

Supplementary information for
Automatic Generation of Mechanistic Pathways of Organic Reactions with Dual Templates

Shuan Chen, Ramil Babazade, Taewan Kim, Jaesik Choi, Sunkyu Han, Yousung Jung

Correspondence: yousung.jung@snu.ac.kr

Contents

RT extension	2
List of special groups used in RT extension.....	3
RT-MT many-to-one correspondence	4
RT-MT one-to-many correspondence	5
Mechanism derivation beyond RT	6
Top-100 RTs.....	8
Labeled data MT distribution table	11
Manual evaluation of 100 randomly sampled reactions.....	12
100 labeled reactions from mech-USPTO-31k	13
100 reactions labeled by ELECTRO	113

S1. RT extension

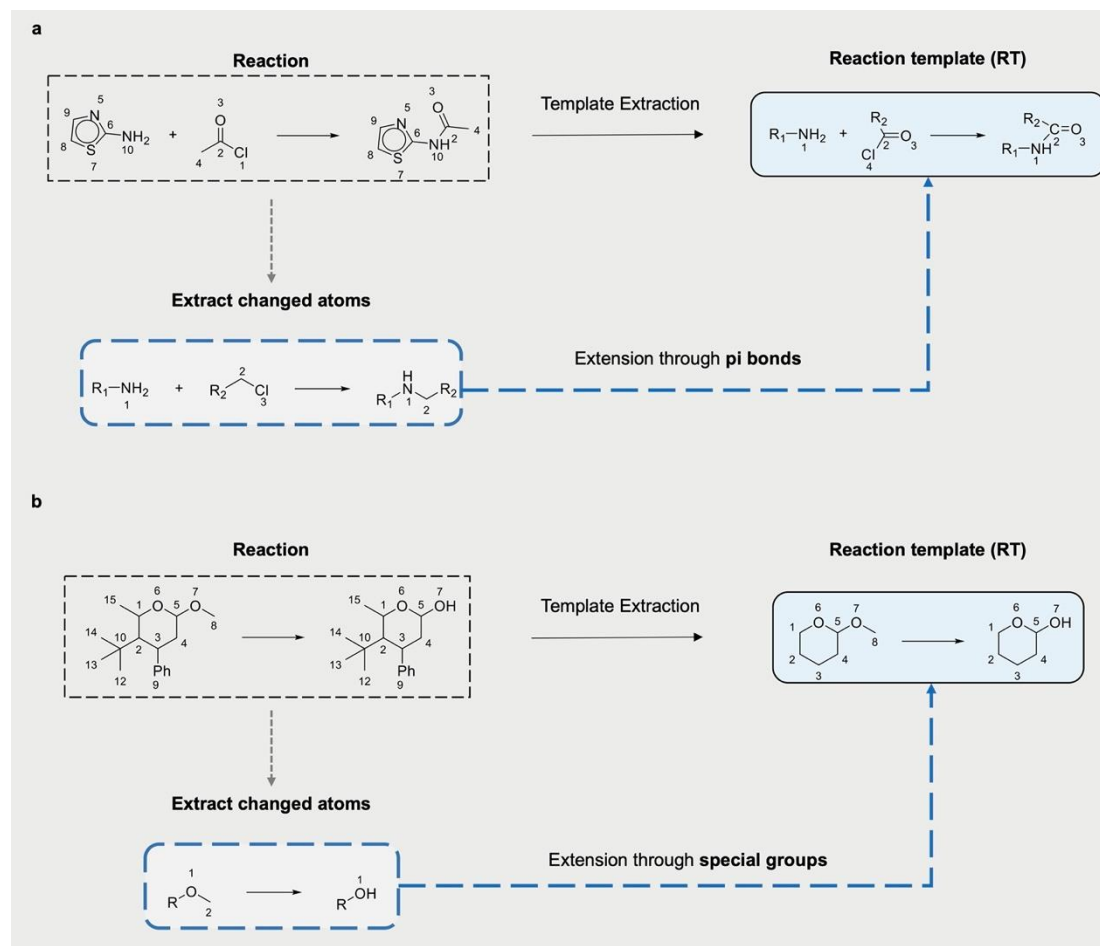


Figure S1. Examples to illustrate the process of obtaining RT. As mentioned in the main text, we extend the original templates comprising changed atoms for mechanism derivation purposes to capture the surrounding environment. Extensions are done through either pi bonds or special groups. (a) Originally, we extract the changed atoms. Since the changed carbon atom is connected to an oxygen through double bond, we include it in the final RT. (b) Changed oxygen atom is one of the special groups we have defined, so whole group THP group is included in the final RT.

S2. List of special groups used in RT extension

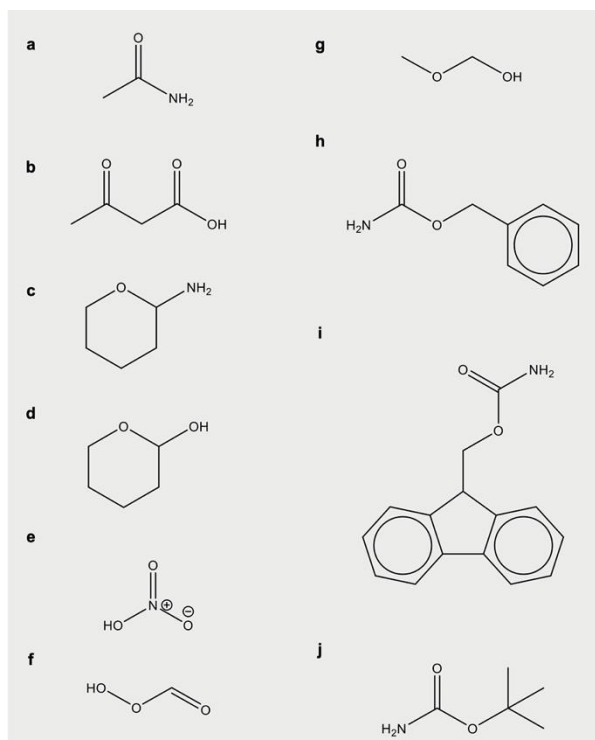


Figure S2. List of special groups used in the extension of originally extracted template to RT. If any changed atom is detected to be part of one of these groups, whole group is included in the RT with respective template atom-map numbers.

S3. RT-MT many-to-one correspondence

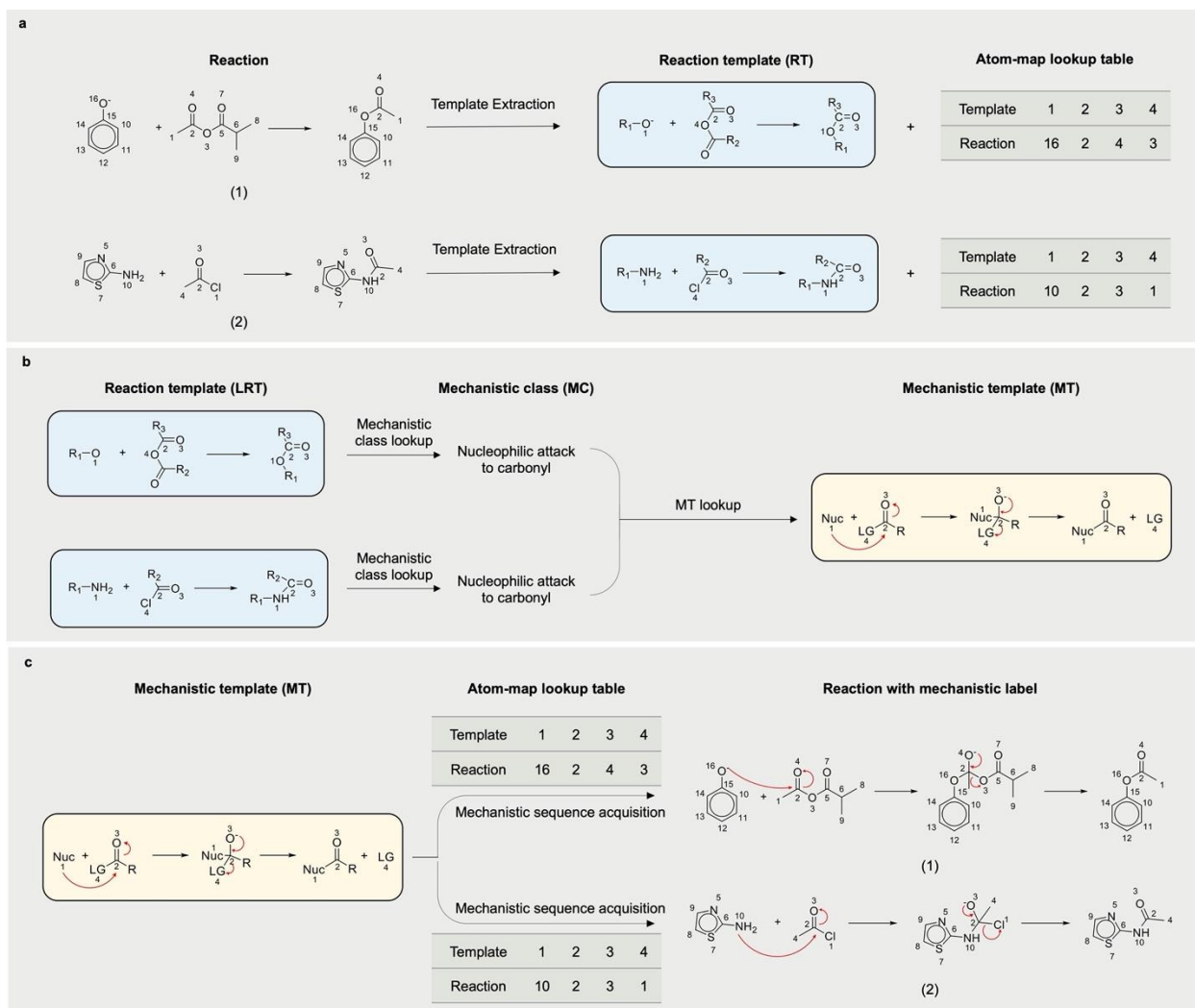


Figure S3. The framework of mechanistic label acquisition. (a) Pair of reactions that follow the same mechanistic pathway is shown as an example to demonstrate the many-to-one correspondence between RTs and an MT. (b) Determination of an MT for extracted RTs. Even though the extracted RTs for both reactions are distinct, the mechanistic sequence that leads to products is the same. Each mechanistic class and MT are unique and there is a one-to-one match between them. (c) Final step in labeling procedure. We convert the MT which shows electron movement in terms of template map numbers to a mechanistic label of the reaction based on the atom-map lookup table.

S4. RT-MT one-to-many correspondence

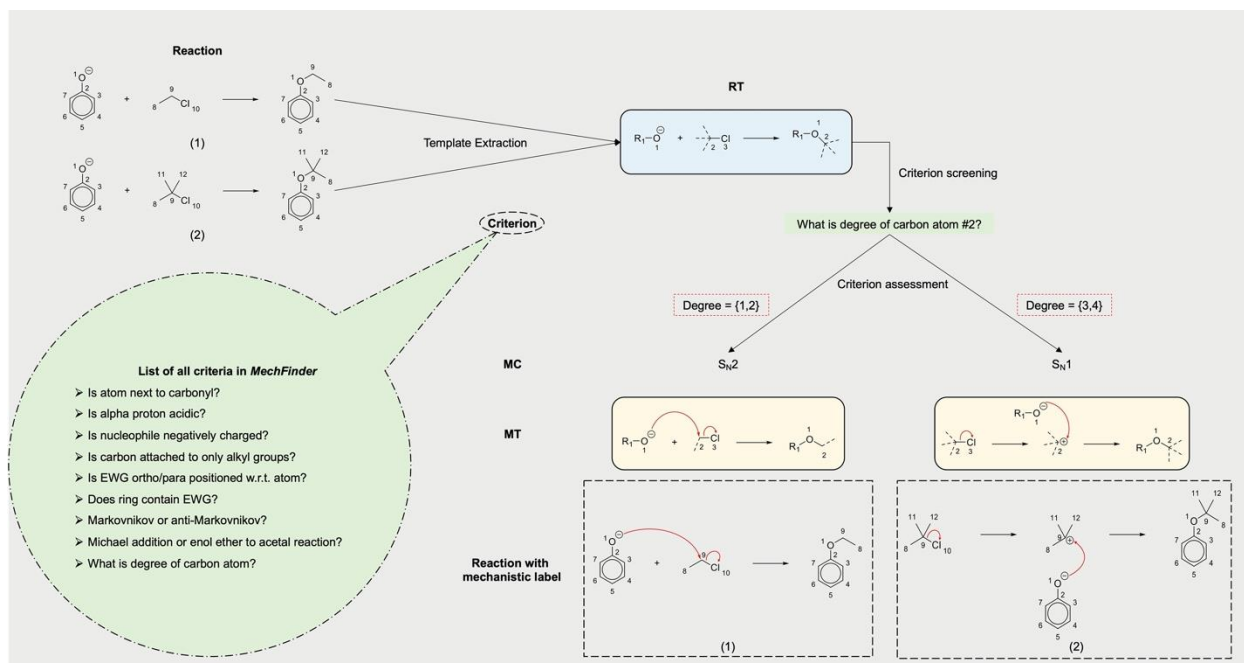


Figure S4. Illustration of one-to-many relationship between extracted RT and labeled MT using two reactions sharing the same RT as examples. For both reactions, RT clearly shows the movement of electrons according to nucleophilic substitution (S_N). Nonetheless, the classification into uni- or bi-molecular types within the S_N class is determined by the degree of electrophilic carbon (atom #2 in the RT) on a high level. Upon extraction of RT, we screen it to assess the applicability of various criteria. Subsequently, we assign the corresponding MT guided by the results of the criterion evaluation. In this case, criterion result {1,2} assign the first reaction into S_N2 MT, whereas the result {3,4} assigns the second reaction into S_N1 MT. These criteria range from examining the presence of certain neighboring functional groups to addressing discreet questions such as whether attached proton is acidic or not. List of all criteria is provided in the green circle. Note that, not all RTs are subject to criterion assessment as the majority of RTs within the labeled dataset exhibit one-to-one correspondence with MTs.

S5. Mechanism derivation beyond RT

Atoms and bonds that must be included in the mechanism but are not present in the RT are introduced based on specific criteria applied to the original reactant molecules. These atom map numbers are denoted by specific placeholders within the MT and are subsequently replaced during the acquisition of the mechanistic sequence. The framework is illustrated in Fig. S5a.

This distinctive feature empowers our method to capture and elucidate crucial mechanistic nuances, such as delocalizations and tautomerization phenomena, which often play pivotal roles in organic reactions. Two illustrative examples, depicted in Fig. S5b and 5c, showcasing the efficacy of our method. These instances, namely nucleophilic aromatic substitution reactions (4.4% of whole dataset) and aldol condensations (0.9% of the whole dataset) prominently feature the vital participation of additional moieties for a comprehensible mechanistic delineation given the RT focusing on narrower reaction center

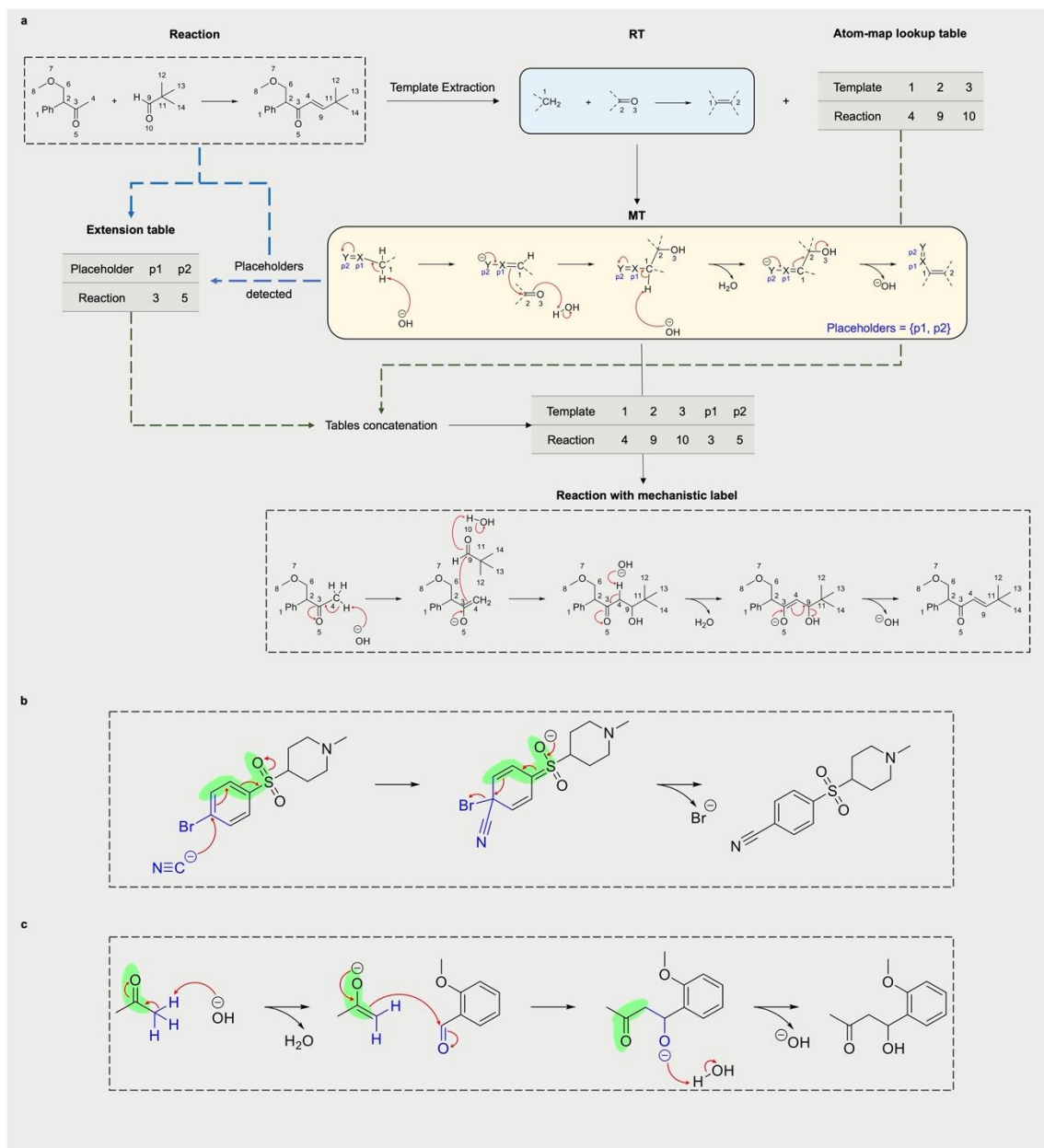


Figure S5. (a) Demonstration of technical manipulation to incorporate functional groups beyond the core atoms in the extracted RT. Once the MT is identified for the reaction, presence of the specific placeholders within the MT is detected which dictates the construction of extension table.

Construction process involves the replacement of these placeholders by the respective atom-map numbers of the atoms present in the original reactant molecule. In this case, upon detection of the presence of p1 and p2, the extension table is built in order to incorporate the respective atom-map numbers in the original reaction. We use original reactant molecules to retrieve corresponding atom-map numbers. The resulting table is then concatenated with the atom-map lookup table generated during RT extraction. This provides complete template map number – reaction map number pairings facilitating the acquisition of mechanistic label for given reaction. (b) Nucleophilic aromatic substitution with cyanide as a nucleophile, bromide as a leaving group and para-positioned sulfonyl group on the benzene ring. The extracted RT for this reaction comprises the nucleophile, leaving group and immediate electrophilic center only (shown in blue). However, the underlying addition-elimination mechanism necessitates electron flow from the ring into the anion-stabilizing sulfonyl group (highlighted in green). Our method captures this pivotal mechanistic element, incorporating it into the resultant label without being constrained by RT limitations. The derived pathway comprehensively includes all requisite atoms and bonds. b) Base-catalyzed aldol condensation. The extracted RT covers the nucleophilic carbon and carbonyl group subject to attack (shown in blue). Nevertheless, the nucleophilicity of the carbon is influenced by the adjacent carbonyl group and should be present in the obtained pathway. The preservation of the enolate intermediate formation is manifested in the mechanism (highlighted in green), notwithstanding the absence of these atoms and bonds in the RT.

S6. Top 100 RTs

Table S1. List of all RTs in SMARTS format along with the number of reactions belonging to each RT.

Reaction Template	Number of reactions
[N:1].[O:4]-[C:2]=[O:3]>>[N:1]-[C:2]=[O:3]	5505
[N:1].[C:2]-[X:3]>>[N:1]-[C:2]	2331
[N:1].[X:4]-[C:2]=[O:3]>>[N:1]-[C:2]=[O:3]	2286
[O:1].[C:2]-[X:3]>>[O:1]-[C:2]	2124
[C:2]-[C:3](-[C:4])(-[C:5])-[O:6]-[C:7](-[N:1])=[O:8]>>[N:1]	1881
[N:1].[C:2]=[O:3]>>[N:1]-[C:2]	1661
[C:1]-[X:5].[a:3].[n:2]:[a:4]>>[C:1]-[n:2](:[a:3]):[a:4]	1078
[N:1].[O:3]=[S:2](=[O:4])-[X:5]>>[N:1]-[S:2](=[O:3])=[O:4]	1027
[N:1].[X:5]-[c:2](:[a:3]):[a:4]>>[N:1]-[c:2](:[a:3]):[a:4]	1022
[C:1]=[O:2]>>[C:1]-[O:2]	657
[C:1]-[O:2]>>[C:1]=[O:2]	550
[N:1].[C:2]=[O:3]>>[N:1]=[C:2]	522
[C:2]-[O:1]>>[O:1]	510
[O:1].[C:2]-[O:3]>>[O:1]-[C:2]	461
[O:1].[X:5]-[c:2](:[a:3]):[a:4]>>[O:1]-[c:2](:[a:3]):[a:4]	412
[N:4].C-C(-C)(-C)-[O:6]-[C:7](=O)-[O:8]-[C:3](=[O:5])-[O:2]-[C:1]>>[C:1]-[O:2]-[C:3](-[N:4])=[O:5]	401
[O:1].[X:4]-[C:2]=[O:3]>>[O:1]-[C:2]=[O:3]	380
[N:1].C-C-[O:4]-[C:2]=[O:3]>>[N:1]-[C:2]=[O:3]	373
[N:1].[N:3]=[C:2]=[O:4]>>[N:1]-[C:2](-[N:3])=[O:4]	342
[N:1].C-[O:4]-[C:2]=[O:3]>>[N:1]-[C:2]=[O:3]	342
[O:1].[O:4]-[C:2]=[O:3]>>[O:1]-[C:2]=[O:3]	320
[C:1].[C:2]=[O:3]>>[C:1]=[C:2]	319
C-[O:3]-[C:1]=[O:2]>>[C:1]-[O:2]	285
[S:1].[C:2]-[X:3]>>[S:1]-[C:2]	267
[N:1]-[C:2](=[O:3])-[O:4]-[C:5]-[a:6]1:[a:7]:[a:8]:[a:9]:[a:10]:[a:11]:1>>[N:1]	262
C-C-[O:3]-[C:1]=[O:2]>>[C:1]-[O:2]	241
[O:1].[O:3]=[S:2](=[O:4])-[X:5]>>[O:1]-[S:2](=[O:3])=[O:4]	240
[C:1]#[N:2]>>[C:1]-[N:2]	225
[N:1].C-C(=O)-[O:4]-[C:2]=[O:3]>>[N:1]-[C:2]=[O:3]	214
C-C(-C)(-C)-[Si:2](-C)(-C)-[O:1]>>[O:1]	198
C-[C:2](-[O:1])=[O:3]>>[O:1]	195
[N:1].[C:2]-[O:3]>>[N:1]-[C:2]	188
[C:1]=[O:3].[C:2]-[P:4](-c1:c:c:c:c:1)(-c1:c:c:c:c:1)-c1:c:c:c:c:1>>[C:1]=[C:2]	176
[N:3].[N:1]=[C:2]=[O:4]>>[N:1]-[C:2](-[N:3])=[O:4]	173
[N:1]=[N:2]=[N:3]>>[N:1]	165
[C:1]-[C:2](-[N:3])=[O:4]>>[C:1]-[C:2]-[N:3]	159

[C:1]-[Mg:4].[C:2]=[O:3]>>[C:1]-[C:2]-[O:3]	153
[C:2]-[C:3](-[N:1])=[O:4]>>[N:1]	144
[O:2]=[C:3]1-[N:1]-[C:4](=[O:5])-[a:6]2:c:c:c:[a:7]:2-1>>[N:1]	140
[N:1].C-S(=O)(=O)-[O:3]-[C:2]>>[N:1]-[C:2]	139
[S:1].Cl-c1:c:c:c(-[C:3](=[O:4])-[O:5]-[O:2]):c:1>>[S:1]=[O:2]	127
[X:6]-[C:2]=[O:1].[a:4]:[c:3]:[a:5]>>[O:1]=[C:2]-[c:3](:[a:4]):[a:5]	121
[N:1].[N:3]=[C:2]=[S:4]>>[N:1]-[C:2](-[N:3])=[S:4]	116
[O:3].[O:1]=[S:2](=[O:4])-[X:5]>>[O:1]=[S:2](-[O:3])=[O:4]	113
[C:1]=[O:3].C-C-O-[P:4](-[C:2])(=[O:5])-[O-C-C]>>[C:1]=[C:2]	111
[O:1].[C:2]=[C:3]>>[O:1]-[C:2]-[C:3]	104
[O:4].[O:1]=[S:2](=[O:3])-[X:5]>>[O:1]=[S:2](=[O:3])-[O:4]	98
[N:1].[N:3].[O:4]-[C:2]=[O:5]>>[n:1]:[c:2]:[n:3]	92
[N:1].F-C(F)(F)-C(=O)-[O:4]-[C:2]=[O:3]>>[N:1]-[C:2]=[O:3]	91
[a:4]:[c:3]:[a:5].C-[N:6](-C)-[C:2]=[O:1]>>[O:1]=[C:2]-[c:3](:[a:4]):[a:5]	87
[S:1].[X:5]-[c:2](:[a:3]):[a:4]>>[S:1]-[c:2](:[a:3]):[a:4]	87
[C:1]=[O:2]>>[C:1]	86
[C:1]-[X:4].[N:2]=[N:3]>>[C:1]-[N:2]=[N:3]	85
[N:2]-[C:1]=[S:5].[X:6]-[C:4]-[C:3]=[O:7]>>[c:1]1:[n:2]:[c:3]:[c:4]:[s:5]:1	72
F-[C:2](-F)(-F)-[C:3](-[N:1])=[O:4]>>[N:1]	71
[C:1]-[O:3].Br-[C:4](-Br)(-Br)-[Br:2]>>[C:1]-[Br:2]	70
[O:1].C-S(=O)(=O)-[O:3]-[C:2]>>[O:1]-[C:2]	66
[a:5]:[n:4]:[a:6].[O:1]=[S:2](=[O:3])-[X:7]>>[O:1]=[S:2](=[O:3])-[n:4](:[a:5]):[a:6]	65
[O:3].[N:1]=[C:2]=[O:4]>>[N:1]-[C:2](-[O:3])=[O:4]	61
[X:6]-[C:2]=[O:1].[a:4]:[n:3]:[a:5]>>[O:1]=[C:2]-[n:3](:[a:4]):[a:5]	58
[N:3]-[C:2](=[O:4])-[a:1]>>[a:1]-[C:2]#[N:3]	56
[a:3]:[n:2]:[a:4].Cl-c1:c:c:c(-[C:5](=[O:6])-[O:7]-[O:1]):c:1>>[O:1]-[n:2](:[a:3]):[a:4]	55
[a:3]:[n:2]:[a:4].C-S(=O)(=O)-[O:5]-[C:1]>>[C:1]-[n:2](:[a:3]):[a:4]	55
[O:1].[O:3].[C:2]=[O:4]>>[O:1]-[C:2]-[O:3]	55
[N:1].C-C(-C)(-C)-[O:4]-[C:2]=[O:3]>>[N:1]-[C:2]=[O:3]	53
[a:6]:[n:5]:[a:7].C-C(-C)(-C)-[O:8]-[C:9](=O)-[O:10]-[C:3](=[O:4])-[O:2]-[C:1]>>[C:1]-[O:2]-[C:3](=[O:4])-[n:5](:[a:6]):[a:7]	53
[N:3].[N:1]=[C:2]=[S:4]>>[N:1]-[C:2](-[N:3])=[S:4]	52
[N:1]-[C:2]=[S:3].[X:6]-[C:4]-[C:5]=[O:7]>>[n:1]1:[c:2]:[s:3]:[c:4]:[c:5]:1	50
[N:1]-[C:2](=[O:4])-[a:3]>>[N:1]-[C:2]-[a:3]	48
[C:1]=[N:2]>>[C:1]-[N:2]	46
[C:1]=[O:3].[C:2]=[P:4](-c1:c:c:c:e:1)(-c1:c:c:c:e:1)-c1:c:c:c:e:1>>[C:1]=[C:2]	45
[a:5]:[n:4]:[a:6].[X:7]-[c:2](:[a:1]):[a:3]>>[a:1]:[c:2](:[a:3])-[n:4](:[a:5]):[a:6]	45
[N:1]-[N:2].[O:6]=[C:3]-[C:4]-[C:5]=[O:7]>>[n:1]1:[n:2]:[c:3]:[c:4]:[c:5]:1	43
[C:1]-[X:4].[C:2]#[N:3]>>[C:1]-[C:2]#[N:3]	43
[S:1].[O:2]-[O:3]>>[S:1]=[O:2]	42
[N:1].[O:6]=[C:2]-[C:3]-[C:4]-[C:5]=[O:7]>>[n:1]1:[c:2]:[c:3]:[c:4]:[c:5]:1	40

[C:2]-[O:3]-[C:4]-[O:1]>>[O:1]	40
[C:1]-[C:2](-[N:3])=[O:4]>>[C:1]-[C:2]#[N:3]	39
[N:1],[C:2]=[O:6],[a:4]:[c:3]:[a:5]>>[N:1]-[C:2]-[c:3](:[a:4]):[a:5]	39
[C:1]=[C:2].Cl-c1:c:c:c(-[C:4])(=[O:5])-[O:6]-[O:3]:c:1>>[C:1]1-[C:2]-[O:3]-1	37
[N:2]=[N:3].C-S(=O)(=O)-[O:4]-[C:1]>>[C:1]-[N:2]=[N:3]	37
[C:4]-[C:5](-[C:6])(-[C:7])-[O:8]-[C:9](=[O:10])-[n:2](:[a:1]):[a:3]>>[a:1]:[n:2]:[a:3]	37
[C:2]=[O:1].[Mg:6]-[c:3](:[a:4]):[a:5]>>[O:1]-[C:2]-[c:3](:[a:4]):[a:5]	36
[N:2],[C:1]-[X:4],[C:3]-[X:5]>>[C:1]-[N:2]-[C:3]	36
[N:3]-[C:2]=[S:1],[X:6]-[C:5]-[C:4]=[O:7]>>[s:1]1:[c:2]:[n:3]:[c:4]:[c:5]:1	36
[O:1]-[C:2]1-[C:3]-[C:4]-[C:5]-[C:6]-[O:7]-1>>[O:1]	34
[a:1]:[n:2]:[a:3],[X:7]-[c:4](:[a:5]):[a:6]>>[a:1]:[n:2](:[a:3])-[c:4](:[a:5]):[a:6]	33
[C:1],[C:2]=[O:3]>>[C:1]-[C:2]-[O:3]	31
[C:1]-[X:10],[C:7]-[C:6](-[C:8])(-[C:9])-[O:5]-[C:3](-[N:2])=[O:4]>>[C:1]-[N:2]-[C:3](=[O:4])-[O:5]-[C:6](-[C:7])(-[C:8])-[C:9]	29
[a:1]:[n:2](:[a:3])-[C:4]1-[C:5]-[C:6]-[C:7]-[C:8]-[O:9]-1>>[a:1]:[n:2]:[a:3]	29
[N:1]-[C:2](=[O:3])-[O:4]-[C:5]-[C:6]1-[a:7]2:[a:8]:[a:9]:[a:10]:[a:11]:[a:12]:2-[a:13]2:[a:14]:[a:15]:[a:16]:[a:17]:[a:18]:2-1>>[N:1]	28
[C:1]-[O:2]-[C:3]1-[C:4]-[C:5]-[C:6]-[C:7]-[O:8]-1>>[C:1]-[O:2]	28
[C:1]-[O:5],[a:3]:[n:2]:[a:4]>>[C:1]-[n:2](:[a:3]):[a:4]	27
[C:1]-[Mg:5].C-O-[N:6](-C)-[C:2](=[O:3])-[a:4]>>[C:1]-[C:2](=[O:3])-[a:4]	27
[C:2]=[O:1],[C:3]#[C:4]>>[O:1]-[C:2]-[C:3]#[C:4]	27
[N:1]-[C:2](=[O:3])-[a:4]1:c:c:c:c:1>>[N:1]	25
[O:1],[C:2]=[N:3]=[N:4]>>[O:1]-[C:2]	25
[N:1],[S:3]=[C:2](-[X:4])-[X:5]>>[N:1]=[C:2]=[S:3]	24
[N:1].F-C(F)(F)-S(=O)(=O)-[O:5]-[c:2](:[a:3]):[a:4]>>[N:1]-[c:2](:[a:3]):[a:4]	21
[C:2]#[N:1],[X:6]-[c:3](:[a:4]):[a:5]>>[N:1]#[C:2]-[c:3](:[a:4]):[a:5]	9

S7. Distribution of mechanistic classes in mech-USPTO-31K dataset

Table S2. Distribution of reactions across mechanistic classes in the labeled dataset.

Mechanistic Class	Number of reactions	Mechanistic Class	Number of reactions
DCC condensation	5816	(hemi)acetal (aminal) hydrolysis	131
Nucleophilic attack to (thio)carbonyl	4963	Sulfide oxidation	127
S _N 2 reaction	3956	Friedel Crafts acylation	121
S _N 2 reaction with alcohol(thiol)	2191	Horner Wadsworth Emmons reaction	111
Boc deprotection	1918	Primary amide dehydration	95
Reductive amination	1661	Imidazole synthesis	92
Alcohol attack to carbonyl or sulfonyl	892	Vilsmeier formylation	87
Nucleophilic attack to iso(thio)cyanate	683	Wolff Kishner reduction	86
Carbonyl reduction	647	Appel reaction	70
S _N Ar reaction (ortho)	599	Acetal formation from enol ether	64
S _N Ar reaction (para)	548	Acetal formation	55
Ester reduction	526	Amine oxidation	55
Imine formation	522	Imine reduction	46
O-demethylation	510	Wittig reaction with ylide	45
Mitsunobu reaction	488	Knorr pyrazole synthesis	43
Swern oxidation	322	Sulfide oxidation by peroxide	42
Aldol condensation	319	Paal Knorr pyrrole synthesis	40
S _N 1 reaction	305	Mannich reaction	39
S _N Ar reaction with alcohol (para)	300	Alkene epoxidation	37
Cbz deprotection	262	Double S _N 2 reaction	36
Carboxylic acid derivative hydrolysis or formation	240	Aldol addition	31
Jones oxidation	228	Fmoc deprotection	28
Nitrile reduction	225	Alkynyl attack to carbonyl	27
Amide reduction	207	Weinreb ketone synthesis	27
Base catalyzed ester hydrolysis	195	Markovnikov addition	26
Grignard reaction	189	Methyl ester synthesis	25
S _N 2 reaction with tosylate	182	Isothiocyanate synthesis	24
S _N Ar reaction with alcohol (ortho)	182	Michael addition	14
Wittig reaction	176	Lactone reduction	10
Staudinger reaction	165	Intramolecular lactonization	9
Hantzsch thiazole synthesis	158	S _N 1 reaction with tosylate	6
Ing Manske	140		

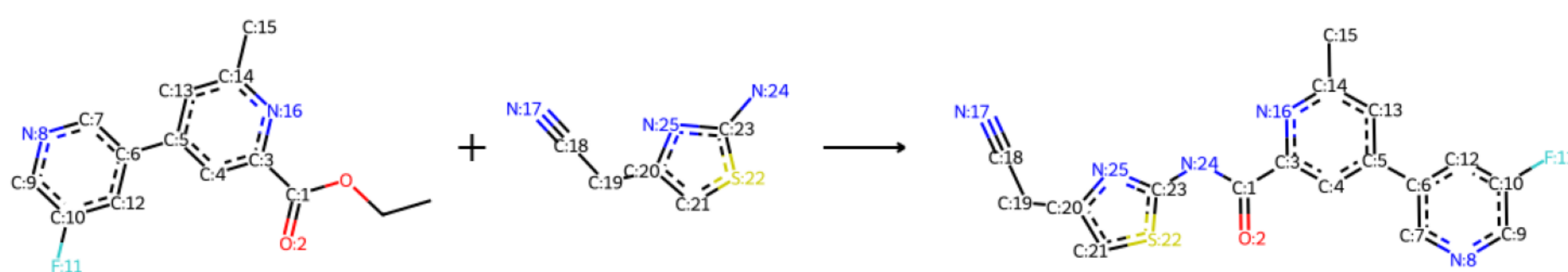
S8. Manual evaluation of 100 randomly sampled reactions

We manually evaluated the 100 randomly sampled reactions from mech-USPTO-31k dataset (see below) and compared the results of reaction mechanism generated by *MechFinder* and ELECTRO labeling method. We found *MechFinder* gives 100% reasonable correct mechanism, while only three of the ELECTRO labels are chemically reasonable, which are S_N2 reactions (reactions 46, 69, and 89).

Reference

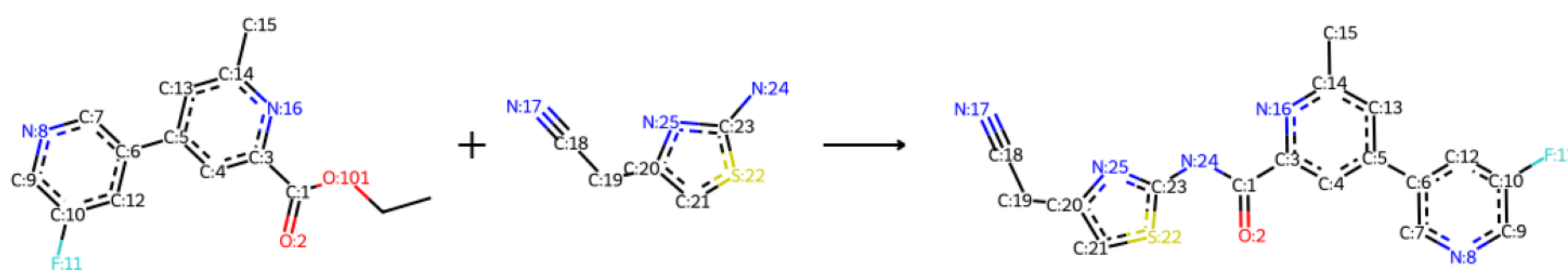
1. Bradshaw, J., Kusner, M. J., Paige, B., Segler, M. H. S. & Hernández-Lobato, J. M. A Generative Model For Electron Paths. *ArXiv180510970 Phys. Stat* (2019).

Original reaction sampled RXN_ID:0)



Identified mechanistic class -
nucleophilic_attack_to_(thio)carbonyl_or_sulfonyl reaction

Reaction with missing reagents recovered

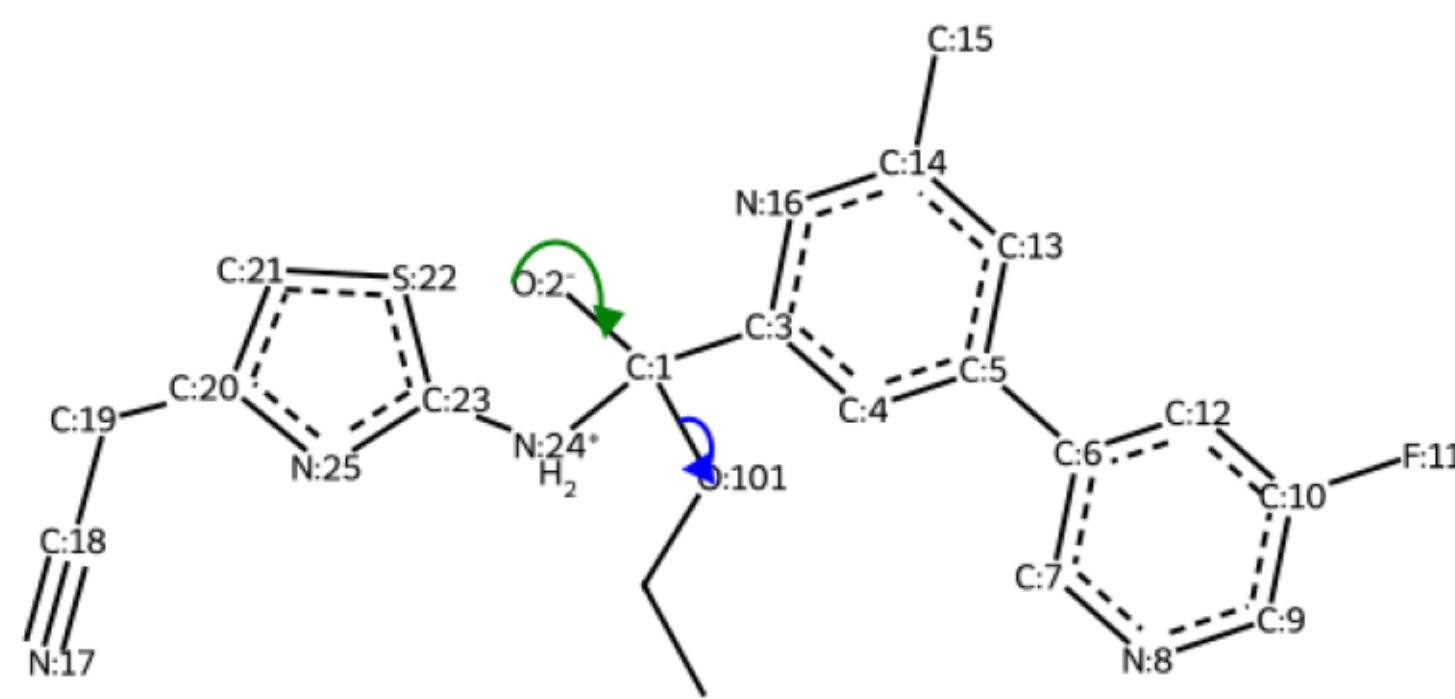
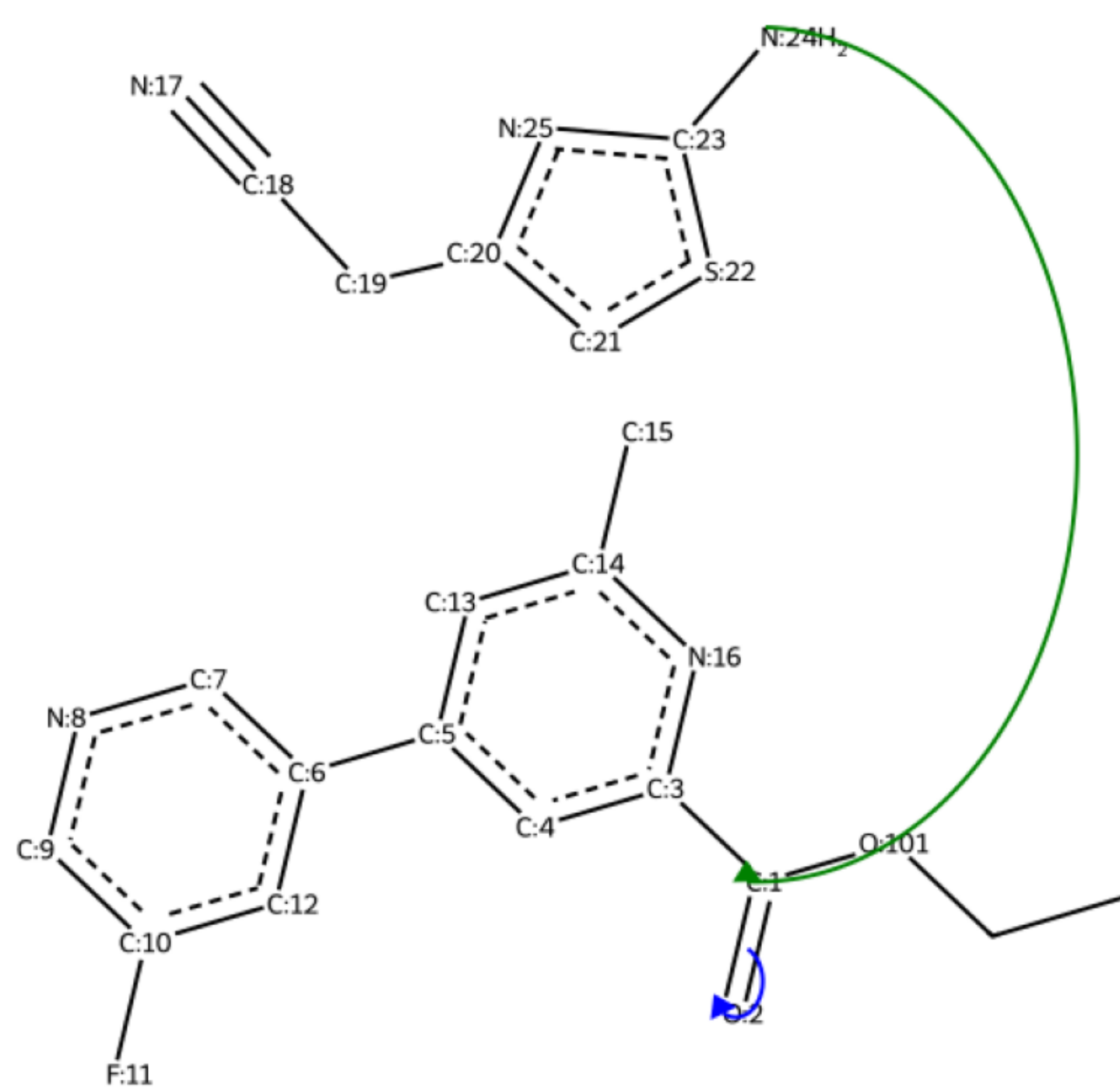


Proposed mechanistic pathway

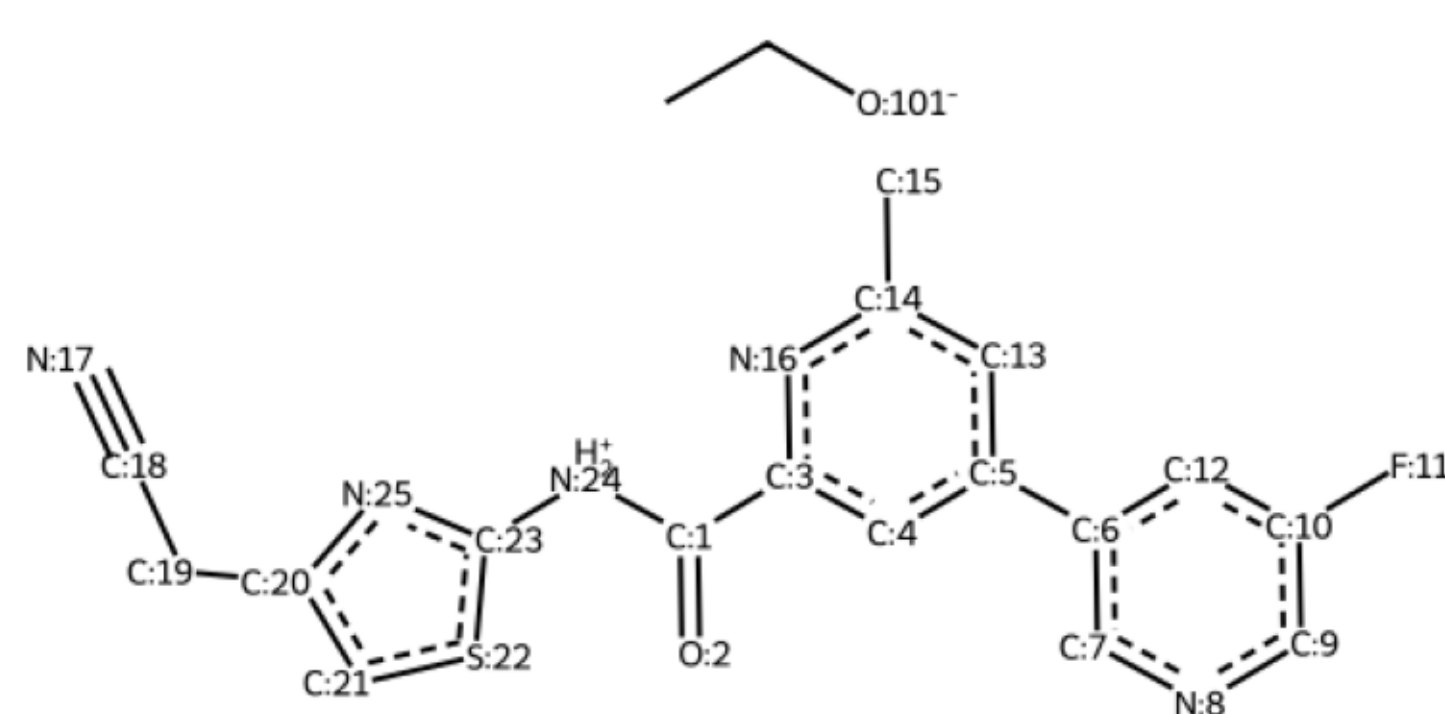
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

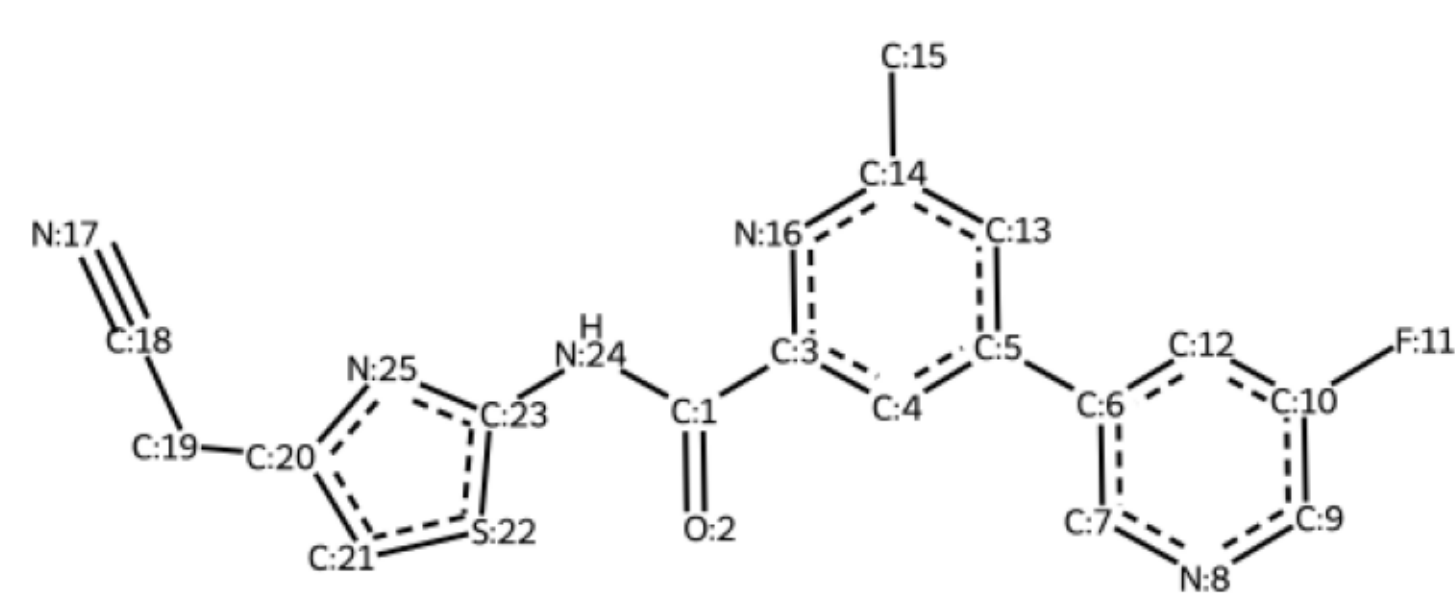
step #2



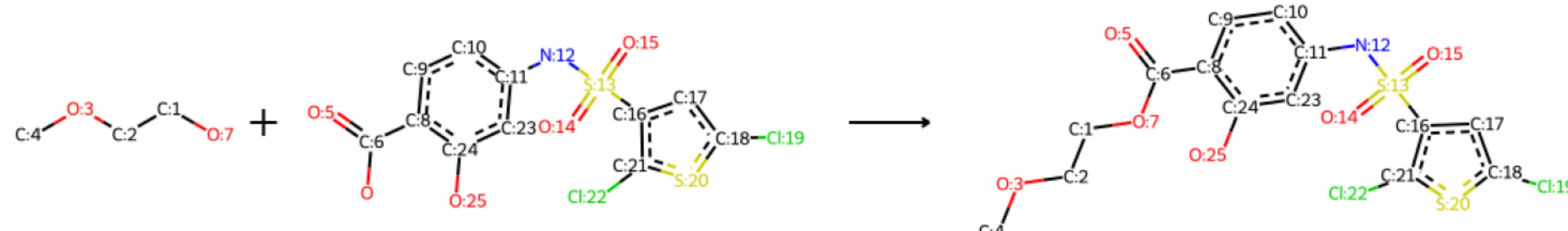
Product(s)



proton transfer

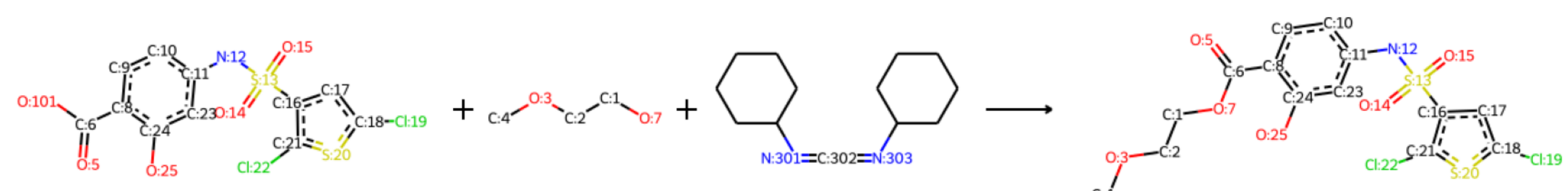


Original reaction sampled RXN_ID:1)



Identified mechanistic class -
DCC_condensation reaction

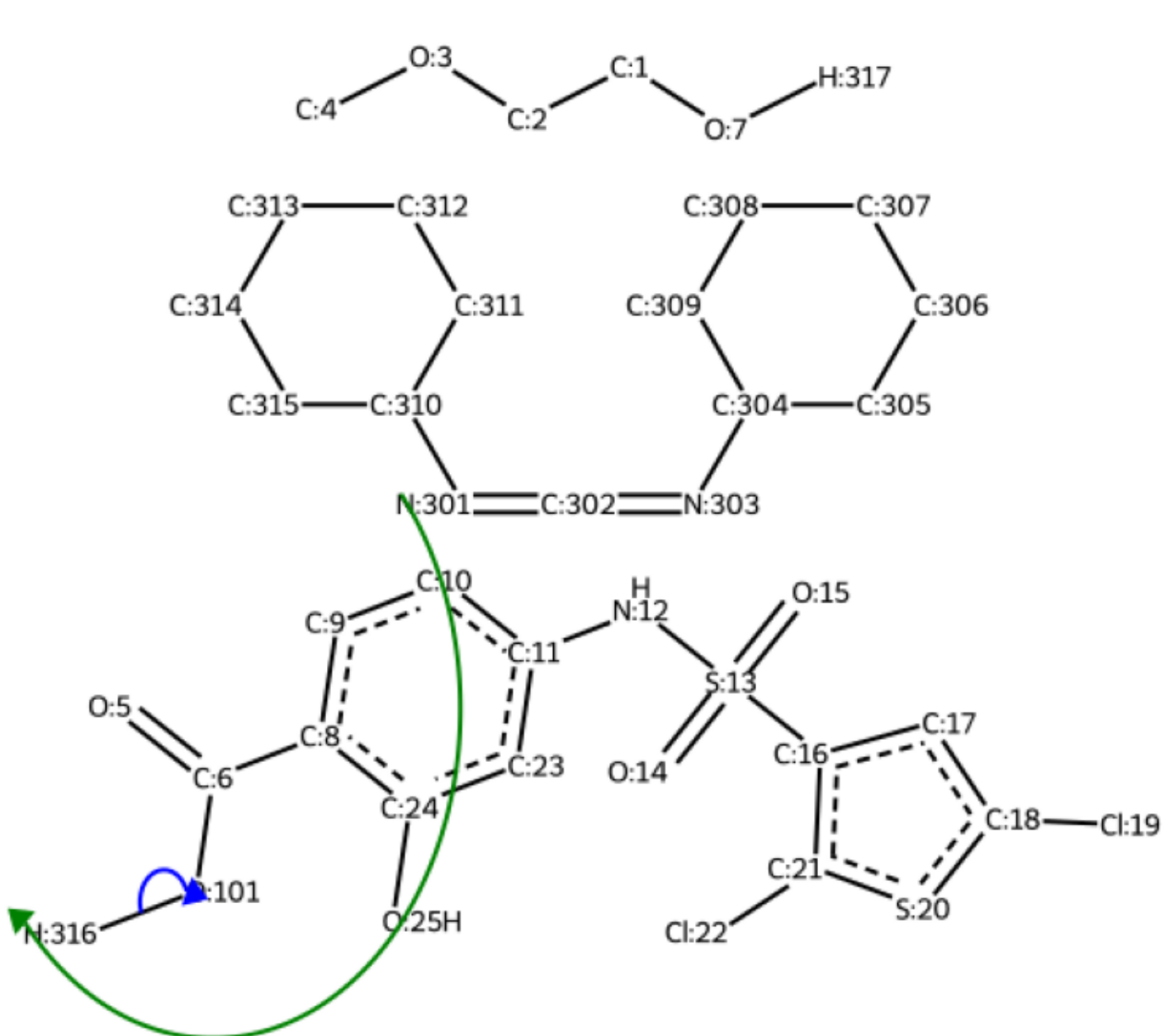
Reaction with missing reagents recovered



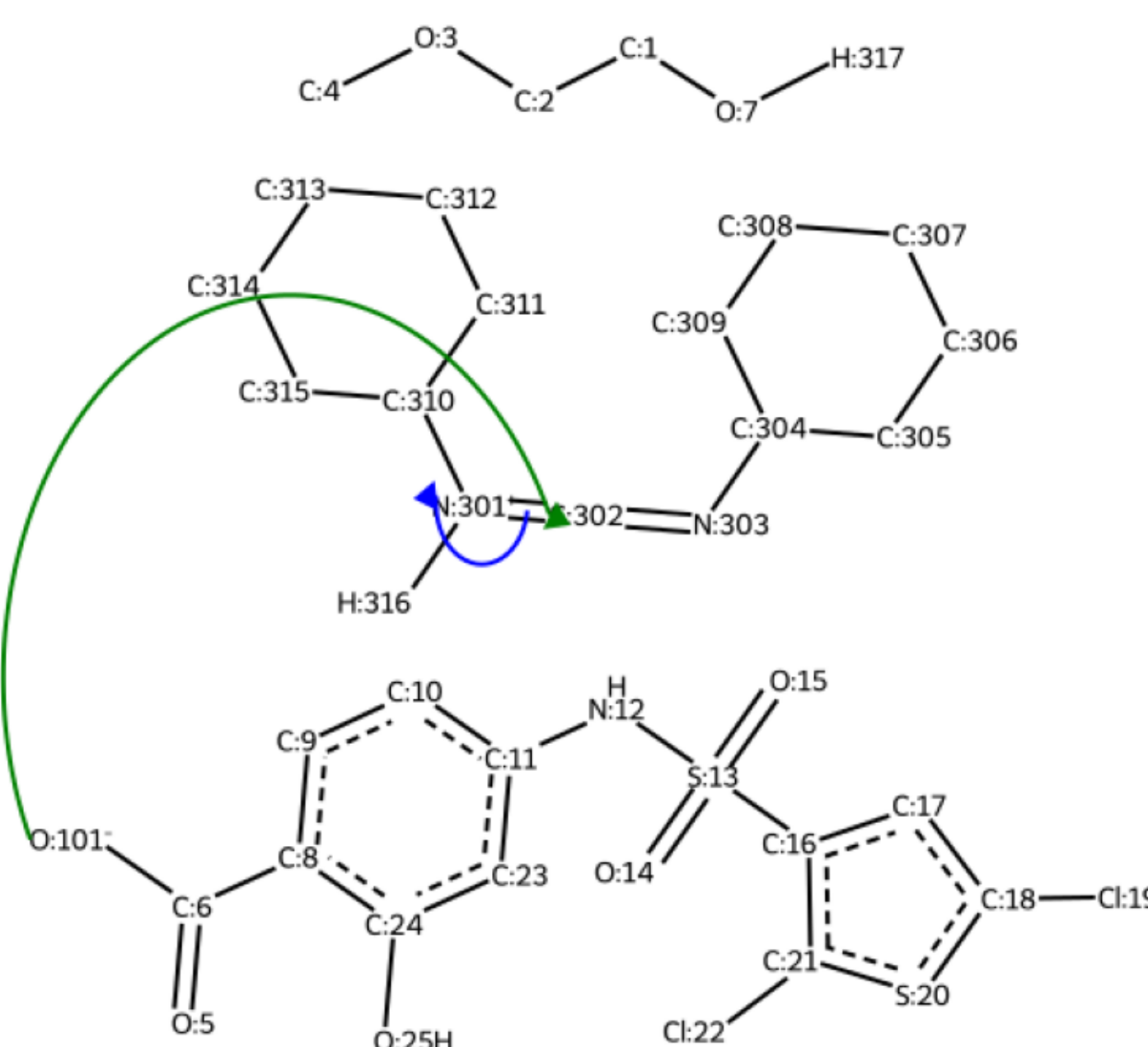
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

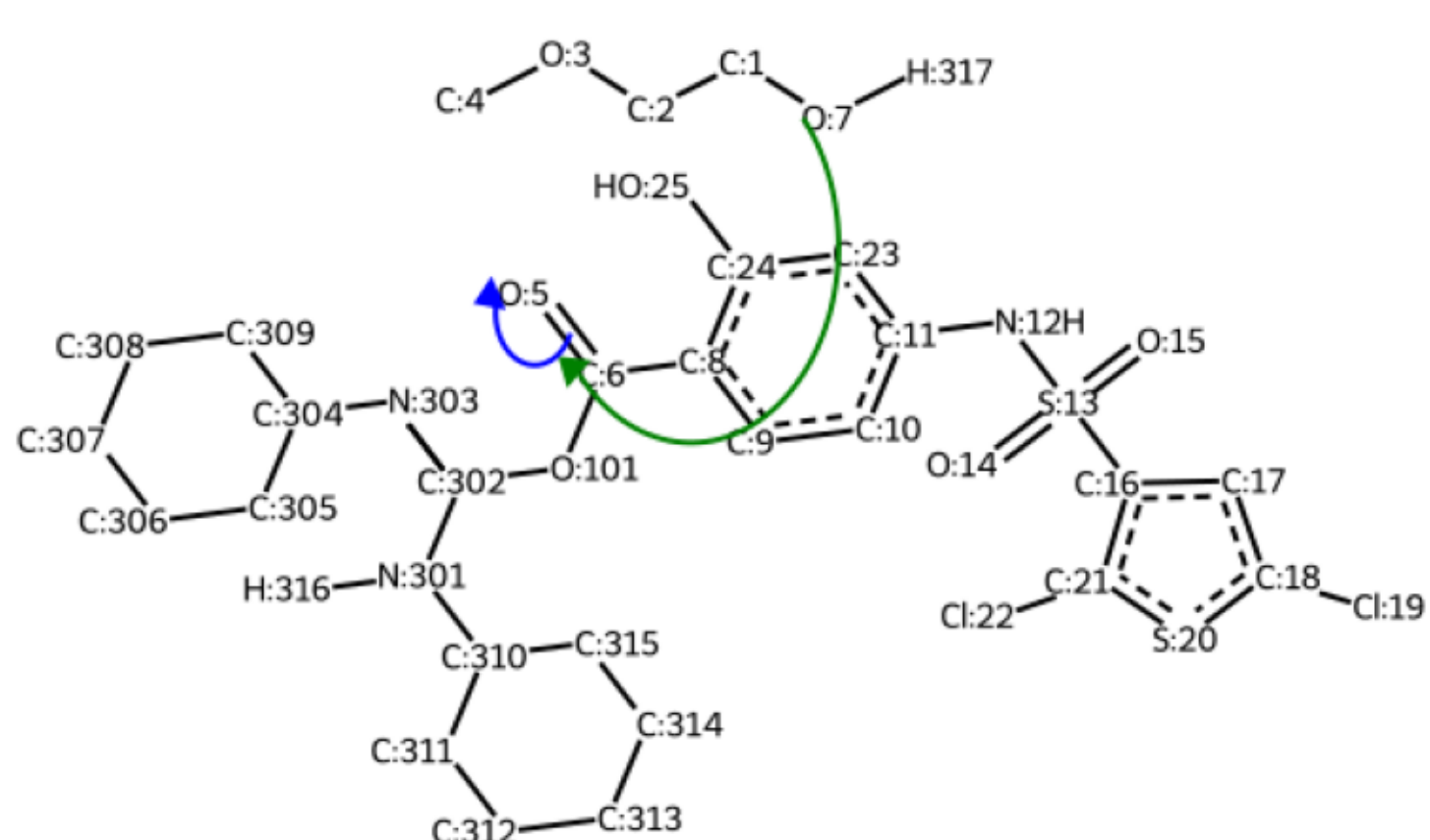
step #1



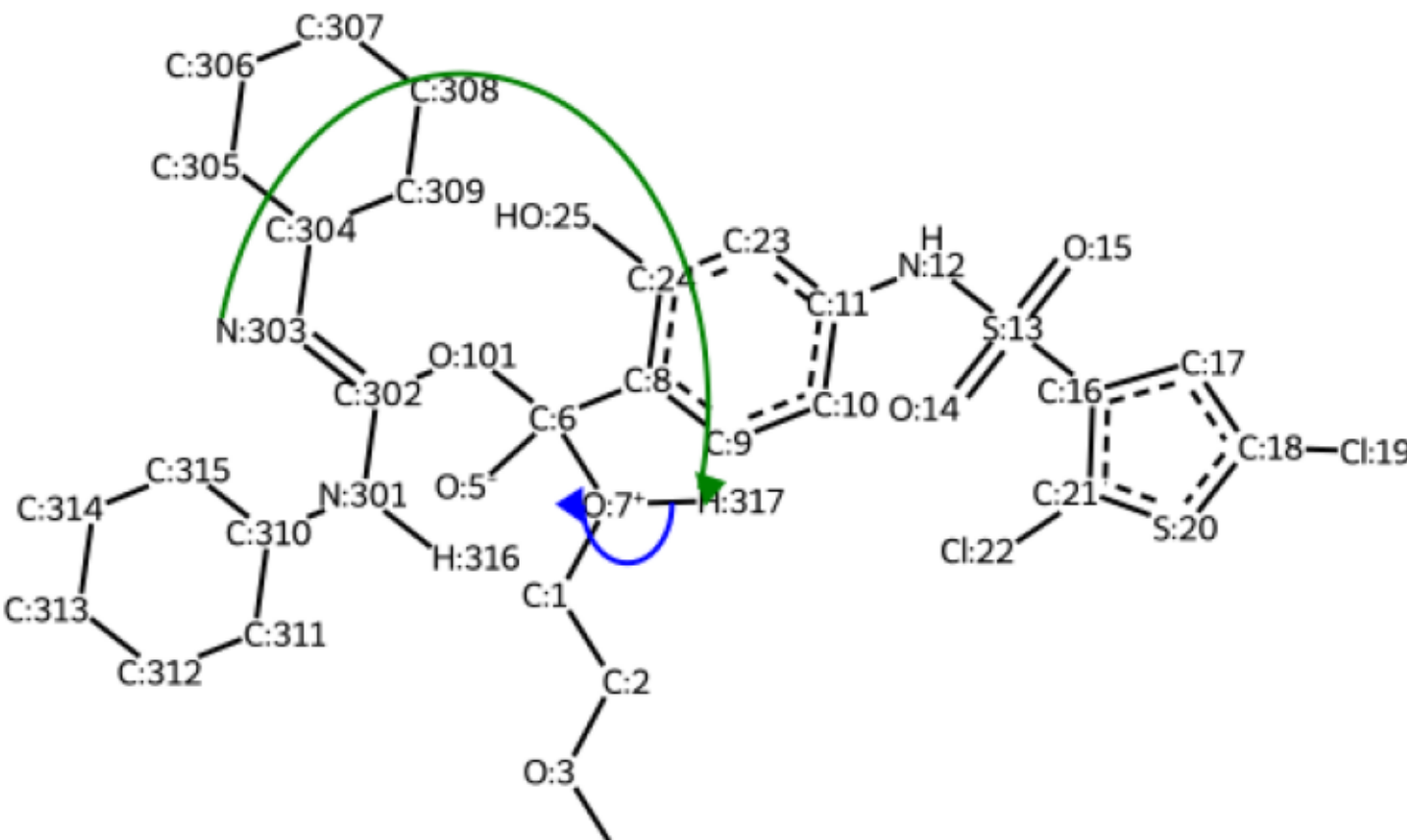
step #2



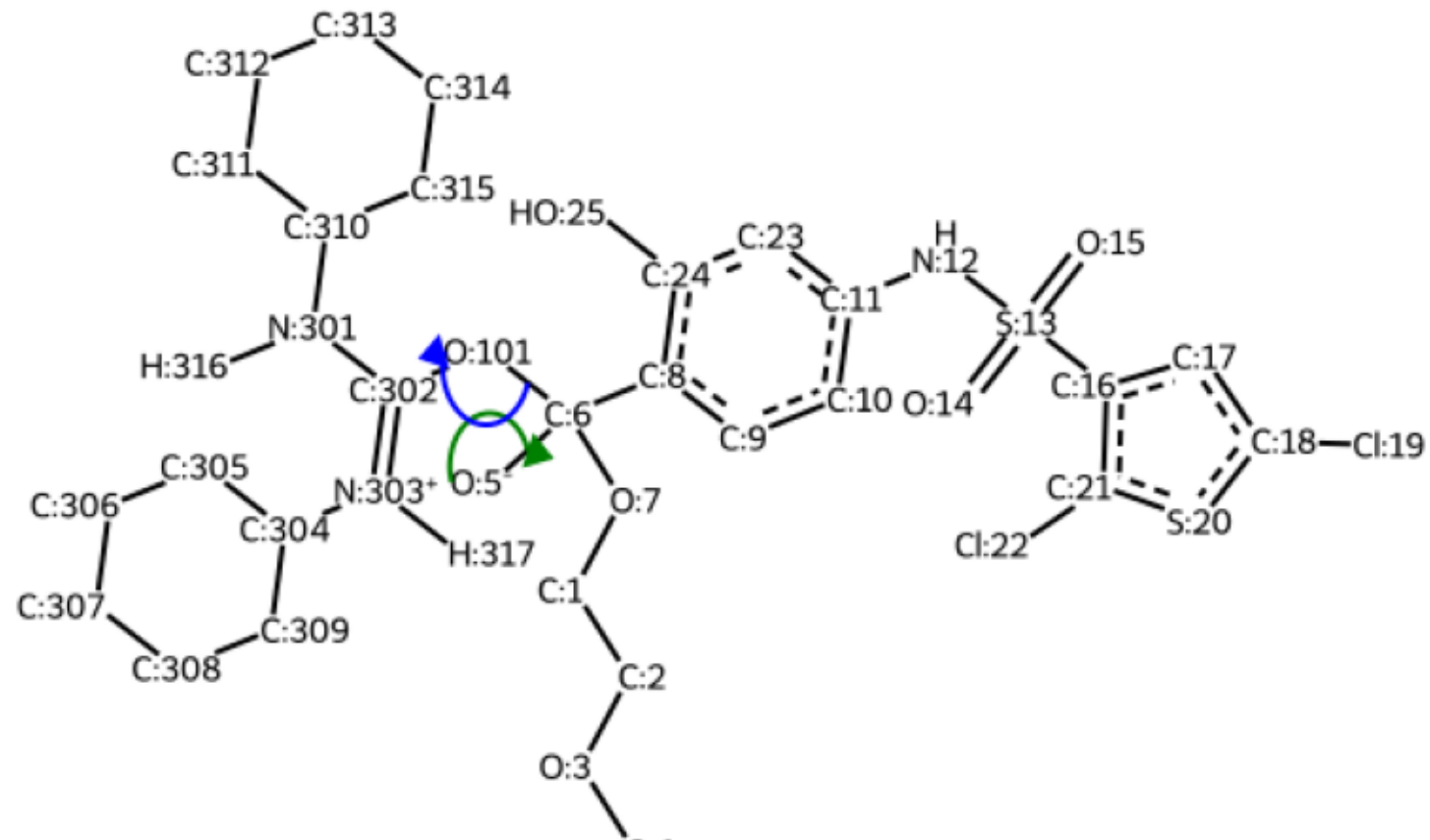
step #3



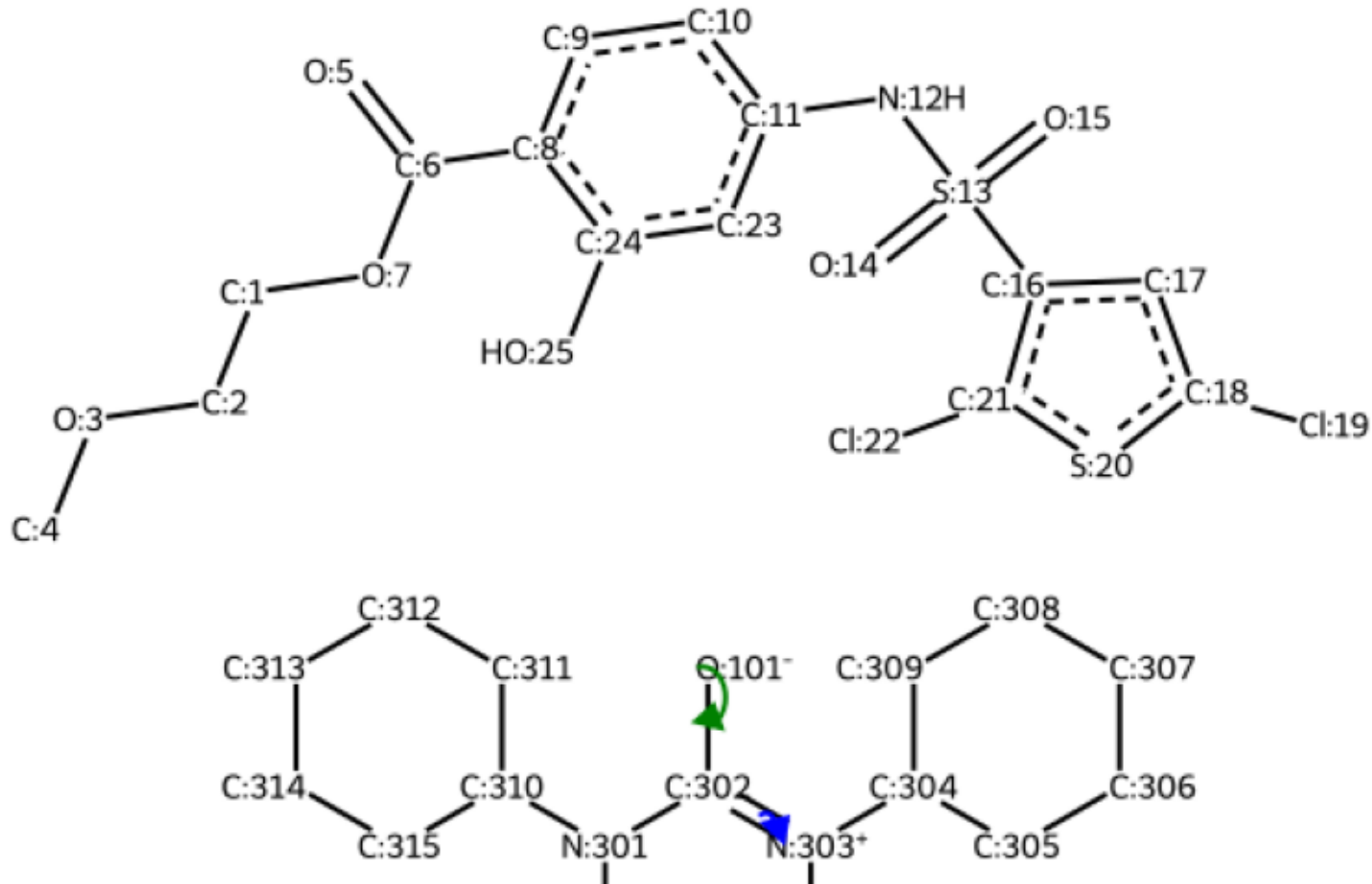
step #4



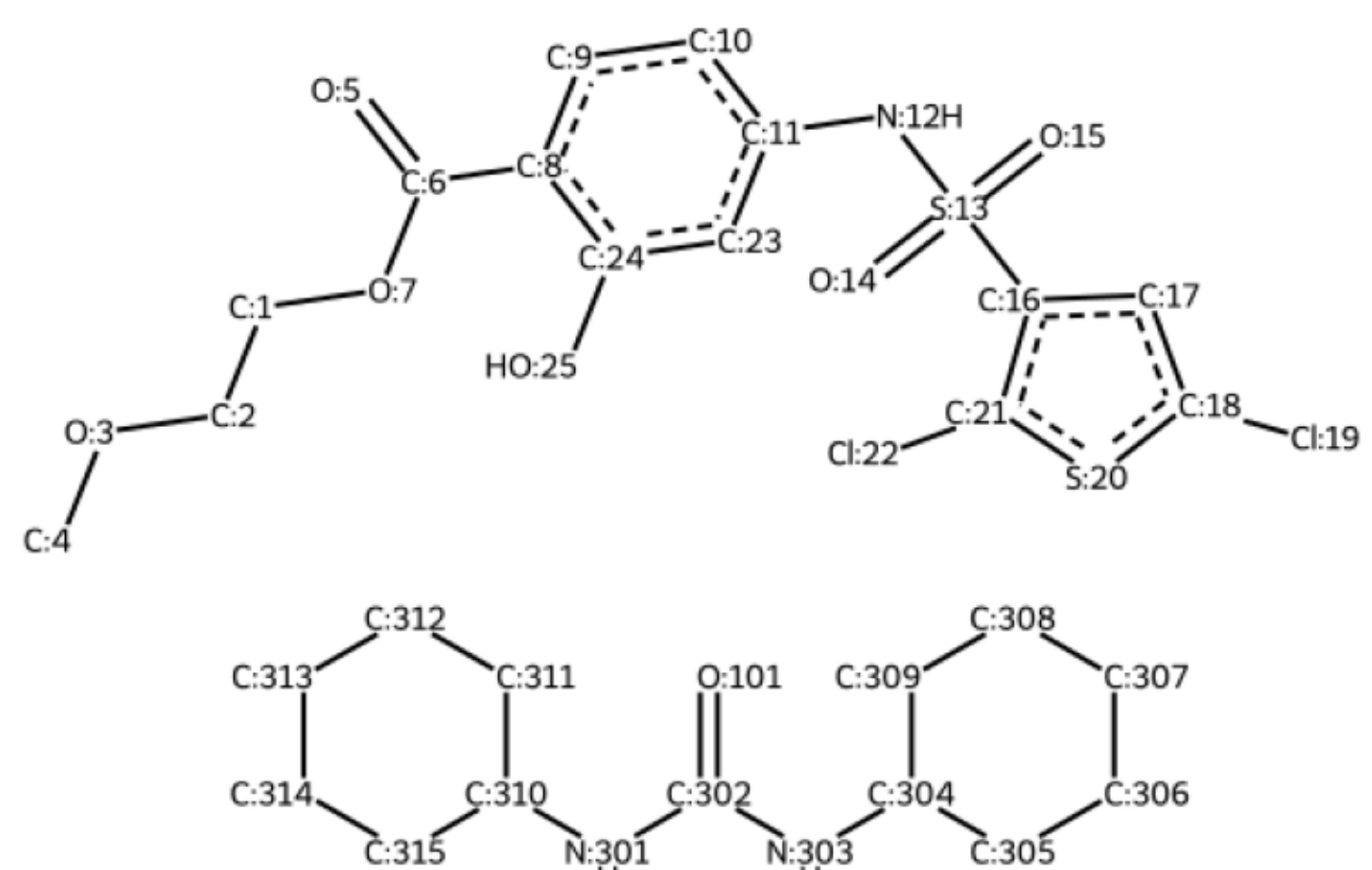
step #5



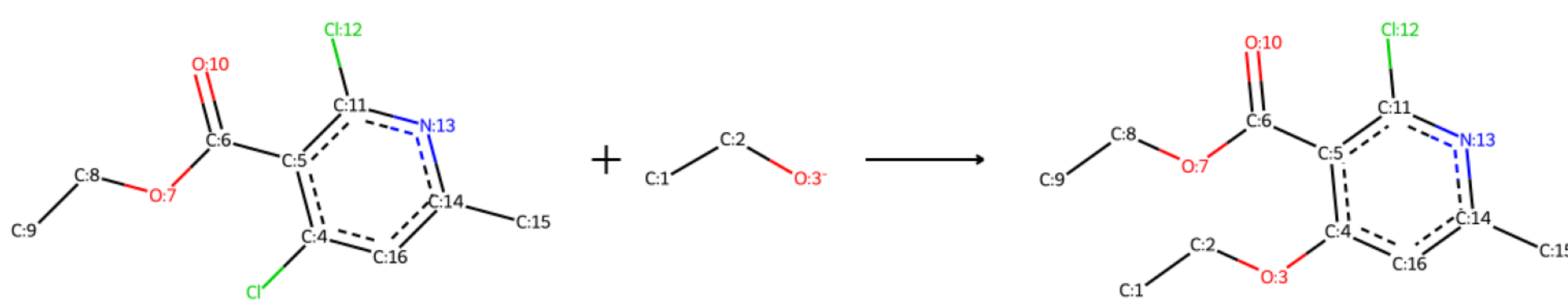
step #6



Product(s)

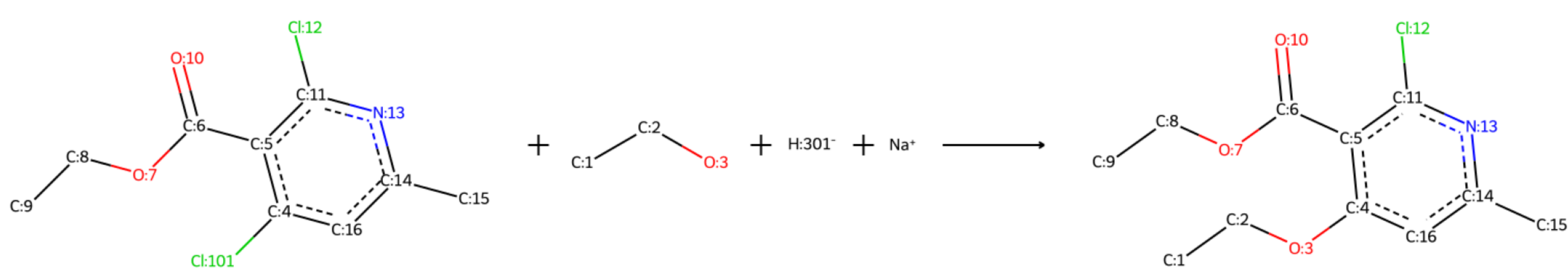


Original reaction sampled RXN_ID:2)



Identified mechanistic class -
S_NAr_{alco(thi)ol(ortho)} reaction

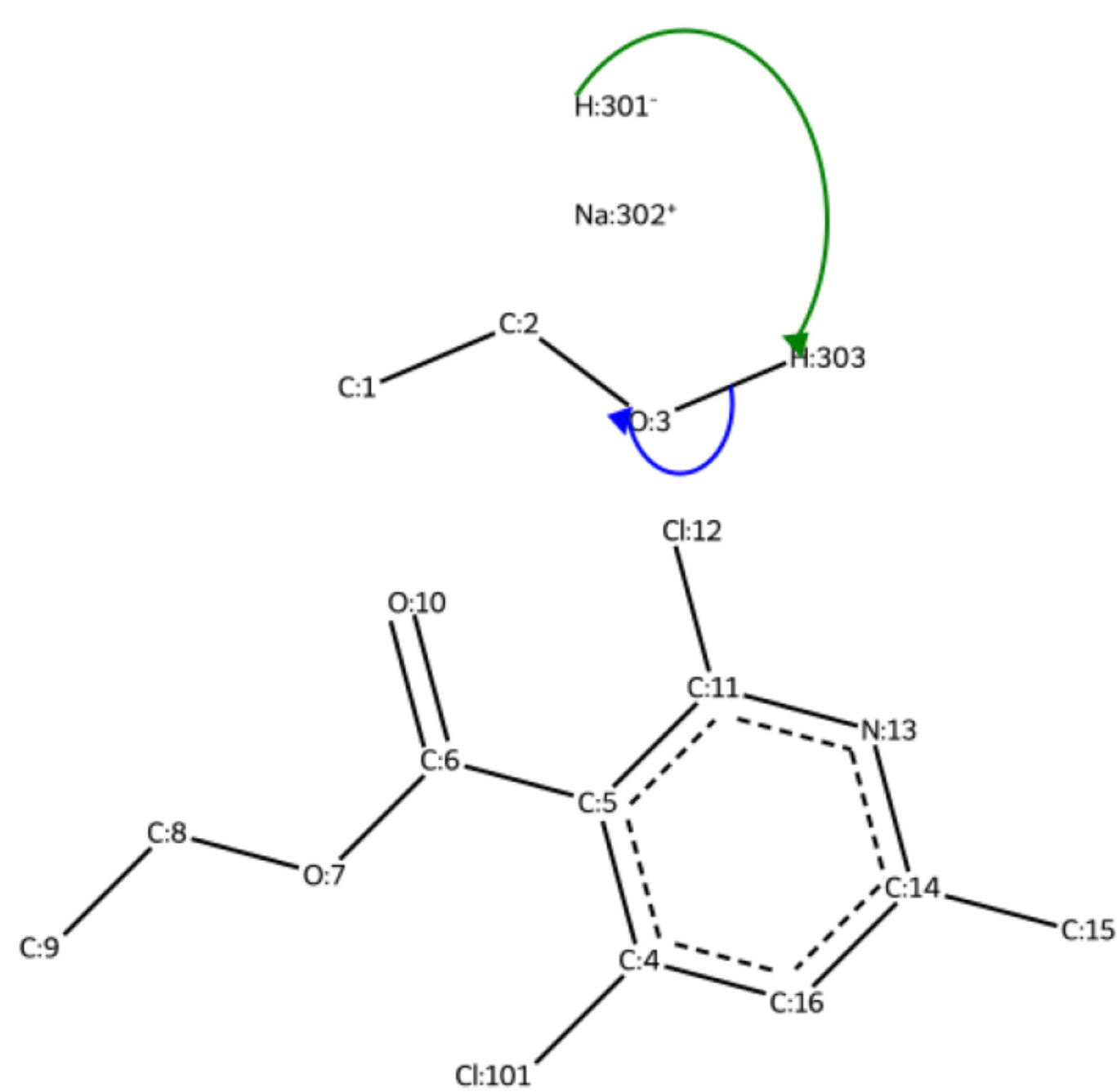
Reaction with missing reagents recovered



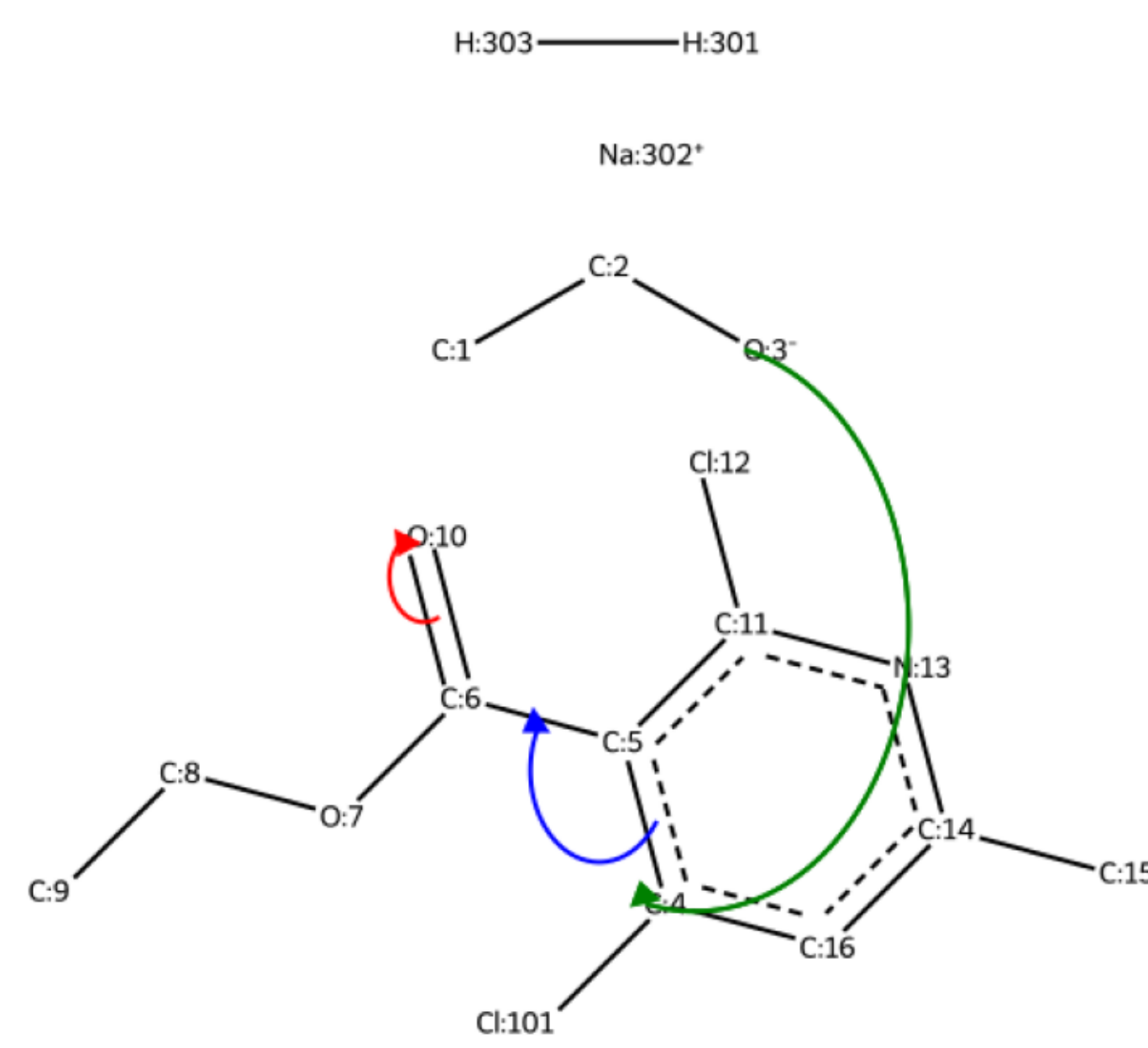
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

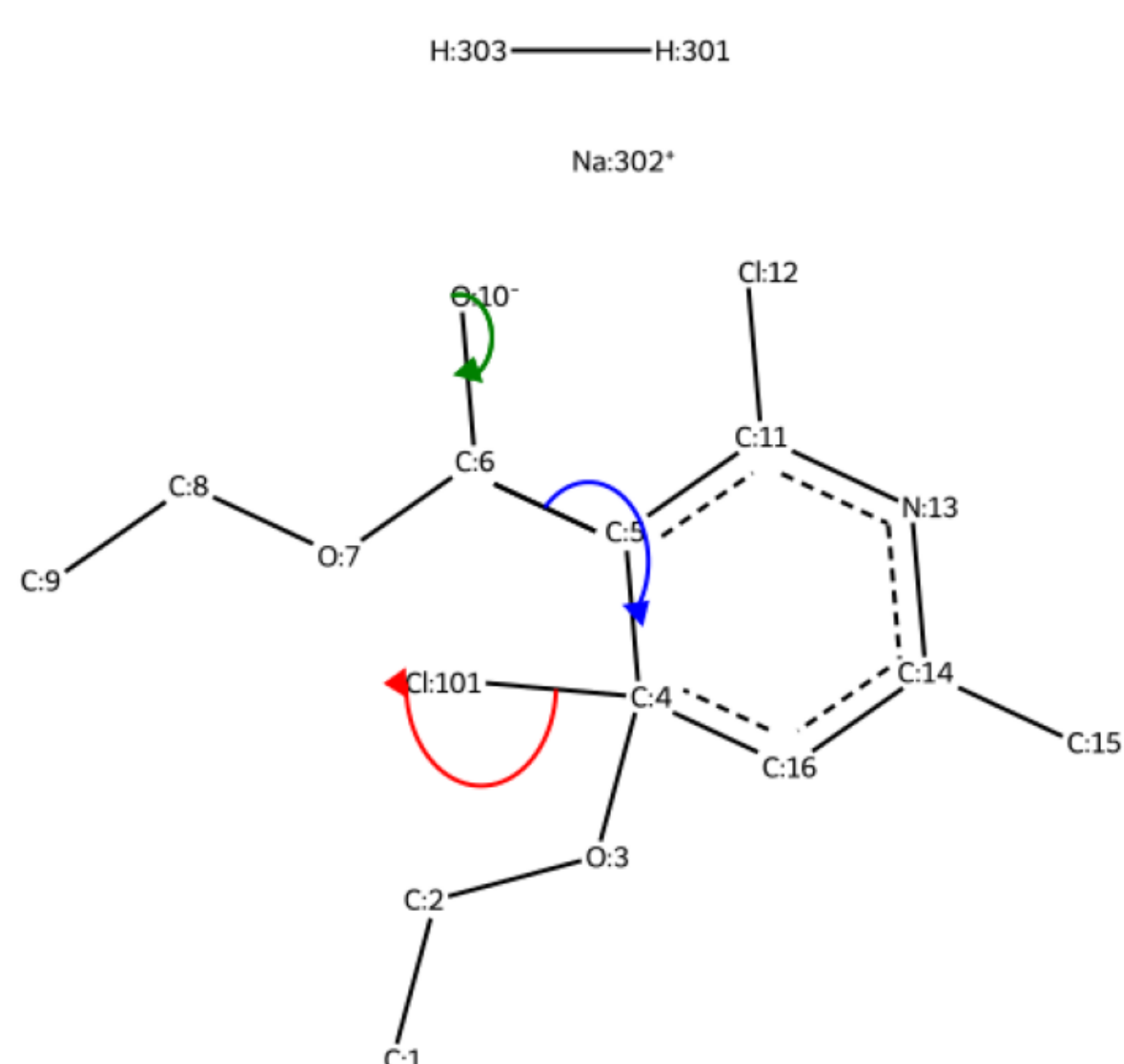
step #1



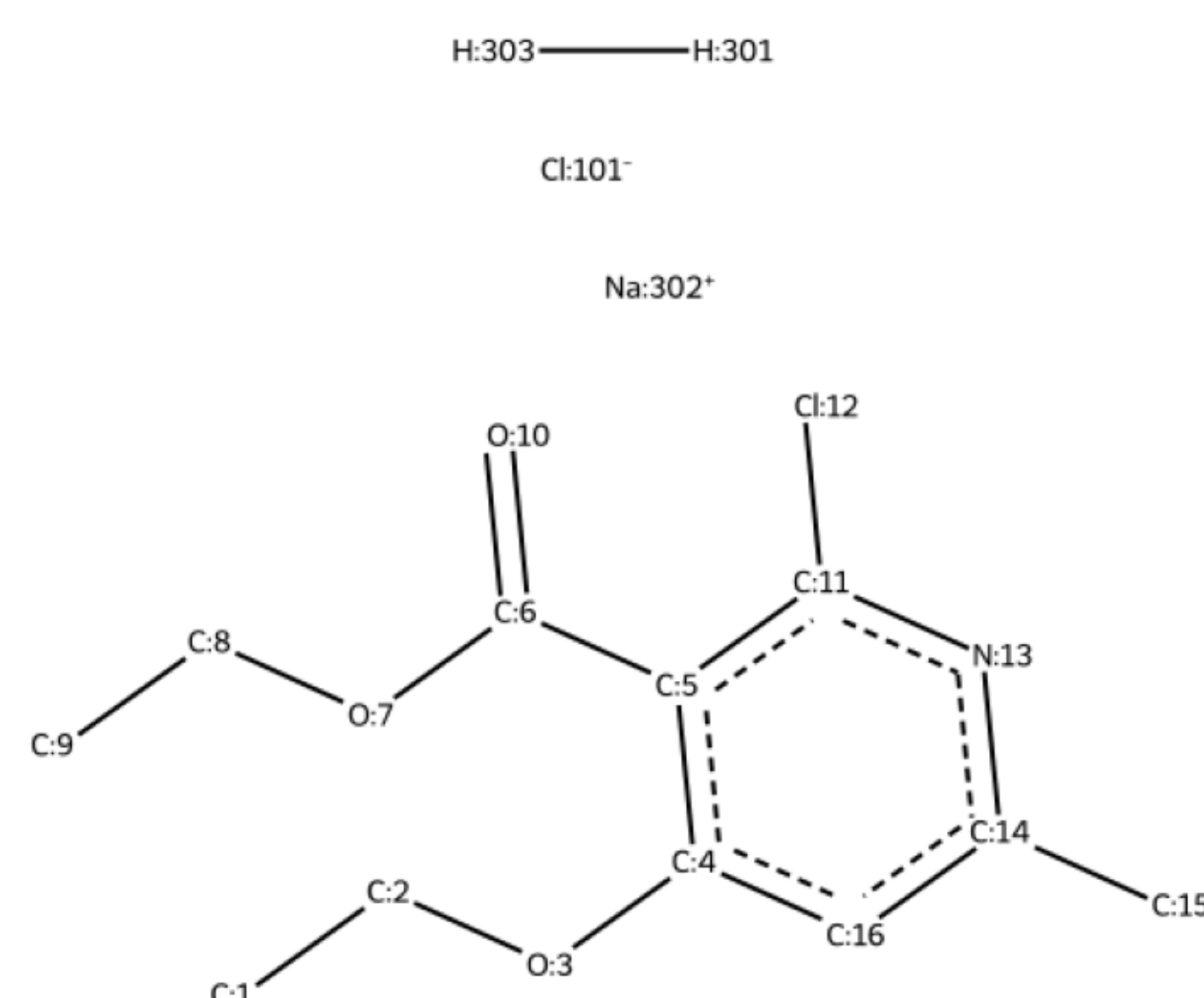
step #2



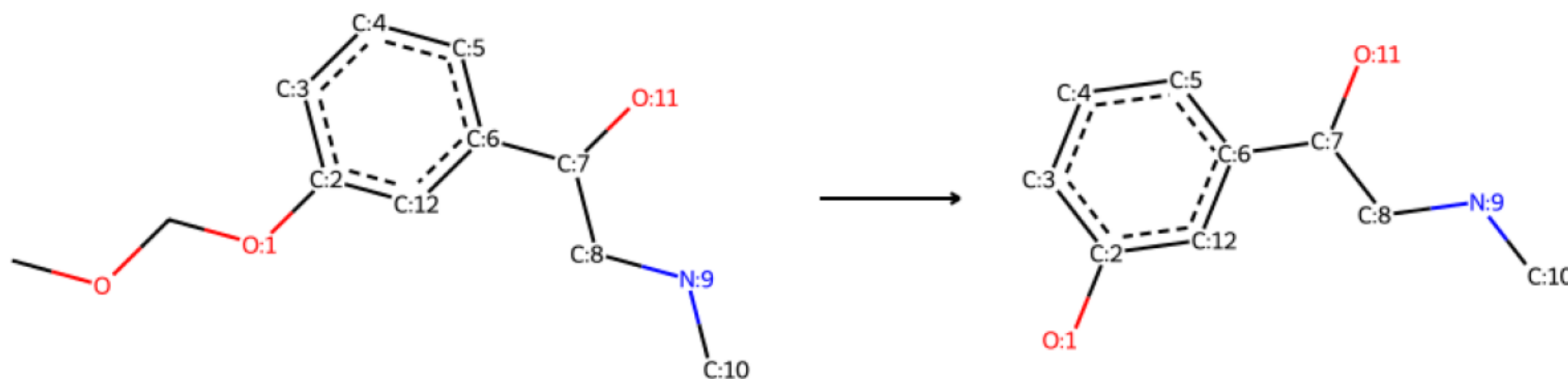
step #3



Product(s)

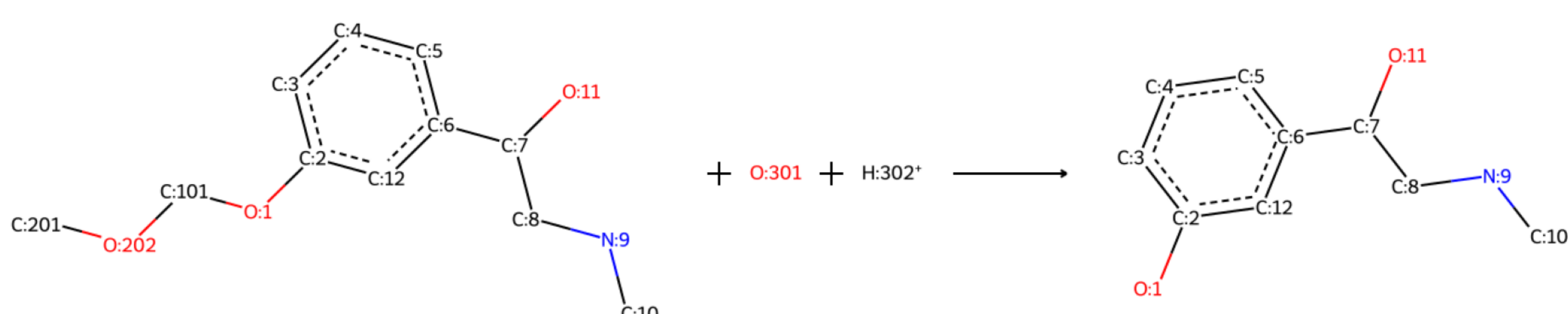


Original reaction sampled RXN_ID:3)



Identified mechanistic class -
(hemi)acetal(amine)_hydrolysis reaction

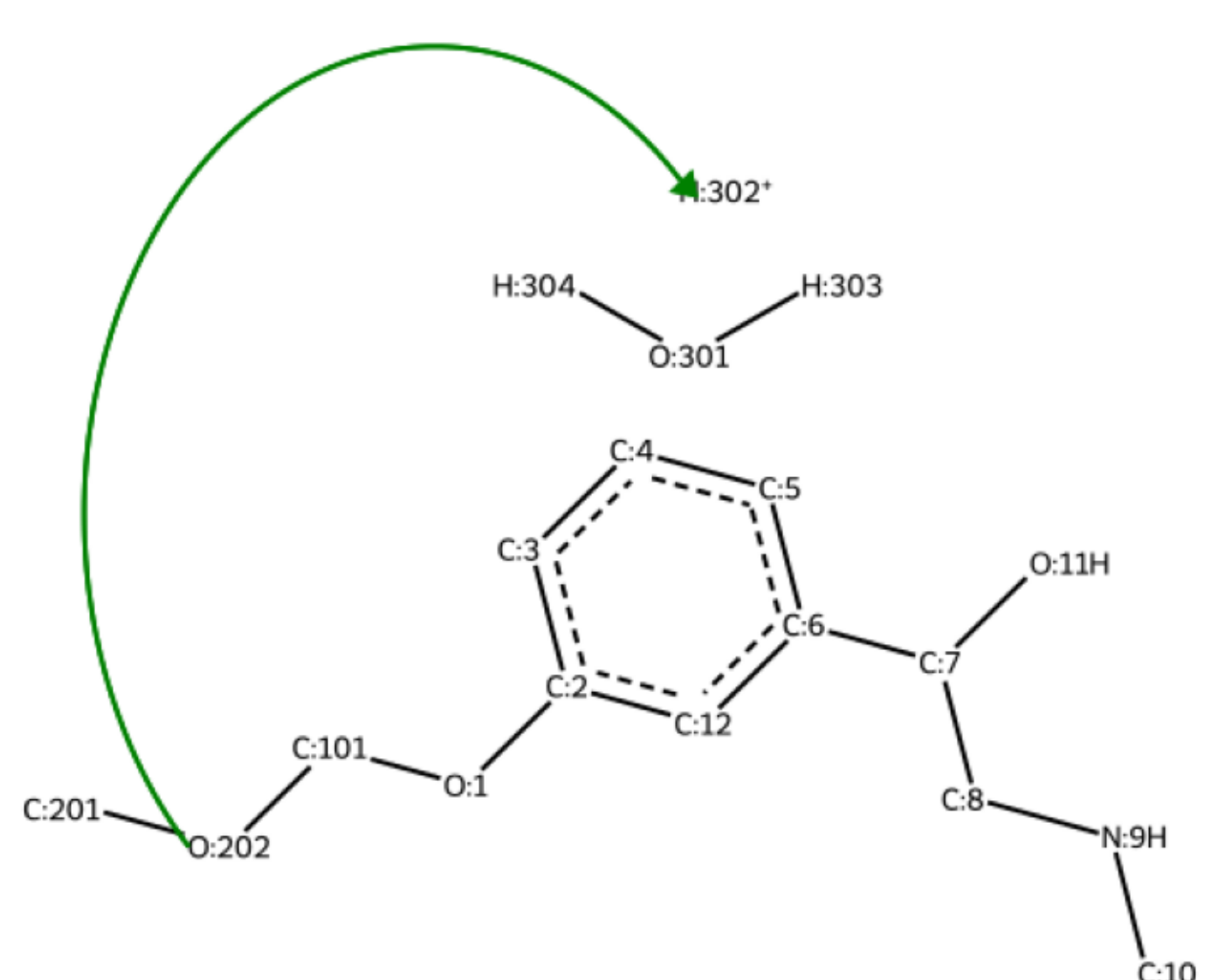
Reaction with missing reagents recovered



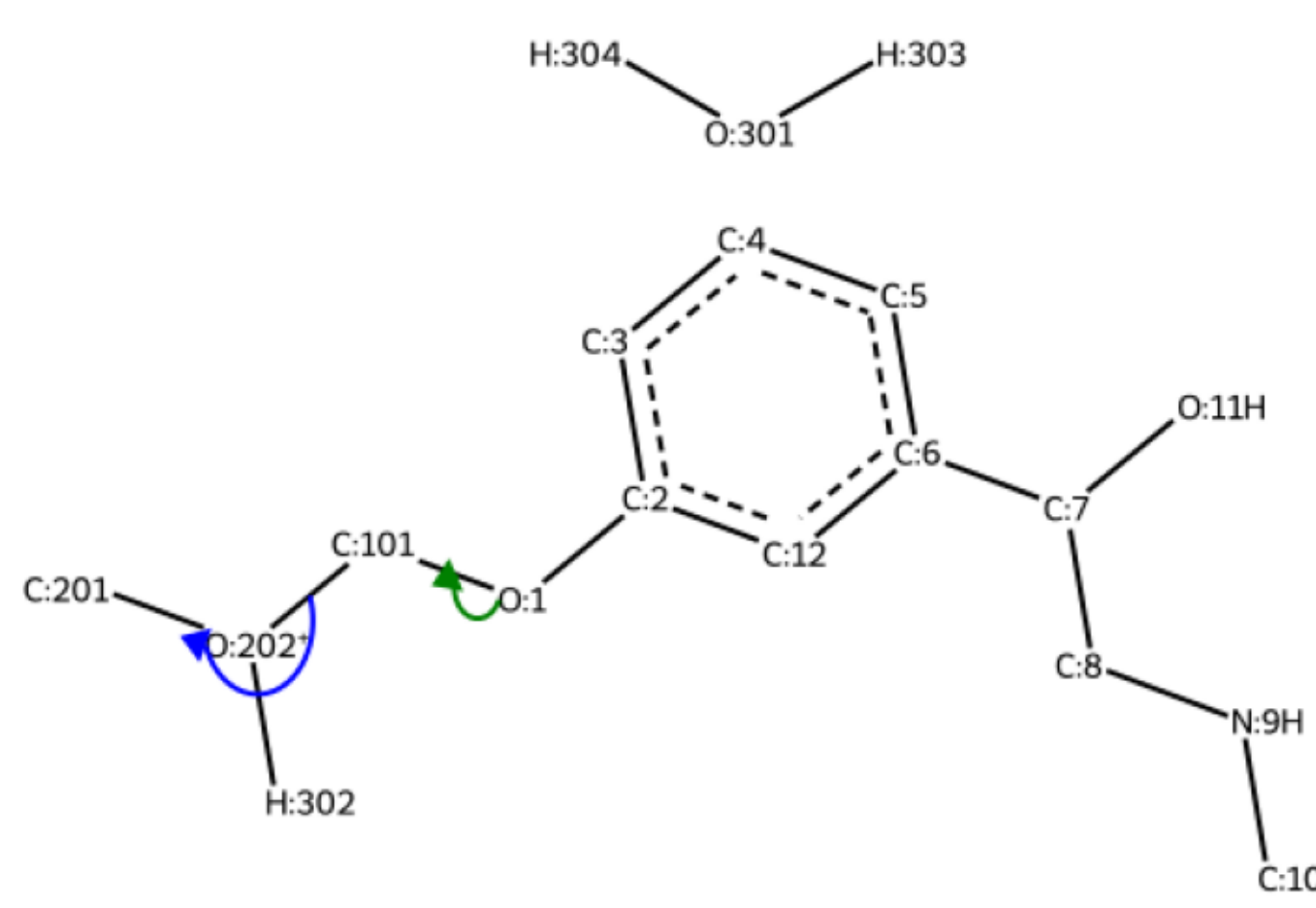
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

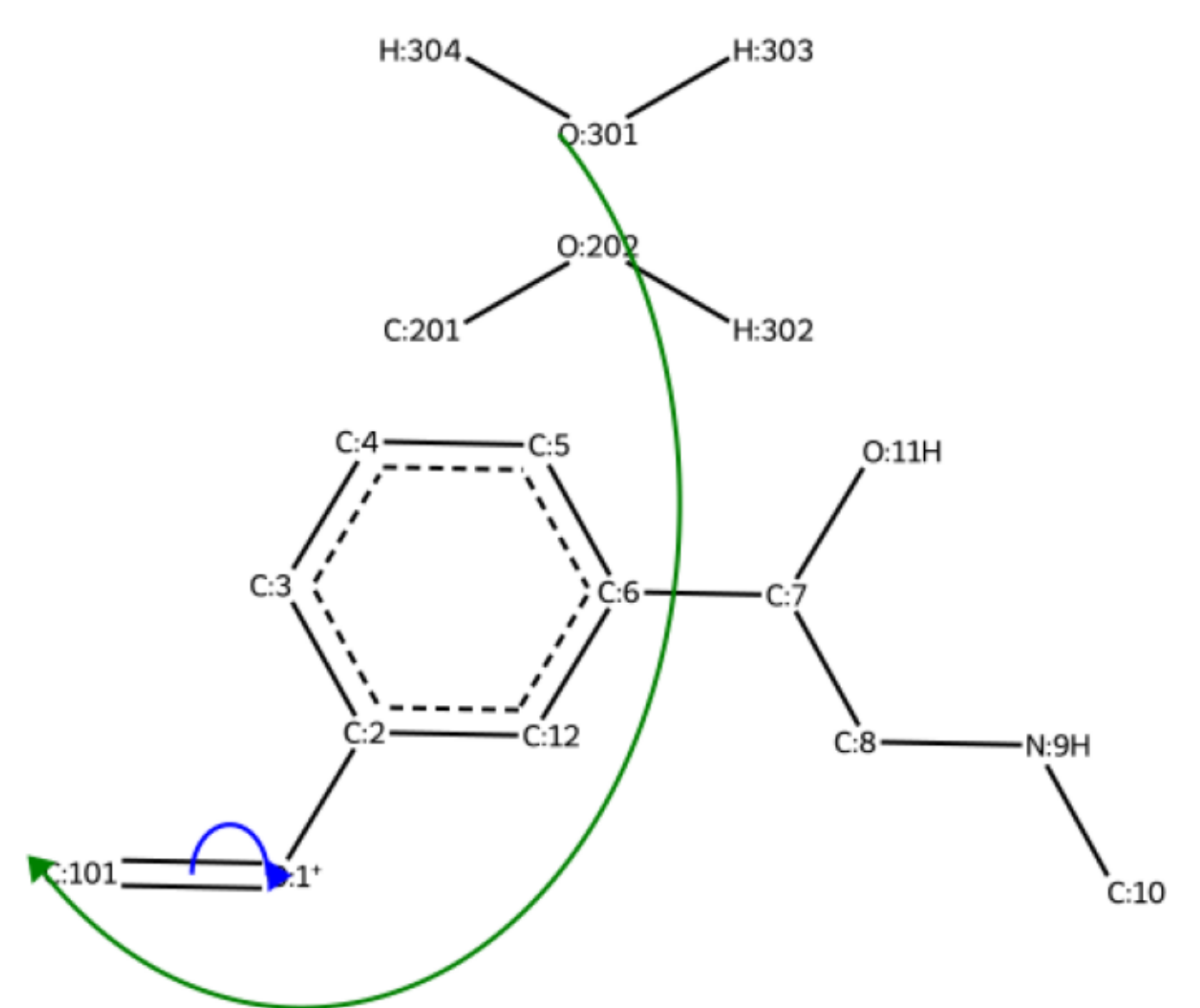
step #1



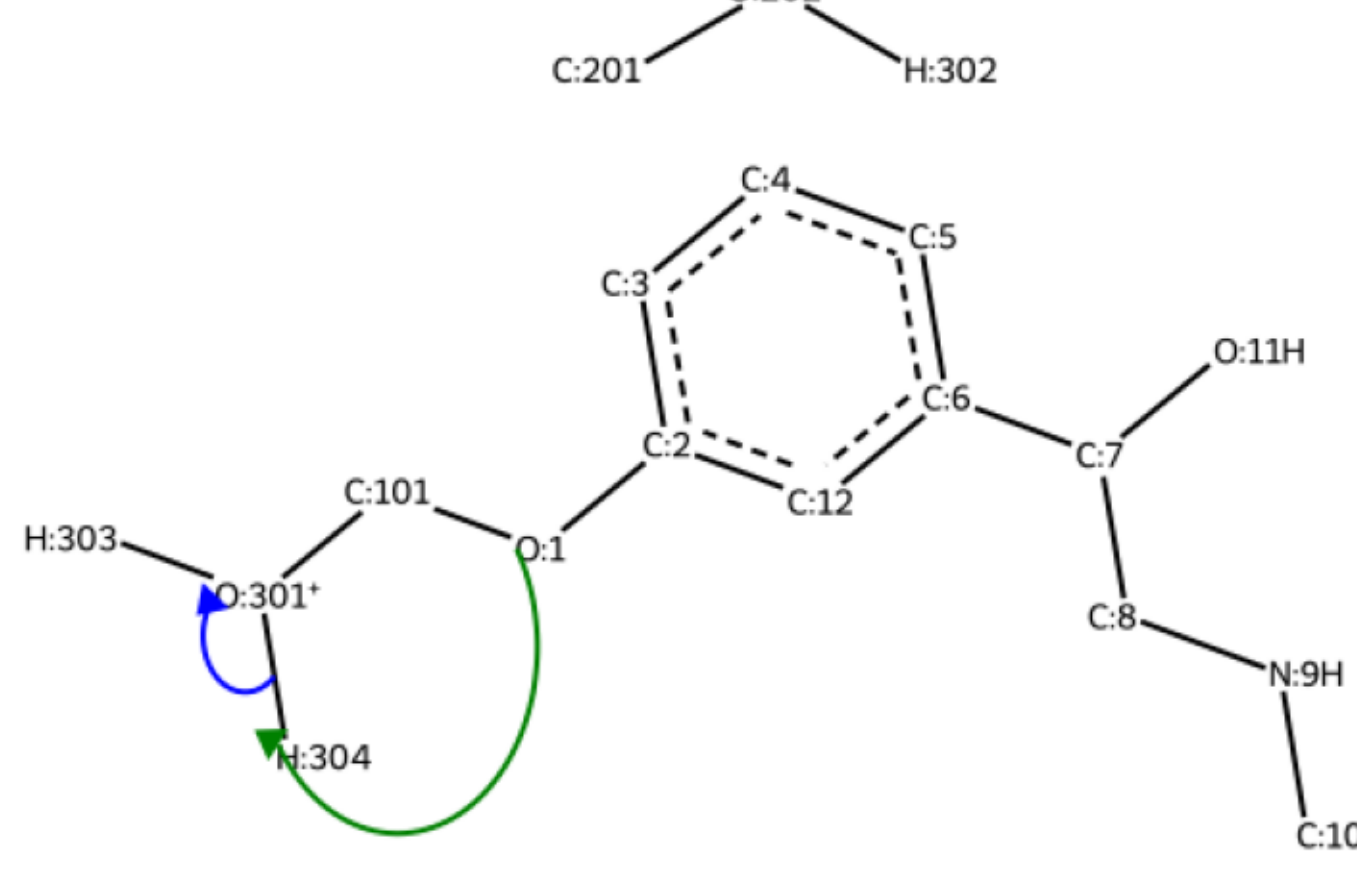
step #2



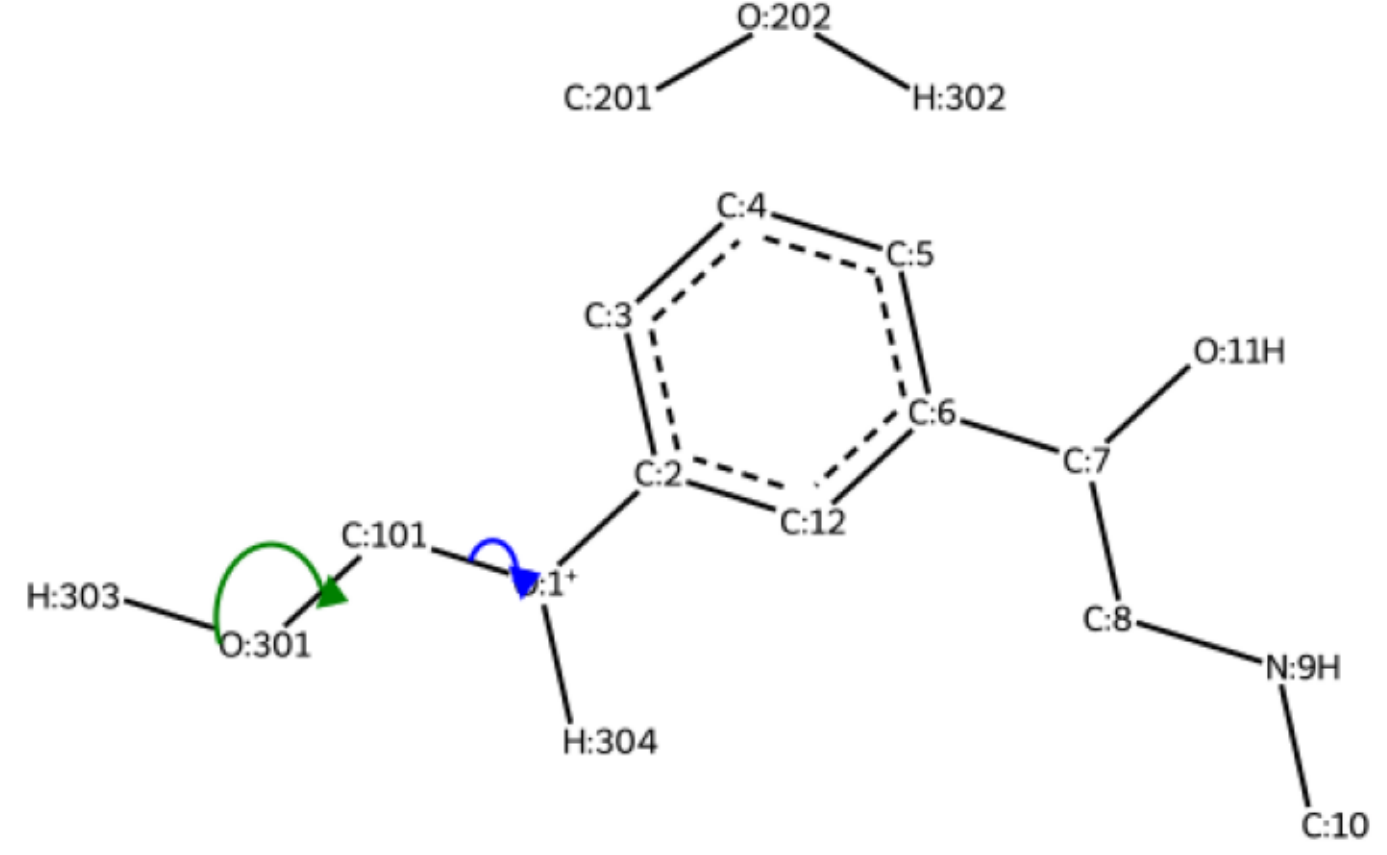
step #3



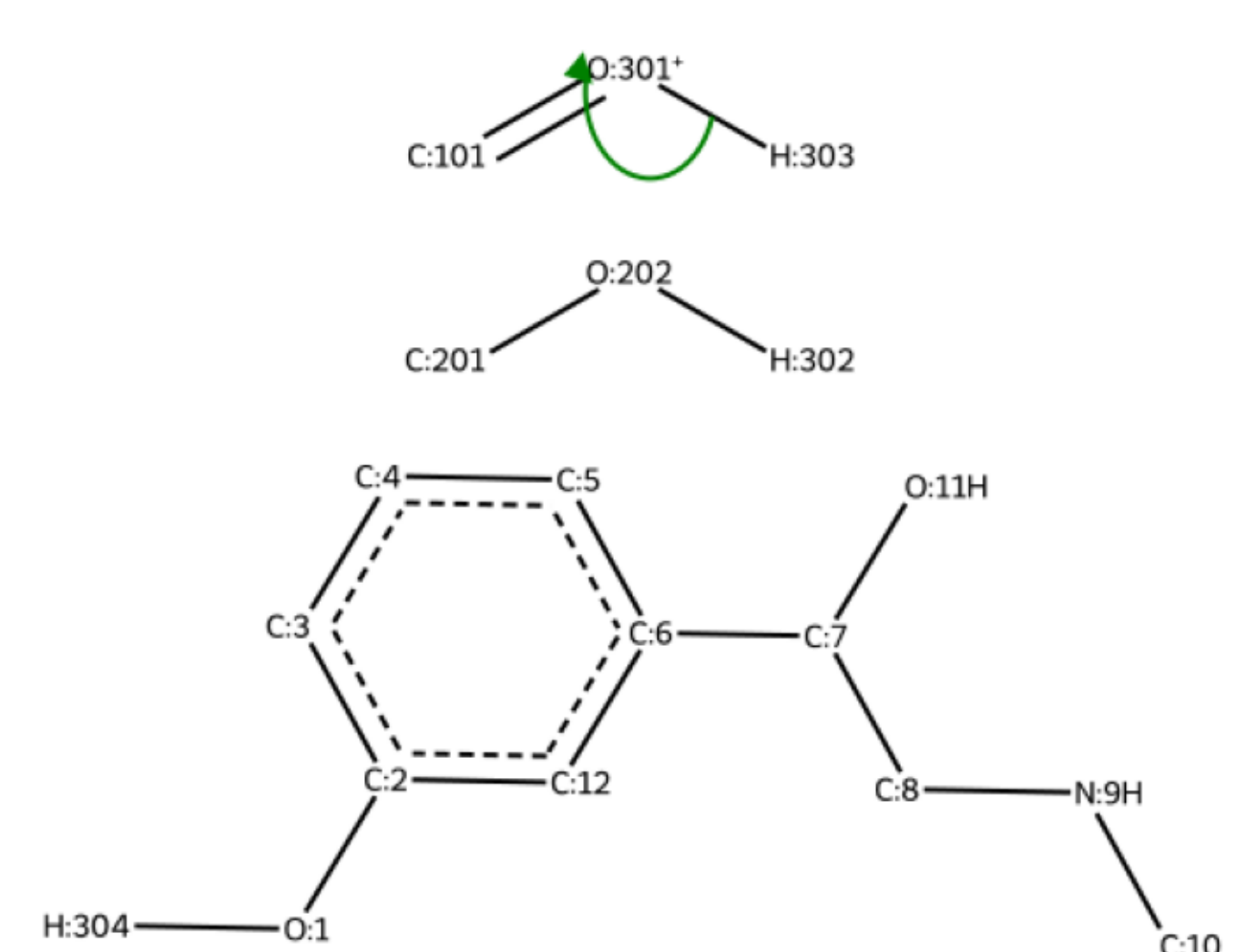
step #4



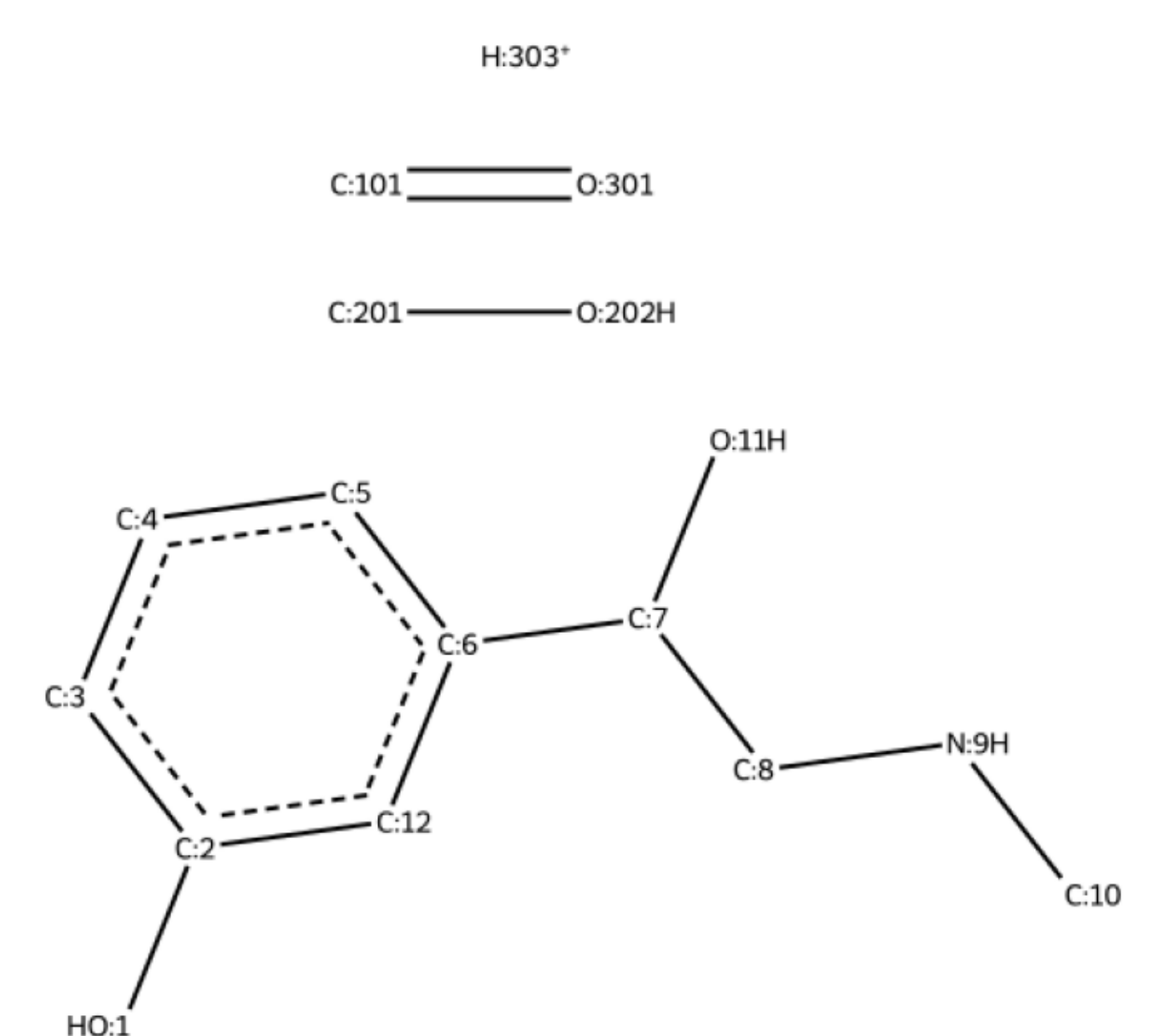
step #5



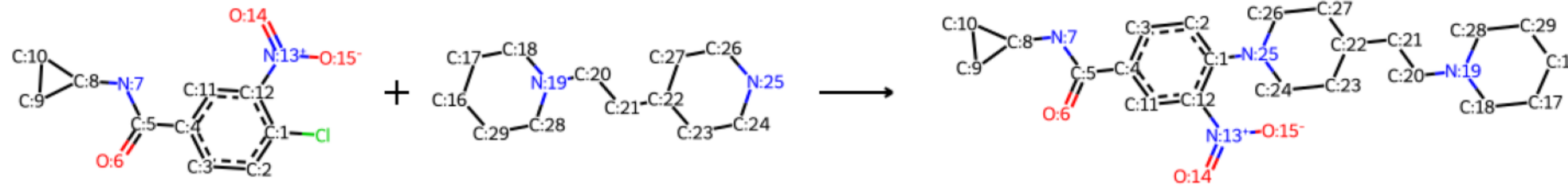
step #6



Product(s)

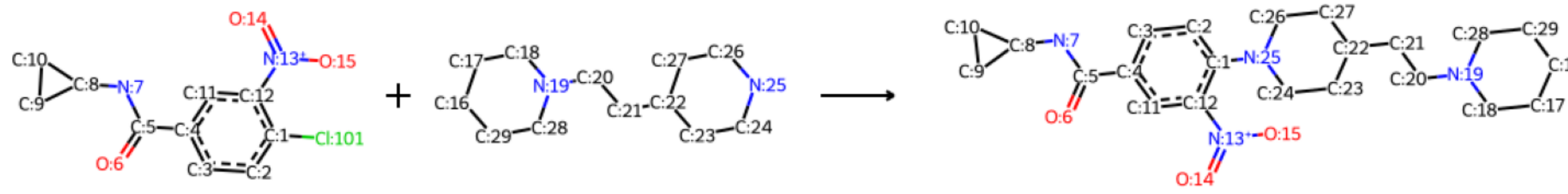


Original reaction sampled RXN_ID:4)



Identified mechanistic class -
S_NAr(ortho) reaction

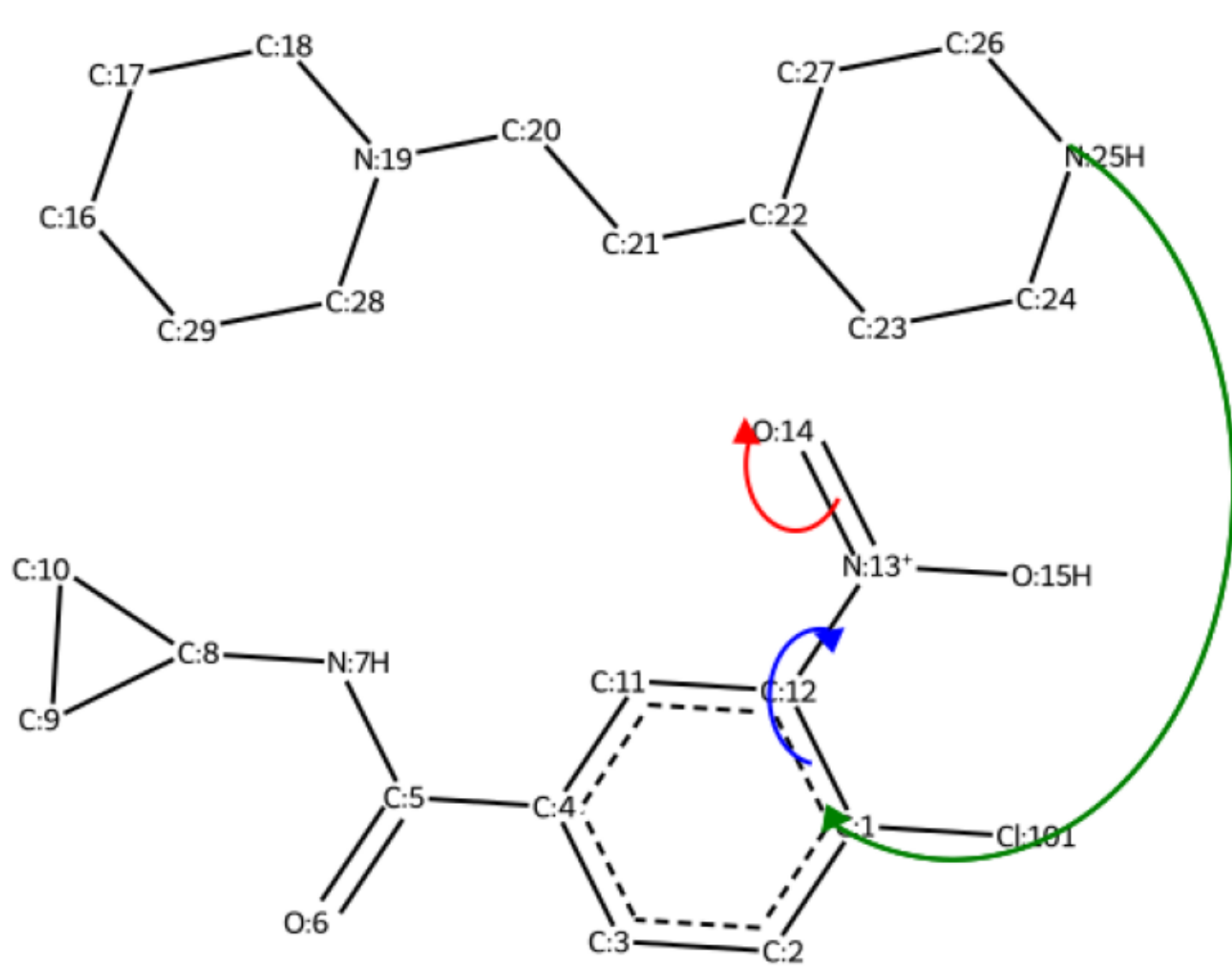
Reaction with missing reagents recovered



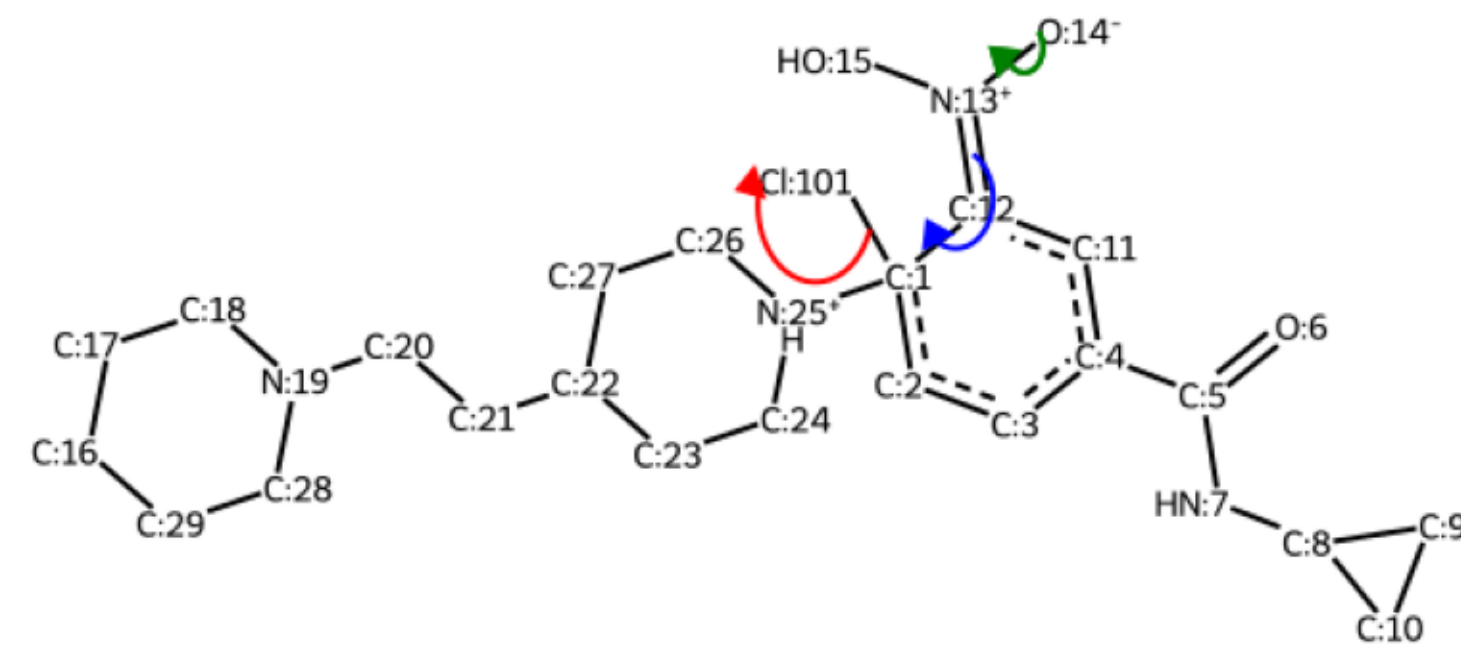
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

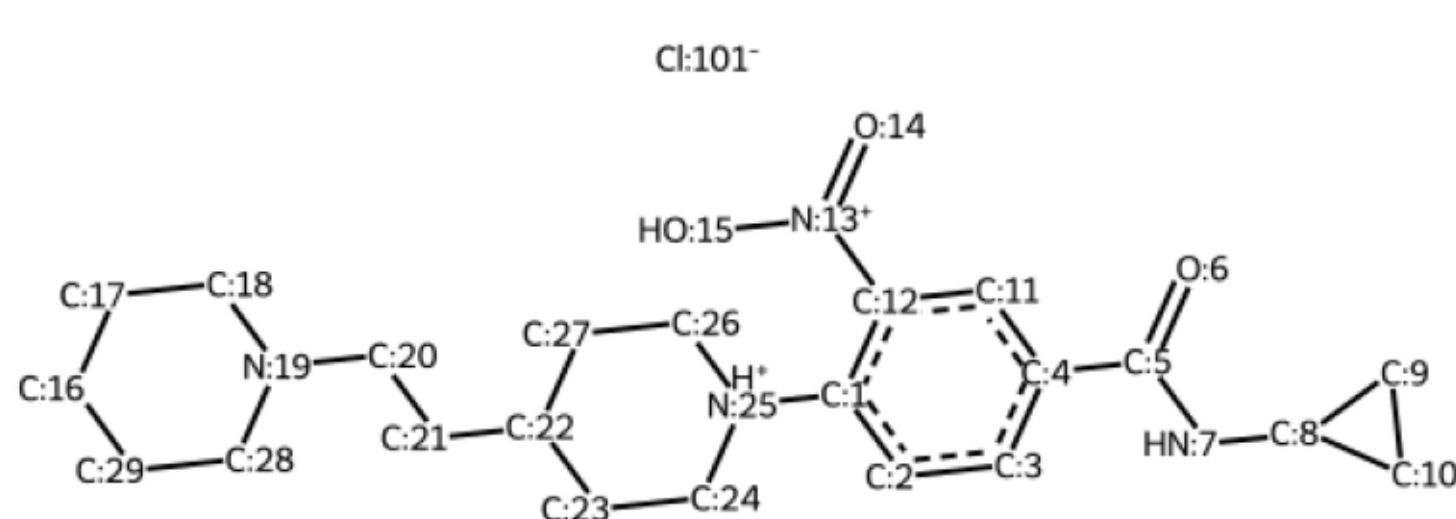
step #1



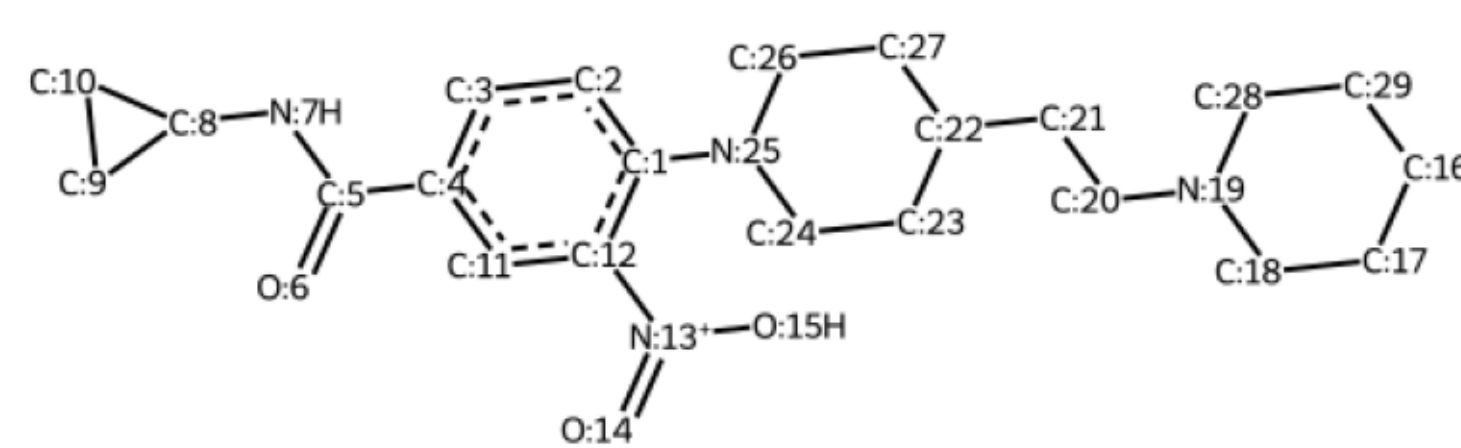
step #2



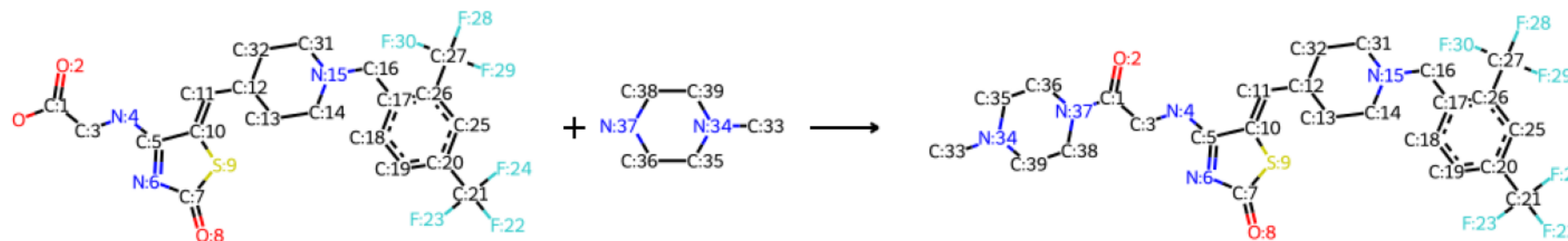
Product(s)



proton transfer

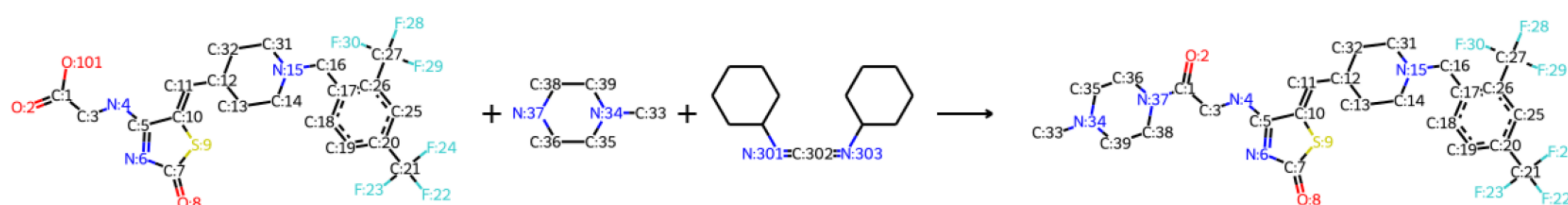


Original reaction
sampled RXN_ID:5)



Identified mechanistic class -
DCC_condensation reaction

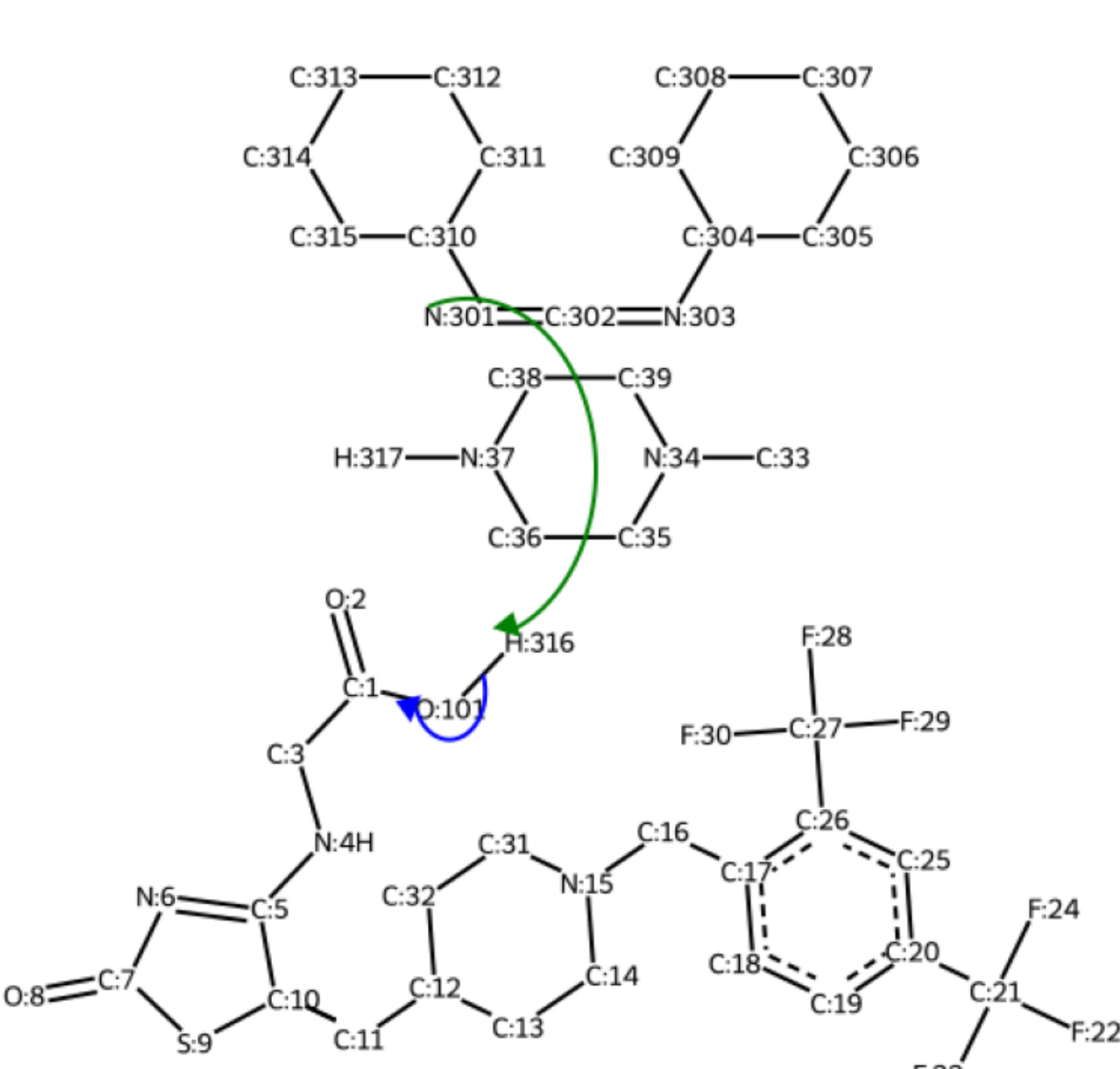
Reaction with missing reagents recovered



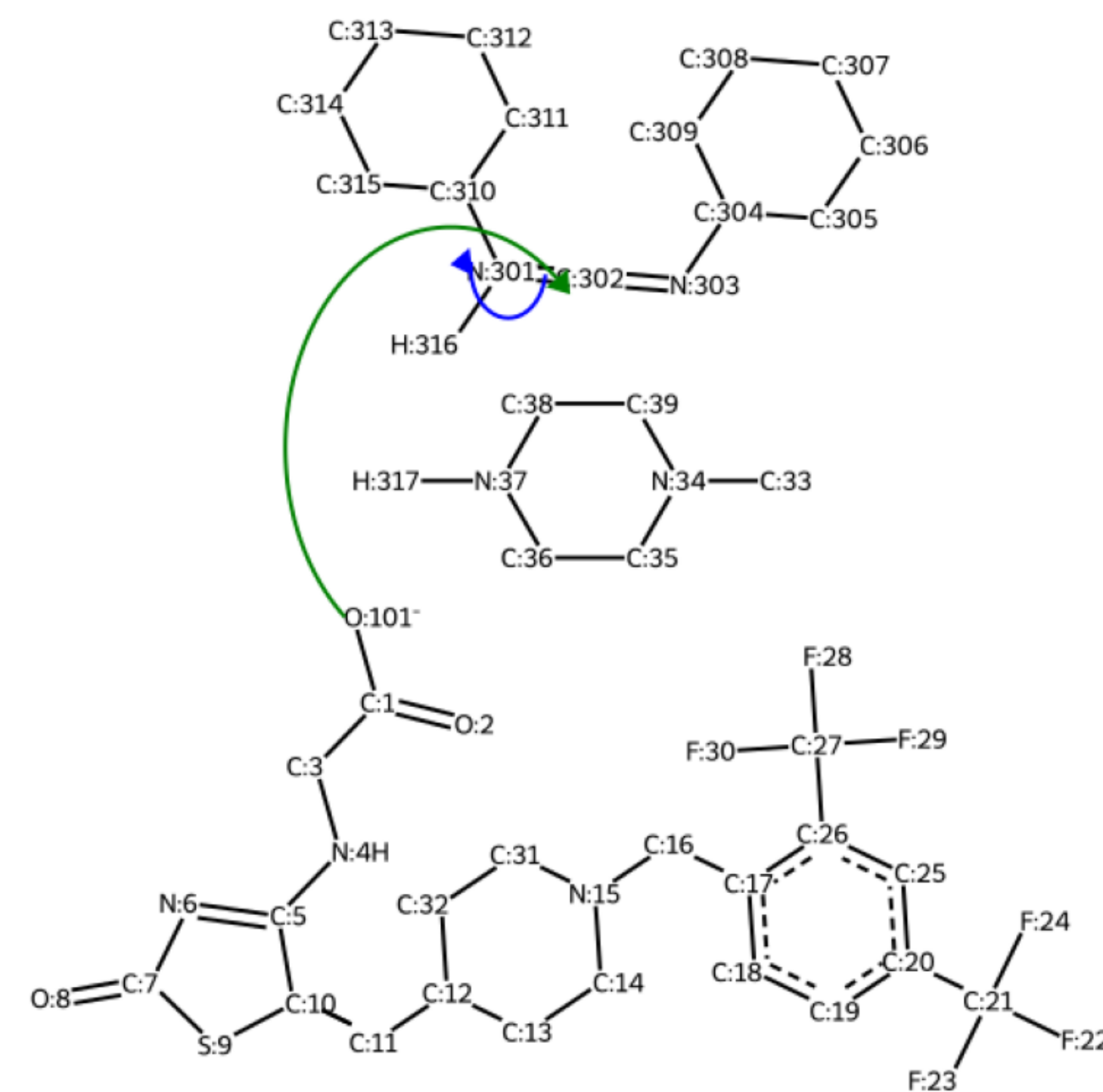
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

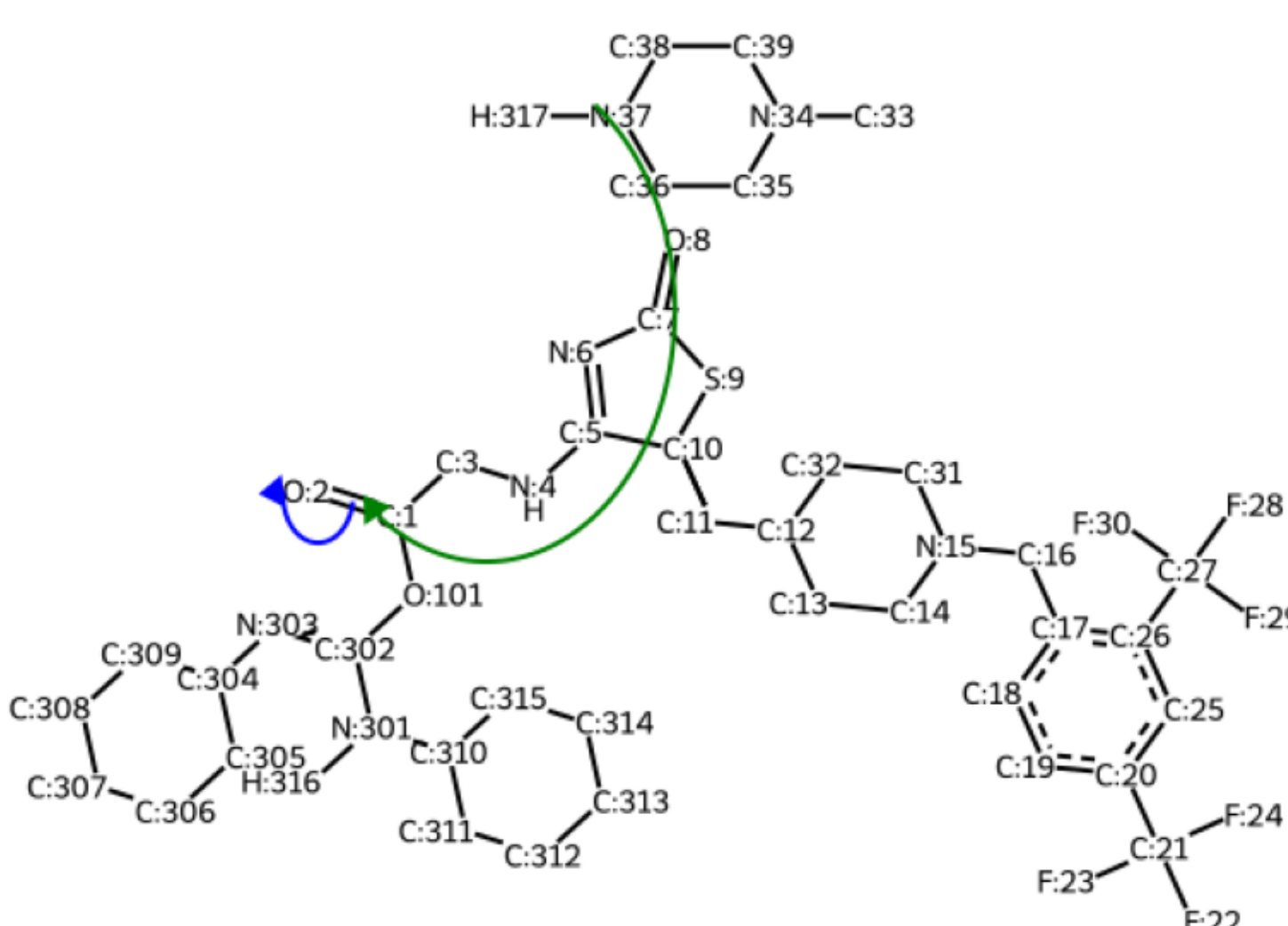
step #1



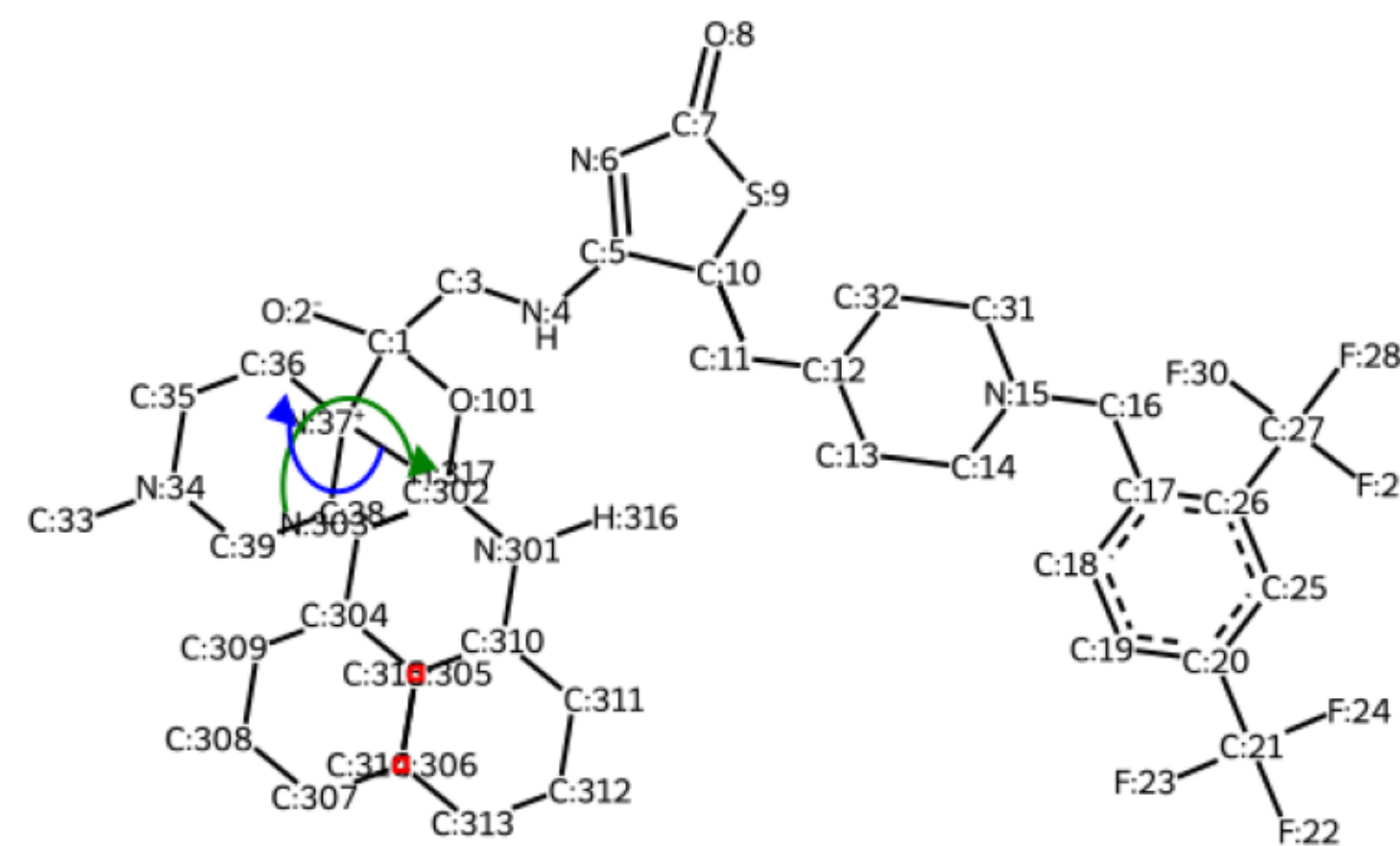
step #2



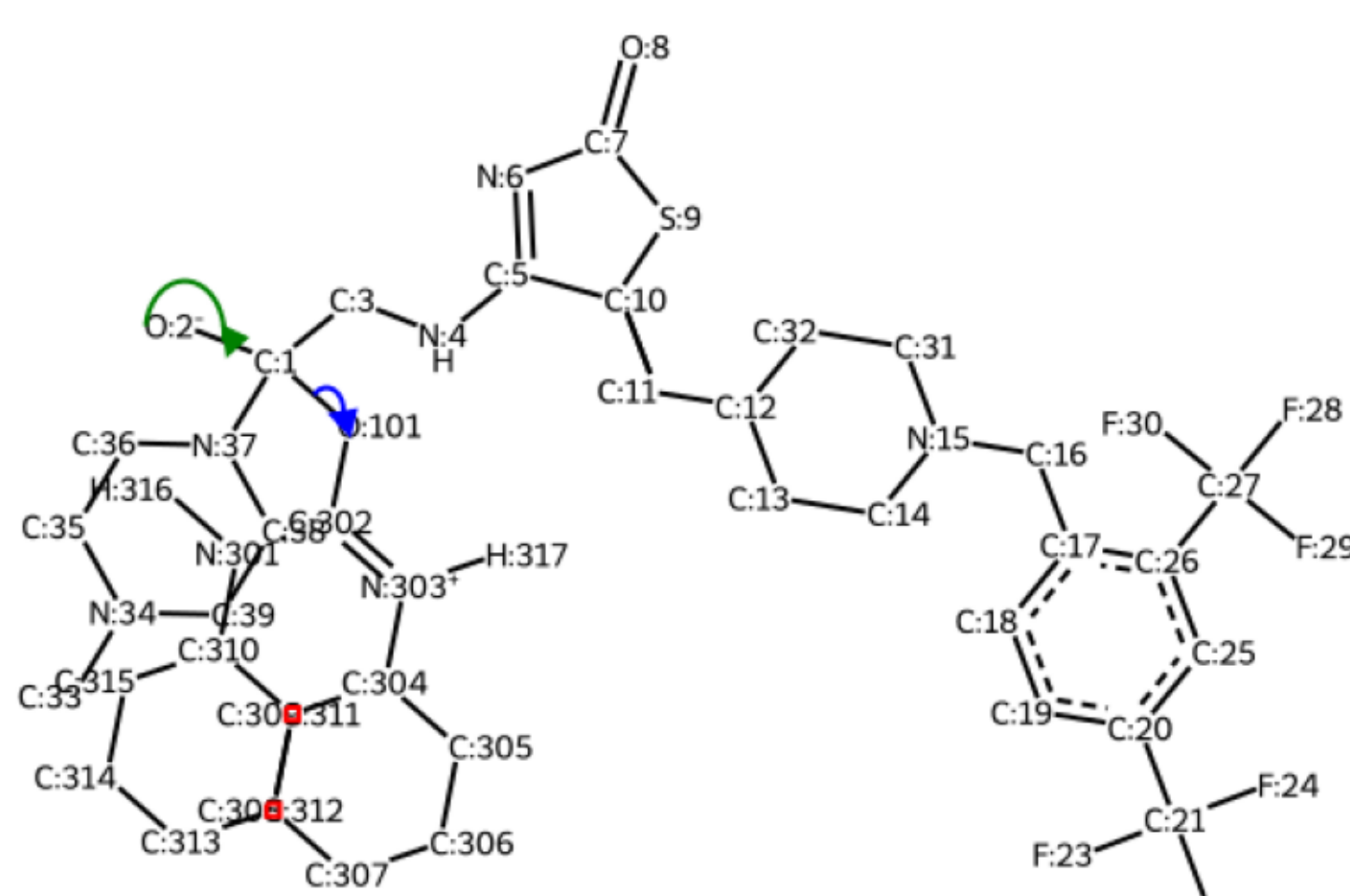
step #3



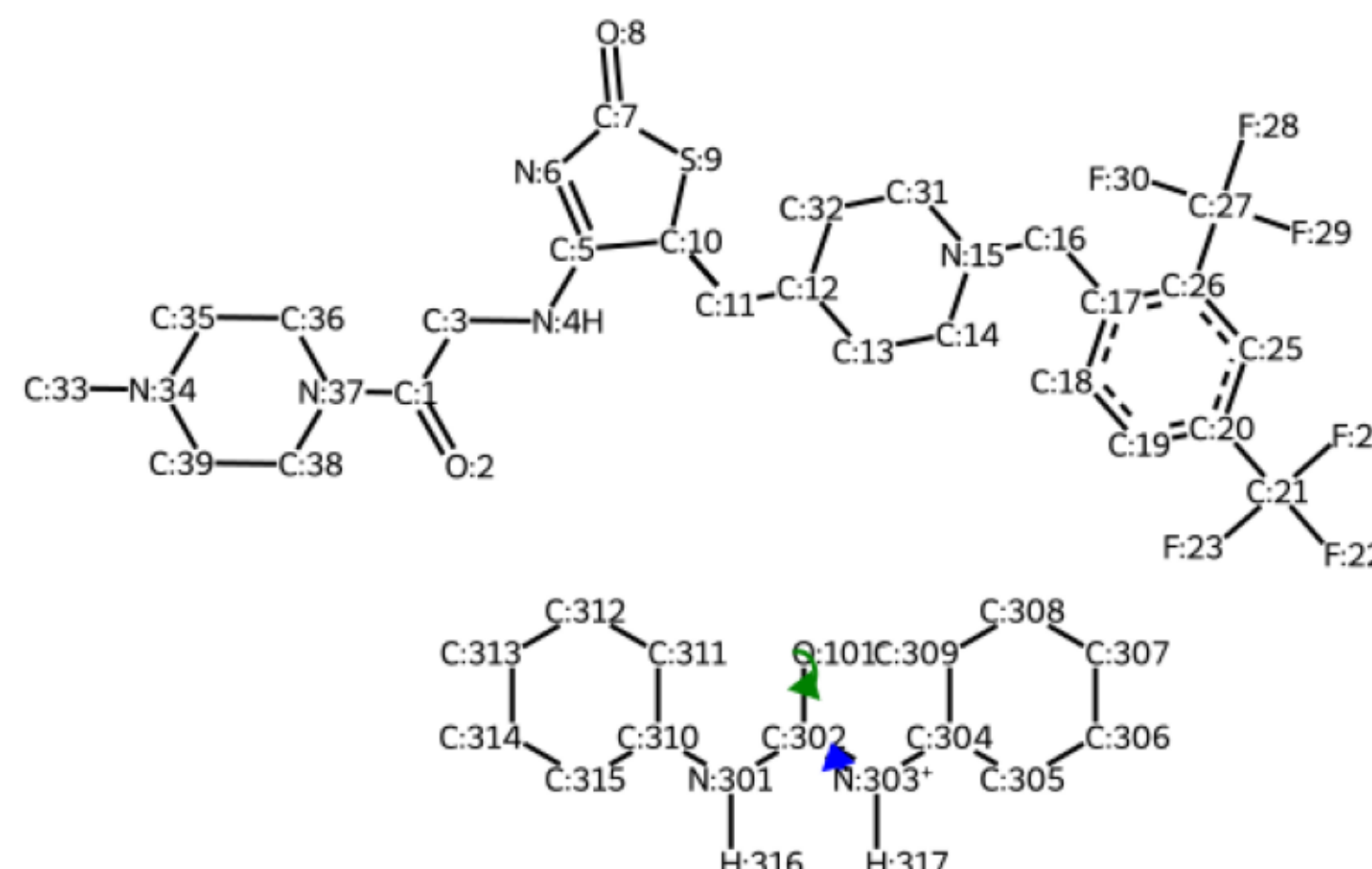
step #4



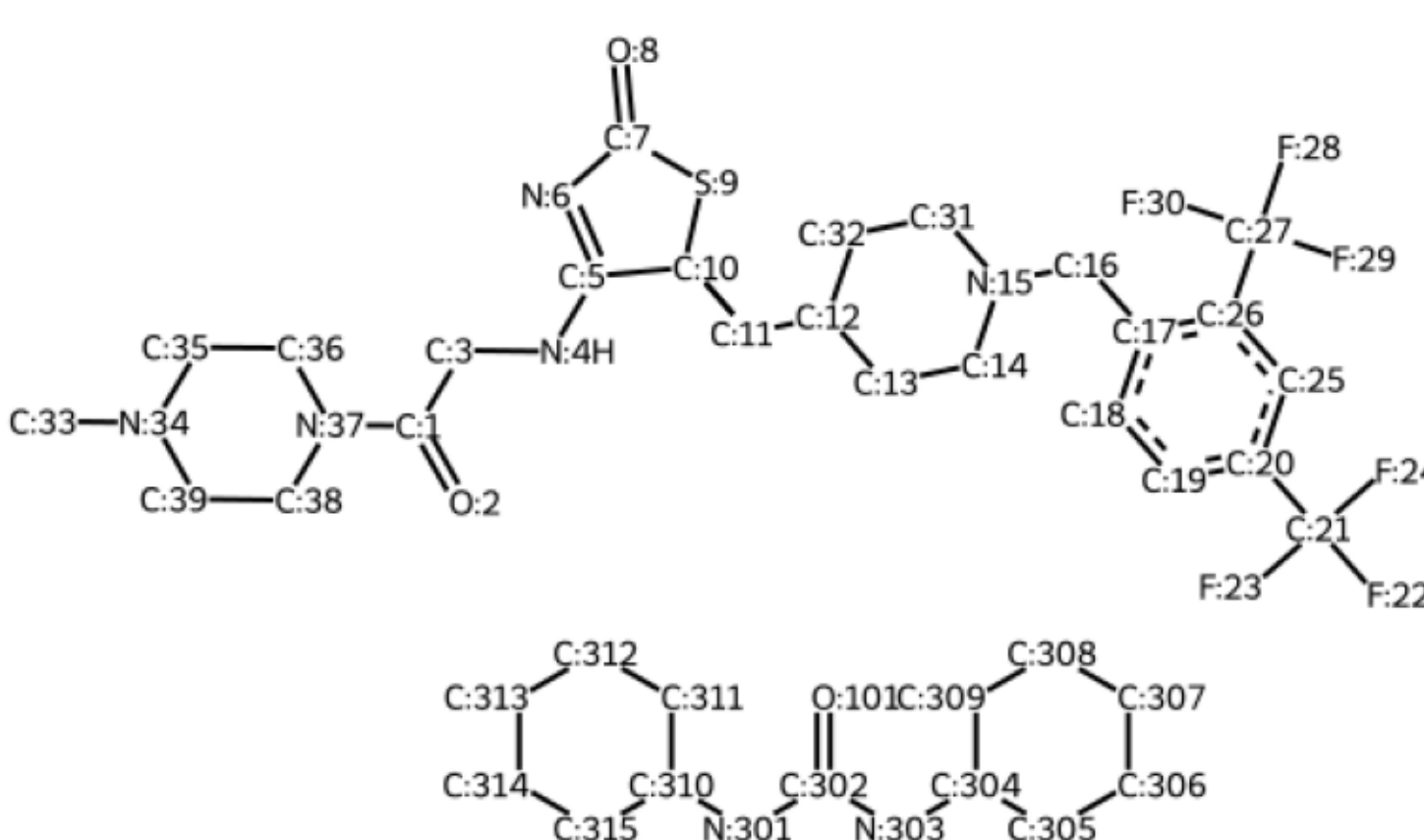
step #5



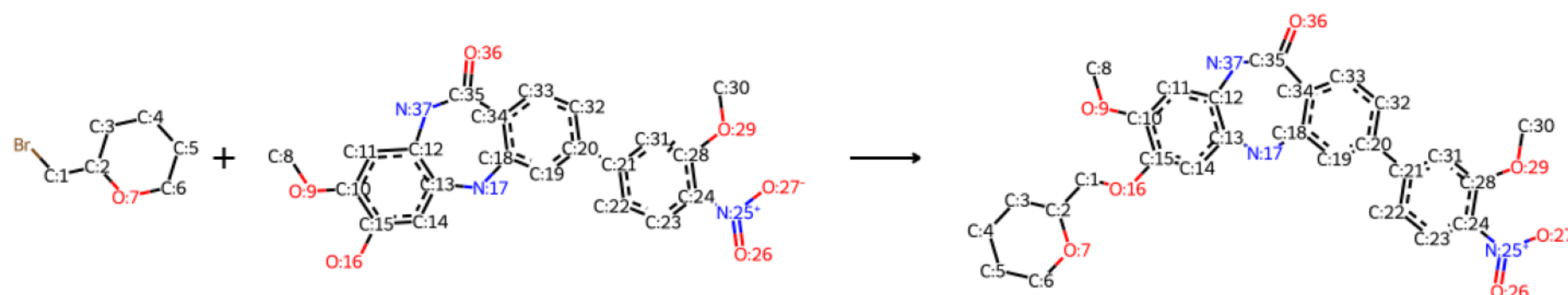
step #6



Product(s)

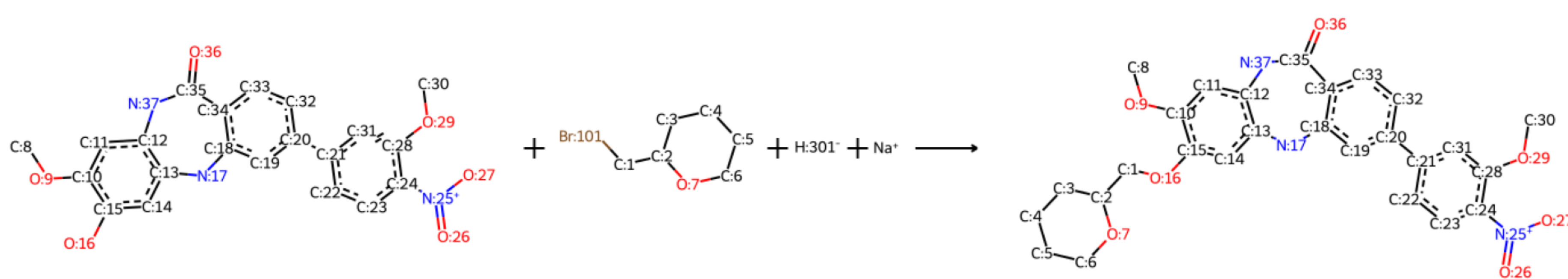


Original reaction sampled RXN_ID:6)



Identified mechanistic class -
SN₂alcohol(thiol) reaction

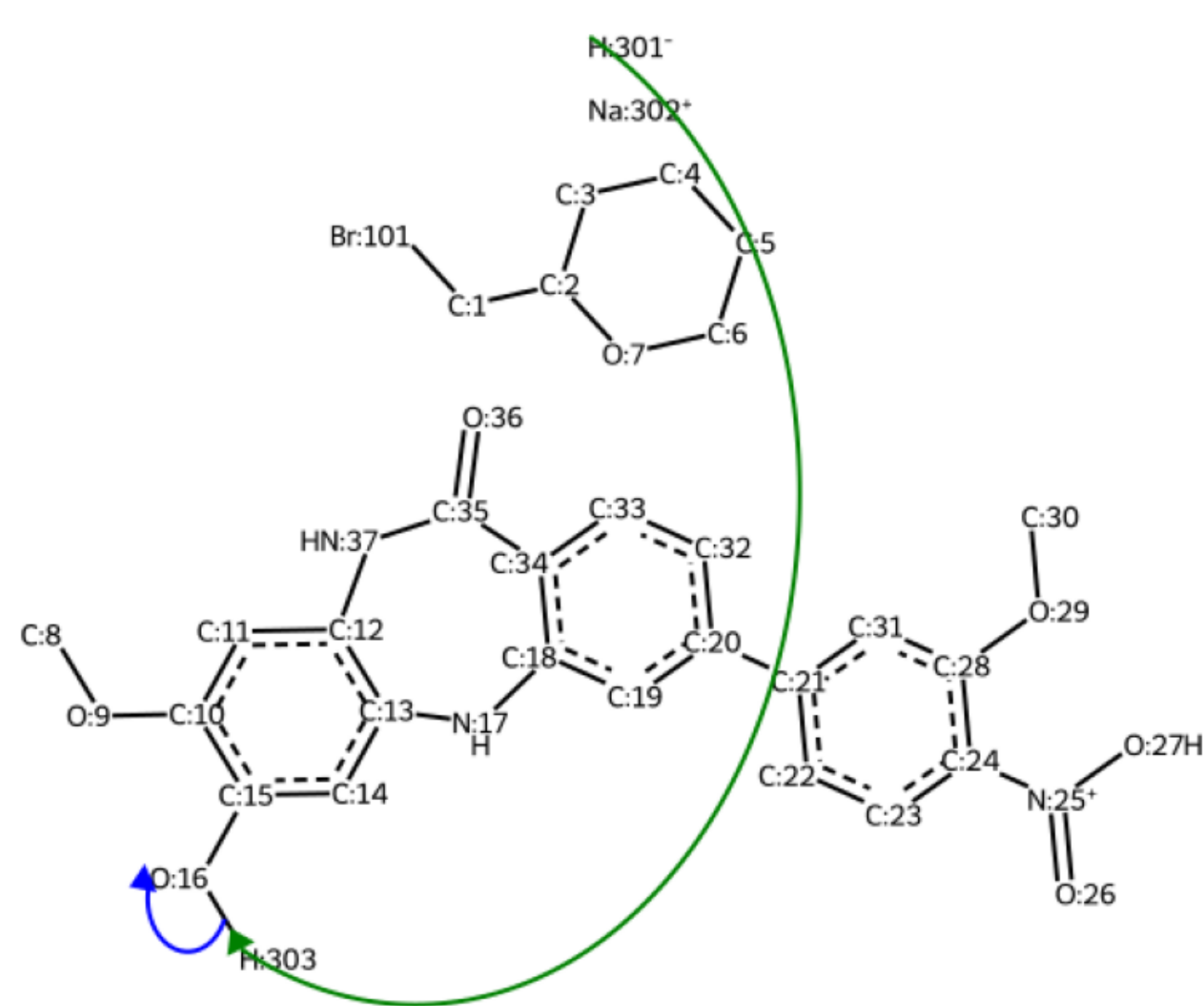
Reaction with missing reagents recovered



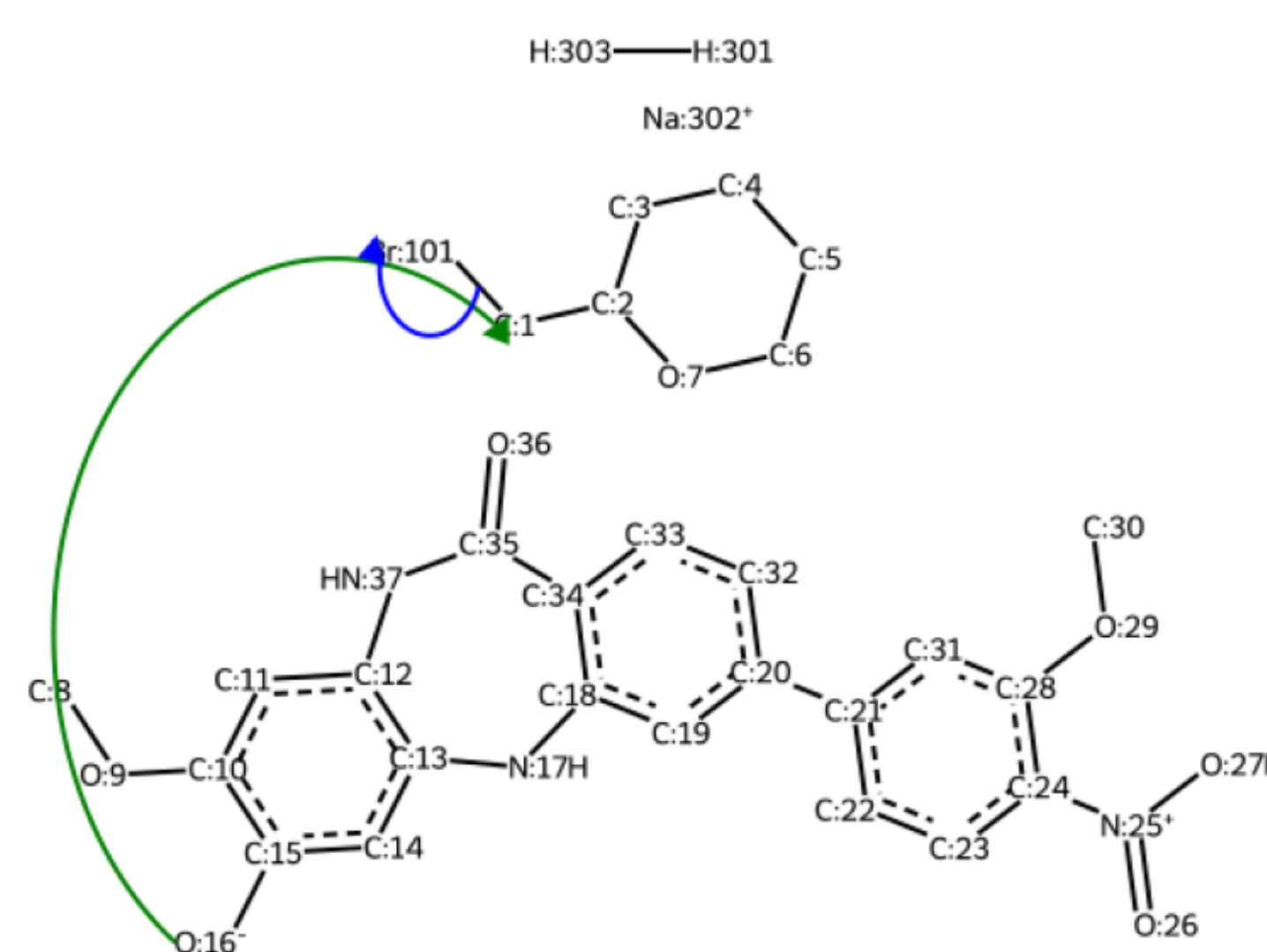
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

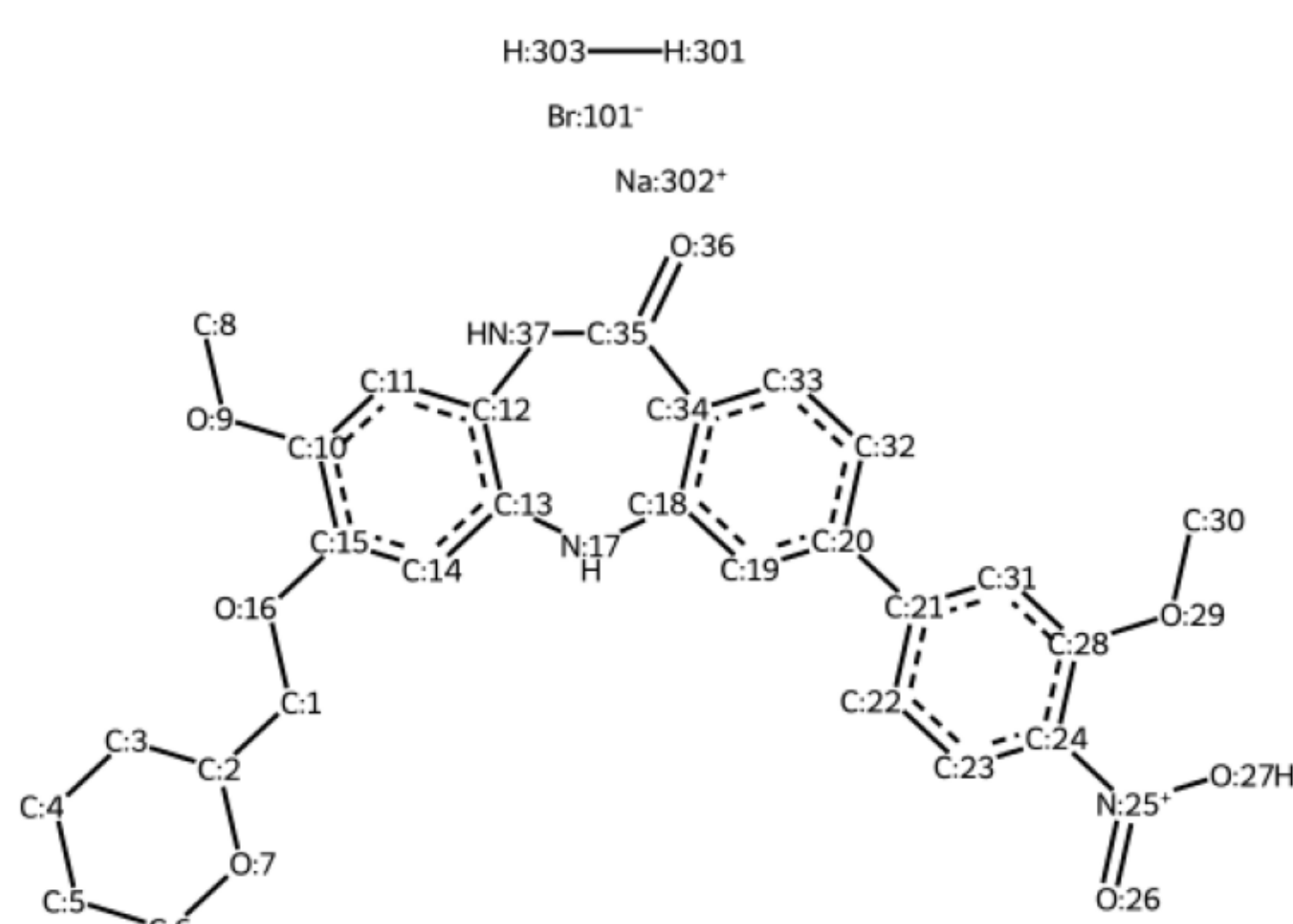
step #1



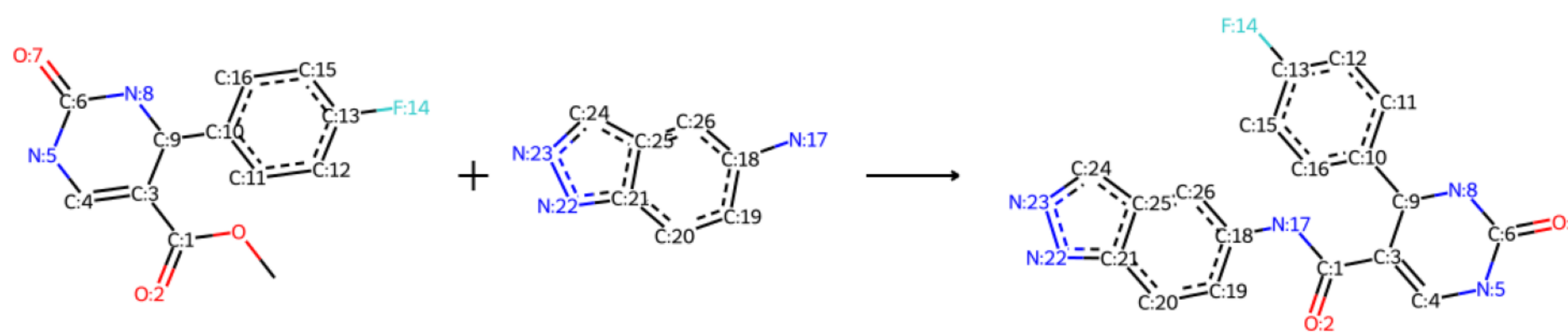
step #2



Product(s)

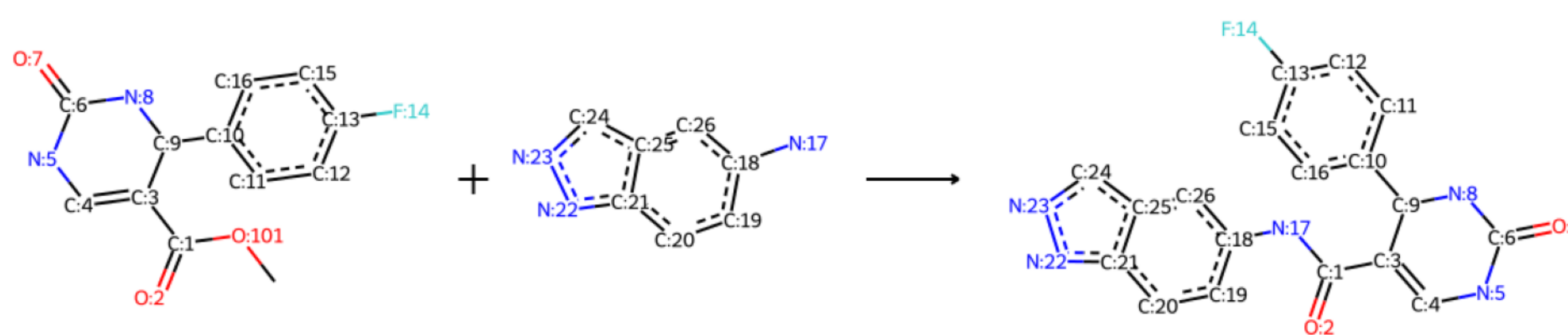


Original reaction
sampled RXN_ID:8)



Identified mechanistic class -
nucleophilic_attack_to_(thio)carbonyl_or_sulfonyl reaction

Reaction with missing reagents recovered

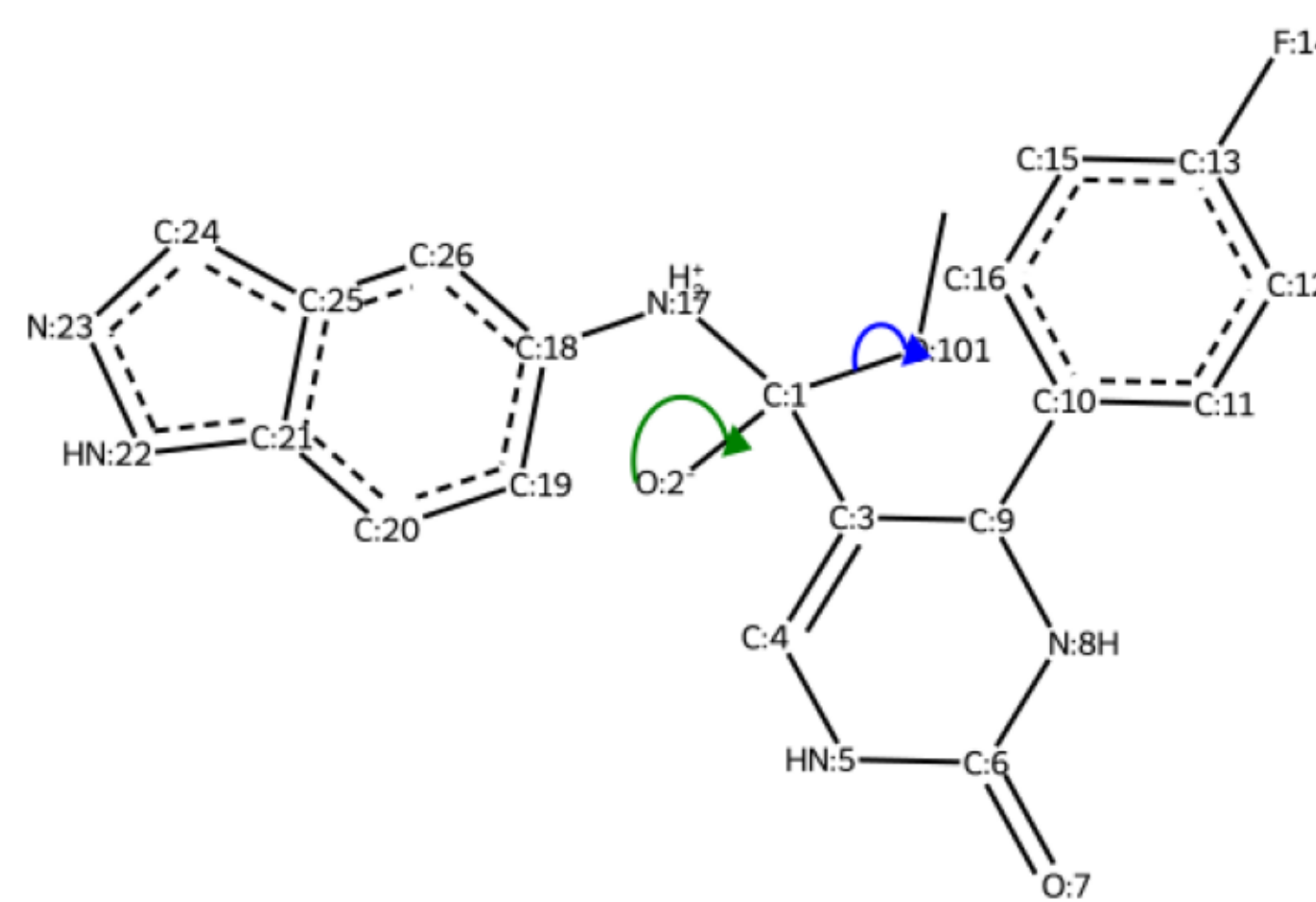
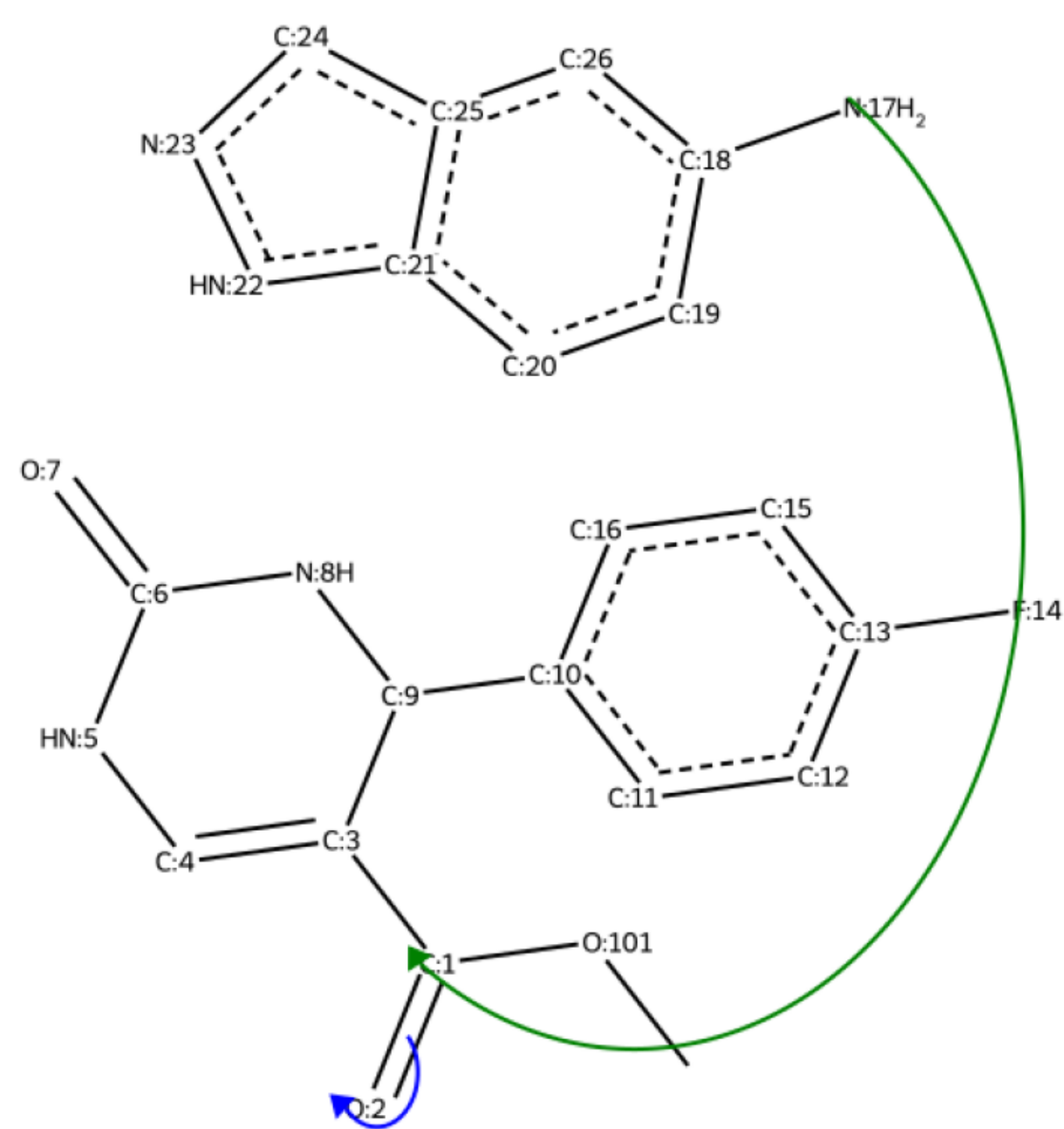


Proposed mechanistic pathway

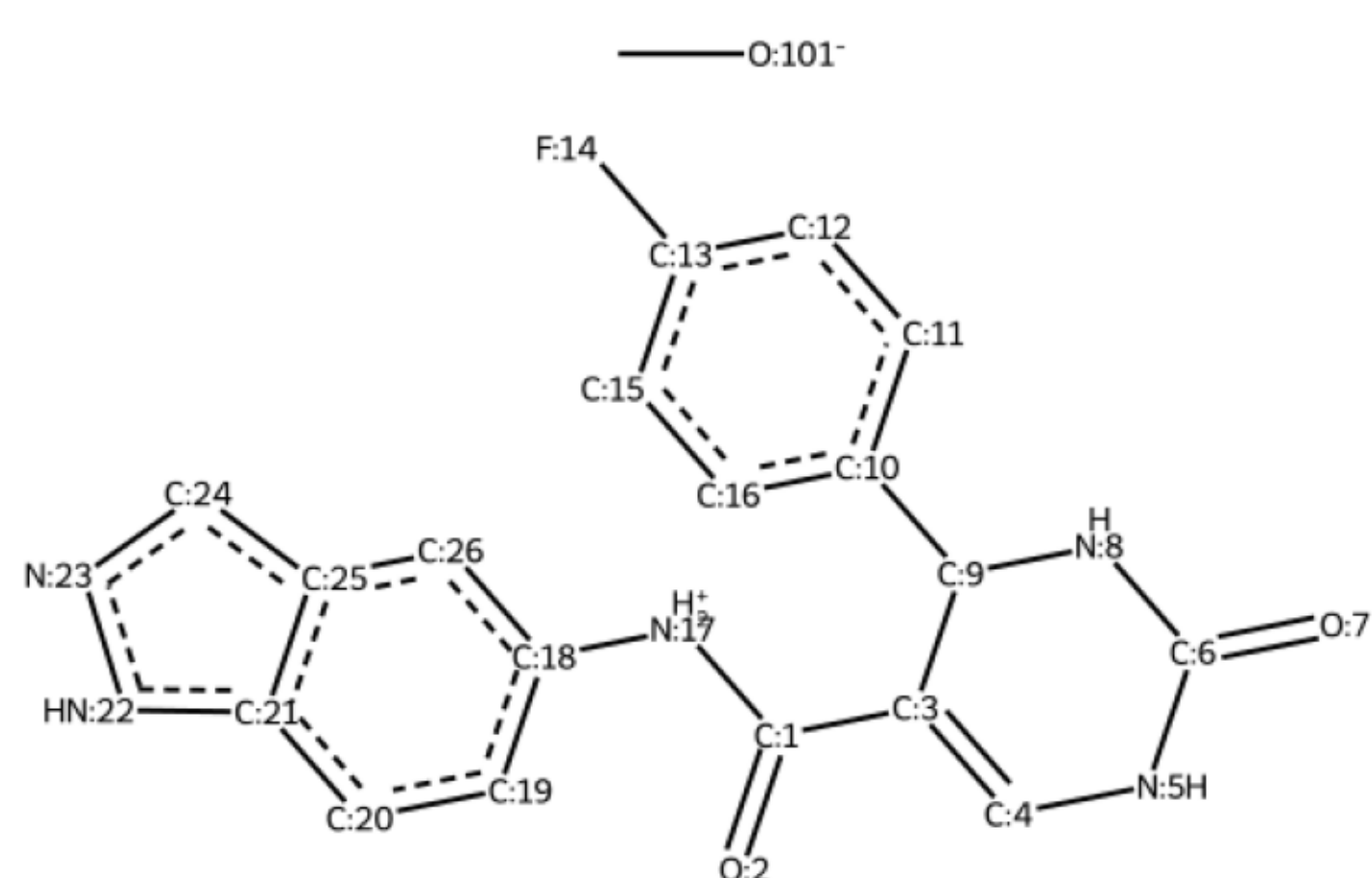
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

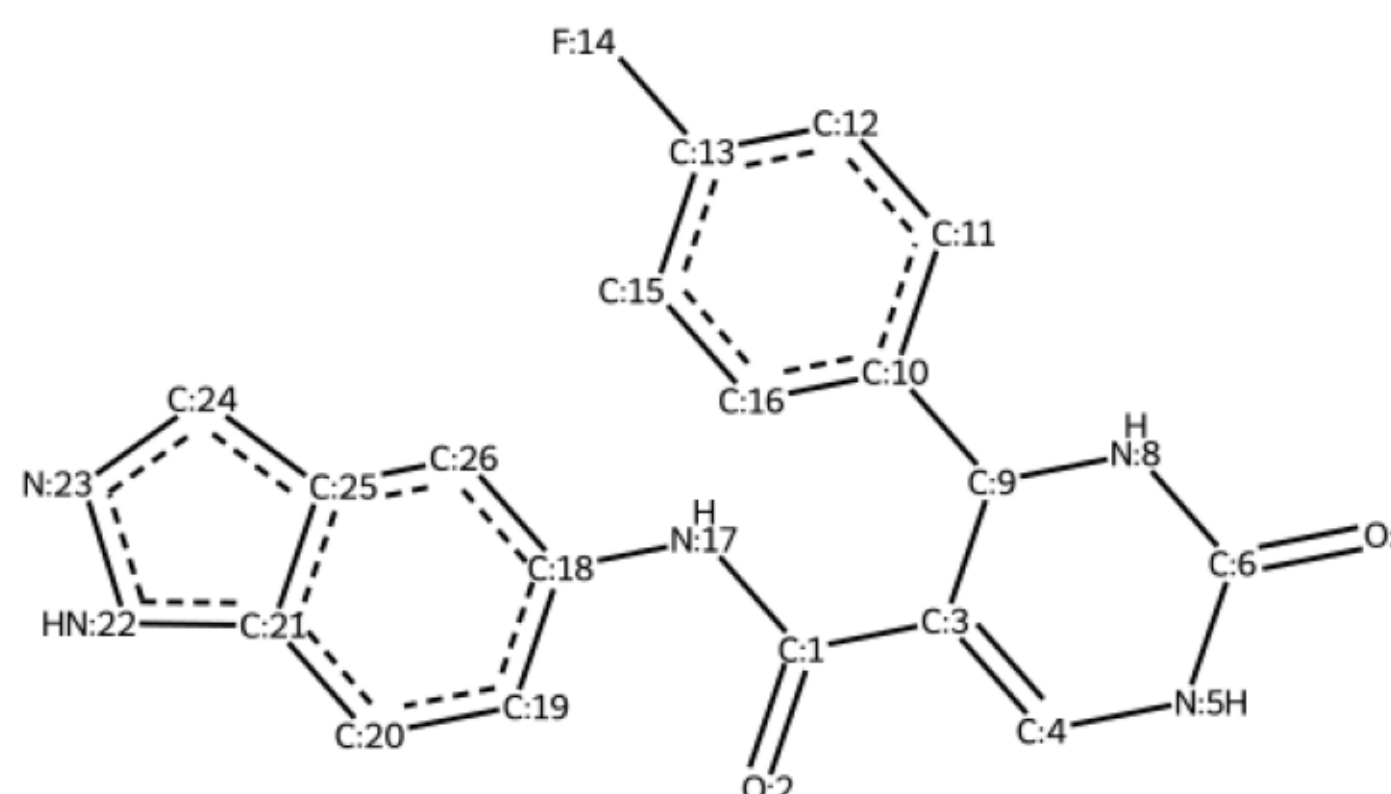
step #2



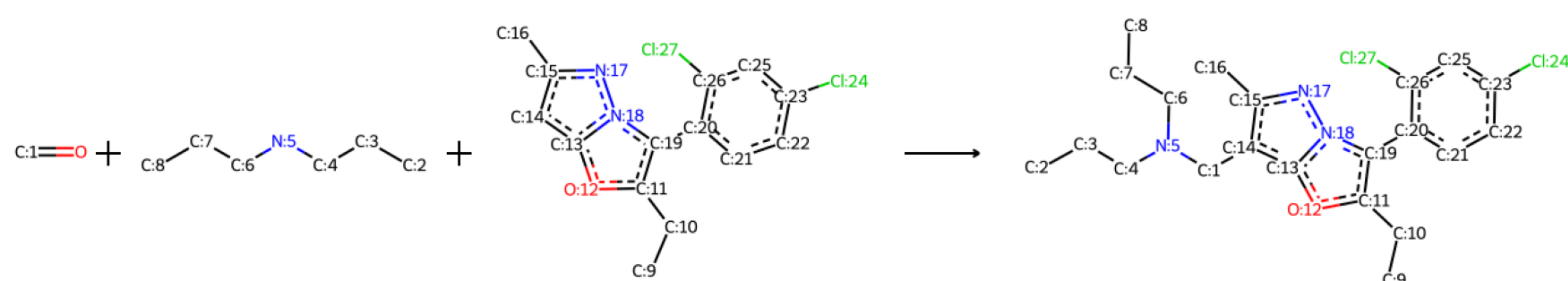
Product(s)



proton transfer

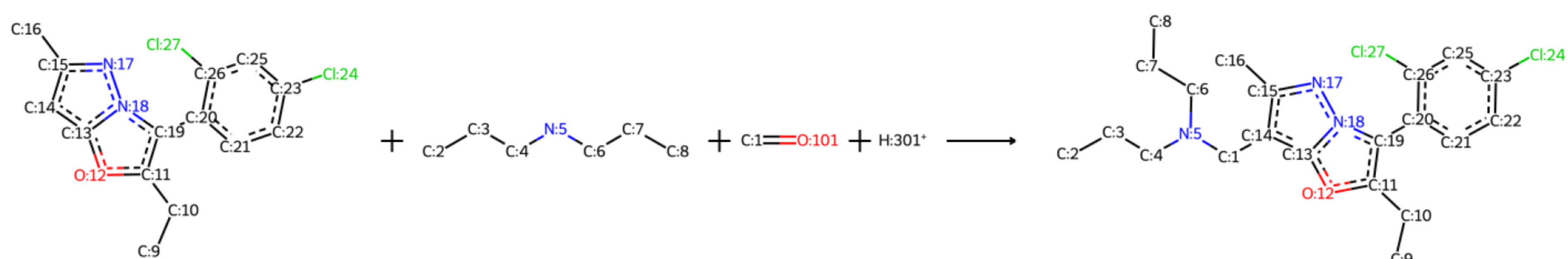


Original reaction
sampled RXN_ID:9)



Identified mechanistic class -
Mannich reaction

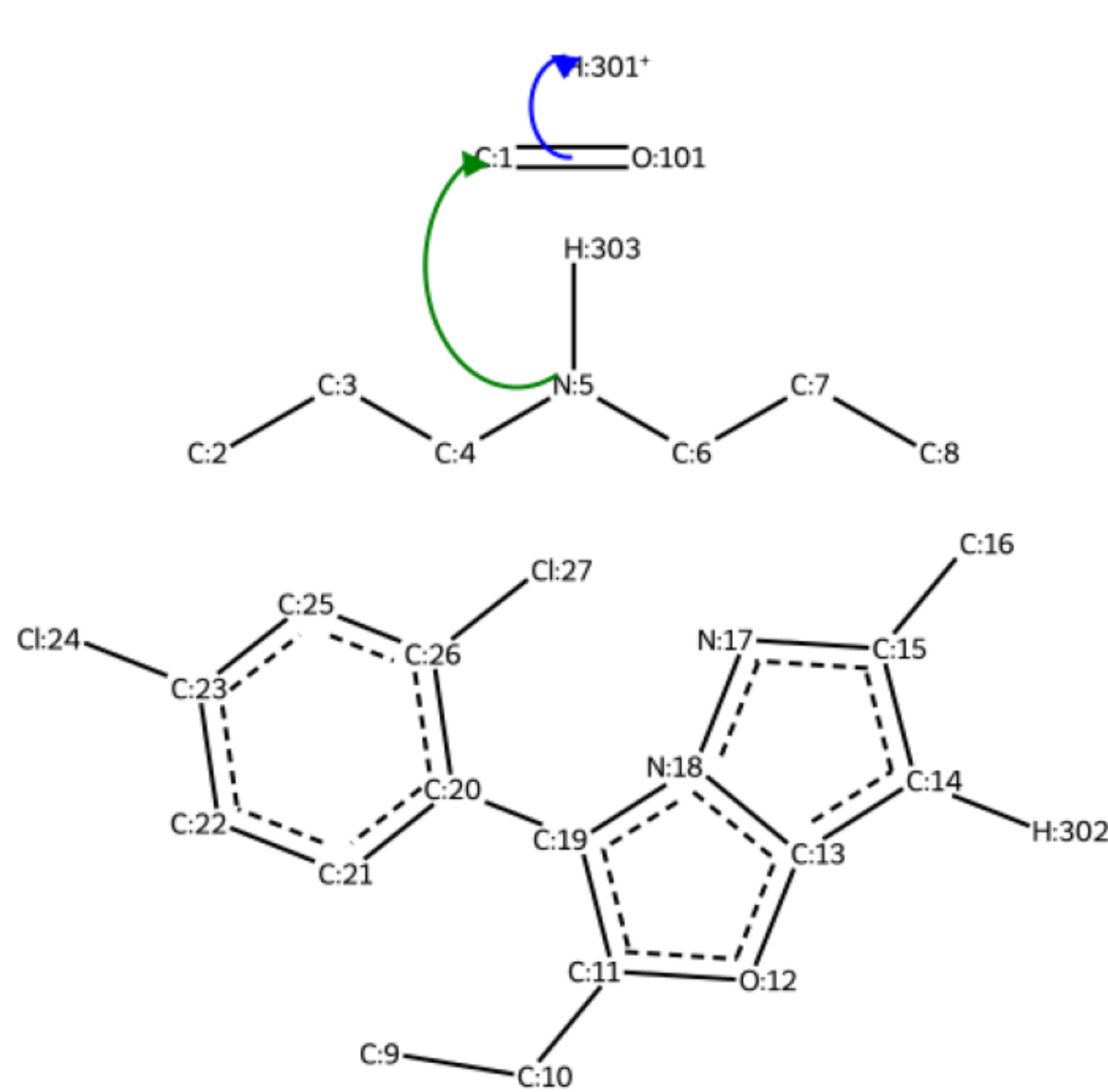
Reaction with missing reagents recovered



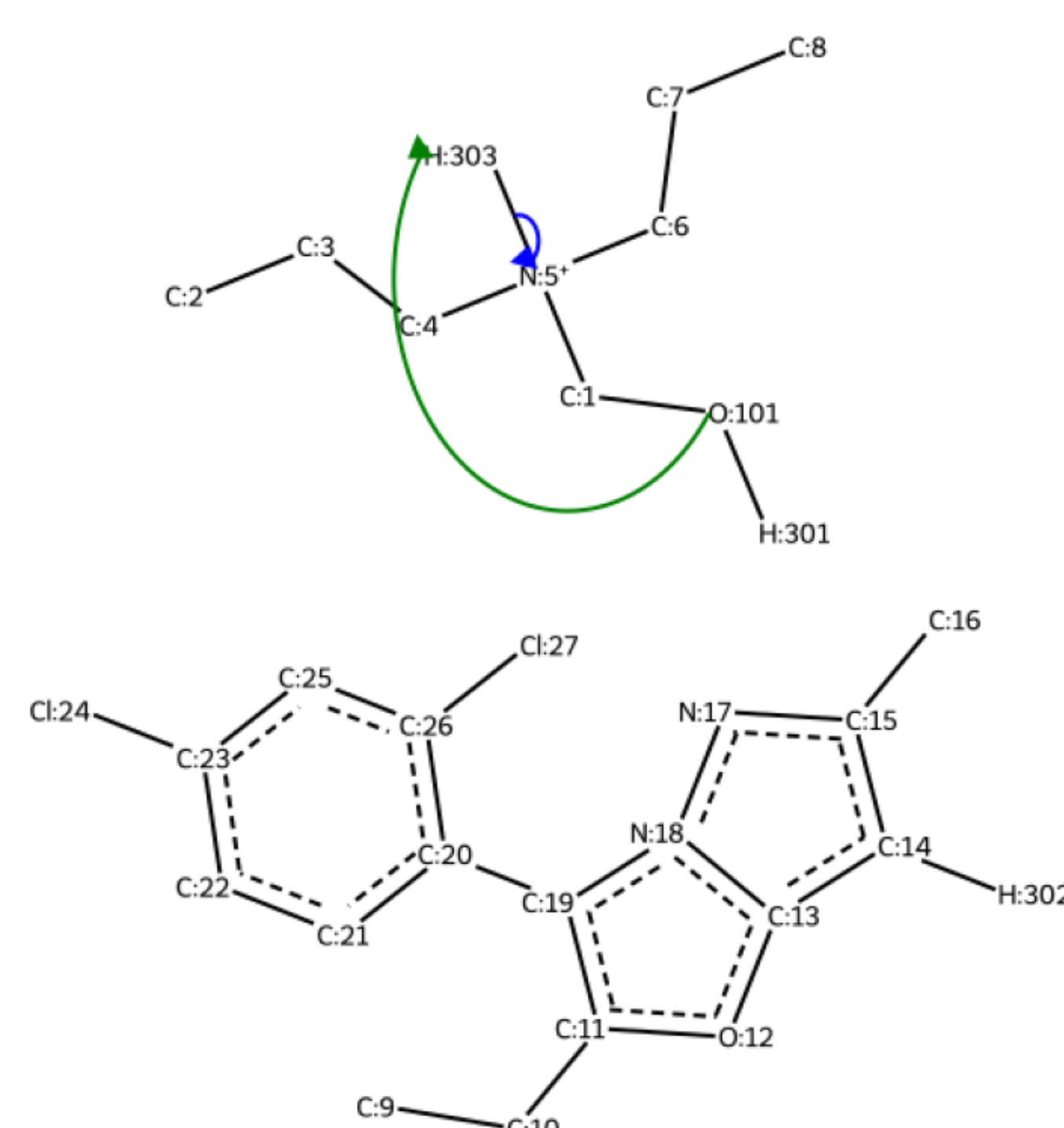
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

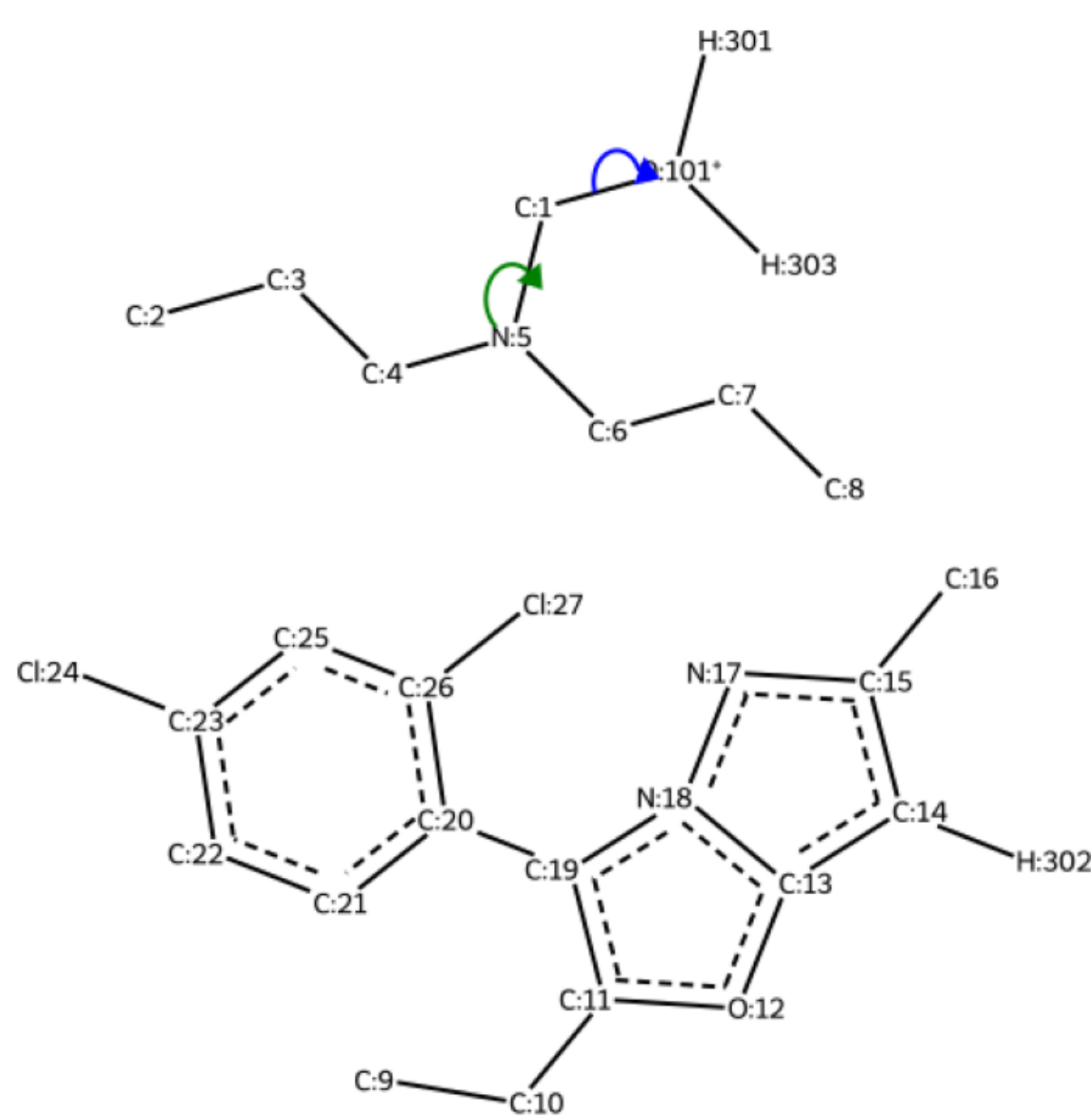
step #1



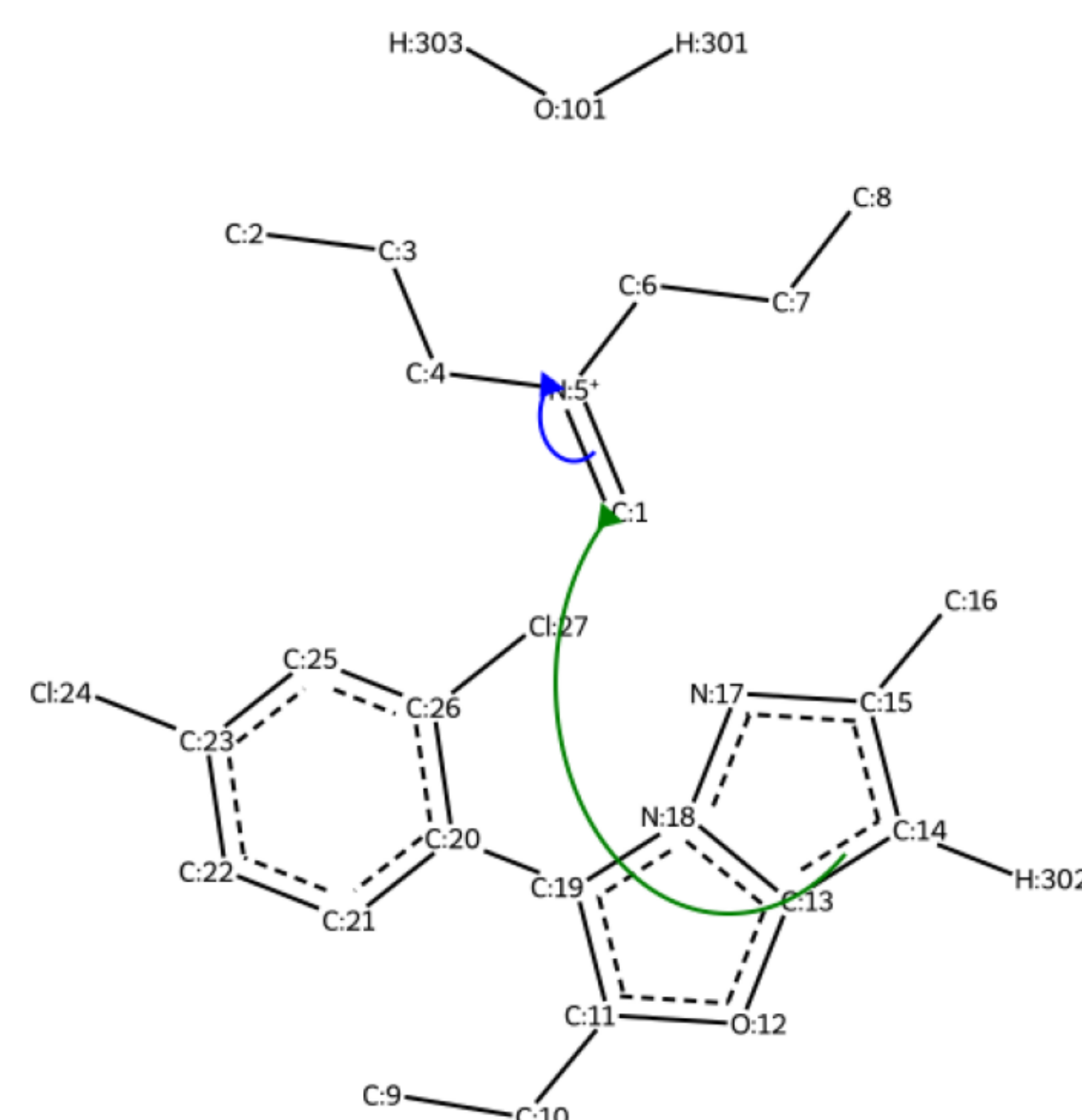
step #2



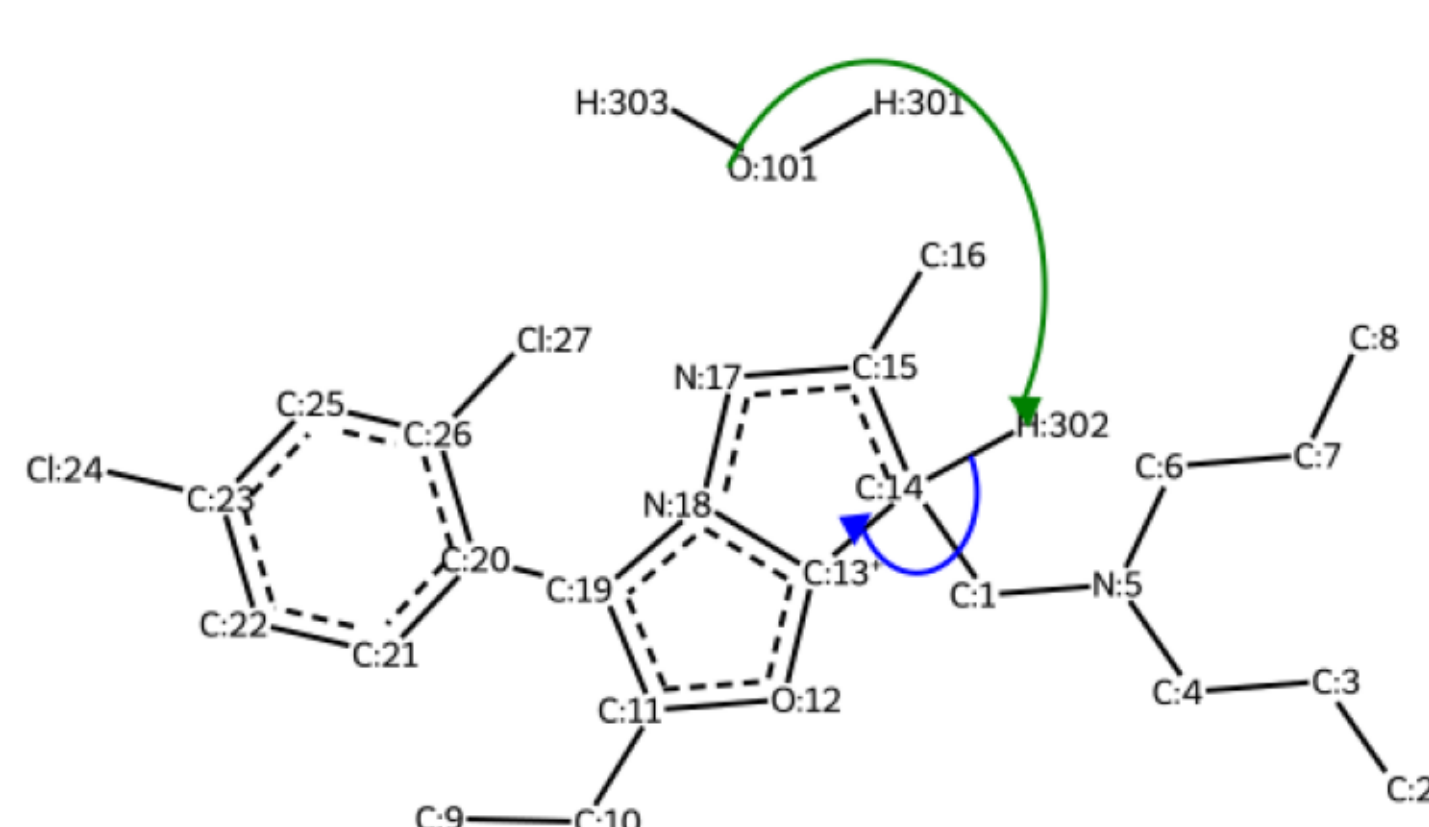
step #3



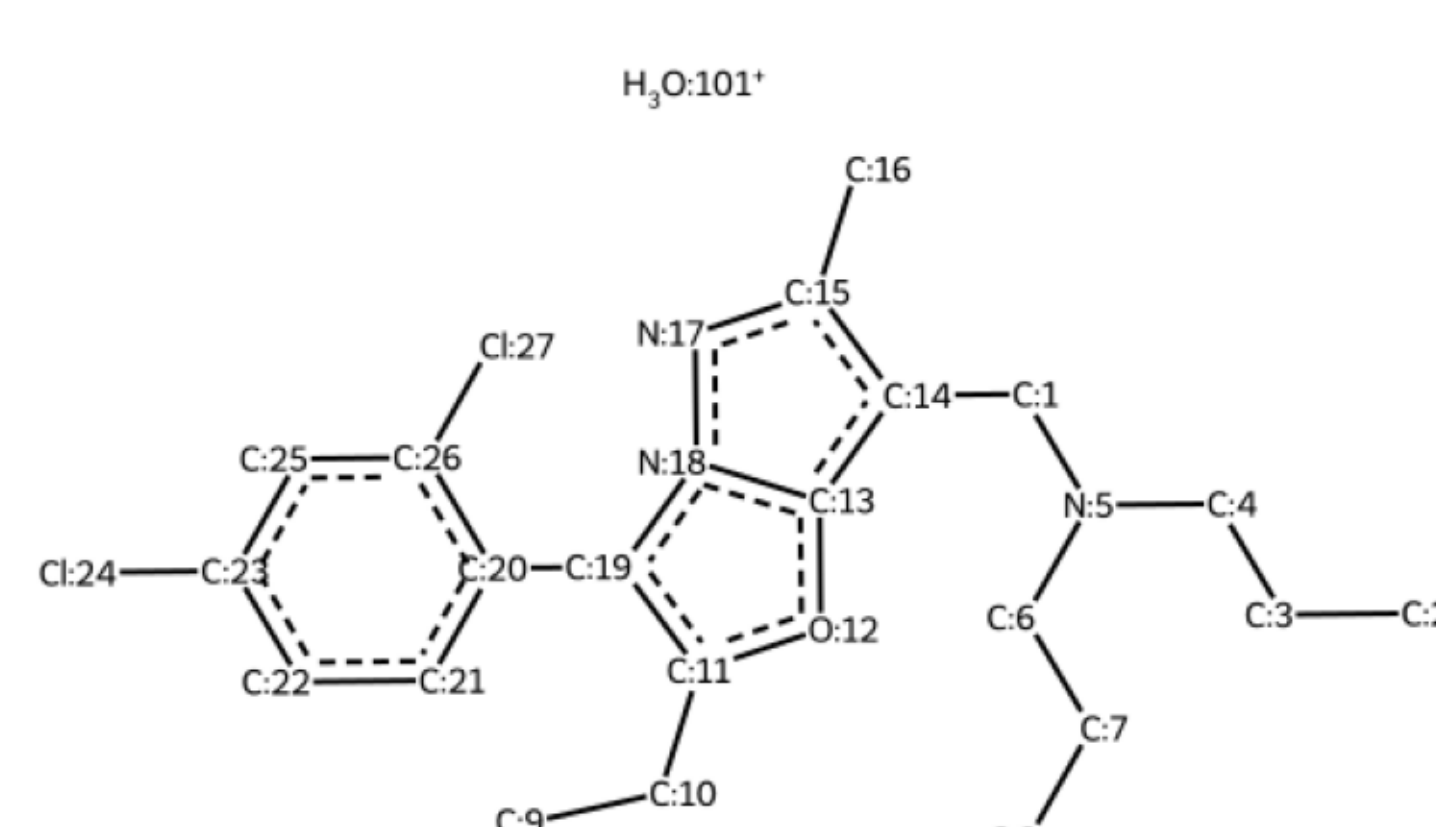
step #4



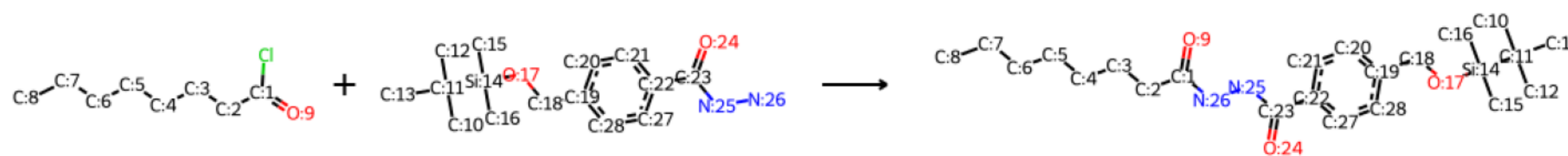
step #5



Product(s)

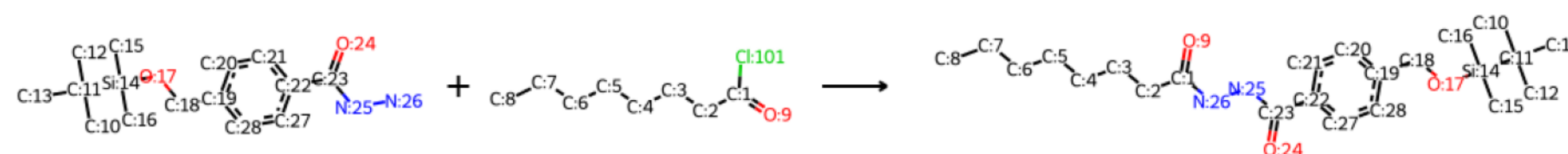


Original reaction
sampled RXN_ID:10)



Identified mechanistic class -
nucleophilic_attack_to_(thio)carbonyl_or_sulfonyl reaction

Reaction with missing reagents recovered

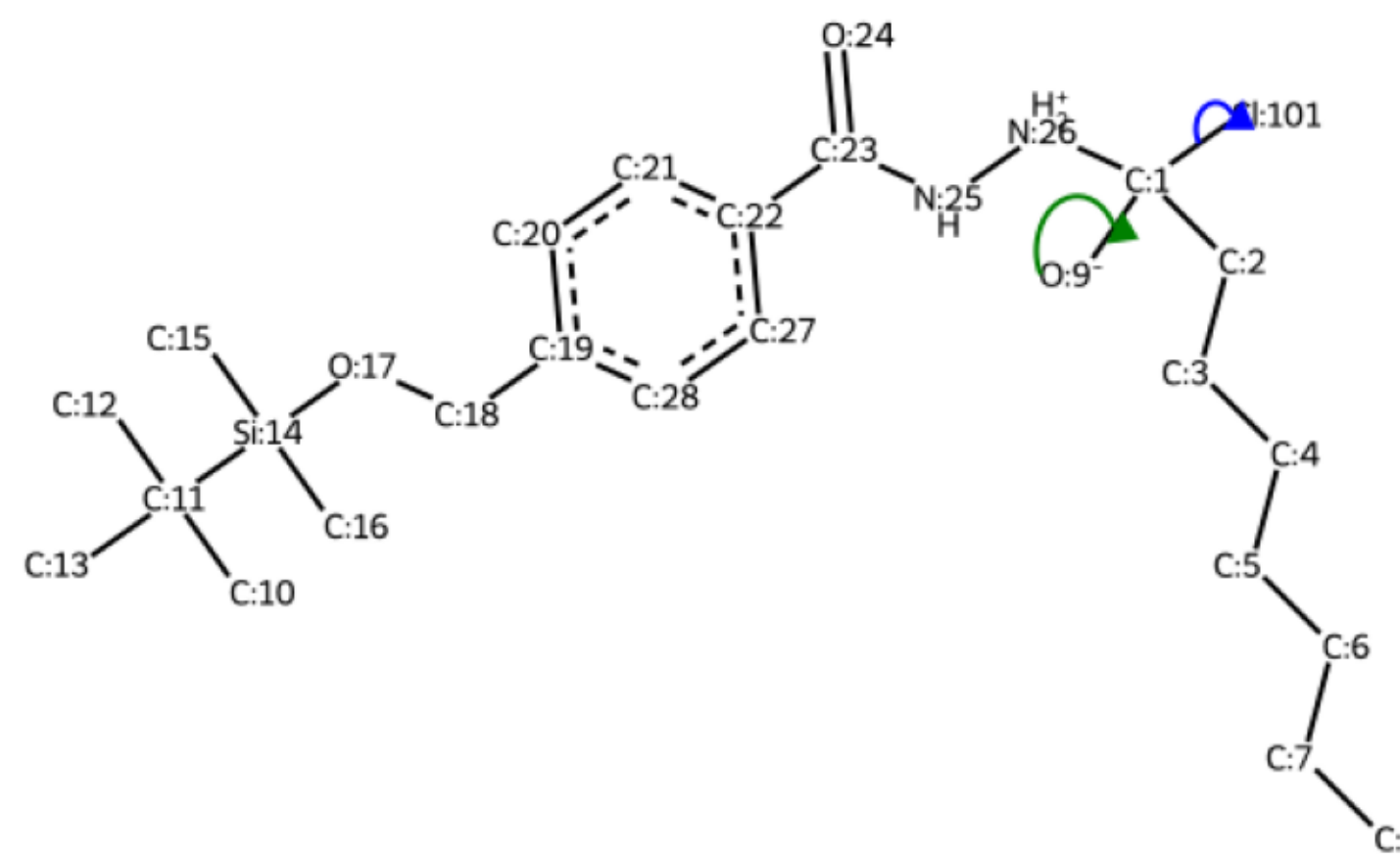
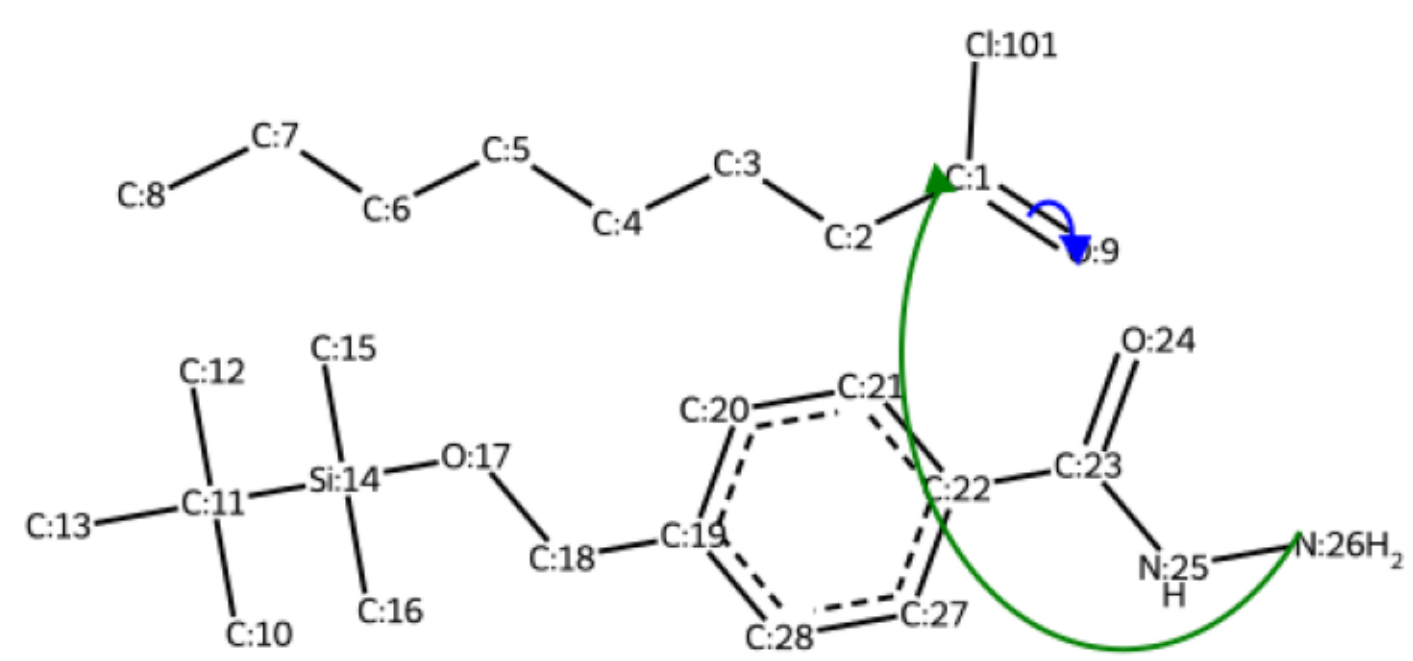


Proposed mechanistic pathway

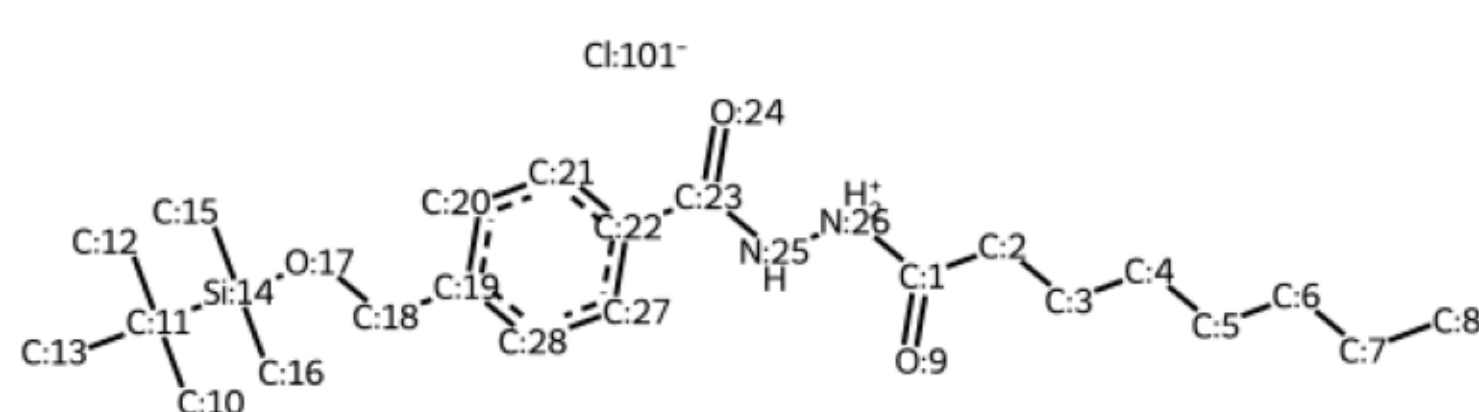
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

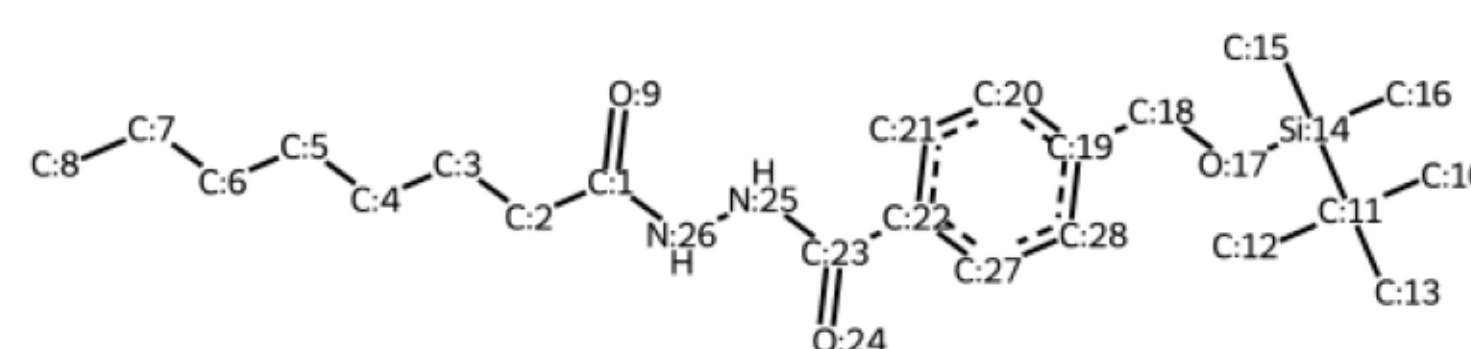
step #2



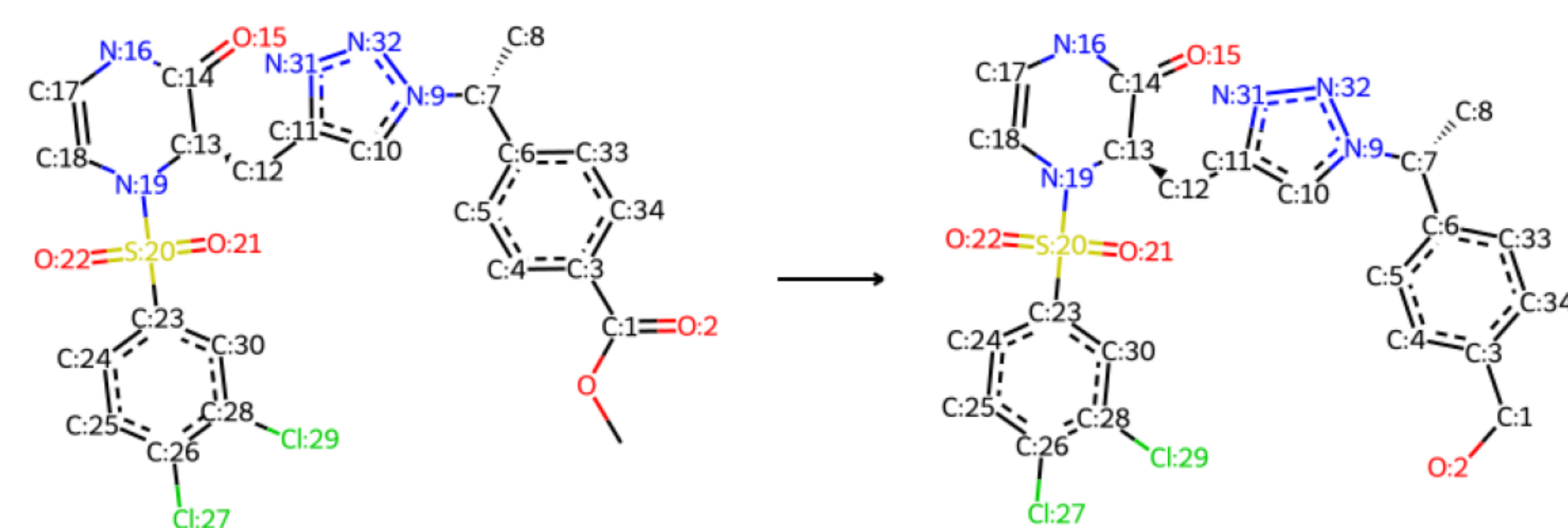
Product(s)



proton transfer

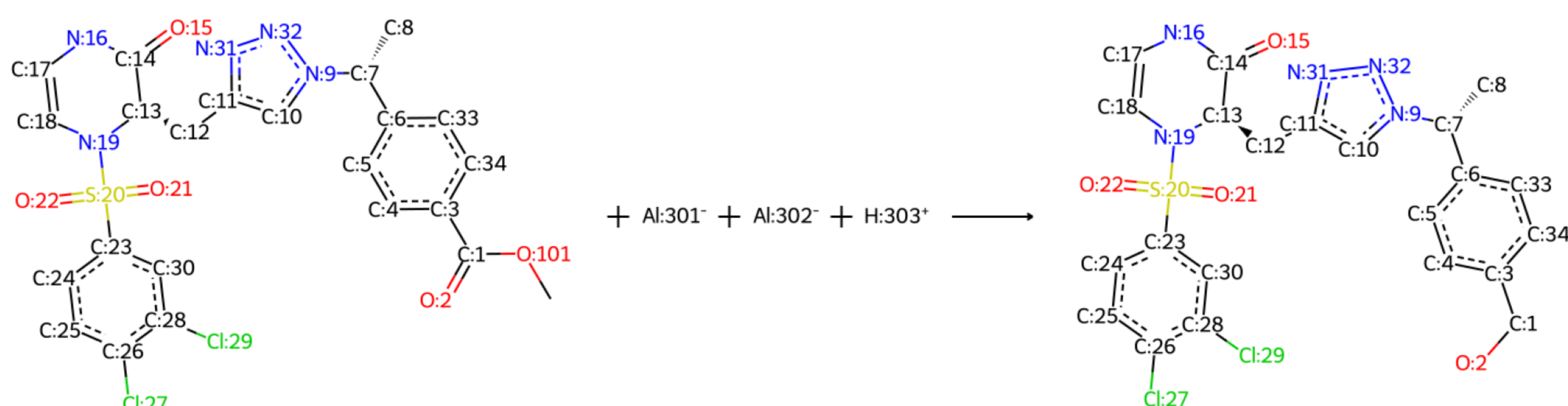


Original reaction
sampled RXN_ID:12)



Identified mechanistic class -
ester_reduction reaction

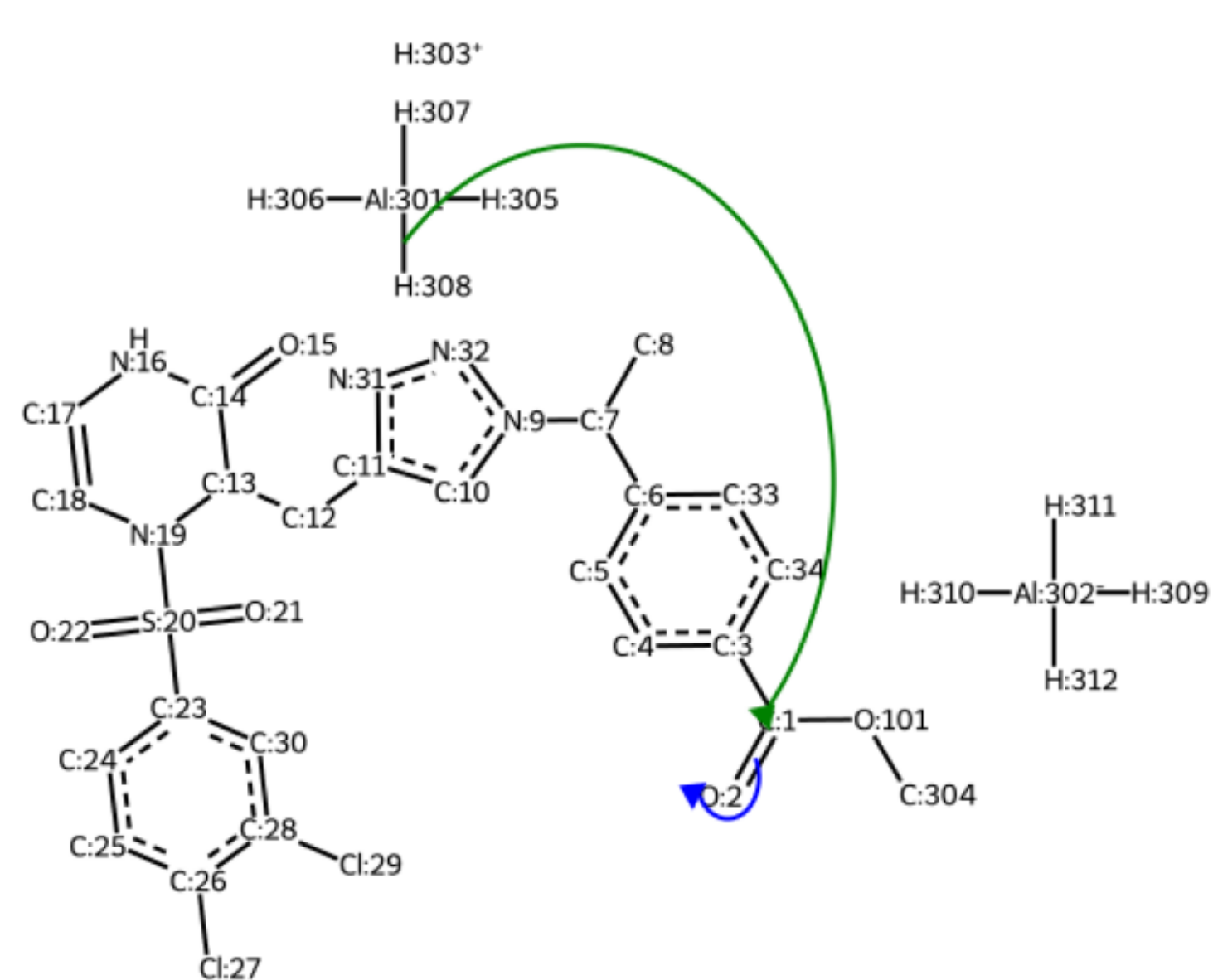
Reaction with missing reagents recovered



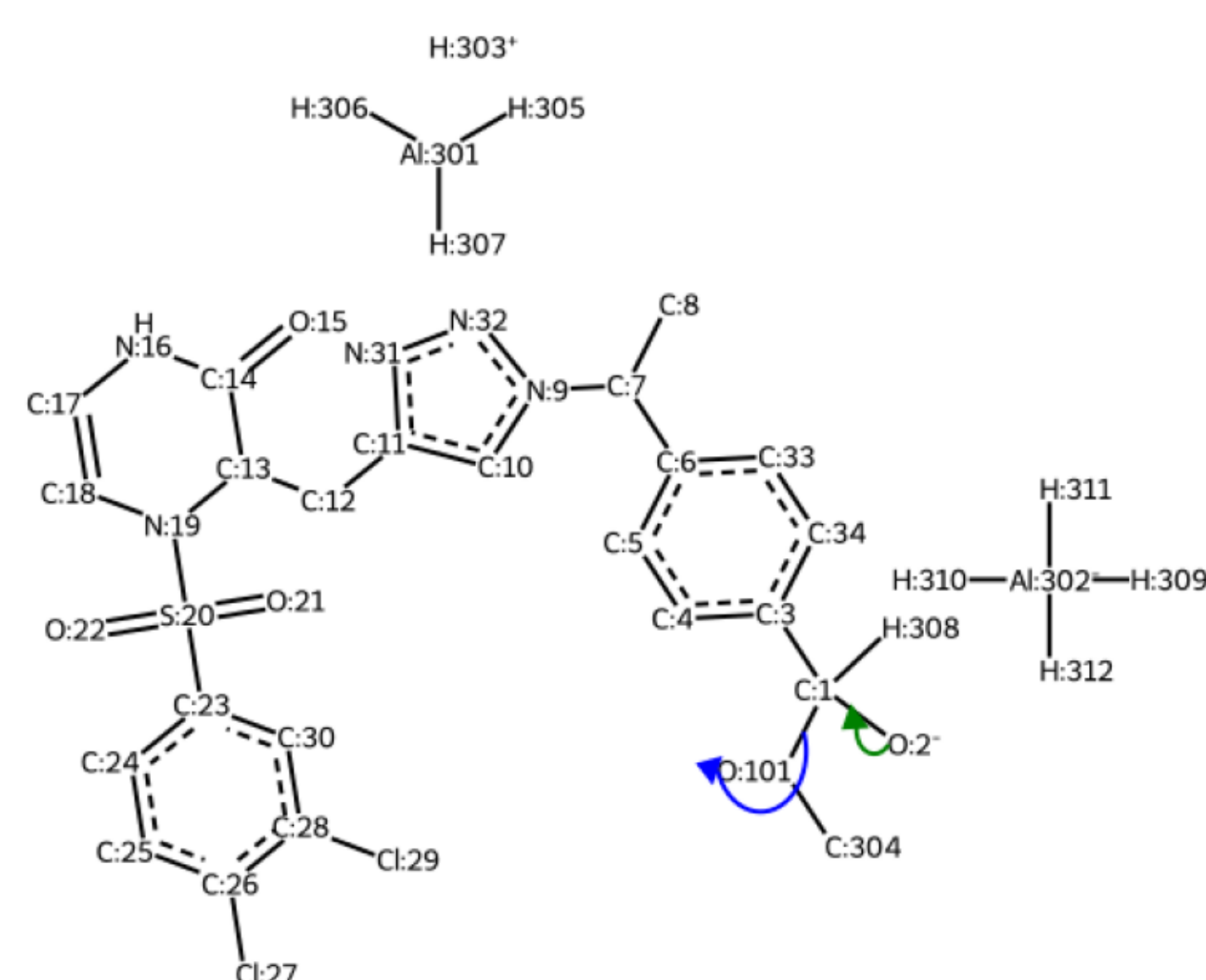
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

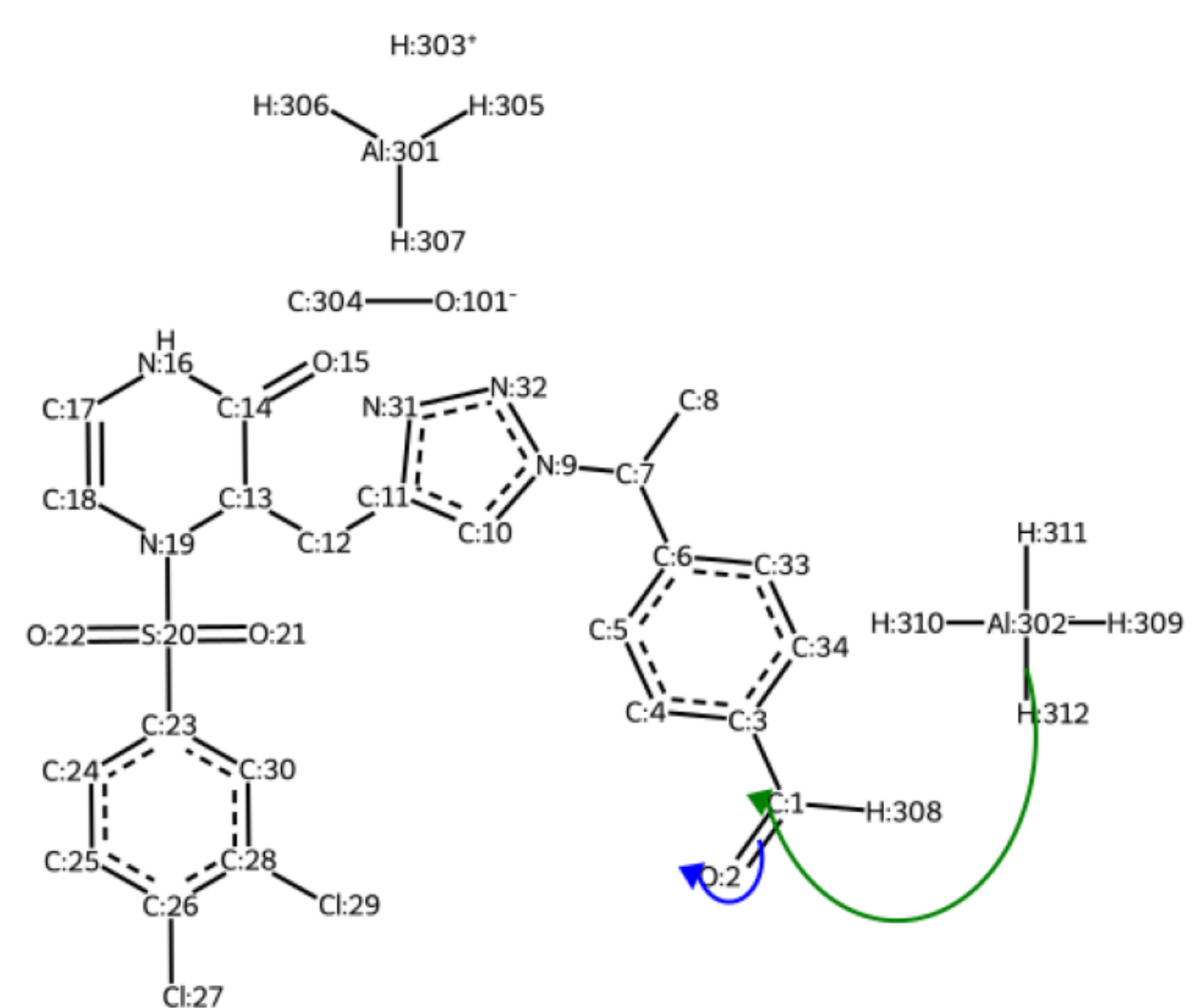
step #1



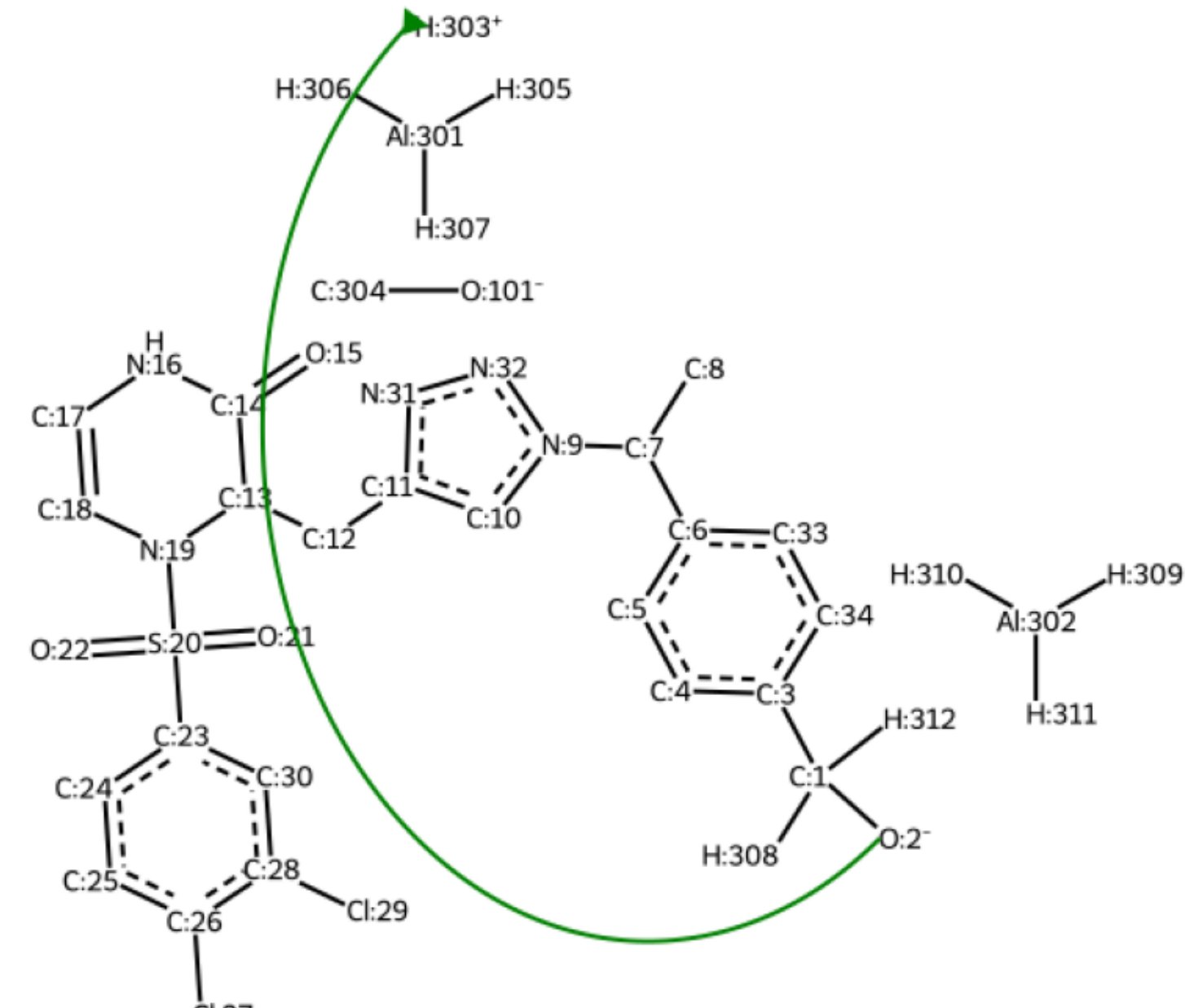
step #2



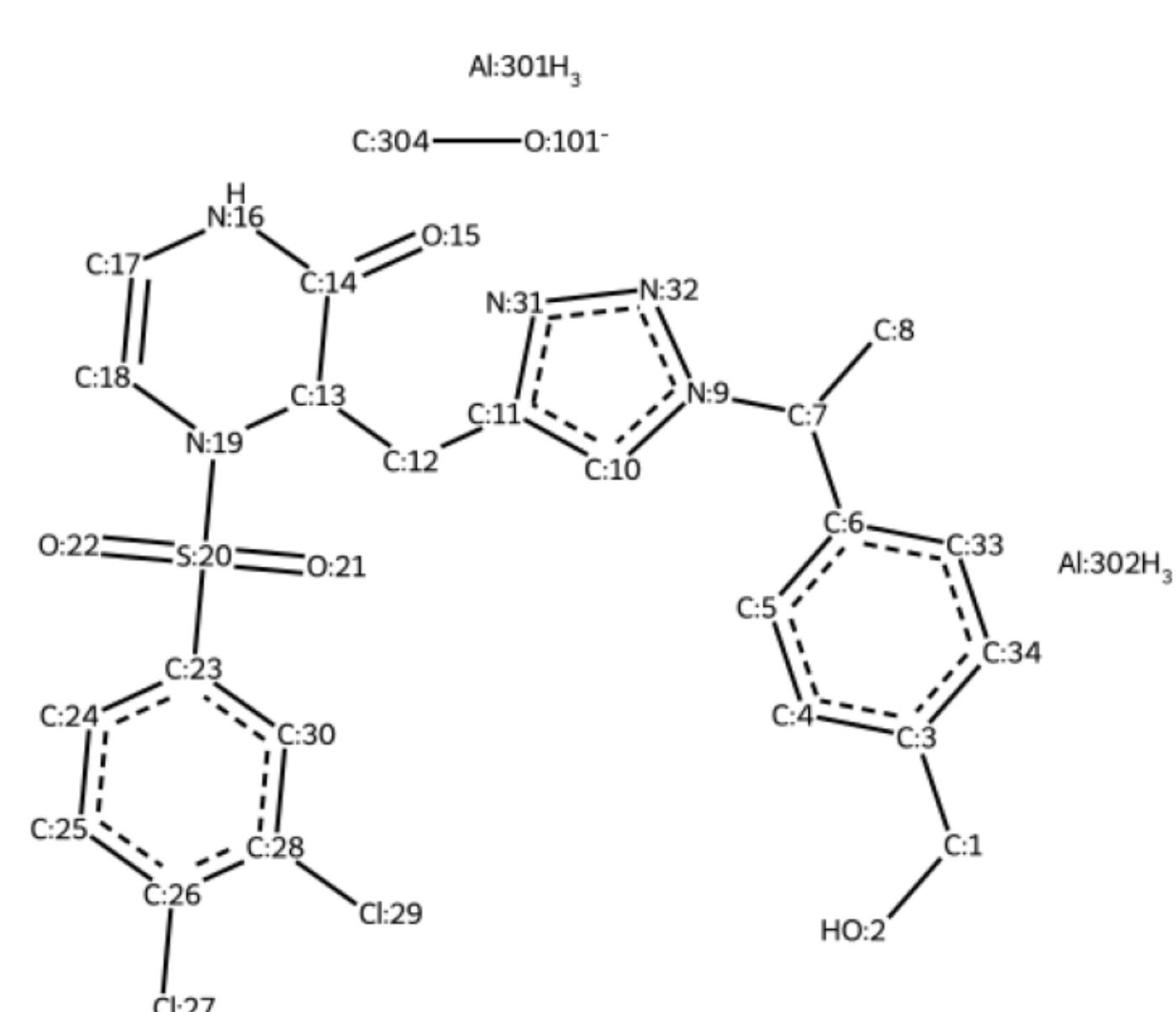
step #3



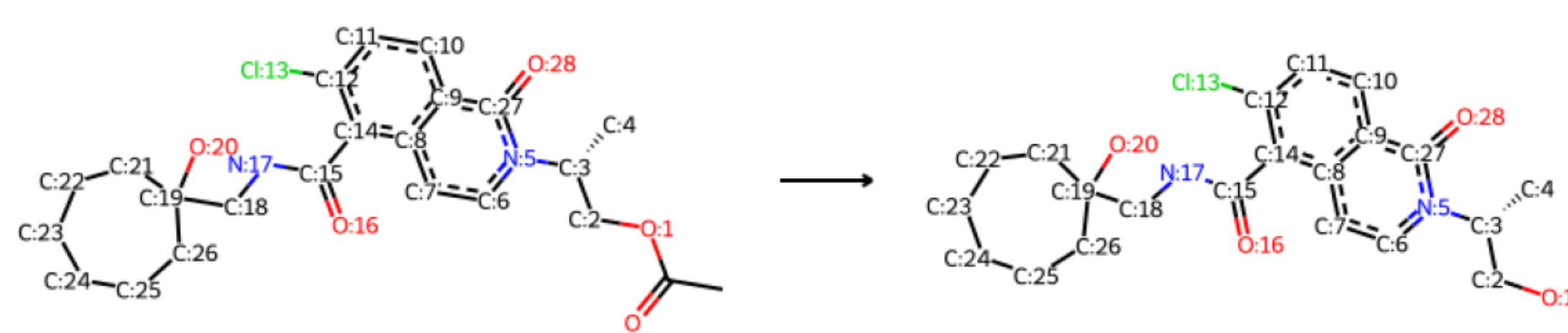
step #4



Product(s)

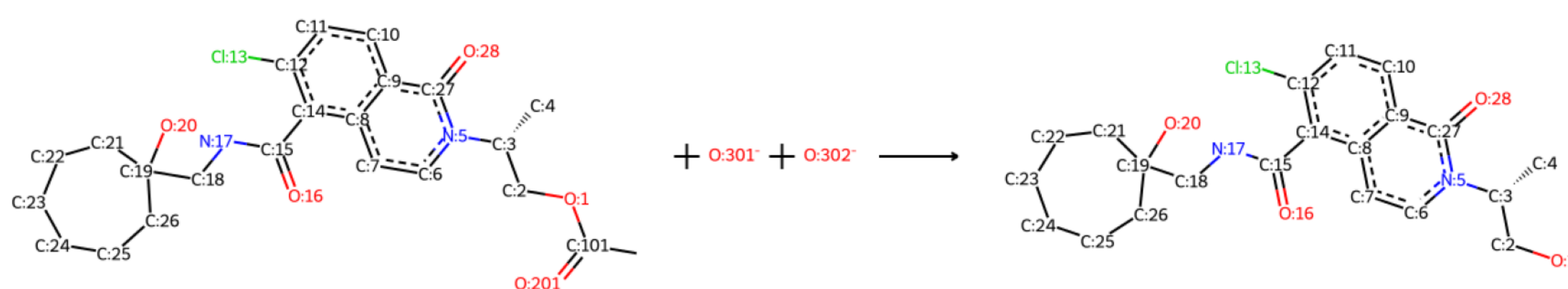


Original reaction
sampled RXN_ID:13)



Identified mechanistic class -
base_cat_ester_hydrolysis reaction

Reaction with missing reagents recovered

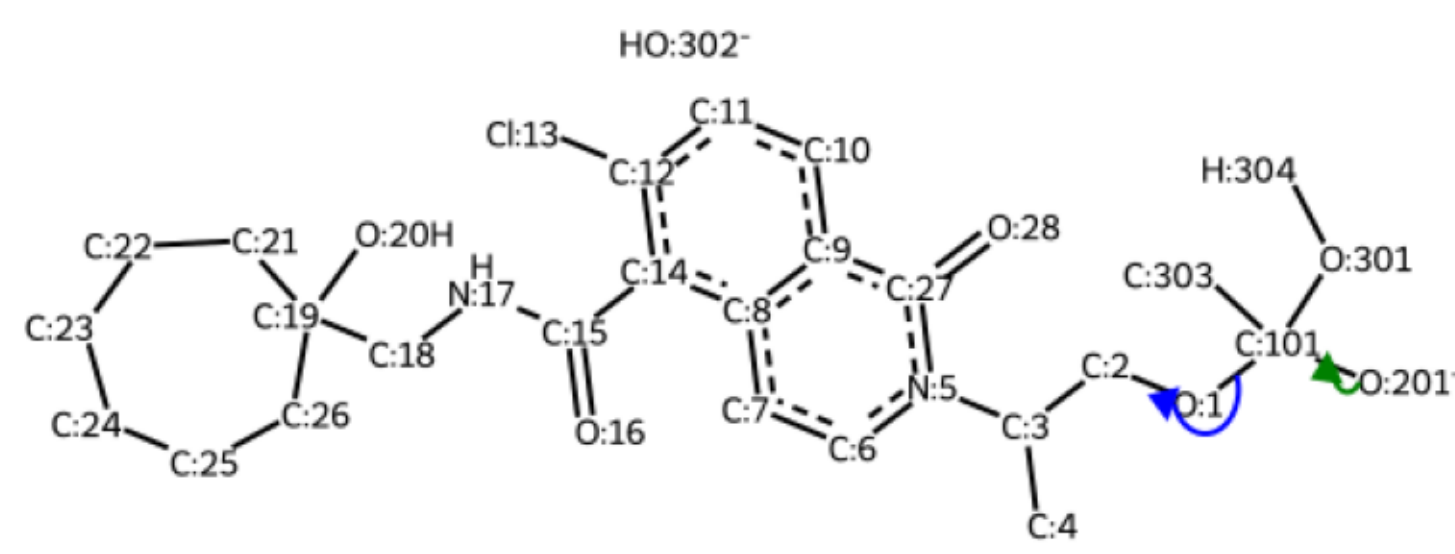
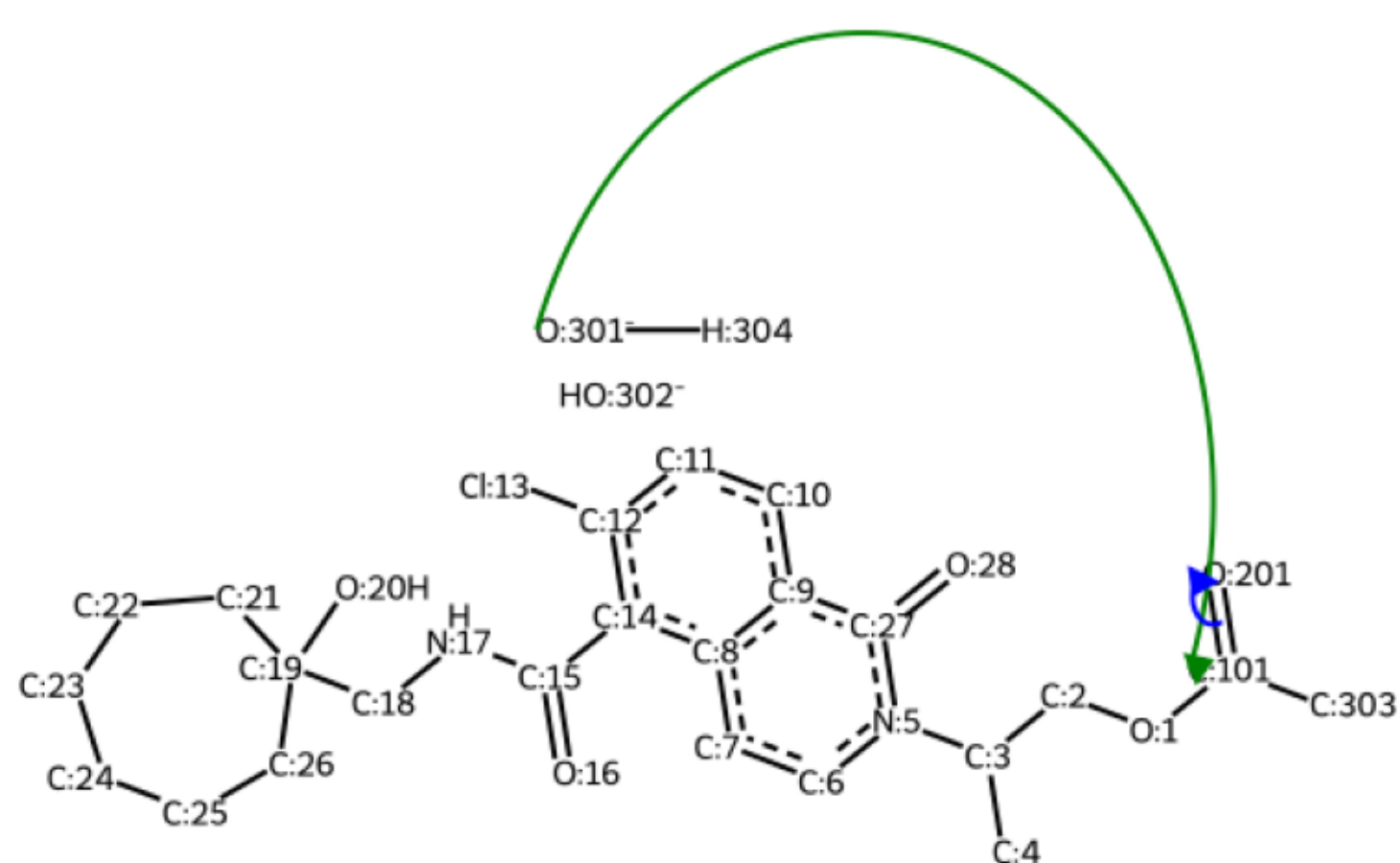


Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

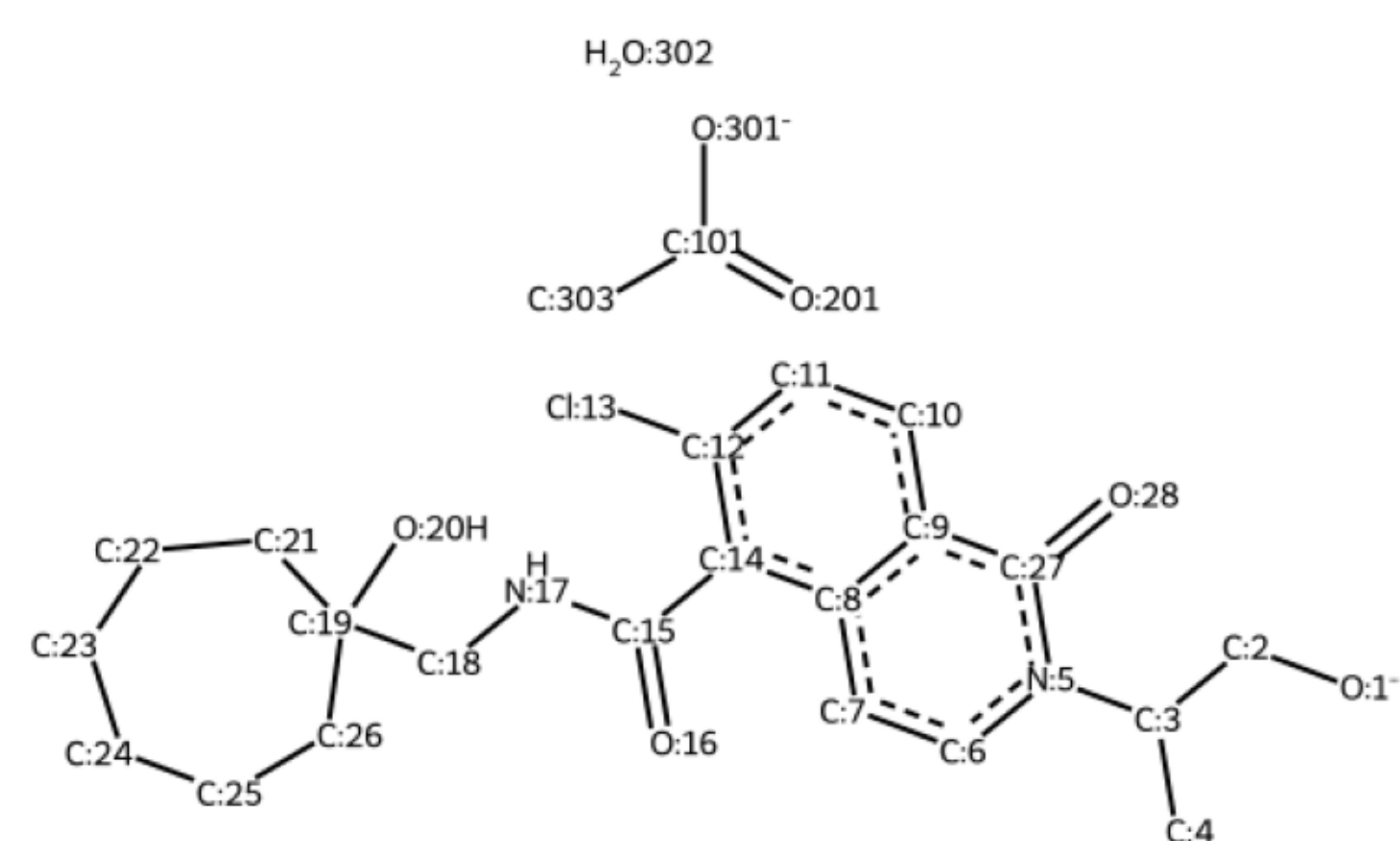
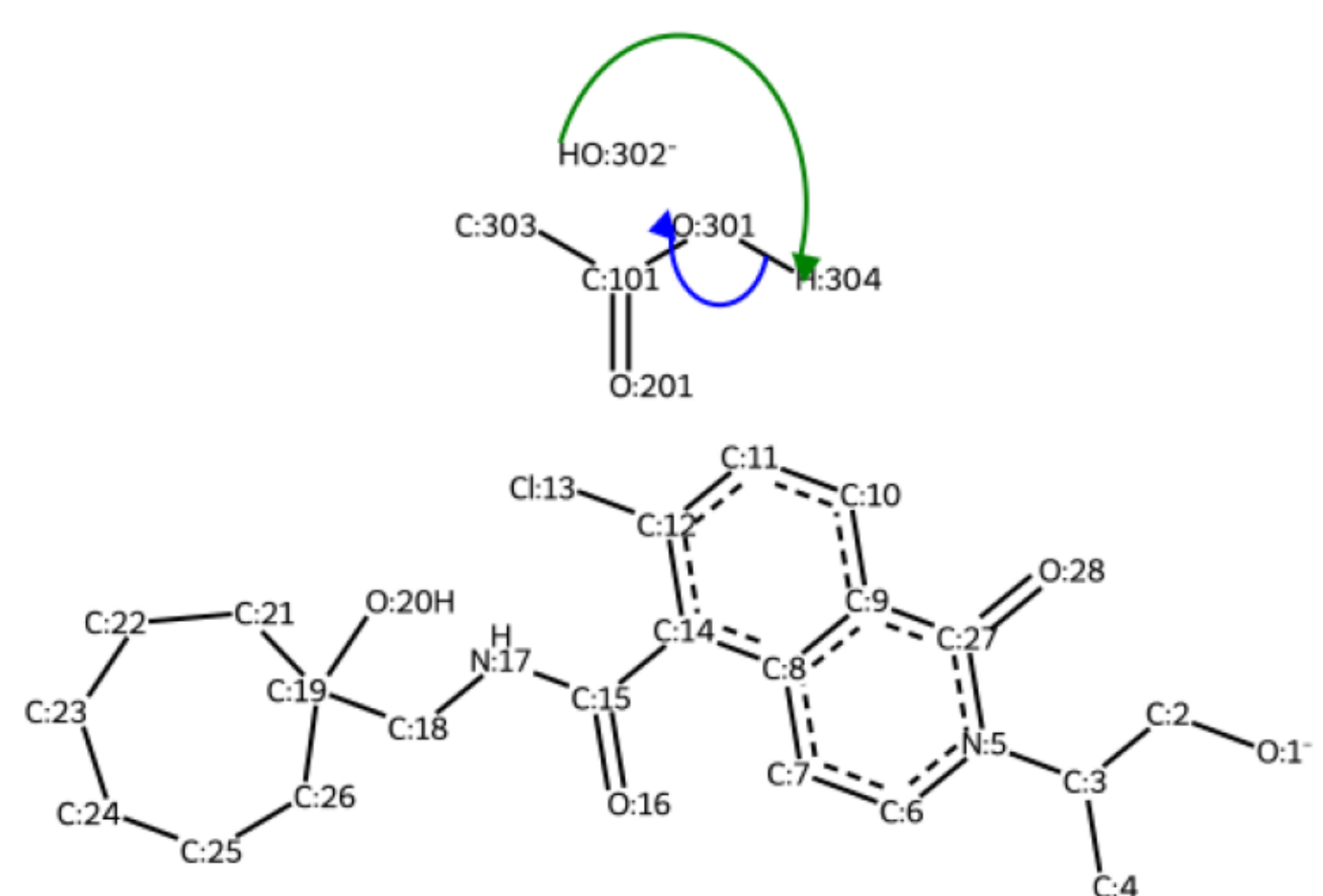
step #1

step #2

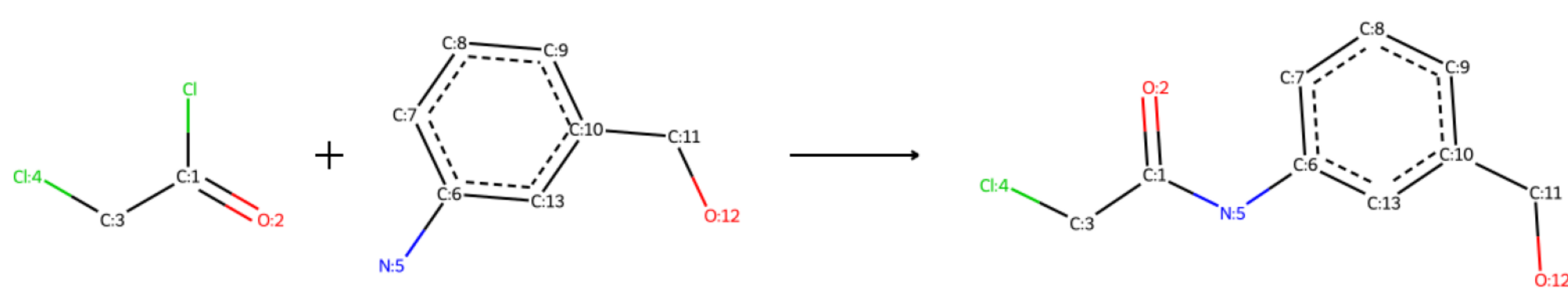


step #3

Product(s)

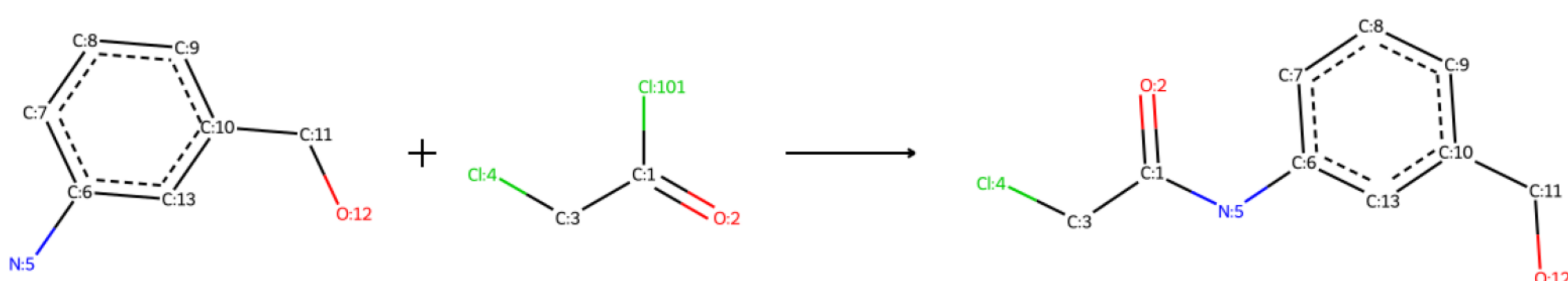


Original reaction sampled RXN_ID:14)



Identified mechanistic class -
nucleophilic_attack_to_(thio)carbonyl_or_sulfonyl reaction

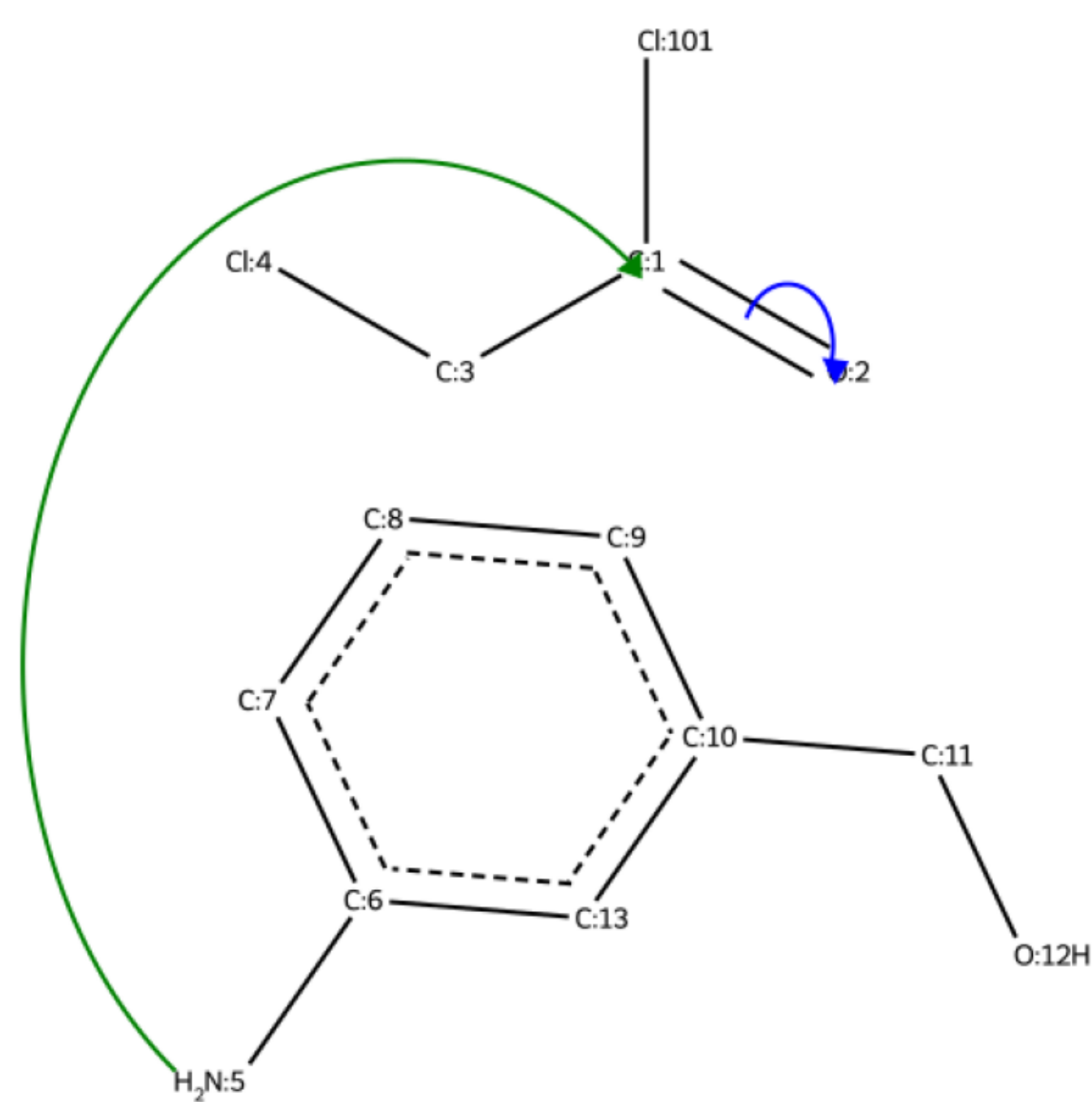
Reaction with missing reagents recovered



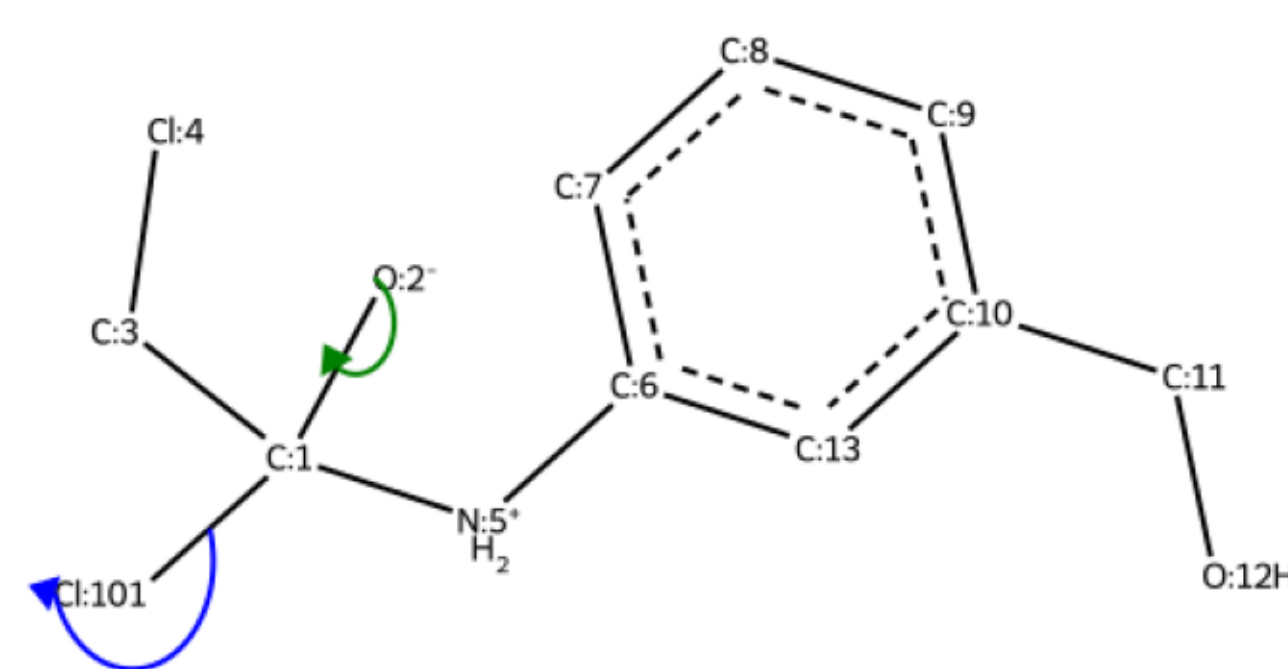
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

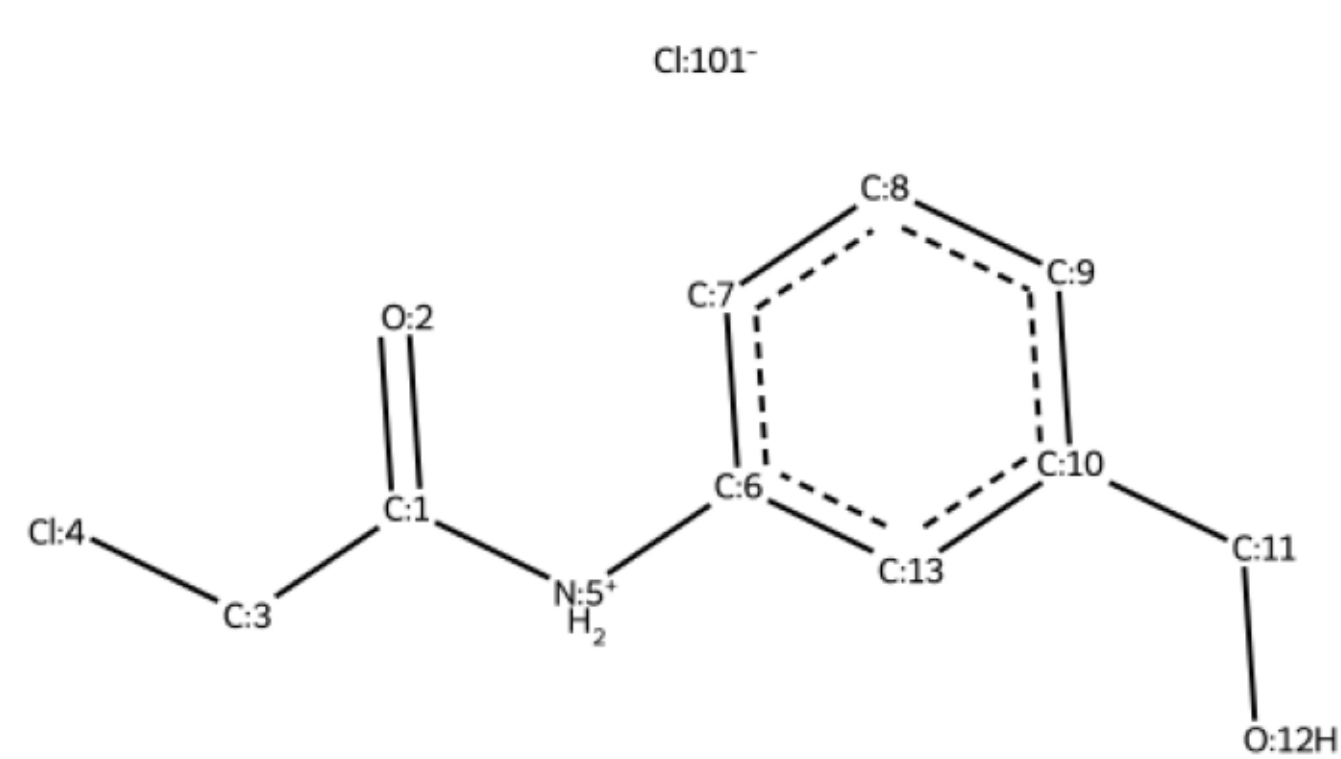
step #1



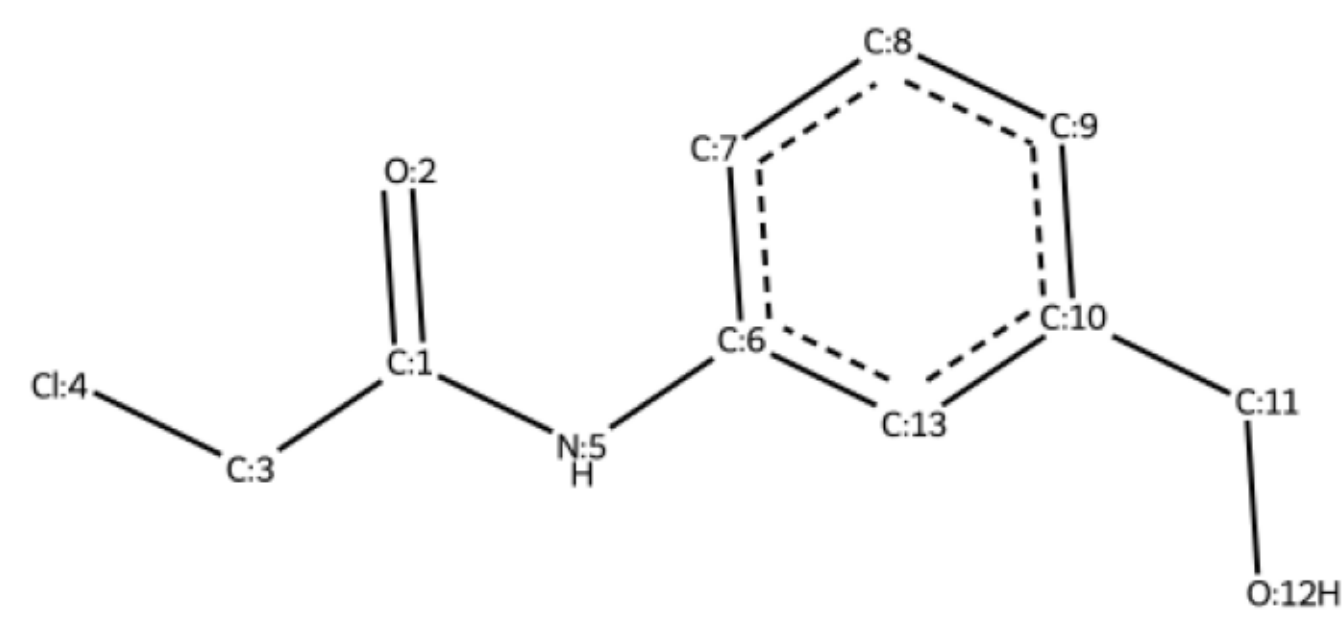
step #2



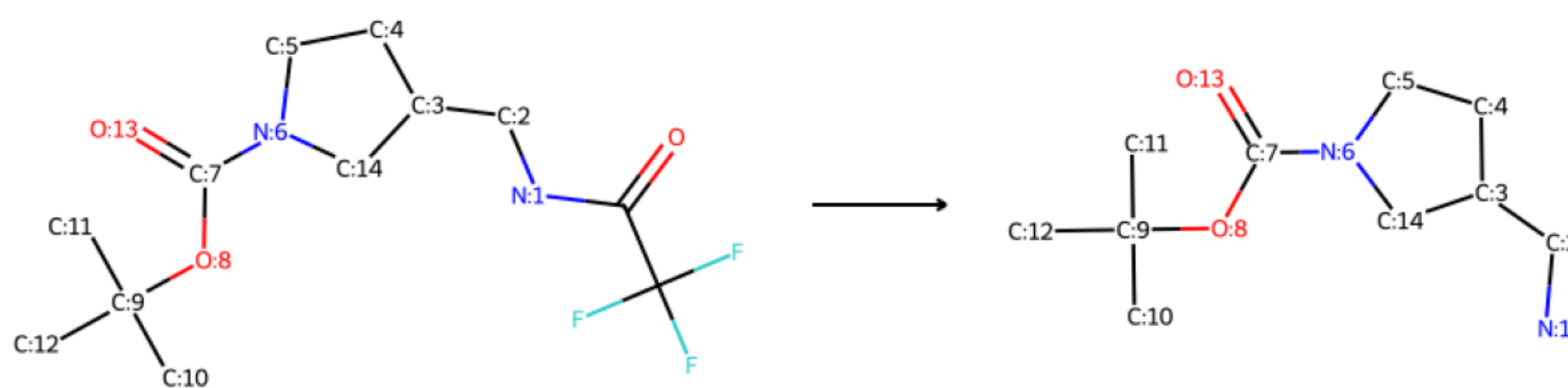
Product(s)



proton transfer

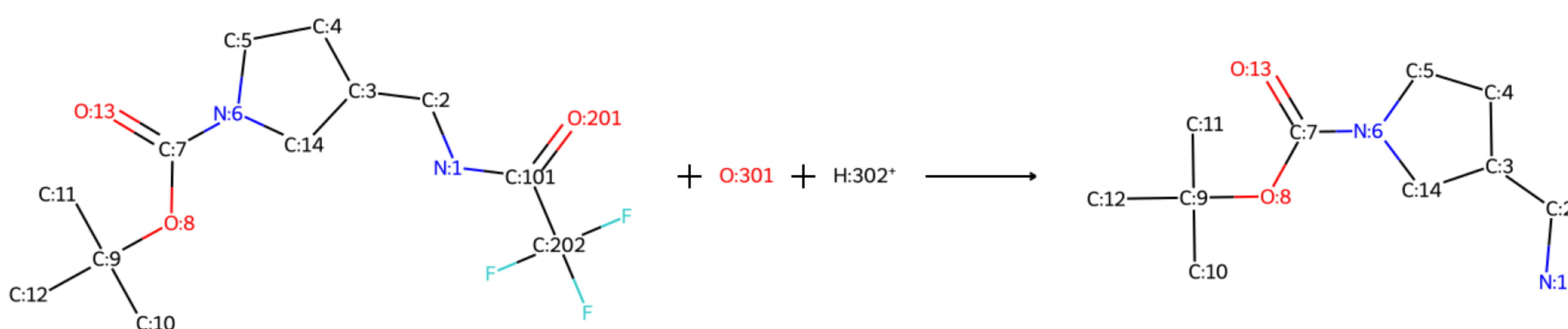


Original reaction
sampled RXN_ID:15)



Identified mechanistic class -
carboxylic_acid_derivative_hydrolysis_or_formation reaction

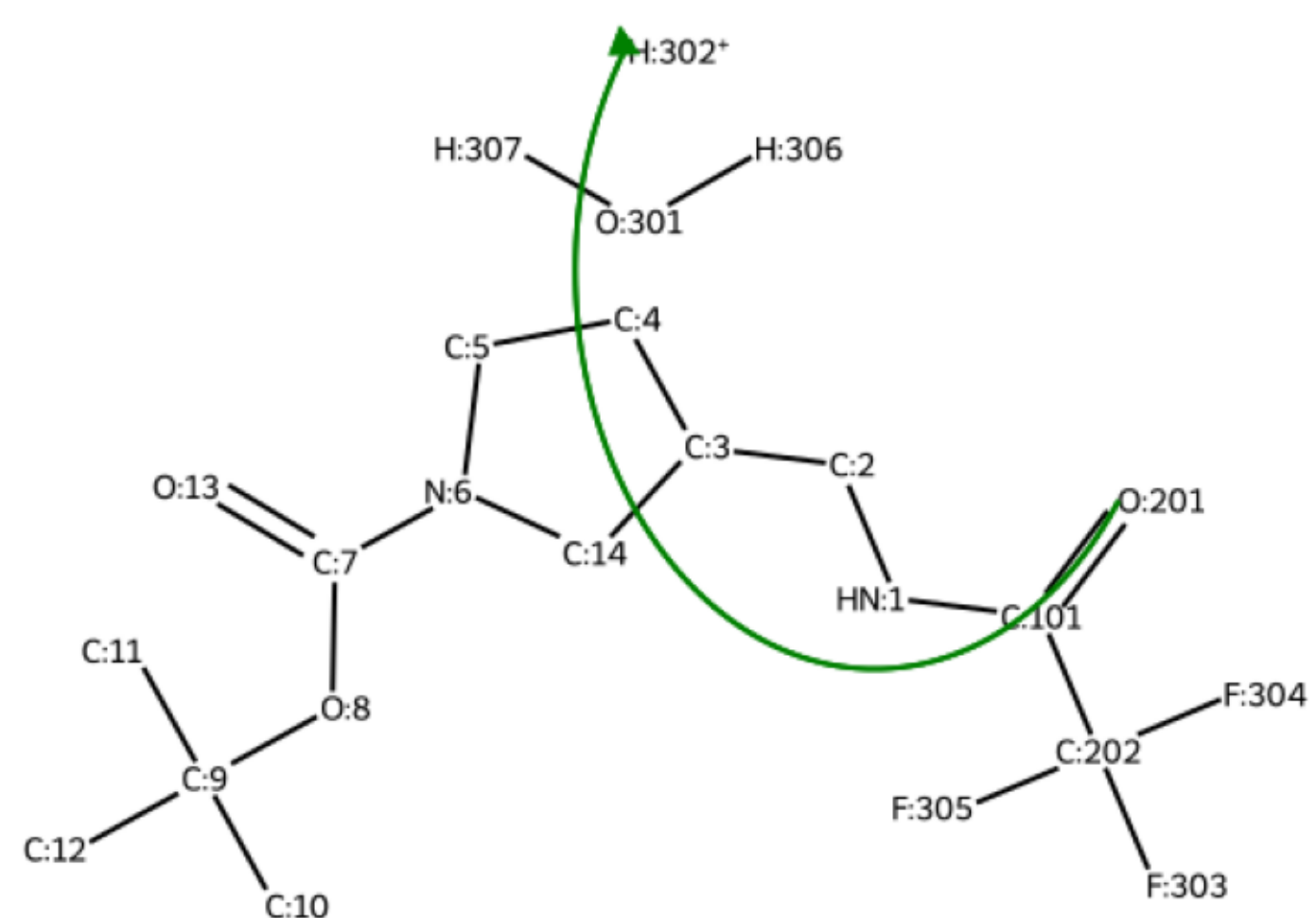
Reaction with missing reagents recovered



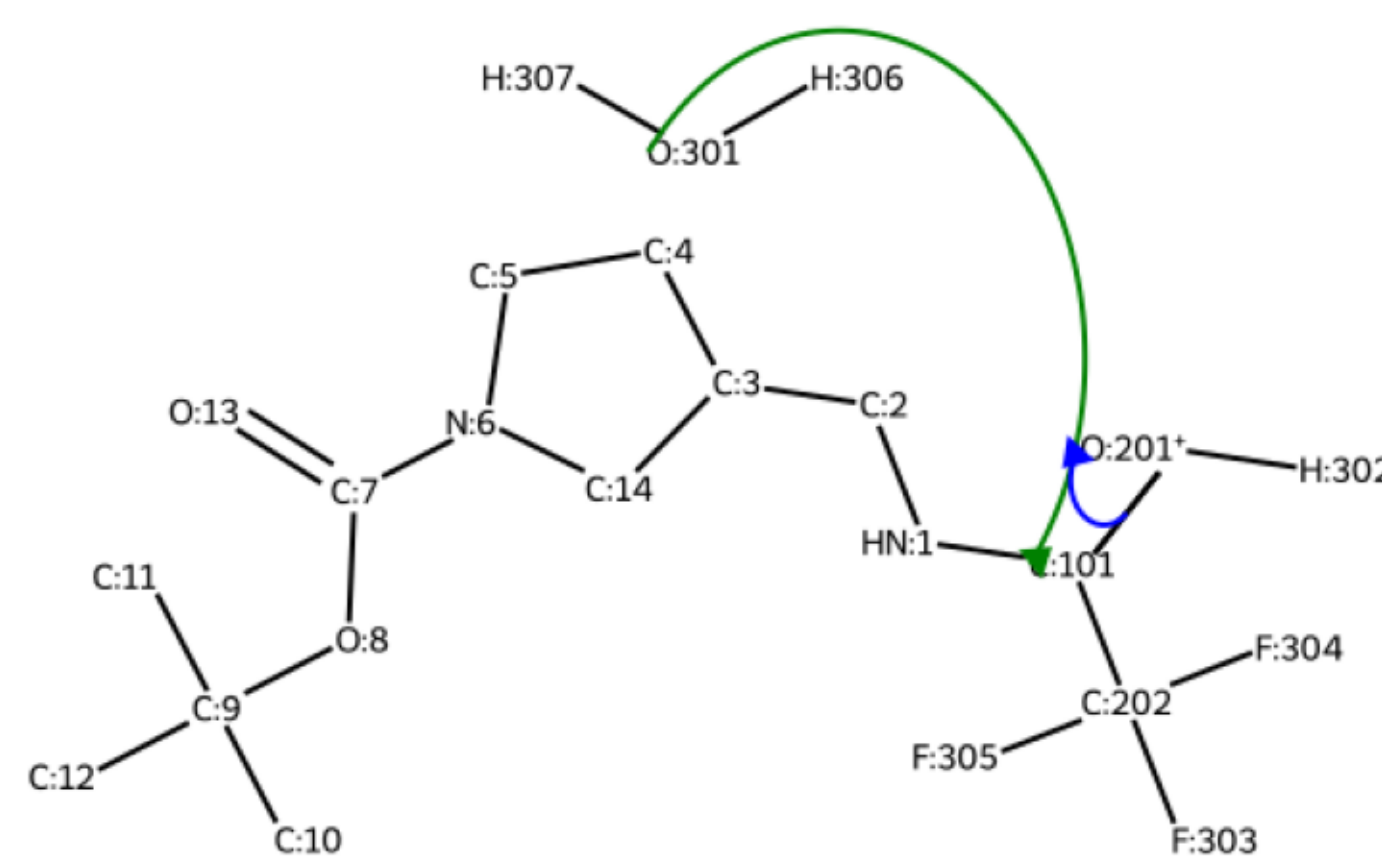
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

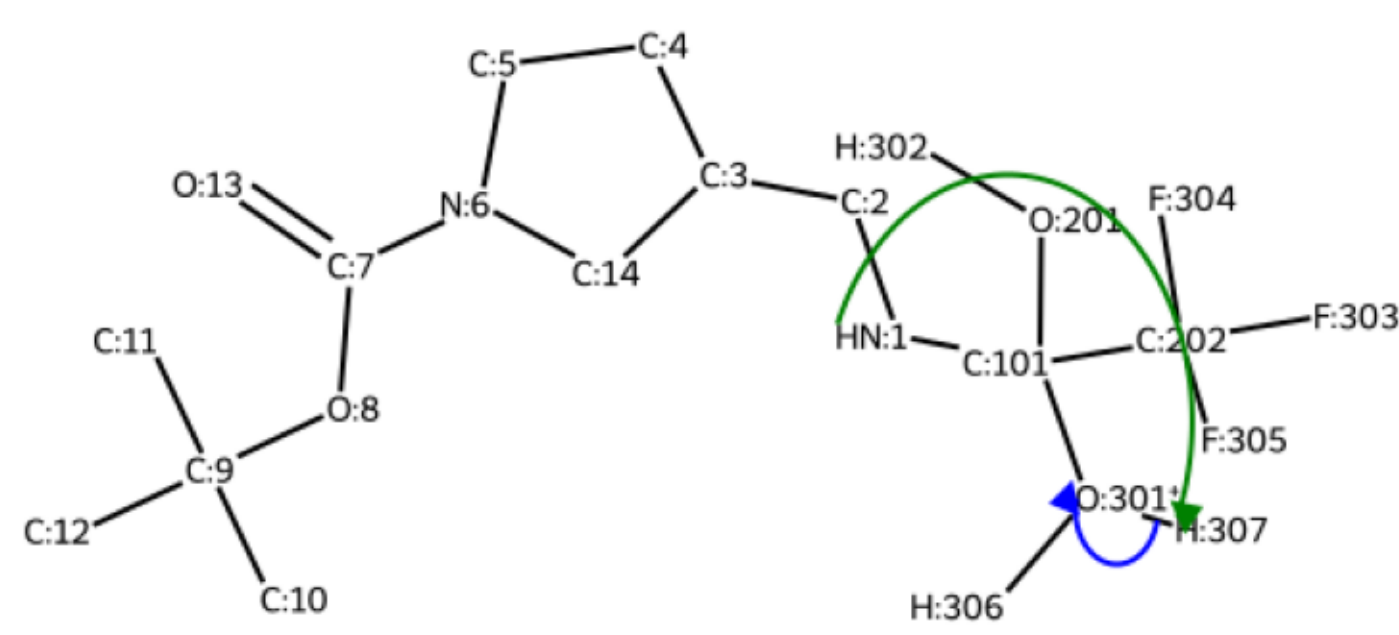
step #1



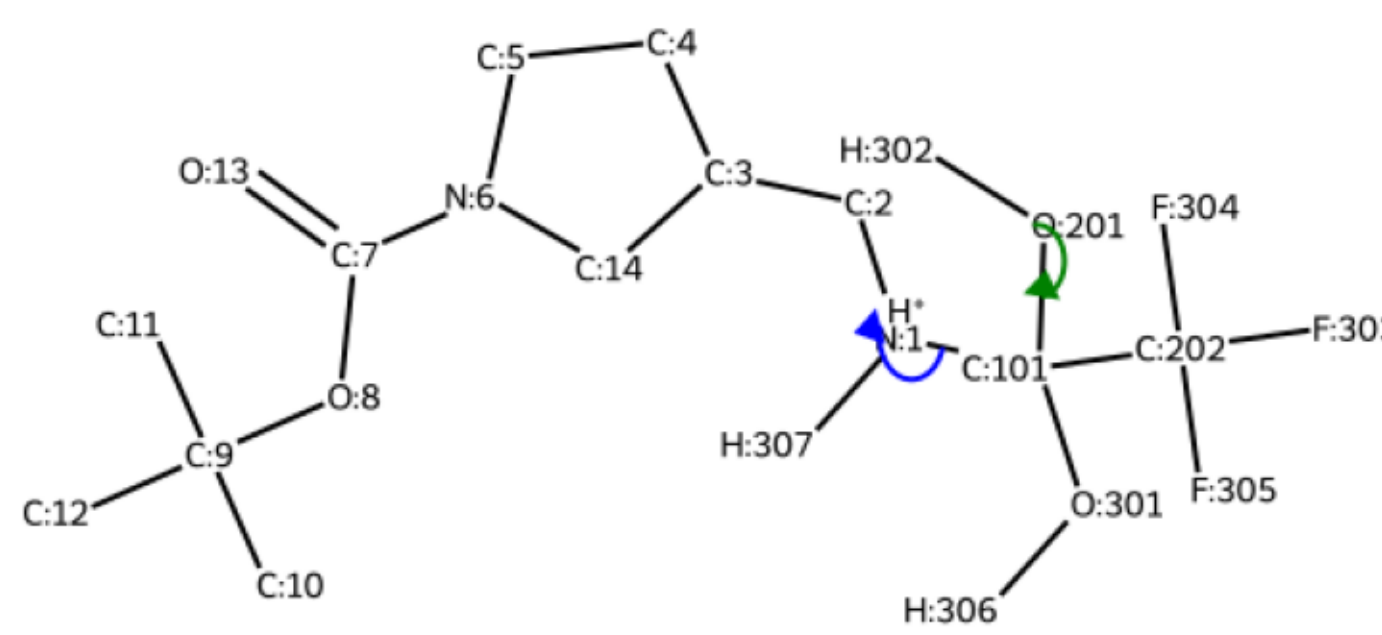
step #2



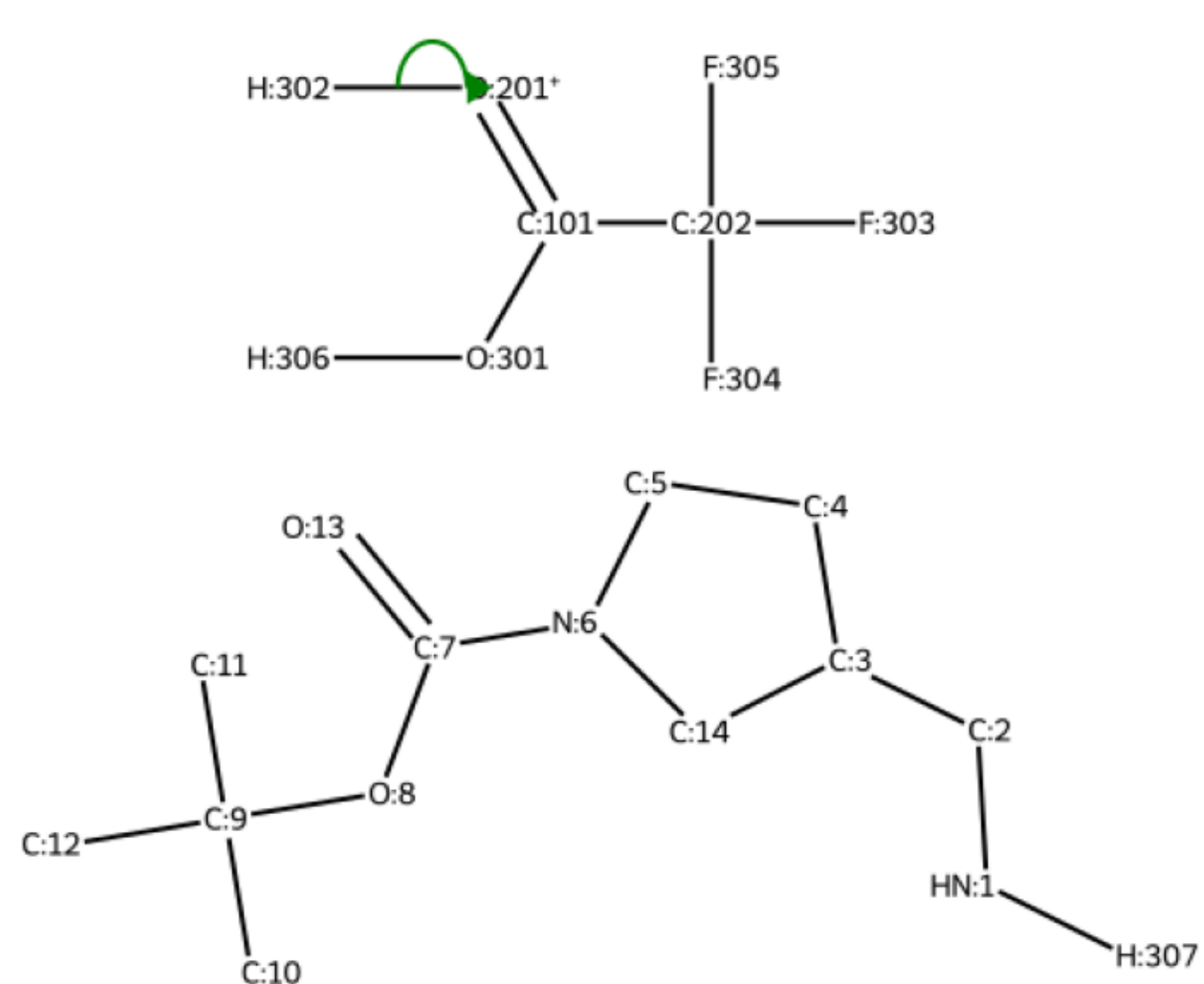
step #3



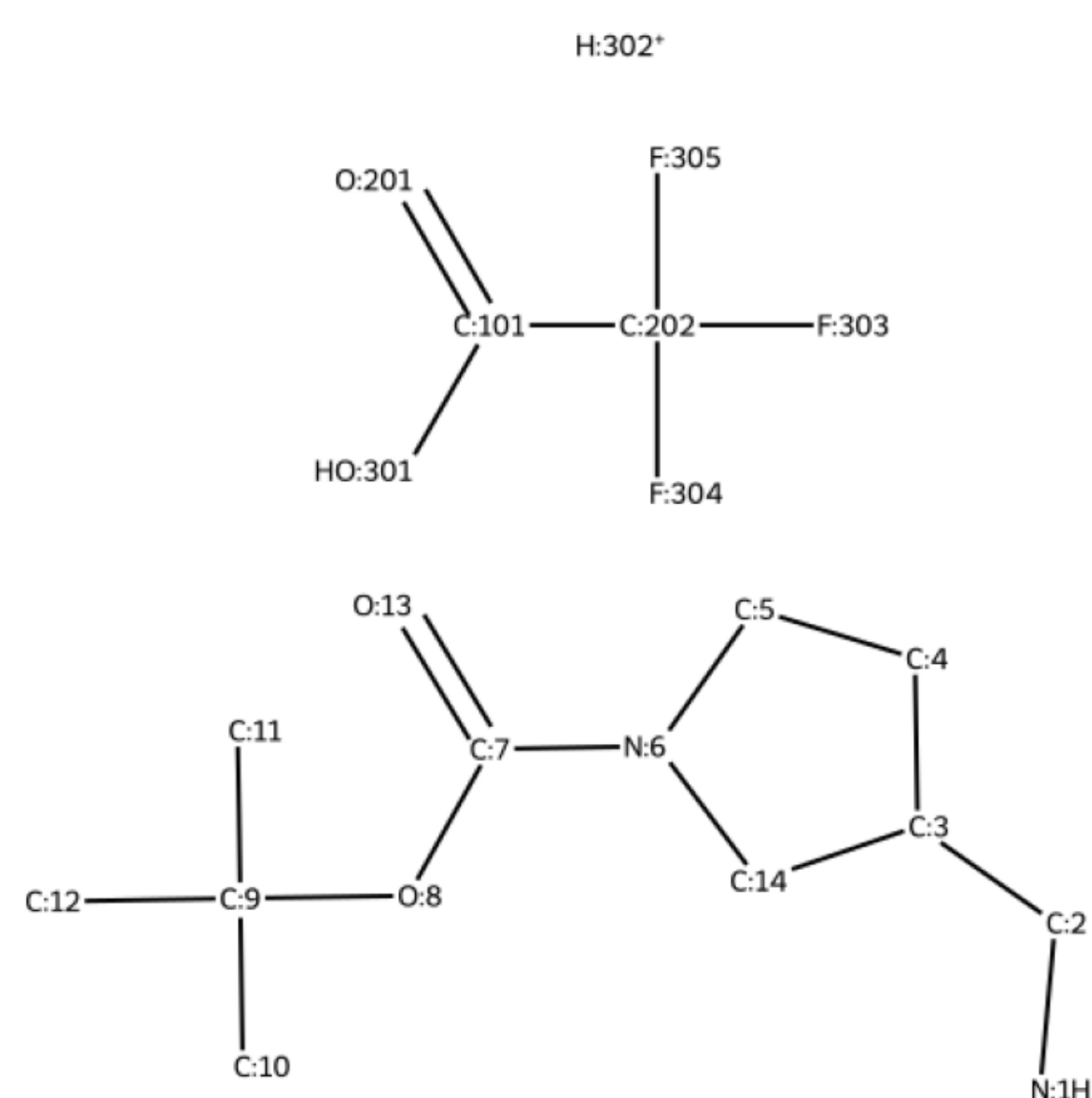
step #4



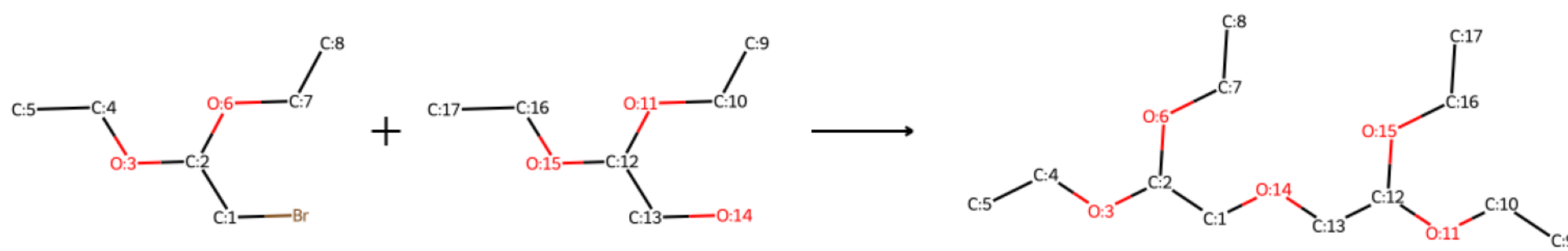
step #5



Product(s)

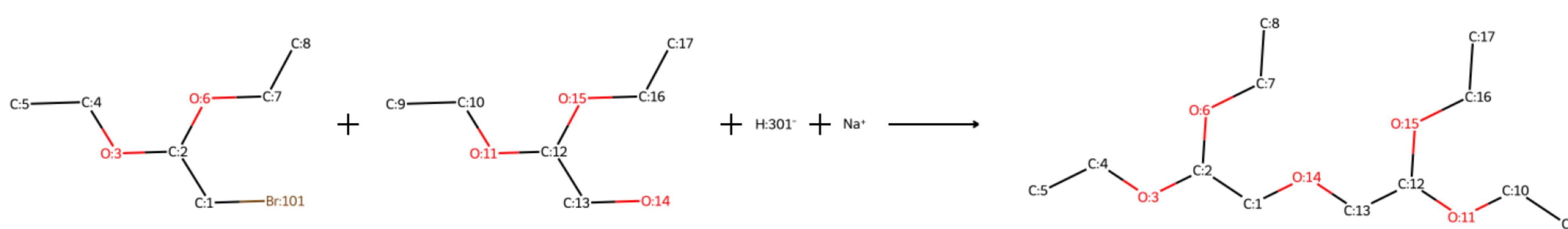


Original reaction
sampled RXN_ID:16)



Identified mechanistic class -
SN2_alcohol(thiol) reaction

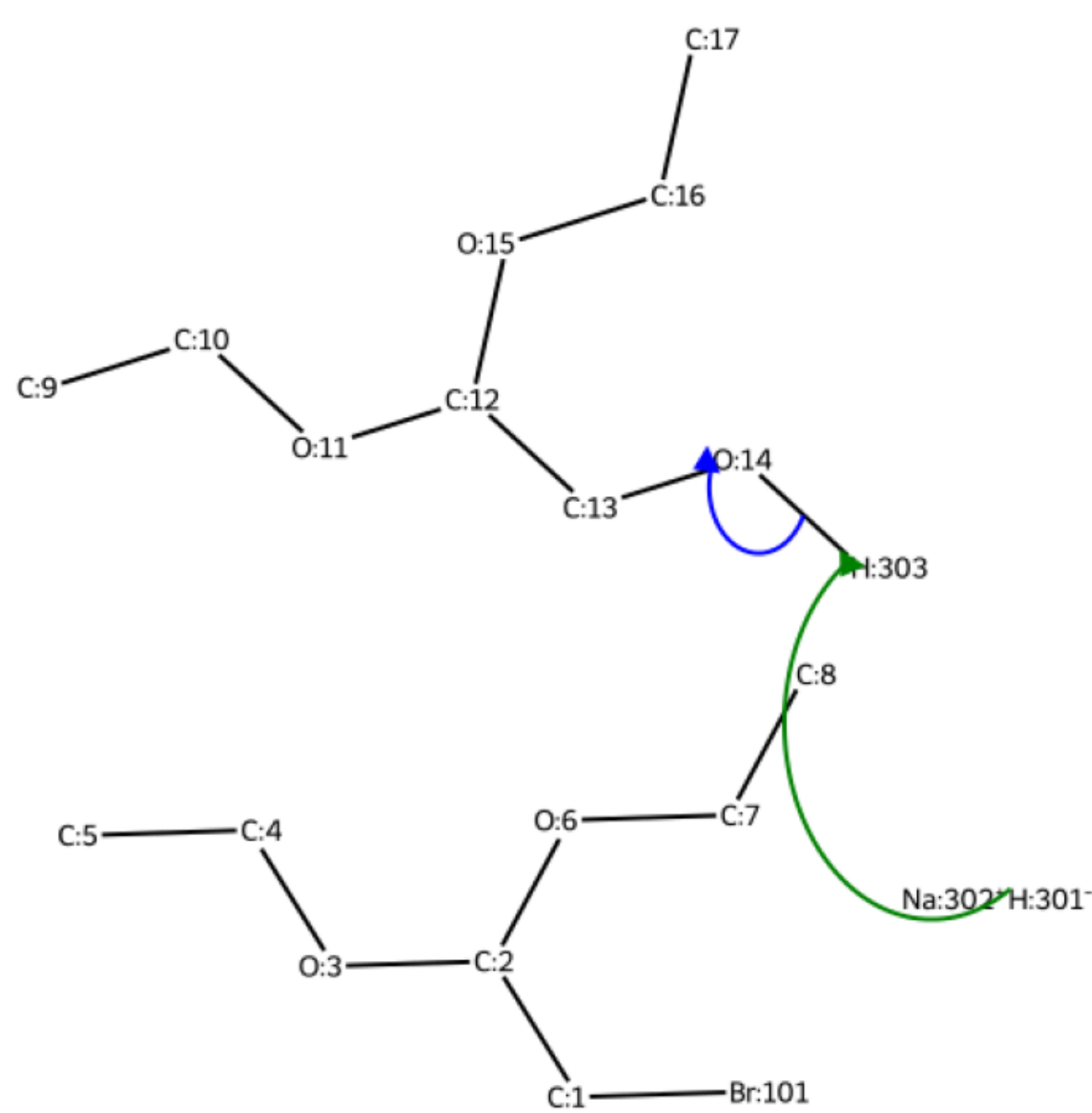
Reaction with missing reagents recovered



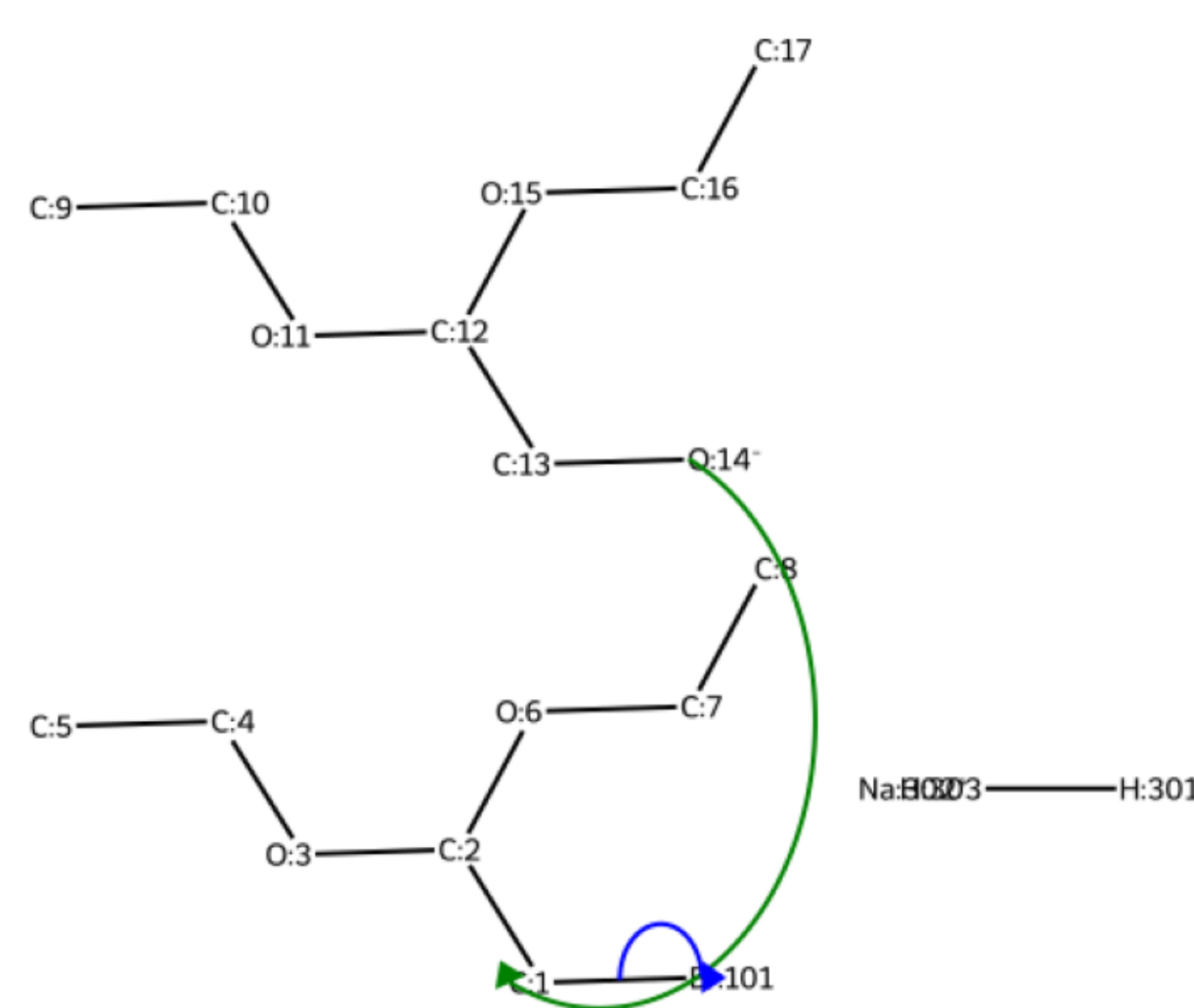
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

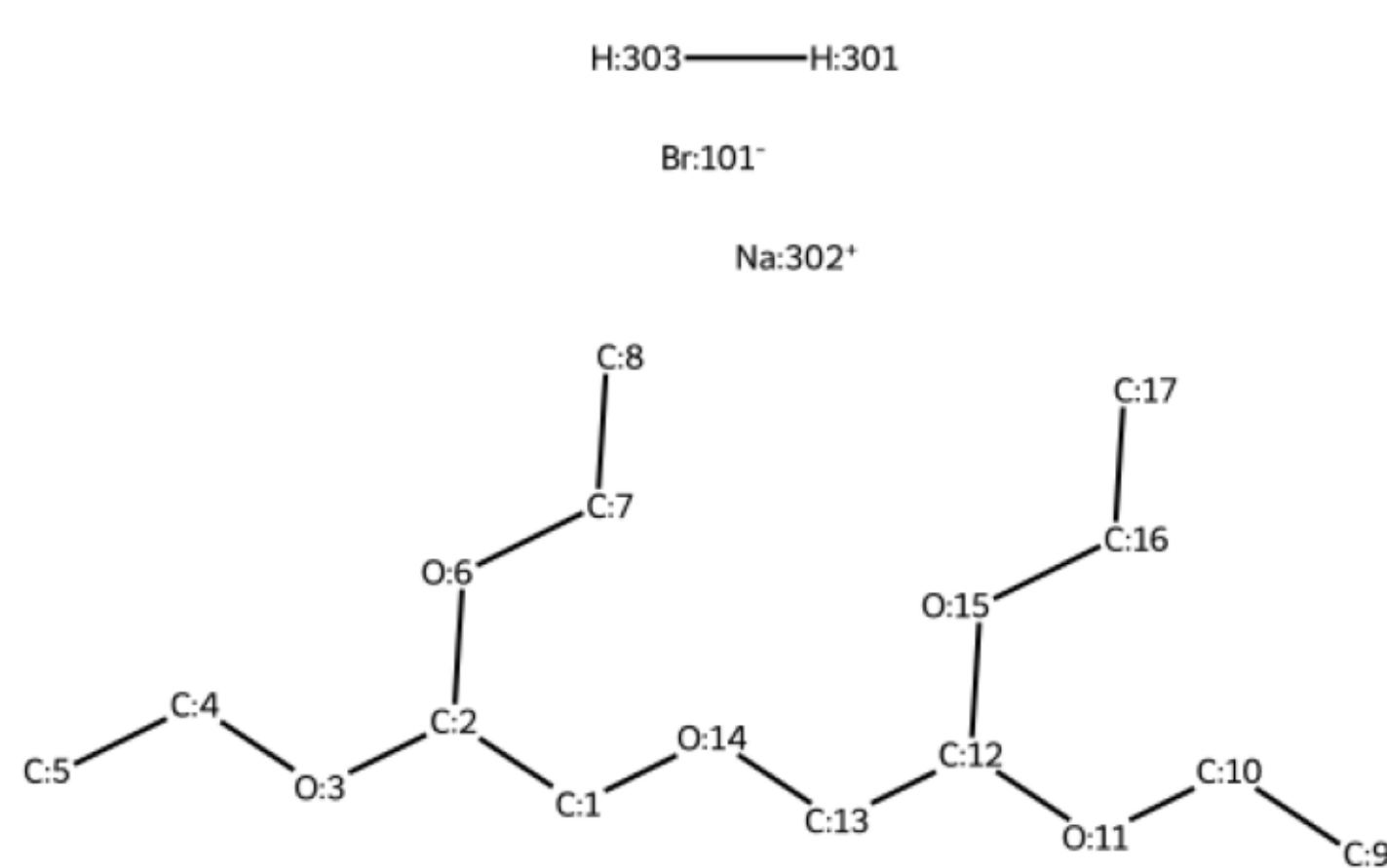
step #1



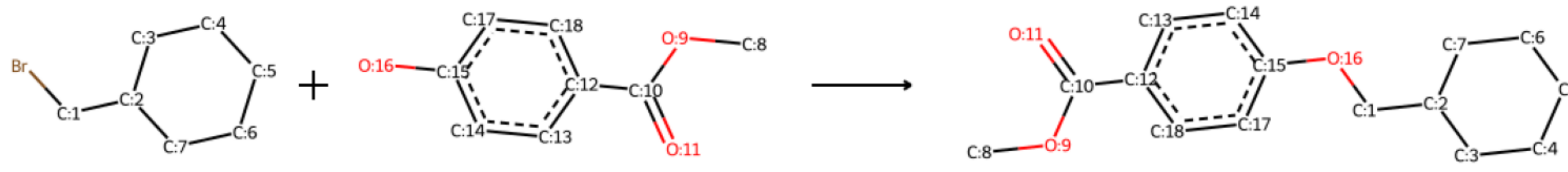
step #2



Product(s)

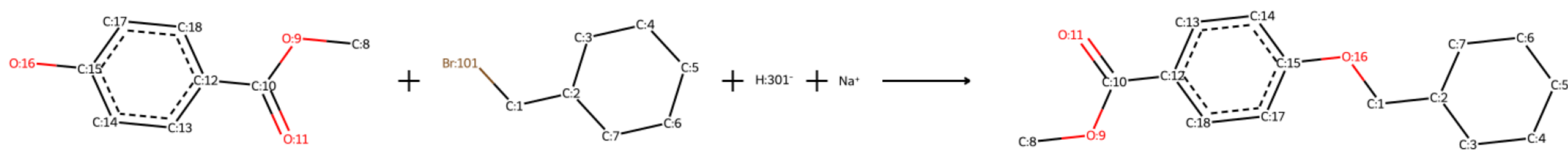


Original reaction
sampled RXN_ID:17)



Identified mechanistic class -
SN2_alcohol(thiol) reaction

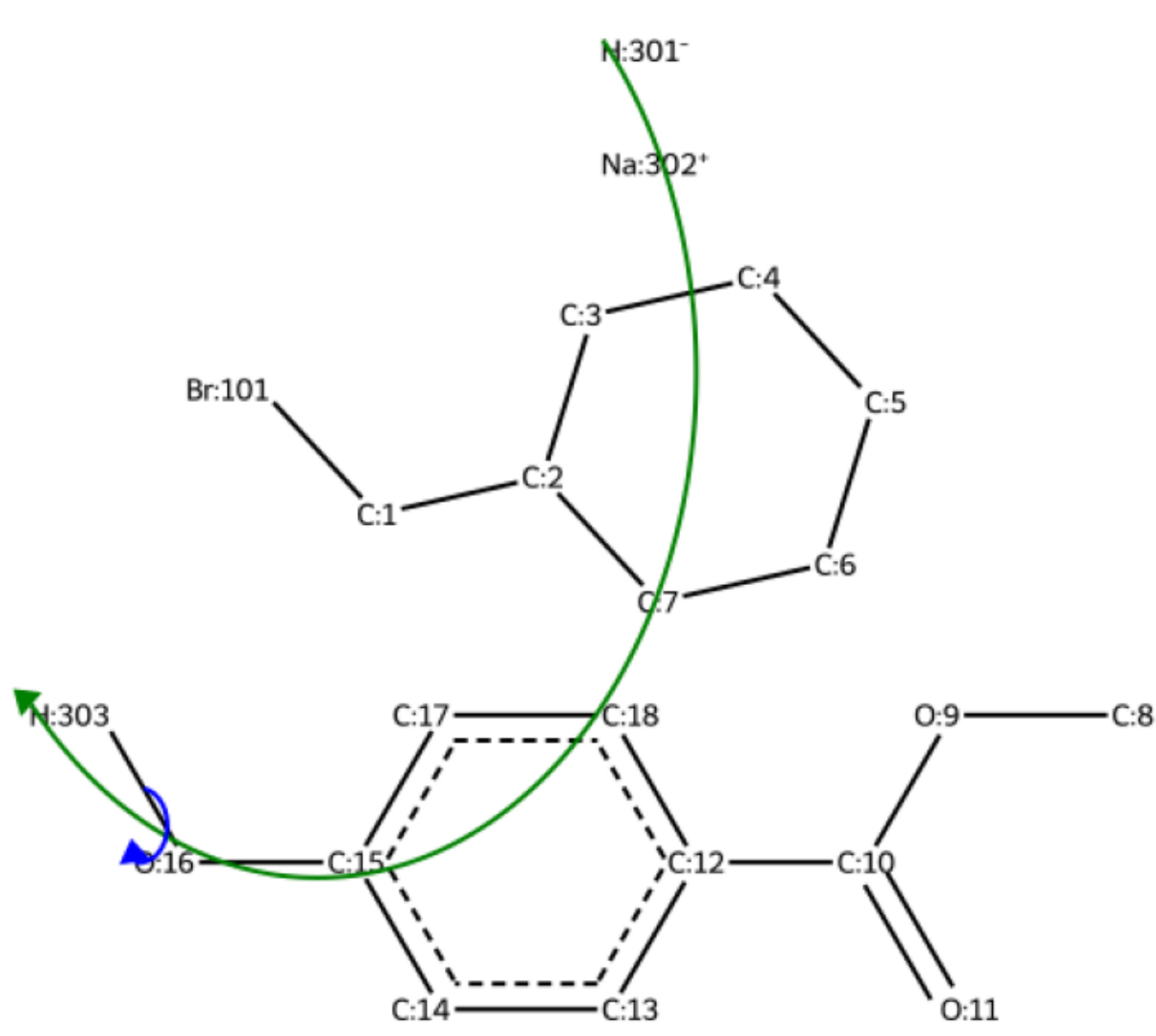
Reaction with missing reagents recovered



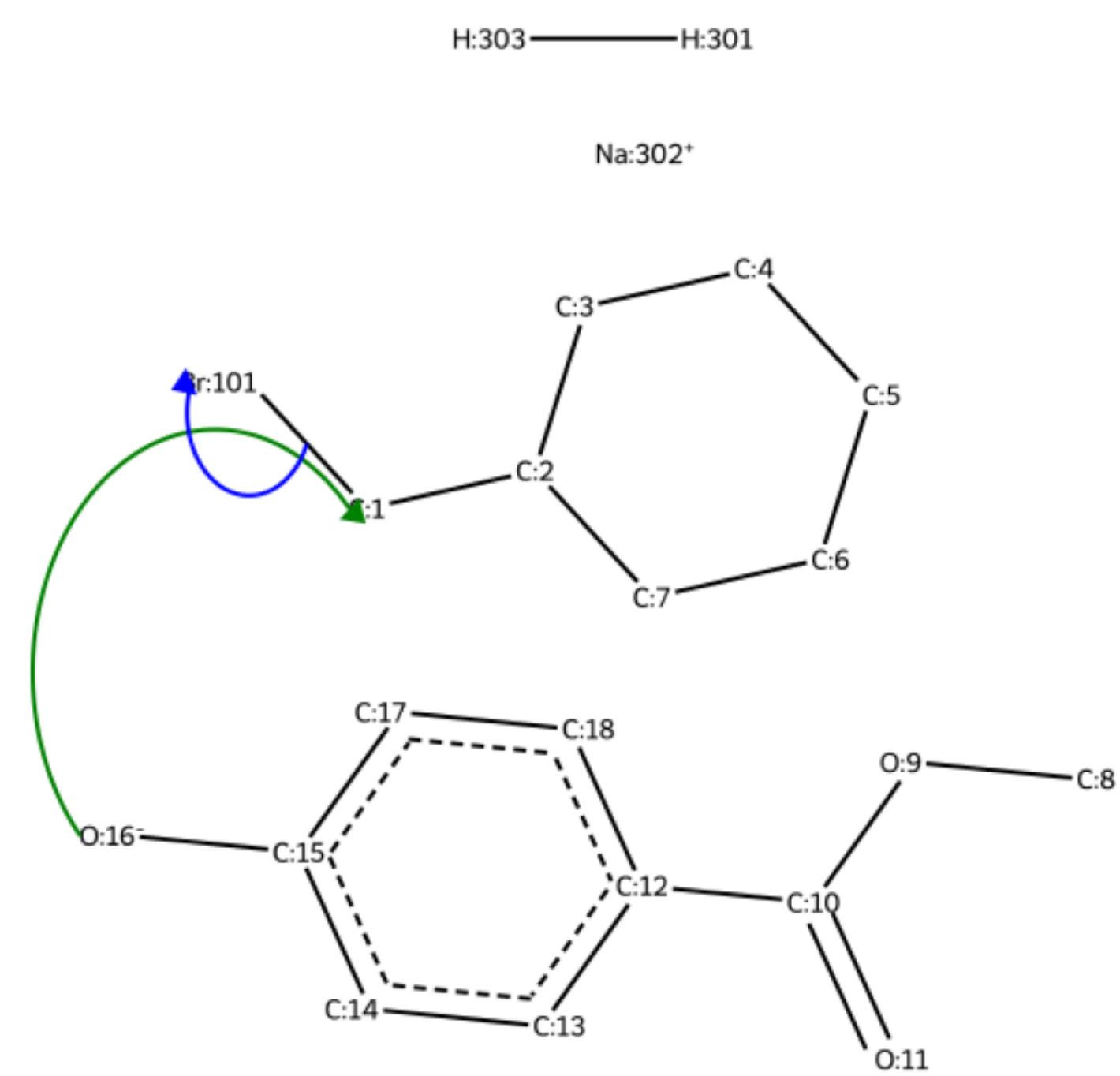
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

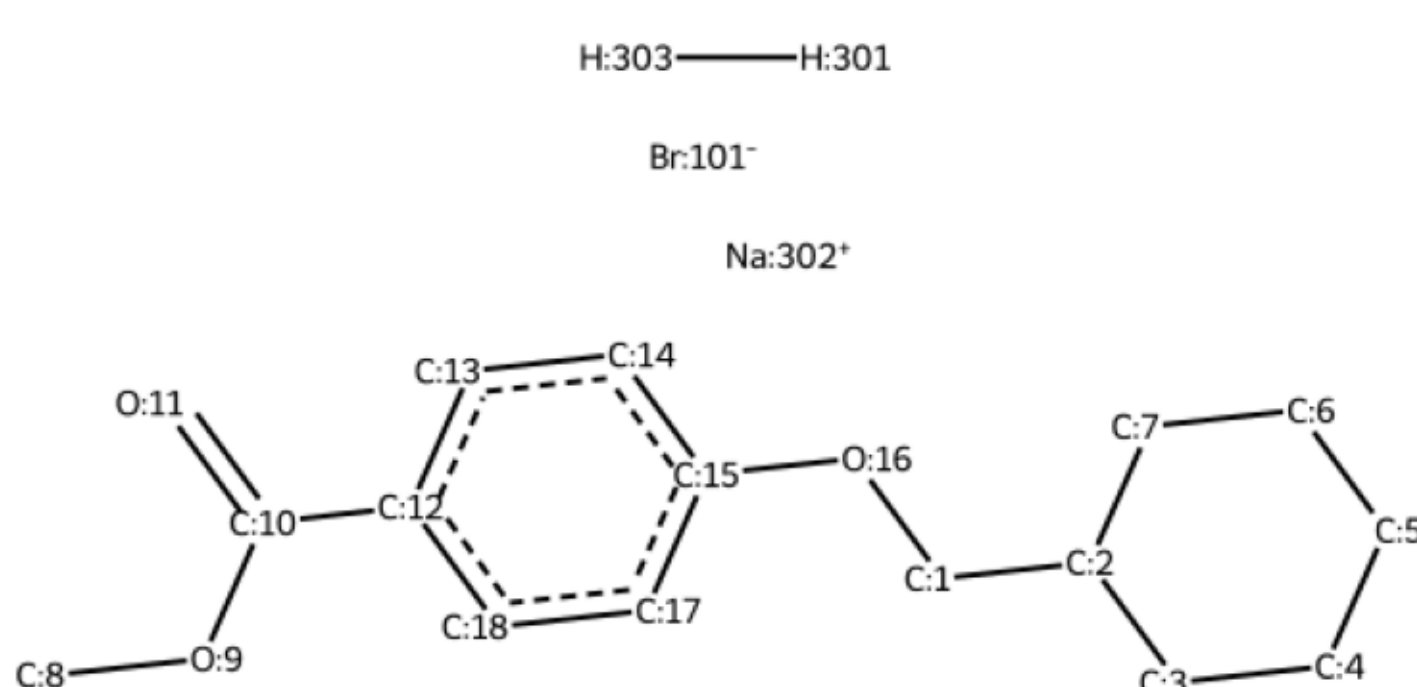
step #1



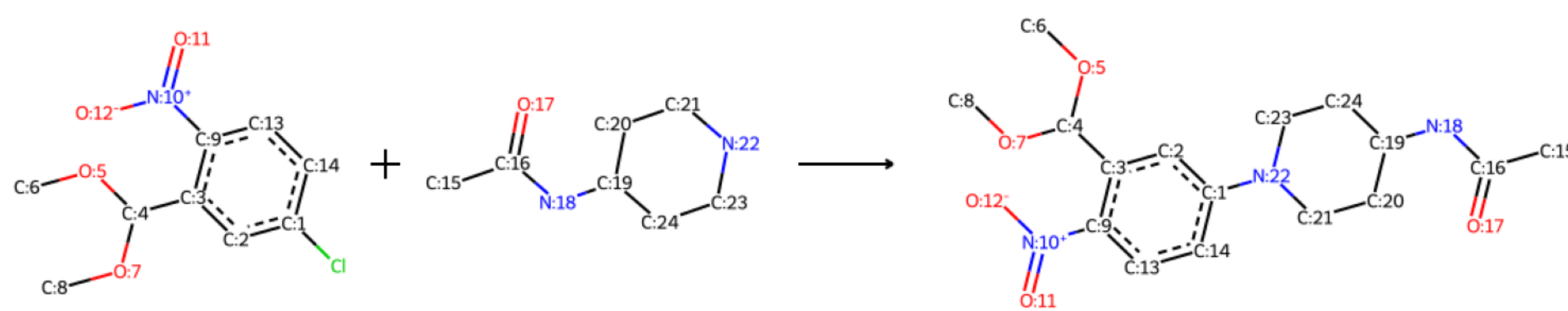
step #2



Product(s)

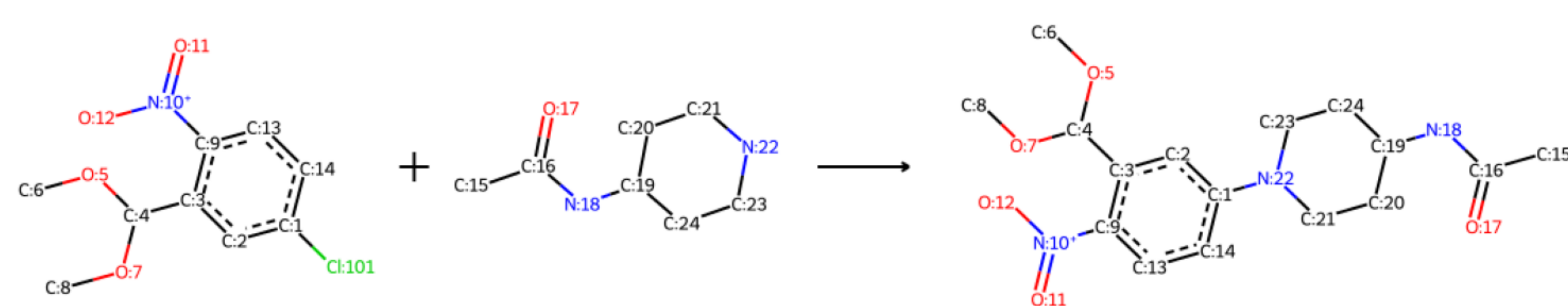


Original reaction
sampled RXN_ID:18)



Identified mechanistic class -
S_NAr(para) reaction

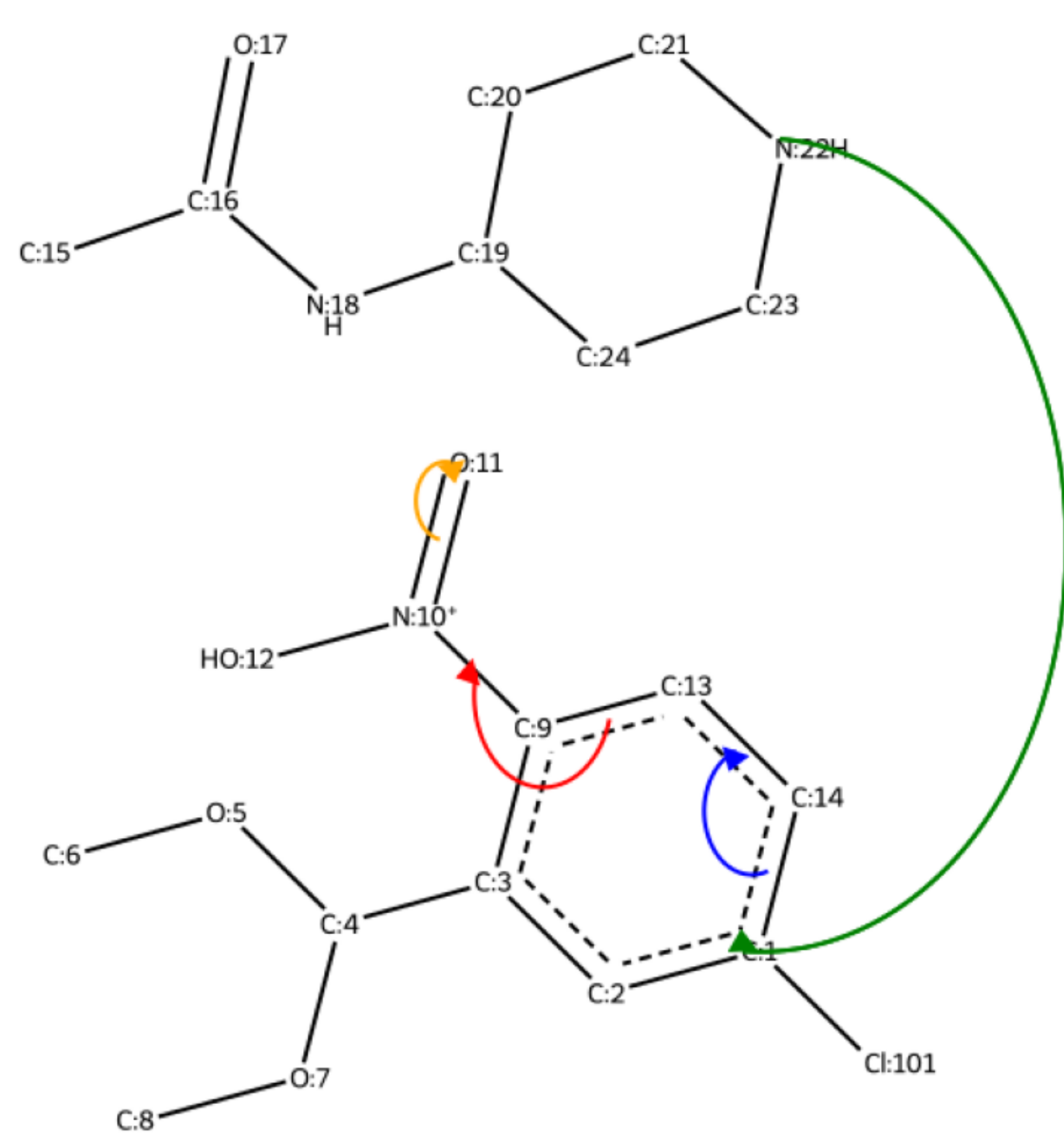
Reaction with missing reagents recovered



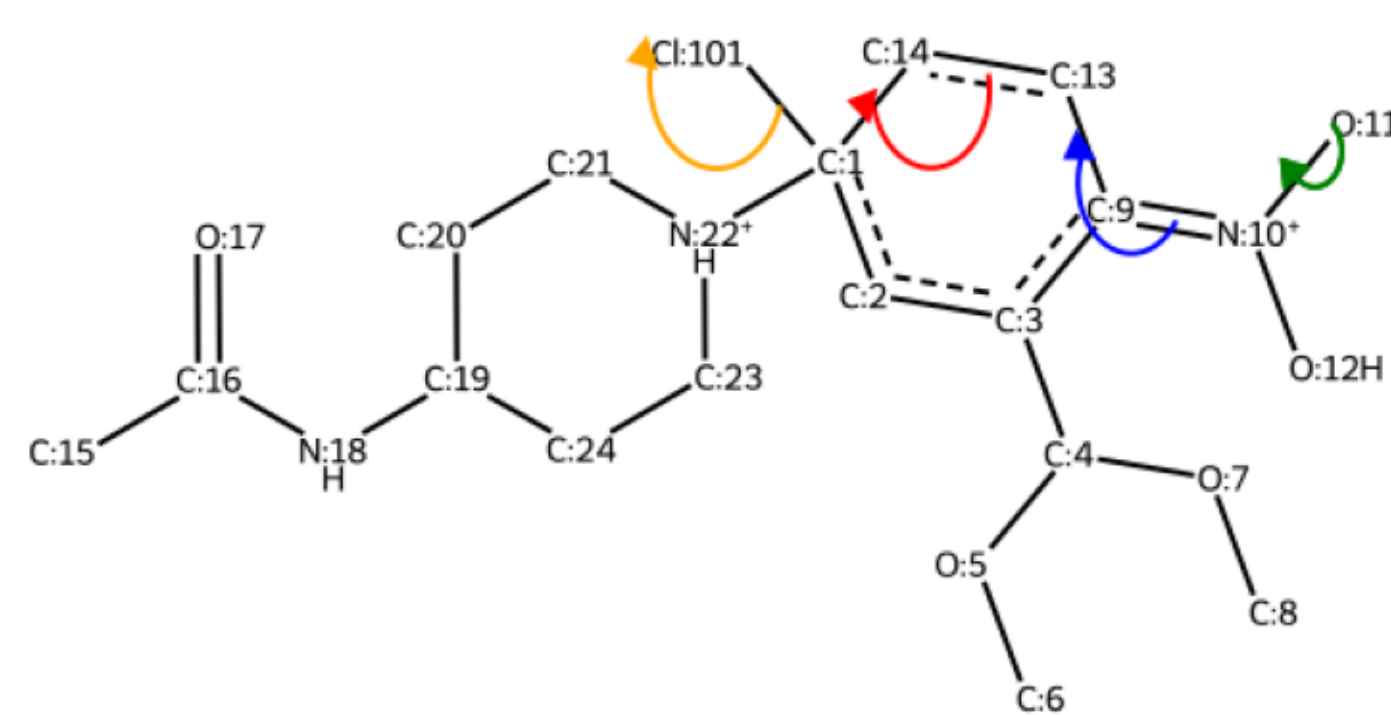
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

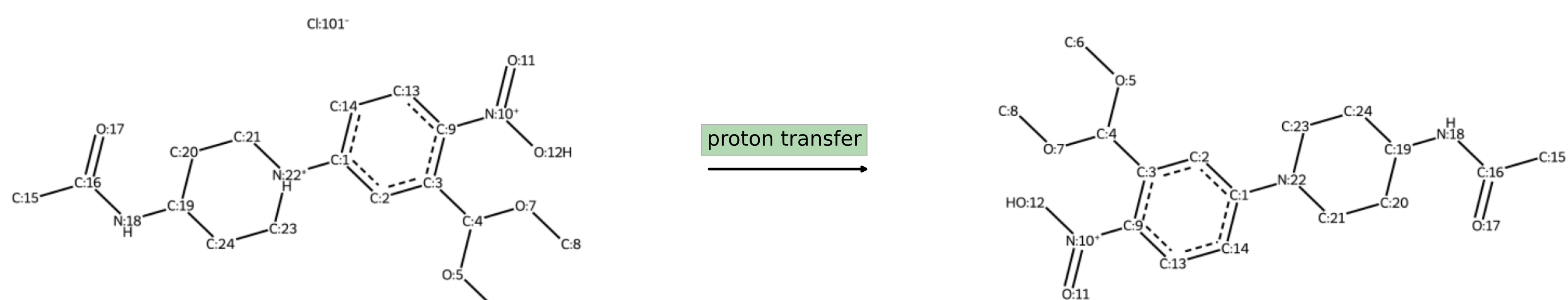
step #1



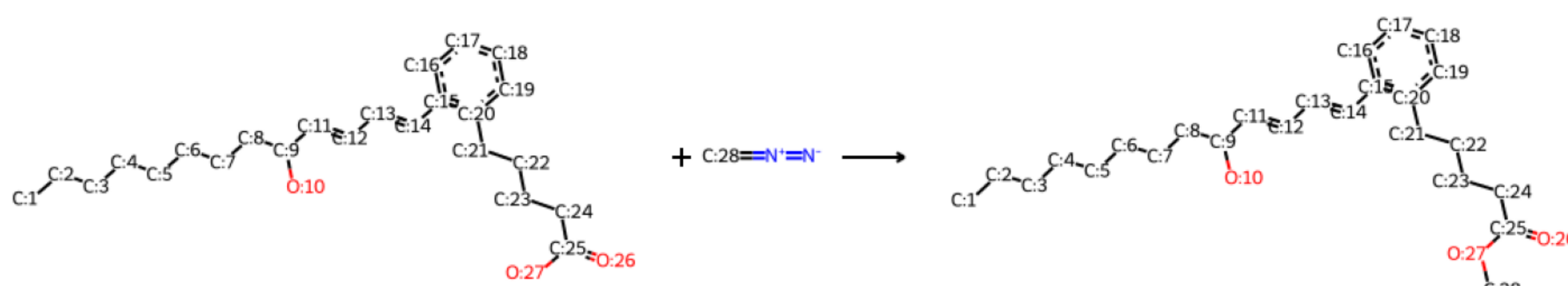
step #2



Product(s)

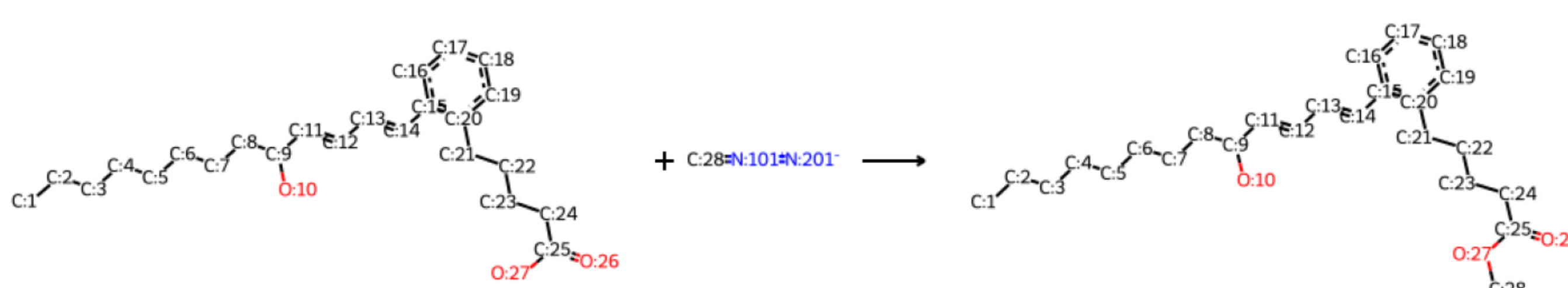


Original reaction sampled RXN_ID:19)



Identified mechanistic class -
methyl_ester_synthesis reaction

Reaction with missing reagents recovered

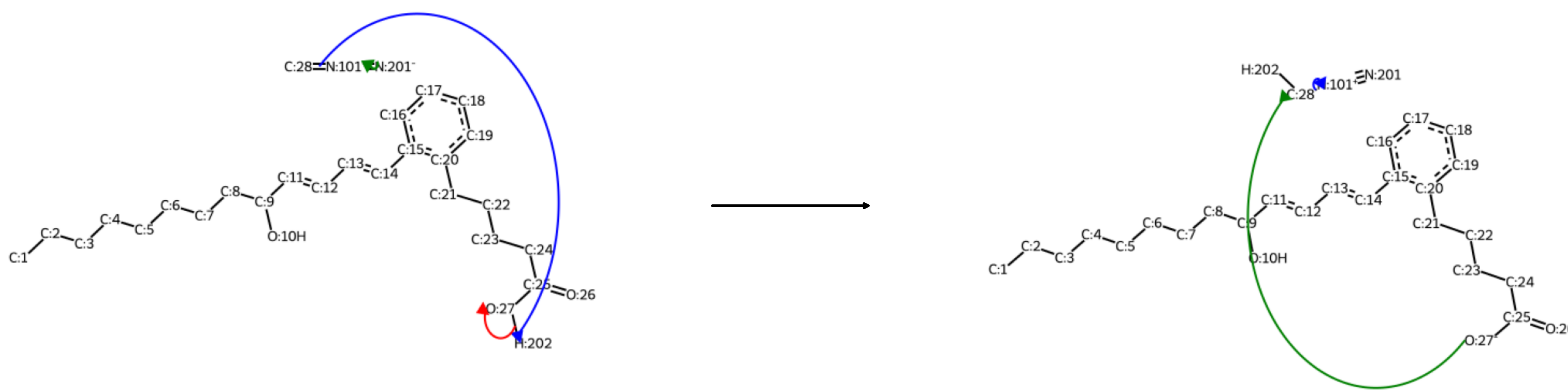


Proposed mechanistic pathway

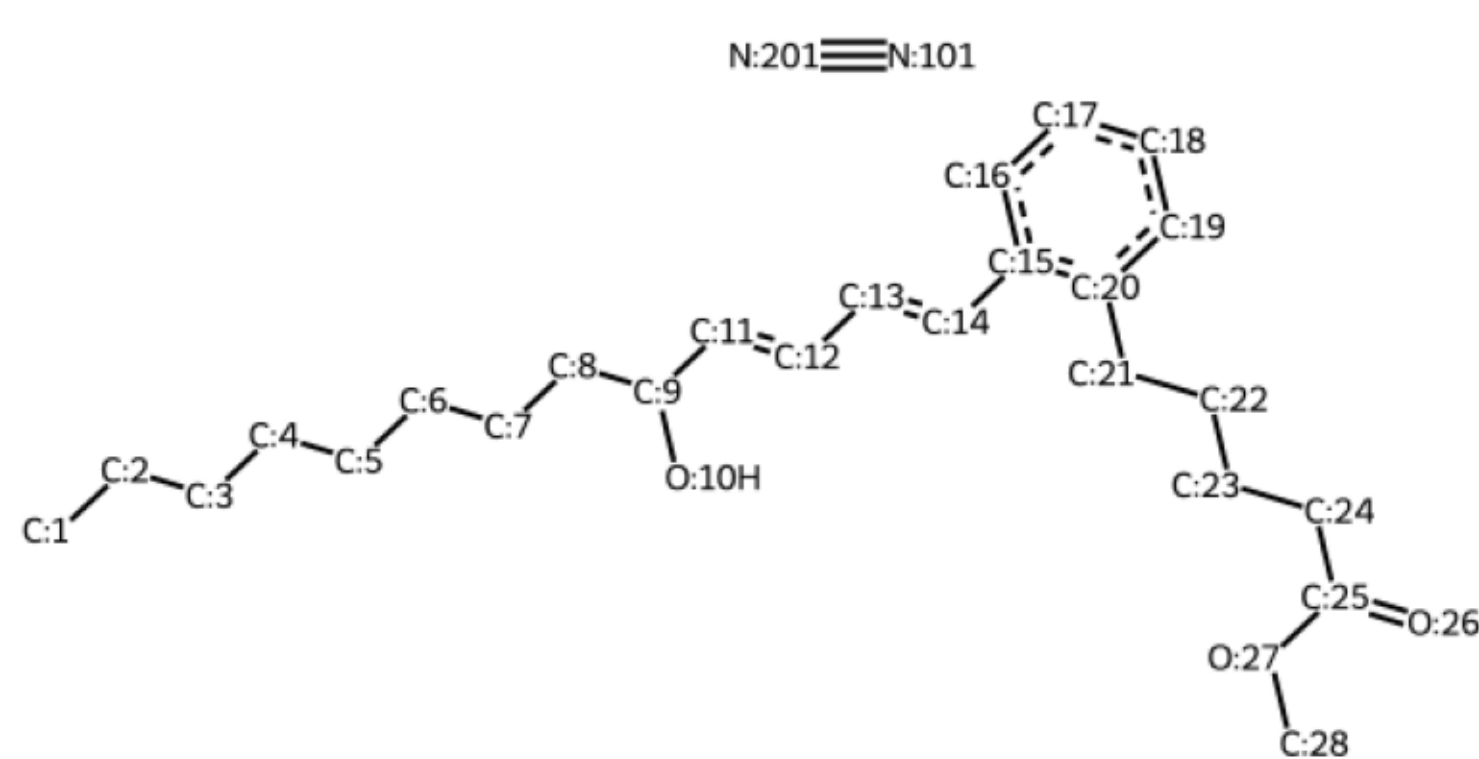
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

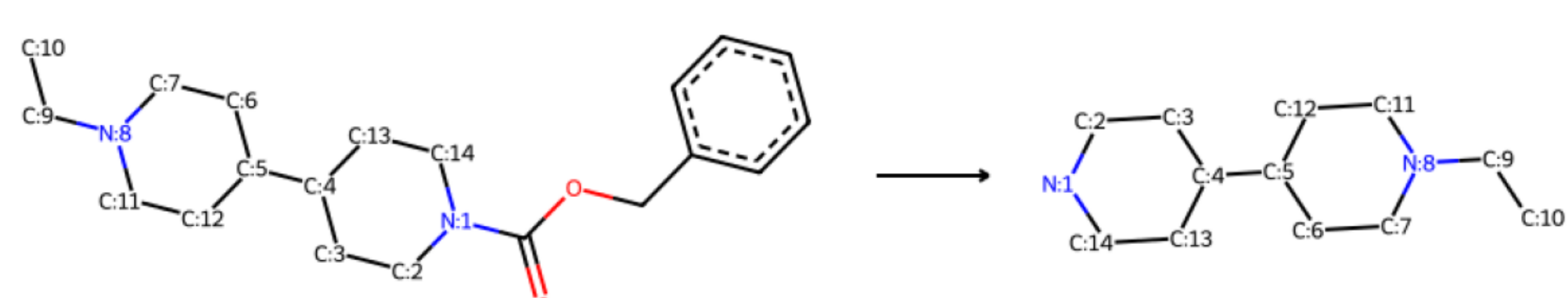
step #2



Product(s)

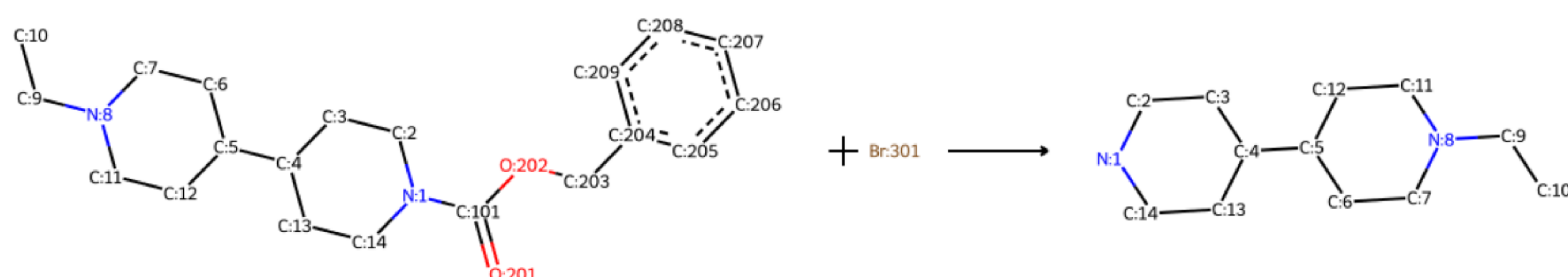


Original reaction
sampled RXN_ID:20)



Identified mechanistic class -
Cbz_deprotection reaction

Reaction with missing reagents recovered

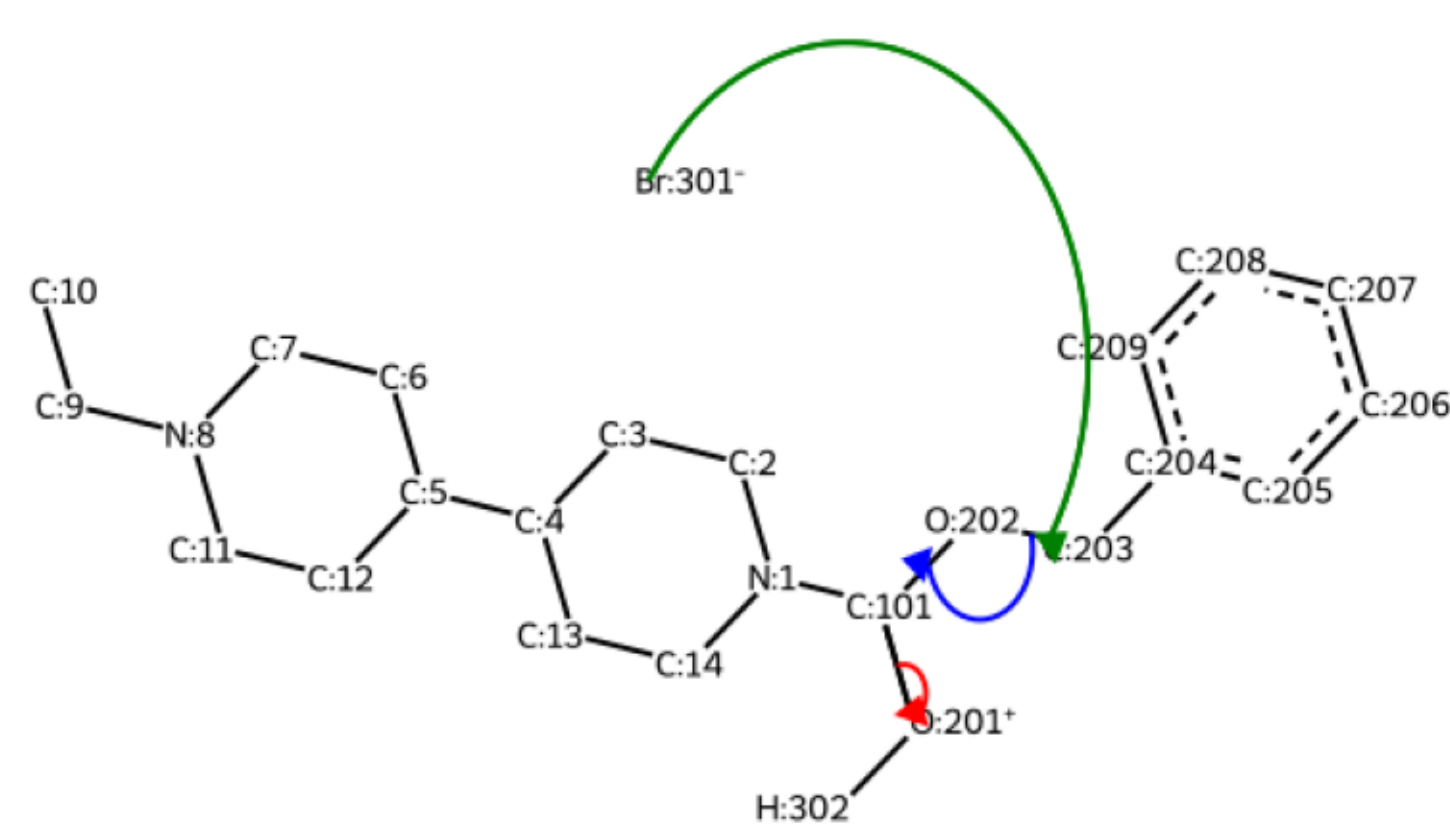
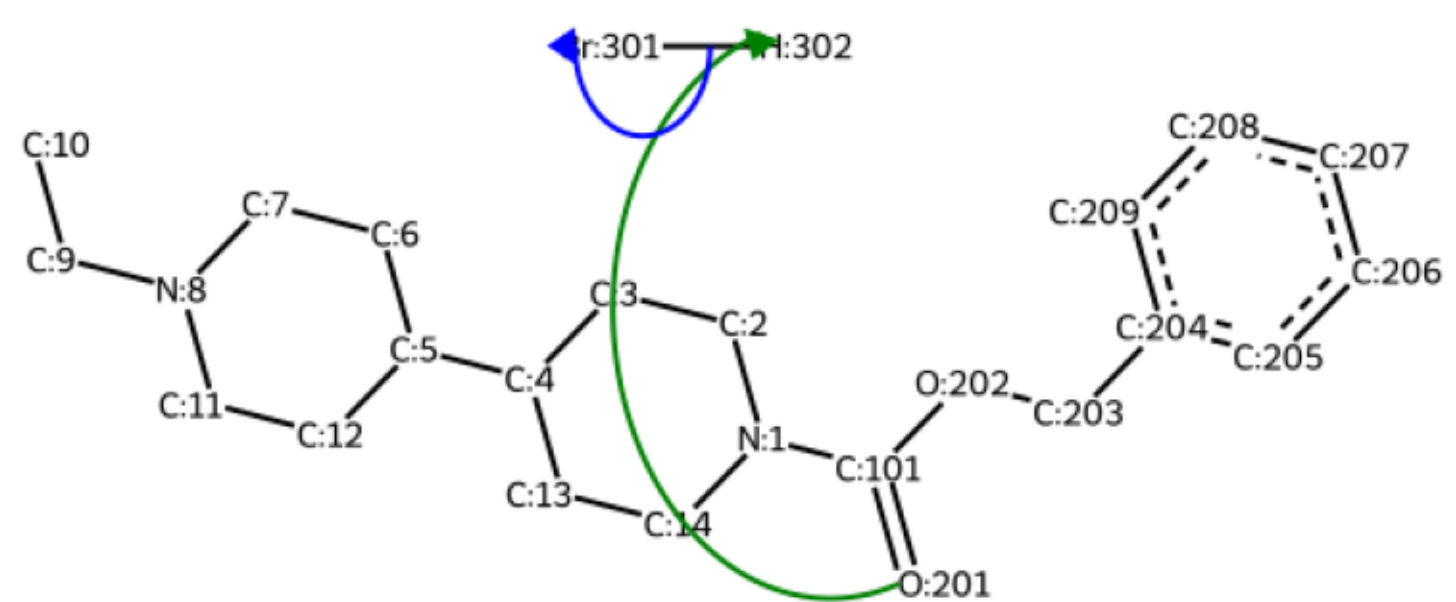


Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

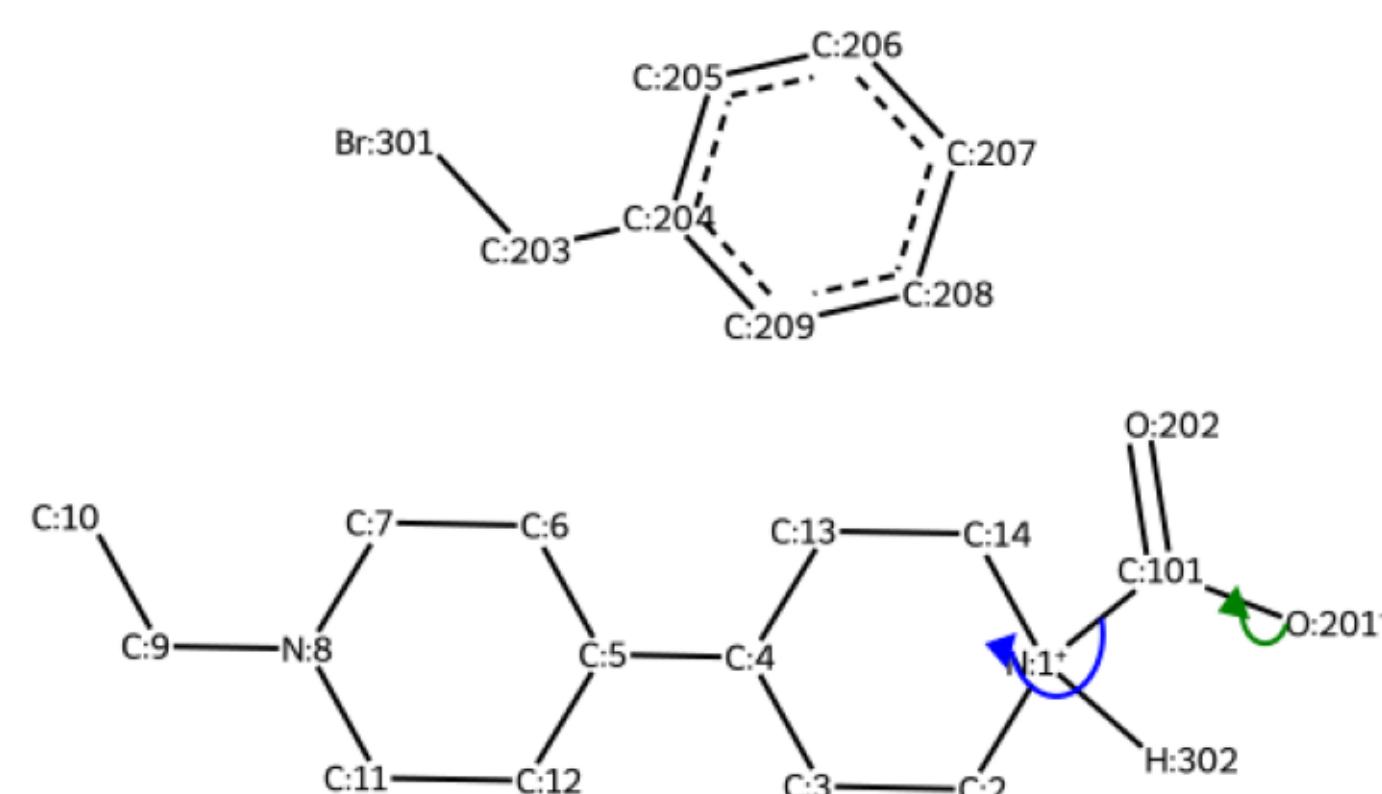
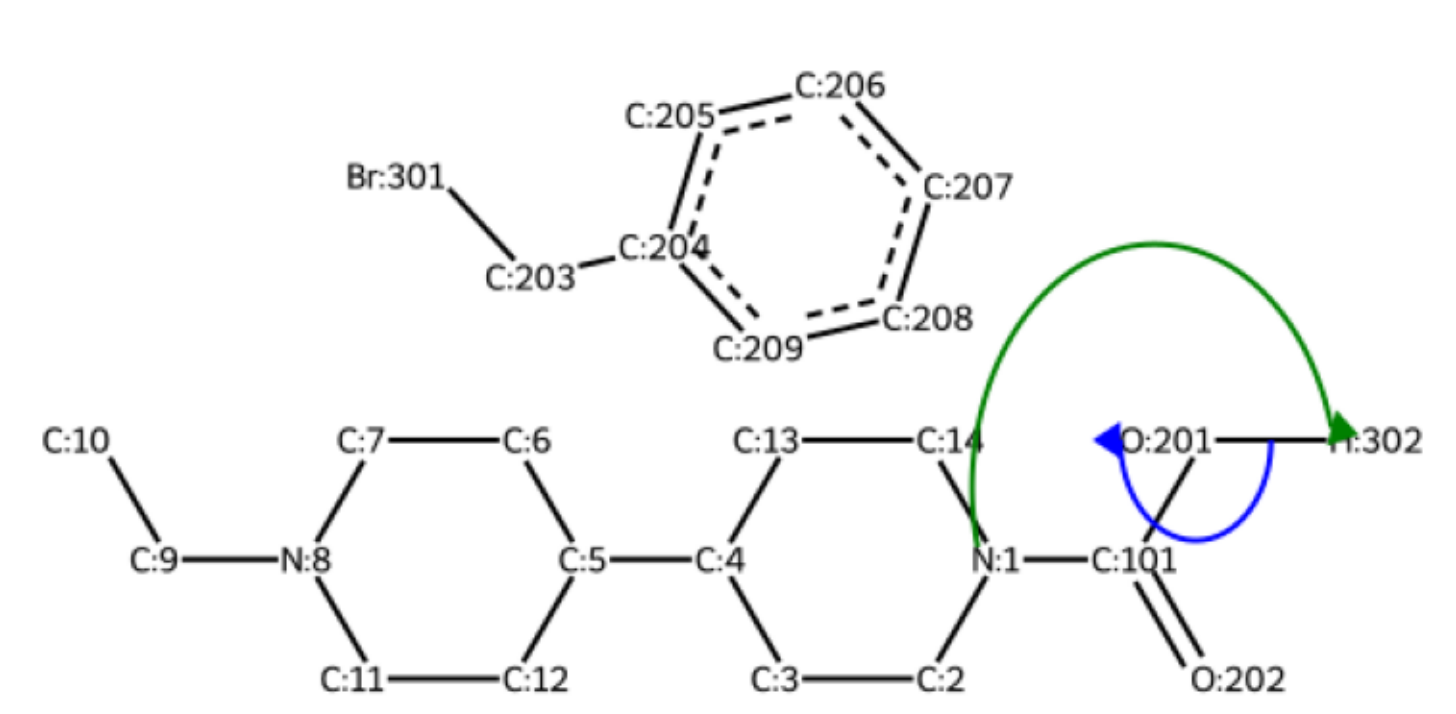
step #1

step #2

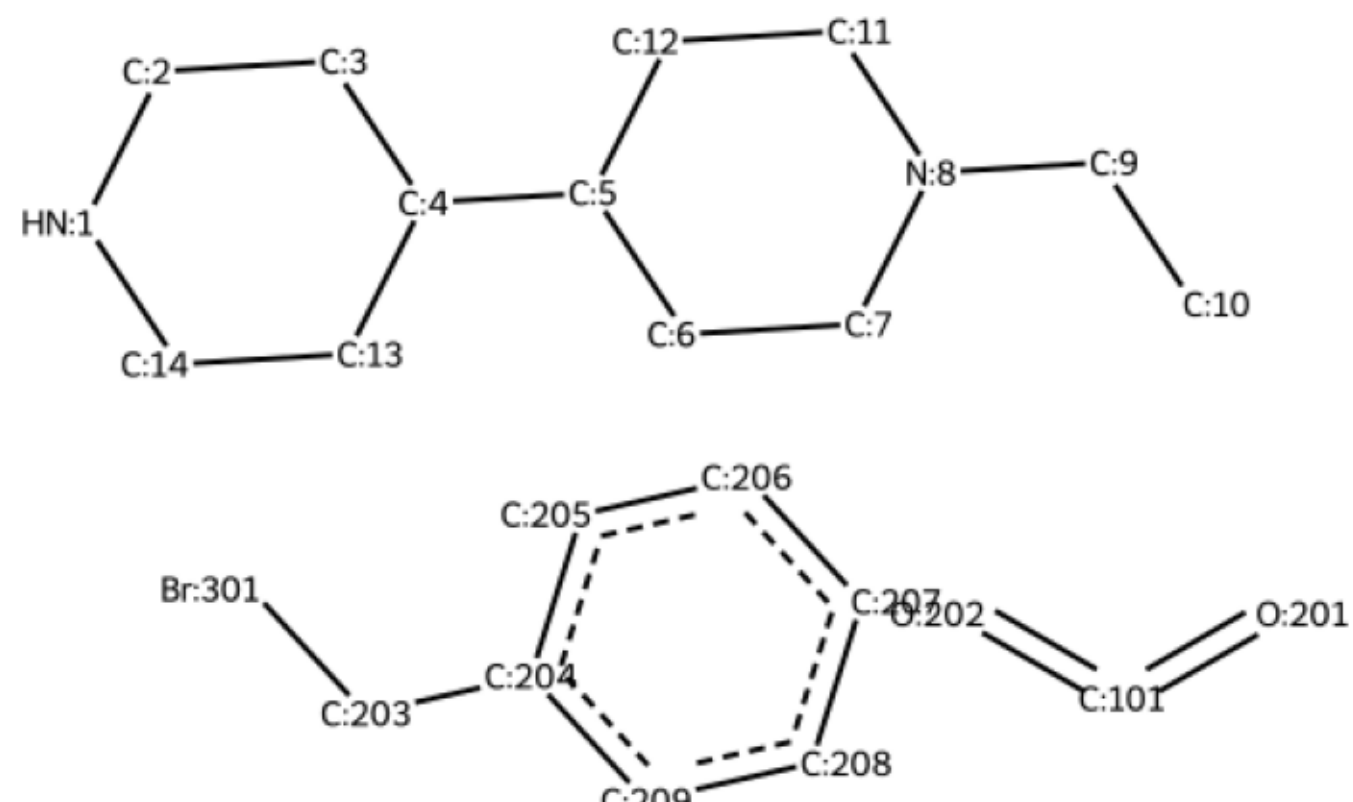


step #3

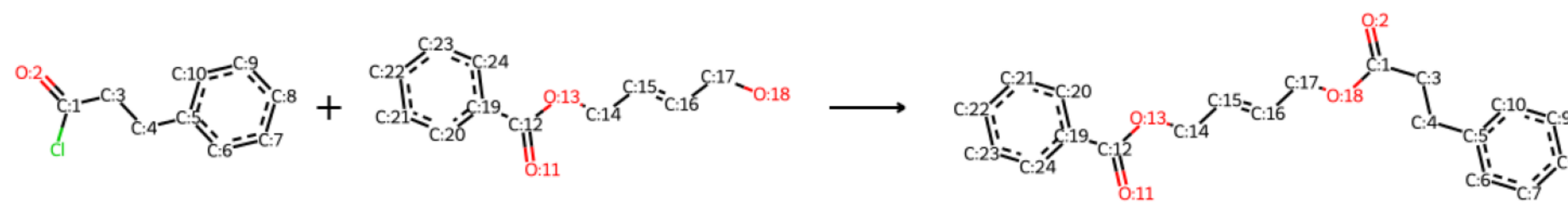
step #4



Product(s)

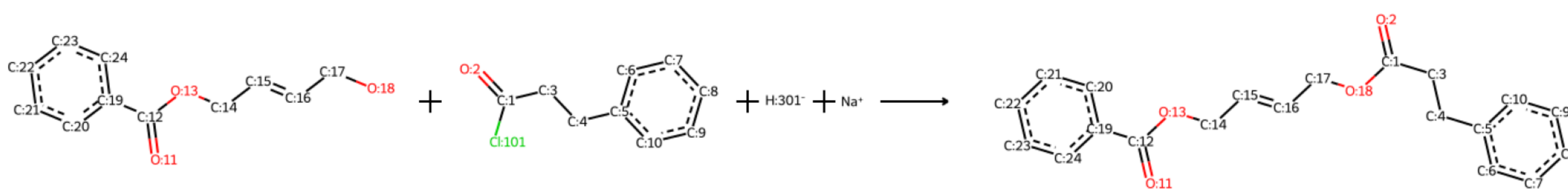


Original reaction
sampled RXN_ID:21)



Identified mechanistic class -
alcohol_attack_to_carbonyl_or_sulfonyl reaction

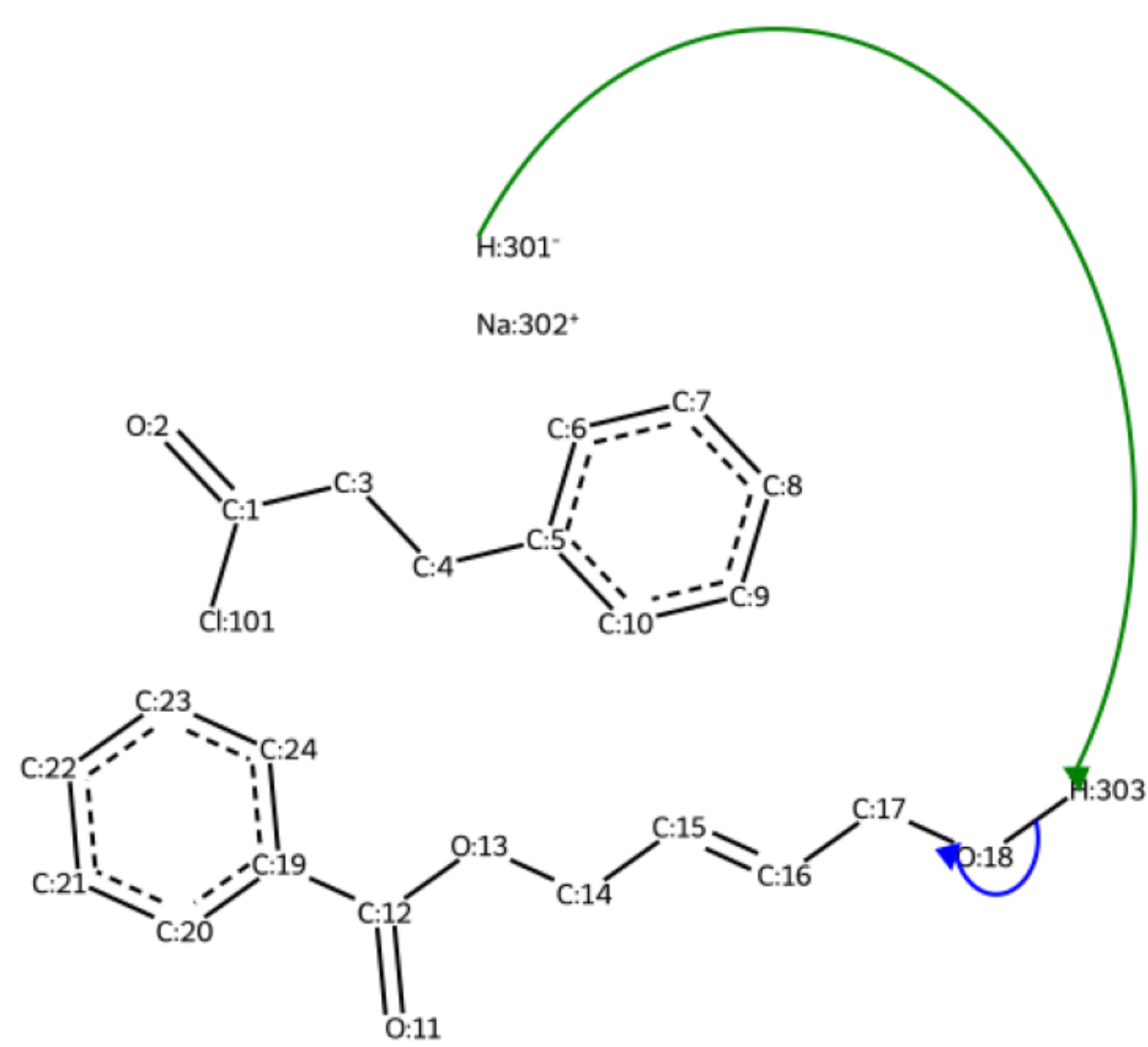
Reaction with missing reagents recovered



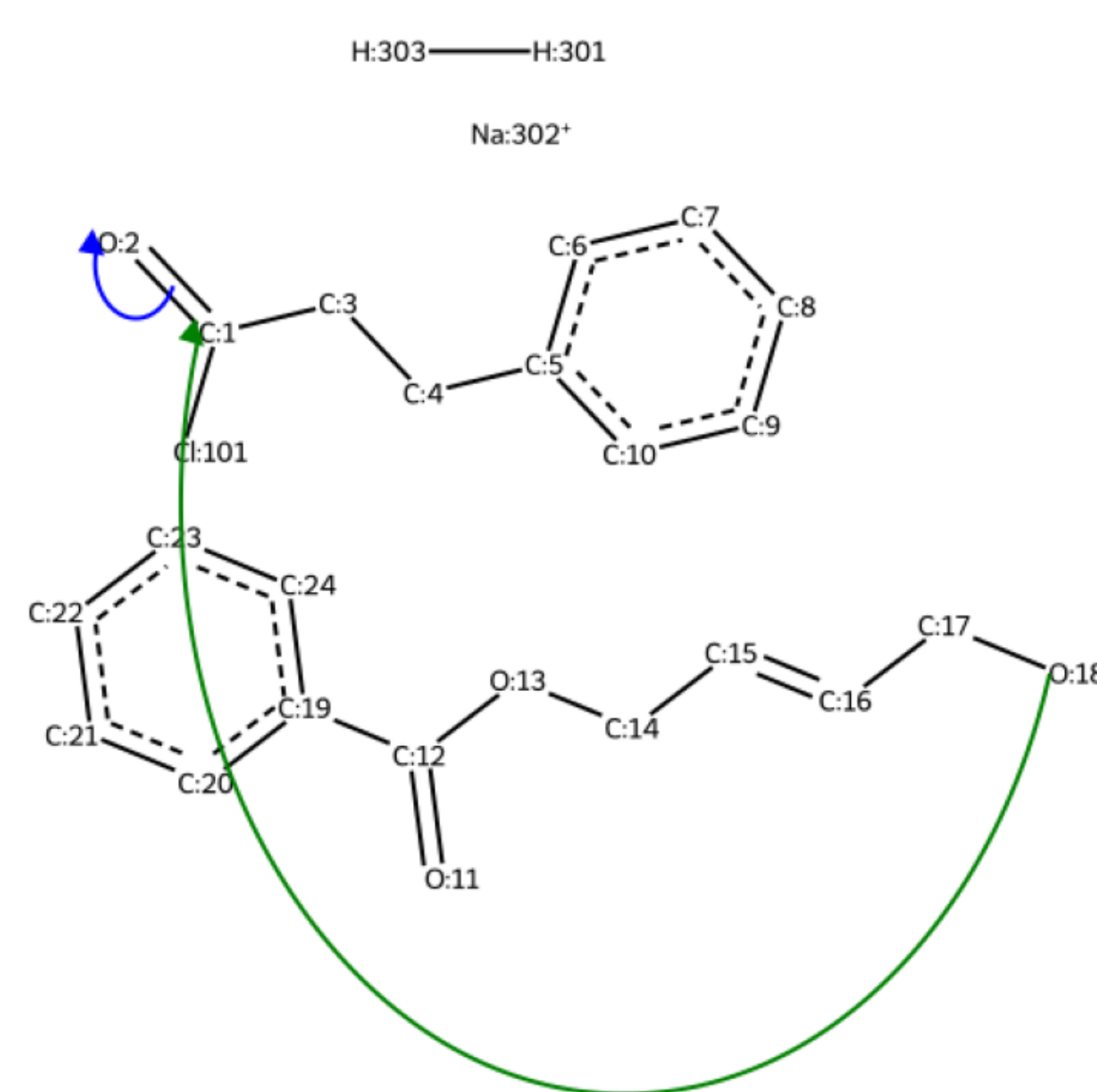
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

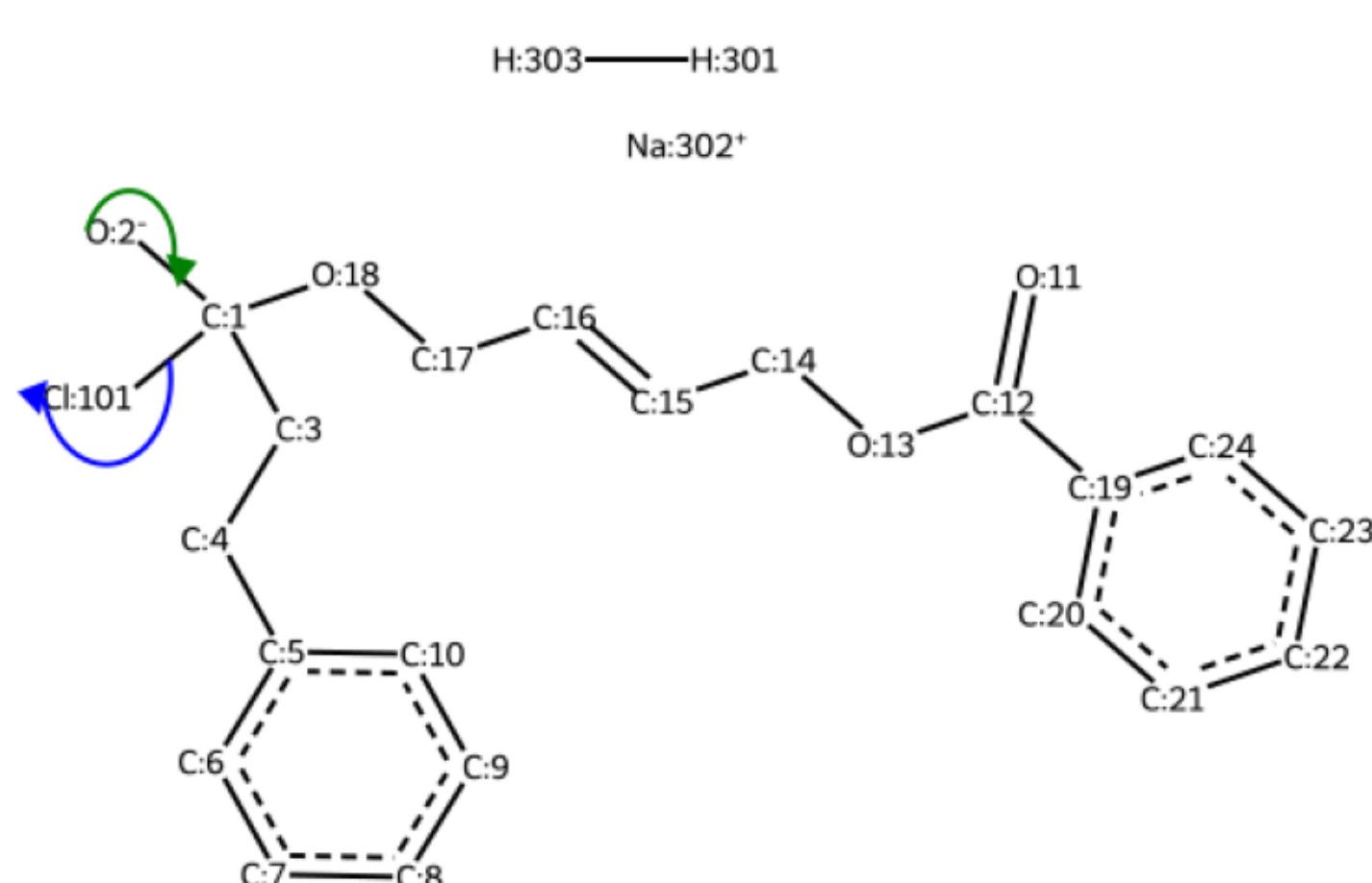
step #1



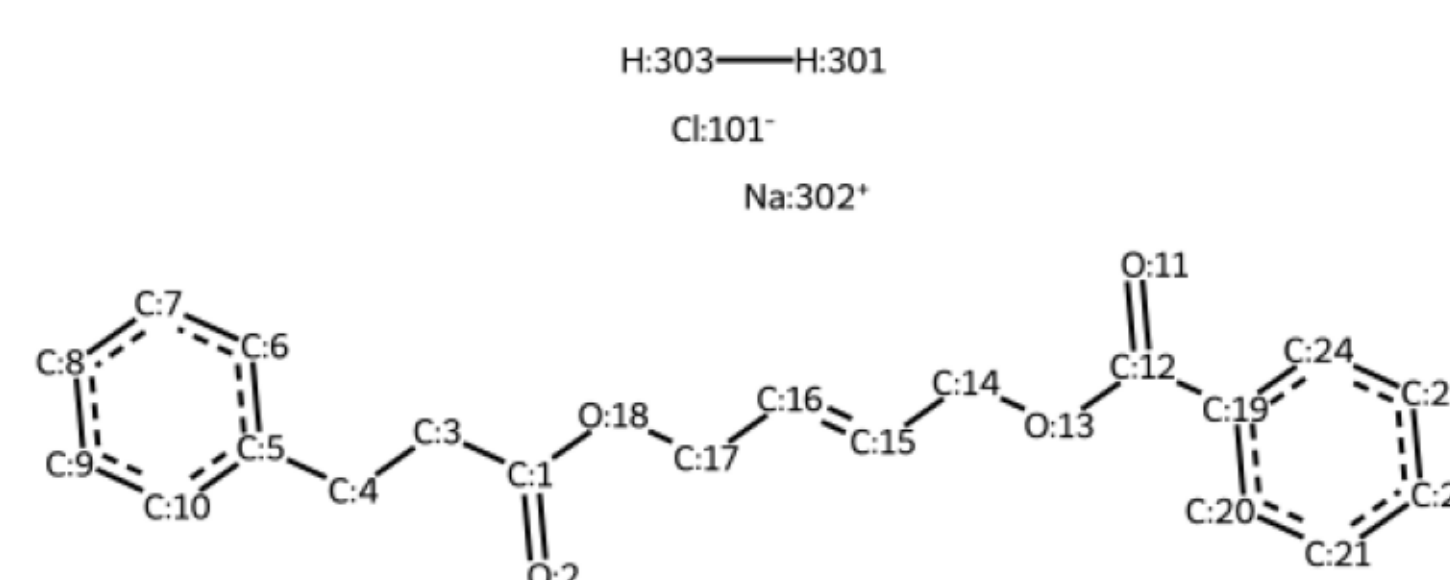
step #2



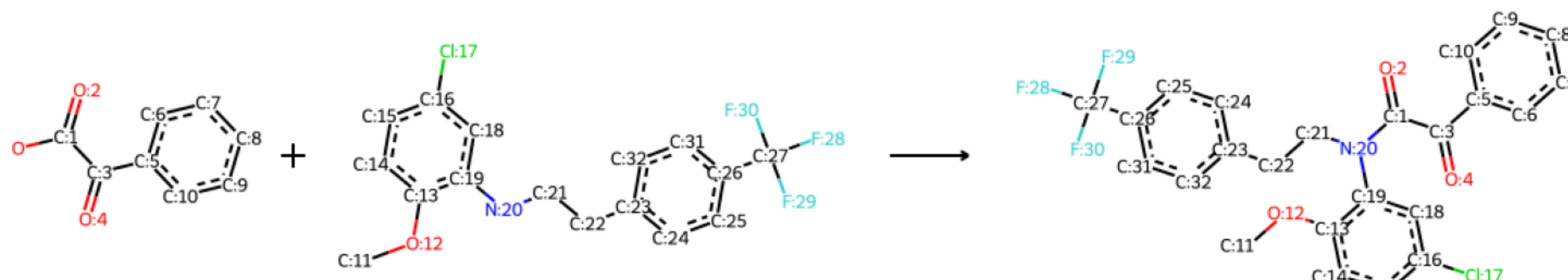
step #3



Product(s)

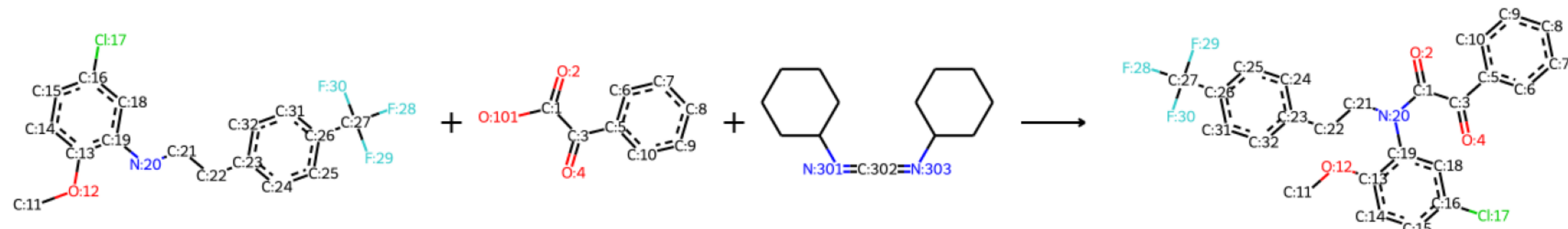


Original reaction
sampled RXN_ID:22)



Identified mechanistic class -
DCC_condensation reaction

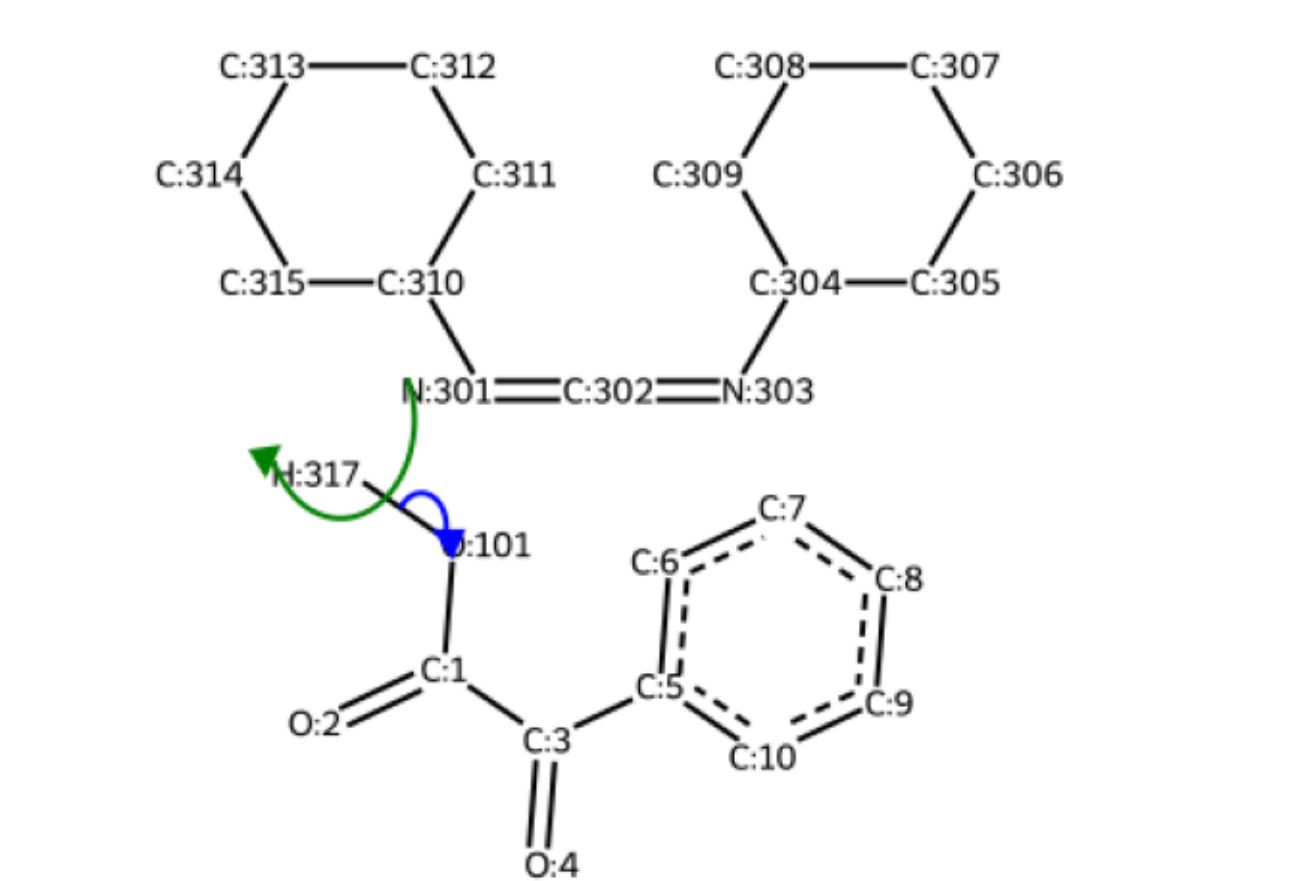
Reaction with missing reagents recovered



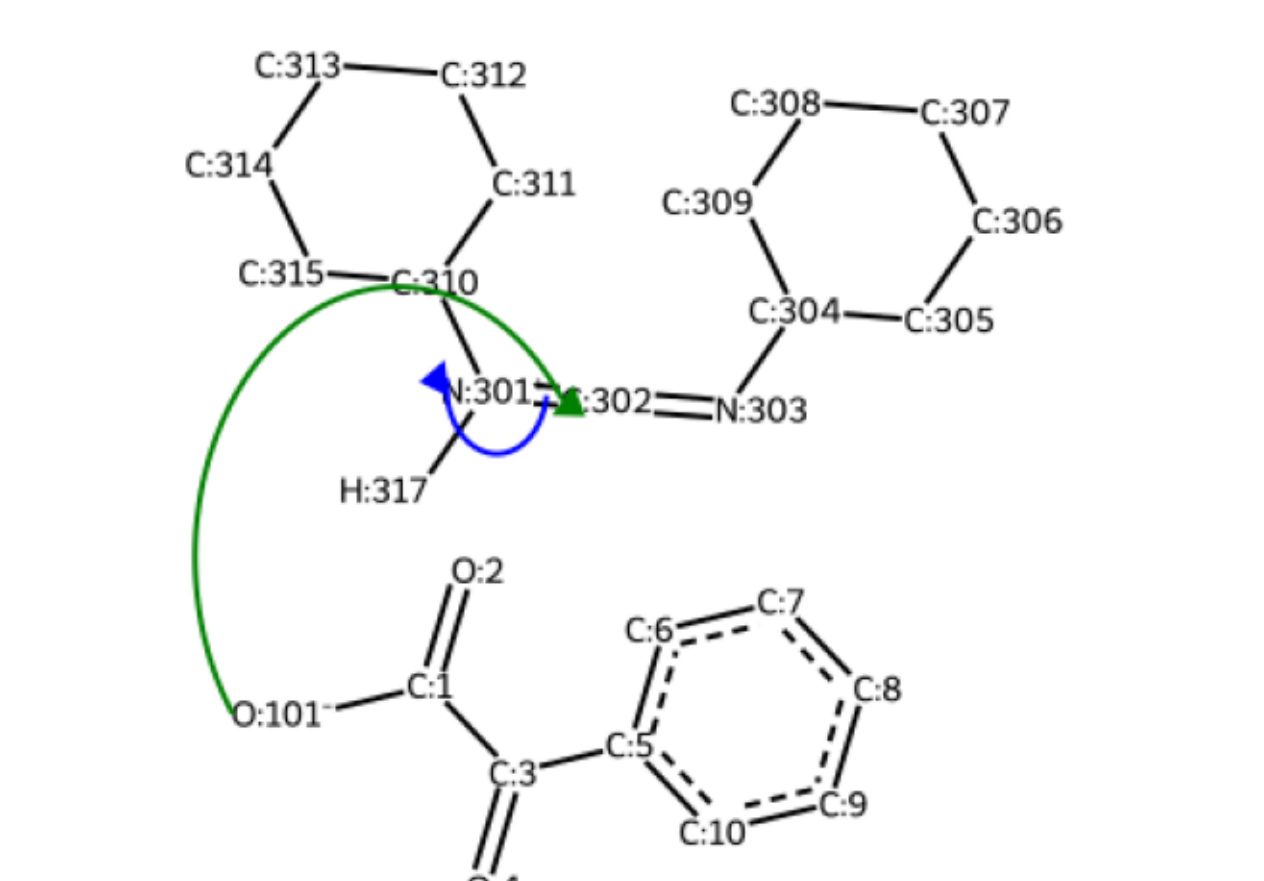
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

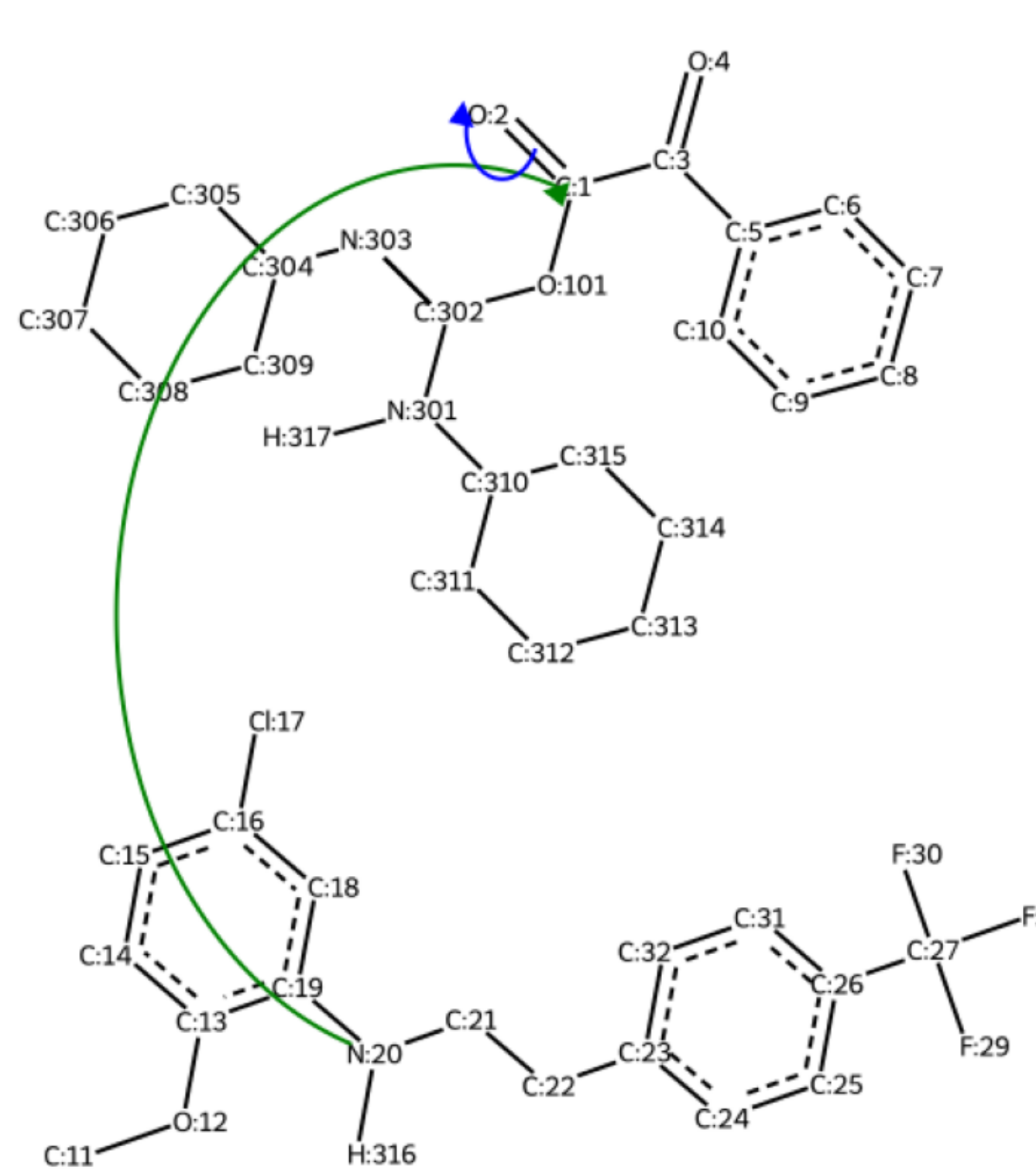
step #1



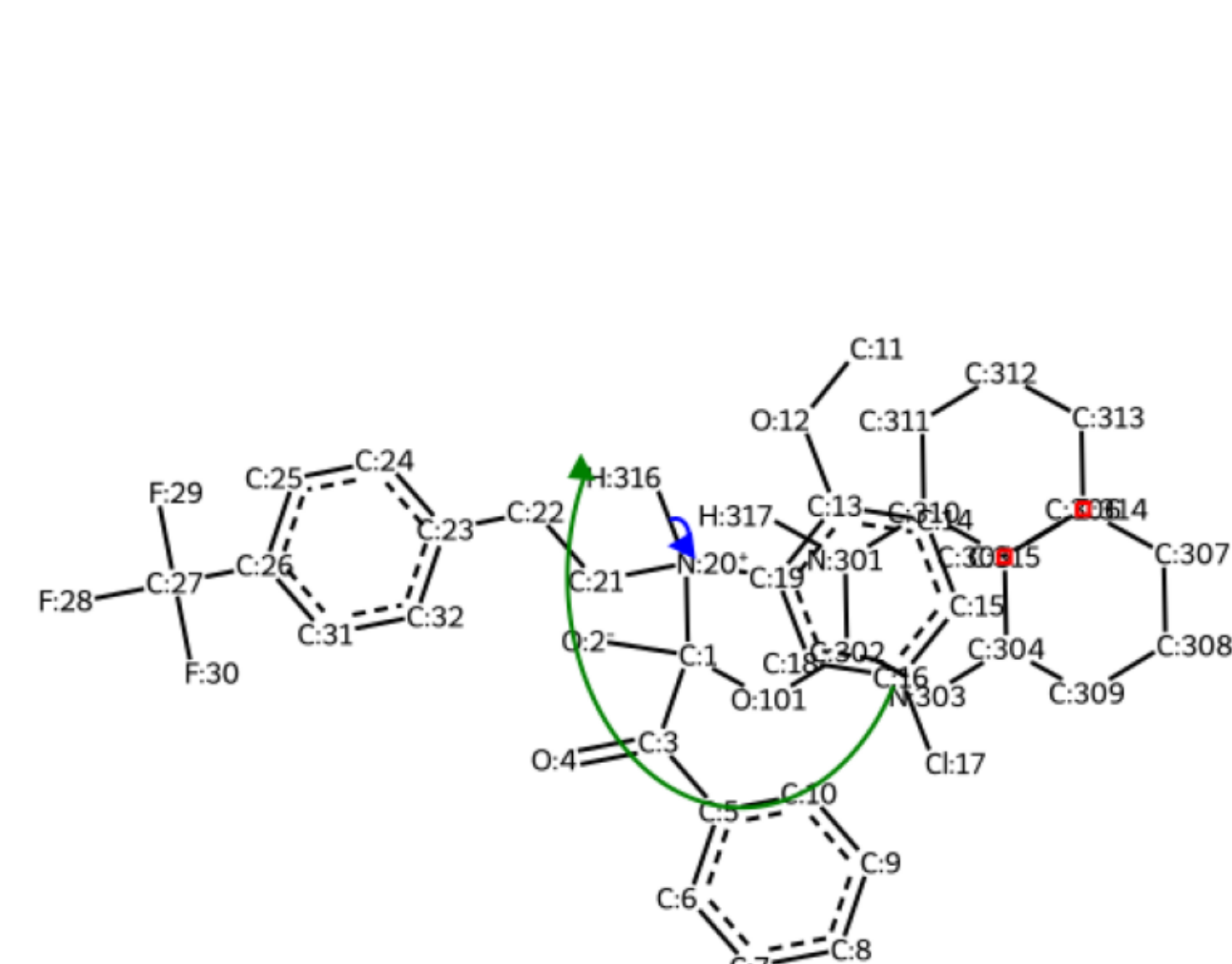
step #2



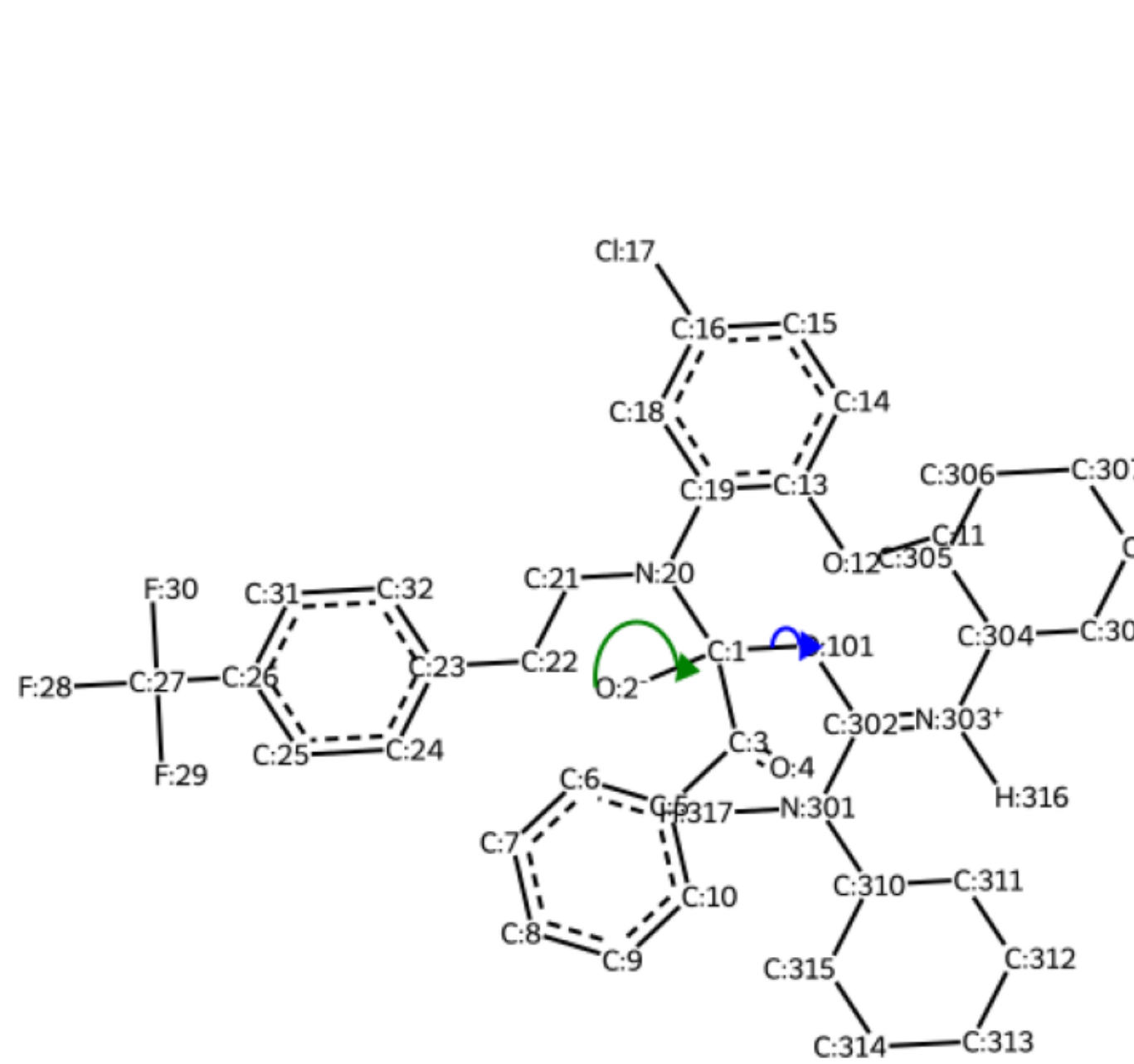
step #3



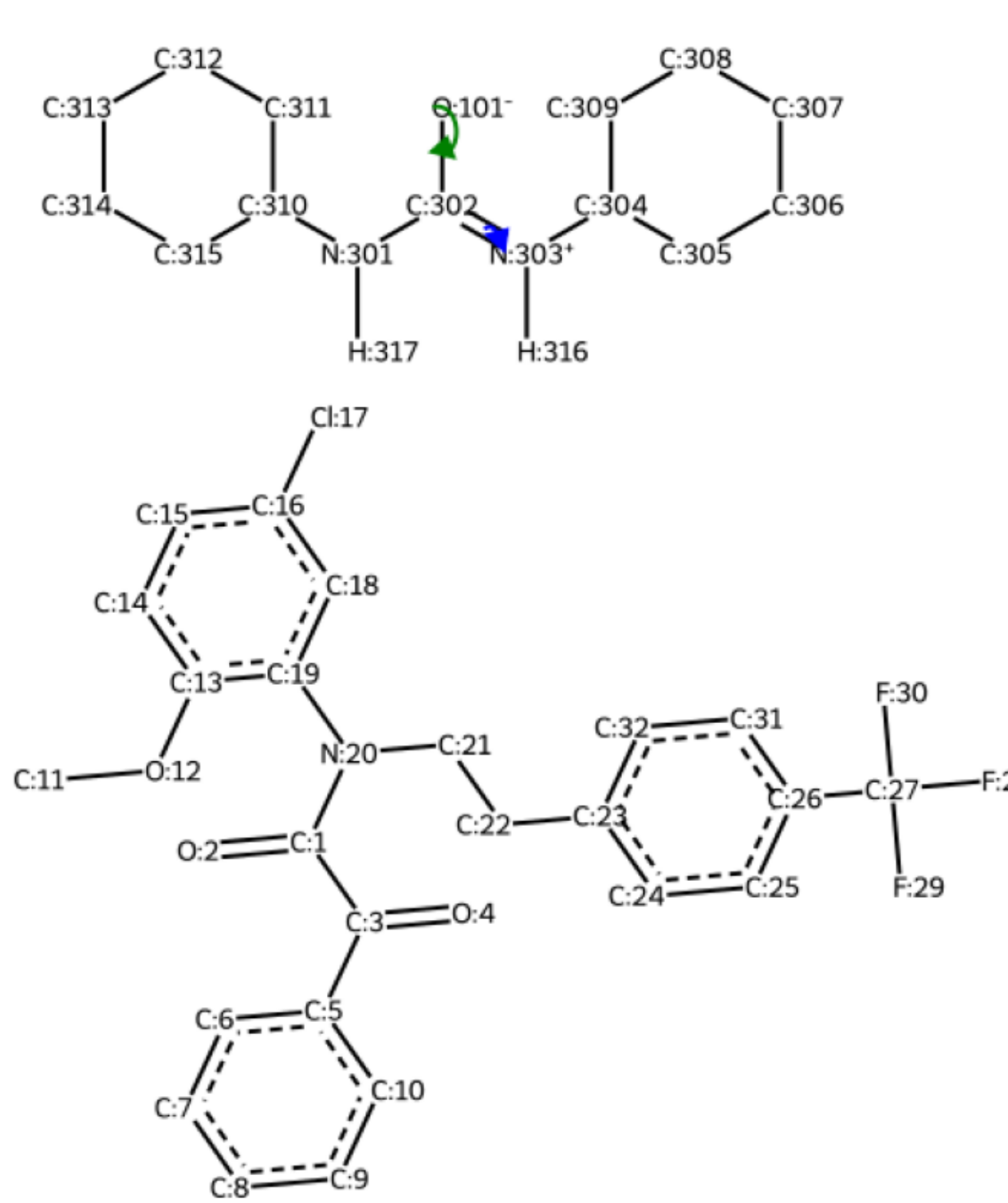
step #4



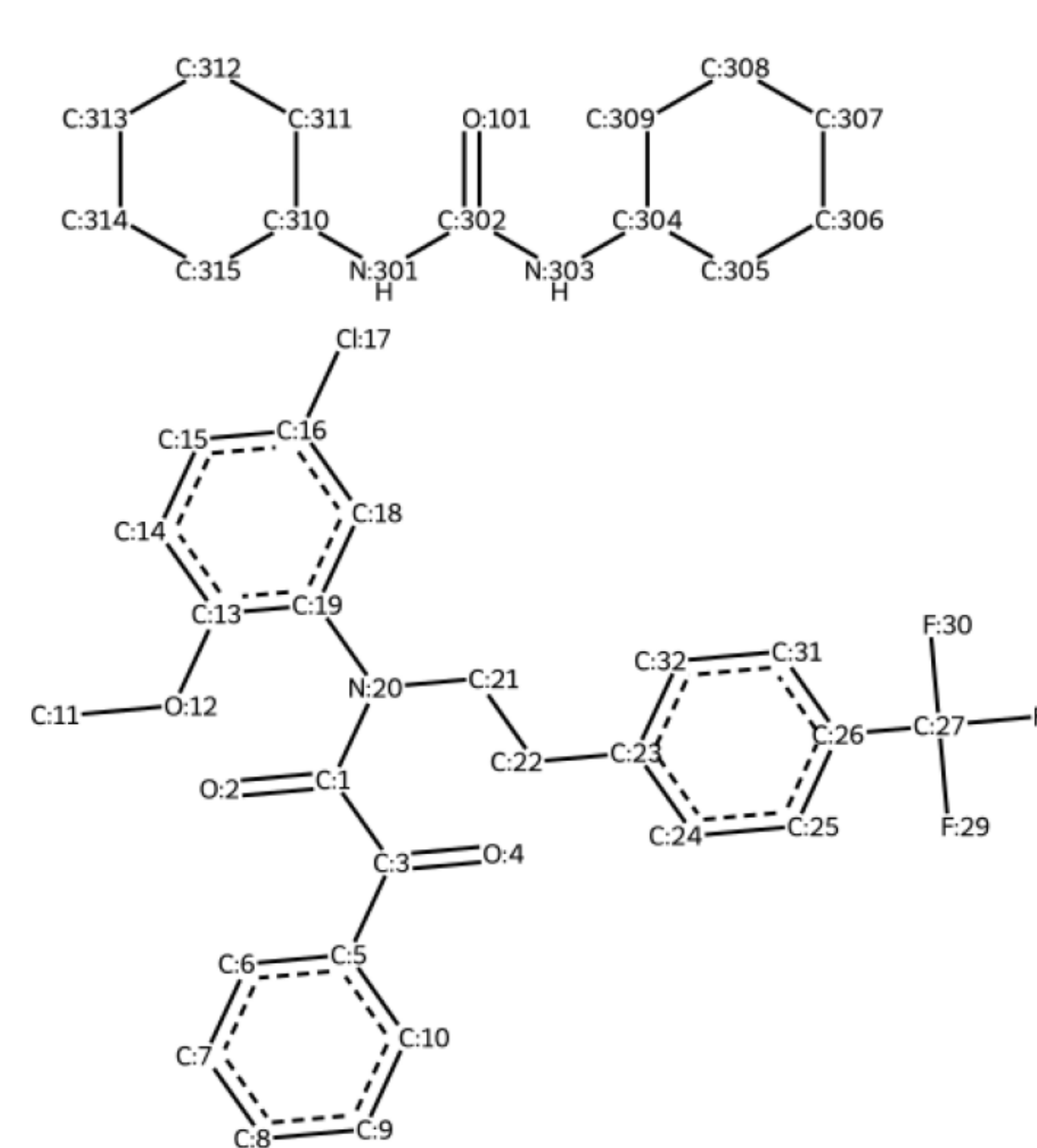
step #5



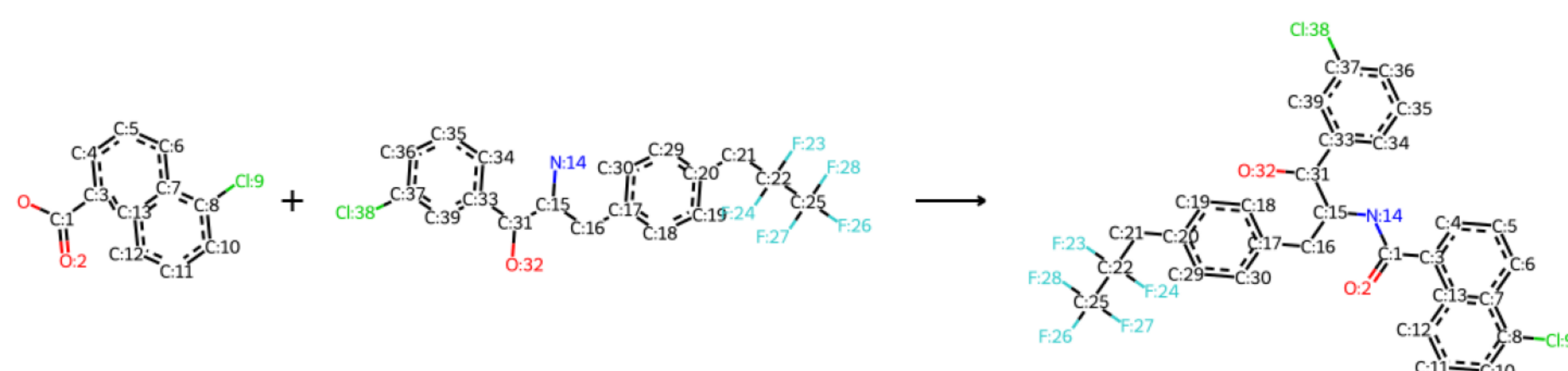
step #6



Product(s)

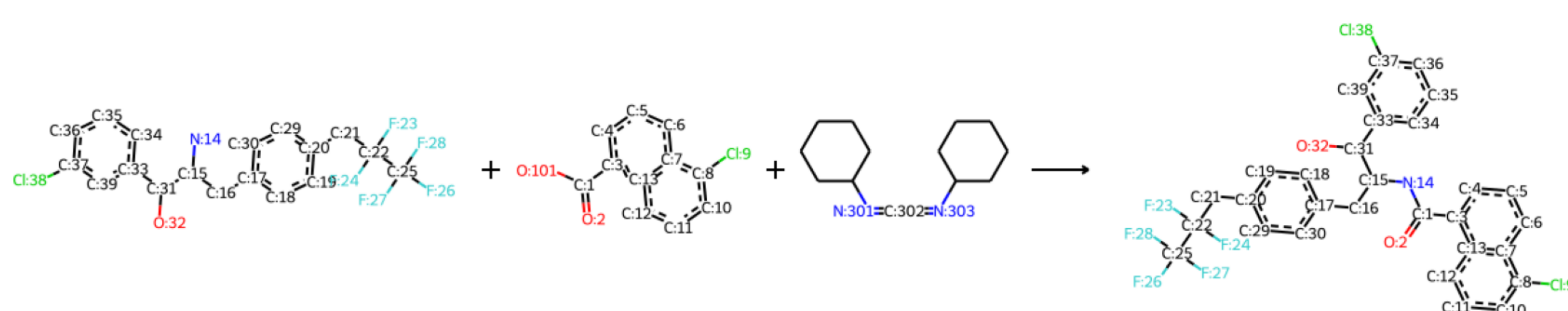


Original reaction
sampled RXN_ID:23)



Identified mechanistic class -
DCC_condensation reaction

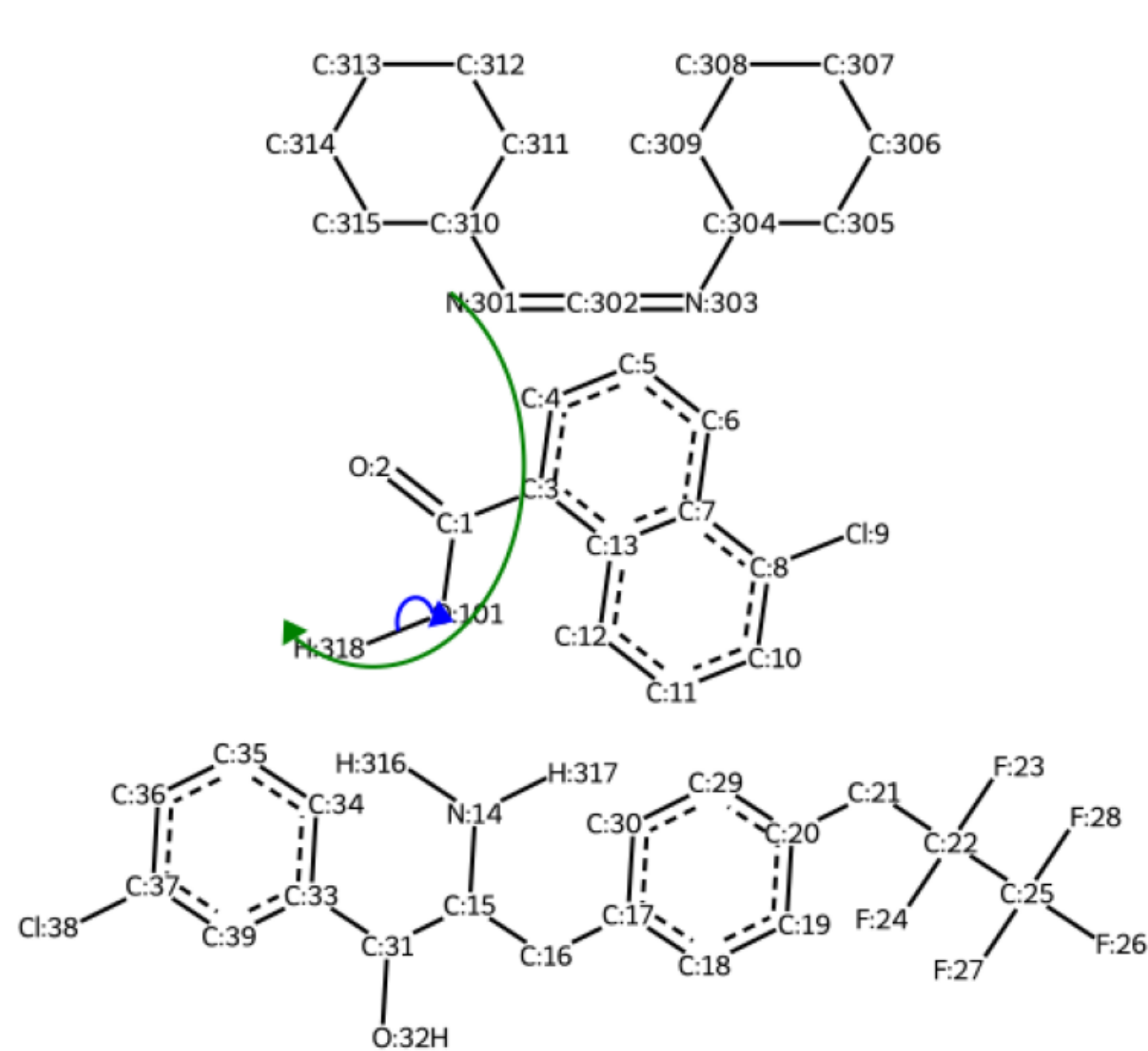
Reaction with missing reagents recovered



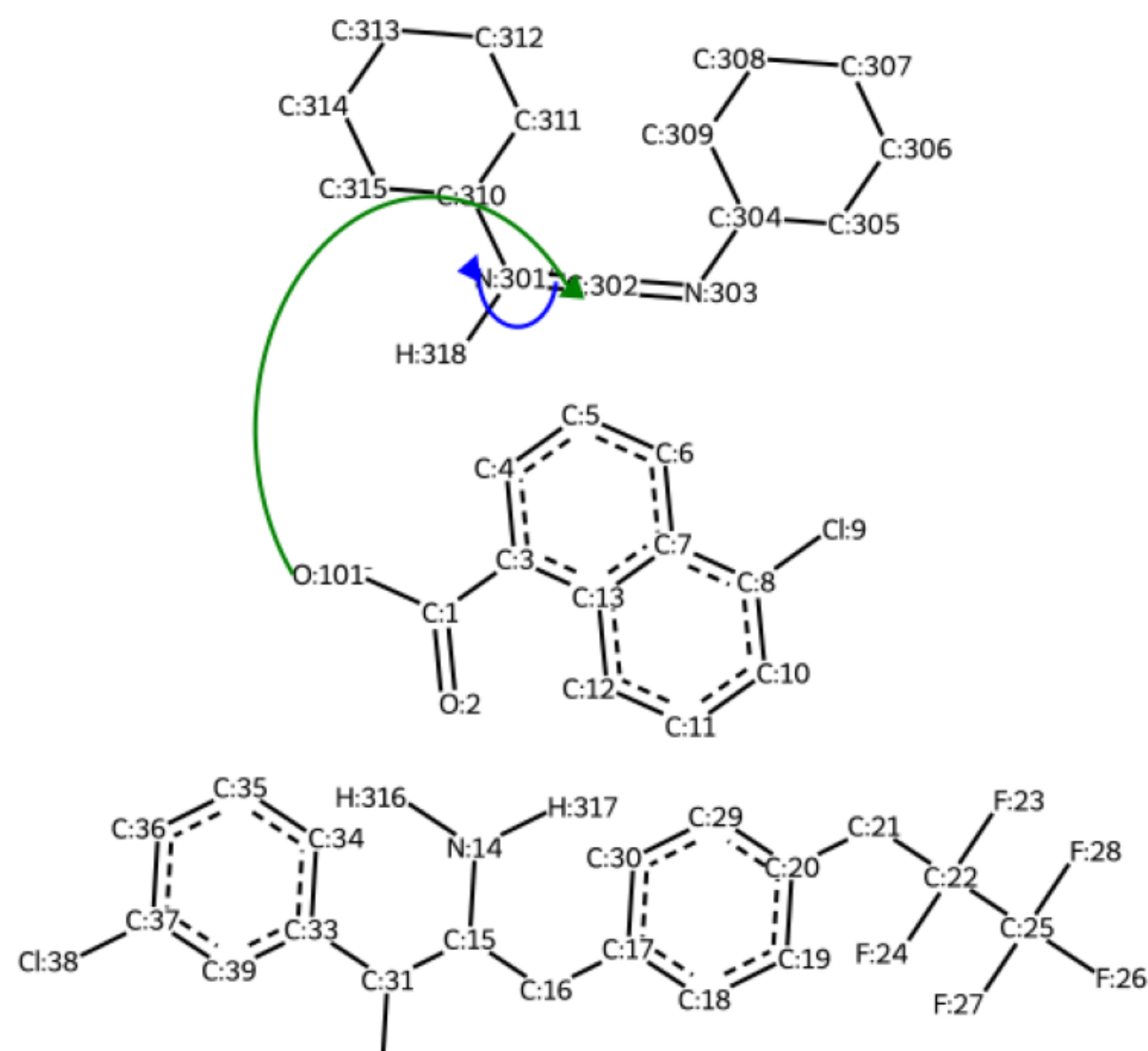
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

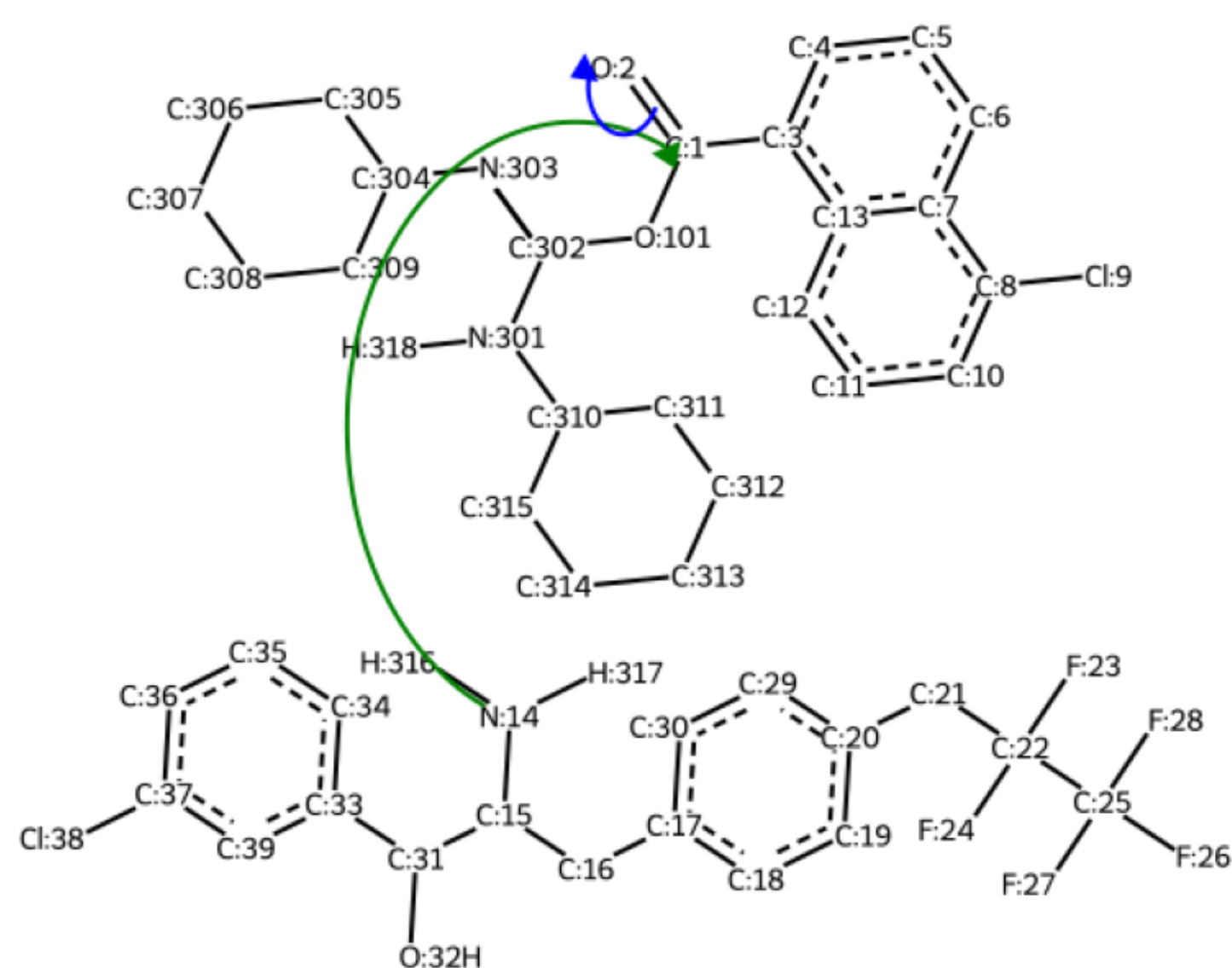
step #1



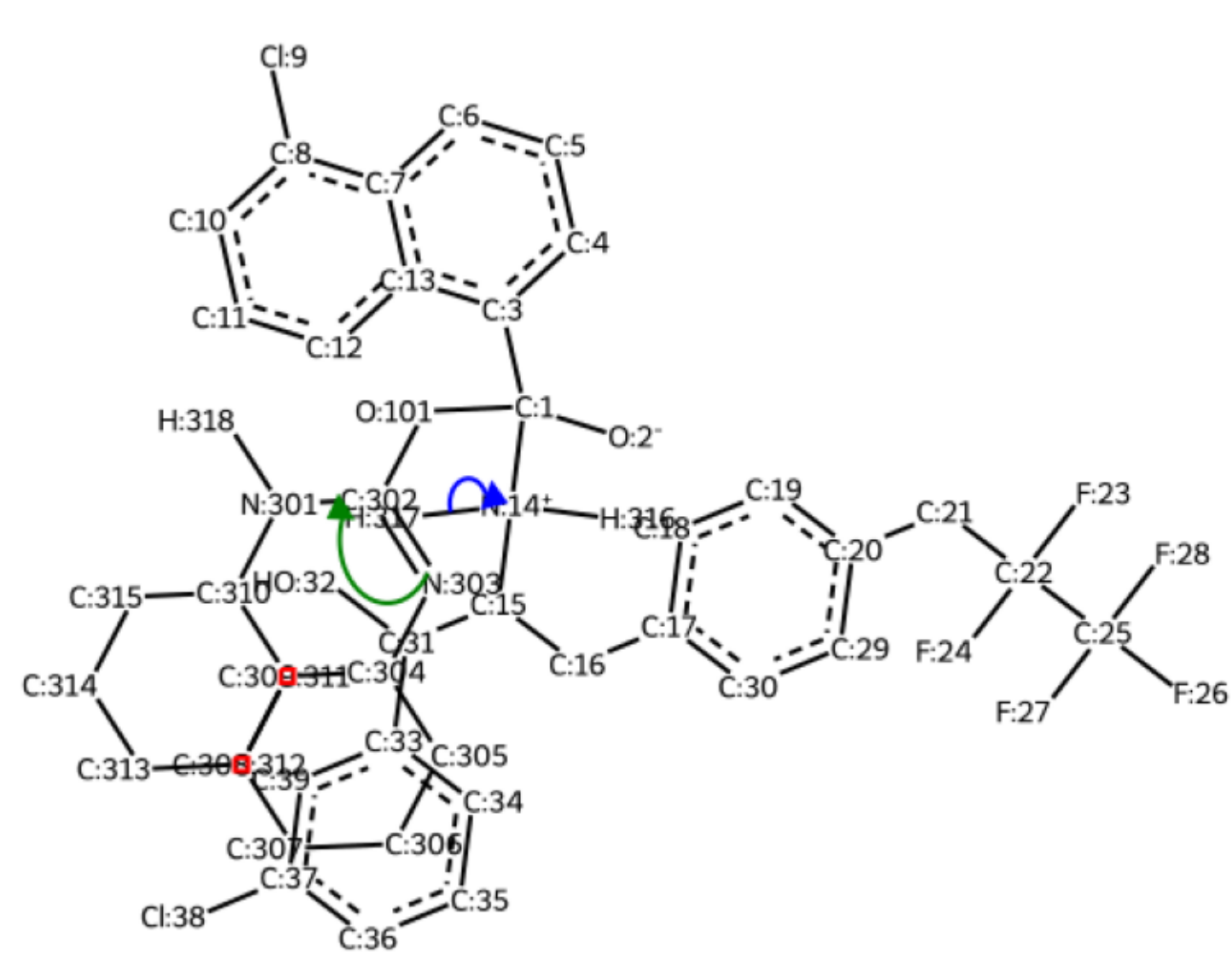
step #2



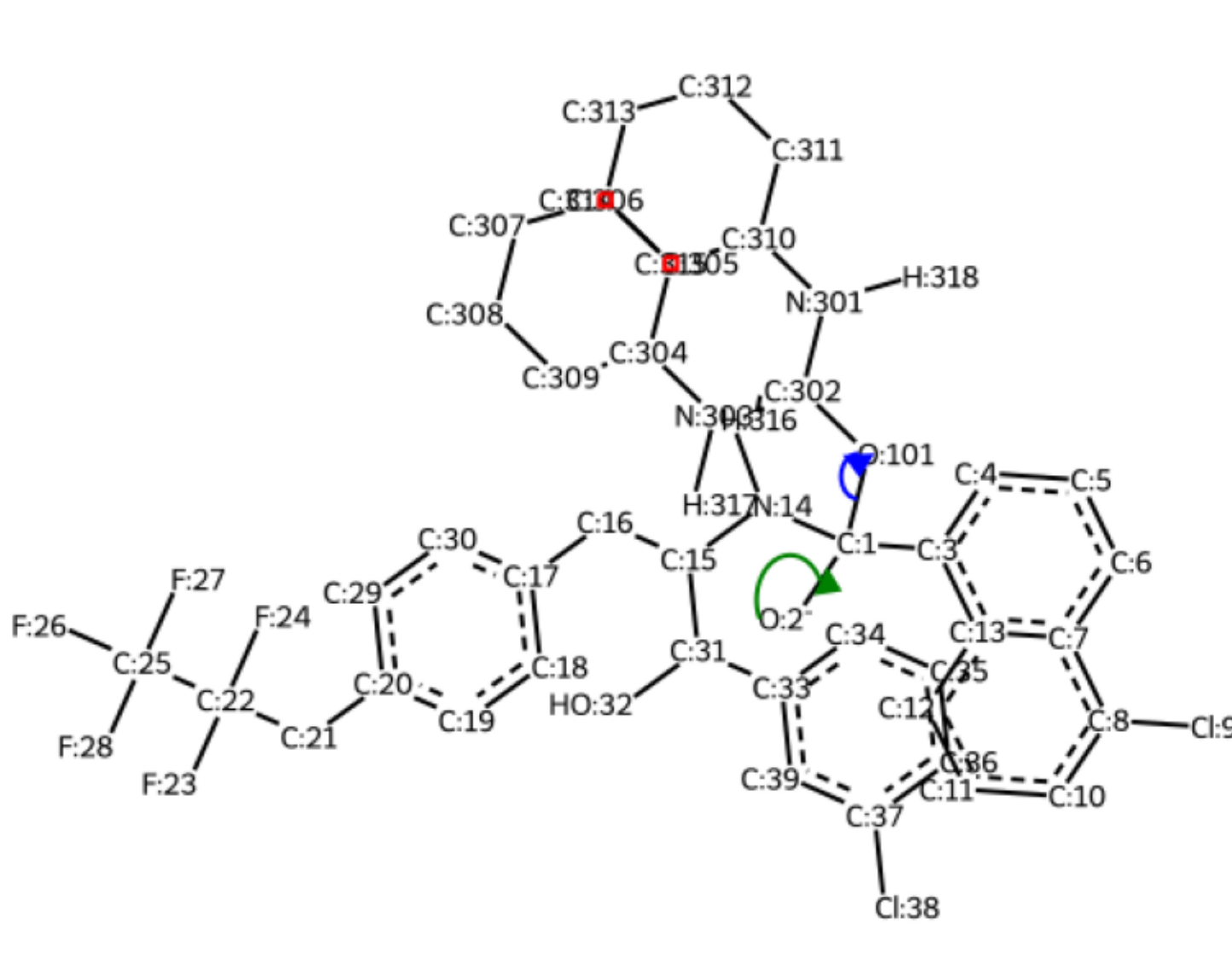
step #3



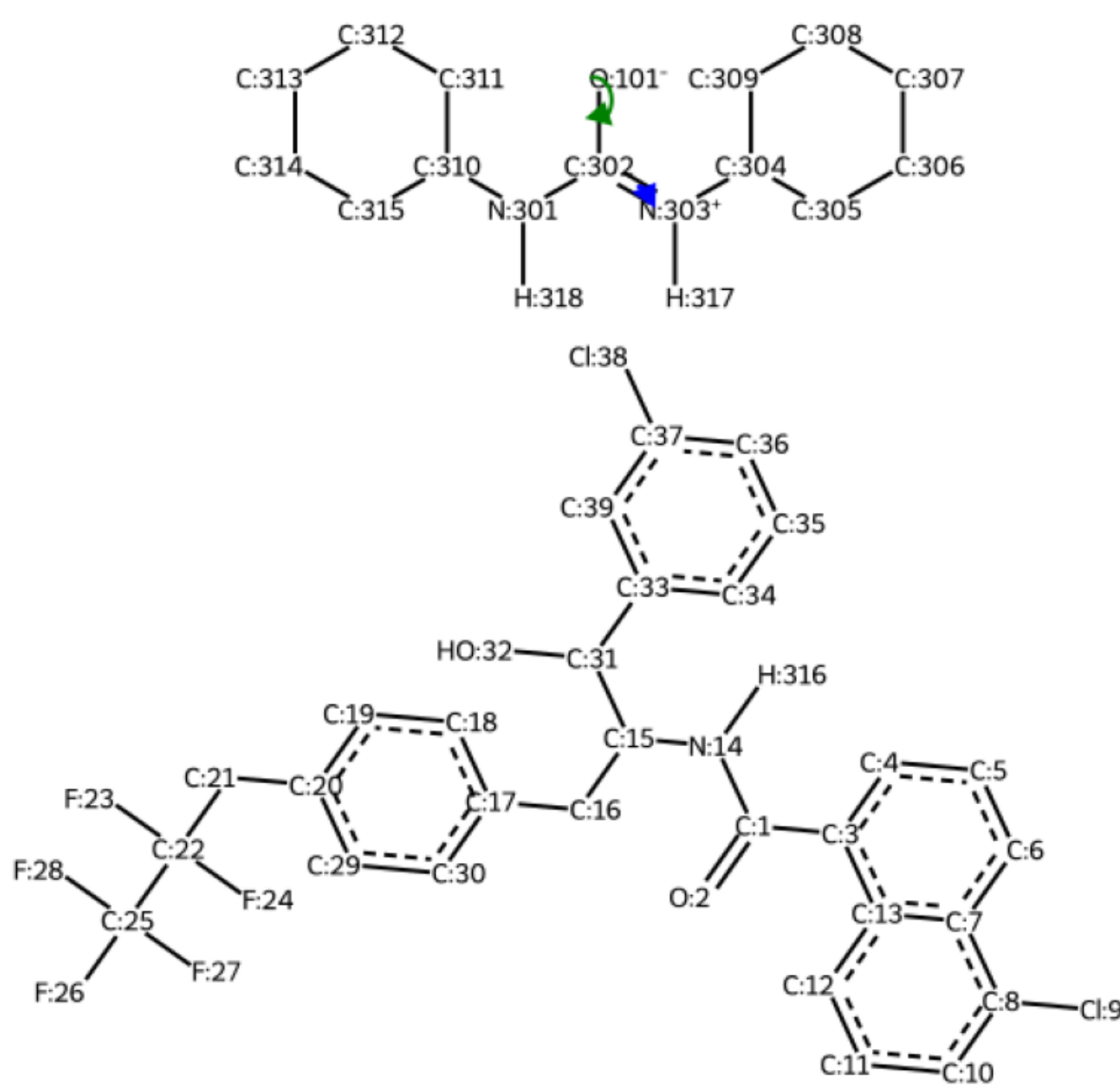
step #4



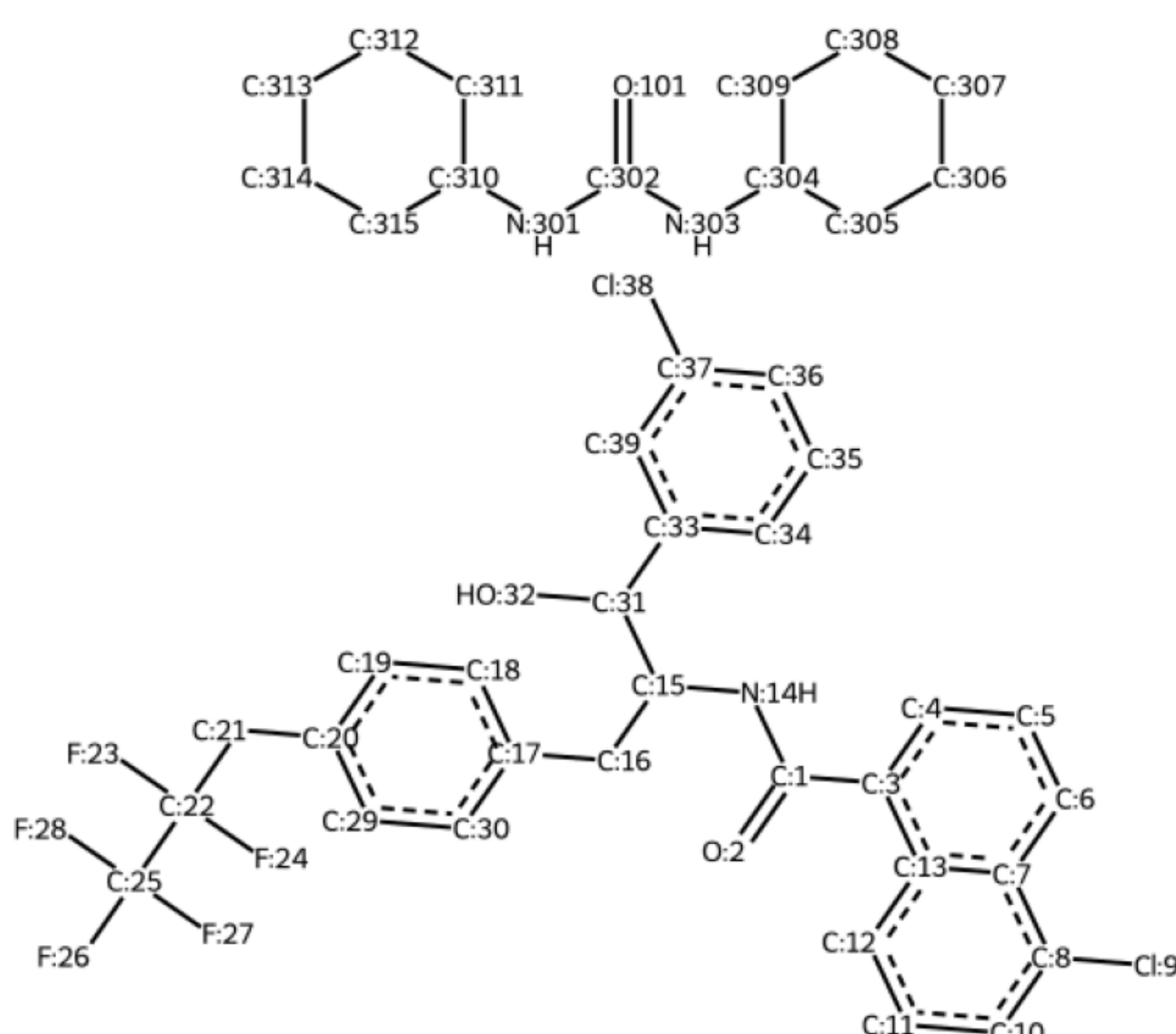
step #5



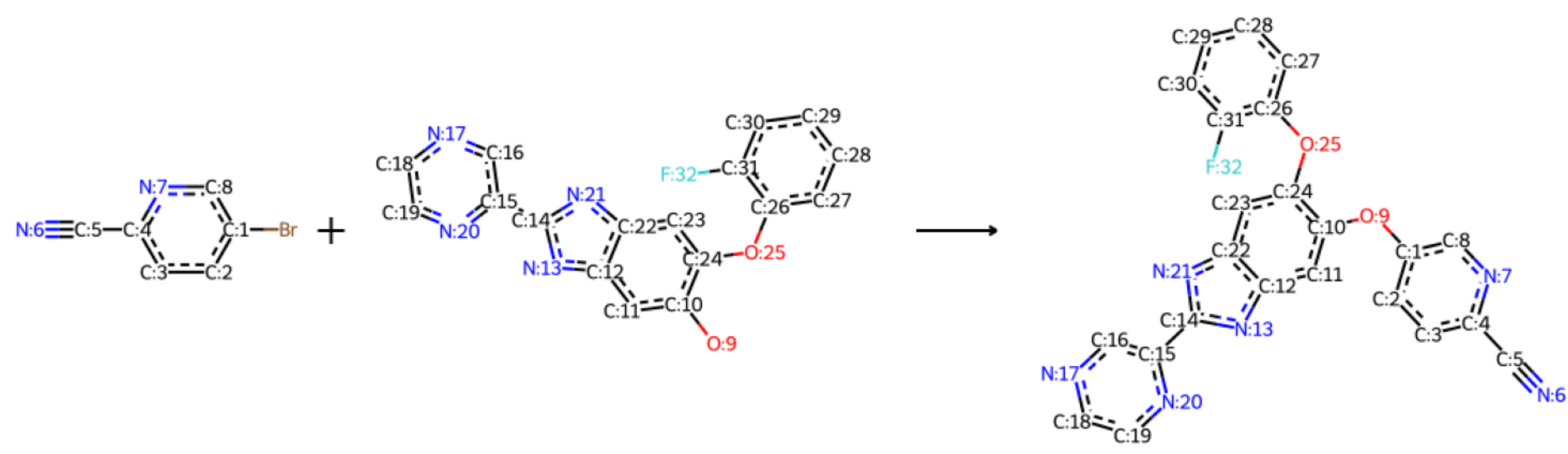
step #6



Product(s)

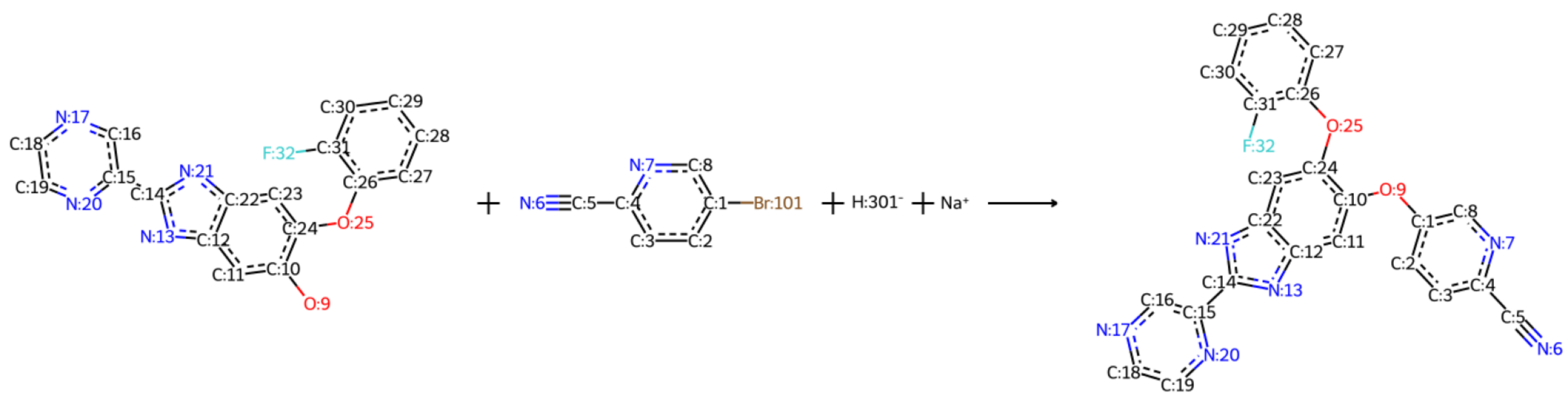


Original reaction
sampled RXN_ID:24)



Identified mechanistic class -
S_NAr_{alco(thi)ol(para)} reaction

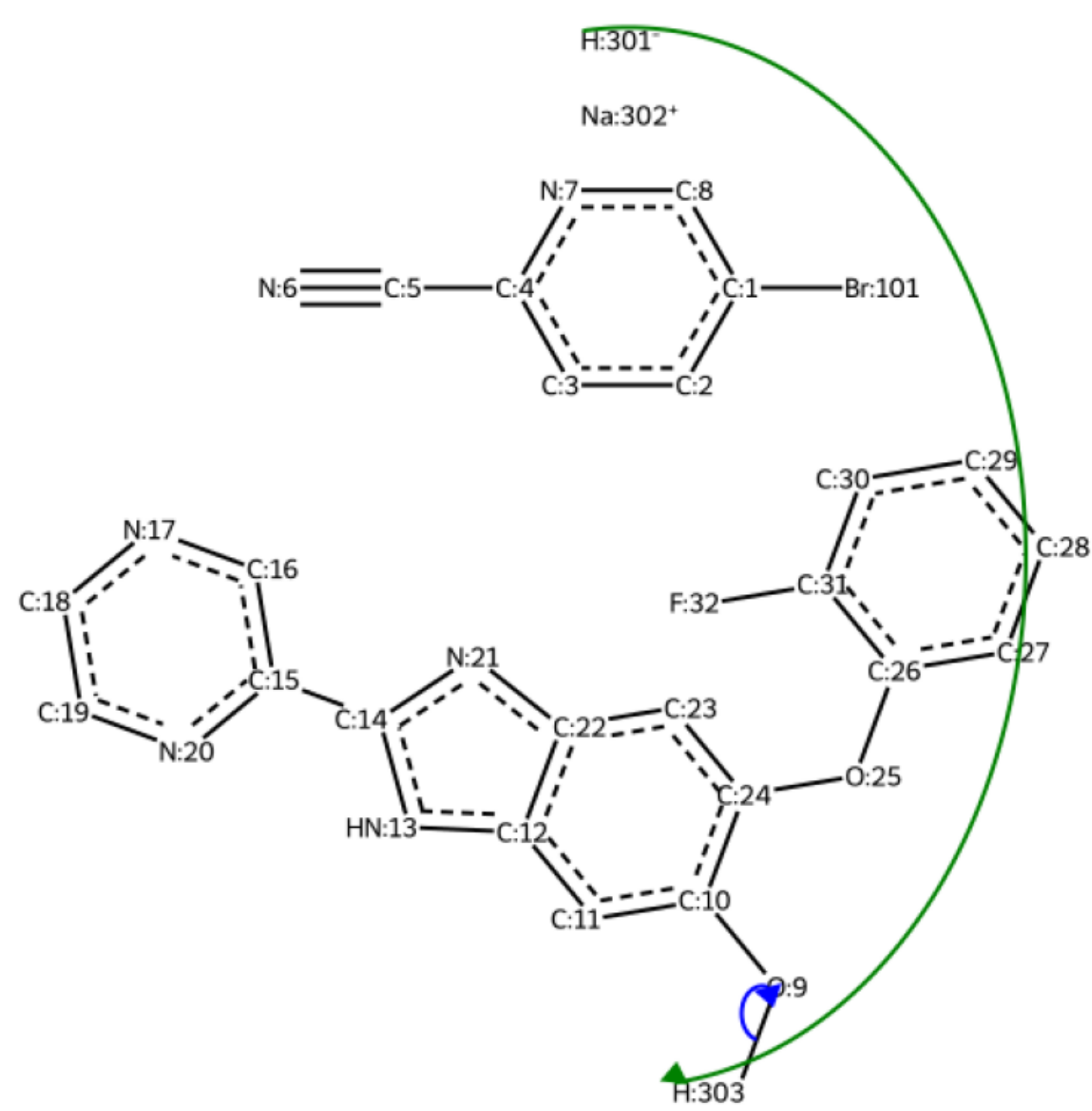
Reaction with missing reagents recovered



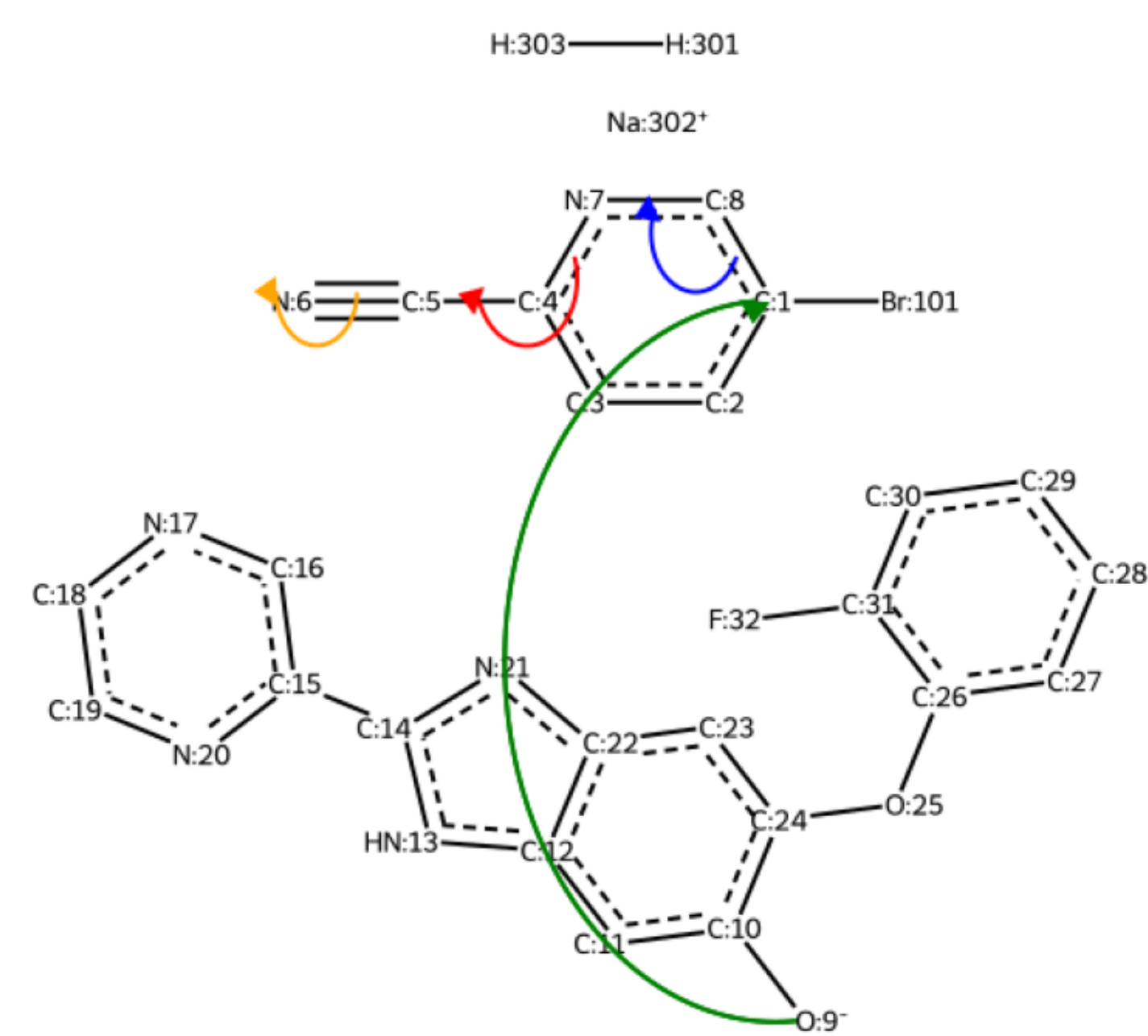
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

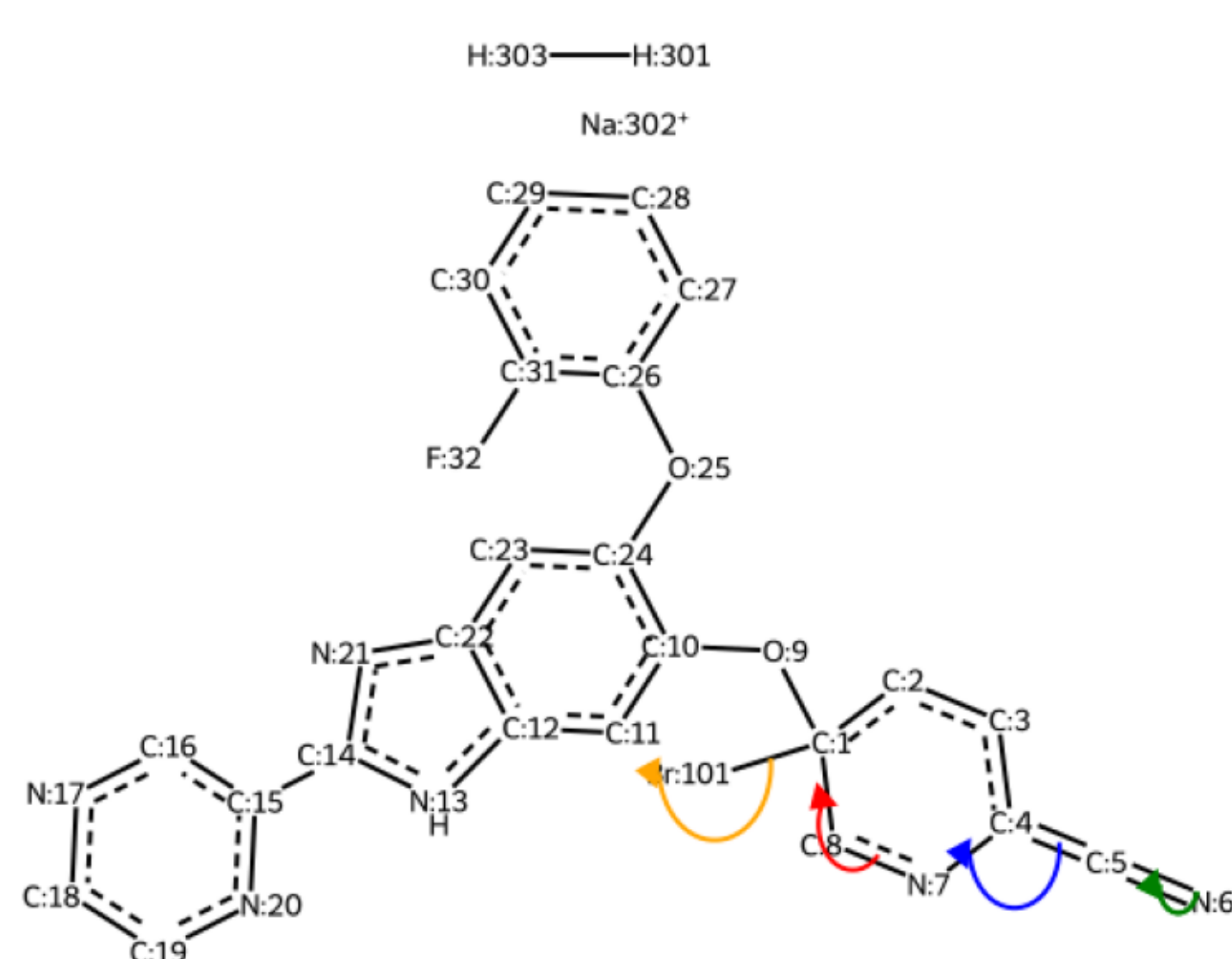
step #1



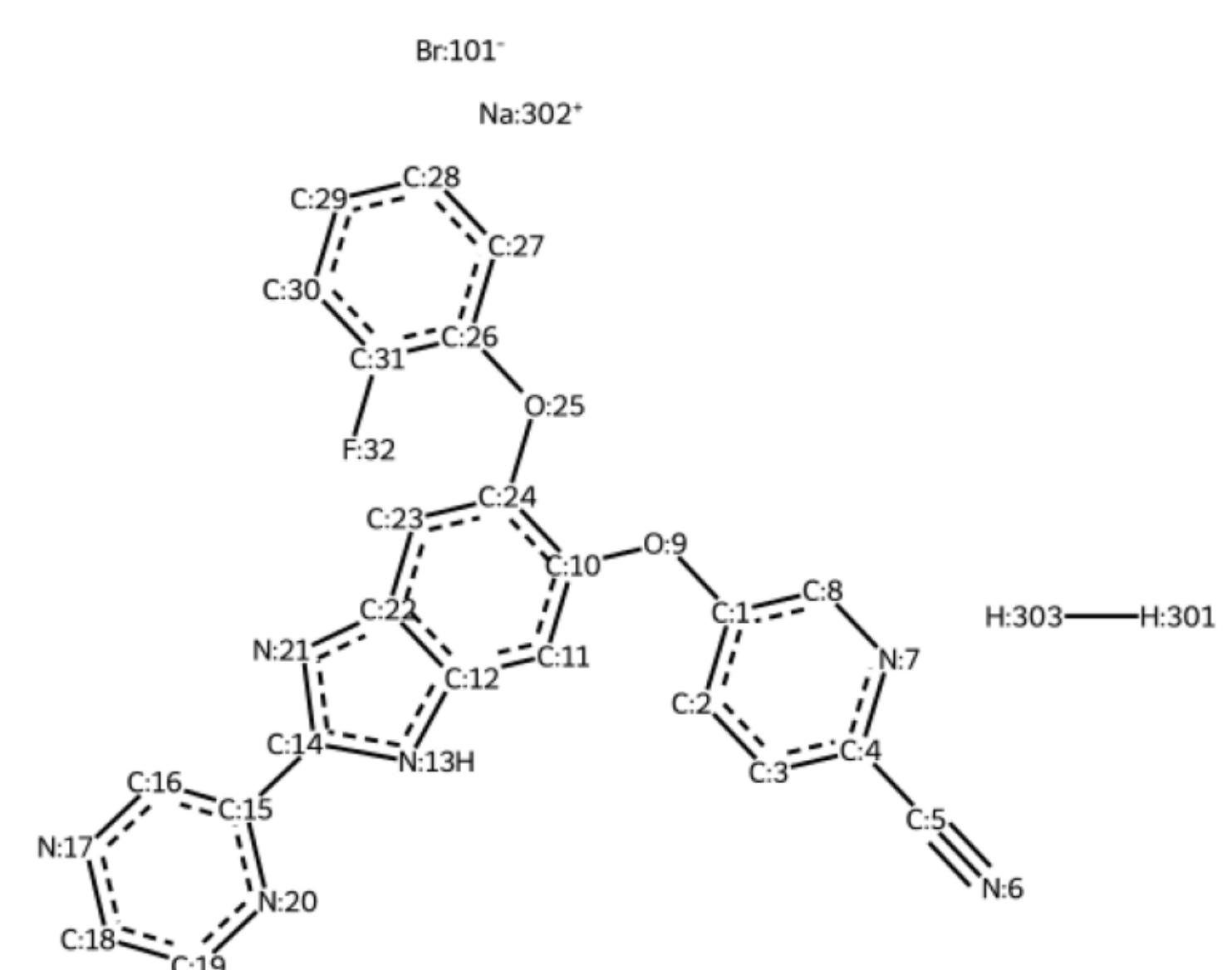
step #2



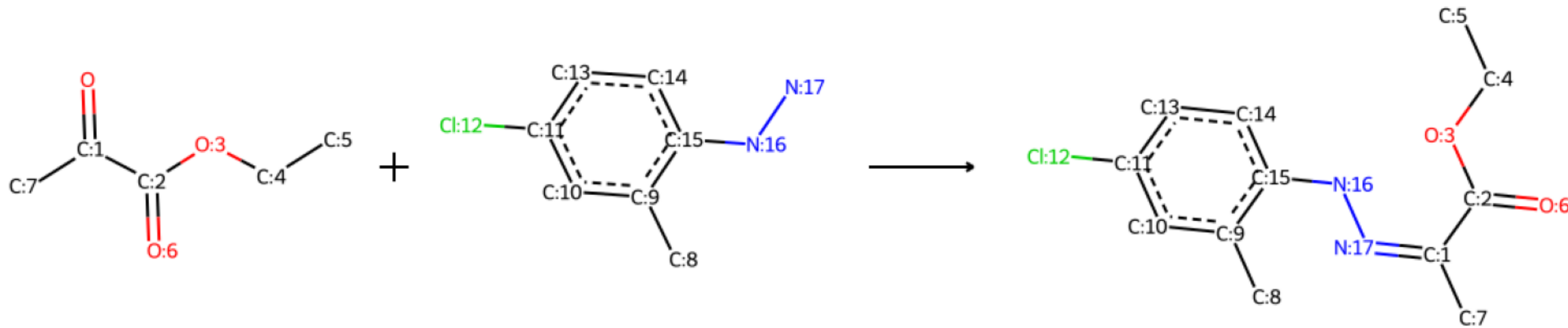
step #3



Product(s)

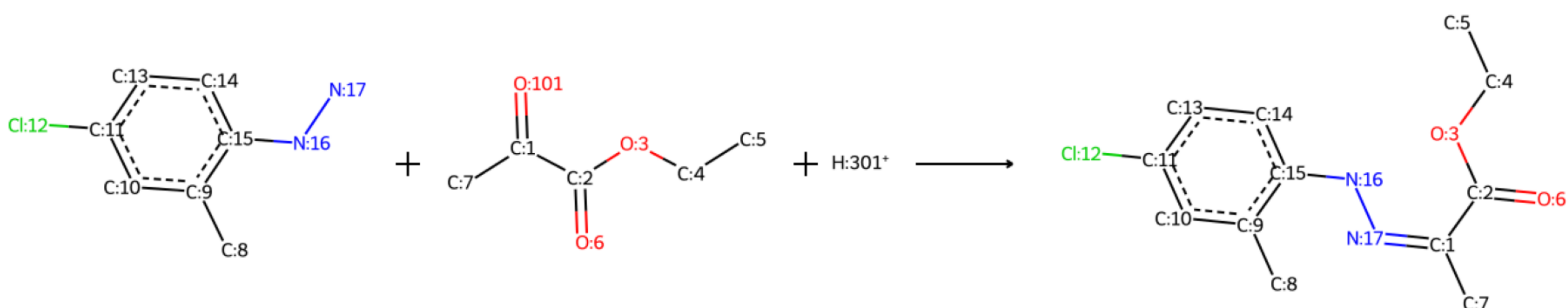


Original reaction
sampled RXN_ID:25)



Identified mechanistic class -
imine_formation reaction

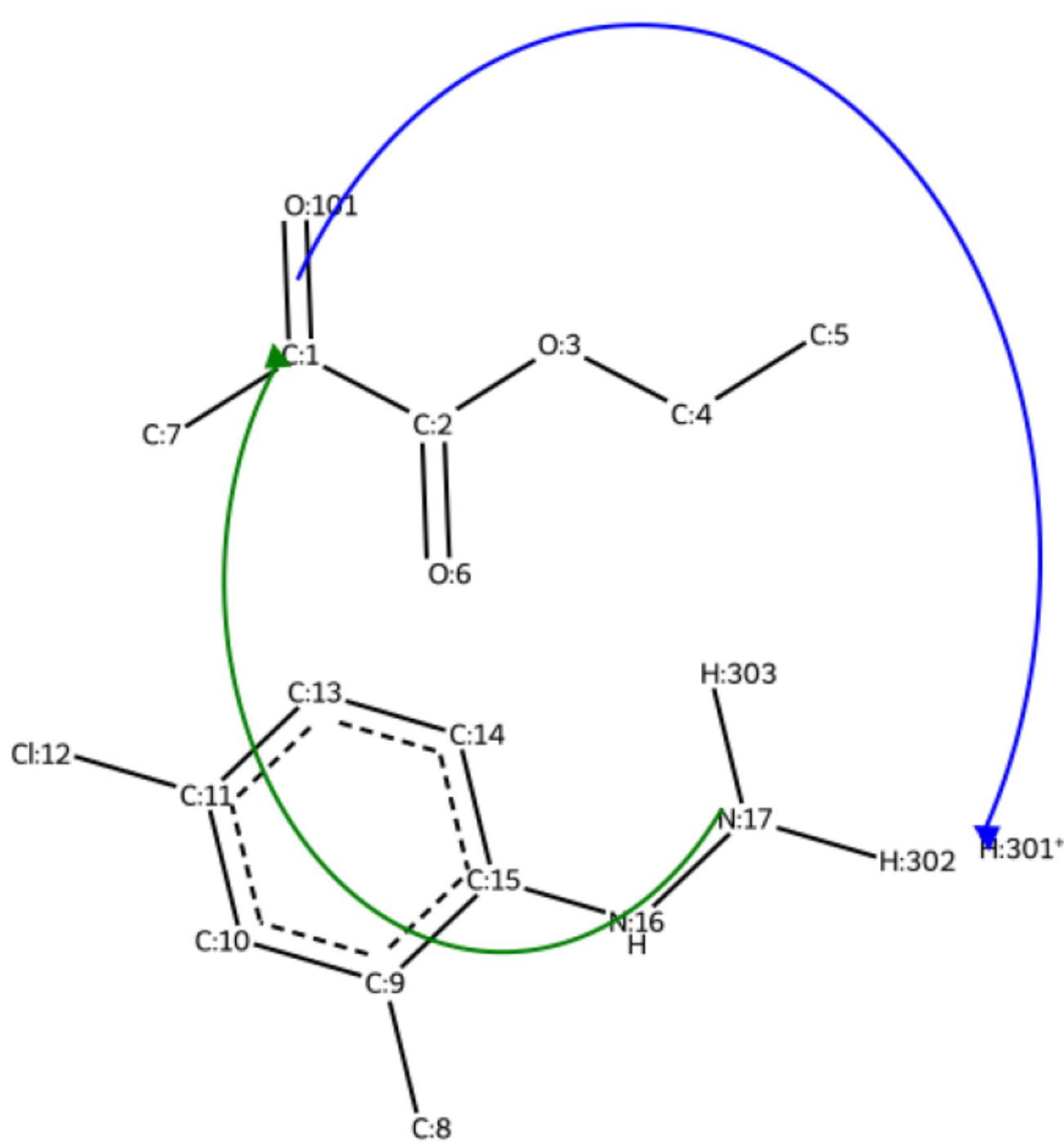
Reaction with missing reagents recovered



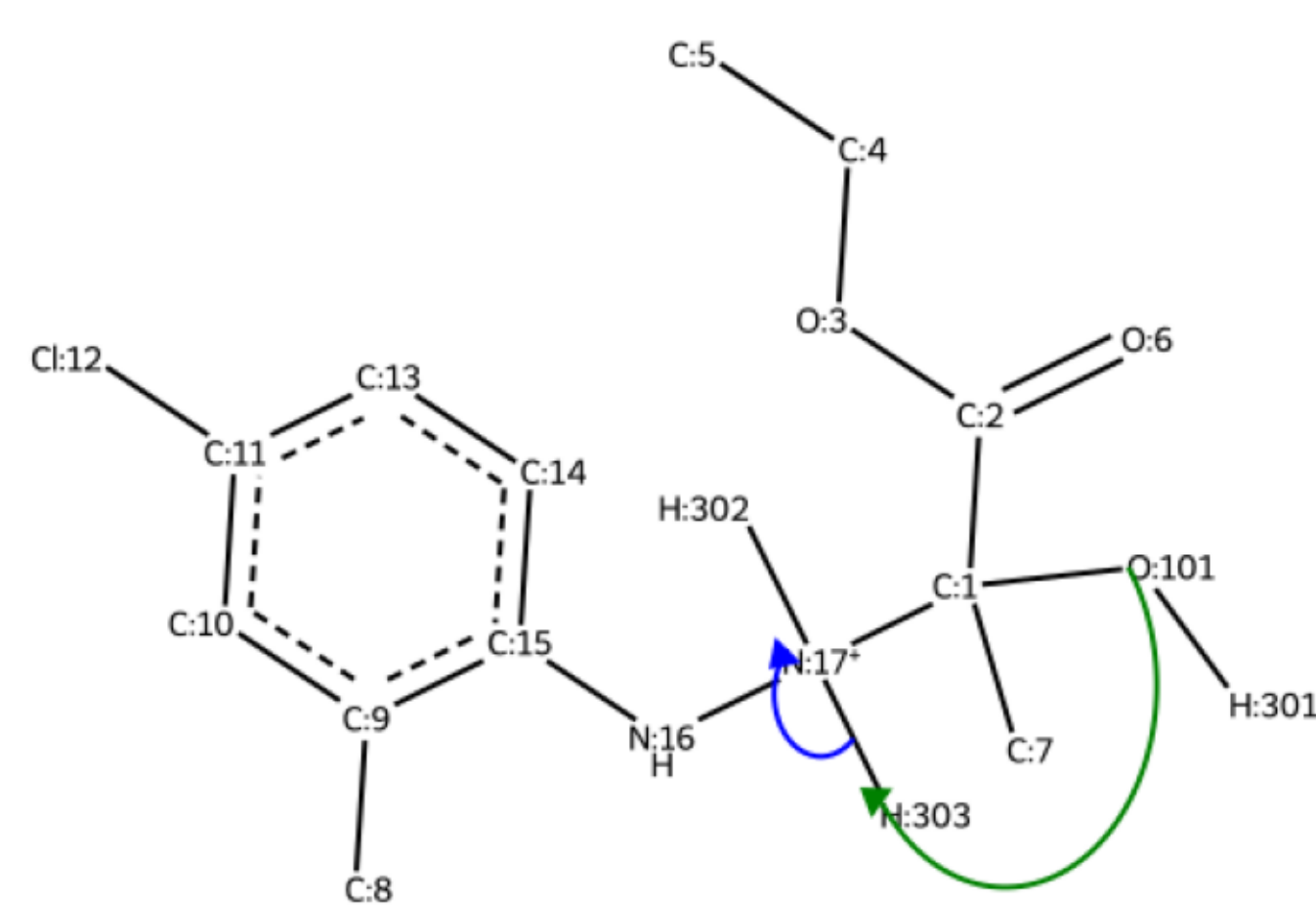
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

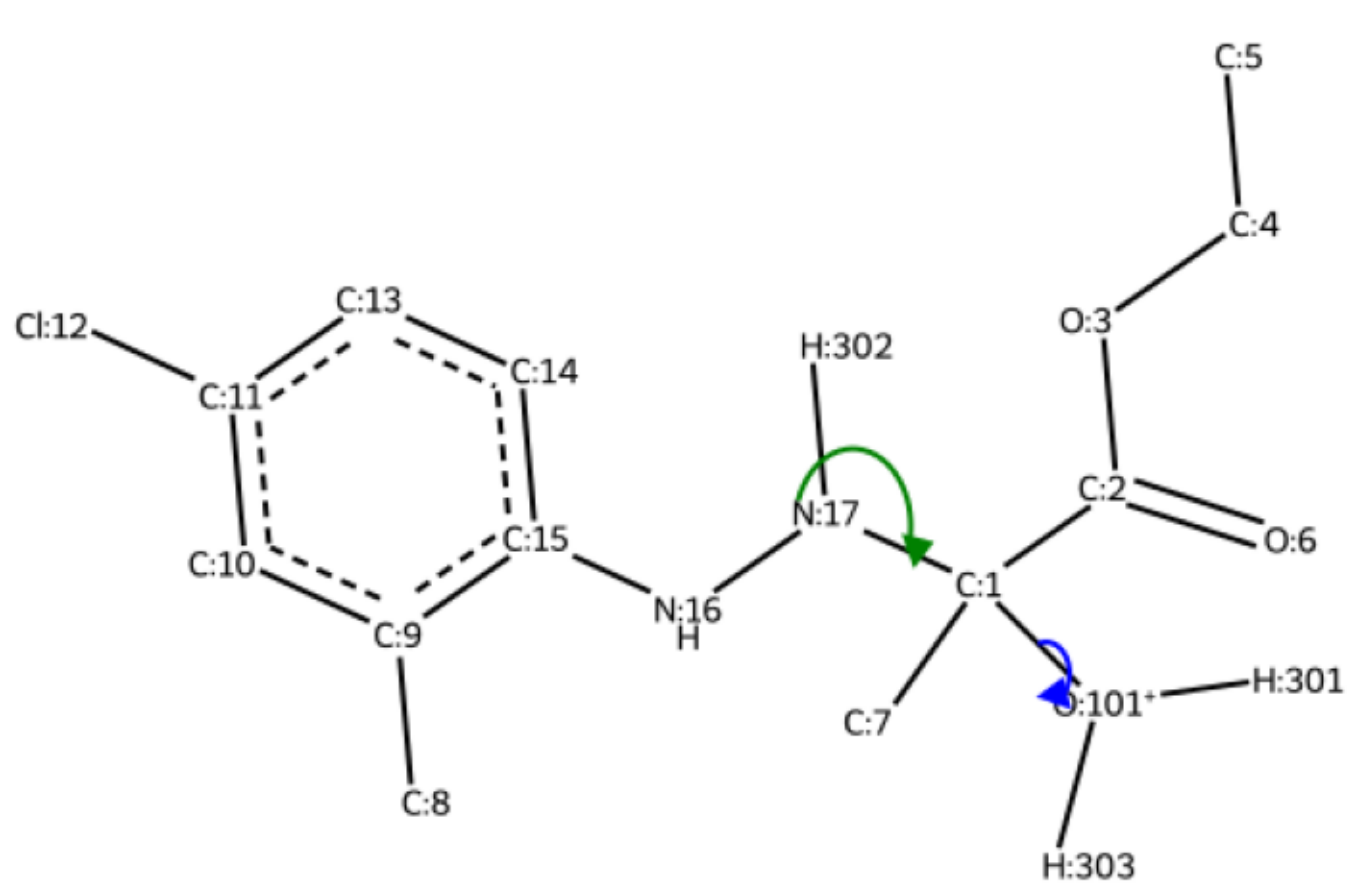
step #1



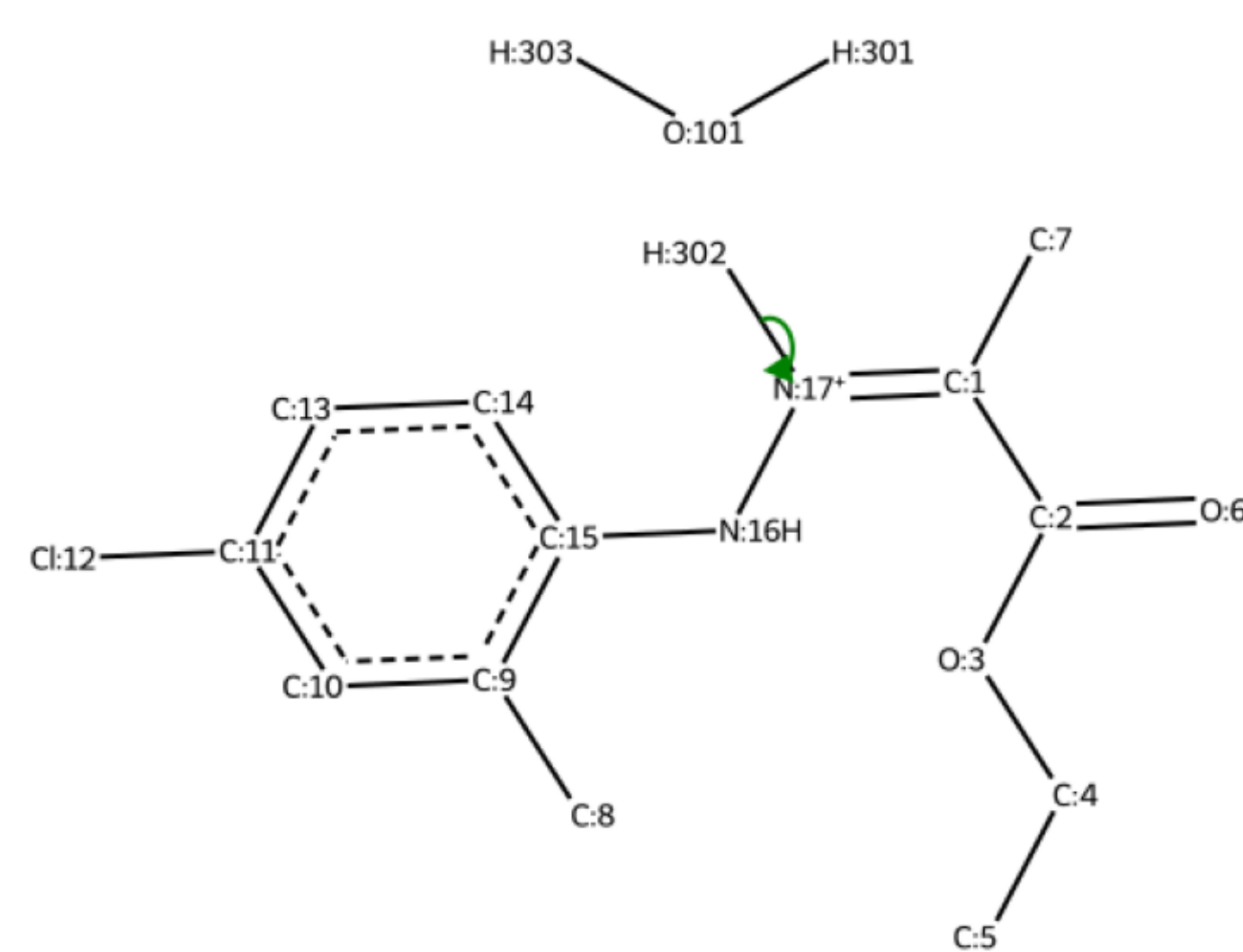
step #2



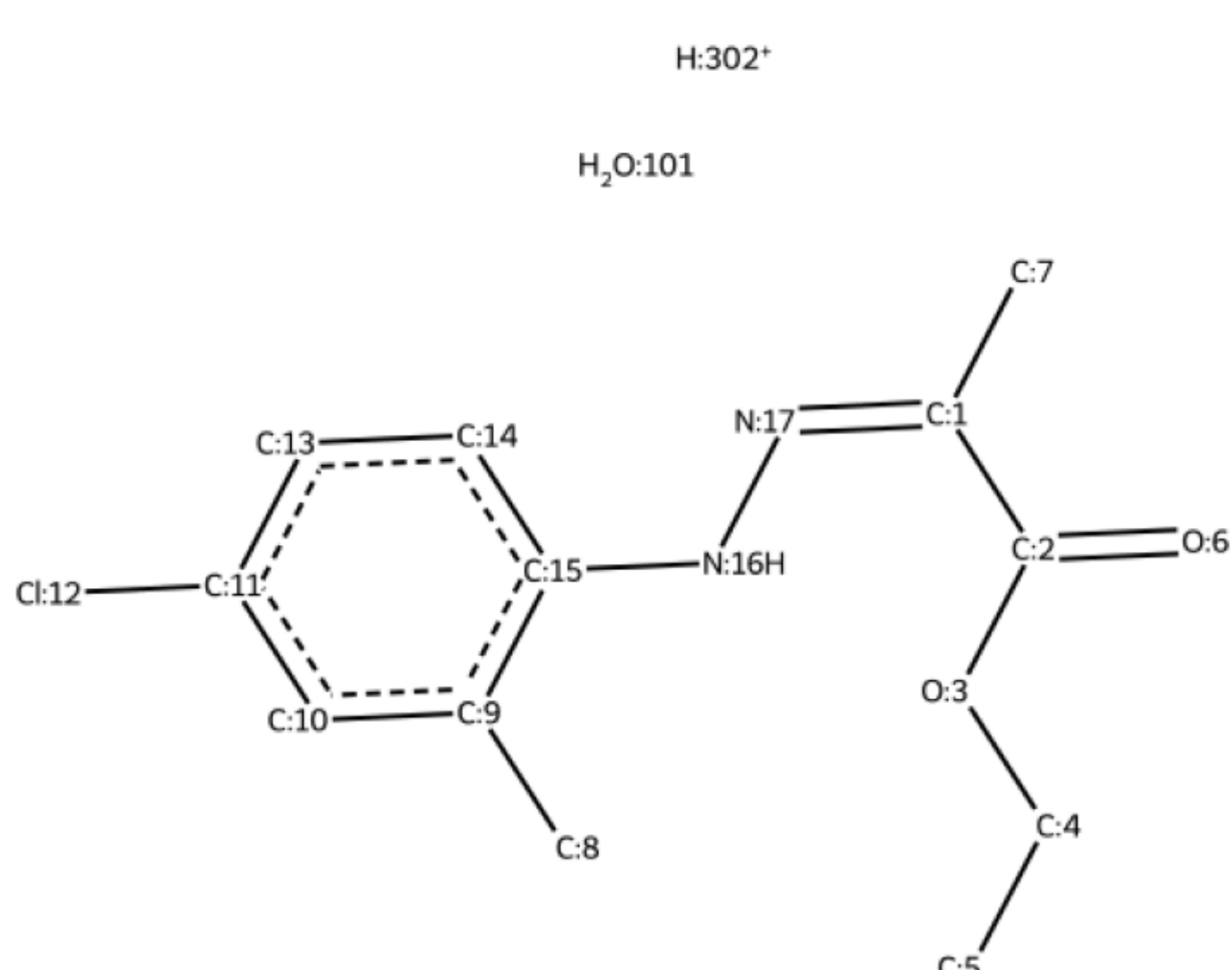
step #3



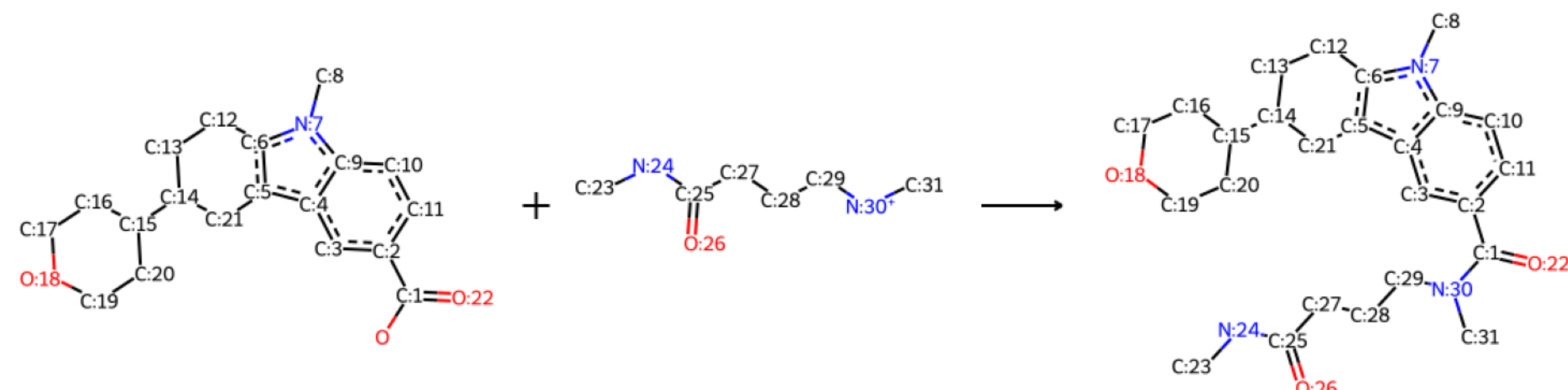
step #4



Product(s)

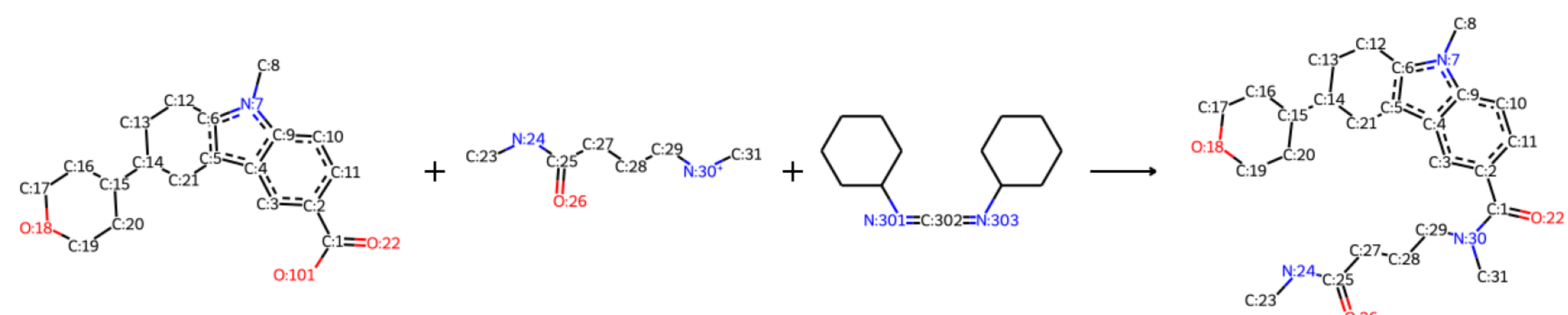


Original reaction
sampled RXN_ID:26)



Identified mechanistic class -
DCC_condensation reaction

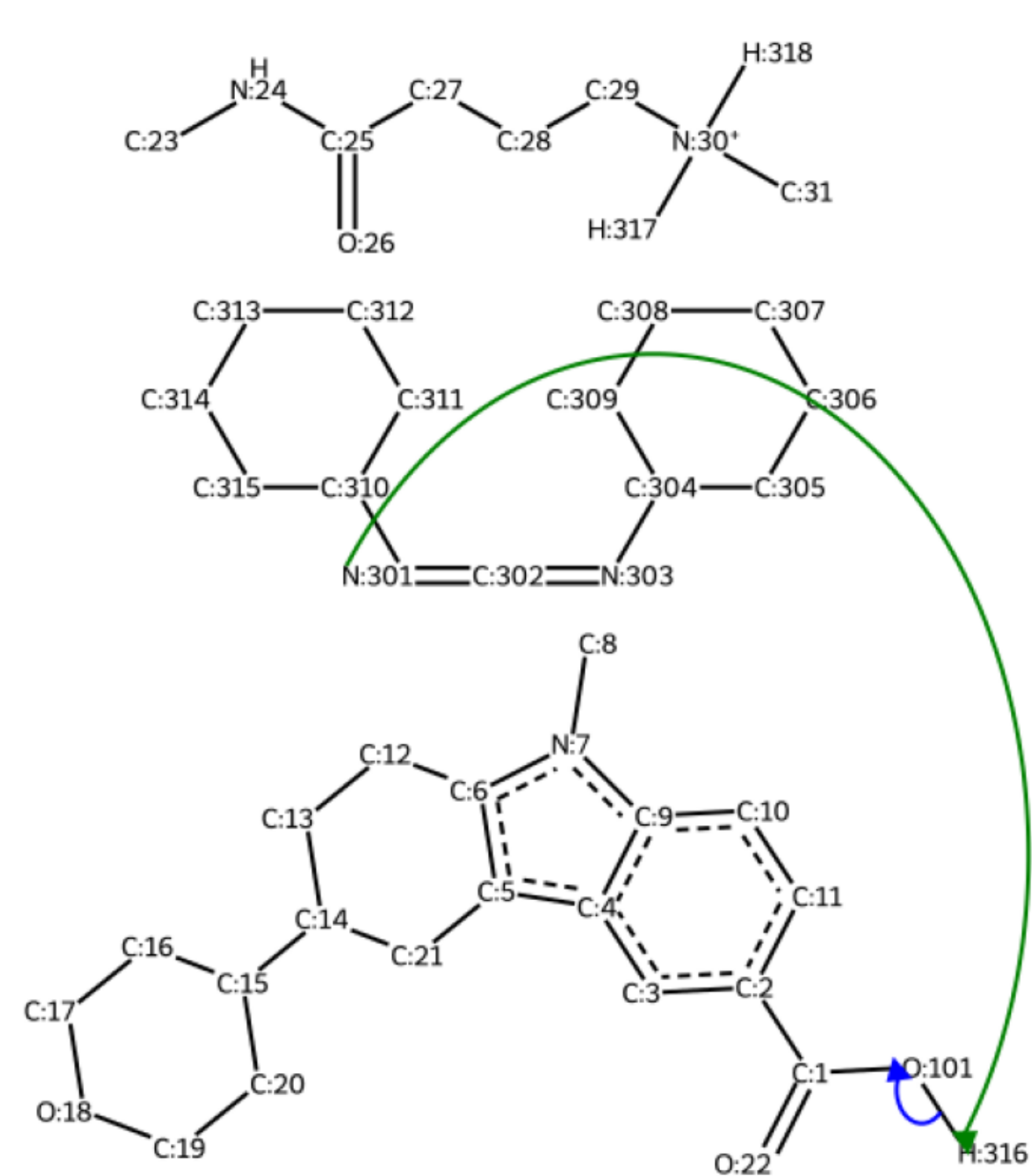
Reaction with missing reagents recovered



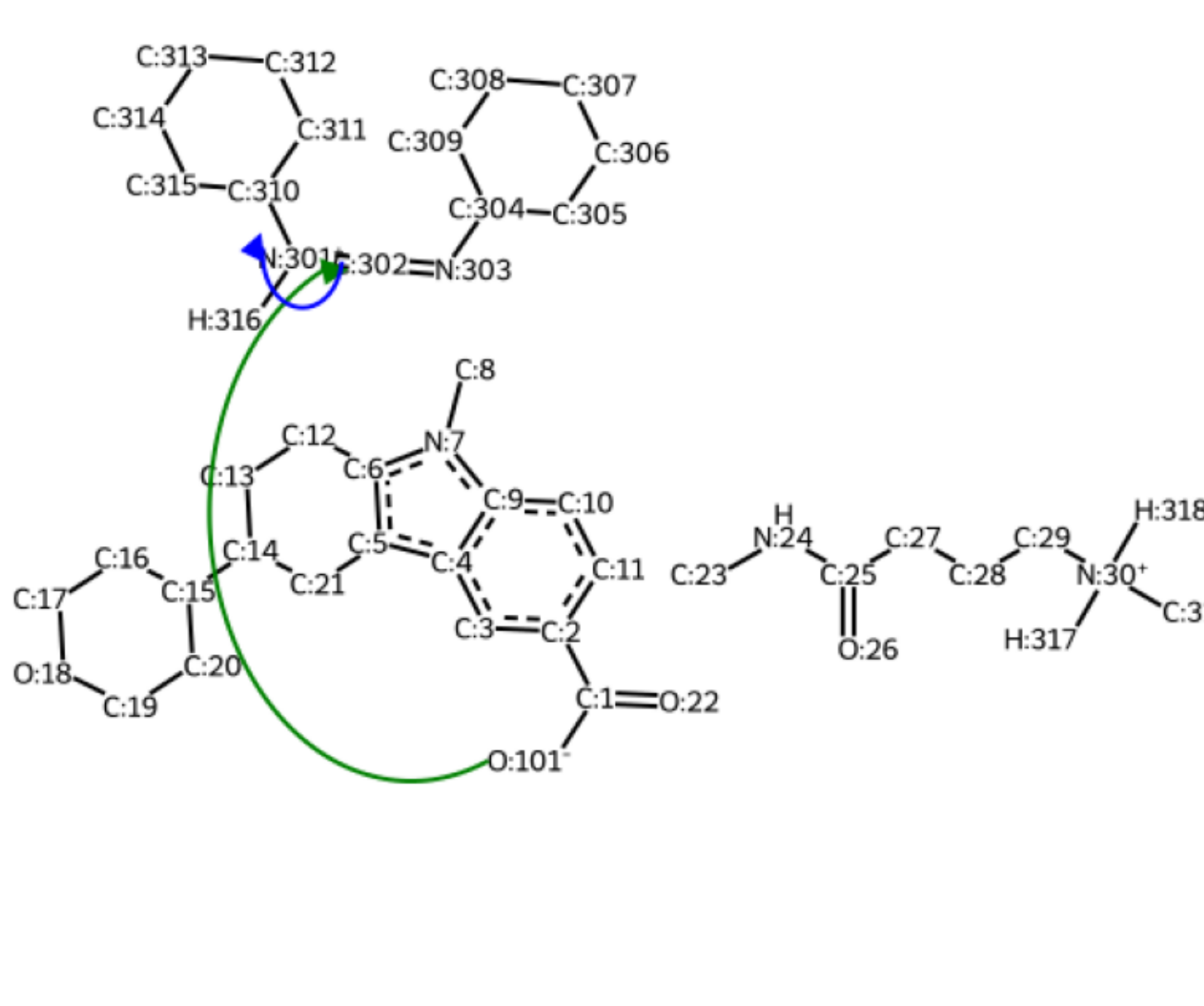
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

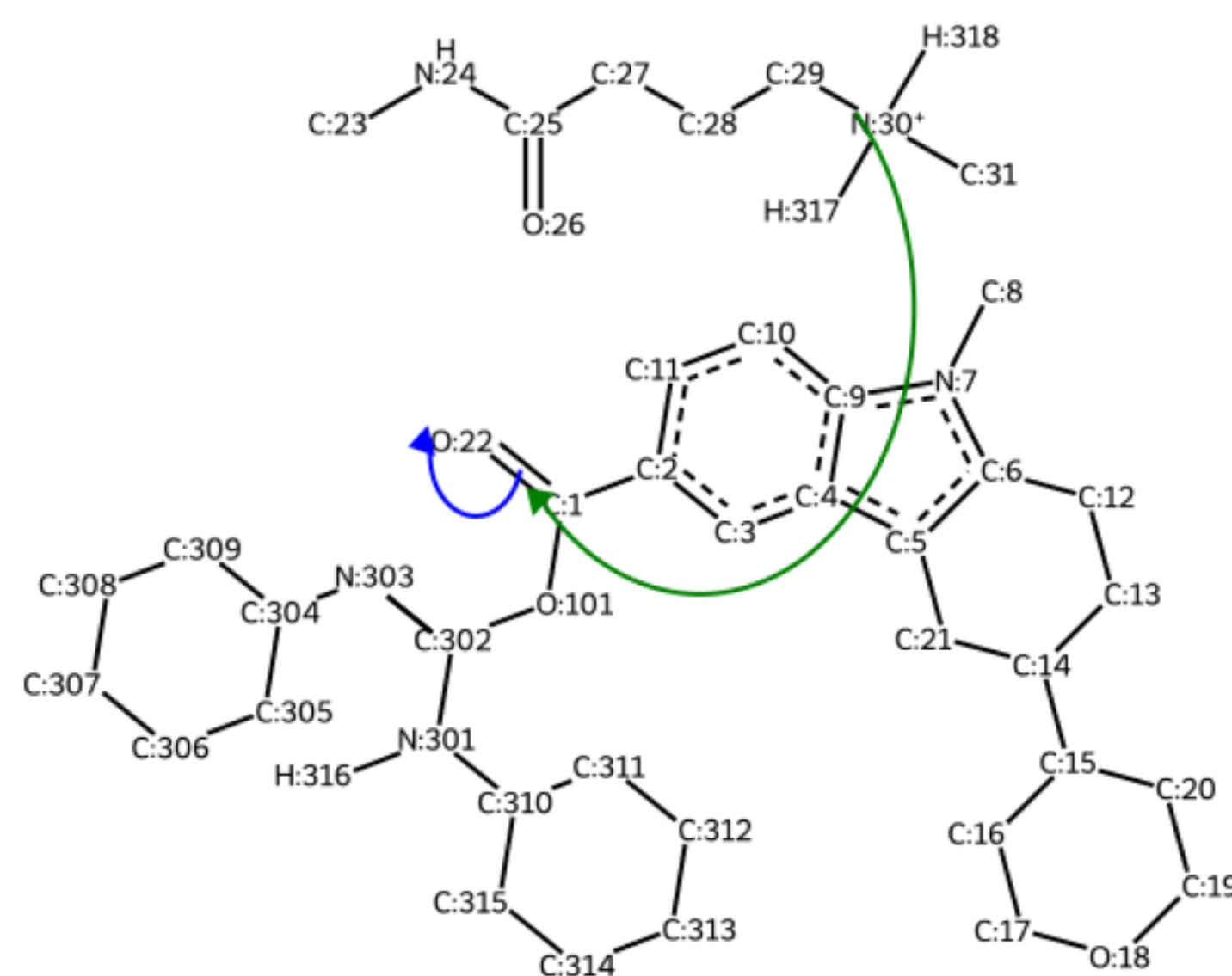
step #1



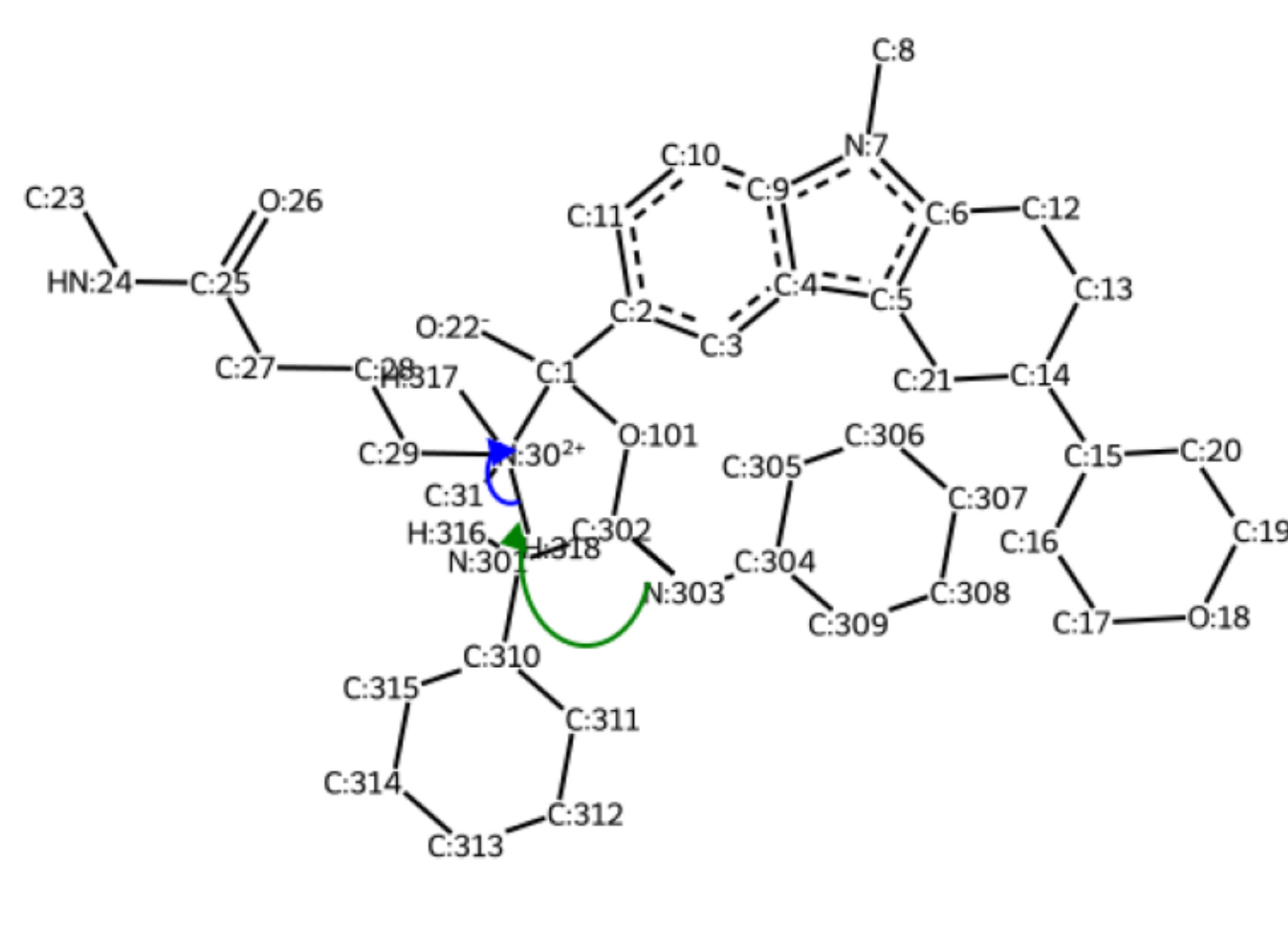
step #2



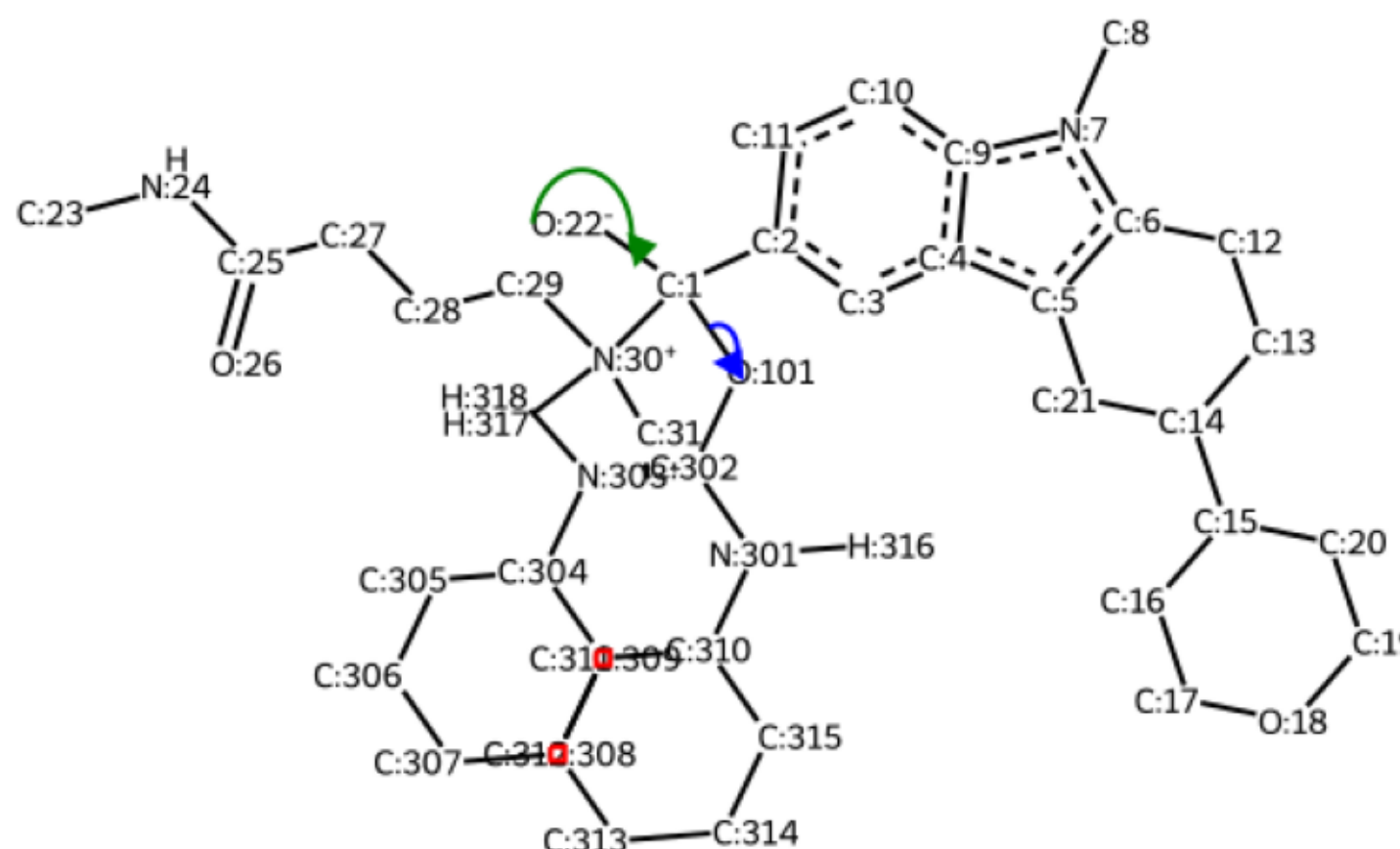
step #3



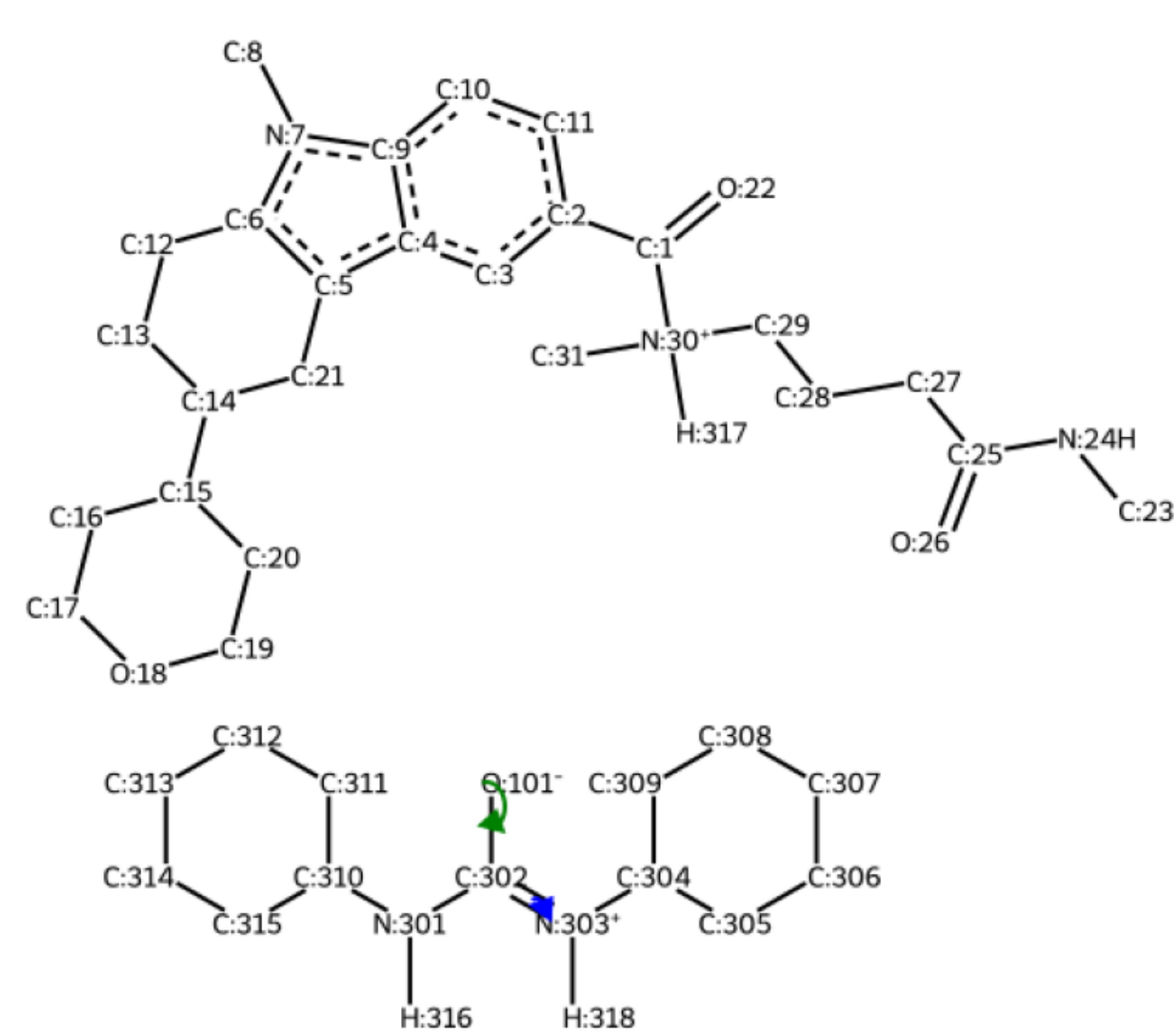
step #4



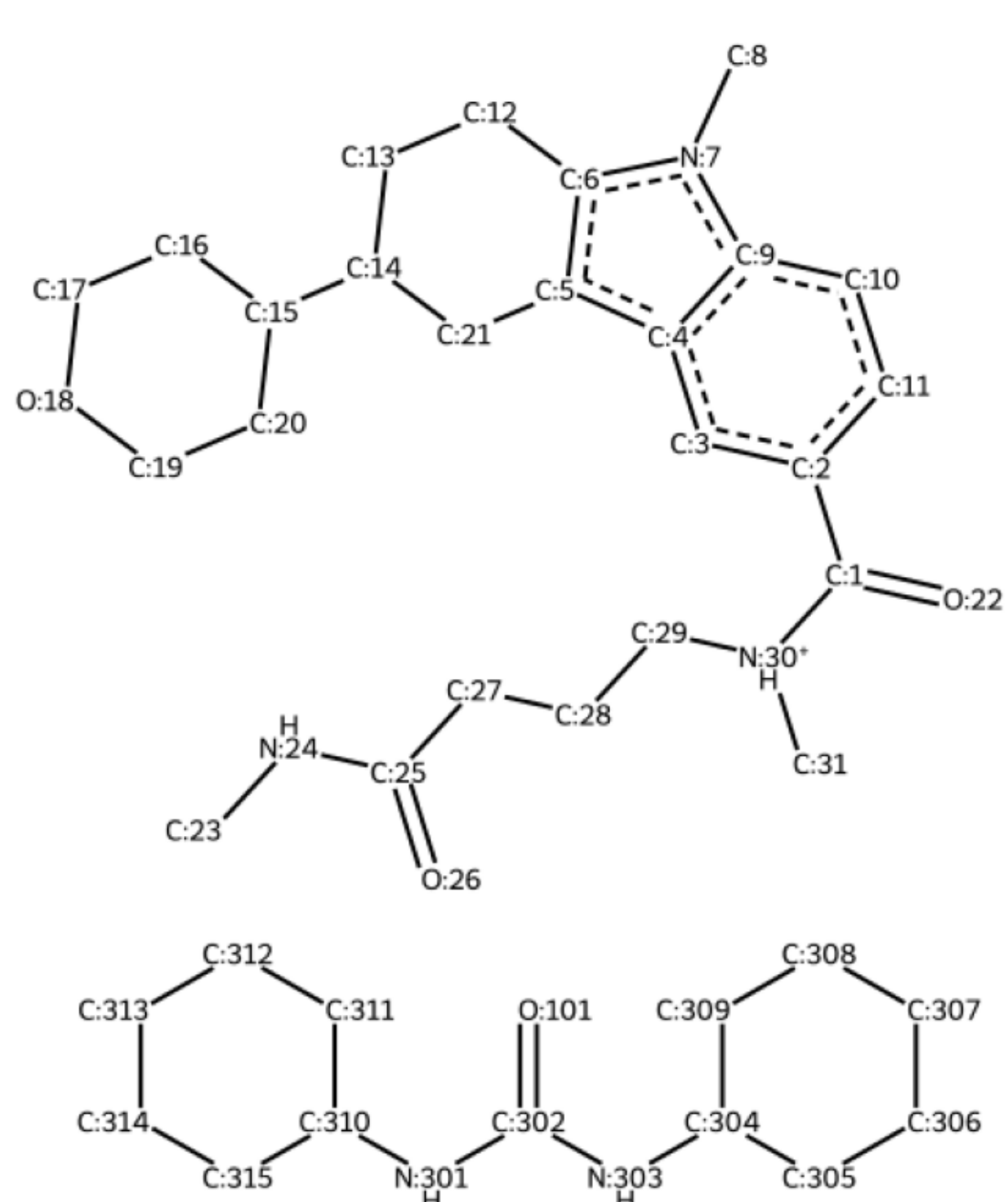
step #5



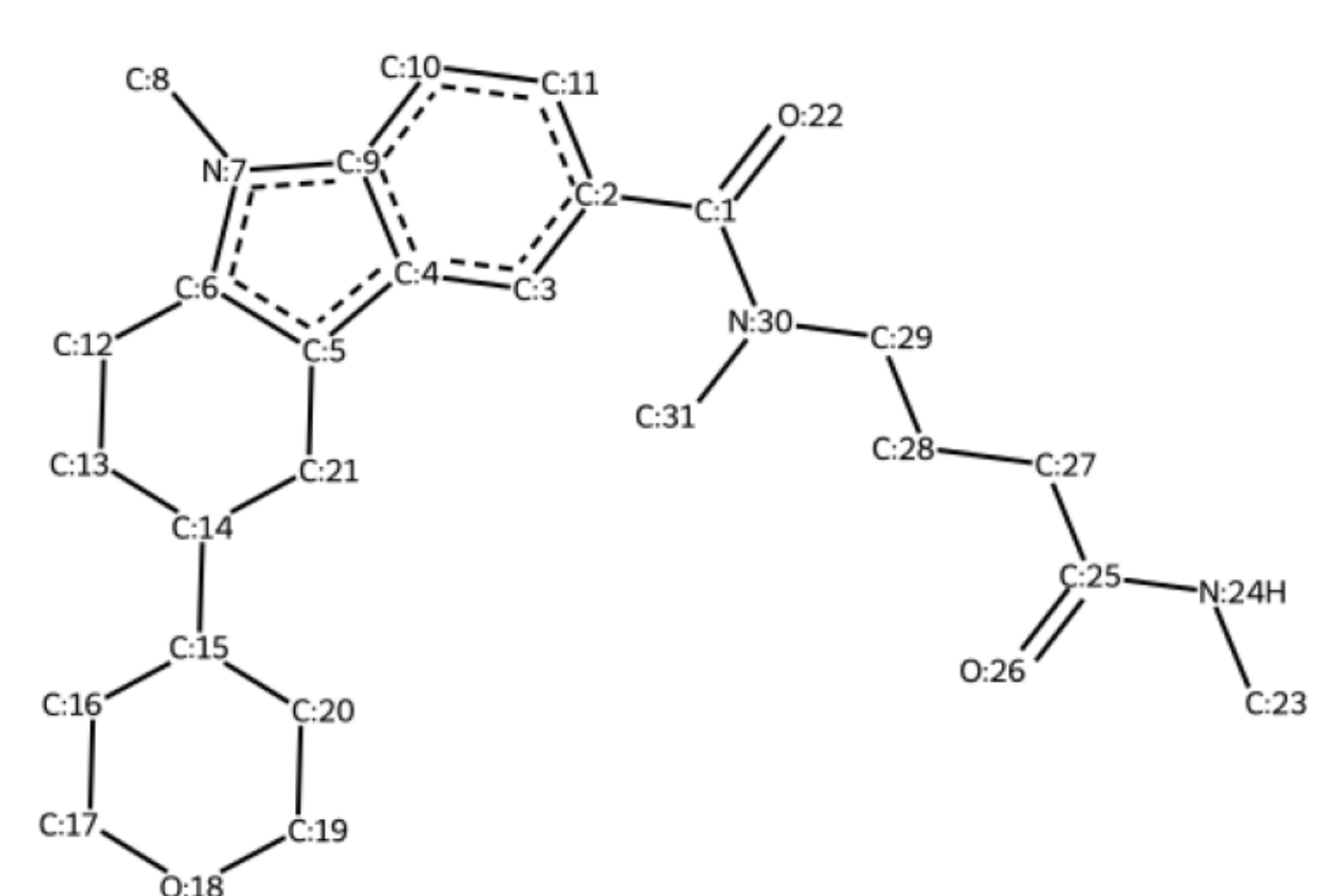
step #6



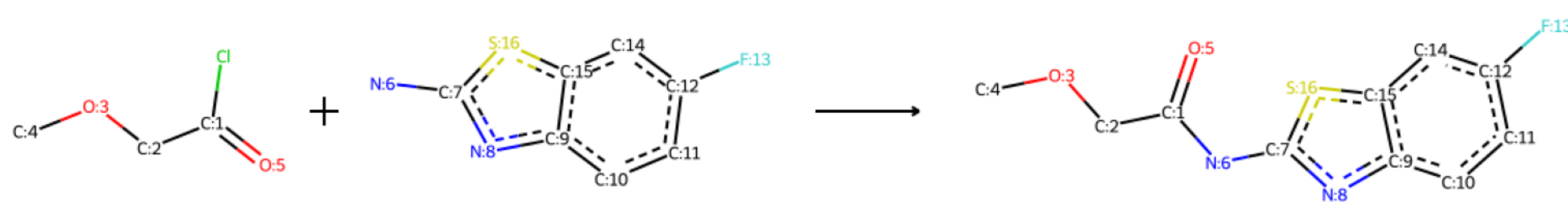
Product(s)



proton transfer

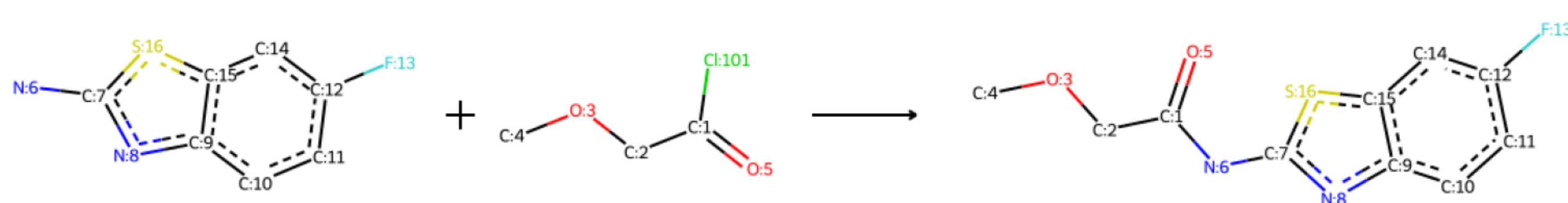


Original reaction
sampled RXN_ID:27)



Identified mechanistic class -
nucleophilic_attack_to_(thio)carbonyl_or_sulfonyl reaction

Reaction with missing reagents recovered

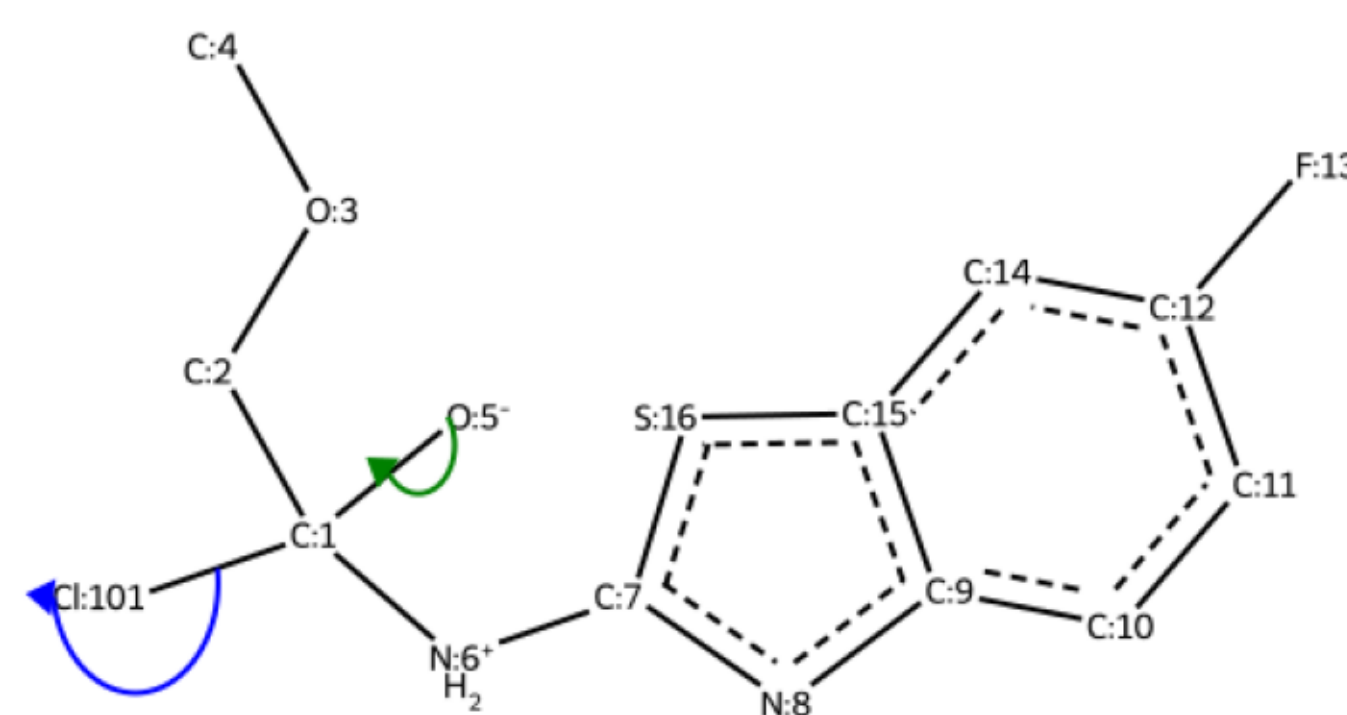
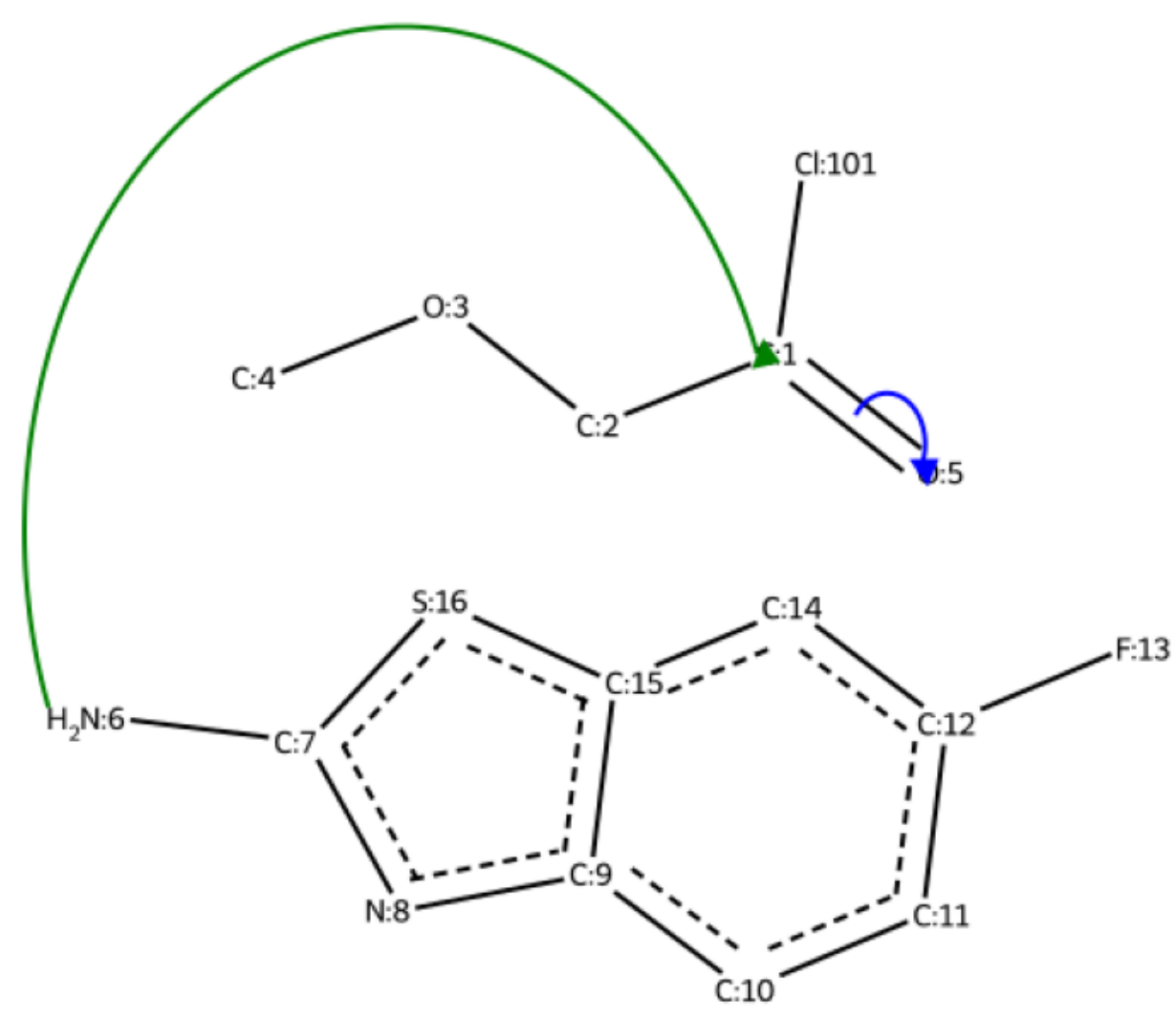


Proposed mechanistic pathway

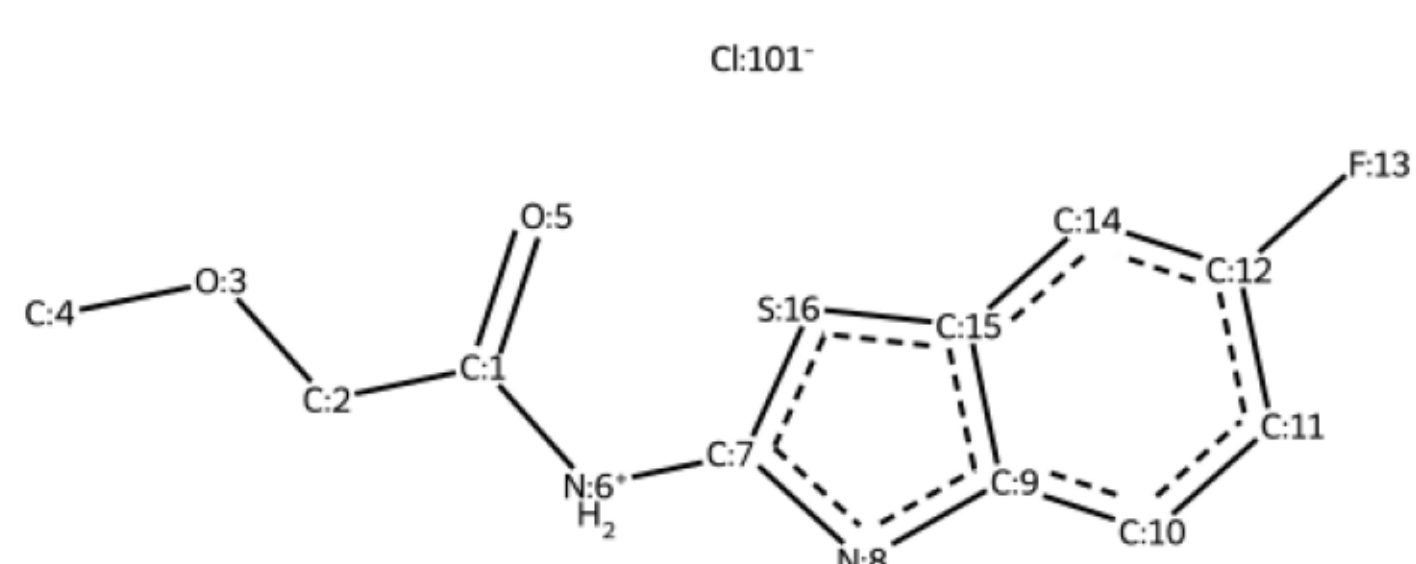
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

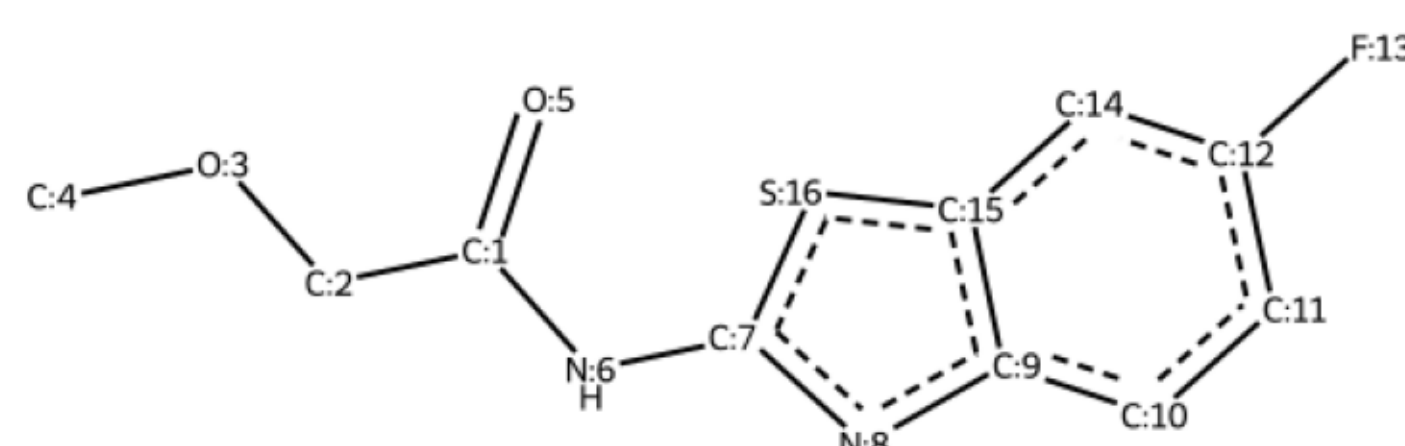
step #2



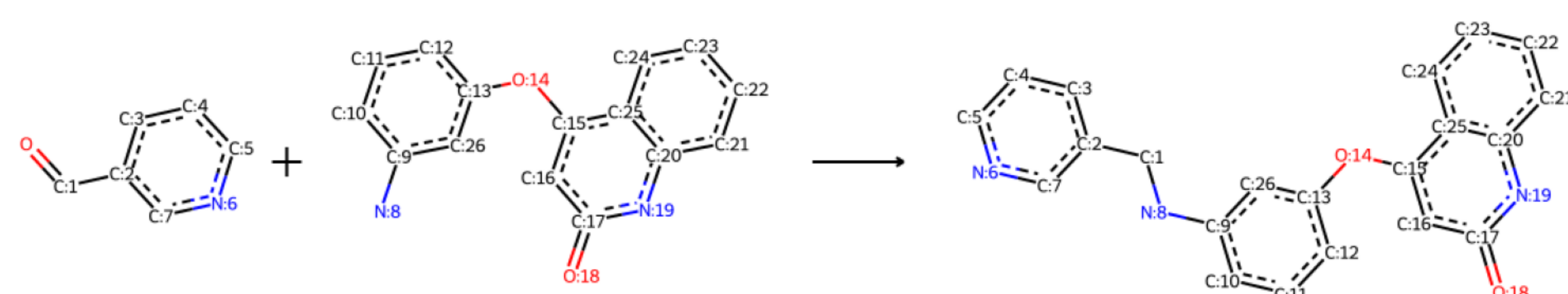
Product(s)



proton transfer

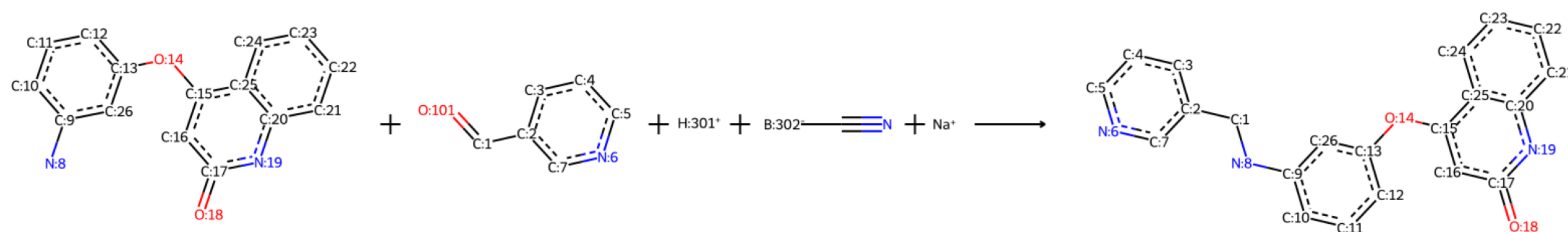


Original reaction
sampled RXN_ID:28)



Identified mechanistic class -
reductive_amination reaction

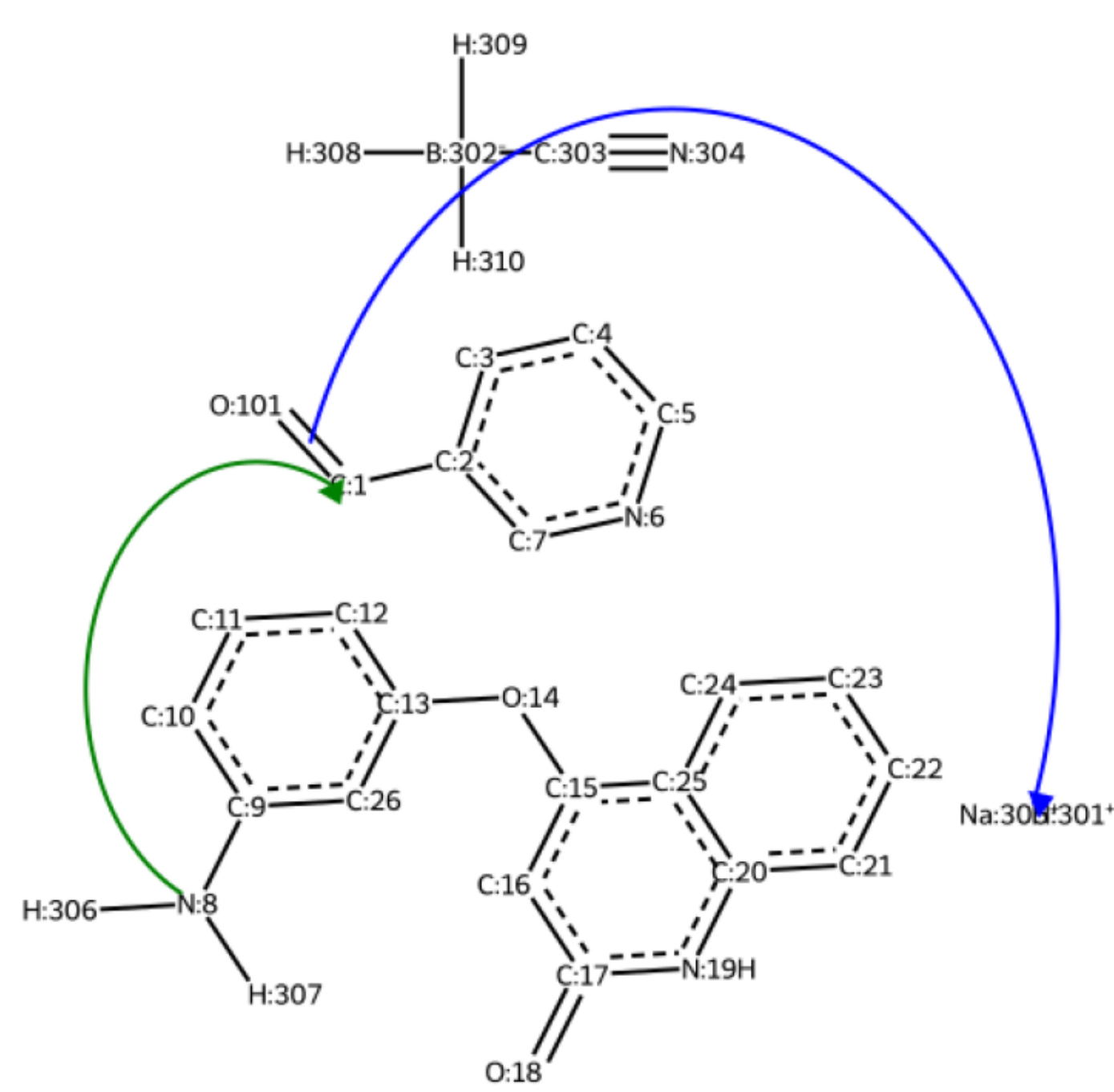
Reaction with missing reagents recovered



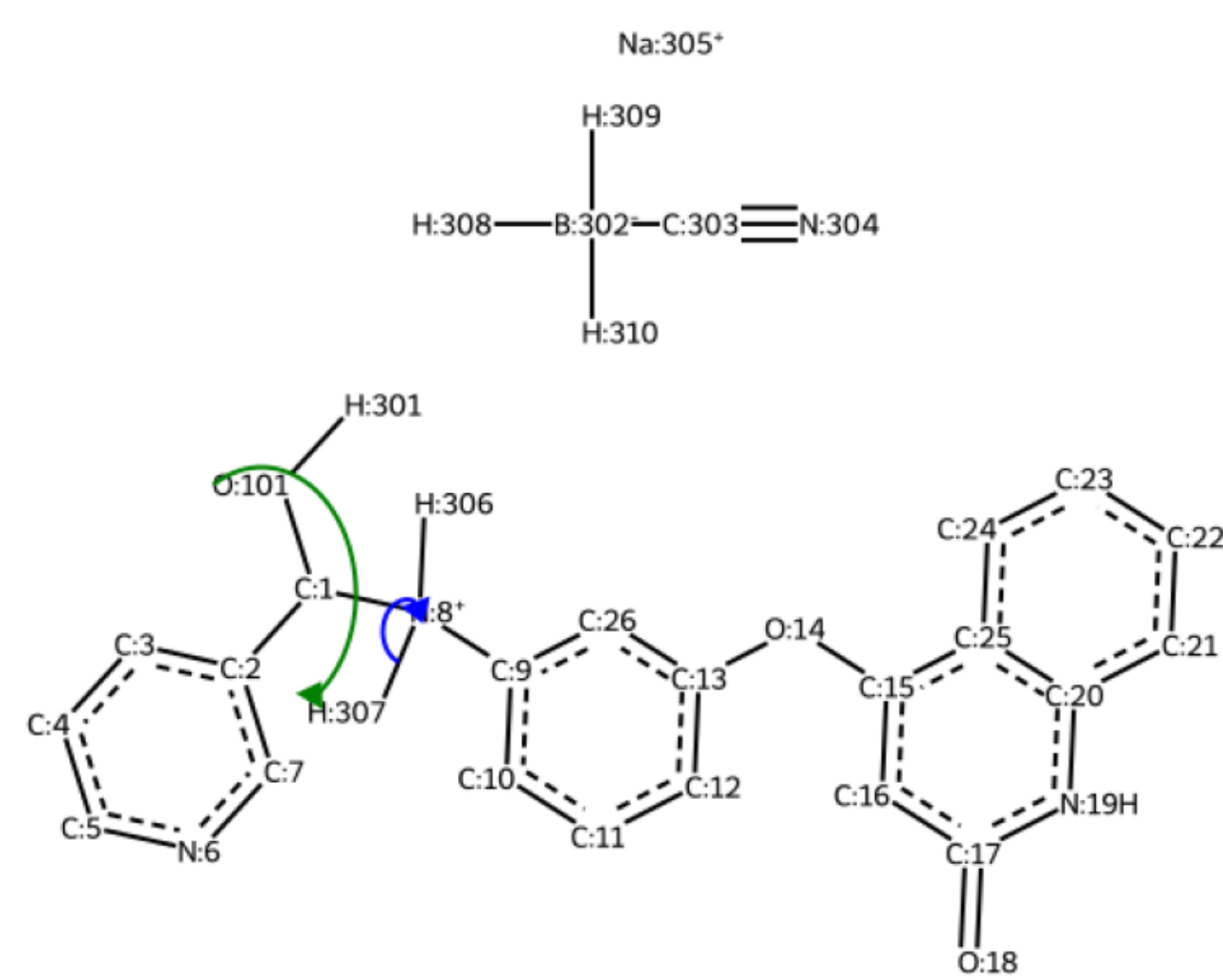
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

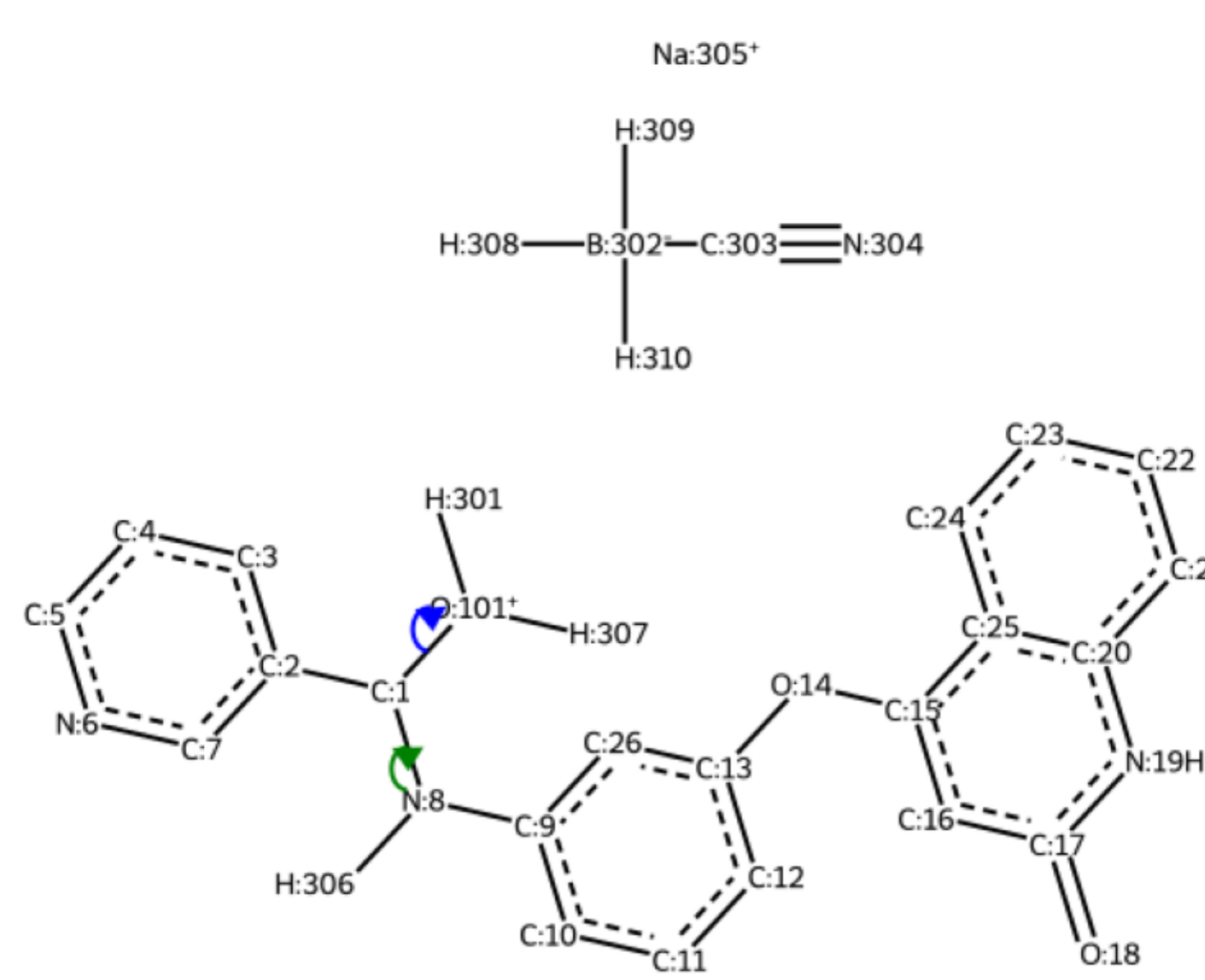
step #1



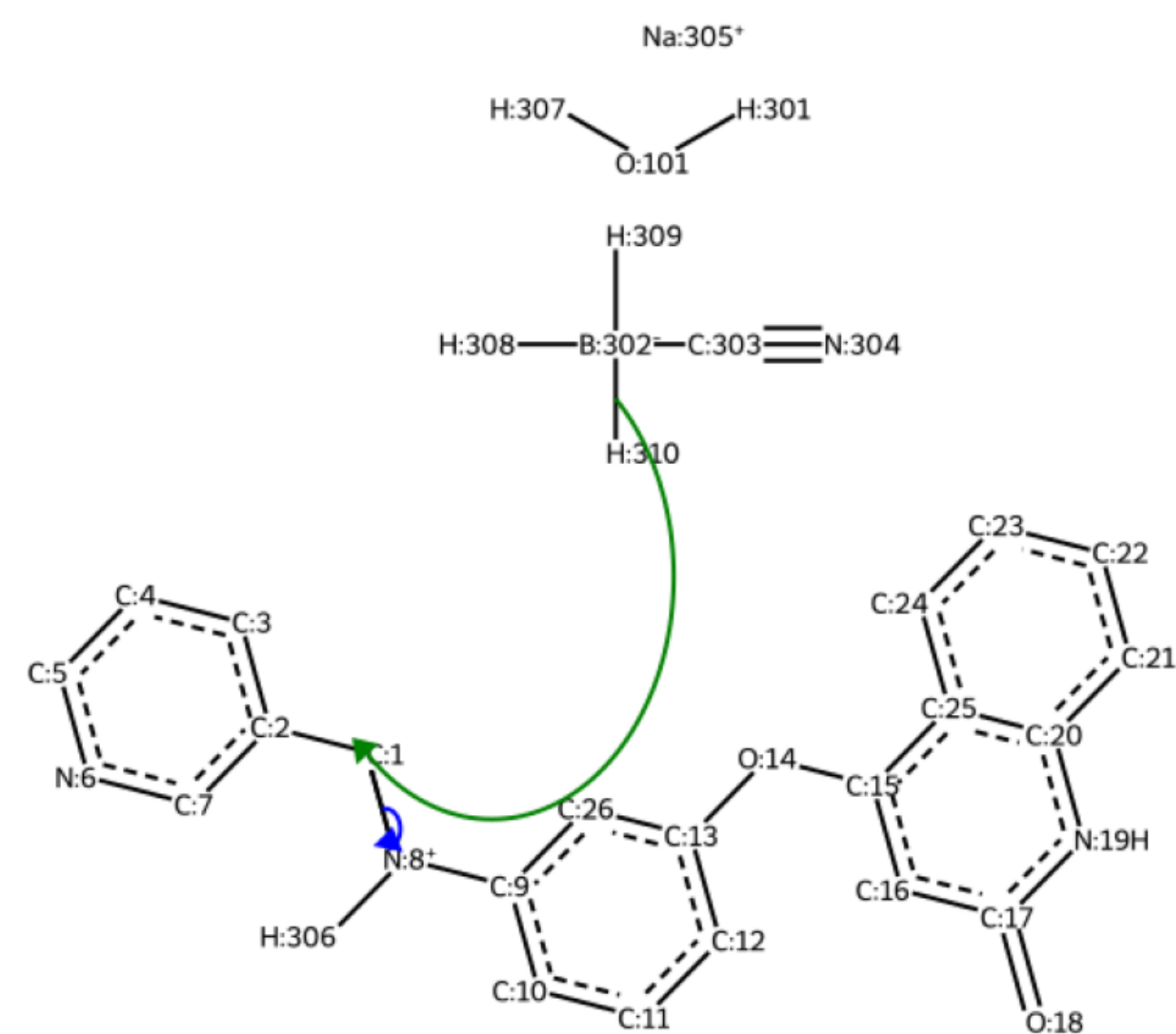
step #2



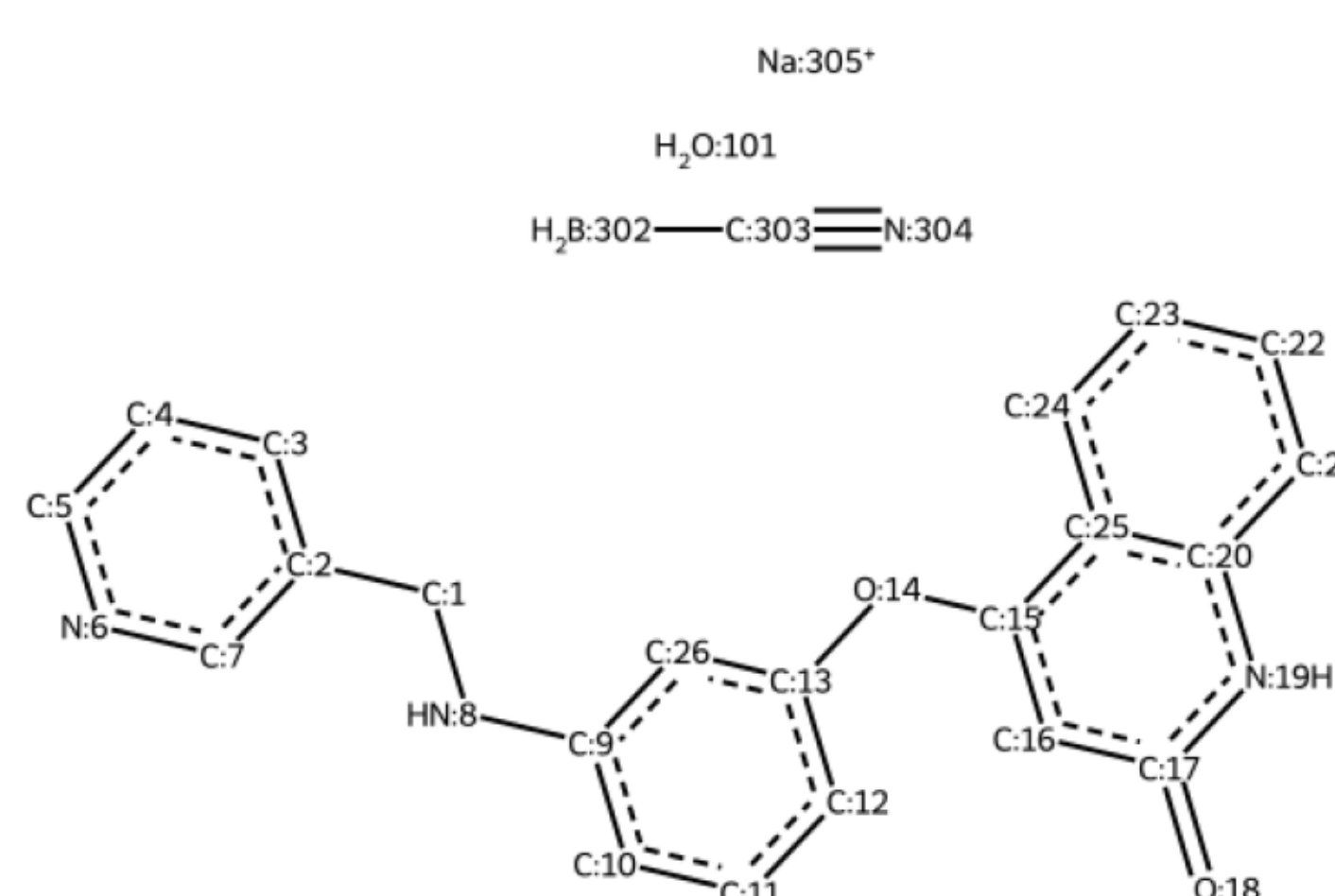
step #3



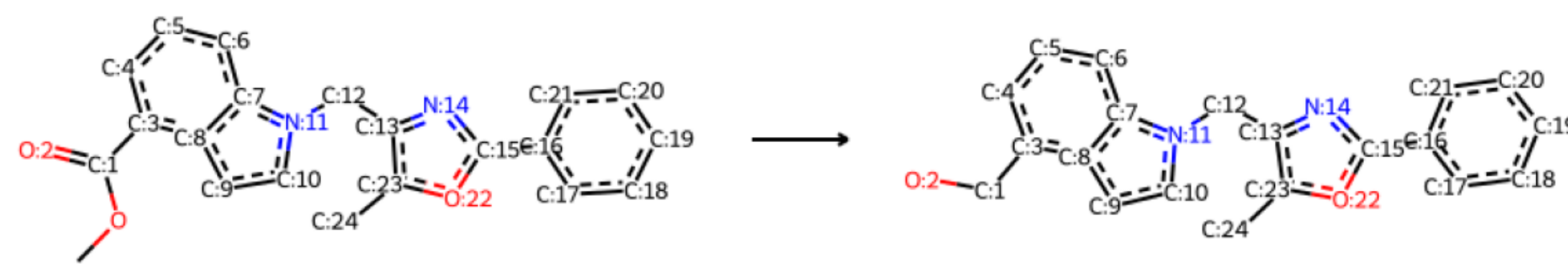
step #4



Product(s)

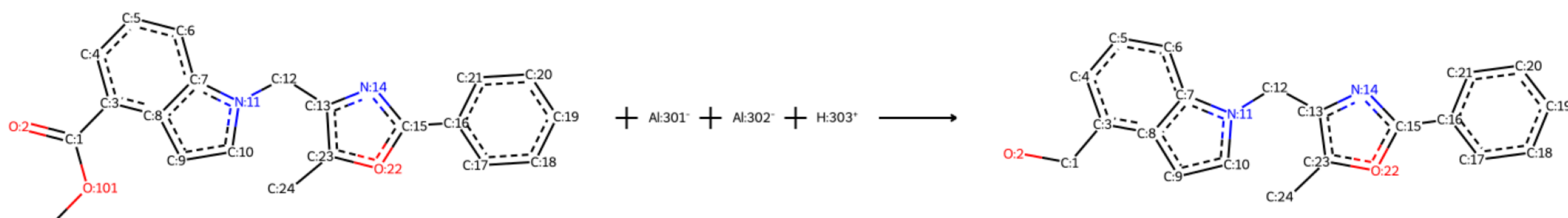


Original reaction
sampled RXN_ID:29)



Identified mechanistic class -
ester_reduction reaction

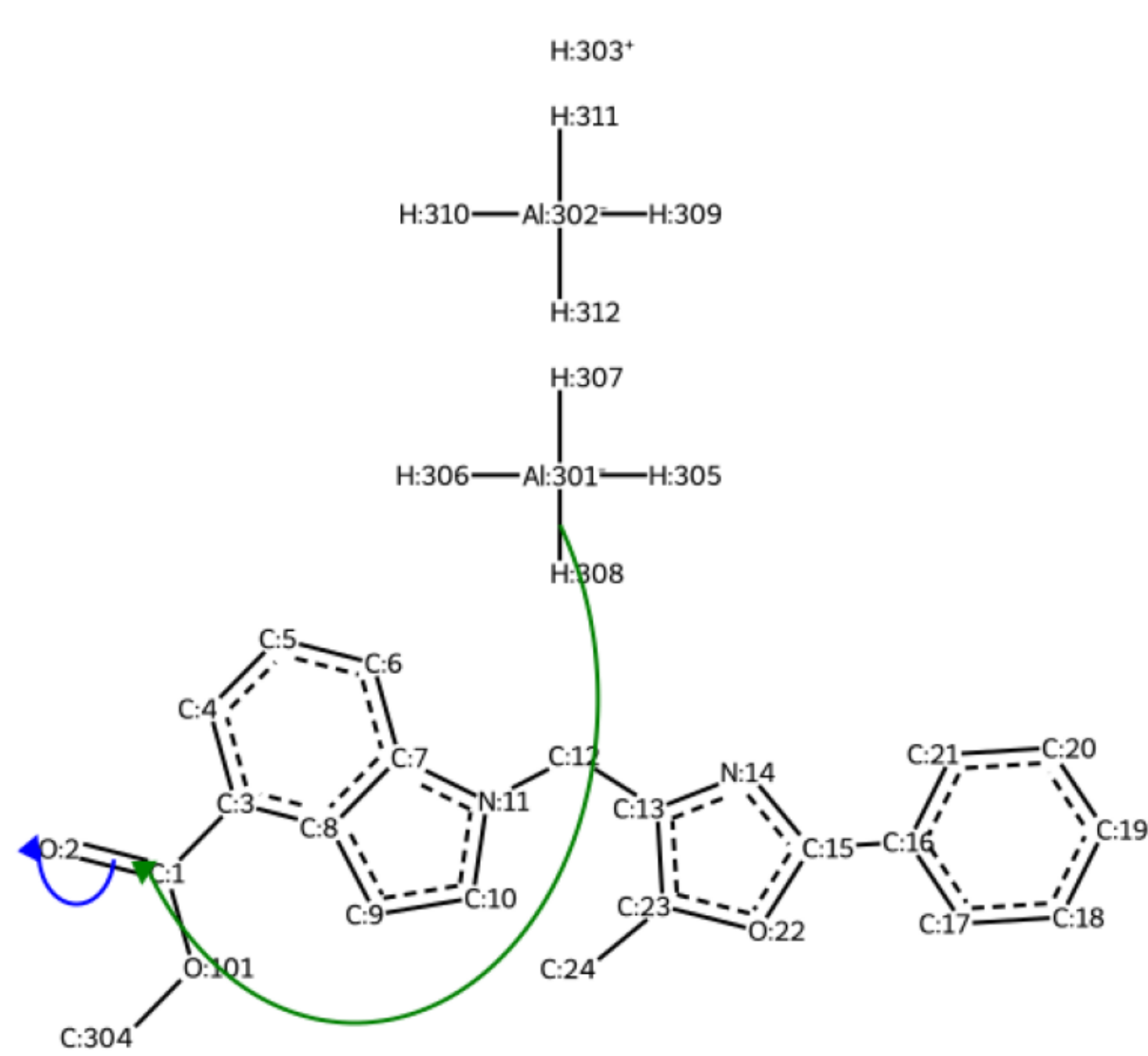
Reaction with missing reagents recovered



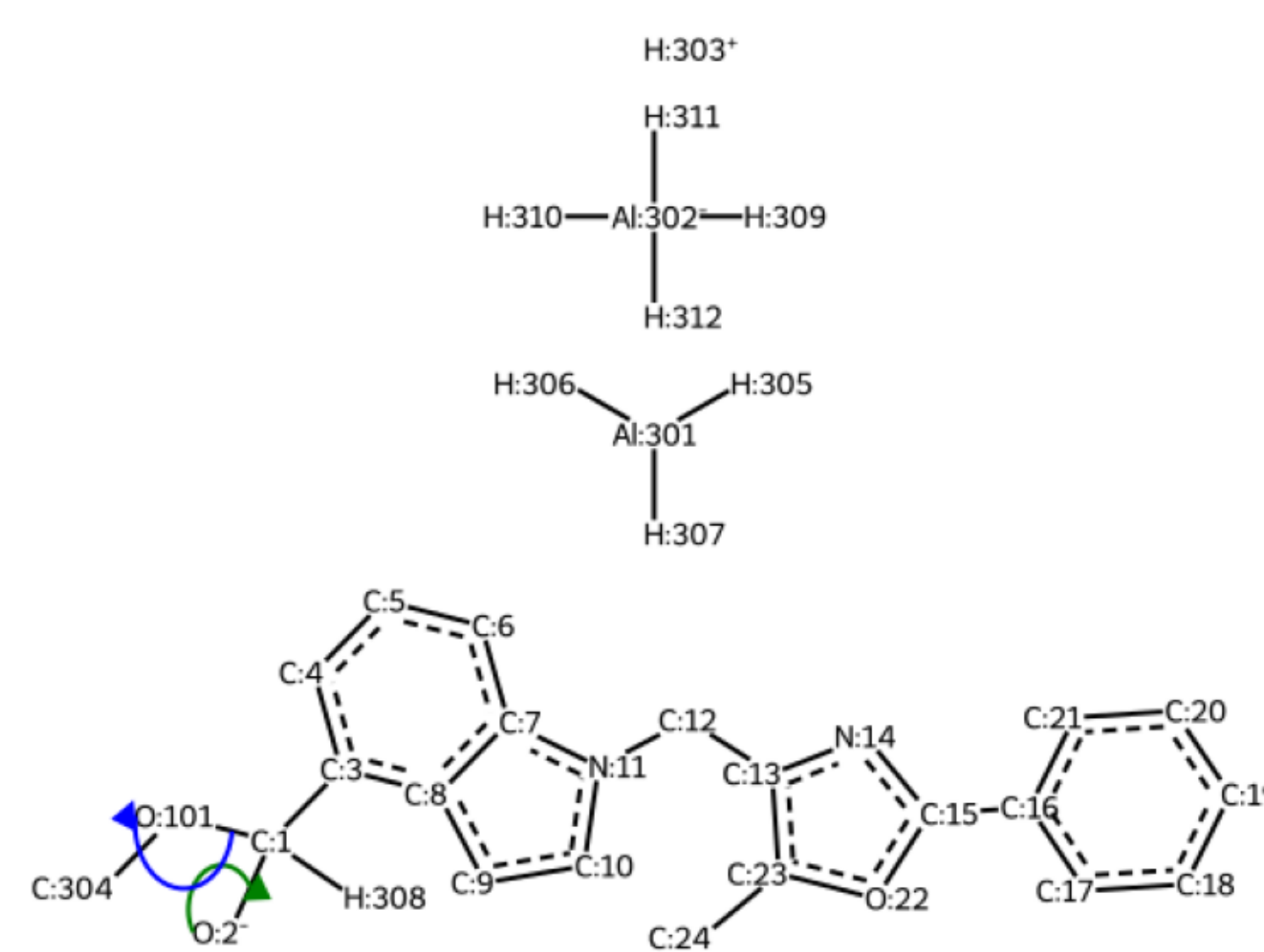
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

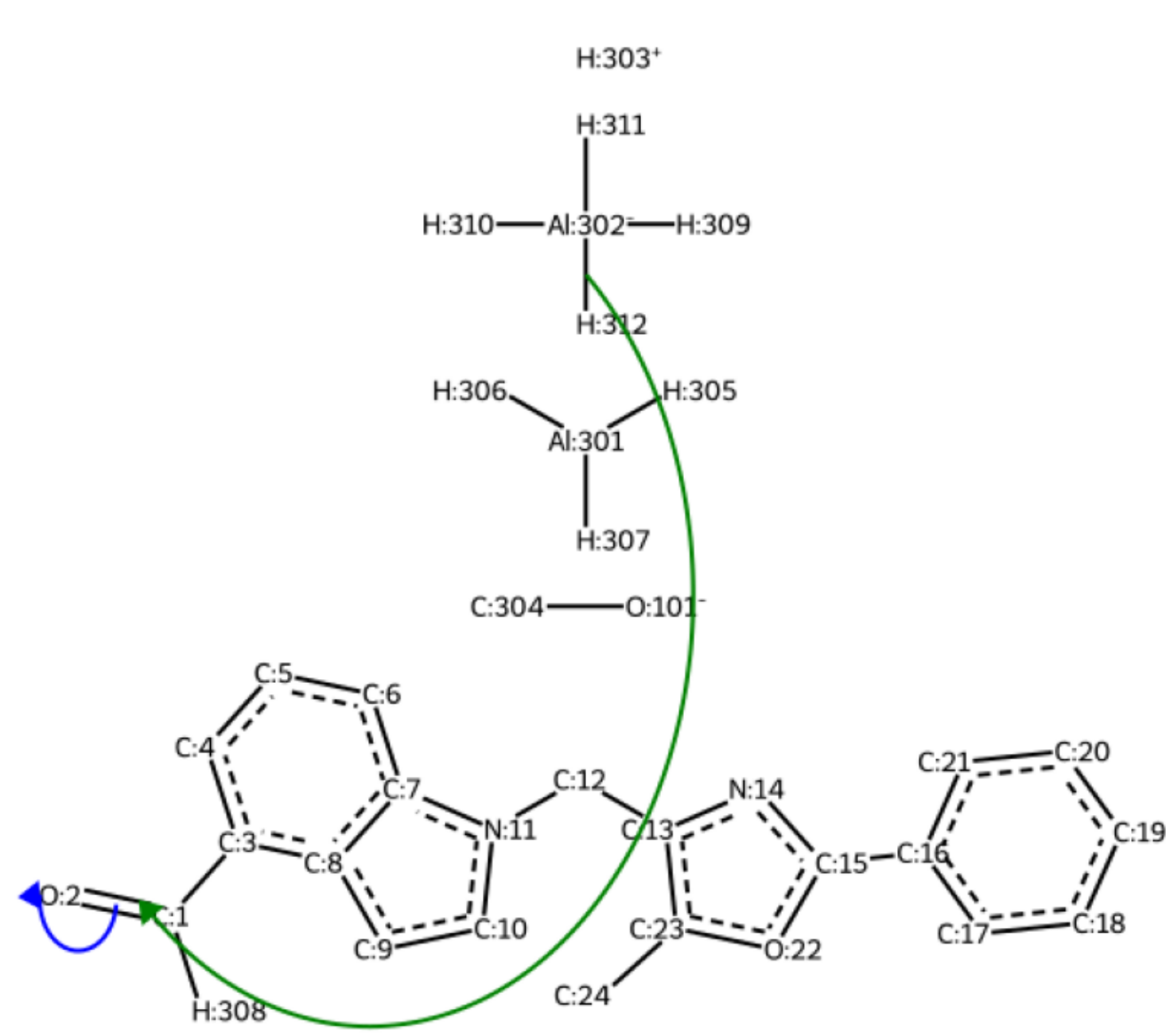
step #1



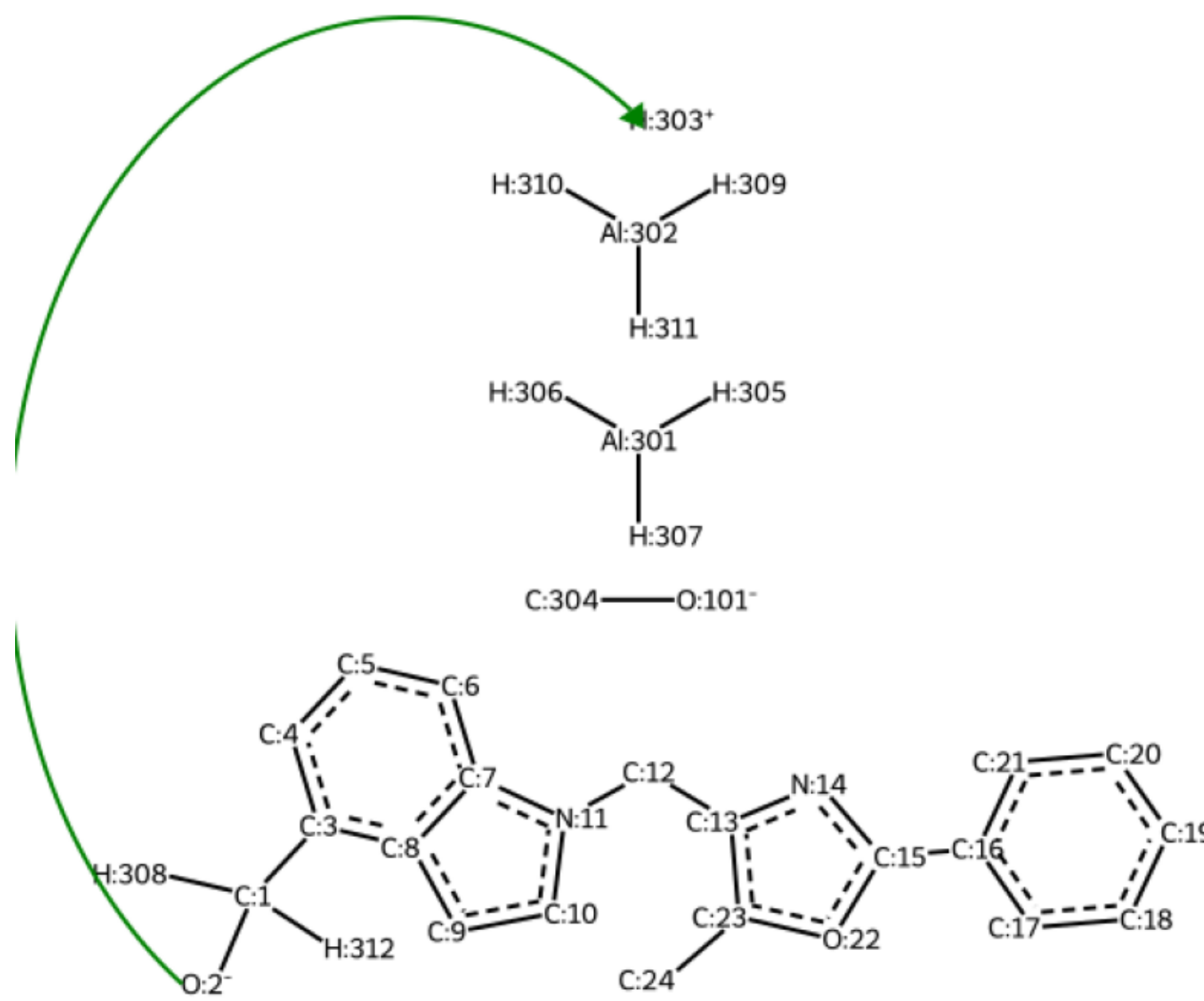
step #2



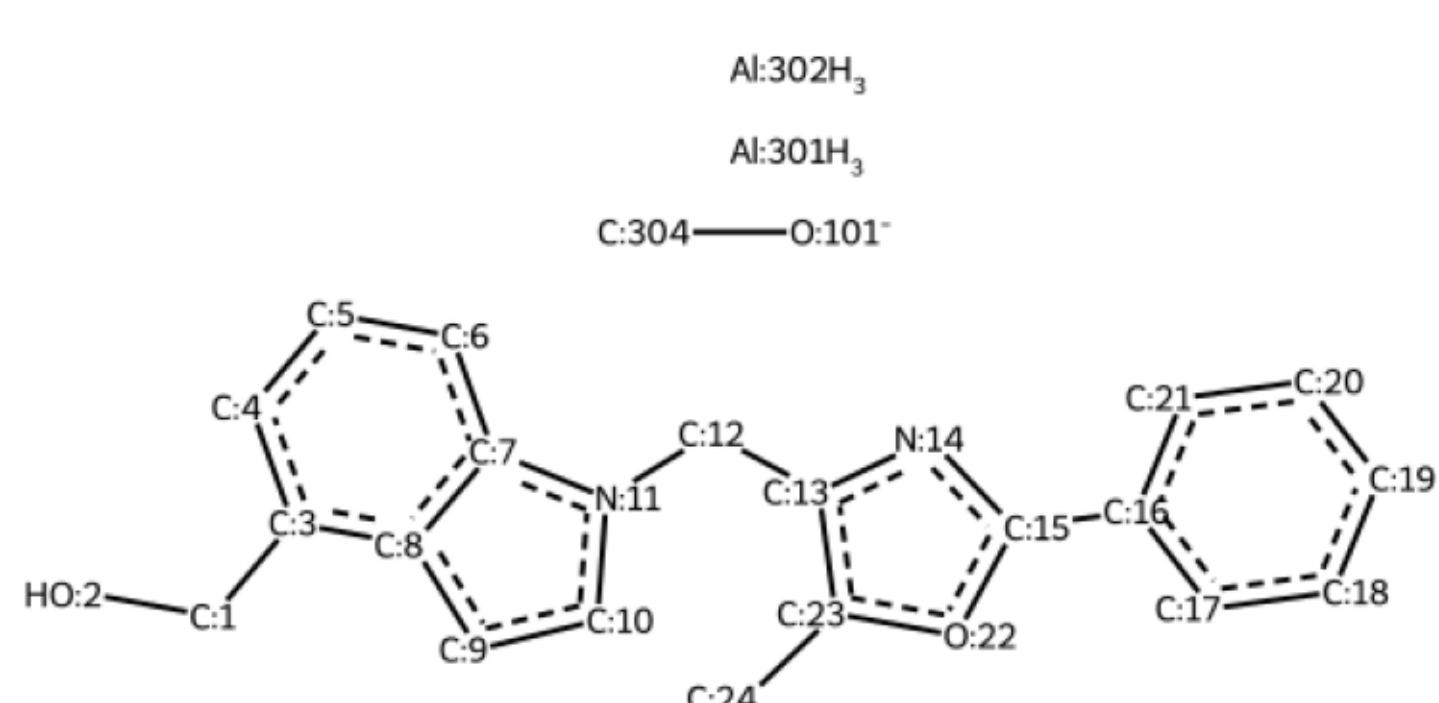
step #3



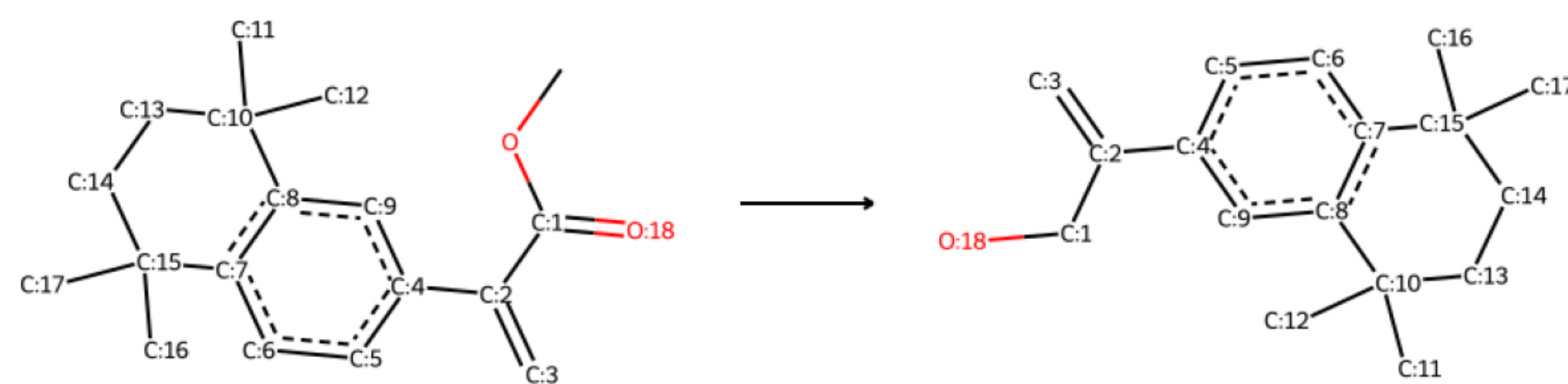
step #4



Product(s)

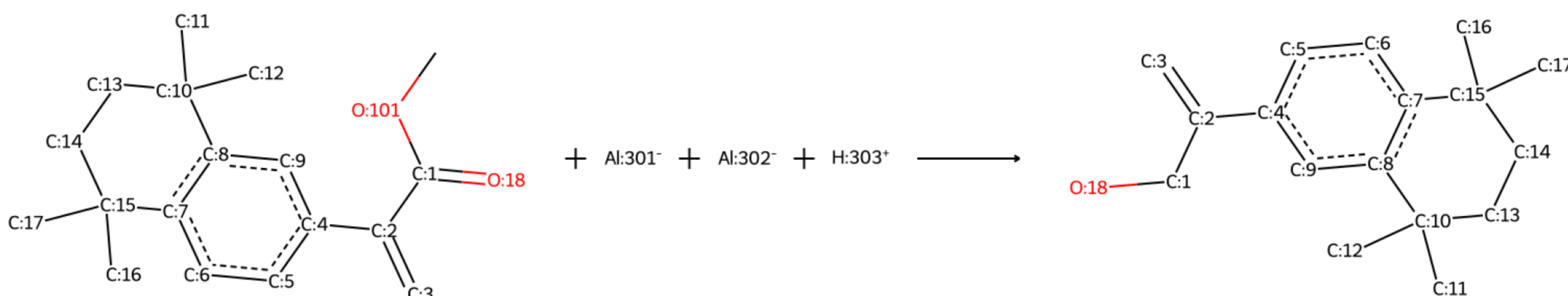


Original reaction
sampled RXN_ID:30)



Identified mechanistic class -
ester_reduction reaction

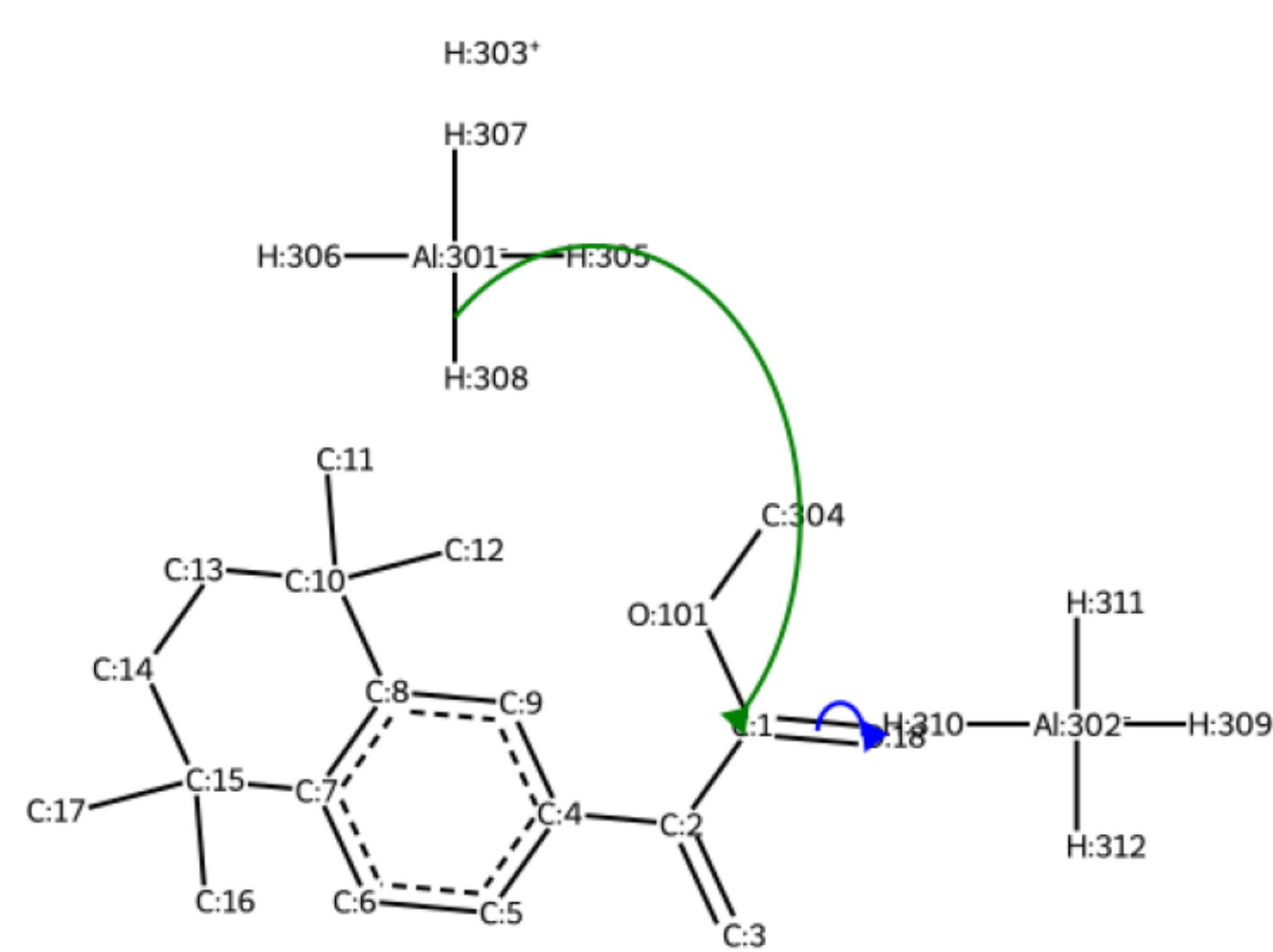
Reaction with missing reagents recovered



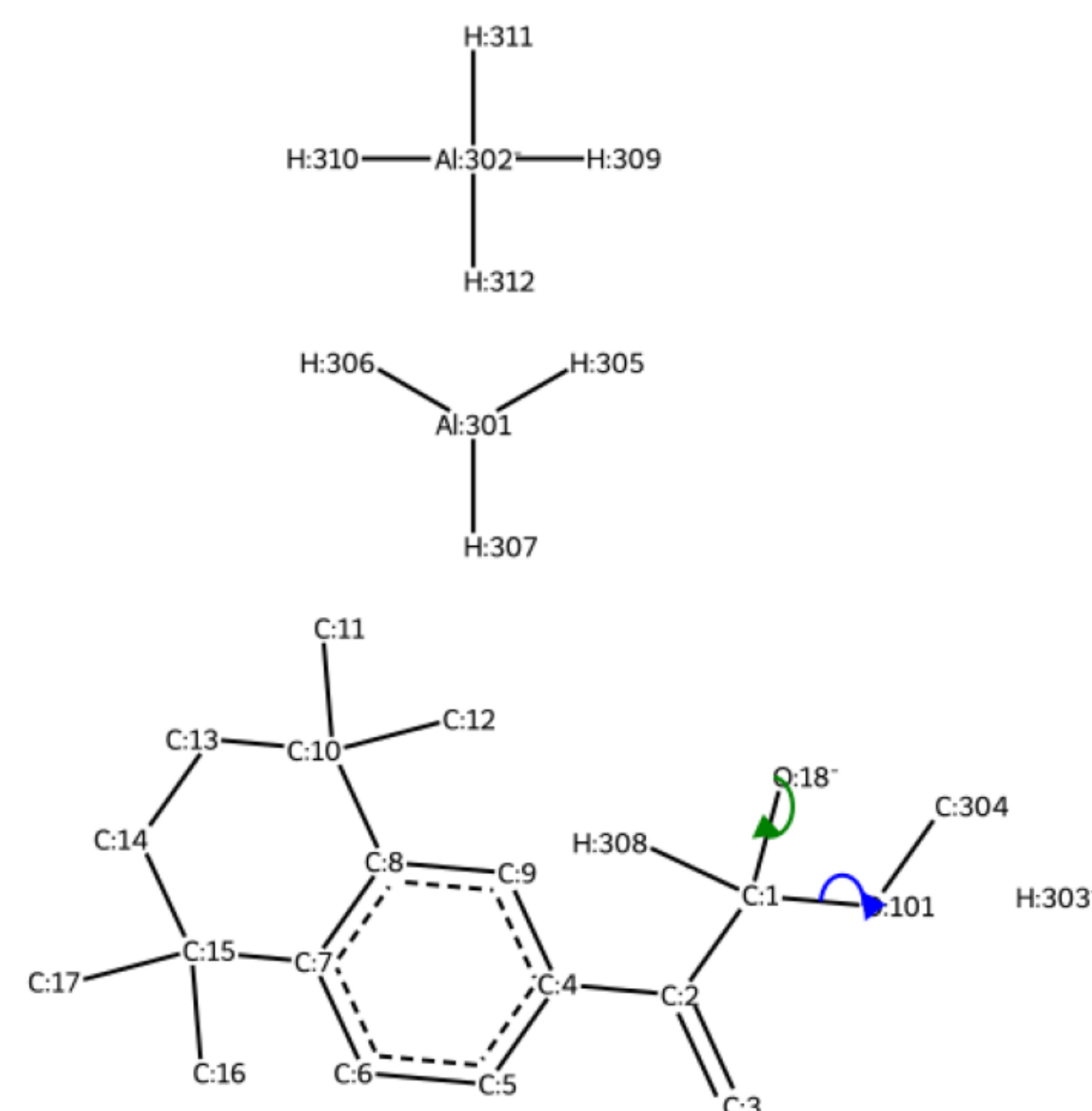
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

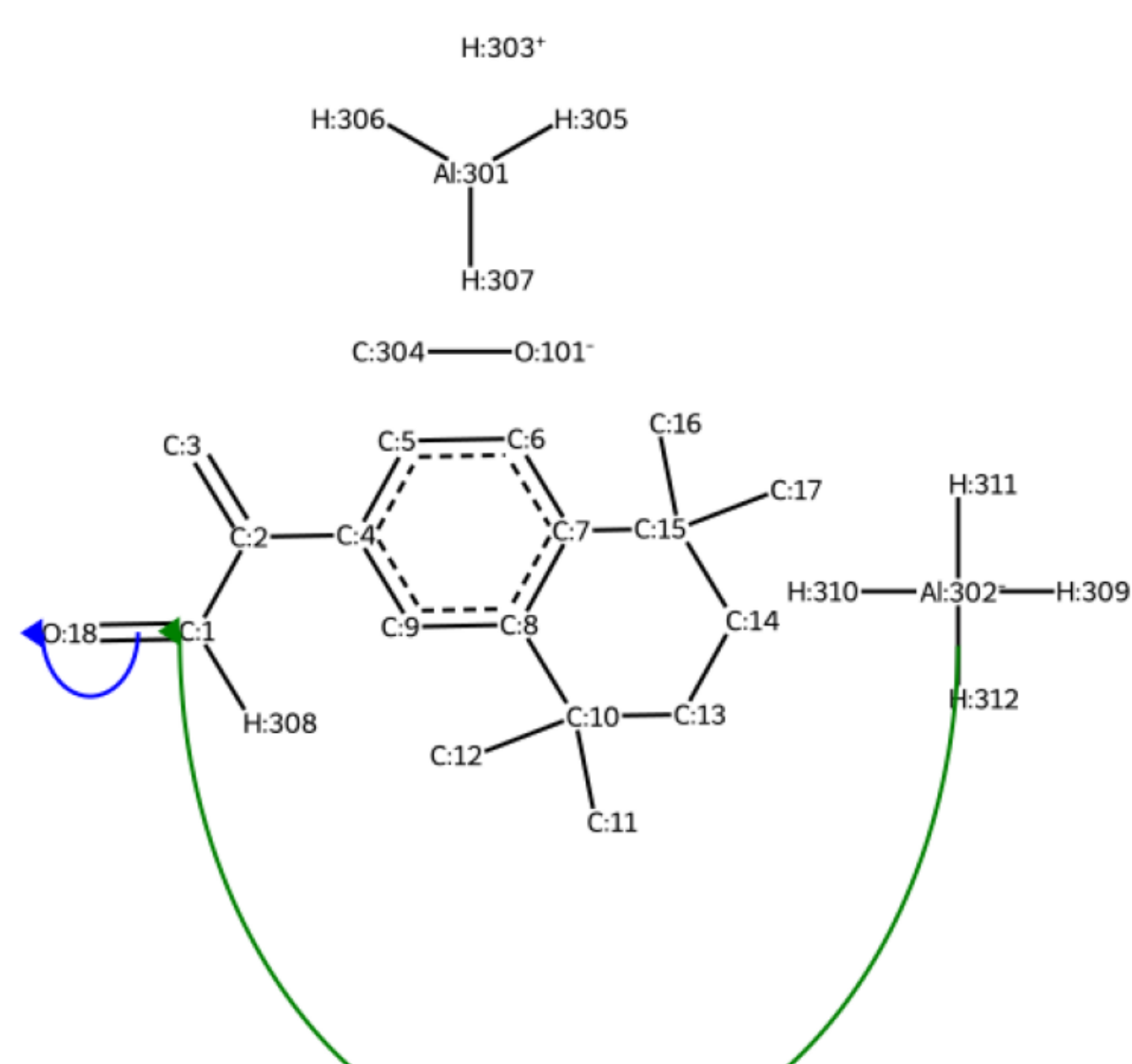
step #1



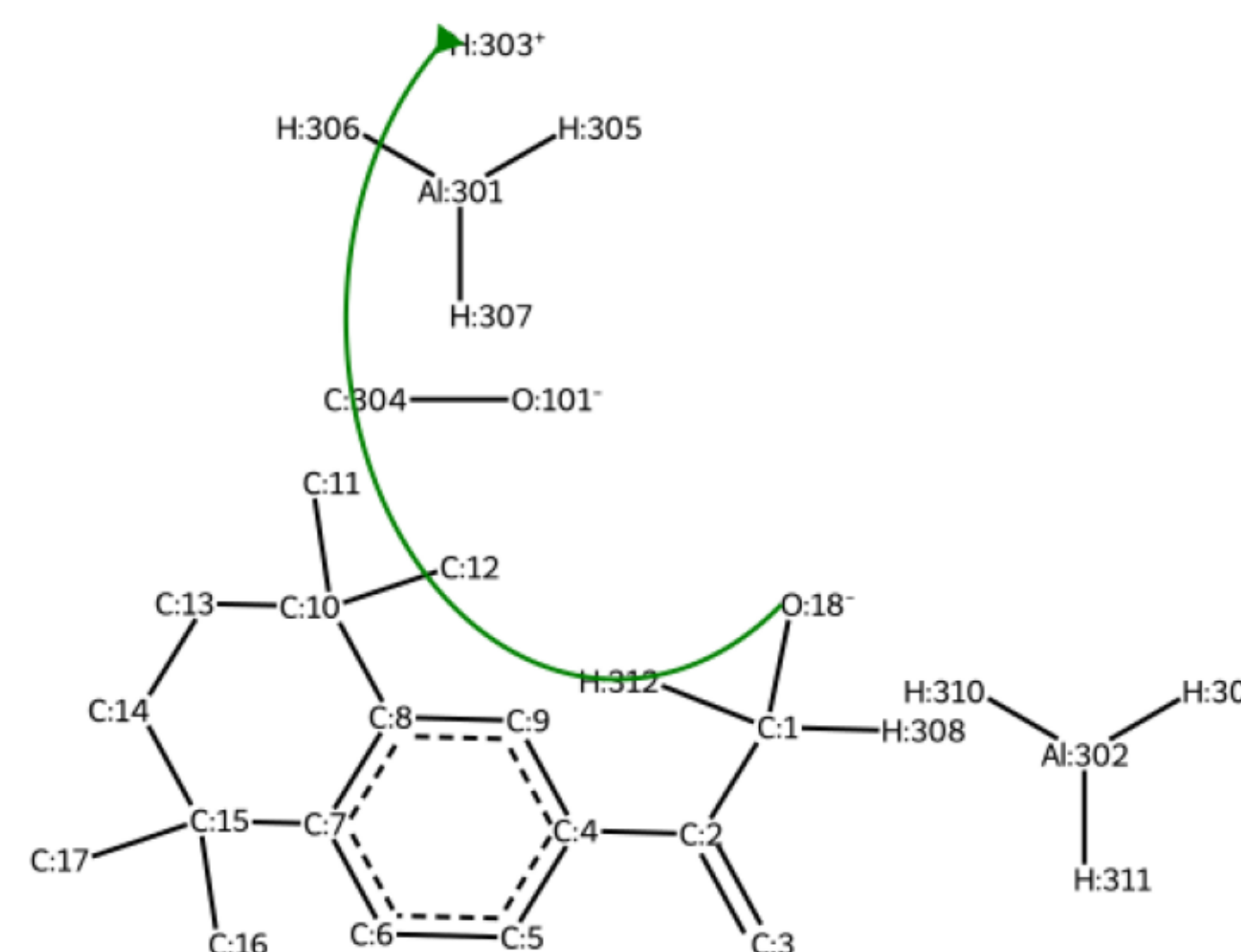
step #2



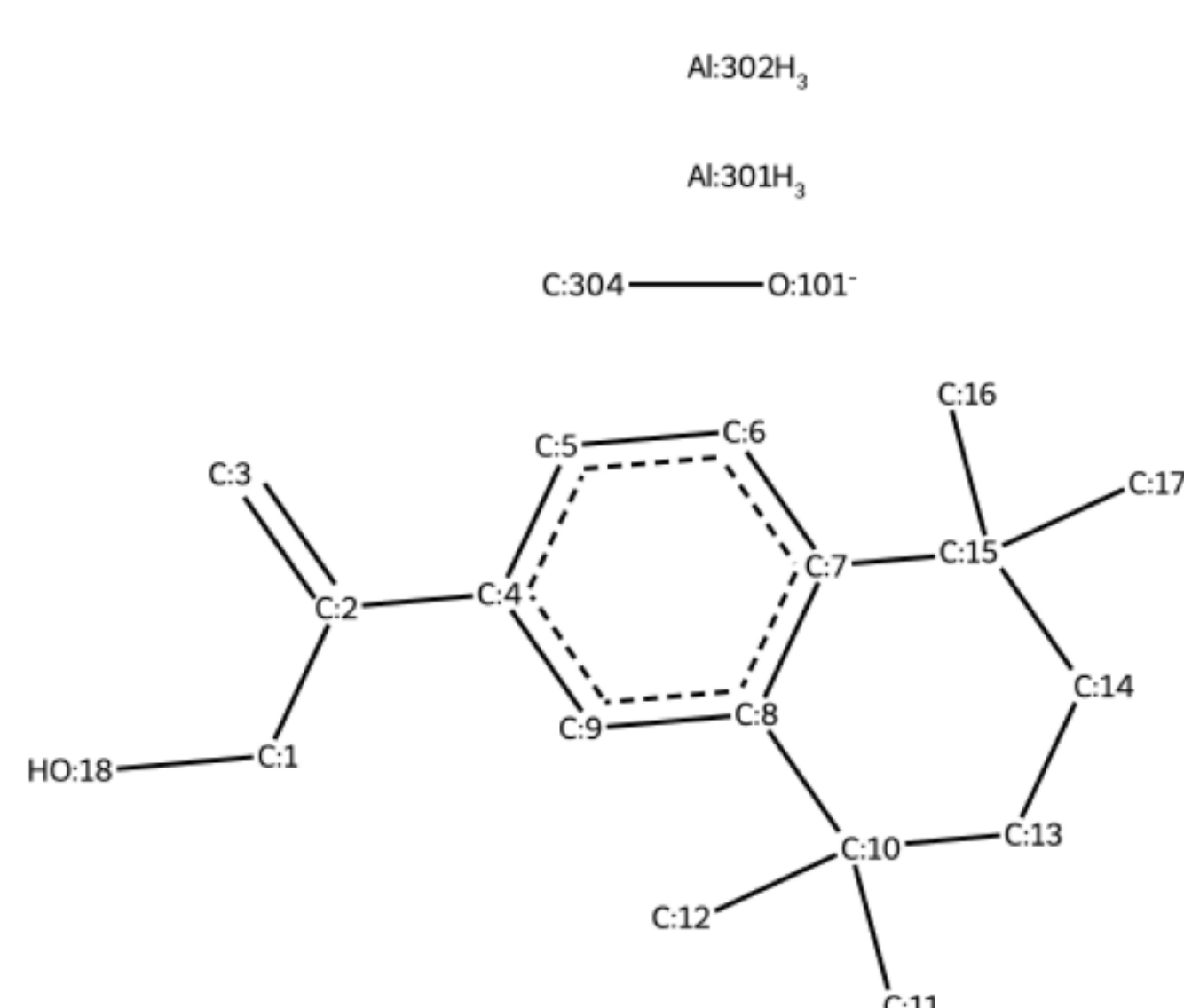
step #3



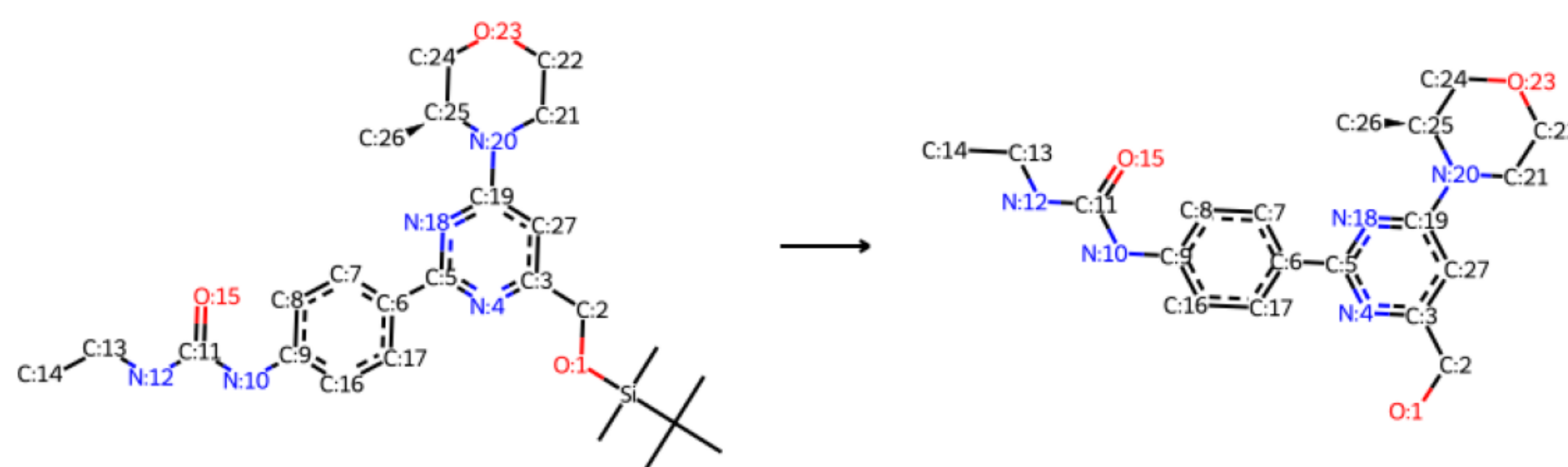
step #4



Product(s)

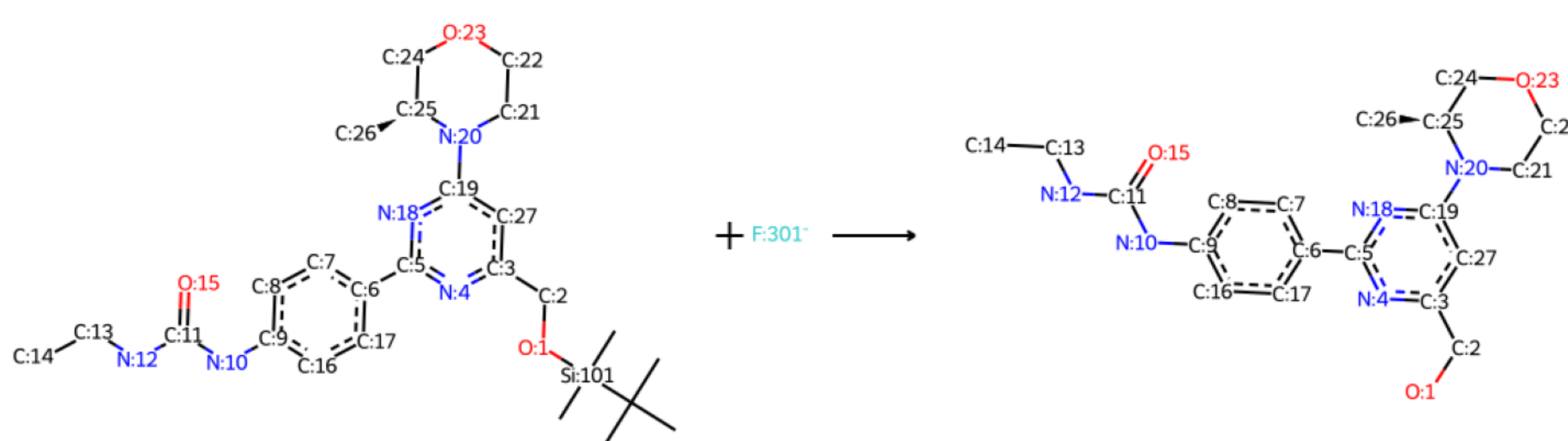


Original reaction sampled RXN_ID:31)



Identified mechanistic class -
SN2 reaction

Reaction with missing reagents recovered

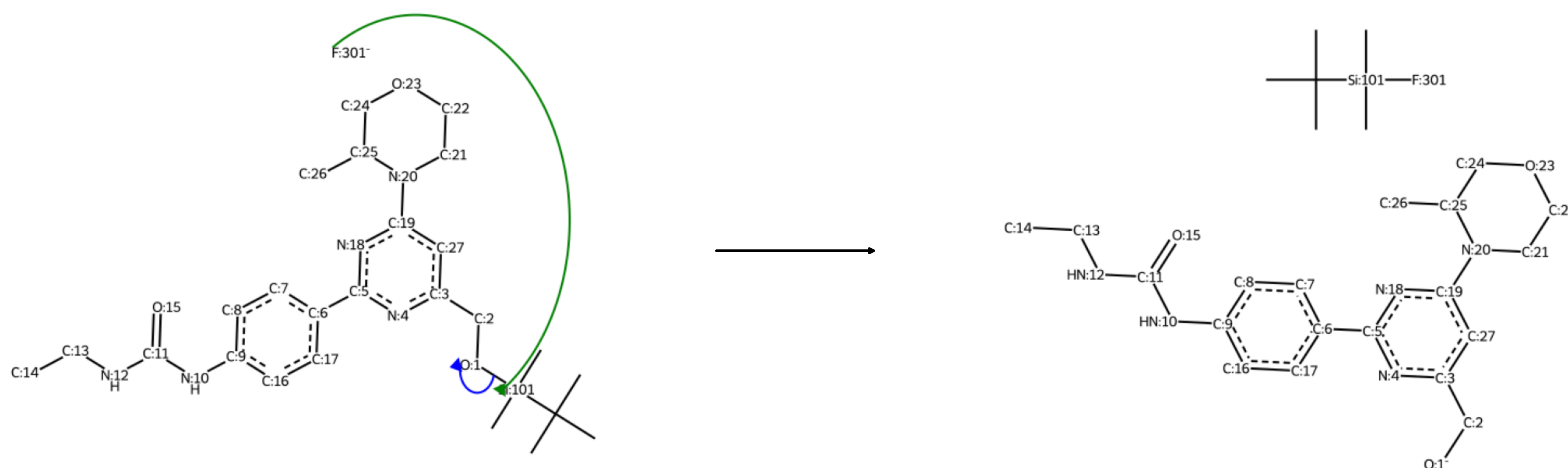


Proposed mechanistic pathway

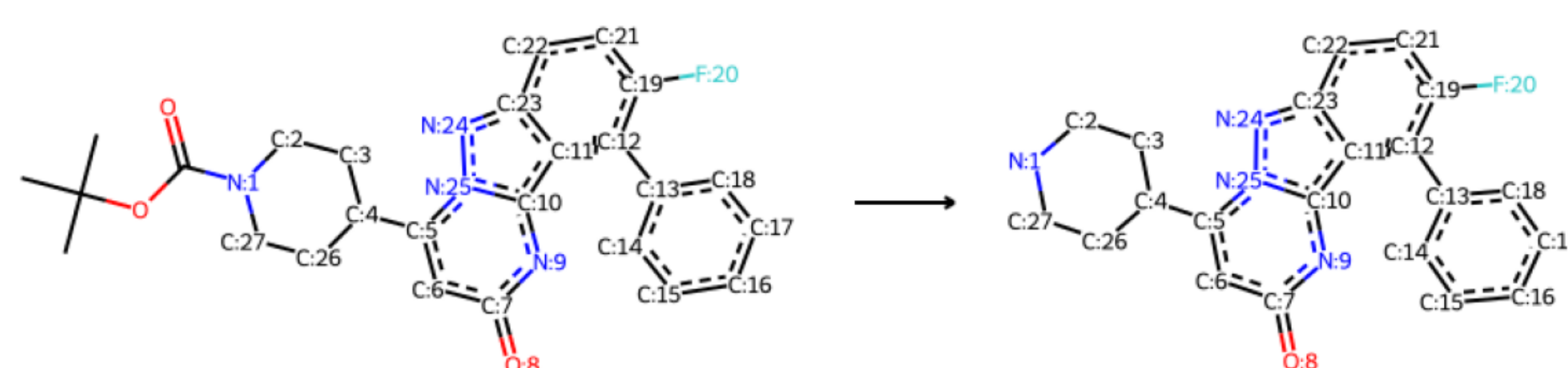
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)

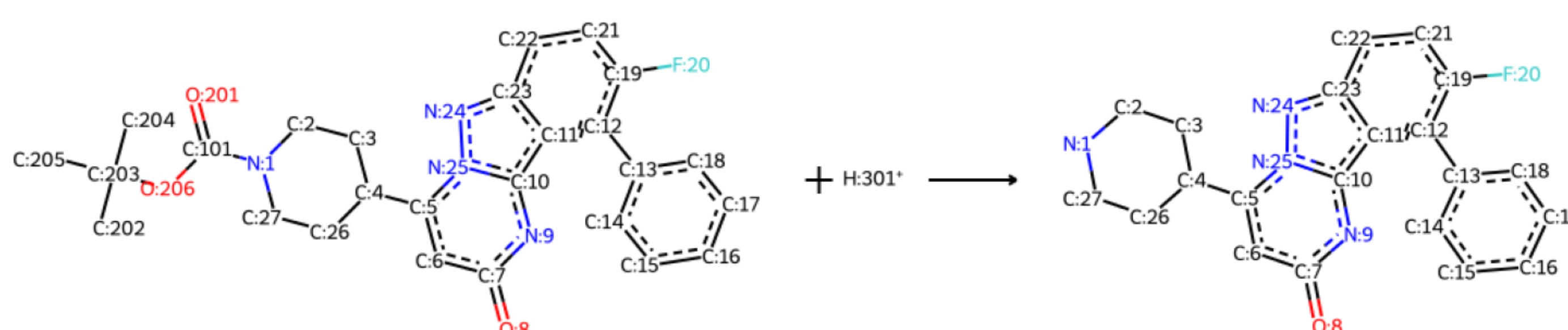


Original reaction
sampled RXN_ID:32)



Identified mechanistic class -
Boc_deprotection reaction

Reaction with missing reagents recovered

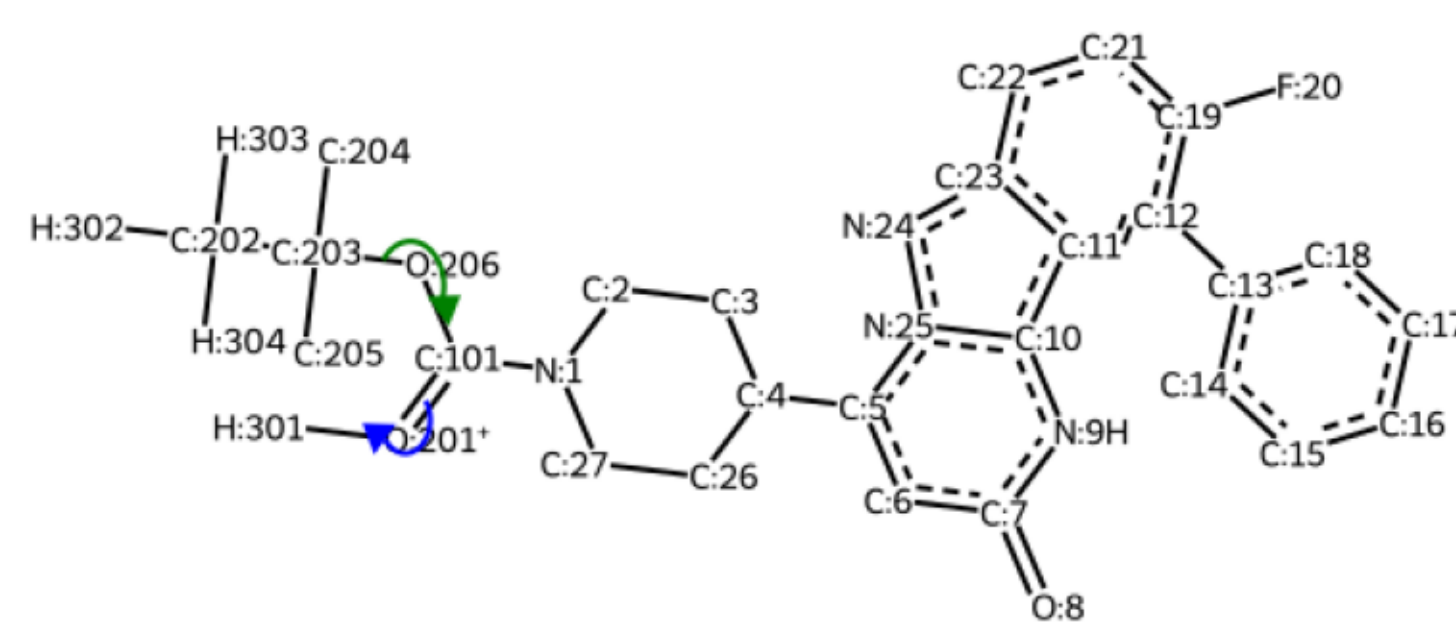
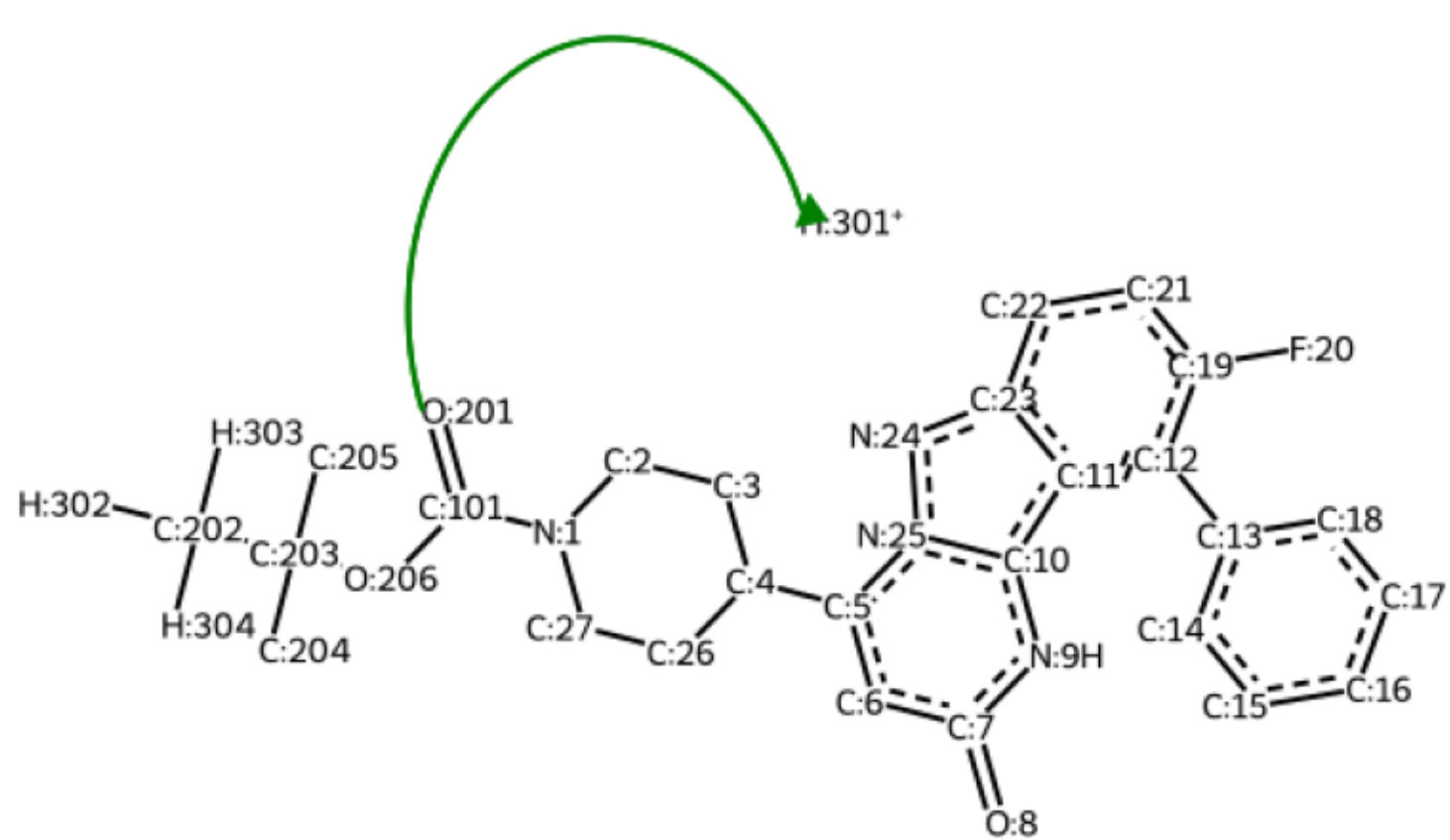


Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

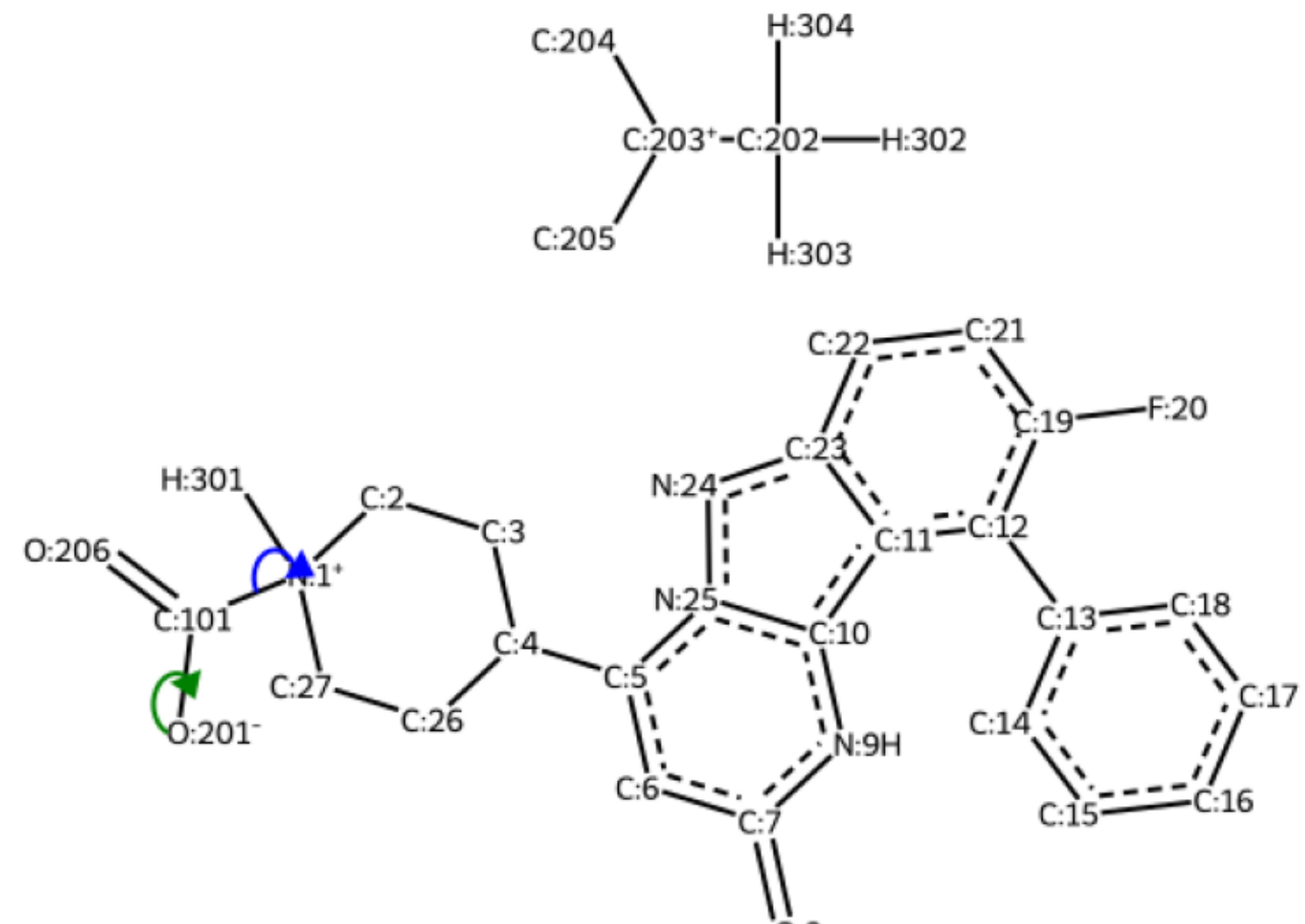
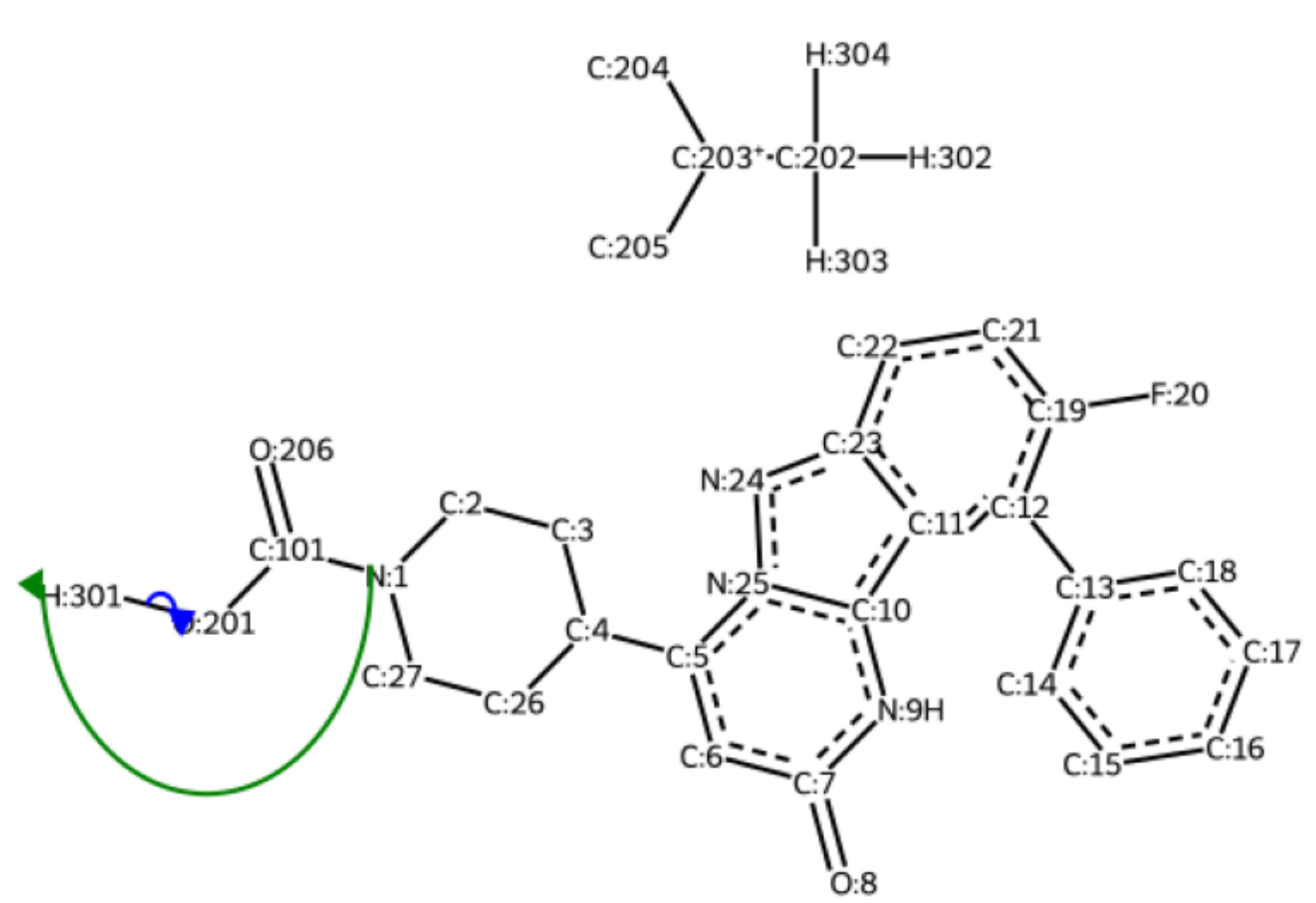
step #1

step #2



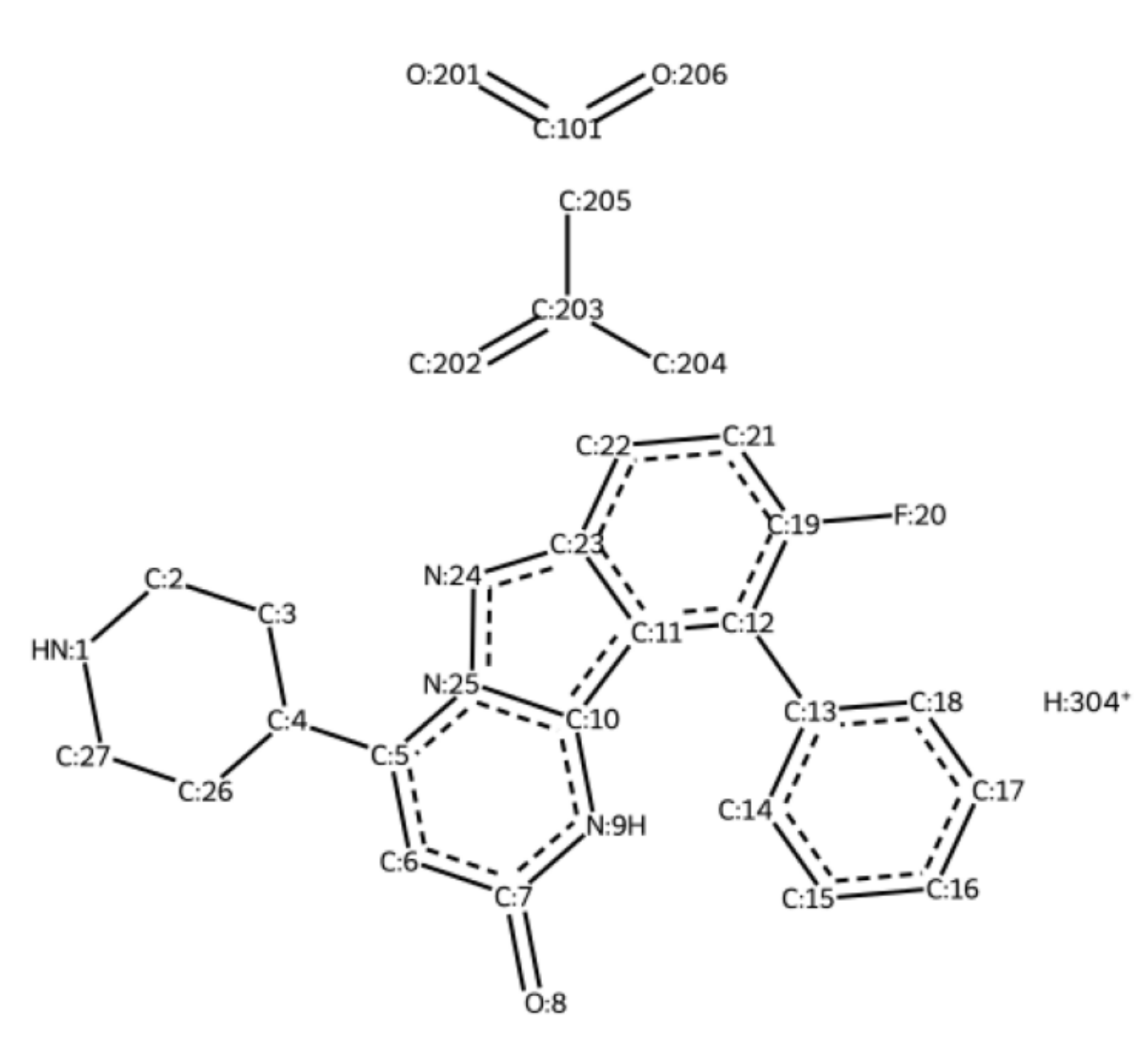
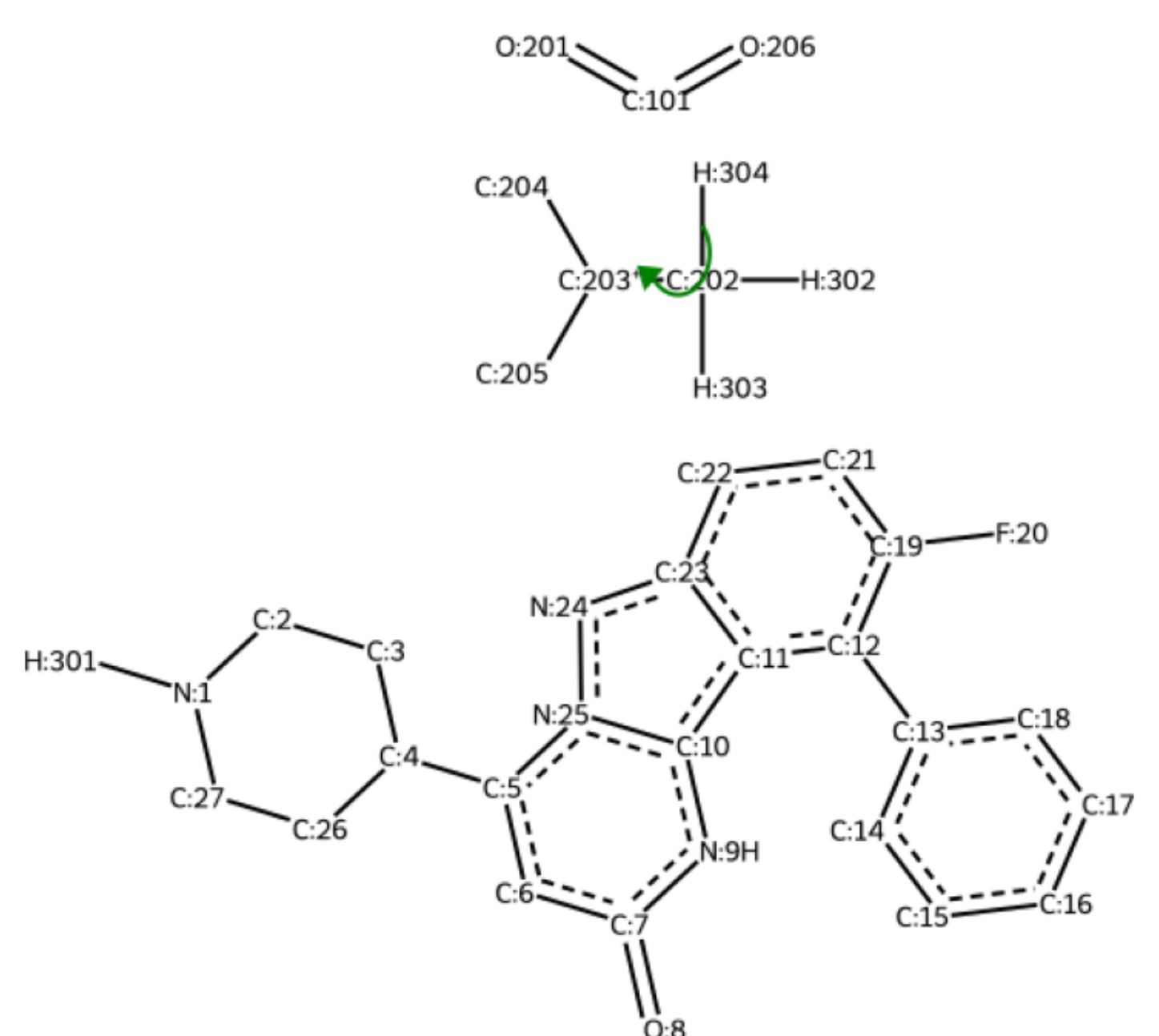
step #3

step #4

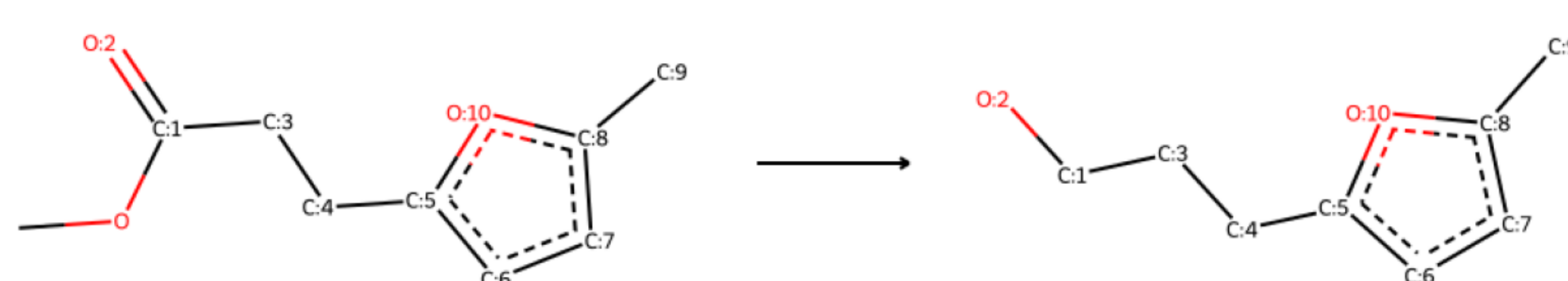


step #5

Product(s)

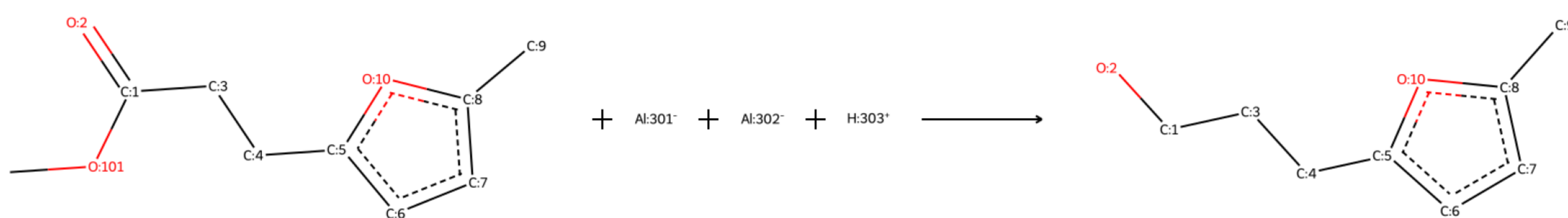


Original reaction
sampled RXN_ID:33)



Identified mechanistic class -
ester_reduction reaction

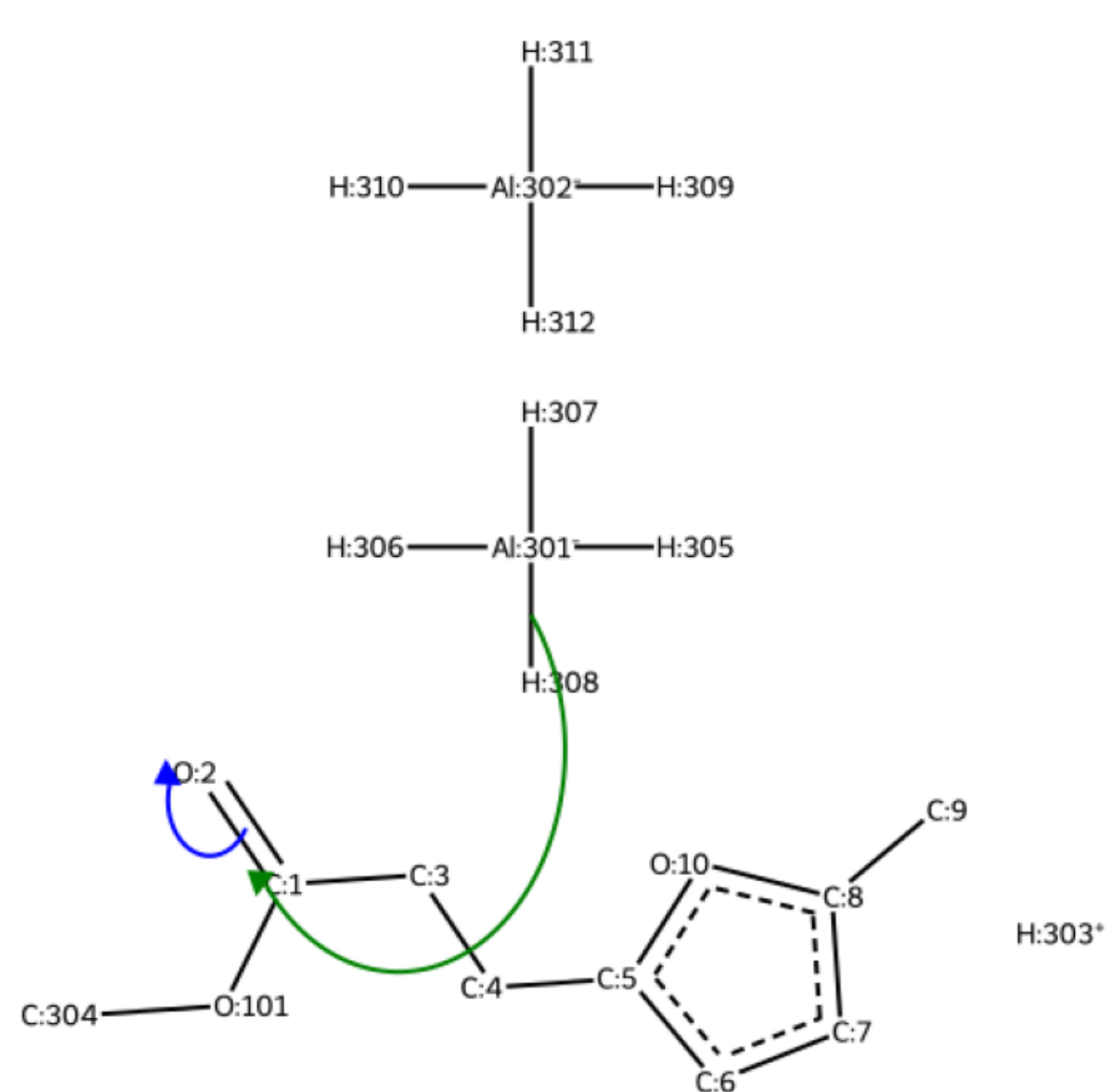
Reaction with missing reagents recovered



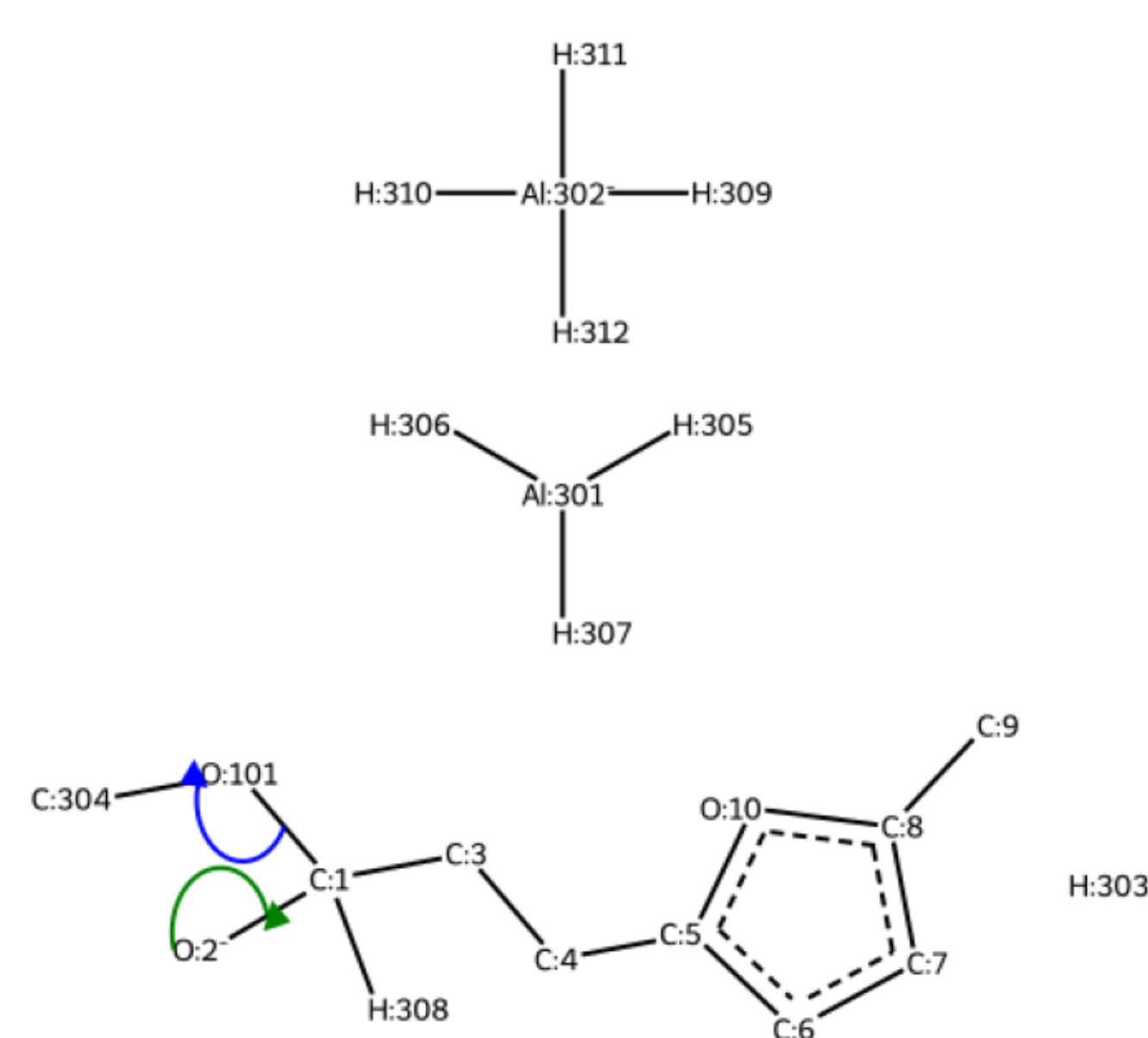
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

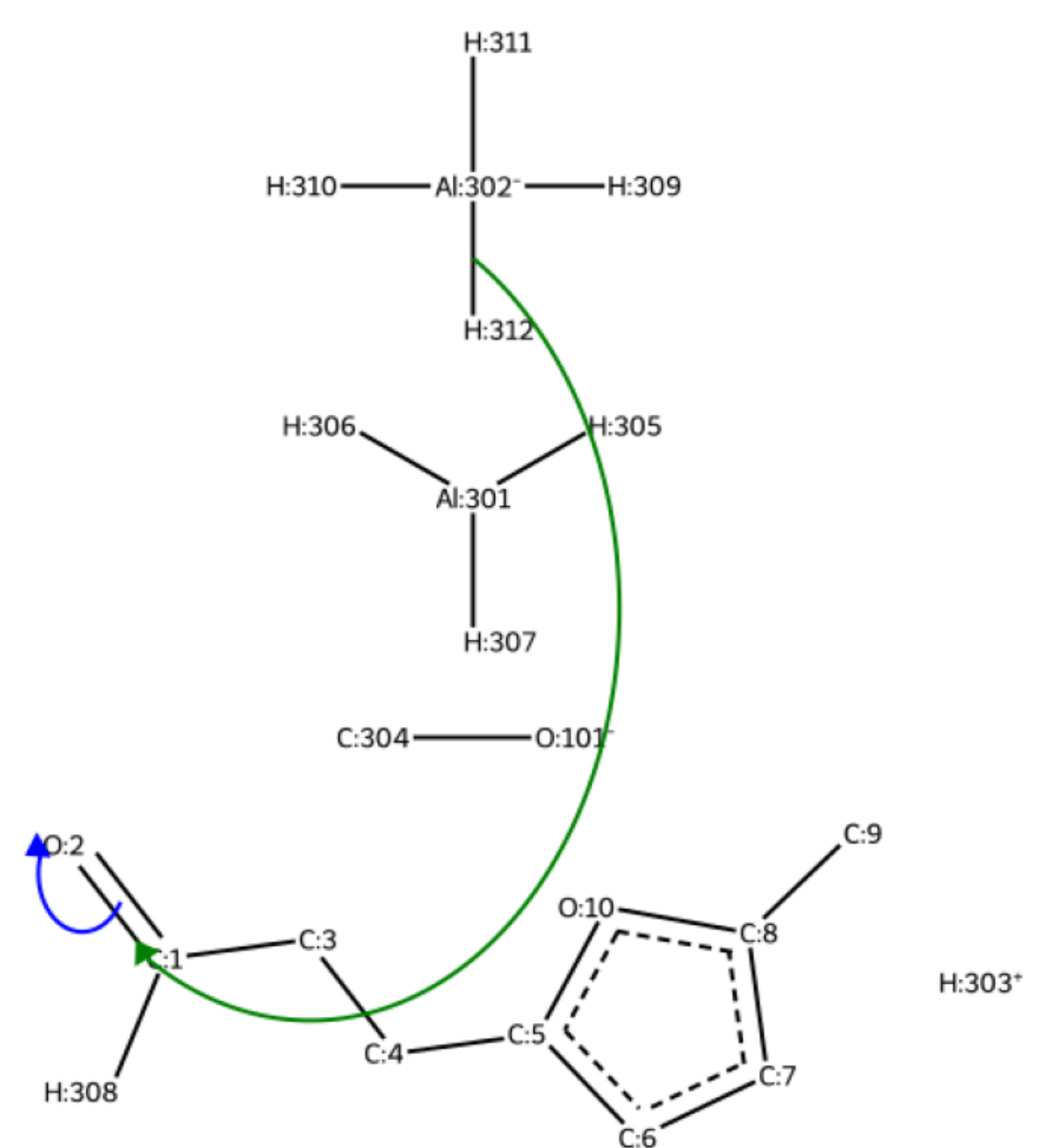
step #1



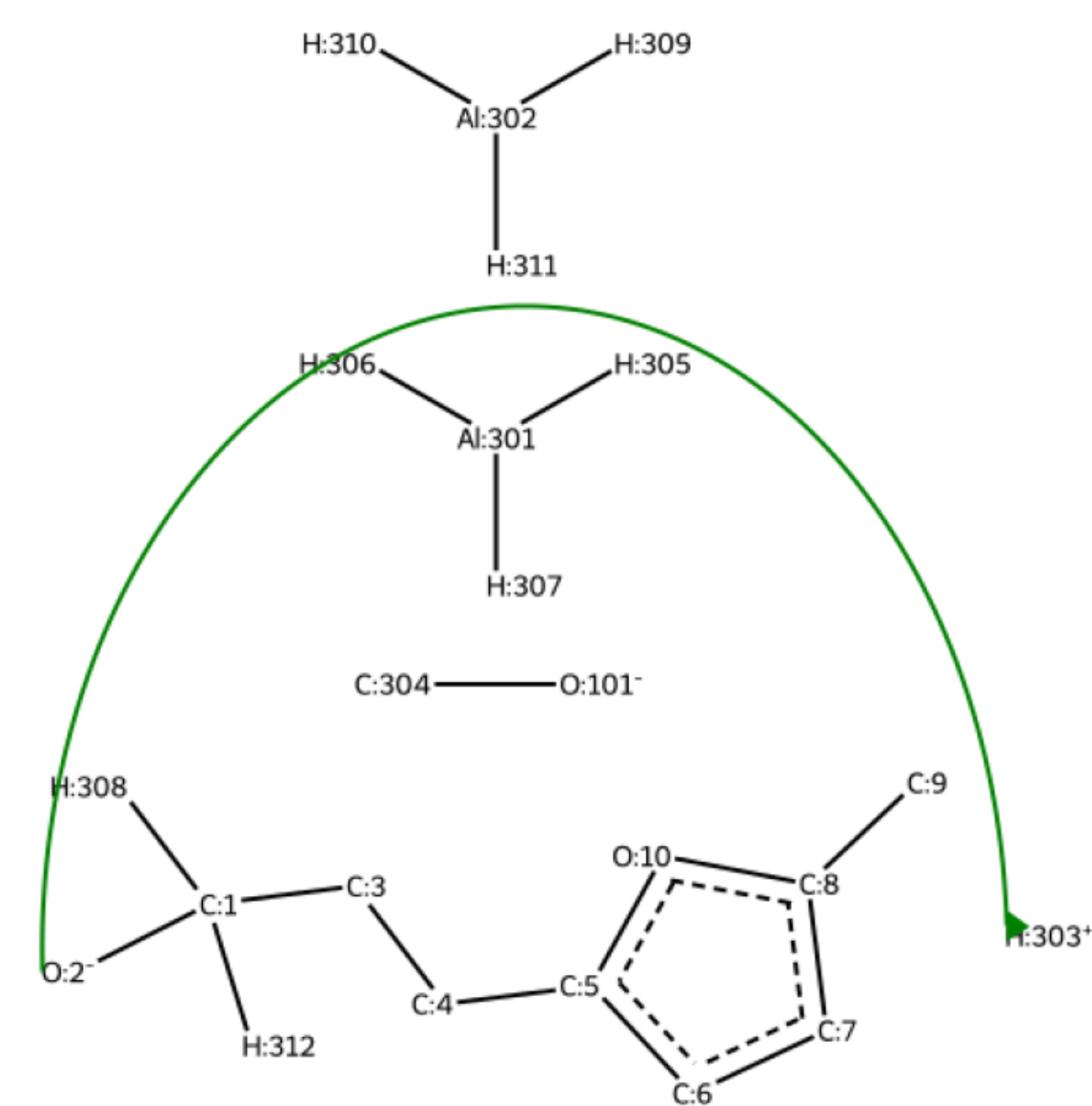
step #2



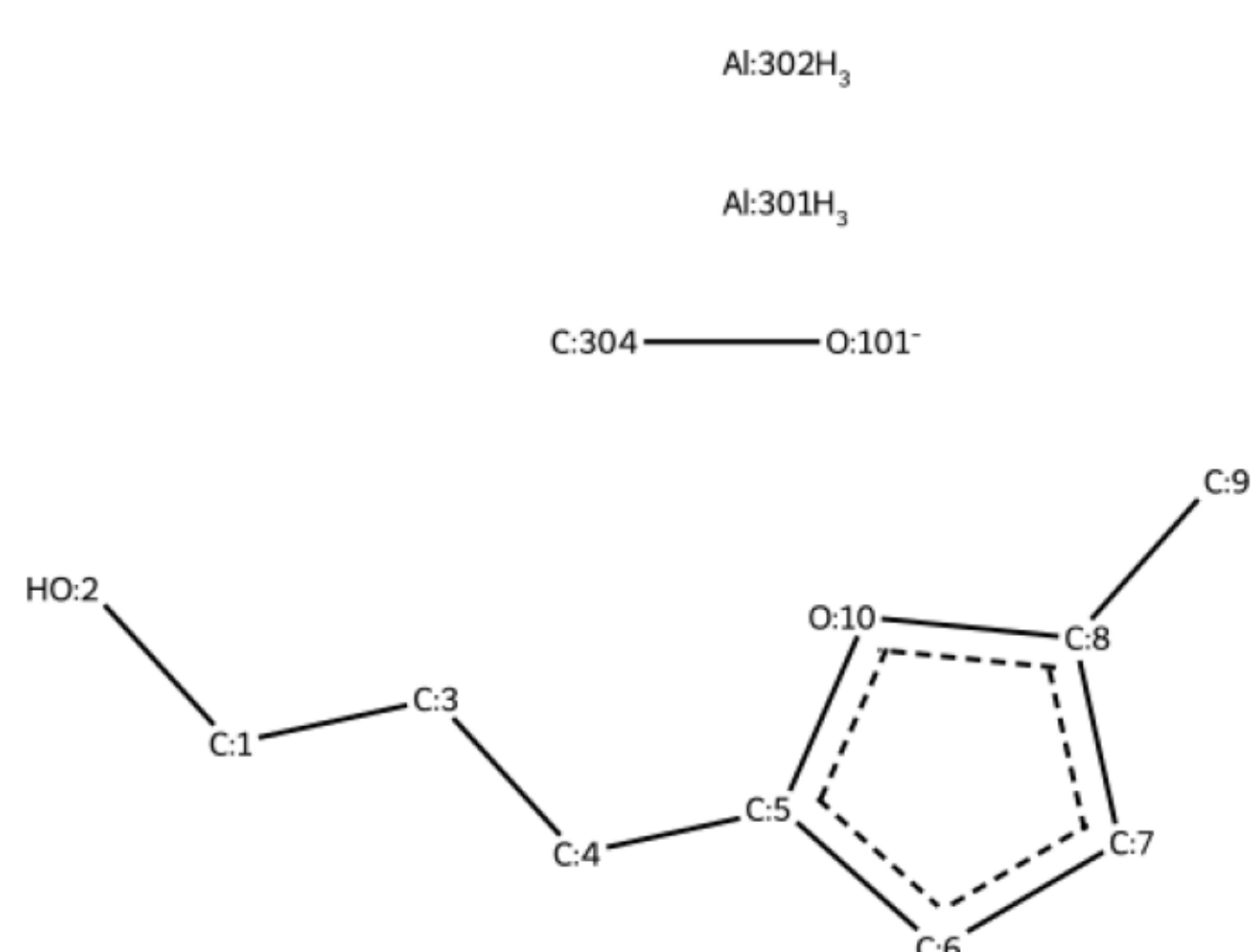
step #3



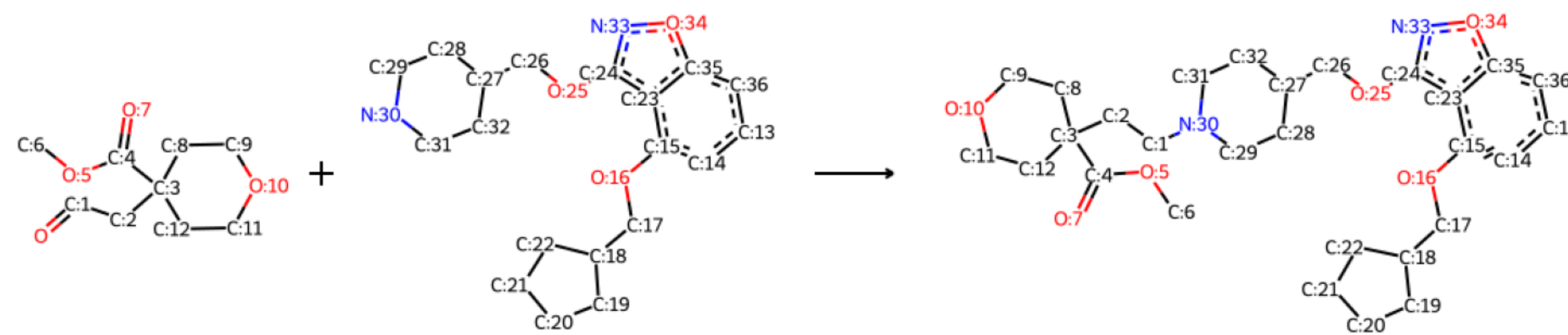
step #4



Product(s)

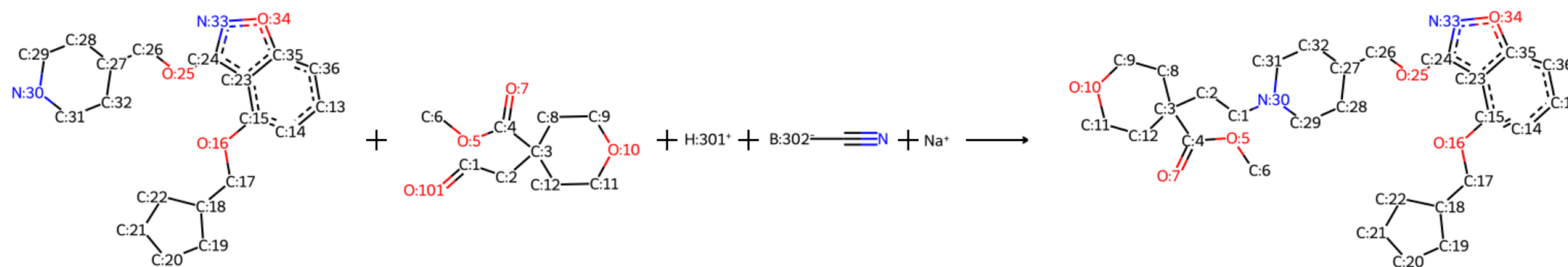


Original reaction
sampled RXN_ID:34)



Identified mechanistic class -
reductive_amination reaction

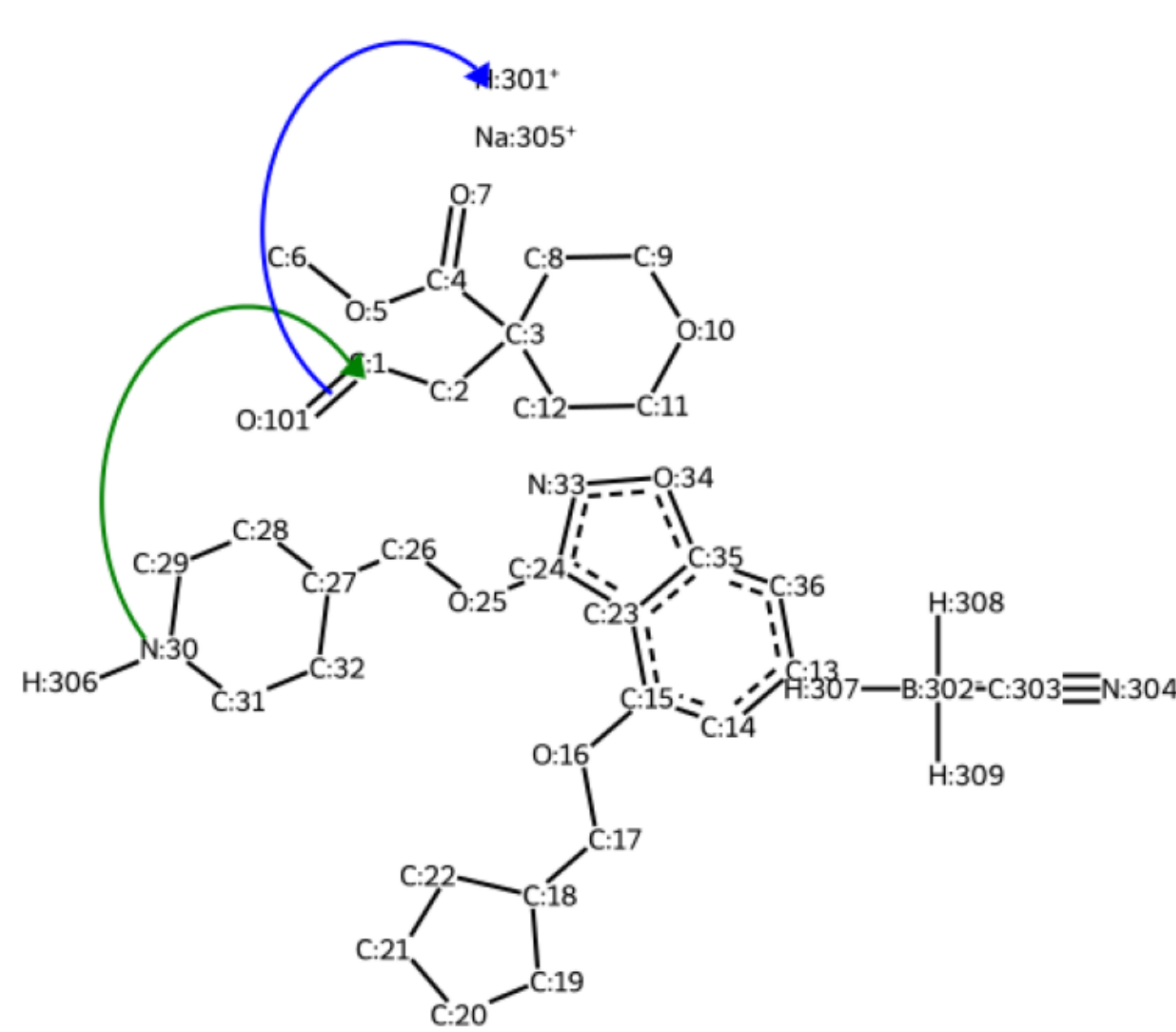
Reaction with missing reagents recovered



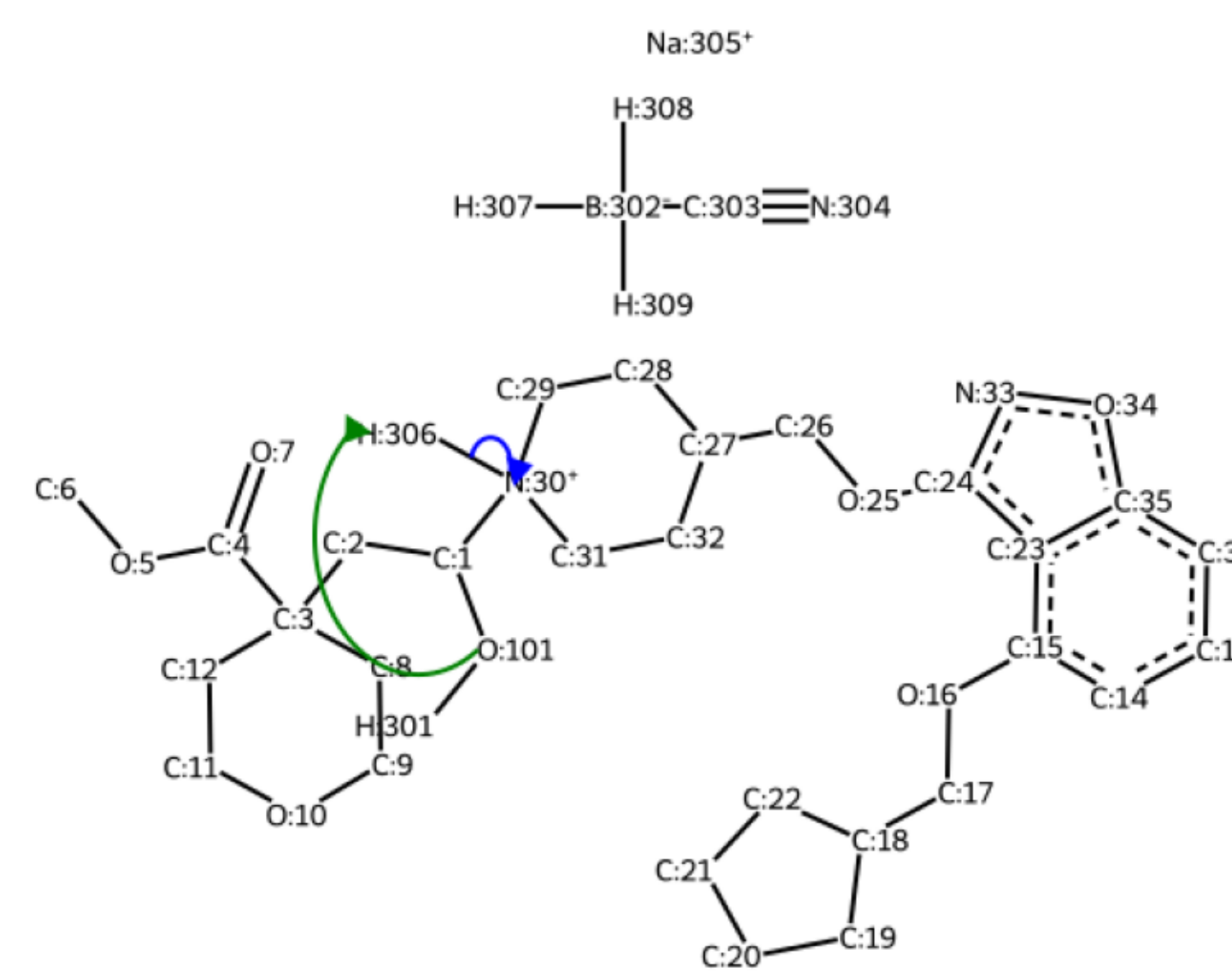
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

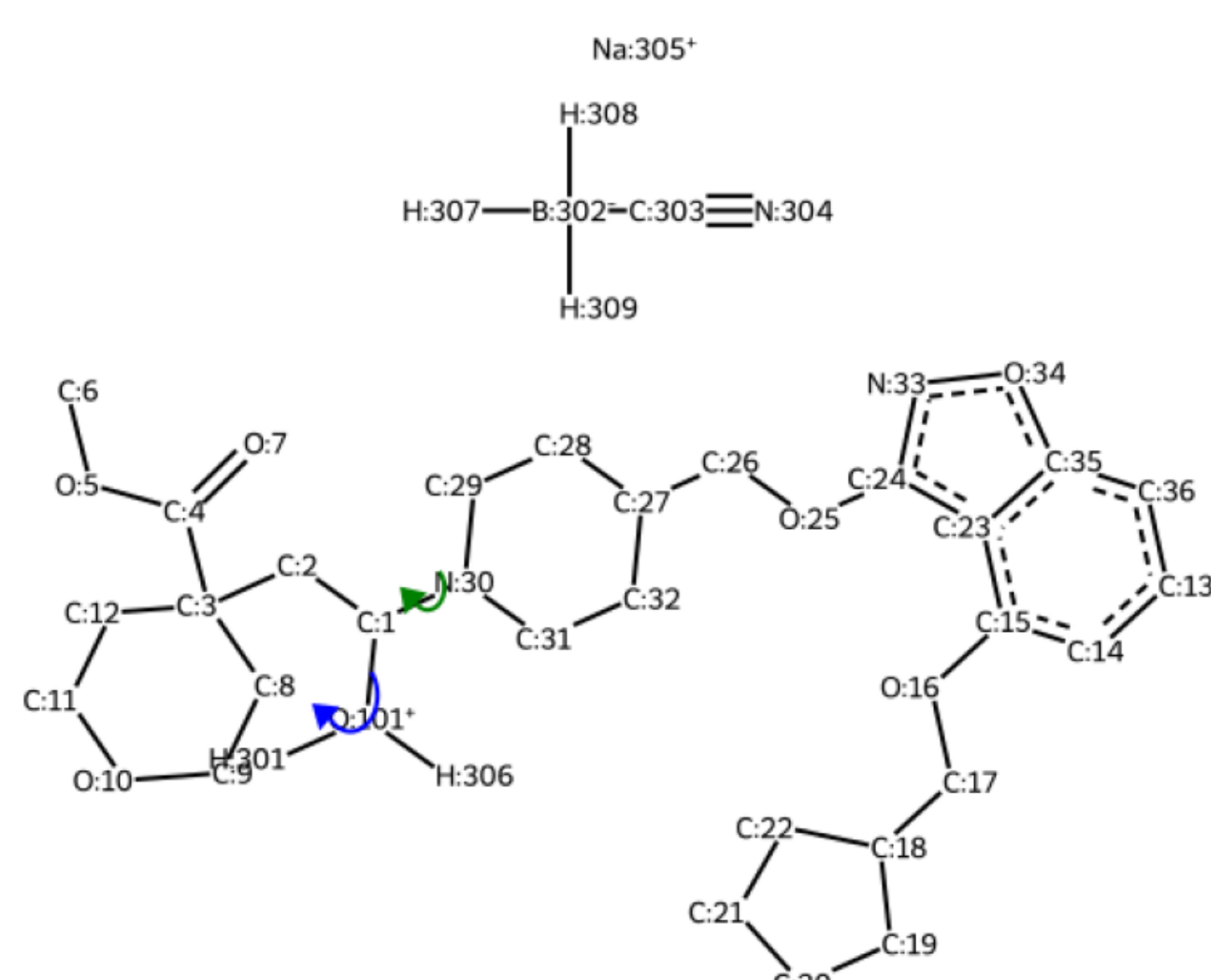
step #1



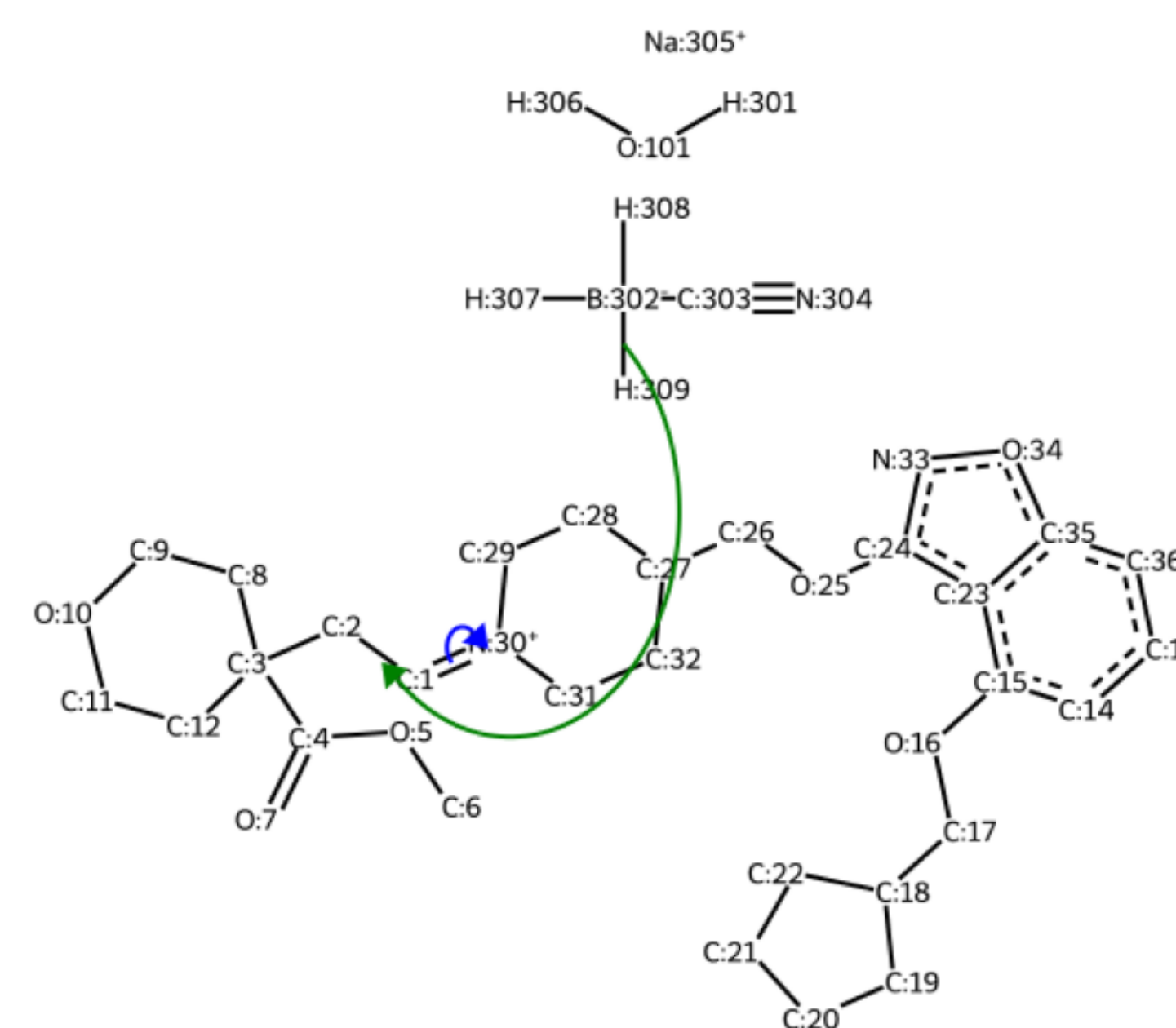
step #2



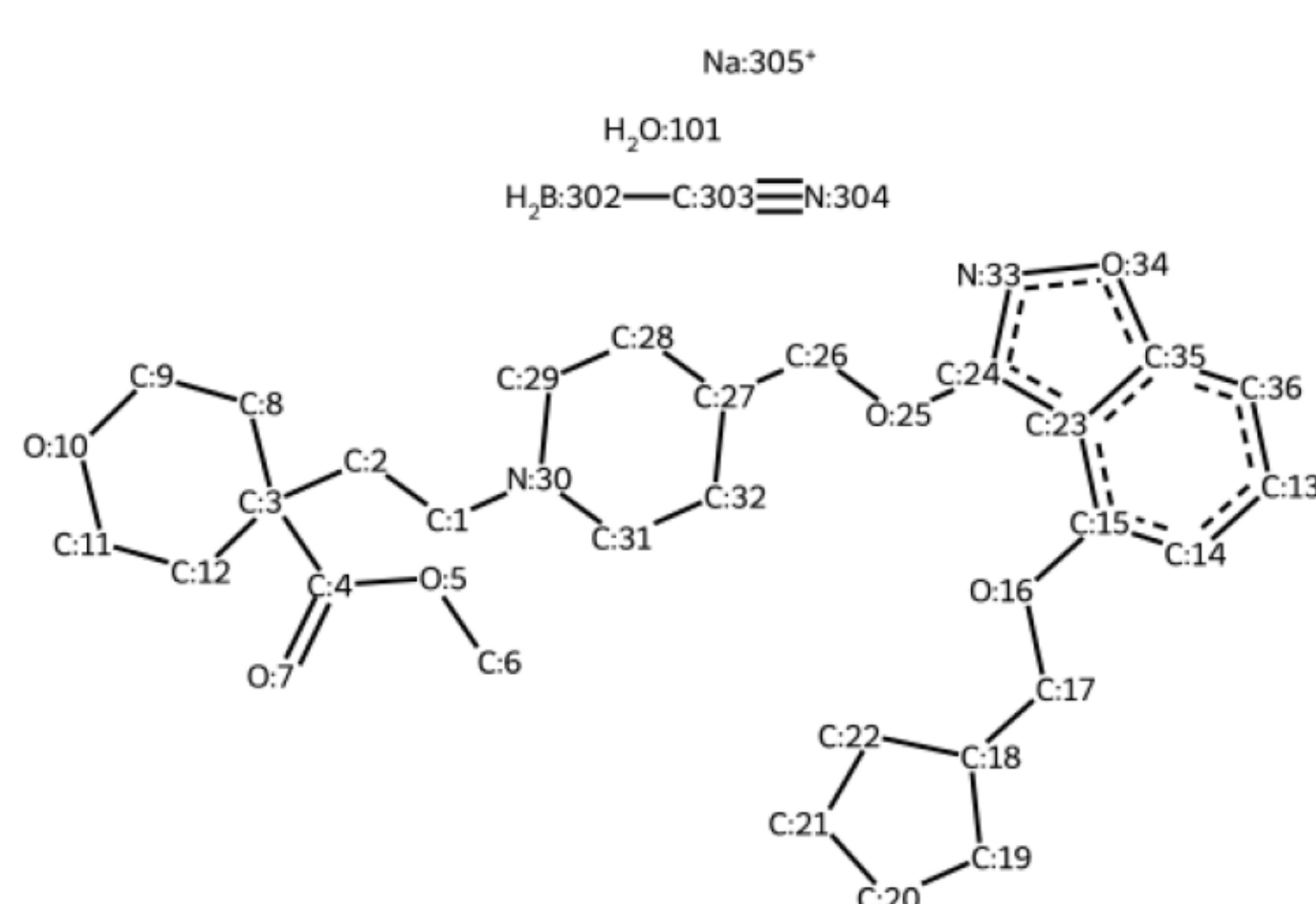
step #3



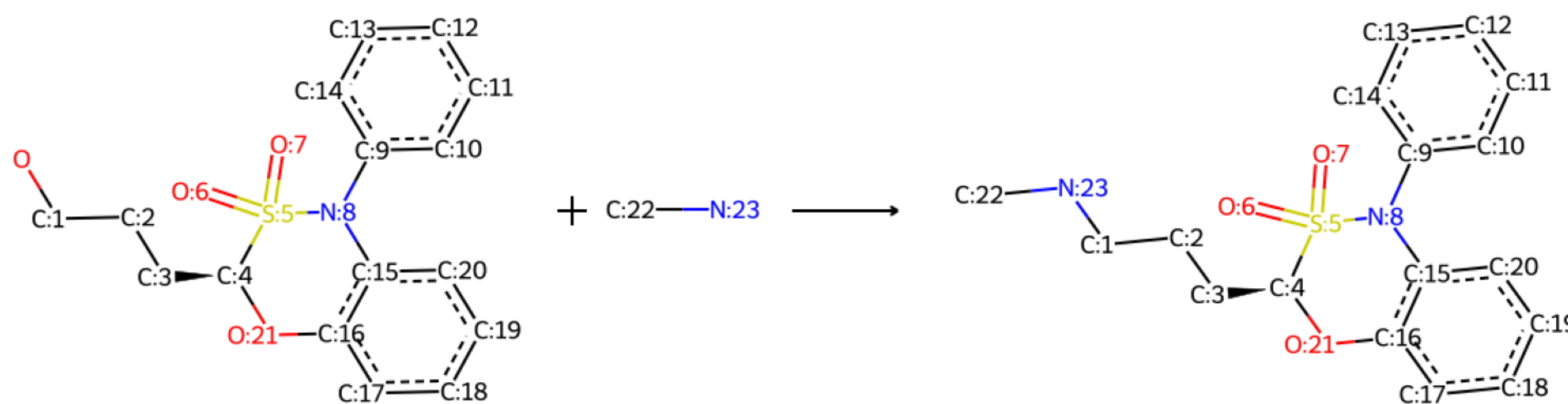
step #4



Product(s)

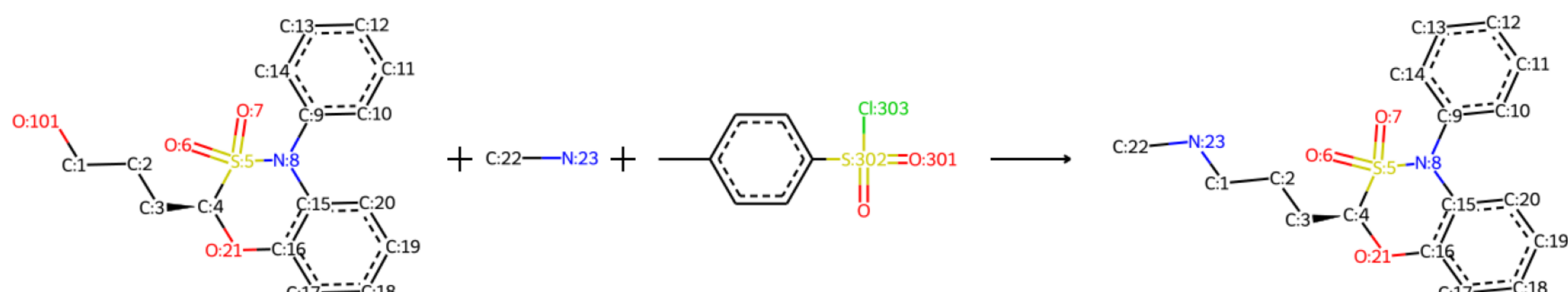


Original reaction
sampled RXN_ID:35)



Identified mechanistic class -
SN2_with_tosylate reaction

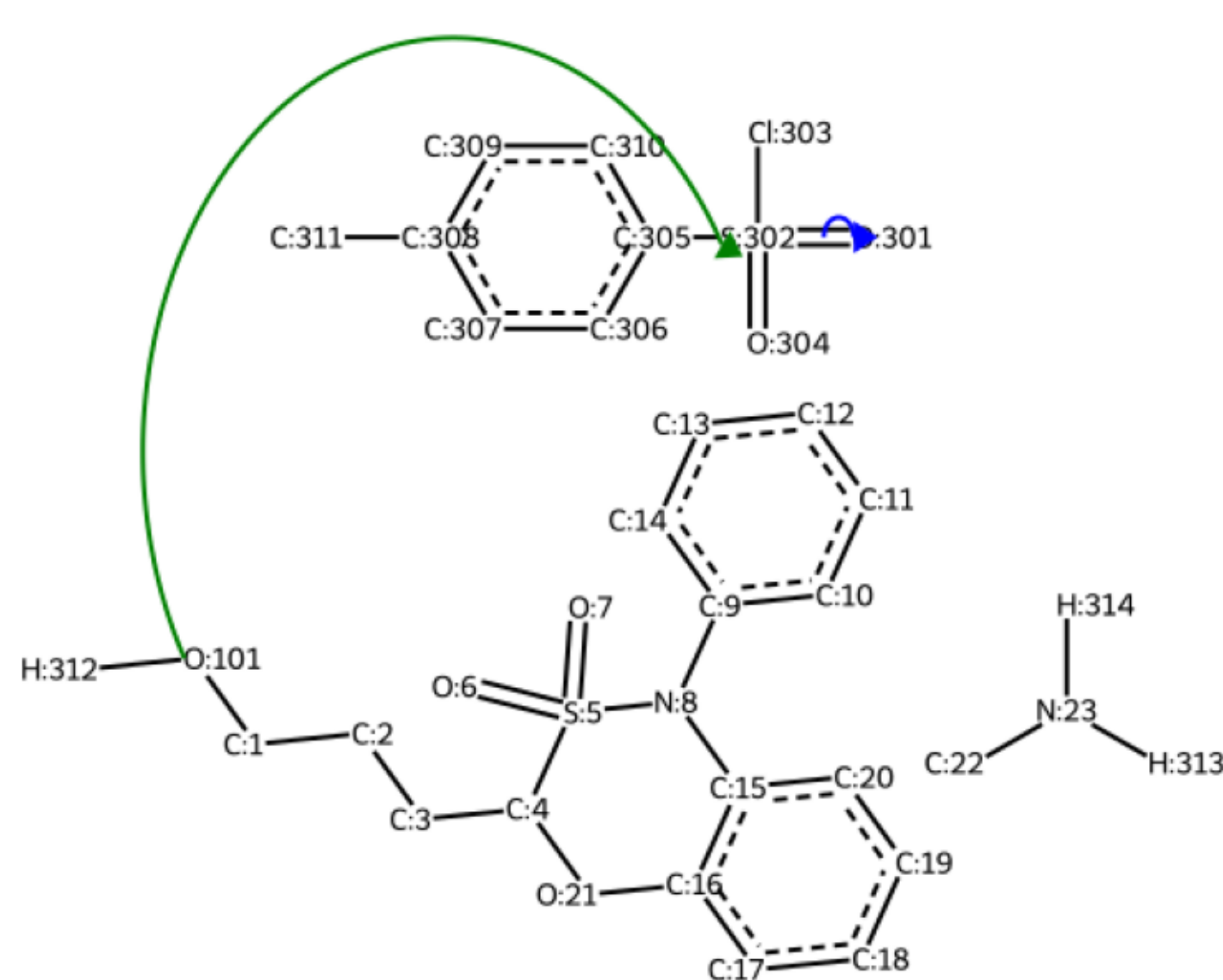
Reaction with missing reagents recovered



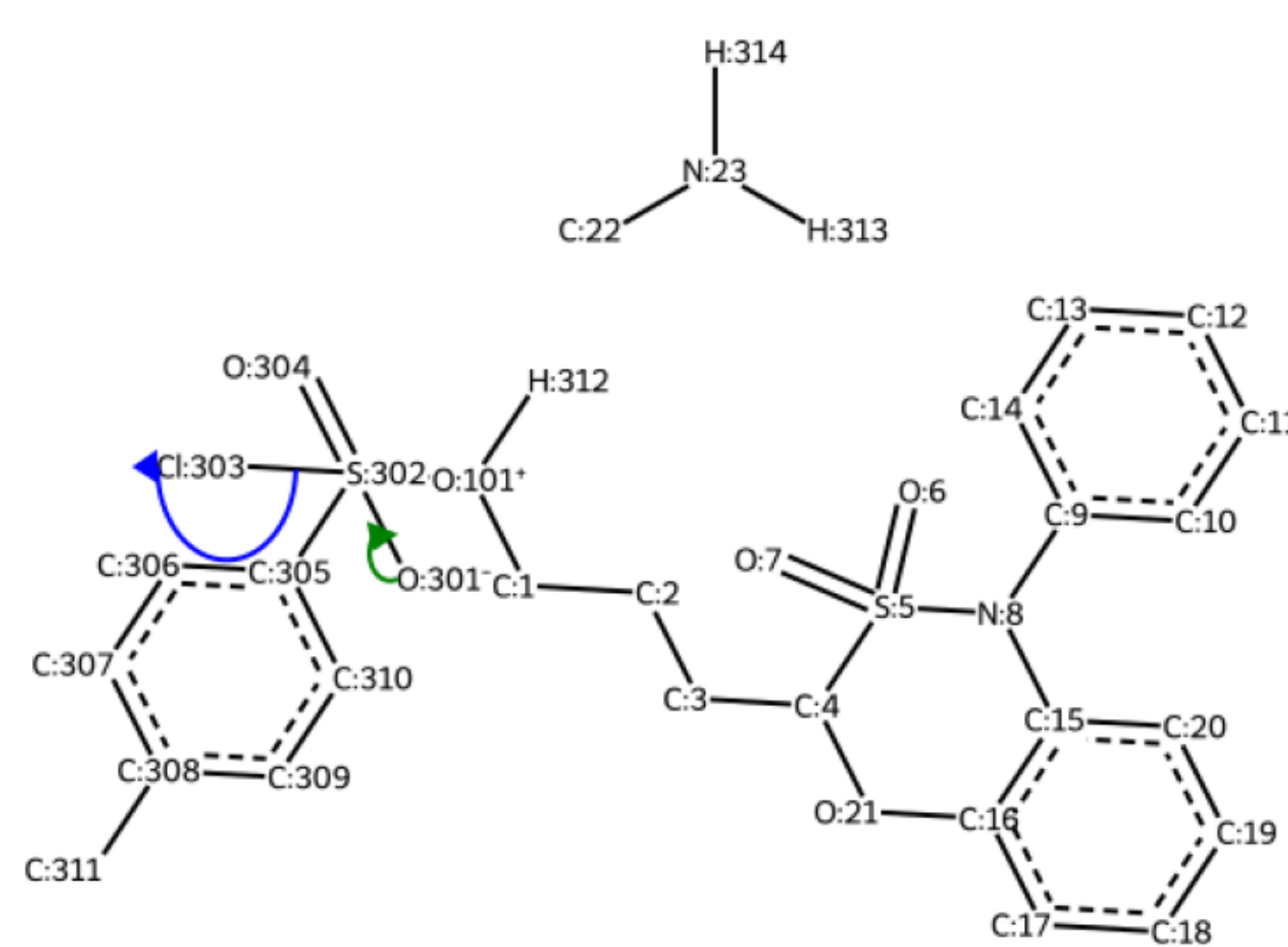
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

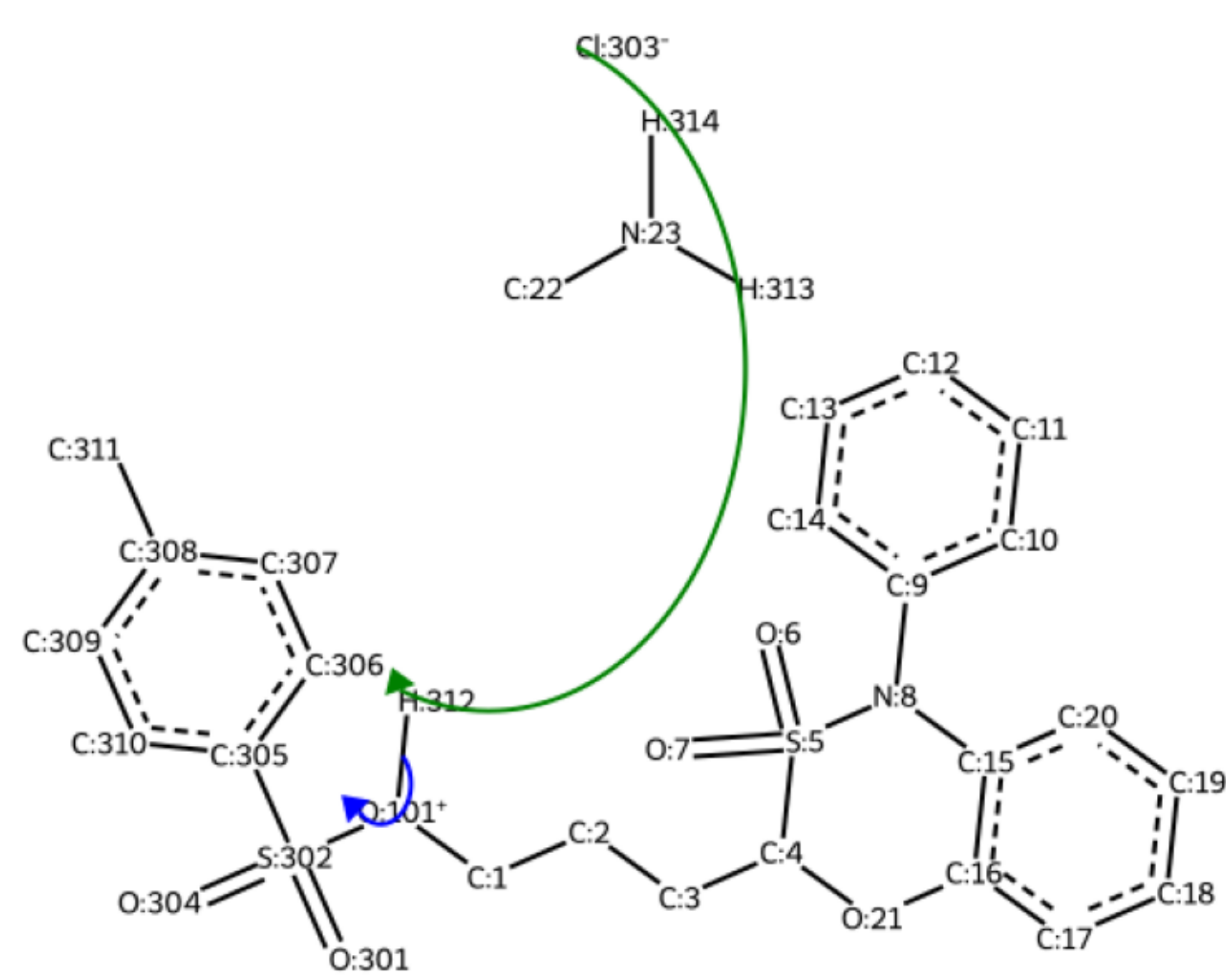
step #1



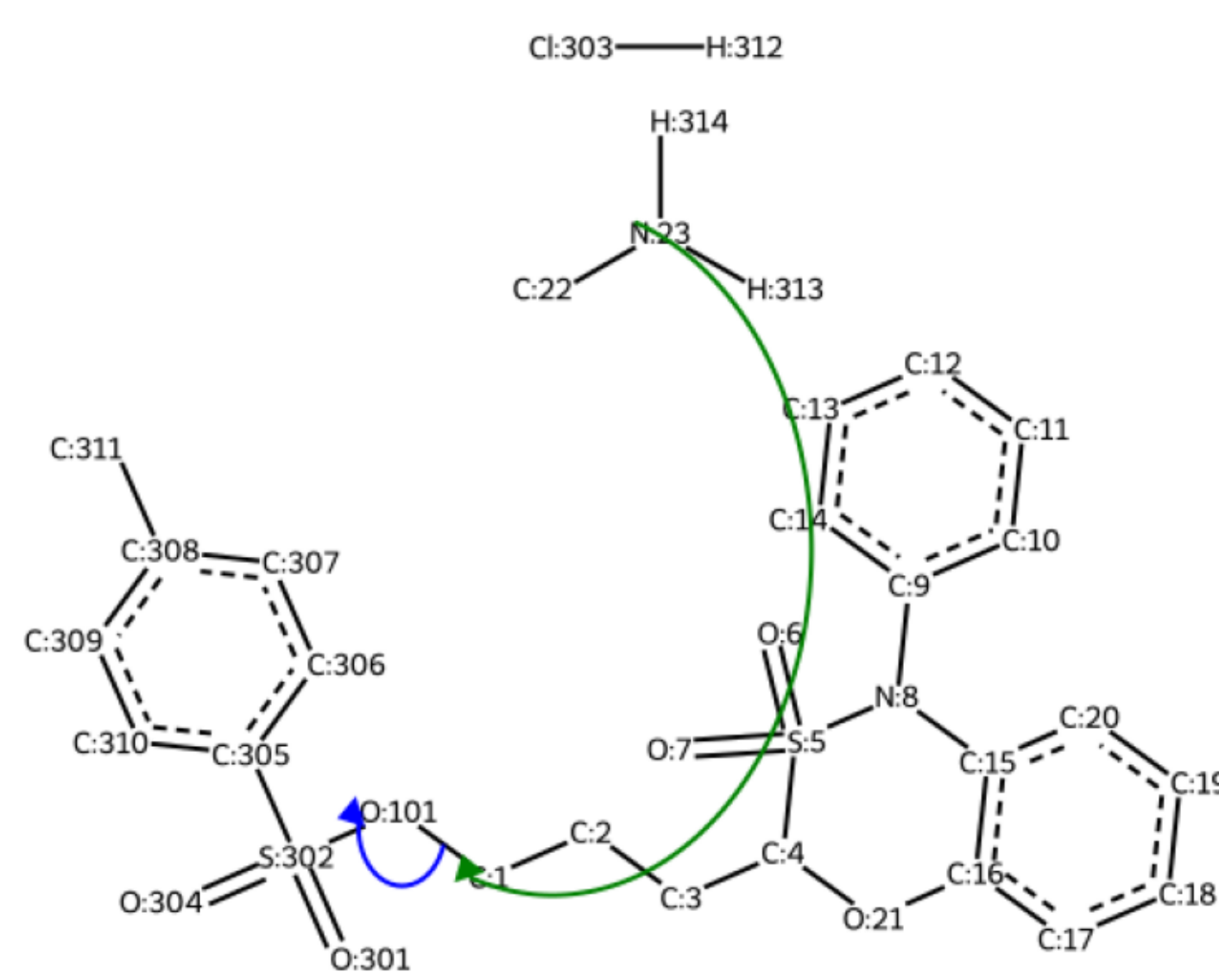
step #2



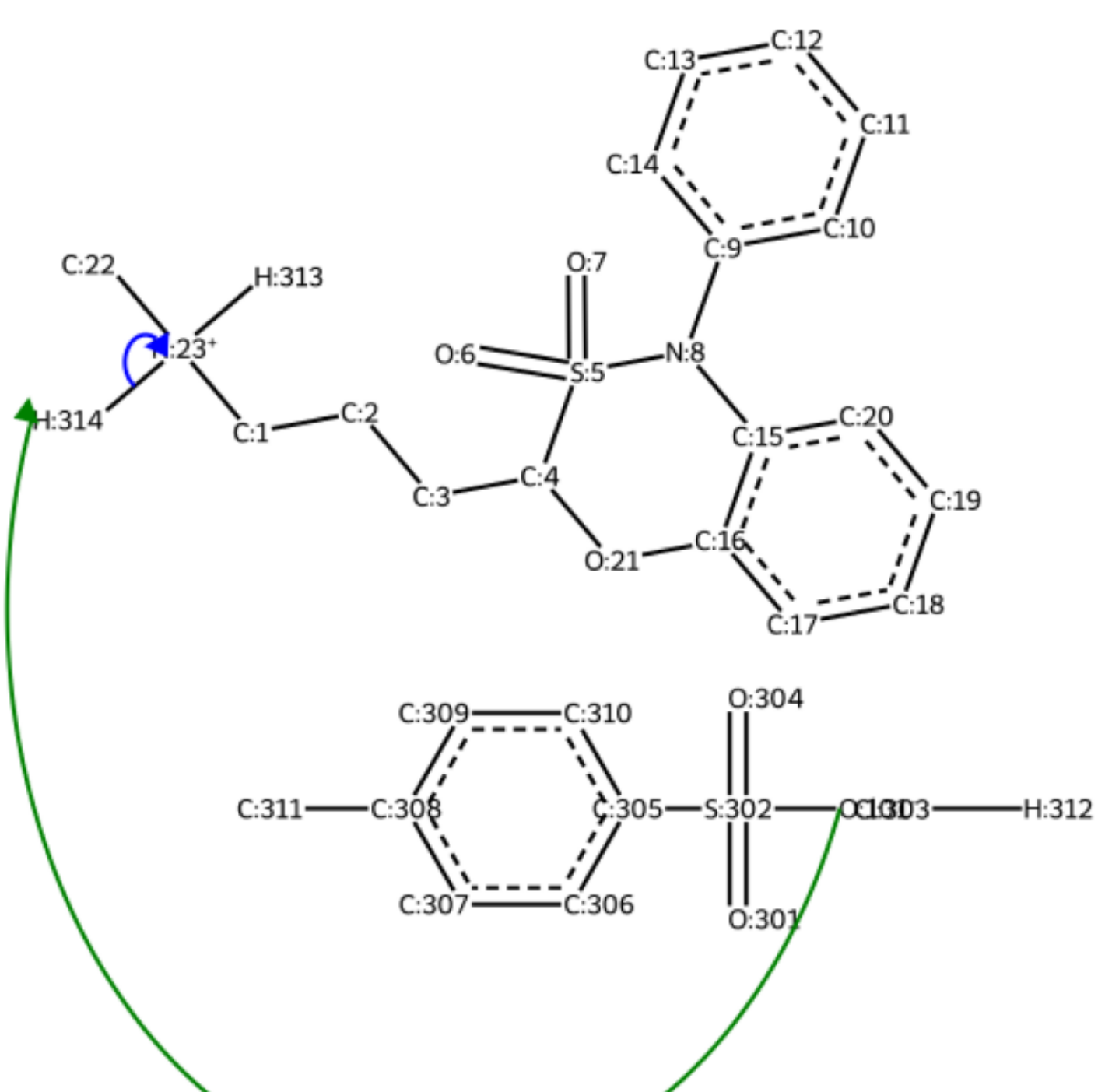
step #3



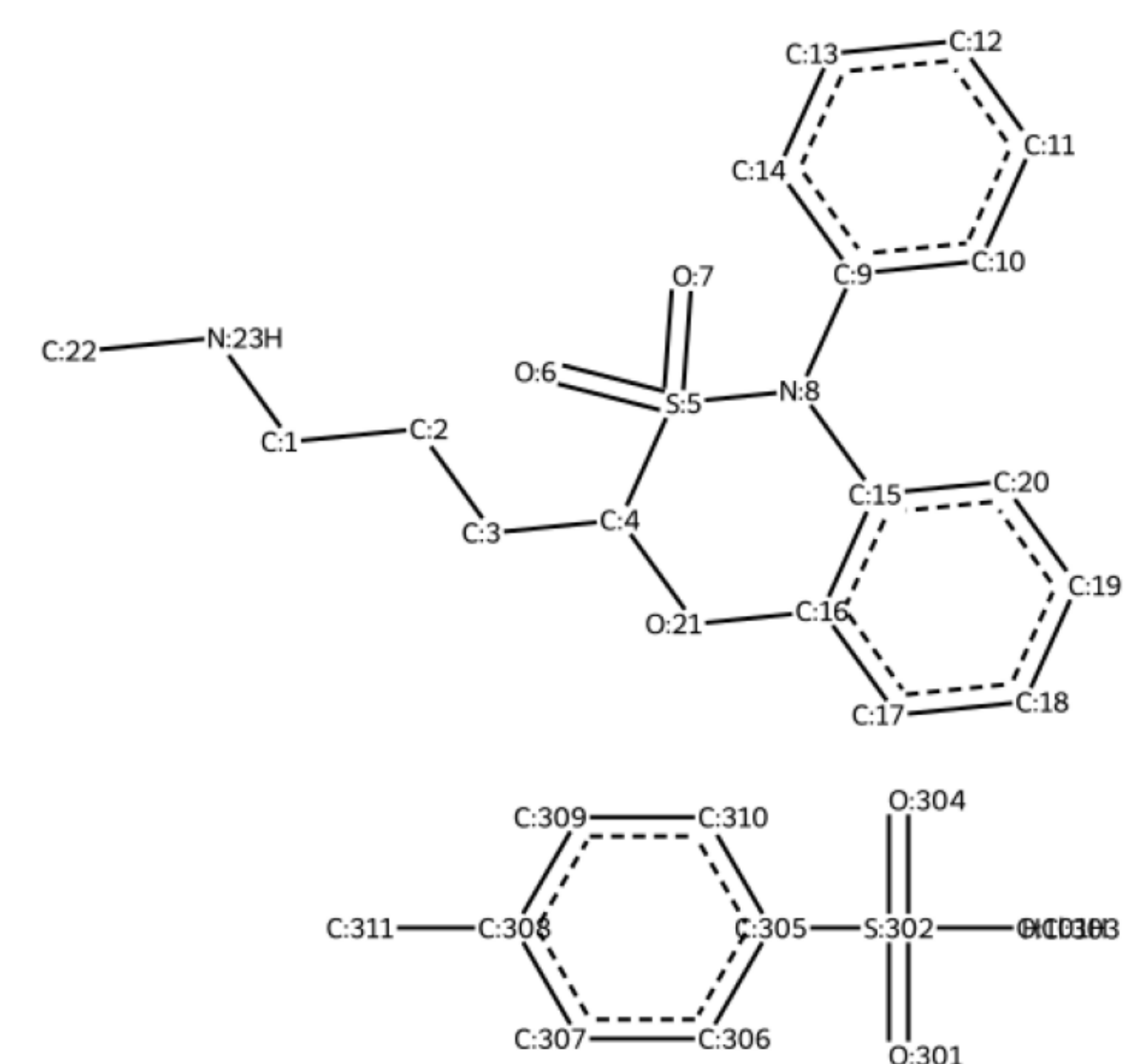
step #4



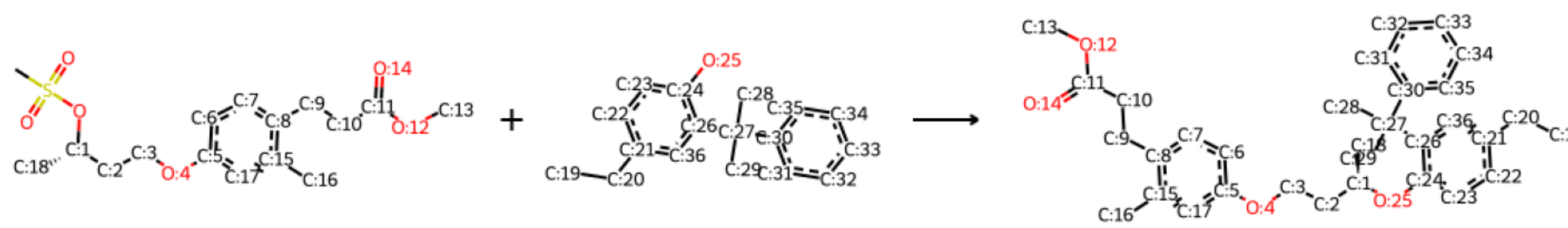
step #5



Product(s)

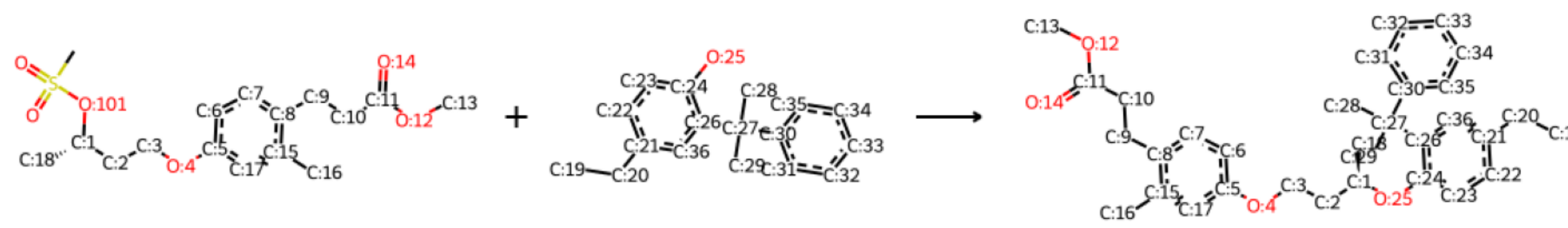


Original reaction
sampled RXN_ID:36)



Identified mechanistic class -
SN1 reaction

Reaction with missing reagents recovered

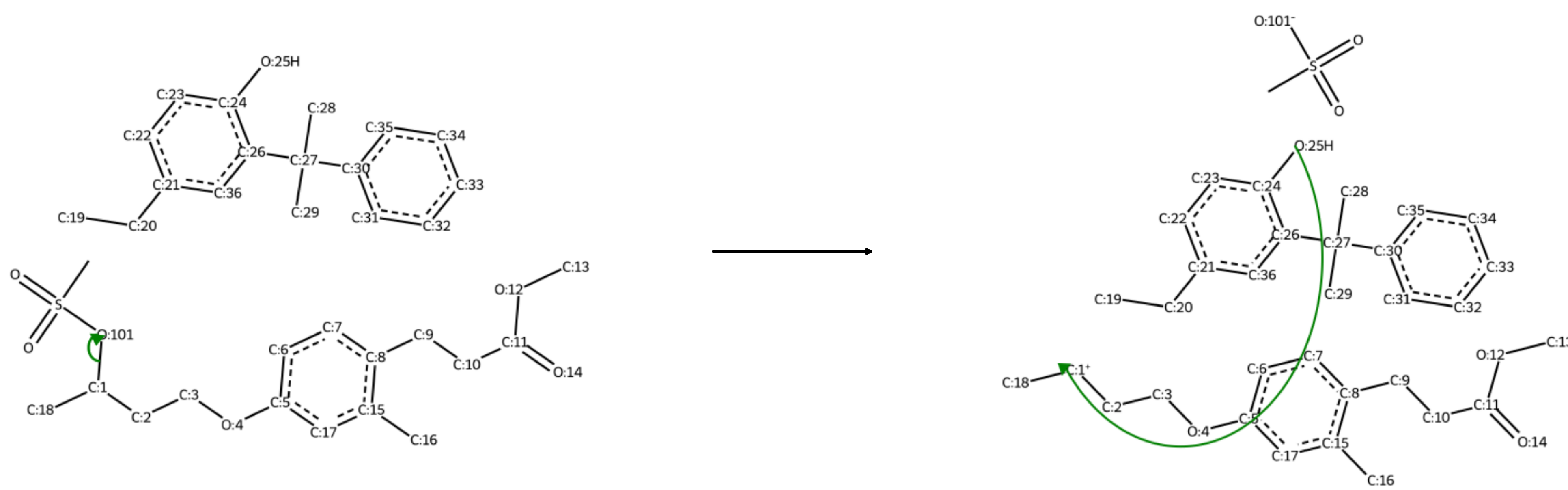


Proposed mechanistic pathway

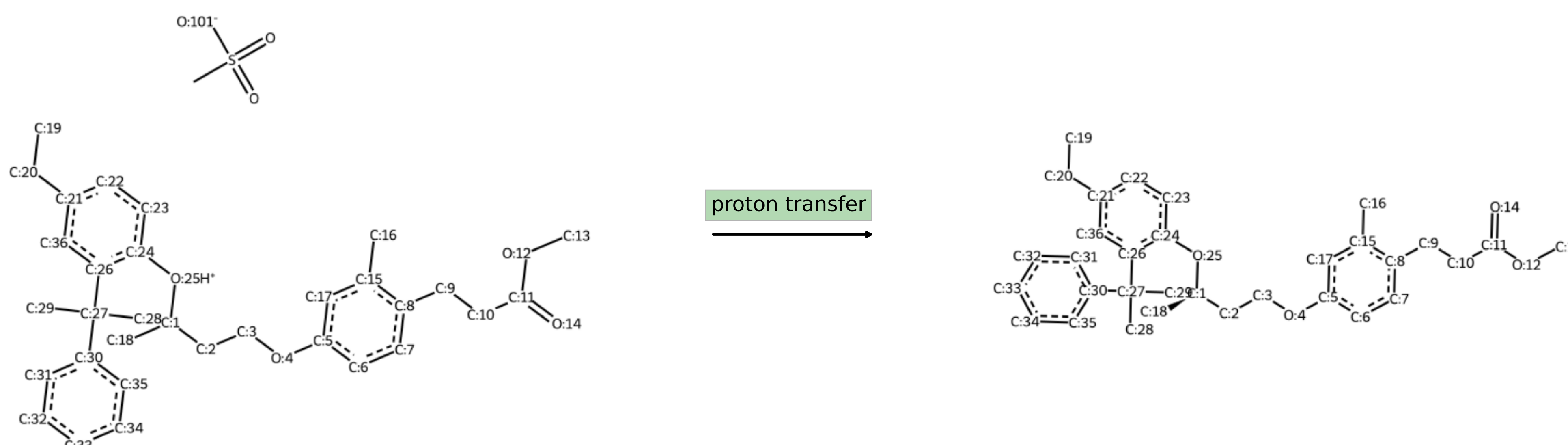
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

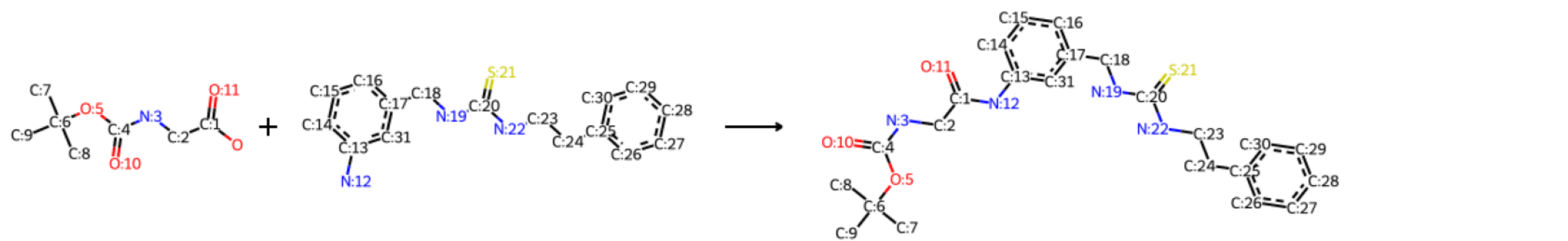
step #2



Product(s)

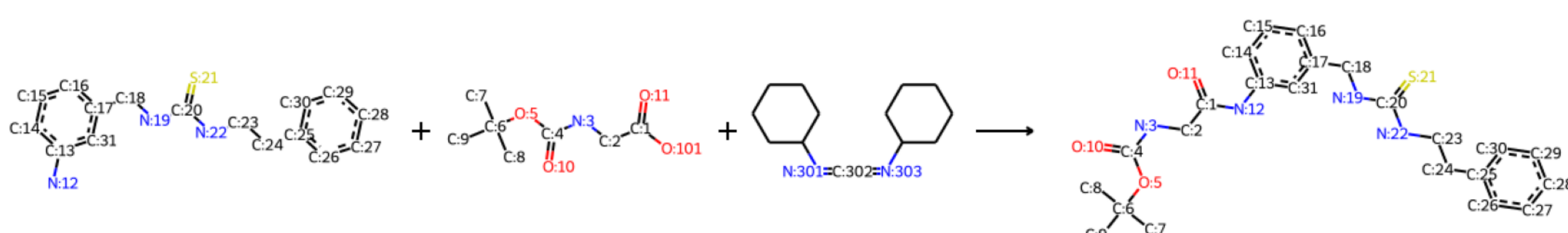


Original reaction sampled RXN_ID:37)



Identified mechanistic class -
DCC_condensation reaction

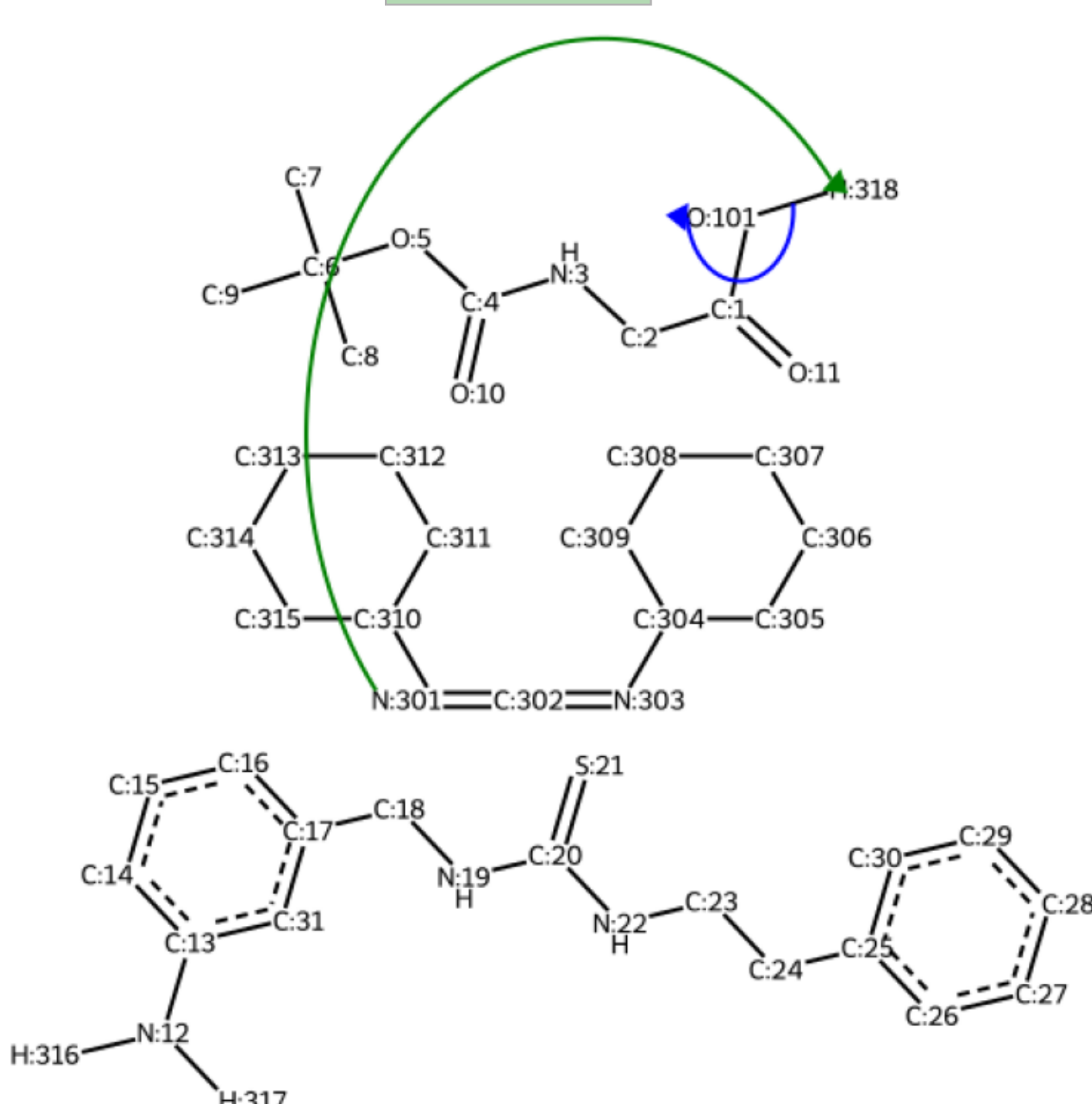
Reaction with missing reagents recovered



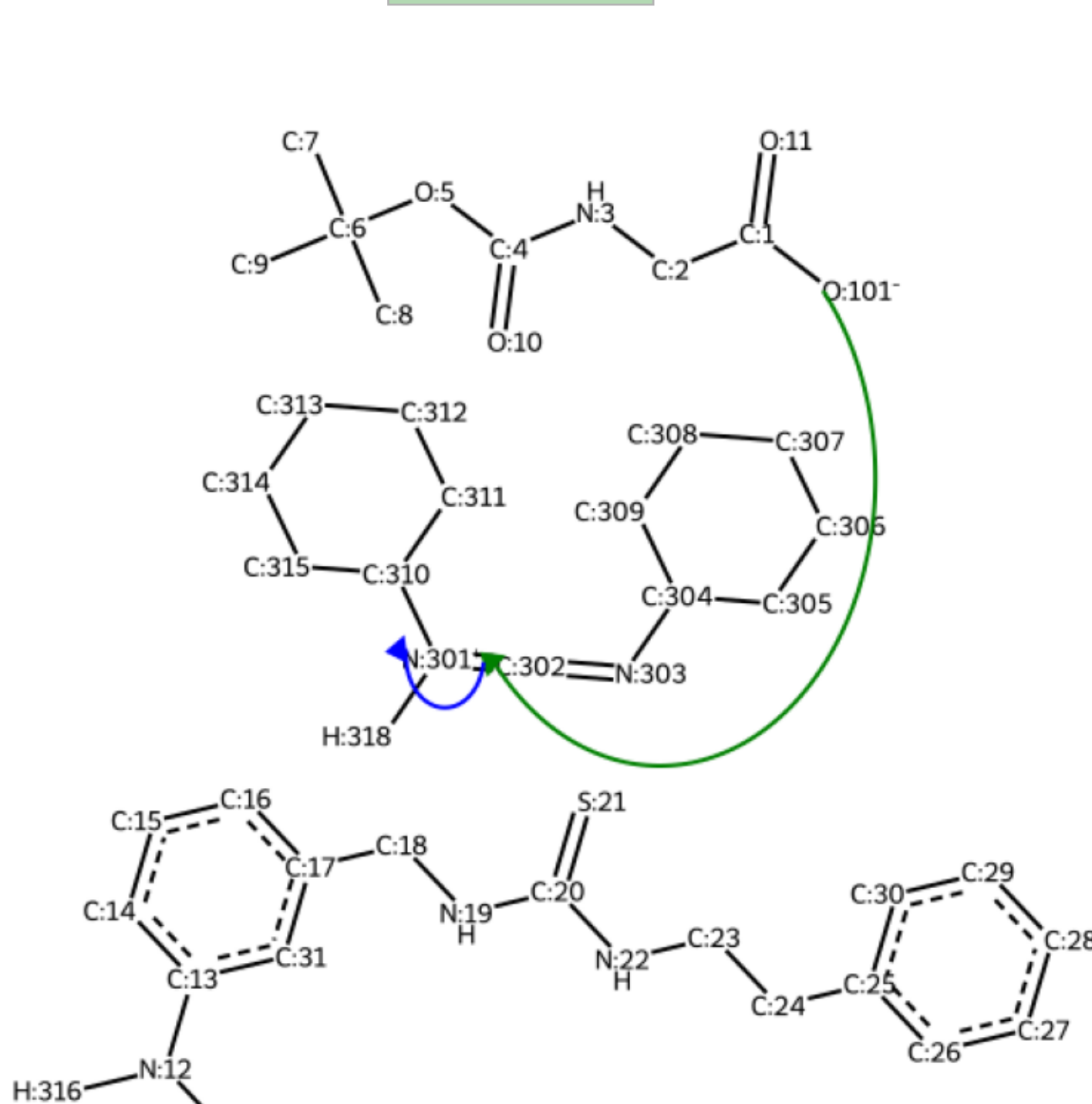
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

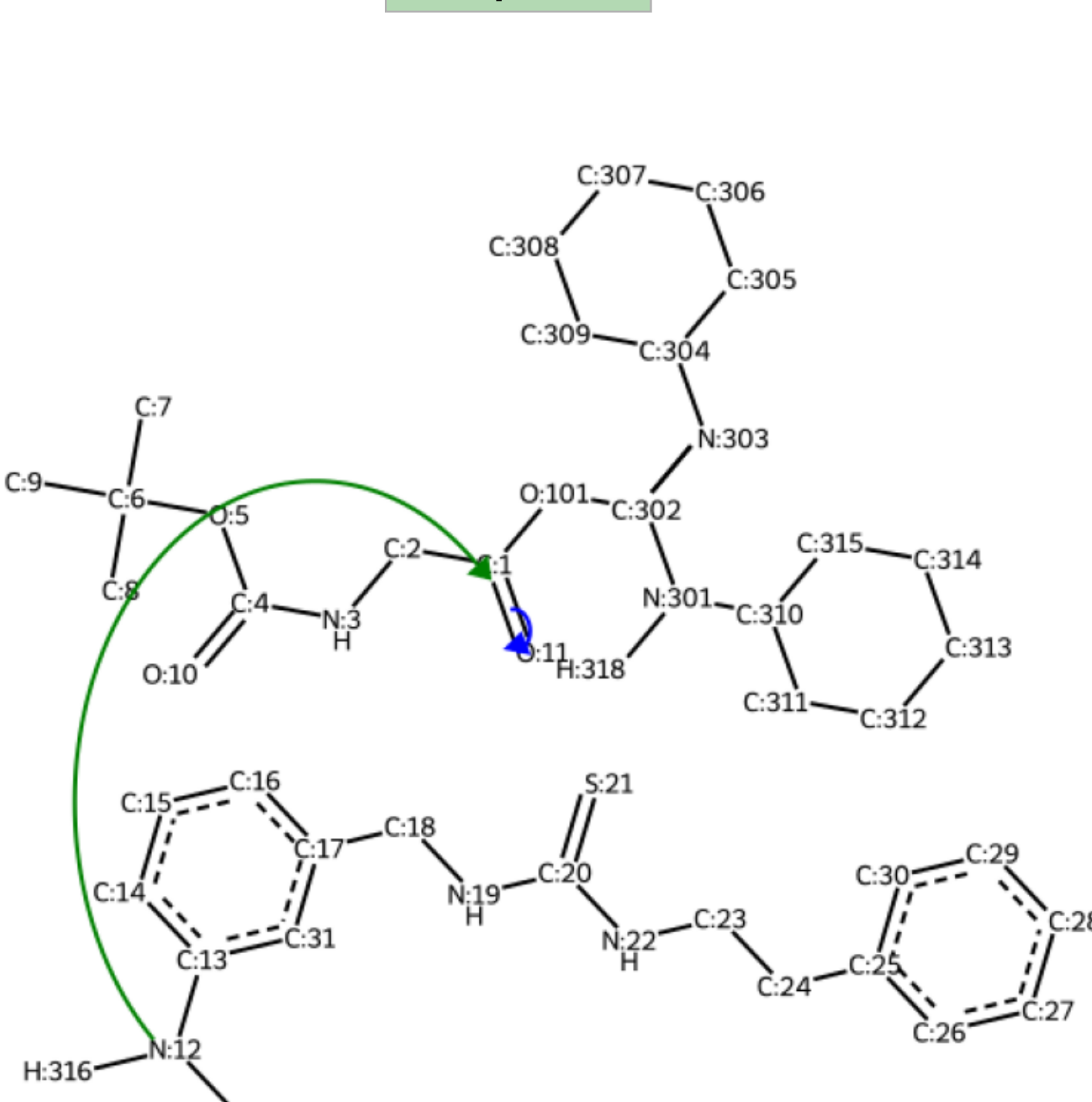
step #1



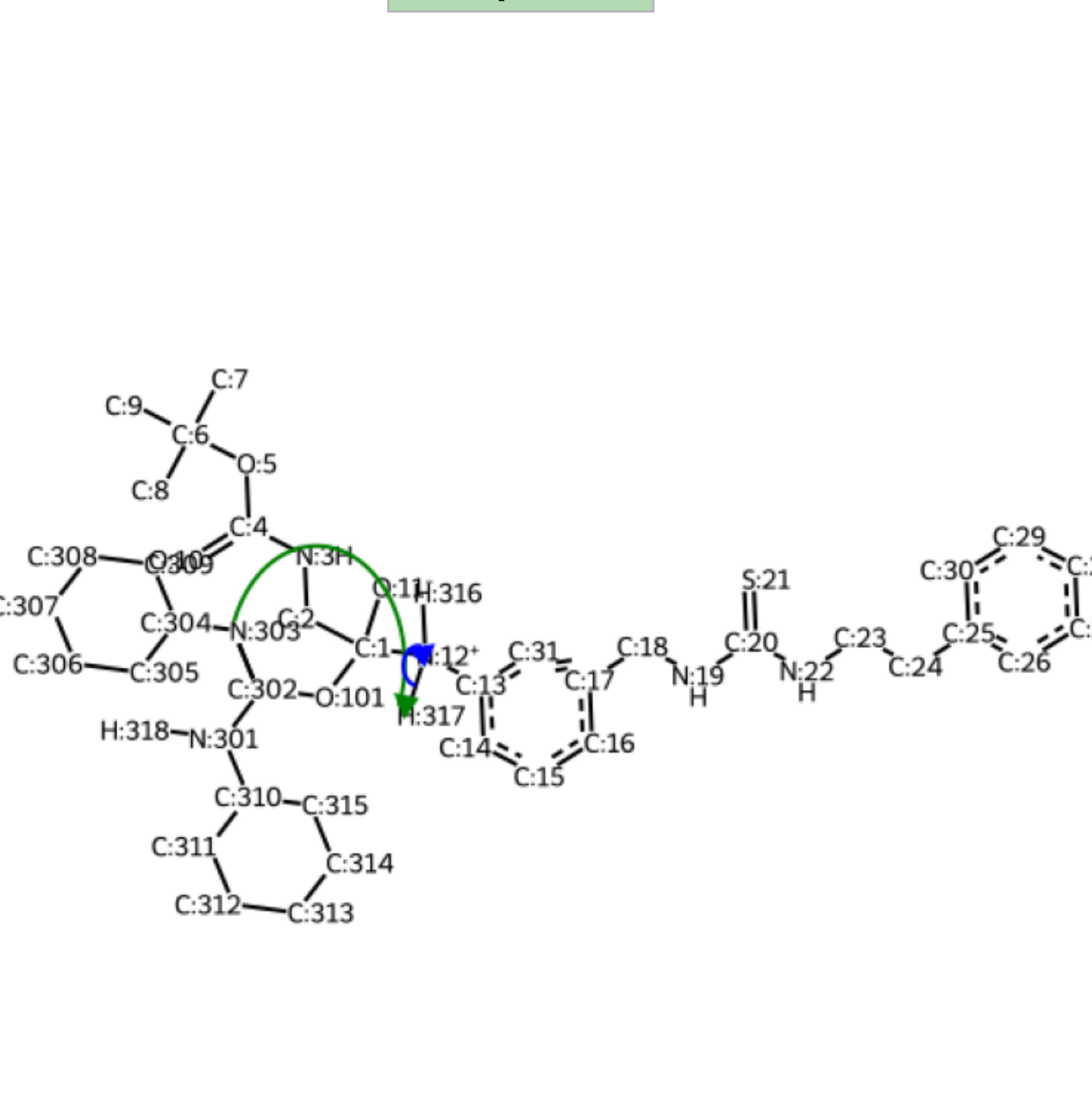
step #2



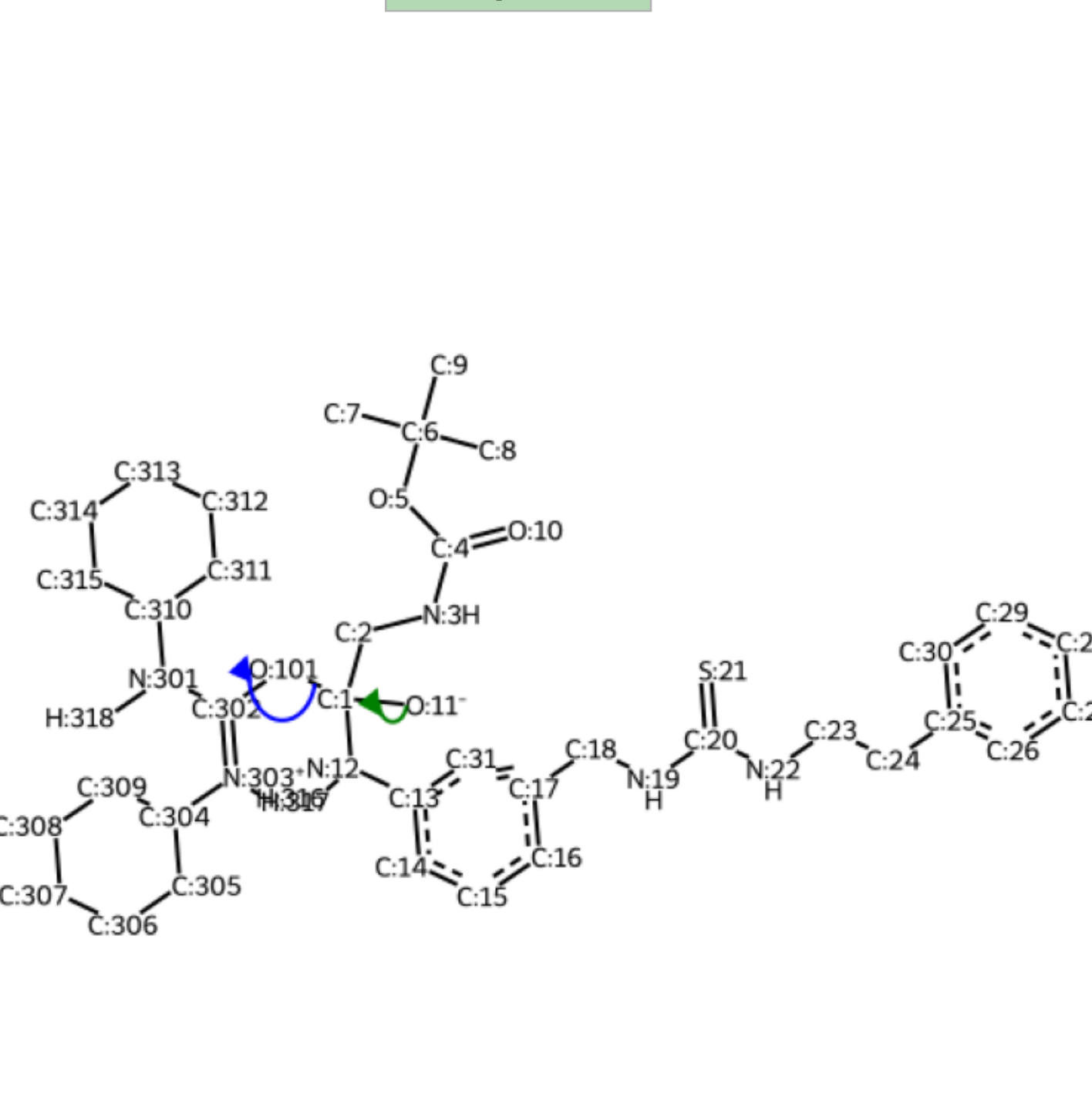
step #3



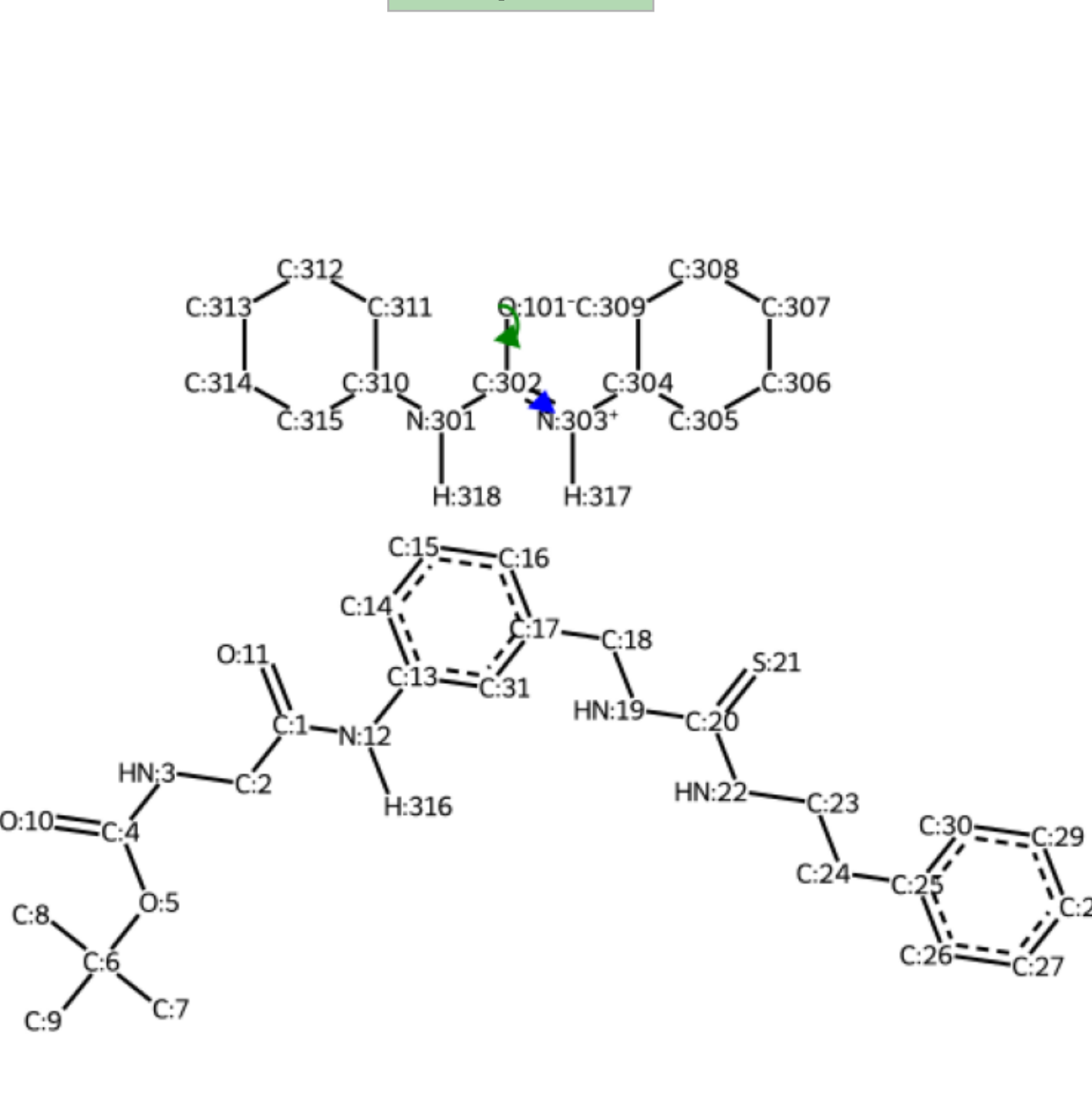
step #4



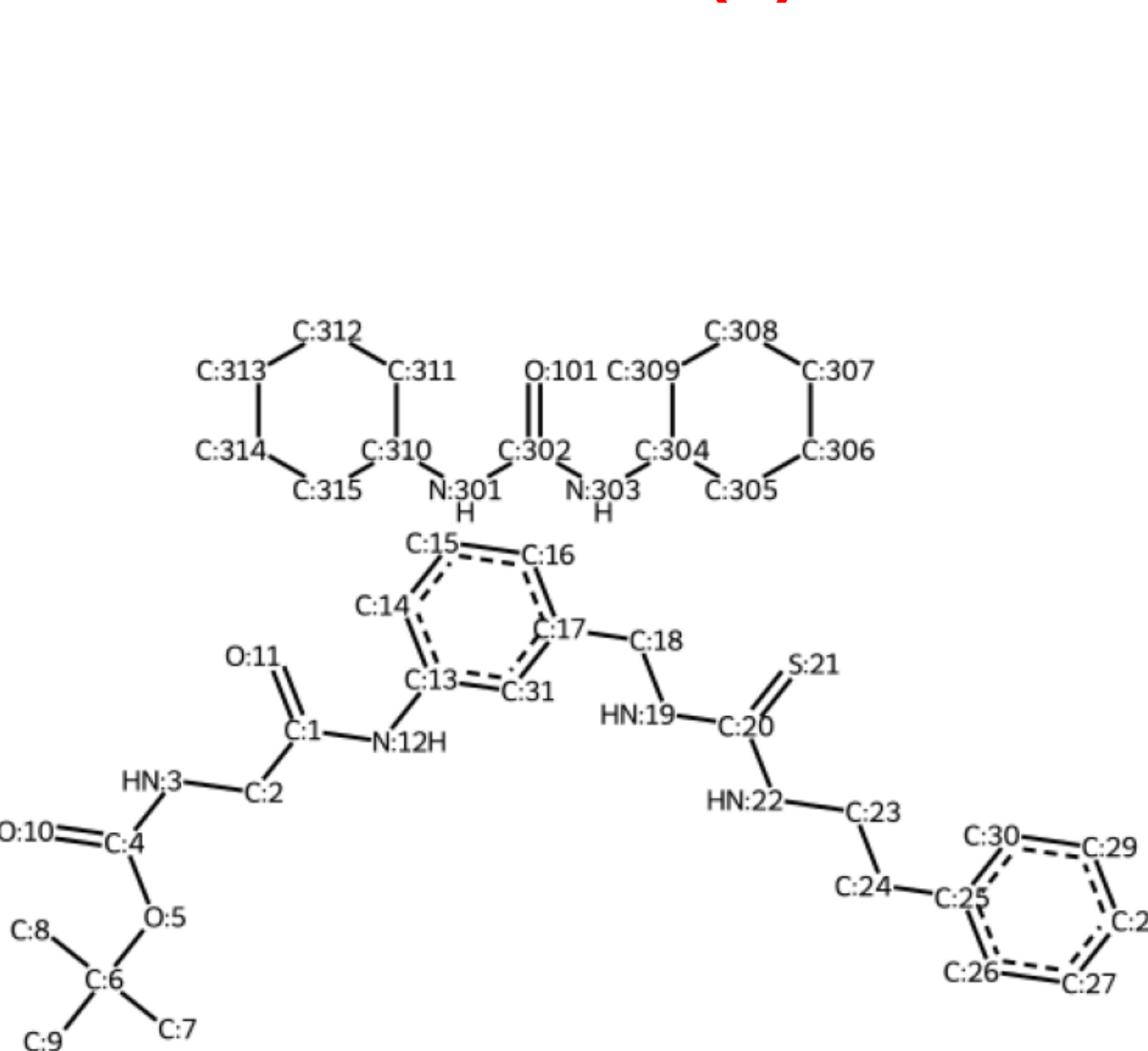
step #5



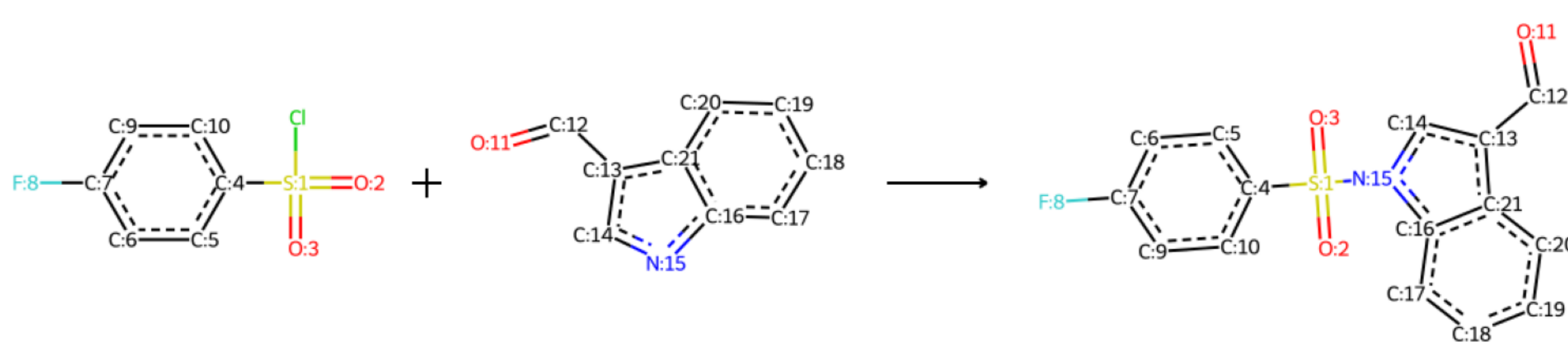
step #6



Product(s)

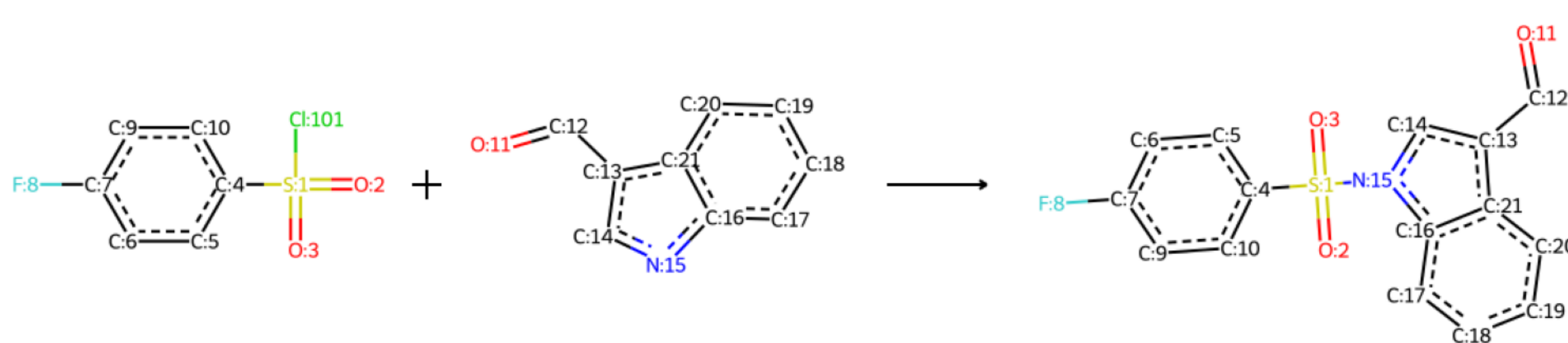


Original reaction
sampled RXN_ID:38)



Identified mechanistic class -
nucleophilic_attack_to_(thio)carbonyl_or_sulfonyl reaction

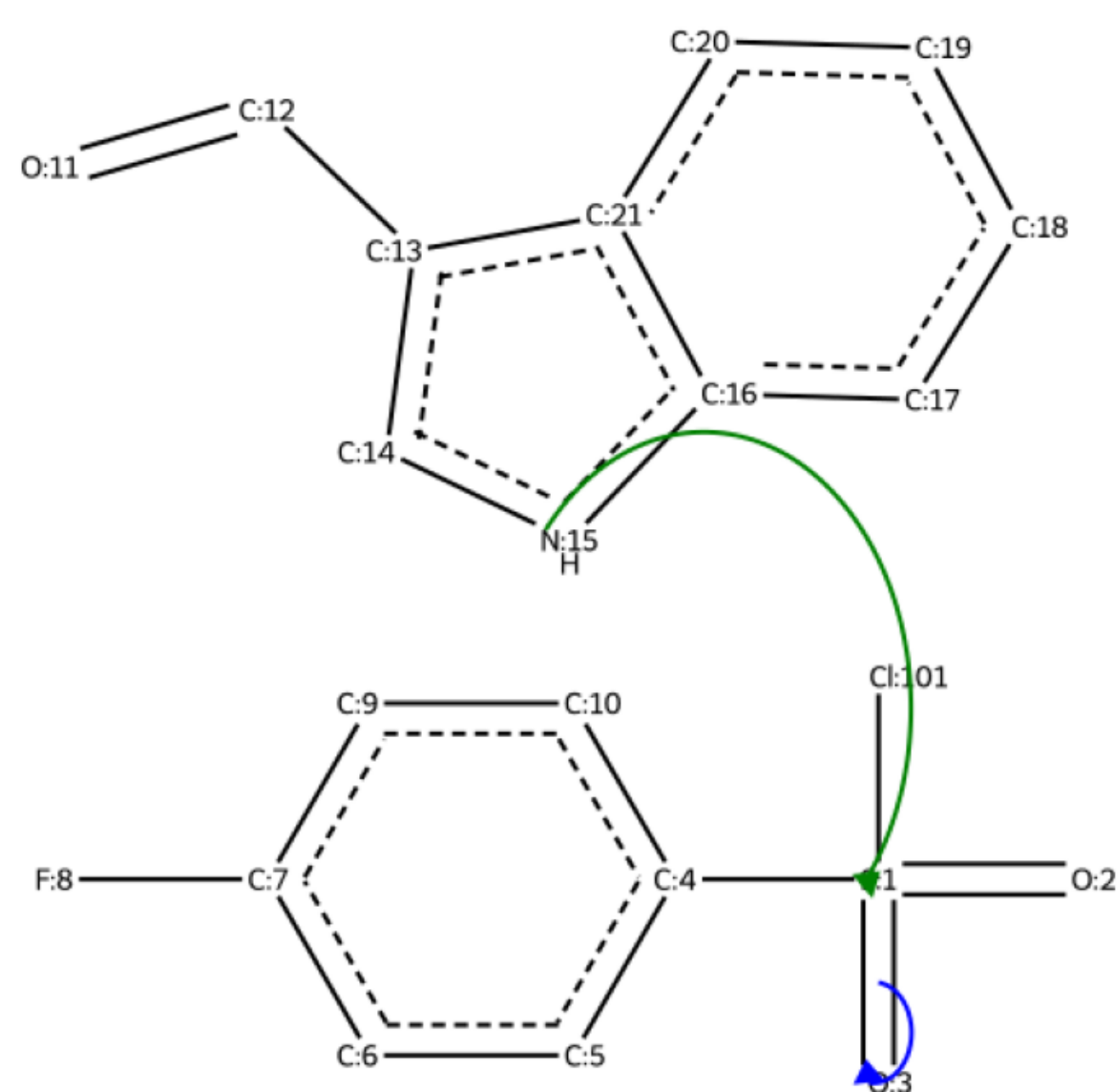
Reaction with missing reagents recovered



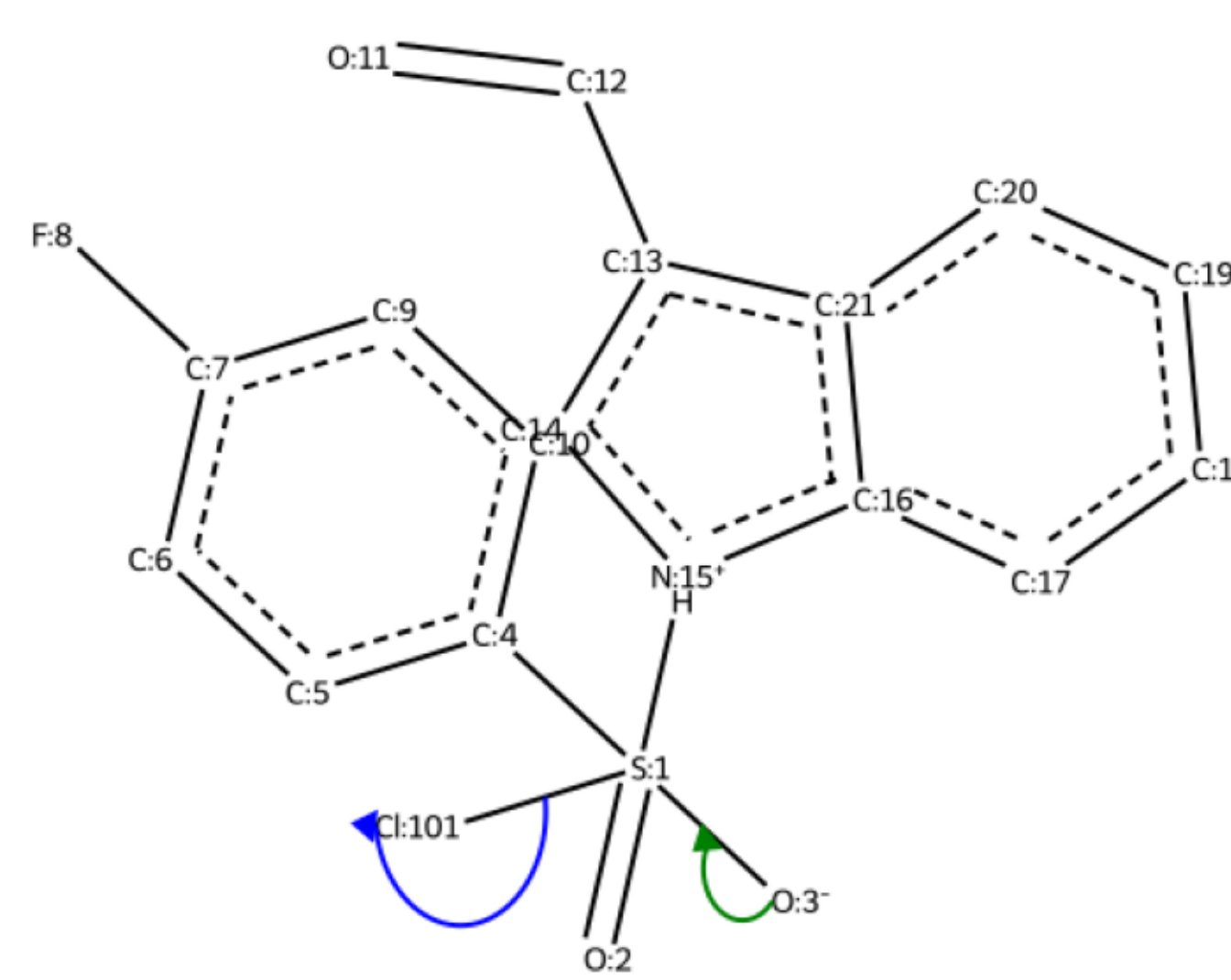
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

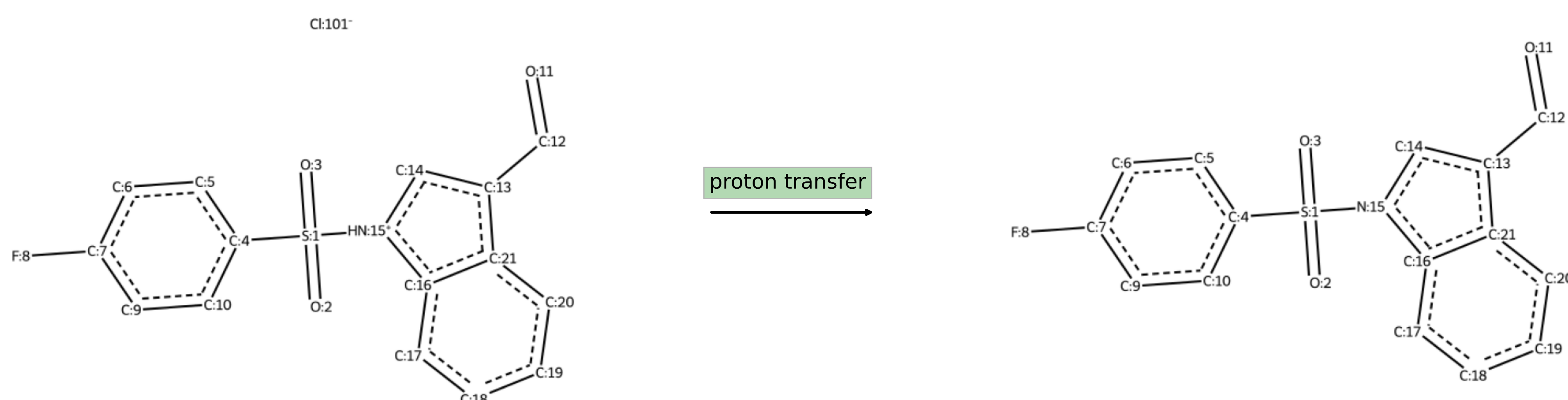
step #1



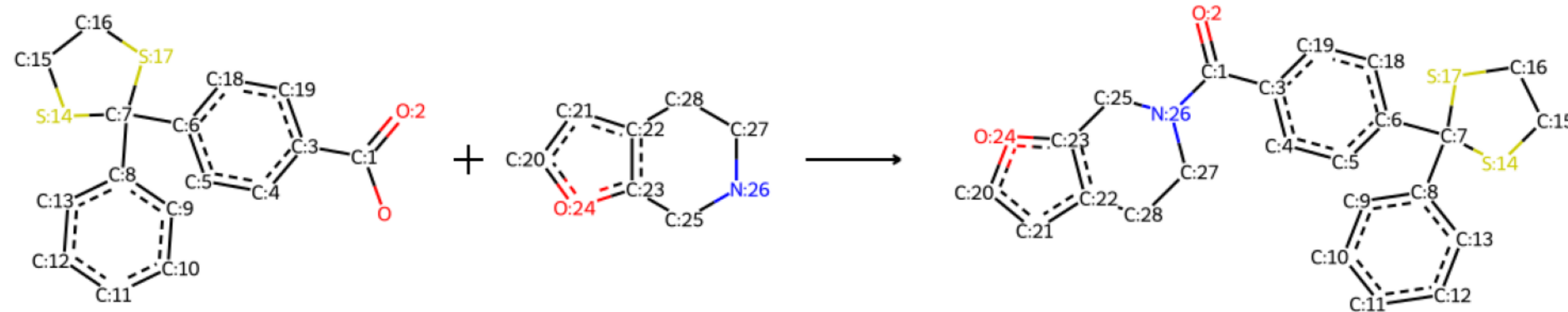
step #2



Product(s)

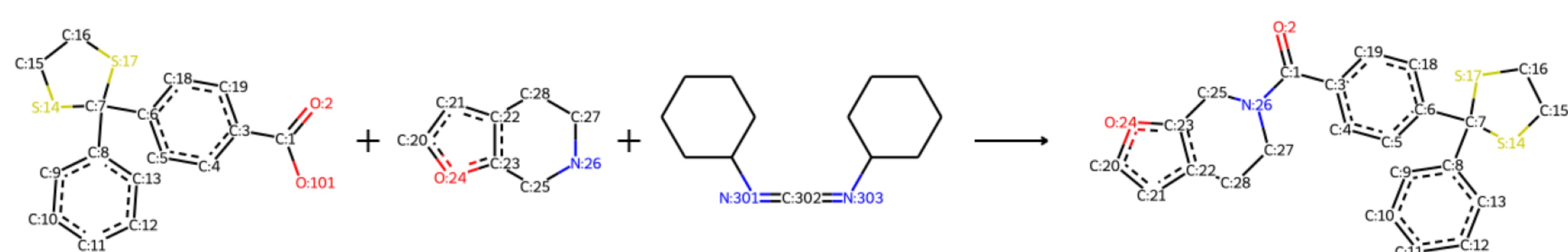


Original reaction sampled RXN_ID:39)



Identified mechanistic class -
DCC_condensation reaction

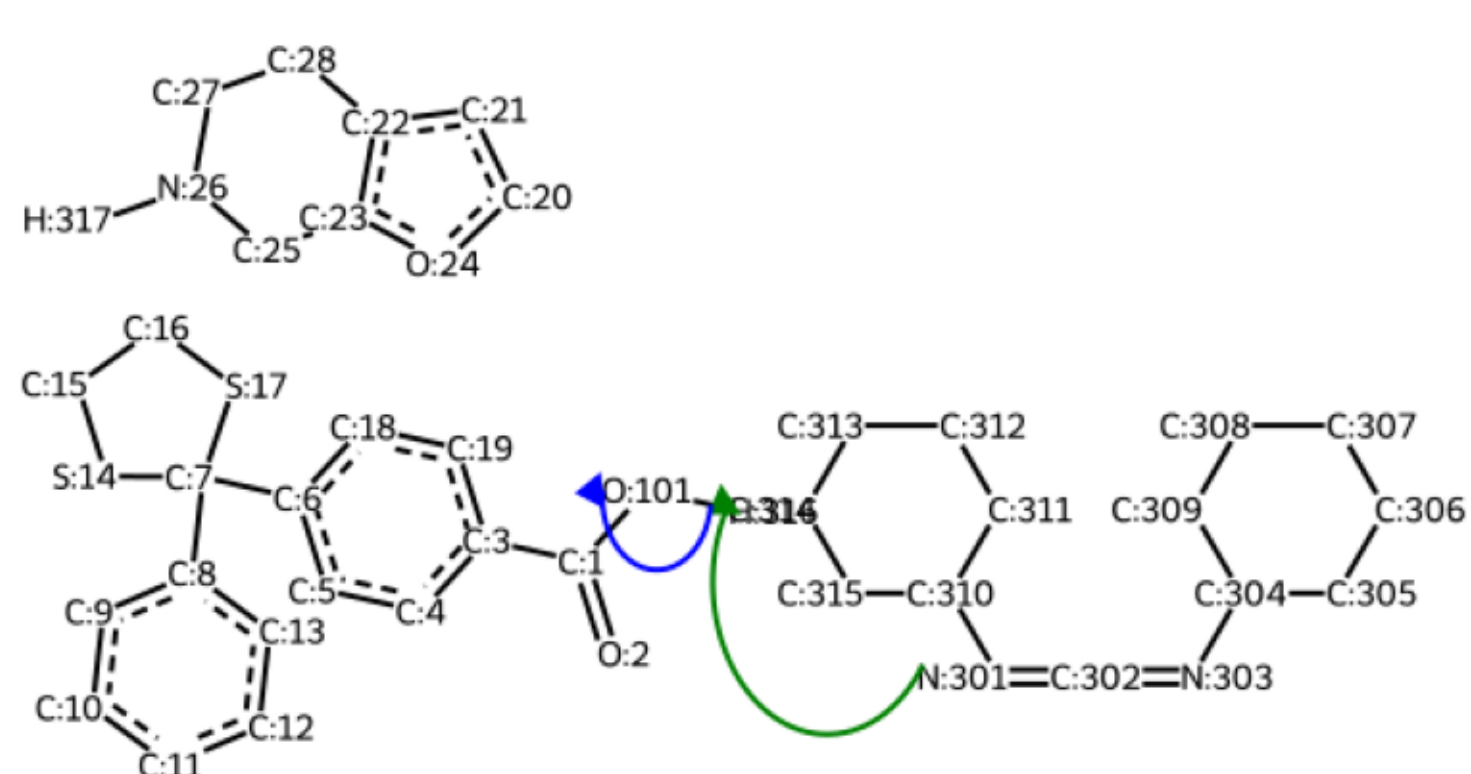
Reaction with missing reagents recovered



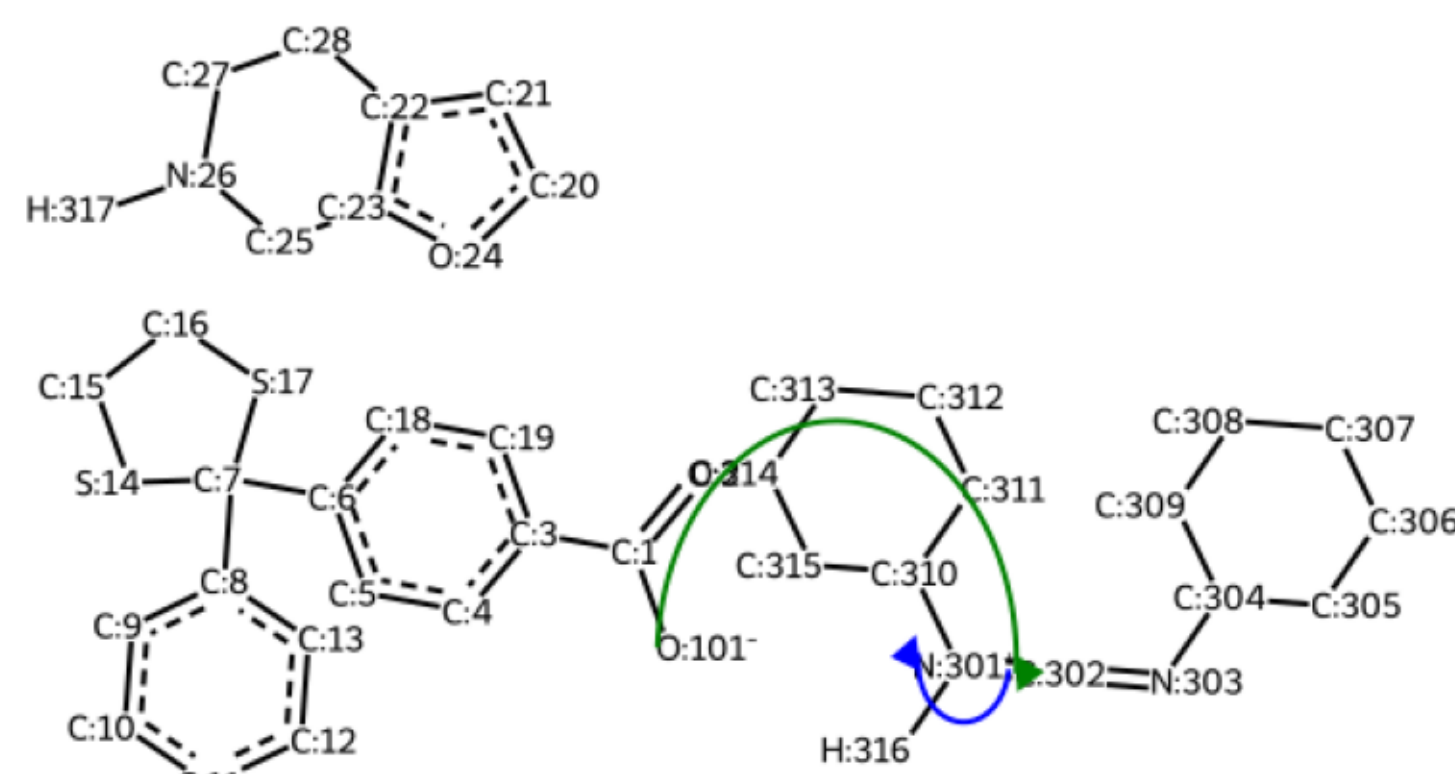
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

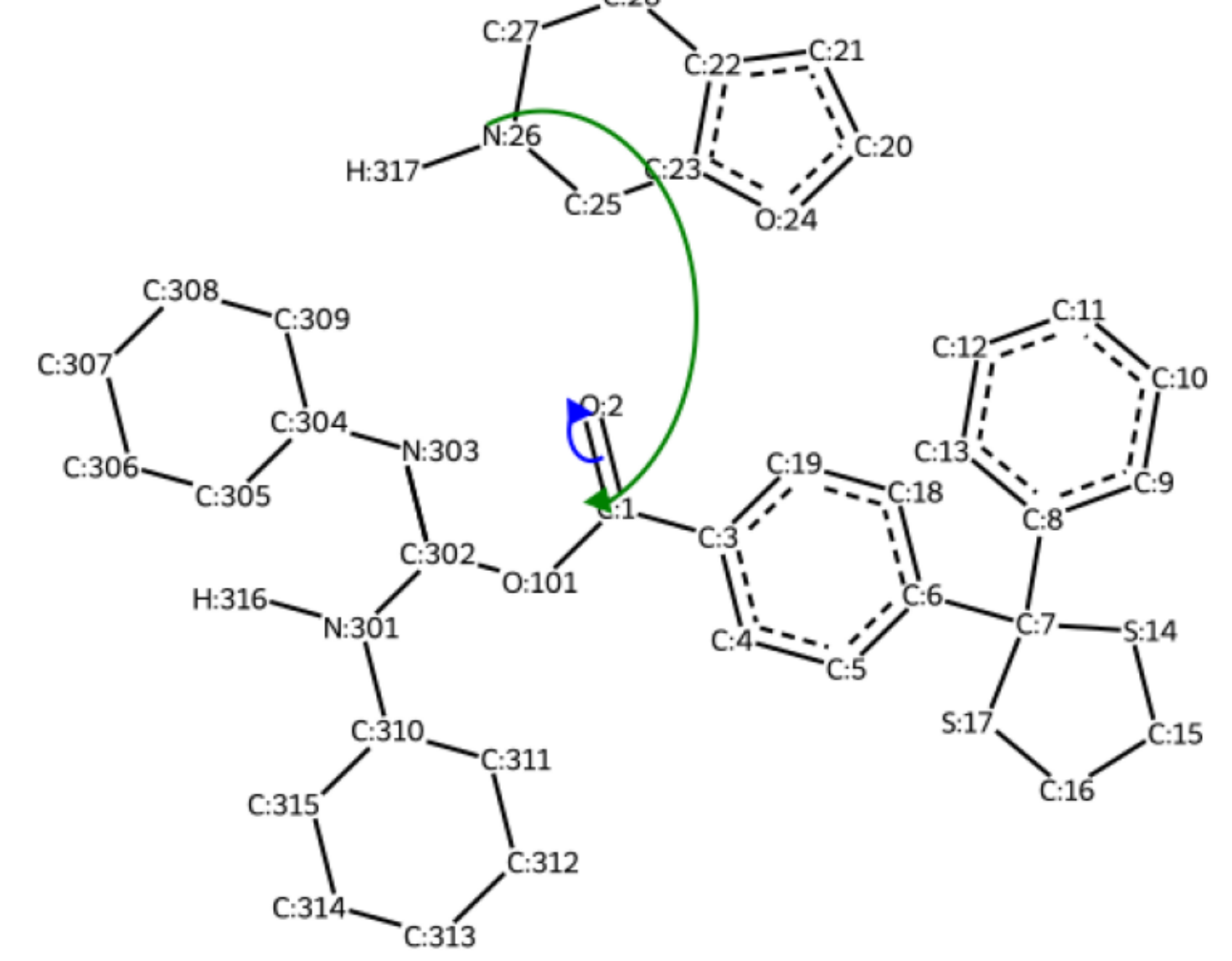
step #1



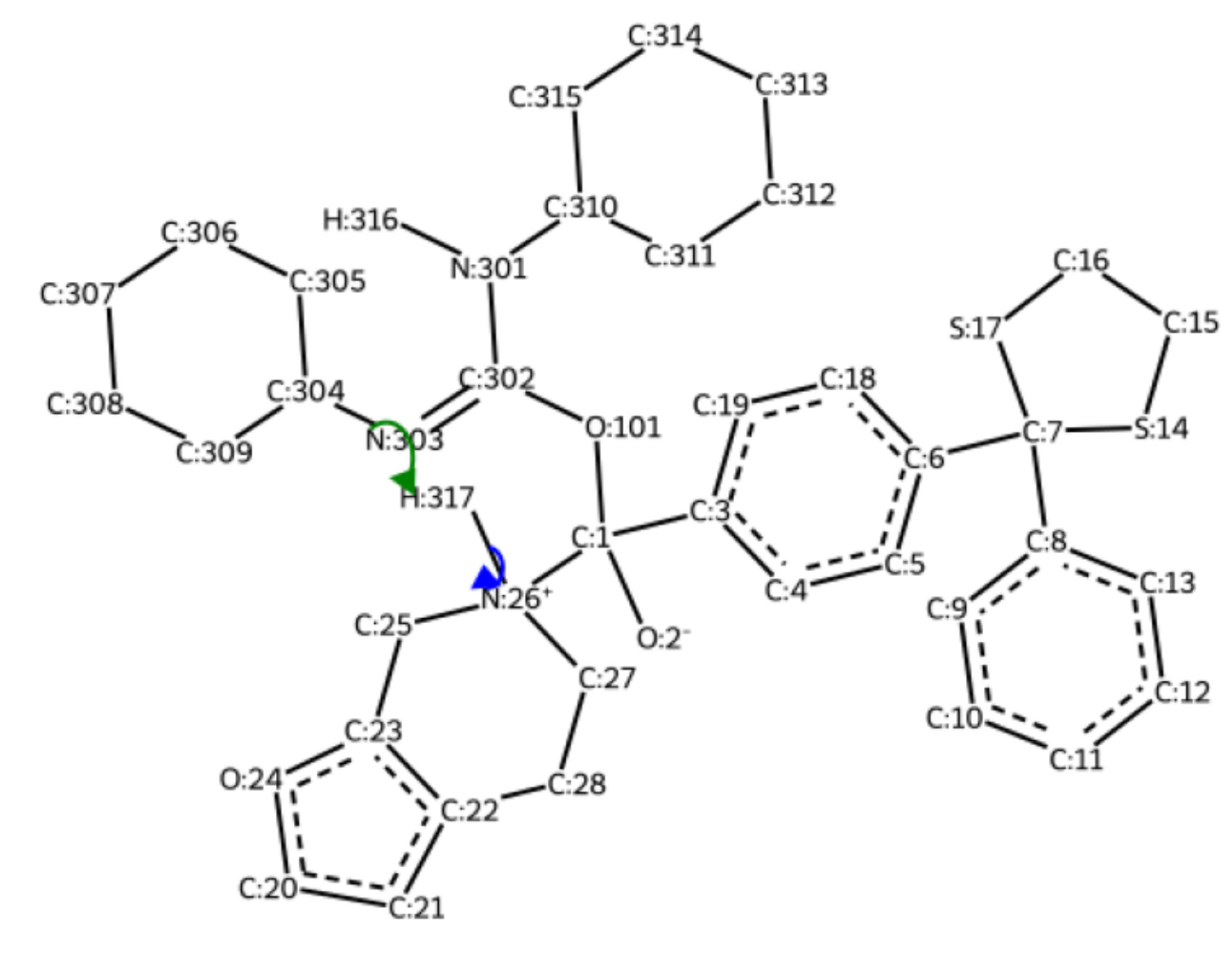
step #2



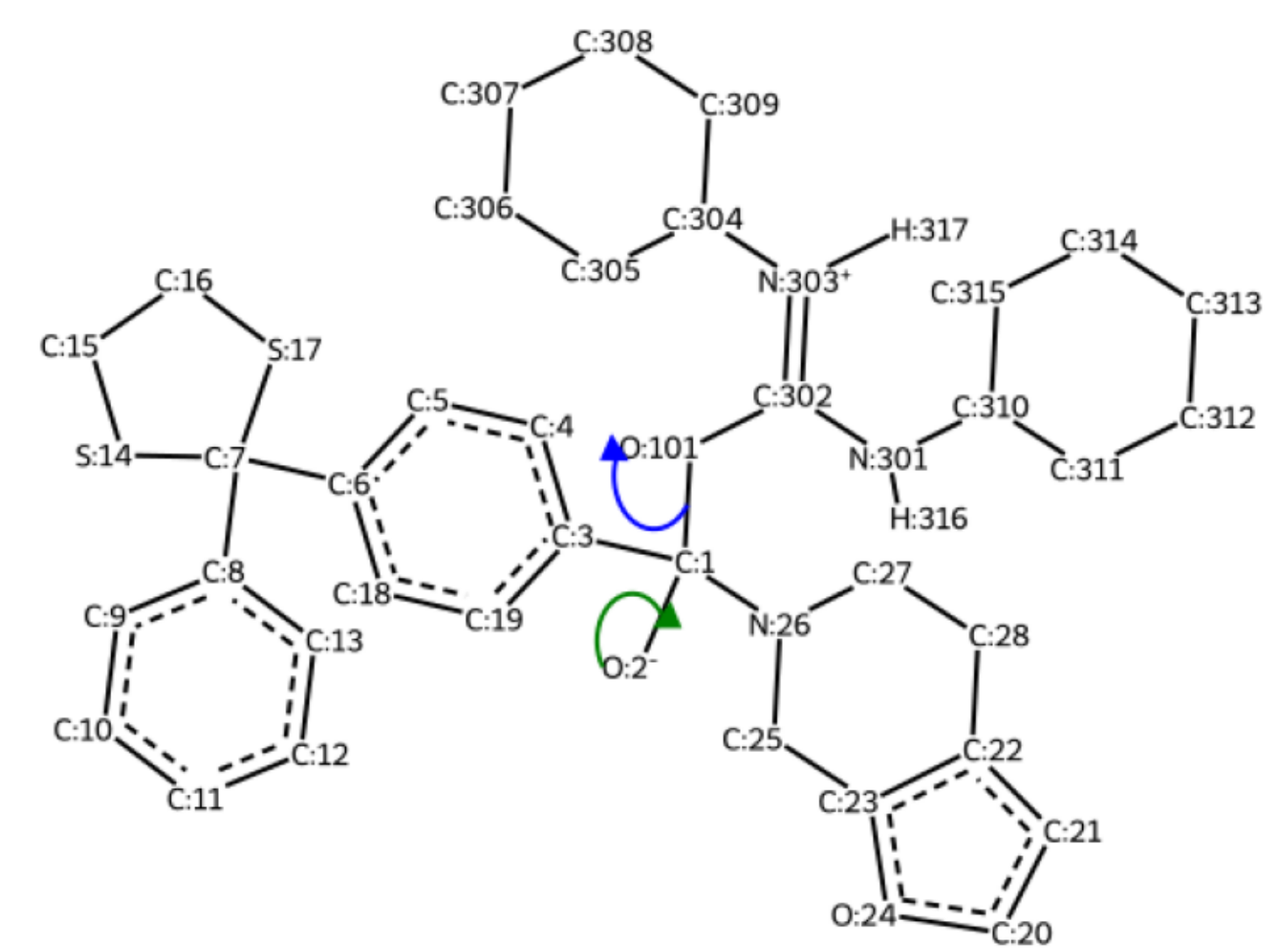
step #3



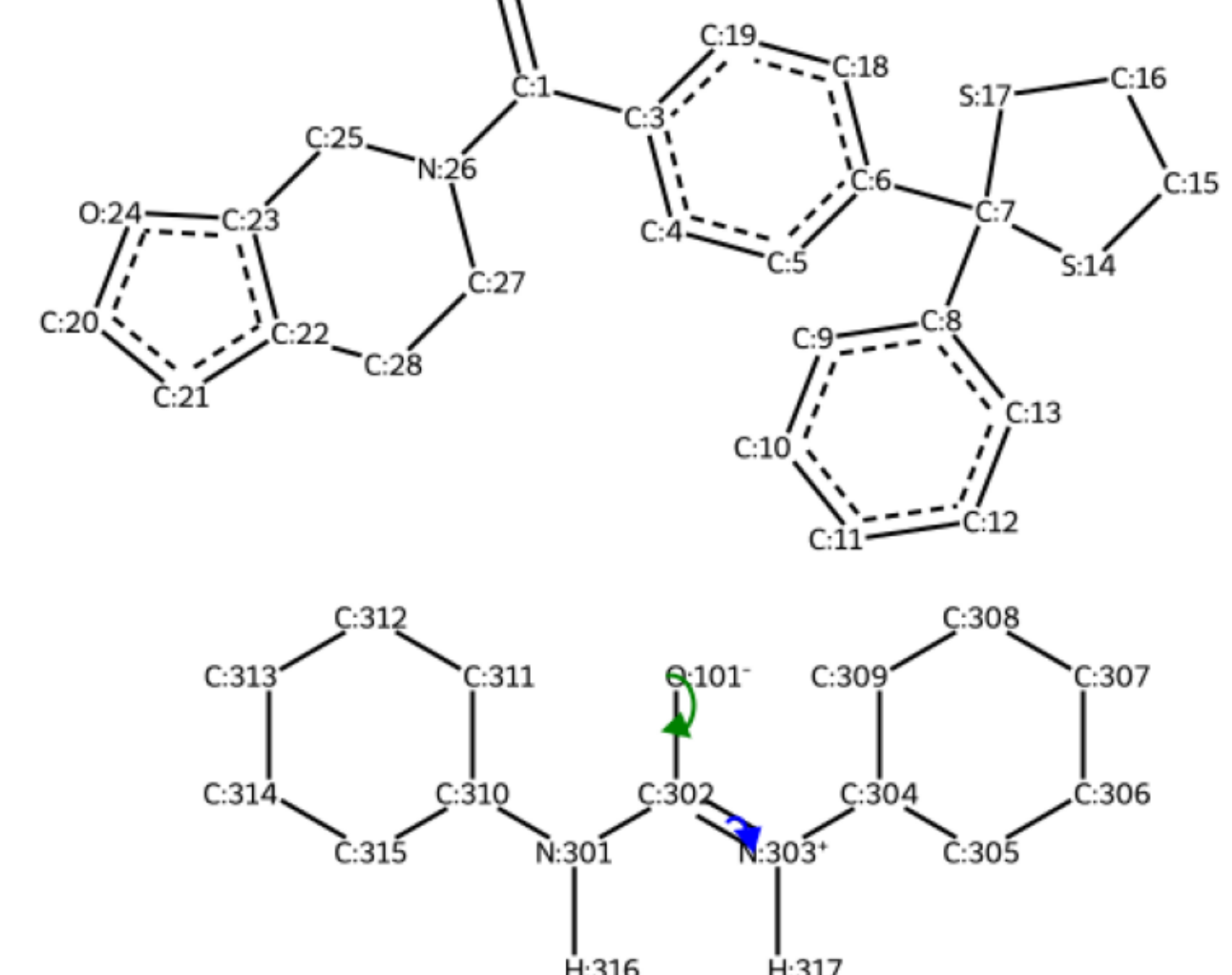
step #4



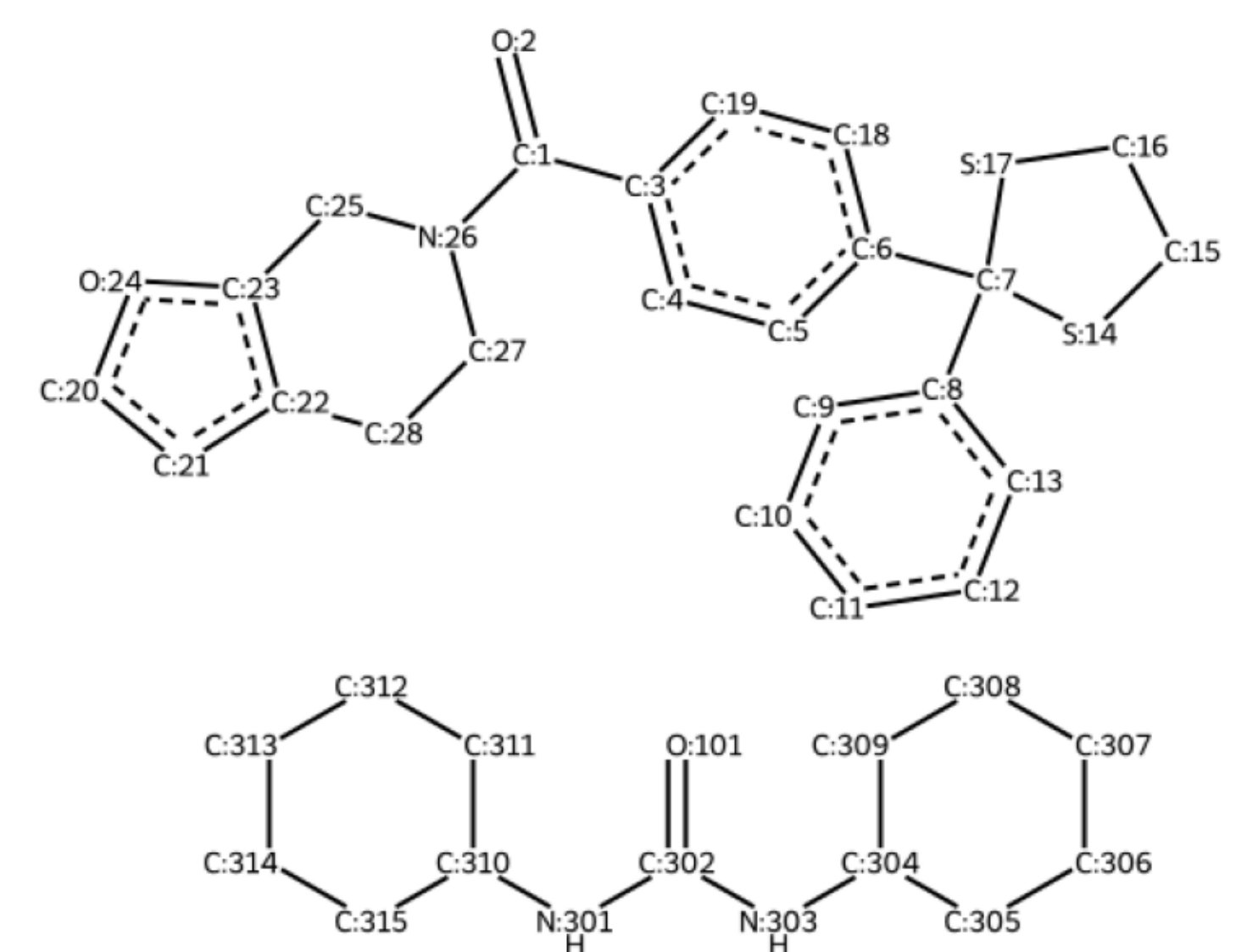
step #5



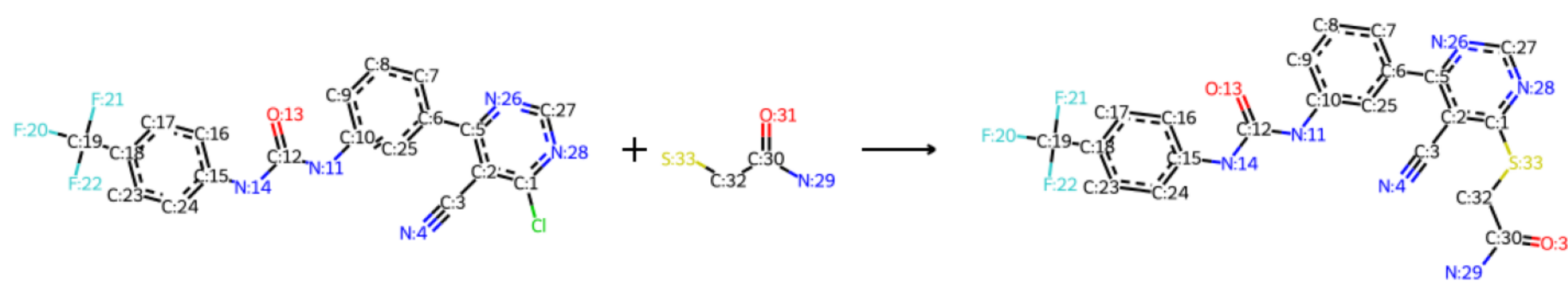
step #6



Product(s)

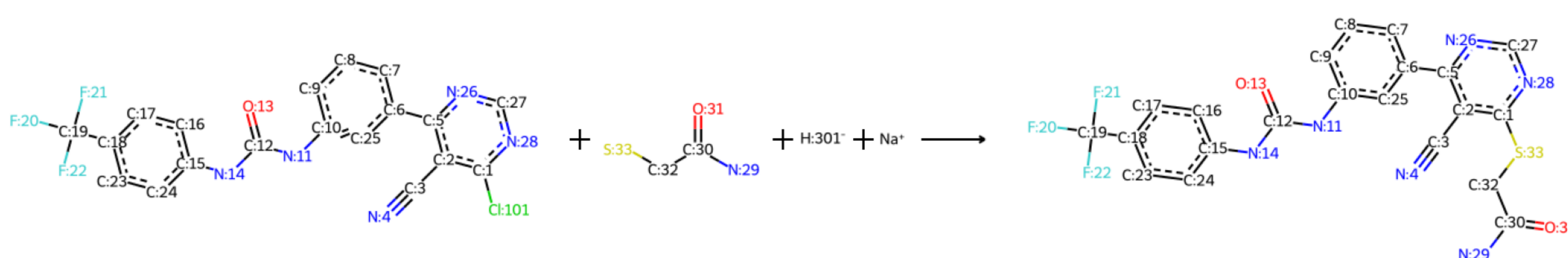


Original reaction
sampled RXN_ID:40)



Identified mechanistic class -
S_NAr_{alco}(thi)ol(ortho) reaction

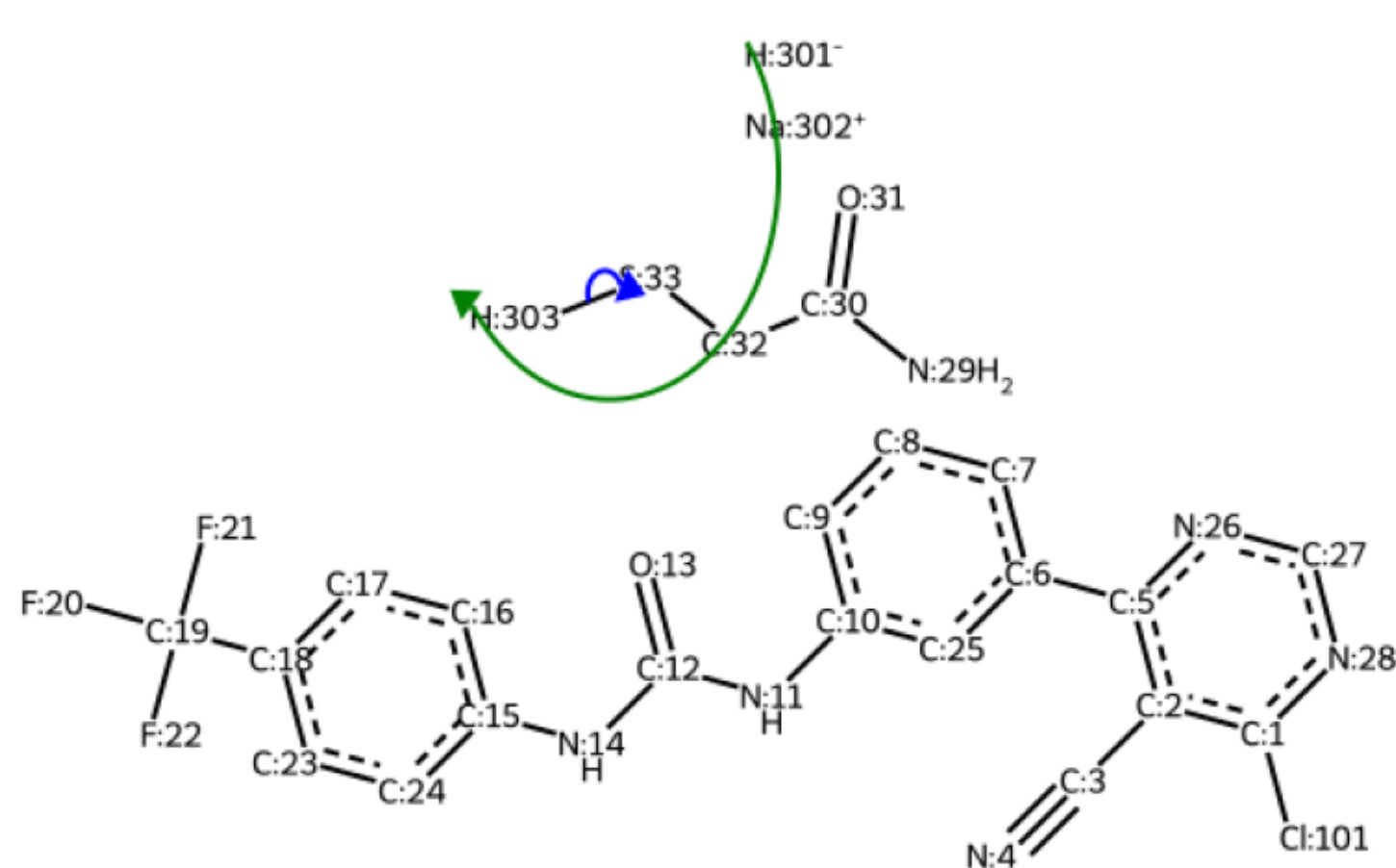
Reaction with missing reagents recovered



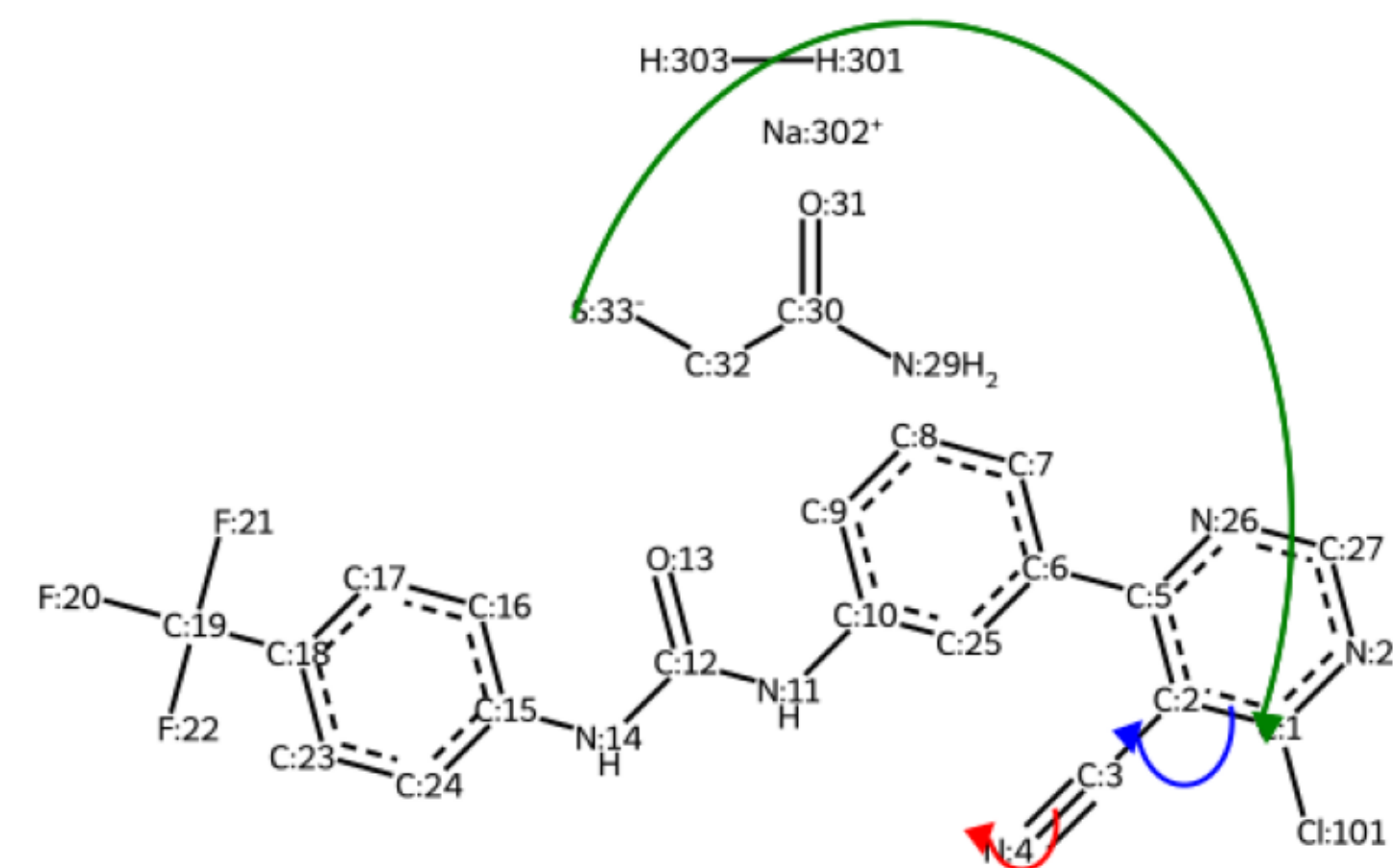
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

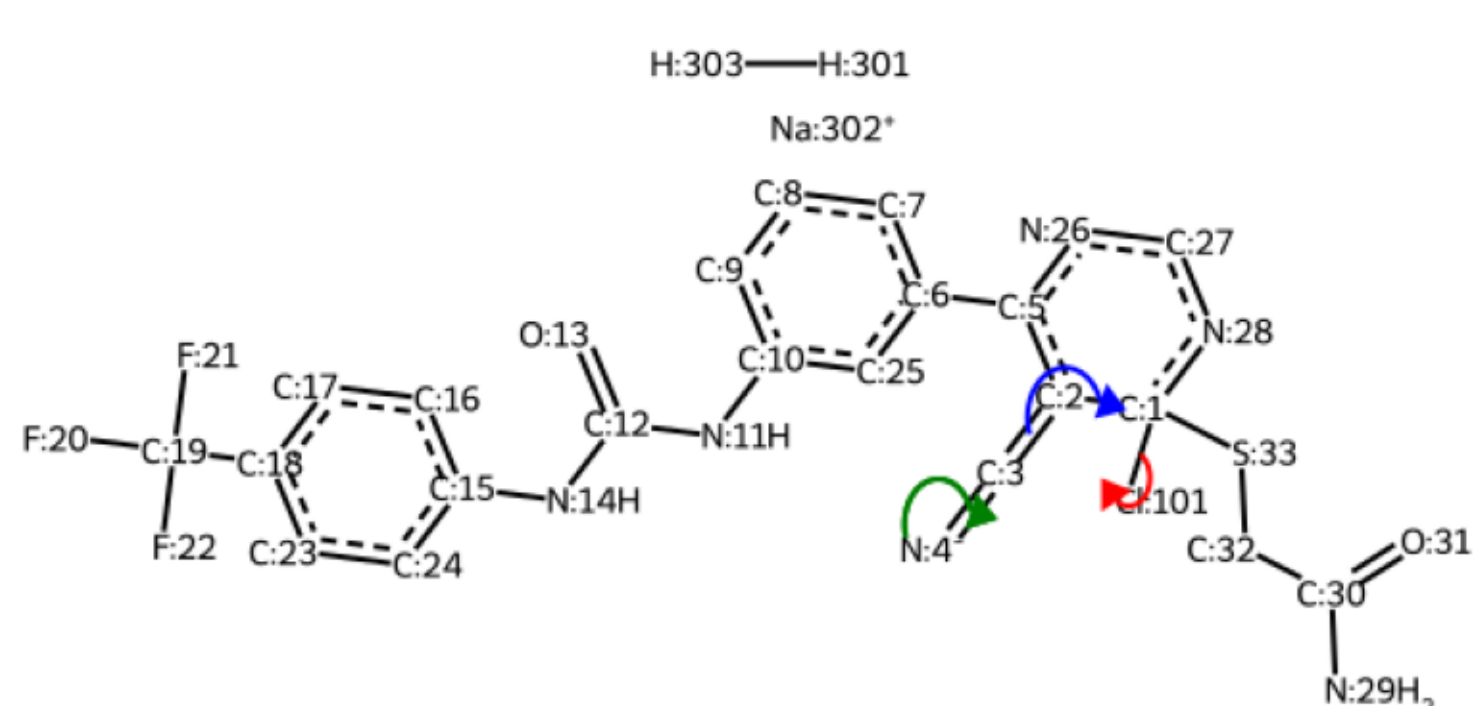
step #1



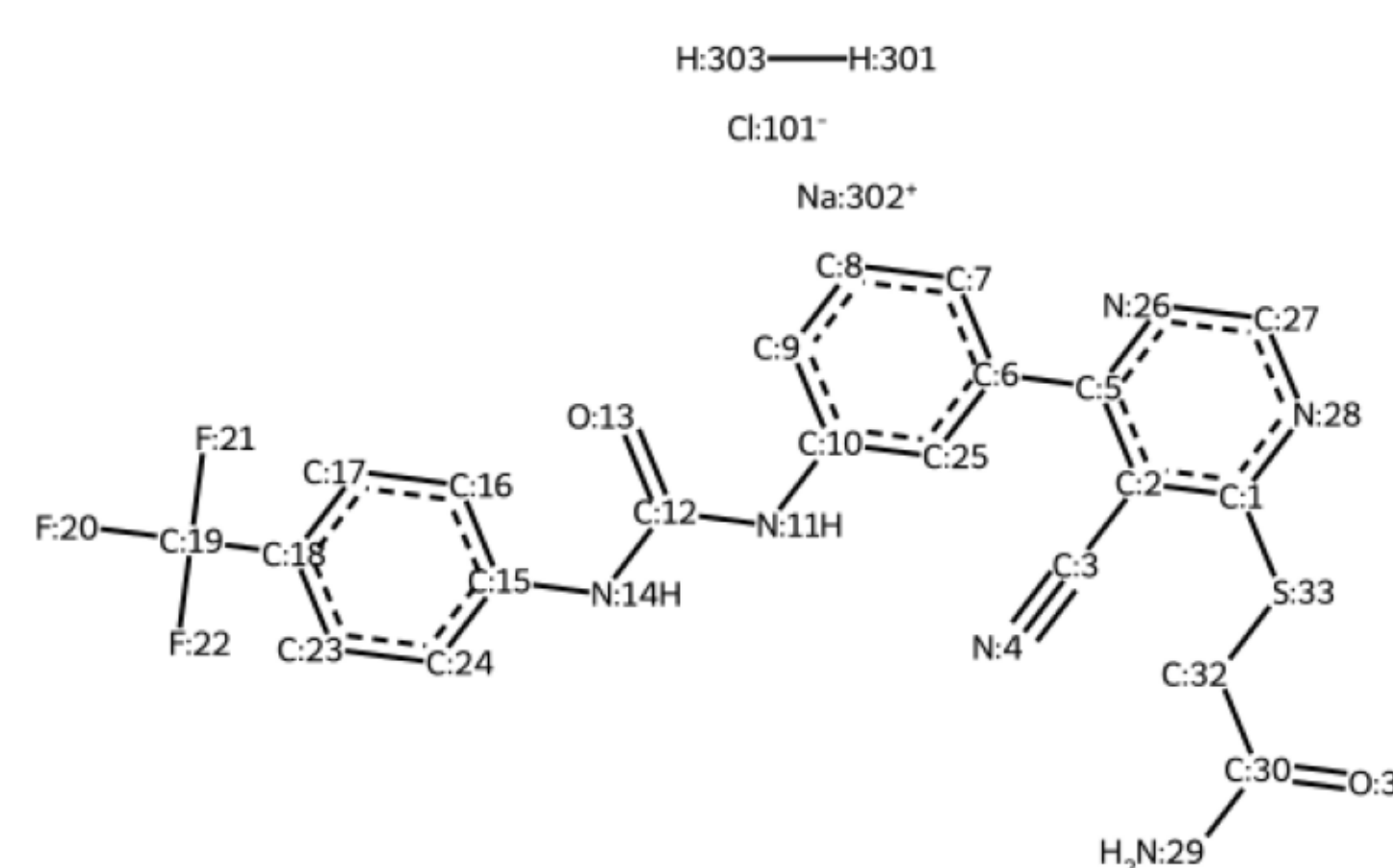
step #2



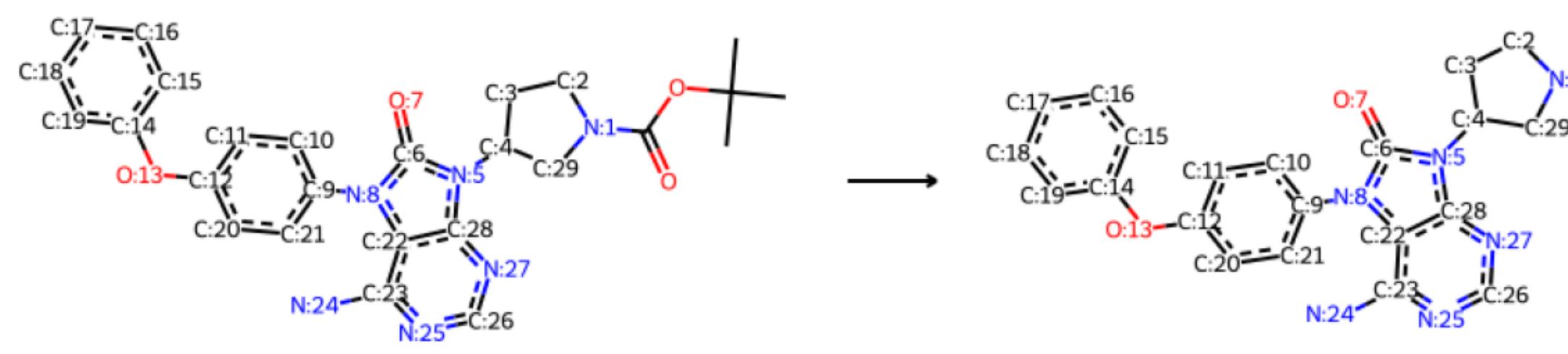
step #3



Product(s)

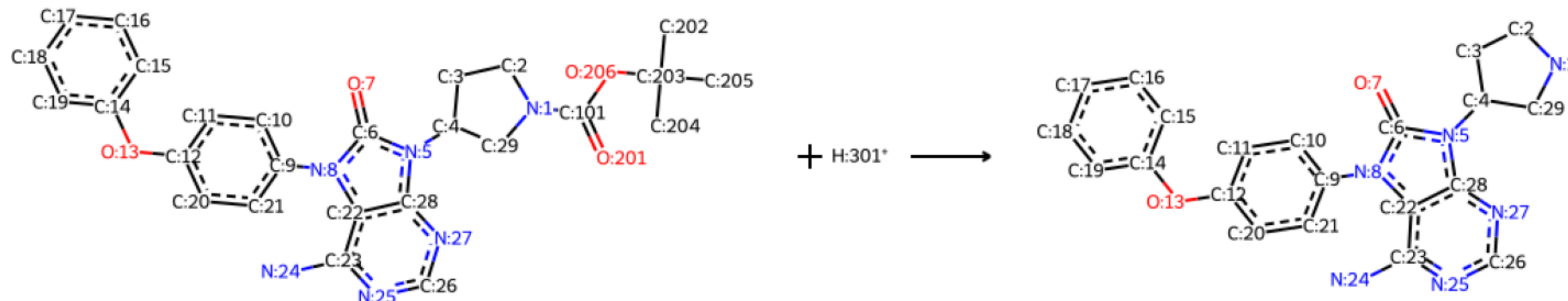


Original reaction
sampled RXN_ID:41)



Identified mechanistic class -
Boc_deprotection reaction

Reaction with missing reagents recovered

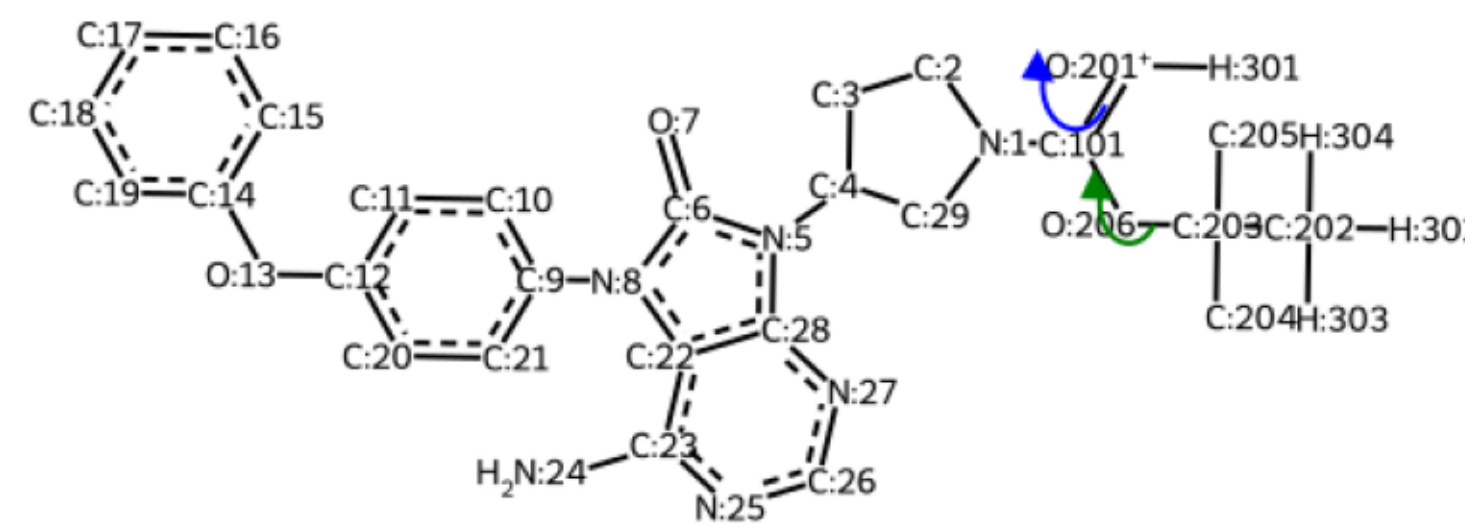
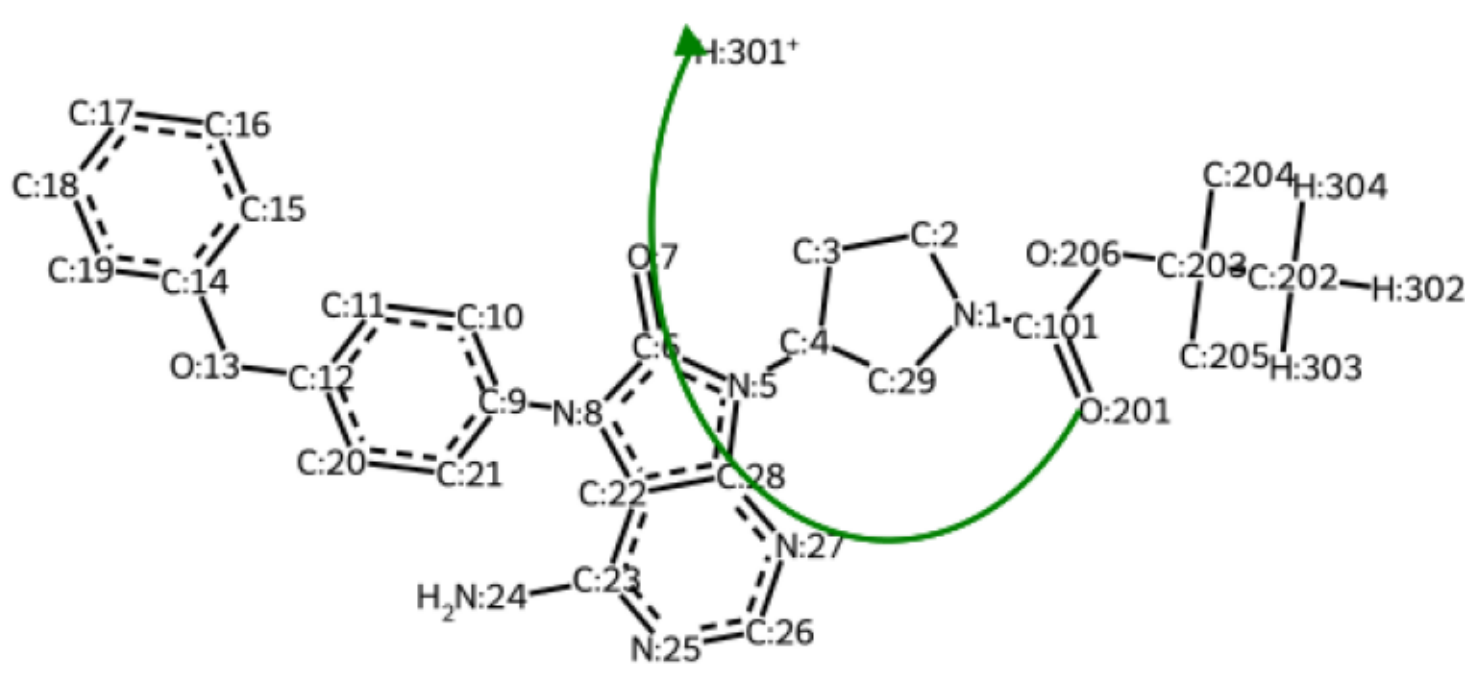


Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

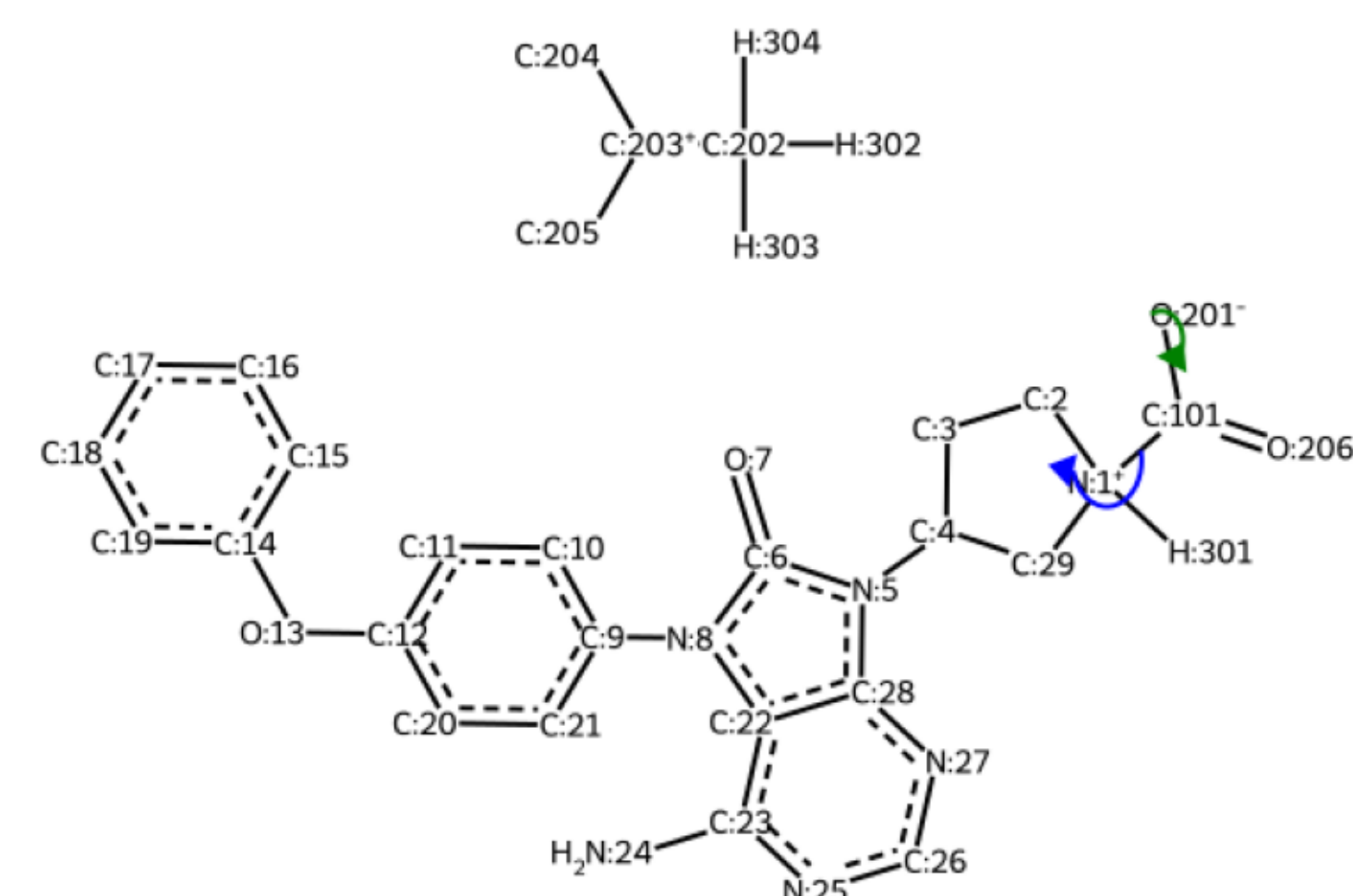
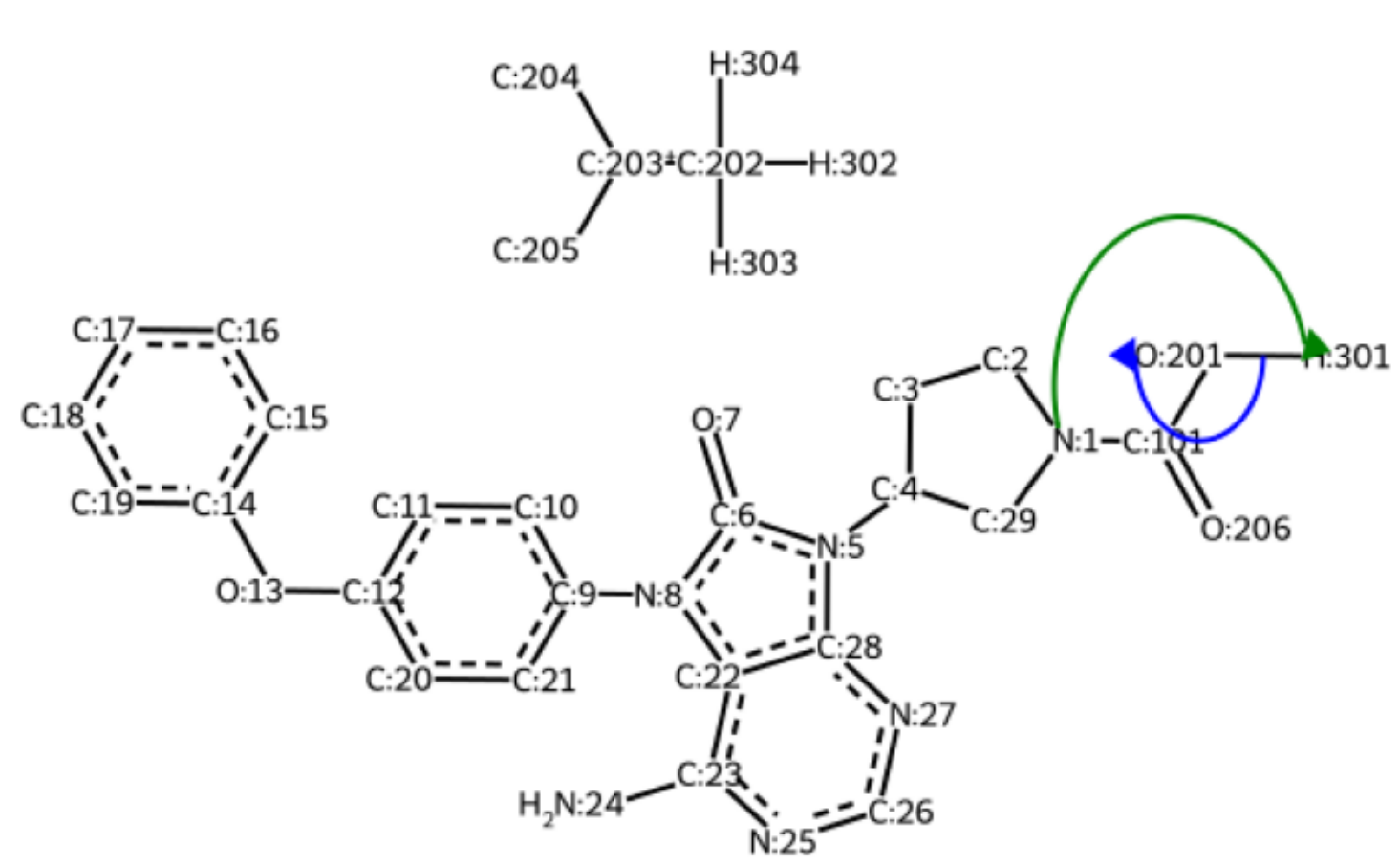
step #1

step #2



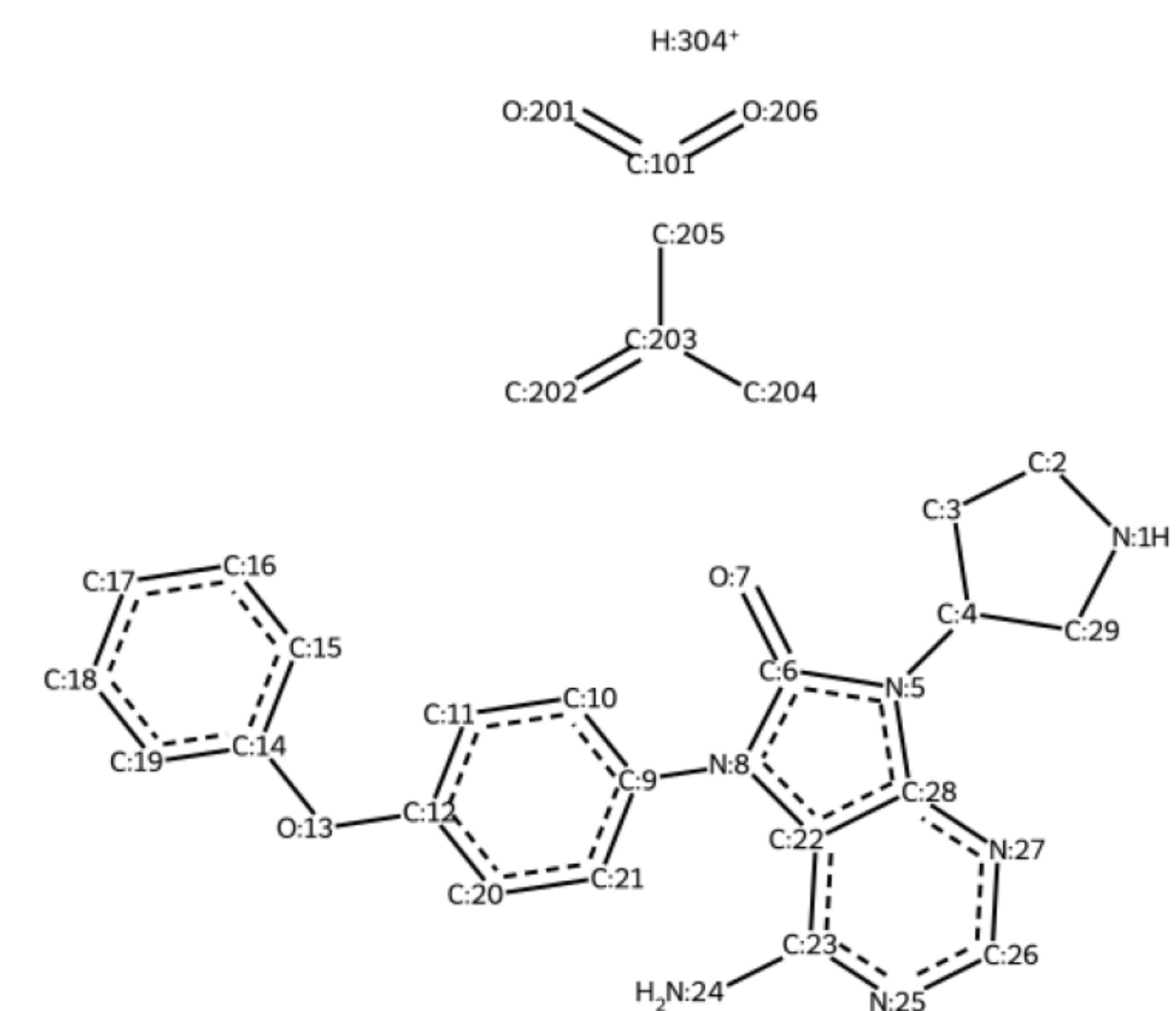
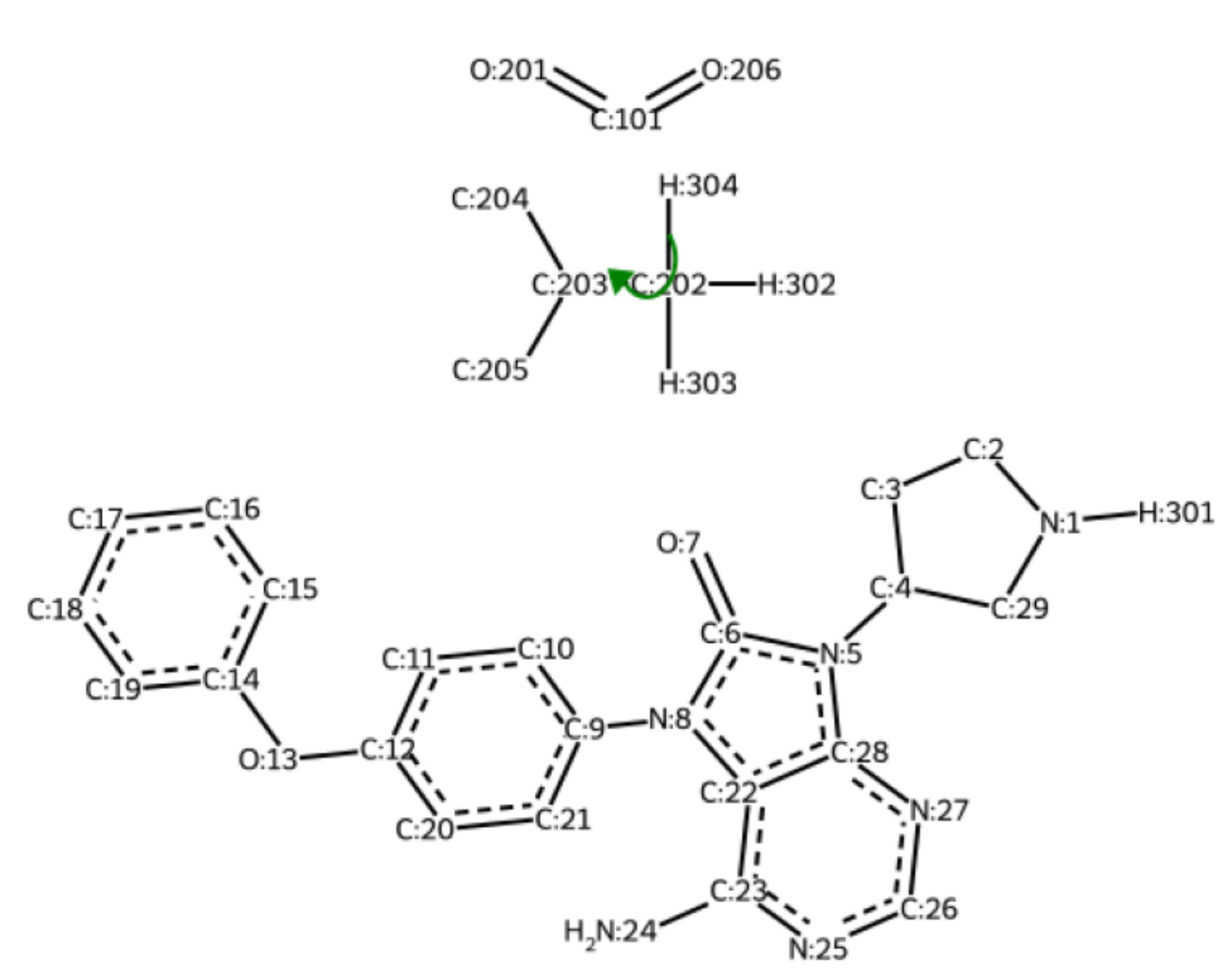
step #3

step #4

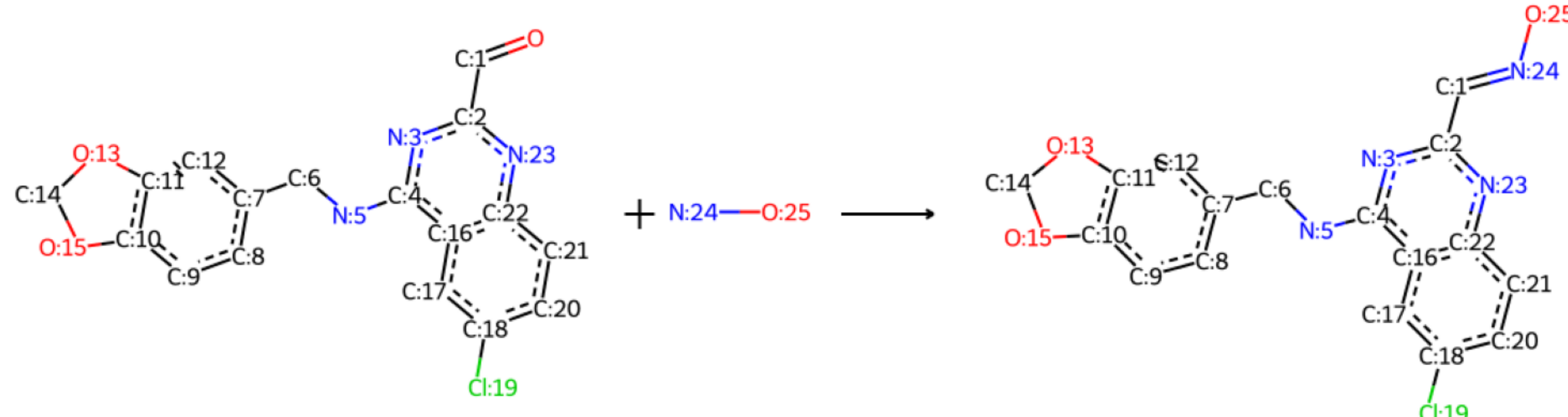


step #5

Product(s)

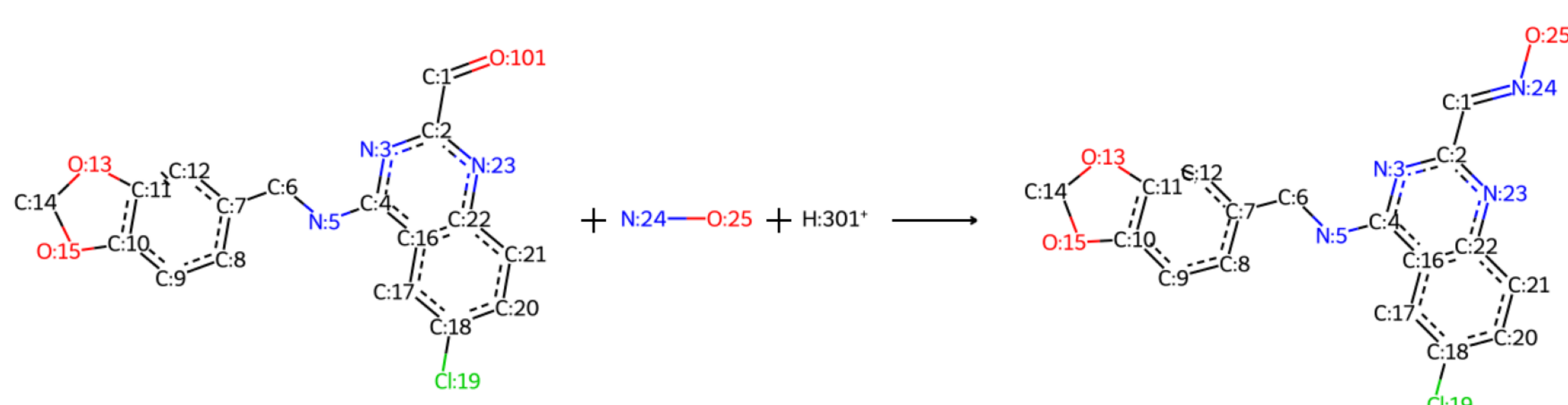


Original reaction
sampled RXN_ID:42)



Identified mechanistic class -
imine_formation reaction

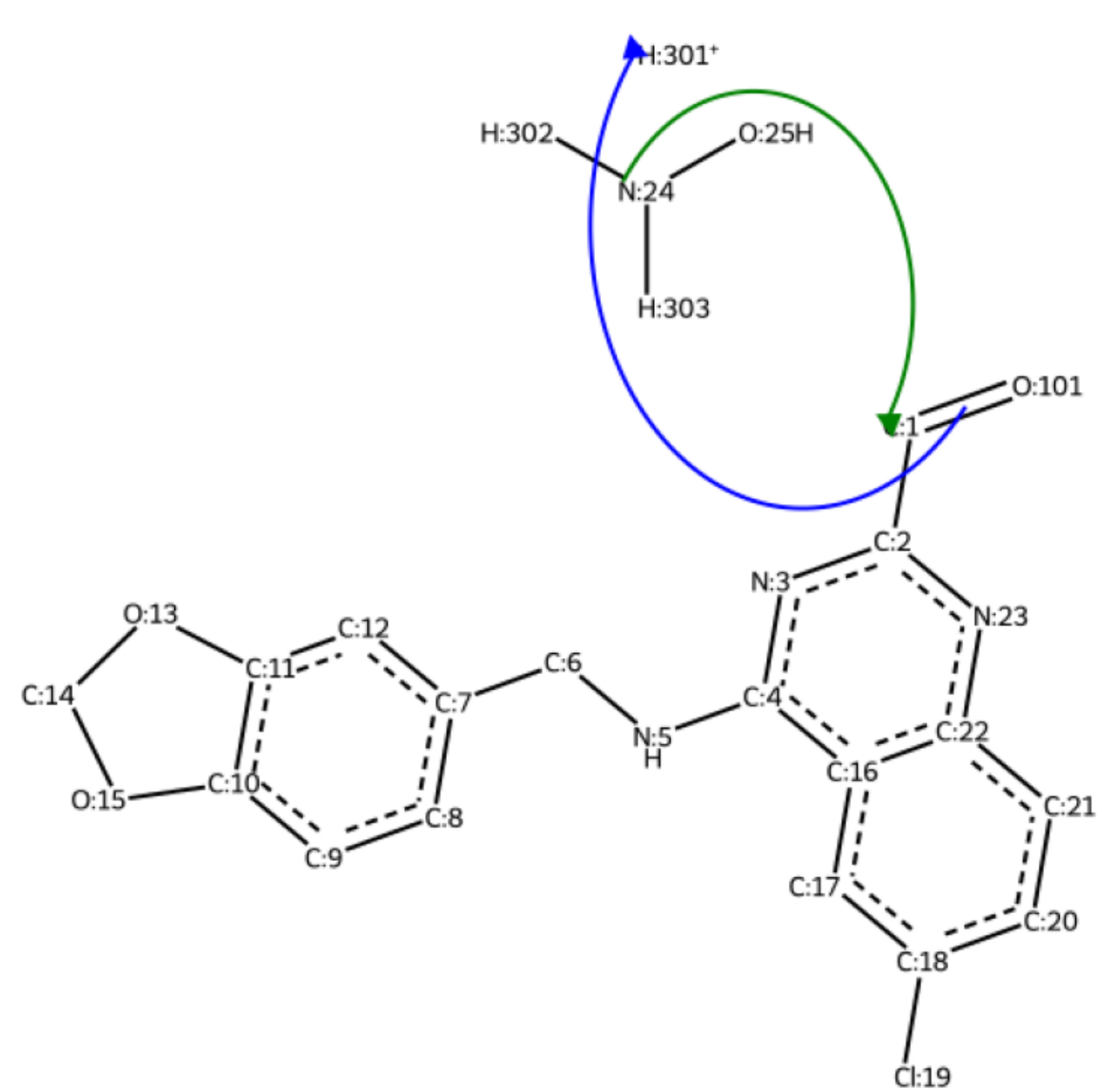
Reaction with missing reagents recovered



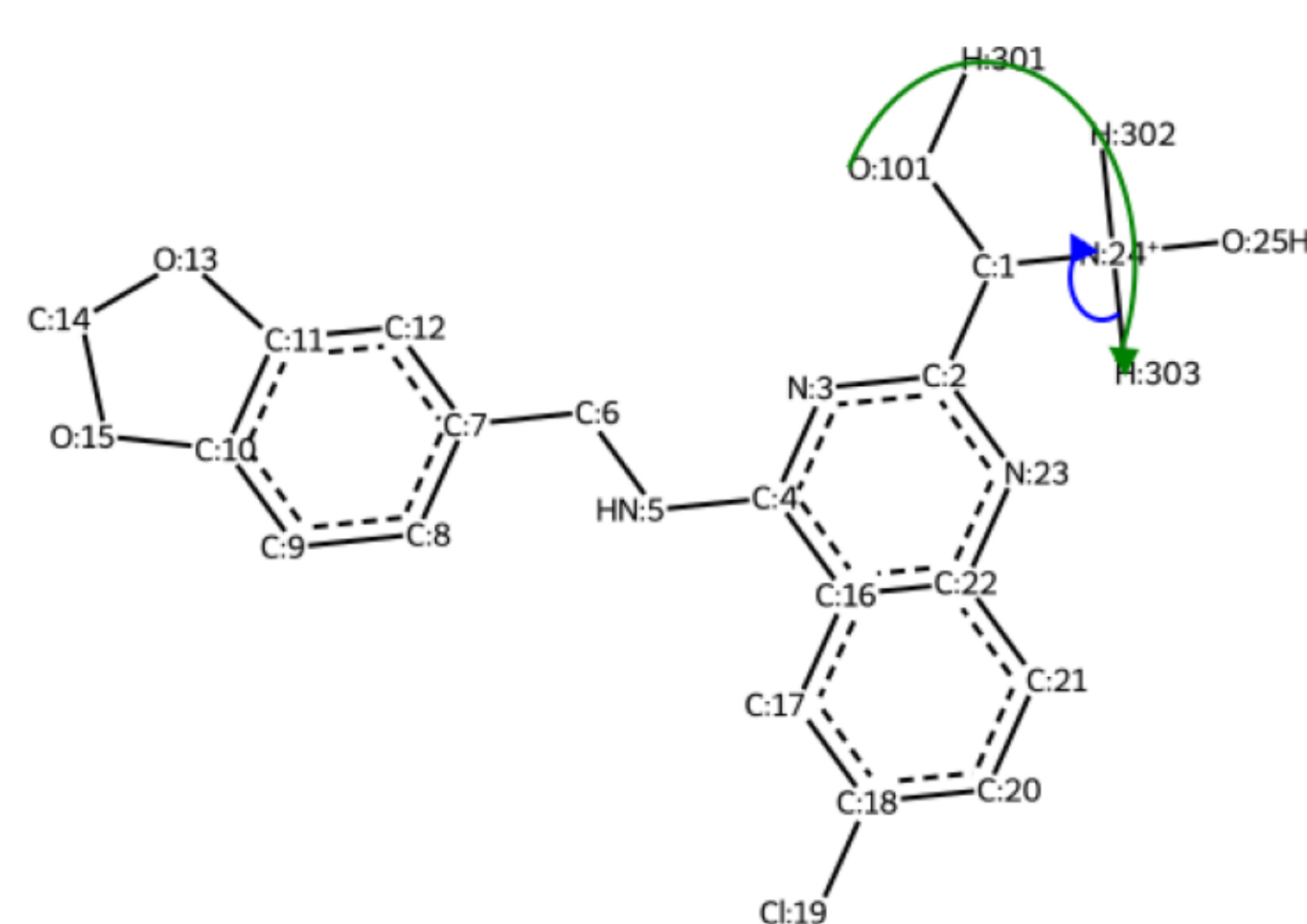
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

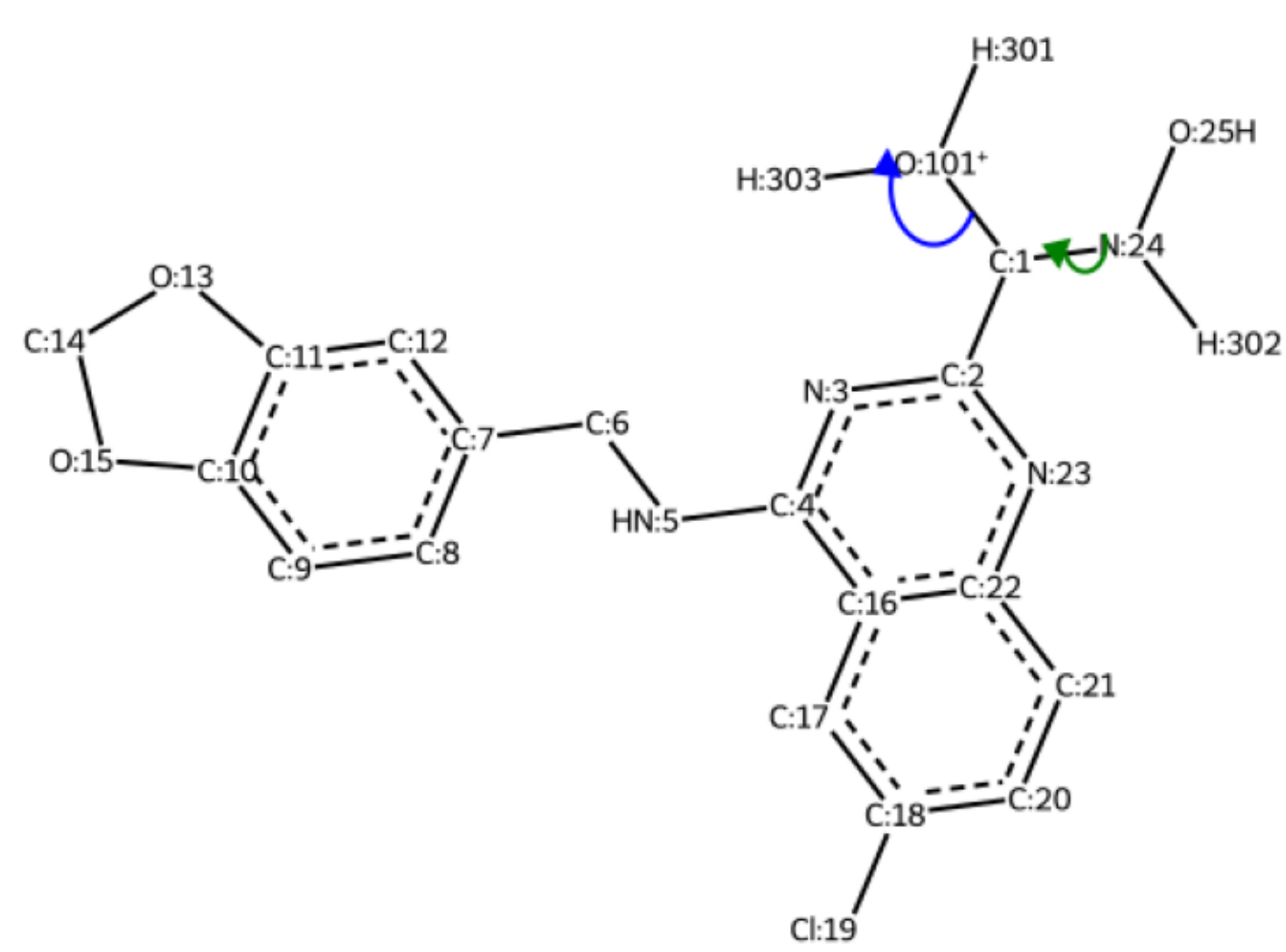
step #1



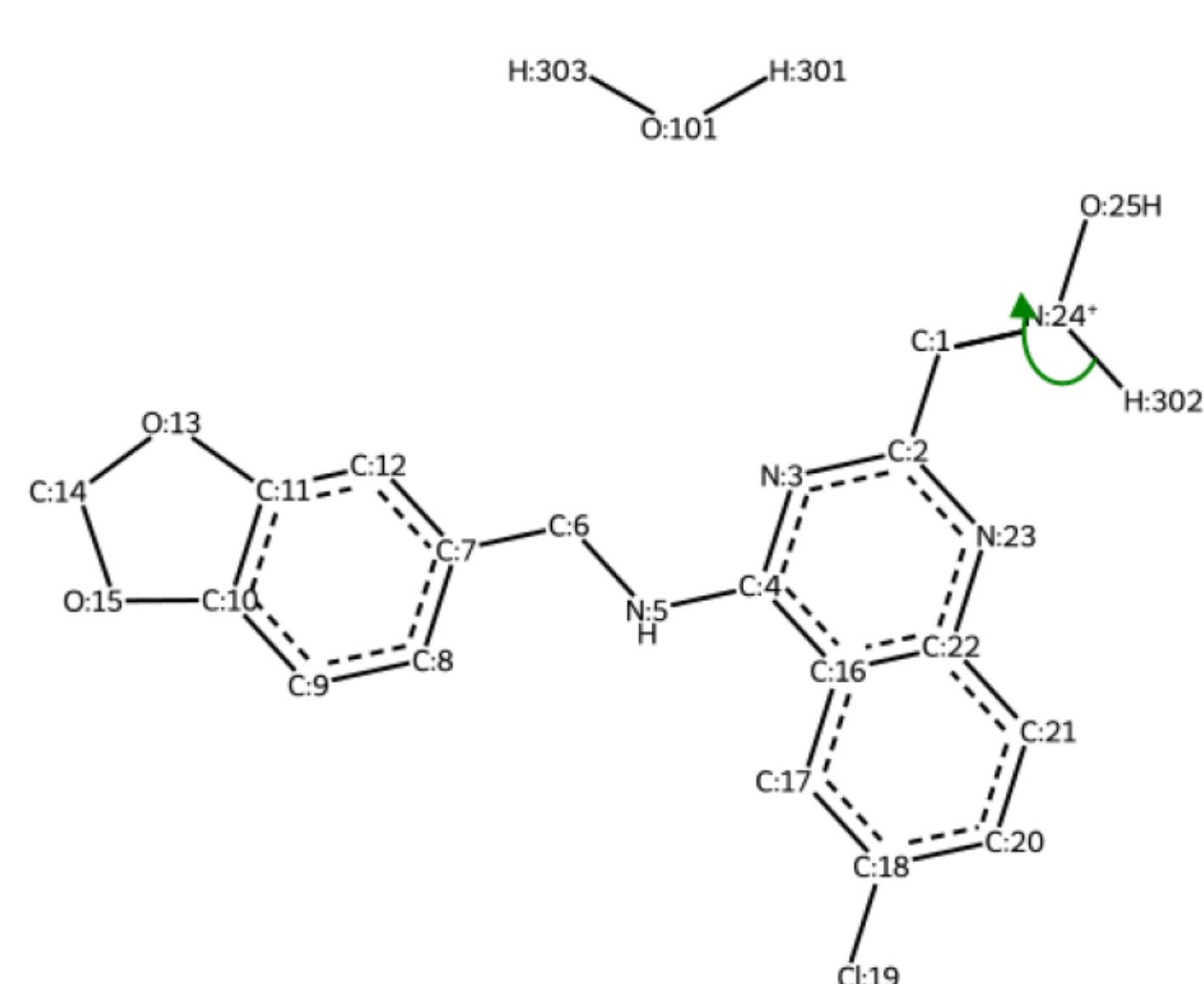
step #2



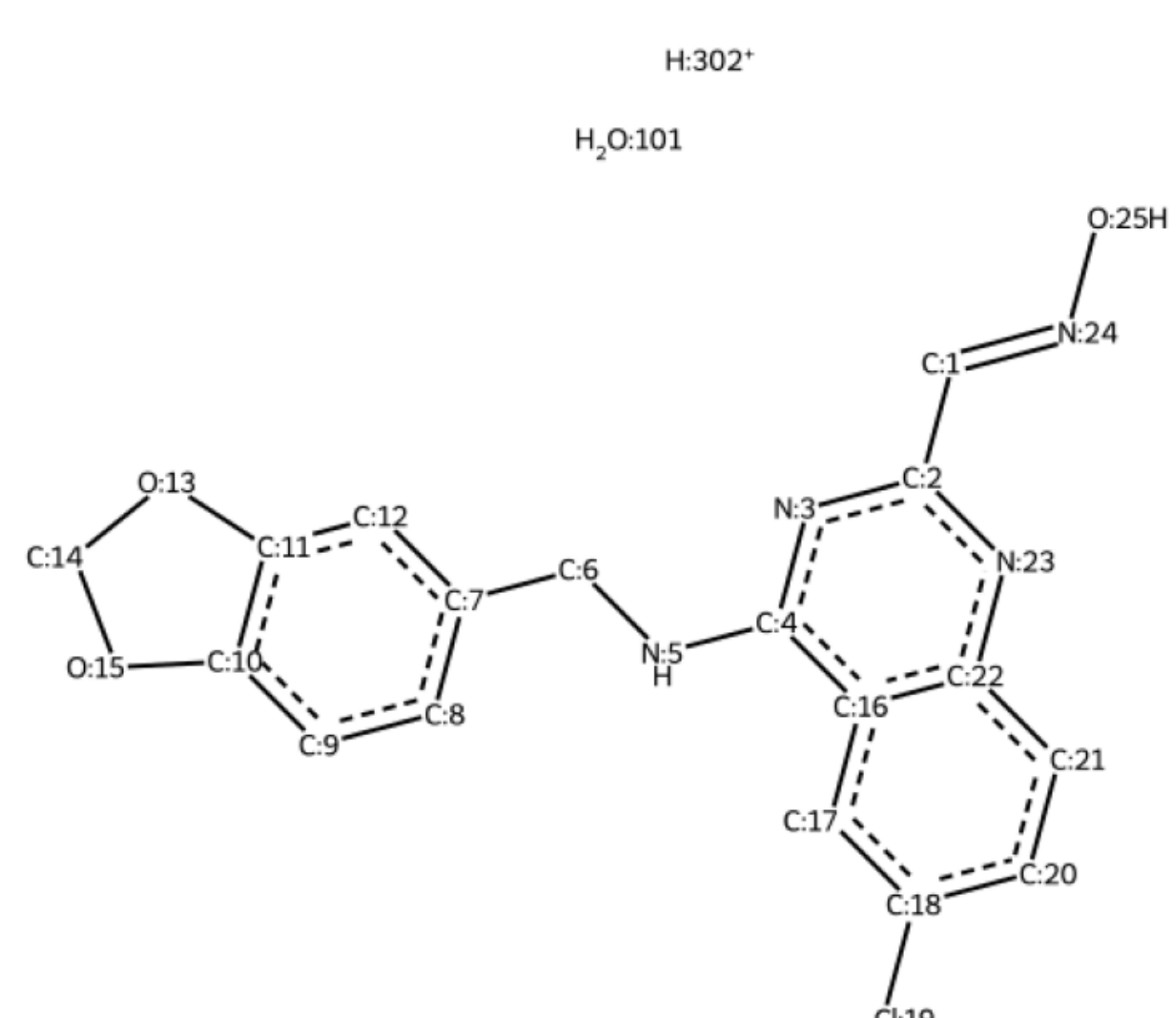
step #3



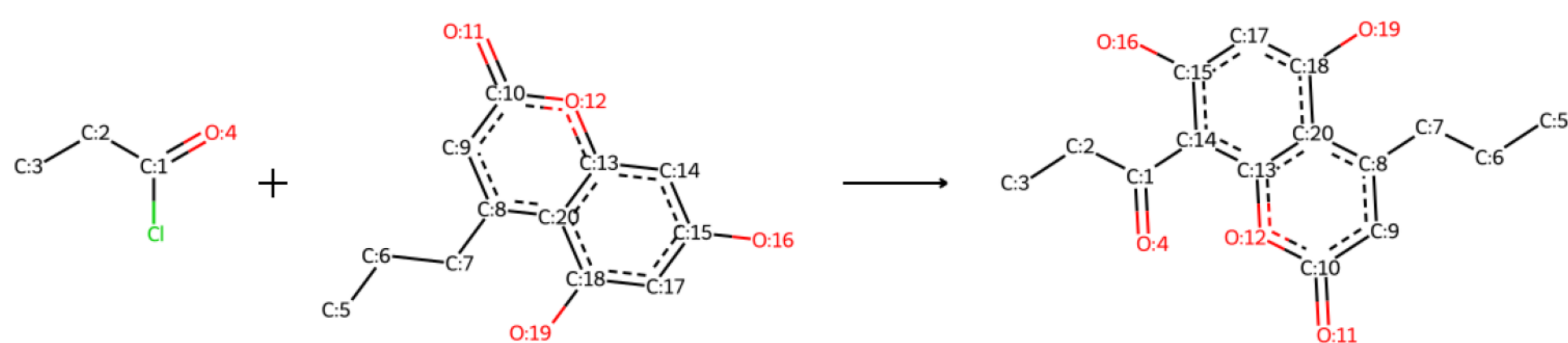
step #4



Product(s)

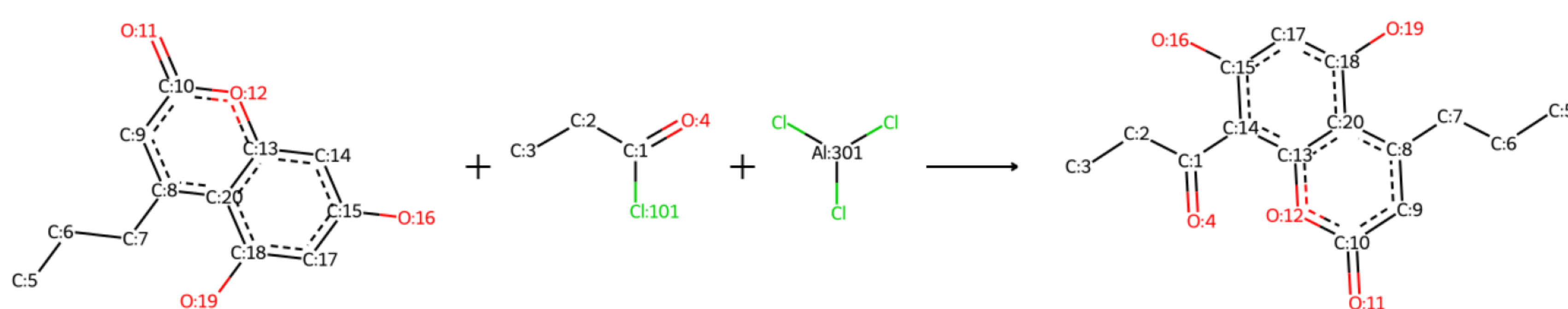


Original reaction
sampled RXN_ID:43)



Identified mechanistic class -
Friedel_Crafts_acylation reaction

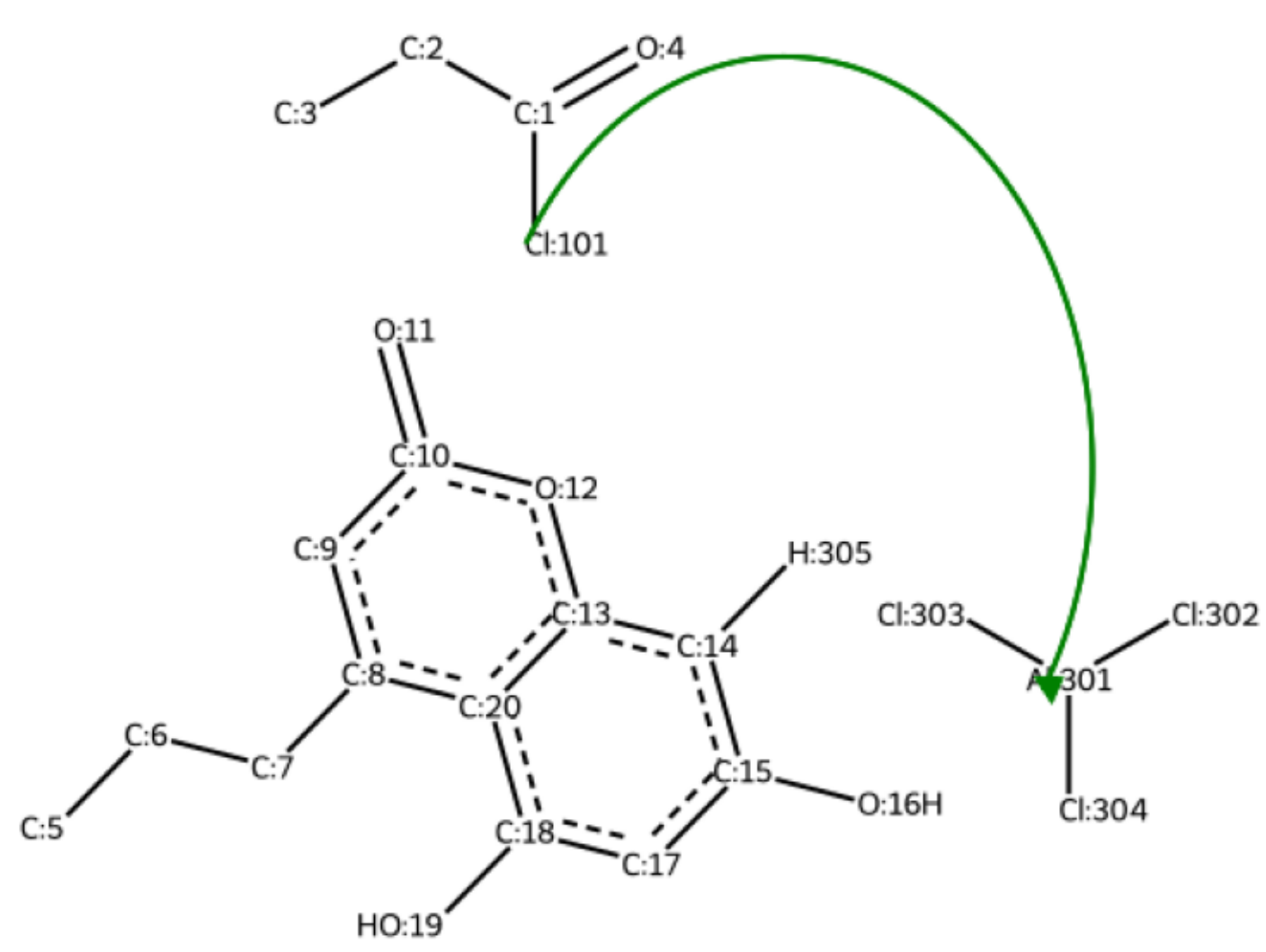
Reaction with missing reagents recovered



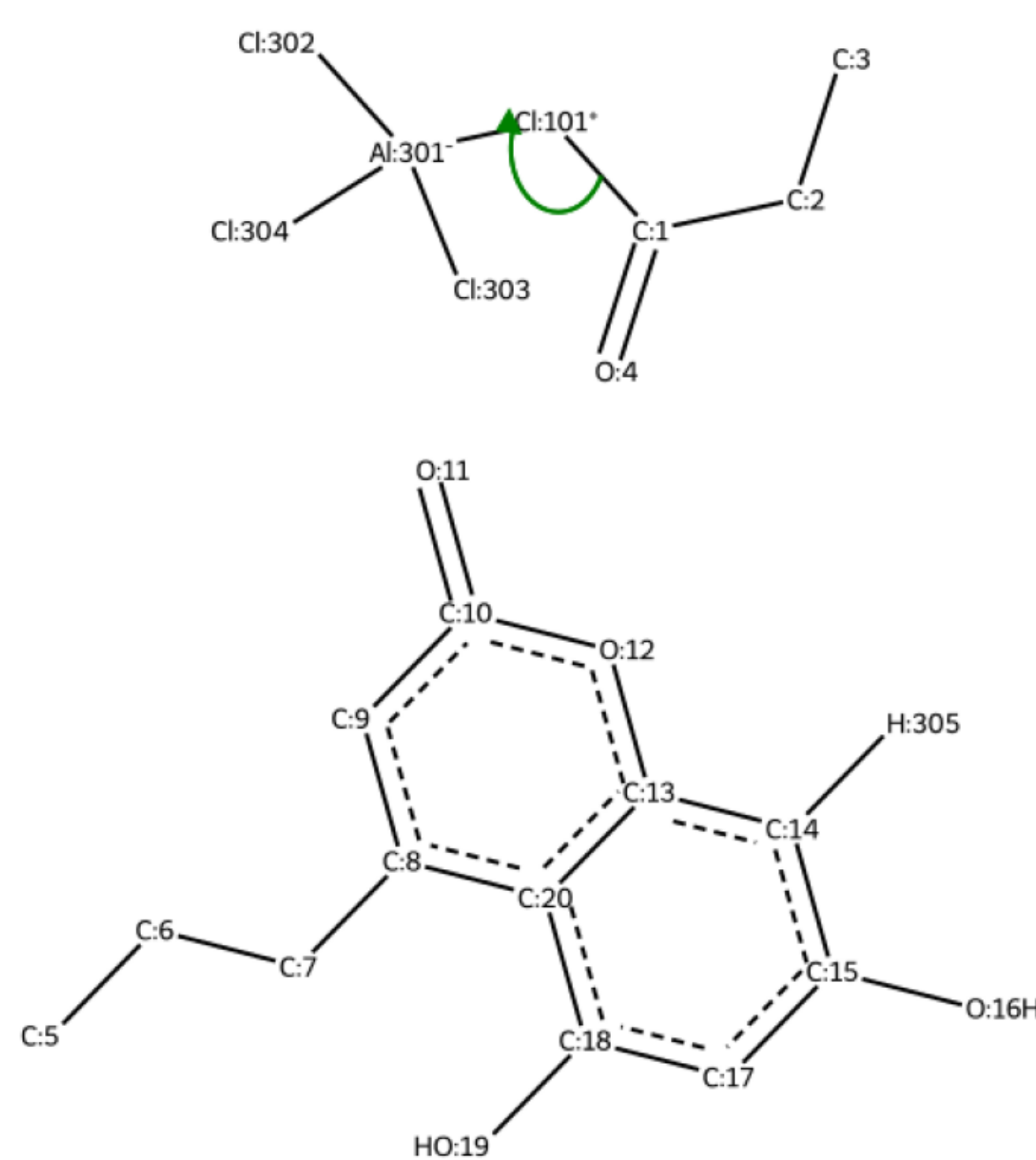
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

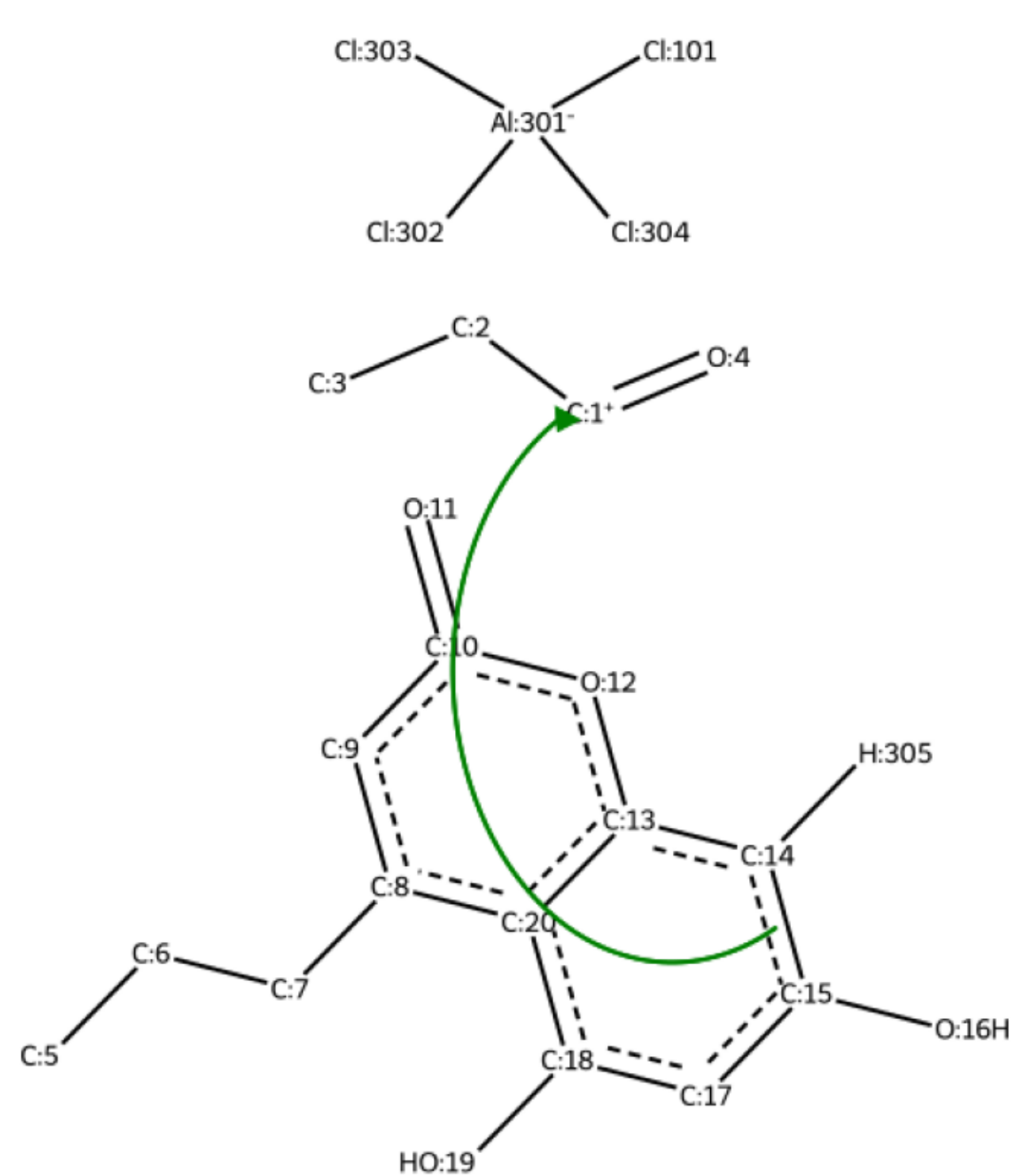
step #1



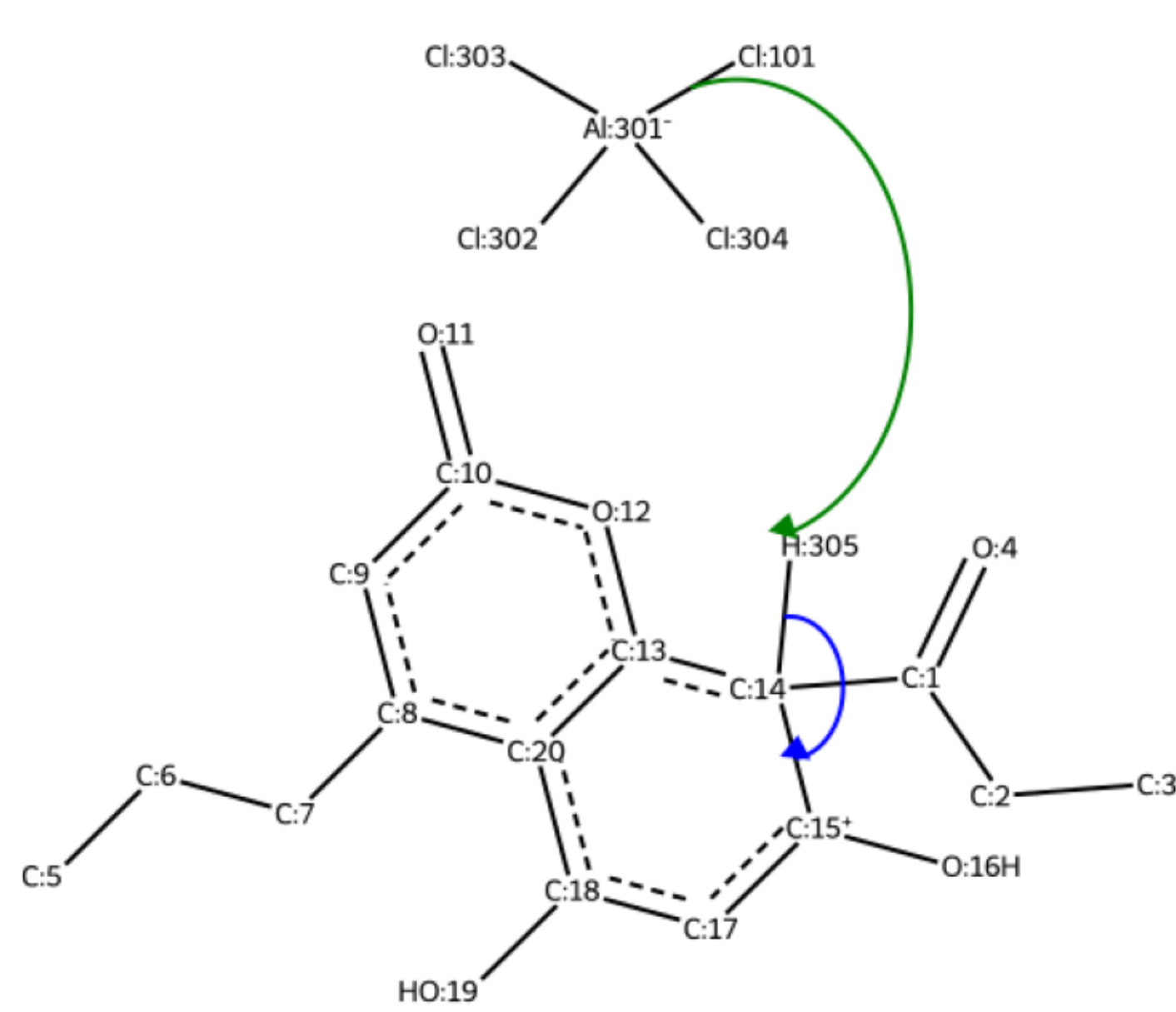
step #2



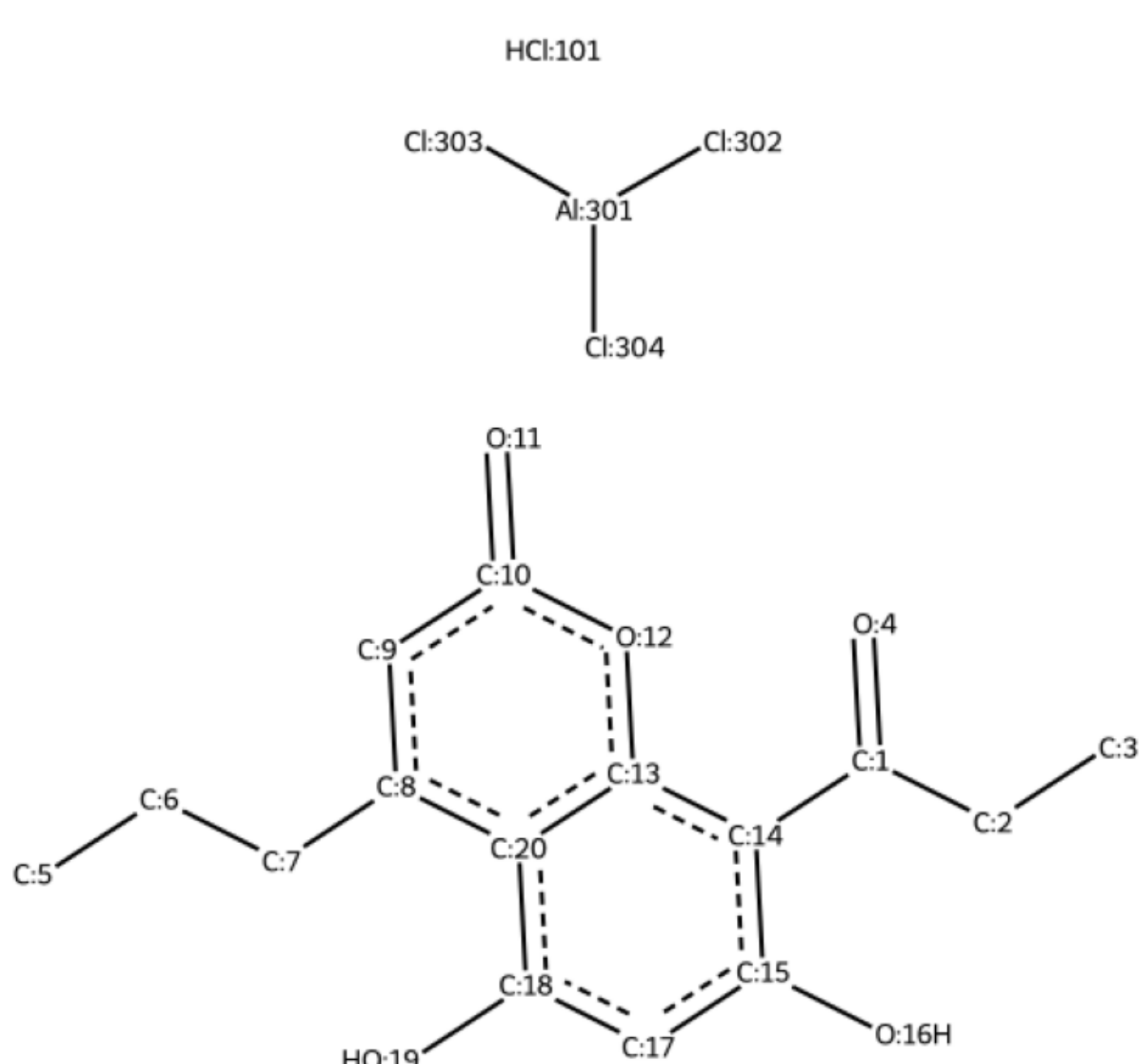
step #3



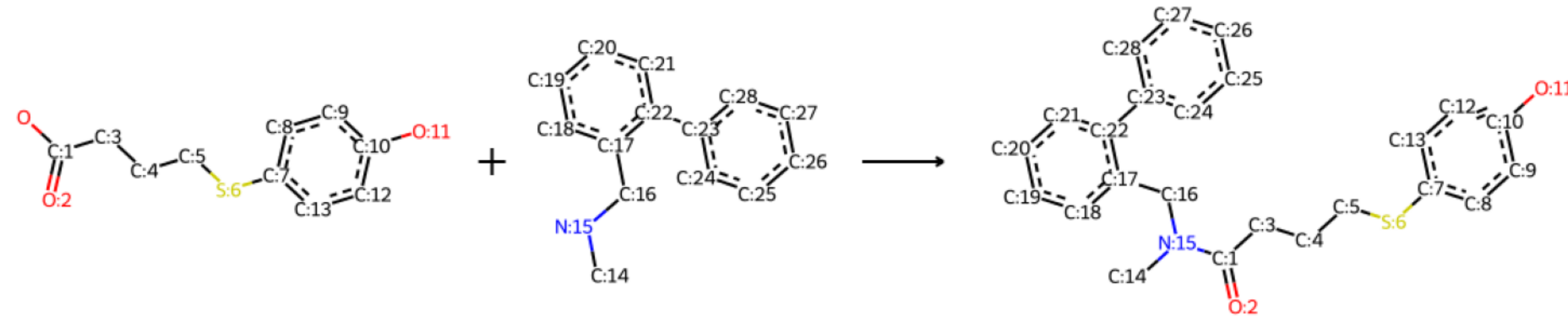
step #4



Product(s)

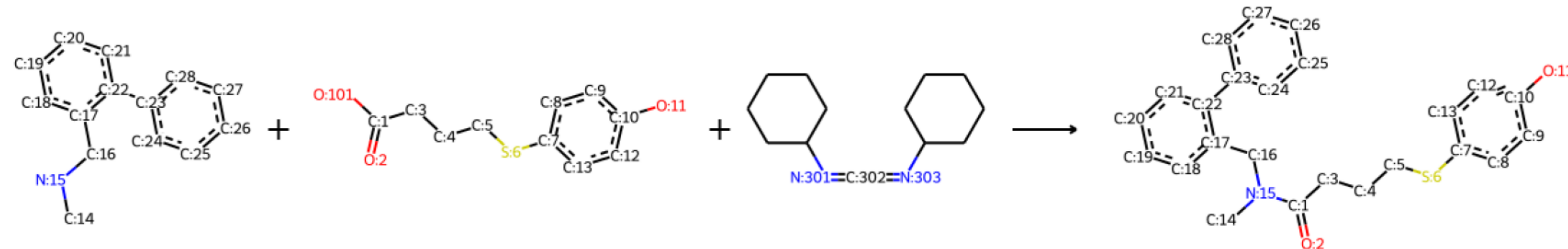


Original reaction
sampled RXN_ID:44)



Identified mechanistic class -
DCC_condensation reaction

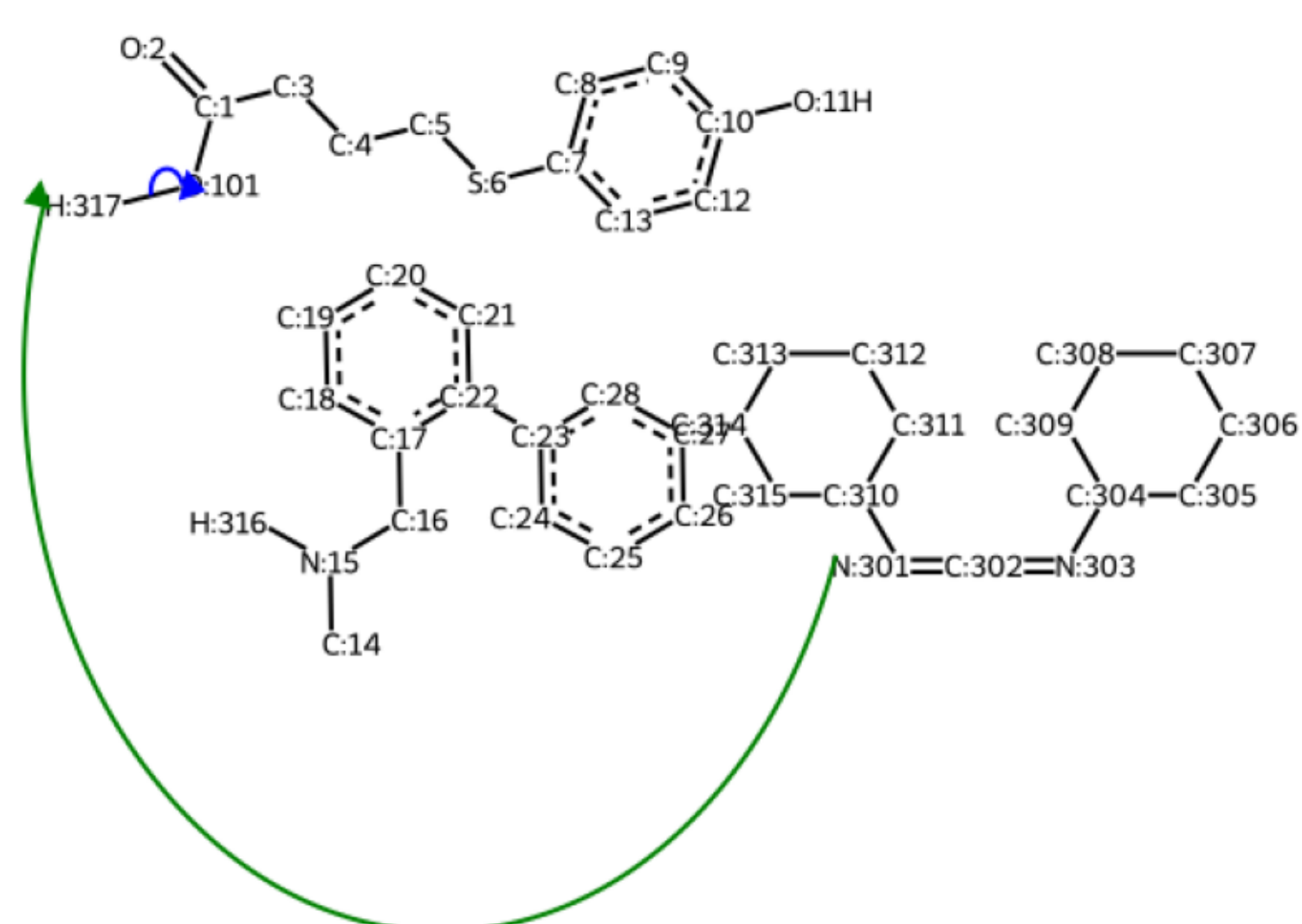
Reaction with missing reagents recovered



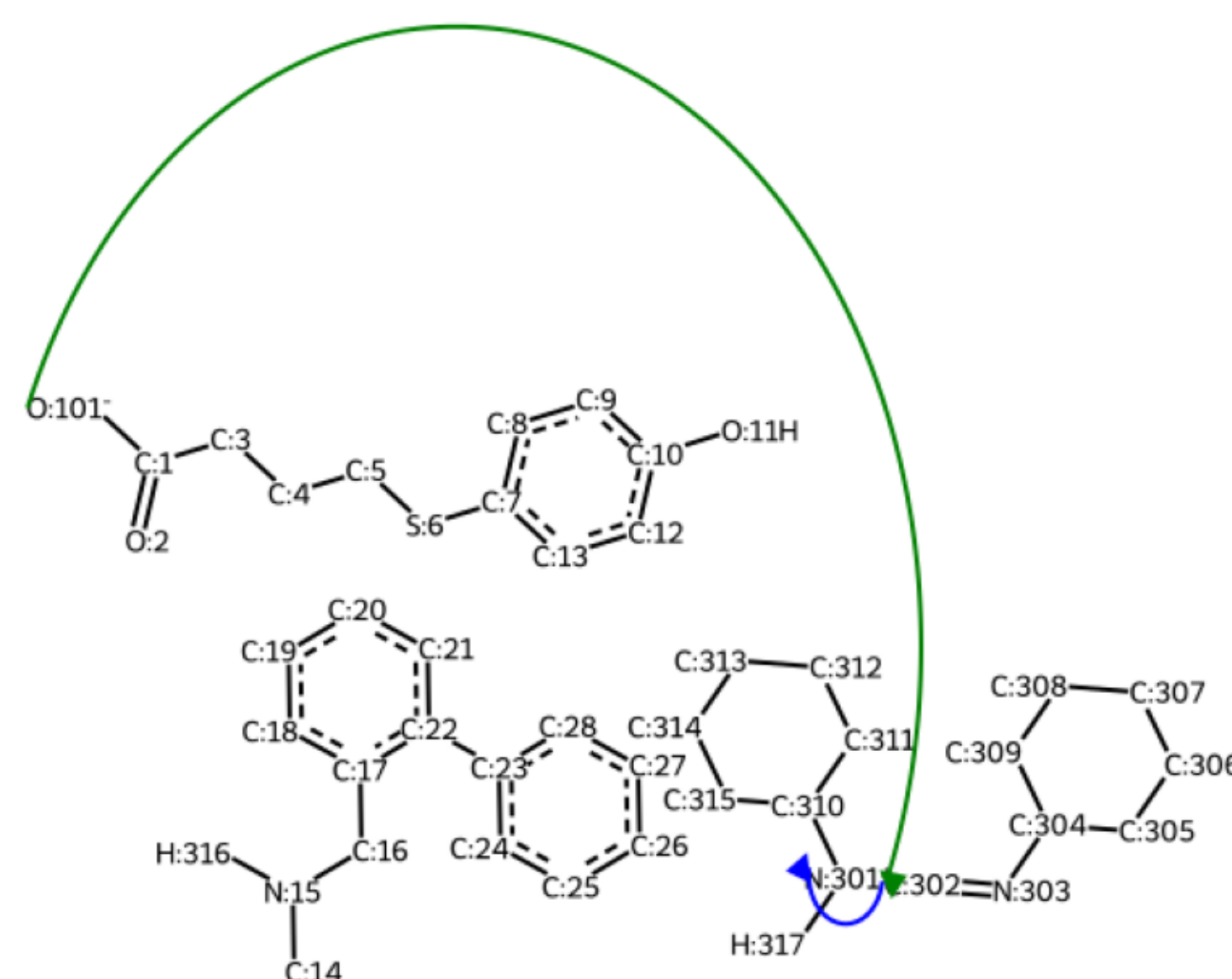
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

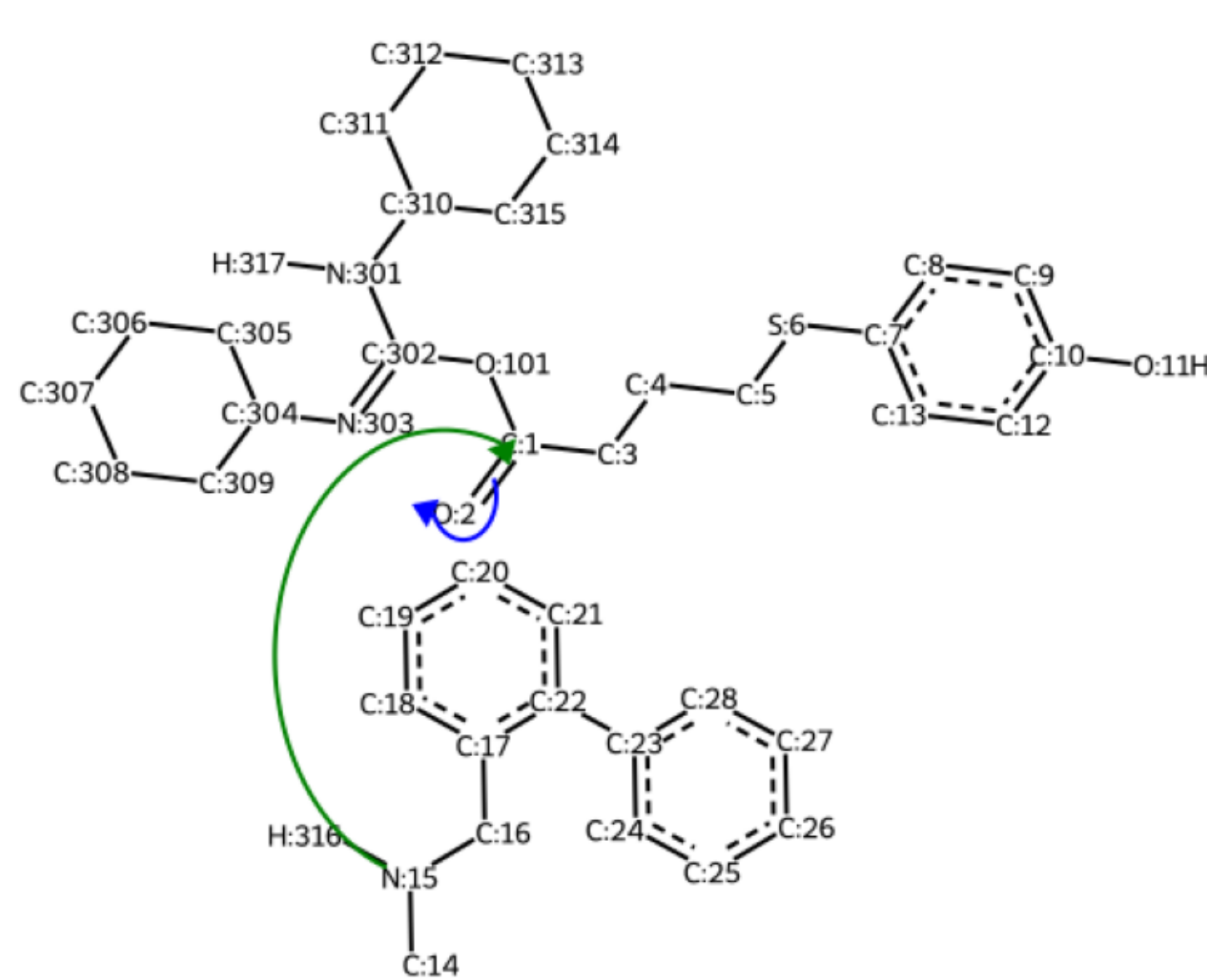
step #1



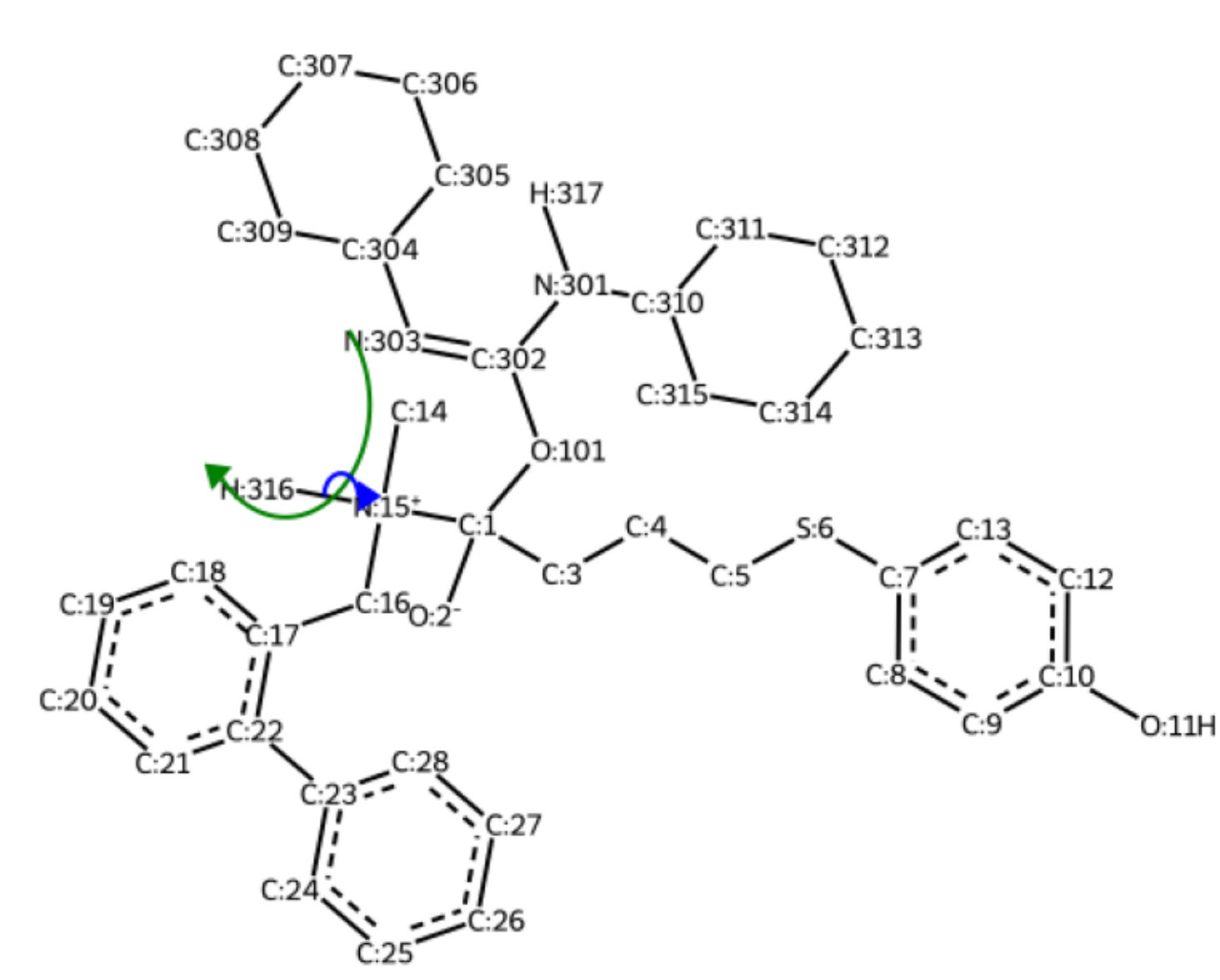
step #2



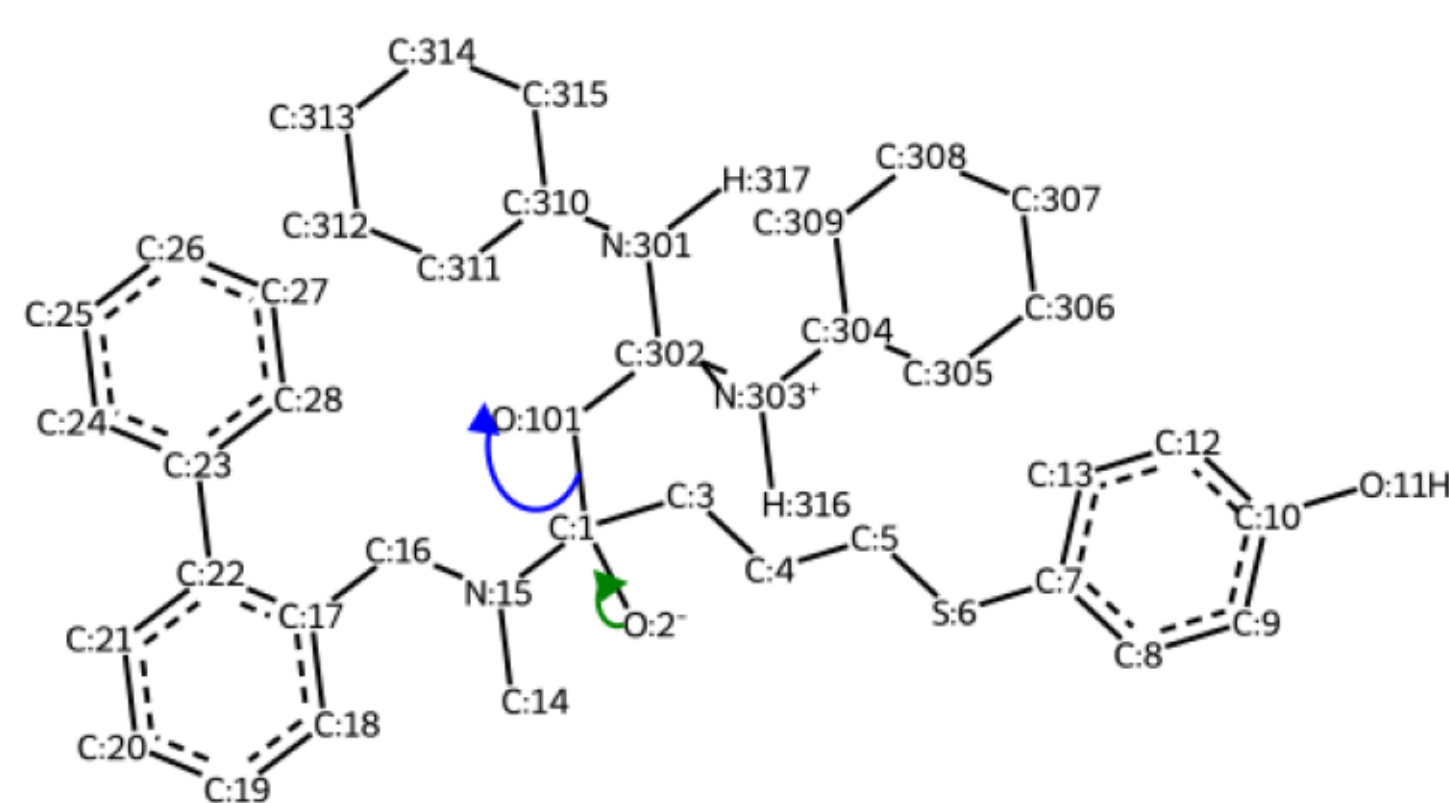
step #3



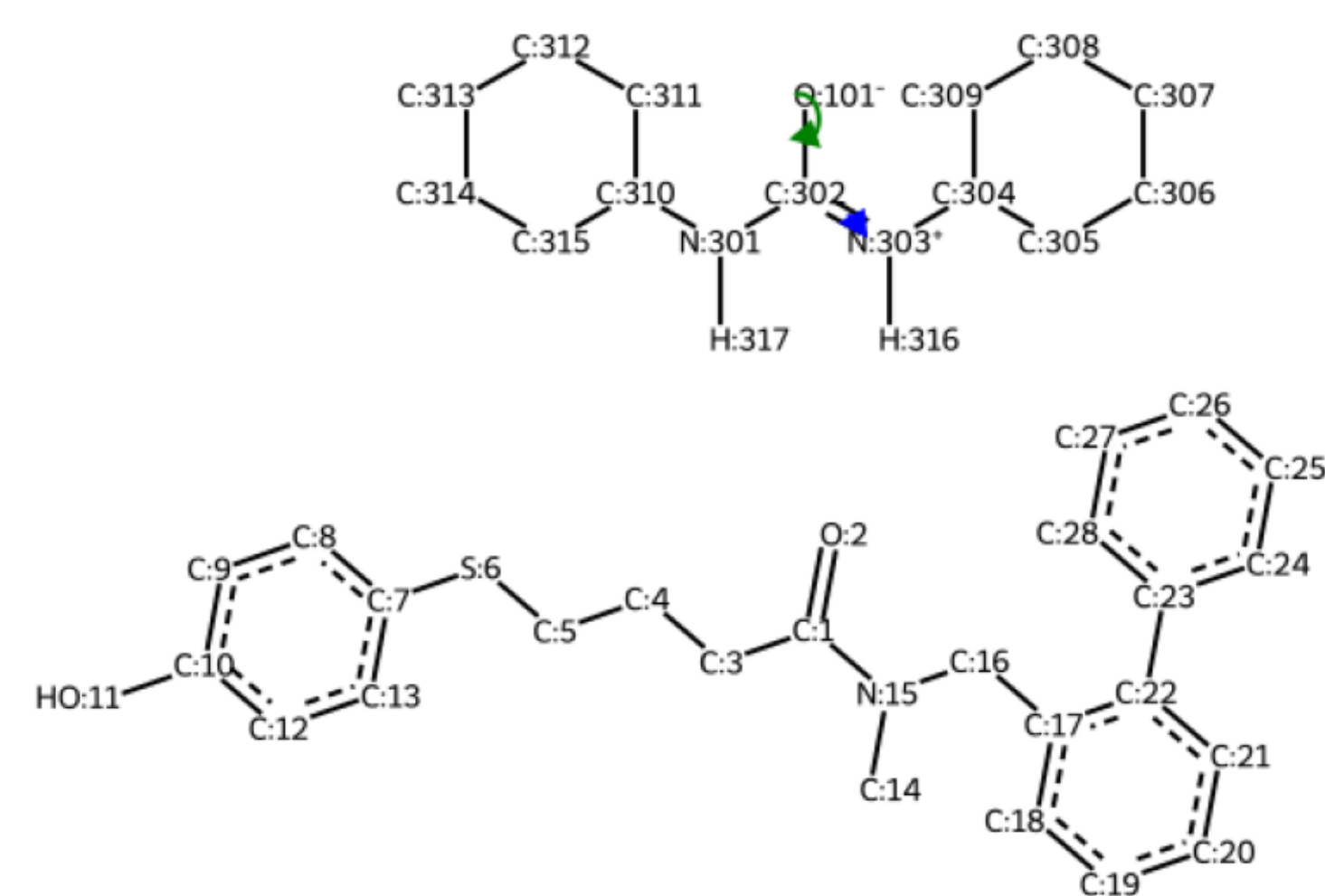
step #4



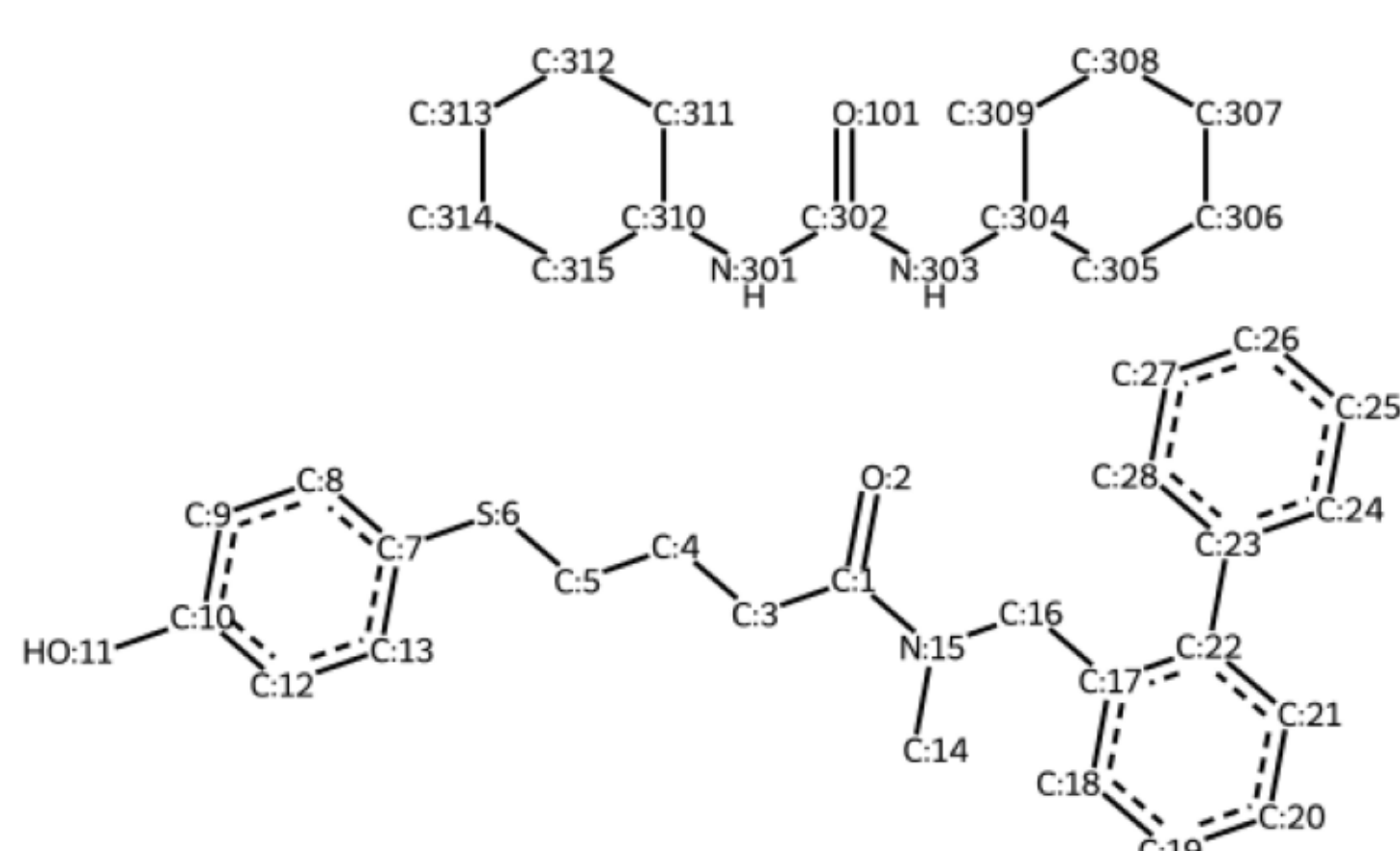
step #5



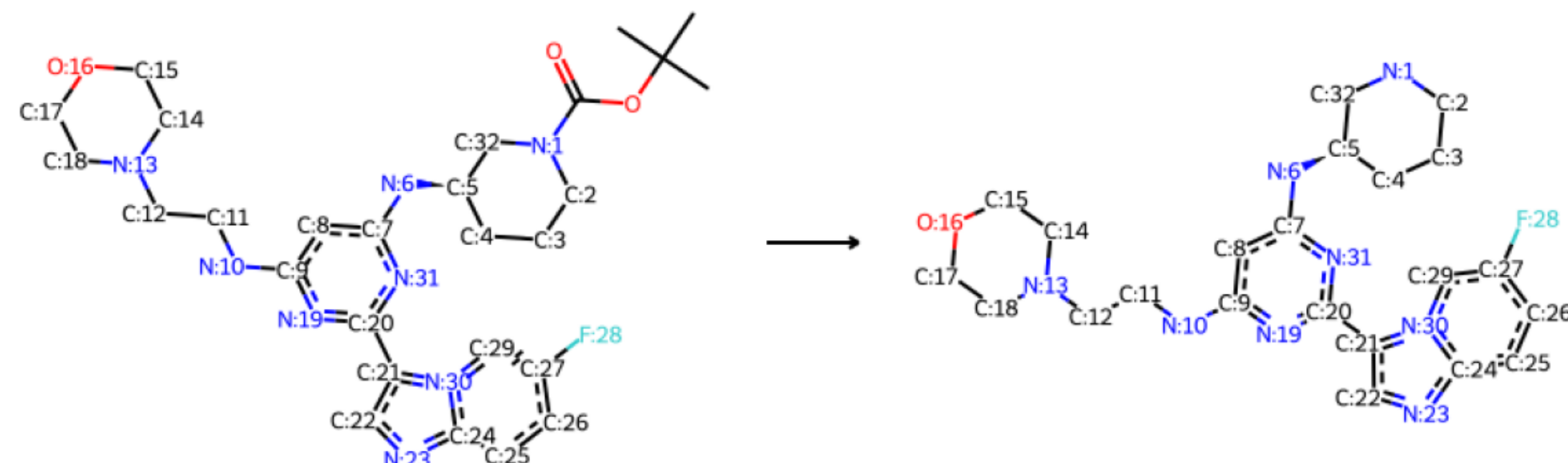
step #6



Product(s)

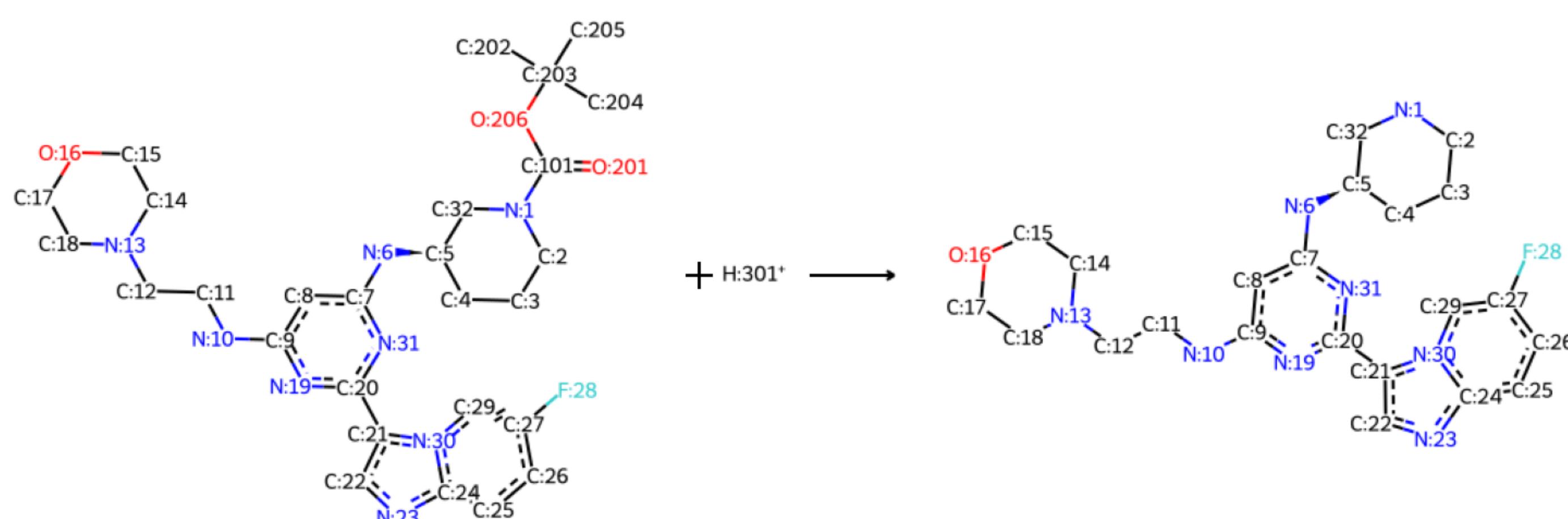


Original reaction
sampled RXN_ID:45)



Identified mechanistic class -
Boc_deprotection reaction

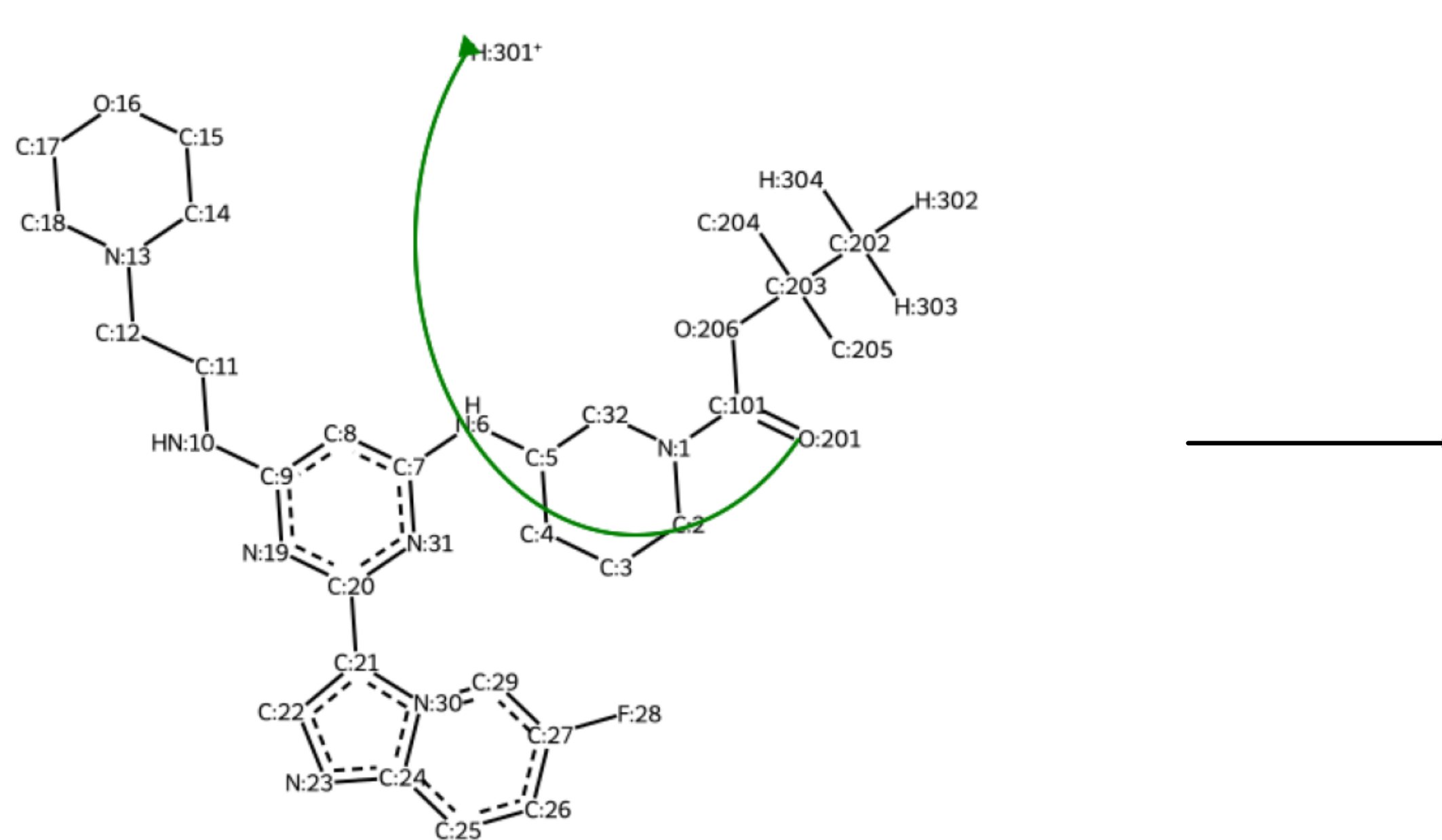
Reaction with missing reagents recovered



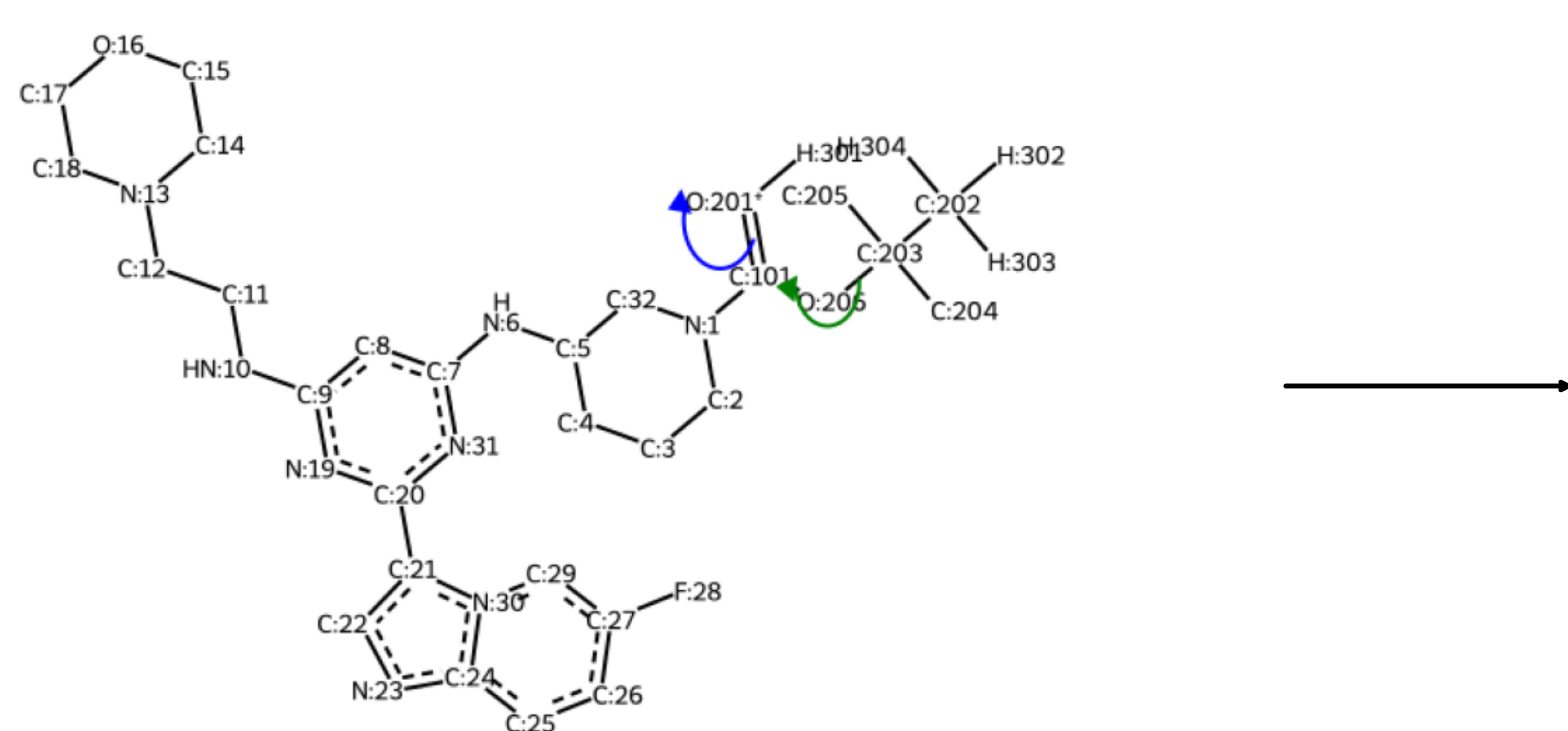
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

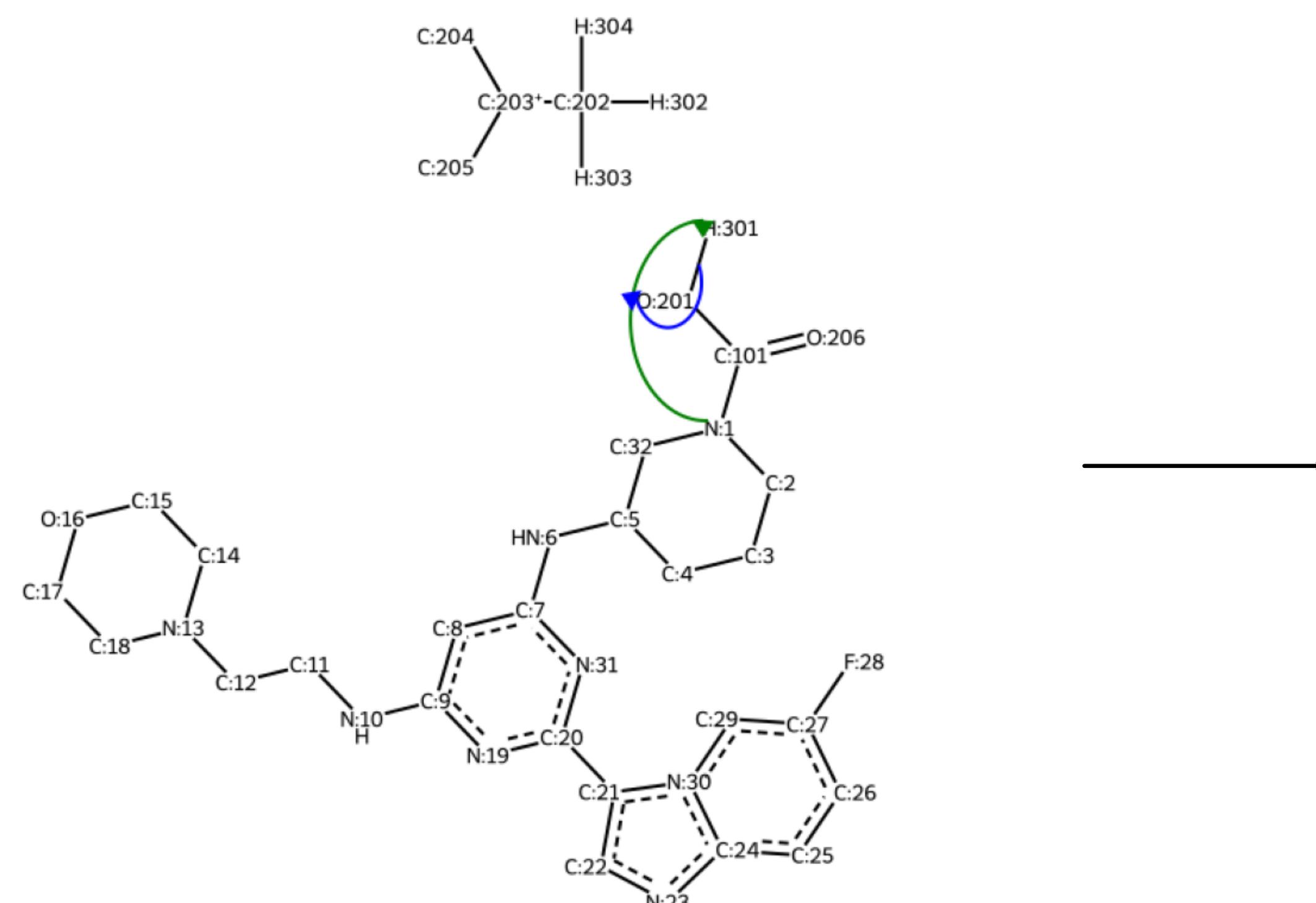
step #1



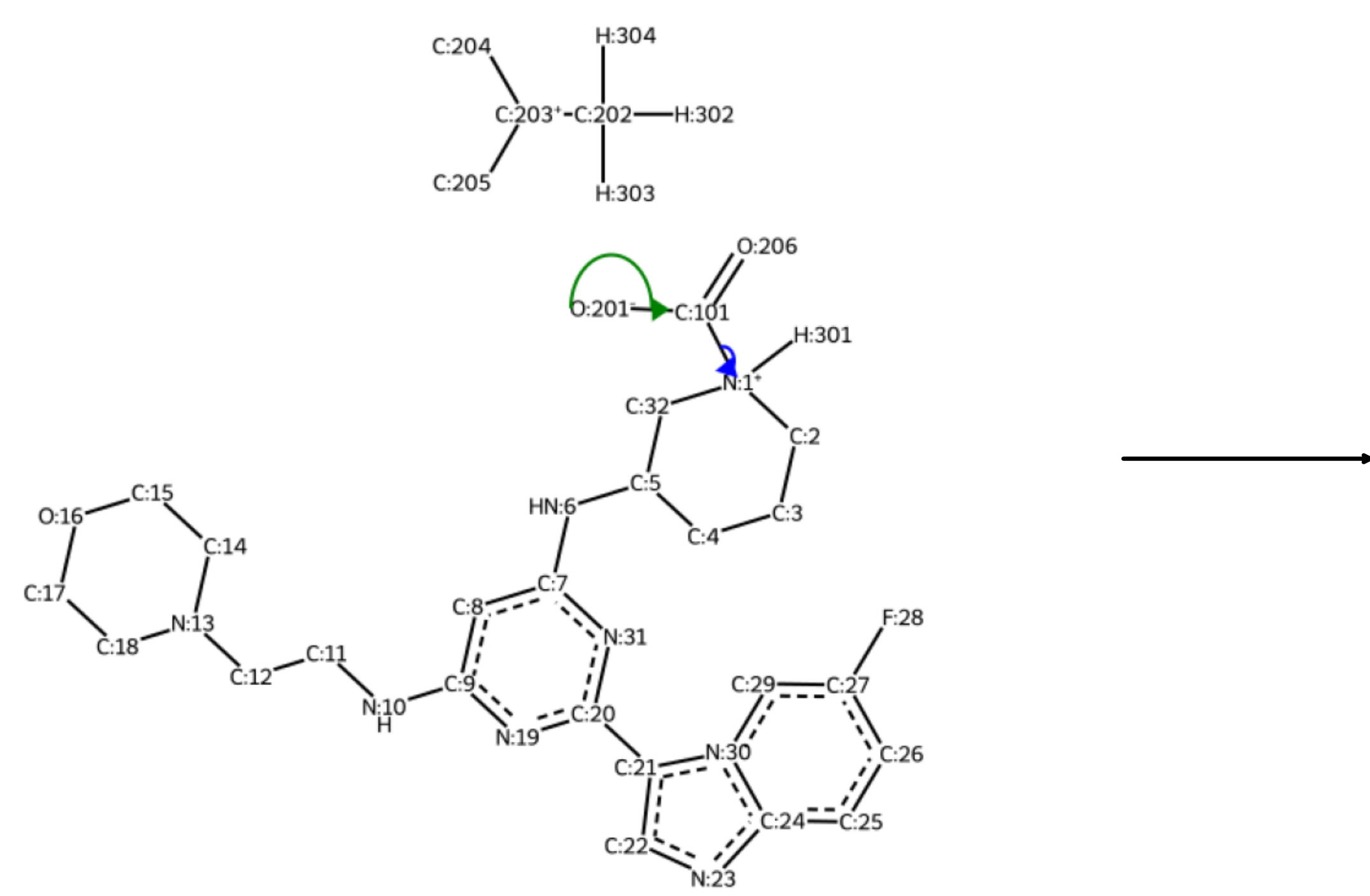
step #2



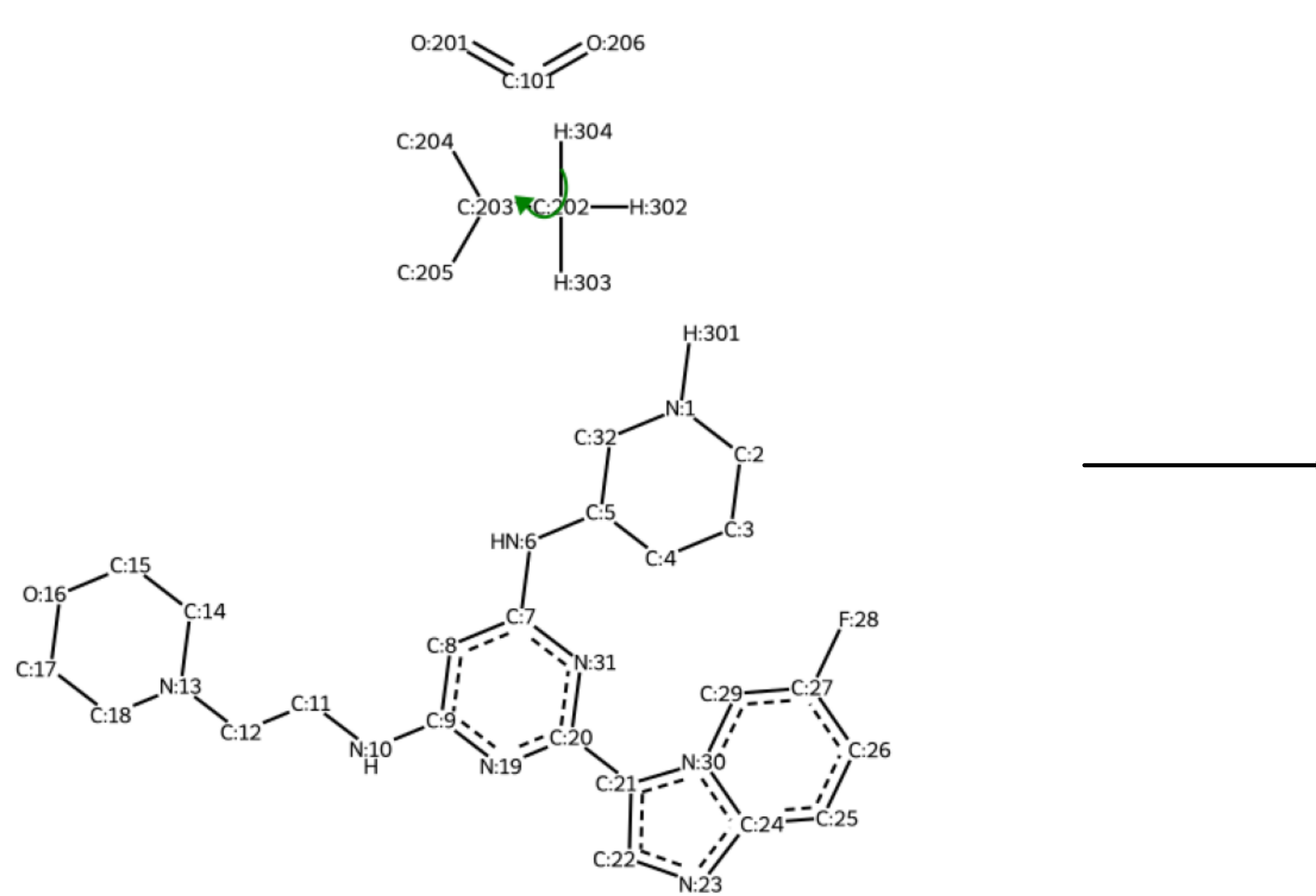
step #3



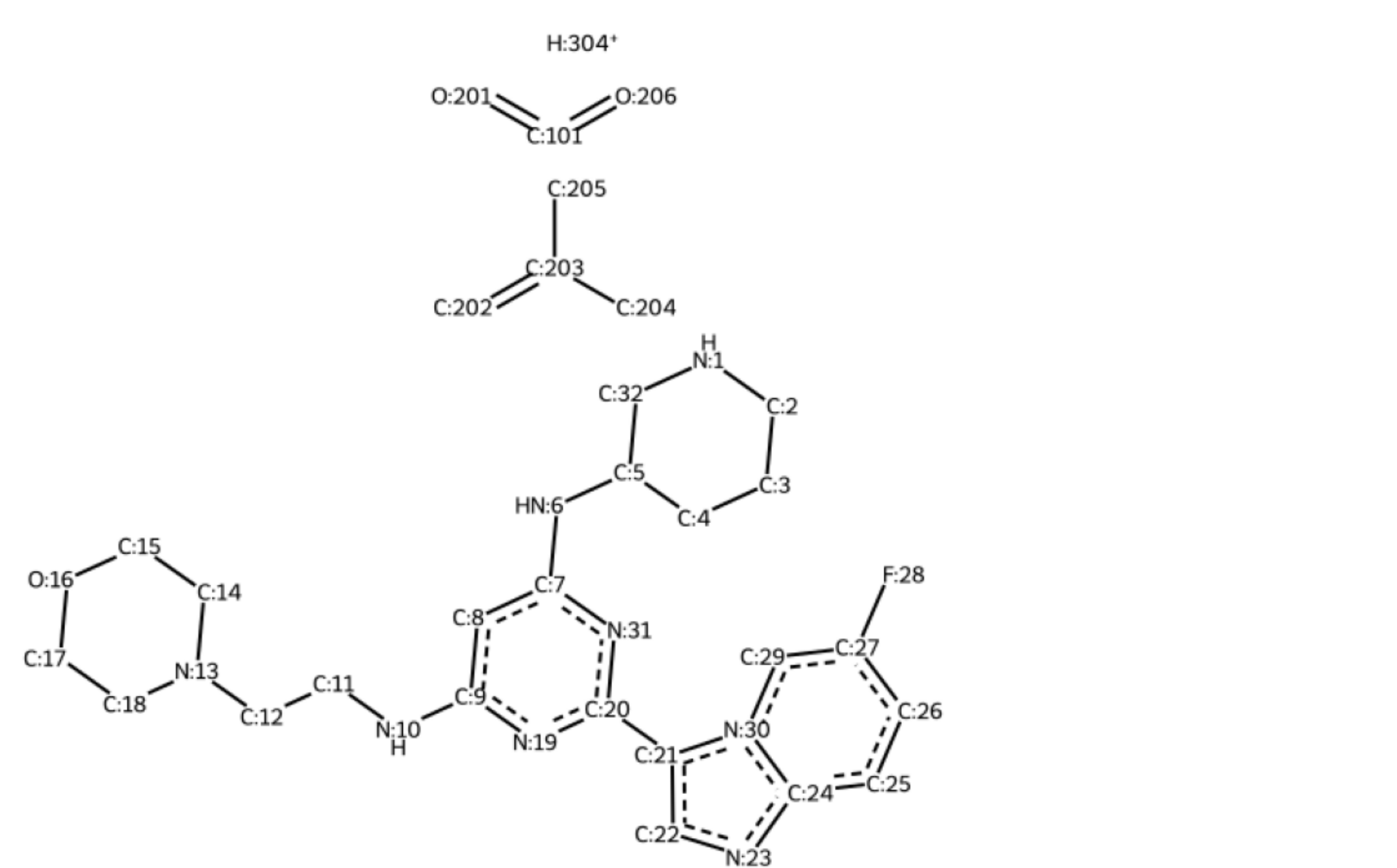
step #4



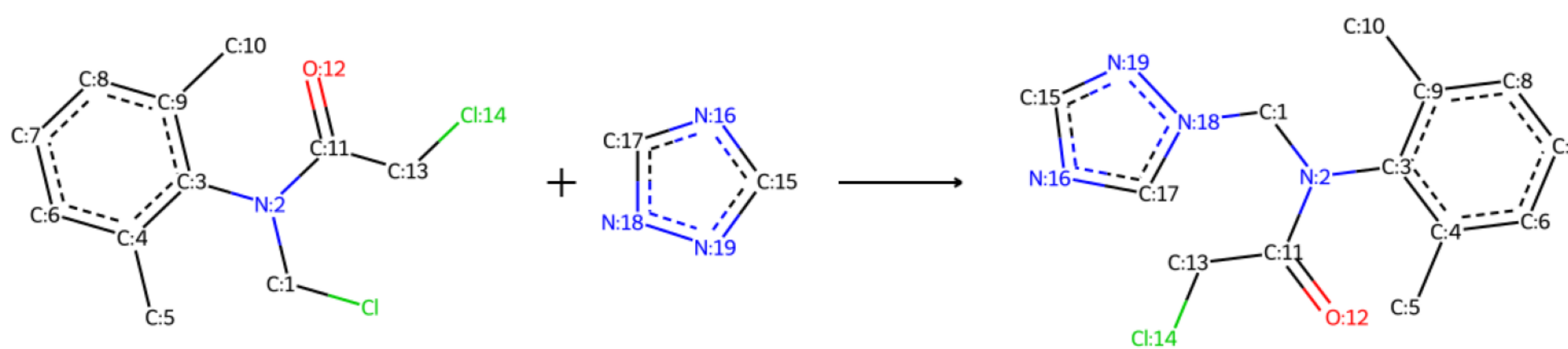
step #5



Product(s)

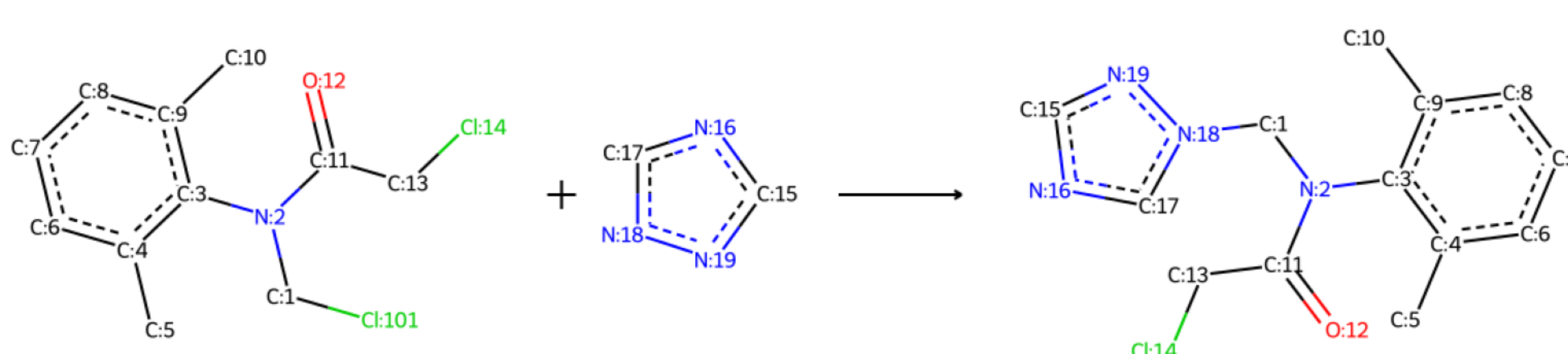


Original reaction
sampled RXN_ID:46)



Identified mechanistic class -
SN2 reaction

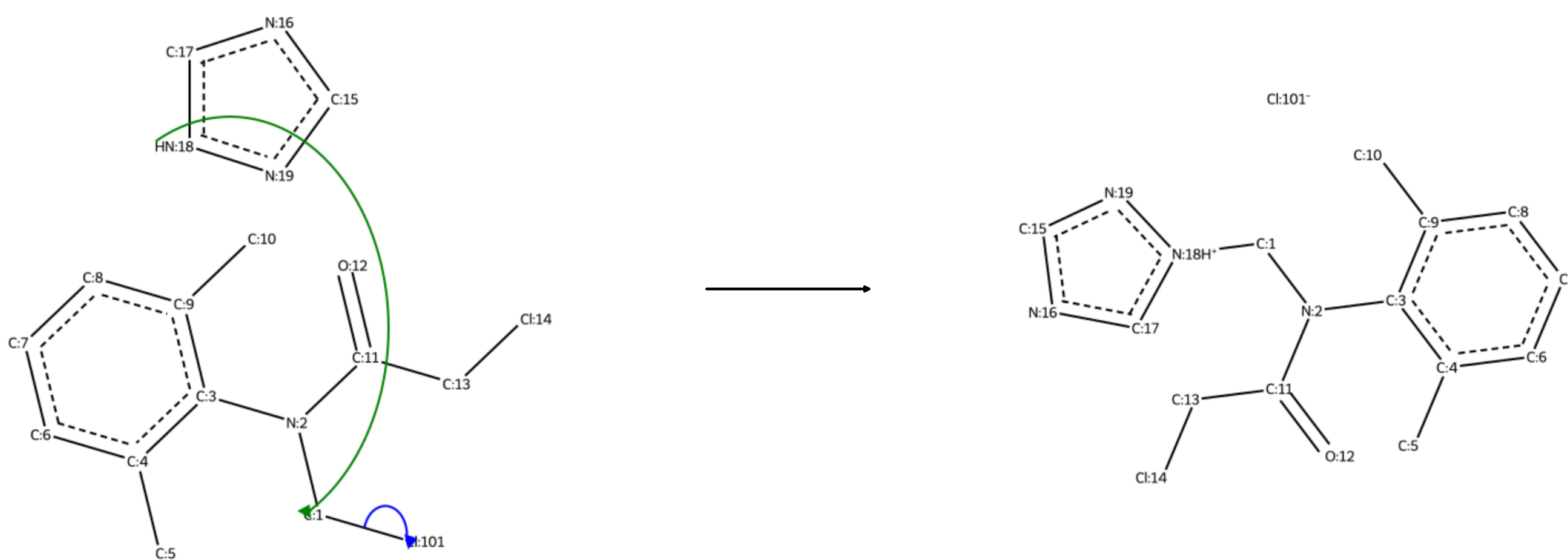
Reaction with missing reagents recovered



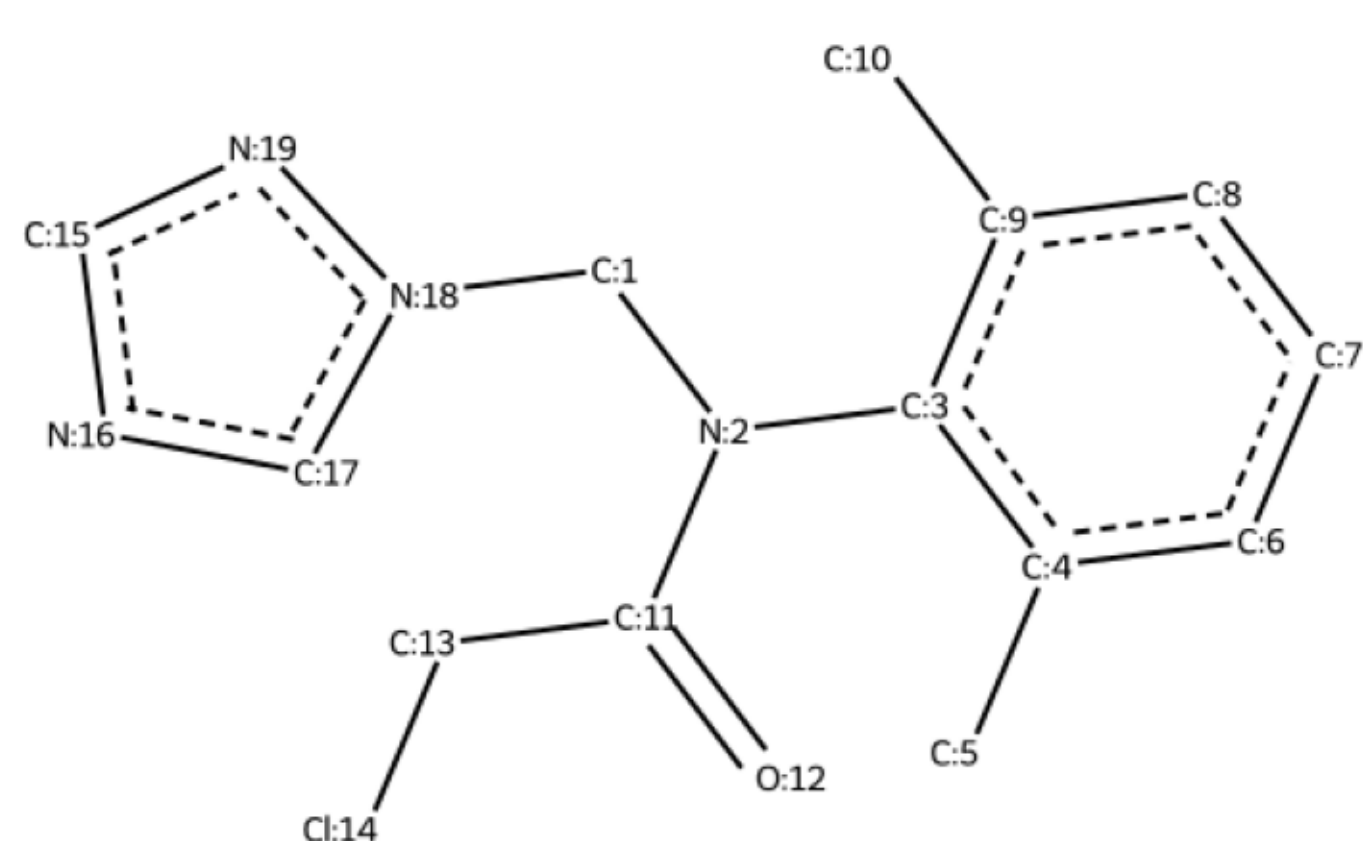
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

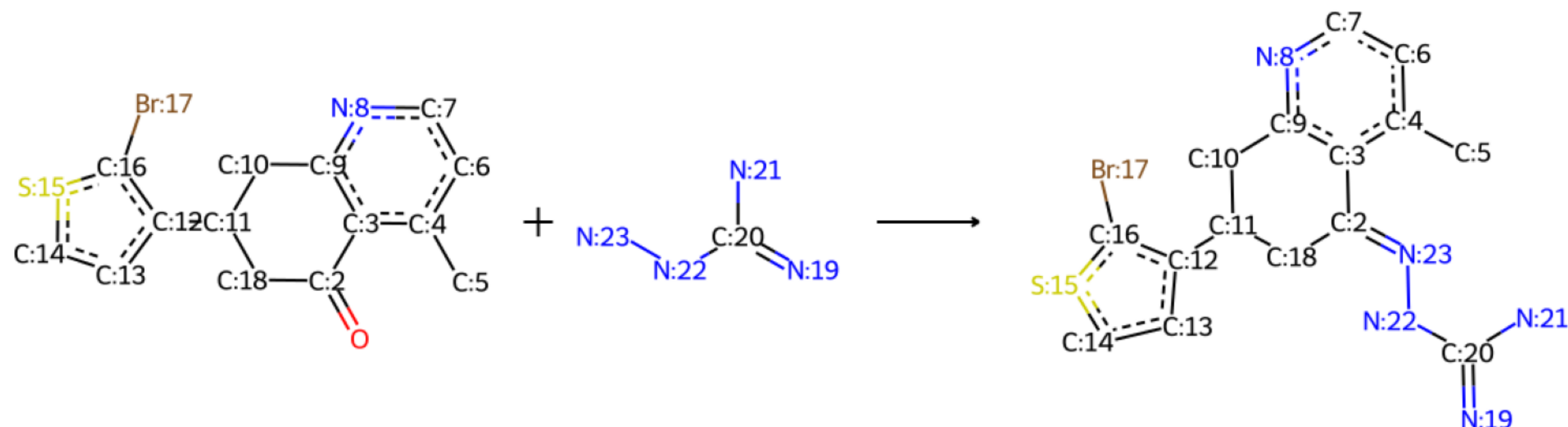
step #1



Product(s)

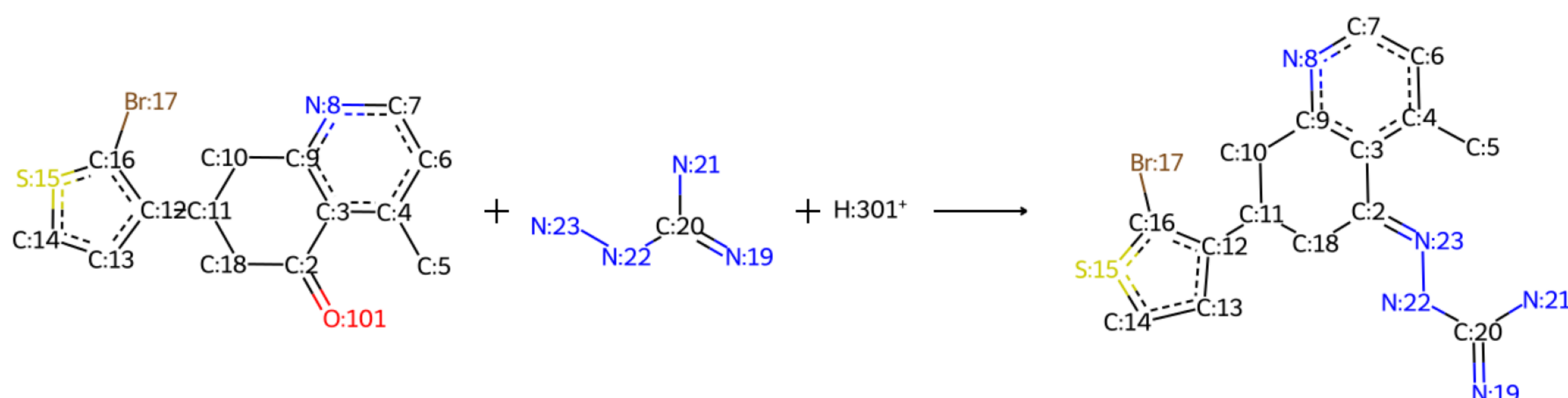


Original reaction
sampled RXN_ID:47)



Identified mechanistic class -
imine_formation reaction

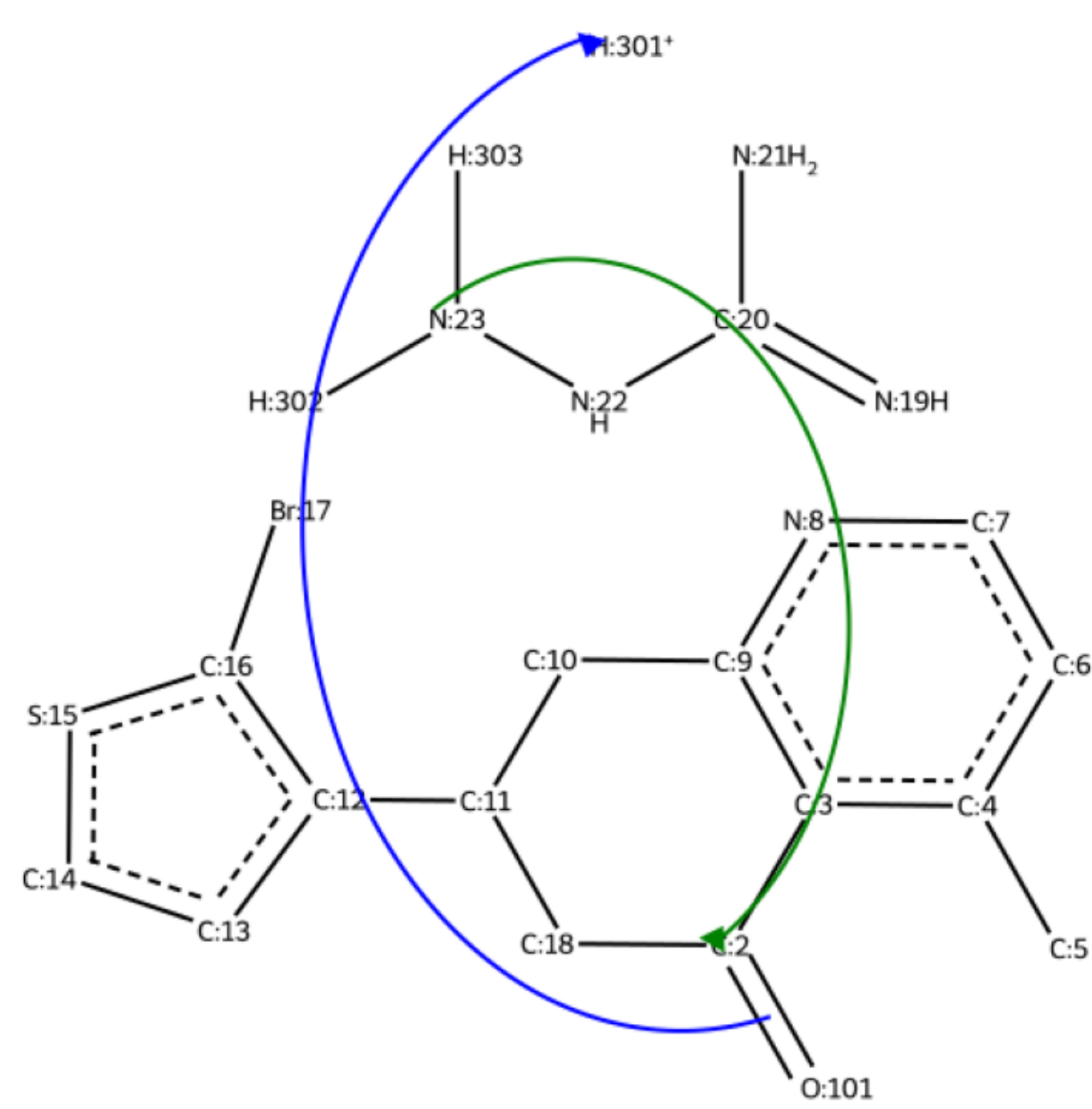
Reaction with missing reagents recovered



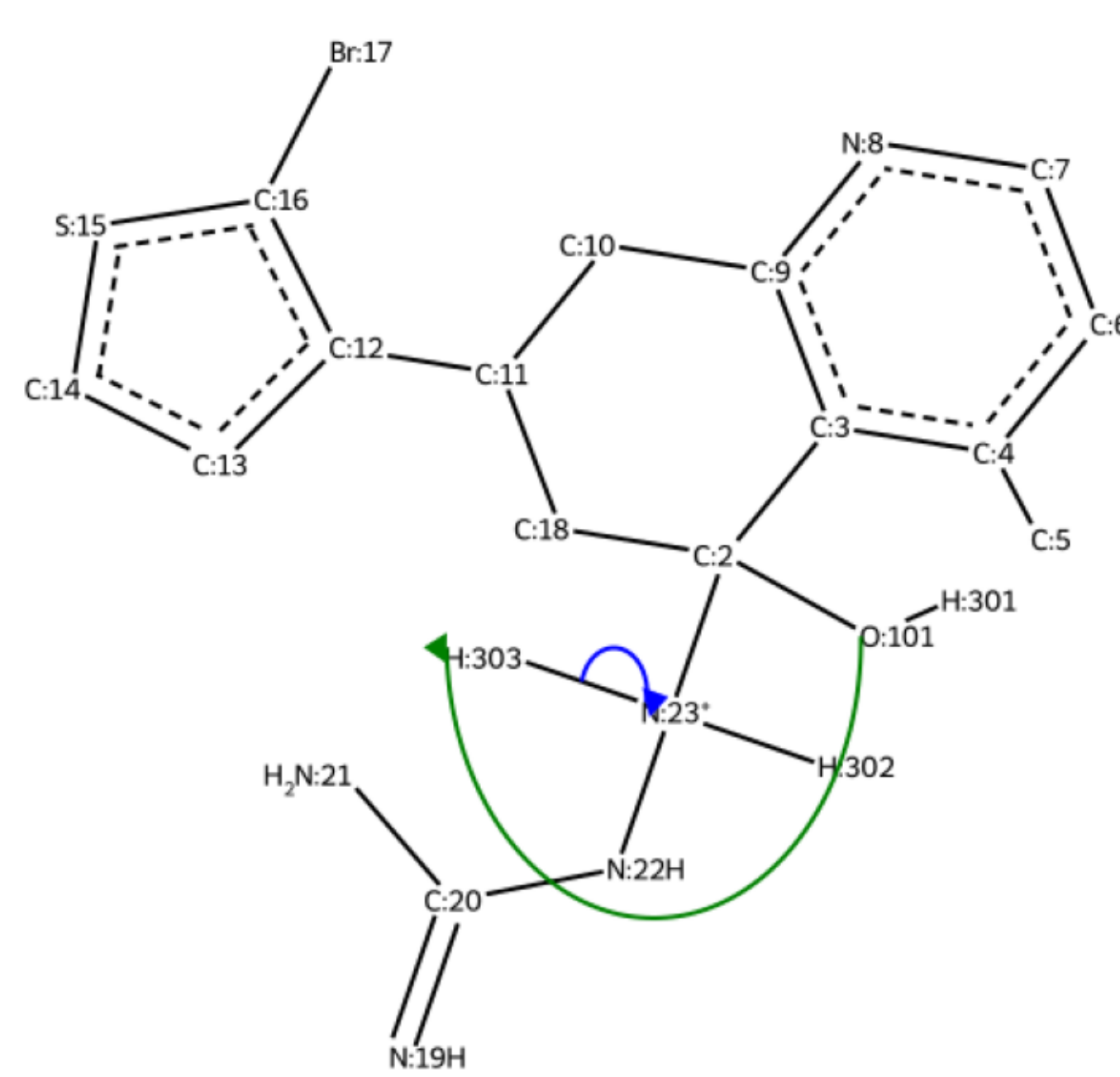
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

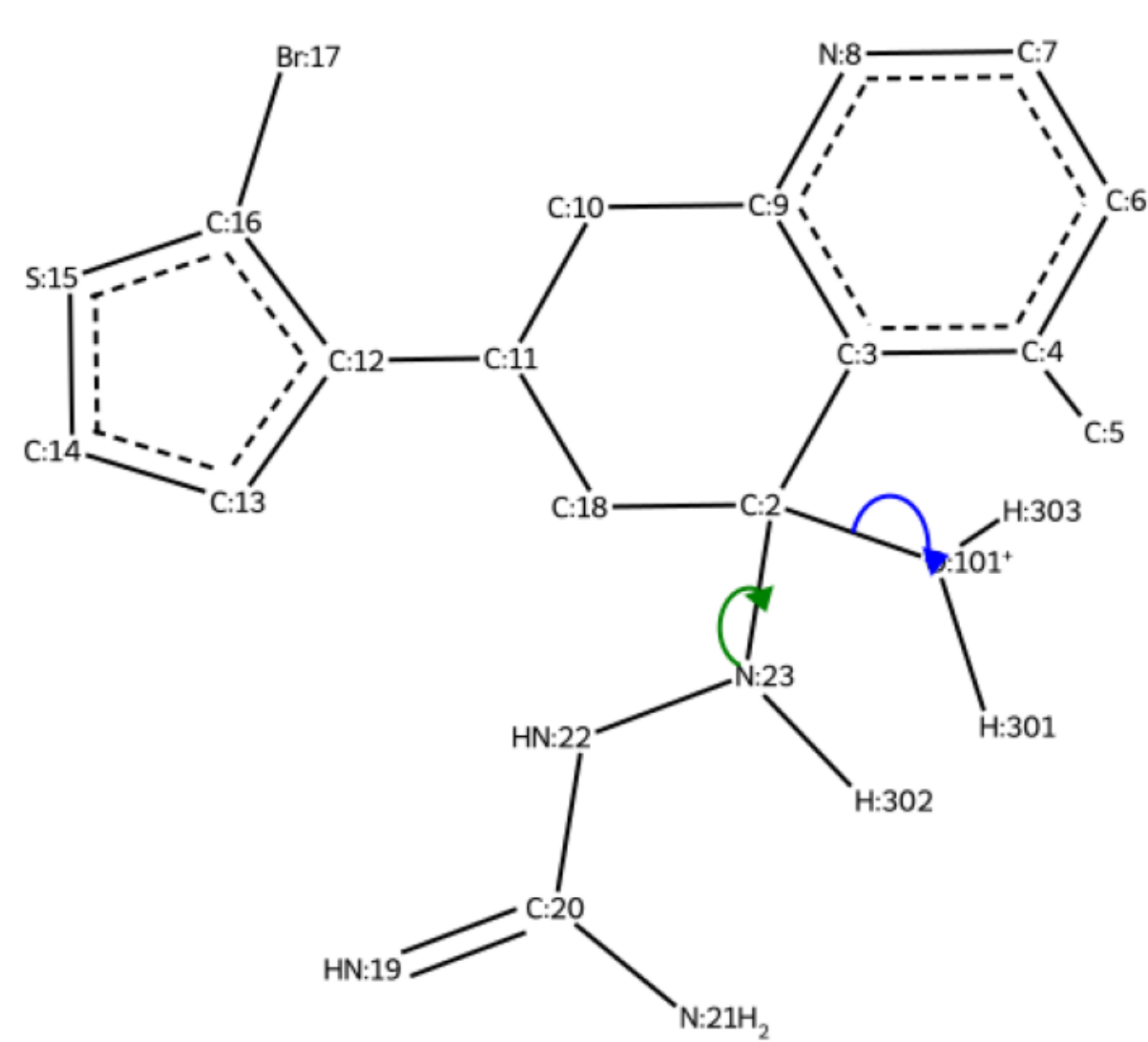
step #1



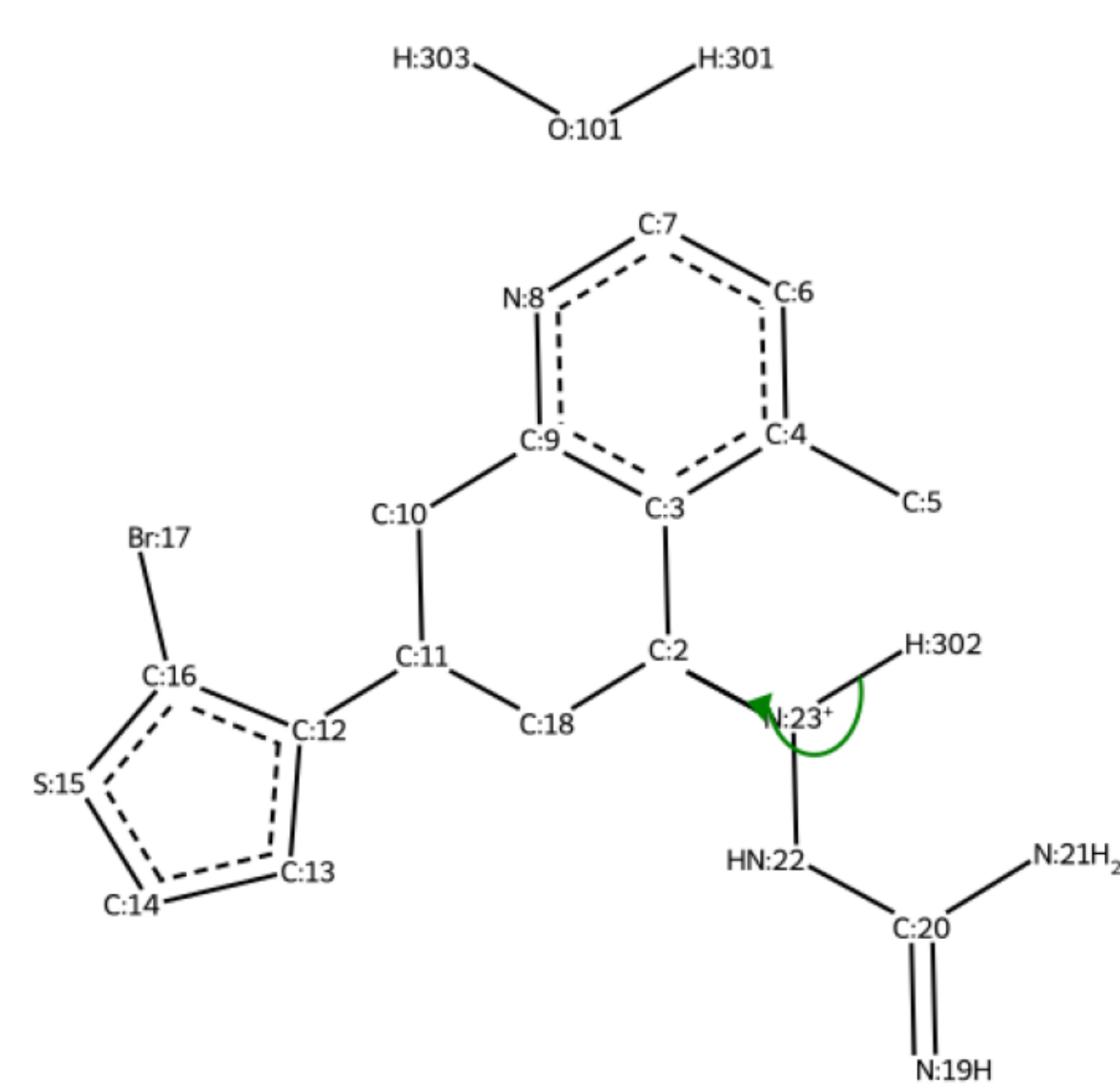
step #2



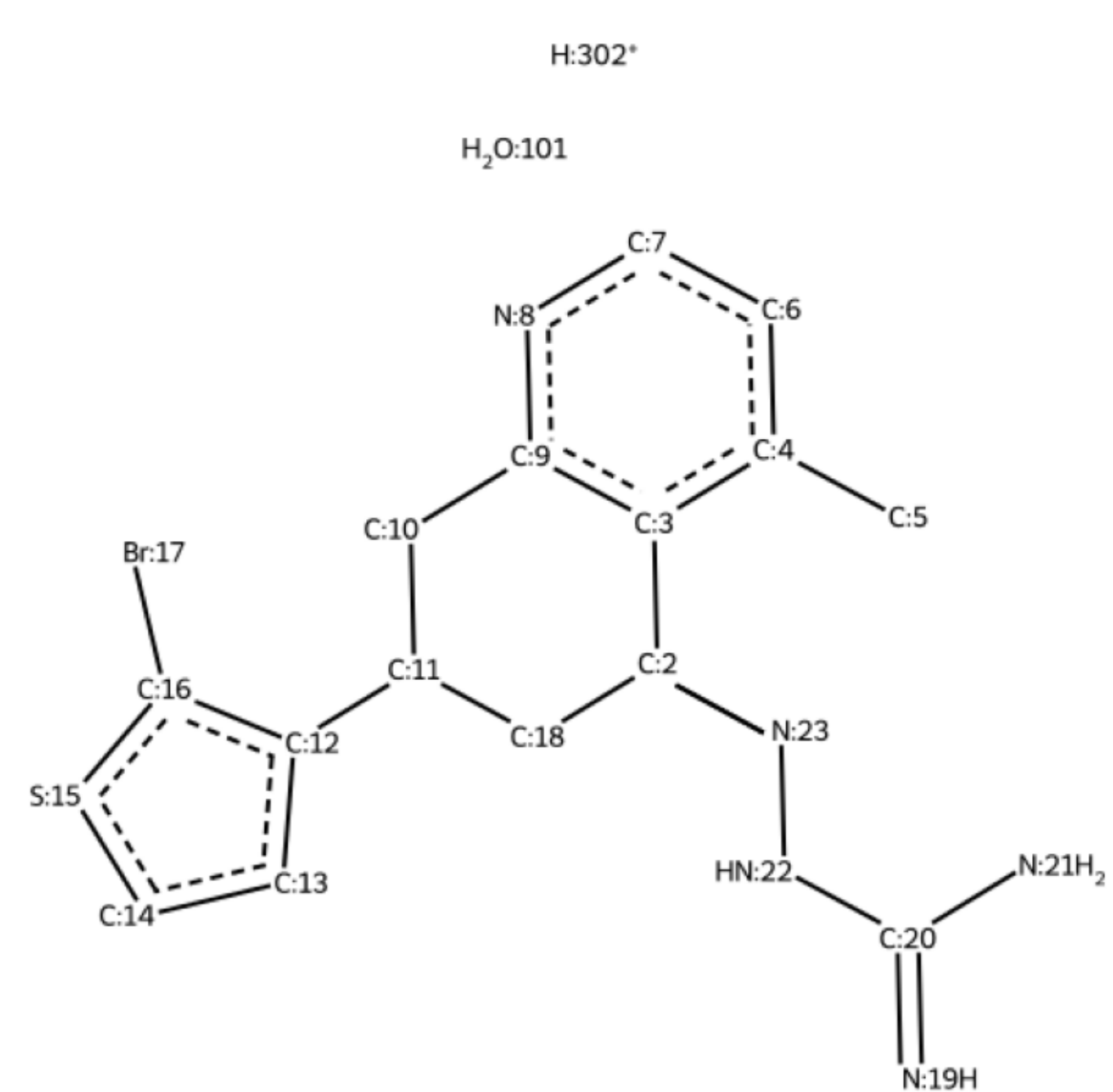
step #3



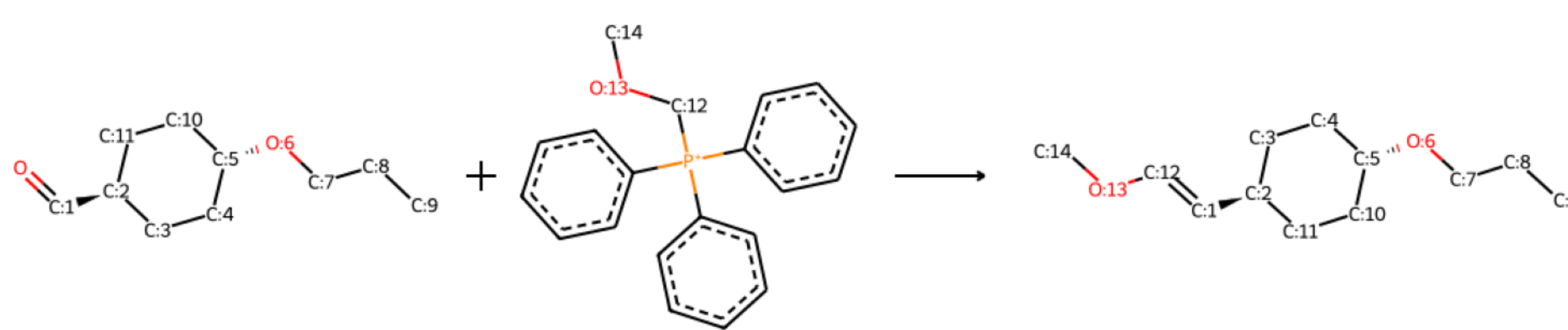
step #4



Product(s)

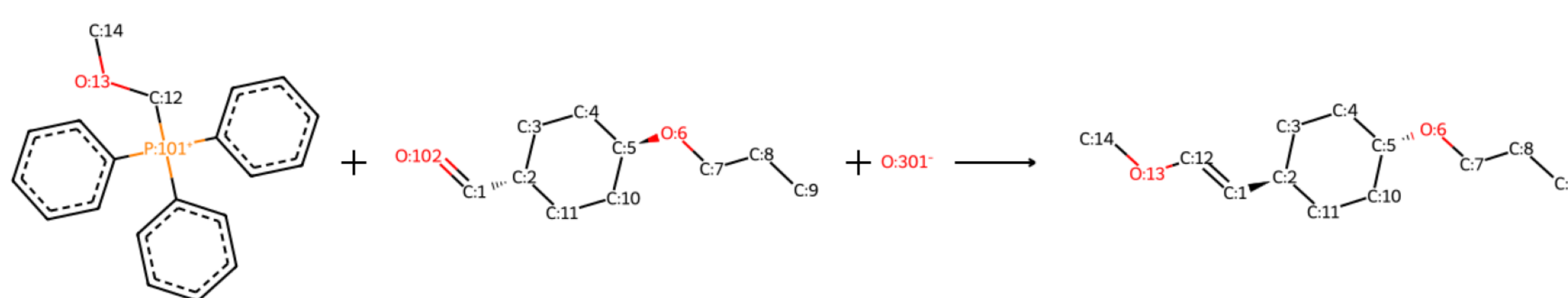


Original reaction
sampled RXN_ID:48)



Identified mechanistic class -
Wittig reaction

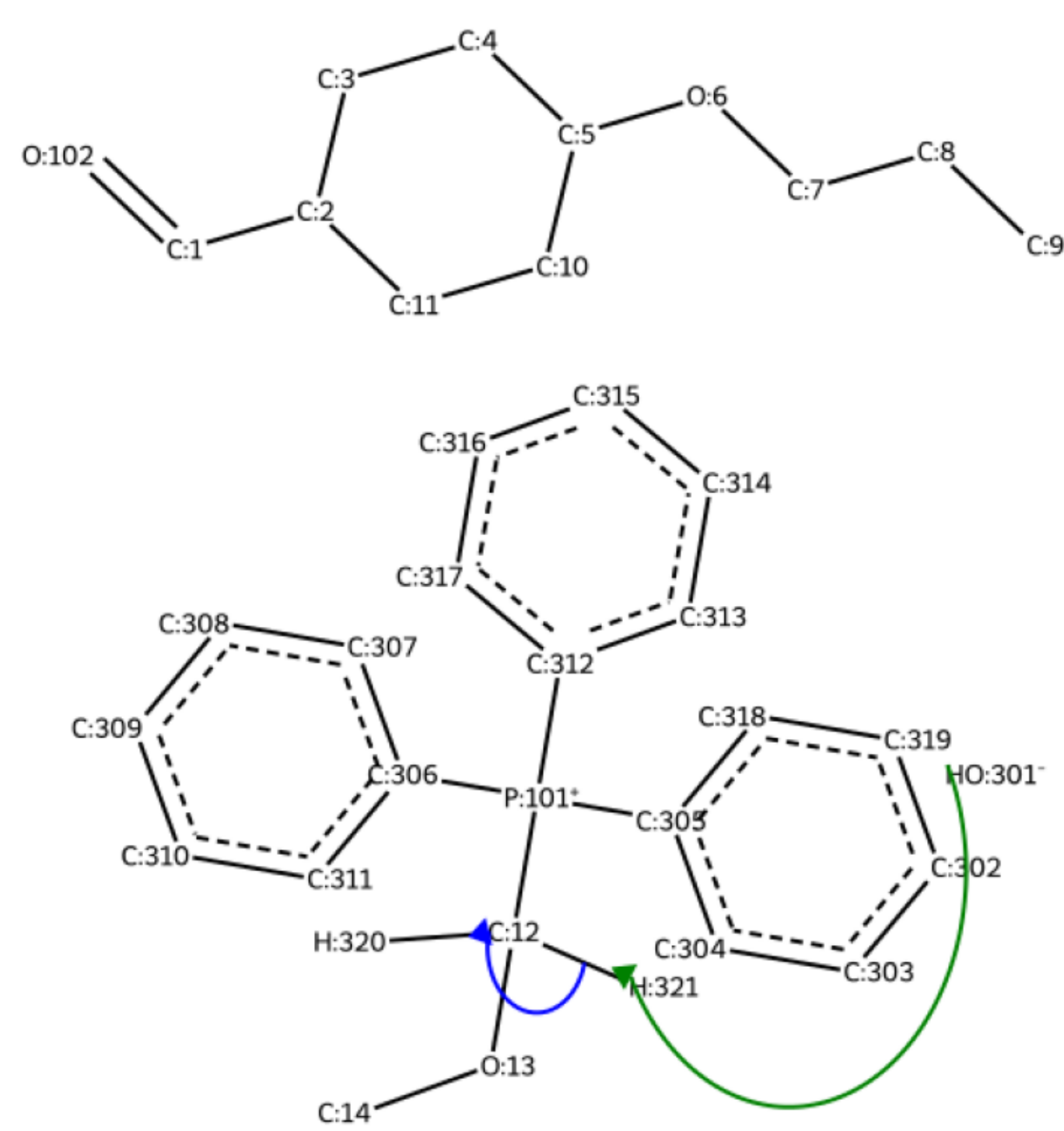
Reaction with missing reagents recovered



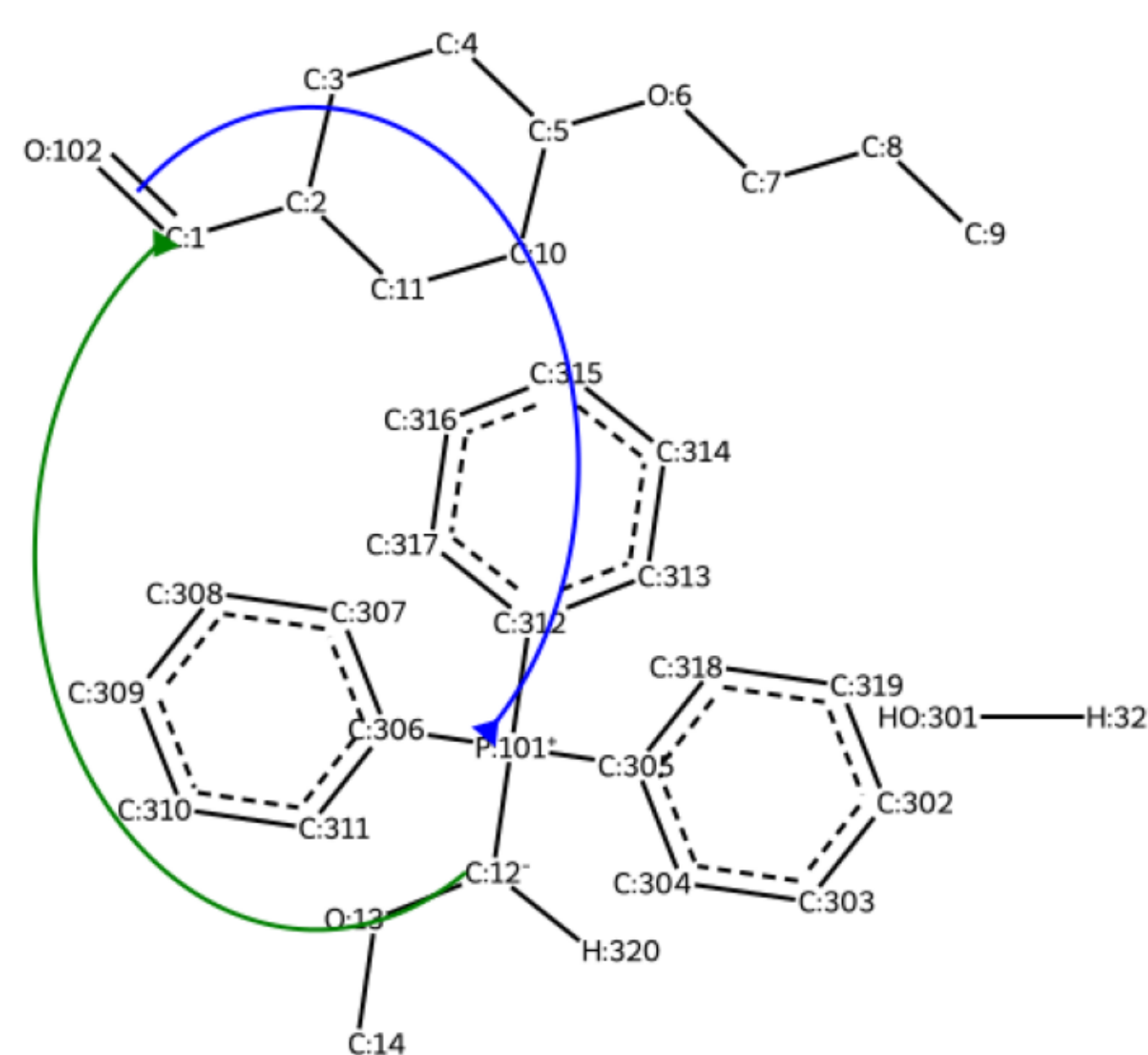
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

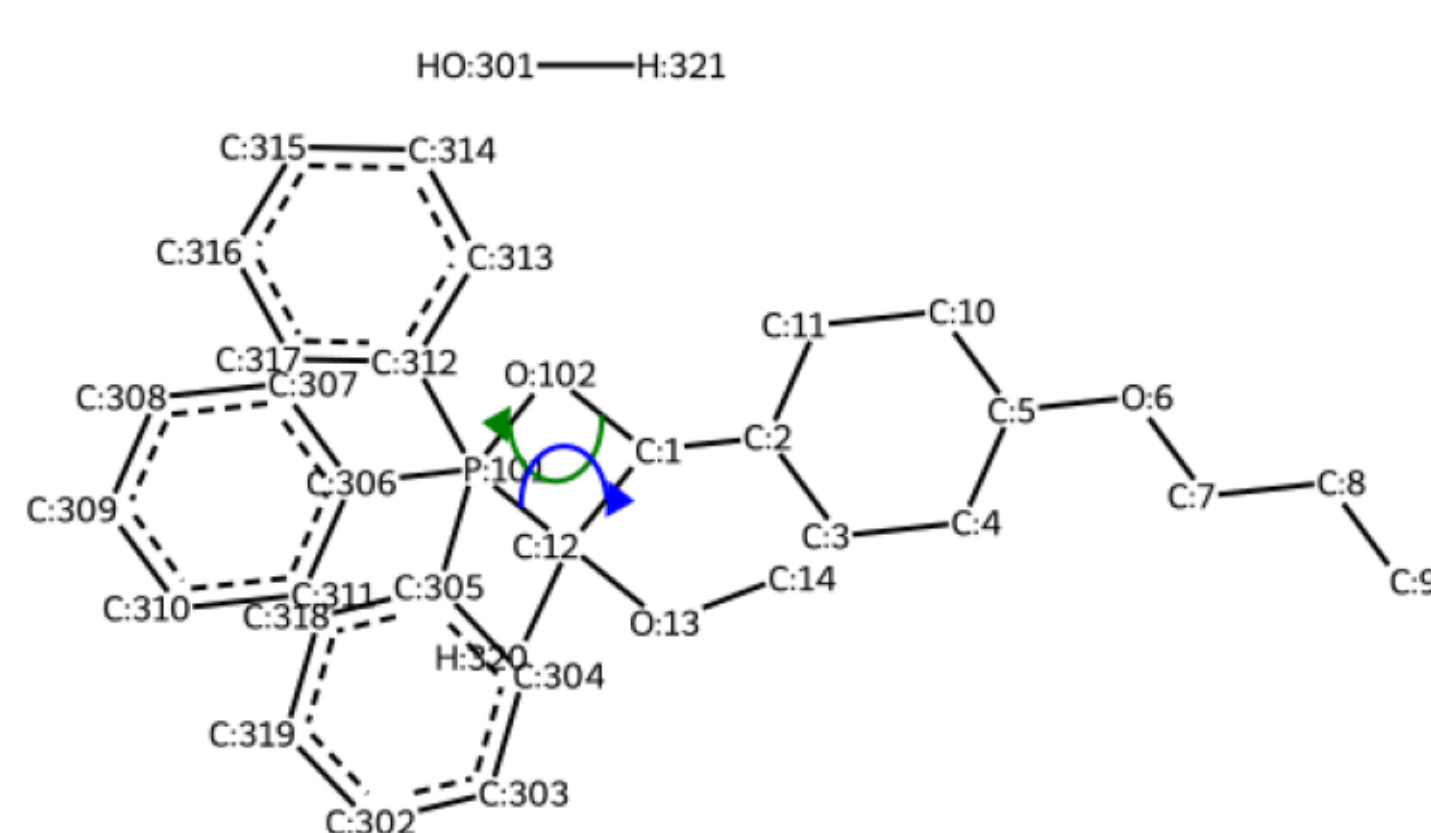
step #1



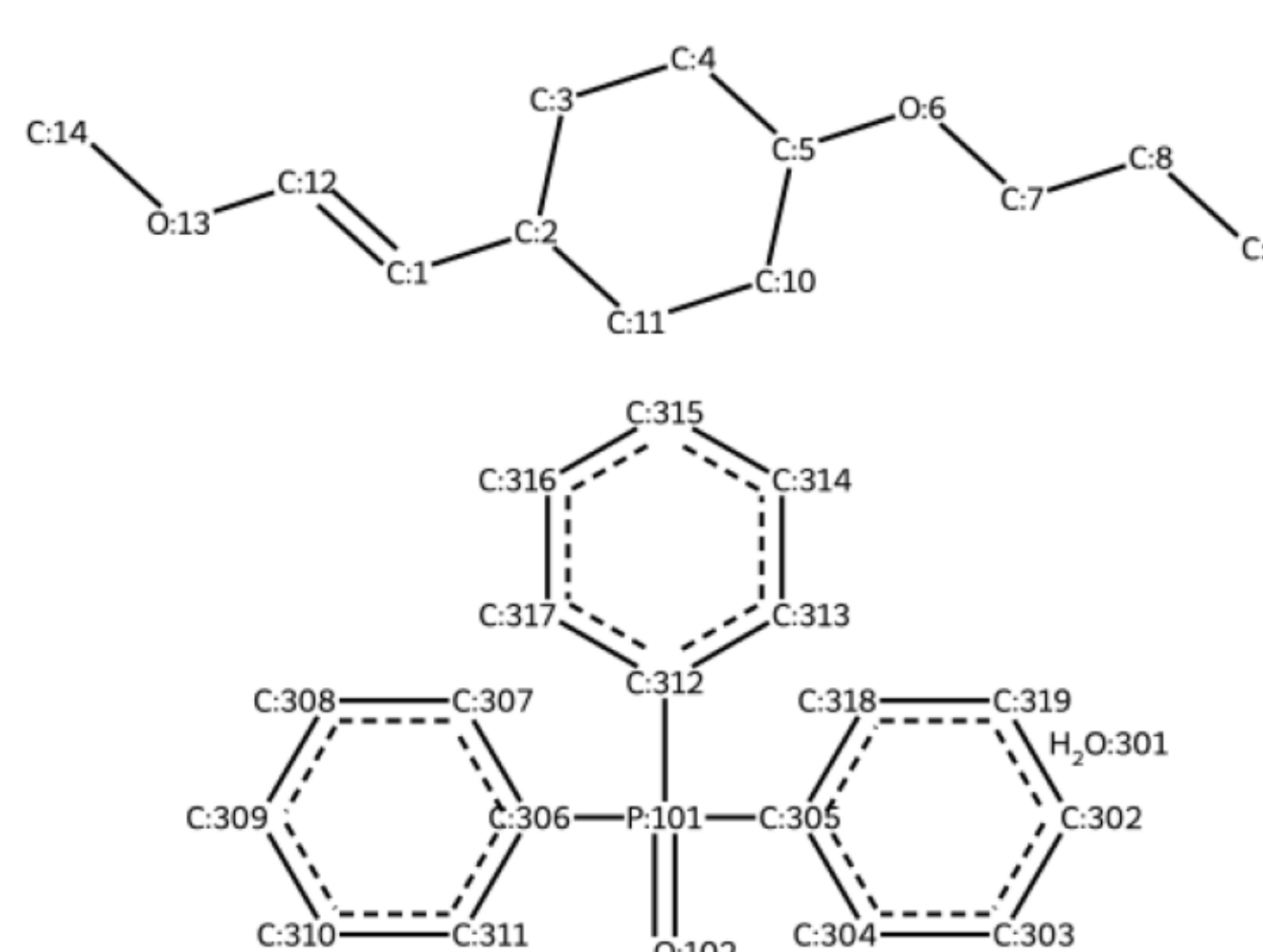
step #2



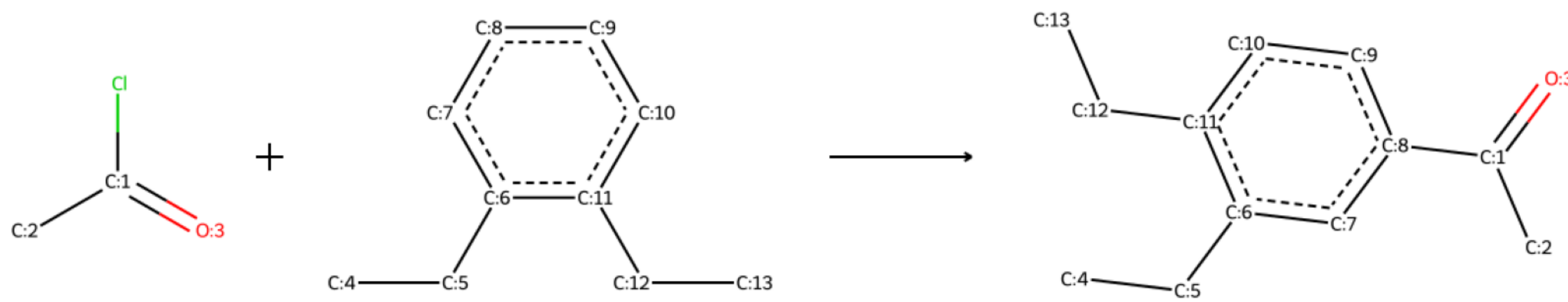
step #3



Product(s)

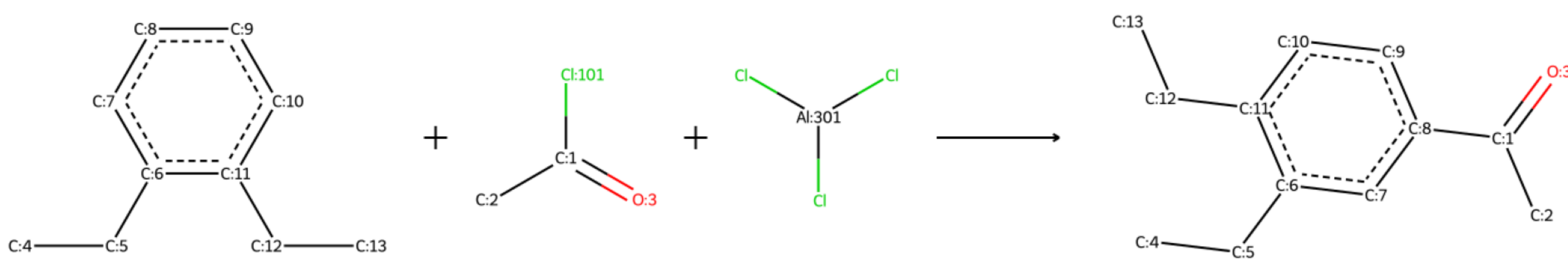


Original reaction
sampled RXN_ID:49)



Identified mechanistic class -
Friedel_Crafts_acylation reaction

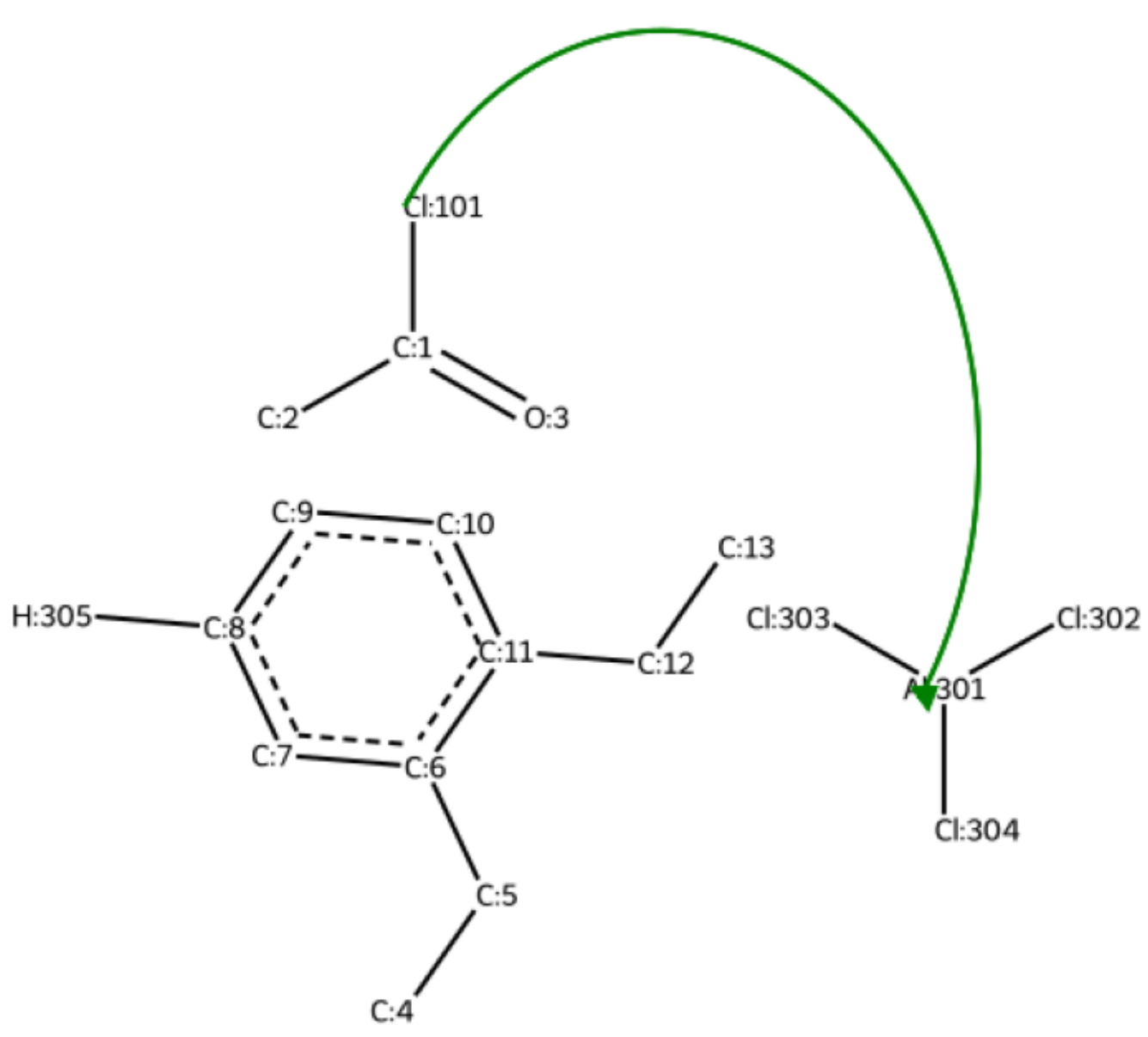
Reaction with missing reagents recovered



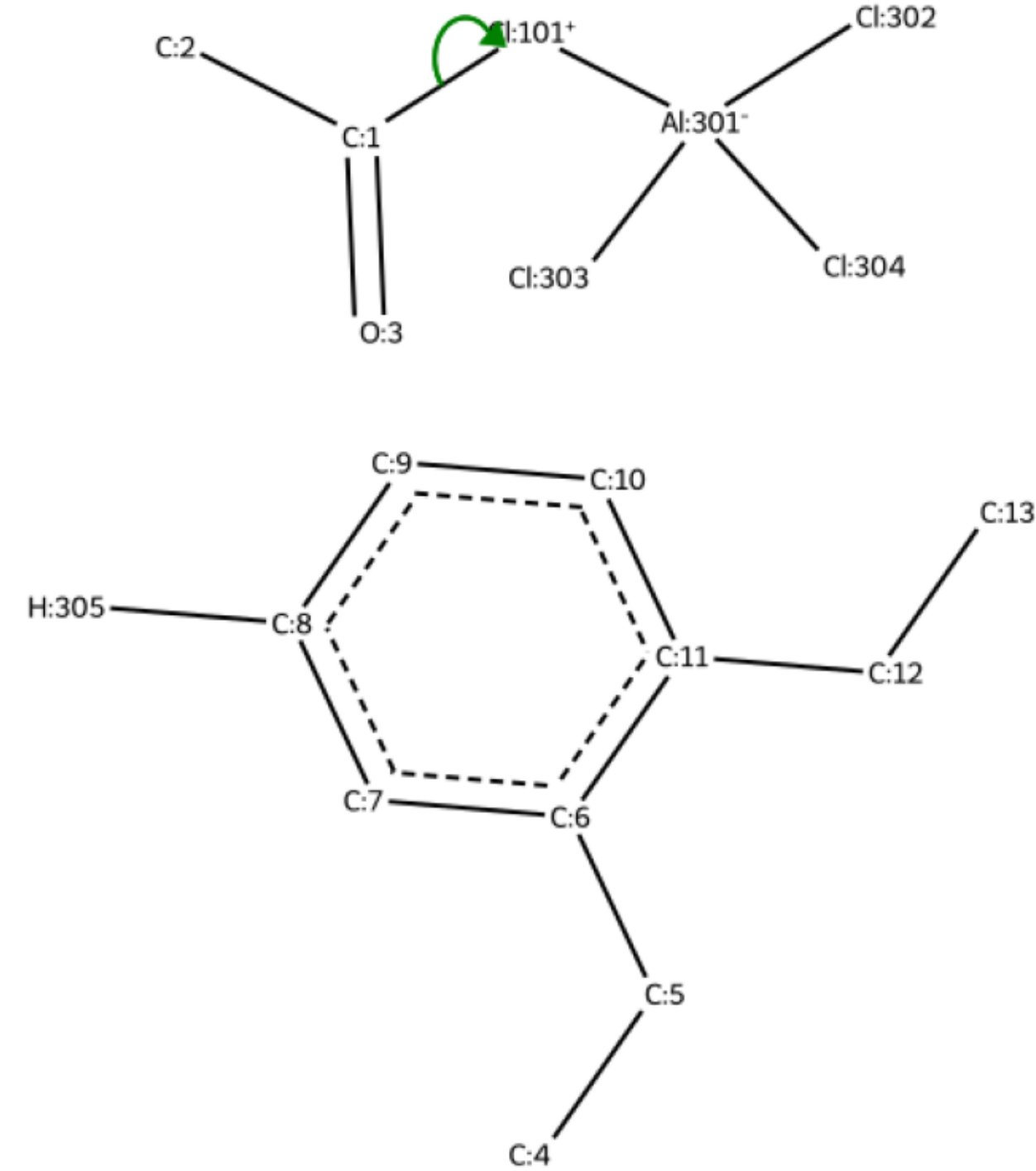
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

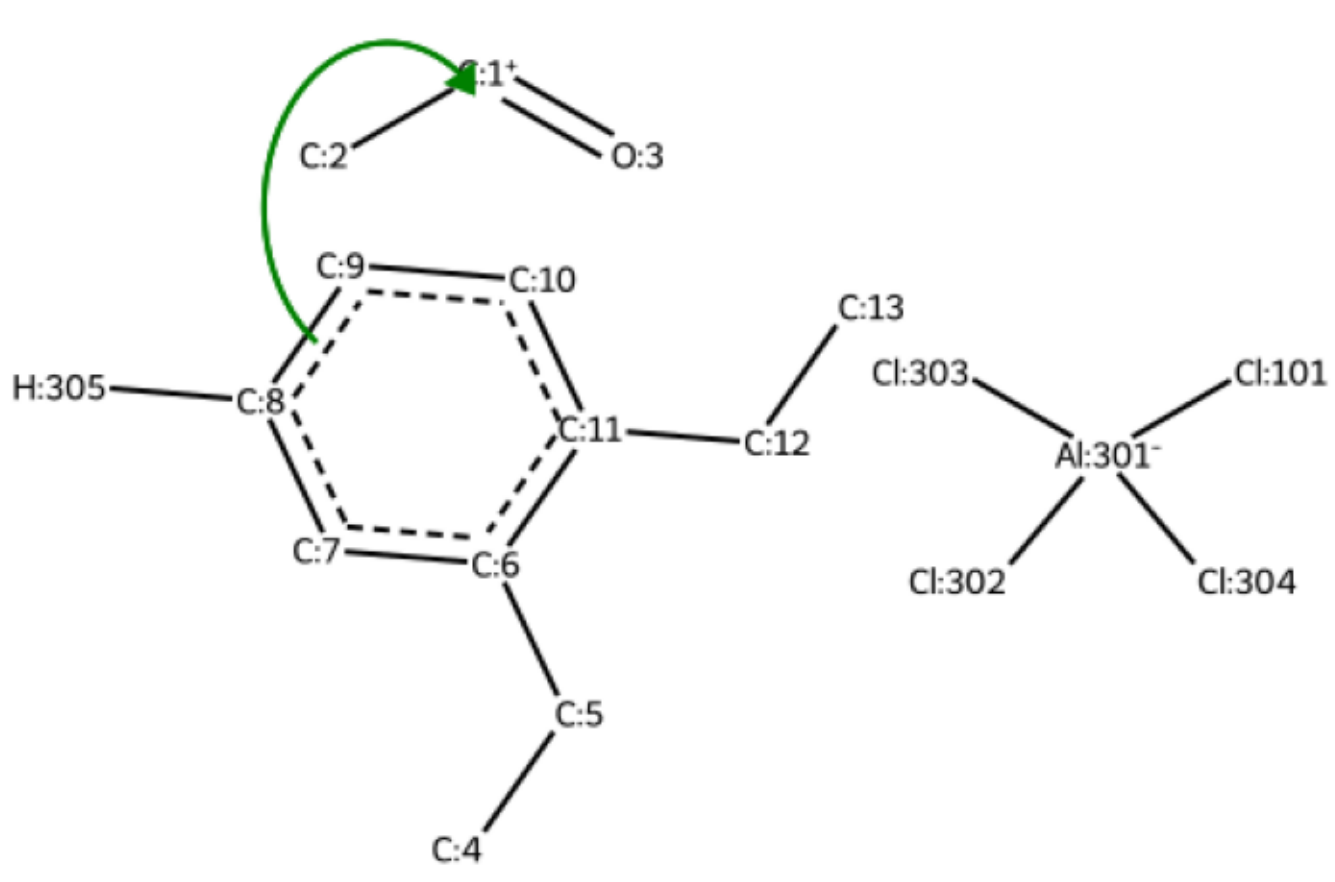
step #1



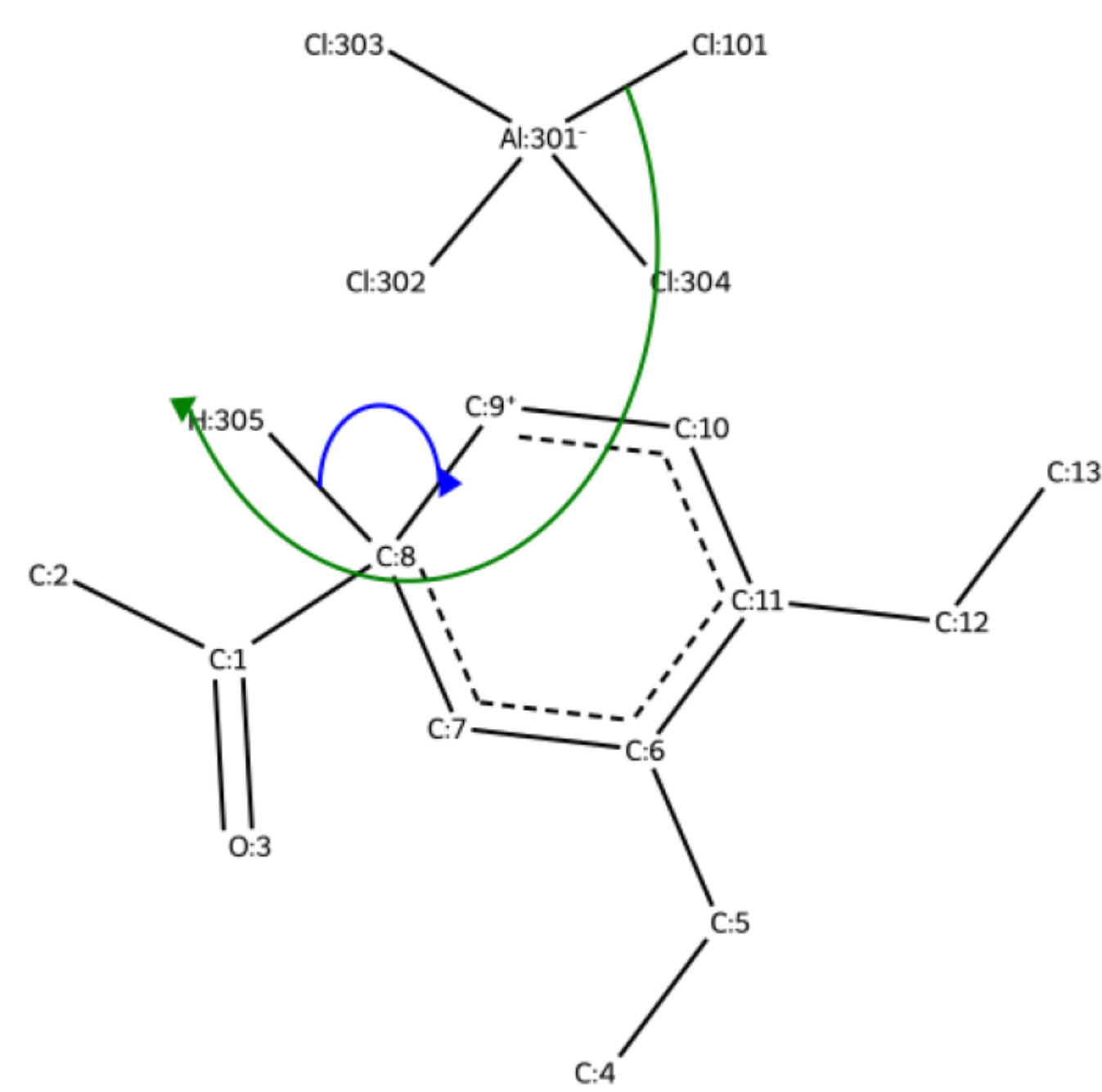
step #2



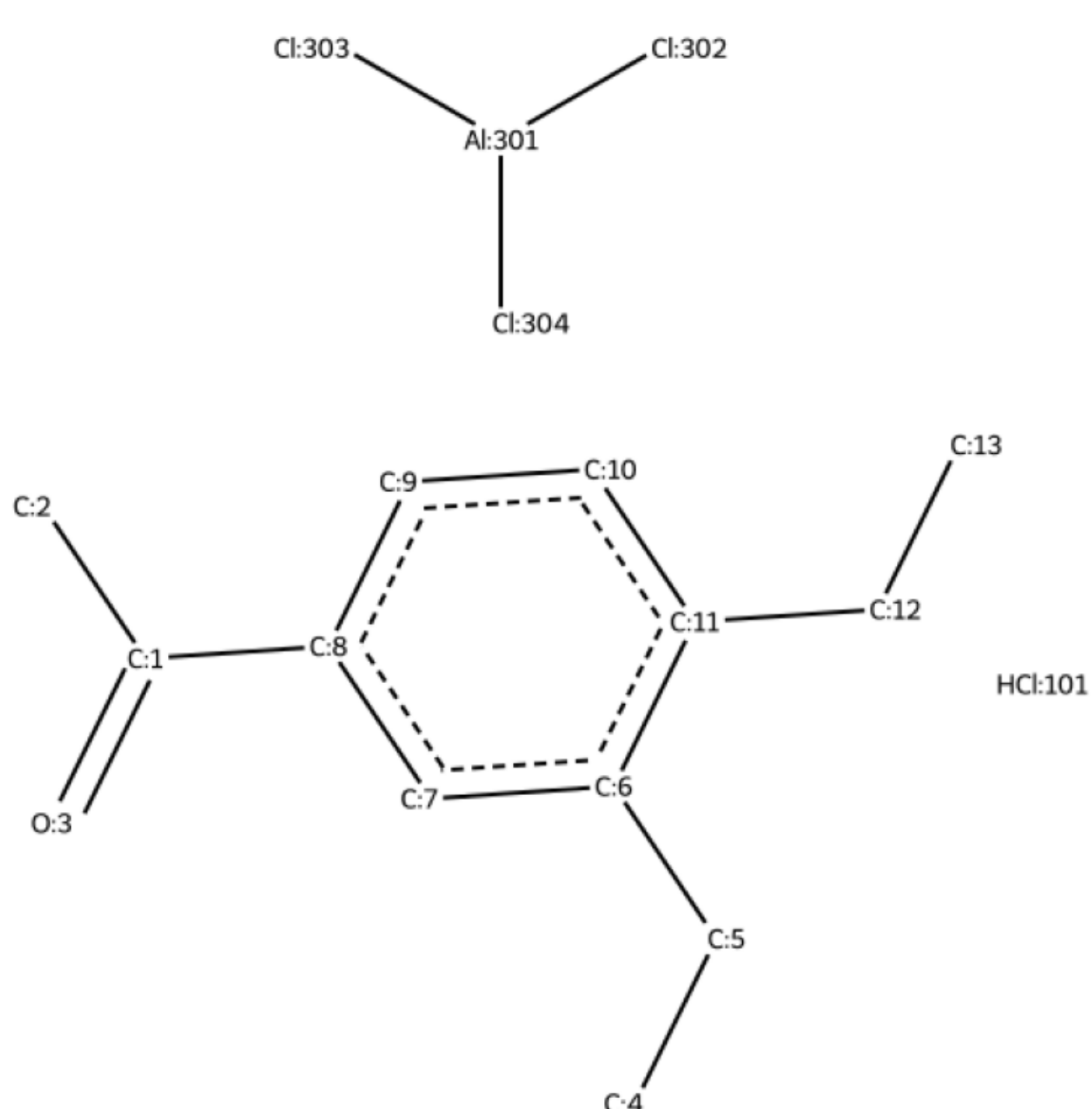
step #3



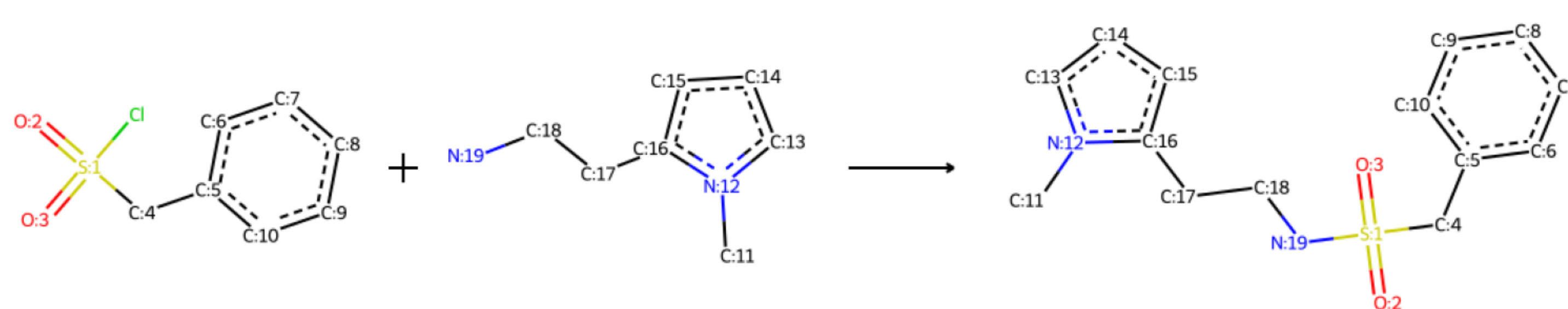
step #4



Product(s)

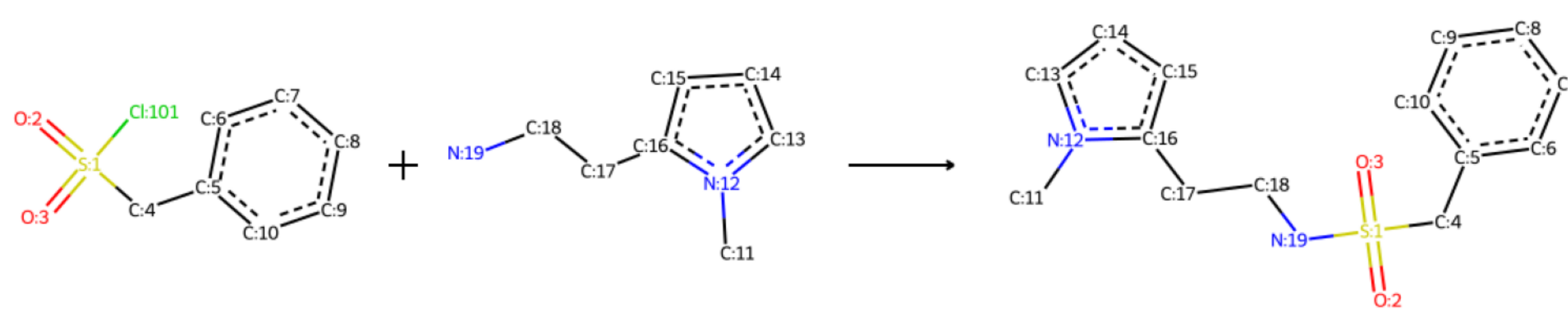


Original reaction
sampled RXN_ID:50)



Identified mechanistic class -
nucleophilic_attack_to_(thio)carbonyl_or_sulfonyl reaction

Reaction with missing reagents recovered

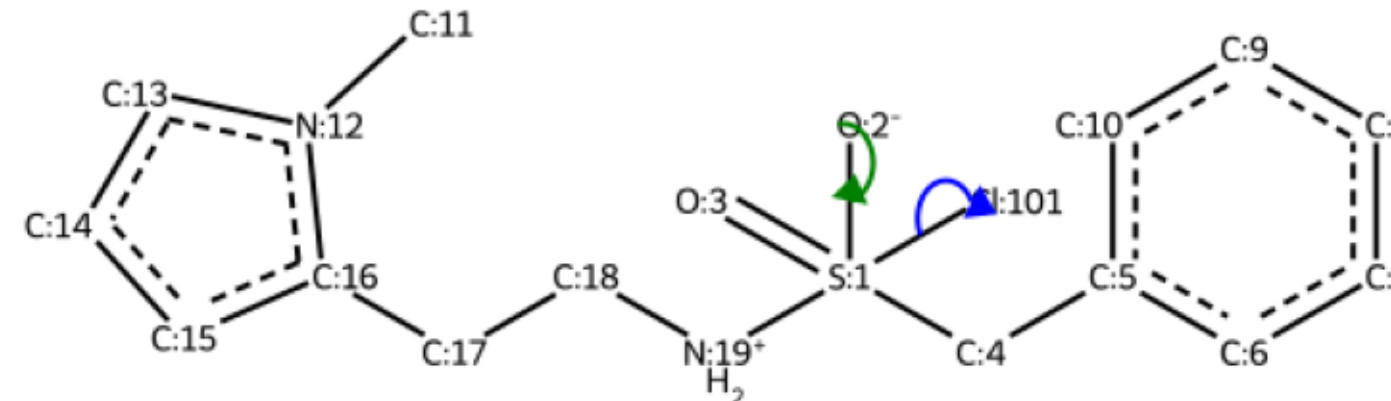
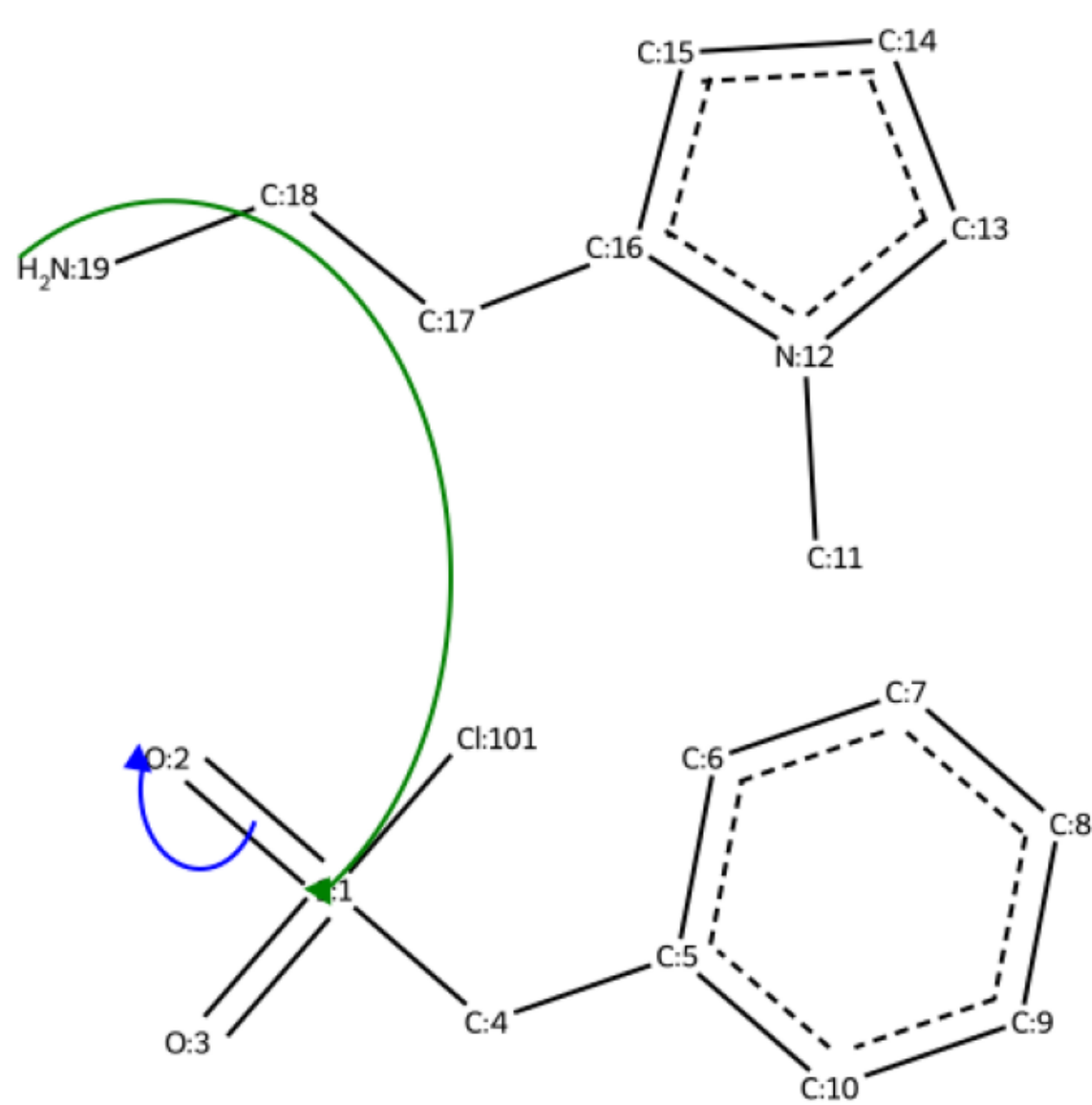


Proposed mechanistic pathway

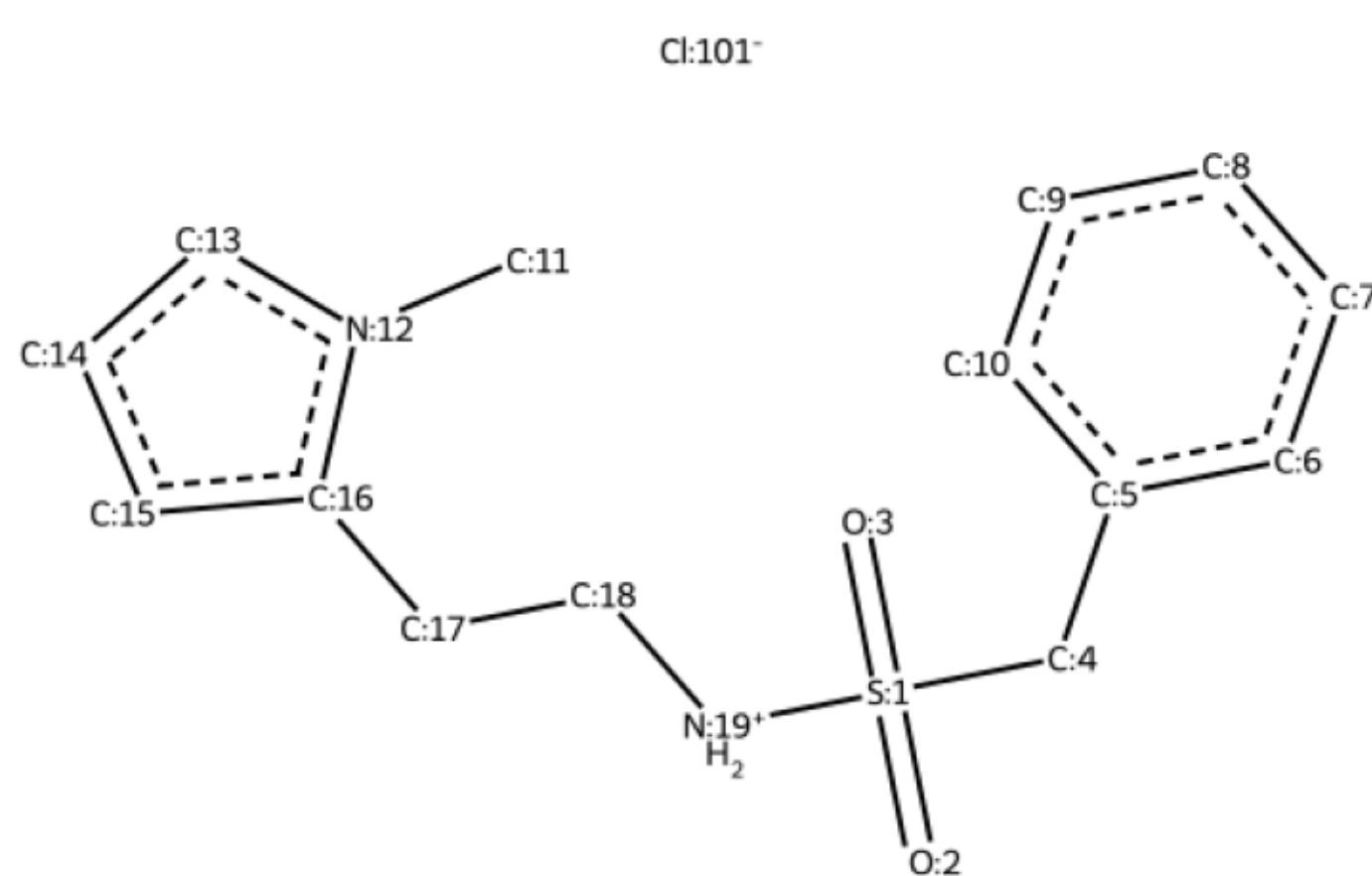
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

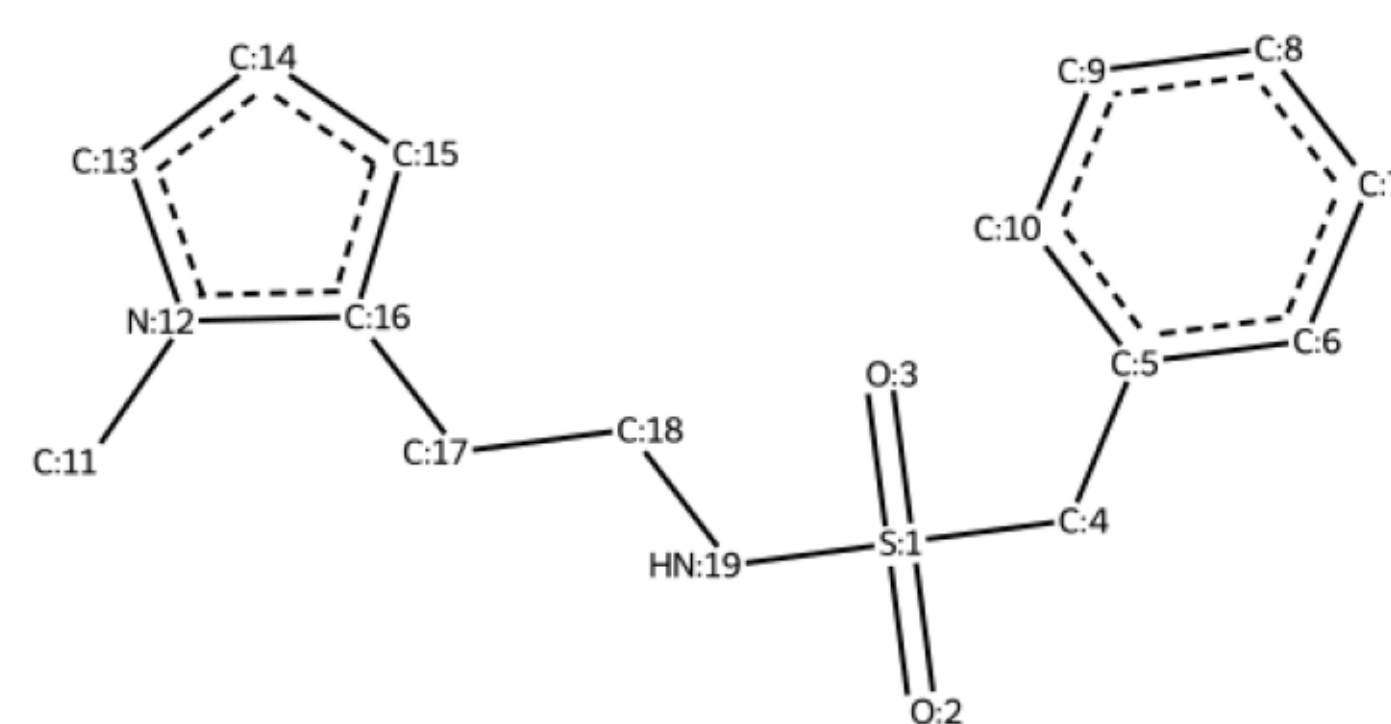
step #2



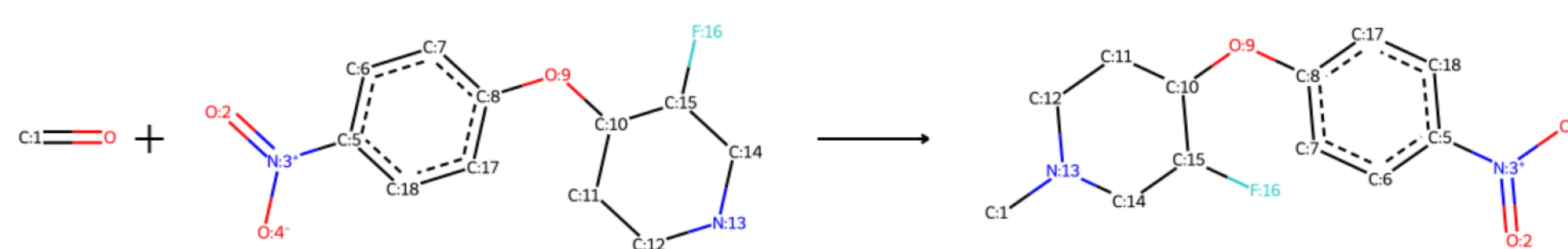
Product(s)



proton transfer

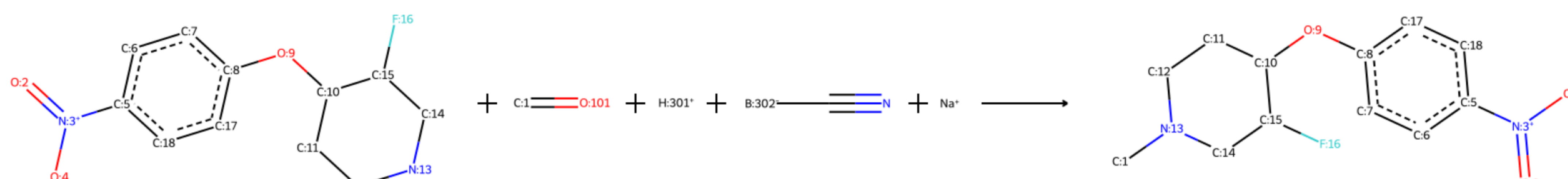


Original reaction
sampled RXN_ID:51)



Identified mechanistic class -
reductive_amination reaction

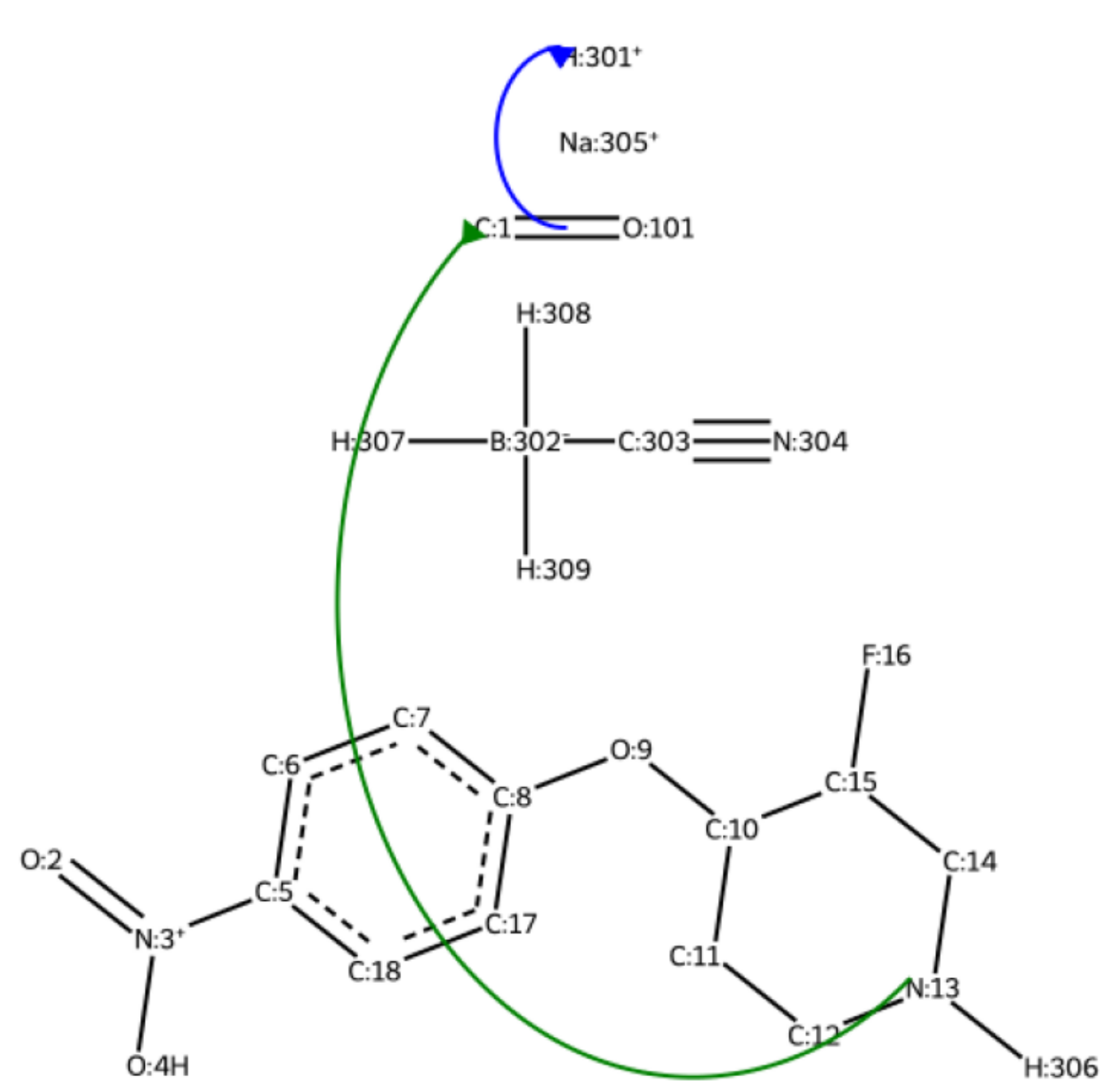
Reaction with missing reagents recovered



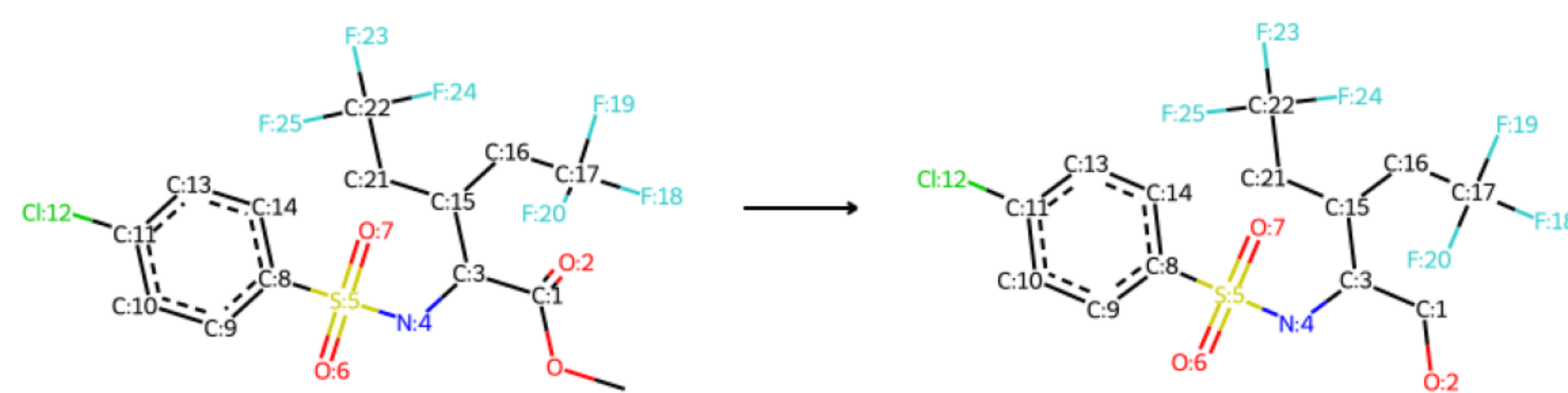
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

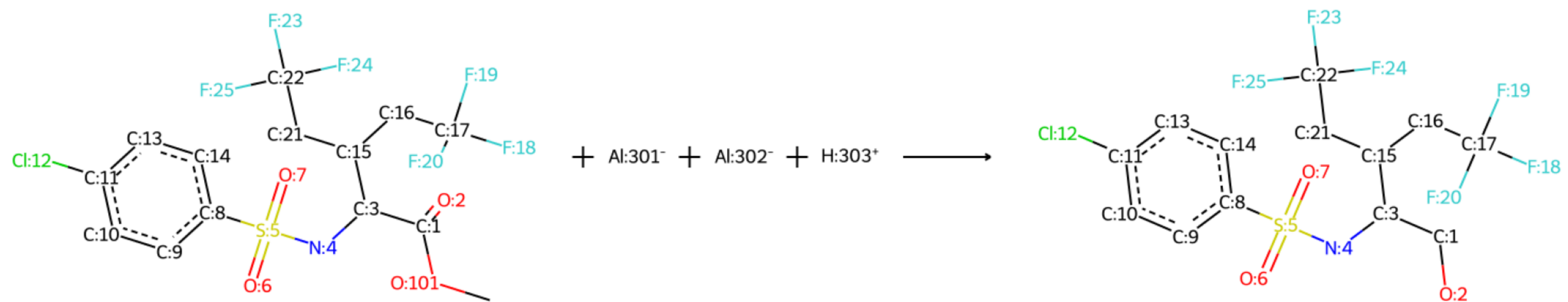


Original reaction
sampled RXN_ID:52)



Identified mechanistic class -
ester_reduction reaction

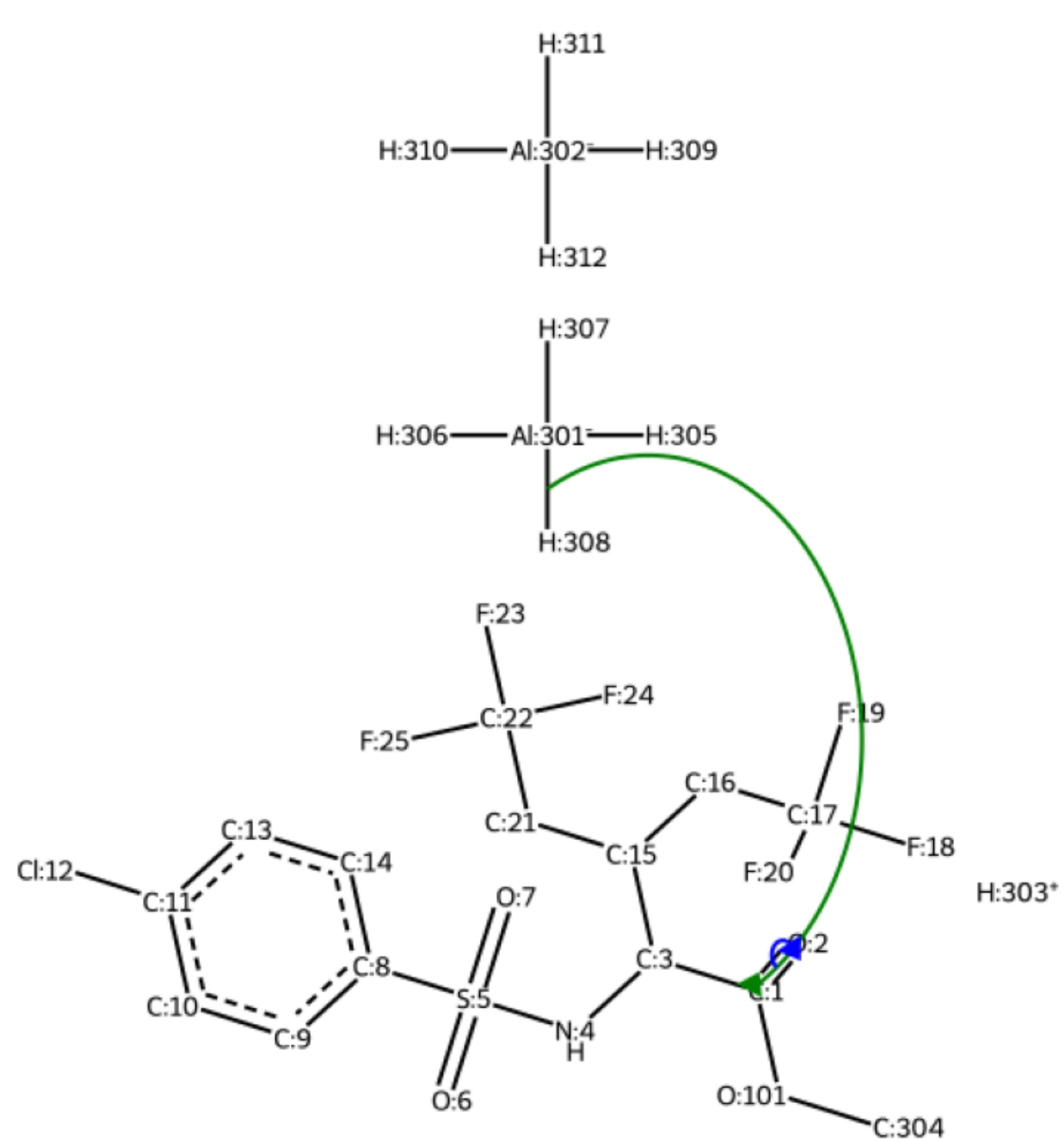
Reaction with missing reagents recovered



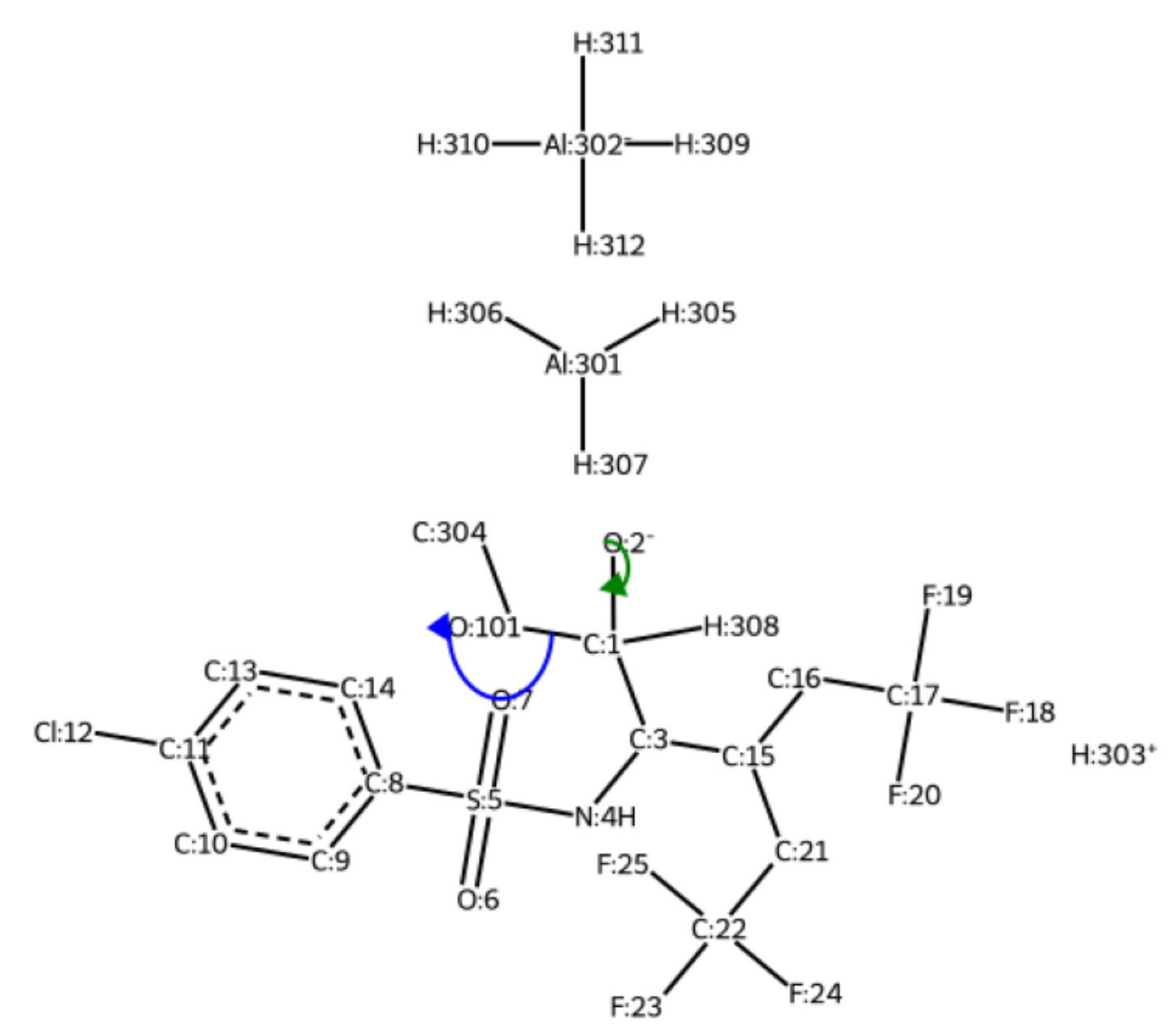
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

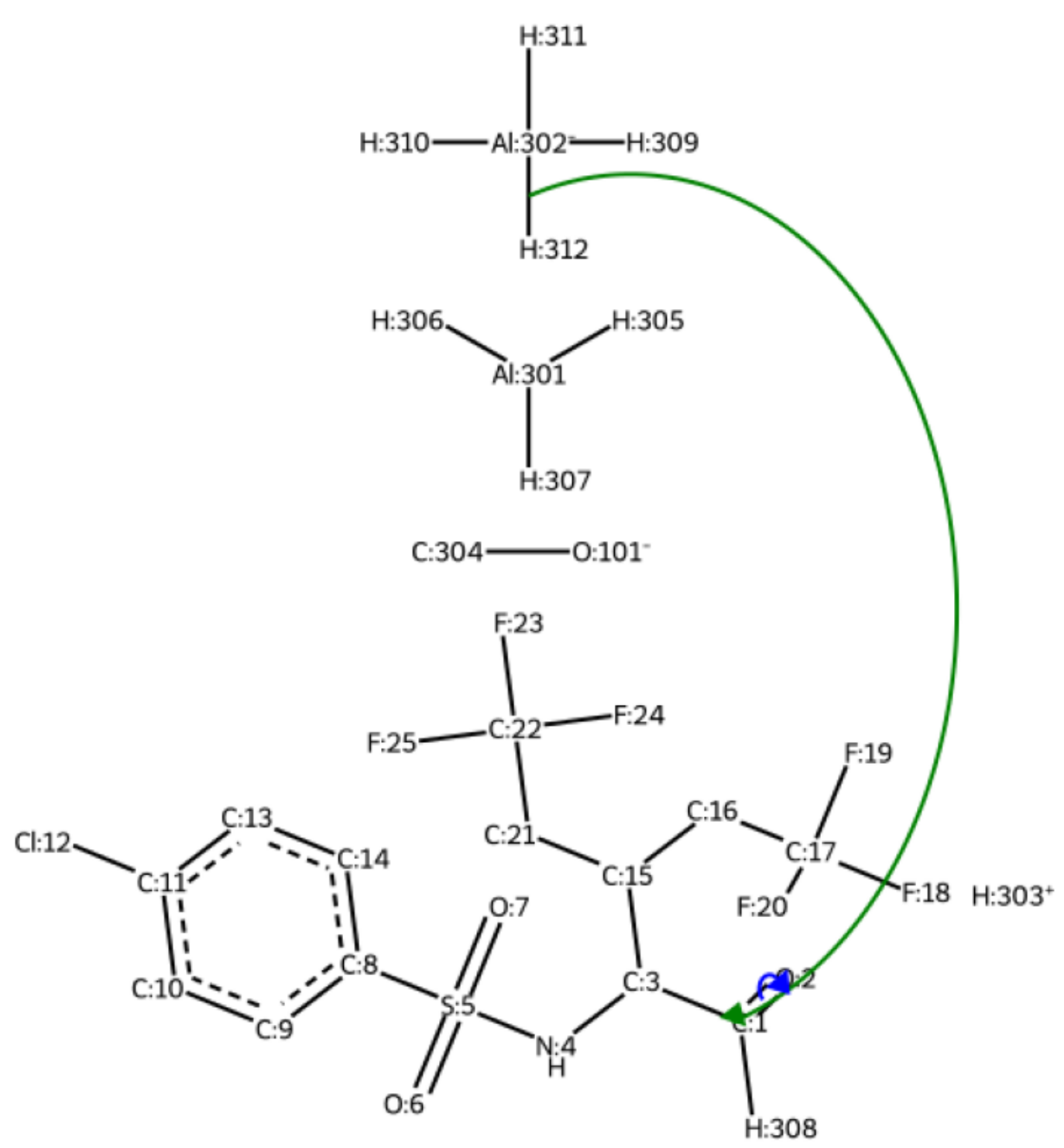
step #1



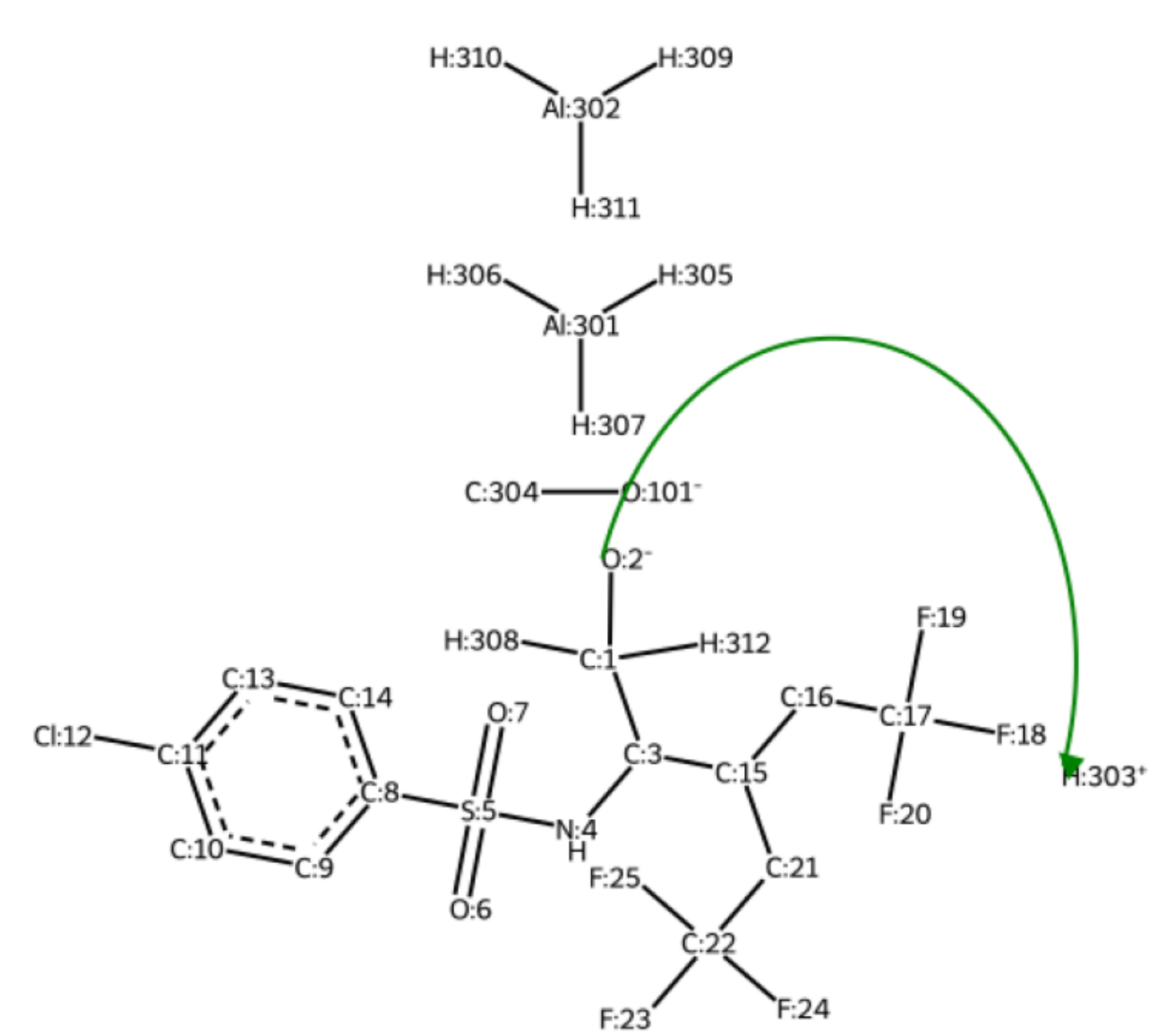
step #2



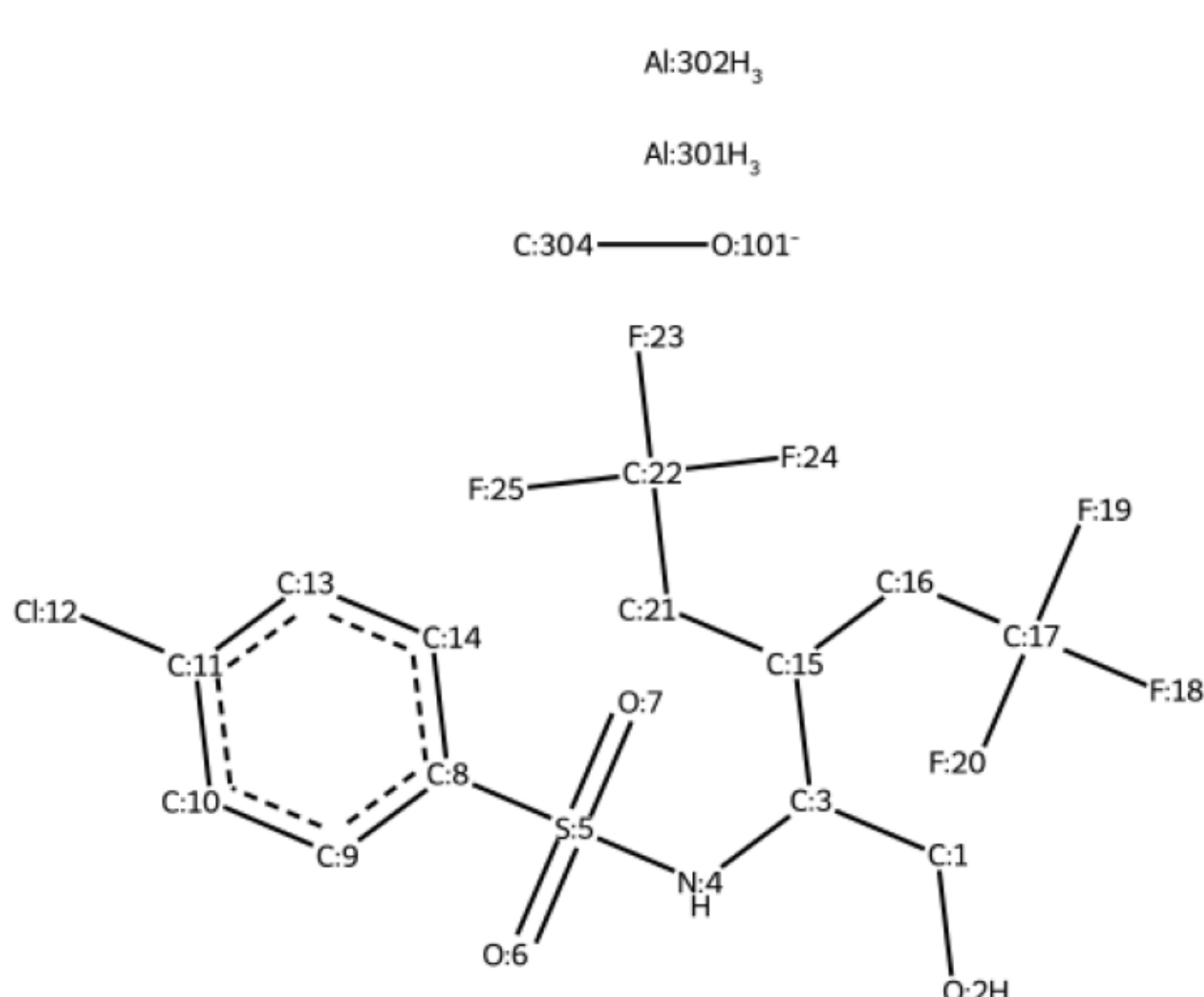
step #3



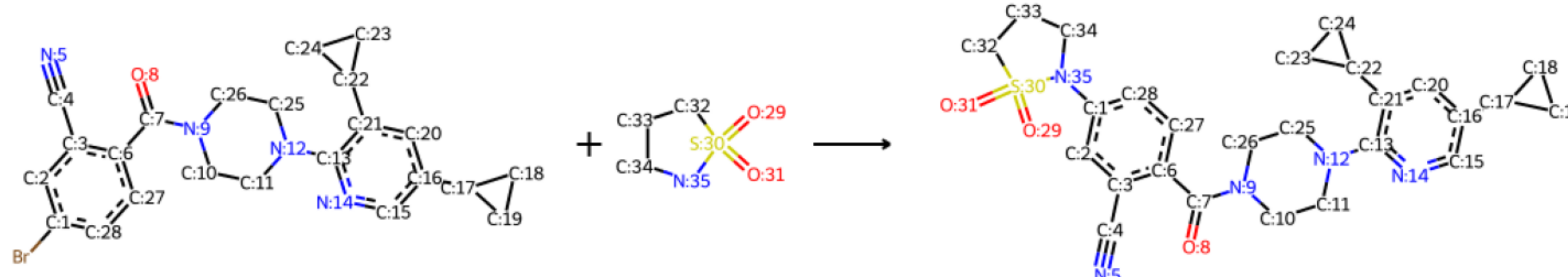
step #4



Product(s)

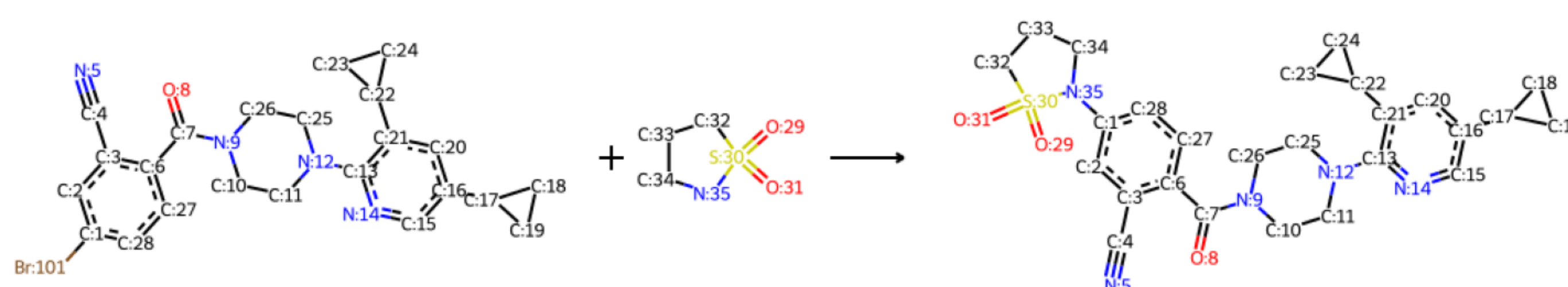


Original reaction
sampled RXN_ID:53)



Identified mechanistic class -
S_NAr(para) reaction

Reaction with missing reagents recovered

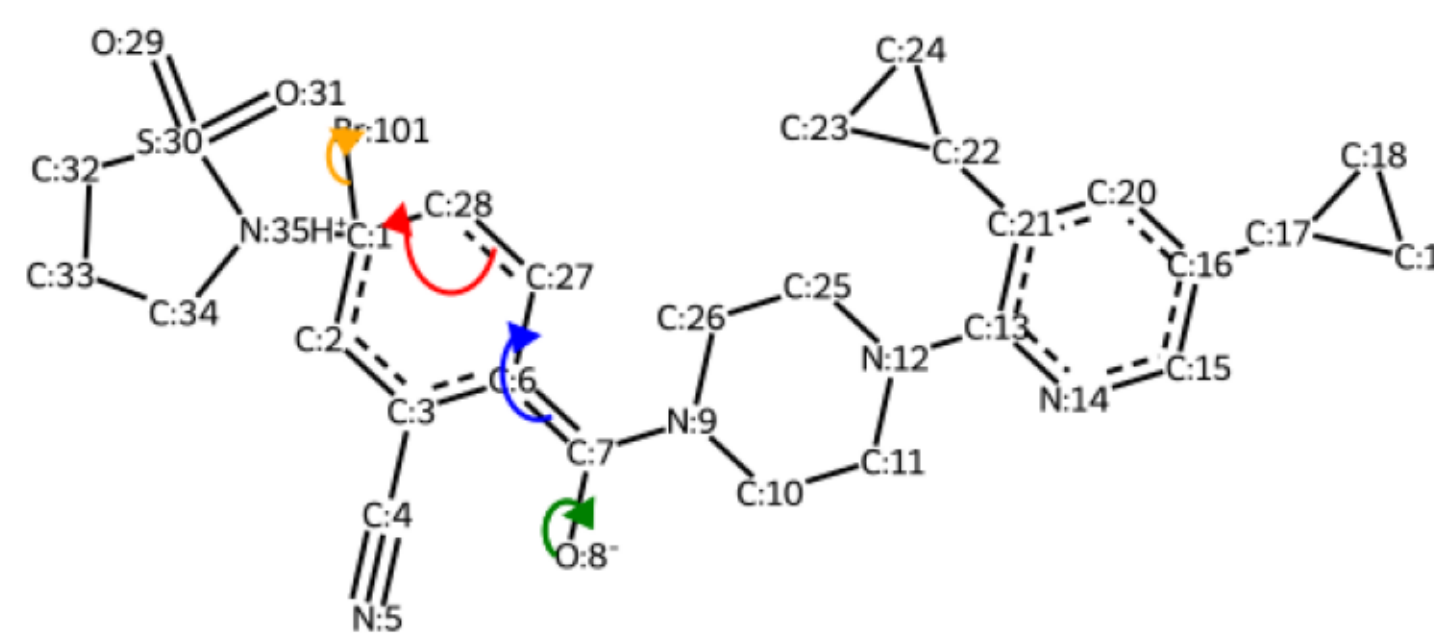
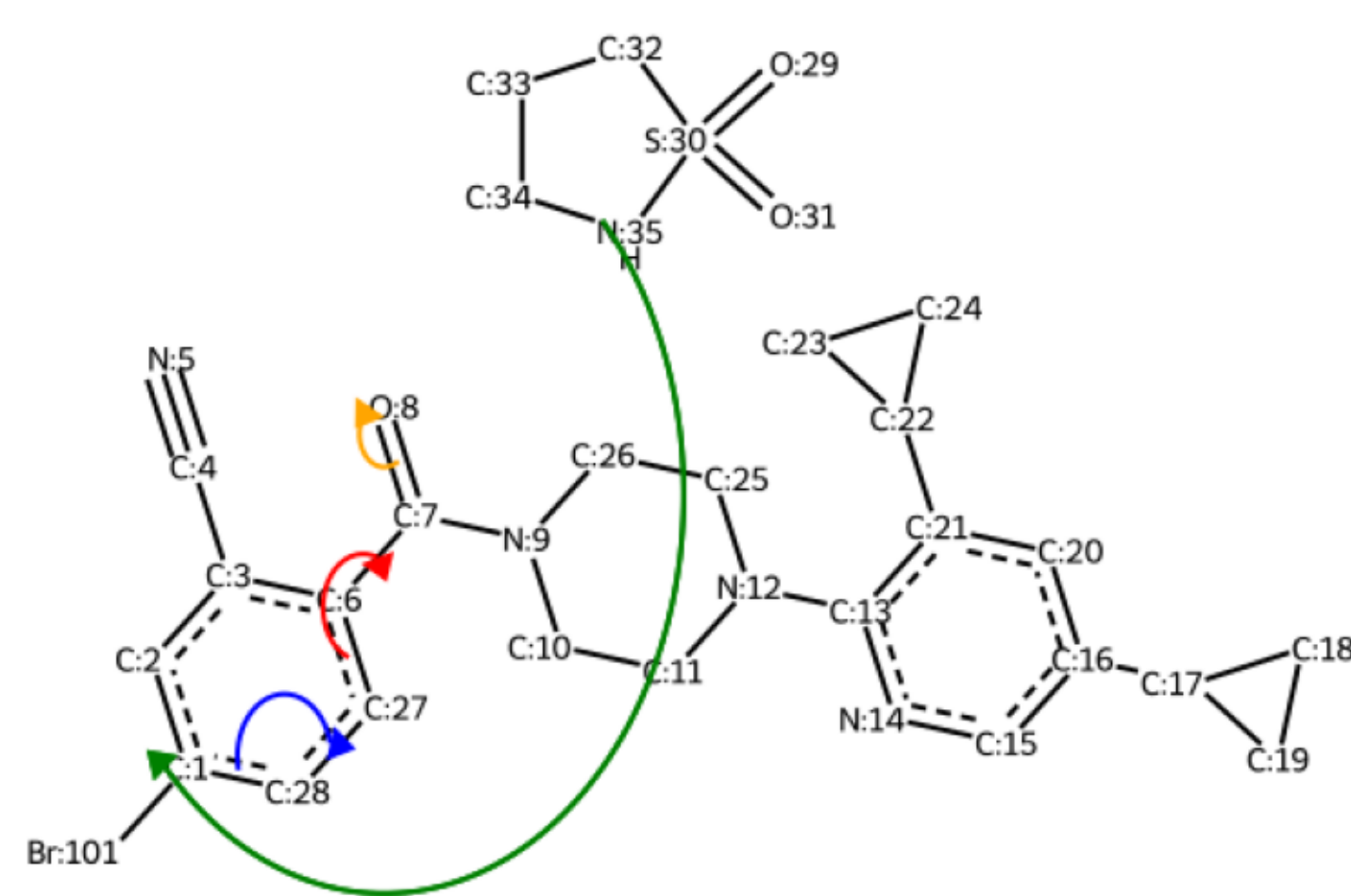


Proposed mechanistic pathway

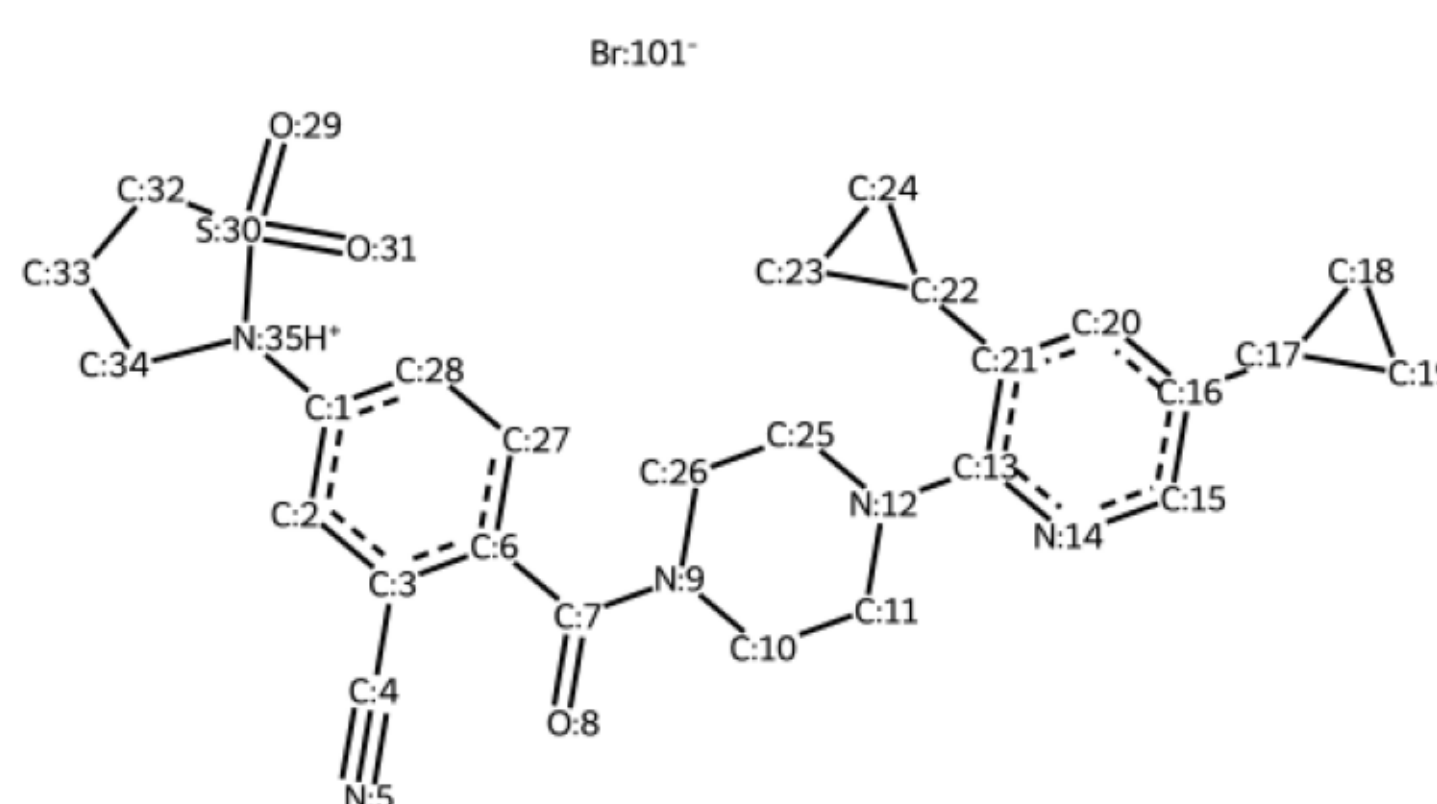
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

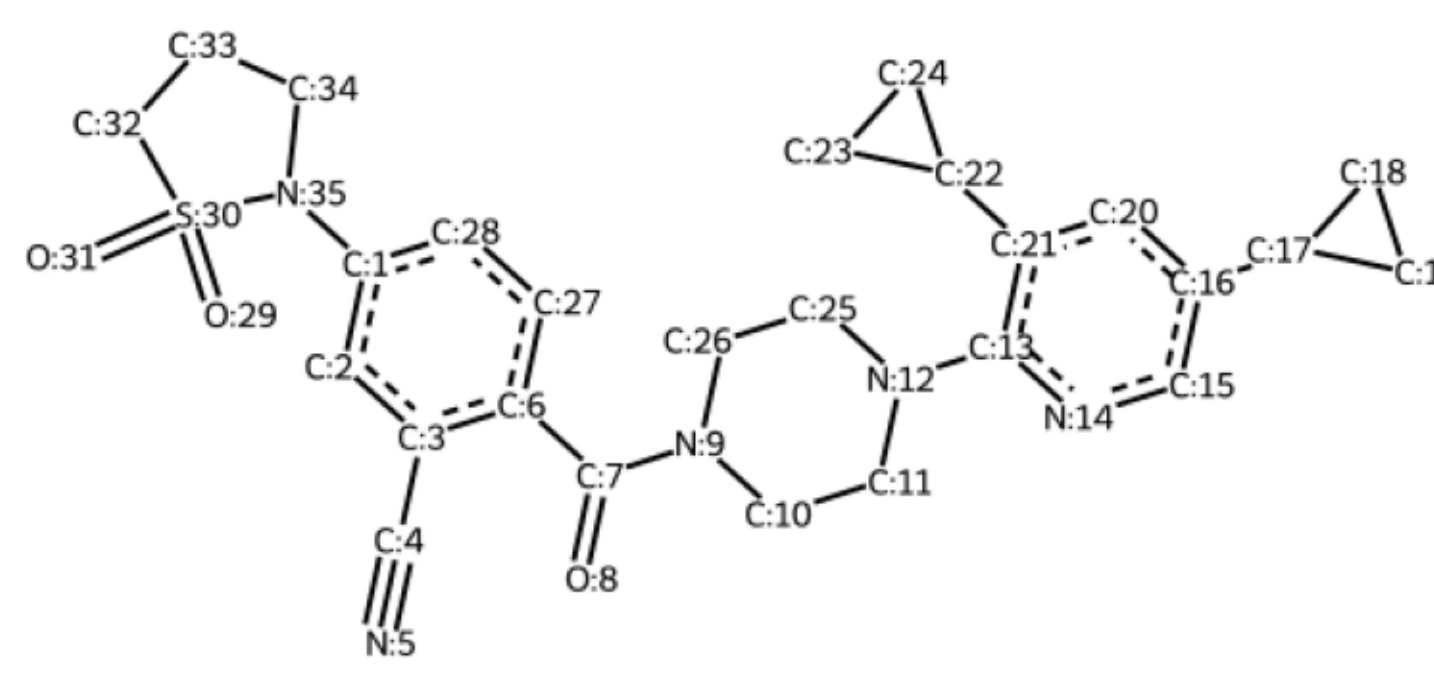
step #2



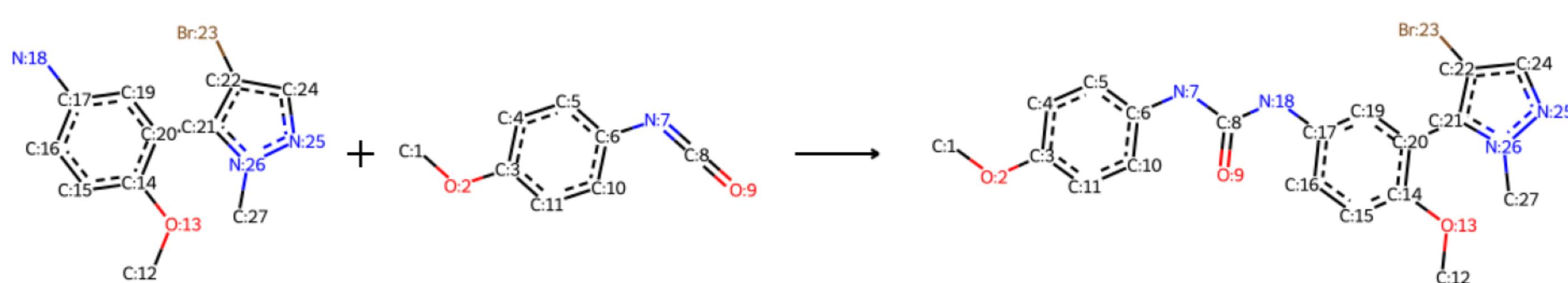
Product(s)



proton transfer

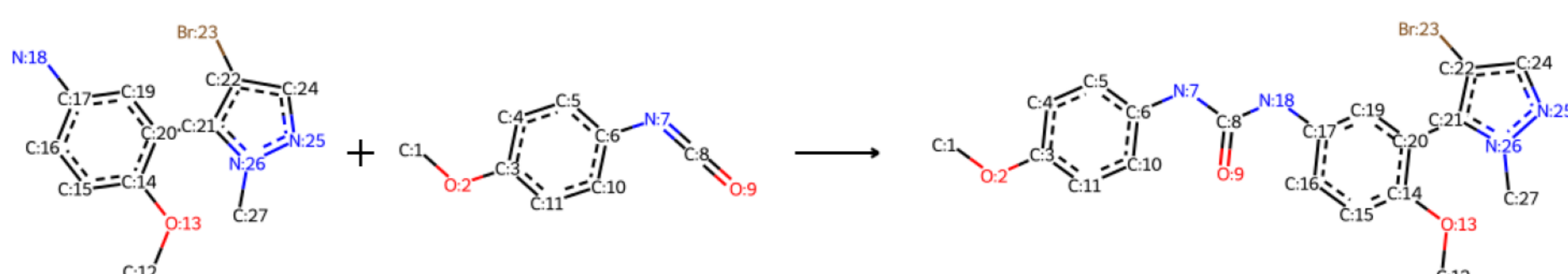


Original reaction
sampled RXN_ID:54)



Identified mechanistic class -
nucleophilic_attack_to_iso(thio)cyanate reaction

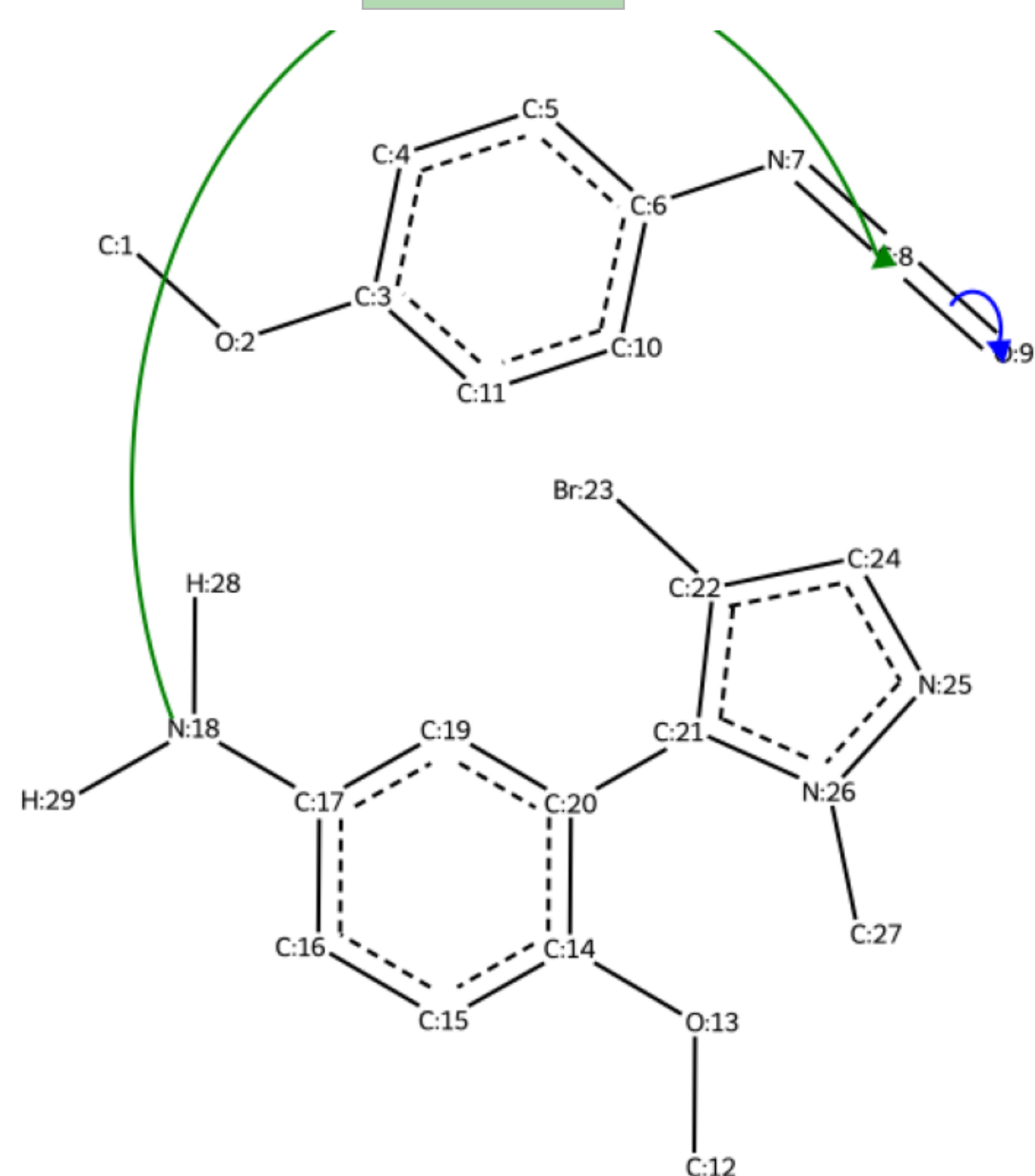
Reaction with missing reagents recovered



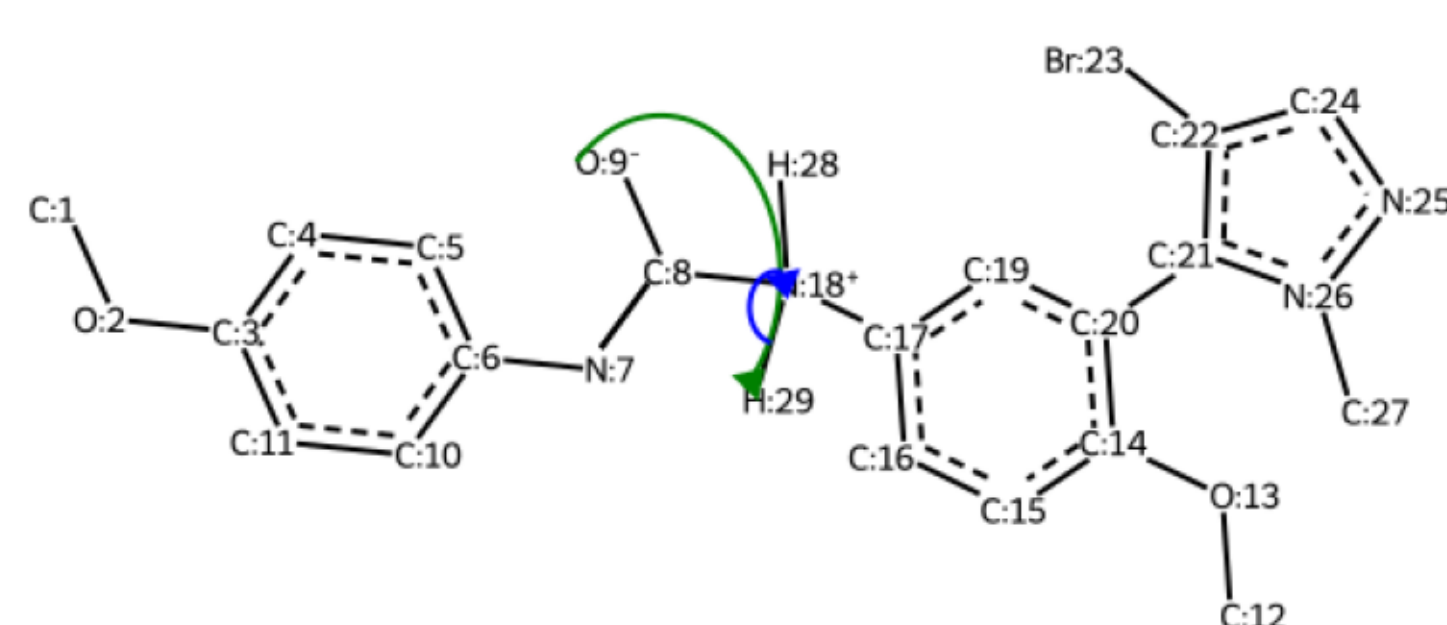
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

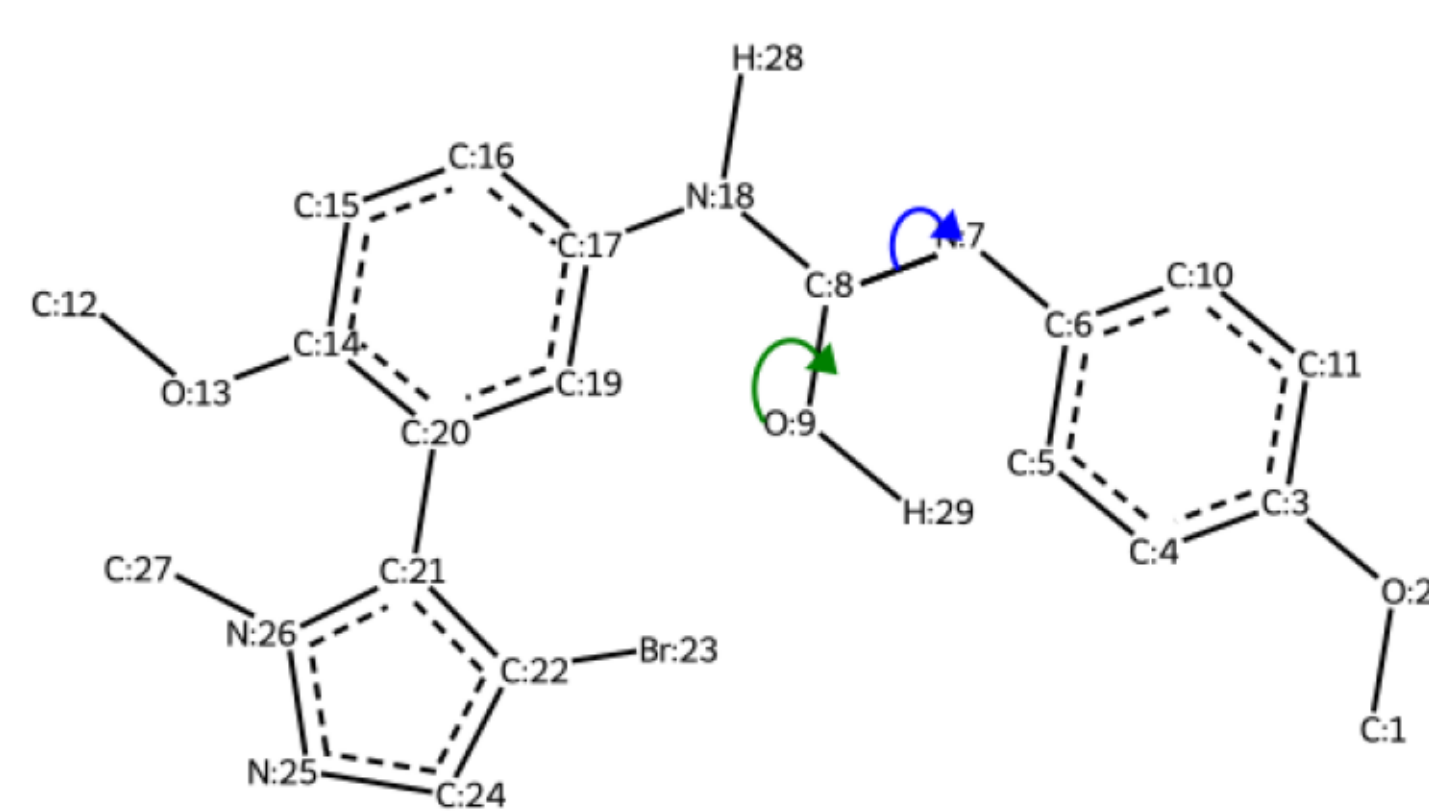
step #1



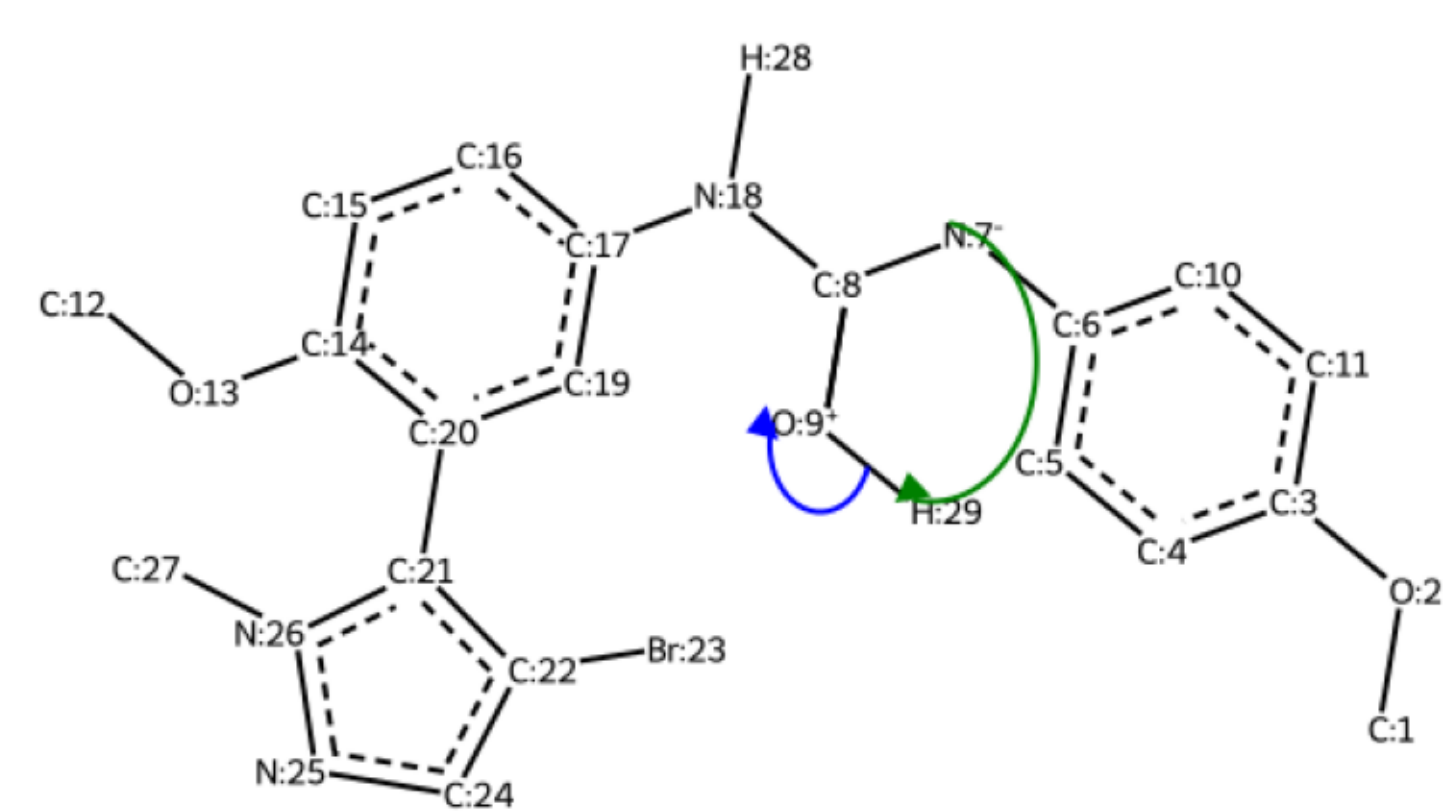
step #2



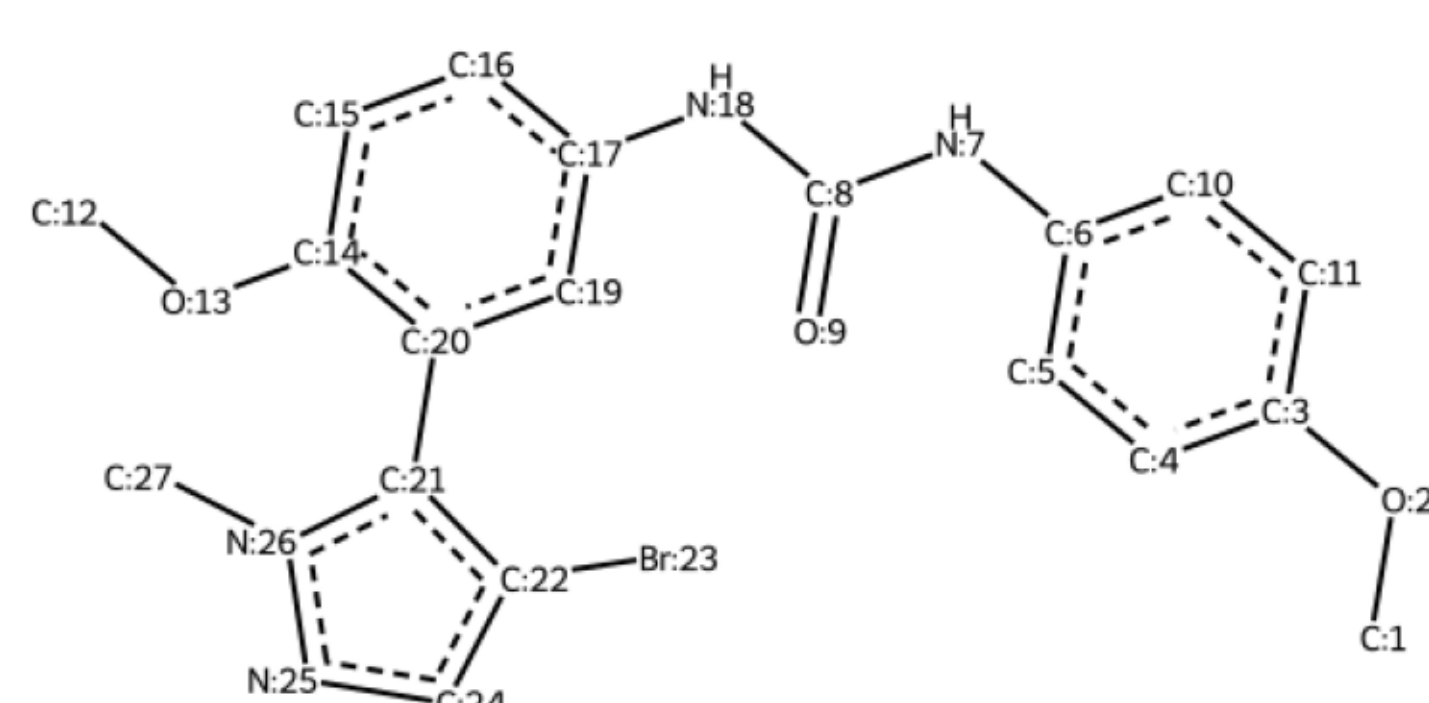
step #3



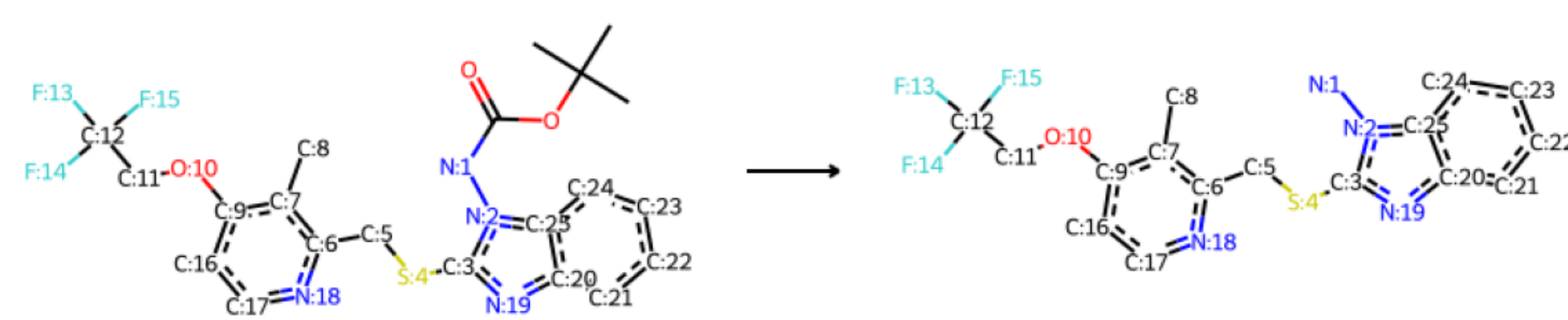
step #4



Product(s)

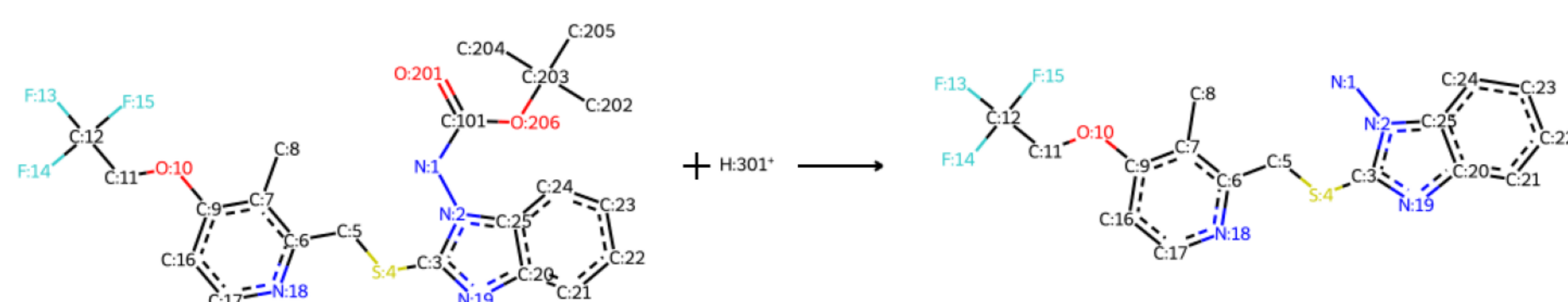


Original reaction
sampled RXN_ID:55)



Identified mechanistic class -
Boc_deprotection reaction

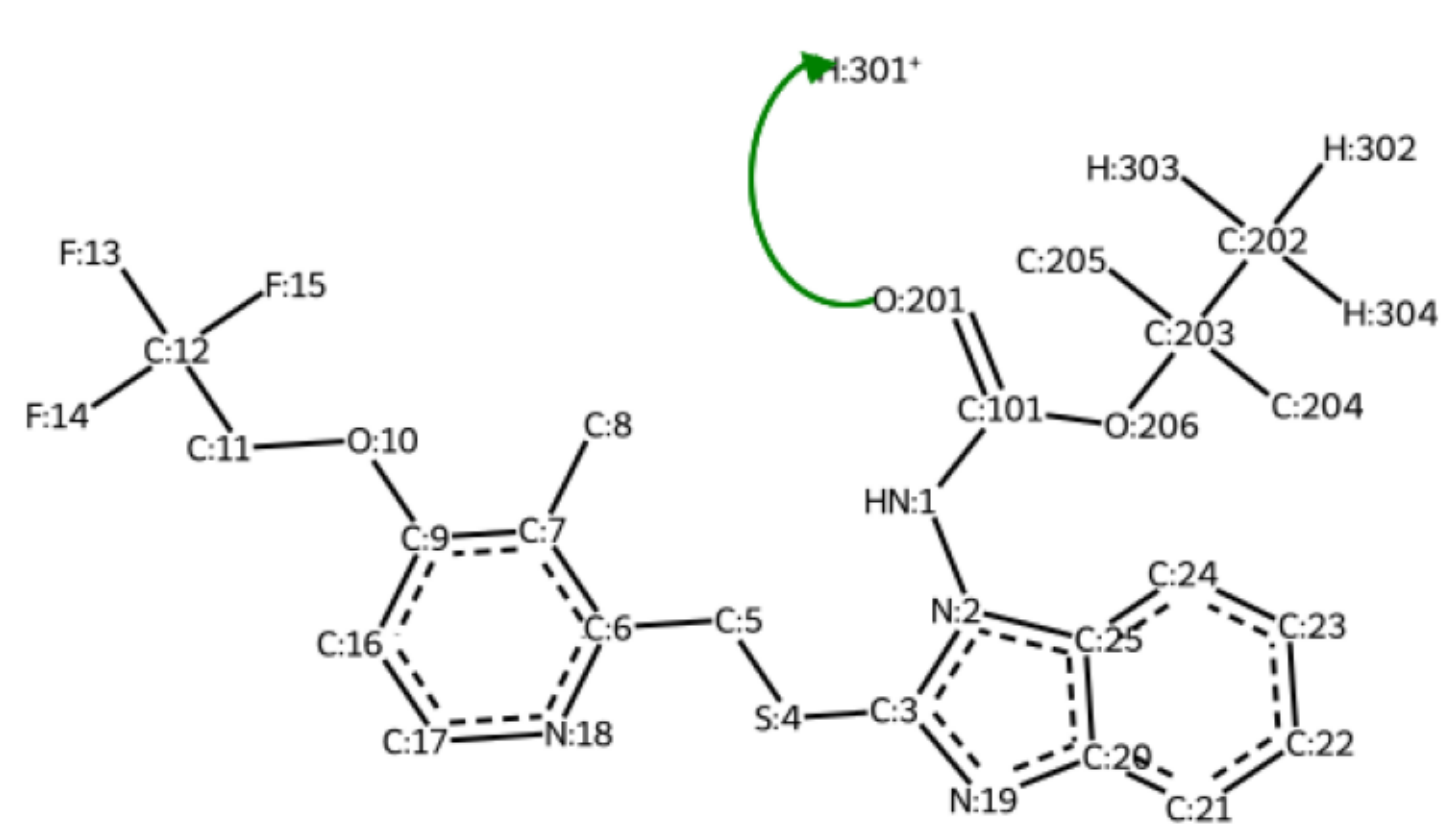
Reaction with missing reagents recovered



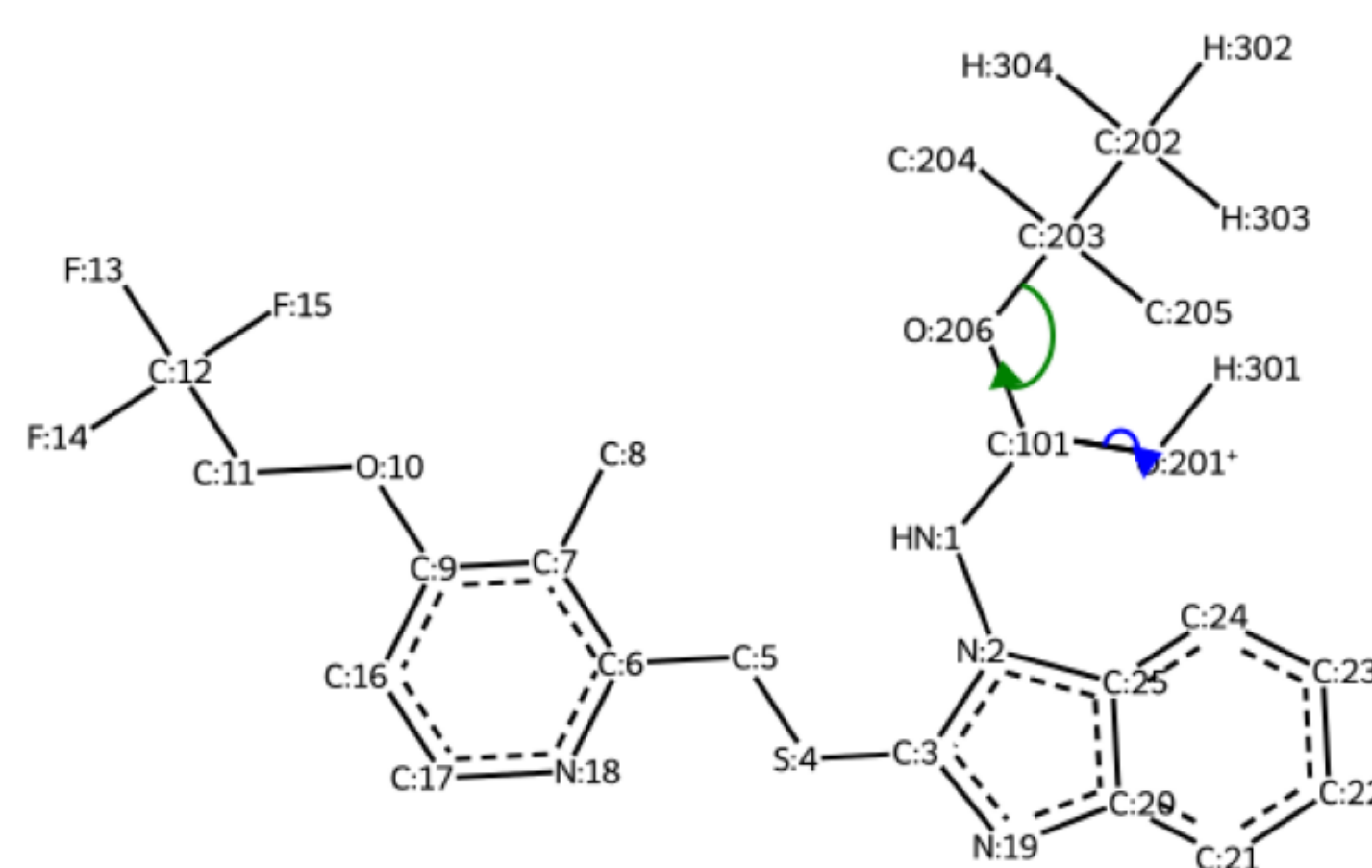
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

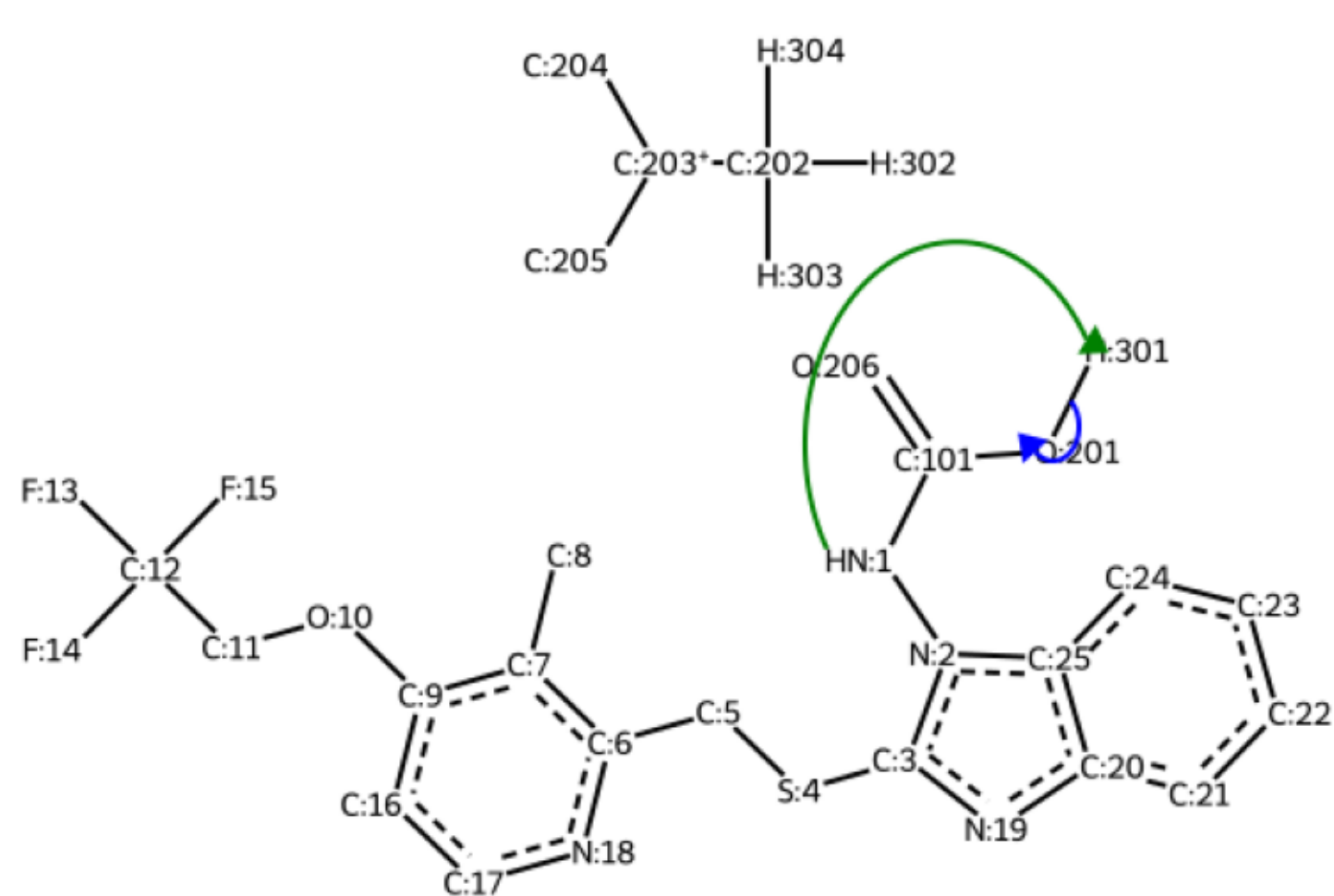
step #1



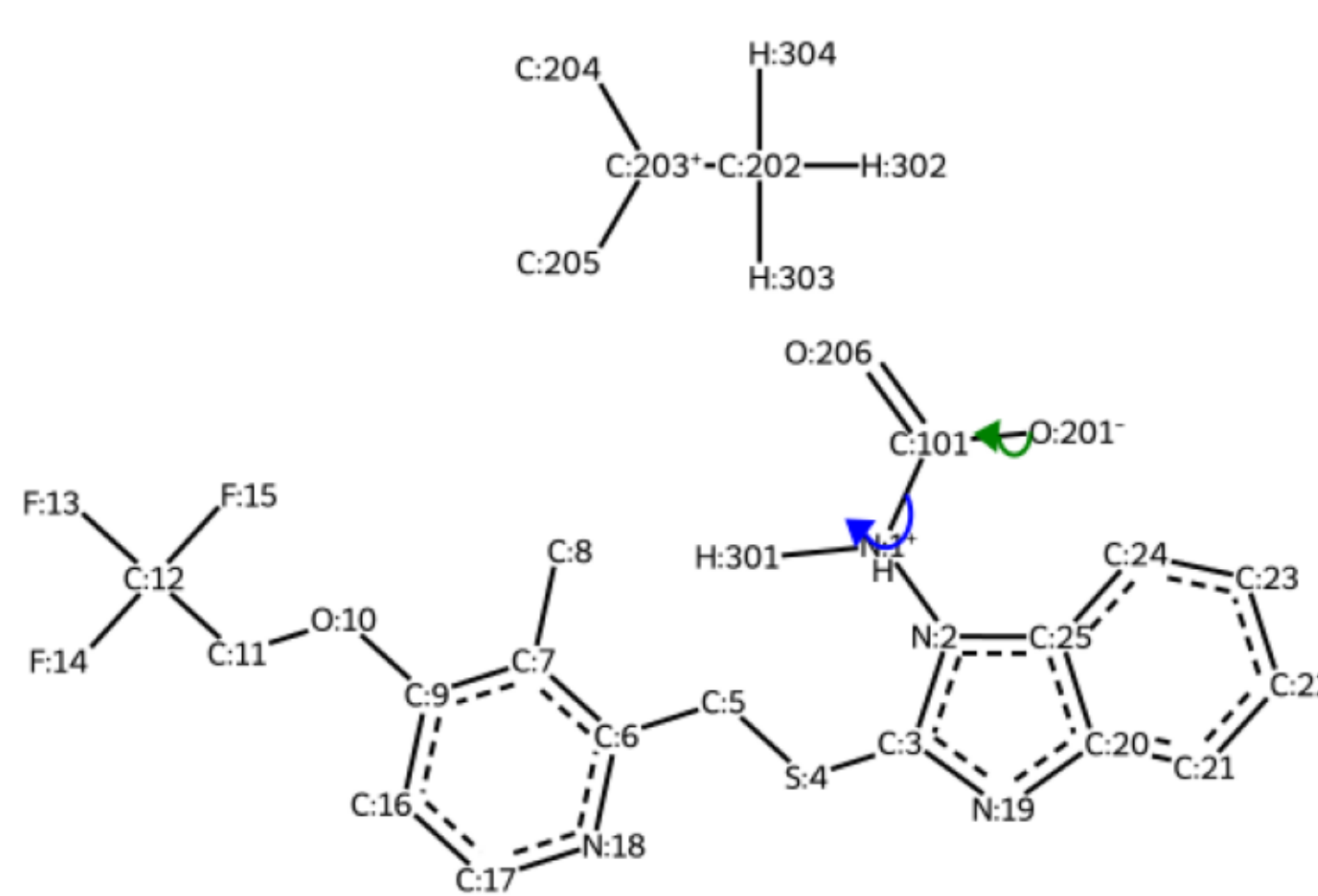
step #2



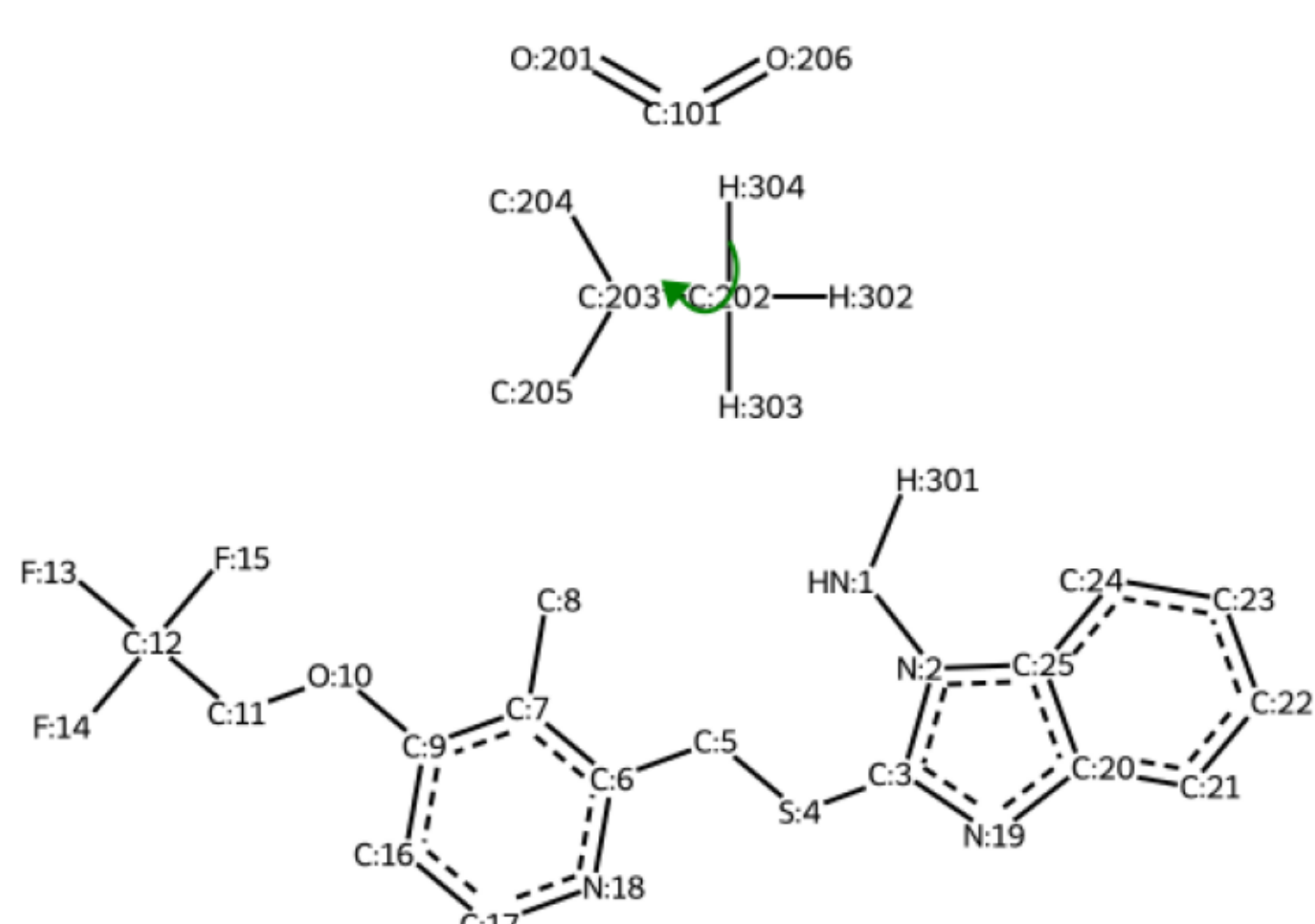
step #3



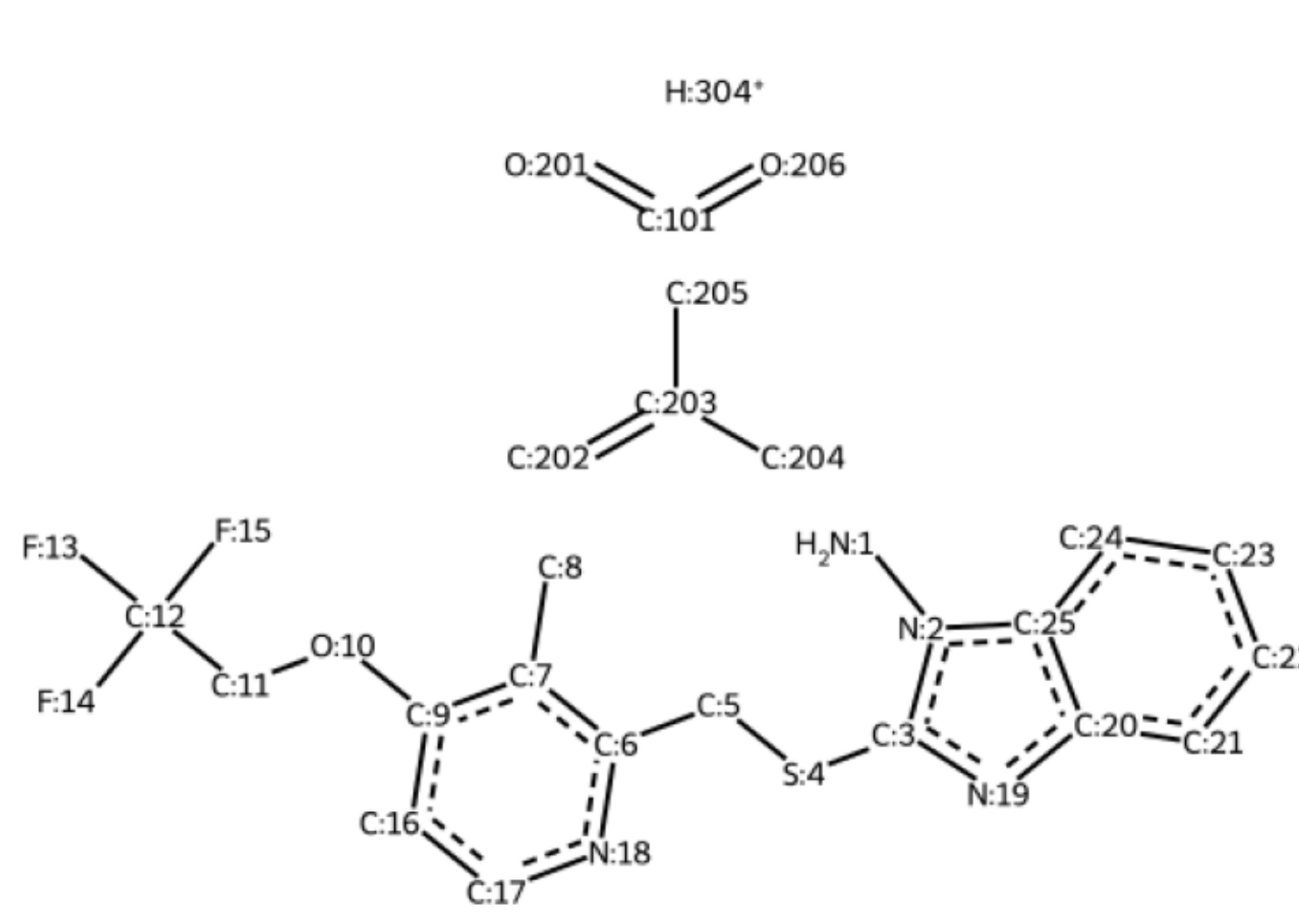
step #4



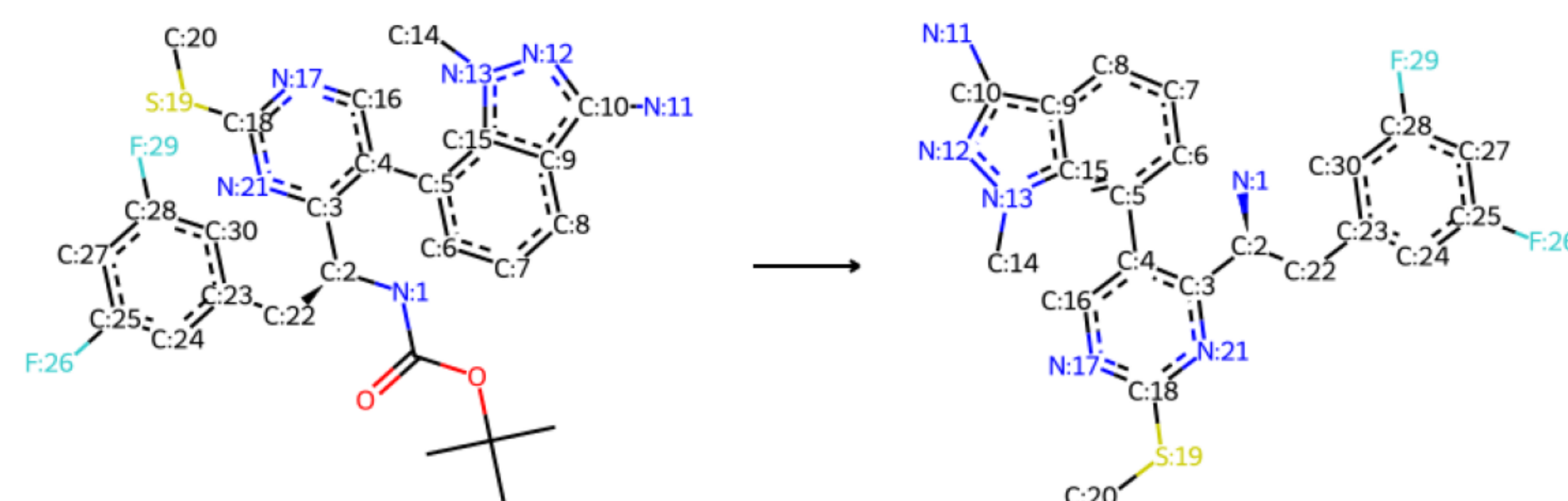
step #5



Product(s)

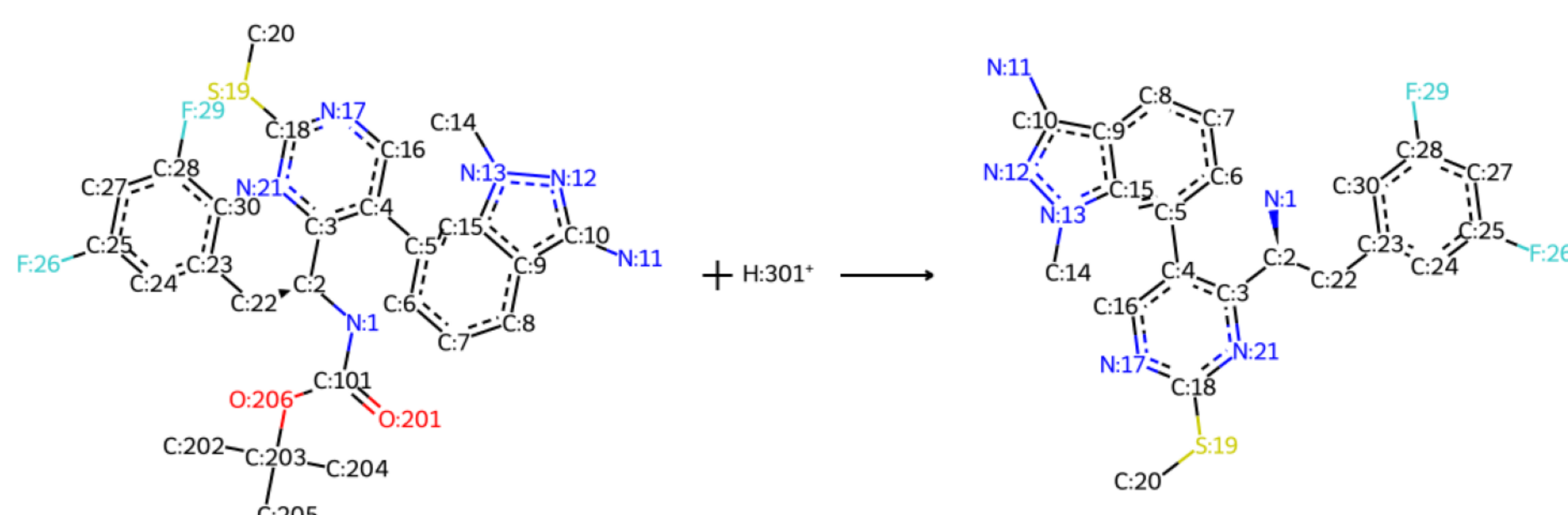


Original reaction
sampled RXN_ID:56)



Identified mechanistic class -
Boc_deprotection reaction

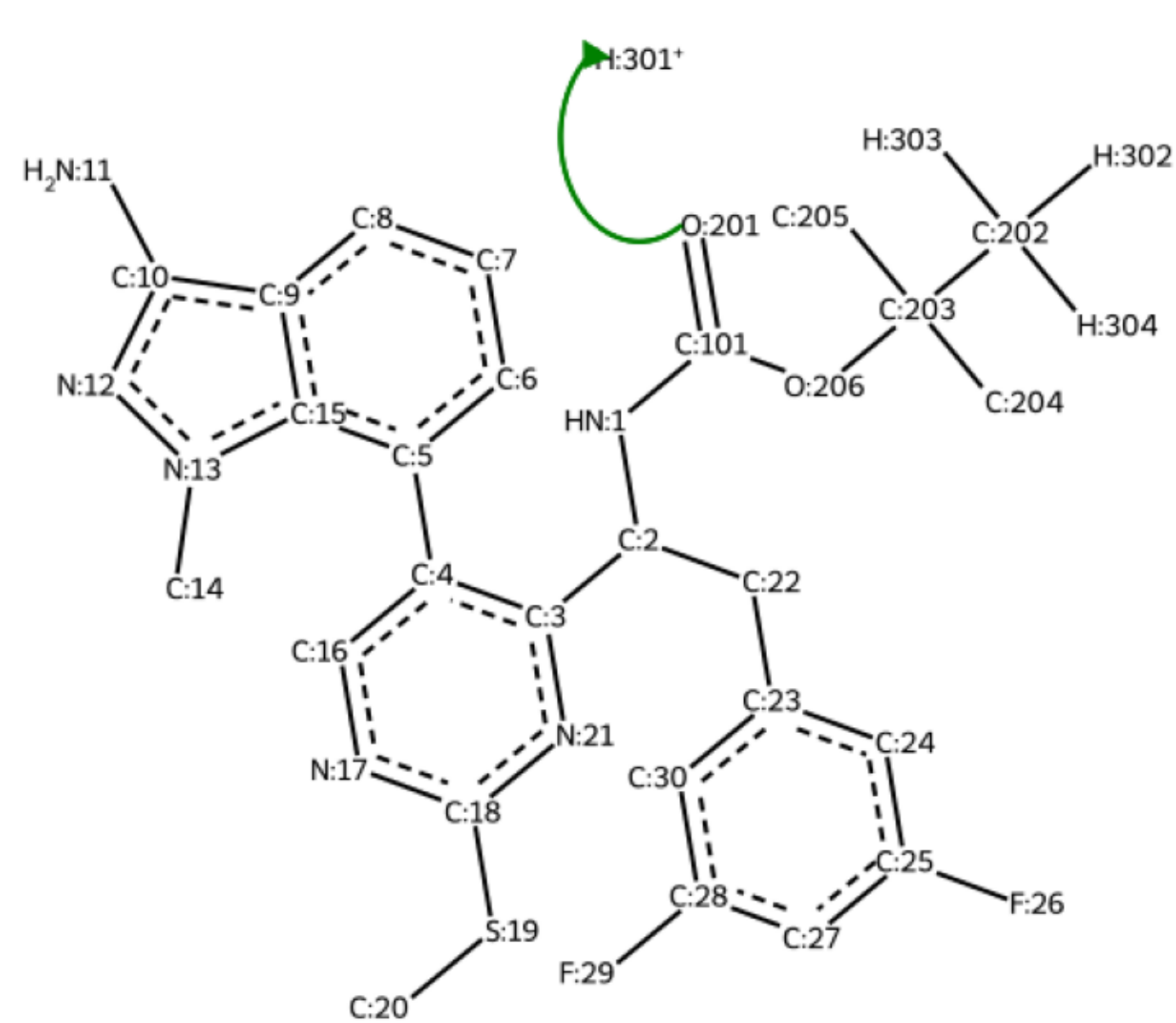
Reaction with missing reagents recovered



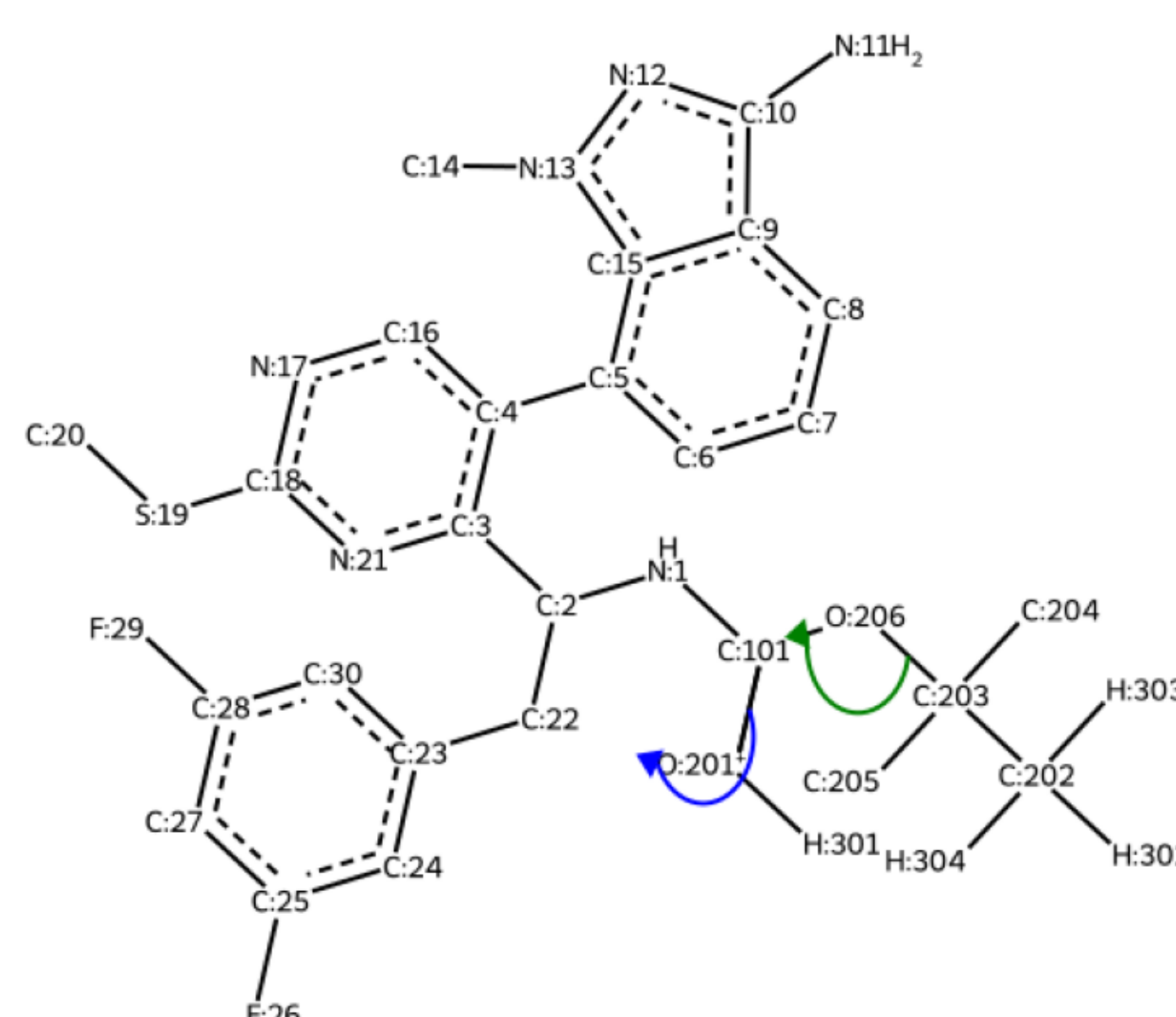
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

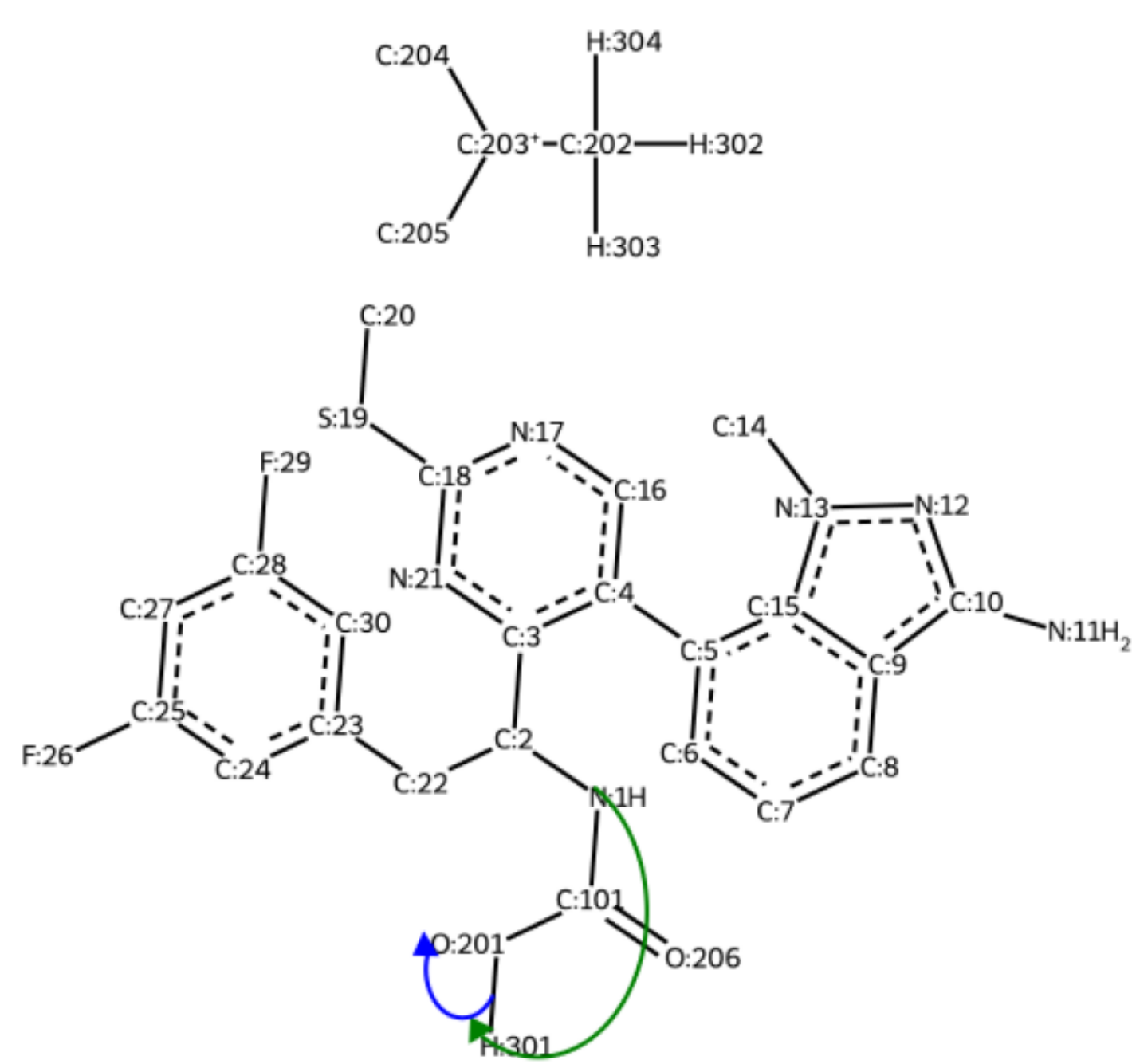
step #1



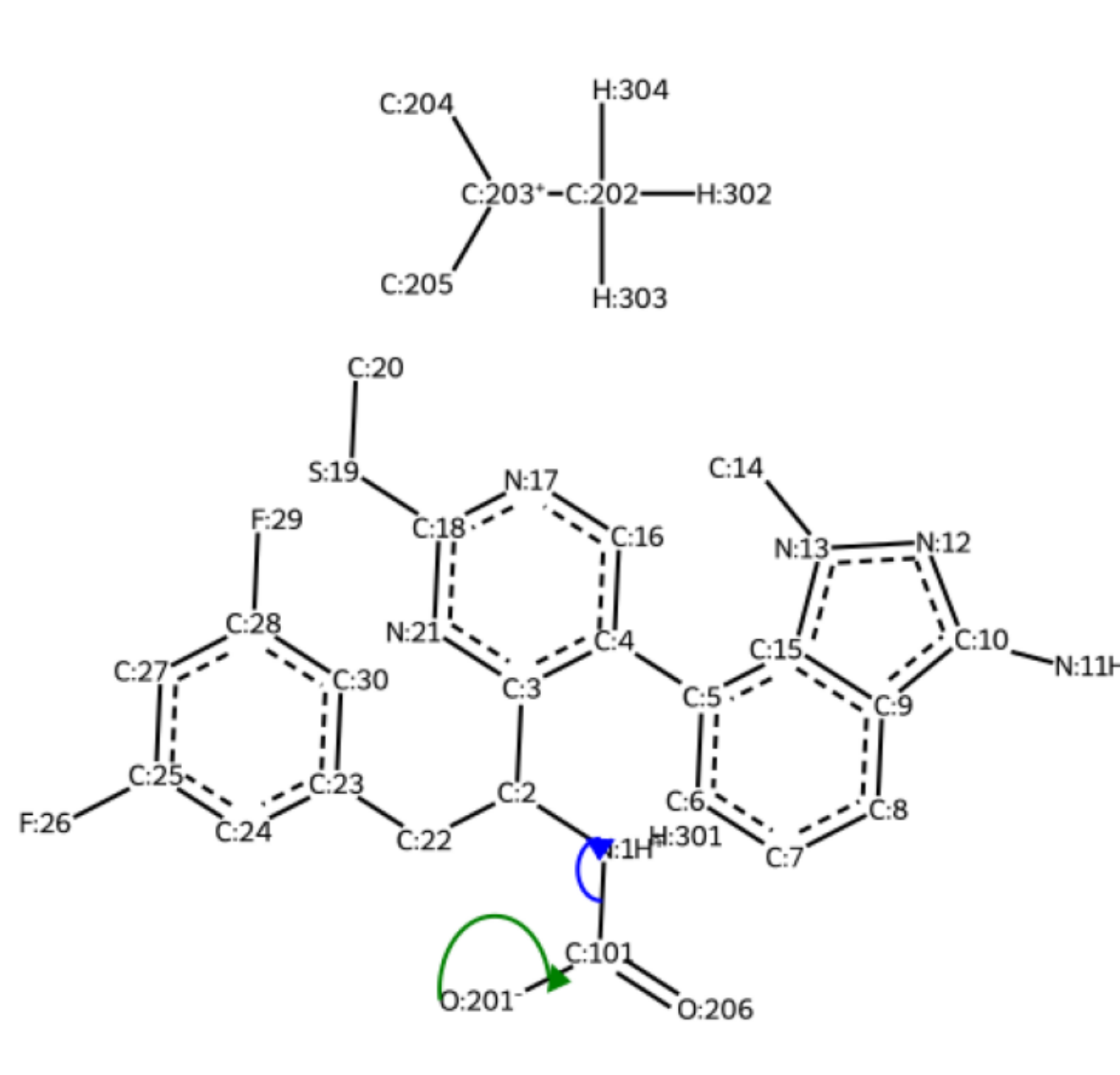
step #2



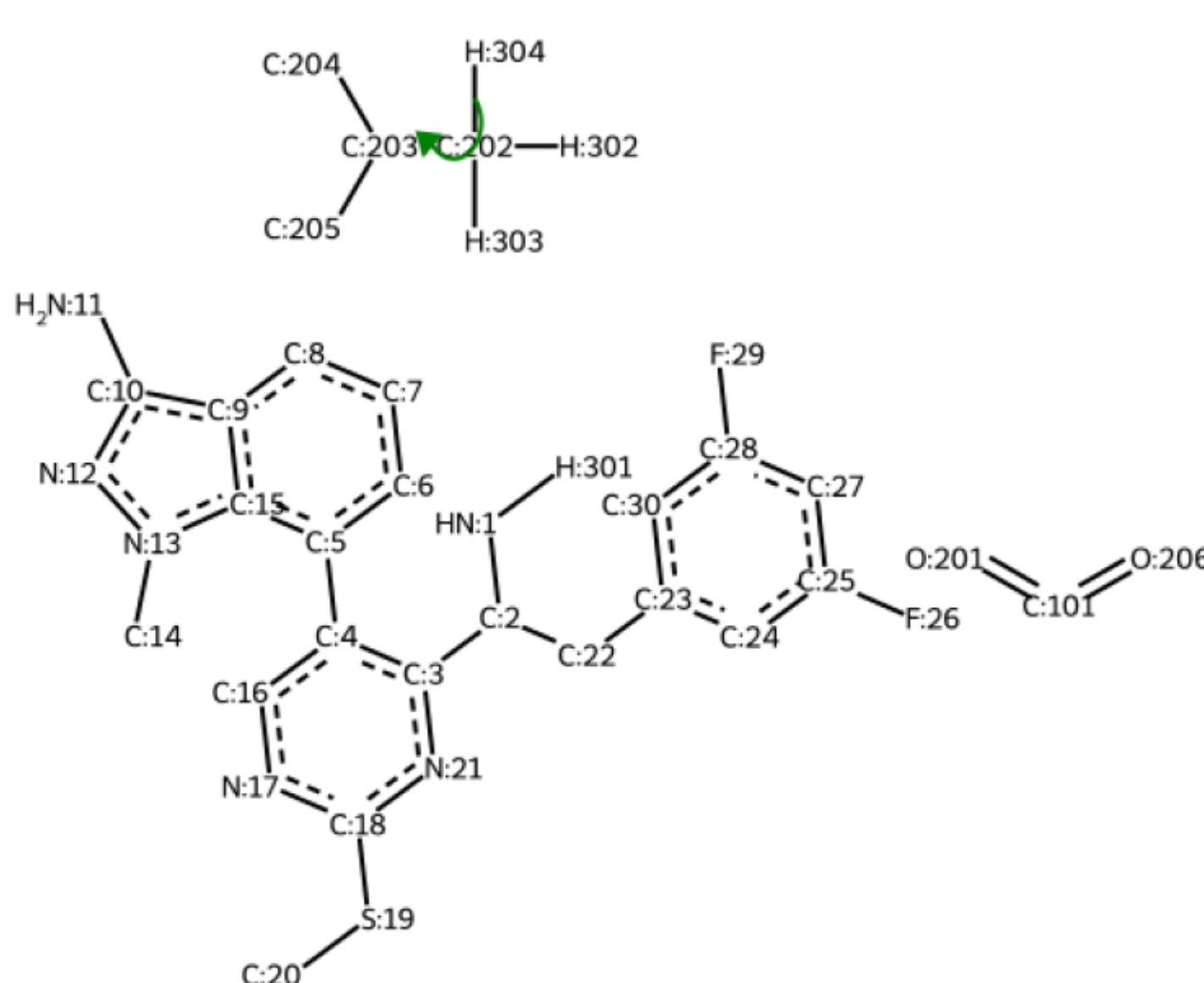
step #3



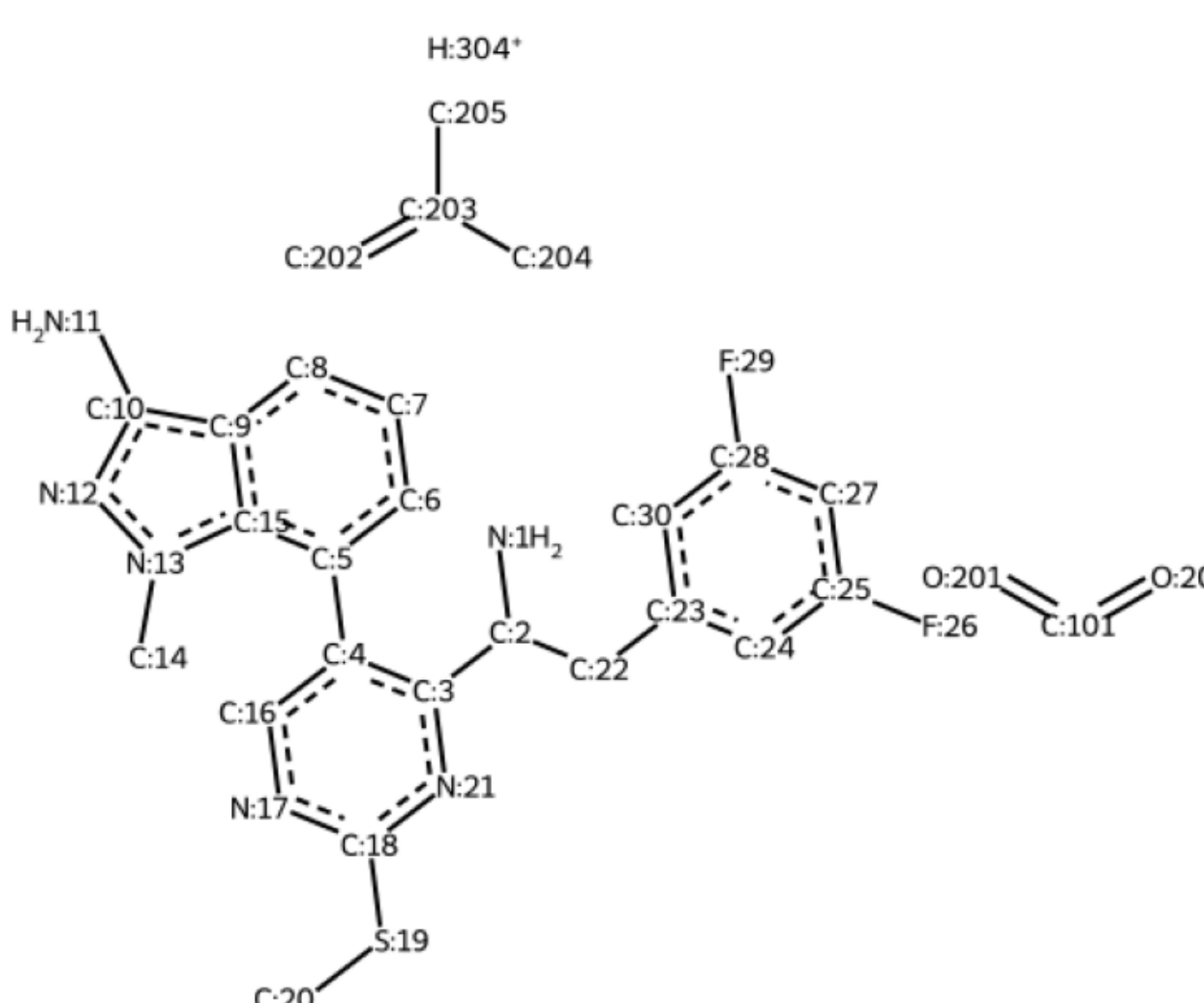
step #4



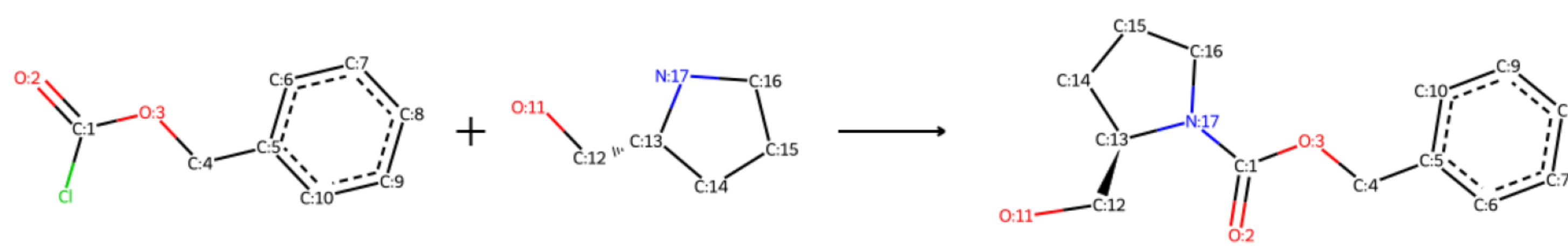
step #5



Product(s)

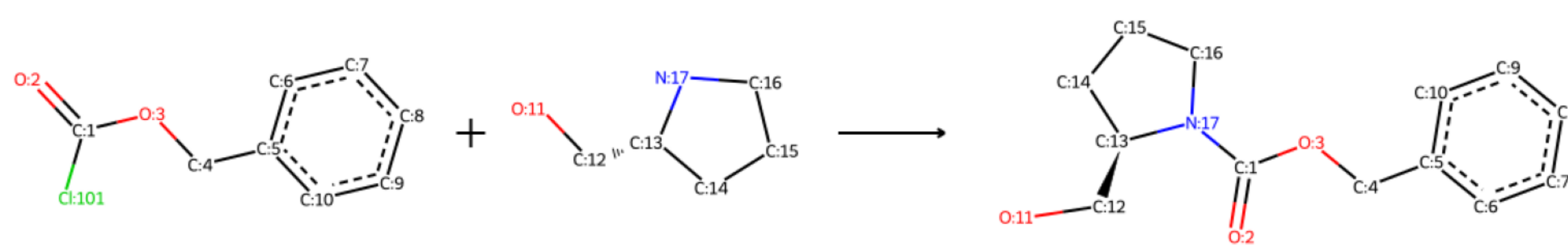


Original reaction sampled RXN_ID:57)



Identified mechanistic class -
nucleophilic_attack_to_(thio)carbonyl_or_sulfonyl reaction

Reaction with missing reagents recovered

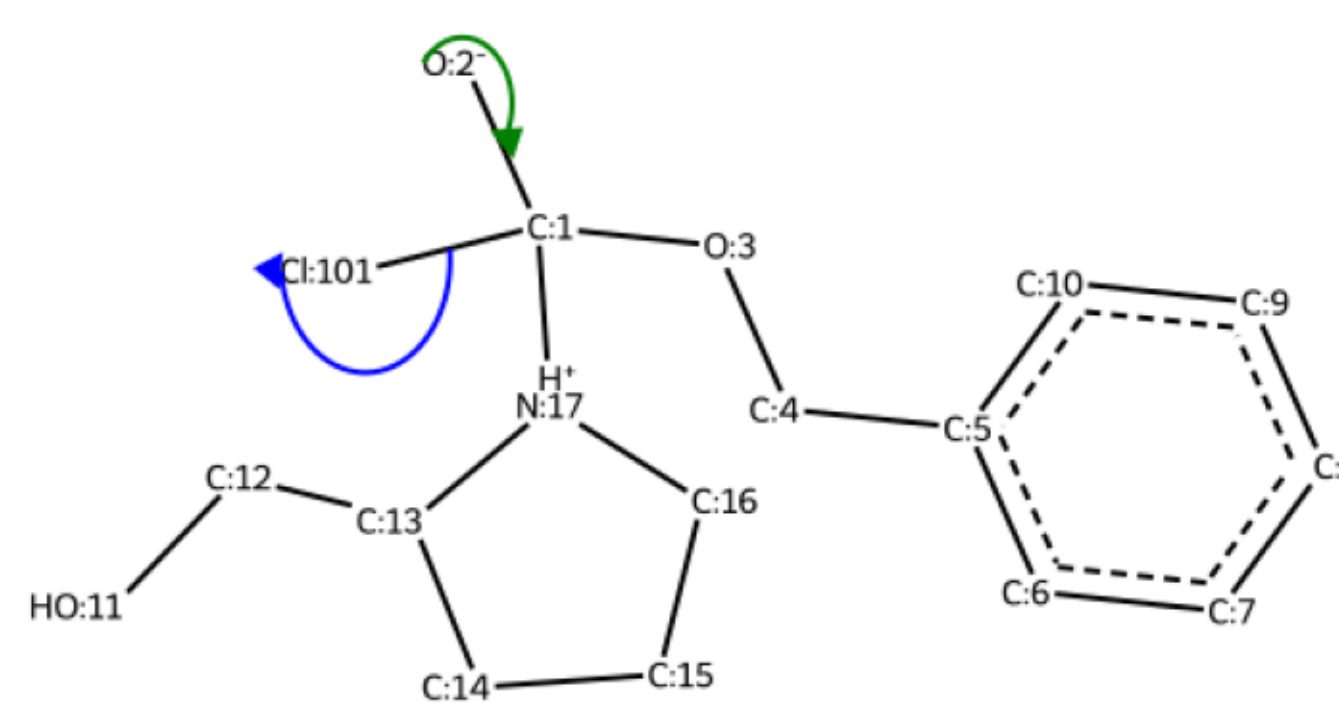
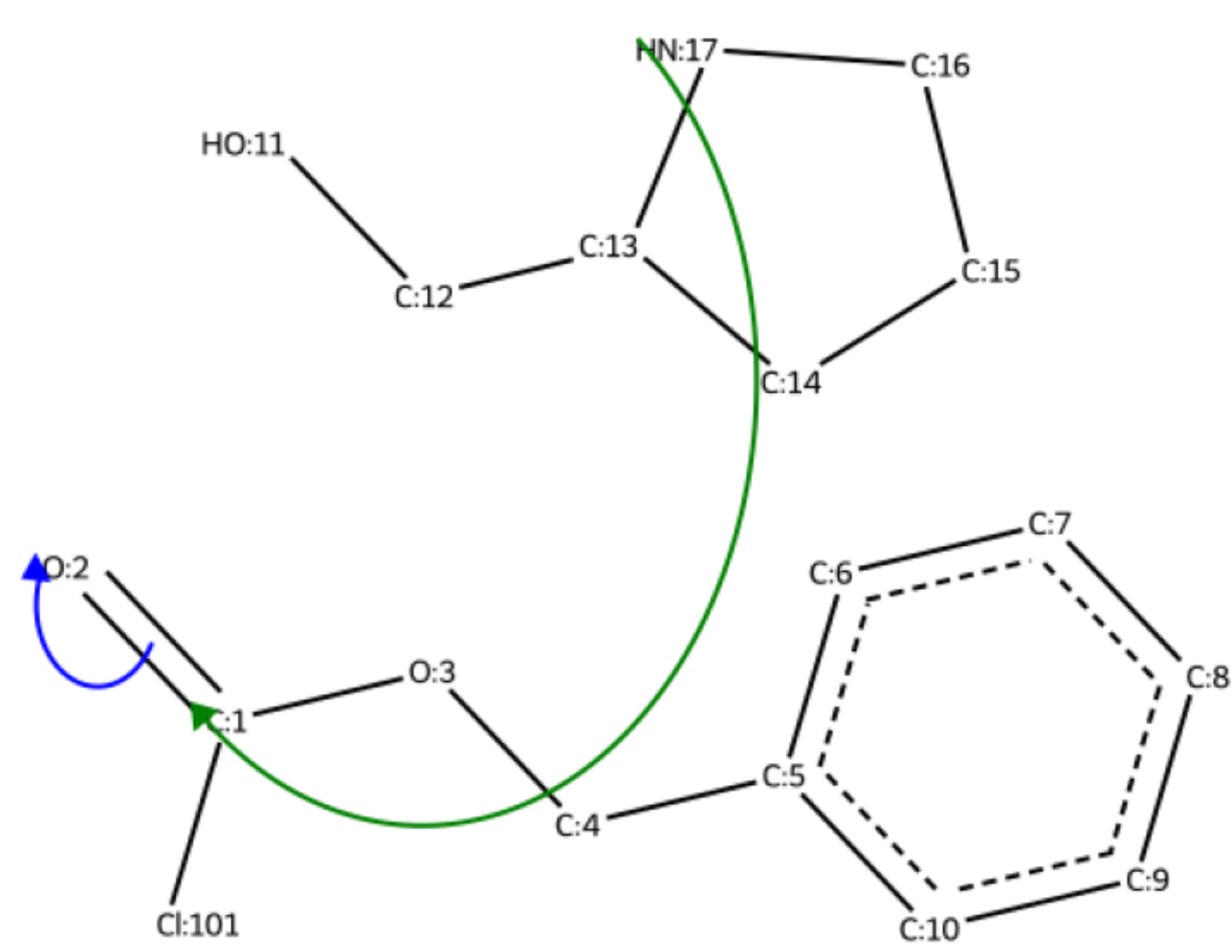


Proposed mechanistic pathway

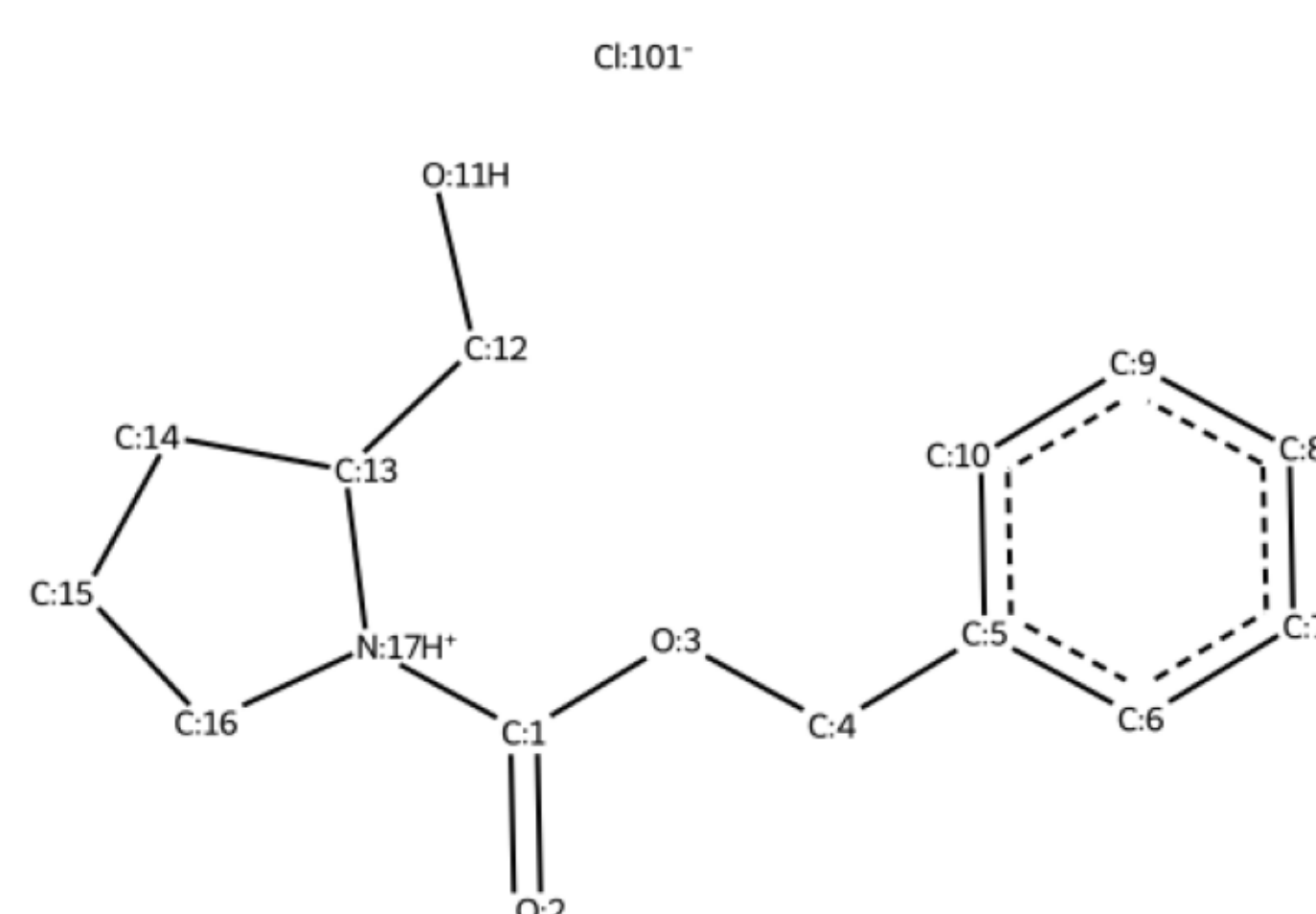
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

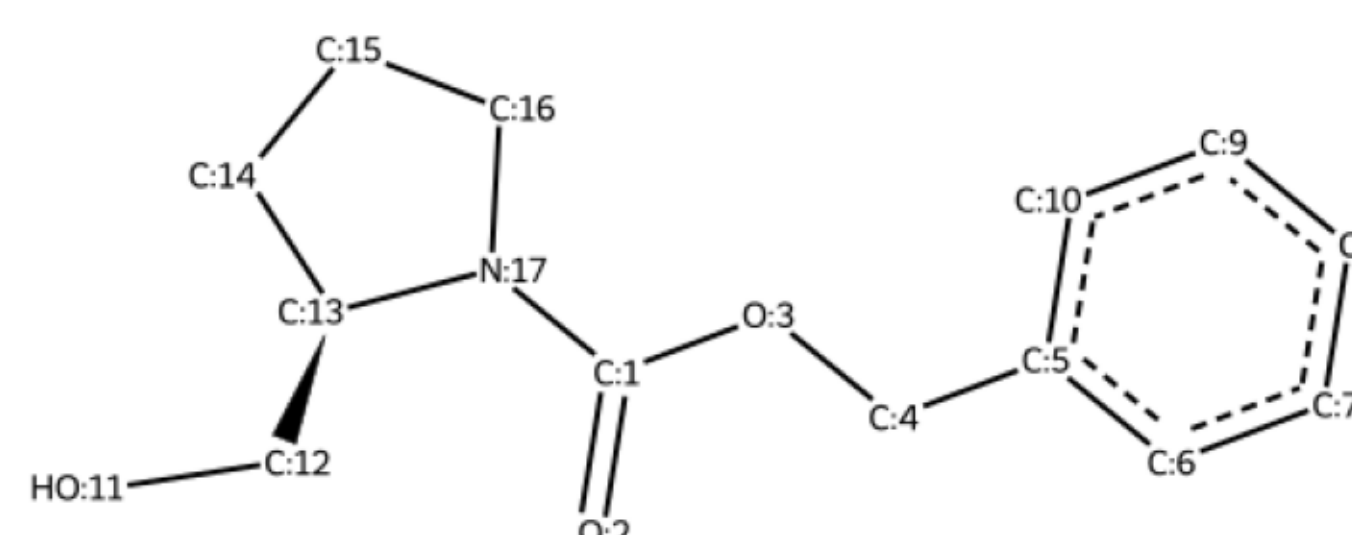
step #2



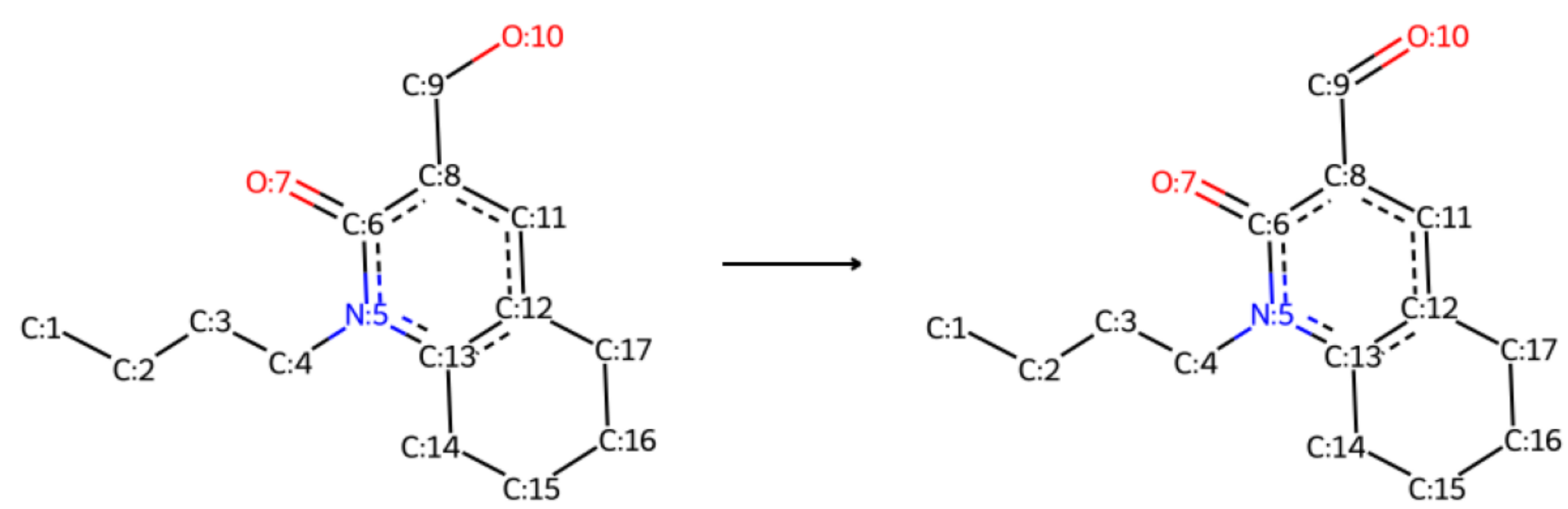
Product(s)



proton transfer

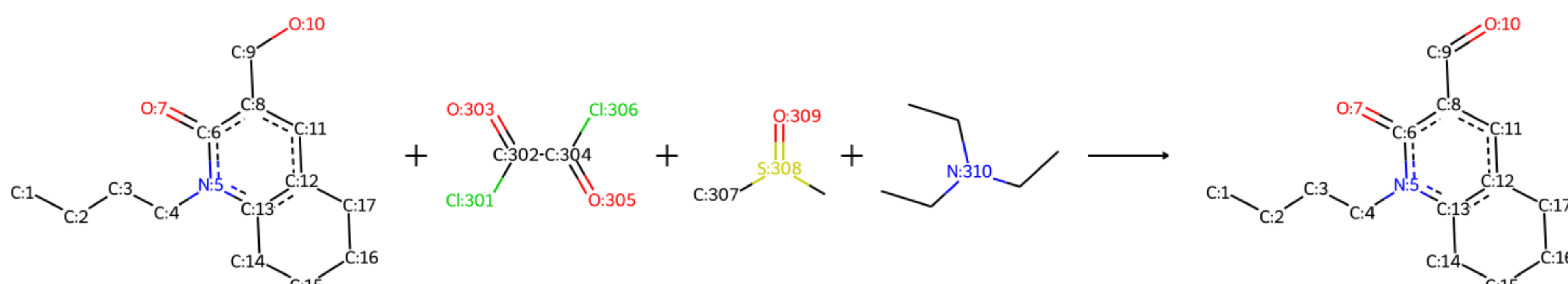


Original reaction
sampled RXN_ID:58)



Identified mechanistic class -
Swern_oxidation reaction

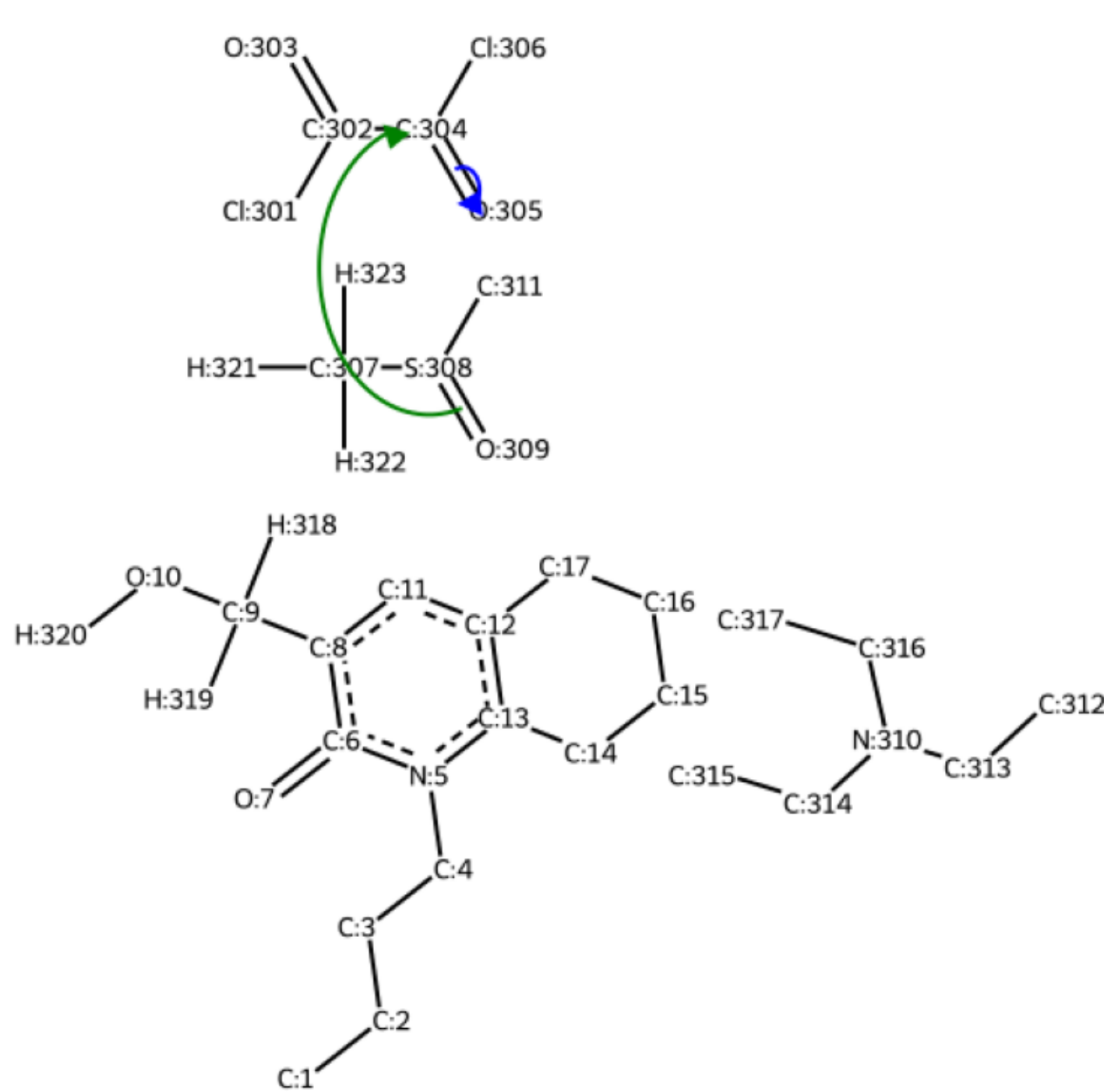
Reaction with missing reagents recovered



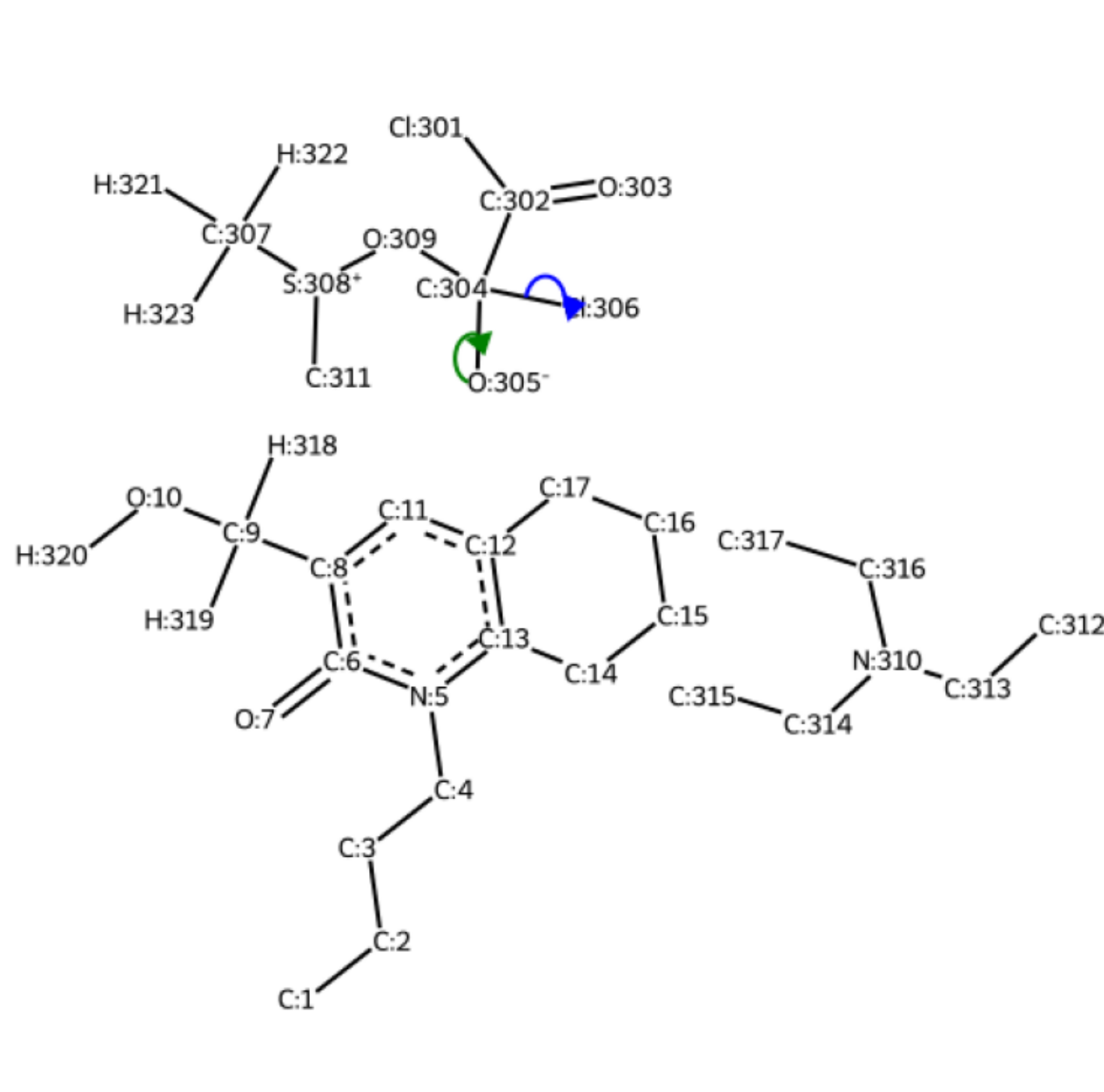
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

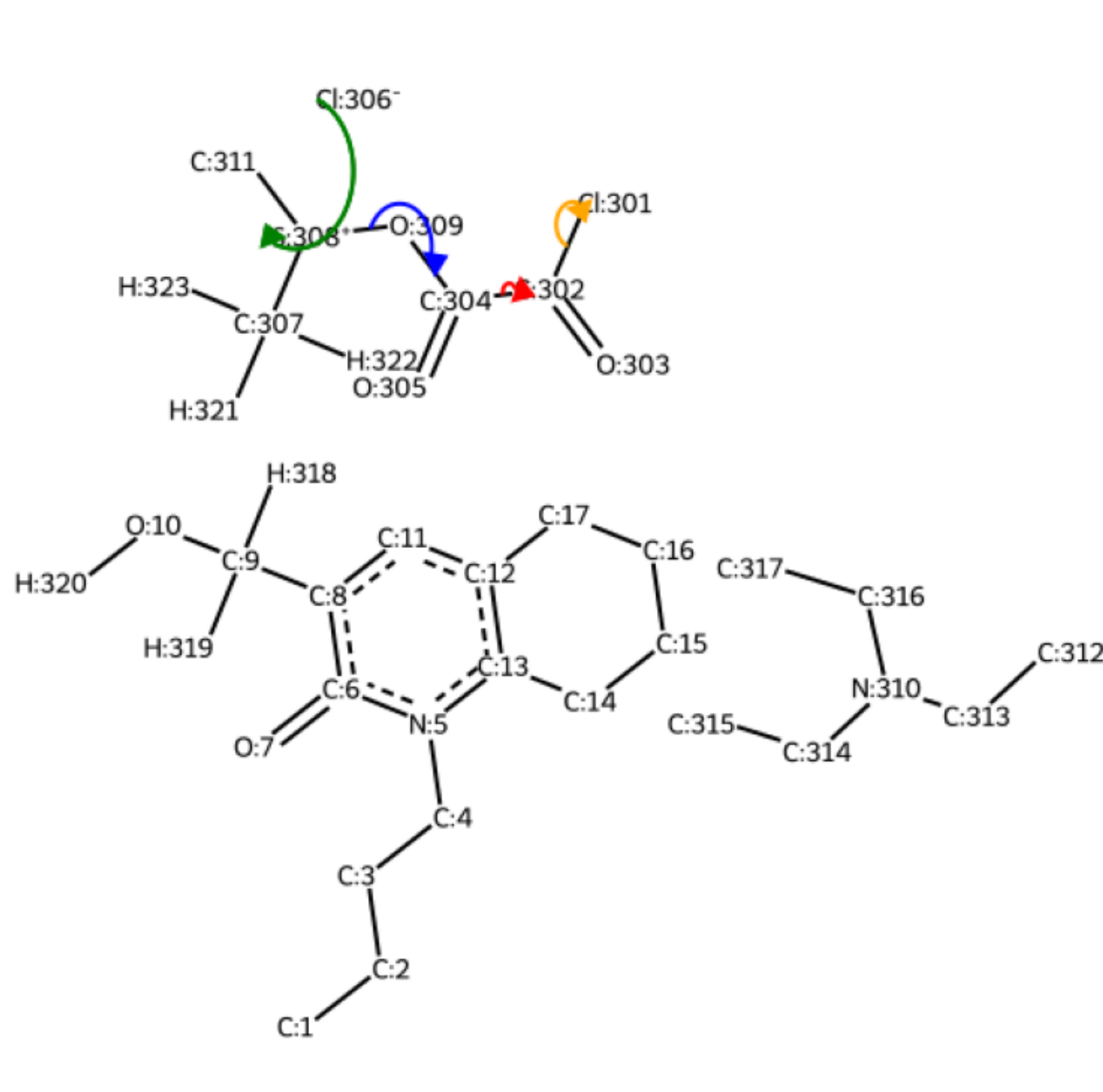
step #1



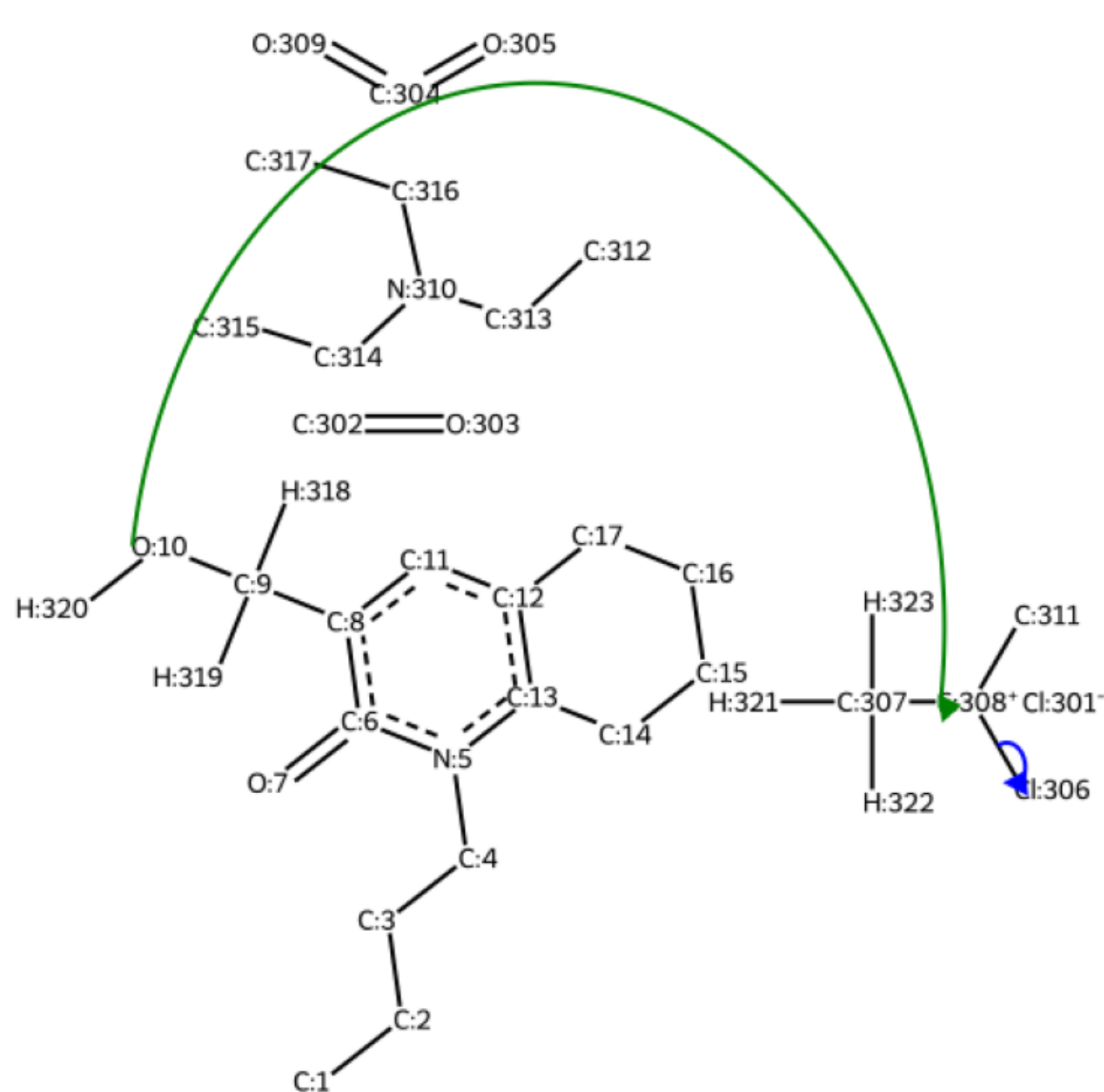
step #2



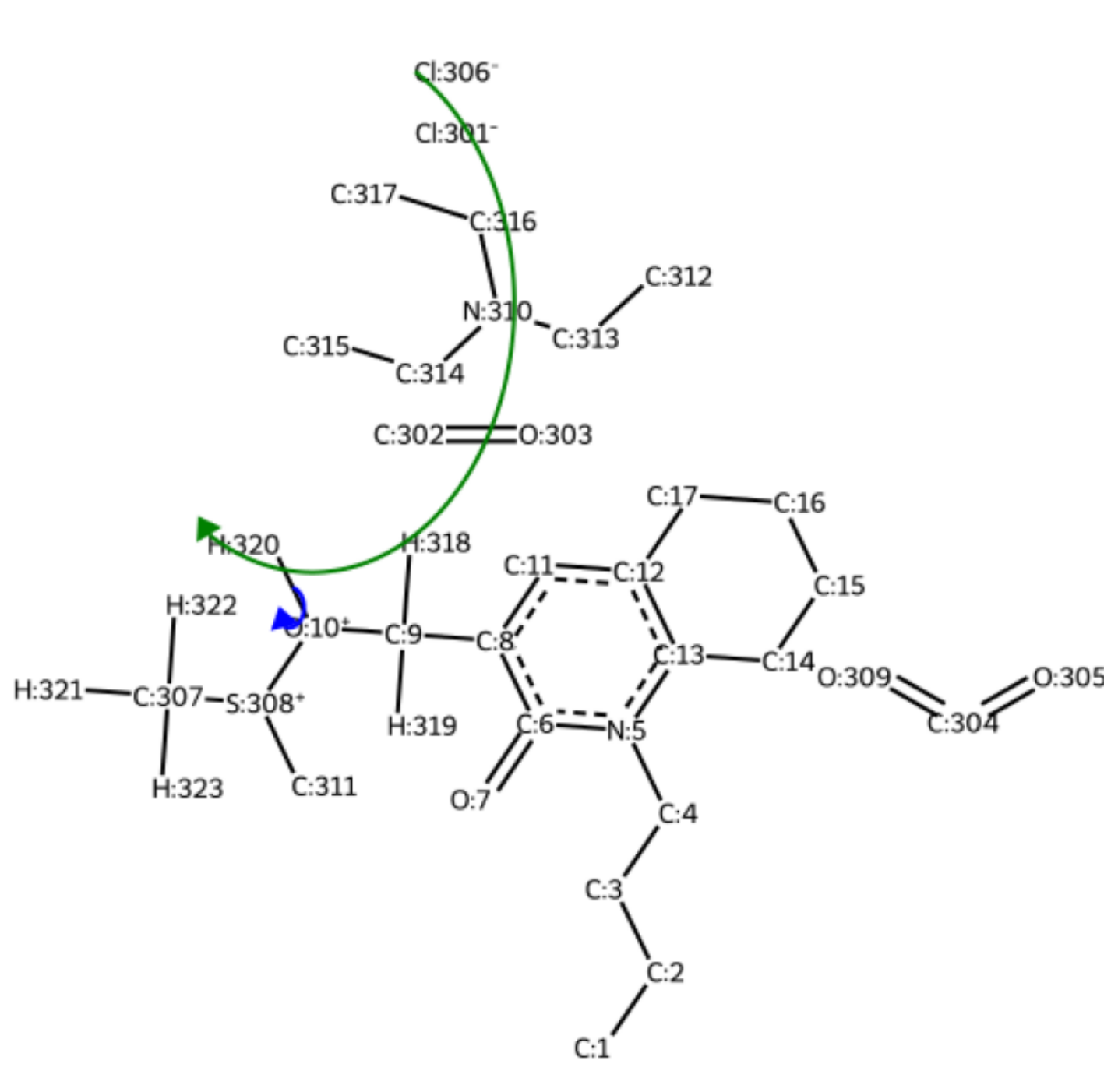
step #3



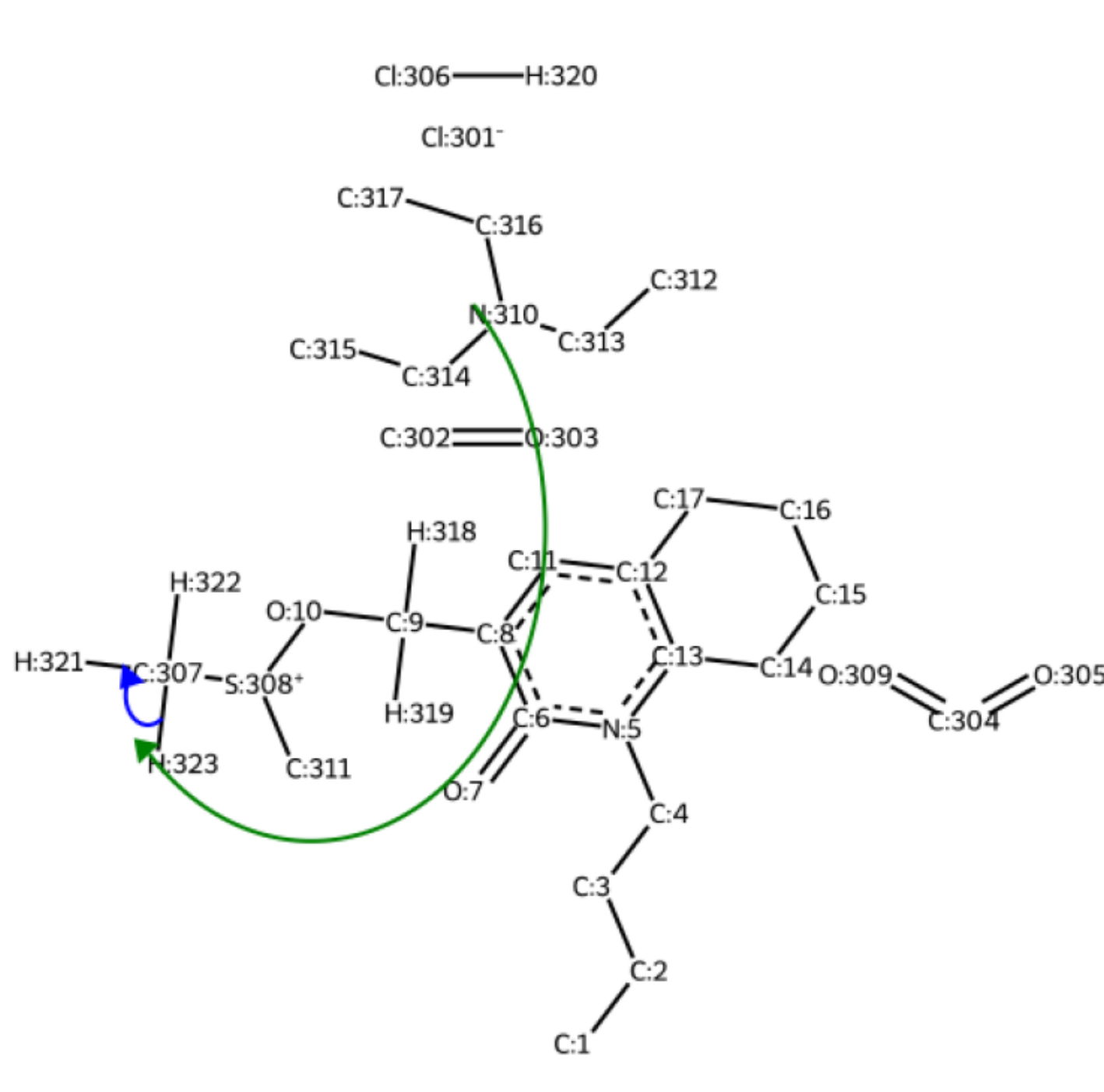
step #4



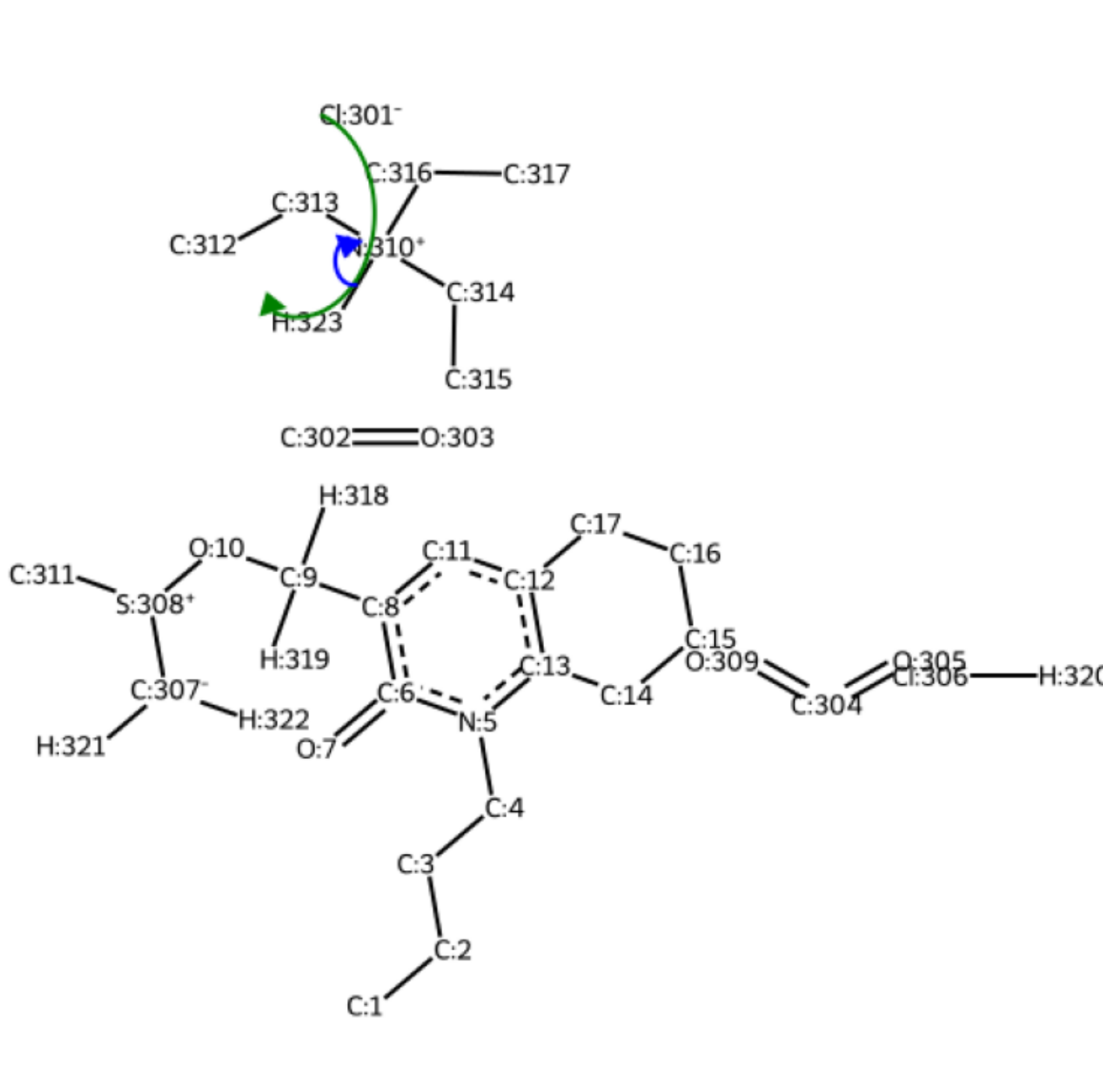
step #5



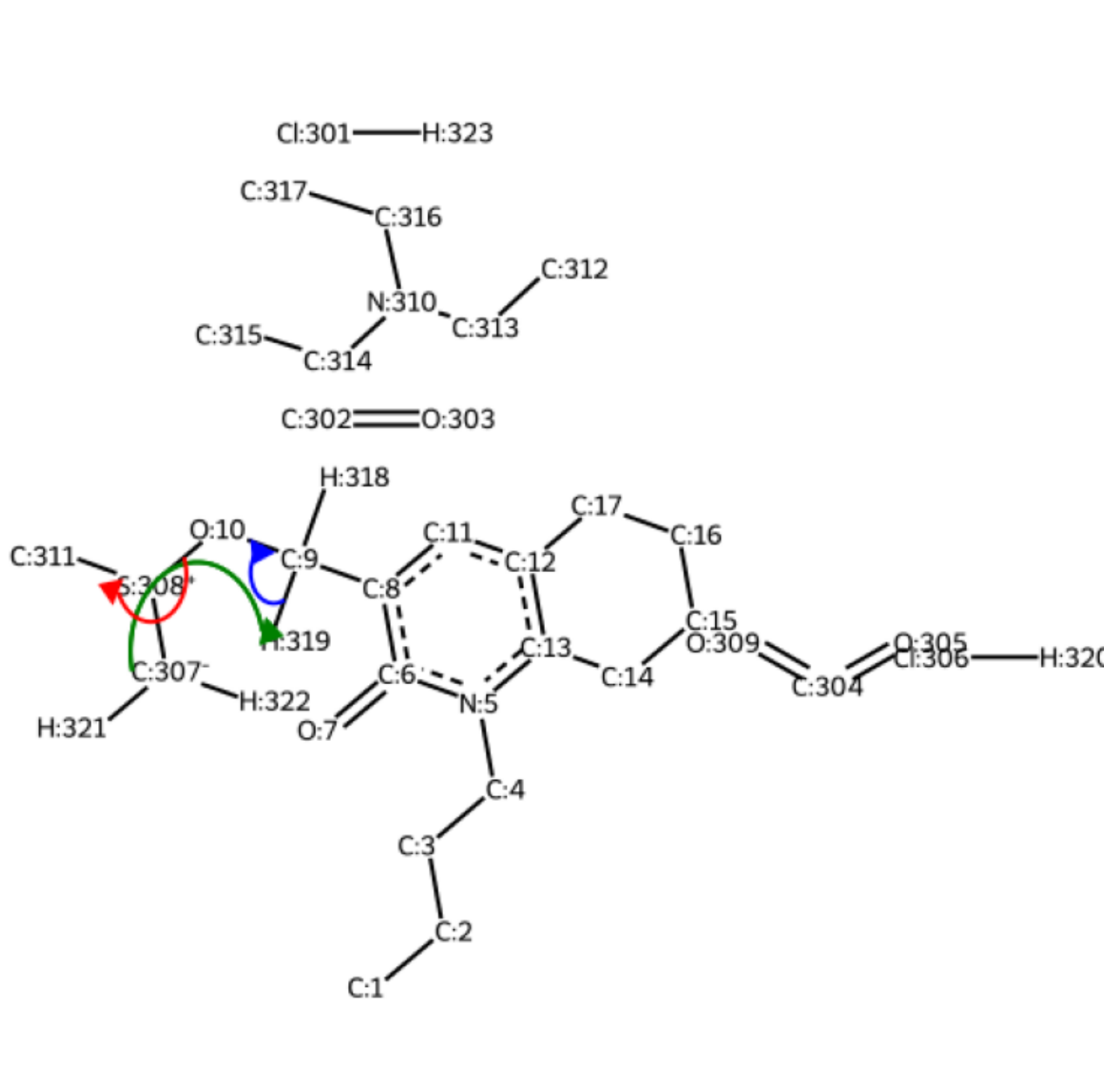
step #6



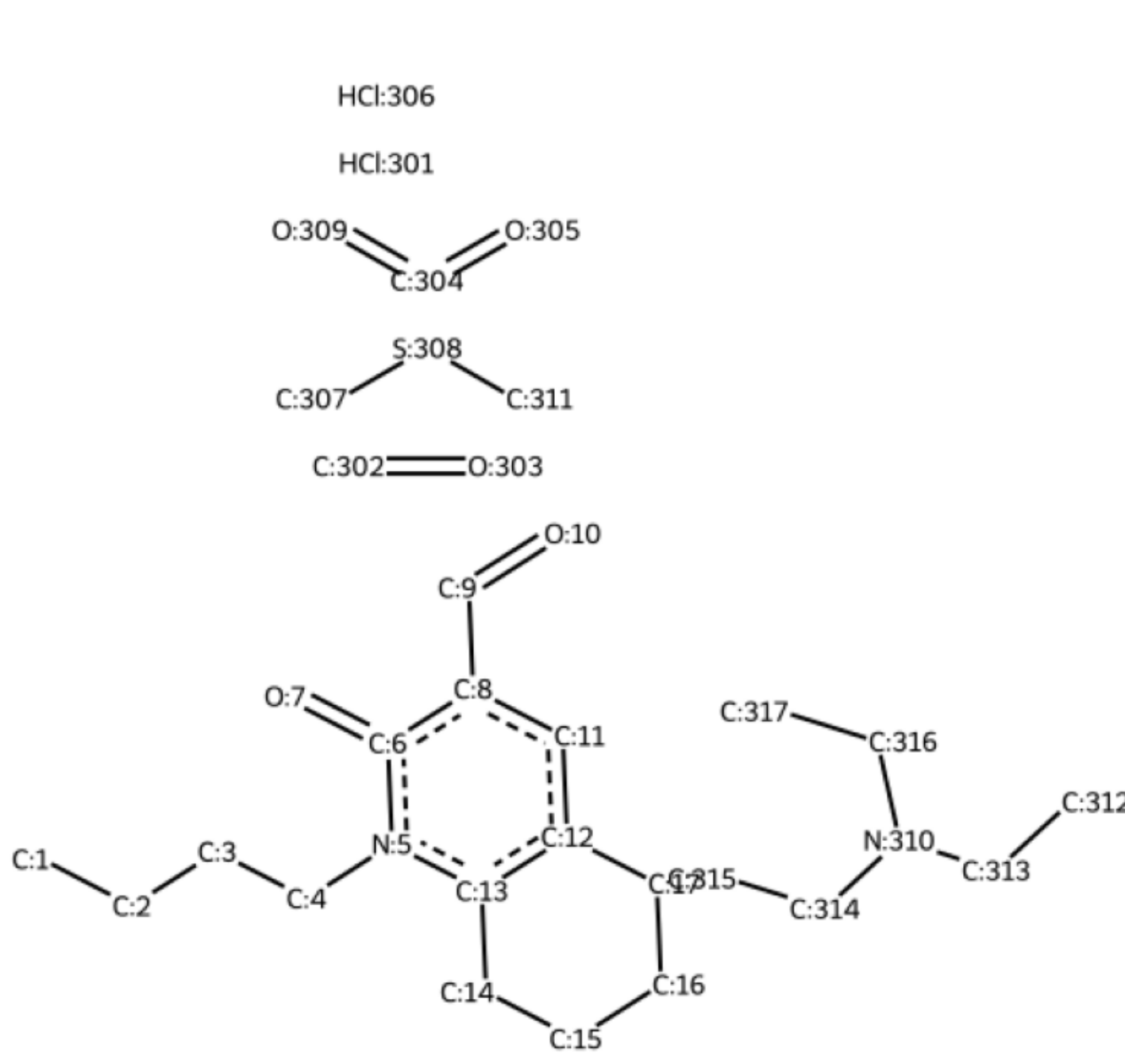
step #7



step #8



Product(s)

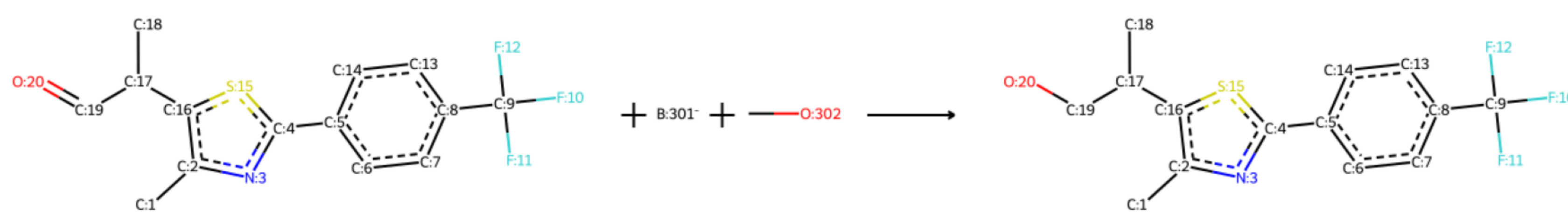


Original reaction
sampled RXN_ID:59)



Identified mechanistic class -
carbonyl_reduction reaction

Reaction with missing reagents recovered

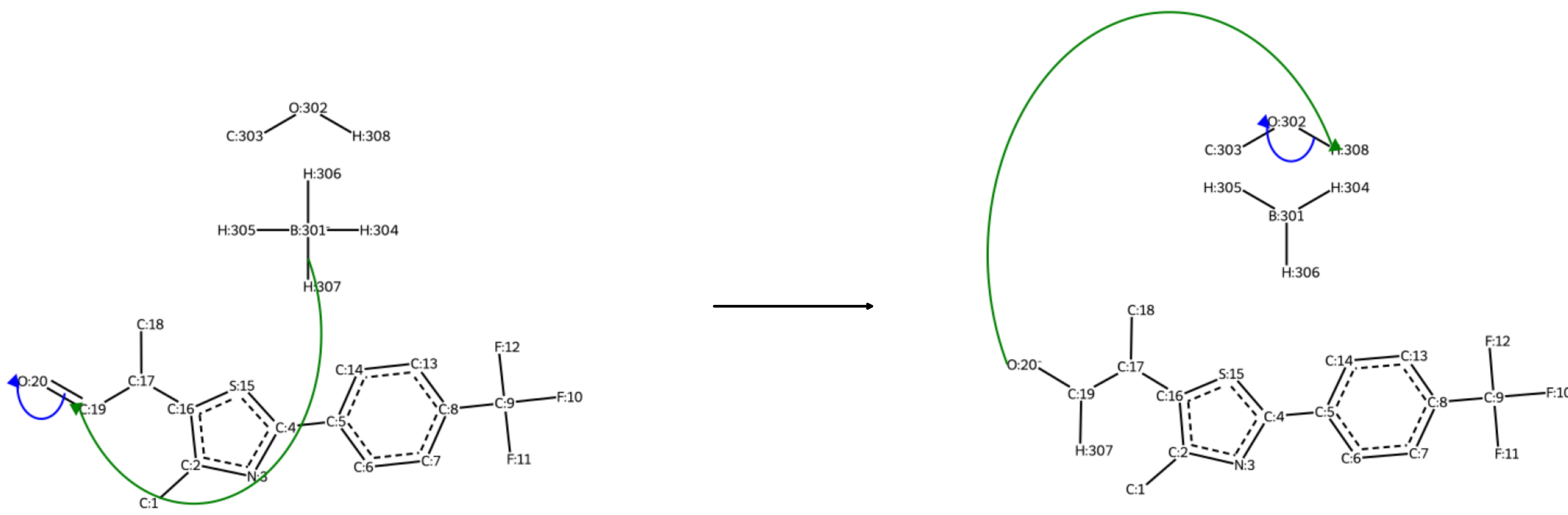


Proposed mechanistic pathway

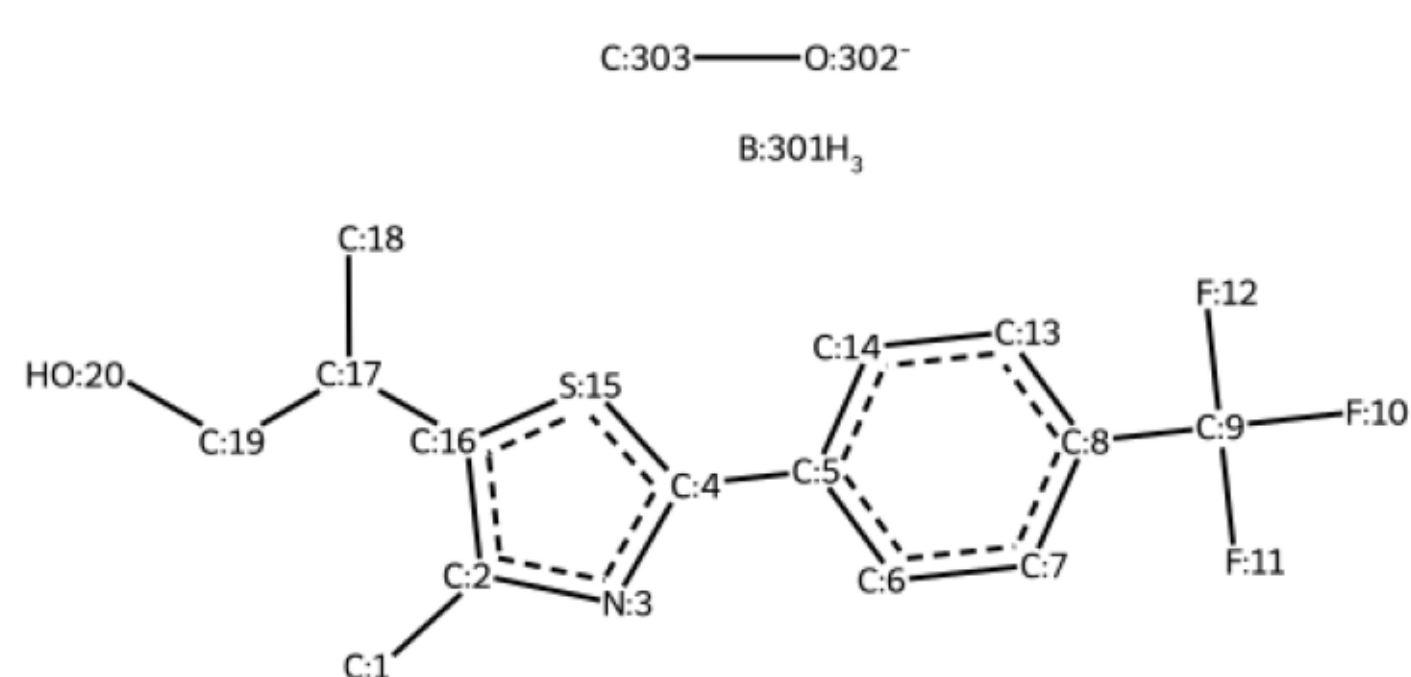
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

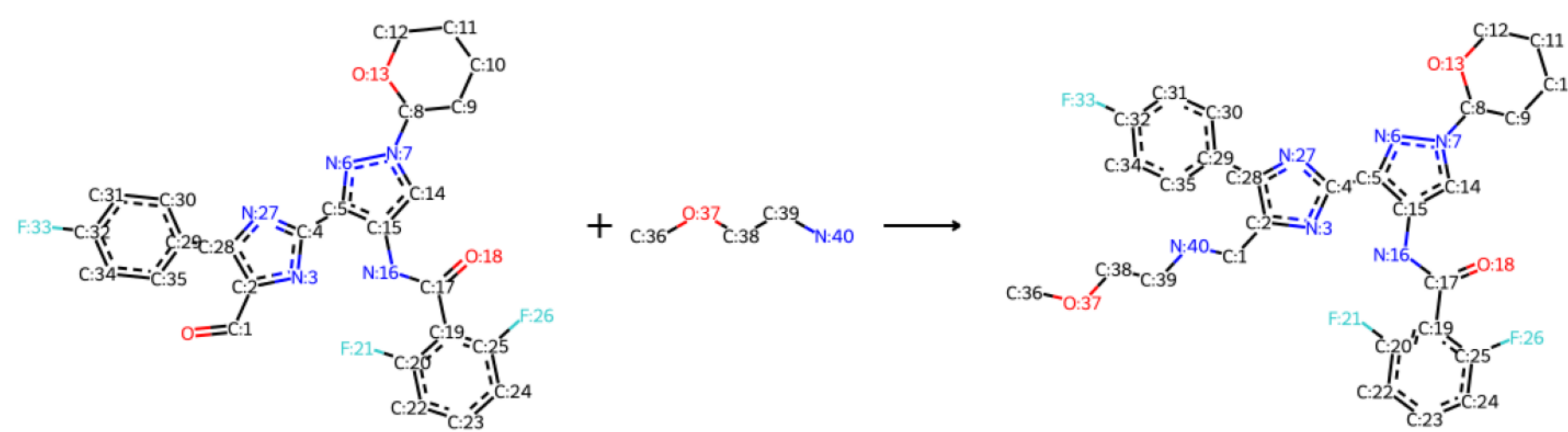
step #2



Product(s)

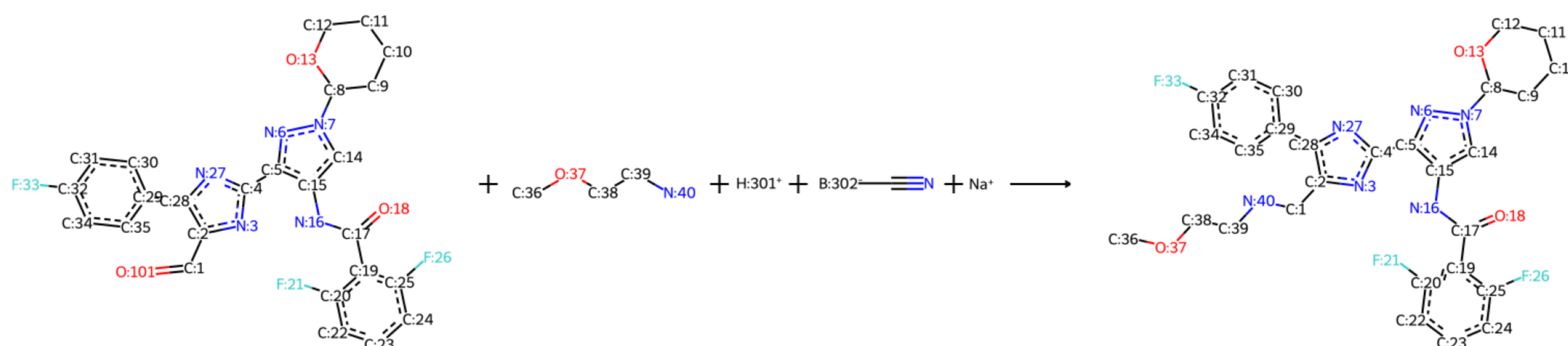


Original reaction
sampled RXN_ID:60)



Identified mechanistic class -
reductive_amination reaction

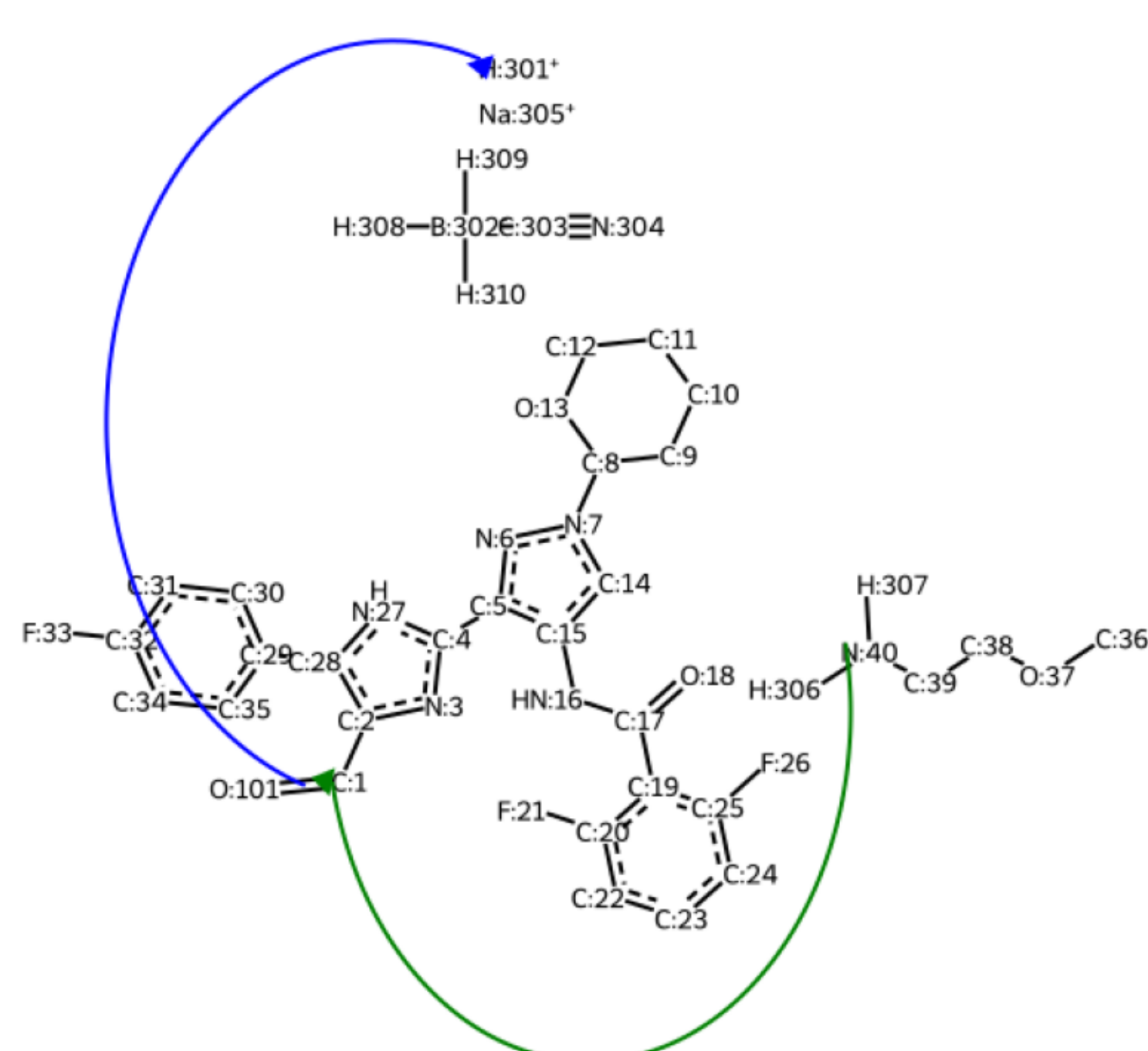
Reaction with missing reagents recovered



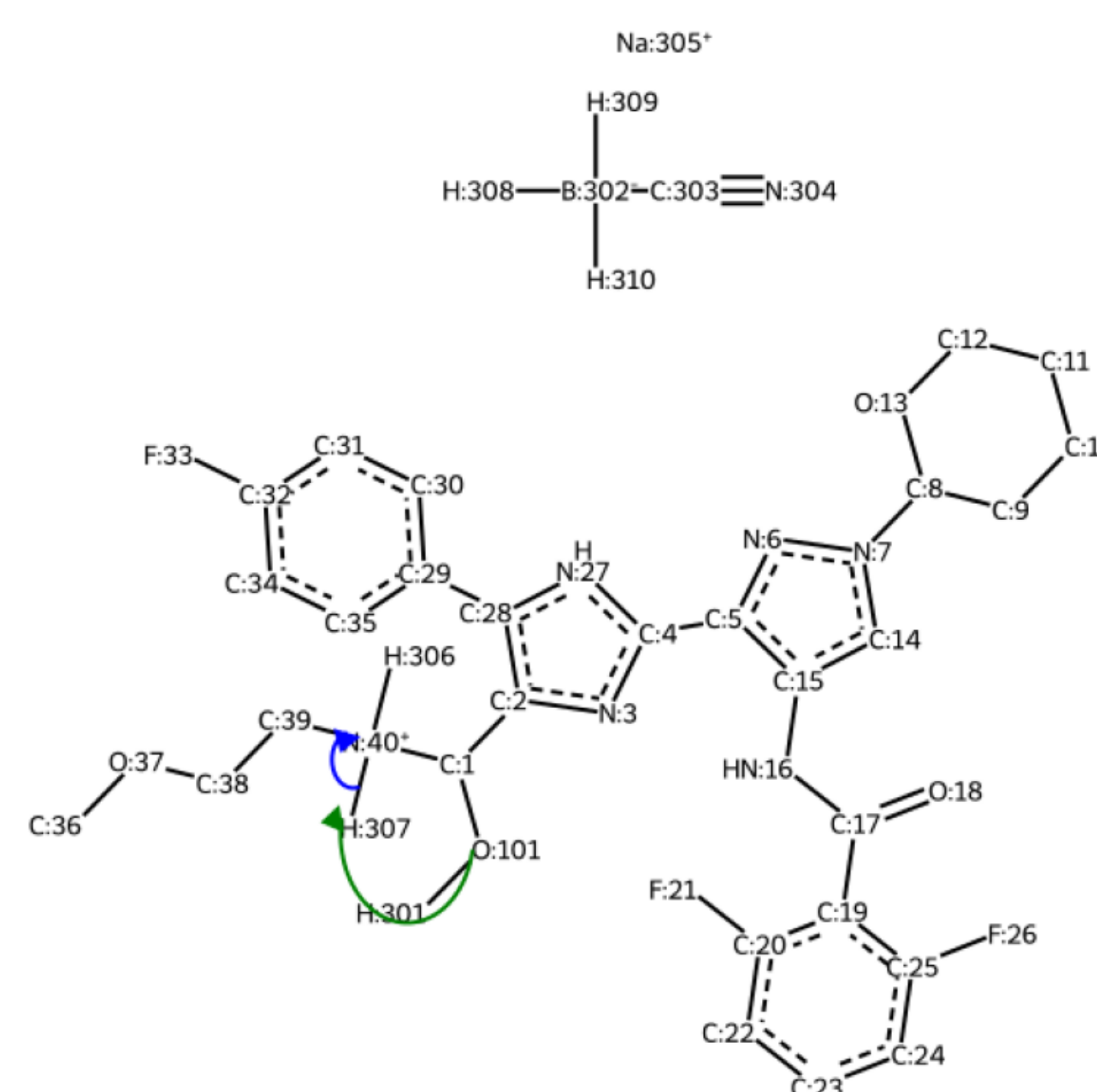
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

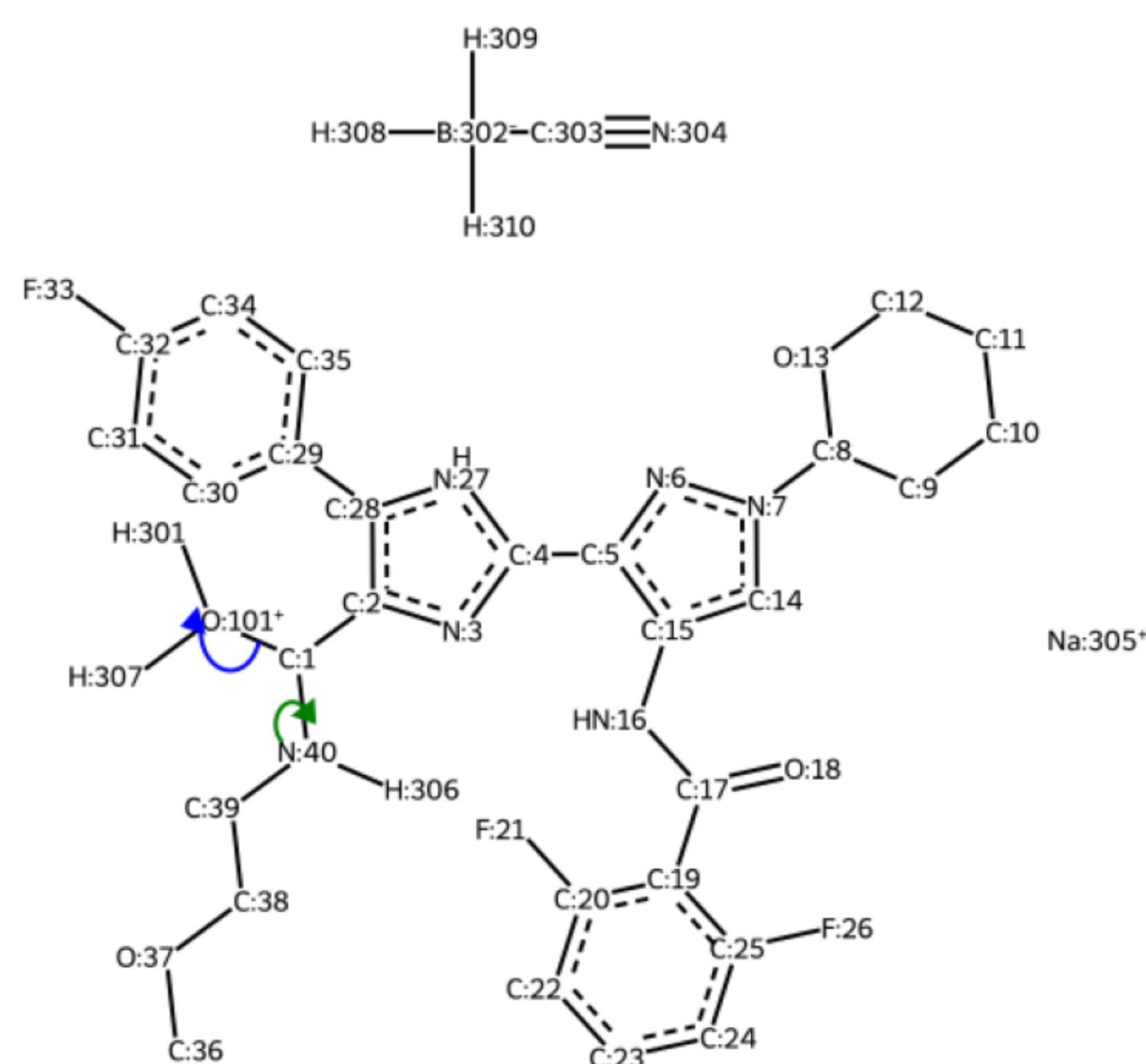
step #1



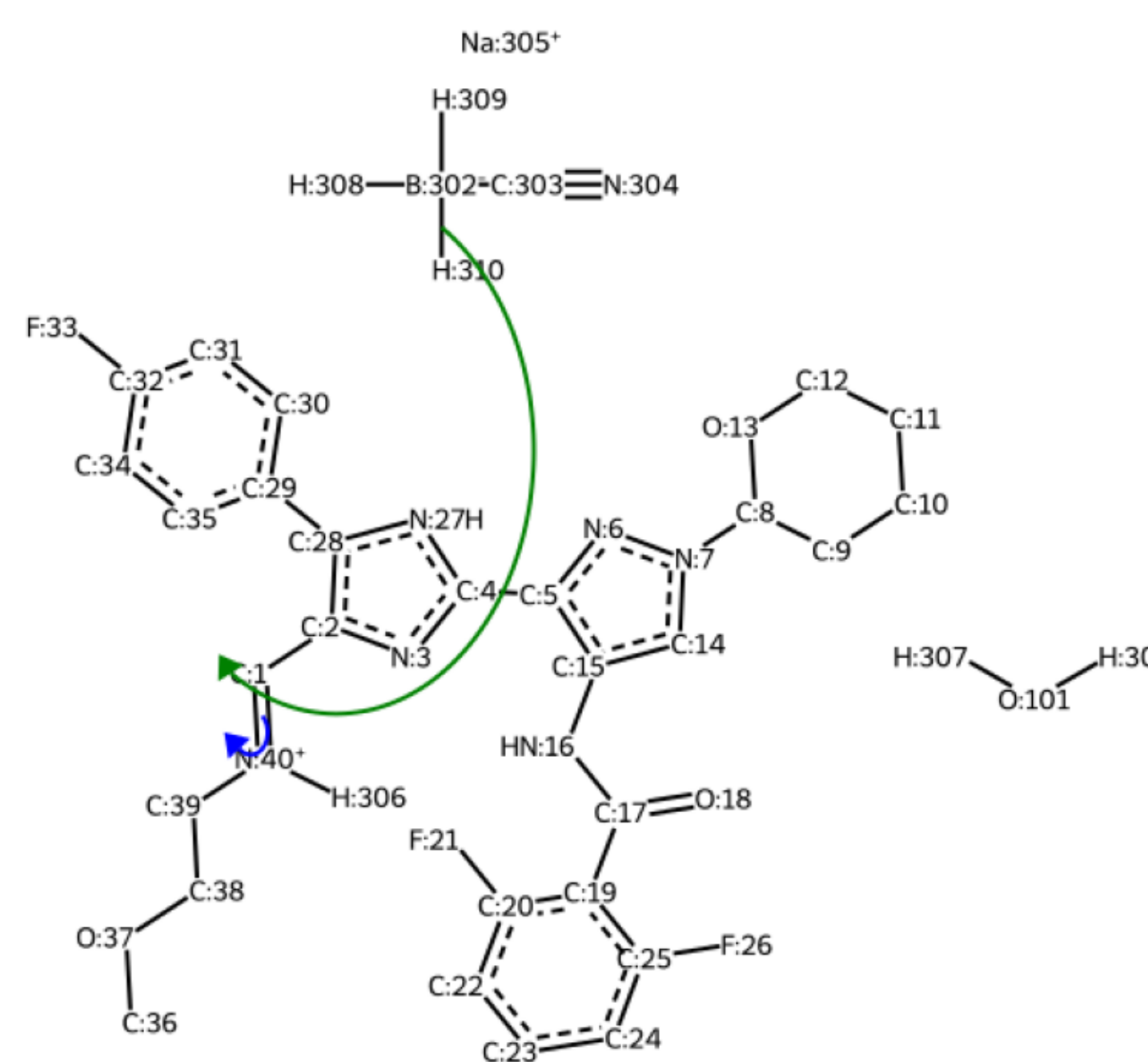
step #2



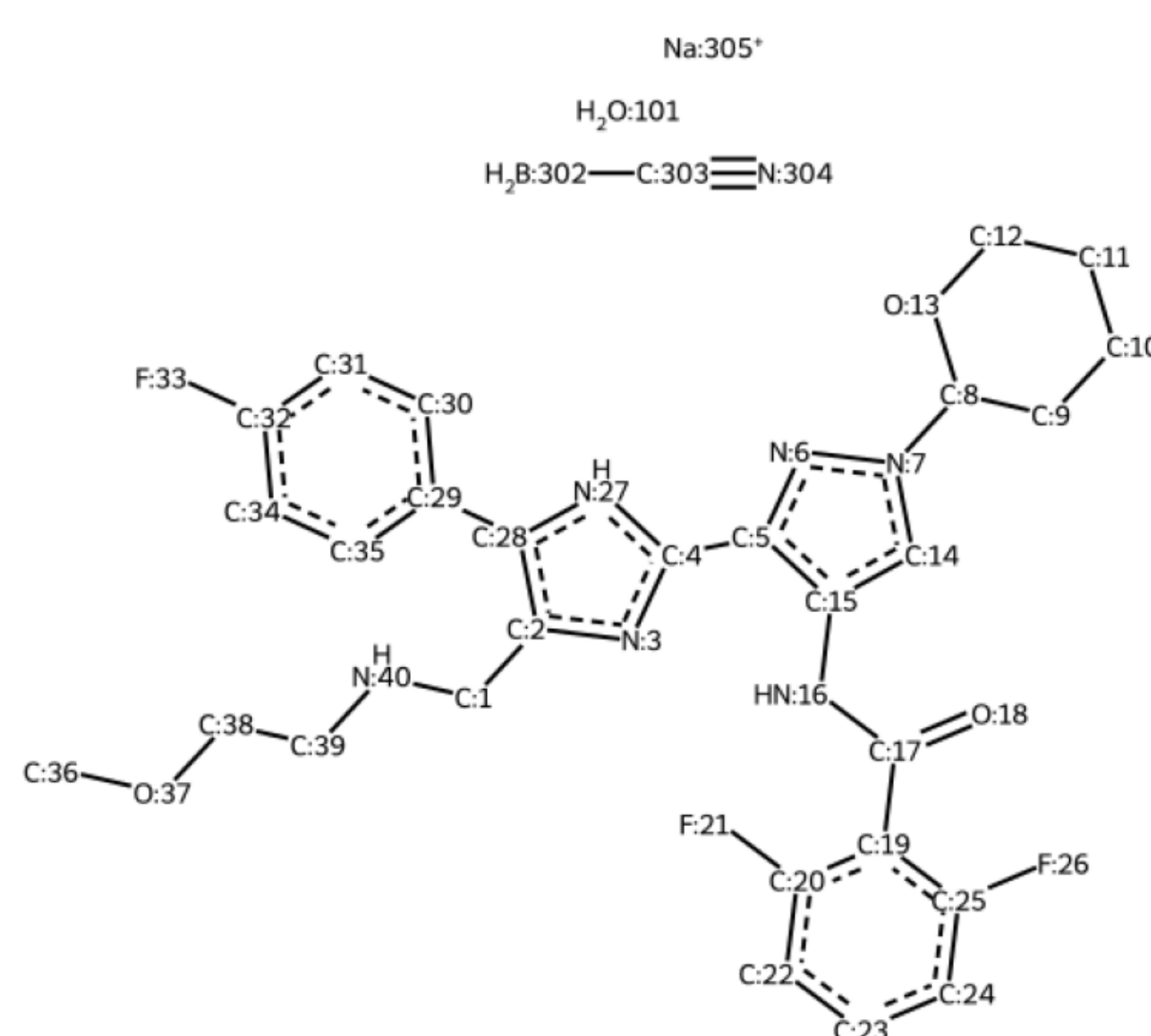
step #3



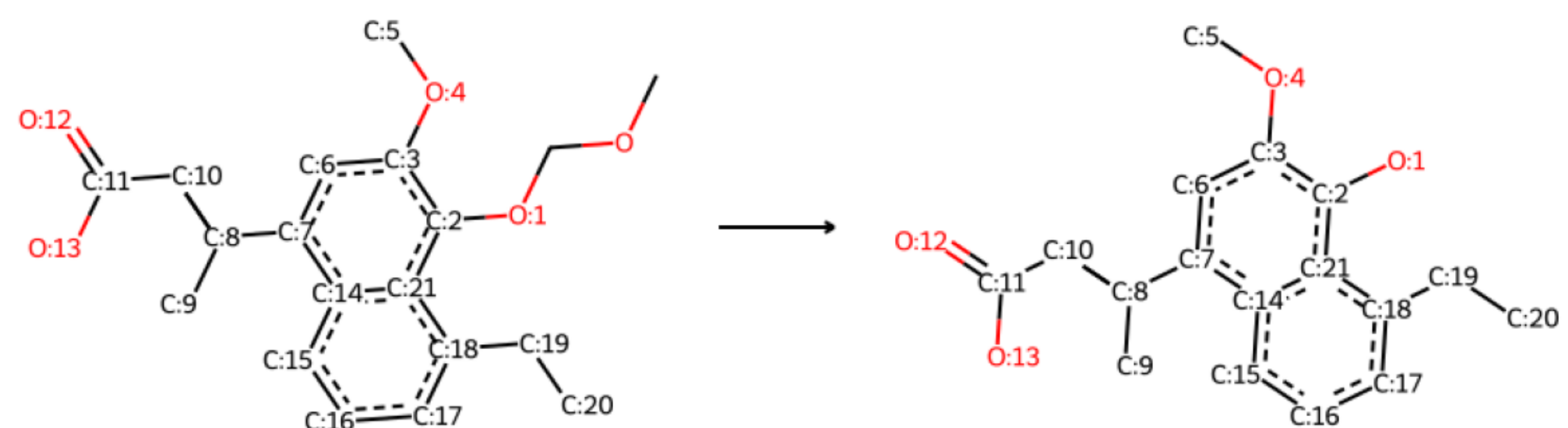
step #4



Product(s)

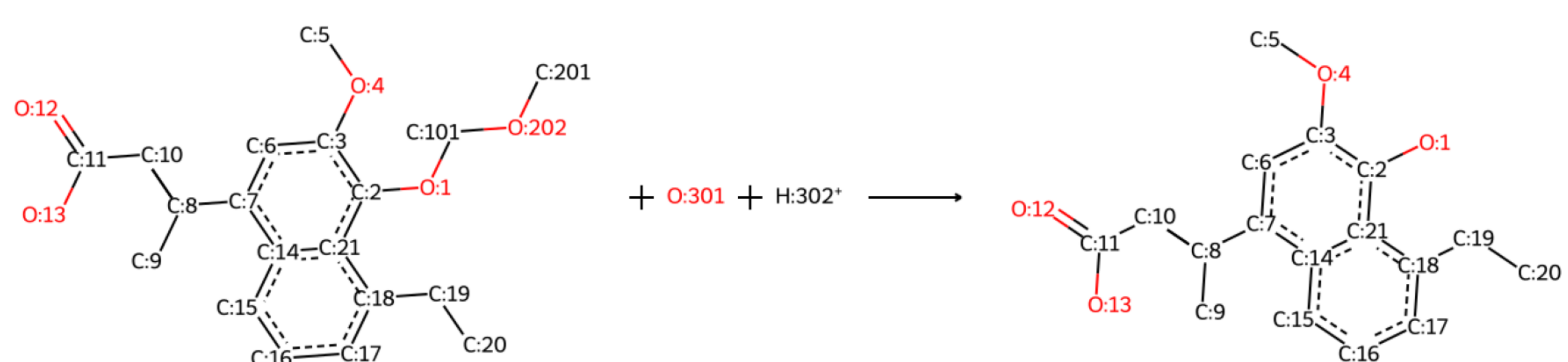


Original reaction
sampled RXN_ID:61)



Identified mechanistic class -
(hemi)acetal(aminal)_hydrolysis reaction

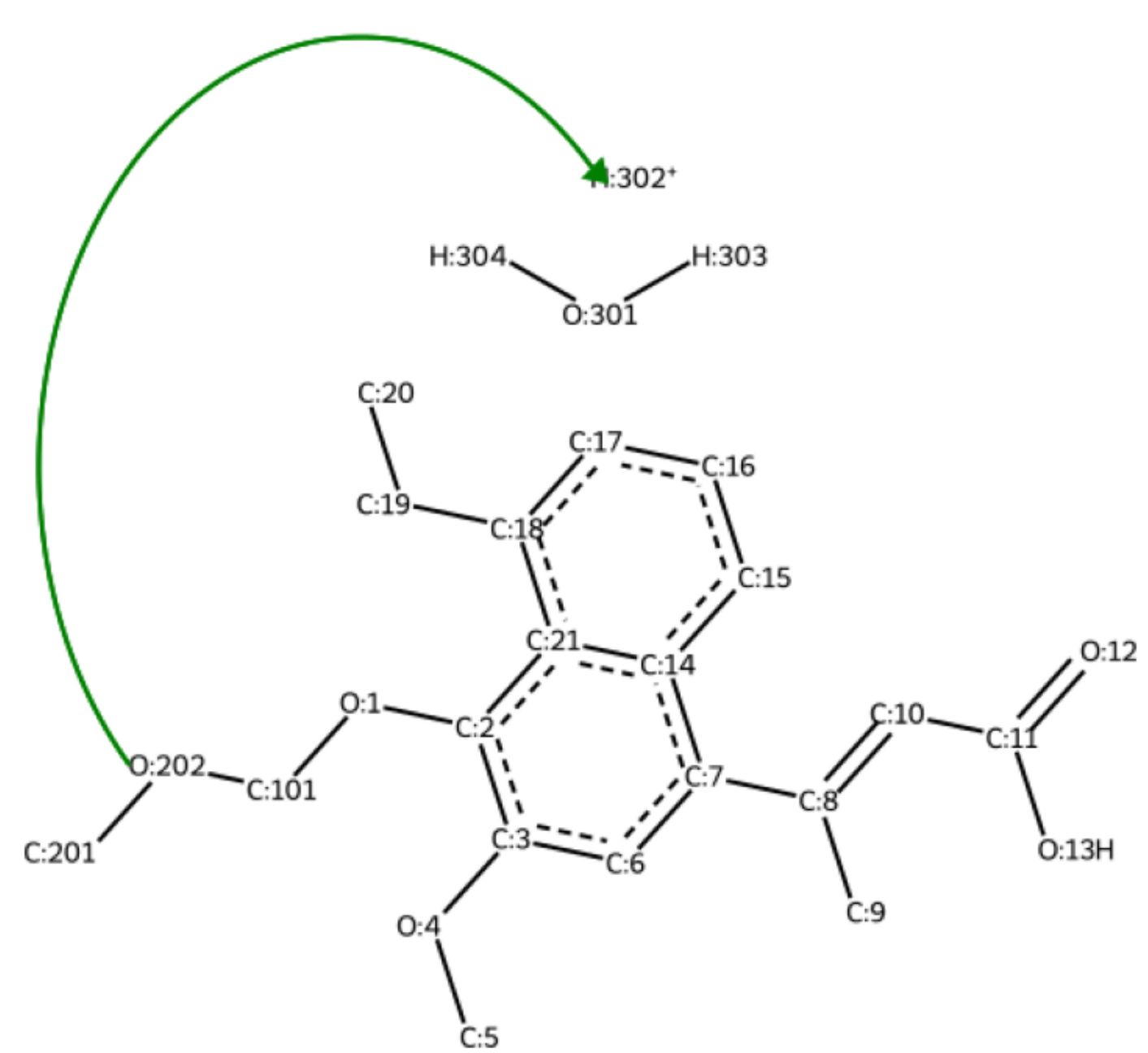
Reaction with missing reagents recovered



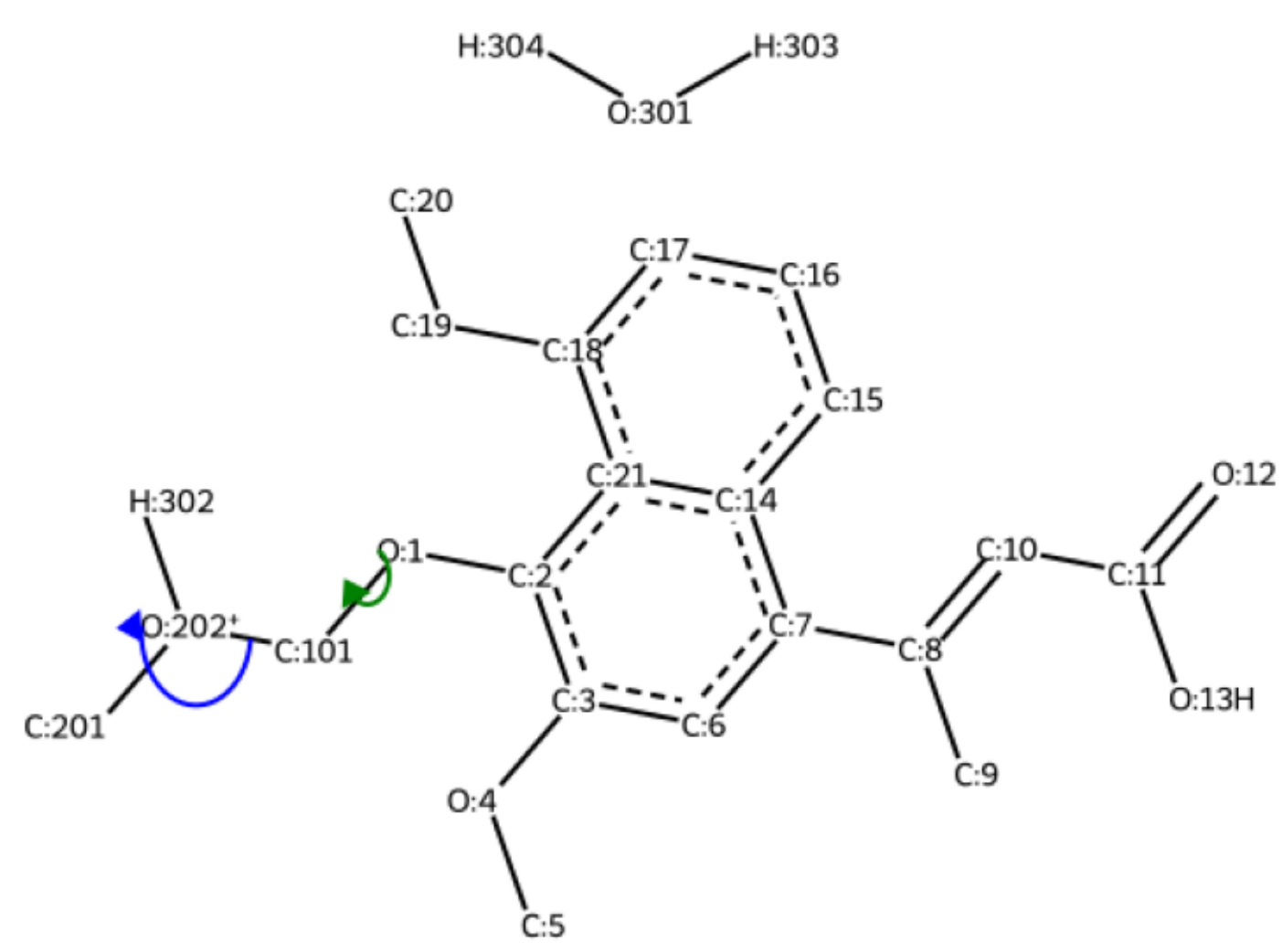
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

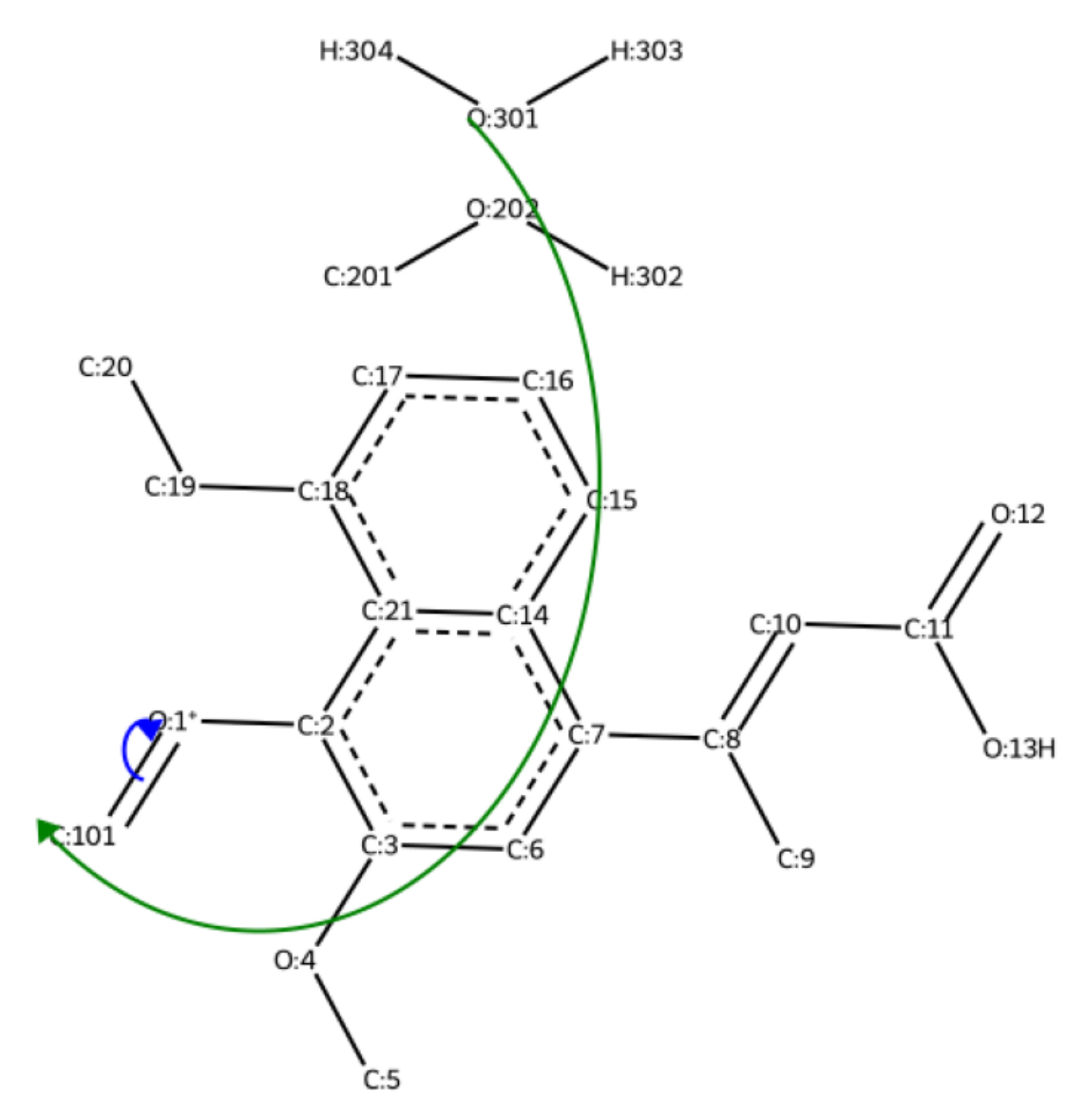
step #1



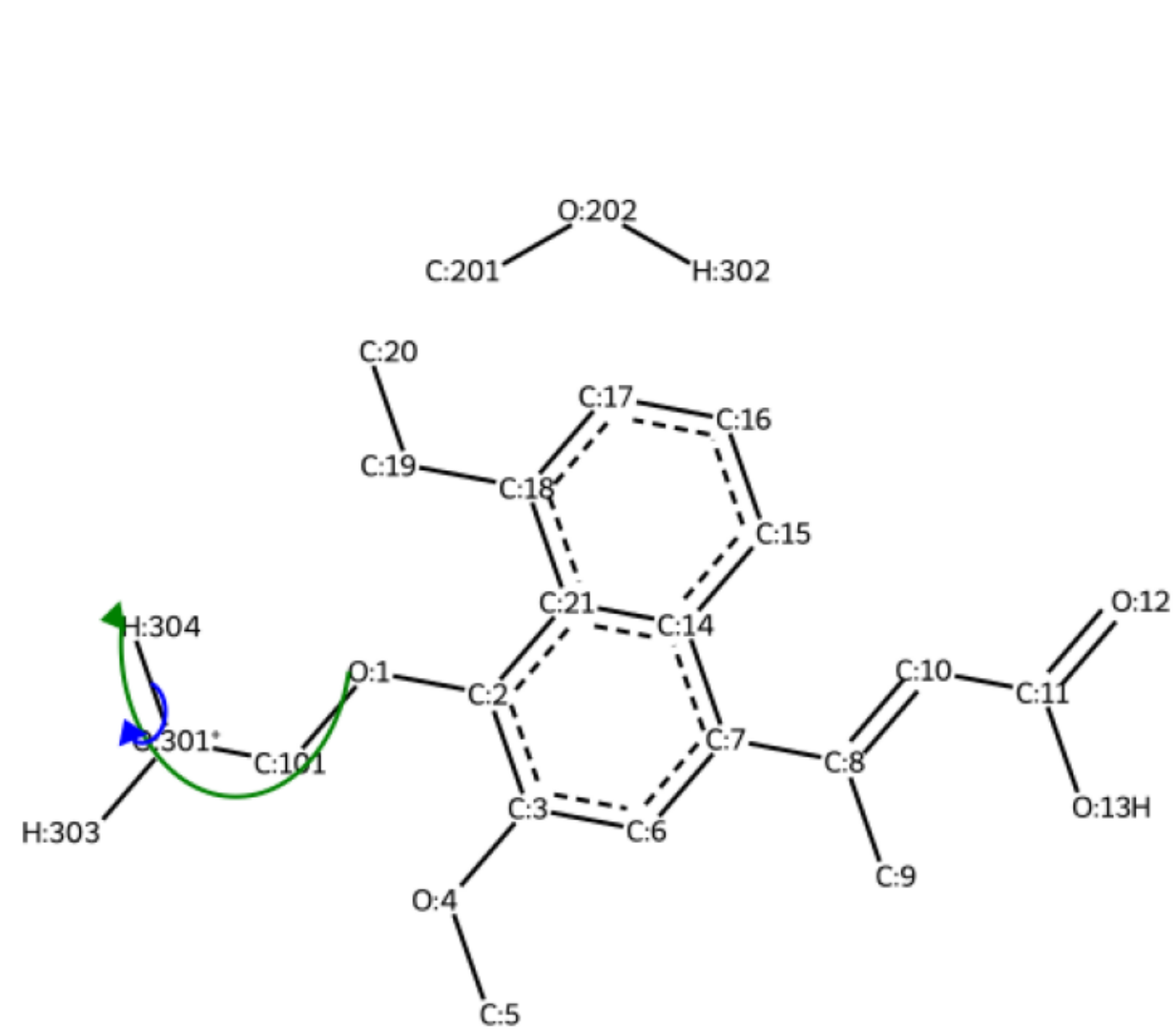
step #2



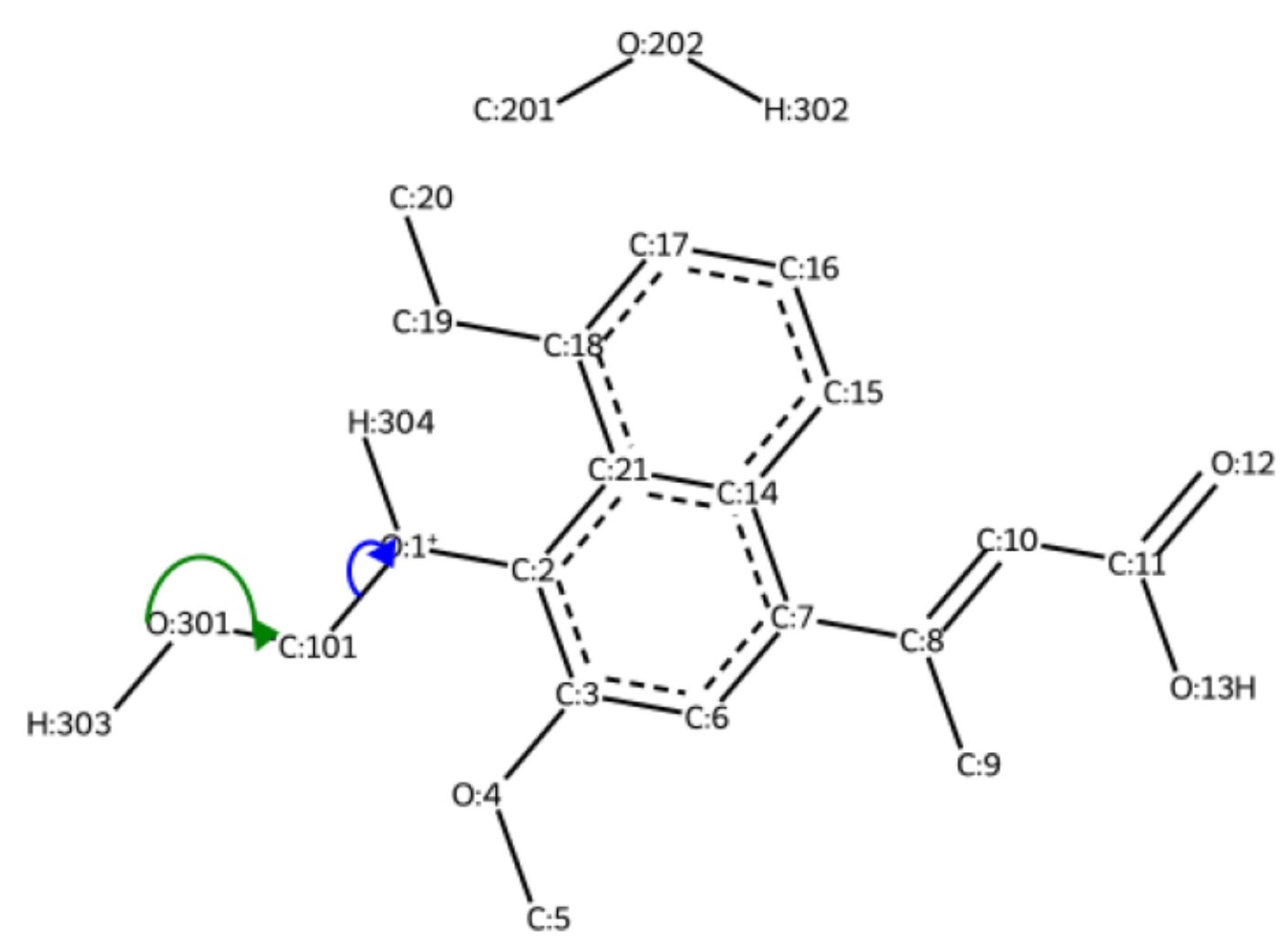
step #3



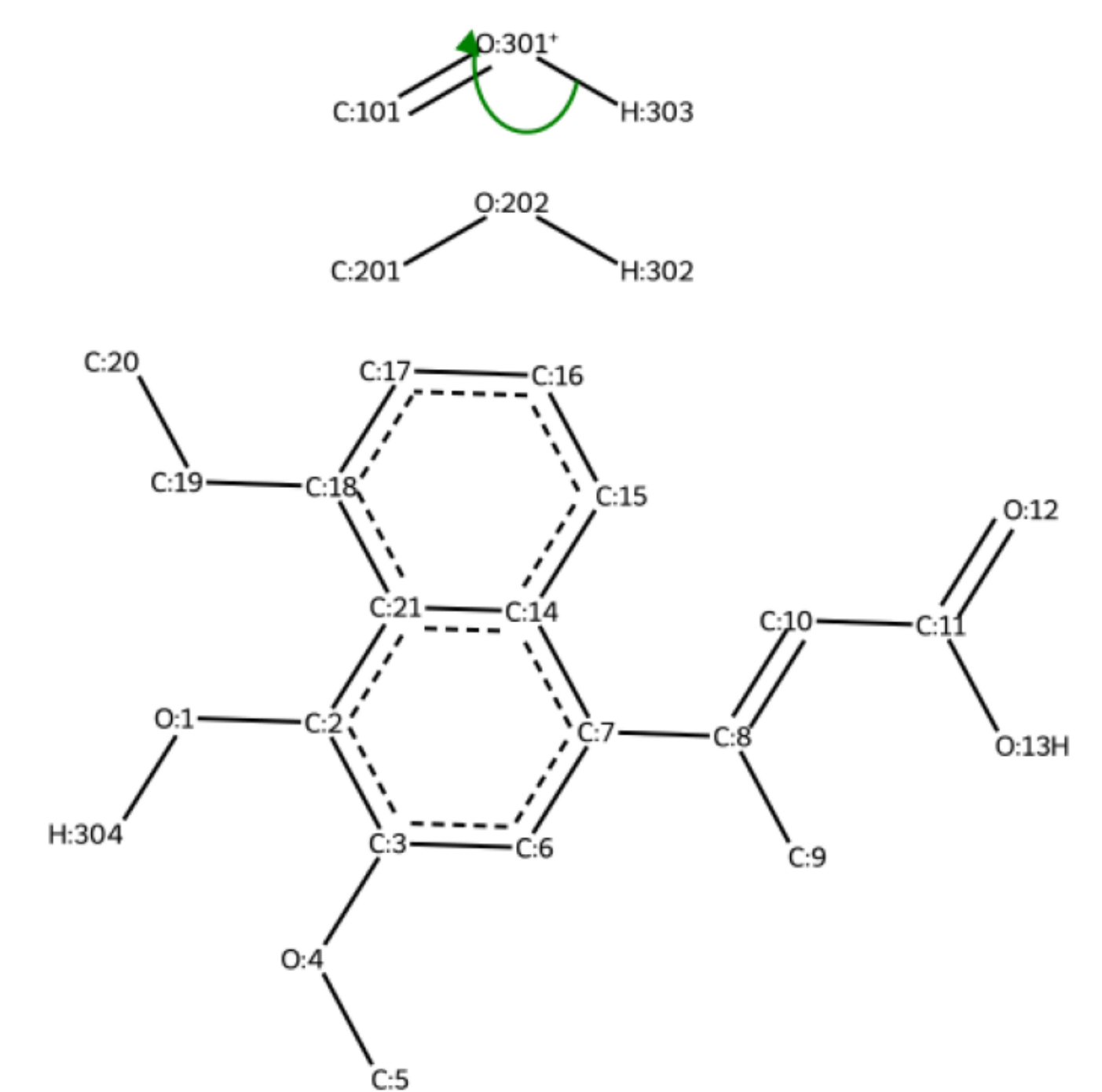
step #4



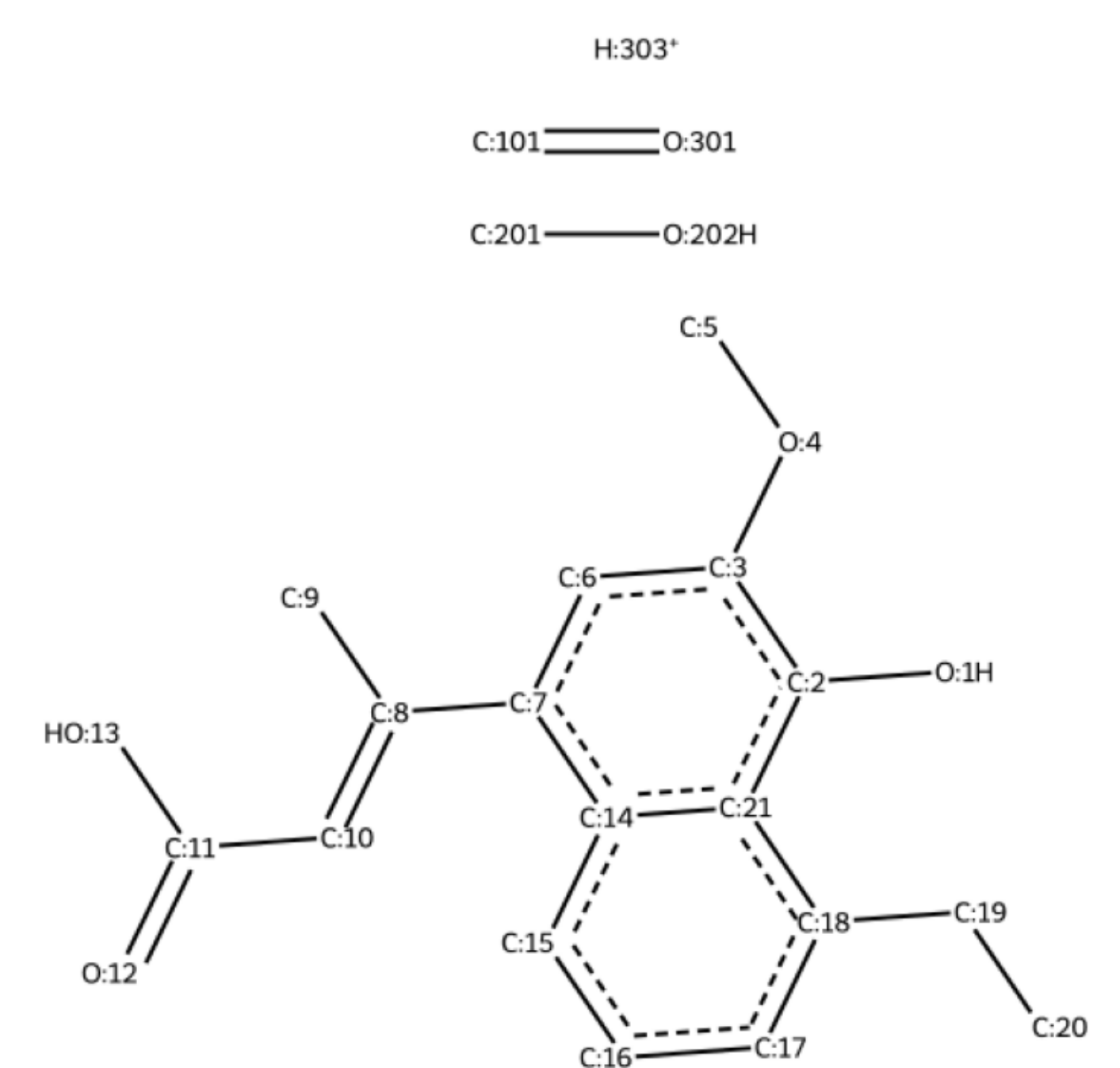
step #5



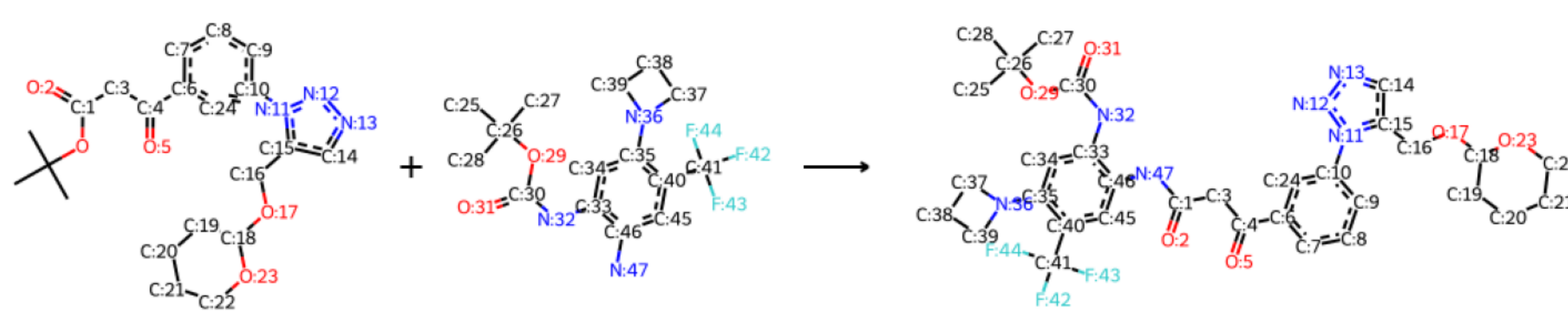
step #6



Product(s)

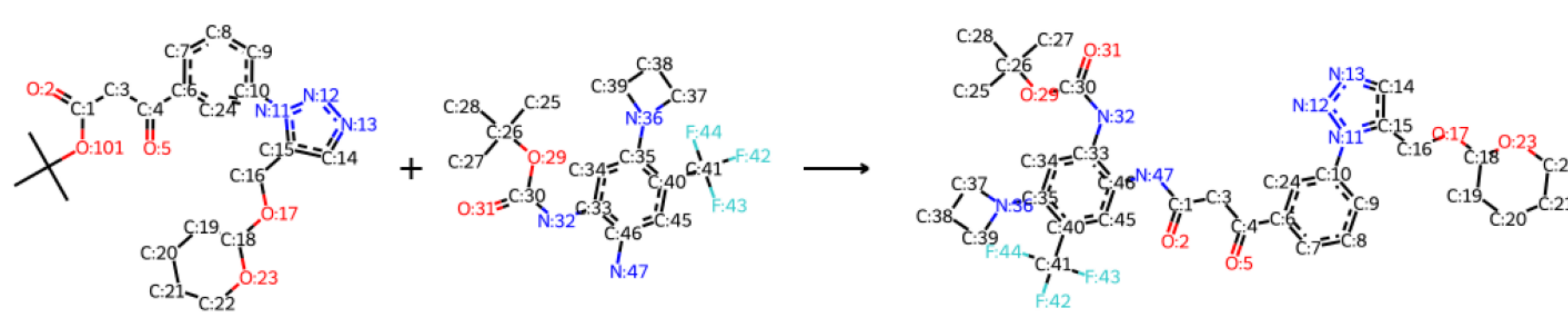


Original reaction
sampled RXN_ID:62)



Identified mechanistic class -
nucleophilic_attack_to_(thio)carbonyl_or_sulfonyl reaction

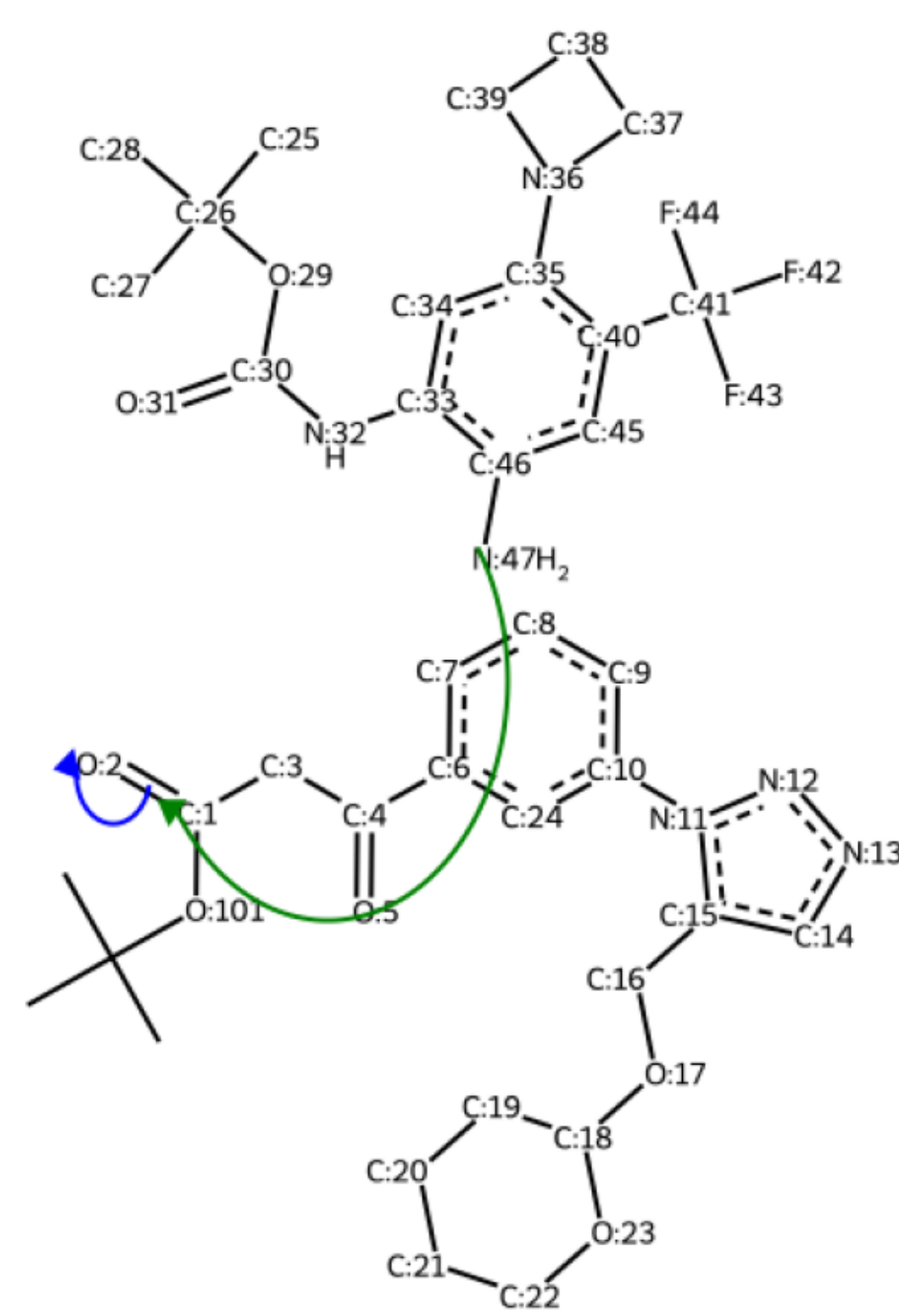
Reaction with missing reagents recovered



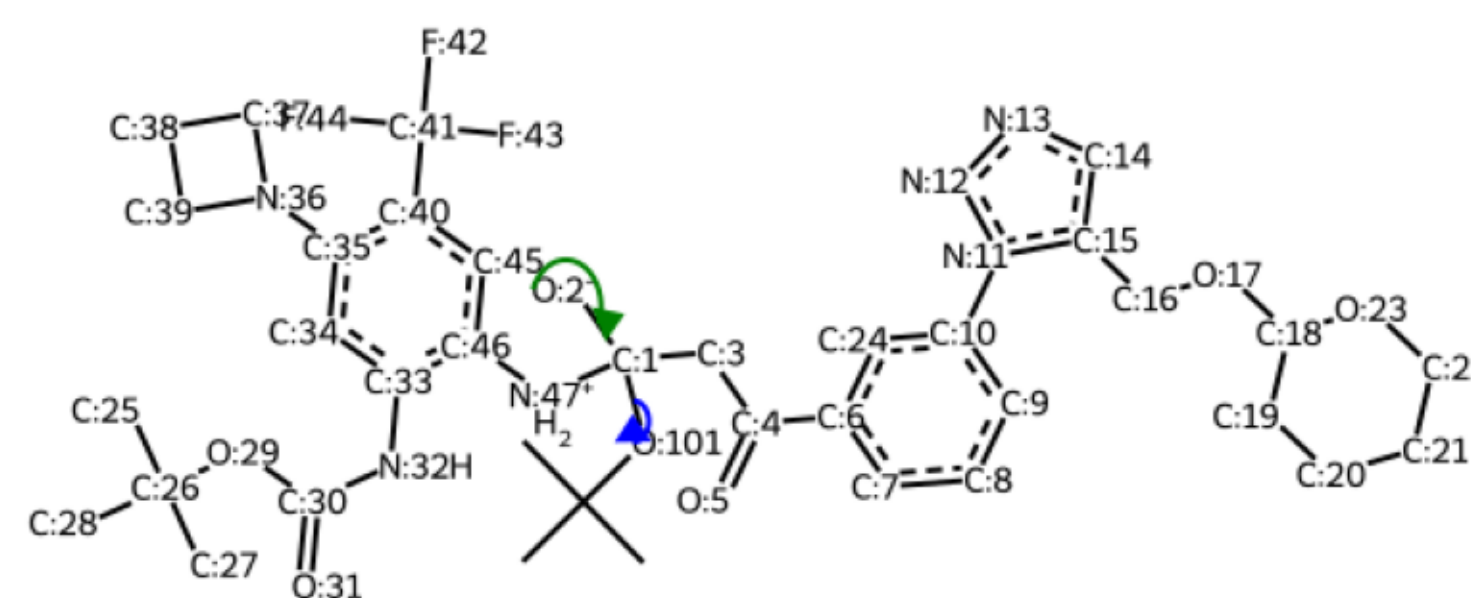
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

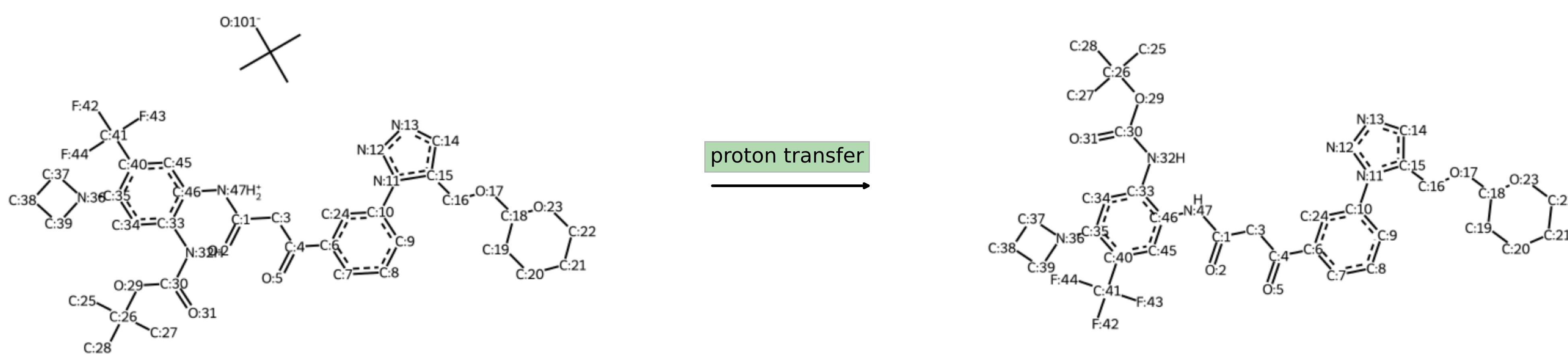
step #1



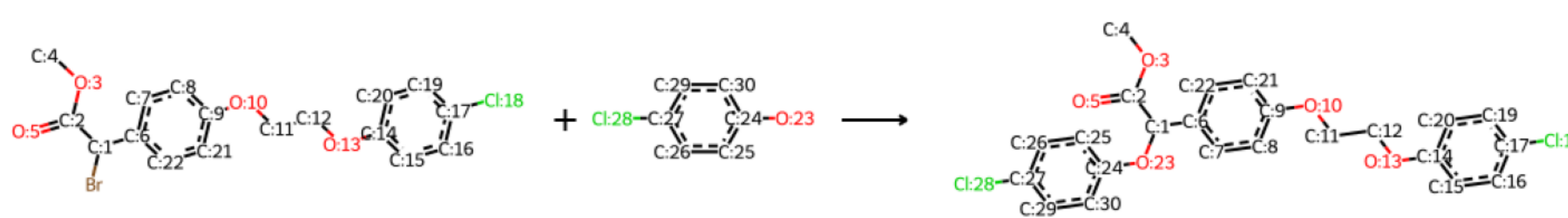
step #2



Product(s)

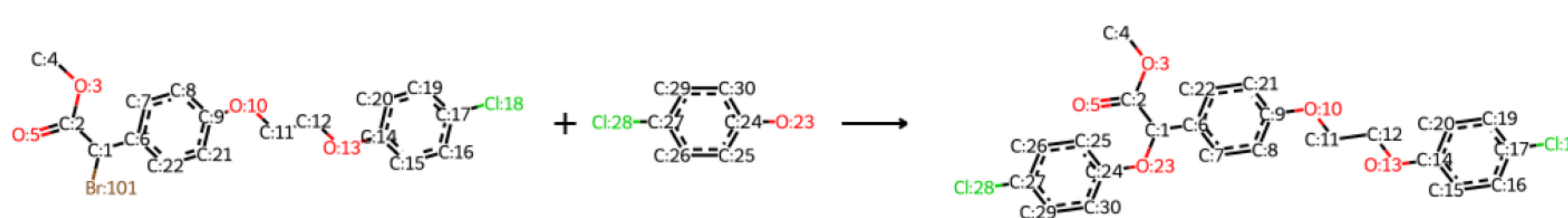


Original reaction
sampled RXN_ID:63)



Identified mechanistic class -
SN1 reaction

Reaction with missing reagents recovered

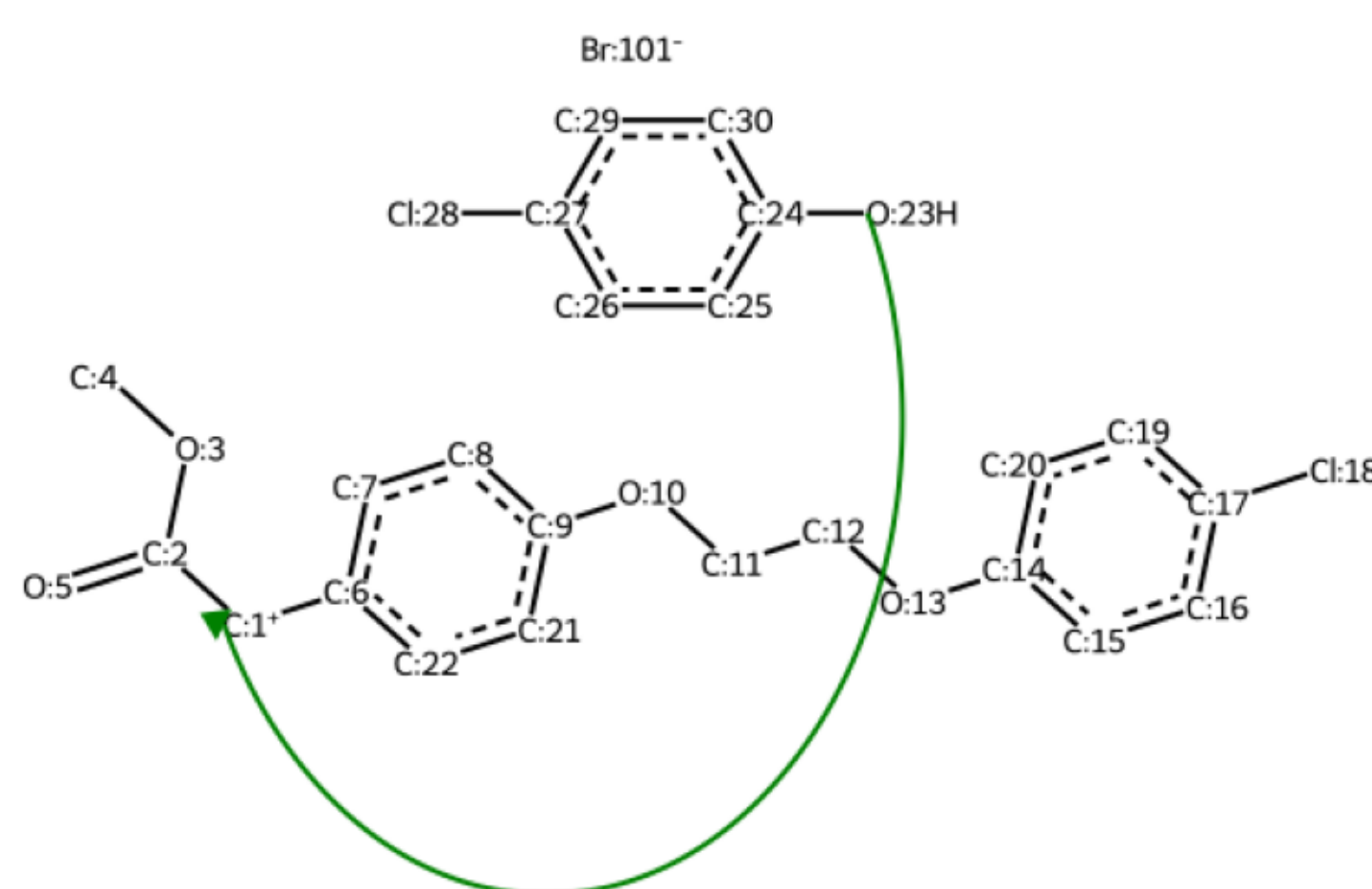
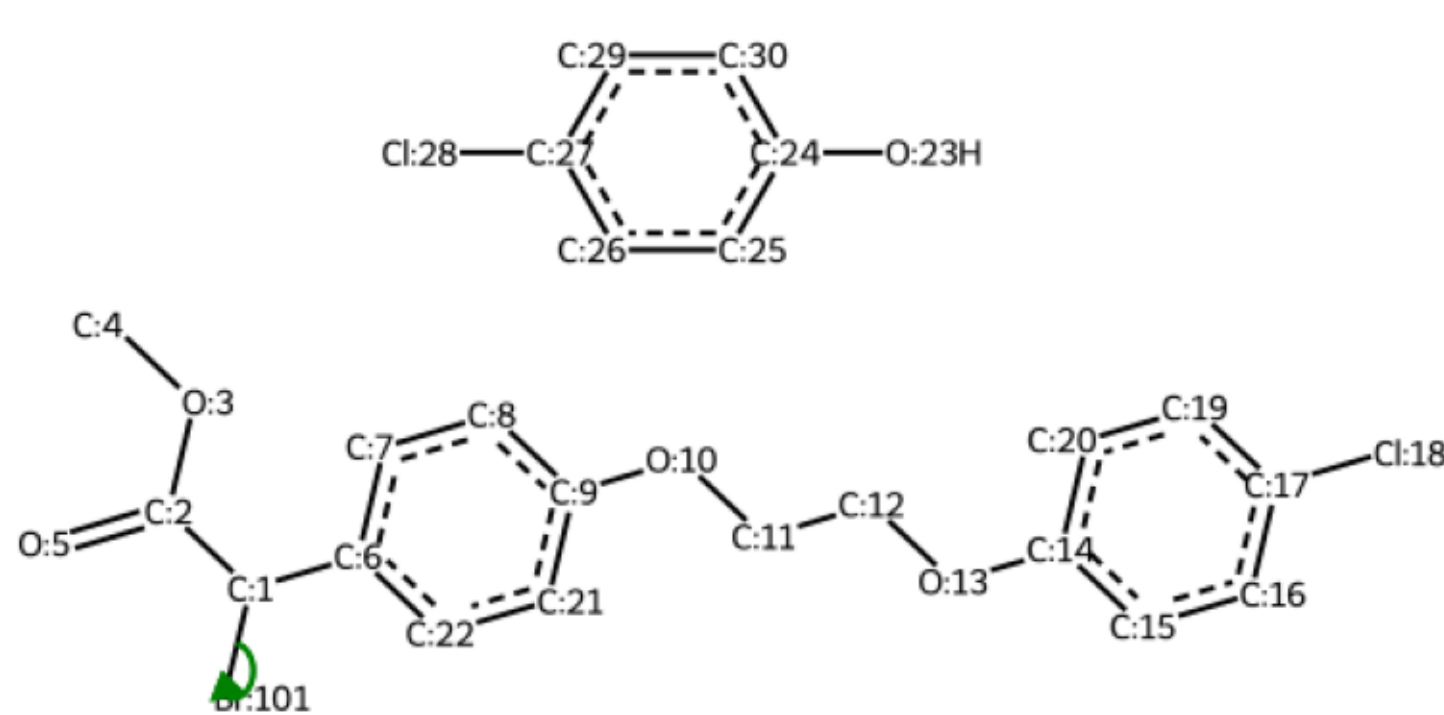


Proposed mechanistic pathway

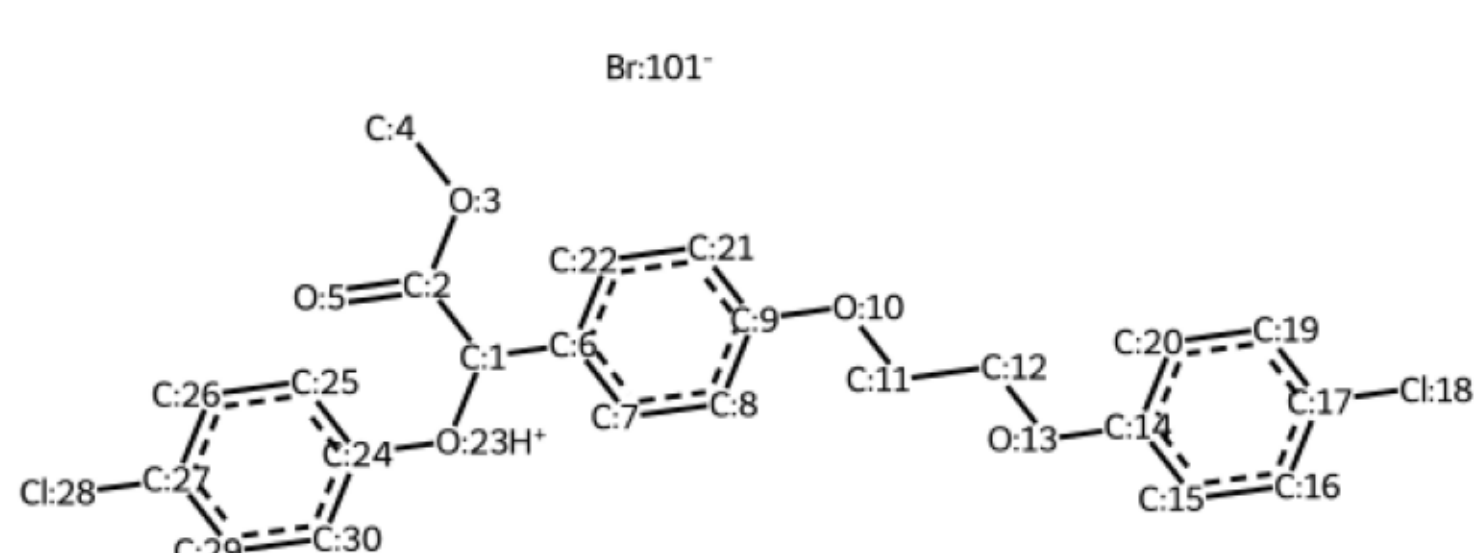
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

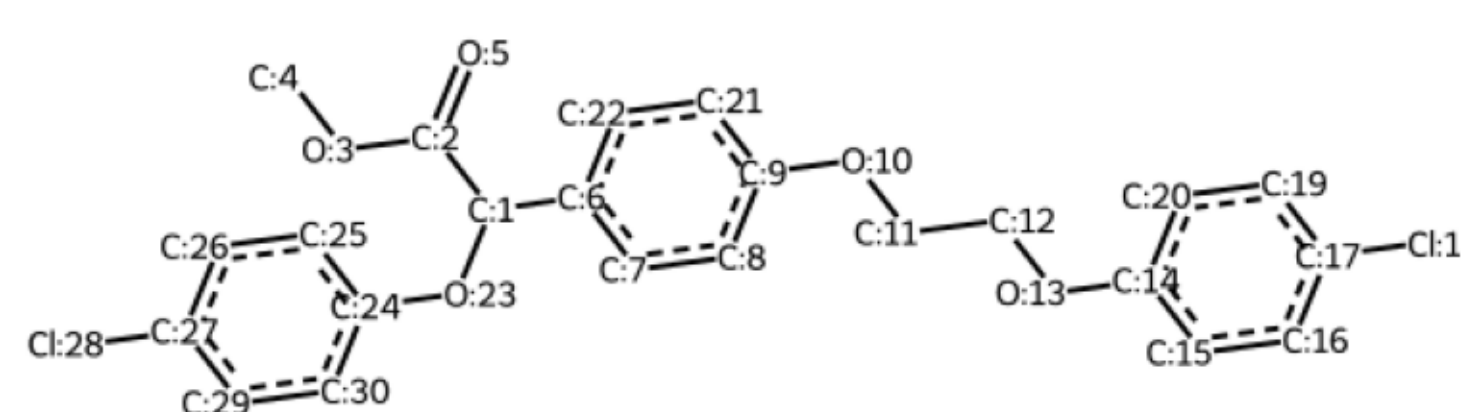
step #2



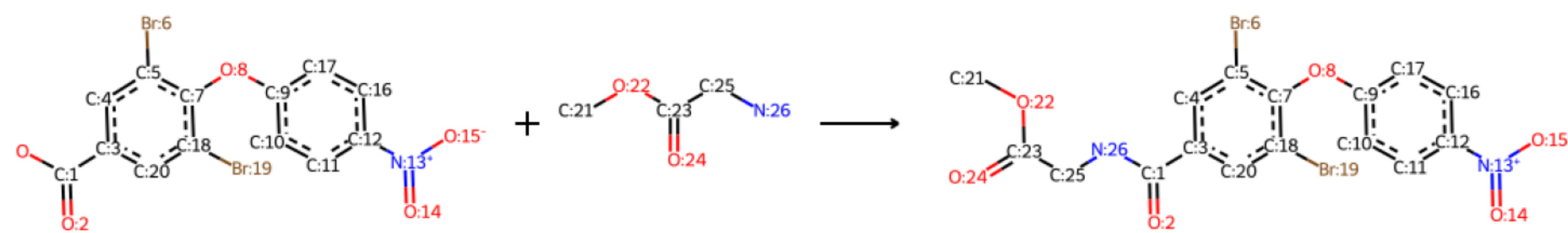
Product(s)



proton transfer

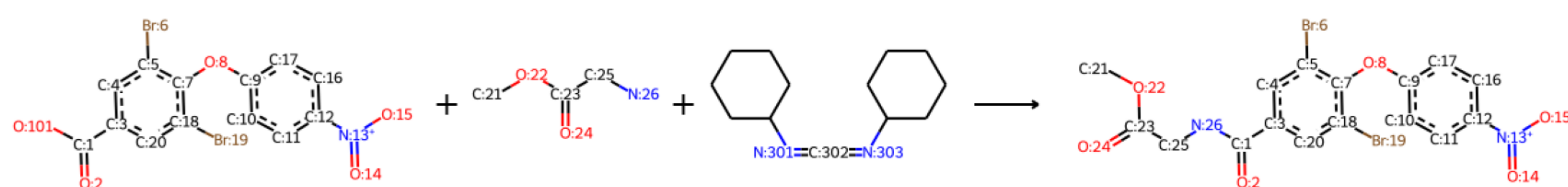


Original reaction
sampled RXN_ID:64)



Identified mechanistic class -
DCC_condensation reaction

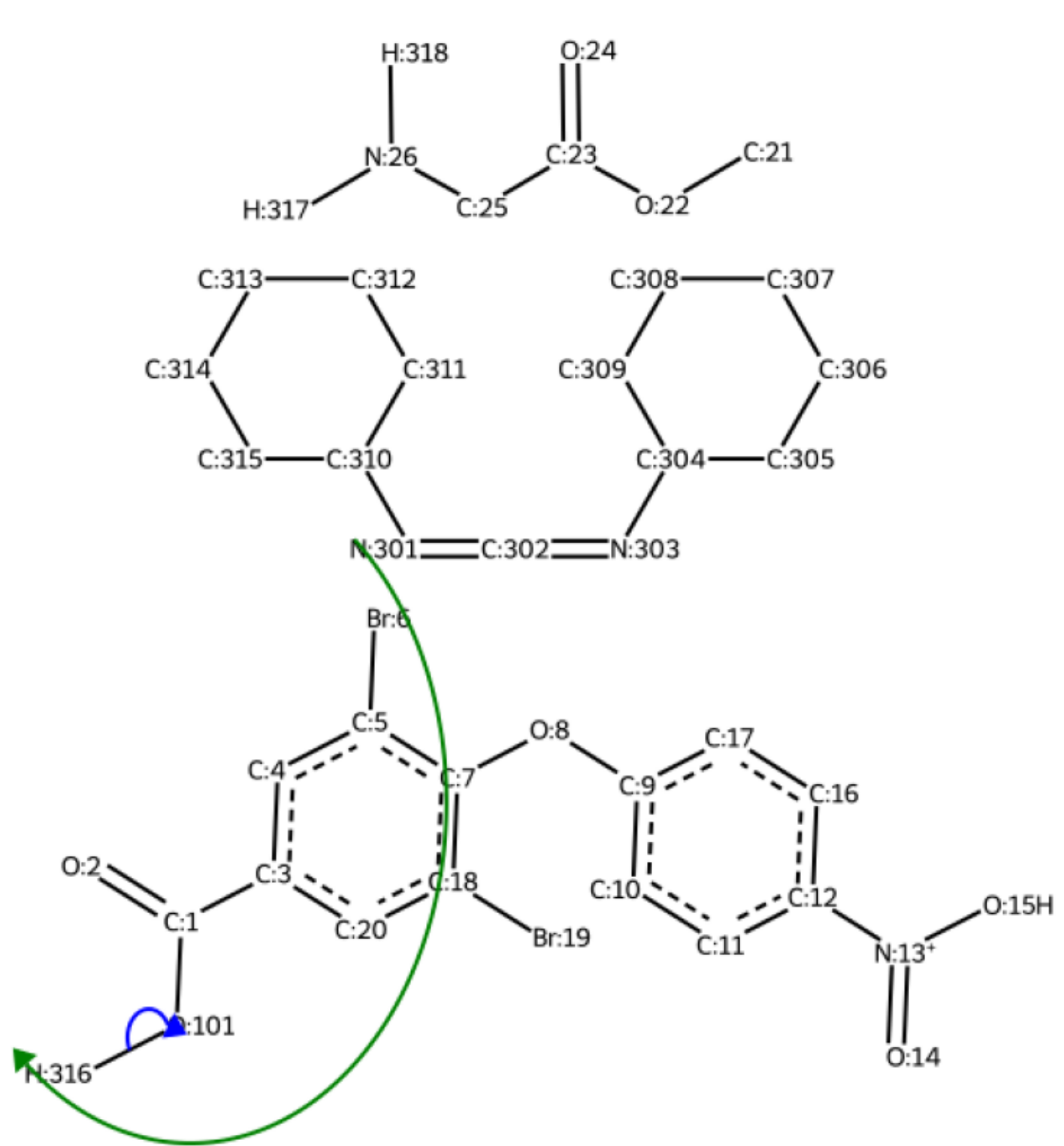
Reaction with missing reagents recovered



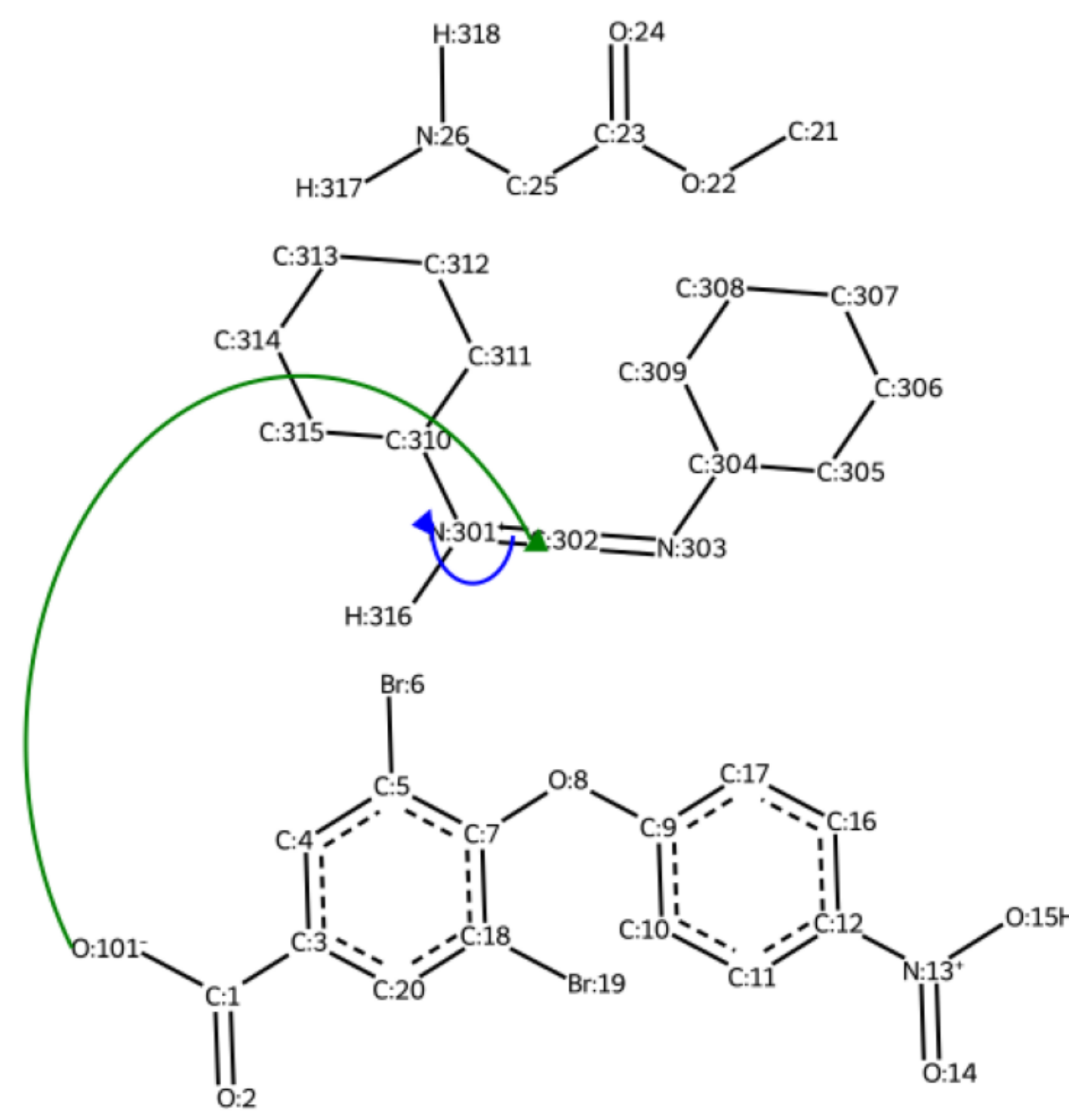
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

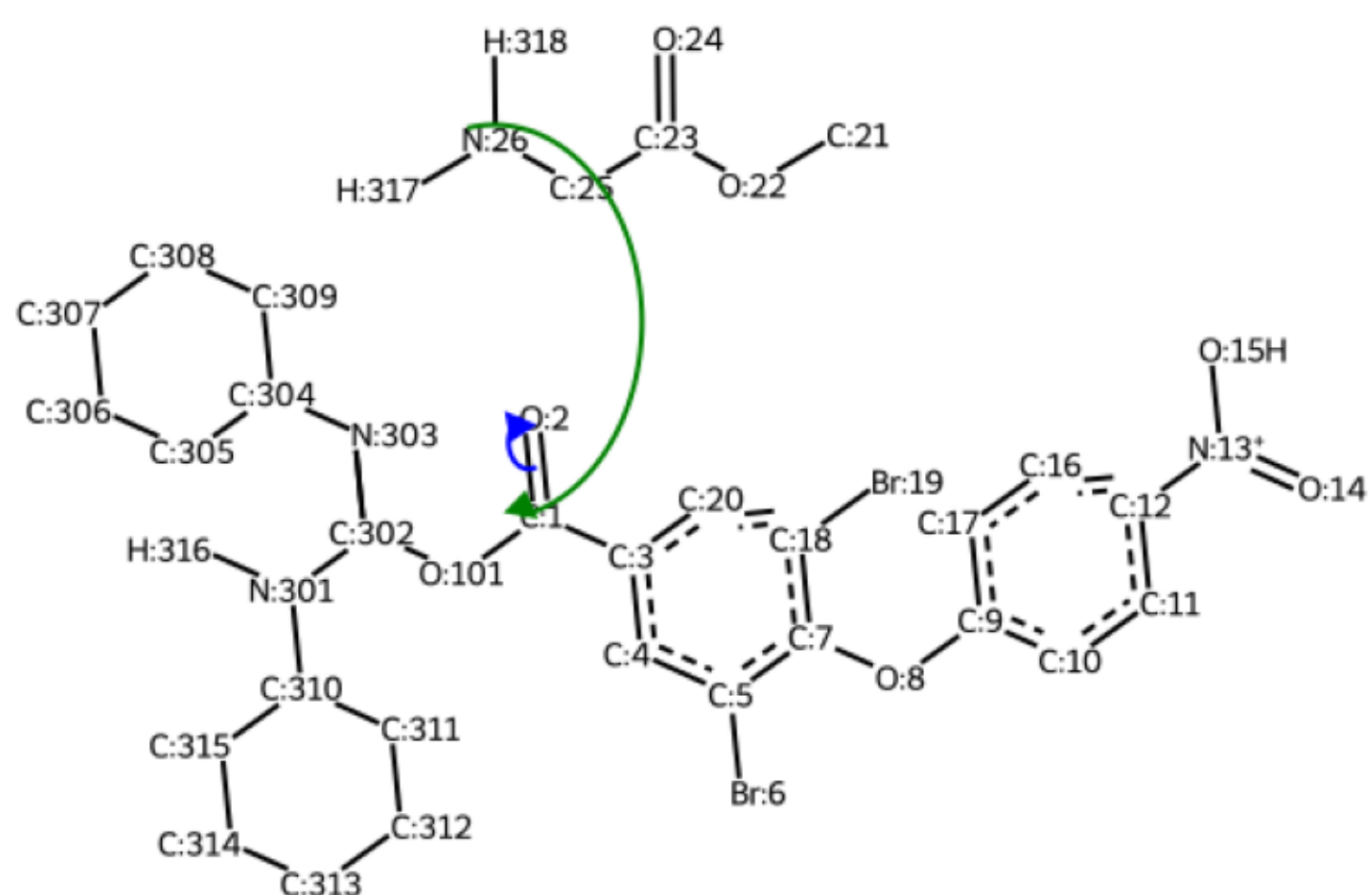
step #1



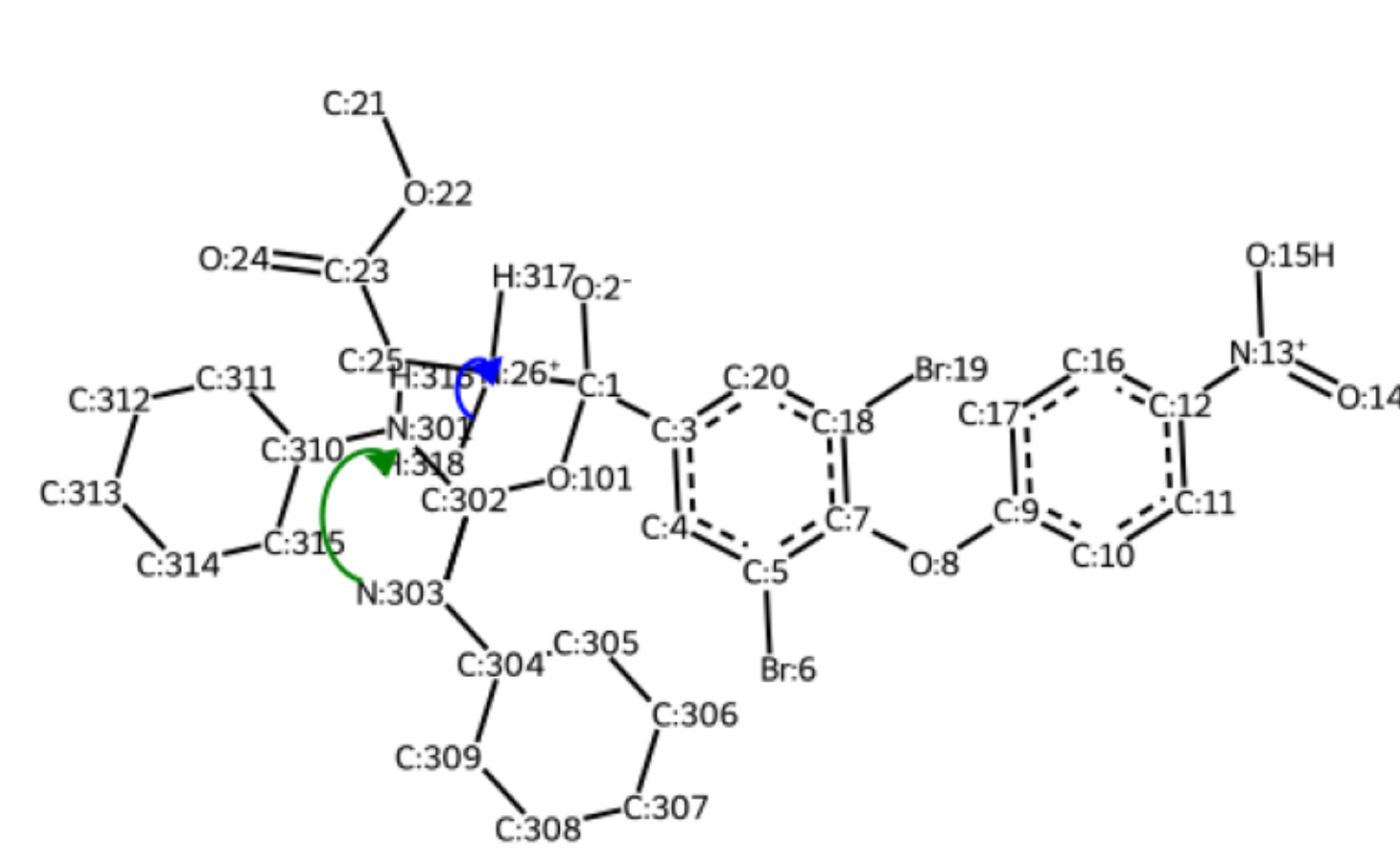
step #2



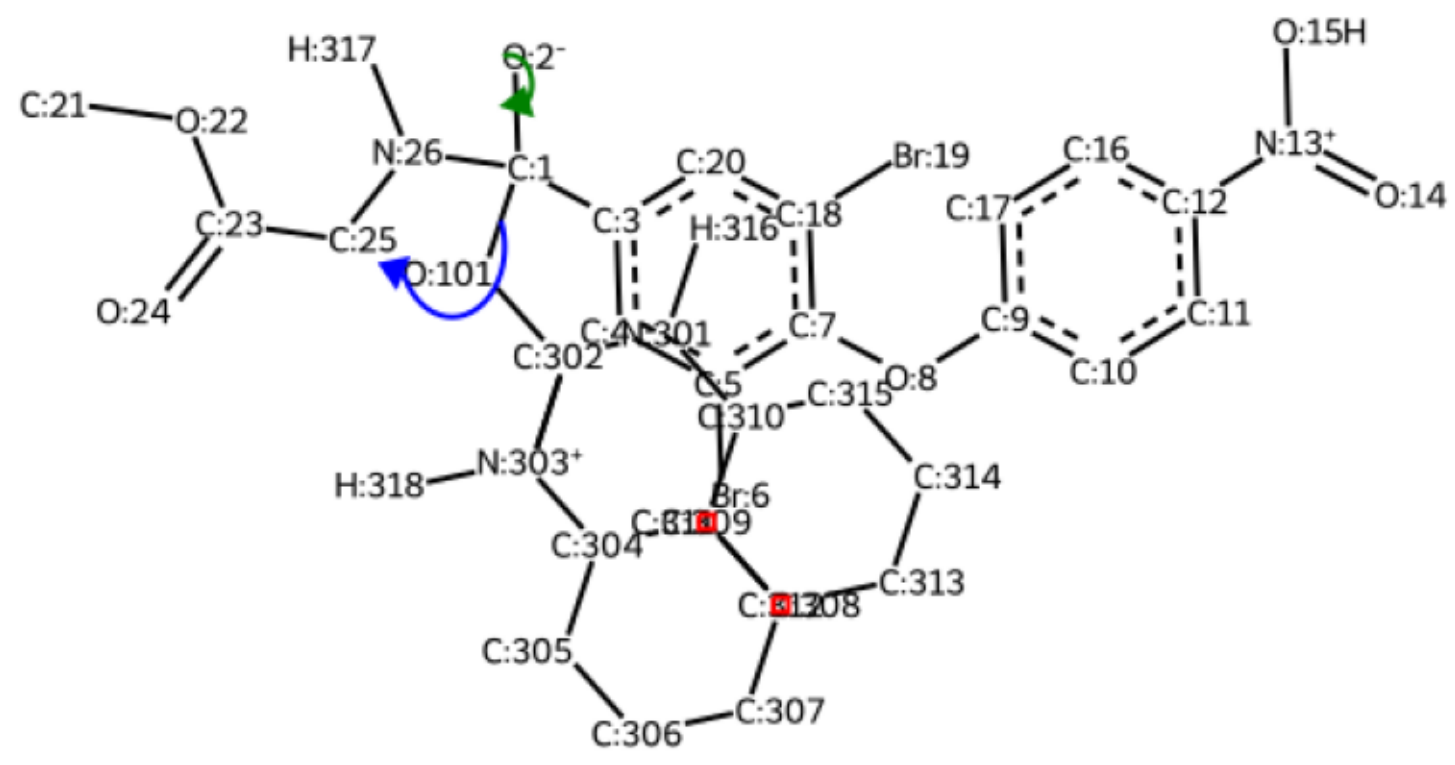
step #3



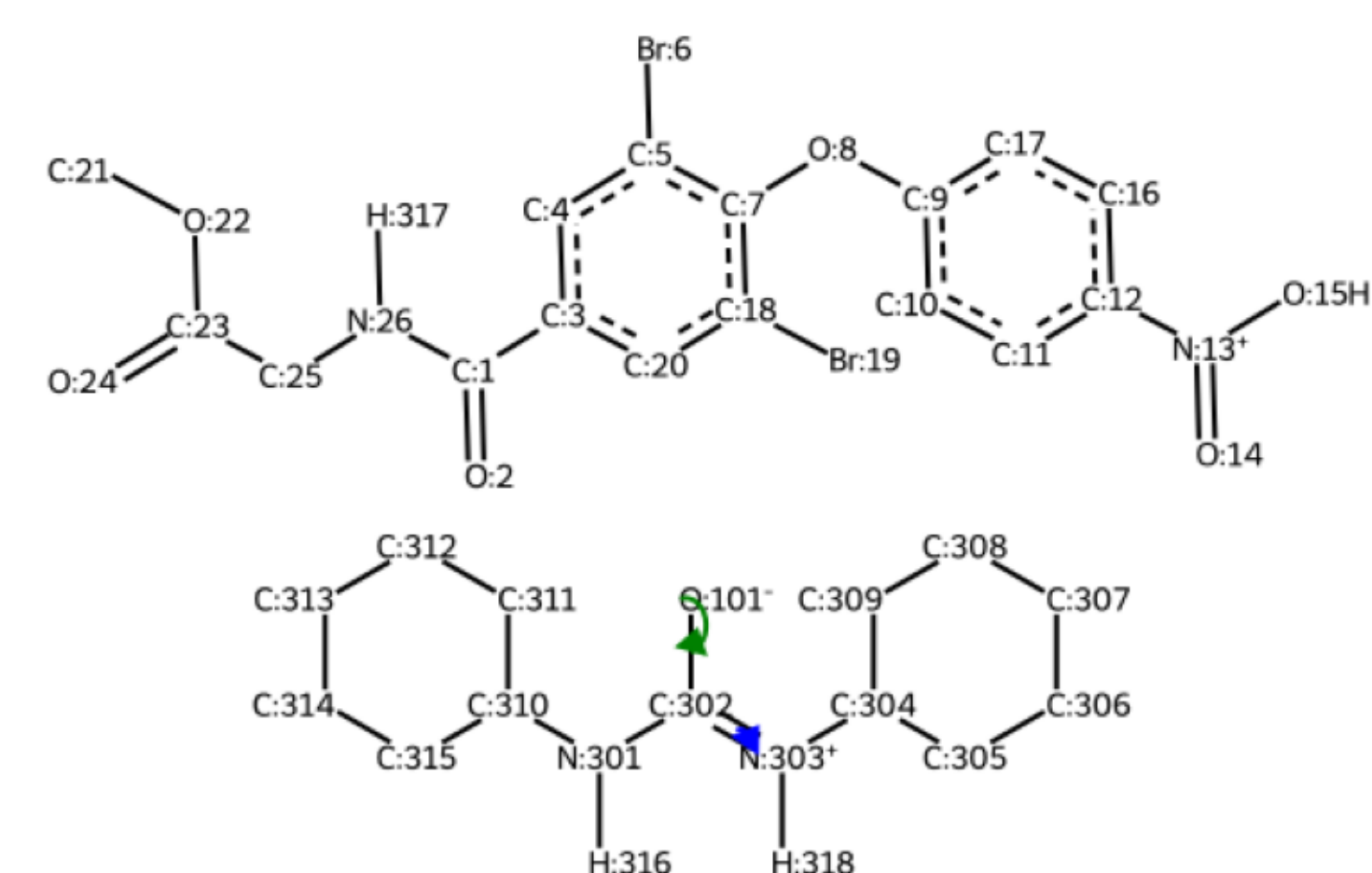
step #4



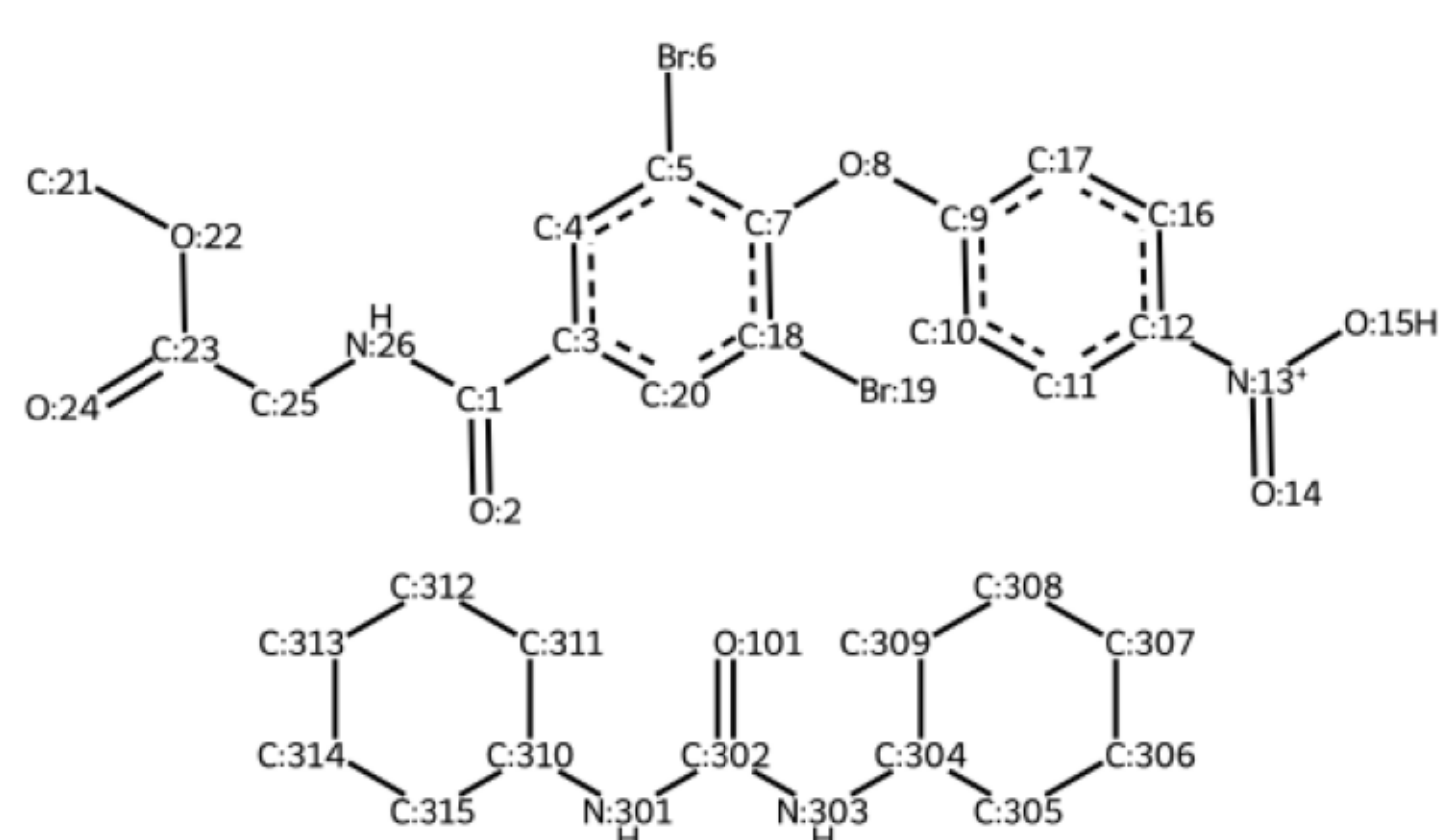
step #5



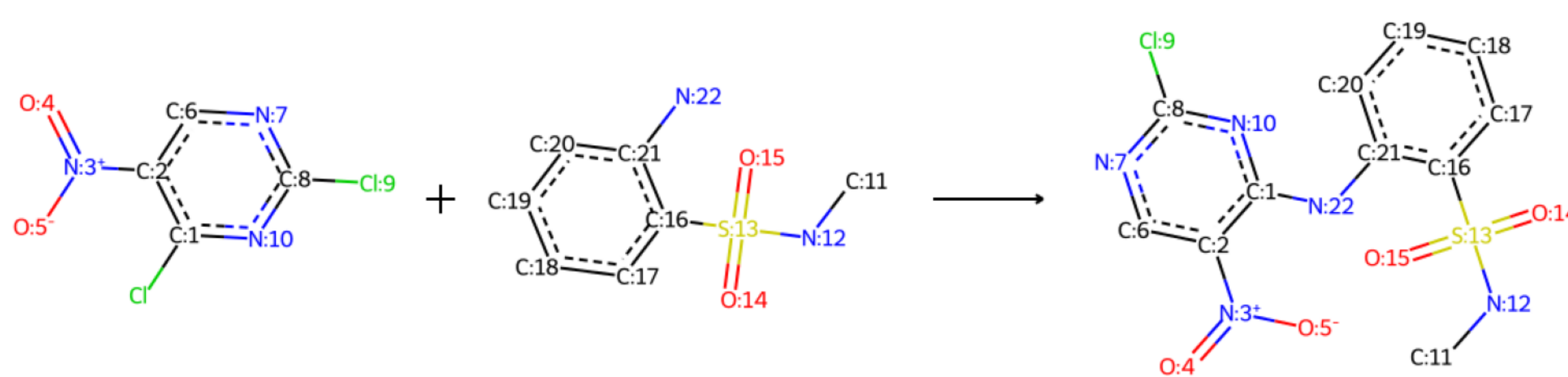
step #6



Product(s)

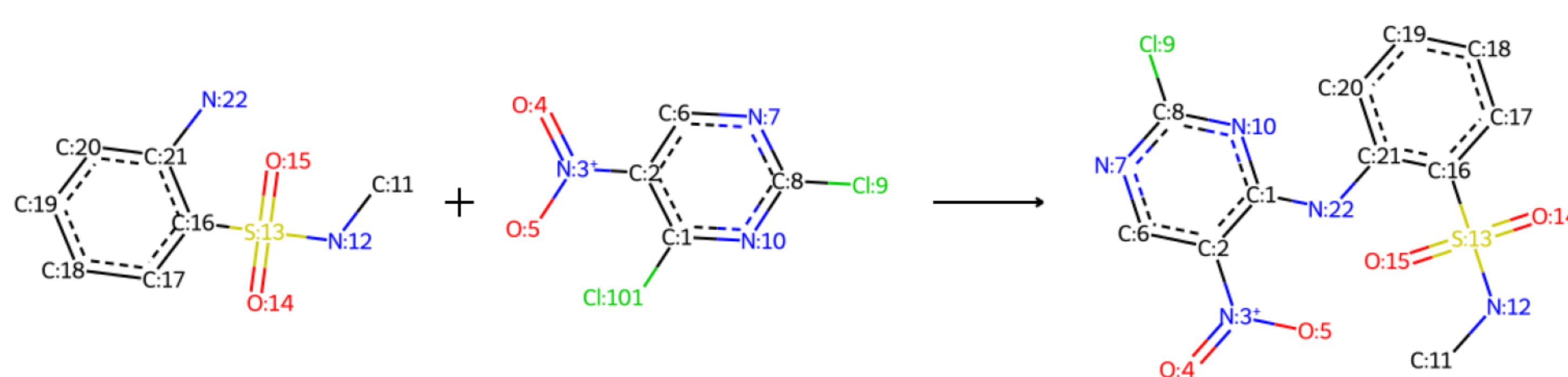


Original reaction
sampled RXN_ID:66)



Identified mechanistic class -
S_NAr(ortho) reaction

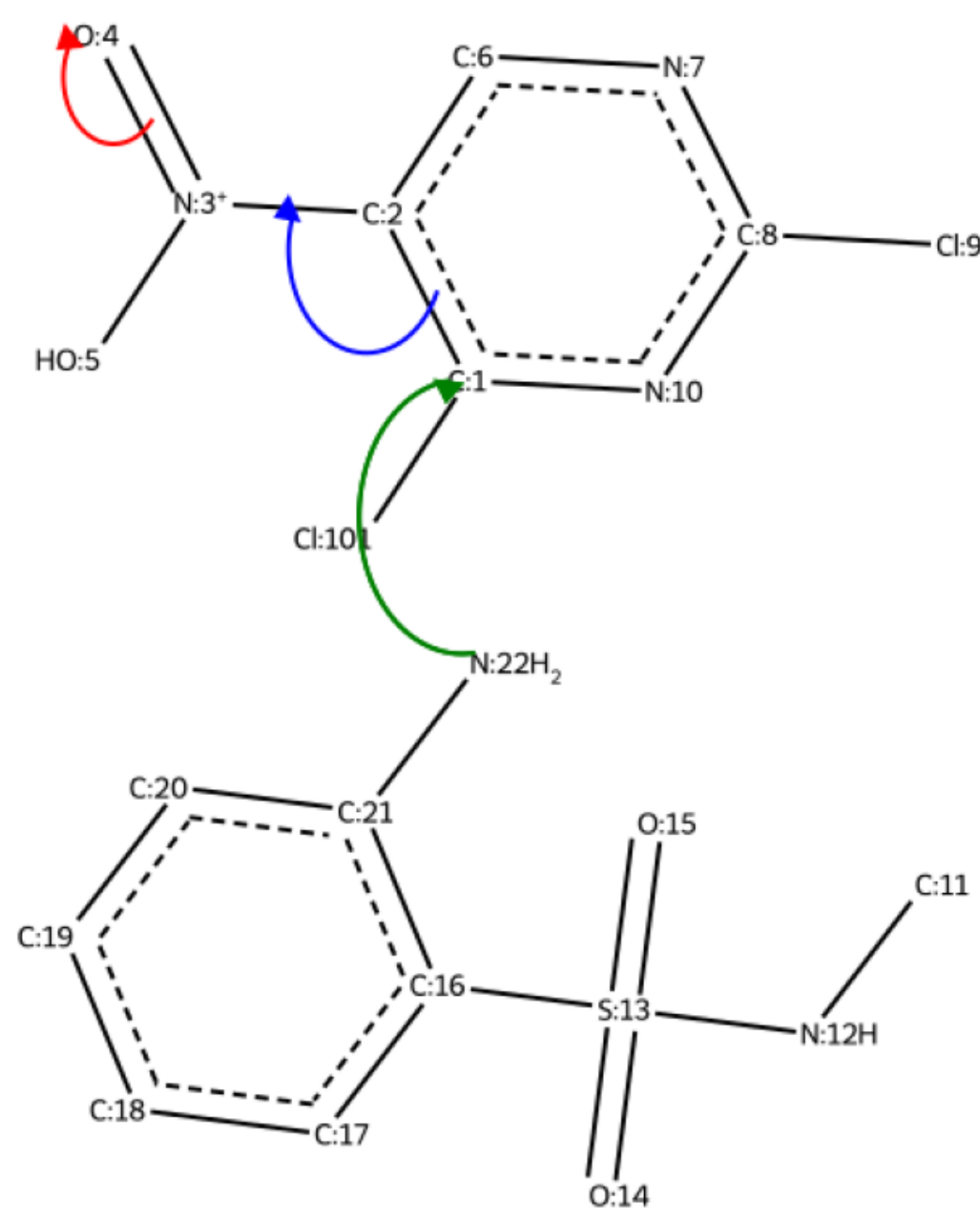
Reaction with missing reagents recovered



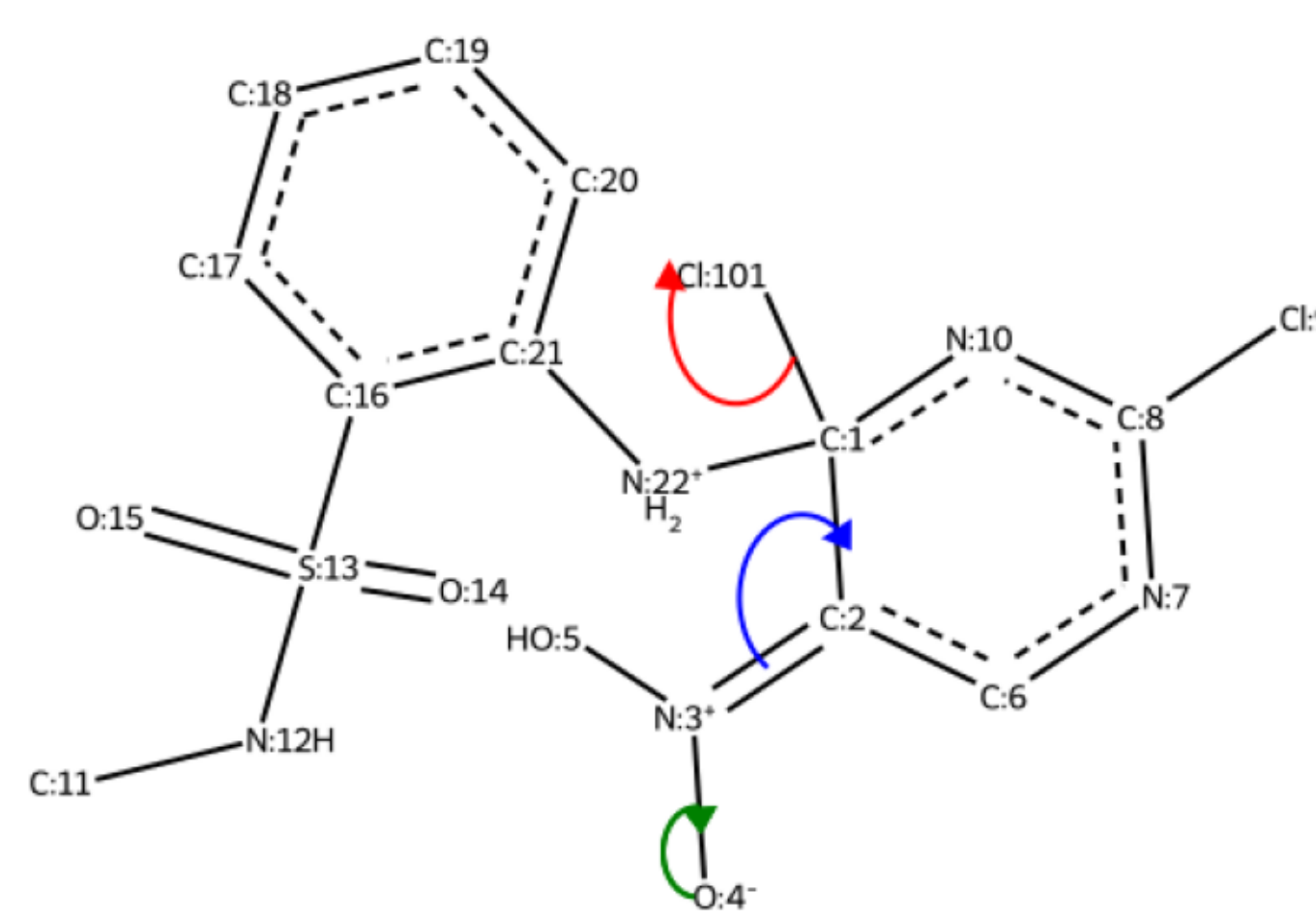
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

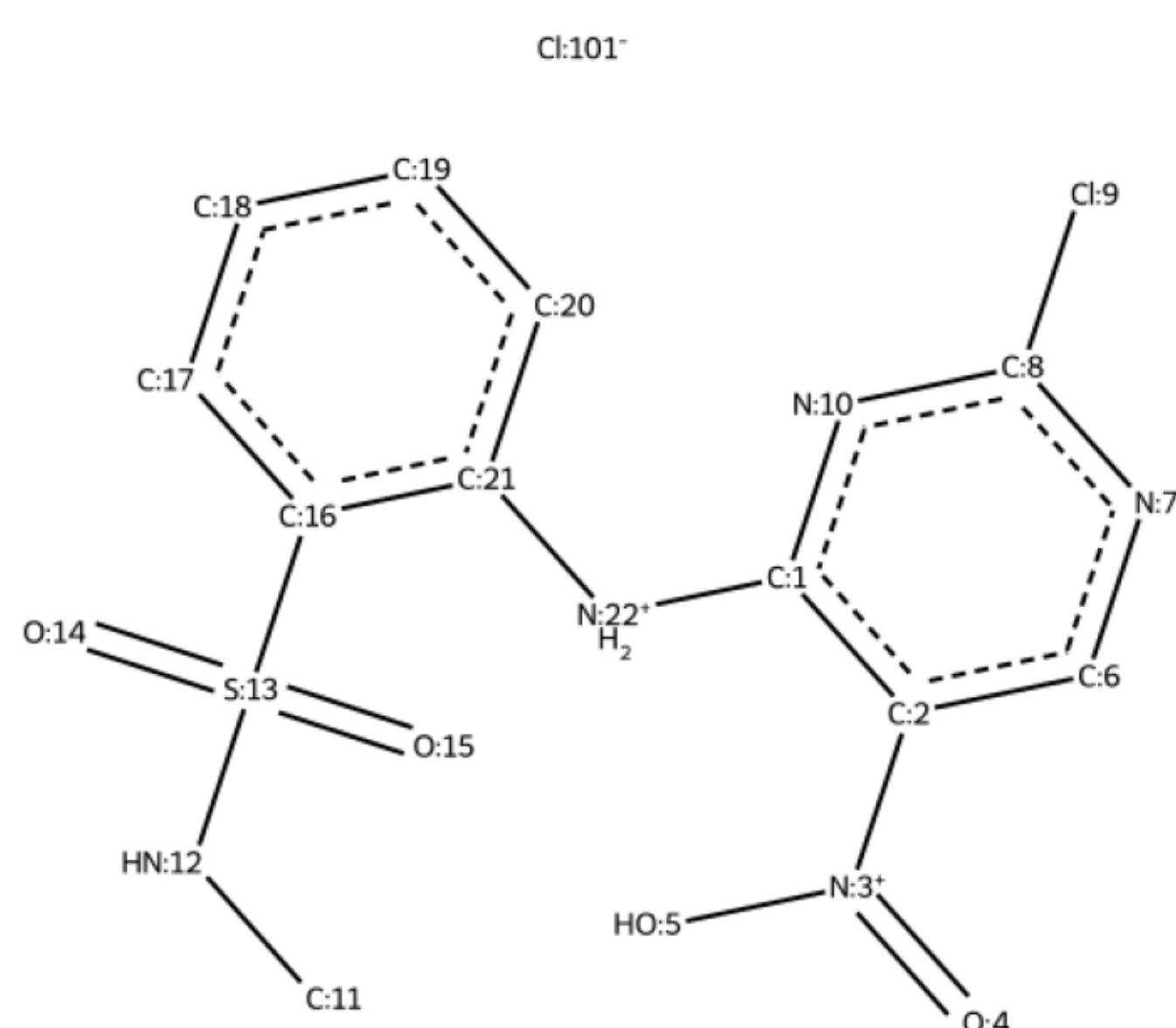
step #1



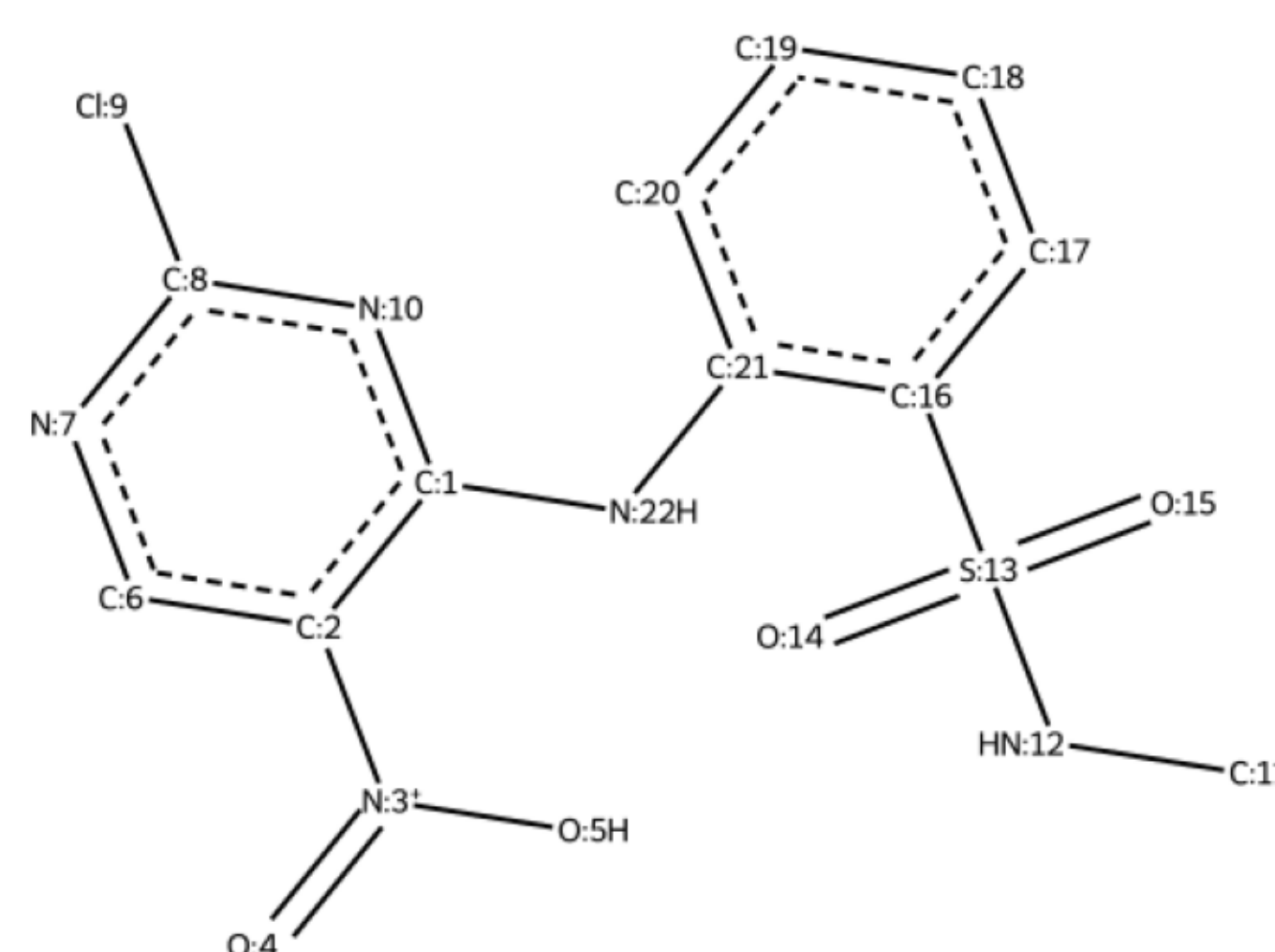
step #2



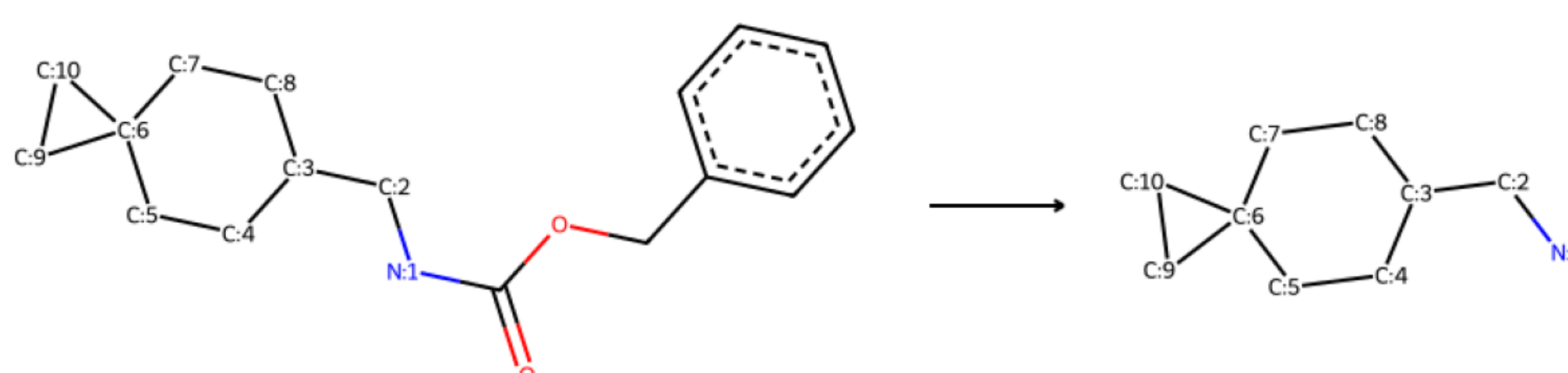
Product(s)



proton transfer

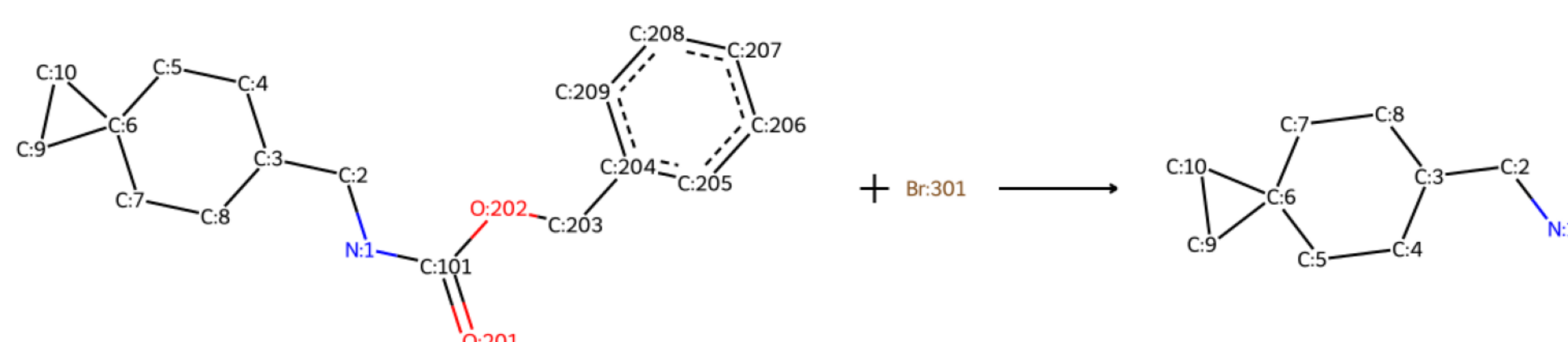


Original reaction
sampled RXN_ID:67)



Identified mechanistic class -
Cbz_deprotection reaction

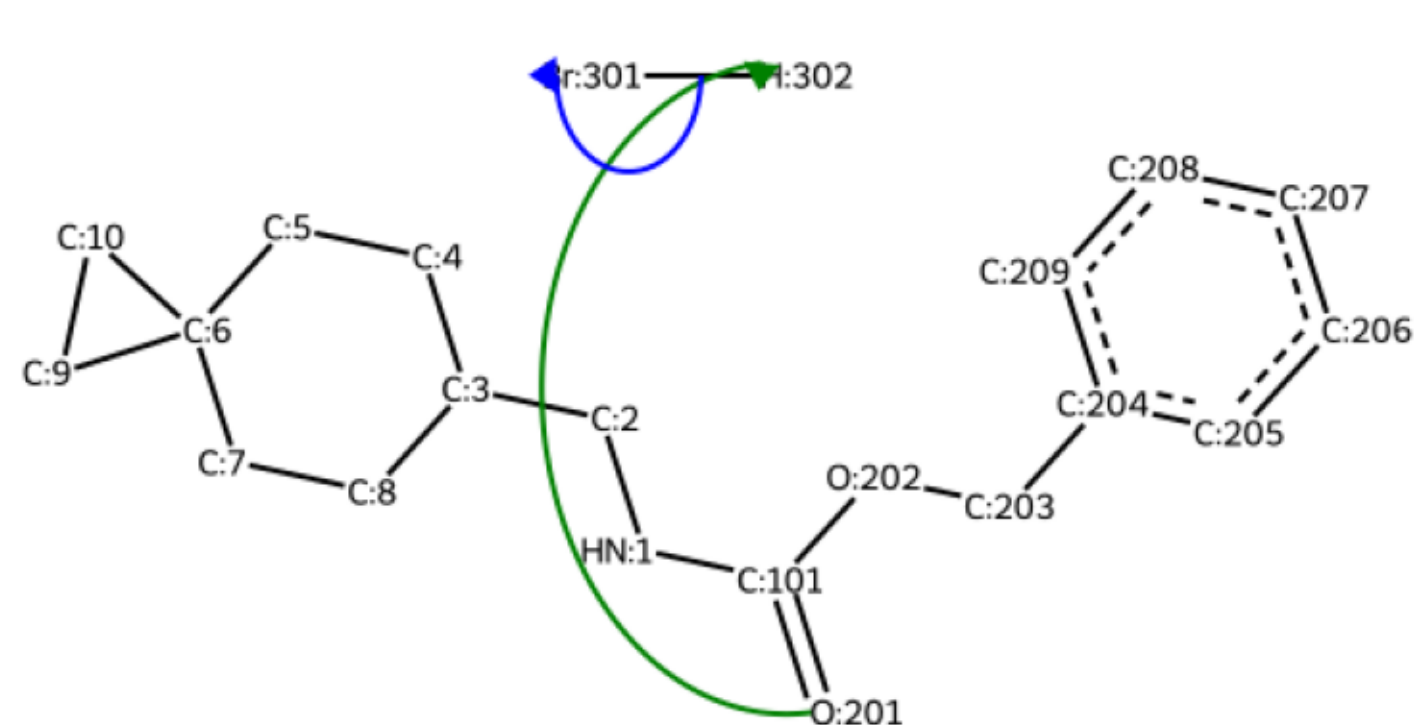
Reaction with missing reagents recovered



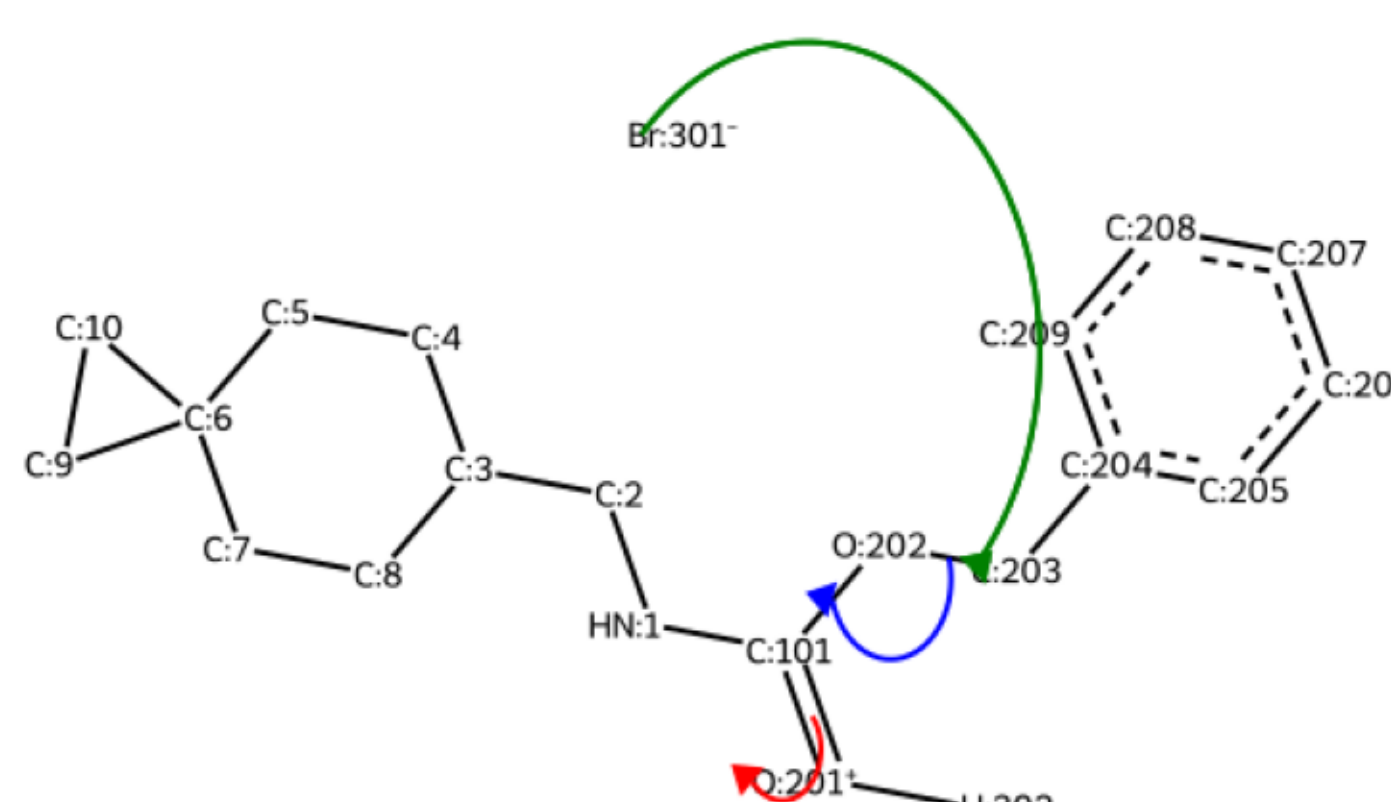
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

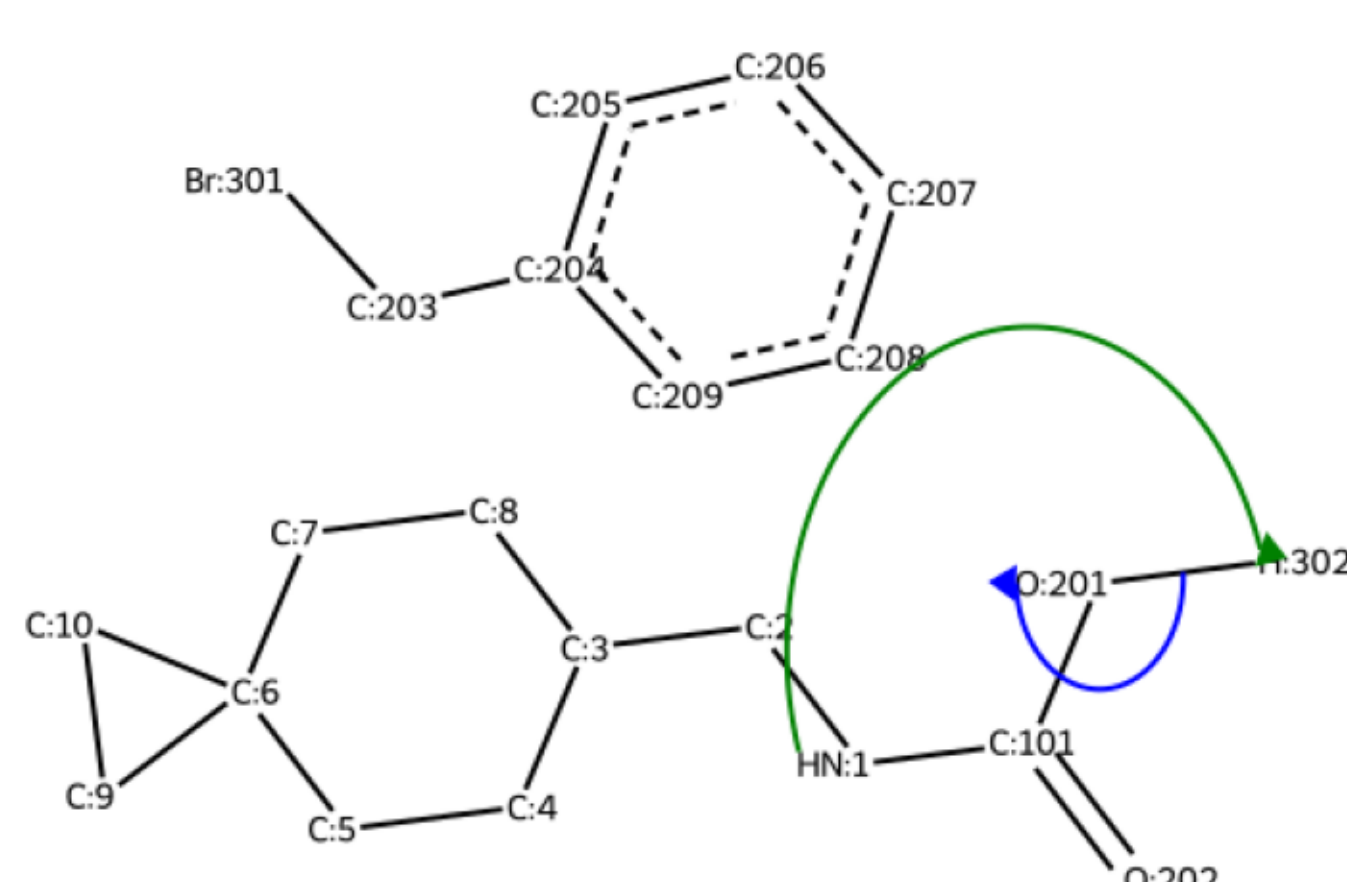
step #1



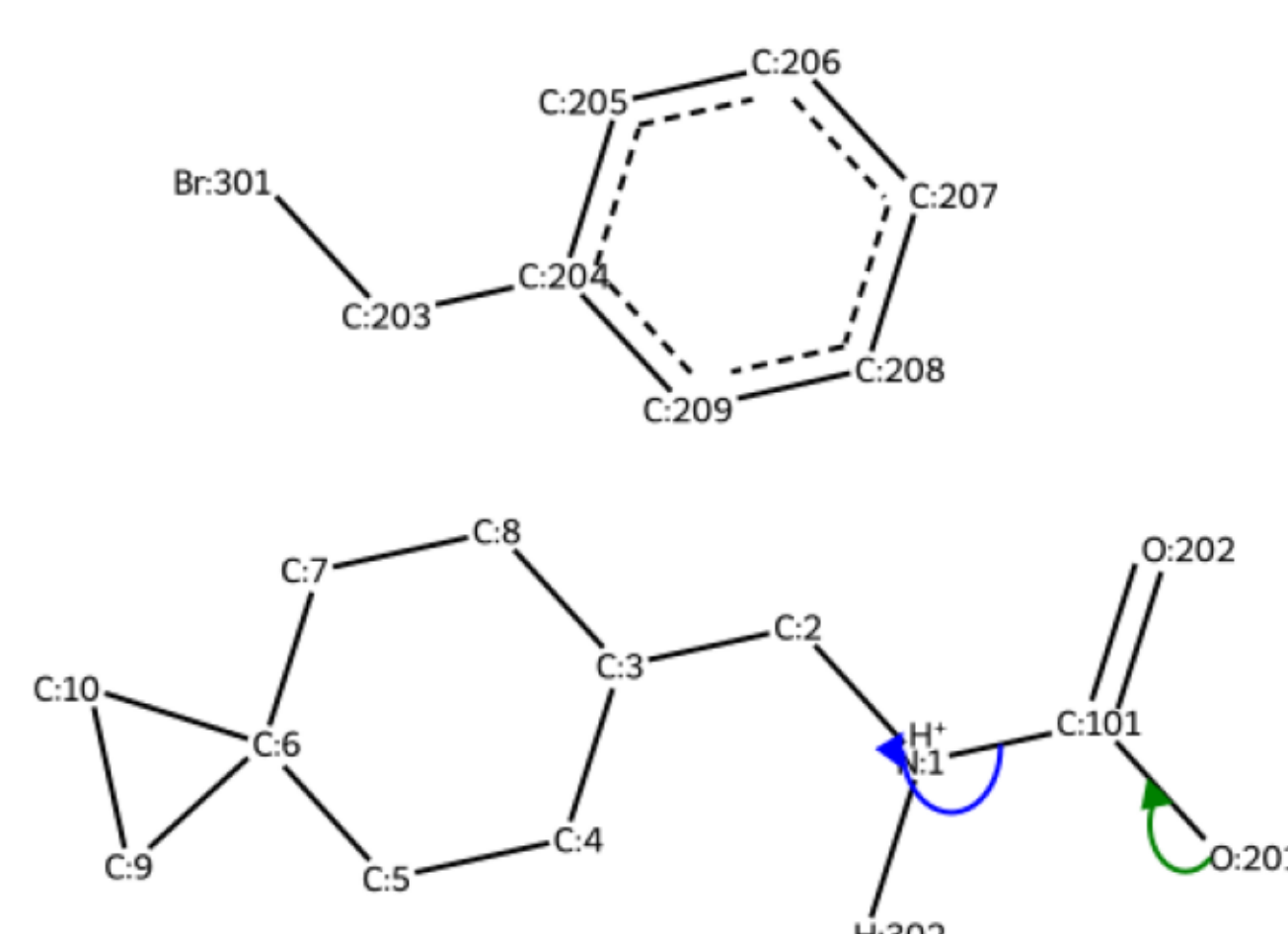
step #2



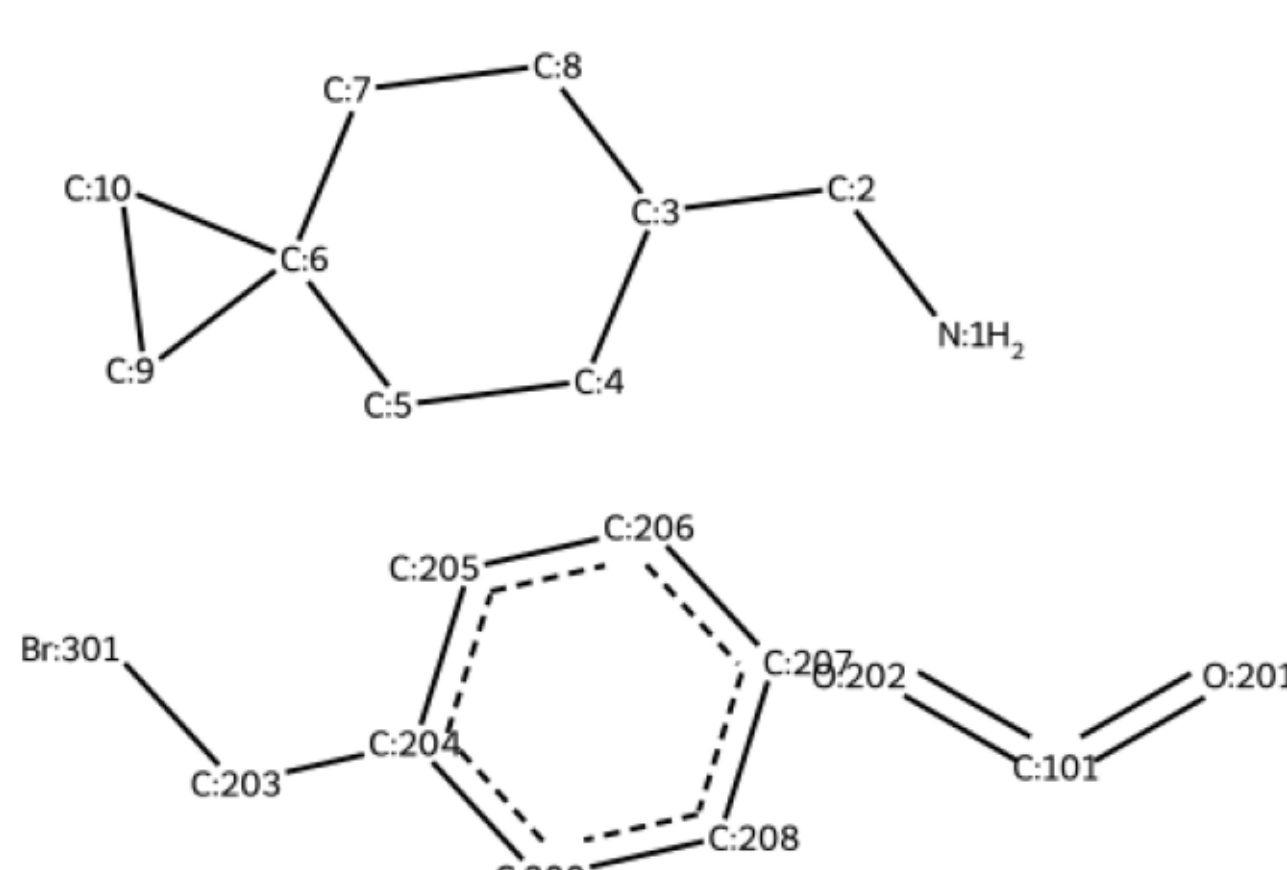
step #3



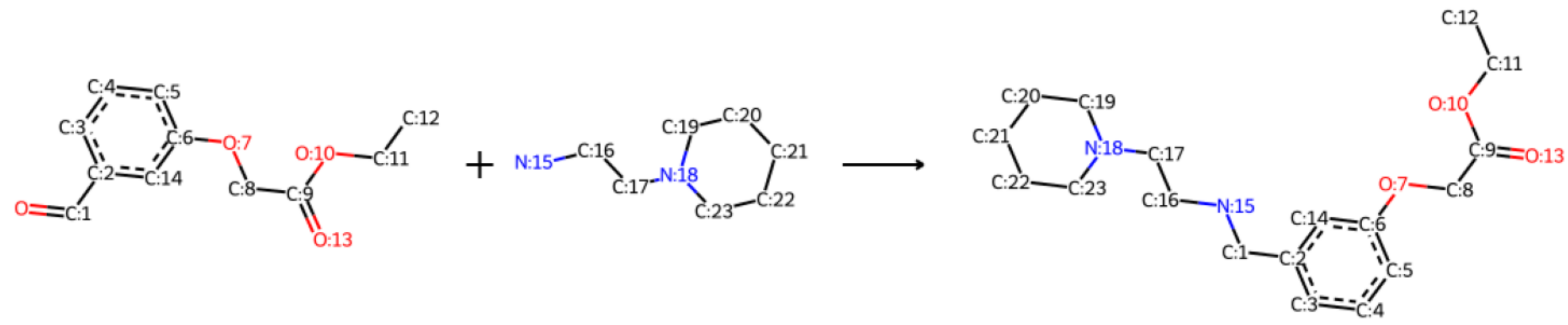
step #4



Product(s)

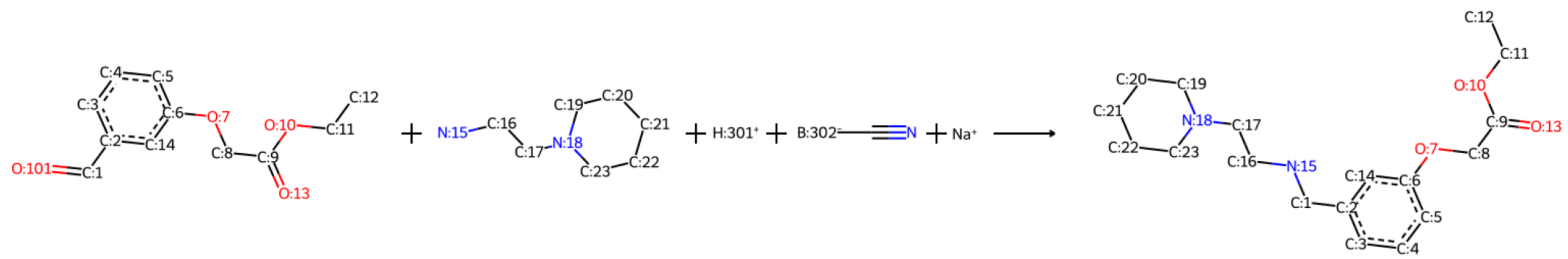


Original reaction
sampled RXN_ID:68)



Identified mechanistic class -
reductive_amination reaction

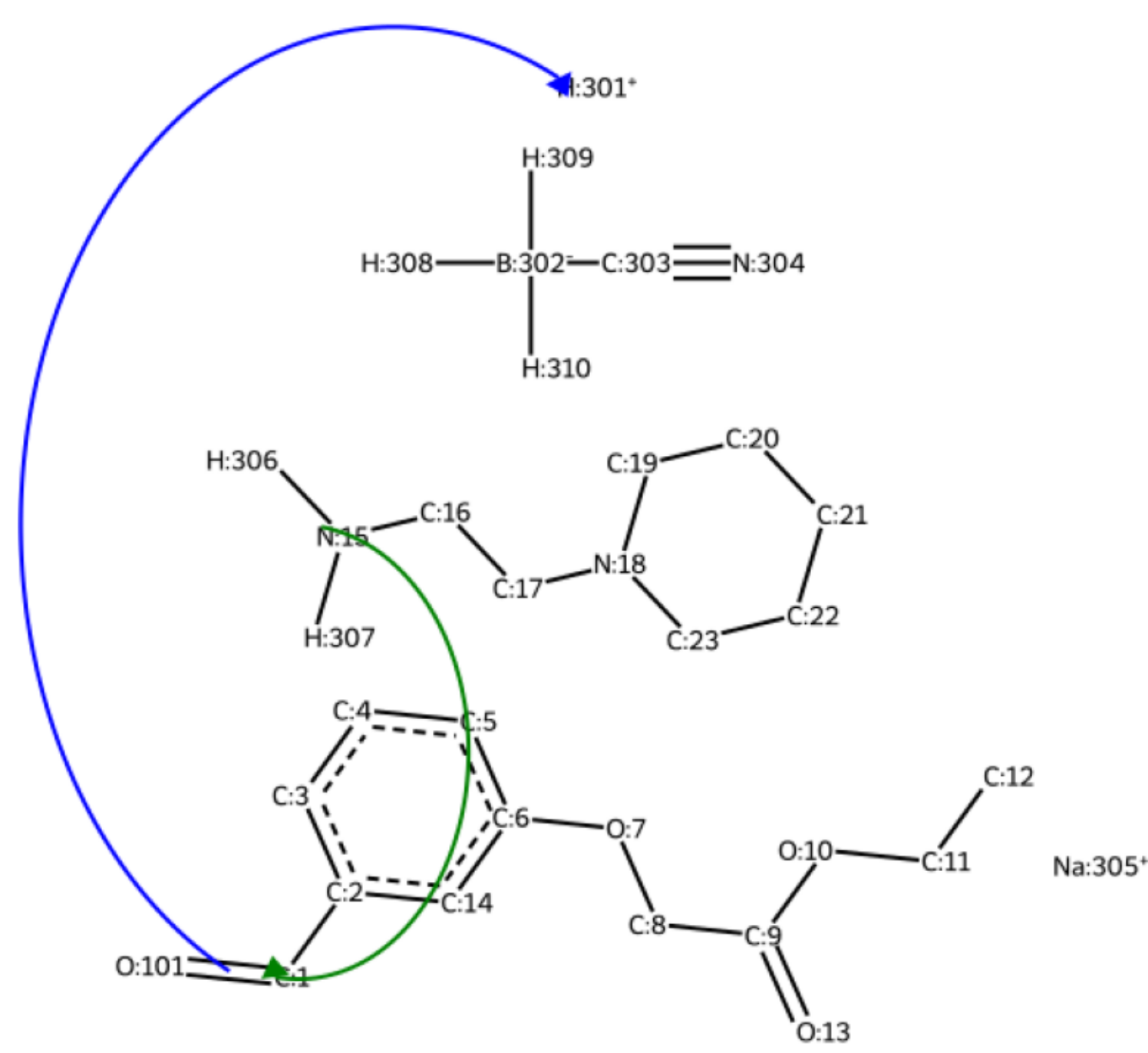
Reaction with missing reagents recovered



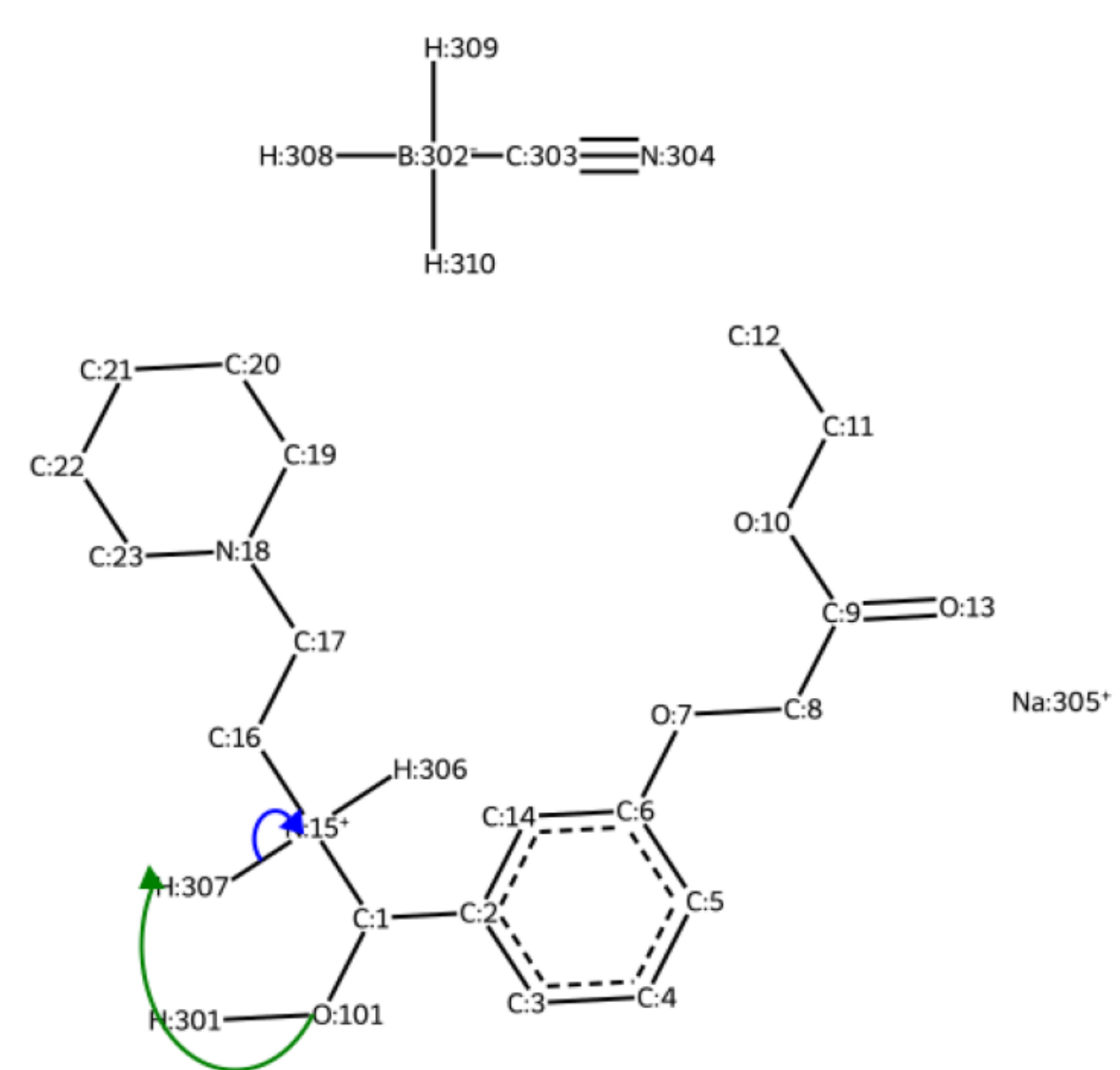
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

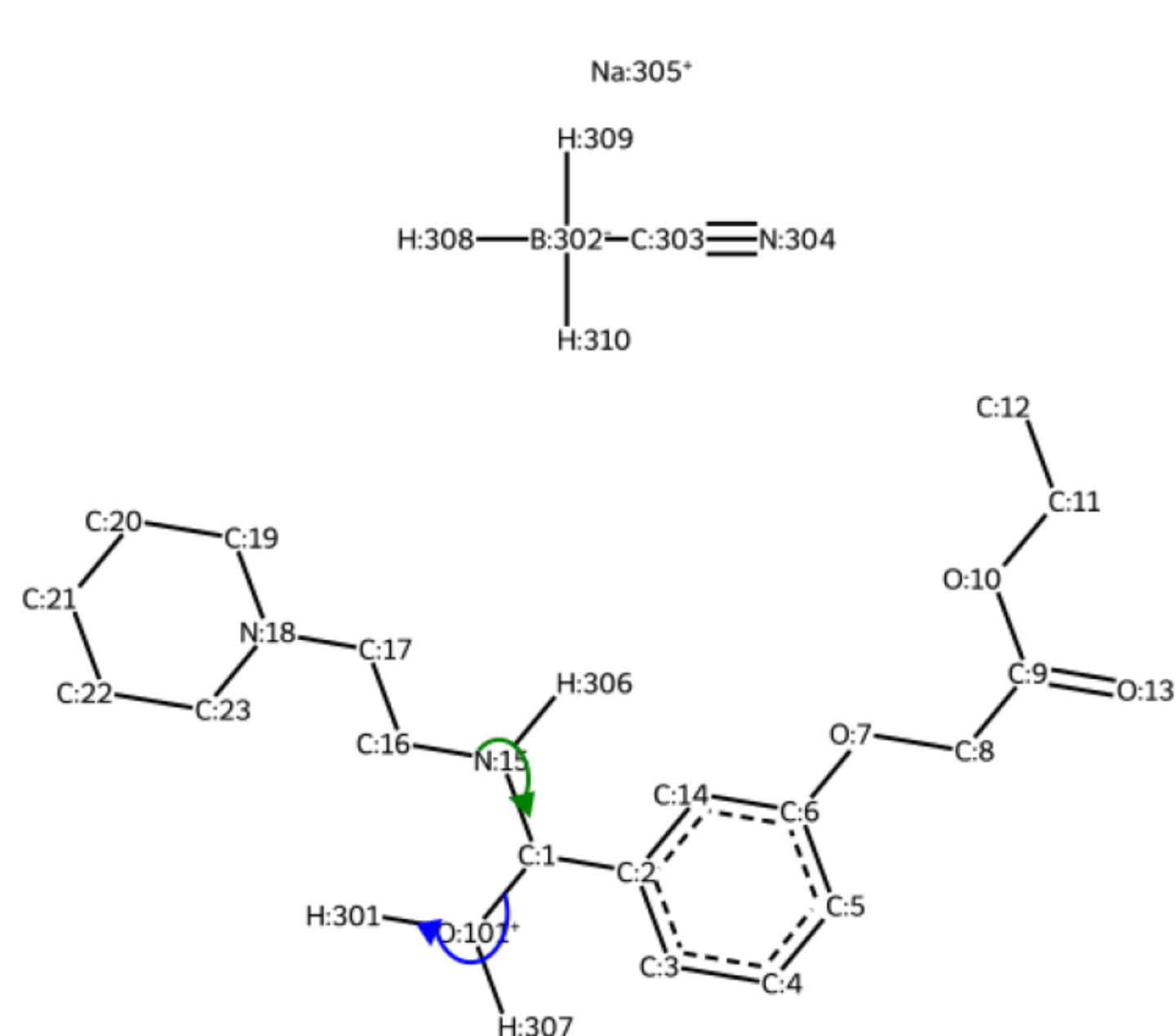
step #1



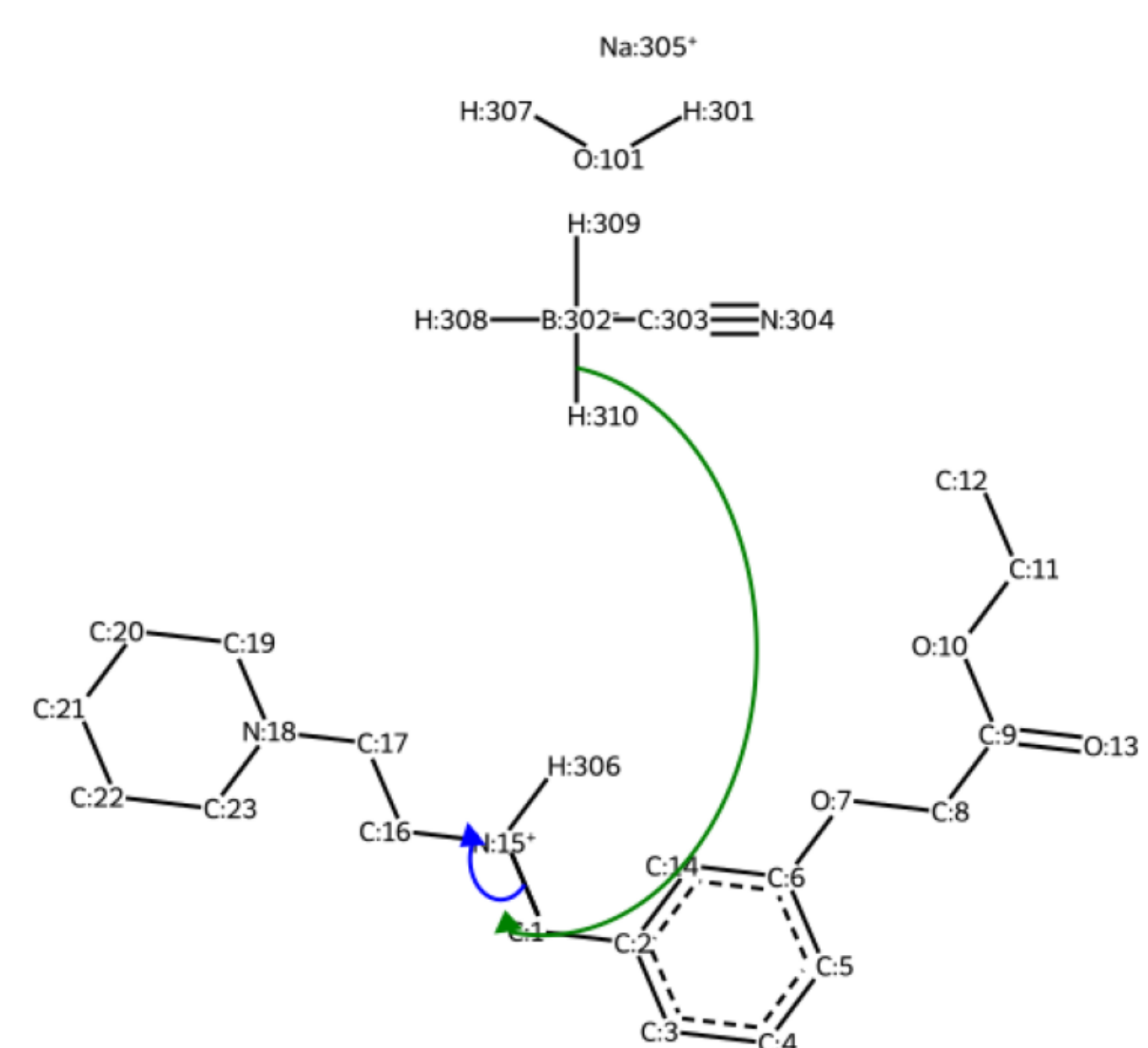
step #2



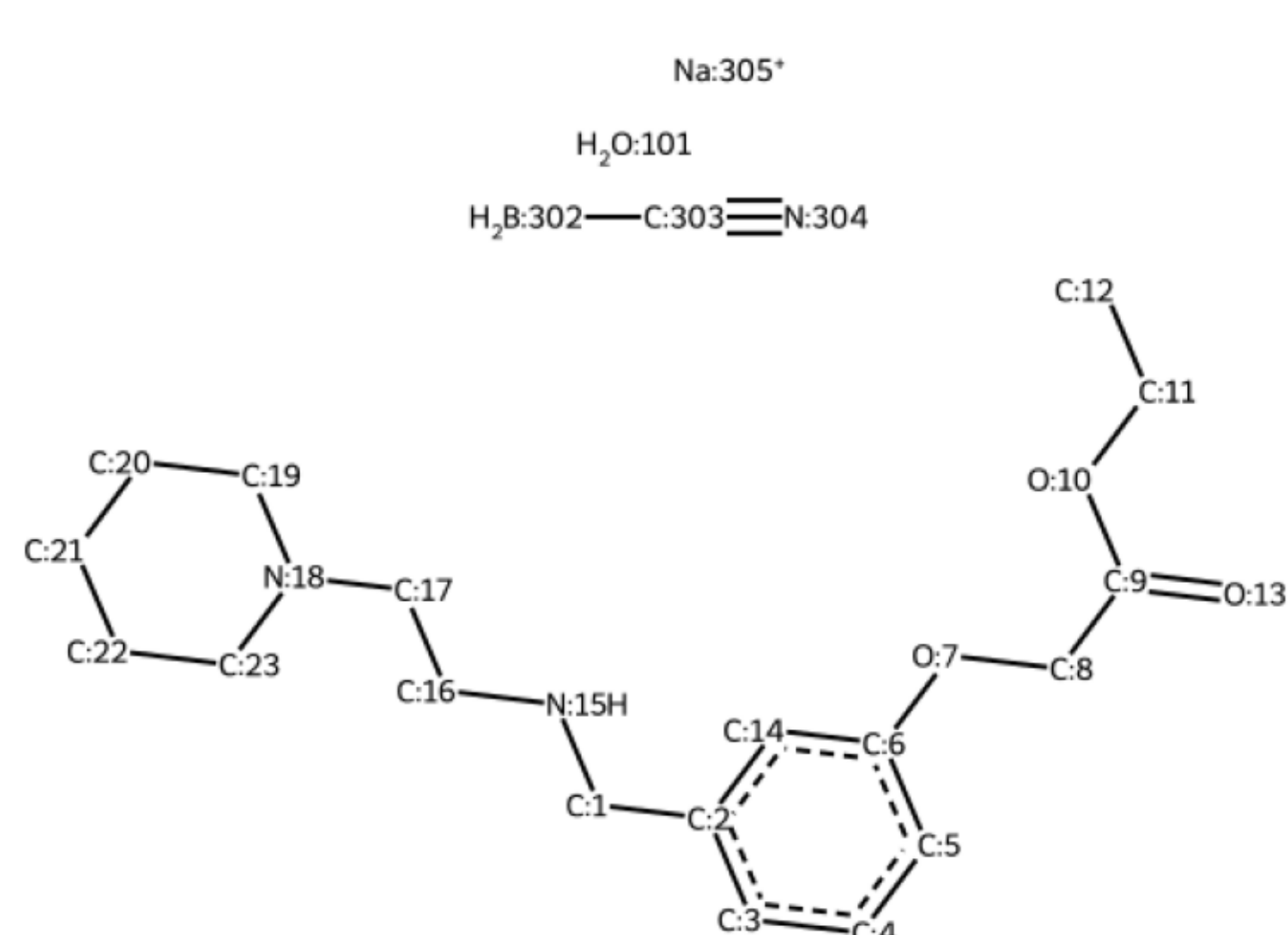
step #3



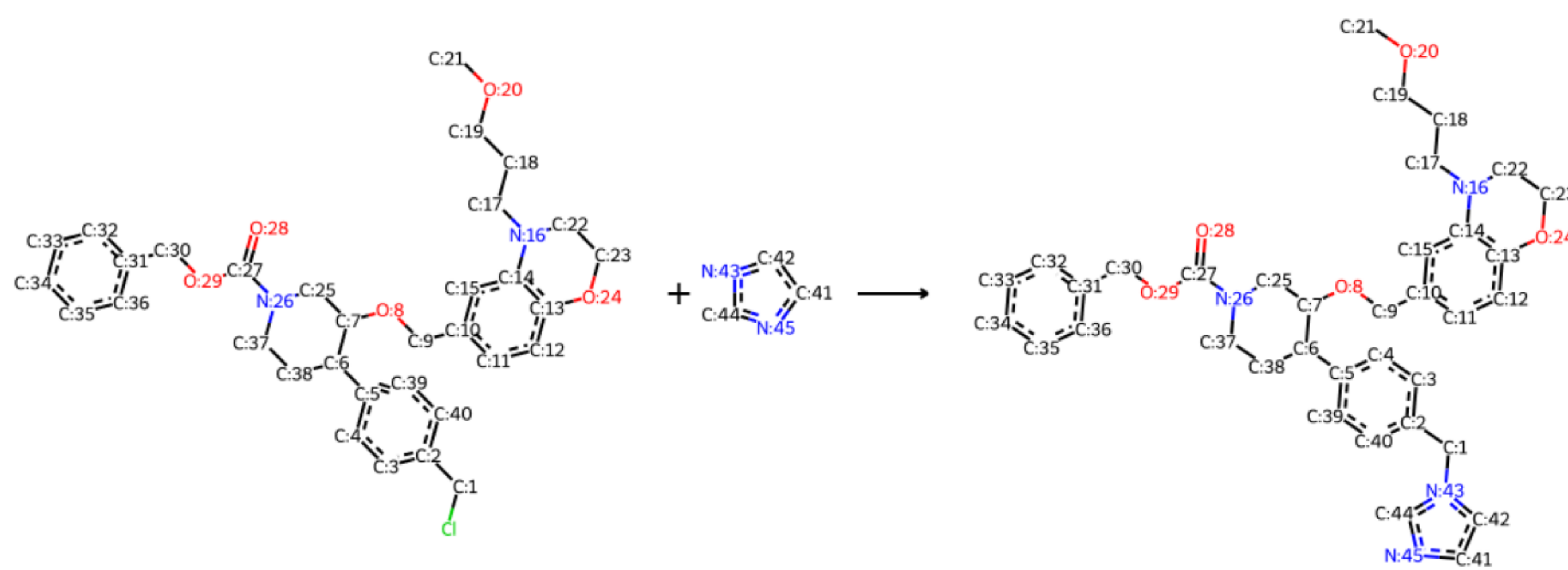
step #4



Product(s)

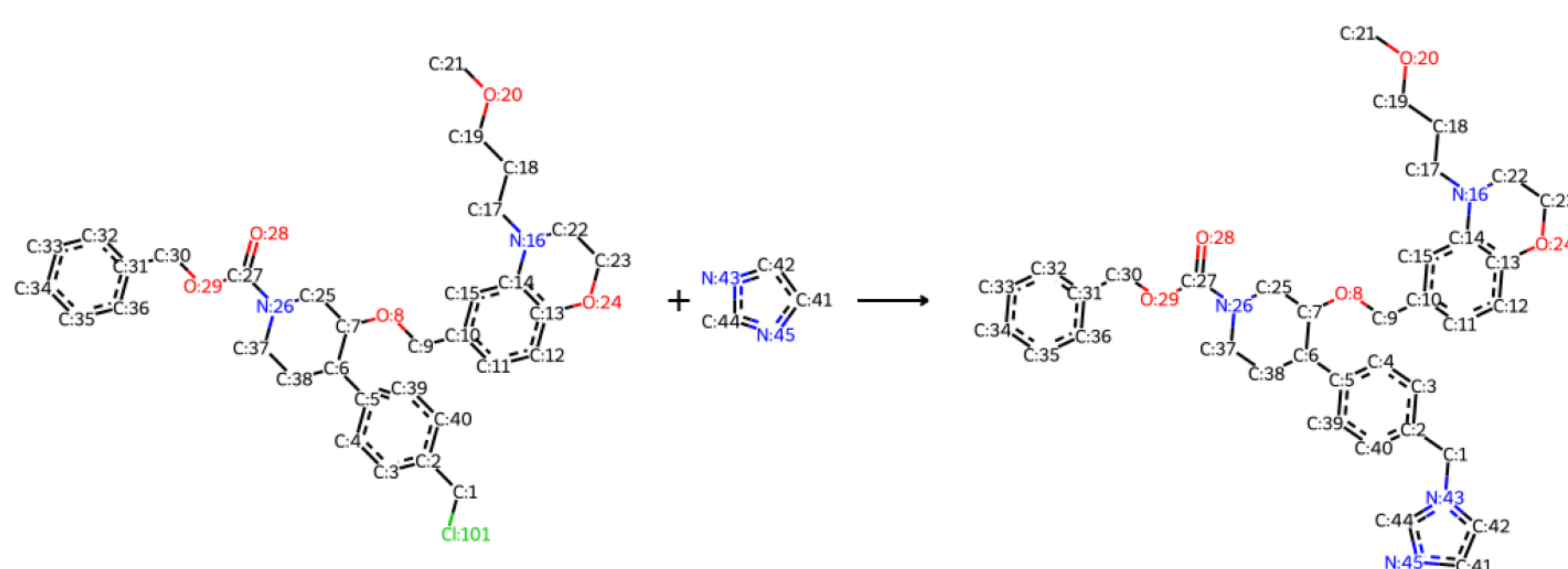


Original reaction
sampled RXN_ID:69)



Identified mechanistic class -
SN2 reaction

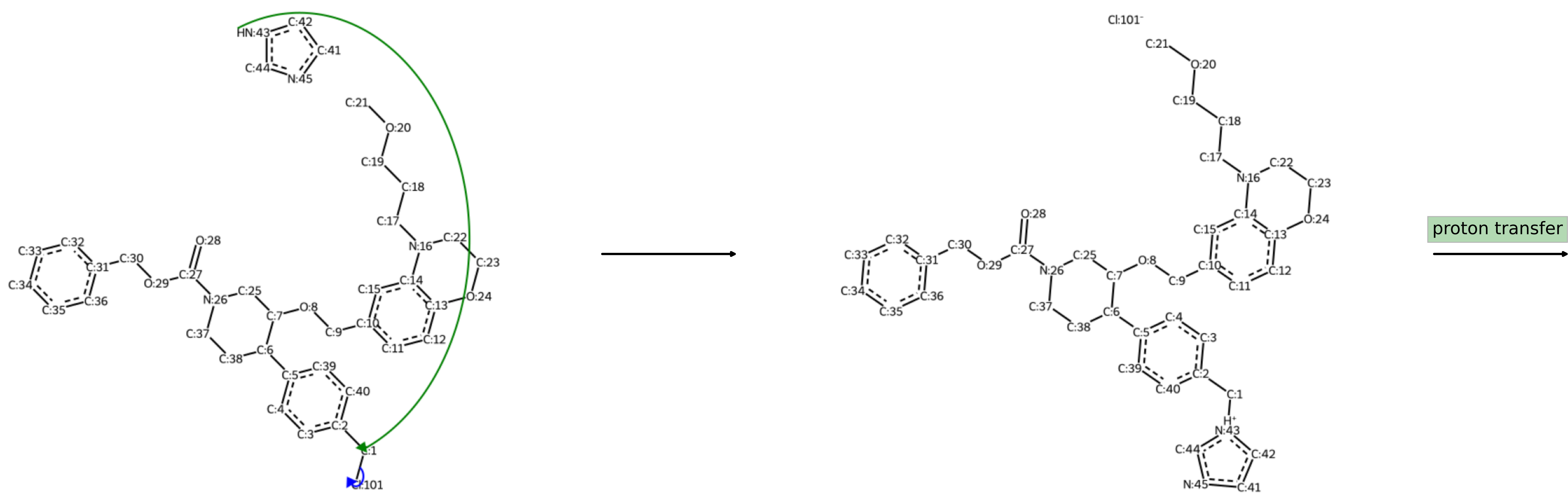
Reaction with missing reagents recovered



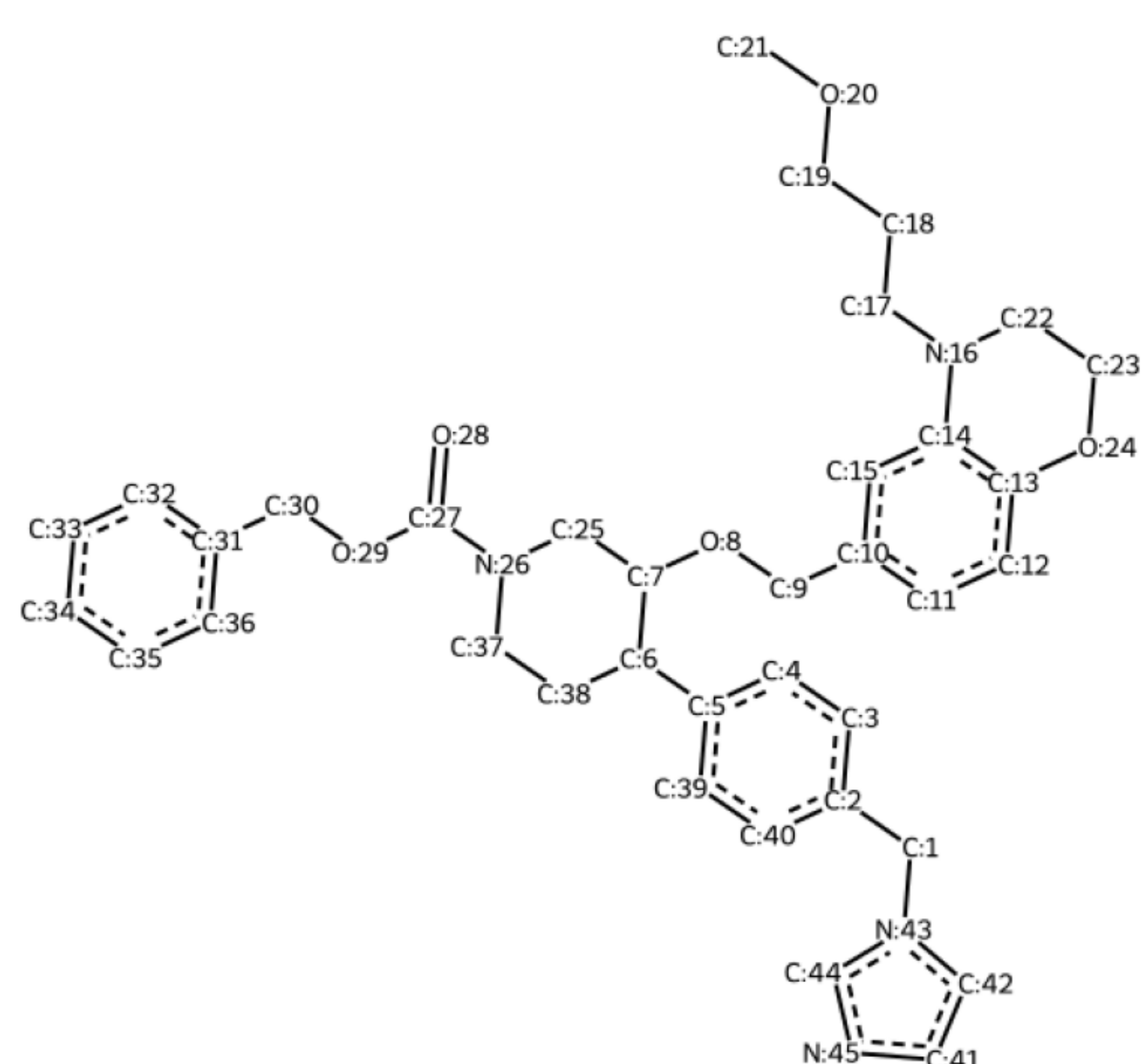
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

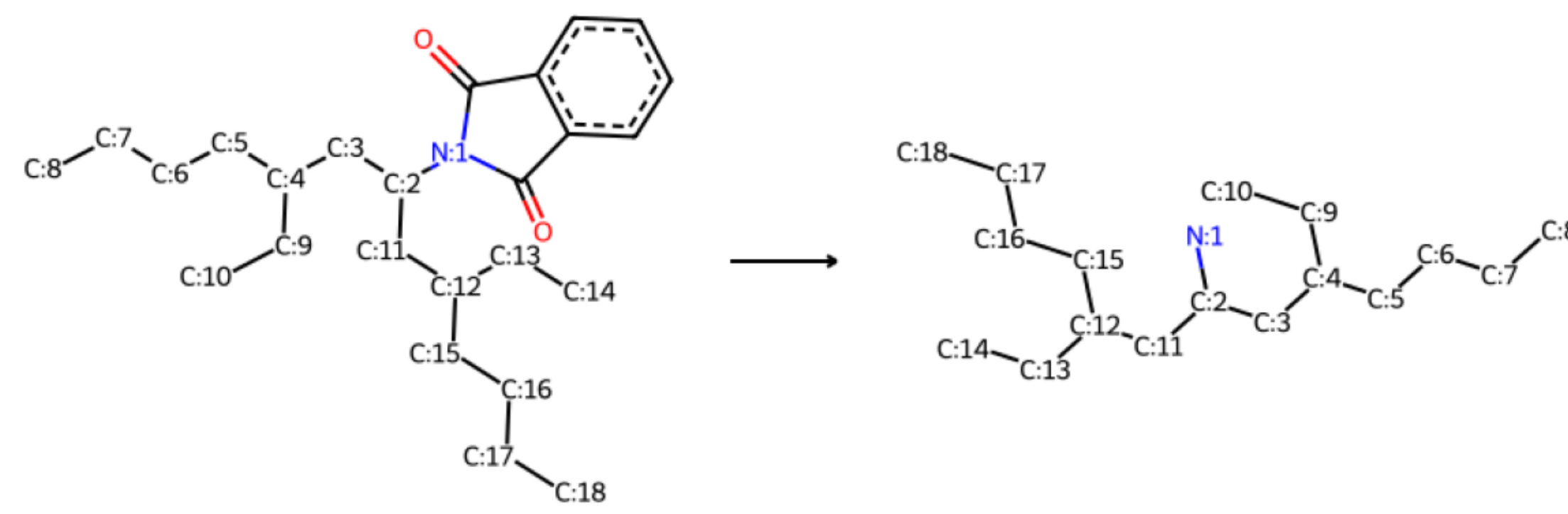
step #1



Product(s)

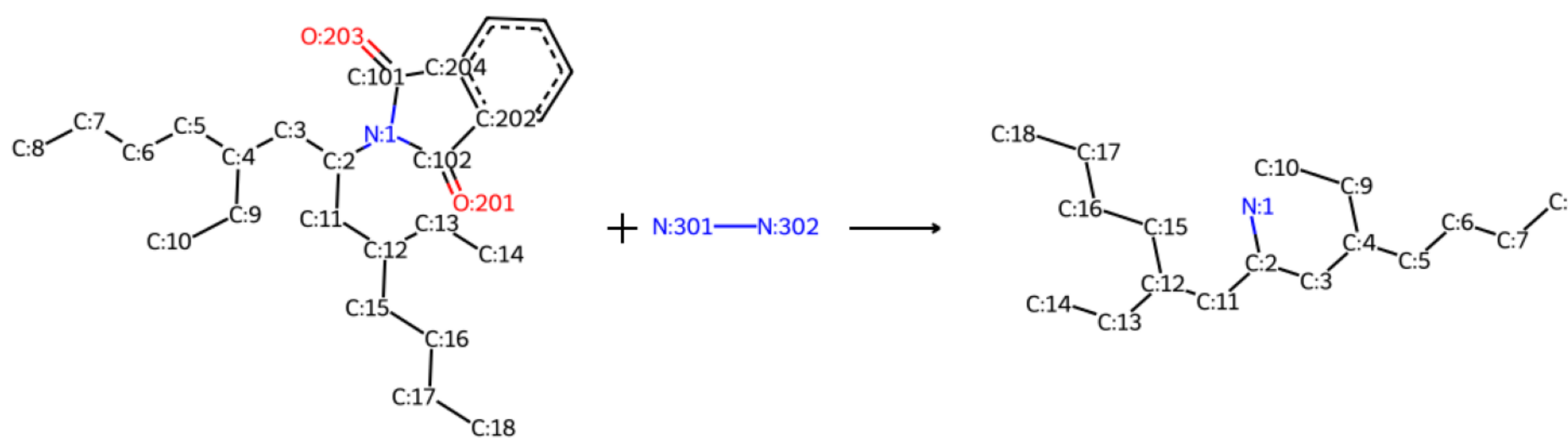


Original reaction sampled RXN_ID:70)



Identified mechanistic class -
Ing_Manske reaction

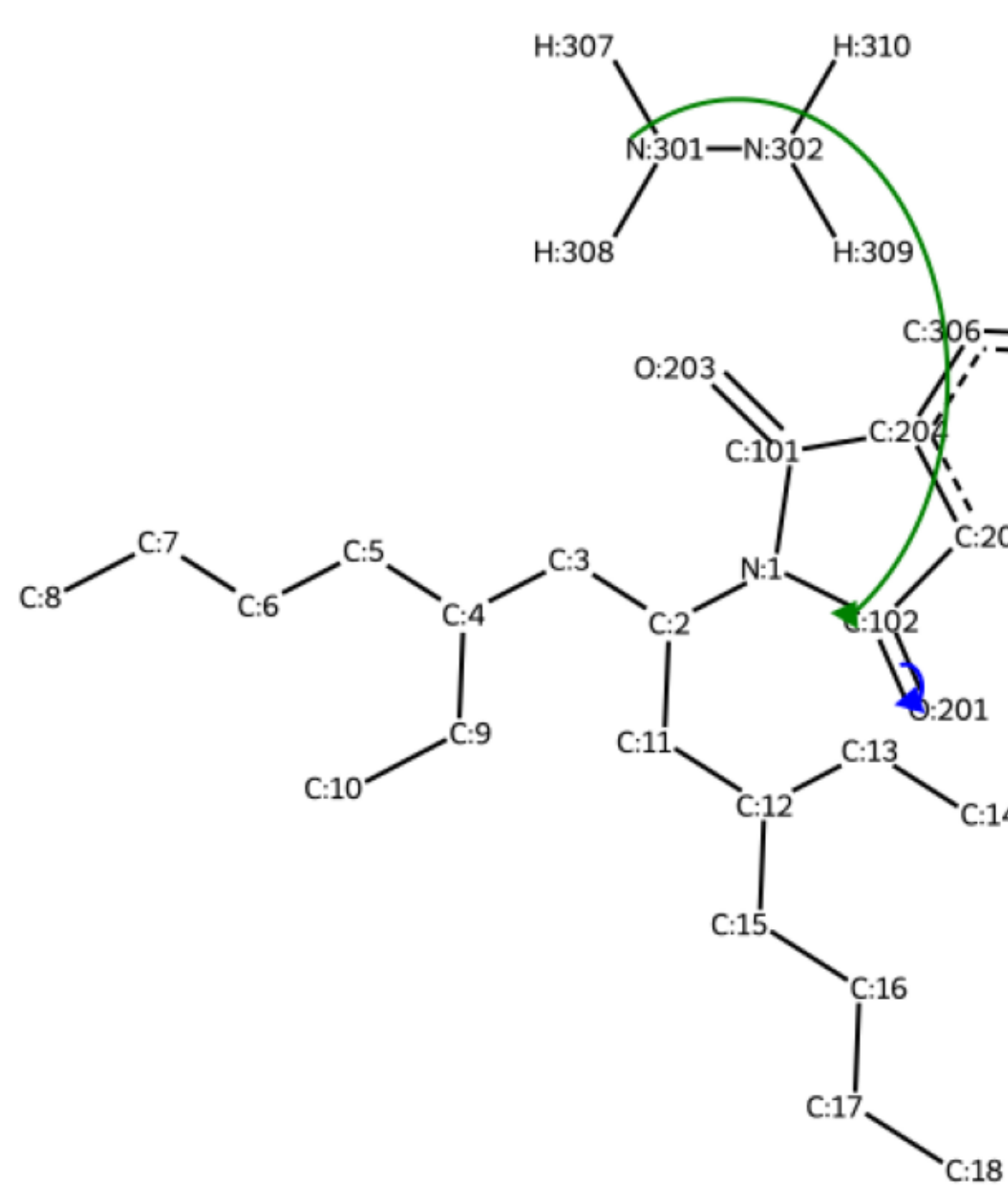
Reaction with missing reagents recovered



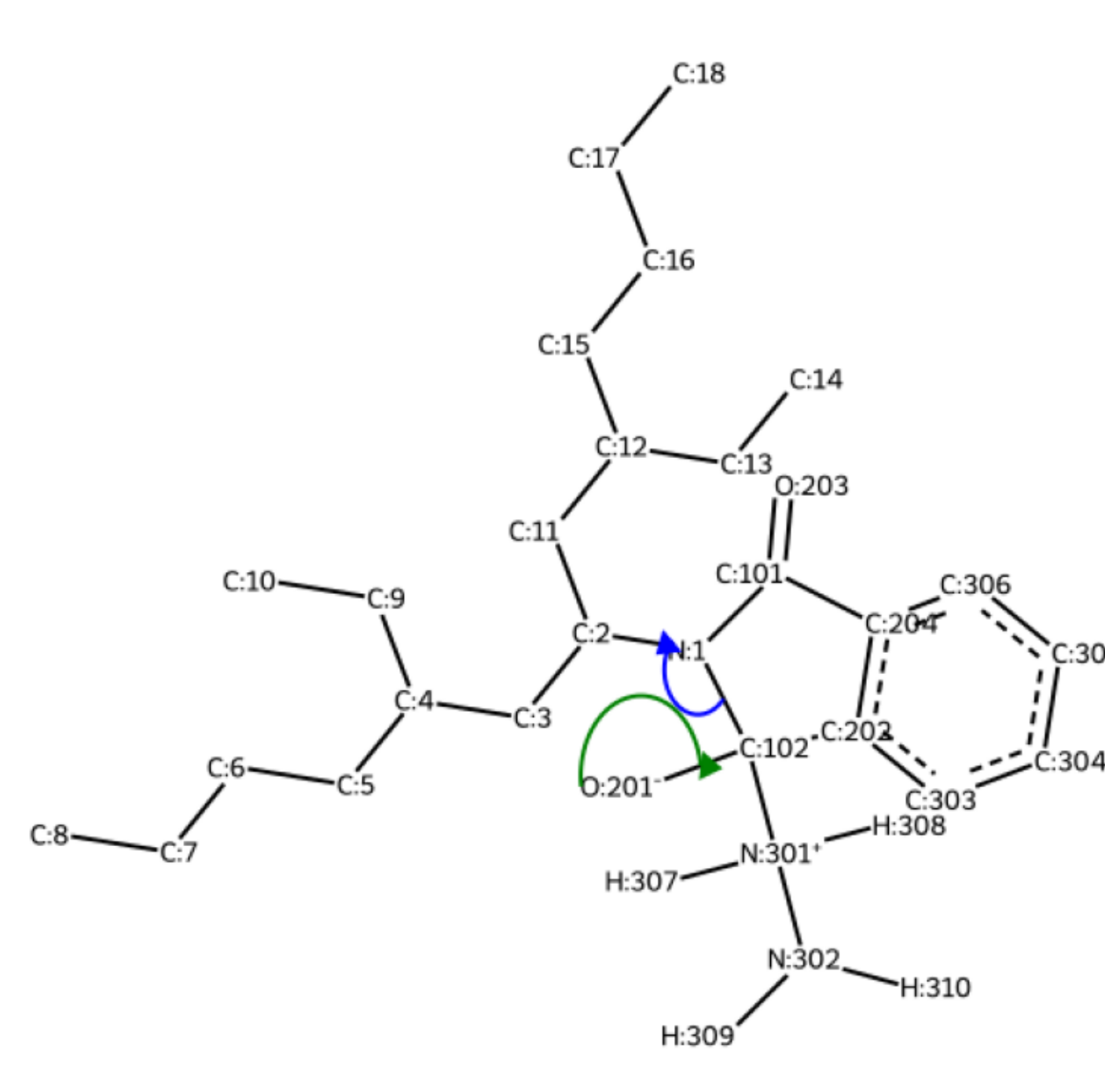
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

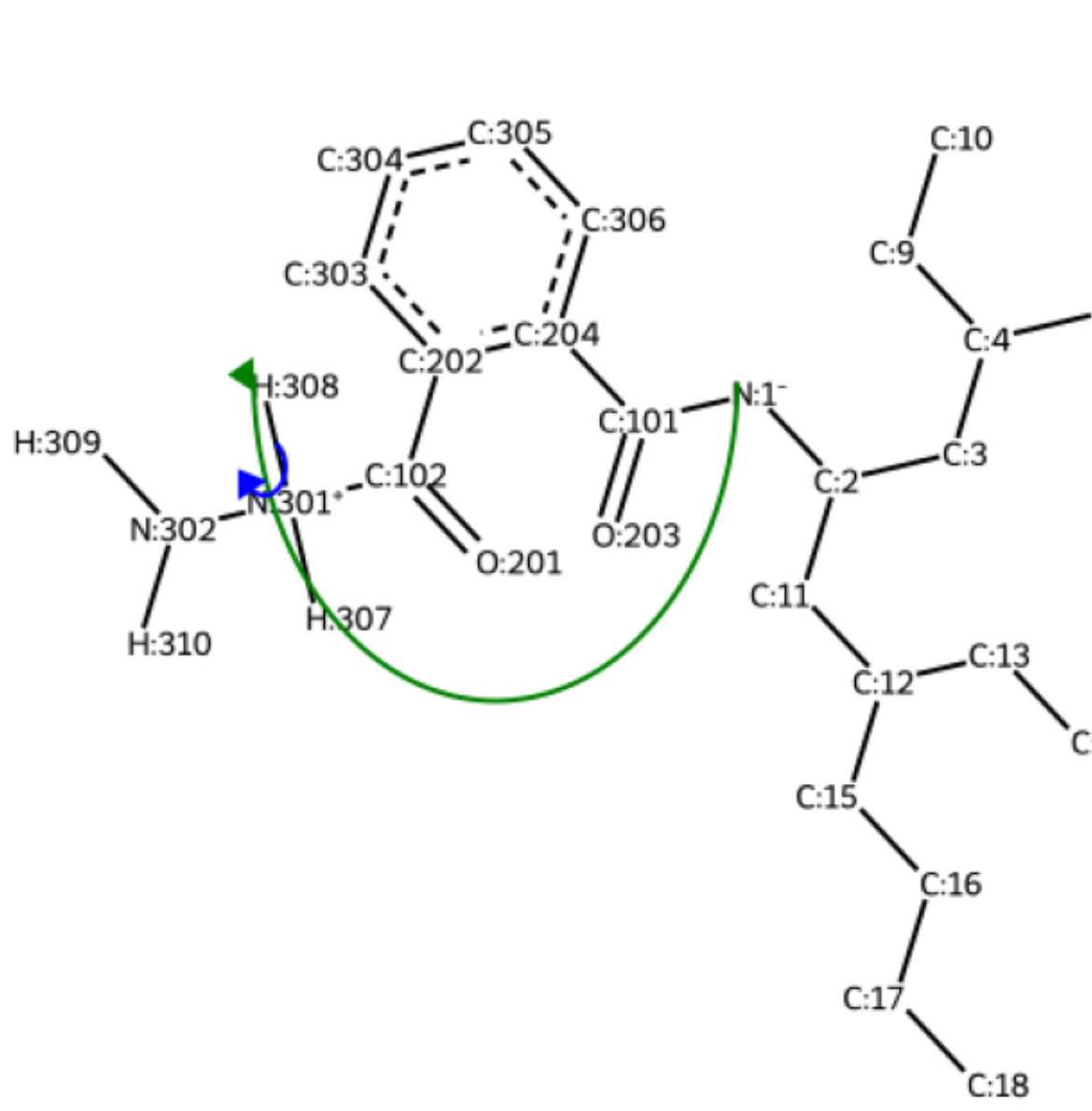
step #1



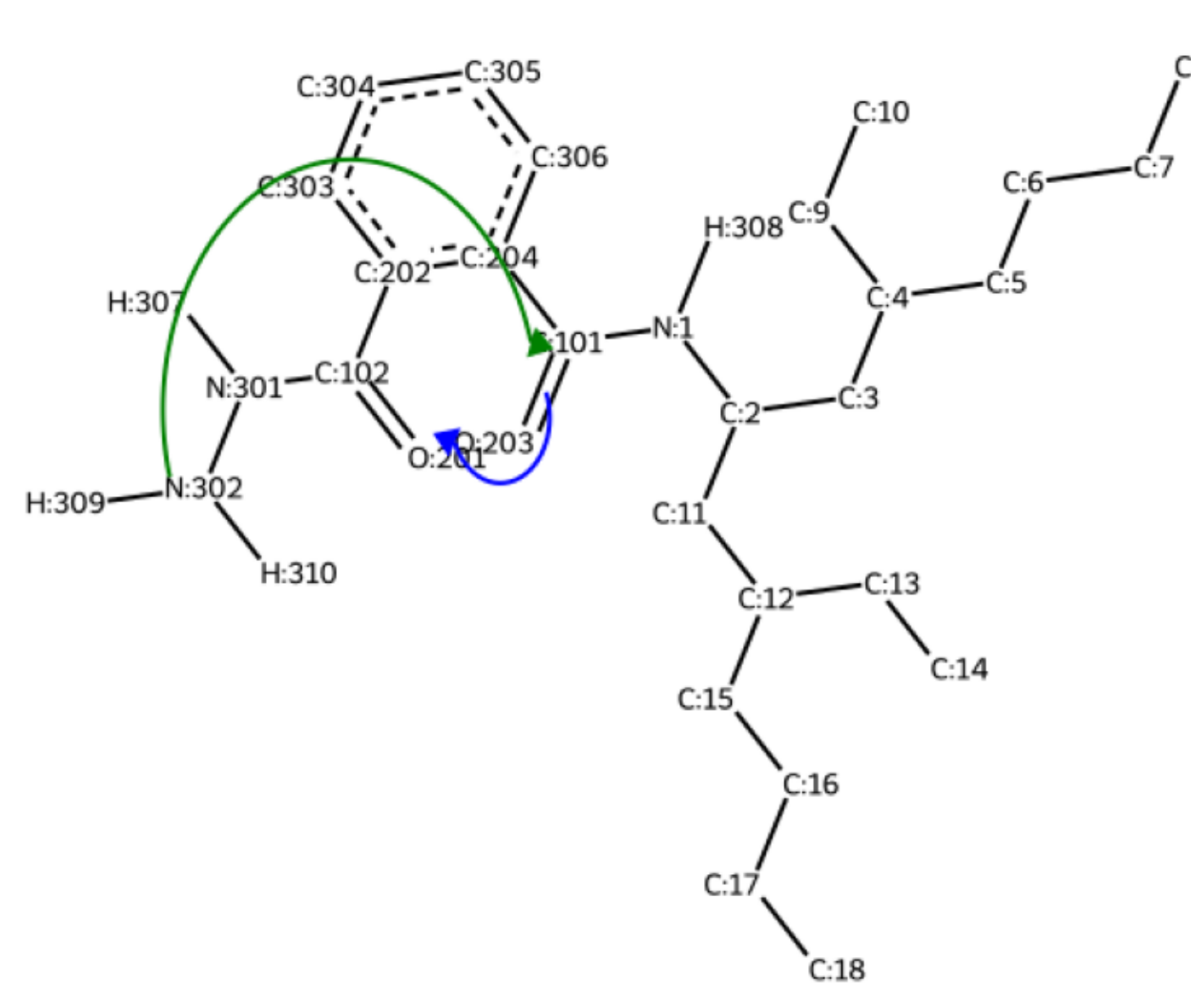
step #2



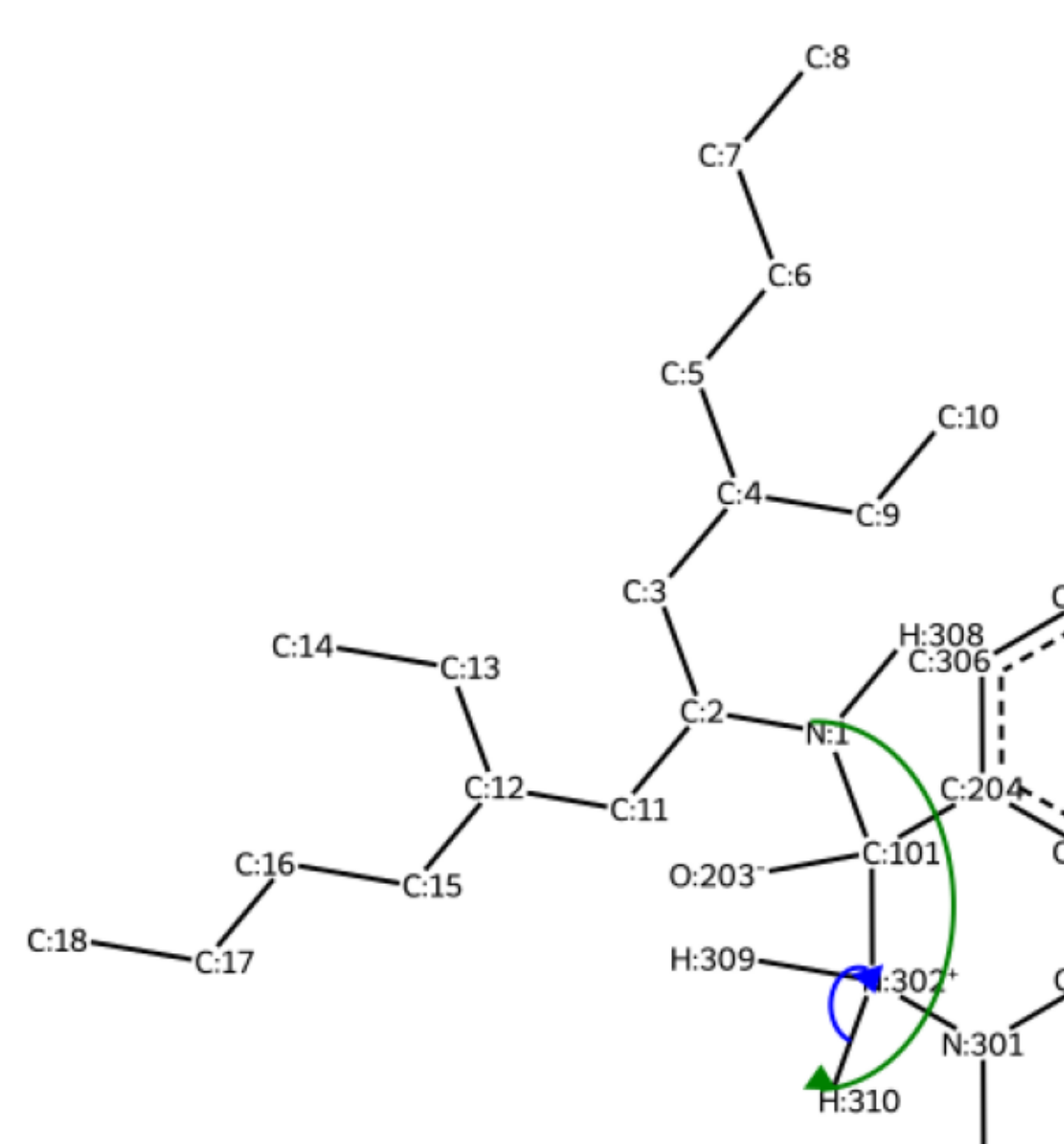
step #3



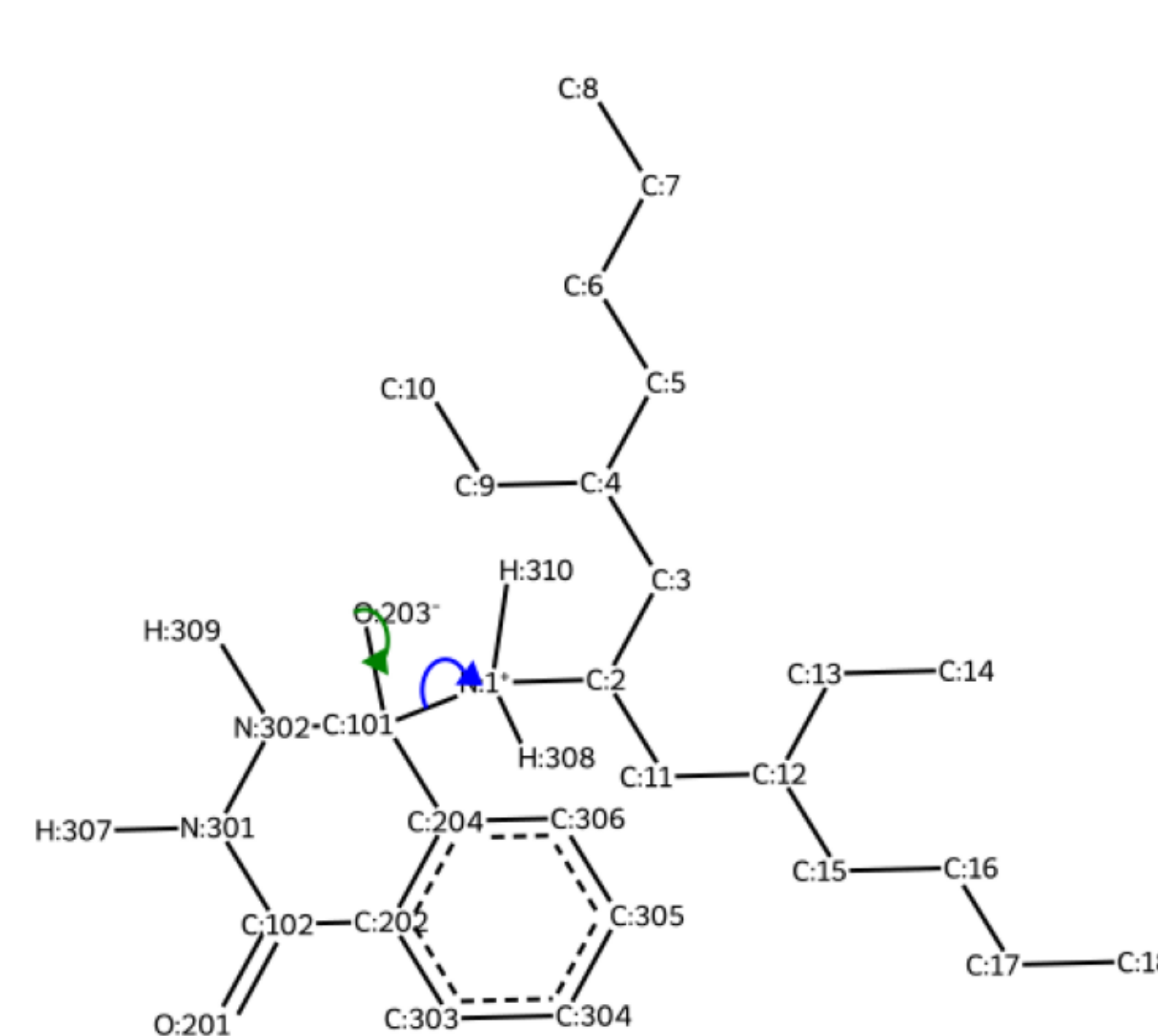
step #4



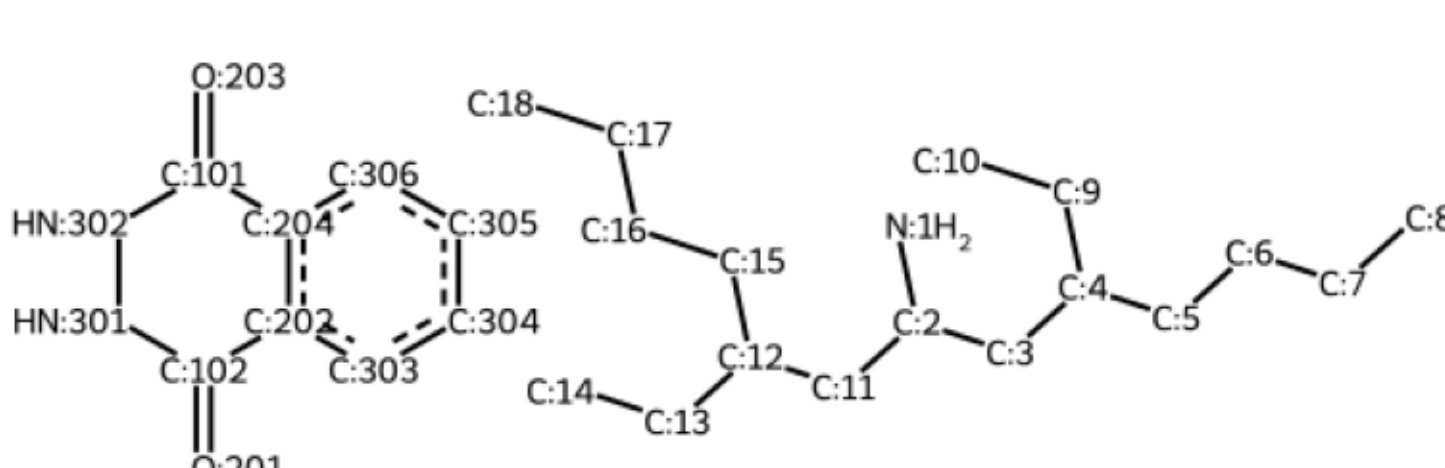
step #5



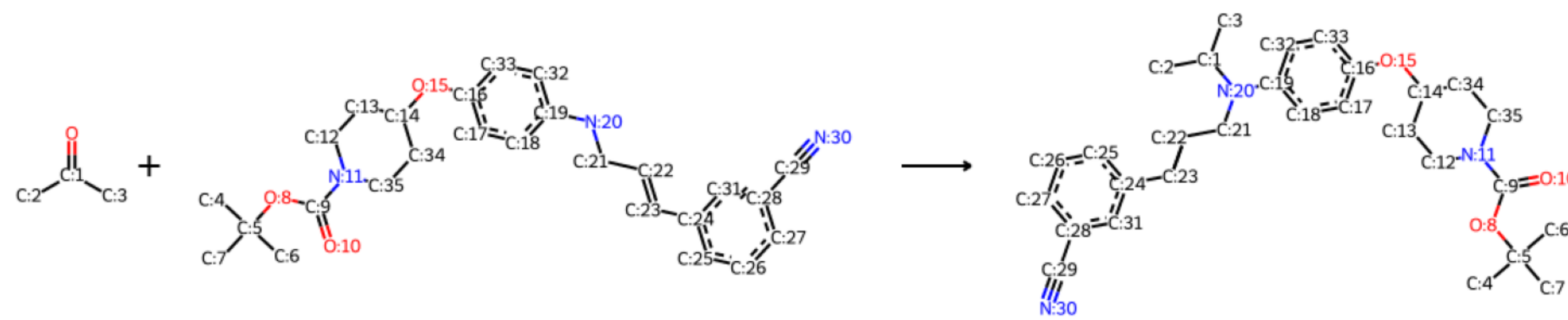
step #6



Product(s)

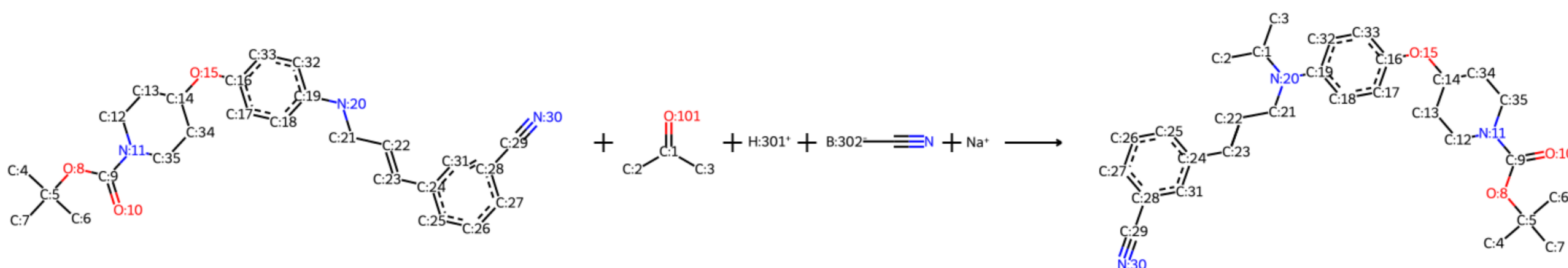


Original reaction
sampled RXN_ID:71)



Identified mechanistic class -
reductive_amination reaction

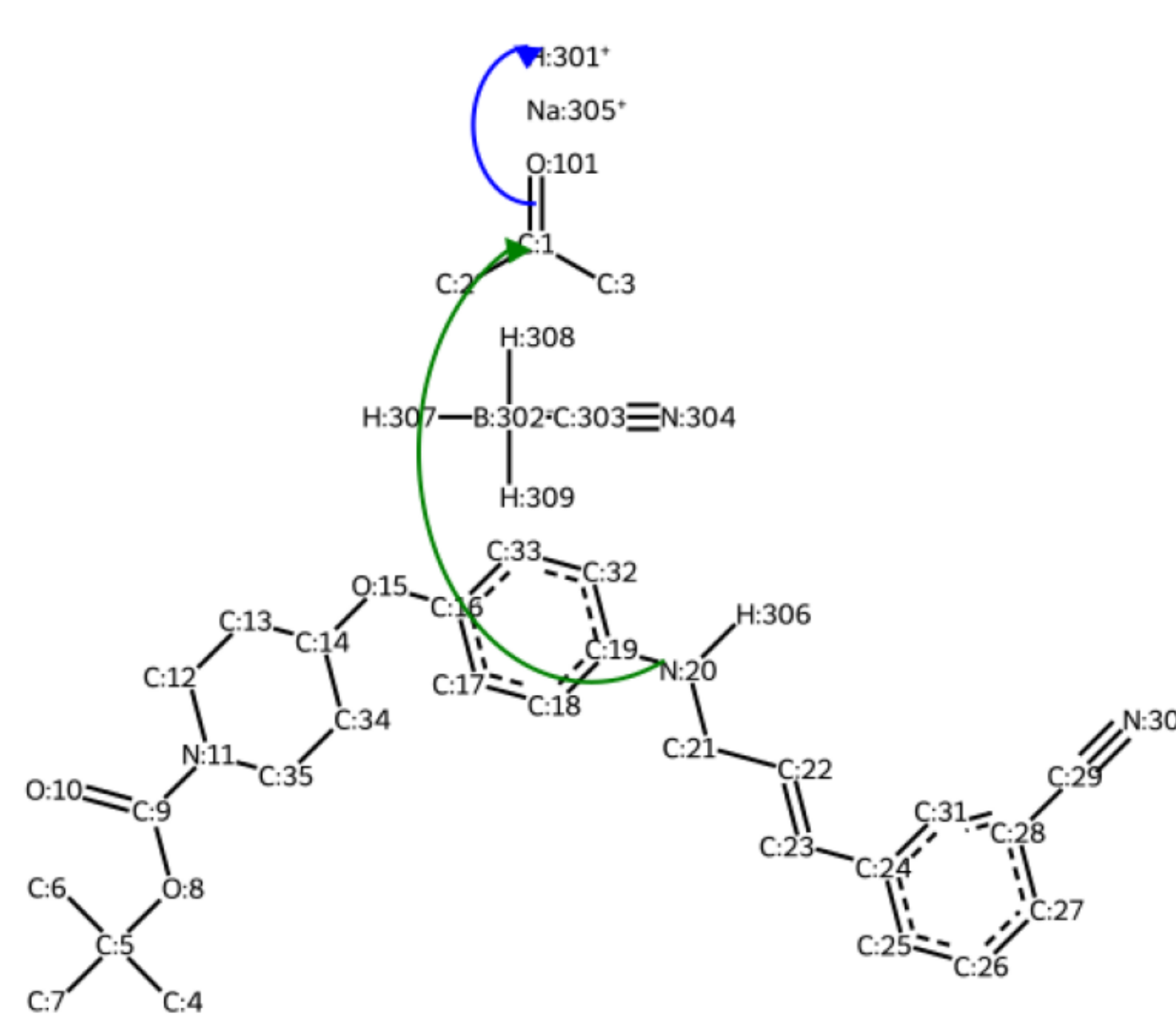
Reaction with missing reagents recovered



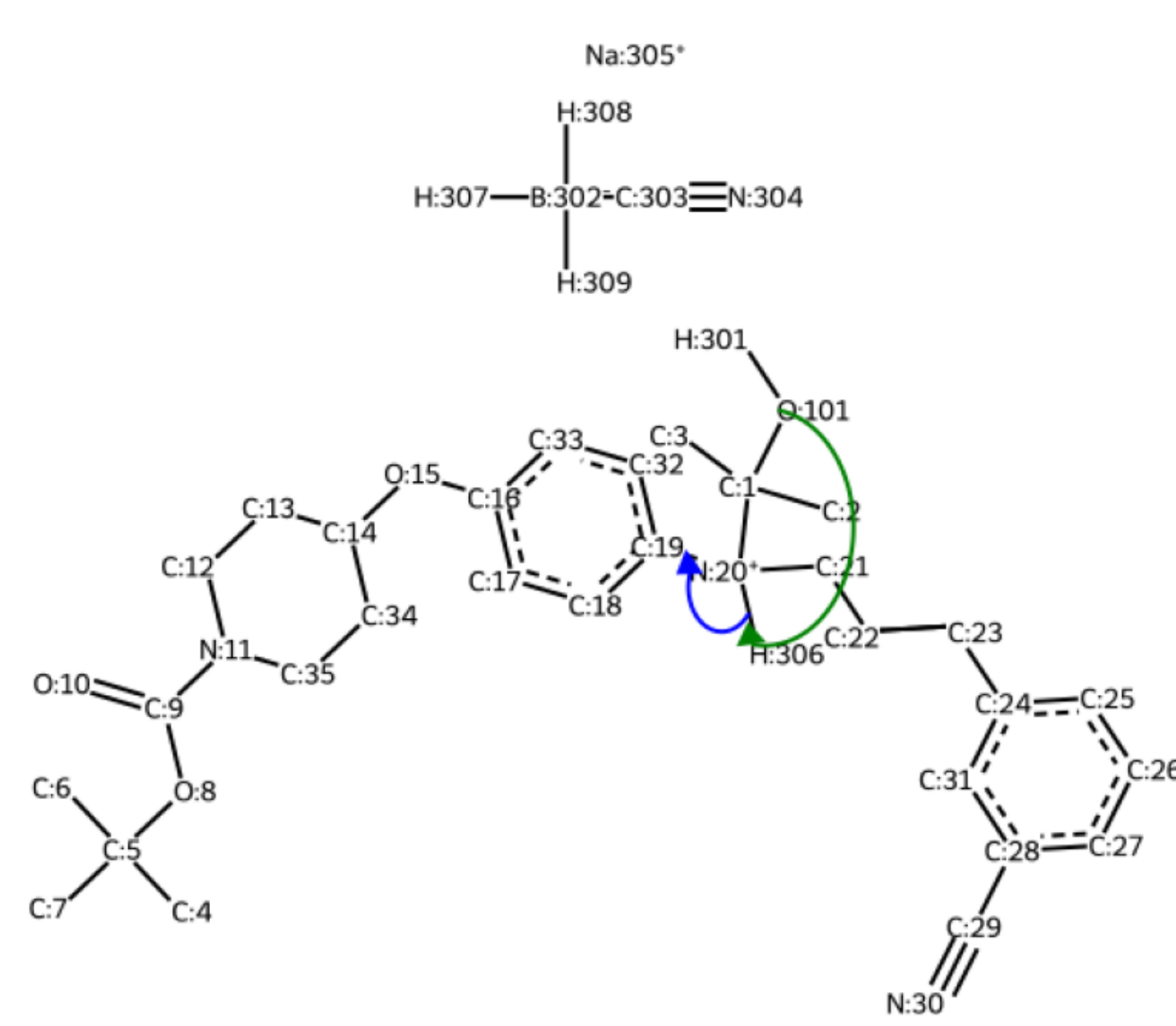
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

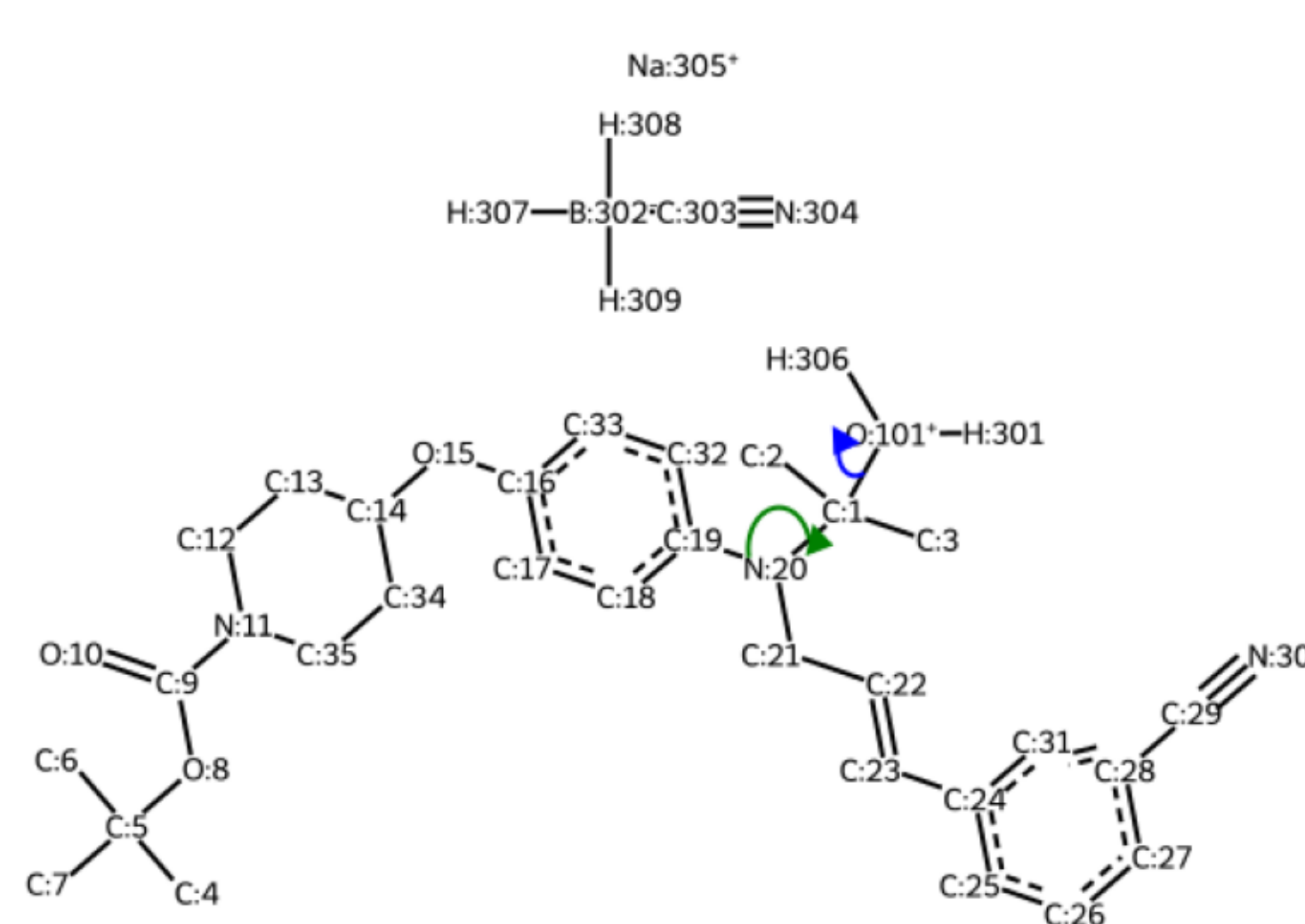
step #1



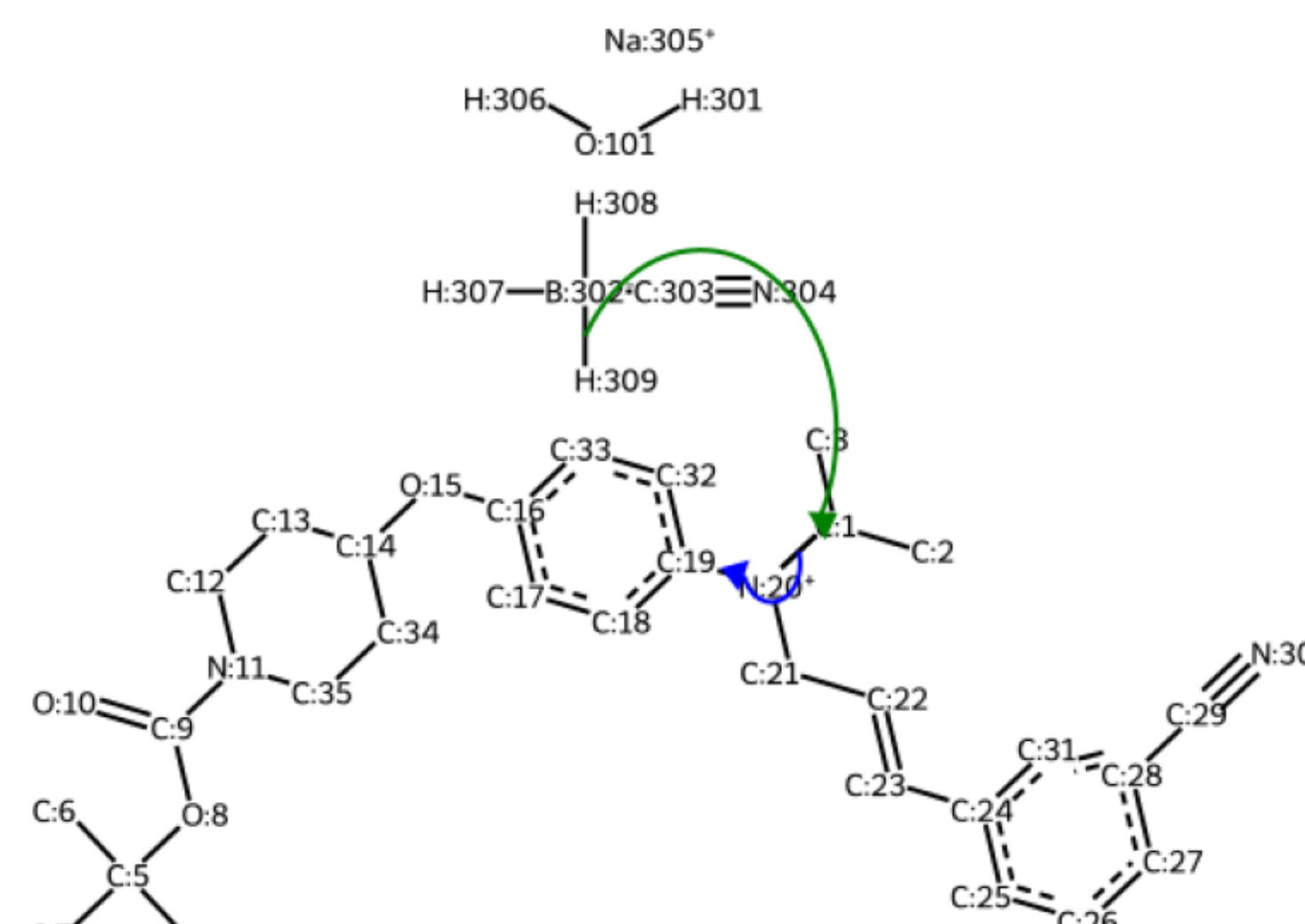
step #2



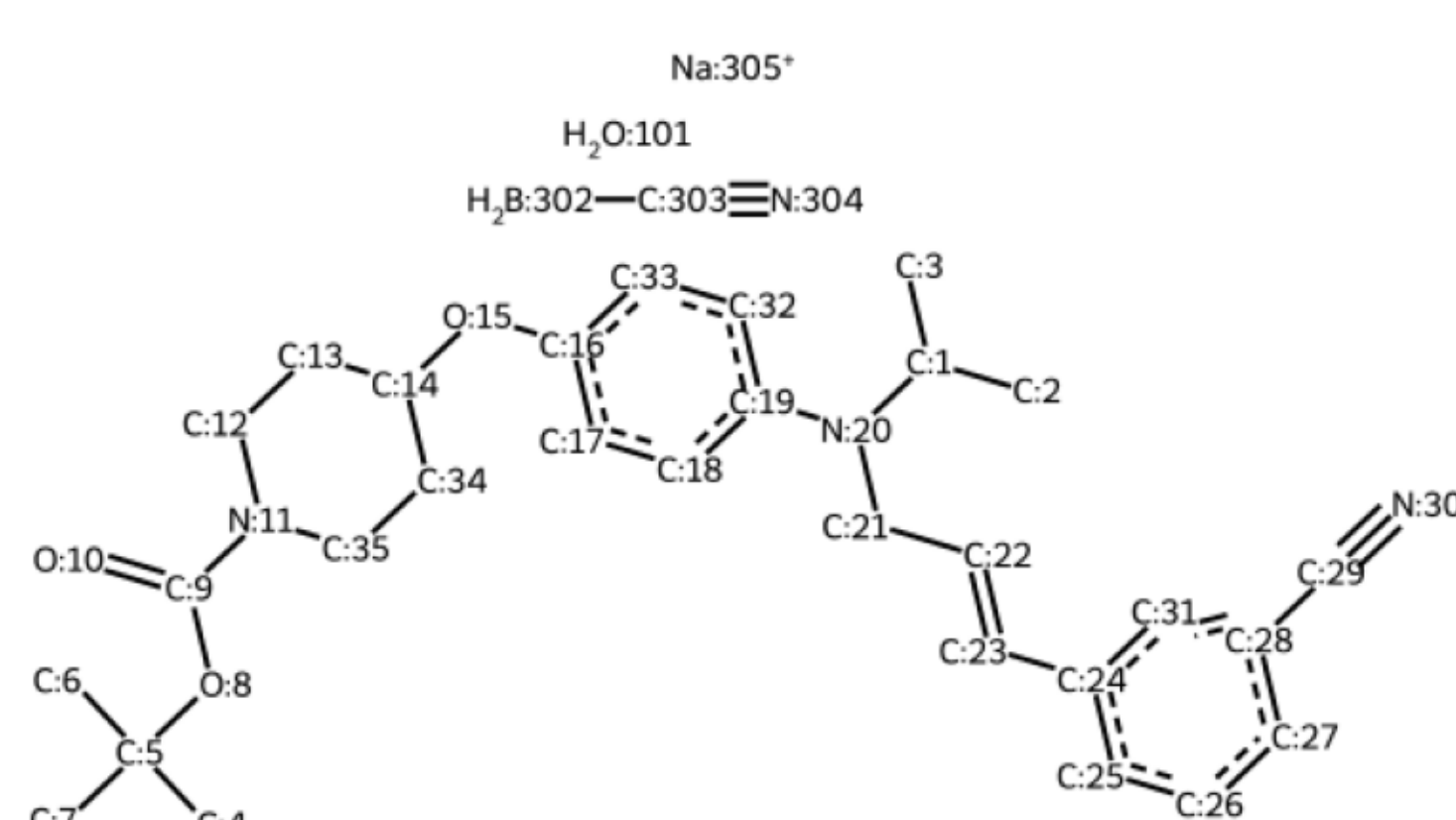
step #3



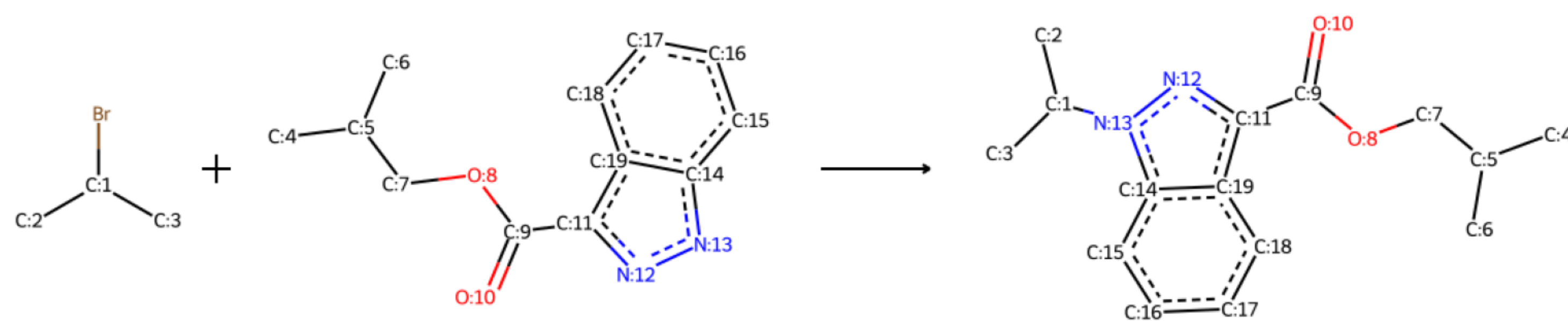
step #4



Product(s)

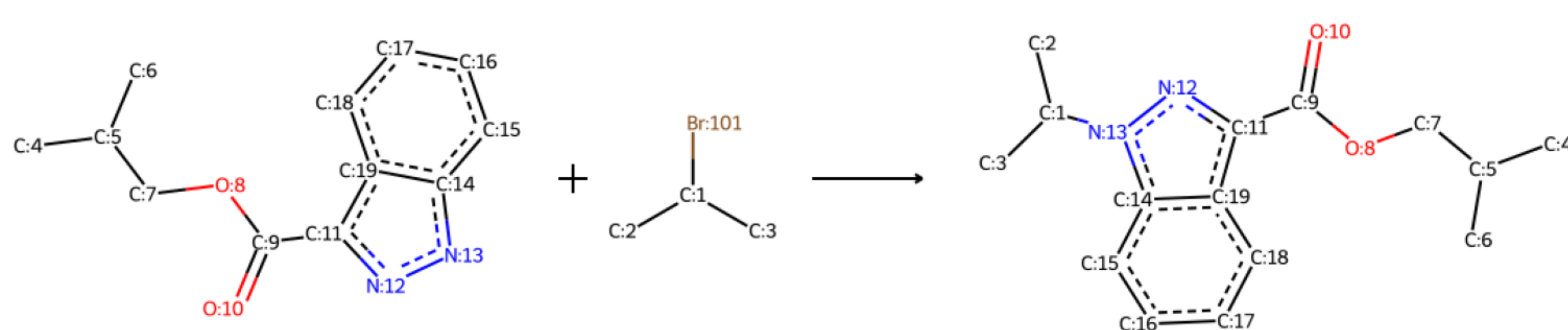


Original reaction sampled RXN_ID:72)



Identified mechanistic class -
SN2 reaction

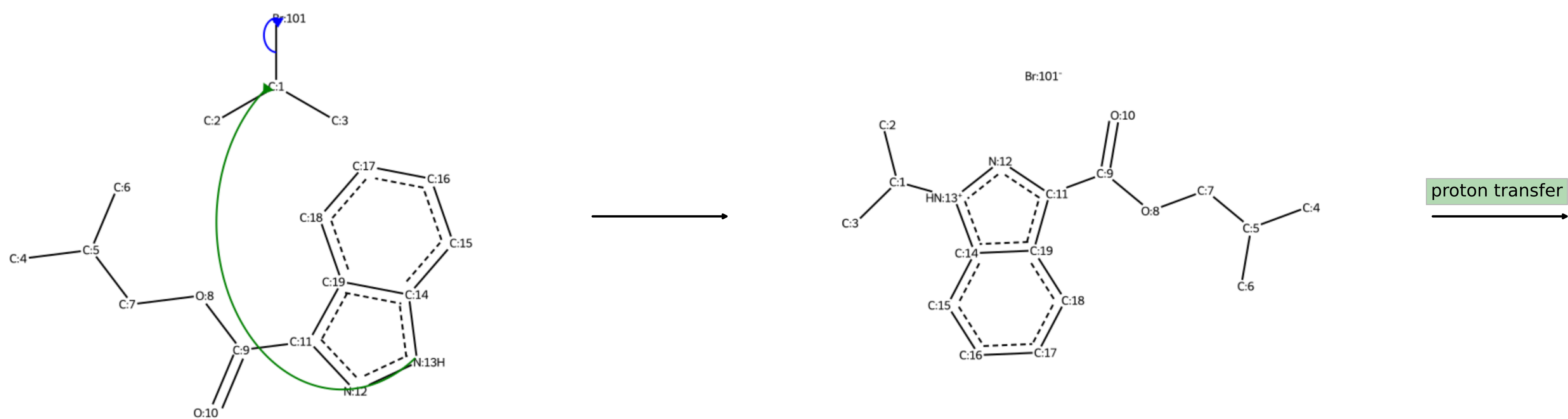
Reaction with missing reagents recovered



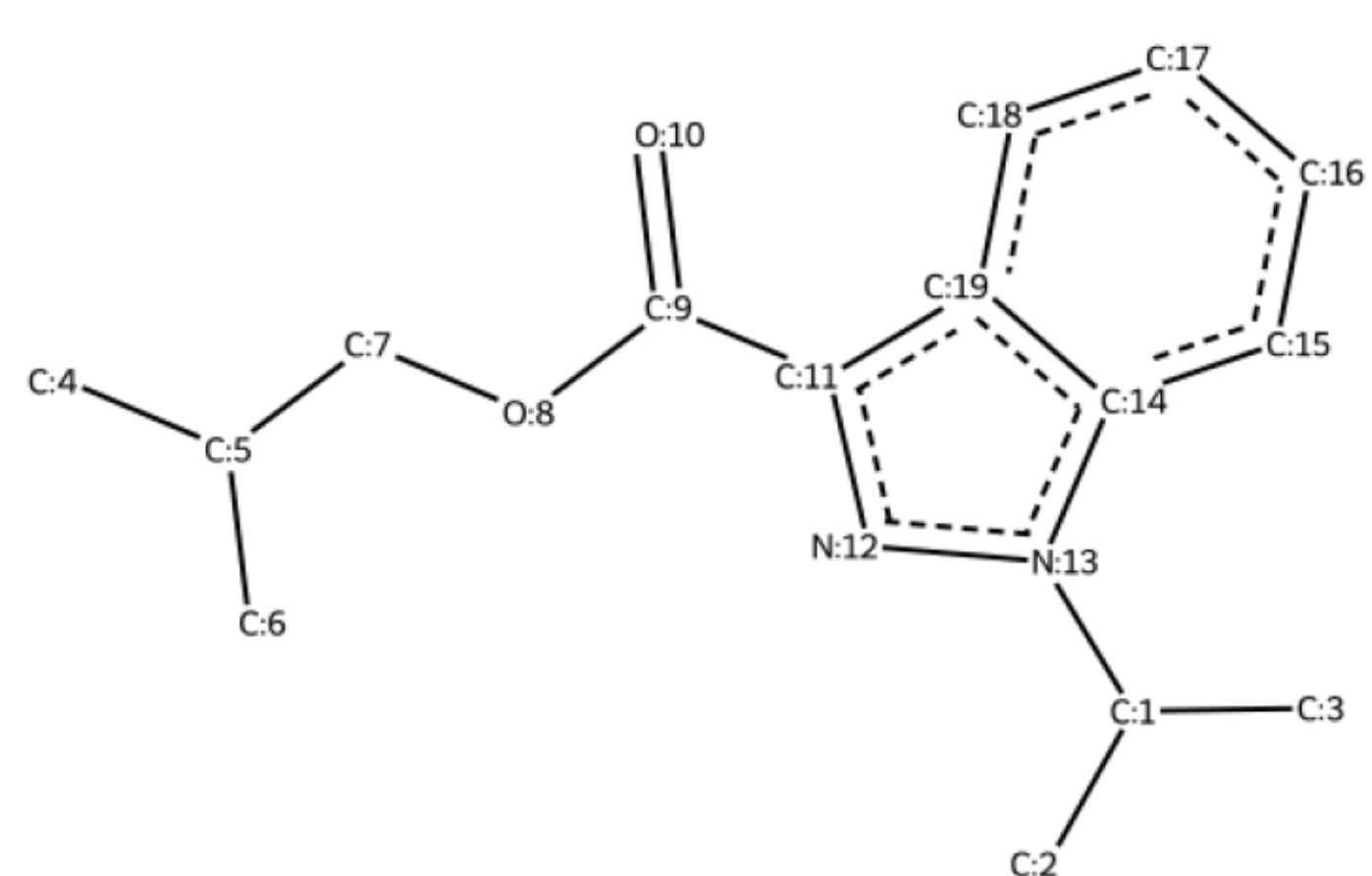
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

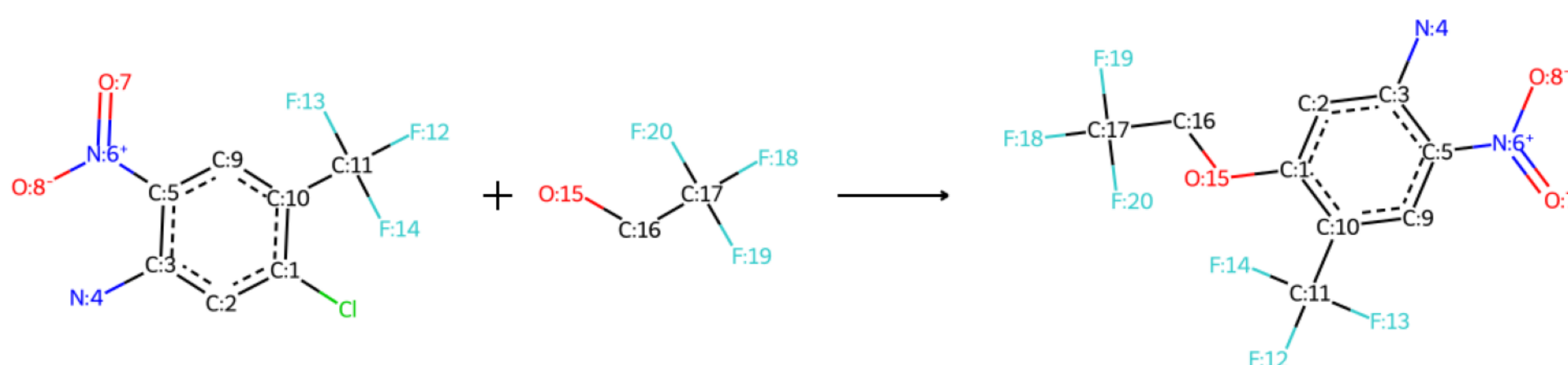
step #1



Product(s)

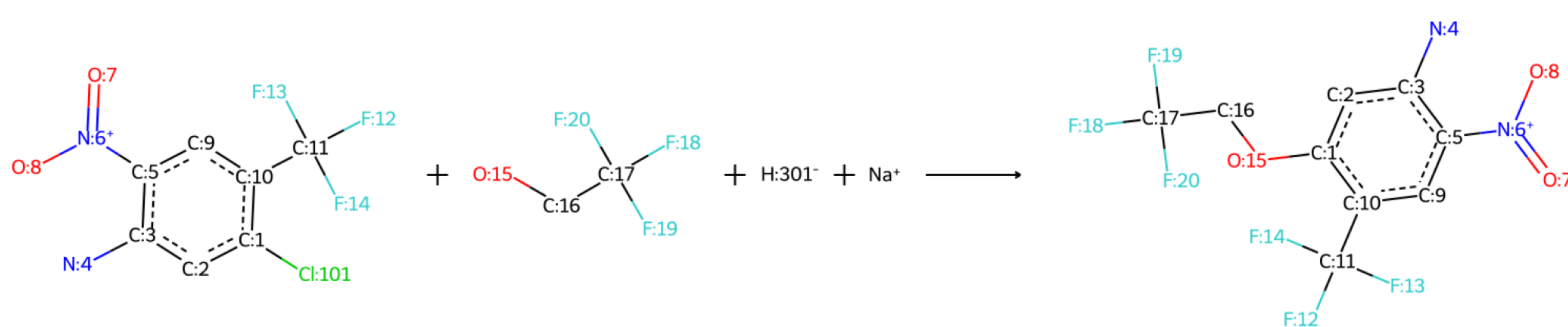


Original reaction
sampled RXN_ID:73)



Identified mechanistic class -
S_NAr_{alco(thi)ol(para)} reaction

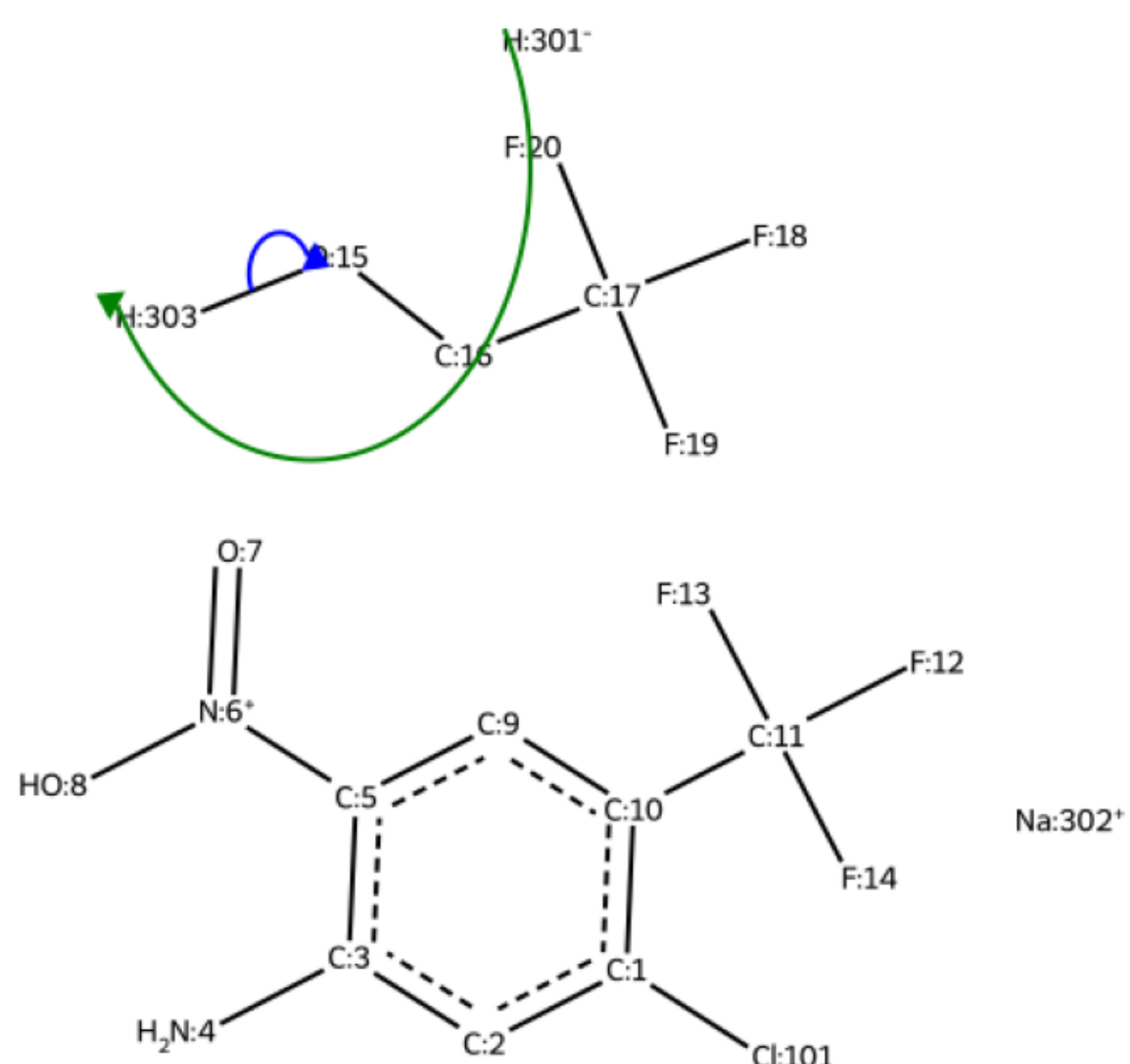
Reaction with missing reagents recovered



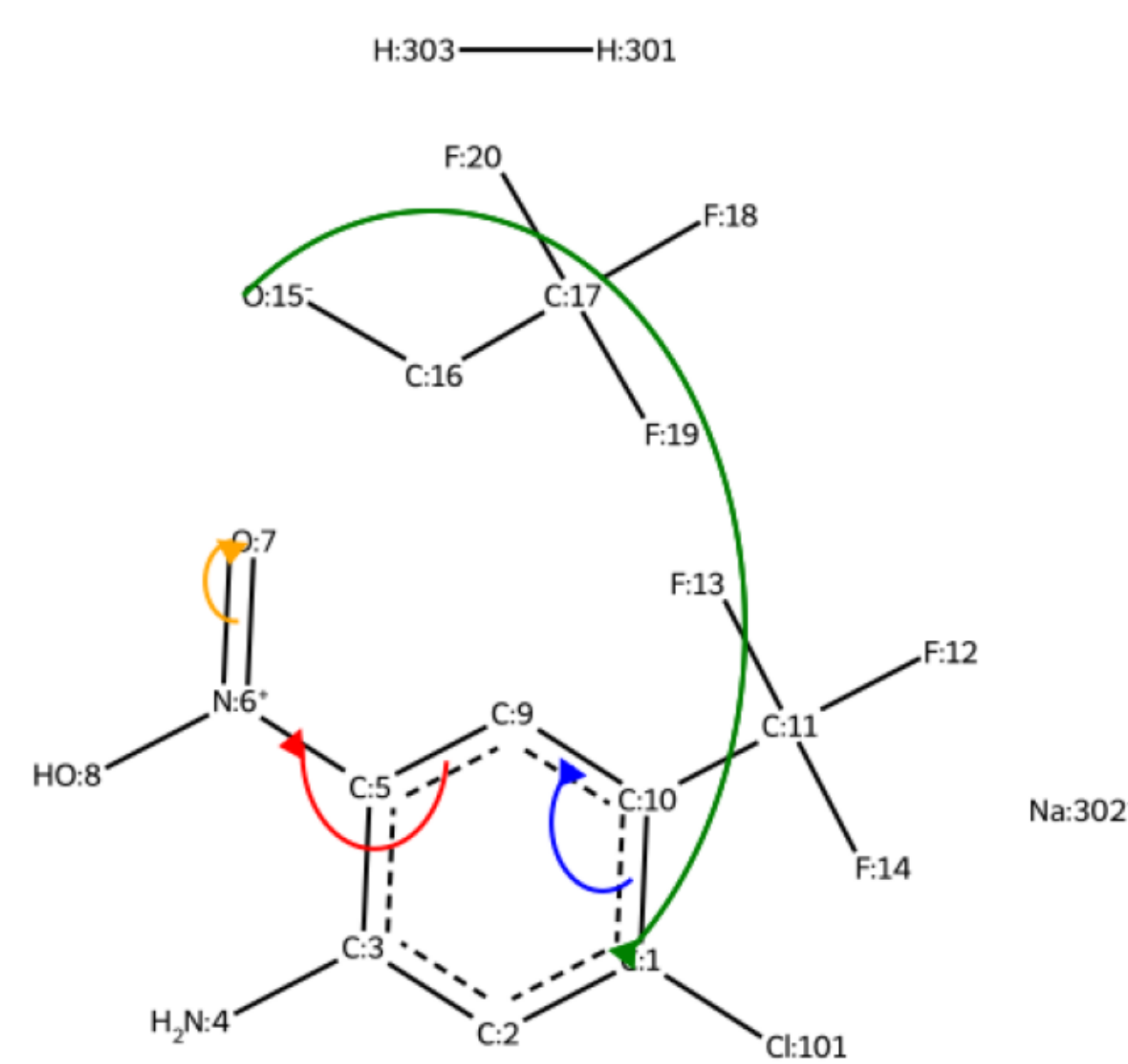
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

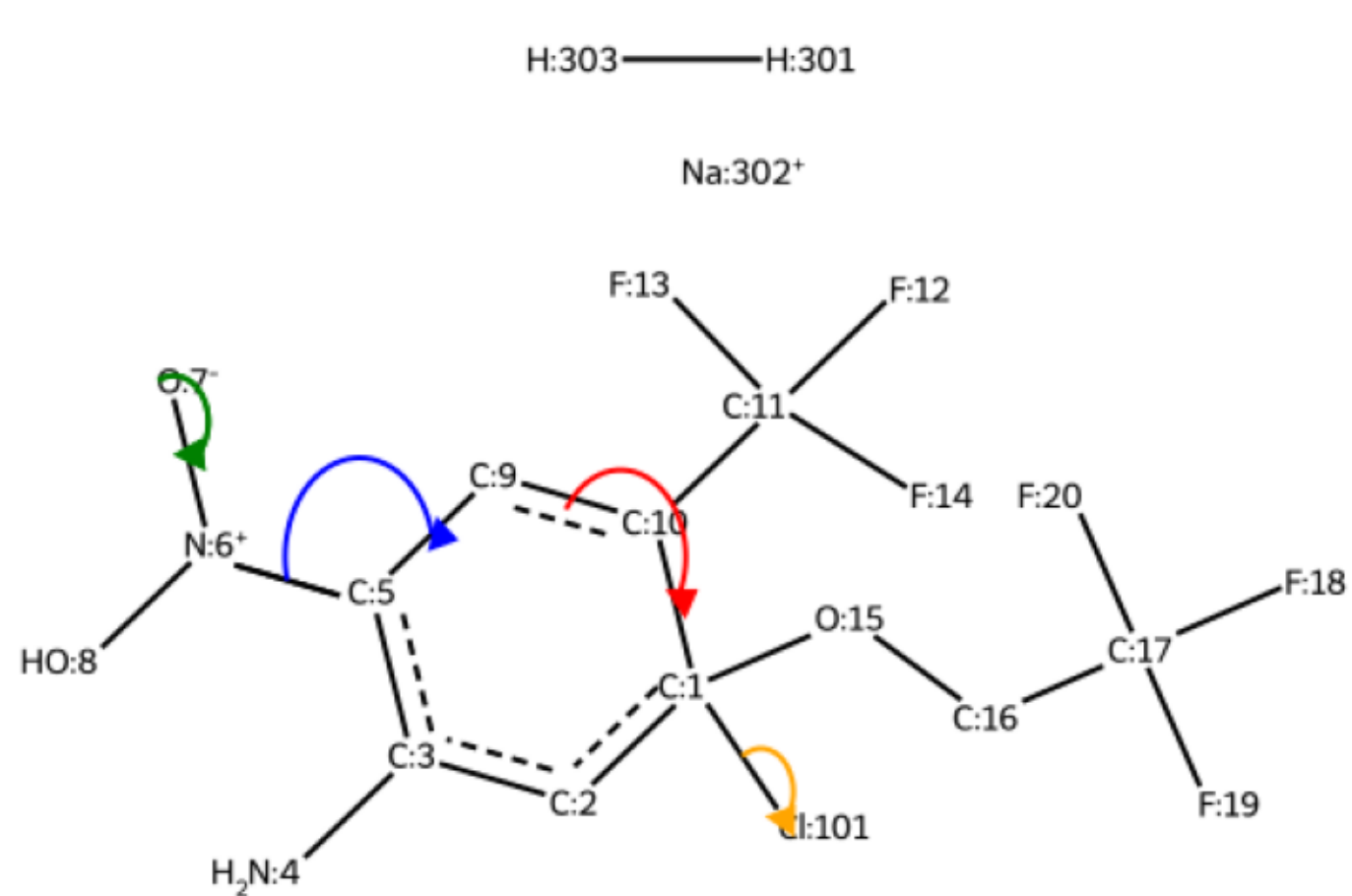
step #1



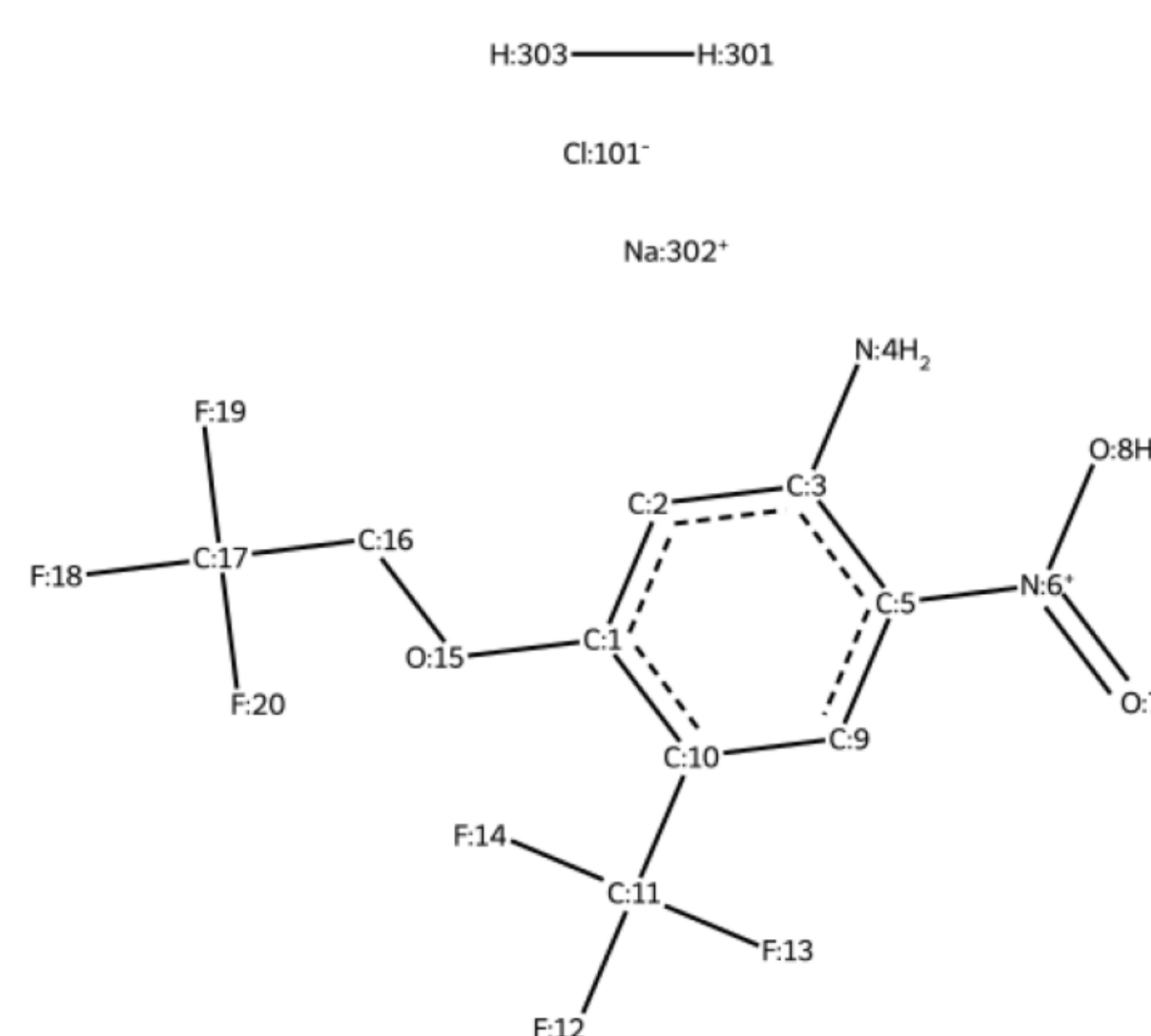
step #2



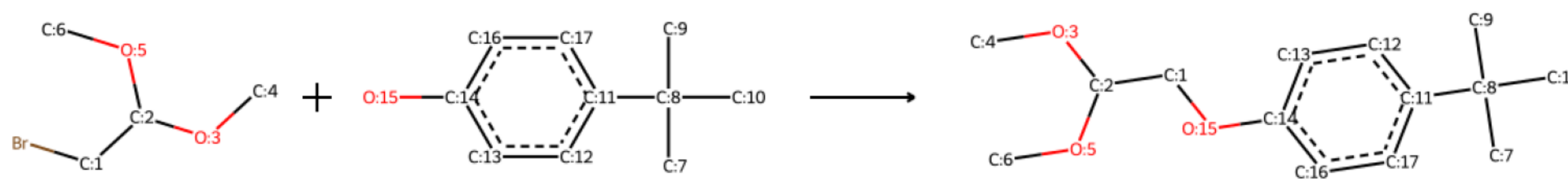
step #3



Product(s)

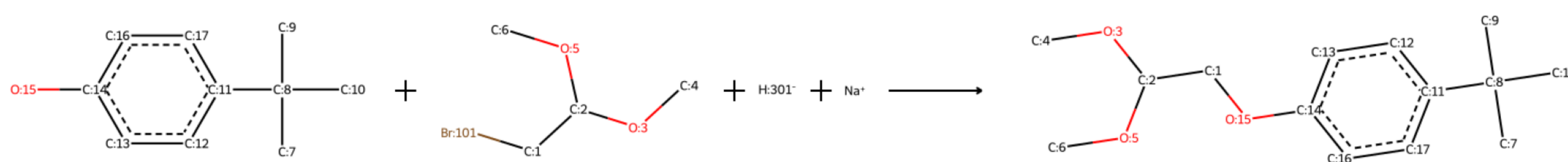


Original reaction
sampled RXN_ID:74)



Identified mechanistic class -
SN2_alcohol(thiol) reaction

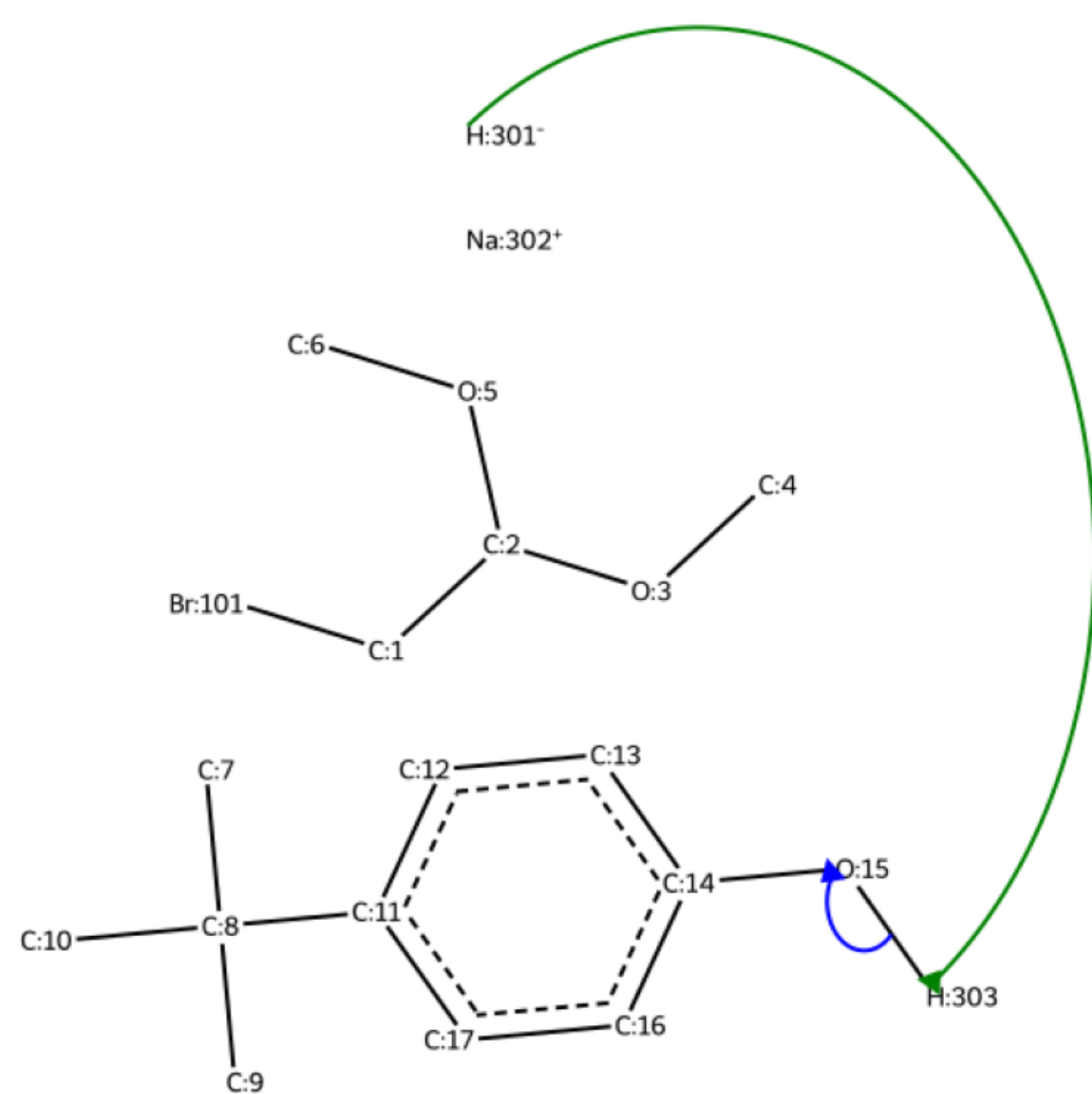
Reaction with missing reagents recovered



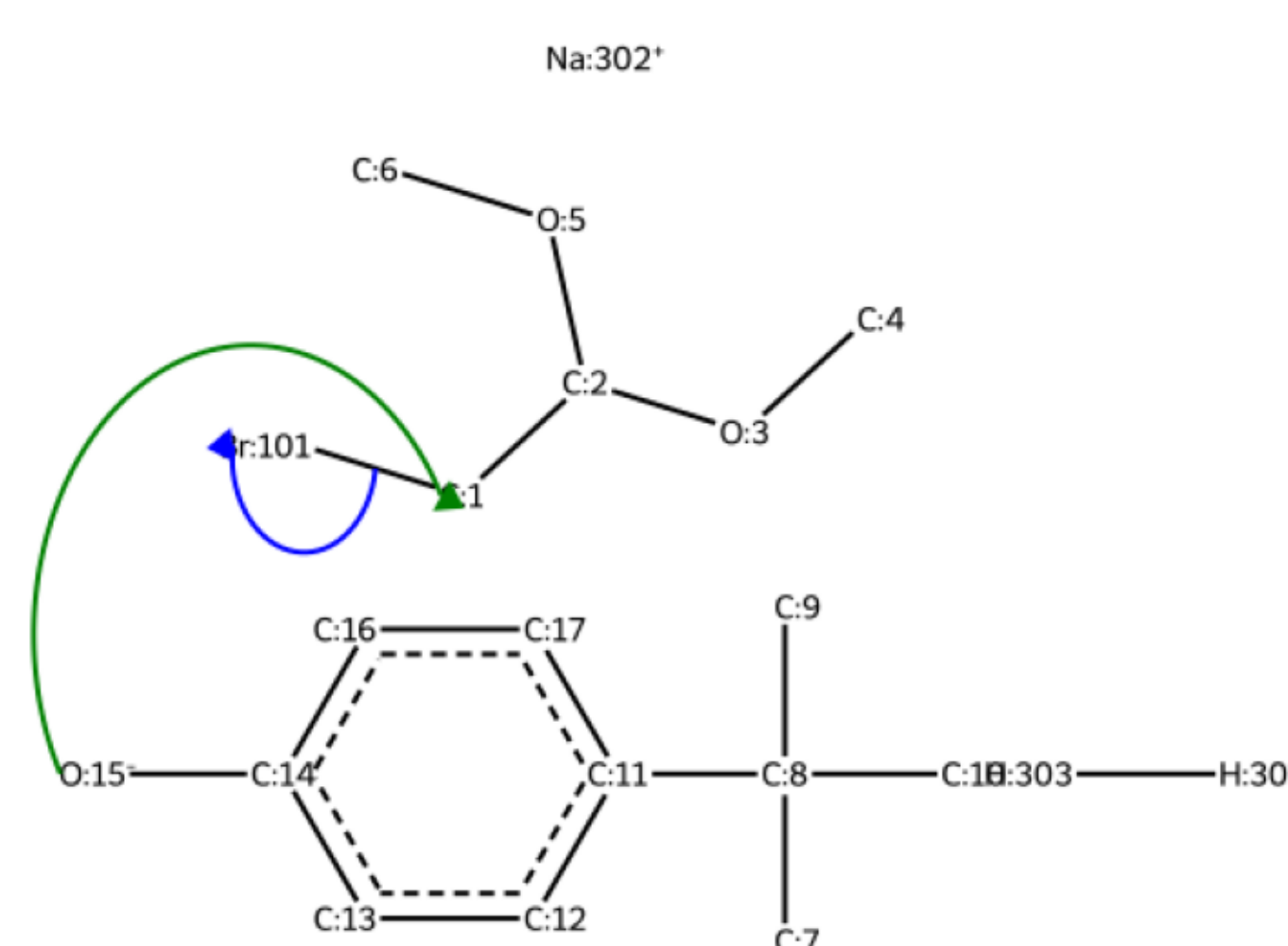
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

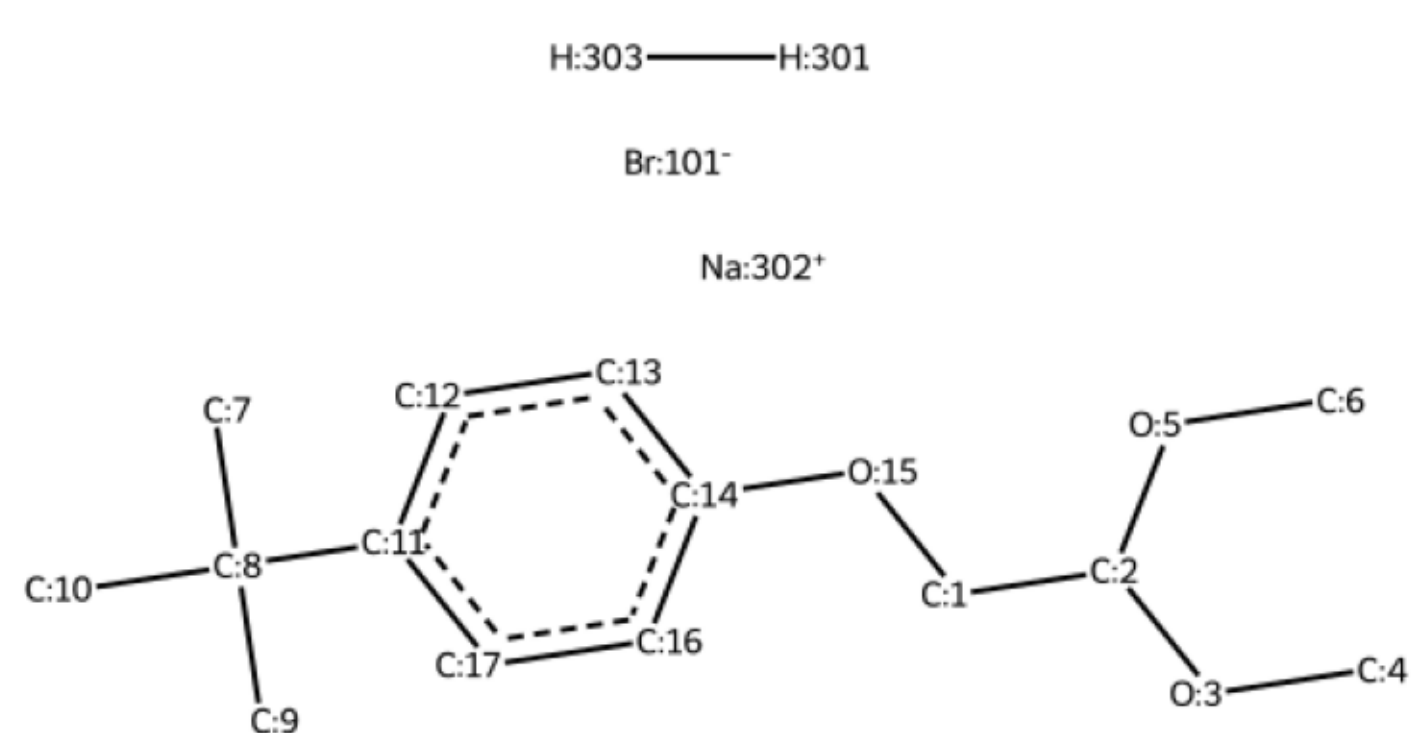
step #1



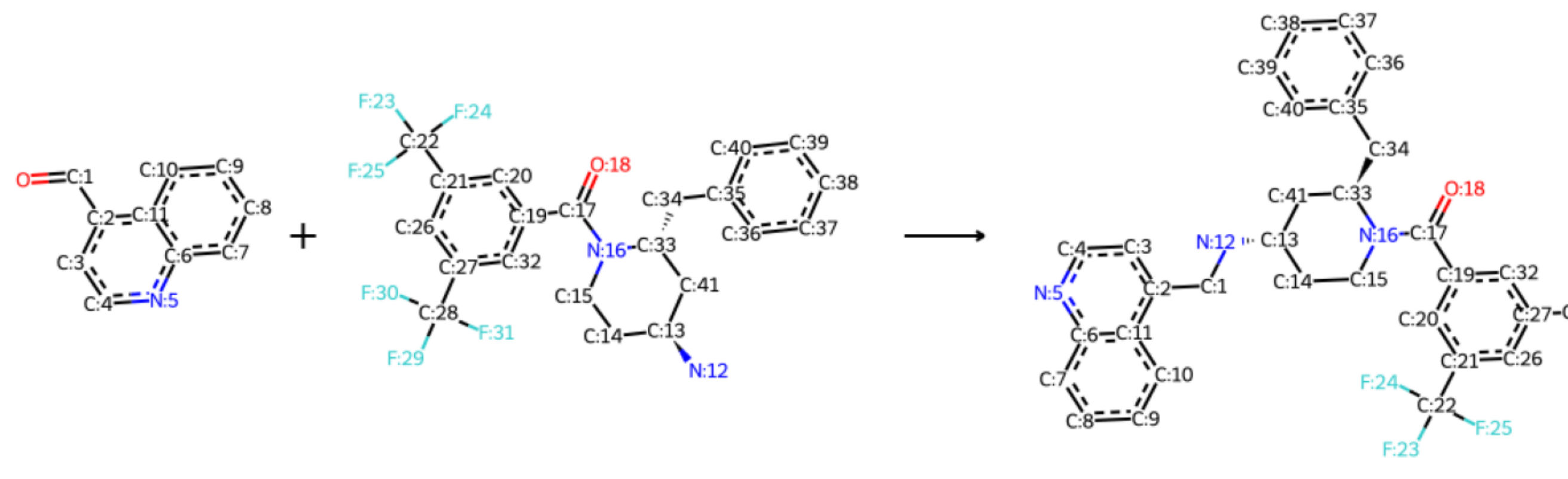
step #2



Product(s)

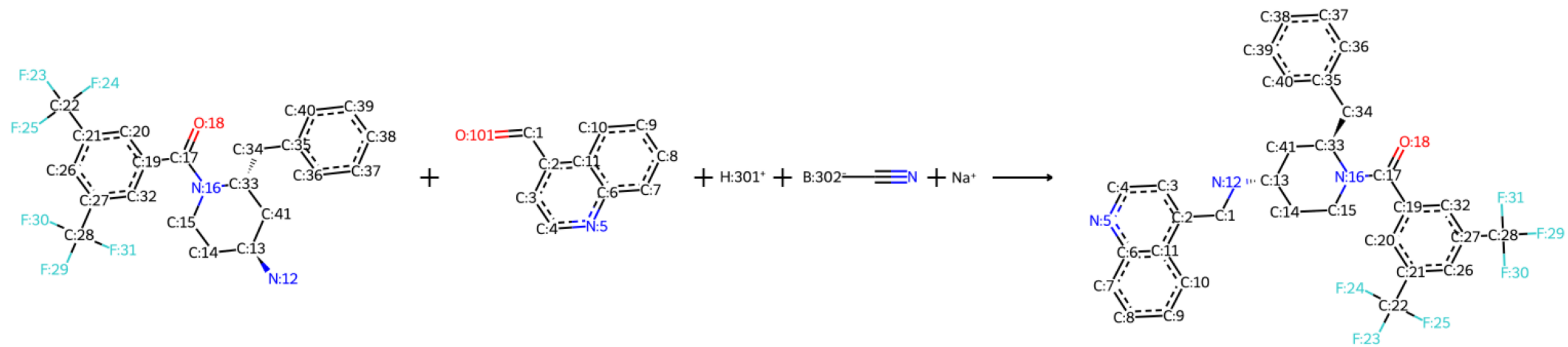


Original reaction
sampled RXN_ID:75)



Identified mechanistic class -
reductive_amination reaction

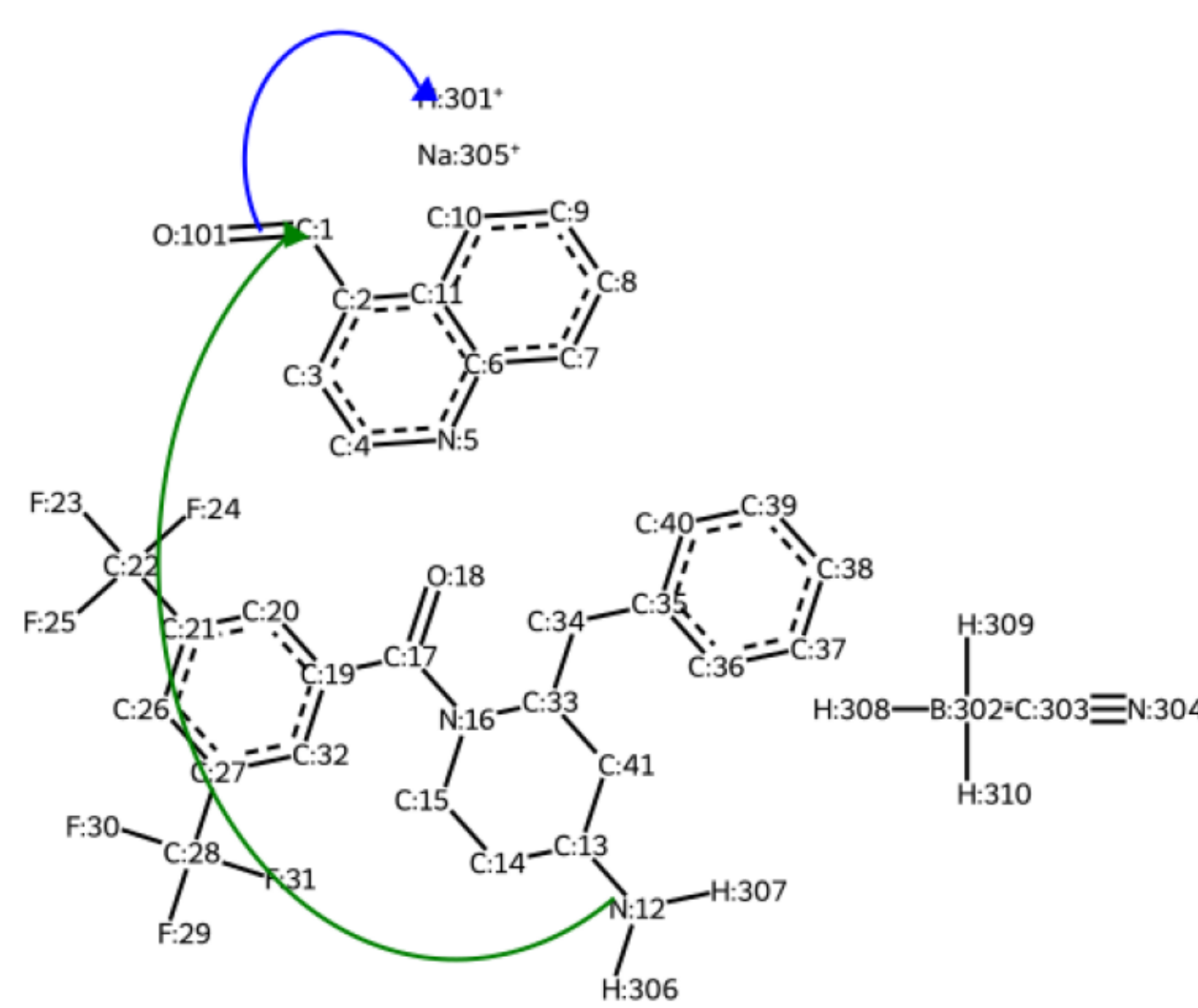
Reaction with missing reagents recovered



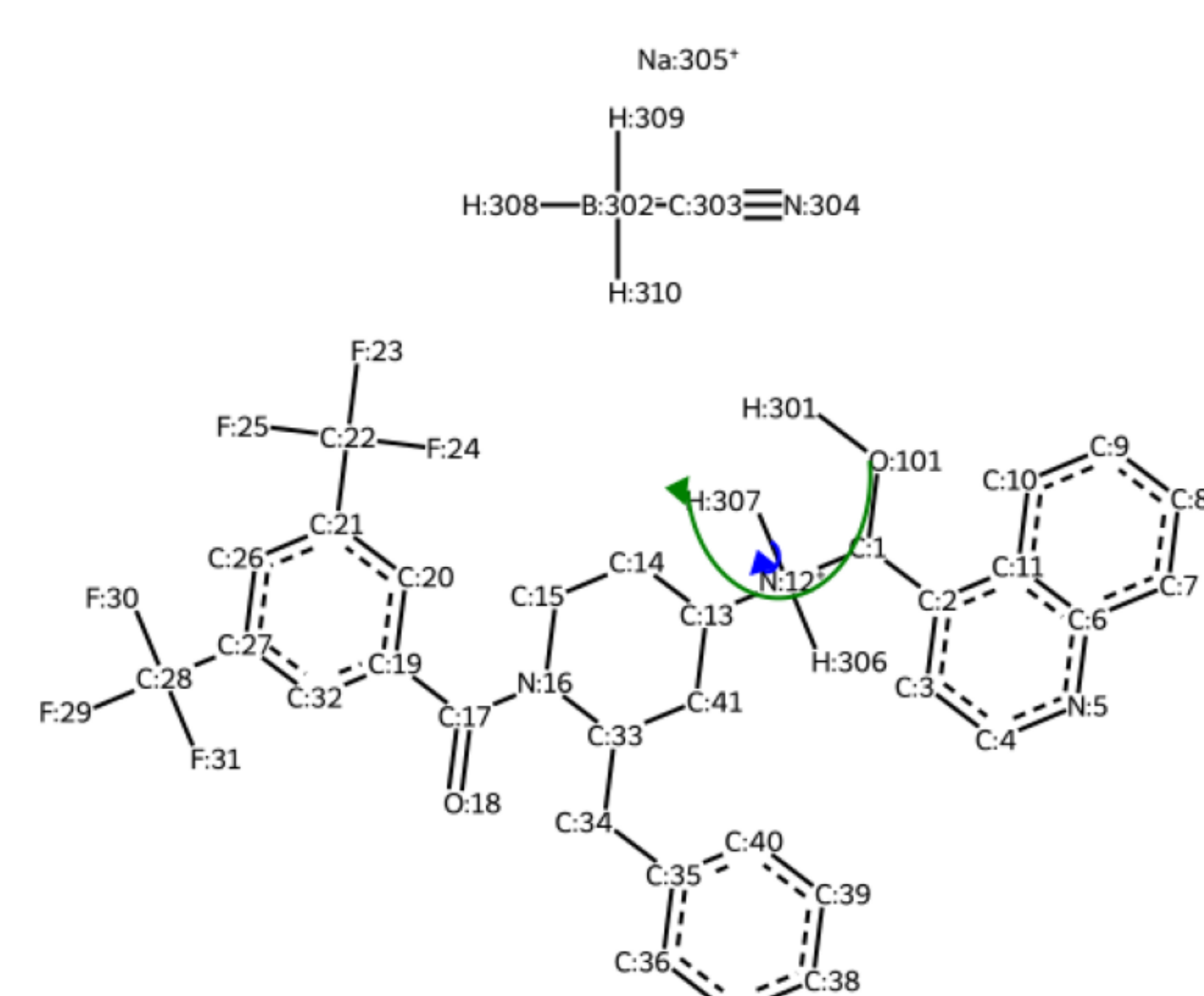
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

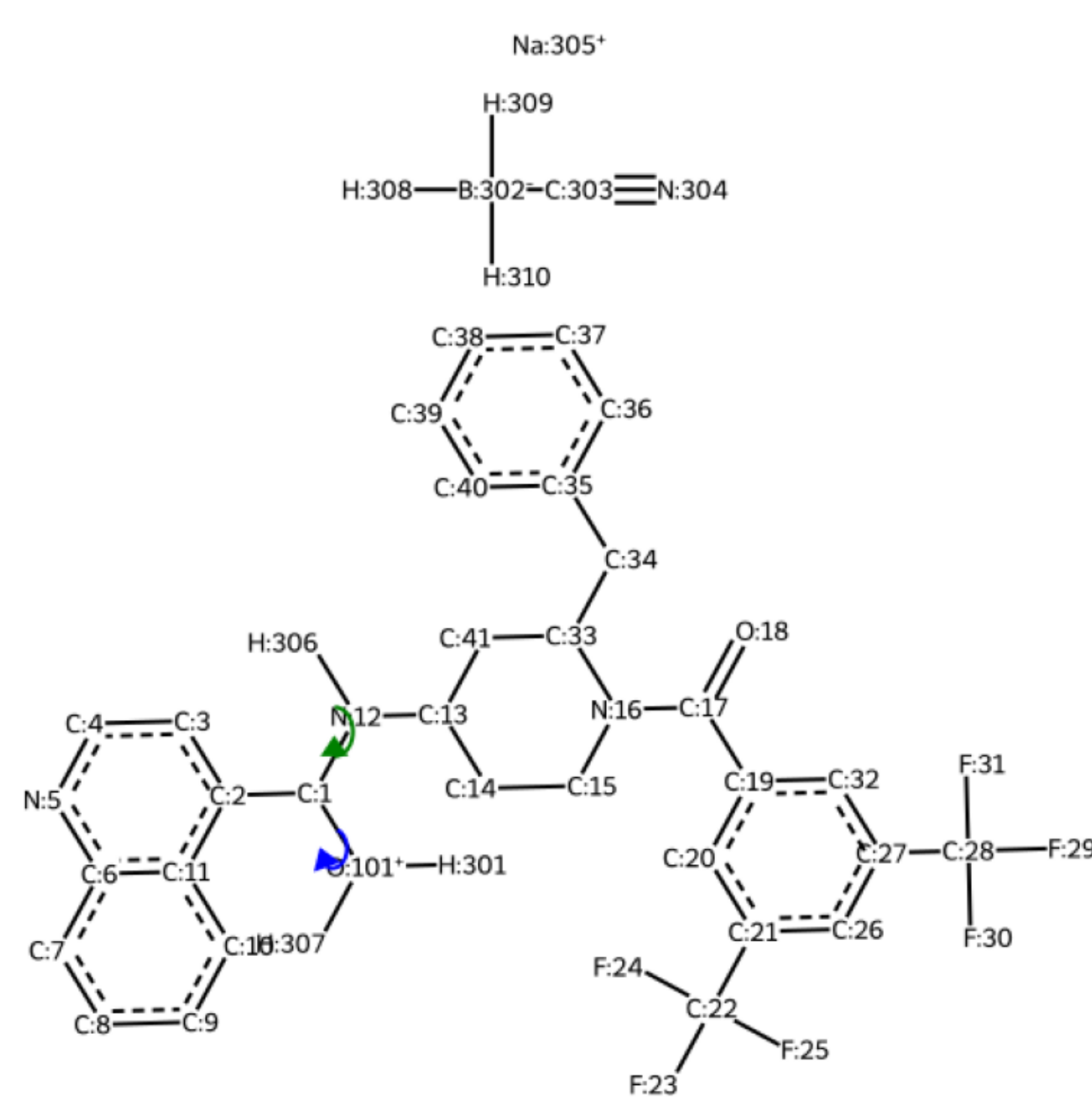
step #1



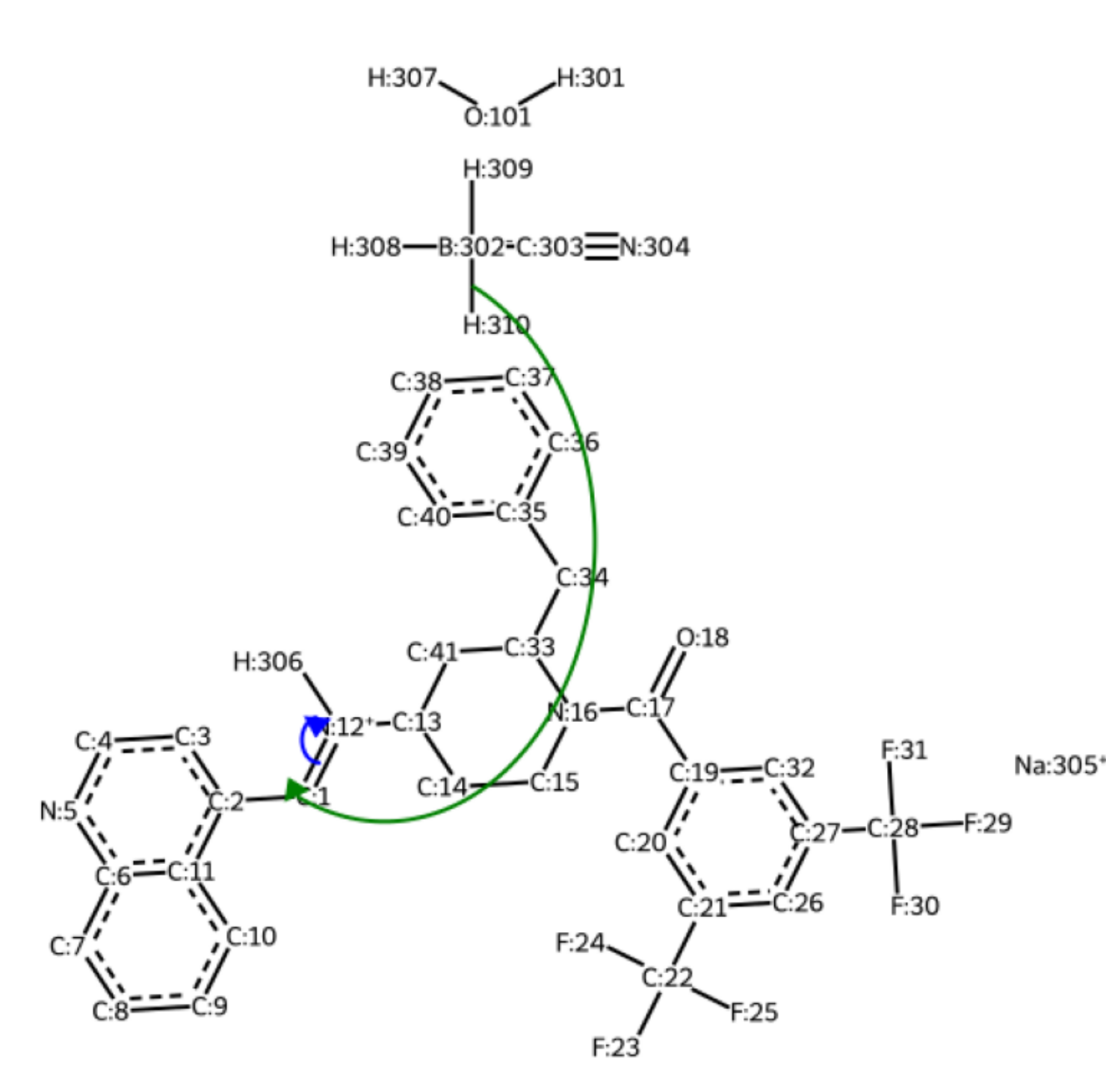
step #2



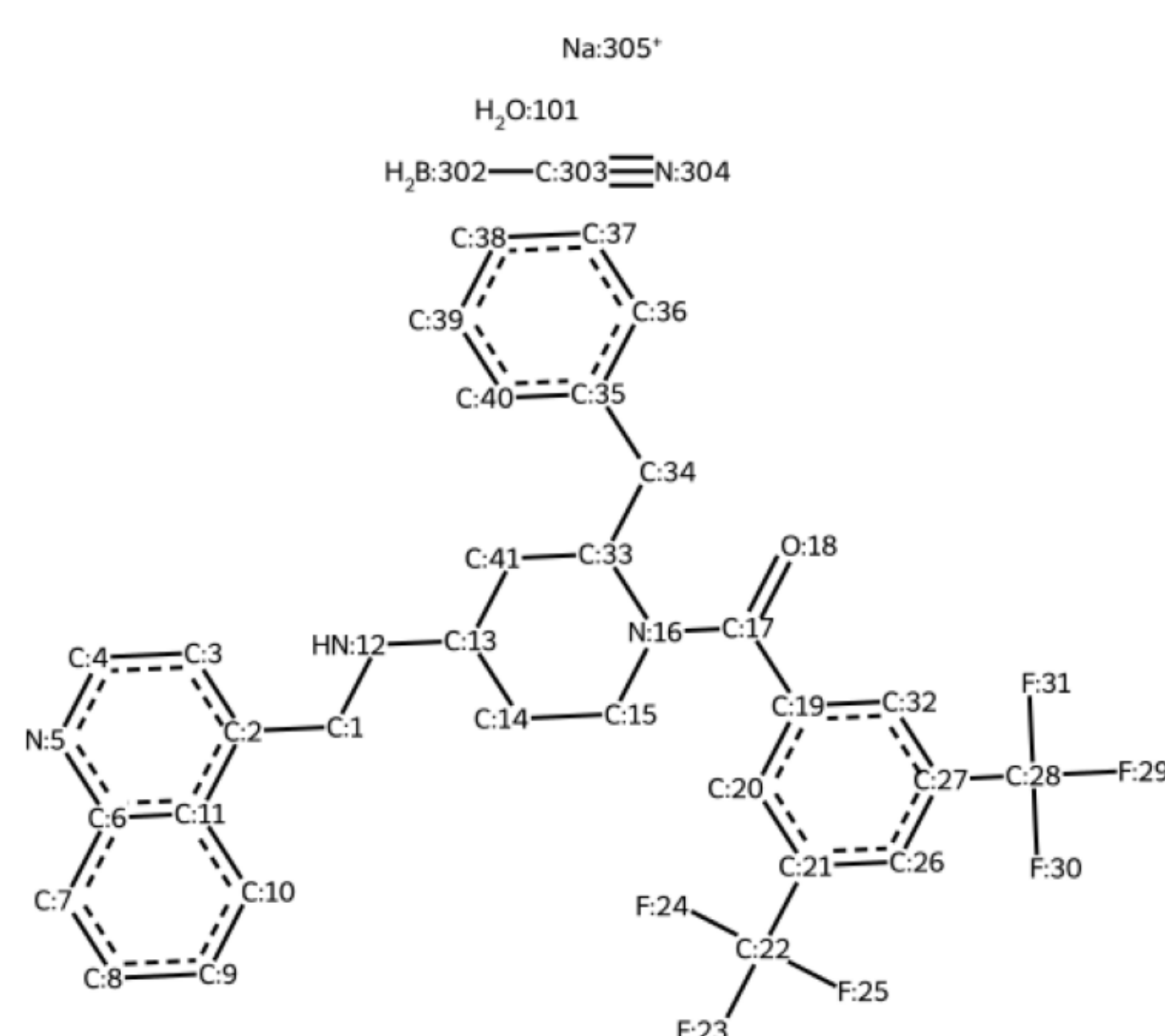
step #3



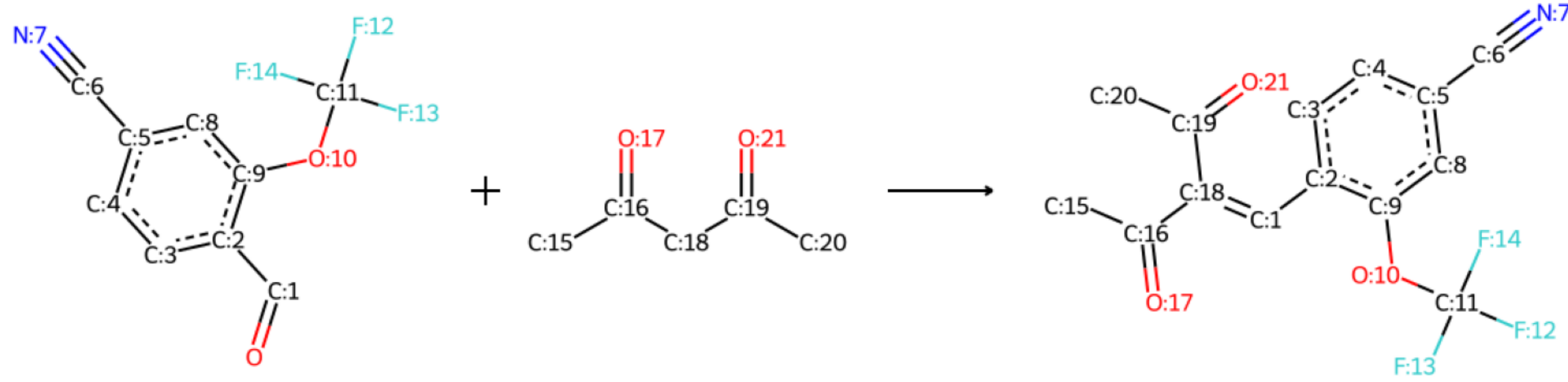
step #4



Product(s)

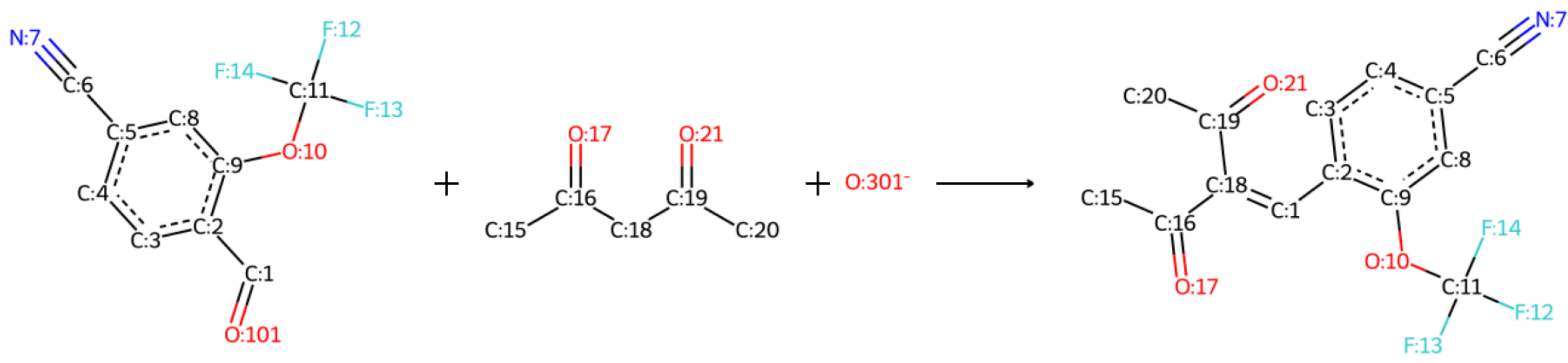


Original reaction
sampled RXN_ID:76)



Identified mechanistic class -
aldol_condensation reaction

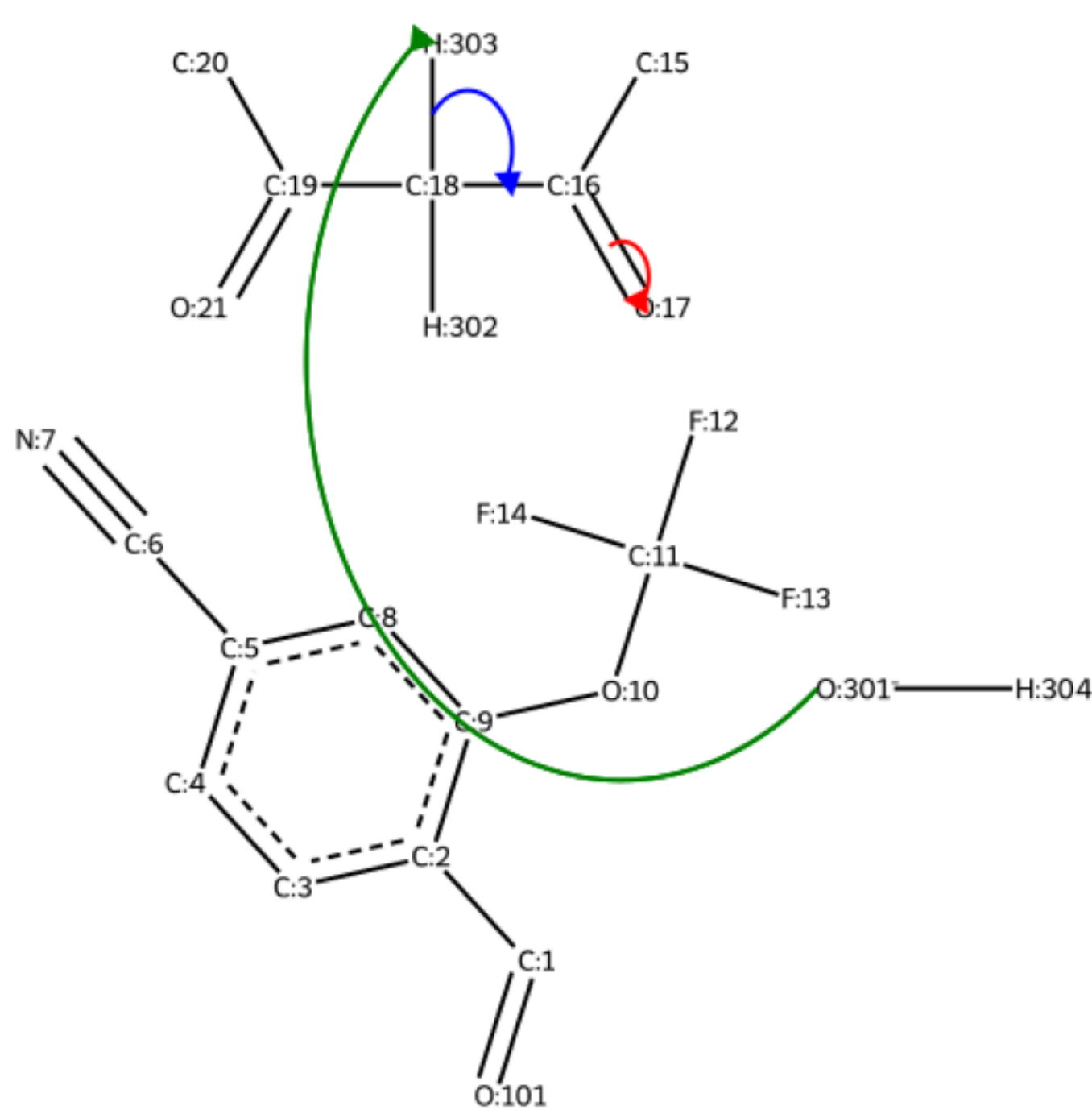
Reaction with missing reagents recovered



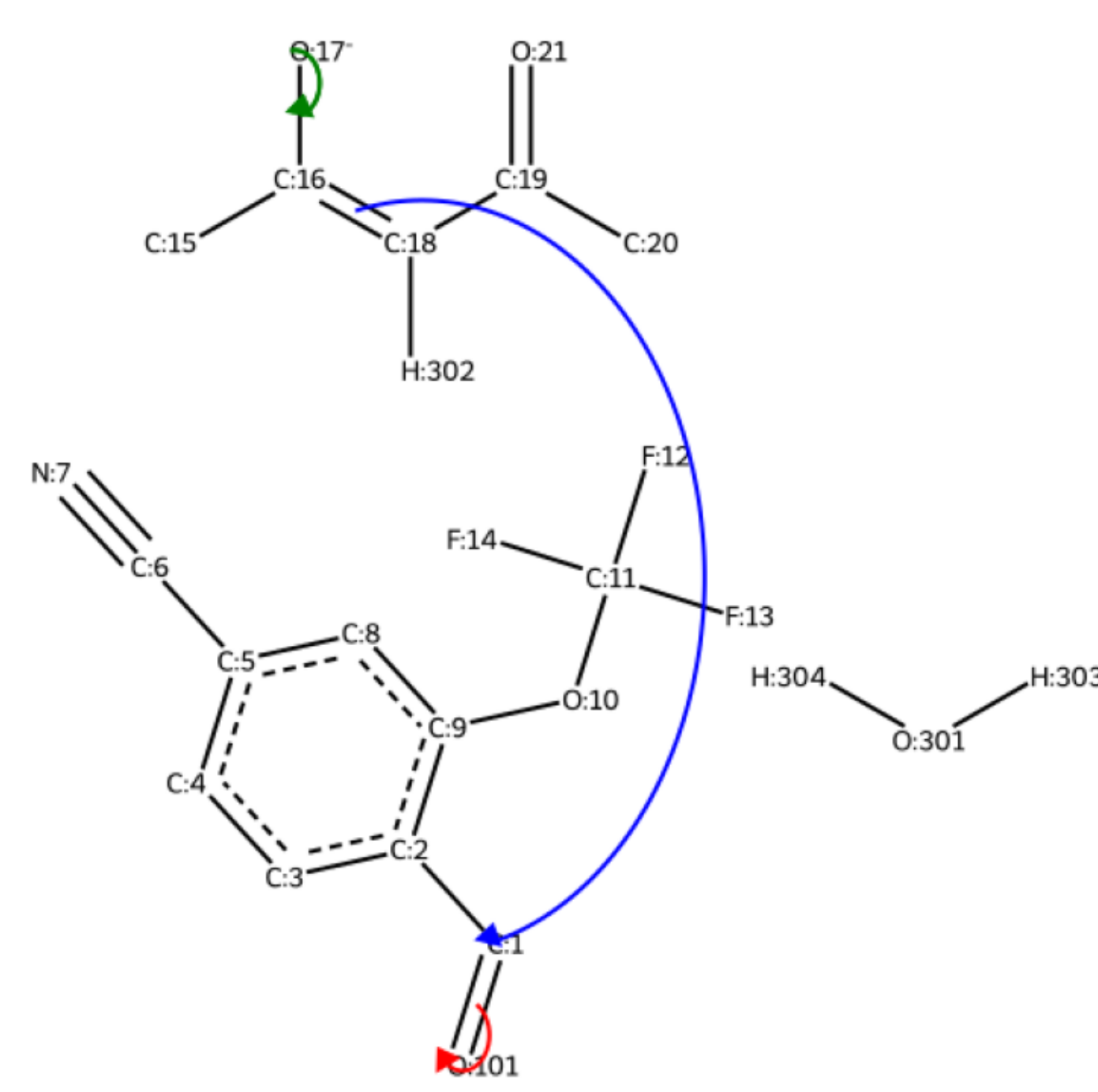
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

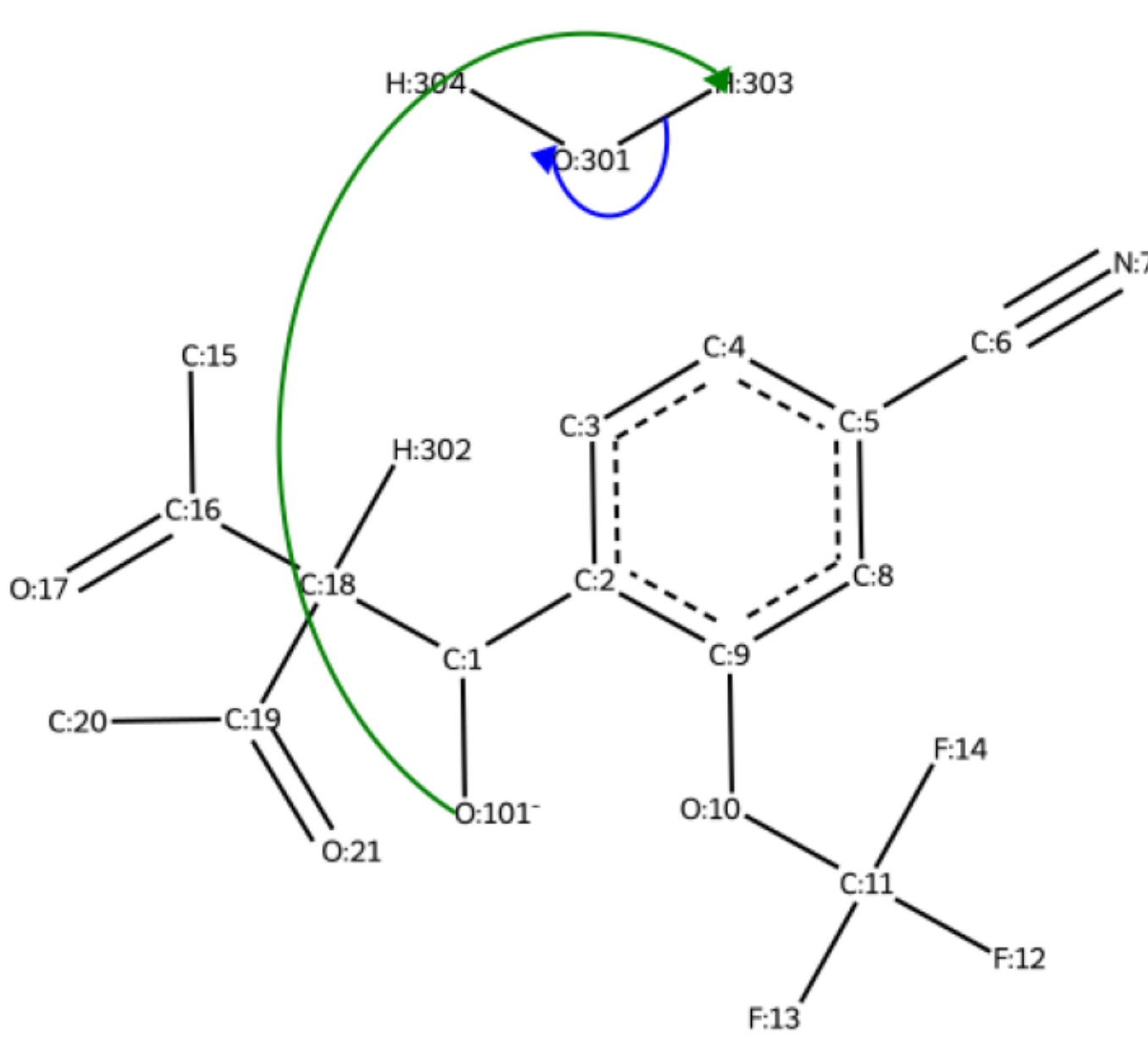
step #1



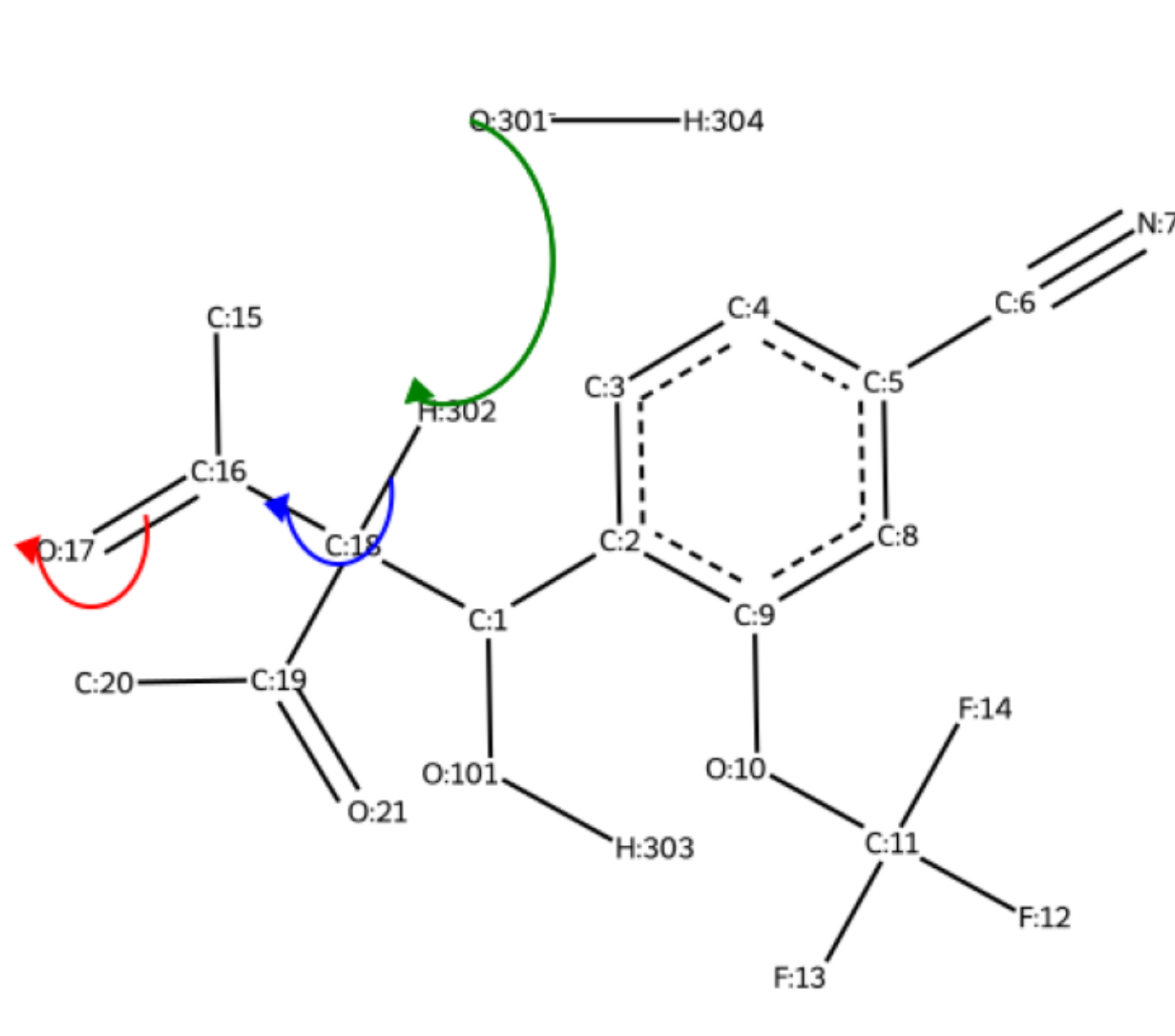
step #2



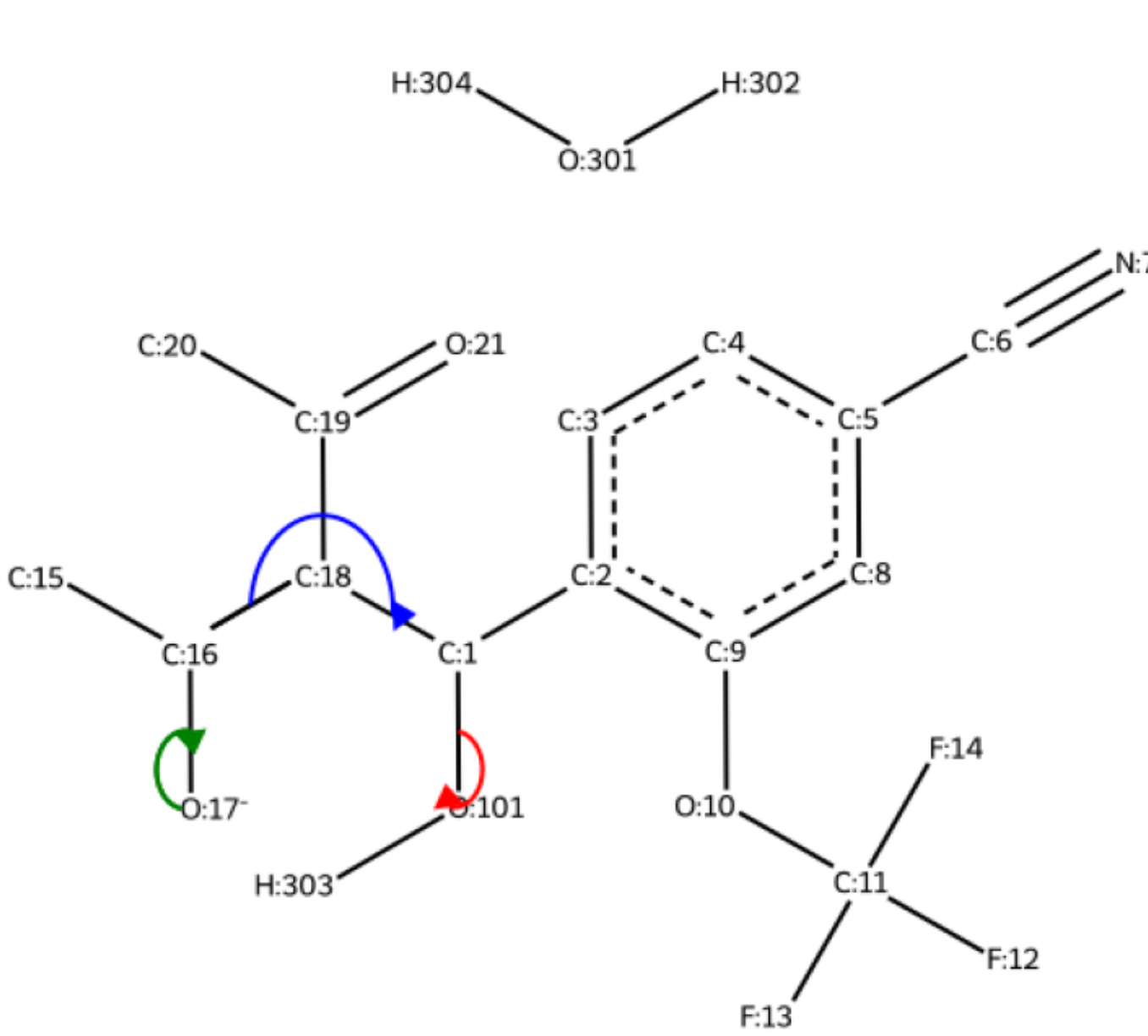
step #3



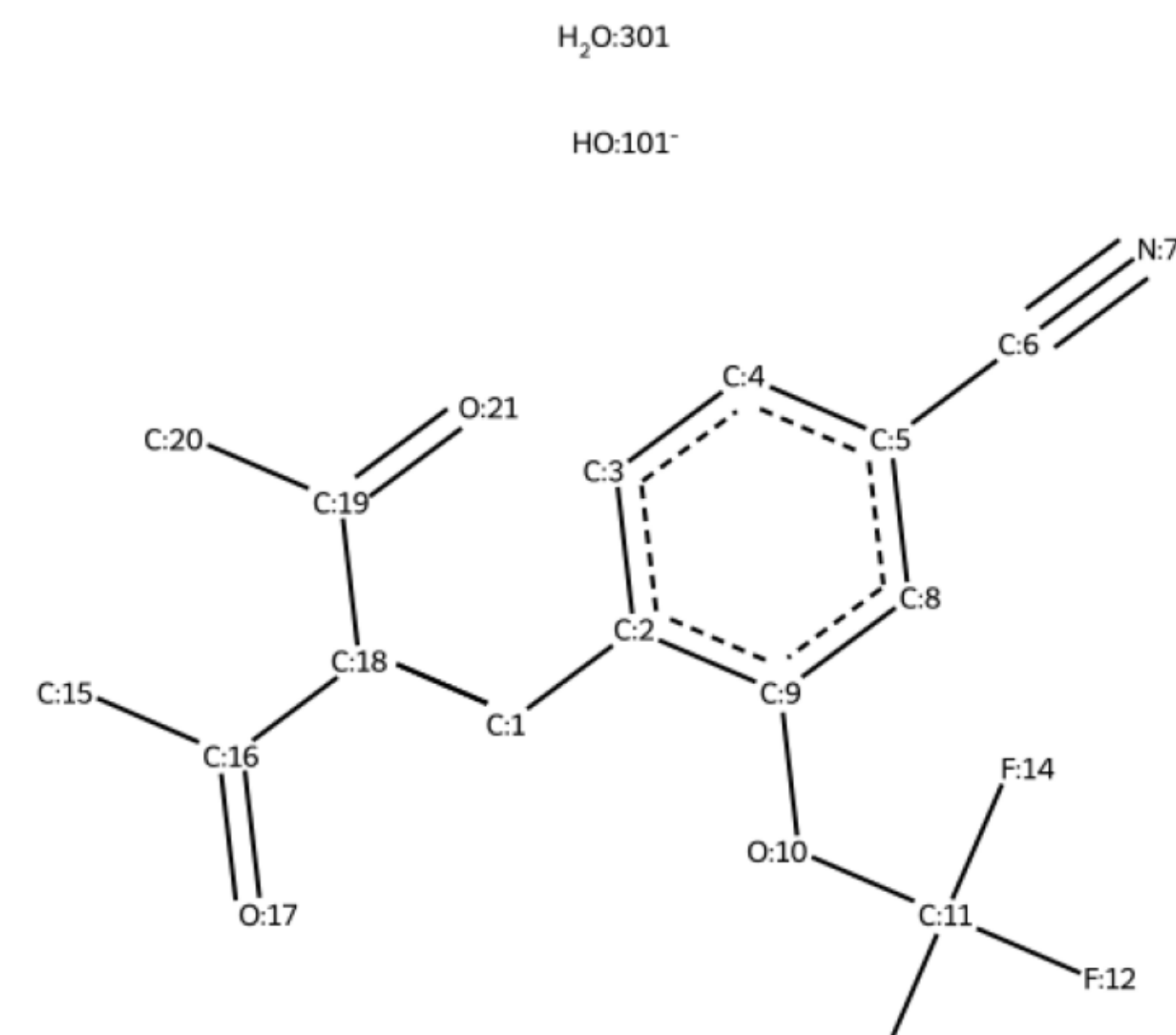
step #4



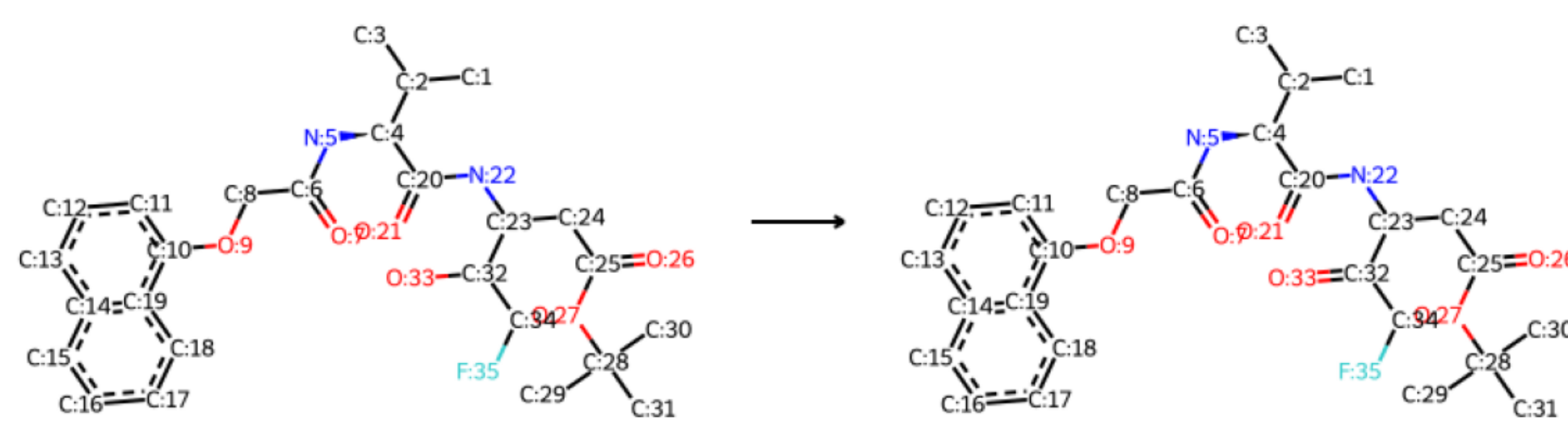
step #5



Product(s)

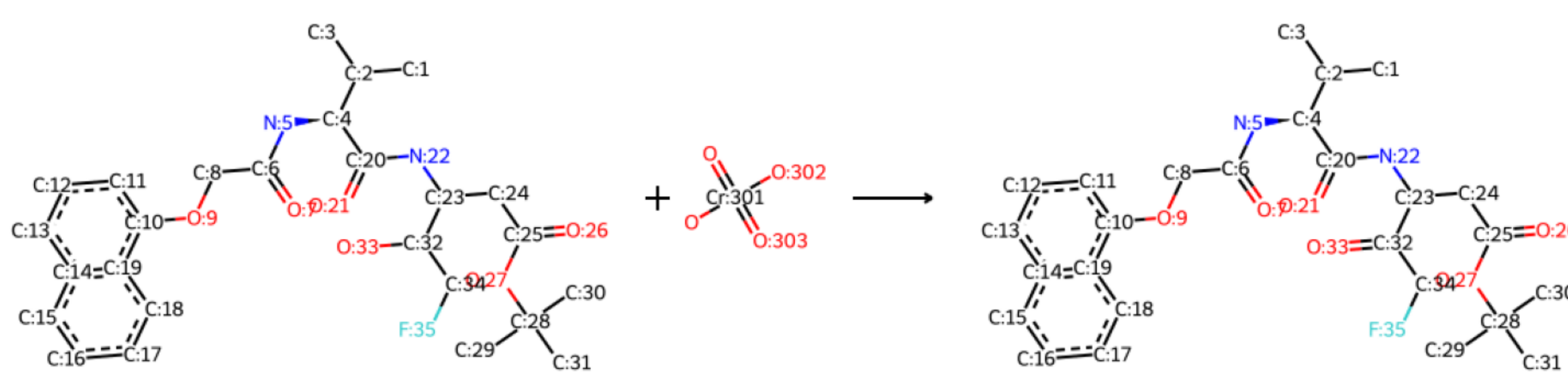


Original reaction
sampled RXN_ID:77)



Identified mechanistic class -
Jones_oxidation reaction

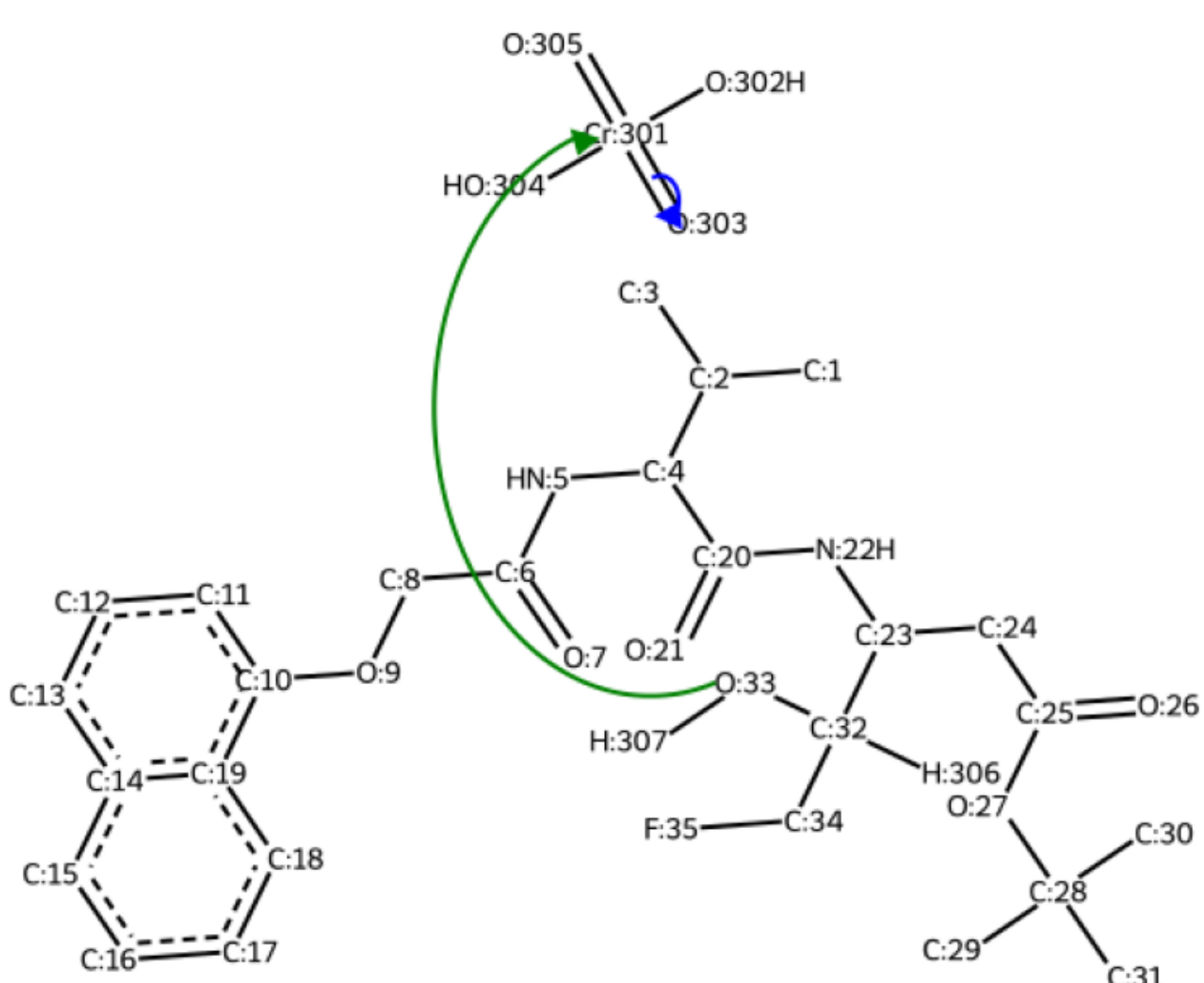
Reaction with missing reagents recovered



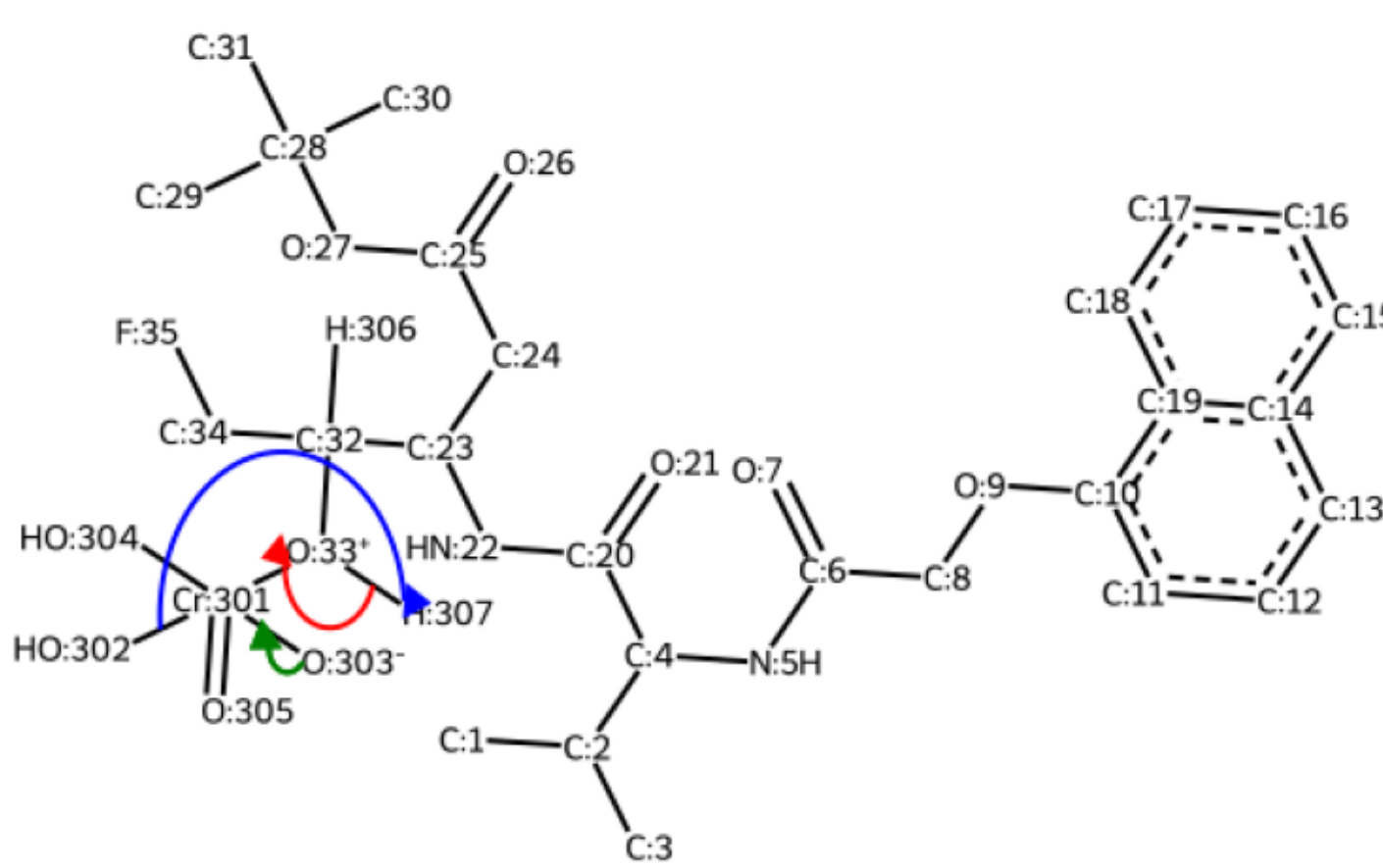
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

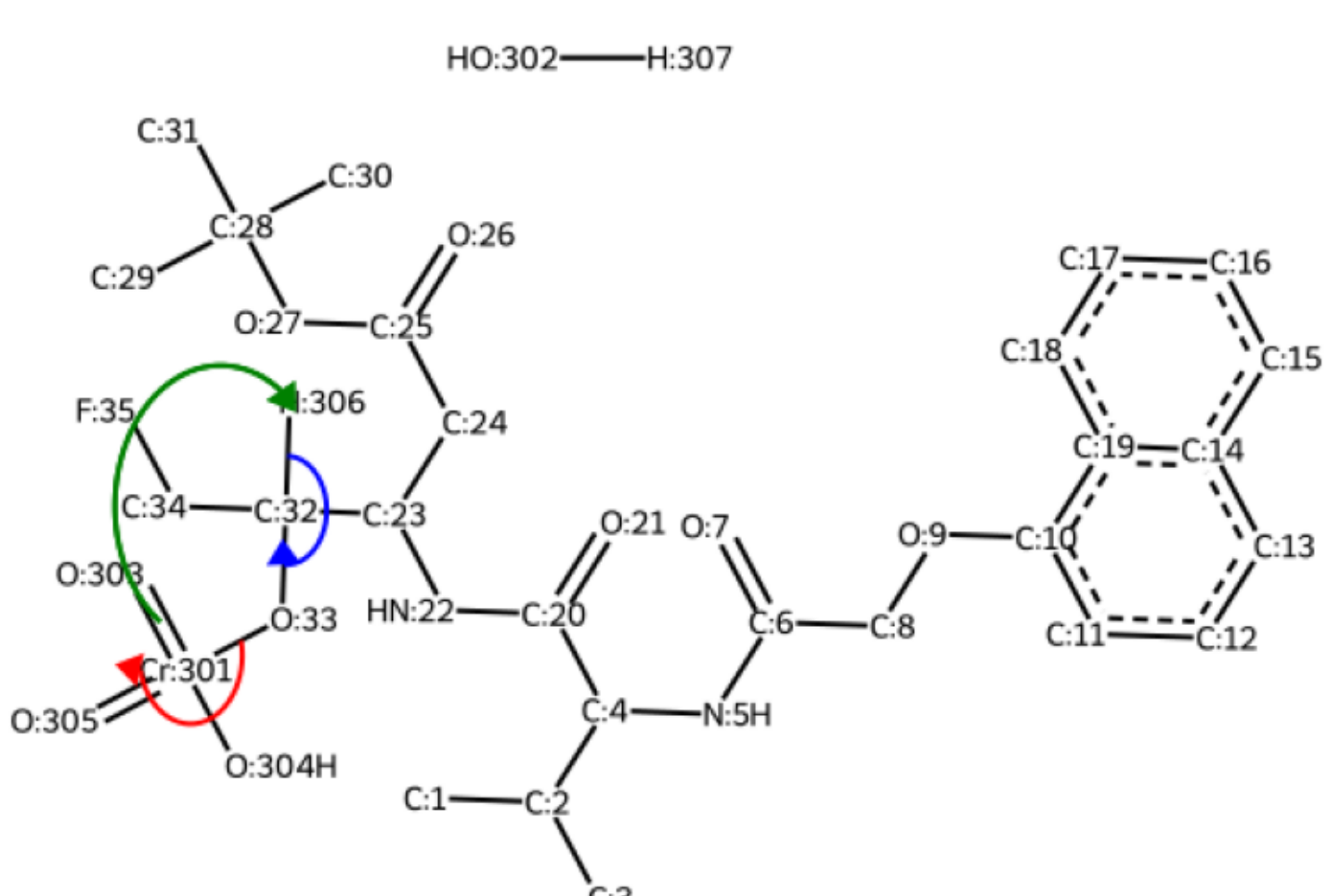
step #1



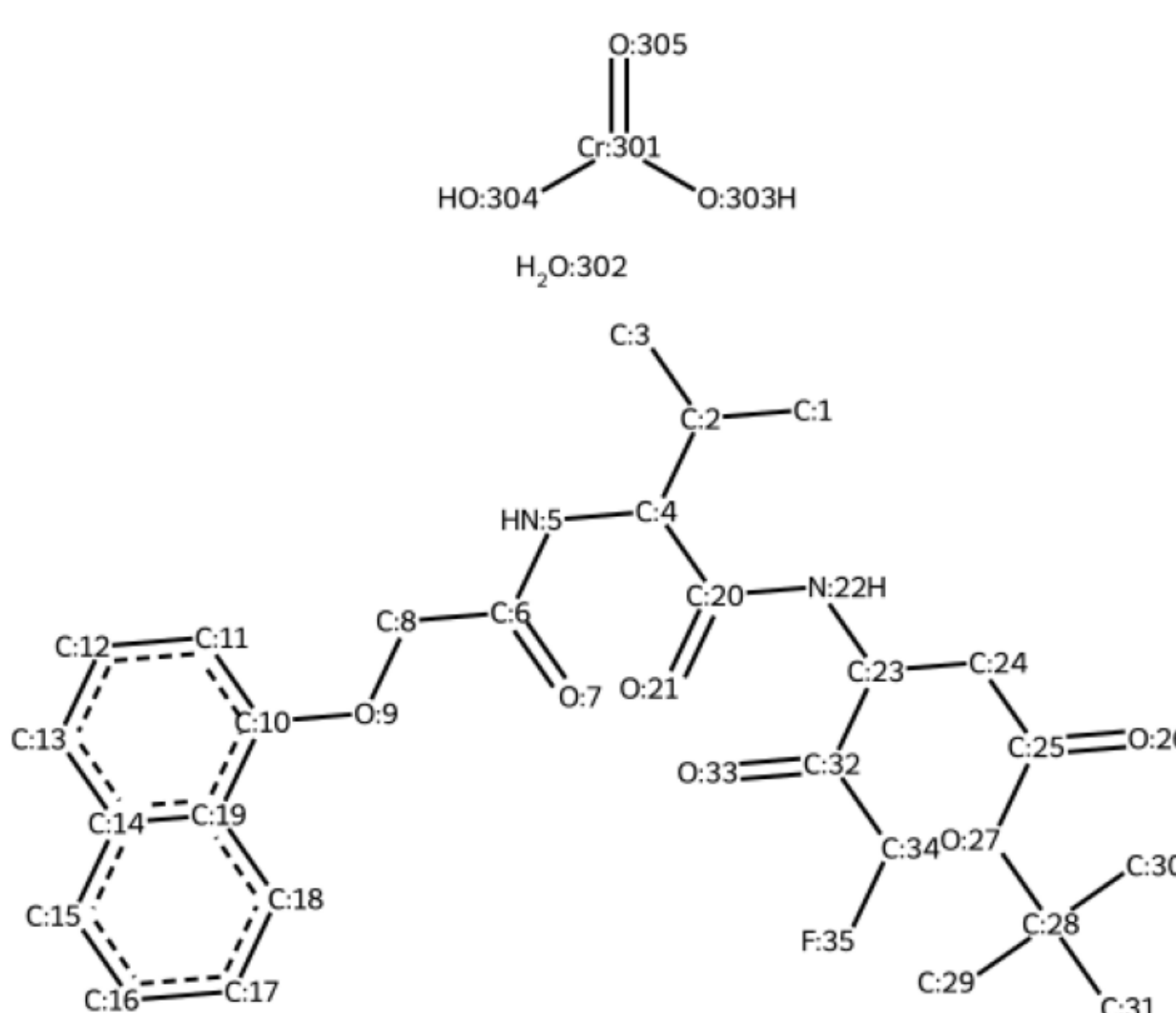
step #2



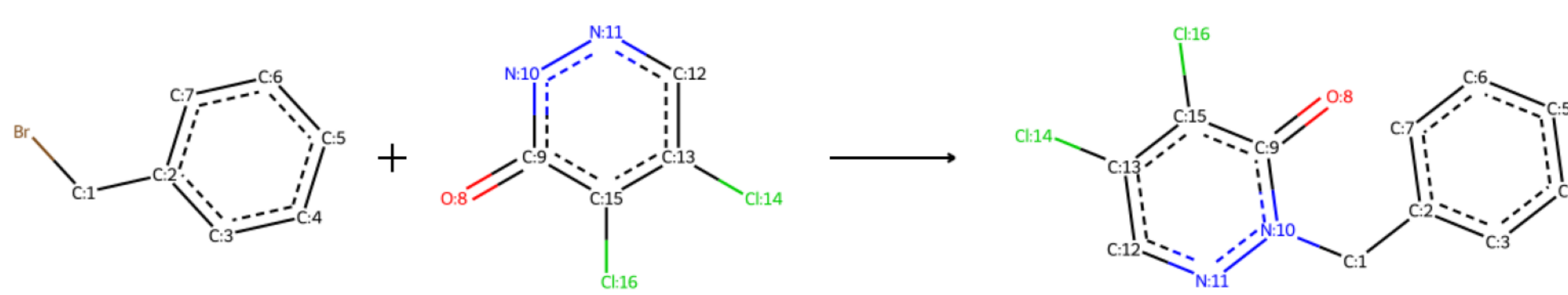
step #3



Product(s)

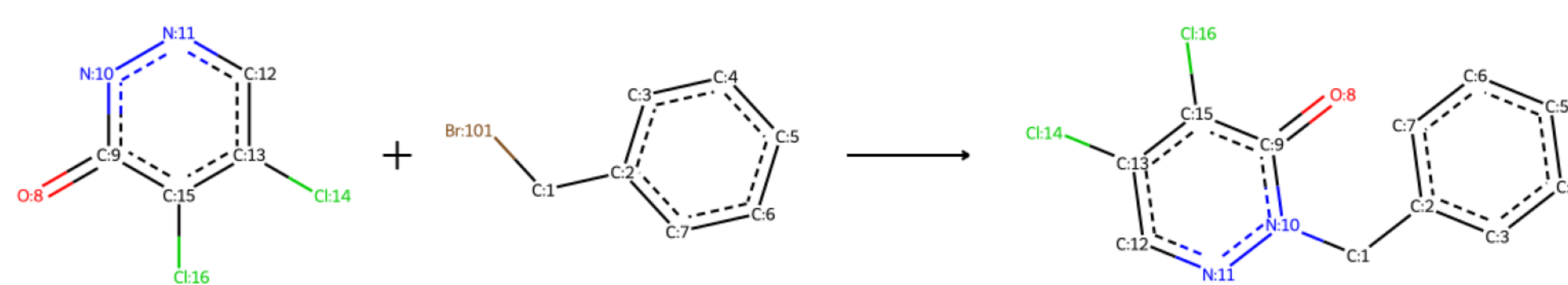


Original reaction sampled RXN_ID:78)



Identified mechanistic class -
SN2 reaction

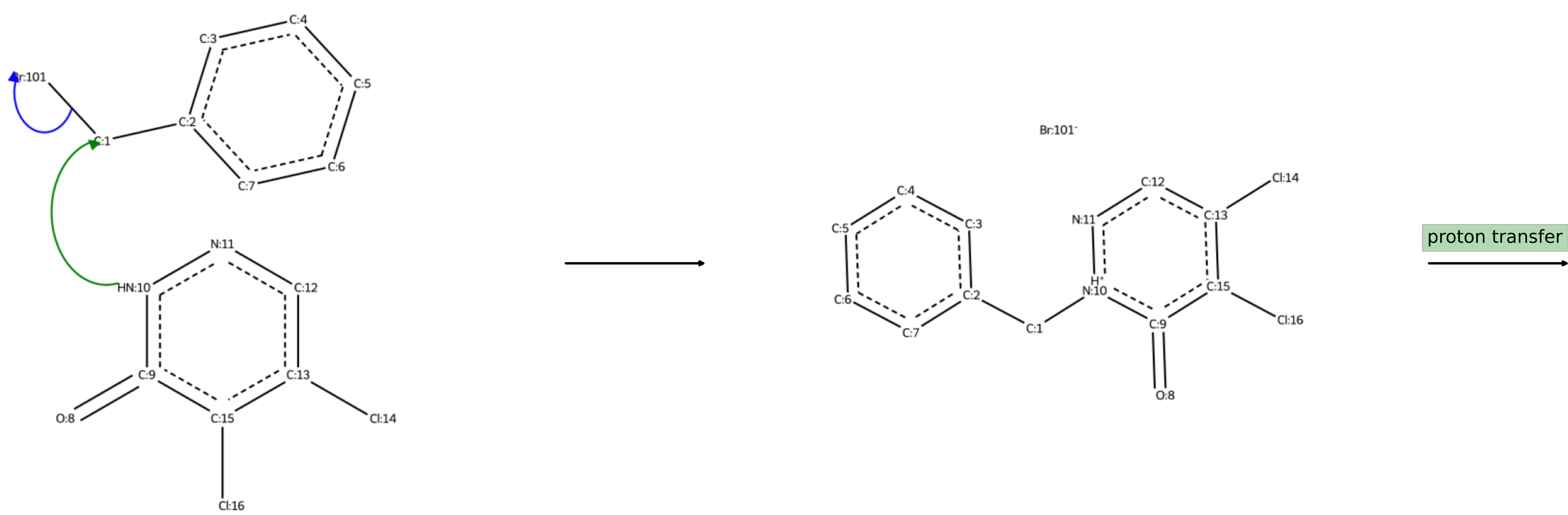
Reaction with missing reagents recovered



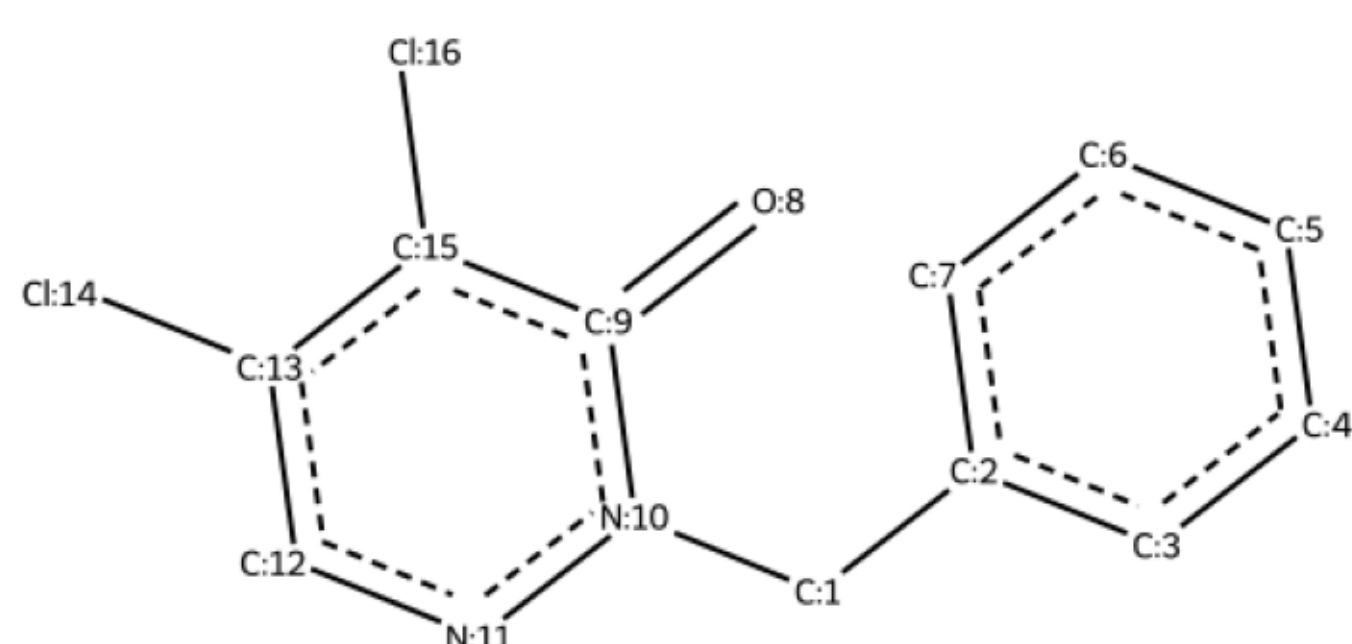
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

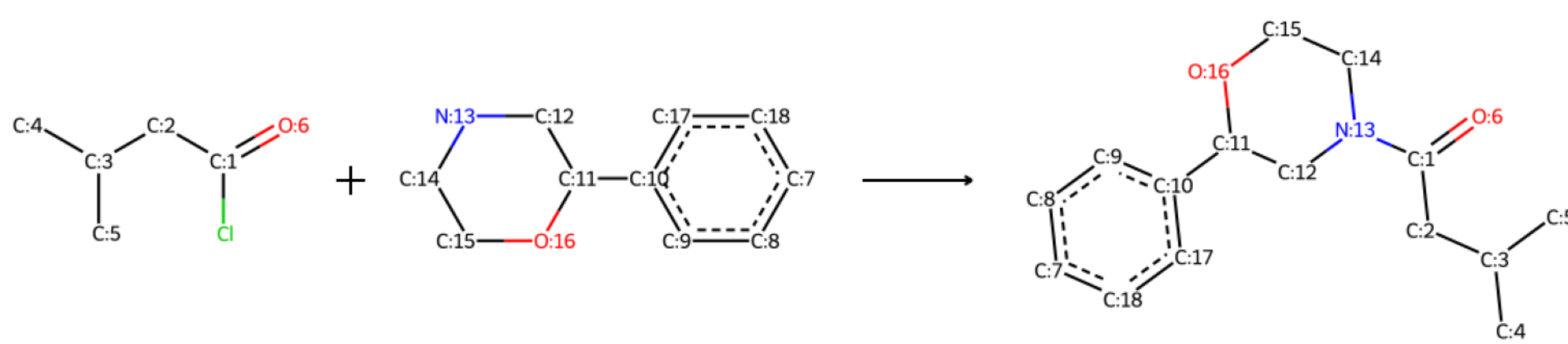
step #1



Product(s)

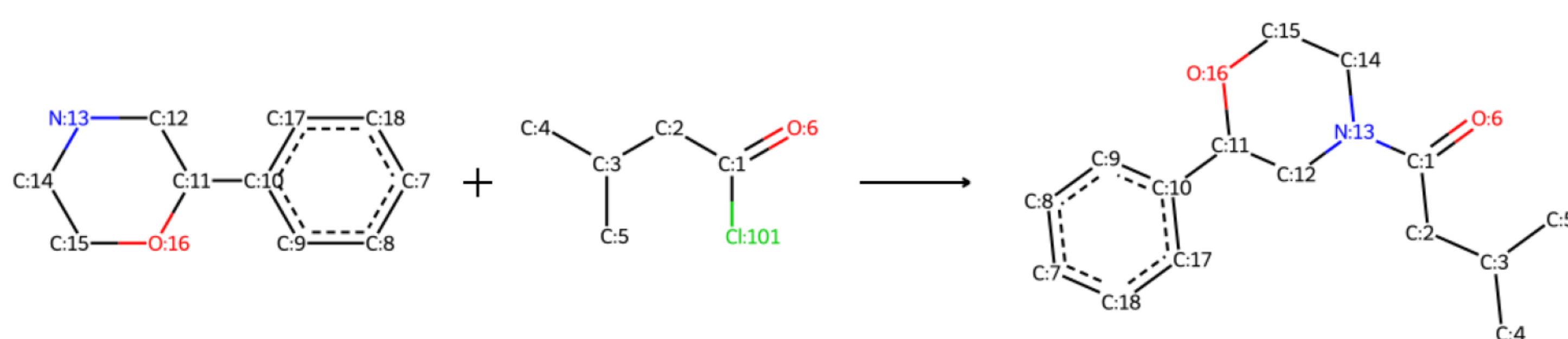


Original reaction sampled RXN_ID:79)



Identified mechanistic class -
nucleophilic_attack_to_(thio)carbonyl_or_sulfonyl reaction

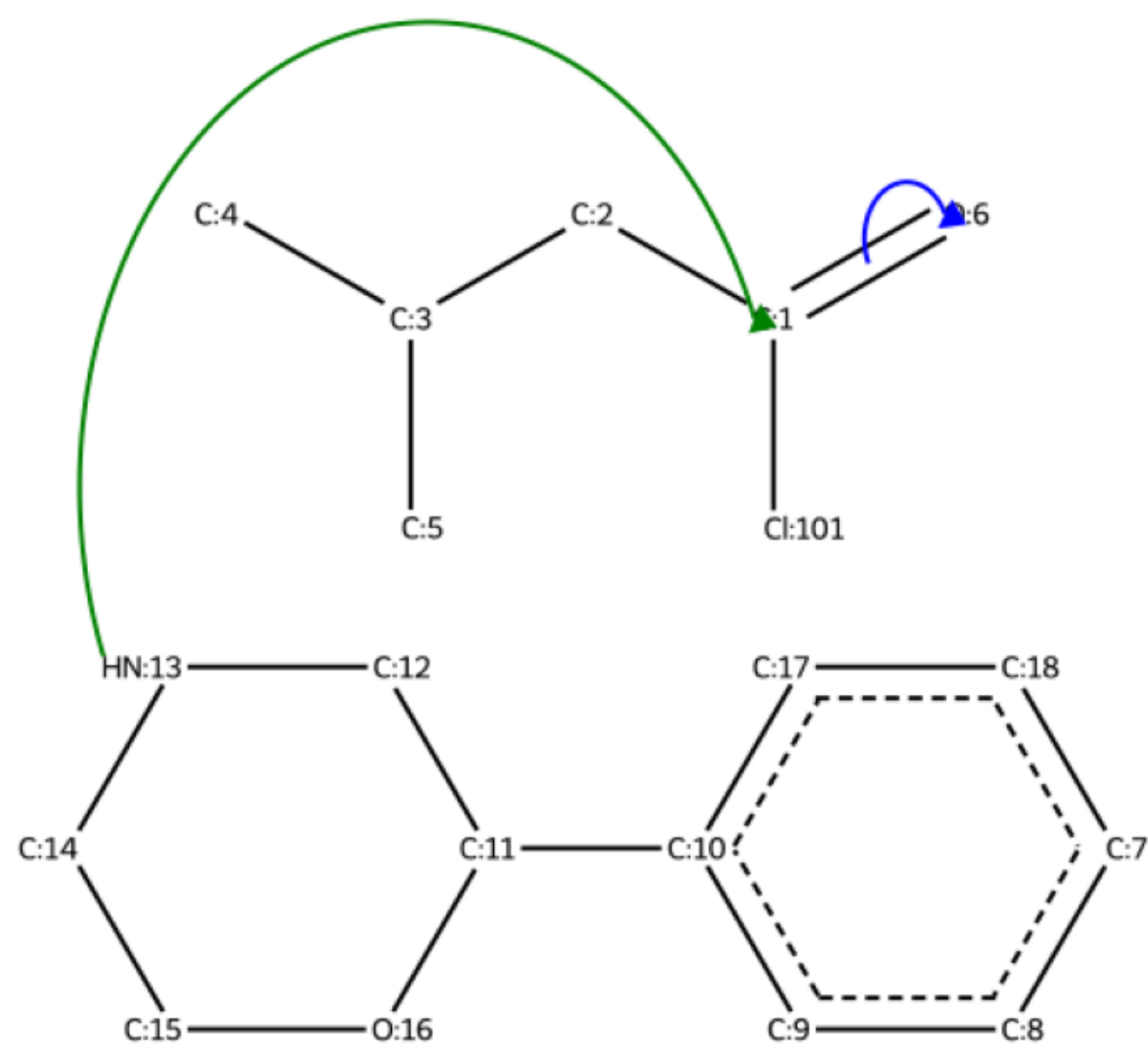
Reaction with missing reagents recovered



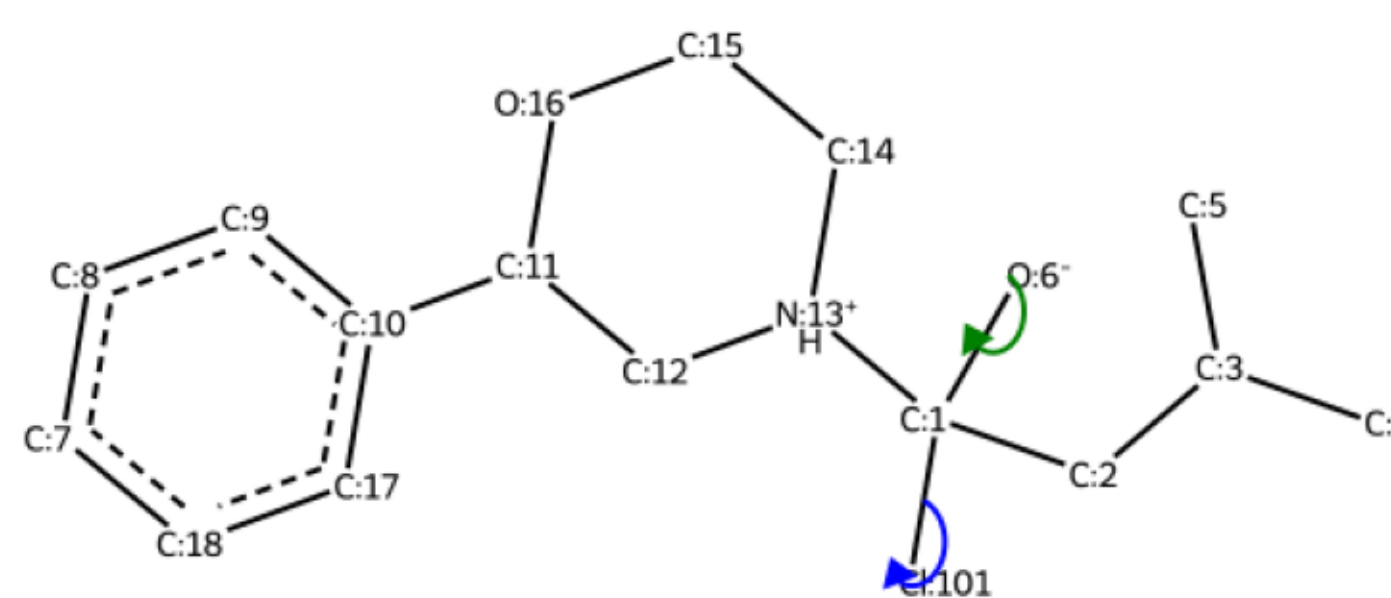
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

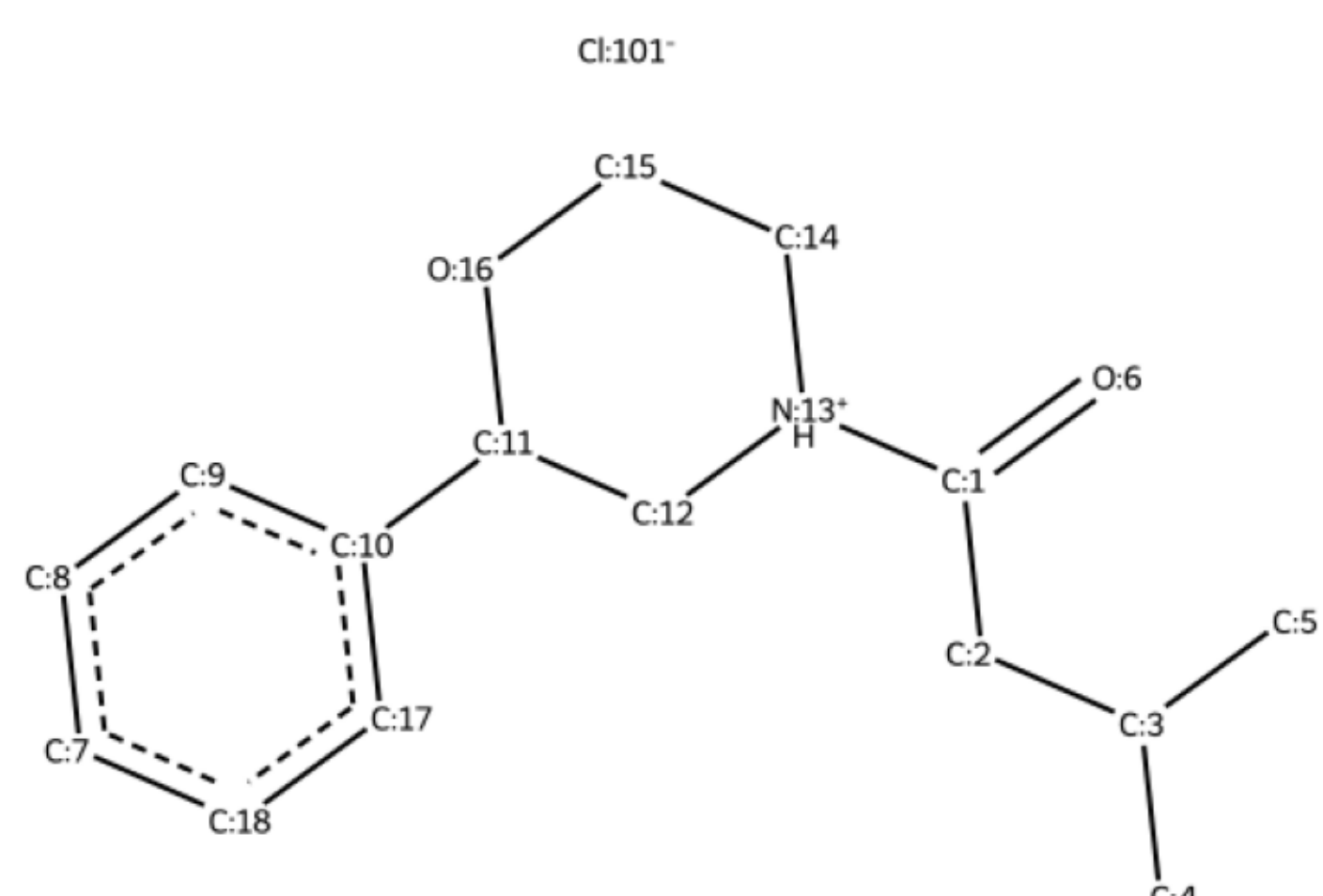
step #1



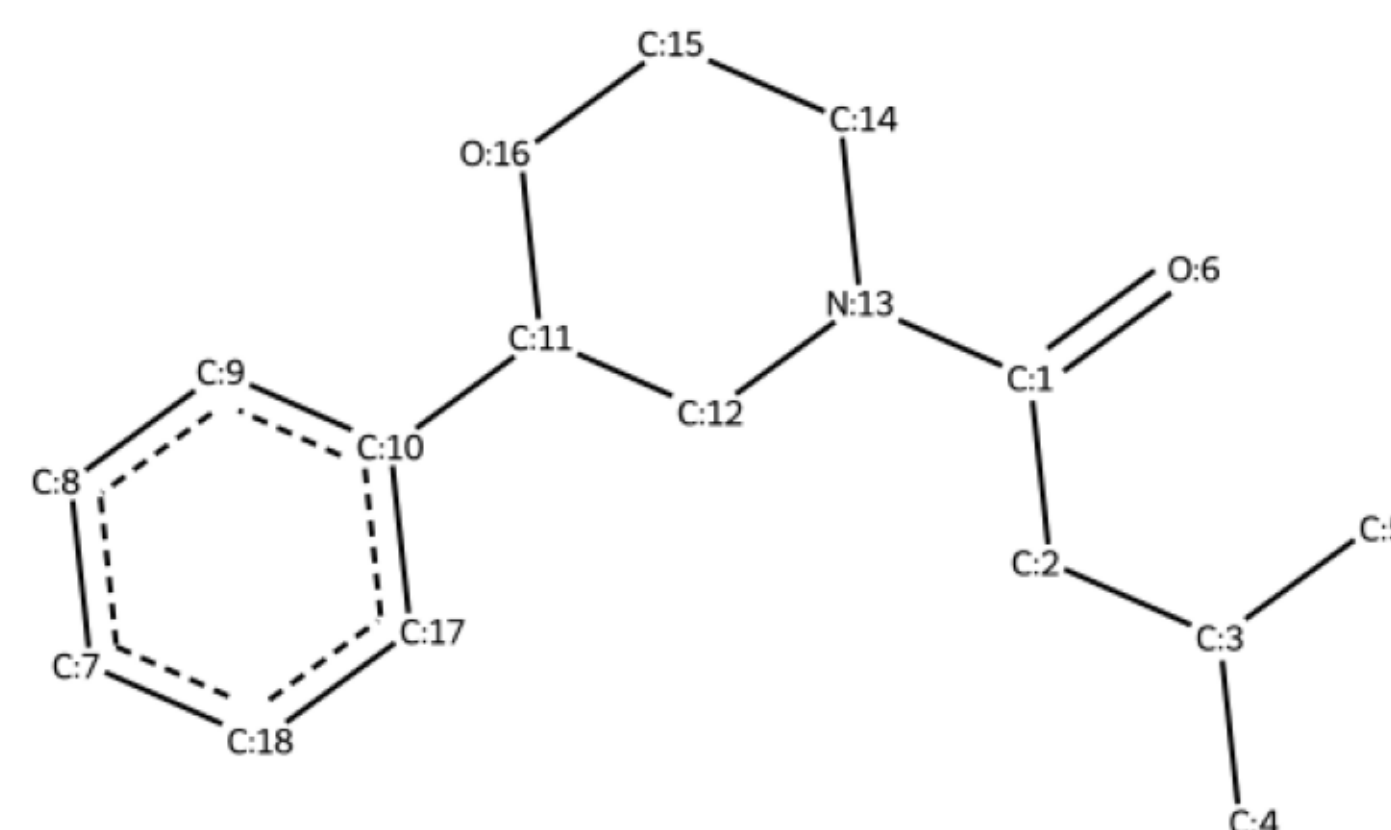
step #2



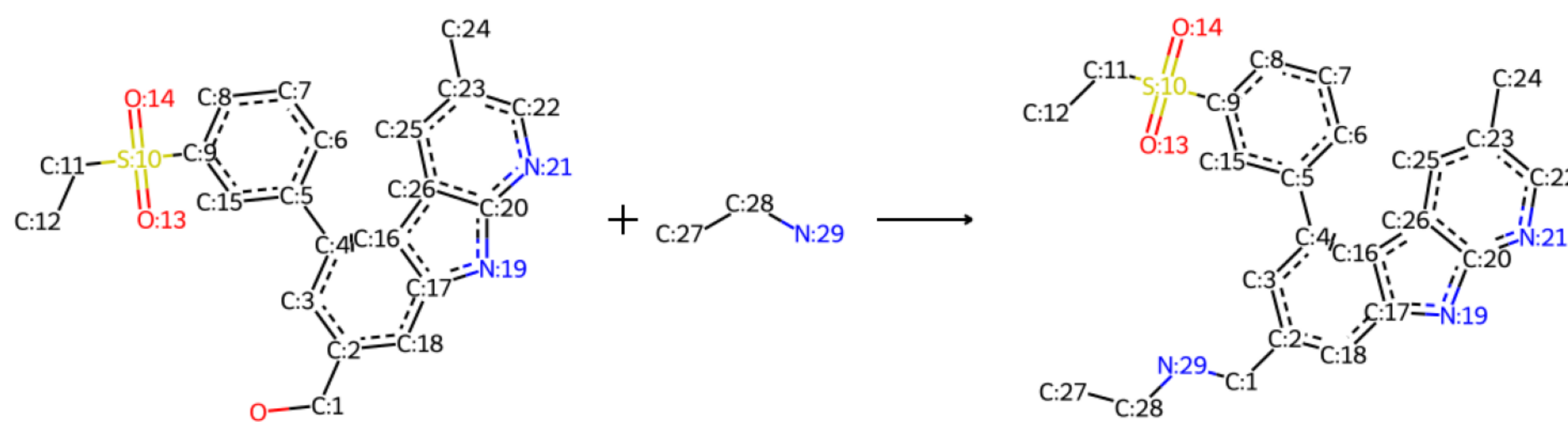
Product(s)



proton transfer

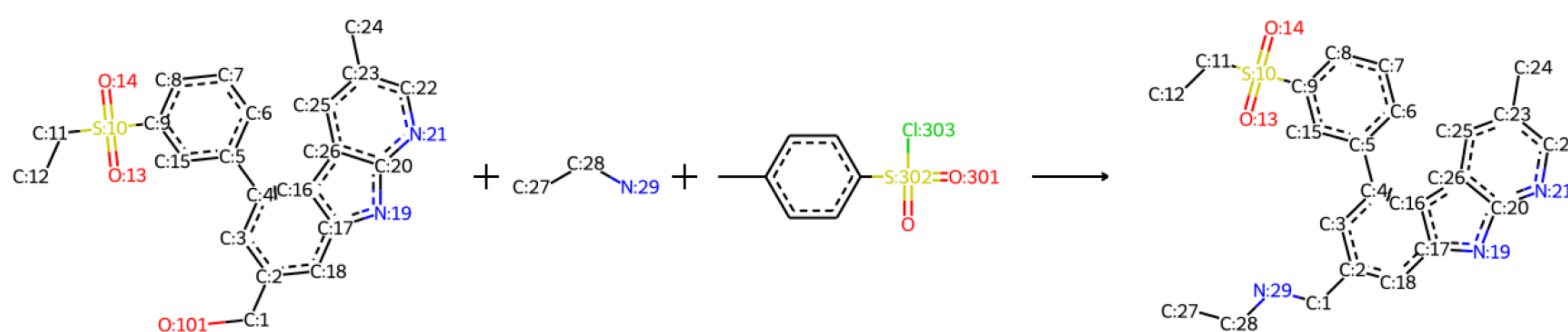


Original reaction
sampled RXN_ID:80)



Identified mechanistic class -
SN₂_with_tosylate reaction

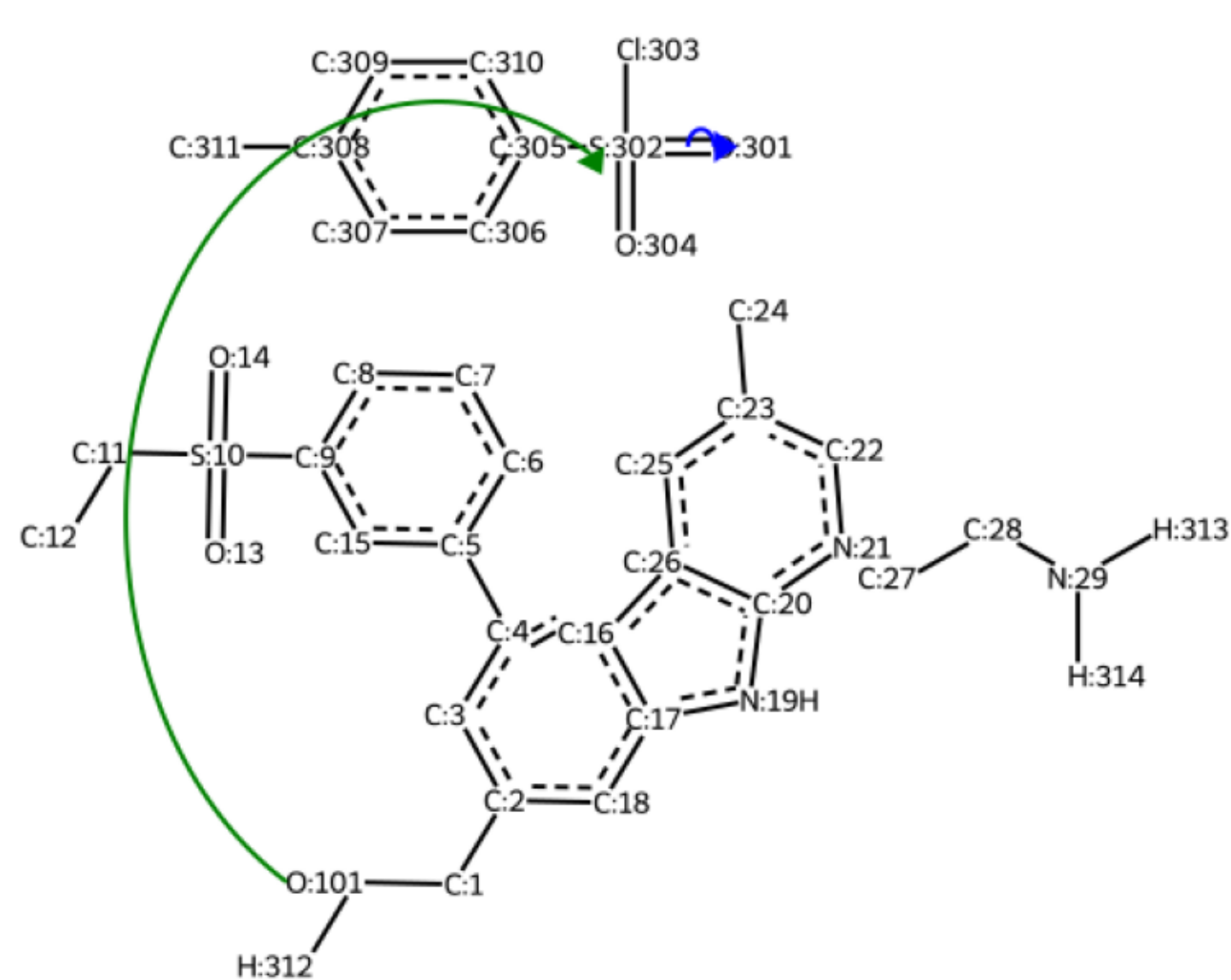
Reaction with missing reagents recovered



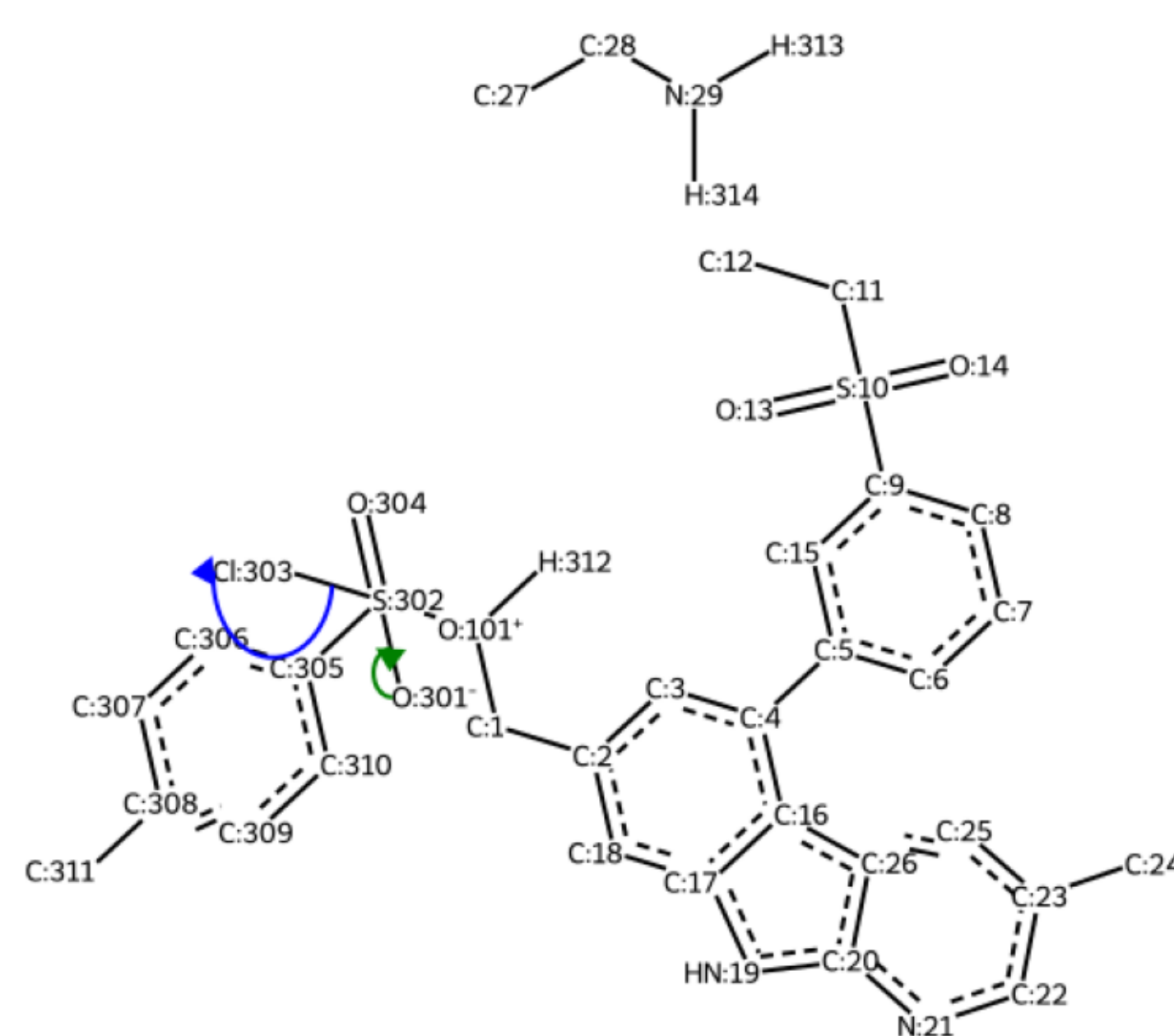
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

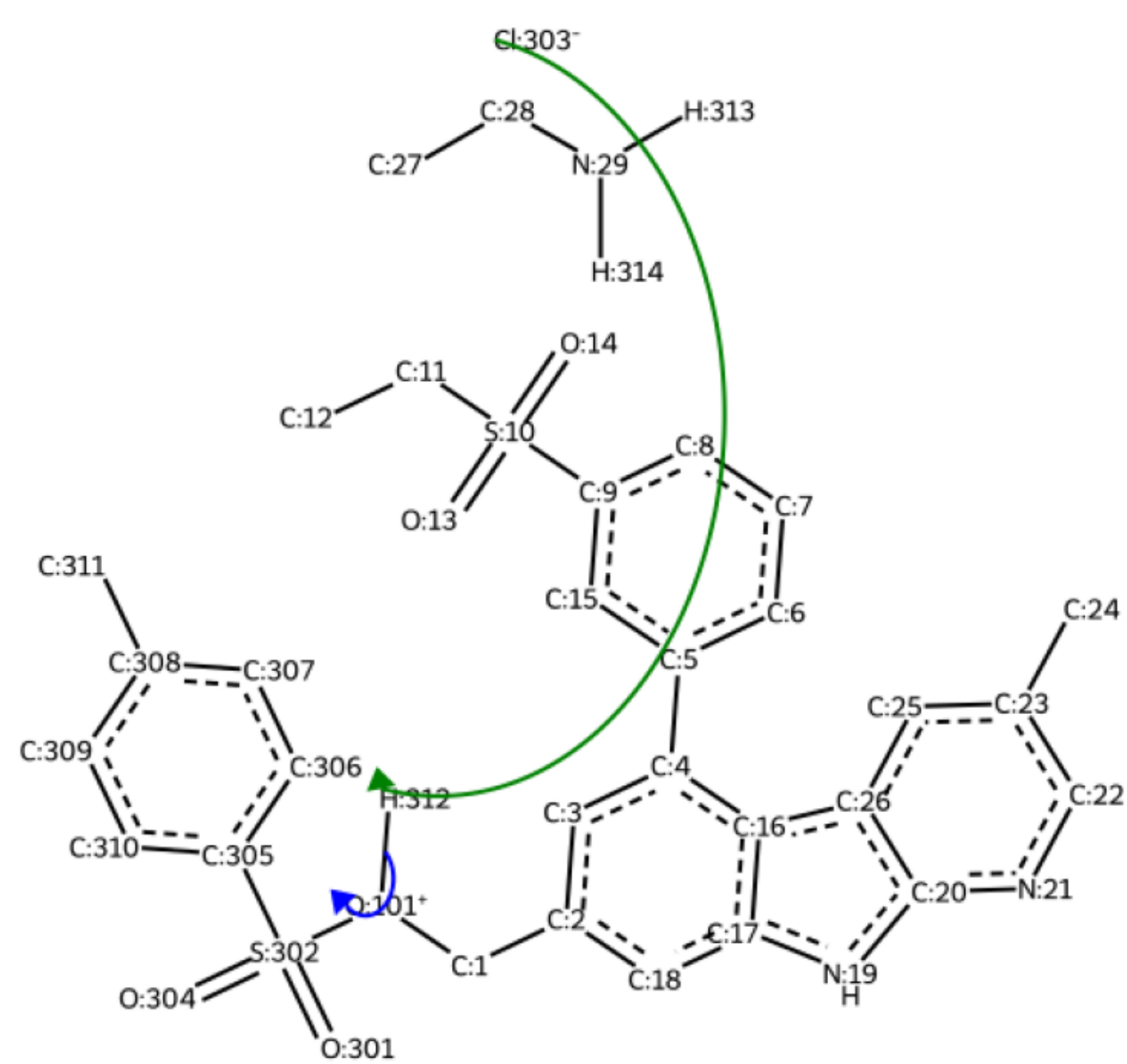
step #1



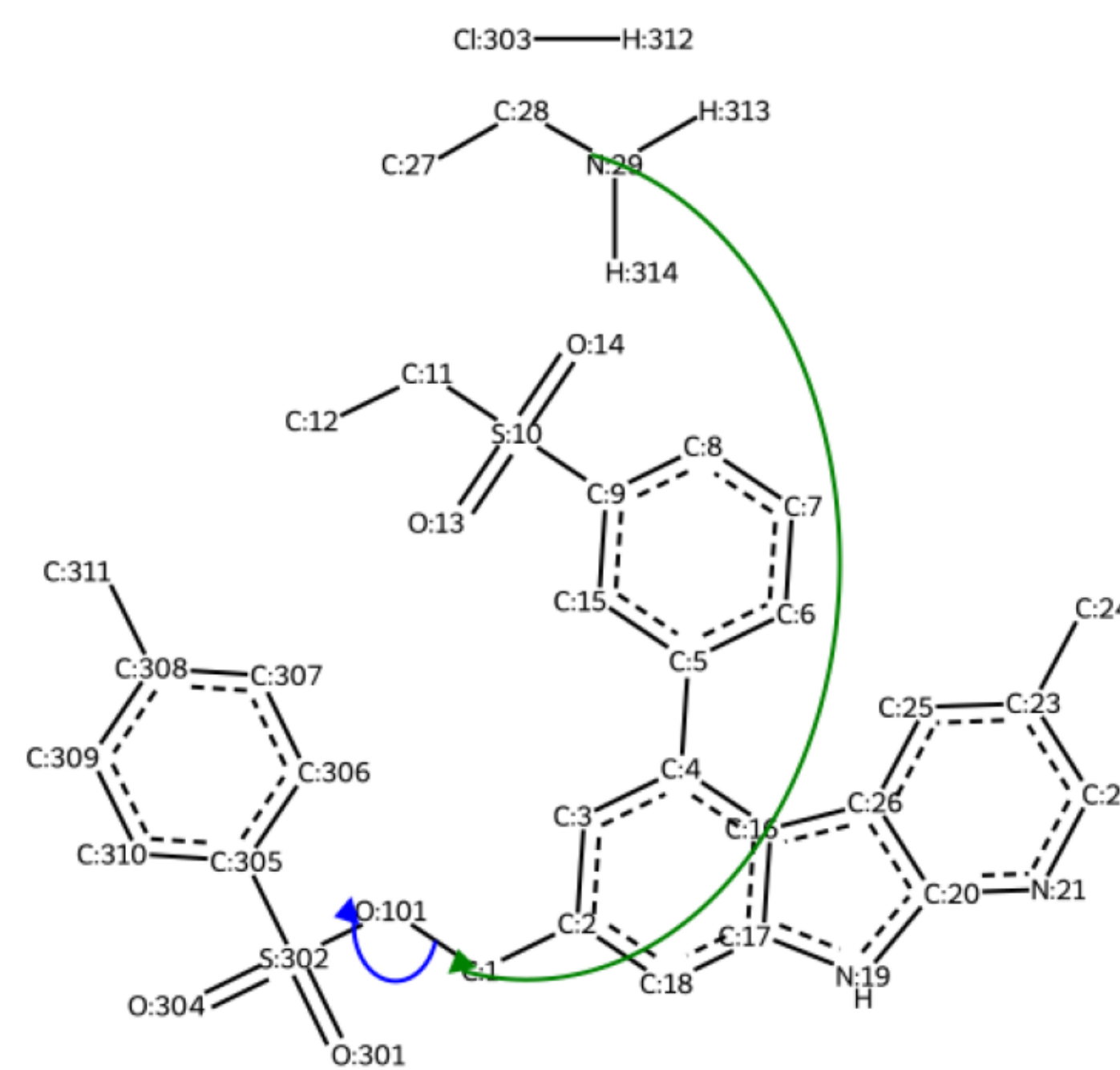
step #2



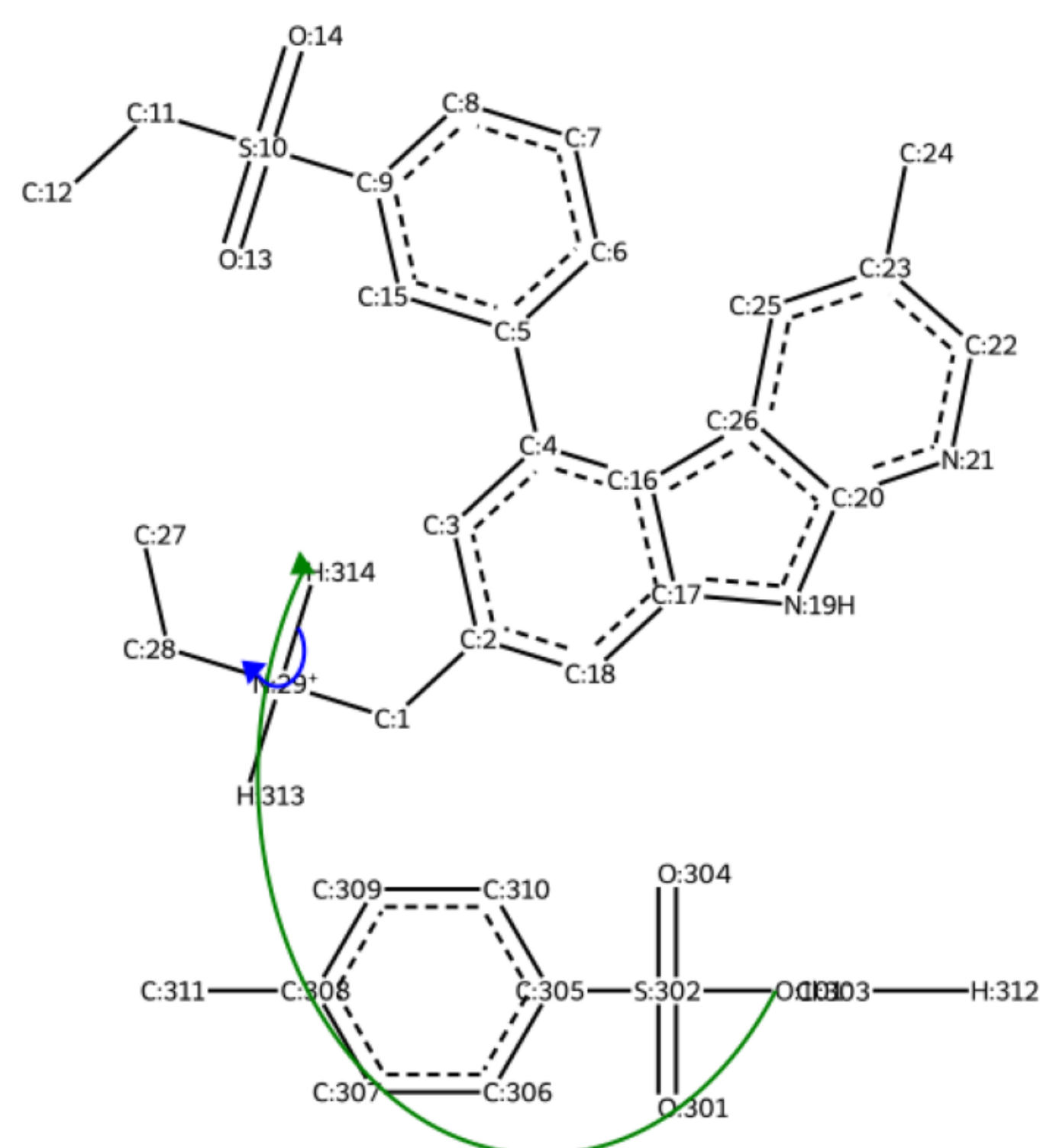
step #3



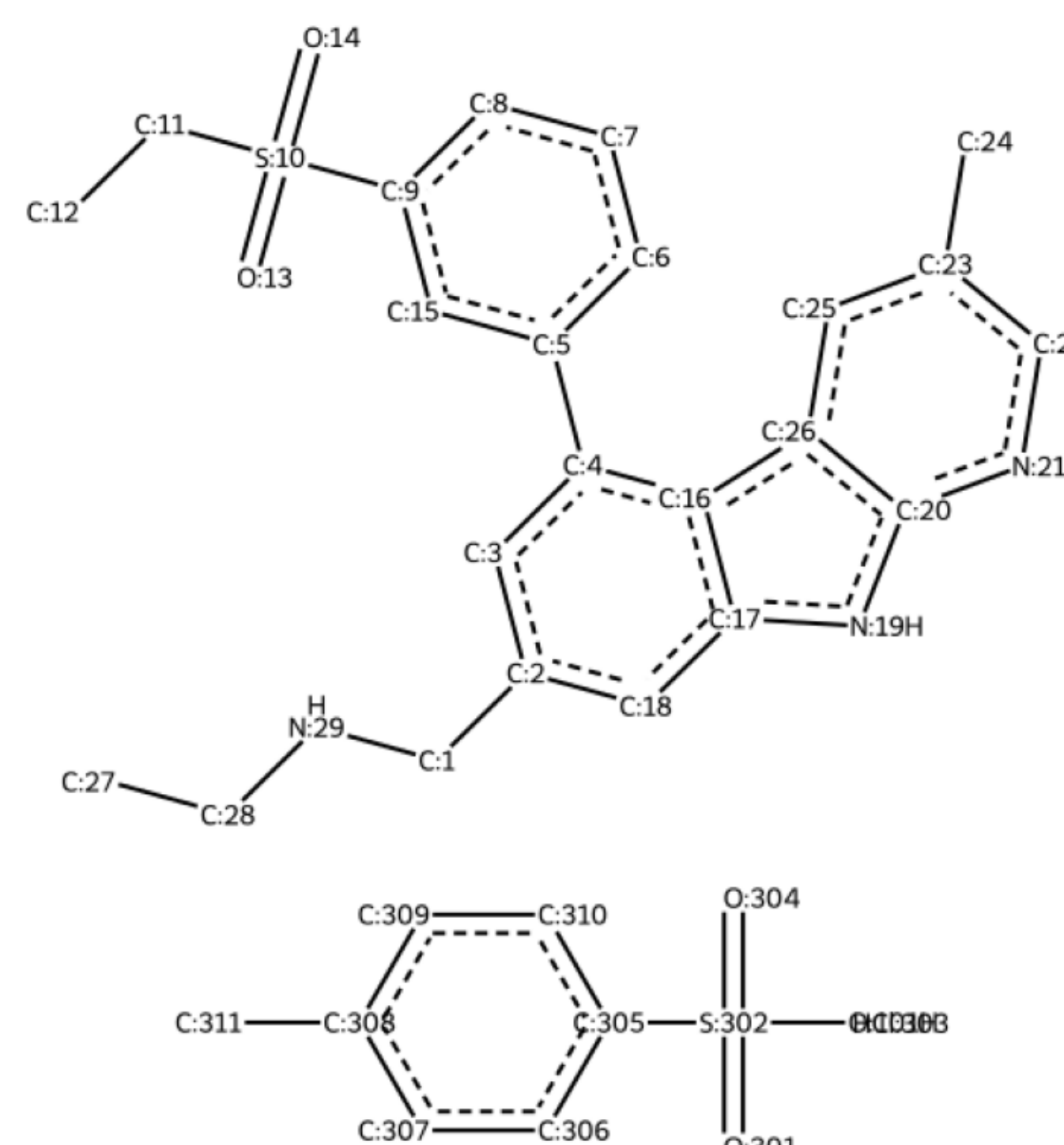
step #4



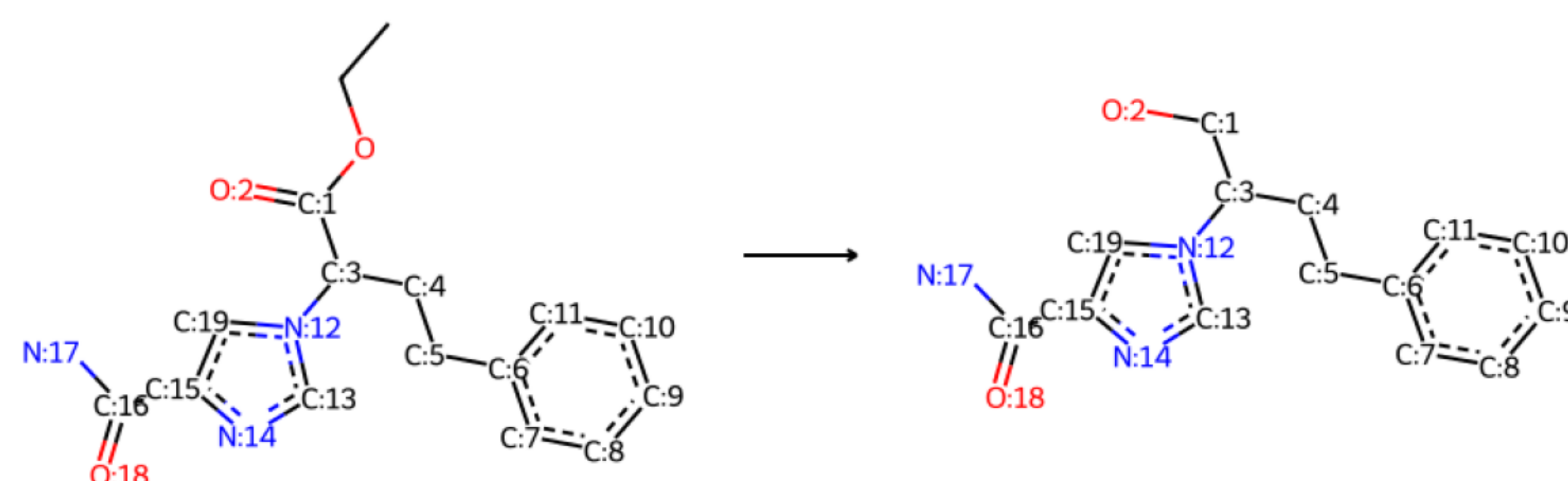
step #5



Product(s)

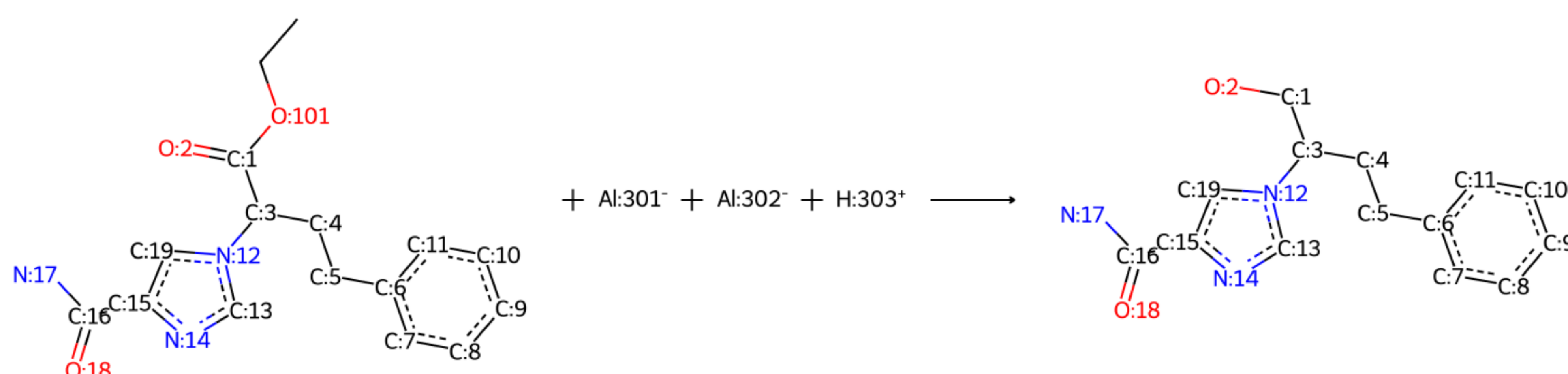


Original reaction
sampled RXN_ID:81)



Identified mechanistic class -
ester_reduction reaction

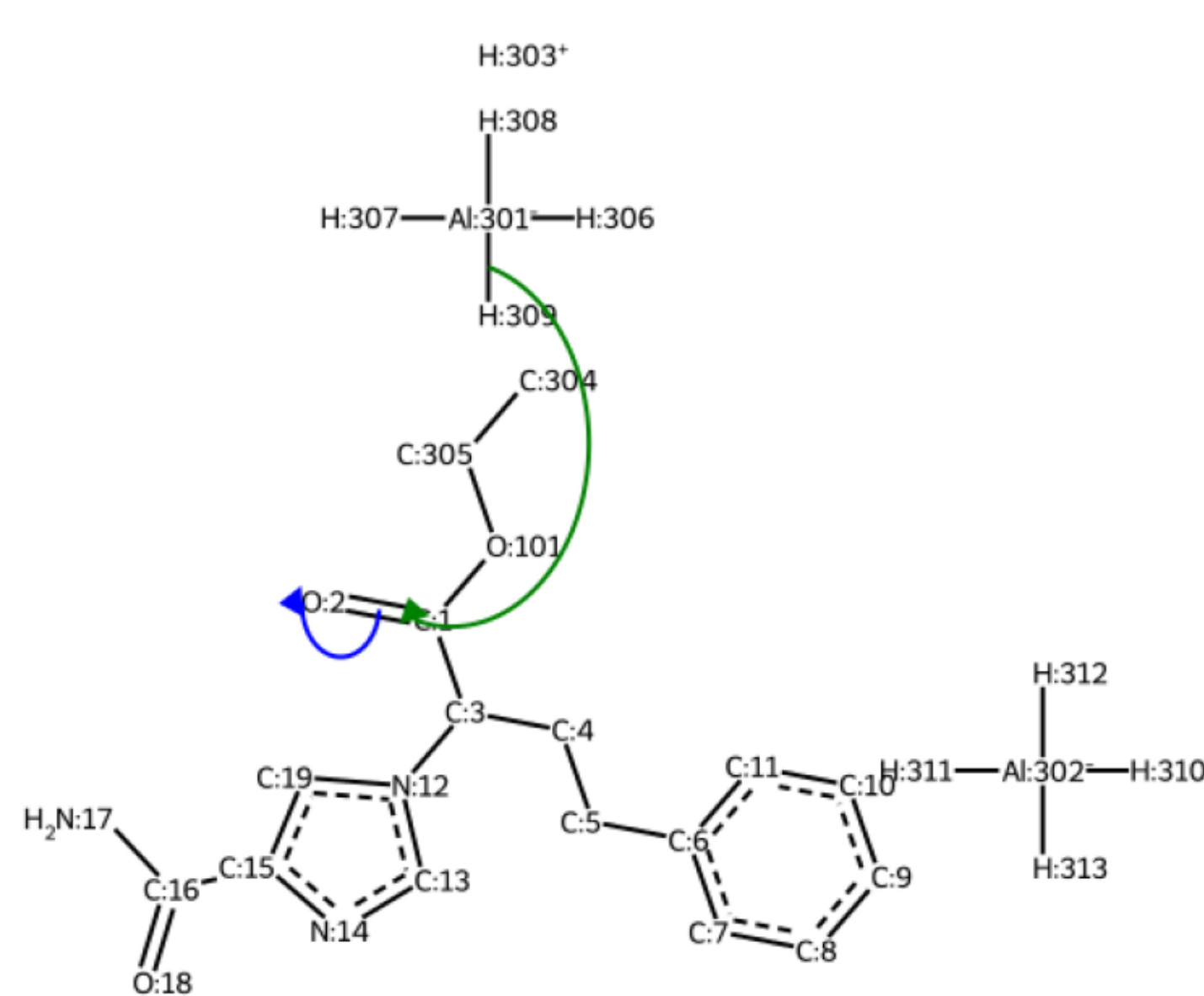
Reaction with missing reagents recovered



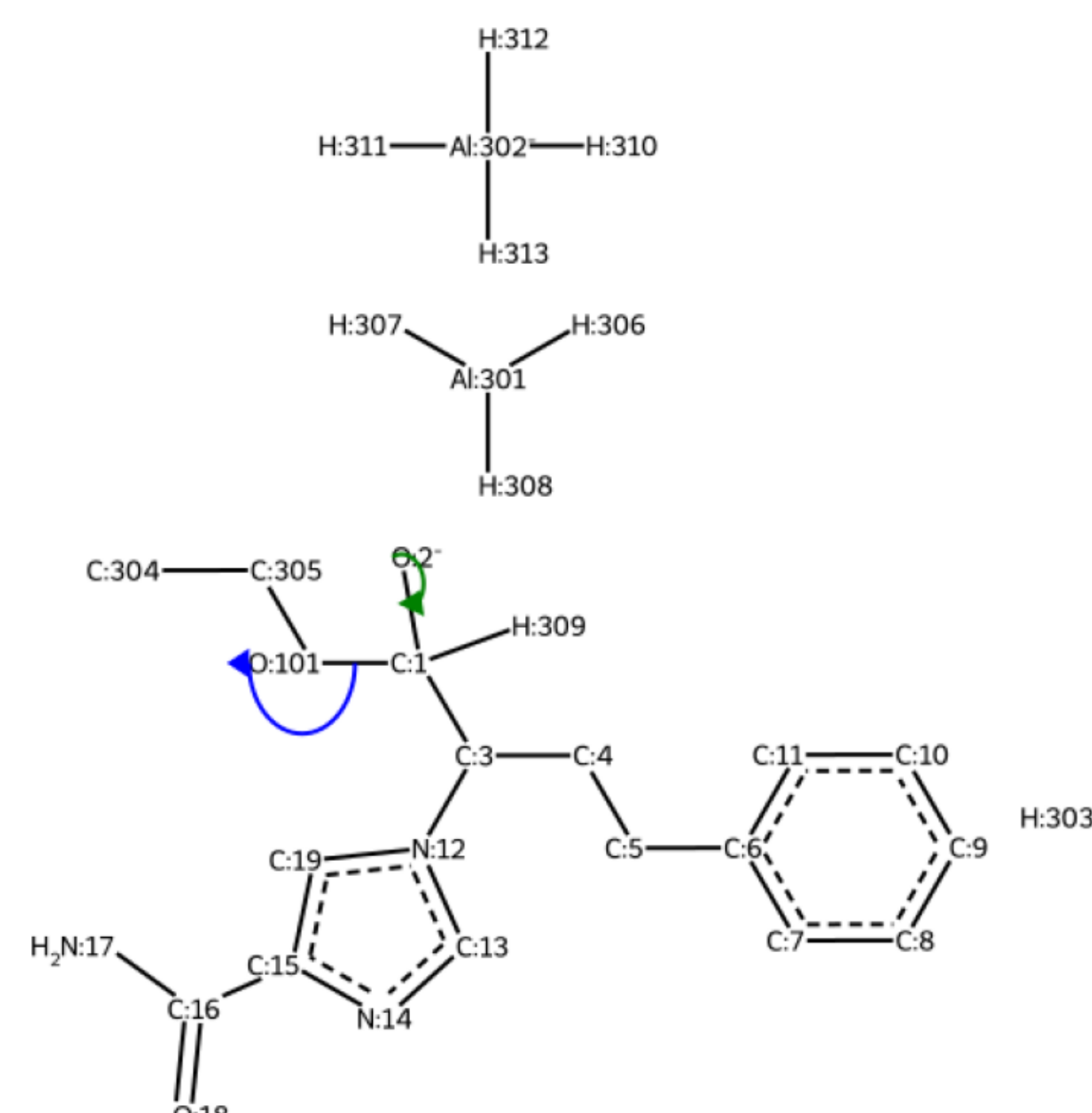
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

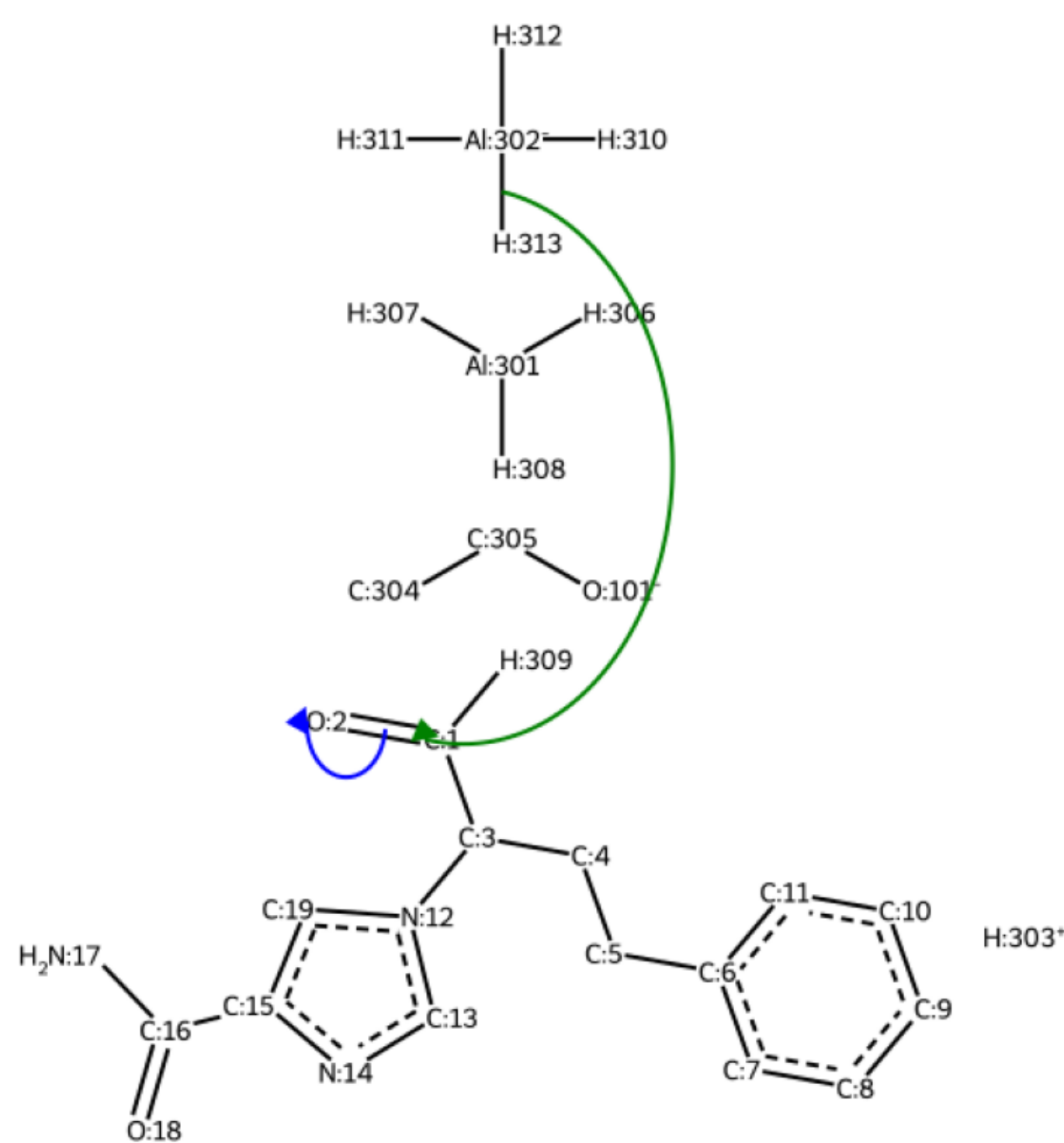
step #1



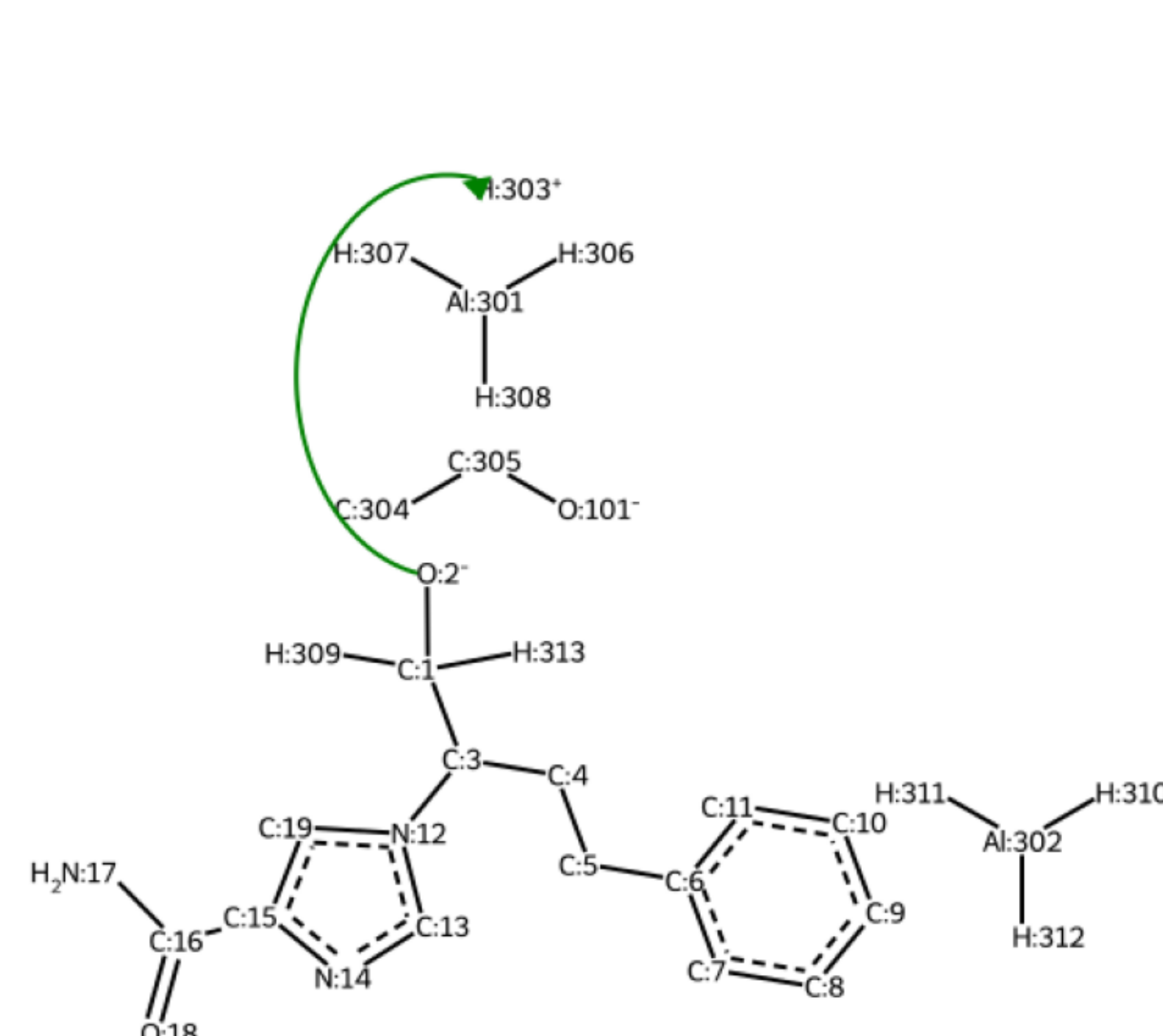
step #2



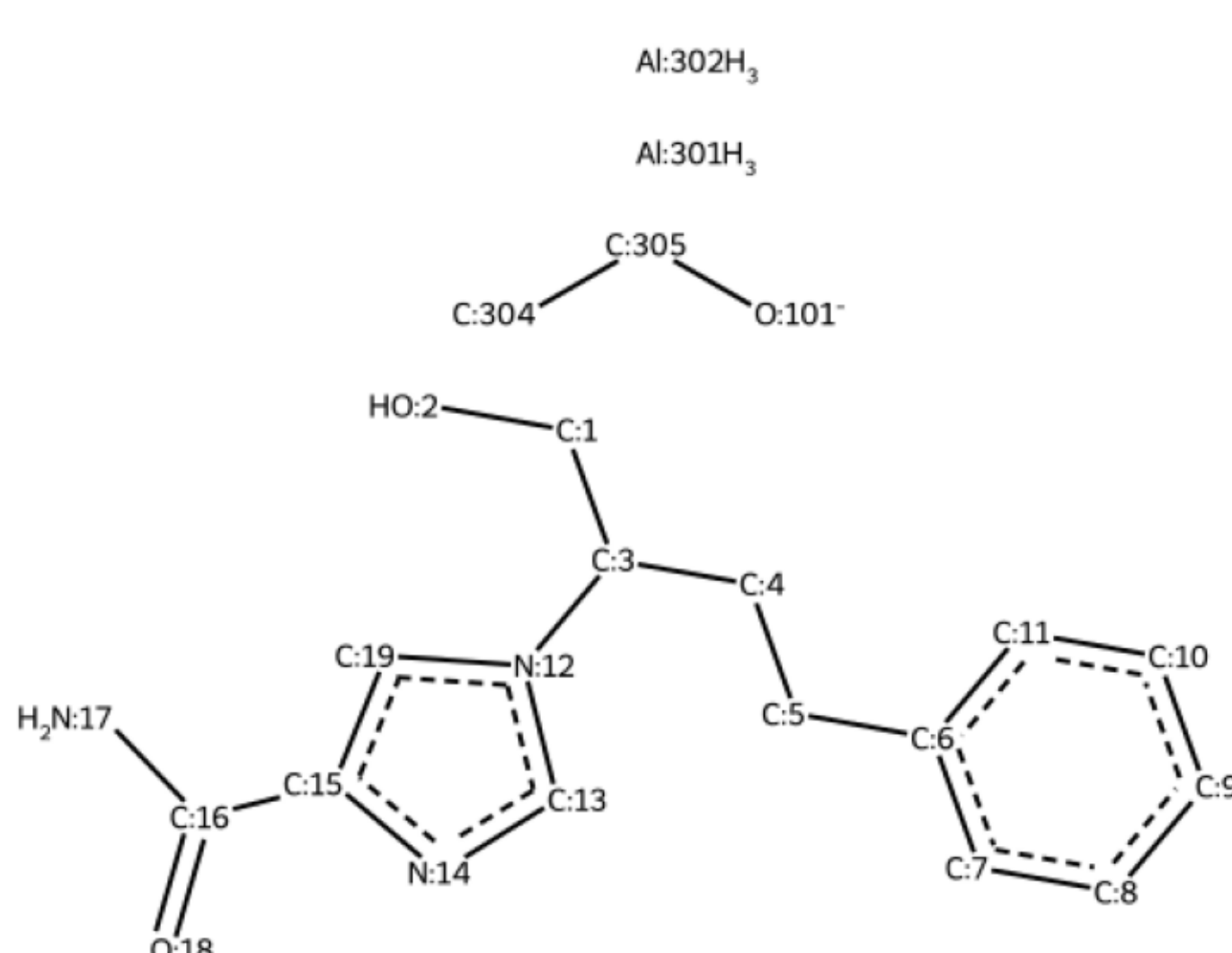
step #3



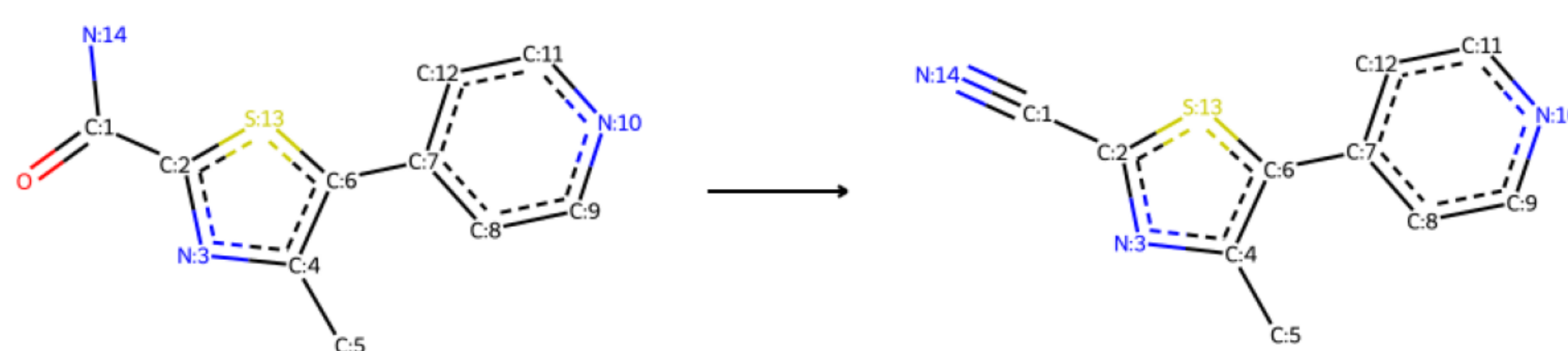
step #4



Product(s)

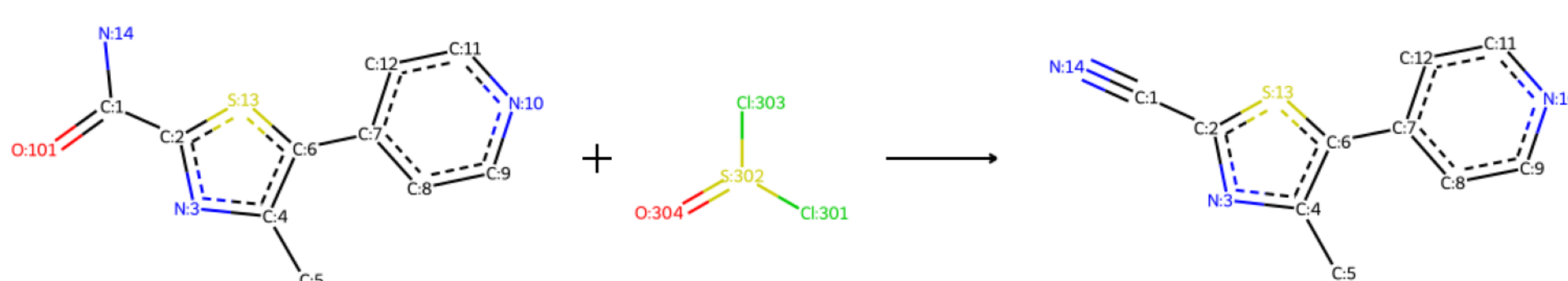


Original reaction
sampled RXN_ID:82)



Identified mechanistic class -
primary_amide_dehydration reaction

Reaction with missing reagents recovered

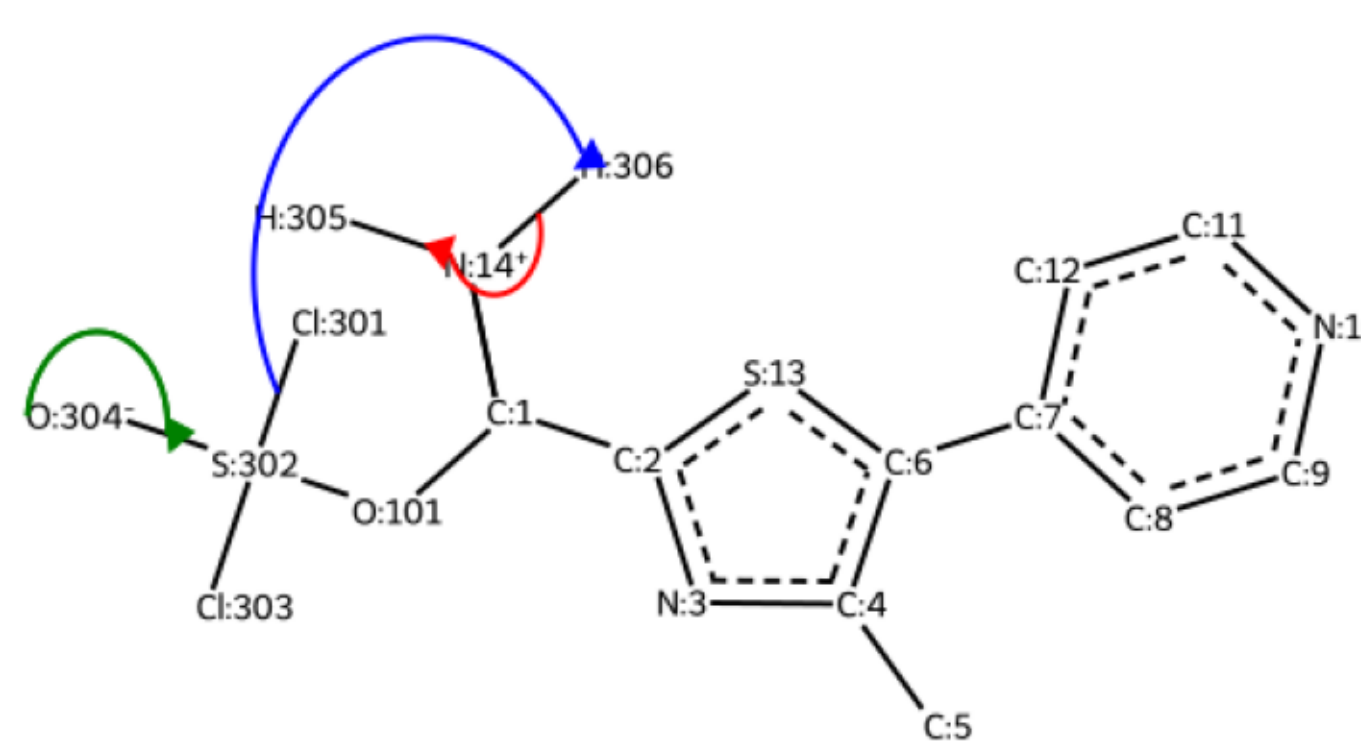
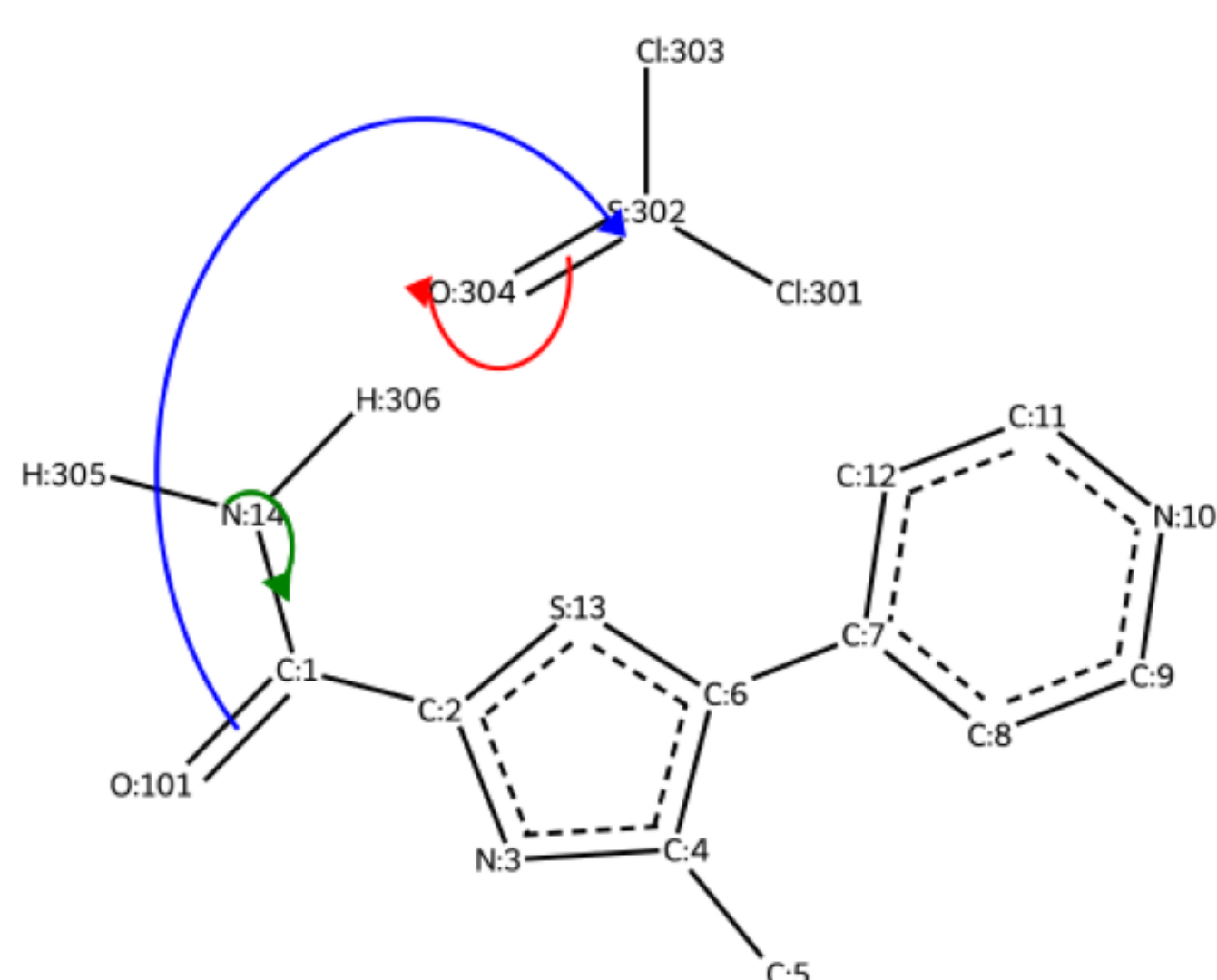


Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

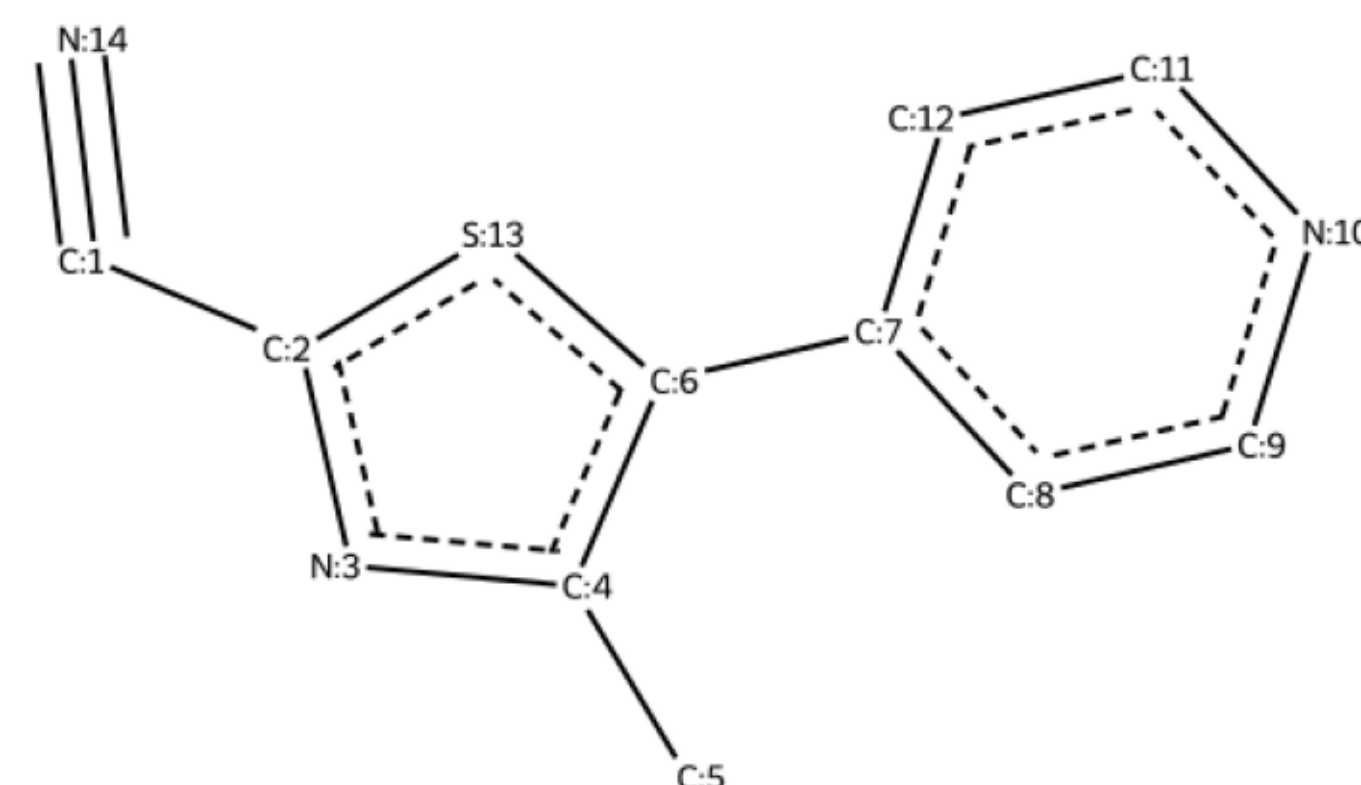
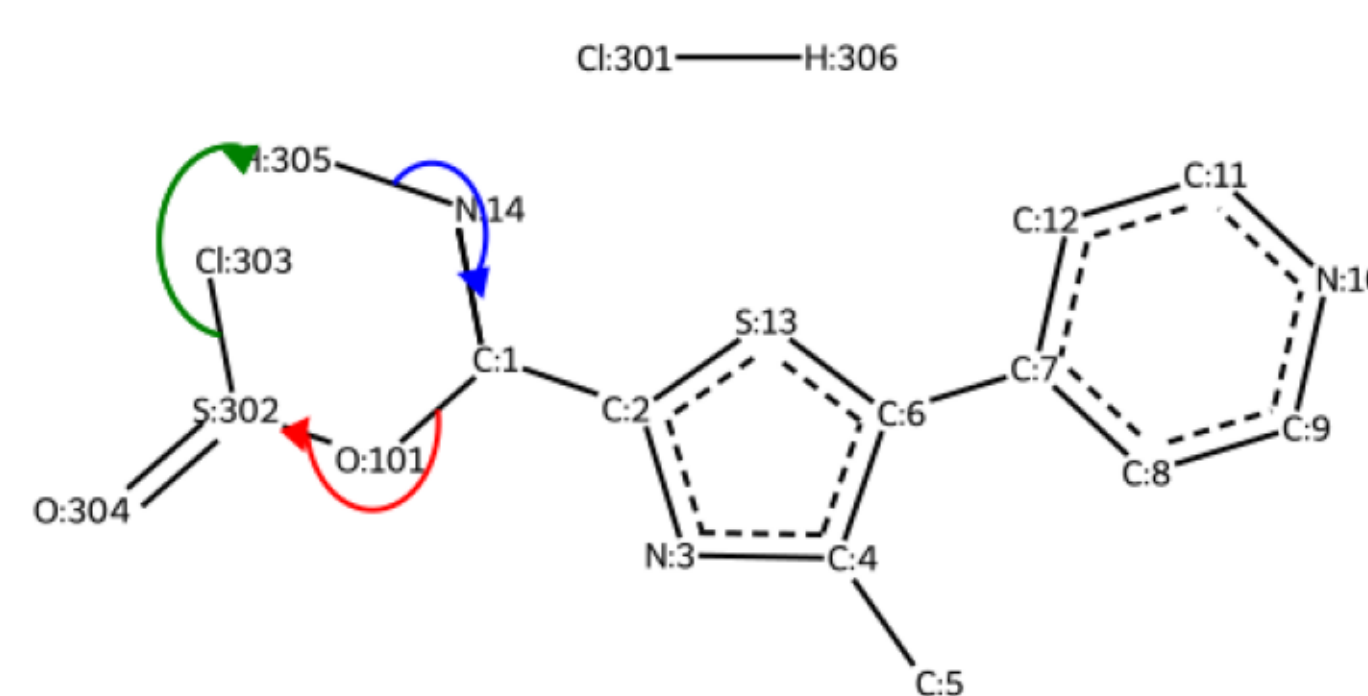
step #1

step #2

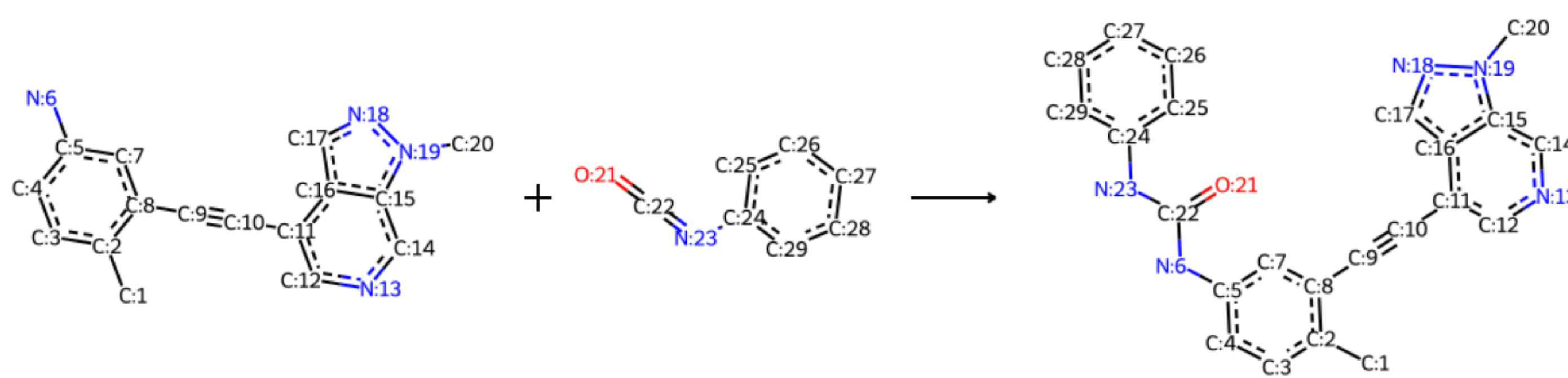


step #3

Product(s)

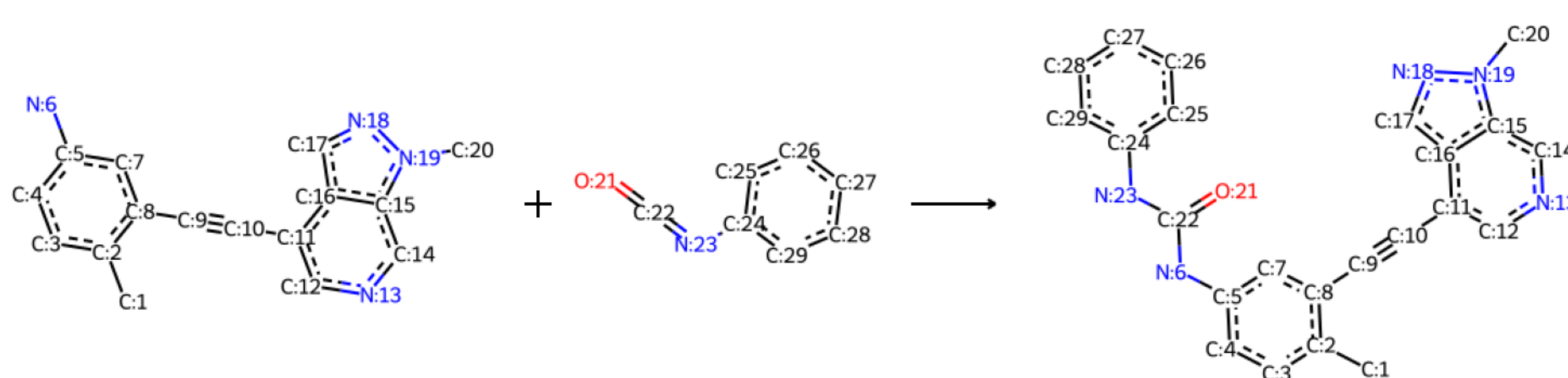


Original reaction
sampled RXN_ID:83)



Identified mechanistic class -
nucleophilic_attack_to_iso(thio)cyanate reaction

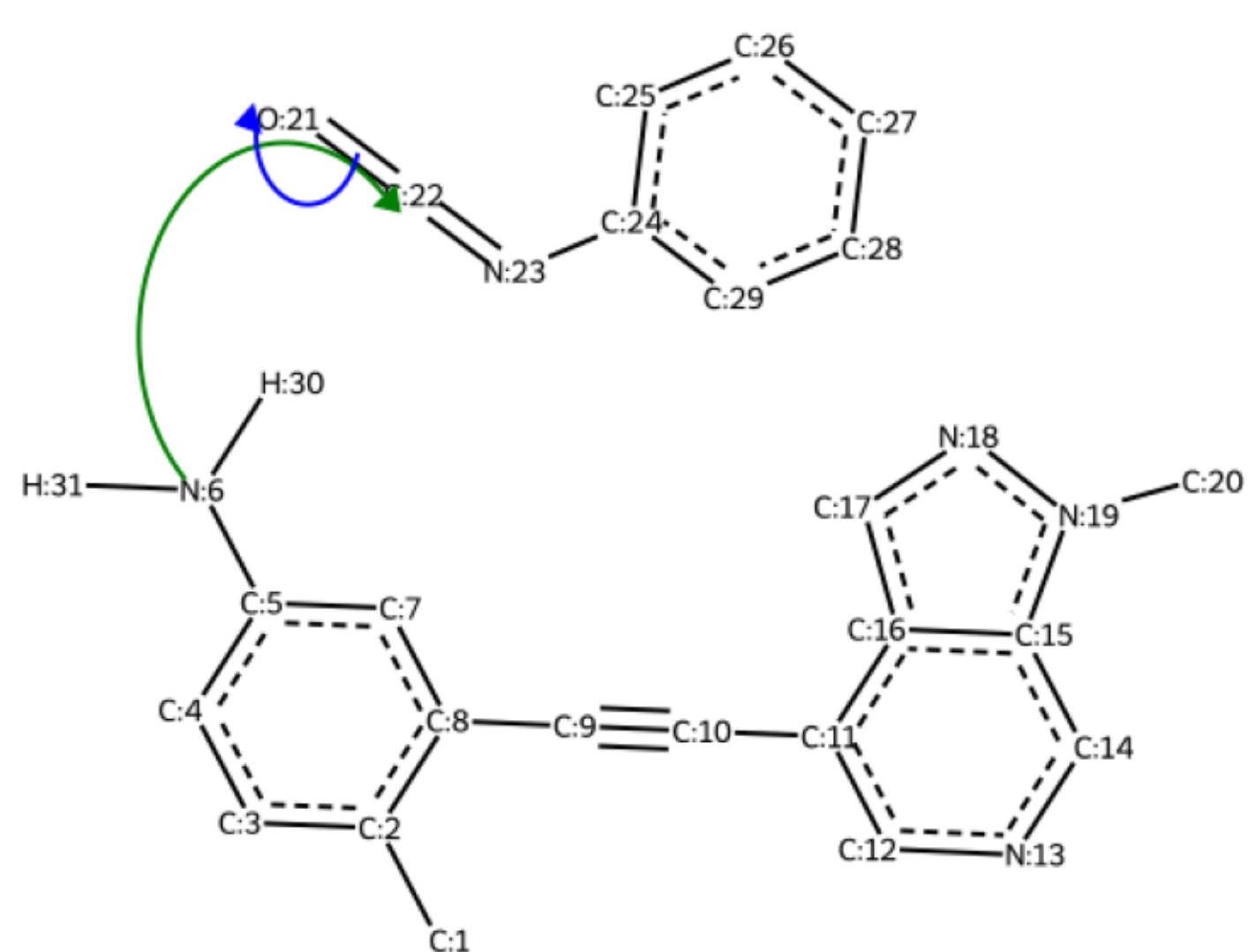
Reaction with missing reagents recovered



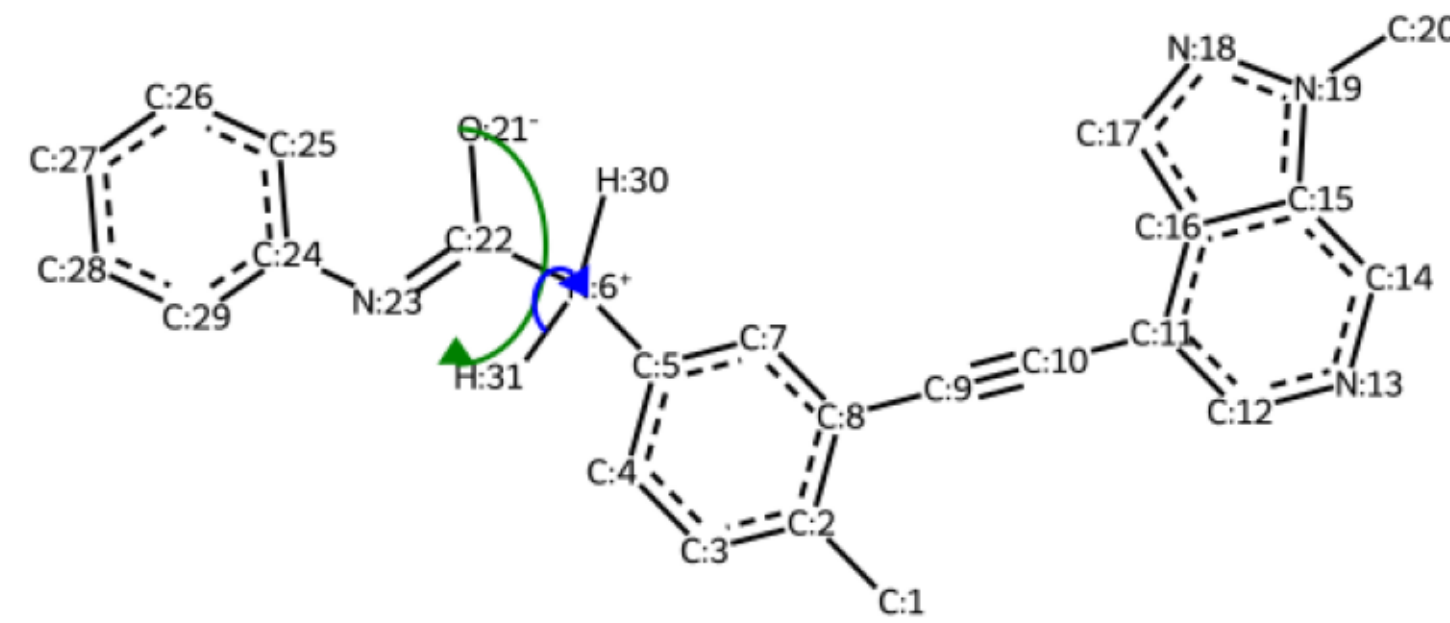
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

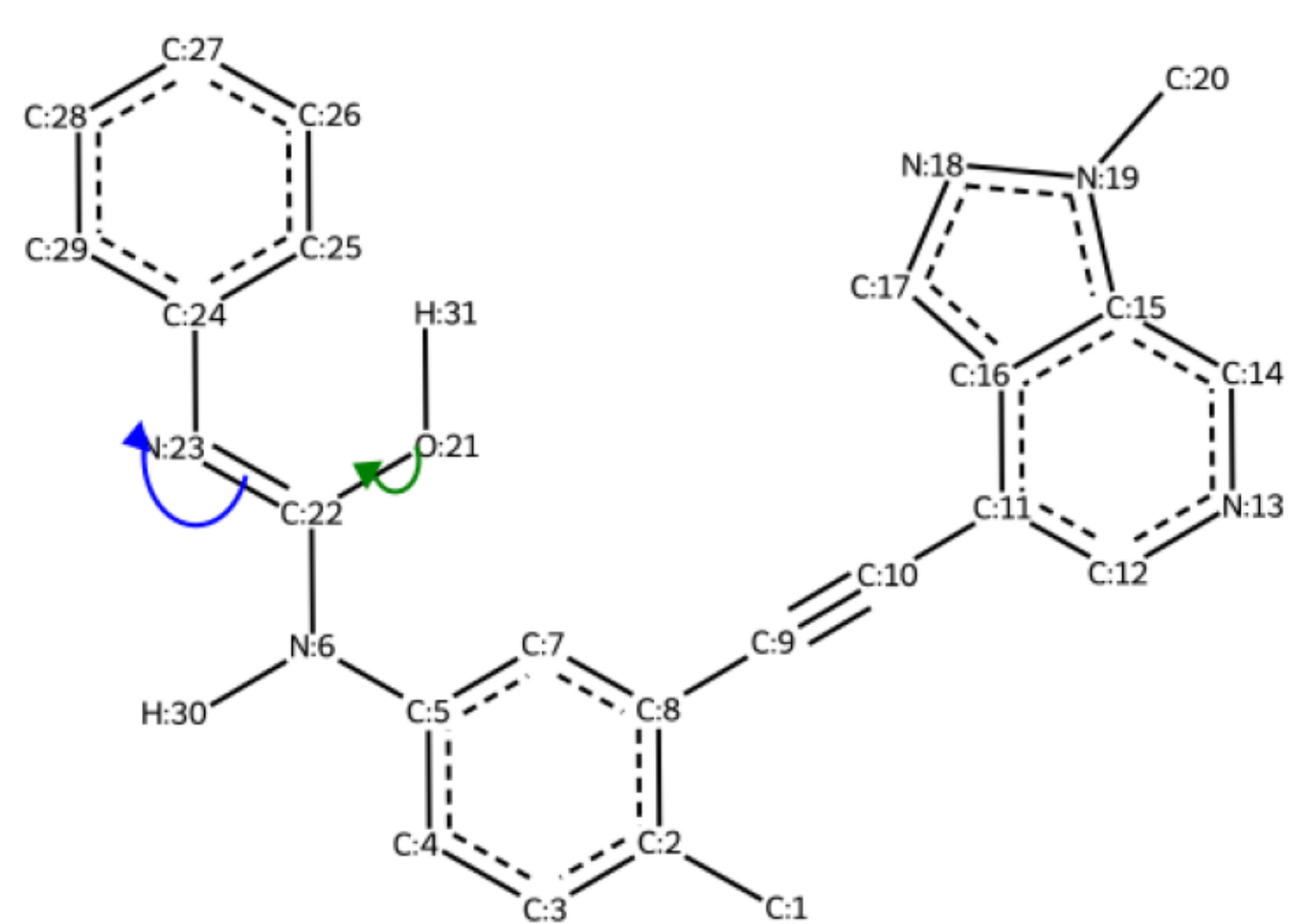
step #1



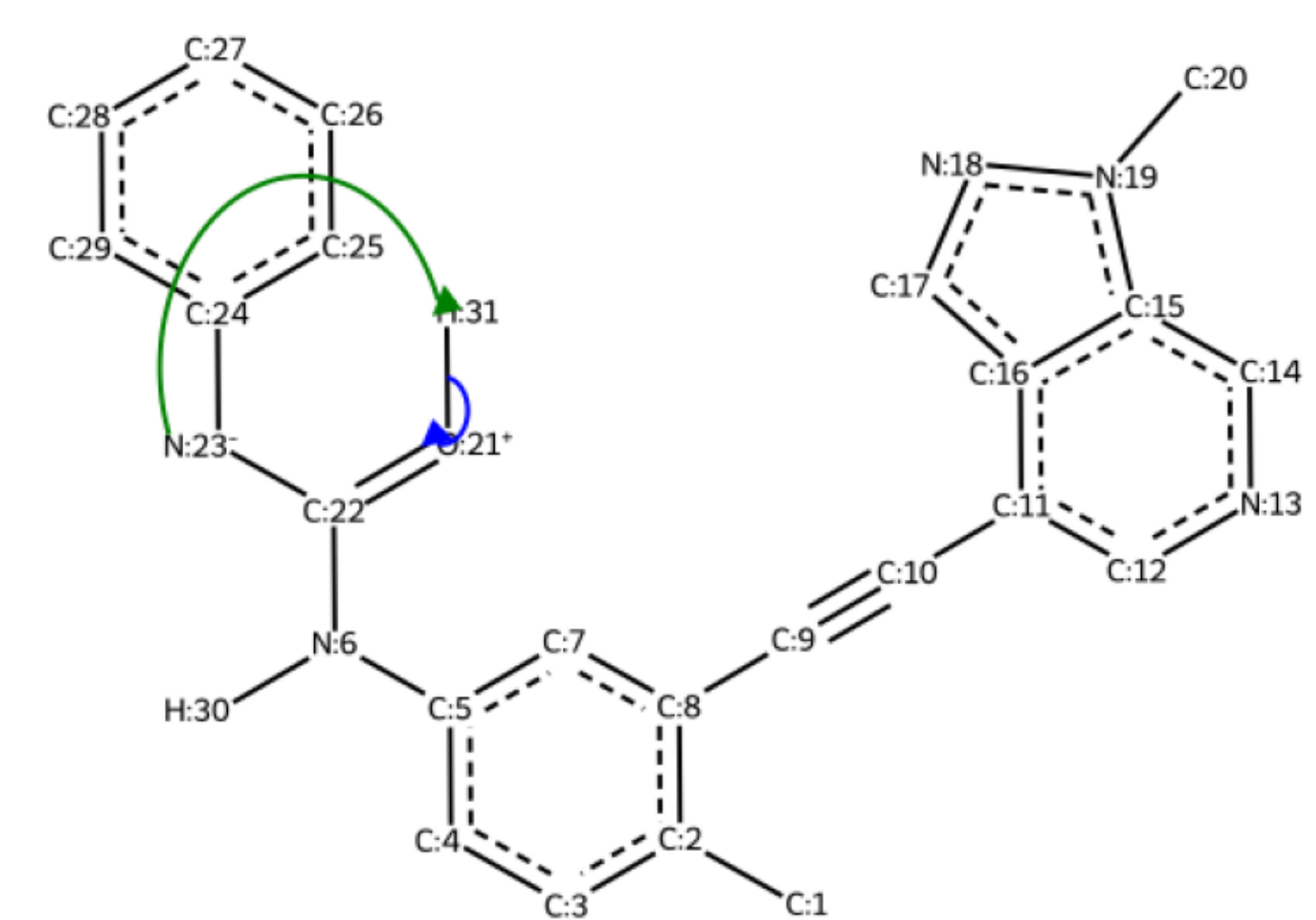
step #2



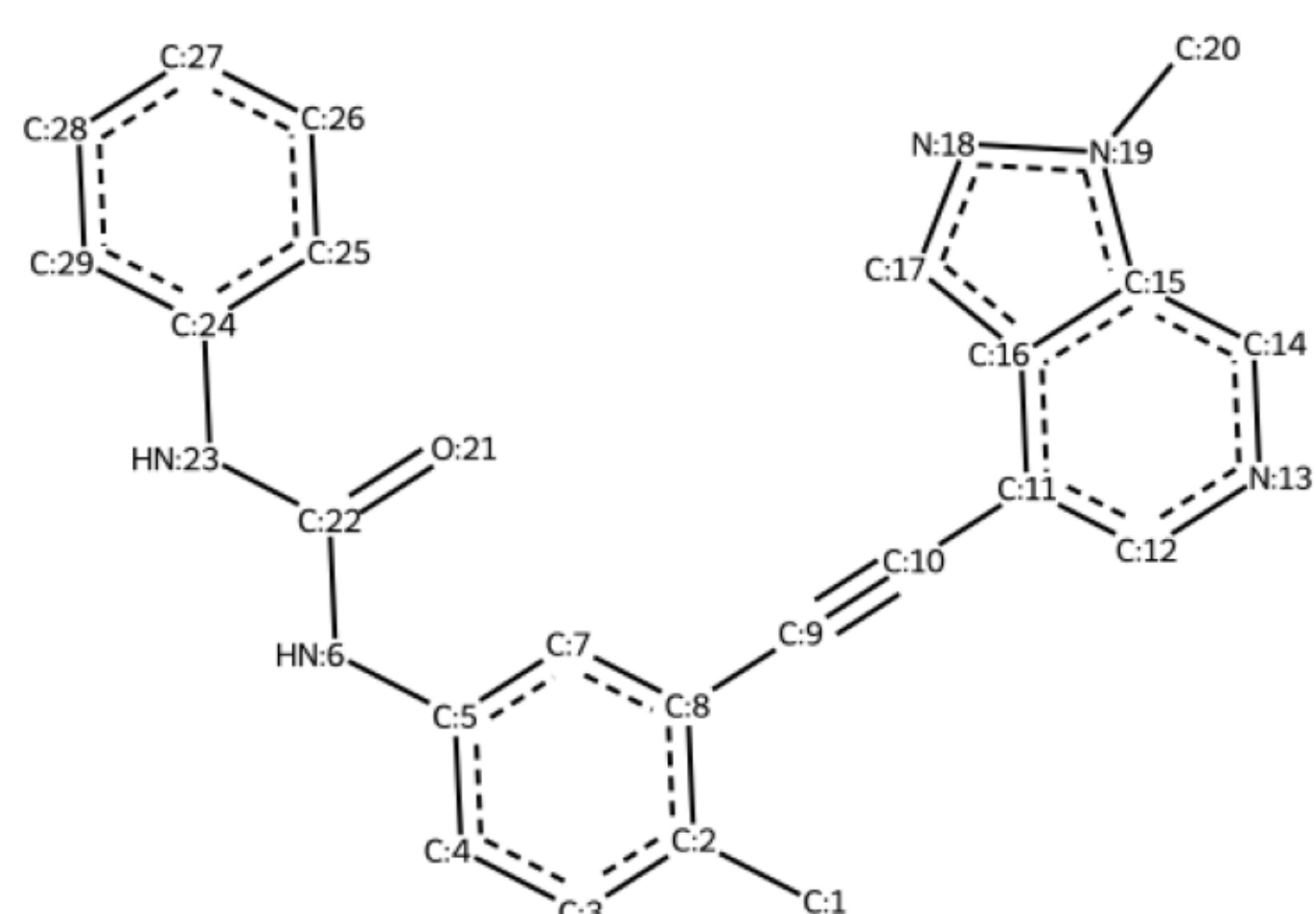
step #3



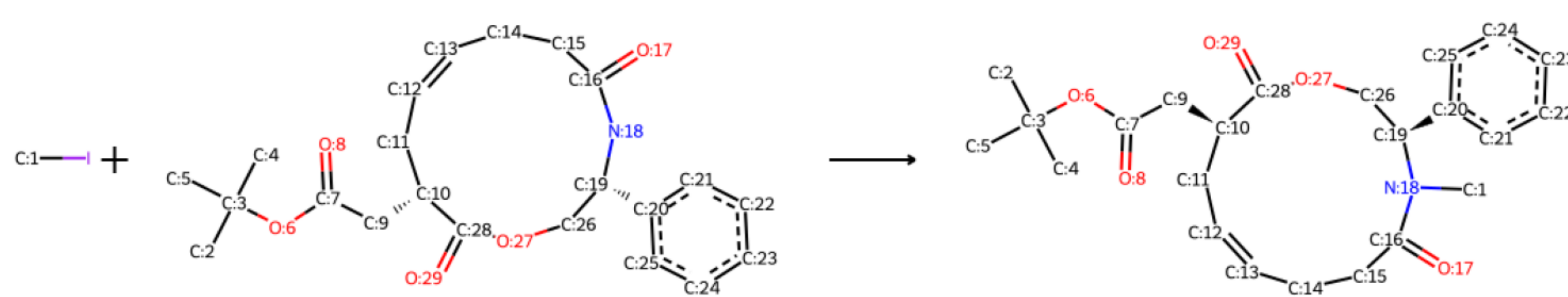
step #4



Product(s)

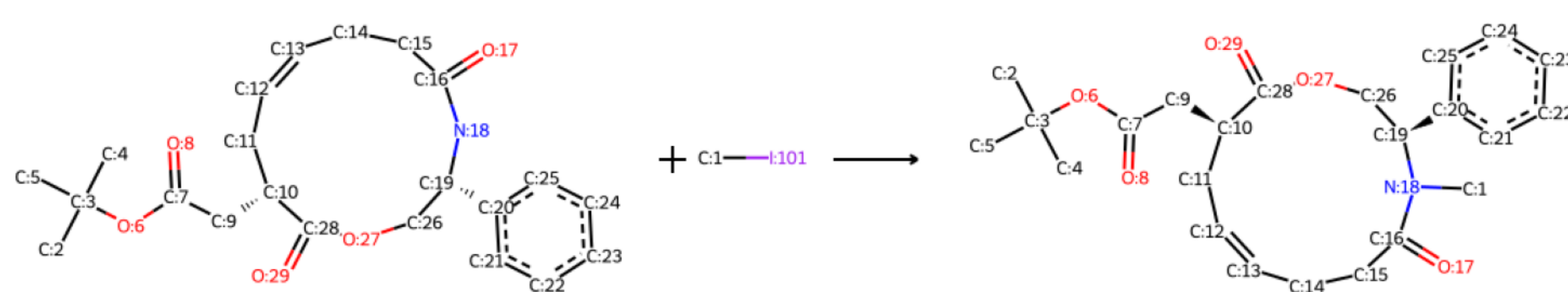


Original reaction sampled RXN_ID:84)



Identified mechanistic class -
SN2 reaction

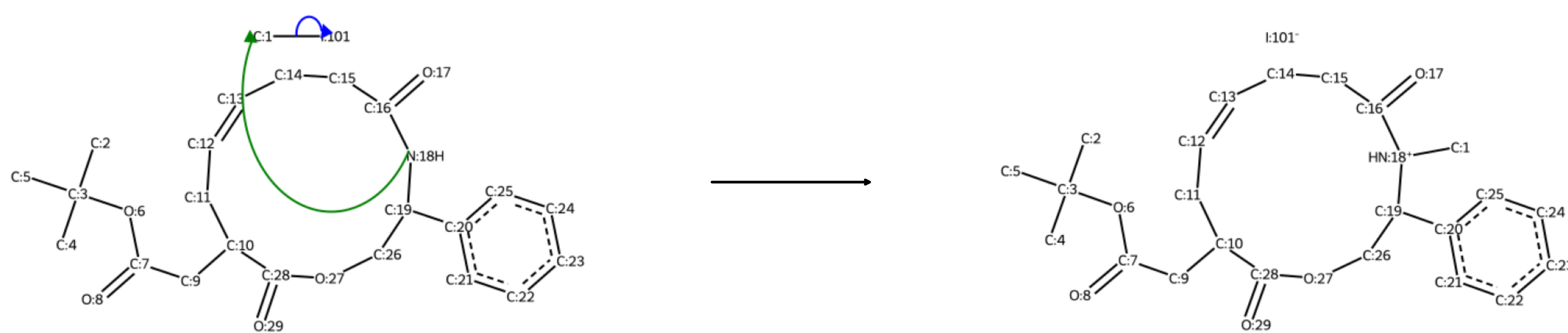
Reaction with missing reagents recovered



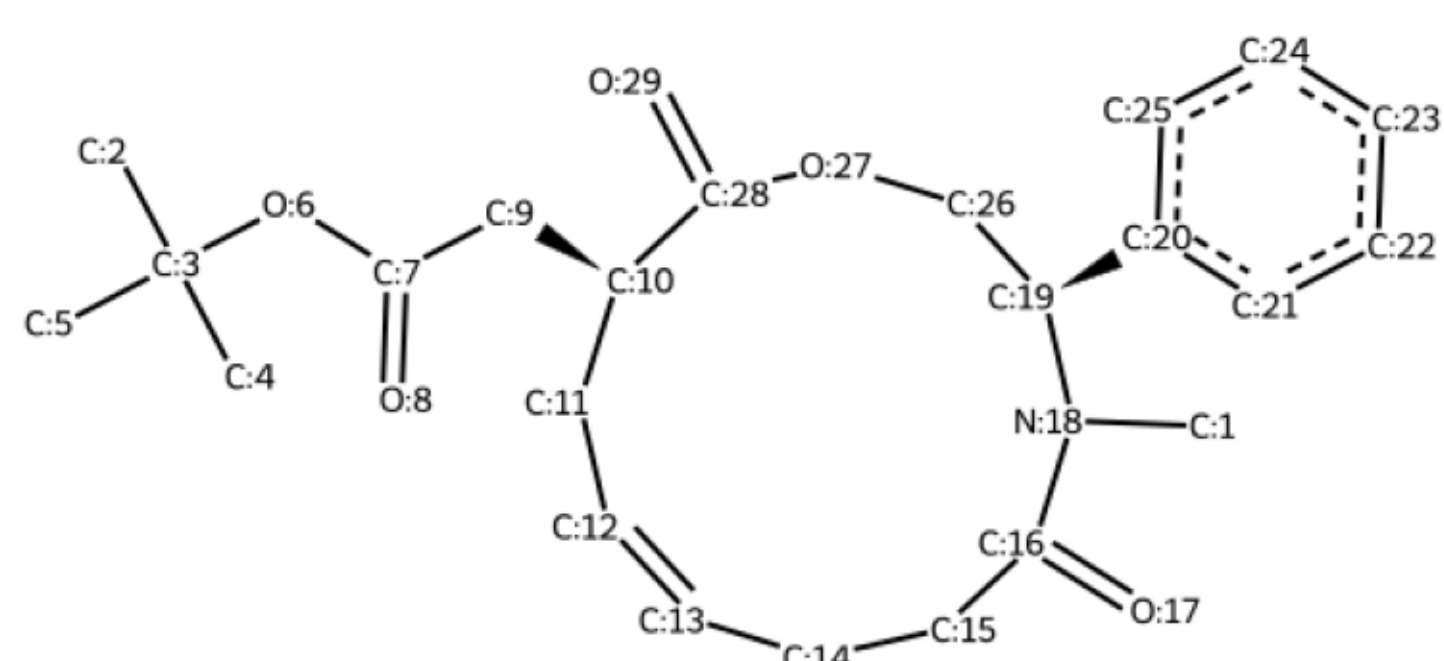
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

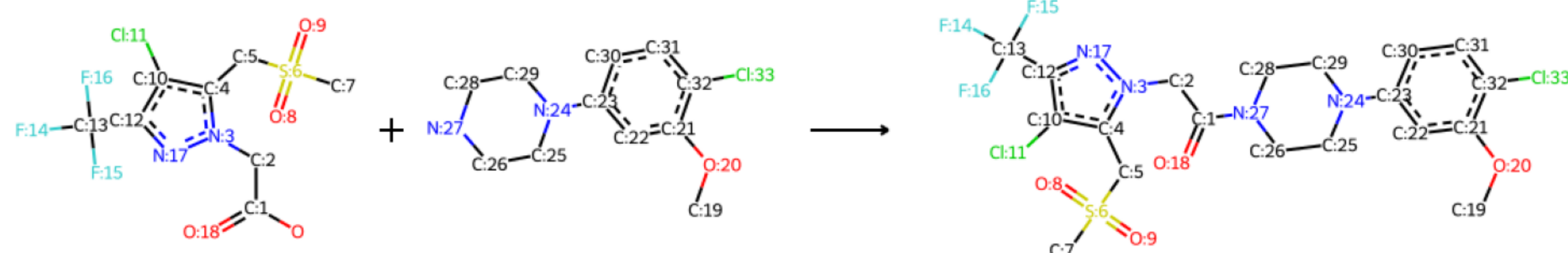
step #1



Product(s)

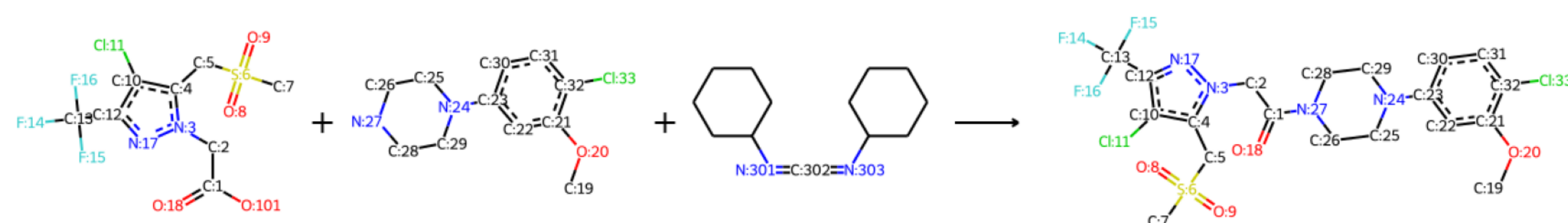


Original reaction
sampled RXN_ID:85)



Identified mechanistic class -
DCC_condensation reaction

Reaction with missing reagents recovered

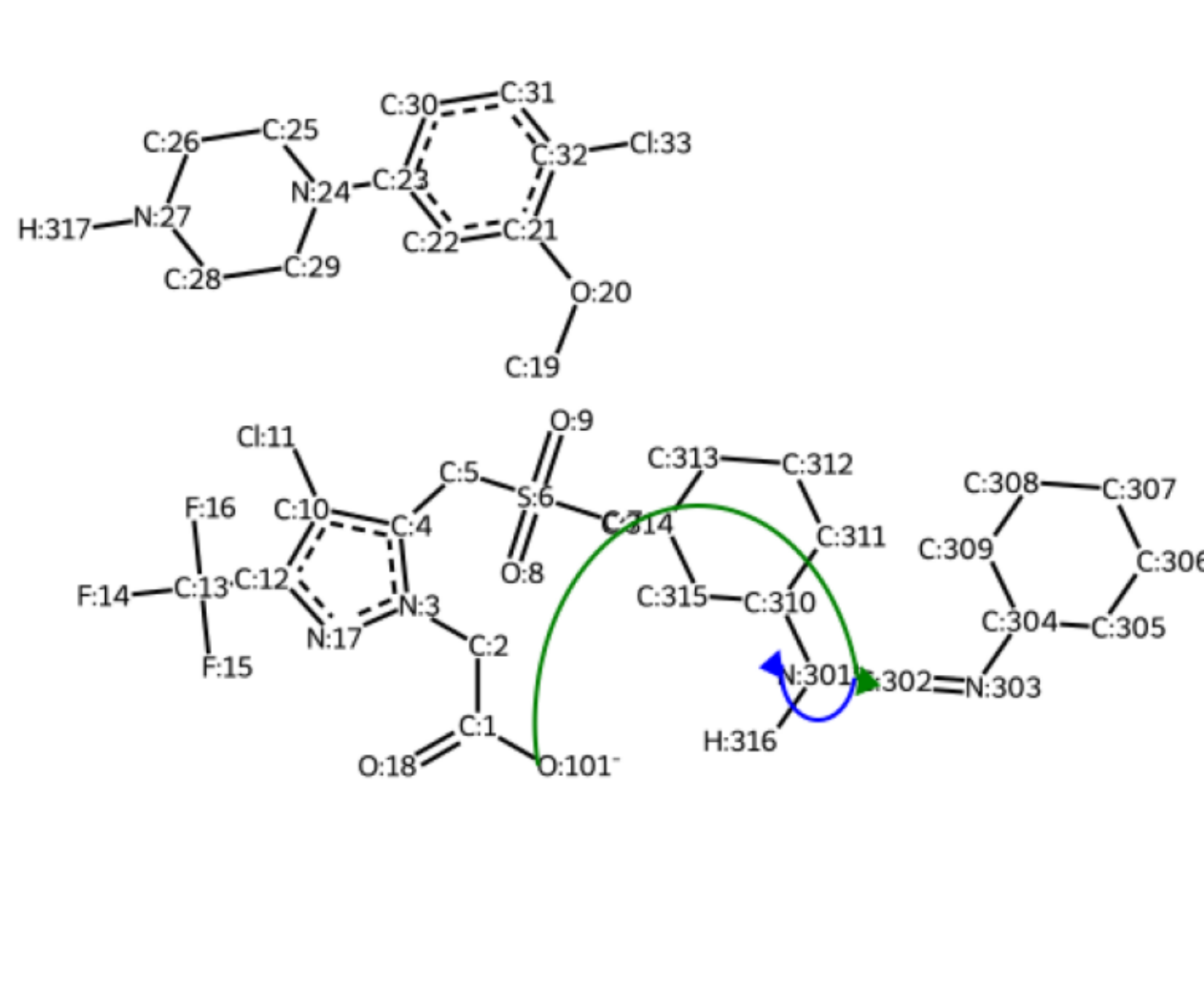
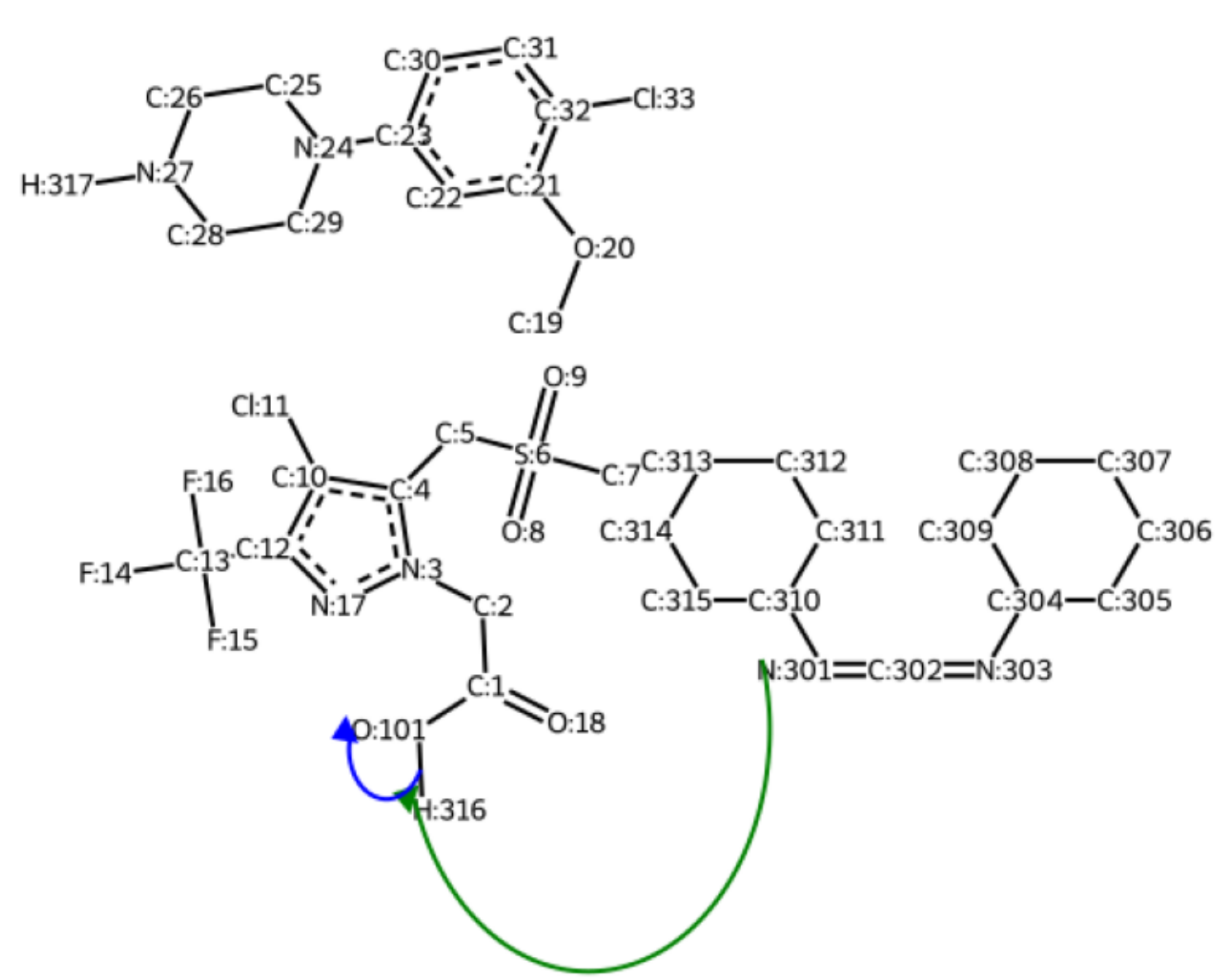


Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

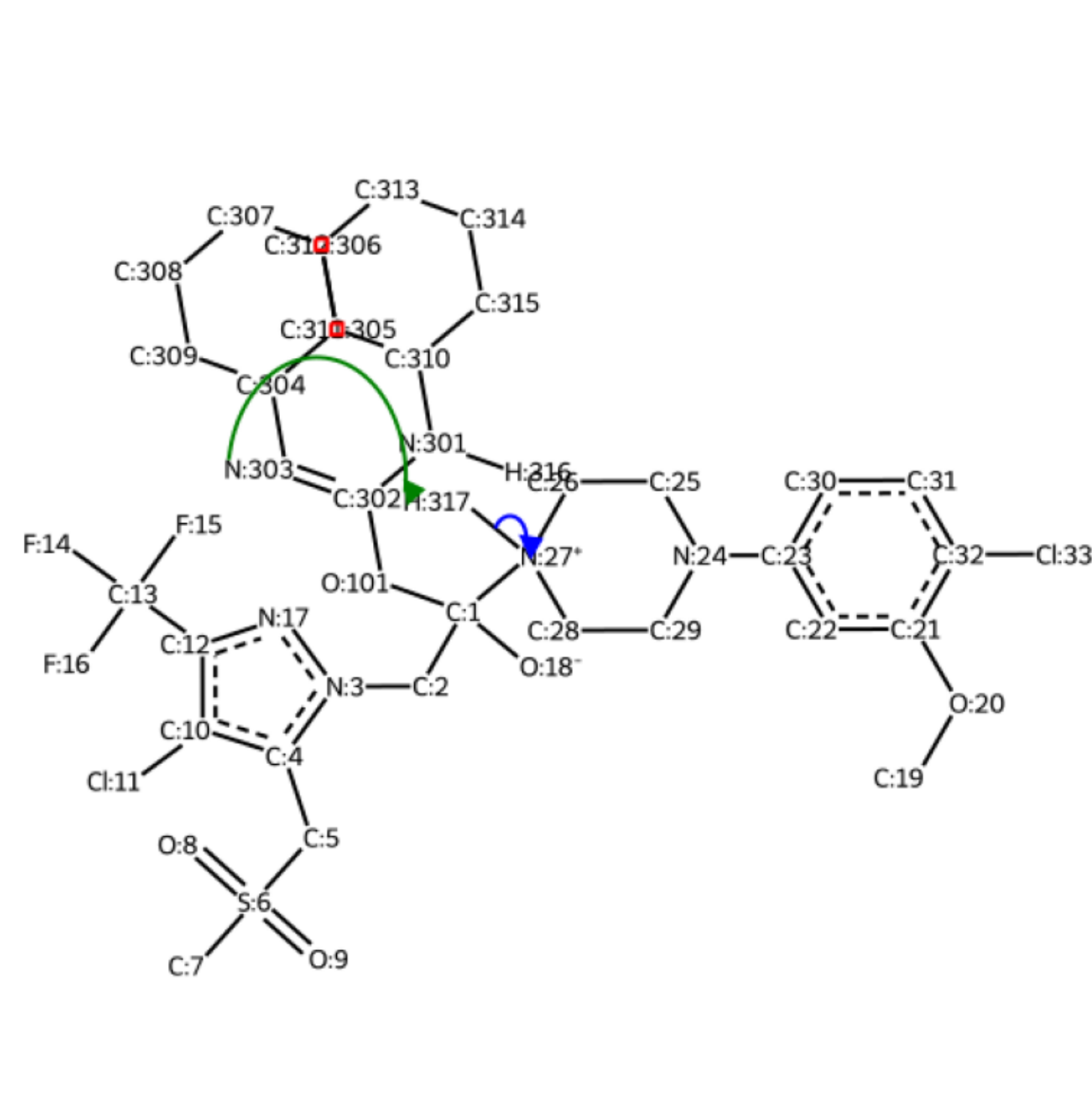
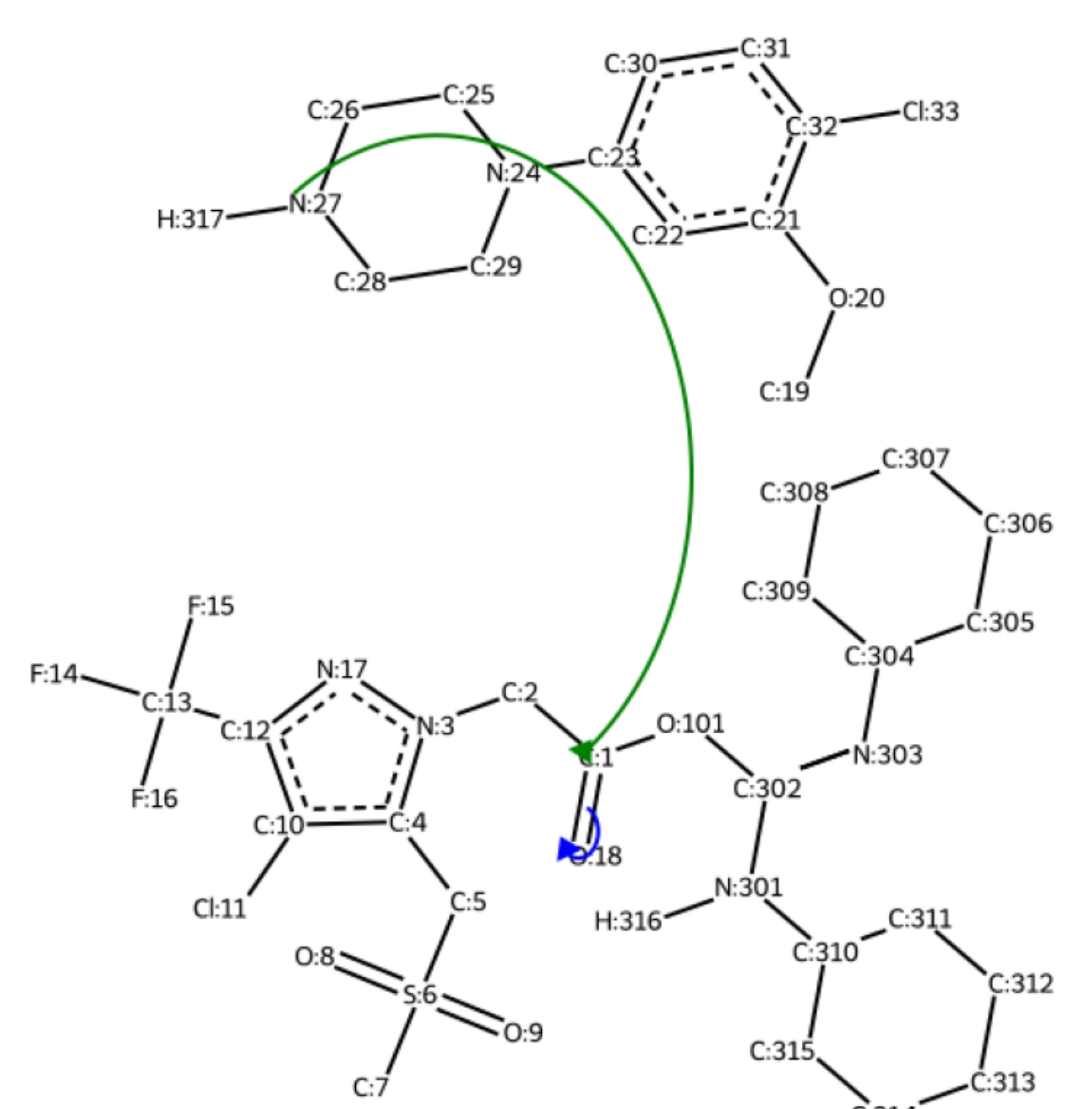
step #1

step #2



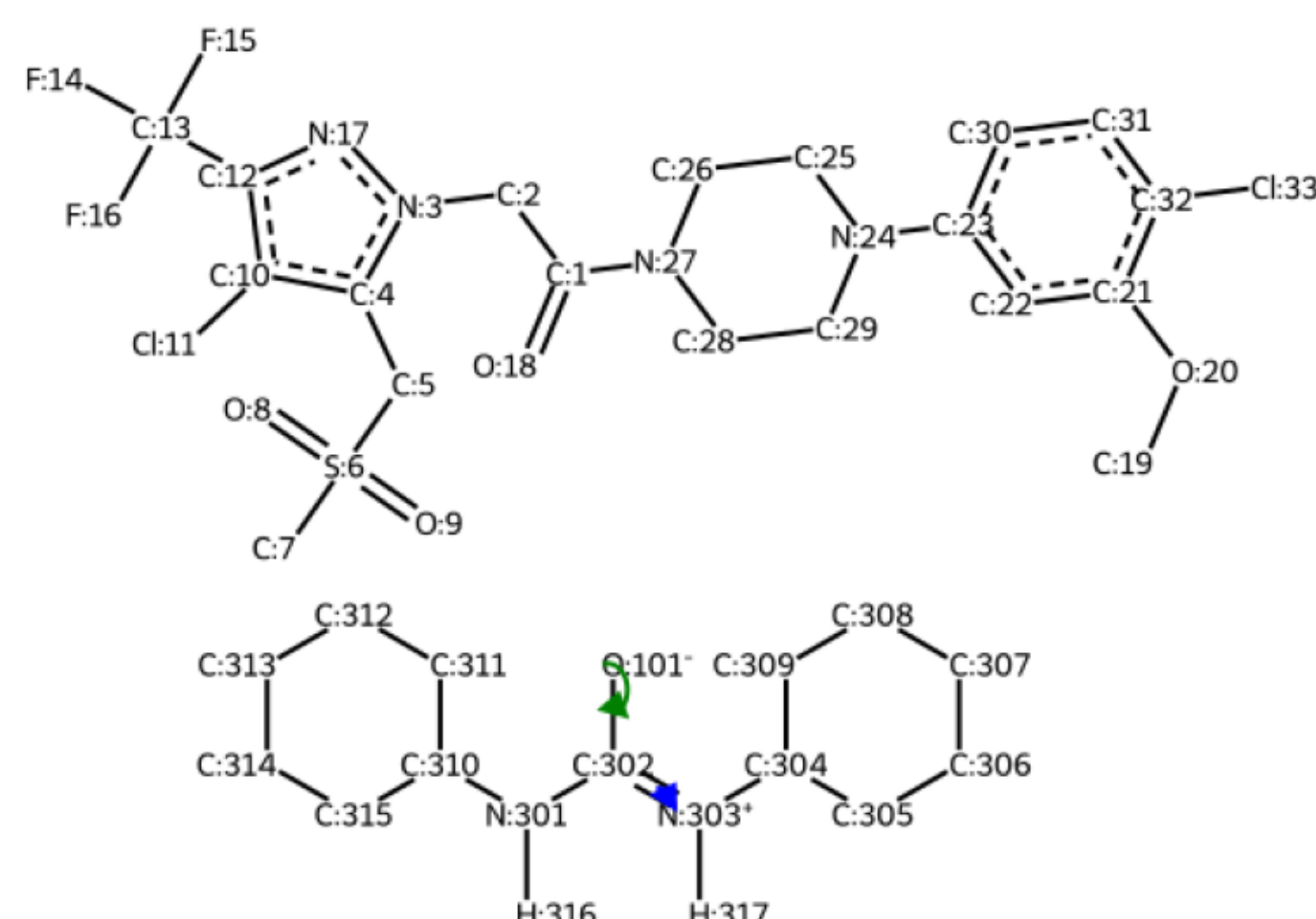
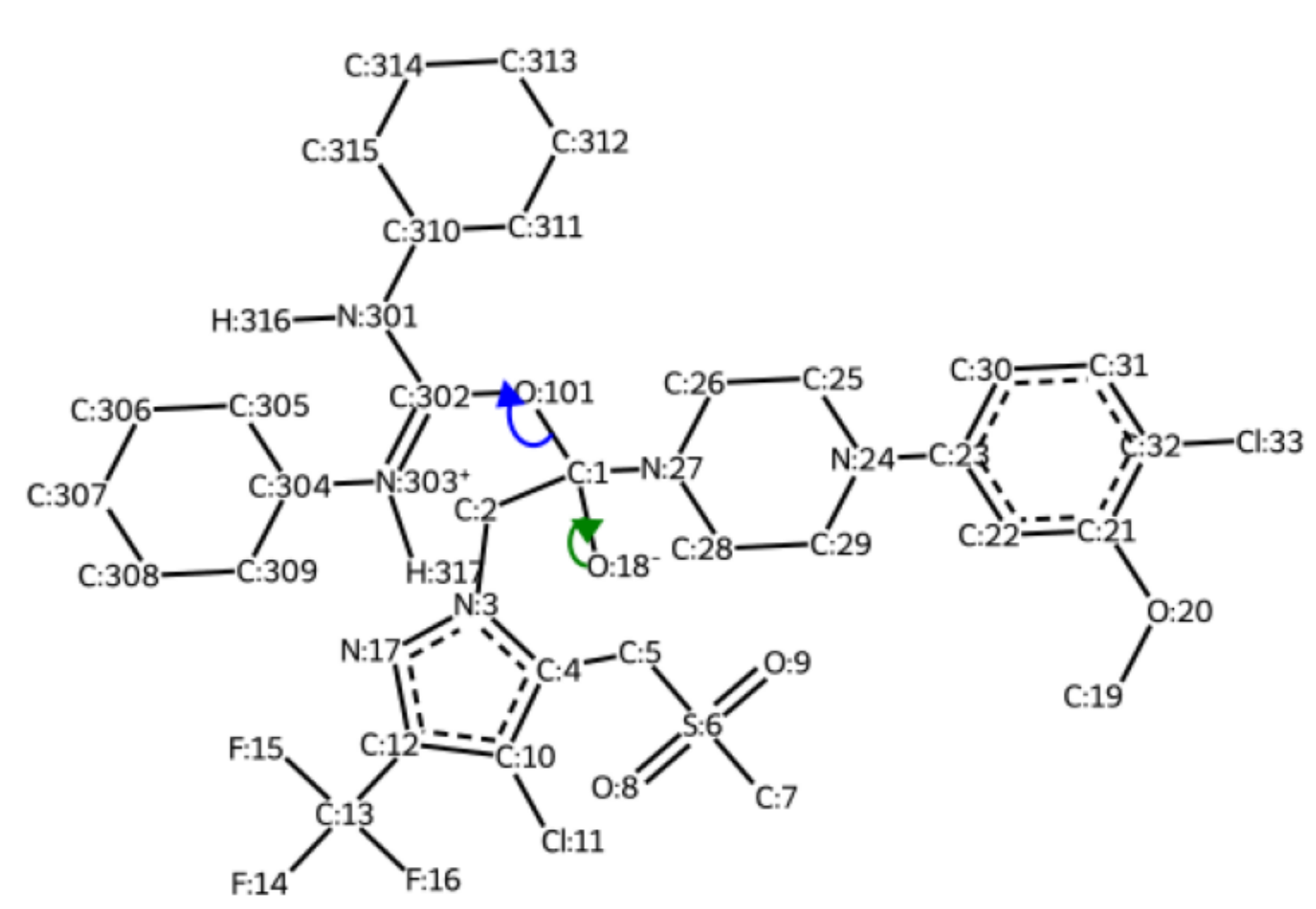
step #3

step #4

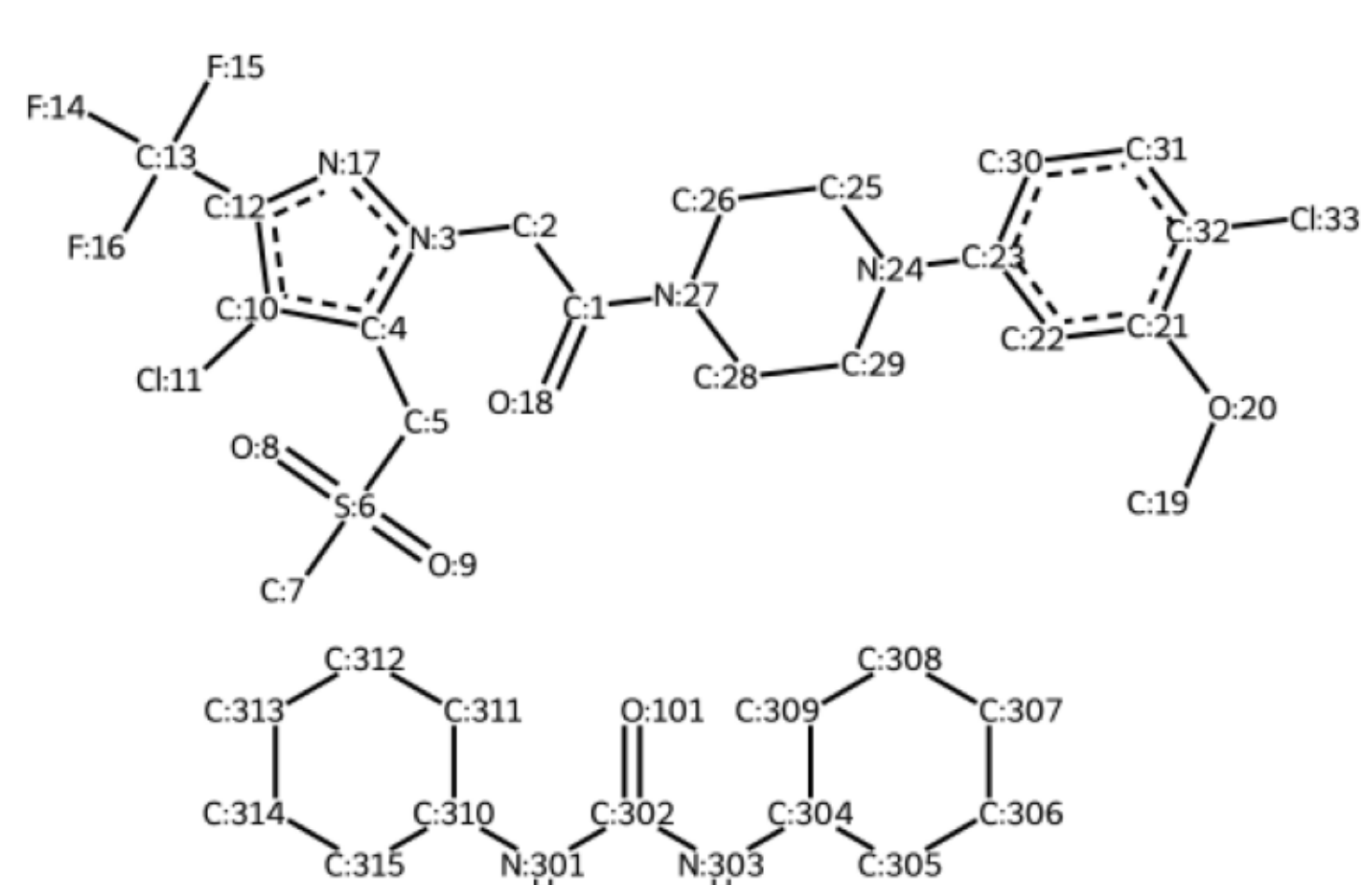


step #5

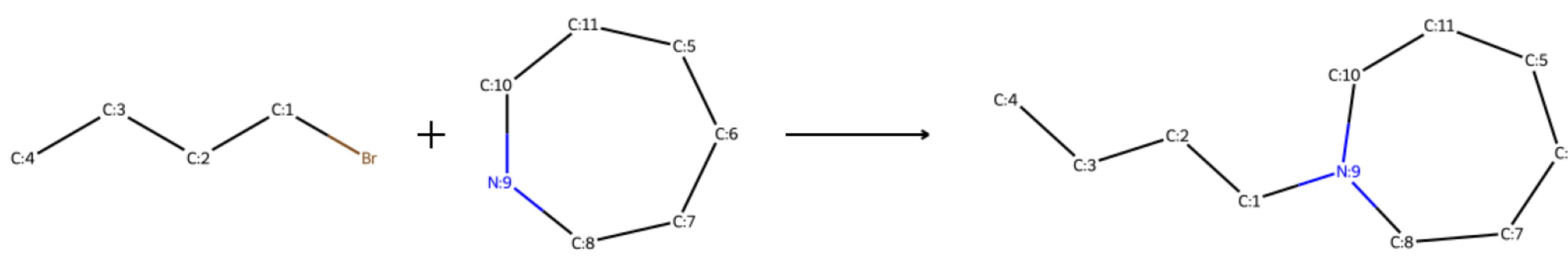
step #6



Product(s)

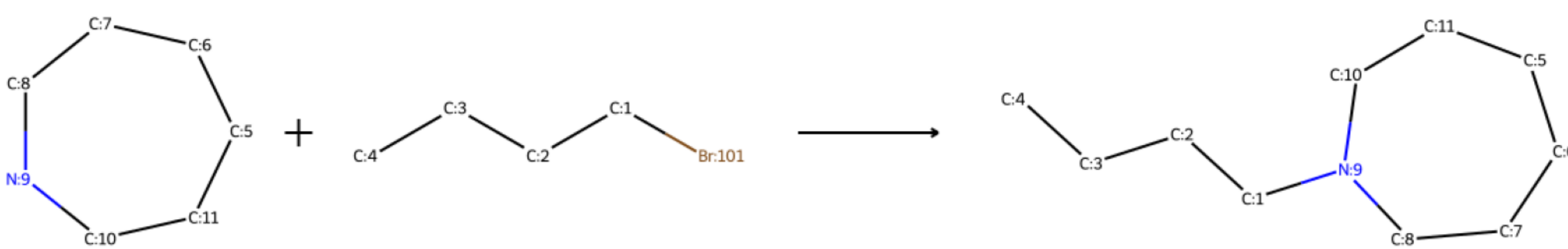


Original reaction
sampled RXN_ID:86)



Identified mechanistic class -
SN2 reaction

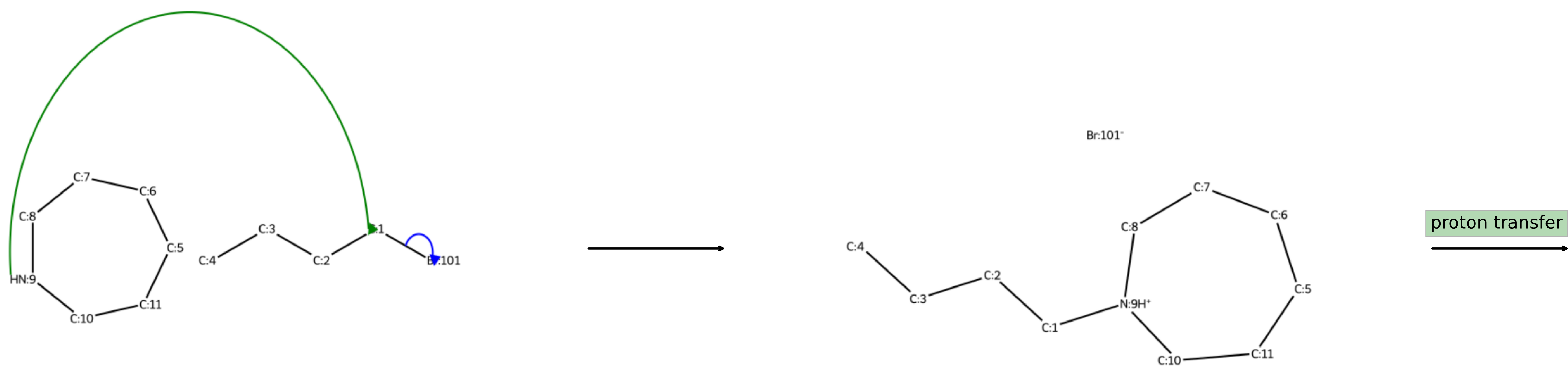
Reaction with missing reagents recovered



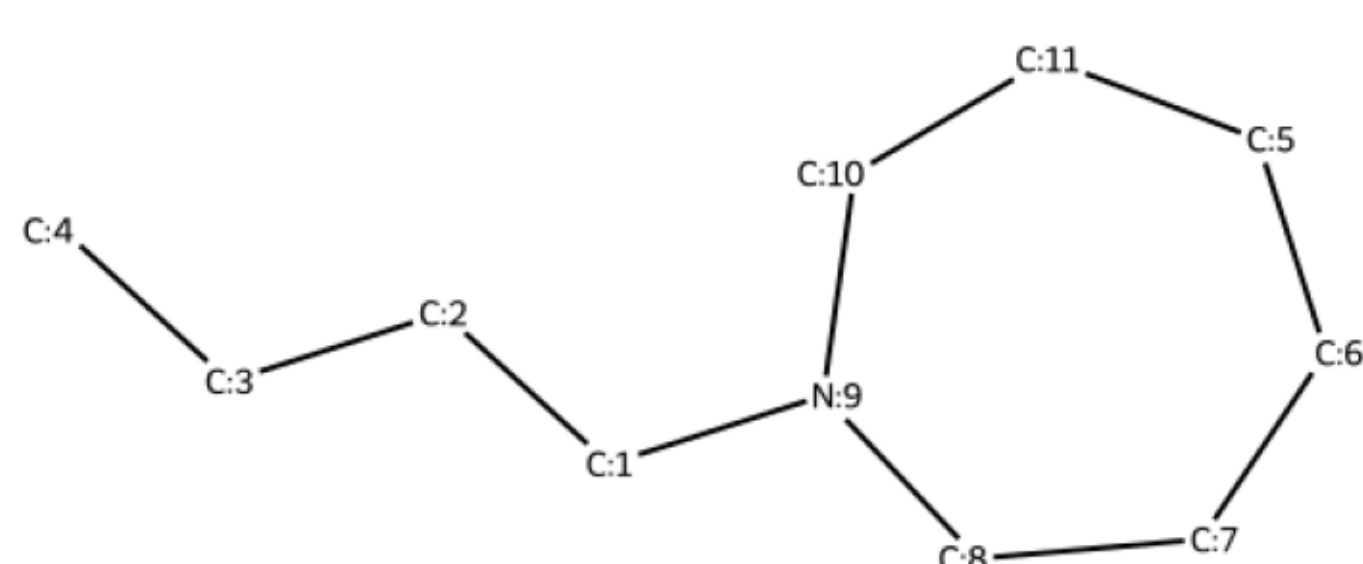
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1



Product(s)

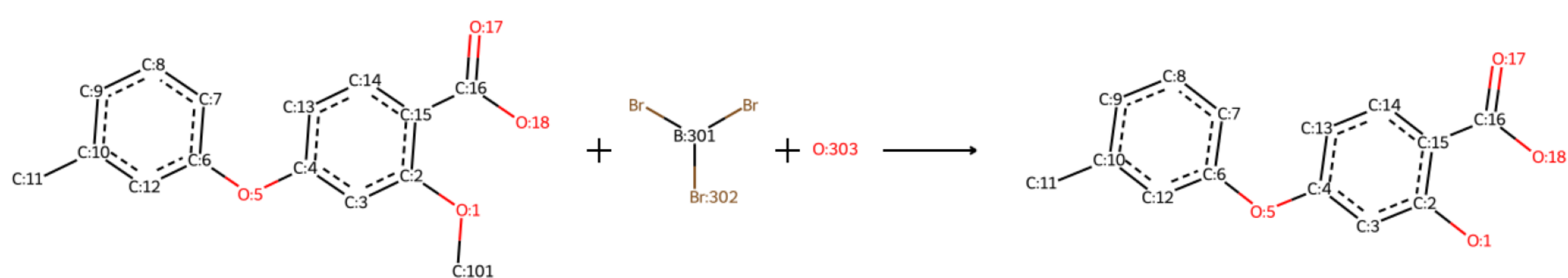


Original reaction
sampled RXN_ID:87)



Identified mechanistic class -
O_demethylation reaction

Reaction with missing reagents recovered

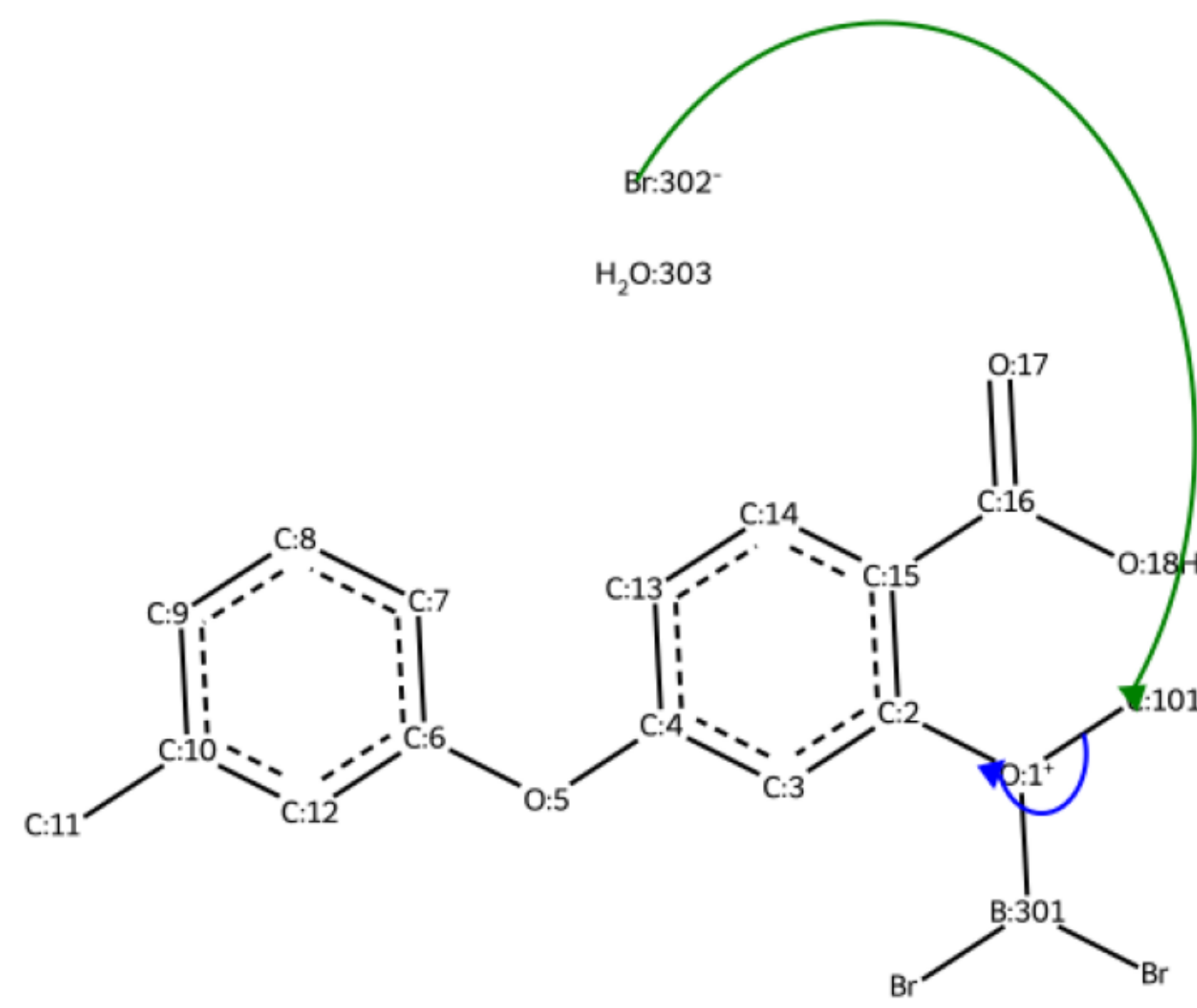
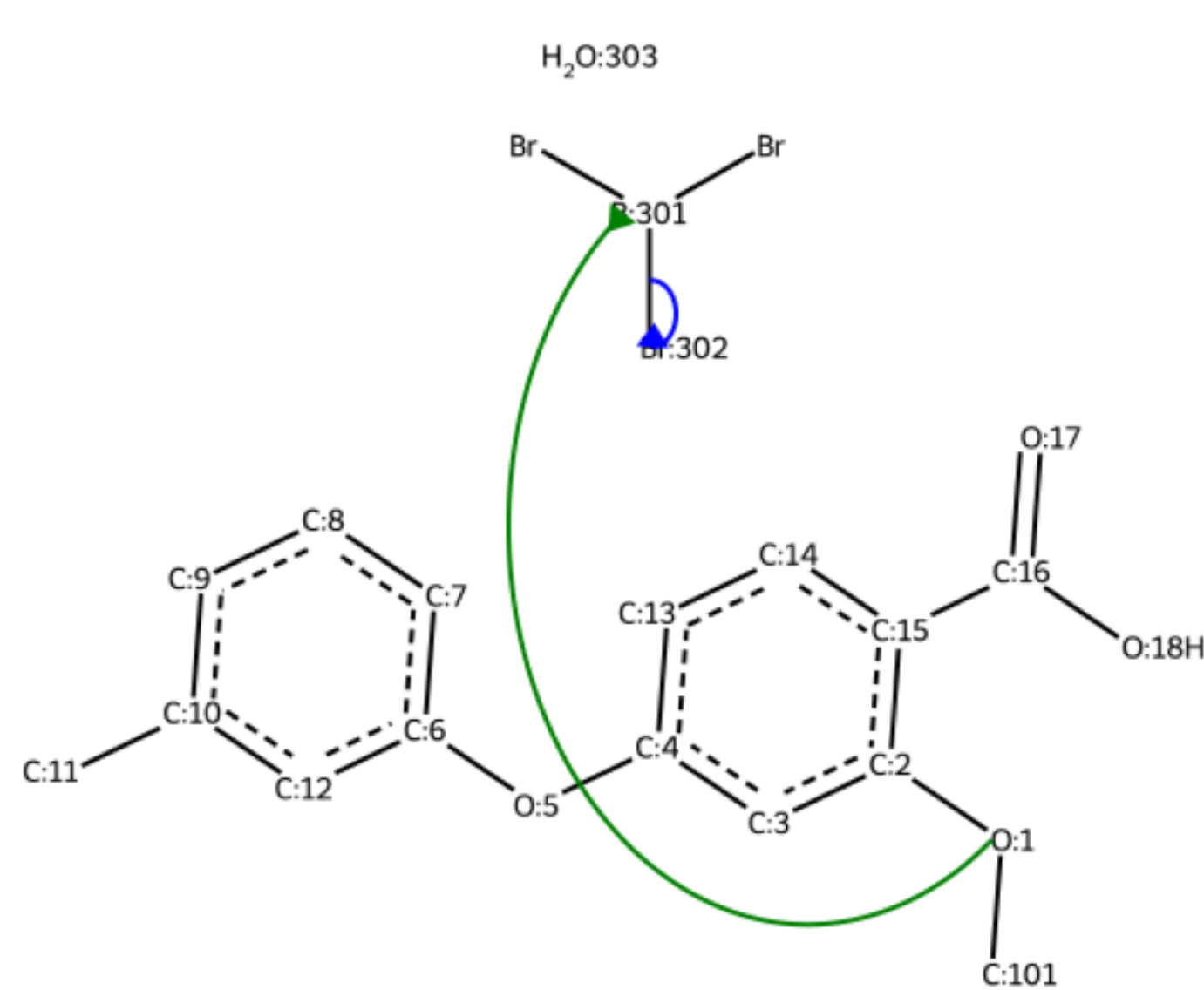


Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

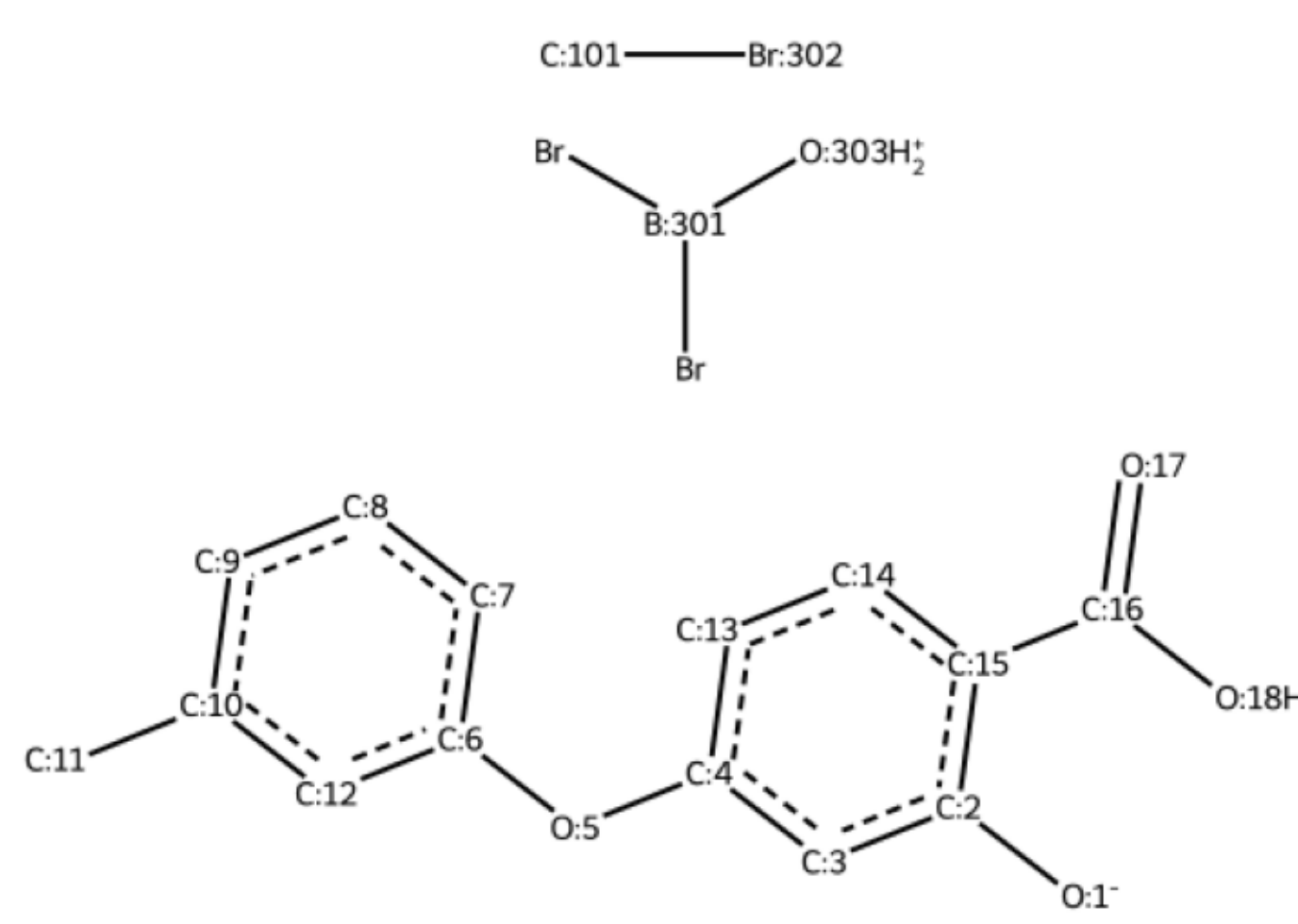
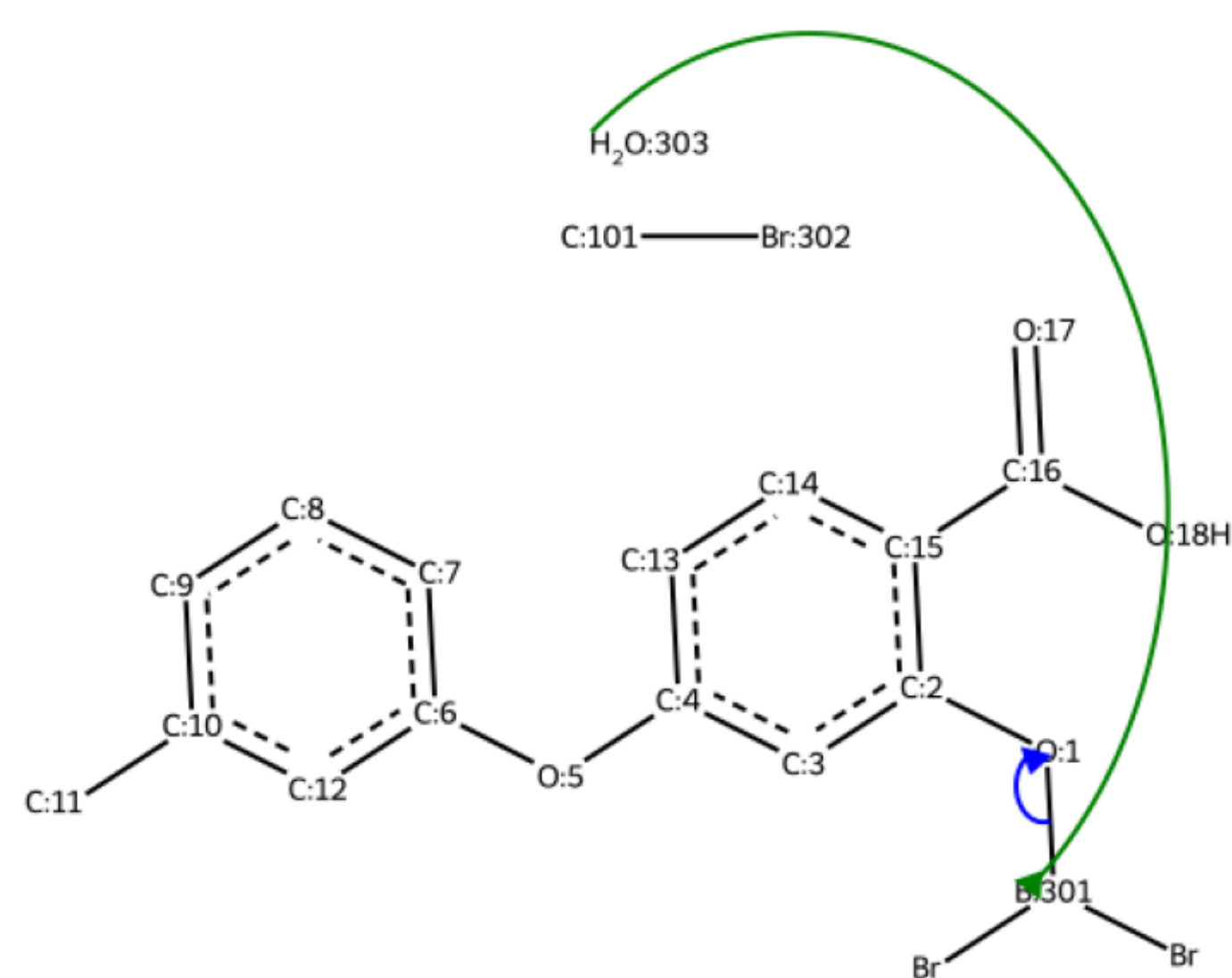
step #1

step #2

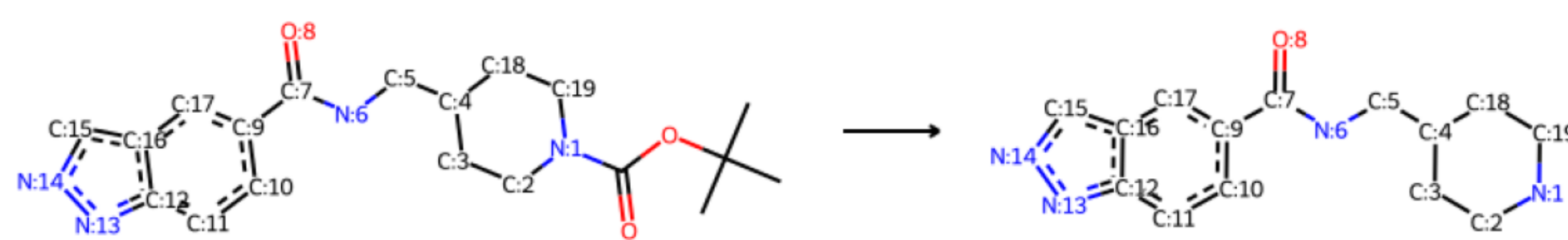


step #3

Product(s)

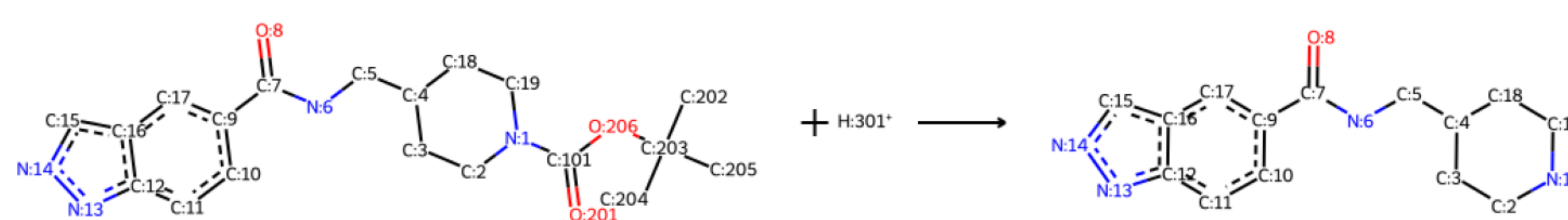


Original reaction
sampled RXN_ID:88)



Identified mechanistic class -
Boc_deprotection reaction

Reaction with missing reagents recovered

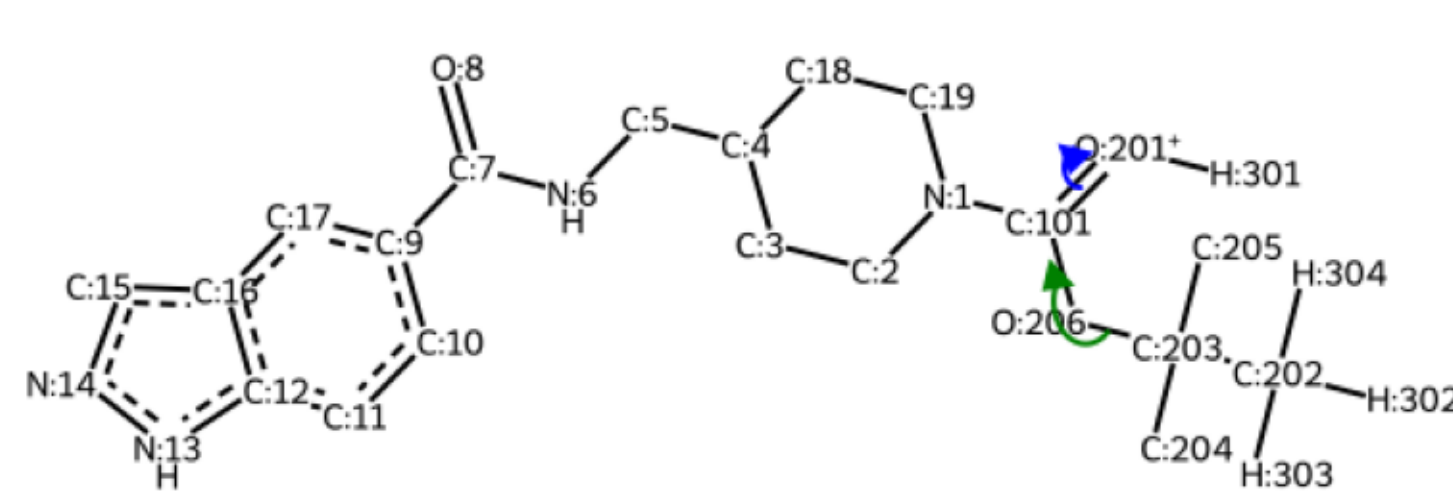
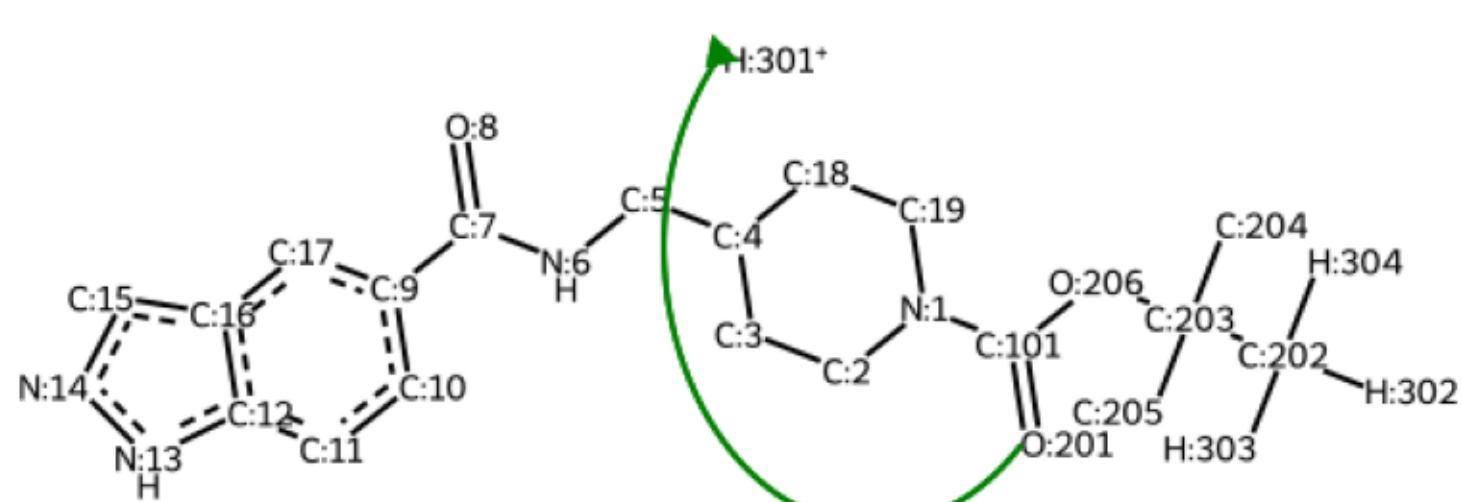


Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

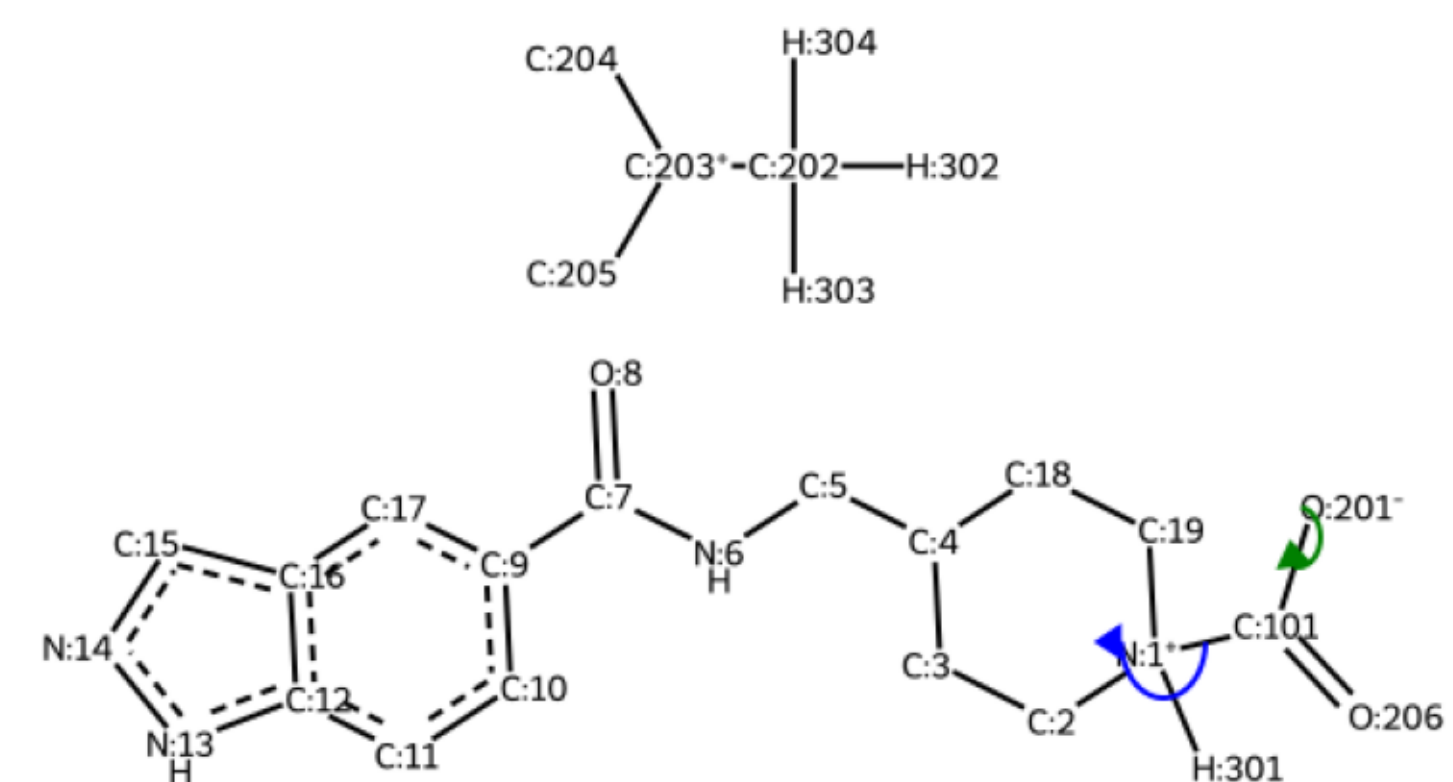
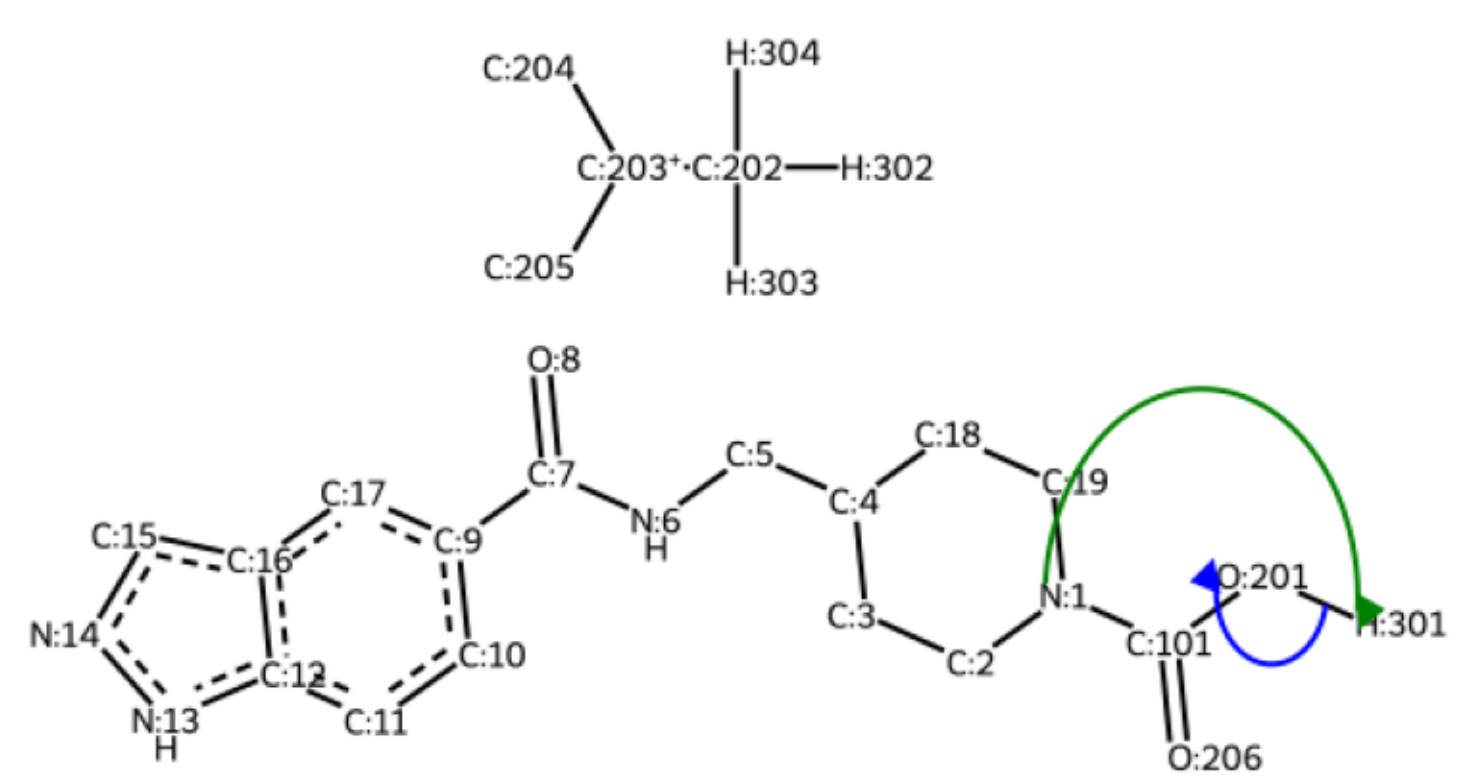
step #1

step #2



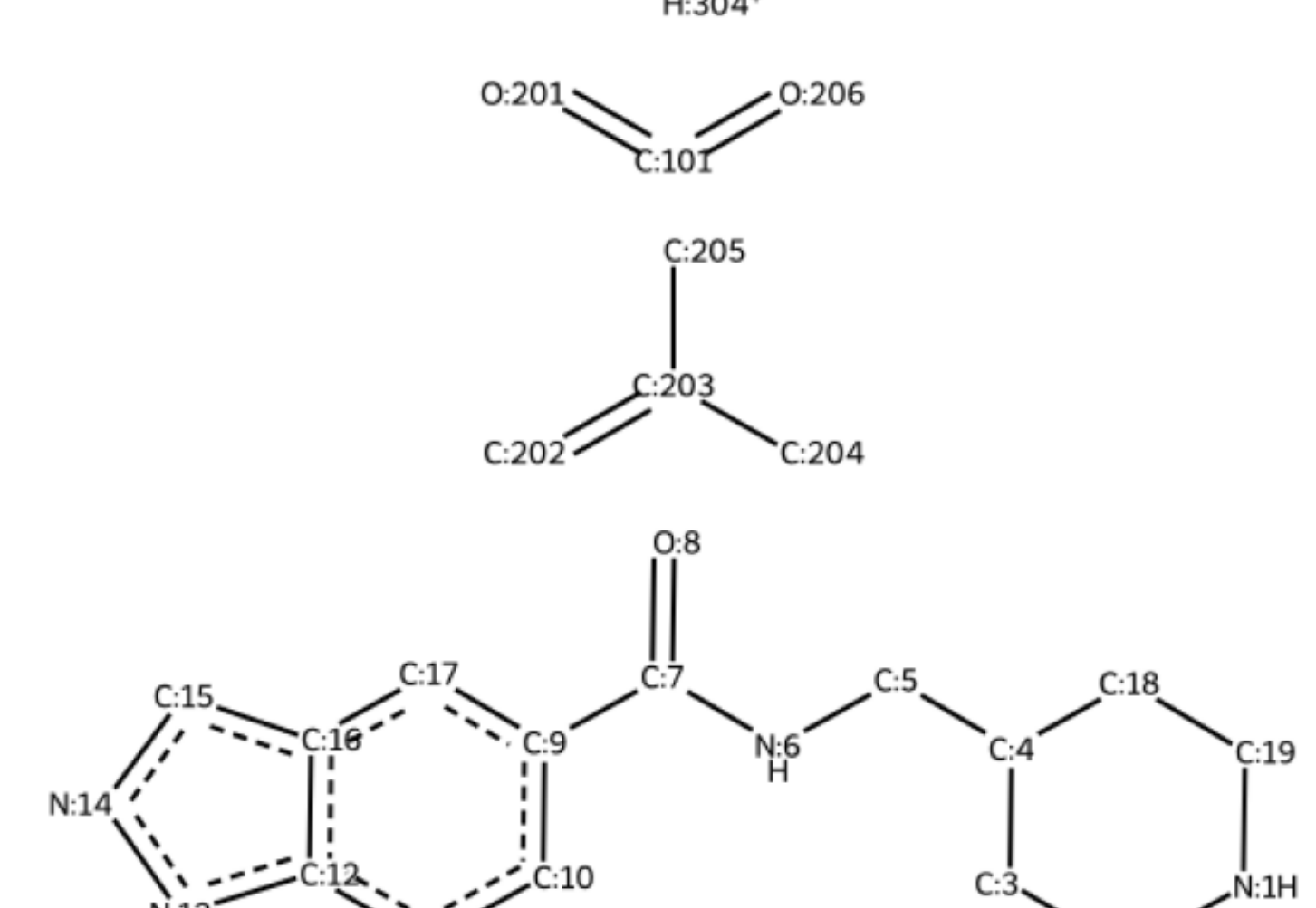
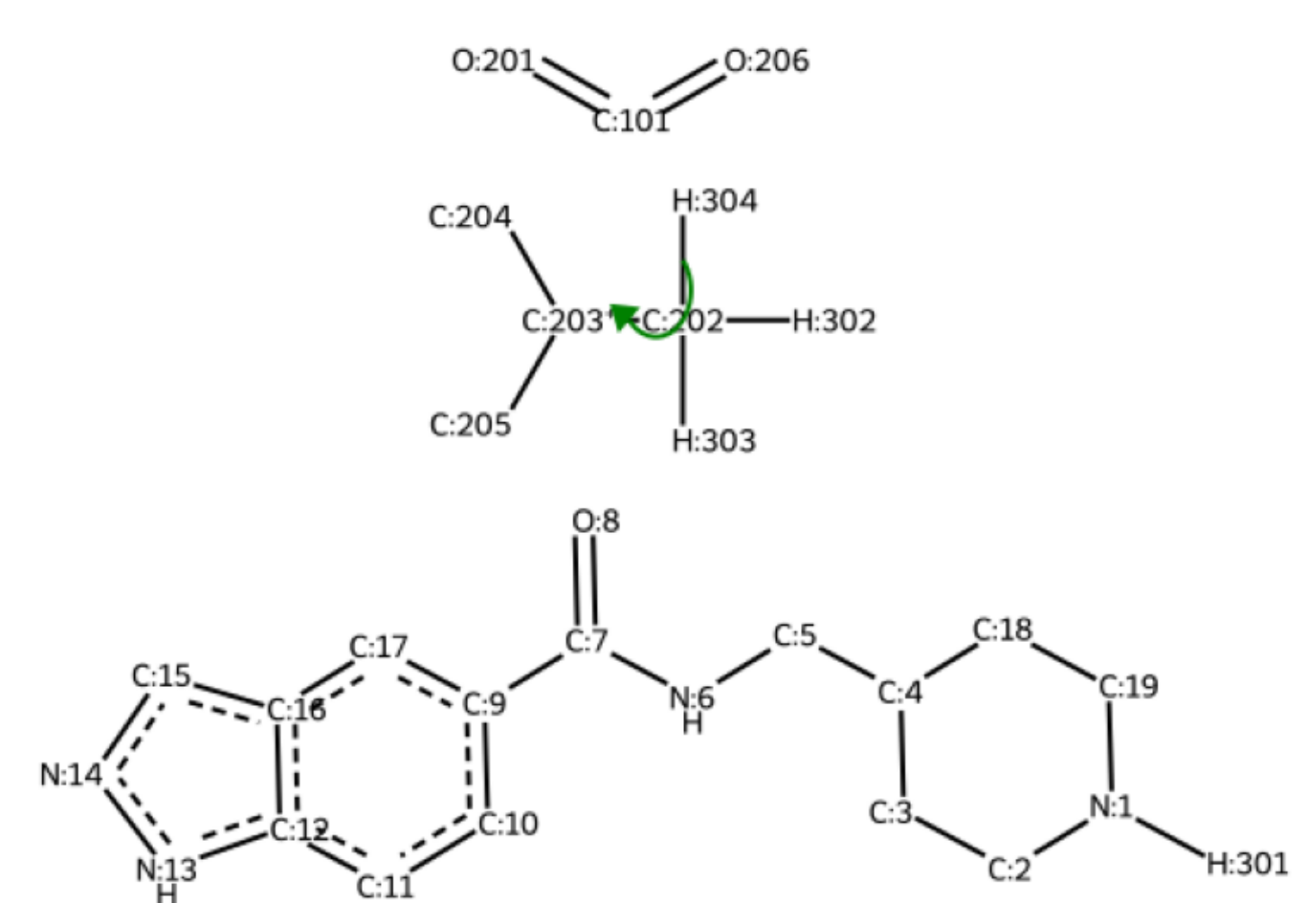
step #3

step #4

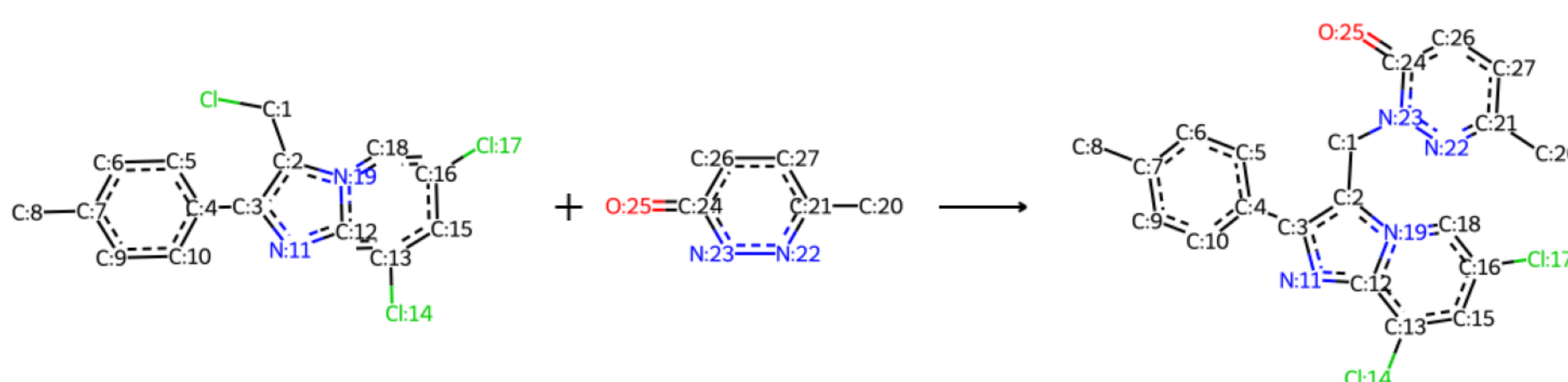


step #5

Product(s)

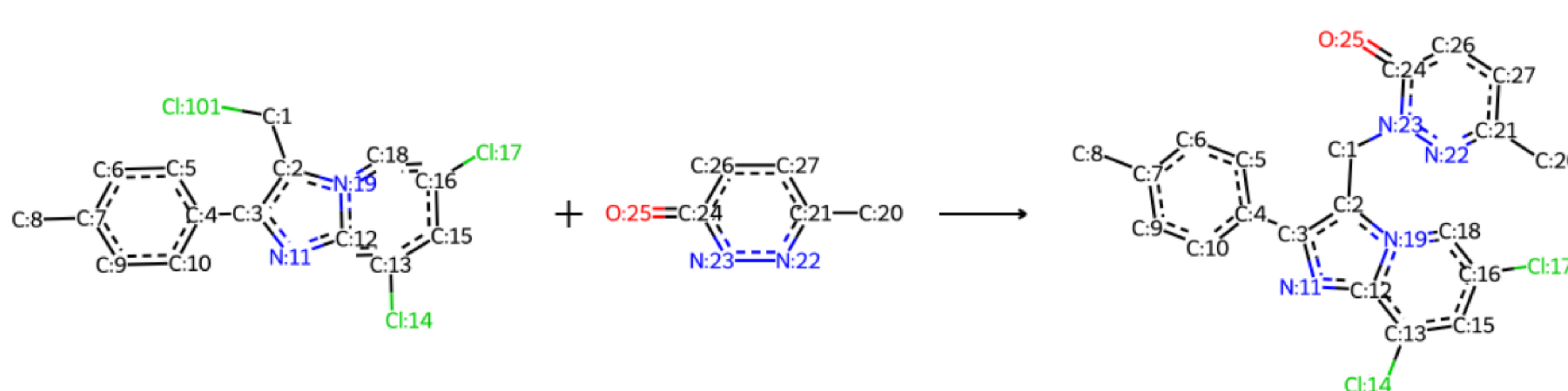


Original reaction sampled RXN_ID:89)



Identified mechanistic class -
SN2 reaction

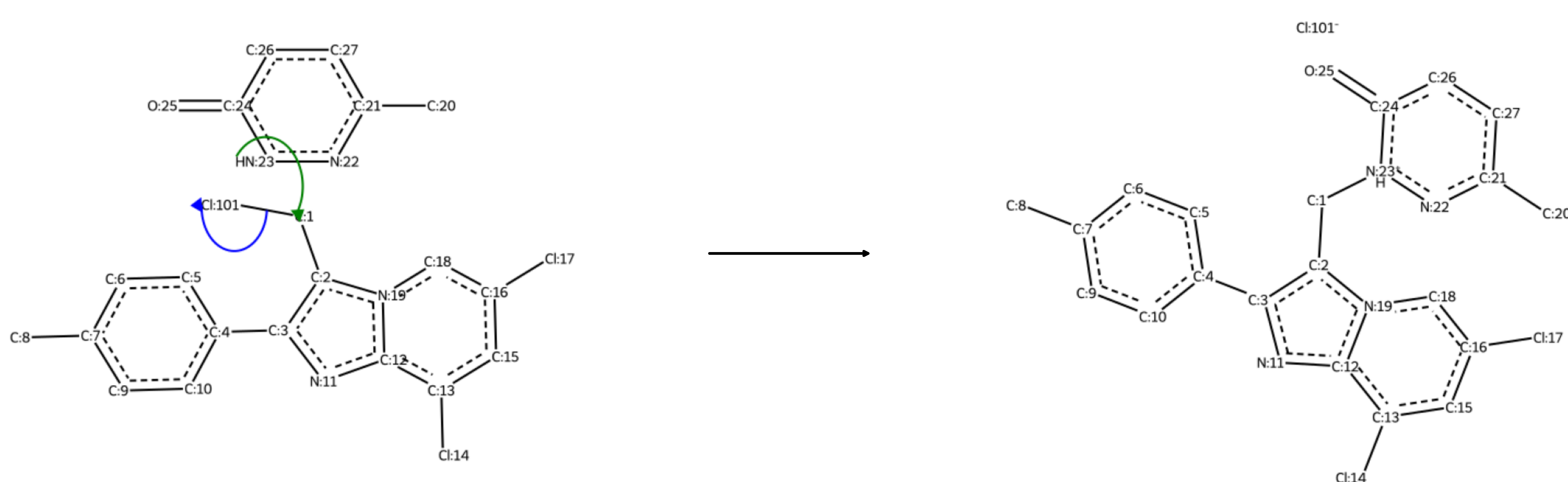
Reaction with missing reagents recovered



Proposed mechanistic pathway

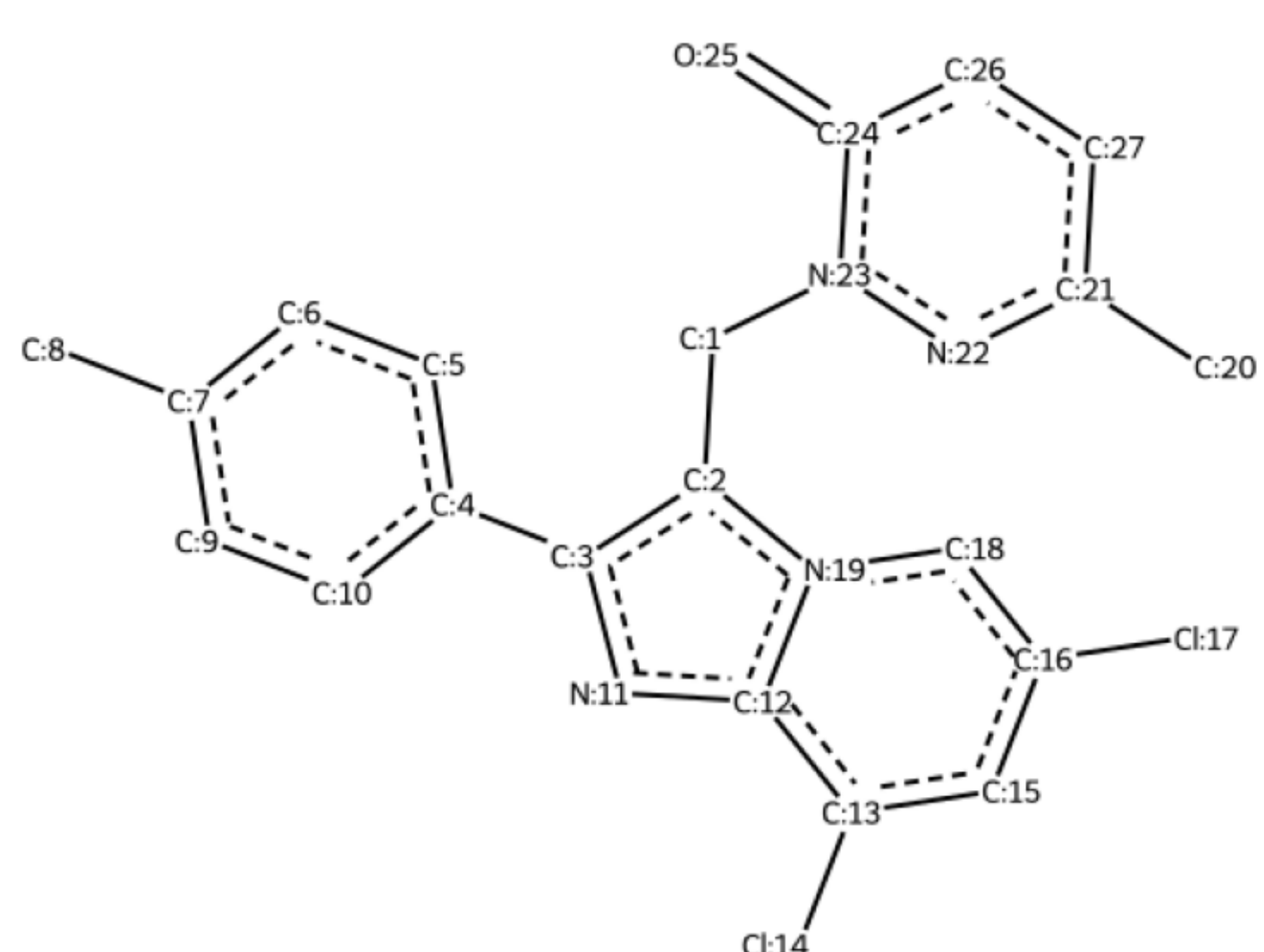
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

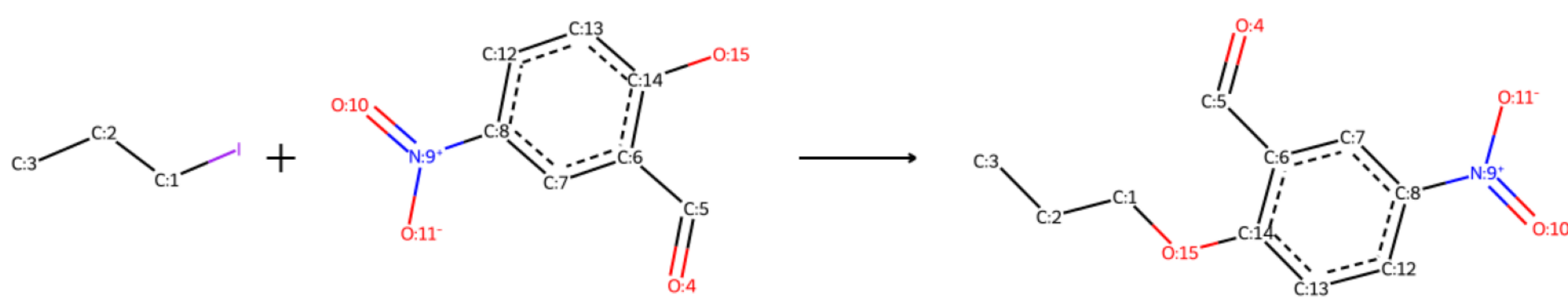


proton transfer

Product(s)

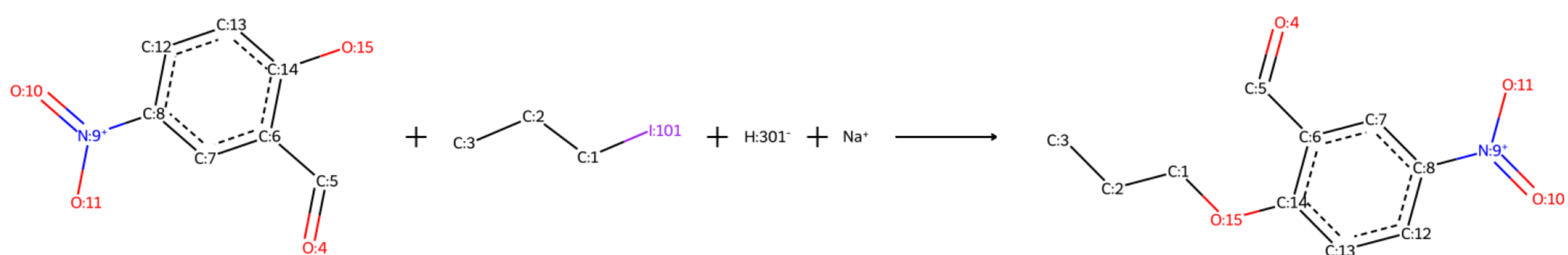


Original reaction sampled RXN_ID:90)



Identified mechanistic class -
SN₂_alcohol(thiol) reaction

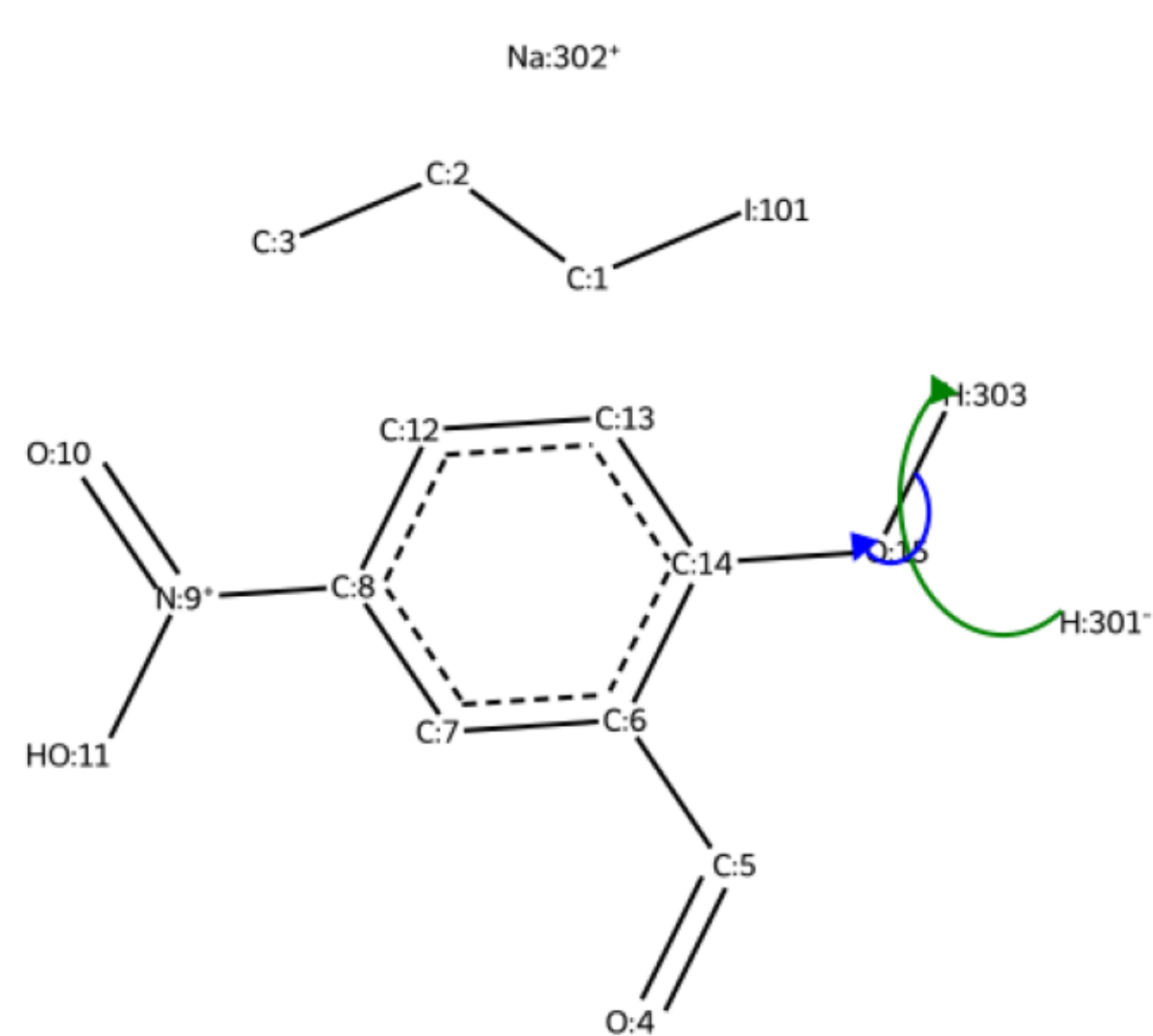
Reaction with missing reagents recovered



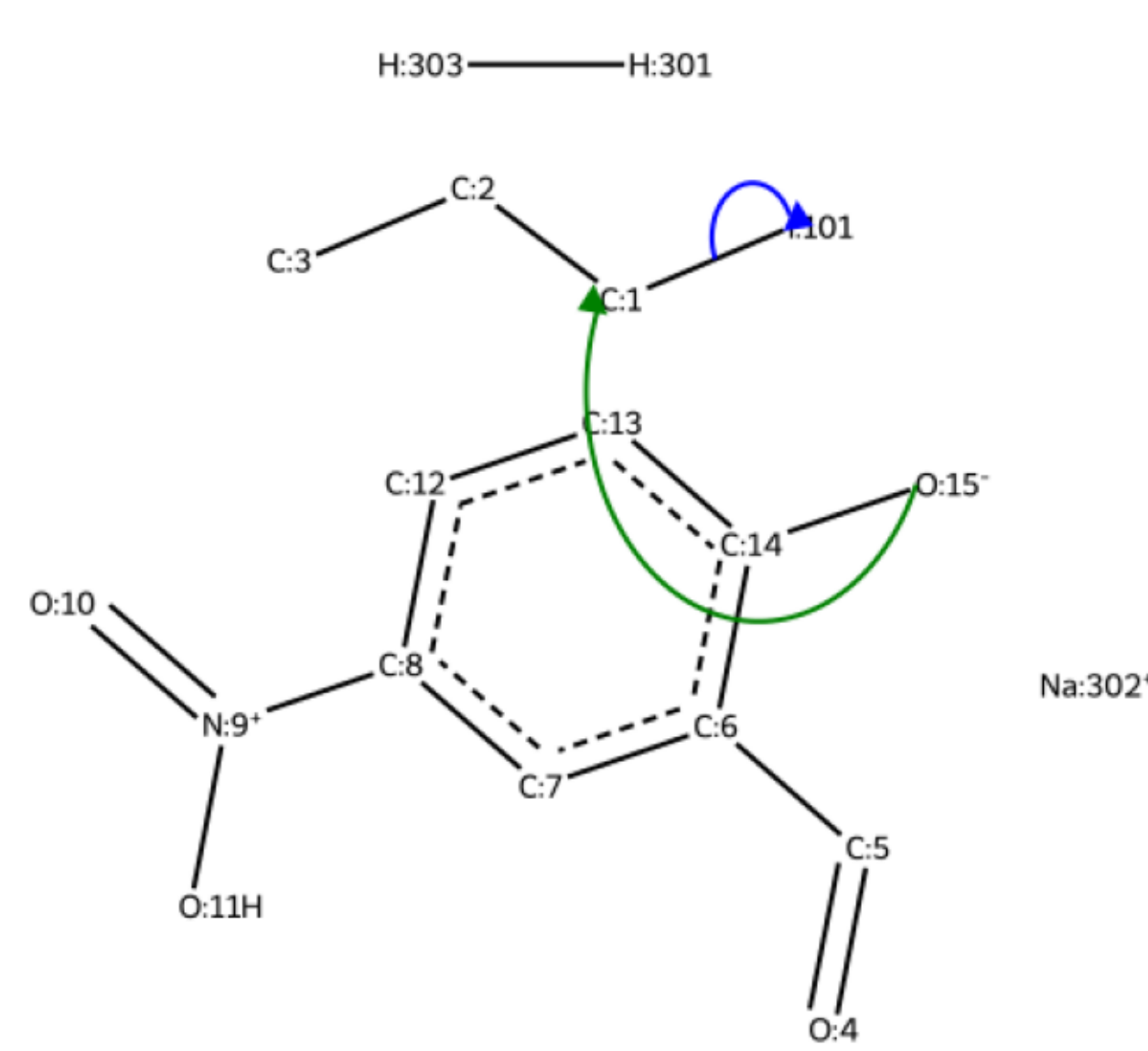
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

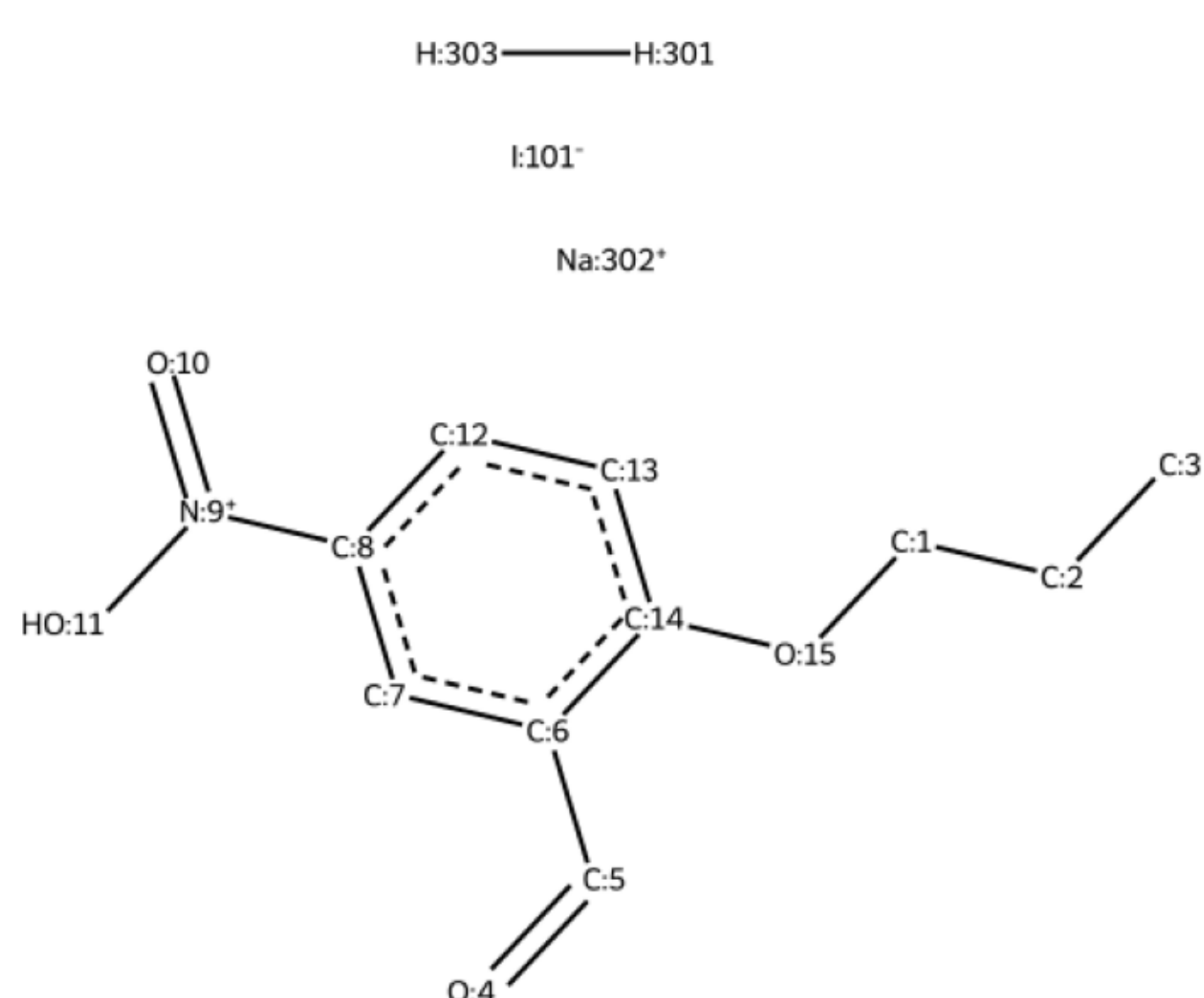
step #1



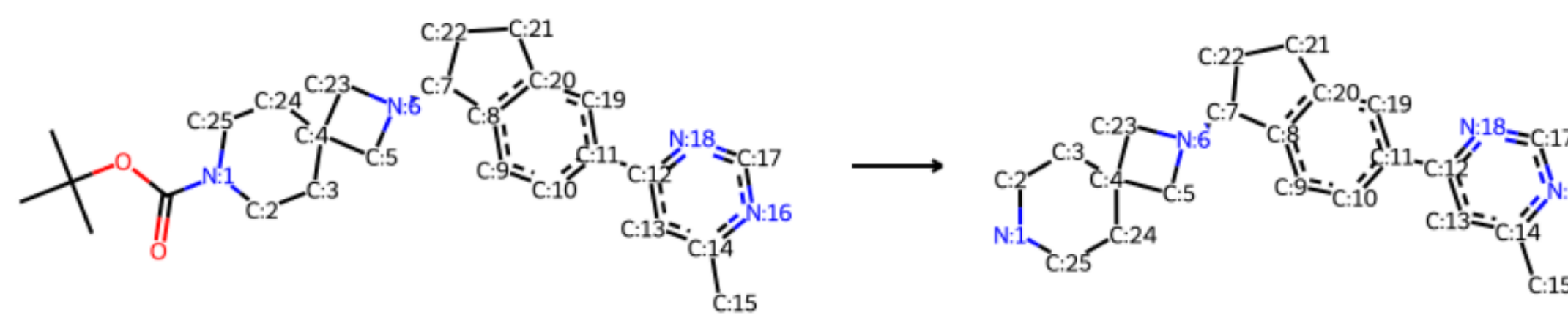
step #2



Product(s)

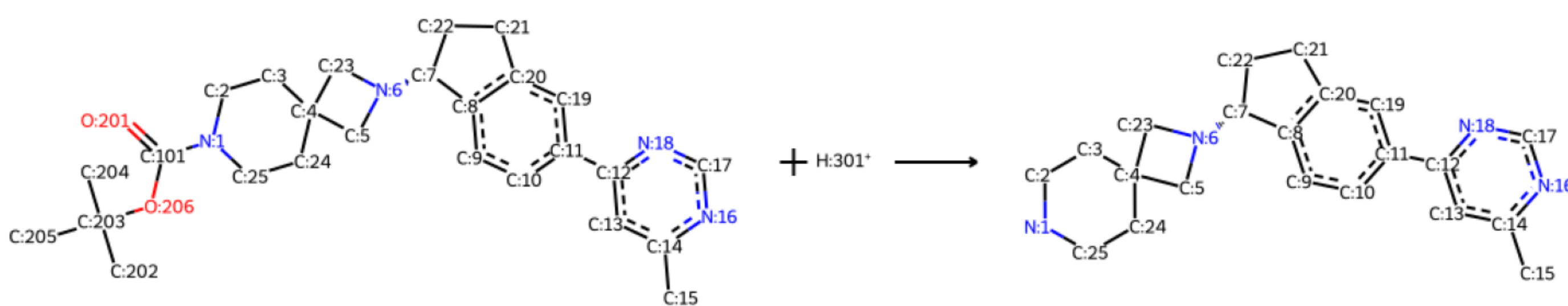


Original reaction
sampled RXN_ID:91)



Identified mechanistic class -
Boc_deprotection reaction

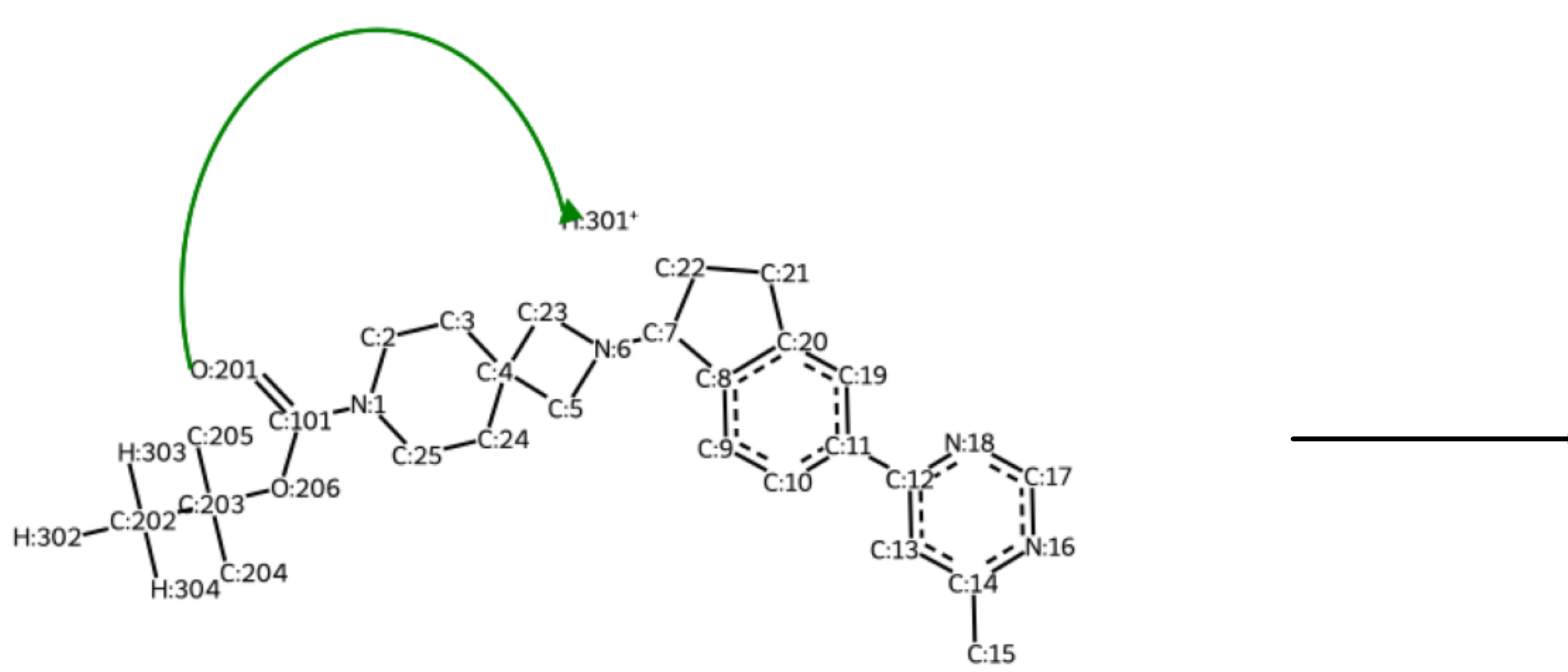
Reaction with missing reagents recovered



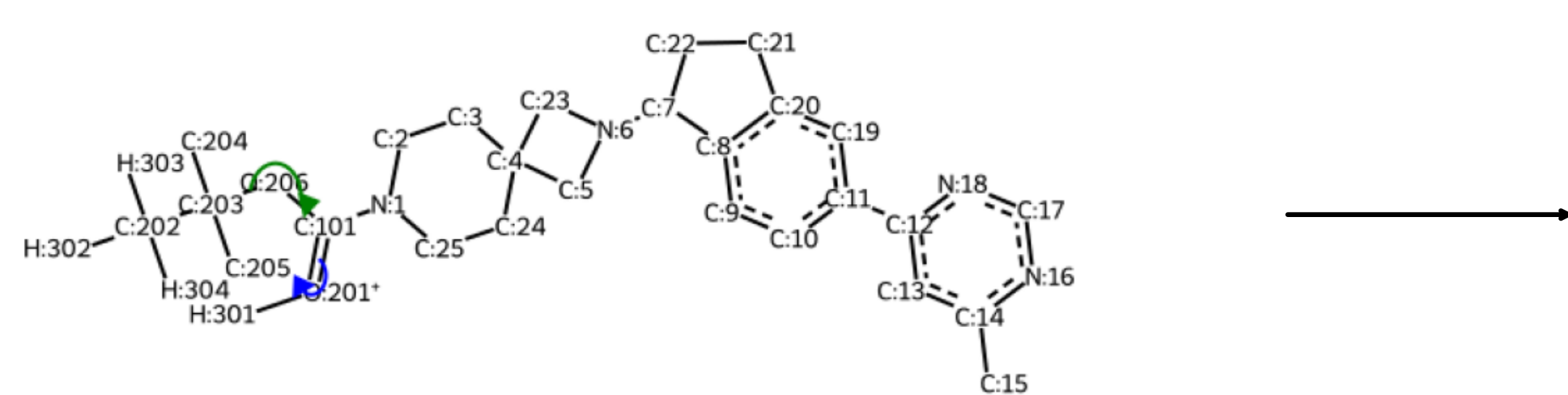
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

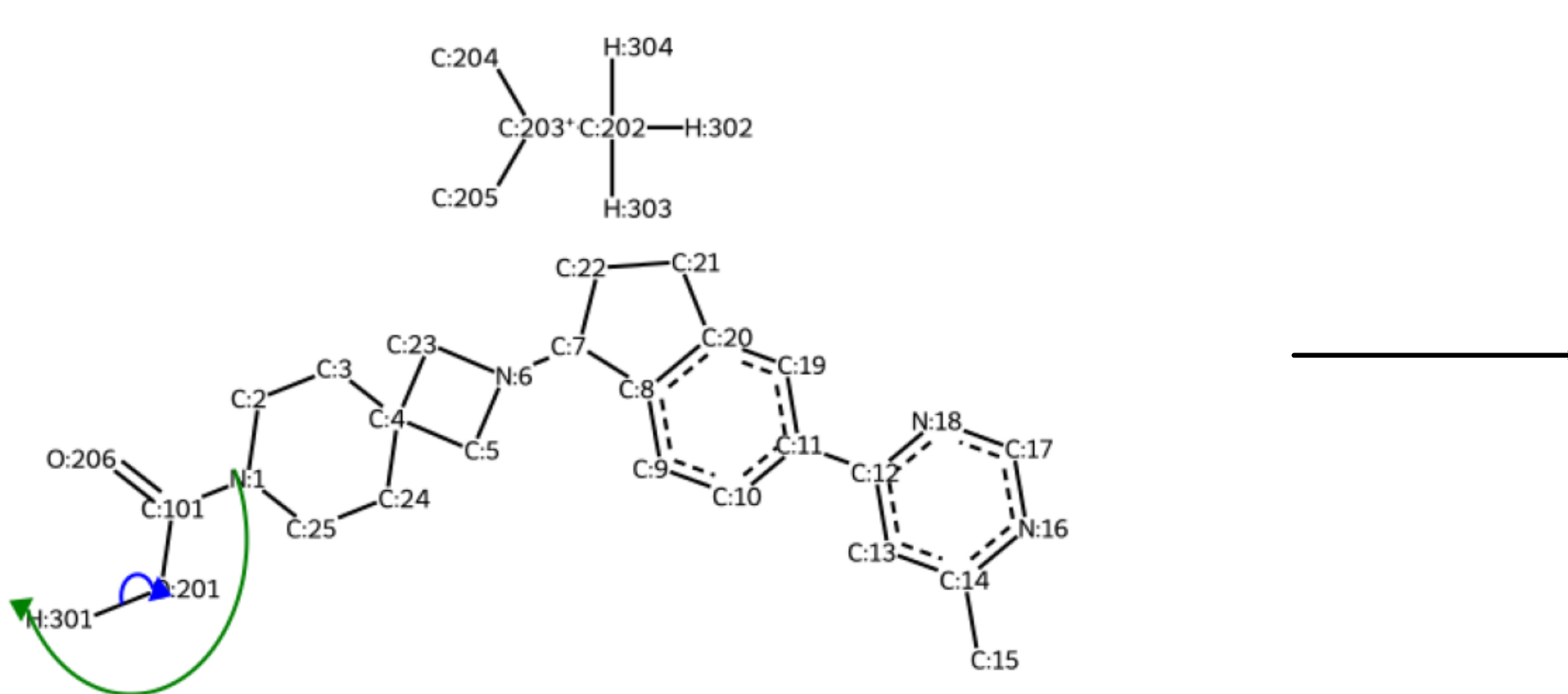
step #1



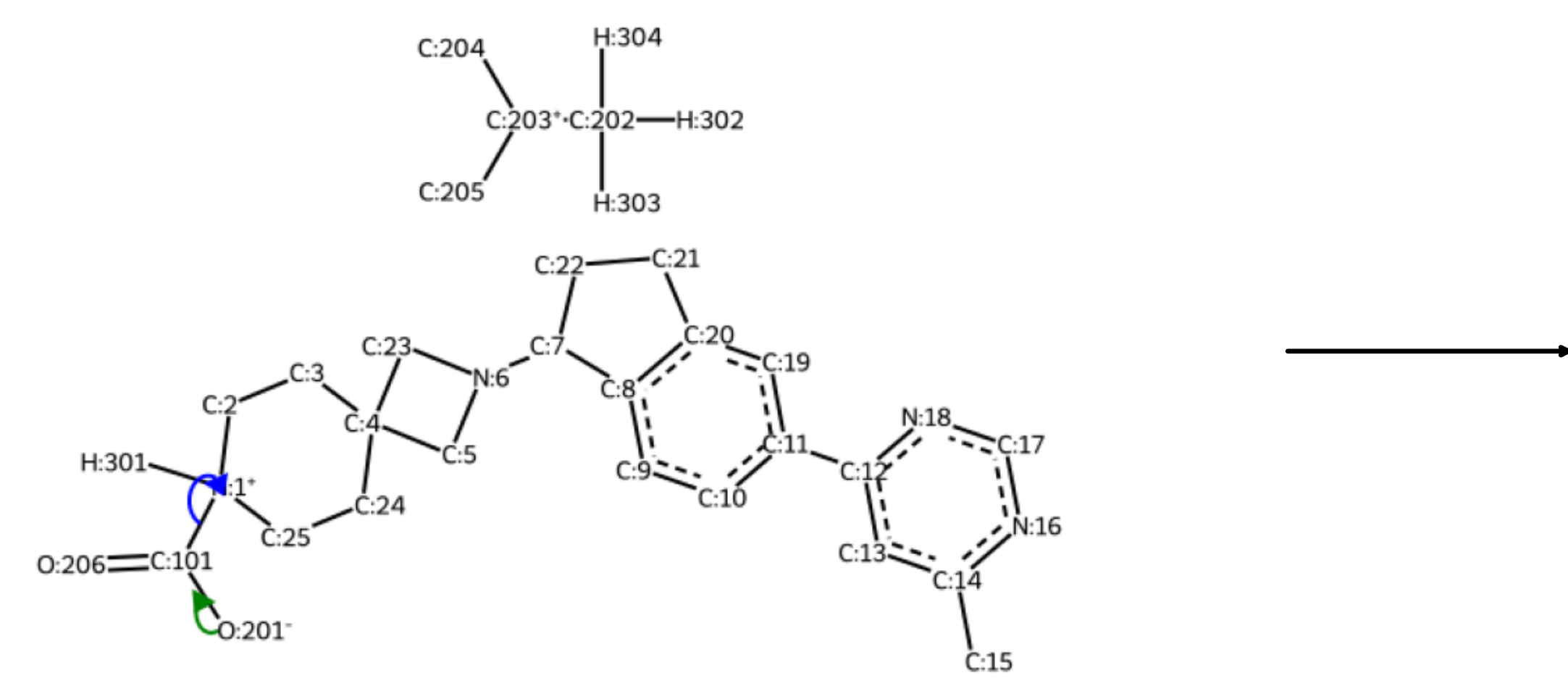
step #2



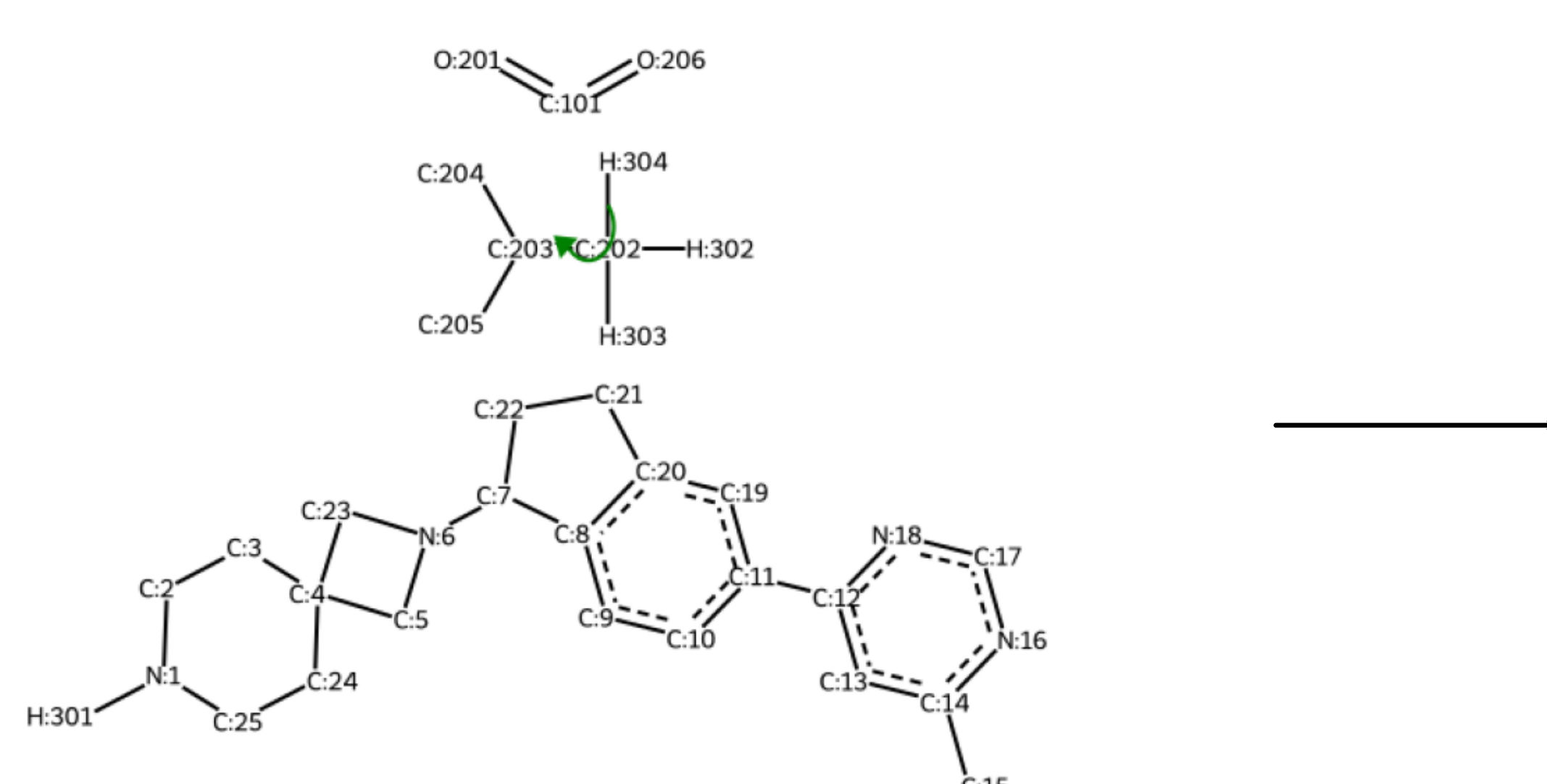
step #3



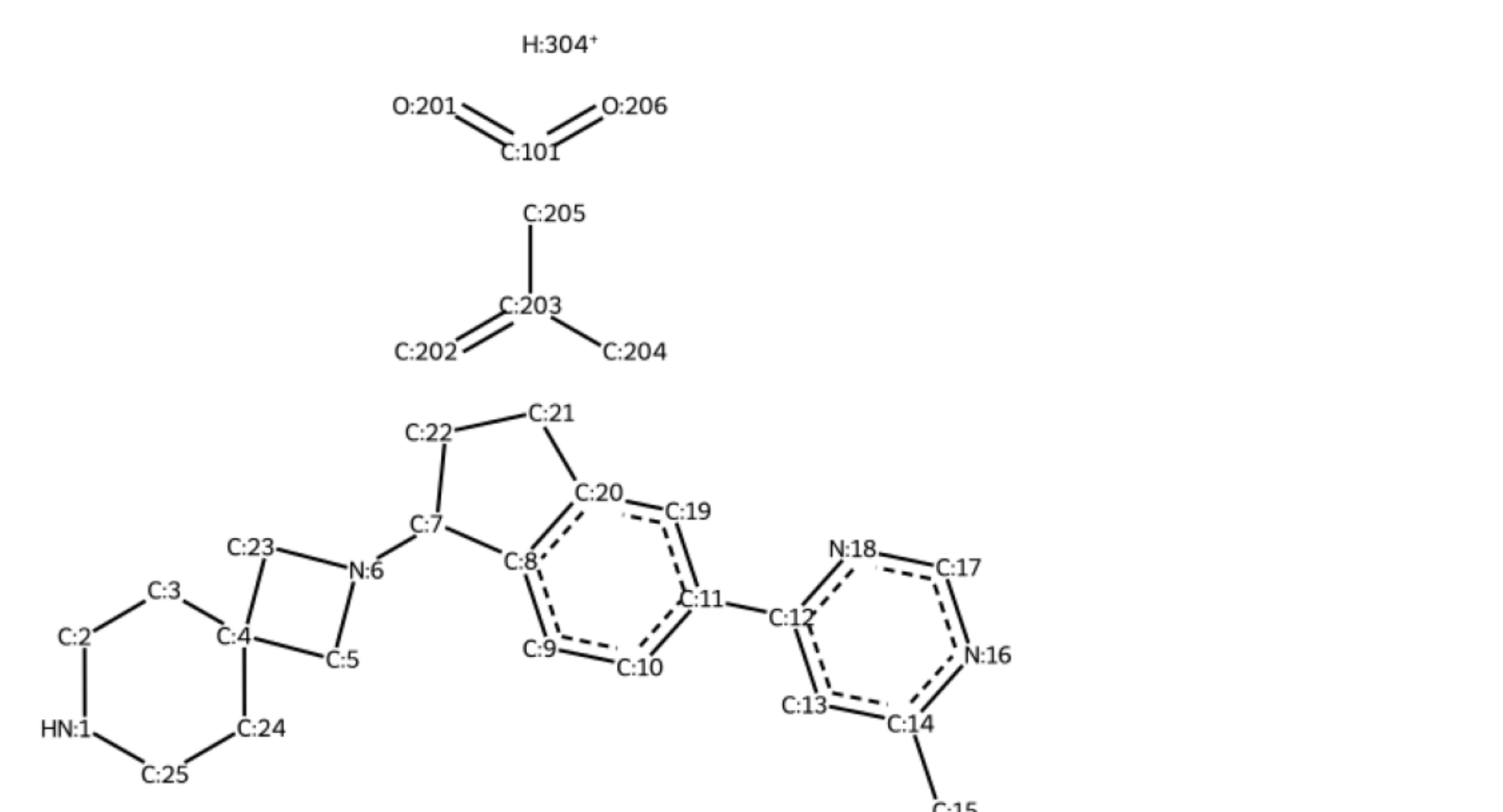
step #4



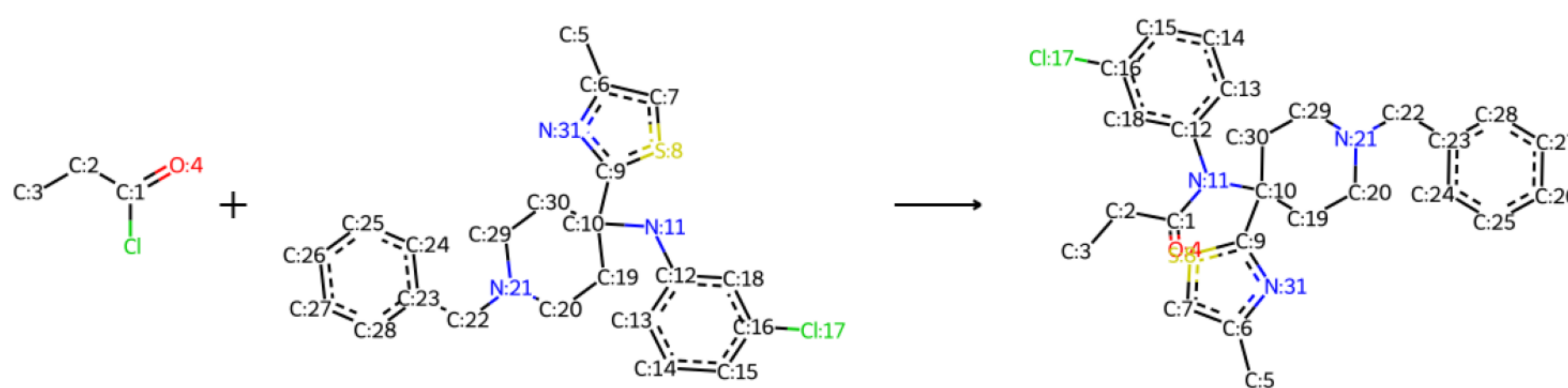
step #5



Product(s)

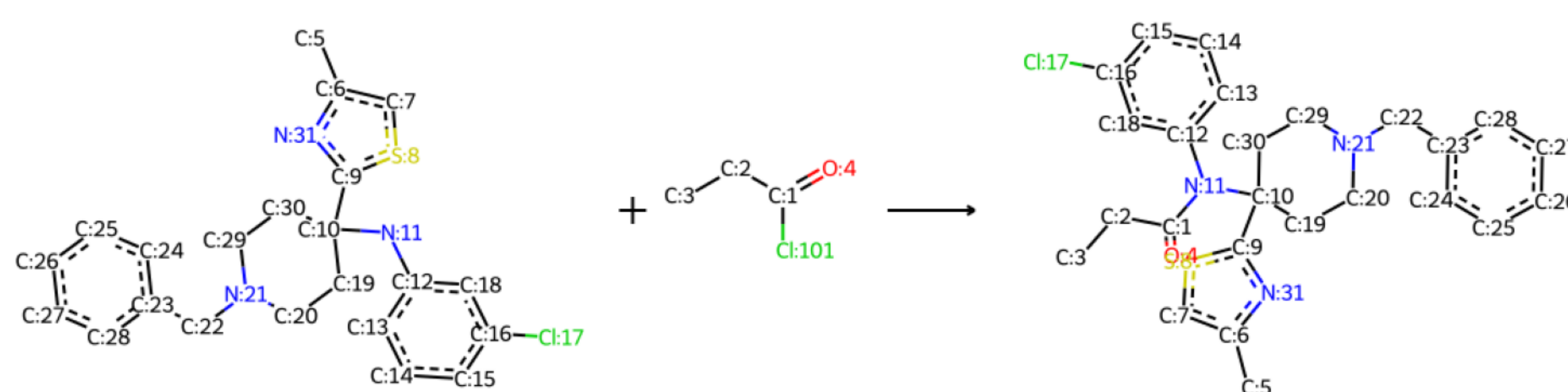


Original reaction
sampled RXN_ID:92)



Identified mechanistic class -
nucleophilic_attack_to_(thio)carbonyl_or_sulfonyl reaction

Reaction with missing reagents recovered

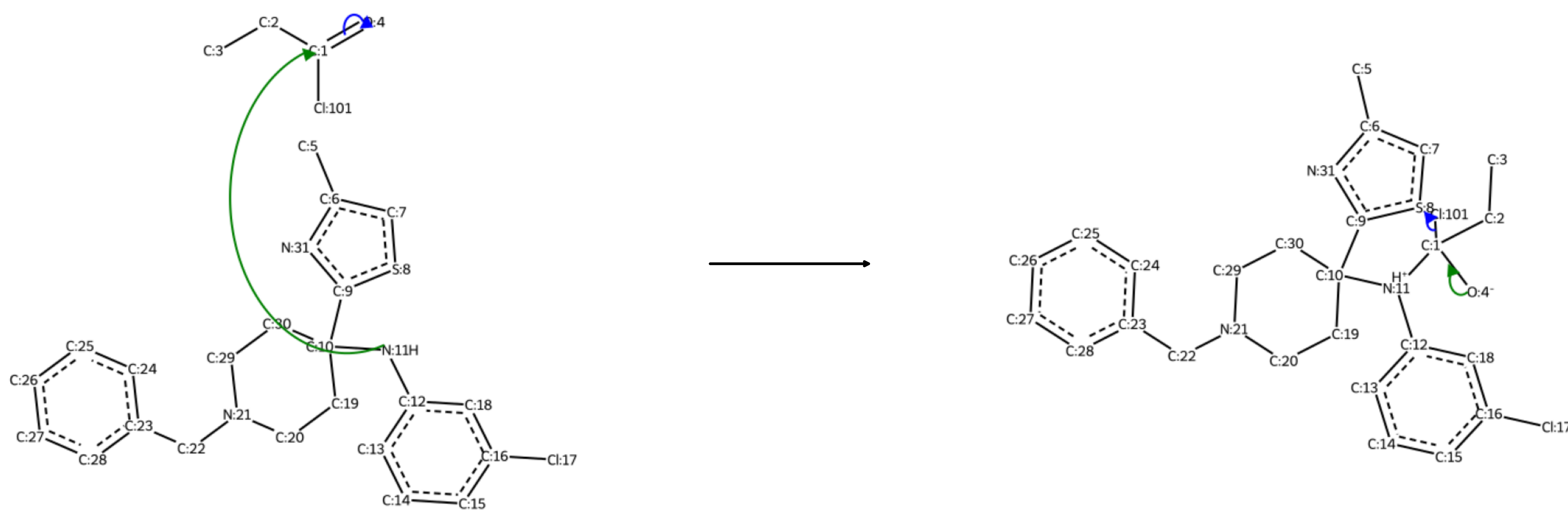


Proposed mechanistic pathway

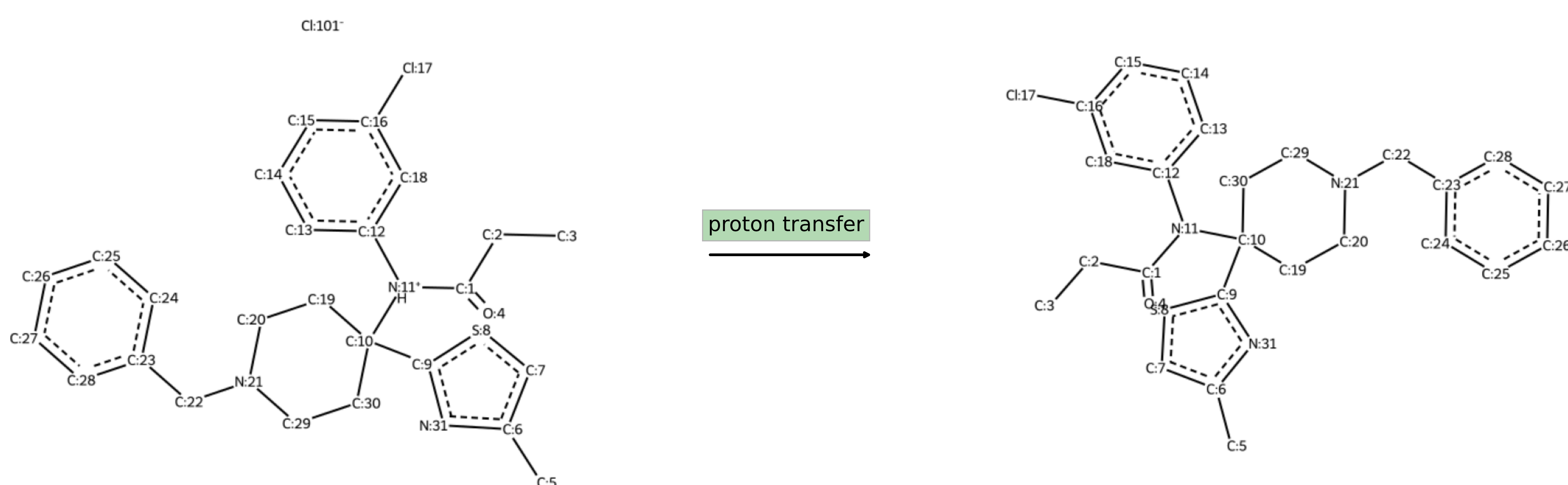
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

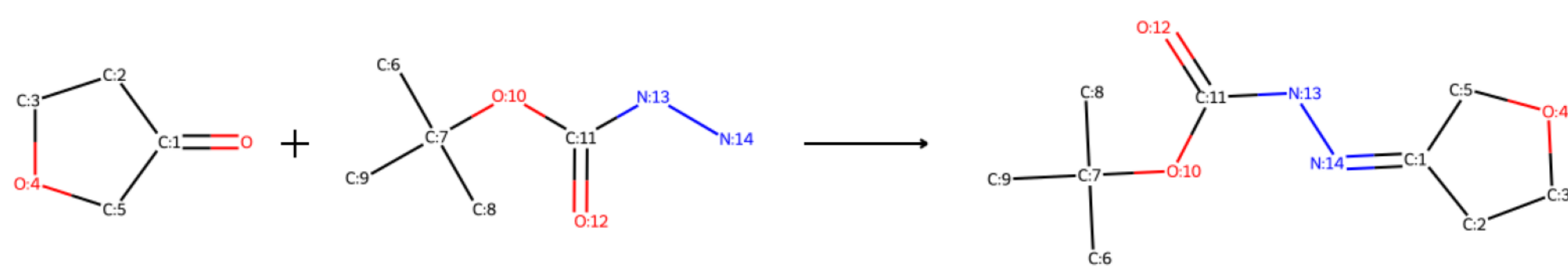
step #2



Product(s)

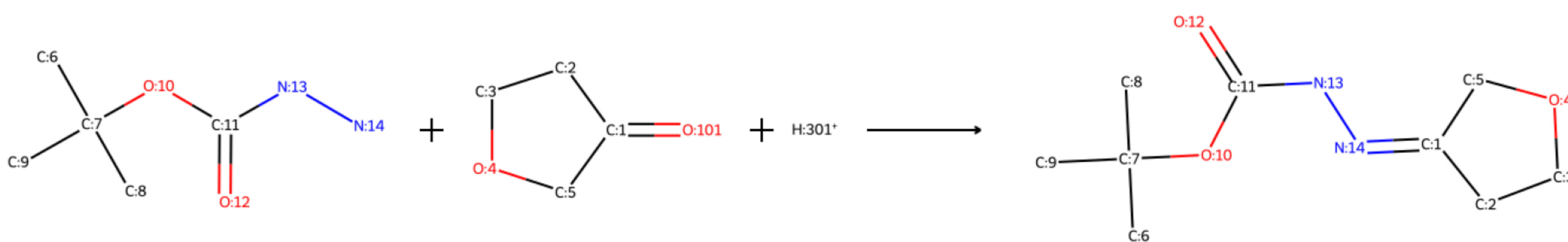


Original reaction
sampled RXN_ID:93)



Identified mechanistic class -
imine_formation reaction

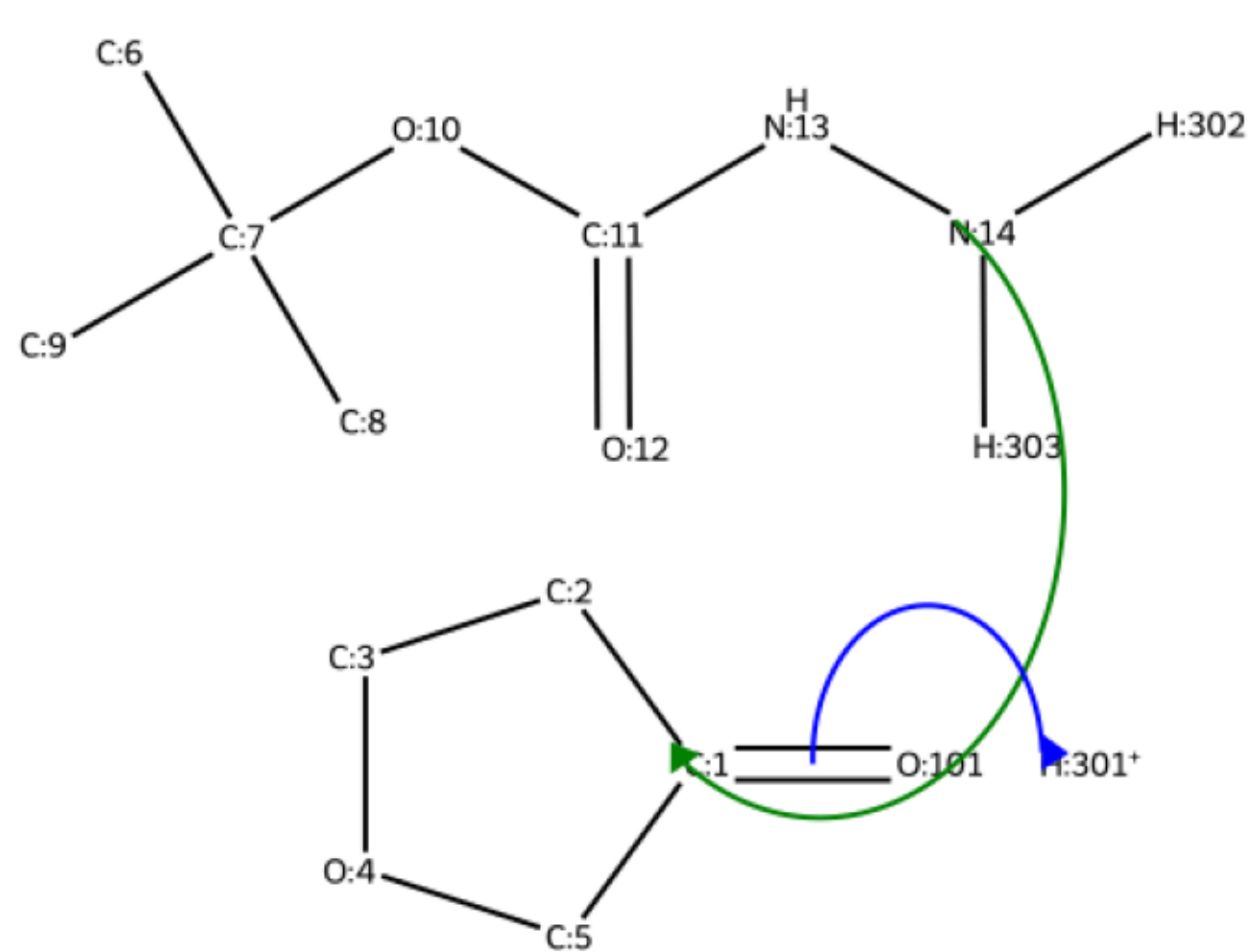
Reaction with missing reagents recovered



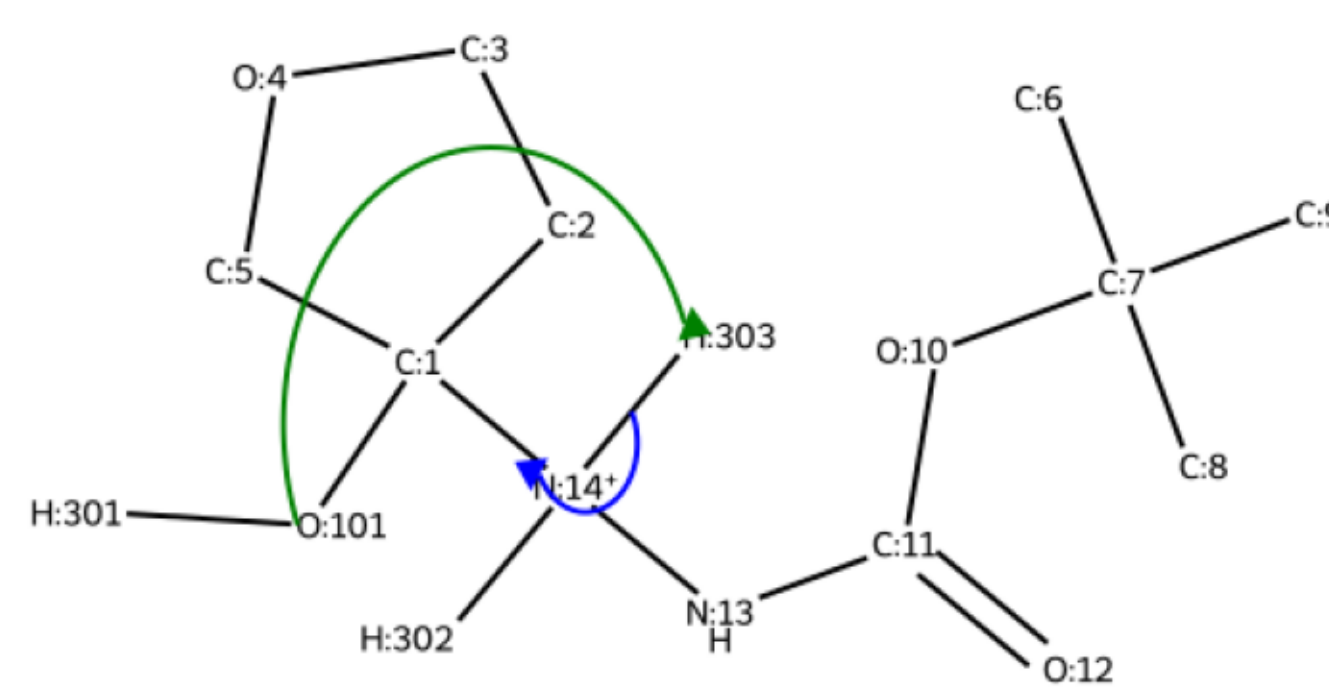
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

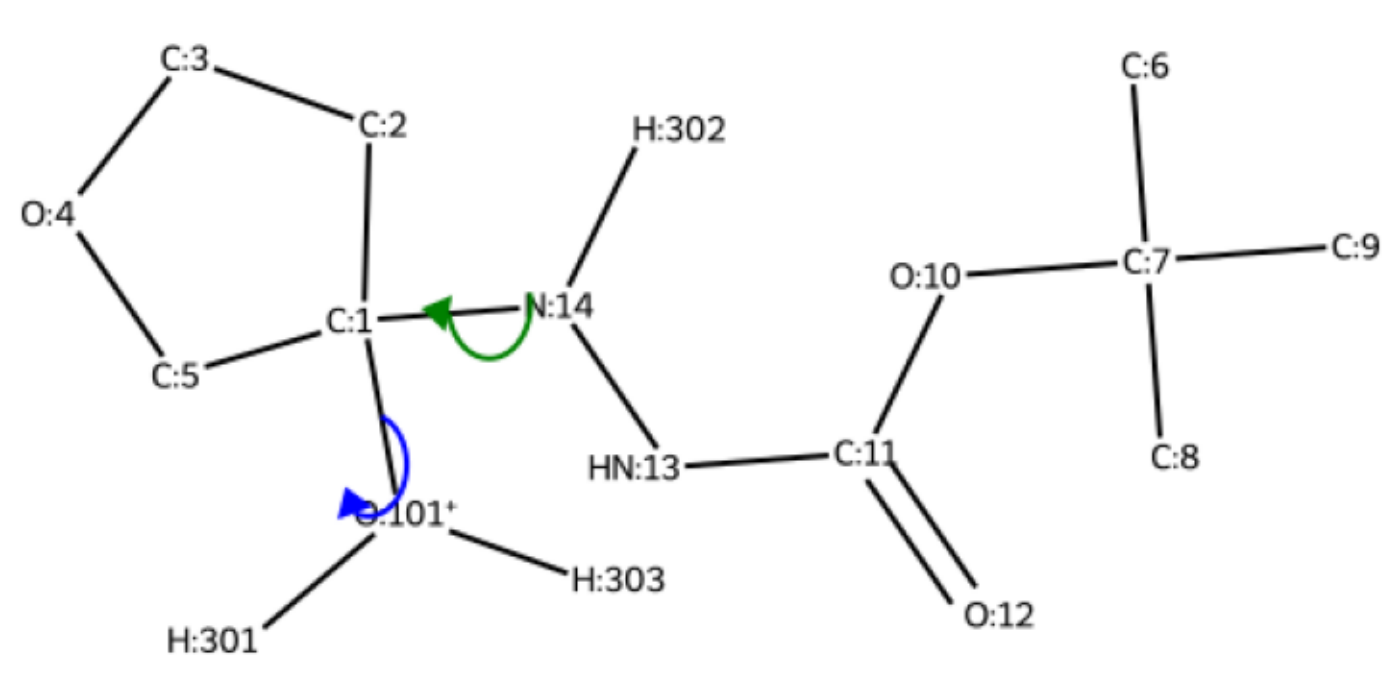
step #1



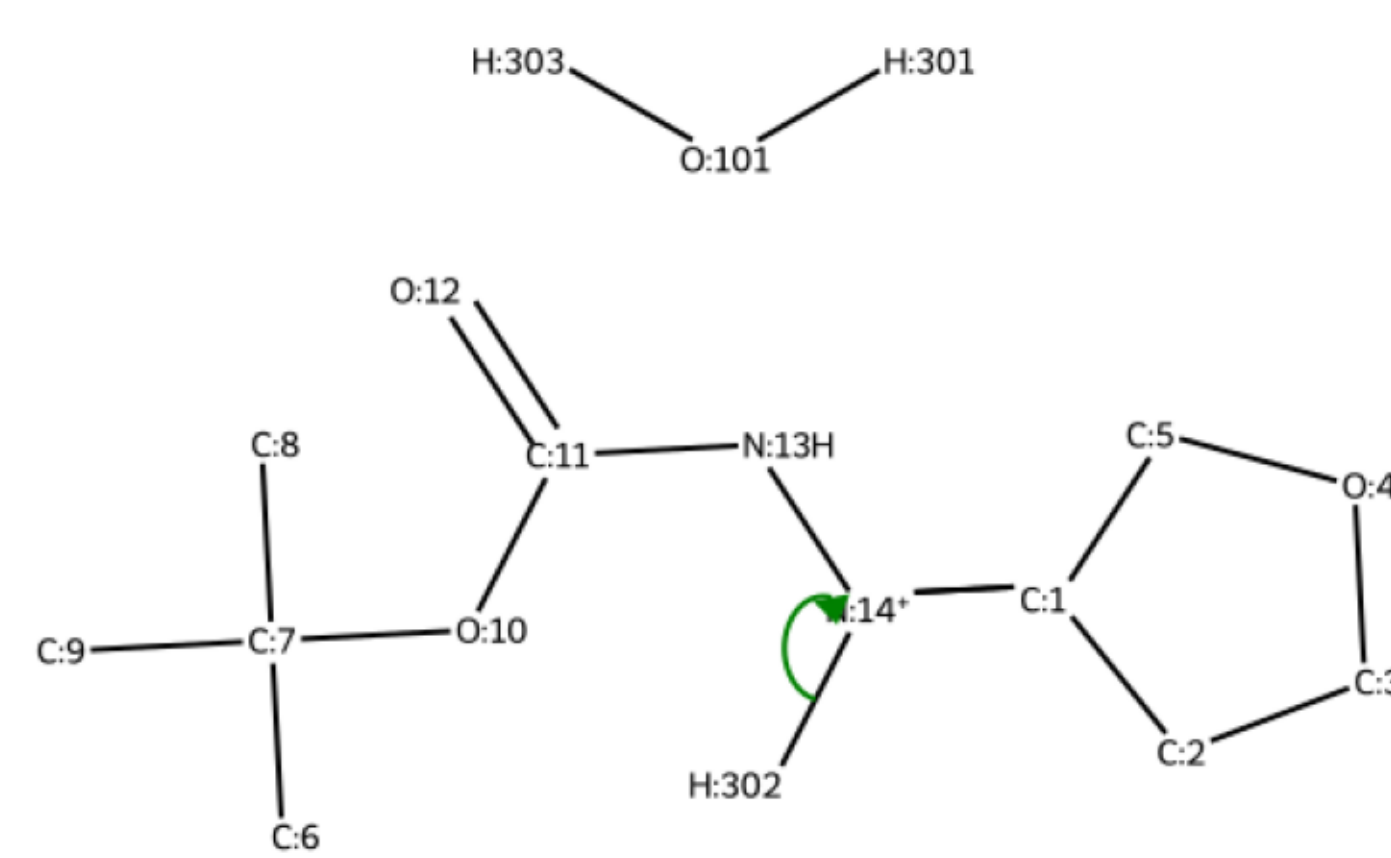
step #2



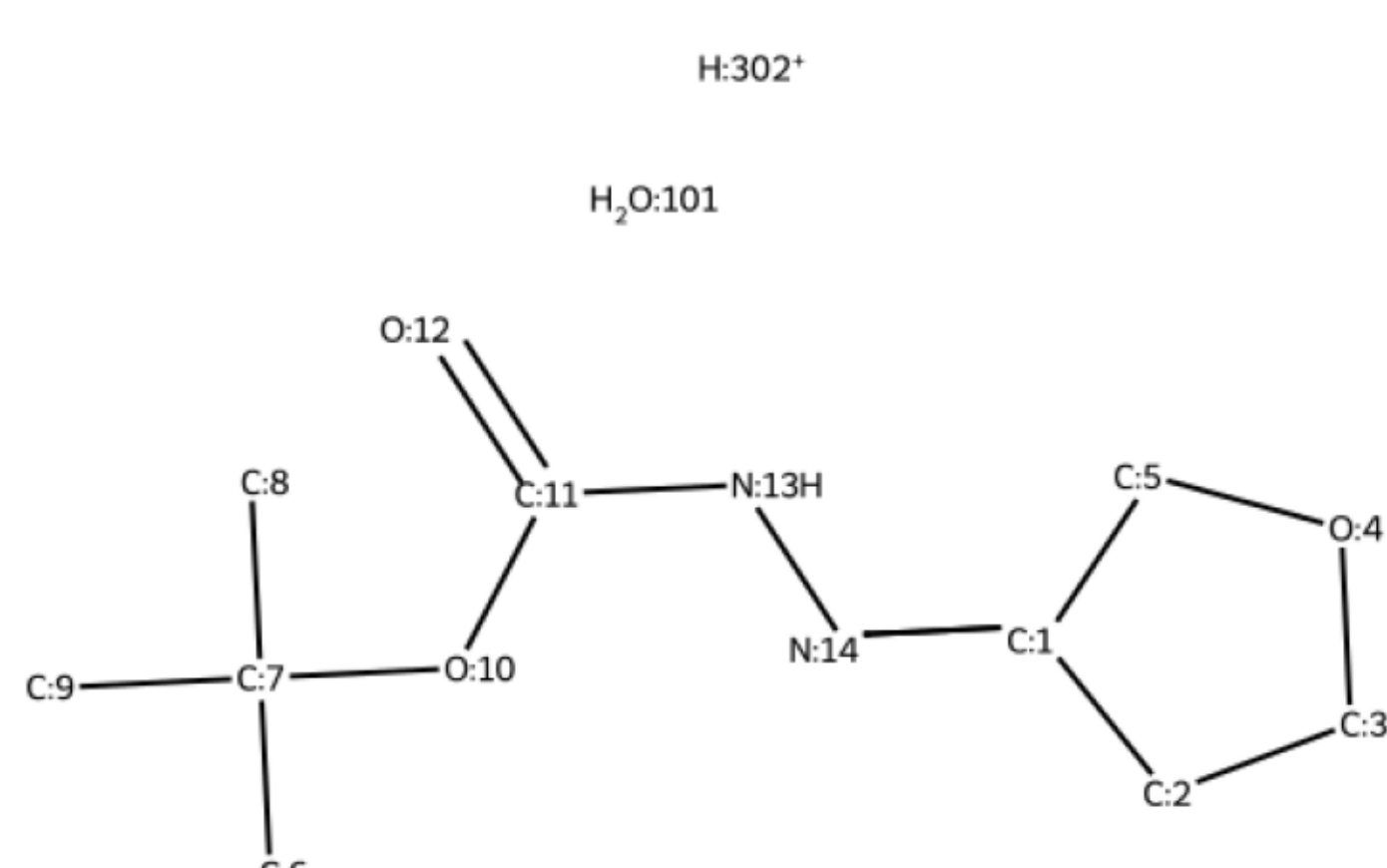
step #3



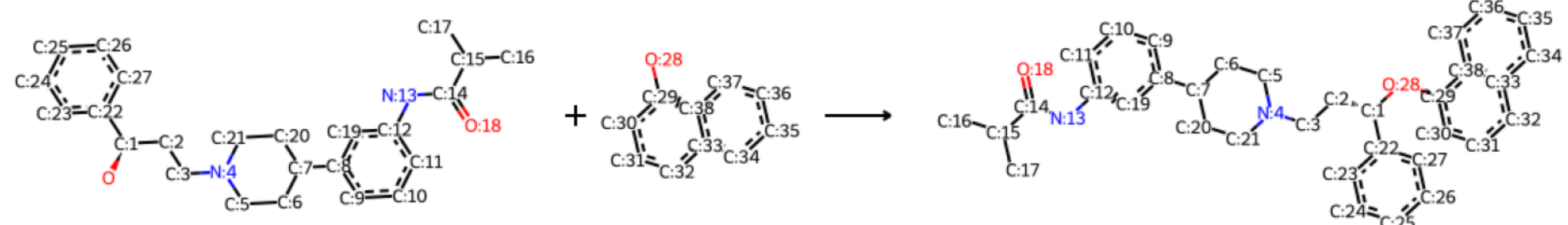
step #4



Product(s)

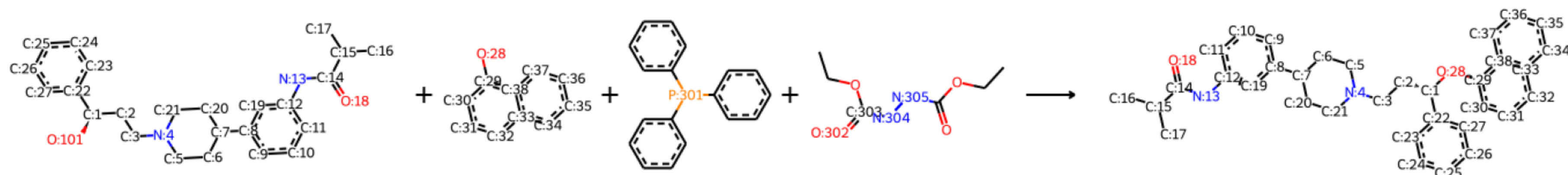


Original reaction
sampled RXN_ID:94)



Identified mechanistic class -
Mitsunobu reaction

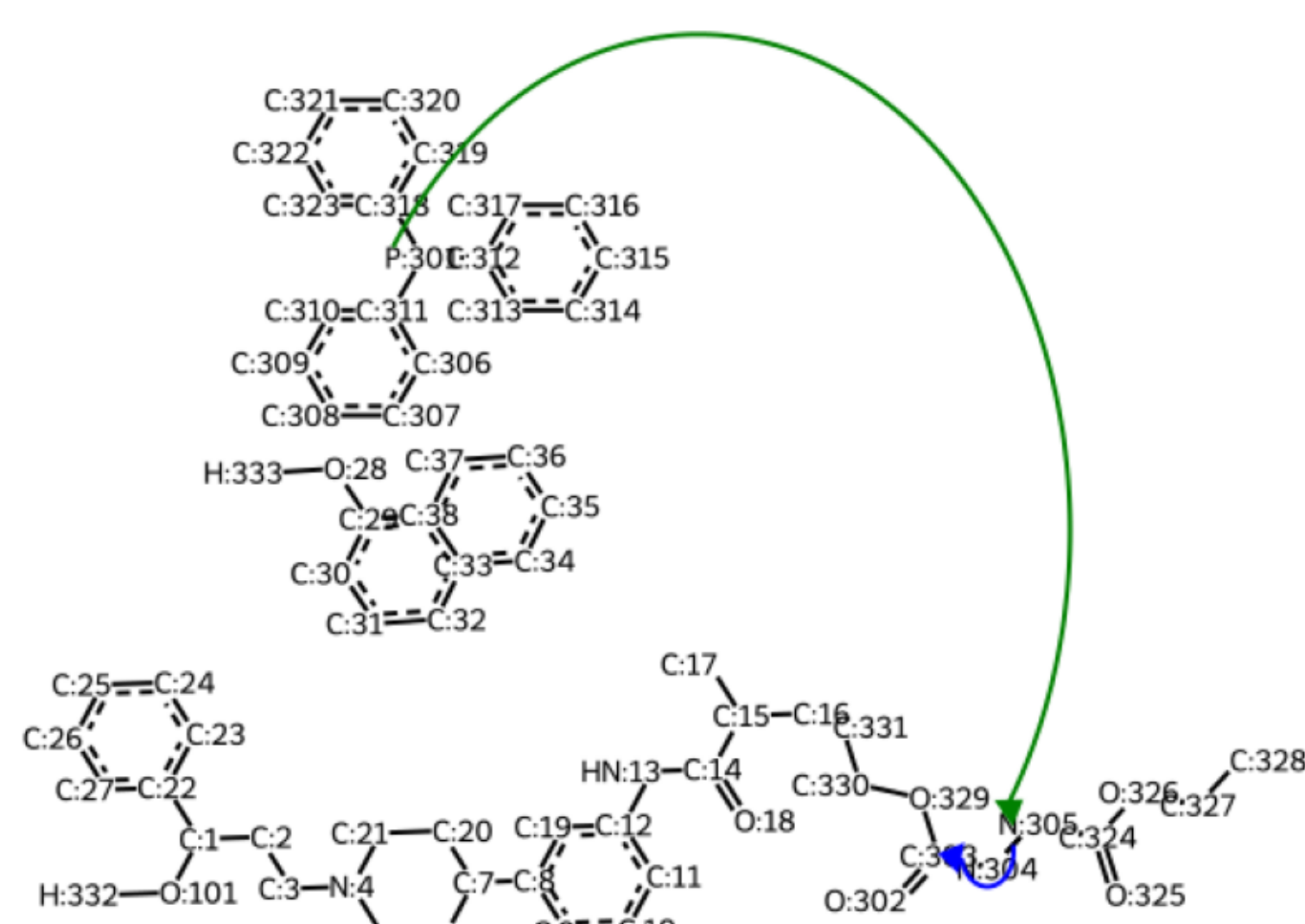
Reaction with missing reagents recovered



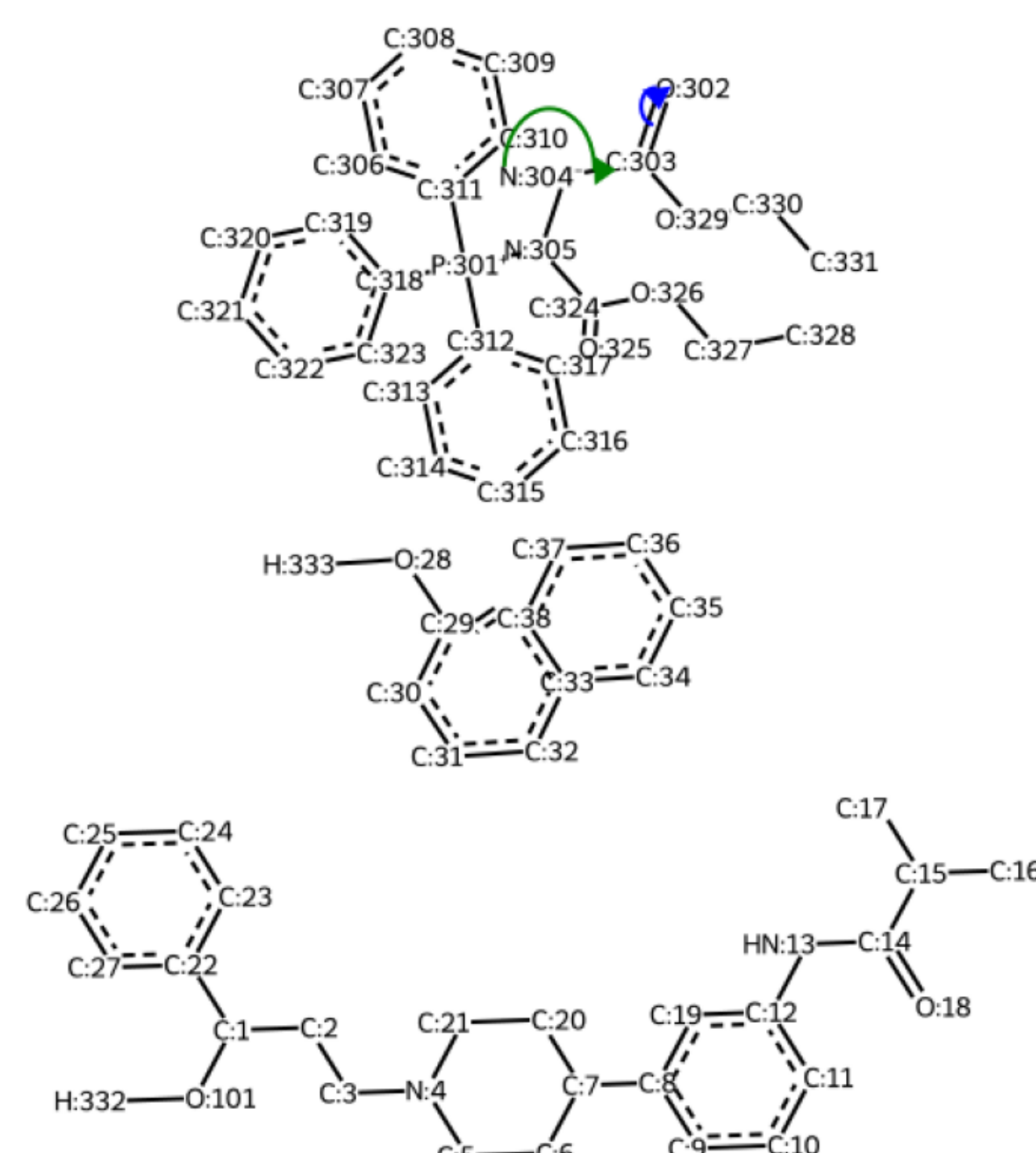
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

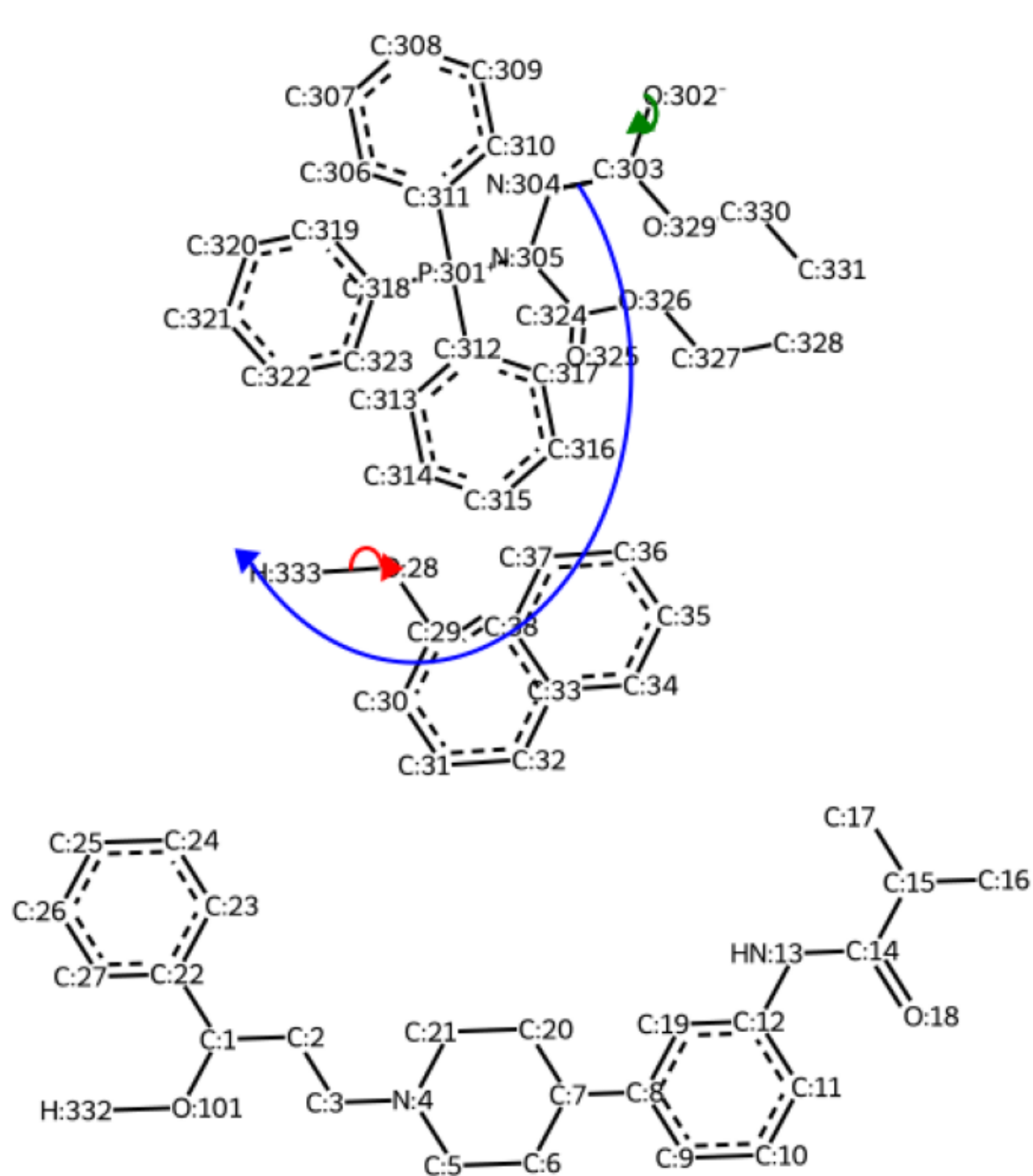
step #1



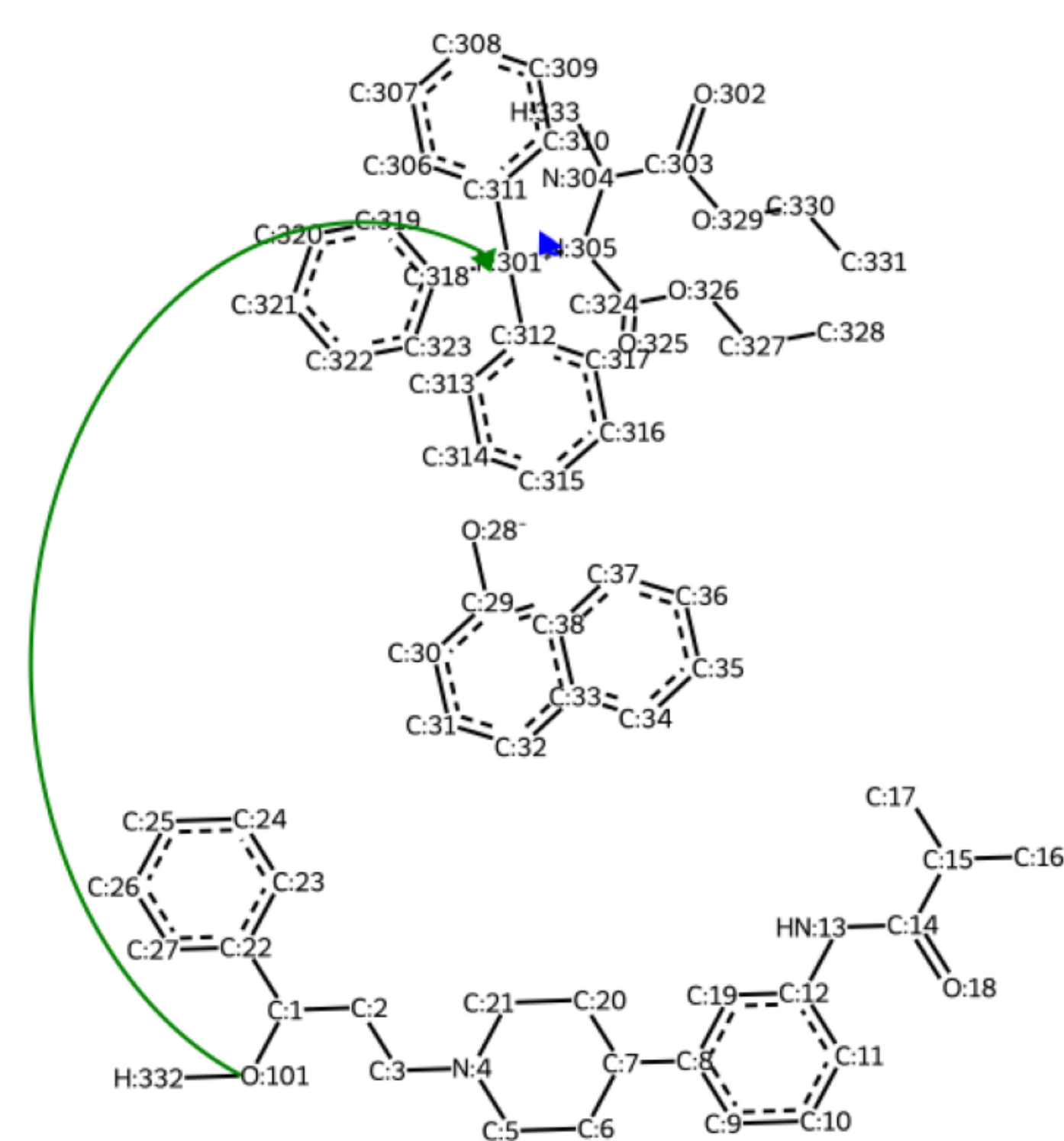
step #2



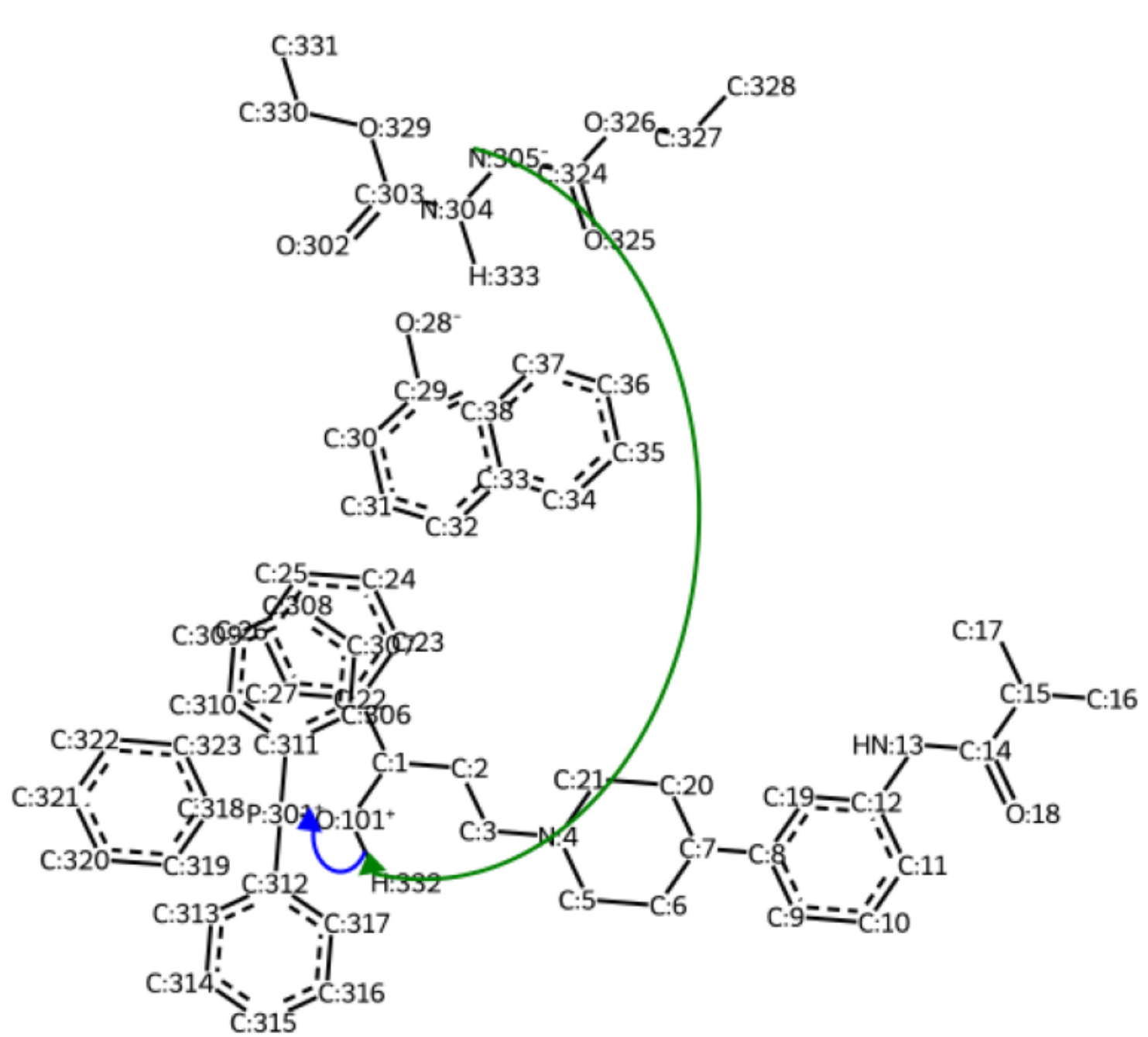
step #3



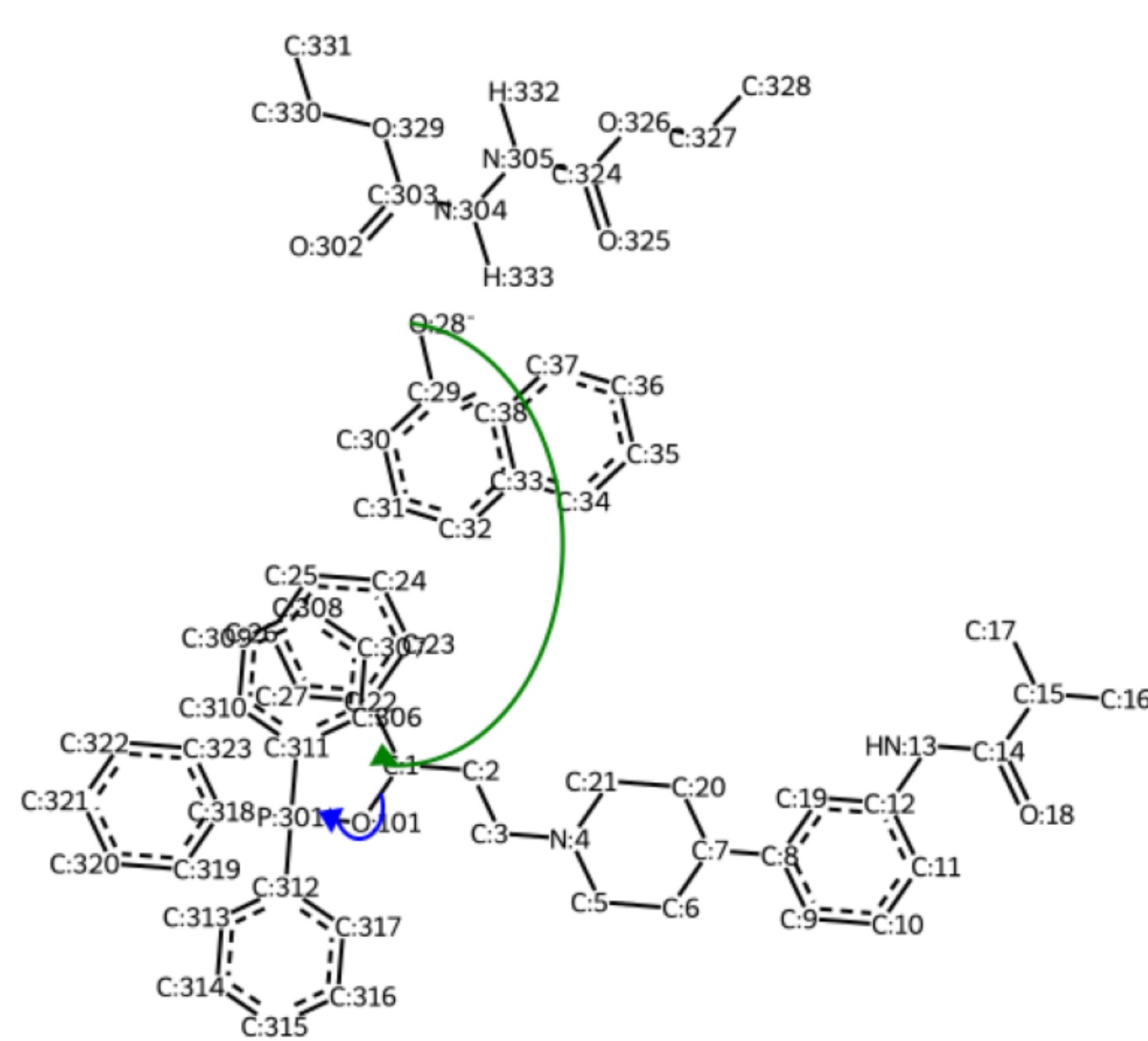
step #4



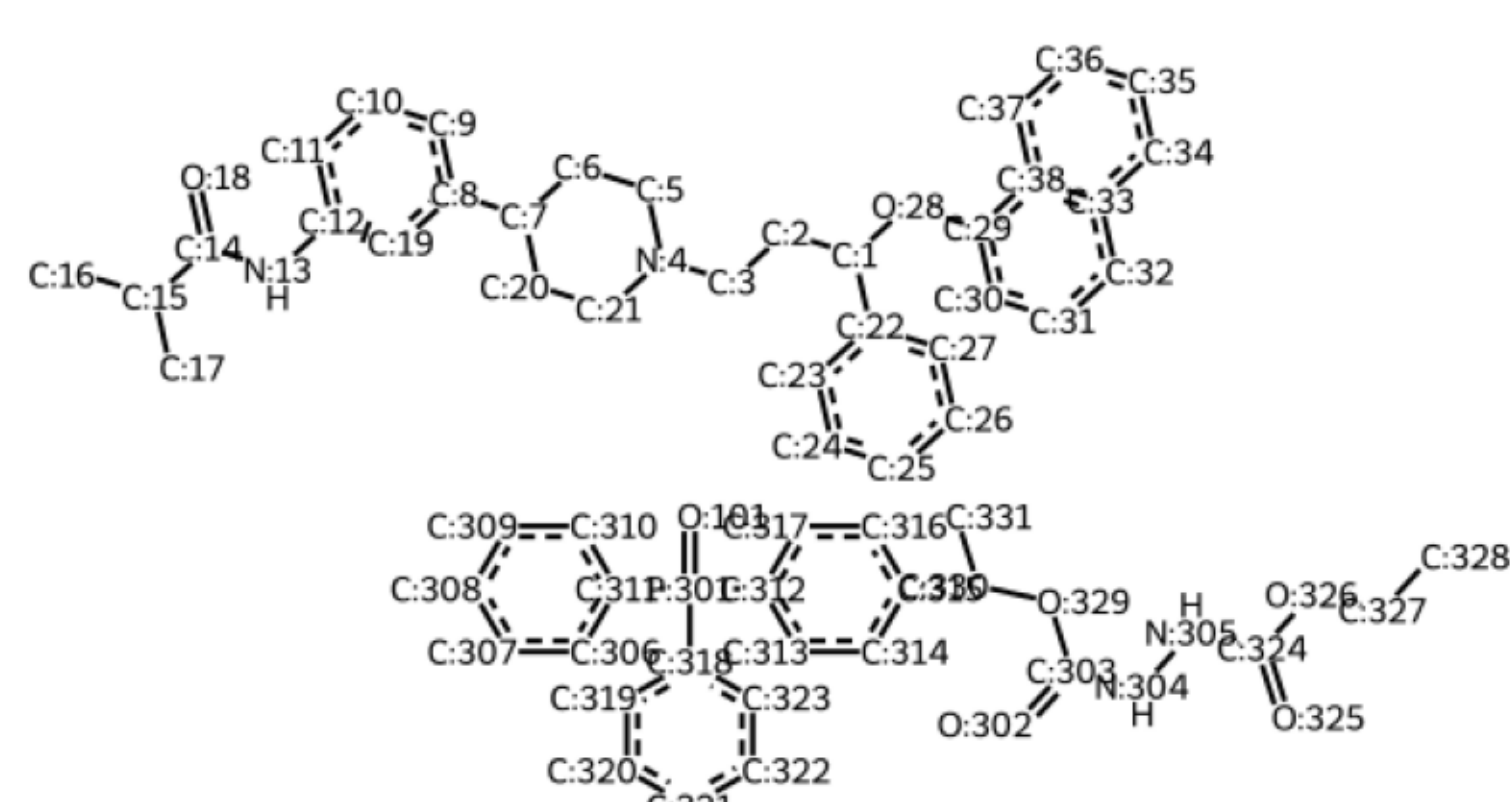
step #5



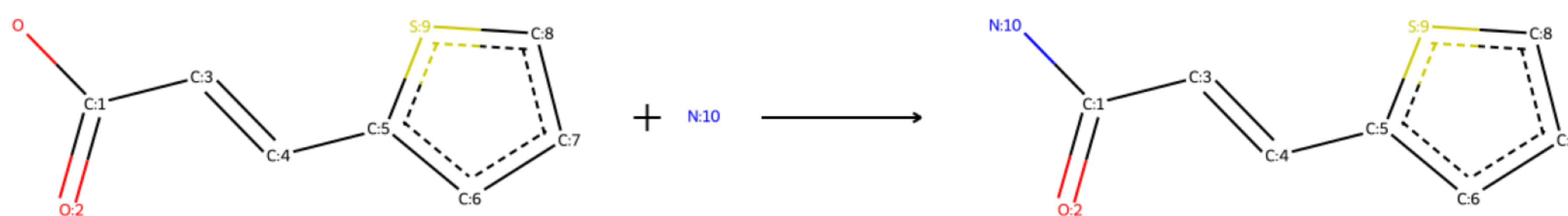
step #6



Product(s)



Original reaction
sampled RXN_ID:95)



Identified mechanistic class -
DCC_condensation reaction

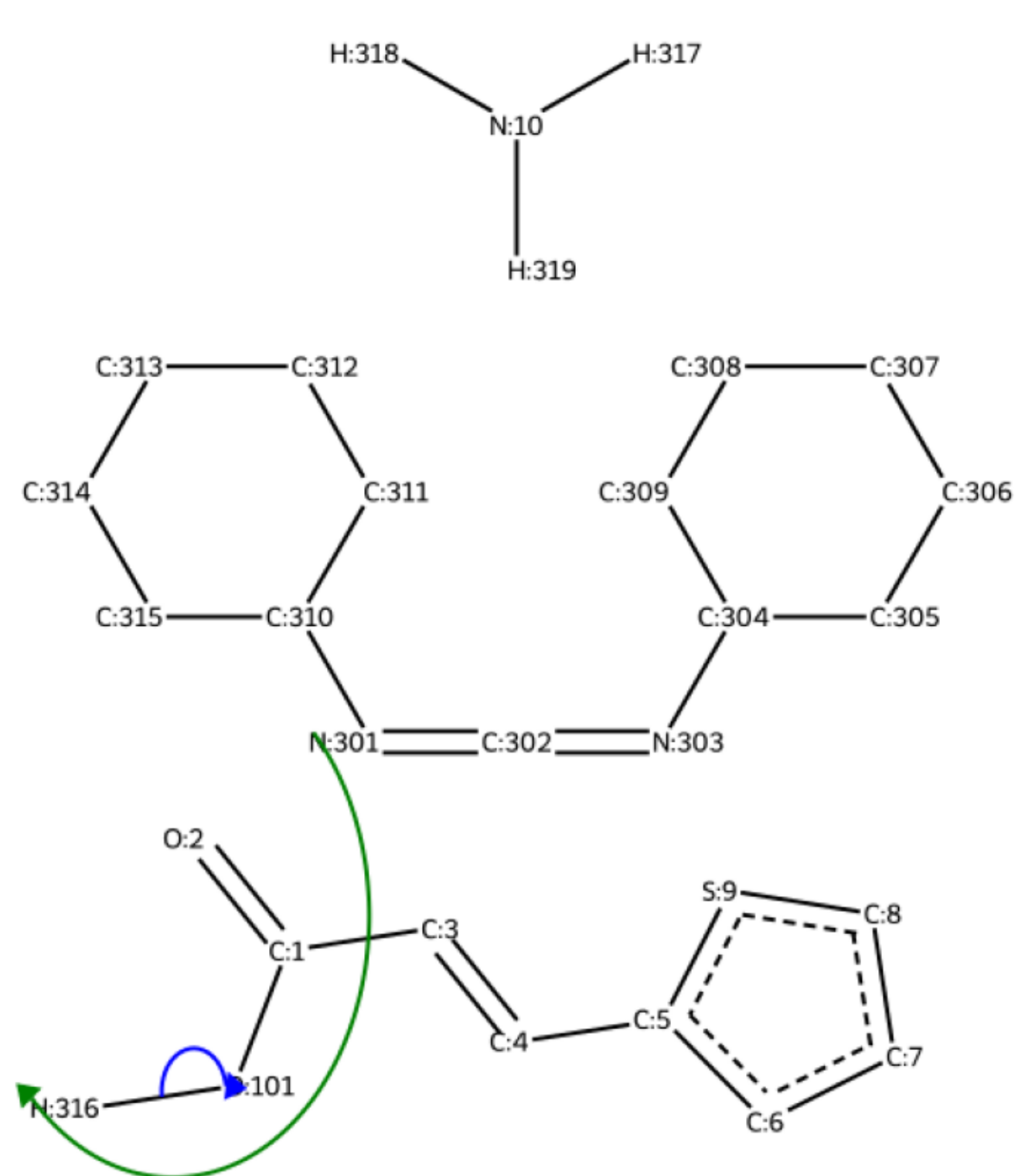
Reaction with missing reagents recovered



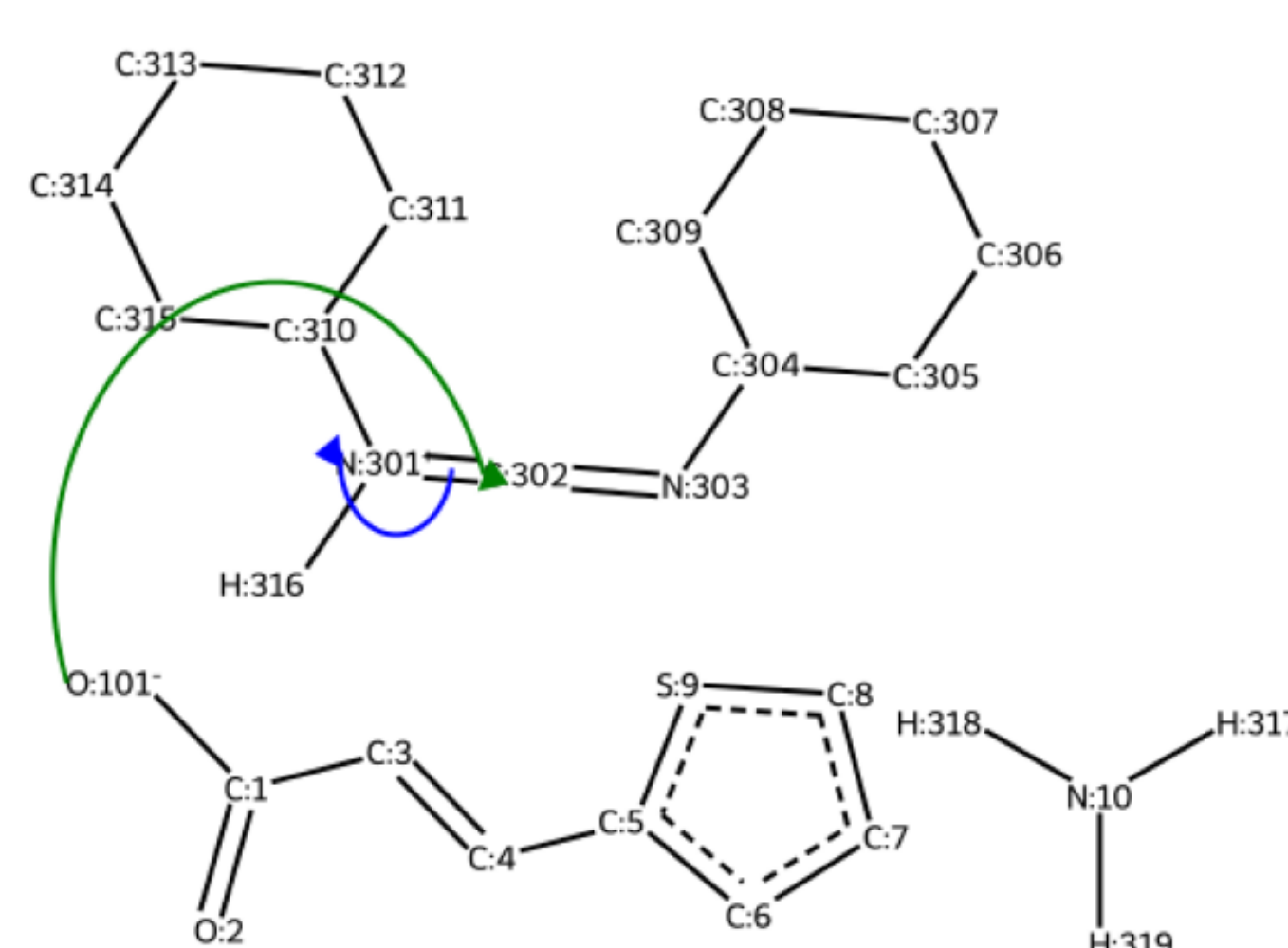
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

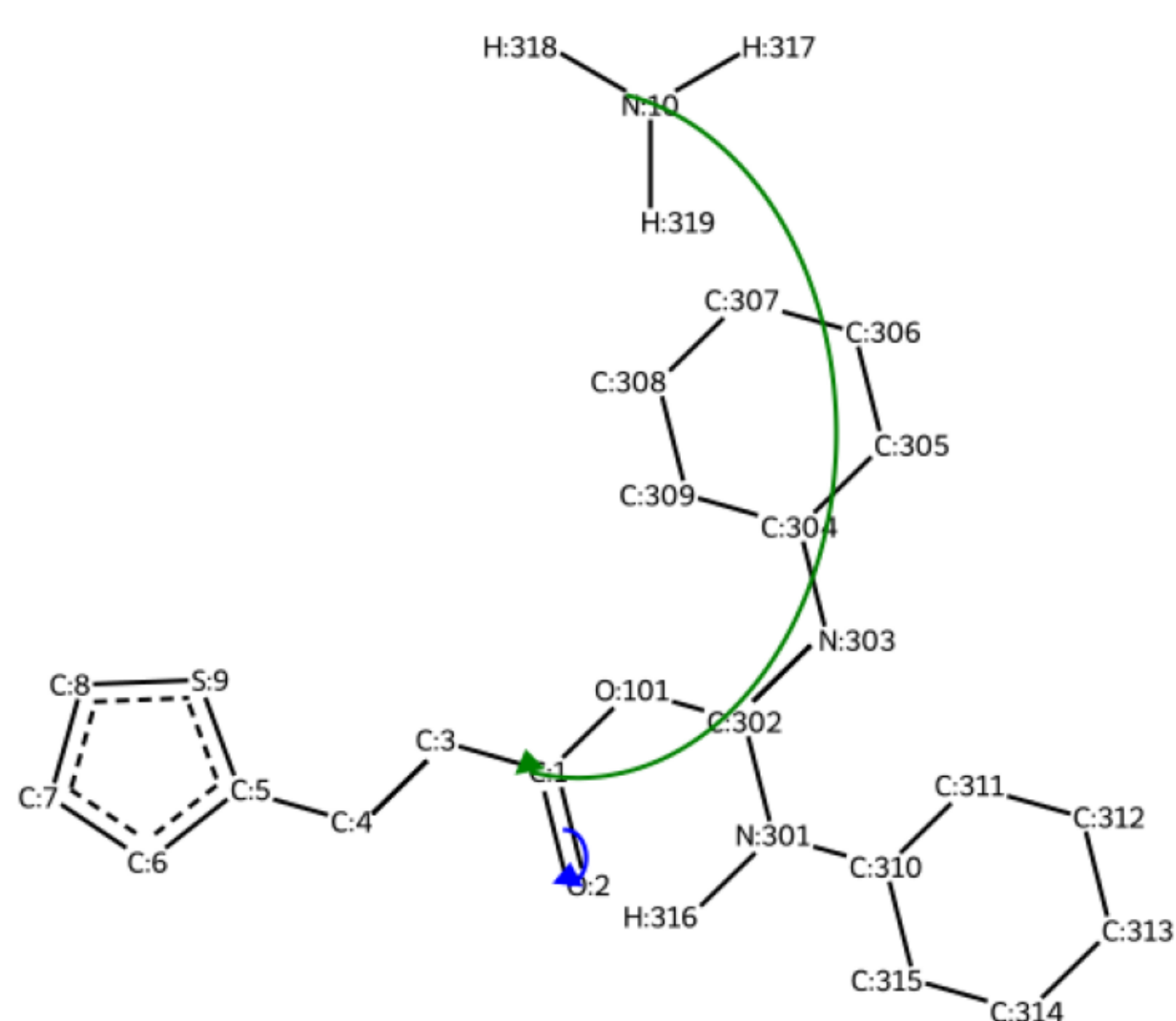
step #1



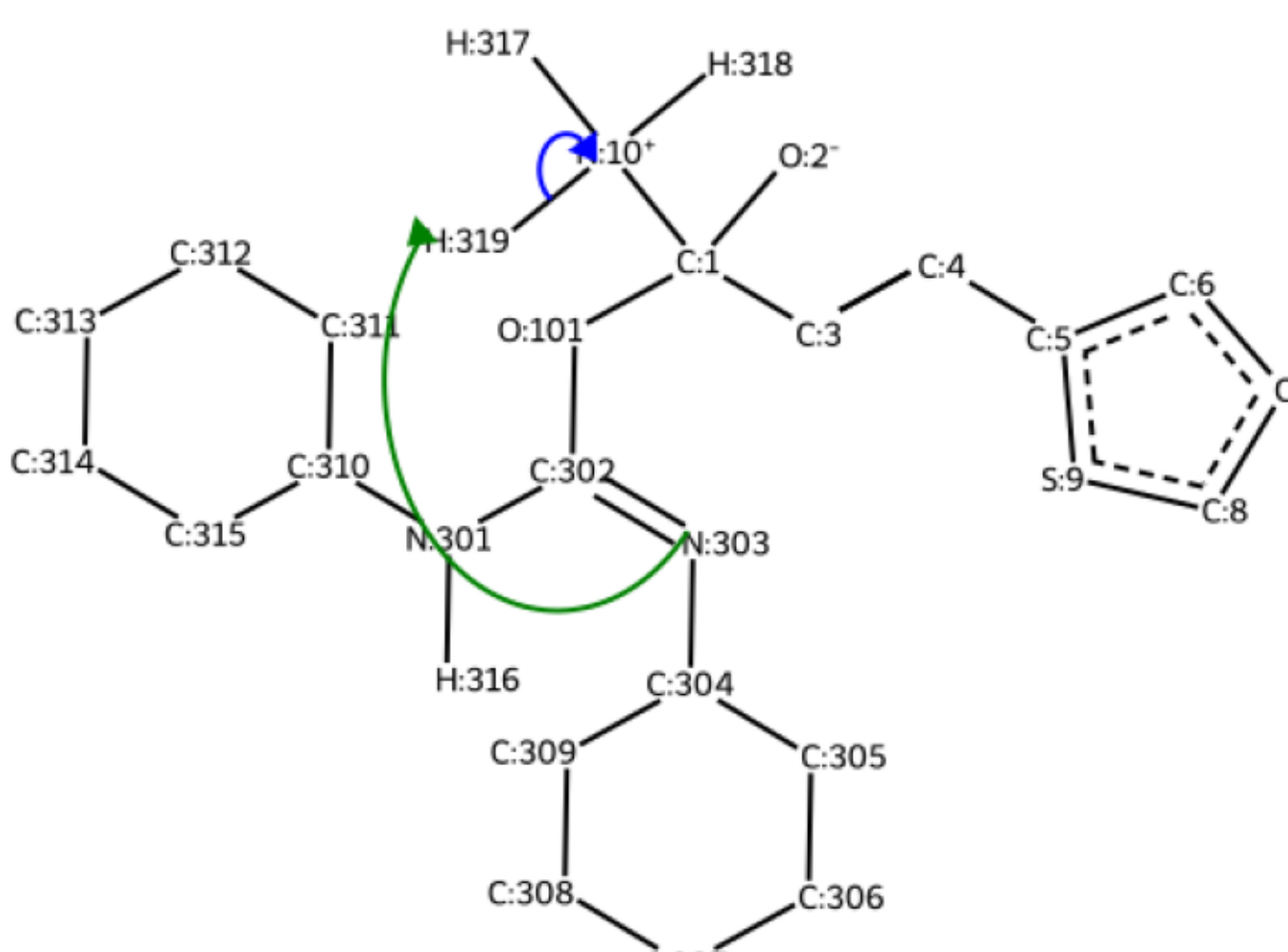
step #2



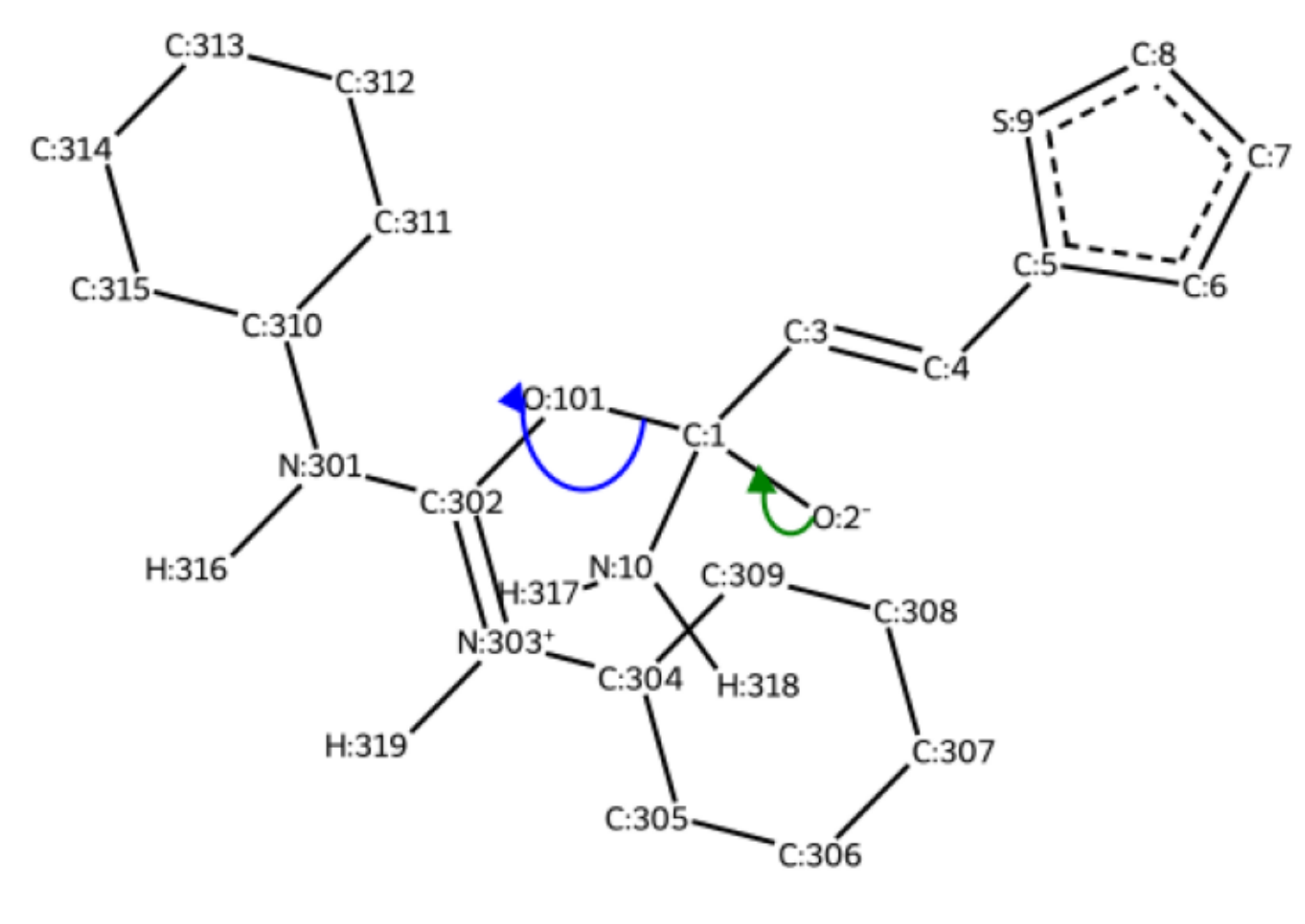
step #3



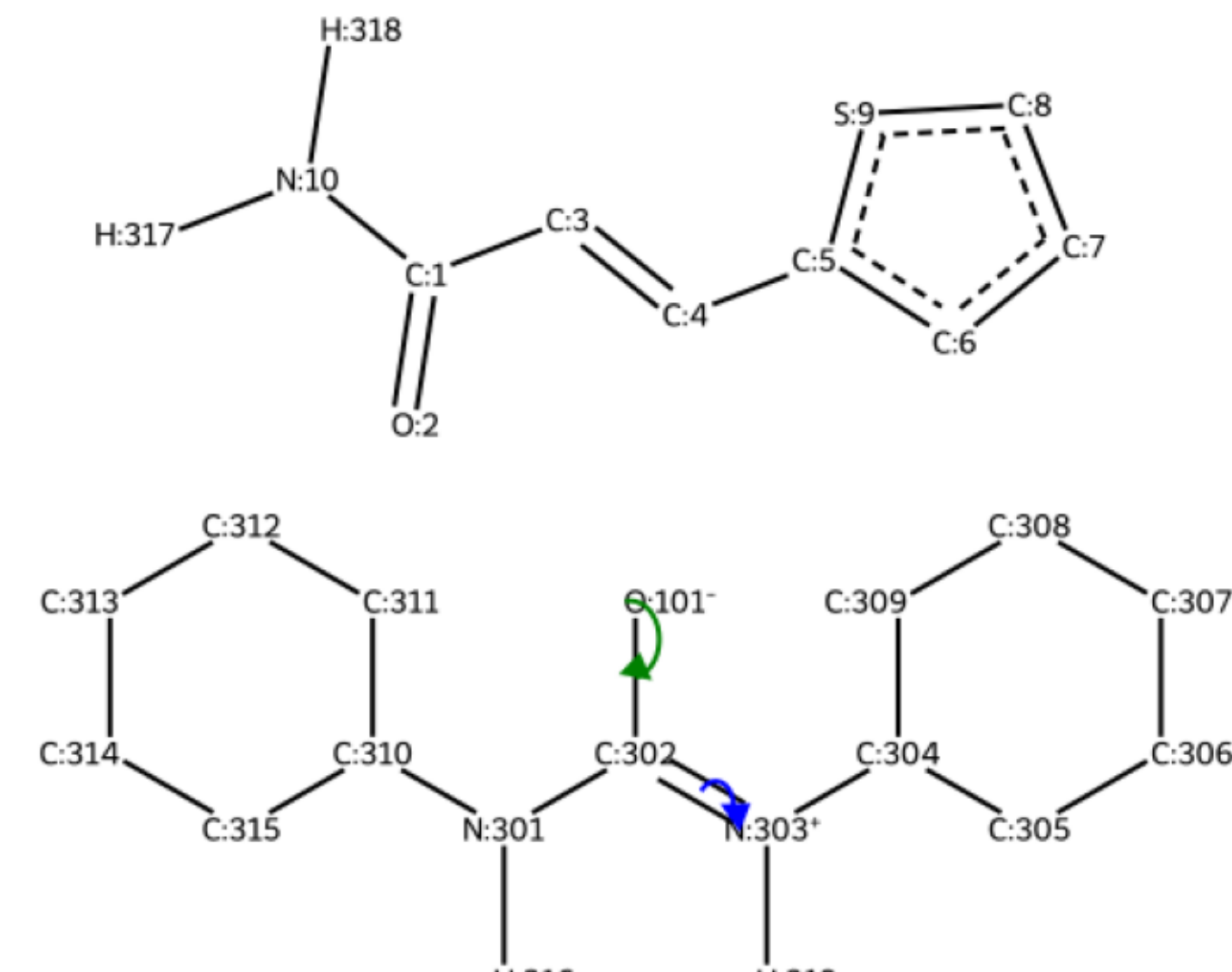
step #4



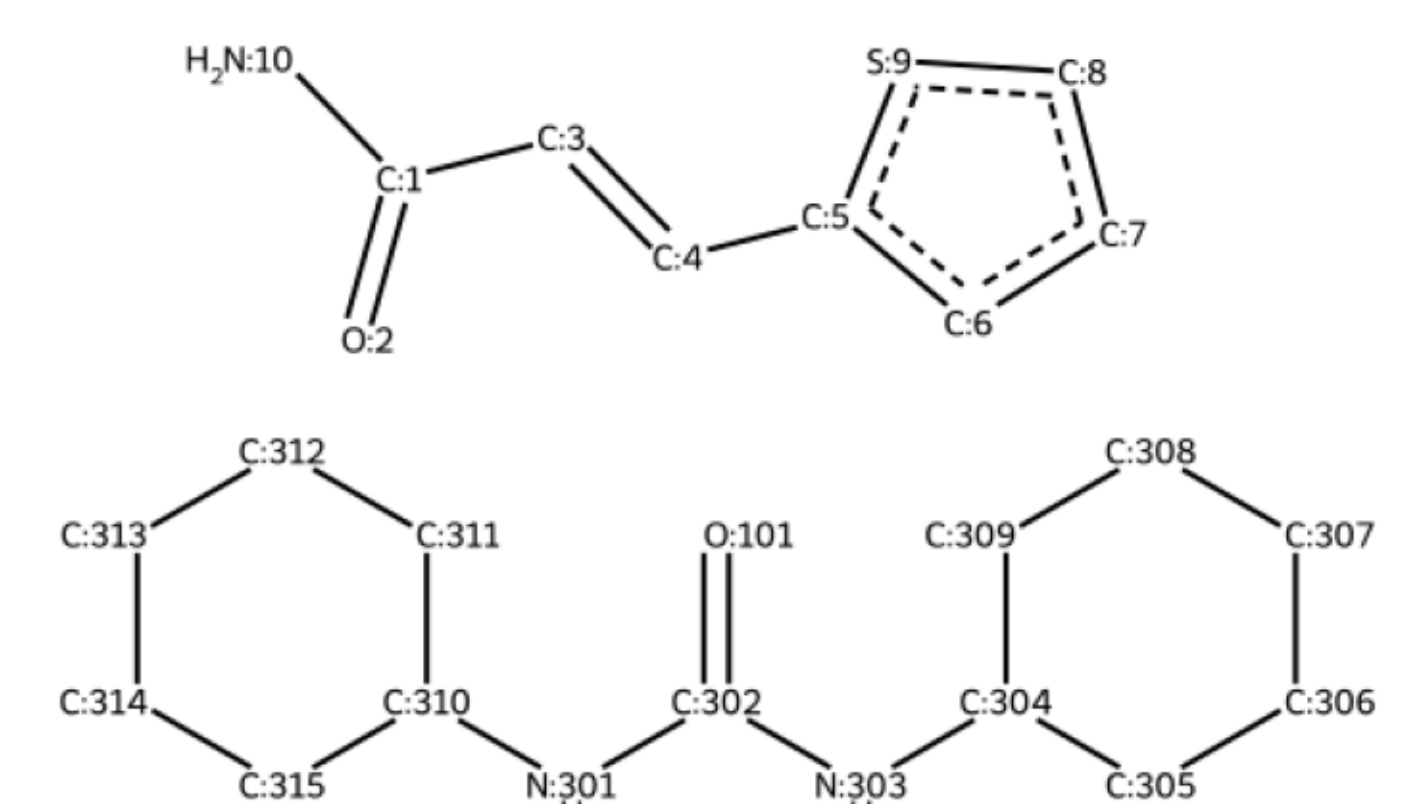
step #5



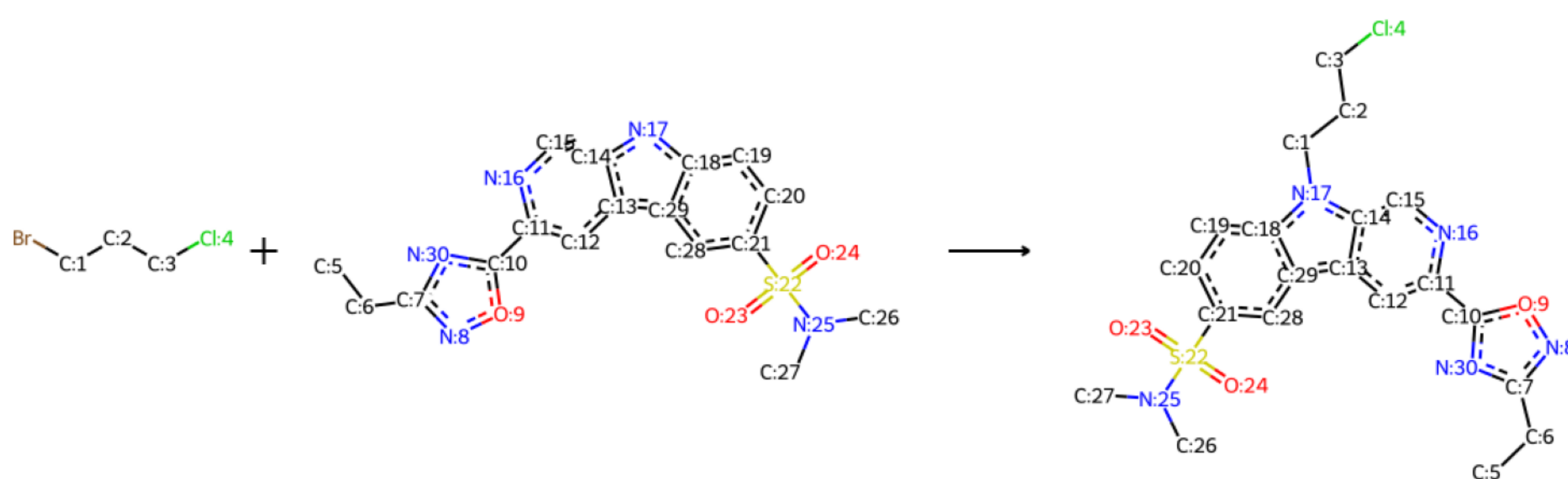
step #6



Product(s)

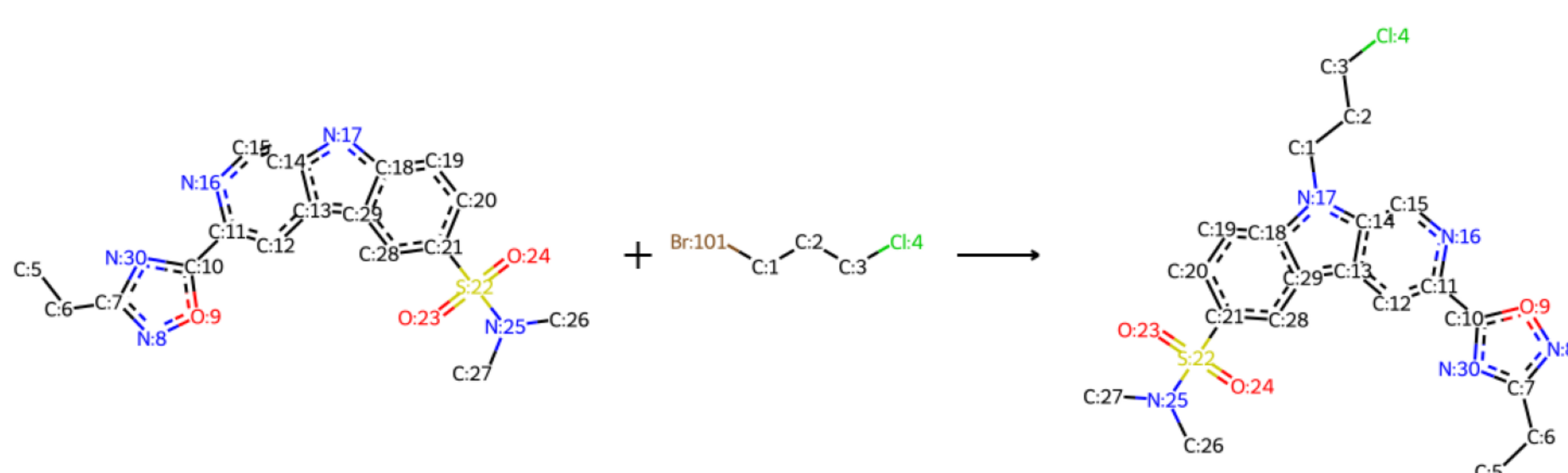


Original reaction sampled RXN_ID:96)



Identified mechanistic class -
SN2 reaction

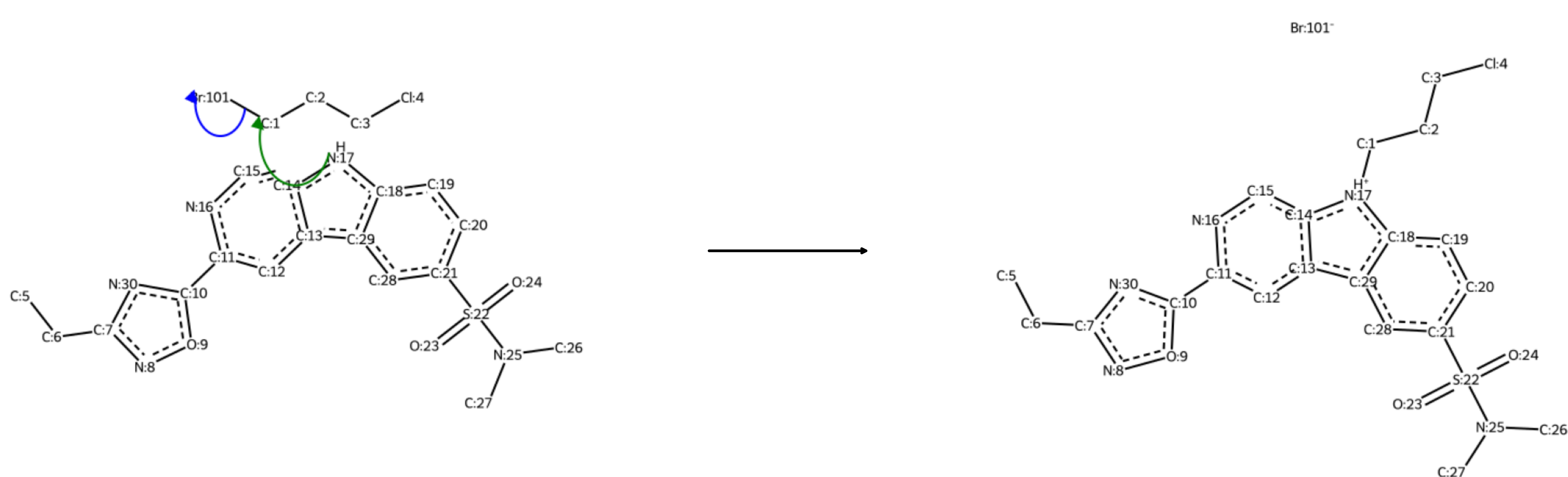
Reaction with missing reagents recovered



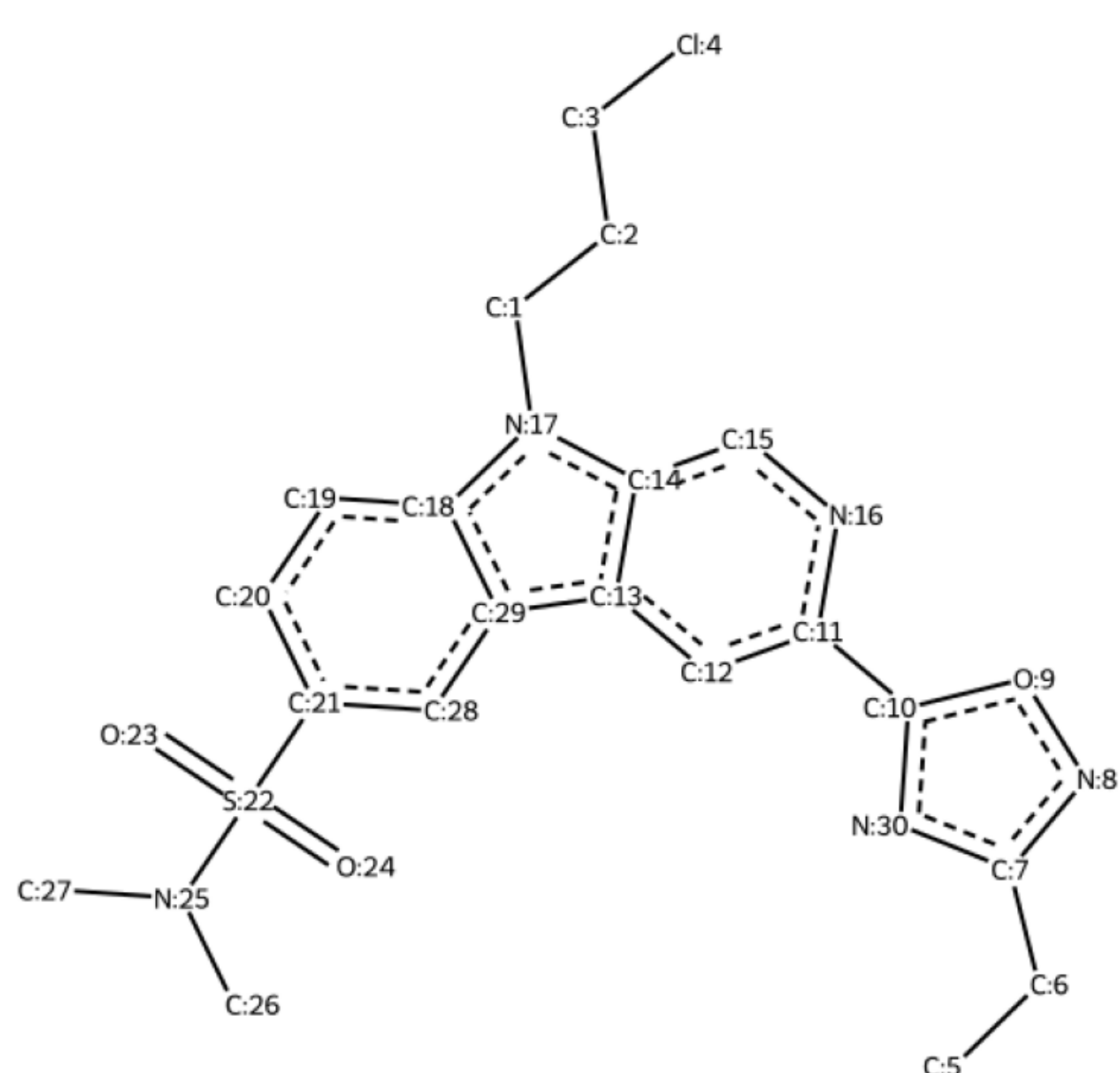
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

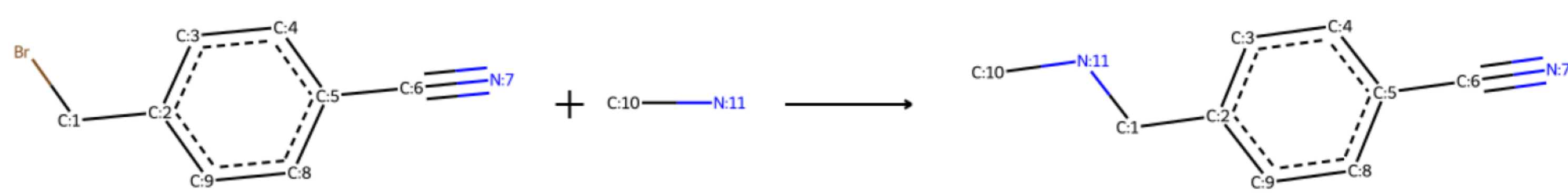
step #1



Product(s)

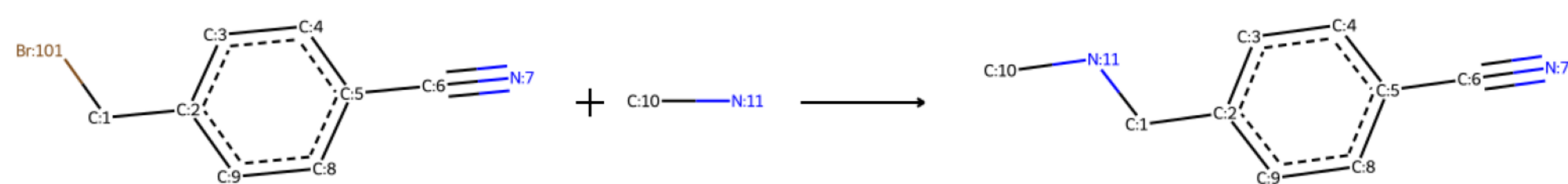


Original reaction
sampled RXN_ID:97)



Identified mechanistic class -
SN2 reaction

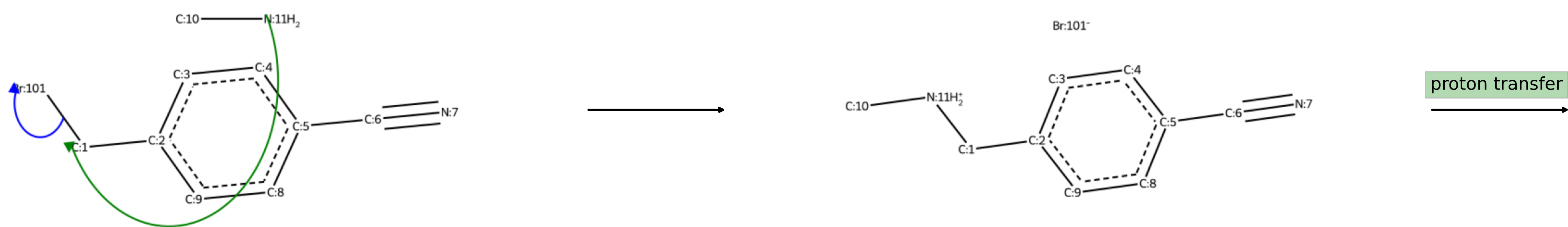
Reaction with missing reagents recovered



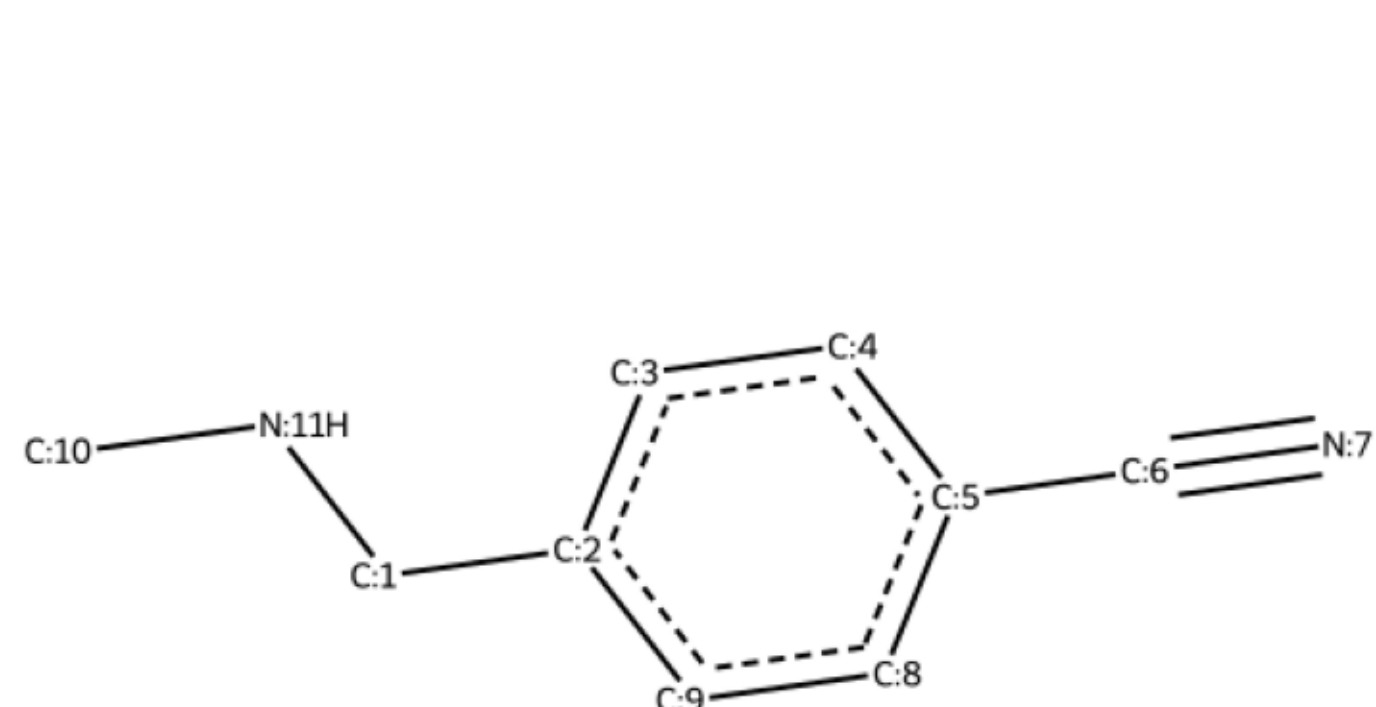
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

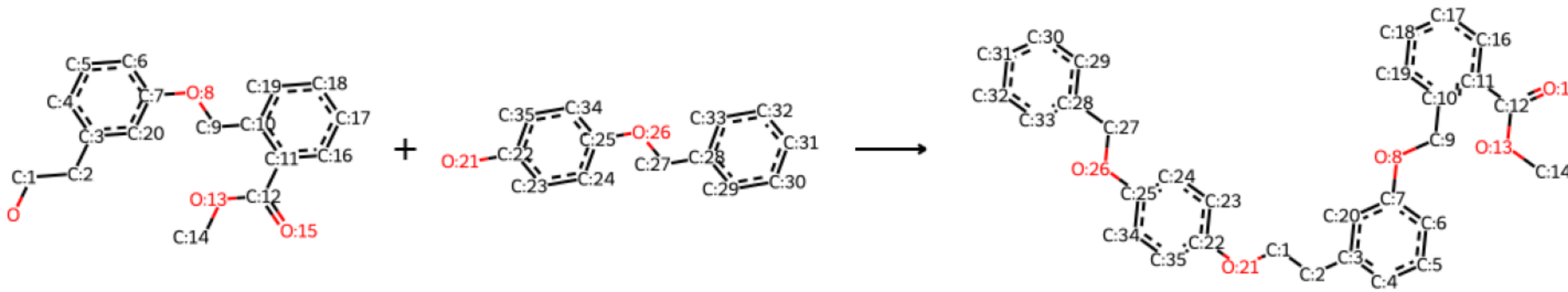
step #1



Product(s)

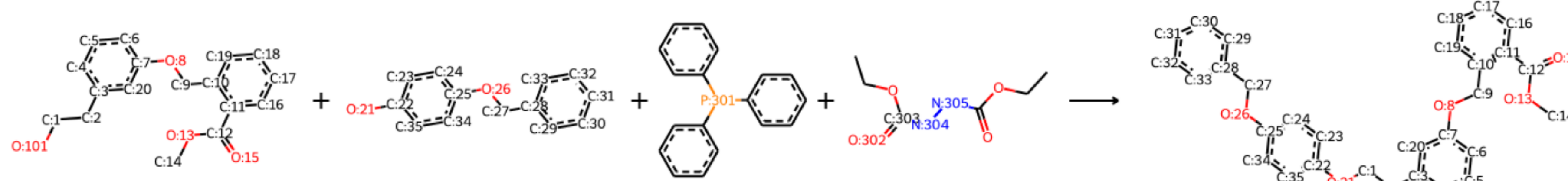


Original reaction
sampled RXN_ID:98)



Identified mechanistic class -
Mitsunobu reaction

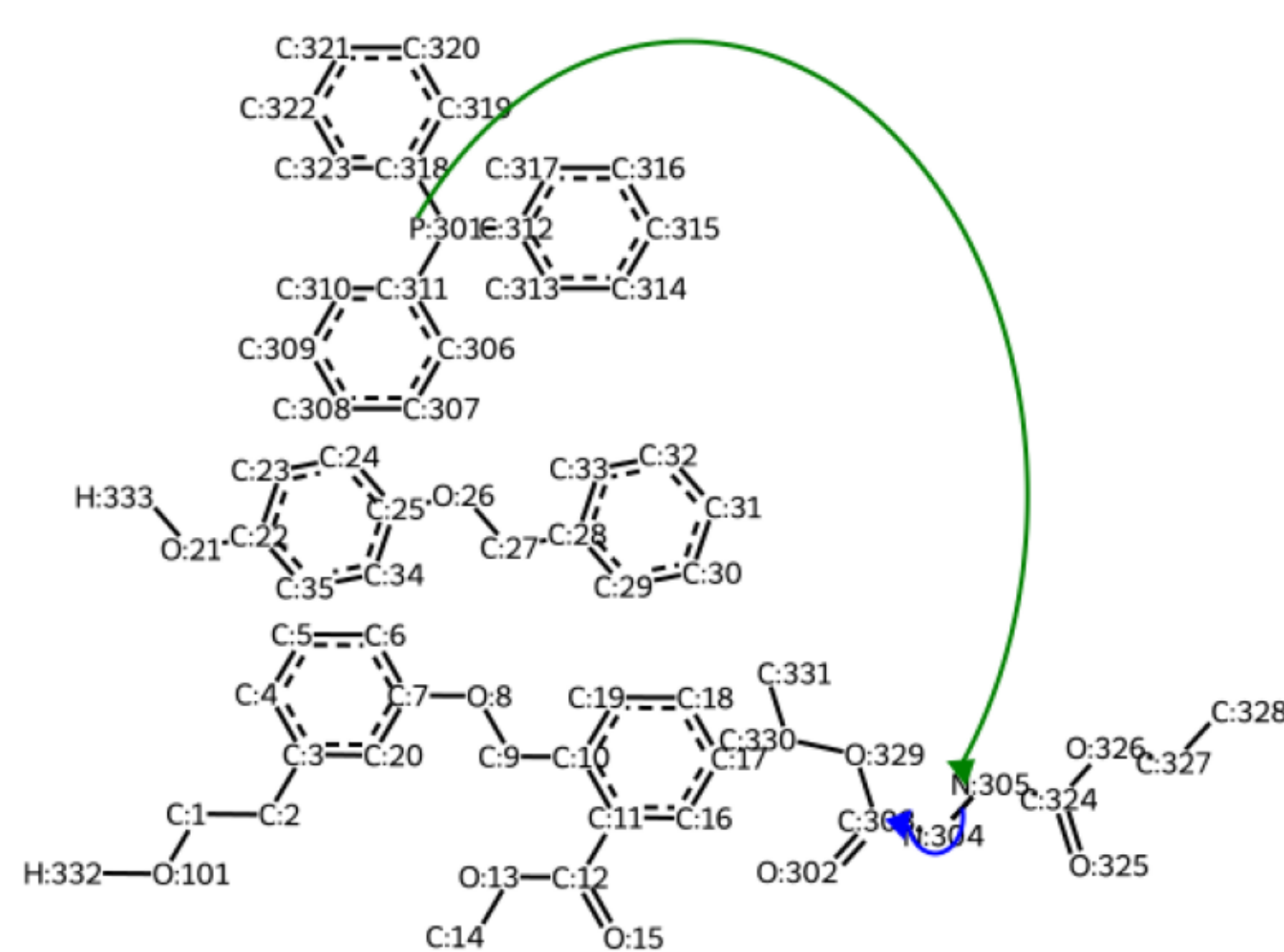
Reaction with missing reagents recovered



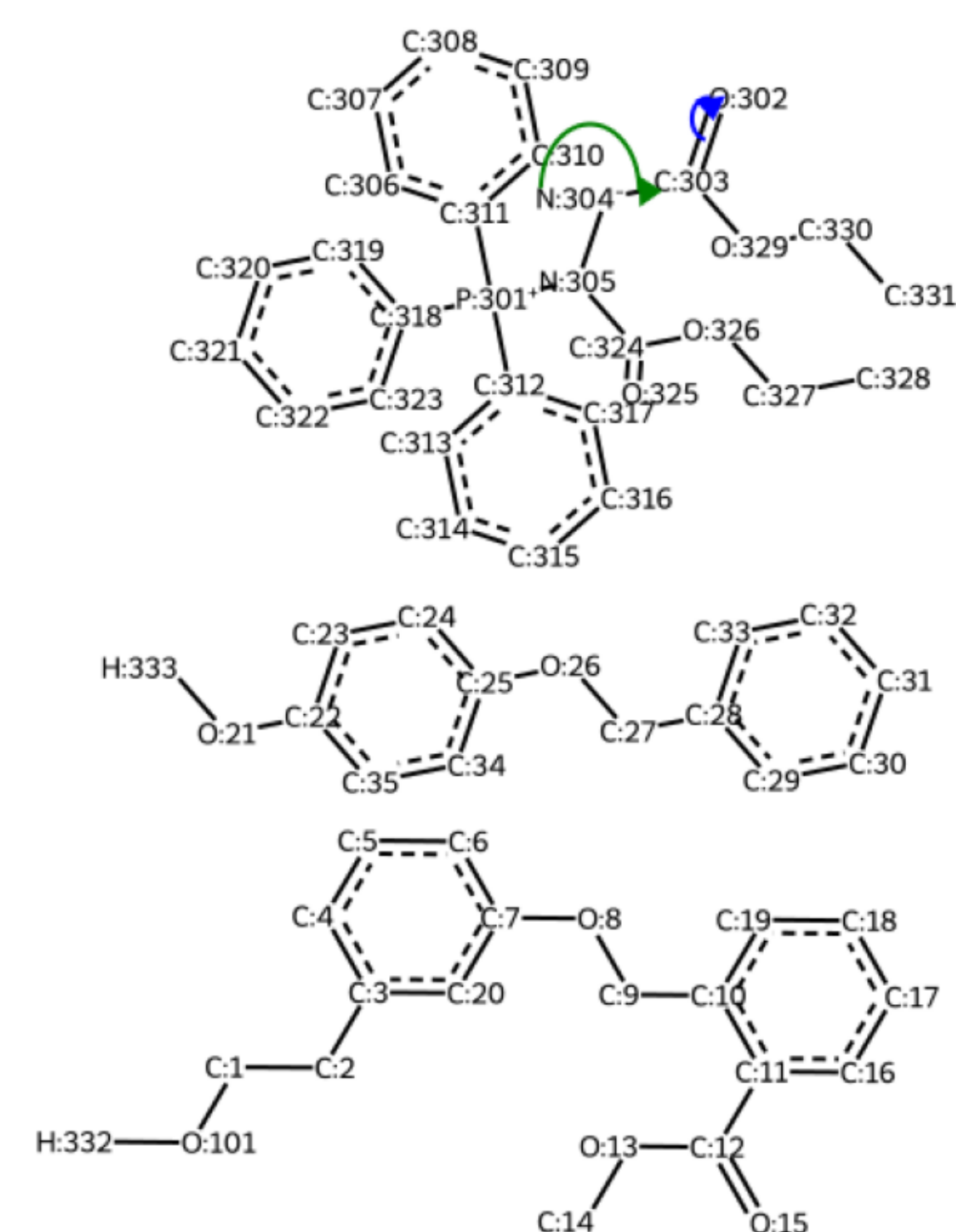
Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

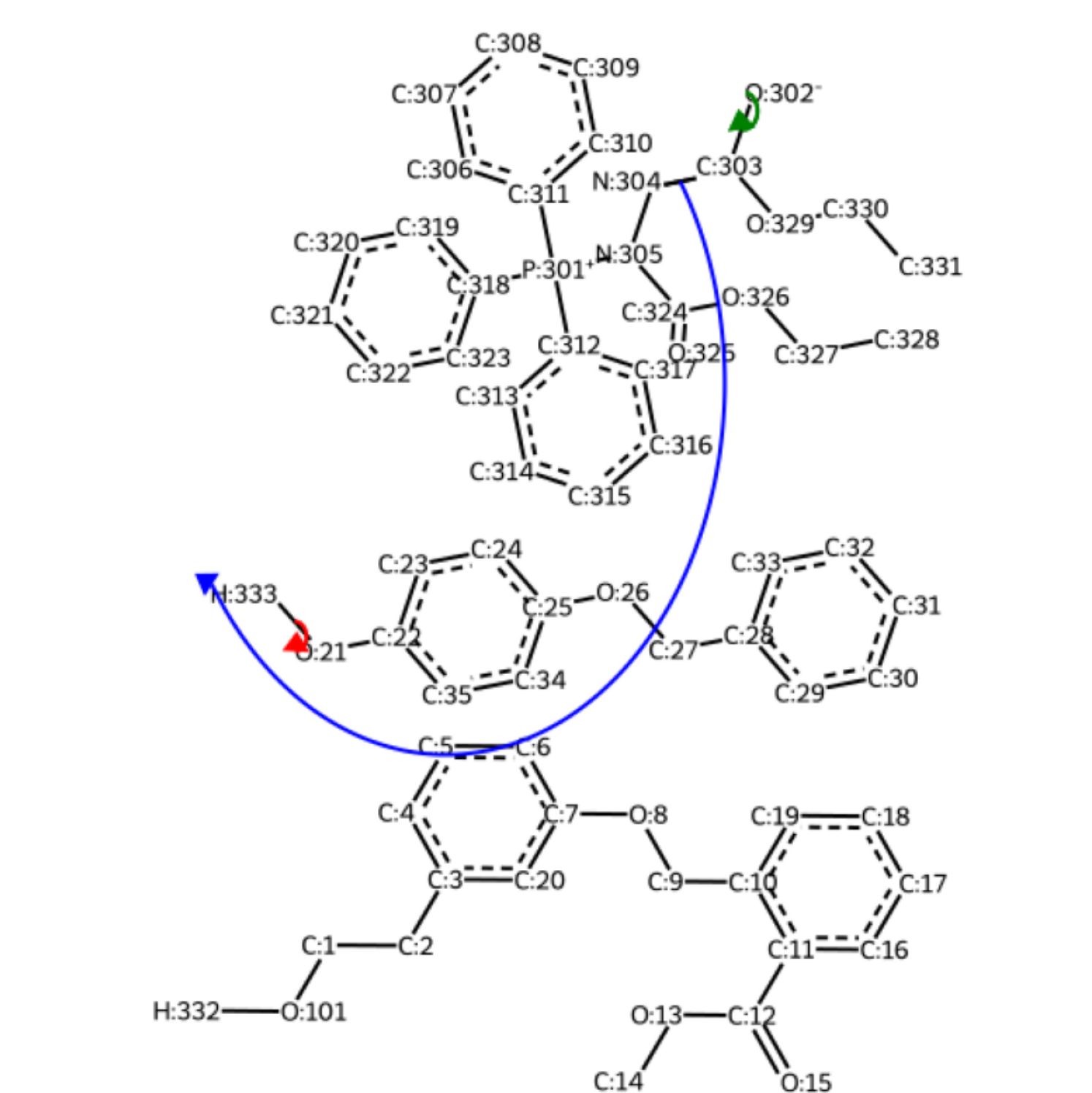
step #1



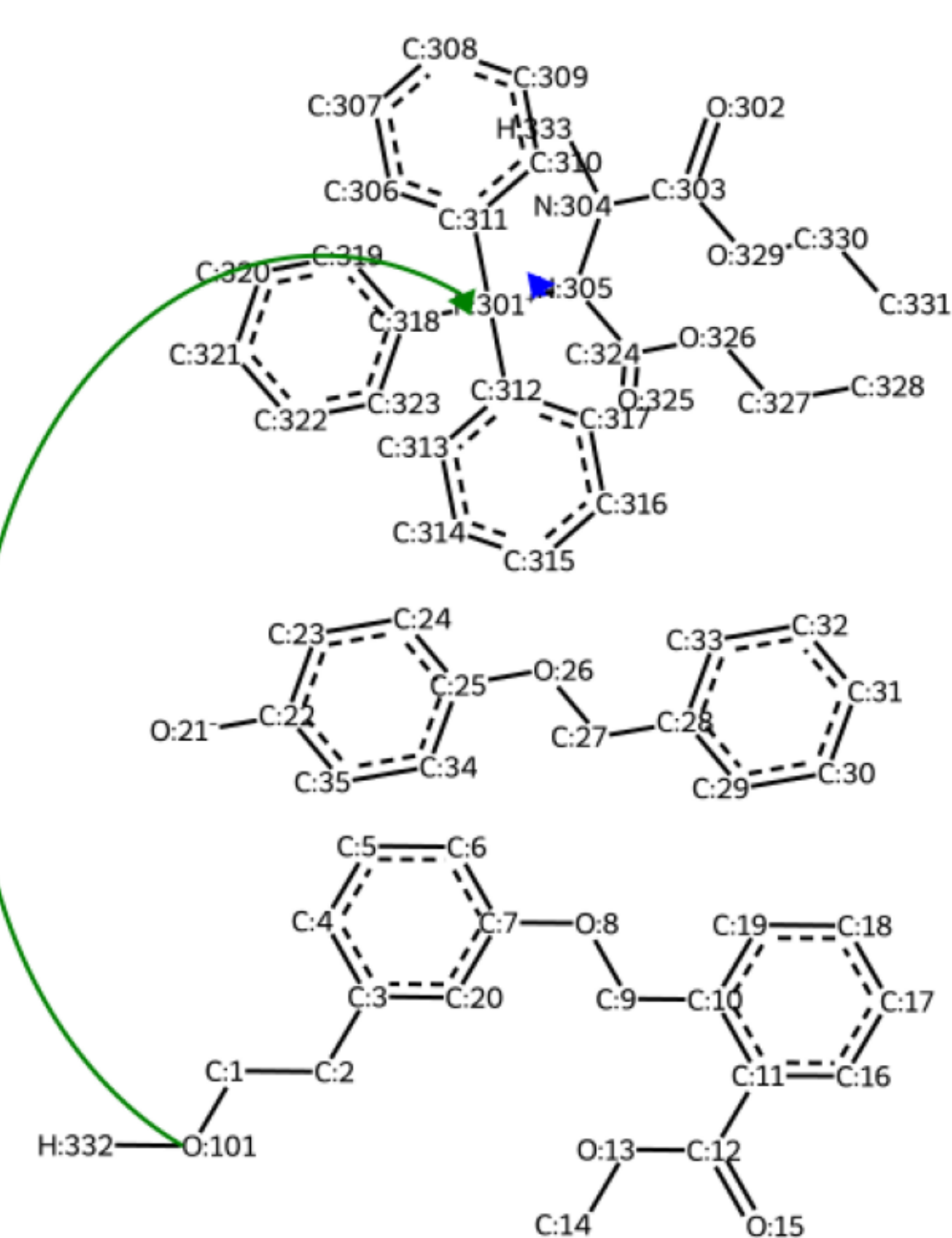
step #2



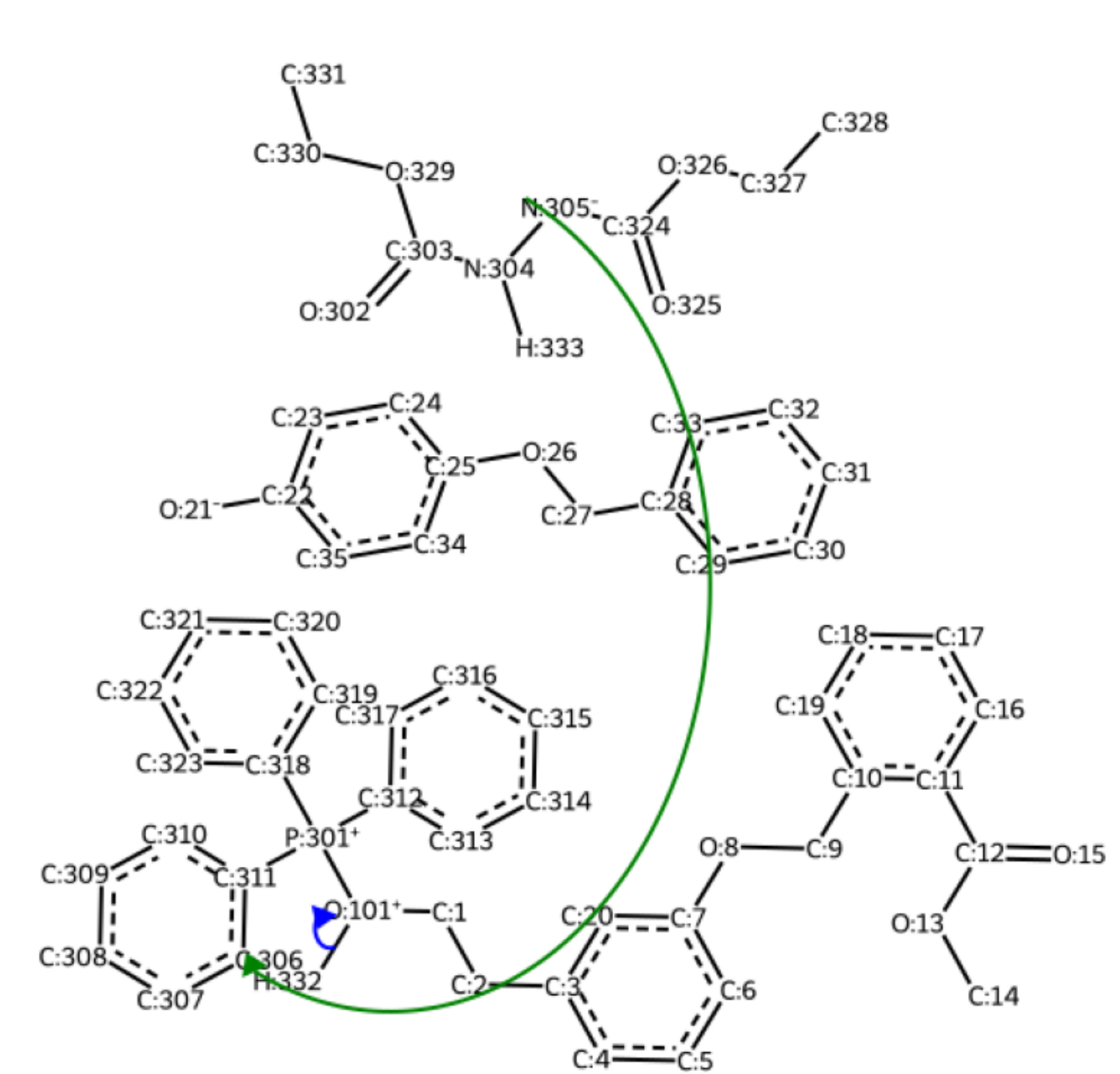
step #3



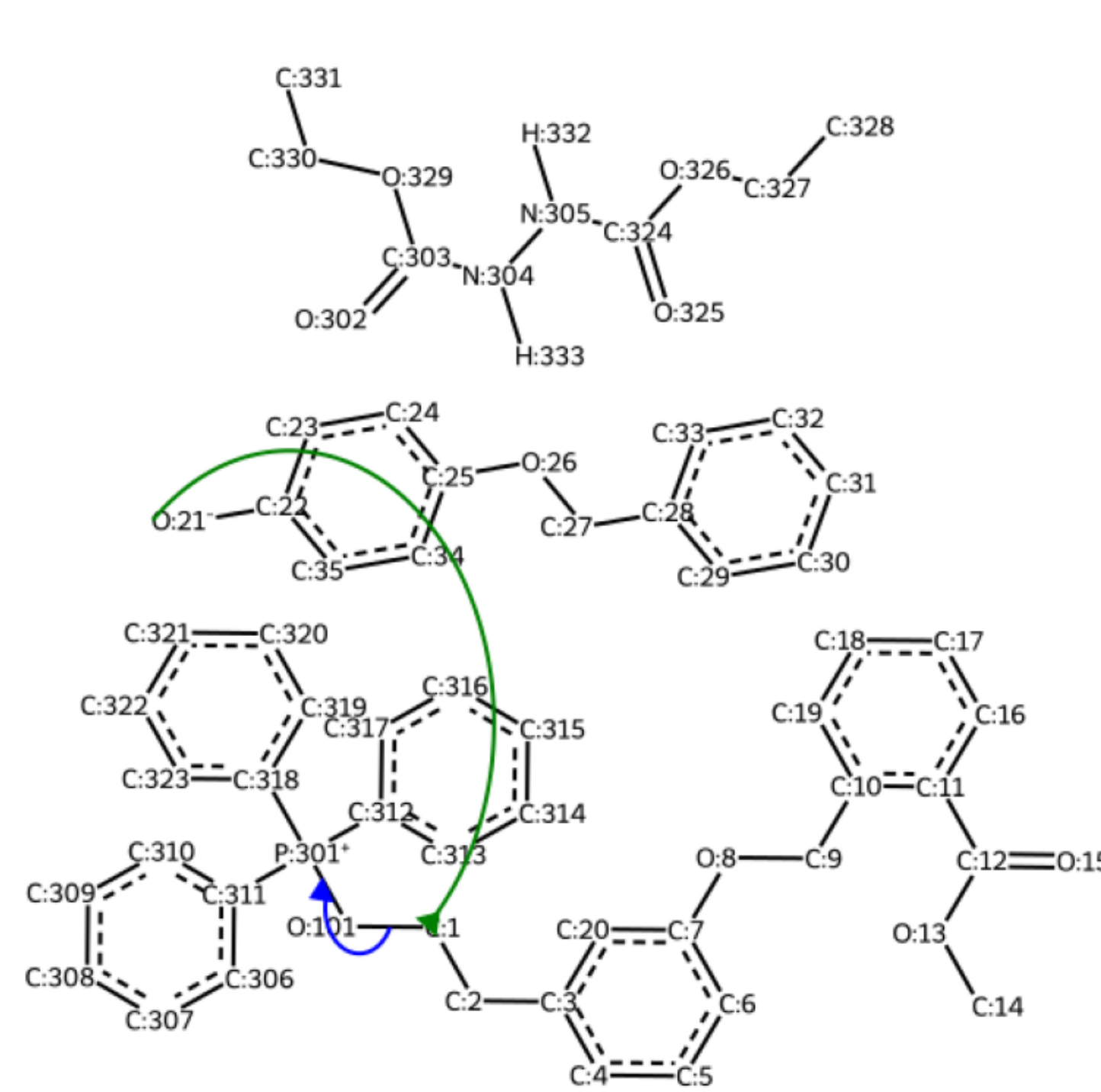
step #4



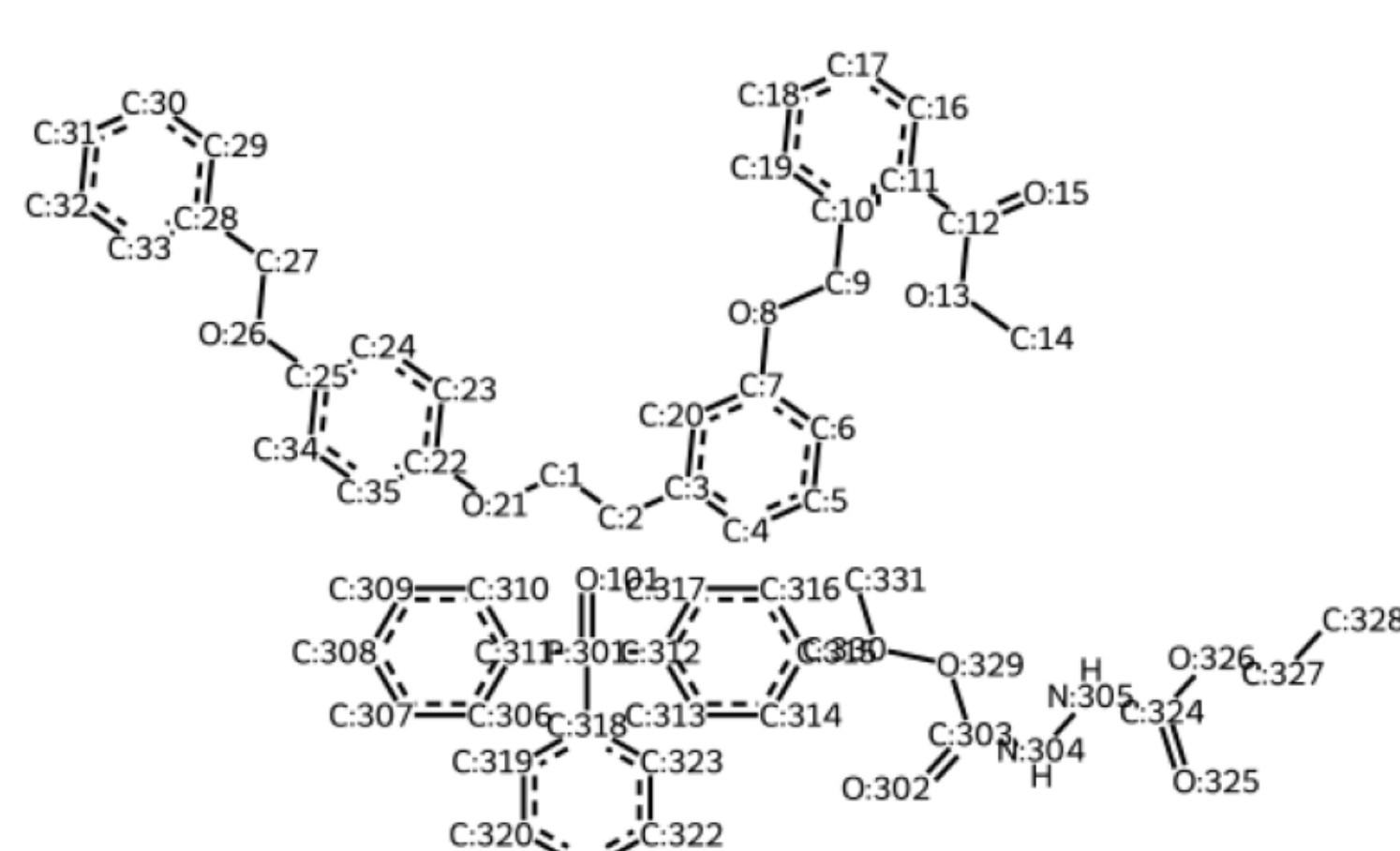
step #5



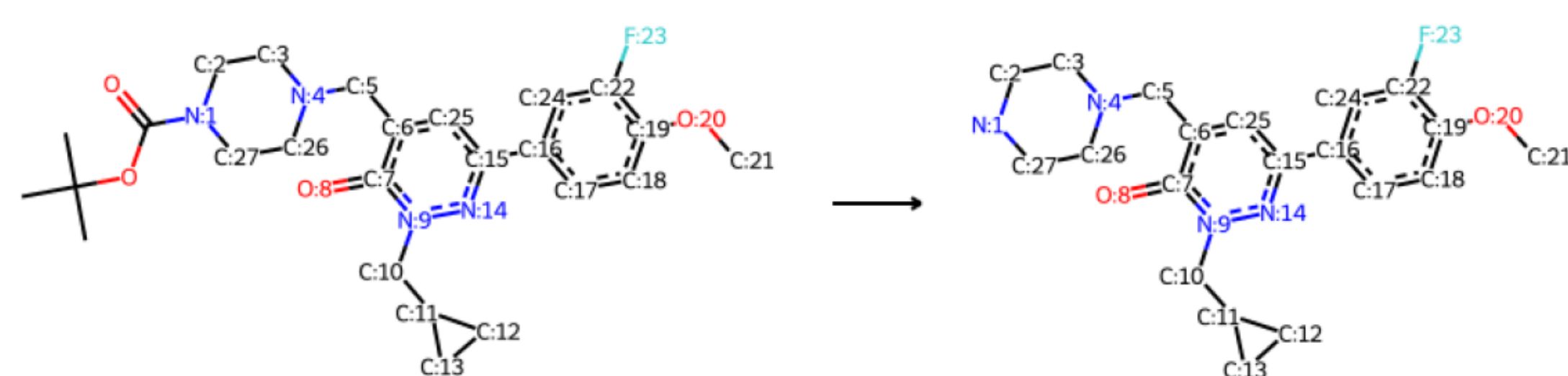
step #6



Product(s)

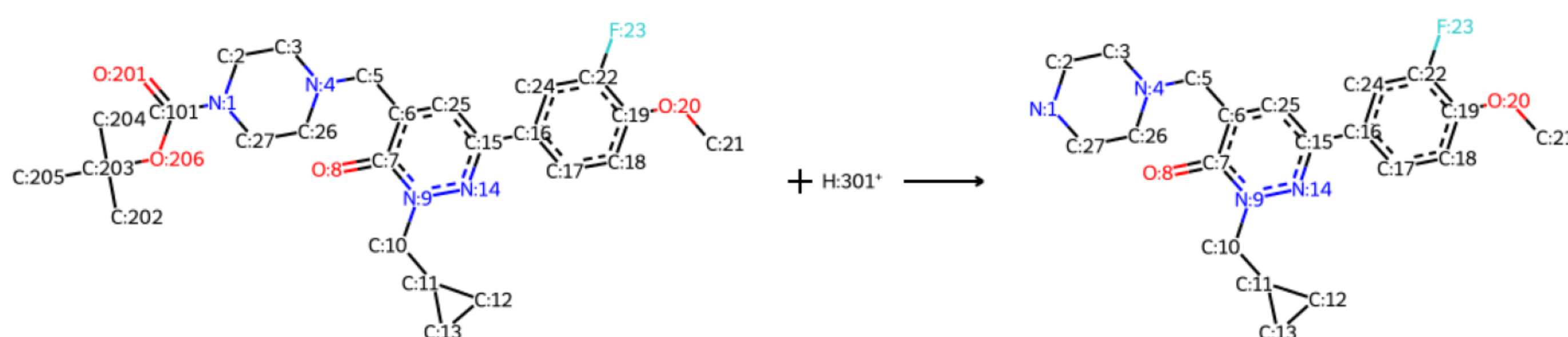


Original reaction
sampled RXN_ID:99)



Identified mechanistic class -
Boc_deprotection reaction

Reaction with missing reagents recovered

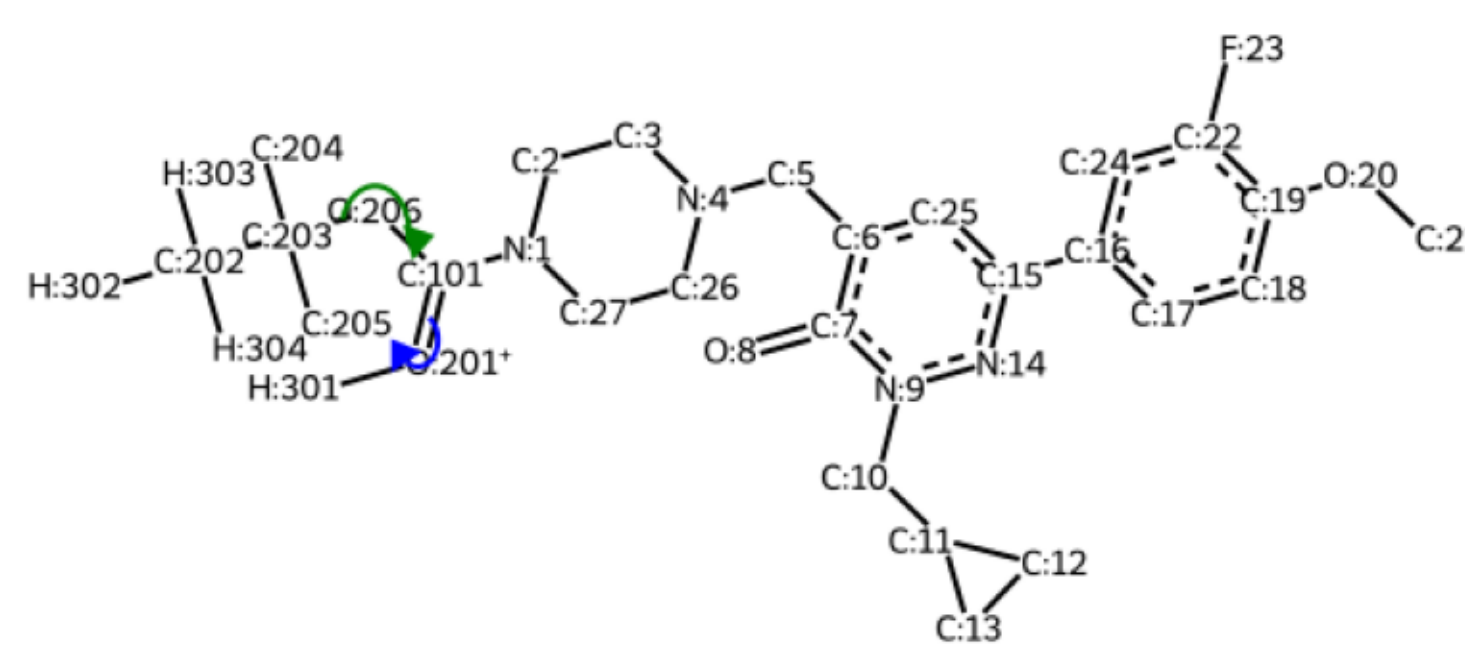
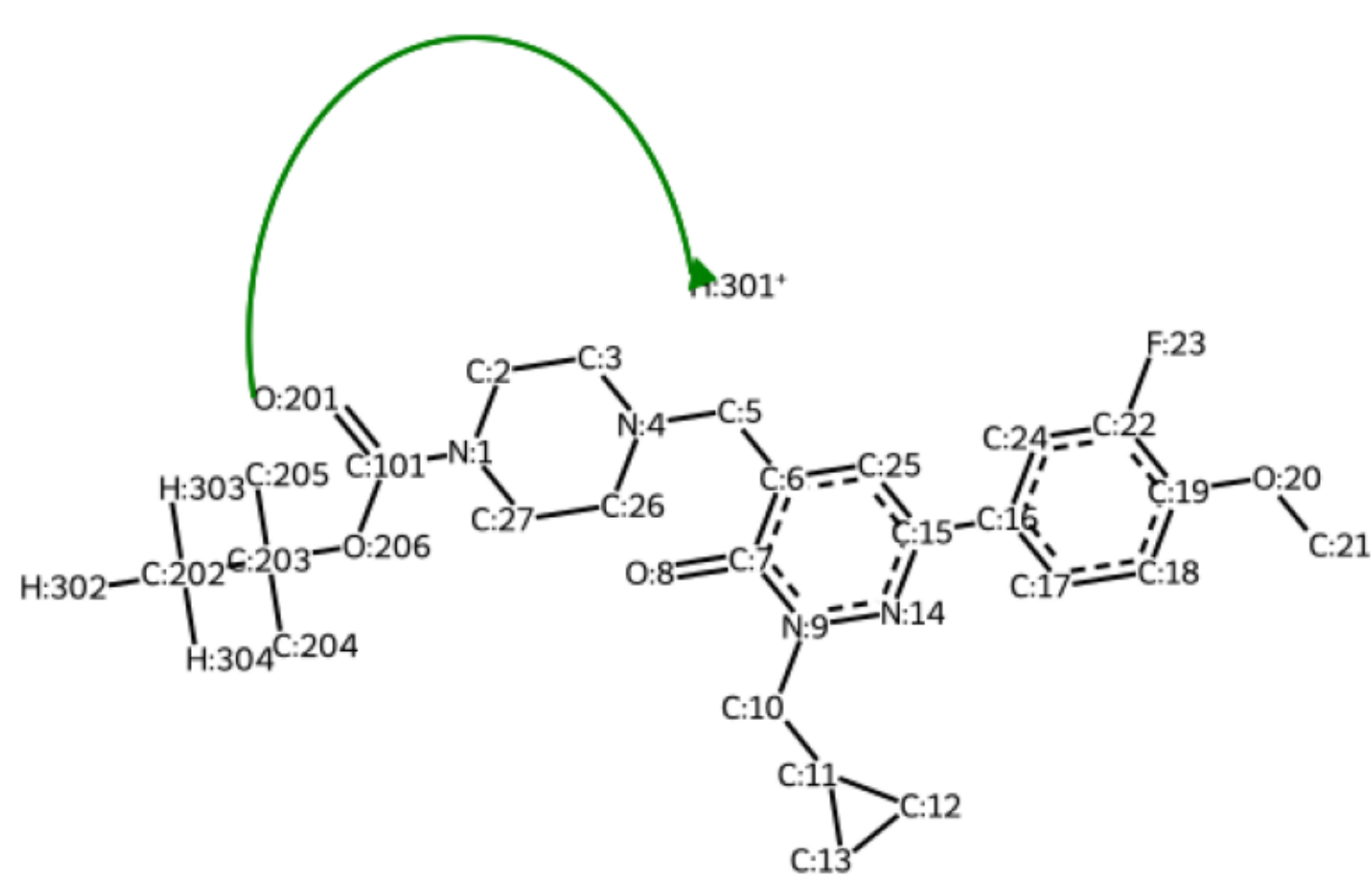


Proposed mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

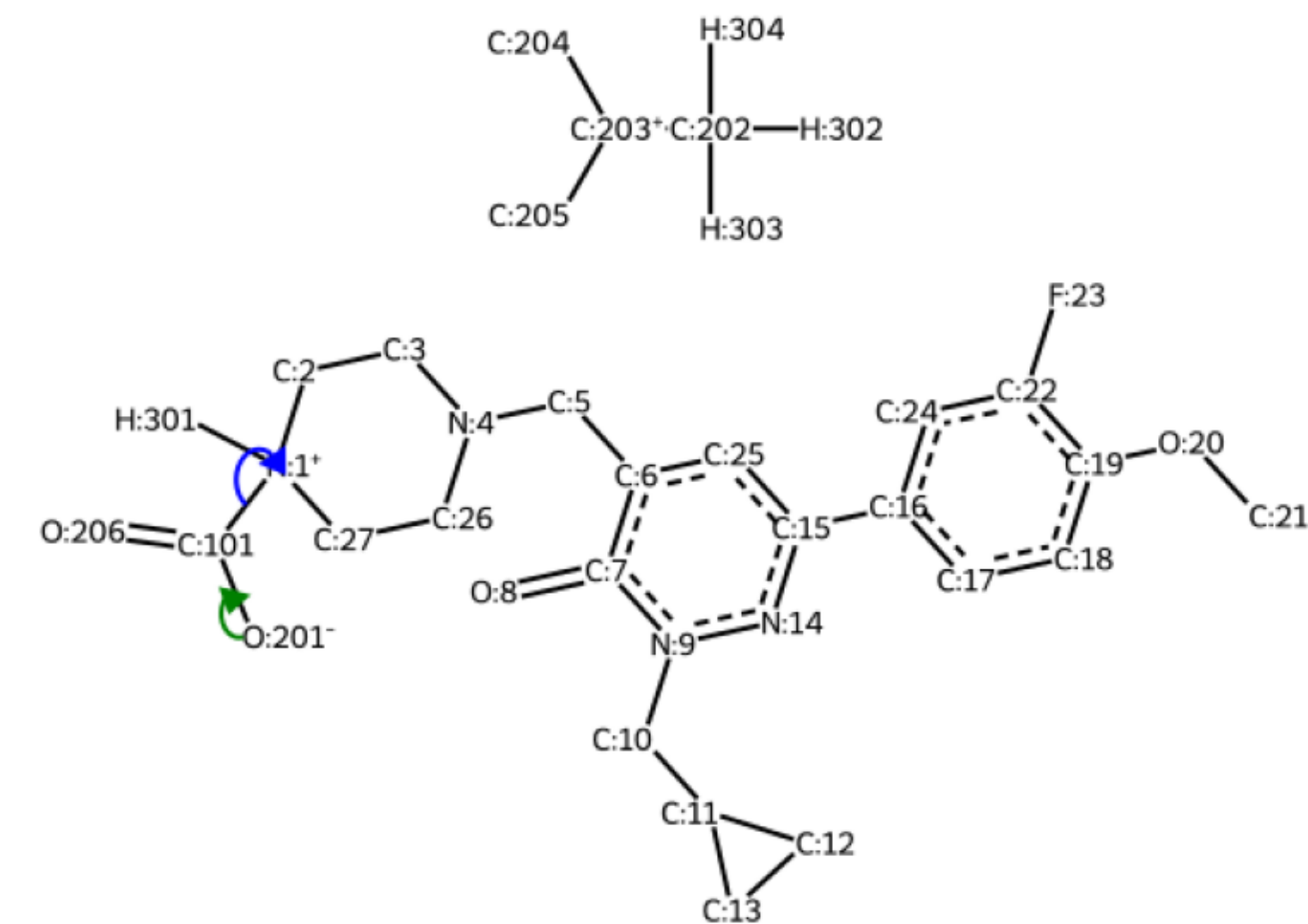
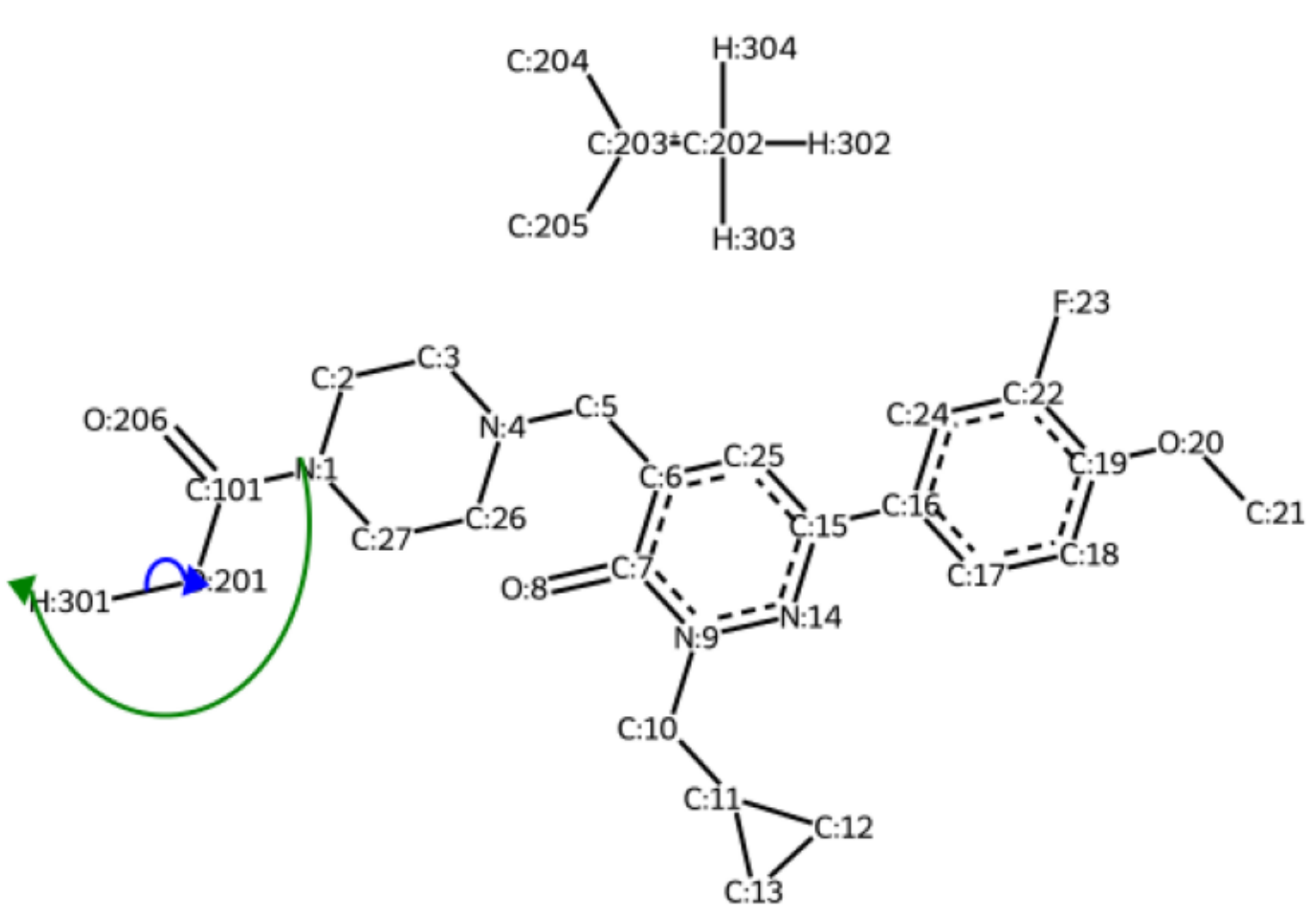
step #1

step #2



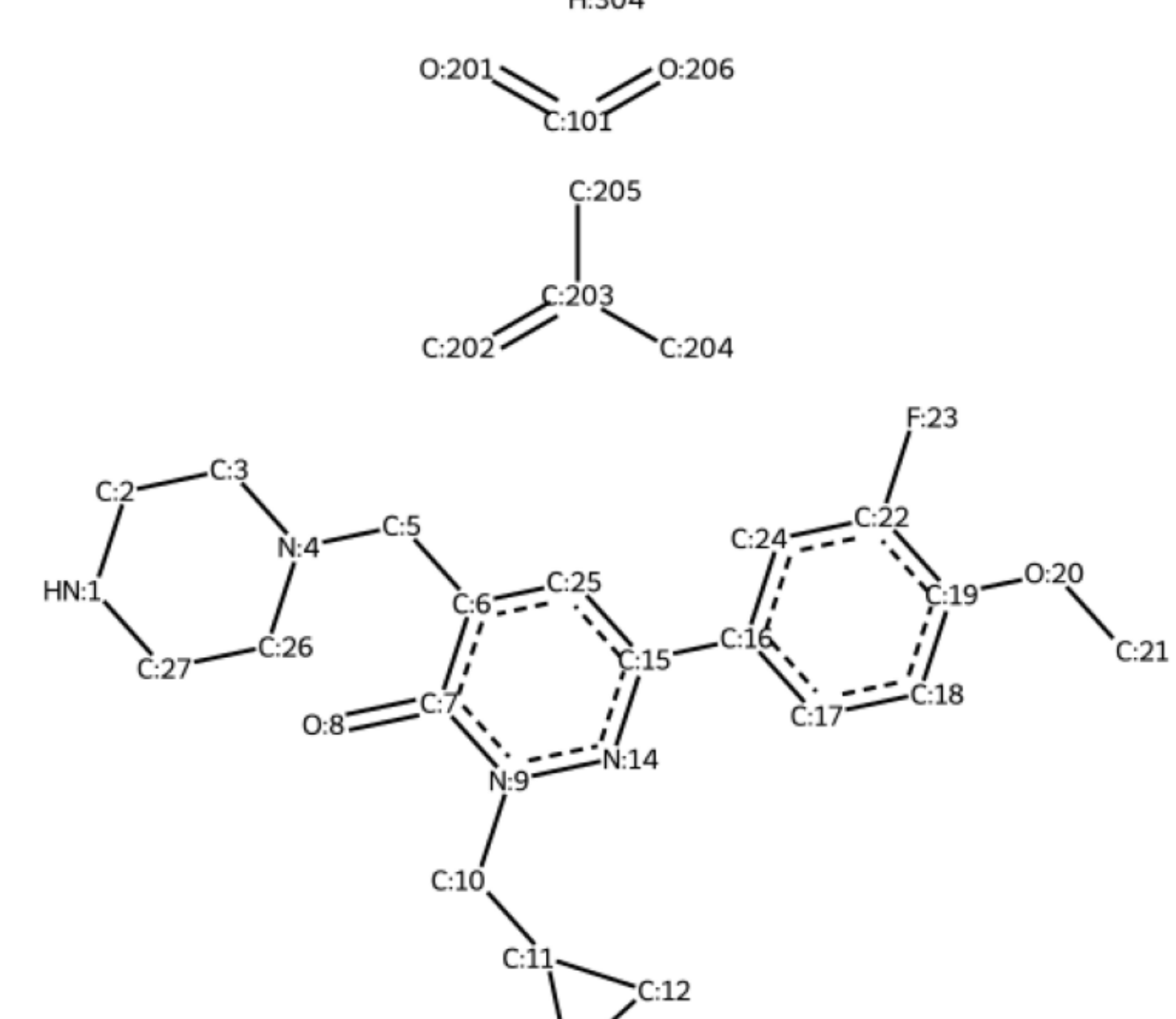
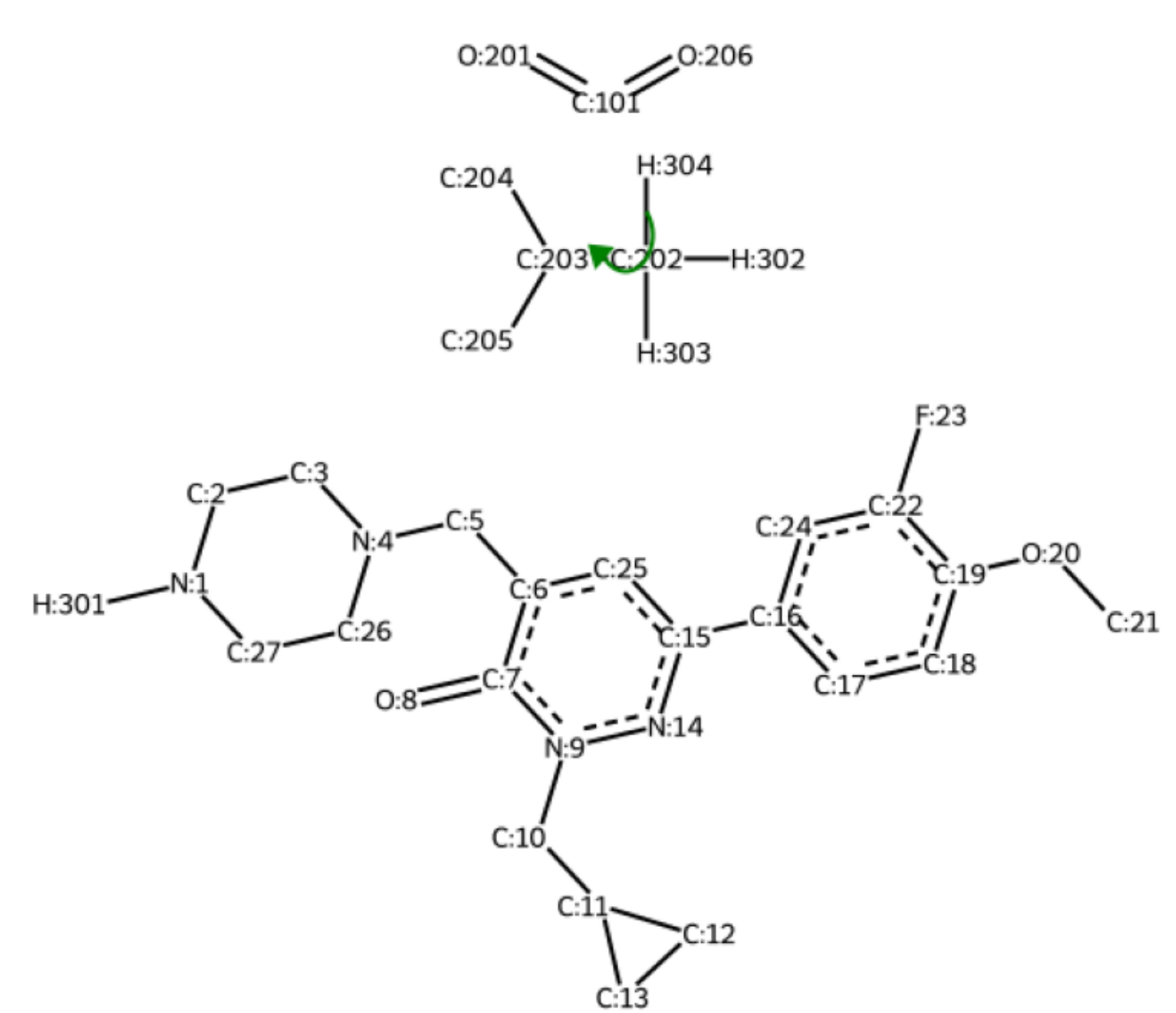
step #3

step #4

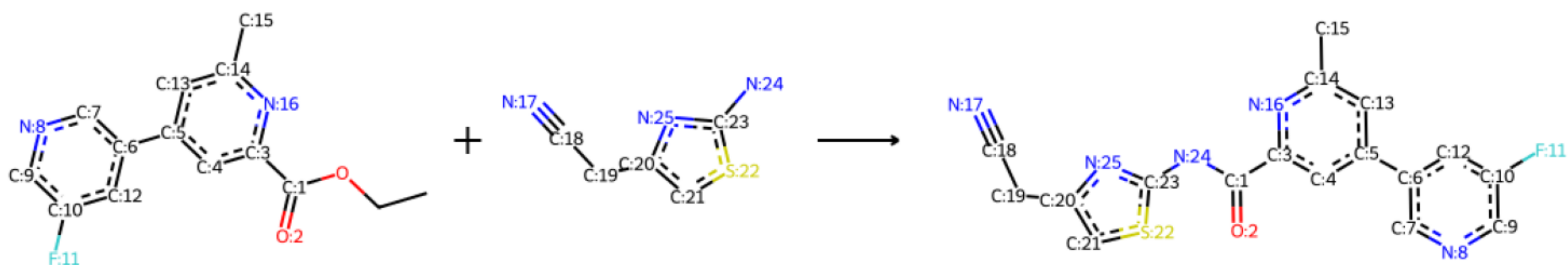


step #5

Product(s)



Original reaction RXN_ID:0

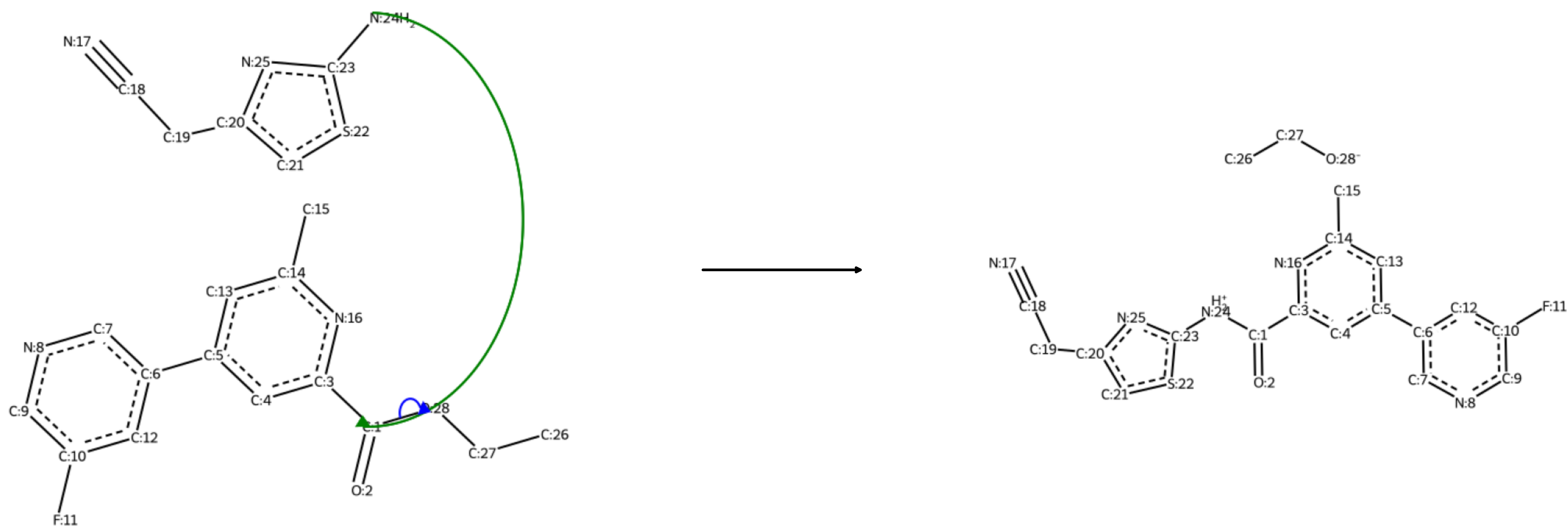


ELECTRO-generated mechanistic pathway

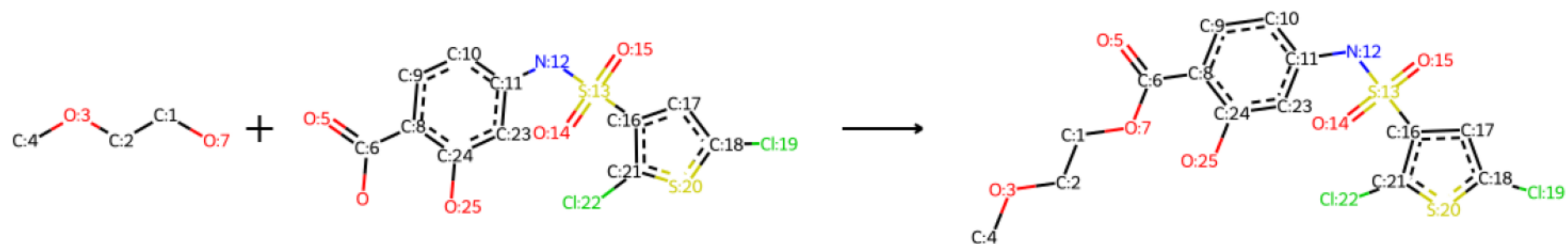
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:1

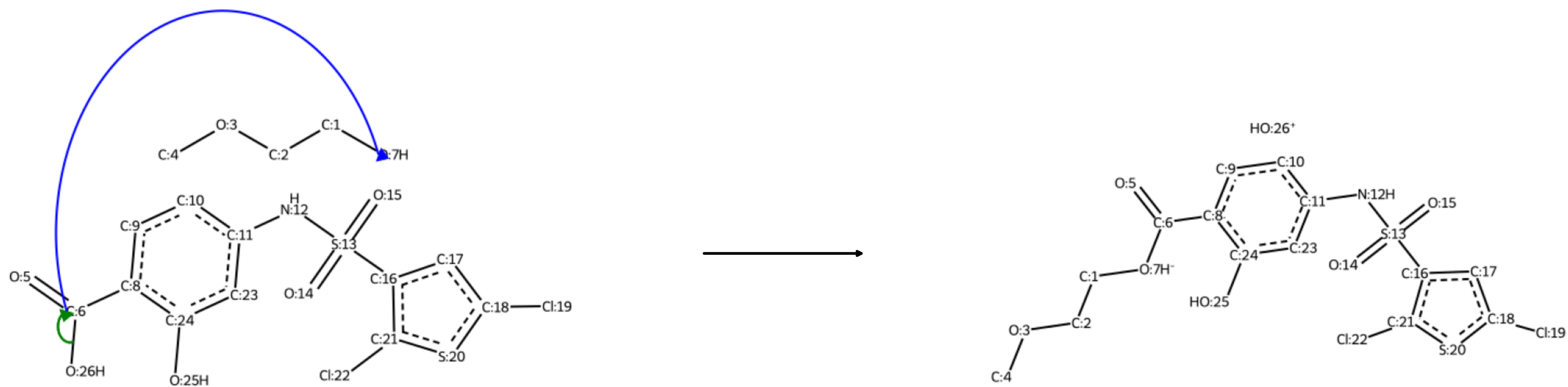


ELECTRO-generated mechanistic pathway

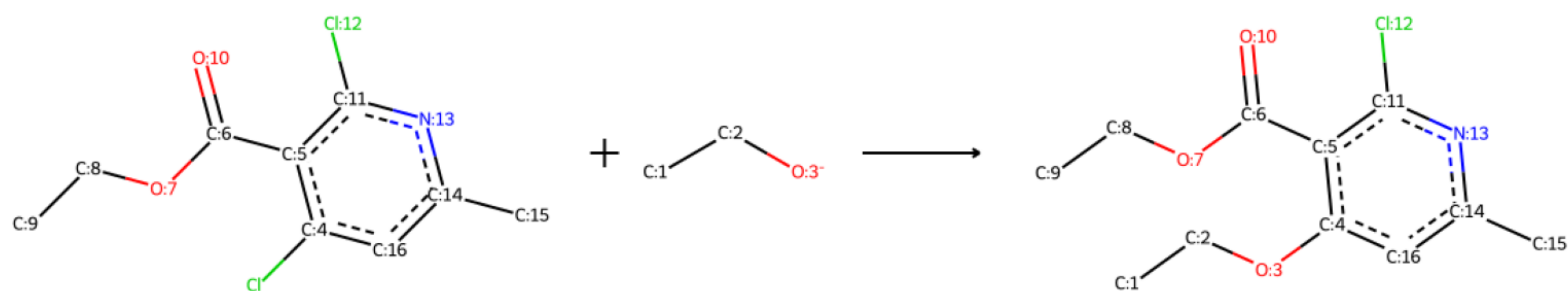
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:2

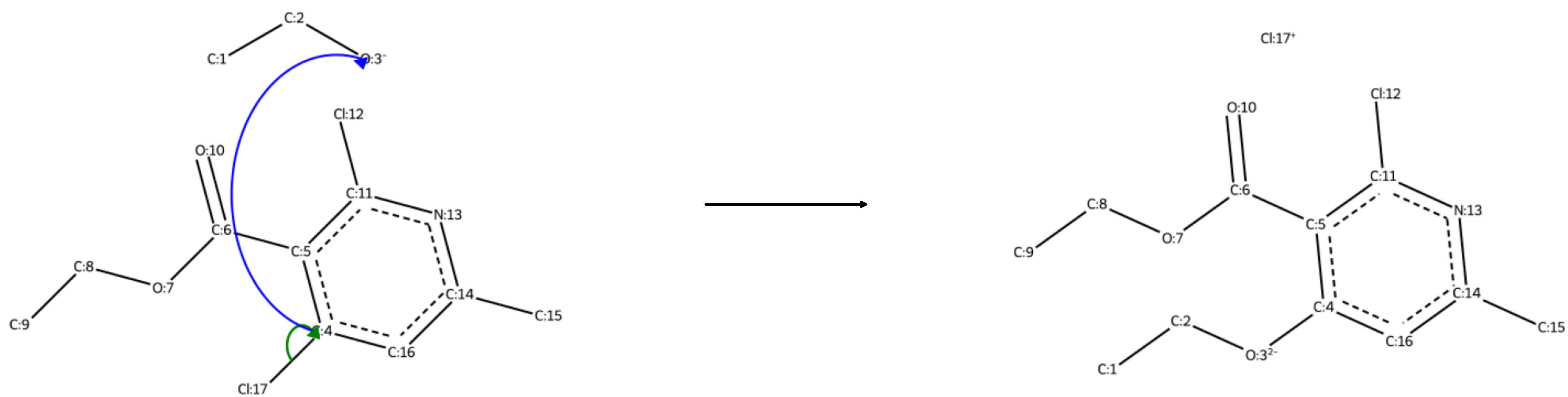


ELECTRO-generated mechanistic pathway

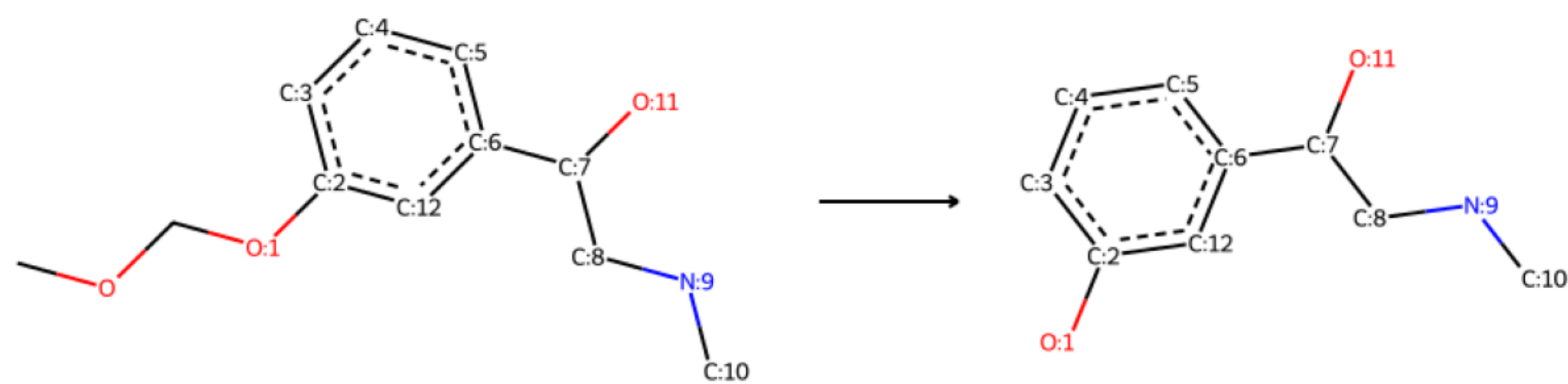
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:3

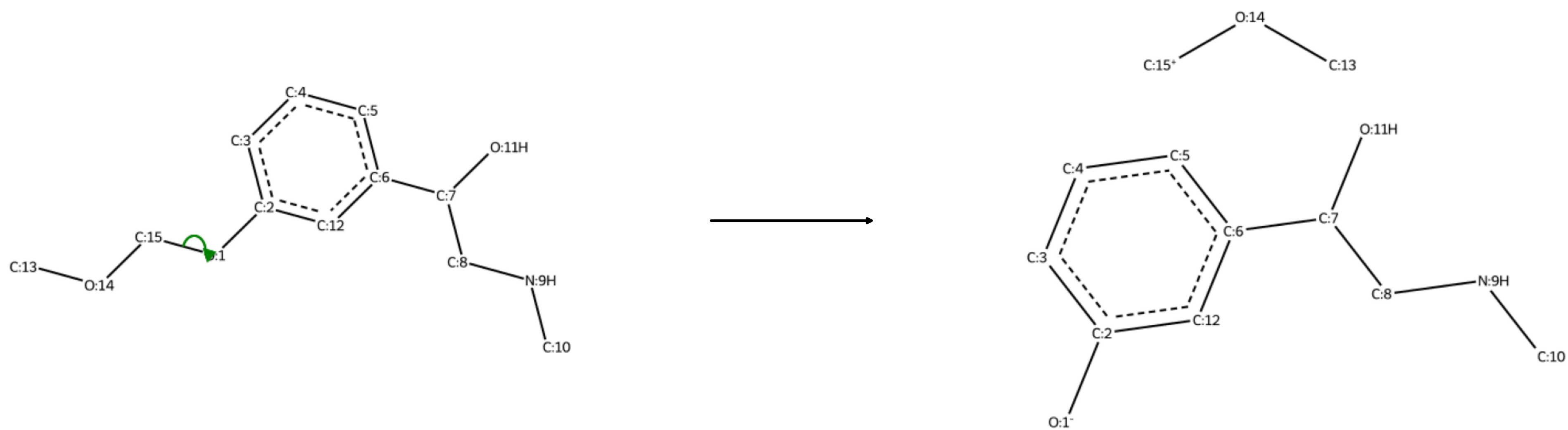


ELECTRO-generated mechanistic pathway

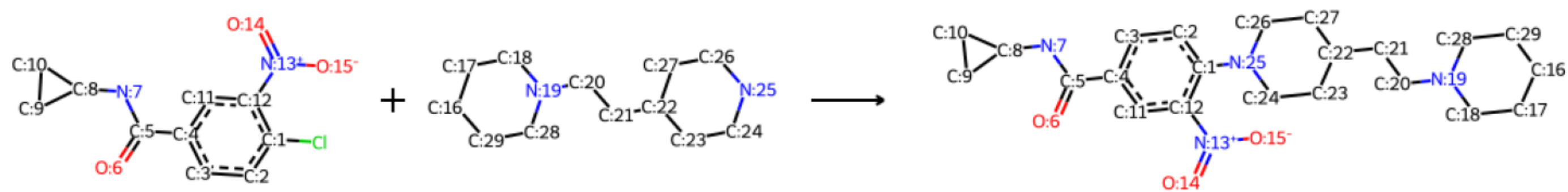
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:4

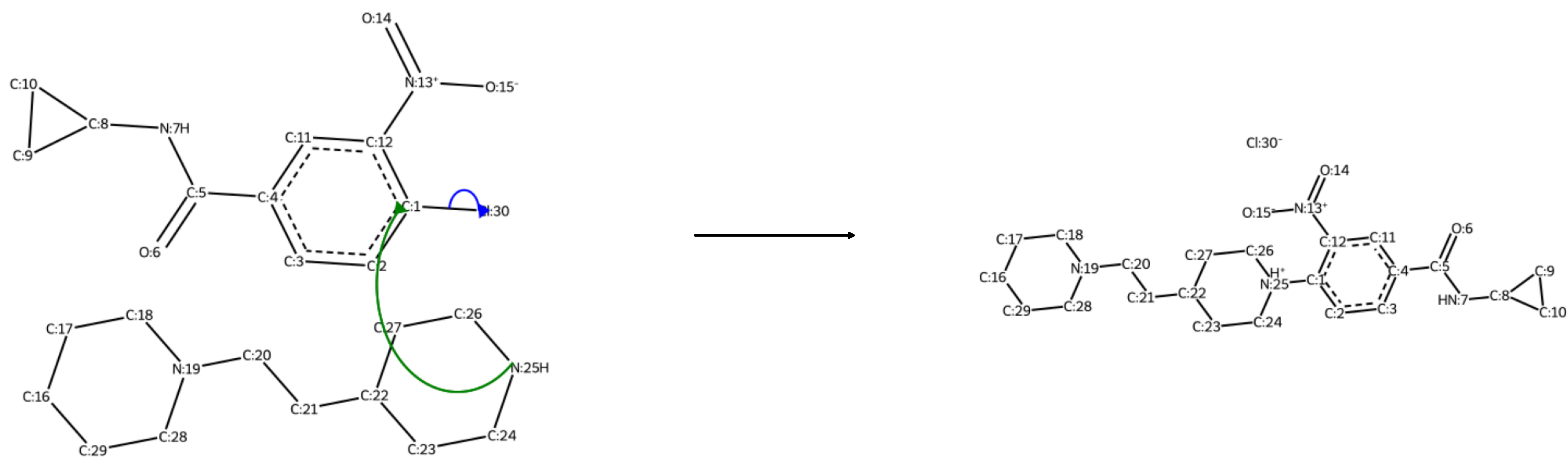


ELECTRO-generated mechanistic pathway

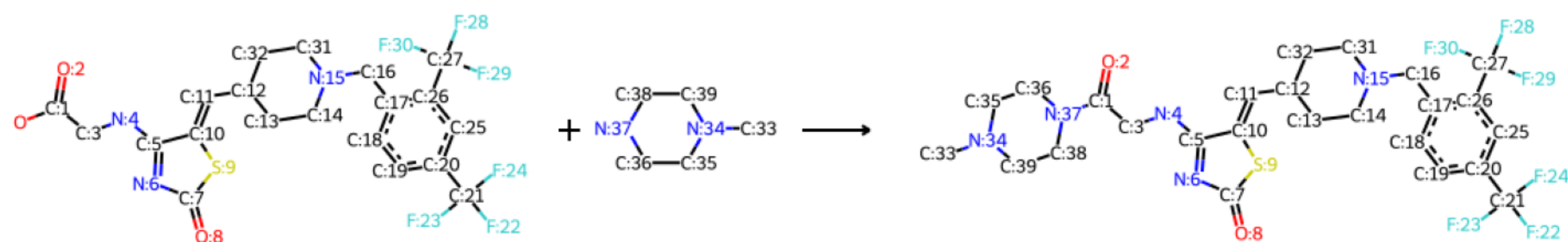
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:5

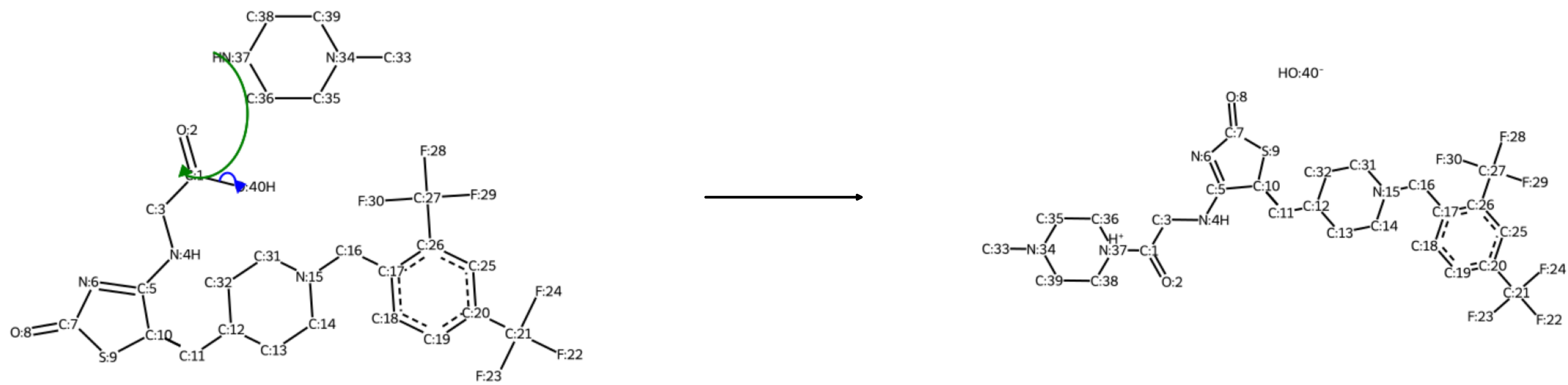


ELECTRO-generated mechanistic pathway

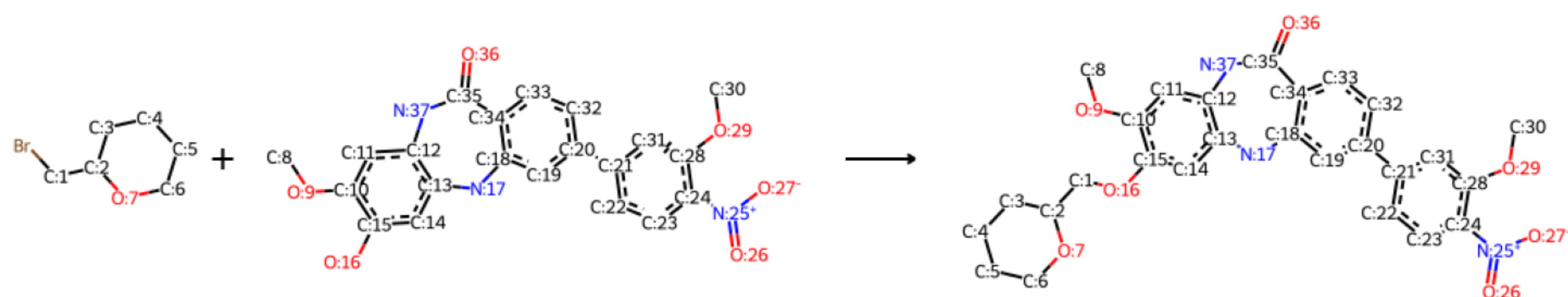
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:6

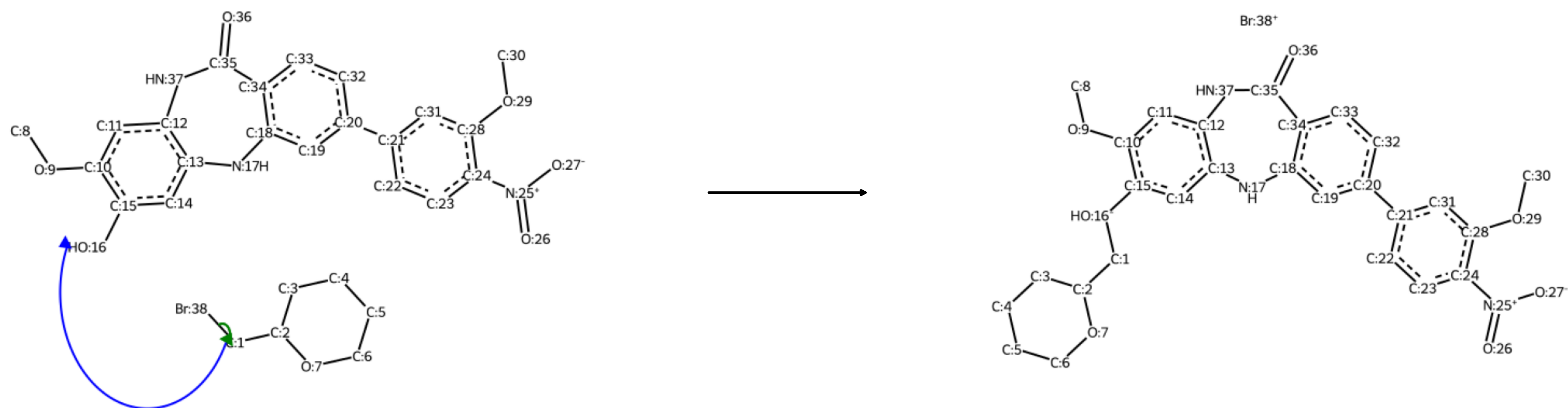


ELECTRO-generated mechanistic pathway

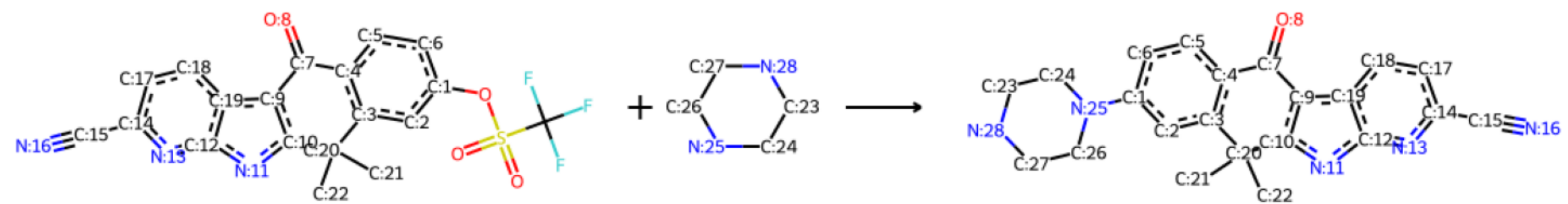
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:7

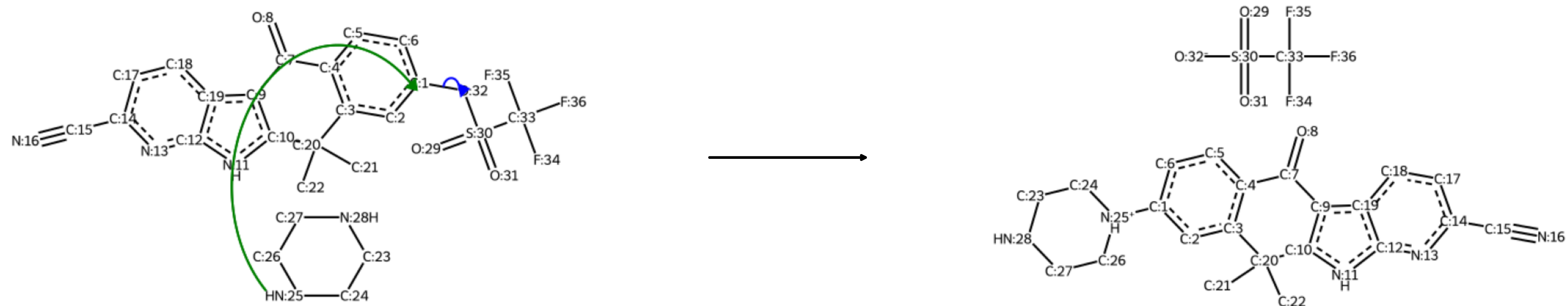


ELECTRO-generated mechanistic pathway

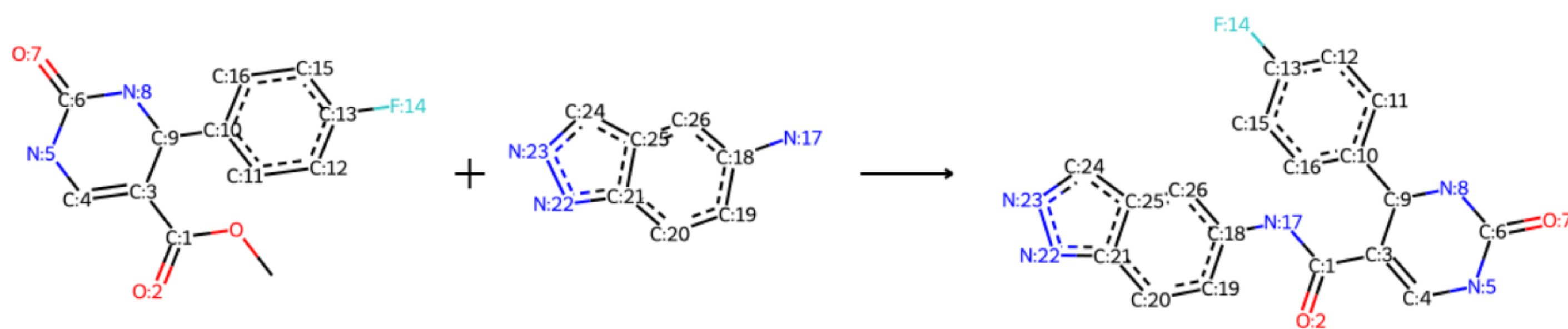
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:8

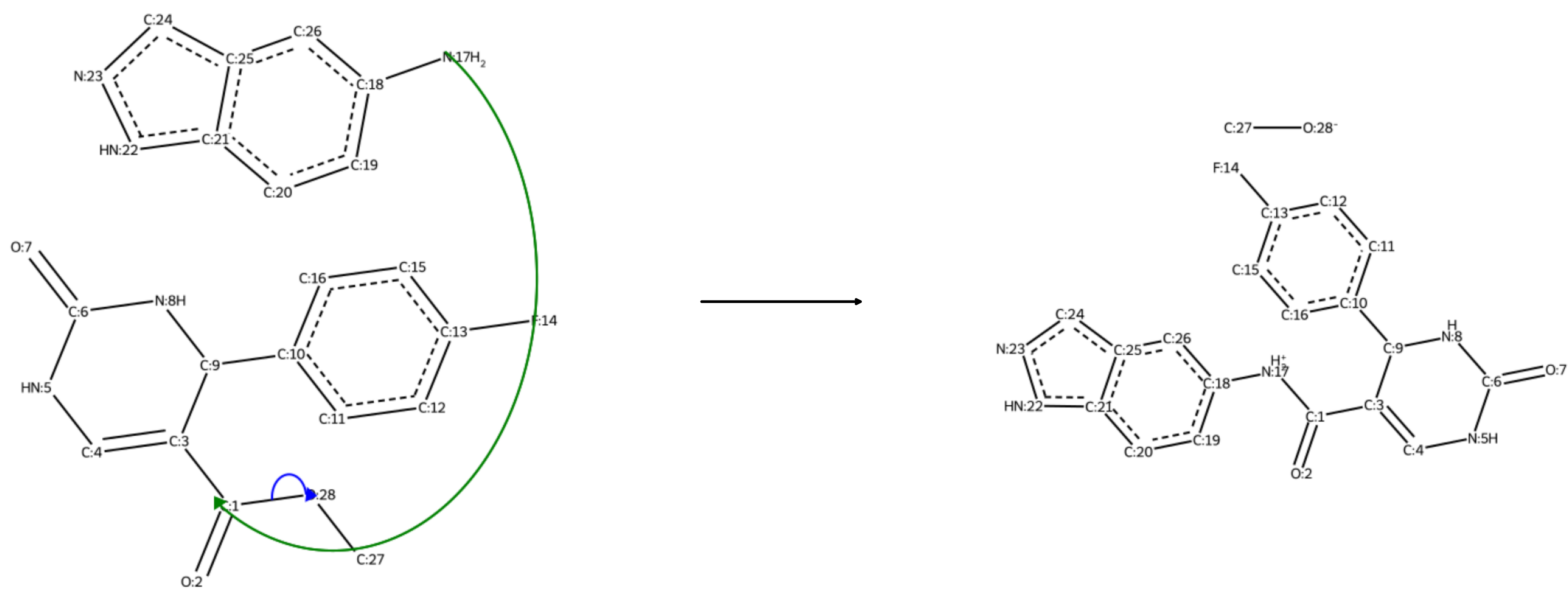


ELECTRO-generated mechanistic pathway

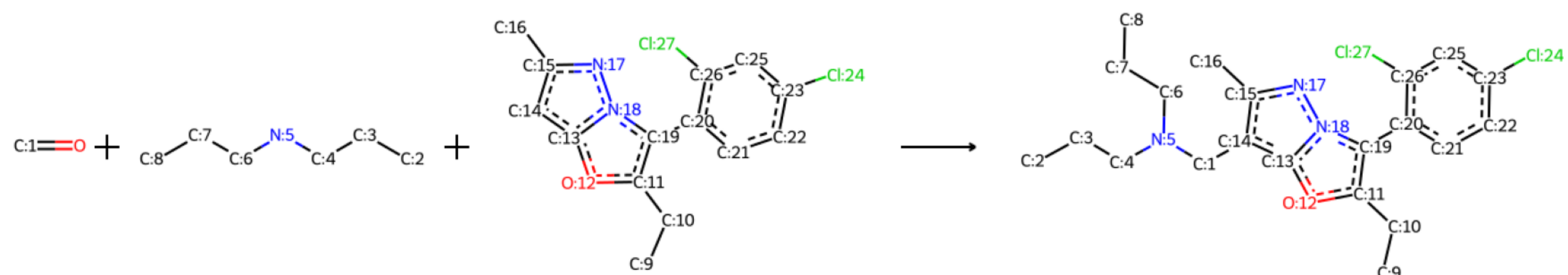
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



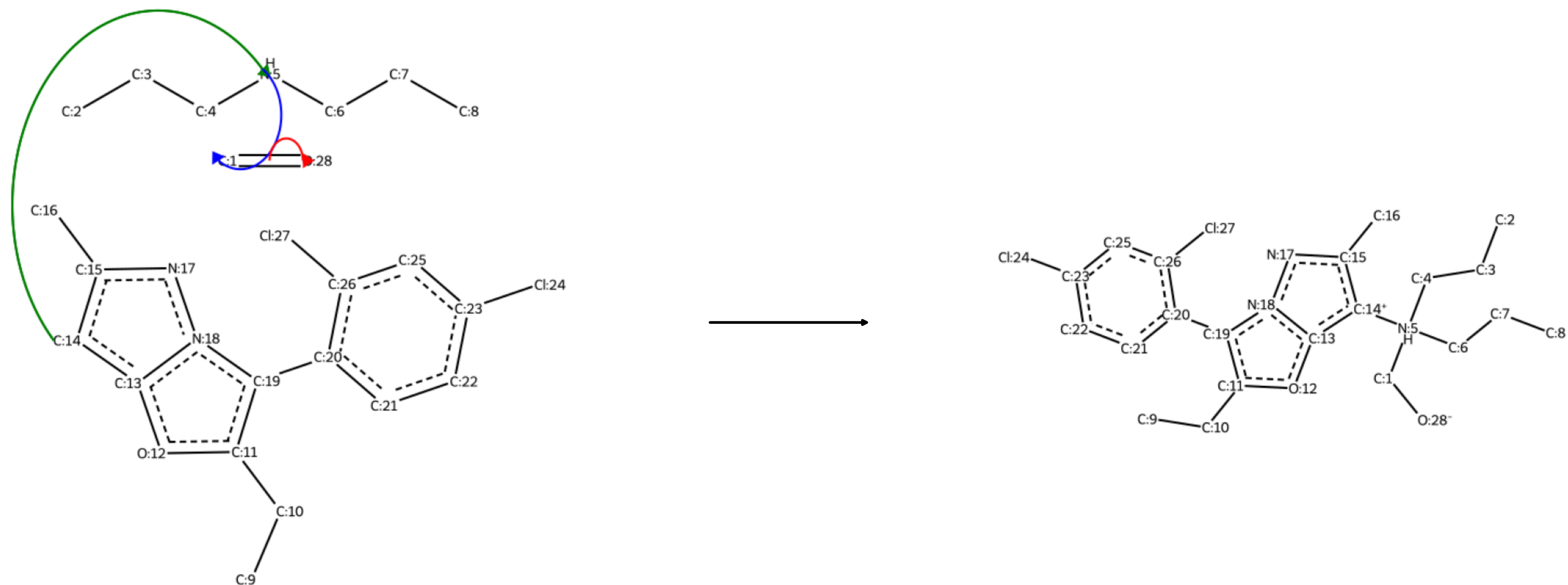
Original reaction RXN_ID:9



ELECTRO-generated mechanistic pathway

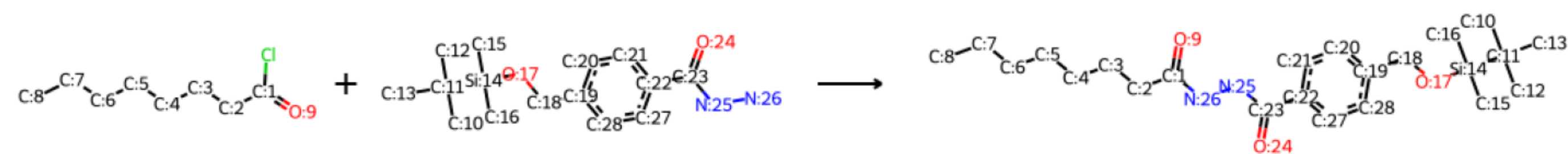
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1



Product(s)

Original reaction RXN_ID:10

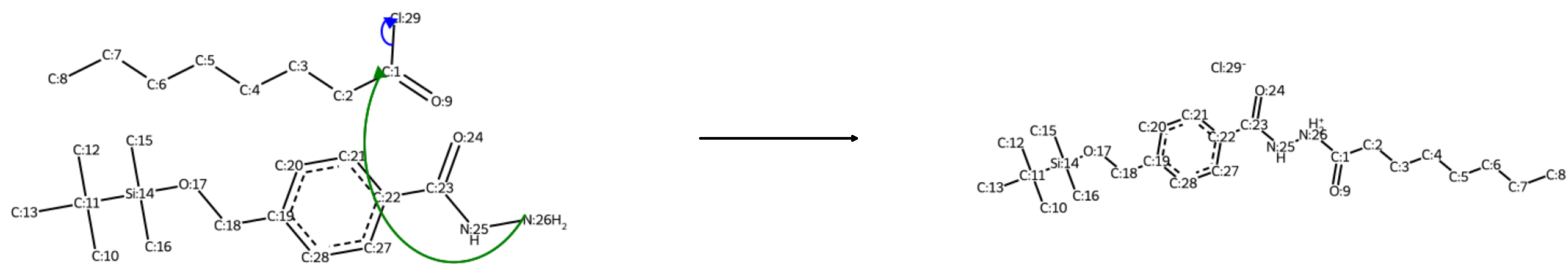


ELECTRO-generated mechanistic pathway

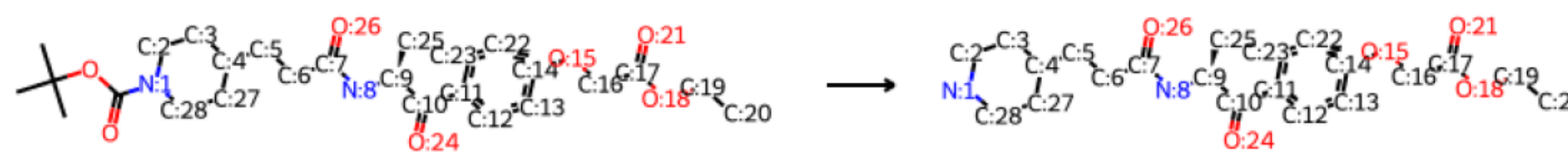
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:11

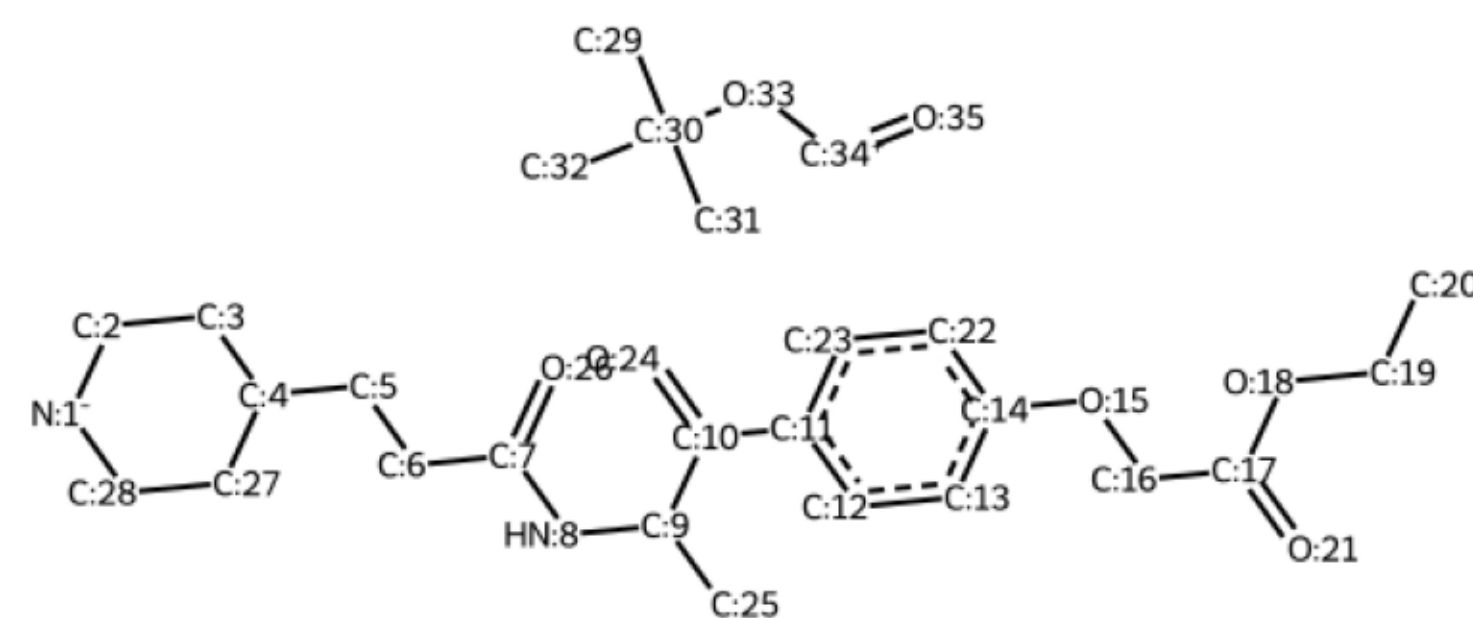
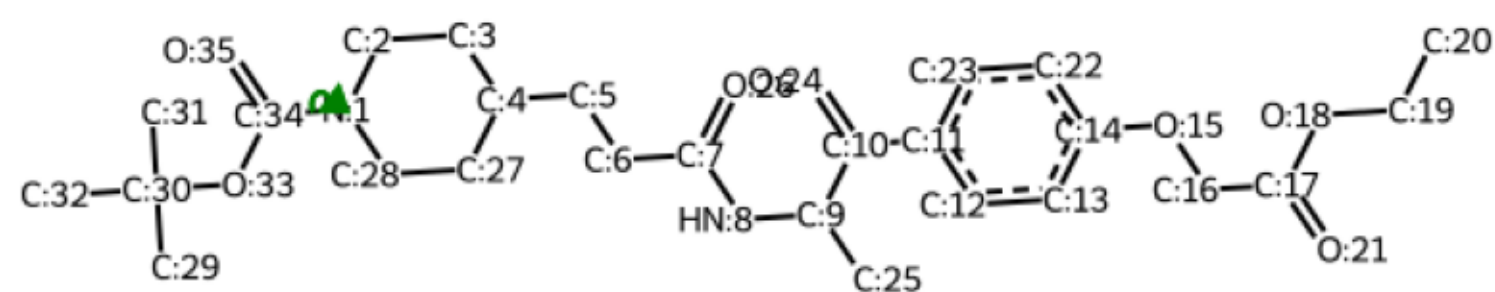


ELECTRO-generated mechanistic pathway

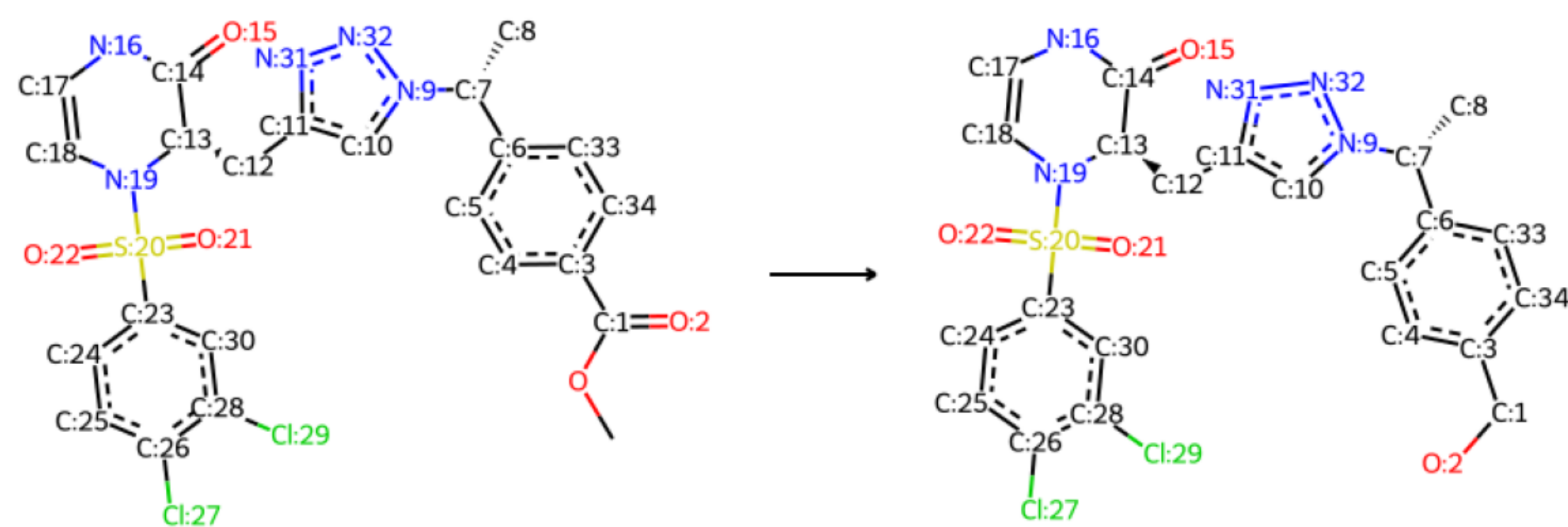
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:12

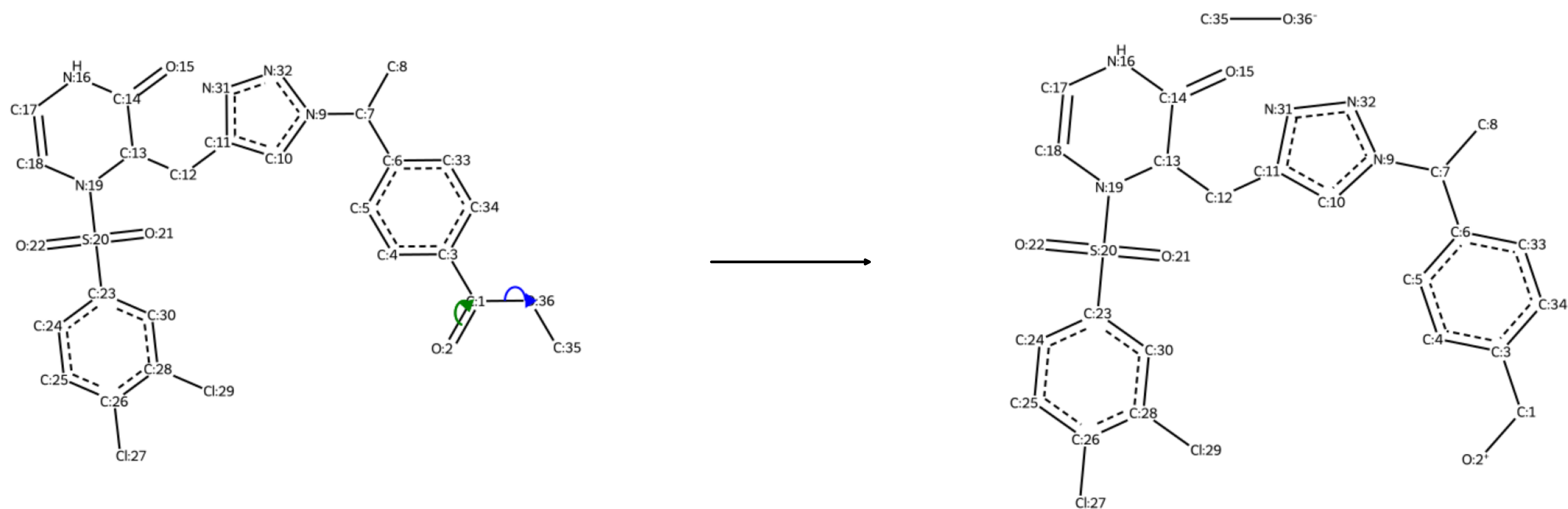


ELECTRO-generated mechanistic pathway

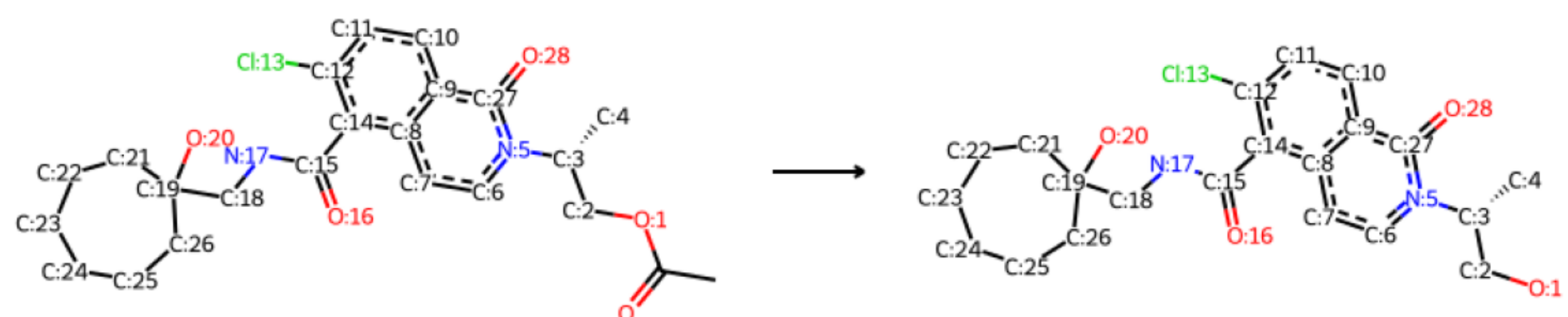
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:13

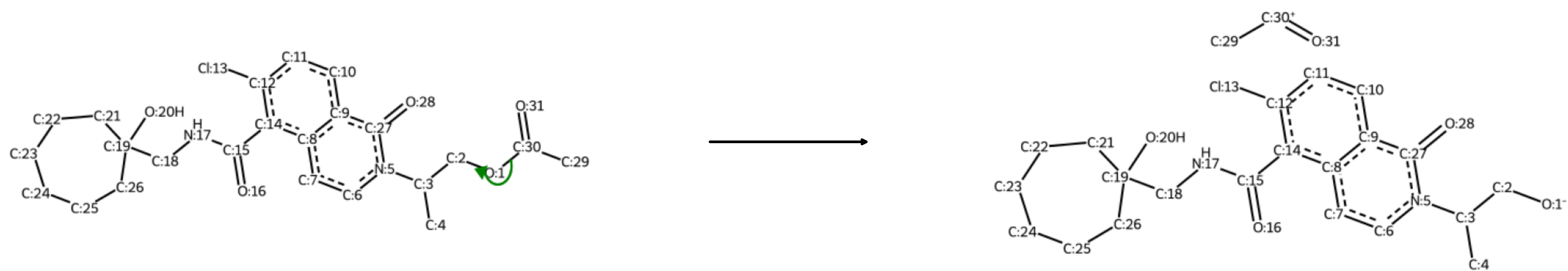


ELECTRO-generated mechanistic pathway

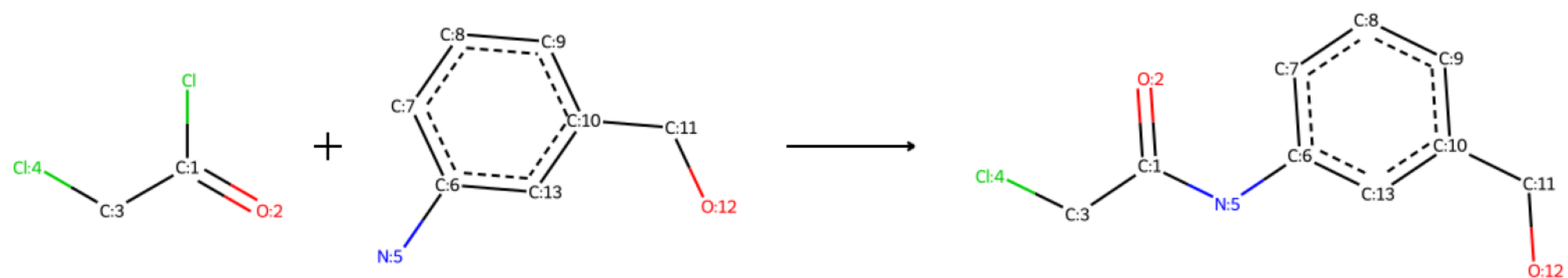
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:14

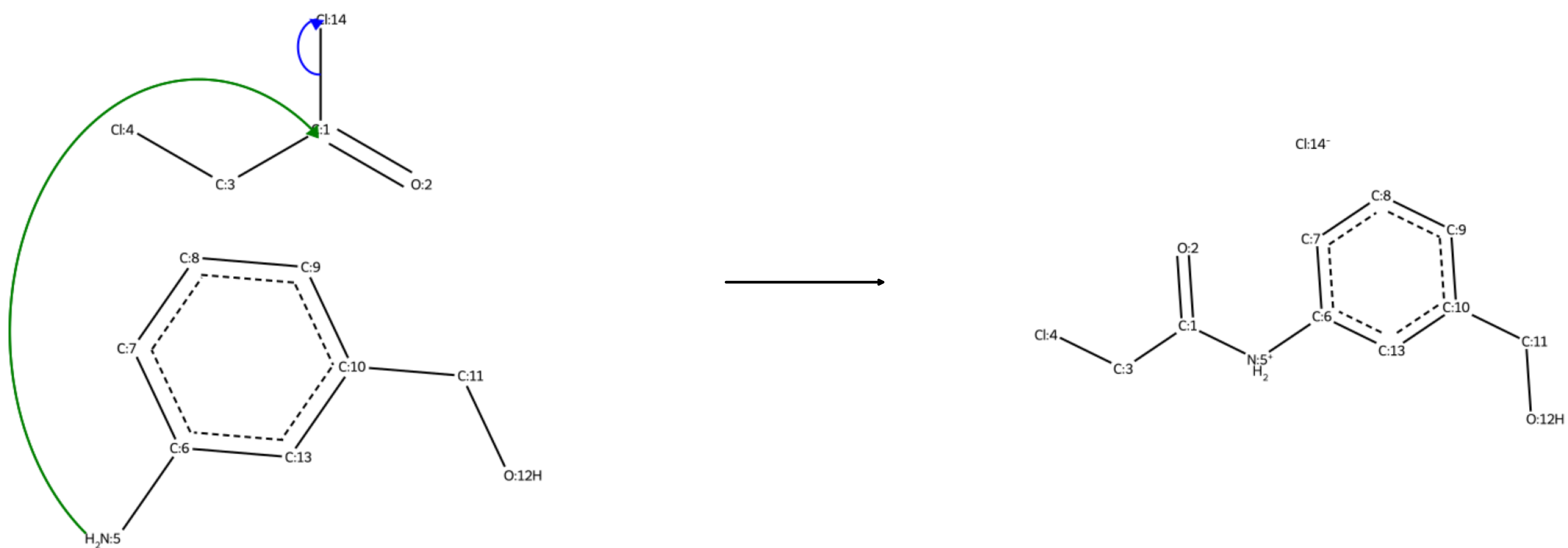


ELECTRO-generated mechanistic pathway

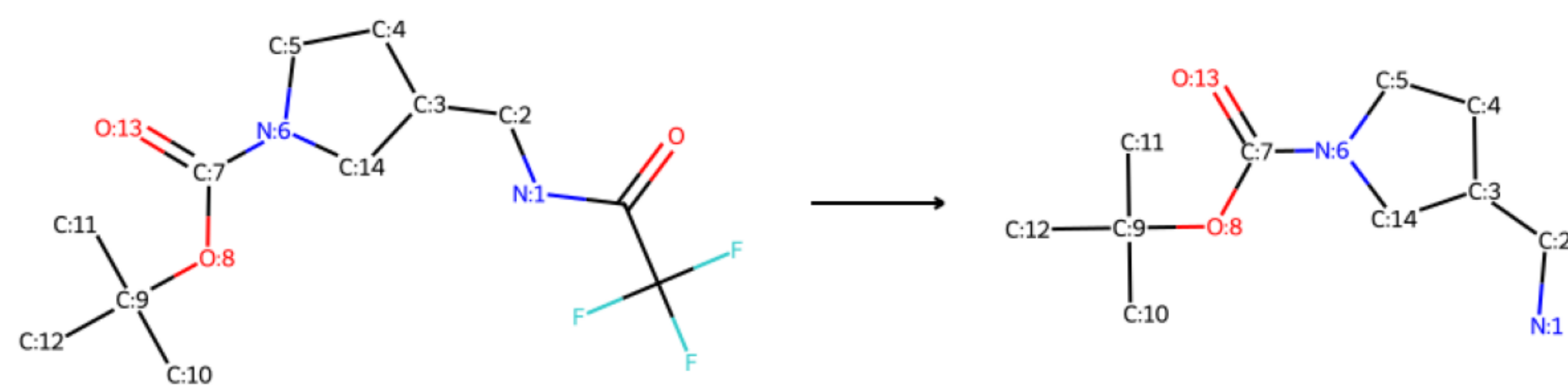
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:15

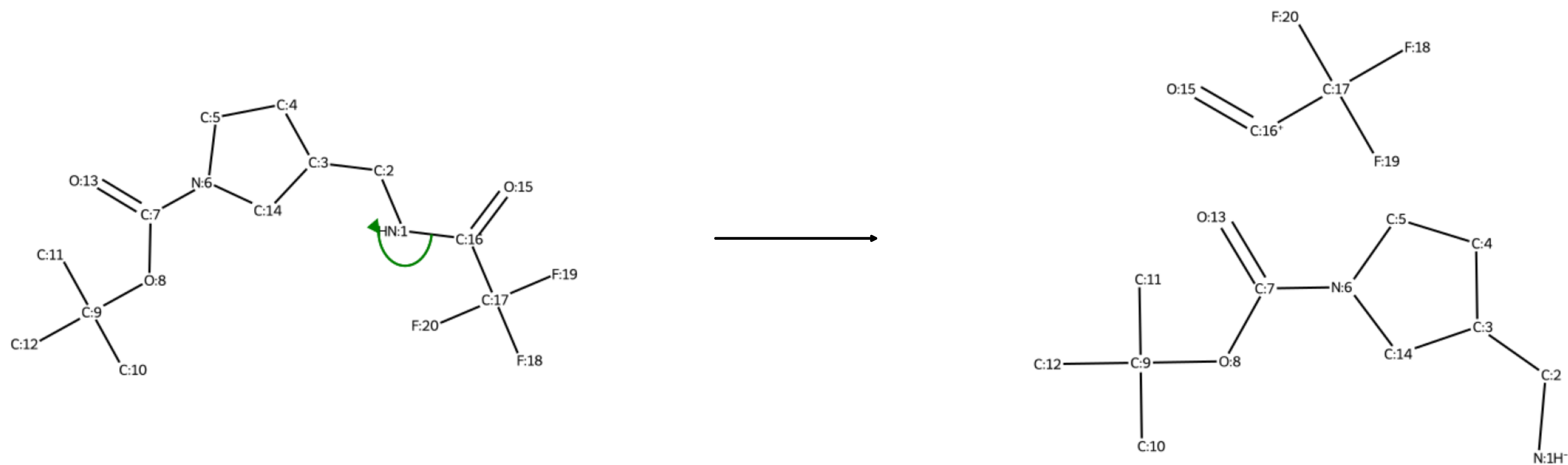


ELECTRO-generated mechanistic pathway

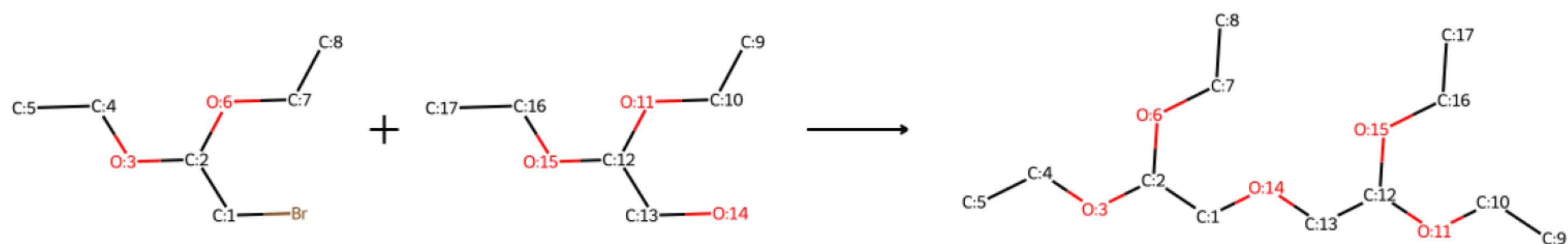
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:16

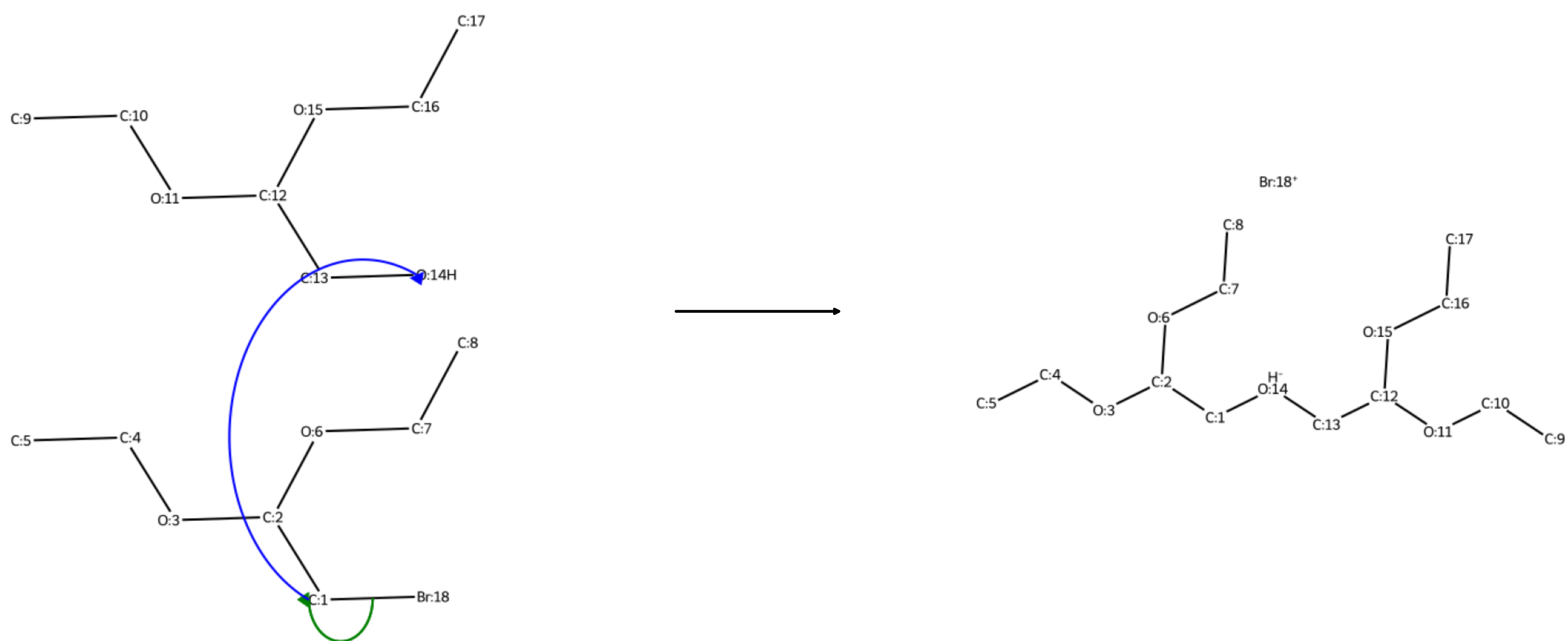


ELECTRO-generated mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:17

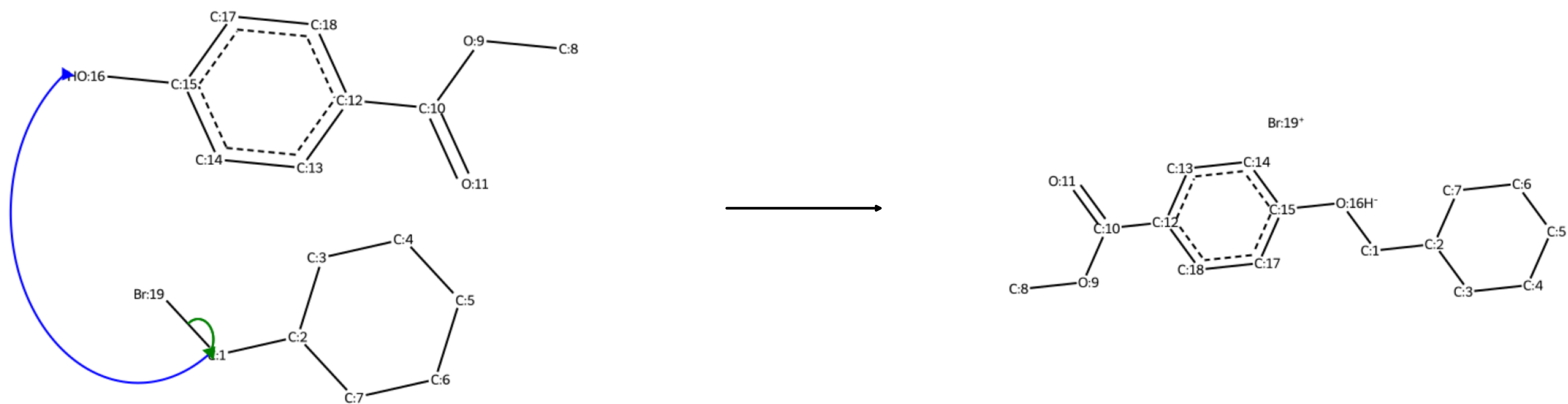


ELECTRO-generated mechanistic pathway

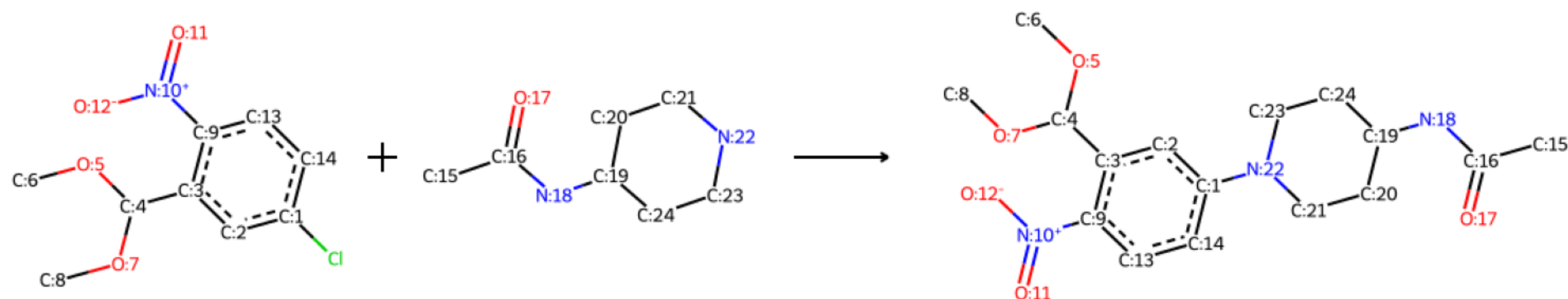
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



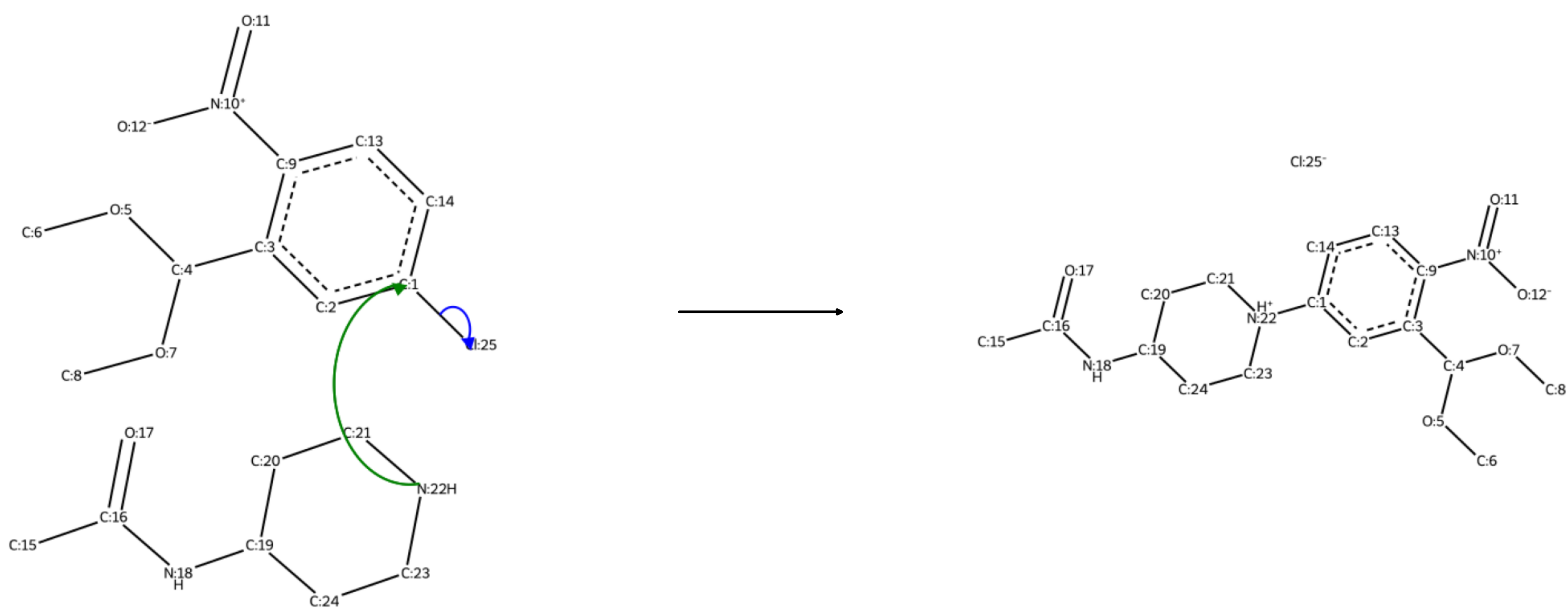
Original reaction RXN_ID:18



ELECTRO-generated mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1



Product(s)

Original reaction RXN_ID:19

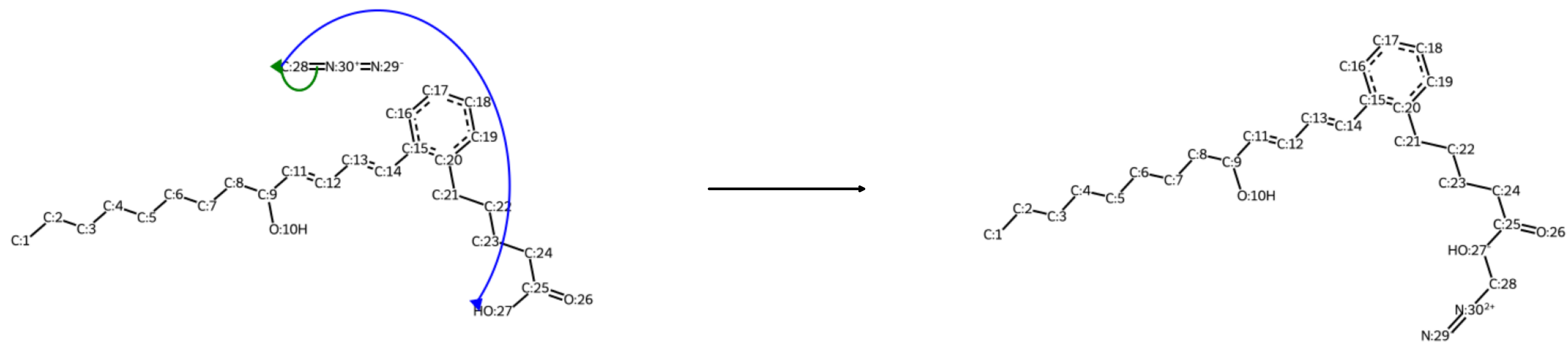


ELECTRO-generated mechanistic pathway

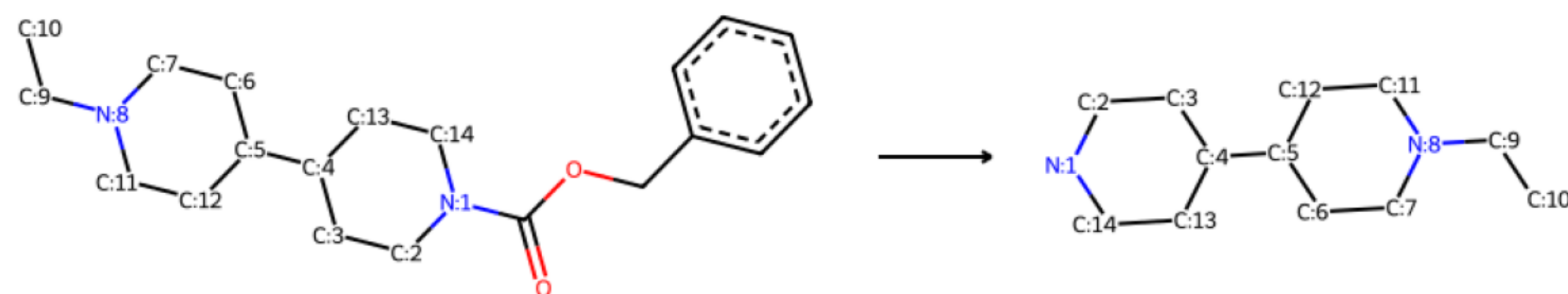
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:20

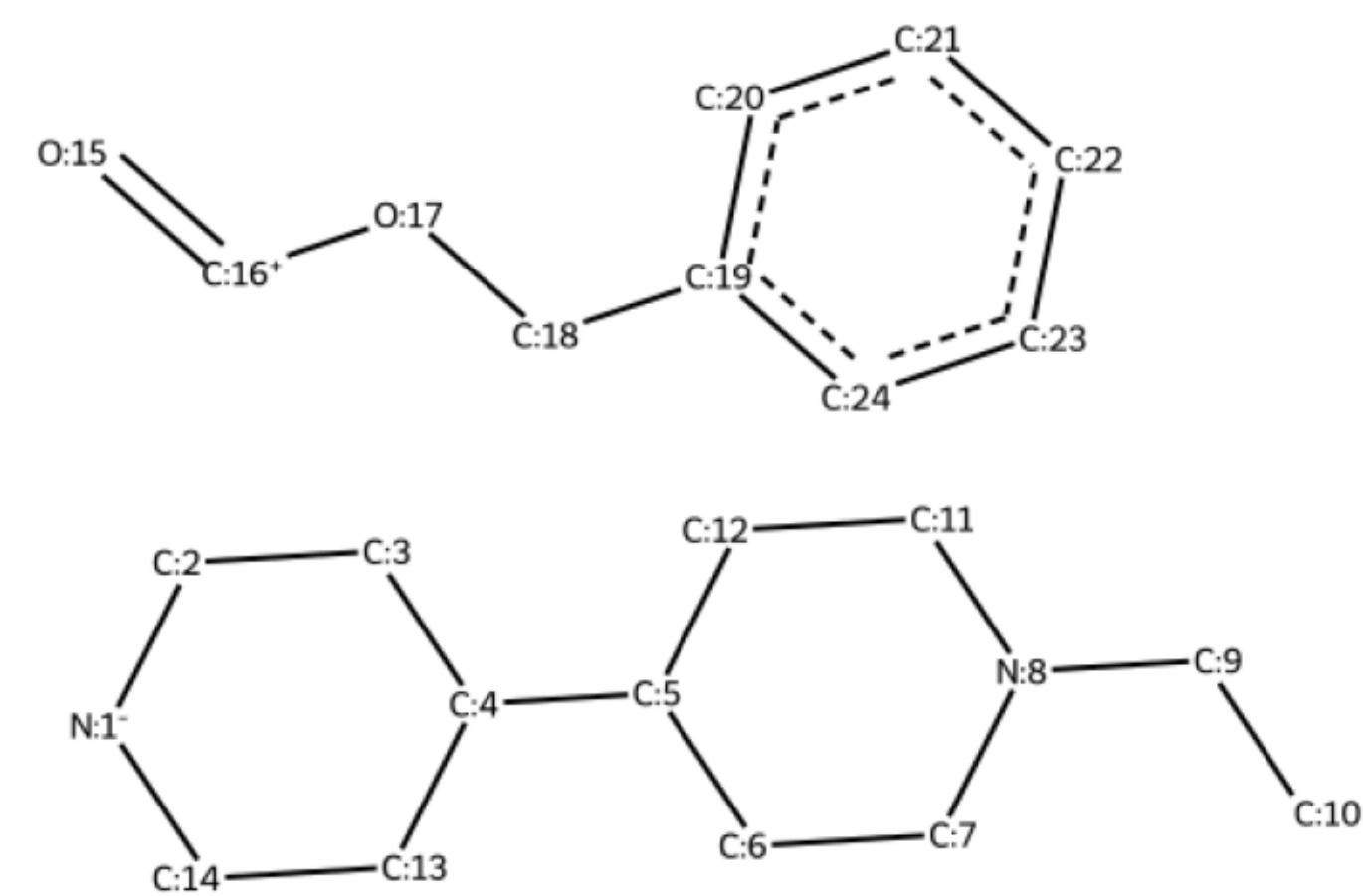
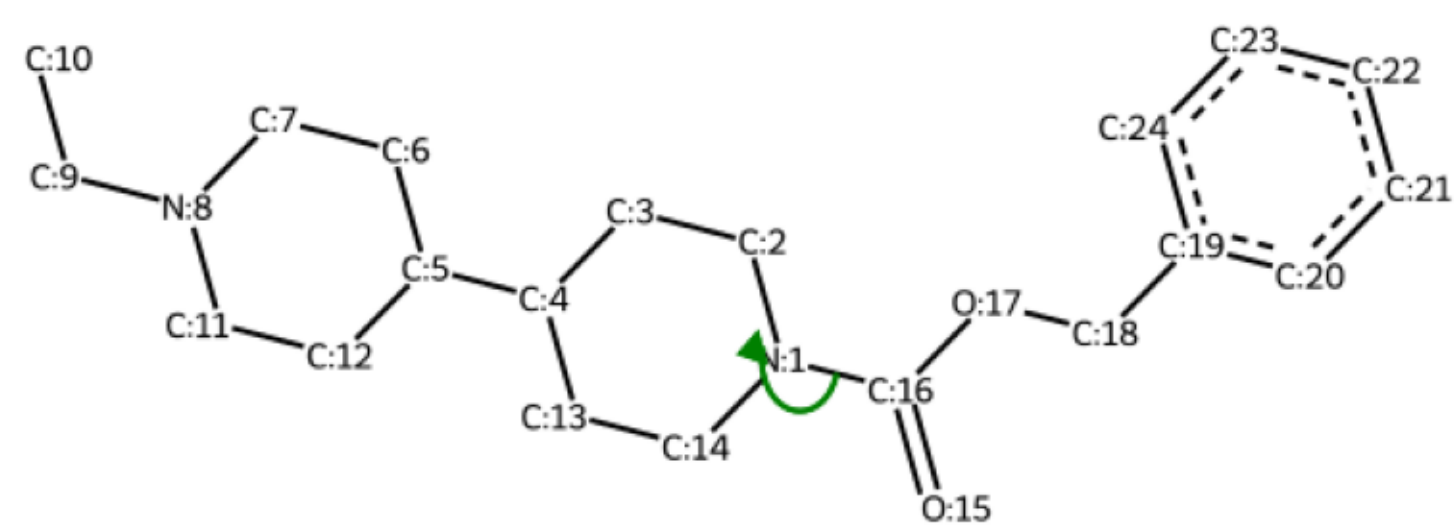


ELECTRO-generated mechanistic pathway

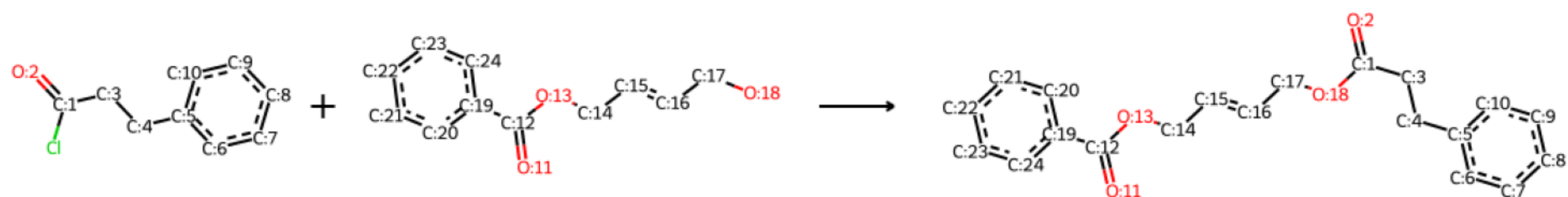
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:21

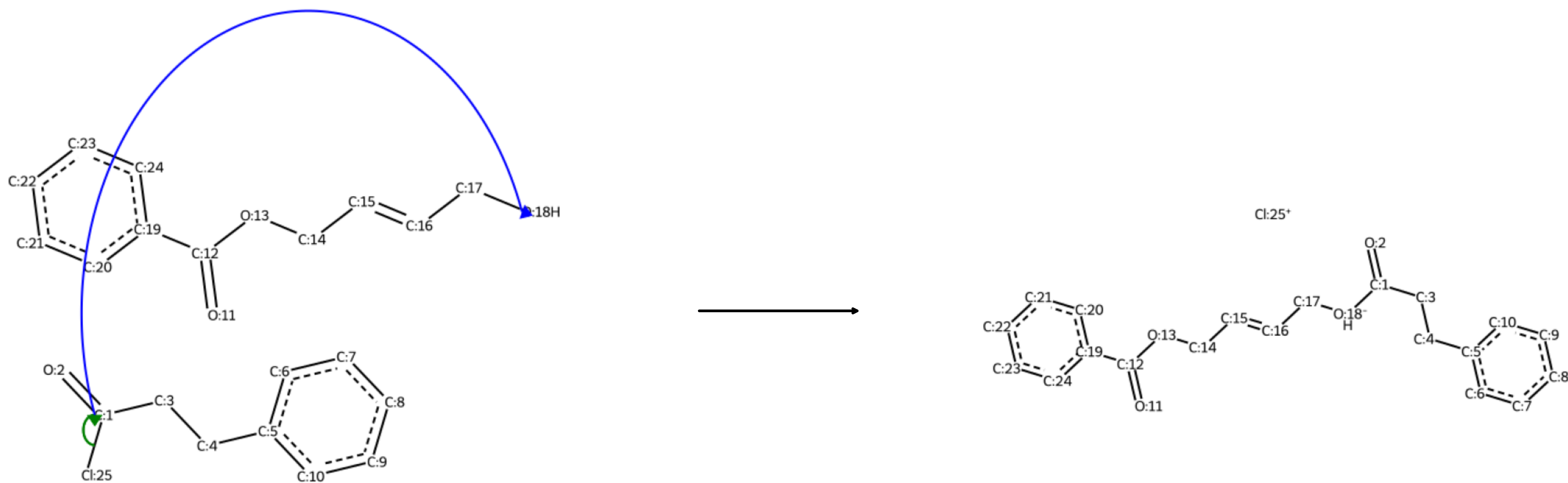


ELECTRO-generated mechanistic pathway

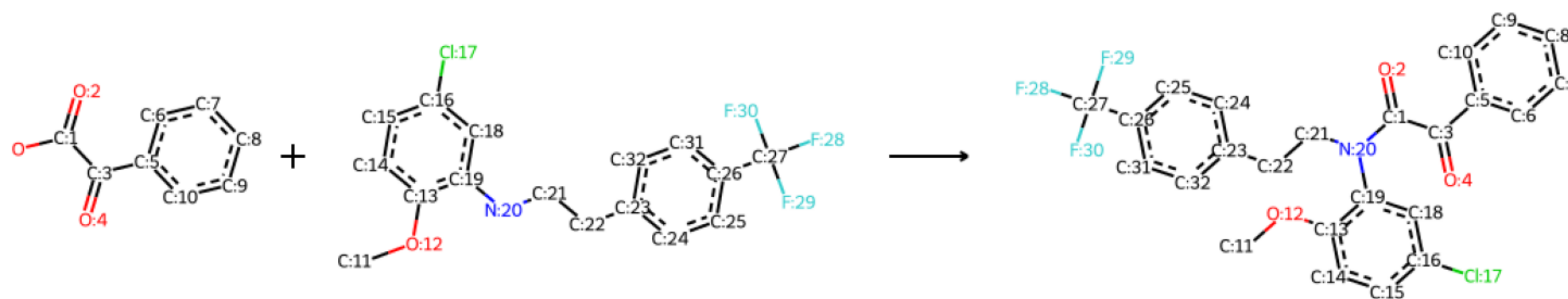
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:22

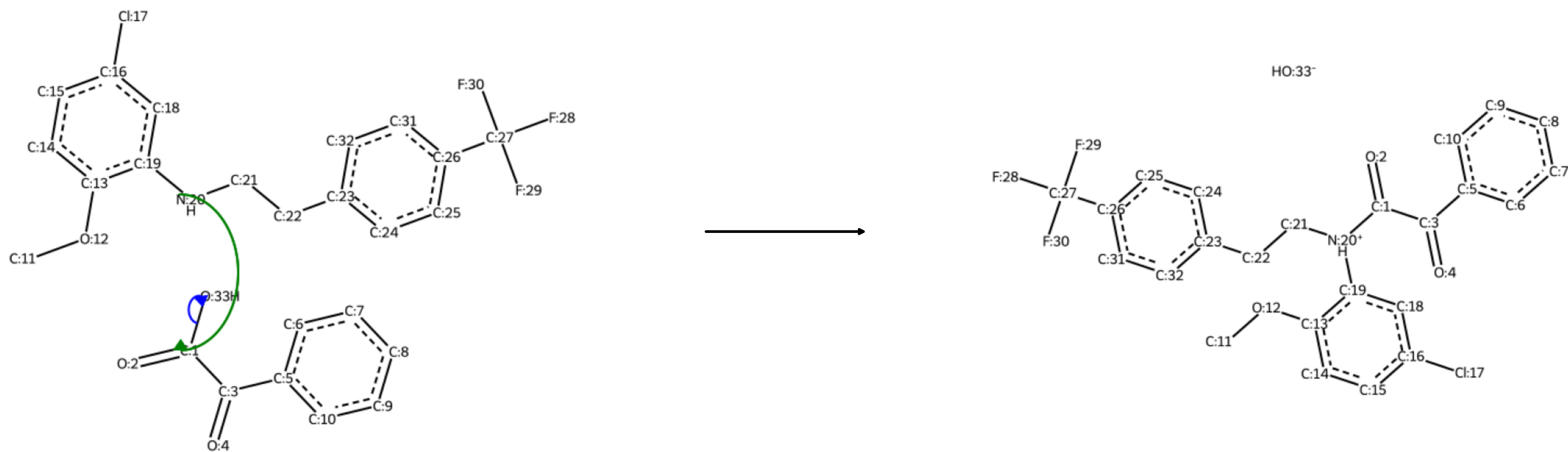


ELECTRO-generated mechanistic pathway

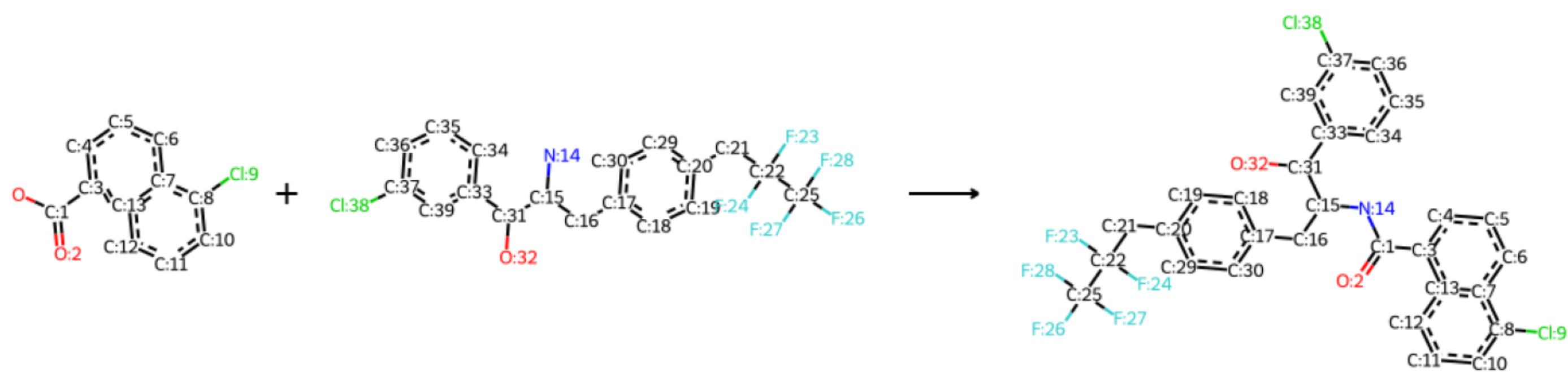
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:23

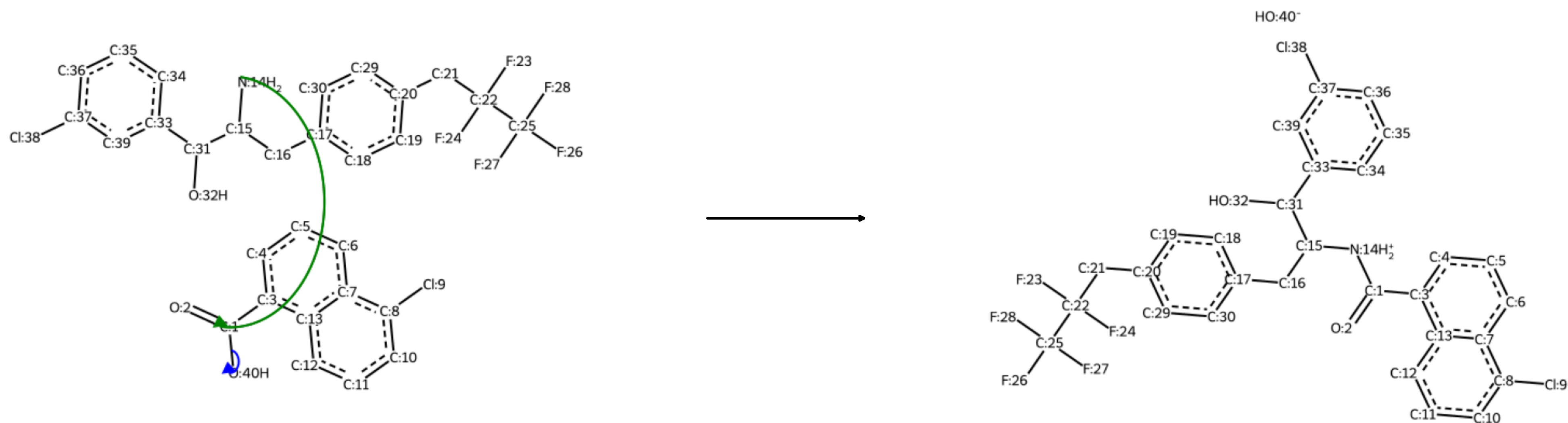


ELECTRO-generated mechanistic pathway

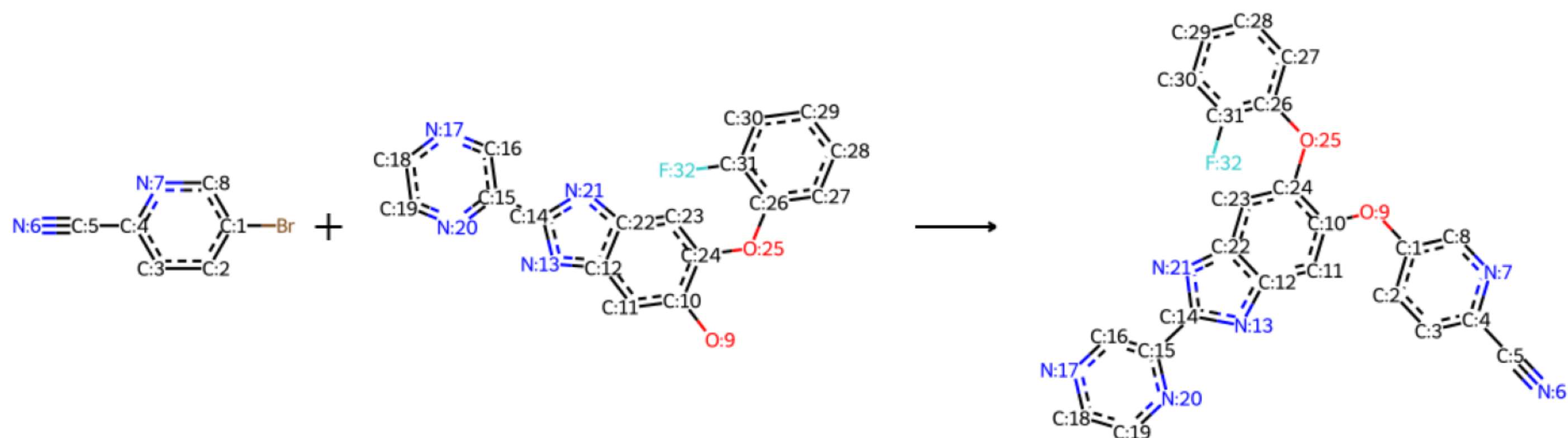
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:24

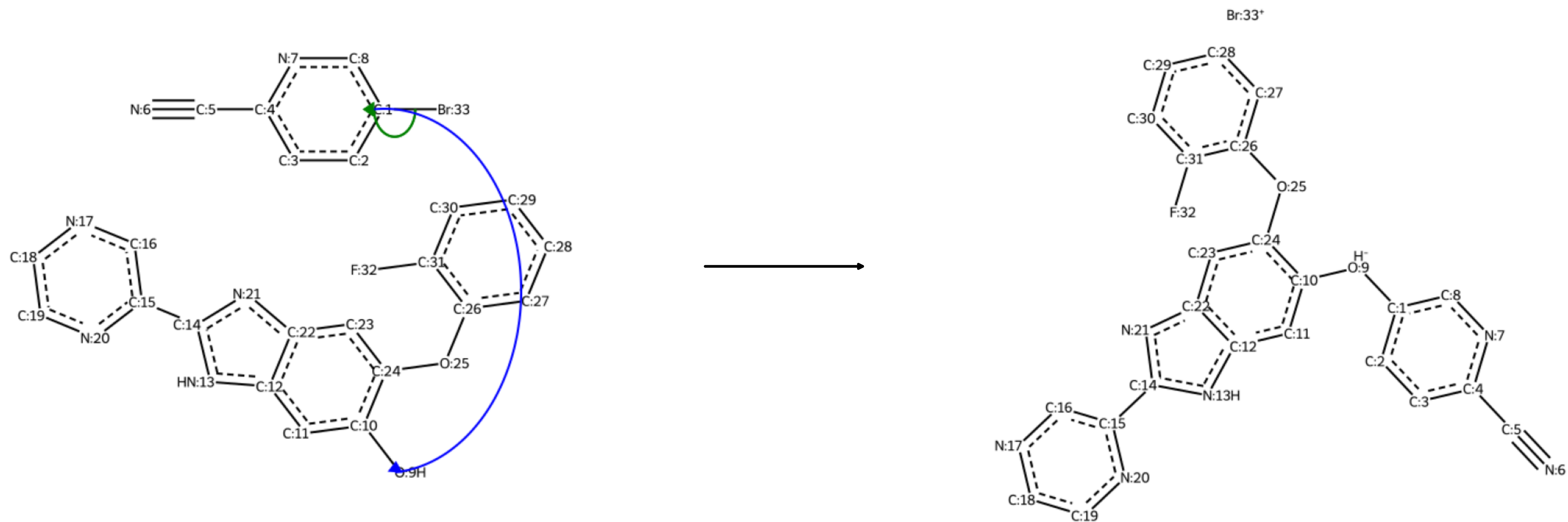


ELECTRO-generated mechanistic pathway

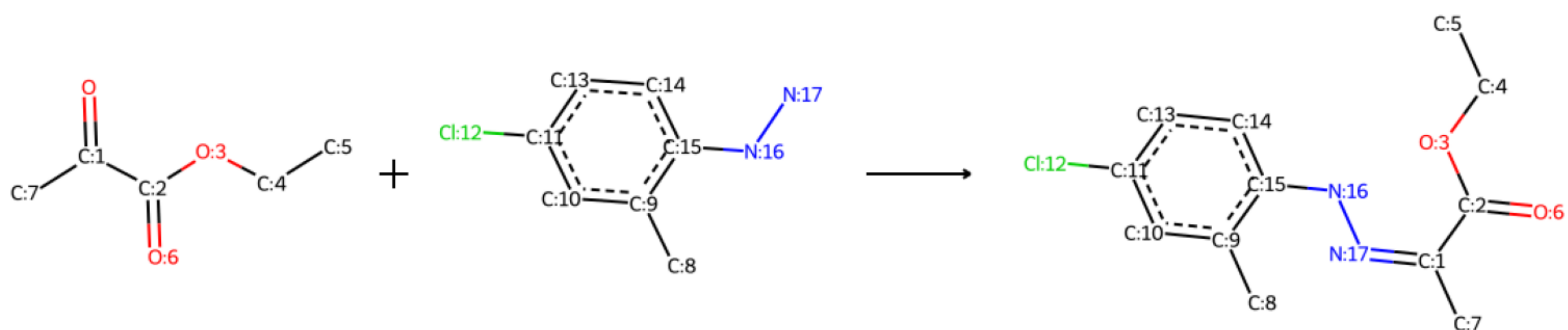
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:25

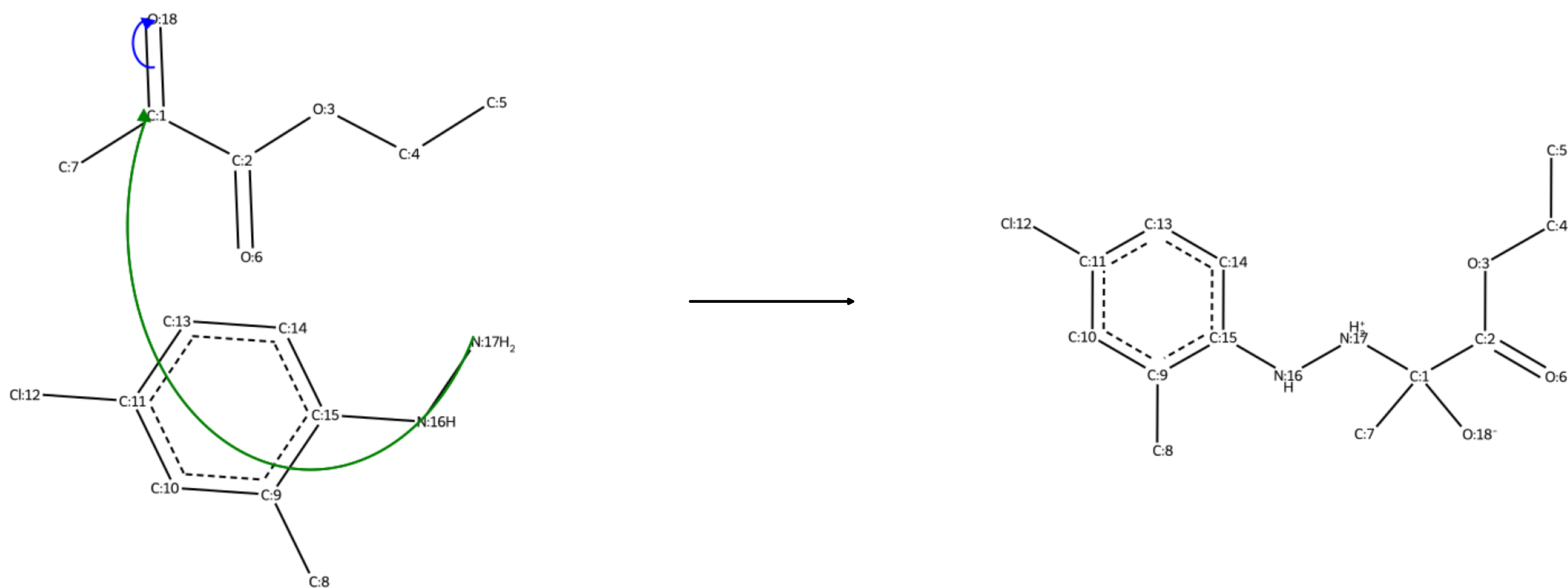


ELECTRO-generated mechanistic pathway

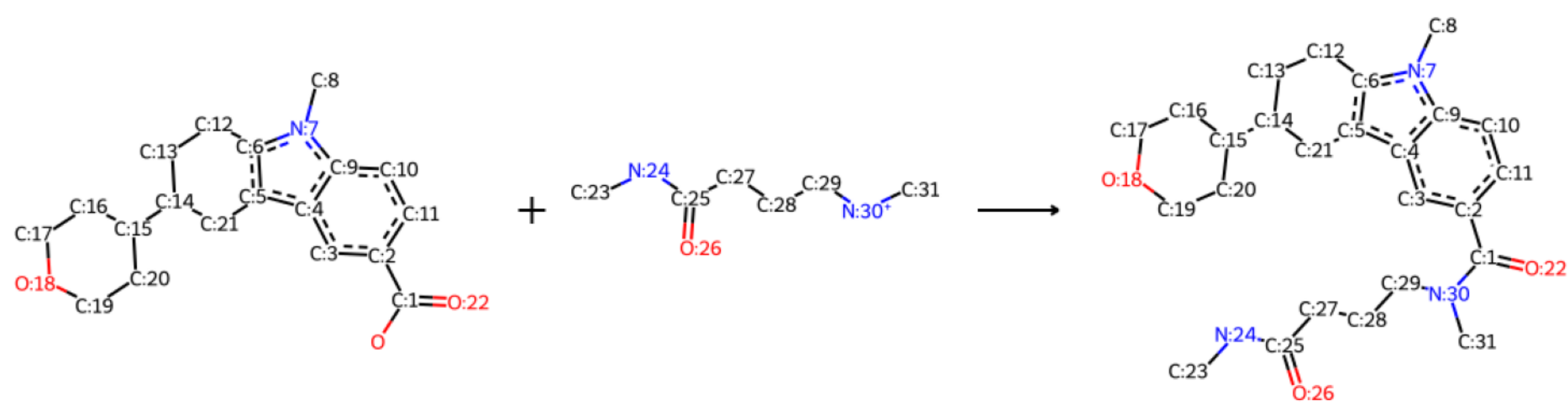
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:26

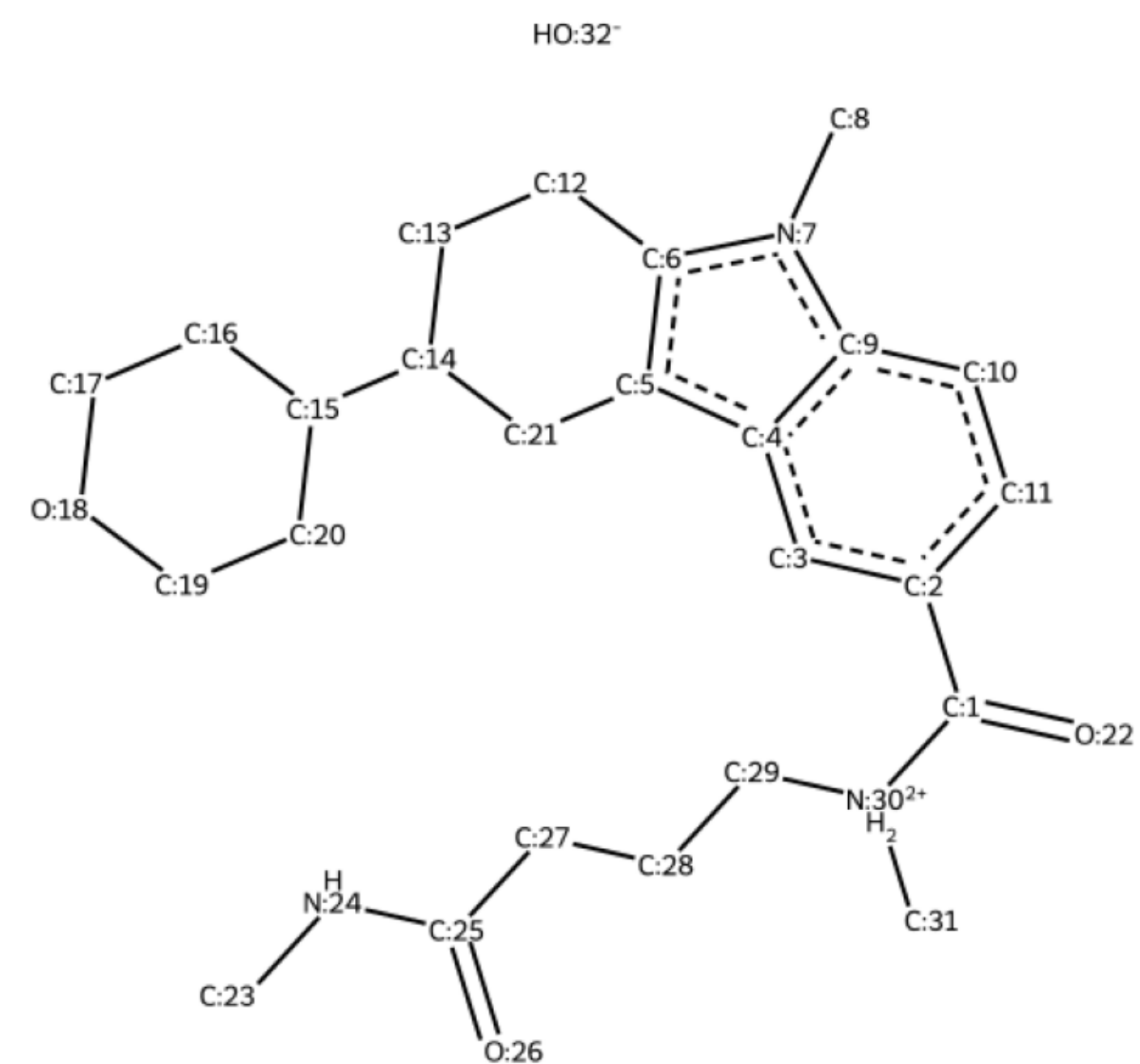
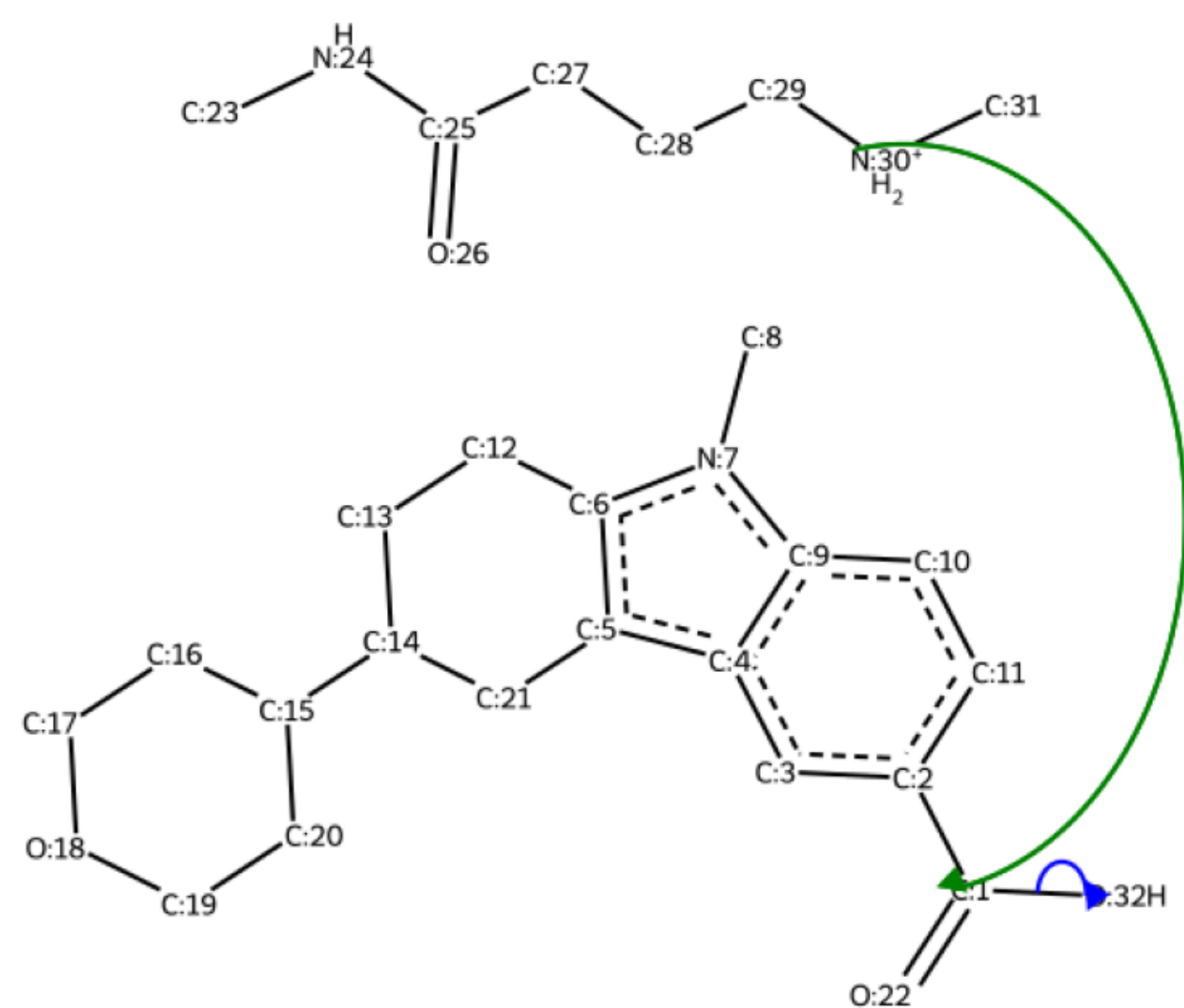


ELECTRO-generated mechanistic pathway

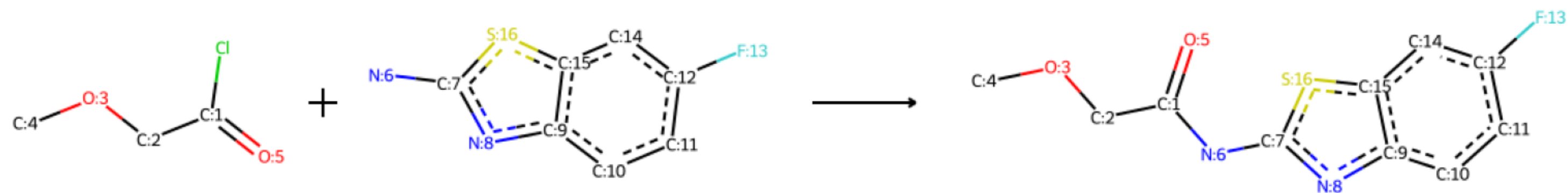
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:27

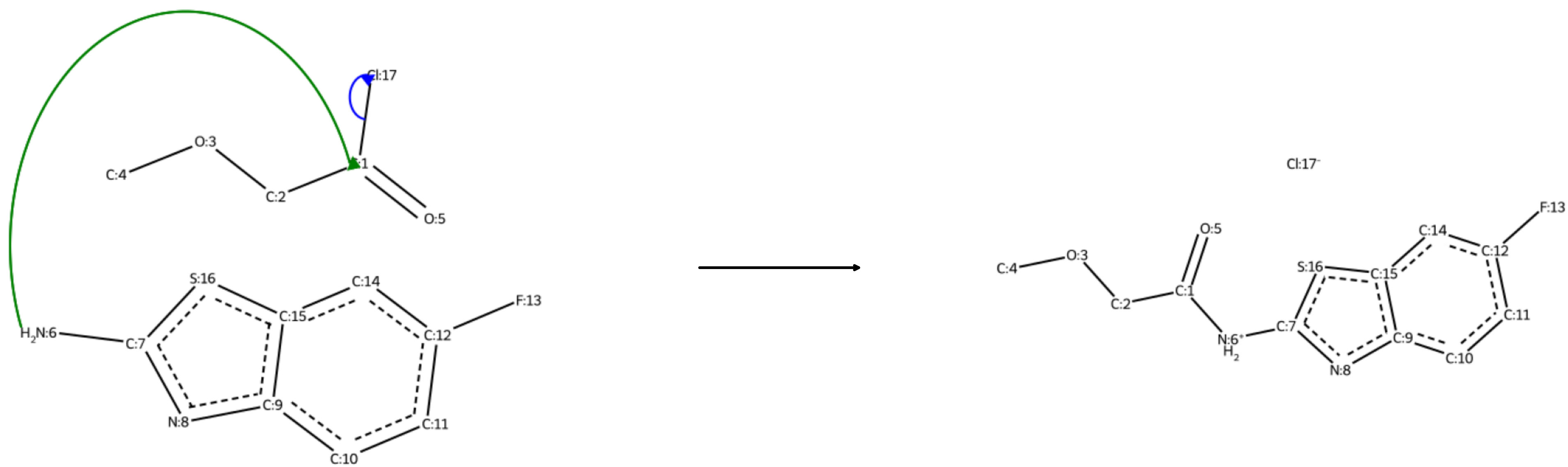


ELECTRO-generated mechanistic pathway

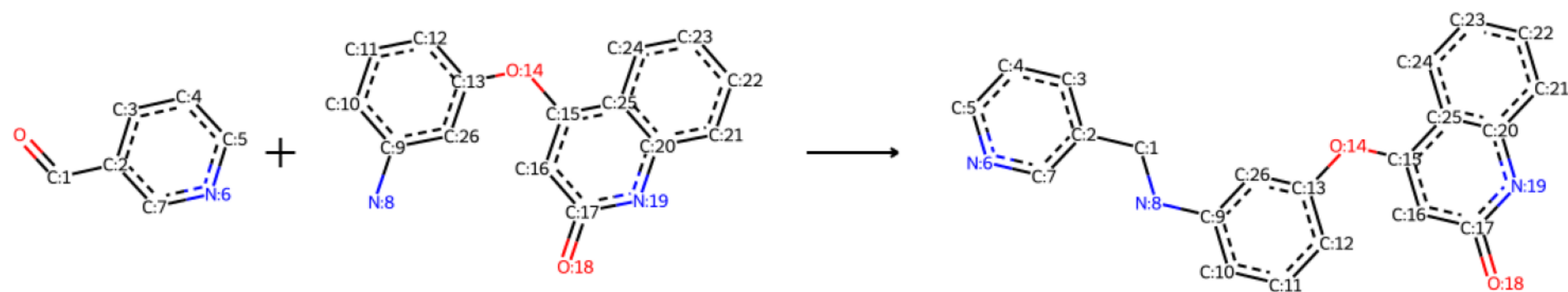
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:28

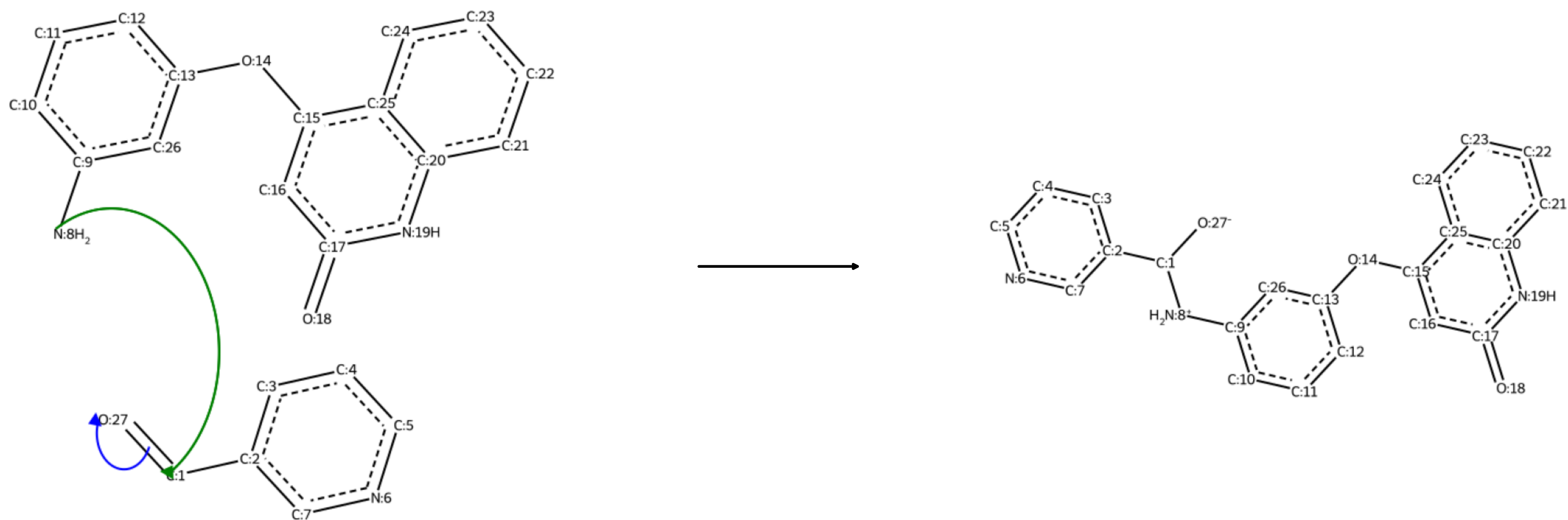


ELECTRO-generated mechanistic pathway

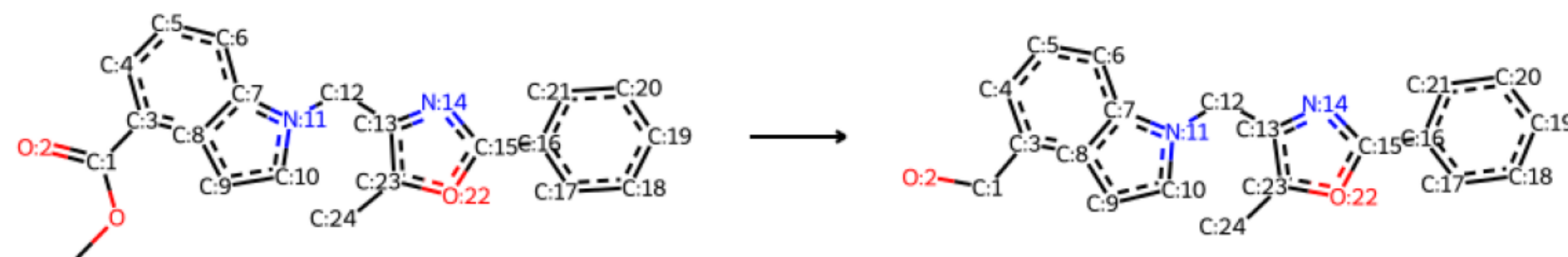
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:29

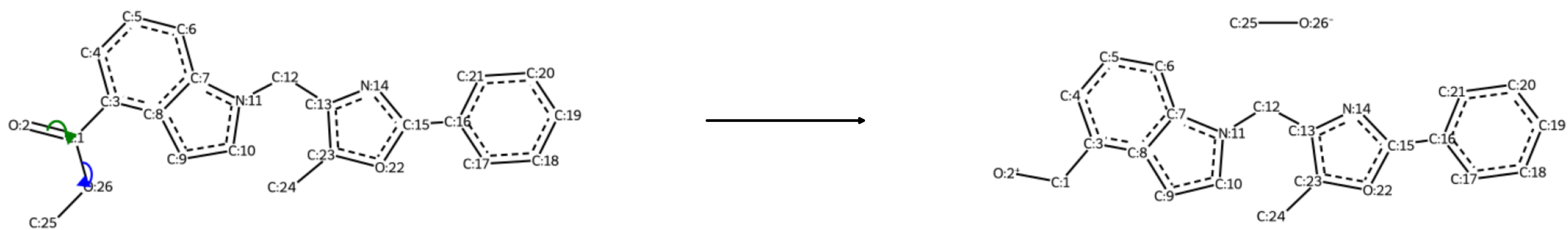


ELECTRO-generated mechanistic pathway

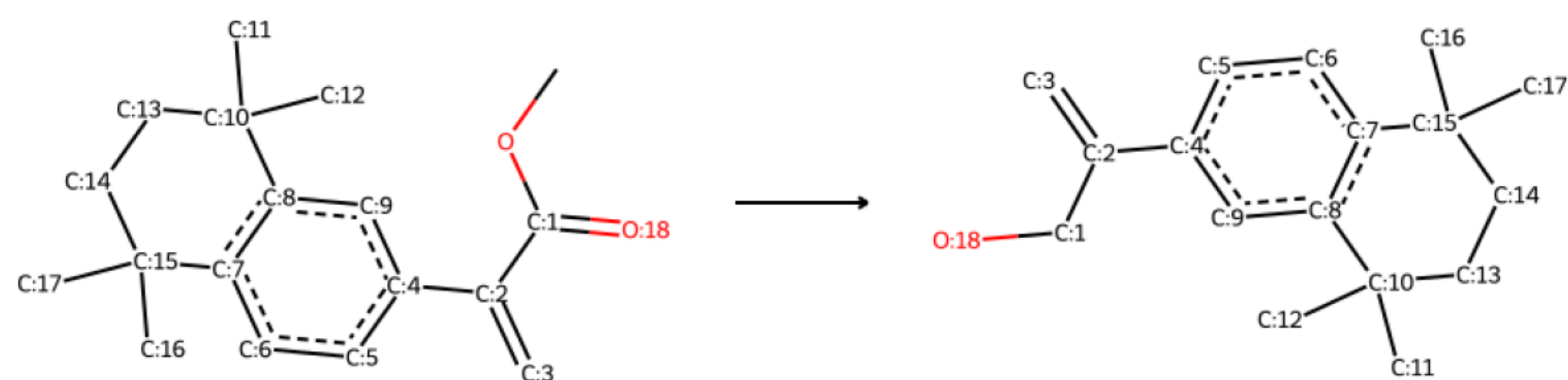
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:30

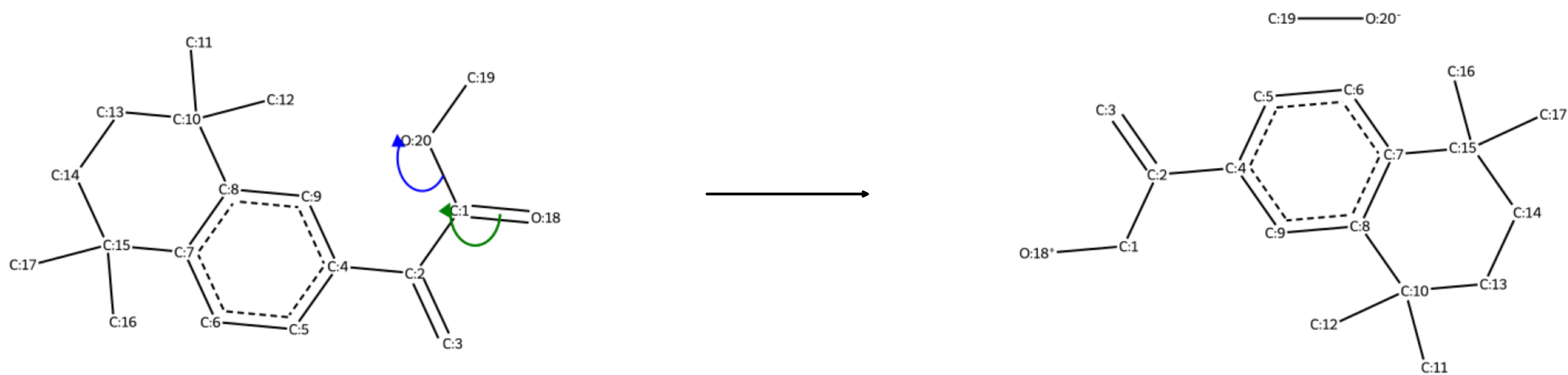


ELECTRO-generated mechanistic pathway

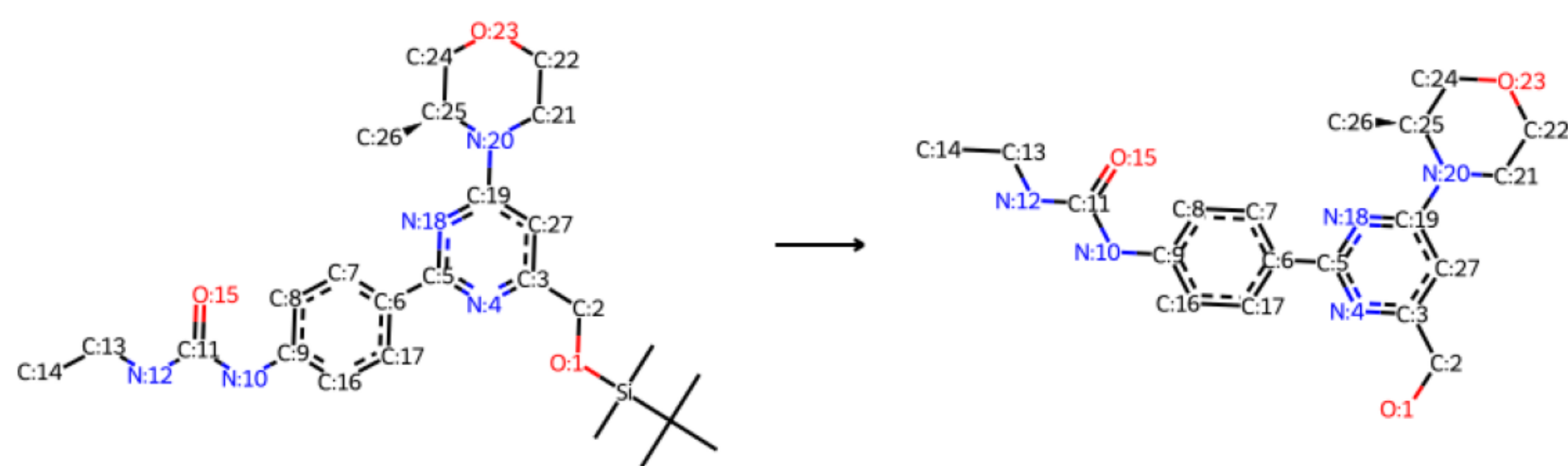
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



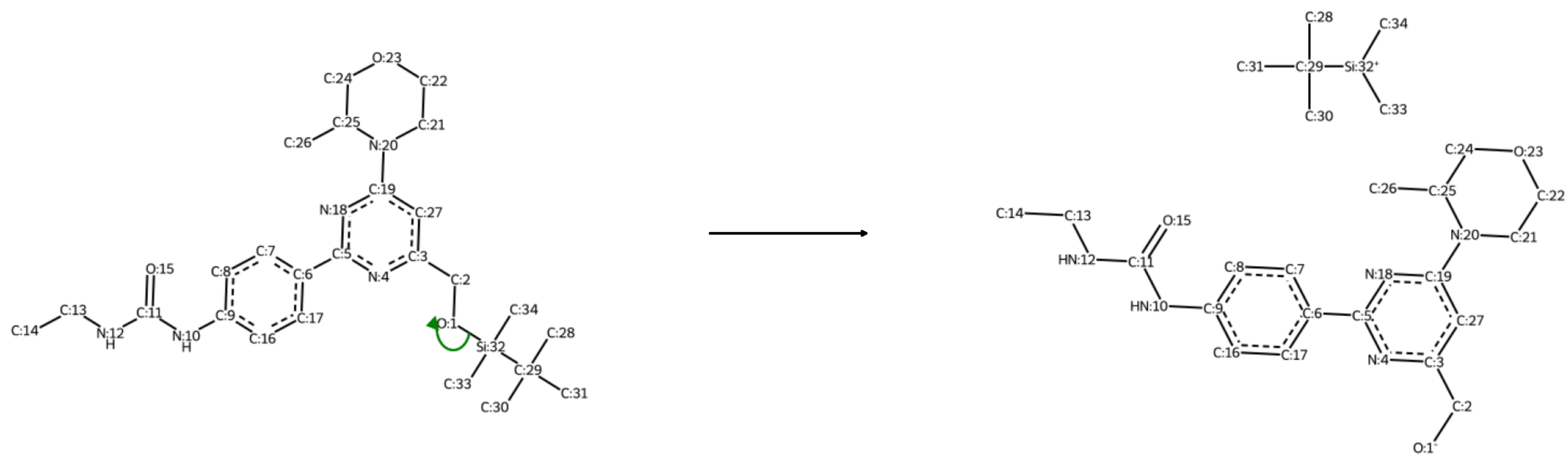
Original reaction RXN_ID:31



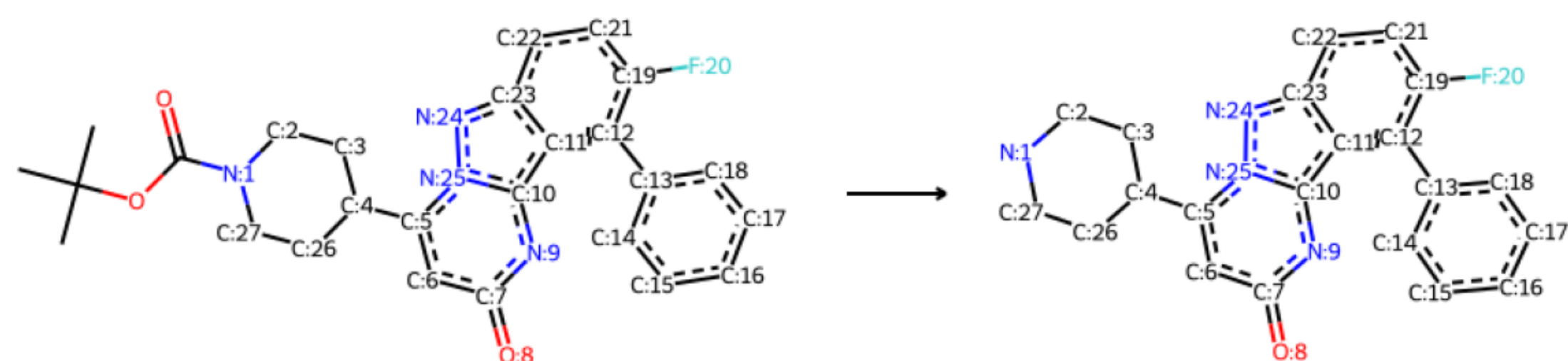
ELECTRO-generated mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1



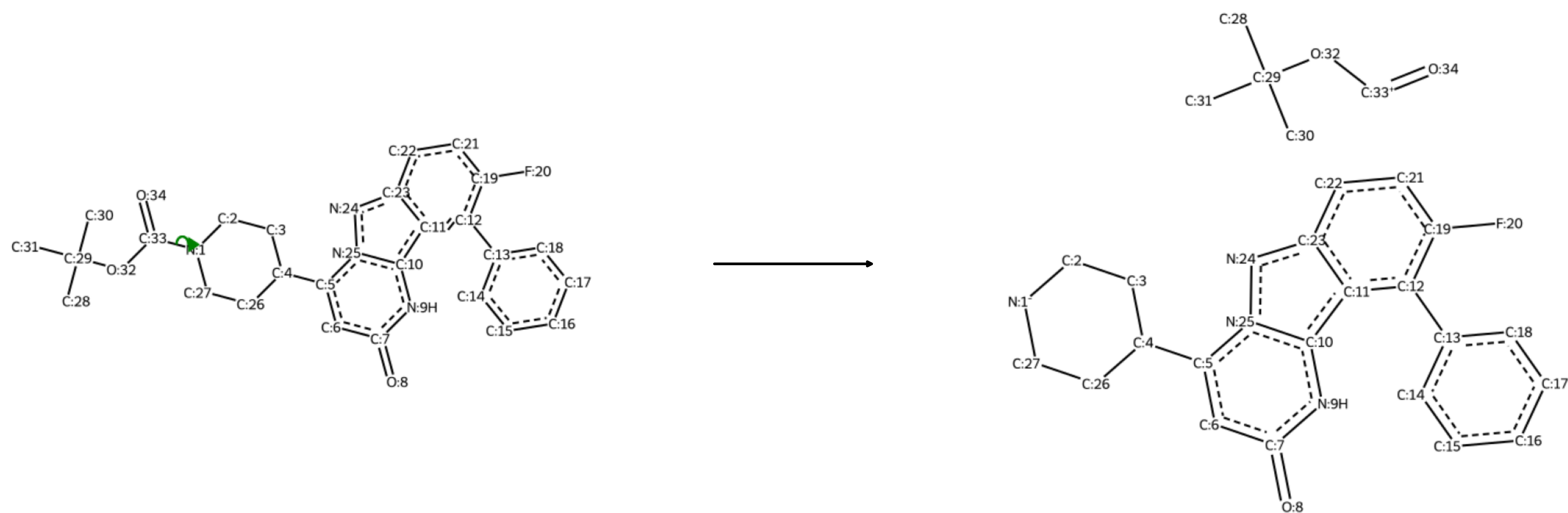
Original reaction RXN_ID:32



ELECTRO-generated mechanistic pathway

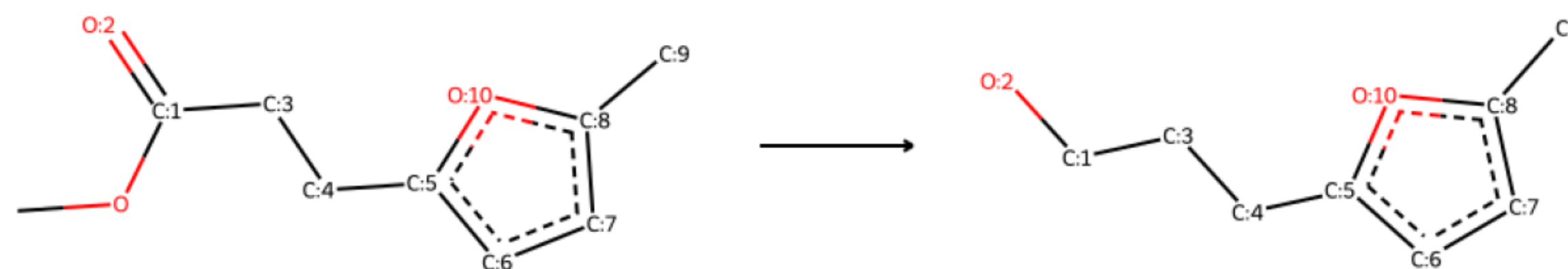
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1



Product(s)

Original reaction RXN_ID:33

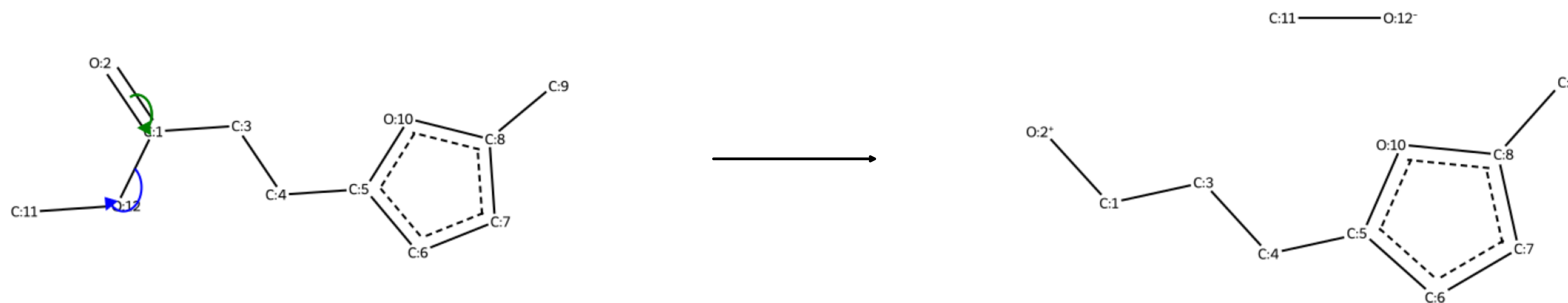


ELECTRO-generated mechanistic pathway

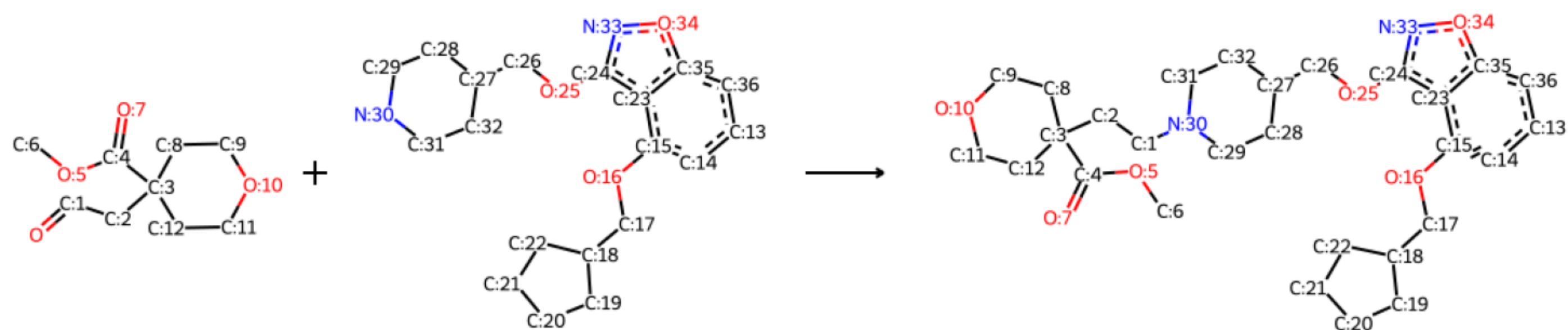
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:34

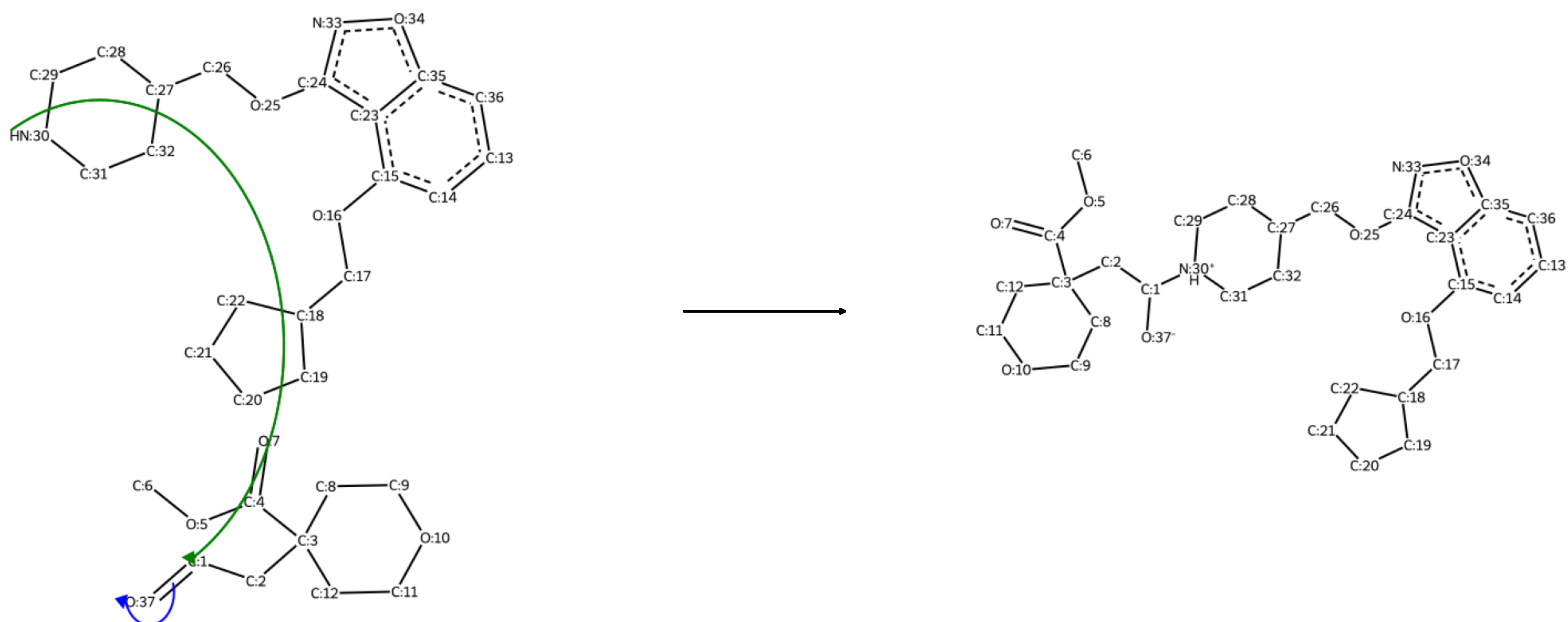


ELECTRO-generated mechanistic pathway

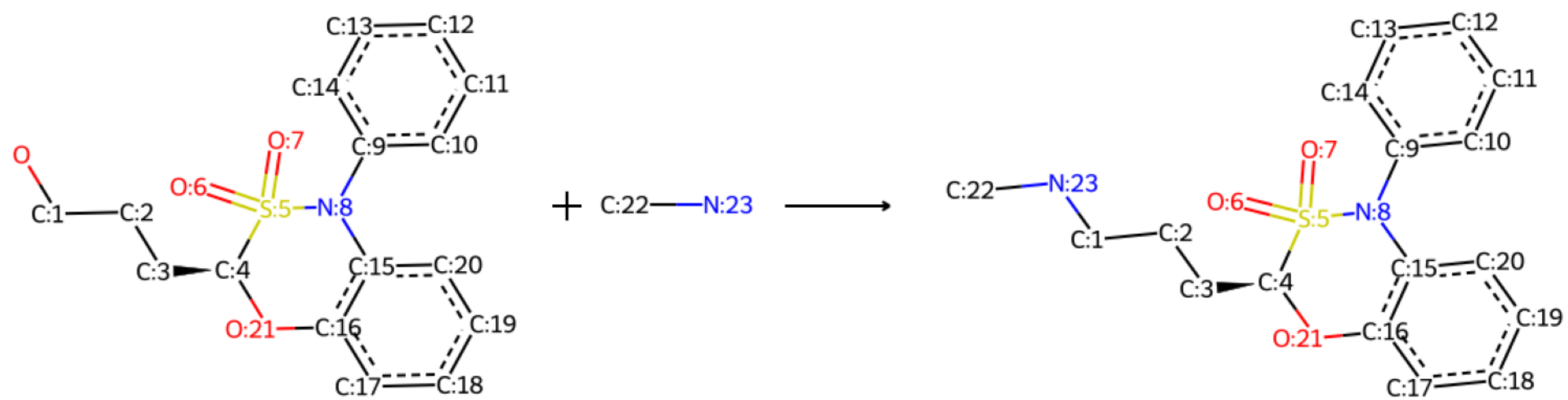
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:35

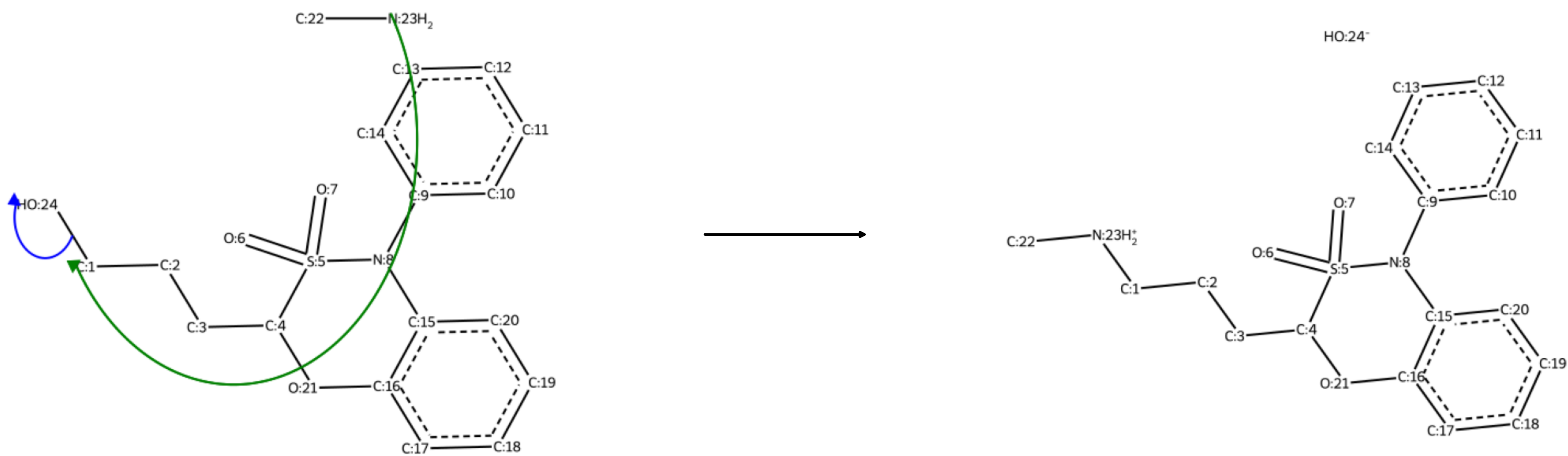


ELECTRO-generated mechanistic pathway

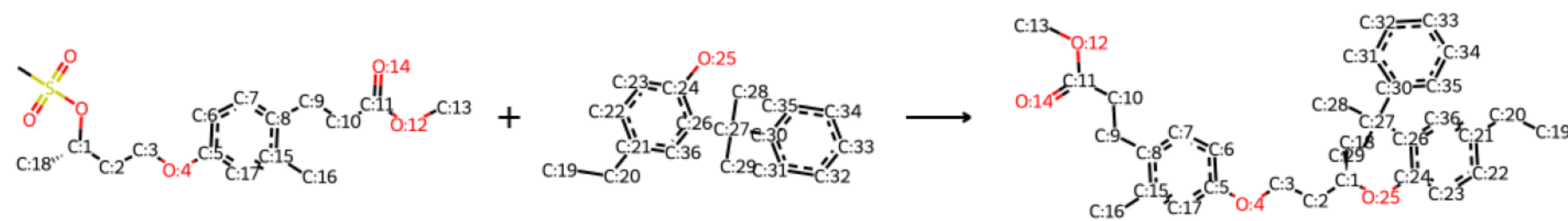
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:36

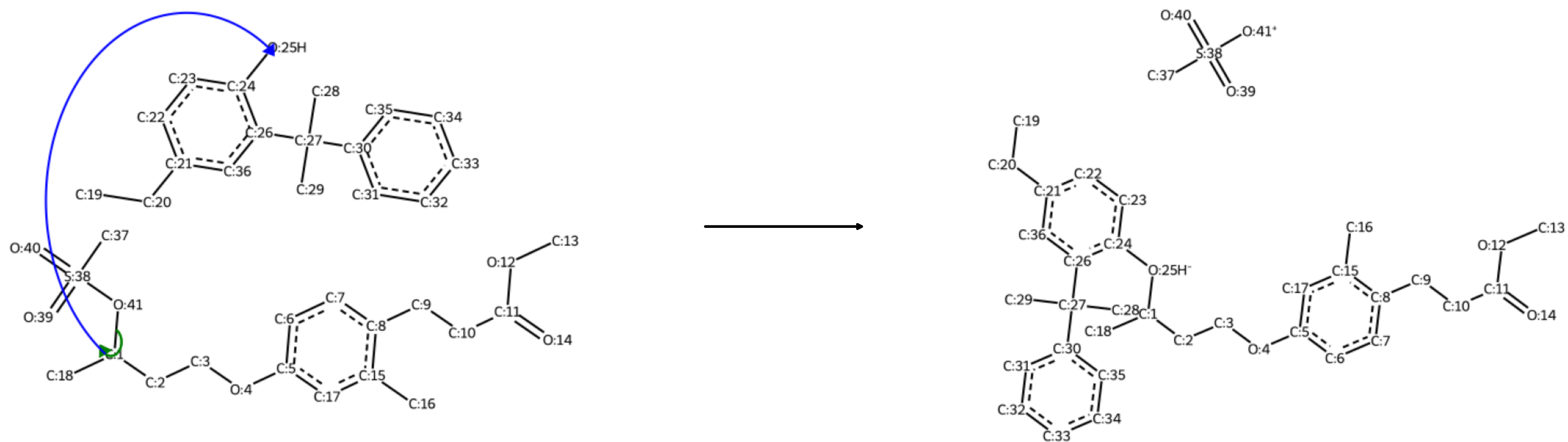


ELECTRO-generated mechanistic pathway

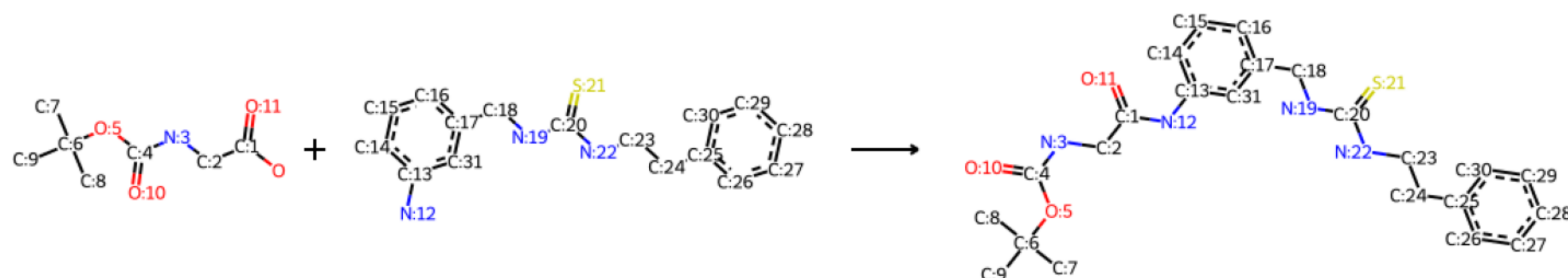
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:37

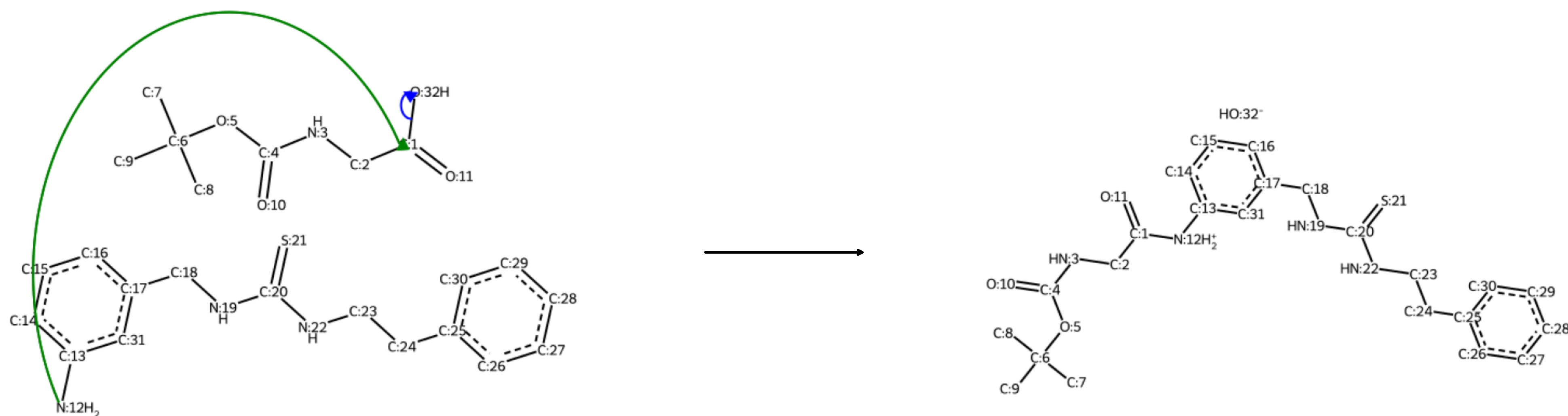


ELECTRO-generated mechanistic pathway

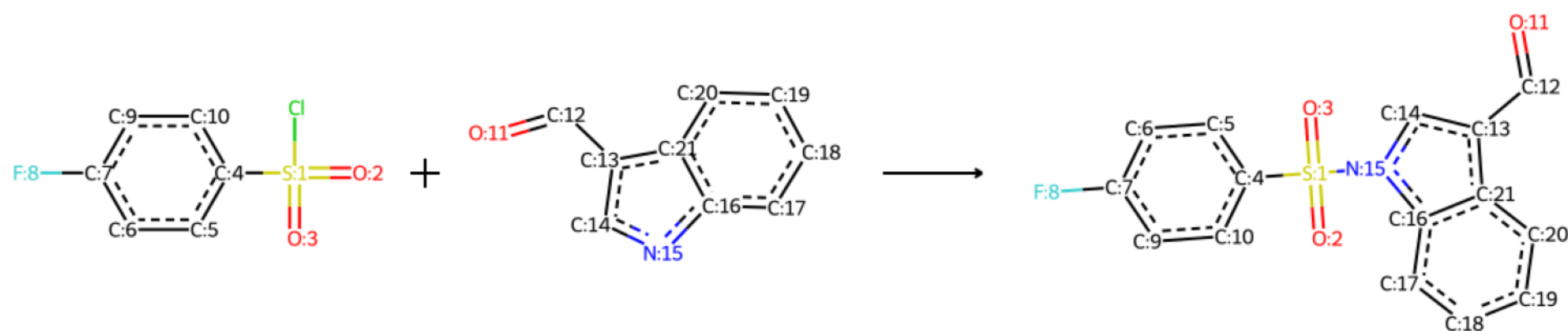
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:38

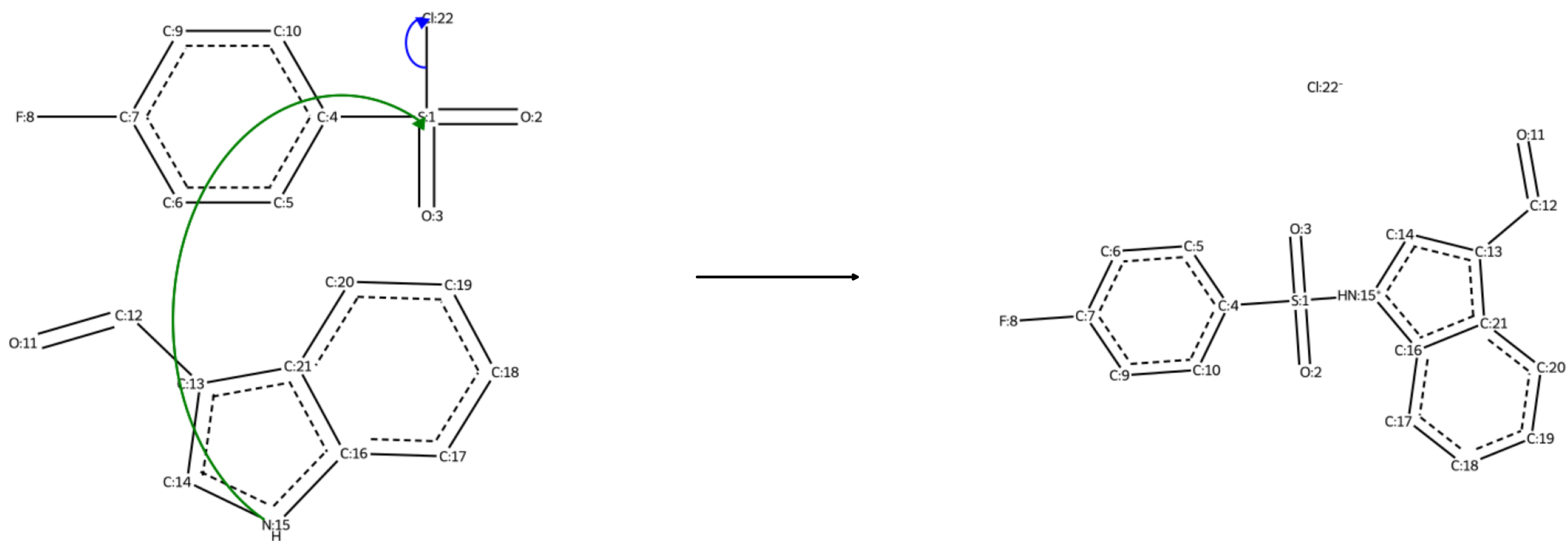


ELECTRO-generated mechanistic pathway

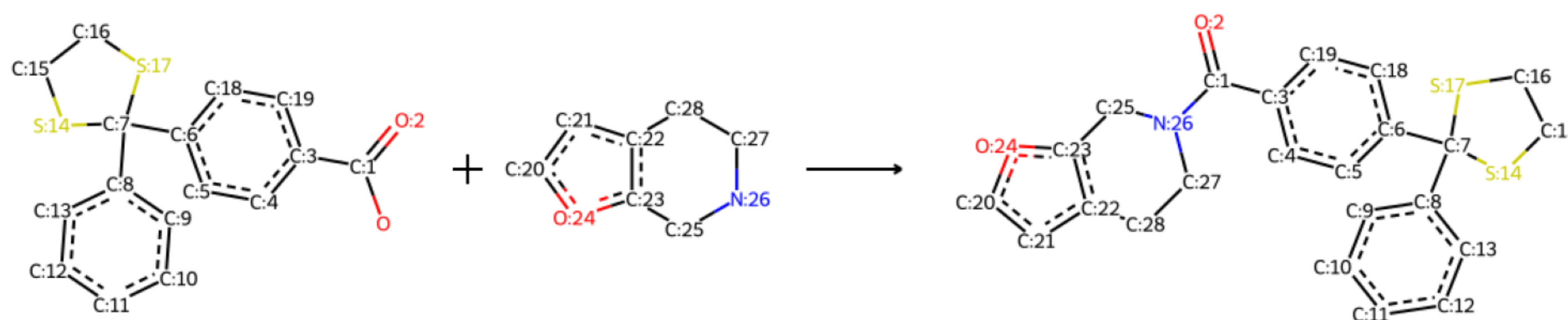
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



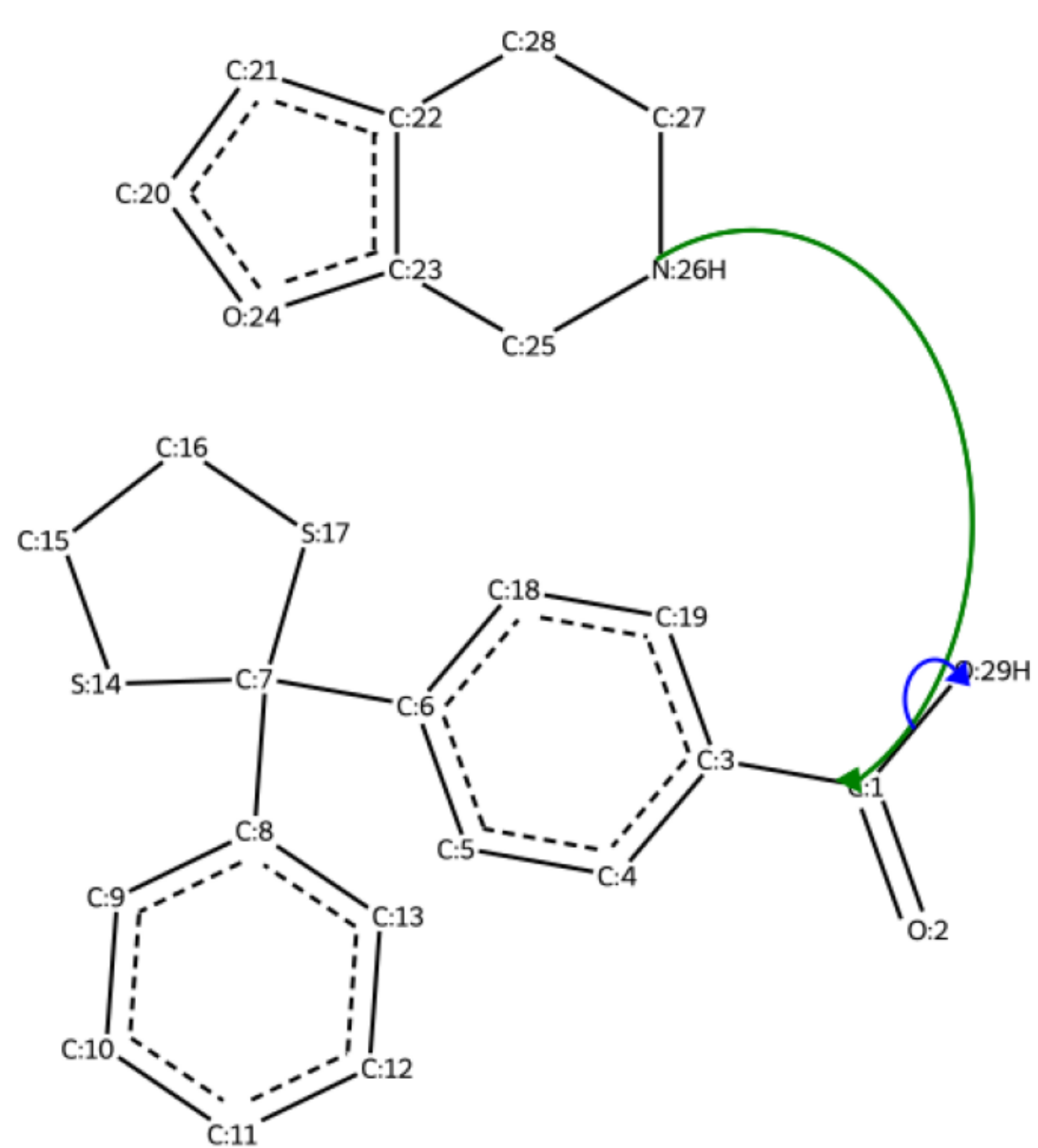
Original reaction RXN_ID:39



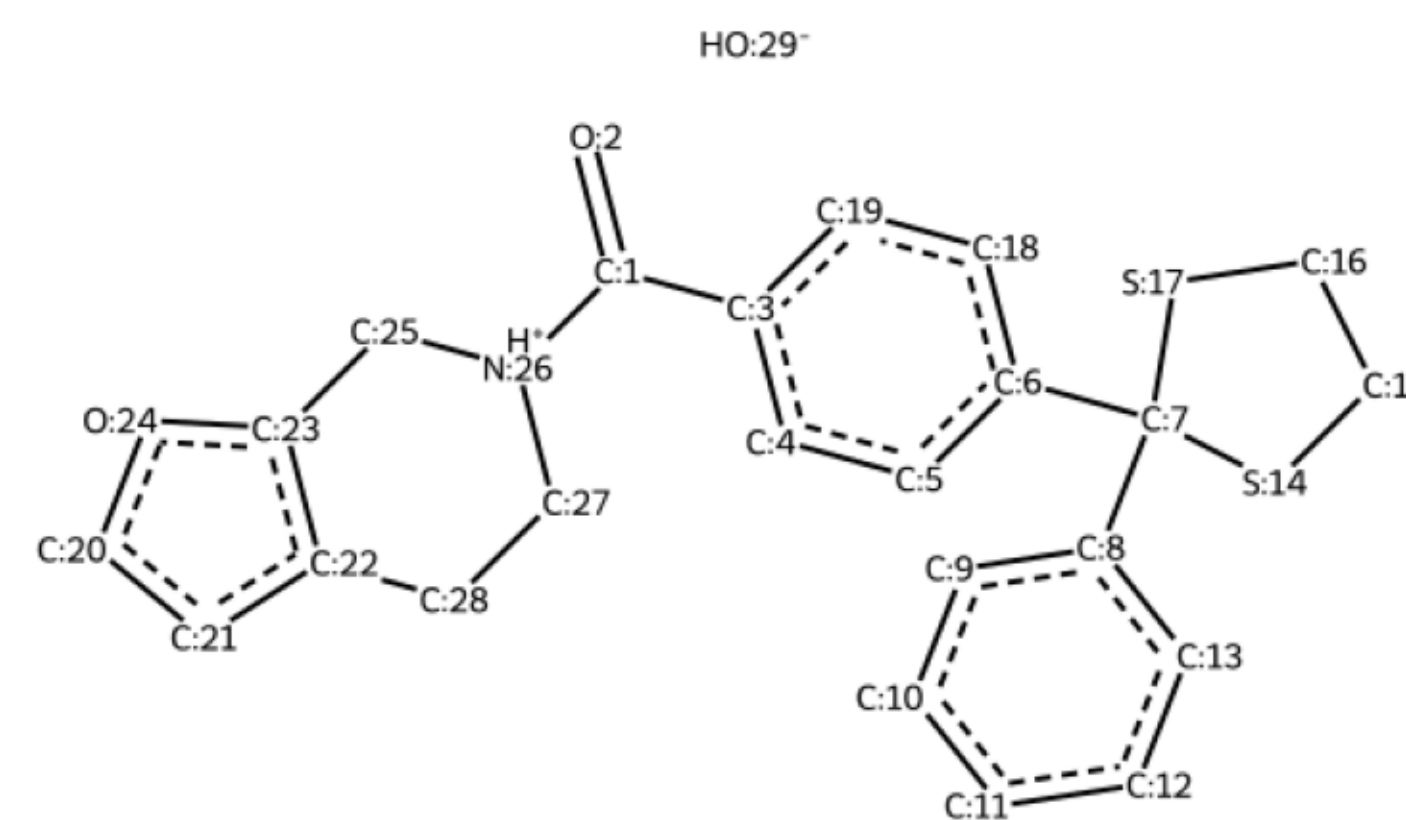
ELECTRO-generated mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

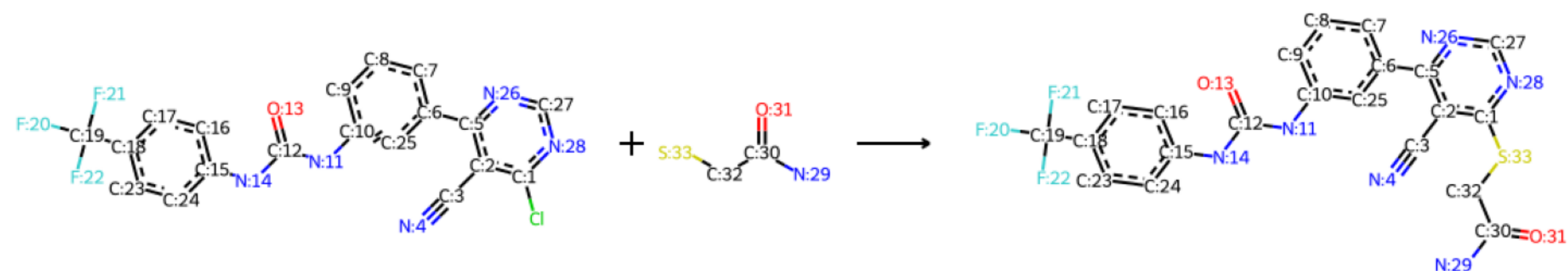
step #1



Product(s)



Original reaction RXN_ID:40

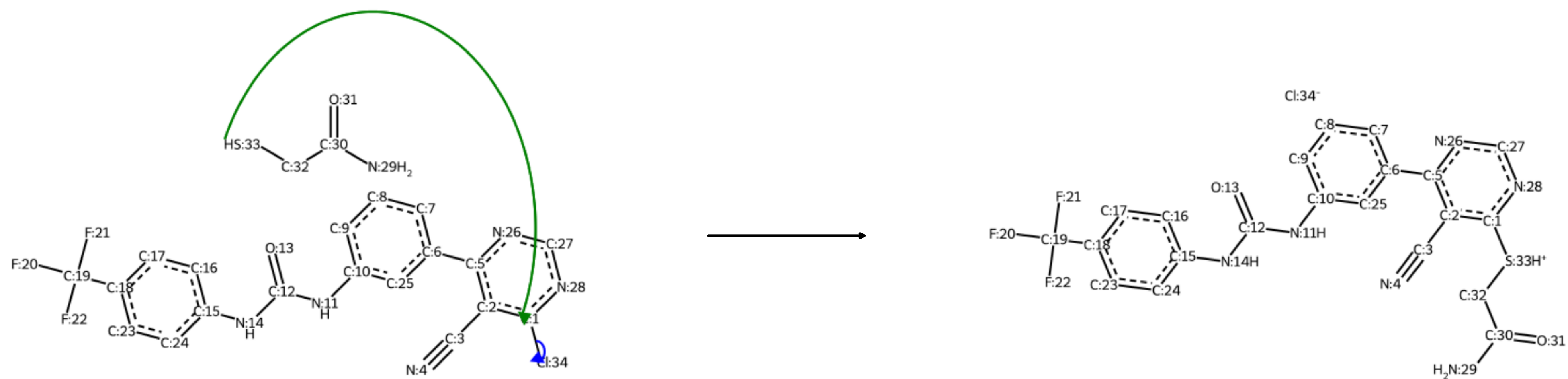


ELECTRO-generated mechanistic pathway

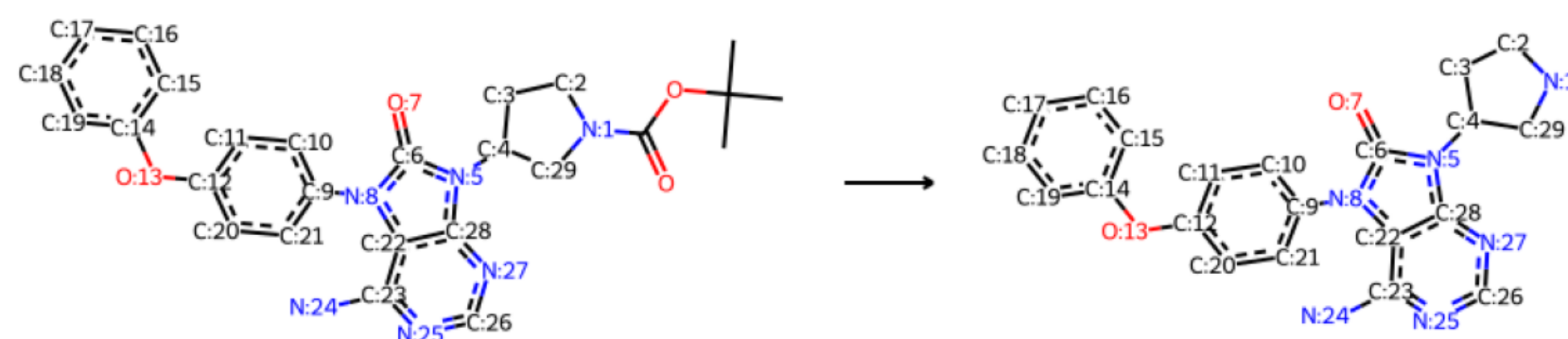
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



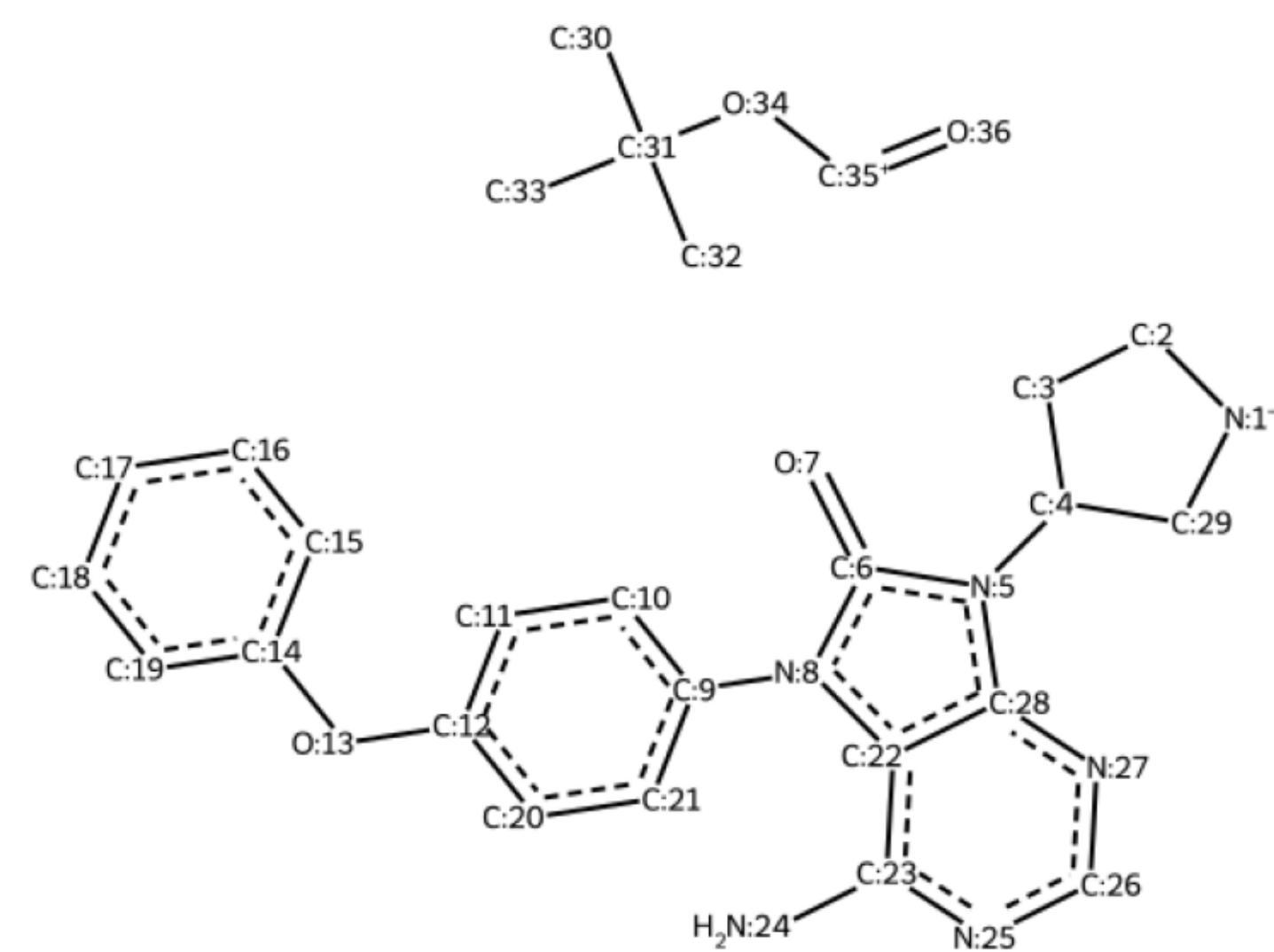
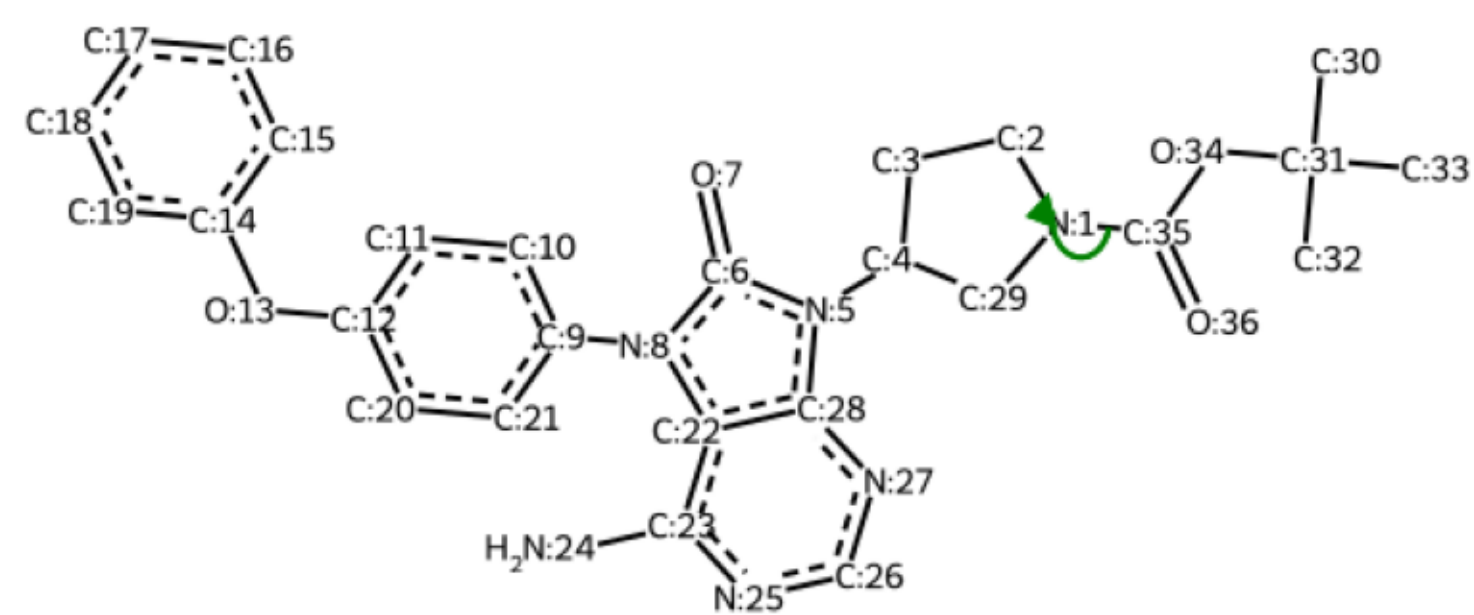
Original reaction RXN_ID:41



ELECTRO-generated mechanistic pathway

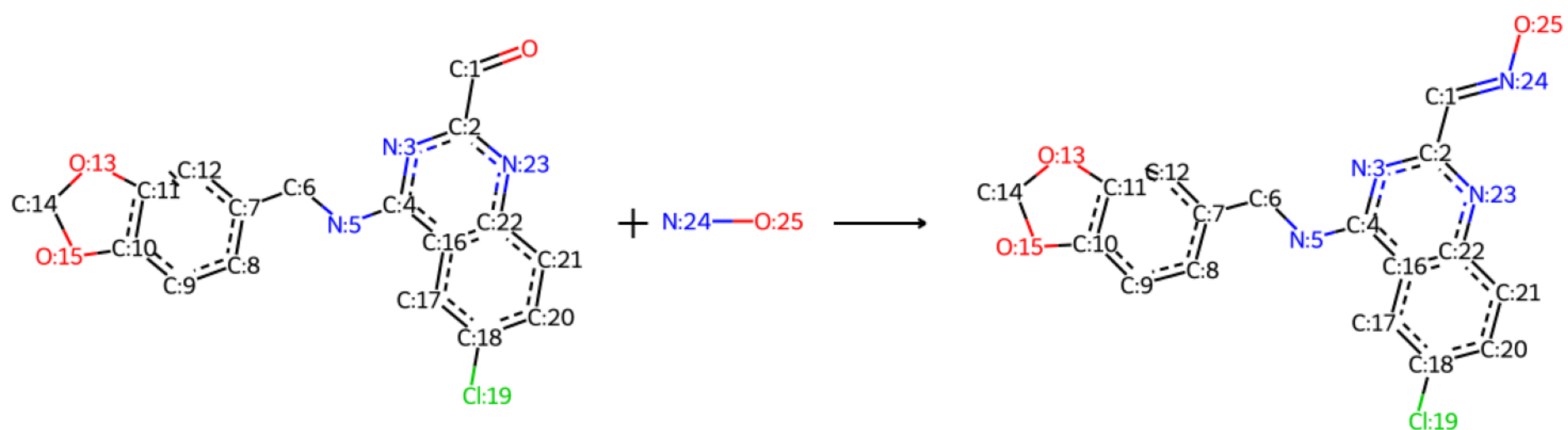
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1



Product(s)

Original reaction RXN_ID:42

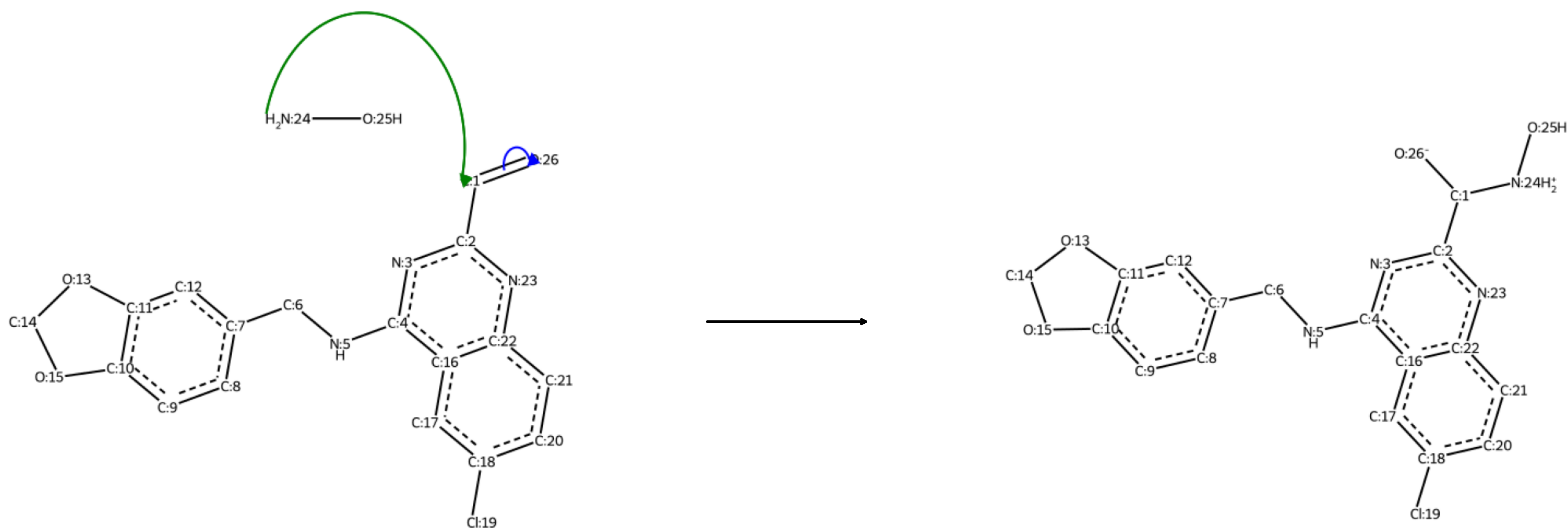


ELECTRO-generated mechanistic pathway

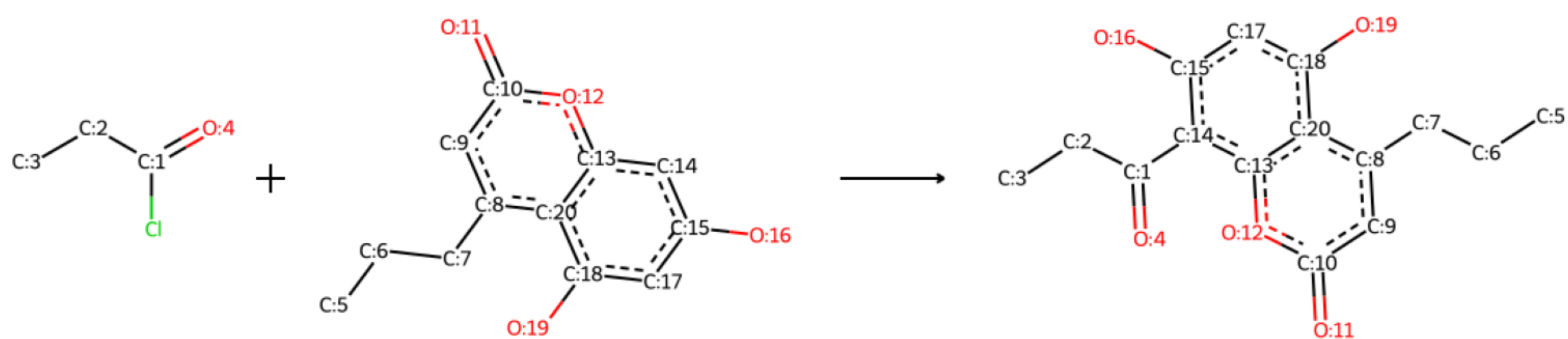
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:43

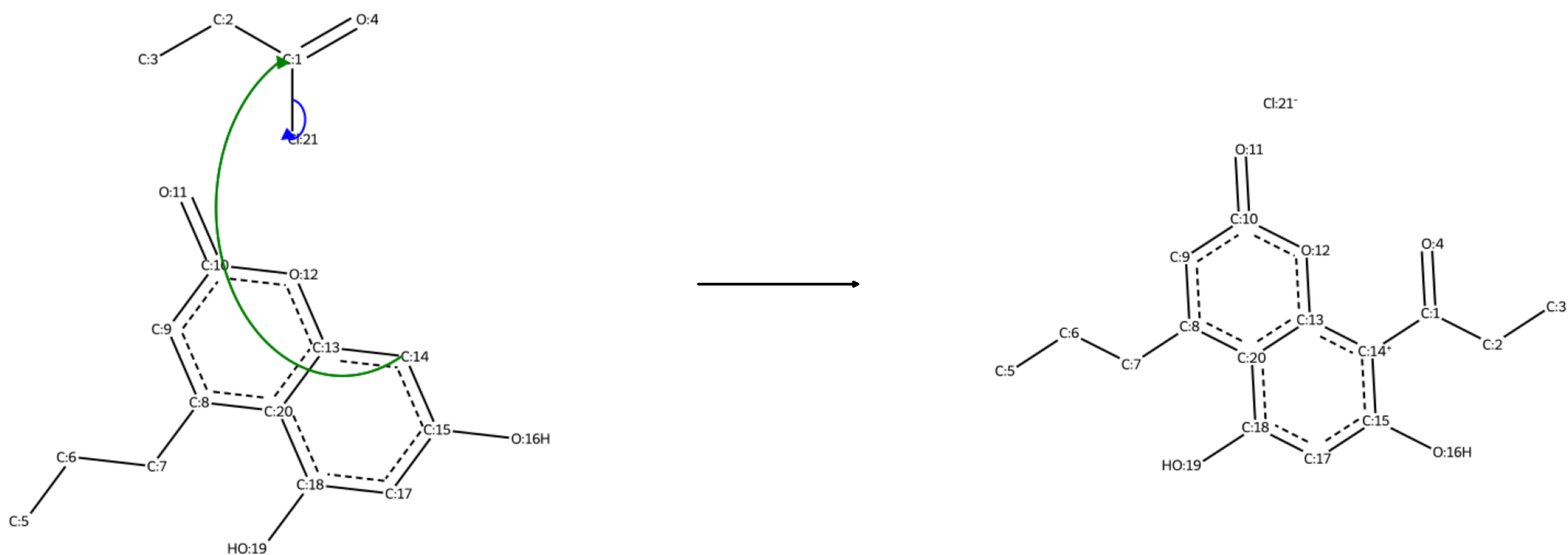


ELECTRO-generated mechanistic pathway

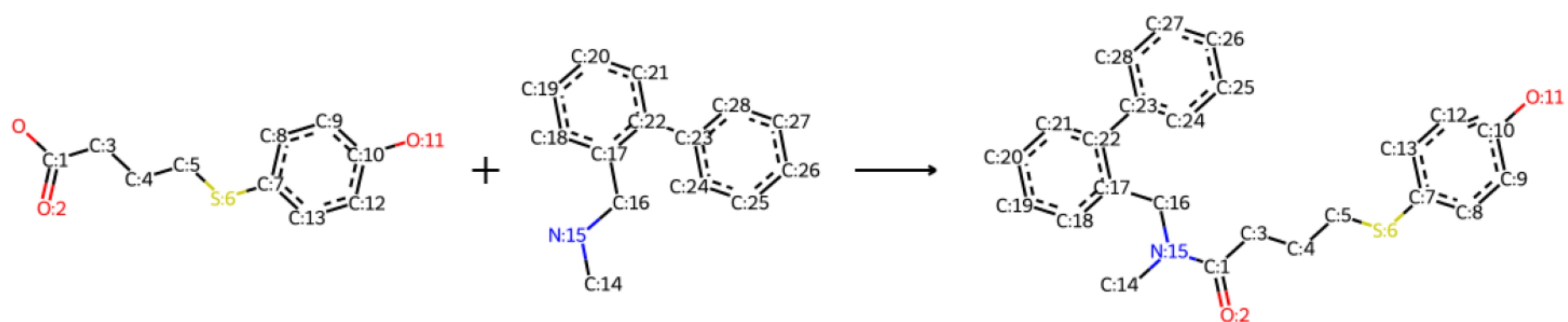
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:44

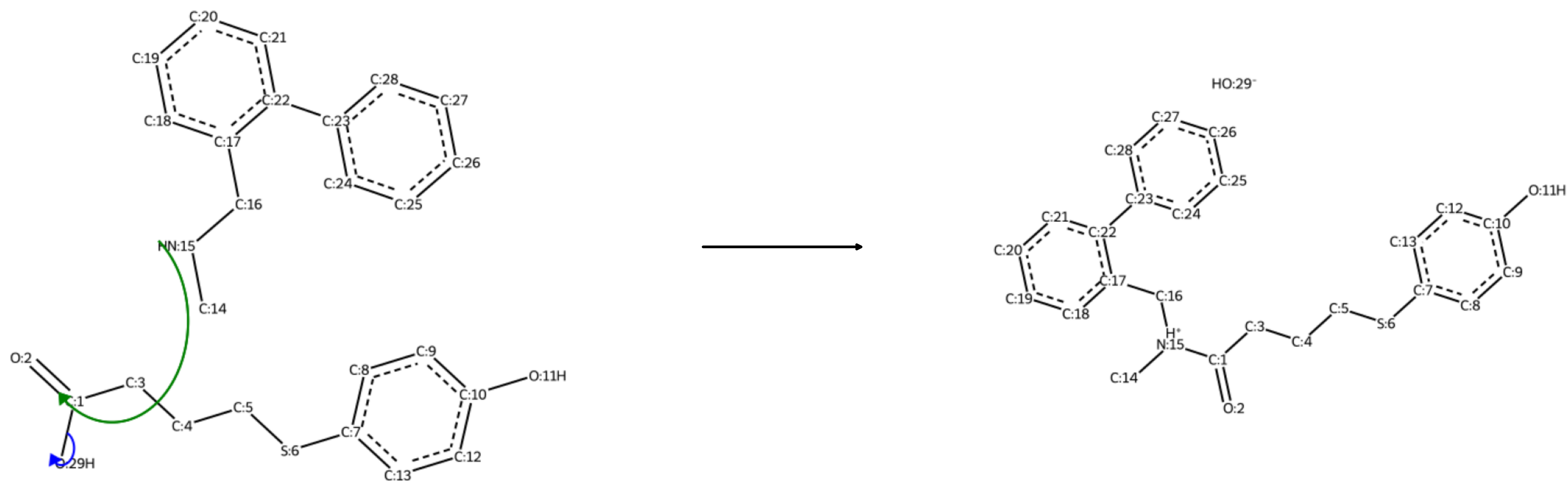


ELECTRO-generated mechanistic pathway

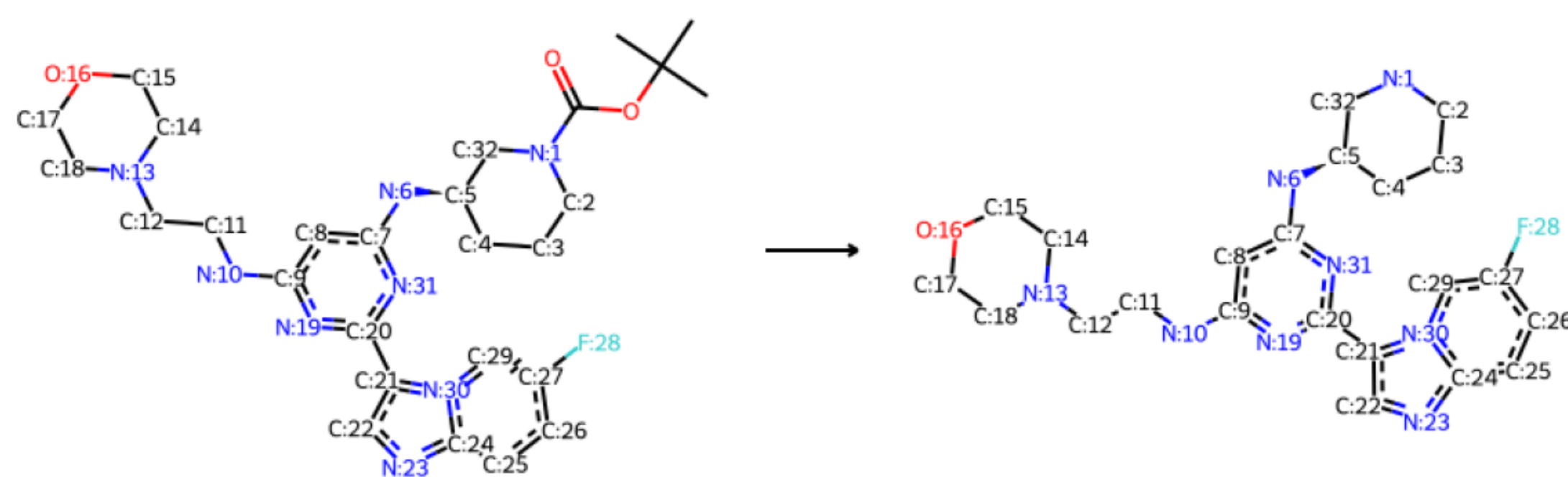
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:45

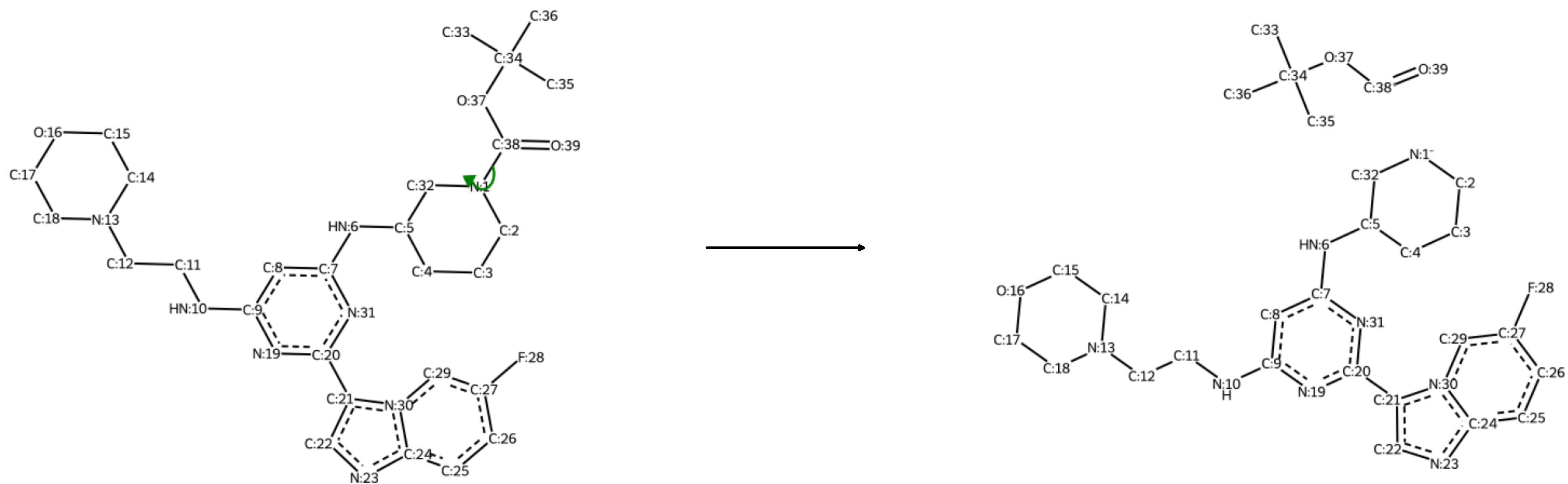


ELECTRO-generated mechanistic pathway

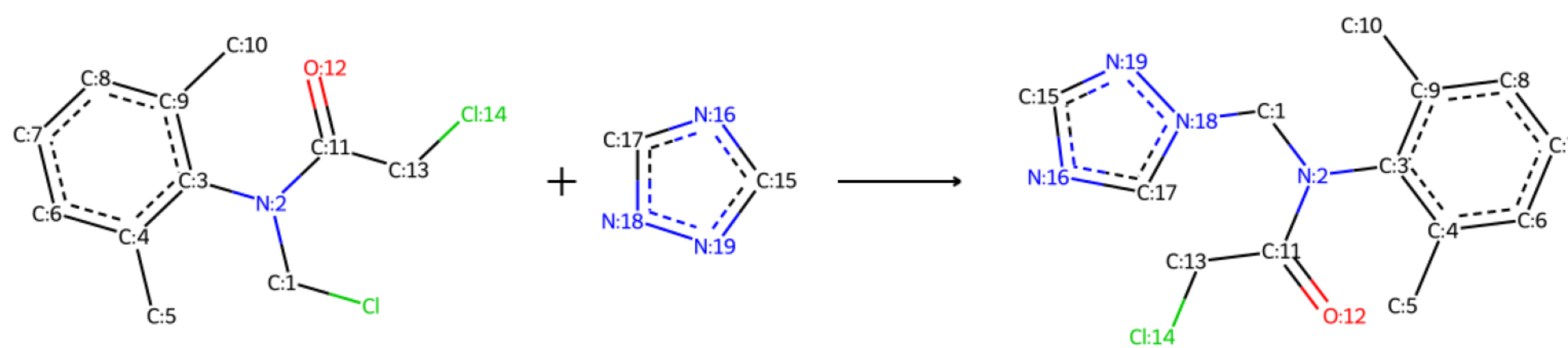
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:46

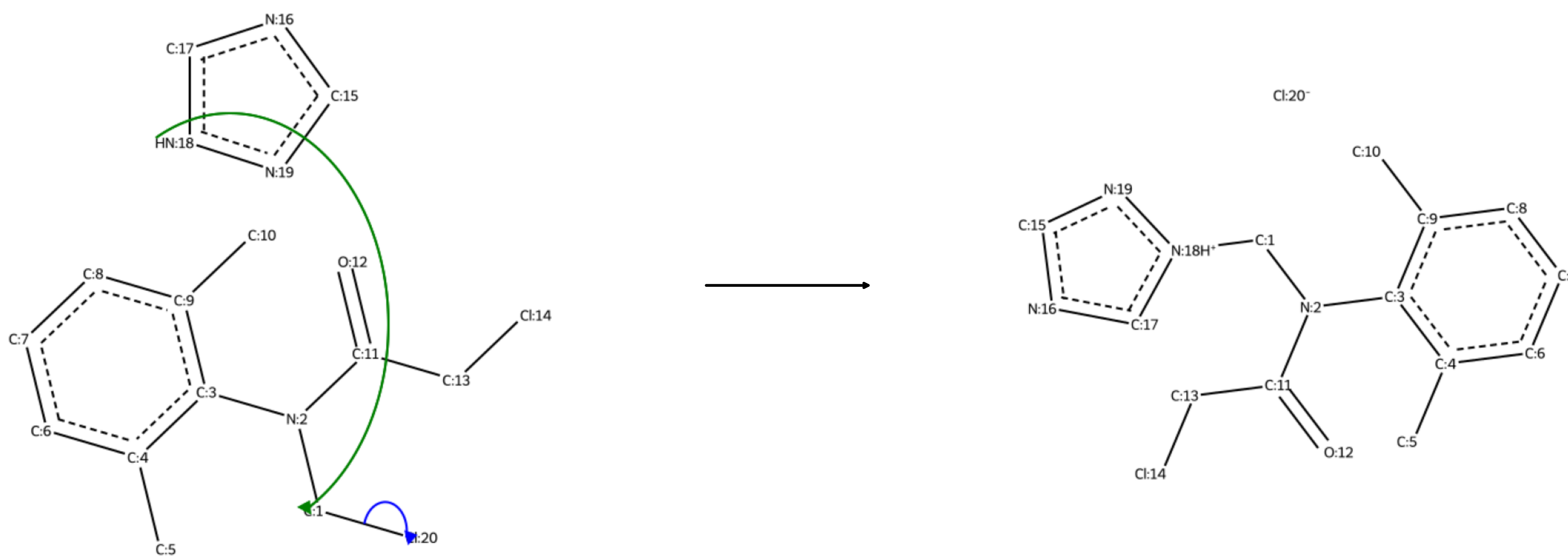


ELECTRO-generated mechanistic pathway

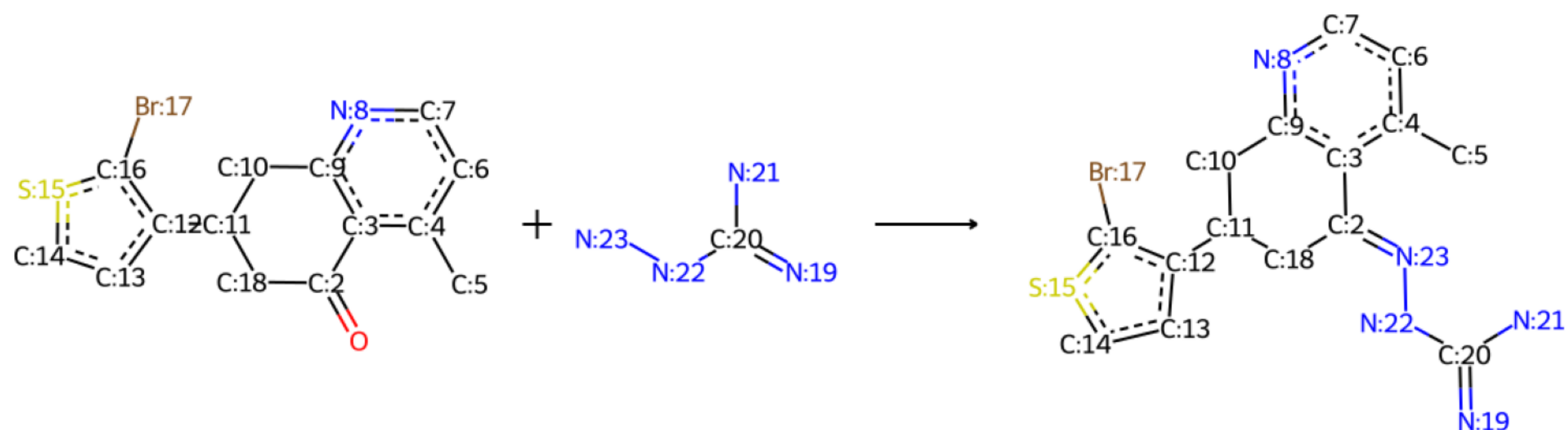
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:47

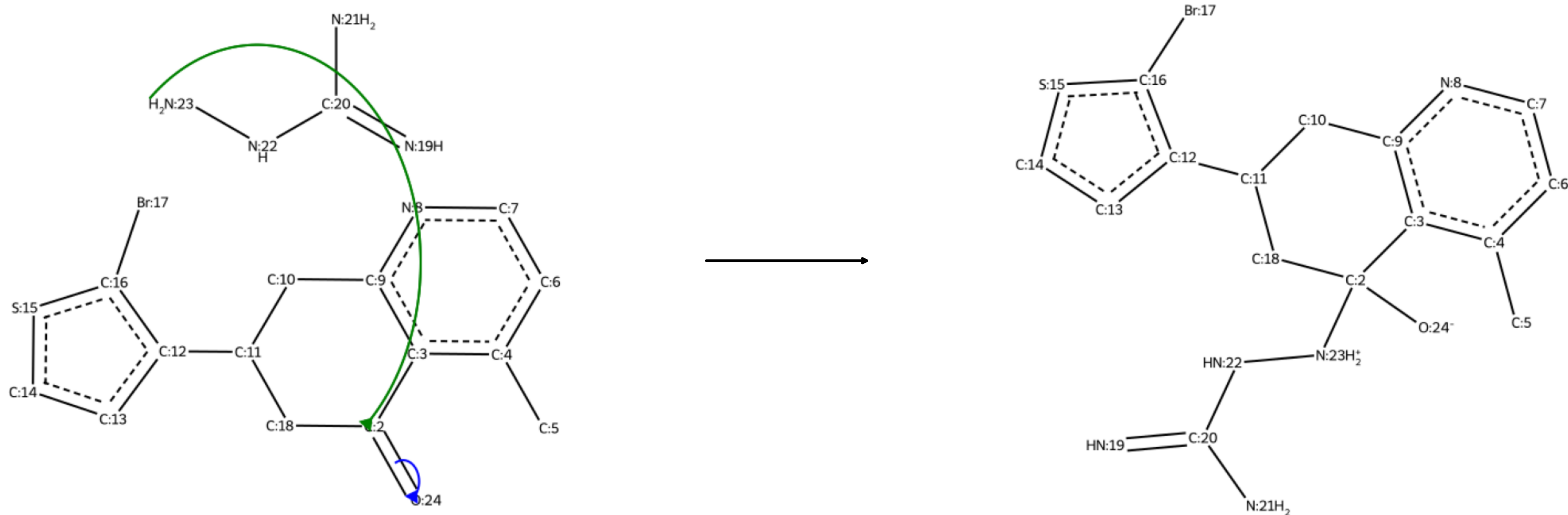


ELECTRO-generated mechanistic pathway

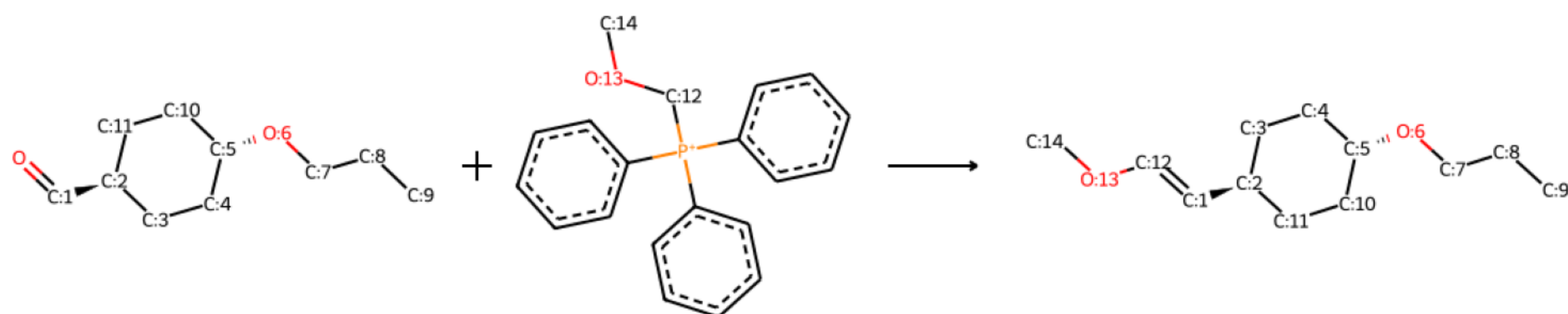
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



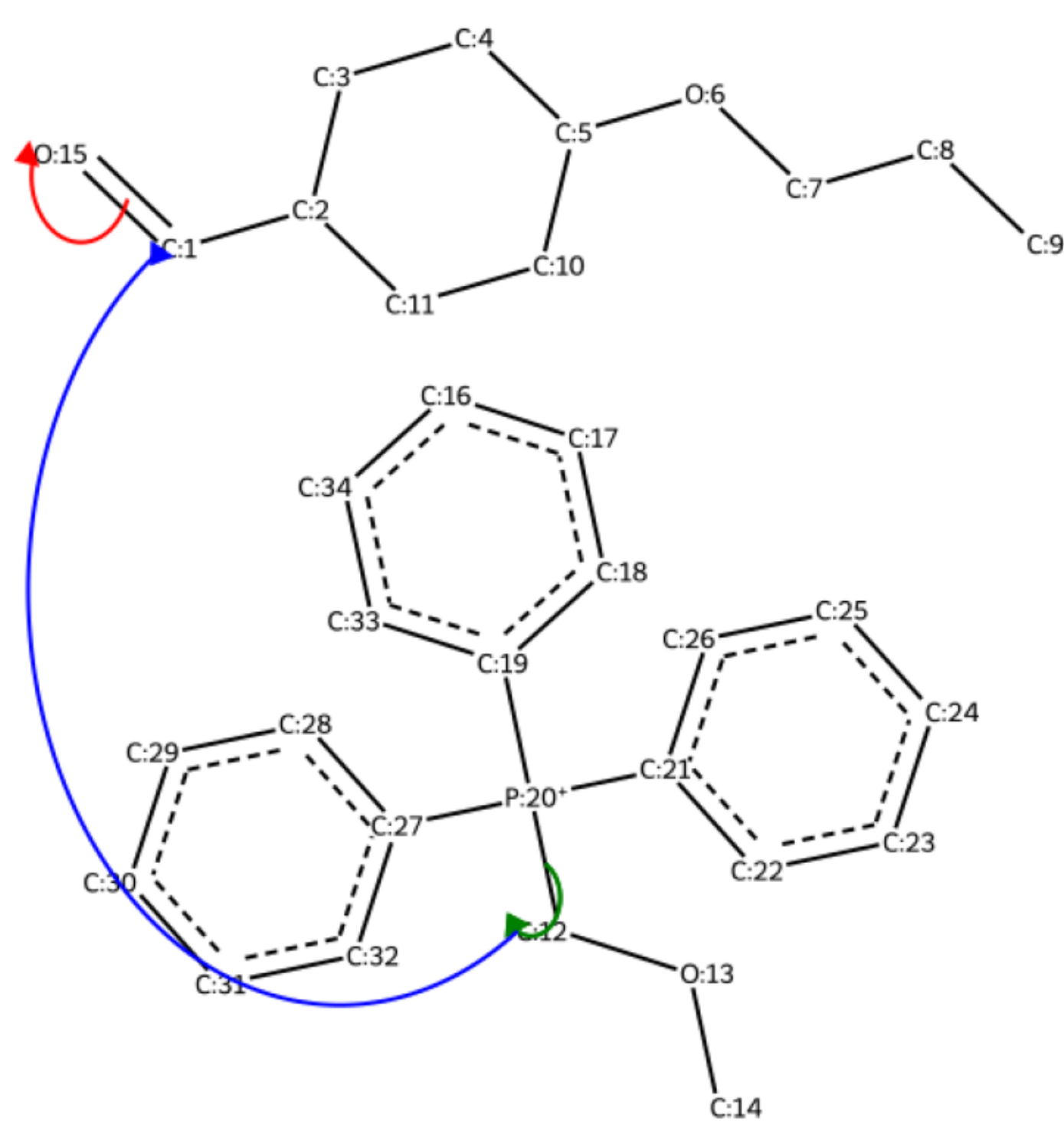
Original reaction RXN_ID:48



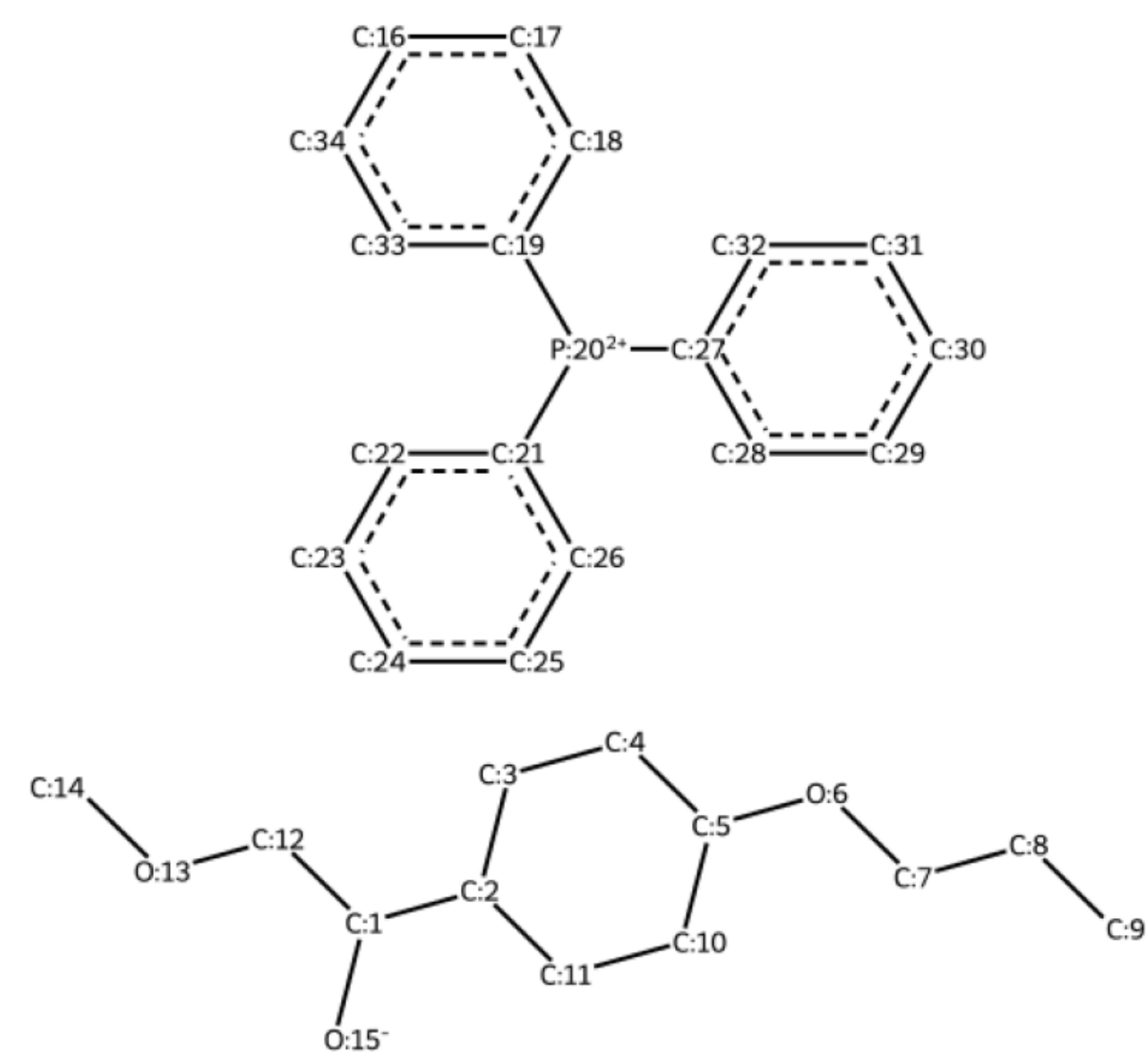
ELECTRO-generated mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

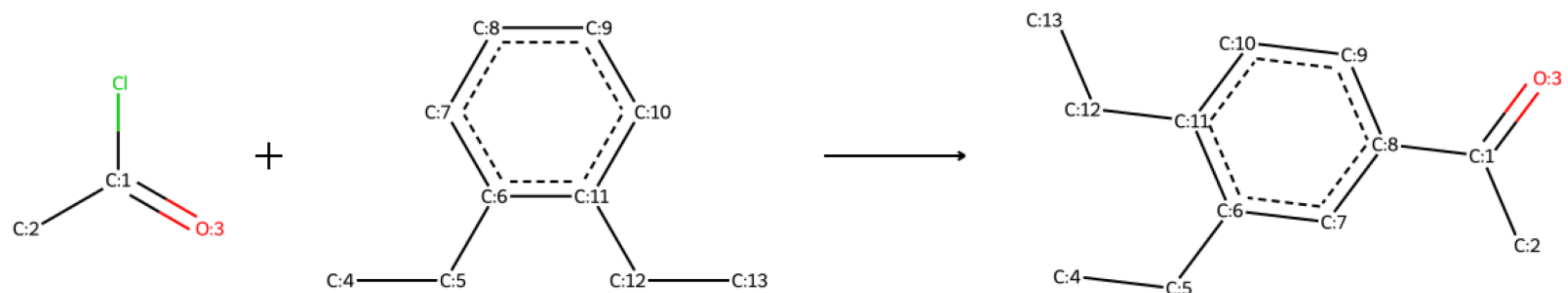
step #1



Product(s)



Original reaction RXN_ID:49

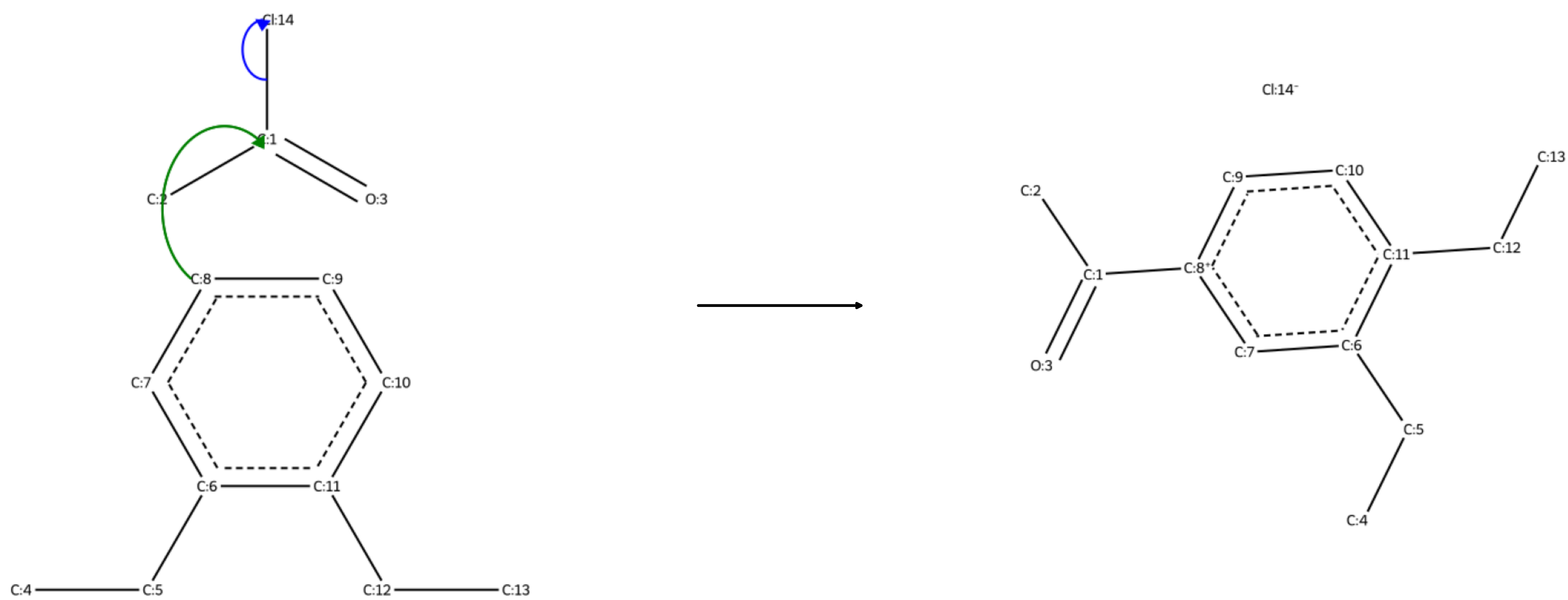


ELECTRO-generated mechanistic pathway

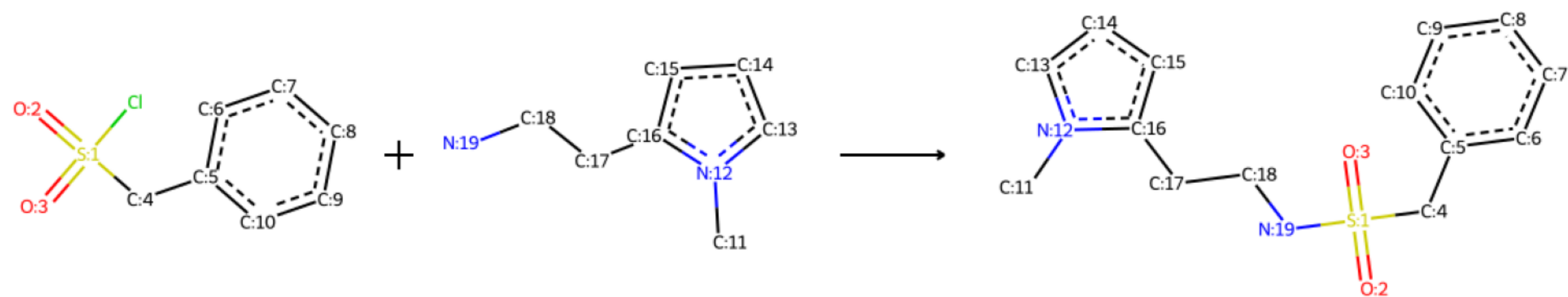
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:50

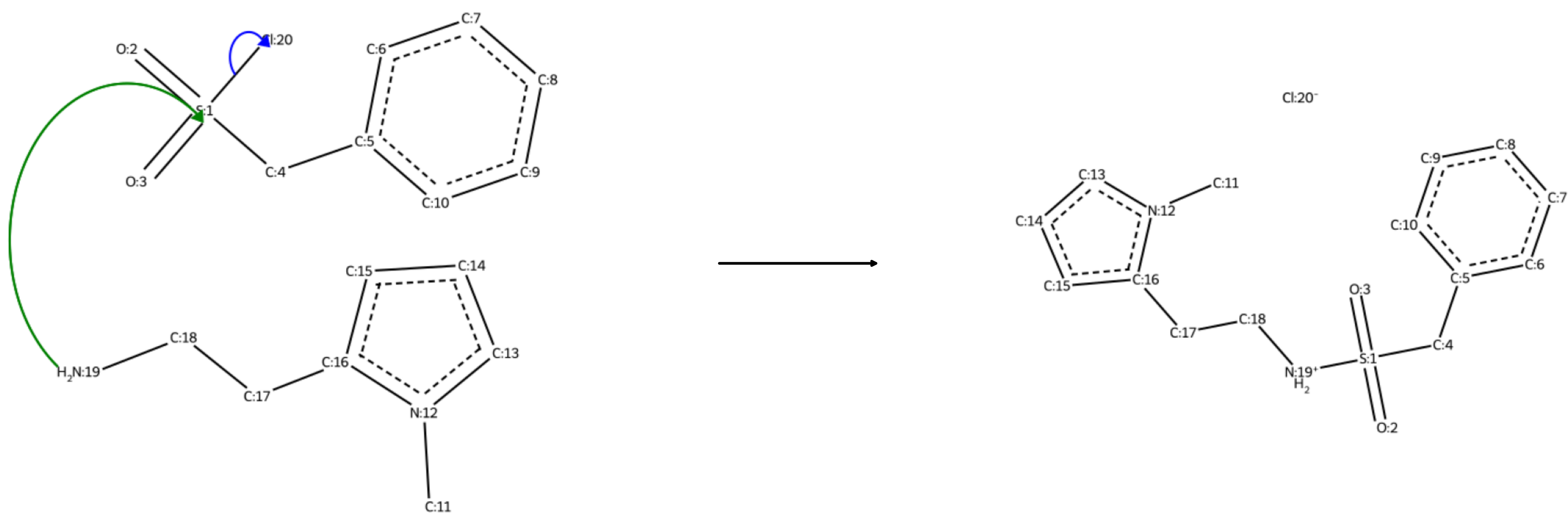


ELECTRO-generated mechanistic pathway

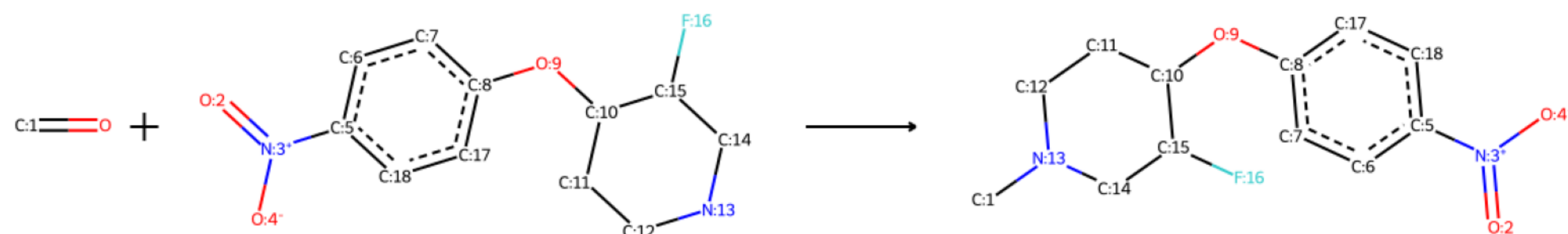
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:51

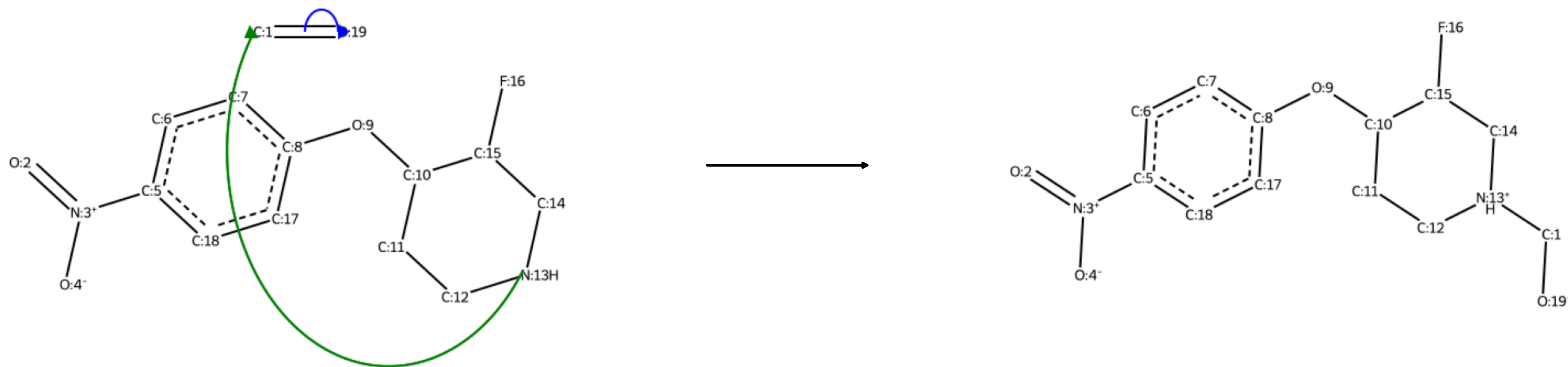


ELECTRO-generated mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:52

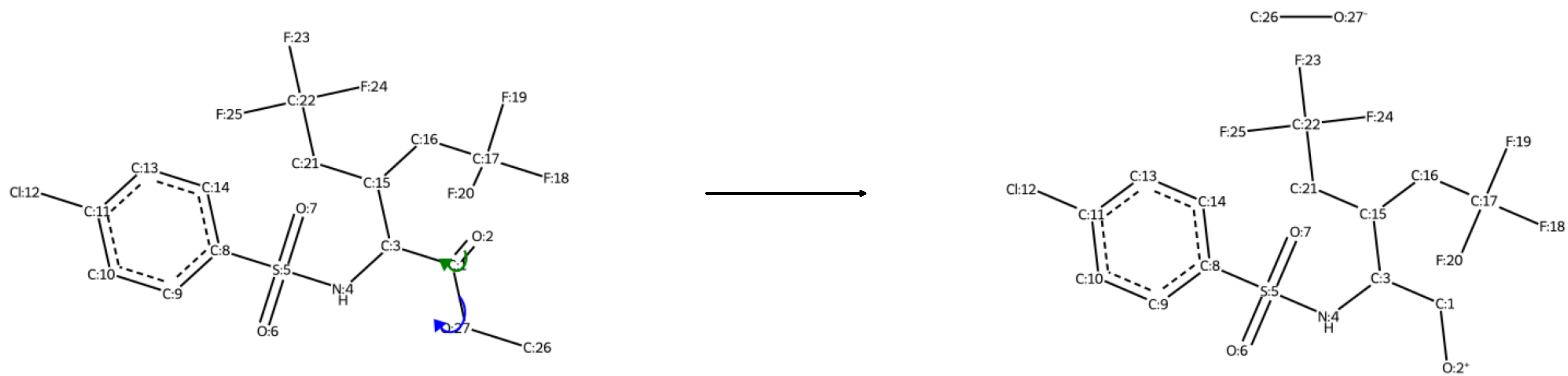


ELECTRO-generated mechanistic pathway

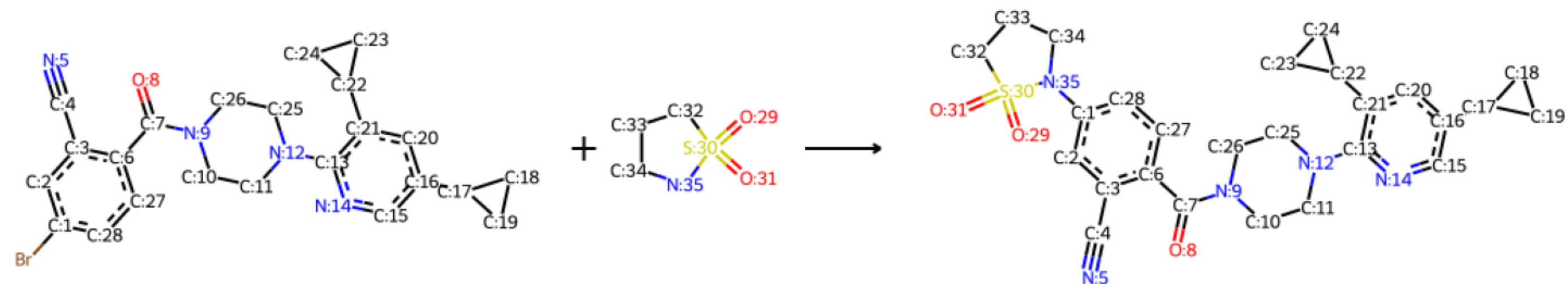
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:53

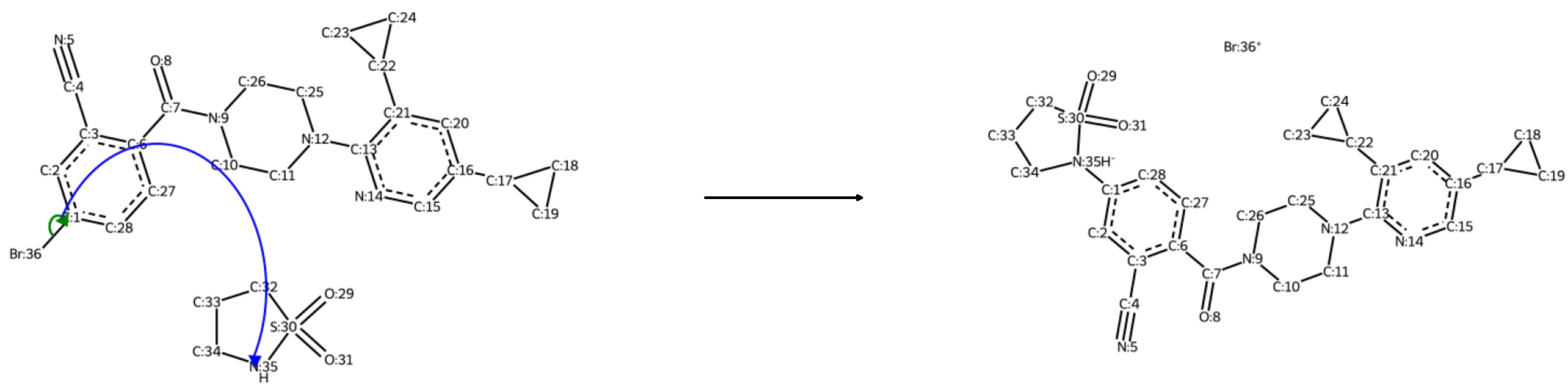


ELECTRO-generated mechanistic pathway

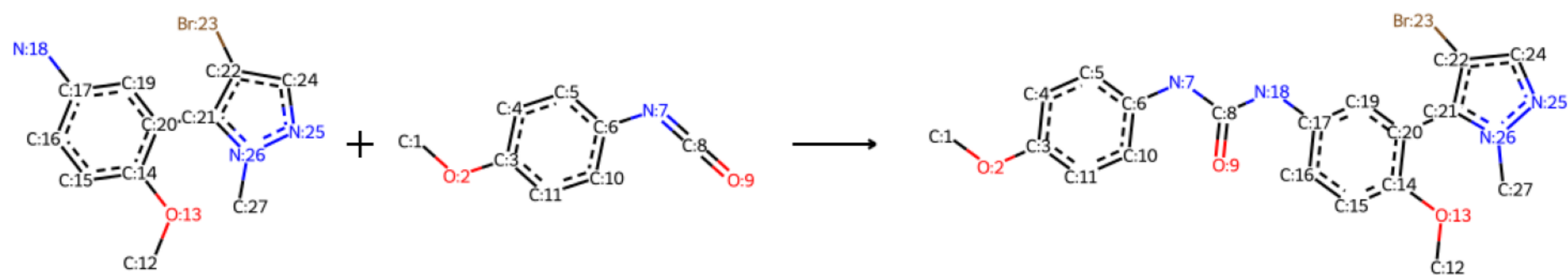
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



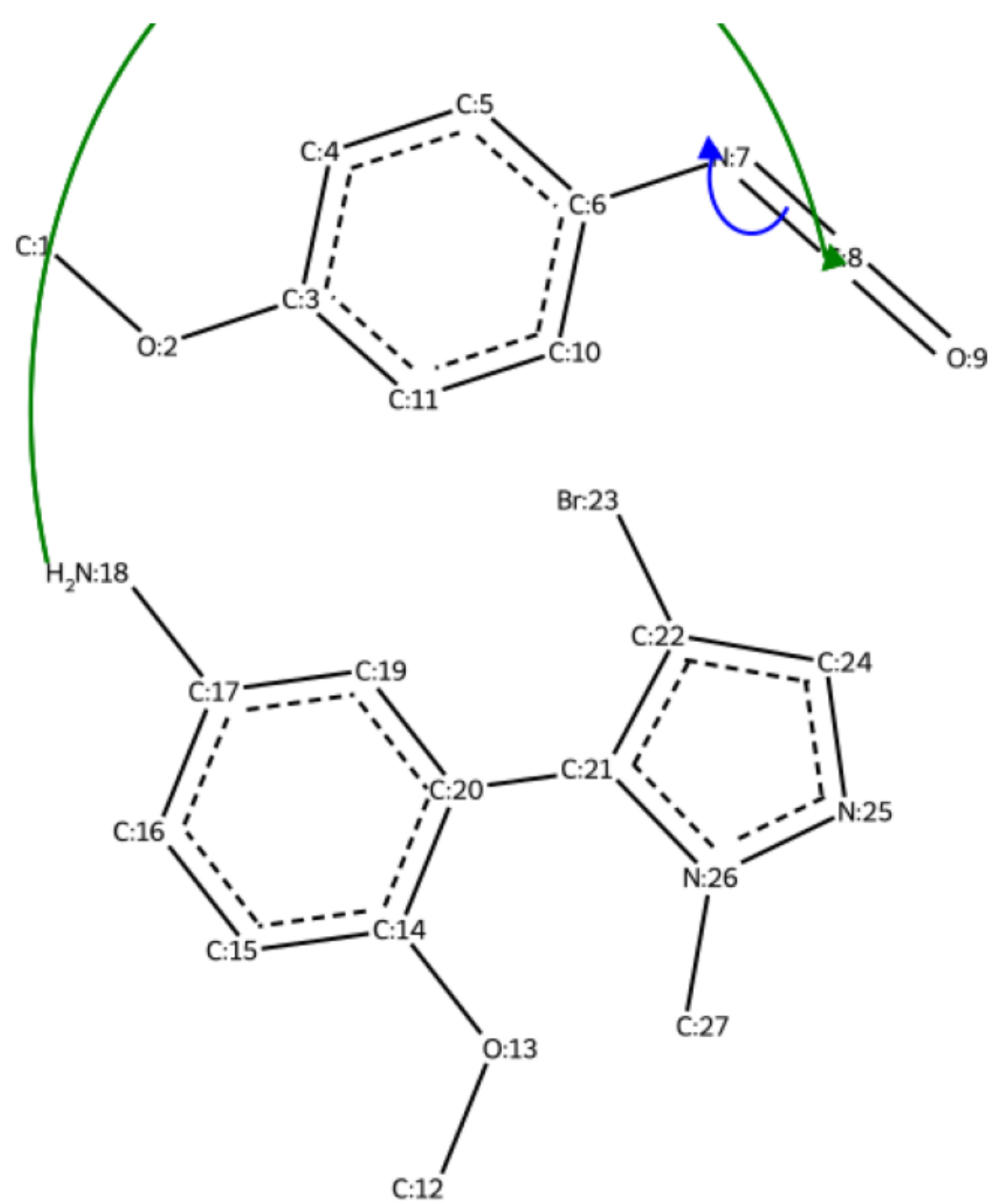
Original reaction RXN_ID:54



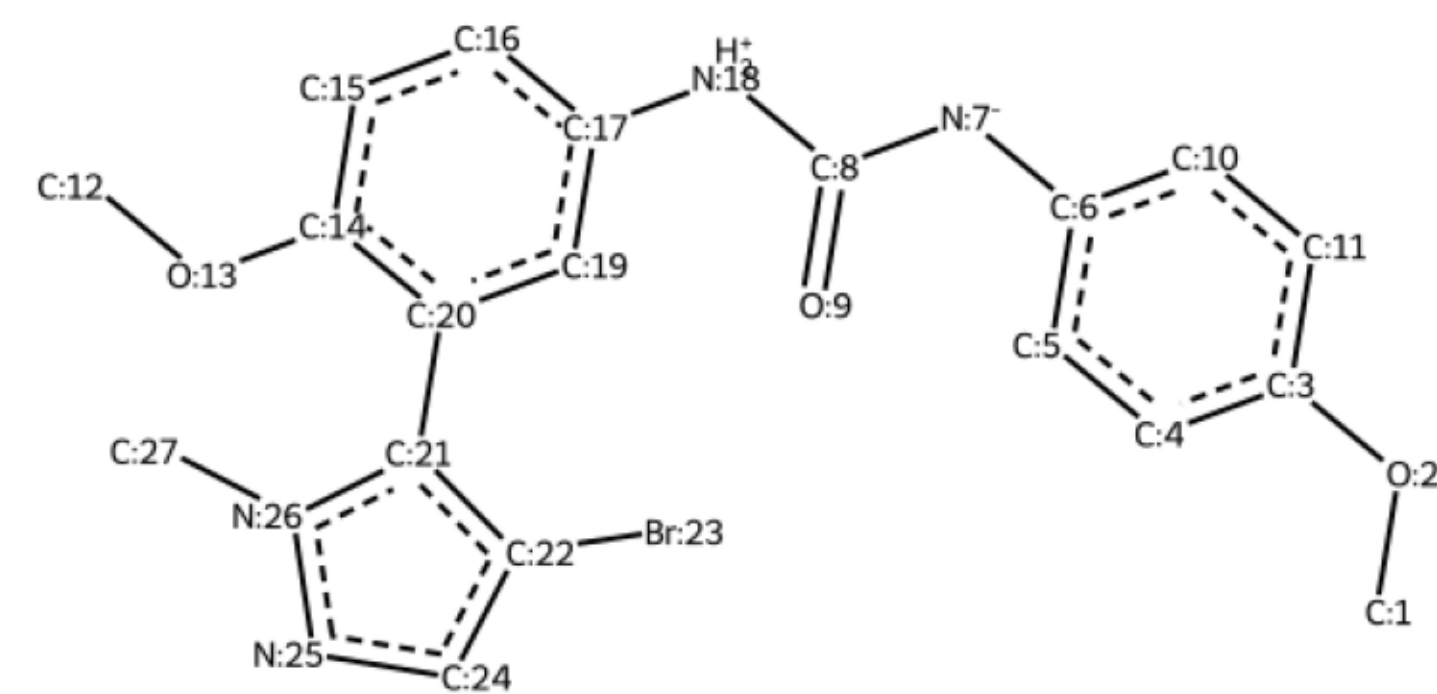
ELECTRO-generated mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1



Product(s)



Original reaction RXN_ID:55

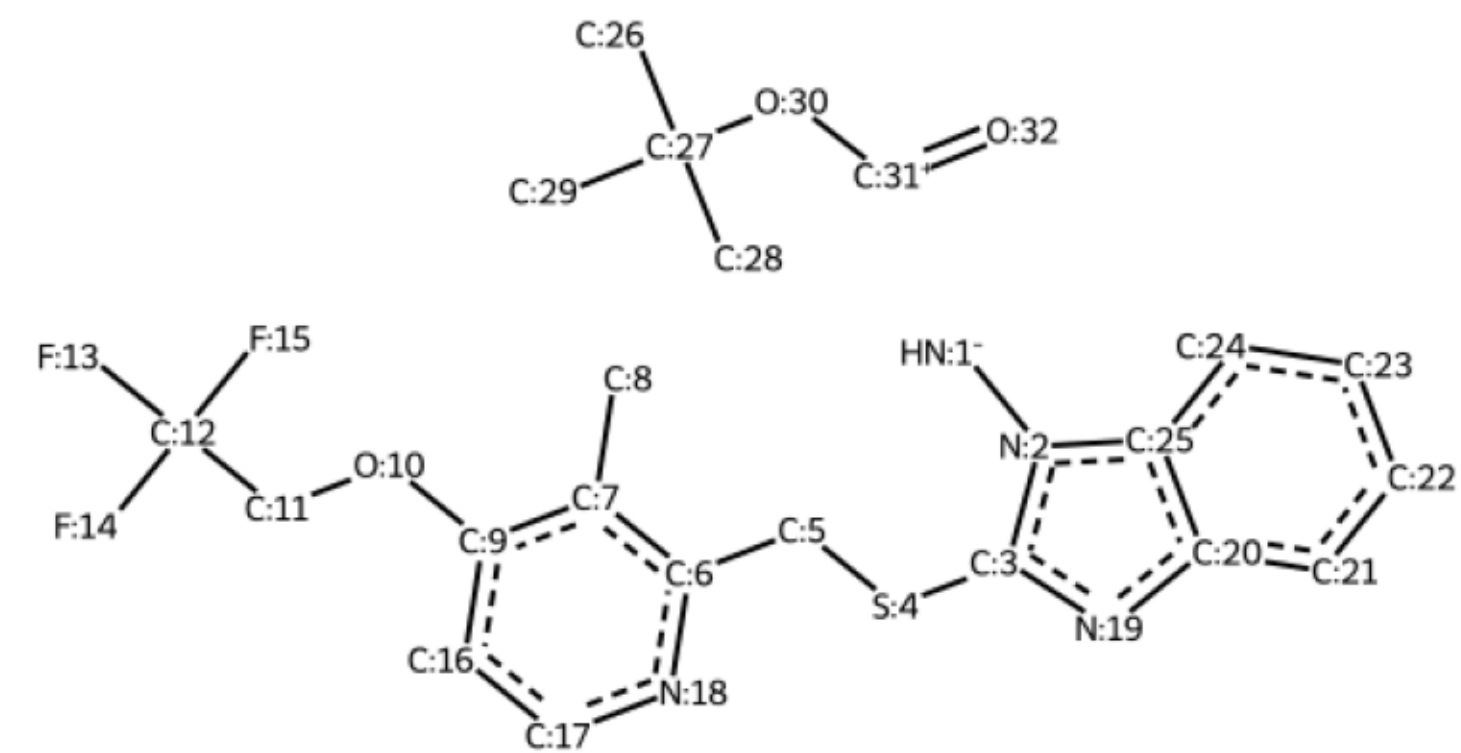
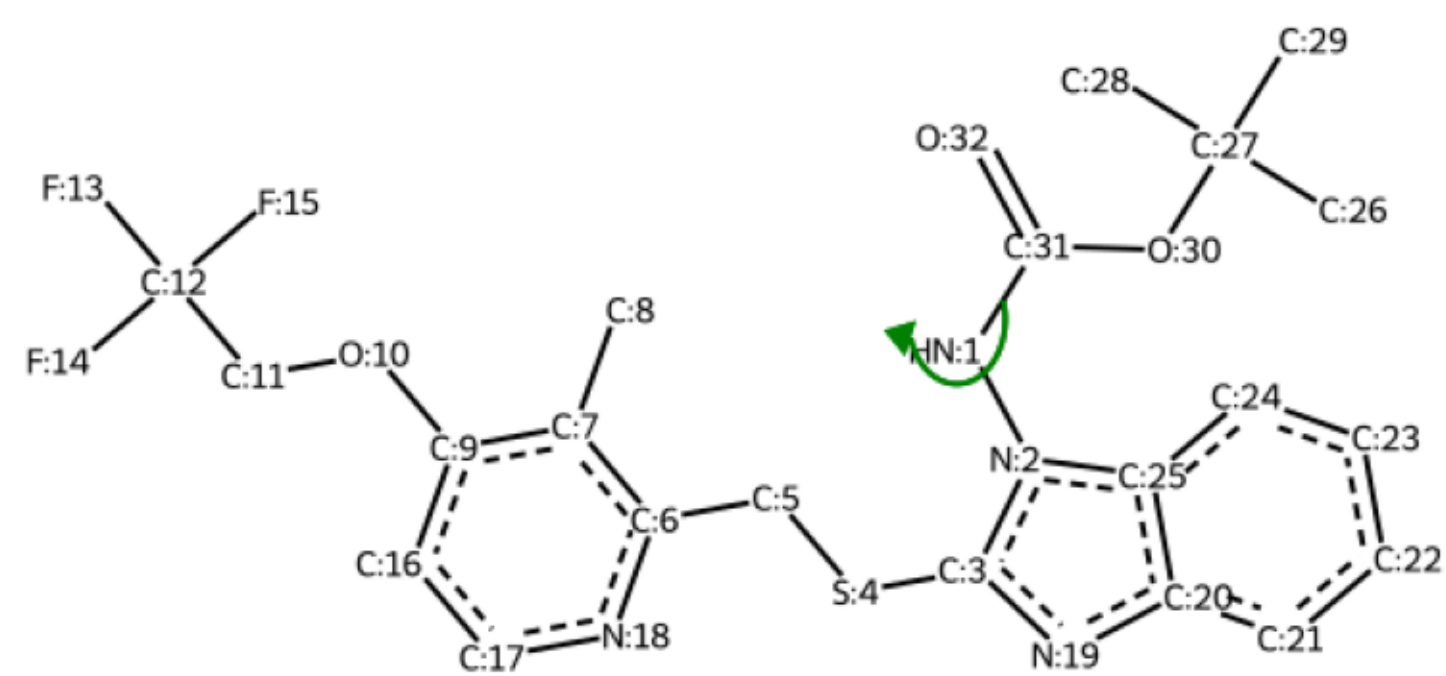


ELECTRO-generated mechanistic pathway

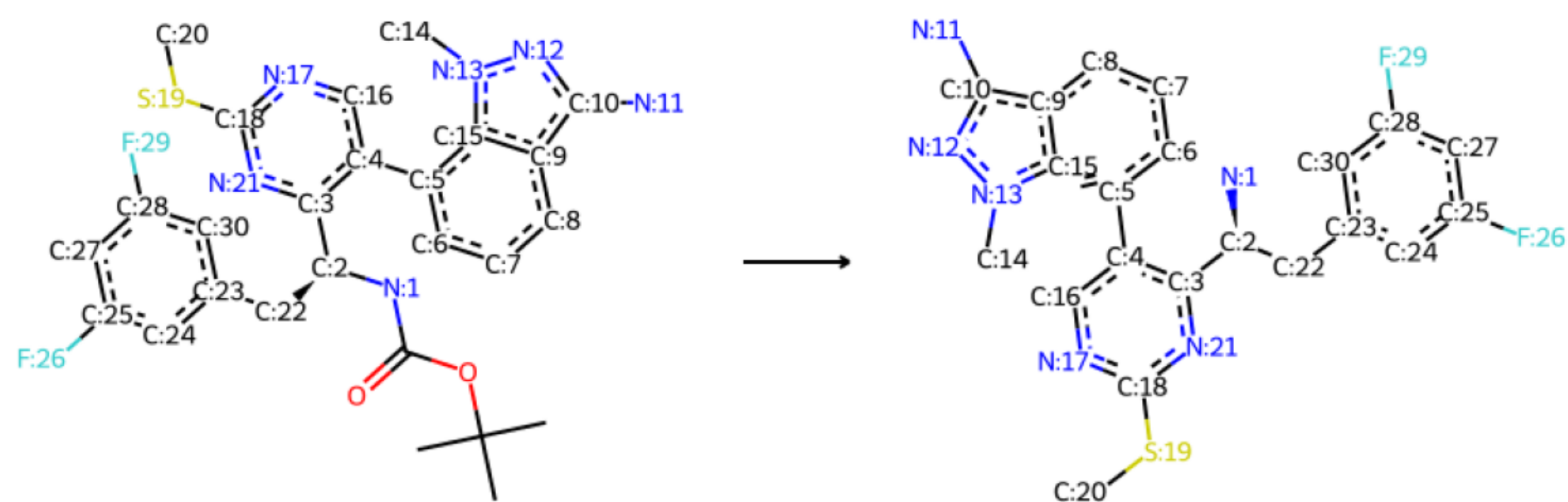
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:56

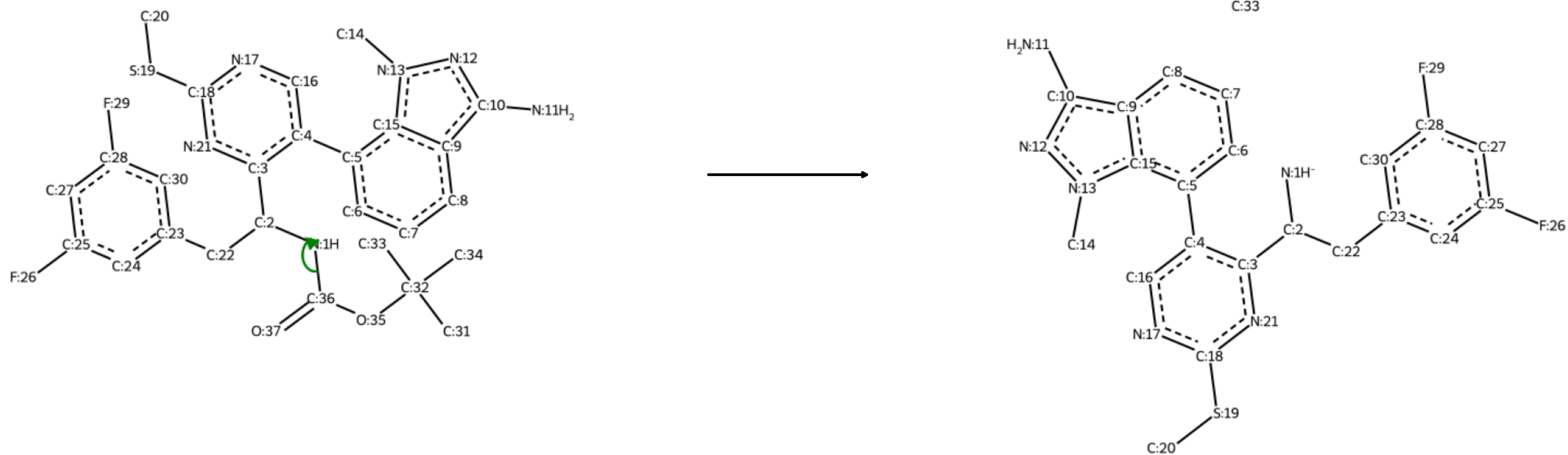


ELECTRO-generated mechanistic pathway

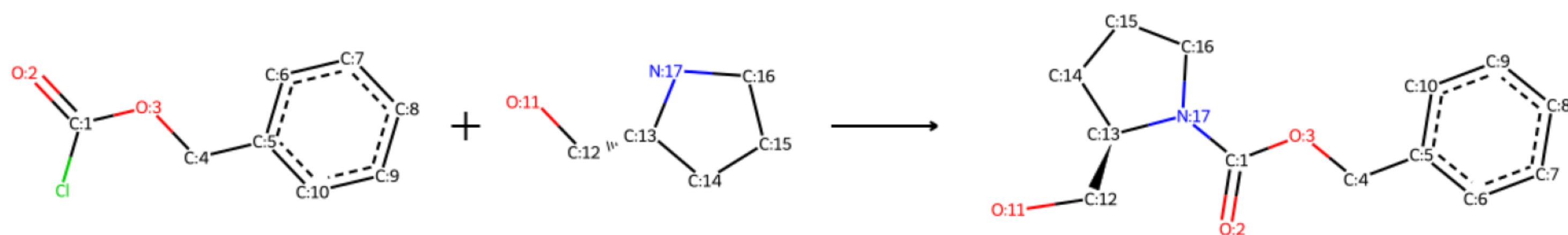
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:57

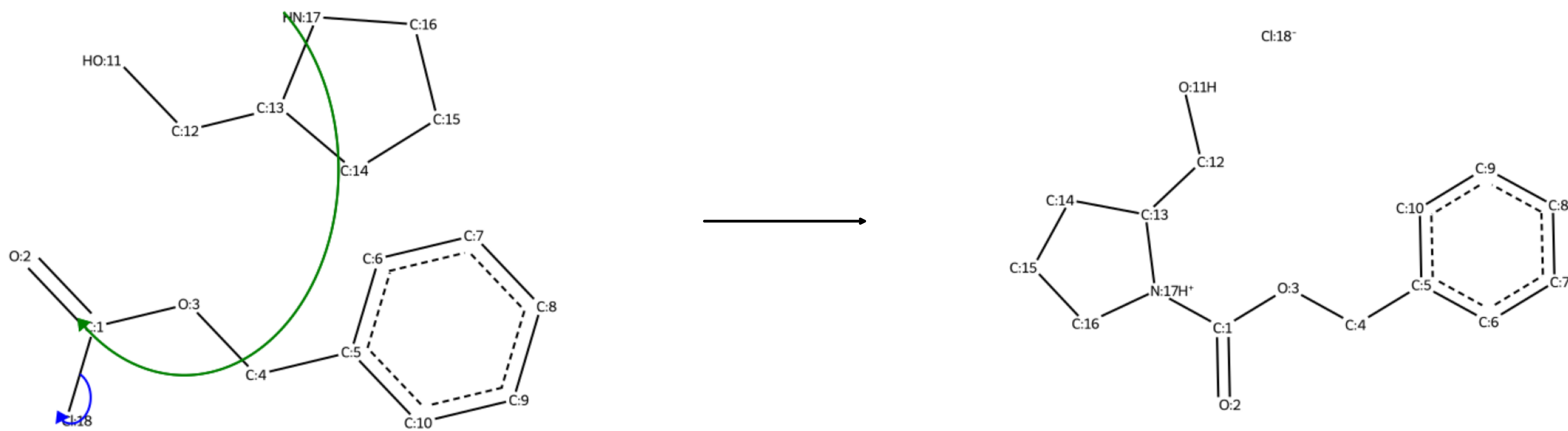


ELECTRO-generated mechanistic pathway

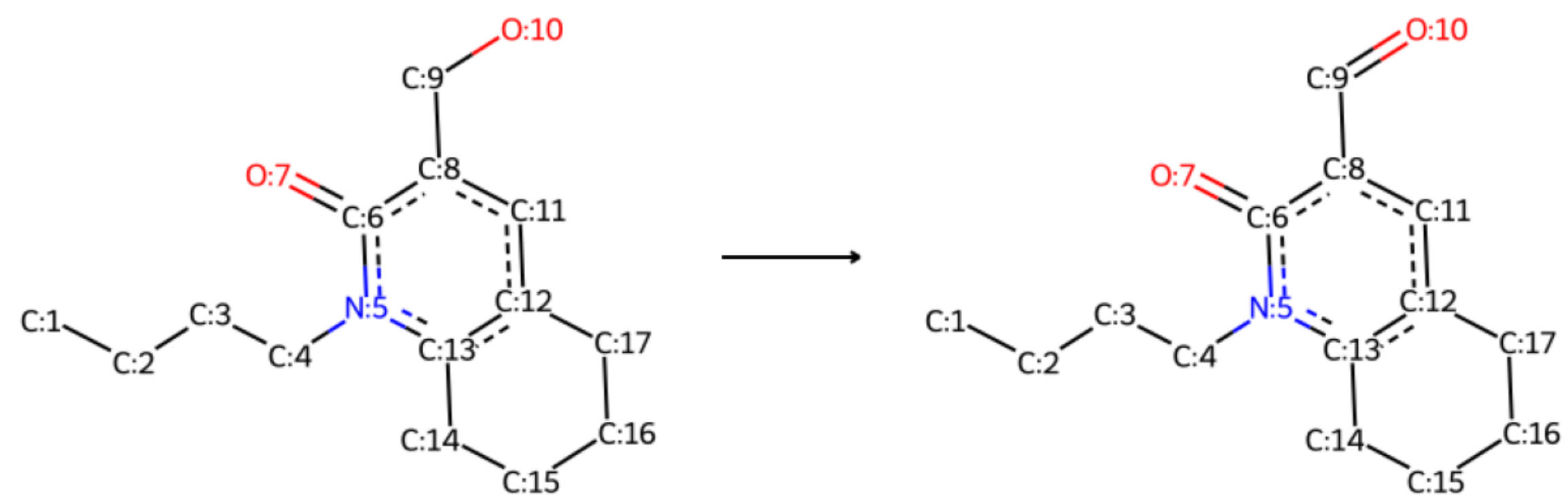
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:58

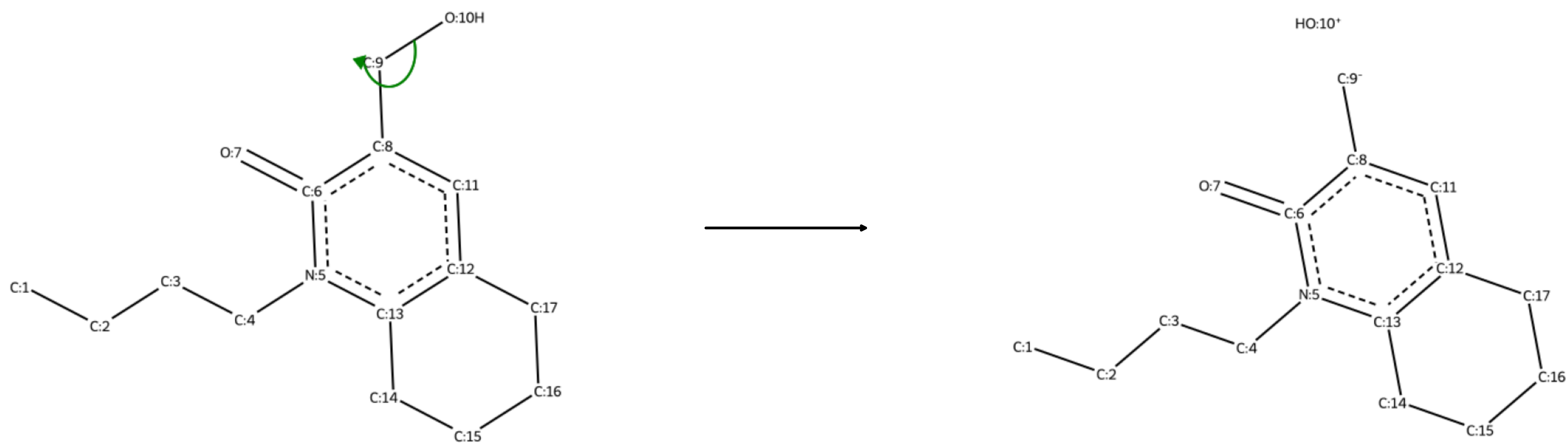


ELECTRO-generated mechanistic pathway

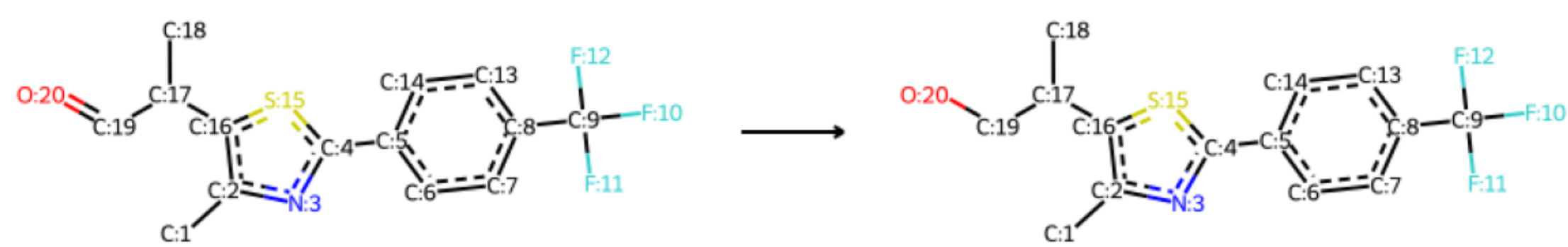
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:59

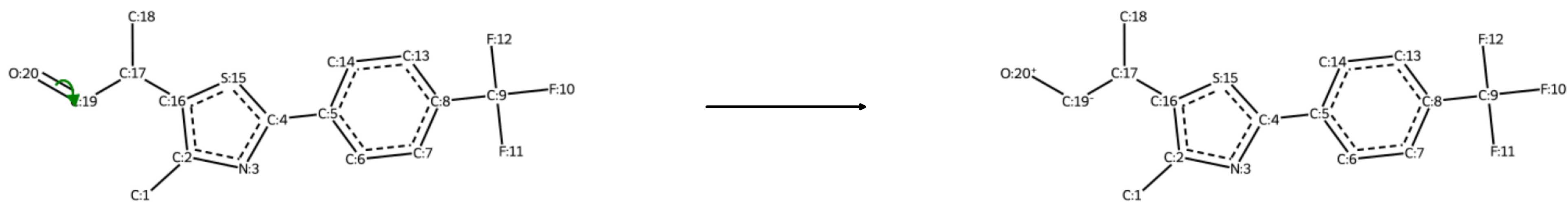


ELECTRO-generated mechanistic pathway

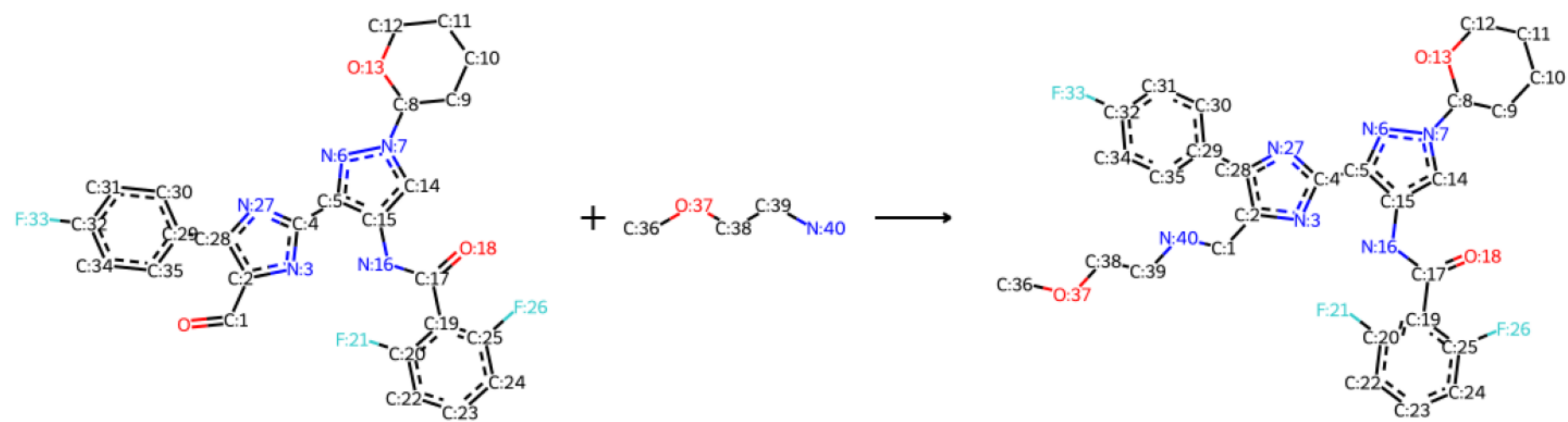
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:60

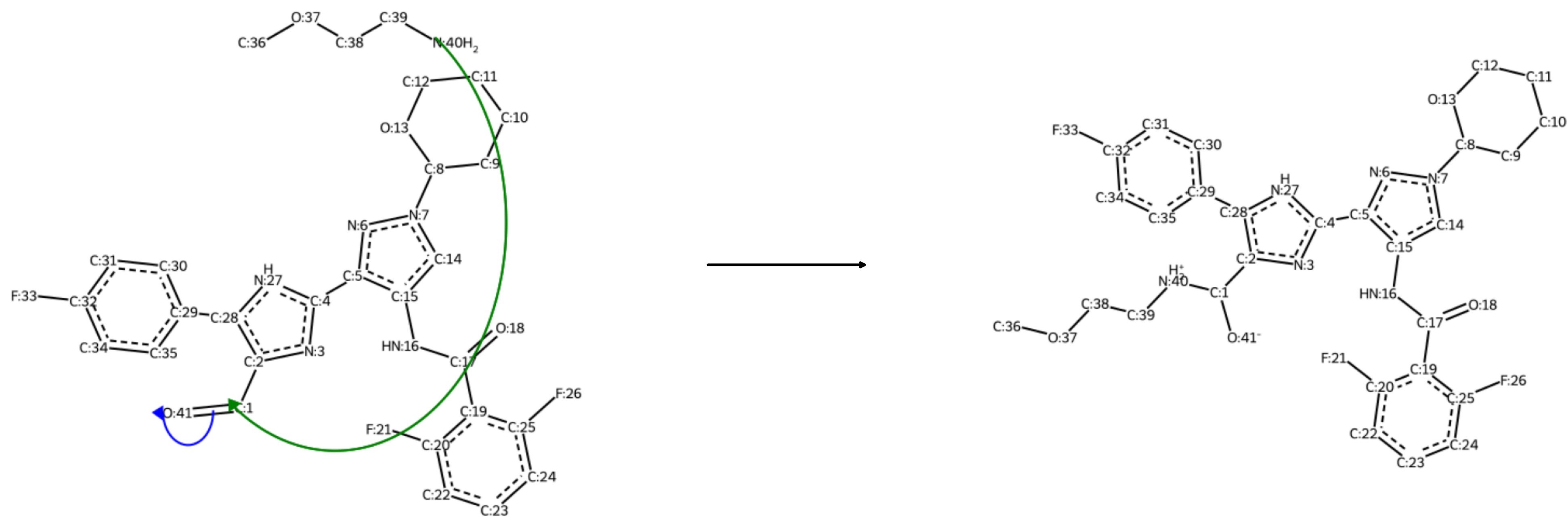


ELECTRO-generated mechanistic pathway

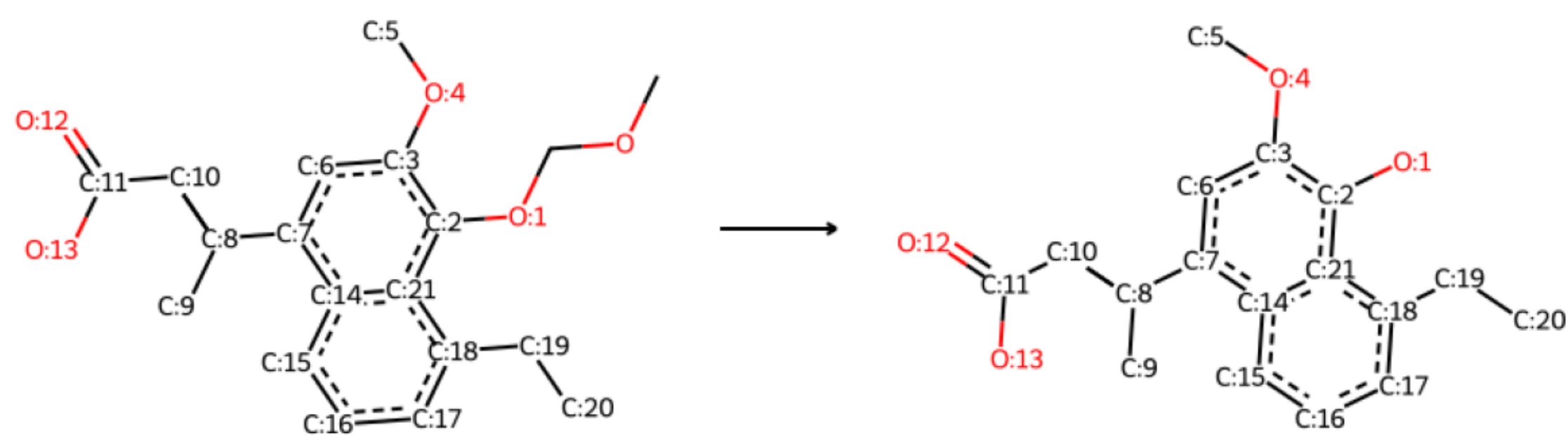
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:61

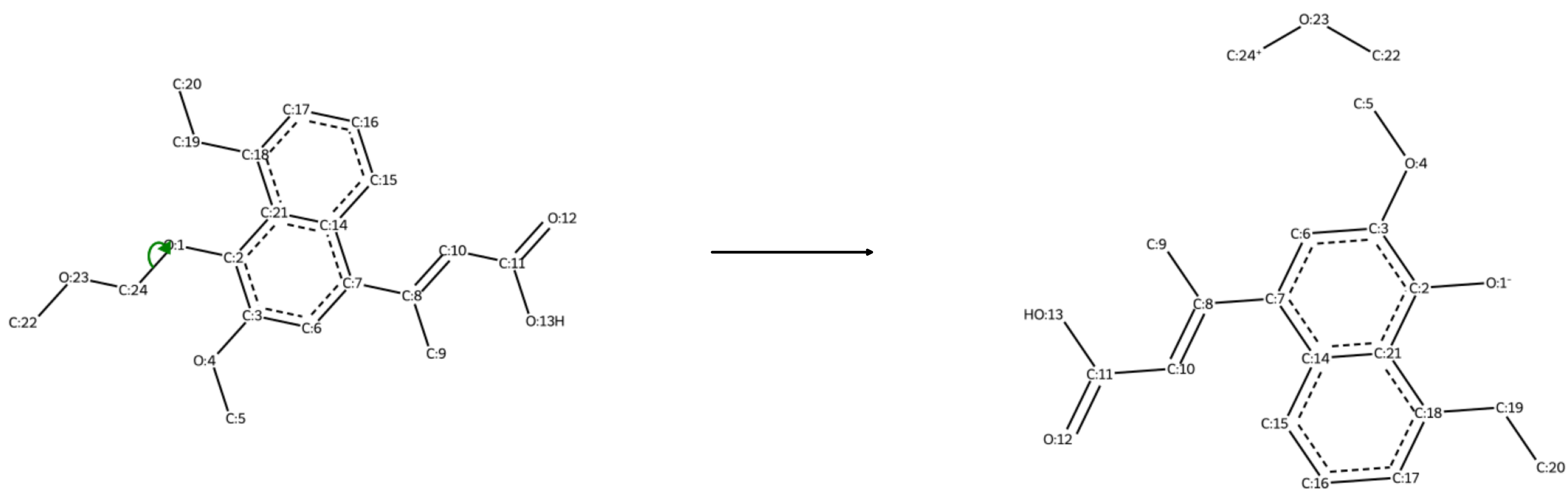


ELECTRO-generated mechanistic pathway

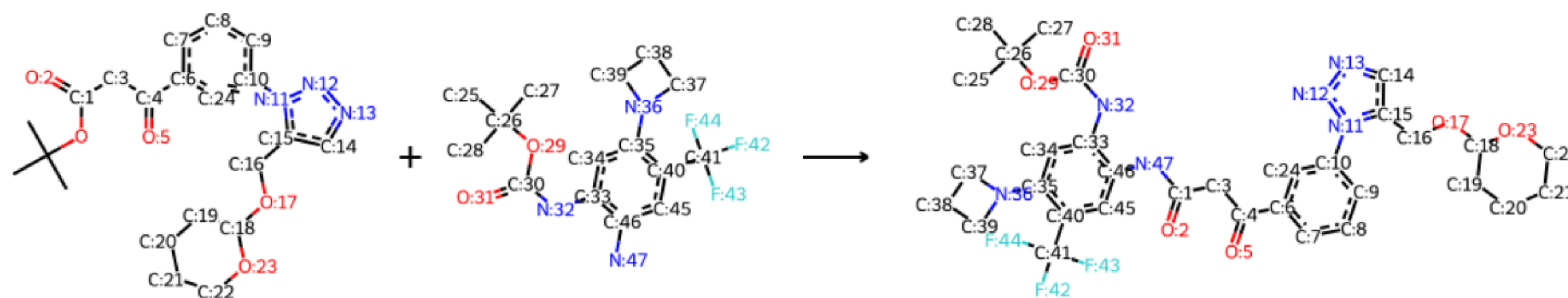
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:62

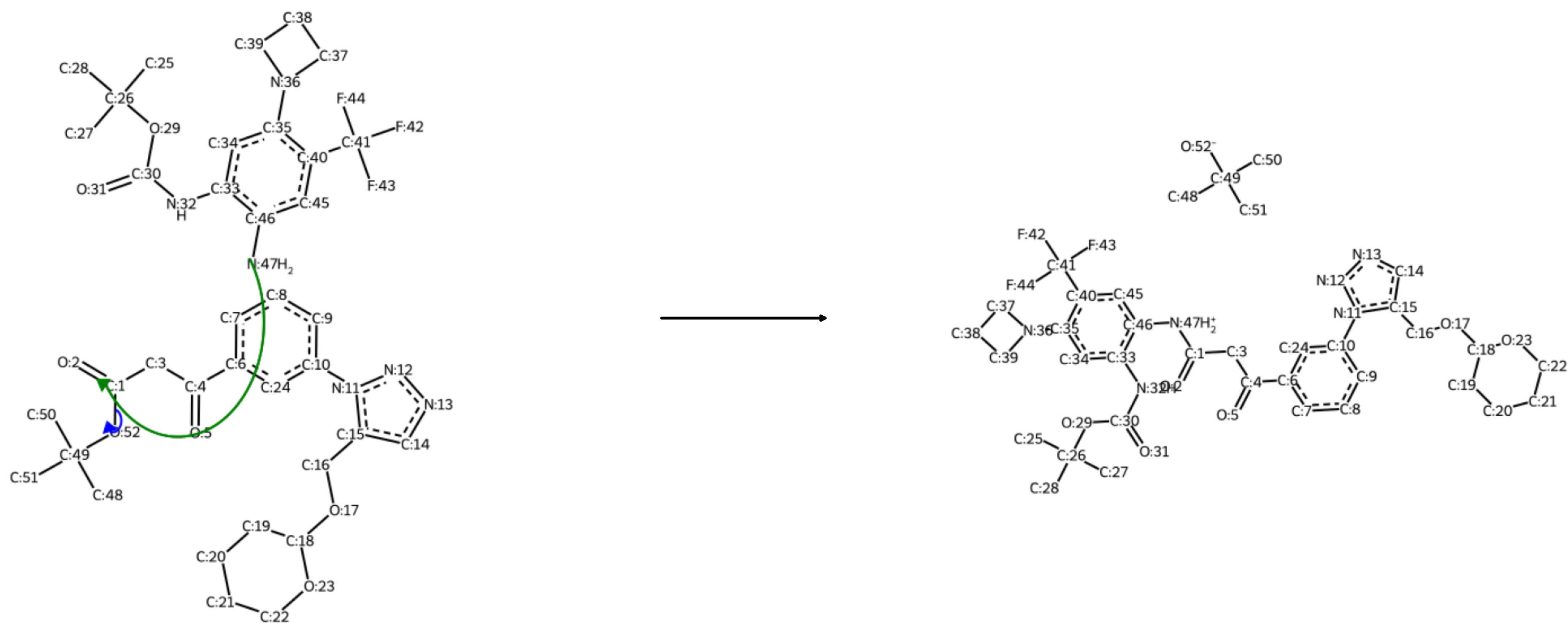


ELECTRO-generated mechanistic pathway

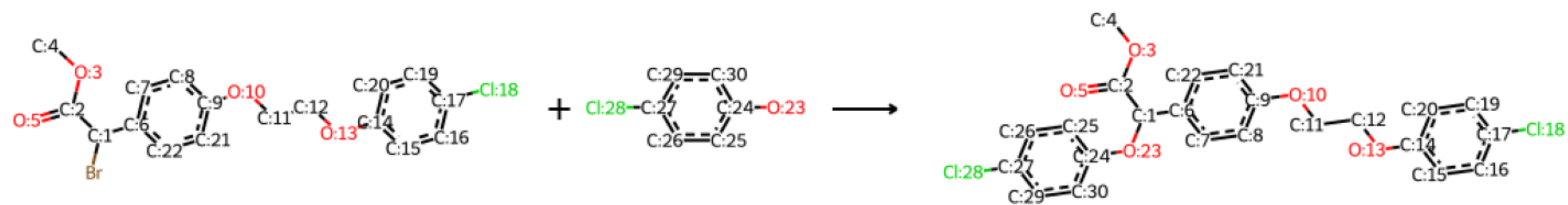
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:63

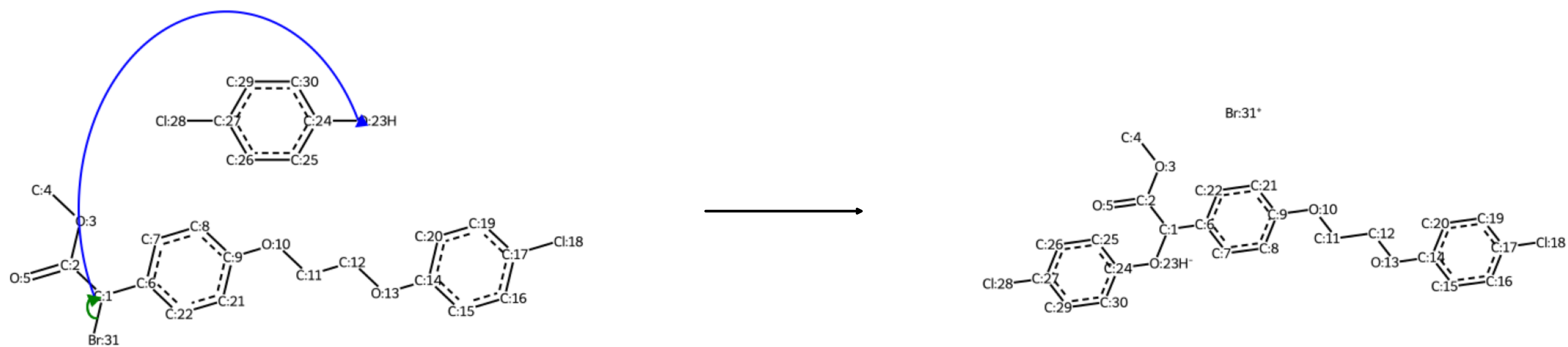


ELECTRO-generated mechanistic pathway

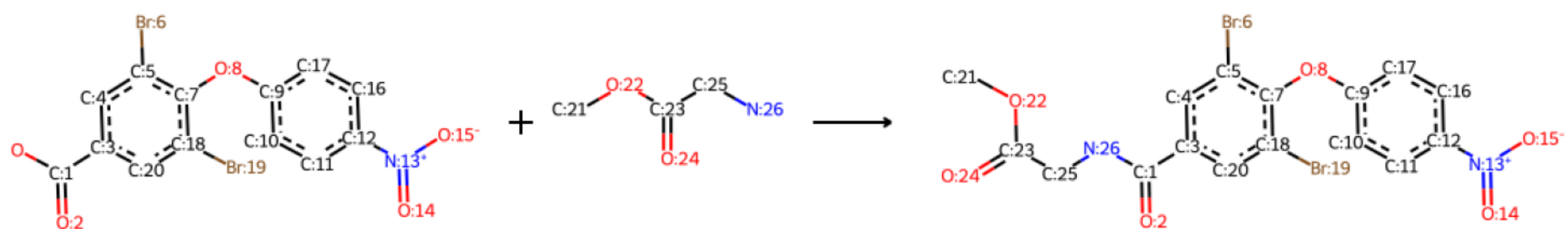
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:64

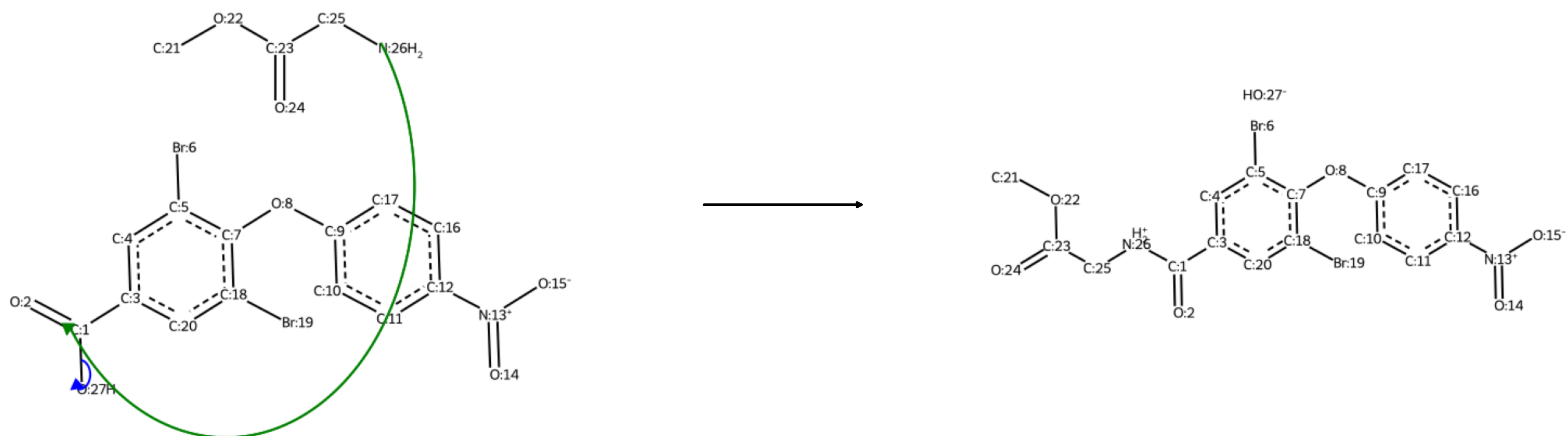


ELECTRO-generated mechanistic pathway

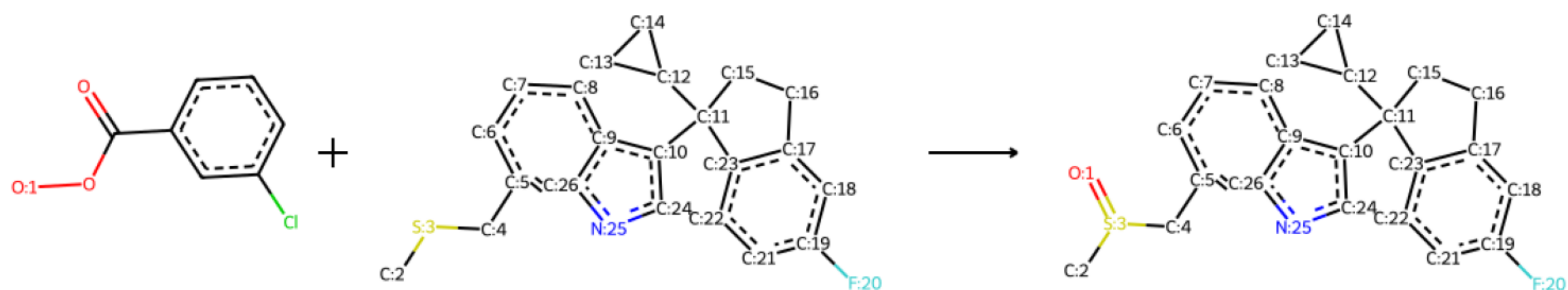
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:65

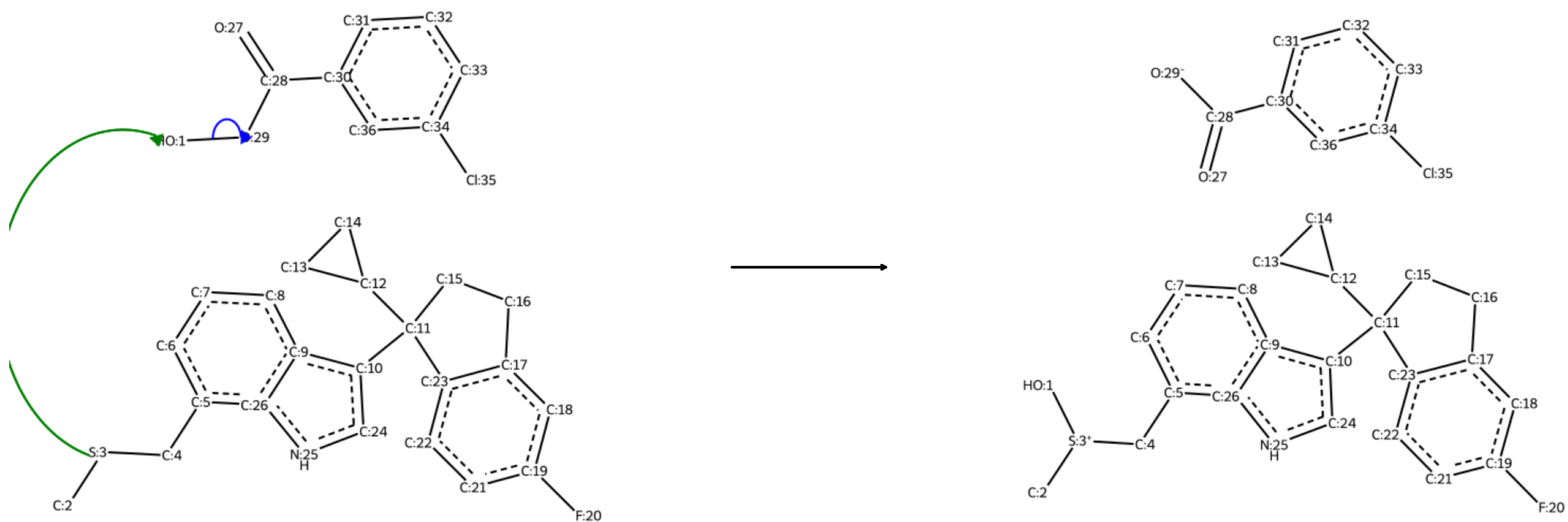


ELECTRO-generated mechanistic pathway

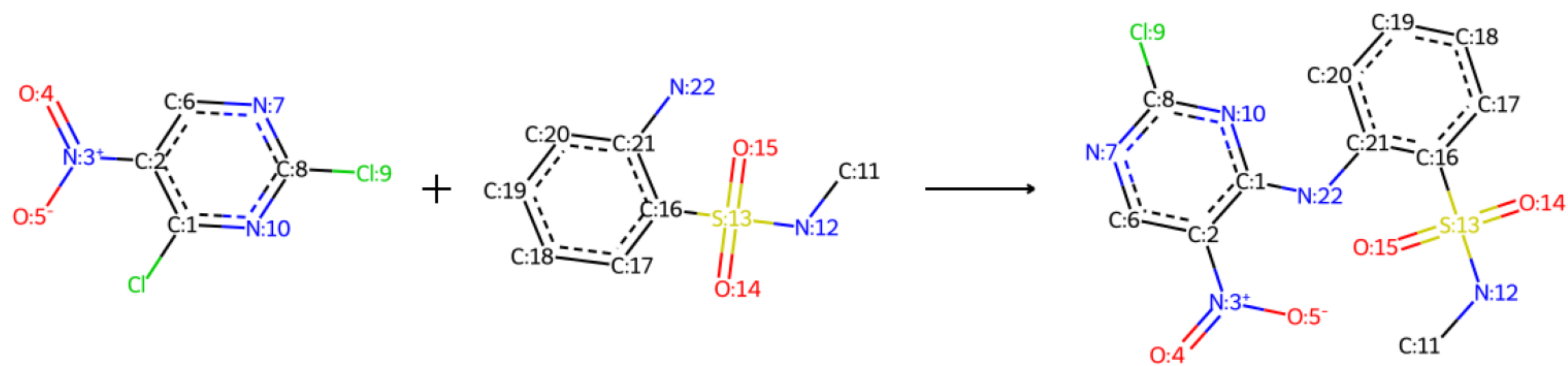
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:66

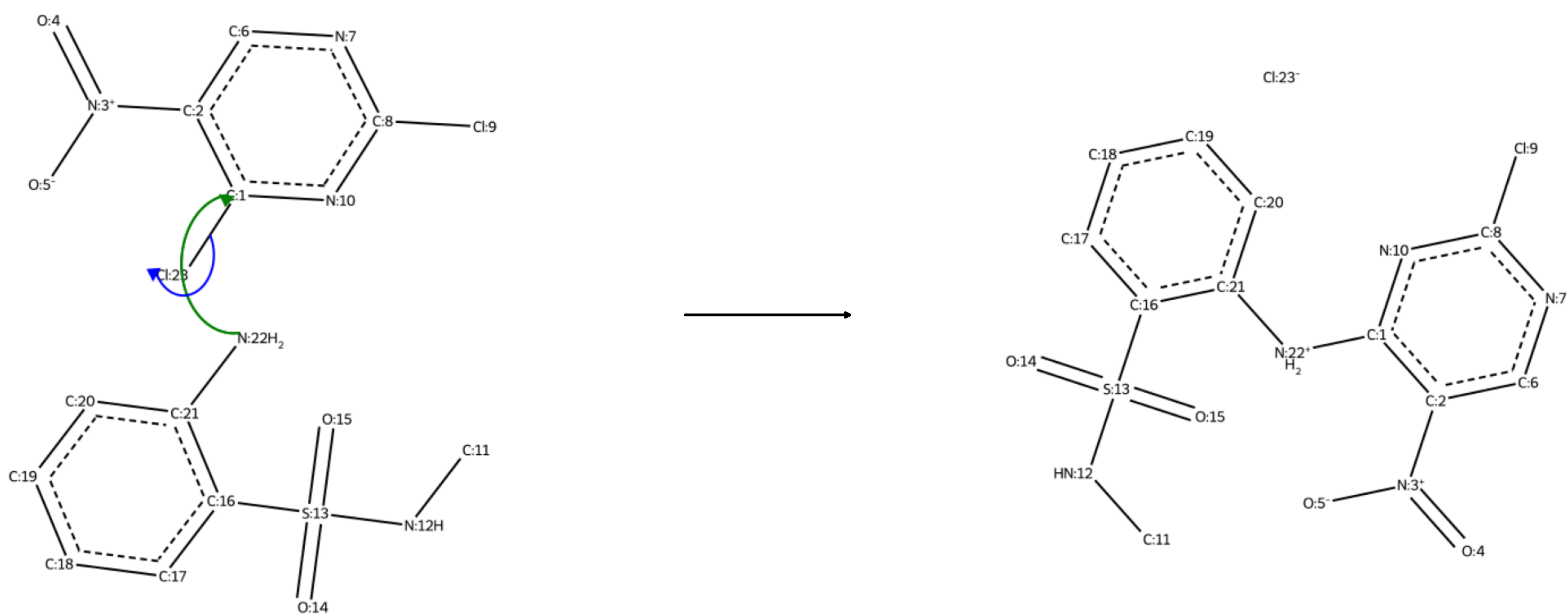


ELECTRO-generated mechanistic pathway

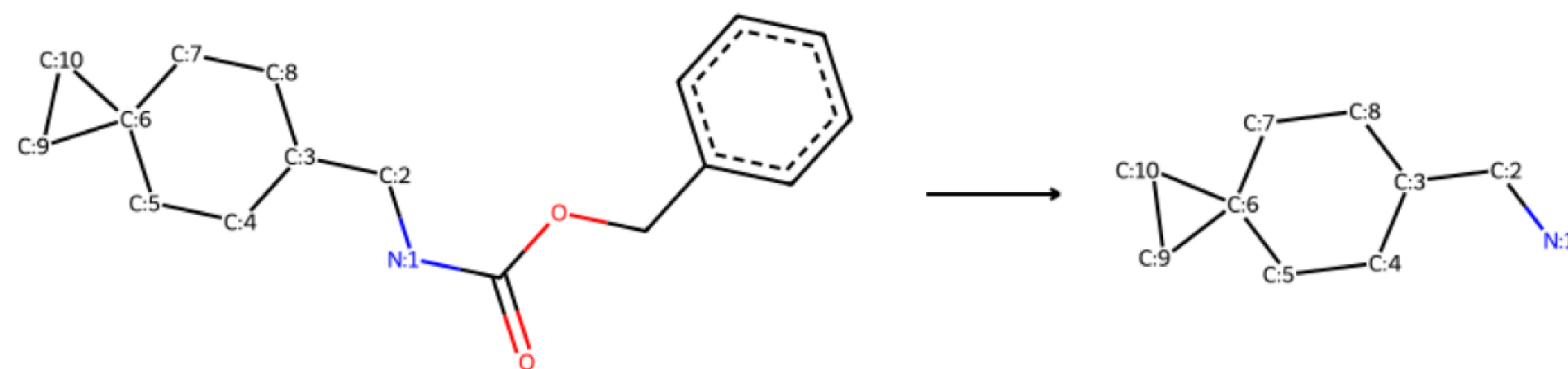
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:67

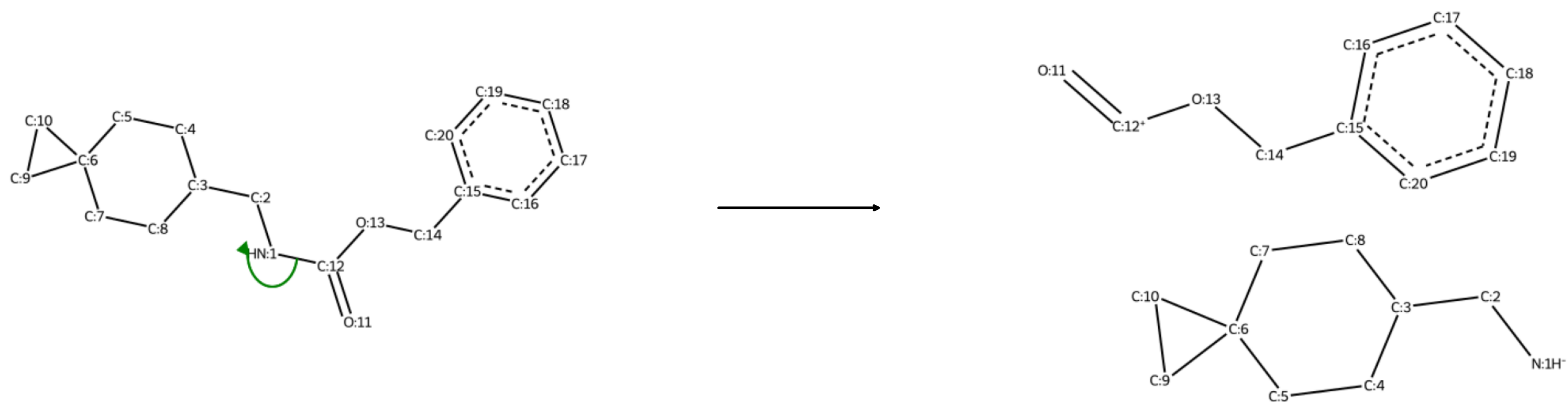


ELECTRO-generated mechanistic pathway

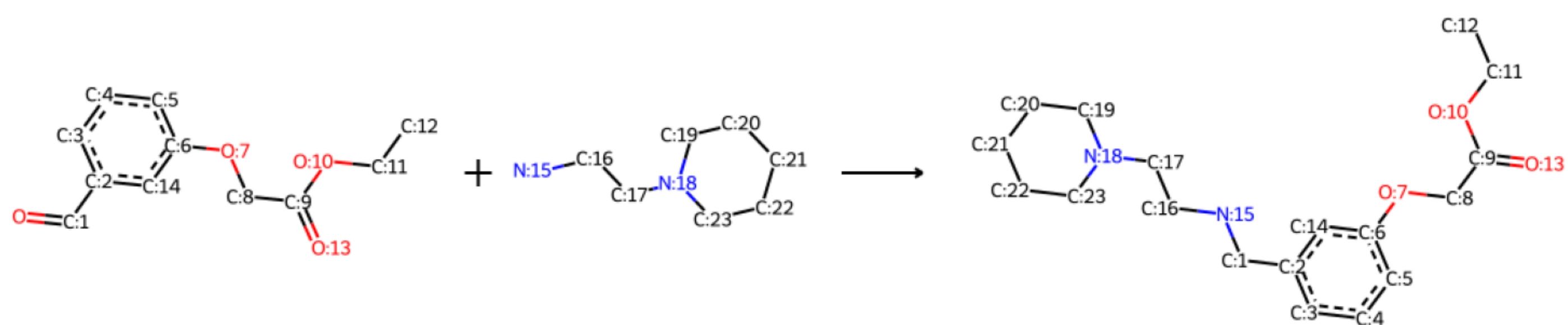
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:68

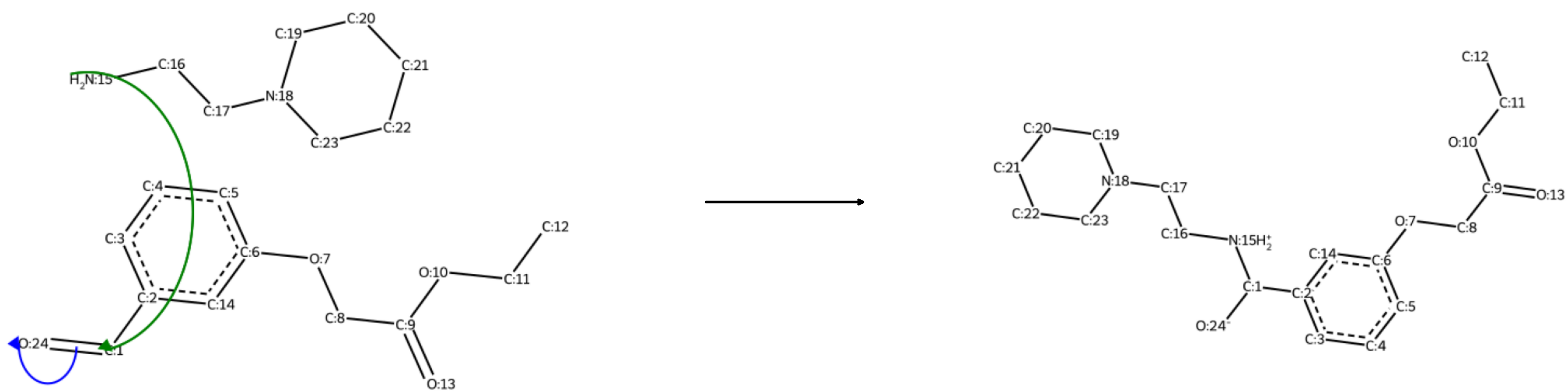


ELECTRO-generated mechanistic pathway

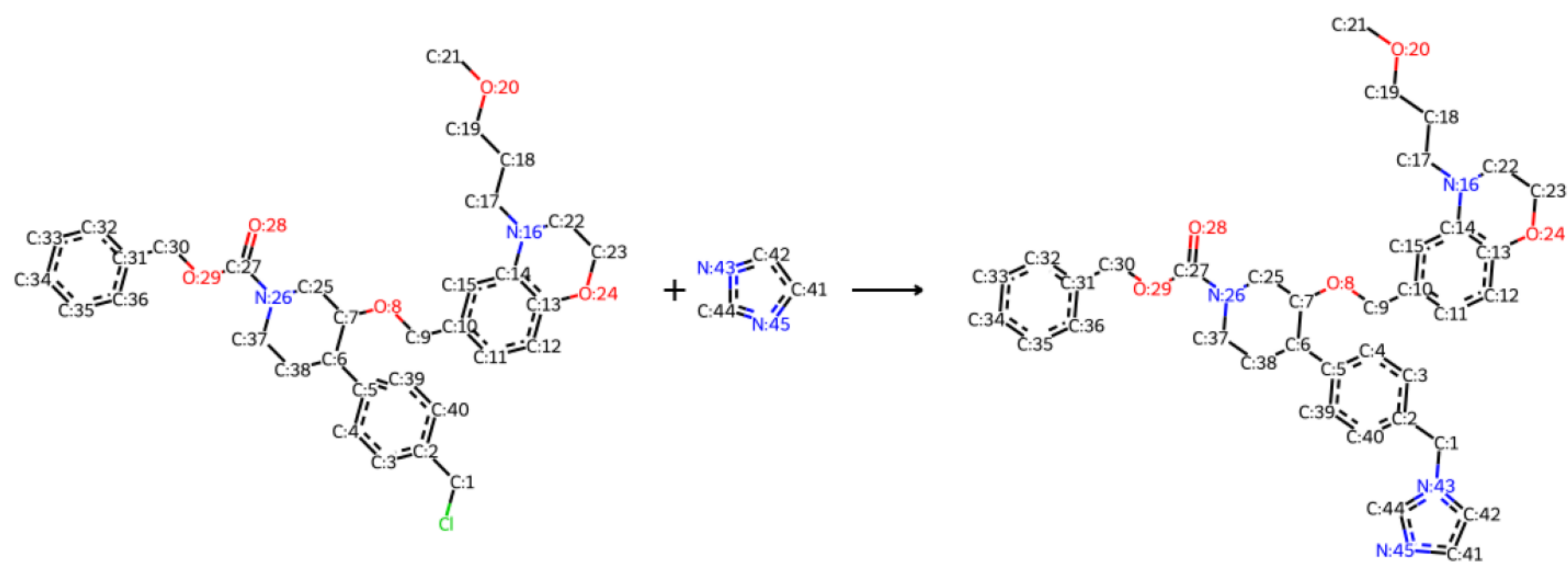
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



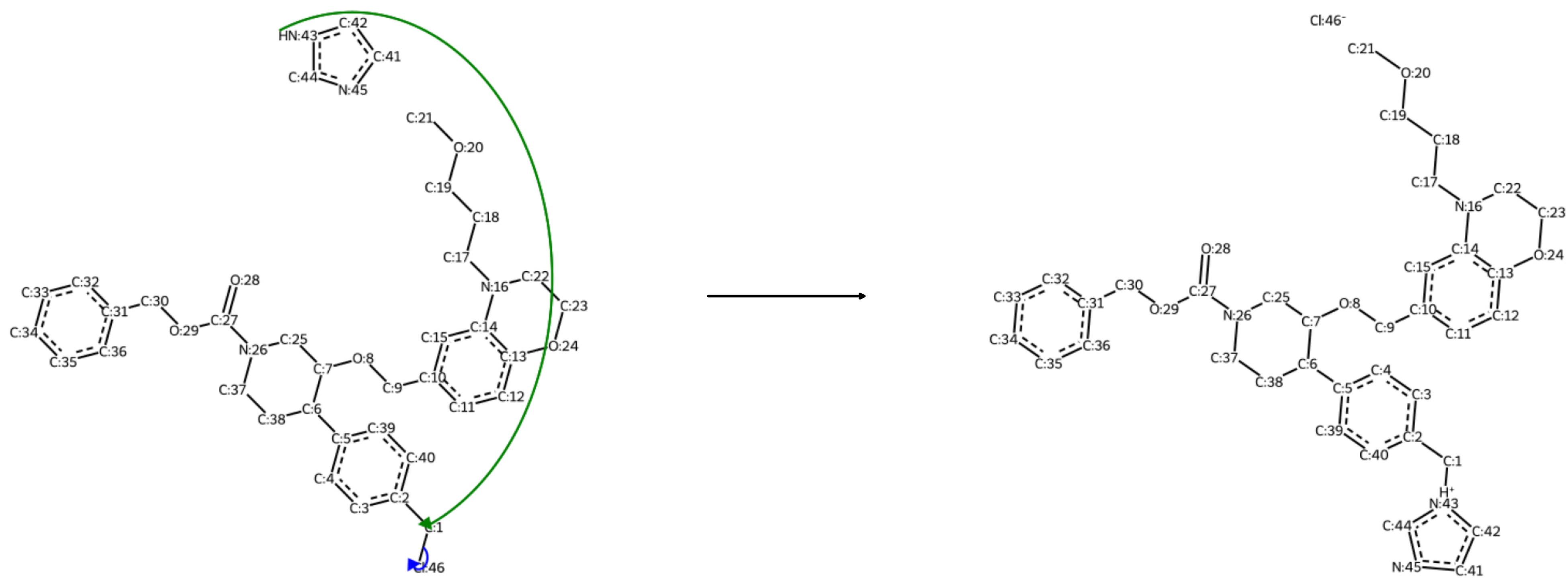
Original reaction RXN_ID:69



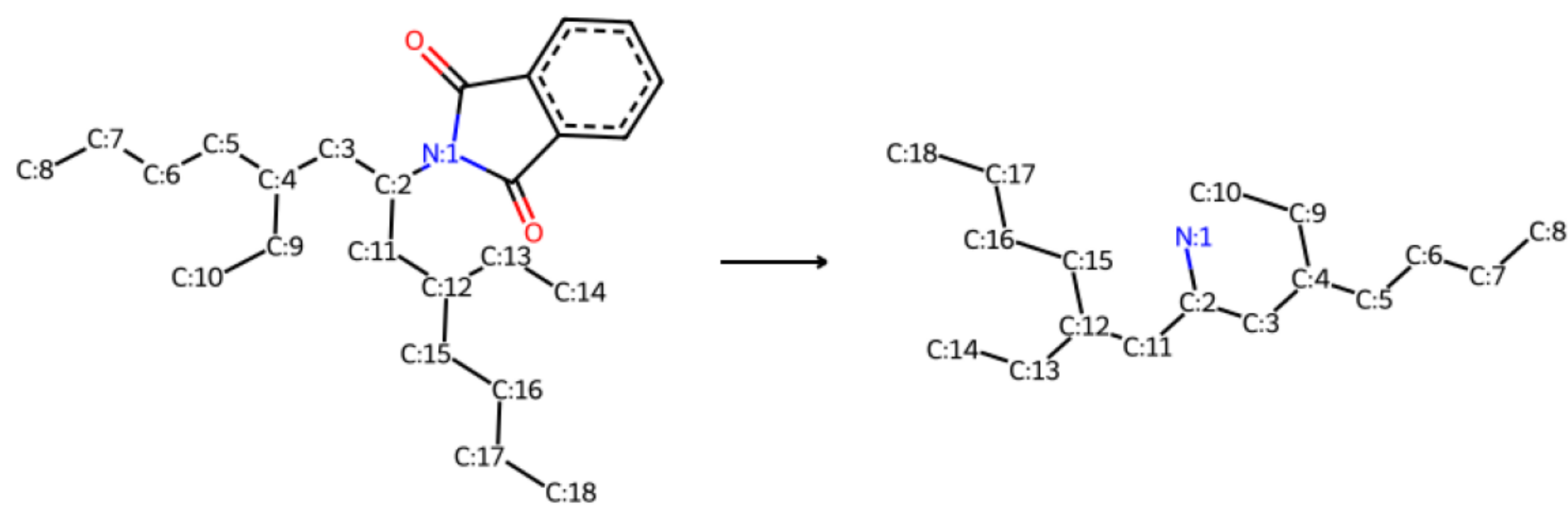
ELECTRO-generated mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1



Original reaction RXN_ID:70

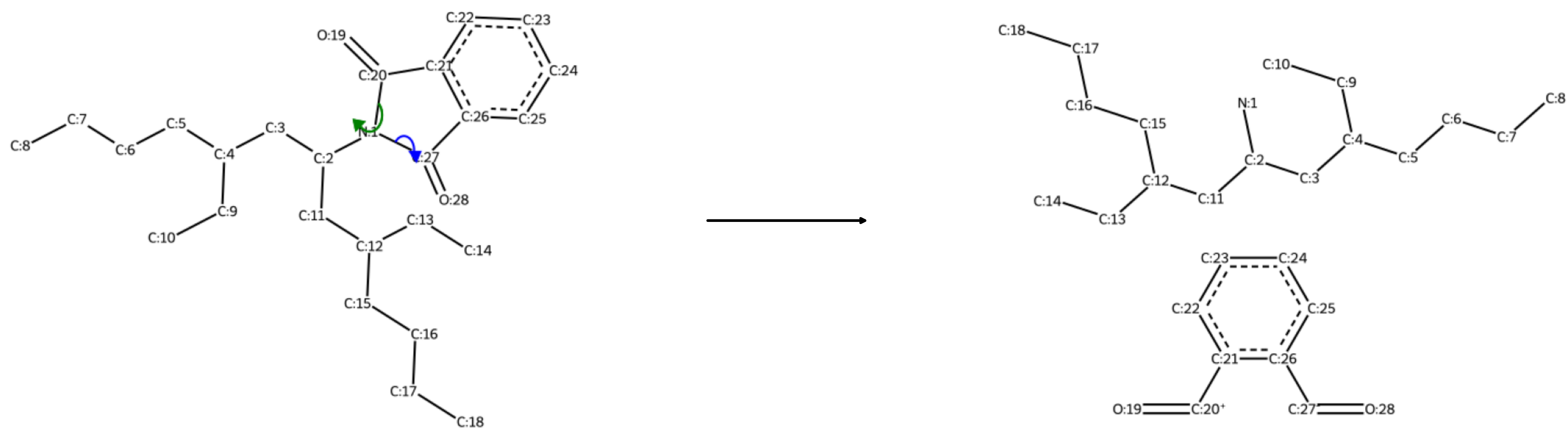


ELECTRO-generated mechanistic pathway

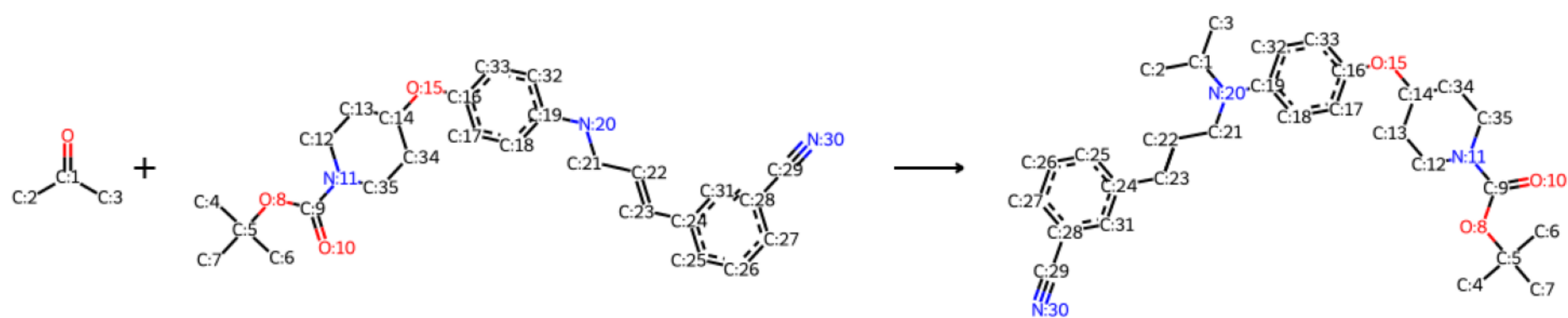
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:71

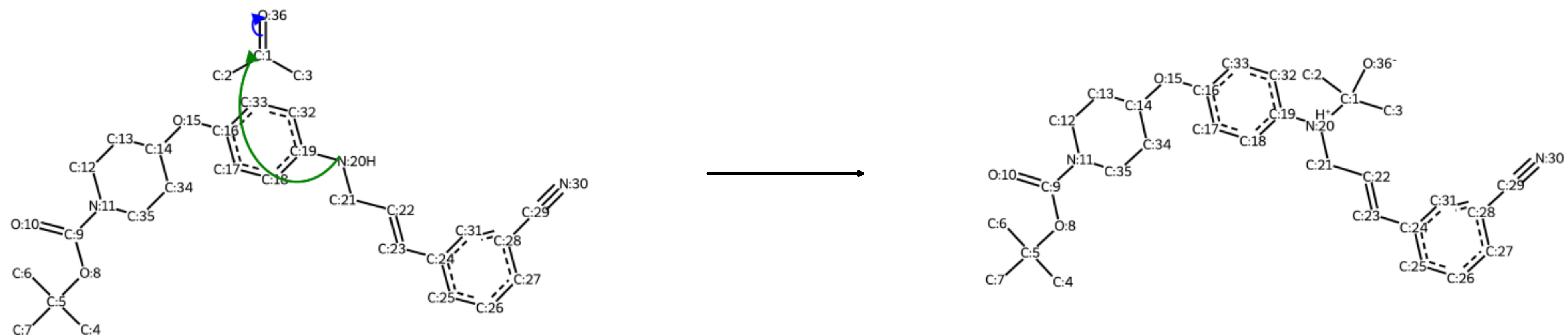


ELECTRO-generated mechanistic pathway

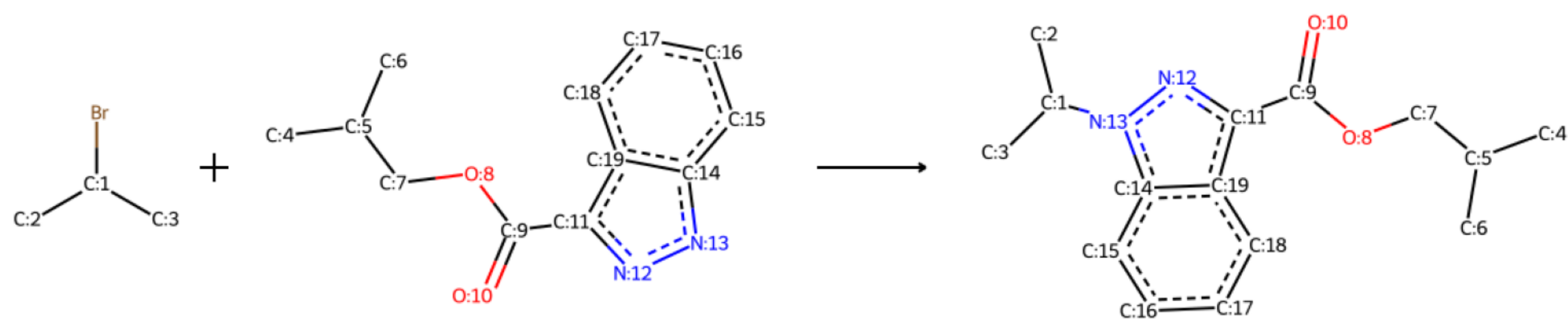
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:72

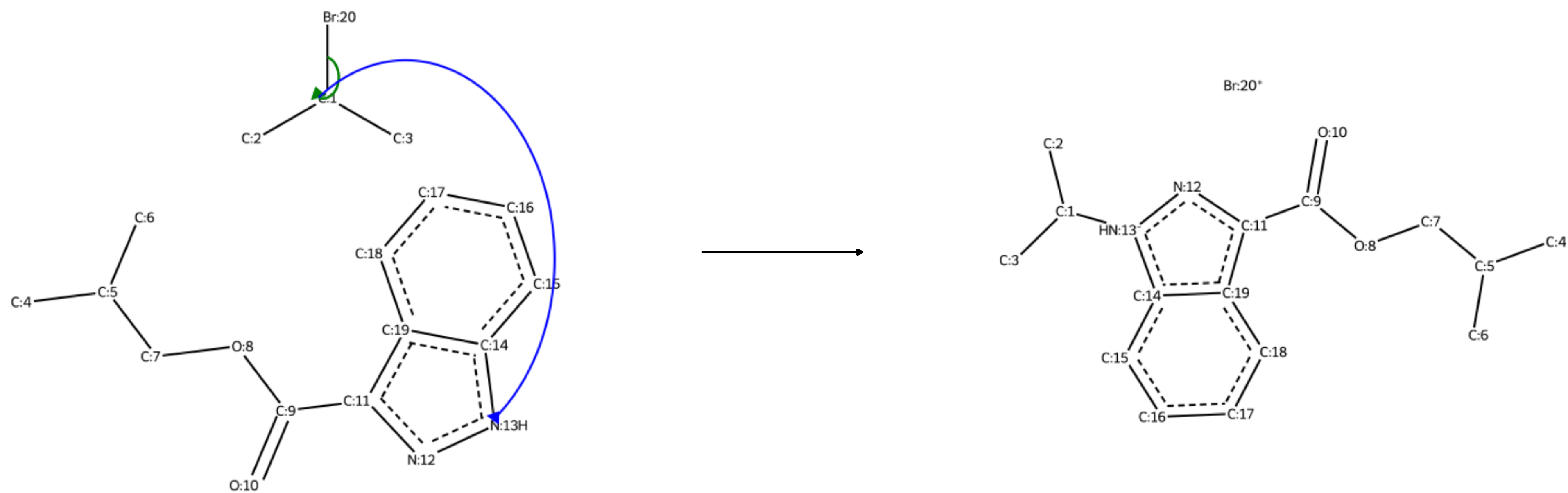


ELECTRO-generated mechanistic pathway

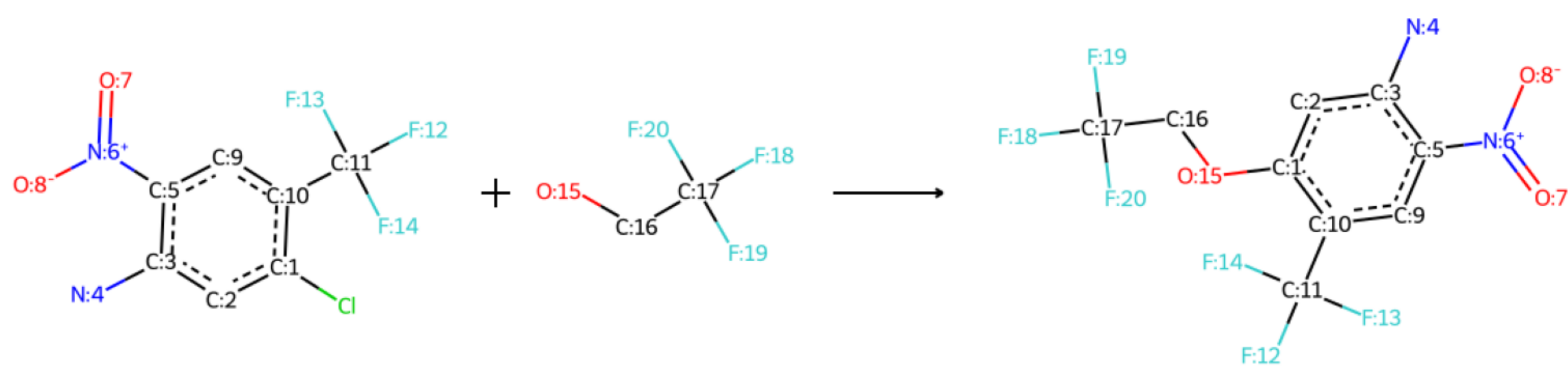
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:73

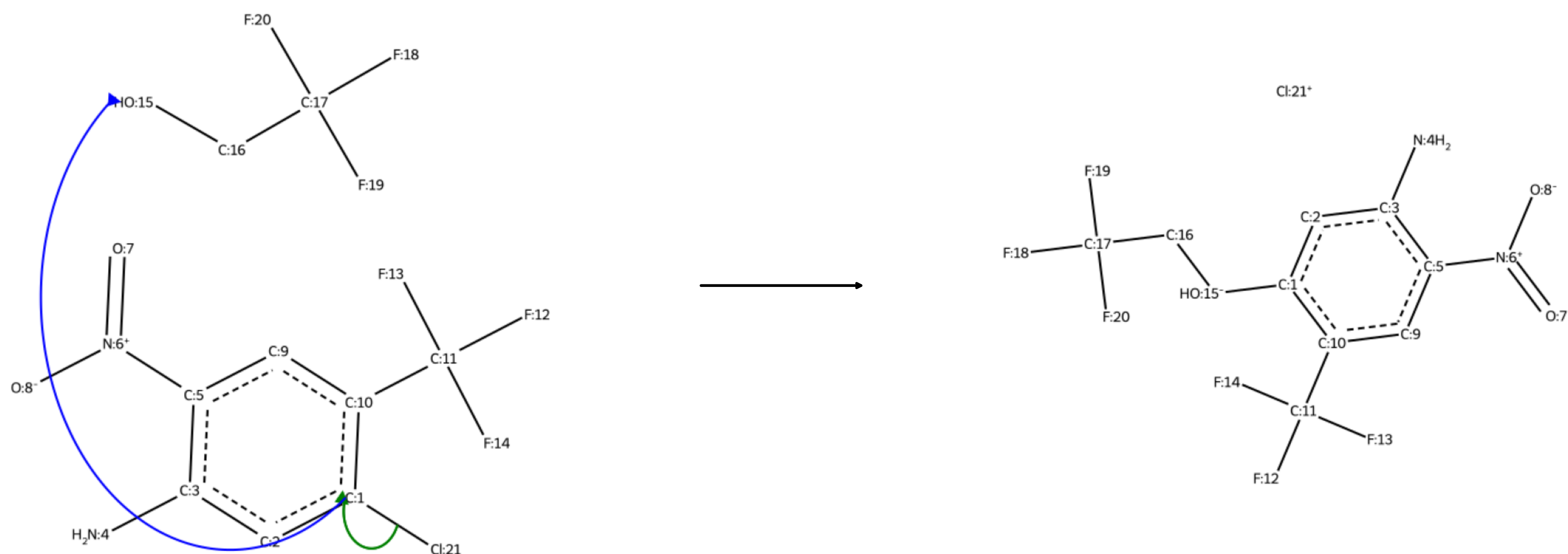


ELECTRO-generated mechanistic pathway

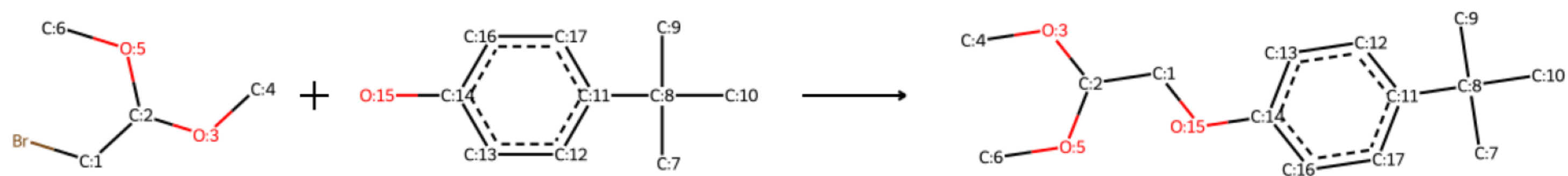
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:74

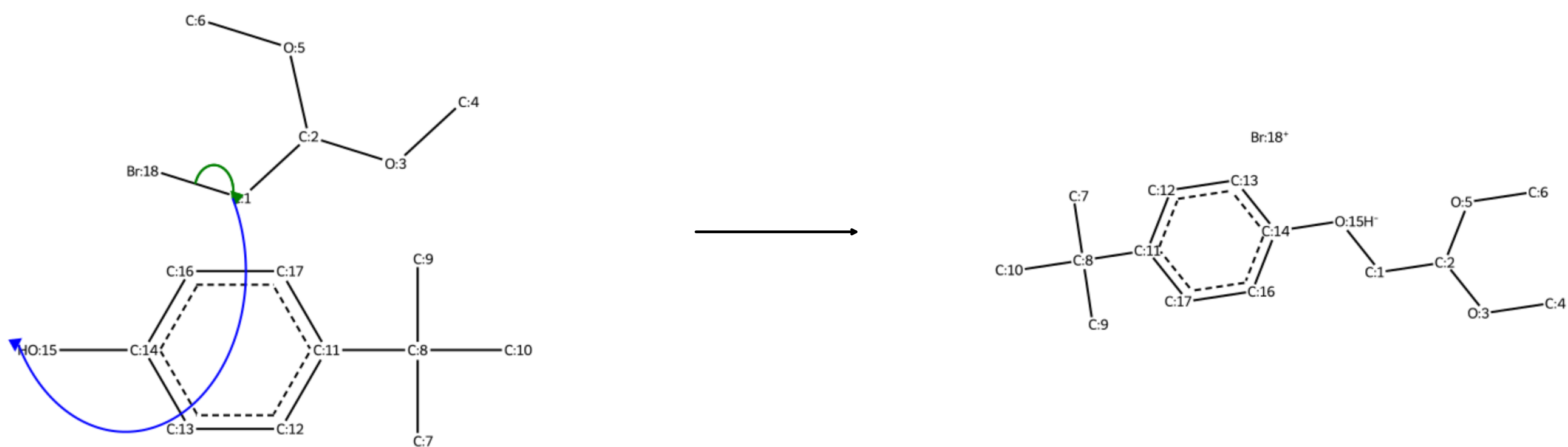


ELECTRO-generated mechanistic pathway

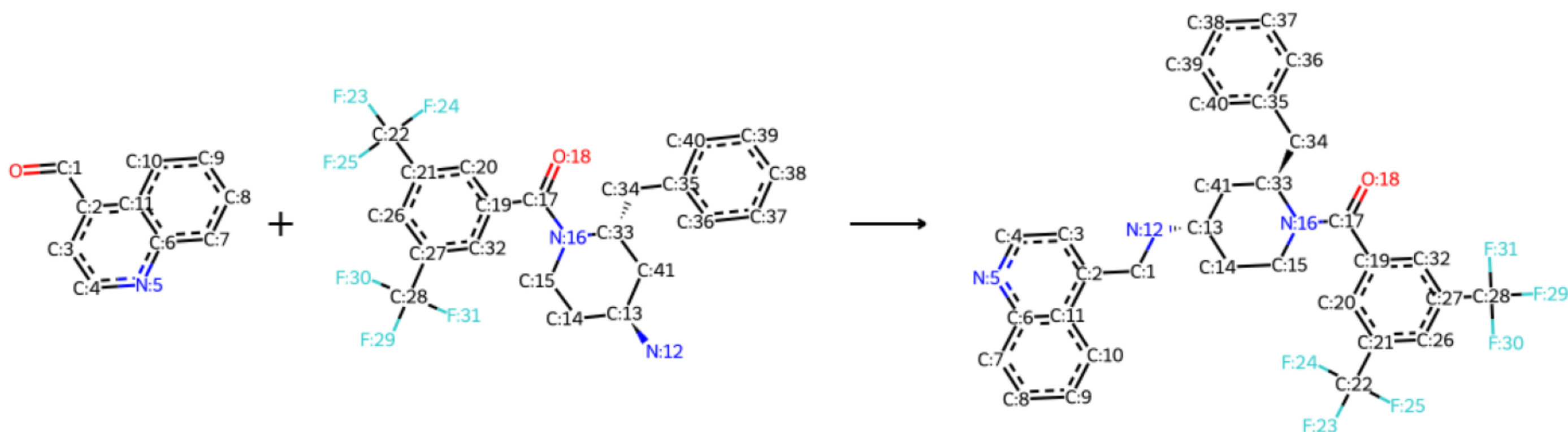
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:75

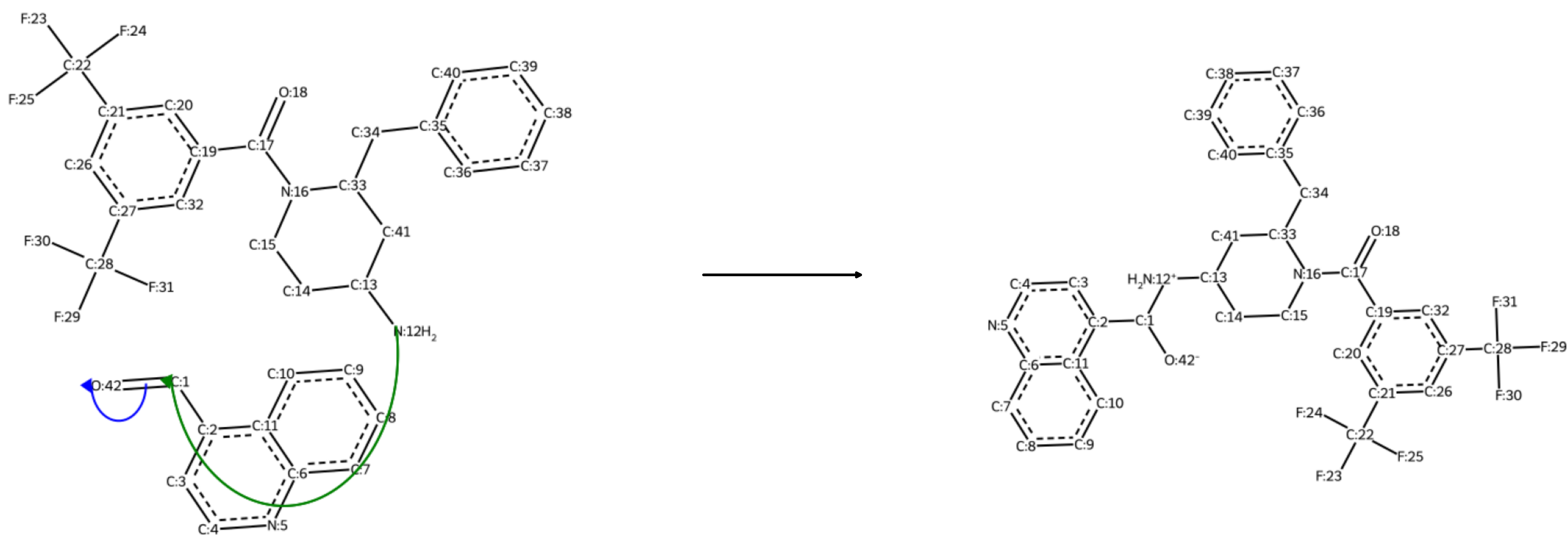


ELECTRO-generated mechanistic pathway

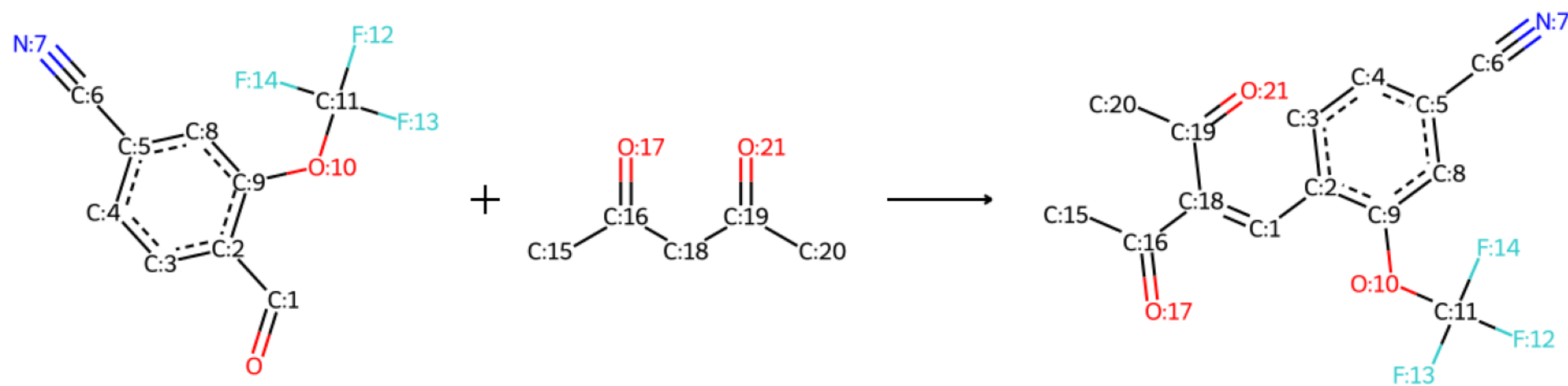
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:76

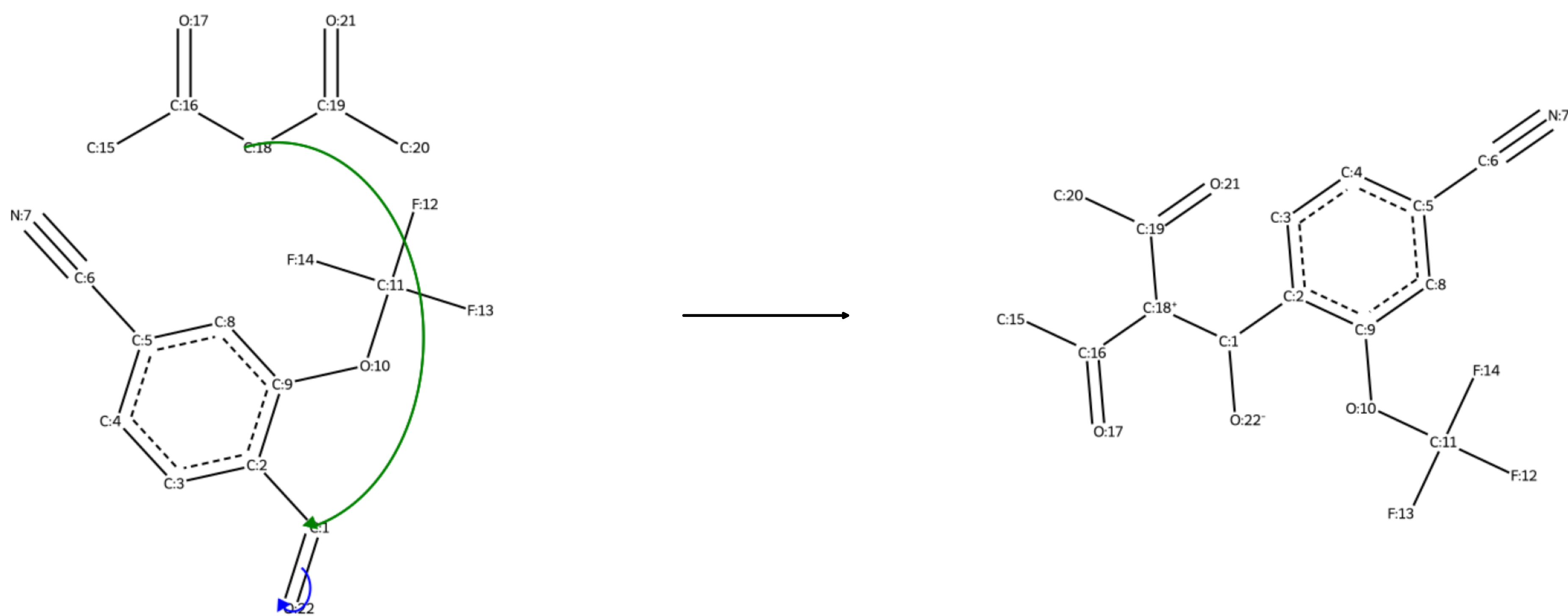


ELECTRO-generated mechanistic pathway

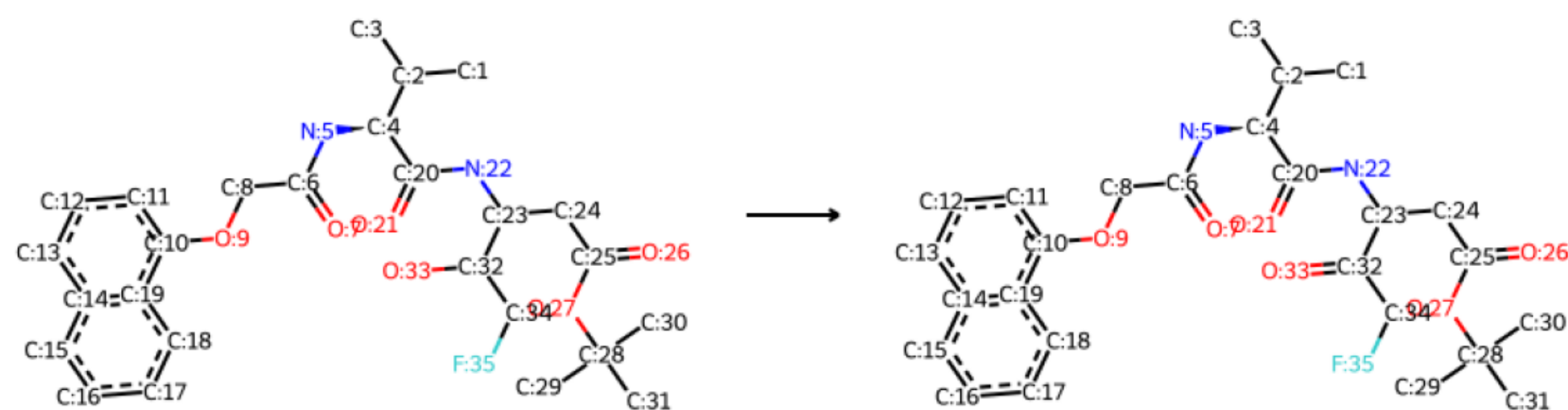
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:77

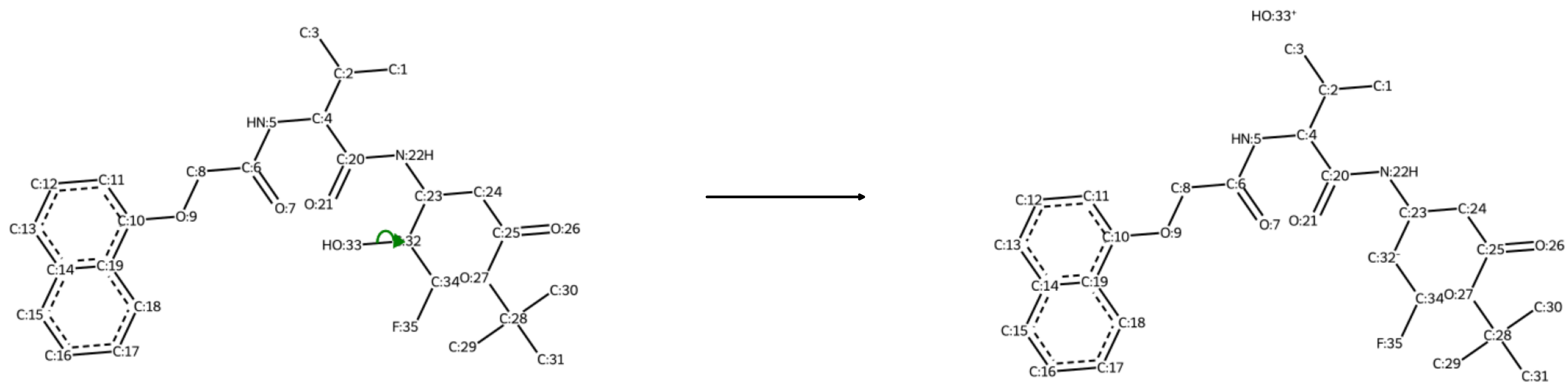


ELECTRO-generated mechanistic pathway

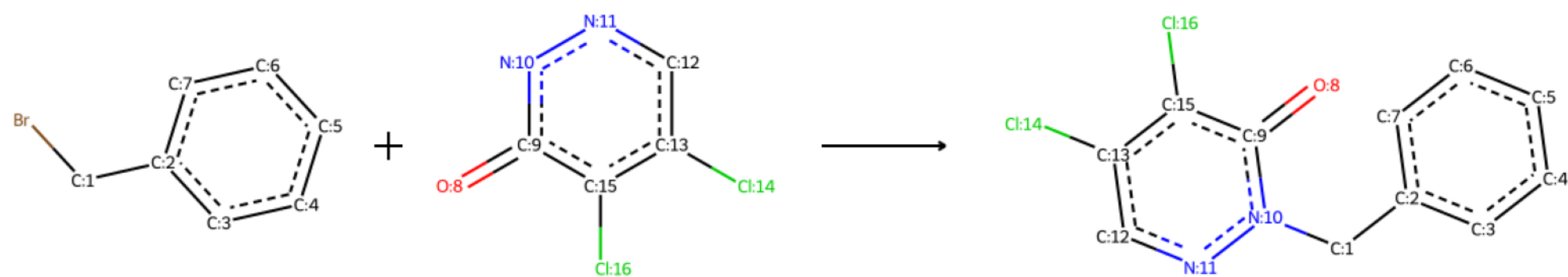
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



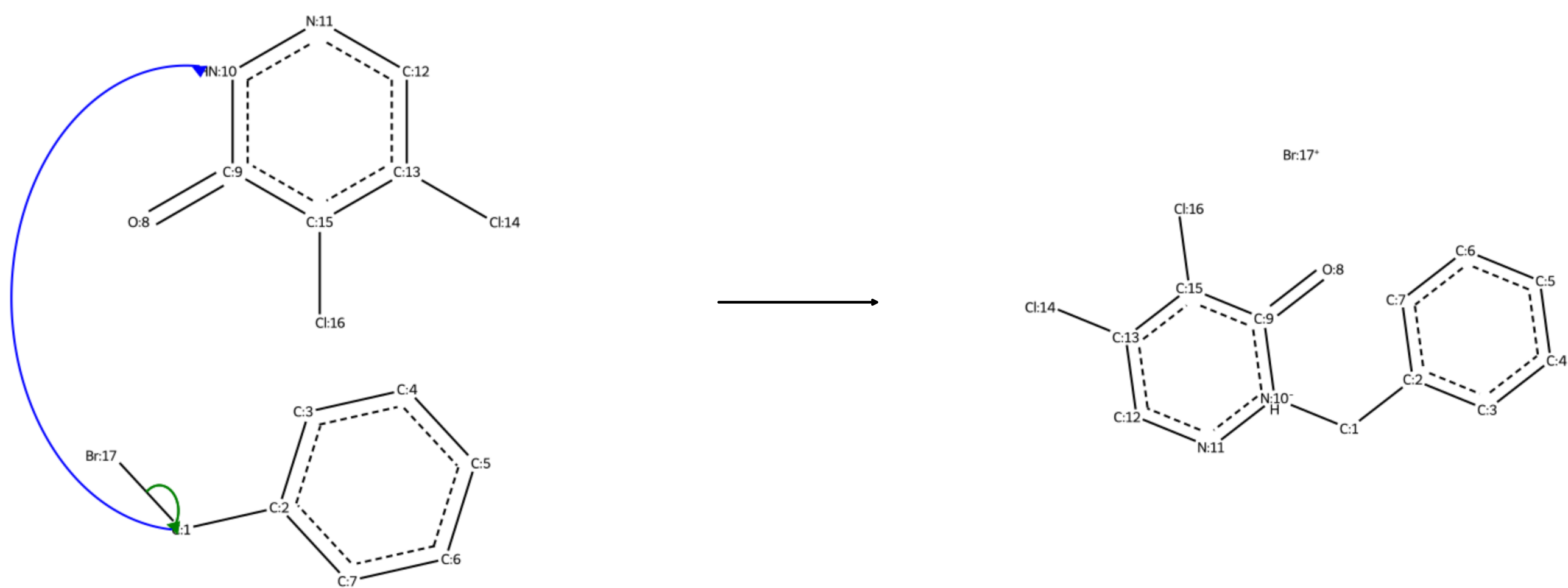
Original reaction RXN_ID:78



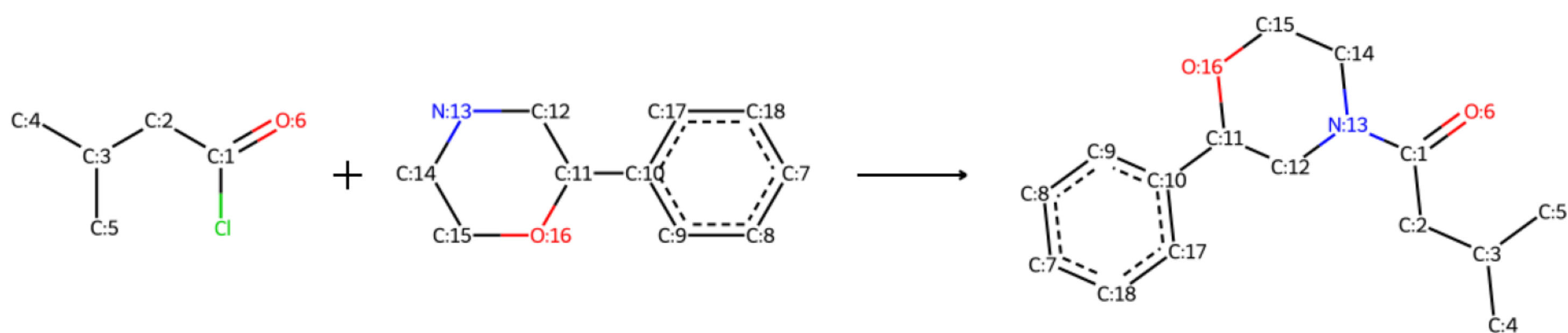
ELECTRO-generated mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1



Original reaction RXN_ID:79

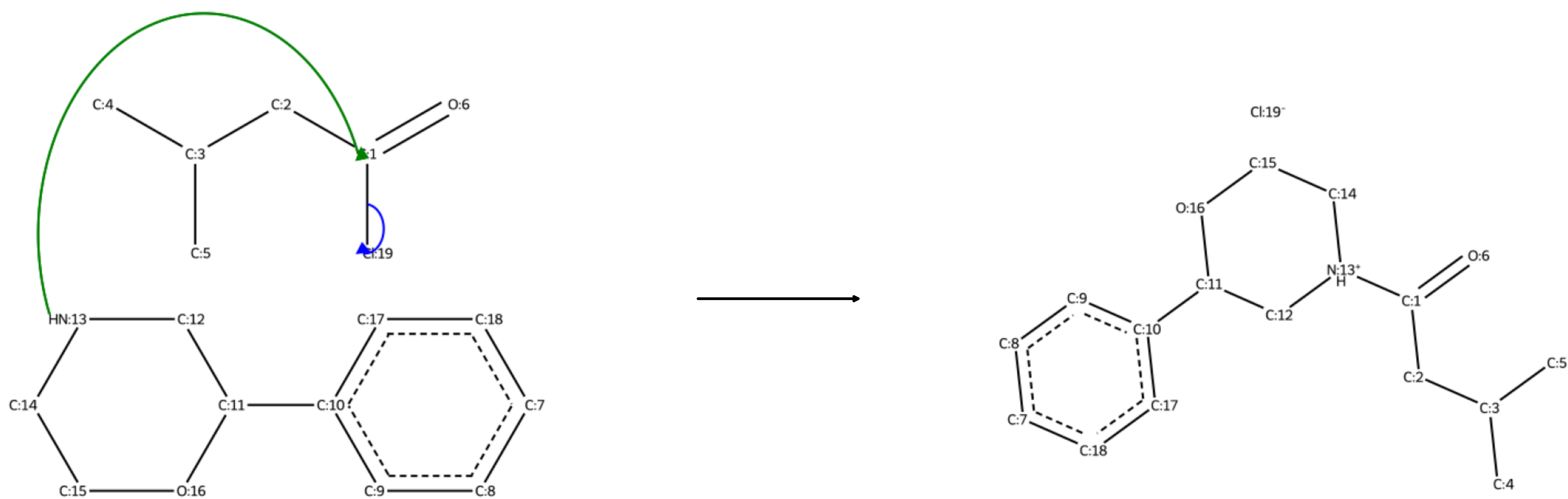


ELECTRO-generated mechanistic pathway

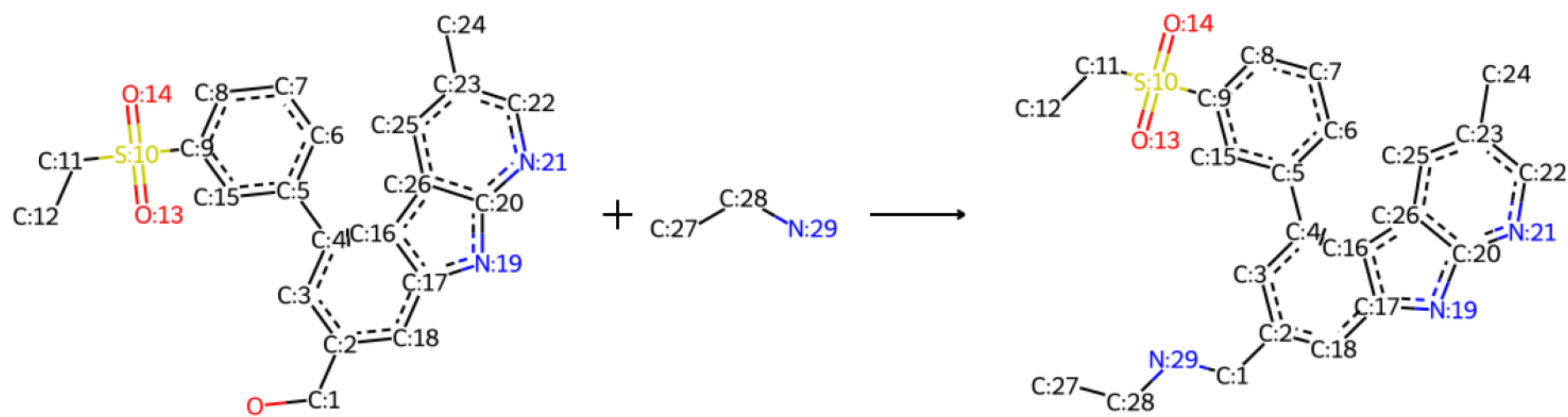
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:80

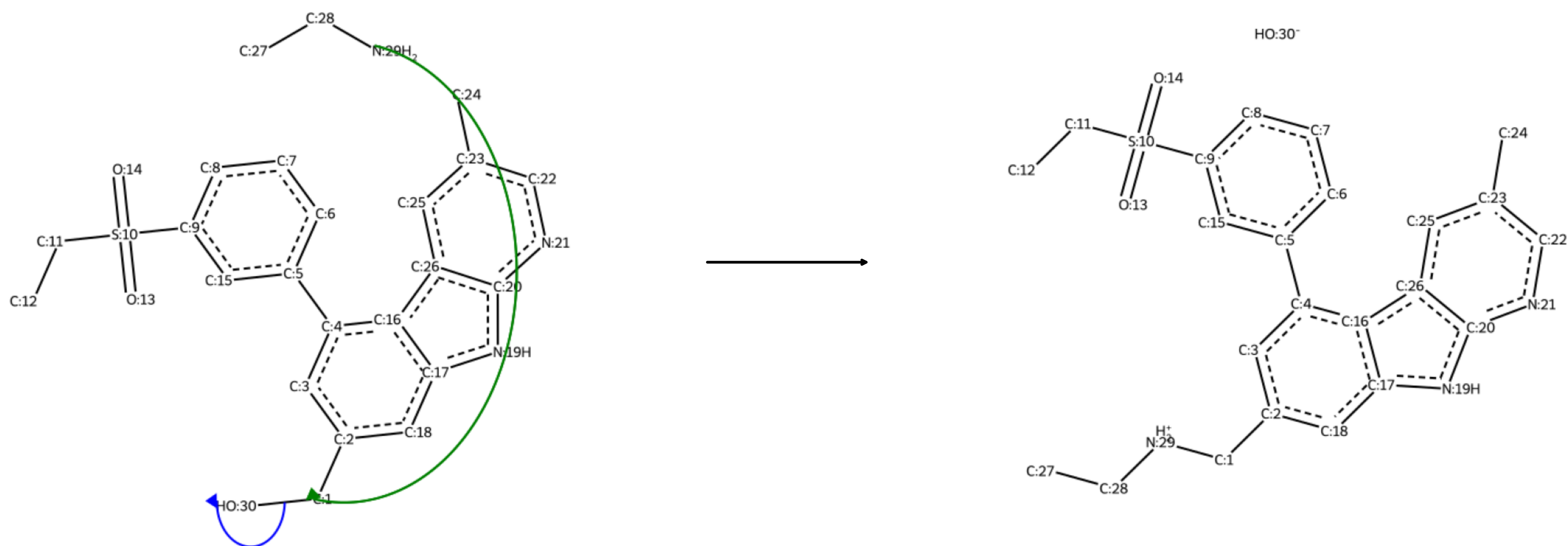


ELECTRO-generated mechanistic pathway

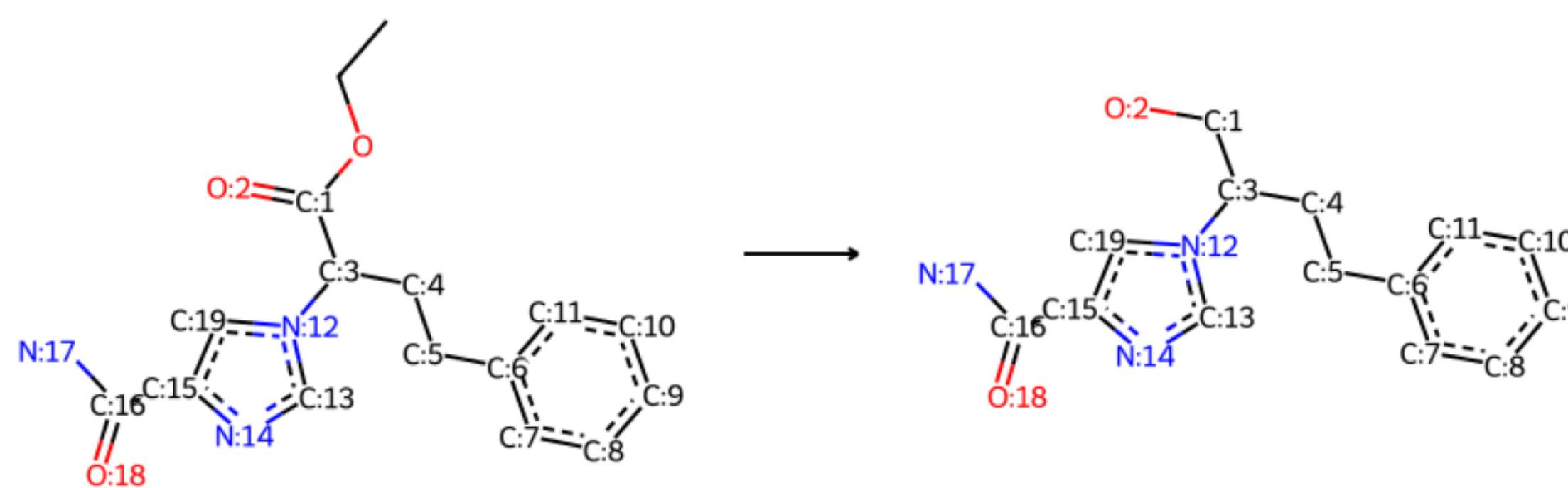
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:81

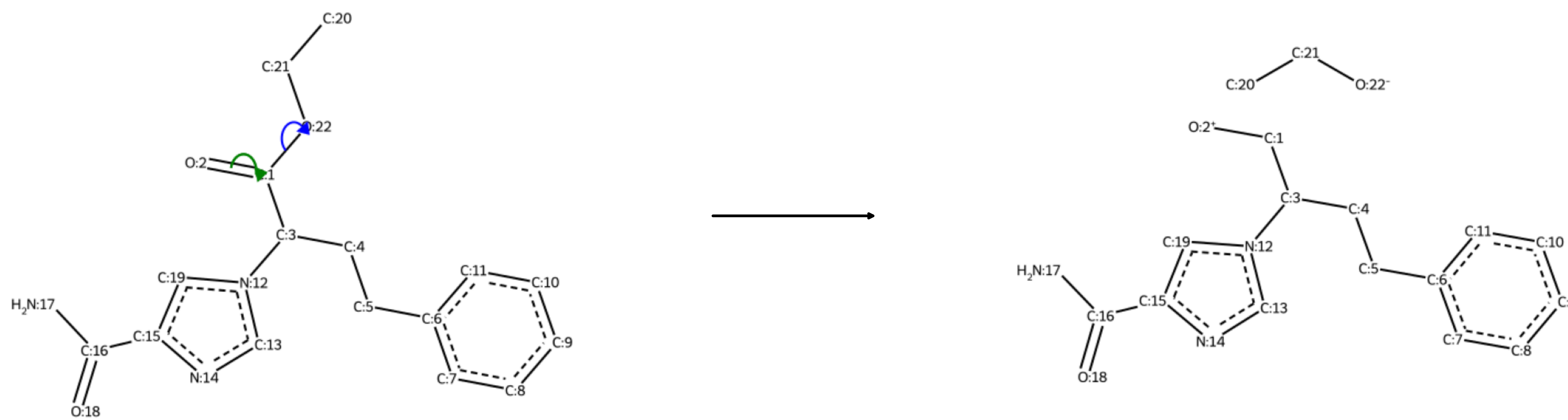


ELECTRO-generated mechanistic pathway

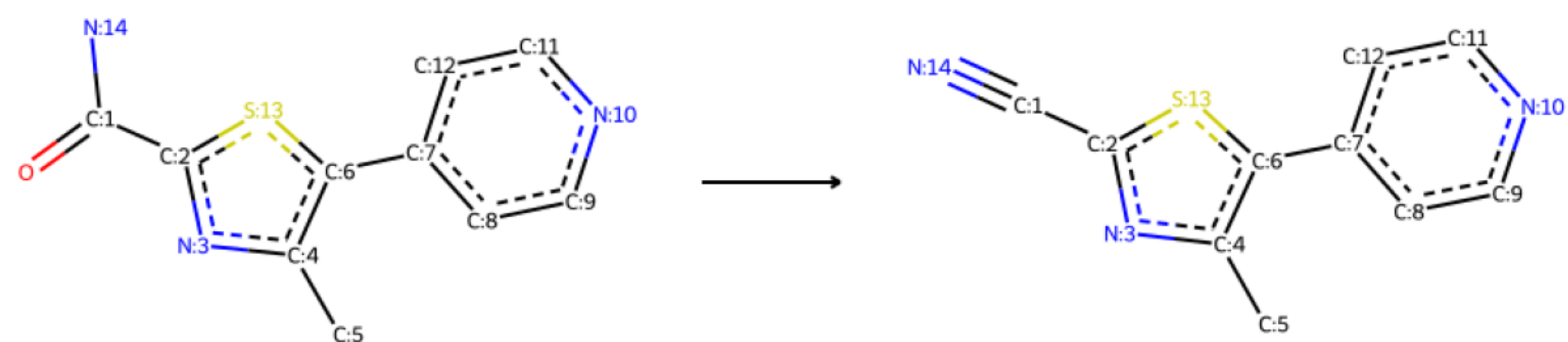
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:82

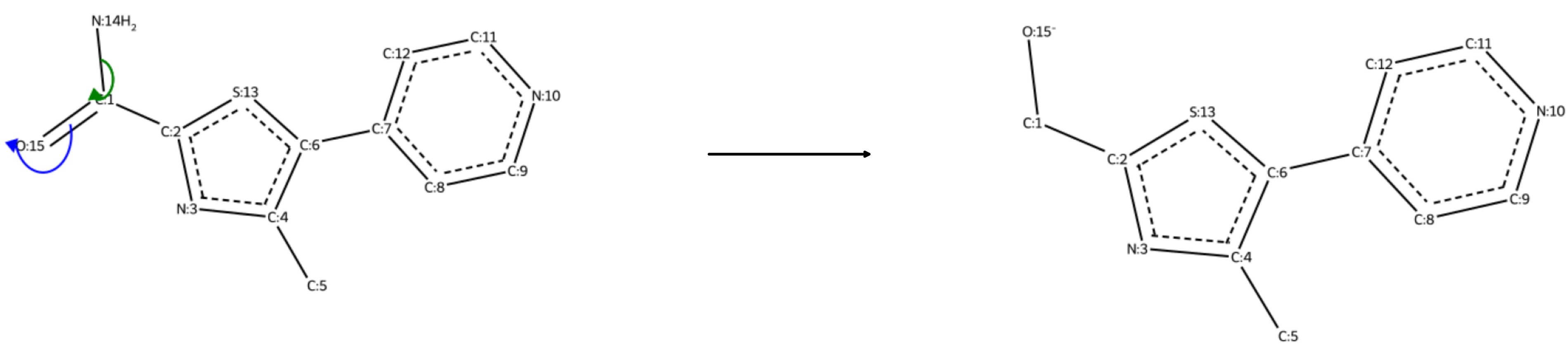


ELECTRO-generated mechanistic pathway

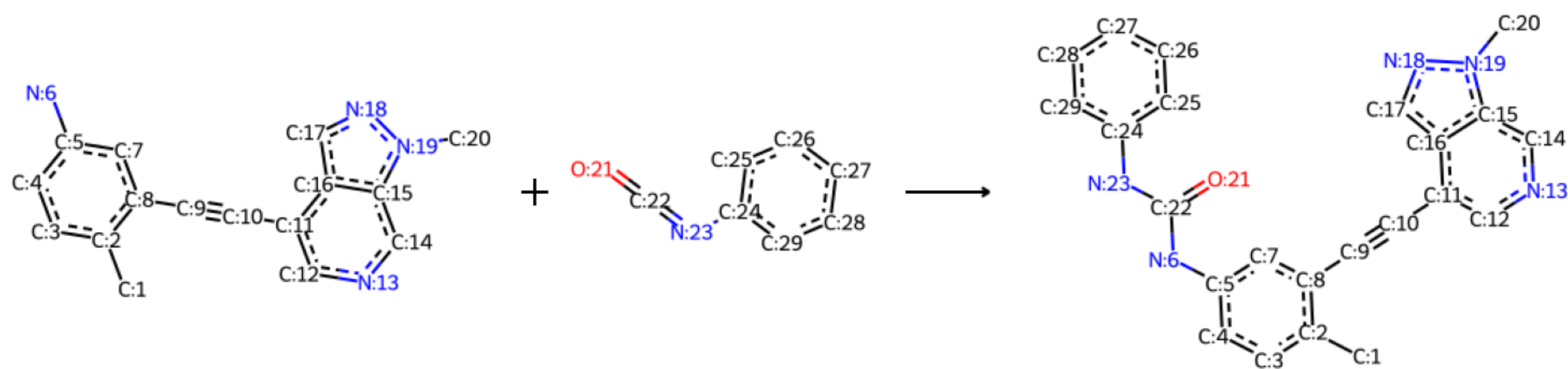
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:83

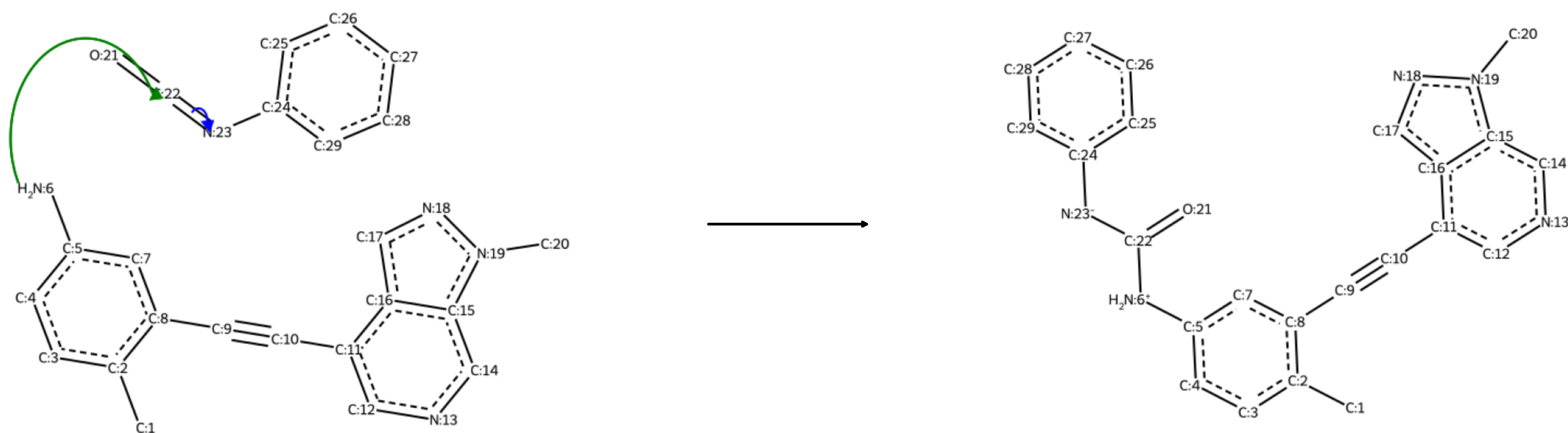


ELECTRO-generated mechanistic pathway

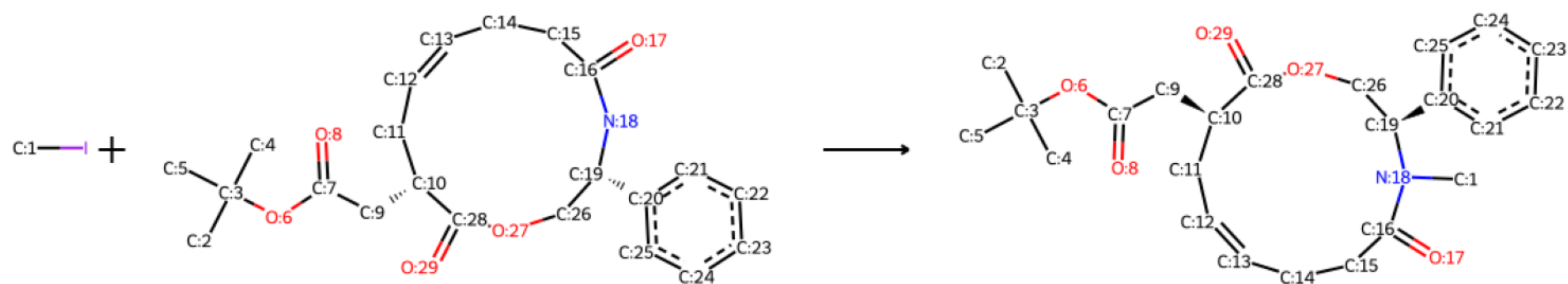
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:84

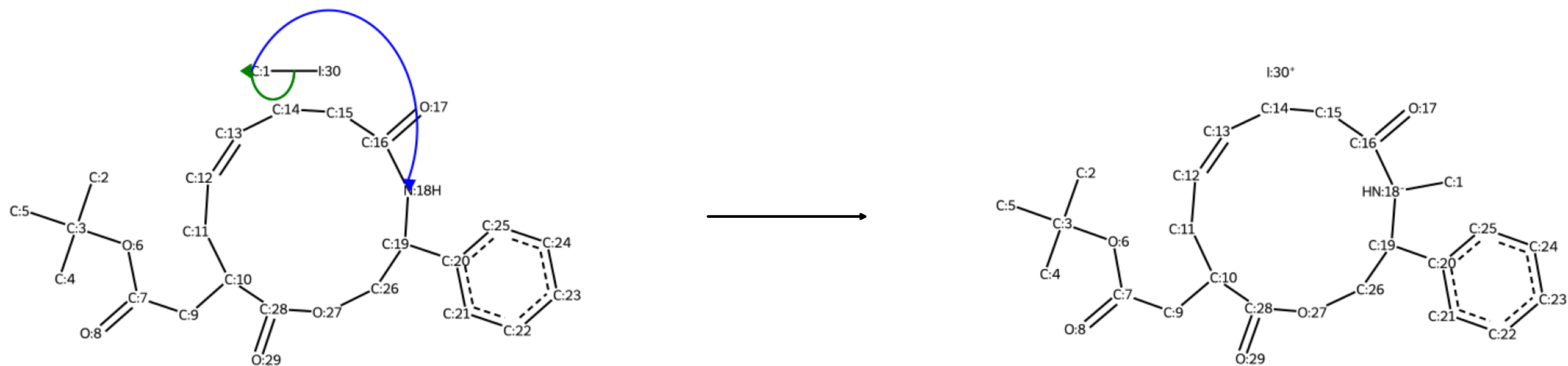


ELECTRO-generated mechanistic pathway

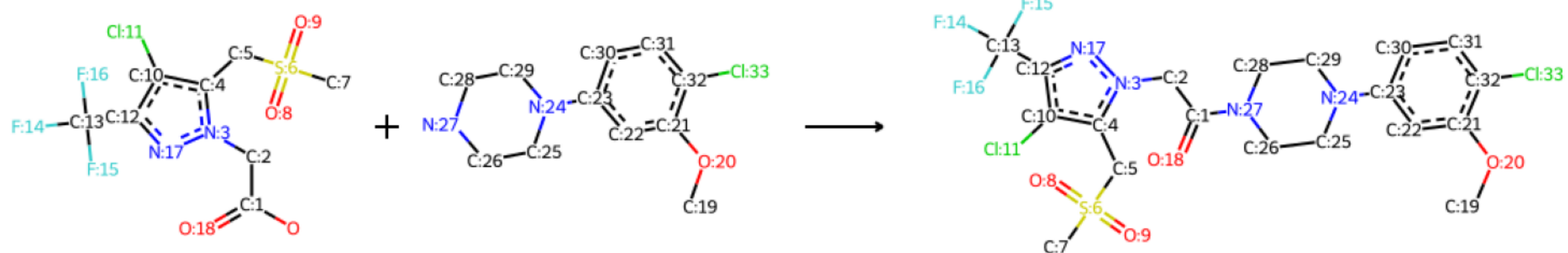
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:85

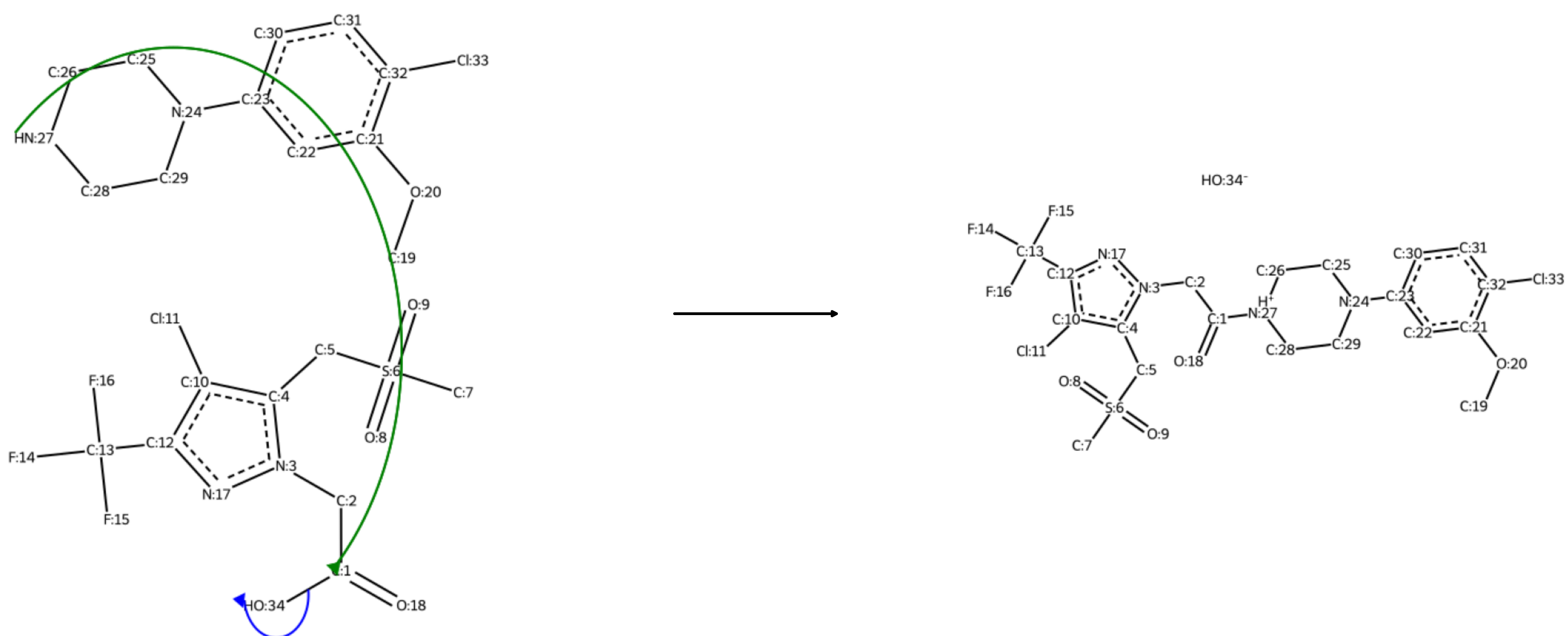


ELECTRO-generated mechanistic pathway

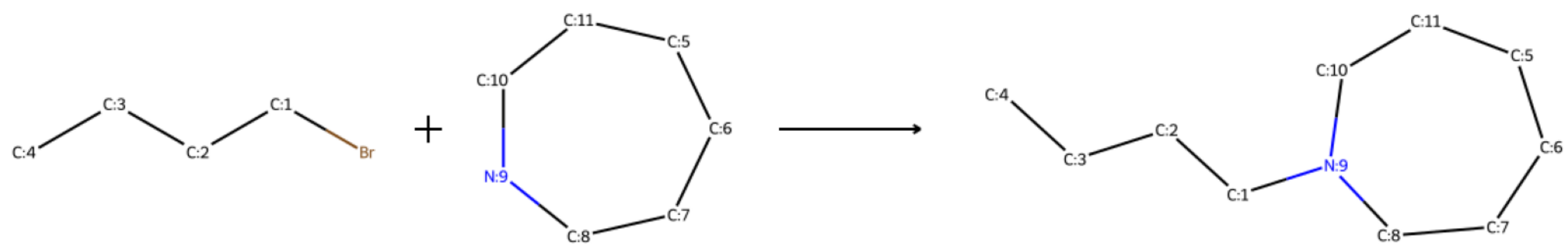
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:86

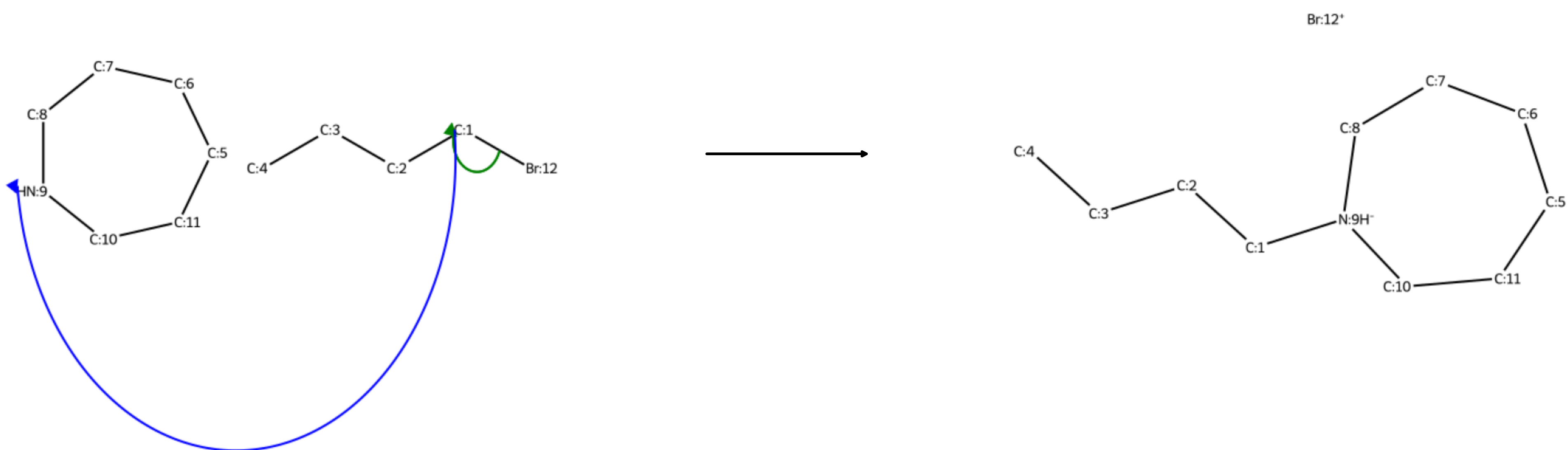


ELECTRO-generated mechanistic pathway

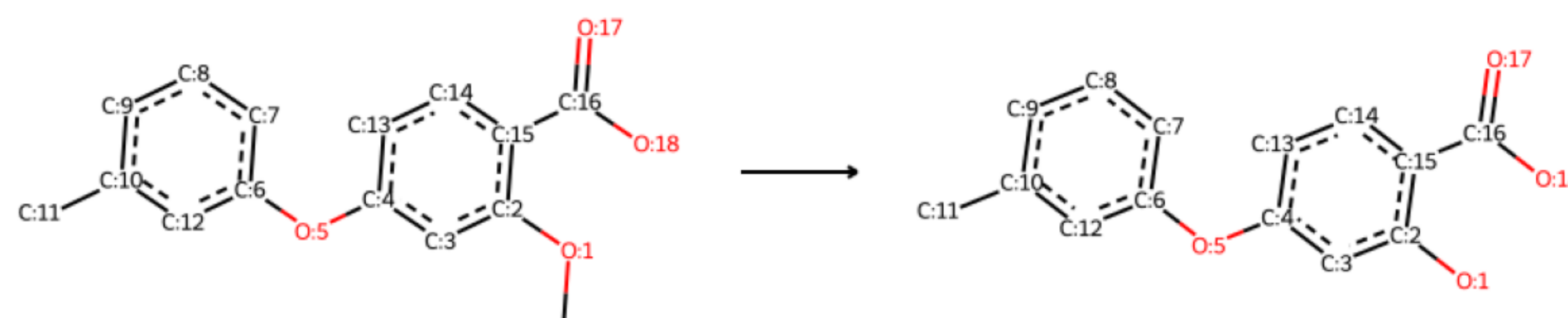
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:87

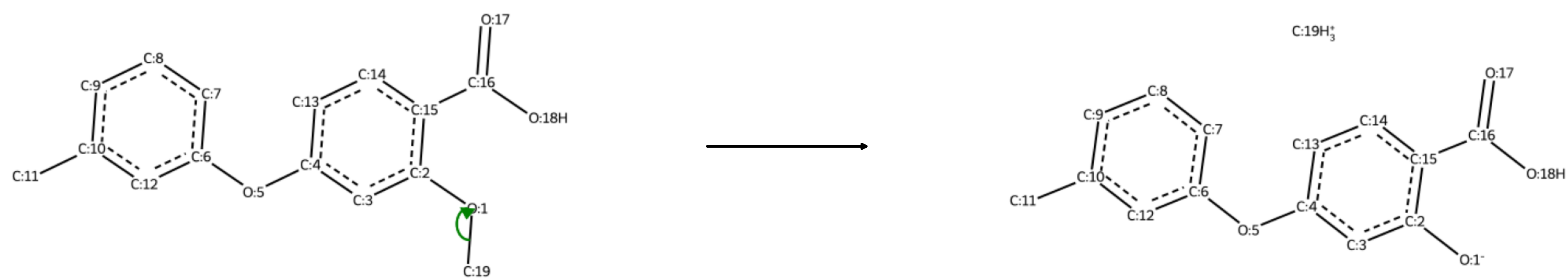


ELECTRO-generated mechanistic pathway

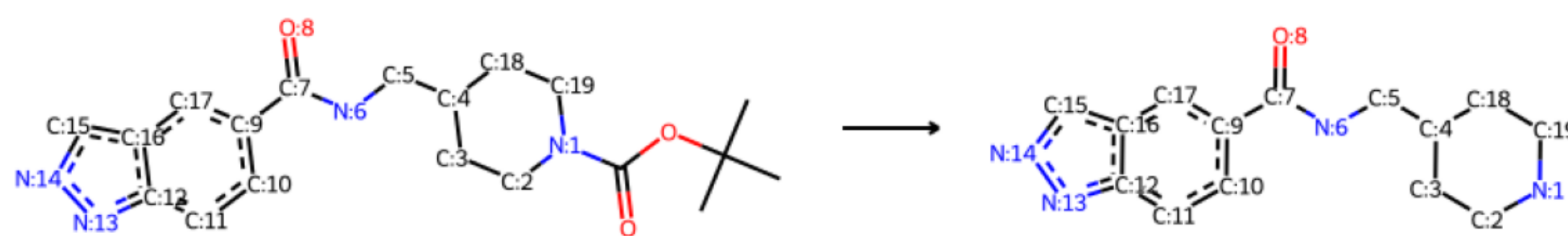
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:88

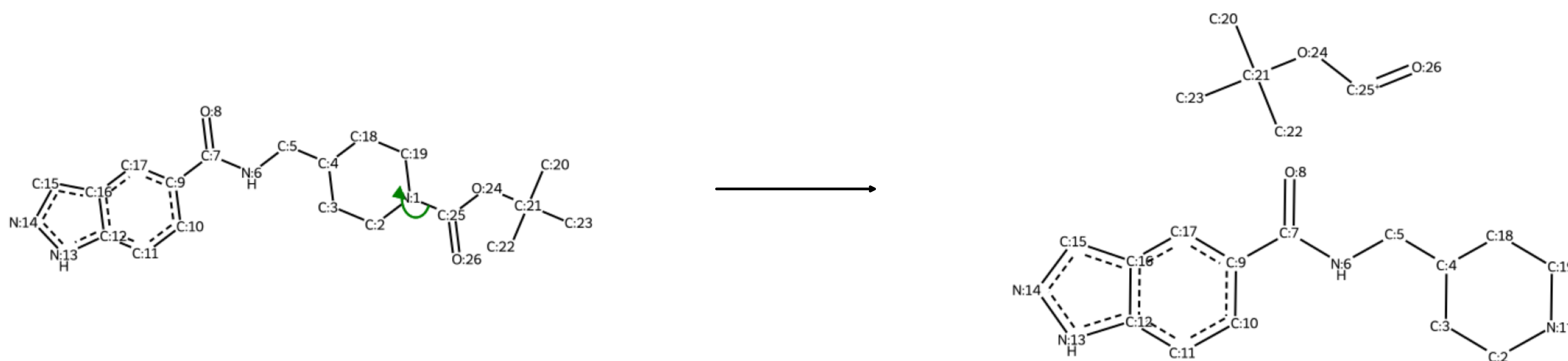


ELECTRO-generated mechanistic pathway

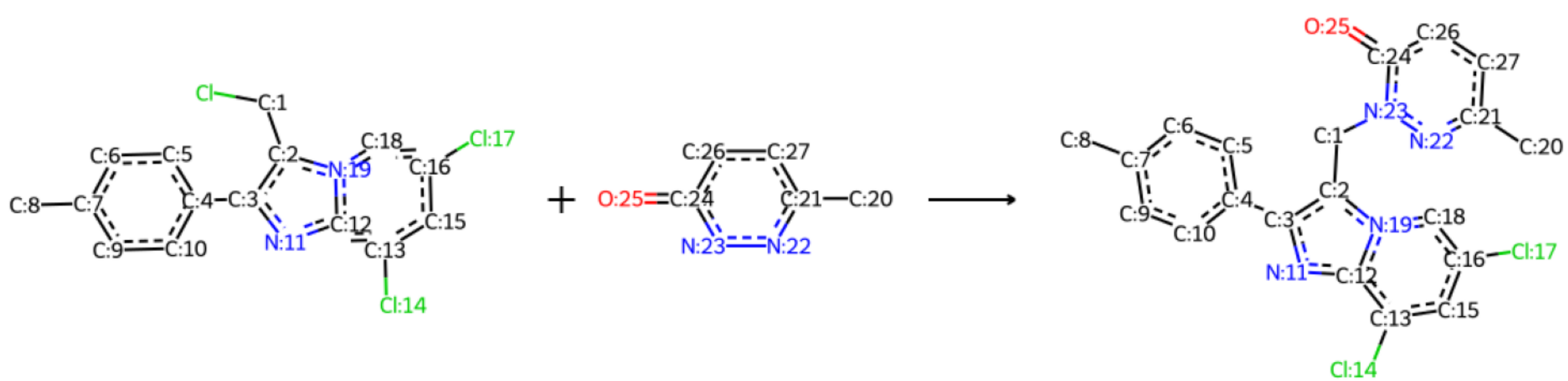
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:89

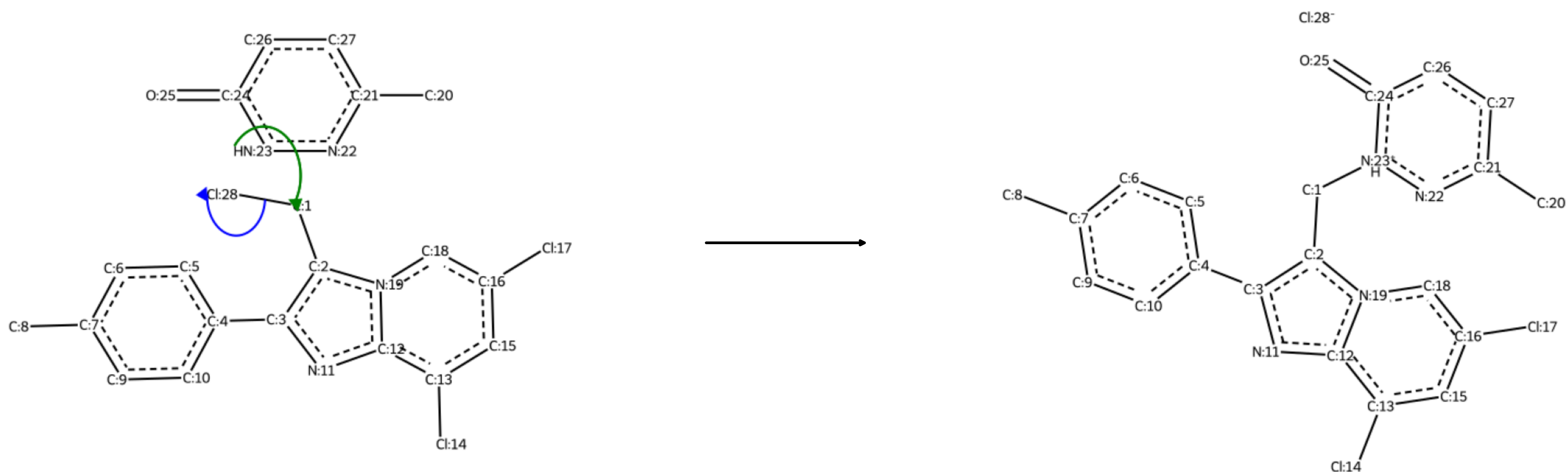


ELECTRO-generated mechanistic pathway

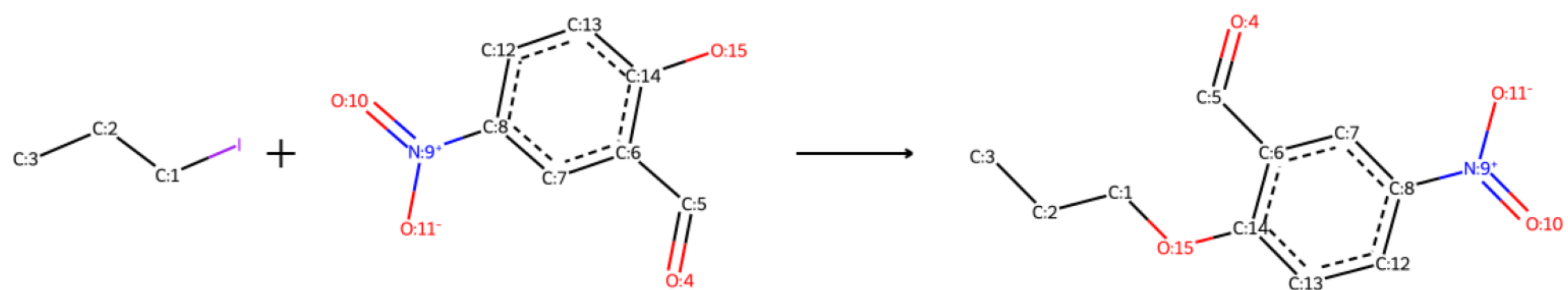
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:90

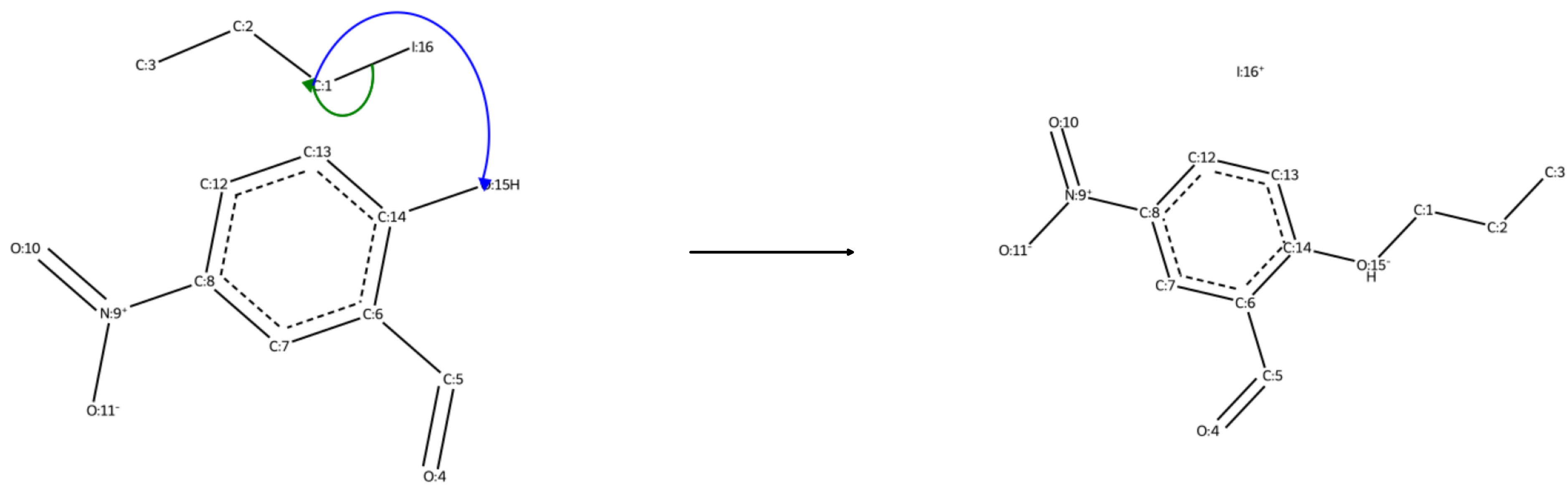


ELECTRO-generated mechanistic pathway

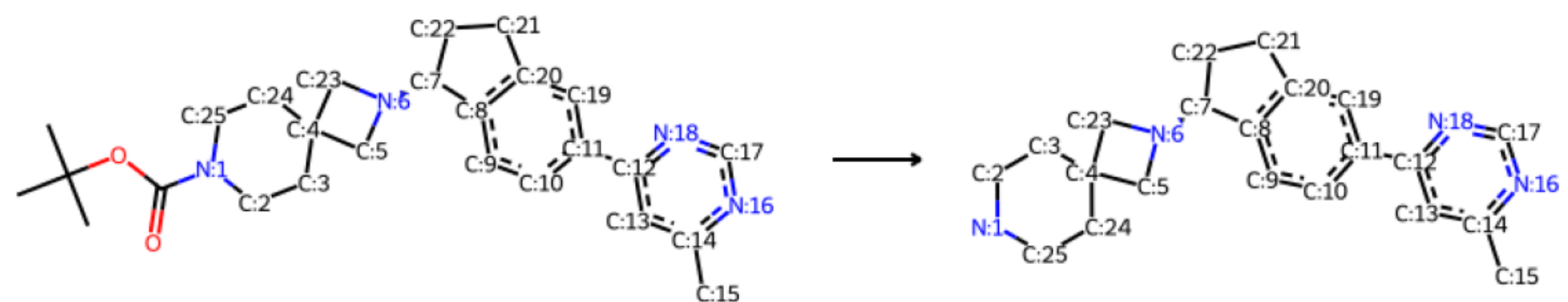
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:91

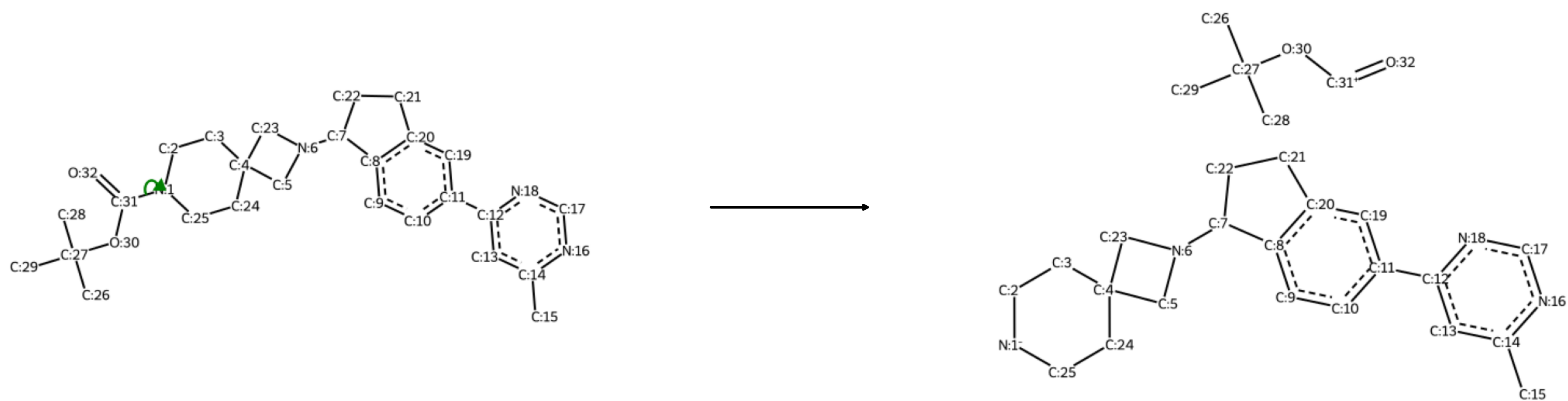


ELECTRO-generated mechanistic pathway

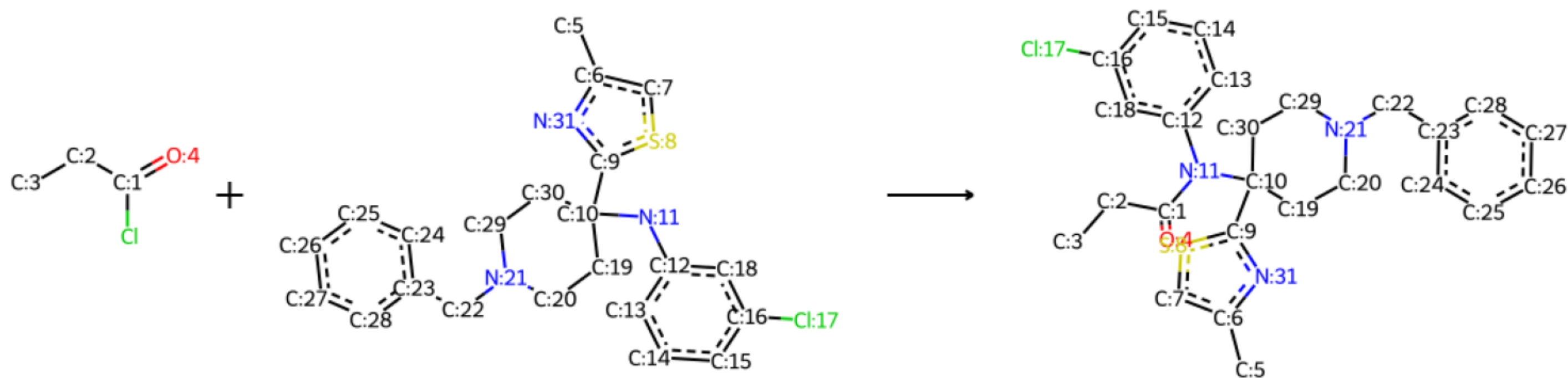
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:92

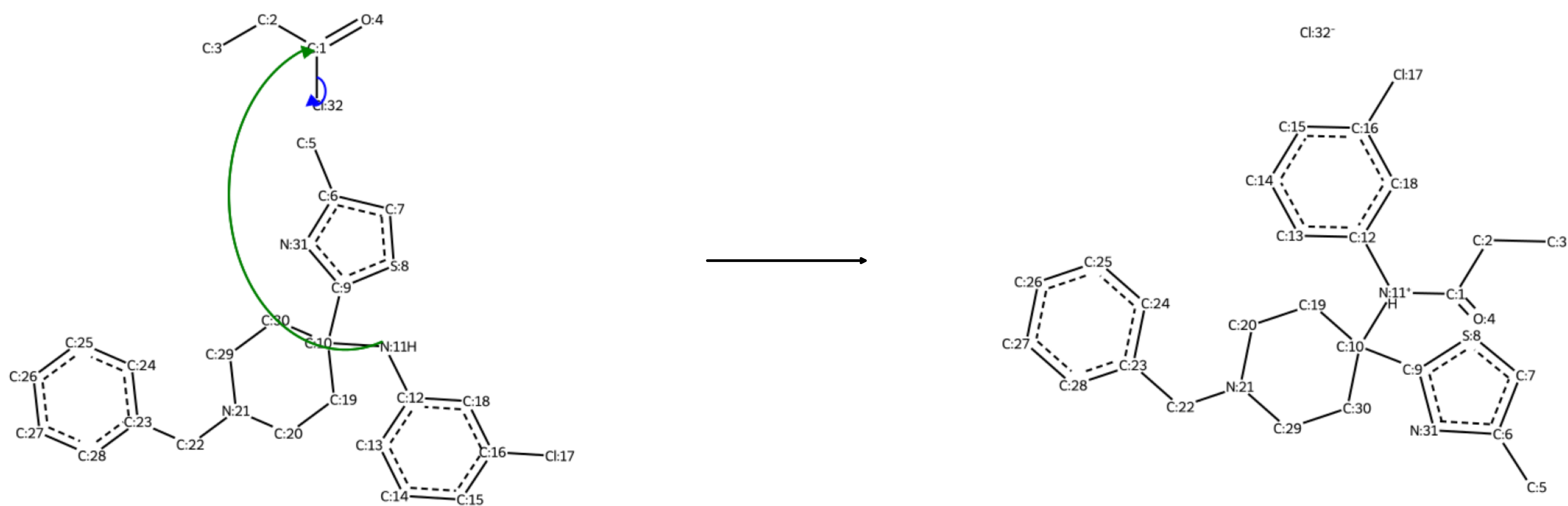


ELECTRO-generated mechanistic pathway

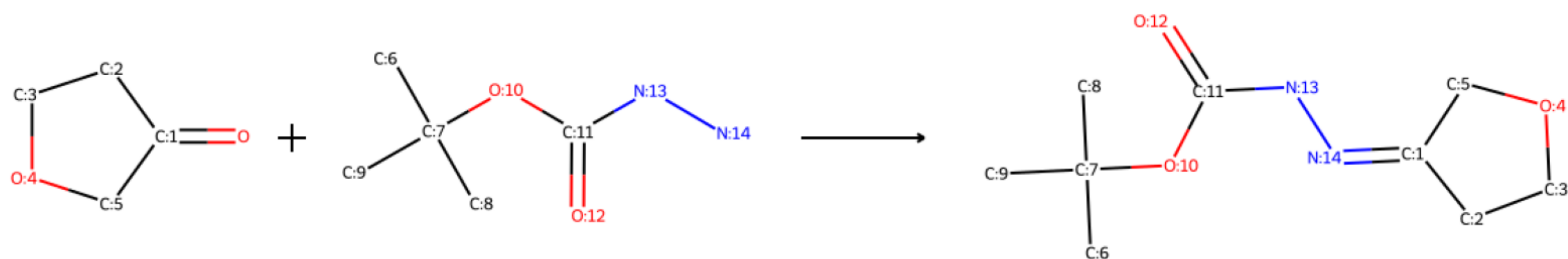
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:93

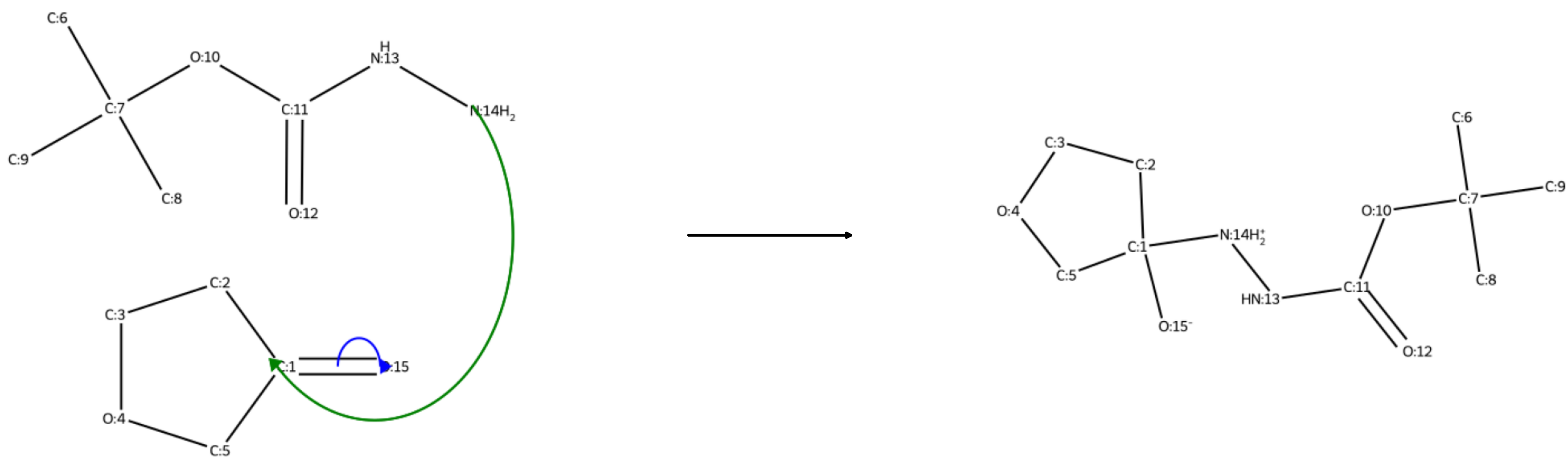


ELECTRO-generated mechanistic pathway

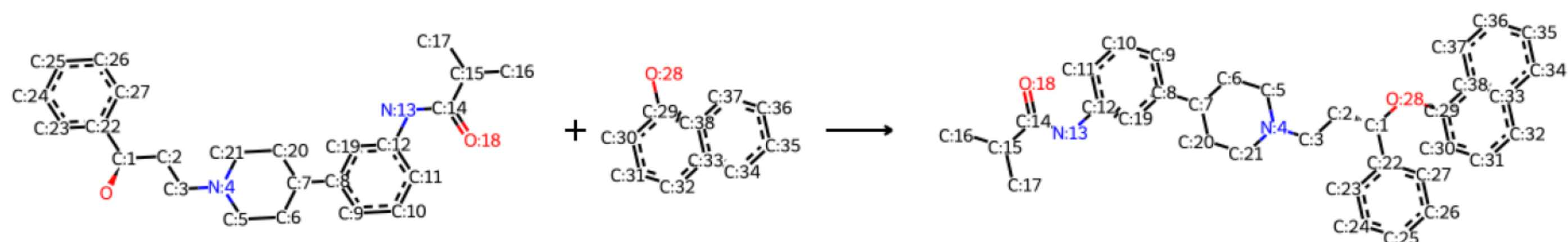
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:94

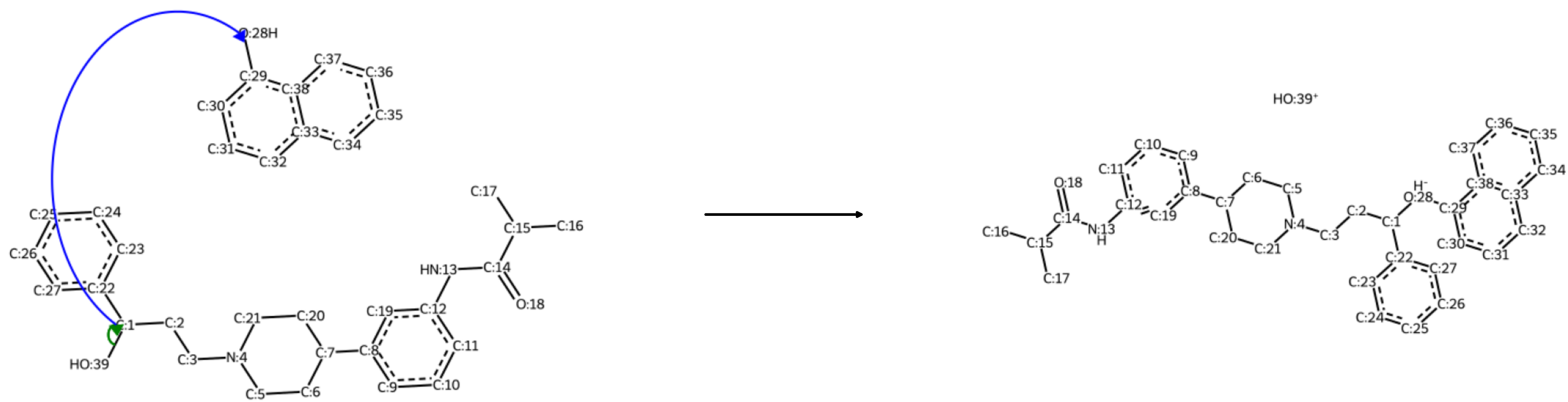


ELECTRO-generated mechanistic pathway

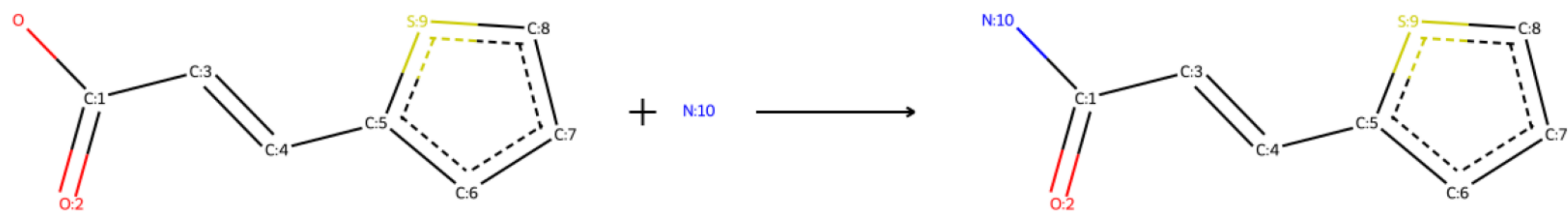
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:95

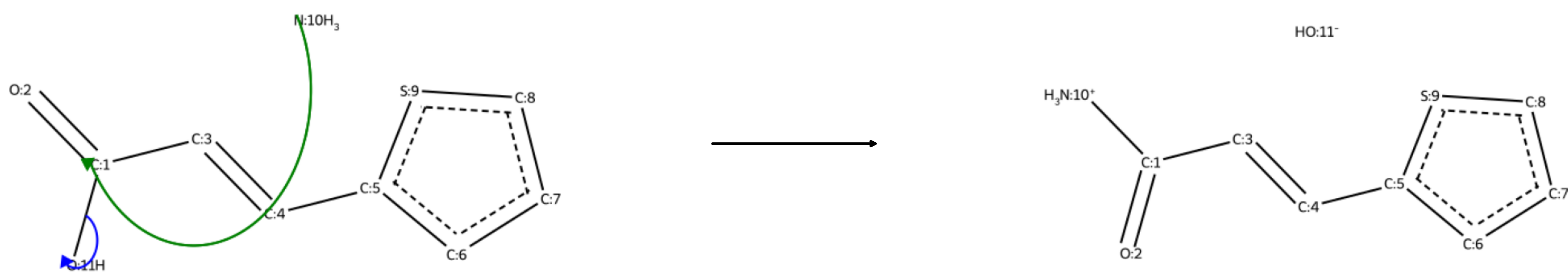


ELECTRO-generated mechanistic pathway

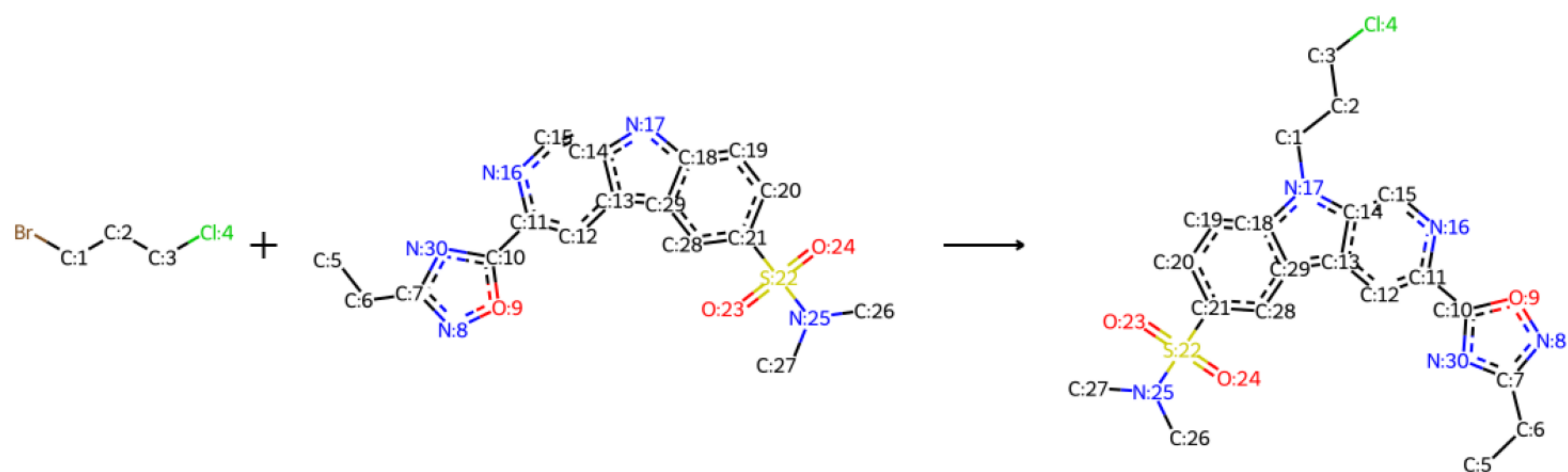
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:96

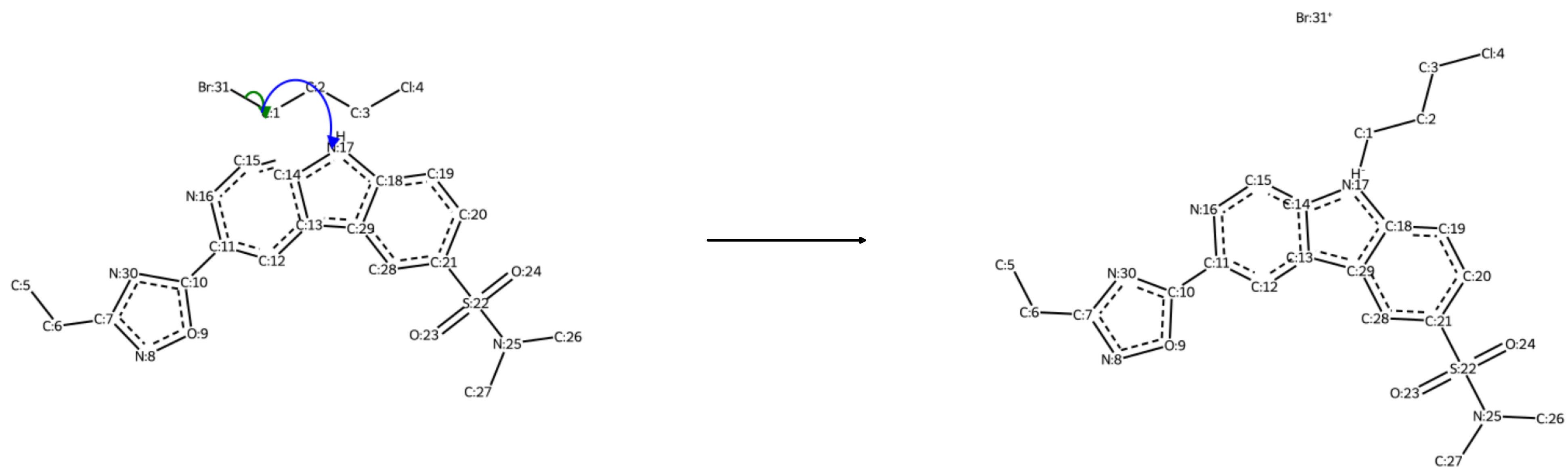


ELECTRO-generated mechanistic pathway

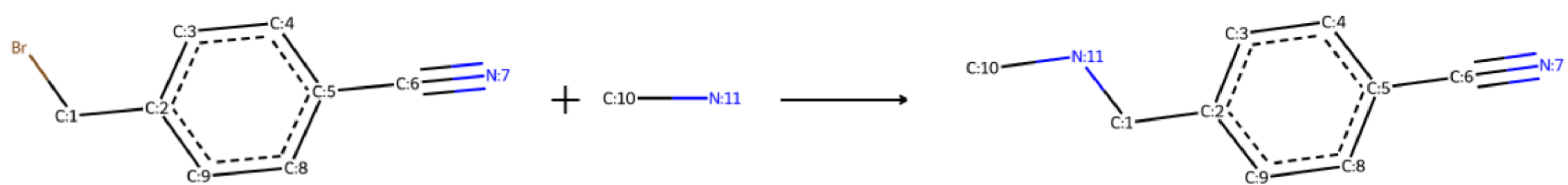
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:97

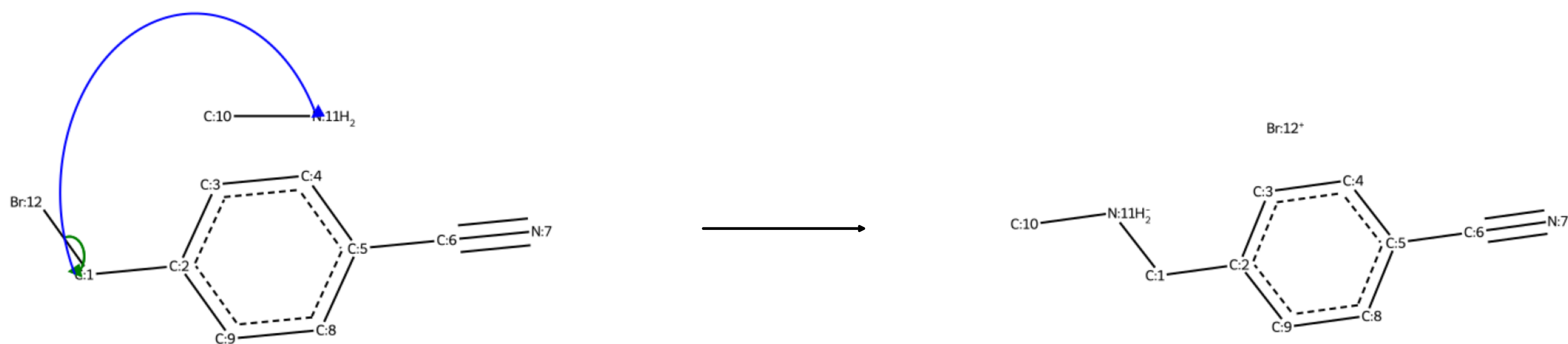


ELECTRO-generated mechanistic pathway

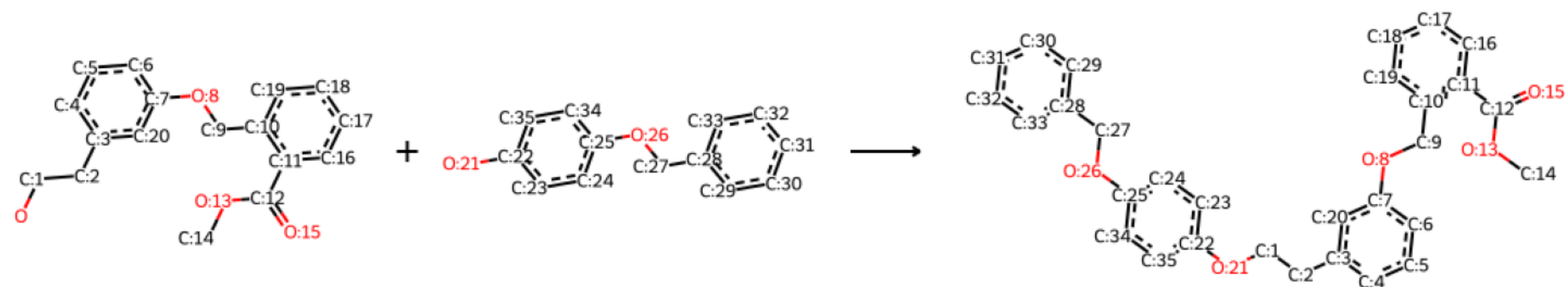
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:98

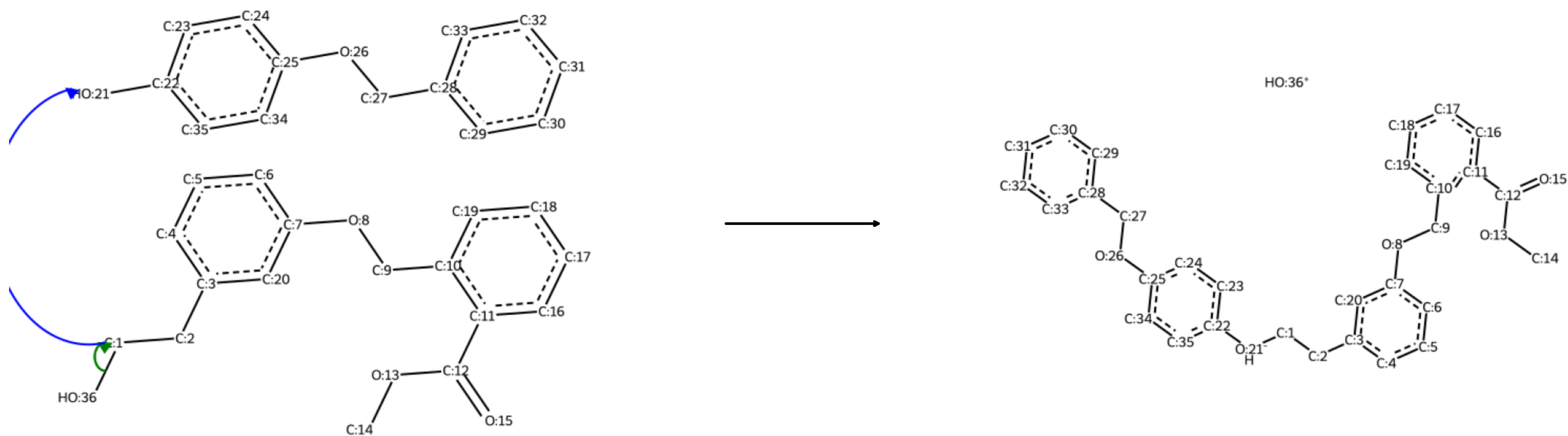


ELECTRO-generated mechanistic pathway

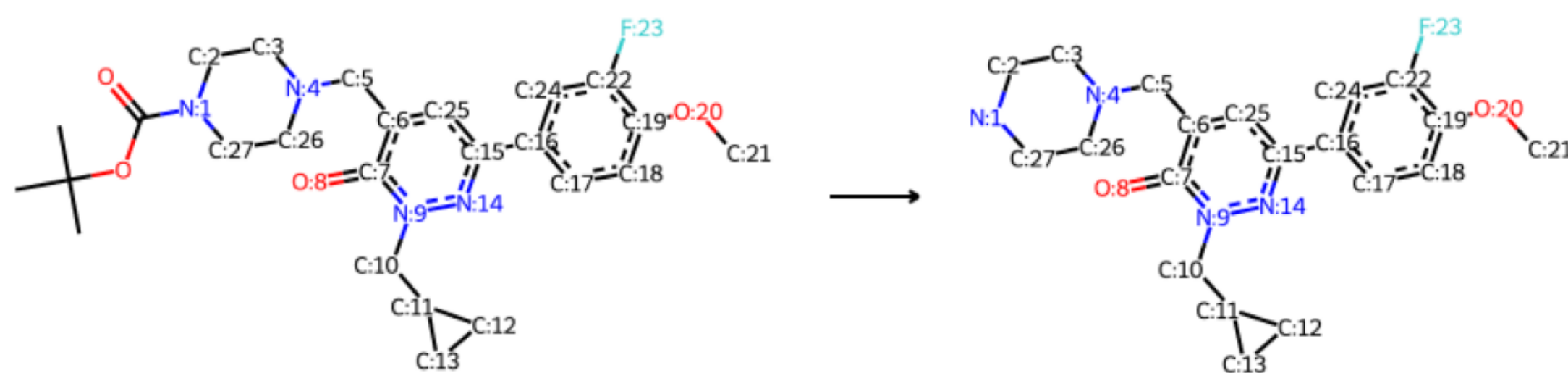
[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)



Original reaction RXN_ID:99



ELECTRO-generated mechanistic pathway

[Arrow order: (1) green, (2) blue, (3) red, (4) orange]

step #1

Product(s)

