Electronic Supplementary Material (ESI) for Chemical Science.

Section S1: Supporting links and supplementary data

Supporting links and supplementary data

RegioSQM is distributed on GitHub under the MIT license
https://github.com/jensengroup/RegioSQM/releases/tag/v1.0.

The SMILES strings, references, experimental EAS sites, etc can be found at
github.com/jensengroup/db-regioselectivity.

The study Kruszyk et al. contained 130 unique reactions. Several reactions had no yields reported and after removing these there are 118 left. These were used to test the performance of several methods.

As described in the main text PM3/chloroform or PM3/DMF have the highest success rate (Table S1 and S2) and that proton affinity is a better probe for reactivity than Br cation affinity at least using semiempirical methods (Table 3).

The high failure rate for PM6 Br cation calculations appears to be due to a strong large attraction between Br^+ and sp^2 nitrogen atoms, which leads to unphysically short Br^+-N distances and small Br^+-X-N angles compared to PM3.

One possible reason that newer methods such as PM6 perform worse is that the radii used in the COSMO calculations were optimized for AM1 and PM3, which means that PM6/COSMO calculations are less accurate (Table S4).

Table 1: Number of incorrect predictions of regioselectivity by the PM3 method in the gas phase, chloroform and DMF using a 1 kcal/mol cutoff. A maximum of 20 conformations per isomer is used.

	gas	chloroform	DMF
incorrect	11	2	2

Table 2: Number of incorrect predictions of regioselectivity by the PM3 method in the gas phase, chloroform and DMF using a 1 kcal/mol cutoff. A maximum of 20 conformations per isomer is used.

	PM3	AM1	PM6	PM6-DH+	PM7
incorrect	2	8	6	6	7

Table 3: Number of incorrect predictions using a maximum of 20 (“20 H”) and 50 (“50 H”) conformers and proton and Bromide cation (20 Br) affinity as a measure of reactivity.

	PM3	PM6
20 H	2	6
50 H	2	
20 Br	4	46

Table 4: Mean absolute error (MAE) and mean error (ME) of aqueous solvation energies computed using the COSMO method and the MNSOLV data set.

	AM1	PM3	PM6
MAE	3.6	3.4	3.9
ME	0	0.5	1.8

Section S2: Table listing numbering used in the paper and SI.

Table 5: This table lists numbering used in the paper and SI.

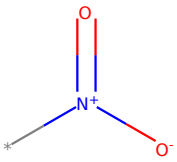
Paper	SI	Reference
1	1	[312]
2	15	[168]
3	170	[64]
4	199	[128]
5	514	[318]
6	75	[105]
7	373	[420]
8	367	[261]
9	163	[227, 366]
10	547	[180]
11	125	[59]
12	137	[269]
13	13	[394]
14	419	[283]

Section S3: Figure S1 Substituents of the compounds

subst1

subst2

subst3



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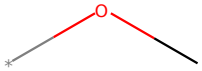

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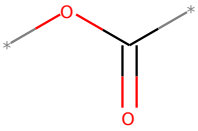

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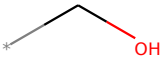

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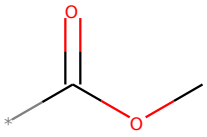

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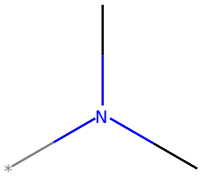

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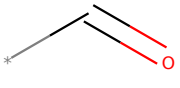

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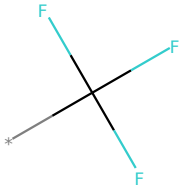

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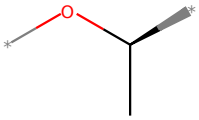

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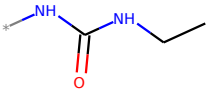

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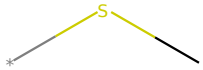

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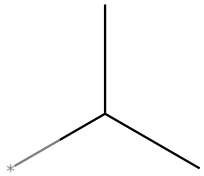

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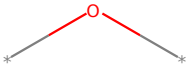

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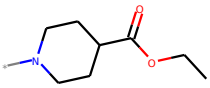

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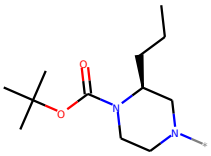

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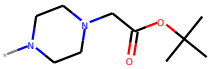

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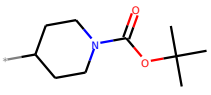

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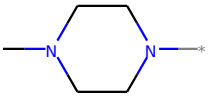

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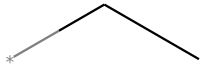

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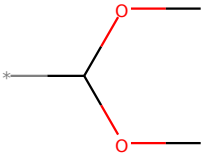

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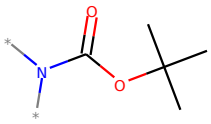

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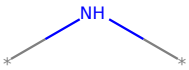

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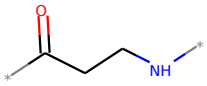

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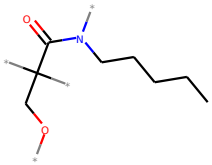

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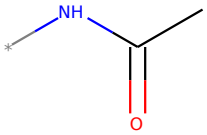

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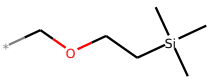

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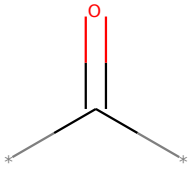

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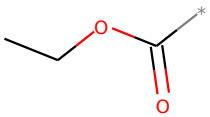

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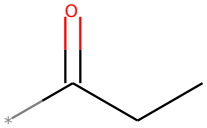

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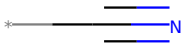

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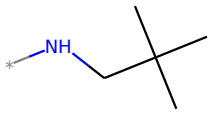

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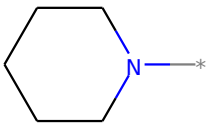

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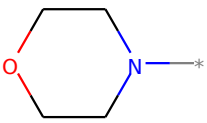

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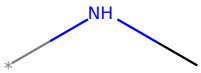

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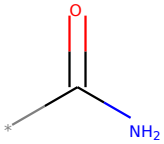

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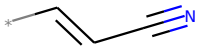

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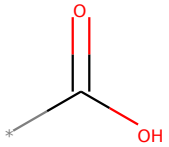

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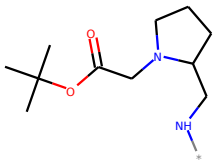

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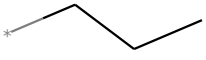

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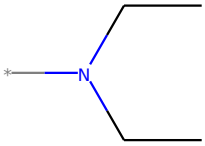

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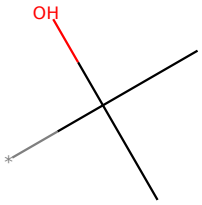

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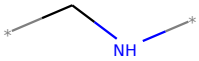

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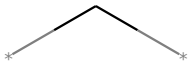

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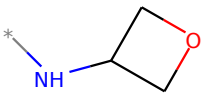

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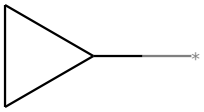

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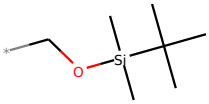

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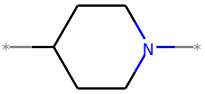

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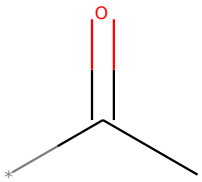

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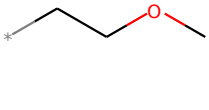

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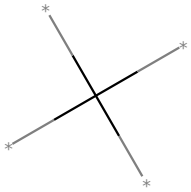

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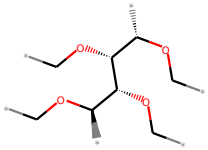

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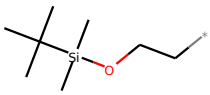

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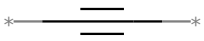

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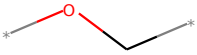

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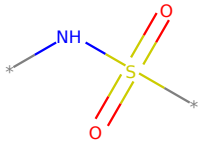

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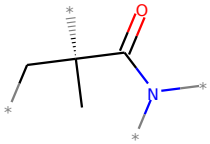

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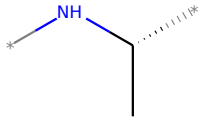

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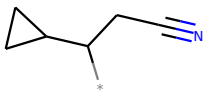

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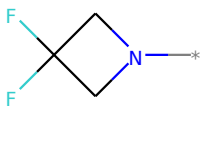

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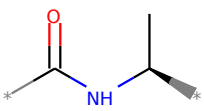

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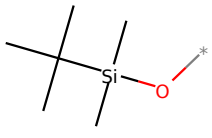

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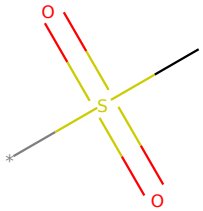

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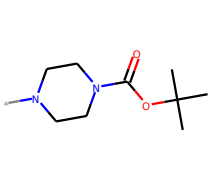

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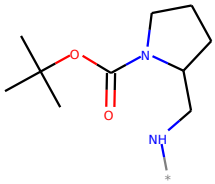

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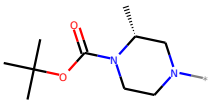

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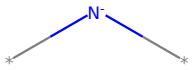

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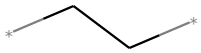

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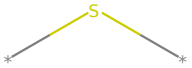

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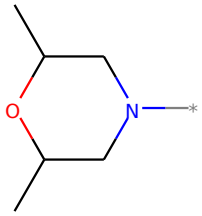

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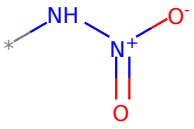

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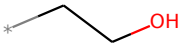

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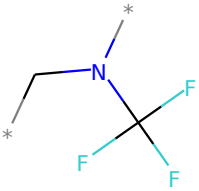

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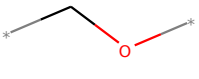

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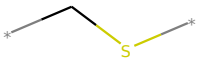

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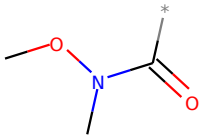

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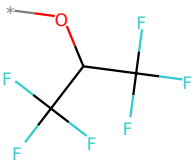

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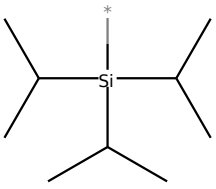

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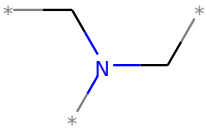

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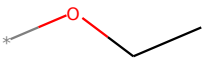

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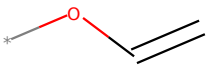

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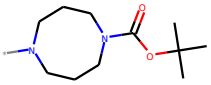

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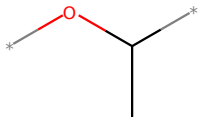

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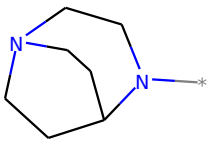

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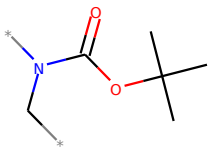

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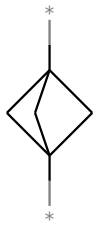

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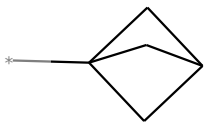

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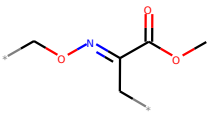

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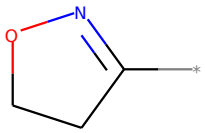

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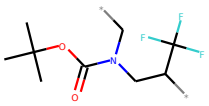

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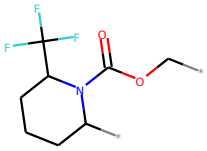

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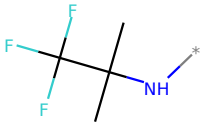

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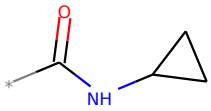

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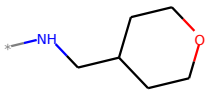

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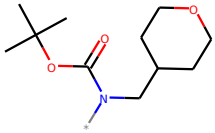

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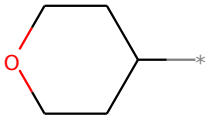

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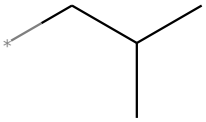

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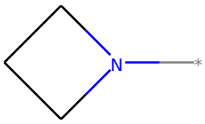

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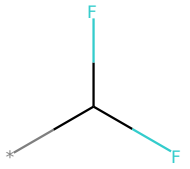

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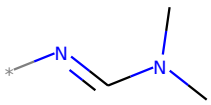

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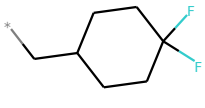

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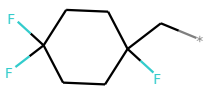

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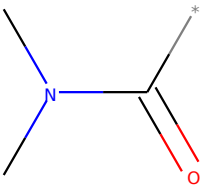

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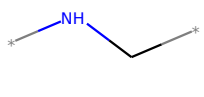

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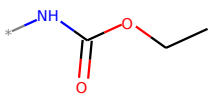

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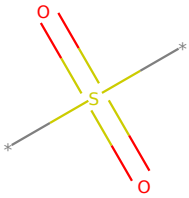

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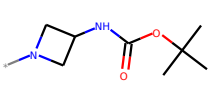

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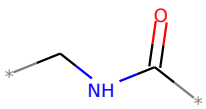

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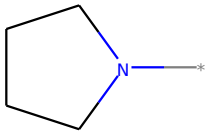

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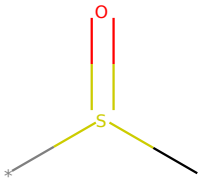

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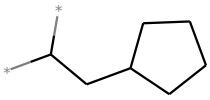

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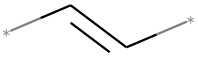

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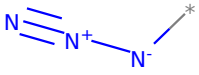

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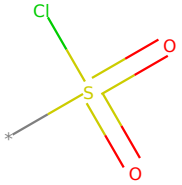

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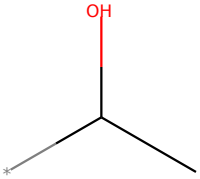

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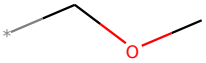

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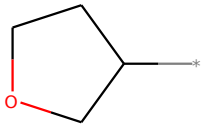

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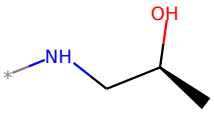

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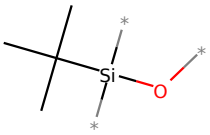

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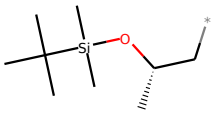

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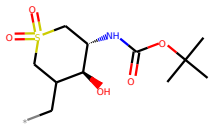

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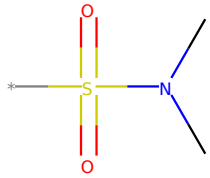

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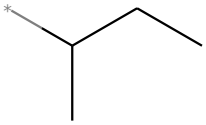

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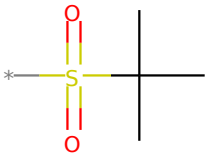

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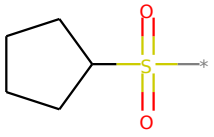

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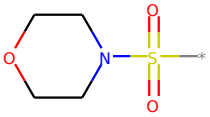

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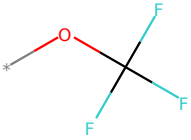

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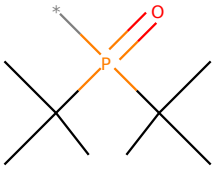

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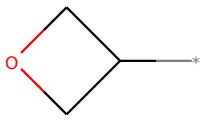

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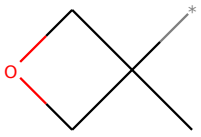

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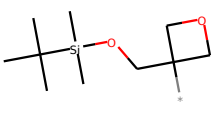

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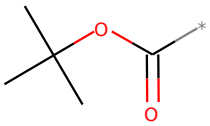

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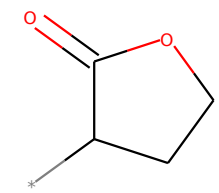

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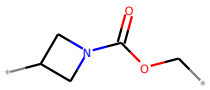

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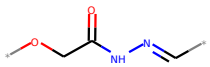

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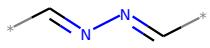

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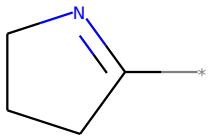

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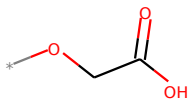

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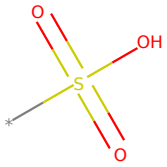

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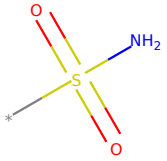

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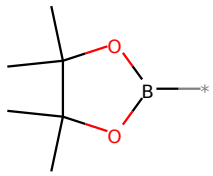

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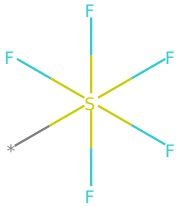

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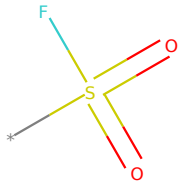

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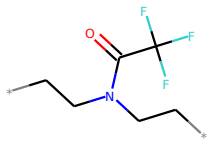

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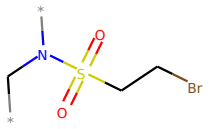

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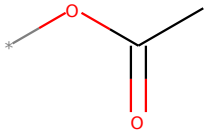

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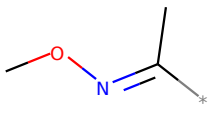

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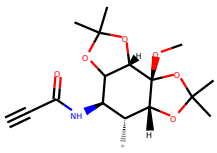

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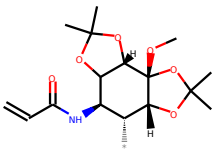

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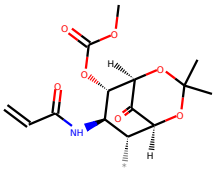

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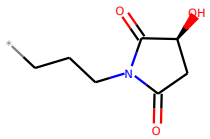

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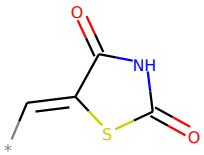

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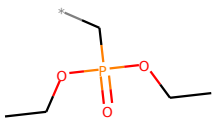

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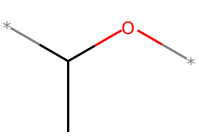

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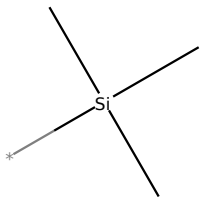

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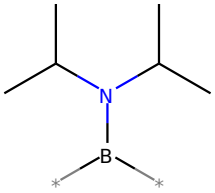

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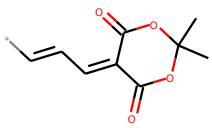

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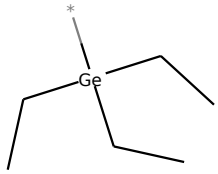

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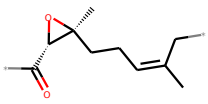

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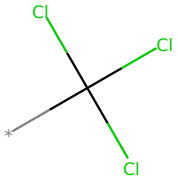

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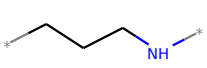

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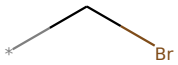

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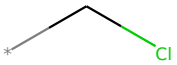

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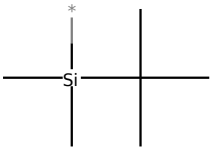

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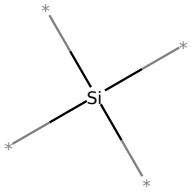

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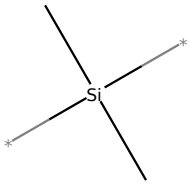

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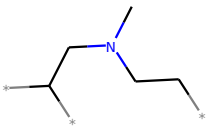

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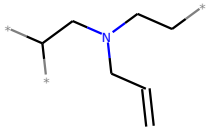

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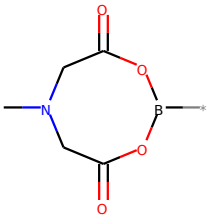

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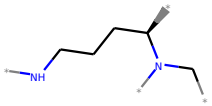

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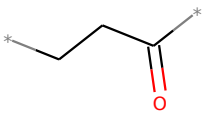

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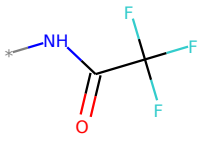

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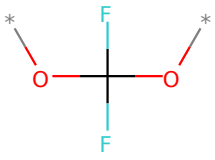

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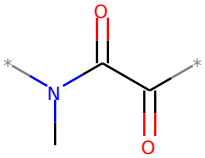

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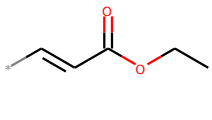

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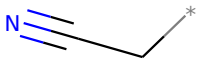

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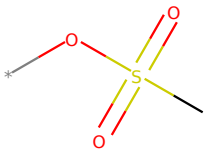

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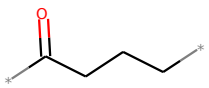

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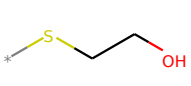

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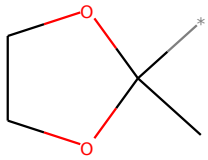

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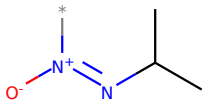

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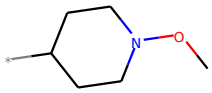

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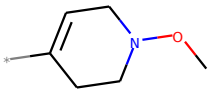

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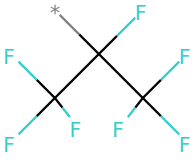

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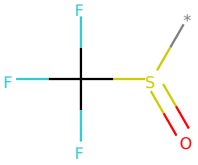

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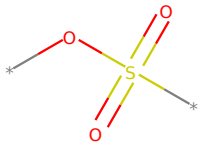

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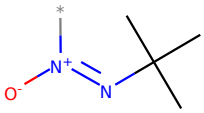

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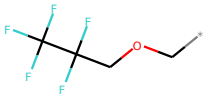

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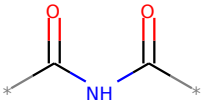

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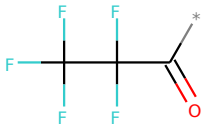

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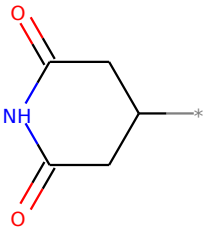

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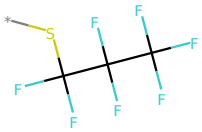

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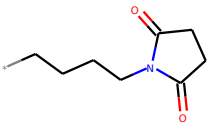

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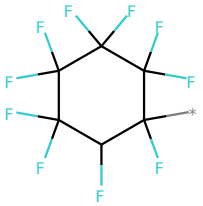

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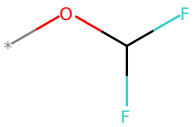

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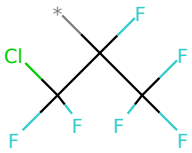

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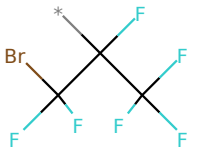

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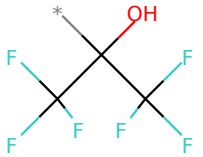

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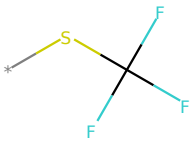

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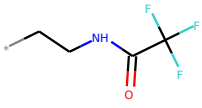

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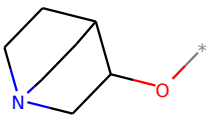

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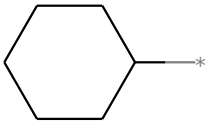

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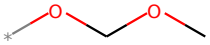

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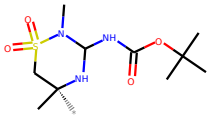

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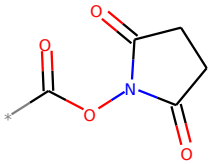

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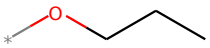

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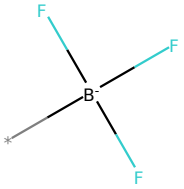
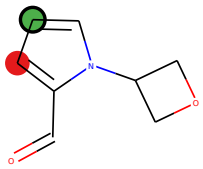


subst222

Section S4: Figure S2 Compounds sorted into EAS groups

Contents

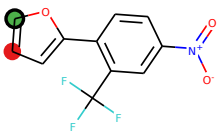
1 Pyrroles



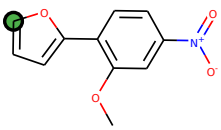
402 [111]

58% (NBS)

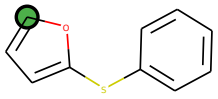
2 Furans



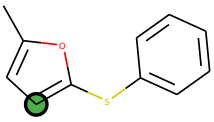
434 [457]
85% (NBS)



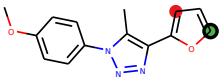
435 [457]
85% (NBS)



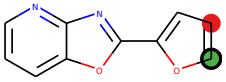
437 [264]
75% (NBS)



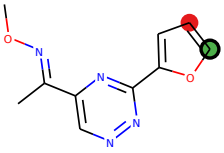
438 [436]
43% (NBS)



441 [343]
45% (NCS)

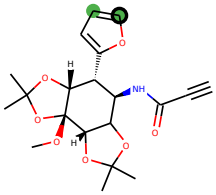


442 [170]
66% (Br_2)

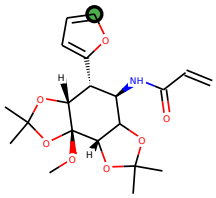


444 [84]
45% (NBS)

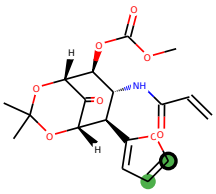
446 [444]
2xBr 65%, NBSD



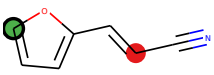
449 [320]
77% (NCS)



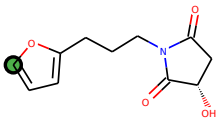
450 [320]
84% (NCS)



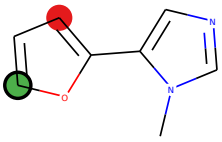
451 [321]
95% (NCS)



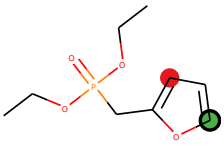
452 [376]
72% (NBS)



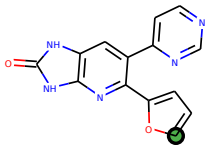
453 [376]
71% (NBS)



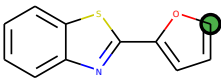
454 [1]
68% (Br_2)



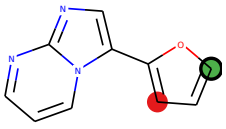
465 [344]
69% (Br_2)



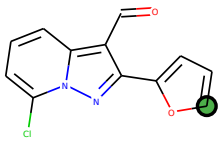
466 [383]
92% (Br_2)



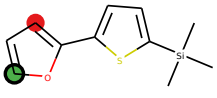
469 [300]
86% (Br_2)



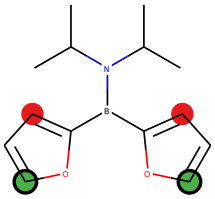
474 [365]
50% (Br_2)



476 [190]
80% (NBS)

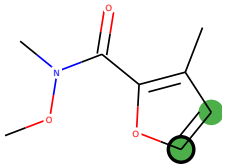


477 [308]
92% (NBS)



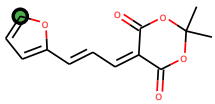
478 [237]

2xBr 70% (NBS)



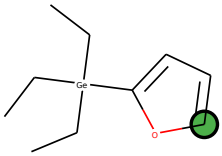
479 [401]

58% (Br_2)



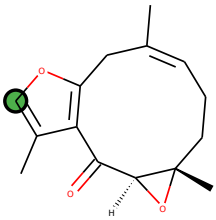
483 [265]

86% (NBS)



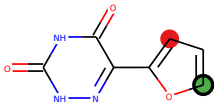
484 [289]

43% (NBS)



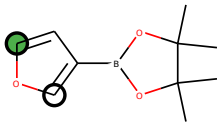
485 [379]

50% (NBS)



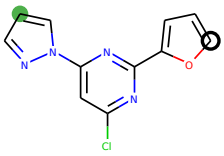
486 [3]

12, 76%



443 [241]

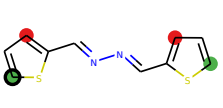
48% (NCS)



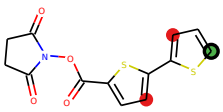
475 [137]

99% (NCS)

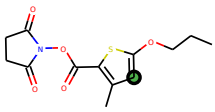
3 Thiophenes



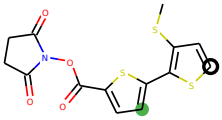
413 [303]
41% (NBS)



586 [47]
73% (NBS)

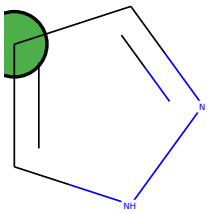


588 [182]
91% (Br_2)

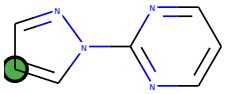


587 [447]
64% (NBS)

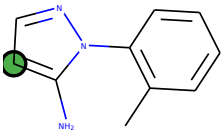
4 Pyrazoles



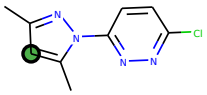
1 [313]
100% (NBS)



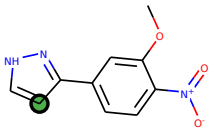
2 [393]
85% (Br_2)



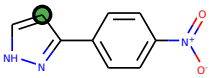
3 [49]
82% (Br_2)



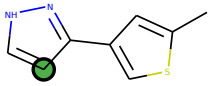
4 [397]
74% (SO_2Cl_2)



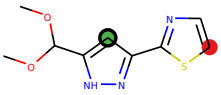
5 [12]
89% (NBS)



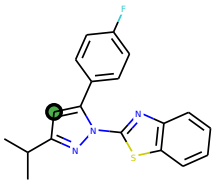
50 [13]
90% (NBS)



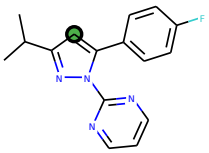
51 [388]
55% (NBS)



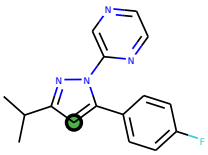
52 [219]
93% (Br_2, AcOH)



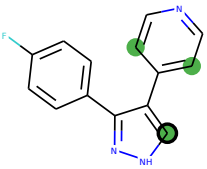
53 [345]
91% (NBS)



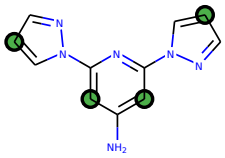
54 [345]
83% (NBS)



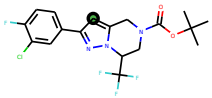
55 [345]
88% (NBS)



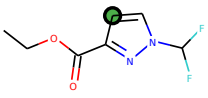
56 [255]
72% (NBS)



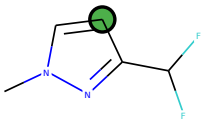
216 [103]
99% (I_2, 4xI)



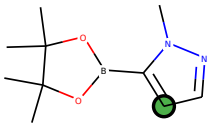
278 [407]
83% (NIS)



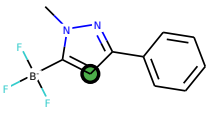
392 [85]
56% (NCS), 84% (NCS)



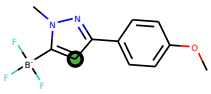
397 [459]
88% (NCS), 95% (NBS)



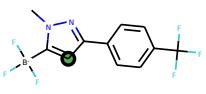
421 [127]
95% (NCS)



599 [178]
75% (NCS), 83% (NBS), 50% (NIS)

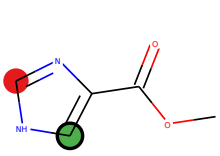


600 [178]
81% (NCS)

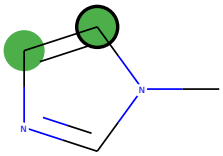


601 [178]
96% (NCS)

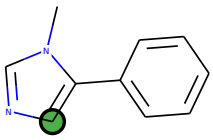
5 Imidazoles



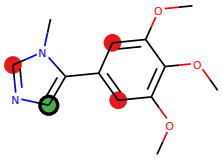
14 [120]
70% (NBS)



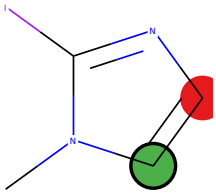
15 [168]
42% (NBS)



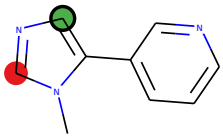
16 [61]
71% (NBS)



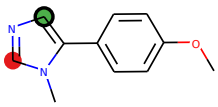
17 [59]
72% (NBS)



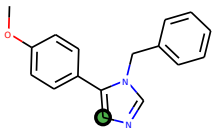
58 [76]
87% (NBS)



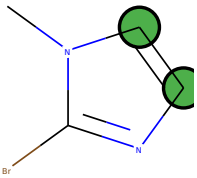
125 [59]
71% (NBS)



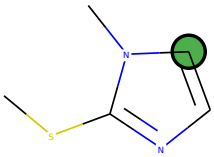
126 [58]
55% (NBS)



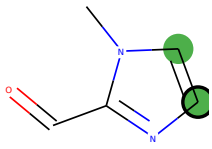
127 [60]
80% (NBS), 84% (NIS, TFA)



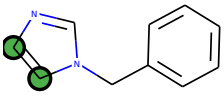
155 [167]
69% (I_2)



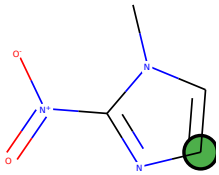
156 [121]
58% (NBS)



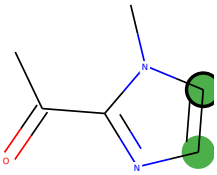
157 [382]
50% (HNO_3), 40% (NBS)



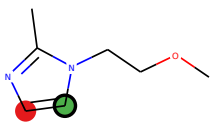
158 [16]
30% & 30% (NBS)



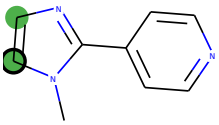
160 [336]
85% (NBS)



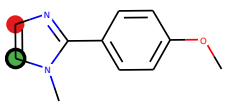
161 [380]
64% (NBS)



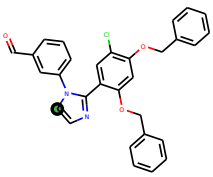
162 [208]
64% (NBS, K_2NO_3)



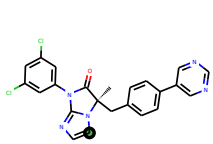
165 [251]
84% (NBS)



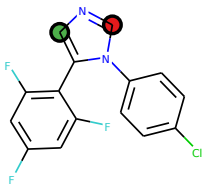
166 [306]
62% (Br_2)



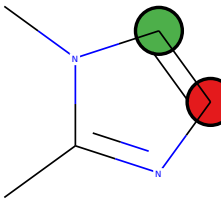
171 [254]
60% (NCS)



173 [425]
63% (NIS)

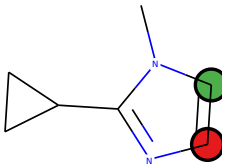


137 [270]
61% (Br_2), 68% (NCS)



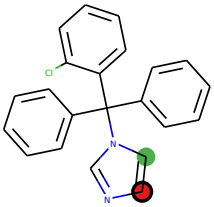
154 [62]

89% (NBS), b 50% (NBS)



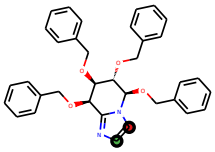
159 [181]

4-pos. 88% (NBS), 5-pos. 86% (NBS, K_2NO_3)



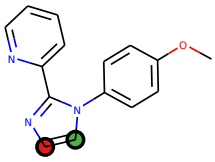
163 [228]

84% (NBS), 58% (NCS)



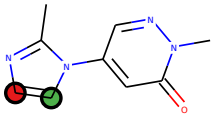
164 [402]

5-pos. 56%, 4+5-pos. 23% (NBS)



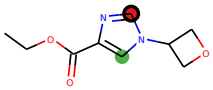
168 [342]

98% (Br_2)



169 [222]

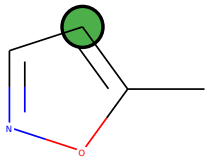
76% (NIS)



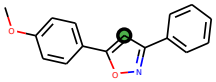
401 [71]

50% (NBS)

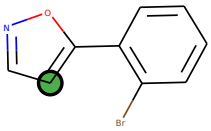
6 Isoxazoles



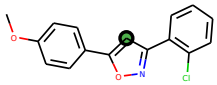
6 [455]
88% (NBS)



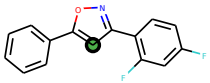
7 [387]
97% (NIS, TFA)



8 [276]
84% (NBS)

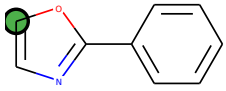


9 [150]
73% (NBS)

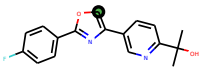


141 [377]
77% (NBS)

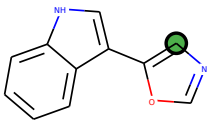
7 Oxazoles



43 [89]
56% (Br_2)

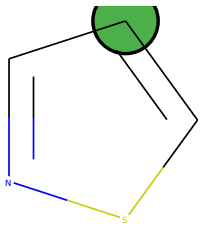


119 [114]
66% (NBS)

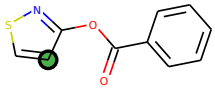


122 [450]
83% (NBS)

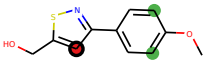
8 Isothiazoles



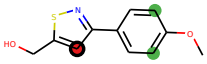
10 [351]
40% (Br_2)



11 [235]
88% (NBS)

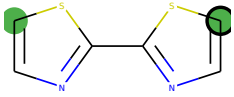


13 [396]
34% (NBS)



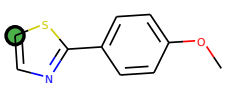
598 [?]
55% (NCS)

9 Thiazoles



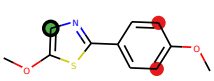
18 [395]

97% (NBS)



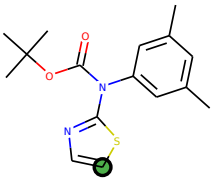
19 [333]

94% (NBS)



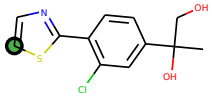
20 [398]

80% (NBS)



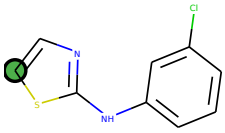
59 [372]

90% (NBS)



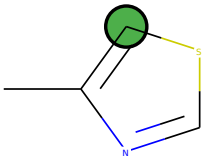
60 [399]

100% (NBS)



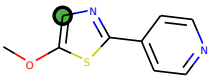
61 [177]

65% (NBS)



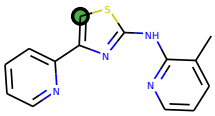
62 [110]

37% (Br_2, AcOH)



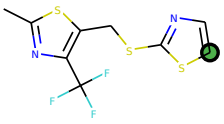
64 [454]

96% (NBS)



66 [211]

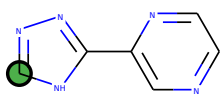
85% (NBS), 93% (NCS)



67 [149]

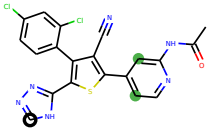
96% (NBS), 63% (NIS), 73% (HNO_3)

10 1,2,4-triazoles



147 [346]

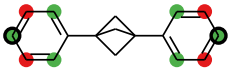
65% (Br_2/NaOH)



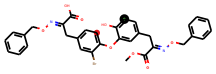
149 [46]

80% (NBS)

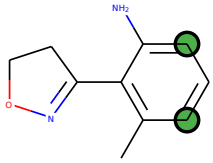
11 Benzenes



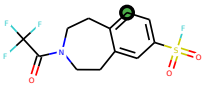
274 [146]
63% 2x para (I_2)



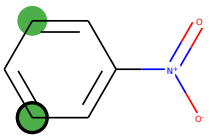
276 [134]
100% (NBS)



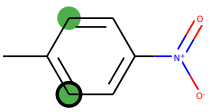
277 [285]
4-Br 75%, 6-Br 2%, 4+6-diBr 3%



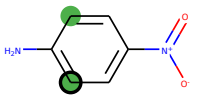
428 [189]
50% (NIS)



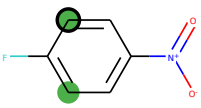
488 [281]
91% (NBS)



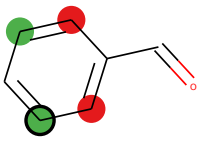
489 [421]
93% (NBS)



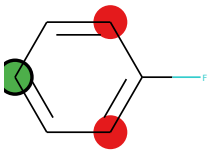
490 [141]
98% (NBS)



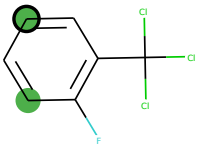
493 [6]
91% (NBS), 91% (NBS)



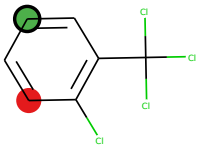
494 [159]
84% (NBS)



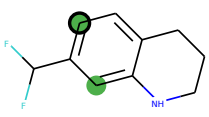
495 [349]
96% (NBS)



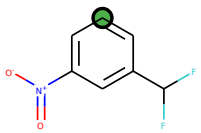
496 [400]
C12 96%



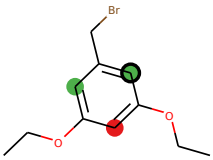
497 [400]
Cl2 82% 3-pos + 6-pos 8%



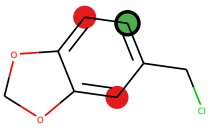
498 [359]
60% (NBS)



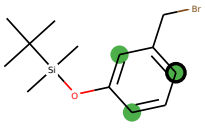
499 [25]
56% (NBS)



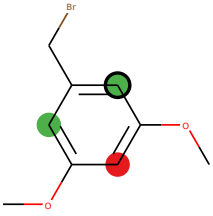
500 [442]
91% (NBS)



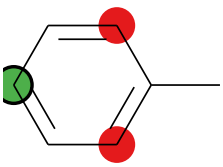
501 [249]
99% (NBS)



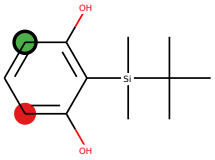
502 [277]
96% (NBS)



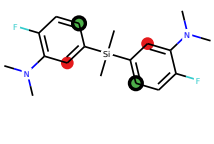
503 [117]
86% (NBS)



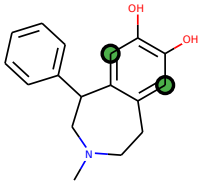
504 [247]
74% (Br_2)



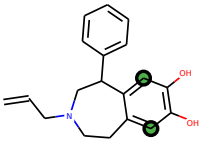
509 [215]
75% (NBS)



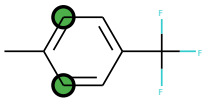
511 [95]
83% (NBS)



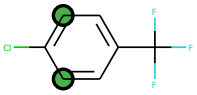
514 [318]
2xCl 55% ($AcOH/SO_2Cl_2$)



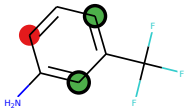
515 [318]
2xCl 55% ($AcOH/SO_2Cl_2$)



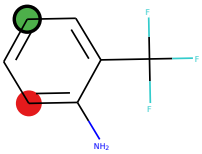
516 [126]
59% (NBS)



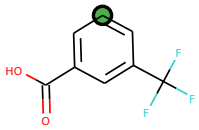
517 [159]
86% (NBS)



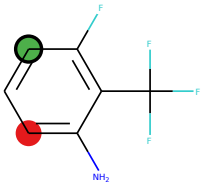
518 [169]
92% (NBS)



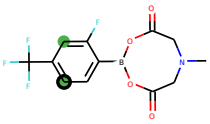
519 [112]
90% (NBS)



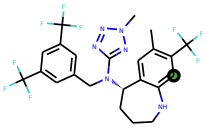
520 [288]
90% (NBS)



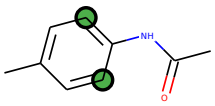
521 [96]
98% (NBS)



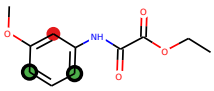
522 [124]
99% (NBS)



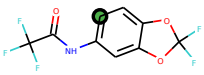
523 [109]
92% (NBS)



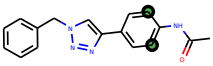
526 [5]
92% (NBS), 92% (NBS)



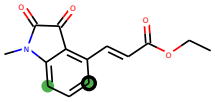
529 [65]
2xBr 98% (NBS)



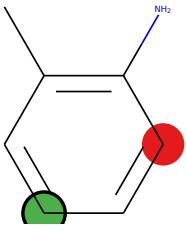
530 [97]
64% (NBS)



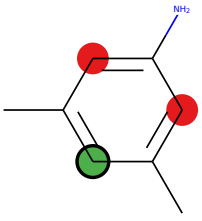
531 [185]
74% (NBS)



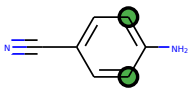
532 [391]
95% (NBS)



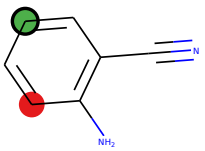
534 [327]
71% (NBS)



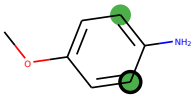
535 [460]
94% (NBS)



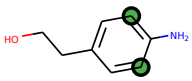
536 [390]
69% (NBS)



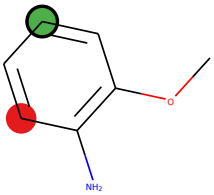
537 [238]
2xBr 77% (NBS)



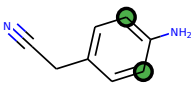
539 [290]
62% (NBS)



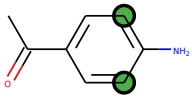
540 [363]
95% (NBS)



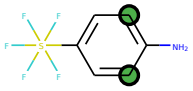
541 [422]
85% (NBS)



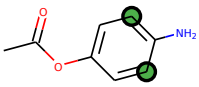
542 [176]
74% (NBS)



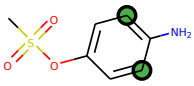
543 [315]
100% (NBS)



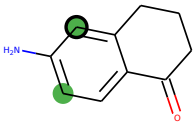
546 [180]
79% (NBS)



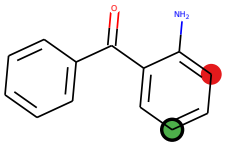
549 [30]
83% (NBS)



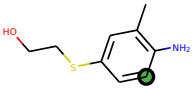
550 [322]
99% (NBS)



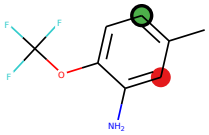
551 [358]
87% (NBS)



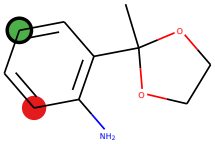
552 [287]
100% (NBS)



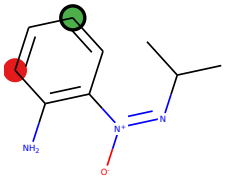
553 [4]
91% (NBS)



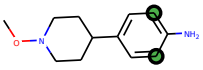
554 [451]
99% (NBS)



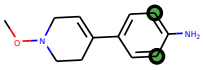
555 [259]
96% (NBS)



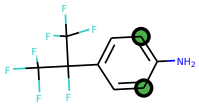
556 [282]
2xBr 92% (NBS)



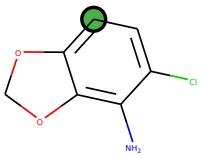
558 [43]
75% (NBS)



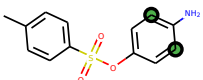
559 [216]
75% (NBS)



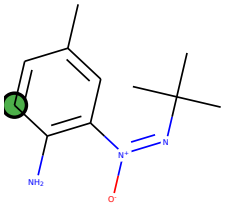
560 [260]
90% (NBS)



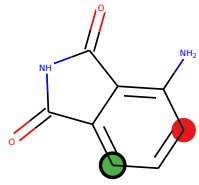
562 [386]
85% (NBS)



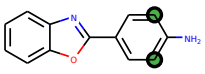
563 [123]
95% (NBS)



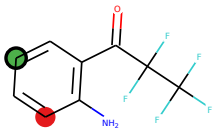
564 [282]
91% (NBS)



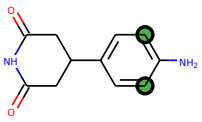
566 [27]
74% (NBS)



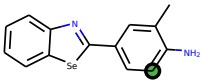
567 [307]
96% (NBS)



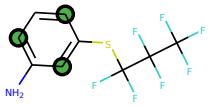
568 [452]
94% (NBS)



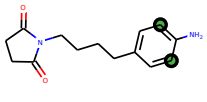
569 [217]
67% (NBS)



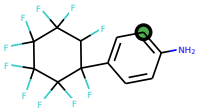
570 [8]
83% (NBS)



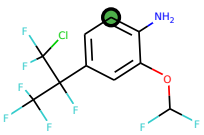
571 [325]
3xBr 89% (NBS)



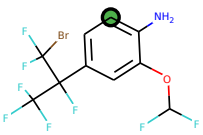
572 [256]
2xBr 90% (NBS), 1xBr 80% (NBS)



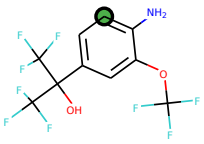
573 [304]
2xBr 96% (NBS)



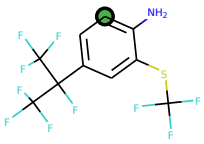
575 [385]
96% (NBS)



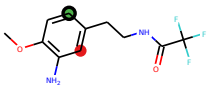
576 [304]
96% (NBS)



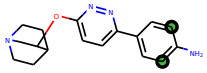
577 [324]
92% (NBS)



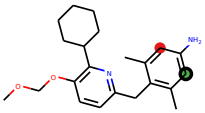
578 [326]
73% (NBS)



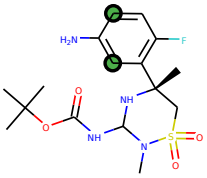
579 [252]
72% (NBS)



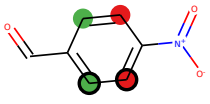
582 [226]
53% (NBS)



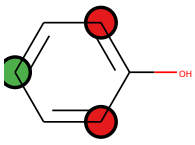
583 [244]
91% (NBS)



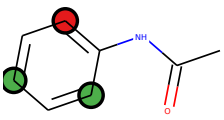
584 [373]
86% (NBS)



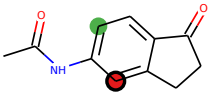
492 [352]
2xBr 96% (NBS)



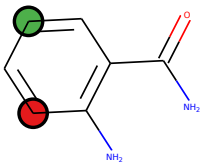
505 [341]
ortho + para 90% (Br_2), para 98% (NBS), 3xBr 97% (Br_2)



524 [5]
92% (NBS)

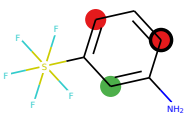


528 [428]
74% (NBS)



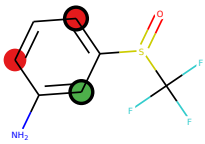
545 [55]

2xBr 91% (NBS), 2xBr 78% (NBS)



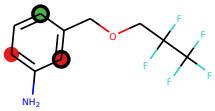
547 [180]

79% (NBS)



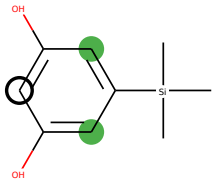
561 [66]

1xBr (1:1) 73% (NBS)



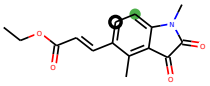
565 [239]

2xBr 77% (NBS)



508 [278]

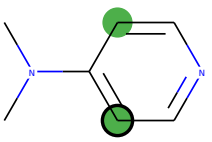
98% (NBS)



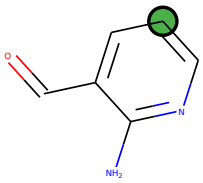
533 [391]

92% (NBS)

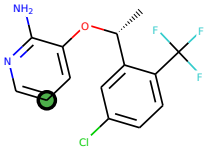
12 Pyridines



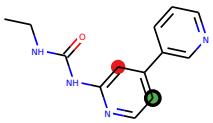
21 [340]
93% (Br_2, K_2CO_3)



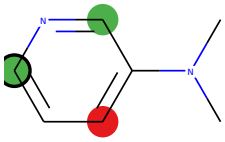
22 [158]
88% (Br_2)



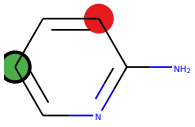
23 [424]
69% (NBS)



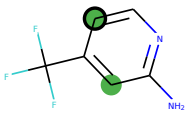
24 [54]
91% (NBS)



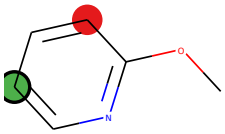
48 [347]
68% (NBS)



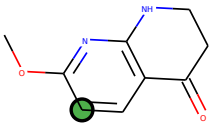
68 [271]
98% (NBS), 80% (NBS), 93% (I_2)



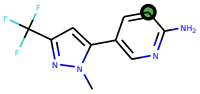
69 [93]
80% (NBS), 83% (NBS)



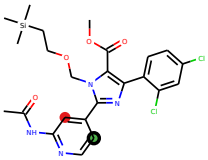
70 [295]
90% (Br_2, AcOH, NaOAc), 81% (5-Br; NBS), 73% (3,5-diBr; Br_2), 80% (NBS)



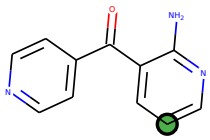
71 [100]
85% (NBS)



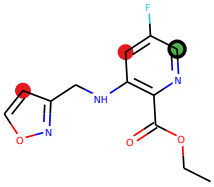
73 [173]
30% (NBS)



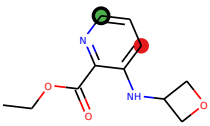
75 [106]
87% (NBS)



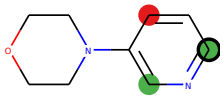
76 [195]
80% (NBS)



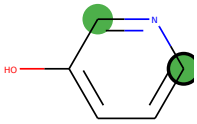
124 [72]
34% (NBS)



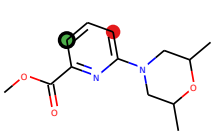
128 [72]
76% (NBS)



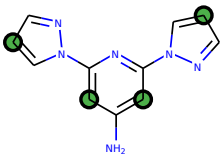
129 [207]
74% (NBS)



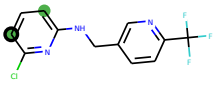
130 [164]
75% (NaI, NaOCl)



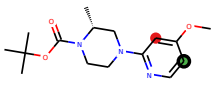
215 [430]
91% (NBS)



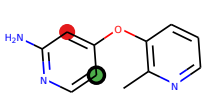
216 [103]
99% (I_2, 4xI)



217 [448]
80% (NBS)

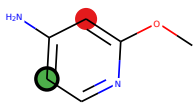


218 [136]
89% (NBS)



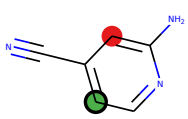
221 [17]

92% (Br_2)



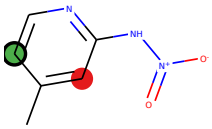
223 [311]

98% (NBS)



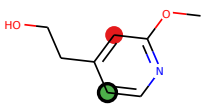
224 [39]

78% (NBS)



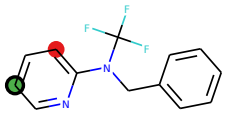
225 [148]

83% (Br_2))



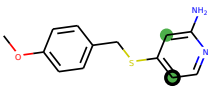
228 [426]

91% (Br_2)



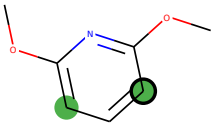
229 [242]

94% (Br_2)



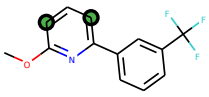
234 [19]

54% (Br_2)



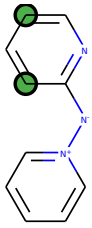
236 [98]

80% (NBS)



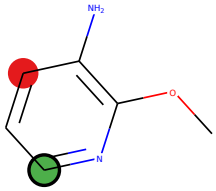
237 [240]

32% (3-Cl) + 50% (5-Cl) NCS



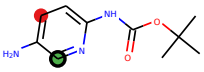
238 [94]

a 61% (2xI, NIS), 73% (2xBr, NBS), b 90% (NIS), 71% (NBS))



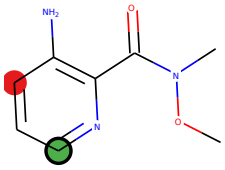
239 [243]

80% (NBS)



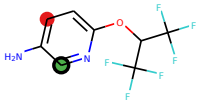
241 [101]

66% (NBS)



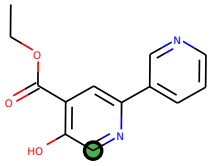
242 [138]

59% (Br_2)



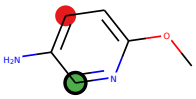
243 [323]

90% (NBS), 86% (NCS))



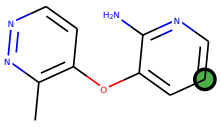
244 [63]

80% (NBS)



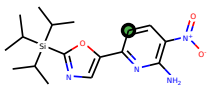
247 [81]

100% (Br_2)



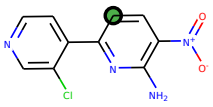
248 [18]

95% (NBS)



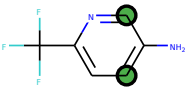
249 [414]

88% (NBS)



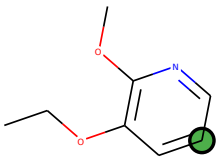
250 [414]

93% (NBS)



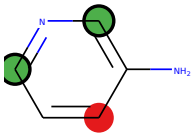
252 [233]

85% (NCS then NBS)



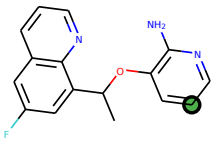
253 [67]

2-Br 56%, 3-Br (Br_2)



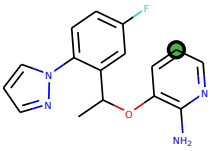
255 [98]

2-Br 40%, 6-Br 32%, 2+6-diBr 14% (NBS)



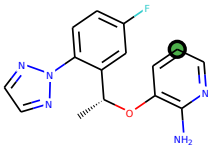
256 [91]

99% (NBS)



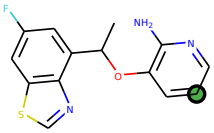
257 [91]

93% (NBS)



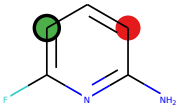
258 [91]

73% (NBS)



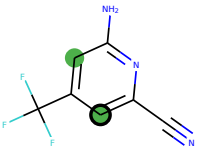
259 [91]

51% (NBS)



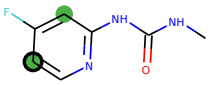
296 [51]

98% (NBS)



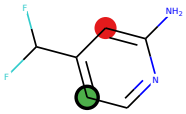
297 [431]

70% (NBS)



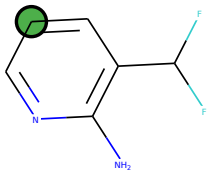
298 [157]

72% (NBS)



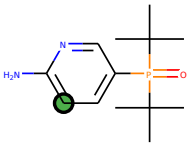
391 [125]

79% (NBS)



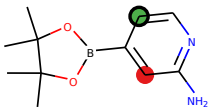
395 [174]

64% (NBS)



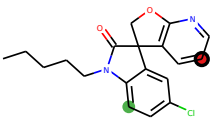
400 [4]

68% (NBS)



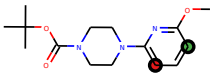
420 [283]

85% (NBS)



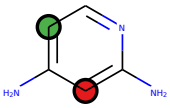
74 [80]

76% (NBS)



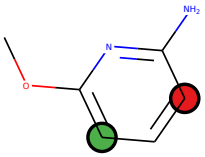
219 [136]

58% (a-to-OMe), 13% (a-to-N) NBS



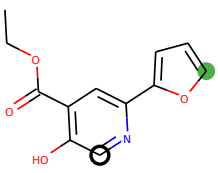
220 [319]

90% (a-to-2xN), 9% regioisomer, I_2



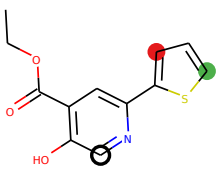
235 [52]

73% (3-pos), 11% (5-pos), NCS



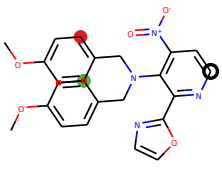
245 [63]

91% (NBS)



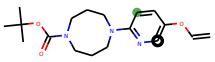
246 [63]

71% (NBS)



251 [415]

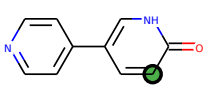
52% (NBS)



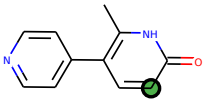
254 [38]

52% (NBS)

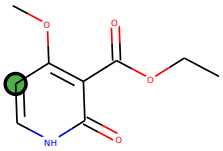
13 2-Pyridones



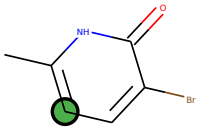
77 [378]
90% (NBS)



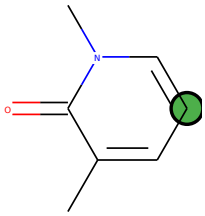
78 [236]
82% (NBS), 93% (NIS)



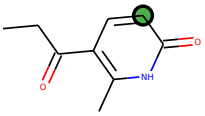
79 [225]
90% (NBS, NH_4NO_3)



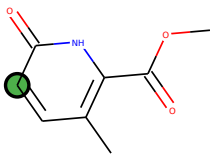
80 [368]
91% (NIS)



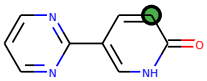
81 [187]
96% (NBS)



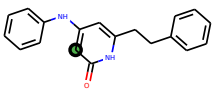
82 [381]
82% (NBS)



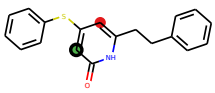
83 [155]
70% (NBS)



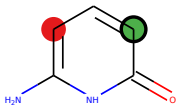
84 [330]
51% (NBS)



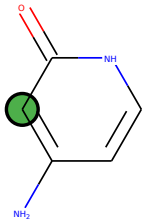
213 [99]
92%(NIS)



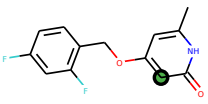
214 [99]
75% (NBS), 91% (NIS)



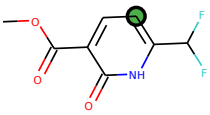
227 [317]
65% (NBS)



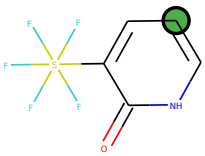
230 [299]
70% (NBS)



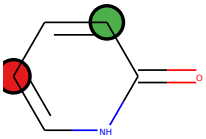
233 [26]
85% (NCS)



398 [458]
65% (NBS)

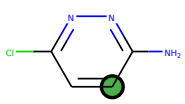


427 [230]
74% (NBS)



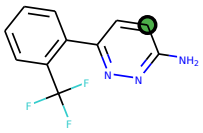
226 [369]
95% (NBS), 34% (2xBr) + 29% (4-Br) + 3% (3-Br) NBS, 76% (5-Br) + 11% (3-Br)

14 Pyridazines



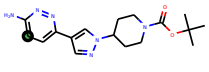
32 [272]

82% (Br_2, $NaHCO_3$)



33 [102]

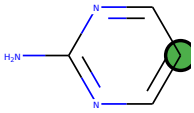
95% (Br_2, $NaHCO_3$)



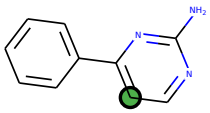
34 [7]

57% (Br_2, $NaHCO_3$)

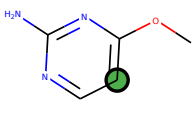
15 Pyrimidines



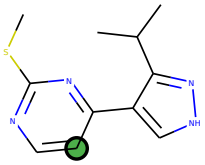
25 [198]
100% (NBS, NH_4OAC)



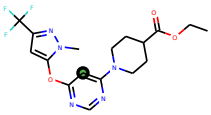
26 [56]
51% (NBS)



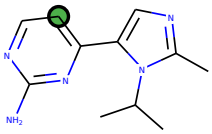
27 [93]
96% (NBS)



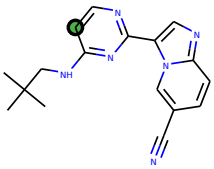
28 [113]
90% (NBS)



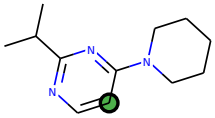
29 [234]
57% (NBS)



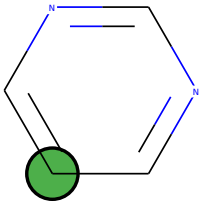
85 [231]
74% (NIS)



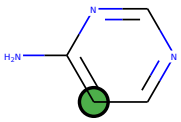
86 [162]
98% (NBS)



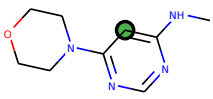
87 [87]
82% (NBS)



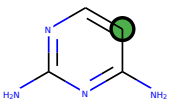
88 [266]
88% (Br_2)



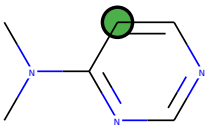
89 [130]
59% (NBS)



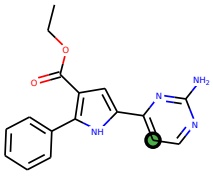
90 [246]
78% (Br_2)



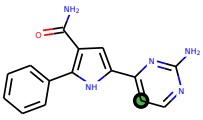
91 [93]
74% (NBS), 87% (Br_2)



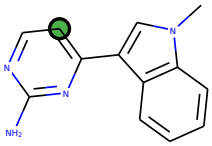
92 [340]
91% (NBS)



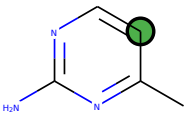
93 [406]
58% (NCS), 65% (NBS)



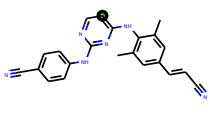
94 [406]
72% (NCS), 75% (NBS)



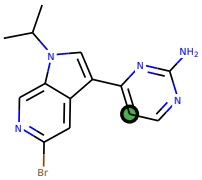
96 [360]
94% (NBS)



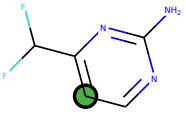
97 [93]
99% (NBS)



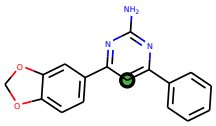
98 [191]
86% (NBS)



324 [213]
69% (NIS), 79% (NCS)

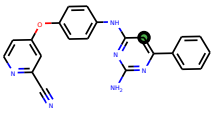


390 [125]
98% (NBS)



593 [405]

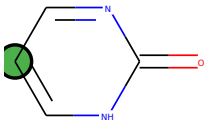
70% (Br_2)



597 [153]

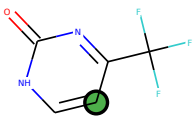
83% (Br_2)

16 Pyrimidin-2(1H)-ones



99 [416]

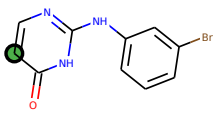
50% (Br_2), 84% (Br_2)



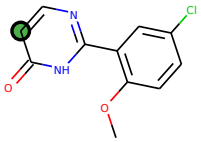
100 [331]

80% (Br_2, KOAc)

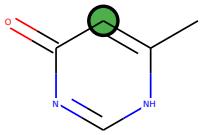
17 Pyrimidin-4(3H)-ones



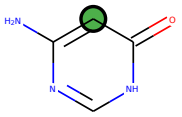
101 [293]
82% (NCS), 73% (NBS), 97% (NIS)



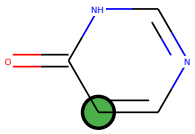
102 [355]
86% (Br_2)



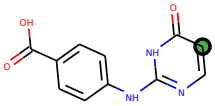
103 [143]
74% (NCS), 94% (NBS), 100% (ICI, AcOH)



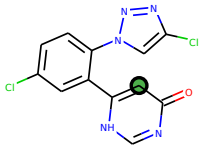
104 [356]
47% (Br_2)



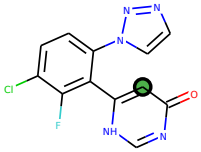
105 [70]
92% (Br_2)



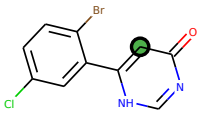
106 [446]
95% (Br_2, AcOH)



594 [133]
93% (NBS)

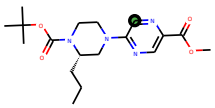


595 [132]
54% (NCS)

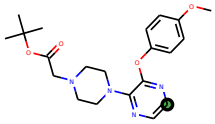


596 [133]
94% (NCS)

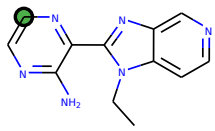
18 Pyrazines



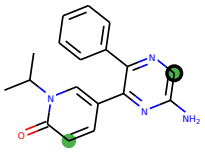
30 [253]
98% (NBS)



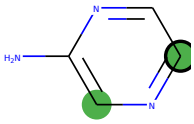
31 [129]
70% (NBS)



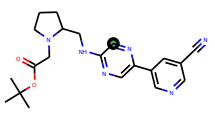
49 [21]
79% (NBS), 78% (NBS)



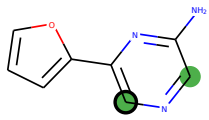
107 [439]
79% (NBS)



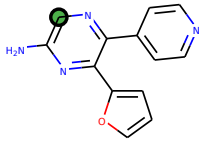
108 [275]
82% (NBS), 5-Br 62% + 3,5diBr 12% (NBS), 72% (NBS), 90% (NBS); 83% (NBS), 77% (NBS)



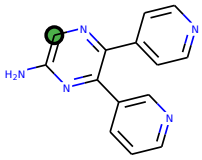
109 [129]
66% (NBS)



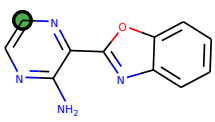
131 [410]
44% (NBS)



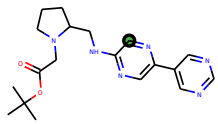
132 [411]
75% (NBS), 75% (NBS)



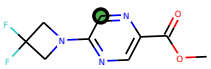
133 [412]
30% (NBS)



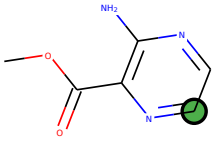
134 [50]
62% (NBS)



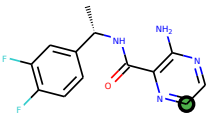
135 [129]
77% (NBS)



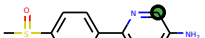
192 [68]
77% (NBS)



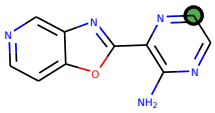
193 [267]
88% (NIS), 88% (NIS), 96% (NBS), 70% (Br_2), 72% (NCS)



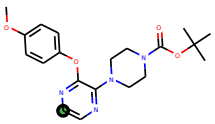
194 [33]
84% (NBS)



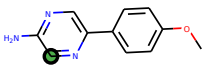
196 [104]
84% (NBS), 65% (NIS)



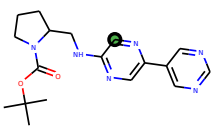
198 [15]
95% (NBS)



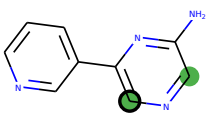
199 [128]
70% (NBS)



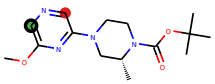
200 [184]
70% (Br_2)



201 [128]
77% (NBS)

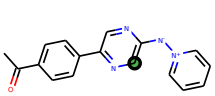


202 [161]
72% (NBS)



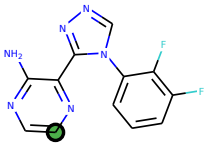
203 [136]

26%/26% (NBS) two mono-Br



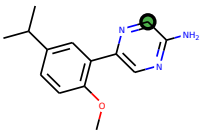
205 [10]

84% (NBS)



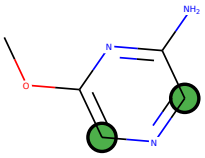
206 [34]

78% (NBS)



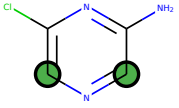
207 [20]

74% (NBS)



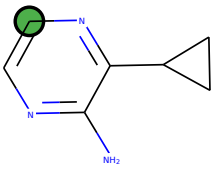
211 [52]

45% (3-Br), 16% (5-Br), 10% (3+5-Br_2)



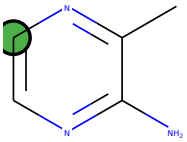
212 [166]

15% (3-Br), 43% (5-Br), 88% (NIS), 2xBr 95% (NBS)



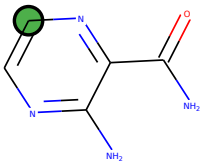
284 [188]

64% (NBS)



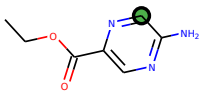
285 [429]

80% (NCS)



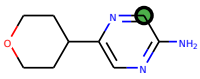
286 [438]

95% (Br_2)



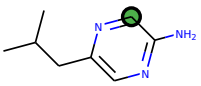
289 [210]

78% (NBS)



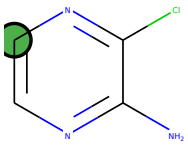
290 [40]

97% (NBS)



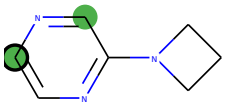
291 [314]

77% (Br_2)



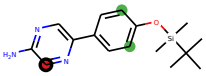
292 [186]

76% (NIS), 71% (NIS)



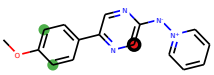
293 [232]

73% (NBS)



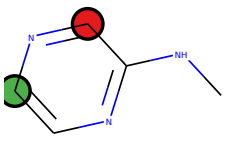
195 [218]

81% (NBS)



209 [10]

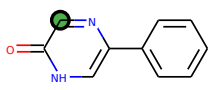
86% (NBS)



283 [165]

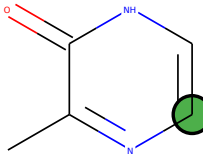
65% (NIS)

19 Pyrazinones



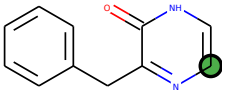
190 [370]

59% (Br_2), 76% also p-phenyl (Br_2)



197 [108]

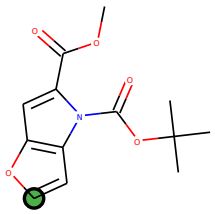
77% (NBS)



204 [23]

74% (NBS)

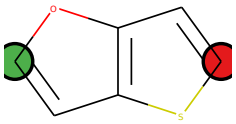
20 4H-Furo[3,2-b]pyrroles



472 [205]

65% (NBS)

21 4H-Thieno[3,2-b]pyrroles

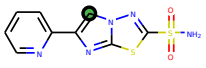


471 [206]

2xBr 92% (NBS), 67% (96:4)

mono-O over mono-S

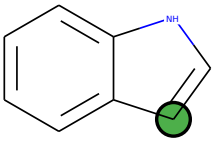
22 Imidazo[2,1-b][1,3,4]thiadiazoles



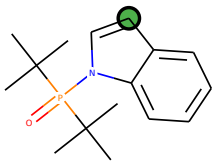
418 [224]

84% (Br_2)

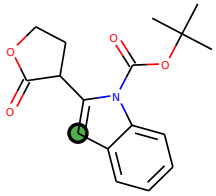
23 Indoles



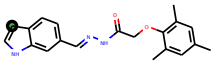
35 [364]
96% (Br_2)



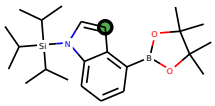
399 [437]
I2, 1xI, 3pos, 48%, NCS, 1xCl 3 pos, 81% + 2,3-diCl, 10%



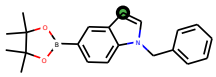
407 [78]
95% (NBS)



412 [115]
32% (NBS)

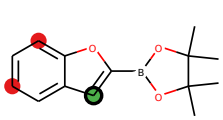


425 [245]
98% (NCS)

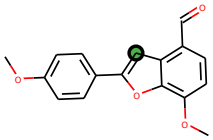


426 [11]
82% (NCS)

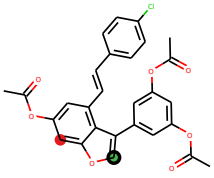
24 Benzofurans



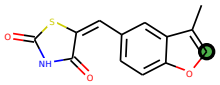
424 [241]
39% (NCS)



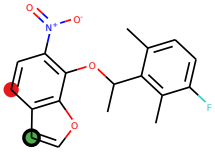
430 [417]
60% (NBS)



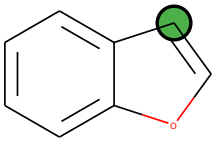
431 [417]
70% (NBS)



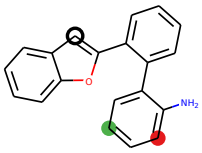
461 [361]
66% (Br_2)



468 [274]
84% (Br_2)

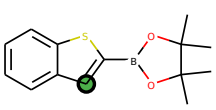


470 [212]
3xBr 76% (Br_2),2xBr (2+3 positions), 84% (Br_2)



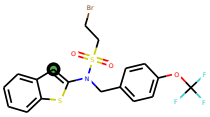
433 [196]
12, 94%

25 Benzo[b]thiophenes



423 [241]

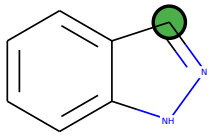
70% (NCS)



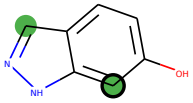
429 [291]

96% (NBS), 100% (NCS)

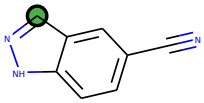
26 Indazoles



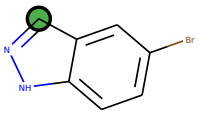
353 [294]
82% (NBS), 60% (NCS)



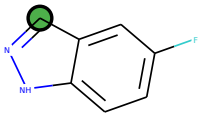
354 [44]
54% (NCS), 95% (HNO_3)



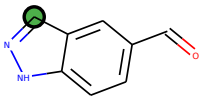
355 [443]
89% (NBS)



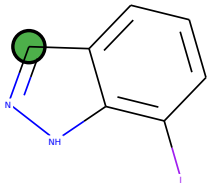
356 [367]
91% (NCS)



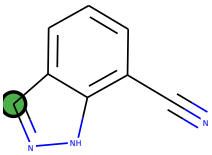
357 [192]
59% (NBS)



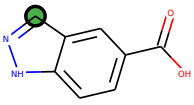
358 [302]
97% (NCS), 82% (NBS)



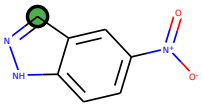
359 [310]
79% (NBS)



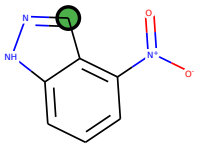
360 [310]
74% (NBS)



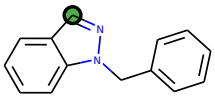
361 [131]
84% (NCS)



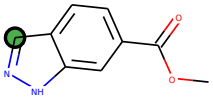
362 [353]
90% (NBS)



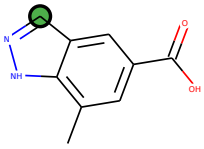
363 [9]
84% (NBS), 90% (NBS)



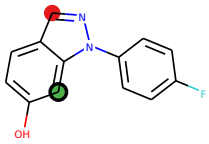
364 [440]
90% (NBS)



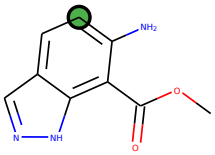
365 [413]
96% (NBS)



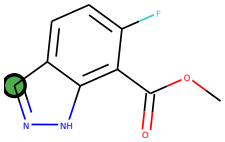
366 [131]
98% (NCS)



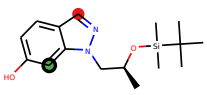
370 [179]
63% (NBS)



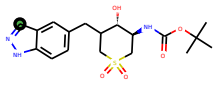
371 [286]
90% (NIS), 82% (NBS)



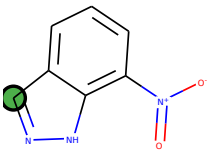
372 [83]
69% (NBS)



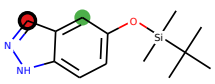
374 [298]
77% (NBS)



375 [362]
97% (NBS)

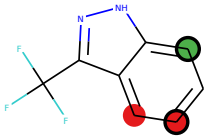


383 [353]
90% (NBS), 84% (NBS), 90% (NBS)



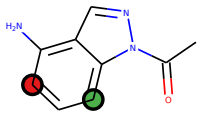
367 [261]

98% (NIS)



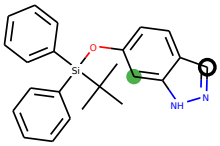
368 [456]

5-Br 35%, 7-Br 6%



369 [90]

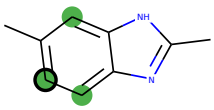
5-Br 66%, 7-Br 11%



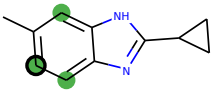
373 [420]

57% (NCS)

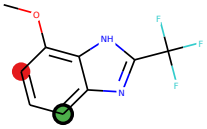
27 1H-benzo[d]imidazoles



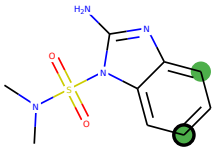
377 [250]
58% (NCS)



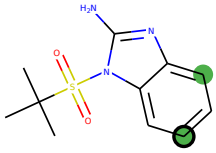
378 [250]
68% (NCS)



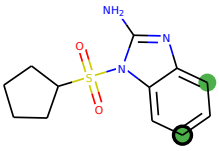
381 [328]
63% (NBS)



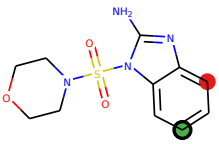
382 [75]
99% (NIS)



385 [145]
72% (NIS)

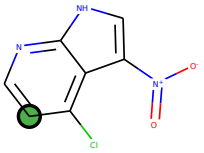


387 [145]
94% (NIS)

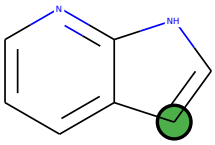


388 [79]
89% (NIS)

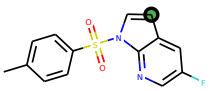
28 7-Azaindoles



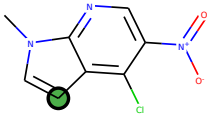
334 [194]
90% (NBS)



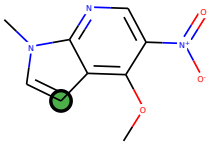
335 [44]
NBS



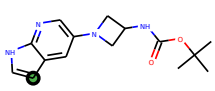
336 [175]
97% (NBS)



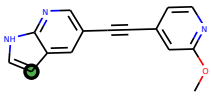
337 [69]
100% (NIS)



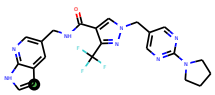
338 [69]
63% (NIS)



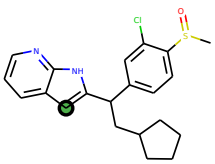
339 [220]
99% (NIS)



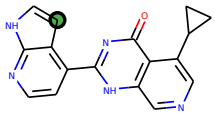
340 [280]
80% (NIS)



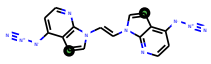
341 [384]
80% (NCS)



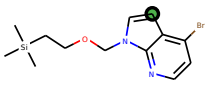
342 [334]
98% (NBS)



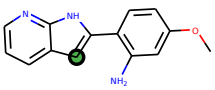
343 [156]
48% (NBS)



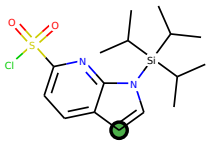
344 [427]
2xBr 49% (NBS), 2xCl 78% (NCS)



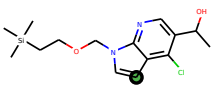
345 [171]
76% (NBS)



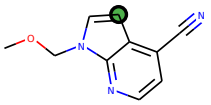
346 [337]
84% (NBS)



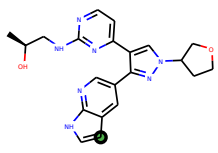
347 [151]
84% (NBS)



348 [203]
54% (NBS)

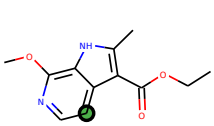


349 [32]
80% (NIS)

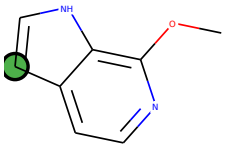


351 [139]
40% (NCS)

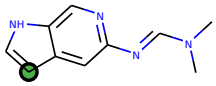
29 6-azaindoles



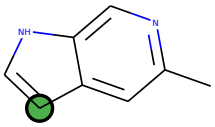
316 [14]
80% (NBS)



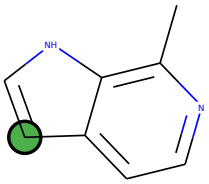
322 [202]
93% (NIS)



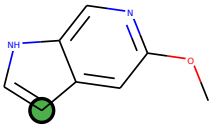
323 [73]
52% (NIS)



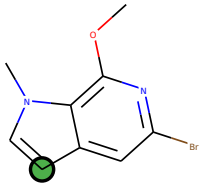
325 [248]
92% (NBS)



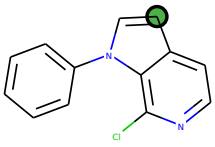
326 [248]
78% (NBS)



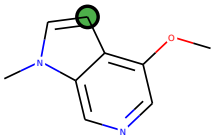
327 [154]
100% (NIS)



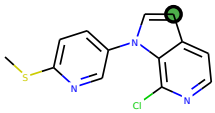
328 [423]
94% (NIS)



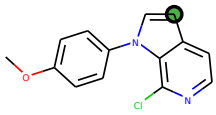
329 [116]
90% (NBS)



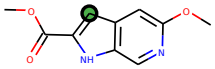
330 [36]
91% (NIS)



331 [389]
97% (NIS)

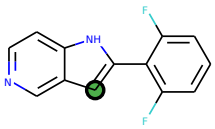


332 [389]
88% (NBS)

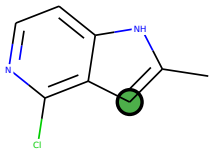


333 [29]
86% (NIS)

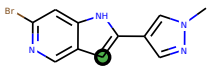
30 5-azaindoles



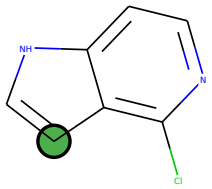
317 [419]
86% (NBS)



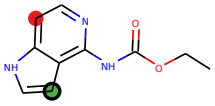
318 [409]
91% (NIS)



319 [37]
76% (NCS)

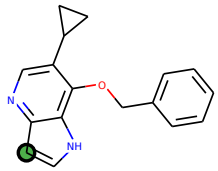


320 [229]
68% (NBS)

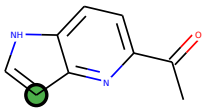


321 [77]
72% (NIS)

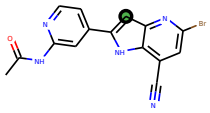
31 4-azaindoles



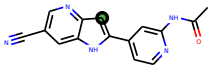
300 [445]
68% (NIS)



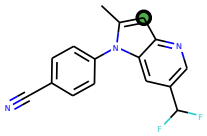
301 [273]
96% (NCS)



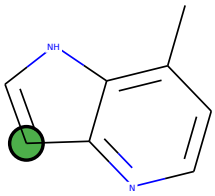
302 [339]
83% (NIS)



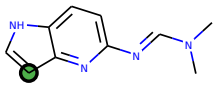
303 [339]
71% (NIS)



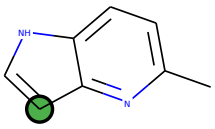
304 [140]
94% (NIS), 94% (NIS)



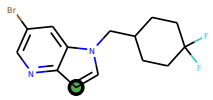
305 [118]
94% (NIS)



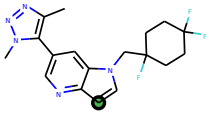
306 [73]
100% (NIS)



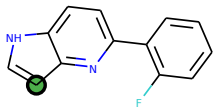
307 [24]
92% (NBS)



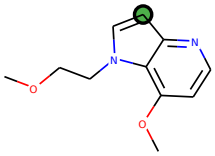
308 [449]
98% (NIS)



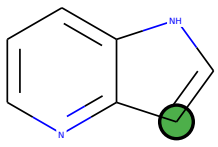
309 [449]
70% (NBS)



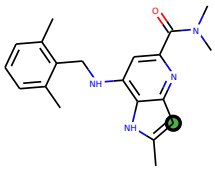
310 [305]
73% (NIS)



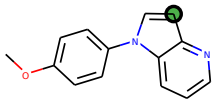
311 [119]
66% (NIS)



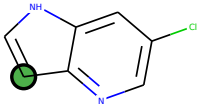
312 [31]
89% (NBS), 67% (NBS)



313 [335]
71% (NBS)

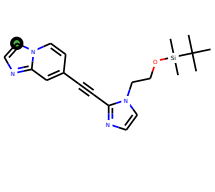


314 [389]
95% (NBS)

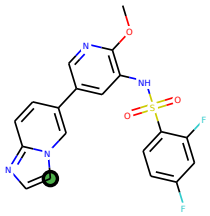


315 [142]
86% (NBS)

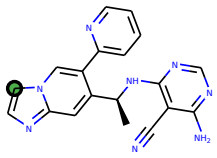
32 Imidazo[1,2-a]pyridines



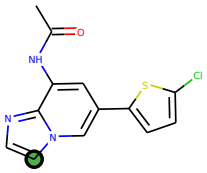
170 [64]
100% (NIS)



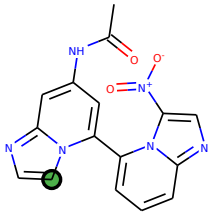
172 [432]
90% (NIS)



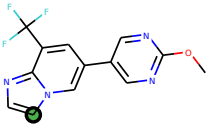
174 [284]
69% (NCS)



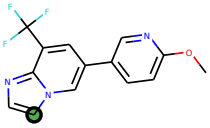
176 [160]
98% (NBS)



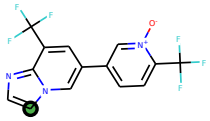
177 [197]
98% (HNO_3)



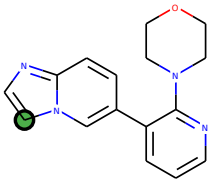
178 [375]
79% (NBS)



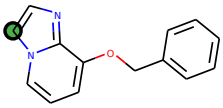
179 [375]
75% (NBS)



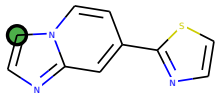
180 [375]
77% (NBS)



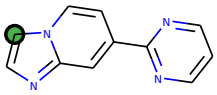
182 [375]
81% (NBS)



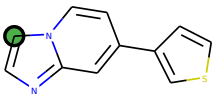
184 [163]
83% (NBS)



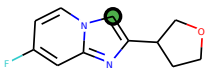
187 [48]
67% (NBS)



188 [371]
96% (NIS)

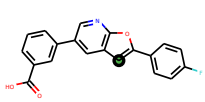


189 [172]
98% (NBS)

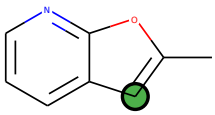


408 [199]
85% (NIS)

33 Furo[2,3-b]pyridines

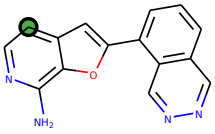


455 [348]
53% (NBS)

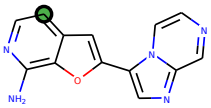


462 [316]
54% (Br_2)

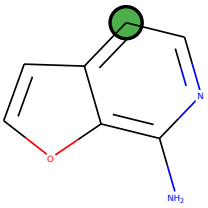
34 Furo[2,3-c]pyridines



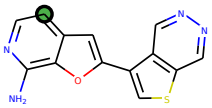
268 [209]
85% (NIS)



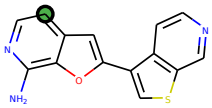
269 [209]
67% (NIS)



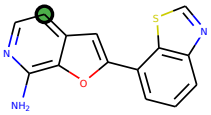
270 [209]
86% (NIS)



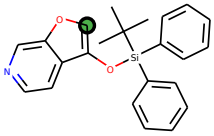
271 [209]
88% (NIS)



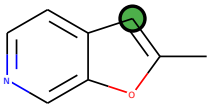
272 [209]
77% (NIS)



273 [209]
92% (NIS)

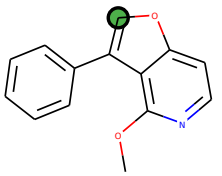


473 [90]
90% (Br_2)



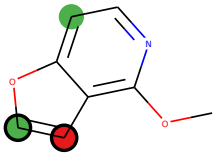
480 [435]
57% (Br_2)

35 Furo[3,2-c]pyridines



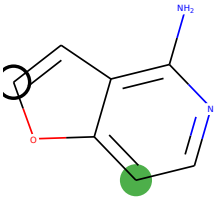
459 [57]

86% (Br_2)



460 [57]

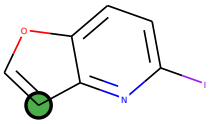
2xBr 99% (Br_2)



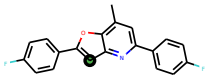
482 [404]

12, 68%

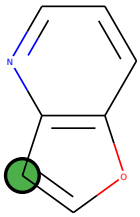
36 furo[3,2-b]pyridines



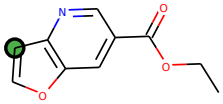
439 [338]
72% (Br_2)



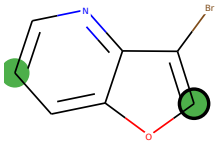
440 [436]
43% (NBS)



447 [357]
46% (Br_2)

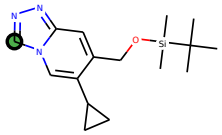


448 [357]
51% (Br_2)

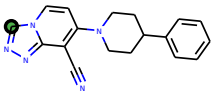


481 [434]
85% (Br_2)

37 [1,2,4]Triazolo[4,3-a]pyridines

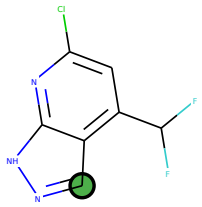


143 [262]
80% (NBS)



150 [122]
78% (NBS)

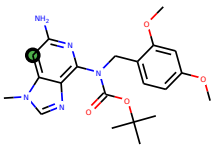
38 1H-Pyrazolo[3,4-b]pyridines



394 [22]

70% (NIS)

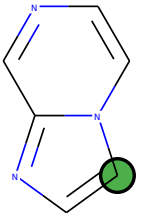
39 1H-Imidazo[4,5-c]pyridines



265 [350]

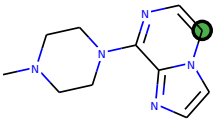
82% (NIS)

40 Imidazo[1,2-a]pyrazines



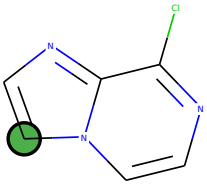
38 [200]

86% (NBS), 95% (Br_2)



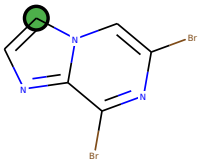
39 [301]

55% (NBS), 59% (NBS)



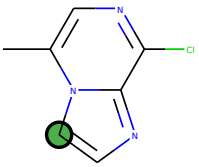
40 [53]

99% (NBS)



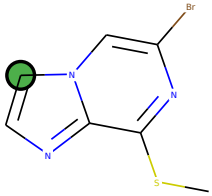
111 [82]

75% (NIS)



112 [292]

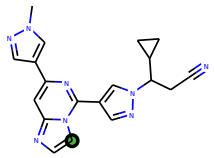
69% (NBS)



186 [258]

96% (NIS)

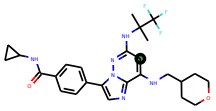
41 Imidazo[1,2-c]pyrimidines



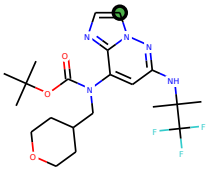
175 [392]

75% (NIS)

42 Imidazo[1,2-b]pyridazines

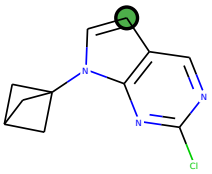


280 [268]
68% (NCS)

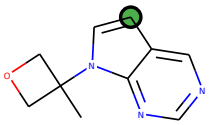


281 [214]
95% (NIS)

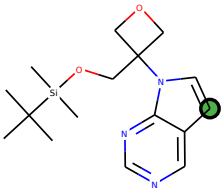
43 7H-Pyrrolo[2,3-d]pyrimidines



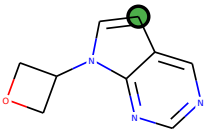
275 [134]
72% (NIS)



403 [28]
78% (NIS)

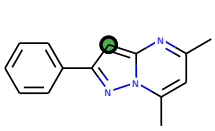


404 [28]
75% (NIS)



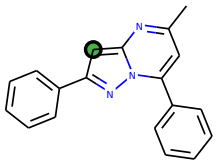
405 [28]
49% (NIS)

44 Pyrazolo[1,5-c]pyrimidines



36 [193]

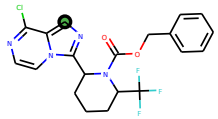
87% (Br_2)



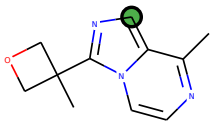
115 [279]

87% (NBS), 60% (NIS)

45 Imidazo[1,5-a]pyrazines

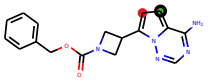


279 [144]
100% (NIS)



406 [296]
78% (NBS)

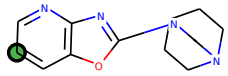
46 Pyrrolo[2,1-f][1,2,4]triazines



411 [11]

Br_2Me_2-hydantion, 100%

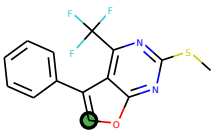
47 Oxazolo[4,5-b]pyridines



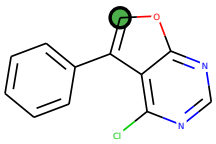
264 [329]

78% (Br_2)

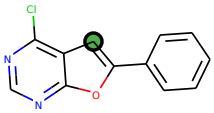
48 Furo[2,3-d]pyrimidines



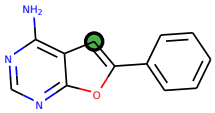
457 [57]
93% (Br_2)



463 [135]
68% (NBS)

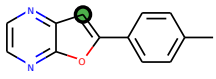


464 [135]
68% (NBS)



467 [403]
78% (NBS)

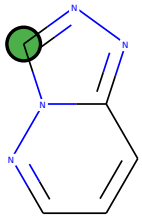
49 Furo[2,3-b]pyrazines



487 [2]

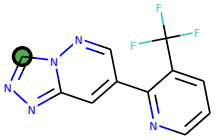
80% (Br_2)

50 [1,2,4]Triazolo[4,3-b]pyridazines



41 [263]

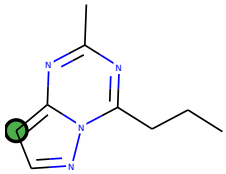
100% (Br_2)



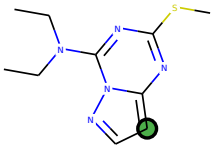
116 [88]

100% (Br_2, AcOH), 100% (Br_2, NaOAc, AcOH)

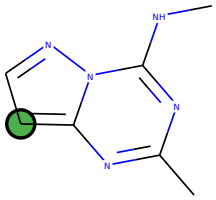
51 Pyrazolo[1,5-a][1,3,5]triazines



113 [374]
41% (NBS)

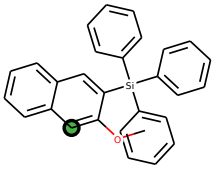


114 [374]
75% (NBS)

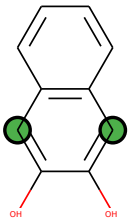


117 [418]
73% (Br_2, AcOH)

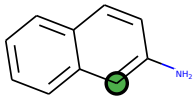
52 Naphthalenes



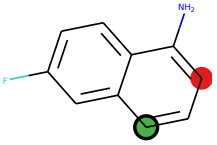
510 [257]
96% (NBS)



512 [453]
81% (Br_2)

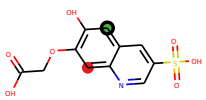


538 [332]
98% (NBS)

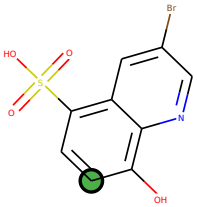


544 [433]
70% (NBS)

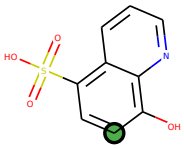
53 Quinolines



415 [152]
70% (Br_2)

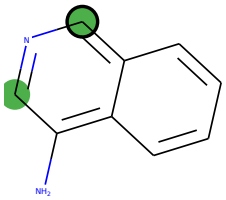


416 [183]
56% (NBS)



417 [183]
95% (NBS)

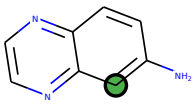
54 Isoquinolines



266 [42]

83% (NBS)

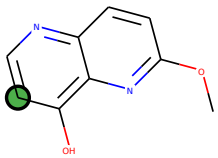
55 Quinoxalines



548 [45]

90% (NBS)

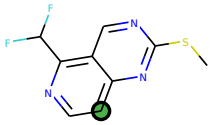
56 1,5-Naphthyridines



260 [91]

97% (NBS)

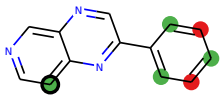
57 Pyrido[4,3-d]pyrimidines



396 [92]

85% (NIS)

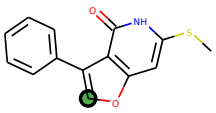
58 Pyrido[3,4-b]pyrazines



262 [297]

75% (NBS)

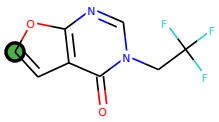
59 Furo[3,2-c]pyridin-4(5H)-ones



456 [57]

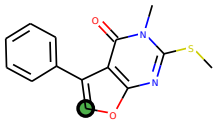
68% (Br_2)

60 Furo[2,3-d]pyrimidin-4(3H)-ones



445 [201]

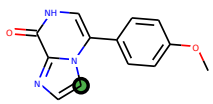
77% (Br_2)



458 [57]

84% (Br_2)

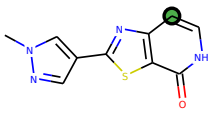
61 Imidazo[1,2-a]pyrazin-8(7H)-ones



181 [223]

96% (NIS)

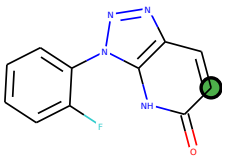
62 Thiazolo[5,4-b]pyridin-5(4H)-ones



585 [74]

84% (NCS)

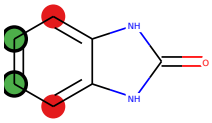
63 3,4-Dihydro-5H-[1,2,3]triazolo[4,5-b]pyridin-5-ones



267 [86]

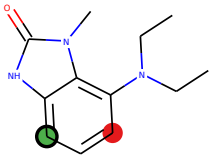
91% (Br_2)

64 1,3-Dihydro-2H-benzo[d]imidazol-2-ones



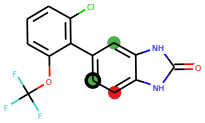
376 [147]

2xCl 97% (NCS)



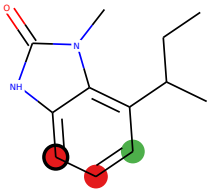
386 [309]

67% (NBS)



389 [354]

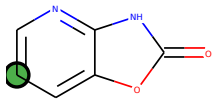
37% (NBS)



384 [35]

68% (NCS)

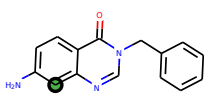
65 Oxazolo[4,5-b]pyridin-2(3H)-ones



261 [408]

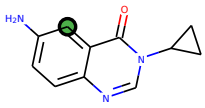
90% (Br_2)

66 Quinazolin-4(3H)-ones



580 [204]

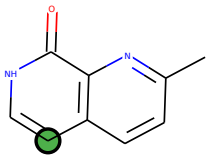
84% (NBS)



581 [441]

93% (NBS), 76% (NBS)

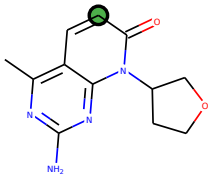
67 1,7-Naphthyridin-8(7H)-ones



263 [221]

80% (NBS)

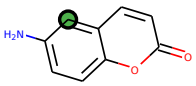
68 Pyrido[2,3-d]pyrimidin-7(8H)-ones



409 [41]

100% (Br_2)

69 2H-Chromen-2-ones



557 [107]

83% (NBS)

Section S5: Figure S3 Screenshot of webinterface

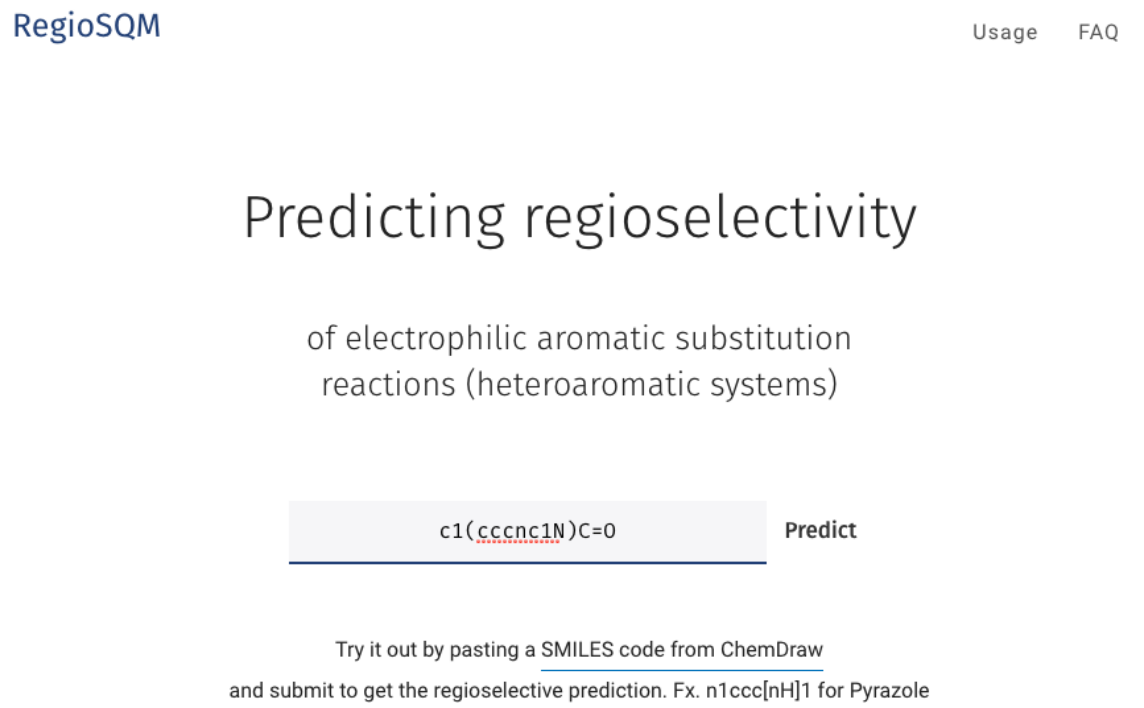


Figure 93: Screenshot of the RegioSQM webserver. The user simply enters the SMILES string of a molecule and pressed the Enter key. The SMILES string can be obtained from ChemDraw by highlighting the molecule and selecting Edit → Copy As → SMILES, which can then be pasted directly into the web interface.

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