Supporting Information: A Fast *Ab Initio* Predictor Tool for Covalent Reactivity Estimation of Acrylamides

Ferruccio Palazzesi, Marc A. Grundl, Alexander Pautsch, Alexander Weber and Christofer S. Tautermann.*

Medicinal Chemistry, Boehringer Ingelheim Pharma GmbH & Co. KG, Birkendorfer Strasse 65, 88397 Biberach an der Riß, Germany

*ferruccio.palazzesi@boehringer-ingelheim.com

Functional groups and rings dictionary

Table S1. List of considered functional groups based on[1] and ring systems in the truncation algorithm reported in the main paper.

Label	**Name**
-C(=O)N	Amide
-C(=O)	Carboxyl
-C(=O)O	Carboxylic acid
-C(=O)OC	Carbonyl methyl ester
-N=C=O	Isocyanate
-N=C=S	Isothiocyanate
-NO2	Nitro
-N=O	Nitroso
=N-O	Oximes
-N=CH2	Imines
-N=NCH3	Terminal azo
-N=N	Hydrazines
-N#N	Diazo

-C#N	Cyano
-SO2NH2	Sulfonamide
-NHSO2CH3	Methyl-sulfonamide
-SO3H	Sulfonic acid
-SO3CH3	Methyl ester sulfonyl
-SO2CH3	Methyl sulfonyl
-SO2Cl	Sulfonyl chloride
-SOCH3	Methyl sulfinyl
-SCH3	Methylthio
=S	Thiocarbonyls
-X	Halogens
-CF3	Trifluoromethyl
-C#CH	Acetylenes
-OMe	Methoxy
-C(=N)N	Acetamide
-N=N(+)=N(-)	Azide
-R	Ring systems (aromatic and not)

The electrophilicity index in comparison with other methods

Activation energies. GSH experimental data and compounds are taken from ref. 2. Calculated electrophilicity indices for compounds 88-108 are reported in Figure S1.

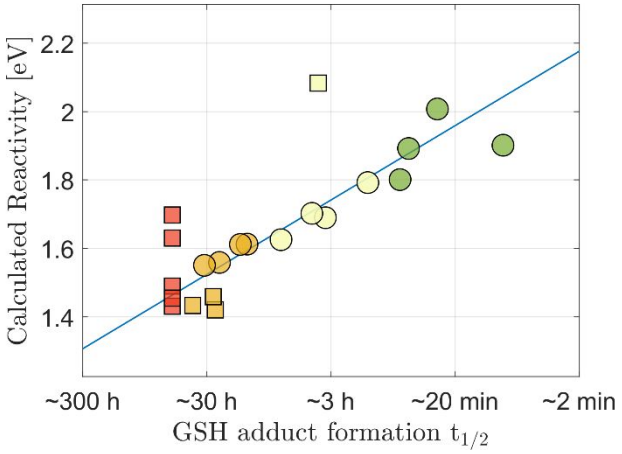


Figure S1. The electrophilicity index calculated for acrylamide compounds 88-108. Circles indicate unsubstituted acrylamide compounds, while squares highlight substituted ones. Color code is based on experimental data: green high reactivity (<1 h t1/2), yellow moderate reactivity (1 h< t1/2 <10 h), orange low reactivity (10 h< t1/2 <100 h) and red not reactive at all. Experimental GSH adduct formation t1/2 axis is in log units.

Hammett method. GSH Experimental data and compounds are taken from ref. 3. Calculated electrophilicity indices for compounds 31-64 are reported in Figure S2. The three higher values

belong to molecules with a nitro-group substituted in meta (38), ortho (39), and para (40) position. The agreement with experimental data is still remarkable even with these very high values of electrophilicity.

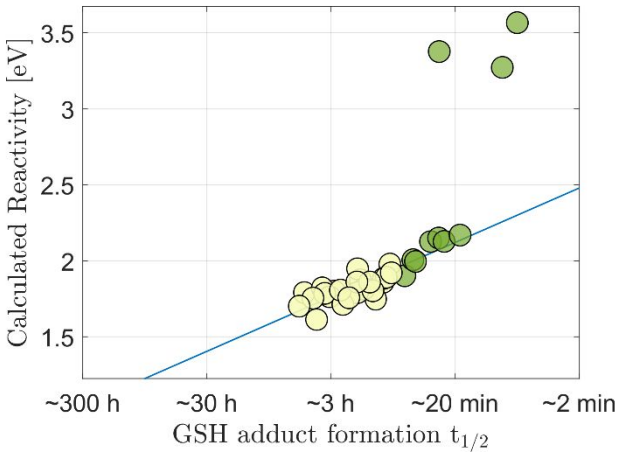


Figure S2. The electrophilicity index calculated for compounds 31-64. Color code is based on experimental data: green high reactivity (<1 h t1/2), yellow moderate reactivity (1 h< t1/2 <10 h), orange low reactivity (10 h< t1/2 <100 h) and red not reactive at all. Experimental GSH adduct formation t1/2 axis is in log units.

Comparison of basis set/functional combinations

Electrophilicity index calculated using different QM functionals and basis sets. In Table S2, we reported R^2 and Spearman correlation calculated for compound 1-10 to 29-30 from ref. 4 with respect to experimental GSH data for all the tested combinations.

Table S2. Performances comparison of different functionals/basis sets.

Functionals/ Basis sets	B3LYP	B2-PLYPD	LC-BLYP	PBE0	wB97XD
6-31+g(d,p)	0.78/0.96	0.70/0.89	0.62/0.82	0.80/0.96	0.69/0.85
6-311+g(d,p)	0.82/0.96	0.70/0.89	0.64/0.85	0.80/0.96	0.68/0.87
cc-pVDZ	0.80/0.96	0.69/0.93	0.65/0.86	0.78/0.94	0.71/0.92
cc-pVTZ	0.81/0.97	0.71/0.93	0.65/0.86	0.80/0.95	0.68/0.86

Conformational search analysis. Electrophilicity index calculated from lowest QM energy configuration after thorough conformational search for compound 1-14 and 29-30[4] (see Table S4). R^2 equal to 0.81, and Spearman correlation equal to 0.96 calculated for compound 1-10 and 29-30.

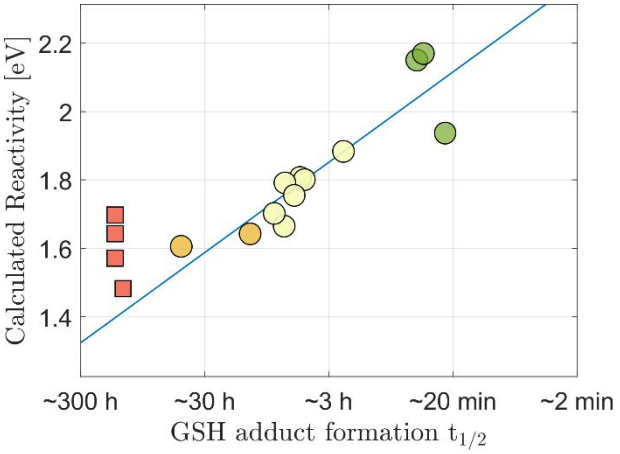


Figure S3. The electrophilicity index calculated for acrylamide compounds 1-14 and 29-30. Circles indicate unsubstituted acrylamide compounds, while squares highlight substituted ones. Color code is based on experimental data: green high reactivity (<1 h t1/2), yellow moderate reactivity (1 h< t1/2 <10 h), orange low reactivity (10 h< t1/2 <100 h) and red not reactive at all. Experimental GSH adduct formation t1/2 axis is in log units.

Table S3. Number of generated configurations for each compound, averaged electrophilicity index calculated from each configurations and associated standard deviation.

Compound	Number of generated configurations	Electrophilicity index [eV]	Standard Deviation [eV]
29	3	1.60	0.05
30	3	1.77	0.03
1	22	1.59	0.02
2	11	1.60	0.11
3	3	1.76	0.03
4	3	1.75	0.04
5	6	1.66	0.03
6	3	2.11	0.04
7	6	1.84	0.03
8	3	1.72	0.03
9	3	1.90	0.04
10	3	2.12	0.04
11	14	1.42	0.03
12	2	1.64	0.09
13	4	1.51	0.07
14	3	1.60	0.03

HOMO orbital before and after truncation

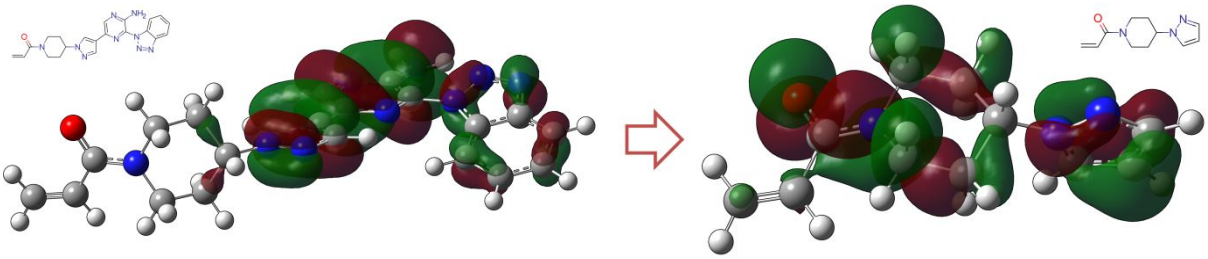


Figure S4. Graphical representation of the HOMO orbital for compound 19 of ref. 4. On the left, the HOMO localization considering the whole molecule. On the right, the HOMO position after molecule truncation.

Comparison of compounds and experimental GSH data

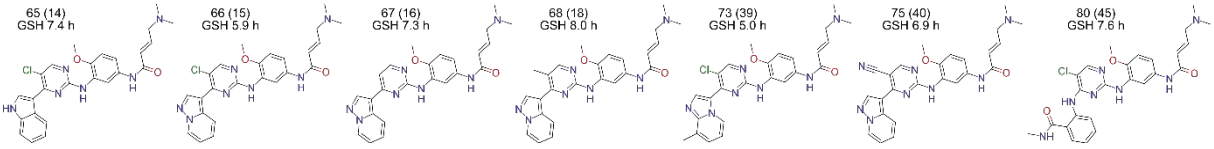


Figure S5. Examples of compounds sharing same structure near to warhead moiety and relative experimental GSH data. In parenthesis compound names from ref. 5.

The electrophilicity index calculated for lead-like molecules

GSH experimental data and compounds are taken from ref. 5. In Figure S6 we reported the electrophilicity index calculated before (left panel) and after truncation (right panel) for compounds 65-87. The agreement between calculations and experimental GSH data improves: R^2 from 0.23 to 0.52, and Spearman coefficient from 0.54 to 0.63. As highlighted in the main paper, the presence of substituents in the acrylamide double bond can influence compound reactivity. This effect could not be accurately predicted by our approach.

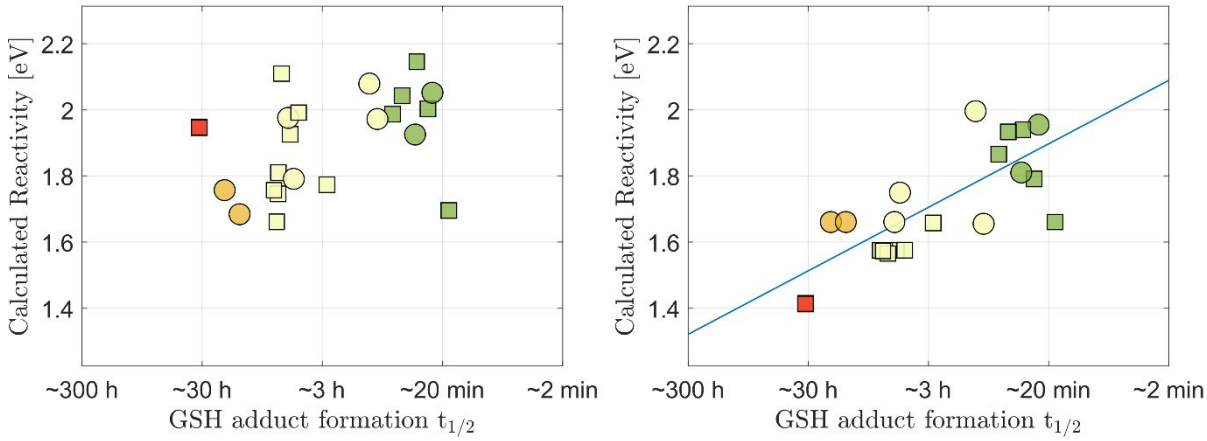
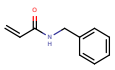
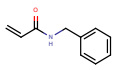
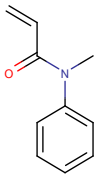
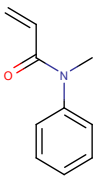
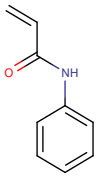
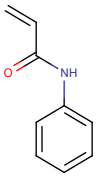
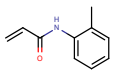
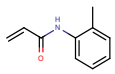
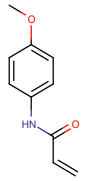
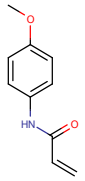
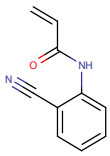
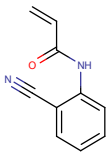
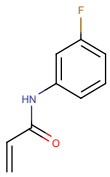
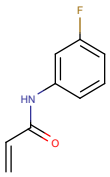
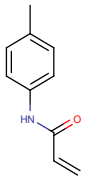
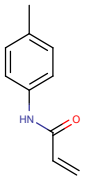
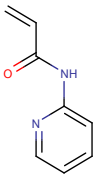
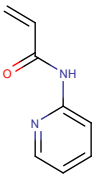
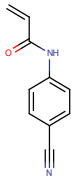
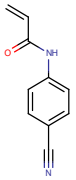
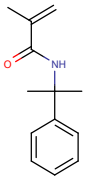
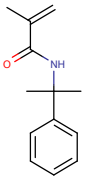
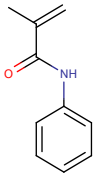
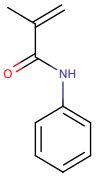
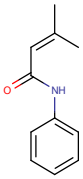
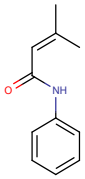
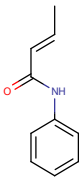
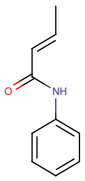
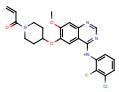
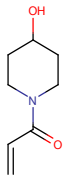
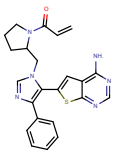
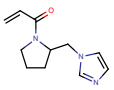
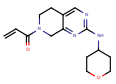
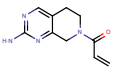
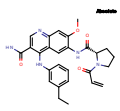


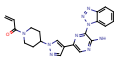
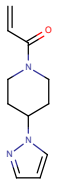
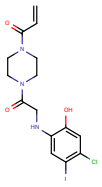
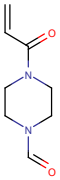
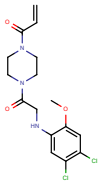
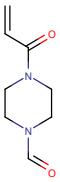
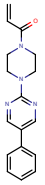
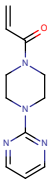
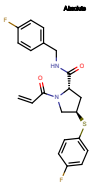
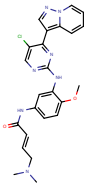
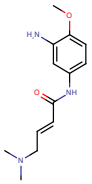
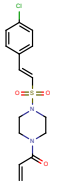
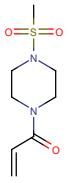
Figure S6. The electrophilicity index calculated for acrylamide compounds 65-87. On the left, results before truncation, on the right after. Circles indicate unsubstituted acrylamide compounds, while squares highlight substituted ones. Color code is based on experimental data: green high reactivity (<1 h t1/2), yellow moderate reactivity (1 h< t1/2 <10 h), orange low reactivity (10 h< t1/2 <100 h) and red not reactive at all. Experimental GSH adduct formation t1/2 axis is in log units.

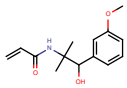
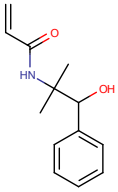
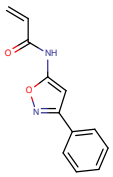
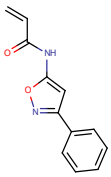
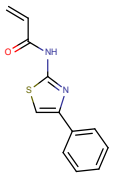
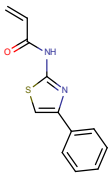
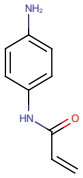
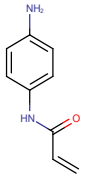
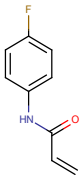
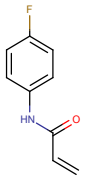
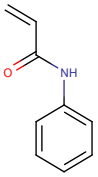
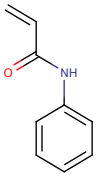
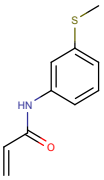
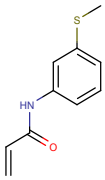
Table S4. List of compound structures employed in this work and associated experimental GSH and LYS adduct formation data obtained from literature.

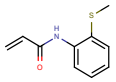
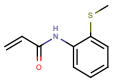
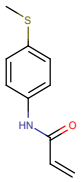
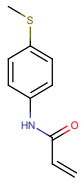
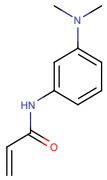
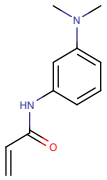
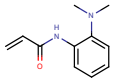
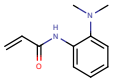
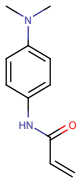
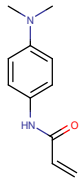
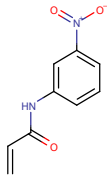
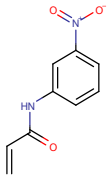
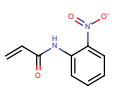
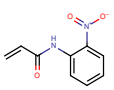
Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
R. Lonsdale et al. [4] - 10		49.00		10	1
R. Lonsdale et al. [4] - 11		7.27		11	2
R. Lonsdale et al. [4] - 12		4.98		12	3
R. Lonsdale et al. [4] - 13		7.13		13	4

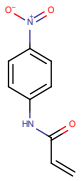
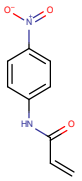
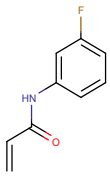
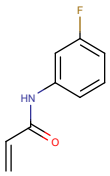
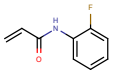
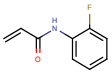
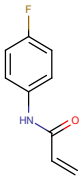
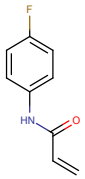
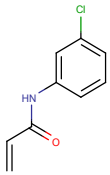
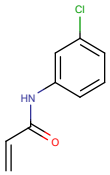
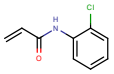
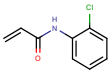
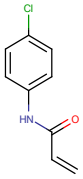
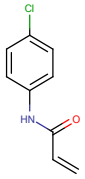
Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
R. Lonsdale et al. [4] - 14		8.73		14	5
R. Lonsdale et al. [4] - 15		0.62		15	6
R. Lonsdale et al. [4] - 16		2.42		16	7
R. Lonsdale et al. [4] - 17		6.02		17	8
R. Lonsdale et al. [4] - 18		0.37		18	9
R. Lonsdale et al. [4] - 19		0.55		19	10
R. Lonsdale et al. [4] - 20		>144.00		20	11

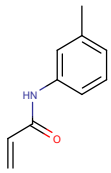
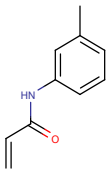
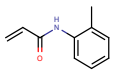
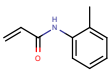
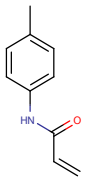
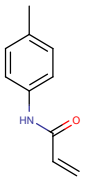
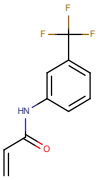
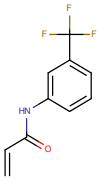
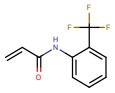
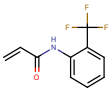
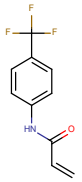
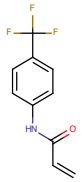
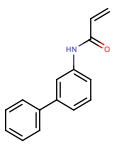
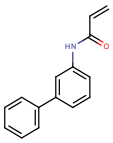
Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
R. Lonsdale et al. [4] - 21		>166.66		21	12
R. Lonsdale et al. [4] - 22		>166.66		22	13
R. Lonsdale et al. [4] - 23		>166.66		23	14
R. Lonsdale et al. [4] - 24		27.33		24	15
R. Lonsdale et al. [4] - 25		28.33		25	16
R. Lonsdale et al. [4] - 26		4.20		26	17
R. Lonsdale et al. [4] - 27		3.52		27	18

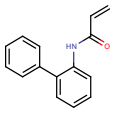
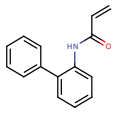
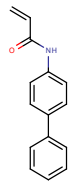
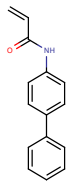
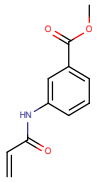
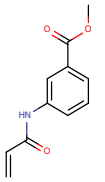
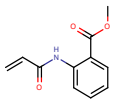
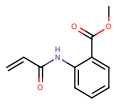
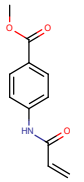
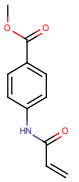
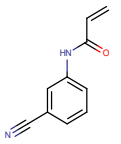
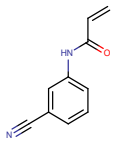
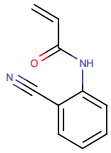
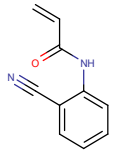
Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
R. Lonsdale et al. [4] - 28		15.82		28	19
R. Lonsdale et al. [4] - 29		6.12		29	20
R. Lonsdale et al. [4] - 30		6.67		30	21
R. Lonsdale et al. [4] - 31		11.52		31	22
R. Lonsdale et al. [4] - 32		1.51		32	23
R. Lonsdale et al. [4] - 34		5.87		34	24
R. Lonsdale et al. [4] - 35		4.72		35	25

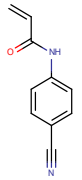
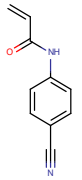
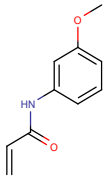
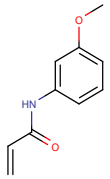
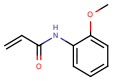
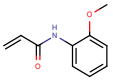
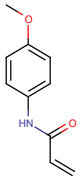
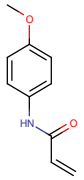
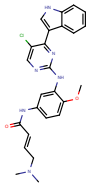
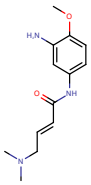
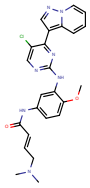
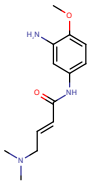
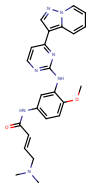
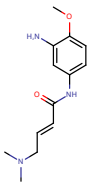
Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
R. Lonsdale et al. [4] - 36		52.67		36	26
R. Lonsdale et al. [4] - 51		0.07		51	27
R. Lonsdale et al. [4] - 52		0.07		52	28
R. Lonsdale et al. [4] - 8		13.60		8	29
R. Lonsdale et al. [4] - 9		5.38		9	30
V. J. Cee et al. [3]- 1		2.98		1	31
V. J. Cee et al. [3]- 10m		1.46		10m	32

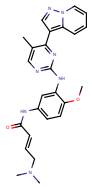
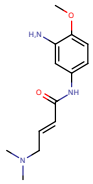
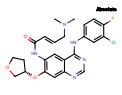
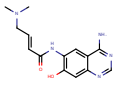
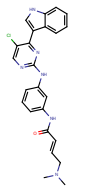
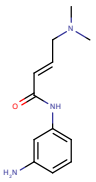
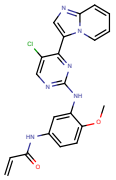
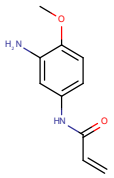
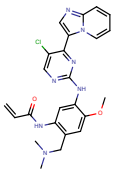
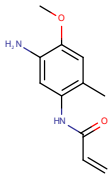
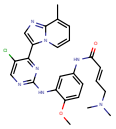
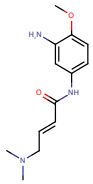
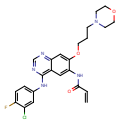
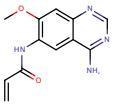
Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
V. J. Cee et al. [3]- 10o		1.21		10o	33
V. J. Cee et al. [3]- 10p		2.27		10p	34
V. J. Cee et al. [3]- 11m		2.53		11m	35
V. J. Cee et al. [3]- 11o		1.38		11o	36
V. J. Cee et al. [3]- 11p		4.12		11p	37
V. J. Cee et al. [3]- 12m		0.43		12m	38
V. J. Cee et al. [3]- 12o		0.10		12o	39

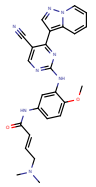
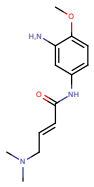
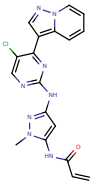
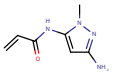
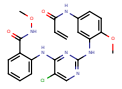
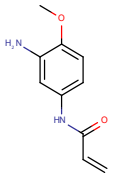
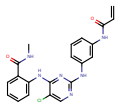
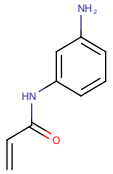
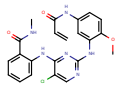
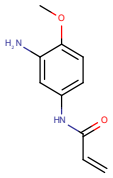
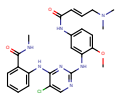
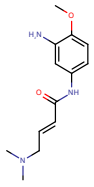
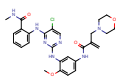
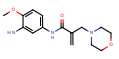
Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
V. J. Cee et al. [3]- 12p		0.13		12p	40
V. J. Cee et al. [3]- 2m		1.19		2m	41
V. J. Cee et al. [3]- 2o		1.83		2o	42
V. J. Cee et al. [3]- 2p		2.65		2p	43
V. J. Cee et al. [3]- 3m		1.13		3m	44
V. J. Cee et al. [3]- 3o		0.80		3o	45
V. J. Cee et al. [3]- 3p		1.54		3p	46

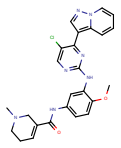
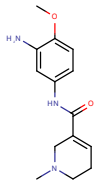
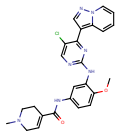
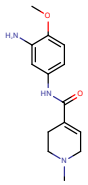
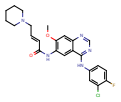
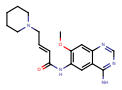
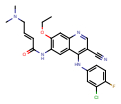
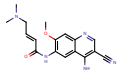
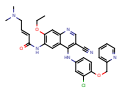
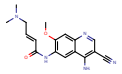
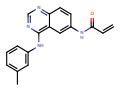
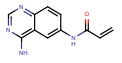
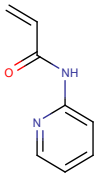
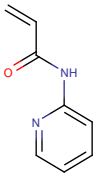
Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
V. J. Cee et al. [3]- 4m		3.55		4m	47
V. J. Cee et al. [3]- 4o		5.18		4o	48
V. J. Cee et al. [3]- 4p		4.42		4p	49
V. J. Cee et al. [3]- 5m		1.03		5m	50
V. J. Cee et al. [3]- 5o		1.06		5o	51
V. J. Cee et al. [3]- 5p		0.66		5p	52
V. J. Cee et al. [3]- 6m		1.72		6m	53

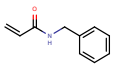
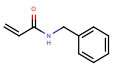
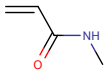
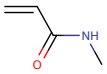
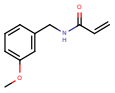
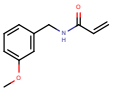
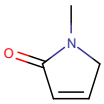
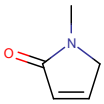
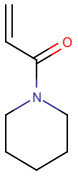
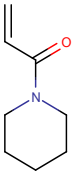
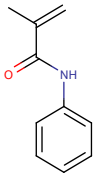
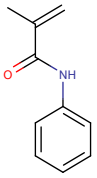
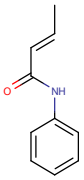
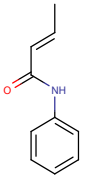
Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
V. J. Cee et al. [3]- 6o		3.72		6o	54
V. J. Cee et al. [3]- 6p		1.95		6p	55
V. J. Cee et al. [3]- 7m		1.93		7m	56
V. J. Cee et al. [3]- 7o		0.50		7o	57
V. J. Cee et al. [3]- 7p		0.39		7p	58
V. J. Cee et al. [3]- 8m		0.69		8m	59
V. J. Cee et al. [3]- 8o		0.43		8o	60

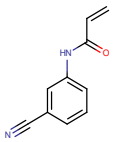
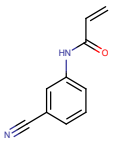
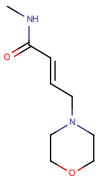
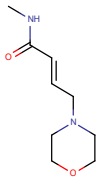
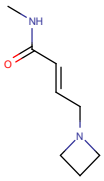
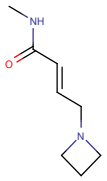
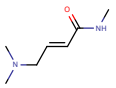
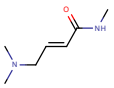
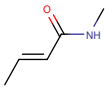
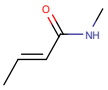
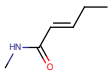
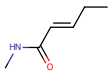
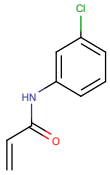
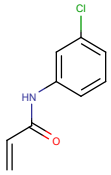
Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
V. J. Cee et al. [3]- 8p		0.29		8p	61
V. J. Cee et al. [3]- 9m		1.93		9m	62
V. J. Cee et al. [3]- 9o		3.23		9o	63
V. J. Cee et al. [3]- 9p		5.70		9p	64
R. A. Ward et al. [5] - 14		7.37		14	65
R. A. Ward et al. [5] - 15		5.87		15	66
R. A. Ward et al. [5] - 16		7.33		16	67

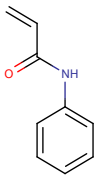
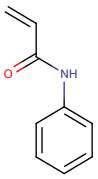
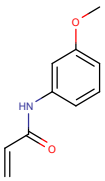
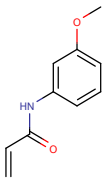
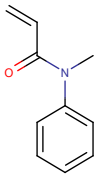
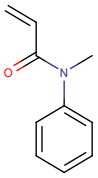
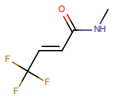
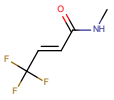
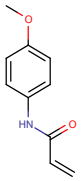
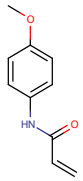
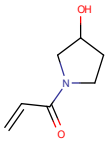
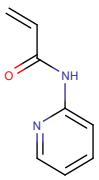
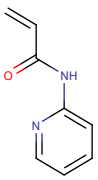
Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
R. A. Ward et al. [5] - 18		7.98		18	68
R. A. Ward et al. [5] - 3		0.42		3	69
R. A. Ward et al. [5] - 36		2.88		36	70
R. A. Ward et al. [5] - 37		6.07		37	71
R. A. Ward et al. [5] - 38		<1.10		38	72
R. A. Ward et al. [5] - 39		4.97		39	73
R. A. Ward et al. [5] - 4		0.38		4	74

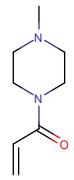
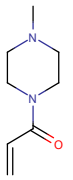
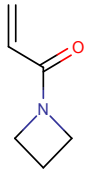
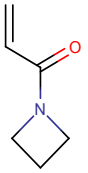
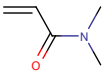
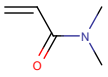
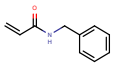
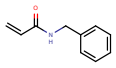
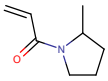
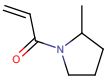
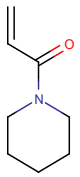
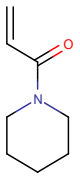
Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
R. A. Ward et al. [5] - 40		6.88		40	75
R. A. Ward et al. [5] - 41		0.53		41	76
R. A. Ward et al. [5] - 42		20.52		42	77
R. A. Ward et al. [5] - 43		5.47		43	78
R. A. Ward et al. [5] - 44		15.40		44	79
R. A. Ward et al. [5] - 45		7.55		45	80
R. A. Ward et al. [5] - 46		0.28		46	81

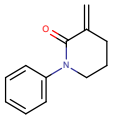
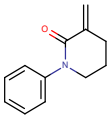
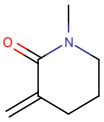
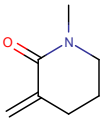
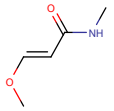
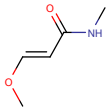
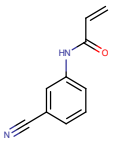
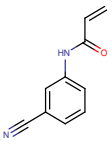
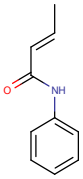
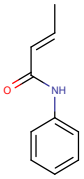
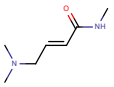
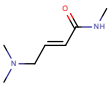
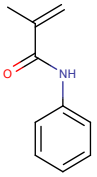
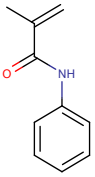
Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
R. A. Ward et al. [5] - 47		>33.33		47	82
R. A. Ward et al. [5] - 48		>33.33		48	83
R. A. Ward et al. [5] - 5		0.82		5	84
R. A. Ward et al. [5] - 53		0.52		53	85
R. A. Ward et al. [5] - 54		0.68		54	86
R. A. Ward et al. [5] - 55		1.28		55	87
M. E. Flanagan et al. [2] - 1		0.13		1	88

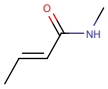
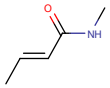
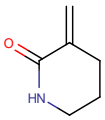
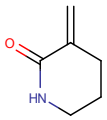
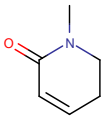
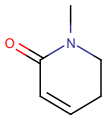
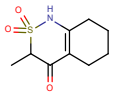
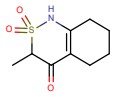
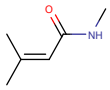
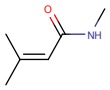
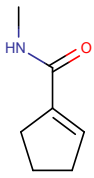
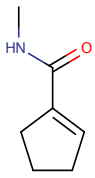
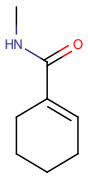
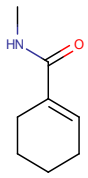
Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
M. E. Flanagan et al. [2] - 10		15.00		10	89
M. E. Flanagan et al. [2] - 11		17.00		11	90
M. E. Flanagan et al. [2] - 12		25.00		12	91
M. E. Flanagan et al. [2] - 13		27.00		13	92
M. E. Flanagan et al. [2] - 14		33.00		14	93
M. E. Flanagan et al. [2] - 15		>60.00		15	94
M. E. Flanagan et al. [2] - 16		>60.00		16	95

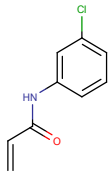
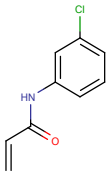
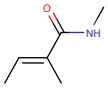
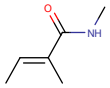
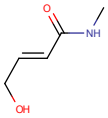
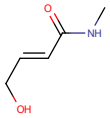
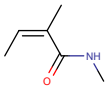
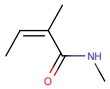
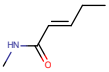
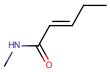
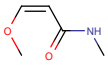
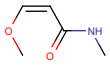
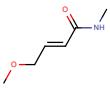
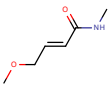
Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
M. E. Flanagan et al. [2] - 2		0.44		2	96
M. E. Flanagan et al. [2] - 21		28.00		21	97
M. E. Flanagan et al. [2] - 22		41.00		22	98
M. E. Flanagan et al. [2] - 23		>60.00		23	99
M. E. Flanagan et al. [2] - 24		>60.00		24	100
M. E. Flanagan et al. [2] - 25		>60.00		25	101
M. E. Flanagan et al. [2] - 3		0.75		3	102

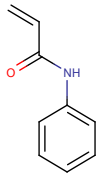
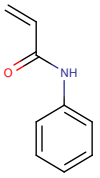
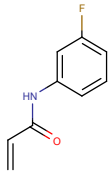
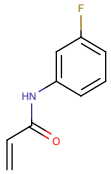
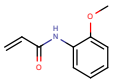
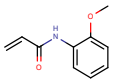
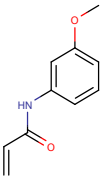
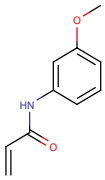
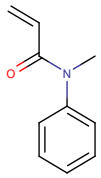
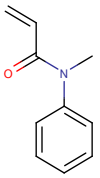
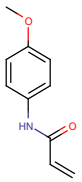
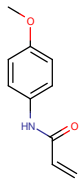
Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
M. E. Flanagan et al. [2] - 4		0.88		4	103
M. E. Flanagan et al. [2] - 5		1.60		5	104
M. E. Flanagan et al. [2] - 6		3.50		6	105
M. E. Flanagan et al. [2] - 7		4.00		7	106
M. E. Flanagan et al. [2] - 8		4.50		8	107
M. E. Flanagan et al. [2] - 9		8.00		9	108
U. P. Dahal et al. [6] - 1		0.67		1	109

Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
U. P. Dahal et al. [6] - 10		3.53		10	110
U. P. Dahal et al. [6] - 11		5.71		11	111
U. P. Dahal et al. [6] - 12		6.17		12	112
U. P. Dahal et al. [6] - 13		11.20		13	113
U. P. Dahal et al. [6] - 14		14.40		14	114
U. P. Dahal et al. [6] - 15		16.90		15	115
U. P. Dahal et al. [6] - 16		26.10		16	116

Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
U. P. Dahal et al. [6] - 17		5.51		17	117
U. P. Dahal et al. [6] - 18		45.90		18	118
U. P. Dahal et al. [6] - 19		47.50		19	119
U. P. Dahal et al. [6] - 2		1.13		2	120
U. P. Dahal et al. [6] - 20		68.80		20	121
U. P. Dahal et al. [6] - 21		71.30		21	122
U. P. Dahal et al. [6] - 22		77.00		22	123

Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
U. P. Dahal et al. [6] - 23		>100.00		23	124
U. P. Dahal et al. [6] - 24		>100.00		24	125
U. P. Dahal et al. [6] - 25		>100.00		25	126
U. P. Dahal et al. [6] - 26		>100.00		26	127
U. P. Dahal et al. [6] - 27		>100.00		27	128
U. P. Dahal et al. [6] - 28		>100.00		28	129
U. P. Dahal et al. [6] - 29		>100.00		29	130

Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
U. P. Dahal et al. [6] - 3		1.88		3	131
U. P. Dahal et al. [6] - 30		>100.00		30	132
U. P. Dahal et al. [6] - 31		>100.00		31	133
U. P. Dahal et al. [6] - 32		>100.00		32	134
U. P. Dahal et al. [6] - 33		>100.00		33	135
U. P. Dahal et al. [6] - 34		>100.00		34	136
U. P. Dahal et al. [6] - 35		>100.00		35	137

Reference - Ref. Name	Whole Molecule	GSH [h]	Frag. Molecule	Ref. Name	Internal Number
U. P. Dahal et al. [6] - 4		2.06		4	138
U. P. Dahal et al. [6] - 5		2.24		5	139
U. P. Dahal et al. [6] - 6		2.85		6	140
U. P. Dahal et al. [6] - 7		3.58		7	141
U. P. Dahal et al. [6] - 8		3.76		8	142
U. P. Dahal et al. [6] - 9		5.94		9	143

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