Supporting Information

BH9, a New Comprehensive Benchmark Dataset for Barrier Heights and Reaction Energies: Assessment of Density Functional Approximations and Basis Set Incompleteness Potentials

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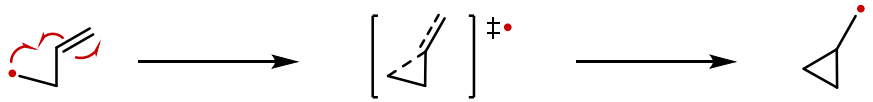
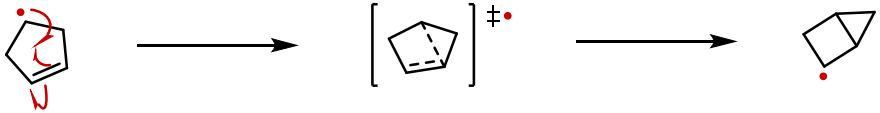
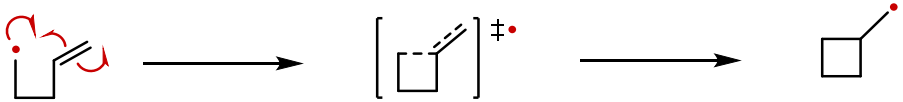
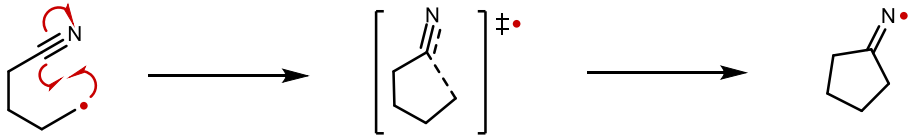
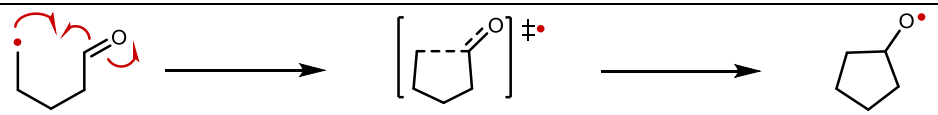
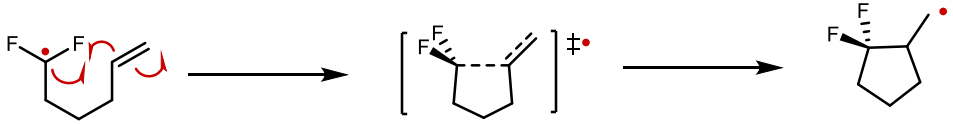
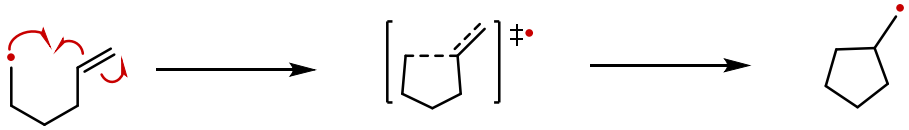
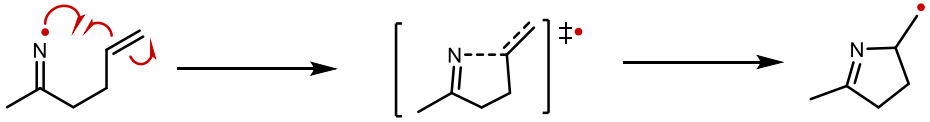
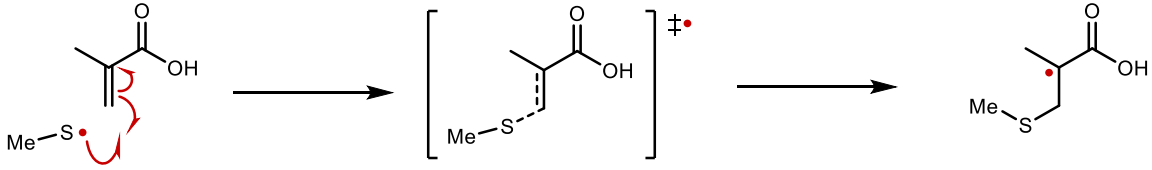
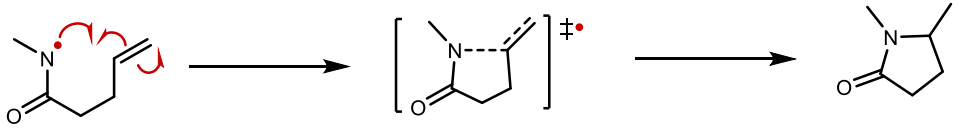
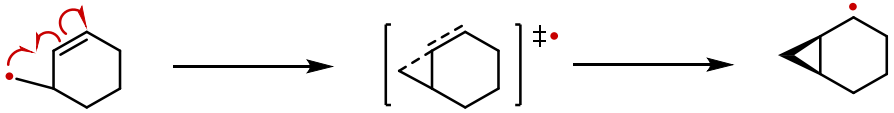
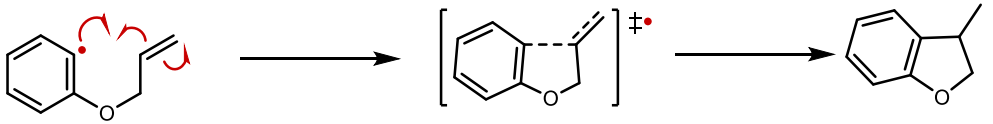
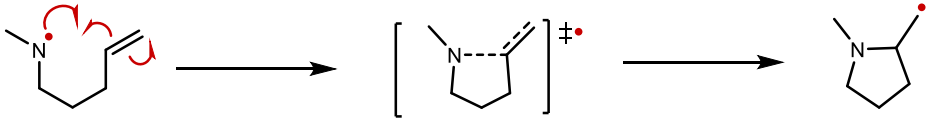
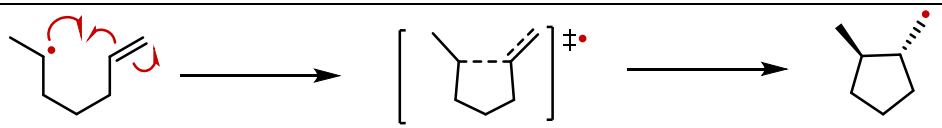
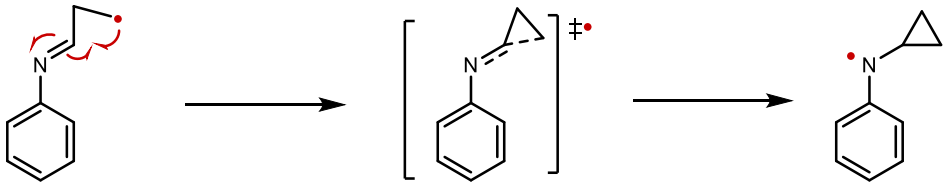
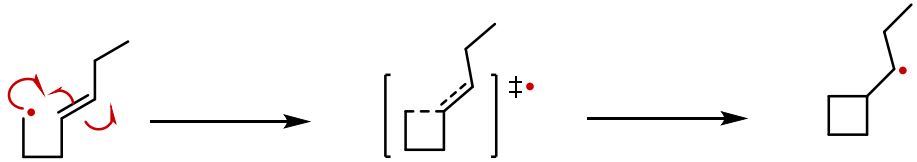
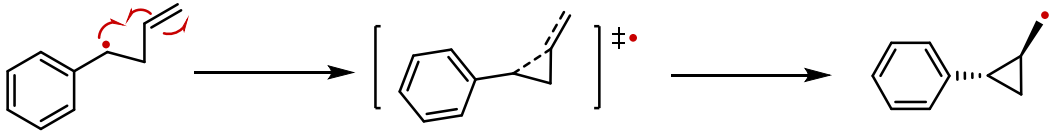
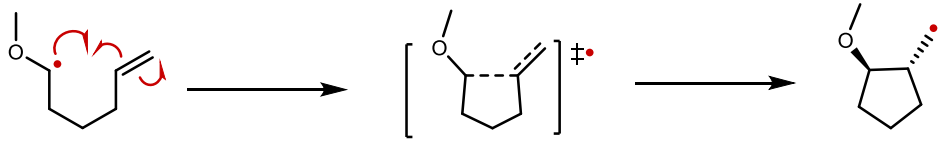
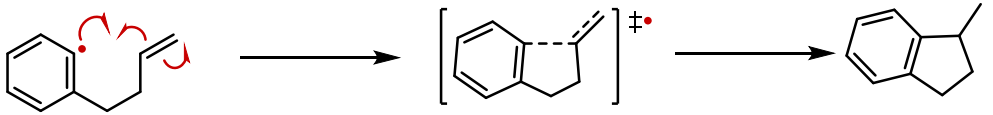
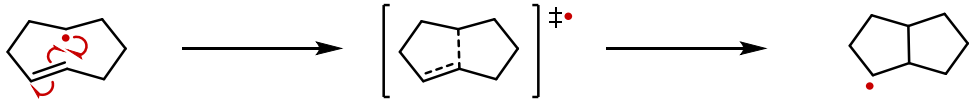
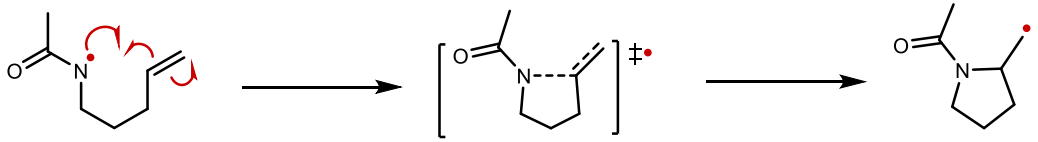
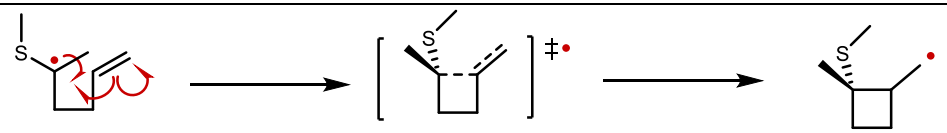
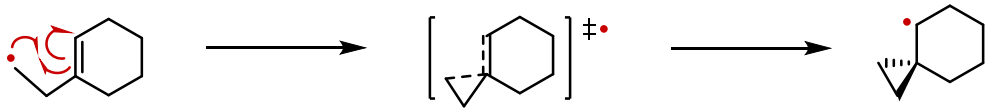
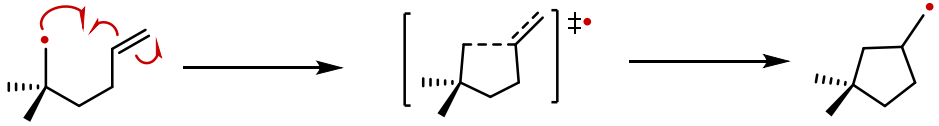
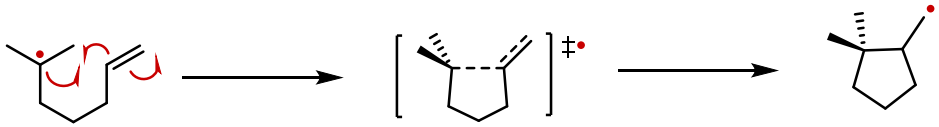
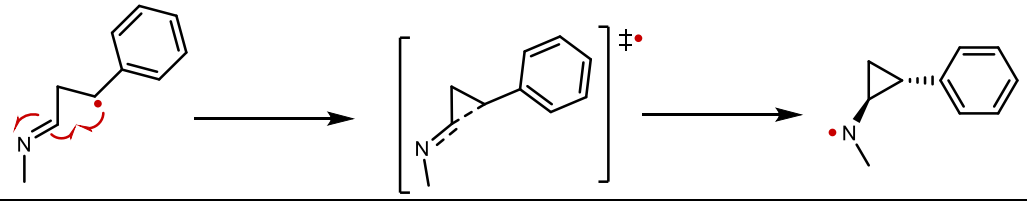
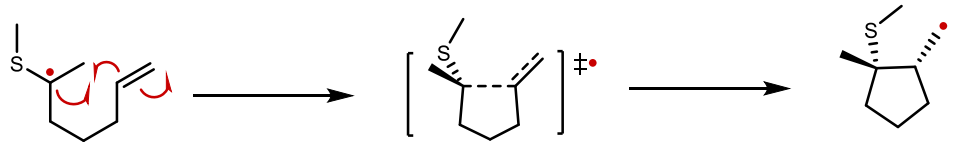
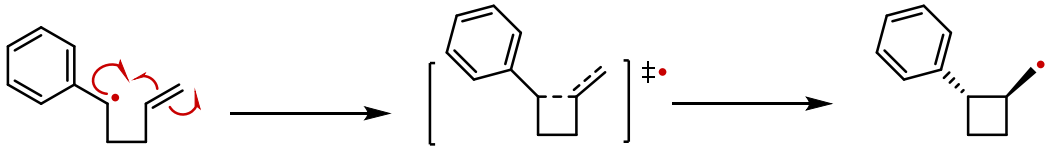
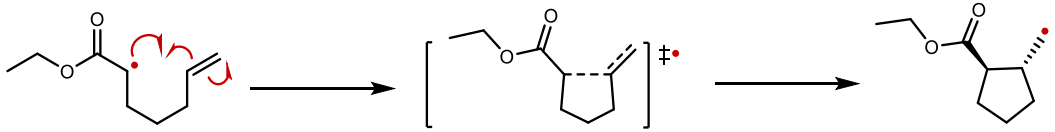
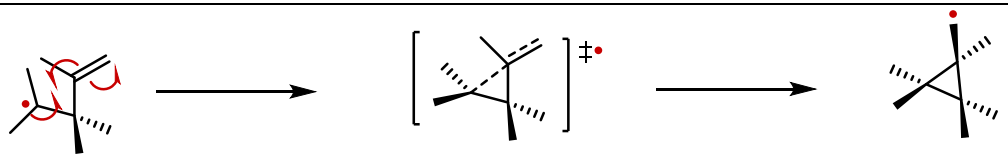
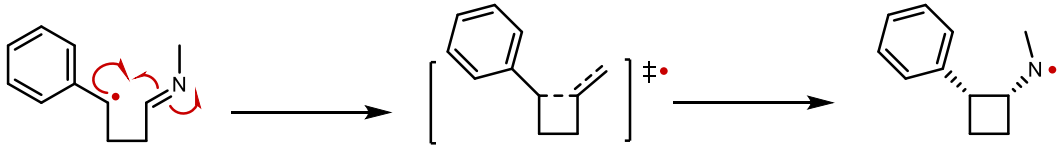
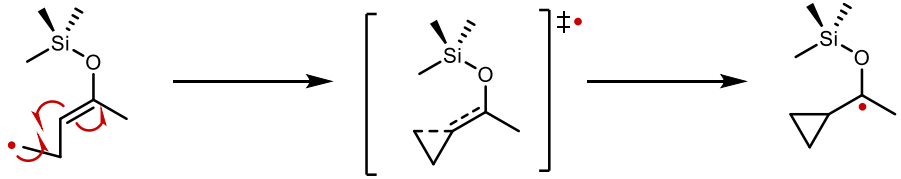
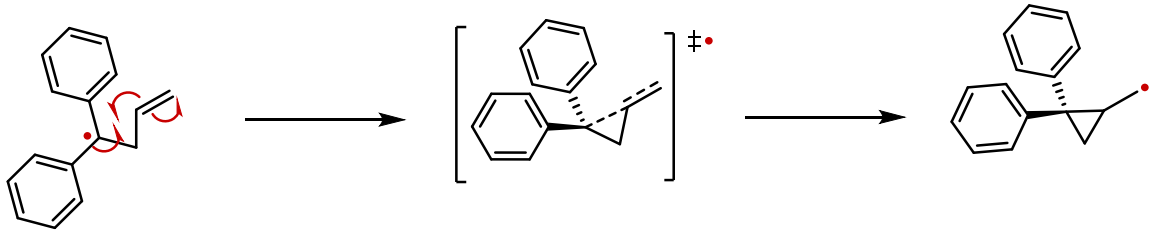
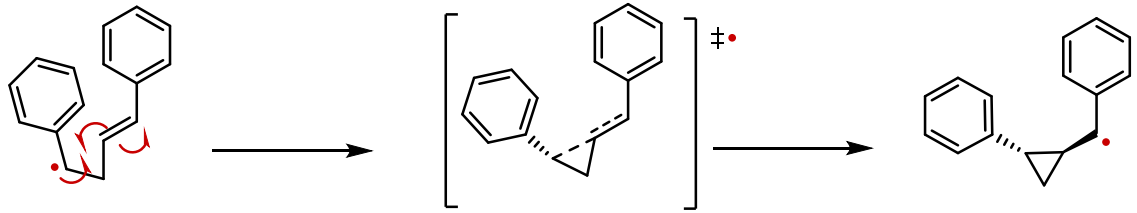
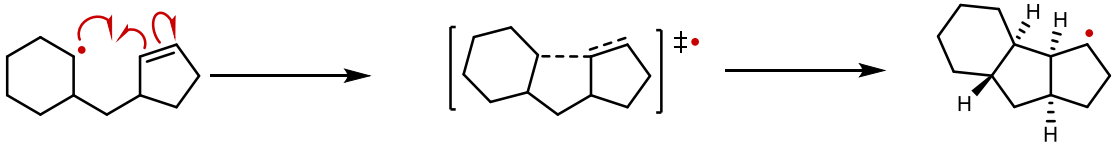
I. Radical rearrangement and addition

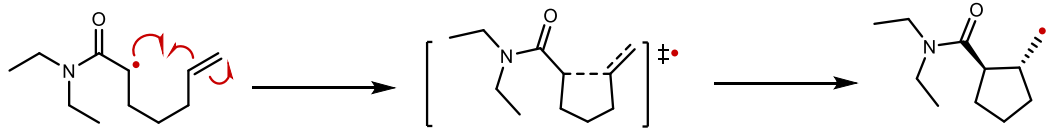
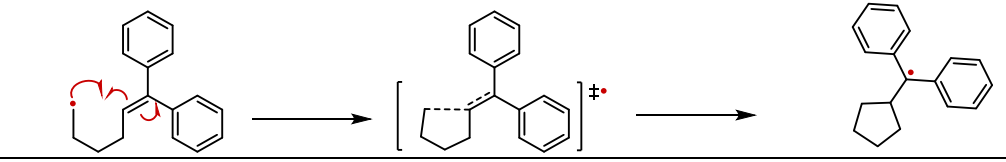
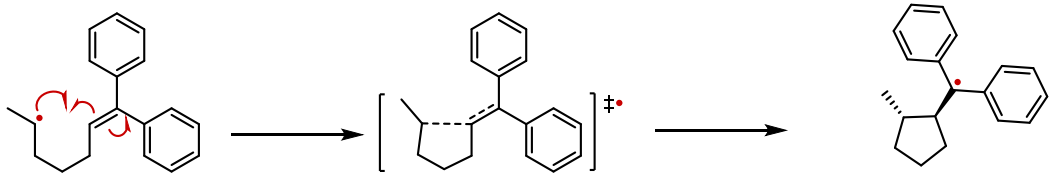
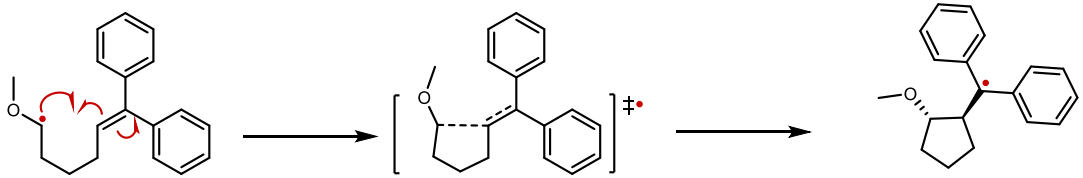
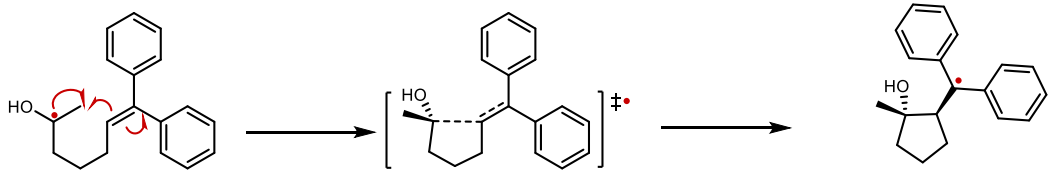
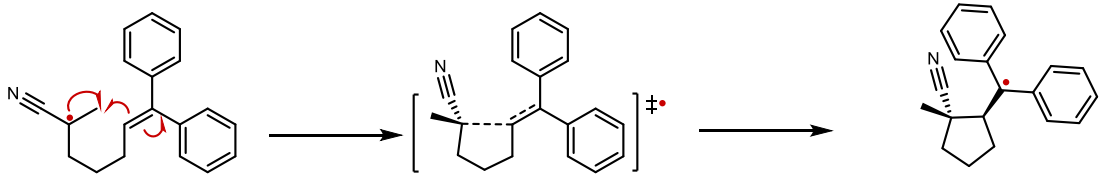
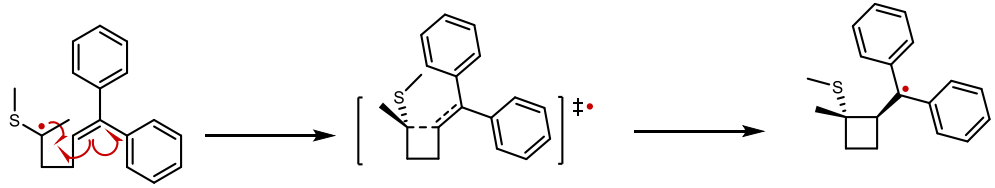
#	Mechanism	Forward barrier height (in kcal/mol)	Reverse barrier height (in kcal/mol)	Reaction energy (in kcal/mol)
1		11.74	9.01	2.74
2		38.51	6.56	31.94
3		17.10	15.18	1.92
4		10.80	20.54	-9.74

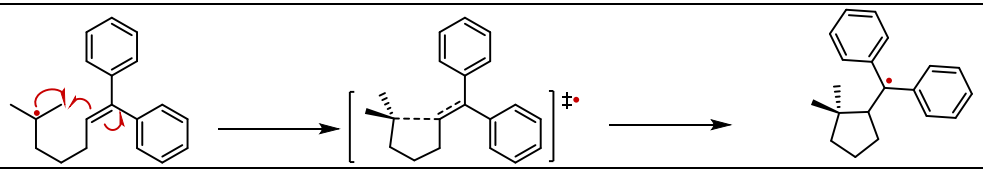
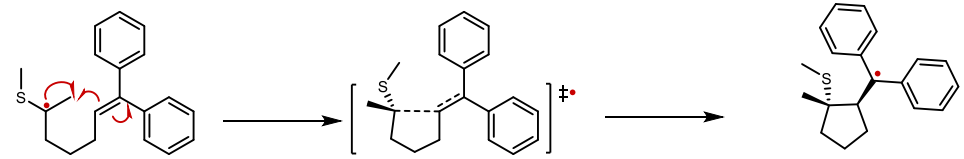
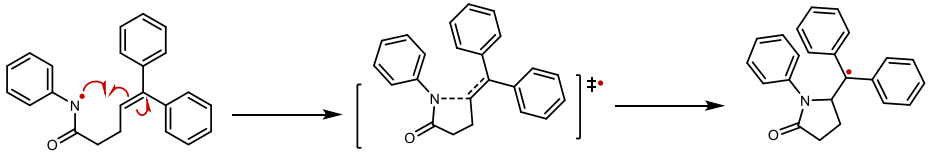
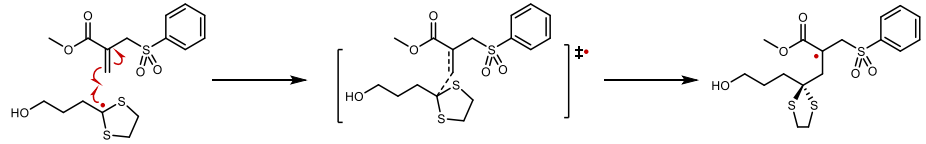
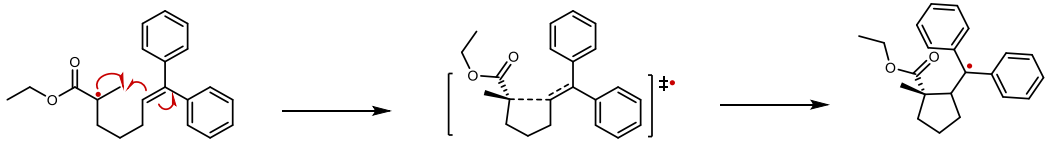
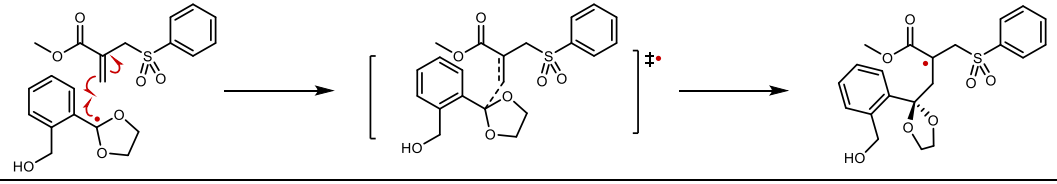
5		8.56	10.84	-2.28
6		6.92	26.65	-19.73
7		7.94	24.57	-16.63
8		13.67	20.45	-6.77
9		-0.79	15.79	-16.58
10		7.64	31.53	-23.89
11		10.88	8.30	2.58
12		3.37	36.53	-33.16
13		14.83	20.64	-5.81

14		7.96	23.95	-15.99
15		9.35	11.72	-2.37
16		17.04	15.20	1.85
17		16.96	3.87	13.09
18		7.76	19.98	-12.22
19		4.25	36.12	-31.88
20		5.78	30.88	-25.10
21		5.42	25.97	-20.55

22		16.38	9.26	7.13
23		12.96	9.63	3.33
24		7.11	24.94	-17.82
25		6.75	21.05	-14.30
26		18.76	2.40	16.36
27		9.78	18.83	-9.05
28		22.46	9.64	12.82
29		7.92	18.08	-10.16

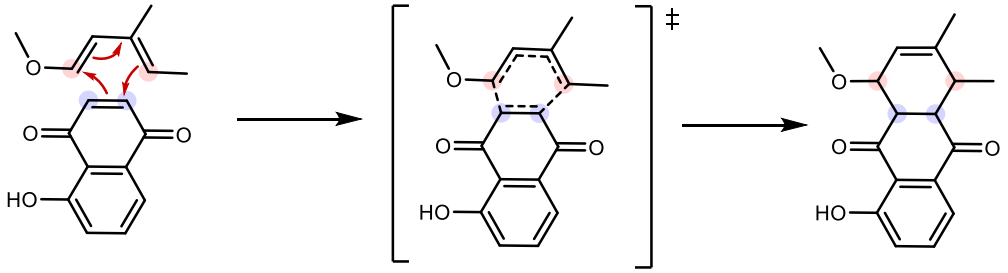
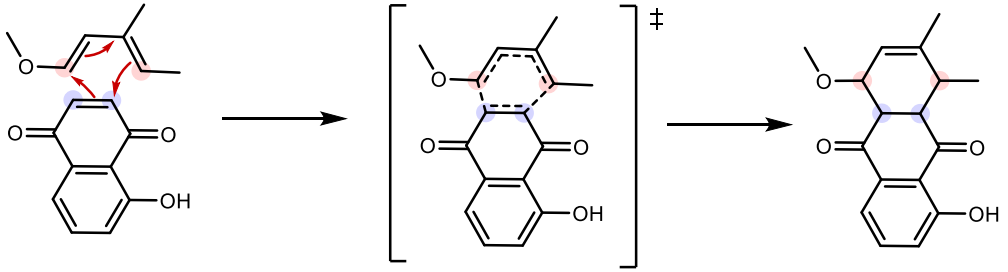
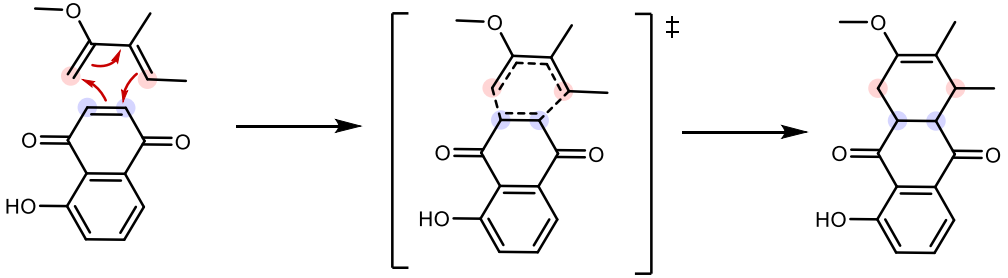
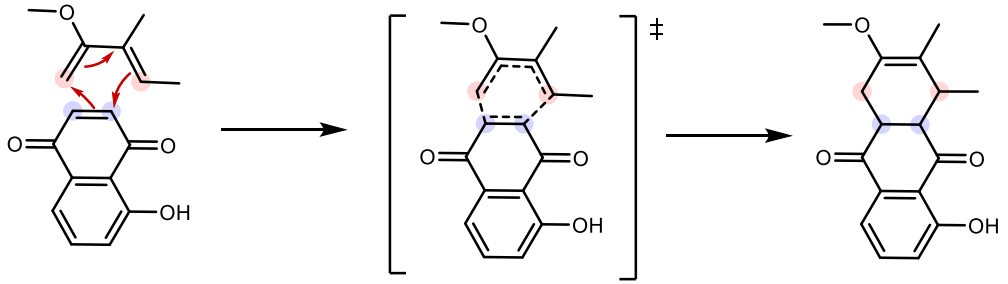
30		14.29	6.03	8.26
31		24.18	7.64	16.54
32		11.47	10.55	0.92
33		20.07	3.03	17.04
34		13.02	8.08	4.94
35		9.68	27.80	-18.12

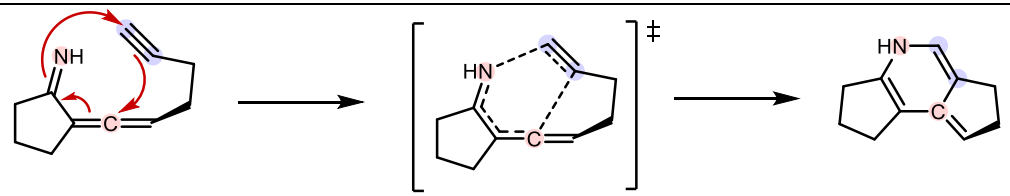
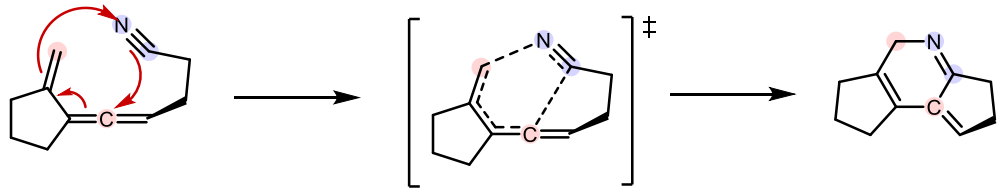
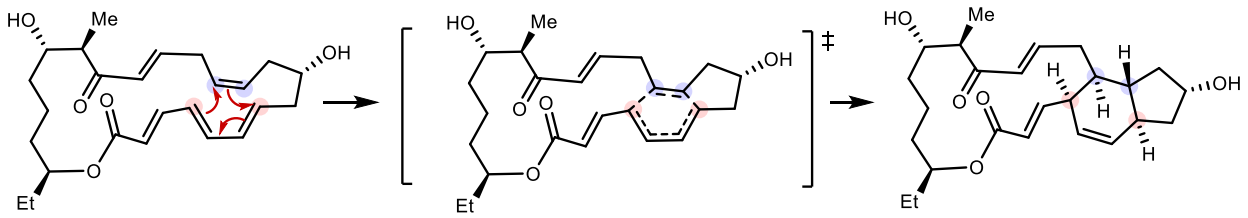
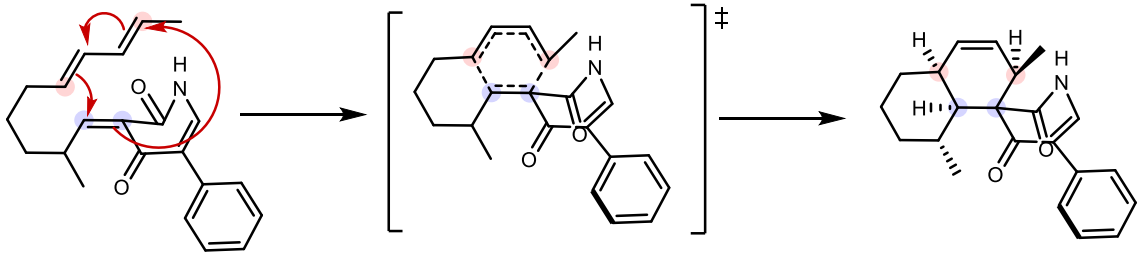
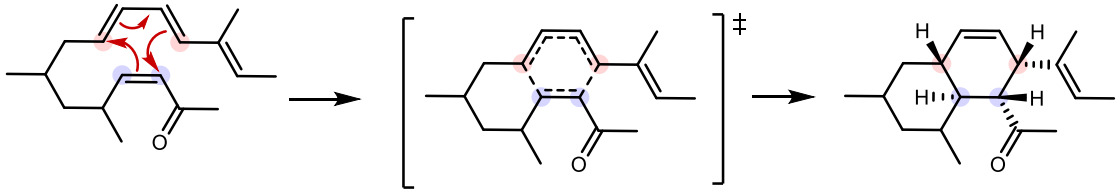
36		7.82	18.49	-10.67
37		6.15	31.91	-25.76
38		6.29	30.93	-24.64
39		5.30	27.45	-22.15
40		5.71	24.84	-19.13
41		7.58	-15.38	22.96
42		13.31	13.52	-0.22

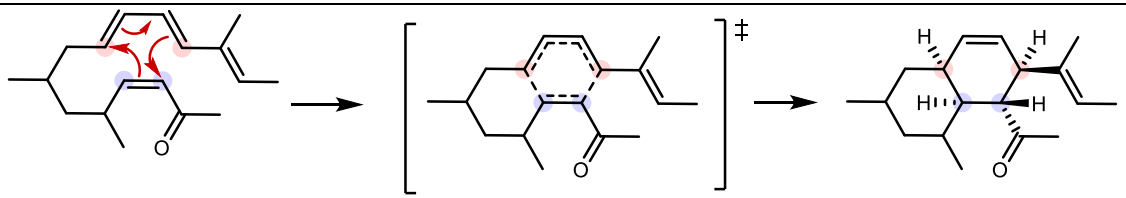
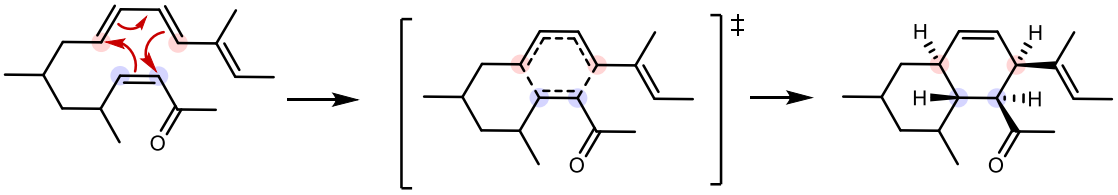
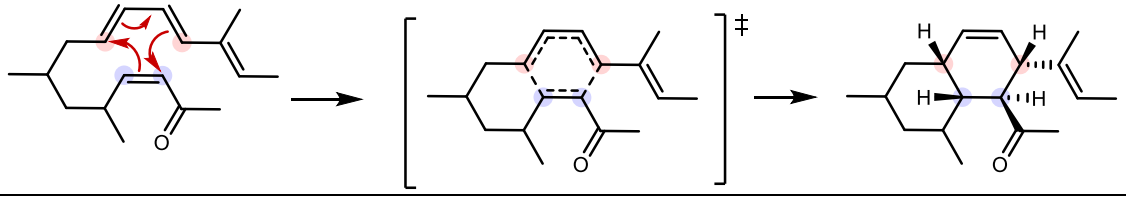
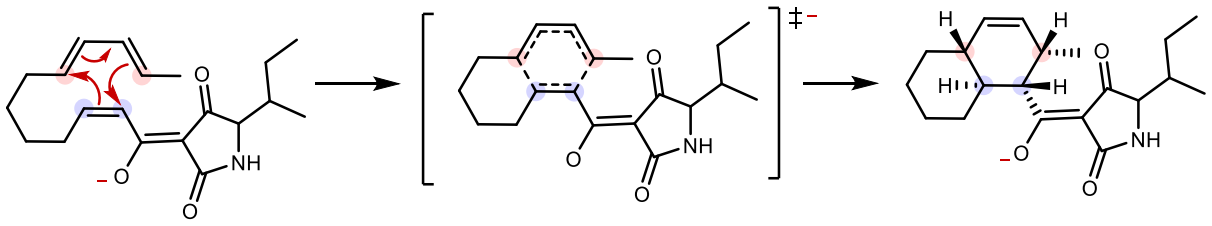
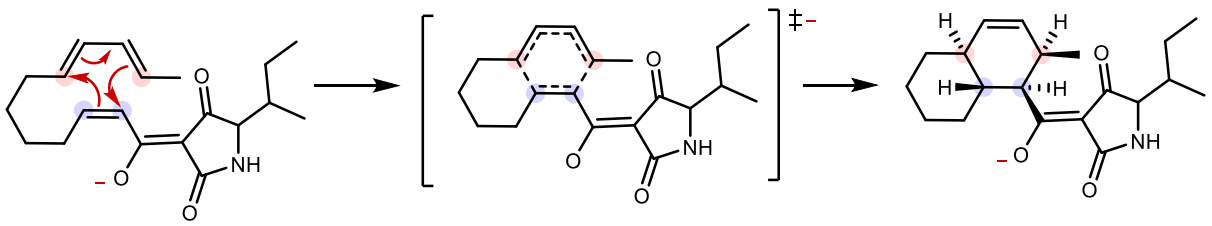
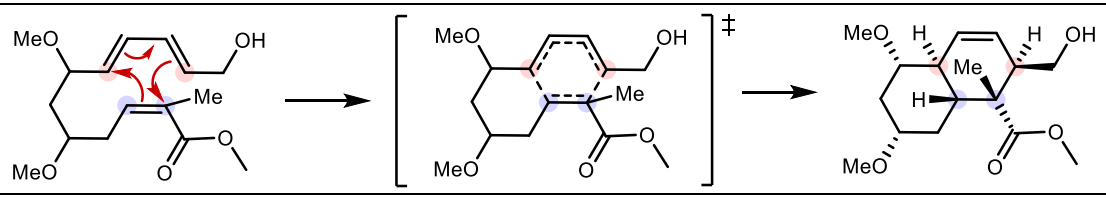
43		5.45	25.56	-20.11
44		6.10	22.21	-16.11
45		-26.78	-5.68	-21.10
46		0.01	19.72	-19.71
47		7.47	58.28	-50.81
48		0.37	22.46	-22.09

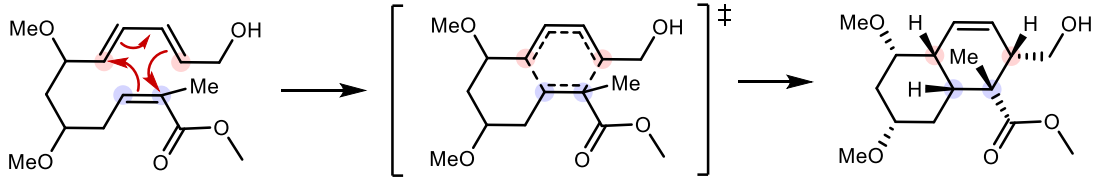
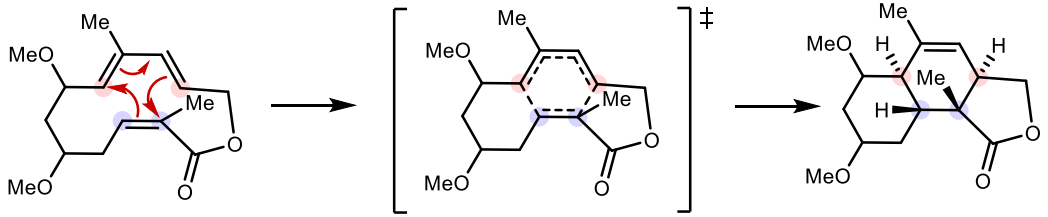
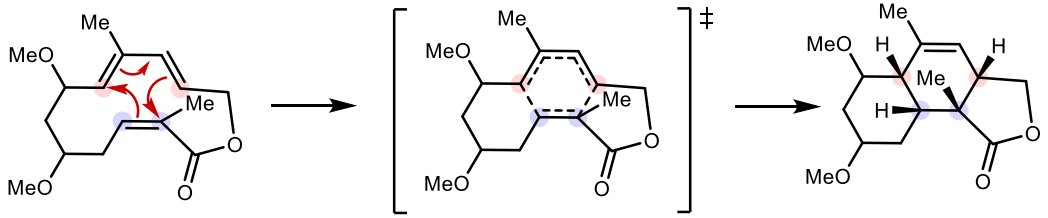
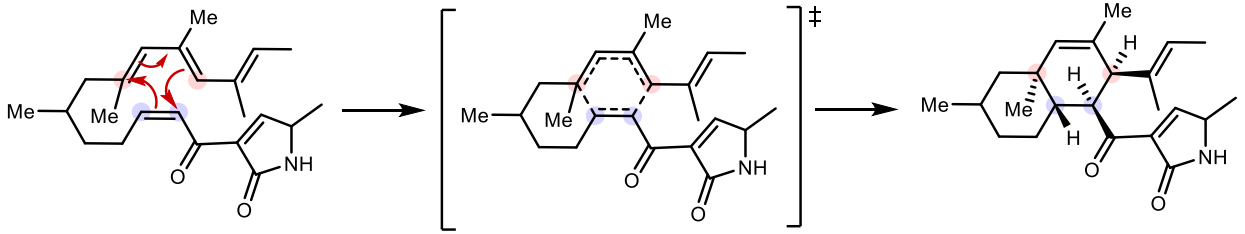
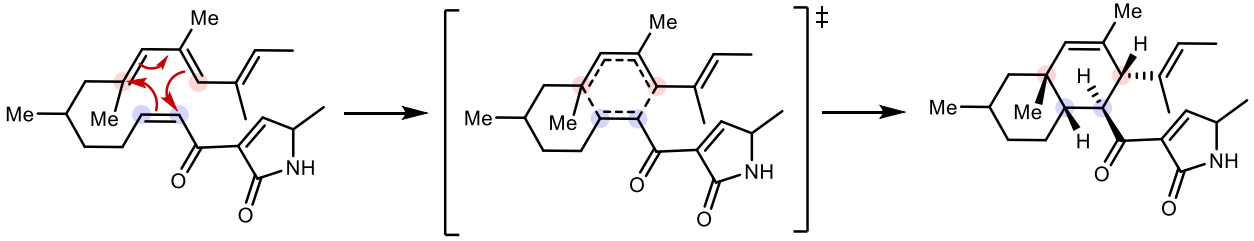
II. Pericyclic

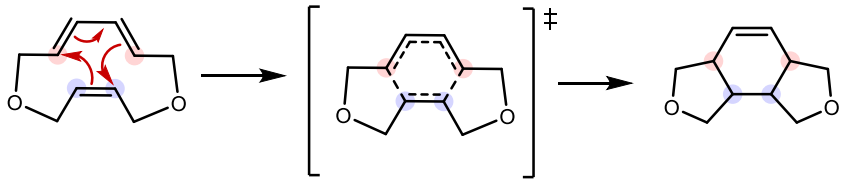
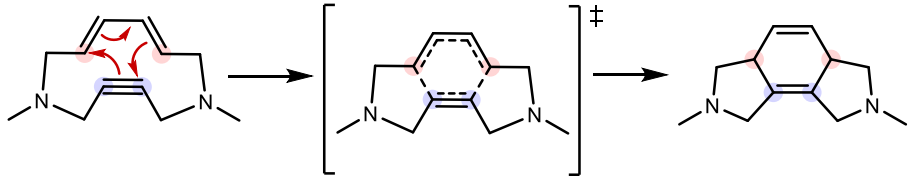
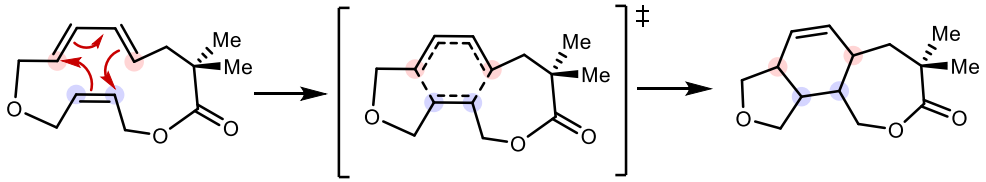
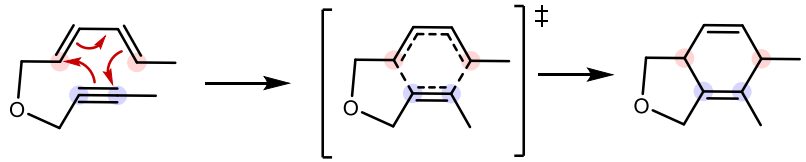
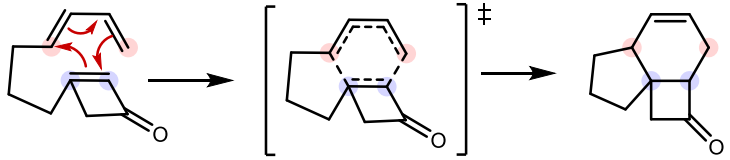
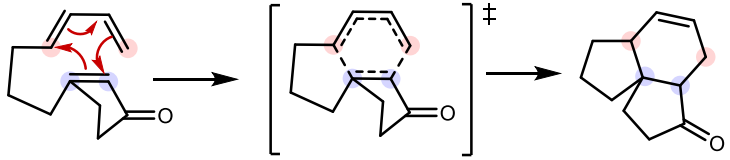
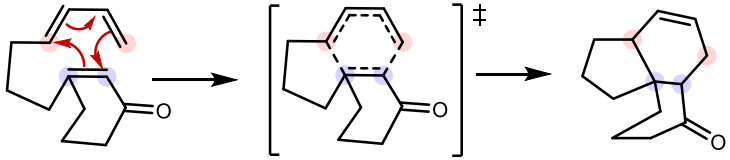
#	Mechanism	Forward barrier height (in	Reverse barrier height (in	Reaction energy (in kcal/mol)

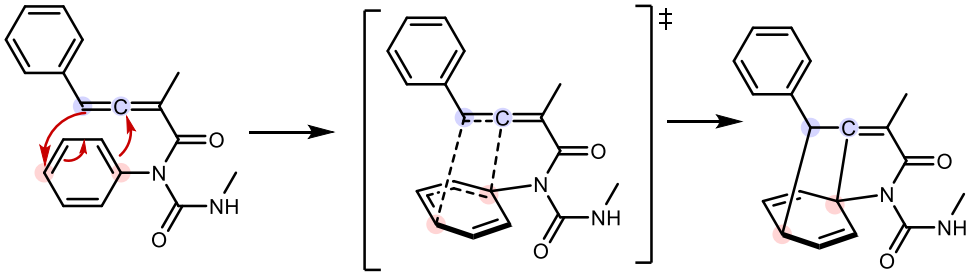
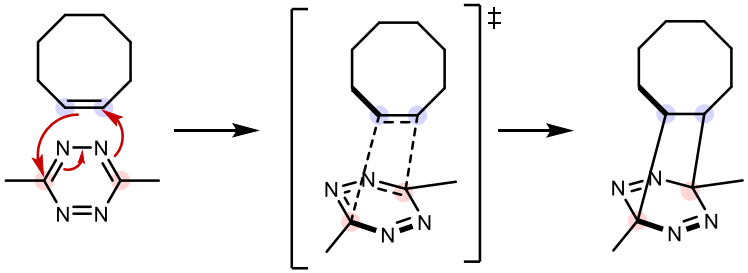
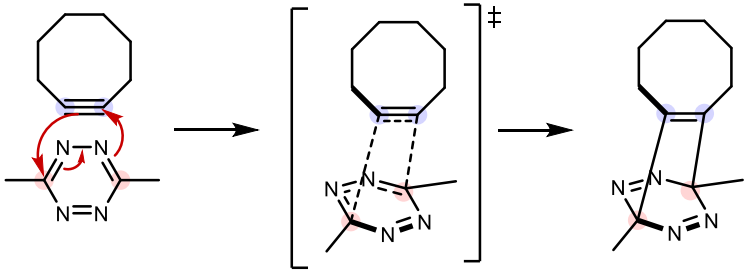
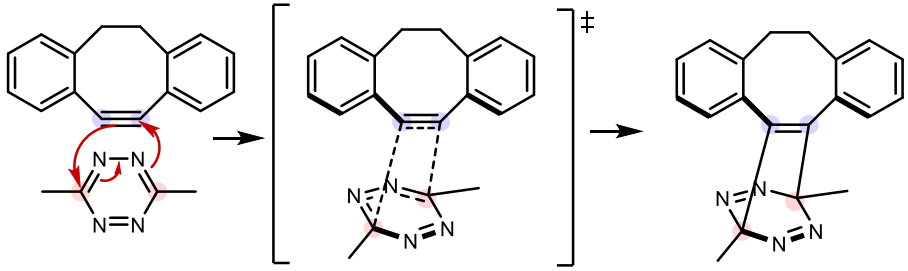
		kcal/mol)	kcal/mol)	
1		8.10	43.77	-35.66
2		8.85	43.49	-34.63
3		11.45	47.83	-36.38
4		10.15	47.06	-36.92

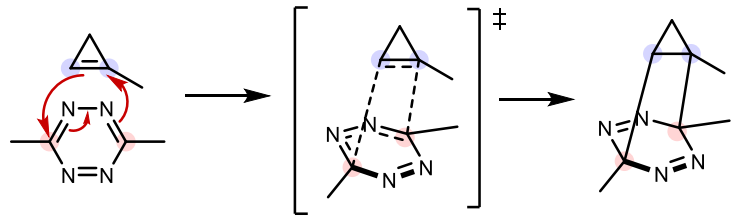
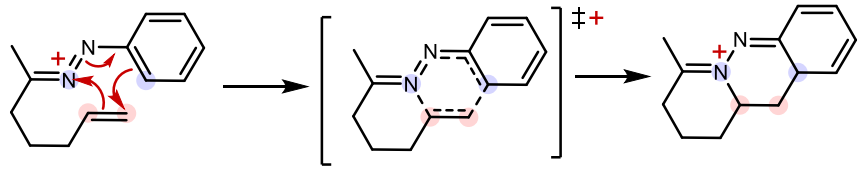
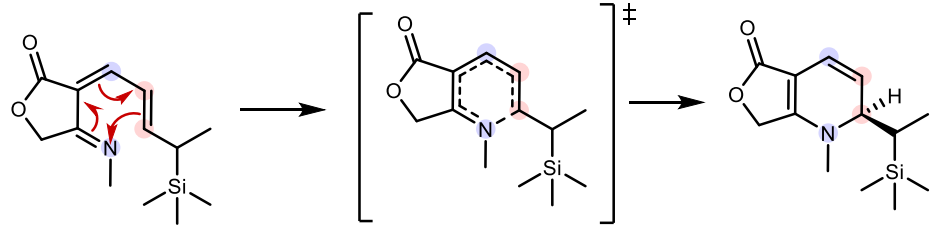
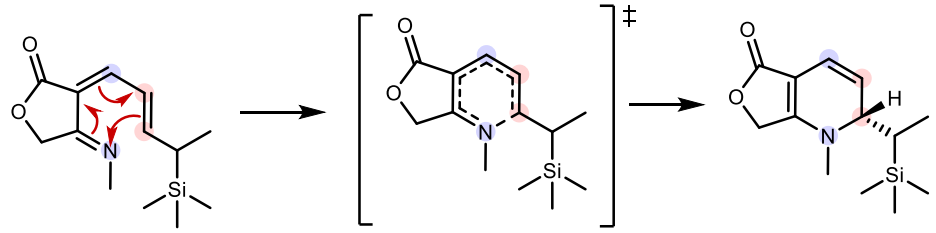
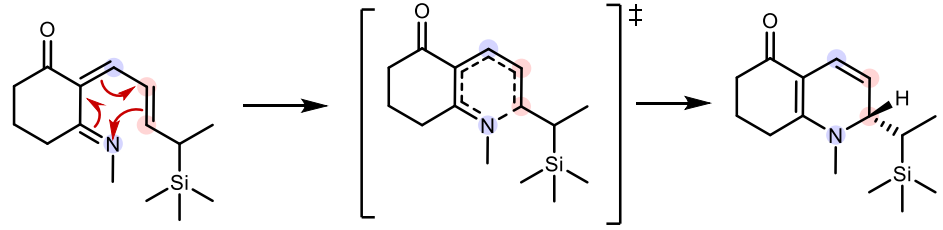
5		26.57	93.72	-67.15
6		26.77	62.05	-35.27
7		19.07	39.40	-20.32
8		12.20	36.77	-24.57
9		17.83	47.85	-30.02

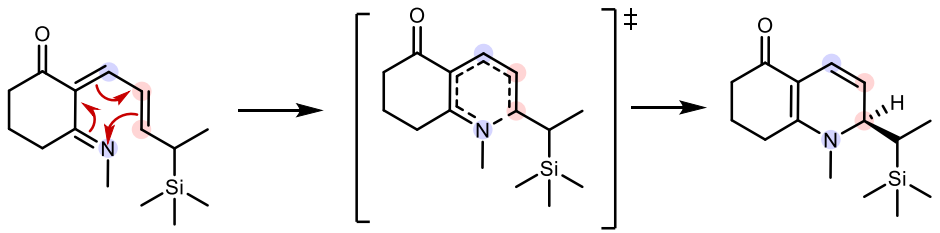
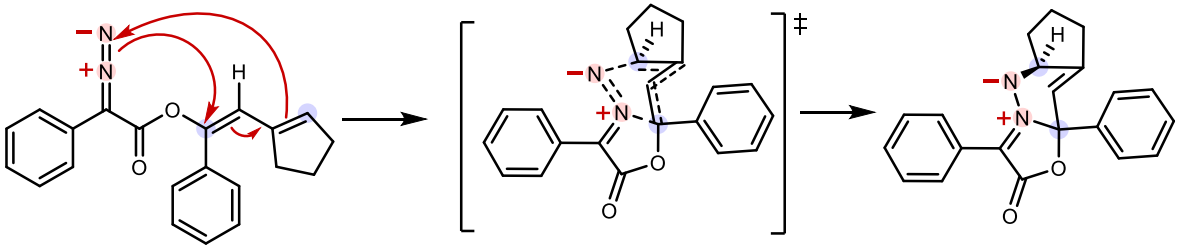
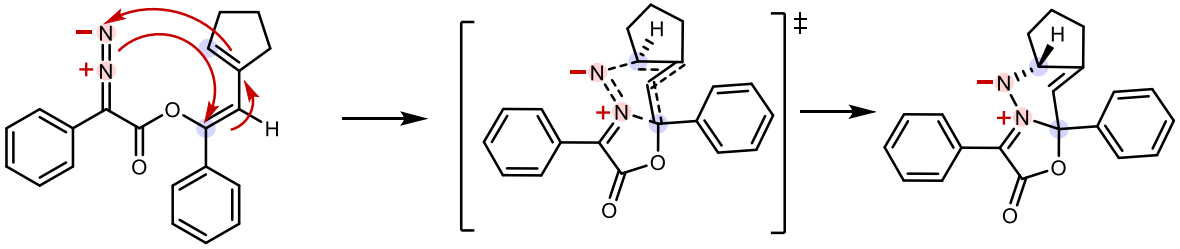
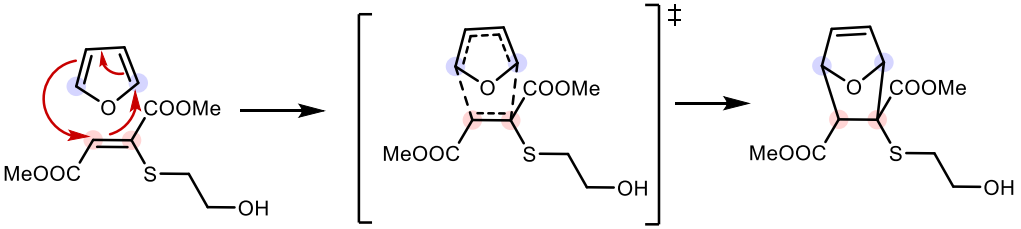
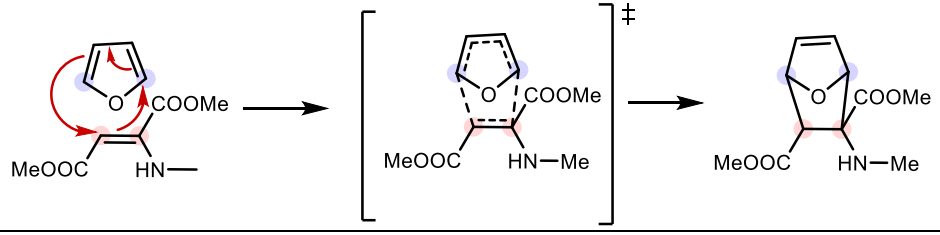
10		19.75	50.92	-31.17
11		23.08	45.70	-22.62
12		24.51	44.87	-20.36
13		24.90	60.92	-36.03
14		21.97	60.48	-38.51
15		25.29	60.68	-35.39

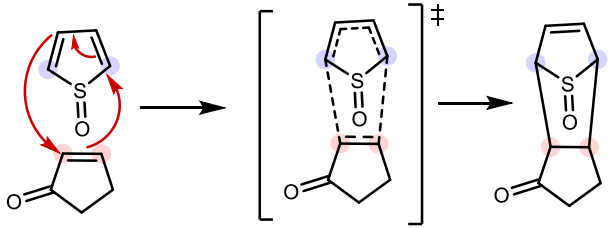
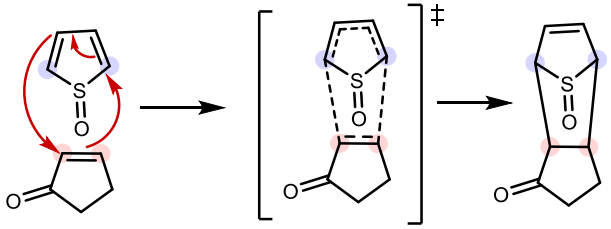
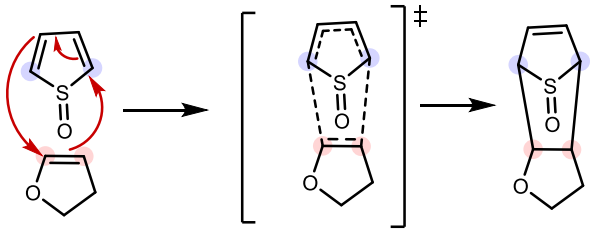
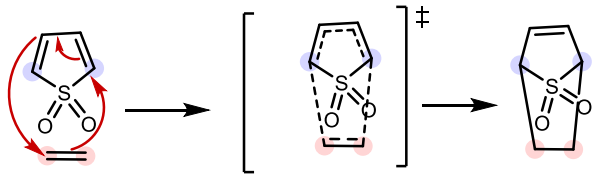
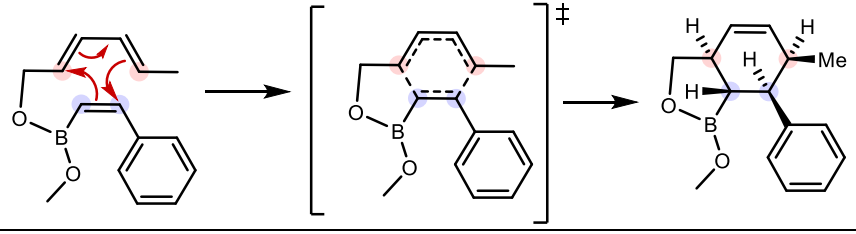
16		23.43	53.32	-29.89
17		15.27	59.46	-44.18
18		19.86	70.40	-50.54
19		22.04	59.33	-37.29
20		19.10	56.89	-37.79

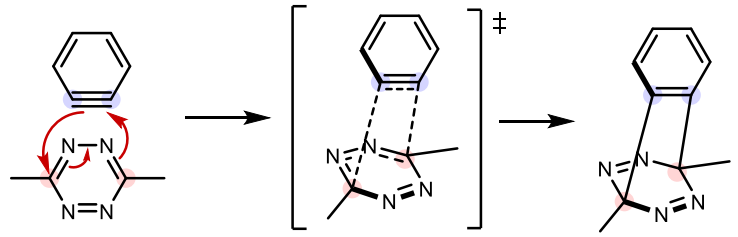
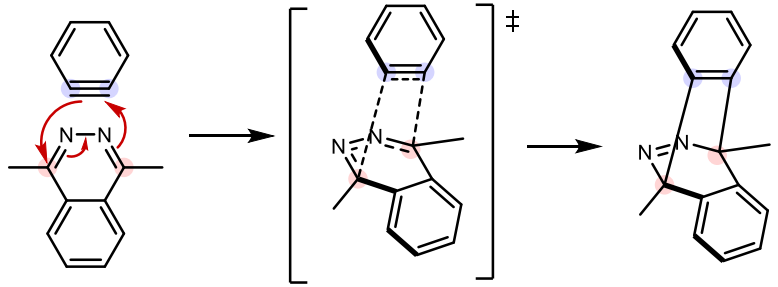
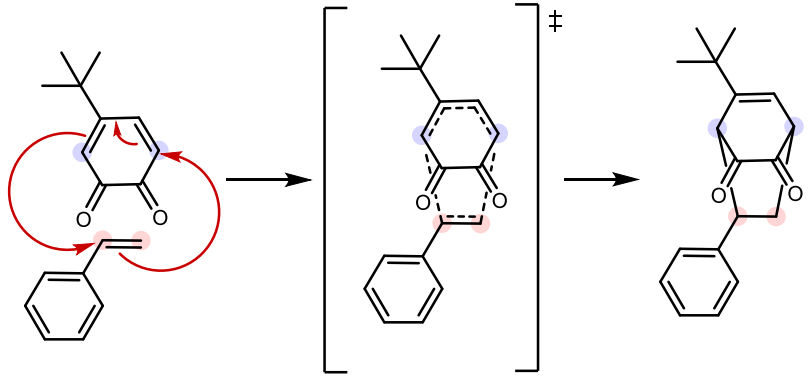
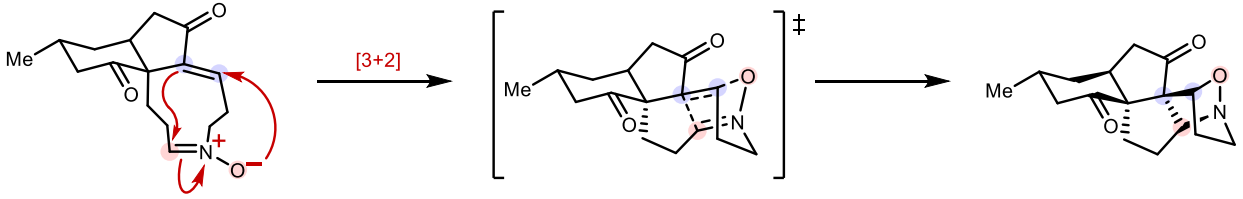
21		12.40	62.14	-49.74
22		8.83	68.85	-60.01
23		24.81	57.02	-32.21
24		26.62	73.95	-47.33
25		23.55	54.52	-30.97
26		27.83	47.79	-19.96
27		29.60	50.22	-20.62

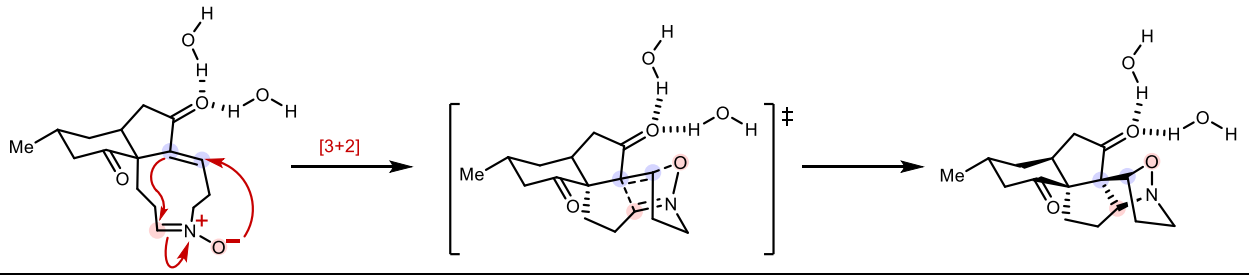
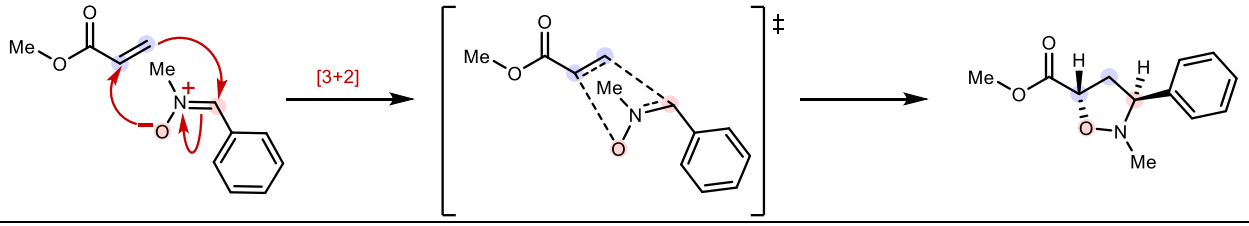
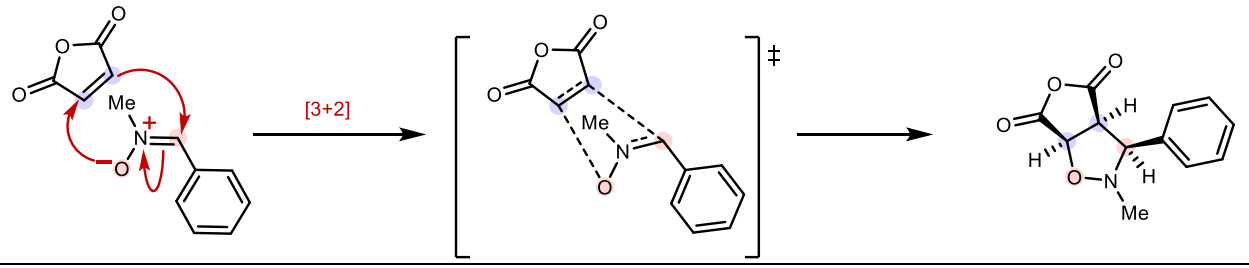
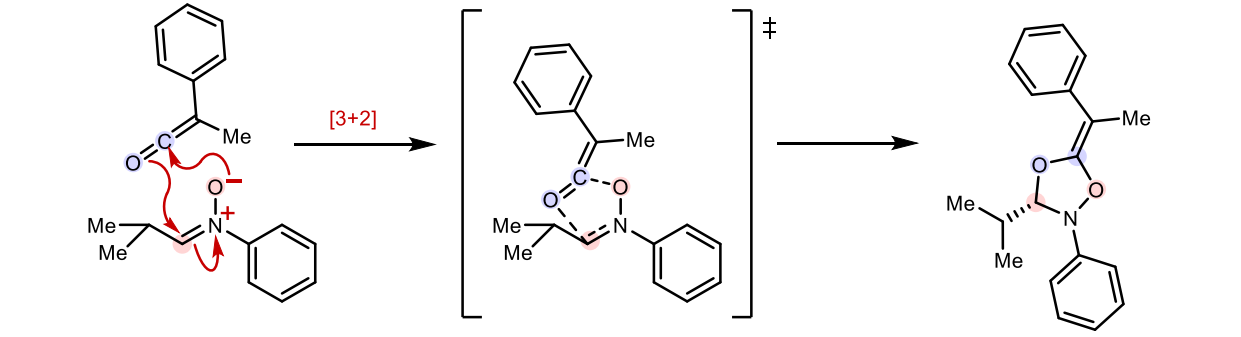
28		21.69	38.32	-16.63
29		1.65	35.57	-33.92
30		7.98	55.02	-47.04
31		15.12	36.68	-21.56

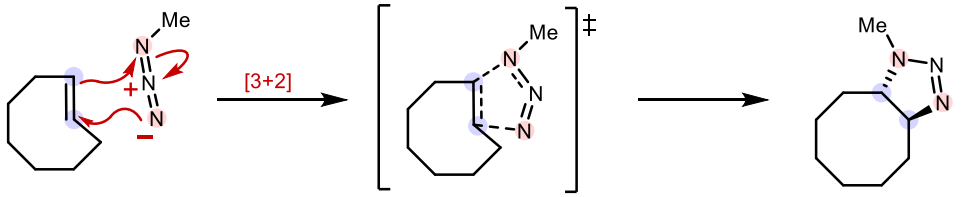
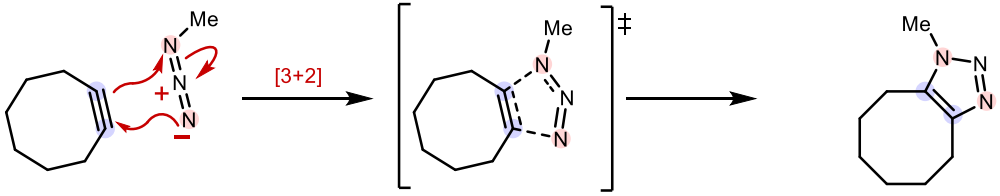
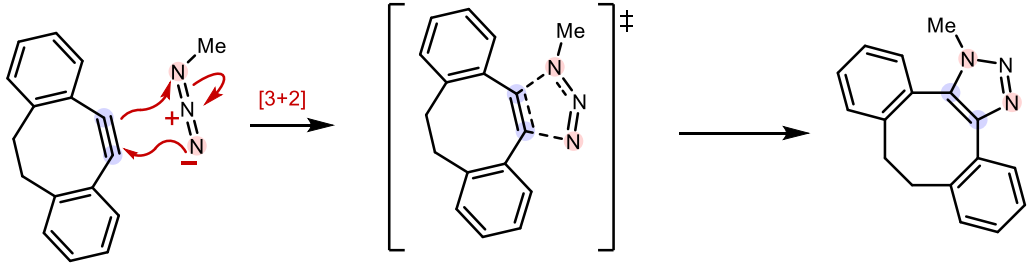
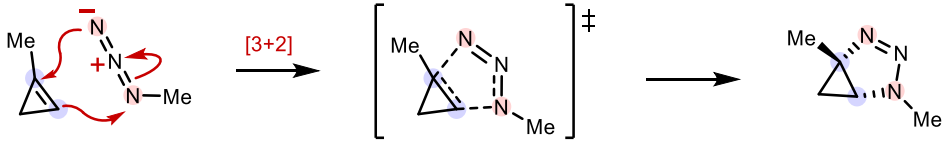
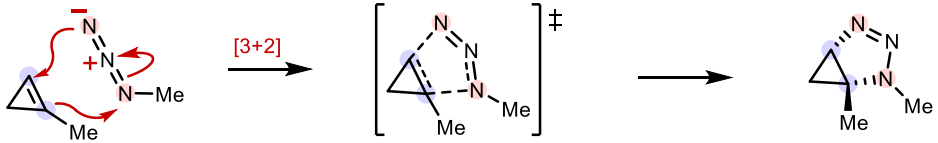
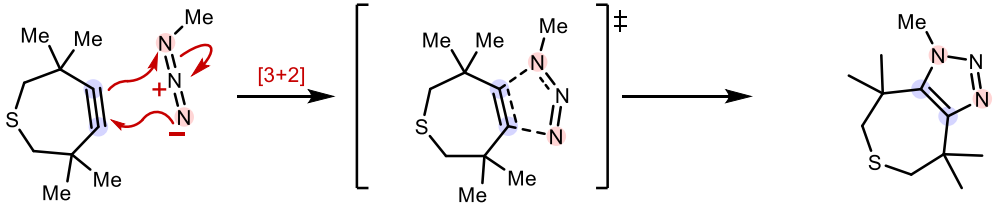
32		6.61	54.79	-48.18
33		11.62	53.25	-41.63
34		18.28	30.48	-12.21
35		16.53	29.81	-13.28
36		15.49	33.65	-18.16

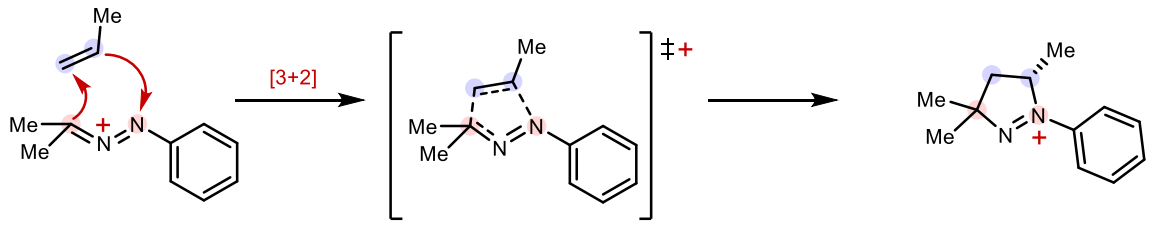
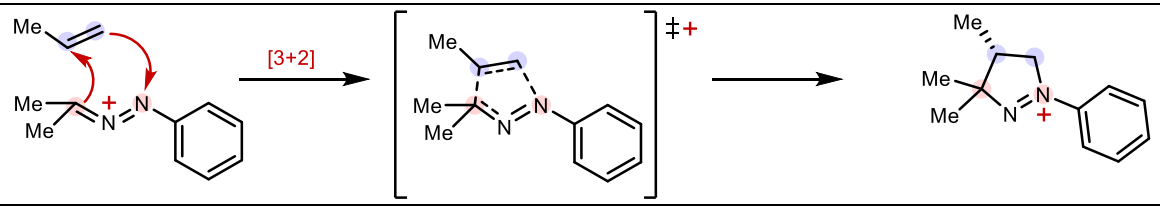
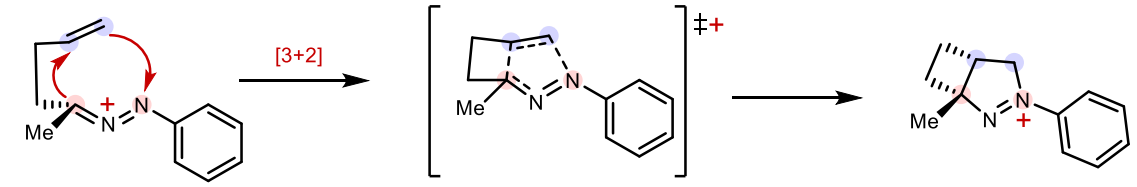
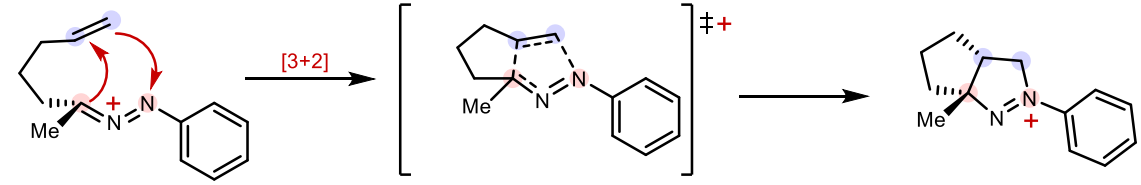
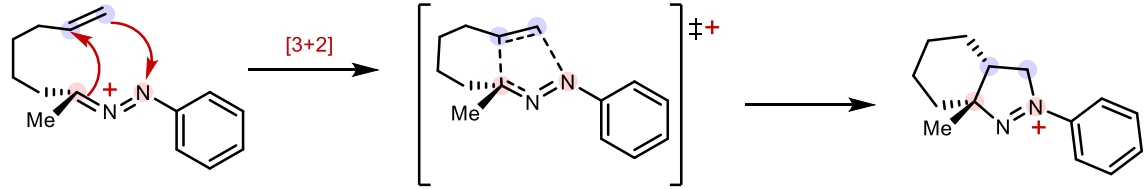
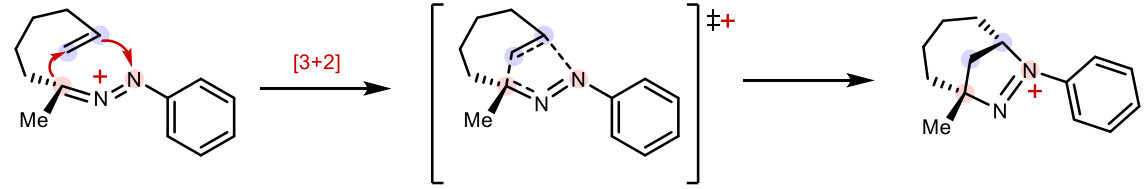
37		17.00	34.43	-17.43
38		22.73	36.09	-13.36
39		37.42	39.32	-1.90
40		14.26	27.77	-13.51
41		28.06	31.78	-3.72

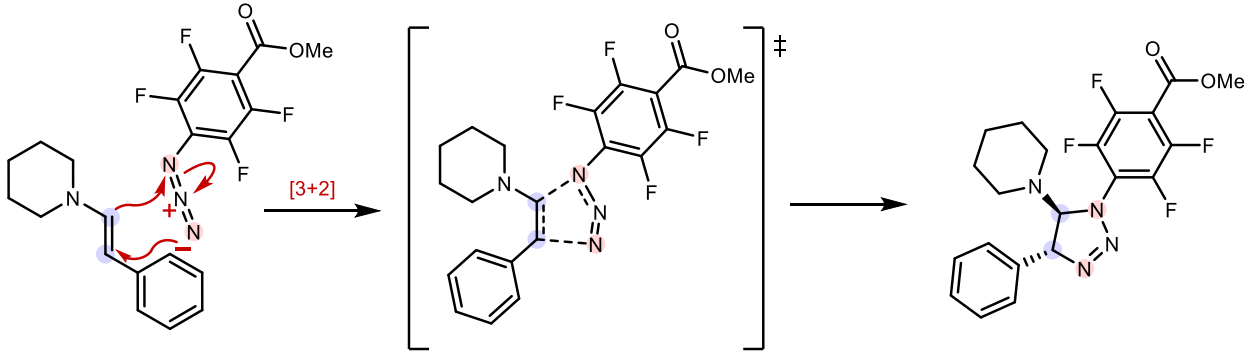
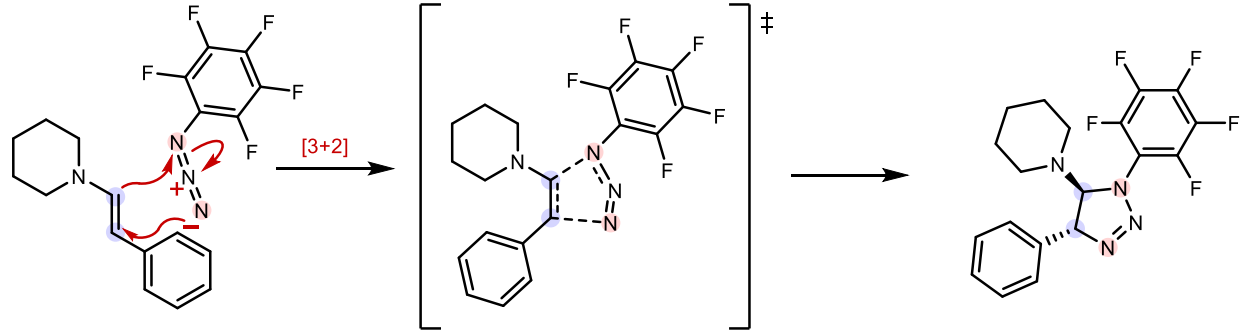
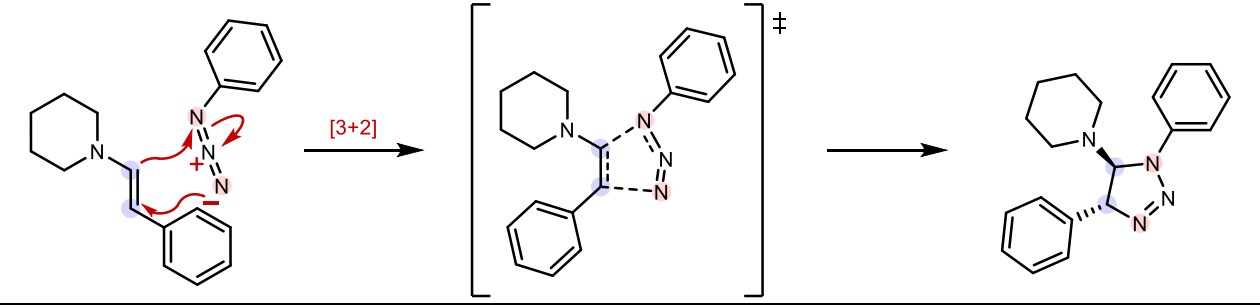
42	 *Syn* adduct	8.58	47.74	-39.15
43	 *Anti* adduct	16.35	48.76	-32.41
44	 *Anti* adduct	16.64	53.18	-36.54
45		16.98	59.46	-42.48
46		26.48	51.36	-24.88

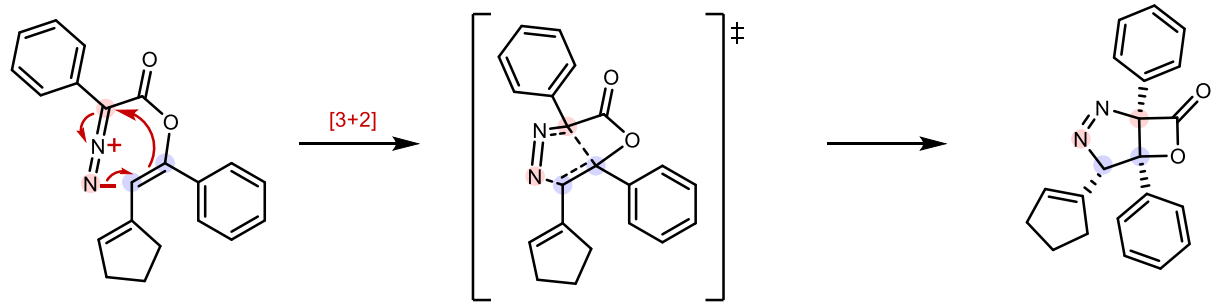
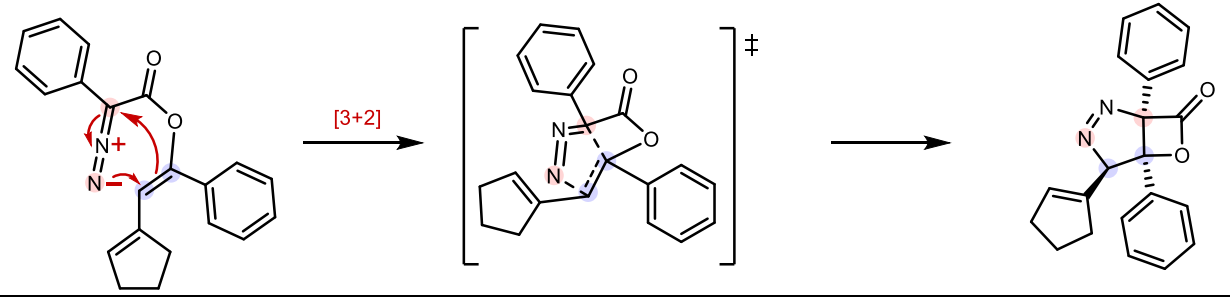
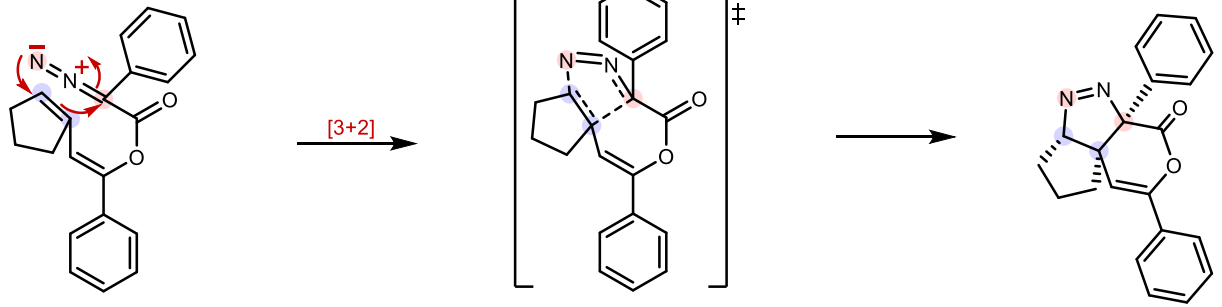
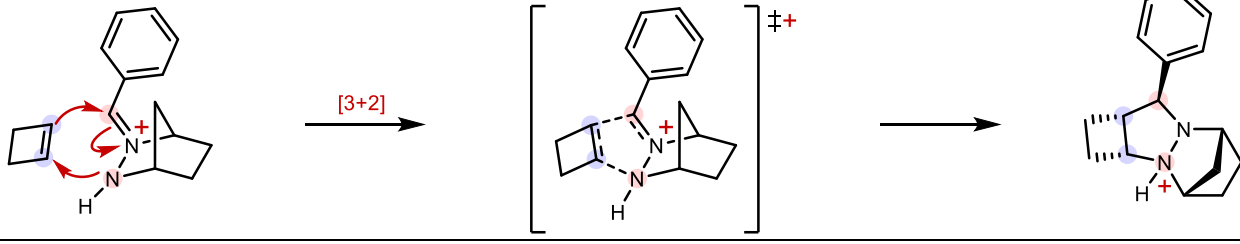
47		-1.34	88.51	-89.85
48		1.98	86.44	-84.47
49		13.95	47.20	-33.24
50		18.44	35.48	-17.04

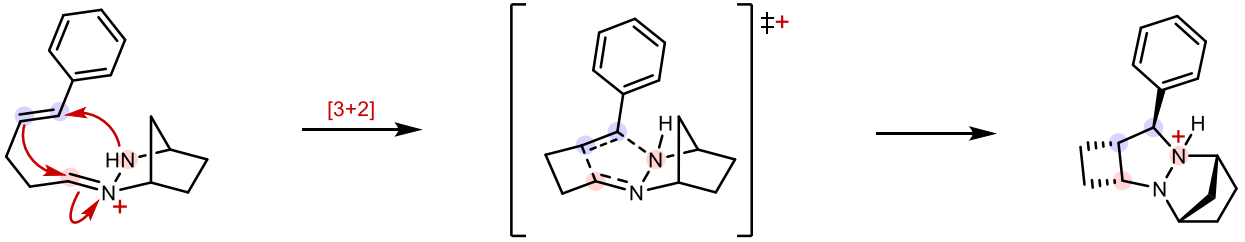
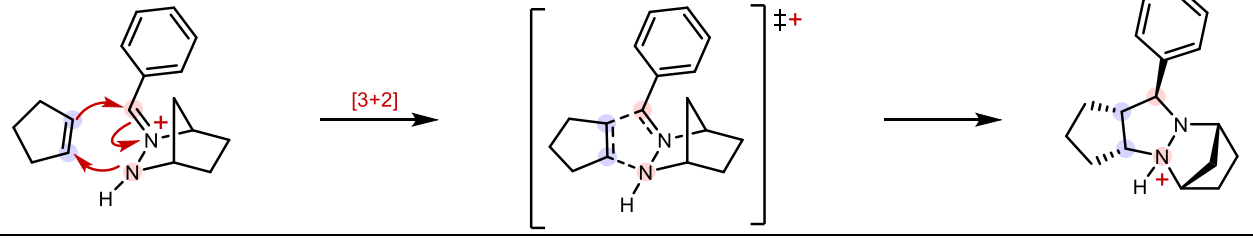
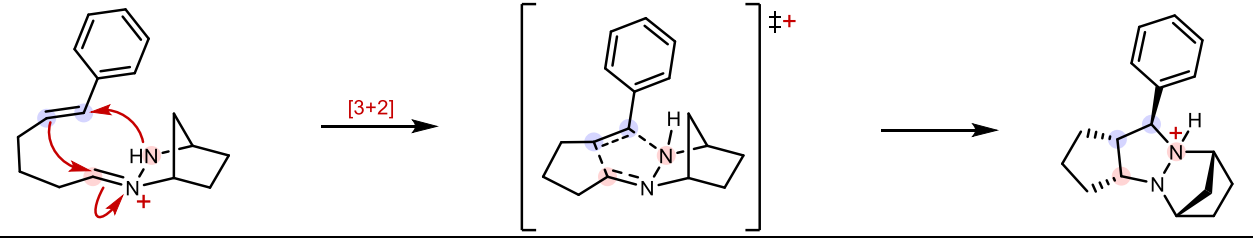
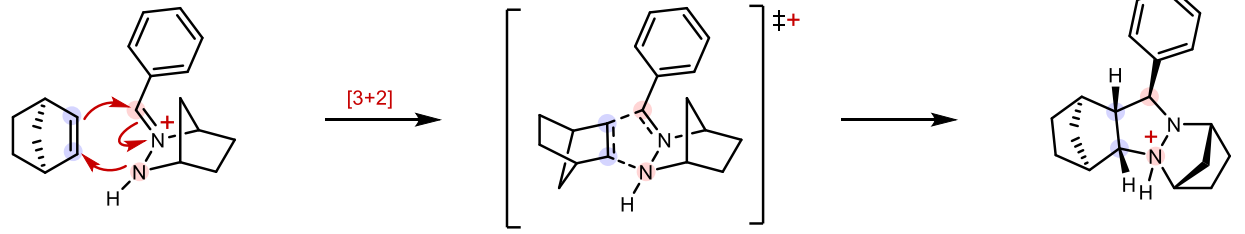
51		-1.95	24.26	-26.21
52		12.39	36.11	-23.72
53		10.45	35.89	-25.44
54		-0.12	26.38	-26.50

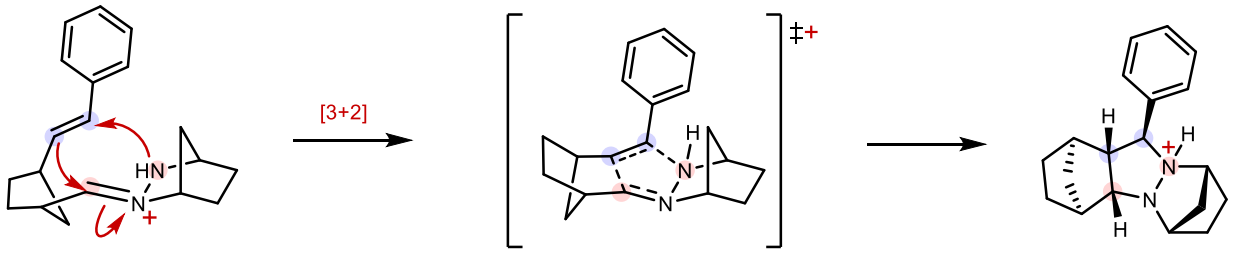
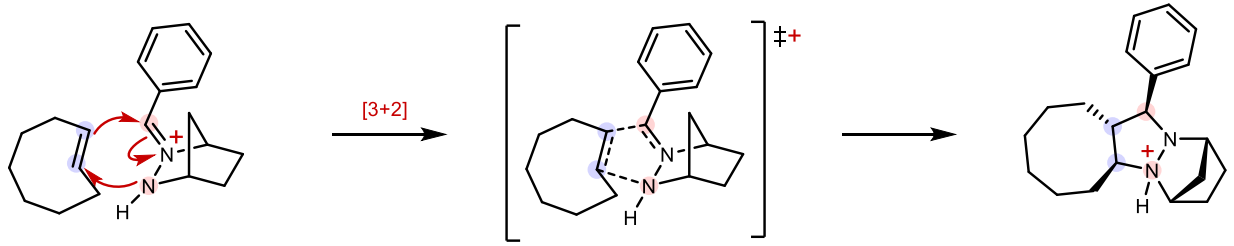
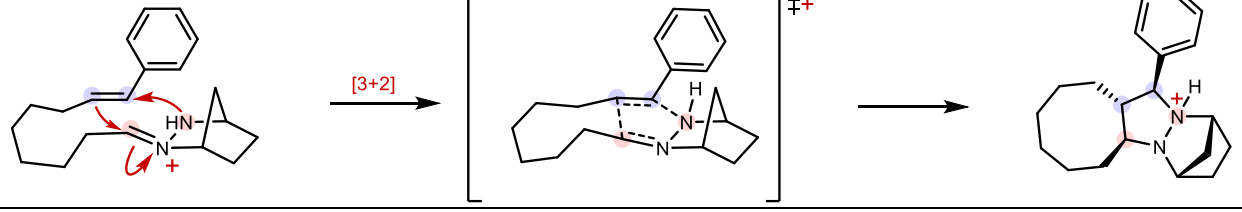
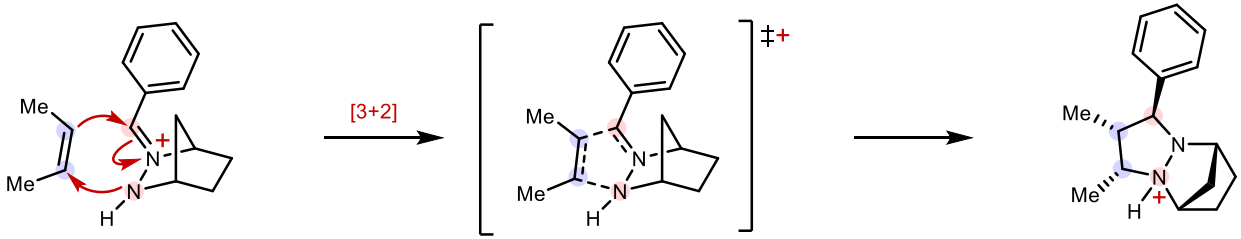
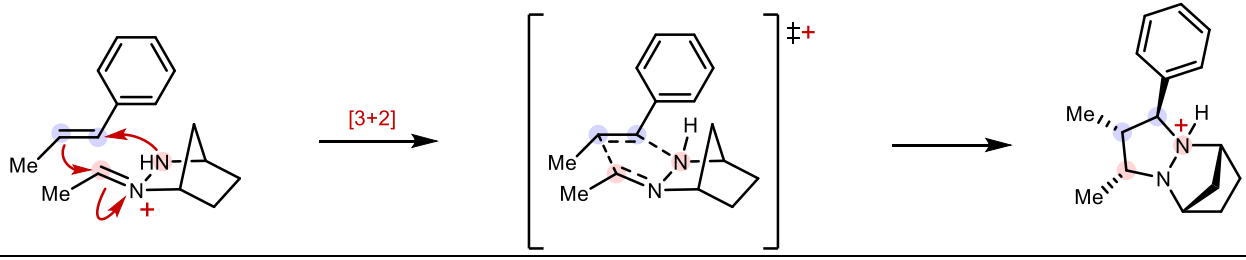
55		12.65	52.78	-40.12
56		11.60	91.82	-80.21
57		8.10	84.96	-76.87
58		15.43	68.29	-52.86
59		15.30	67.99	-52.69
60		5.93	86.94	-81.00

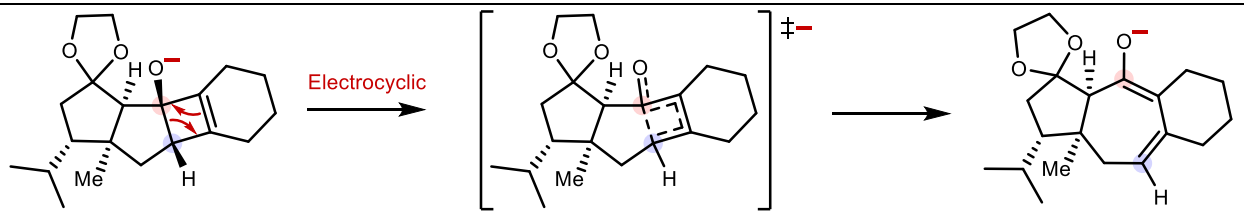
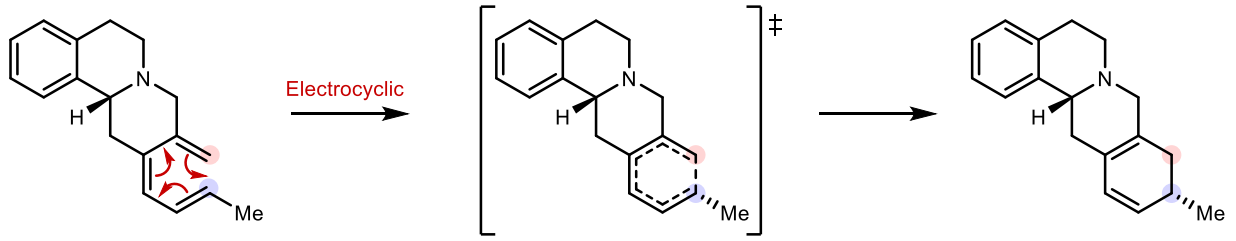
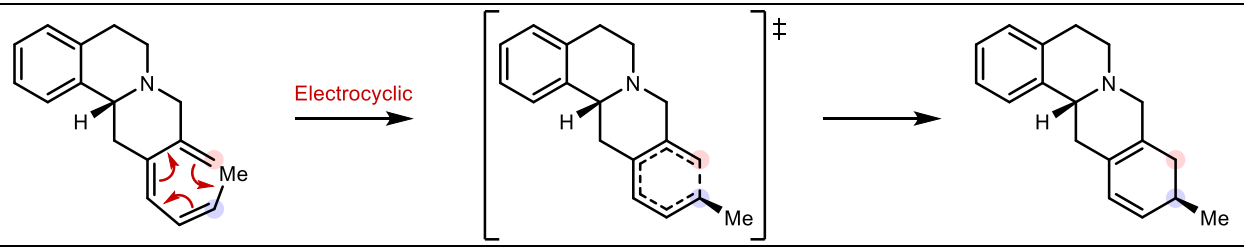
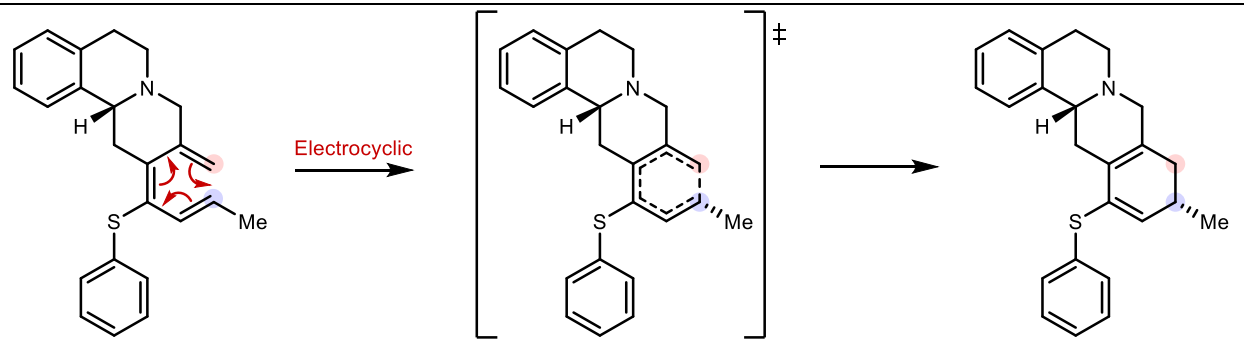
61		0.41	56.60	-56.19
62		3.87	58.42	-54.55
63		16.87	41.50	-24.63
64		5.38	50.91	-45.54
65		8.08	56.87	-48.79
66		6.79	55.77	-48.98

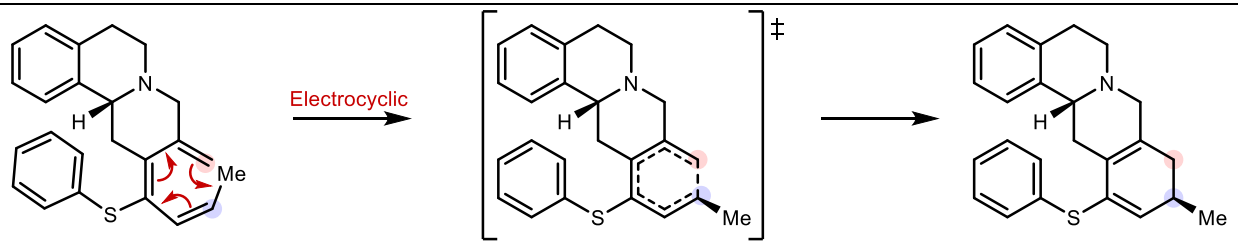
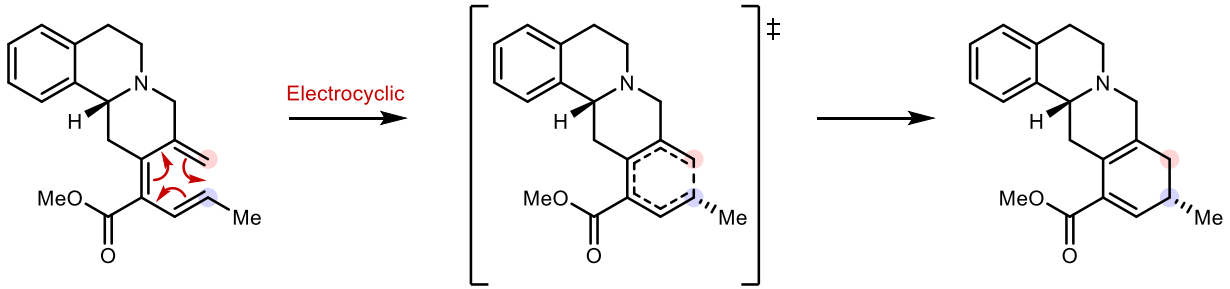
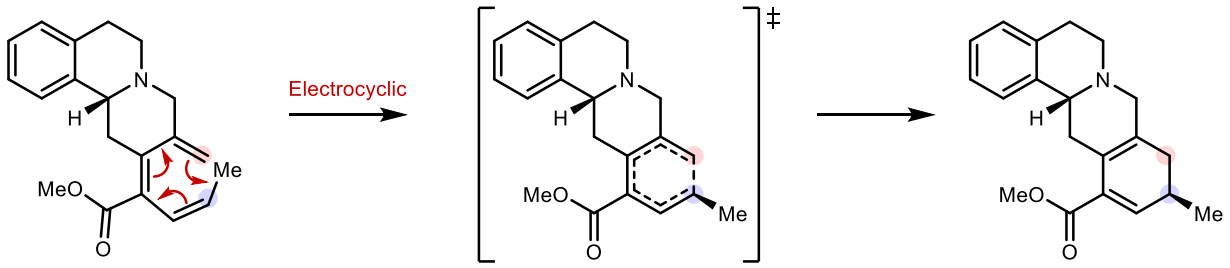
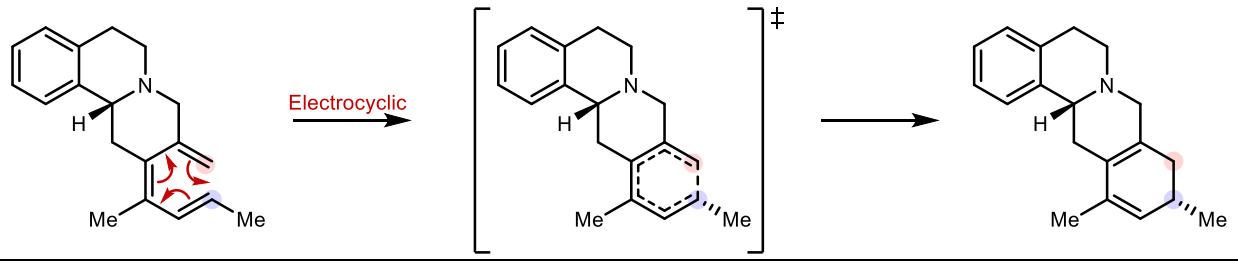
67		6.93	34.09	-27.16
68		8.70	35.15	-26.45
69		13.35	38.42	-25.07

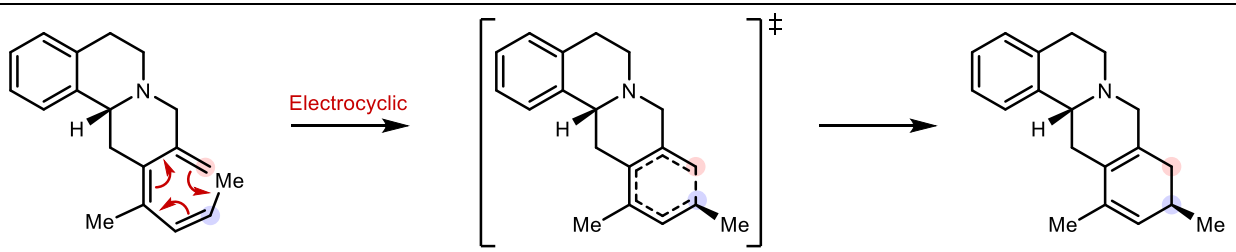
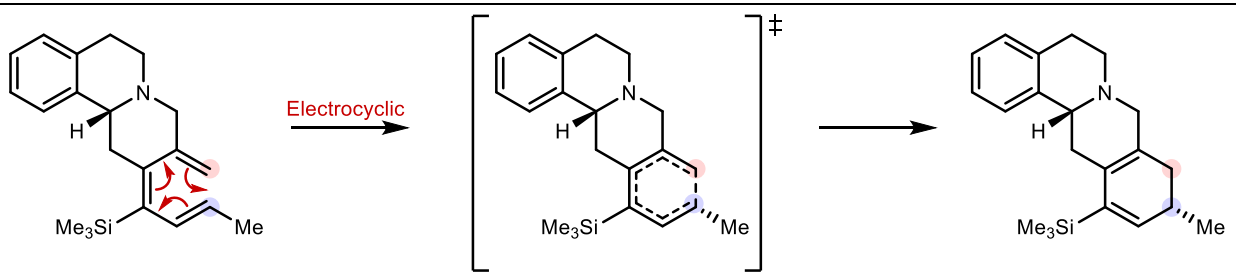
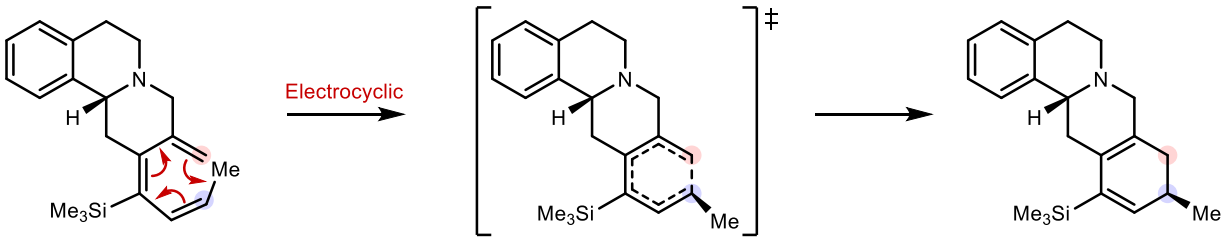
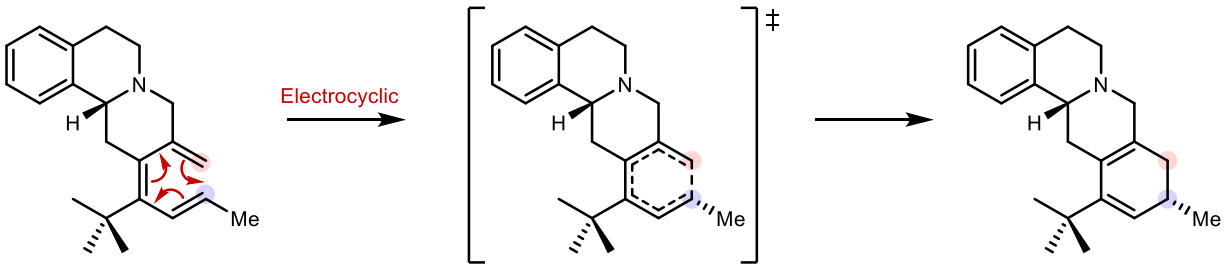
70		33.30	41.80	-8.51
71		34.78	40.16	-5.38
72		26.38	51.44	-25.06
73		10.06	45.53	-35.47

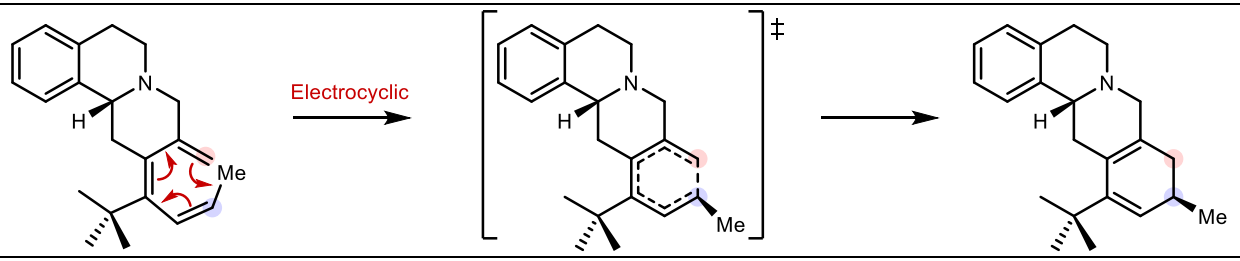
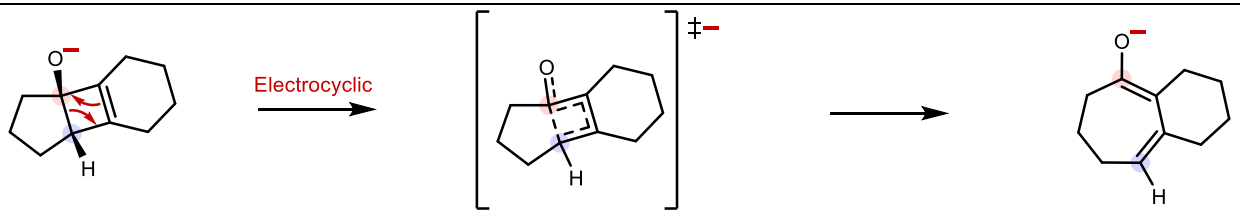
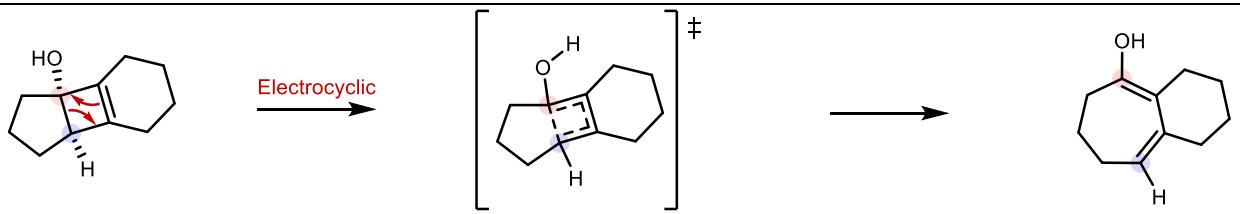
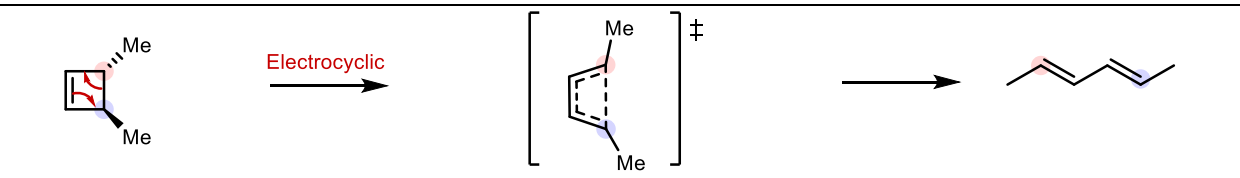
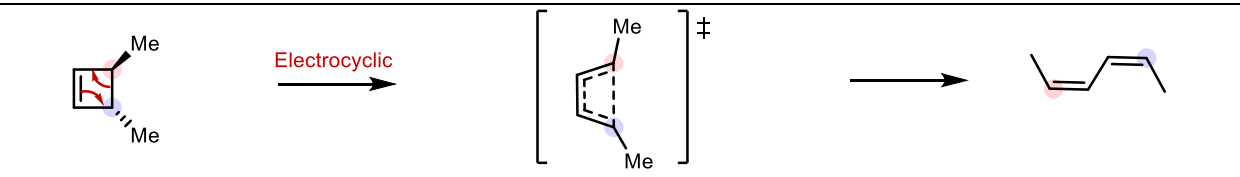
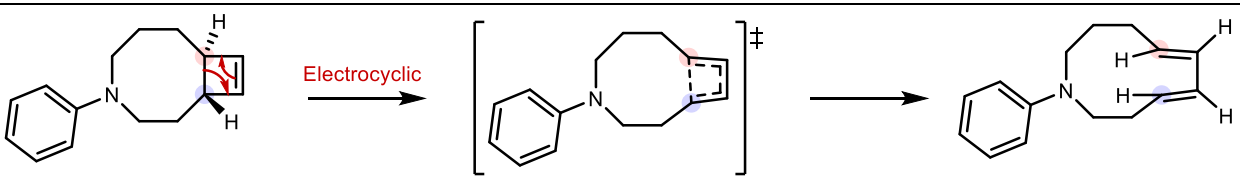
74		27.86	26.23	1.63
75		9.79	41.83	-32.04
76		20.35	37.37	-17.02
77		6.99	46.28	-39.30

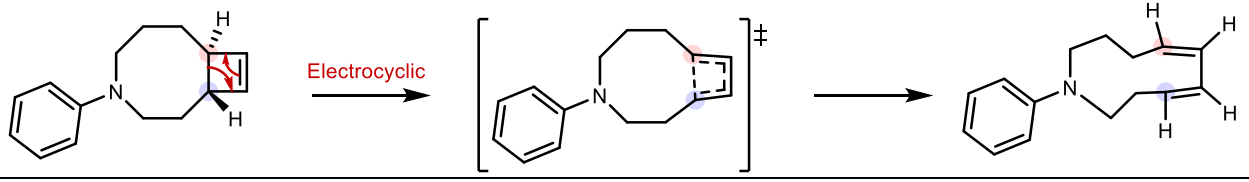
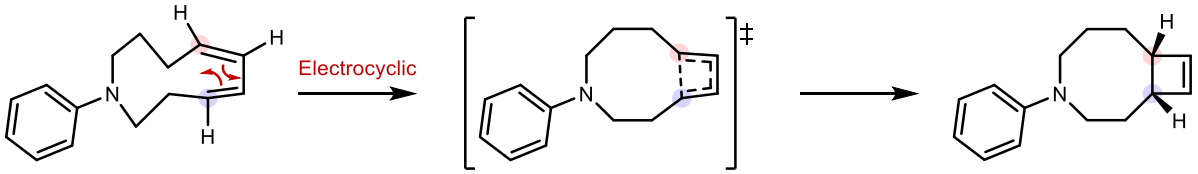
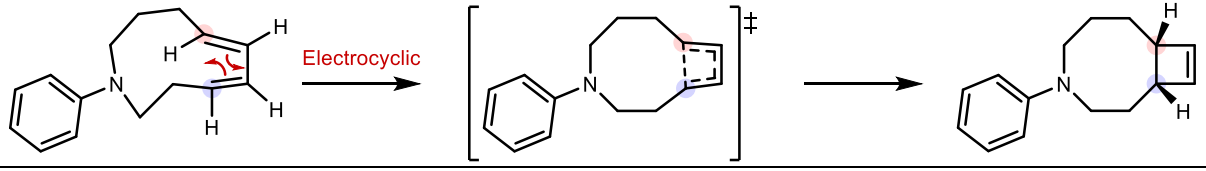
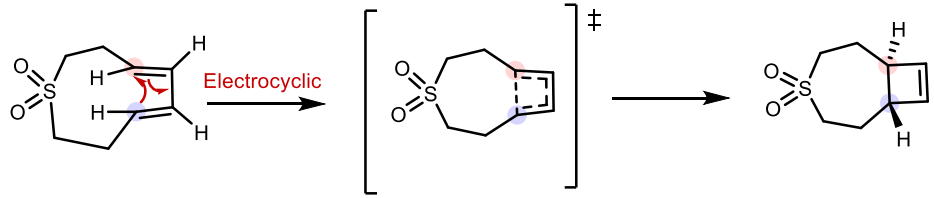
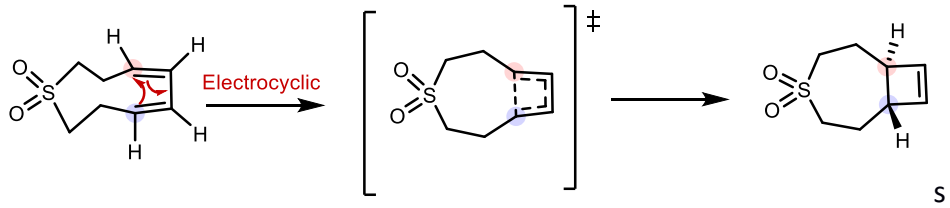
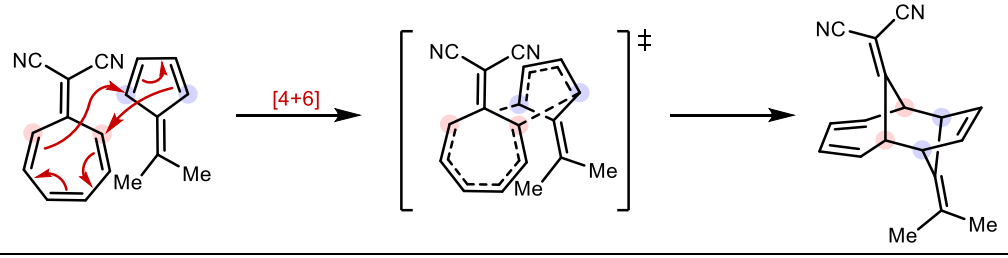
78		19.13	38.27	-19.14
79		1.94	42.25	-40.31
80		28.38	41.25	-12.87
81		11.14	43.06	-31.92
82		10.61	37.95	-27.34

83		17.65	44.98	-27.33
84		26.68	50.51	-23.83
85		30.66	51.43	-20.78
86		27.74	52.70	-24.96

87		30.73	53.65	-22.91
88		24.91	51.36	-26.45
89		28.62	52.88	-24.26
90		27.43	52.17	-24.74

91		31.00	54.55	-23.55
92		23.66	53.48	-29.82
93		28.69	54.95	-26.26
94		25.60	54.46	-28.86

95		28.02	55.88	-27.86
96		11.39	15.19	-3.80
97		43.52	21.76	21.76
98		33.08	45.42	-12.34
99		44.28	54.35	-10.07
100		36.07	19.79	16.28

101		41.80	45.81	-4.01
102		38.73	36.55	2.18
103		36.24	36.68	-0.44
104		13.10	40.49	-27.39
105		48.25	42.24	6.01
106		11.53	29.79	-18.26

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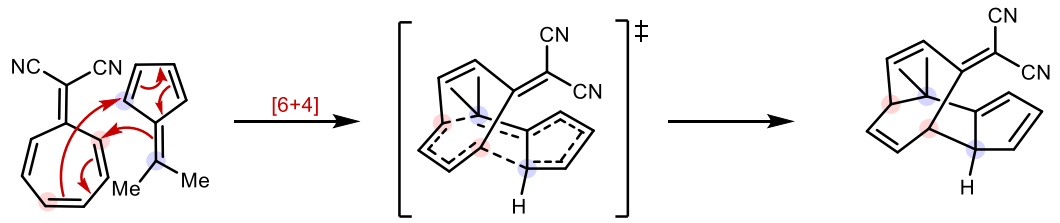
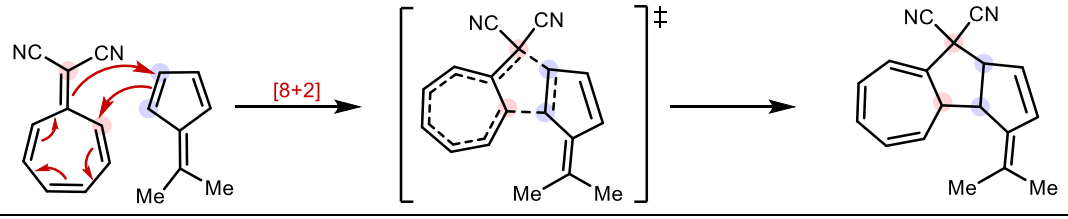
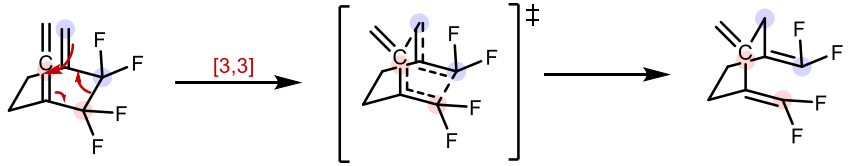
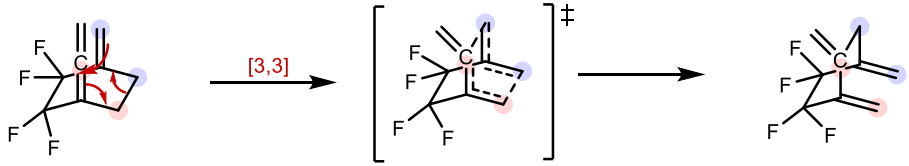
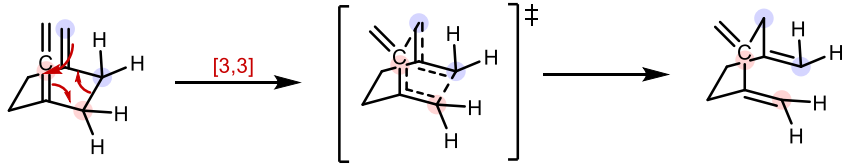
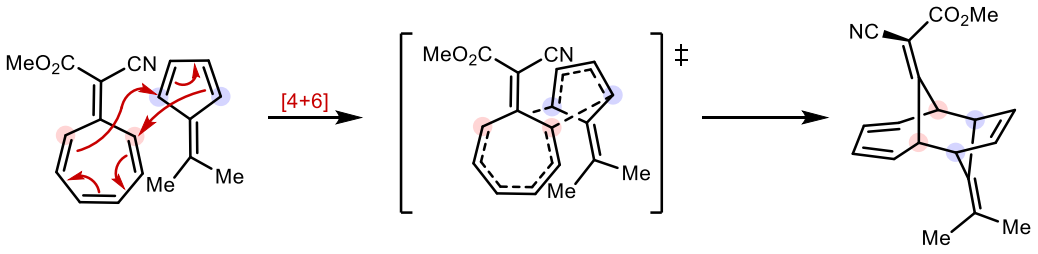
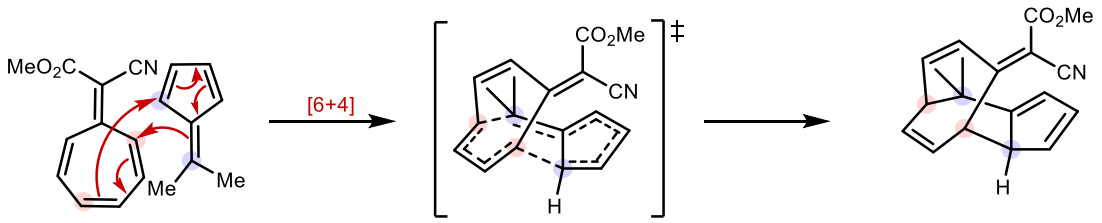
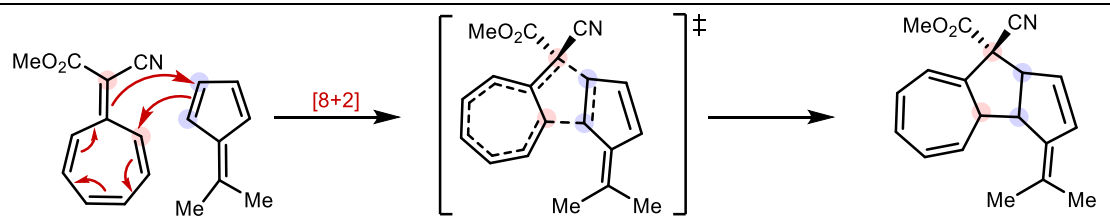
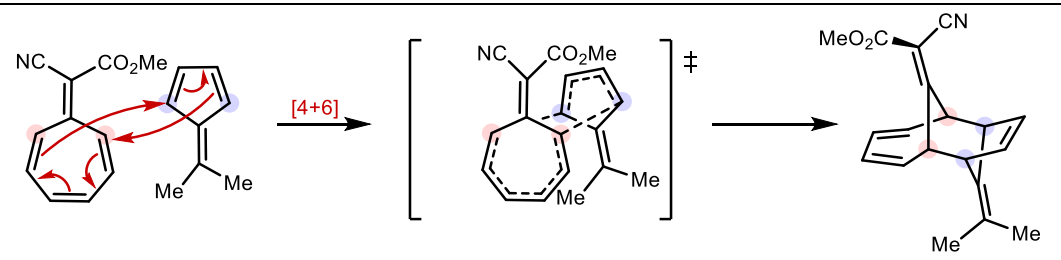
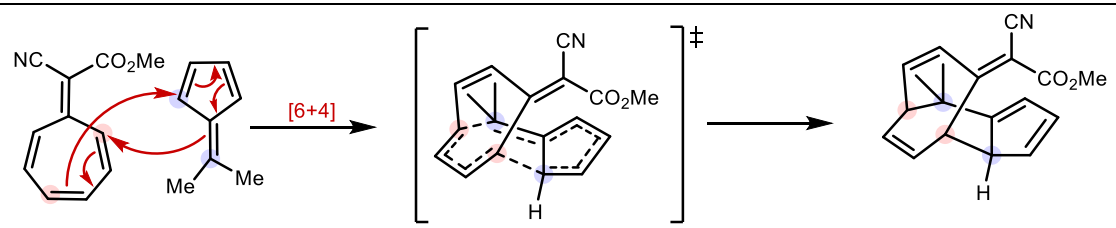
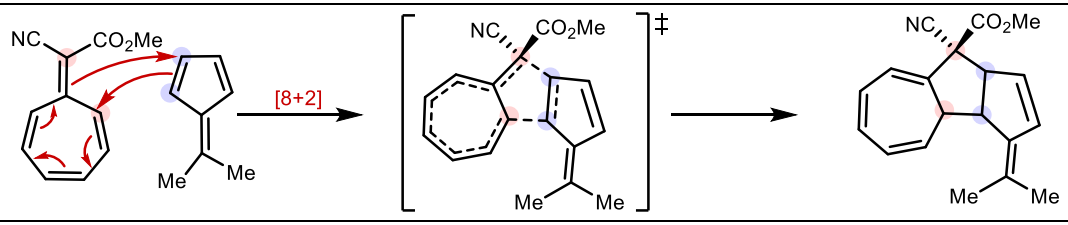
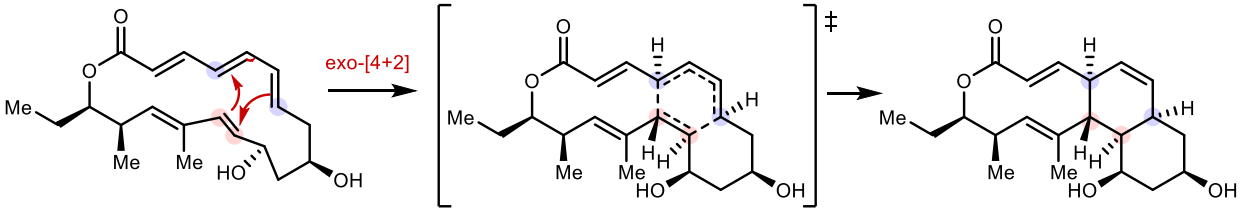
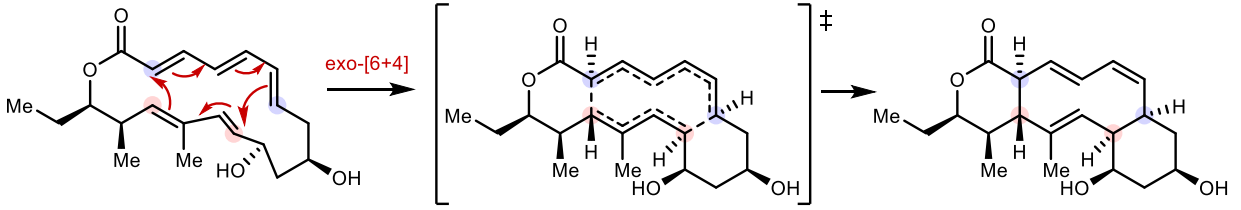
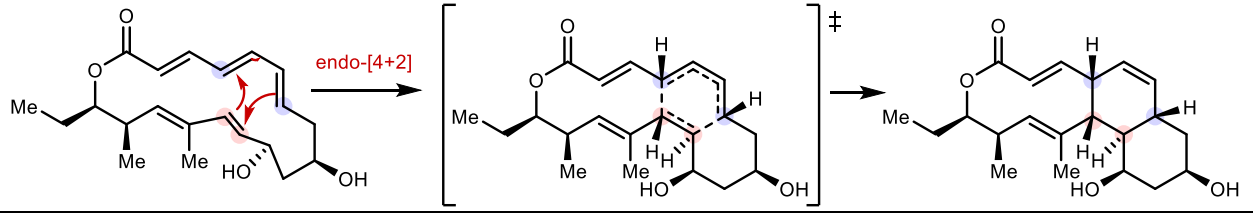
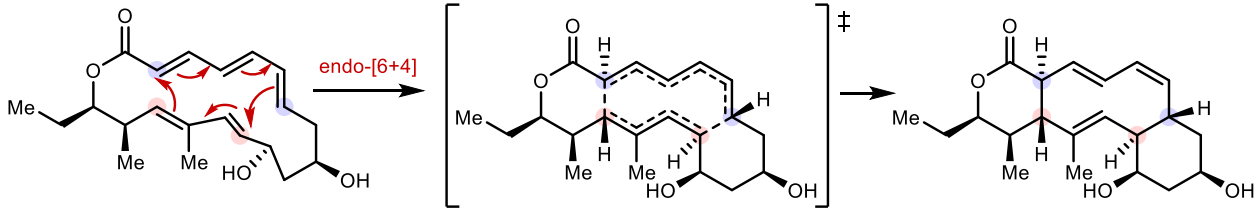
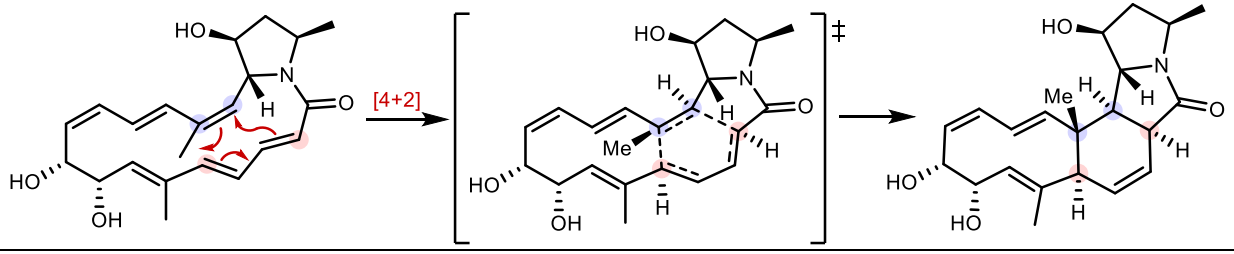
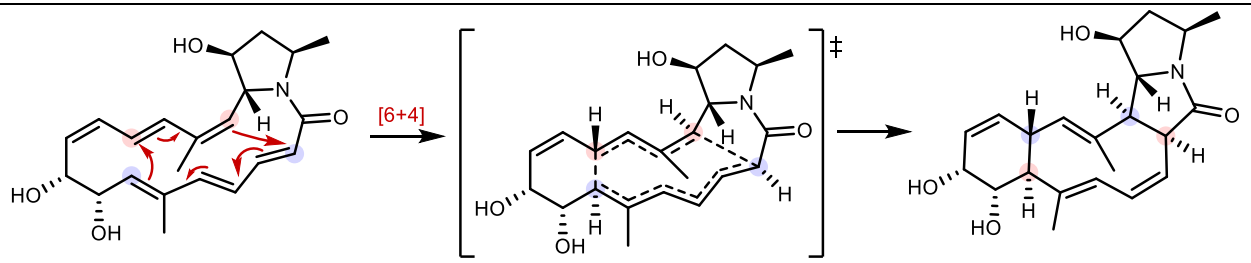
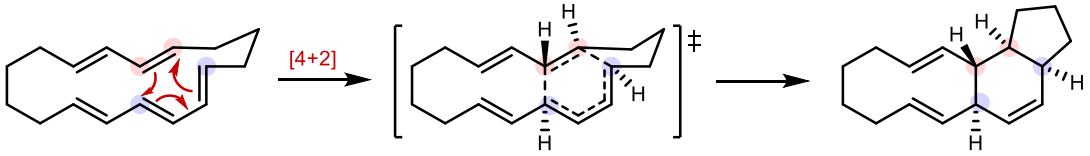
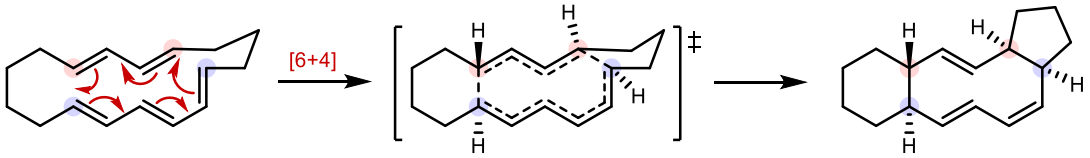
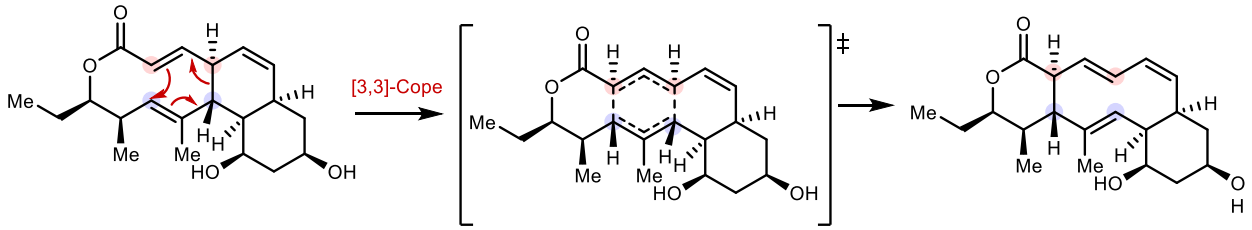
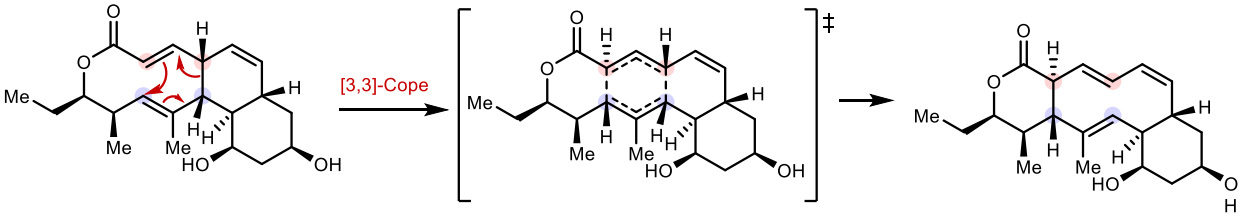
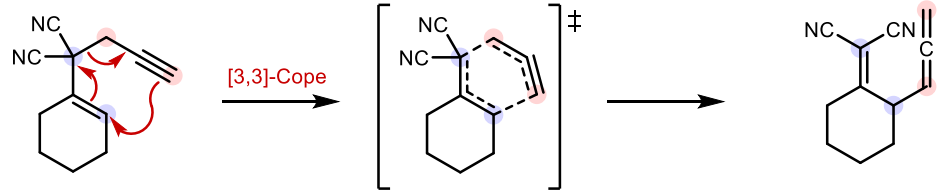
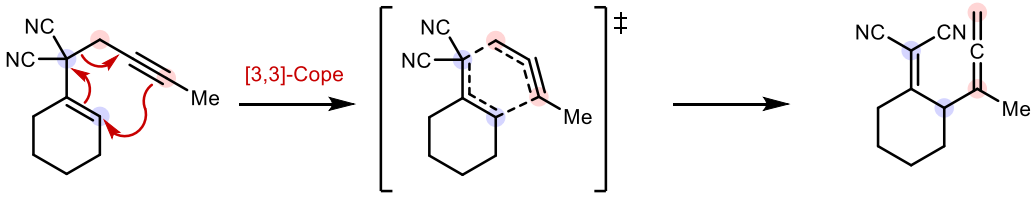
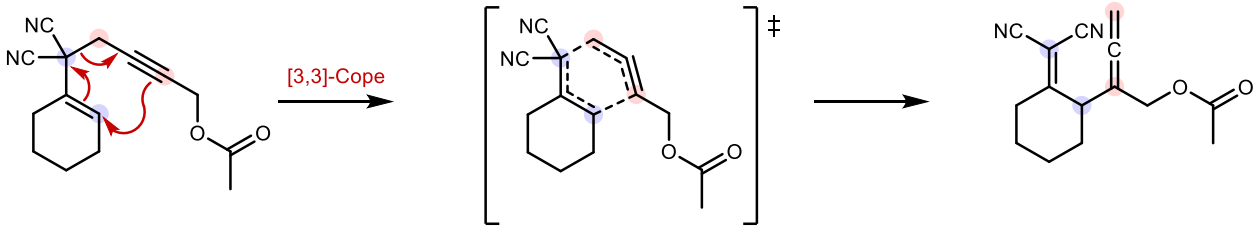
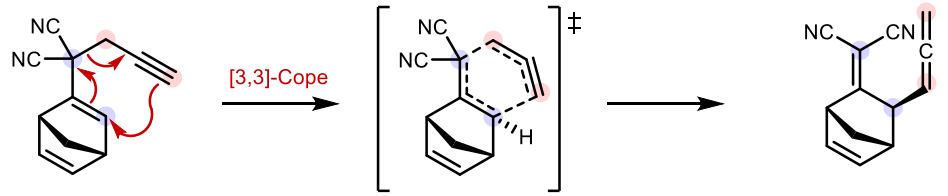
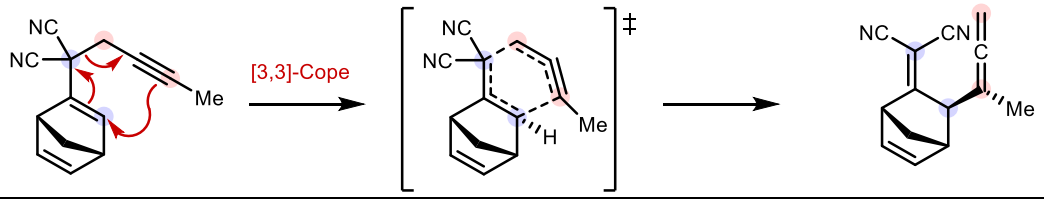
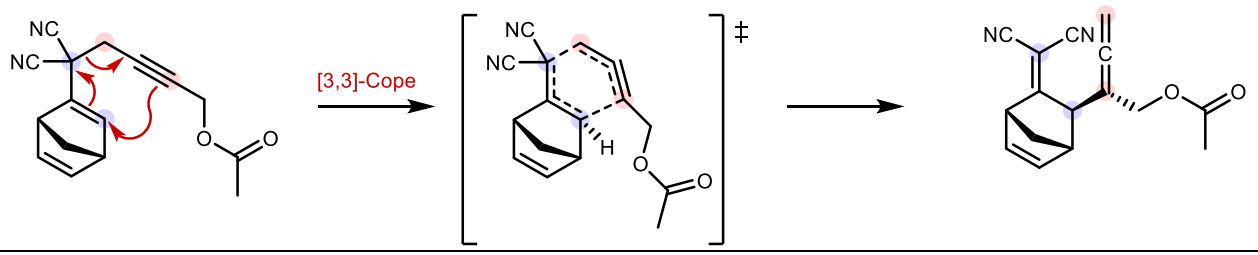
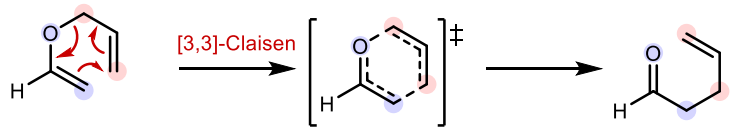
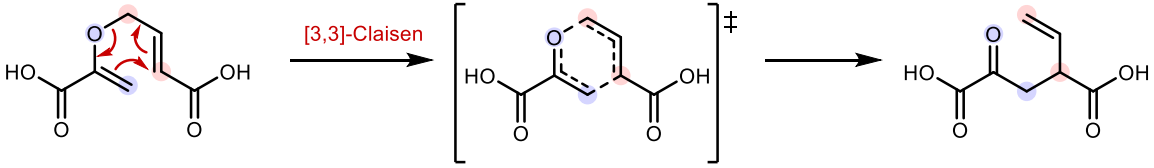
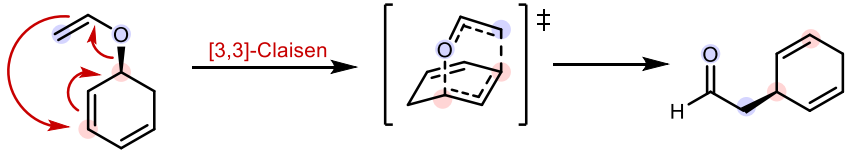
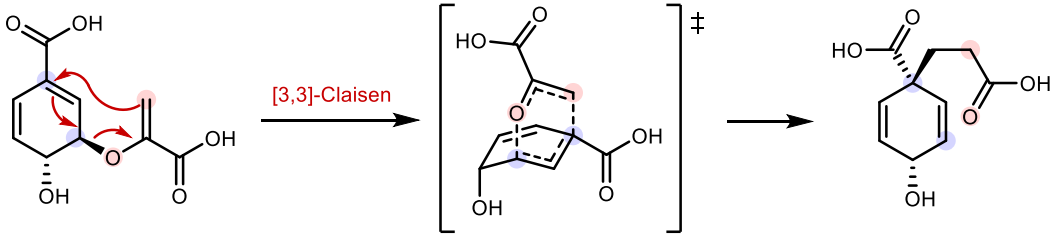
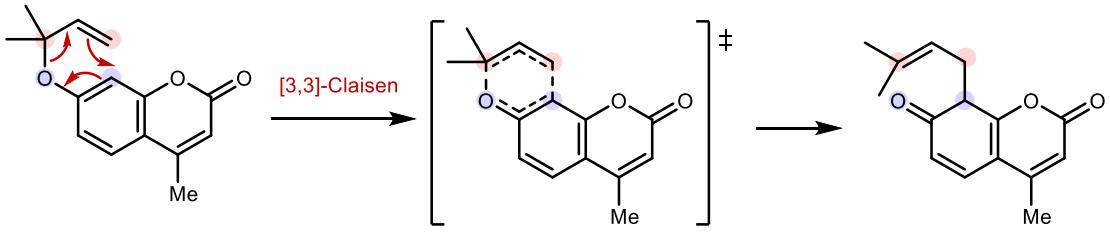
107		11.53	36.38	-24.85
108		11.53	35.01	-23.48
109		43.45	50.58	-7.13
110		43.45	57.37	-13.92
111		36.96	51.17	-14.22
112		12.84	31.12	-18.28

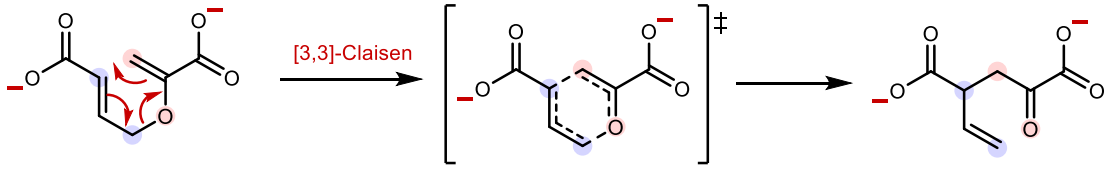
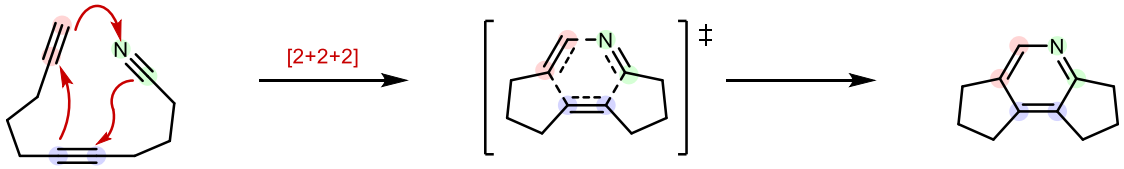
113		12.84	36.75	-23.91
114		12.84	37.94	-25.10
115		11.83	30.11	-18.28
116		11.83	35.81	-23.98
117		11.83	40.21	-28.38

118		22.52	41.61	-19.09
119		18.91	47.58	-28.67
120		16.79	43.12	-26.33
121		16.79	54.33	-37.54
122		19.29	37.46	-18.17

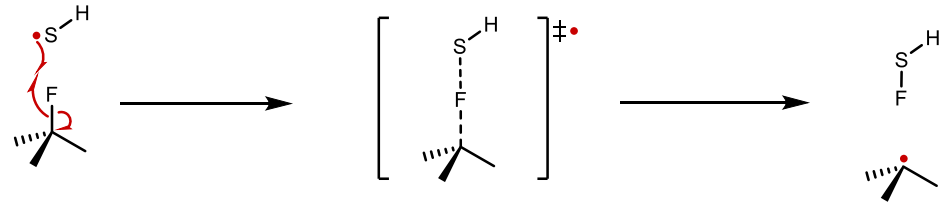
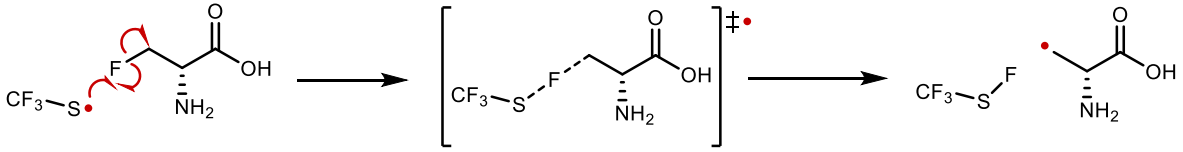
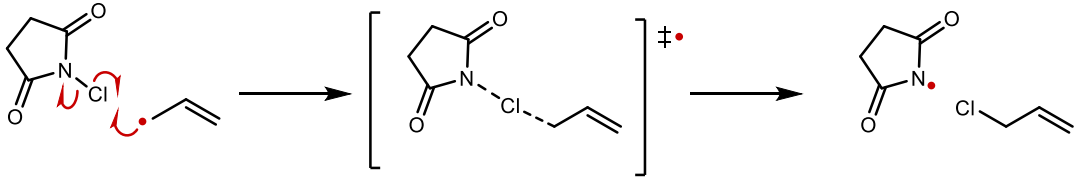
123		19.29	41.95	-22.66
124		21.68	46.02	-24.34
125		21.68	47.32	-25.64
126		20.25	26.19	-5.95
127		20.95	32.16	-11.21

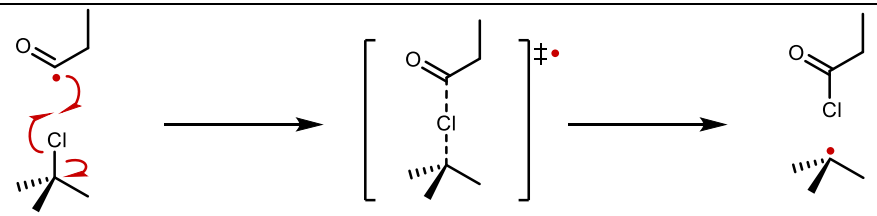
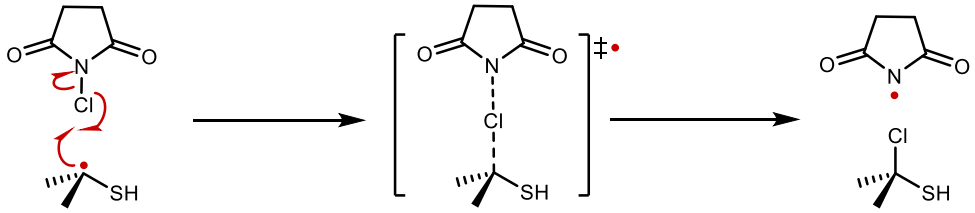
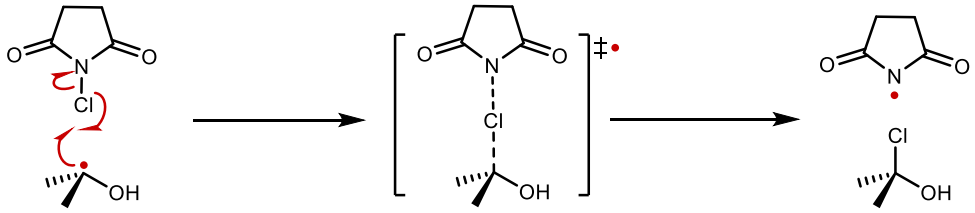
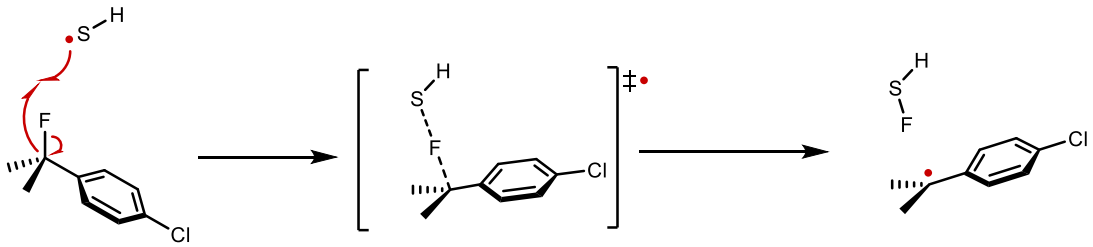
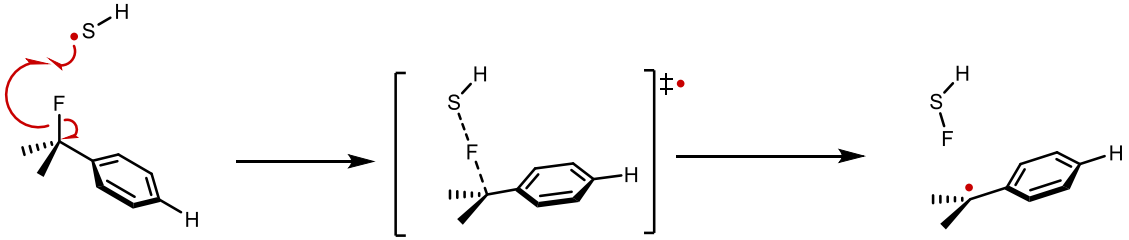
128		32.74	41.45	-8.71
129		34.42	40.15	-5.73
130		35.40	43.32	-7.92
131		32.39	43.38	-10.99
132		32.92	41.10	-8.18

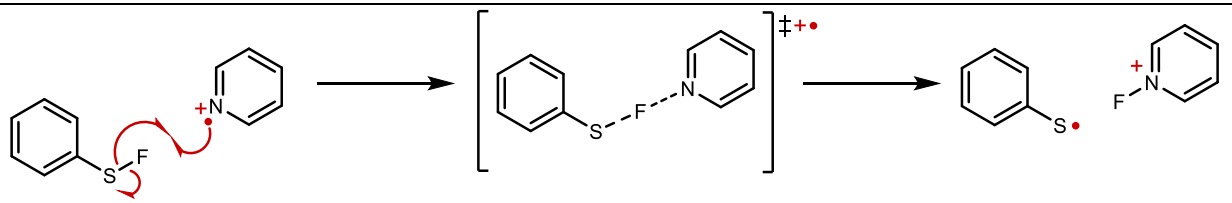
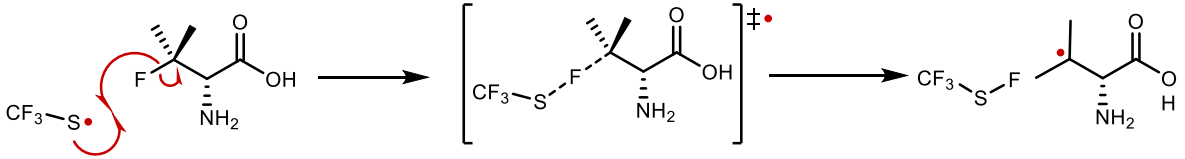
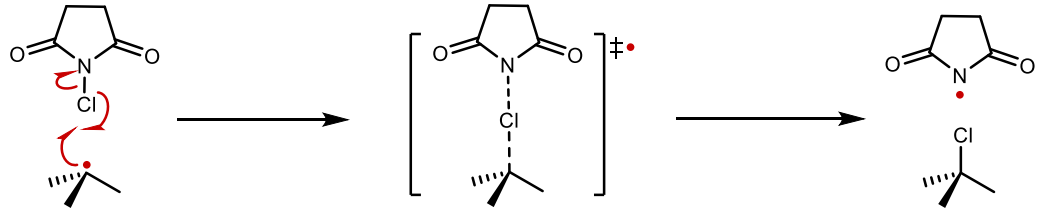
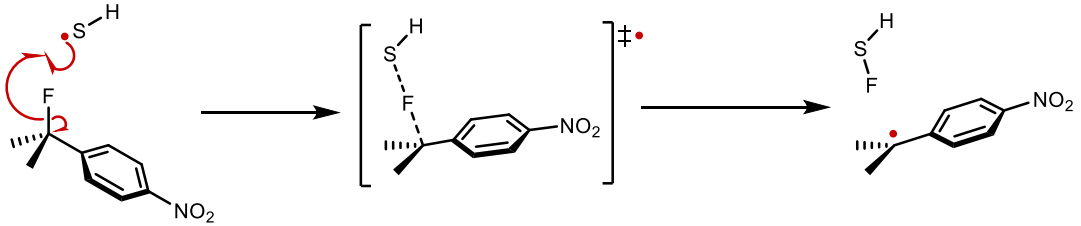
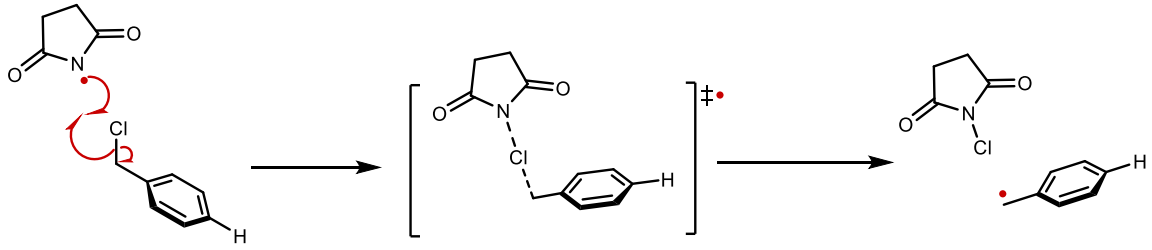
133		33.84	44.83	-10.99
134		32.08	49.61	-17.53
135		28.35	44.42	-16.07
136		29.79	45.83	-16.04
137		25.98	41.35	-15.37
138		31.94	28.09	3.85

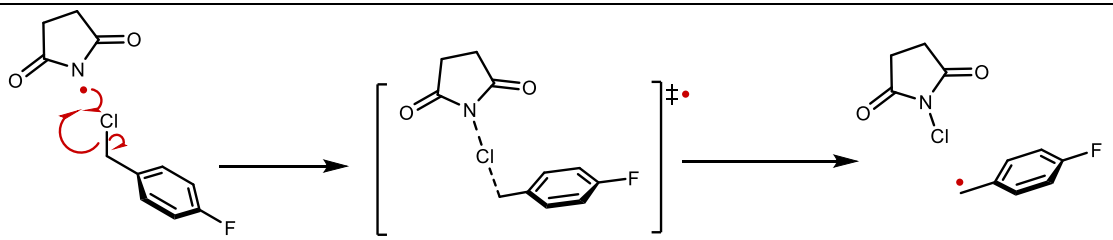
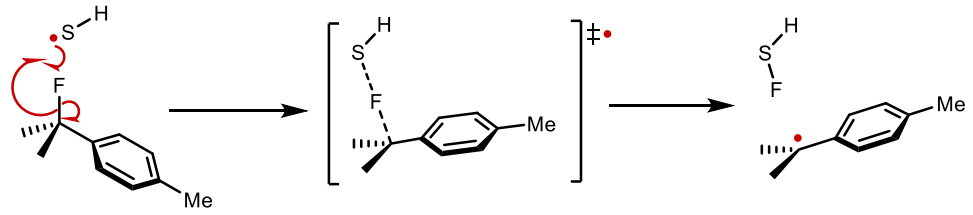
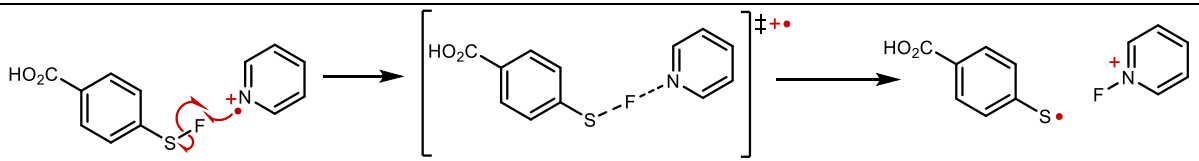
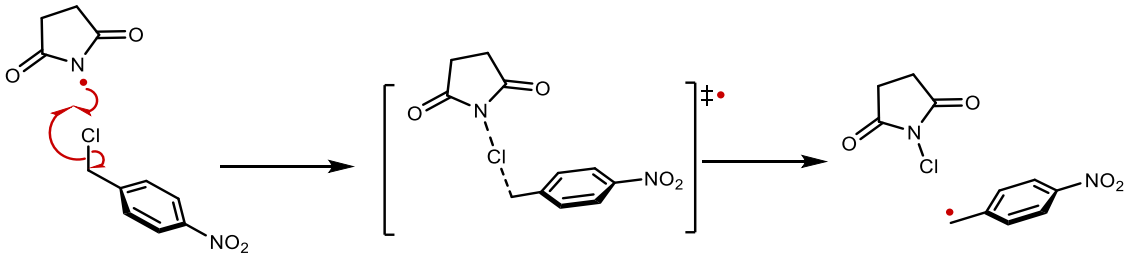
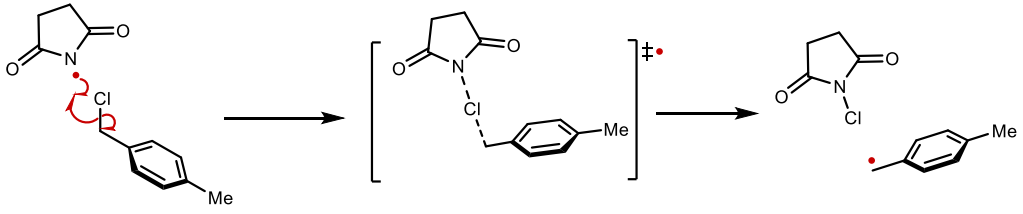
139		34.37	50.96	-16.59
140		54.84	144.39	-89.55

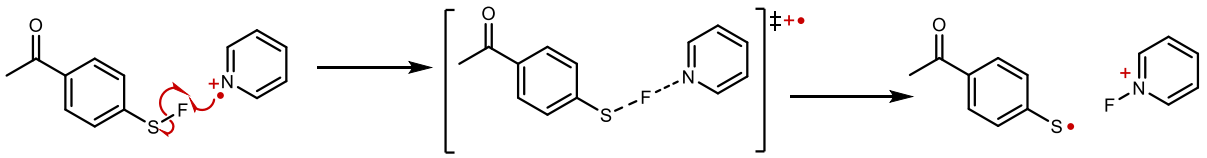
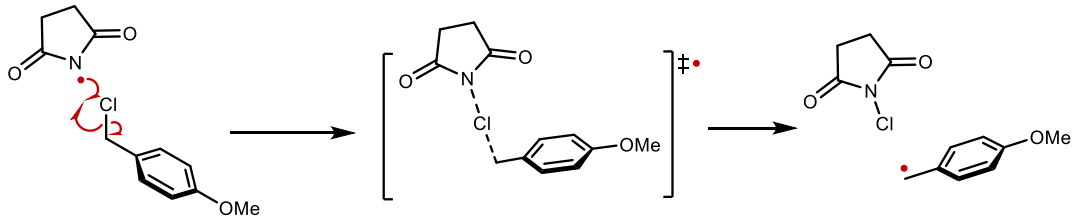
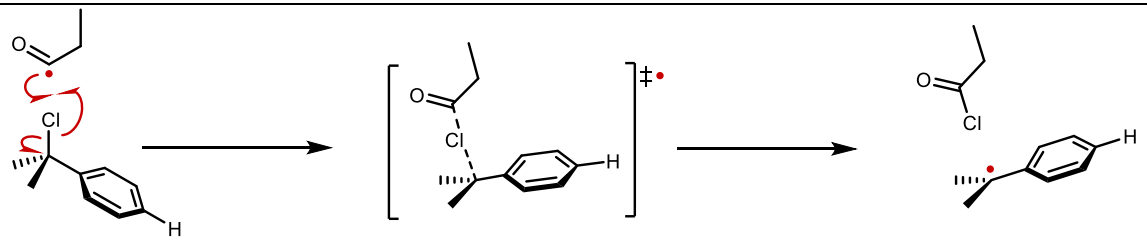
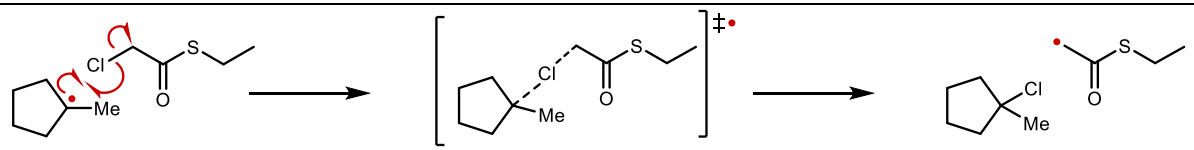
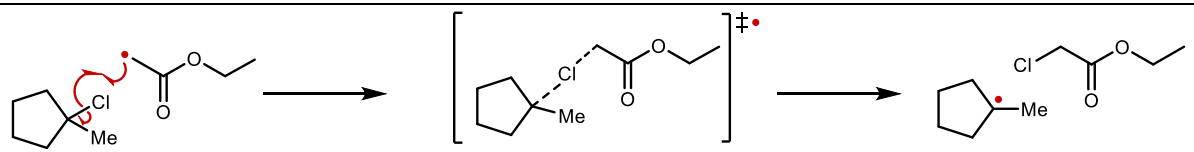
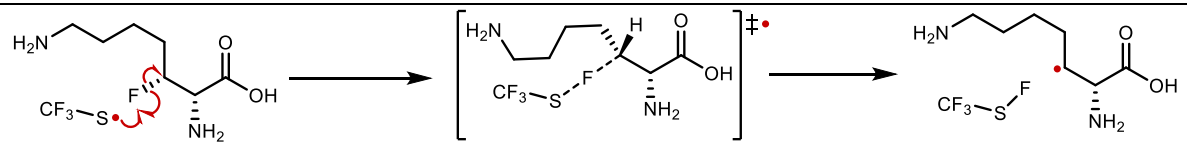
III. Halogen atom transfer

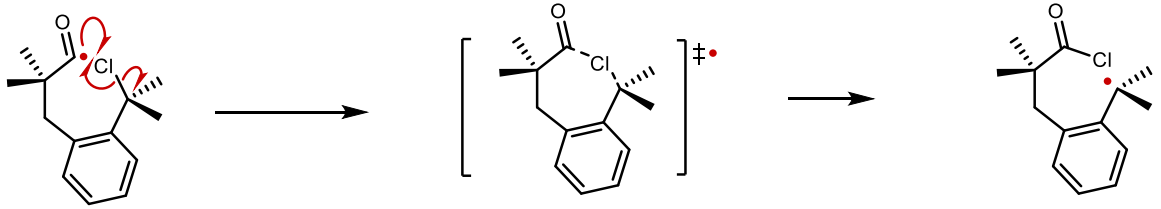
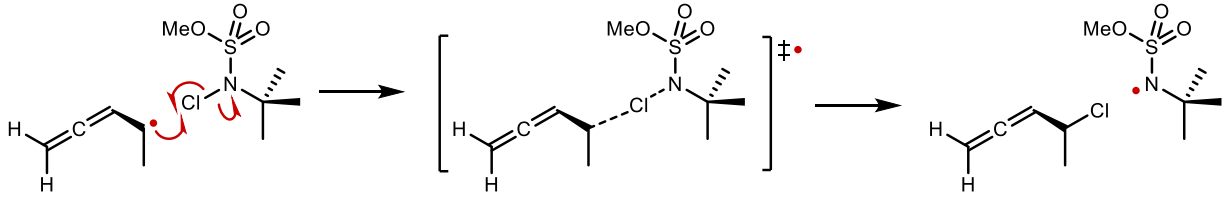
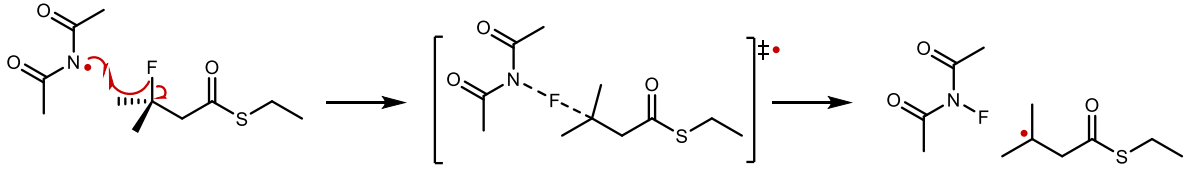
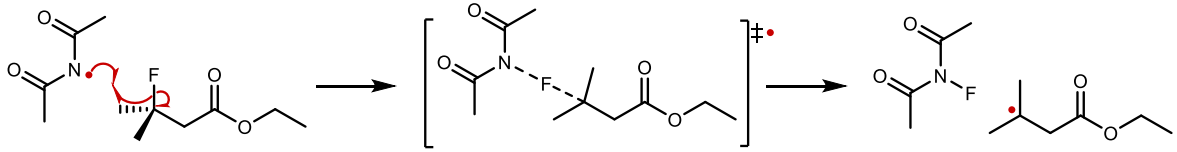
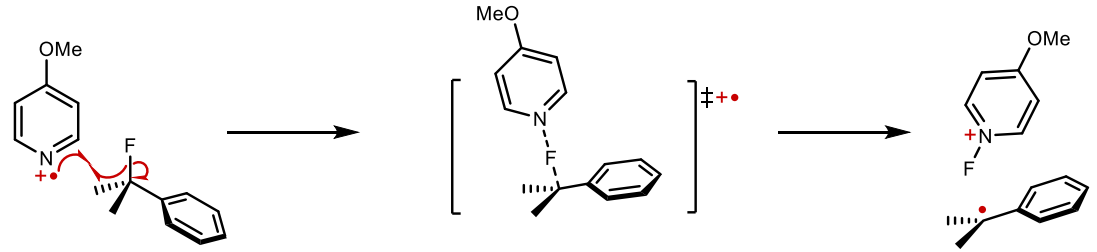
#	Mechanism	Forward barrier height (in kcal/mol)	Reverse barrier height (in kcal/mol)	Reaction energy (in kcal/mol)
1		47.62	11.46	36.16
2		45.08	13.69	31.39
3		15.39	4.08	11.31

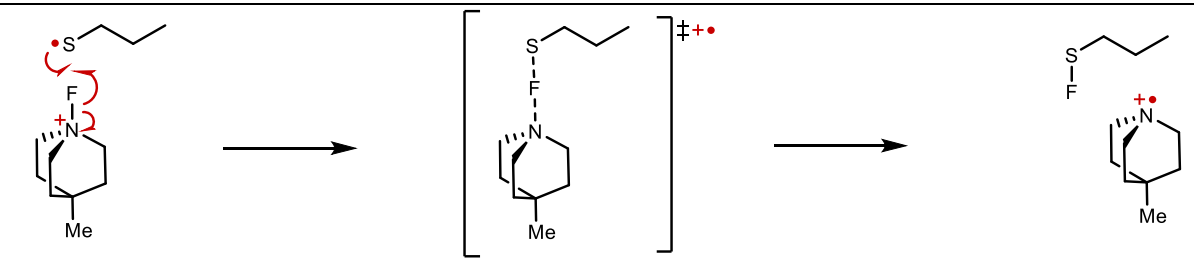
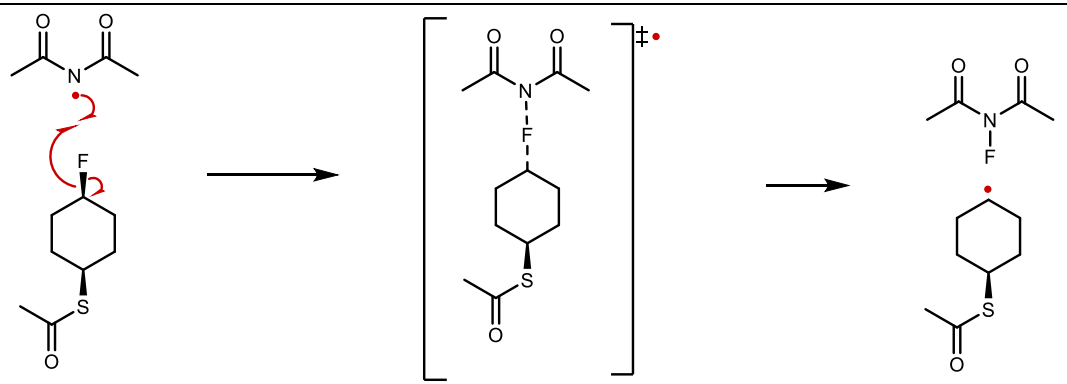
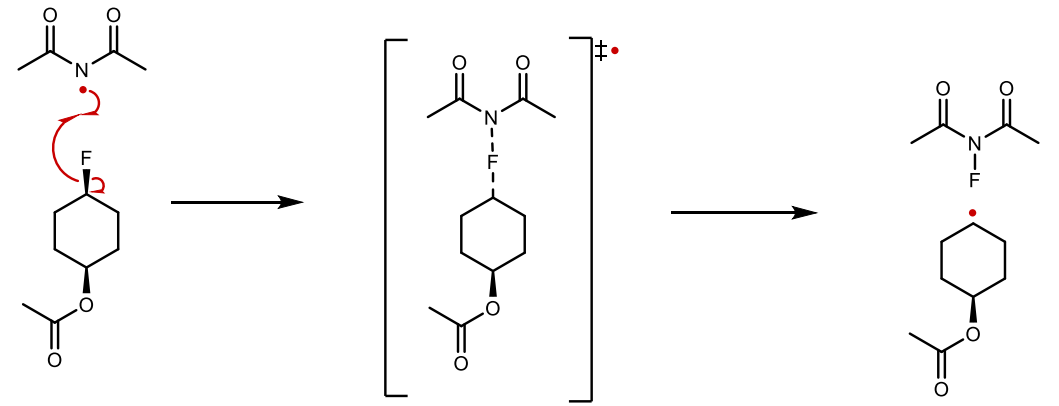
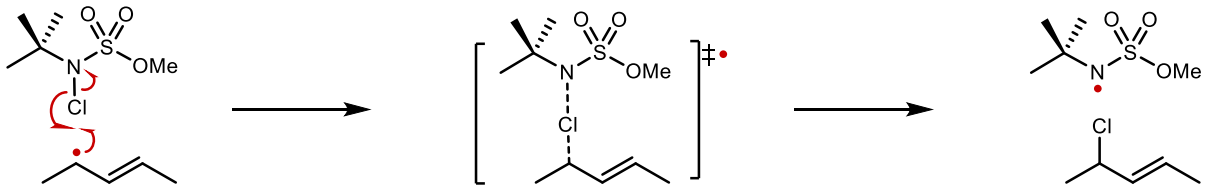
4		15.91	13.98	1.93
5		4.23	4.65	-0.42
6		-1.35	1.80	-3.16
7		42.38	17.76	24.62
8		42.36	17.42	24.94

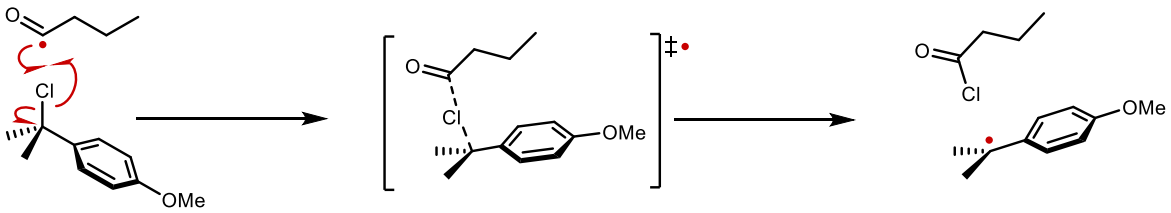
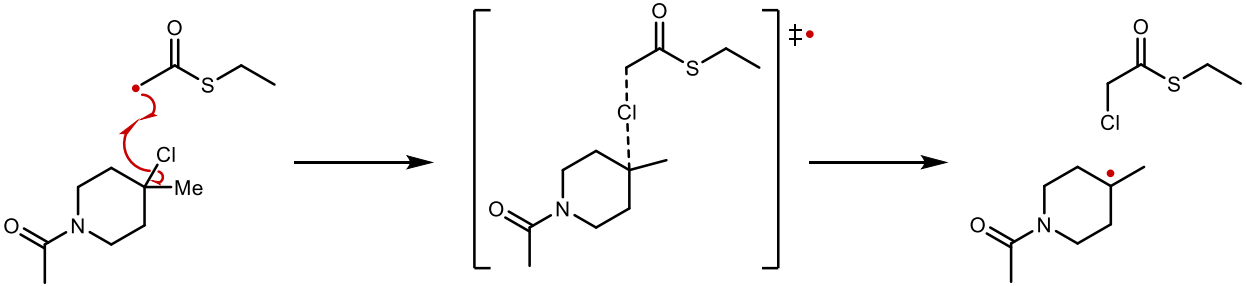
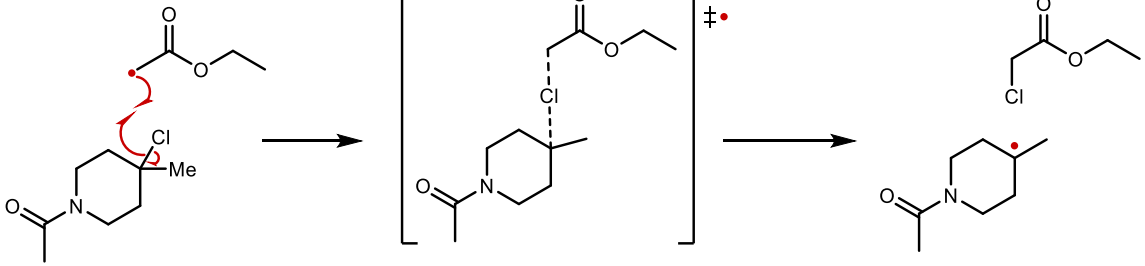
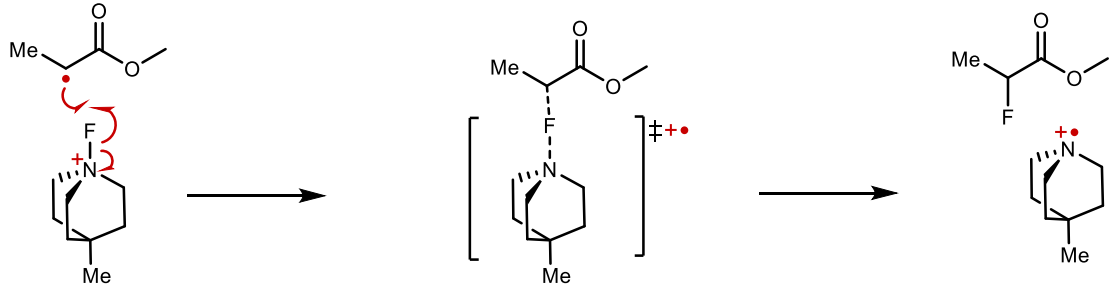
9		-67.71	-62.16	-5.55
10		41.34	7.92	33.42
11		0.50	5.21	-4.70
12		43.97	20.13	23.84
13		3.23	11.60	-8.37

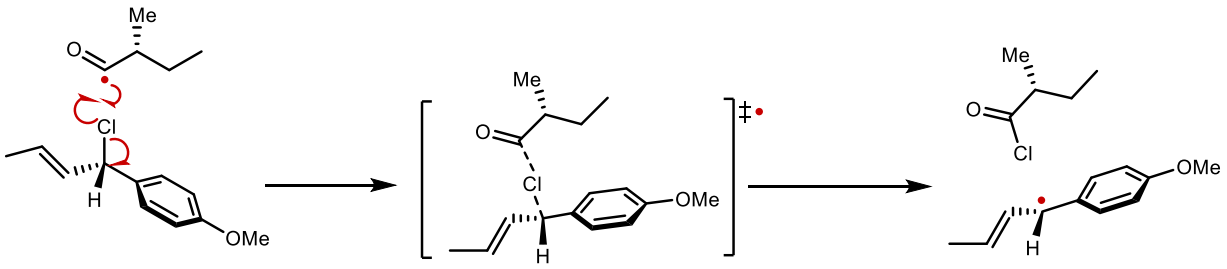
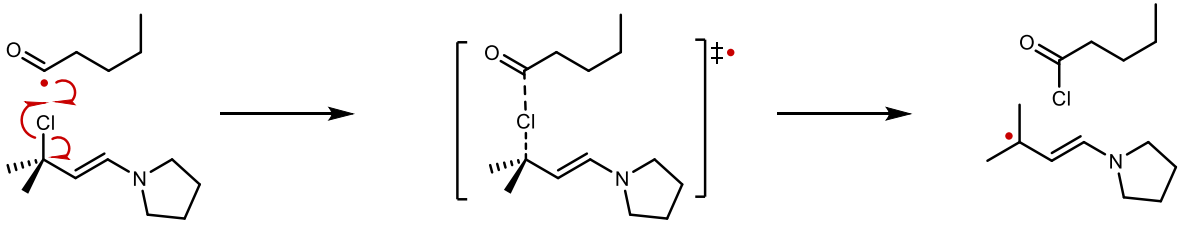
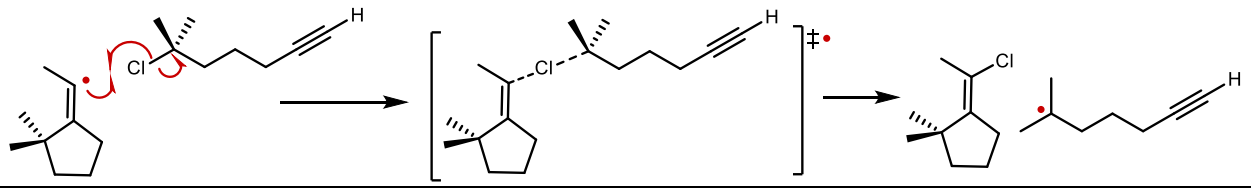
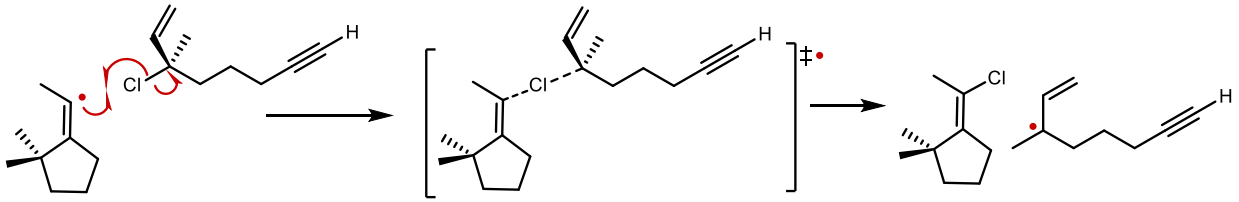
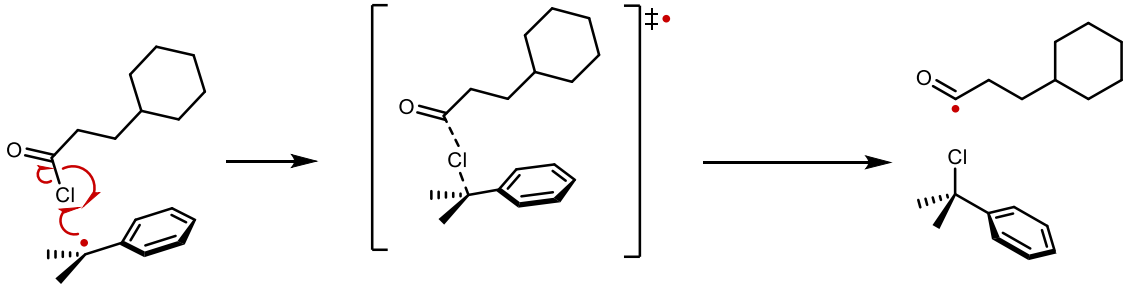
14		3.48	11.59	-8.11
15		41.94	16.76	25.18
16		77.42	81.94	-4.52
17		9.22	14.73	-5.52
18		2.95	11.10	-8.15

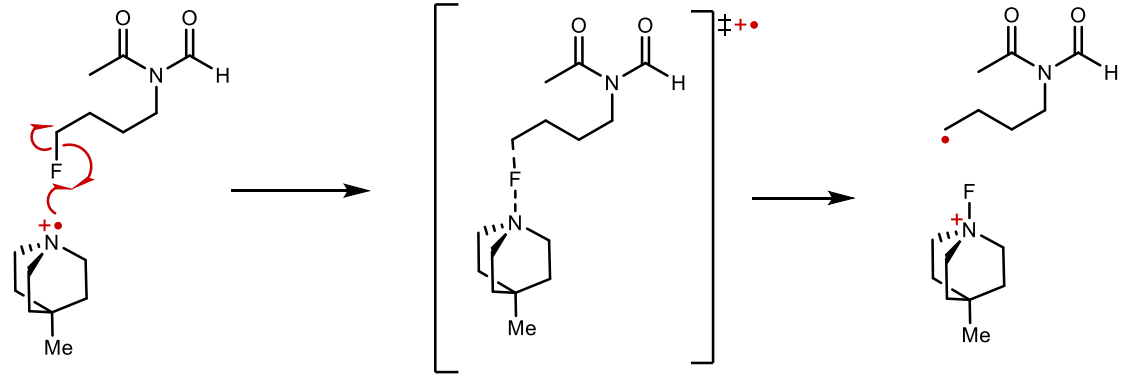
19		-0.68	3.87	-4.54
20		2.41	10.55	-8.14
21		12.96	23.34	-10.38
22		10.47	18.30	-7.83
23		18.66	10.80	7.85
24		41.74	8.44	33.31

25		26.26	34.43	-8.17
26		5.84	26.05	-20.21
27		53.90	10.31	43.59
28		56.10	11.62	44.48
29		26.77	1.36	25.42

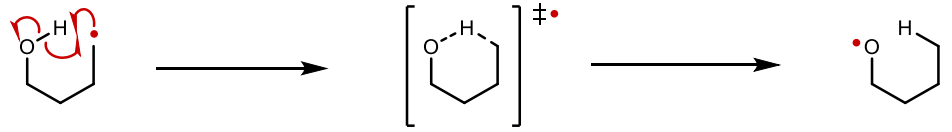
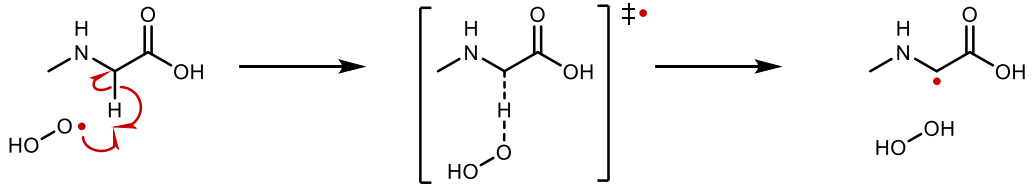
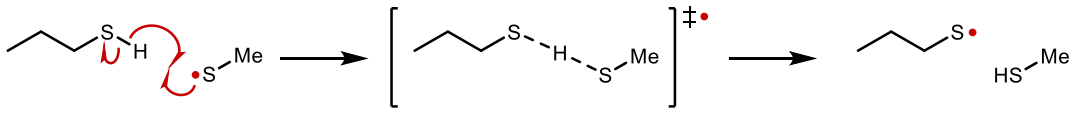
30		14.71	34.21	-19.50
31		51.57	12.40	39.17
32		52.03	12.75	39.29
33		6.22	25.32	-19.10

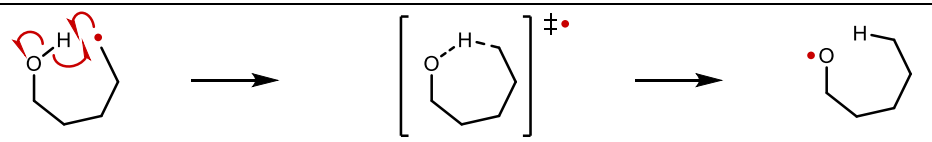
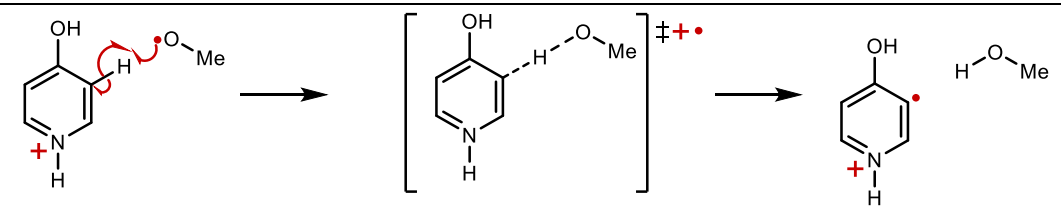
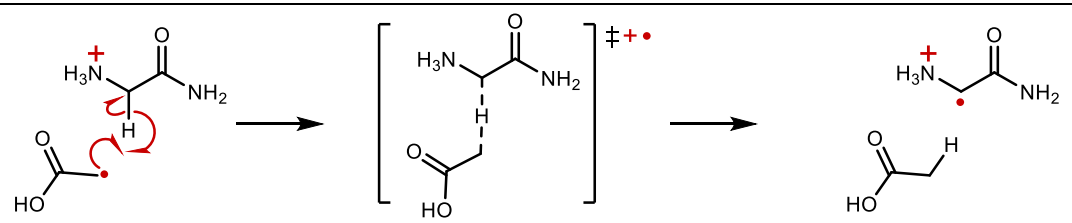
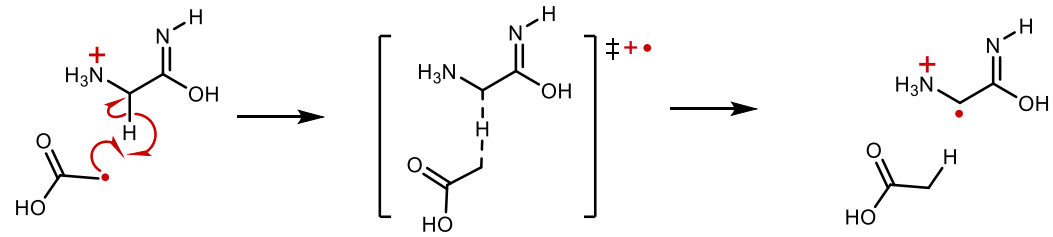
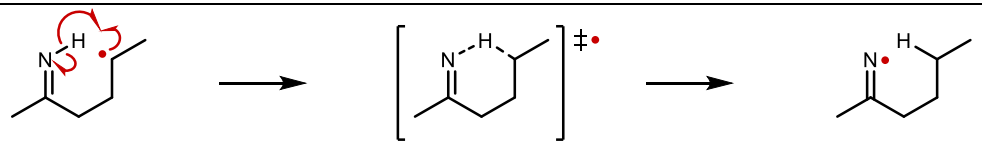
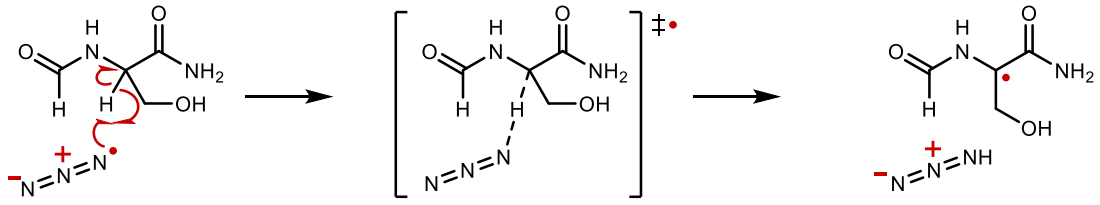
34		12.79	22.60	-9.81
35		16.87	8.88	7.99
36		16.65	8.64	8.02
37		8.00	47.09	-39.09

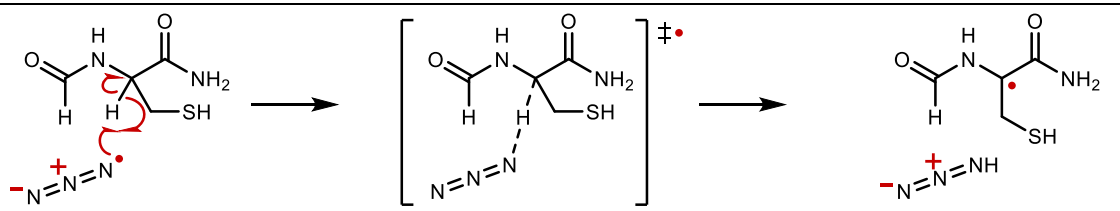
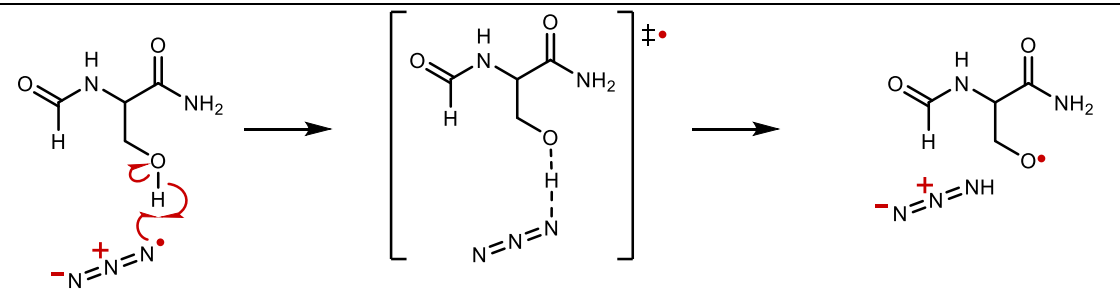
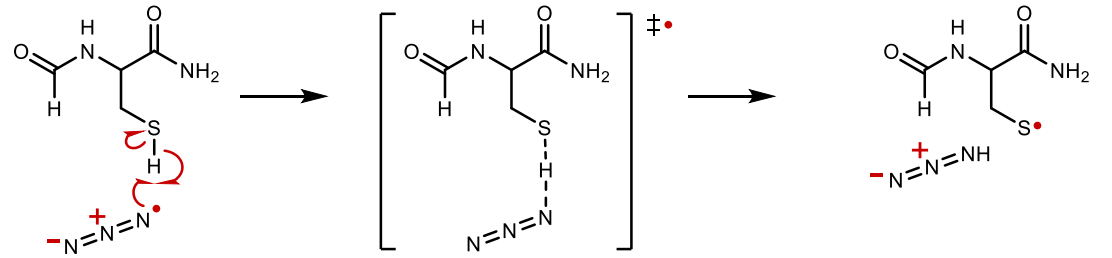
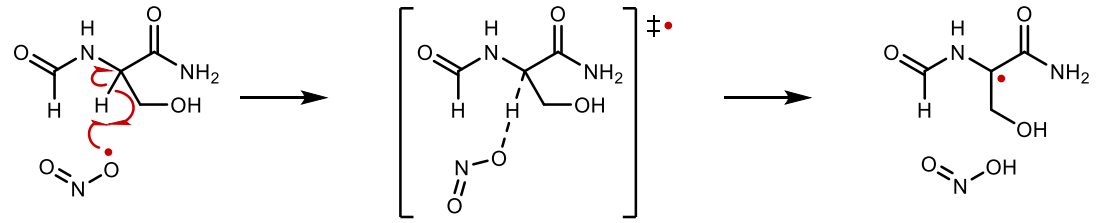
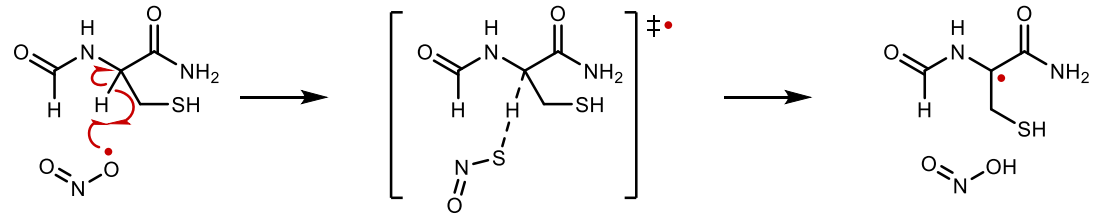
38		10.67	31.39	-20.71
39		11.00	24.57	-13.57
40		10.04	20.95	-10.91
41		7.96	35.40	-27.43
42		21.33	10.29	11.03

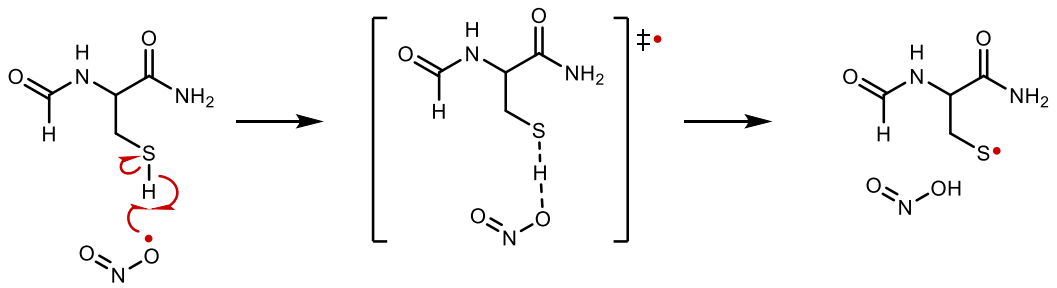
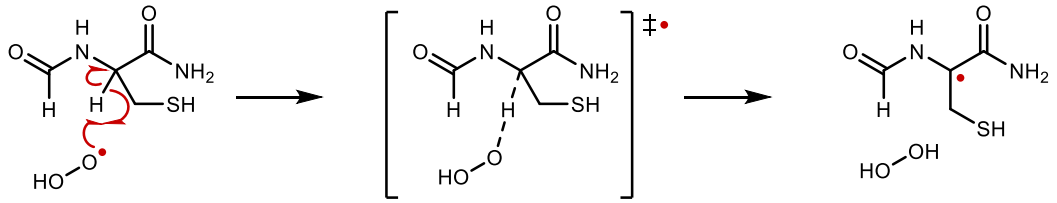
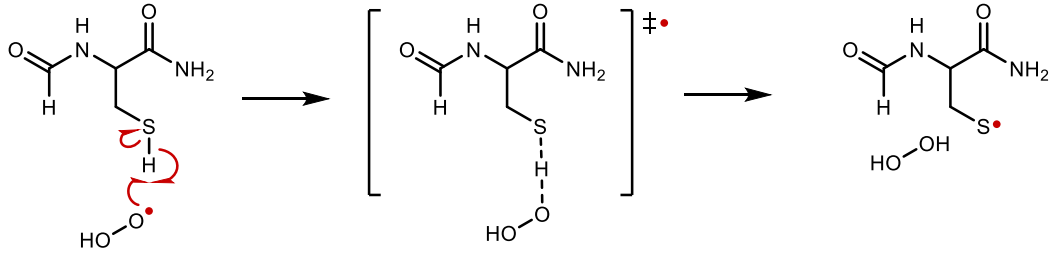
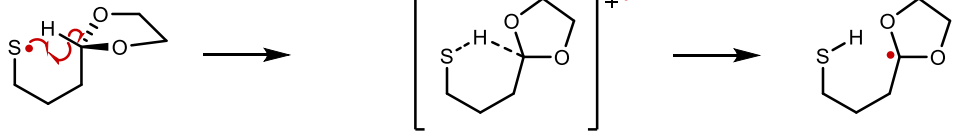
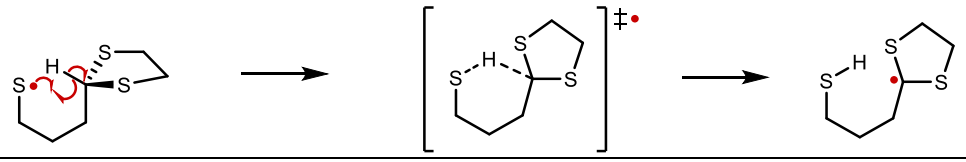
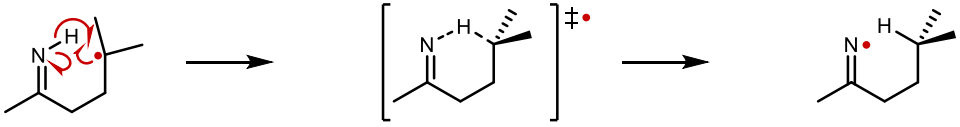
43		46.53	-3.19	49.72

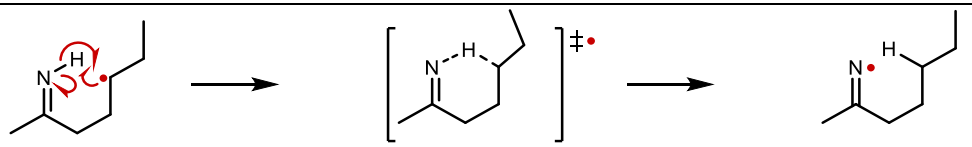
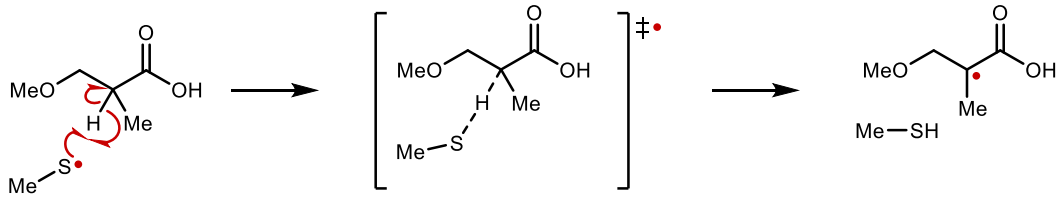
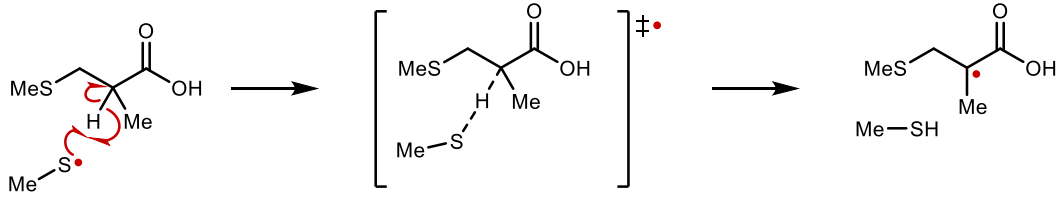
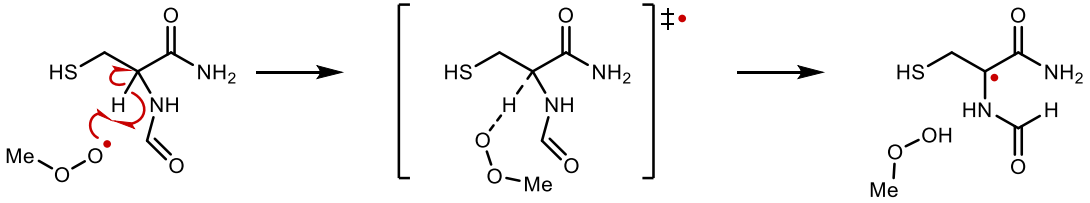
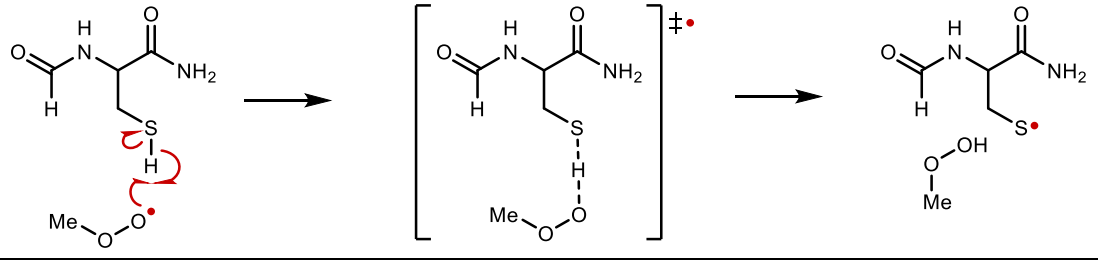
IV. Hydrogen atom transfer

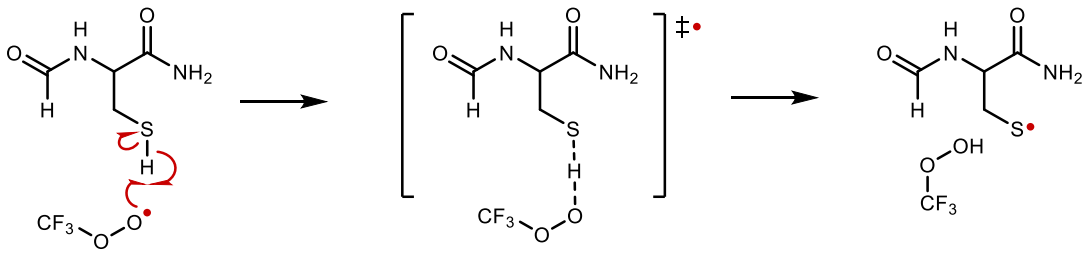
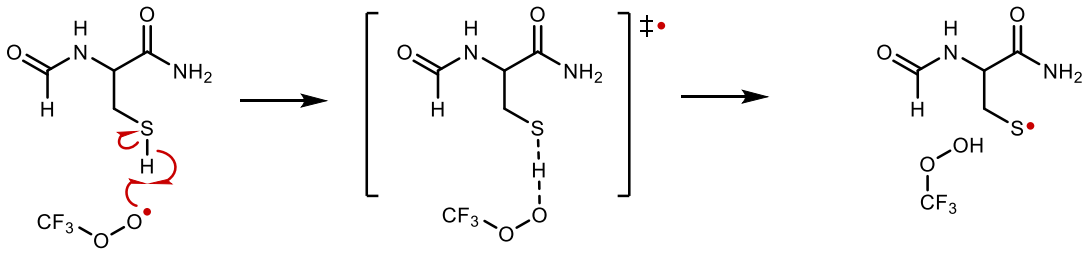
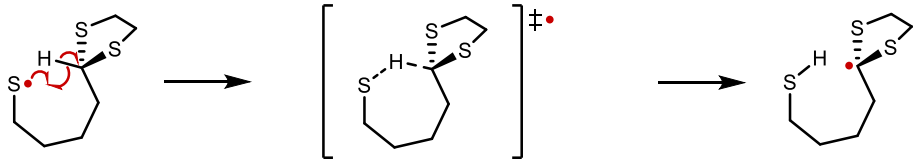
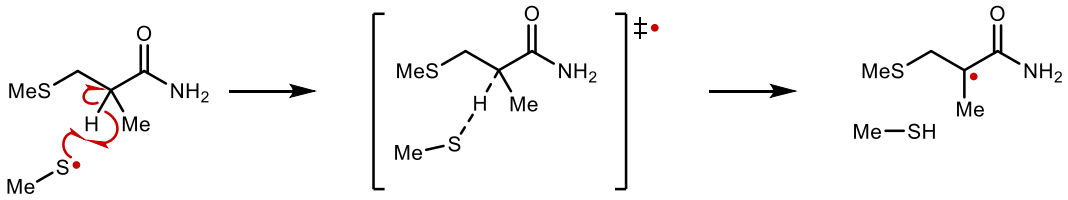
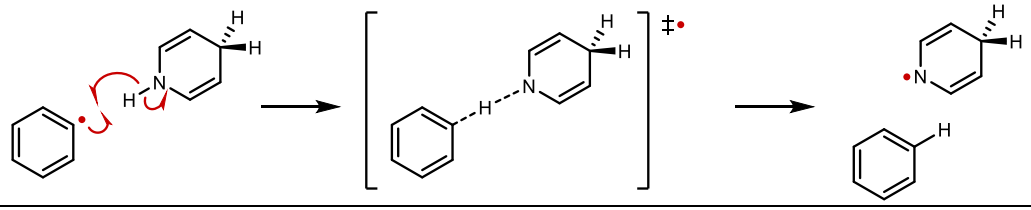
#	Mechanism	Forward barrier height (in kcal/mol)	Reverse barrier height (in kcal/mol)	Reaction energy (in kcal/mol)
1		16.42	12.36	4.06
2		11.89	19.47	-7.58
3		4.80	4.58	0.22

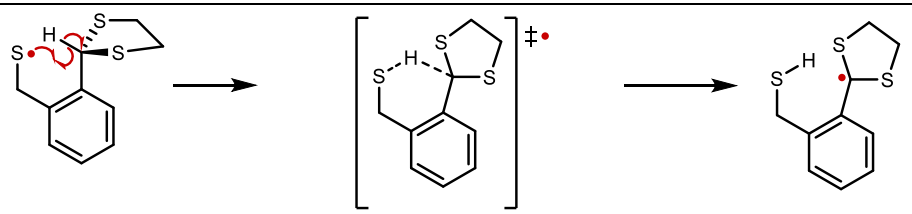
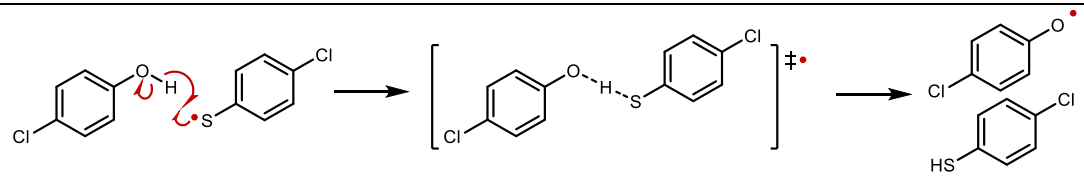
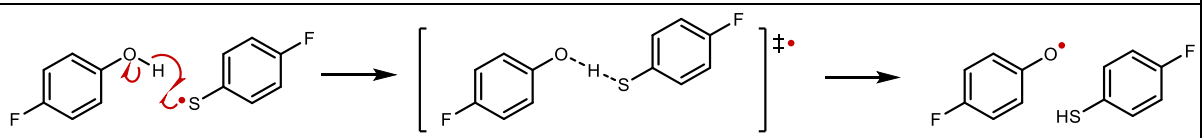
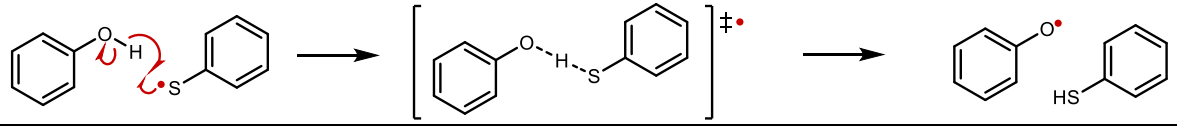
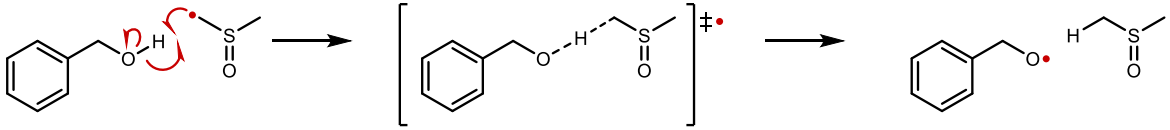
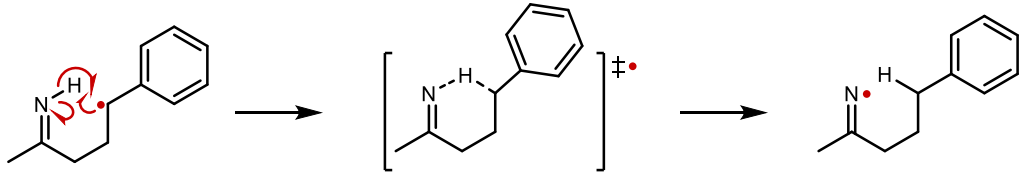
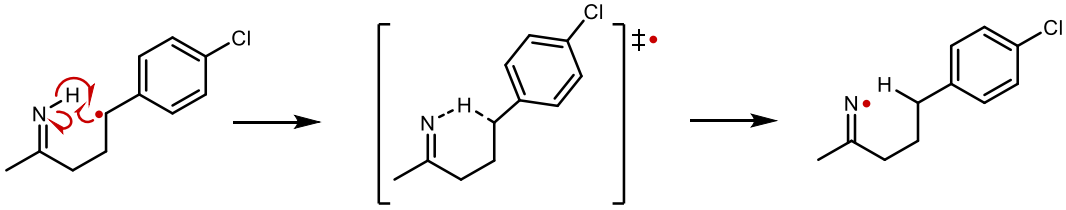
4		16.44	12.67	3.77
5		13.93	0.17	13.76
6		6.44	2.44	4.01
7		4.00	4.61	-0.61
8		12.36	21.11	-8.75
9		17.45	17.15	0.30

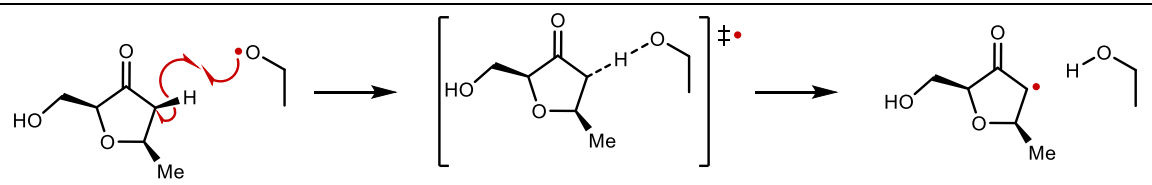
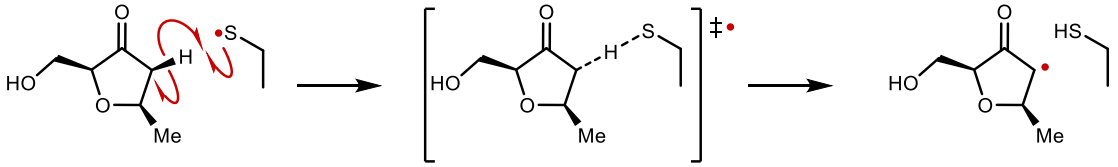
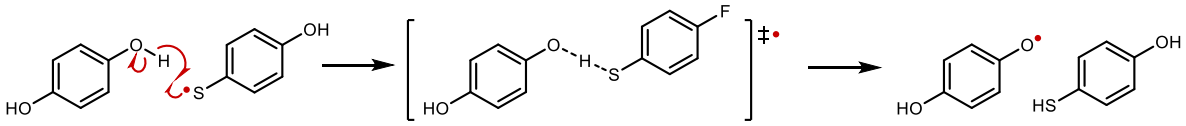
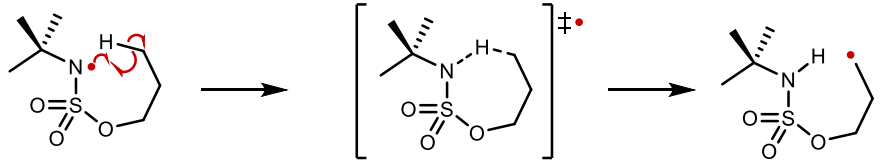
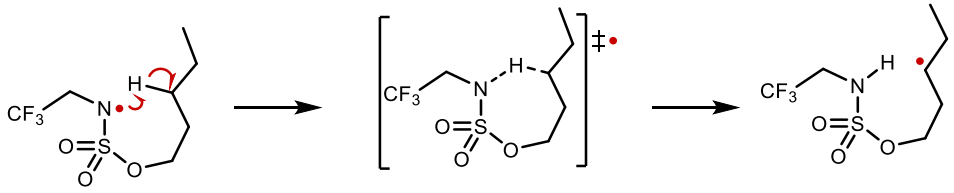
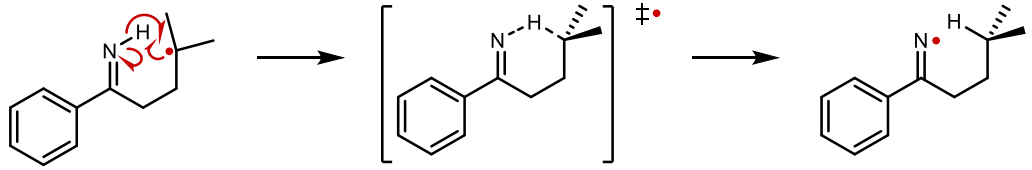
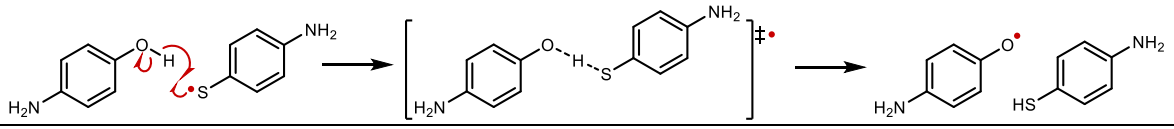
10		16.29	17.84	-1.56
11		34.10	12.51	21.59
12		12.97	15.74	-2.77
13		30.51	19.78	10.73
14		27.87	18.89	8.98

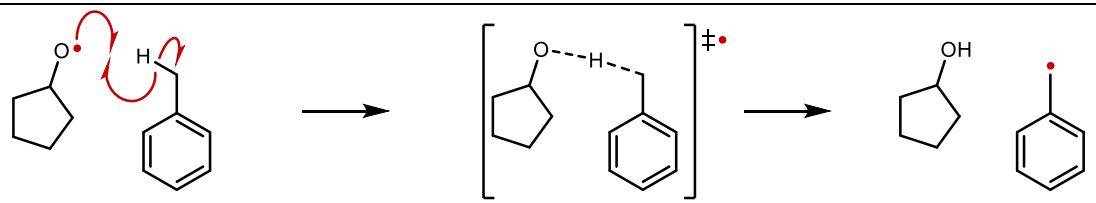
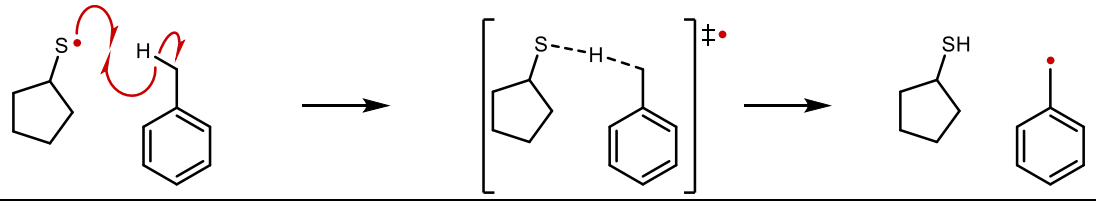
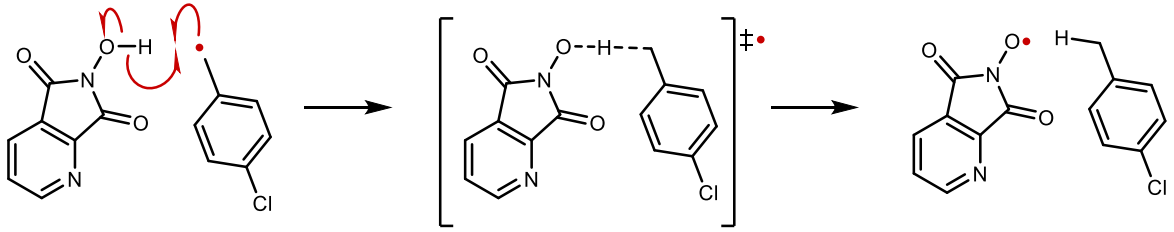
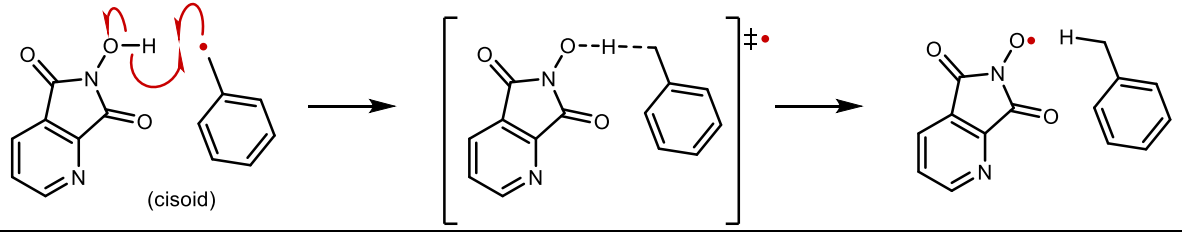
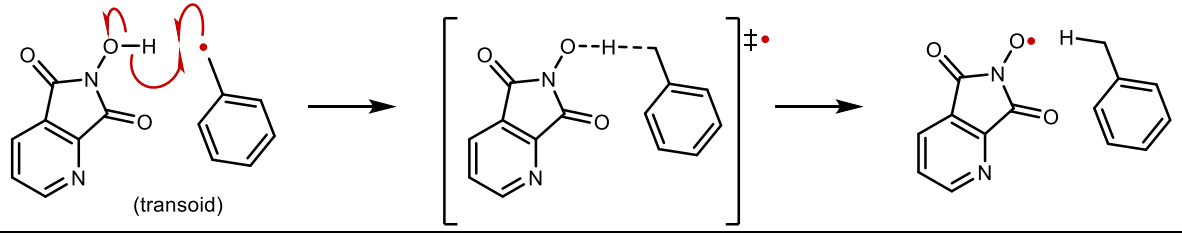
15		23.98	16.31	7.67
16		14.52	13.49	1.02
17		9.08	9.37	-0.29
18		12.84	3.23	9.61
19		10.35	9.72	0.63
20		12.19	19.25	-7.06

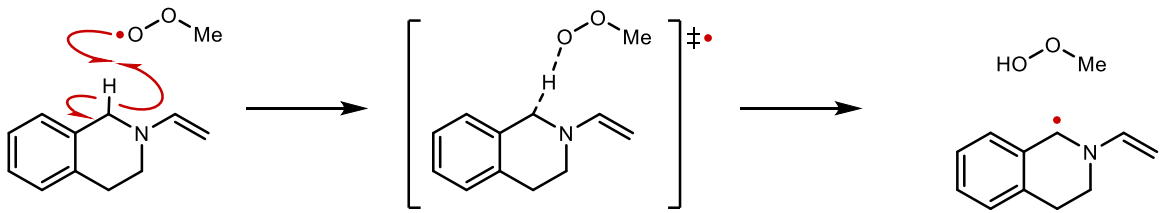
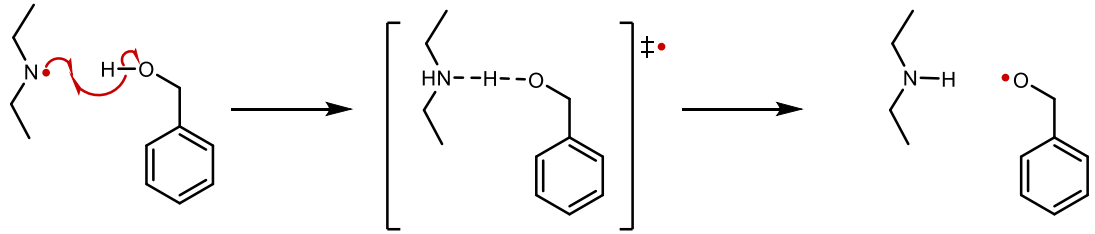
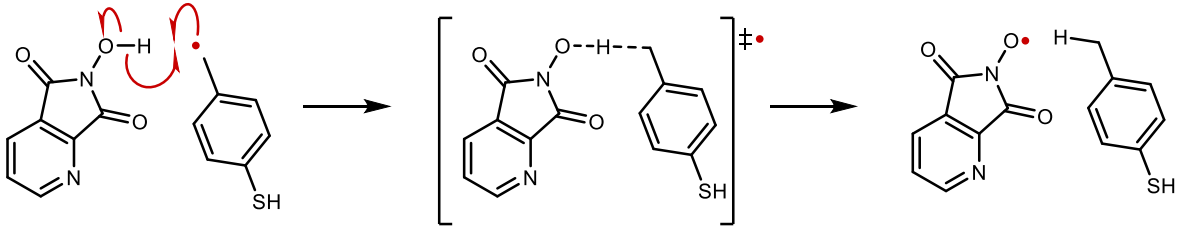
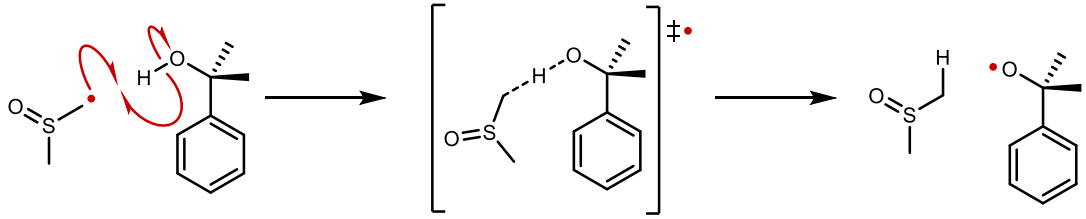
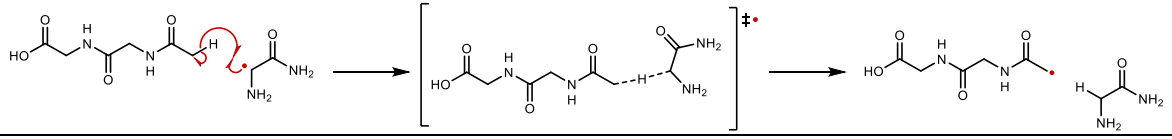
21		11.81	20.88	-9.06
22		13.47	6.04	7.43
23		11.29	6.86	4.43
24		18.51	15.80	2.71
25		14.12	12.73	1.39

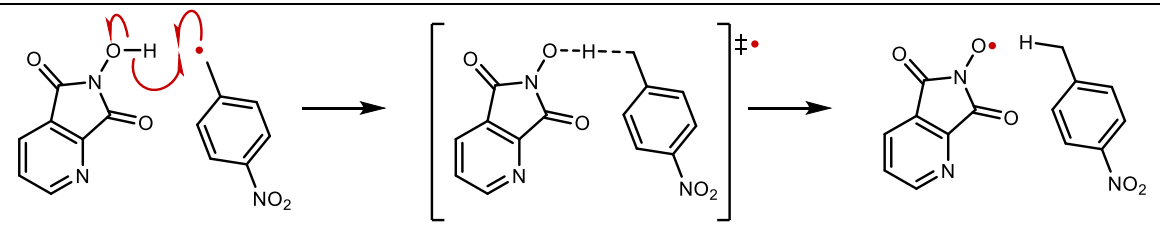
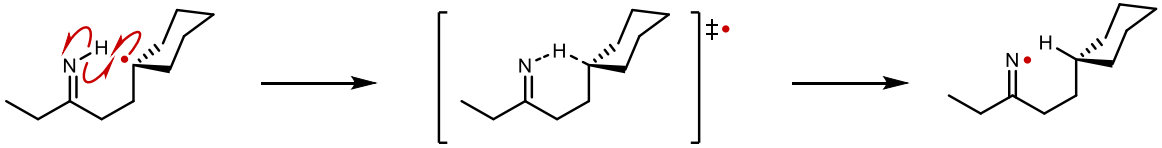
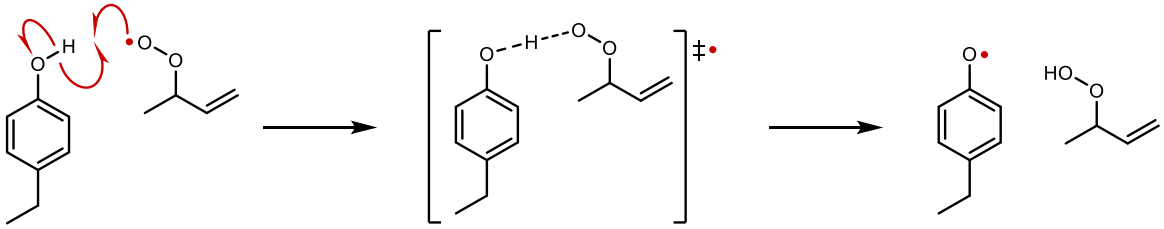
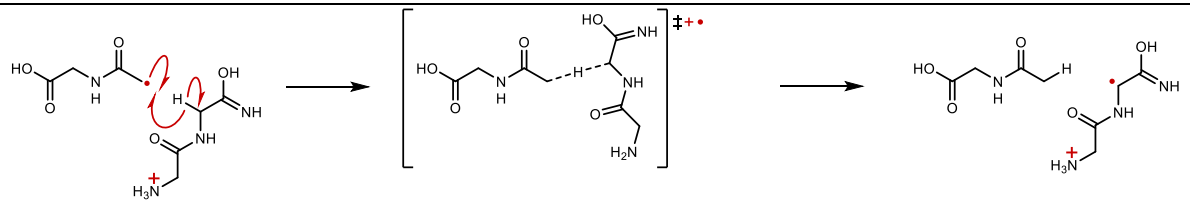
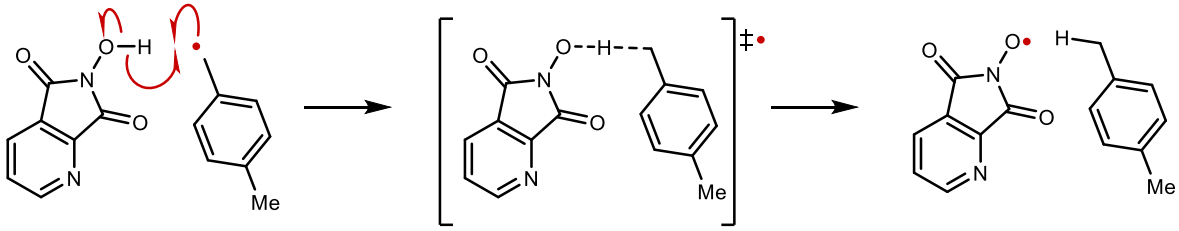
26		14.83	20.51	-5.68
27		13.20	18.89	-5.69
28		10.10	8.71	1.38
29		11.34	5.16	6.19
30		3.48	35.56	-32.09

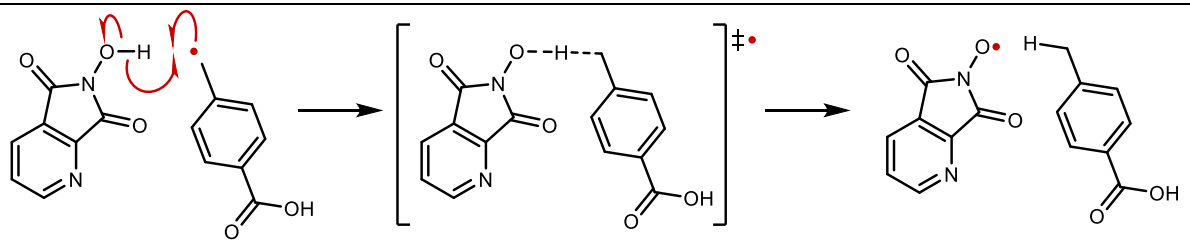
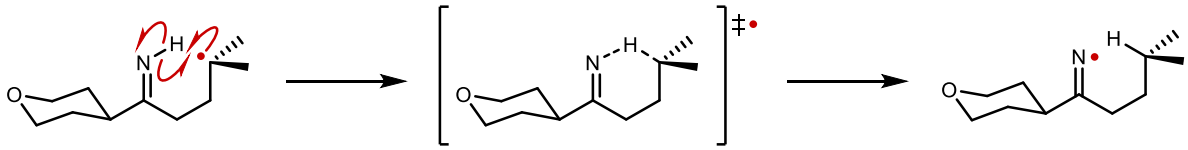
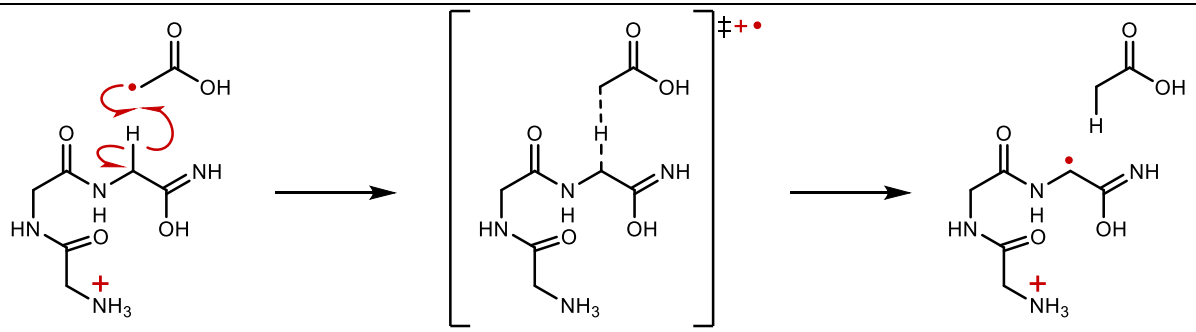
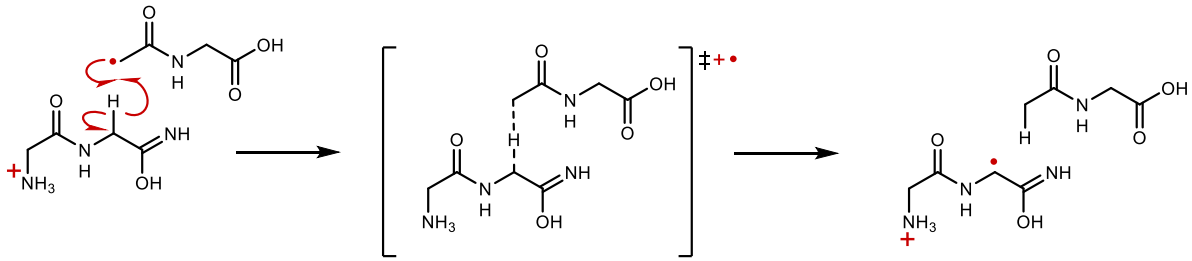
31		10.13	11.96	-1.83
32		29.28	18.90	10.38
33		30.75	20.43	10.31
34		31.27	20.17	11.10
35		12.23	7.14	5.09
36		21.30	19.97	1.33
37		21.57	19.91	1.66

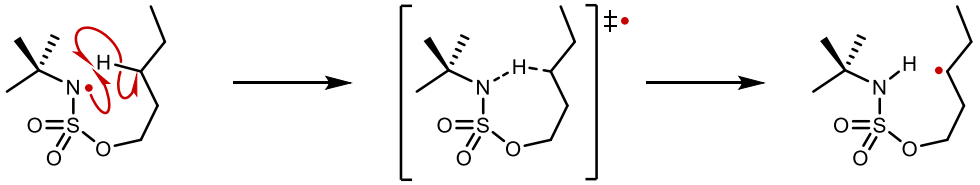
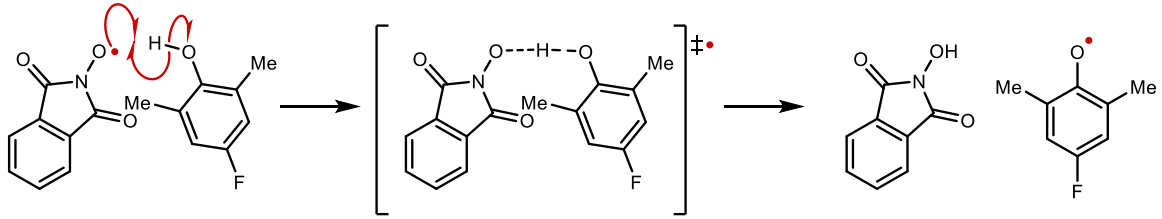
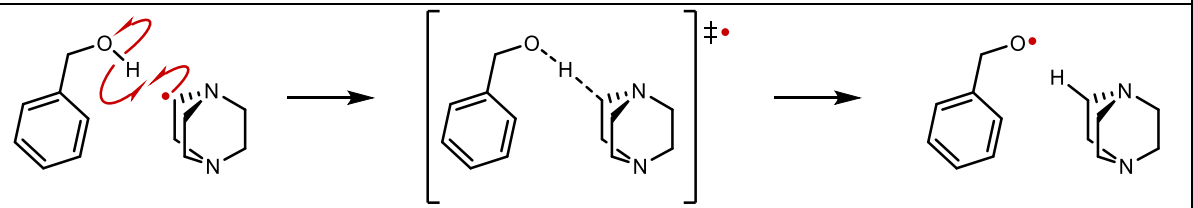
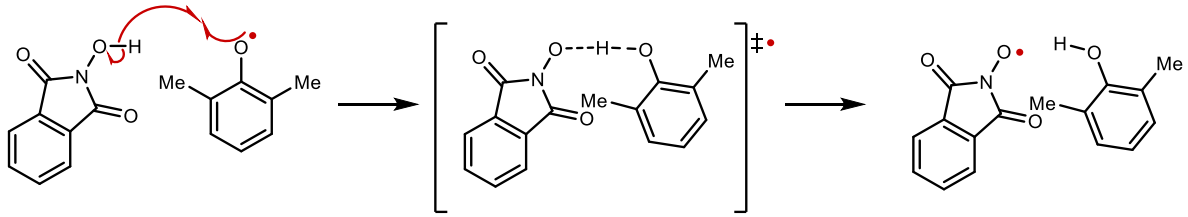
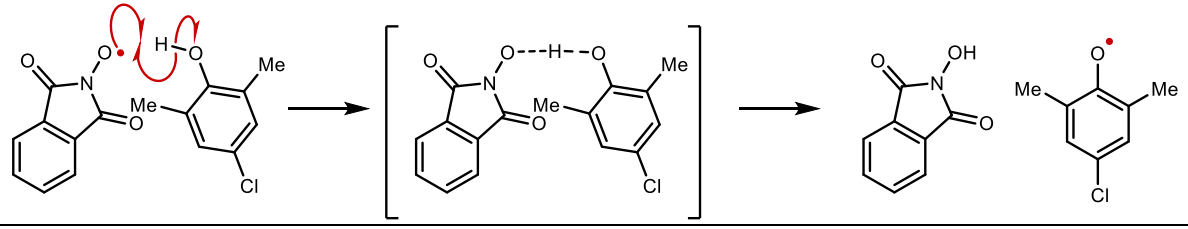
38		6.68	17.92	-11.24
39		13.24	3.28	9.96
40		27.97	19.50	8.47
41		18.43	18.66	-0.24
42		12.15	16.10	-3.95
43		13.68	18.76	-5.08
44		22.68	15.83	6.85

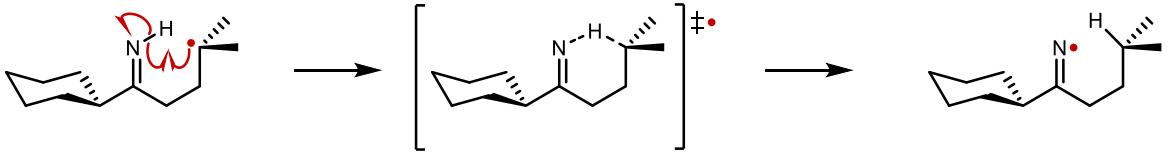
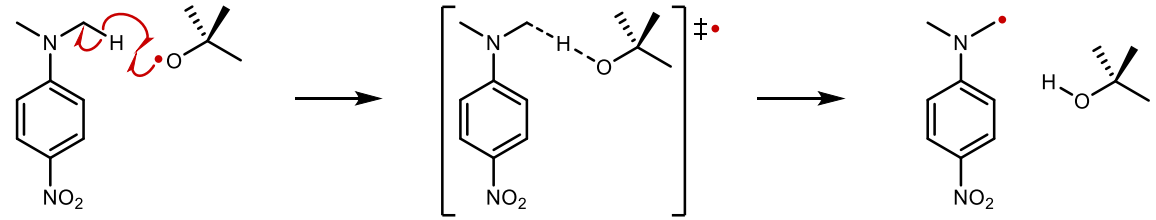
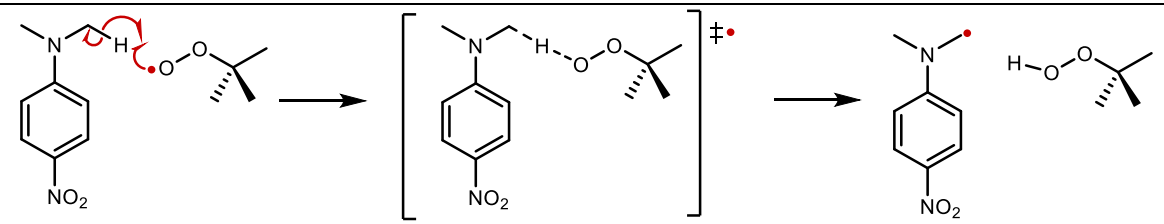
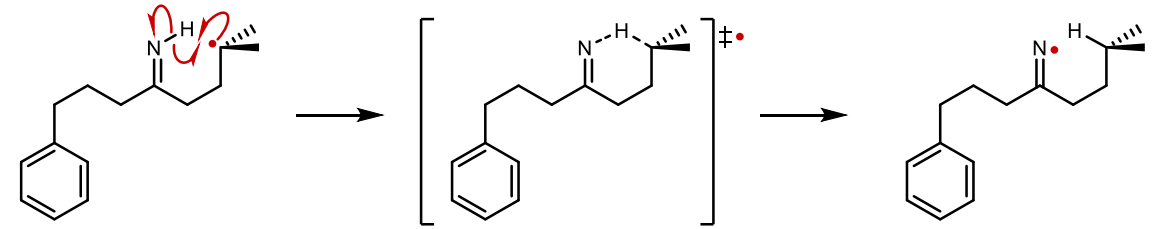
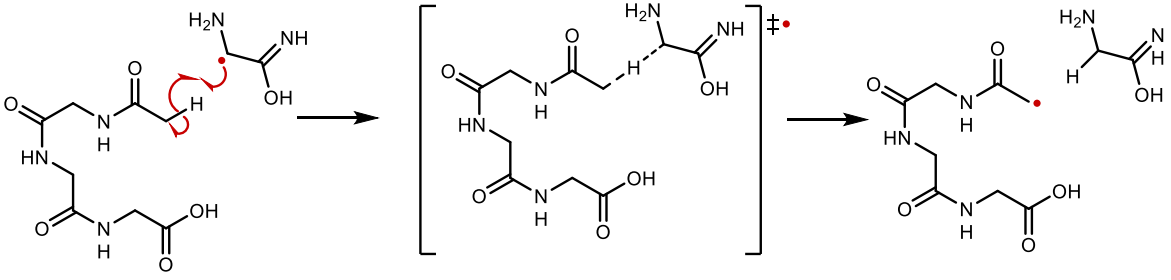
45		7.33	22.38	-15.05
46		11.46	6.32	5.14
47		5.60	11.33	-5.72
48	 (cisoid)	5.93	11.61	-5.68
49	 (transoid)	12.58	18.27	-5.69

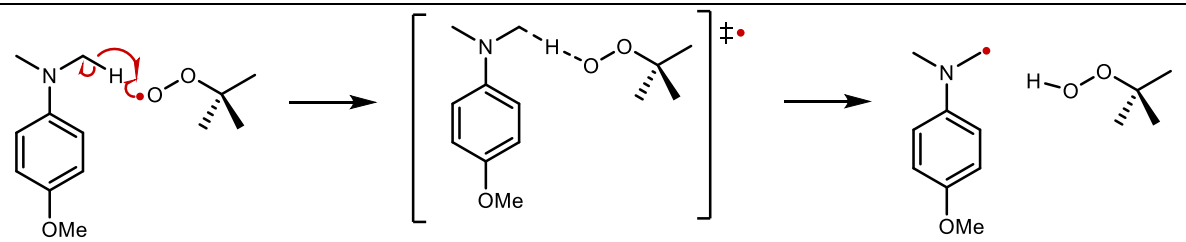
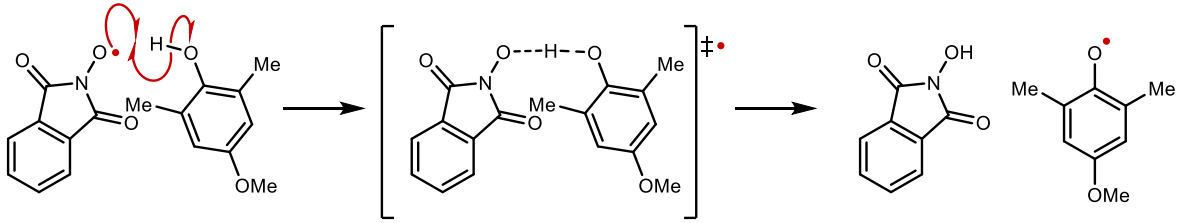
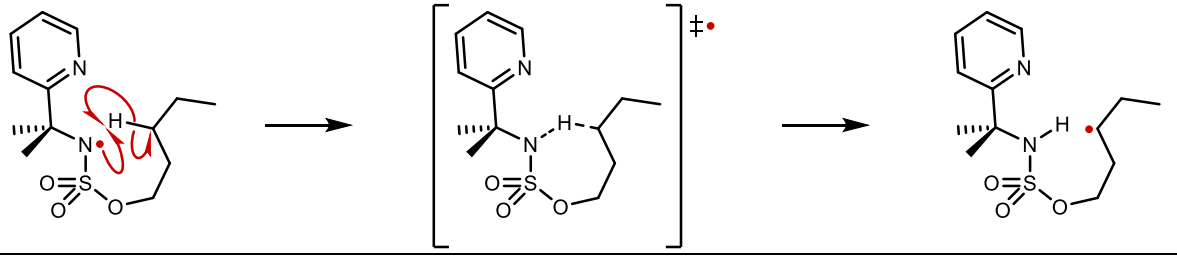
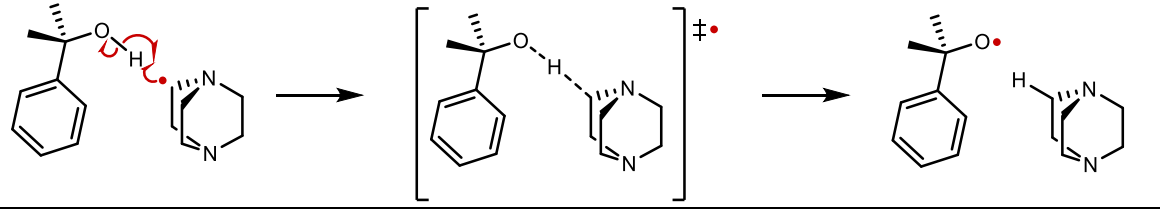
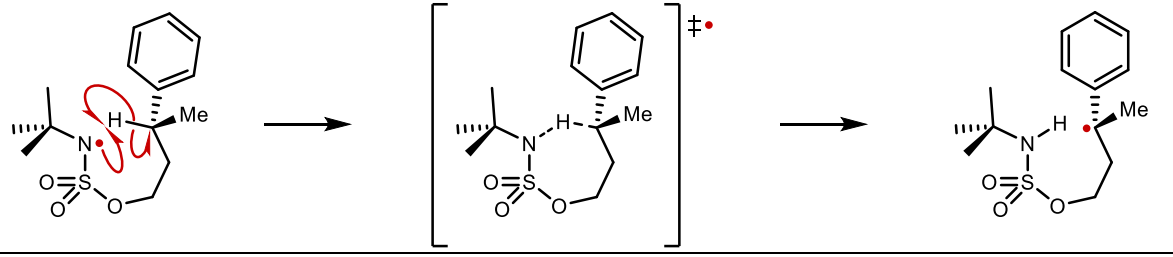
50		12.73	18.65	-5.92
51		11.99	-0.34	12.34
52		4.82	9.92	-5.10
53		12.35	7.34	5.02
54		19.94	2.71	17.22

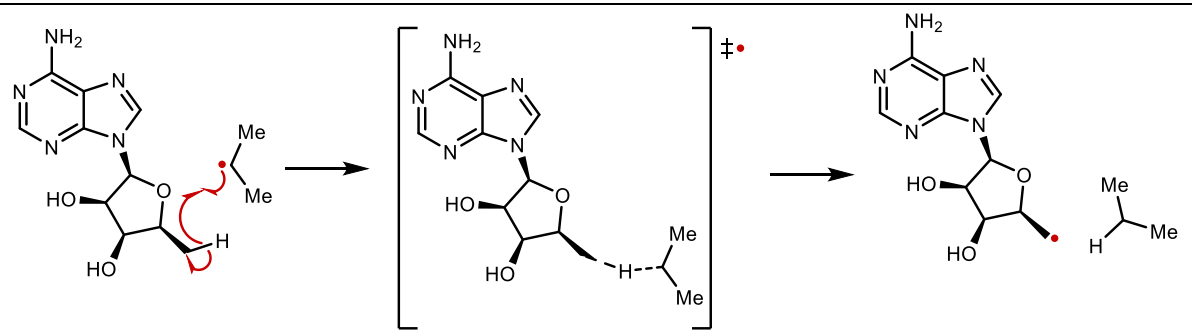
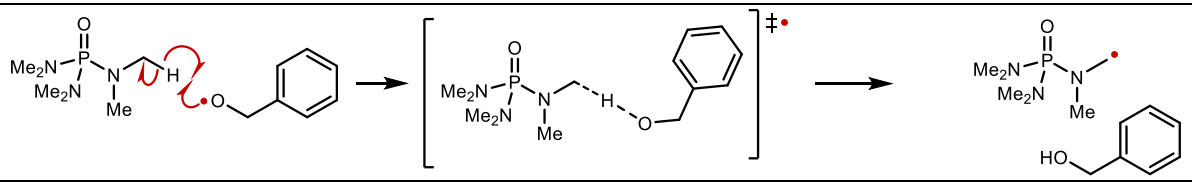
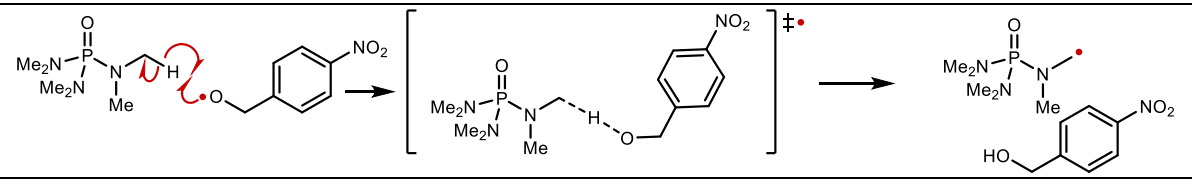
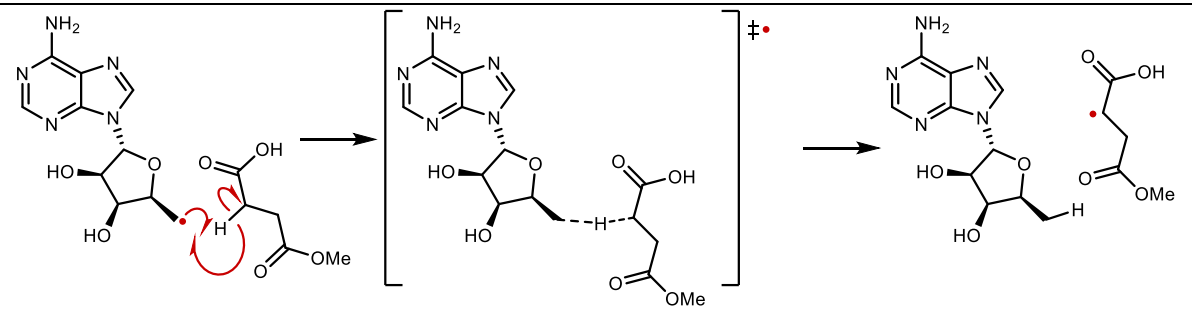
55		6.94	12.94	-6.00
56		12.91	18.25	-5.35
57		14.38	12.67	1.71
58		12.42	2.71	9.71
59		5.02	10.66	-5.64

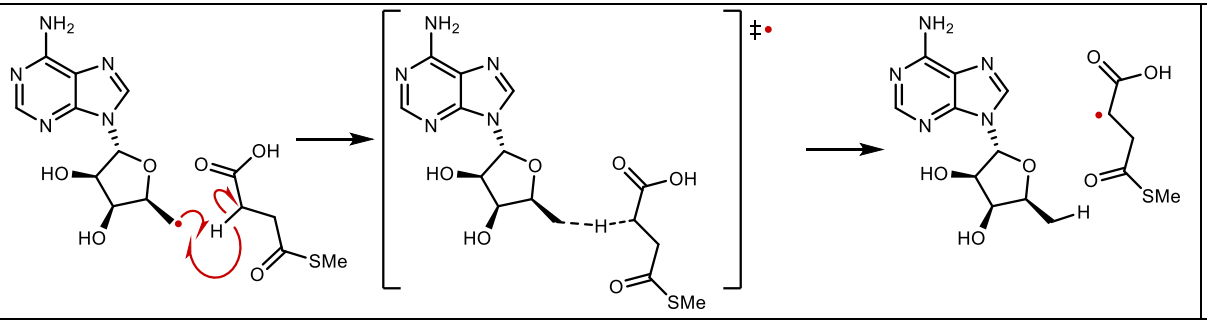
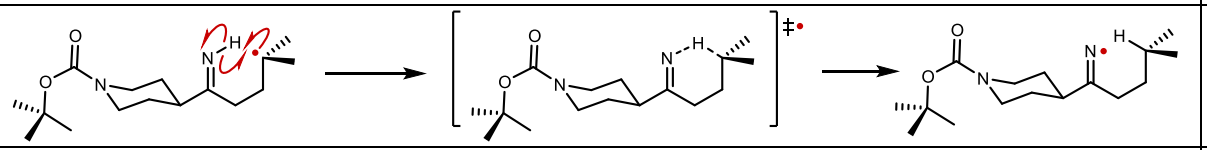
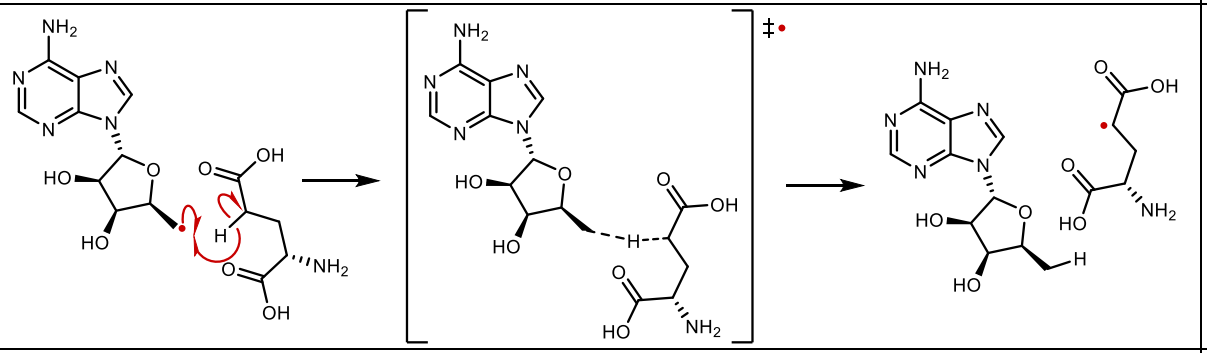
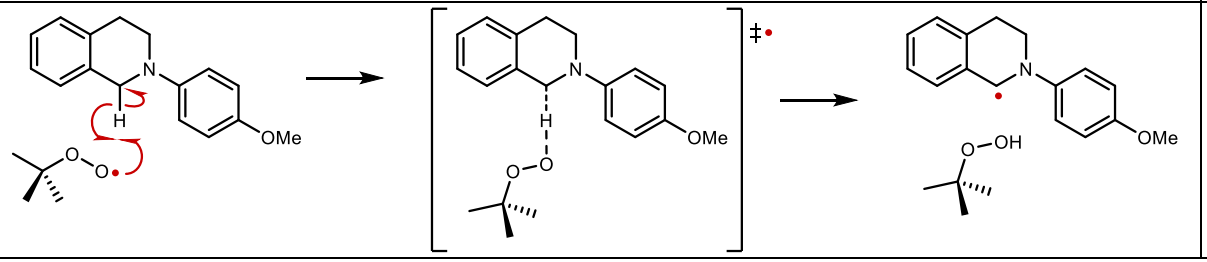
60		6.68	12.22	-5.55
61		11.91	19.00	-7.09
62		25.06	34.50	-9.44
63		12.43	20.69	-8.26

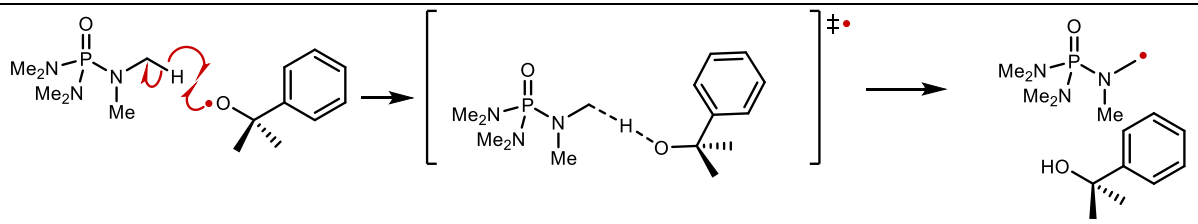
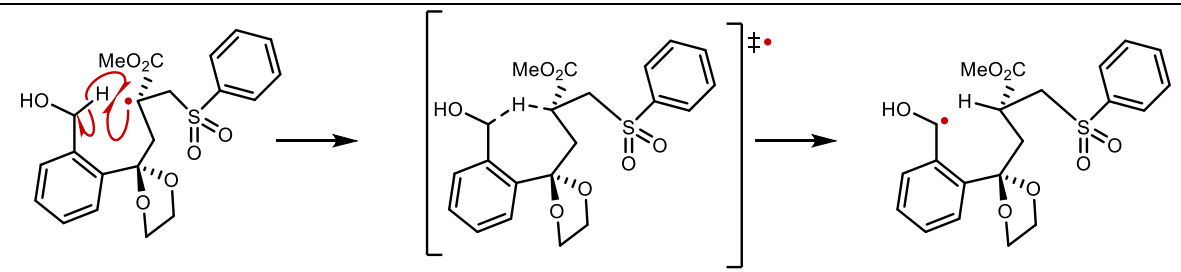
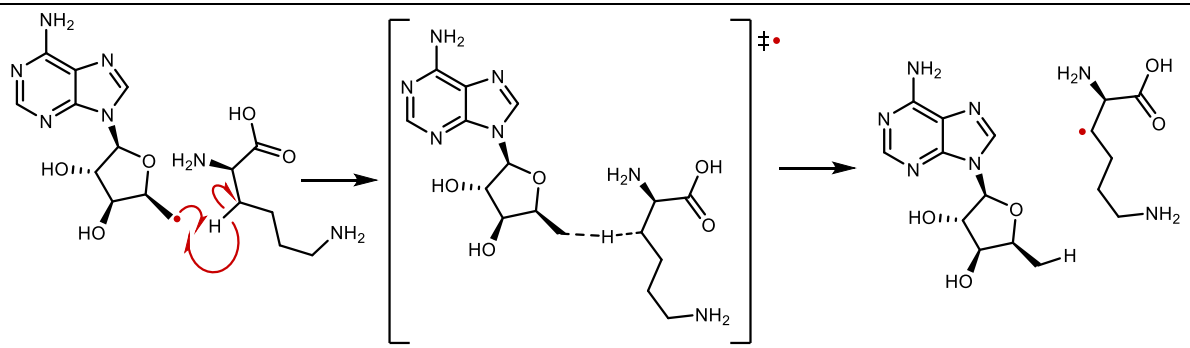
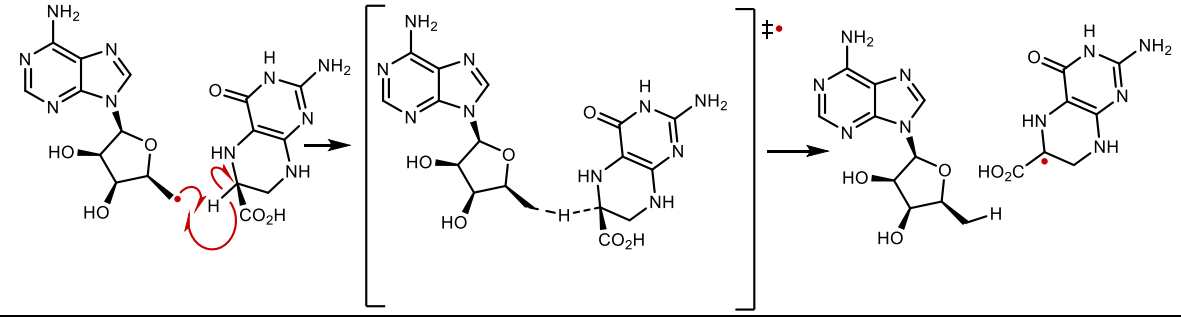
64		14.37	17.61	-3.24
65		3.46	3.34	0.12
66		12.91	5.36	7.55
67		3.55	5.23	-1.69
68		3.62	2.75	0.87

69		11.97	19.19	-7.22
70		5.16	19.31	-14.15
71		16.88	8.08	8.80
72		11.57	19.48	-7.91
73		30.00	12.73	17.28

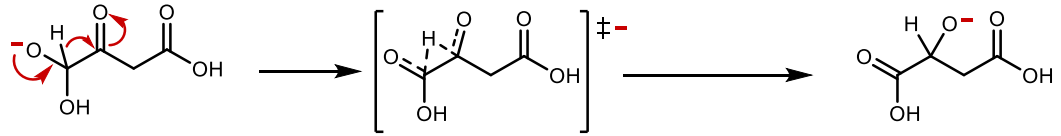
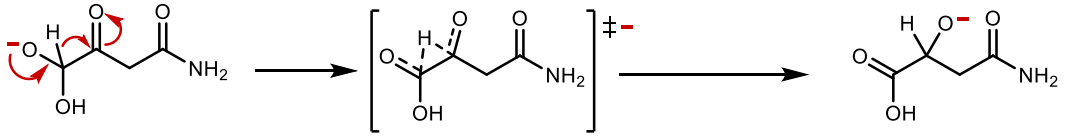
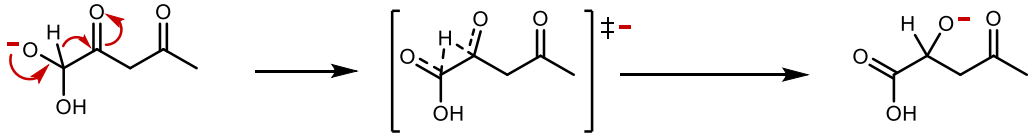
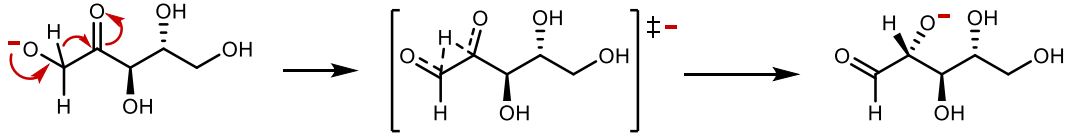
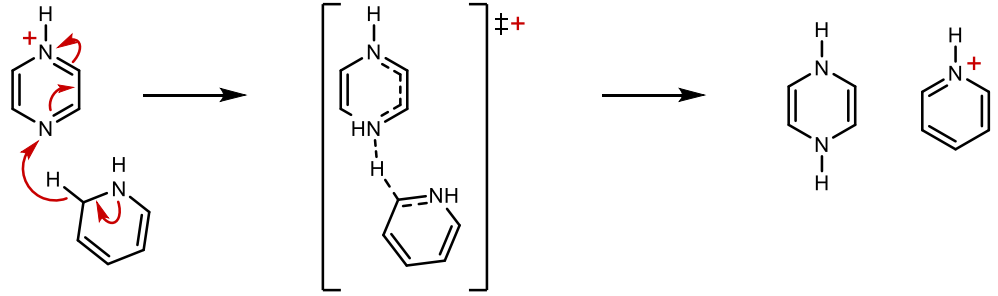
74		14.37	7.11	7.26
75		3.66	6.58	-2.91
76		13.85	18.38	-4.54
77		12.93	5.40	7.53
78		13.54	29.68	-16.14

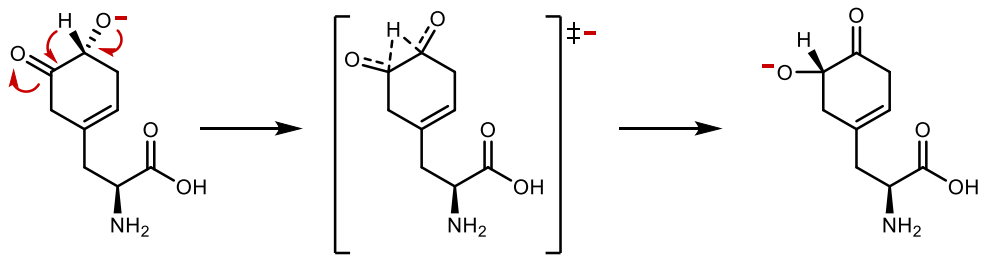
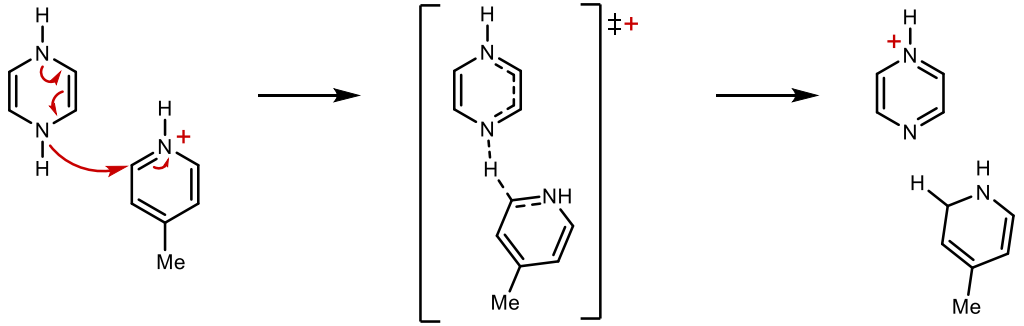
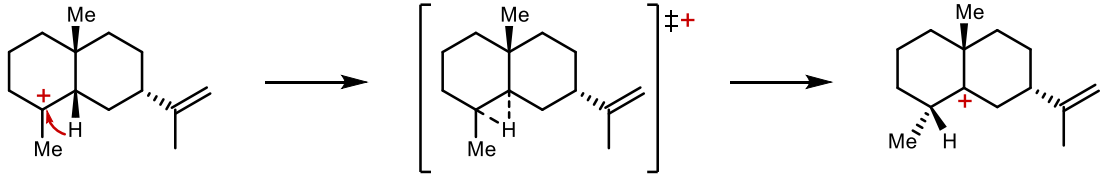
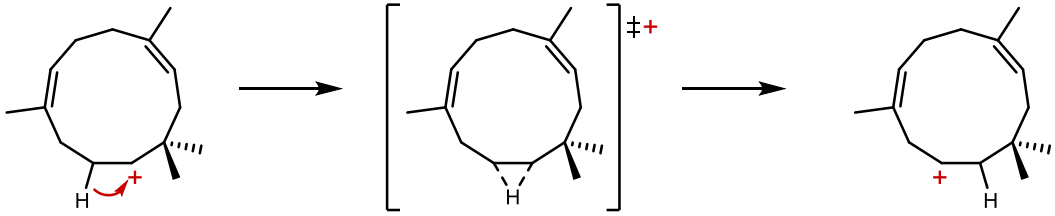
79		18.60	11.78	6.82
80		1.14	15.53	-14.39
81		-0.11	14.46	-14.57
82		16.39	25.48	-9.09

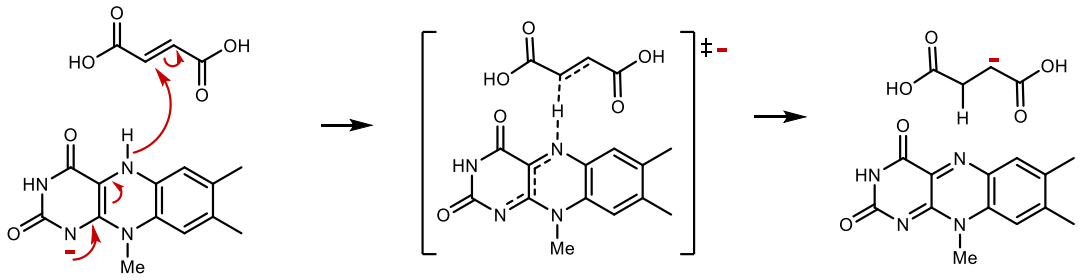
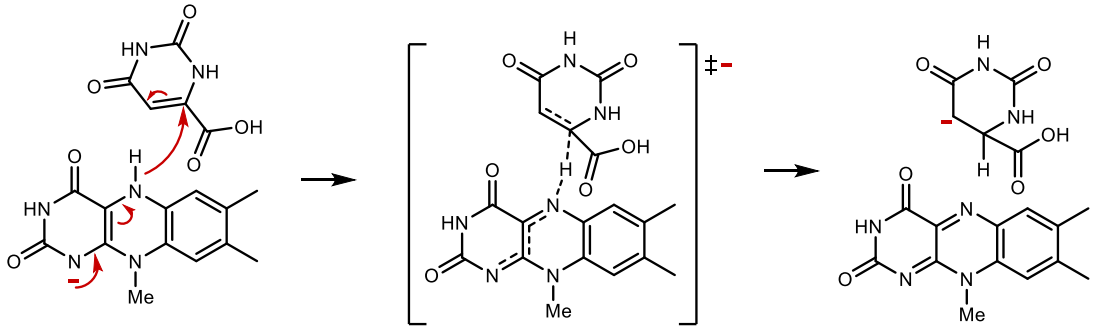
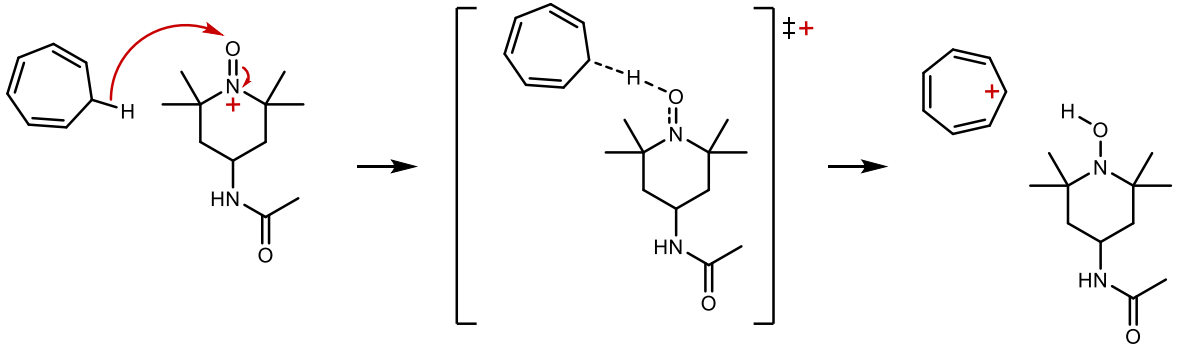
83		15.83	25.03	-9.20
84		11.86	18.34	-6.48
85		15.58	27.22	-11.63
86		15.31	20.29	-4.98

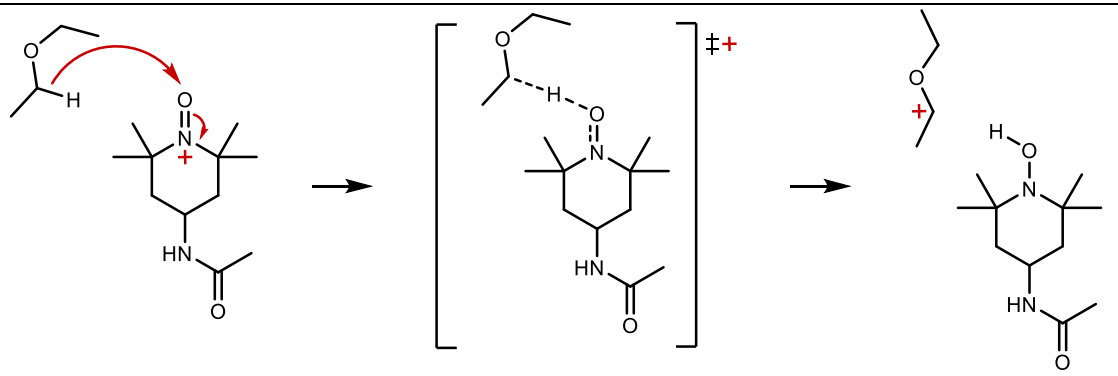
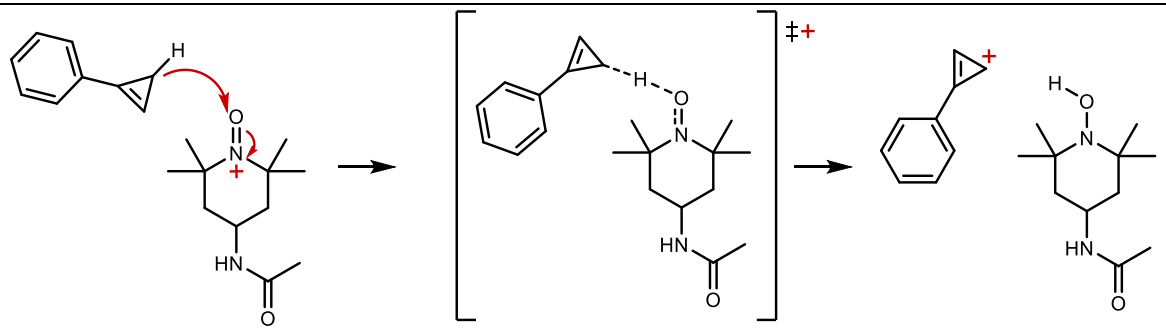
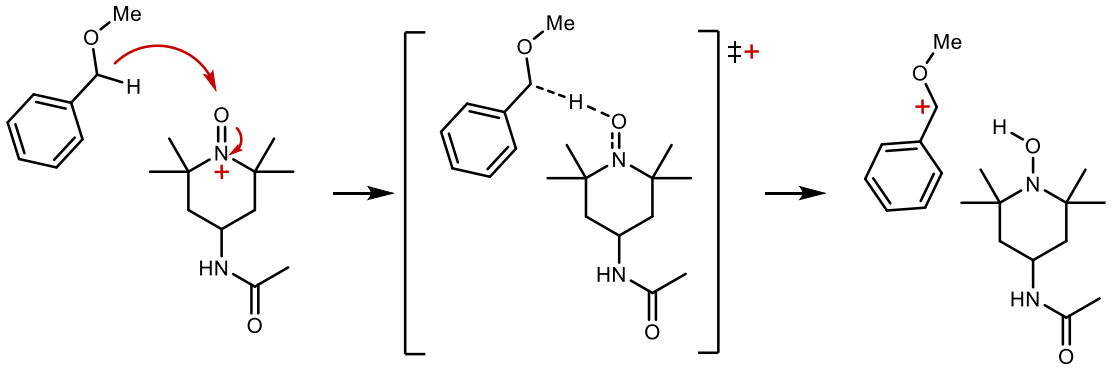
87		3.84	18.14	-14.29
88		33.51	40.20	-6.69
89		13.47	22.19	-8.72
90		0.28	28.62	-28.35

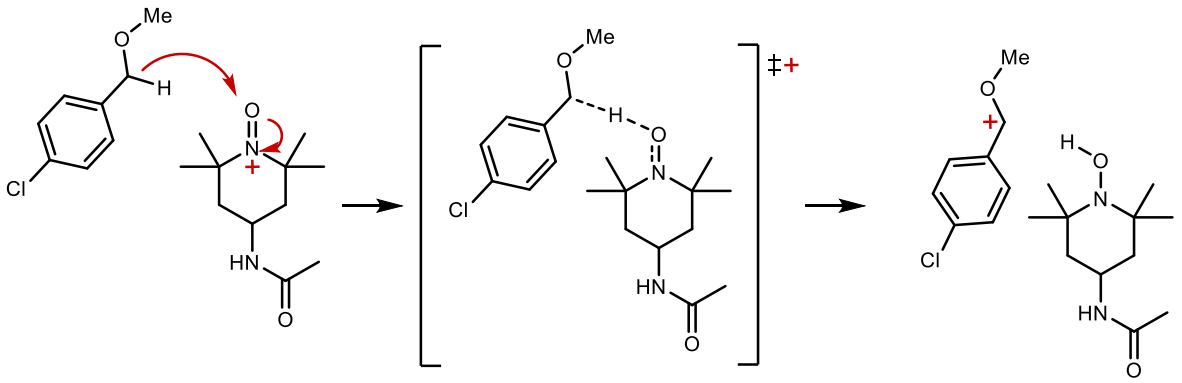
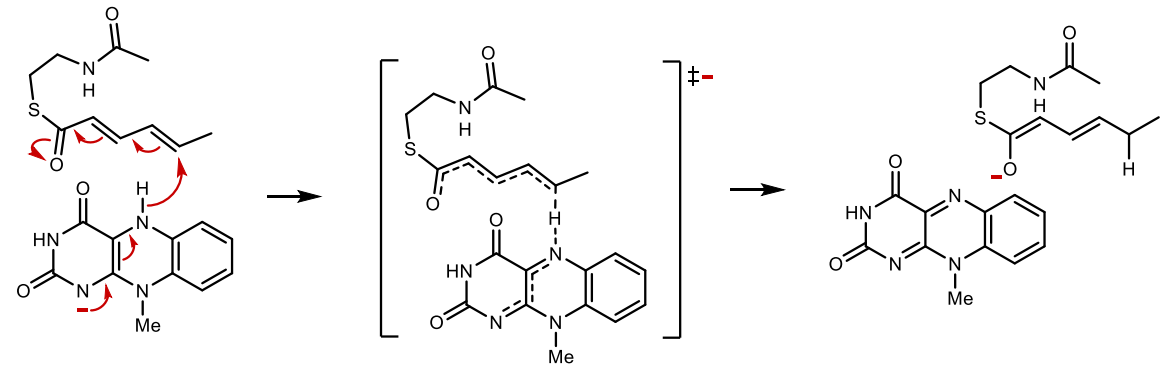
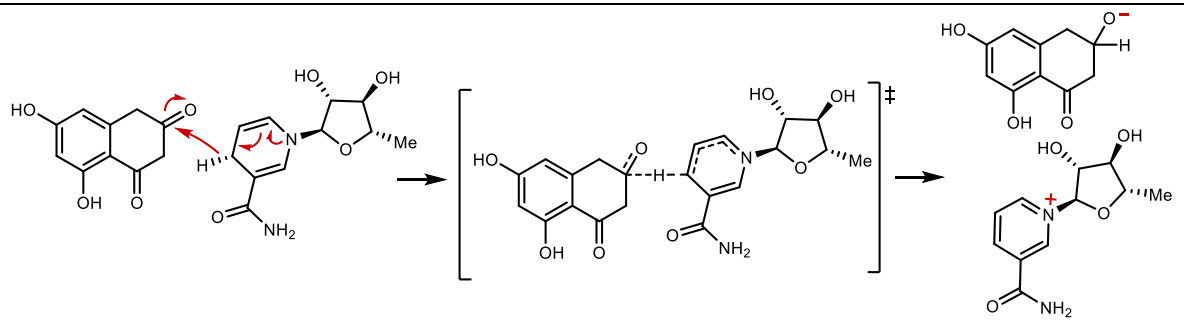
V. Hydride transfer

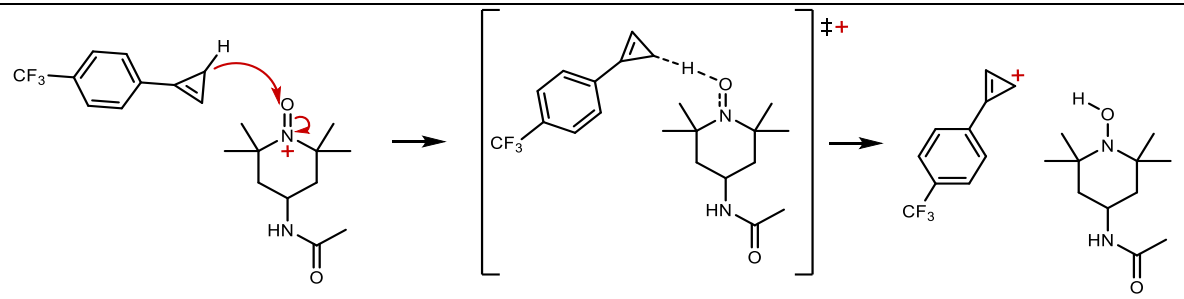
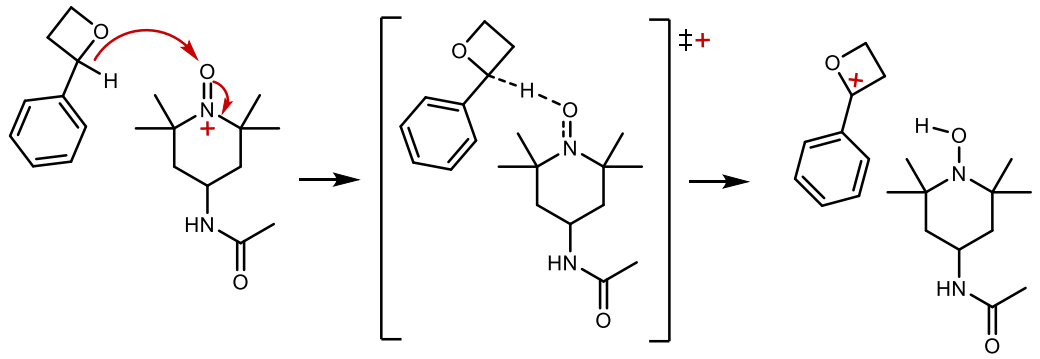
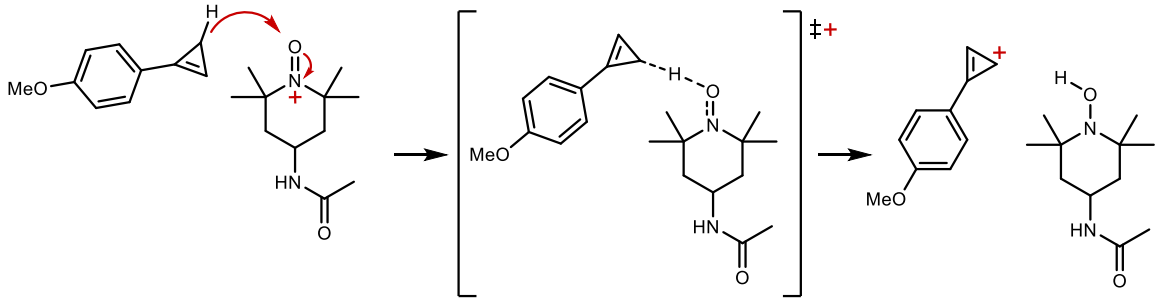
#	Mechanism	Forward barrier height (in kcal/mol)	Reverse barrier height (in kcal/mol)	Reaction energy (in kcal/mol)
1		0.85	6.50	-5.65
2		22.01	23.81	-1.79
3		14.75	18.57	-3.82
4		5.49	25.25	-19.76
5		1.51	15.07	-13.56

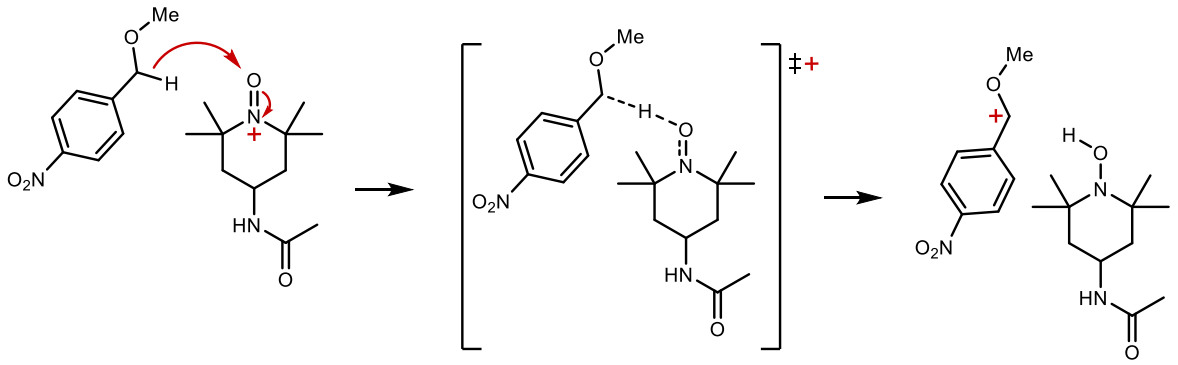
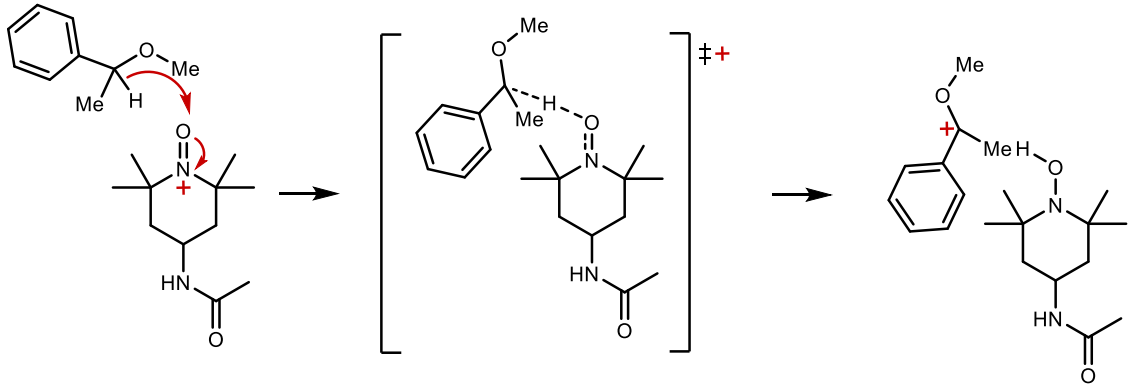
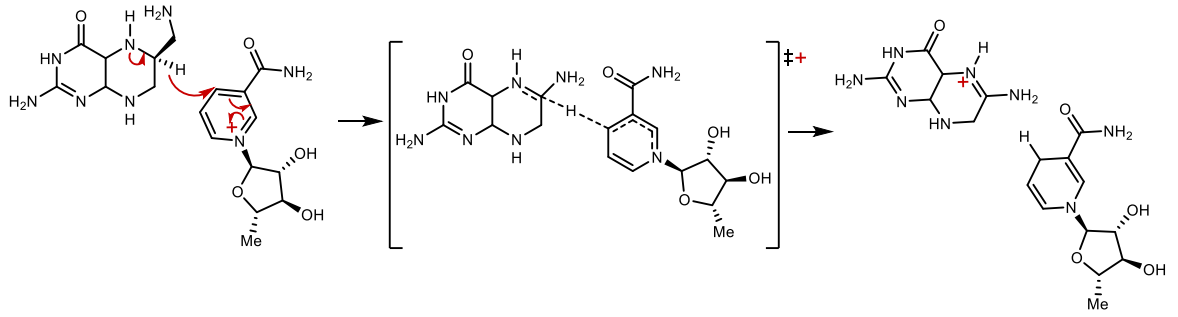
6		10.00	11.94	-1.94
7		16.81	-0.50	17.31
8		1.04	8.07	-7.03
9		-2.46	8.58	-11.04

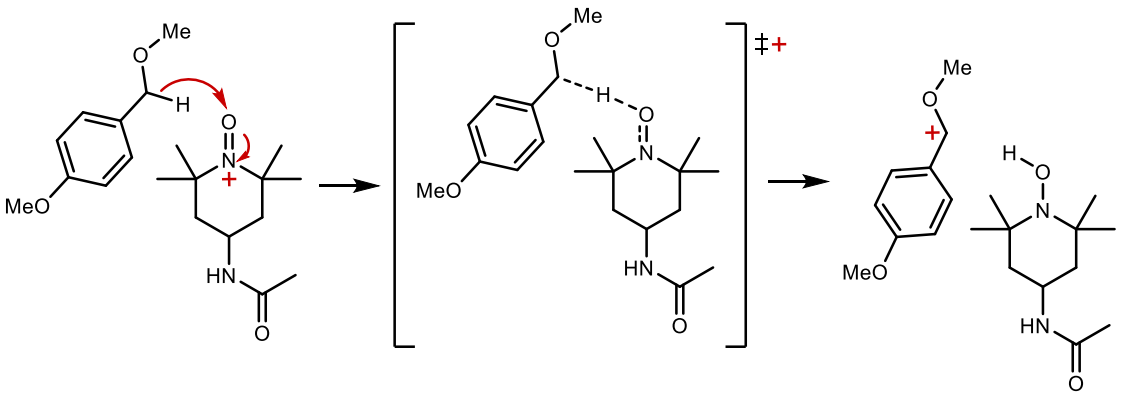
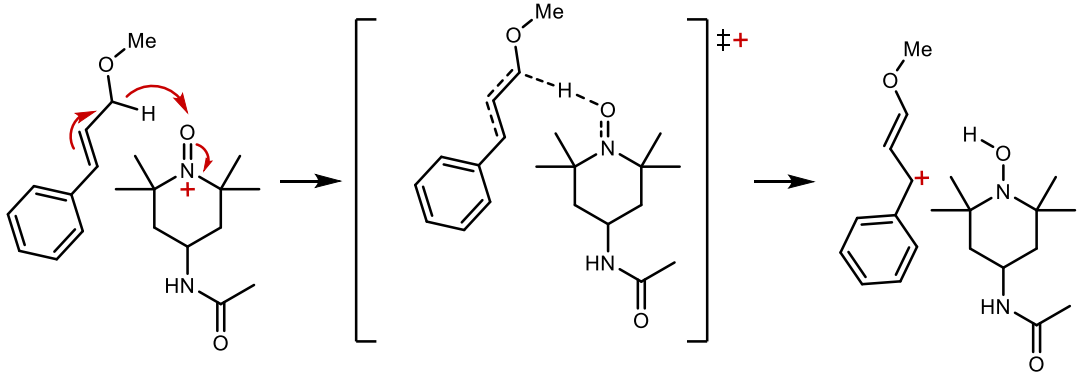
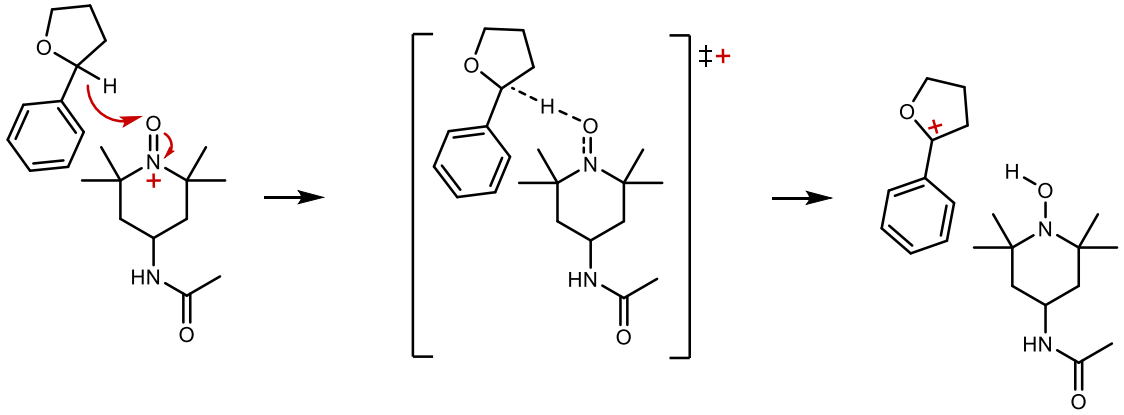
10		14.88	5.63	9.25
11		14.99	-4.21	19.20
12		5.79	20.17	-14.38

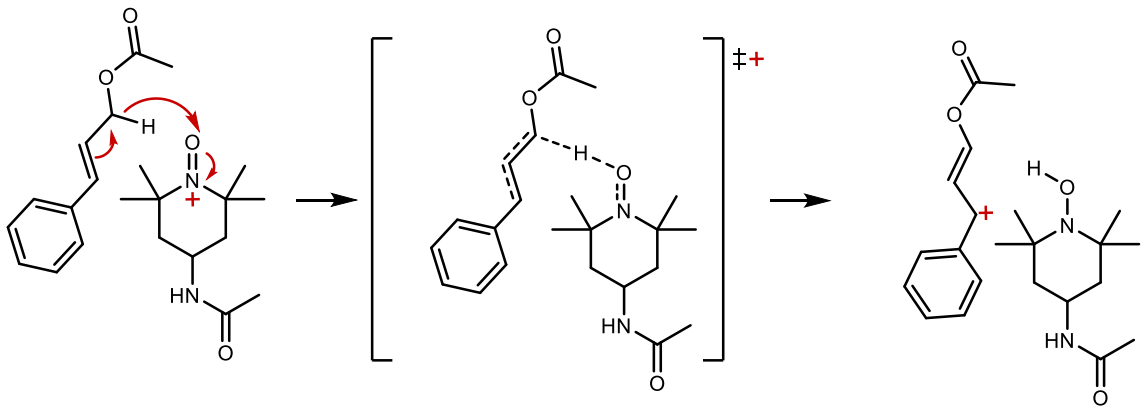
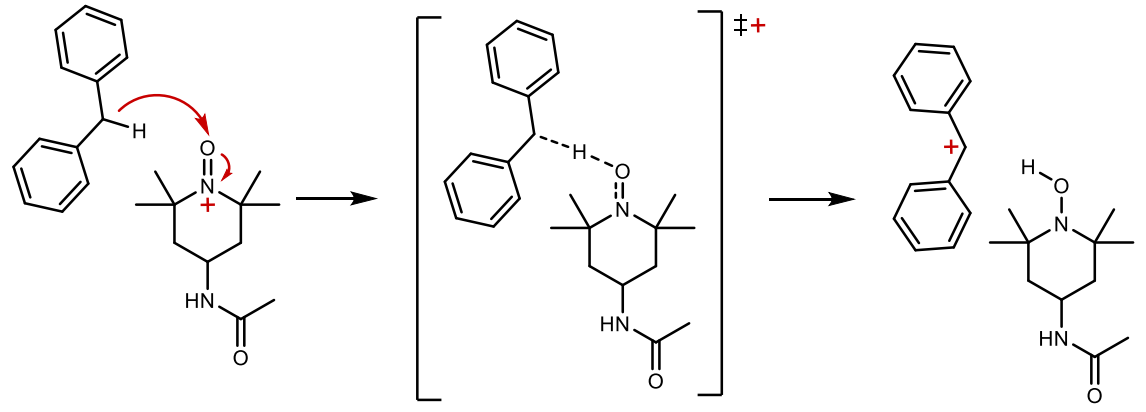
13		17.06	10.36	6.70
14		7.58	16.78	-9.21
15		13.40	18.28	-4.88

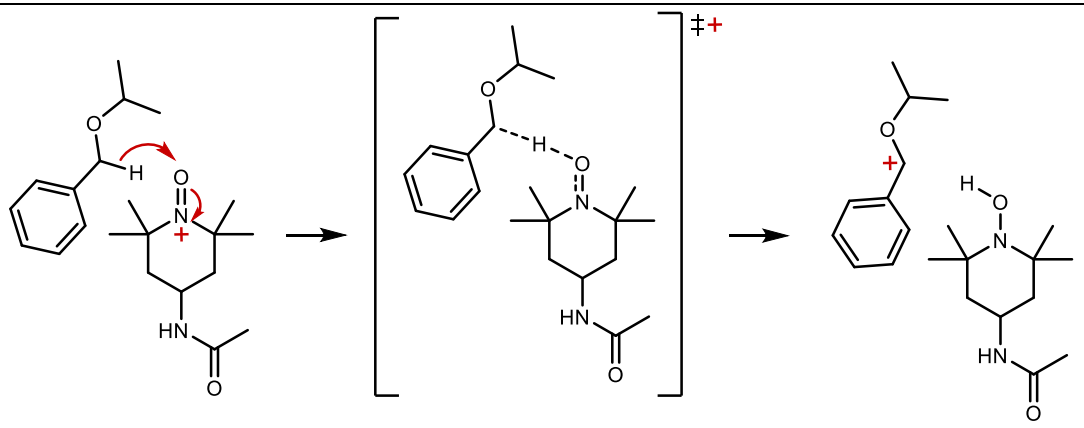
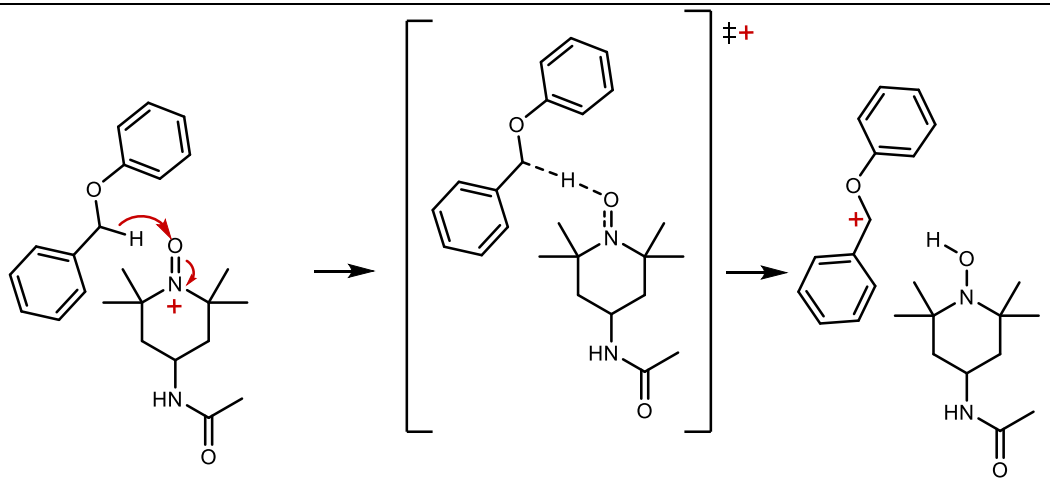
16		16.06	18.89	-2.83
17		14.02	3.43	10.58
18		20.63	-96.26	116.88

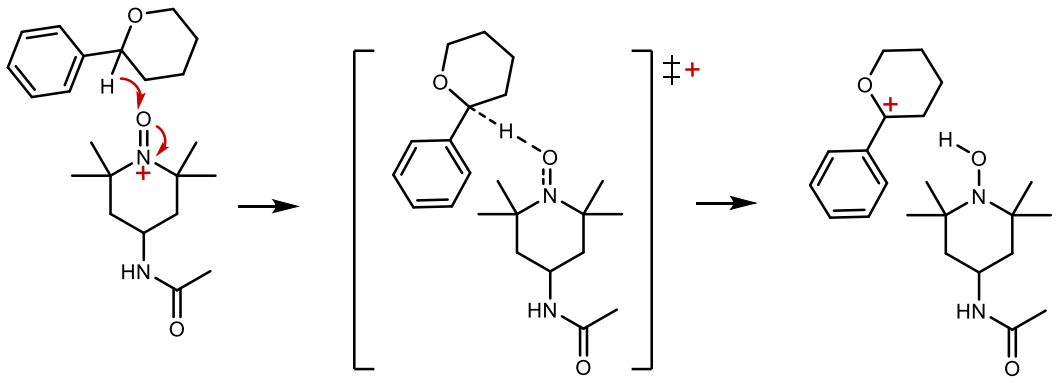
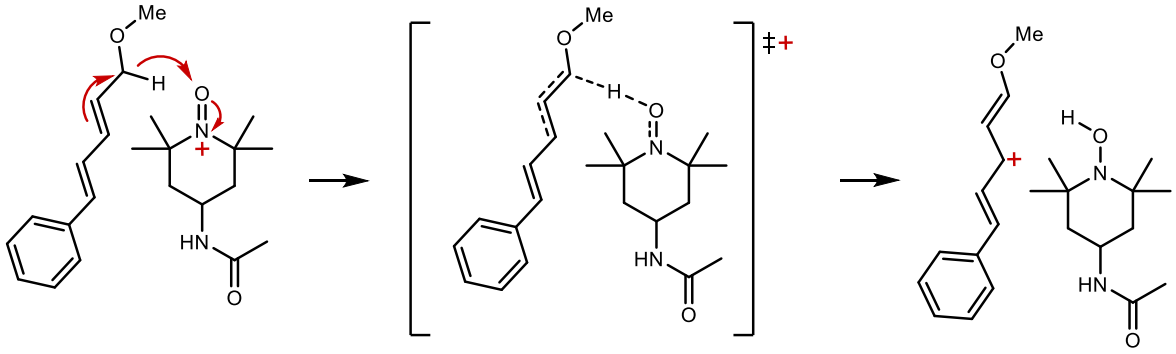
19		12.54	14.68	-2.14
20		5.38	16.10	-10.72
21		3.60	19.57	-15.96

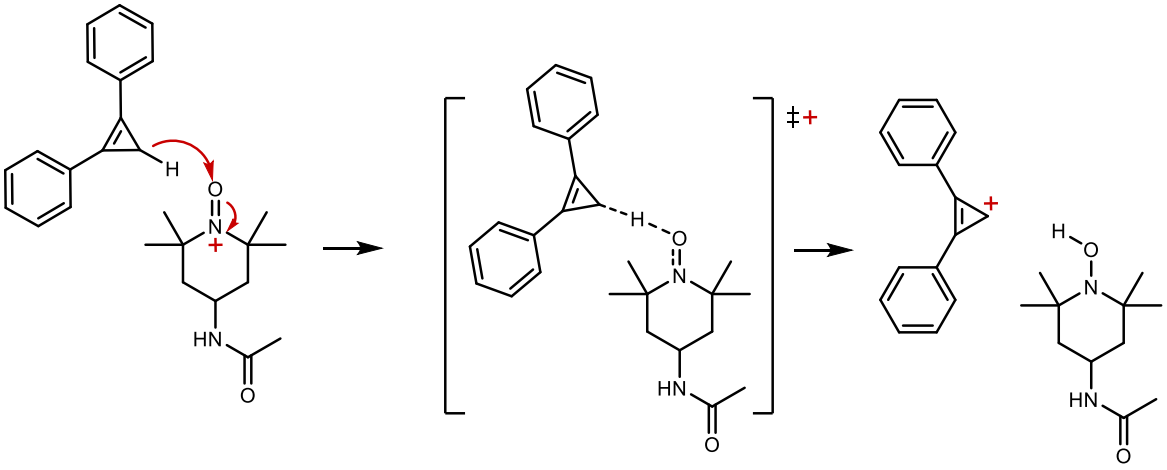
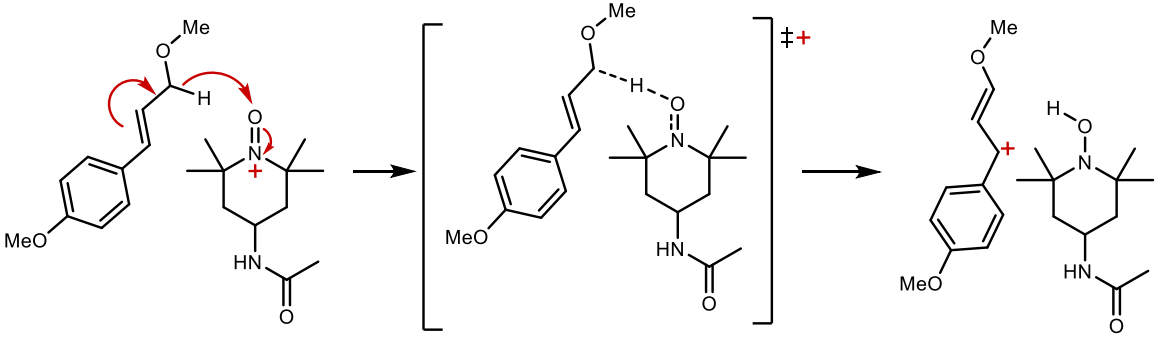
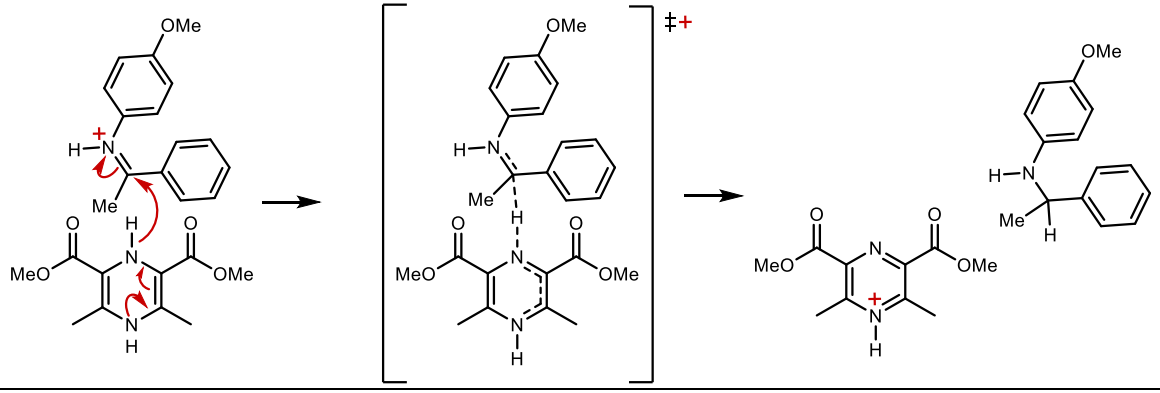
22		21.77	13.81	7.95
23		12.53	21.75	-9.23
24		14.19	5.33	8.86

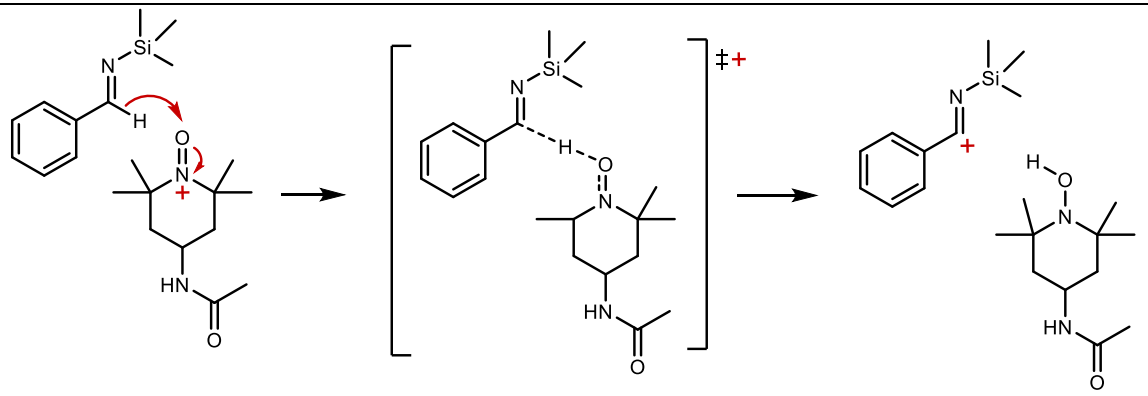
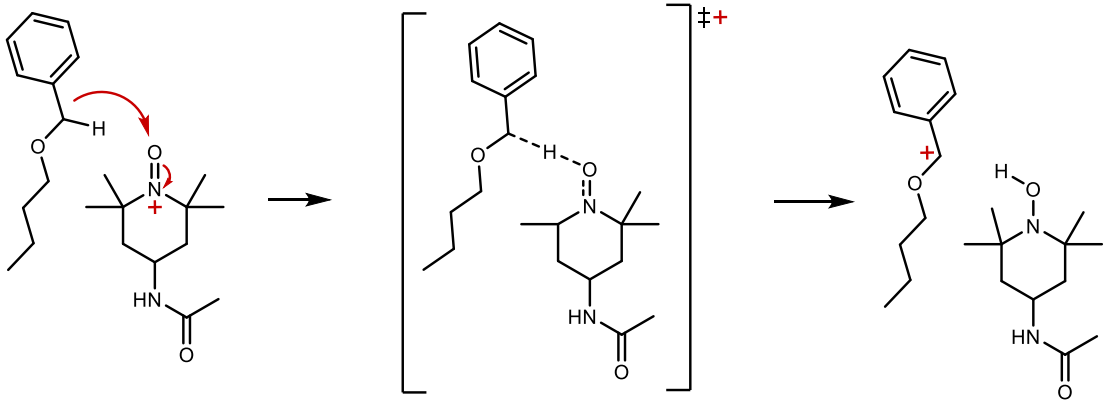
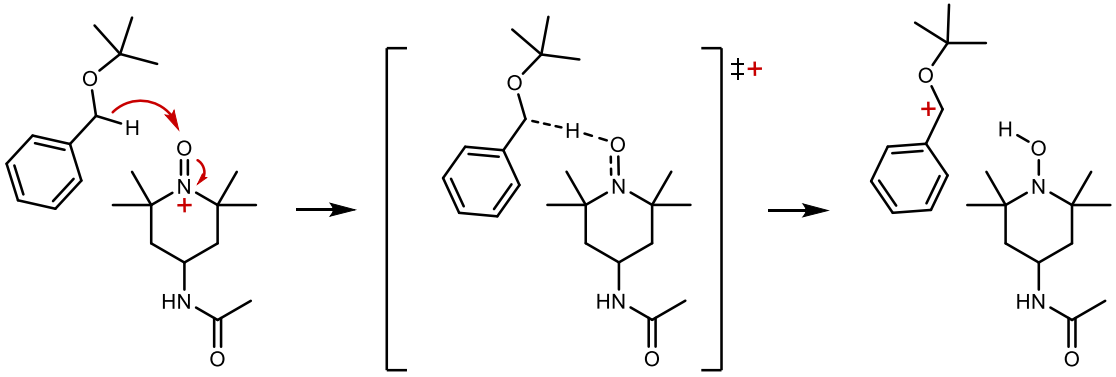
25		9.50	23.84	-14.33
26		4.49	17.53	-13.03
27		1.54	18.71	-17.17

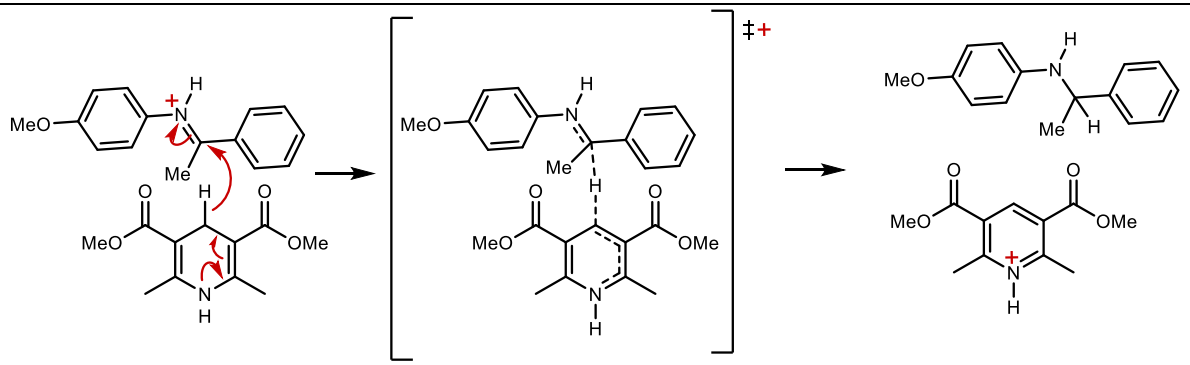
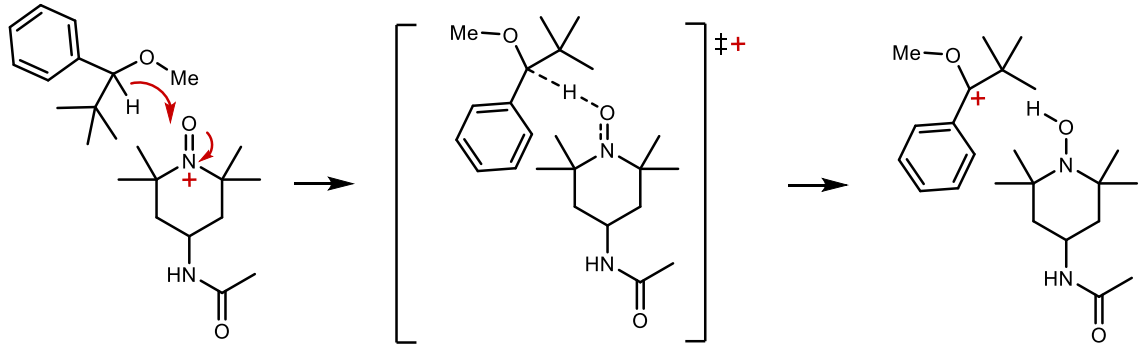
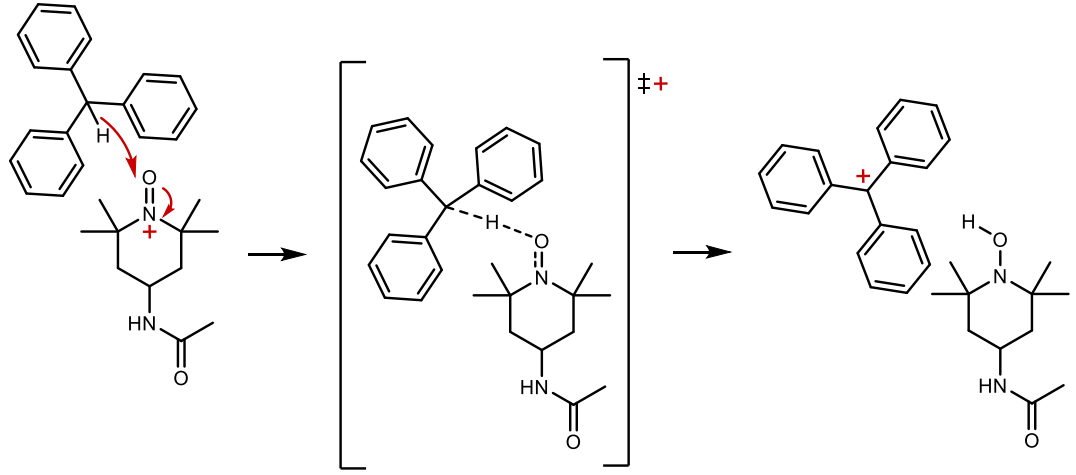
28		9.84	12.24	-2.39
29		12.06	8.00	4.06

30		8.70	19.21	-10.52
31		15.27	18.26	-2.99

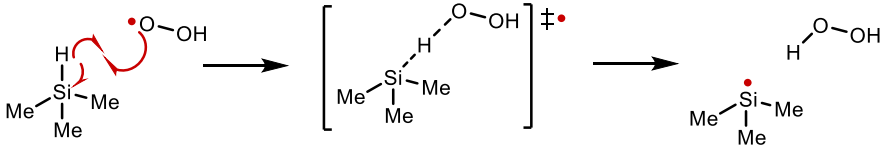
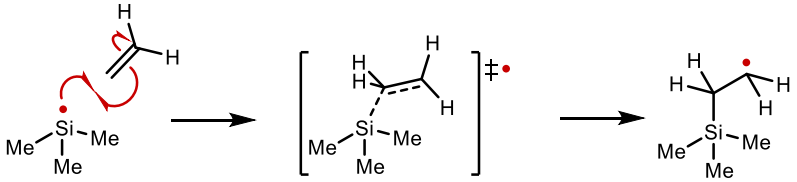
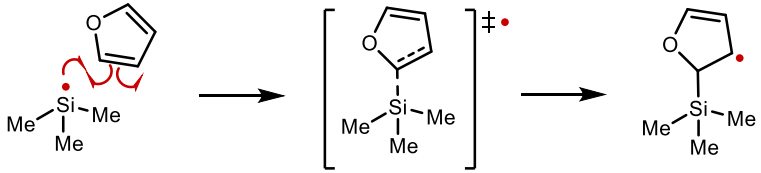
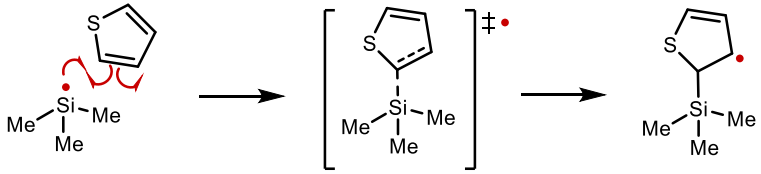
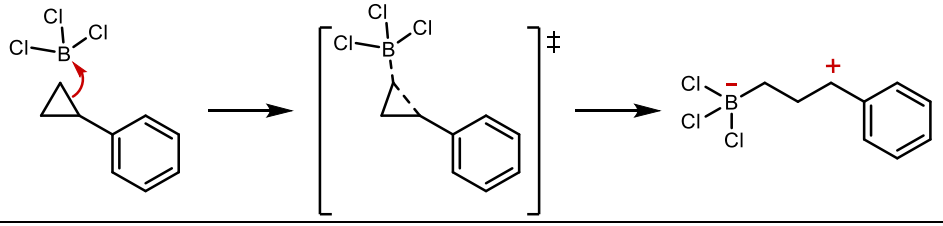
32		4.56	19.64	-15.08
33		1.97	19.13	-17.16

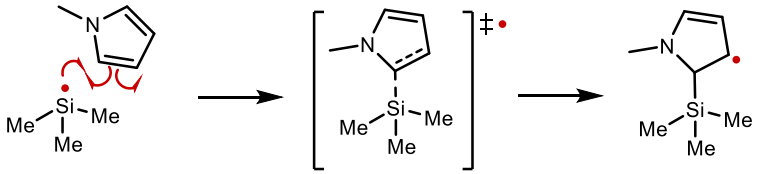
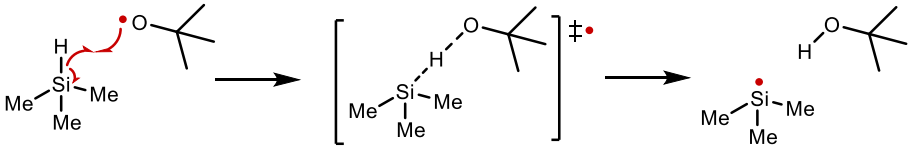
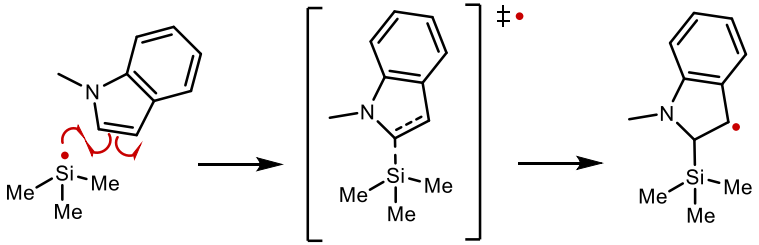
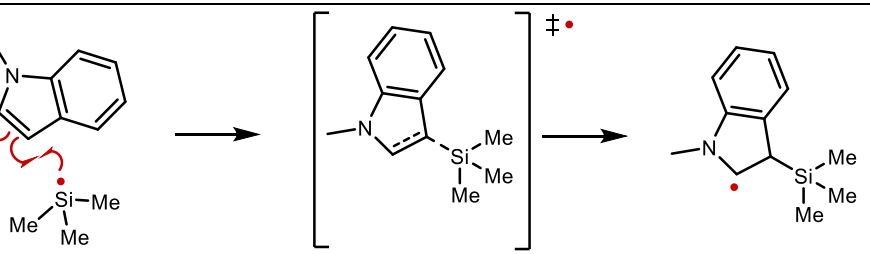
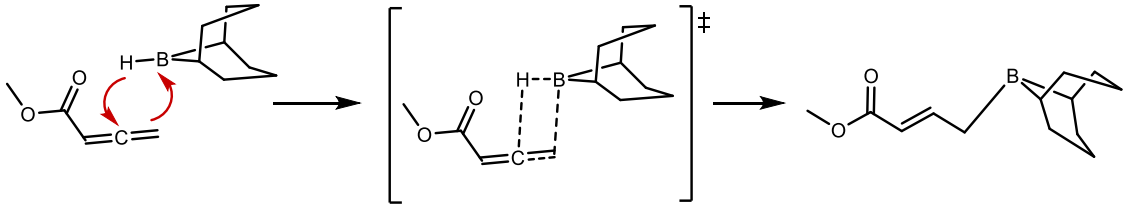
34		1.14	20.97	-19.83
35		0.74	20.87	-20.12
36		10.15	10.19	-0.04

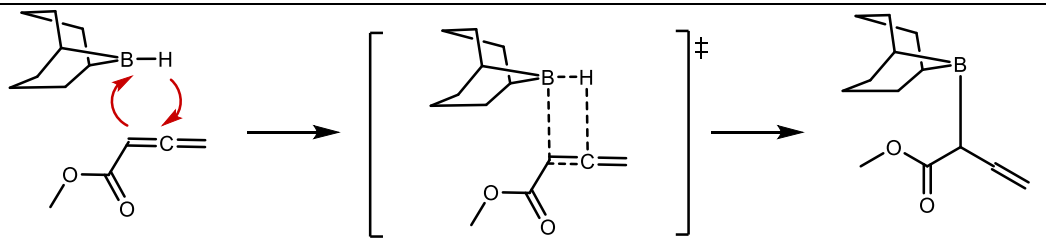
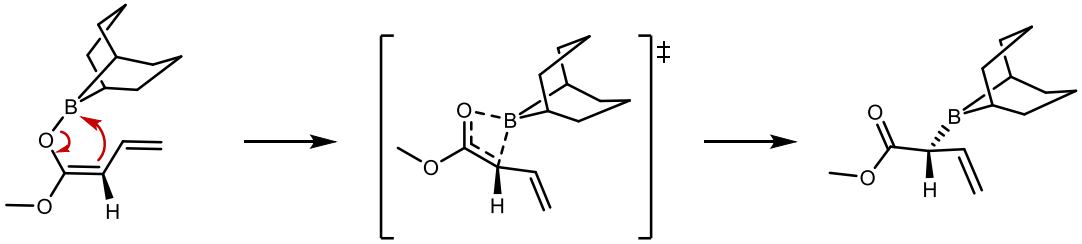
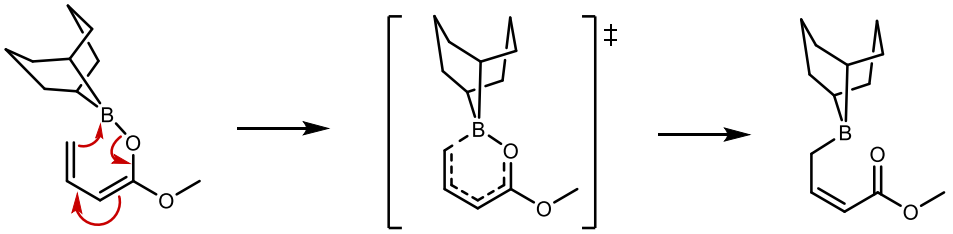
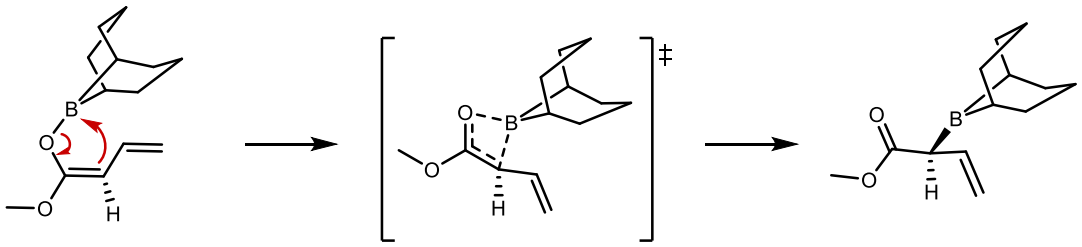
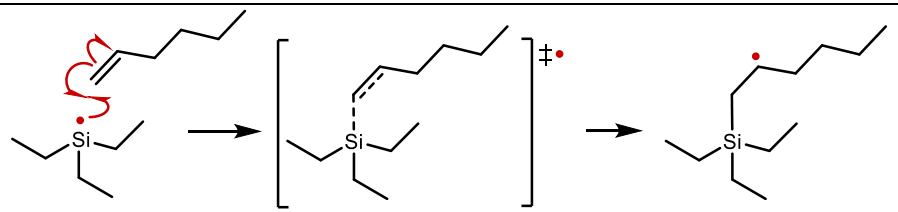
37		-0.57	30.56	-31.13
38		8.26	17.27	-9.02
39		5.34	18.84	-13.50

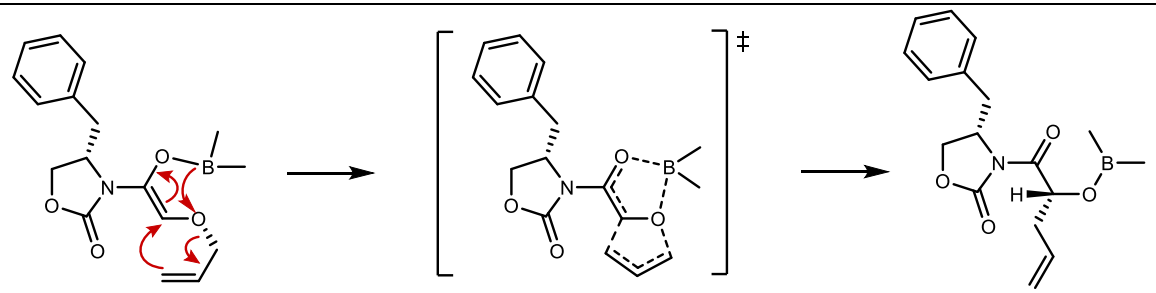
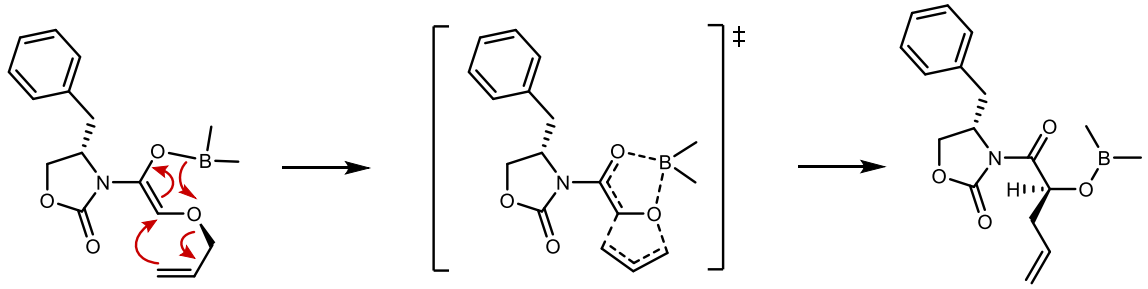
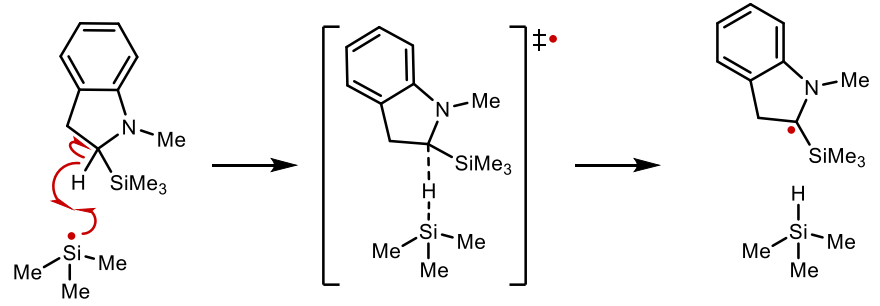
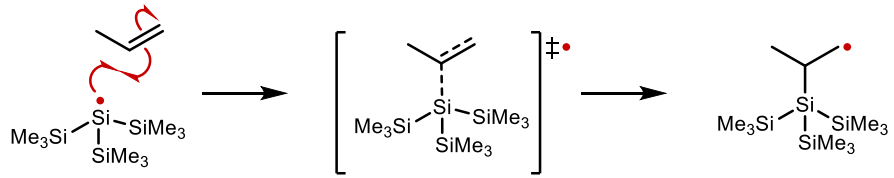
40		-1.16	7.89	-9.05
41		15.49	19.55	-4.06
42		7.36	18.18	-10.82

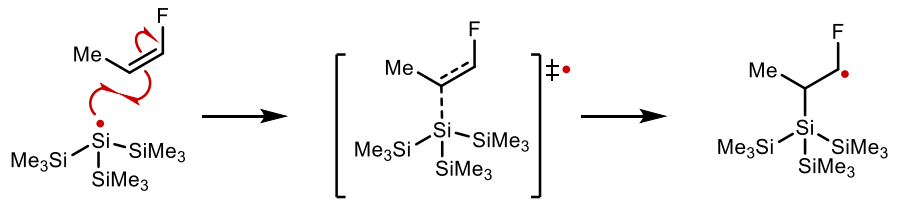
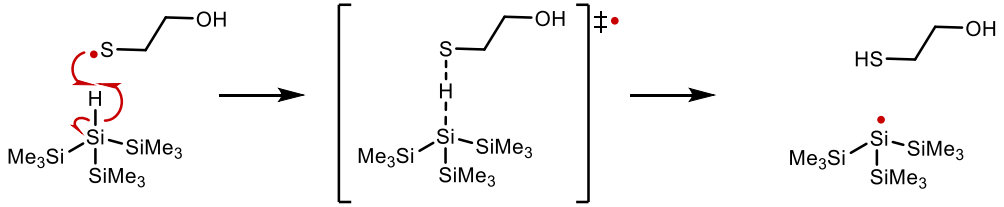
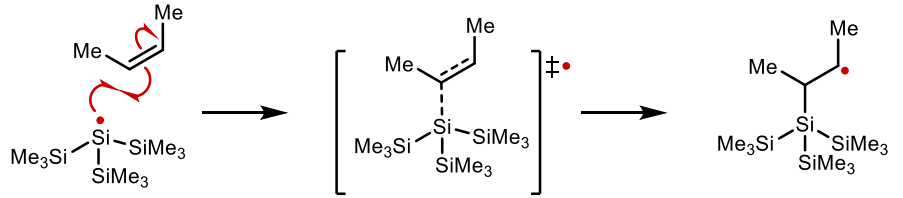
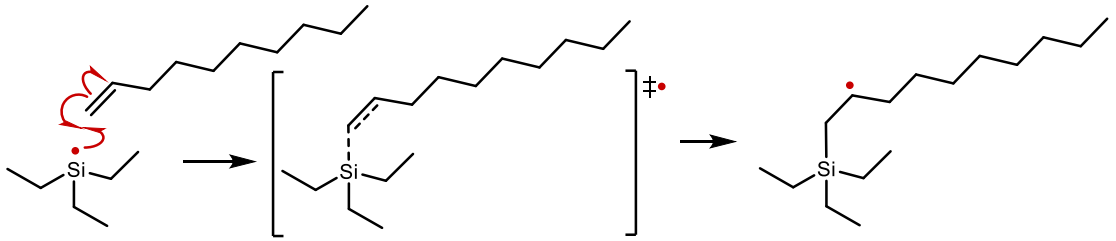
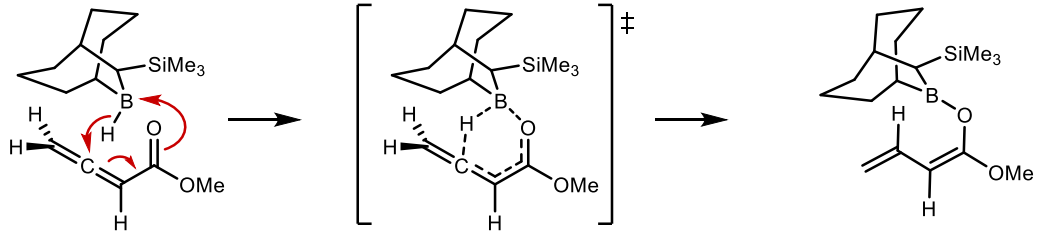
VI. B- and Si-containing

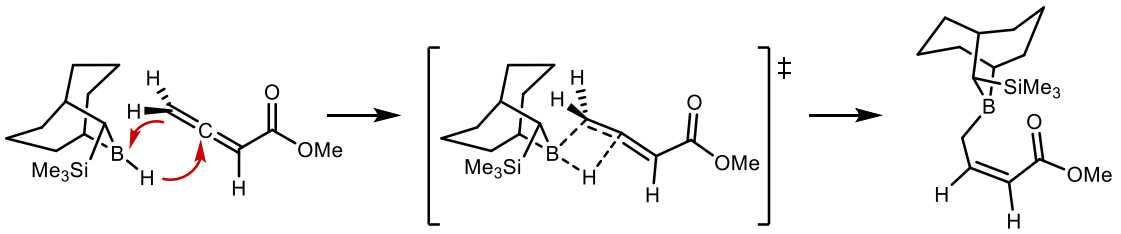
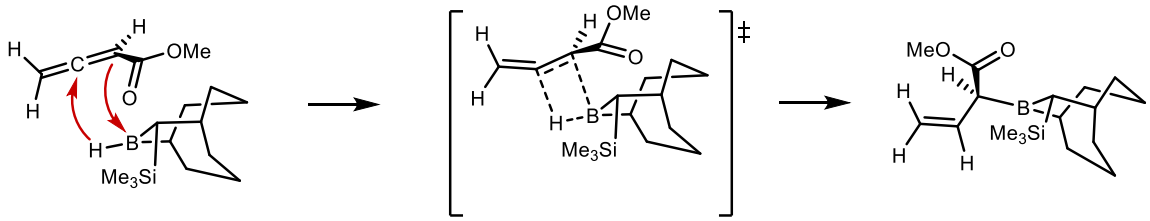
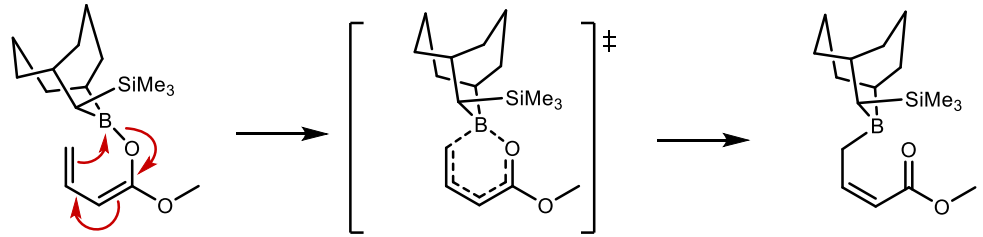
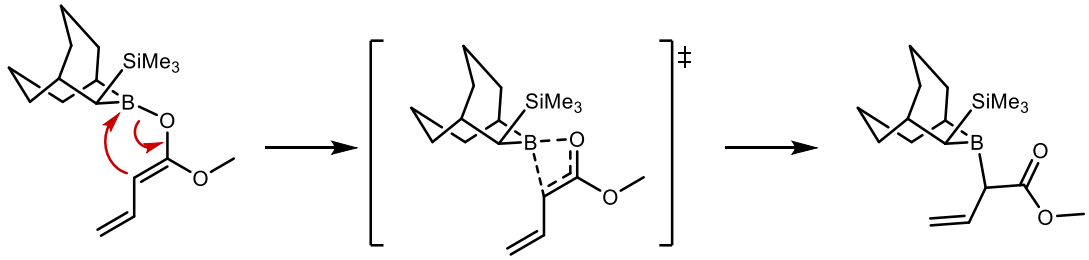
#	Mechanism	Forward barrier height (in kcal/mol)	Reverse barrier height (in kcal/mol)	Reaction energy (in kcal/mol)
1		15.72	10.68	5.04
2		2.24	28.35	-26.12
3		4.81	25.87	-21.06
4		4.62	29.54	-24.91
5		14.75	-1.06	15.80

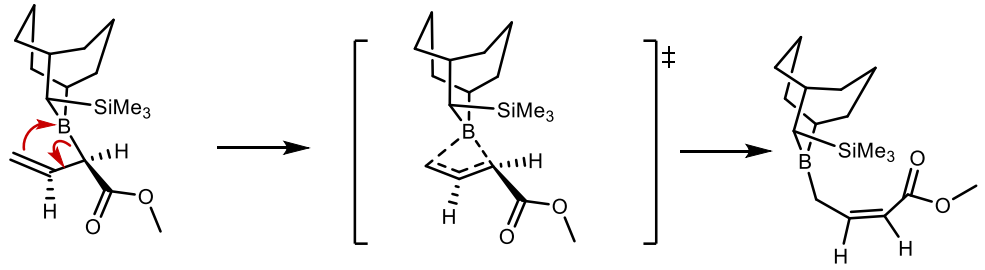
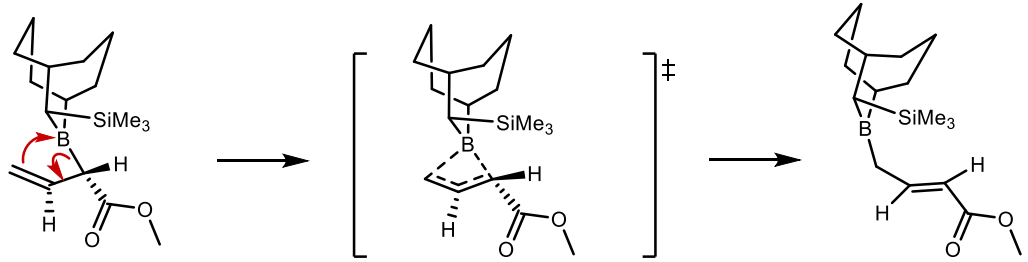
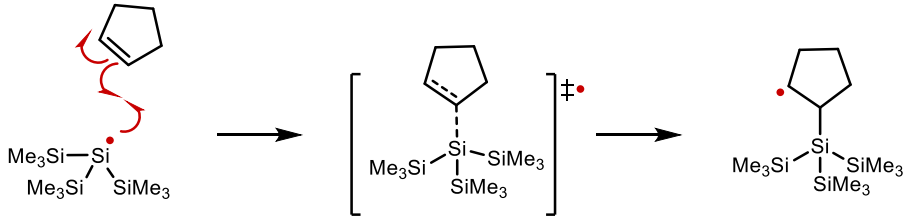
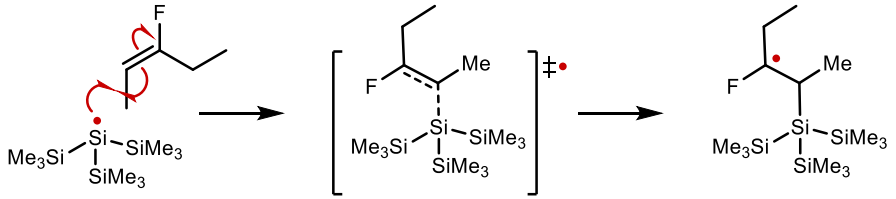
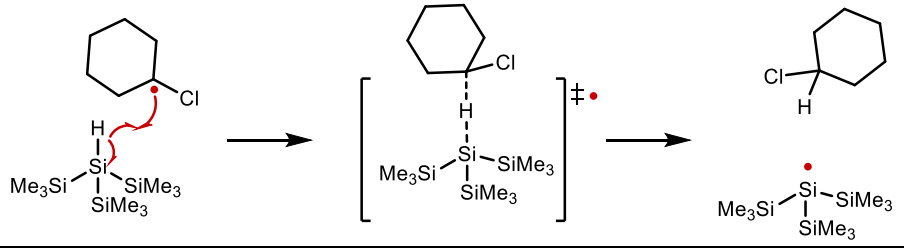
6		4.04	19.53	-15.48
7		3.89	19.12	-15.24
8		3.36	21.63	-18.27
9		5.78	21.11	-15.32
10		3.49	52.87	-49.38

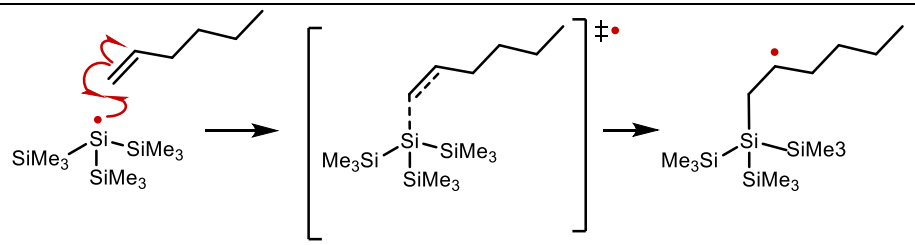
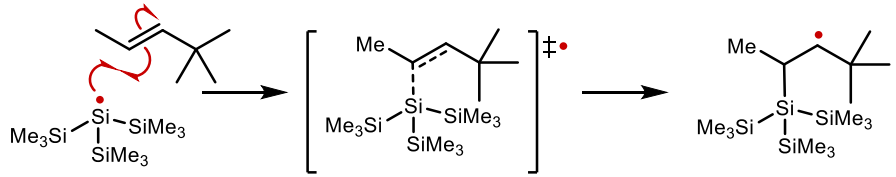
11		1.31	50.23	-48.92
12		20.32	14.77	5.54
13		11.81	16.75	-4.95
14		13.62	10.81	2.80
15		1.33	27.06	-25.73

16		18.86	53.61	-34.76
17		20.99	54.73	-33.74
18		7.60	15.41	-7.82
19		4.39	13.75	-9.36

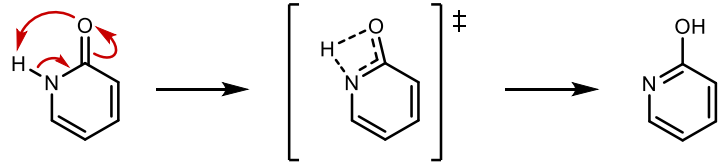
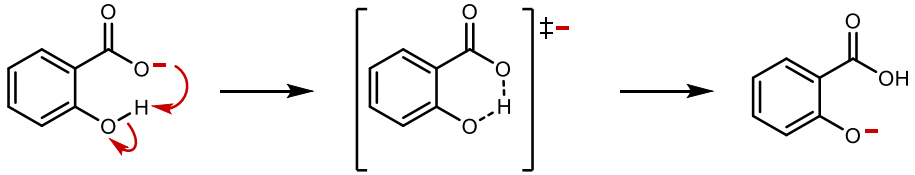
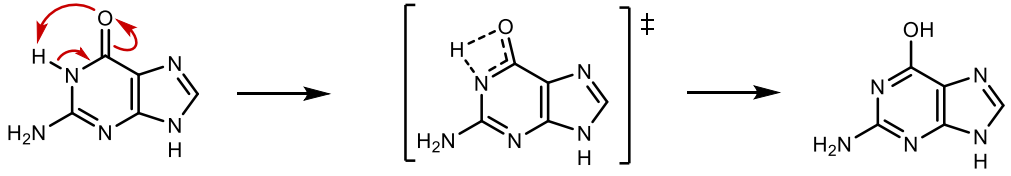
20		4.00	14.18	-10.18
21		-1.69	2.54	-4.23
22		2.98	12.74	-9.76
23		1.07	26.52	-25.45
24		7.84	61.88	-54.04

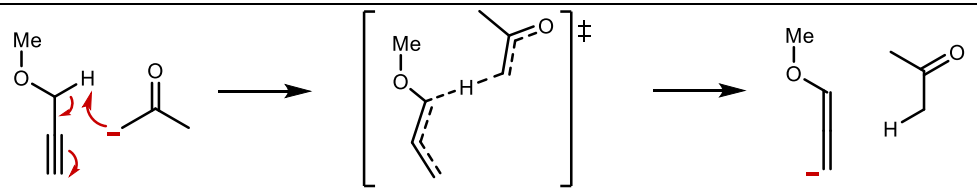
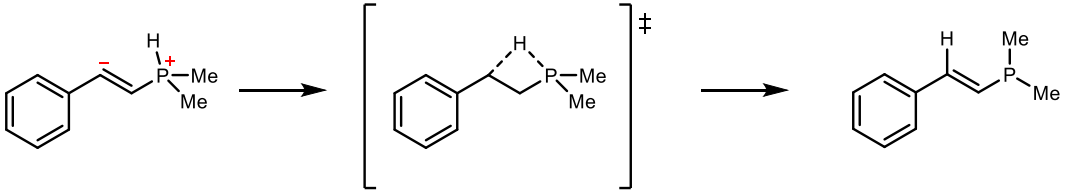
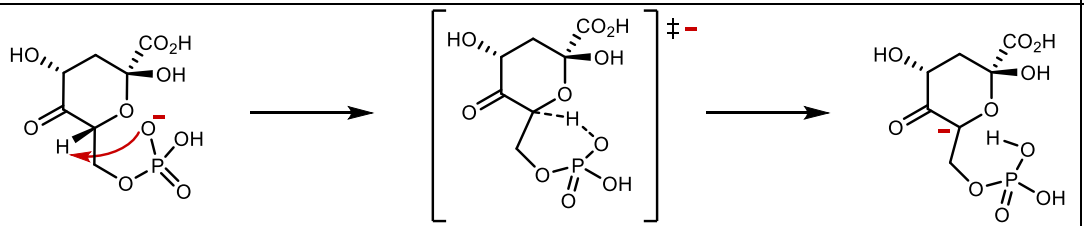
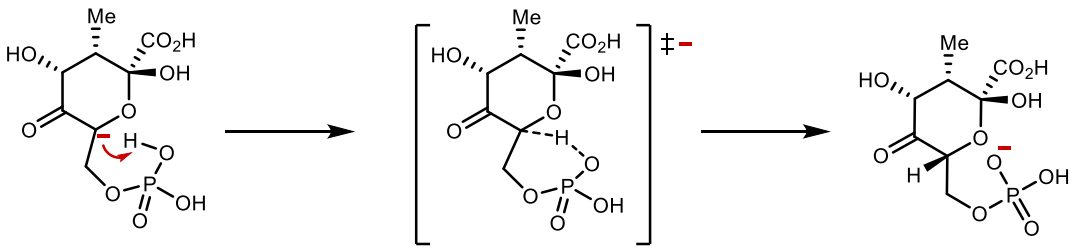
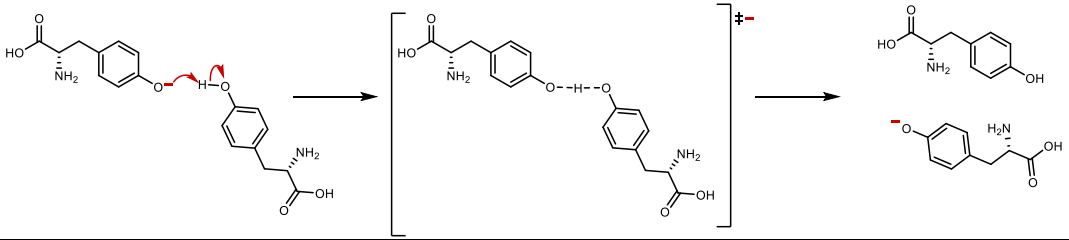
25		8.11	56.40	-48.28
26		8.68	55.38	-46.70
27		21.41	15.51	5.90
28		20.08	15.35	4.73

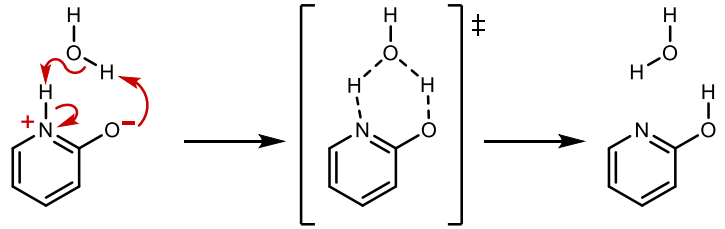
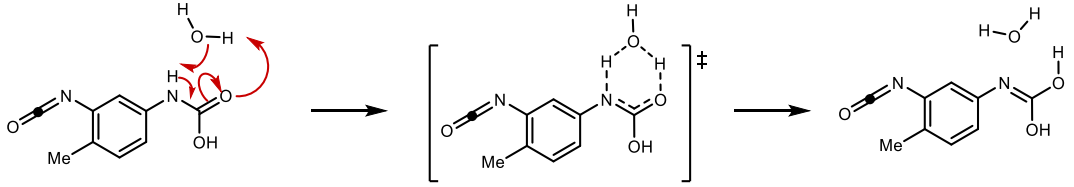
29		18.58	20.49	-1.91
30		13.88	15.61	-1.73
31		2.21	13.33	-11.12
32		2.61	13.62	-11.00
33		1.43	17.74	-16.31

34		1.41	13.67	-12.26
35		5.79	13.34	-7.55

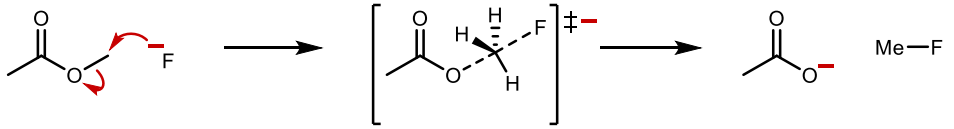
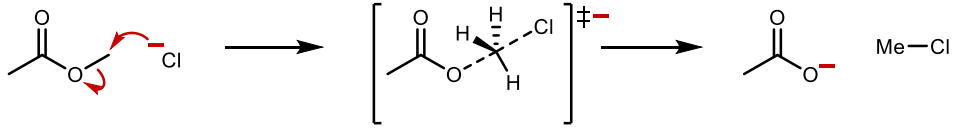
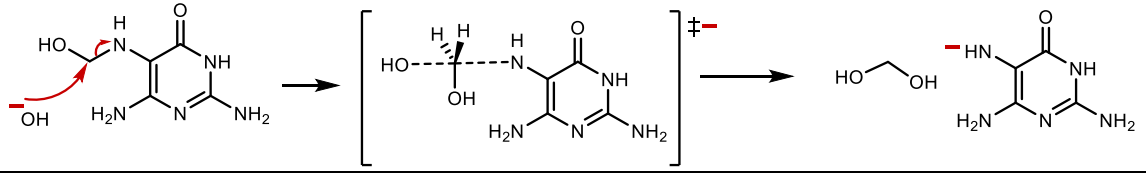
VII. Proton transfer

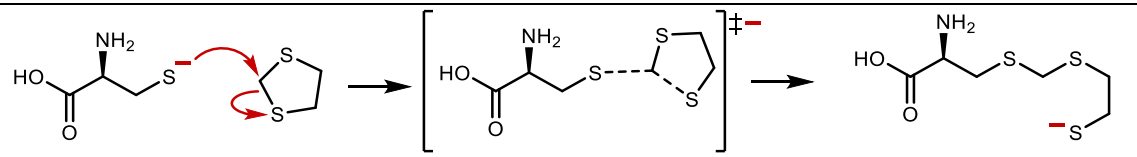
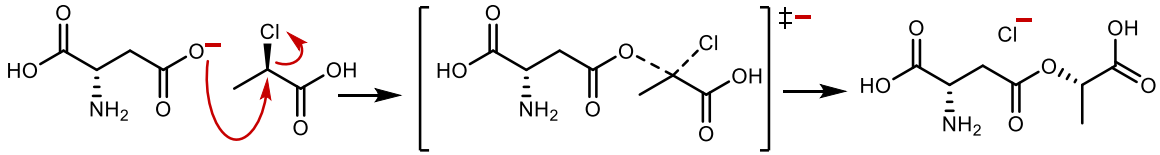
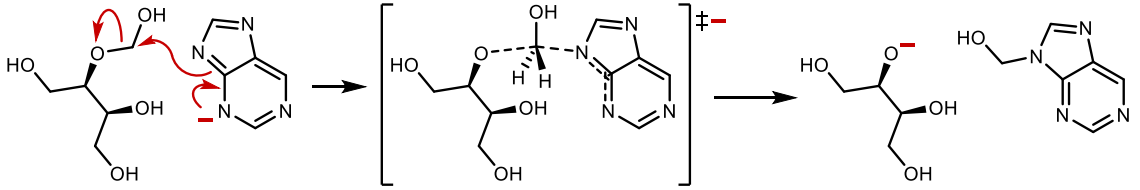
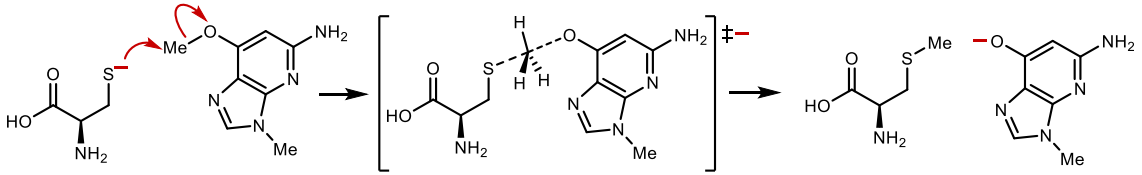
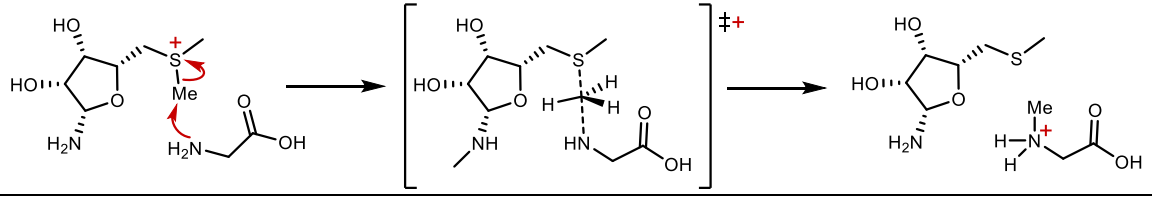
#	Mechanism	Forward barrier height (in kcal/mol)	Reverse barrier height (in kcal/mol)	Reaction energy (in kcal/mol)
1		37.29	38.20	-0.91
2		0.84	0.75	0.09
3		37.38	37.14	0.24

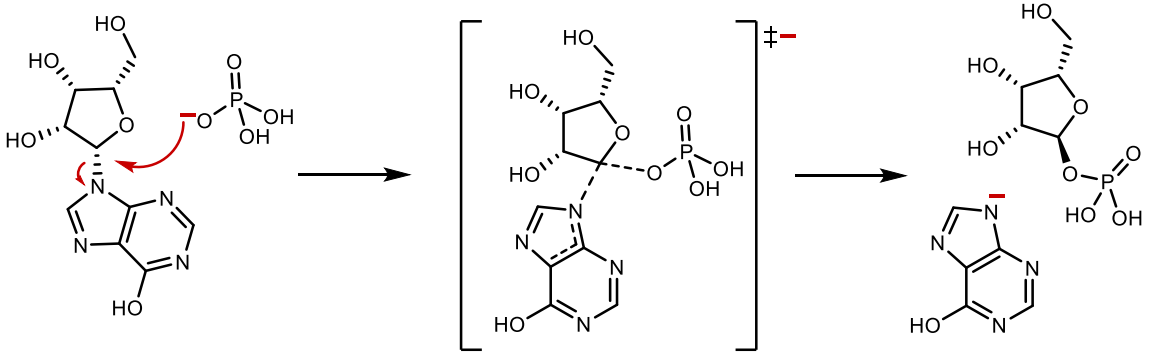
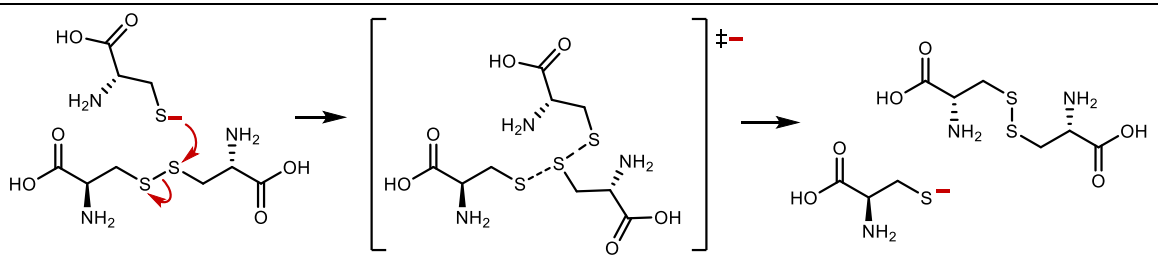
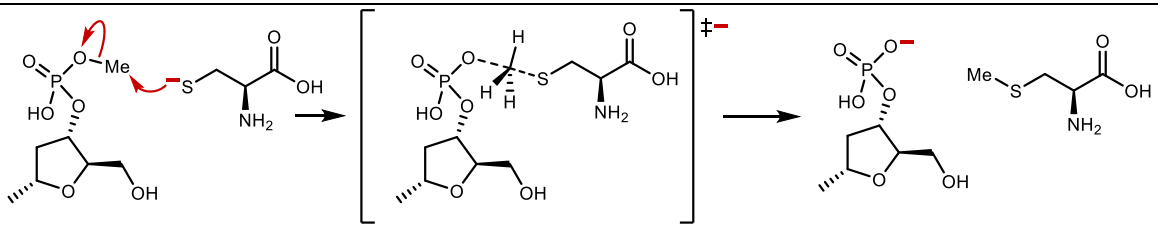
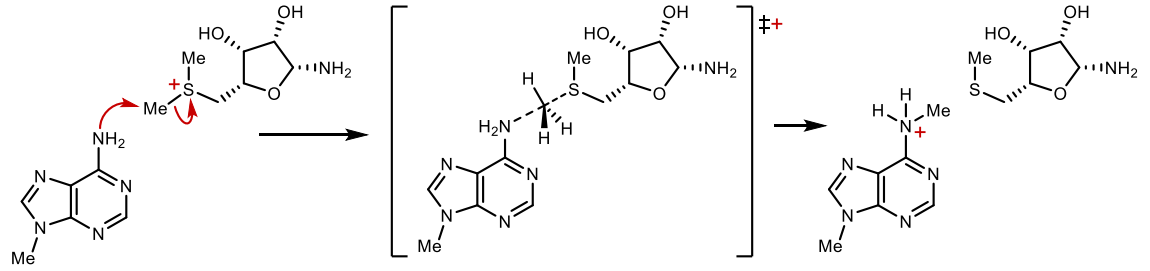
4		12.73	0.08	12.64
5		11.94	71.12	-59.18
6		30.60	3.14	27.46
7		3.08	32.75	-29.68
8		-31.63	-30.51	-1.12

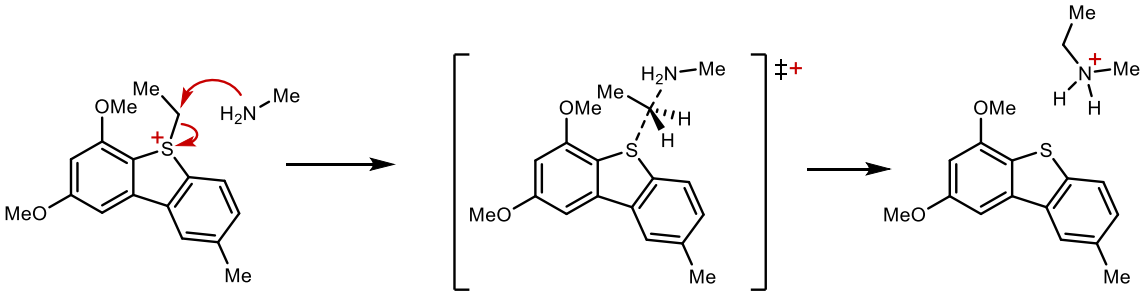
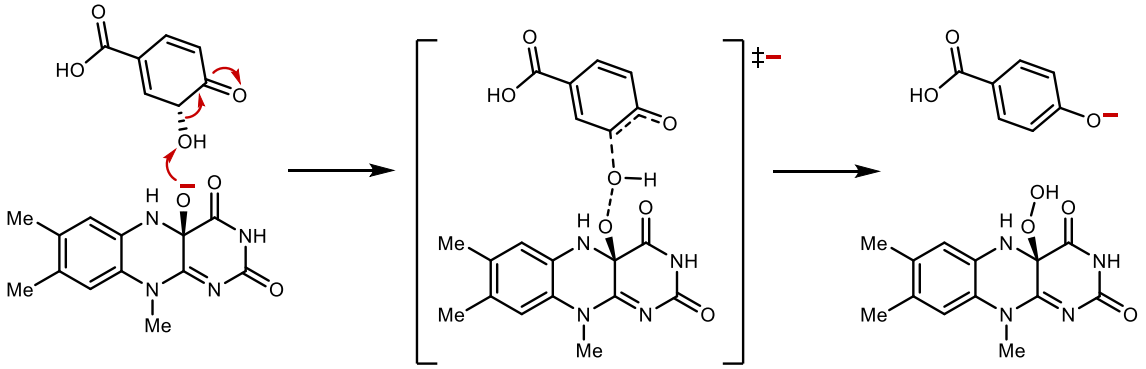
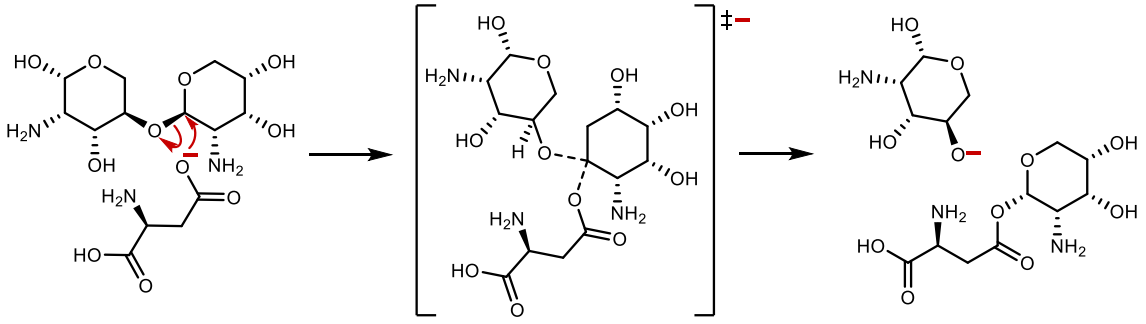
9		4.73	5.64	-0.91
10		17.32	-0.47	17.79

VIII. Nucleophilic substitution

#	Mechanism	Forward barrier height (in kcal/mol)	Reverse barrier height (in kcal/mol)	Reaction energy (in kcal/mol)
1		-3.21	15.07	-18.28
2		14.28	-0.05	14.33
3		13.63	28.04	-14.41

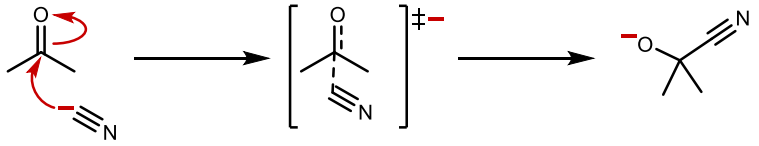
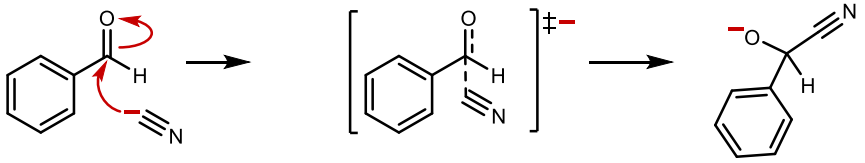
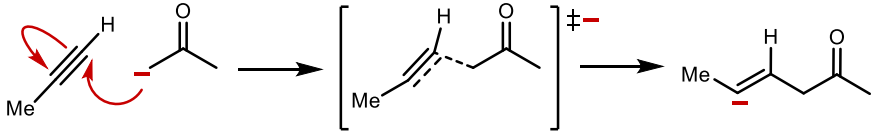
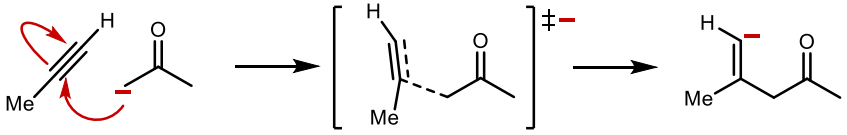
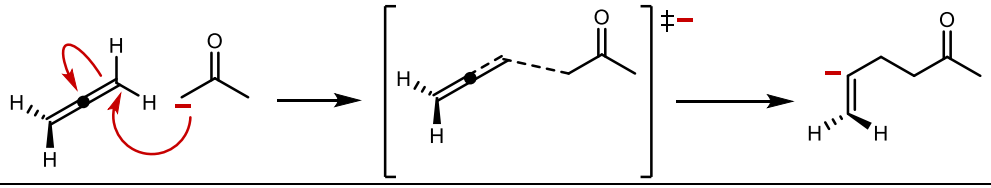
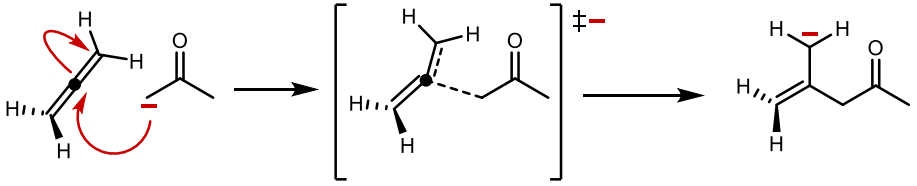
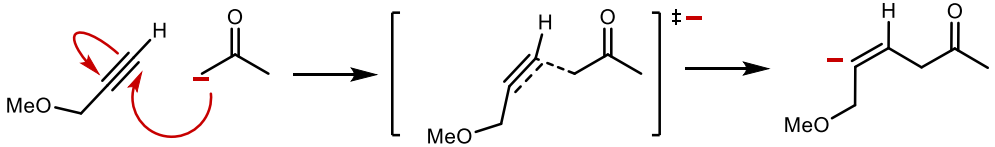
4		23.74	29.96	-6.22
5		-4.00	4.56	-8.56
6		20.98	10.61	10.37
7		9.10	11.86	-2.76
8		17.89	15.80	2.09

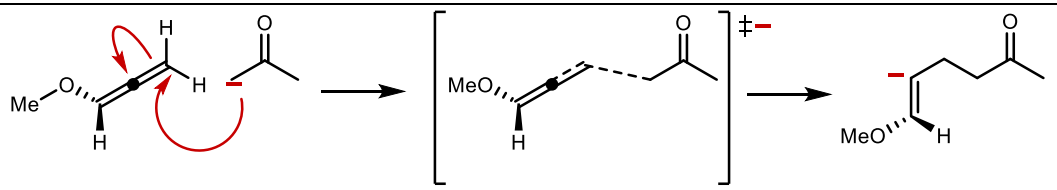
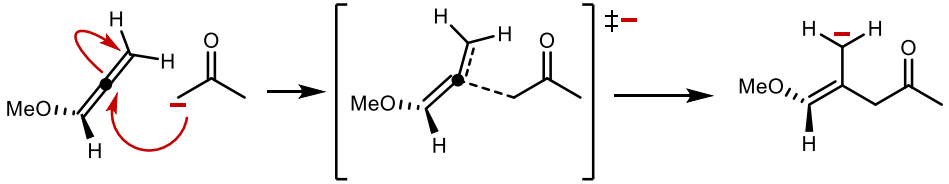
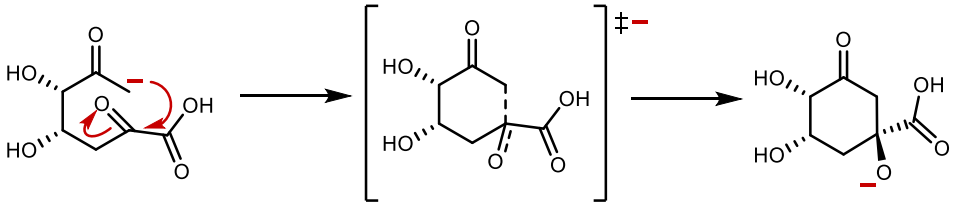
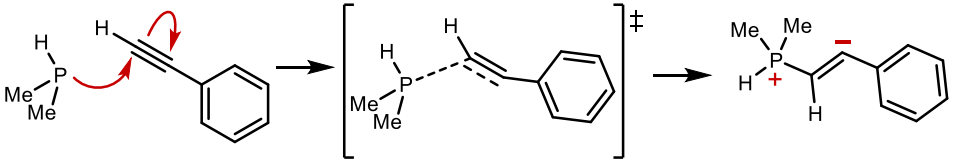
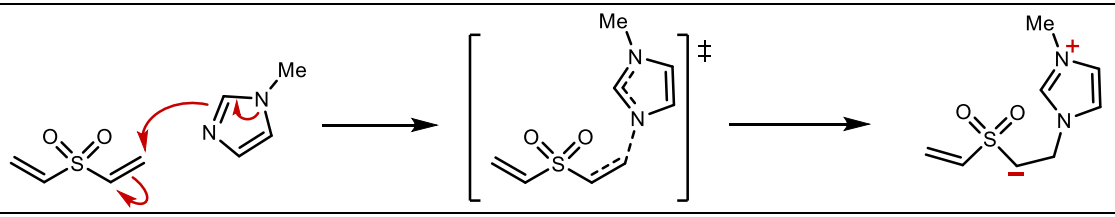
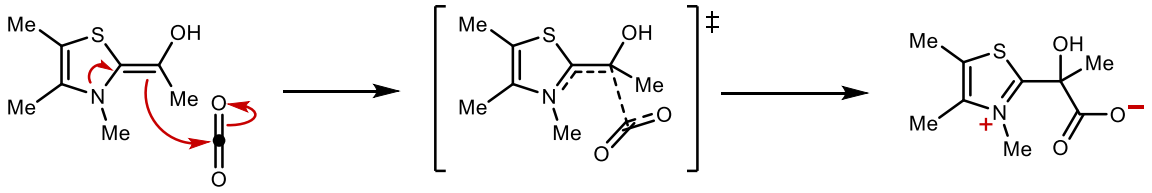
9		3.08	-5.70	8.78
10		3.14	6.09	-2.95
11		-2.99	19.74	-22.72
12		14.76	6.60	8.16

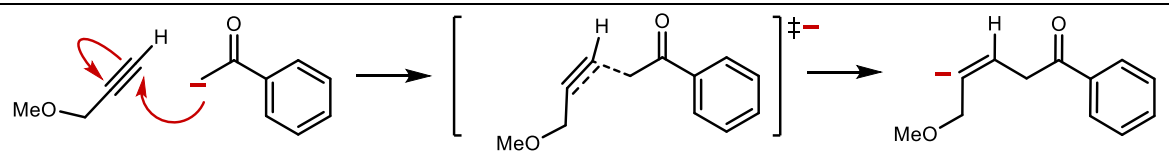
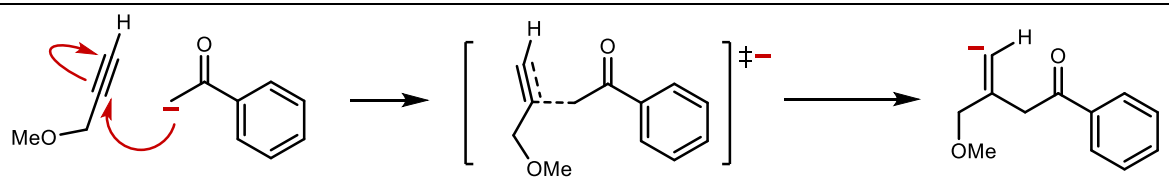
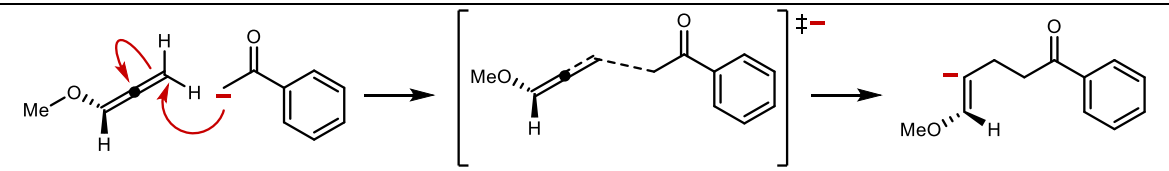
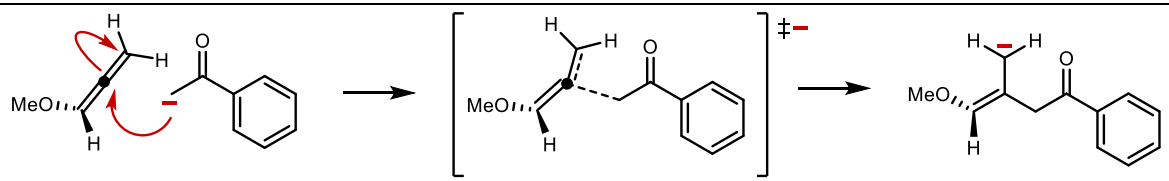
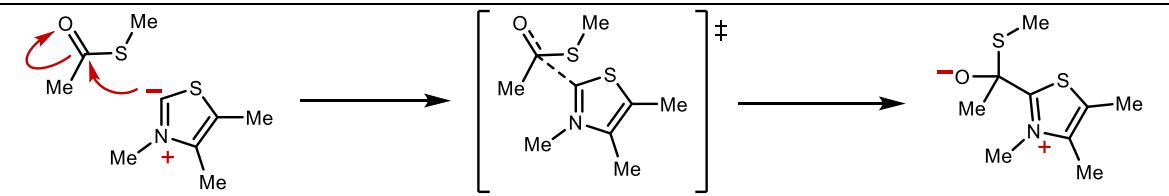
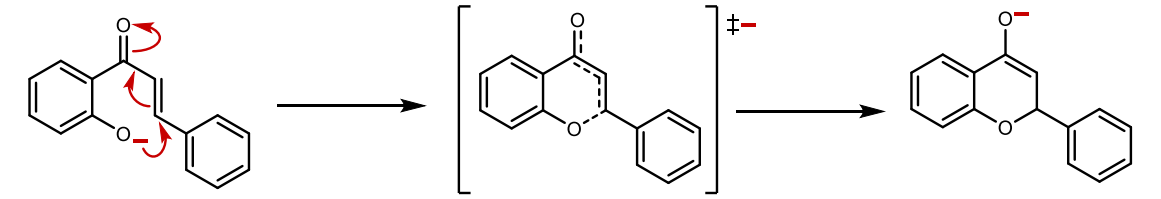
13		12.46	18.94	-6.48
14		32.38	-2.33	34.71
15		18.15	2.87	15.27

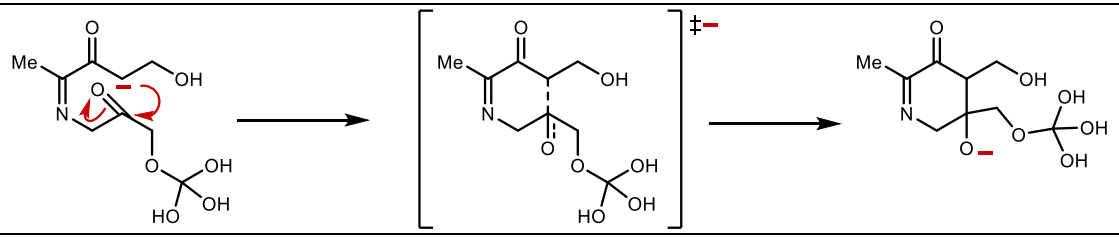
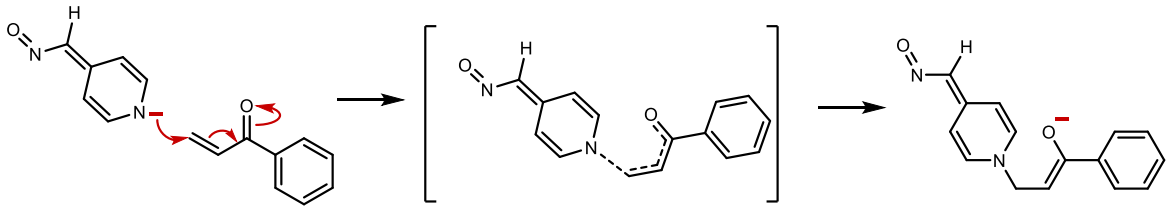
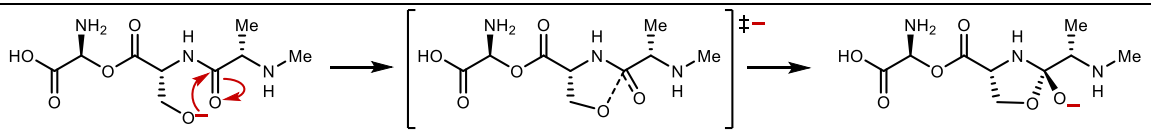
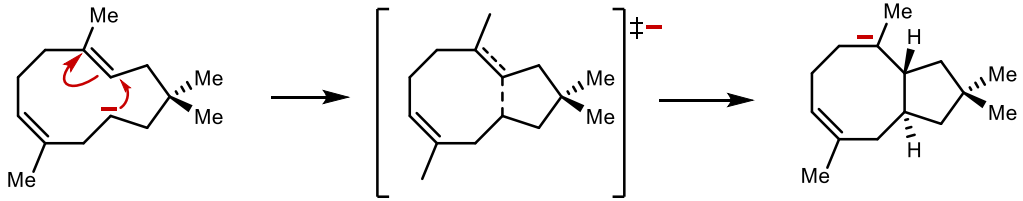
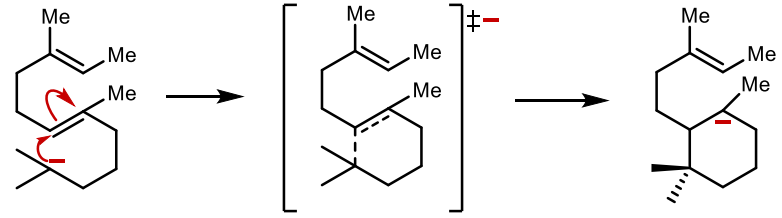
IX. Nucleophilic addition

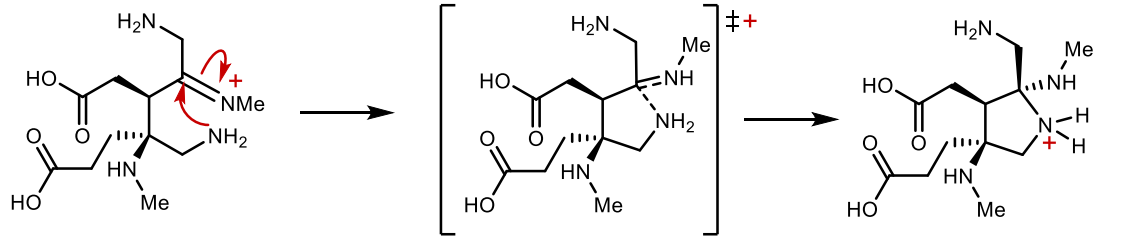
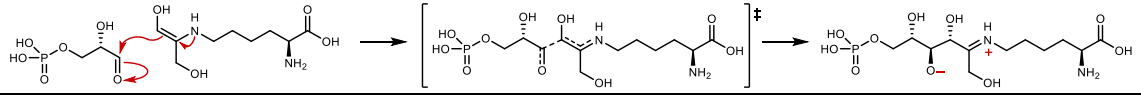
#	Mechanism	Forward barrier height (in	Reverse barrier height	Reaction energy (in

		kcal/mol)	(in kcal/mol)	kcal/mol)
1		-0.94	4.81	-5.76
2		-4.35	6.35	-10.71
3		20.11	29.26	-9.15
4		17.01	24.61	-7.59
5		18.75	26.00	-7.24
6		7.22	32.29	-25.06
7		2.72	17.07	-14.35

8		1.90	15.44	-13.54
9		7.30	33.00	-25.70
10		0.22	7.33	-7.11
11		31.22	14.12	17.10
12		13.77	0.34	13.43
13		7.18	9.50	-2.31

14		4.89	13.69	-8.80
15		5.42	8.25	-2.83
16		3.82	12.73	-8.92
17		9.95	30.33	-20.38
18		6.92	24.11	-17.19
19		20.06	9.65	10.41

20		1.46	11.03	-9.57
21		1.23	11.93	-10.69
22		12.21	3.51	8.69
23		6.35	13.38	-7.03
24		7.58	22.45	-14.87

25		3.76	8.69	-4.93
26		6.41	5.53	0.88