Supporting Information

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

Viki Kumar Prasad¹, Zhipeng Pei¹, Simon Edelmann¹, Alberto Otero-de-la-Roza², and Gino A. DiLabio¹

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

¹ Department of Chemistry, Irving K. Barber Faculty of Science, University of British Columbia, 3247 University Way, Kelowna, British Columbia, Canada V1V 1V7

² Departmento de Química Física y Analítica, Facultad de Química, Universidad de Oviedo, MALTA Consolider Team, 33006 Oviedo, Spain

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	Me S OH Me S OH	-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	$\left[\begin{array}{c} \begin{array}{c} \\ \\ \end{array}\right]^{\ddagger \bullet} \\ \end{array}$	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	HO	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	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.01	19.72	-19.71
47		7.47	58.28	-50.81
48	HO H	0.37	22.46	-22.09

II. Pericyclic

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

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

5	THE CONTRACTOR OF THE CONTRACT	26.57	93.72	-67.15
6		26.77	62.05	-35.27
7	HO Me	19.07	39.40	-20.32
8		12.20	36.77	-24.57
9	→ [→] [‡] → H H H H H H H H H H H H H H H H H H	17.83	47.85	-30.02

10	$- \left[\begin{array}{c} \\ \\ \\ \end{array} \right]^{\ddagger} - \left[\begin{array}{c} \\ \\ \\ \end{array} \right]^{H}$	19.75	50.92	-31.17
11	# H H H H H H H H H H H H H H H H H H H	23.08	45.70	-22.62
12		24.51	44.87	-20.36
13		24.90	60.92	-36.03
14	#- H N N N N N N N N N N N N N N N N N N	21.97	60.48	-38.51
15	MeO OH MeO OH H MeO H H OH MeO MeO O	25.29	60.68	-35.39

16	MeO OH ME	23.43	53.32	-29.89
17	MeO	15.27	59.46	-44.18
18	MeO	19.86	70.40	-50.54
19	Me M	22.04	59.33	-37.29
20	Me Me Me Me H Me NH	19.10	56.89	-37.79

21		12.40	62.14	-49.74
22		8.83	68.85	-60.01
23	Me Me Me Me Me	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	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	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	# H H H H H H H H H H H H H H H H H H H	37.42	39.32	-1.90
40	MeOOC S—OH	14.26	27.77	-13.51
41	MeOOC HN—Me MeOOC HN—Me MeOOC HN—Me	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	$\longrightarrow \left[\begin{array}{c} \downarrow \\ \downarrow \downarrow \\ \downarrow \downarrow \downarrow \downarrow \\ \downarrow \downarrow \downarrow \downarrow \\ \downarrow \downarrow \downarrow \downarrow \downarrow \\ \downarrow \downarrow \downarrow \downarrow \downarrow \\ \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \\ \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \\ \downarrow \downarrow$	16.98	59.46	-42.48
46	# H H Me	26.48	51.36	-24.88

47	The second secon	-1.34	88.51	-89.85
48		1.98	86.44	-84.47
49		13.95	47.20	-33.24
50	Me (3+2) Me (3+2) Me (3+2)	18.44	35.48	-17.04

51	Me (3+2) Me (3+2) Me (3+2)	-1.95	24.26	-26.21
52	Me Me Me Me Me Me Me Me	12.39	36.11	-23.72
53	# # # # # # # # # # # # # # # # # # #	10.45	35.89	-25.44
54	# Me	-0.12	26.38	-26.50

55	Me Me N N N N N N N N N N N N N N N N N	12.65	52.78	-40.12
56	Me Me Me Me N N N N N N N N N N N N N N	11.60	91.82	-80.21
57	Me M	8.10	84.96	-76.87
58	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	15.43	68.29	-52.86
59	N—Me [3+2] Me Me Me Me Me	15.30	67.99	-52.69
60	Me M	5.93	86.94	-81.00

61	Me M	0.41	56.60	-56.19
62	Me M	3.87	58.42	-54.55
63	[3+2]	16.87	41.50	-24.63
64	[3+2] Me N + Me N +	5.38	50.91	-45.54
65	[3+2] Me Me Me Me Me Me Me Me Me M	8.08	56.87	-48.79
66	[3+2] Me N Me Me	6.79	55.77	-48.98

67	F OME	6.93	34.09	-27.16
68	F [3+2] N F [3+2] N N F N N F N N N N N N N N N N N N N	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	[3+2] H (3+2) (3+2)	10.06	45.53	-35.47

74	HN-N+	[3+2]	‡+	→	The state of the s	27.86	26.23	1.63
75	H H	[3+2] ➤	‡+		H. H. M.	9.79	41.83	-32.04
76	HN- N+	[3+2]	‡+		\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\	20.35	37.37	-17.02
77	H N N	[3+2]	#+ N N N N N N N N N N N N N N N N N N N			6.99	46.28	-39.30

78	HN- N+	[3+2]	#+ H N N N N N N N N N N N N N N N N N N		H H N H	19.13	38.27	-19.14
79	N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-	[3+2]		~		1.94	42.25	-40.31
80	HN-N+	[3+2]	‡+		N H	28.38	41.25	-12.87
81	Me N	[3+2]	Me N N N N N N N N N N N N N N N N N N N		Me,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	11.14	43.06	-31.92
82	Me HN-	[3+2]	#+		Me, H	10.61	37.95	-27.34

83	Electrocyclic HO	17.65	44.98	-27.33
84	Electrocyclic H Me Electrocyclic H Me	26.68	50.51	-23.83
85	Electrocyclic H Me	30.66	51.43	-20.78
86	Electrocyclic S Me	27.74	52.70	-24.96

87	Electrocyclic Ne Signature Me	30.73	53.65	-22.91
88	Electrocyclic MeO MeO MeO MeO MeO MeO MeO Me	24.91	51.36	-26.45
89	Electrocyclic MeO MeO MeO MeO MeO MeO MeO Me	28.62	52.88	-24.26
90	Electrocyclic Me Me Me Me Me Me Me Me Me	27.43	52.17	-24.74

91	Electrocyclic Me Me Me Me	31.00	54.55	-23.55
92	Electrocyclic Me ₃ Si Me Me ₃ Si Me	23.66	53.48	-29.82
93	Electrocyclic Me ₃ Si Me Me ₃ Si Me	28.69	54.95	-26.26
94	Electrocyclic Me Electrocyclic Me	25.60	54.46	-28.86

95	H N Elect	trocyclic	‡	H N Me	28.02	55.88	-27.86
96	Electrocy	yclic +-		о -	11.39	15.19	-3.80
97	HO Electroc	tyclic H		H	43.52	21.76	21.76
98	Me Electro	cyclic ## Me ## ## Me ## ## Me		~~~	33.08	45.42	-12.34
99	Me Electro	ocyclic Me			44.28	54.35	-10.07
100	H Ele	ectrocyclic		N H H	36.07	19.79	16.28

101	Electrocyclic HHHH	41.80	45.81	-4.01
102	Electrocyclic The state of the	38.73	36.55	2.18
103	Electrocyclic #	36.24	36.68	-0.44
104	H Electrocyclic	13.10	40.49	-27.39
105	# Electrocyclic	48.25	42.24	6.01
106	NC CN NC CN NC CN NC CN NC Me Me Me	11.53	29.79	-18.26

107	NC CN CN CN CN CN CN H	11.53	36.38	-24.85
108	NC CN TO THE ME ME ME ME ME ME ME	11.53	35.01	-23.48
109	$\begin{bmatrix} F & & & & & & & & & & & & & & & & & & $	43.45	50.58	-7.13
110	[3,3] 	43.45	57.37	-13.92
111	[3,3] † H H H H H	36.96	51.17	-14.22
112	MeO ₂ C CN Me Me Me Me Me Me Me	12.84	31.12	-18.28

113	MeO ₂ C CN CN CN H	12.84	36.75	-23.91
114	MeO ₂ C CN	12.84	37.94	-25.10
115	NC CO ₂ Me	11.83	30.11	-18.28
116	$\begin{array}{c} \text{NC} \\ \text{CO}_2\text{Me} \\ \text{Me} \end{array}$	11.83	35.81	-23.98
117	NC CO ₂ Me NC CO ₂ Me NC CO ₂ Me NC Me Me Me	11.83	40.21	-28.38

118	Me Me HO OH EXO-[4+2] Me Me HO OH Me Me HO OH	22.52	41.61	-19.09
119	Me Me HO OH EXO-[6+4] Me Me HO OH Me Me HO OH	18.91	47.58	-28.67
120	endo-[4+2] Me Me HO OH Me Me HO OH Me Me HO OH	16.79	43.12	-26.33
121	endo-[6+4] Me Me Me Me Me Me Me Me Me M	16.79	54.33	-37.54
122	HO H	19.29	37.46	-18.17

123	HOW HO (6+4) HOW	19.29	41.95	-22.66
124	[4+2] \$\frac{\frac{1}{H}}{\frac{1}{H}}\frac{1}{H}\$	21.68	46.02	-24.34
125		21.68	47.32	-25.64
126	Me Me HO OH [3,3]-Cope Me Me HO OH HO OH	20.25	26.19	-5.95
127	Me Me HO OH (3,3)-Cope Me HO OH Me HO OH	20.95	32.16	-11.21

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

133	NC N	33.84	44.83	-10.99
134	[3,3]-Claisen H	32.08	49.61	-17.53
135	HO OH (3,3]-Claisen HO OH HO OH	28.35	44.42	-16.07
136	[3,3]-Claisen	29.79	45.83	-16.04
137	OH (3,3)-Claisen OH OH OH	25.98	41.35	-15.37
138	[3,3]-Claisen Me [3,3]-Claisen Me Me	31.94	28.09	3.85

139	[3,3]-Claisen [3,3]-Claisen	34.37	50.96	-16.59
140	[2+2+2] [‡]	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	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	45.08	13.69	31.39
3		15.39	4.08	11.31

4		15.91	13.98	1.93
5	The second secon	4.23	4.65	-0.42
6	The state of the s	-1.35	1.80	-3.16
7		42.38	17.76	24.62
8		42.36	17.42	24.94

9	$\begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\ddagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\ddagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \end{bmatrix}^{\dagger + \bullet} \end{bmatrix}^{\dagger + \bullet} \begin{bmatrix} \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \end{bmatrix}^{\dagger + \bullet} \end{bmatrix}^{\dagger + \bullet} \end{bmatrix}^{\bullet} \begin{bmatrix} \vdots \\ \vdots \end{bmatrix}^{\dagger + \bullet} \end{bmatrix}^{\bullet} \end{bmatrix}^{\dagger + \bullet} \end{bmatrix}^{\bullet} \end{bmatrix}^{\dagger + \bullet} \end{bmatrix}^{\bullet} \end{bmatrix}^{\dagger + \bullet} \end{bmatrix}^{\dagger +$	-67.71	-62.16	-5.55
10	$\begin{bmatrix} & & & & & & & & & & & & & & & & & & &$	41.34	7.92	33.42
11		0.50	5.21	-4.70
12	NO ₂ H NO ₂ NO ₂ NO ₂	43.97	20.13	23.84
13	$\begin{bmatrix} C \\ C \\ C \end{bmatrix} = \begin{bmatrix} C \\ C \\ C \end{bmatrix}$	3.23	11.60	-8.37

14	$\begin{bmatrix} & & & & & & & & & & & & & & & & & & &$	3.48	11.59	-8.11
15	Me Me	41.94	16.76	25.18
16	HO_2C S F N HO_2C S F N	77.42	81.94	-4.52
17	$\begin{bmatrix} C_1 & \cdots & $	9.22	14.73	-5.52
18	CI Me Me	2.95	11.10	-8.15

19	S. F. N.	-0.68	3.87	-4.54
20	OMe CI OME OME	2.41	10.55	-8.14
21	CI CI H	12.96	23.34	-10.38
22	CI S S S S S S S S S S S S S S S S S S S	10.47	18.30	-7.83
23	CI CI Me O	18.66	10.80	7.85
24	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	41.74	8.44	33.31

25		26.26	34.43	-8.17
26	MeO NeO NeO NeO NeO NeO NeO NeO NeO NeO N	5.84	26.05	-20.21
27	$\begin{array}{c} \begin{array}{c} \begin{array}{c} \\ \\ \\ \end{array} \end{array} \\ \begin{array}{c} \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \end{array} \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	53.90	10.31	43.59
28	$\begin{array}{c} \begin{array}{c} \\ \\ \\ \end{array} \end{array} \longrightarrow \begin{array}{c} \\ \\ \end{array} \end{array} \longrightarrow \begin{array}{c} \\ \\ \\ \end{array} \longrightarrow \begin{array}{c} \\ \\ \end{array} \longrightarrow \begin{array}{c} \\ \\ \\ \\ \\ \end{array} \longrightarrow \begin{array}{c} \\ \\\\ \\ \end{array} \longrightarrow \begin{array}{c} \\ \\\\ \\ \end{array} \longrightarrow \begin{array}{c} \\\\ \\\\ \\\\ \end{array} \longrightarrow \begin{array}{c} \\\\ \\\\ \\\\ \end{array} \longrightarrow \begin{array}{c} \\$	56.10	11.62	44.48
29	OMe OMe	26.77	1.36	25.42

30	The state of the s	14.71	34.21	-19.50
31		51.57	12.40	39.17
32		52.03	12.75	39.29
33	NS OME CI CI CI CI CI CI CI CI CI C	6.22	25.32	-19.10

34	OMe CI OMe OMe	12.79	22.60	-9.81
35	\$\circ{\circ}{\circ}\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\	16.87	8.88	7.99
36	CI NMe	16.65	8.64	8.02
37	Me Me Me Me	8.00	47.09	-39.09

38	Me Me OMe OMe OMe	10.67	31.39	-20.71
39	* · · · · · · · · · · · · · · · · · · ·	11.00	24.57	-13.57
40	H CC	10.04	20.95	-10.91
41	$\begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	7.96	35.40	-27.43
42		21.33	10.29	11.03

43	F Me	THE SHAPE OF THE S	F Me	46.53	-3.19	49.72
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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	S. Me S. Me HS. Me	4.80	4.58	0.22

4		16.44	12.67	3.77
5	OH HOME OH HOME HOME HOME HOME	13.93	0.17	13.76
6	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	6.44	2.44	4.01
7	$\begin{array}{c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$	4.00	4.61	-0.61
8	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	12.36	21.11	-8.75
9	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	17.45	17.15	0.30

10	0 + N + N + N + N + N + N + N + N + N +	$\begin{bmatrix} & & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & $	0 + N + N + N + N + N + N + N + N + N +	16.29	17.84	-1.56
11	O H NH ₂	+ NH ₂ + NH ₂	0 + N + N + N + N + N + N + N + N + N +	34.10	12.51	21.59
12	NH ₂	** O NH2 N NH2 N NH2	0 + N + N + N + N + N + N + N + N + N +	12.97	15.74	-2.77
13	NH ₂ O N O N O N O N O N O N O N O N O N O	$\begin{bmatrix} & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & \\ & & & & \\ & & \\ & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ $	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	30.51	19.78	10.73
14	$0 \longrightarrow H \longrightarrow NH_2$ $0 \longrightarrow N \longrightarrow NH_2$ $0 \longrightarrow N \longrightarrow NH_2$		$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	27.87	18.89	8.98

15	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	23.98	16.31	7.67
16	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	14.52	13.49	1.02
17	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	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	MeO OH MeO OH MeO OH Me Me-SH	13.47	6.04	7.43
23	Mes OH Mes OH Mes OH Me Me SH	11.29	6.86	4.43
24	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	18.51	15.80	2.71
25	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	14.12	12.73	1.39

26	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	14.83	20.51	-5.68
27	$\begin{array}{c} & & & \\ & &$	13.20	18.89	-5.69
28	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	10.10	8.71	1.38
29	MeS NH ₂ MeS NH ₂ MeS NH ₂ Me NH ₂	11.34	5.16	6.19
30	# # # # # # # # # # # # # # # # # # #	3.48	35.56	-32.09

31	$\begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}^{\sharp \bullet} $	10.13	11.96	-1.83
32		29.28	18.90	10.38
33		30.75	20.43	10.31
34	$\left[\bigcirc^{\circ}_{H_{s}} \bigcirc^{\circ} \right]^{\ddagger \bullet} \longrightarrow \left[\bigcirc^{\circ}_{H_{s}} \bigcirc^{\circ} \right]$	31.27	20.17	11.10
35	PH S	12.23	7.14	5.09
36		21.30	19.97	1.33
37		21.57	19.91	1.66

38	HO Me HO Me	6.68	17.92	-11.24
39	HO Me HS Me	13.24	3.28	9.96
40	HO HO HS OH	27.97	19.50	8.47
41		18.43	18.66	-0.24
42	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	12.15	16.10	-3.95
43	NST - [N-H-10] **	13.68	18.76	-5.08
44	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	22.68	15.83	6.85

45	$ \longrightarrow $	7.33	22.38	-15.05
46	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	11.46	6.32	5.14
47		5.60	11.33	-5.72
48	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	5.93	11.61	-5.68
49	(transoid)	12.58	18.27	-5.69

50	HO Me HO Me	12.73	18.65	-5.92
51	$\begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	11.99	-0.34	12.34
52	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	4.82	9.92	-5.10
53		12.35	7.34	5.02
54	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	19.94	2.71	17.22

55	$\begin{bmatrix} O & O & H & O & H & O & H & O & H & O & H & O & H & O & H & O & O$	6.94	12.94	-6.00
56		12.91	18.25	-5.35
57		14.38	12.67	1.71
58	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	12.42	2.71	9.71
59	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	5.02	10.66	-5.64

60	О—Н О—Н О— О— Н— О— О— Н— О— О— Н— О— О— Н— О— О— О— Н— О—	6.68	12.22	-5.55
61		11.91	19.00	-7.09
62	EH CHANGE TO THE CHANGE THE CHANG	25.06	34.50	-9.44
63	$\begin{bmatrix} & & & & & & & & & & & & & & & & & & &$	12.43	20.69	-8.26

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

69	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	11.97	19.19	-7.22
70	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	5.16	19.31	-14.15
71	$\begin{bmatrix} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	16.88	8.08	8.80
72		11.57	19.48	-7.91
73	$\begin{array}{c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$	30.00	12.73	17.28

74	OMe H-OOLING	14.37	7.11	7.26
75	Me OMe OMe OMe OMe	3.66	6.58	-2.91
76	*•	13.85	18.38	-4.54
77		12.93	5.40	7.53
78	The state of the s	13.54	29.68	-16.14

79	NH2 NH2 NH2 NH2 NH2 NH2 NH2 NH2 NH4	18.60	11.78	6.82
80	$\begin{array}{c} O \\ H \\ Me_2N \\$	1.14	15.53	-14.39
81	$\begin{bmatrix} O & & & & & & & & & & & & & & & & & & $	-0.11	14.46	-14.57
82	NH2 NH2 NH2 NH2 NH2 NH2 NH2 NH2 NH2 NH2	16.39	25.48	-9.09

83	NH ₂	15.83	25.03	-9.20
84		11.86	18.34	-6.48
85	$\begin{array}{c} NH_2 \\ NH_2 \\$	15.58	27.22	-11.63
86	OME OME OME OME OME	15.31	20.29	-4.98

87	$\begin{array}{c} O \\ Me_2N - P \\ Me_2N -$	3.84	18.14	-14.29
88	$\begin{array}{c} \text{MeO}_2\text{C} \\ \text{HO} \\ $	33.51	40.20	-6.69
89	$\begin{array}{c} NH_2 \\ NH$	13.47	22.19	-8.72
90	$\begin{array}{c} & & & \\ & &$	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	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.85	6.50	-5.65
2	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	22.01	23.81	-1.79
3		14.75	18.57	-3.82
4	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	5.49	25.25	-19.76
5	## ## ## ## ## ## ## ## ## ##	1.51	15.07	-13.56

6	$\begin{array}{c} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \end{array} \end{array} \begin{array}{c} \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	10.00	11.94	-1.94
7		16.81	-0.50	17.31
8	Me M	1.04	8.07	-7.03
9	##	-2.46	8.58	-11.04

10	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	14.88	5.63	9.25
11	HN NH OH HN	14.99	-4.21	19.20
12	## ## ## ## ## ## ## ## ## ## ## ## ##	5.79	20.17	-14.38

13	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	17.06	10.36	6.70
14		7.58	16.78	-9.21
15		13.40	18.28	-4.88

16	CI HO	16.06	18.89	-2.83
17	THE STATE OF THE S	14.02	3.43	10.58
18	HO, OH HO	20.63	-96.26	116.88

19	$CF_{3} \longrightarrow \begin{pmatrix} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	12.54	14.68	-2.14
20	## OF THE	5.38	16.10	-10.72
21	MeO	3.60	19.57	-15.96

22	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	21.77	13.81	7.95
23	Me H O H O H O H O H O H O H O H O H O H	12.53	21.75	-9.23
24	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	14.19	5.33	8.86

25	MeO HO	9.50	23.84	-14.33
26	Me M	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	# + O + H O - Z + H O O + H O O O O O O O O O O O O O O	4.56	19.64	-15.08
33	Me Me H O H O H O H O H O H O H O H O H O H	1.97	19.13	-17.16

34	## ##	1.14	20.97	-19.83
35	MeO HN MeO HN MeO HN MeO Neo	0.74	20.87	-20.12
36	OMe H Me Me Me Me Me Me Me Me M	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	MeO	-1.16	7.89	-9.05
41	Me-o H H H H H H H H H H H H H	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	Me Me Me Me Me Me Me Me	15.72	10.68	5.04
2	H H H H H H H H H H H H H H H H H H H	2.24	28.35	-26.12
3	Me Si Me Me Me Me Me Me	4.81	25.87	-21.06
4	Me Si Me Me Me Me Me Me	4.62	29.54	-24.91
5	$ \begin{array}{c} C_{CI} \\ C_{CI} \\ B \end{array} $ $ \begin{array}{c} C_{CI} \\ C_{CI} \\ C_{CI} \end{array} $ $ \begin{array}{c} C_{CI} \\ C_{CI} \end{array} $	14.75	-1.06	15.80

6	Me Si Me Me Me Me Me	4.04	19.53	-15.48
7	Me Me Me Me Me Me Me	3.89	19.12	-15.24
8	Me Si Me Me Me Me Me	3.36	21.63	-18.27
9	#• We Si Me Me Me Me	5.78	21.11	-15.32
10	H-B O O O O O O O O O O O O O	3.49	52.87	-49.38

11	$\begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	1.31	50.23	-48.92
12		20.32	14.77	5.54
13	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	11.81	16.75	-4.95
14	□ B □ B □ B □ B □ B □ B □ B □ B □ B □ B	13.62	10.81	2.80
15	$\begin{array}{c} \vdots \\ \vdots \\ \vdots \\ \vdots \\ \end{array}$	1.33	27.06	-25.73

16	#	18.86	53.61	-34.76
17		20.99	54.73	-33.74
18	N-Me N-Me SiMe ₃ SiMe ₃ H SiMe Me Me Me Me Me	7.60	15.41	-7.82
19	Me ₃ Si SiMe ₃	4.39	13.75	-9.36

	The state of the s			1
20	Me ₃ Si SiMe ₃ SiMe ₃ SiMe ₃ SiMe ₃ Me ₃ Si SiMe ₃	4.00	14.18	-10.18
21	Me ₃ Si SiMe ₃ SiMe ₃ SiMe ₃ SiMe ₃ SiMe ₃	-1.69	2.54	-4.23
22	$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Si} \\ \text{SiMe}_3 \\ \text{SiMe}_3 \\ \end{array} \\ \begin{array}{c} \text{Me} \\ \text{Me} \\ \text{Me}_3 \\ \text{Si} \\ \text{SiMe}_3 \\ \text{SiMe}_3 \\ \end{array} \\ \begin{array}{c} \text{Me} \\ \text{Me}_3 \\ \text{SiMe}_3 \\ \text{SiMe}_3 \\ \end{array} \\ \begin{array}{c} \text{Me} \\ \text{Me}_3 \\ \text{SiMe}_3 \\ \text{SiMe}_3 \\ \end{array}$	2.98	12.74	-9.76
23		1.07	26.52	-25.45
24	SiMe ₃ H H OMe H OMe H OMe	7.84	61.88	-54.04

25	Me ₃ Si B H OMe To Me	8.11	56.40	-48.28
26	H OMe H OMe H H B Me ₃ Si Me ₃ Si	8.68	55.38	-46.70
27	# SiMe ₃ B O O O O O O O O O O O O O O O O O O	21.41	15.51	5.90
28	SiMe ₃ BO BO BO	20.08	15.35	4.73

29	SiMe ₃ B SiMe ₃ B SiMe ₃ B SiMe ₃ B H H	18.58	20.49	-1.91
30	# SiMe ₃ B SiMe ₃ H O H O H O H O H O H O H O H O H O H	13.88	15.61	-1.73
31		2.21	13.33	-11.12
32	Me ₃ Si SiMe ₃ SiMe ₃ SiMe ₃ SiMe ₃ SiMe ₃	2.61	13.62	-11.00
33	Me ₃ Si SiMe ₃ SiMe ₃ SiMe ₃ CI H Me ₃ Si SiMe ₃ SiMe ₃ SiMe ₃	1.43	17.74	-16.31

34	SiMe ₃ Si-SiMe ₃ Si-SiMe ₃ Si-SiMe ₃ Si-SiMe ₃ SiMe ₃	1.41	13.67	-12.26
35	Me ₃ Si SiMe ₃ SiMe ₃ SiMe ₃ SiMe ₃	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	$\begin{array}{c} \downarrow \\ \downarrow $	37.38	37.14	0.24

4	Me O H O H O H O H O H O H O H O H O H O	12.73	0.08	12.64
5	# P Me Me Me Me Me	11.94	71.12	-59.18
6	HO, CO_2H	30.60	3.14	27.46
7	$\begin{array}{c} \text{Me} \\ \text{E} \\ \text{CO}_2\text{H} \\ \text{OH} \\ $	3.08	32.75	-29.68
8	$\begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	-31.63	-30.51	-1.12

9	+ - - - - - - - - - - - - -	4.73	5.64	-0.91
10	# H H H H H H H H H H H H H H H H H H H	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	$\begin{bmatrix} & & & & & & & & & & & & & & & & & & &$	-3.21	15.07	-18.28
2	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	14.28	-0.05	14.33
3	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	13.63	28.04	-14.41

4	$\begin{array}{c c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$	23.74	29.96	-6.22
5	$\begin{array}{c} O \\ O $	-4.00	4.56	-8.56
6	$\begin{array}{c} OH \\ OH $	20.98	10.61	10.37
7	$\begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	9.10	11.86	-2.76
8	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	17.89	15.80	2.09

9	HO HO HO OH	3.08	-5.70	8.78
10	$\begin{array}{c} & & & \\ & &$	3.14	6.09	-2.95
11	$\begin{array}{c} \begin{array}{c} \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	-2.99	19.74	-22.72
12	HO, OH HO	14.76	6.60	8.16

13	Me Me Me Me Me Me	12.46	18.94	-6.48
14	HO HO HO HO HO ME ME ME ME ME	32.38	-2.33	34.71
15	$\begin{array}{c} HO \\ H_2N \\ HO \\ \end{array}$ $\begin{array}{c} HO \\ H_2N \\ \end{array}$ $\begin{array}{c} HO \\ HO \\ \end{array}$	18.15	2.87	15.27

IX. Nucleophilic addition

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

		kcal/mol)	(in kcal/mol)	kcal/mol)
1		-0.94	4.81	-5.76
2		-4.35	6.35	-10.71
3	$\begin{bmatrix} & & & \\ & $	20.11	29.26	-9.15
4	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	17.01	24.61	-7.59
5	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	18.75	26.00	-7.24
6		7.22	32.29	-25.06
7	MeO MeO MeO MeO	2.72	17.07	-14.35

8	MeO, H	1.90	15.44	-13.54
9	MeOH MeOH MeOH MeOH	7.30	33.00	-25.70
10	HO,	0.22	7.33	-7.11
11	H Me	31.22	14.12	17.10
12	Me M	13.77	0.34	13.43
13	Me OH	7.18	9.50	-2.31

14	$\begin{array}{c c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$	4.89	13.69	-8.80
15	MeO	5.42	8.25	-2.83
16	MeO,, Heo, Heo, Heo, Heo, Heo, Heo, Heo, He	3.82	12.73	-8.92
17	MeO,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	9.95	30.33	-20.38
18	Me Me Me Me Me Me Me Me	6.92	24.11	-17.19
19		20.06	9.65	10.41

20	Me HOOH OH HOOH OH OH OH OH	1.46	11.03	-9.57
21		1.23	11.93	-10.69
22	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	12.21	3.51	8.69
23	Me Me Me Me Me Me Me Me	6.35	13.38	-7.03
24	Me Me Me Me Me Me	7.58	22.45	-14.87

25	HO NMe NH ₂	HO Me HO Me HO Me HO Me HO Me HO Me HO Me	3.76	8.69	-4.93
26	$\begin{array}{cccccccccccccccccccccccccccccccccccc$		6.41	5.53	0.88