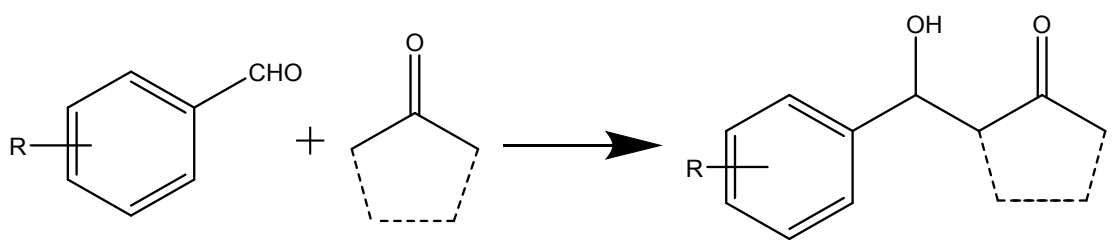
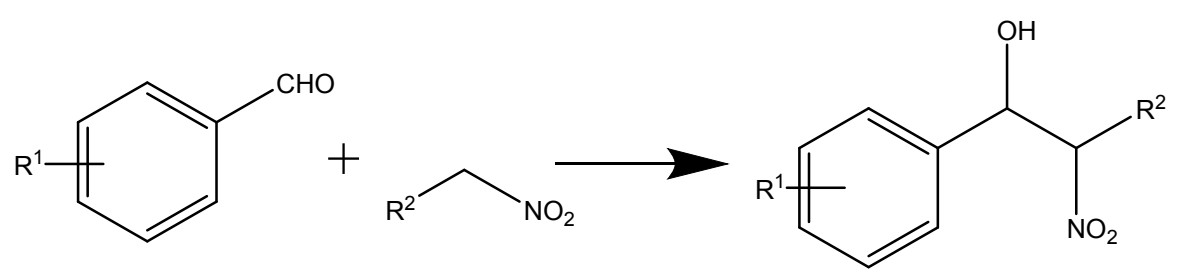
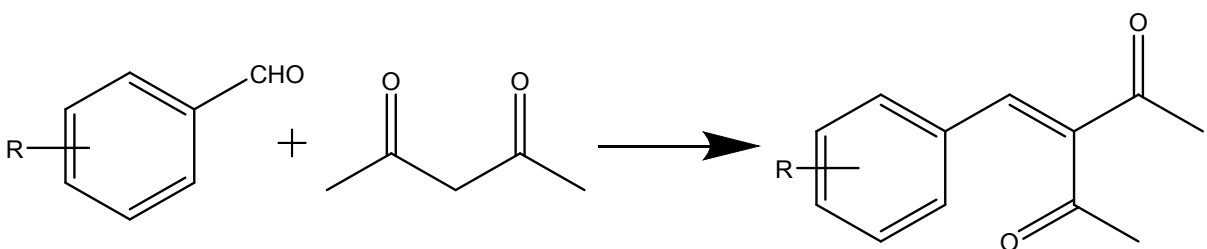
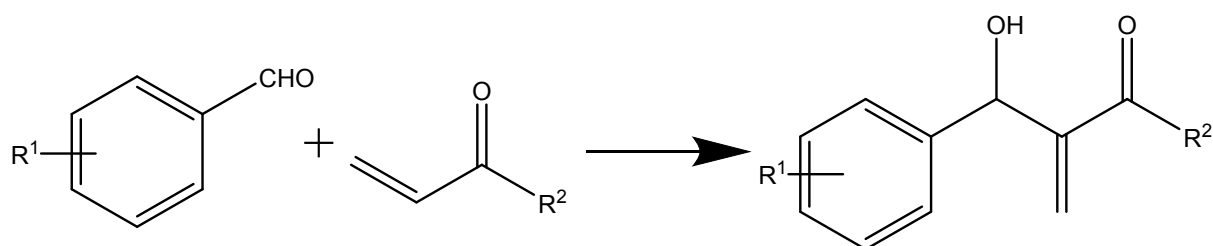


Table S1 The structure of two substrates in different reactions

		
No.1-29		
No.	Substrate 1	Substrate 2
1-25	R=4-NO ₂	Acetone
26	R=2-NO ₂	Acetone
27	R=4-NO ₂	Cyclopentanone
28	R=3-NO ₂	Cyclopentanone
29	R=4-CN	Cyclopentanone

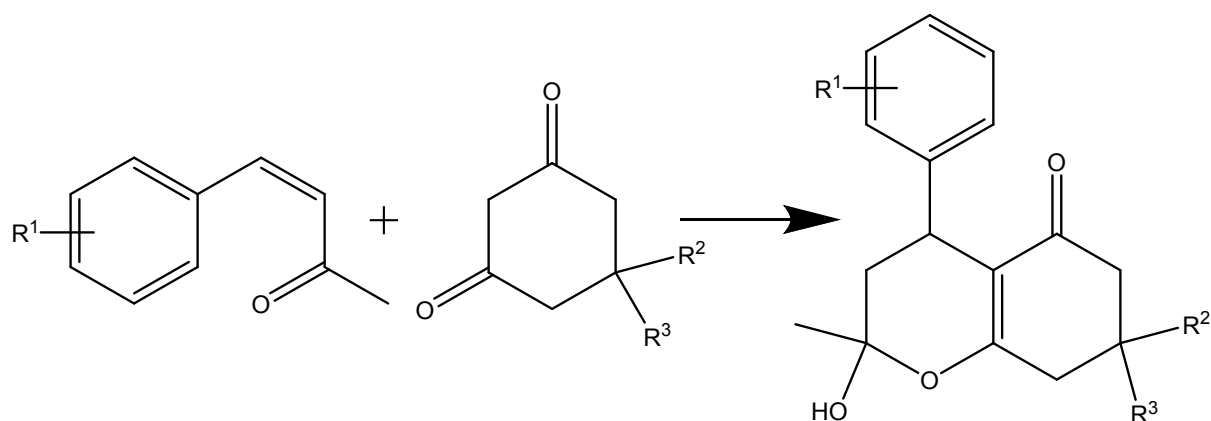
		
No.30-53		
No.	Substrate 1	Substrate 2
30-49	R¹=4-NO ₂	R²=H
50	R¹=3-NO ₂	R²=H
51	R¹=2-NO ₂	R²=H
52	R¹=4-NO ₂	R²=Me
53	R¹=3-NO ₂	R²=Me

		
No.54-75		
No.	Substrate 1	Substrate 2
54-70	R=4-NO ₂	Acetylacetone
71	R=3-NO ₂	Acetylacetone
72	R=4-CH ₃	Acetylacetone
73	R=4-F	Acetylacetone
74	R=4-Cl	Acetylacetone
75	R=2-Cl	Acetylacetone



No.76-101

No.	Substrate 1	Substrate 2
76-93	R ¹ =4-NO ₂	R ² =Me
94	R ¹ =3-NO ₂	R ² =Me
95	R ¹ =2-NO ₂	R ² =Me
96	R ¹ =4-CN	R ² =Me
97	R ¹ =4-NO ₂	R ² =OMe
98	R ¹ =3-NO ₂	R ² =OMe
99	R ¹ =2-NO ₂	R ² =OMe
100	R ¹ =4-NO ₂	R ² =OEt
101	R ¹ =3-NO ₂	R ² =OEt



No.102-125

No.	Substrate 1	Substrate 2
102-115	R ¹ =4-NO ₂	R ² =H; R ³ =H
116	R ¹ =3-NO ₂	R ² =H; R ³ =H
117	R ¹ =4-H	R ² =H; R ³ =H
118	R ¹ =4-NO ₂	R ² =H; R ³ =H
119	R ¹ =3-NO ₂	R ² =Me; R ³ =Me
120	R ¹ =2-NO ₂	R ² =Me; R ³ =Me
121	R ¹ =4-F	R ² =Me; R ³ =Me
122	R ¹ =4-Me	R ² =Me; R ³ =Me
123	R ¹ =4-MeO	R ² =Me; R ³ =Me
124	R ¹ =2-Cl	R ² =Me; R ³ =Me
125	R ¹ =2-F	R ² =Me; R ³ =Me

Table S2 Quantum chemical descriptors of the substrates

No.	Substrate 1				Substrate 2			
	S^1_{COSMO}	V^1_{COSMO}	E^1_{HOMO}	E^1_{LUMO}	S^2_{COSMO}	V^2_{COSMO}	E^2_{HOMO}	E^2_{LUMO}
1	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
2	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
3	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
4	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
5	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
6	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
7	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
8	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
9	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
10	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
11	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
12	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
13	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
14	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
15	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
16	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
17	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
18	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
19	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
20	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
21	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
22	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
23	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
24	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
25	169.35	165.06	-10.897	-1.907	100.78	83.79	-10.233	0.922
26	167.32	167.76	-10.727	-1.431	100.78	83.79	-10.233	0.922
27	169.35	165.06	-10.897	-1.907	124.68	113.08	-10.112	0.958
28	169.73	165.68	-10.801	-1.667	124.68	113.08	-10.112	0.958
29	166.57	160.49	-10.642	-1.527	124.68	113.08	-10.112	0.958
30	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
31	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
32	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
33	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
34	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
35	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
36	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097

37	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
38	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
39	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
40	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
41	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
42	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
43	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
44	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
45	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
46	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
47	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
48	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
49	169.35	165.06	-10.897	-1.907	87.76	69.03	-11.242	-0.097
50	169.9	165.59	-10.841	-1.638	87.76	69.03	-11.242	-0.097
51	165.8	163.33	-10.61	-1.826	87.76	69.03	-11.242	-0.097
52	169.35	165.06	-10.897	-1.907	106.15	89.98	-11.047	0.002
53	169.9	165.59	-10.841	-1.638	106.15	89.98	-11.047	0.002
54	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
55	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
56	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
57	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
58	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
59	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
60	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
61	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
62	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
63	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
64	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
65	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
66	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
67	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
68	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
69	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
70	169.35	165.06	-10.897	-1.907	140.73	129.36	-10.299	0.477
71	169.68	165.24	-10.841	-1.639	140.73	129.36	-10.299	0.477
72	161.26	156.02	-9.81	-0.587	140.73	129.36	-10.299	0.477
73	149.65	142.99	-10.306	-0.956	140.73	129.36	-10.299	0.477
74	161.13	156.62	-10.142	-1.078	140.73	129.36	-10.299	0.477
75	158.78	155.67	-10.166	-1.055	140.73	129.36	-10.299	0.477
76	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183

77	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
78	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
79	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
80	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
81	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
82	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
83	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
84	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
85	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
86	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
87	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
88	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
89	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
90	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
91	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
92	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
93	169.35	165.06	-10.897	-1.907	115.29	99.64	-10.209	-0.183
94	169.73	165.68	-10.801	-1.667	115.29	99.64	-10.209	-0.183
95	167.32	167.76	-10.727	-1.431	115.29	99.64	-10.209	-0.183
96	166.57	160.49	-10.642	-1.527	115.29	99.64	-10.209	-0.183
97	169.35	165.06	-10.897	-1.907	126.69	111.38	-10.892	-0.279
98	169.73	165.68	-10.801	-1.667	126.69	111.38	-10.892	-0.279
99	167.32	167.76	-10.727	-1.431	126.69	111.38	-10.892	-0.279
100	169.35	165.06	-10.897	-1.907	146.78	131.82	-10.823	-0.216
101	169.73	165.68	-10.801	-1.667	146.78	131.82	-10.823	-0.216
102	222.39	220.68	-10.264	-1.865	142.83	136.67	-10.443	0.467
103	222.39	220.68	-10.264	-1.865	142.83	136.67	-10.443	0.467
104	222.39	220.68	-10.264	-1.865	142.83	136.67	-10.443	0.467
105	222.39	220.68	-10.264	-1.865	142.83	136.67	-10.443	0.467
106	222.39	220.68	-10.264	-1.865	142.83	136.67	-10.443	0.467
107	222.39	220.68	-10.264	-1.865	142.83	136.67	-10.443	0.467
108	222.39	220.68	-10.264	-1.865	142.83	136.67	-10.443	0.467
109	222.39	220.68	-10.264	-1.865	142.83	136.67	-10.443	0.467
110	222.39	220.68	-10.264	-1.865	142.83	136.67	-10.443	0.467
111	222.39	220.68	-10.264	-1.865	142.83	136.67	-10.443	0.467
112	222.39	220.68	-10.264	-1.865	142.83	136.67	-10.443	0.467
113	222.39	220.68	-10.264	-1.865	142.83	136.67	-10.443	0.467
114	222.39	220.68	-10.264	-1.865	142.83	136.67	-10.443	0.467
115	222.39	220.68	-10.264	-1.865	142.83	136.67	-10.443	0.467
116	218.47	220.17	-10.124	-1.725	142.83	136.67	-10.443	0.467

117	195.46	190.71	-9.518	-0.87	142.83	136.67	-10.443	0.467
118	222.39	220.68	-10.264	-1.865	142.83	136.67	-10.443	0.467
119	222.75	221.35	-10.186	-1.605	172.96	182.48	-10.366	0.535
120	218.47	220.17	-10.124	-1.725	172.96	182.48	-10.366	0.535
121	202.43	198.66	-9.638	-1.07	172.96	182.48	-10.366	0.535
122	214.17	212.13	-9.247	-0.77	172.96	182.48	-10.366	0.535
123	224.27	223.45	-8.937	-0.714	172.96	182.48	-10.366	0.535
124	211.07	211.2	-9.661	-1.129	172.96	182.48	-10.366	0.535
125	201.24	198.04	-9.689	-1.077	172.96	182.48	-10.366	0.535

Table S3 conditions of reaction

No.	<i>mr</i>	Solvent	Log <i>P</i>	W	<i>c</i>	<i>T</i>	<i>H</i>	Exp. Yield	Pre. Yield
1	15	cyclohexane	3.35	20	1.5	37	168	89	66
2	15	Tetrahydrofuran	0.46	20	1.5	37	168	15	30
3	15	1,4-dioxane	-0.5	20	1.5	37	168	18	23
4	15	Dimethyl formamide	-1.3	20	1.5	37	168	15	21
5	15	tert-butyl methyl ether	0.94	20	1.5	37	168	28	35
6	15	Acetonitrile	-0.33	20	1.5	37	168	50	24
7	15	cyclohexane	3.35	0	1.875	37	168	31	49
8	15	cyclohexane	3.35	5	1.5	37	168	47	49
9	15	cyclohexane	3.35	10	1.6875	37	168	58	58
10	15	cyclohexane	3.35	15	1.59375	37	168	77	62
11	15	cyclohexane	3.35	25	1.40625	37	168	82	69
12	15	cyclohexane	3.35	30	1.3125	37	168	73	72
13	15	cyclohexane	3.35	35	1.21875	37	168	66	75
14	1	cyclohexane	3.35	20	1.5	37	168	21	21
15	5	cyclohexane	3.35	20	1.5	37	168	35	36
16	10	cyclohexane	3.35	20	1.5	37	168	85	82
17	20	cyclohexane	3.35	20	1.5	37	168	87	85
18	25	cyclohexane	3.35	20	1.5	37	168	82	82
19	30	cyclohexane	3.35	20	1.5	37	168	86	84
20	15	cyclohexane	3.35	20	0.5	37	168	10	46
21	15	cyclohexane	3.35	20	1	37	168	44	56
22	15	cyclohexane	3.35	20	1.5	37	168	89	66
23	15	cyclohexane	3.35	20	2	37	168	87	75
24	15	cyclohexane	3.35	20	4	37	168	82	93
25	15	cyclohexane	3.35	20	6	37	168	86	86
26	15	cyclohexane	3.35	20	1.5	37	168	62	64
27	15	cyclohexane	3.35	20	1.5	37	168	56	52
28	15	cyclohexane	3.35	20	1.5	37	168	47	45
29	15	cyclohexane	3.35	20	1.5	37	168	36	41
30	5	toluene	2.56	50	3	37	24	78	72
31	5	1,4-dioxane	-0.5	50	3	37	24	94	89
32	5	cyclohexane	3.35	50	3	37	24	55	61
33	5	tert-butyl methyl ether	0.94	50	3	37	24	87	87
34	5	1,2-dimethoxyethane	-0.44	50	3	37	24	91	89
35	5	Tetrahydrofuran	0.46	50	3	37	24	88	89
36	5	Dimethyl formamide	-1.3	50	3	37	24	95	85
37	5	Dimethyl formamide	-1.3	0	6	37	24	10	9

38	5	Dimethyl formamide	-1.3	15	5.1	37	24	22	37
39	5	Dimethyl formamide	-1.3	25	4.5	37	24	51	55
40	5	Dimethyl formamide	-1.3	35	3.9	37	24	79	70
41	5	Dimethyl formamide	-1.3	45	3.3	37	24	85	81
42	5	Dimethyl formamide	-1.3	60	2.4	37	24	85	87
43	5	Dimethyl formamide	-1.3	80	1.2	37	24	71	75
44	5	Dimethyl formamide	-1.3	50	0.5	37	24	40	58
45	5	Dimethyl formamide	-1.3	50	1	37	24	75	64
46	5	Dimethyl formamide	-1.3	50	2	37	24	92	76
47	5	Dimethyl formamide	-1.3	50	4	37	24	93	89
48	5	Dimethyl formamide	-1.3	50	6	37	24	89	84
49	5	Dimethyl formamide	-1.3	50	3	37	24	95	85
50	5	Dimethyl formamide	-1.3	50	3	37	24	82	76
51	5	Dimethyl formamide	-1.3	50	3	37	24	40	80
52	5	Dimethyl formamide	-1.3	50	3	37	24	37	32
53	5	Dimethyl formamide	-1.3	50	3	37	24	21	26
54	15	Dimethyl formamide	-1.3	20	3	37	168	57	43
55	15	Tetrahydrofuran	0.46	20	3	37	168	20	32
56	15	Dimethyl sulfoxide	-1.35	20	3	37	168	46	19
57	15	Acetonitrile	-0.33	20	3	37	168	36	44
58	15	hexane	3.9	20	3	37	168	6	31
59	15	tert-butyl methyl ether	0.94	20	3	37	168	12	5
60	15	Dimethyl formamide	-1.3	0	3.75	37	168	33	14
61	15	Dimethyl formamide	-1.3	10	3.375	37	168	42	44
62	15	Dimethyl formamide	-1.3	30	2.625	37	168	54	45
63	15	Dimethyl formamide	-1.3	40	2.25	37	168	30	39
64	15	Dimethyl formamide	-1.3	50	1.875	37	168	20	34
65	15	Dimethyl formamide	-1.3	60	1.5	37	168	15	26
66	15	Dimethyl formamide	-1.3	20	1	37	168	13	18
67	15	Dimethyl formamide	-1.3	20	2	37	168	31	18
68	15	Dimethyl formamide	-1.3	20	4	37	168	61	31
69	15	Dimethyl formamide	-1.3	20	5	37	168	65	53
70	15	Dimethyl formamide	-1.3	20	6	37	168	56	59
71	15	Dimethyl formamide	-1.3	20	3	37	168	48	62
72	15	Dimethyl formamide	-1.3	20	3	37	200	35	44
73	15	Dimethyl formamide	-1.3	20	3	37	200	43	44
74	15	Dimethyl formamide	-1.3	20	3	37	200	41	36
75	15	Dimethyl formamide	-1.3	20	3	37	200	38	40
76	1	Dimethyl sulfoxide	-1.35	0	3	30	96	37	40
77	1	Tetrahydrofuran	0.46	0	3	30	96	5	38

78	1	cyclohexane	3.35	0	3	30	96	5	26
79	1	hexane	3.9	0	3	30	96	6	6
80	1	toluene	2.56	0	3	30	96	10	5
81	1	Dimethyl formamide	-1.3	0	3	30	96	22	10
82	1	Acetonitrile	-0.33	0	3	30	96	46	38
83	1	Acetonitrile	-0.33	0	1	30	96	14	33
84	1	Acetonitrile	-0.33	0	2	30	96	31	18
85	1	1,2-dimethoxyethane	-0.44	0	3	30	96	46	25
86	1	1,2-dimethoxyethane	-0.44	0	4	30	96	48	33
87	1	1,2-dimethoxyethane	-0.44	0	5	30	96	51	41
88	1	1,2-dimethoxyethane	-0.44	0	6	30	96	53	49
89	1	1,2-dimethoxyethane	-0.44	0	3	10	96	25	54
90	1	1,2-dimethoxyethane	-0.44	0	3	20	96	37	25
91	1	1,2-dimethoxyethane	-0.44	0	3	40	96	44	37
92	1	1,2-dimethoxyethane	-0.44	0	3	50	96	19	44
93	1	1,2-dimethoxyethane	-0.44	0	3	60	96	9	20
94	1	1,2-dimethoxyethane	-0.44	0	3	30	120	38	10
95	1	1,2-dimethoxyethane	-0.44	0	3	30	120	36	37
96	1	1,2-dimethoxyethane	-0.44	0	3	30	96	35	37
97	1	1,2-dimethoxyethane	-0.44	0	3	30	120	34	35
98	1	1,2-dimethoxyethane	-0.44	0	3	30	144	30	34
99	1	1,2-dimethoxyethane	-0.44	0	3	30	144	27	29
100	1	1,2-dimethoxyethane	-0.44	0	3	30	168	22	28
101	1	1,2-dimethoxyethane	-0.44	0	3	30	168	21	22
102	1	Dimethyl formamide	-1.3	0	1	37	120	46	22
103	1	Dimethyl formamide	-1.3	0	0.25	37	120	10	35
104	1	Dimethyl formamide	-1.3	0	0.5	37	120	24	24
105	1	Dimethyl formamide	-1.3	0	0.75	37	120	37	28
106	1	Dimethyl formamide	-1.3	0	1.25	37	120	46	31
107	1	Dimethyl formamide	-1.3	0	1.5	37	120	47	39
108	1	Dimethyl formamide	-1.3	0	1.75	37	120	47	42
109	1	Dimethyl formamide	-1.3	0	1	15	120	17	46
110	1	Dimethyl formamide	-1.3	0	1	25	120	29	18
111	1	Dimethyl formamide	-1.3	0	1	30	120	41	29
112	1	Dimethyl formamide	-1.3	0	1	40	120	45	40
113	1	Dimethyl formamide	-1.3	0	1	45	120	28	44
114	1	Dimethyl formamide	-1.3	0	1	50	120	18	29
115	1	Dimethyl formamide	-1.3	0	1	37	120	28	18
116	1	Dimethyl formamide	-1.3	0	1	37	120	17	28
117	1	Dimethyl formamide	-1.3	0	1	37	120	14	14

118	1	Dimethyl formamide	-1.3	0	1	37	144	76	74
119	1	Dimethyl formamide	-1.3	0	1	37	144	66	66
120	1	Dimethyl formamide	-1.3	0	1	37	168	47	46
121	1	Dimethyl formamide	-1.3	0	1	37	144	69	68
122	1	Dimethyl formamide	-1.3	0	1	37	168	32	28
123	1	Dimethyl formamide	-1.3	0	1	37	168	19	24
124	1	Dimethyl formamide	-1.3	0	1	37	168	36	37
125	1	Dimethyl formamide	-1.3	0	1	37	168	41	39
