Supporting information 1

On Benchmarking of Automated Methods for Performing Exhaustive Reaction Path Search

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Table SI1. A full list of discovered channels and relative energy values of the best (energetically most preferable) TSs in kcal/mol.

		SC-AFIR1	SC-AFIR1+	SC-AFIR2	FSM	GSM	SSM	KinBot1	KinBot2	Attribute[a]
1	[H]OC1([H])OOC([H])([H])C1([H])[H]	34.2	34.2	34.2	39.1	35.3	39.1	34.9	34.9	R37, R38
2	[H]C(=O)C([H])([H])[H].[H]OC([H])=O	37.7	37.7	37.7	38.8	38.8	38.8	48.8	48.8	R69
3	[H]OOC([H])([H])C([H])=C([H])O[H]	43.8	43.8	43.8	68.8	45.8	45.8	70.6	70.6	R47, R53
4	[H]OC([H])=C([H])[H].[H]C([H])OO	-	48.1	48.8	-	-	-	48.7	48.7	R17
5	[H]C([H])=C=O.[H]C([H])=O.[H]O[H]	49.8	49.8	49.8	50.5	50.5	50.5	50.5	50.5	R10[b], R28
6	[H]C(=O)C([H])([H])C([H])=O.[H]O[H]	50.1	50.1	50.1	51.0	53.1	51.0	52.6	52.6	R1-R5
7	[H]C(=O)C([H])([H])C([H])([H])O([H])O	50.2	50.7	50.2	51.7	53.0	51.4	52.7	52.7	R18, R19, R26
8	[H]C(=O)C([H])=C([H])[H].[H]OO[H]	53.1	53.1	53.1	55.9	56.5	56.8	55.4	55.4	R74
9	[H]OOC([H])=O.[H]C([H])=C([H])[H]	54.8	-	54.8	56.6	58.5	56.6	56.6	56.6	R20[b], R71, R72
10	[H]C(=O)C([H])=C([H])[H].[H]O([H])O	55.4	55.4	55.4						
11	[H]OC1([H])O(O)C([H])([H])C1([H])[H]	-	-	55.4						
12	[H]C1([H])OC(=O)C1([H])[H].[H]O[H]	57.6	57.6	57.6	76.0	58.1	58.1	58.3	58.3	R35, R36
13	[H]OC([H])=C([H])C([H])=O.[H]O[H]	59.6	59.6	59.6	61.6	-	61.6	60.3	60.3	R63
14	[H]OC([H])(O[H])C([H])([H])C([H])=O	64.7	62.5	64.7	65.8	63.6	63.6	-	-	R54, R57
15	[H]OOC([H])=C([H])[H].[H]C([H])=O	62.7	62.7	62.7	69.9	72.8	66.4	63.4	63.4	R67, R68, R73
16	[H]C1([H])OC1([H])[H].[H]OC([H])=O	63.4	-	63.4	-	65.5	-	-	-	R43
17	[H]C1([H])OOC(=O)C1([H])[H].[H][H]	-	-	64.3	66.8	65.4	66.4	-	65.9	R39
18	[H]C(=O)C([H])([H])[H].[H]C([H])OO	64.4	65.9	64.4	65.6	65.6	67.1	65.1	65.1	R16
19	[H]OC([H])([H])OC([H])([H])C([H])=O	65.6	65.6	65.6	66.8	67.2	66.8	-	-	R52
20	[H]C(=O)C([H])([H])C([H])OO.[H][H]	66.5	66.8	66.5	69.9	67.4	70.0	69.5	69.5	R15
21	[H]C(=O)C([H])([H])[H].[H]C=O.[H]O	67.2	67.2	67.2	71.0	75.2	69.4	68.6	68.6	R14[b]
22	[H]OC([H])=C([H])[H].[H]O[H].C=O	67.3	68.4	67.3						
23	[H]OOC([H])([H])OC([H])=C([H])[H]	67.6	-	67.6	-	78.2	68.7	-	78.8	R56
24	[H]OC([H])([H])C([H])([H])C([H])OO	68.6	68.5	68.6						
25	[H]C([H])=C([H])[H].[H]OO[H].C=O	69.2	-	69.2	69.7	69.7	70.3	69.9	69.9	R30
26	[H]OOC([H])([H])[H].[H]C([H])=C=O	-	-	69.6	-	89.6	-	80.4	80.4	R65, R66
27	[H]OOC1([H])OC([H])([H])C1([H])[H]	70.1	-	70.1	-	-	71.6	-	-	R44
28	[H]C(=O)C([H])([H])[H].[H]COO[H]	-	76.4	70.2						
29	[H]OC([H])=C([H])[H].[H]OC([H])=O	71.7	-	71.7						
30	[H]OC([H])=C([H])[H].[H]C=O.[H]O	-	-	73.3						
31	[H]OC([H])([H])C([H])=O.[H]C([H])=O	74.3	-	74.3	76.4	74.7	77.7	76.8	76.8	R64
32	[H]OOC([H])=C([H])[H].C=O.[H][H]	74.9	74.9	74.9	75.2	-	78.2	75.5	75.5	R29
33	[H]OOC([H])([H])C(=O)C([H])([H])[H]	79.9	-	74.9	80.5	80.0	80.5	-	-	R50
34	[H]OC([H])([H])C1([H])O(O)C1([H])[H]	-	-	75.1						
35	[H]C1([H])OO1.[H]OC([H])=C([H])[H]	-	-	75.2						

36	[H]C1([H])C(=O)O(O)C1([H])[H].[H][H]	-	-	75.7	-	-	-	-	76.4	R27
37	[H]OC([H])([H])C([H])C([H])([H])OO	-	-	76.0						
38	[H]OC([H])([H])C1([H])OOC1([H])[H]	-	-	76.7	77.8	77.8	-	-	-	R32[c]
39	[H]C([H])=C=O.[H]O[H].C=O.[H][H]	77.1	78.1	77.1	-	88.4	78.2	79.9	79.9	R31[b], R62[b]
40	[H]C([H])(O)C([H])([H])C([H])([H])OO	-	-	77.1						
41	[H]C(=O)C([H])([H])C=O.[H]O.[H][H]	77.7	80.1	77.7						
42	[H]C(=O)OOC([H])([H])C([H])([H])[H]	-	-	135.0	80.0	80.0	80.0	78.9	78.9	R51
43	[H]OC1([H])OO1.[H]C([H])=C([H])[H]	-	-	78.8						
44	[H]OOC([H])([H])C([H])=C=O.[H][H]	79.3	79.3	79.3	-	84.7	82.2	81.8	81.8	R12[b], R59-R61
45	[H]C(=O)C([H])(O([H])O)C([H])([H])[H]	-	-	80.3	-	80.5	80.4	-	-	R21
46	[H]OOC([H])([H])C([H])([H])[H].C=O	84.0	79.9	79.9	86.6	-	86.3	83.8	83.8	R70
47	[H]OOC([H])([H])C1([H])OC1([H])[H]	82.5	85.9	81.2	85.3	87.5	86.6	-	102.7	R33, R34
48	[H]OOC([H])=C([H])C([H])([H])O[H]	-	-	81.3						
49	[H]OCC([H])([H])C([H])([H])OO[H]	84.6	84.2	84.2	85.8	87.0	-	-	85.8	R6
50	[H]C([H])=C([H])[H].[H]O([H])O.C=O	-	-	-	-	-	85.6	-	-	R23
51	[H]C1=C([H])C([H])([H])O1.[H]OO[H]	86.5	-	86.5	-	89.3	-	-	-	R42
52	[H]OOC([H])(C([H])=O)C([H])([H])[H]	-	-	88.3	-	87.2	87.4	-	87.4	R55
53	[H]OC([H])([H])OOC([H])=C([H])[H]	-	-	87.4						
54	[H]OOOC1([H])C([H])([H])C1([H])[H]	-	-	-	-	-	-	-	88.3	R46
55	[H]C1([H])OOOC([H])([H])C1([H])[H]	-	-	96.0	-	-	-	89.0	89.0	R45
56	[H]OC(=O)C([H])([H])C([H])=O.[H][H]	-	-	88.6						
57	[H]CC([H])([H])C([H])=O.[H]OO[H]	-	-	-	89.0	-	-	-	-	R7
58	[H]OOCC([H])([H])C([H])=O.[H][H]	-	-	89.7						
59	[H]OC([H])(C([H])OO)C([H])([H])[H]	90.3	90.3	90.3						
60	[H]C(=O)C([H])C([H])([H])OO.[H][H]	-	-	90.8	-	109.6	-	-	91.5	R11
61	[H]C1([H])O(O)C1([H])[H].[H]C([H])=O	-	-	91.3						
62	[H]C(=O)C([H])OC([H])([H])[H].[H]O	-	-	92.2	-	-	-	-	92.8	R13[b]
63	[H]O(O)C1([H])OC([H])([H])C1([H])[H]	-	92.7	-	-	-	94.3	-	101.8	R24, R25
64	[H]OOC1([H])C([H])([H])C1([H])O[H]	-	-	95.4	93.8	-	96.1	-	96.1	R40
65	[H]C(=O)C([H])=C([H])[H].O=O.[H][H]	-	-	94.9						
66	[H]OC1([H])O(O)C1([H])C([H])([H])[H]	-	-	95.4						
67	[H]OCC([H])([H])C([H])([H])O([H])O	-	95.4	95.4						
68	[H]OC([H])(OC([H])([H])[H])C([H])=O	-	-	95.6						
69	[H]C(=C=O)C([H])([H])[H].[H]OO[H]	95.9	97.4	95.9	-	-	97.6	-	-	R75
70	[H]C(=O)C([H])([H])C1([H])OO1.[H][H]	-	-	96.6						
71	[H]OOC([H])=C([H])C([H])=O.[H][H]	96.9	97.5	96.9	99.7	99.7	107.6	103.5	103.5	R58
72	[H]C([H])(O)C1([H])OC1([H])[H].[H]O	-	-	97.2						
73	[H]OOC([H])([H])CC([H])=O.[H][H]	-	-	98.8						
74	[H]O(O)C(=O)C([H])([H])C([H])([H])[H]	98.9	-	98.9	-	100.0	-	-	-	R22
75	[H]C(=O)C([H])([H])C([H])([H])O.[H]O	-	-	99.3						
76	[H]C(OO)C([H])([H])[H].[H]C([H])=O	-	-	100.7						
77	[H]OC1([H])OC1([H])[H].[H]C([H])=O	103.4	-	103.2						
78	[H]C(=O)C1OC1([H])[H].[H]O.[H][H]	-	-	103.7						
79	[H]C(=O)C([H])([H])C([H])([H])[H].O=O	-	-	104.1						
80	[H]COC([H])([H])C([H])([H])OO[H]	110.5	110.7	110.5	106.8	106.8	107.4	-	112.0	R8, R9
81	[H]OOC1([H])C(=O)C1([H])[H].[H][H]	-	-	105.4						
82	[H]C1([H])OOC2([H])OC12[H].[H][H]	-	-	-	-	106.8	106.8	-	-	R41

83	[H]OOC(=O)C([H])([H])C([H])([H])[H]	110.6	-	110.2
84	[H]COC([H])(OO[H])C([H])([H])[H]	-	-	111.2
85	[H]C1([H])OOC1([H])[H].[H]C([H])=O	-	-	114.7

[a]Corresponding labels defined in Ref. 4.

[b]The IRC calculation reached a product minimum different from the label in Ref. 4 after it completely terminated.

[c]Using the attribution in the SI of Ref. 4.