Supplementary Information for

Electrochemical and Theoretical Analysis of the Reactivity of Shikonin Derivatives: Dissociative Electron Transfer in Esterified Compounds

By

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Internal coordinates Z-matrices and calculated harmonic frequencies obtained for the minimum energy conformers for the neutral structures of Shikonin derivatives, 1,4-naphthoquinone and 5,8-dihydroxy-1,4-naphthoquinone at the BHandHLYP/6-311++G(2d,2p) level considering solvation by the Marenich, Cramer and Truhlar model in Z-matrices

Shikonin Neutral

Atom number	Symbol	NA	Bond	NB	Angle	NC	Dihedral
1	C						
2	C	1	1.4636611				
3	C	2	1.4580151	1	118.516989		
4	C	3	1.4160284	2	119.545726	1	0.5023941
5	C	4	1.4593177	3	120.164772	2	-0.0948625
6	C	1	1.3318876	2	122.907847	3	0.2951661
7	H	1	1.0760132	6	121.149033	5	178.927896
8	C	3	1.3854939	2	120.356831	1	-179.45036
9	C	4	1.3872714	3	119.750357	2	179.880354
10	C	9	1.404941	4	119.336412	3	0.3758299
11	C	10	1.3622446	9	120.832683	4	-0.3178861
12	H	10	1.0761339	9	118.438901	4	179.771665
13	H	11	1.0761389	10	120.706419	9	-179.949715
14	C	6	1.5088655	1	122.774274	2	178.630025
15	H	14	1.0869891	6	107.932402	1	138.541703
16	C	14	1.5296913	6	110.747645	1	-102.481598
17	H	16	1.084441	14	107.941978	6	66.0699535
18	H	16	1.0874186	14	107.80699	6	-49.3345686
19	C	16	1.4969441	14	112.425593	6	-169.637779
20	H	19	1.0823443	16	114.367238	14	55.7552072
21	C	19	1.3297958	16	128.189015	14	-125.267244
22	C	21	1.5011477	19	120.792733	16	-178.710081
23	H	22	1.0890192	21	110.717087	19	-121.674008
24	H	22	1.0850946	21	111.937147	19	-0.6554584
25	H	22	1.08901	21	110.718528	19	120.313782
26	C	21	1.4995113	19	125.058553	16	0.8237576
27	H	26	1.0823087	21	113.501298	19	0.7886503
28	H	26	1.0887839	21	110.187694	19	122.223582
29	H	26	1.0889725	21	110.185583	19	-120.517803
30	O	14	1.4083067	6	111.506486	1	17.4665527
31	H	30	0.9542136	14	109.292883	6	73.7736095
32	O	9	1.3326196	4	123.358189	3	-179.752674

33	H	32	0.9690552	9	107.96237	4	0.5736496
34	O	8	1.3330536	3	123.140019	2	-0.1377409
35	H	34	0.9697539	8	107.882647	3	-0.0153301
36	O	5	1.2236392	4	121.400018	3	178.57106
37	O	2	1.2253583	1	119.789404	6	-179.440659

List of calculated harmonic frequencies for each vibrational normal mode

Mode	Frequency / cm^{-1}
1	23.71
2	34.56
3	41.13
4	64.44
5	95.19
6	111.56
7	112.89
8	140.34
9	160.40
10	173.77
11	190.52
12	209.62
13	214.80
14	277.11
15	295.45
16	302.52
17	316.93
18	334.01
19	381.61
20	386.34
21	401.82
22	431.96
23	444.32
24	448.29
25	477.99
26	479.61
27	492.20
28	502.35
29	508.34
30	546.59
31	569.47
32	615.48

33	658.44
34	716.24
35	721.98
36	736.94
37	741.21
38	744.18
39	770.86
40	813.11
41	820.01
42	837.02
43	873.29
44	896.93
45	940.62
46	953.66
47	981.54
48	996.66
49	998.07
50	1030.31
51	1038.84
52	1051.10
53	1071.37
54	1081.80
55	1123.39
56	1145.39
57	1165.00
58	1189.06
59	1205.19
60	1213.35
61	1250.01
62	1288.87
63	1290.22
64	1331.79
65	1342.67
66	1351.29
67	1364.17
68	1402.22
69	1410.06
70	1421.98
71	1439.78
72	1449.17
73	1458.44
74	1464.91
75	1481.86

76	1486.78
77	1504.97
78	1508.90
79	1517.74
80	1522.87
81	1526.96
82	1543.00
83	1565.63
84	1684.12
85	1694.95
86	1740.85
87	1745.06
88	1794.84
89	1801.86
90	3092.45
91	3099.82
92	3130.77
93	3138.48
94	3139.65
95	3141.55
96	3182.91
97	3184.11
98	3203.40
99	3212.34
100	3285.74
101	3293.31
102	3298.44
103	3608.41
104	3621.90
105	3983.54

Deoxyshikonin Neutral

Atom Number	Symbol	NA	Bond	NB	Angle	NC	Dihedral
1	C						
2	C	1	1.4622716				
3	C	2	1.4589269	1	118.487322		
4	C	3	1.4155547	2	119.515324	1	0.4371711
5	C	4	1.4603598	3	120.154274	2	-0.1217896
6	C	1	1.3342833	2	123.266808	3	0.2587884
7	H	1	1.0774818	6	121.09212	5	179.125646
8	C	3	1.3855482	2	120.370463	1	-179.67003
9	C	4	1.387408	3	119.735836	2	179.772513
10	C	9	1.4046036	4	119.347009	3	0.3134757
11	C	10	1.3625894	9	120.822592	4	-0.2723584
12	H	10	1.0761355	9	118.478243	4	179.770474
13	H	11	1.0761195	10	120.706252	9	-179.934035
14	C	6	1.4946671	1	122.838548	2	178.131307
15	H	14	1.0857763	6	109.146042	1	137.312339
16	C	14	1.5387259	6	112.503408	1	-101.386766
17	H	16	1.0838965	14	108.951769	6	61.4516694
18	H	16	1.0877315	14	108.650654	6	-54.7606327
19	C	16	1.4970706	14	111.519492	6	-174.819168
20	H	19	1.0823064	16	114.413982	14	64.5713339
21	C	19	1.3307095	16	128.342698	14	-114.76772
22	C	21	1.5012447	19	120.763185	16	179.993012
23	H	22	1.0889974	21	110.753884	19	-121.330543
24	H	22	1.0850199	21	111.88721	19	-0.2864096
25	H	22	1.0890324	21	110.683988	19	120.655412
26	C	21	1.4996061	19	125.130333	16	-0.3838661
27	H	26	1.0825118	21	113.548185	19	1.0214524
28	H	26	1.0887776	21	110.141117	19	122.424359
29	H	26	1.0889032	21	110.174089	19	-120.363939
30	O	9	1.3330588	4	123.322585	3	-179.773189
31	H	30	0.9693606	9	107.853805	4	0.4335127
32	O	8	1.3335228	3	123.109025	2	-0.0231718
33	H	32	0.9699207	8	107.788586	3	-0.0960699
34	O	5	1.2230766	4	121.252892	3	178.833308
35	O	2	1.2260489	1	119.911357	6	-179.57524
36	H	14	1.0847144	6	108.815975	1	19.7829364

List of calculated harmonic frequencies for each vibrational normal mode

Mode	Frequency / cm^{-1}
1	31.26
2	35.35
3	52.95
4	74.31
5	89.73
6	112.51
7	129.07
8	162.69
9	169.72
10	187.99
11	213.25
12	226.05
13	254.05
14	316.02
15	328.81
16	349.69
17	378.65
18	385.00
19	403.24
20	424.86
21	444.97
22	445.42
23	471.68
24	484.09
25	500.03
26	506.18
27	531.21
28	557.88
29	603.55
30	628.55
31	701.98
32	717.10
33	725.00
34	740.69
35	741.63
36	766.28
37	774.79
38	796.86
39	831.44
40	846.69
41	897.39
42	901.19

43	952.67
44	964.55
45	991.22
46	997.29
47	1033.37
48	1039.63
49	1052.03
50	1058.98
51	1077.90
52	1096.02
53	1144.77
54	1165.23
55	1185.04
56	1200.66
57	1227.35
58	1254.59
59	1289.80
60	1292.55
61	1335.55
62	1340.98
63	1353.97
64	1380.16
65	1402.73
66	1408.67
67	1427.18
68	1431.87
69	1455.37
70	1464.96
71	1465.89
72	1480.21
73	1507.26
74	1514.75
75	1520.26
76	1523.45
77	1527.35
78	1542.77
79	1543.68
80	1566.00
81	1684.31
82	1696.10
83	1737.83
84	1744.43
85	1791.77

86	1798.07
87	3093.09
88	3100.76
89	3121.84
90	3139.11
91	3140.52
92	3142.73
93	3173.89
94	3184.06
95	3193.12
96	3203.63
97	3211.90
98	3275.23
99	3284.77
100	3297.53
101	3604.12
102	3613.97

Isobutyrylshikonin Neutral

Atom Number	Symbol	NA	Bond	NB	Angle	NC	Dihedral
1	C						
2	C	1	1.4650818				
3	C	2	1.4570875	1	118.506453		
4	C	3	1.4162363	2	119.596	1	0.3530911
5	C	4	1.4580423	3	120.193303	2	-0.0215221
6	C	1	1.3309216	2	122.753784	3	-0.0865791
7	H	1	1.0760476	6	121.63526	5	179.390233
8	C	3	1.3853951	2	120.322059	1	-179.598203
9	C	4	1.3872387	3	119.770034	2	179.934877
10	C	9	1.405248	4	119.321471	3	0.2069975
11	C	10	1.3619549	9	120.830349	4	-0.1751546
12	H	10	1.0760781	9	118.438494	4	179.930208
13	H	11	1.0760777	10	120.725918	9	-179.911359
14	C	6	1.5043979	1	123.492393	2	178.575015
15	H	14	1.0818393	6	108.686651	1	139.785152
16	C	14	1.5283896	6	111.583612	1	-98.9111101
17	H	16	1.0836986	14	108.426627	6	64.9847407
18	H	16	1.0873066	14	107.1205	6	-50.2820971
19	C	16	1.49689	14	112.265314	6	-170.129533
20	H	19	1.0820229	16	114.356766	14	59.4167597
21	C	19	1.3297832	16	128.096697	14	-121.239565
22	C	21	1.5008787	19	120.692714	16	-179.138859
23	H	22	1.0888804	21	110.757201	19	121.186668
24	H	22	1.0888737	21	110.57884	19	-120.826479
25	H	22	1.0849445	21	111.933683	19	0.148932
26	C	21	1.499297	19	125.150786	16	0.7303175
27	H	26	1.0823907	21	113.60036	19	2.6036369
28	H	26	1.0886408	21	110.012925	19	123.978336
29	H	26	1.0889738	21	110.177267	19	-118.821626
30	O	14	1.4262609	6	110.776186	1	20.1899678
31	O	9	1.3321309	4	123.399173	3	-179.835618
32	H	31	0.9688083	9	108.064691	4	0.3349226
33	O	8	1.3325934	3	123.15128	2	-0.0611871
34	H	33	0.9696164	8	107.936491	3	-0.1466975
35	O	5	1.2233727	4	121.600885	3	179.244065
36	O	2	1.2249245	1	119.671217	6	-179.888144
37	C	30	1.3360632	14	118.606045	6	84.8390892
38	C	37	1.5071295	30	111.399087	14	178.573291
39	H	38	1.0868485	37	106.396927	30	-44.262902
40	O	37	1.1976333	30	122.861743	14	-2.0313651

41	C	38	1.530834	37	109.561405	30	72.3304643
42	H	41	1.0870193	38	110.95698	37	61.3894721
43	H	41	1.0855036	38	109.449466	37	-179.52372
44	H	41	1.0846487	38	111.746513	37	-59.8765352
45	C	38	1.5188696	37	111.294464	30	-163.514321
46	H	45	1.0855283	38	111.550406	37	57.4578203
47	H	45	1.0858802	38	109.568443	37	177.165283
48	H	45	1.0857639	38	111.206149	37	-63.3229209

List of calculated harmonic frequencies for each vibrational normal mode

Mode	**Frequency / cm^{-1}**
1	19.08
2	22.19
3	28.36
4	330.7
5	39.34
6	50.92
7	67.30
8	85.02
9	113.03
10	125.45
11	140.43
12	147.66
13	159.92
14	171.18
15	184.02
16	200.08
17	220.18
18	224.85
19	240.56
20	259.05
21	285.48
22	297.84
23	328.76
24	329.38
25	337.61
26	364.52
27	380.01
28	387.27
29	397.02
30	425.20

31	440.06
32	445.37
33	464.62
34	478.35
35	490.14
36	501.84
37	512.86
38	518.61
39	559.60
40	569.95
41	617.12
42	660.01
43	675.32
44	719.53
45	728.40
46	739.80
47	743.72
48	746.70
49	775.68
50	799.91
51	812.30
52	825.08
53	840.56
54	877.95
55	890.56
56	896.18
57	927.84
58	956.20
59	971.12
60	978.06
61	990.06
62	996.57
63	997.24
64	1010.49
65	1037.83
66	1042.72
67	1049.94
68	1080.23
69	1109.41
70	1117.90
71	1142.79
72	1159.47
73	1167.81

74	1177.98
75	1188.43
76	1208.83
77	1225.05
78	1250.23
79	1253.50
80	1268.49
81	1292.19
82	1312.83
83	1337.43
84	1348.25
85	1363.79
86	1373.51
87	1402.05
88	1404.48
89	1417.18
90	1430.27
91	1440.05
92	1444.35
93	1454.13
94	1455.75
95	1464.37
96	1464.84
97	1483.33
98	1491.50
99	1506.02
100	1511.72
101	1518.69
102	1523.17
103	1523.47
104	1525.76
105	1532.06
106	1532.90
107	1542.31
108	1543.66
109	1565.57
110	1684.06
111	1694.19
112	1744.91
113	1746.63
114	1797.20
115	1801.33
116	1850.62

17	3094.08
118	3101.45
119	3133.79
120	3118.79
121	3134.18

Isovalerylshikonin Neutral

Atom Number	Symbol	NA	Bond	NB	Angle	NC	Dihedral
1	C						
2	C	1	1.4652784				
3	C	2	1.4572867	1	118.507417		
4	C	3	1.4163082	2	119.61078	1	0.6787348
5	C	4	1.457736	3	120.164776	2	-0.2232668
6	C	1	1.3309896	2	122.712828	3	-0.1849216
7	H	1	1.0761125	6	121.632449	5	179.28567
8	C	3	1.3853866	2	120.324953	1	-179.487041
9	C	4	1.3872118	3	119.788748	2	179.840478
10	C	9	1.4052563	4	119.312593	3	0.1960729
11	C	10	1.3619682	9	120.825548	4	-0.2000874
12	H	10	1.0760427	9	118.463533	4	179.84993
13	H	11	1.0761	10	120.719867	9	-179.954599
14	C	6	1.504473	1	123.453162	2	178.573538
15	H	14	1.0816116	6	108.732196	1	139.2833
16	C	14	1.528168	6	111.756043	1	-99.3366525
17	H	16	1.0836911	14	108.443439	6	65.4996837
18	H	16	1.0873075	14	107.14971	6	-49.7938163
19	C	16	1.4970832	14	112.149338	6	-169.576774
20	H	19	1.0820952	16	114.282307	14	58.1637912
21	C	19	1.3297276	16	128.195163	14	-122.596598
22	C	21	1.5008919	19	120.653126	16	-179.04489
23	H	22	1.0888477	21	110.640657	19	-121.135662
24	H	22	1.0848868	21	111.914187	19	-0.0950505
25	H	22	1.0889228	21	110.742611	19	120.886703
26	C	21	1.499212	19	125.166402	16	0.5914271
27	H	26	1.0823648	21	113.569193	19	2.4403669
28	H	26	1.0885763	21	110.11354	19	123.905343
29	H	26	1.0889737	21	110.125331	19	-118.90156
30	O	14	1.4266455	6	110.492536	1	19.758916
31	O	9	1.3321762	4	123.394473	3	-179.859952
32	H	31	0.968822	9	108.063411	4	0.4485945
33	O	8	1.3325405	3	123.163462	2	-0.023082
34	H	33	0.9695379	8	107.951857	3	-0.0862368
35	O	5	1.2233497	4	121.605289	3	179.054723
36	O	2	1.2248989	1	119.657708	6	-179.889137
37	C	30	1.336096	14	118.592336	6	85.371425
38	C	37	1.4997473	30	111.495933	14	-178.319476
39	H	38	1.0856507	37	109.013829	30	-26.6205236
40	H	38	1.0900631	37	105.387793	30	87.5545721

41	C	38	1.5259496	37	114.253987	30	-151.479515
42	H	41	1.0873548	38	107.845017	37	-51.3997883
43	C	41	1.5238813	38	111.306663	37	67.4124271
44	H	43	1.0866712	41	111.807376	38	-58.0332099
45	H	43	1.0885274	41	110.718964	38	62.3461448
46	H	43	1.086878	41	110.80686	38	-178.123846
47	C	41	1.52315	38	109.90305	37	-169.291138
48	H	47	1.0867453	41	110.81167	38	179.483767
49	H	47	1.0884609	41	110.954558	38	-60.86556
50	H	47	1.087215	41	111.360472	38	59.2825398
51	O	37	1.1977173	30	122.930887	14	-0.1926816

List of calculated harmonic frequencies for each vibrational normal mode

Mode	**Frequency / cm^{-1}**
1	16.43
2	26.57
3	29.66
4	31.94
5	37.43
6	45.57
7	52.20
8	78.55
9	92.74
10	111.87
11	129.13
12	136.43
13	151.15
14	164.84
15	171.11
16	185.53
17	202.79
18	214.82
19	227.05
20	236.77
21	244.91
22	266.27
23	306.96
24	312.56
25	331.35
26	341.50
27	377.00

28	380.21
29	386.82
30	393.93
31	414.01
32	437.53
33	440.65
34	444.91
35	466.49
36	477.19
37	488.08
38	501.33
39	509.75
40	512.74
41	555.45
42	570.84
43	616.30
44	623.72
45	664.04
46	719.55
47	727.11
48	739.41
49	743.36
50	745.28
51	767.19
52	776.88
53	812.17
54	823.96
55	841.02
56	865.09
57	884.03
58	897.77
59	925.85
60	934.48
61	954.92
62	961.97
63	979.55
64	986.67
65	996.97
66	997.45
67	1004.77
68	1027.59
69	1039.17
70	1043.78

71	1051.81
72	1081.40
73	1110.36
74	1122.36
75	1144.07
76	1167.67
77	1169.32
78	1181.42
79	1188.47
80	1209.70
81	1228.47
82	1249.26
83	1252.91
84	1259.09
85	1291.86
86	1302.47
87	1312.35
88	1337.60
89	1350.14
90	1362.21
91	1373.86
92	1401.91
93	1404.17
94	1410.07
95	1417.36
96	1434.92
97	1443.41
98	1448.08
99	1456.43
100	1457.65
101	1461.67
102	1464.71
103	1483.60
104	1490.69
105	1496.69
106	1504.91
107	1513.09
108	1519.22
109	1522.99
110	1524.17
111	1525.77
112	1531.26
113	1532.69

114	1540.07
115	1542.79
116	1565.13
17	1683.99
118	1693.86
119	1744.22
120	1747.04
121	1796.74
122	1802.13
123	1850.08
124	3094.46
125	3096.41
126	3100.88
127	3101.21
128	3114.92
129	3122.20
130	3134.97
131	3140.99
132	3143.79
133	3158.25
134	3163.68
135	3169.39
136	3171.31
137	3175.66
138	3185.33
139	3189.25
140	3204.61
141	3208.71
142	3215.37
143	3286.71
144	3293.11
145	3299.31
146	3612.69
147	3627.24

1,4-naphthoquinone Neutral

Atom Number	Symbol	NA	Bond	NB	Angle	NC	Dihedral
1	C						
2	C	1	1.327305				
3	C	1	1.475517	2	122.085118		
4	C	2	1.4755175	1	122.085064	3	-0.000973
5	C	4	1.4834179	2	117.577367	1	0.0004569
6	C	5	1.396302	4	120.337566	2	-0.0004651
7	C	6	1.3864005	5	119.843295	4	-180
8	C	7	1.3834128	6	120.015682	5	0
9	C	8	1.386821	7	120.141064	6	0
10	C	9	1.3834128	8	120.141064	7	0
11	H	8	1.0763183	7	119.84616	6	-180
12	H	9	1.0763188	8	120.012822	7	-180
13	O	4	1.207859	2	120.332603	1	-180
14	O	3	1.2078589	1	120.332617	2	-179.999354
15	H	1	1.0769421	2	121.870479	4	179.999557
16	H	2	1.0769415	1	121.87052	3	179.999576
17	H	7	1.075406	6	119.336678	5	-180
18	H	10	1.075406	9	120.647694	8	180

List of calculated harmonic frequencies for each vibrational normal mode

Mode	Frequency / cm^{-1}
1	82.56
2	119.92
3	198.19
4	267.24
5	278.66
6	389.73
7	436.26
8	465.92
9	471.15
10	486.85
11	574.88
12	625.97
13	638.97
14	716.96
15	727.96
16	793.11
17	812.64

18	82270
19	829.20
20	912.06
21	956.69
22	1050.98
23	1059.70
24	1071.33
25	1075.49
26	1109.09
27	1118.01
28	1170.92
29	1202.92
30	1216.90
31	1294.63
32	1352.86
33	1360.94
34	1389.16
35	1449.58
36	1541.90
37	1567.91
38	1687.93
39	1704.12
40	1747.76
41	1812.23
42	1827.24
43	3276.12
44	3277.28
45	3287.86
46	3293.37
47	3298.55
48	3301.95

5,8-dihydroxy-1,4-naphthoquinone Neutral

Atom Number	Symbol	NA	Bond	NB	Angle	NC	Dihedral
1	C						
2	C	1	1.328097				
3	C	1	1.4694498	2	121.785951		
4	C	2	1.469448	1	121.786051	3	-0.0250039
5	C	4	1.4593348	2	118.238176	1	0.0049798
6	C	5	1.417888	4	119.975811	2	0.0050754
7	C	6	1.3863903	5	119.882606	4	-179.996401
8	C	7	1.4048997	6	119.354494	5	0
9	C	8	1.36218	7	120.762896	6	-0.0026181
10	C	5	1.3863906	4	120.14156	2	-179.993219
11	H	8	1.0760123	7	118.551352	6	-179.998119
12	H	9	1.076013	8	120.685748	7	-179.99951
13	O	4	1.2237753	2	119.808163	1	179.974855
14	O	3	1.2237758	1	119.808083	2	179.938167
15	O	10	1.3326093	5	123.189844	4	0.0047541
16	H	15	0.9692063	10	108.006865	5	0.0071848
17	O	7	1.3326084	6	123.189746	5	-179.988703
18	H	17	0.9692081	7	108.006866	6	0.0118939
19	H	1	1.0765152	2	121.983948	4	179.984321
20	H	2	1.0765153	1	121.983841	3	179.983051

List of calculated harmonic frequencies for each vibrational normal mode

Mode	Frequency / cm^{-1}
1	103.30
2	109.69
3	171.93
4	197.26
5	279.46
6	298.04
7	369.65
8	379.32
9	418.87
10	442.04
11	461.89
12	470.15
13	488.47
14	516.21
15	574.12

16	642.20
17	671.13
18	671.33
19	707.12
20	736.92
21	740.99
22	764.82
23	779.97
24	796.72
25	895.06
26	908.40
27	990.76
28	998.38
29	1035.97
30	1060.16
31	1151.23
32	1155.21
33	1199.09
34	1271.12
35	1297.37
36	1341.42
37	1396.05
38	1412.90
39	1424.91
40	1469.84
41	1481.06
42	1543.43
43	1565.14
44	1684.25
45	1695.21
46	1732.14
47	1753.25
48	1798.31
49	3284.20
50	3286.62
51	3299.21
52	3299.46
53	3618.05
54	3618.68