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Hydrogen Bonding Processes During Self-protonation of Natural α-hydroxyquinones

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Supplementary Information

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Optimized neutral structures of the studied compounds at the BHandHLYP/6-311++G- (2d,2p) level considering solvation in DMSO by the Marenich, Cramer and Truhlar model

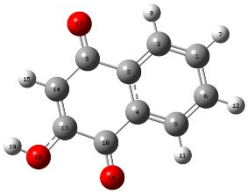

Fig. S1. Optimized structure of 2-hydroxy-1,4-naphtoquinone (1).

Table S1. XYZ coordinates of 2-hydroxy-1,4-naphtoquinone (neutral species).

Atom number	Symbol	X	Y	Z
1	C	-3.069207	0.094219	0.000103
2	C	-2.070317	1.04777	0.000051
3	C	-0.743879	0.659451	0.000021
4	C	-0.420299	-0.69328	0.000021
5	C	-1.424662	-1.645589	0.000055
6	C	-2.746951	-1.251685	0.000111
7	H	-4.098601	0.399032	0.00014
8	H	-2.310956	2.092855	0.000041
9	C	0.328703	1.686651	-0.000012
10	C	0.990446	-1.129106	0.000022
11	H	-1.164592	-2.686009	0.00006
12	H	-3.52548	-1.990849	0.000167
13	C	2.032026	-0.059556	0.000159
14	C	1.711331	1.23378	0.00009
15	H	2.470726	1.994907	0.000099
16	O	1.31475	-2.285255	-0.00057
17	O	0.065171	2.867493	-0.000301
18	O	3.270303	-0.537914	0.000297
19	H	3.903973	0.17954	0.000358

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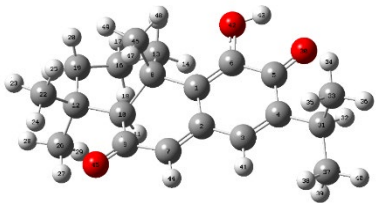

Fig. S2. Optimized structure of taxodione (2).

Table S2. XYZ coordinates of taxodione (neutral species).

Atom number	Symbol	X	Y	Z
1	C	0.297883	0.421013	0.031066
2	C	0.795326	-0.940396	-0.043745
3	C	2.215859	-1.214446	-0.174343
4	C	3.14454	-0.260231	-0.223341
5	C	2.674286	1.11899	-0.121658
6	C	1.230635	1.385538	0.037042
7	C	-0.034063	-1.987992	0.048755
8	C	-1.189946	0.687623	0.255508
9	C	-1.487126	-1.853324	0.129322
10	C	-2.051928	-0.508157	-0.253194
11	H	-1.883787	-0.510929	-1.330384
12	C	-3.595504	-0.363085	-0.074991
13	C	-1.637782	1.955987	-0.528898
14	H	-0.934175	2.158097	-1.32378
15	H	-1.589651	2.803371	0.140724
16	C	-3.037188	1.867951	-1.128641
17	H	-3.401522	2.871247	-1.317758
18	H	-2.999924	1.373675	-2.093805
19	C	-3.984163	1.121106	-0.216726
20	H	-3.992217	1.600245	0.756048
21	H	-5.001721	1.174442	-0.58789
22	C	-4.151694	-0.878858	1.254608
23	H	-5.189986	-0.57378	1.337709
24	H	-4.113966	-1.955104	1.317364
25	H	-3.627475	-0.474273	2.109078
26	C	-4.272583	-1.142258	-1.206832
27	H	-3.964274	-2.17905	-1.213922
28	H	-5.349818	-1.114309	-1.084435
29	H	-4.038185	-0.714311	-2.175367
30	O	3.417313	2.083672	-0.154318
31	C	4.625978	-0.491728	-0.348926
32	H	4.996656	0.259931	-1.037281
33	C	5.322123	-0.263842	0.992754
34	H	5.099665	0.714458	1.397282
35	H	5.010389	-1.010025	1.715469
36	H	6.396592	-0.340336	0.873484
37	C	4.979348	-1.85986	-0.908089
38	H	4.693974	-2.657446	-0.231613

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39	H	4.500683	-2.040127	-1.86338
40	H	6.050544	-1.927277	-1.054902
41	H	2.486624	-2.251074	-0.239329
42	O	0.962692	2.686477	0.201985
43	H	1.809546	3.139023	0.143569
44	H	0.350824	-2.990725	0.061689
45	O	-2.151076	-2.828855	0.39113
46	C	-1.346255	0.906896	1.769757
47	H	-1.109076	0.006848	2.325759
48	H	-0.671142	1.687701	2.095511
49	H	-2.346483	1.213817	2.033222

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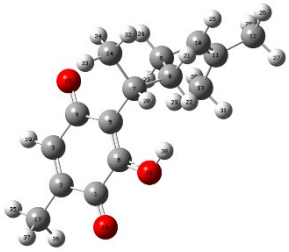

Fig. S3. Optimized structure of perezone (3).

Table S3. XYZ coordinates of perezone (neutral species).

Atom number	Symbol	X	Y	Z
1	C	-2.803558	-0.643502	0.813087
2	C	-3.104679	-1.020585	-0.583613
3	C	-2.359771	-0.494686	-1.543166
4	C	-1.244214	0.436769	-1.28599
5	C	-0.972788	0.890237	0.088496
6	C	-1.703857	0.335039	1.065669
7	C	0.095317	1.919966	0.398992
8	C	1.4713	1.297365	0.689061
9	C	2.148159	0.558106	-0.462043
10	C	3.541724	0.148984	-0.100816
11	C	4.040114	-1.074856	0.023399
12	C	5.476017	-1.285473	0.39856
13	C	3.271051	-2.341951	-0.189978
14	C	0.169043	3.080565	-0.590527
15	O	-0.571945	0.7934	-2.227383
16	O	-3.427107	-1.099842	1.73349
17	C	-4.221835	-1.974697	-0.811603
18	O	-1.567703	0.580283	2.369221
19	H	-2.518858	-0.736633	-2.577784
20	H	-0.202238	2.390861	1.332183
21	H	2.121151	2.100641	1.02332
22	H	1.378495	0.613215	1.527274
23	H	1.552944	-0.295536	-0.752219
24	H	2.193386	1.210619	-1.32751
25	H	4.213345	0.972991	0.088719
26	H	5.997197	-0.347832	0.54182
27	H	5.554825	-1.863357	1.315148
28	H	5.996898	-1.850941	-0.369086
29	H	2.230152	-2.178509	-0.42537
30	H	3.713074	-2.919305	-0.997063
31	H	3.321217	-2.965853	0.69764
32	H	0.795607	3.859102	-0.170879
33	H	-0.813015	3.505824	-0.761309
34	H	0.575207	2.789678	-1.545086
35	H	-4.352062	-2.160425	-1.868142
36	H	-4.029922	-2.916962	-0.311872
37	H	-5.147965	-1.58421	-0.40679
38	H	-0.857533	1.198231	2.527213

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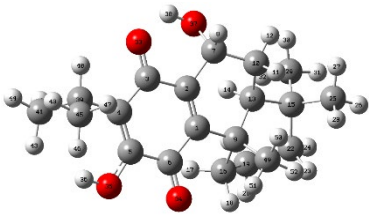

Fig. S4. Optimized structure of horminone (4).

Table S4. XYZ coordinates of horminone (neutral species).

Atom number	Symbol	X	Y	Z
1	C	-0.068429	-0.393224	0.214217
2	C	-0.505721	0.865203	0.229763
3	C	-1.947345	1.200294	0.067308
4	C	-2.967335	0.151035	-0.015298
5	C	-2.535082	-1.11117	0.038437
6	C	-1.092149	-1.473452	0.193869
7	C	0.392907	2.06127	0.40245
8	H	-0.019195	2.664176	1.204072
9	C	1.403372	-0.787116	0.275263
10	C	1.802049	1.659537	0.75974
11	H	1.842807	1.440325	1.818866
12	H	2.440656	2.515938	0.59088
13	C	2.253368	0.462953	-0.058629
14	H	2.001745	0.69414	-1.089227
15	C	3.794904	0.246264	-0.055516
16	C	1.708694	-1.876715	-0.795909
17	H	0.944577	-1.865648	-1.563203
18	H	1.649527	-2.847241	-0.324979
19	C	3.072998	-1.719788	-1.467846
20	H	3.378661	-2.679992	-1.867922
21	H	2.994662	-1.050294	-2.317638
22	C	4.120453	-1.188285	-0.509738
23	H	4.187045	-1.848107	0.348462
24	H	5.101041	-1.198055	-0.973866
25	C	4.455231	0.513378	1.296837
26	H	5.513193	0.279946	1.233511
27	H	4.37315	1.554101	1.586817
28	H	4.037012	-0.088852	2.091441
29	C	4.39903	1.223661	-1.067284
30	H	4.115879	2.247695	-0.851998
31	H	5.482158	1.171193	-1.04561
32	H	4.075482	0.997122	-2.077019
33	O	-2.25449	2.372325	-0.019316
34	O	-0.808726	-2.632215	0.329065
35	O	-3.302245	-2.197954	-0.024861
36	H	-4.222063	-1.962512	-0.111635
37	O	0.423896	2.843222	-0.783012
38	H	-0.462691	3.163266	-0.922118

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39	C	-4.411151	0.575263	-0.159457
40	H	-4.386418	1.653921	-0.192694
41	C	-5.043692	0.112188	-1.471024
42	H	-4.439511	0.404937	-2.320878
43	H	-5.188425	-0.96193	-1.526369
44	H	-6.021613	0.564896	-1.583134
45	C	-5.262958	0.193954	1.050873
46	H	-5.399969	-0.876683	1.161248
47	H	-4.823416	0.563866	1.96898
48	H	-6.250427	0.629259	0.95282
49	C	1.66767	-1.34375	1.685071
50	H	1.545345	-0.585459	2.447526
51	H	0.97701	-2.145761	1.901863
52	H	2.66541	-1.74627	1.768016

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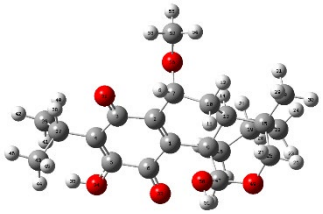

Fig. S5. Optimized structure of 7 α-O-methyl-conacytone.

Table S5. XYZ coordinates of 7 α-O-methyl-conacytone (neutral species).

Tag	Symbol	X	Y	Z
1	C	0.212466	-0.433464	0.027089
2	C	0.691274	0.781687	-0.226243
3	C	2.157168	1.036724	-0.326227
4	C	3.125835	-0.021846	0.003672
5	C	2.637389	-1.242523	0.233118
6	C	1.179942	-1.550656	0.162875
7	C	-0.182872	1.978858	-0.46042
8	H	0.241332	2.541659	-1.282759
9	C	-1.265192	-0.754865	0.139255
10	C	-1.609408	1.589567	-0.787946
11	H	-1.650317	1.2317	-1.80652
12	H	-2.219354	2.480498	-0.730626
13	C	-2.095356	0.544976	0.202091
14	H	-1.920041	0.978427	1.1788
15	C	-3.589778	0.176636	0.131741
16	C	-1.56495	-1.579885	1.431873
17	H	-0.696367	-1.583691	2.076244
18	H	-1.740123	-2.611306	1.157764
19	C	-2.754919	-1.060481	2.230474
20	H	-3.043297	-1.814007	2.955135
21	H	-2.456879	-0.193584	2.808373
22	C	-3.950289	-0.705365	1.359795
23	H	-4.421254	-1.618154	1.013916
24	H	-4.686556	-0.192535	1.96722
25	C	-3.824216	-0.621371	-1.1393
26	H	-4.856016	-0.940378	-1.201975
27	H	-3.604624	-0.026786	-2.01957
28	C	-4.483828	1.408277	0.102122
29	H	-4.354962	1.989506	-0.802354
30	H	-5.525898	1.112922	0.156772
31	H	-4.279335	2.053943	0.949309
32	O	2.538461	2.123686	-0.693928
33	O	0.826049	-2.698608	0.205341
34	O	3.354302	-2.333205	0.510357
35	H	4.28554	-2.131076	0.53762
36	O	-0.109858	2.77143	0.713991
37	C	4.592518	0.343433	0.000294
38	H	4.620042	1.401844	-0.210011
39	C	5.261318	0.150092	1.360517

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40	H	4.718803	0.671794	2.139354
41	H	5.345054	-0.889113	1.661282
42	H	6.268338	0.548646	1.328539
43	C	5.368159	-0.343506	-1.123076
44	H	5.43031	-1.420339	-1.005609
45	H	4.913165	-0.146524	-2.086081
46	H	6.384214	0.032121	-1.148716
47	C	-1.67864	-1.623214	-1.074946
48	H	-1.272637	-2.614247	-0.946829
49	O	-3.053668	-1.809864	-1.152909
50	O	-1.177157	-1.06119	-2.255817
51	H	-1.367511	-1.664093	-2.969139
52	C	-0.264762	4.146201	0.479916
53	H	0.524399	4.526539	-0.162326
54	H	-1.225443	4.377014	0.028627
55	H	-0.206772	4.645563	1.437252

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Calculated properties from electron structure calculations of the studied compounds at the BHandHLYP/6-311++G- (2d,2p) level considering solvation in DMSO by the Marenich, Cramer and Truhlar model

Table S6. Vertical ionization Potentials (I), vertical electron affinities (A) and global electroaccepting powers (ω^+) for compounds 1 - 5.

	Calculated property (eV)		
Compound	**I**	**A**	**ω^+**
1	7.1137	3.0037	4.0275
2	6.1755	3.0097	4.5640
3	6.7804	3.0177	4.1643
4	6.7828	3.0140	4.1531
5	6.7518	2.9058	3.8887

Table S7. Calculated charges from Hirshfeld population analysis for N+1 and N electron structures, condensed-to-atom Fukui function $f^+[\rho_{N_0}; r]$ and local electroaccepting powers $\omega^+(r)$ for 2-hydroxy-1,4-napthoquinone (1).

		Calculated property			
Number	**Atom**	$\mathbf{q_i(N+1)}$	$\mathbf{q_i(N)}$	$f^+[\rho_{N_0}; r]$	$\omega_i^+(r)$
1	C	0.0252	-0.0179	0.0431	0.1738
2	C	-0.0004	-0.0231	0.0227	0.0915
3	C	0.0118	-0.0152	0.0270	0.1087
4	C	0.0130	-0.0184	0.0314	0.1265
5	C	0.0038	-0.0198	0.0237	0.0953
6	C	0.0189	-0.0212	0.0401	0.1615
7	H	0.0798	0.0625	0.0173	0.0696
8	H	0.0682	0.0546	0.0137	0.0550
9	C	0.1932	0.1573	0.0359	0.1444
10	C	0.1899	0.1704	0.0195	0.0787
11	H	0.0699	0.0564	0.0135	0.0542
12	H	0.0787	0.0621	0.0166	0.0670
13	C	0.2400	0.1074	0.1326	0.5339
14	C	0.1461	-0.0631	0.2092	0.8427
15	H	0.1322	0.0688	0.0634	0.2554
16	O	-0.2360	-0.2753	0.0393	0.1583
17	O	-0.2360	-0.3086	0.0726	0.2923
18	O	-0.0480	-0.1815	0.1336	0.5380
19	H	0.2492	0.2042	0.0450	0.1811

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Table S8. Calculated charges from Hirshfeld population analysis for N+1 and N electron structures, condensed-to-atom Fukui function $f^{+}[\rho_{N_0};r]$ and local electroaccepting powers $\omega^{+}(r)$ for taxodione (2)

		Calculated property			
Number	**Atom**	$\mathbf{q_i(N+1)}$	$\mathbf{q_i(N)}$	$f^{+}[\rho_{N_0};r]$	$\omega_i^{+}(r)$
1	C	0.1045	-0.0124	0.1169	0.5335
2	C	0.0520	0.0124	0.0396	0.1808
3	C	0.0191	-0.0104	0.0295	0.1348
4	C	0.0135	-0.0047	0.0182	0.0832
5	C	0.1872	0.1528	0.0345	0.1573
6	C	0.1938	0.0722	0.1217	0.5552
7	C	0.0877	-0.0220	0.1097	0.5007
8	C	0.0281	0.0199	0.0082	0.0376
9	C	0.1896	0.1715	0.0182	0.0830
10	C	-0.0172	-0.0235	0.0062	0.0284
11	H	0.0649	0.0534	0.0115	0.0527
12	C	0.0178	0.0158	0.0020	0.0089
13	C	-0.0446	-0.0515	0.0069	0.0316
14	H	0.0340	0.0248	0.0092	0.0418
15	H	0.0361	0.0274	0.0087	0.0396
16	C	-0.0431	-0.0497	0.0067	0.0304
17	H	0.0381	0.0308	0.0073	0.0334
18	H	0.0343	0.0291	0.0052	0.0236
19	C	-0.0484	-0.0513	0.0029	0.0132
20	H	0.0334	0.0298	0.0036	0.0164
21	H	0.0353	0.0300	0.0053	0.0243
22	C	-0.0901	-0.0929	0.0028	0.0129
23	H	0.0310	0.0263	0.0047	0.0214
24	H	0.0210	0.0184	0.0026	0.0119
25	H	0.0296	0.0267	0.0029	0.0133
26	C	-0.0837	-0.0871	0.0034	0.0157
27	H	0.0248	0.0223	0.0024	0.0110
28	H	0.0327	0.0281	0.0046	0.0212
29	H	0.0320	0.0289	0.0032	0.0144
30	O	-0.2184	-0.2841	0.0657	0.2999
31	C	-0.0101	-0.0150	0.0049	0.0224
32	H	0.0423	0.0360	0.0063	0.0288
33	C	-0.0772	-0.0814	0.0042	0.0192
34	H	0.0290	0.0264	0.0026	0.0119
35	H	0.0335	0.0299	0.0036	0.0166
36	H	0.0383	0.0335	0.0049	0.0222
37	C	-0.0739	-0.0782	0.0043	0.0195
38	H	0.0376	0.0343	0.0033	0.0151
39	H	0.0353	0.0321	0.0032	0.0147
40	H	0.0392	0.0347	0.0045	0.0205
41	H	0.0826	0.0641	0.0185	0.0843
42	O	-0.0861	-0.1892	0.1030	0.4701
43	H	0.1879	0.1516	0.0363	0.1657
44	H	0.0992	0.0613	0.0379	0.1731
45	O	-0.2425	-0.2865	0.0440	0.2007
46	C	-0.0662	-0.0821	0.0159	0.0725
47	H	0.0453	0.0330	0.0123	0.0562

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48	H	0.0390	0.0288	0.0102	0.0463
49	H	0.0520	0.0363	0.0157	0.0718

Table S9. Calculated charges from Hirshfeld population analysis for N+1 and N electron structures, condensed-to-atom Fukui function $f^{+}[\rho_{N_0};r]$ and local electroaccepting powers $\omega^{+}(r)$ for perezone (3).

		Calculated property			
Number	**Atom**	$\mathbf{q_i(N+1)}$	$\mathbf{q_i(N)}$	$\boldsymbol{f^{+}[\rho_{N_0};r]}$	$\boldsymbol{\omega_i{}^{+}(r)}$
1	C	0.1865	0.1670	0.0195	0.0811
2	C	0.0472	0.0146	0.0326	0.1359
3	C	0.0101	-0.0289	0.0390	0.1622
4	C	0.1859	0.1601	0.0257	0.1072
5	C	0.0998	-0.0294	0.1292	0.5381
6	C	0.1985	0.0921	0.1064	0.4432
7	C	0.0095	-0.0099	0.0195	0.0810
8	C	-0.0214	-0.0452	0.0239	0.0994
9	C	-0.0449	-0.0560	0.0112	0.0465
10	C	-0.0217	-0.0671	0.0454	0.1891
11	C	0.0328	-0.0127	0.0455	0.1894
12	C	-0.0748	-0.0860	0.0112	0.0466
13	C	-0.0728	-0.0829	0.0100	0.0418
14	C	-0.0685	-0.0831	0.0145	0.0606
15	O	-0.2262	-0.2756	0.0494	0.2055
16	O	-0.2339	-0.2724	0.0385	0.1604
17	C	-0.0585	-0.0707	0.0123	0.0511
18	O	-0.0920	-0.1895	0.0975	0.4060
19	H	0.0840	0.0628	0.0212	0.0883
20	H	0.0647	0.0412	0.0235	0.0977
21	H	0.0548	0.0341	0.0206	0.0859
22	H	0.0425	0.0283	0.0142	0.0592
23	H	0.0379	0.0299	0.0080	0.0331
24	H	0.0423	0.0312	0.0111	0.0461
25	H	0.0460	0.0295	0.0165	0.0685
26	H	0.0400	0.0334	0.0066	0.0273
27	H	0.0448	0.0336	0.0112	0.0468
28	H	0.0441	0.0337	0.0104	0.0432
29	H	0.0412	0.0358	0.0054	0.0224
30	H	0.0465	0.0360	0.0105	0.0438
31	H	0.0459	0.0357	0.0101	0.0422
32	H	0.0473	0.0322	0.0151	0.0628
33	H	0.0435	0.0306	0.0129	0.0537
34	H	0.0344	0.0252	0.0092	0.0383
35	H	0.0577	0.0484	0.0092	0.0384
36	H	0.0574	0.0465	0.0109	0.0453
37	H	0.0571	0.0463	0.0109	0.0452
38	H	0.2122	0.1808	0.0314	0.1308

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Table S10. Calculated charges from Hirshfeld population analysis for N+1 and N electron structures, condensed-to-atom Fukui function $f^{+}[\rho_{N_0};r]$ and local electroaccepting powers $\omega^{+}(r)$ for horminone (4)

		Calculated property			
Number	**Atom**	$\mathbf{q_i(N+1)}$	$\mathbf{q_i(N)}$	$f^{+}[\rho_{N_0};r]$	$\omega_i^{+}(r)$
1	C	0.0562	0.0139	0.0423	0.1758
2	C	0.0355	-0.0043	0.0397	0.1650
3	C	0.1967	0.1656	0.0311	0.1292
4	C	0.1355	-0.0334	0.1689	0.7015
5	C	0.2236	0.0949	0.1287	0.5345
6	C	0.1939	0.1728	0.0210	0.0874
7	C	0.0645	0.0565	0.0080	0.0333
8	H	0.0498	0.0378	0.0119	0.0495
9	C	0.0190	0.0146	0.0044	0.0184
10	C	-0.0483	-0.0523	0.0040	0.0165
11	H	0.0443	0.0391	0.0051	0.0214
12	H	0.0442	0.0376	0.0066	0.0273
13	C	-0.0219	-0.0235	0.0015	0.0064
14	H	0.0324	0.0289	0.0035	0.0146
15	C	0.0142	0.0129	0.0013	0.0054
16	C	-0.0472	-0.0510	0.0038	0.0158
17	H	0.0306	0.0266	0.0041	0.0169
18	H	0.0301	0.0256	0.0045	0.0185
19	C	-0.0463	-0.0496	0.0033	0.0138
20	H	0.0327	0.0289	0.0038	0.0156
21	H	0.0302	0.0278	0.0024	0.0101
22	C	-0.0508	-0.0520	0.0013	0.0054
23	H	0.0305	0.0288	0.0017	0.0069
24	H	0.0305	0.0280	0.0025	0.0106
25	C	-0.0841	-0.0855	0.0013	0.0055
26	H	0.0298	0.0279	0.0019	0.0080
27	H	0.0298	0.0283	0.0014	0.0059
28	H	0.0299	0.0287	0.0012	0.0049
29	C	-0.0828	-0.0843	0.0015	0.0064
30	H	0.0296	0.0282	0.0014	0.0057
31	H	0.0291	0.0272	0.0019	0.0081
32	H	0.0298	0.0286	0.0012	0.0049
33	O	-0.2059	-0.2670	0.0611	0.2538
34	O	-0.2027	-0.2454	0.0427	0.1772
35	O	-0.0635	-0.1860	0.1225	0.5088
36	H	0.2090	0.1741	0.0349	0.1451
37	O	-0.2520	-0.2667	0.0147	0.0609
38	H	0.1426	0.1361	0.0065	0.0268
39	C	-0.0016	-0.0193	0.0177	0.0735
40	H	0.0536	0.0334	0.0202	0.0838
41	C	-0.0544	-0.0759	0.0215	0.0892
42	H	0.0506	0.0353	0.0153	0.0634
43	H	0.0441	0.0330	0.0111	0.0462
44	H	0.0599	0.0384	0.0215	0.0891
45	C	-0.0552	-0.0764	0.0212	0.0879
46	H	0.0437	0.0326	0.0111	0.0462
47	H	0.0502	0.0350	0.0152	0.0630

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48	H	0.0589	0.0380	0.0208	0.0865
49	C	-0.0771	-0.0842	0.0071	0.0296
50	H	0.0374	0.0318	0.0056	0.0233
51	H	0.0286	0.0243	0.0043	0.0178
52	H	0.0429	0.0352	0.0077	0.0321

Table S11. Calculated charges q_i from Hirshfeld population analysis for N+1 and N electron structures, condensed-to-atom Fukui function $f^{+}[\rho_{N_0};r]$ and local electroaccepting powers $\omega^{+}(r)$ for 7a-O-methyl-conacytone (5)

		Calculated property			
Number	**Atom**	$\mathbf{q_i(N+1)}$	$\mathbf{q_i(N)}$	$\boldsymbol{f^{+}[\rho_{N_0};r]}$	$\boldsymbol{\omega_i^{+}(r)}$
1	C	0.0432	0.0077	0.0354	0.1378
2	C	0.0363	0.0002	0.0361	0.1405
3	C	0.1943	0.1633	0.0309	0.1202
4	C	0.1384	-0.0315	0.1700	0.6609
5	C	0.2227	0.0900	0.1327	0.5159
6	C	0.1913	0.1701	0.0212	0.0824
7	C	0.0636	0.0572	0.0064	0.0250
8	H	0.0483	0.0384	0.0100	0.0388
9	C	0.0058	0.0027	0.0031	0.0122
10	C	-0.0551	-0.0587	0.0036	0.0139
11	H	0.0342	0.0301	0.0041	0.0159
12	H	0.0439	0.0372	0.0067	0.0259
13	C	-0.0254	-0.0268	0.0014	0.0054
14	H	0.0364	0.0327	0.0037	0.0145
15	C	0.0046	0.0032	0.0014	0.0055
16	C	-0.0445	-0.0484	0.0039	0.0153
17	H	0.0344	0.0302	0.0042	0.0165
18	H	0.0335	0.0288	0.0047	0.0183
19	C	-0.0450	-0.0483	0.0033	0.0129
20	H	0.0355	0.0315	0.0039	0.0153
21	H	0.0308	0.0282	0.0026	0.0102
22	C	-0.0497	-0.0511	0.0014	0.0055
23	H	0.0274	0.0256	0.0019	0.0073
24	H	0.0311	0.0286	0.0025	0.0097
25	C	0.0299	0.0282	0.0017	0.0068
26	H	0.0445	0.0413	0.0031	0.0121
27	H	0.0342	0.0319	0.0023	0.0088
28	C	-0.0765	-0.0785	0.0020	0.0078
29	H	0.0336	0.0320	0.0016	0.0064
30	H	0.0344	0.0322	0.0022	0.0086
31	H	0.0362	0.0346	0.0016	0.0063
32	O	-0.2059	-0.2709	0.0650	0.2527
33	O	-0.2056	-0.2499	0.0443	0.1724
34	O	-0.0637	-0.1893	0.1256	0.4883
35	H	0.2092	0.1733	0.0359	0.1397
36	O	-0.2004	-0.2057	0.0053	0.0206
37	C	-0.0017	-0.0196	0.0179	0.0695
38	H	0.0536	0.0330	0.0205	0.0799
39	C	-0.0548	-0.0758	0.0211	0.0820

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40	H	0.0505	0.0352	0.0153	0.0596
41	H	0.0439	0.0329	0.0110	0.0428
42	H	0.0592	0.0382	0.0210	0.0815
43	C	-0.0547	-0.0769	0.0221	0.0860
44	H	0.0433	0.0319	0.0113	0.0441
45	H	0.0499	0.0345	0.0154	0.0598
46	H	0.0593	0.0375	0.0217	0.0846
47	C	0.1306	0.1276	0.0030	0.0117
48	H	0.0359	0.0320	0.0039	0.0153
49	O	-0.1997	-0.2051	0.0054	0.0210
50	O	-0.2301	-0.2324	0.0023	0.0090
51	H	0.1759	0.1711	0.0048	0.0188
52	C	0.0134	0.0084	0.0050	0.0193
53	H	0.0357	0.0318	0.0039	0.0153
54	H	0.0389	0.0348	0.0042	0.0162
55	H	0.0451	0.0411	0.0041	0.0158