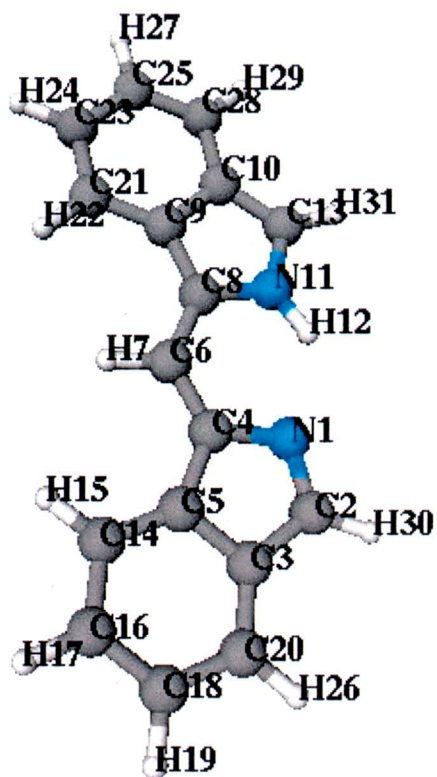


Computational insights into the chemical structures and mechanisms of the chromogenic and neurotoxic effects of aromatic γ -diketones

Chang-Guo Zhan,¹ Peter Spencer,² and David A. Dixon^{1*}

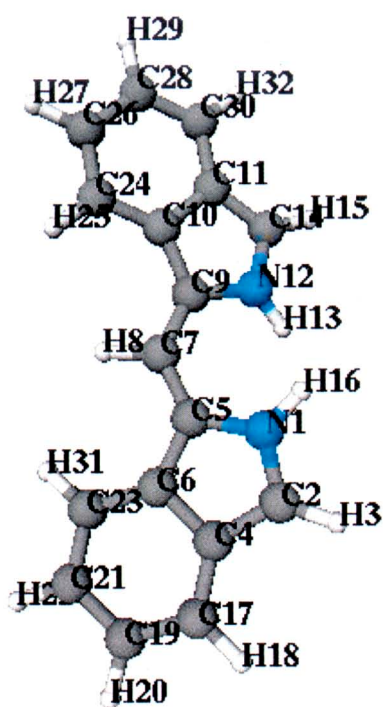
Theory, Modeling & Simulation, William R. Wiley Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, MS K1-83, P.O. Box 999, Richland, Washington 99352¹ and Center for Research on Occupational and Environmental Toxicology, Oregon Health Sciences University, 3181 S.W. Sam Jackson Park Rd. L606, Portland, Oregon 97201.²

Supporting Information Available. Geometries of 3a, 3b, 4a, 4b, 5a, 5b, 6a, 6b, 7a, 7b, 8b, 9a, 10a, and 11a optimized at the B3LYP/6-31+G(d) level.



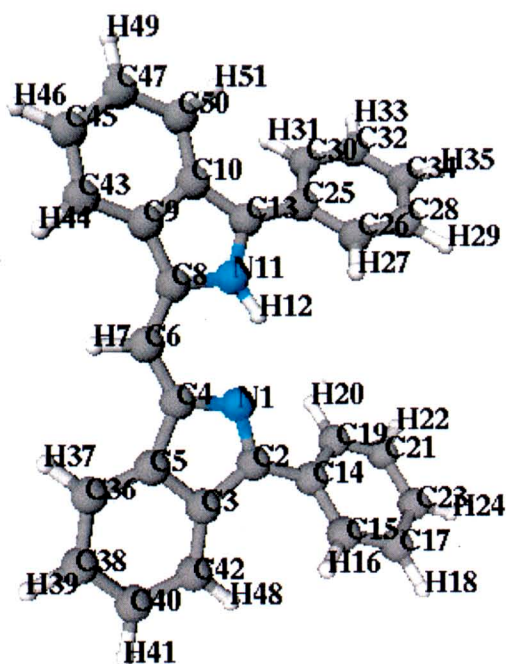
1	7	1.375775	-1.636844	-0.000086
2	6	2.659686	-1.917613	-0.000197
3	6	3.490983	-0.730138	-0.000079
4	6	1.252904	-0.234284	-0.000006
5	6	2.583778	0.362159	0.000014
6	6	0.033004	0.403250	0.000037
7	1	0.036824	1.490894	0.000031
8	6	-1.243528	-0.205511	0.000054
9	6	-2.550888	0.359688	0.000005
10	6	-3.487240	-0.734749	0.000044
11	7	-1.420605	-1.577408	0.000163
12	1	-0.599906	-2.189054	0.000278
13	6	-2.725837	-1.920700	0.000132
14	6	3.066467	1.675934	0.000104
15	1	2.390240	2.527973	0.000173
16	6	4.447605	1.878409	0.000103
17	1	4.839281	2.892601	0.000169
18	6	5.345830	0.792720	0.000019
19	1	6.415642	0.984531	0.000016
20	6	4.875724	-0.520249	-0.000068
21	6	-3.027020	1.689957	-0.000076
22	1	-2.337018	2.530284	-0.000108
23	6	-4.392626	1.906708	-0.000117
24	1	-4.773543	2.924796	-0.000181
25	6	-5.317682	0.824373	-0.000077
26	1	5.570022	-1.357494	-0.000145
27	1	-6.382865	1.039925	-0.000110
28	6	-4.881700	-0.485353	0.000004
29	1	-5.591219	-1.309253	0.000038
30	1	3.007480	-2.947074	-0.000277
31	1	-3.037893	-2.955966	0.000203

3a geometry (coordinates in Å) optimized at the B3LYP/6-31+G(d) level



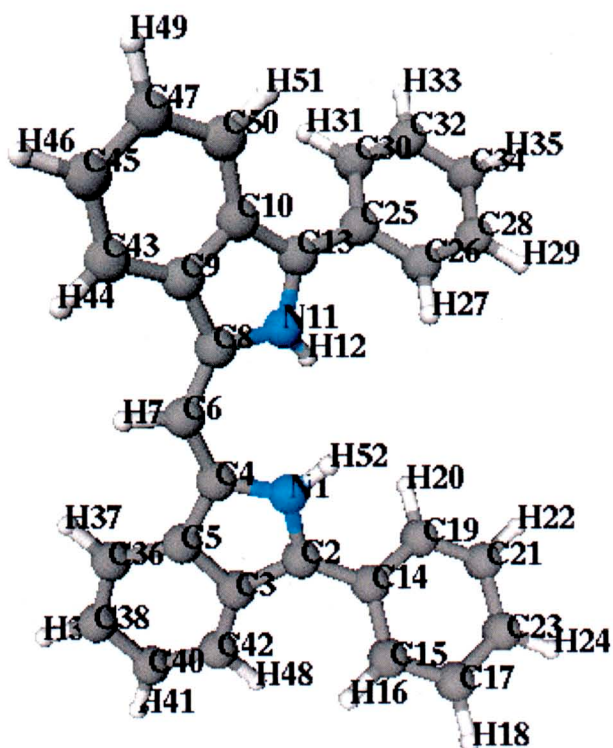
1	7	1.501391	-1.604569	-0.447280
2	6	2.824499	-1.858494	-0.537008
3	1	3.188322	-2.832799	-0.836537
4	6	3.532103	-0.681974	-0.227975
5	6	1.258037	-0.257885	-0.131089
6	6	2.555644	0.339953	0.013085
7	6	0.000029	0.325775	-0.000386
8	1	0.000013	1.413467	-0.000631
9	6	-1.257973	-0.257847	0.130579
10	6	-2.555638	0.339884	-0.013603
11	6	-3.532016	-0.681978	0.228126
12	7	-1.501220	-1.604458	0.447094
13	1	-0.797430	-2.234088	0.813029
14	6	-2.824290	-1.858429	0.537140
15	1	-3.187973	-2.832675	0.837014
16	1	0.797662	-2.234232	-0.813191
17	6	4.916507	-0.403863	-0.143618
18	1	5.653081	-1.181381	-0.323893
19	6	5.299627	0.884227	0.176350
20	1	6.353970	1.133239	0.247184
21	6	4.333282	1.895047	0.421059
22	1	4.673684	2.895610	0.671737
23	6	2.971387	1.639511	0.353289
24	6	-2.971643	1.639447	-0.353482
25	1	-2.254987	2.429468	-0.559036
26	6	-4.333537	1.894905	-0.420871
27	1	-4.674020	2.895479	-0.671426
28	6	-5.299741	0.884049	-0.175822
29	1	-6.354094	1.133075	-0.246363
30	6	-4.916461	-0.403985	0.144200
31	1	2.254621	2.429451	0.558683
32	1	-5.652948	-1.181488	0.324885

3b geometry (coordinates in Å) optimized at the B3LYP/6-31+G(d) level



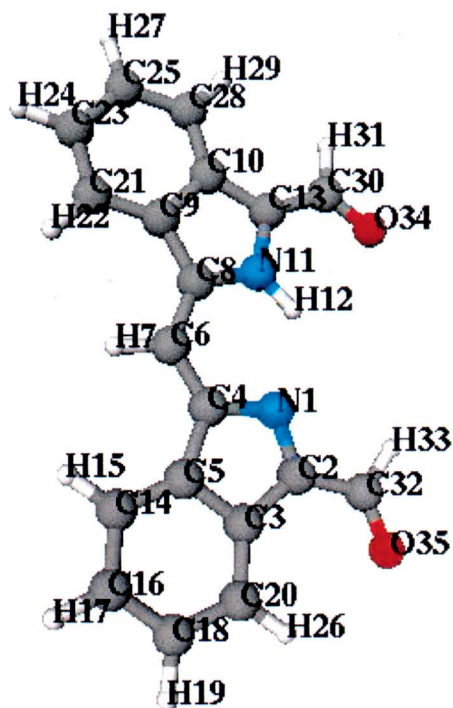
1	7	-1.369653	-0.216026	0.041822
2	6	-2.657415	0.093875	0.037402
3	6	-3.490786	-1.110688	0.036136
4	6	-1.251758	-1.607371	0.024163
5	6	-2.581996	-2.200847	0.025652
6	6	-0.032343	-2.253265	-0.001157
7	1	-0.039557	-3.340513	-0.007010
8	6	1.241047	-1.644050	-0.023910
9	6	2.551078	-2.205919	-0.027768
10	6	3.484947	-1.112757	-0.035327
11	7	1.415320	-0.276007	-0.037537
12	1	0.590248	0.328813	0.000248
13	6	2.722987	0.092465	-0.034570
14	6	-3.103924	1.495112	0.054309
15	6	-4.278967	1.901924	-0.605112
16	1	-4.864186	1.175201	-1.159976
17	6	-4.676130	3.240174	-0.593511
18	1	-5.580488	3.537096	-1.118874
19	6	-2.338882	2.470114	0.723480
20	1	-1.436056	2.162493	1.242193
21	6	-2.740690	3.804704	0.739297
22	1	-2.142264	4.540852	1.270495
23	6	-3.912318	4.196201	0.081820
24	1	-4.225779	5.236978	0.095076
25	6	3.127486	1.496162	-0.057400
26	6	2.327220	2.465863	-0.697417
27	1	1.420403	2.162365	-1.214431
28	6	2.703209	3.808225	-0.706217
29	1	2.074150	4.537024	-1.210881
30	6	4.315336	1.920353	0.571891
31	1	4.926324	1.199554	1.105827
32	6	4.690194	3.263329	0.554686
33	1	5.606435	3.570105	1.052866
34	6	3.887819	4.214239	-0.083637
35	1	4.181750	5.260411	-0.094798
36	6	-3.050375	-3.519440	0.038758
37	1	-2.362668	-4.362104	0.028833
38	6	-4.427354	-3.738197	0.075512
39	1	-4.809658	-4.755850	0.087070
40	6	-5.330628	-2.658942	0.111474
41	1	-6.398522	-2.856204	0.157213
42	6	-4.872587	-1.341497	0.096539
43	6	3.016058	-3.538407	-0.038527
44	1	2.317664	-4.371647	-0.027900
45	6	4.379580	-3.766985	-0.070199
46	1	4.754238	-4.787309	-0.078634
47	6	5.305084	-2.689227	-0.105519
48	1	-5.580601	-0.519892	0.147425
49	1	6.369108	-2.906063	-0.150149
50	6	4.874960	-1.375606	-0.092899
51	1	5.594689	-0.564336	-0.142303

4a geometry (coordinates in Å) optimized at the B3LYP/6-31+G(d) level



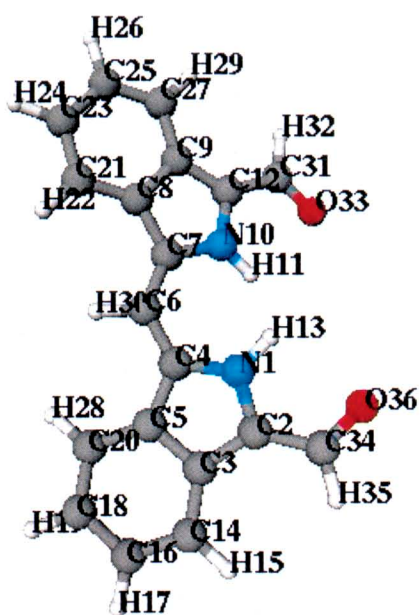
1	7	-1.559117	-0.121116	-0.140516
2	6	-2.893384	0.138059	-0.038466
3	6	-3.526195	-1.074626	0.360669
4	6	-1.261739	-1.470219	0.093800
5	6	-2.514827	-2.083931	0.427867
6	6	0.000000	-2.052273	0.000000
7	1	0.000000	-3.139631	0.000000
8	6	1.261740	-1.470219	-0.093799
9	6	2.514828	-2.083931	-0.427866
10	6	3.526195	-1.074626	-0.360669
11	7	1.559117	-0.121116	0.140516
12	1	0.940390	0.500679	0.647216
13	6	2.893384	0.138059	0.038465
14	6	-3.444429	1.454388	-0.336561
15	6	-4.701295	1.577932	-0.963418
16	1	-5.253452	0.687517	-1.246946
17	6	-5.215247	2.836872	-1.268805
18	1	-6.179309	2.917768	-1.762723
19	6	-2.723303	2.625431	-0.021219
20	1	-1.777715	2.553310	0.511440
21	6	-3.243893	3.881130	-0.327048
22	1	-2.686343	4.775539	-0.063654
23	6	-4.490694	3.990649	-0.952503
24	1	-4.896670	4.970155	-1.188317
25	6	3.444430	1.454388	0.336561
26	6	2.723303	2.625432	0.021218
27	1	1.777716	2.553310	-0.511442
28	6	3.243893	3.881130	0.327048
29	1	2.686343	4.775539	0.063653
30	6	4.701295	1.577932	0.963419
31	1	5.253451	0.687517	1.246947
32	6	5.215246	2.836873	1.268806
33	1	6.179308	2.917768	1.762725
34	6	4.490693	3.990649	0.952504
35	1	4.896669	4.970155	1.188318
36	6	-2.846201	-3.394278	0.819424
37	1	-2.089553	-4.170695	0.889772
38	6	-4.169155	-3.675775	1.123200
39	1	-4.446598	-4.684000	1.417497
40	6	-5.169987	-2.671760	1.078056
41	1	-6.189782	-2.928088	1.349147
42	6	-4.863004	-1.374337	0.710160
43	6	2.846201	-3.394279	-0.819424
44	1	2.089553	-4.170695	-0.889770
45	6	4.169155	-3.675775	-1.123200
46	1	4.446598	-4.684000	-1.417497
47	6	5.169987	-2.671760	-1.078057
48	1	-5.628271	-0.604957	0.707491
49	1	6.189781	-2.928088	-1.349148
50	6	4.863004	-1.374337	-0.710160
51	1	5.628271	-0.604957	-0.707493
52	1	-0.940390	0.500679	-0.647216

4b geometry (coordinates in Å) optimized at the B3LYP/6-31+G(d) level



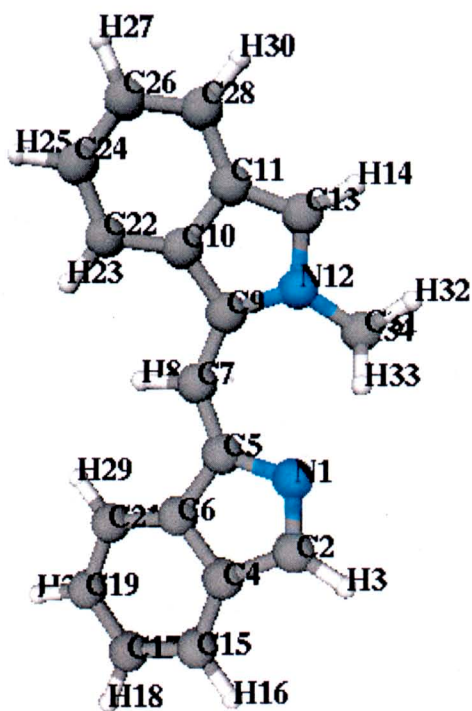
1	7	1.246507	-1.034621	0.000000
2	6	2.522516	-1.381692	0.000000
3	6	3.411843	-0.224389	0.000000
4	6	1.191669	0.359572	0.000000
5	6	2.553249	0.901409	0.000000
6	6	0.000000	1.048728	0.000000
7	1	0.047712	2.134788	0.000000
8	6	-1.304177	0.491832	0.000000
9	6	-2.575818	1.151954	0.000000
10	6	-3.581435	0.130087	0.000000
11	7	-1.562316	-0.850474	0.000000
12	1	-0.812208	-1.544919	0.000000
13	6	-2.897289	-1.119043	0.000000
14	6	3.081129	2.194589	0.000000
15	1	2.438648	3.072015	0.000000
16	6	4.471089	2.340722	0.000000
17	1	4.903409	3.337998	0.000000
18	6	5.320908	1.220200	0.000000
19	1	6.397511	1.367914	0.000000
20	6	4.802574	-0.076948	0.000000
21	6	-2.943488	2.513065	0.000000
22	1	-2.191313	3.297694	0.000000
23	6	-4.289960	2.832370	0.000000
24	1	-4.595368	3.875163	0.000000
25	6	-5.287062	1.820751	0.000000
26	1	5.452290	-0.945640	0.000000
27	1	-6.333934	2.111924	0.000000
28	6	-4.950985	0.479491	0.000000
29	1	-5.724177	-0.283591	0.000000
30	6	-3.391803	-2.481126	0.000000
31	1	-4.493284	-2.589161	0.000000
32	6	2.885187	-2.809408	0.000000
33	1	2.022863	-3.504027	0.000000
34	8	-2.662427	-3.468732	0.000000
35	8	4.036131	-3.217202	0.000000

5a geometry (coordinates in Å) optimized at the B3LYP/6-31+G(d) level



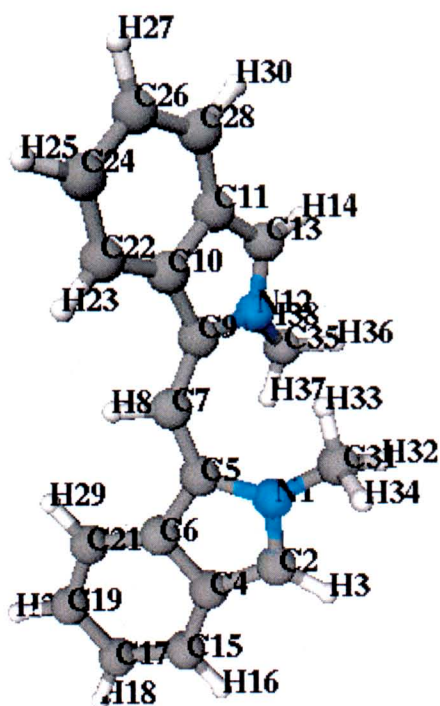
1	7	-1.534990	0.960673	-0.327610
2	6	-2.865917	1.211141	-0.343705
3	6	-3.551630	0.006256	-0.039909
4	6	-1.265109	-0.373935	-0.061246
5	6	-2.550121	-1.004287	0.124635
6	6	-0.000036	-0.958815	0.000329
7	6	1.265058	-0.373959	0.061799
8	6	2.549965	-1.004347	-0.124628
9	6	3.551570	0.006180	0.039430
10	7	1.535056	0.960697	0.327762
11	1	0.884472	1.665258	0.664016
12	6	2.865996	1.211174	0.343149
13	1	-0.884237	1.665217	-0.663552
14	6	-4.922417	-0.301703	0.101156
15	1	-5.687343	0.459702	-0.016417
16	6	-5.264858	-1.608870	0.399200
17	1	-6.310362	-1.878591	0.512520
18	6	-4.273181	-2.607738	0.565275
19	1	-4.582658	-3.621827	0.800375
20	6	-2.920040	-2.320975	0.439696
21	6	2.919868	-2.321196	-0.439119
22	1	2.179002	-3.102354	-0.583163
23	6	4.272929	-2.607982	-0.565108
24	1	4.582303	-3.622181	-0.799891
25	6	5.264654	-1.609051	-0.399781
26	1	6.310103	-1.878841	-0.513375
27	6	4.922315	-0.301779	-0.102034
28	1	-2.179170	-3.101986	0.584398
29	1	5.687252	0.459674	0.015082
30	1	-0.000034	-2.045869	0.000316
31	6	3.323149	2.565448	0.693945
32	1	4.410153	2.747992	0.696545
33	8	2.517636	3.439212	0.971834
34	6	-3.322865	2.565614	-0.693994
35	1	-4.409877	2.748159	-0.697360
36	8	-2.517142	3.439412	-0.971223

5b geometry (coordinates in Å) optimized at the B3LYP/6-31+G(d) level



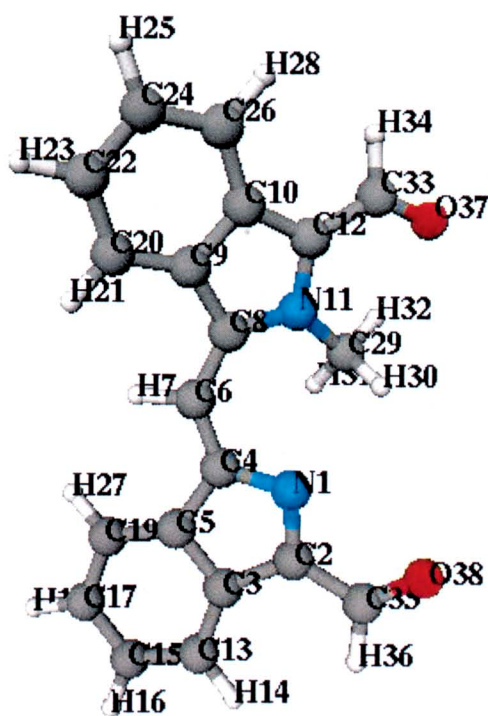
1	7	-1.665396	1.724314	-0.383776
2	6	-2.968811	1.787201	-0.518627
3	1	-3.455433	2.715358	-0.807599
4	6	-3.627129	0.520967	-0.255544
5	6	-1.341648	0.405795	-0.025204
6	6	-2.579214	-0.378247	0.065170
7	6	-0.079457	-0.113777	0.149247
8	1	-0.087664	-1.190708	0.311576
9	6	1.257253	0.372699	0.123727
10	6	2.405003	-0.472785	0.011369
11	6	3.569623	0.364406	-0.004005
12	7	1.749515	1.677460	0.188082
13	6	3.104584	1.681622	0.118489
14	1	3.652343	2.611913	0.184024
15	6	-4.963482	0.104240	-0.268168
16	1	-5.765071	0.796898	-0.514927
17	6	-5.244404	-1.226217	0.044909
18	1	-6.273095	-1.577360	0.043617
19	6	-4.206416	-2.122477	0.365311
20	1	-4.449607	-3.154058	0.607856
21	6	-2.871928	-1.709641	0.380198
22	6	2.554313	-1.874118	-0.108871
23	1	1.689646	-2.532735	-0.118141
24	6	3.827659	-2.401609	-0.219114
25	1	3.955371	-3.477695	-0.305023
26	6	4.981403	-1.566891	-0.229412
27	1	5.963566	-2.022691	-0.323126
28	6	4.865397	-0.195726	-0.127608
29	1	-2.087677	-2.418396	0.637217
30	1	5.745409	0.442746	-0.141983
31	6	0.996223	2.893351	0.503331
32	1	1.606124	3.754280	0.220360
33	1	0.049448	2.895264	-0.035309
34	1	0.793993	2.932002	1.580129

6a geometry (coordinates in Å) optimized at the B3LYP/6-31+G(d) level



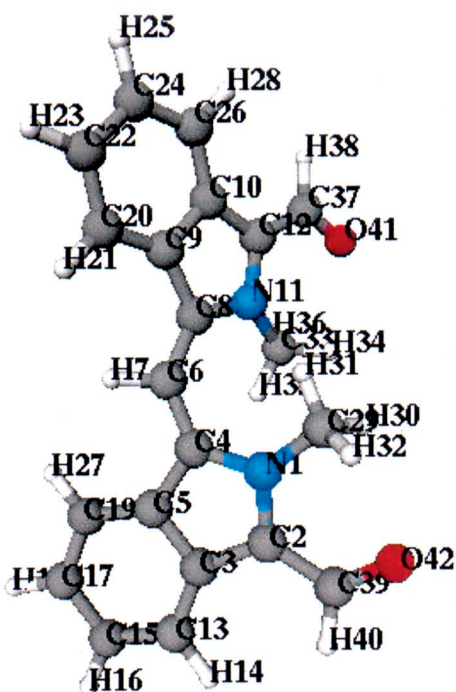
1	7	1.617357	1.369681	0.710487
2	6	2.959446	1.494783	0.772384
3	1	3.407432	2.382359	1.202144
4	6	3.576447	0.323651	0.292197
5	6	1.274715	0.093838	0.209362
6	6	2.521430	-0.581449	-0.040635
7	6	-0.000012	-0.438284	0.000001
8	1	-0.000077	-1.528315	0.000078
9	6	-1.274725	0.093939	-0.209172
10	6	-2.521451	-0.581259	0.041032
11	6	-3.576444	0.323700	-0.292238
12	7	-1.617316	1.369743	-0.710411
13	6	-2.959405	1.494822	-0.772422
14	1	-3.407333	2.382286	-1.202460
15	6	4.932158	-0.038580	0.123981
16	1	5.730200	0.655100	0.372730
17	6	5.208908	-1.301278	-0.367096
18	1	6.239365	-1.614954	-0.503879
19	6	4.163030	-2.198450	-0.704621
20	1	4.418656	-3.181596	-1.089494
21	6	2.826460	-1.850844	-0.563371
22	6	-2.826575	-1.850708	0.563596
23	1	-2.046361	-2.549914	0.851101
24	6	-4.163123	-2.198338	0.704652
25	1	-4.418717	-3.181500	1.089517
26	6	-5.208964	-1.301255	0.366836
27	1	-6.239408	-1.615054	0.503378
28	6	-4.932172	-0.038640	-0.124464
29	1	2.046215	-2.550006	-0.850845
30	1	-5.730170	0.654926	-0.373649
31	6	0.731473	2.274631	1.457665
32	1	0.870495	3.300383	1.107102
33	1	-0.305681	1.980597	1.316538
34	1	0.968004	2.219925	2.524060
35	6	-0.731315	2.274584	-1.457586
36	1	-0.869491	3.300258	-1.106462
37	1	0.305733	1.979826	-1.317121
38	1	-0.968430	2.220534	-2.523879

6b geometry (coordinates in Å) optimized at the B3LYP/6-31+G(d) level



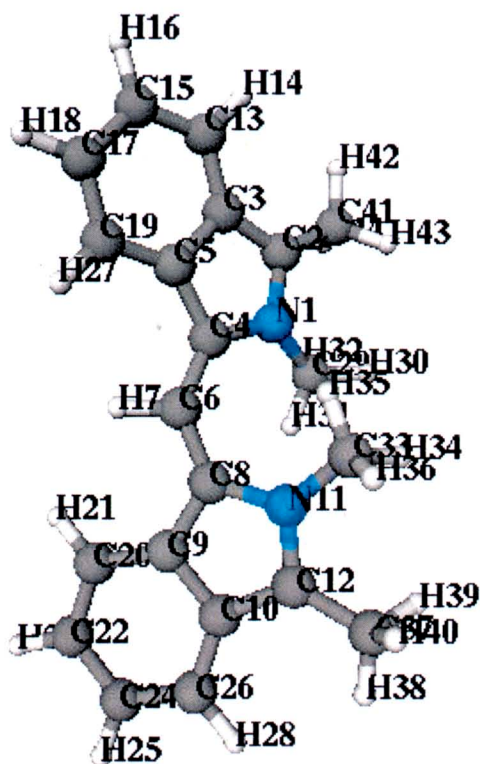
1	7	1.586061	1.061450	0.269161
2	6	2.886320	1.209401	0.421708
3	6	3.628754	-0.017600	0.118963
4	6	1.358028	-0.250298	-0.129643
5	6	2.639688	-0.963721	-0.239873
6	6	0.114253	-0.815630	-0.301042
7	1	0.131715	-1.893614	-0.453806
8	6	-1.215796	-0.310158	-0.233618
9	6	-2.352429	-1.129131	0.073330
10	6	-3.496052	-0.280526	0.090502
11	7	-1.677813	0.975409	-0.425293
12	6	-3.041135	1.028790	-0.236226
13	6	4.984484	-0.363263	0.124033
14	1	5.753719	0.354300	0.396573
15	6	5.335784	-1.666944	-0.234077
16	1	6.382299	-1.959621	-0.238312
17	6	4.353609	-2.606280	-0.592147
18	1	4.653792	-3.613380	-0.869329
19	6	2.998517	-2.263872	-0.601047
20	6	-2.478203	-2.503148	0.366973
21	1	-1.611570	-3.158568	0.378612
22	6	-3.736408	-3.005432	0.648178
23	1	-3.856714	-4.062497	0.869186
24	6	-4.877093	-2.160920	0.663169
25	1	-5.848761	-2.588172	0.895699
26	6	-4.771989	-0.808699	0.393985
27	1	2.252242	-3.000788	-0.888867
28	1	-5.652841	-0.173910	0.418498
29	6	-0.881831	2.105968	-0.930693
30	1	-0.412967	2.638919	-0.103037
31	1	-0.096627	1.714744	-1.575848
32	1	-1.542964	2.773199	-1.477399
33	6	-3.885029	2.203914	-0.360124
34	1	-4.954065	1.983543	-0.169811
35	6	3.484392	2.490670	0.860116
36	1	4.587060	2.470921	0.988001
37	8	-3.539325	3.348532	-0.636215
38	8	2.860670	3.513741	1.074711

7a geometry (coordinates in Å) optimized at the B3LYP/6-31+G(d) level



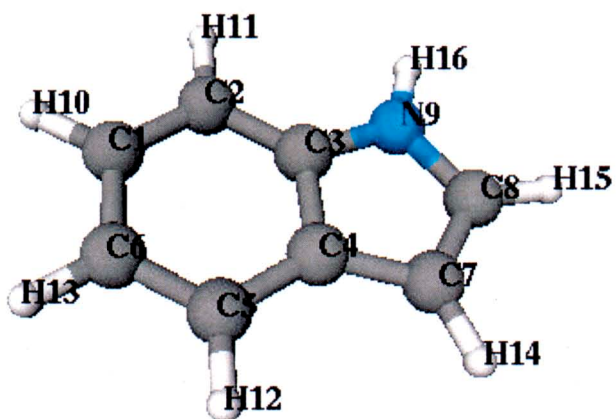
1	7	1.676964	0.849908	0.605645
2	6	3.034661	0.969825	0.552044
3	6	3.588863	-0.217208	-0.006288
4	6	1.291053	-0.401450	0.108879
5	6	2.499738	-1.098472	-0.259705
6	6	-0.000003	-0.932496	0.000016
7	1	-0.000113	-2.022358	0.000030
8	6	-1.291025	-0.401246	-0.108487
9	6	-2.499681	-1.098261	0.260153
10	6	-3.588844	-0.217146	0.006399
11	7	-1.676954	0.849938	-0.605650
12	6	-3.034673	0.969743	-0.552292
13	6	4.914319	-0.599616	-0.307743
14	1	5.752323	0.067838	-0.132399
15	6	5.120401	-1.861188	-0.841584
16	1	6.129062	-2.186668	-1.077694
17	6	4.035770	-2.736020	-1.094753
18	1	4.236413	-3.716743	-1.516250
19	6	2.724396	-2.363996	-0.825197
20	6	-2.724353	-2.363819	0.825582
21	1	-1.905938	-3.041478	1.051913
22	6	-4.035712	-2.735979	1.094844
23	1	-4.236303	-3.716725	1.516328
24	6	-5.120384	-1.861348	0.841205
25	1	-6.129054	-2.187054	1.076927
26	6	-4.914372	-0.599819	0.307199
27	1	1.905973	-3.041631	-1.051475
28	1	-5.752424	0.067401	0.131258
29	6	0.812191	1.750993	1.390538
30	1	0.753983	2.731366	0.917828
31	1	-0.175798	1.304404	1.472446
32	1	1.237101	1.878152	2.387378
33	6	-0.812158	1.750806	-1.390759
34	1	-0.753964	2.731335	-0.918371
35	1	0.175837	1.304203	-1.472516
36	1	-1.237031	1.877649	-2.387650
37	6	-3.780681	2.146867	-1.026736
38	1	-4.877588	2.063308	-0.928204
39	6	3.780618	2.147244	1.025875
40	1	4.877654	2.062982	0.929354
41	8	-3.264573	3.152724	-1.483857
42	8	3.264456	3.152354	1.484604

7b geometry (coordinates in Å) optimized at the B3LYP/6-31+G(d) level



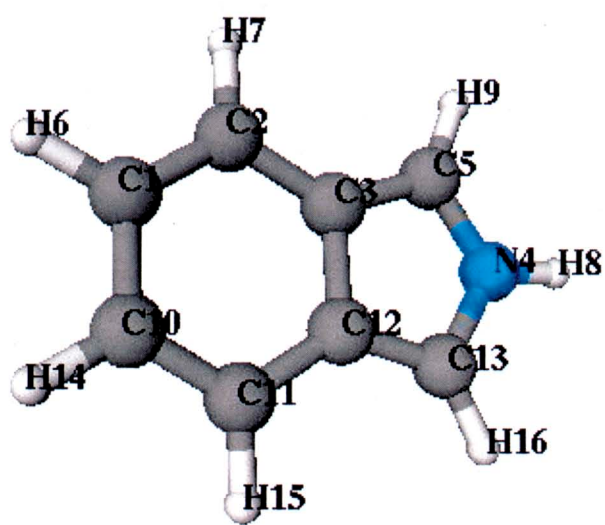
1	7	-1.669606	1.095242	-0.631798
2	6	-3.021403	1.222290	-0.630481
3	6	-3.586766	0.033373	-0.104618
4	6	-1.286674	-0.175205	-0.140646
5	6	-2.510404	-0.858801	0.175984
6	6	0.000017	-0.700869	-0.000054
7	1	0.000093	-1.791053	-0.000006
8	6	1.286669	-0.175034	0.140277
9	6	2.510410	-0.858580	-0.176401
10	6	3.586761	0.033461	0.104653
11	7	1.669544	1.095405	0.631482
12	6	3.021349	1.222417	0.630380
13	6	-4.926209	-0.345117	0.137755
14	1	-5.748277	0.334340	-0.068438
15	6	-5.165559	-1.608628	0.647540
16	1	-6.184566	-1.930450	0.840162
17	6	-4.094849	-2.493952	0.931867
18	1	-4.318606	-3.478088	1.333812
19	6	-2.772968	-2.130462	0.718029
20	6	2.773079	-2.130324	-0.718240
21	1	1.969322	-2.817898	-0.966309
22	6	4.094967	-2.493859	-0.931766
23	1	4.318754	-3.478047	-1.333582
24	6	5.165645	-1.608594	-0.647181
25	1	6.184667	-1.930514	-0.839517
26	6	4.926240	-0.345104	-0.137335
27	1	-1.969149	-2.817939	0.966093
28	1	5.748271	0.334282	0.069193
29	6	-0.806665	1.997266	-1.400988
30	1	-0.809792	2.999757	-0.965007
31	1	0.209101	1.608387	-1.409711
32	1	-1.163324	2.059043	-2.433275
33	6	0.806500	1.997302	1.400702
34	1	0.809426	2.999813	0.964754
35	1	-0.209197	1.608244	1.409462
36	1	1.163190	2.059106	2.432978
37	6	3.717474	2.418027	1.186326
38	1	4.780812	2.383534	0.939763
39	1	3.307218	3.353799	0.788618
40	1	3.634470	2.462223	2.281222
41	6	-3.717513	2.418177	-1.185846
42	1	-4.780793	2.383769	-0.939015
43	1	-3.306999	3.353762	-0.787972
44	1	-3.634785	2.462707	-2.280749

8b geometry (coordinates in Å) optimized at the B3LYP/6-31+G(d) level



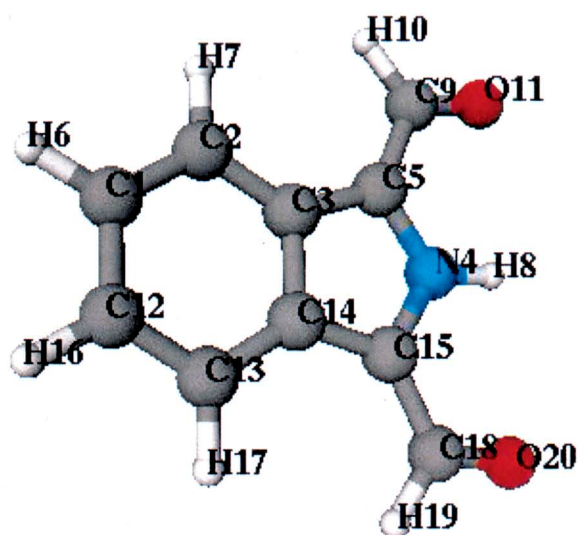
1	6	2.255557	-0.065904	0.000000
2	6	1.369989	1.008033	0.000000
3	6	0.000000	0.716851	0.000000
4	6	-0.495368	-0.618998	0.000000
5	6	0.426845	-1.682999	0.000000
6	6	1.788211	-1.399122	0.000000
7	6	-1.931371	-0.531785	0.000000
8	6	-2.255443	0.801404	0.000000
9	7	-1.096539	1.558296	0.000000
10	1	3.325658	0.124937	0.000000
11	1	1.731465	2.033846	0.000000
12	1	0.077338	-2.712858	0.000000
13	1	2.507850	-2.213830	0.000000
14	1	-2.633143	-1.355306	0.000000
15	1	-3.223572	1.283840	0.000000
16	1	-1.060346	2.566418	0.000000

9a geometry (coordinates in Å) optimized at the B3LYP/6-31+G(d) level



1	6	0.000000	0.716081	-2.159379
2	6	0.000000	1.432762	-0.985313
3	6	0.000000	0.726397	0.251224
4	7	0.000000	0.000000	2.353327
5	6	0.000000	1.135896	1.585946
6	1	0.000000	1.240310	-3.111948
7	1	0.000000	2.520410	-0.996613
8	1	0.000000	0.000000	3.363741
9	1	0.000000	2.118516	2.035180
10	6	0.000000	-0.716081	-2.159379
11	6	0.000000	-1.432762	-0.985313
12	6	0.000000	-0.726397	0.251224
13	6	0.000000	-1.135896	1.585946
14	1	0.000000	-1.240310	-3.111948
15	1	0.000000	-2.520410	-0.996613
16	1	0.000000	-2.118516	2.035180

10a geometry (coordinates in Å) optimized at the B3LYP/6-31+G(d) level



1	6	0.000000	0.711494	-3.057513
2	6	0.000000	1.431300	-1.879107
3	6	0.000000	0.719059	-0.656474
4	7	0.000000	0.000000	1.465095
5	6	0.000000	1.129797	0.704599
6	1	0.000000	1.237827	-4.008129
7	1	0.000000	2.517592	-1.894511
8	1	0.000000	0.000000	2.481561
9	6	0.000000	2.442087	1.322836
10	1	0.000000	3.302286	0.626945
11	8	0.000000	2.613887	2.537629
12	6	0.000000	-0.711494	-3.057513
13	6	0.000000	-1.431300	-1.879107
14	6	0.000000	-0.719059	-0.656474
15	6	0.000000	-1.129797	0.704599
16	1	0.000000	-1.237827	-4.008129
17	1	0.000000	-2.517592	-1.894511
18	6	0.000000	-2.442087	1.322836
19	1	0.000000	-3.302286	0.626945
20	8	0.000000	-2.613887	2.537629

11a geometry (coordinates in Å) optimized at the B3LYP/6-31+G(d) level