Supplementary Information

Computational Design and *in silico* Screening of Selective Chromone-Based COX-2 Inhibitors

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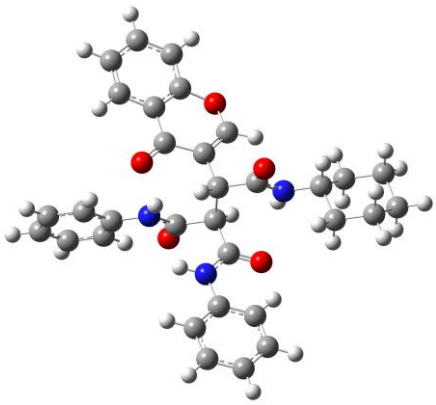
Table S1. Optimized structure for compound (**1**) and cartesian Z-matrix

Compound **1**	

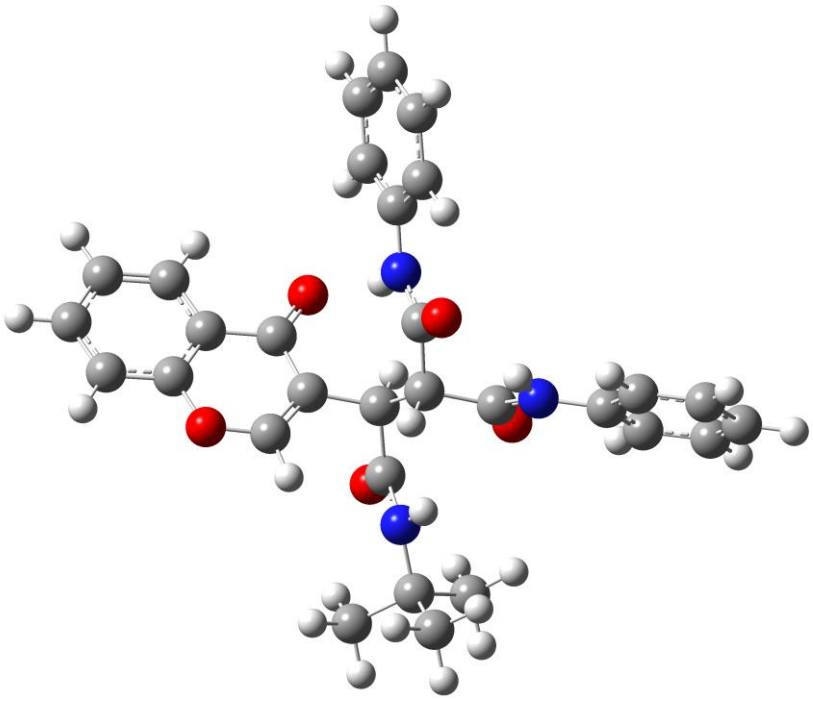
Center number	Atom	Standard orientation: coordinates / Angstroms		
		X	Y	Z
1	C	-1.02223	1.636214	0.082929
2	C	-2.20298	1.456931	0.928802
3	C	-3.23558	2.492916	0.78778
4	C	-3.07462	3.517866	-0.15607
5	C	-0.98014	2.676679	-0.78239
6	H	-4.52051	1.678258	2.291214
7	C	-4.40724	2.476972	1.566569
8	C	-4.04327	4.50911	-0.33869
9	H	-0.13419	2.890466	-1.42639
10	C	-5.18773	4.471028	0.444526
11	C	-5.3723	3.455907	1.400217
12	H	-3.87839	5.281754	-1.0813
13	H	-5.94727	5.235784	0.315235
14	H	-6.27358	3.441172	2.004331
15	O	-1.95678	3.591175	-0.94557
16	O	-2.33101	0.488055	1.695163
17	C	0.159337	0.687423	0.247572
18	H	-0.03387	0.131641	1.170087
19	C	0.292207	-0.30817	-0.94455
20	H	0.562279	0.244466	-1.84667
21	C	1.397023	1.56506	0.597429
22	O	1.37848	2.192671	1.65014
23	C	1.459533	-1.30596	-0.7434
24	O	2.572508	-1.05477	-1.20554
25	C	-0.97504	-1.0864	-1.37057
26	O	-1.10628	-1.39312	-2.54667
27	N	2.383907	1.679597	-0.33541

28	H	2.508919	0.905447	-0.98548
29	N	1.16041	-2.41607	-0.0126
30	H	0.187351	-2.52073	0.25007
31	N	-1.81611	-1.49215	-0.35776
32	H	-1.77598	-0.96891	0.518728
33	C	3.59456	2.455401	-0.04039
34	C	4.605191	1.644293	0.792303
35	C	4.22346	2.952116	-1.35033
36	H	3.26675	3.313854	0.555253
37	C	5.891064	2.444326	1.050529
38	H	4.843935	0.718636	0.250263
39	H	4.134114	1.353673	1.736746
40	C	5.510146	3.750389	-1.08838
41	H	4.457573	2.085507	-1.98609
42	H	3.496093	3.560175	-1.90104
43	C	6.519501	2.942089	-0.25942
44	H	6.606965	1.830363	1.609298
45	H	5.65709	3.306962	1.690205
46	H	5.956233	4.059162	-2.04093
47	H	5.257358	4.674216	-0.54922
48	H	7.408293	3.548913	-0.04962
49	H	6.861585	2.079108	-0.84811
50	C	2.000946	-3.48934	0.369379
51	C	3.365498	-3.55417	0.053504
52	C	1.406661	-4.5253	1.10596
53	C	4.111034	-4.65291	0.481523
54	H	3.819901	-2.75848	-0.5183
55	C	2.165214	-5.61408	1.52433
56	H	0.347941	-4.47569	1.349374
57	C	3.524577	-5.68434	1.214654
58	H	5.167368	-4.69756	0.232928
59	H	1.690251	-6.40773	2.093119
60	H	4.117695	-6.5331	1.54034
61	C	-2.99721	-2.27271	-0.49555
62	C	-3.26242	-3.07597	-1.61422
63	C	-3.90207	-2.25198	0.57775
64	C	-4.42528	-3.8464	-1.64112
65	H	-2.57505	-3.07902	-2.44751
66	C	-5.05626	-3.02926	0.533555
67	H	-3.70027	-1.61464	1.433562
68	C	-5.32543	-3.8328	-0.57574

69	H	-4.62433	-4.46465	-2.51177
70	H	-5.74778	-3.00268	1.370726
71	H	-6.22627	-4.43783	-0.60986

Table S2. Optimized structure for compound (**2**) and cartesian Z-matrix

Compound **2**



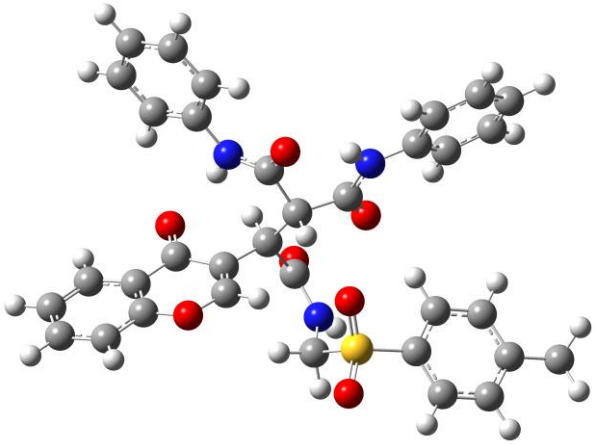
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	1.618278	-1.084274	0.004379
2	C	2.716767	-0.435206	0.726246
3	C	4.065669	-0.75483	0.236123
4	C	4.226787	-1.578559	-0.886925
5	C	1.90831	-1.874831	-1.056669
6	H	5.077868	0.402696	1.722644
7	C	5.216398	-0.234413	0.856148
8	C	5.490549	-1.886988	-1.39887
9	H	1.160942	-2.419022	-1.622657
10	C	6.608644	-1.362369	-0.766772
11	C	6.474859	-0.535916	0.363178
12	H	5.568534	-2.527393	-2.270375
13	H	7.596583	-1.595405	-1.15172
14	H	7.359921	-0.134095	0.845547
15	O	3.146373	-2.118708	-1.534069
16	O	2.522871	0.342366	1.673331
17	C	0.193182	-0.922597	0.523736
18	H	0.270869	-0.503534	1.529107
19	C	-0.685375	0.00564	-0.344295

20	H	-0.789553	-0.419954	-1.350052
21	C	-0.374573	-2.345058	0.785587
22	O	-0.007486	-2.952587	1.780668
23	C	-2.117972	0.121644	0.267266
24	O	-2.396906	-0.427594	1.325989
25	C	-0.189781	1.437475	-0.656999
26	O	-0.676394	2.001633	-1.643892
27	N	-1.154686	-2.893615	-0.198539
28	H	-1.588205	-2.245694	-0.839991
29	N	-2.981785	0.836023	-0.510439
30	H	-2.542057	1.316383	-1.293454
31	N	0.681984	2.008905	0.207371
32	H	1.078195	1.423227	0.942989
33	C	-4.342184	1.134326	-0.274732
34	C	-5.063976	0.643447	0.823799
35	C	-4.982931	1.957841	-1.214057
36	C	-6.410122	0.982943	0.961911
37	H	-4.568191	0.017205	1.551495
38	C	-6.326034	2.287184	-1.059859
39	H	-4.422506	2.339458	-2.063938
40	C	-7.049955	1.800312	0.030159
41	H	-6.96137	0.600642	1.816244
42	H	-6.805832	2.926822	-1.794782
43	H	-8.097772	2.056793	0.151499
44	C	1.222337	3.32075	0.163693
45	C	0.797763	4.308452	-0.737182
46	C	2.224787	3.617177	1.101623
47	C	1.378784	5.575844	-0.683251
48	H	0.032418	4.077171	-1.462954
49	C	2.791117	4.887751	1.140464
50	H	2.55973	2.844115	1.78643
51	C	2.371646	5.876618	0.248656
52	H	1.044062	6.335803	-1.38356
53	H	3.564481	5.10296	1.872051
54	H	2.81388	6.867683	0.279941
55	C	-1.88347	-4.185281	-0.060954
56	C	-2.704039	-4.348295	-1.349785
57	H	-3.252818	-5.293647	-1.328742
58	H	-3.43912	-3.541804	-1.458826
59	H	-2.056586	-4.351832	-2.23357
60	C	-0.8718	-5.33682	0.062392

61	H	-0.220042	-5.373555	-0.816968
62	H	-0.254192	-5.20926	0.951914
63	H	-1.402802	-6.291653	0.133447
64	C	-2.819575	-4.142918	1.160999
65	H	-2.242904	-4.019562	2.078859
66	H	-3.52009	-3.306109	1.080917
67	H	-3.394248	-5.072774	1.227452

Table S3. Optimized structure for compound (**3**) and cartesian Z-matrix

Compound **3**



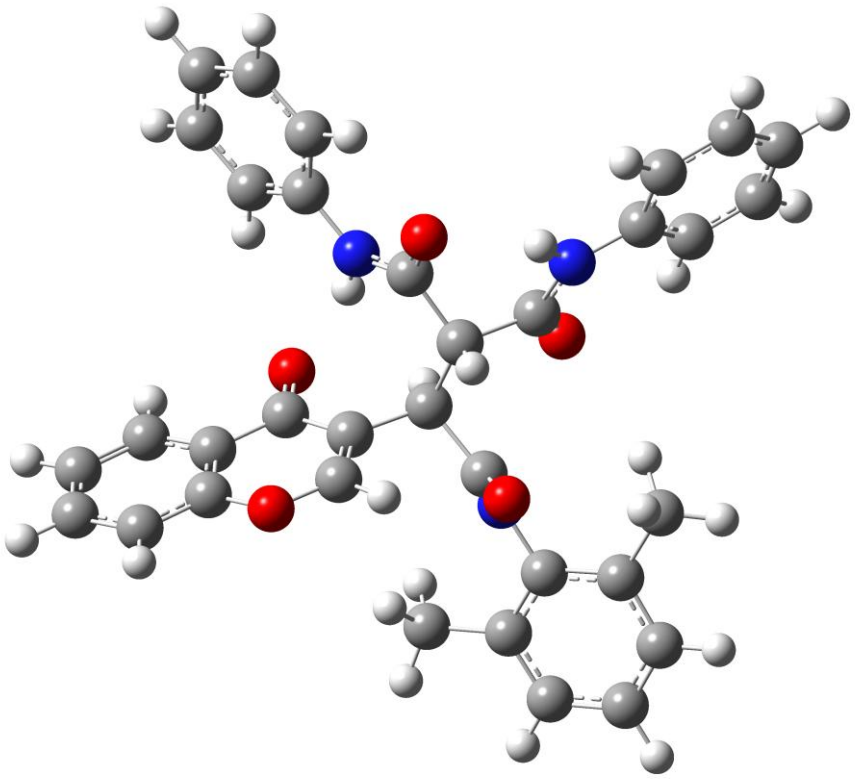
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	1.865386	-1.21009	0.347972
2	C	3.164612	-1.30229	1.036512
3	C	4.115983	-2.2618	0.454506
4	C	3.816954	-2.88858	-0.76272
5	C	1.729327	-1.81633	-0.85806
6	H	5.566869	-2.05143	2.011839
7	C	5.344565	-2.55088	1.075094
8	C	4.700822	-3.78922	-1.36393
9	H	0.86469	-1.70634	-1.50442
10	C	5.901737	-4.06523	-0.72551
11	C	6.226611	-3.44807	0.495561
12	H	4.431444	-4.24702	-2.30922
13	H	6.597218	-4.76463	-1.17898
14	H	7.170909	-3.67426	0.979964
15	O	2.648415	-2.62522	-1.42886
16	O	3.450976	-0.58471	2.00302
17	C	0.805546	-0.30964	0.976297
18	H	1.326384	0.221399	1.775024
19	C	0.285277	0.745974	-0.03874
20	H	-0.03416	0.247476	-0.95867
21	C	-0.21332	-1.05435	1.893039
22	O	-0.20692	-0.79308	3.082203
23	C	-1.00529	1.483681	0.423371

24	O	-1.69385	1.031492	1.334435
25	C	1.369532	1.74569	-0.51111
26	O	1.140155	2.426416	-1.51701
27	N	-1.11498	-2.02865	1.4612
28	H	-1.71548	-2.26972	2.239441
29	N	-1.32445	2.578294	-0.31715
30	H	-0.66716	2.791661	-1.06659
31	N	2.514224	1.846961	0.215939
32	H	2.635508	1.22489	1.007403
33	C	-2.46038	3.408539	-0.21209
34	C	-3.37807	3.343514	0.848131
35	C	-2.64667	4.35824	-1.22963
36	C	-4.46274	4.220982	0.868692
37	H	-3.23047	2.62066	1.637381
38	C	-3.73363	5.225944	-1.19312
39	H	-1.9356	4.409839	-2.05011
40	C	-4.65174	5.162173	-0.14313
41	H	-5.16531	4.166563	1.695675
42	H	-3.86187	5.953195	-1.98946
43	H	-5.50008	5.838947	-0.1138
44	C	3.638531	2.680426	-0.01923
45	C	3.680581	3.679058	-1.00266
46	C	4.751869	2.470744	0.810872
47	C	4.833679	4.453309	-1.13737
48	H	2.826457	3.834507	-1.64455
49	C	5.891787	3.254747	0.662477
50	H	4.719369	1.68631	1.562293
51	C	5.940372	4.252381	-0.31308
52	H	4.859307	5.225555	-1.90083
53	H	6.744564	3.082027	1.312395
54	H	6.829947	4.863861	-0.42893
55	C	-1.14406	-2.93648	0.36541
56	H	-0.16244	-3.13558	-0.06476
57	H	-1.57799	-3.88951	0.676739
58	S	-2.14825	-2.44642	-1.12118
59	O	-1.58848	-1.17036	-1.62057
60	O	-2.15273	-3.63914	-1.98892
61	C	-3.81208	-2.16369	-0.52337
62	C	-4.78583	-3.12548	-0.79785
63	C	-4.11619	-1.00121	0.193511
64	C	-6.08714	-2.91579	-0.34545

65	H	-4.52325	-4.00785	-1.37101
66	C	-5.42201	-0.81805	0.639977
67	H	-3.35694	-0.2556	0.403184
68	C	-6.4245	-1.76552	0.380451
69	H	-6.85325	-3.65408	-0.56547
70	H	-5.66687	0.085019	1.192289
71	C	-7.83009	-1.54959	0.885559
72	H	-8.53614	-2.23946	0.416332
73	H	-7.88469	-1.70422	1.96983
74	H	-8.16967	-0.52777	0.689101

Table S4. Optimized structure for compound (**4**) and cartesian Z-matrix

Compound **4**



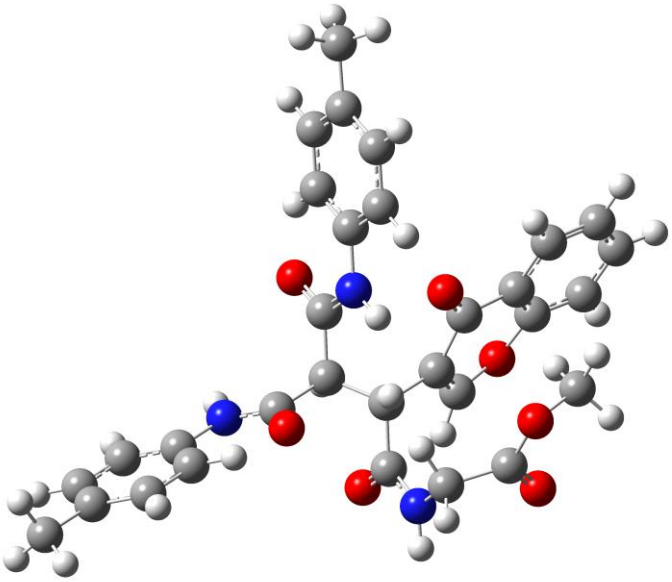
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	-1.39358	0.947822	-0.48366
2	C	-2.50736	0.863274	0.462161
3	C	-3.77994	1.421846	-0.01629
4	C	-3.87403	1.930934	-1.31969
5	C	-1.60857	1.471249	-1.71733
6	H	-4.84251	1.044123	1.801502
7	C	-4.92794	1.444103	0.797122
8	C	-5.07062	2.451958	-1.82145
9	H	-0.82759	1.586354	-2.4594
10	C	-6.18649	2.464404	-0.99732
11	C	-6.1181	1.961816	0.314603
12	H	-5.09886	2.833093	-2.83616
13	H	-7.12189	2.867151	-1.37325
14	H	-7.00102	1.978255	0.945245
15	O	-2.79344	1.938169	-2.1609
16	O	-2.38853	0.342355	1.584177
17	C	-0.01169	0.490327	-0.02886
18	H	-0.05448	0.365181	1.055456

19	C	0.459988	-0.83195	-0.67287
20	H	0.651167	-0.63111	-1.73181
21	C	1.001622	1.599327	-0.38824
22	O	1.370676	1.755964	-1.54904
23	C	1.816815	-1.2648	-0.04633
24	O	2.309437	-0.63912	0.888136
25	C	-0.47904	-2.05223	-0.67172
26	O	-0.29342	-2.92222	-1.5282
27	N	1.365182	2.404948	0.646468
28	H	1.007431	2.160856	1.559487
29	N	2.367676	-2.35421	-0.65029
30	H	1.770092	-2.797	-1.34447
31	N	-1.39862	-2.13542	0.325189
32	H	-1.48789	-1.34027	0.95479
33	C	3.579257	-3.01594	-0.35555
34	C	4.474628	-2.58733	0.635865
35	C	3.881077	-4.15675	-1.11605
36	C	5.652458	-3.3042	0.847713
37	H	4.238806	-1.71285	1.224791
38	C	5.060156	-4.86032	-0.89077
39	H	3.186777	-4.48877	-1.88392
40	C	5.955501	-4.43786	0.093641
41	H	6.340002	-2.9661	1.617794
42	H	5.277605	-5.74107	-1.48784
43	H	6.875896	-4.98584	0.269926
44	C	-2.33175	-3.17359	0.574419
45	C	-2.35837	-4.38322	-0.13533
46	C	-3.25945	-2.95013	1.605111
47	C	-3.30785	-5.34928	0.199349
48	H	-1.64847	-4.55053	-0.93175
49	C	-4.19755	-3.92686	1.925318
50	H	-3.24336	-2.00577	2.141444
51	C	-4.22817	-5.1342	1.224858
52	H	-3.32155	-6.28383	-0.35424
53	H	-4.90759	-3.7405	2.725858
54	H	-4.96023	-5.8959	1.475161
55	C	2.178899	3.579212	0.552795
56	C	1.613187	4.794834	0.986239
57	C	3.506795	3.502772	0.092459
58	C	2.396755	5.950716	0.937676
59	C	4.248975	4.690381	0.048433

60	C	3.706361	5.90243	0.464413
61	H	1.970118	6.894304	1.266766
62	H	5.27503	4.650724	-0.30689
63	H	4.304707	6.808105	0.426124
64	C	0.191491	4.852244	1.492995
65	H	-0.5045	4.376174	0.794609
66	H	0.075656	4.338966	2.45689
67	H	-0.12534	5.887734	1.639403
68	C	4.135834	2.200905	-0.33172
69	H	3.846737	1.379366	0.329595
70	H	3.806084	1.924912	-1.3382
71	H	5.225898	2.284427	-0.33185

Table S5. Optimized structure for compound (**5**) and cartesian Z-matrix

Compound **5**



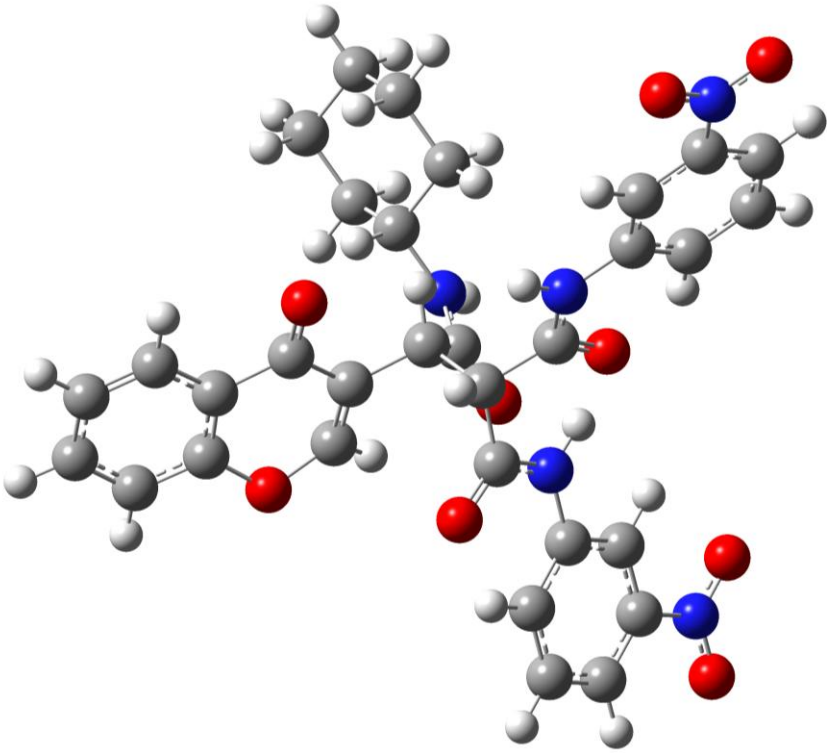
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	-1.60621	1.077401	-0.93967
2	C	-2.57177	0.48891	-0.01296
3	C	-3.93444	0.337322	-0.5389
4	C	-4.21665	0.701015	-1.86332
5	C	-2.00266	1.395777	-2.19715
6	H	-4.74447	-0.47145	1.268104
7	C	-4.9763	-0.18786	0.247507
8	C	-5.4954	0.555173	-2.41035
9	H	-1.34987	1.859783	-2.9264
10	C	-6.50479	0.038887	-1.61151
11	C	-6.24811	-0.33387	-0.27971
12	H	-5.66783	0.848816	-3.43979
13	H	-7.50272	-0.07827	-2.0226
14	H	-7.04878	-0.73826	0.331101
15	O	-3.24729	1.212227	-2.6827
16	O	-2.25609	0.118692	1.133139
17	C	-0.19608	1.368421	-0.43726
18	H	-0.22278	1.26334	0.646692
19	C	0.889938	0.424154	-1.00257
20	H	0.997018	0.64487	-2.06902
21	C	0.178555	2.810192	-0.83821

22	O	0.445794	3.0741	-2.00955
23	C	2.256625	0.751776	-0.33605
24	O	2.338977	1.579393	0.569103
25	C	0.680433	-1.10032	-0.94039
26	O	1.321285	-1.79998	-1.73195
27	N	0.14226	3.782187	0.111735
28	H	0.338726	4.70355	-0.25371
29	N	3.299848	0.060491	-0.8696
30	H	3.028572	-0.65714	-1.53819
31	N	-0.13023	-1.58619	0.03432
32	H	-0.64146	-0.91571	0.606199
33	C	4.666484	0.105409	-0.5175
34	C	5.200659	1.005948	0.414431
35	C	5.523786	-0.79901	-1.16165
36	C	6.568413	0.981672	0.683931
37	H	4.54769	1.707736	0.913027
38	C	6.884831	-0.80512	-0.87721
39	C	7.437435	0.083222	0.054658
40	H	6.96775	1.688363	1.407479
41	H	7.528887	-1.51399	-1.3916
42	C	-0.43582	-2.9403	0.324495
43	C	0.182954	-4.0334	-0.29717
44	C	-1.41472	-3.17216	1.303638
45	C	-0.18128	-5.32764	0.073448
46	H	0.927733	-3.86349	-1.06062
47	C	-1.759	-4.4721	1.657038
48	C	-1.14781	-5.57903	1.053176
49	H	0.305915	-6.16522	-0.41995
50	H	-2.52162	-4.62813	2.416223
51	H	5.119553	-1.49717	-1.8905
52	H	-1.9111	-2.32728	1.772251
53	C	0.002649	3.614846	1.53922
54	H	0.341801	4.530573	2.033229
55	H	0.653634	2.813914	1.901398
56	C	-1.4382	3.348588	1.976835
57	O	-2.41197	3.413174	1.261469
58	O	-1.46575	3.023542	3.281129
59	C	-2.75937	2.651465	3.795585
60	H	-2.60489	2.447507	4.854651
61	H	-3.47602	3.464677	3.660121
62	H	-3.11754	1.759421	3.277158

63	C	8.910726	0.052359	0.385225
64	H	9.129588	-0.68082	1.172037
65	H	9.51195	-0.22188	-0.48732
66	H	9.260534	1.02542	0.742728
67	C	-1.50313	-6.98824	1.463708
68	H	-0.92428	-7.30788	2.339634
69	H	-2.56181	-7.0743	1.728415
70	H	-1.29735	-7.70245	0.660948

Table S6. Optimized structure for compound (**6**) and cartesian Z-matrix

Compound **6**



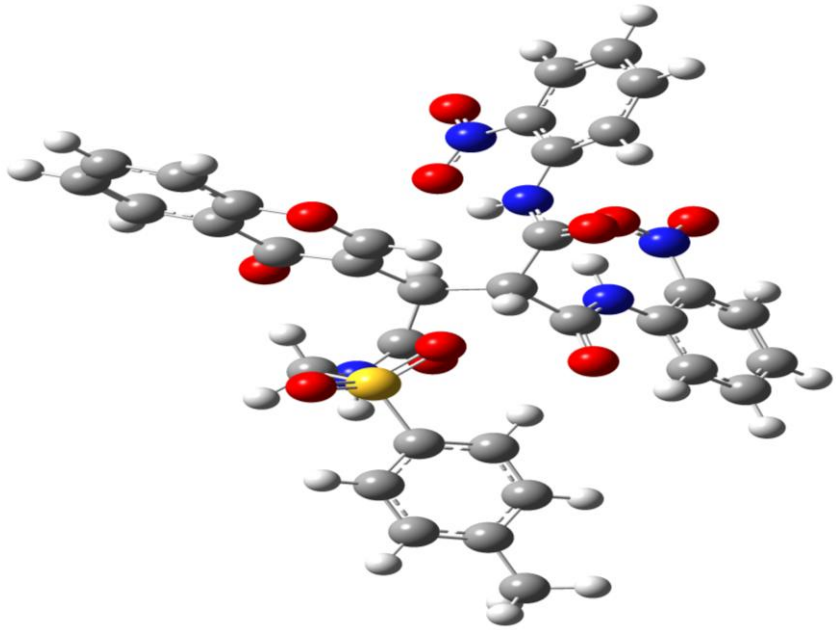
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	-1.01689	1.899225	-0.38078
2	C	-2.07943	1.451932	-1.27888
3	C	-2.77719	2.522485	-2.00109
4	C	-2.36325	3.85384	-1.83852
5	C	-0.6857	3.210917	-0.32981
6	H	-4.15889	1.220451	-2.98888
7	C	-3.85182	2.253751	-2.86919
8	C	-2.99116	4.905471	-2.51245
9	H	0.134361	3.607134	0.255482
10	C	-4.05044	4.613025	-3.3594
11	C	-4.48416	3.287101	-3.53965
12	H	-2.63702	5.919076	-2.36128
13	H	-4.54687	5.420024	-3.8892
14	O	-1.31775	4.182926	-1.01488
15	O	-2.36093	0.248464	-1.42825
16	C	-0.28342	0.812201	0.373284
17	H	-1.05949	0.083297	0.62638
18	C	0.724414	0.065902	-0.57411
19	H	0.306798	0.173831	-1.58024

20	C	0.357085	1.242476	1.704032
21	O	1.569348	1.216093	1.879727
22	C	2.077464	0.805536	-0.68214
23	O	2.063993	1.967803	-1.07611
24	C	0.702373	-1.44788	-0.29473
25	O	1.647243	-2.08956	0.165134
26	N	-0.48868	1.668802	2.691526
27	H	0.013838	1.876934	3.54771
28	N	3.194866	0.069584	-0.42746
29	H	3.006056	-0.8585	-0.04712
30	N	-0.50642	-1.99997	-0.62791
31	H	-1.20854	-1.34697	-0.98358
32	C	4.531853	0.489462	-0.46094
33	C	4.940149	1.773488	-0.86671
34	C	5.501179	-0.44638	-0.0731
35	C	6.29638	2.100028	-0.87884
36	H	4.189157	2.492367	-1.16047
37	C	6.841696	-0.08271	-0.09864
38	C	7.270516	1.181514	-0.49646
39	H	6.595139	3.095081	-1.19343
40	C	-0.93385	-3.33557	-0.49977
41	C	-0.11186	-4.38109	-0.04403
42	C	-2.26104	-3.60611	-0.85989
43	C	-0.62492	-5.67584	0.043964
44	H	0.910195	-4.16915	0.234583
45	C	-2.73328	-4.9085	-0.75792
46	C	-1.94061	-5.96269	-0.31052
47	H	0.020205	-6.47416	0.396442
48	H	5.228668	-1.44505	0.246422
49	H	-2.92259	-2.82389	-1.21372
50	H	-5.31358	3.076747	-4.20687
51	C	-1.93988	1.507242	2.817344
52	C	-2.31489	0.19869	3.540415
53	C	-2.53679	2.72592	3.540946
54	H	-2.35934	1.48266	1.806459
55	C	-3.83557	0.064095	3.716363
56	H	-1.82645	0.193142	4.525137
57	H	-1.91119	-0.65829	2.988276
58	C	-4.05641	2.589524	3.723245
59	H	-2.05844	2.81891	4.527295
60	H	-2.29009	3.636744	2.983997

61	C	-4.42787	1.282596	4.439022
62	H	-4.06554	-0.85641	4.26419
63	H	-4.30706	-0.03754	2.728796
64	H	-4.44076	3.453278	4.277235
65	H	-4.54126	2.613055	2.737182
66	H	-5.51719	1.188017	4.511412
67	H	-4.04751	1.313072	5.469712
68	H	8.326292	1.4172	-0.49942
69	H	-2.35453	-6.96034	-0.24898
70	N	7.844545	-1.07954	0.31204
71	O	7.443707	-2.19254	0.654149
72	O	9.028504	-0.74288	0.289146
73	N	-4.13179	-5.17634	-1.13684
74	O	-4.53624	-6.33458	-1.04432
75	O	-4.8139	-4.22654	-1.52202

Table S7. Optimized structure for compound (**7**) and cartesian Z-matrix

Compound **7**



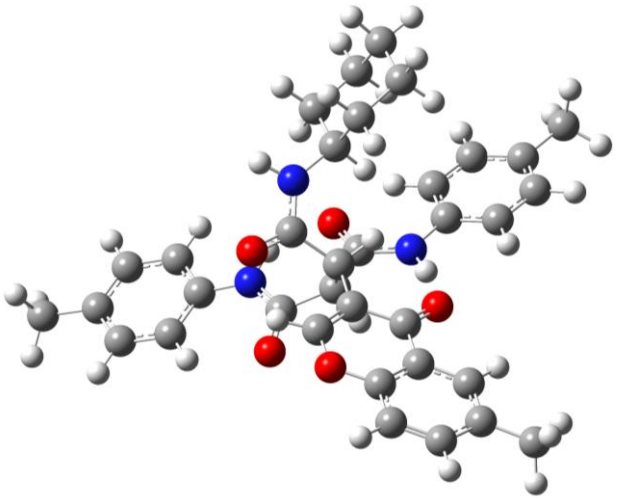
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	-0.0688	-1.9786	0.330555
2	C	0.172563	-2.79723	1.531225
3	C	0.326842	-4.24237	1.275508
4	C	0.204637	-4.74006	-0.02862
5	C	-0.17159	-2.57975	-0.87949
6	H	0.68219	-4.745	3.321559
7	C	0.589831	-5.14753	2.318434
8	C	0.334622	-6.10306	-0.31076
9	H	-0.38372	-2.06849	-1.80965
10	C	0.595349	-6.97574	0.736668
11	C	0.724895	-6.5009	2.053594
12	H	0.228957	-6.44574	-1.33409
13	H	0.699515	-8.03686	0.532071
14	H	0.930102	-7.19684	2.860611
15	O	-0.05295	-3.90909	-1.08958
16	O	0.221559	-2.30447	2.65874
17	C	-0.12947	-0.48011	0.554112
18	H	0.718904	-0.24442	1.206938
19	C	-0.03261	0.366185	-0.7544
20	H	-0.8754	0.117925	-1.40036
21	C	-1.27967	0.068592	1.435126
22	O	-1.06282	1.071439	2.098229

23	C	-0.22104	1.882861	-0.49819
24	O	-1.30195	2.40958	-0.71516
25	C	1.216976	0.119046	-1.62513
26	O	1.127745	0.211089	-2.84056
27	N	-2.55136	-0.47184	1.467824
28	H	-3.14614	0.099503	2.055416
29	N	0.898318	2.545735	-0.04475
30	H	1.759473	2.020211	0.086335
31	N	2.385388	-0.14678	-0.942
32	H	2.355425	-0.29036	0.066147
33	C	1.018821	3.876902	0.34692
34	C	-0.07118	4.770086	0.306024
35	C	2.261879	4.397818	0.80796
36	C	0.07038	6.091749	0.703709
37	H	-1.02021	4.392211	-0.04168
38	C	2.38646	5.735874	1.20521
39	C	1.297592	6.587788	1.156494
40	H	-0.79559	6.745486	0.659734
41	H	3.35556	6.072931	1.547896
42	H	1.400699	7.621788	1.466639
43	C	3.678047	-0.29195	-1.45051
44	C	3.958794	-0.19249	-2.82699
45	C	4.77559	-0.53248	-0.57844
46	C	5.25778	-0.32372	-3.30089
47	H	3.135461	-0.01126	-3.50146
48	C	6.078721	-0.65844	-1.07265
49	C	6.327351	-0.55651	-2.43128
50	H	5.434329	-0.24179	-4.36918
51	H	6.874544	-0.83532	-0.36154
52	H	7.339352	-0.65708	-2.80787
53	C	-3.16159	-1.61479	0.873131
54	H	-2.46733	-2.43656	0.709496
55	H	-3.9882	-1.96678	1.493773
56	S	-3.9089	-1.35435	-0.81247
57	O	-2.81561	-0.9493	-1.72004
58	O	-4.69426	-2.57254	-1.07975
59	C	-5.02753	0.031181	-0.62127
60	C	-6.38085	-0.22541	-0.39033
61	C	-4.53529	1.337433	-0.70188
62	C	-7.25307	0.848731	-0.23128
63	H	-6.73834	-1.24913	-0.36166

64	C	-5.42702	2.394831	-0.53399
65	H	-3.48538	1.52858	-0.90135
66	C	-6.79091	2.171384	-0.29413
67	H	-8.30965	0.657984	-0.06431
68	H	-5.0546	3.413401	-0.59934
69	C	-7.73617	3.330154	-0.09052
70	H	-8.76522	3.056971	-0.33932
71	H	-7.72834	3.661181	0.955333
72	H	-7.45209	4.1897	-0.70438
73	N	3.480543	3.596806	0.899253
74	O	3.437692	2.388937	0.594133
75	O	4.514855	4.141435	1.272065
76	N	4.628204	-0.6704	0.871416
77	O	5.639851	-0.80953	1.549232
78	O	3.486938	-0.66183	1.371175

Table S8. Optimized structure for compound (**8**) and cartesian Z-matrix

Compound **8**



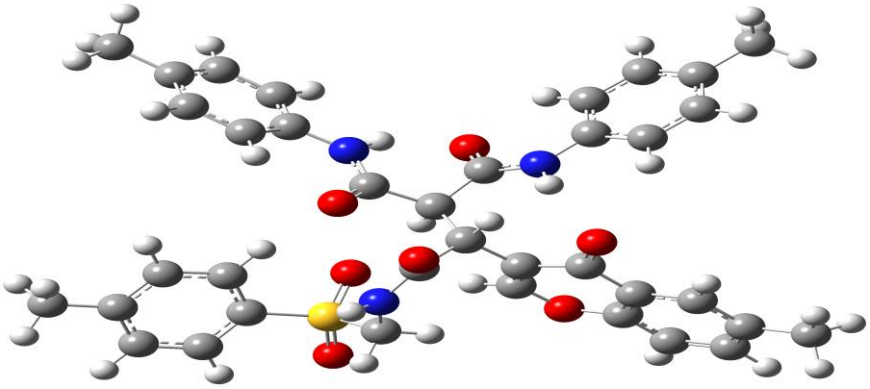
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	-1.26511	1.83237	0.678826
2	C	-2.51763	1.582009	-0.03176
3	C	-3.46159	2.706114	-0.05318
4	C	-3.09698	3.925867	0.529697
5	C	-1.00985	3.068464	1.176627
6	H	-4.98653	1.645502	-1.10736
7	C	-4.72833	2.59885	-0.65754
8	C	-3.96663	5.021982	0.519908
9	H	-0.08118	3.330862	1.663525
10	C	-5.20721	4.88257	-0.07901
11	C	-5.61278	3.668136	-0.67925
12	H	-3.65162	5.953401	0.977355
13	H	-5.88635	5.731119	-0.08912
14	O	-1.87792	4.099729	1.123969
15	O	-2.76851	0.496912	-0.59256
16	C	-0.30673	0.662536	0.723172
17	H	-0.94942	-0.20993	0.851717
18	C	0.380346	0.480996	-0.70017
19	H	-0.33043	0.896509	-1.41684
20	C	0.720527	0.699738	1.862147
21	O	1.287716	1.740295	2.192458
22	C	1.617316	1.389859	-0.85359
23	O	1.433348	2.590306	-1.0268
24	C	0.505815	-1.0145	-1.02669
25	O	1.565747	-1.64965	-0.97561

26	N	1.028349	-0.47483	2.484706
27	H	1.727268	-0.33574	3.20647
28	N	2.825712	0.77063	-0.76195
29	H	2.771801	-0.24714	-0.71656
30	N	-0.70265	-1.56236	-1.33977
31	H	-1.50106	-0.9302	-1.24876
32	C	4.11072	1.343865	-0.84165
33	C	4.345156	2.724695	-0.91736
34	C	5.206228	0.466869	-0.84087
35	C	5.655426	3.194665	-0.98871
36	H	3.505626	3.404845	-0.92589
37	C	6.505363	0.958334	-0.91219
38	C	6.75935	2.333897	-0.98509
39	H	5.819409	4.268007	-1.05023
40	C	-1.02427	-2.91134	-1.61285
41	C	-0.06954	-3.91963	-1.80607
42	C	-2.3877	-3.23152	-1.70895
43	C	-0.49381	-5.21954	-2.08448
44	H	0.982501	-3.68099	-1.74435
45	C	-2.78589	-4.53343	-1.98986
46	C	-1.84801	-5.5577	-2.18027
47	H	0.258317	-5.98968	-2.23711
48	H	5.034718	-0.60563	-0.79021
49	H	-3.13121	-2.45178	-1.56464
50	C	0.462951	-1.82313	2.388488
51	C	1.595638	-2.8634	2.354031
52	C	-0.52199	-2.10606	3.538783
53	H	-0.07978	-1.89894	1.442997
54	C	1.045191	-4.29694	2.300441
55	H	2.214173	-2.74146	3.256162
56	H	2.234931	-2.66172	1.489343
57	C	-1.07147	-3.53952	3.471518
58	H	0.002078	-1.95469	4.493373
59	H	-1.33792	-1.37407	3.510802
60	C	0.062019	-4.57515	3.446991
61	H	1.876441	-5.01083	2.327924
62	H	0.537657	-4.44886	1.338246
63	H	-1.74054	-3.7213	4.320446
64	H	-1.6823	-3.65035	2.564648
65	H	-0.3512	-5.58621	3.354326
66	H	0.600992	-4.54407	4.404702

67	H	7.33683	0.257614	-0.91388
68	H	-3.84732	-4.75671	-2.0637
69	C	8.171499	2.867875	-1.03057
70	H	8.565481	3.048826	-0.02214
71	H	8.850998	2.163827	-1.52111
72	H	8.222728	3.817465	-1.57209
73	C	-2.28724	-6.97603	-2.45595
74	H	-2.54337	-7.50363	-1.52838
75	H	-3.17396	-7.00378	-3.09722
76	H	-1.49728	-7.54998	-2.94888
77	C	-6.97342	3.55662	-1.32412
78	H	-7.77391	3.749085	-0.60069
79	H	-7.0903	4.284875	-2.13466
80	H	-7.13348	2.560447	-1.74358

Table S9. Optimized structure for compound (**9**) and cartesian Z-matrix

Compound **9**



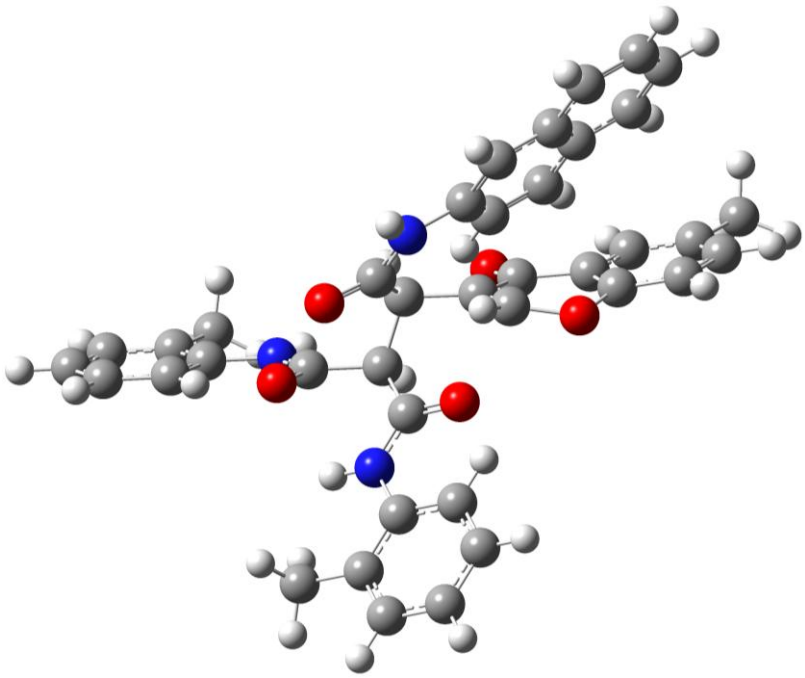
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	1.770791	-1.24992	0.284629
2	C	3.080149	-1.2462	0.959988
3	C	4.103218	-2.10719	0.347119
4	C	3.843784	-2.72864	-0.8793
5	C	1.672754	-1.83907	-0.93392
6	H	5.541651	-1.80223	1.895647
7	C	5.359292	-2.30213	0.94971
8	C	4.8012	-3.53442	-1.5027
9	H	0.794688	-1.78844	-1.56942
10	C	6.024645	-3.71513	-0.87821
11	C	6.327599	-3.10388	0.359734
12	H	4.569481	-3.99647	-2.45601
13	H	6.772438	-4.3424	-1.35627
14	O	2.650394	-2.55405	-1.53078
15	O	3.313738	-0.52866	1.941186
16	C	0.645186	-0.45535	0.941392
17	H	1.127706	0.101299	1.746659
18	C	0.027468	0.573377	-0.04641
19	H	-0.25808	0.068654	-0.97397
20	C	-0.29764	-1.30181	1.850515
21	O	-0.30318	-1.06479	3.044825
22	C	-1.31576	1.190354	0.44184
23	O	-1.95683	0.661185	1.346789

24	C	1.019553	1.670582	-0.50499
25	O	0.724053	2.352171	-1.4935
26	N	-1.11601	-2.3421	1.406087
27	H	-1.68649	-2.64887	2.183758
28	N	-1.73118	2.271194	-0.26917
29	H	-1.10026	2.557444	-1.01703
30	N	2.157945	1.852391	0.214967
31	H	2.3406	1.225054	0.990315
32	C	-2.93151	3.000956	-0.13412
33	C	-3.83613	2.833273	0.923664
34	C	-3.20939	3.959601	-1.12143
35	C	-4.98988	3.616473	0.970947
36	H	-3.6299	2.102538	1.692375
37	C	-4.36464	4.729061	-1.05367
38	C	-5.28147	4.575457	-0.00442
39	H	-5.68023	3.474993	1.799199
40	C	3.203423	2.785556	-0.00939
41	C	3.15473	3.807176	-0.96667
42	C	4.342307	2.65645	0.801031
43	C	4.236666	4.678803	-1.09069
44	H	2.287695	3.905516	-1.60274
45	C	5.406791	3.539285	0.659575
46	C	5.376499	4.572522	-0.28672
47	H	4.185852	5.465295	-1.83969
48	H	-2.51611	4.094631	-1.94777
49	H	4.392547	1.853189	1.531447
50	H	-4.55774	5.461874	-1.83328
51	H	6.279622	3.419469	1.296573
52	C	-6.52196	5.433039	0.07767
53	H	-6.28966	6.439918	0.446851
54	H	-6.99402	5.551931	-0.90328
55	H	-7.26232	4.99992	0.756422
56	C	6.522402	5.547761	-0.41428
57	H	6.435927	6.363328	0.314885
58	H	7.486277	5.05959	-0.23843
59	H	6.551272	6.002866	-1.40862
60	C	7.673214	-3.32463	1.007557
61	H	7.840267	-4.38567	1.22511
62	H	8.488109	-2.998	0.351818
63	H	7.756858	-2.77308	1.946932
64	C	-1.07807	-3.22664	0.291967

65	H	-0.0876	-3.33073	-0.15114
66	H	-1.4246	-4.21988	0.586828
67	S	-2.13787	-2.7962	-1.17476
68	O	-1.69568	-1.46804	-1.65556
69	O	-2.05233	-3.96892	-2.06553
70	C	-3.81258	-2.66737	-0.55425
71	C	-4.70271	-3.70723	-0.83055
72	C	-4.20492	-1.54918	0.188612
73	C	-6.00927	-3.62042	-0.35532
74	H	-4.37118	-4.5564	-1.41796
75	C	-5.51479	-1.48906	0.658124
76	H	-3.50881	-0.7462	0.405747
77	C	-6.4354	-2.51384	0.392659
78	H	-6.70954	-4.42264	-0.57143
79	H	-5.82665	-0.62388	1.236556
80	C	-7.86035	-2.41116	0.87883
81	H	-7.91352	-1.93538	1.862466
82	H	-8.46269	-1.80394	0.192125
83	H	-8.33328	-3.39455	0.947603

Table S10. Optimized structure for compound (**10**) and cartesian Z-matrix

Compound **10**



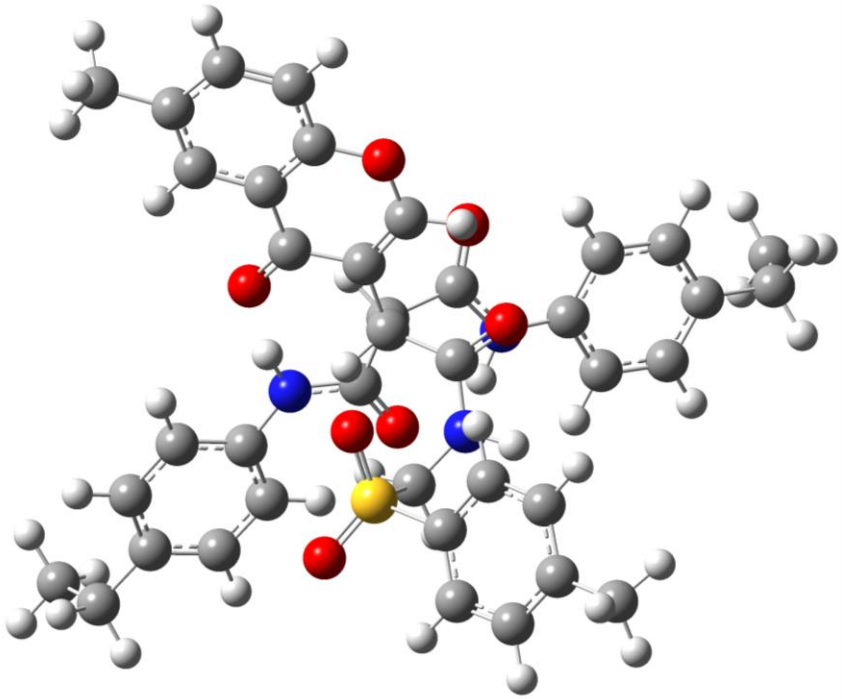
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	0.778751	-0.55509	-0.57883
2	C	1.393307	0.545764	-1.31345
3	C	2.466466	0.158909	-2.23839
4	C	2.787394	-1.19508	-2.39664
5	C	1.149533	-1.82967	-0.84439
6	H	2.912706	2.1556	-2.85041
7	C	3.181945	1.112898	-2.9854
8	C	3.797321	-1.60305	-3.27385
9	H	0.686581	-2.69992	-0.39969
10	C	4.485539	-0.63876	-3.99117
11	C	4.19172	0.737967	-3.8611
12	H	4.018482	-2.65984	-3.37507
13	H	5.271568	-0.95054	-4.67397
14	O	2.121379	-2.17601	-1.71074
15	O	1.017765	1.724784	-1.17808
16	C	-0.32765	-0.17151	0.378824
17	H	-0.02962	0.813116	0.751297
18	C	-1.68745	0.051334	-0.375
19	H	-1.4046	0.348851	-1.39137
20	C	-0.51888	-1.04449	1.626511
21	O	-1.63015	-1.39924	1.991601

22	C	-2.43161	-1.29093	-0.58469
23	O	-1.78728	-2.22726	-1.05682
24	C	-2.45237	1.262781	0.199651
25	O	-3.5593	1.189158	0.734336
26	N	0.585799	-1.41804	2.367528
27	H	0.321929	-2.05579	3.109254
28	N	-3.76119	-1.29997	-0.31343
29	H	-4.07226	-0.46868	0.189638
30	N	-1.77172	2.437943	0.027096
31	H	-0.87974	2.367857	-0.46023
32	C	-4.68144	-2.35988	-0.46114
33	C	-4.34618	-3.57259	-1.08265
34	C	-5.99297	-2.15308	0.02964
35	C	-5.30509	-4.57513	-1.21857
36	H	-3.33779	-3.71326	-1.44314
37	C	-6.92732	-3.18003	-0.12405
38	C	-6.60017	-4.38719	-0.7418
39	H	-5.02925	-5.50844	-1.70148
40	C	-2.16461	3.739624	0.437319
41	C	-3.07974	3.939691	1.480192
42	C	-1.58112	4.844344	-0.22348
43	C	-3.4167	5.233392	1.873354
44	H	-3.52724	3.083508	1.964099
45	C	-1.93575	6.127884	0.202828
46	C	-2.84407	6.334339	1.240277
47	H	-4.12828	5.373427	2.681722
48	H	-7.34832	-5.1673	-0.84645
49	H	-3.10326	7.343811	1.54487
50	H	-7.93497	-3.02357	0.252983
51	C	-6.38579	-0.86116	0.707326
52	H	-5.78371	-0.66602	1.602787
53	H	-6.26062	0.007298	0.049201
54	H	-7.43408	-0.89364	1.013912
55	H	-1.49094	6.981978	-0.30138
56	C	-0.61671	4.663605	-1.37231
57	H	0.299846	4.138785	-1.08059
58	H	-1.06465	4.080655	-2.18611
59	H	-0.32718	5.634827	-1.78092
60	C	4.963673	1.758764	-4.66203
61	H	6.03423	1.718881	-4.43093
62	H	4.859962	1.580846	-5.73837

63	H	4.613885	2.773005	-4.45508
64	C	1.947501	-1.0156	2.331204
65	C	2.931201	-1.97542	2.471366
66	C	2.311675	0.35526	2.237138
67	C	4.303859	-1.62105	2.509479
68	H	2.652522	-3.02326	2.547801
69	C	3.636209	0.722457	2.245456
70	H	1.540153	1.114833	2.186689
71	C	4.669919	-0.24187	2.380151
72	C	5.332046	-2.59149	2.656041
73	H	3.904371	1.772727	2.171264
74	C	6.044767	0.112094	2.404348
75	C	6.655939	-2.2157	2.674051
76	H	5.055274	-3.63791	2.753223
77	C	7.017098	-0.85163	2.54781
78	H	6.316588	1.160003	2.308733
79	H	7.431764	-2.96713	2.787117
80	H	8.065577	-0.56993	2.565729

Table S11. Optimized structure for compound (**11**) and cartesian Z-matrix

Compound **11**



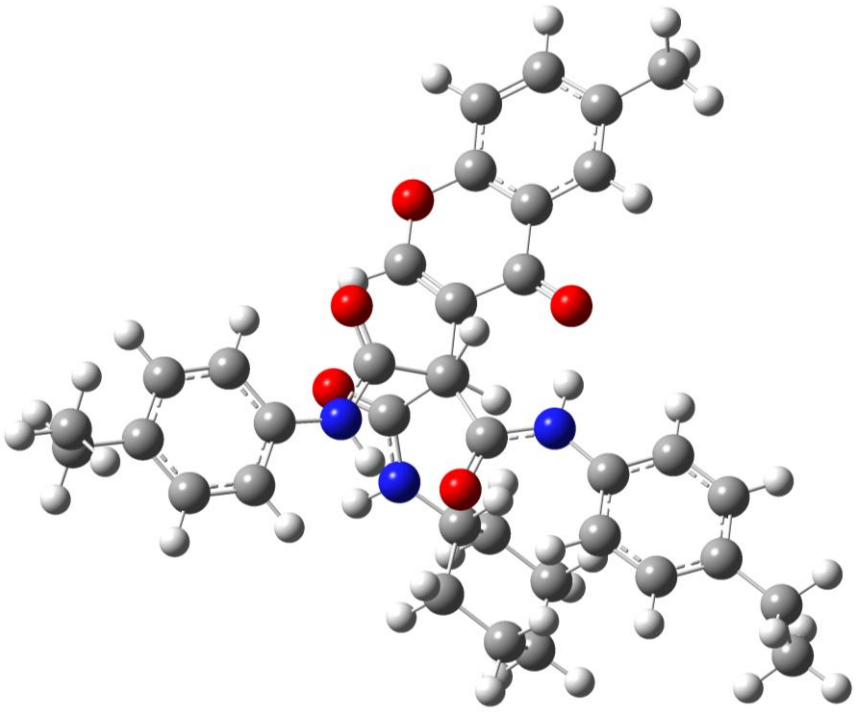
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	-0.73749	1.162171	1.954785
2	C	-2.04	1.795705	1.750007
3	C	-2.6149	2.445099	2.934088
4	C	-1.88247	2.482144	4.126277
5	C	-0.11011	1.29222	3.149785
6	H	-4.43388	3.009299	1.967652
7	C	-3.88635	3.047846	2.903834
8	C	-2.39344	3.101847	5.271769
9	H	0.874721	0.897684	3.353072
10	C	-3.6492	3.682152	5.210505
11	C	-4.4208	3.665811	4.025748
12	H	-1.79854	3.115626	6.178367
13	H	-4.05136	4.164025	6.0979
14	O	-0.63739	1.923921	4.218879
15	O	-2.61901	1.803381	0.647042
16	C	-0.17748	0.450651	0.743416
17	H	-1.04316	-0.04423	0.30129
18	C	0.328828	1.51319	-0.32946
19	H	-0.25343	2.414821	-0.13367
20	C	0.892177	-0.60387	1.028207
21	O	1.728965	-0.49759	1.914133

22	C	1.781469	1.948136	-0.0478
23	O	1.987196	2.698933	0.900328
24	C	-0.04748	1.040613	-1.74281
25	O	0.759936	0.553554	-2.54453
26	N	0.971566	-1.6888	0.168767
27	H	1.735394	-2.30028	0.433537
28	N	2.728466	1.421879	-0.87229
29	H	2.347574	0.894241	-1.6597
30	N	-1.38035	1.175067	-1.98102
31	H	-1.93284	1.496532	-1.18196
32	C	4.123424	1.620498	-0.84158
33	C	4.788021	2.326357	0.172477
34	C	4.87447	1.058567	-1.88573
35	C	6.174761	2.456548	0.120383
36	H	4.214891	2.758248	0.980324
37	C	6.257647	1.200835	-1.91659
38	C	6.938876	1.904662	-0.91497
39	H	6.675728	3.003217	0.916234
40	C	-2.12324	0.804696	-3.12733
41	C	-1.54286	0.385406	-4.33238
42	C	-3.52067	0.880721	-3.0265
43	C	-2.36662	0.052728	-5.40721
44	H	-0.46766	0.317813	-4.41562
45	C	-4.32095	0.544551	-4.11239
46	C	-3.76205	0.124042	-5.32684
47	H	-1.90402	-0.27516	-6.33523
48	H	4.367883	0.506688	-2.67378
49	H	-3.97315	1.194436	-2.08942
50	H	6.817969	0.753752	-2.73447
51	H	-5.40179	0.603448	-4.01077
52	C	8.439303	2.096083	-0.97286
53	H	8.901792	1.223828	-1.45091
54	H	8.841586	2.139525	0.046532
55	C	-4.63577	-0.20331	-6.51858
56	H	-4.14595	-0.97019	-7.13042
57	H	-5.57929	-0.64083	-6.17067
58	C	-5.78656	4.308903	3.999372
59	H	-6.46022	3.841871	4.726855
60	H	-5.72987	5.374144	4.250504
61	H	-6.24736	4.221284	3.012547
62	C	-0.03475	-2.25665	-0.67035

63	H	-0.62583	-1.51304	-1.20528
64	H	0.410012	-2.93034	-1.40493
65	S	-1.2996	-3.24762	0.267459
66	O	-1.76493	-2.38738	1.372069
67	O	-2.22947	-3.79354	-0.73546
68	C	-0.36166	-4.60385	0.977713
69	C	-0.28494	-5.81474	0.286584
70	C	0.291483	-4.4269	2.200199
71	C	0.463249	-6.85646	0.829753
72	H	-0.81895	-5.93527	-0.64997
73	C	1.039049	-5.47952	2.724024
74	H	0.202638	-3.48664	2.733391
75	C	1.13588	-6.70662	2.051614
76	H	0.523073	-7.80292	0.299399
77	H	1.551073	-5.34766	3.673181
78	C	1.919297	-7.85123	2.646155
79	H	2.757483	-7.49198	3.249678
80	H	1.282978	-8.45935	3.300709
81	H	2.314234	-8.51252	1.869951
82	C	8.855968	3.367587	-1.73341
83	H	9.945849	3.4749	-1.75488
84	H	8.496599	3.34102	-2.76726
85	H	8.435503	4.261215	-1.26107
86	C	-4.94125	1.023922	-7.39574
87	H	-4.01886	1.465501	-7.78653
88	H	-5.57479	0.75108	-8.24637
89	H	-5.45989	1.797718	-6.82052

Table S12. Optimized structure compound (**12**) and cartesian Z-matrix

Compound **12**



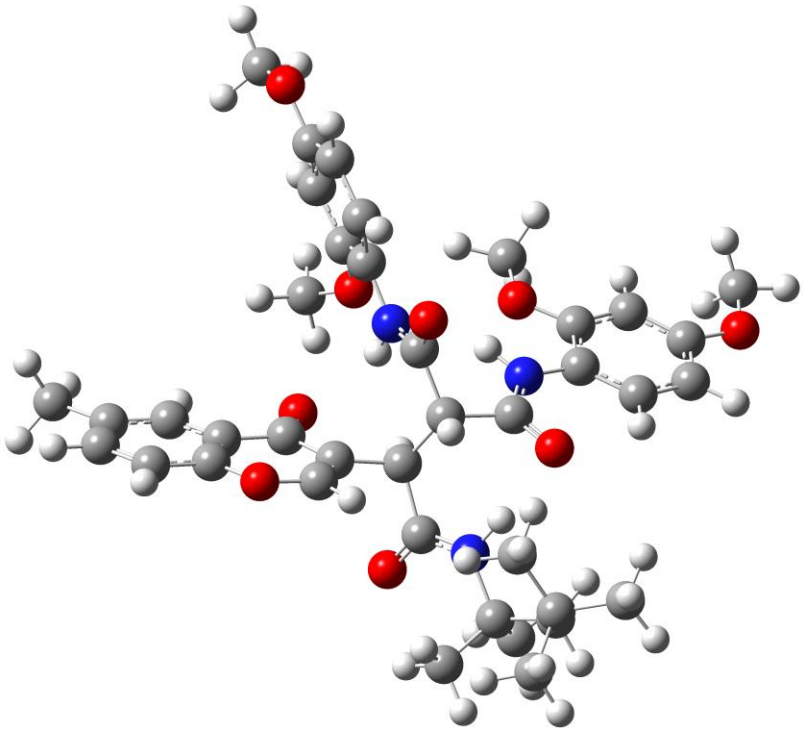
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	-0.41221	2.402564	0.687899
2	C	-1.61388	2.726237	-0.07863
3	C	-1.94563	4.154441	-0.15077
4	C	-1.0917	5.092947	0.441306
5	C	0.354976	3.402775	1.189803
6	H	-3.74281	3.869529	-1.26911
7	C	-3.09907	4.614963	-0.81326
8	C	-1.37023	6.46298	0.384297
9	H	1.282221	3.23014	1.717799
10	C	-2.51511	6.883158	-0.27137
11	C	-3.40237	5.967465	-0.88286
12	H	-0.6861	7.163455	0.850479
13	H	-2.73582	7.946384	-0.3184
14	O	0.049963	4.713068	1.090826
15	O	-2.30651	1.857012	-0.64401
16	C	-0.08885	0.927654	0.783185
17	H	-1.06096	0.442762	0.886048
18	C	0.497602	0.419136	-0.6056
19	H	0.081633	1.093039	-1.35682
20	C	0.799084	0.526541	1.968344

21	O	1.762125	1.207366	2.318536
22	C	2.017142	0.665994	-0.70342
23	O	2.404367	1.814548	-0.89225
24	C	-0.05481	-0.97912	-0.91997
25	O	0.600723	-2.02303	-0.82015
26	N	0.518976	-0.64412	2.611081
27	H	1.177748	-0.81653	3.362839
28	N	2.809031	-0.42995	-0.54743
29	H	2.298194	-1.3119	-0.50203
30	N	-1.36775	-0.92921	-1.28382
31	H	-1.79659	-0.00246	-1.23109
32	C	4.21631	-0.50131	-0.56134
33	C	5.052699	0.623461	-0.61936
34	C	4.79498	-1.77837	-0.49754
35	C	6.435509	0.449451	-0.61504
36	H	4.612202	1.60907	-0.66424
37	C	6.177724	-1.92784	-0.49393
38	C	7.029277	-0.8171	-0.55442
39	H	7.070515	1.331703	-0.65539
40	C	-2.25468	-1.99312	-1.56489
41	C	-1.85186	-3.32836	-1.71375
42	C	-3.6107	-1.66461	-1.71758
43	C	-2.80734	-4.30208	-2.00498
44	H	-0.80832	-3.58825	-1.60868
45	C	-4.54409	-2.65291	-2.01031
46	C	-4.1641	-3.9937	-2.15842
47	H	-2.47989	-5.33226	-2.12422
48	H	4.154334	-2.65544	-0.44674
49	H	-3.9254	-0.62987	-1.60854
50	H	6.602306	-2.92763	-0.43972
51	H	-5.58848	-2.37495	-2.12968
52	C	8.533345	-0.98296	-0.59337
53	H	9.008097	-0.12697	-0.09863
54	H	8.819099	-1.87102	-0.01634
55	C	-5.18874	-5.07252	-2.43631
56	H	-5.99832	-4.65855	-3.04942
57	H	-4.72698	-5.86986	-3.03076
58	C	-4.63963	6.465519	-1.59048
59	H	-5.2942	7.018004	-0.90677
60	H	-4.38229	7.146182	-2.40992
61	H	-5.21645	5.638331	-2.01116

62	C	9.089292	-1.11047	-2.02284
63	H	10.17836	-1.22779	-2.01364
64	H	8.658401	-1.97711	-2.53473
65	H	8.847872	-0.22312	-2.61686
66	C	-5.78638	-5.67992	-1.15467
67	H	-6.52242	-6.45489	-1.39317
68	H	-5.0056	-6.13236	-0.53475
69	H	-6.28409	-4.91297	-0.55231
70	C	-0.59009	-1.59497	2.498323
71	C	-0.04787	-3.03471	2.503701
72	C	-1.6288	-1.38409	3.616234
73	H	-1.08144	-1.43329	1.535587
74	C	-1.184	-4.06698	2.435878
75	H	0.533398	-3.18913	3.425406
76	H	0.637763	-3.15773	1.660091
77	C	-2.76336	-2.41731	3.535561
78	H	-1.11968	-1.46856	4.587063
79	H	-2.02593	-0.36362	3.559422
80	C	-2.21827	-3.85287	3.550626
81	H	-0.7651	-5.07828	2.492168
82	H	-1.67854	-3.99027	1.458102
83	H	-3.46549	-2.26352	4.363035
84	H	-3.33347	-2.25668	2.609815
85	H	-3.04027	-4.57066	3.447488
86	H	-1.74987	-4.0516	4.525186

Table S13. Optimized structure for compound (**13**) and cartesian Z-matrix

Compound **13**



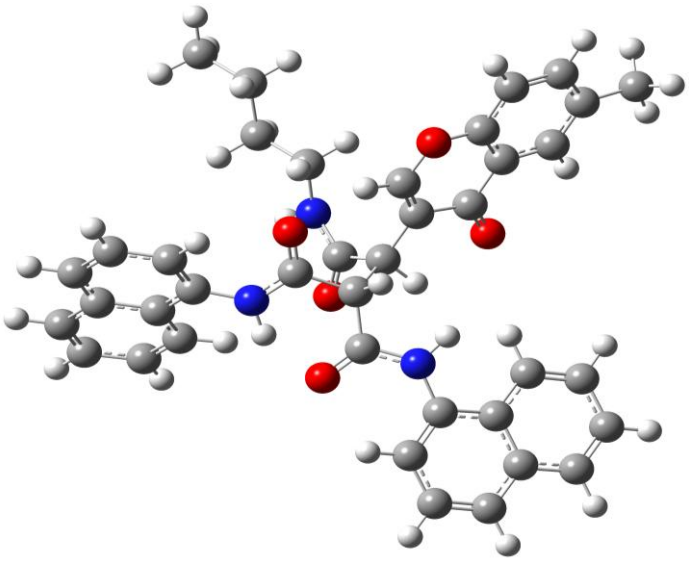
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	-0.58289	2.27524	0.26009
2	C	-1.84332	2.079825	0.983182
3	C	-2.81623	3.17644	0.83554
4	C	-2.52738	4.261879	0.000306
5	C	-0.42334	3.374226	-0.51205
6	H	-4.25414	2.307604	2.151139
7	C	-4.05177	3.157625	1.507498
8	C	-3.43988	5.307243	-0.17458
9	H	0.479108	3.595103	-1.07114
10	C	-4.64681	5.258365	0.502997
11	C	-4.97566	4.183316	1.359194
12	H	-3.18405	6.13145	-0.83131
13	H	-5.35831	6.069587	0.372515
14	O	-1.34282	4.347543	-0.68266
15	O	-2.08083	1.063827	1.649263
16	C	0.535765	1.255242	0.431405
17	H	0.190224	0.570233	1.212795
18	C	0.790242	0.460699	-0.88693
19	H	1.21994	1.132857	-1.63231
20	C	1.729119	2.003591	1.105406

21	O	1.500638	2.56348	2.175552
22	C	1.847772	-0.65763	-0.73196
23	O	3.031121	-0.42734	-1.00545
24	C	-0.47304	-0.08616	-1.59153
25	O	-0.52697	-0.06861	-2.81497
26	N	2.911771	2.048213	0.442783
27	H	3.060636	1.355255	-0.28697
28	N	1.392155	-1.84414	-0.26285
29	H	0.392967	-1.94133	-0.11955
30	N	-1.42695	-0.64966	-0.78214
31	H	-1.40076	-0.45932	0.217945
32	C	2.121452	-3.02117	0.021189
33	C	3.493571	-3.1924	-0.18466
34	C	1.374575	-4.09264	0.553487
35	C	4.108303	-4.40003	0.132706
36	H	4.065663	-2.37228	-0.59396
37	C	1.983574	-5.30729	0.871243
38	C	3.361526	-5.45771	0.658007
39	H	5.171711	-4.53969	-0.02481
40	C	-2.63286	-1.27365	-1.18695
41	C	-3.11673	-1.31303	-2.50177
42	C	-3.39778	-1.87884	-0.1718
43	C	-4.33673	-1.91558	-2.78788
44	H	-2.52761	-0.86066	-3.28618
45	C	-4.63053	-2.47325	-0.45103
46	C	-5.10357	-2.48853	-1.7684
47	H	-4.71655	-1.9415	-3.80316
48	H	1.392078	-6.11606	1.275884
49	H	-5.19377	-2.9278	0.352911
50	C	-6.30025	4.166147	2.083679
51	H	-6.40845	5.040193	2.735879
52	H	-7.13978	4.183935	1.379399
53	H	-6.40192	3.272105	2.70371
54	C	4.153823	2.664631	0.984969
55	C	4.530974	1.9625	2.310309
56	H	4.741016	0.901621	2.139012
57	H	5.425775	2.422544	2.742593
58	H	3.713118	2.047952	3.027224
59	C	3.917946	4.160109	1.257565
60	H	3.529558	4.671177	0.373553
61	H	3.191446	4.278702	2.06253

62	H	4.855289	4.642534	1.551282
63	C	5.303757	2.373829	-0.02427
64	H	6.237895	2.579695	0.513505
65	H	5.292728	1.286933	-0.18192
66	C	5.44044	3.043548	-1.42832
67	C	6.535793	2.245712	-2.17315
68	H	6.238159	1.201417	-2.31642
69	H	6.727476	2.679023	-3.16106
70	H	7.480617	2.253035	-1.61731
71	C	4.148725	2.975527	-2.26646
72	H	3.808332	1.942041	-2.39049
73	H	3.336952	3.55089	-1.81168
74	H	4.327975	3.386857	-3.26659
75	C	5.917581	4.508502	-1.33411
76	H	5.166797	5.170189	-0.89819
77	H	6.827718	4.589111	-0.72846
78	H	6.151835	4.892815	-2.33351
79	O	0.04334	-3.82841	0.721781
80	O	4.054801	-6.60261	0.935036
81	C	3.347916	-7.70971	1.466493
82	H	4.08651	-8.5003	1.606677
83	H	2.888512	-7.47264	2.435251
84	H	2.569494	-8.06439	0.778068
85	C	-0.80927	-4.83004	1.254221
86	H	-0.4897	-5.13257	2.259297
87	H	-1.79569	-4.37002	1.306618
88	H	-0.84447	-5.71263	0.603617
89	O	-2.8369	-1.87774	1.082818
90	O	-6.29334	-3.04459	-2.15068
91	C	-3.70166	-1.70395	2.203309
92	H	-4.39474	-0.87396	2.03539
93	H	-4.26622	-2.61837	2.425063
94	H	-3.05482	-1.4656	3.0478
95	C	-7.10888	-3.63806	-1.15613
96	H	-7.41319	-2.91105	-0.39144
97	H	-7.99705	-4.00529	-1.6725
98	H	-6.6051	-4.4818	-0.66578

Table S14. Optimized structure for compound (**14**) and cartesian Z-matrix

Compound **14**



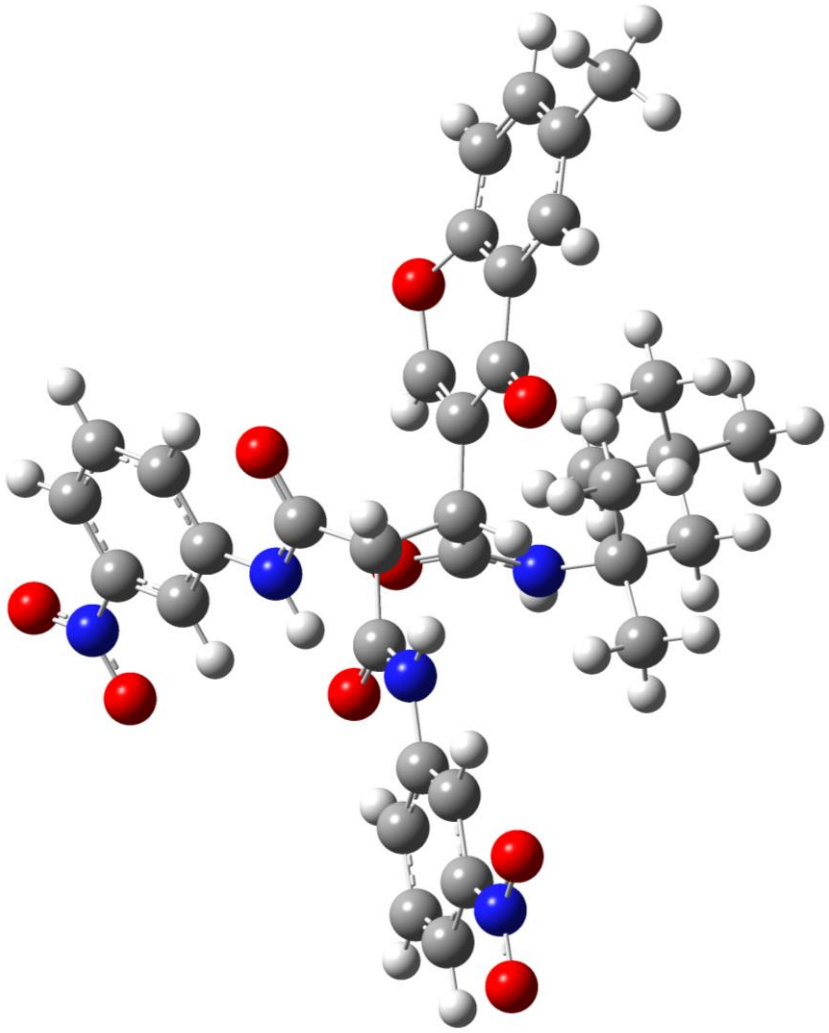
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	1.277442	1.497735	0.371535
2	C	2.537416	1.728362	-0.35803
3	C	3.282967	2.932574	0.054807
4	C	2.823446	3.707111	1.124846
5	C	0.961291	2.303666	1.415108
6	H	4.805492	2.699256	-1.42132
7	C	4.46752	3.319472	-0.59705
8	C	3.516232	4.846774	1.546135
9	H	0.078668	2.162493	2.030176
10	C	4.677189	5.204534	0.879723
11	C	5.175525	4.448363	-0.20501
12	H	5.218597	6.09027	1.201934
13	O	1.685194	3.375081	1.811922
14	O	2.953141	0.961653	-1.23272
15	C	0.490221	0.273835	-0.05316
16	H	1.248834	-0.35607	-0.52417
17	C	-0.15464	-0.5774	1.108394
18	H	0.430329	-0.37402	2.011905
19	C	-0.52357	0.353857	-1.22534
20	O	-0.7452	-0.69471	-1.82915
21	C	-1.57555	-0.06667	1.440313
22	O	-1.69515	1.010508	2.034192
23	C	0.004486	-2.08907	0.820878
24	O	-0.93401	-2.86518	0.654439

25	N	-1.14984	1.505183	-1.58718
26	H	-1.77117	1.337627	-2.37009
27	N	-2.6039	-0.81119	0.976201
28	H	-2.31948	-1.72077	0.603964
29	N	1.312392	-2.49046	0.814782
30	H	2.005115	-1.76772	0.941894
31	C	-6.54179	-2.18275	-1.94052
32	C	-7.07021	-1.45041	-0.90268
33	C	-6.23213	-0.86999	0.086884
34	C	-4.81539	-1.07694	0.003405
35	C	-4.29691	-1.81261	-1.09856
36	C	-5.14172	-2.35252	-2.0438
37	H	-7.83871	0.075184	1.188026
38	H	-7.1957	-2.61948	-2.6897
39	H	-8.14365	-1.29781	-0.82584
40	C	-6.76427	-0.07912	1.139607
41	C	-3.98451	-0.51014	1.028198
42	H	-3.22484	-1.91867	-1.22823
43	H	-4.72571	-2.90447	-2.88122
44	C	-4.53481	0.270319	2.028367
45	C	-5.92988	0.488112	2.073289
46	H	-3.88815	0.70725	2.776467
47	H	-6.33932	1.09975	2.871872
48	C	1.126527	-4.92618	0.884462
49	C	1.832612	-3.78427	0.557558
50	C	3.146407	-3.87264	-0.01362
51	C	3.727998	-5.17524	-0.16859
52	C	2.978617	-6.3267	0.189403
53	C	1.703292	-6.1997	0.685097
54	H	3.465101	-1.74596	-0.42985
55	H	0.129556	-4.83752	1.292559
56	C	3.895104	-2.74284	-0.44707
57	C	5.042322	-5.28417	-0.69649
58	H	3.428001	-7.30668	0.05575
59	H	1.127758	-7.08189	0.948358
60	C	5.751866	-4.16914	-1.07748
61	C	5.164481	-2.88868	-0.96262
62	H	5.475851	-6.27532	-0.80069
63	H	6.754513	-4.26996	-1.48211
64	H	5.70848	-2.01134	-1.29864
65	C	6.444204	4.869516	-0.90716

66	H	6.344804	5.870329	-1.34267
67	H	7.291247	4.903666	-0.21262
68	H	6.699682	4.177851	-1.71348
69	H	3.133671	5.423557	2.381172
70	C	-1.29335	2.802376	-0.91896
71	H	-1.49395	2.652385	0.145468
72	H	-0.37014	3.386576	-1.01276
73	C	-2.45423	3.576525	-1.54869
74	H	-2.27208	3.6889	-2.62697
75	H	-3.37507	2.987915	-1.44178
76	C	-2.65216	4.959521	-0.91775
77	H	-2.82546	4.842756	0.159912
78	H	-1.72558	5.540425	-1.01836
79	C	-3.81417	5.738104	-1.54129
80	H	-4.76005	5.197714	-1.42526
81	H	-3.93196	6.719567	-1.07146
82	H	-3.65425	5.899292	-2.61329

Table S15. Optimized structure for compound (**15**) and cartesian Z-matrix

Compound **15**



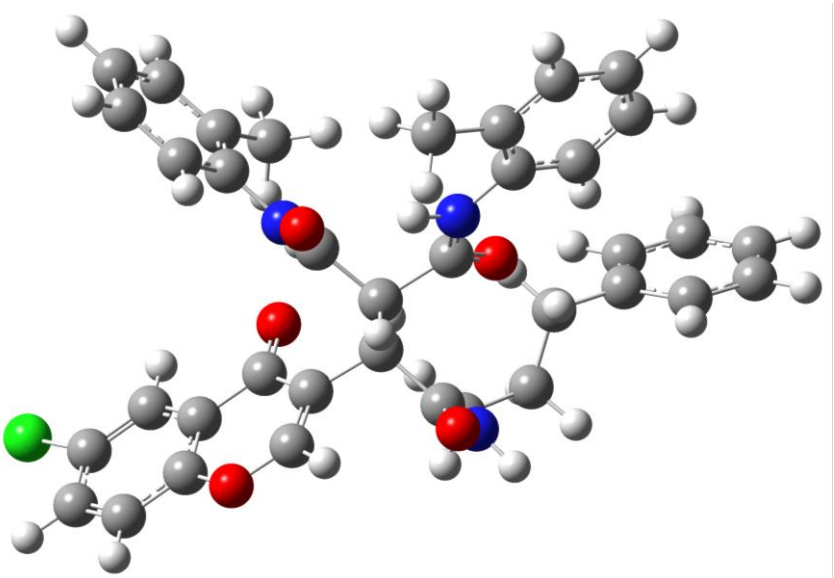
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	1.04648	-1.81582	-0.60423
2	C	2.313658	-1.39355	-1.19702
3	C	3.122007	-2.47451	-1.77079
4	C	2.622503	-3.78394	-1.77376
5	C	0.652399	-3.10919	-0.69563
6	H	4.753643	-1.21114	-2.32492
7	C	4.389213	-2.23337	-2.33452
8	C	3.360028	-4.83853	-2.32121
9	H	-0.30397	-3.47034	-0.3384
10	C	4.604982	-4.56831	-2.86439
11	C	5.144588	-3.26126	-2.88158
12	H	2.943619	-5.83974	-2.31136

13	H	5.181891	-5.38461	-3.29098
14	O	1.39295	-4.08743	-1.2507
15	O	2.672355	-0.20015	-1.22241
16	C	0.209599	-0.71384	0.00796
17	H	0.926173	-0.03663	0.466938
18	C	-0.48218	0.123757	-1.14531
19	H	0.180524	0.020571	-2.00677
20	C	-0.76054	-1.23263	1.071683
21	O	-1.74118	-1.90117	0.740601
22	C	-1.7994	-0.50082	-1.65065
23	O	-1.73341	-1.48623	-2.37472
24	C	-0.4656	1.610715	-0.7677
25	O	-1.4492	2.239401	-0.37177
26	N	-0.52204	-0.99319	2.394041
27	H	-1.25777	-1.41616	2.945104
28	N	-2.94696	0.132002	-1.26855
29	H	-2.80091	0.987921	-0.73366
30	N	0.789677	2.14402	-0.89154
31	H	1.525425	1.475483	-1.13172
32	C	-4.27083	-0.24188	-1.53647
33	C	-4.6241	-1.40545	-2.24442
34	C	-5.28151	0.603074	-1.05774
35	C	-5.9692	-1.70388	-2.46183
36	H	-3.84027	-2.05246	-2.61083
37	C	-6.60971	0.270691	-1.29429
38	C	-6.9849	-0.8744	-1.99297
39	H	-6.22616	-2.60533	-3.00916
40	C	1.228342	3.447738	-0.58893
41	C	0.364018	4.502119	-0.24608
42	C	2.609137	3.678009	-0.65515
43	C	0.889039	5.766382	0.024467
44	H	-0.69966	4.320148	-0.19289
45	C	3.091575	4.951087	-0.37916
46	C	2.25808	6.013266	-0.03726
47	H	0.21142	6.572439	0.286844
48	C	6.504942	-3.00846	-3.4851
49	H	7.280599	-3.58929	-2.97343
50	H	6.530079	-3.29786	-4.54169
51	H	6.77865	-1.95284	-3.41998
52	C	0.523417	-0.28163	3.180387
53	C	0.42155	1.240436	2.933915

54	H	-0.57029	1.61263	3.205364
55	H	1.167078	1.772864	3.532876
56	H	0.600115	1.496308	1.887617
57	C	1.943372	-0.76946	2.831005
58	H	1.997563	-1.85936	2.803517
59	H	2.282567	-0.39077	1.863703
60	H	2.653738	-0.407	3.578932
61	C	0.168652	-0.50351	4.685032
62	H	0.758236	0.23183	5.24534
63	H	-0.87528	-0.17716	4.7934
64	C	0.314499	-1.86147	5.444734
65	C	-0.39251	-1.65508	6.804798
66	H	-1.45789	-1.4359	6.673384
67	H	-0.31037	-2.55529	7.422935
68	H	0.053484	-0.82515	7.364331
69	C	-0.35971	-3.04904	4.72981
70	H	-1.43076	-2.87429	4.569577
71	H	0.096964	-3.26826	3.76086
72	H	-0.27575	-3.95087	5.34607
73	C	1.787761	-2.2173	5.739332
74	H	2.343151	-2.49995	4.843155
75	H	2.312098	-1.37885	6.21162
76	H	1.83515	-3.06574	6.430702
77	H	-5.05163	1.507696	-0.50764
78	H	-8.03287	-1.0903	-2.15236
79	N	-7.65678	1.169309	-0.7813
80	O	-7.30161	2.173214	-0.16221
81	O	-8.82952	0.865732	-1.00018
82	H	2.682542	6.986929	0.168321
83	H	3.303593	2.887121	-0.91394
84	N	4.545965	5.178139	-0.4501
85	O	4.959297	6.309725	-0.20047
86	O	5.261349	4.223357	-0.75319

Table S16. Optimized structure for compound (**16**) and cartesian Z-matrix

Compound **16**



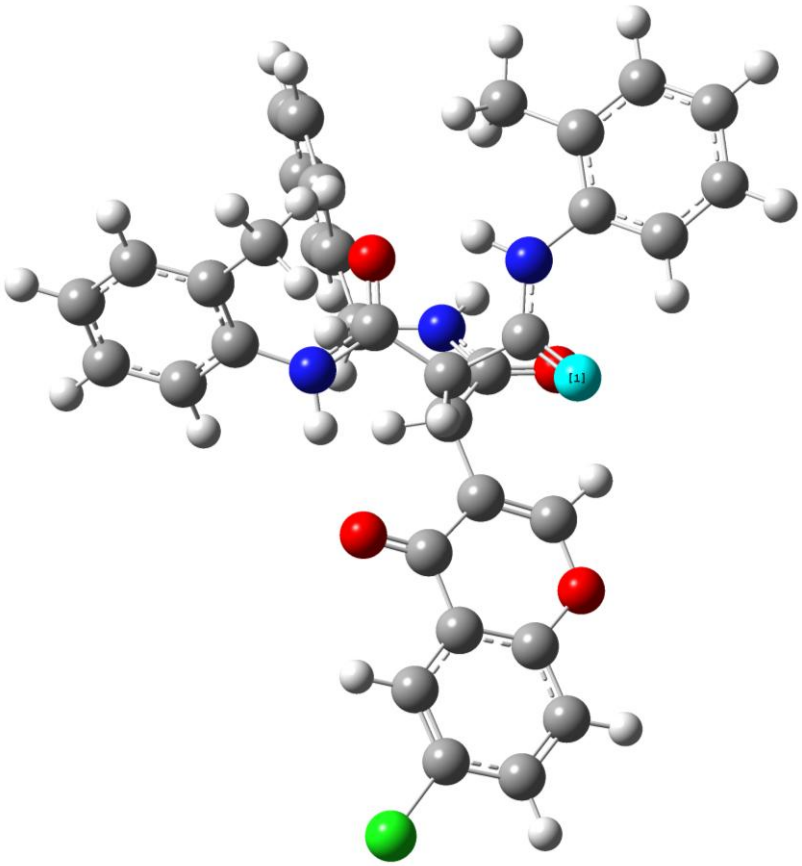
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	-1.66219	0.549503	-1.42129
2	C	-2.52101	0.969392	-0.31399
3	C	-3.94045	1.15195	-0.66286
4	C	-4.37763	0.904778	-1.97136
5	C	-2.20329	0.356007	-2.64961
6	H	-4.53088	1.746177	1.312328
7	C	-4.87681	1.56116	0.30238
8	C	-5.72023	1.056097	-2.33304
9	H	-1.62135	0.078263	-3.52109
10	C	-6.63349	1.461845	-1.37311
11	C	-6.20338	1.71313	-0.05818
12	H	-6.0234	0.855072	-3.35437
13	H	-7.67926	1.586605	-1.62959
14	O	-3.51023	0.507406	-2.95168
15	O	-2.08863	1.155569	0.832666
16	C	-0.16862	0.383452	-1.17457
17	H	0.050161	0.781568	-0.18412
18	C	0.301251	-1.08316	-1.24592
19	H	0.21132	-1.4121	-2.28458
20	C	0.588533	1.192492	-2.24616
21	O	0.865689	0.674128	-3.32777
22	C	1.809399	-1.17706	-0.88065
23	O	2.427538	-0.19266	-0.48954

24	C	-0.45821	-2.14093	-0.42755
25	O	-0.4324	-3.30875	-0.82293
26	N	0.866146	2.499721	-1.99956
27	H	1.326918	2.942804	-2.7859
28	N	2.323362	-2.42791	-1.05237
29	H	1.63161	-3.12825	-1.29989
30	N	-1.04121	-1.73757	0.736265
31	H	-1.00861	-0.74863	0.958806
32	C	3.633057	-2.89851	-0.79856
33	C	4.684426	-2.0374	-0.4544
34	C	3.855516	-4.2903	-0.91422
35	C	5.957406	-2.55568	-0.22221
36	H	4.490646	-0.9782	-0.36711
37	C	5.144375	-4.7732	-0.6751
38	C	6.195797	-3.92372	-0.33088
39	H	6.763007	-1.8783	0.045643
40	C	-1.71571	-2.55343	1.688294
41	C	-2.30997	-3.76894	1.324416
42	C	-1.7881	-2.08908	3.020347
43	C	-2.98267	-4.52818	2.279911
44	H	-2.22726	-4.11443	0.303998
45	C	-2.47751	-2.87258	3.950975
46	C	-3.07344	-4.08219	3.59657
47	H	-3.43758	-5.46949	1.986136
48	H	7.186679	-4.32878	-0.14944
49	H	-3.59734	-4.67037	4.343931
50	Cl	-7.38119	2.225924	1.136207
51	C	0.530532	3.361424	-0.86849
52	H	-0.1639	4.139168	-1.21504
53	H	-0.00878	2.778448	-0.11899
54	C	1.763764	4.027777	-0.24338
55	H	2.336505	4.534319	-1.03206
56	H	1.418176	4.819452	0.433118
57	C	2.683763	3.05625	0.520105
58	H	2.123589	2.629941	1.362009
59	H	2.944897	2.215274	-0.1284
60	C	3.936473	3.733081	1.03325
61	C	3.945002	4.395041	2.268698
62	C	5.110376	3.743442	0.267656
63	C	5.088789	5.05038	2.725557
64	H	3.046556	4.389884	2.88187

65	C	6.257034	4.39779	0.719351
66	H	5.125895	3.225652	-0.68847
67	C	6.249749	5.055005	1.950604
68	H	5.075043	5.552889	3.688773
69	H	7.157992	4.388958	0.112185
70	H	7.142517	5.561454	2.305842
71	H	5.321159	-5.84228	-0.76095
72	C	2.740241	-5.23931	-1.2884
73	H	1.884372	-5.16867	-0.60632
74	H	2.359985	-5.04845	-2.30056
75	H	3.093921	-6.27265	-1.26601
76	H	-2.5371	-2.52348	4.978489
77	C	-1.13427	-0.79593	3.447879
78	H	-0.06625	-0.78287	3.198802
79	H	-1.59146	0.076725	2.967732
80	H	-1.22256	-0.66405	4.528874

Table S17. Optimized structure for compound (**17**) and cartesian Z-matrix

Compound **17**



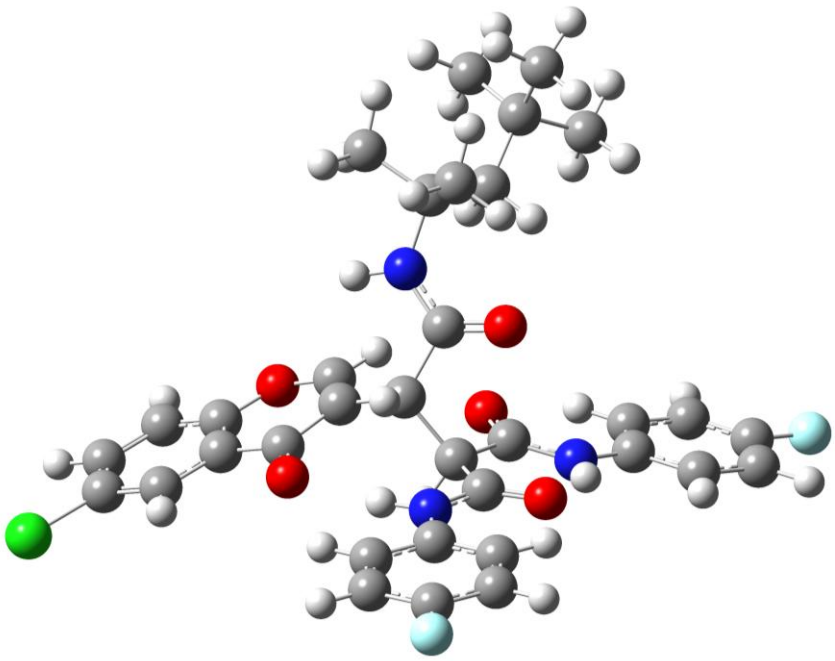
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	-2.04858	0.743041	0.853846
2	C	-3.02573	-0.18649	0.290627
3	C	-4.43101	0.224308	0.433675
4	C	-4.73683	1.461098	1.01726
5	C	-2.46292	1.9283	1.366786
6	H	-5.23326	-1.54797	-0.47184
7	C	-5.48008	-0.59609	-0.01695
8	C	-6.06063	1.891379	1.160734
9	H	-1.78571	2.680907	1.746122
10	C	-7.08648	1.072641	0.717261
11	C	-6.78707	-0.16982	0.130509
12	H	-6.26071	2.855939	1.613549
13	H	-8.11975	1.3844	0.818197
14	O	-3.75737	2.301091	1.463614
15	O	-2.70219	-1.24313	-0.2802
16	C	-0.60472	0.31044	0.725755
17	H	-0.62707	-0.77071	0.876969

18	C	-0.1234	0.523908	-0.77546
19	H	-1.02552	0.453938	-1.38442
20	C	0.353377	0.947307	1.740107
21	O	0.304174	2.144966	2.01439
22	C	0.367613	1.96664	-1.01992
23	O	-0.47905	2.839735	-1.17888
24	C	0.783395	-0.64303	-1.17568
25	O	2.018182	-0.59656	-1.13973
26	N	1.304476	0.149486	2.304925
27	H	1.893799	0.657338	2.954156
28	N	1.718427	2.140792	-1.01512
29	H	2.24337	1.27145	-0.93839
30	N	0.076213	-1.75644	-1.51999
31	H	-0.92095	-1.72539	-1.30385
32	C	2.454382	3.337919	-1.15602
33	C	1.835031	4.584942	-1.32663
34	C	3.865434	3.242571	-1.11784
35	C	2.612051	5.734024	-1.46214
36	H	0.756132	4.633855	-1.34904
37	C	4.61161	4.415186	-1.25789
38	C	4.002566	5.658093	-1.43021
39	H	2.11878	6.692862	-1.59338
40	C	0.632422	-3.04927	-1.76724
41	C	1.552692	-3.27339	-2.8091
42	C	0.174755	-4.1078	-0.97318
43	C	2.021023	-4.58319	-2.98205
44	C	0.644106	-5.4019	-1.17952
45	C	1.583047	-5.63785	-2.18343
46	H	2.734061	-4.77584	-3.77926
47	Cl	-8.10683	-1.18683	-0.42263
48	H	5.696171	4.345856	-1.22887
49	H	0.282612	-6.21503	-0.5577
50	H	-0.55481	-3.90321	-0.19432
51	C	1.478688	-1.30893	2.279681
52	H	0.801186	-1.78727	3.000522
53	H	1.231848	-1.68882	1.287701
54	C	2.912205	-1.67137	2.607978
55	C	3.88769	-1.67784	1.60144
56	C	3.283892	-1.97275	3.922909
57	C	5.212856	-1.98149	1.911951
58	H	3.597898	-1.45527	0.578153

59	C	4.611308	-2.27397	4.233462
60	H	2.530232	-1.97797	4.707022
61	C	5.57781	-2.27765	3.227526
62	H	5.96134	-1.99164	1.125016
63	H	4.887524	-2.50932	5.2571
64	H	6.610426	-2.51516	3.466026
65	H	4.608886	6.552609	-1.53645
66	C	4.561633	1.9155	-0.92458
67	H	4.293938	1.444061	0.02954
68	H	4.312637	1.19628	-1.71448
69	H	5.646163	2.048276	-0.93115
70	H	1.963334	-6.64054	-2.35388
71	C	2.00419	-2.17513	-3.73634
72	H	1.160135	-1.55138	-4.04921
73	H	2.722293	-1.51367	-3.24306
74	H	2.469272	-2.59416	-4.63222

Table S18. Optimized structure for compound (**18**) and cartesian Z-matrix

Compound **18**



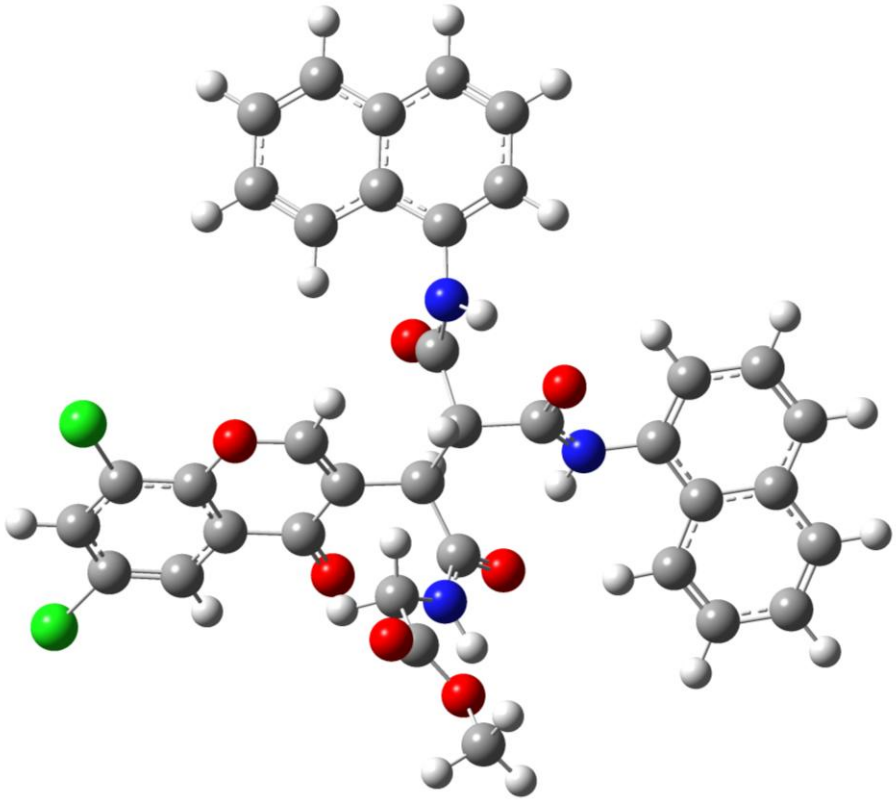
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	-1.25216	1.228172	-0.31994
2	C	-2.7024	1.036328	-0.36422
3	C	-3.46045	2.134152	-0.98586
4	C	-2.77513	3.215019	-1.55737
5	C	-0.70236	2.296235	-0.95104
6	H	-5.38706	1.272478	-0.59652
7	C	-4.86519	2.11506	-1.03429
8	C	-3.4586	4.270974	-2.16897
9	H	0.363989	2.444004	-1.05605
10	C	-4.84365	4.244263	-2.2047
11	C	-5.53923	3.163354	-1.63435
12	H	-2.89634	5.088917	-2.60519
13	H	-5.39547	5.051704	-2.67216
14	O	-1.40827	3.277498	-1.55258
15	O	-3.25684	0.013328	0.069714
16	C	-0.44863	0.121826	0.330566
17	H	-1.13036	-0.30523	1.073462
18	C	-0.10501	-1.02672	-0.68199
19	H	-0.82409	-0.92913	-1.50604
20	C	0.791028	0.489453	1.175763
21	O	1.664073	-0.35631	1.347697

22	C	1.258856	-0.73911	-1.35274
23	O	1.476359	0.413632	-1.73424
24	C	-0.38068	-2.43246	-0.0989
25	O	0.444233	-3.34906	-0.08972
26	N	0.77609	1.710062	1.76867
27	H	-0.01484	2.306214	1.575806
28	N	2.079493	-1.79668	-1.54482
29	H	1.77412	-2.64397	-1.05858
30	N	-1.66369	-2.57016	0.343679
31	H	-2.26884	-1.75423	0.248229
32	C	3.345903	-1.82134	-2.16245
33	C	3.928432	-0.71242	-2.79717
34	C	4.039116	-3.04283	-2.14061
35	C	5.181901	-0.83448	-3.39615
36	H	3.398538	0.228748	-2.80926
37	C	5.290206	-3.16452	-2.73714
38	C	5.845631	-2.05324	-3.35971
39	H	5.647167	0.011805	-3.89005
40	C	-2.29338	-3.70659	0.903899
41	C	-1.64167	-4.9267	1.139684
42	C	-3.65118	-3.57122	1.236825
43	C	-2.34878	-5.99096	1.698946
44	H	-0.59744	-5.03321	0.885767
45	C	-4.35543	-4.63381	1.793991
46	C	-3.6907	-5.83368	2.01774
47	H	-1.86255	-6.94162	1.888807
48	Cl	-7.29177	3.155555	-1.69455
49	H	5.832937	-4.10319	-2.7236
50	H	-5.40395	-4.54091	2.054187
51	C	1.784164	2.231226	2.74025
52	C	1.826225	1.274457	3.948225
53	H	2.177846	0.287544	3.644867
54	H	2.479934	1.657825	4.732712
55	H	0.821198	1.167832	4.370004
56	C	1.23726	3.596577	3.184762
57	H	1.208242	4.311601	2.355632
58	H	0.222674	3.486228	3.585632
59	H	1.853971	4.021745	3.977928
60	C	3.139367	2.318219	1.967208
61	H	2.904296	2.761216	0.990917
62	H	3.420588	1.282217	1.757476

63	C	4.407194	3.062575	2.494601
64	C	5.560901	2.620854	1.563744
65	H	5.331185	2.839738	0.515029
66	H	6.488851	3.144183	1.81956
67	H	5.746839	1.54478	1.645153
68	C	4.279956	4.596886	2.377043
69	H	4.004625	4.893092	1.358317
70	H	3.536772	5.01478	3.060202
71	H	5.238154	5.074582	2.610865
72	C	4.796667	2.695893	3.939305
73	H	4.086646	3.088983	4.673635
74	H	4.863448	1.611757	4.076521
75	H	5.777069	3.121445	4.181891
76	H	3.592889	-3.9034	-1.65011
77	F	7.061372	-2.1634	-3.94267
78	H	-4.1552	-2.62564	1.056652
79	F	-4.36854	-6.87007	2.558899

Table S19. Optimized structure for compound (**19**) and cartesian Z-matrix

Compound **19**



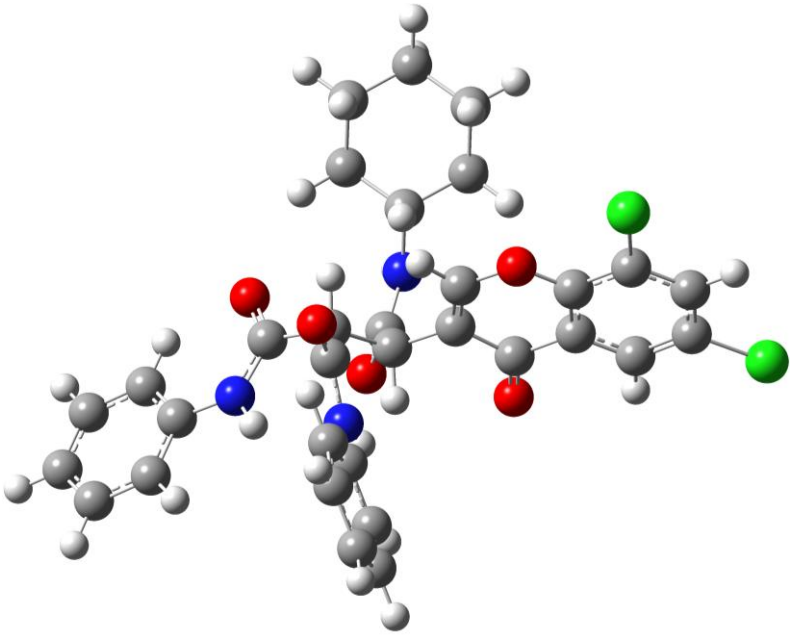
Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	-1.35185	-0.75308	-0.24059
2	C	-2.09727	-1.68807	-1.09916
3	C	-3.57105	-1.6397	-0.95414
4	C	-4.14891	-0.75739	-0.03382
5	C	-2.04068	0.047246	0.603184
6	H	-3.91588	-3.14703	-2.43737
7	C	-4.38798	-2.47414	-1.73159
8	C	-5.5455	-0.70428	0.115824
9	H	-1.60094	0.780169	1.267688
10	C	-6.35082	-1.53031	-0.6544
11	C	-5.76115	-2.41081	-1.57458
12	H	-7.42732	-1.49141	-0.54255
13	O	-3.38941	0.066985	0.738378
14	O	-1.54036	-2.46246	-1.87436
15	C	0.157509	-0.70822	-0.43608
16	H	0.303988	-0.41416	-1.47974
17	C	0.864575	0.351192	0.443037
18	H	0.553183	0.24218	1.486904
19	C	0.833984	-2.09103	-0.37097

20	O	1.681489	-2.37233	-1.22244
21	C	2.412783	0.431734	0.572276
22	O	2.836507	1.098452	1.520393
23	C	0.432111	1.777817	-0.04206
24	O	-0.03102	1.964706	-1.15328
25	N	0.578461	-2.96272	0.638918
26	H	1.090699	-3.83212	0.555713
27	N	3.199673	-0.12215	-0.38641
28	H	2.762313	-0.77913	-1.03209
29	N	0.60859	2.739033	0.923453
30	C	-0.32922	-2.86511	1.764722
31	H	-0.3559	-1.85423	2.173777
32	H	-1.36205	-3.12605	1.492883
33	C	7.121456	-3.10735	-1.87173
34	C	7.65336	-1.87583	-1.57039
35	C	6.833075	-0.81714	-1.09593
36	C	5.422671	-1.04228	-0.94033
37	C	4.907292	-2.3325	-1.24599
38	C	5.73656	-3.33421	-1.70131
39	H	8.456586	0.597395	-0.885
40	H	7.761097	-3.90638	-2.23495
41	H	8.717728	-1.69029	-1.68861
42	C	7.387002	0.447043	-0.76765
43	C	4.612998	0.0479	-0.47733
44	H	3.852882	-2.54506	-1.1157
45	H	5.319055	-4.31045	-1.9298
46	C	5.190826	1.264626	-0.16683
47	C	6.580907	1.459609	-0.30593
48	H	4.56868	2.073196	0.190712
49	H	7.004381	2.42703	-0.05367
50	C	1.725123	4.869186	0.936914
51	C	0.573997	4.148726	0.684754
52	C	-0.62415	4.81231	0.275397
53	C	-0.57708	6.236607	0.099955
54	C	0.629254	6.940302	0.354821
55	C	1.753898	6.271064	0.7755
56	H	-1.91116	3.072082	0.191475
57	H	2.620043	4.341466	1.254624
58	C	-1.85978	4.144689	0.062467
59	C	-1.75574	6.919375	-0.30648
60	H	0.644219	8.018321	0.220761

61	H	2.673641	6.811158	0.977683
62	C	-2.93333	6.240768	-0.51262
63	C	-2.98426	4.840044	-0.3186
64	H	-1.70798	7.996174	-0.44518
65	H	-3.82665	6.776039	-0.8204
66	H	-3.91877	4.309378	-0.47431
67	Cl	-6.80304	-3.4435	-2.53316
68	Cl	-6.26025	0.396063	1.263607
69	C	0.048238	-3.78376	2.922225
70	O	-0.43526	-3.67663	4.024722
71	O	0.927147	-4.73562	2.560391
72	C	1.305943	-5.66197	3.600135
73	H	2.014435	-6.3466	3.136686
74	H	1.770454	-5.12646	4.430325
75	H	0.427946	-6.19872	3.964916
76	H	1.272737	2.44744	1.639186

Table S20. Optimized structure for compound (**20**) and cartesian Z-matrix

Compound **20**



Center number	Atom	Standard orientation: coordinates / Angstroms		
		x	y	z
1	C	0.911252	0.07633	-0.25356
2	C	1.822346	-0.19582	-1.37959
3	C	3.218229	-0.51268	-0.99398
4	C	3.563227	-0.59145	0.360519
5	C	1.371773	-0.06577	1.011229
6	H	3.896428	-0.67693	-3.01926
7	C	4.190945	-0.74087	-1.97857
8	C	4.882647	-0.89572	0.737976
9	H	0.775068	0.043233	1.908478
10	C	5.843352	-1.11786	-0.23774
11	C	5.485905	-1.03786	-1.59238
12	H	6.8609	-1.35167	0.049969
13	O	2.645645	-0.3885	1.345277
14	O	1.45476	-0.17721	-2.55122
15	C	-0.51856	0.4359	-0.61675
16	H	-0.82237	-0.28349	-1.38466
17	C	-1.51309	0.362122	0.579404
18	H	-1.16059	1.003843	1.388775
19	C	-0.67206	1.744004	-1.45568
20	O	-1.38875	1.701928	-2.44546
21	C	-2.89158	0.993505	0.237891
22	O	-3.0223	2.206658	0.329907

23	C	-1.59965	-1.0328	1.226168
24	O	-1.5558	-1.1516	2.443216
25	N	0.02166	2.872972	-1.12265
26	H	-0.19101	3.617641	-1.77871
27	N	-3.87787	0.130339	-0.14292
28	H	-3.6526	-0.8547	-0.11294
29	N	-1.76771	-2.0861	0.35274
30	H	-1.63854	-1.87436	-0.62788
31	C	-5.21162	0.42142	-0.51745
32	C	-5.70104	1.724866	-0.68131
33	C	-6.06007	-0.6738	-0.73917
34	C	-7.03029	1.908643	-1.06206
35	H	-5.0455	2.566099	-0.51082
36	C	-7.38328	-0.47231	-1.11979
37	H	-5.68098	-1.68528	-0.6106
38	C	-7.87754	0.822788	-1.28302
39	H	-7.40299	2.920937	-1.18837
40	H	-8.02691	-1.33068	-1.28746
41	H	-8.90954	0.982273	-1.57941
42	C	-1.85418	-3.47391	0.640641
43	C	-1.98887	-3.98284	1.939866
44	C	-1.82036	-4.3517	-0.45311
45	C	-2.08402	-5.36297	2.121503
46	H	-2.00893	-3.3051	2.780784
47	C	-1.91765	-5.72558	-0.25334
48	H	-1.71607	-3.95693	-1.46146
49	C	-2.05018	-6.23996	1.037491
50	H	-2.1862	-5.75183	3.13032
51	H	-1.88863	-6.39222	-1.10981
52	H	-2.12552	-7.31119	1.195107
53	Cl	6.720139	-1.32363	-2.80383
54	Cl	5.308579	-0.99337	2.425954
55	C	0.535645	3.324414	0.174177
56	C	1.989663	3.808819	0.043336
57	C	-0.36557	4.421543	0.77157
58	H	0.520655	2.467418	0.851611
59	C	2.537735	4.329904	1.381022
60	H	2.023239	4.612631	-0.70611
61	H	2.61343	2.995955	-0.34533
62	C	0.187087	4.940279	2.108178
63	H	-0.42048	5.254139	0.054128

64	H	-1.37957	4.027153	0.883949
65	C	1.638345	5.424158	1.974752
66	H	3.558814	4.704121	1.244334
67	H	2.608153	3.494579	2.092714
68	H	-0.45277	5.745993	2.485626
69	H	0.140773	4.135702	2.856193
70	H	2.024881	5.744066	2.949426
71	H	1.666421	6.308104	1.321999

Table S21. Predicted biological activity of the compound (**1**-**20**) using PASS

Biological activity						
	Analgesic		Analgesic, non-opioid		Muscular dystrophy treatment	
Ligand	Pa[a]	Pi[b]	Pa[a]	Pi[b]	Pa[a]	Pi[b]
C1	–	–	–	–	0.563	0.009
C2	–	–	–	–	0.495	0.018
C3	0.617	0.014	0.646	0.010	0.349	0.063
C4	–	–	–	–	0.585	0.006
C5	–	–	–	–	–	–
C6	–	–	–	–	0.605	0.005
C7	–	–	–	–	0.547	0.010
C8	–	–	–	–	0.547	0.010
C9	0.645	0.014	0.650	0.009	0.333	0.074
C10	–	–	–	–	0.391	0.041
C11	0.578	0.023	0.561	0.017	0.303	0.105
C12	–	–	–	–	0.316	0.091
C13	–	–	–	–	–	–
C14	–	–	–	–	0.526	0.014
C15	–	–	–	–	0.258	0.172
C16	–	–	–	–	0.515	0.015
C17	–	–	–	–	0.424	0.031
C18	0.305	0.124	0.250	0.139	0.274	0.146
C19	–	–	–	–	0.340	0.069
C20	–	–	–	–	0.402	0.038
Celecoxib	0.412	0.067	0.439	0.041	–	–

[a]Pa: probability ‘to be active’. [b]Pi: probability ‘to be inactive’.

Table S22. The active site residues of proteins (PDB: 1P60) and (PDB: 1X2J)

Active Site of PDB: 1X2J	
Pocket Surface area / Å^2	402.149
Pocket Volume (SA) / Å^3	419.304
Active site residues	324 Val, 364 Gly, 365 Leu, 366 Ala, 367 Gly, 368 Cys, 369 Val, 415 Arg, 416 Ile, 17 Gly, 418 Val, 419 Gly, 420 Val, 462 Gly, 463 Val, 464 Gly, 465 Val, 466 Ala, 467 Val, 509 Gly, 510 Ala, 511 Gly, 512 Val, 513 Cys, 514 Val, 556 Ala, 557 Leu, 558 Gly, 559 Ile, 560 Thr, 561 Val, 603 Gly, 604 Val, 606 Gly, 607 Ala, 608 Val
Active Site of PDB: 1P60	
Pocket Surface area / Å^2	320.855
Pocket Volume (SA) / Å^3	356.089
Active site residues	61 Val, 62 Gly, 63 Ser, 64 Thr, 65 Gly, 66 Asp, 69 Glu, 73 Met, 7 Ser, 75 Gln, 76 Lys, 78 Gly, 79 Gly, 134 Arg, 135 Tyr, 149 Glu, 150 Thr, 152 Trp, 153 Thr, 156 Gln, 160 Thr, 222 Asp, 223 Lys, 223 Thr, 224 Asp
Active Site of PDB: 4UV7	
Pocket Surface area / Å^2	3220.564
Pocket Volume (SA) / Å^3	6125.590
Active site residues	1 Leu, 2 Glu, 3 Glu, 4 Lys, 6 Val, 6 Gln, 9 Gly, 10 Thr, 11 Ser, 13 Lys, 36 Val, 38 Leu, 39 Gly, 40 Asn, 60 Glu, 62 Ala, 63 Gly, 64 Tyr, 8 Arg, 86 Asn, 87 Met, 88 Tyr, 89 Tyr, 90 Glu, 91 Asn, 118 Glu, 120 Leu, 121 His, 134 Ile, 144 Val, 145 Ser, 188 Lys, 197 Gly, 198 Arg, 209 His, 210 Asn, 211 Gly, 212 Cys, 221 Glu, 225 Leu, 226 Val, 227 Cys, 228 Arg, 229 Lys, 230 Phe, 231 Arg, 237 Lys, 241 Pro 242 Pro 243 Leu 244 Met 245 Lys, 509 Arg, 511 Cys, 524 Glu, 532 Ile, 533 Glu, 580 Asn, 582 Leu, 584 Trp, 601 Trp, 602 Tyr
Active Site of PDB: 1V40	
Pocket Surface area / Å^2	4123.958
Pocket Volume (SA) / Å^3	5317.225
Active site residues	208 Tyr, 209 Phe, 211 Met, 212 Rg, 213 Gly, 214 Arg, 217 Ile, 236 Gln, 239 Trp, 243 Lys, 244 Ser, 246 Leu, 247 Pro, 248 Phe, 249 Gly, 250 Lys, 251 Ile, 252 His, 263 Glu, 264 Ser, 265 Leu, 293 Asp, 294 Thr, 296 Asp, 297 Asp, 230 Phe, 299 Met, 300 Ser, 301 Cys, 302 Phe, 303 Pro, 304 Trp, 305 Ala, 306 Glu, 318 Glu 319 Leu, 322 Tyr, 323 Asn, 326 His, 327 Leu, 330 Asp, 352 Tyr, 355 Ile, 356 Cys, 399 Leu, 408 Tyr, 630 Glu, 631 Asp, 632 His, 632 Arg, 635 Ile, 636 Glu, 790 Trp, 793 Arg, 794 Arg, 795 Pro, 796 Gln, 797 Thr

Active Site of PDB: 1YQ7	
Pocket Surface area / Å^2	851.723
Pocket Volume (SA) / Å^3	437.561
Active site residues	27 Glu, 67 Ala, 69 Gly, 70 Gly, 71 Lys, 72 Tyr, 73 Asn, 74 Arg, 76 Leu, 77 Thr, 79 Val 80 Ala 54 Glu, 107 Glu, 110 Gln, 113 Phe, 114 Leu, 117 Asp, 118 Asp, 120 Met, 121 Asp, 125 Thr, 129 Arg, 257 Asp, 258 Asp, 260 Leu, 261 Asp, 264 Gly, 266 Pro, 268 Val, 270 Gly, 271 Lys, 280 Lys, 281 Cys, 282 Ser, 361 Lys, 362 Ile
Color code	

Gln: glutamine, GLU: glutamic acid, Leu: leucine, His: histidine, Val: valine, Asn: asparagine, Thr: threonine, Phe: phenylalanine, Tyr: tyrosine, Ile: isoleucine, Ala: alanine, Trp: tryptophan, Cys: cysteine, Gly: glycine, Arg: arginine, Lys: lysine, Asp: asparagine, Ser: serine, Pro: proline, Met: methionine, PDB: Protein Data Bank.

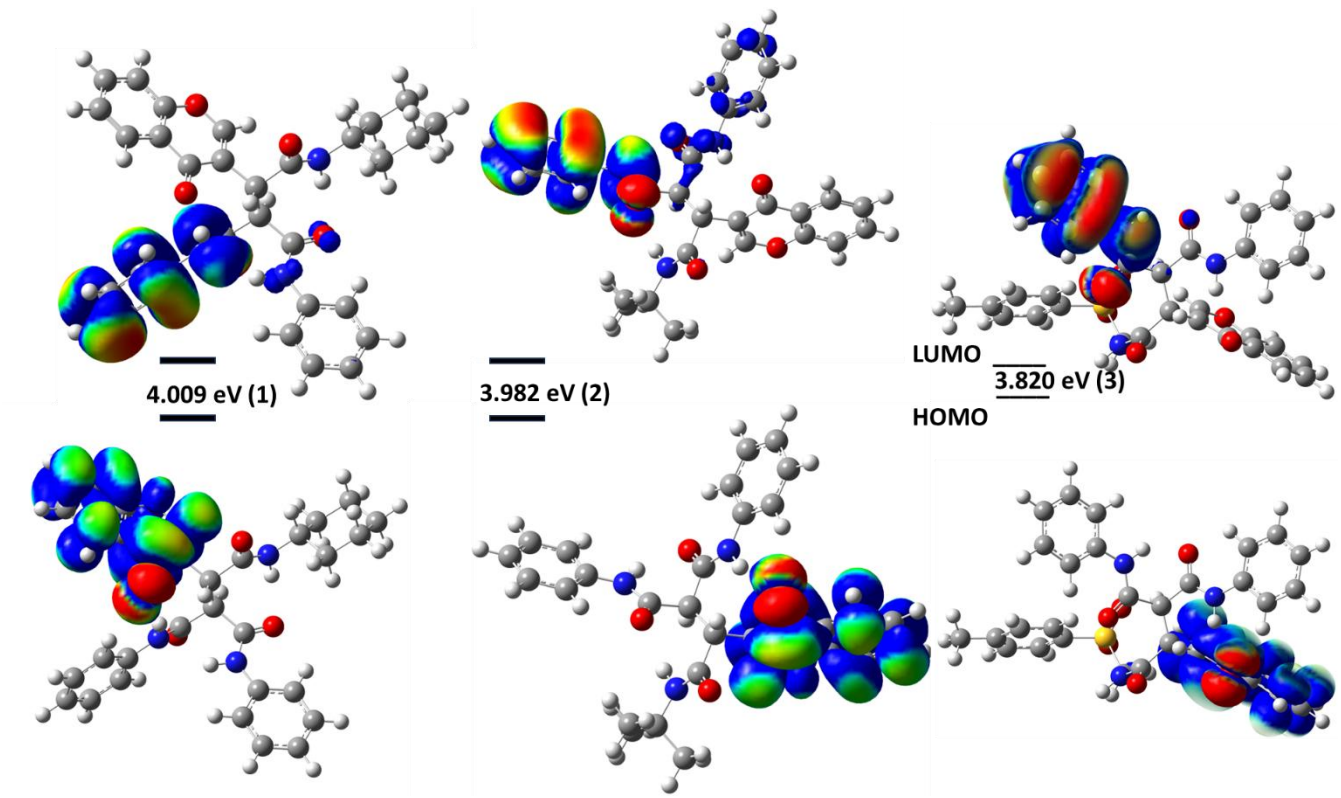


Figure S1. Molecular orbitals (MO) of HOMO and LUMO gap for compounds (**1-3**).

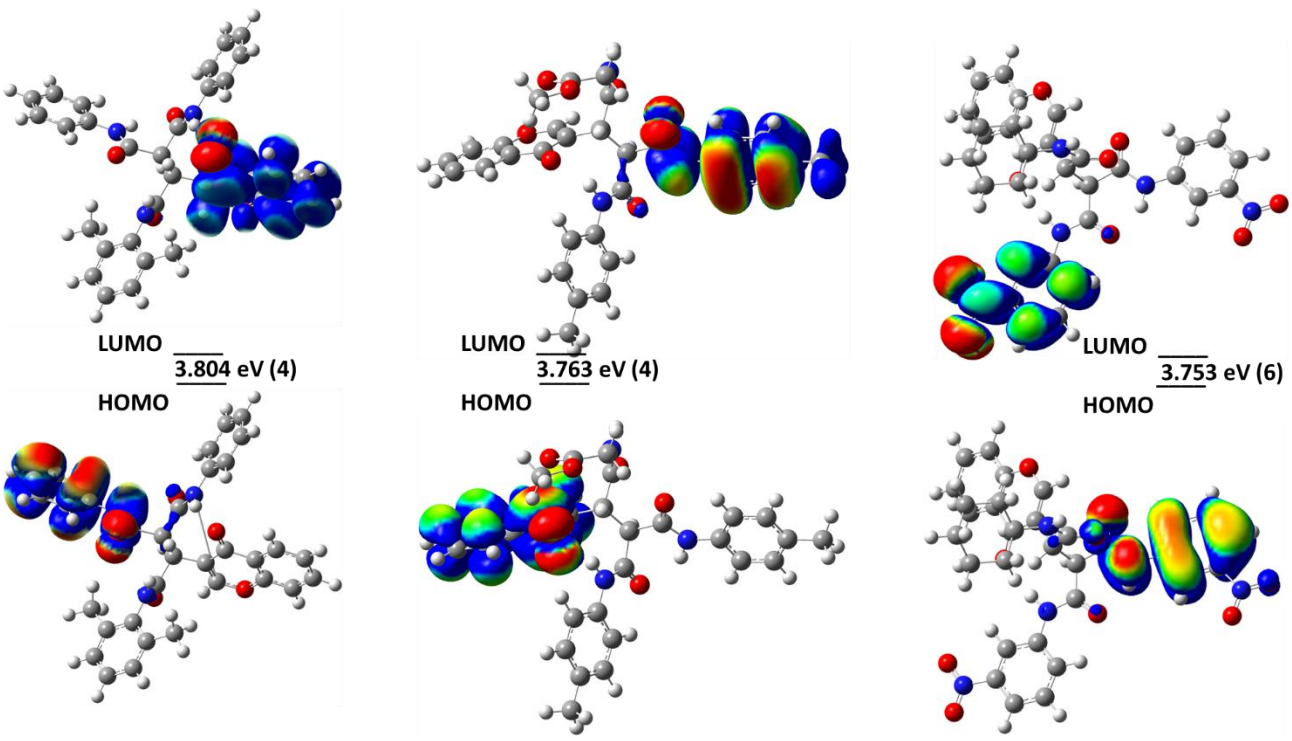


Figure S2. Molecular orbitals (MO) of HOMO and LUMO gap for compounds (**4-6**).

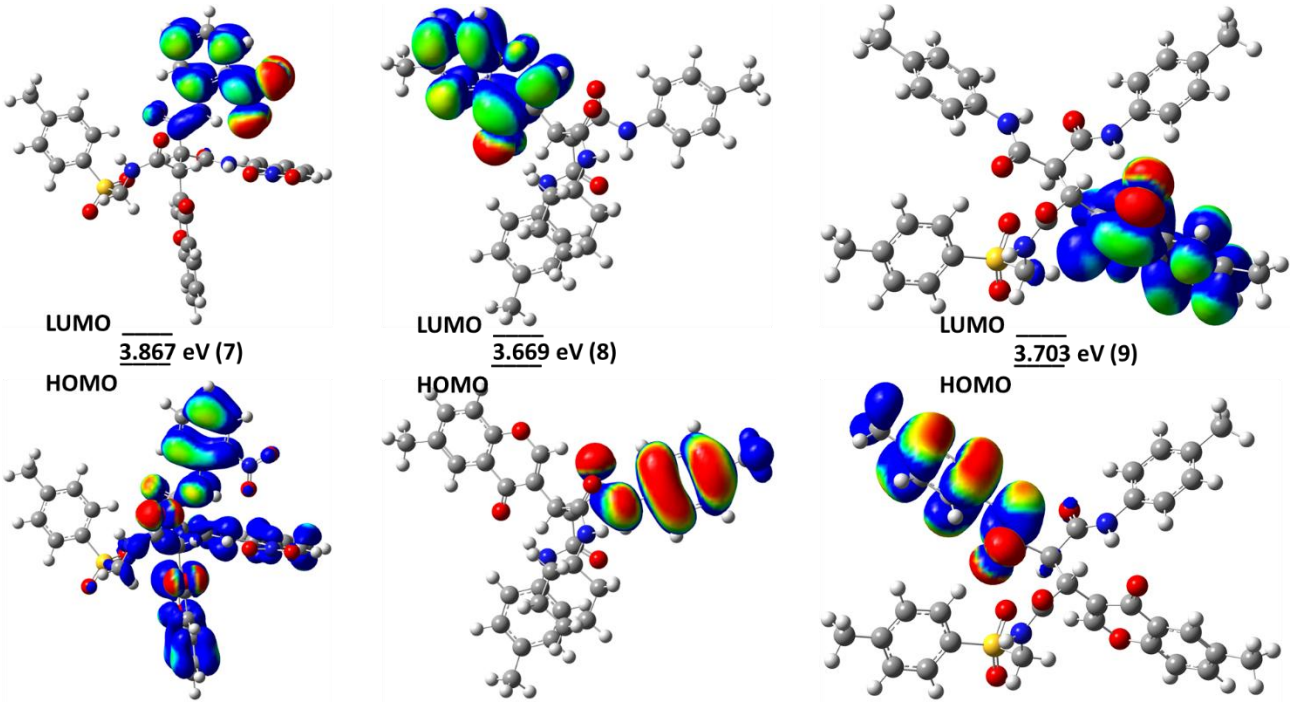


Figure S3. Molecular orbitals (MO) of HOMO and LUMO gap for compounds (**7-9**).

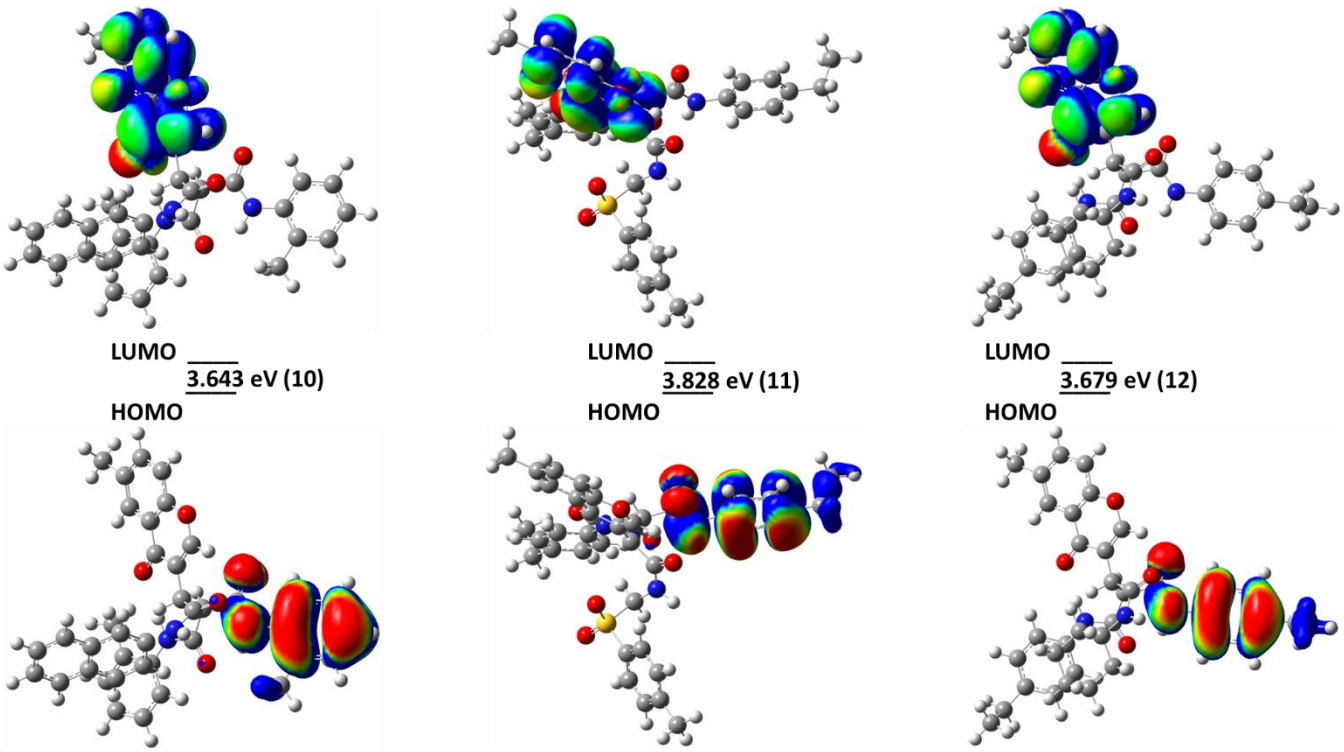


Figure S4. Molecular orbitals (MO) of HOMO and LUMO gap for compounds (**10-12**).

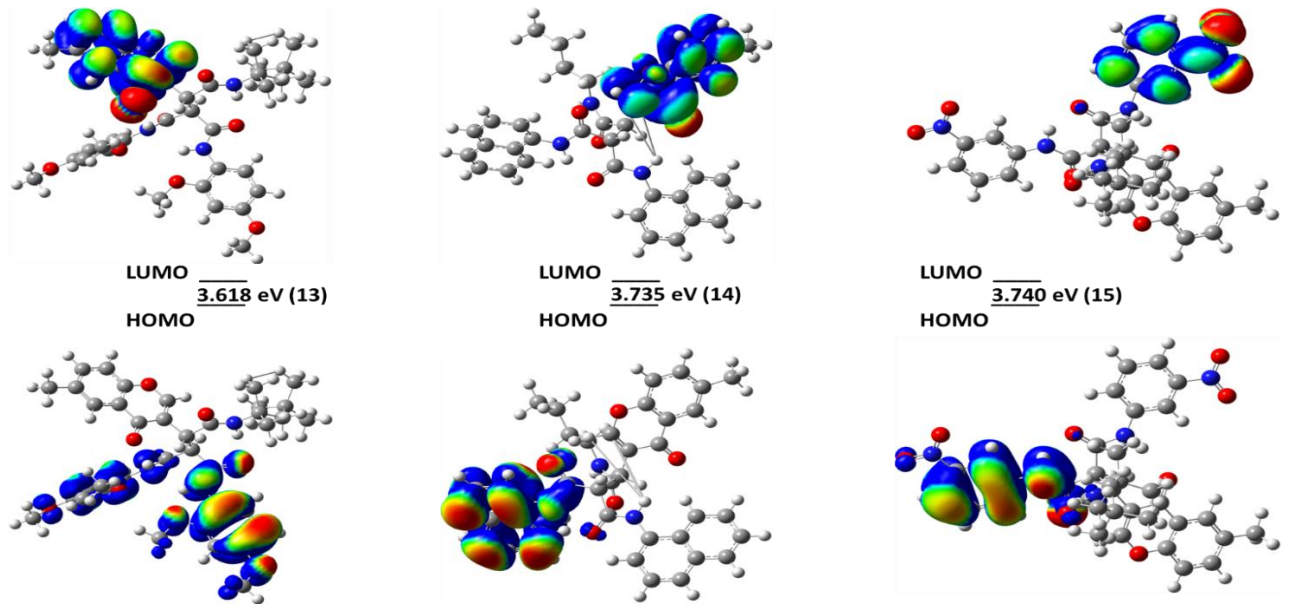


Figure S5. Molecular orbitals (MO) of HOMO and LUMO gap for compounds (**13-15**).

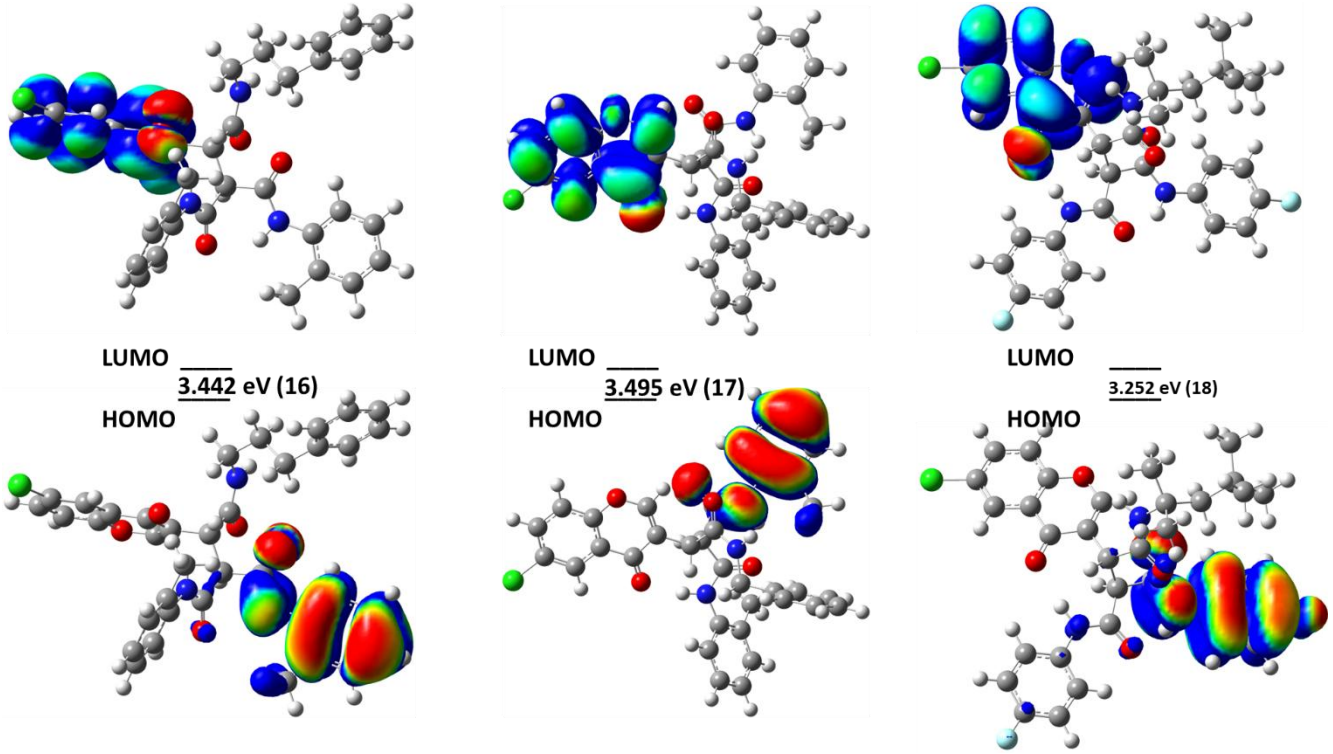


Figure S6. Molecular orbitals (MO) of HOMO and LUMO gap for compounds (**13-15**).

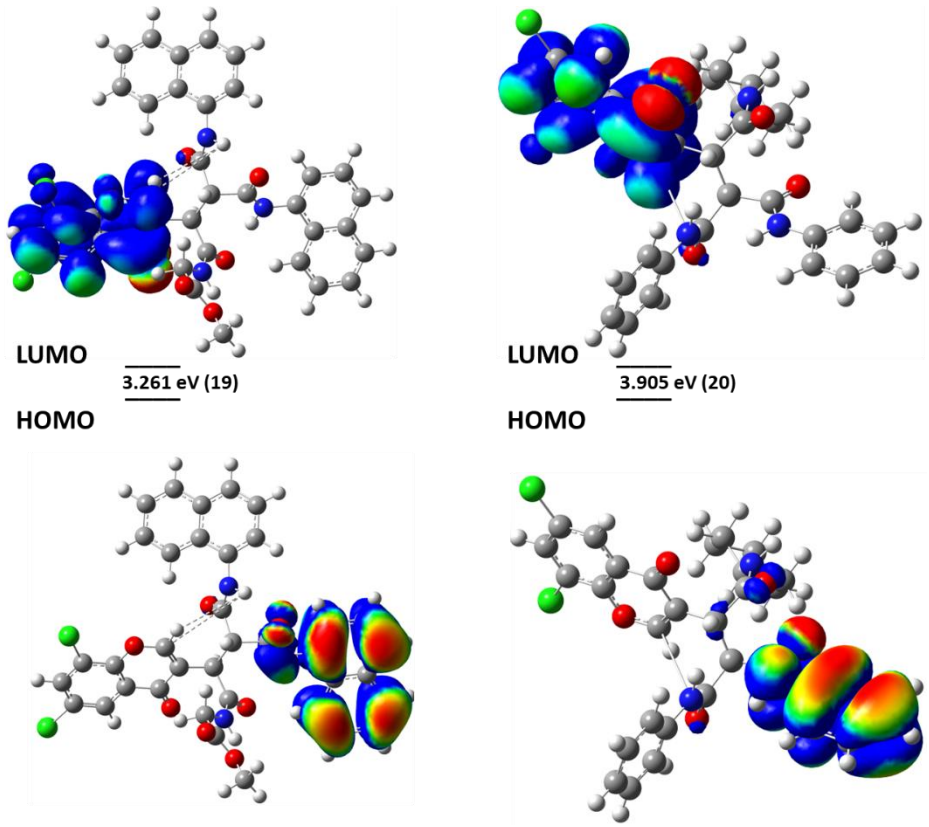


Figure S7. Molecular orbitals (MO) of HOMO and LUMO gap for compounds (**13-15**).

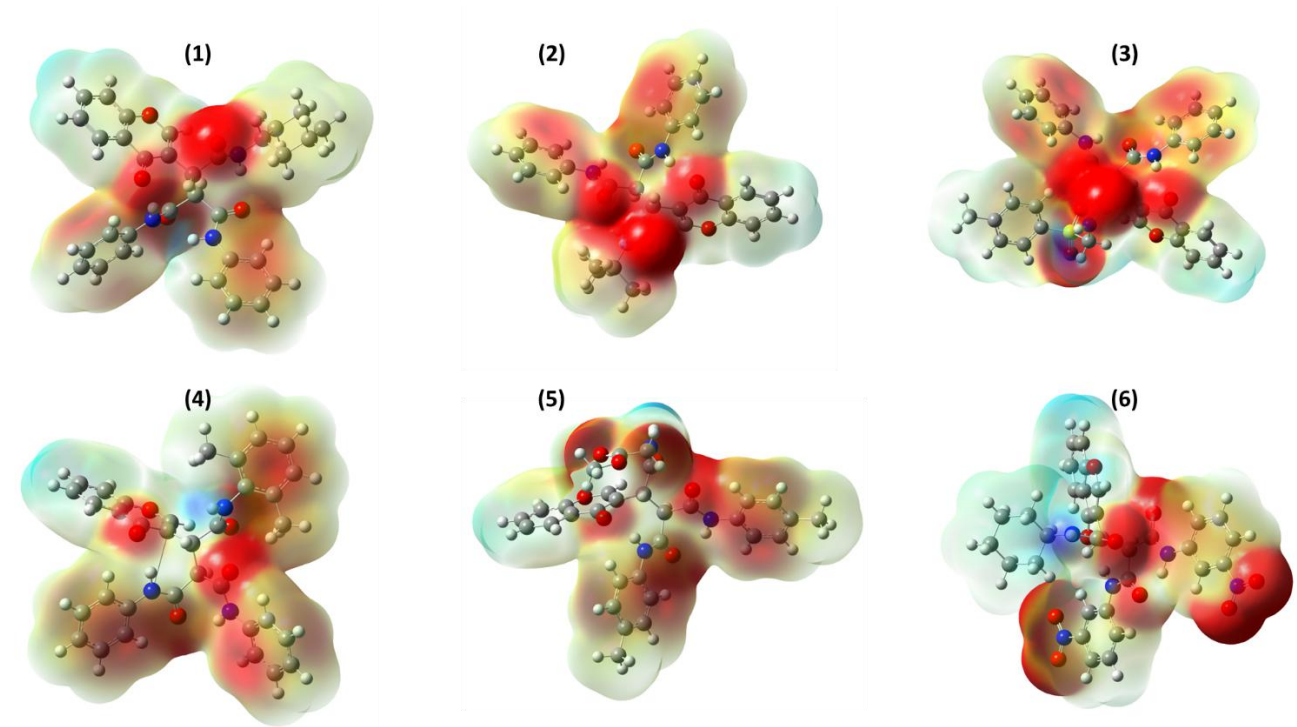


Figure S8. Maps of electrostatic potential (0.02 electrons Bohr^{-3} surface) (red = electron-rich, blue = electron-deficient) for compounds **1** to **6**.

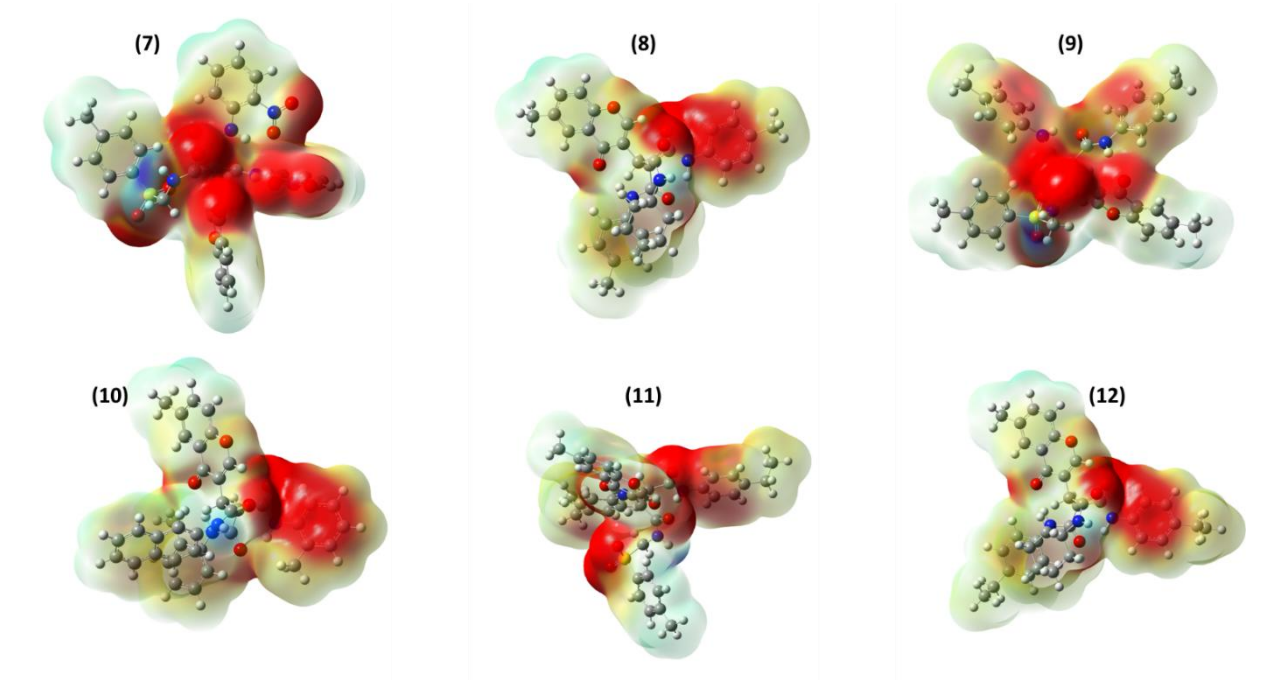


Figure S9. Maps of electrostatic potential (0.02 electrons $Bohr^{-3}$ surface) (red = electron-rich, blue = electron-deficient) for compounds **7** to **12**.

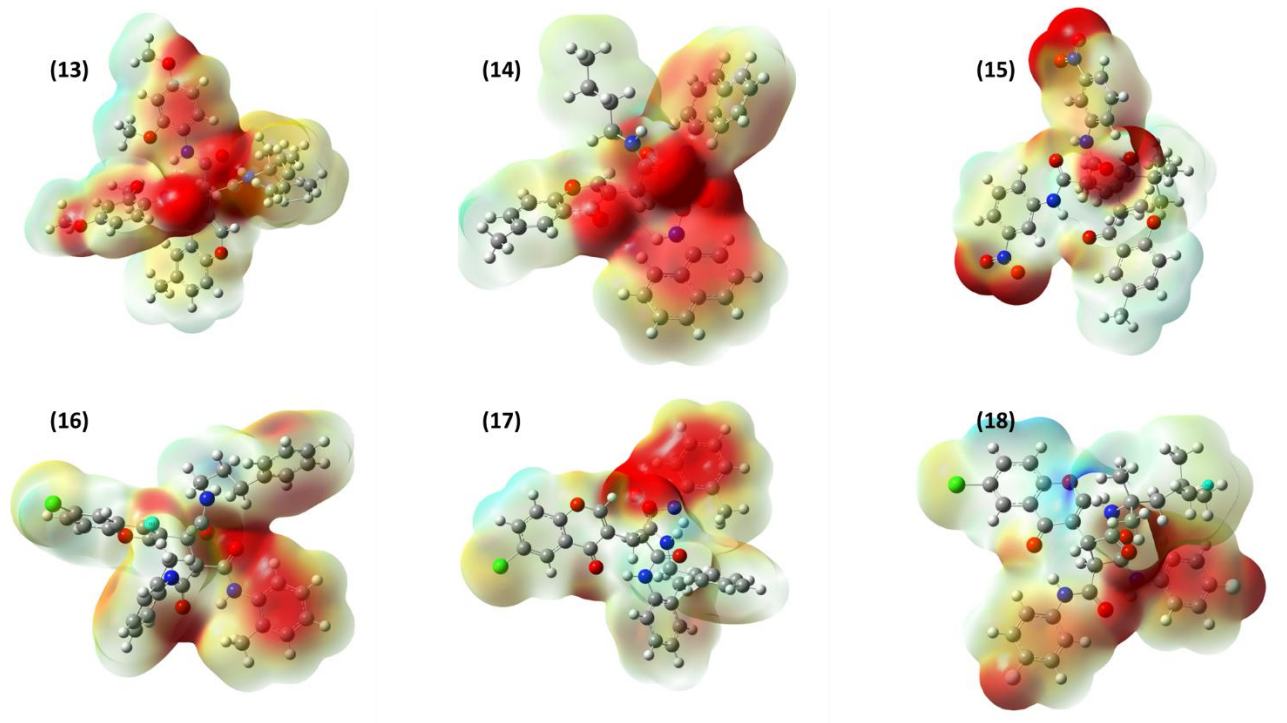


Figure S10. Maps of electrostatic potential (0.02 electrons $Bohr^{-3}$ surface) (red = electron-rich, blue = electron-deficient) for compounds **13** to **18**.

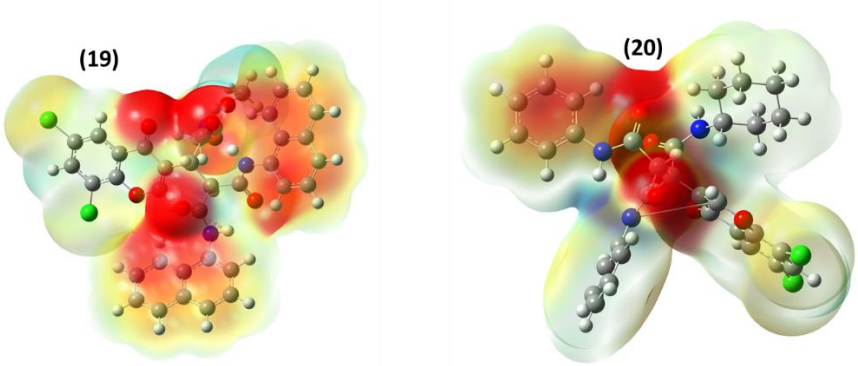


Figure S11. Maps of electrostatic potential (0.02 electrons $Bohr^{-3}$ surface) (red = electron-rich, blue = electron-deficient) for compounds **19** to **20**.

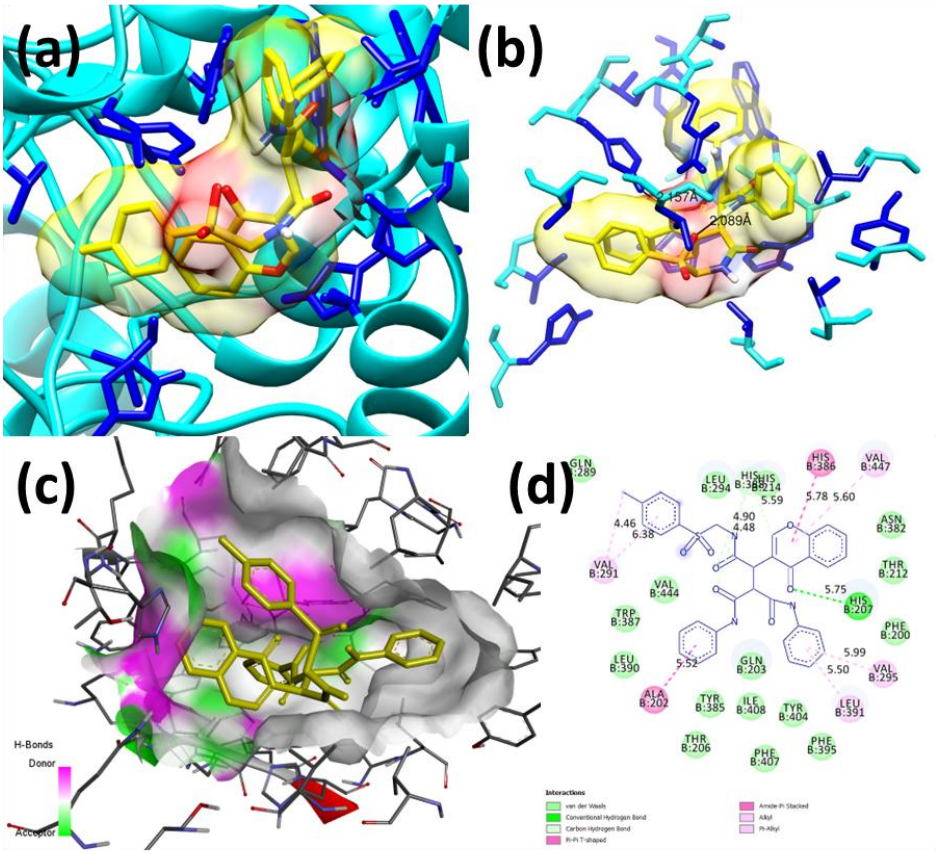


Figure S12. The Molecular docking poses: (a) ligand in protein pocket; (b) active site; (c) hydrogen bonding in solid; (d) ligand-protein interaction for 2D diagram of compound **3** with PDB (**5F19**).

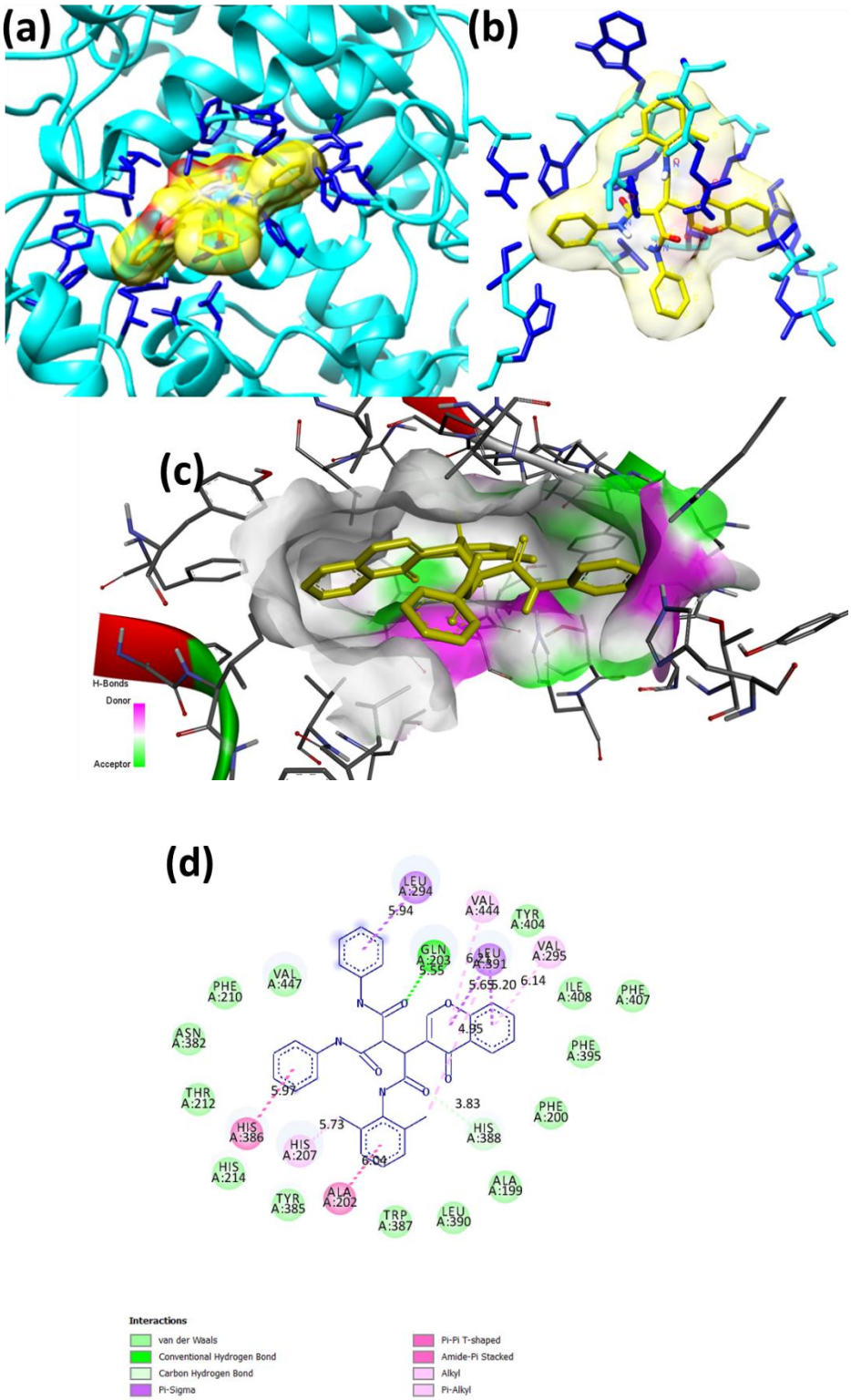


Figure S13. The molecular docking poses: (a) ligand in protein pocket; (b) active site; (c) hydrogen bonding in solid; (d) ligand-protein interaction for 2D diagram of compound **4** with PDB (**5F19**).

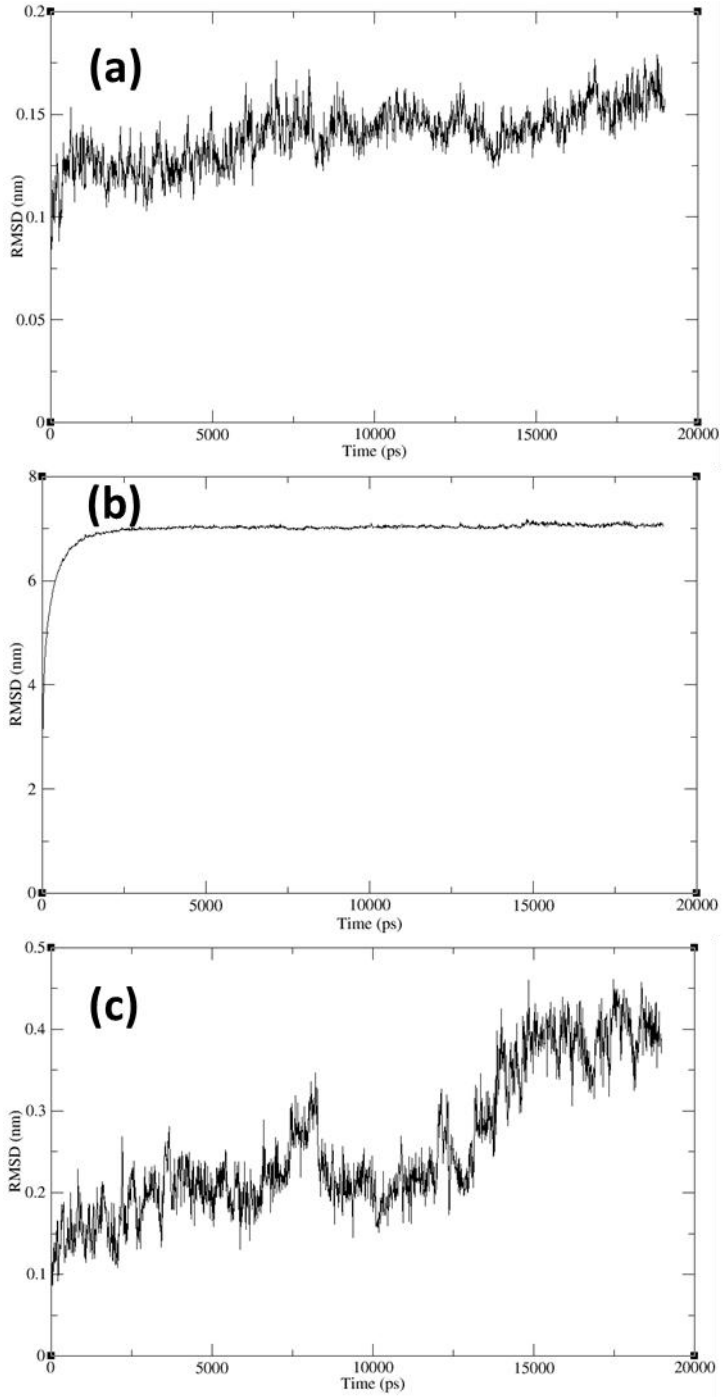


Figure S14. RMSD evolution for (a) the protein (**5F19**), (b) ligand (**3**), and protein-ligand complex (black) during 20 ns MD simulation.

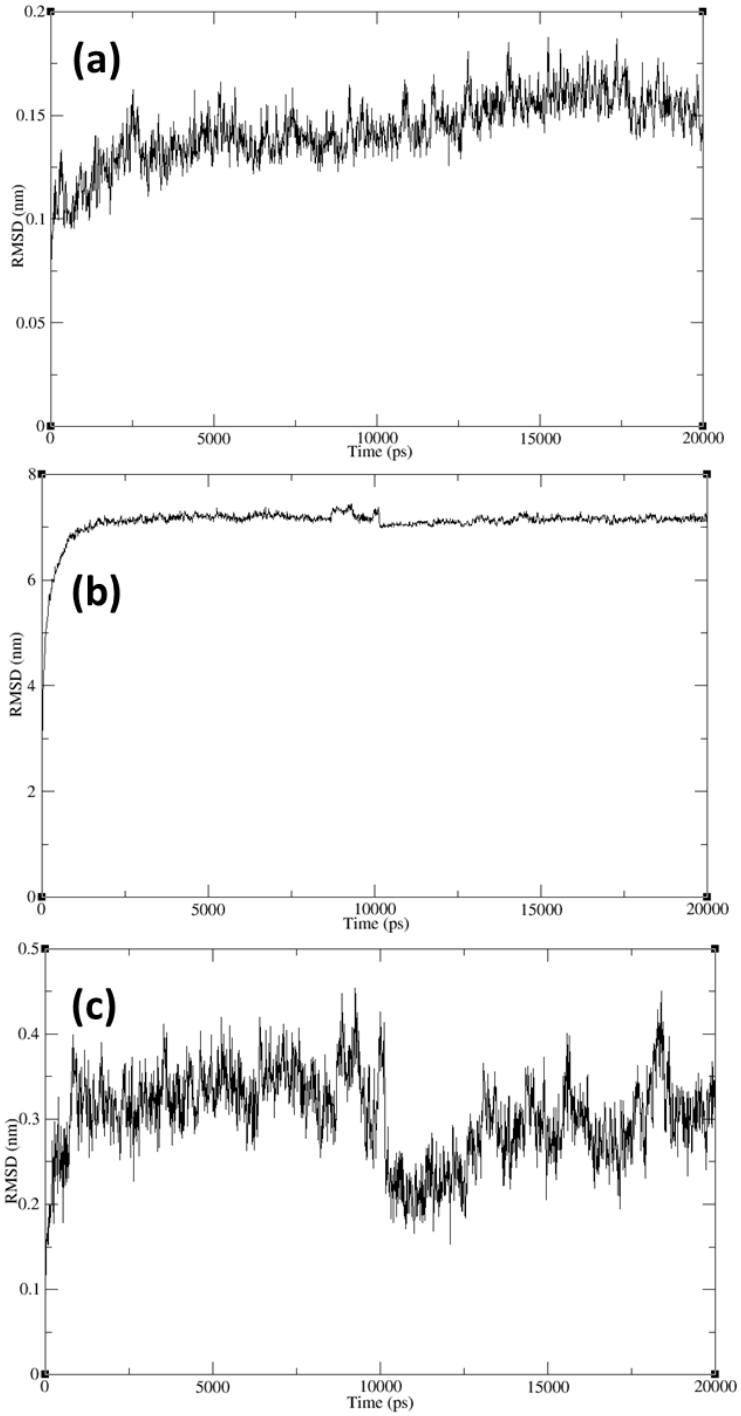


Figure S15. RMSD evolution for (a) the protein (**5F19**), (b) ligand (**4**), and protein-ligand complex (black) during 20 ns MD simulation.