Supplementary Materials

Theoretical Insight and Molecular Recognition of Fluconazole Molecularly Imprinted Polymers: A Combined Computational and Experimental Analysis

Computational settings and scripts S1. Geometry optimization calculation

```
nprocshared= [number of processor want to used, ie: 12]
%chk= [name of chk file that want to used, ie: 7_complex.chk]
#p b3lyp/6-311++g(d,p) opt EmpiricalDispersion=GD3 scrf=(smd,solvent=name of solvent)

[name of the molecule, ie: 7_complex]

[multiplicity of molecule, ie: 0 1]
[coordinate of atom in molecule]
```

Computational settings and scripts S2. Frequency calculation

```
nprocshared= [number of processor want to used, ie: 12]
%chk=[name of chk file that want to used, ie: 7_complex.chk]
#p b3lyp/6-311++g(d,p) freq EmpiricalDispersion=GD3 scrf=(smd,solvent=name of solvent)

[name of the molecule, ie: 7_complex]

[multiplicity of molecule, ie: 0 1]
[coordinate of atom in molecule]
```

Computational settings and scripts S3. NBO and NCI calculation

```
nprocshared= [number of processor want to used, ie: 12]
%chk=[name of chk file that want to used, ie: 7_complex.chk]
#p b3lyp/6-311++g(d,p) EmpiricalDispersion=GD3 pop=nbo output=wfn scrf=(smd,solvent=name of solvent)

[name of the molecule, ie: 7_complex]

[multiplicity of molecule, ie: 0 1]
[coordinate of atom in molecule]
```

Table S1. Type of intermolecular interactions of all complexes
(+ available, - not available)

Complex	Hydrogen bond	Hydrophobic bond	Halogen Bond	Complex	Hydrogen bond	Hydrophobic bond	Halogen Bond
1	+	+	+	21	-	+	-
2	+	-	+	22	+	-	-
3	+	+	+	23	-	+	-
4	-	+	-	24	+	+	+
5	-	+	+	25	-	+	-
6	+	-	+	26	+	+	-
7	+	+	-	27	+	+	-
8	+	+	-	28	-	+	+
9	+	+	-	29	+	+	-
10	+	+	+	30	+	+	-
11	+	+	+	31	+	+	+
12	+	+	+	32	+	+	+
13	+	+	-	33	+	+	-
14	-	+	-	34	-	+	-
15	+	+	+	35	-	+	+
16	+	+	+	36	-	+	-
17	+	+	+	37	-	+	-
18	+	+	-	38	+	+	+
19	-	+	-	39	-	+	+
20	-	-	-				

Table S2. Thermodynamics parameter (ΔG, ΔH, ΔS) of all complexes at different solvents

Complex	Condition	ΔG (kcal/mol)	ΔH (kcal/mol)	ΔS (cal/mol-kelvin)
1_complex	vacuum	0.91	-9.99	-36.55
	acetone	3.46	-6.87	-34.63
	acetonitrile	4.86	-6.66	-38.66
	chloroform	3.50	-6.94	-35.05
	dichloromethane	4.84	-6.58	-38.33
	dmso	3.48	-7.29	-36.10
2_complex	vacuum	-0.17	-12.29	-40.64
	acetone	5.55	-7.17	-42.66
	acetonitrile	4.75	-6.71	-38.42
	chloroform	3.84	-7.84	-39.17
	dichloromethane	5.41	-7.30	-42.64
	dmso	4.95	-7.60	-42.09
3_complex	vacuum	0.32	-9.46	-32.80
	acetone	3.16	-7.12	-34.49
	acetonitrile	3.55	-7.11	-35.75
	chloroform	3.67	-7.34	-36.92
	dichloromethane	3.60	-7.14	-36.01
	dmso	3.72	-8.00	-39.32
4_complex	vacuum	-0.20	-9.63	-31.60
	acetone	3.39	-7.45	-36.35
	acetonitrile	3.61	-7.43	-37.04
	chloroform	3.34	-7.60	-36.68

	dichloromethane	4.73	-8.05	-42.87
	dmso	3.06	-7.70	-36.07
5_complex	vacuum	-1.60	-10.64	-30.34
	acetone	2.23	-8.53	-36.08
	acetonitrile	2.55	-8.53	-37.18
	chloroform	2.14	-8.53	-35.76
	dichloromethane	2.61	-8.32	-36.66
	dmso	1.73	-8.81	-35.36
6_complex	vacuum	-2.67	-15.45	-42.86
	acetone	5.25	-8.23	-45.22
	acetonitrile	4.65	-8.42	-43.85
	chloroform	3.67	-10.17	-46.41
	dichloromethane	4.23	-9.35	-45.55
	dmso	3.14	-8.38	-38.63
7_complex	vacuum	-8.57	-23.08	-48.65
	acetone	-1.90	-17.44	-52.13
	acetonitrile	-2.33	-17.40	-50.54
	chloroform	-2.78	-18.94	-54.23
	dichloromethane	-0.44	-17.36	-56.79
	dmso	-2.91	-17.97	-50.48
8_complex	vacuum	-1.12	-8.05	-23.27
	acetone	5.98	-1.78	-26.04
	acetonitrile	5.33	-1.80	-23.91
	chloroform	5.36	-1.99	-24.66
	dichloromethane	6.21	-1.80	-26.88
	dmso	6.22	-1.08	-24.48
9_complex	vacuum	4.72	-8.01	-42.68
	acetone	6.62	-3.31	-33.33
	acetonitrile	6.98	-3.35	-34.65
	chloroform	7.11	-3.81	-36.63
	dichloromethane	7.69	-3.97	-39.10
	dmso	11.67	-2.37	-47.09
10_complex	vacuum	3.67	-7.34	-36.94
	acetone	5.90	-4.76	-35.76
	acetonitrile	6.40	-4.73	-37.33
	chloroform	6.12	-4.74	-36.40
	dichloromethane	6.38	-4.51	-36.53
	dmso	5.04	-5.46	-35.22
11_complex	vacuum	3.62	-8.31	-40.01
	acetone	5.94	-5.62	-38.79
	acetonitrile	5.67	-5.89	-38.80
	chloroform	6.21	-5.43	-39.04
	dichloromethane	6.34	-5.30	-39.06
	dmso	7.37	-7.63	-50.32
12_complex	vacuum	-0.74	-15.43	-49.26
	acetone	5.21	-8.73	-46.75

	acetonitrile	5.02	-9.02	-47.11
	chloroform	4.58	-9.86	-48.42
	dichloromethane	4.63	-9.17	-46.29
	dmso	5.49	-9.04	-48.73
13_complex	vacuum	-0.47	-10.22	-32.70
	acetone	5.11	-6.17	-37.83
	acetonitrile	4.48	-7.61	-40.55
	chloroform	5.10	-6.94	-40.38
	dichloromethane	5.54	-4.71	-34.39
	dmso	4.56	-6.39	-36.73
14_complex	vacuum	3.69	-7.30	-36.88
	acetone	5.64	-5.13	-36.14
	acetonitrile	5.57	-5.18	-36.05
	chloroform	5.03	-4.66	-32.50
	dichloromethane	5.71	-4.59	-34.53
	dmso	5.09	-6.12	-37.62
15_complex	vacuum	2.18	-7.75	-33.31
	acetone	5.76	-5.90	-39.13
	acetonitrile	5.90	-5.92	-39.62
	chloroform	5.34	-4.72	-33.72
	dichloromethane	6.66	-4.43	-37.19
	dmso	4.77	-6.78	-38.72
16_complex	vacuum	3.84	-4.85	-29.12
	acetone	5.69	-2.73	-28.25
	acetonitrile	8.72	-3.36	-40.50
	chloroform	9.37	-2.83	-40.94
	dichloromethane	8.42	-2.58	-36.92
	dmso	5.77	-4.31	-33.82
17_complex	vacuum	1.97	-8.06	-33.65
	acetone	4.54	-6.27	-36.25
	acetonitrile	5.29	-6.59	-39.82
	chloroform	5.50	-4.68	-34.16
	dichloromethane	6.56	-4.26	-36.31
	dmso	5.26	-7.22	-41.86
18_complex	vacuum	0.74	-12.12	-43.13
	acetone	4.21	-7.21	-38.30
	acetonitrile	5.42	-7.89	-44.66
	chloroform	3.39	-7.64	-36.98
	dichloromethane	5.34	-6.90	-41.05
	dmso	4.35	-8.31	-42.46
19_complex	vacuum	-2.99	-14.96	-40.14
	acetone	3.66	-9.33	-43.55
	acetonitrile	3.86	-9.22	-43.88
	chloroform	2.57	-10.07	-42.41
	dichloromethane	3.88	-9.19	-43.85
	dmso	2.42	-10.29	-42.63

20_complex	vacuum	-9.42	-23.16	-46.11
	acetone	-2.80	-16.76	-46.84
	acetonitrile	-3.20	-16.93	-46.06
	chloroform	-4.73	-17.56	-43.05
	dichloromethane	-3.50	-17.42	-46.69
	dmso	-3.65	-17.41	-46.13
21_complex	vacuum	-2.89	-14.18	-37.87
	acetone	4.24	-6.35	-35.51
	acetonitrile	5.00	-6.30	-37.90
	chloroform	2.26	-8.25	-35.26
	dichloromethane	4.37	-7.09	-38.44
	dmso	4.28	-6.33	-35.58
22_complex	vacuum	-5.45	-14.26	-29.56
	acetone	-1.22	-12.30	-37.17
	acetonitrile	-0.85	-12.17	-37.98
	chloroform	-2.04	-12.46	-34.97
	dichloromethane	-0.17	-12.29	-40.67
	dmso	-1.50	-12.43	-36.69
23_complex	vacuum	-0.02	-12.14	-40.63
	acetone	3.23	-8.17	-38.24
	acetonitrile	5.14	-8.13	-44.50
	chloroform	4.26	-8.28	-42.06
	dichloromethane	5.64	-7.83	-45.19
	dmso	3.09	-8.66	-39.40
24_complex	vacuum	0.39	-9.43	-32.95
	acetone	3.46	-7.17	-35.65
	acetonitrile	3.60	-7.27	-36.43
	chloroform	3.37	-7.21	-35.49
	dichloromethane	4.05	-7.05	-37.23
	dmso	4.13	-8.02	-40.74
25_complex	vacuum	2.46	-8.24	-35.89
	acetone	3.20	-7.49	-35.88
	acetonitrile	3.84	-7.63	-38.47
	chloroform	3.79	-7.20	-36.83
	dichloromethane	4.18	-7.14	-37.96
	dmso	2.98	-8.25	-37.67
26_complex	vacuum	-4.57	-18.58	-46.98
	acetone	4.12	-11.97	-53.97
	acetonitrile	2.97	-11.32	-47.91
	chloroform	1.72	-12.62	-48.09
	dichloromethane	2.77	-11.65	-48.38
	dmso	2.28	-11.93	-47.65
27_complex	vacuum	2.03	-9.13	-37.41
	acetone	5.35	-6.18	-38.67
	acetonitrile	5.49	-6.26	-39.41
	chloroform	4.54	-6.59	-37.31

	dichloromethane	4.57	-6.26	-36.31
	dmso	4.70	-6.77	-38.46
28_complex	vacuum	1.39	-10.87	-41.15
	acetone	9.65	-6.13	-52.95
	acetonitrile	4.66	-8.01	-42.50
	chloroform	6.85	-7.18	-47.04
	dichloromethane	5.55	-6.22	-39.48
	dmso	6.72	-9.26	-53.59
29_complex	vacuum	-0.29	-12.92	-42.38
	acetone	7.33	-5.07	-41.61
	acetonitrile	7.77	-5.04	-42.97
	chloroform	6.13	-6.58	-42.63
	dichloromethane	7.48	-5.57	-43.78
	dmso	6.42	-5.15	-38.80
30_complex	vacuum	-7.08	-16.39	-31.24
	acetone	3.62	-10.21	-46.40
	acetonitrile	2.07	-10.02	-40.56
	chloroform	1.94	-10.52	-41.82
	dichloromethane	2.98	-10.82	-46.28
	dmso	2.31	-10.02	-41.38
31_complex	vacuum	-0.12	-14.01	-46.58
	acetone	5.58	-7.57	-44.11
	acetonitrile	6.15	-7.58	-46.04
	chloroform	4.70	-8.45	-44.12
	dichloromethane	5.43	-7.78	-44.30
	dmso	5.54	-8.11	-45.78
32_complex	vacuum	1.36	-6.96	-27.91
	acetone	4.29	-4.34	-28.96
	acetonitrile	4.74	-5.66	-34.88
	chloroform	3.62	-3.88	-25.17
	dichloromethane	4.50	-5.31	-32.89
	dmso	3.98	-6.11	-33.83
33_complex	vacuum	-6.33	-20.78	-48.49
	acetone	1.70	-11.77	-45.21
	acetonitrile	1.06	-11.85	-43.32
	chloroform	4.27	-9.55	-46.39
	dichloromethane	2.03	-11.64	-45.86
	dmso	1.65	-11.90	-45.48
34_complex	vacuum	-2.47	-14.97	-41.94
	acetone	4.52	-6.97	-38.54
	acetonitrile	4.67	-6.95	-38.98
	chloroform	3.59	-8.06	-39.07
	dichloromethane	4.45	-7.11	-38.79
	dmso	3.67	-7.64	-37.93
35_complex	vacuum	-4.80	-18.05	-44.46
	acetone	2.21	-10.08	-41.25

	acetonitrile	1.47	-10.80	-41.18
	chloroform	2.55	-11.00	-45.47
	dichloromethane	1.39	-10.80	-40.92
	dmso	2.03	-10.41	-41.74
36_complex	vacuum	4.22	-4.64	-29.70
	acetone	7.69	-1.68	-31.42
	acetonitrile	7.77	-1.68	-31.71
	chloroform	6.49	-2.17	-29.03
	dichloromethane	7.33	-1.80	-30.63
	dmso	7.31	-1.94	-31.04
37_complex	vacuum	2.04	-10.73	-42.83
	acetone	5.59	-6.56	-40.74
	acetonitrile	5.97	-6.72	-42.56
	chloroform	9.22	-5.45	-49.22
	dichloromethane	6.80	-5.81	-42.30
	dmso	4.13	-7.90	-40.34
38_complex	vacuum	1.97	-8.06	-33.65
	acetone	7.30	-6.86	-47.50
	acetonitrile	5.35	-6.58	-40.03
	chloroform	5.50	-4.68	-34.17
	dichloromethane	6.56	-4.26	-36.31
	dmso	5.22	-7.22	-41.71
39_complex	vacuum	-2.43	-15.18	-42.76
	acetone	2.83	-10.83	-45.82
	acetonitrile	2.87	-11.03	-46.60
	chloroform	0.51	-11.57	-40.55
	dichloromethane	1.60	-11.02	-42.32
	dmso	2.72	-11.54	-47.81

Table S3. FMO analysis all complexes at different solvents

Complex	Condition	Eg	IP	IEA	η	S	ω	SE	μ	X
1_complex	vacuum	5.9550	7.5014	1.5464	2.9775	0.1679	3.4368	-3.4368	-4.5239	4.5239
	acetone	5.6222	7.0835	1.4613	2.8111	0.1779	3.2466	-3.2466	-4.2724	4.2724
	acetonitrile	5.5944	7.0731	1.4787	2.7972	0.1787	3.2681	-3.2681	-4.2759	4.2759
	chloroform	5.6908	7.1455	1.4547	2.8454	0.1757	3.2493	-3.2493	-4.3001	4.3001
	dichloromethane	5.6391	7.0987	1.4596	2.8195	0.1773	3.2472	-3.2472	-4.2792	4.2792
	dmso	5.6086	7.0688	1.4602	2.8043	0.1783	3.2425	-3.2425	-4.2645	4.2645
2_complex	vacuum	5.8627	7.5213	1.6585	2.9314	0.1706	3.5934	-3.5934	-4.5899	4.5899
	acetone	5.6720	7.1338	1.4618	2.8360	0.1763	3.2565	-3.2565	-4.2978	4.2978
	acetonitrile	5.6399	7.1123	1.4724	2.8199	0.1773	3.2668	-3.2668	-4.2924	4.2924
	chloroform	5.7876	7.2195	1.4319	2.8938	0.1728	3.2330	-3.2330	-4.3257	4.3257
	dichloromethane	5.7223	7.1626	1.4403	2.8612	0.1748	3.2334	-3.2334	-4.3015	4.3015
	dmso	5.6622	7.1161	1.4539	2.8311	0.1766	3.2428	-3.2428	-4.2850	4.2850
3_complex	vacuum	5.9792	7.5349	1.5557	2.9896	0.1672	3.4553	-3.4553	-4.5453	4.5453
	acetone	5.5806	7.1218	1.5413	2.7903	0.1792	3.3621	-3.3621	-4.3315	4.3315
	acetonitrile	5.5591	7.1112	1.5521	2.7795	0.1799	3.3753	-3.3753	-4.3317	4.3317
	chloroform	5.6674	7.1983	1.5309	2.8337	0.1764	3.3613	-3.3613	-4.3646	4.3646
	dichloromethane	5.6170	7.1531	1.5361	2.8085	0.1780	3.3604	-3.3604	-4.3446	4.3446
	dmso	5.5650	7.1069	1.5418	2.7825	0.1797	3.3602	-3.3602	-4.3243	4.3243
4_complex	vacuum	4.6428	6.5955	1.9527	2.3214	0.2154	3.9347	-3.9347	-4.2741	4.2741
	acetone	4.6039	6.5365	1.9326	2.3020	0.2172	3.8948	-3.8948	-4.2345	4.2345
	acetonitrile	4.5993	6.5438	1.9445	2.2997	0.2174	3.9165	-3.9165	-4.2442	4.2442
	chloroform	4.6094	6.5196	1.9103	2.3047	0.2169	3.8543	-3.8543	-4.2149	4.2149
	dichloromethane	4.6050	6.5283	1.9233	2.3025	0.2172	3.8779	-3.8779	-4.2258	4.2258
	dmso	4.6045	6.5419	1.9375	2.3022	0.2172	3.9038	-3.9038	-4.2397	4.2397
5_complex	vacuum	5.4695	7.6269	2.1573	2.7348	0.1828	4.3756	-4.3756	-4.8921	4.8921
	acetone	5.1493	7.1368	1.9875	2.5746	0.1942	4.0420	-4.0420	-4.5622	4.5622
	acetonitrile	5.1386	7.1235	1.9848	2.5693	0.1946	4.0361	-4.0361	-4.5541	4.5541
	chloroform	5.2083	7.2258	2.0175	2.6042	0.1920	4.1010	-4.1010	-4.6216	4.6216

	dichloromethane	5.1737	7.1716	1.9979	2.5869	0.1933	4.0628	-4.0628	-4.5847	4.5847
	dmso	5.1433	7.1194	1.9761	2.5716	0.1944	4.0212	-4.0212	-4.5477	4.5477
6_complex	vacuum	5.6665	7.3833	1.7168	2.8333	0.1765	3.6535	-3.6535	-4.5501	4.5501
	acetone	5.6606	7.0674	1.4068	2.8303	0.1767	3.1716	-3.1716	-4.2371	4.2371
	acetonitrile	5.6437	7.0494	1.4058	2.8218	0.1772	3.1668	-3.1668	-4.2276	4.2276
	chloroform	5.6995	7.1507	1.4512	2.8497	0.1755	3.2456	-3.2456	-4.3009	4.3009
	dichloromethane	5.6693	7.1001	1.4308	2.8346	0.1764	3.2092	-3.2092	-4.2654	4.2654
	dmso	5.6793	7.0478	1.3685	2.8397	0.1761	3.1180	-3.1180	-4.2081	4.2081
7_complex	vacuum	5.7283	7.3324	1.6041	2.8642	0.1746	3.4854	-3.4854	-4.4683	4.4683
	acetone	5.8140	7.0745	1.2604	2.9070	0.1720	2.9872	-2.9872	-4.1675	4.1675
	acetonitrile	5.7944	7.0639	1.2651	2.8972	0.1726	2.9961	-2.9961	-4.1666	4.1666
	chloroform	5.8758	7.1409	1.2694	2.9379	0.1702	3.0064	-3.0064	-4.2030	4.2030
	dichloromethane	5.8143	7.0701	1.2558	2.9072	0.1720	2.9806	-2.9806	-4.1630	4.1630
	dmso	5.8067	7.0513	1.2447	2.9033	0.1722	2.9631	-2.9631	-4.1480	4.1480
8_complex	vacuum	4.6831	6.7115	2.0284	2.3416	0.2135	4.0777	-4.0777	-4.3699	4.3699
	acetone	4.7833	6.4736	1.6904	2.3916	0.2091	3.4836	-3.4836	-4.0820	4.0820
	acetonitrile	4.7784	6.4581	1.6798	2.3892	0.2093	3.4649	-3.4649	-4.0690	4.0690
	chloroform	4.7658	6.5093	1.7434	2.3829	0.2098	3.5727	-3.5727	-4.1264	4.1264
	dichloromethane	4.7245	6.4328	1.7083	2.3622	0.2117	3.5072	-3.5072	-4.0706	4.0706
	dmso	4.7800	6.4551	1.6751	2.3900	0.2092	3.4572	-3.4572	-4.0651	4.0651
9_complex	vacuum	5.5166	7.0407	1.5241	2.7583	0.1813	3.3244	-3.3244	-4.2824	4.2824
	acetone	5.7626	7.0396	1.2770	2.8813	0.1735	3.0007	-3.0007	-4.1583	4.1583
	acetonitrile	5.7495	7.0361	1.2866	2.8748	0.1739	3.0118	-3.0118	-4.1613	4.1613
	chloroform	5.7299	7.0364	1.3064	2.8650	0.1745	3.0368	-3.0368	-4.1714	4.1714
	dichloromethane	5.7569	7.0410	1.2841	2.8784	0.1737	3.0098	-3.0098	-4.1626	4.1626
	dmso	5.7721	7.0369	1.2648	2.8861	0.1732	2.9850	-2.9850	-4.1509	4.1509
10_complex	vacuum	5.5596	7.2152	1.6556	2.7798	0.1799	3.5384	-3.5384	-4.4354	4.4354
	acetone	5.8900	7.0459	1.1559	2.9450	0.1698	2.8553	-2.8553	-4.1009	4.1009
	acetonitrile	5.8690	7.0312	1.1622	2.9345	0.1704	2.8596	-2.8596	-4.0967	4.0967
	chloroform	5.9188	7.1147	1.1959	2.9594	0.1690	2.9173	-2.9173	-4.1553	4.1553

	dichloromethane	5.9221	7.0973	1.1753	2.9610	0.1689	2.8890	-2.8890	-4.1363	4.1363
	dmso	5.8720	7.0149	1.1429	2.9360	0.1703	2.8333	-2.8333	-4.0789	4.0789
11_complex	vacuum	5.4630	7.2884	1.8254	2.7315	0.1830	3.8010	-3.8010	-4.5569	4.5569
	acetone	5.4423	6.9863	1.5440	2.7212	0.1837	3.3426	-3.3426	-4.2651	4.2651
	acetonitrile	5.4254	6.9735	1.5481	2.7127	0.1843	3.3461	-3.3461	-4.2608	4.2608
	chloroform	5.4842	7.0576	1.5734	2.7421	0.1823	3.3958	-3.3958	-4.3155	4.3155
	dichloromethane	5.4608	7.0222	1.5614	2.7304	0.1831	3.3731	-3.3731	-4.2918	4.2918
	dmso	5.4434	6.9373	1.4939	2.7217	0.1837	3.2648	-3.2648	-4.2156	4.2156
12_complex	vacuum	5.9128	7.3134	1.4006	2.9564	0.1691	3.2105	-3.2105	-4.3570	4.3570
	acetone	5.6532	7.0154	1.3622	2.8266	0.1769	3.1038	-3.1038	-4.1888	4.1888
	acetonitrile	5.6309	7.0045	1.3736	2.8154	0.1776	3.1165	-3.1165	-4.1891	4.1891
	chloroform	5.7308	7.0862	1.3554	2.8654	0.1745	3.1087	-3.1087	-4.2208	4.2208
	dichloromethane	5.6834	7.0437	1.3603	2.8417	0.1760	3.1067	-3.1067	-4.2020	4.2020
	dmso	5.6388	6.9991	1.3603	2.8194	0.1773	3.0982	-3.0982	-4.1797	4.1797
13_complex	vacuum	5.3114	6.9512	1.6398	2.6557	0.1883	3.4739	-3.4739	-4.2955	4.2955
	acetone	5.7933	6.9776	1.1842	2.8967	0.1726	2.8747	-2.8747	-4.0809	4.0809
	acetonitrile	5.8236	7.0454	1.2218	2.9118	0.1717	2.9340	-2.9340	-4.1336	4.1336
	chloroform	5.8214	7.0024	1.1810	2.9107	0.1718	2.8759	-2.8759	-4.0917	4.0917
	dichloromethane	5.8317	7.0413	1.2096	2.9159	0.1715	2.9184	-2.9184	-4.1254	4.1254
	dmso	5.7754	6.9531	1.1777	2.8877	0.1731	2.8617	-2.8617	-4.0654	4.0654
14_complex	vacuum	4.9370	6.4086	1.4716	2.4685	0.2026	3.1445	-3.1445	-3.9401	3.9401
	acetone	5.0012	6.2777	1.2765	2.5006	0.2000	2.8526	-2.8526	-3.7771	3.7771
	acetonitrile	5.0061	6.2878	1.2817	2.5031	0.1998	2.8613	-2.8613	-3.7847	3.7847
	chloroform	5.0026	6.2481	1.2455	2.5013	0.1999	2.8062	-2.8062	-3.7468	3.7468
	dichloromethane	4.9947	6.2614	1.2667	2.4973	0.2002	2.8366	-2.8366	-3.7640	3.7640
	dmso	5.0064	6.2864	1.2800	2.5032	0.1997	2.8589	-2.8589	-3.7832	3.7832
15_complex	vacuum	4.6284	7.0309	2.4025	2.3142	0.2161	4.8067	-4.8067	-4.7167	4.7167
	acetone	4.6050	6.6032	1.9981	2.3025	0.2172	4.0164	-4.0164	-4.3007	4.3007
	acetonitrile	4.5903	6.6078	2.0175	2.2952	0.2178	4.0517	-4.0517	-4.3126	4.3126
	chloroform	4.6034	6.6633	2.0599	2.3017	0.2172	4.1325	-4.1325	-4.3616	4.3616

	dichloromethane	4.6039	6.6298	2.0259	2.3020	0.2172	4.0684	-4.0684	-4.3279	4.3279
	dmso	4.6039	6.6298	2.0259	2.3020	0.2172	4.0684	-4.0684	-4.3279	4.3279
16_complex	vacuum	5.6246	7.4584	1.8338	2.8123	0.1778	3.8378	-3.8378	-4.6461	4.6461
	acetone	5.4336	7.0179	1.5843	2.7168	0.1840	3.4046	-3.4046	-4.3011	4.3011
	acetonitrile	5.4331	7.0143	1.5813	2.7165	0.1841	3.3998	-3.3998	-4.2978	4.2978
	chloroform	5.5482	7.1137	1.5655	2.7741	0.1802	3.3942	-3.3942	-4.3396	4.3396
	dichloromethane	5.5114	7.0796	1.5682	2.7557	0.1814	3.3923	-3.3923	-4.3239	4.3239
	dmso	5.4475	7.0181	1.5707	2.7237	0.1836	3.3854	-3.3854	-4.2944	4.2944
17_complex	vacuum	5.2423	6.4897	1.2474	2.6212	0.1908	2.8548	-2.8548	-3.8685	3.8685
	acetone	5.3762	6.3033	0.9271	2.6881	0.1860	2.4310	-2.4310	-3.6152	3.6152
	acetonitrile	5.4059	6.3123	0.9064	2.7029	0.1850	2.4099	-2.4099	-3.6093	3.6093
	chloroform	5.2984	6.2391	0.9407	2.6492	0.1887	2.4323	-2.4323	-3.5899	3.5899
	dichloromethane	5.3389	6.2317	0.8928	2.6695	0.1873	2.3768	-2.3768	-3.5623	3.5623
	dmso	5.3928	6.2891	0.8964	2.6964	0.1854	2.3935	-2.3935	-3.5927	3.5927
18_complex	vacuum	4.8197	6.3591	1.5394	2.4099	0.2075	3.2359	-3.2359	-3.9492	3.9492
	acetone	4.8477	6.1261	1.2784	2.4239	0.2063	2.8275	-2.8275	-3.7023	3.7023
	acetonitrile	4.8502	6.1218	1.2716	2.4251	0.2062	2.8175	-2.8175	-3.6967	3.6967
	chloroform	4.8418	6.1313	1.2896	2.4209	0.2065	2.8435	-2.8435	-3.7104	3.7104
	dichloromethane	4.8442	6.1294	1.2852	2.4221	0.2064	2.8372	-2.8372	-3.7073	3.7073
	dmso	4.8486	6.1134	1.2648	2.4243	0.2062	2.8069	-2.8069	-3.6891	3.6891
19_complex	vacuum	4.4866	6.2138	1.7271	2.2433	0.2229	3.5136	-3.5136	-3.9704	3.9704
	acetone	4.4537	5.7689	1.3151	2.2269	0.2245	2.8169	-2.8169	-3.5420	3.5420
	acetonitrile	4.4515	5.7553	1.3037	2.2258	0.2246	2.7984	-2.7984	-3.5295	3.5295
	chloroform	4.4652	5.8377	1.3726	2.2326	0.2240	2.9108	-2.9108	-3.6051	3.6051
	dichloromethane	4.4578	5.7917	1.3339	2.2289	0.2243	2.8475	-2.8475	-3.5628	3.5628
	dmso	4.4507	5.7512	1.3004	2.2254	0.2247	2.7931	-2.7931	-3.5258	3.5258
20_complex	vacuum	5.7544	7.4527	1.6983	2.8772	0.1738	3.6381	-3.6381	-4.5755	4.5755
	acetone	5.5022	7.0217	1.5195	2.7511	0.1817	3.3147	-3.3147	-4.2706	4.2706
	acetonitrile	5.4766	7.0064	1.5298	2.7383	0.1826	3.3263	-3.3263	-4.2681	4.2681
	chloroform	5.5816	7.0992	1.5176	2.7908	0.1792	3.3256	-3.3256	-4.3084	4.3084

	dichloromethane	5.5367	7.0473	1.5105	2.7684	0.1806	3.3068	-3.3068	-4.2789	4.2789
	dmso	5.4918	6.9996	1.5078	2.7459	0.1821	3.2947	-3.2947	-4.2537	4.2537
21_complex	vacuum	4.3811	6.5822	2.2011	2.1905	0.2283	4.4023	-4.4023	-4.3917	4.3917
	acetone	4.4954	6.2315	1.7361	2.2477	0.2225	3.5304	-3.5304	-3.9838	3.9838
	acetonitrile	4.5071	6.2298	1.7228	2.2535	0.2219	3.5080	-3.5080	-3.9763	3.9763
	chloroform	4.4371	6.2617	1.8245	2.2186	0.2254	3.6841	-3.6841	-4.0431	4.0431
	dichloromethane	4.4662	6.2396	1.7734	2.2331	0.2239	3.5941	-3.5941	-4.0065	4.0065
	dmso	4.5190	6.2317	1.7127	2.2595	0.2213	3.4916	-3.4916	-3.9722	3.9722
22_complex	vacuum	1.6466	4.4532	2.8066	0.8233	0.6073	8.0021	-8.0021	-3.6299	3.6299
	acetone	1.6888	4.1715	2.4828	0.8444	0.5922	6.5551	-6.5551	-3.3272	3.3272
	acetonitrile	1.6939	4.1645	2.4705	0.8470	0.5903	6.4972	-6.4972	-3.3175	3.3175
	chloroform	1.6806	4.1906	2.5100	0.8403	0.5950	6.6789	-6.6789	-3.3503	3.3503
	dichloromethane	1.6839	4.1789	2.4950	0.8419	0.5939	6.6130	-6.6130	-3.3370	3.3370
	dmso	1.6950	4.1729	2.4779	0.8475	0.5900	6.5240	-6.5240	-3.3254	3.3254
23_complex	vacuum	4.8766	6.7014	1.8248	2.4383	0.2051	3.7268	-3.7268	-4.2631	4.2631
	acetone	4.8869	6.1953	1.3083	2.4435	0.2046	2.8803	-2.8803	-3.7518	3.7518
	acetonitrile	4.8858	6.1792	1.2934	2.4429	0.2047	2.8572	-2.8572	-3.7363	3.7363
	chloroform	4.8856	6.2905	1.4049	2.4428	0.2047	3.0303	-3.0303	-3.8477	3.8477
	dichloromethane	4.8935	6.2413	1.3478	2.4467	0.2044	2.9424	-2.9424	-3.7945	3.7945
	dmso	4.9008	6.1770	1.2762	2.4504	0.2040	2.8338	-2.8338	-3.7266	3.7266
24_complex	vacuum	4.6548	6.9387	2.2839	2.3274	0.2148	4.5681	-4.5681	-4.6113	4.6113
	acetone	4.6328	6.8015	2.1688	2.3164	0.2159	4.3422	-4.3422	-4.4852	4.4852
	acetonitrile	4.6284	6.8059	2.1775	2.3142	0.2161	4.3590	-4.3590	-4.4917	4.4917
	chloroform	4.6333	6.8149	2.1816	2.3167	0.2158	4.3670	-4.3670	-4.4982	4.4982
	dichloromethane	4.6317	6.8051	2.1734	2.3158	0.2159	4.3512	-4.3512	-4.4892	4.4892
	dmso	4.6341	6.7988	2.1647	2.3171	0.2158	4.3344	-4.3344	-4.4818	4.4818
25_complex	vacuum	5.8021	7.2386	1.4365	2.9010	0.1724	3.2427	-3.2427	-4.3375	4.3375
	acetone	5.9629	6.8802	0.9173	2.9814	0.1677	2.5491	-2.5491	-3.8987	3.8987
	acetonitrile	5.9773	6.8761	0.8988	2.9887	0.1673	2.5283	-2.5283	-3.8874	3.8874
	chloroform	5.9025	6.9556	1.0531	2.9512	0.1694	2.7166	-2.7166	-4.0043	4.0043

	dichloromethane	5.9376	6.9101	0.9725	2.9688	0.1684	2.6162	-2.6162	-3.9413	3.9413
	dmso	5.9751	6.8628	0.8876	2.9876	0.1674	2.5133	-2.5133	-3.8752	3.8752
26_complex	vacuum	5.0595	6.6864	1.6270	2.5297	0.1976	3.4150	-3.4150	-4.1567	4.1567
	acetone	5.6788	6.6734	0.9946	2.8394	0.1761	2.5885	-2.5885	-3.8340	3.8340
	acetonitrile	5.6701	6.6862	1.0161	2.8350	0.1764	2.6157	-2.6157	-3.8511	3.8511
	chloroform	5.6132	6.6946	1.0814	2.8066	0.1782	2.6930	-2.6930	-3.8880	3.8880
	dichloromethane	5.6902	6.6892	0.9989	2.8451	0.1757	2.5969	-2.5969	-3.8440	3.8440
	dmso	5.6608	6.6630	1.0022	2.8304	0.1767	2.5948	-2.5948	-3.8326	3.8326
27_complex	vacuum	5.2801	6.8187	1.5385	2.6401	0.1894	3.3069	-3.3069	-4.1786	4.1786
	acetone	5.7626	6.8723	1.1097	2.8813	0.1735	2.7640	-2.7640	-3.9910	3.9910
	acetonitrile	5.7580	6.8951	1.1372	2.8790	0.1737	2.8013	-2.8013	-4.0162	4.0162
	chloroform	5.7384	6.8647	1.1263	2.8692	0.1743	2.7819	-2.7819	-3.9955	3.9955
	dichloromethane	5.7667	6.8783	1.1116	2.8833	0.1734	2.7675	-2.7675	-3.9949	3.9949
	dmso	5.7561	6.8617	1.1056	2.8780	0.1737	2.7570	-2.7570	-3.9836	3.9836
28_complex	vacuum	5.2355	6.6323	1.3968	2.6178	0.1910	3.0783	-3.0783	-4.0145	4.0145
	acetone	4.6154	6.1384	1.5230	2.3077	0.2167	3.1795	-3.1795	-3.8307	3.8307
	acetonitrile	4.6238	6.1327	1.5089	2.3119	0.2163	3.1572	-3.1572	-3.8208	3.8208
	chloroform	4.5950	6.1229	1.5279	2.2975	0.2176	3.1847	-3.1847	-3.8254	3.8254
	dichloromethane	4.6072	6.1006	1.4934	2.3036	0.2171	3.1292	-3.1292	-3.7970	3.7970
	dmso	4.6271	6.1305	1.5034	2.3135	0.2161	3.1487	-3.1487	-3.8170	3.8170
29_complex	vacuum	5.2355	6.6323	1.3968	2.6178	0.1910	3.0783	-3.0783	-4.0145	4.0145
	acetone	5.3974	6.3893	0.9919	2.6987	0.1853	2.5235	-2.5235	-3.6906	3.6906
	acetonitrile	5.3857	6.3852	0.9995	2.6929	0.1857	2.5314	-2.5314	-3.6923	3.6923
	chloroform	5.4203	6.4192	0.9989	2.7101	0.1845	2.5381	-2.5381	-3.7091	3.7091
	dichloromethane	5.4154	6.4002	0.9848	2.7077	0.1847	2.5177	-2.5177	-3.6925	3.6925
	dmso	5.3944	6.3708	0.9764	2.6972	0.1854	2.5017	-2.5017	-3.6736	3.6736
30_complex	vacuum	4.0298	5.9065	1.8768	2.0149	0.2482	3.7583	-3.7583	-3.8917	3.8917
	acetone	4.6290	6.0072	1.3783	2.3145	0.2160	2.9459	-2.9459	-3.6928	3.6928
	acetonitrile	4.2820	5.7806	1.4985	2.1410	0.2335	3.0935	-3.0935	-3.6396	3.6396
	chloroform	4.2676	5.7678	1.5002	2.1338	0.2343	3.0944	-3.0944	-3.6340	3.6340

	dichloromethane	4.2534	5.7582	1.5048	2.1267	0.2351	3.1005	-3.1005	-3.6315	3.6315
	dmso	4.2839	5.7844	1.5004	2.1420	0.2334	3.0970	-3.0970	-3.6424	3.6424
31_complex	vacuum	4.7691	6.2309	1.4618	2.3846	0.2097	3.1022	-3.1022	-3.8464	3.8464
	acetone	4.6290	6.0072	1.3783	2.3145	0.2160	2.9459	-2.9459	-3.6928	3.6928
	acetonitrile	4.6262	6.0091	1.3829	2.3131	0.2162	2.9528	-2.9528	-3.6960	3.6960
	chloroform	4.6303	6.0249	1.3946	2.3152	0.2160	2.9722	-2.9722	-3.7098	3.7098
	dichloromethane	4.6254	6.0121	1.3867	2.3127	0.2162	2.9588	-2.9588	-3.6994	3.6994
	dmso	4.6330	6.0045	1.3715	2.3165	0.2158	2.9357	-2.9357	-3.6880	3.6880
32_complex	vacuum	5.4328	6.9444	1.5116	2.7164	0.1841	3.2904	-3.2904	-4.2280	4.2280
	acetone	5.5174	6.5297	1.0123	2.7587	0.1812	2.5773	-2.5773	-3.7710	3.7710
	acetonitrile	5.5381	6.5232	0.9851	2.7691	0.1806	2.5448	-2.5448	-3.7541	3.7541
	chloroform	5.4875	6.5735	1.0860	2.7437	0.1822	2.6728	-2.6728	-3.8298	3.8298
	dichloromethane	5.5035	6.5743	1.0708	2.7518	0.1817	2.6550	-2.6550	-3.8225	3.8225
	dmso	5.5373	6.5169	0.9796	2.7686	0.1806	2.5372	-2.5372	-3.7483	3.7483
33_complex	vacuum	1.1521	2.5998	1.4477	0.5761	0.8680	3.5547	-3.5547	-2.0237	2.0237
	acetone	1.7927	2.8050	1.0123	0.8964	0.5578	2.0320	-2.0320	-1.9086	1.9086
	acetonitrile	2.0684	2.8531	0.7848	1.0342	0.4835	1.5996	-1.5996	-1.8190	1.8190
	chloroform	2.1056	2.7922	0.6865	1.0528	0.4749	1.4368	-1.4368	-1.7394	1.7394
	dichloromethane	2.0327	2.7661	0.7334	1.0164	0.4920	1.5061	-1.5061	-1.7497	1.7497
	dmso	2.0474	2.8199	0.7725	1.0237	0.4884	1.5759	-1.5759	-1.7962	1.7962
34_complex	vacuum	5.1014	6.5305	1.4292	2.5507	0.1960	3.1049	-3.1049	-3.9798	3.9798
	acetone	5.0121	5.9849	0.9728	2.5061	0.1995	2.4147	-2.4147	-3.4789	3.4789
	acetonitrile	5.0061	5.9632	0.9570	2.5031	0.1998	2.3915	-2.3915	-3.4601	3.4601
	chloroform	5.0331	6.1036	1.0705	2.5165	0.1987	2.5565	-2.5565	-3.5870	3.5870
	dichloromethane	5.0126	6.0293	1.0166	2.5063	0.1995	2.4760	-2.4760	-3.5229	3.5229
	dmso	5.0107	5.9618	0.9510	2.5054	0.1996	2.3842	-2.3842	-3.4564	3.4564
35_complex	vacuum	5.1694	7.1735	2.0041	2.5847	0.1934	4.0735	-4.0735	-4.5888	4.5888
	acetone	5.1403	6.8783	1.7380	2.5701	0.1945	3.6107	-3.6107	-4.3081	4.3081
	acetonitrile	5.1487	6.8772	1.7285	2.5744	0.1942	3.5959	-3.5959	-4.3028	4.3028
	chloroform	5.1449	6.9322	1.7873	2.5724	0.1944	3.6943	-3.6943	-4.3597	4.3597

	dichloromethane	5.1414	6.8981	1.7568	2.5707	0.1945	3.6424	-3.6424	-4.3275	4.3275
	dmso	5.1370	6.8628	1.7258	2.5685	0.1947	3.5898	-3.5898	-4.2943	4.2943
36_complex	vacuum	4.9950	6.7648	1.7698	2.4975	0.2002	3.6457	-3.6457	-4.2673	4.2673
	acetone	4.8494	6.6192	1.7698	2.4247	0.2062	3.6281	-3.6281	-4.1945	4.1945
	acetonitrile	4.8537	6.6236	1.7698	2.4269	0.2060	3.6286	-3.6286	-4.1967	4.1967
	chloroform	4.8366	6.6064	1.7698	2.4183	0.2068	3.6266	-3.6266	-4.1881	4.1881
	dichloromethane	4.8404	6.6102	1.7698	2.4202	0.2066	3.6271	-3.6271	-4.1900	4.1900
	dmso	4.8548	6.6247	1.7698	2.4274	0.2060	3.6288	-3.6288	-4.1973	4.1973
37_complex	vacuum	4.6194	6.3893	1.7698	2.3097	0.2165	3.6028	-3.6028	-4.0796	4.0796
	acetone	4.3315	6.1014	1.7698	2.1658	0.2309	3.5759	-3.5759	-3.9356	3.9356
	acetonitrile	4.3299	6.0998	1.7698	2.1650	0.2310	3.5757	-3.5757	-3.9348	3.9348
	chloroform	4.3487	6.1185	1.7698	2.1743	0.2300	3.5773	-3.5773	-3.9442	3.9442
	dichloromethane	4.3375	6.1074	1.7698	2.1688	0.2305	3.5764	-3.5764	-3.9386	3.9386
	dmso	4.3228	6.0927	1.7698	2.1614	0.2313	3.5752	-3.5752	-3.9313	3.9313
38_complex	vacuum	4.7199	6.4897	1.7698	2.3599	0.2119	3.6135	-3.6135	-4.1298	4.1298
	acetone	4.5329	6.3028	1.7698	2.2665	0.2206	3.5941	-3.5941	-4.0363	4.0363
	acetonitrile	4.5427	6.3125	1.7698	2.2714	0.2201	3.5951	-3.5951	-4.0412	4.0412
	chloroform	4.4692	6.2391	1.7698	2.2346	0.2238	3.5880	-3.5880	-4.0045	4.0045
	dichloromethane	4.4619	6.2317	1.7698	2.2309	0.2241	3.5873	-3.5873	-4.0008	4.0008
	dmso	4.5193	6.2891	1.7698	2.2597	0.2213	3.5928	-3.5928	-4.0295	4.0295
39_complex	vacuum	4.4254	6.1953	1.7698	2.2127	0.2260	3.5840	-3.5840	-3.9826	3.9826
	acetone	4.3955	6.1653	1.7698	2.1977	0.2275	3.5813	-3.5813	-3.9676	3.9676
	acetonitrile	4.4023	6.1721	1.7698	2.2011	0.2272	3.5819	-3.5819	-3.9710	3.9710
	chloroform	4.3756	6.1455	1.7698	2.1878	0.2285	3.5796	-3.5796	-3.9577	3.9577
	dichloromethane	4.3887	6.1585	1.7698	2.1943	0.2279	3.5807	-3.5807	-3.9642	3.9642
	dmso	4.3966	6.1664	1.7698	2.1983	0.2274	3.5814	-3.5814	-3.9681	3.9681

Table S4. QTAIM analysis of all systems in complex 7 at different solvents

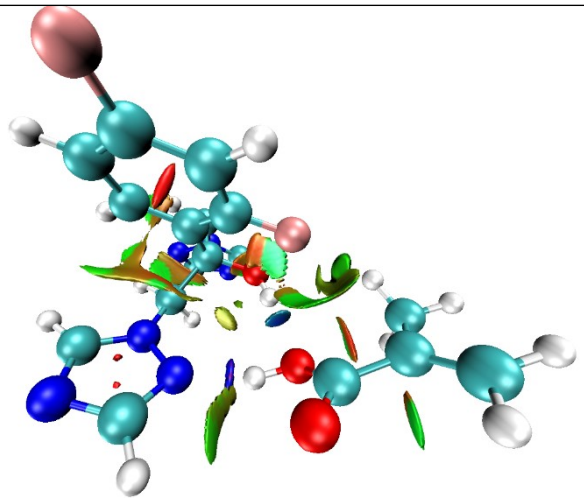
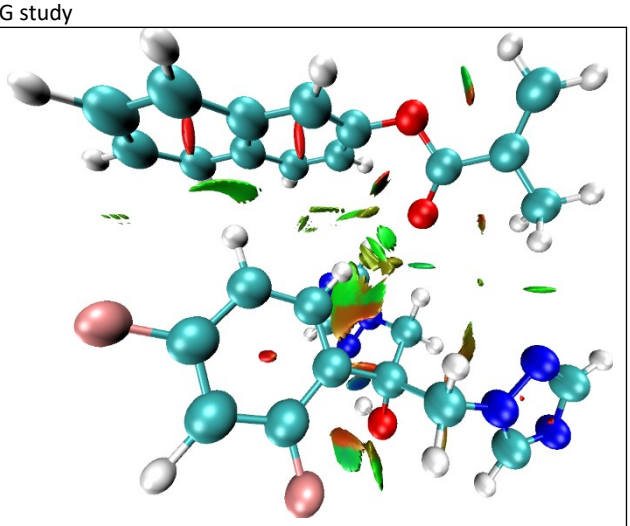
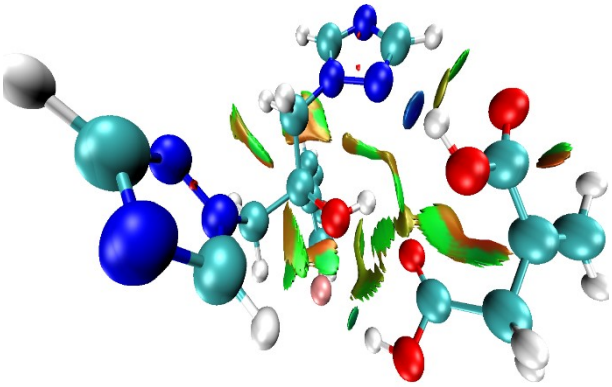
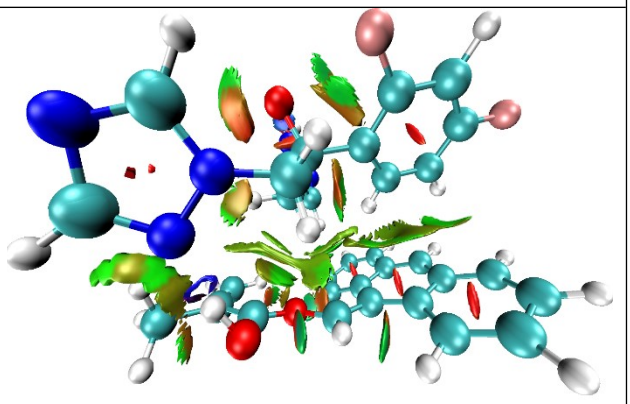
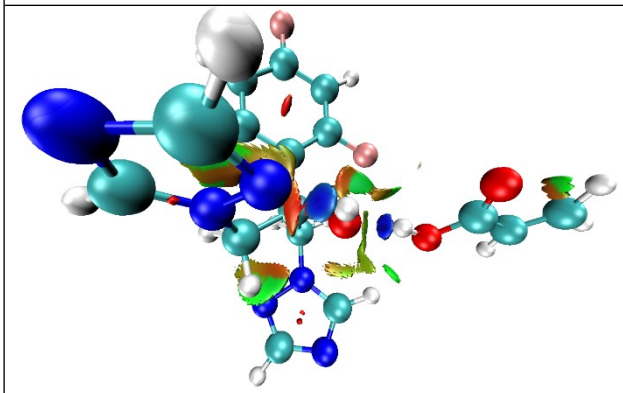
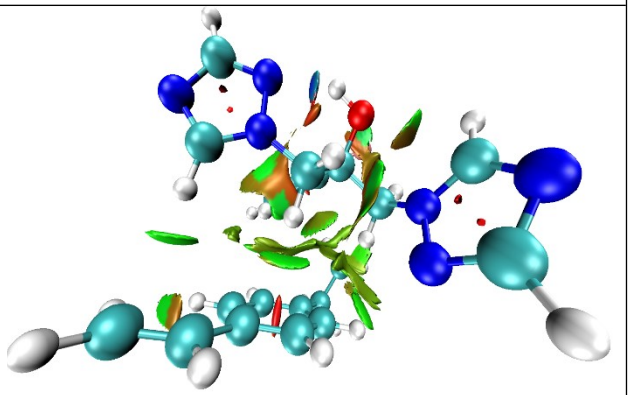
System	Interaction	BCP	Condition	*P*	G_{BCP}	V_{BCP}	H_{BCP}	$(\nabla^2 r)$	λ1	λ2	λ3	|V/G|
1	38(O) - 30(H)	108	Vacuum	0.0129	0.0103	-0.0083	0.0019	0.0486	0.0305	0.0247	-0.0066	0.8138
		111	Acetone	0.0080	0.0061	-0.0049	0.0011	0.0289	0.0263	0.0033	-0.0007	0.8108
		113	Acetonitrile	0.0081	0.0061	-0.0049	0.0011	0.0290	0.0268	0.0032	-0.0010	0.8114
		69	Chloroform	0.0099	0.0075	-0.0061	0.0014	0.0355	0.0317	0.0039	-0.0002	0.8183
		69	Dichloromethane	0.0104	0.0080	-0.0065	0.0015	0.0378	0.0307	0.0086	-0.0015	0.8173
		110	DMSO	0.0070	0.0053	-0.0042	0.0010	0.0252	0.0235	0.0022	-0.0004	0.8023
2	39(O) - 25(H)	56	Vacuum	0.0085	0.0063	-0.0052	0.0011	0.0296	0.0166	-0.0045	0.0176	0.8259
		NA	Acetone	NA	NA	NA	NA	NA	NA	NA	NA	NA
		NA	Acetonitrile	NA	NA	NA	NA	NA	NA	NA	NA	NA
		NA	Chloroform	NA	NA	NA	NA	NA	NA	NA	NA	NA
		NA	Dichloromethane	NA	NA	NA	NA	NA	NA	NA	NA	NA
		NA	DMSO	NA	NA	NA	NA	NA	NA	NA	NA	NA
3	40(N) - 13(O)	83	Vacuum	0.0092	0.0073	-0.0061	0.0012	0.0342	0.0238	0.0148	-0.0044	0.8334
		NA	Acetone	NA	NA	NA	NA	NA	NA	NA	NA	NA
		NA	Acetonitrile	NA	NA	NA	NA	NA	NA	NA	NA	NA
		103	Chloroform	0.0080	0.0064	-0.0053	0.0011	0.0299	0.0269	0.0071	-0.0041	0.8338
		NA	Dichloromethane	NA	NA	NA	NA	NA	NA	NA	NA	NA
		86	DMSO	0.0063	0.0047	-0.0040	0.0008	0.0219	0.0233	0.0025	-0.0039	0.8405
4	43(C) - 34(N)	69	Vacuum	0.0069	0.0052	-0.0040	0.0012	0.0260	0.0065	0.0088	0.0107	0.7623
		NA	Acetone	NA	NA	NA	NA	NA	NA	NA	NA	NA
		NA	Acetonitrile	NA	NA	NA	NA	NA	NA	NA	NA	NA
		NA	Chloroform	NA	NA	NA	NA	NA	NA	NA	NA	NA
		NA	Dichloromethane	NA	NA	NA	NA	NA	NA	NA	NA	NA
		NA	DMSO	NA	NA	NA	NA	NA	NA	NA	NA	NA
5	44(C) - 34(N)	NA	Vacuum	NA	NA	NA	NA	NA	NA	NA	NA	NA
		67	Acetone	0.0045	0.0028	-0.0021	0.0006	0.0137	0.0048	-0.0001	0.0090	0.7661
		67	Acetonitrile	0.0046	0.0028	-0.0022	0.0007	0.0139	0.0049	-0.0001	0.0091	0.7675
		121	Chloroform	0.0039	0.0025	-0.0018	0.0007	0.0128	0.0030	0.0020	0.0078	0.7310
		118	Dichloromethane	0.0044	0.0027	-0.0021	0.0006	0.0134	0.0043	0.0000	0.0091	0.7652
		67	DMSO	0.0048	0.0029	-0.0022	0.0006	0.0141	0.0049	-0.0003	0.0095	0.7746
6	48(H) - 33(N)	NA	Vacuum	NA	NA	NA	NA	NA	NA	NA	NA	NA
		92	Acetone	0.0063	0.0038	-0.0033	0.0005	0.0175	-0.0032	0.0248	-0.0040	0.8594
		93	Acetonitrile	0.0062	0.0038	-0.0033	0.0005	0.0173	-0.0031	0.0243	-0.0039	0.8585
		82	Chloroform	0.0066	0.0040	-0.0034	0.0006	0.0183	-0.0034	0.0260	-0.0043	0.8601
		82	Dichloromethane	0.0057	0.0036	-0.0030	0.0005	0.0164	-0.0023	0.0223	-0.0037	0.8476

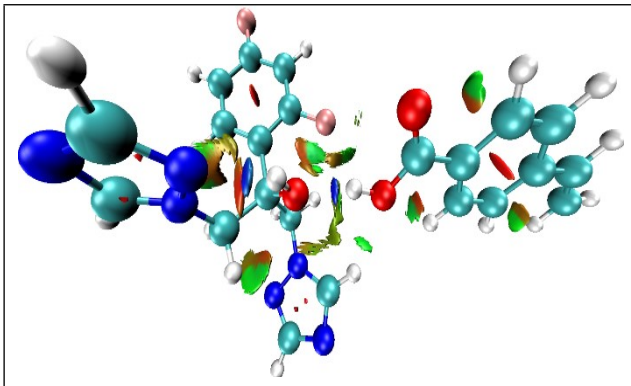
		92	DMSO	0.0044	0.0028	-0.0023	0.0005	0.0129	-0.0017	0.1718	-0.0025	0.8295
7	50(H) - 13(O)	NA	Vacuum	NA	NA	NA	NA	NA	NA	NA	NA	NA
		87	Acetone	0.0070	0.0053	-0.0045	0.0008	0.0247	0.0264	0.0029	-0.0046	0.8440
		87	Acetonitrile	0.0073	0.0056	-0.0047	0.0009	0.0256	0.0281	0.0026	-0.0050	0.8468
		NA	Chloroform	NA	NA	NA	NA	NA	NA	NA	NA	NA
		98	Dichloromethane	0.0068	0.0052	-0.0044	0.0008	0.0241	0.0261	0.0025	-0.0045	0.8416
		NA	DMSO	NA	NA	NA	NA	NA	NA	NA	NA	NA
8	50(H) - 30(H)	NA	Vacuum	NA	NA	NA	NA	NA	NA	NA	NA	NA
		87	Acetone	0.0030	0.0023	-0.0015	0.0008	0.0122	-0.0005	0.0138	-0.0012	0.6705
		90	Acetonitrile	0.0032	0.2367	-0.0016	0.0008	0.0125	-0.0007	0.0146	-0.0014	0.0068
		NA	Chloroform	NA	NA	NA	NA	NA	NA	NA	NA	NA
		NA	Dichloromethane	NA	NA	NA	NA	NA	NA	NA	NA	NA
		98	DMSO	0.0031	0.0023	-0.0015	0.0007	0.0121	-0.0007	0.0140	-0.0012	0.6754
9	51(H) - 33(N)	113	Vacuum	0.0623	0.0422	-0.0598	-0.0176	0.0983	0.1644	0.0463	-0.1124	1.4171
		115	Acetone	0.0832	0.0539	-0.0867	-0.0329	0.0840	0.3479	-0.1121	-0.1518	1.6099
		116	Acetonitrile	0.0779	0.0510	-0.0798	-0.0288	0.0889	0.2910	-0.0659	-0.1363	1.5643
		66	Chloroform	0.0868	0.0555	-0.0914	-0.0359	0.0786	0.3623	-0.1186	-0.1651	1.6461
		65	Dichloromethane	0.0873	0.0570	-0.0931	-0.0362	0.0735	0.3585	-0.1194	-0.1558	1.6347
		114	DMSO	0.0837	0.0542	-0.0875	-0.3332	0.0834	0.3565	-0.1184	-0.1547	1.6151
10	52(H) - 13(O)	NA	Vacuum	NA	NA	NA	NA	NA	NA	NA	NA	NA
		80	Acetone	0.0050	0.0040	-0.0029	0.0010	0.0202	0.0029	0.0106	0.0066	0.7386
		80	Acetonitrile	0.0052	0.0042	-0.0031	0.0011	0.0210	0.0031	0.0110	0.0069	0.7452
		111	Chloroform	0.0054	0.0044	-0.0033	0.0011	0.0220	0.0028	0.0111	0.0081	0.7525
		110	Dichloromethane	0.0052	0.0042	-0.0031	0.0011	0.0210	-0.0003	0.0133	0.0080	0.7456
		NA	DMSO	NA	NA	NA	NA	NA	NA	NA	NA	NA

Table S5. NBO analysis of complex 7 at different solvents

System	Interaction	Donor NBO (i)	Acceptor NBO (j)	$E^{(2)}$ (kcal/mol)					
				Vacuum	Acetone	Acetonitrile	Chloroform	Dichloromethane	DMSO
1	38(O) - 30(H)	BD C28 - H30	BD* S35 - O38	0.06	NA	NA	NA	NA	NA
		BD* S35 - O38	BD* C28 - H30	0.48	0.21	0.21	0.34	0.31	0.16
		LP O38	BD* C28 - H30	1.21	0.51	0.53	0.81	0.74	0.41
2	39(O) - 25(H)	BD C24 - H25	BD* O39 - C43	0.07	NA	NA	NA	NA	NA
		BD* O39 - C43	BD* C24 - H25	0.07	NA	NA	NA	NA	NA
		LP O39	BD* C24 - H25	0.29	NA	NA	NA	NA	NA
3	43(C) - 34 (N)	BD N40 - H50	BD* O13 - H14	0.07	NA	NA	NA	NA	NA
		LP O13	BD* N40 - H50	0.18	0.36	0.44	0.36	0.39	0.28
		LP N40	BD* C12 - O13	0.15	NA	NA	0.09	NA	NA
		LP N40	BD* O13 - H14	0.47	0.11	0.11	0.16	0.10	0.09
4	43(C) - 34 (N)	BD O39 - C43	BD* N21 - N34	0.09	NA	NA	NA	NA	NA
		BD* C24 - N34	BD* O39 - C43	NA	0.11	NA	NA	NA	0.12
		LP N34	BD* O39 - C43	0.42	0.11	0.11	0.11	0.09	0.12
5	44(C) - 34(N)	BD C44 - C45	BD* N21 - N34	NA	0.05	0.05	NA	NA	0.06
		LP N34	BD* C44 - C45	NA	NA	0.10	NA	NA	0.07
6	48(H) - 33(N)	BD C28 - N33	BD* C42 - H48	0.05	0.25	0.24	0.15	0.19	0.26
7	50(H) - 13 (O)	BD N40 - H50	BD* O13 - H14	0.07	NA	NA	NA	NA	NA
		LP O13	BD* N40 - H50	0.18	0.36	0.44	0.36	0.39	0.28
8	50(H) - 30 (H)	BD C28 - H30	BD* N40 - H50	NA	0.10	0.11	0.07	0.11	0.10
9	51(H) - 33(N)	BD C28 - N33	LP* H51	3.54	2.64	2.89	2.83	2.89	2.57
		BD C29 - N33	LP* H51	0.63	1.45	1.60	1.19	1.52	0.38
		BD* C28 - N33	LP* H51	3.22	1.14	1.27	1.60	1.16	1.05
		LP N33	LP* H51	60.13	93.21	98.86	104.67	99.11	94.26
		LP* H51	BD* C28 - N33	0.71	1.27	1.30	1.00	1.17	1.35
		LP* H51	BD* C29- N33	2.52	2.35	2.35	2.57	2.70	2.25
		CR N33	LP* H51	0.60	1.25	1.39	1.07	1.38	1.28
10	52(H) - 13(O)	BD C44 - H52	BD* O13 - H14	NA	0.13	0.14	0.11	0.15	0.11
		LP O13	BD* C44 - H52	NA	0.05	0.06	0.05	0.07	NA
Total				75.21	105.66	112.20	117.54	112.47	105.20

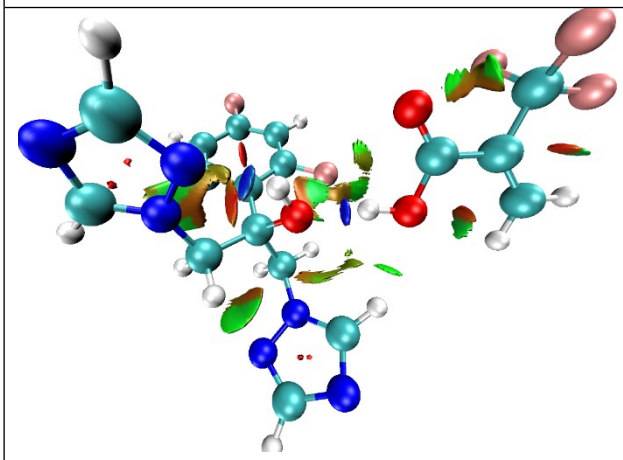
Table S6. Intermolecular interactions of all complexes from NBO, QTAIM, and NCI-RDG study

 Complex 1	 Complex 21
 Complex 2	 Complex 22
 Complex 3	 Complex 23



Complex 4

Complex 24



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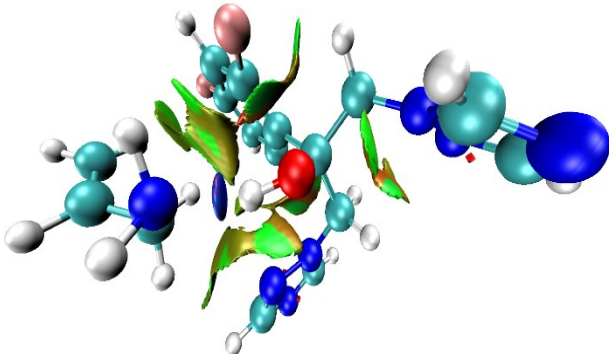

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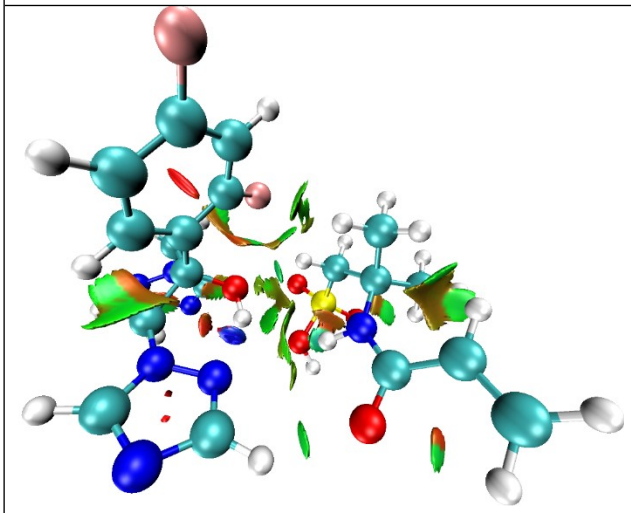

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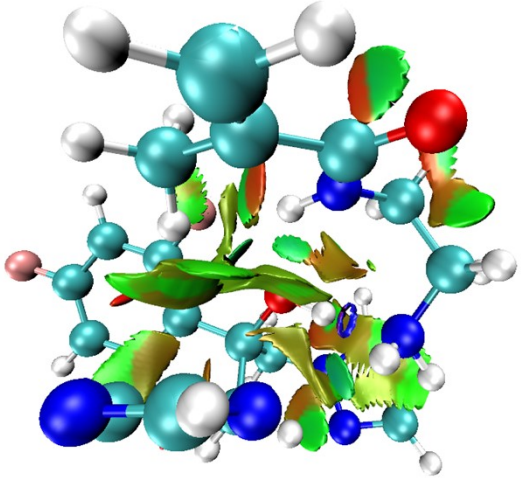
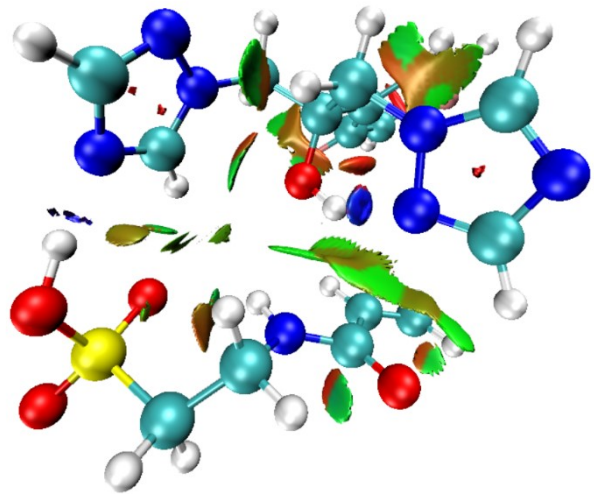
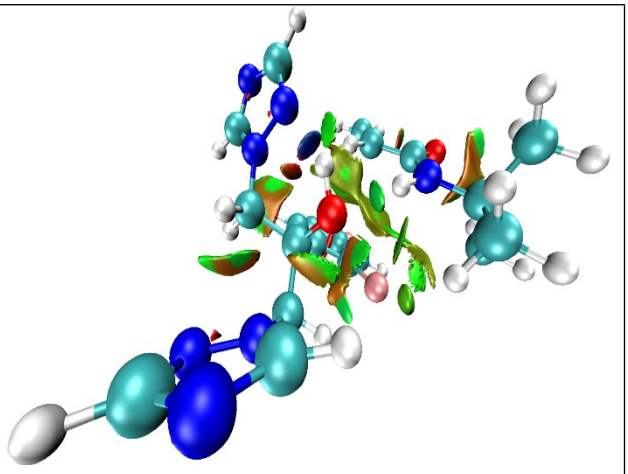
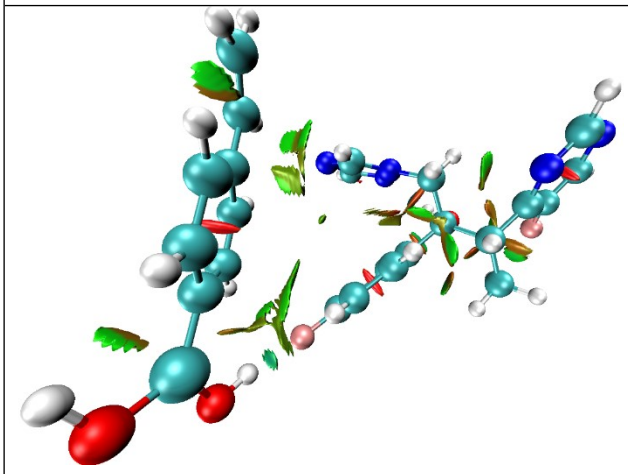
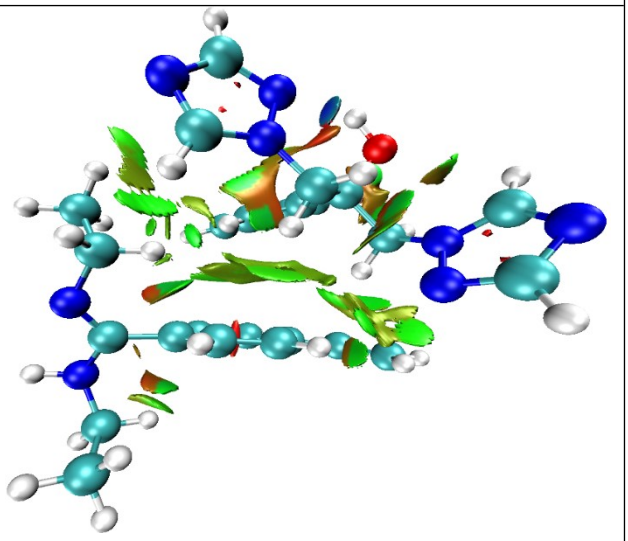
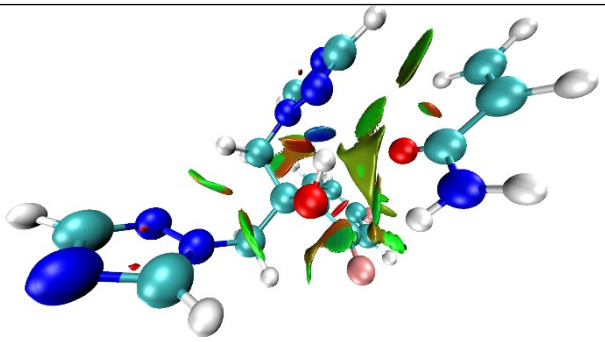
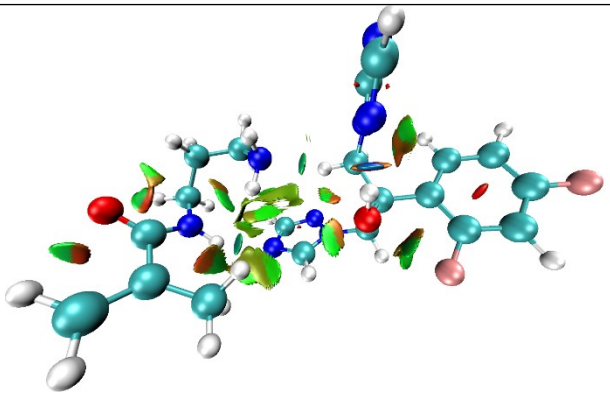
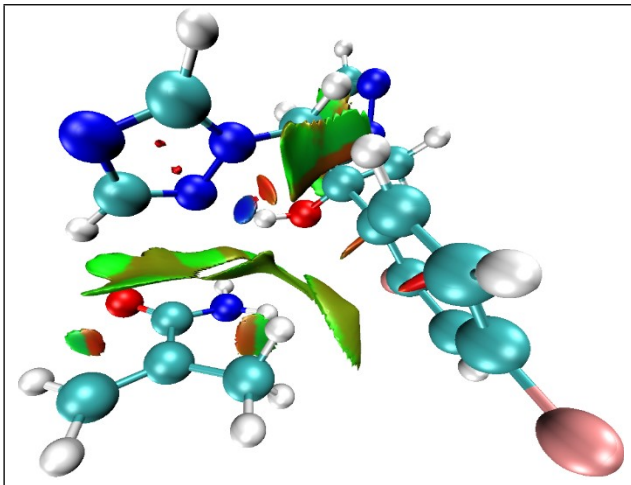


Complex 26

 Complex 7	 Complex 27
 Complex 8	 Complex 28
 Complex 9	 Complex 29



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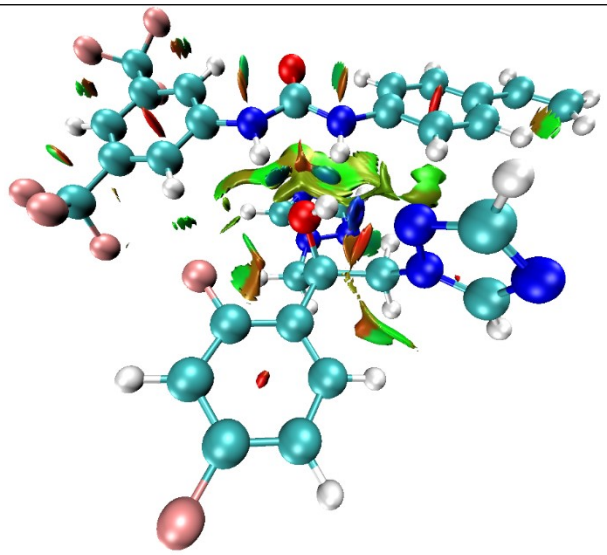

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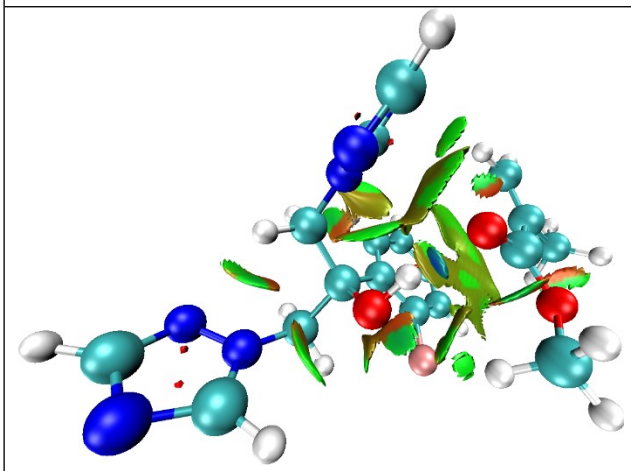

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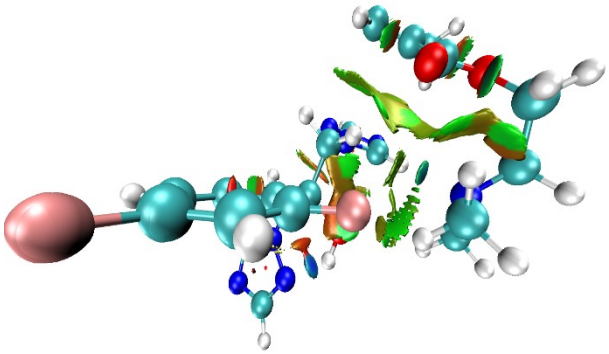

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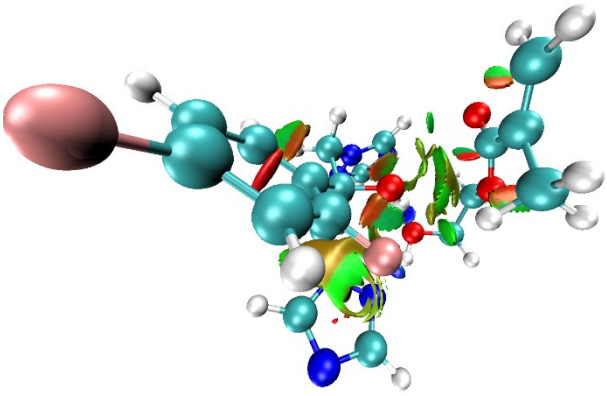

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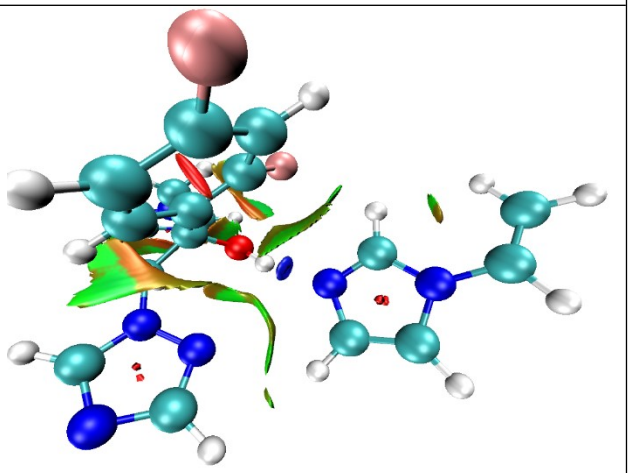

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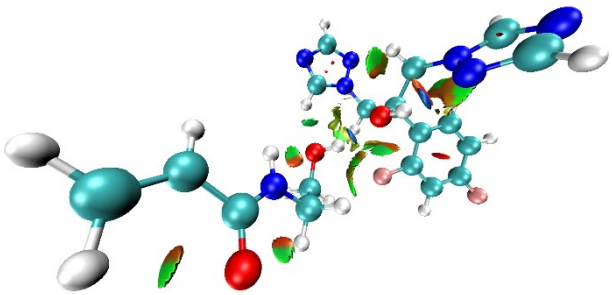
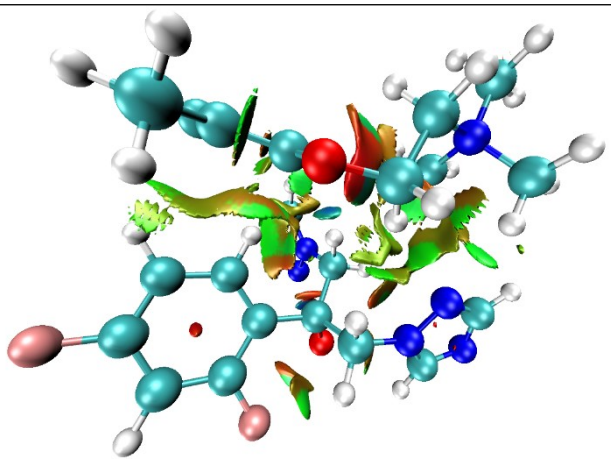
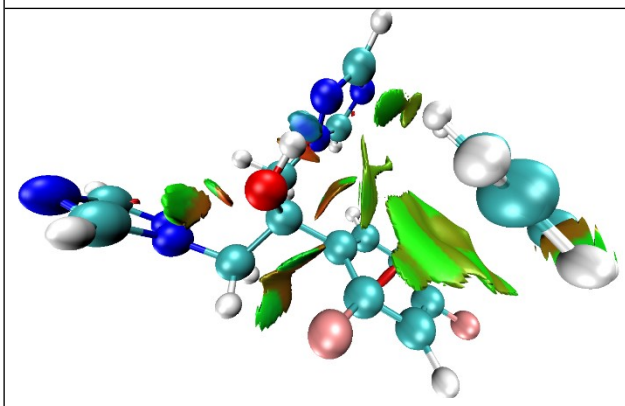
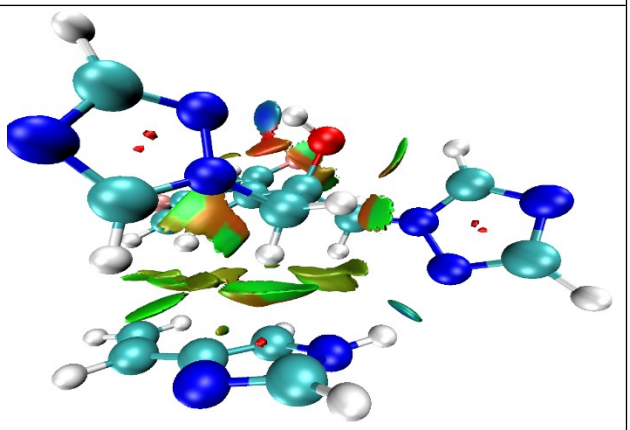
	
Complex 13	Complex 33
	
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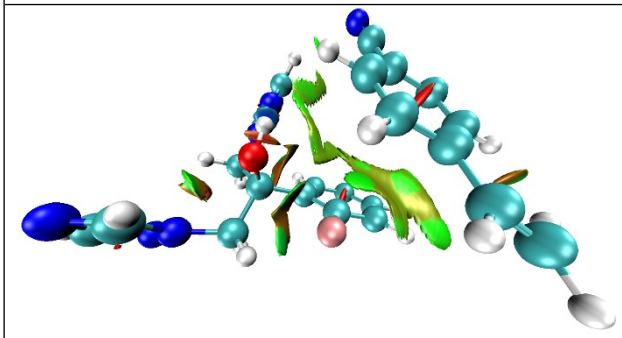	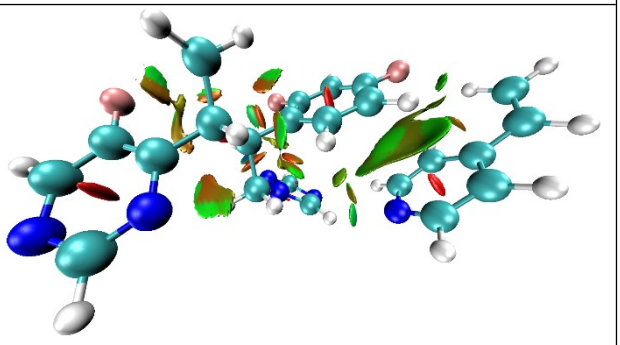
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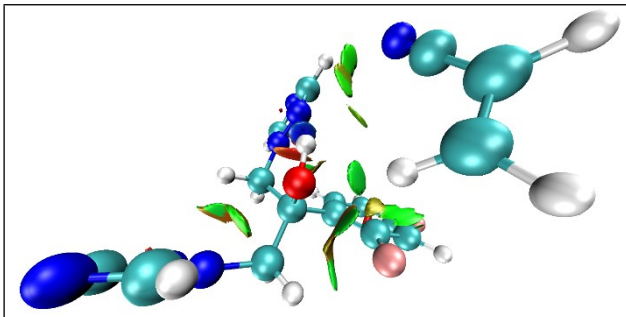

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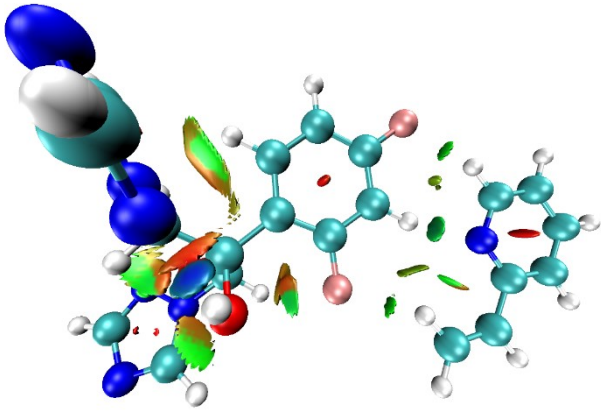

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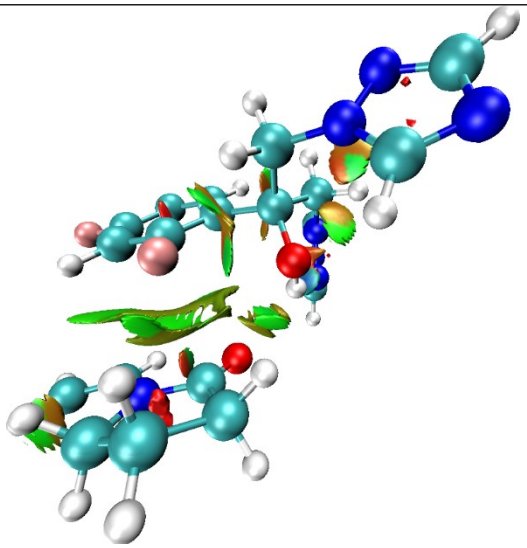

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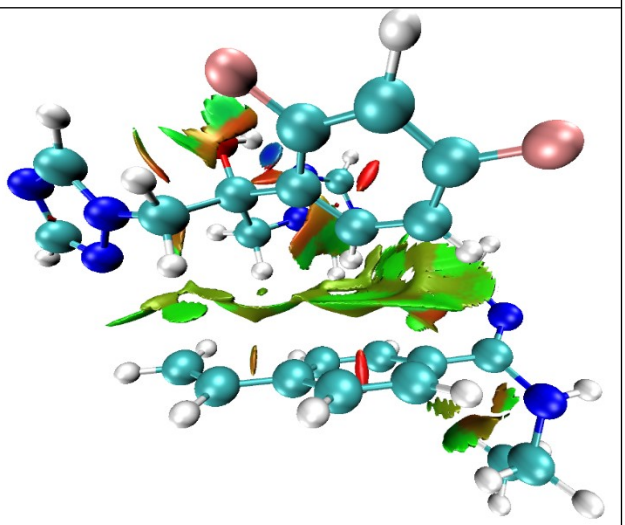

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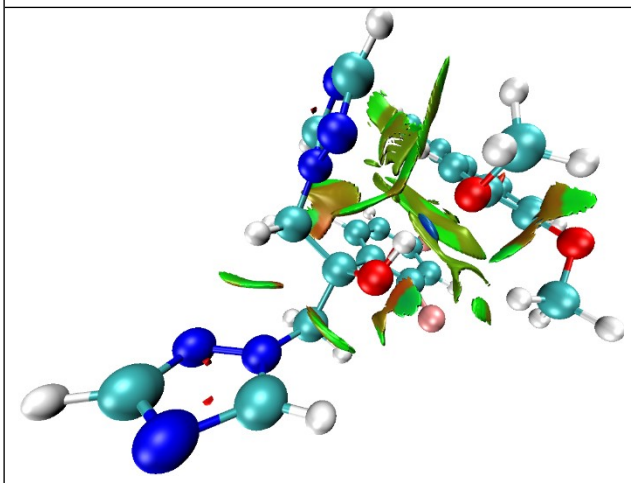

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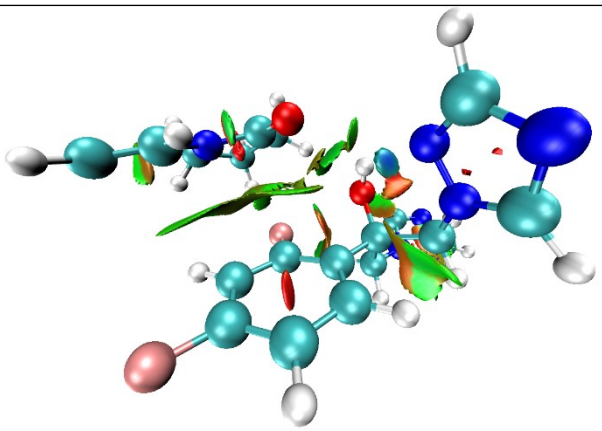

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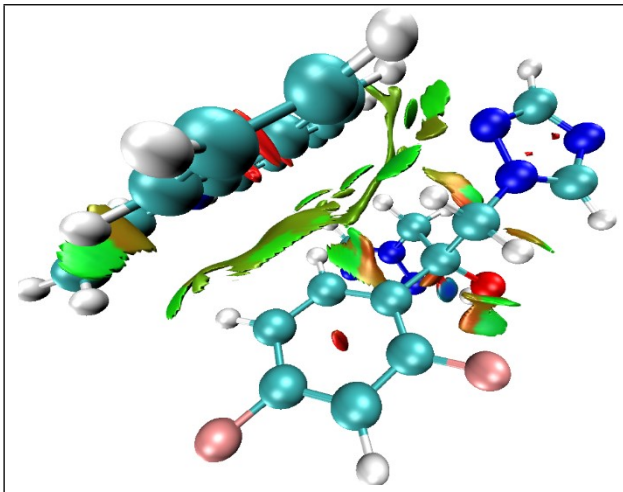

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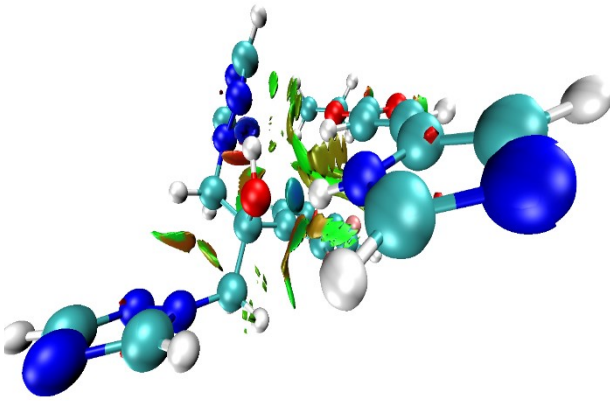

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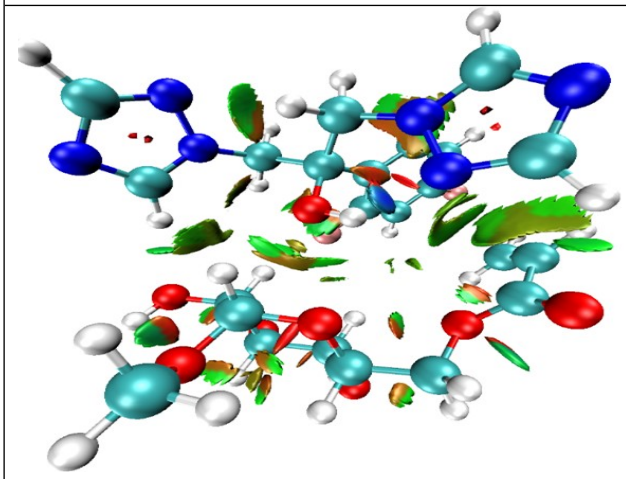

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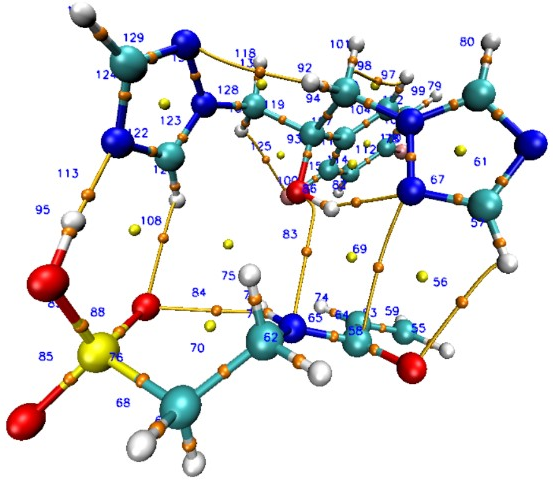
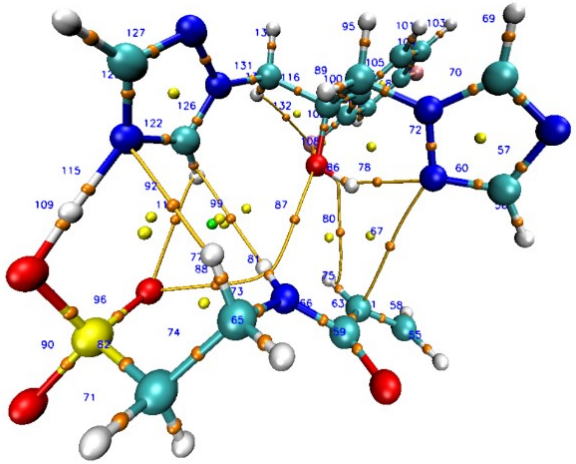
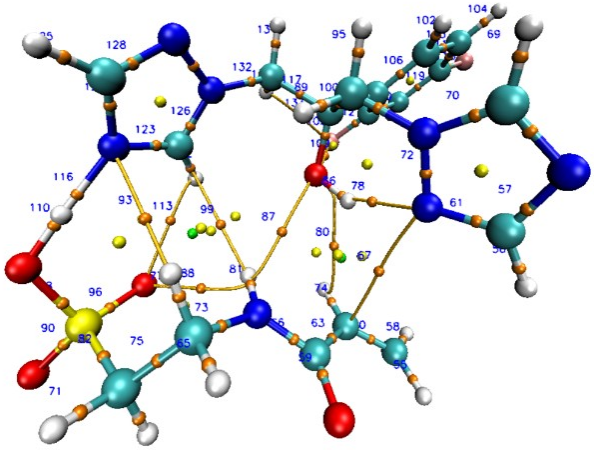


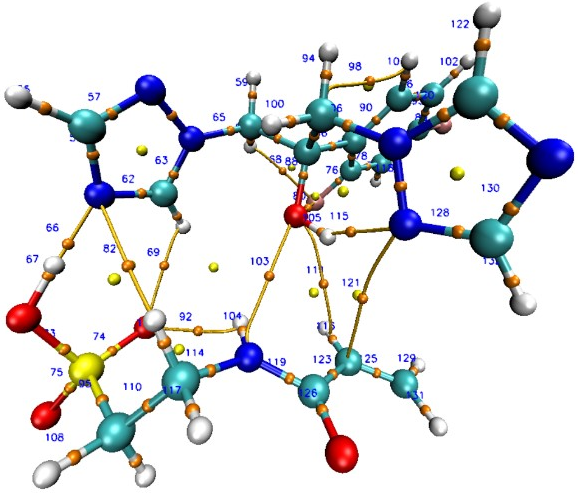
Vacuum



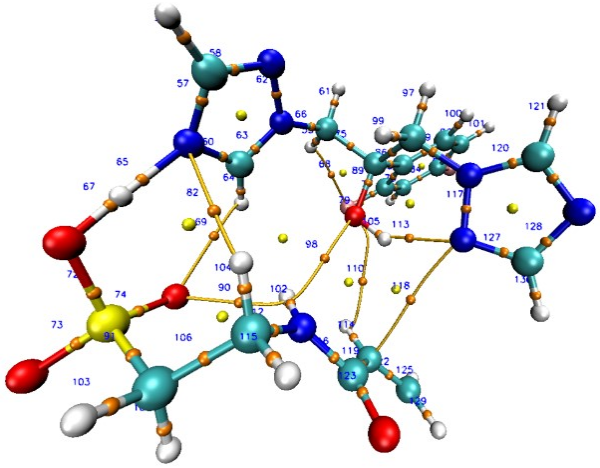
Acetone



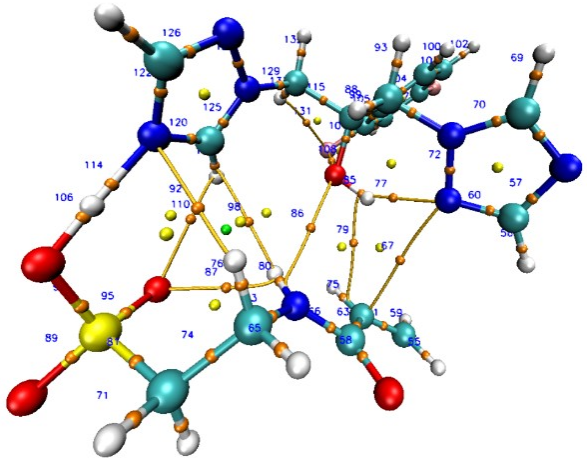
Acetonitrile



Chloroform



Dichloromethane



DMSO

Figure S1. Bond critical point of complex 7 in all conditions

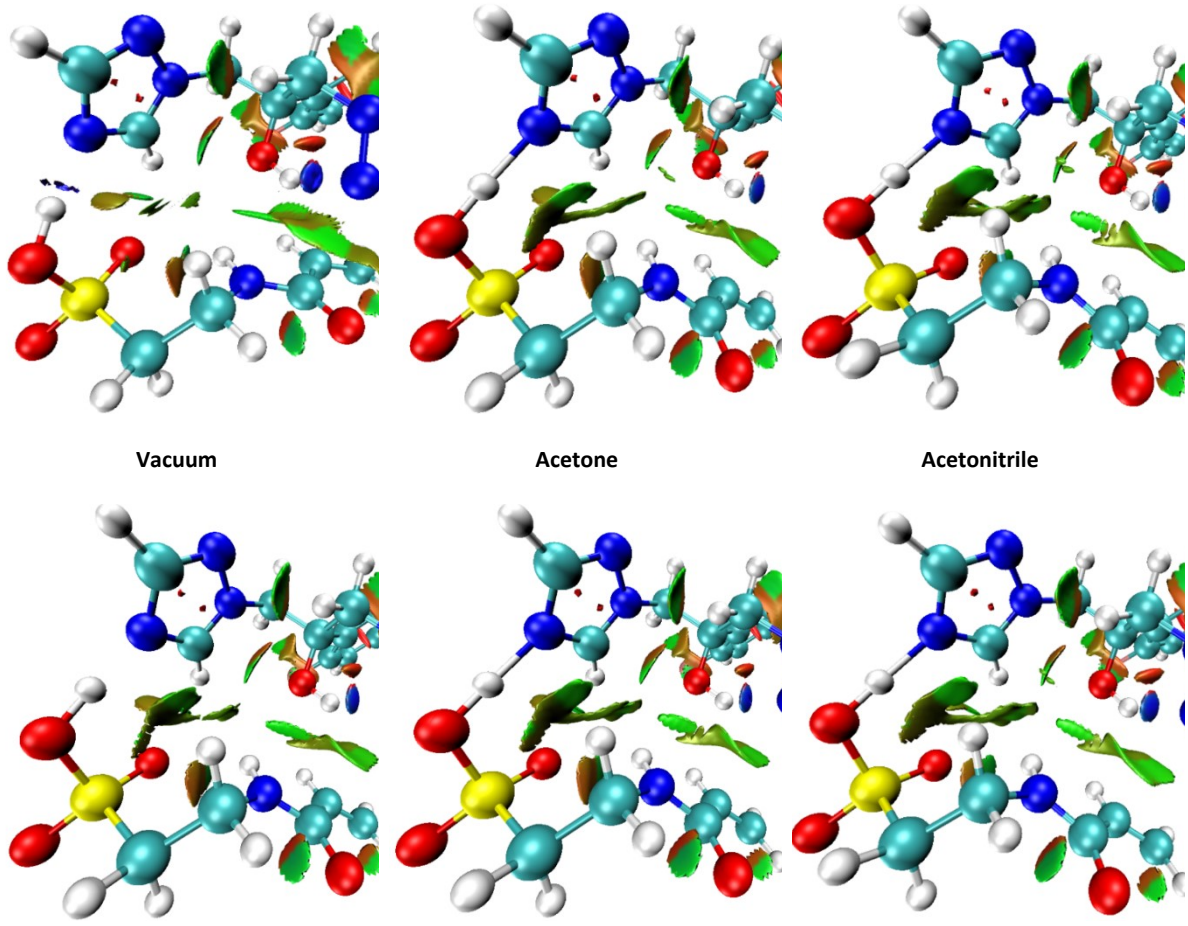
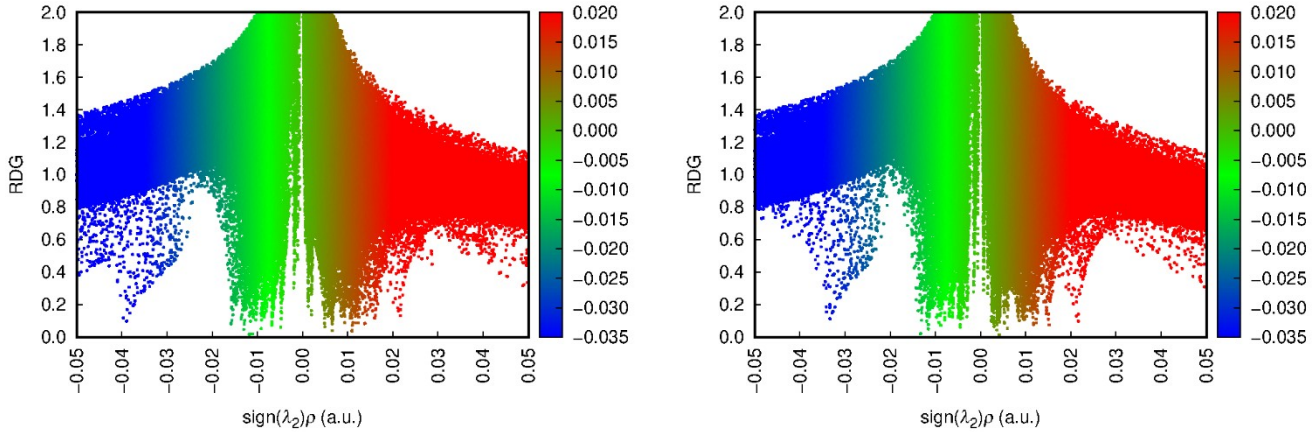
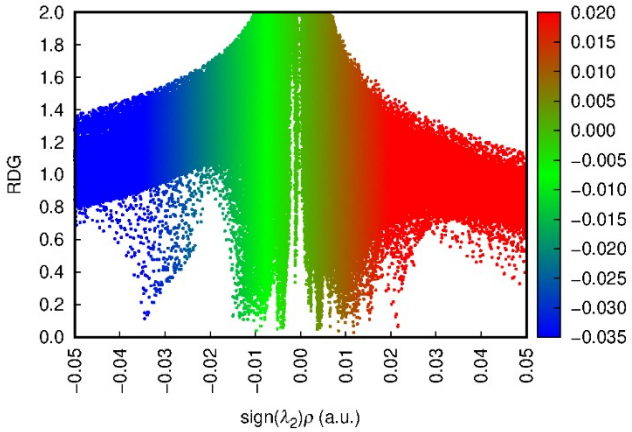


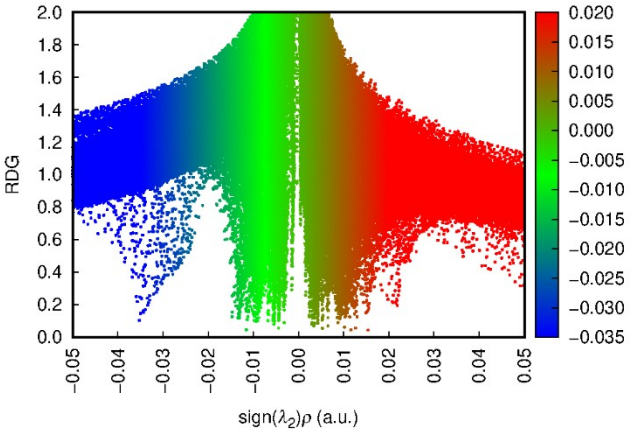
Figure S2. RDG isosurface of complex 7 in all conditions



Vacuum **Acetone**



Chloroform



Dichloromethane

Figure S3. 2D scatter plot of complex 7 in all conditions