

Table 1. Some descriptors of studied molecules calculated by B3LYP/6-31G(d,p)

No	E _{HOMO} (eV)	E _{LUMO} (eV)	ΔE^1 (eV)	μ (eV)	η (eV)	s (eV ⁻¹)	ω (eV)	Dipole Moment (D)	Polarizability (au)	E ² (eV)	Activity, EC ₅₀ (μg/mL)
1	-6.23	-0.83	5.40	-3.53	2.70	0.370	2.308	4.688	201.866	-34446.716	0.06
2	-5.57	-1.47	4.10	-3.52	2.05	0.488	3.022	4.343	218.214	-43837.695	NA
3	-5.39	-1.24	4.15	-3.32	2.08	0.482	2.648	4.914	206.415	-31331.256	NA
4	-5.37	-0.94	4.43	-3.16	2.21	0.451	2.247	4.651	215.477	-32400.419	NA
5	-5.35	-1.17	4.18	-3.26	2.09	0.478	2.542	4.578	218.693	-32400.500	NA
6	-5.52	-1.37	4.15	-3.45	2.08	0.482	2.860	4.378	206.709	-34031.715	NA
7	-5.63	-1.55	4.08	-3.59	2.04	0.490	3.159	4.183	218.167	-40502.313	NA
8	-5.33	-1.20	4.13	-3.27	2.06	0.484	2.581	4.883	221.285	-32400.500	NA
9	-5.31	-0.93	4.38	-3.12	2.19	0.457	2.222	4.533	229.960	-33469.663	NA
10	-5.32	-0.85	4.47	-3.09	2.24	0.447	2.129	5.511	227.938	-33469.663	NA
11	-5.31	-1.12	4.19	-3.22	2.10	0.477	2.467	4.802	231.914	-33469.718	NA
12	-5.21	-0.89	4.32	-3.05	2.16	0.463	2.153	5.427	220.327	-34446.716	NA
13	-6.14	-0.52	5.62	-3.33	2.81	0.356	1.973	3.796	189.490	-24590.122	0.05
14	-5.25	-0.99	4.26	-3.12	2.13	0.469	2.285	5.341	208.909	-33378.179	4.5
15	-5.96	-0.48	5.48	-3.22	2.74	0.365	1.892	3.526	202.541	-25659.340	0.03
16	-5.21	-0.95	4.26	-3.08	2.13	0.469	2.227	5.114	221.965	-34447.396	0.4
17	-5.43	-1.20	4.23	-3.32	2.12	0.473	2.598	5.445	221.314	-45884.618	0.9
18	-6.29	-0.92	5.37	-3.61	2.68	0.372	2.420	5.819	202.737	-32400.473	0.2
19	-5.60	-1.51	4.09	-3.56	2.05	0.489	3.090	5.603	218.612	-43837.695	0.02
20	-5.41	-1.27	4.14	-3.34	2.07	0.483	2.695	5.902	206.868	-31331.229	0.05
21	-5.39	-1.00	4.39	-3.20	2.20	0.456	2.325	6.274	216.142	-32400.419	0.065±0.035
22	-5.36	-1.22	4.14	-3.29	2.07	0.483	2.615	5.448	219.254	-32400.473	0.015±0.007

23	-5.53	-1.41	4.12	-3.47	2.06	0.485	2.923	5.634	207.330	-34031.688	0.038
24	-5.65	-1.61	4.04	-3.63	2.02	0.495	3.262	5.466	219.123	-40502.313	0.09
25	-5.35	-1.23	4.12	-3.29	2.06	0.485	2.627	5.985	221.665	-32400.473	NA
26	-5.33	-0.94	4.39	-3.14	2.20	0.456	2.239	5.846	230.238	-33469.636	0.15
27	-5.35	-0.94	4.41	-3.15	2.20	0.454	2.243	5.773	229.057	-33469.636	0.023±0.011
28	-5.33	-1.14	4.19	-3.24	2.10	0.477	2.498	5.891	232.385	-33469.691	0.03±0.07
29	-5.21	-0.81	4.40	-3.01	2.20	0.455	2.059	6.019	220.888	-34446.743	1.0
30	-6.18	-0.56	5.62	-3.37	2.81	0.356	2.021	5.645	190.082	-24590.122	25
31	-5.25	-1.00	4.25	-3.13	2.12	0.471	2.298	6.959	209.719	-33378.179	2
35	-5.79	-1.80	3.99	-3.80	2.00	0.501	3.610	5.358	203.427	-25659.312	2.5
36	-5.82	-2.61	3.21	-4.22	1.60	0.623	5.535	6.839	222.728	-34447.396	NA
32	-6.00	-0.54	5.46	-3.27	2.73	0.366	1.958	7.183	222.223	-45884.618	0.15±0.071
33	-5.22	-0.92	4.30	-3.07	2.15	0.465	2.192	6.196	223.645	-33841.262	0.5
34	-5.44	-1.19	4.25	-3.32	2.12	0.471	2.586	5.788	224.483	-36895.850	1.8
37	-5.55	-1.55	4.00	-3.55	2.00	0.500	3.151	6.039	237.697	-37531.100	NA
38	-5.69	-0.76	4.93	-3.23	2.46	0.406	2.110	3.037	217.341	-38029.477	1-3
39	-5.61	-0.37	5.24	-2.99	2.62	0.382	1.706	3.108	227.124	-39097.606	NA
40	-5.64	-0.60	5.04	-3.12	2.52	0.397	1.931	2.272	210.664	-35982.364	NA
41	-5.79	-0.90	4.89	-3.35	2.44	0.409	2.288	5.019	193.240	-24016.996	1.6-3.1
42	-5.43	-0.49	4.94	-2.96	2.47	0.405	1.774	4.677	206.585	-25523.011	NA
43	-5.77	-1.14	4.63	-3.46	2.32	0.432	2.578	4.734	193.871	-26717.373	0.4-0.8
44	-5.72	-1.23	4.49	-3.48	2.24	0.445	2.689	4.658	204.948	-36523.435	0.8
45	-5.86	-1.19	4.67	-3.53	2.34	0.428	2.661	4.637	212.752	-93980.543	0.8
46	-5.61	-0.86	4.75	-3.24	2.38	0.421	2.203	5.025	205.793	-25086.186	0.2-0.3
47	-5.26	-0.91	4.35	-3.09	2.18	0.460	2.188	4.777	211.977	-27132.401	0.6
48	-5.31	-0.95	4.36	-3.13	2.18	0.459	2.247	4.482	198.384	-26063.647	NA

49	-5.73	-1.28	4.45	-3.51	2.22	0.449	2.761	4.522	206.365	-33188.107	NA
50	-6.00	-1.24	4.76	-3.62	2.38	0.420	2.753	5.018	223.292	-26122.342	2
51	-5.61	-1.23	4.38	-3.42	2.19	0.457	2.670	4.988	223.443	-28468.318	0.5
52	-5.61	-0.86	4.75	-3.24	2.38	0.421	2.203	5.357	238.473	-28293.376	NA
53	-5.55	-0.97	4.58	-3.26	2.29	0.437	2.320	5.182	260.960	-30302.366	NA
54	-5.75	-1.58	4.17	-3.67	2.08	0.480	3.221	6.949	269.471	-33385.907	NA
55	-5.71	-0.79	4.92	-3.25	2.46	0.407	2.147	5.107	207.681	-25086.240	4
56	-6.05	-1.52	4.53	-3.79	2.26	0.442	3.163	5.905	236.566	-40974.621	NA
57	-5.40	-1.43	3.97	-3.42	1.98	0.504	2.938	5.441	243.748	-28196.612	NA
58	-5.57	-1.30	4.27	-3.44	2.14	0.468	2.763	4.466	236.051	-28196.530	NA
59	-5.53	-0.78	4.75	-3.16	2.38	0.421	2.096	5.435	281.753	-32537.428	NA
60	-5.66	-0.80	4.86	-3.23	2.43	0.412	2.147	4.878	206.332	-25086.240	8
61	-5.79	-1.50	4.29	-3.65	2.14	0.466	3.097	6.677	218.098	-49029.765	10-20
62	-5.42	-0.79	4.63	-3.11	2.32	0.432	2.082	5.410	198.501	-26063.483	NA
63	-5.74	-0.99	4.75	-3.37	2.38	0.421	2.384	4.229	194.494	-26717.536	10
64	-5.27	-0.62	4.65	-2.95	2.32	0.430	1.865	2.306	197.190	-23475.979	5-10
65	-5.83	-1.05	4.78	-3.44	2.39	0.418	2.476	6.665	223.564	-27628.900	NA

$$^1\Delta E^1 = E_{\text{HOMO}} - E_{\text{LUMO}}$$

²Sum of electronic and zero-point Energies

Table 2. Mulliken charges on some atoms of studied molecules calculated by B3LYP/6-31G(d,p)

No	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	C ₈	N ₉	(O/S) ₃₉
1	0.007	-0.095	-0.089	-0.093	-0.130	0.348	0.107	-0.444	-0.263
2	0.080	-0.102	-0.087	-0.064	-0.102	-0.074	0.073	-0.451	-0.239
3	0.081	0.106	0.088	0.079	0.091	0.091	0.075	0.453	-0.254
4	0.023	-0.094	-0.090	-0.076	-0.128	0.119	0.071	-0.444	-0.260
5	0.084	-0.111	-0.086	-0.115	0.116	-0.127	0.075	-0.452	-0.258
6	0.077	0.105	0.090	0.132	0.352	0.146	0.075	0.451	-0.243
7	0.071	-0.094	-0.093	-0.092	-0.049	-0.106	-0.075	-0.452	-0.237
8	0.082	-0.106	-0.123	0.129	-0.125	-0.092	0.074	-0.453	-0.258
9	0.021	-0.094	-0.127	0.137	-0.168	0.124	0.071	-0.444	-0.263
10	0.025	-0.133	0.123	-0.111	-0.127	0.115	0.715	-0.444	-0.262
11	0.089	-0.150	0.124	-0.148	0.119	-0.134	0.072	-0.450	-0.258
12	0.011	-0.094	-0.089	-0.092	-0.131	0.346	0.106	-0.446	-0.265
13	0.013	-0.125	-0.103	-0.082	-0.103	0.302	0.549	-0.543	-0.569
14	0.068	-0.117	-0.097	-0.083	-0.101	0.294	0.080	-0.469	-0.278
15	0.019	-0.170	0.115	-0.118	-0.100	0.296	0.548	-0.542	-0.578
16	0.075	-0.163	0.122	-0.118	-0.098	0.287	0.079	-0.469	-0.281
17	0.071	-0.103	-0.107	-0.069	-0.098	0.297	0.082	-0.468	-0.266
18	0.082	-0.111	-0.086	-0.115	0.117	-0.123	0.078	-0.454	-0.261
19	0.073	-0.099	-0.087	-0.064	-0.103	-0.070	0.083	-0.463	-0.250
20	0.083	-0.106	-0.088	-0.079	-0.089	-0.089	0.075	-0.452	-0.256
21	0.021	-0.093	-0.090	-0.077	-0.127	0.122	0.072	-0.444	-0.262
22	0.084	-0.112	-0.087	-0.112	0.116	-0.125	0.077	-0.454	-0.261
23	0.076	-0.106	-0.090	-0.132	0.352	0.143	0.078	-0.453	-0.247
24	0.073	-0.095	-0.093	-0.091	-0.048	-0.104	0.074	-0.452	-0.239
25	0.083	-0.107	-0.124	0.130	-0.123	-0.089	0.074	-0.453	-0.261
26	0.021	-0.094	-0.127	0.137	-0.166	0.127	0.072	-0.444	-0.265
27	0.025	-0.132	0.122	-0.112	-0.126	0.118	0.072	-0.444	-0.264
28	0.087	-0.152	0.126	-0.148	0.120	-0.130	0.076	-0.453	-0.262
29	0.021	-0.095	-0.091	-0.092	-0.134	0.344	0.103	-0.447	-0.275
30	0.013	-0.123	-0.104	-0.083	-0.103	0.302	0.552	-0.545	-0.580
31	0.067	-0.115	-0.097	-0.083	-0.101	0.294	0.08	-0.469	-0.276
32	0.019	-0.169	0.115	-0.118	-0.100	0.296	0.550	-0.543	-0.579
33	0.075	-0.162	0.122	-0.118	-0.098	0.288	0.080	-0.469	-0.282
34	0.070	-0.100	-0.108	-0.070	-0.098	0.298	0.083	-0.468	-0.266
35	0.074	-0.093	-0.090	-0.072	0.095	-0.083	0.075	-0.455	-0.233
36	0.057	-0.084	-0.099	-0.083	0.234	-0.089	0.081	-0.459	-0.231

37	0.065	-0.078	-0.101	-0.091	0.013	-0.115	0.086	-0.458	-0.261
38	0.010	-0.129	-0.154	0.334	-0.141	0.302	0.620	-0.568	-0.604
39	-0.007	-0.116	-0.143	0.325	-0.151	0.327	0.544	-0.541	-0.528
40	0.037	-0.117	-0.148	0.326	-0.116	-0.101	0.568	-0.563	-0.534
41	0.012	-0.137	-0.100	-0.083	-0.103	0.301	0.616	-0.563	-0.597
42	0.003	-0.142	-0.126	0.298	-0.146	0.300	0.613	-0.568	-0.607
43	0.013	-0.198	0.342	-0.135	-0.105	0.304	0.621	-0.563	-0.595
44	0.014	-0.120	-0.113	-0.070	-0.099	0.306	0.622	-0.563	-0.594
45	0.012	-0.141	0.039	-0.088	-0.102	0.308	0.624	-0.563	-0.595
46	0.019	-0.180	0.119	-0.119	-0.100	0.295	0.617	-0.564	-0.599
47	0.014	-0.180	0.344	-0.129	-0.116	0.300	0.616	-0.562	-0.595
48	0.012	-0.162	0.318	-0.128	-0.108	0.298	0.615	-0.562	-0.596
49	0.006	-0.156	-0.053	-0.097	-0.106	0.312	0.631	-0.565	-0.599
50	0.017	-0.200	0.131	-0.121	-0.103	0.301	0.624	-0.565	-0.600
51	0.006	-0.152	0.256	-0.092	-0.116	0.309	0.624	-0.563	-0.595
52	0.013	-0.142	-0.134	0.153	-0.157	0.293	0.620	-0.567	-0.602
53	0.010	-0.174	0.058	-0.115	-0.108	0.302	0.619	-0.564	-0.597
54	0.002	-0.174	0.035	-0.094	-0.107	0.311	0.625	-0.565	-0.598
55	0.009	-0.135	-0.131	0.129	-0.145	0.303	0.619	-0.565	-0.602
56	0.023	-0.132	-0.133	0.297	-0.118	0.305	0.627	-0.566	-0.595
57	0.016	-0.203	0.103	0.113	-0.173	0.307	0.615	-0.559	-0.589
58	-0.059	0.067	0.095	-0.123	-0.099	0.303	0.592	-0.554	-0.597
59	0.021	-0.187	0.091	0.096	-0.150	0.290	0.619	-0.566	-0.600
60	0.024	-0.143	-0.095	-0.122	0.092	0.260	0.617	-0.565	-0.601
61	0.018	-0.118	-0.110	-0.056	-0.140	0.339	0.627	-0.563	-0.592
62	0.024	-0.117	-0.100	-0.124	0.303	0.263	0.597	-0.582	-0.546
63	-0.063	0.301	-0.141	-0.087	-0.102	0.303	0.646	-0.577	-0.606
64	0.022	-0.143	-0.103	-0.084	-0.116	0.275	0.585	-0.556	-0.566
65	0.018	-0.142	-0.088	-0.093	-0.094	0.285	0.582	-0.549	-0.548

Table 3. Fukui functions of studied molecules calculated by B3LYP/6-31G(d,p)

[illegible]

[illegible]