Supplementary Material for *Journal of Materials Chemistry*

Enhanced electron injection and efficiency in blended-layer organic light emitting diodes with aluminium cathodes: new 2,5-diaryl-1,3,4-oxadiazole–fluorene hybrids incorporating pyridine units

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X-Ray Molecular Structure of 11.

The asymmetric unit comprises two molecules, A and B, each having one *t*-Bu and one *n*-hexyl group conformationally disordered (Figure S1). The conformations of the molecular 'rod' are somewhat different. In molecule B, as in **8**, the central fluorene moiety is planar with the mean deviation δ=0.013 Å (max. δ=0.025 Å), whilst in molecule A it is substantially puckered (mean δ=0.08, max. 0.16 Å). The interplanar angles between the fluorene moiety (or rather its outer 6-membered rings, **i** and **v**, Figure S1a) and the adjacent thiophene rings **ii** and **vi** varies from 4.6 to 36.4°, but on average are smaller than the corresponding angles in **8**, which has benzene rings instead of thiophene. In both molecules of **11**, the mutual orientation of the two thiophene rings is *transoid*, that of oxadiazole rings also *transoid*, and each adjacent pair of thiophene and oxadiazole rings has the S and O atoms in *trans*-positions relative to the connecting C–C bond. The dihedral angles between these and other rings along the chain are also mostly small. Overall, the 'rod' acquires some out-of-plane bending. Thus, the two outlying C(benzene)−C(*t*-Bu) bonds deviate from the fluorene mean plane by ca. 1° and 22° in molecule A, 17° and 25° in B.

The single-crystal X-ray diffraction experiment was carried out on a Bruker SMART 3-circle diffractometer with an APEX CCD area detector, using graphite monochromated Mo-K_α radiation ($\bar{\lambda}$=0.71073 Å) from 60W Mo-target microfocus Bede Microsource® X-ray generator with glass polycapillary X-ray optics and a Cryostream-Plus open-flow N_2 cryostat. The structure was solved by direct methods and refined by full-matrix least squares against F^2 of all reflections, using SHELXTL 6.14 software (Bruker-Nonius AXS, Madison, WI, USA, 2003). *Crystal data*: $C_{57}H_{62}N_4O_2S_2$, M=899.23, T=120 K, triclinic, space group $P\bar{1}$ (No. 2), a=16.095(2), b=16.647(2), c=19.390(2) Å, α=82.61(1), β=87.70(1), γ=72.94(1)º, U= 4925(1) Å^3, Z=4, D_c=1.213 g cm^{-3}, μ=0.15 mm^{-1}, 47733 reflections (2θ≤50º), 17322 unique, R_{int}=0.093, R=0.048 [6940 data with $F^2 \geq 2\sigma(F^2)$], w$R(F^2)$=0.147 (all data).

Table S1. Angles (°) between ring planes in **11** (molecules A and B) and corresponding angles in **8**

	A	B	**8**		A	B	**8**
i/v	9.7	1.0	0				
i/ii	8.2	12.9	21.9	v/vi	36.4	4.6	30.3
ii/iii	11.3	5.8	5.0	vi/vii	7.4	7.5	11.4
iii/iv	23.6	12.4	6.7	vii/viii	11.5	31.4	9.5

Ring notation for **11** see in Fig. S1a. In **8,** rings ii and vi are benzene instead of thiophene

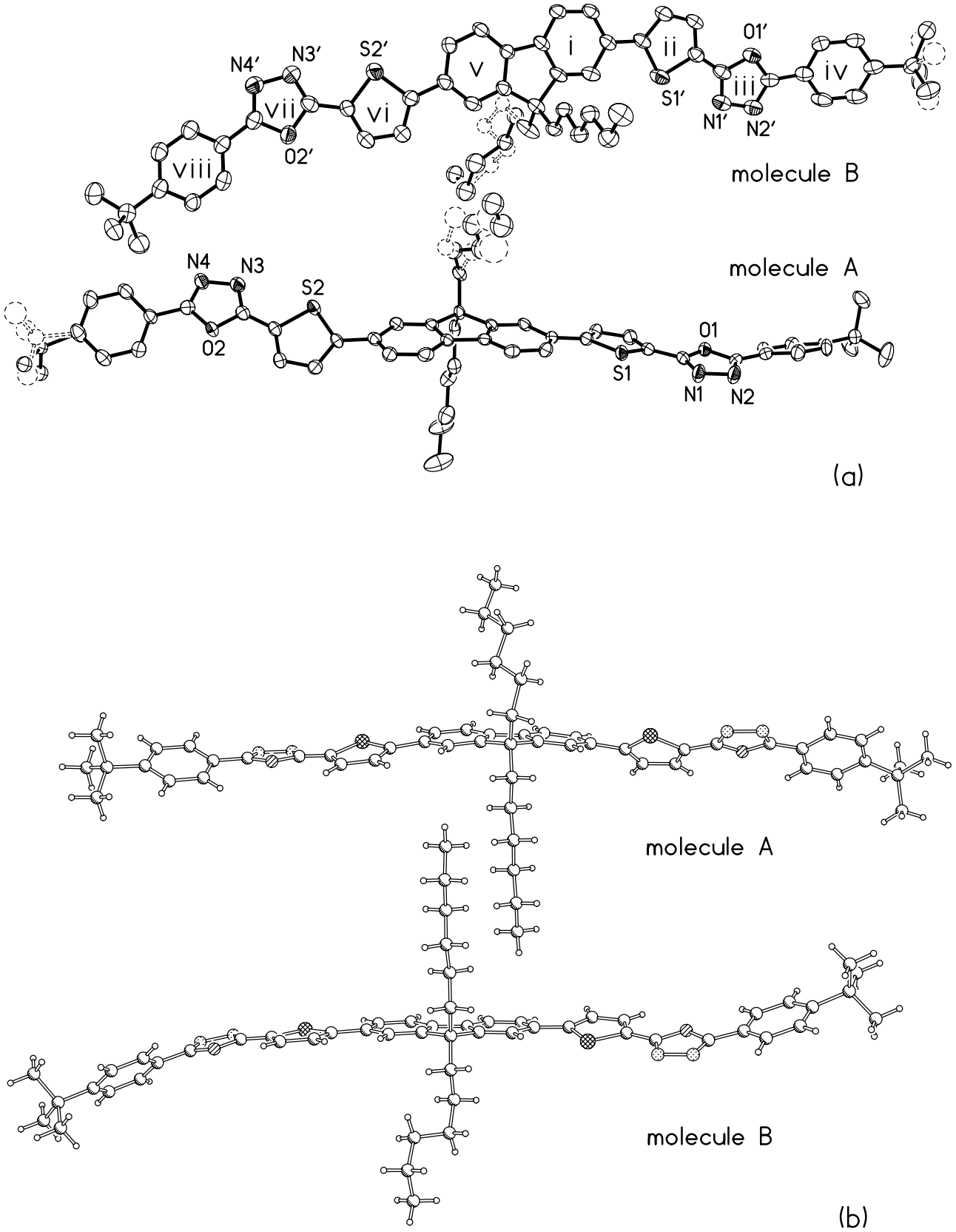
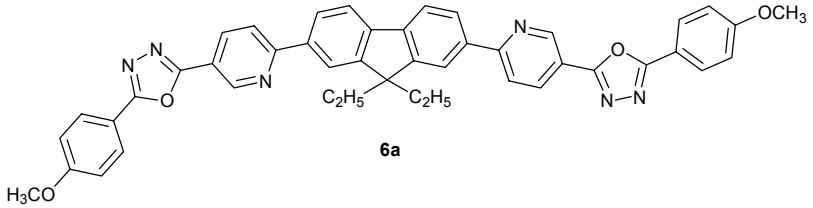
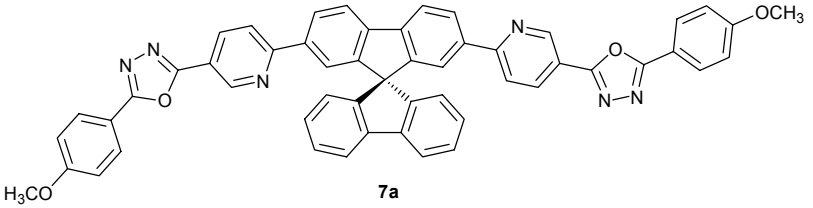


Figure S1. X-Ray molecular structure of compound **11**: (a) the asymmetric unit, showing thermal ellipsoids at the 50% probability level and the disorder; H atoms are omitted for clarity; (b) two independent molecules shown in the same orientation; minor positions of the disordered atoms are omitted.

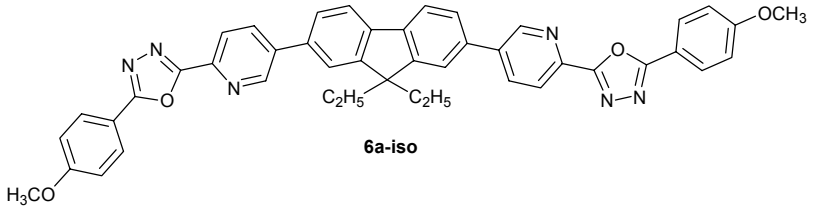
Theoretical Calculations



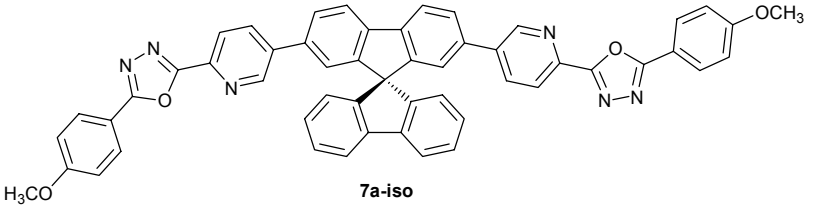
6a



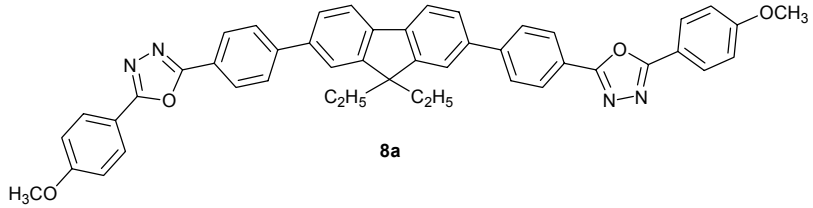
7a



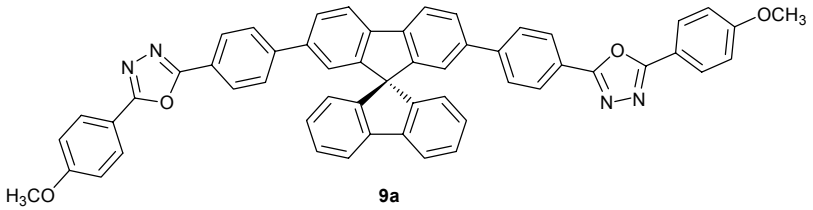
6a-iso



7a-iso



8a



9a

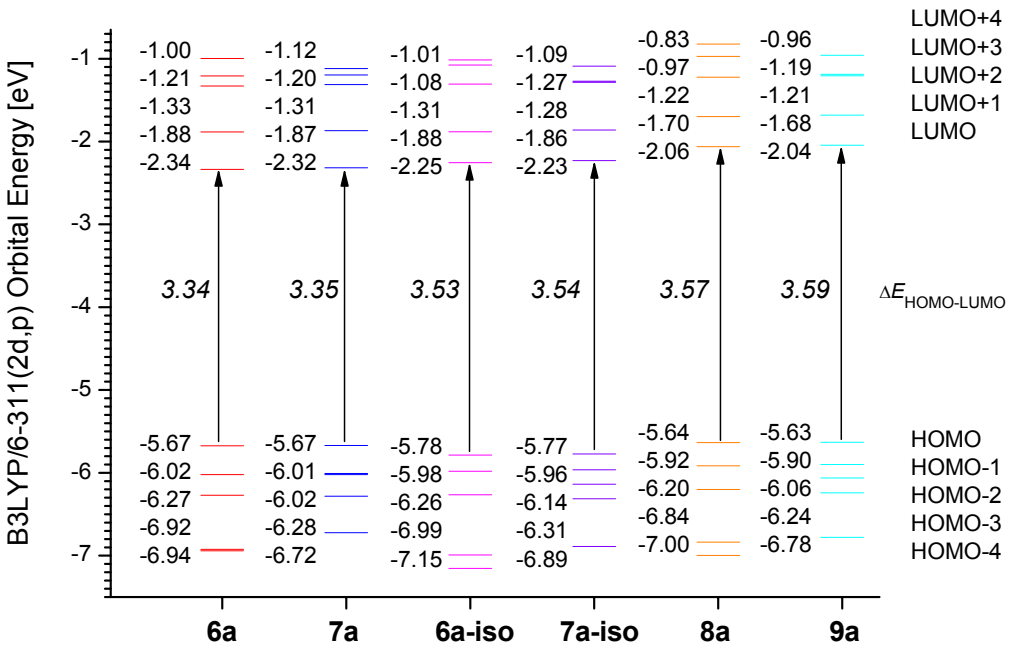


Figure S2. B3LYP/6-311G(2d,p)//B3LYP/6-31G(d) orbital energy level diagram for compounds **6a, 7a** and a comparison with isomers **6a-iso** and **7a-iso**, and with phenylene analogues **8a** and **9a**.

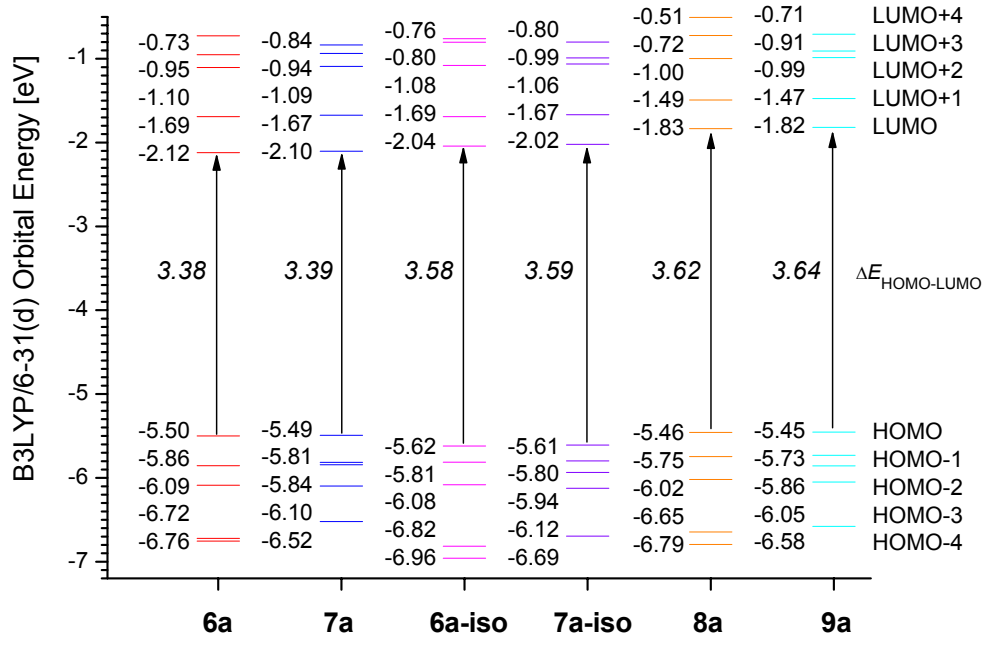


Figure S3. B3LYP/6-31G(d) orbital energy level diagram for compounds **6a, 7a** and a comparison with isomers **6a-iso** and **7a-iso**, and with phenylene analogues **8a** and **9a**.

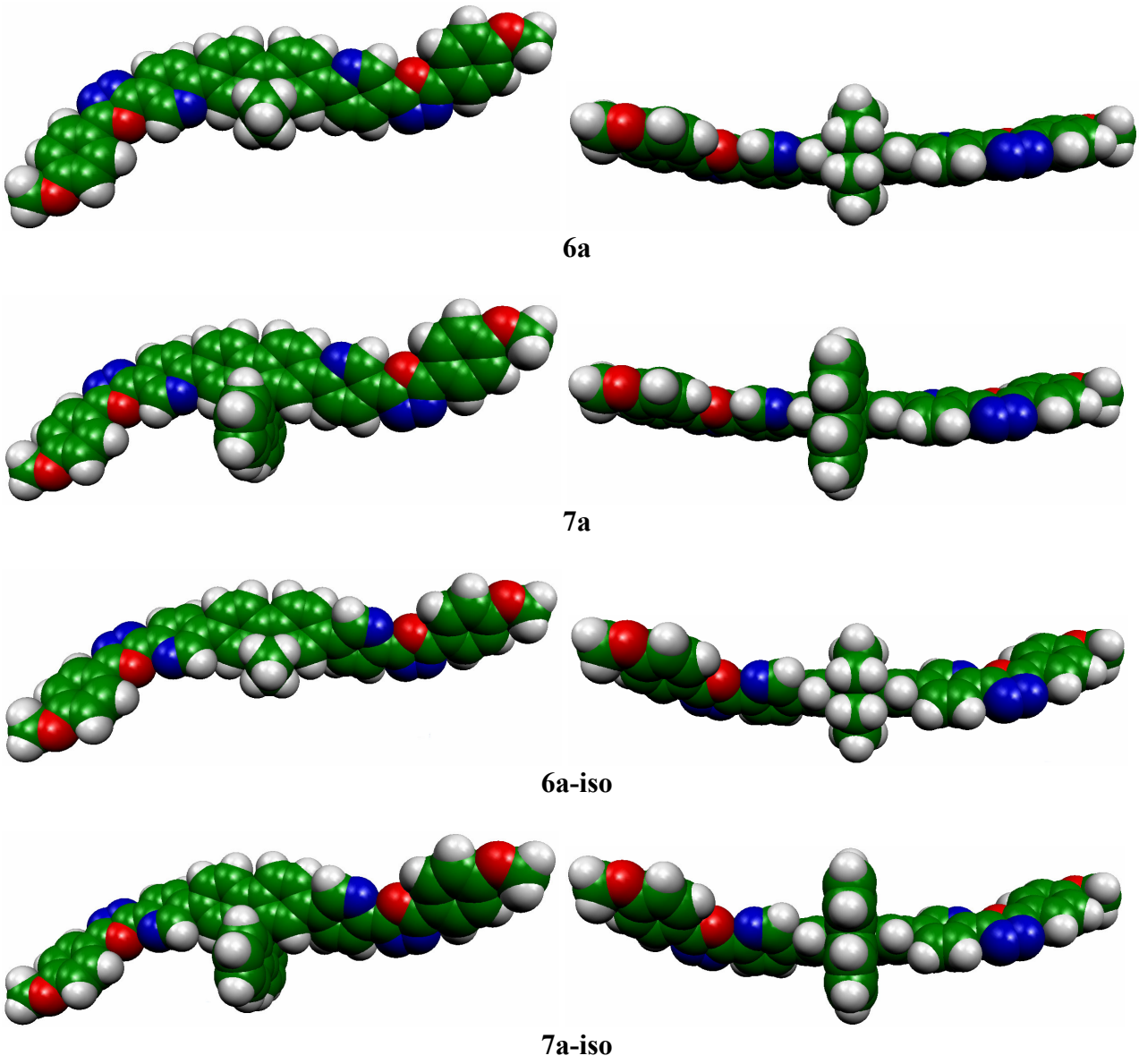
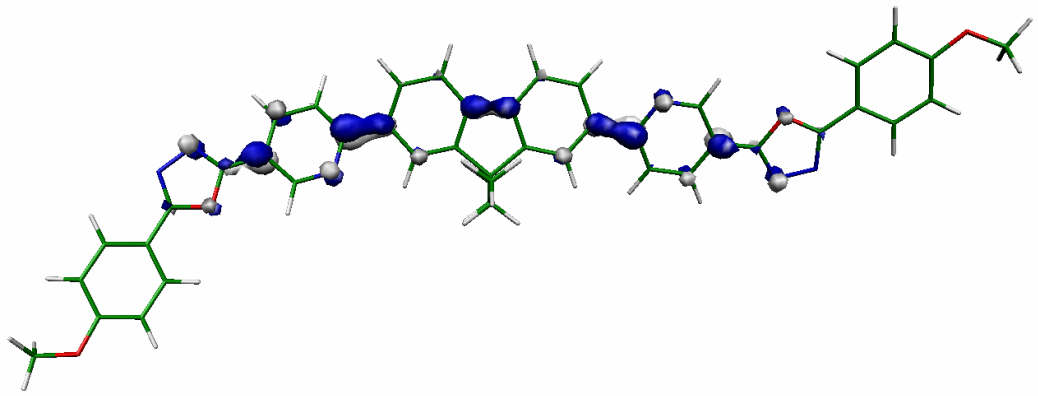
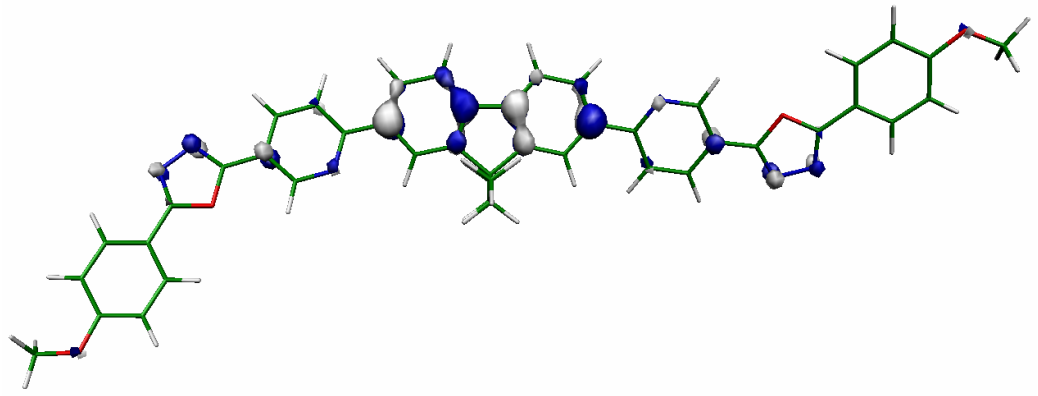


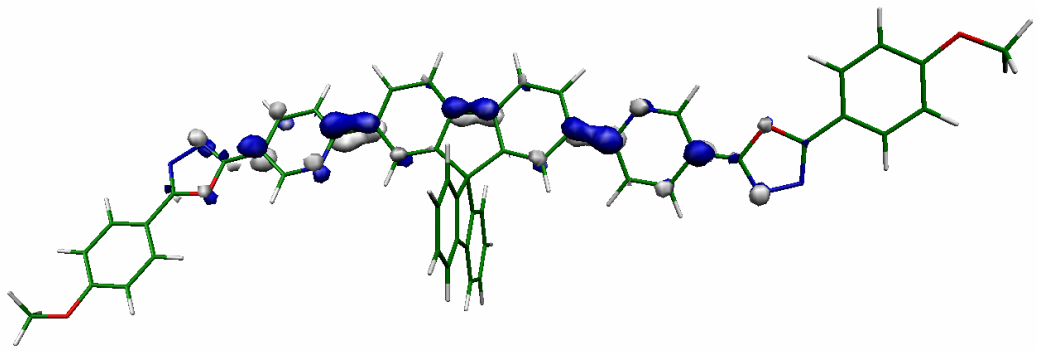
Figure S4. B3LYP/6-31G(d) optimised geometries of compound **6a**, **7a, 6a-iso** and **7a-iso**.



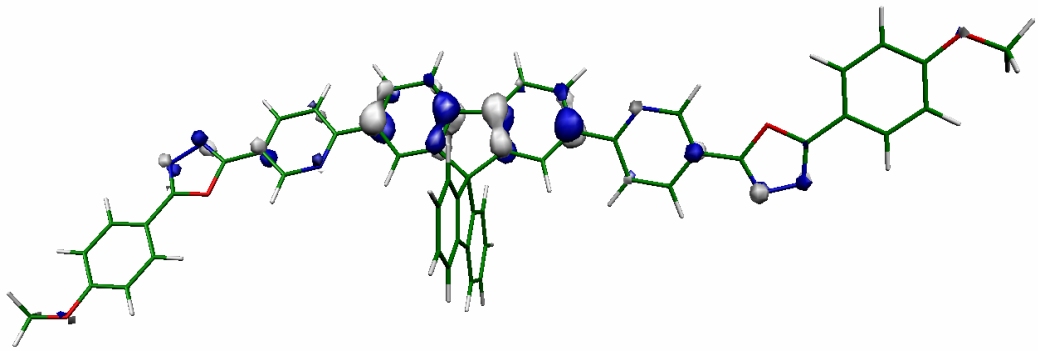
6a, LUMO = –2.34 eV



6a, HOMO = –5.67 eV

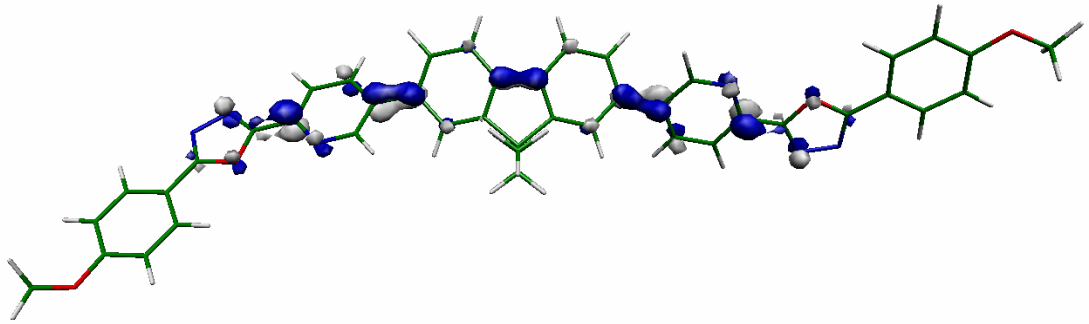


7a, LUMO = –2.32 eV

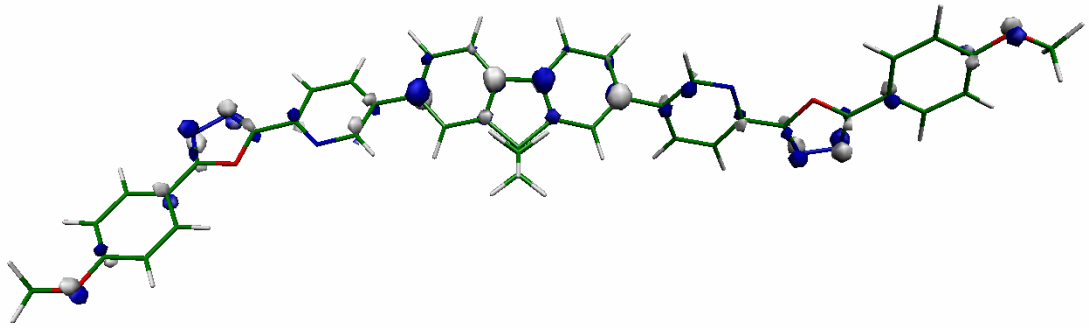


7a, HOMO = –5.67 eV

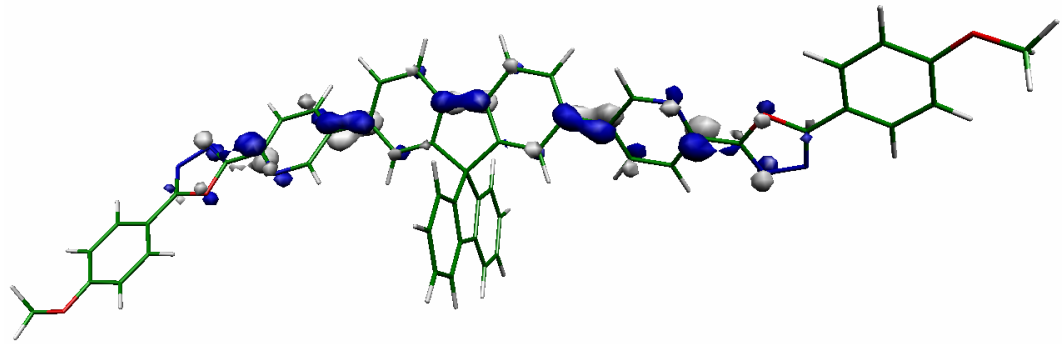
Figure S5. Frontier orbitals of compounds **6a** (E_{total} = –2366.5004319 Hartree) and **7a** (E_{total} = –2670.2215067 Hartree) calculated by DFT method at B3LYP/6-311G(2d,p)//B3LYP6031G(d) level.



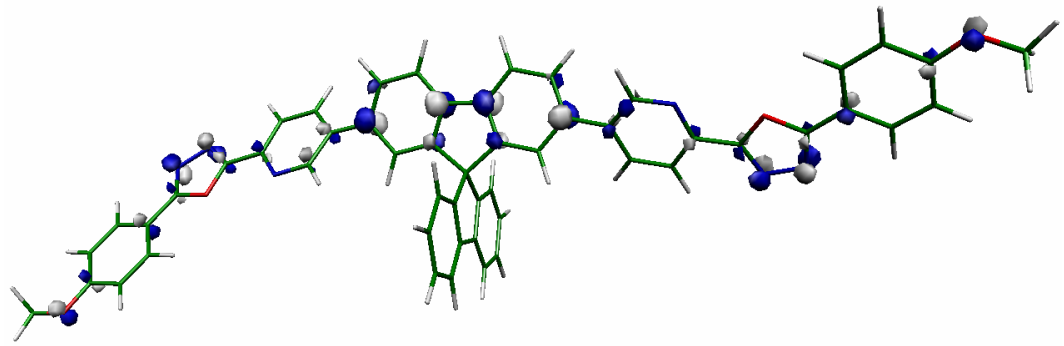
6a-iso, LUMO = –2.25 eV



6a-iso, HOMO = –5.78 eV



7a-iso, LUMO = –2.23 eV



7a-iso, HOMO = –5.77 eV

Figure S6. Frontier orbitals of compounds **6a-iso** (E_{total} = –2366.4931201 Hartree), **7a-iso** (E_{total} = –2670.2148323 Hartree) calculated by DFT method at B3LYP/6-311G(2d,p)//B3LYP6031G(d) DFT level.

Table S1. B3LYP/6-31G(d) optimised geometry of compound **6a**.
E_{total} = –2365.8768971 Hartree
Dipole moment (Debye): X = 0.3933 Y = 1.1267 Z = –0.8190 Tot = 1.4474

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.388573	-0.523010	0.331791
2	6	0	2.255730	0.311373	0.427260
3	6	0	0.982581	-0.233064	0.347139
4	6	0	0.812677	-1.621634	0.170018
5	6	0	1.926615	-2.459409	0.065793
6	6	0	3.200862	-1.906715	0.142855
7	6	0	-0.620940	-1.910744	0.118545
8	6	0	-1.329682	-0.698931	0.258171
9	6	0	-2.714949	-0.689144	0.243888
10	6	0	-3.427800	-1.897359	0.094833
11	6	0	-2.705328	-3.097827	-0.051966
12	6	0	-1.312728	-3.113422	-0.041020
13	6	0	-0.368310	0.479905	0.412923
14	6	0	-0.533646	1.517570	-0.736449
15	6	0	-0.376574	0.973936	-2.159763
16	6	0	-0.572997	1.219708	1.767306
17	6	0	-0.440730	0.361244	3.028896
18	6	0	4.766291	0.018599	0.415843
19	6	0	-4.910670	-1.869969	0.088049
20	7	0	5.758724	-0.778164	-0.032898
21	6	0	7.012442	-0.338158	0.012712
22	6	0	7.379894	0.924491	0.503770
23	6	0	6.353324	1.749986	0.987811
24	6	0	5.046414	1.293439	0.947954
25	6	0	-5.693088	-3.032480	0.242078
26	6	0	-7.074494	-2.940646	0.214511
27	6	0	-7.672515	-1.682582	0.043091
28	6	0	-6.817772	-0.576248	-0.080980
29	7	0	-5.491134	-0.660731	-0.061403
30	6	0	8.760219	1.373721	0.528095
31	6	0	-9.118006	-1.553437	0.006733
32	7	0	9.234773	2.503362	0.969040
33	7	0	10.607585	2.462647	0.776155
34	6	0	10.877132	1.309375	0.229778
35	8	0	9.746877	0.560619	0.041670
36	7	0	-10.014710	-2.493227	0.098566
37	7	0	-11.252592	-1.874522	0.010560
38	6	0	-11.026472	-0.597655	-0.129738
39	8	0	-9.686467	-0.317886	-0.140848
40	6	0	12.166330	0.774276	-0.174044
41	6	0	-11.986406	0.484676	-0.265582
42	6	0	12.283935	-0.496678	-0.766080
43	6	0	13.524631	-0.983814	-1.143811
44	6	0	14.680555	-0.212608	-0.939065
45	6	0	14.573709	1.056065	-0.349684
46	6	0	13.324218	1.539088	0.027013
47	6	0	-11.574972	1.824021	-0.393530
48	6	0	-12.511050	2.837504	-0.520099
49	6	0	-13.883304	2.537821	-0.522456
50	6	0	-14.303613	1.205297	-0.395787
51	6	0	-13.357853	0.192565	-0.268772
52	8	0	15.847061	-0.781687	-1.343478
53	8	0	-14.718246	3.602793	-0.652088
54	6	0	-16.120236	3.369224	-0.660834
55	6	0	17.055403	-0.055590	-1.162668
56	1	0	2.375856	1.385514	0.537279
57	1	0	1.807645	-3.530831	-0.074148
58	1	0	4.080042	-2.534917	0.057860
59	1	0	-3.280288	0.231390	0.344336
60	1	0	-3.231820	-4.034968	-0.200987
61	1	0	-0.780127	-4.052918	-0.163063
62	1	0	-1.523801	1.980677	-0.630469

63	1	0	0.196760	2.321569	-0.571024
64	1	0	-0.504316	1.781367	-2.889456
65	1	0	0.614895	0.536077	-2.315921
66	1	0	-1.123739	0.204406	-2.379567
67	1	0	0.148782	2.046987	1.812095
68	1	0	-1.567081	1.686093	1.746852
69	1	0	-0.600074	0.974527	3.922956
70	1	0	-1.179077	-0.447216	3.043402
71	1	0	0.554057	-0.090045	3.106208
72	1	0	7.773812	-1.019059	-0.361889
73	1	0	6.597506	2.727131	1.392225
74	1	0	4.251319	1.914113	1.345158
75	1	0	-5.227087	-3.998242	0.400164
76	1	0	-7.700385	-3.819678	0.330579
77	1	0	-7.233509	0.421569	-0.204283
78	1	0	11.396740	-1.099925	-0.928745
79	1	0	13.629147	-1.962244	-1.601362
80	1	0	15.451084	1.669594	-0.181693
81	1	0	13.234646	2.519697	0.483014
82	1	0	-10.517024	2.065327	-0.392703
83	1	0	-12.207196	3.874550	-0.619122
84	1	0	-15.356698	0.949781	-0.395201
85	1	0	-13.676091	-0.840185	-0.170482
86	1	0	-16.584173	4.350542	-0.771905
87	1	0	-16.415593	2.729872	-1.502533
88	1	0	-16.456973	2.911847	0.278229
89	1	0	17.847951	-0.695929	-1.553074
90	1	0	17.043538	0.889442	-1.720510
91	1	0	17.244532	0.151273	-0.101592

Table S2. B3LYP/6-31G(d) optimised geometry of compound **7a**.
E_{total} = –2669.5300258 Hartree
Dipole moment (Debye): X= –0.4242 Y= –0.9557 Z= –0.9529 Tot= 1.4147

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.316780	2.282052	0.133007
2	6	0	2.592525	3.487261	0.040944
3	6	0	1.200006	3.501035	0.041735
4	6	0	0.509276	2.290807	0.137091
5	6	0	1.224180	1.079010	0.221611
6	6	0	2.608529	1.066182	0.215167
7	6	0	-0.924383	1.995758	0.165865
8	6	0	-2.043054	2.831551	0.098325
9	6	0	-3.313985	2.268235	0.145804
10	6	0	-3.496242	0.875600	0.268623
11	6	0	-2.361775	0.042662	0.326422
12	6	0	-1.095147	0.602412	0.275246
13	6	0	0.631821	-1.560162	3.886728
14	6	0	0.888710	-2.889996	3.535182
15	6	0	0.935846	-3.275426	2.193634
16	6	0	0.722479	-2.310878	1.206651
17	6	0	0.463935	-0.974019	1.564268
18	6	0	0.417161	-0.592126	2.899530
19	6	0	0.710555	-2.416475	-0.259065
20	6	0	0.909882	-3.513079	-1.100259
21	6	0	0.839801	-3.324560	-2.482197
22	6	0	0.574534	-2.058899	-3.016684
23	6	0	0.374545	-0.958741	-2.175755
24	6	0	0.444142	-1.144580	-0.800472
25	6	0	0.261086	-0.109788	0.315036
26	6	0	4.799906	2.260650	0.138017
27	6	0	-4.871830	0.324475	0.327728
28	6	0	-5.143722	-0.976950	0.795242
29	6	0	-6.448994	-1.439410	0.818781
30	6	0	-7.480808	-0.594094	0.382306

31	6	0	-7.120443	0.692593	-0.047544
32	7	0	-5.868459	1.139266	-0.076451
33	7	0	5.385978	1.070848	-0.108223
34	6	0	6.713013	0.992908	-0.120560
35	6	0	7.561314	2.087760	0.107812
36	6	0	6.956478	3.324433	0.380367
37	6	0	5.574206	3.408809	0.400193
38	6	0	-8.859787	-1.048244	0.393275
39	7	0	-9.328993	-2.197385	0.786978
40	7	0	-10.702913	-2.152195	0.603463
41	6	0	-10.978506	-0.976896	0.109650
42	8	0	-9.851342	-0.217371	-0.051709
43	6	0	9.007716	1.965962	0.078291
44	7	0	9.900561	2.893144	0.275487
45	7	0	11.141252	2.287739	0.143648
46	6	0	10.920298	1.030776	-0.125597
47	8	0	9.581471	0.752034	-0.183210
48	6	0	-12.271555	-0.428742	-0.263310
49	6	0	11.884284	-0.032082	-0.354828
50	6	0	-12.395839	0.863833	-0.804900
51	6	0	-13.640187	1.362690	-1.154418
52	6	0	-14.793202	0.581837	-0.971039
53	6	0	-14.679693	-0.708408	-0.431935
54	6	0	-13.426590	-1.203097	-0.083449
55	6	0	11.476777	-1.349115	-0.635969
56	6	0	12.416241	-2.344611	-0.850071
57	6	0	14.204265	-0.738604	-0.508784
58	6	0	13.255169	0.256269	-0.294964
59	8	0	-15.963832	1.163562	-1.344595
60	6	0	13.787933	-2.048857	-0.788405
61	8	0	14.626590	-3.095092	-1.012899
62	6	0	16.028166	-2.864272	-0.964186
63	6	0	-17.169302	0.428475	-1.182092
64	1	0	3.119803	4.430659	-0.058416
65	1	0	0.665811	4.444038	-0.038462
66	1	0	3.168018	0.139137	0.272688
67	1	0	-1.929241	3.908982	0.010660
68	1	0	-4.196281	2.895300	0.089157
69	1	0	-2.466699	-1.036229	0.386254
70	1	0	0.599021	-1.276131	4.935053
71	1	0	1.053716	-3.630153	4.313631
72	1	0	1.136581	-4.309803	1.926469
73	1	0	0.217855	0.440251	3.174754
74	1	0	1.116910	-4.498363	-0.690320
75	1	0	0.993229	-4.168956	-3.148869
76	1	0	0.523801	-1.928336	-4.094202
77	1	0	0.169358	0.023235	-2.593795
78	1	0	-4.344083	-1.614326	1.154890
79	1	0	-6.687526	-2.436647	1.174514
80	1	0	-7.886085	1.388226	-0.384427
81	1	0	7.134081	0.010713	-0.324275
82	1	0	7.577421	4.192043	0.579403
83	1	0	5.100682	4.354778	0.637104
84	1	0	-11.510889	1.474613	-0.950868
85	1	0	-13.749723	2.357805	-1.573171
86	1	0	-15.554712	-1.329789	-0.281323
87	1	0	-13.331922	-2.200452	0.333530
88	1	0	10.419292	-1.587367	-0.685296
89	1	0	12.115472	-3.364290	-1.067749
90	1	0	15.256885	-0.486538	-0.456063
91	1	0	13.570299	1.271773	-0.078283
92	1	0	16.495352	-3.828851	-1.168895
93	1	0	16.342491	-2.139041	-1.725573
94	1	0	16.342718	-2.510487	0.025943
95	1	0	-17.966120	1.081267	-1.542003
96	1	0	-17.159884	-0.494886	-1.775196
97	1	0	-17.349792	0.181285	-0.128150

Table S3. B3LYP/6-31G(d) optimised geometry of compound **6a-iso**.
E_{total} = –2365.869631 Hartree
Dipole moment (Debye): X= 0.4132 Y= 1.0338 Z= -1.3336 Tot= 1.7372

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.425874	-0.864894	0.305306
2	6	0	2.334215	-0.087879	0.745310
3	6	0	1.035564	-0.512561	0.505474
4	6	0	0.797159	-1.721497	-0.179902
5	6	0	1.867050	-2.502750	-0.620957
6	6	0	3.168745	-2.071004	-0.375358
7	6	0	-0.650544	-1.914840	-0.291991
8	6	0	-1.296901	-0.820525	0.318001
9	6	0	-2.682357	-0.756772	0.356064
10	6	0	-3.453549	-1.788222	-0.218785
11	6	0	-2.790596	-2.873635	-0.824107
12	6	0	-1.399983	-2.944603	-0.864710
13	6	0	-0.278938	0.171005	0.881731
14	6	0	-0.413587	1.576984	0.225455
15	6	0	-0.292731	1.621758	-1.300834
16	6	0	-0.424553	0.340001	2.423018
17	6	0	-0.325164	-0.944062	3.251965
18	6	0	4.815106	-0.421311	0.554191
19	6	0	-4.931647	-1.732039	-0.190215
20	6	0	5.836010	-0.639574	-0.390477
21	7	0	7.107282	-0.275580	-0.232472
22	6	0	7.437375	0.353258	0.907554
23	6	0	6.506881	0.640760	1.917347
24	6	0	5.190135	0.245237	1.733178
25	6	0	-5.723370	-2.882318	-0.031155
26	6	0	-7.106118	-2.775291	-0.015648
27	6	0	-7.678645	-1.502070	-0.155540
28	7	0	-6.948407	-0.385811	-0.312629
29	6	0	-5.622789	-0.513687	-0.331108
30	6	0	8.834039	0.746020	1.082017
31	6	0	-9.133034	-1.361712	-0.134592
32	7	0	9.366248	1.368105	2.095572
33	7	0	10.712883	1.516883	1.808540
34	6	0	10.905045	0.972395	0.636260
35	8	0	9.751628	0.462323	0.116029
36	7	0	-10.021612	-2.305771	-0.005248
37	7	0	-11.262440	-1.692558	-0.045538
38	6	0	-11.040060	-0.413826	-0.197314
39	8	0	-9.706522	-0.132496	-0.261179
40	6	0	12.140087	0.858936	-0.120951
41	6	0	-12.004213	0.668578	-0.298900
42	6	0	12.170865	0.234190	-1.381468
43	6	0	13.359778	0.134227	-2.085550
44	6	0	14.547664	0.656224	-1.547609
45	6	0	14.526615	1.281414	-0.291963
46	6	0	13.328835	1.378449	0.410213
47	6	0	-11.592252	2.005548	-0.449992
48	6	0	-12.529484	3.021444	-0.544535
49	6	0	-13.901750	2.726538	-0.490854
50	6	0	-14.321890	1.396529	-0.340530
51	6	0	-13.375211	0.380819	-0.245947
52	8	0	15.658365	0.505868	-2.317912
53	8	0	-14.737910	3.794272	-0.593050
54	6	0	-16.139465	3.565313	-0.544833
55	6	0	16.894811	1.009885	-1.831847
56	1	0	2.519508	0.858012	1.248418
57	1	0	1.696880	-3.441606	-1.141464
58	1	0	4.002464	-2.691443	-0.690530
59	1	0	-3.181965	0.071334	0.852206
60	1	0	-3.376583	-3.658713	-1.293514
61	1	0	-0.913600	-3.789728	-1.344846
62	1	0	-1.382993	1.996051	0.527468
63	1	0	0.349426	2.230056	0.670373

64	1	0	-0.404078	2.651241	-1.658915
65	1	0	0.682393	1.254919	-1.637696
66	1	0	-1.065855	1.014947	-1.783717
67	1	0	0.343566	1.050881	2.756847
68	1	0	-1.390253	0.825835	2.618069
69	1	0	-0.442383	-0.717200	4.317472
70	1	0	-1.105058	-1.661217	2.975561
71	1	0	0.644974	-1.434509	3.119408
72	1	0	5.599563	-1.119976	-1.338140
73	1	0	6.831135	1.149131	2.818758
74	1	0	4.454999	0.429167	2.511440
75	1	0	-5.252935	-3.852113	0.103173
76	1	0	-7.745907	-3.641511	0.112453
77	1	0	-5.064433	0.407215	-0.489416
78	1	0	11.256773	-0.171357	-1.802762
79	1	0	13.398668	-0.345013	-3.058413
80	1	0	15.430492	1.691560	0.142940
81	1	0	13.305077	1.860196	1.382319
82	1	0	-10.533627	2.240173	-0.492557
83	1	0	-12.226523	4.056948	-0.661154
84	1	0	-15.375098	1.145187	-0.296731
85	1	0	-13.692738	-0.650342	-0.129853
86	1	0	-16.604731	4.547418	-0.643316
87	1	0	-16.470239	2.921907	-1.370202
88	1	0	-16.440371	3.114504	0.409528
89	1	0	17.633018	0.779217	-2.601631
90	1	0	16.854668	2.096234	-1.680752
91	1	0	17.185471	0.523354	-0.891976

Table S4. B3LYP/6-31G(d) optimised geometry of compound **7a-iso**.
E(RB+HF-LYP) = –2669.5231617 Hartree
Dipole moment (Debye): X= 0.4313 Y= 0.8057 Z= -1.5820 Tot= 1.8270

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.373431	-2.179870	-0.026913
2	6	0	-2.711019	-3.367683	-0.396103
3	6	0	-1.320680	-3.448648	-0.422252
4	6	0	-0.568631	-2.324109	-0.074570
5	6	0	-1.219207	-1.131737	0.296963
6	6	0	-2.602896	-1.053562	0.323519
7	6	0	0.879704	-2.108640	-0.009505
8	6	0	1.953458	-2.959290	-0.281591
9	6	0	3.252936	-2.479489	-0.132734
10	6	0	3.505914	-1.157063	0.283797
11	6	0	2.413494	-0.309609	0.554345
12	6	0	1.120120	-0.785472	0.408499
13	6	0	-0.457032	0.554063	4.459769
14	6	0	-0.658101	1.938600	4.431075
15	6	0	-0.705056	2.626347	3.216451
16	6	0	-0.547828	1.909056	2.028679
17	6	0	-0.345550	0.516194	2.061695
18	6	0	-0.299107	-0.166818	3.270961
19	6	0	-0.550829	2.351278	0.627079
20	6	0	-0.714402	3.619698	0.066452
21	6	0	-0.674593	3.753267	-1.323122
22	6	0	-0.474112	2.636309	-2.141816
23	6	0	-0.309733	1.364375	-1.582442
24	6	0	-0.349297	1.229936	-0.199957
25	6	0	-0.199006	-0.042089	0.641787
26	6	0	-4.851639	-2.116480	-0.011872
27	6	0	4.893297	-0.666839	0.439404
28	6	0	5.260437	0.226591	1.460206
29	6	0	6.575165	0.656252	1.564219
30	6	0	7.510483	0.173850	0.636417
31	7	0	7.187645	-0.674721	-0.353331

32	6	0	5.918200	-1.068938	-0.437659
33	6	0	-5.538626	-0.952640	-0.406122
34	7	0	-6.863914	-0.820737	-0.415861
35	6	0	-7.597158	-1.876617	-0.026855
36	6	0	-7.028595	-3.093702	0.377575
37	6	0	-5.645960	-3.205669	0.384697
38	6	0	8.904596	0.601416	0.732804
39	7	0	9.430111	1.410161	1.608739
40	7	0	10.775962	1.511746	1.299352
41	6	0	10.974773	0.754541	0.253090
42	8	0	9.826492	0.144886	-0.160429
43	6	0	-9.050973	-1.728214	-0.033791
44	7	0	-9.944019	-2.612669	0.309305
45	7	0	-11.181810	-2.016275	0.135758
46	6	0	-10.952940	-0.806613	-0.302400
47	8	0	-9.618408	-0.556015	-0.433323
48	6	0	12.212693	0.512084	-0.468307
49	6	0	-11.910757	0.231446	-0.644027
50	6	0	12.254214	-0.336800	-1.589746
51	6	0	13.446150	-0.551527	-2.262543
52	6	0	14.626248	0.076435	-1.831323
53	6	0	14.594656	0.923926	-0.713874
54	6	0	13.394013	1.135444	-0.042670
55	6	0	-11.490867	1.489643	-1.113840
56	6	0	-12.421640	2.464118	-1.435287
57	6	0	-14.223188	0.954671	-0.826671
58	6	0	-13.282926	-0.020011	-0.505782
59	8	0	15.740554	-0.200325	-2.560337
60	6	0	-13.795123	2.205794	-1.294974
61	8	0	-14.624096	3.228009	-1.638065
62	6	0	-16.026701	3.032912	-1.521920
63	6	0	16.968520	0.403962	-2.178447
64	1	0	-3.298103	-4.231612	-0.694235
65	1	0	-0.835736	-4.374764	-0.719486
66	1	0	-3.092513	-0.136465	0.638289
67	1	0	1.786533	-3.986237	-0.595729
68	1	0	4.089285	-3.148025	-0.314314
69	1	0	2.586345	0.720969	0.851579
70	1	0	-0.423823	0.033609	5.412988
71	1	0	-0.779499	2.484071	5.363036
72	1	0	-0.862104	3.701778	3.200363
73	1	0	-0.143690	-1.242254	3.295708
74	1	0	-0.870719	4.490931	0.697308
75	1	0	-0.800665	4.734395	-1.772908
76	1	0	-0.445632	2.756973	-3.221247
77	1	0	-0.154252	0.498463	-2.220629
78	1	0	4.521076	0.562311	2.181647
79	1	0	6.894193	1.338479	2.344504
80	1	0	5.687022	-1.733527	-1.268083
81	1	0	-4.977543	-0.086928	-0.753039
82	1	0	-7.670728	-3.911760	0.685080
83	1	0	-5.178249	-4.127166	0.719479
84	1	0	11.346117	-0.824851	-1.928504
85	1	0	13.493234	-1.203107	-3.129083
86	1	0	15.492455	1.418879	-0.362576
87	1	0	13.361802	1.789858	0.822381
88	1	0	-10.431282	1.695940	-1.224646
89	1	0	-12.112638	3.438654	-1.799241
90	1	0	-15.277495	0.732790	-0.710099
91	1	0	-13.606584	-0.990308	-0.143288
92	1	0	-16.484828	3.968167	-1.847778
93	1	0	-16.373503	2.214662	-2.165968
94	1	0	-16.319701	2.827119	-0.484399
95	1	0	17.710922	0.046398	-2.893796
96	1	0	16.911176	1.498789	-2.230647
97	1	0	17.266166	0.104318	-1.165380
