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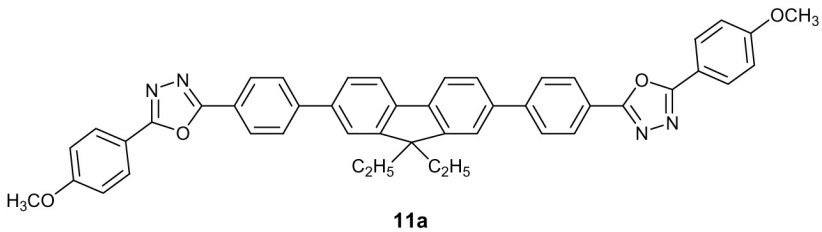
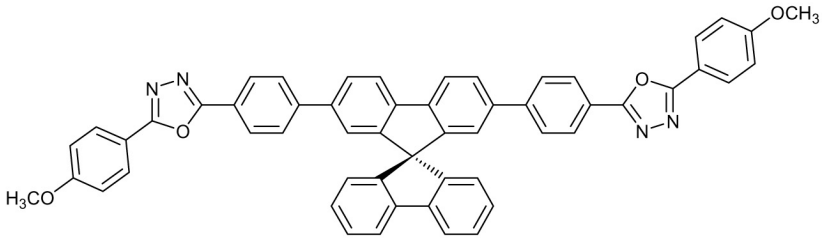
New 2,5-diaryl-1,3,4-oxadiazole–fluorene hybrids as electron transporting materials for blended-layer organic light emitting diodes

Stephen Oyston,[a] Changsheng Wang,[a] Gregory Hughes,[a] Andrei S. Batsanov,[a] Igor F. Perepichka,[a] Martin R. Bryce,*[a] Jin H. Ahn,[b] Christopher Pearson[b] and Michael C. Petty*[b]

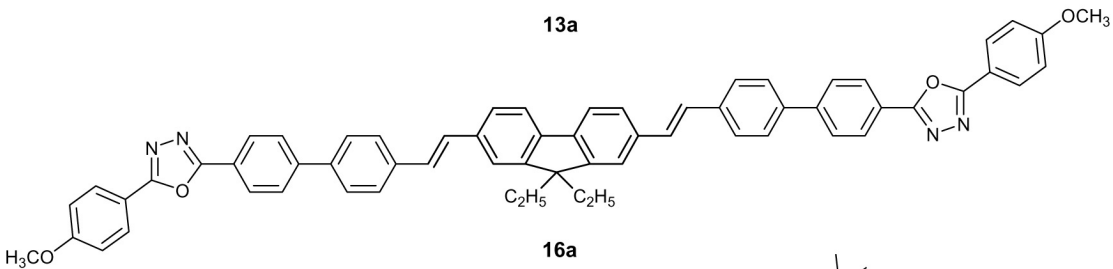
[a] *Department of Chemistry and Centre for Molecular and Nanoscale Electronics, University of Durham, Durham, UK DH1 3LE. E-mail m.r.bryce@durham.ac.uk*
[b] *School of Engineering and Centre for Molecular and Nanoscale Electronics, University of Durham, Durham, UK DH1 3LE. E-mail m.c.petty@durham.ac.uk*



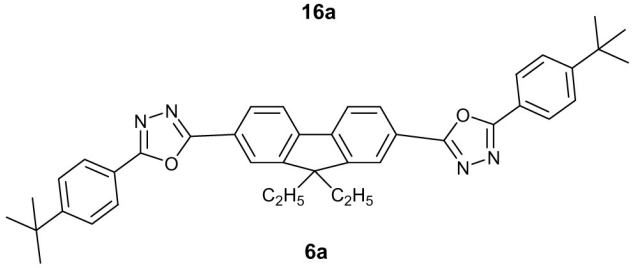
11a



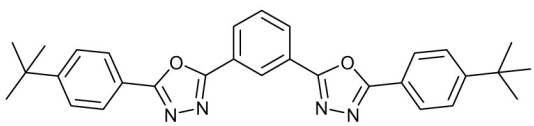
13a



16a



6a



OXD-7

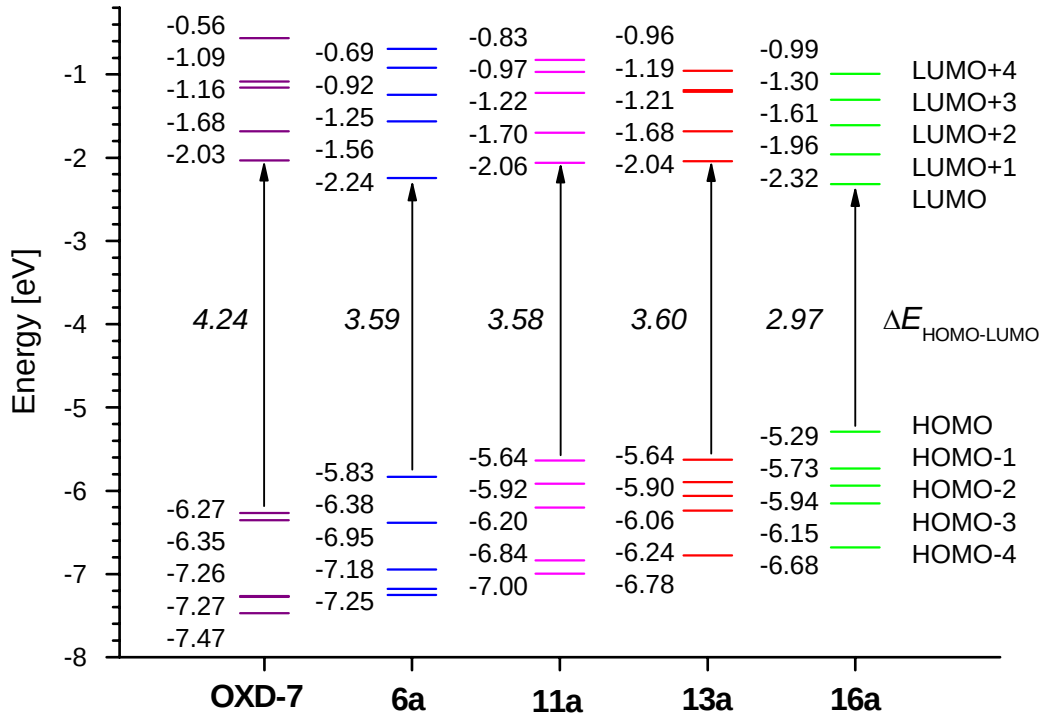


Figure S1. B3LYP/6-311G(2d,p)//B3LYP/6-31G(d) orbital energy level diagrams for compounds **OXD-7**, **6a**, **11a**, **13a** and **16a**.

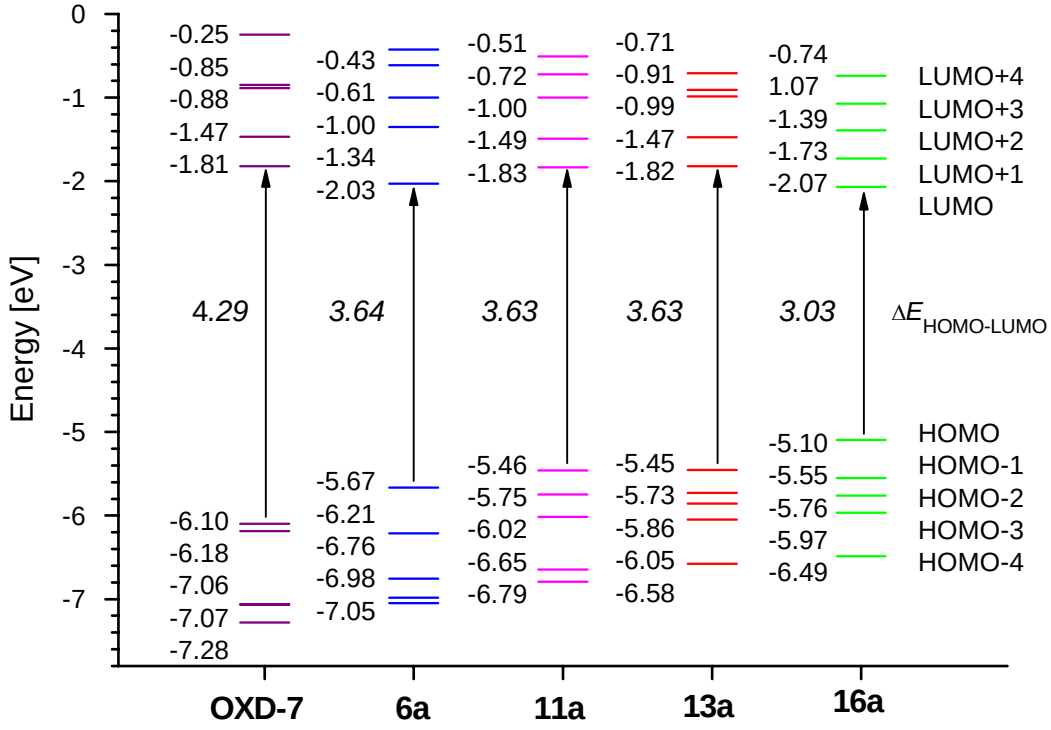


Figure S2. B3LYP/6-31G(d) orbital energy level diagrams for compounds **OXD-7**, **6a**, **11a**, **13a** and **16a**.

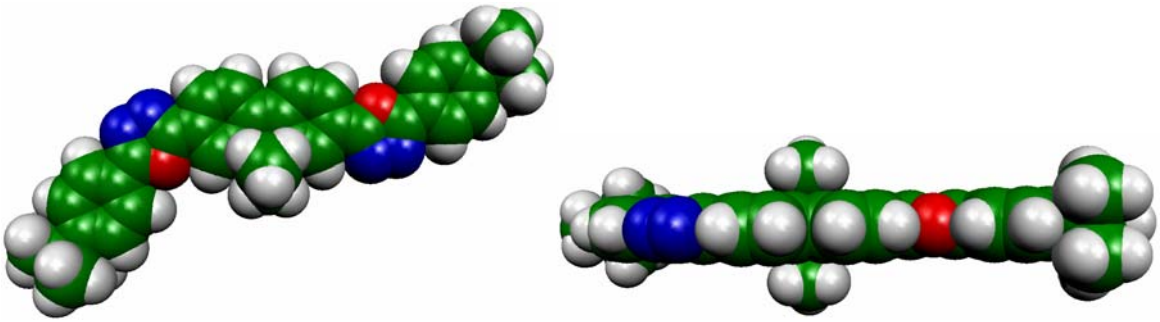


Figure S3. B3LYP/6-31G(d) optimized geometry of compound **6a**.

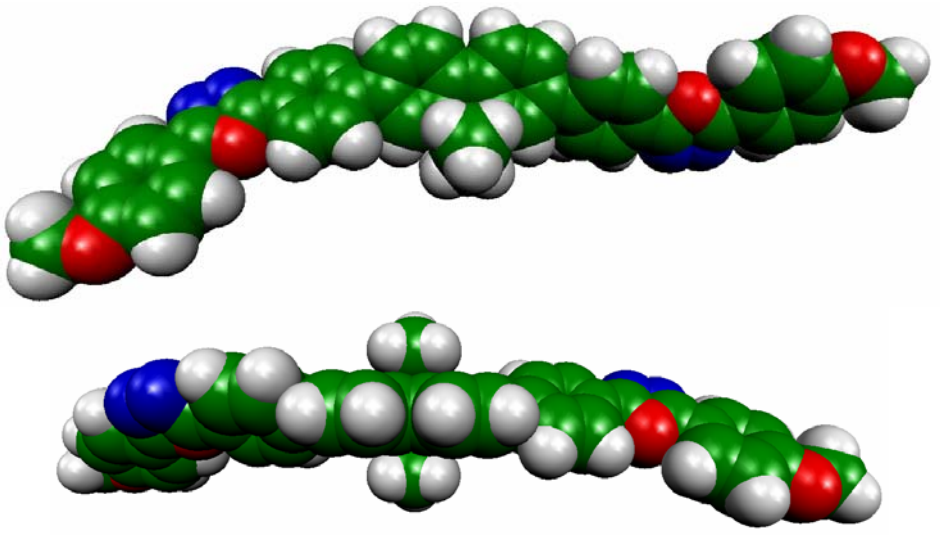


Figure S4. B3LYP/6-31G(d) optimized geometry of compound **11a**.

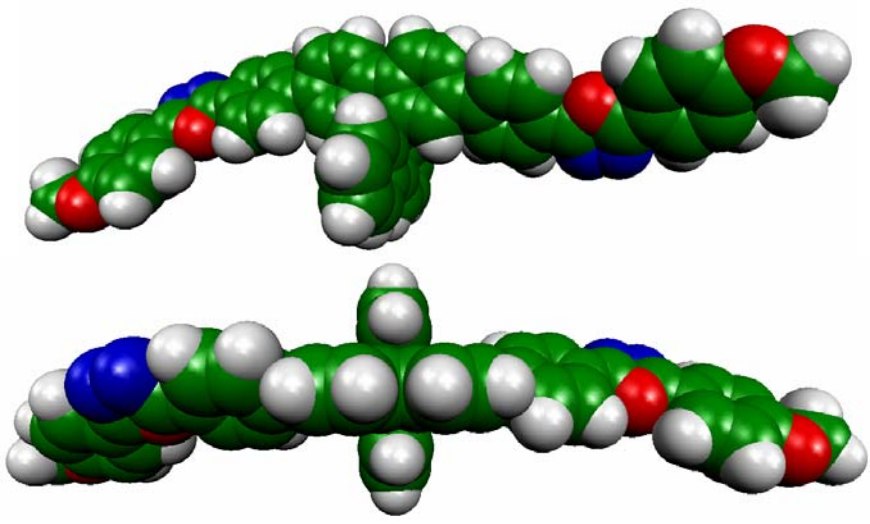


Figure S5. B3LYP/6-31G(d) optimized geometry of compound **13a**.

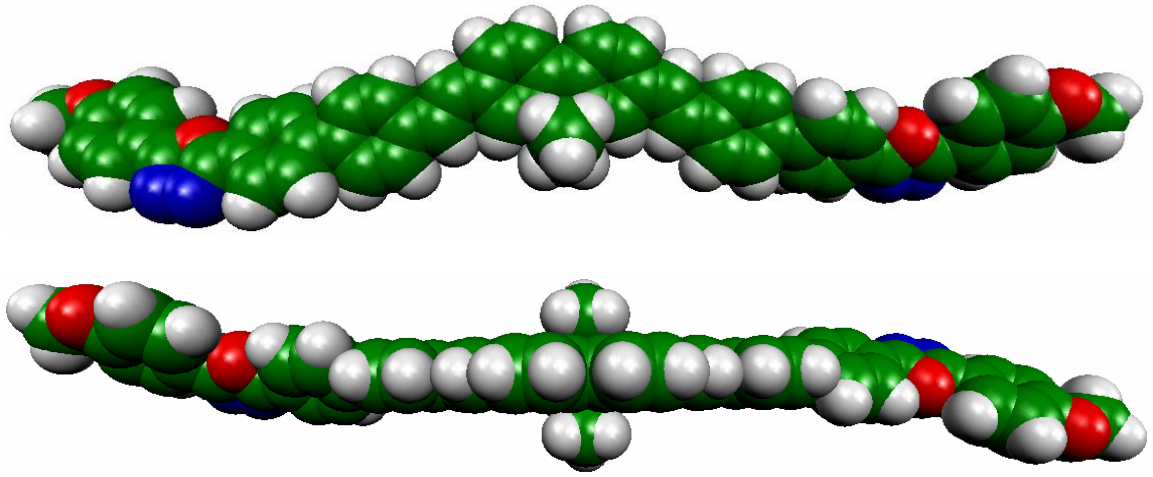


Figure S6. B3LYP/6-31G(d) optimized geometry of compound **16a**.

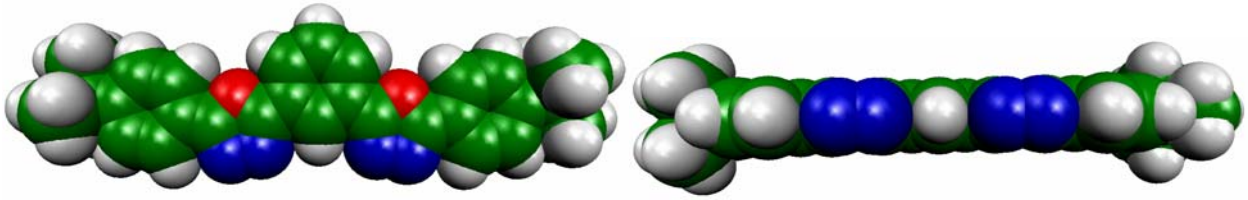
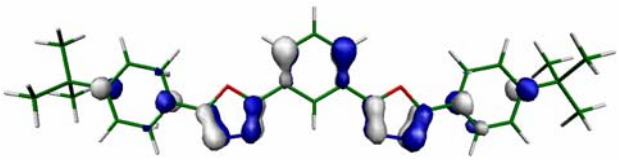
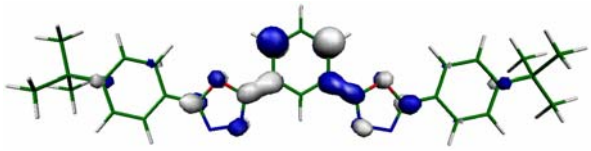


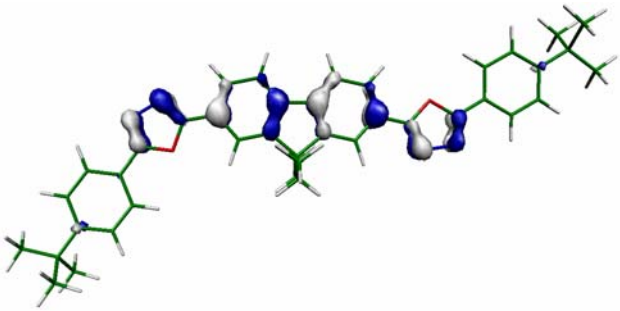
Figure S7. B3LYP/6-31G(d) optimized geometry of compound **OXD-7**.



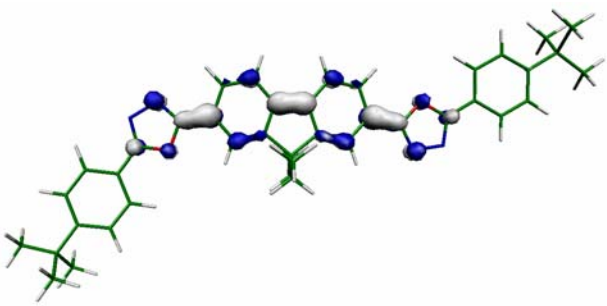
OXD-7, HOMO = –6.27 eV



OXD-7, LUMO = –2.03 eV

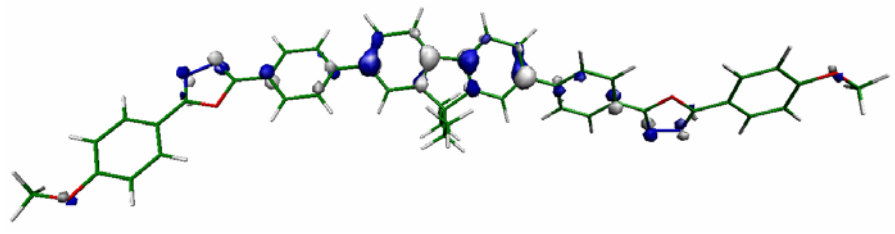


6a, HOMO = –5.83 eV

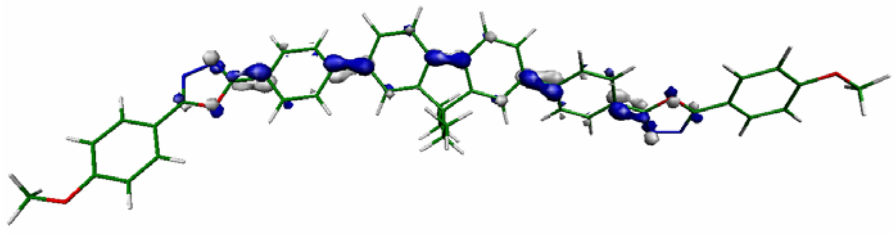


6a, LUMO = –2.34 eV

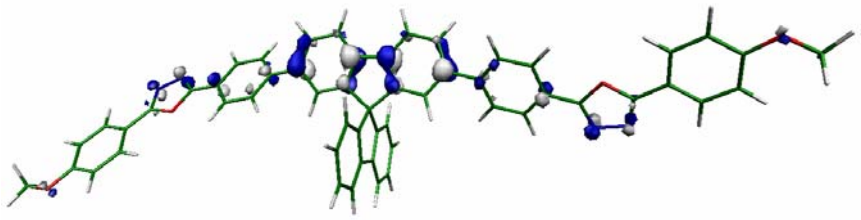
Figure S8. Frontier orbitals of compounds **OXD-7** and **6a** calculated by B3LYP/6-311G(2d,p)//B3LYP6031G(d) DFT method.



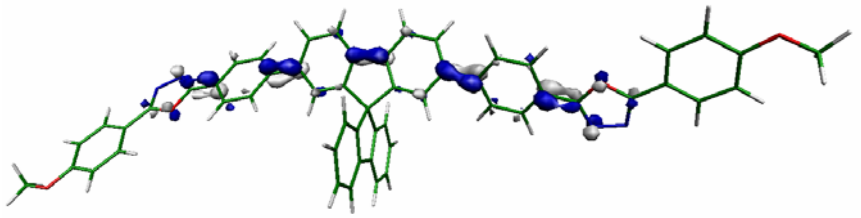
11a, HOMO = – 5.64 eV



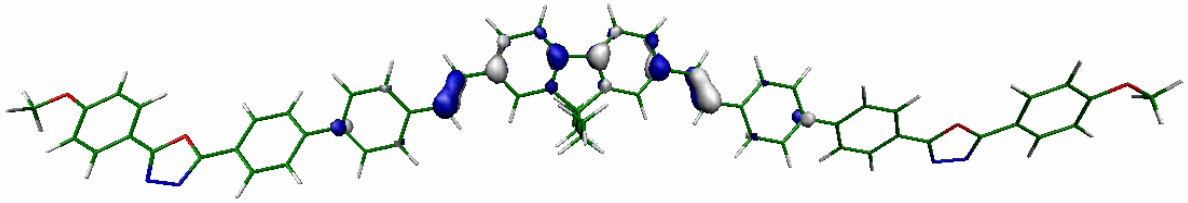
11a, LUMO = – 2.06 eV



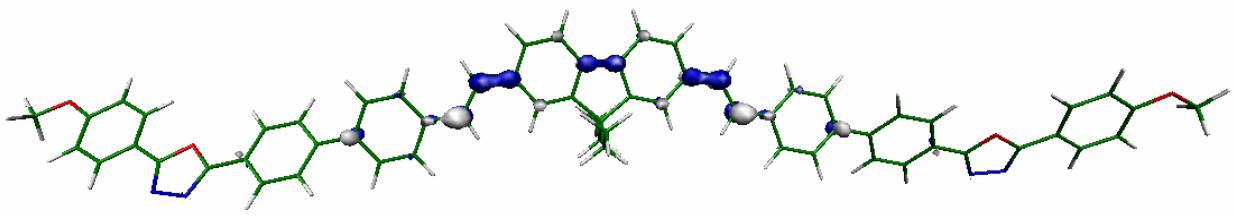
13a, HOMO = – 5.64 eV



13a, LUMO = – 2.04 eV



16a, HOMO = –5.29 eV



16a, LUMO = –2.32 eV

Figure S9. Frontier orbitals of compounds **11a**, **13a** and **16a** calculated by B3LYP/6-311G(2d,p)//B3LYP6031G(d) DFT method.

Table S1. B3LYP/6-31G(d) optimised geometry of compound **6a**.
E(RB+HF-LYP) = –1957.1475651 Hartree
Dipole moment (Debye): X= 1.2814 Y= -0.7816 Z= -0.0001 Tot= 1.5010

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.341225	1.974013	-0.000082
2	6	0	-2.778116	0.683572	-0.000045
3	6	0	-1.398018	0.546300	-0.000051
4	6	0	-0.569230	1.687797	-0.000098
5	6	0	-1.125867	2.971307	-0.000139
6	6	0	-2.508907	3.110208	-0.000130
7	6	0	0.826813	1.247609	-0.000086
8	6	0	0.850425	-0.164609	-0.000029
9	6	0	2.056040	-0.845199	-0.000001
10	6	0	3.260029	-0.111740	-0.000029
11	6	0	3.231534	1.294285	-0.000088
12	6	0	2.018051	1.977531	-0.000116
13	6	0	-0.566482	-0.735616	-0.000003
14	6	0	-0.839800	-1.607751	-1.261388
15	6	0	-0.628863	-0.919959	-2.613648
16	6	0	-0.839794	-1.607650	1.261453
17	6	0	-0.628856	-0.919748	2.613657
18	6	0	-4.784148	2.162201	-0.000060
19	6	0	4.521697	-0.836526	0.000007
20	7	0	-5.458250	3.277796	-0.000026
21	7	0	-6.801061	2.934702	-0.000001
22	6	0	-6.857416	1.632601	-0.000025
23	8	0	-5.609720	1.071132	-0.000061
24	7	0	4.715259	-2.125571	0.000067
25	7	0	6.086962	-2.324871	0.000085
26	6	0	6.639108	-1.144288	0.000035
27	8	0	5.702807	-0.146559	-0.000019
28	6	0	-8.033136	0.774906	-0.000009
29	6	0	8.054036	-0.803769	0.000034
30	6	0	-7.923779	-0.623998	-0.000132
31	6	0	-9.067194	-1.413972	-0.000113
32	6	0	-10.357173	-0.853849	0.000032
33	6	0	-10.446004	0.547114	0.000153
34	6	0	-9.310334	1.352190	0.000132
35	6	0	8.489818	0.530067	-0.000028
36	6	0	9.848957	0.820697	-0.000023
37	6	0	10.825015	-0.191881	0.000042
38	6	0	10.369388	-1.519564	0.000100
39	6	0	9.011717	-1.827062	0.000097
40	6	0	-11.593107	-1.770219	0.000055
41	6	0	12.318319	0.179589	0.000043
42	6	0	12.638936	1.015317	1.262710
43	6	0	13.231384	-1.061027	0.000074
44	6	0	12.638944	1.015266	-1.262656
45	6	0	-11.568502	-2.665221	1.262538
46	6	0	-12.912637	-0.975302	0.000243
47	6	0	-11.568720	-2.664991	-1.262595
48	1	0	-3.429178	-0.185356	-0.000007
49	1	0	-0.492760	3.854438	-0.000175
50	1	0	-2.968819	4.092730	-0.000157
51	1	0	2.103677	-1.929980	0.000045
52	1	0	4.165527	1.846297	-0.000110
53	1	0	2.007811	3.064090	-0.000160
54	1	0	-0.196933	-2.496004	-1.199751
55	1	0	-1.872758	-1.975956	-1.196779

56	1	0	-0.841651	-1.618943	-3.430060
57	1	0	-1.290428	-0.055616	-2.733654
58	1	0	0.403256	-0.574169	-2.732319
59	1	0	-1.872750	-1.975864	1.196877
60	1	0	-0.196924	-2.495906	1.199887
61	1	0	-0.841633	-1.618668	3.430126
62	1	0	0.403260	-0.573938	2.732294
63	1	0	-1.290430	-0.055401	2.733597
64	1	0	-6.943232	-1.089279	-0.000245
65	1	0	-8.947130	-2.493484	-0.000212
66	1	0	-11.415619	1.031676	0.000268
67	1	0	-9.401233	2.433587	0.000227
68	1	0	7.762889	1.336022	-0.000078
69	1	0	10.152743	1.863562	-0.000074
70	1	0	11.078564	-2.339181	0.000152
71	1	0	8.680619	-2.860540	0.000144
72	1	0	13.699364	1.295046	1.273543
73	1	0	12.051041	1.938163	1.302300
74	1	0	12.428523	0.445112	2.174624
75	1	0	14.280544	-0.745462	0.000097
76	1	0	13.074059	-1.683398	0.888171
77	1	0	13.074105	-1.683411	-0.888023
78	1	0	13.699366	1.295020	-1.273479
79	1	0	12.428564	0.445013	-2.174548
80	1	0	12.051026	1.938095	-1.302299
81	1	0	-12.441316	-3.329187	1.273729
82	1	0	-10.672564	-3.293544	1.301194
83	1	0	-11.591311	-2.058201	2.174616
84	1	0	-13.759999	-1.669846	0.000242
85	1	0	-13.007297	-0.340188	0.888317
86	1	0	-13.007442	-0.340011	-0.887689
87	1	0	-12.441530	-3.328965	-1.273749
88	1	0	-11.591700	-2.057806	-2.174559
89	1	0	-10.672783	-3.293296	-1.301525

Table S2. B3LYP/6-31G(d) optimised geometry of compound **11a**.
E(RB+HF-LYP) = –2333.7994071 Hartree
Dipole moment (Debye): X= 0.8701 Y= 2.1239 Z= -2.8745 Tot= 3.6784

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.448829	-0.913622	0.196578
2	6	0	2.383766	-0.092332	0.621368
3	6	0	1.070738	-0.492765	0.420192
4	6	0	0.788805	-1.722269	-0.209339
5	6	0	1.831418	-2.548623	-0.633350
6	6	0	3.147326	-2.139636	-0.427975
7	6	0	-0.665080	-1.880737	-0.291489
8	6	0	-1.272662	-0.744616	0.280843
9	6	0	-2.655158	-0.640012	0.332719
10	6	0	-3.464622	-1.671330	-0.187128
11	6	0	-2.839439	-2.799257	-0.753629
12	6	0	-1.451801	-2.911100	-0.810249
13	6	0	-0.219204	0.239550	0.790376
14	6	0	-0.327180	1.623432	0.085115
15	6	0	-0.231994	1.607880	-1.443660
16	6	0	-0.334003	0.468474	2.326550
17	6	0	-0.254917	-0.787654	3.199416
18	6	0	4.856044	-0.495683	0.401932
19	6	0	-4.942801	-1.569879	-0.142937
20	6	0	5.848693	-0.792781	-0.548914
21	6	0	7.169751	-0.403153	-0.360632
22	6	0	7.541349	0.304447	0.792629
23	6	0	6.560131	0.609935	1.750735
24	6	0	5.244342	0.214163	1.554568
25	6	0	-5.744348	-2.705706	0.082507
26	6	0	-7.128848	-2.617058	0.118611
27	6	0	-7.763974	-1.377929	-0.069774
28	6	0	-6.978471	-0.236752	-0.291957
29	6	0	-5.592177	-0.336380	-0.327730
30	6	0	8.915693	0.725751	1.016373
31	6	0	-9.216628	-1.307732	-0.034075
32	7	0	9.408865	1.389578	2.022658
33	7	0	10.765036	1.544263	1.775520
34	6	0	11.007768	0.963622	0.633637
35	8	0	9.876238	0.419502	0.090386
36	7	0	-10.071713	-2.274556	0.140650
37	7	0	-11.335878	-1.706417	0.090478
38	6	0	-11.166637	-0.429682	-0.112799
39	8	0	-9.841505	-0.101264	-0.202101
40	6	0	12.272268	0.841203	-0.072763
41	6	0	-12.174856	0.608825	-0.246282
42	6	0	12.364891	0.173385	-1.307499
43	6	0	13.582506	0.067374	-1.960239
44	6	0	14.739835	0.626966	-1.394831
45	6	0	14.658051	1.295601	-0.164390
46	6	0	13.431630	1.398067	0.485502
47	6	0	-11.824860	1.957096	-0.443122
48	6	0	-12.806218	2.927477	-0.567461
49	6	0	-14.163758	2.574463	-0.498308
50	6	0	-14.523144	1.232816	-0.301738
51	6	0	-13.532113	0.263762	-0.177718
52	8	0	15.883124	0.466948	-2.114065
53	8	0	-15.046952	3.600067	-0.632670
54	6	0	-16.436837	3.310418	-0.571734
55	6	0	17.090920	1.008731	-1.597282

56	1	0	2.601176	0.868305	1.081693
57	1	0	1.628771	-3.504283	-1.110068
58	1	0	3.959870	-2.793688	-0.730597
59	1	0	-3.124767	0.222739	0.798548
60	1	0	-3.453574	-3.585904	-1.182127
61	1	0	-0.996518	-3.788686	-1.262047
62	1	0	-1.279364	2.080545	0.387189
63	1	0	0.461292	2.271014	0.492152
64	1	0	-0.318822	2.626096	-1.839236
65	1	0	0.725855	1.199044	-1.781716
66	1	0	-1.030848	1.006362	-1.890032
67	1	0	0.458990	1.169117	2.621646
68	1	0	-1.283065	0.987172	2.519142
69	1	0	-0.349355	-0.520431	4.257869
70	1	0	-1.057310	-1.493010	2.959686
71	1	0	0.700151	-1.307394	3.069698
72	1	0	5.575682	-1.313408	-1.462003
73	1	0	7.915864	-0.637177	-1.113104
74	1	0	6.849079	1.148523	2.647304
75	1	0	4.506061	0.434017	2.320018
76	1	0	-5.270720	-3.667051	0.257904
77	1	0	-7.735936	-3.497738	0.300822
78	1	0	-7.456989	0.724652	-0.448249
79	1	0	-5.002533	0.552705	-0.530964
80	1	0	11.476079	-0.262427	-1.751953
81	1	0	13.667391	-0.445531	-2.912814
82	1	0	15.537324	1.735444	0.291415
83	1	0	13.361389	1.913387	1.437886
84	1	0	-10.778522	2.239519	-0.497540
85	1	0	-12.549518	3.970852	-0.719609
86	1	0	-15.563863	0.936053	-0.244821
87	1	0	-13.803053	-0.775941	-0.025783
88	1	0	-16.945776	4.266820	-0.701931
89	1	0	-16.740071	2.625119	-1.373564
90	1	0	-16.715358	2.879536	0.398490
91	1	0	17.863088	0.764572	-2.328603
92	1	0	17.027317	2.098728	-1.485963
93	1	0	17.351062	0.559747	-0.630186

Table S3. B3LYP/6-31G(d) optimised geometry of compound **13a**.
E(RB+HF-LYP) = –2637.4530028 Hartree
Dipole moment (Debye): X= 0.9149 Y= 1.4455 Z= -3.2690 Tot= 3.6896

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.400831	-2.065711	-0.011190
2	6	0	-2.775928	-3.288373	-0.328439
3	6	0	-1.388655	-3.412145	-0.362197
4	6	0	-0.599742	-2.296343	-0.073713
5	6	0	-1.211960	-1.069015	0.245500
6	6	0	-2.592364	-0.948645	0.277954
7	6	0	0.854752	-2.121704	-0.028276
8	6	0	1.901588	-3.014950	-0.267020
9	6	0	3.215388	-2.566264	-0.149647
10	6	0	3.512383	-1.234902	0.204283
11	6	0	2.446318	-0.345190	0.442603
12	6	0	1.138383	-0.788760	0.326025
13	6	0	-0.367868	0.795480	4.315942
14	6	0	-0.527157	2.182449	4.220540
15	6	0	-0.562353	2.810778	2.973778
16	6	0	-0.436013	2.031500	1.821874
17	6	0	-0.275851	0.636381	1.921850
18	6	0	-0.240917	0.012709	3.163177
19	6	0	-0.435114	2.404416	0.400336
20	6	0	-0.561696	3.648566	-0.221036
21	6	0	-0.525560	3.712870	-1.615666
22	6	0	-0.365691	2.551317	-2.379456
23	6	0	-0.238817	1.303604	-1.759046
24	6	0	-0.273921	1.237979	-0.371433
25	6	0	-0.156620	0.004722	0.530791
26	6	0	-4.879022	-1.956552	0.014691
27	6	0	4.917843	-0.779335	0.326480
28	6	0	5.296510	0.150219	1.314198
29	6	0	6.610535	0.580570	1.434047
30	6	0	7.598086	0.090730	0.562787
31	6	0	7.235373	-0.835776	-0.426523
32	6	0	5.916196	-1.260003	-0.539154
33	6	0	-5.527517	-0.787051	-0.419717
34	6	0	-6.913503	-0.680110	-0.399457
35	6	0	-7.698977	-1.748609	0.058869
36	6	0	-7.064380	-2.923074	0.497119
37	6	0	-5.680024	-3.019783	0.473884
38	6	0	8.969908	0.553548	0.705891
39	7	0	9.455157	1.400926	1.567874
40	7	0	10.811441	1.513109	1.300733
41	6	0	11.062532	0.725770	0.292242
42	8	0	9.936471	0.080680	-0.140635
43	6	0	-9.151192	-1.666775	0.089156
44	7	0	-10.007751	-2.564398	0.485609
45	7	0	-11.270614	-2.015462	0.318906
46	6	0	-11.098916	-0.818512	-0.168805
47	8	0	-9.773772	-0.526431	-0.342096
48	6	0	12.331255	0.481600	-0.373812
49	6	0	-12.103744	0.169610	-0.525004
50	6	0	12.434577	-0.399647	-1.465518
51	6	0	13.656219	-0.613359	-2.083624
52	6	0	14.806916	0.048587	-1.625486
53	6	0	14.714599	0.928965	-0.537273
54	6	0	13.484305	1.138816	0.078353
55	6	0	-11.749014	1.426120	-1.048904

56	6	0	-12.726103	2.350467	-1.381847
57	6	0	-14.448238	0.792119	-0.677408
58	6	0	-13.461328	-0.131316	-0.345428
59	8	0	15.954825	-0.230212	-2.299748
60	6	0	-14.083953	2.042317	-1.199084
61	8	0	-14.962346	3.017417	-1.556405
62	6	0	-16.352242	2.770910	-1.393493
63	6	0	17.155881	0.406266	-1.885638
64	1	0	-3.391310	-4.147271	-0.579795
65	1	0	-0.934249	-4.365454	-0.619396
66	1	0	-3.051977	-0.003259	0.551891
67	1	0	1.702365	-4.050222	-0.531556
68	1	0	4.030935	-3.266258	-0.306284
69	1	0	2.651574	0.692201	0.690832
70	1	0	-0.342830	0.321536	5.293383
71	1	0	-0.624315	2.776499	5.125281
72	1	0	-0.685503	3.888657	2.905743
73	1	0	-0.117814	-1.064414	3.239957
74	1	0	-0.685677	4.554181	0.367236
75	1	0	-0.622008	4.674571	-2.112467
76	1	0	-0.339068	2.618240	-3.463674
77	1	0	-0.114469	0.402729	-2.354171
78	1	0	4.552540	0.518997	2.014035
79	1	0	6.892990	1.290204	2.204731
80	1	0	7.986780	-1.213770	-1.112202
81	1	0	5.649177	-1.955571	-1.329253
82	1	0	-4.938184	0.040091	-0.804081
83	1	0	-7.391630	0.229222	-0.748880
84	1	0	-7.671373	-3.745528	0.861132
85	1	0	-5.206259	-3.924684	0.842754
86	1	0	11.550966	-0.915613	-1.826822
87	1	0	13.749251	-1.290216	-2.926778
88	1	0	15.588607	1.450751	-0.165438
89	1	0	13.405759	1.818463	0.920626
90	1	0	-10.702409	1.673443	-1.193593
91	1	0	-12.465744	3.323057	-1.786789
92	1	0	-15.489384	0.531295	-0.527753
93	1	0	-13.736086	-1.100363	0.058301
94	1	0	-16.856849	3.674929	-1.738233
95	1	0	-16.682845	1.916956	-1.998517
96	1	0	-16.607799	2.590695	-0.341449
97	1	0	17.933973	0.037835	-2.556113
98	1	0	17.084504	1.497739	-1.976612
99	1	0	17.413286	0.144572	-0.851290

Table S4. B3LYP/6-31G(d) optimised geometry of compound **16a**
E(RB+HF-LYP) = –2950.7243769 Hartree
Dipole moment (Debye): X= -0.0019 Y= 4.6058 Z= 0.0124 Tot= 4.6058

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.480540	1.820133	-0.198187
2	6	0	2.530897	0.773216	-0.143577
3	6	0	1.179540	1.061682	-0.068168
4	6	0	0.729424	2.401094	-0.045197
5	6	0	1.650930	3.449081	-0.099312
6	6	0	3.008404	3.149956	-0.174591
7	6	0	-0.729736	2.401046	0.038149
8	6	0	-1.179473	1.061607	0.065991
9	6	0	-2.530744	0.773034	0.142466
10	6	0	-3.480699	1.819870	0.193128
11	6	0	-3.008928	3.149734	0.164891
12	6	0	-1.651534	3.448963	0.088548
13	6	0	0.000178	0.090170	0.000752
14	6	0	4.923226	1.595937	-0.275371
15	6	0	5.566617	0.408339	-0.305620
16	6	0	-4.923336	1.595508	0.270844
17	6	0	-5.566487	0.407802	0.302012
18	6	0	-7.010362	0.188622	0.375437
19	6	0	7.010571	0.189452	-0.378467
20	6	0	-7.499080	-1.131819	0.389637
21	6	0	-8.859952	-1.406101	0.454909
22	6	0	-9.806599	-0.369255	0.507870
23	6	0	-9.321799	0.952999	0.495515
24	6	0	-7.962945	1.226299	0.432326
25	6	0	7.963135	1.227372	-0.431099
26	6	0	9.322048	0.954374	-0.494227
27	6	0	9.806942	-0.367801	-0.510595
28	6	0	8.860338	-1.404879	-0.461627
29	6	0	7.499397	-1.130905	-0.396435
30	6	0	-11.257889	-0.654401	0.573058
31	6	0	11.258305	-0.652601	-0.575693
32	6	0	11.750927	-1.765601	-1.284467
33	6	0	13.110165	-2.038275	-1.346664
34	6	0	14.031058	-1.198869	-0.697111
35	6	0	13.555305	-0.085741	0.012391
36	6	0	12.191687	0.178316	0.069654
37	6	0	-12.191809	0.178523	-0.068918
38	6	0	-13.555349	-0.085964	-0.011706
39	6	0	-14.030466	-1.201575	0.694314
40	6	0	-13.109037	-2.042960	1.340539
41	6	0	-11.749891	-1.769822	1.278449
42	6	0	-15.450968	-1.505407	0.771523
43	7	0	-16.036765	-2.500151	1.374770
44	7	0	-17.399174	-2.353003	1.161137
45	6	0	-17.552901	-1.277193	0.440683
46	8	0	-16.354429	-0.683217	0.153367
47	6	0	15.451690	-1.501990	-0.774707
48	7	0	16.038247	-2.493403	-1.382683
49	7	0	17.400452	-2.346964	-1.167247
50	6	0	17.553305	-1.274878	-0.441079
51	8	0	16.354431	-0.682783	-0.151563
52	6	0	18.784858	-0.685167	0.057341
53	6	0	-18.785040	-0.685272	-0.053648
54	6	0	20.011121	-1.295305	-0.242345
55	6	0	21.208921	-0.756255	0.217300
56	6	0	21.193987	0.413634	0.991245
57	6	0	19.969293	1.029574	1.296216
58	6	0	18.780504	0.487148	0.834964
59	6	0	-20.010714	-1.298449	0.242230

60	6	0	-21.209088	-0.757345	-0.213480
61	6	0	-21.195344	0.417753	-0.979522
62	6	0	-19.971250	1.036755	-1.280667
63	6	0	-18.781878	0.492236	-0.823398
64	8	0	22.301794	1.025664	1.489386
65	8	0	-22.303801	1.032164	-1.473259
66	6	0	-23.575492	0.462626	-1.194581
67	6	0	23.574016	0.458764	1.207768
68	6	0	-0.071126	-0.825293	-1.256402
69	6	0	-0.145531	-0.107116	-2.607209
70	6	0	0.071651	-0.820530	1.261358
71	6	0	0.146233	-0.097246	2.609427
72	1	0	2.864641	-0.260884	-0.160445
73	1	0	1.321579	4.484874	-0.082987
74	1	0	3.731718	3.960981	-0.216285
75	1	0	-2.864162	-0.261096	0.163414
76	1	0	-3.732468	3.960702	0.203650
77	1	0	-1.322469	4.484782	0.068552
78	1	0	5.514652	2.509794	-0.308942
79	1	0	4.978462	-0.507465	-0.271993
80	1	0	-5.514946	2.509281	0.303511
81	1	0	-4.978179	-0.507893	0.268216
82	1	0	-6.791862	-1.956572	0.338202
83	1	0	-9.195531	-2.439071	0.434921
84	1	0	-10.023888	1.779058	0.566015
85	1	0	-7.637696	2.262359	0.436811
86	1	0	7.637850	2.263429	-0.431979
87	1	0	10.024152	1.780704	-0.561336
88	1	0	9.195998	-2.437877	-0.444732
89	1	0	6.792196	-1.955865	-0.348197
90	1	0	11.057200	-2.409579	-1.816724
91	1	0	13.478901	-2.893557	-1.903341
92	1	0	14.255355	0.564745	0.526648
93	1	0	11.841230	1.027965	0.648102
94	1	0	-11.841847	1.030135	-0.644774
95	1	0	-14.255831	0.566080	-0.523394
96	1	0	-13.477288	-2.900169	1.894565
97	1	0	-11.055731	-2.415415	1.808171
98	1	0	20.015585	-2.199631	-0.842074
99	1	0	22.141193	-1.249926	-0.030773
100	1	0	19.979567	1.933544	1.896574
101	1	0	17.839175	0.970552	1.075285
102	1	0	-20.014264	-2.206788	0.835871
103	1	0	-22.140880	-1.253483	0.031471
104	1	0	-19.982441	1.944749	-1.874905
105	1	0	-17.841027	0.978056	-1.060705
106	1	0	-23.772225	0.428256	-0.115380
107	1	0	-23.663452	-0.548799	-1.611616
108	1	0	-24.305605	1.116120	-1.674758
109	1	0	23.771457	0.431605	0.128491
110	1	0	23.662359	-0.555320	1.618219
111	1	0	24.303415	1.109554	1.692678
112	1	0	-0.944485	-1.482418	-1.145179
113	1	0	0.807225	-1.485110	-1.242379
114	1	0	0.732572	0.525292	-2.774324
115	1	0	-1.035656	0.526819	-2.676154
116	1	0	-0.191413	-0.837668	-3.422715
117	1	0	0.944965	-1.478110	1.152520
118	1	0	-0.806732	-1.480349	1.249944
119	1	0	-0.732262	0.535117	2.774633
120	1	0	1.035916	0.537612	2.675514
121	1	0	0.193097	-0.824707	3.427636

Table S5. B3LYP/6-31G(d) optimised geometry of compound **OXD-7**
E(RB+HF-LYP) = –1530.7162 316 Hartree
Dipole moment (Debye): X= -0.0225 Y= 6.5750 Z= 0.0004 Tot= 6.5751

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.218743	1.699185	-0.000150
2	6	0	1.216608	0.294627	-0.000071
3	6	0	0.002135	-0.402037	-0.000021
4	6	0	-1.207381	0.303170	-0.000043
5	6	0	-1.199709	1.707709	-0.000123
6	6	0	0.011951	2.394882	-0.000177
7	6	0	-2.461890	-0.440973	0.000029
8	6	0	2.465782	-0.458421	-0.000042
9	8	0	-3.647698	0.239928	-0.000058
10	6	0	-4.574787	-0.766323	0.000062
11	7	0	-4.011812	-1.941813	0.000212
12	7	0	-2.641706	-1.729759	0.000165
13	7	0	2.636307	-1.748487	-0.000017
14	7	0	4.004749	-1.970559	0.000031
15	6	0	4.576328	-0.799253	-0.000029
16	8	0	3.656525	0.213798	-0.000064
17	6	0	5.996961	-0.481801	-0.000027
18	6	0	-5.993189	-0.439594	0.000038
19	6	0	-6.940626	-1.477080	0.000342
20	6	0	-8.296262	-1.181239	0.000327
21	6	0	-8.768902	0.145293	0.000012
22	6	0	-7.808634	1.166467	-0.000294
23	6	0	-6.442762	0.885795	-0.000281
24	6	0	6.454524	0.844532	-0.000075
25	6	0	7.818269	1.112523	-0.000065
26	6	0	8.777258	0.083791	-0.000008
27	6	0	8.299668	-1.236108	0.000034
28	6	0	6.937011	-1.521128	0.000028
29	6	0	-10.282492	0.419229	0.000036
30	6	0	-10.917143	-0.211273	1.263020
31	6	0	-10.607384	1.924993	-0.000397
32	6	0	-10.917361	-0.212028	-1.262458
33	6	0	10.276365	0.430869	0.000003
34	6	0	10.610344	1.261286	1.262608
35	6	0	11.169214	-0.824340	0.000007
36	6	0	10.610371	1.261289	-1.262591
37	1	0	2.161108	2.236537	-0.000189
38	1	0	-0.001698	-1.486388	0.000040
39	1	0	-2.138303	2.251614	-0.000140
40	1	0	0.015783	3.480903	-0.000237
41	1	0	-6.597515	-2.506587	0.000589
42	1	0	-9.003986	-2.005122	0.000575
43	1	0	-8.117616	2.205532	-0.000553
44	1	0	-5.725281	1.700281	-0.000520
45	1	0	5.741356	1.662749	-0.000119
46	1	0	8.139675	2.150058	-0.000103
47	1	0	8.994970	-2.067483	0.000074
48	1	0	6.588966	-2.549028	0.000066
49	1	0	-11.999260	-0.033546	1.272680
50	1	0	-10.757458	-1.293671	1.304489
51	1	0	-10.493187	0.224238	2.174966
52	1	0	-11.693771	2.066874	-0.000412
53	1	0	-10.209768	2.429843	0.887463
54	1	0	-10.209805	2.429316	-0.888573
55	1	0	-11.999472	-0.034262	-1.272050

56	1	0	-10.493536	0.222901	-2.174743
57	1	0	-10.757738	-1.294460	-1.303294
58	1	0	11.675514	1.522306	1.274421
59	1	0	10.038891	2.194513	1.301365
60	1	0	10.389147	0.695471	2.174717
61	1	0	12.223416	-0.525960	0.000015
62	1	0	11.002234	-1.444335	0.888022
63	1	0	11.002243	-1.444330	-0.888013
64	1	0	11.675539	1.522320	-1.274370
65	1	0	10.389208	0.695473	-2.174708
66	1	0	10.038914	2.194513	-1.301368