Electronic Supporting Information (ESI)

Stereo-electronic effect of perfluoropropyl group on solid state molecular packing of isomeric dibenzo [a,c]phenazine derivatives

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1. Synthesis of compound 1 and 3.

Compound 1:

A mixture of 10,13-dibromo-dibenzo[a,c] phenazine (0.125 g, 0.28 mmol), Cu powder (0.178 g, 2.8 mmol) DMSO (1 mL), HFE-7200 (1 mL) were added to pressure tube. To this, n-perfluoropropyl iodide (0.42 g, 1.42 mmol) was added and the reaction was heated to 130 °C and continued at this temperature with stirring for 24 hours. The reaction tube was cooled to room temperature, slowly release the pressure. Dichloromethane (2 x 30 mL) was added, sonicated for 15 minutes to dissolve the product and filtered the mixture. The filtrate was extracted with dichloromethane (30 mL), deionized water (3 x 30 mL) to remove any residual DMSO. Organic layer was dried over Na_2SO_4, filtered and rotovapored to get crude product. Crude product was subjected to column chromatography with eluent hexane: chloroform in 3 : 1 ratio to get yellow powder. Yellow powder was recrystallized with chloroform to get pure yellow crystalline material in a yield of 94 mg (54%) with mp 246-250 °C. Compound **1** was characterized by ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.32 (dd, J = 7.9, 1.3 Hz, 2H), 8.60 (d, J = 8.1 Hz, 2H), 8.28 (s, 2H), 7.89 (m, 2H), 7.82 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -80.04 (t, J = 9.5 Hz, 6F), -105.88 (m, 4F), -123.50 (m, 4F); EI-MS : m/z ($m^{+\cdot}$) 616.0 (calcd for C26H10F14N2 : 616.36).

Compound 3: Compound 3 was prepared in three steps.

Step1: 3,6-dibromophenanthrene-9,10-di(ethyleneglycol)ketal (1 g, 2.2 mmol) was transferred to an oven-dried pressure tube with a magnetic spin bar. Copper powder (1.4 g, 22 mmol), HFE-7200 (7 mL) and DMSO (7 mL) were then added to it followed by heptaperfluoro-iodopropane (3.2 g, 11 mmol). The reaction was carried out at 135 °C for 20 hours. After completion of reaction, the pressure tube was left for cooling down to room temperature and the pressure was slowly released.

30 mL dichloromethane was added to the pressure tube and sonicated for 5 minutes to dissolve the target product. It was then filtered through small silica pad. The filtrate was extracted with dichloromethane (50 mL) and water (2 × 200 mL) to remove the residual DMSO. The organic phase was dried over anhydrous sodium sulfate and filtered to get crude compound (b) in 89% yield. This crude product was characterized by ^{1}H and ^{19}F NMR and used for next step without further purification. ^{1}H NMR ($CDCl_3$, 400 MHZ) δ (ppm) 8.08 (s, 2H), 7.97 (d, J_1 = 8.28 Hz, 2H), 7.72 (d, J_1 = 8.28 Hz, 2H), 4.28 (bs, 4H), 3.68 (bs, 4H); ^{19}F NMR (376 MHZ, $CDCl_3$); δ -79.83 (t, J = 9.58 Hz, 6F), -111.88 (m, 4F), -125.92 (m, 4F).

Step2: The crude product from step 1 (2.5 g, 3.95 mmol) was transferred to an oven dried 500 mL round bottom flask with a magnetic spin bar. Dichloromethane (150 mL) was added to the flask followed by 25 mL of concentrated perchloric acid. The reaction mixture was stirred at 0 °C for 5 hours and then at room temperature overnight. After completion of the reaction, the resulting yellow colored reaction mixture was carefully transferred to a separatory funnel containing 200 mL of distilled water. The target compound was then extracted with dichloromethane (20 mL). The organic phase was dried over anhydrous sodium sulfate and filtered. The solvent was evaporated until some turbidity of the product was observed. It was then directly transferred to refrigerator for cooling which cause the precipitation of compound in the form of yellow crystalline material. This yellow crystalline material was then transferred to vacuum filter to remove residual solution. Recrystallization from dichloromethane afforded yellow crystals of 3,6-bisperfluoropropylphenanthrene-9,10-dione in a yield of 2.0 g (92%) with melting point of 135-137 °C. ^{1}H NMR (400 Hz, $CDCl_3$) δ (ppm) 8.42 (d, J = 8.26 Hz, 2H), 8.23 (s, 2H), 7.81 (d, J = 8.26 Hz, 2H); ^{19}F NMR (376 MHz, $CDCl_3$); δ -79.74 (t, J = 9.60 Hz, 6F), -112.71 (m, 4F), -125.80 (m, 4F).ESI-MS; m/z ($m^{+\cdot}$) 544.0 (Calculated for C20H6F14O2: 544.23).

Step3: 3,6-bisperfluoropropylphenanthrene-9,10-dione (0.1257 g, 0.23 mmol) and 1,2-phenylenediamine (0.027 g, 0.25 mmol) was transferred to an oven dried 50 mL round bottom flask with a magnetic spin bar. Glacial acetic acid (12 mL) and ethanol mixture in (1:3) ratio was added to it and the reaction was carried out at 35 °C for 10 hours. After completion of the reaction, reaction mixture was filtered through a plastic funnel to recover yellowish white solid target product. The crude product was thoroughly washed with water to remove residual acetic acid and then with 15 mL of methanol. Recrystallization from dichloromethane afforded compound 3 as yellowish white crystalline material in yield of 0.135 g (95%) with melting point 184-186 °C. ^{1}H NMR (400 Hz, $CDCl_3$) δ (ppm) 9.63 (d, J = 8.50 Hz, 2H), 8.77 (s, 2H), 8.41 (m, 2H), 8.02 (d, J = 8.50 Hz, 2H), 7.98 (m, 2H); ^{19}F NMR (376 Hz, CDCl3) δ -79.76 (t, J = 9.50 Hz, 6F), -111.52 (m, 4F), -125.85 (m, 4F); FTMS (p ESI sim MS); m/z $(M+H)^+$ 617.0679.(cald for C26H11F14N2: 617.0698).

1. ^{1}H NMR, ^{19}F NMR and Mass spectra for compounds 1 and 3

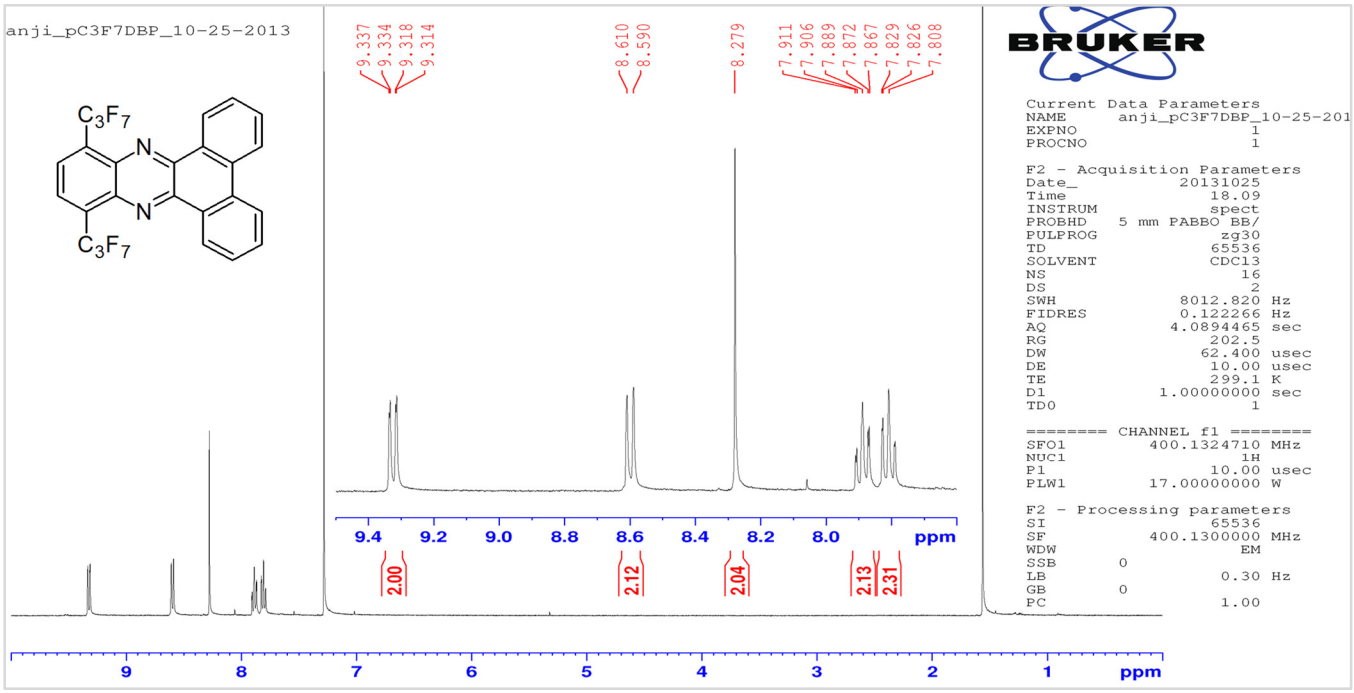


Figure S1: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **1**.

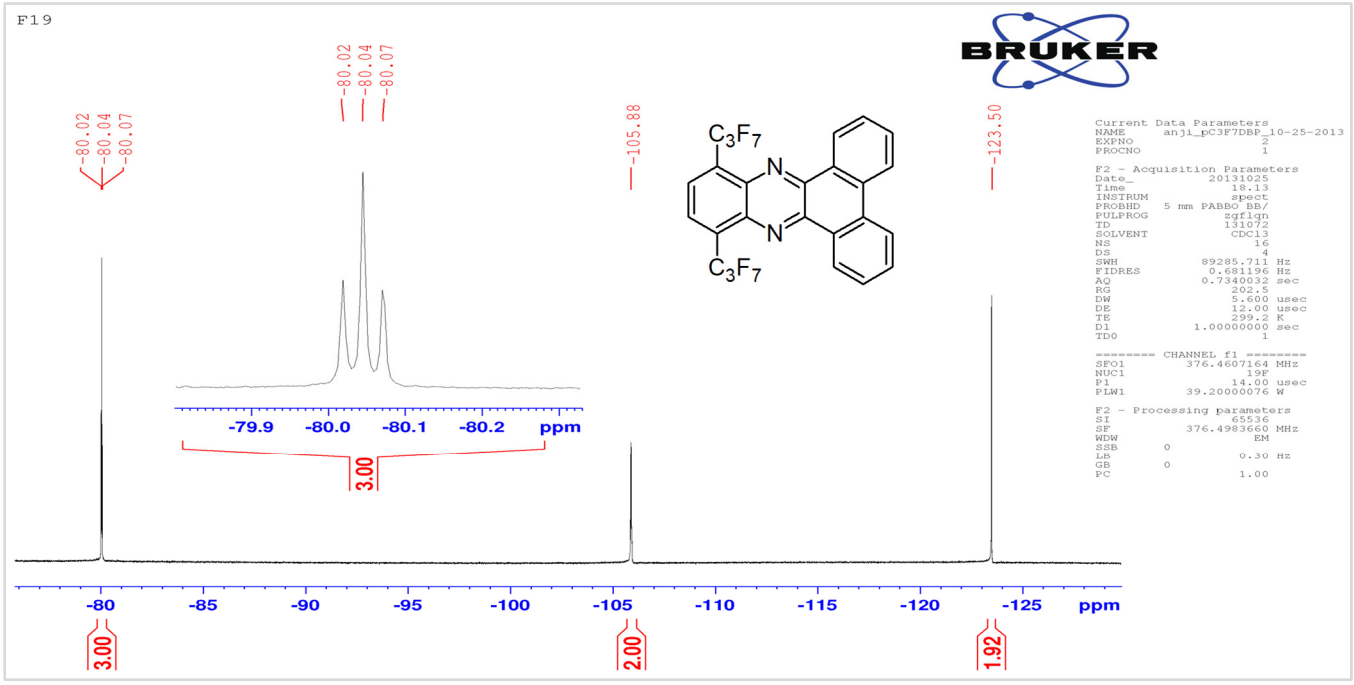


Figure S2: ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of compound **1**.

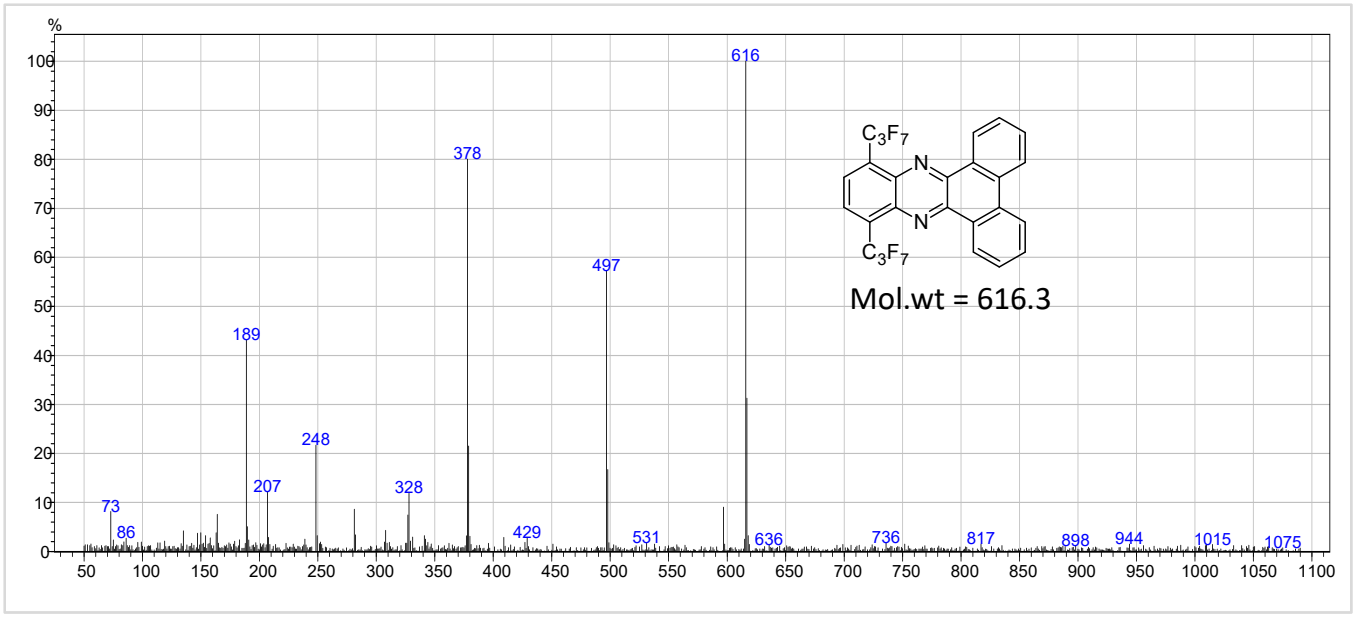


Figure S3: EI-MS spectrum of compound **1**.

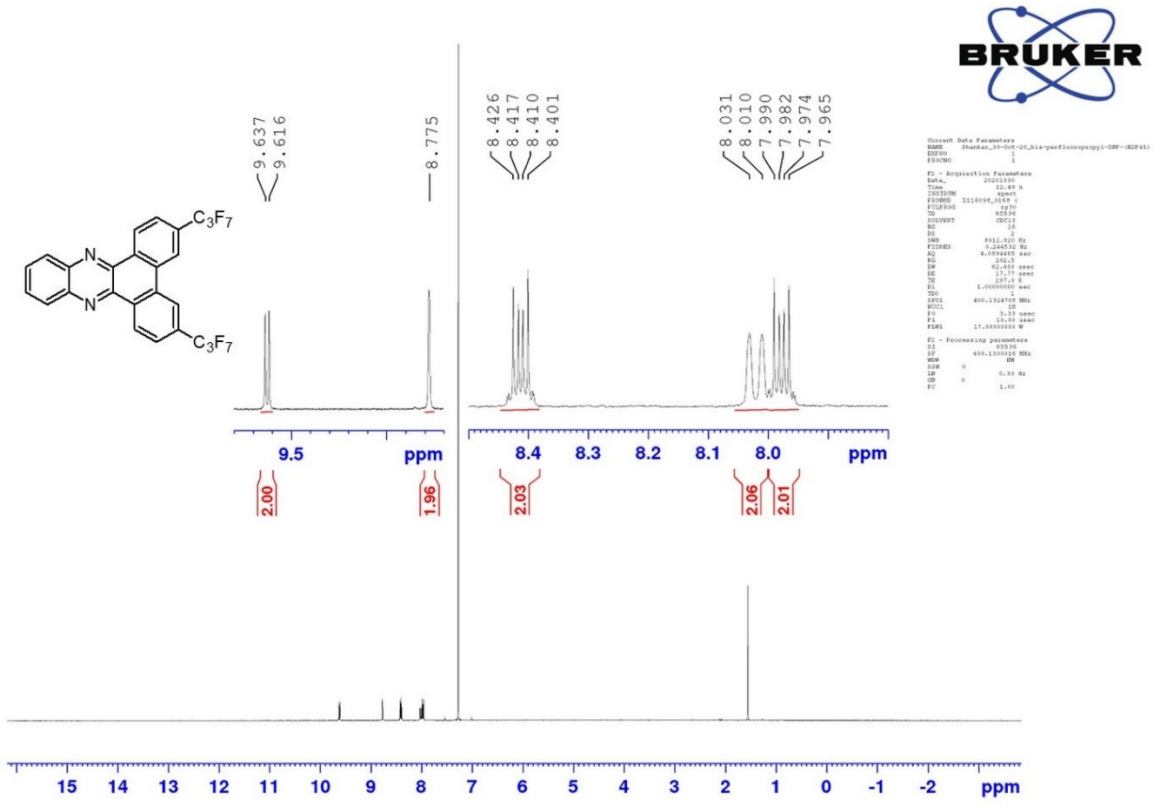


Figure S4: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3**.

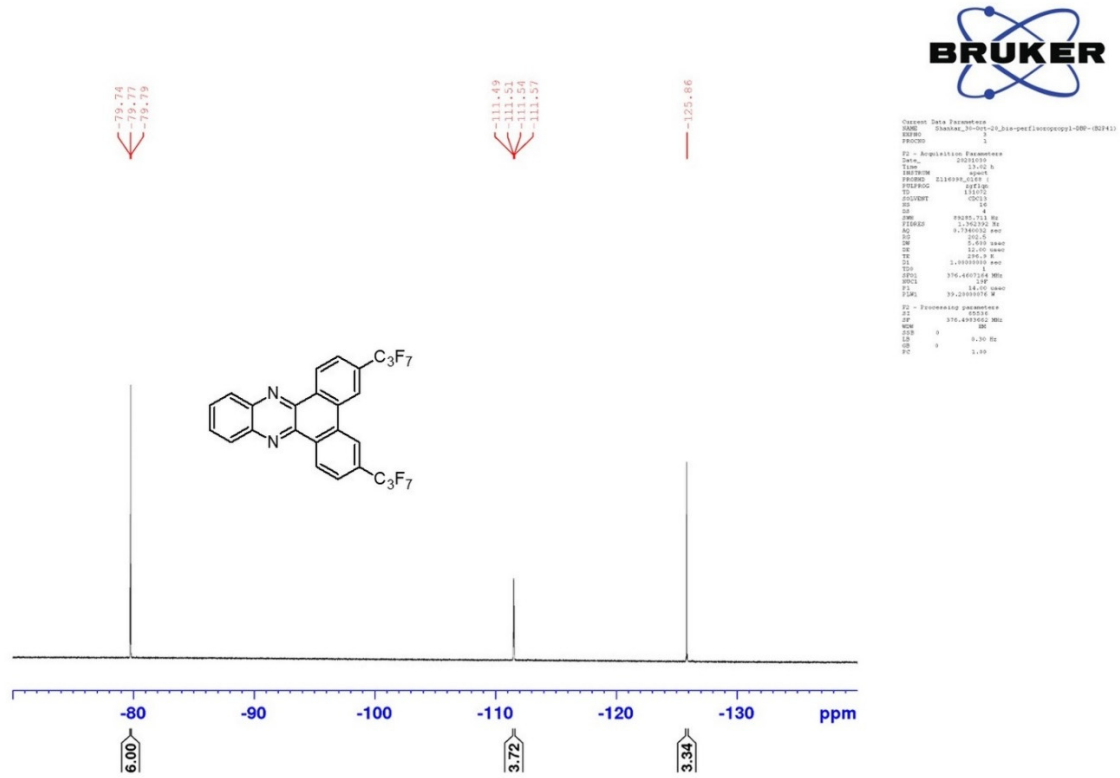


Figure S5: ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of compound **3**.

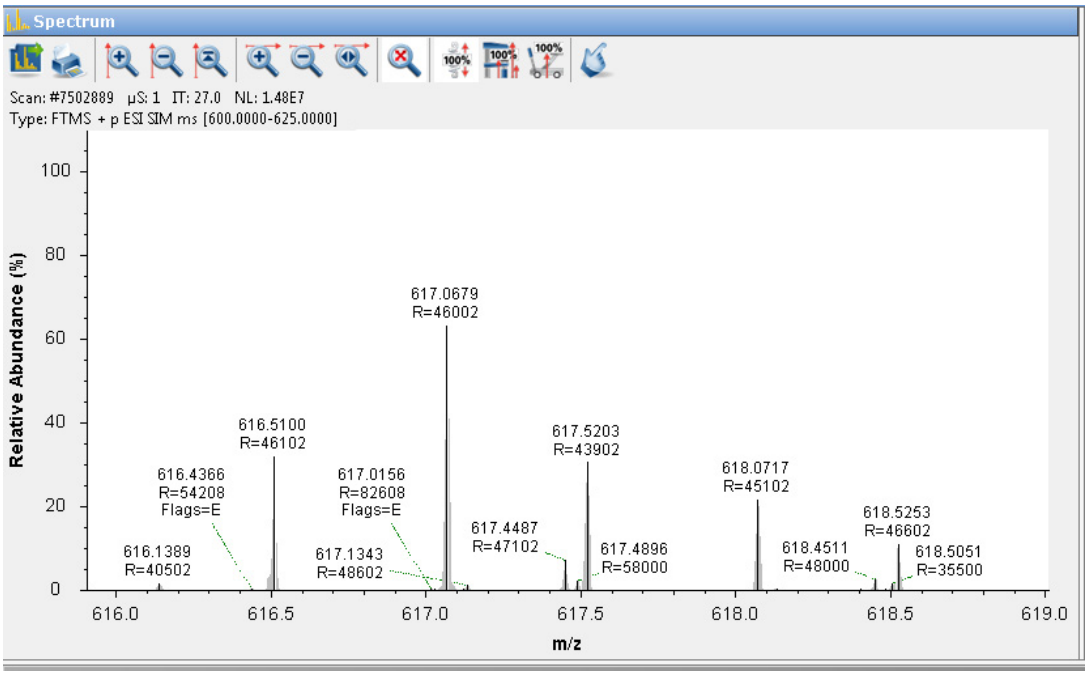


Figure S6: ESI-MS spectrum of compound **3**

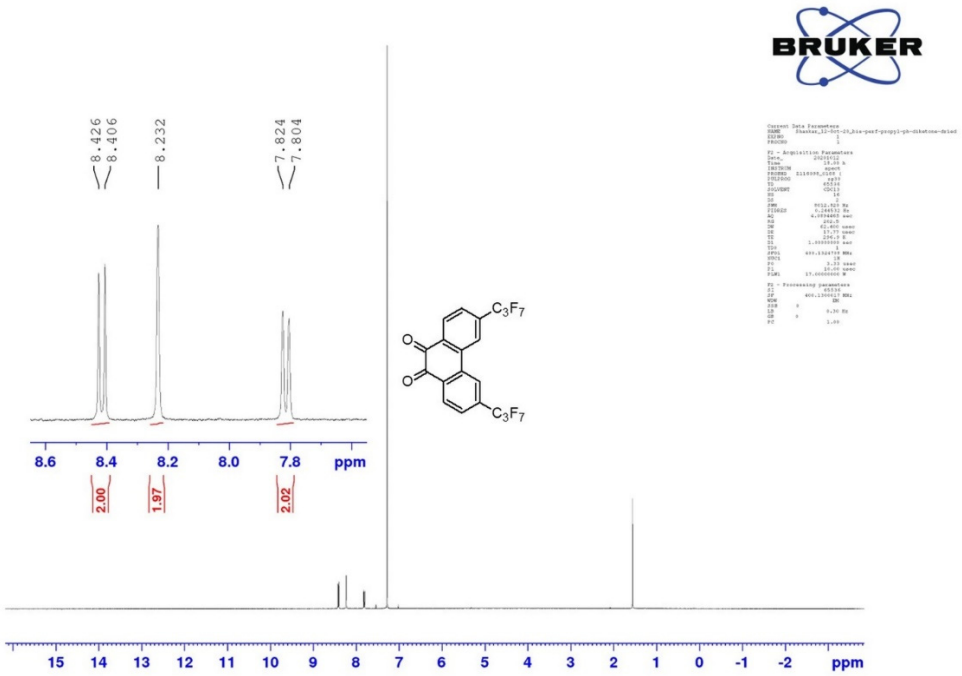


Figure S7: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3,6-bisperfluoropropylphenanthrene-9,10-dione.

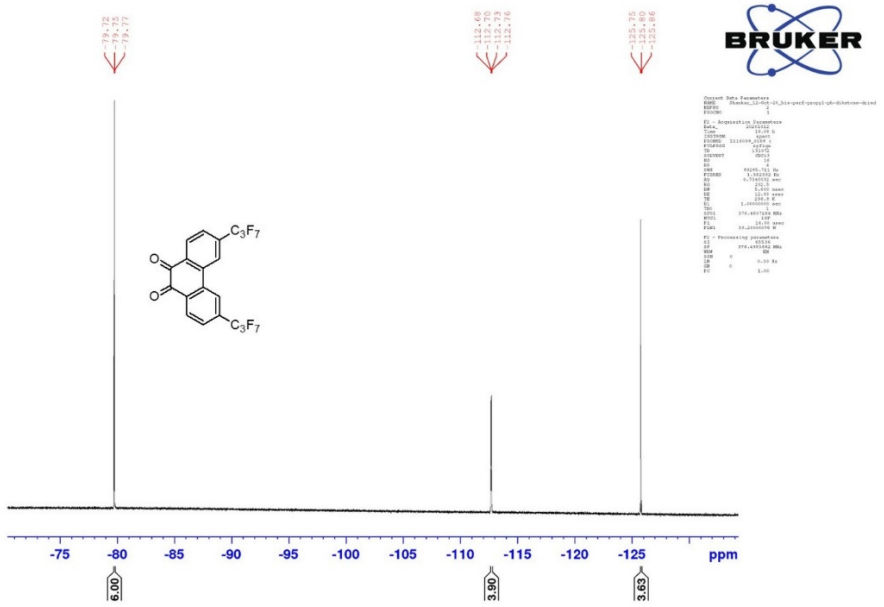


Figure S8: ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 3,6-bisperfluoropropylphenanthrene-9,10-dione.

3. Crystal structure analysis:

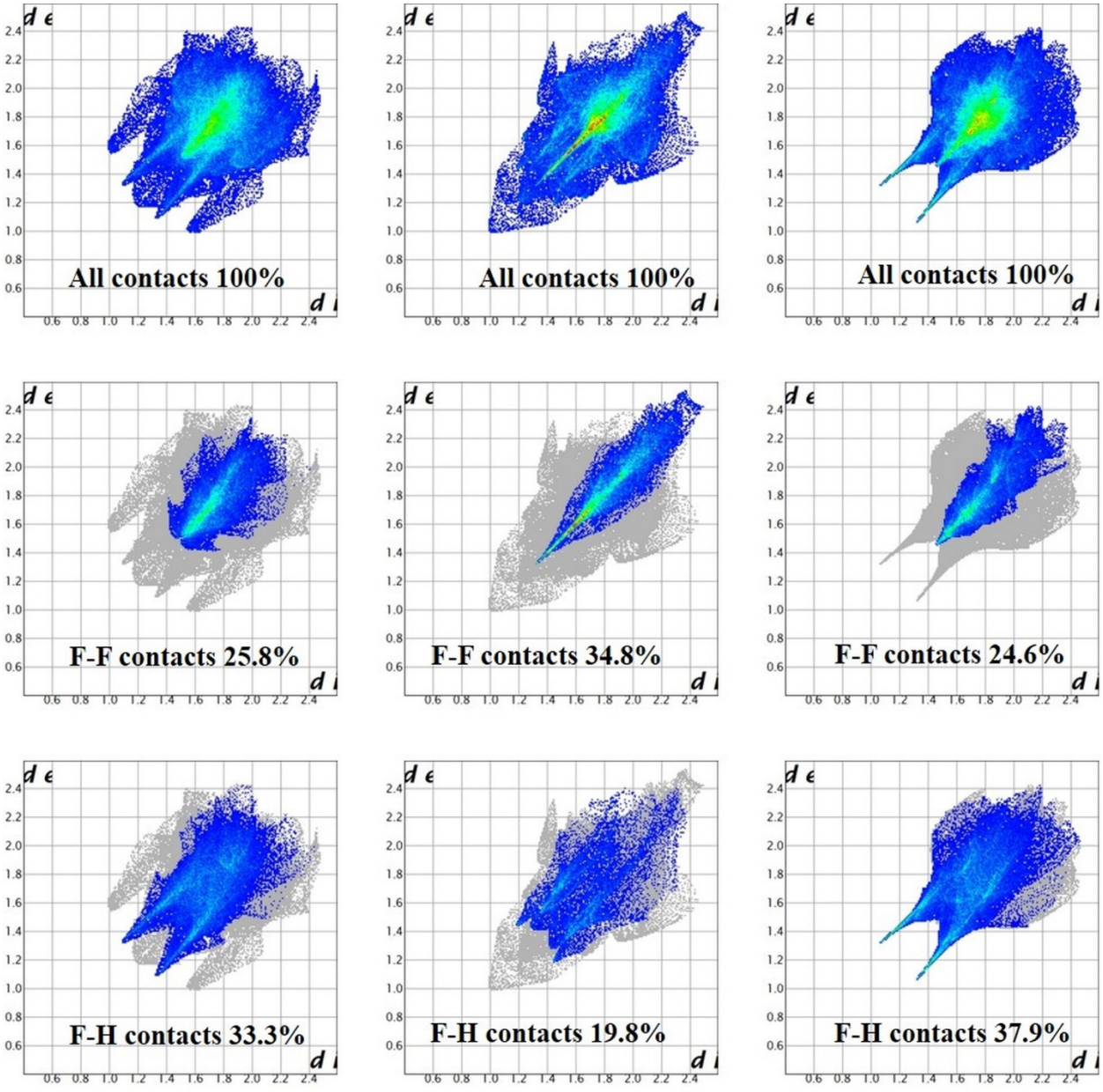


Figure S9: Comparison of 2D finger print plots of all, F-F, F-H contacts of compound **1**,**2** and **3**.

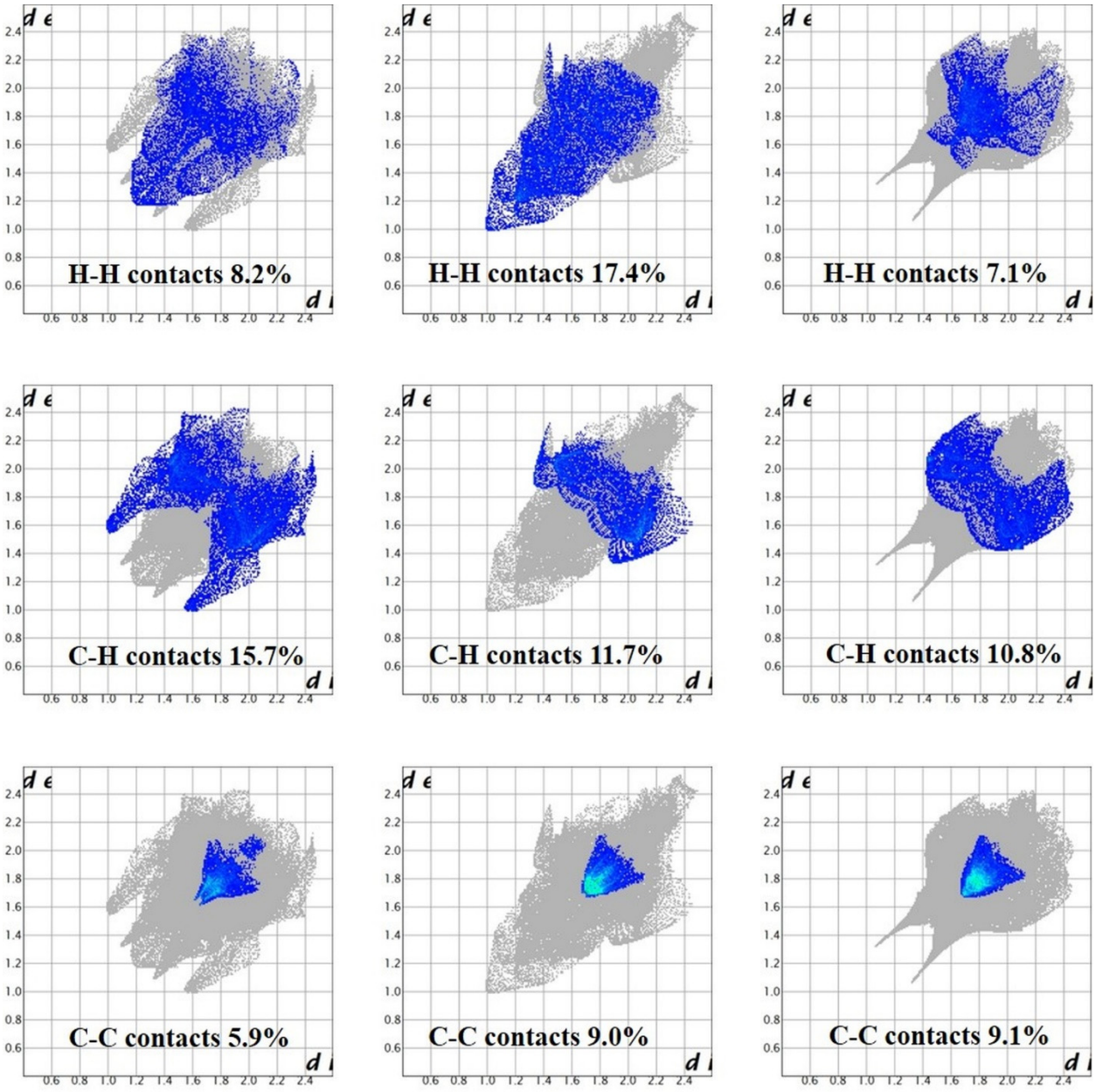


Figure S10: Comparison of 2D finger print plots of H-H, C-H, C-C contacts of compound **1**,**2** and **3**.

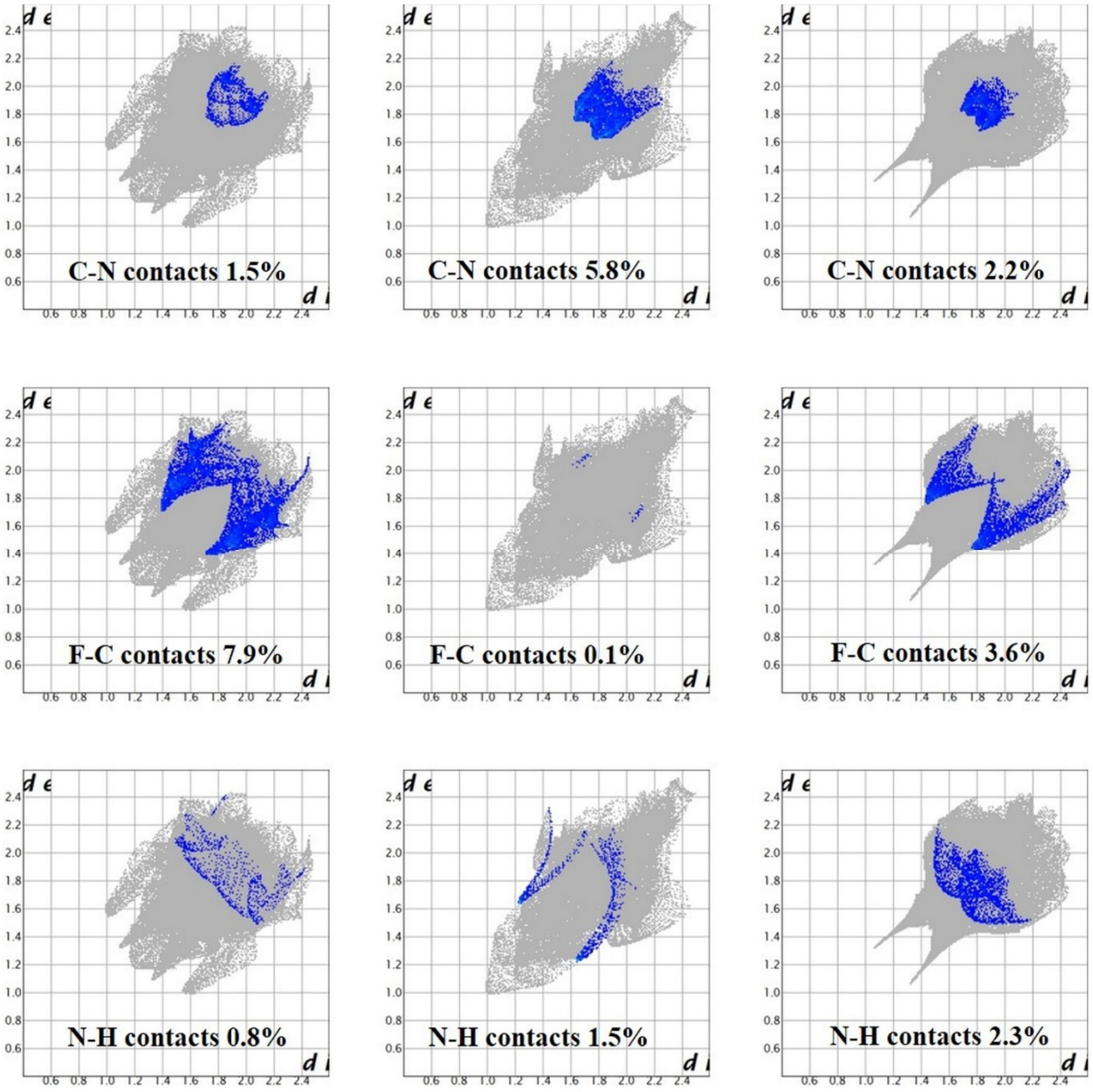


Figure S11: Comparison of 2D finger print plots of C-N, F-C, N-H contacts of compound **1**,**2** and **3**.

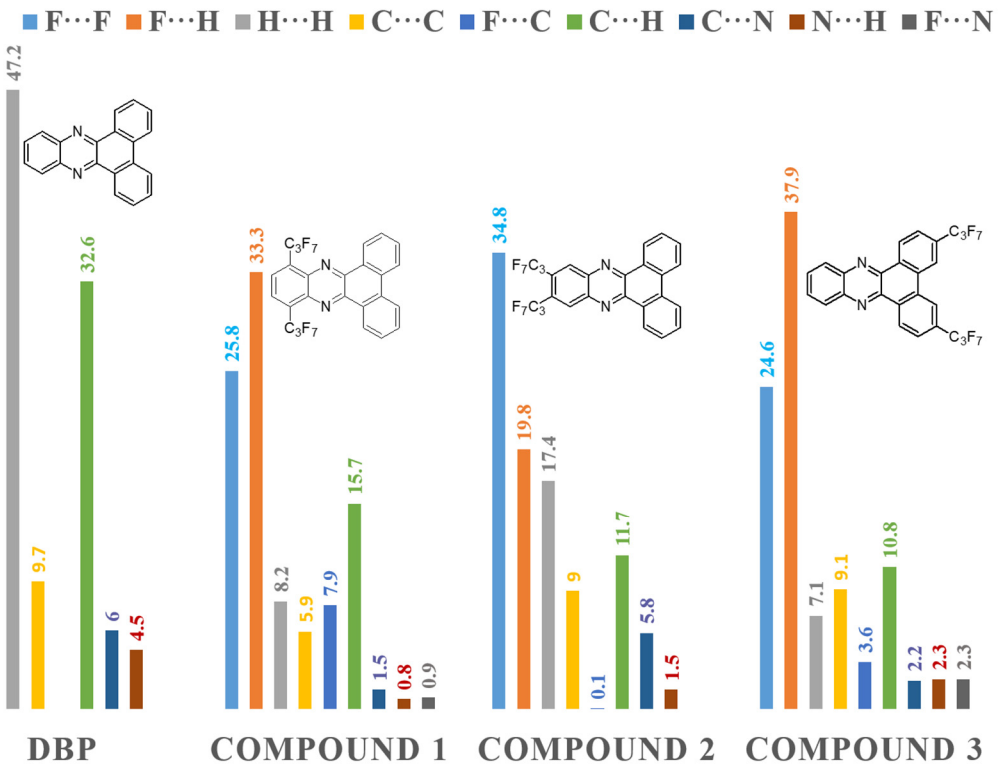


Figure S12: Short contact distributions of different intermolecular interactions in DBP, compounds **1-3** obtained from the Hirshfeld surface finger print plots.

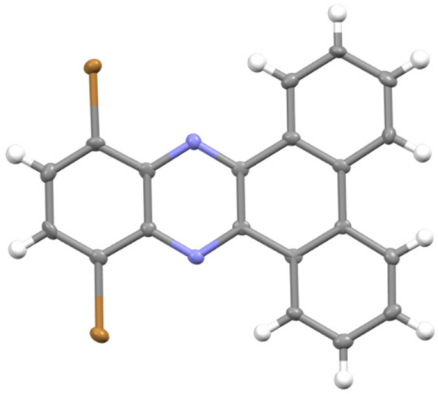


Figure S13: Crystal structure of 10,13-dibromo-dibenzo [a,c]phenazine (PBrDBP) with CCDC deposition number 2053442.

4. Computational work:

Geometry optimization was done with DFT method at B3LYP/6-311G(d,p) level of theory. All calculated geometries were checked with frequency calculation at B3LYP/6-311G(d,p) level of theory to make sure the optimized geometry is a local minimum. Dimer interaction energy calculations were performed using M06-2X/TZVP method and basis set with BSSE correction. Neutral, anion, cation structures were optimized under fully relaxed conditions followed by frequency calculations to make sure local minima was achieved and no imaginary frequency was observed in the vibrational spectra. Electron affinity (EA), ionization potential (IP) and reorganization energy (λ) were calculated under adiabatic conditions using the below formula.[1]

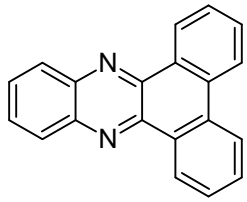
EA= Neutral Energy of the molecule ($E_{neutral}$) - Anion Energy of the molecule (E_{anion})

IP = Cation Energy of the molecule (E_{cation}) - Neutral Energy of the molecule ($E_{neutral}$)

Adiabatic reorganization energy was calculated according to the following formula.

Reorganization energy for electron transfer (λ_i^e) = $\lambda_1 + \lambda_2$
λ_1 = Anion Energy with neutral state structure – Anion Energy with anion state structure
λ_2 = Neutral Energy with anion state structure – Neutral Energy with neutral state structure

Reorganization energy for hole transfer (λ_i^h) = $\lambda_1 + \lambda_2$
λ_1 = Cation Energy with neutral state structure – Cation Energy with cation state structure
λ_2 = Neutral Energy with cation state structure – Neutral Energy with neutral state structure
XYZ coordinates of optimized geometry of DBP_neutral



C	6	2.209754	0.736041	-0.000065
C	6	2.209755	-0.736038	0.000065
C	6	0.985315	1.445923	0.000081
C	6	0.985317	-1.445922	-0.000082
N	7	-1.418052	1.404895	0.000571
N	7	-1.418046	-1.404911	-0.000572
C	6	-3.816875	1.410459	0.000800
C	6	-3.816877	-1.410437	-0.000800
H	1	-3.790770	2.493468	0.001411
C	6	-2.578587	0.715647	0.000159
C	6	-2.578585	-0.715658	-0.000159
C	6	-0.285408	0.718946	0.000300
C	6	-0.285408	-0.718951	-0.000302
C	6	0.985185	2.851598	-0.000057
C	6	0.985188	-2.851596	0.000057
H	1	0.029058	3.357717	0.000062

H	1	0.029061	-3.357716	-0.000063
C	6	3.387642	2.869014	-0.000424
C	6	3.387645	-2.869010	0.000425
H	1	4.324339	3.415089	-0.000638
H	1	4.324343	-3.415084	0.000639
C	6	3.402554	1.485211	-0.000310
C	6	3.402555	-1.485207	0.000310
H	1	4.359270	0.980950	-0.000454
H	1	4.359271	-0.980945	0.000455
C	6	2.171218	3.560544	-0.000303
C	6	2.171222	-3.560542	0.000303
H	1	2.158580	4.644402	-0.000400
H	1	2.158586	-4.644400	0.000401
C	6	-4.996213	0.709858	0.000640
C	6	-4.996220	-0.709856	-0.000639
H	1	-5.941676	-1.240425	-0.000618
H	1	-3.790767	-2.493521	-0.001410
H	1	-5.941671	1.240423	0.000620

Total electronic energy = -879.104531840

XYZ coordinates of optimized geometry of DBP_anion

C	6	2.231706	0.728331	-0.000008
C	6	2.231706	-0.728331	0.000008
C	6	0.986989	1.423865	0.000006
C	6	0.986990	-1.423865	-0.000006
N	7	-1.422435	1.427698	0.000039
N	7	-1.422435	-1.427698	-0.000039
C	6	-3.825655	1.396432	0.000053
C	6	-3.825655	-1.396432	-0.000053
H	1	-3.798949	2.481366	0.000090
C	6	-2.587351	0.719473	0.000026
C	6	-2.587351	-0.719473	-0.000026
C	6	-0.278503	0.709969	0.000014
C	6	-0.278503	-0.709969	-0.000014
C	6	0.990533	2.838896	0.000005
C	6	0.990533	-2.838896	-0.000005
H	1	0.025708	3.329651	0.000022
H	1	0.025708	-3.329651	-0.000022
C	6	3.399464	2.874917	-0.000051
C	6	3.399464	-2.874917	0.000050
H	1	4.332687	3.429732	-0.000083
H	1	4.332687	-3.429732	0.000083
C	6	3.419000	1.492929	-0.000045
C	6	3.419000	-1.492929	0.000045
H	1	4.378802	0.990312	-0.000080

H	1	4.378802	-0.990312	0.000080
C	6	2.167959	3.555104	-0.000020
C	6	2.167959	-3.555104	0.000020
H	1	2.145435	4.640878	-0.000022
H	1	2.145435	-4.640878	0.000022
C	6	-5.030213	0.700150	0.000026
C	6	-5.030213	-0.700150	-0.000026
H	1	-5.970218	-1.244427	-0.000049
H	1	-3.798949	-2.481367	-0.000090
H	1	-5.970218	1.244427	0.000049

Total electronic energy = -879.146550551

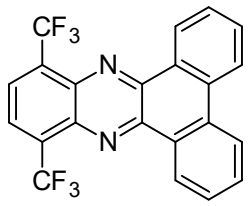
XYZ coordinates of optimized geometry of DBP_cation

C	6	2.215613	-0.718348	-0.000023
C	6	2.215615	0.718346	0.000042
C	6	0.969979	-1.442268	-0.000020
C	6	0.969985	1.442268	0.000034
N	7	-1.425558	-1.405655	-0.000020
N	7	-1.425554	1.405659	0.000017
C	6	-3.818368	-1.412550	-0.000034
C	6	-3.818364	1.412554	0.000003
H	1	-3.797941	-2.495240	-0.000047
C	6	-2.584977	-0.716980	-0.000018
C	6	-2.584975	0.716986	-0.000002
C	6	-0.294511	-0.715583	-0.000004
C	6	-0.294509	0.715586	0.000017
C	6	0.978349	-2.839125	-0.000032
C	6	0.978358	2.839123	0.000044
H	1	0.030437	-3.359433	-0.000019
H	1	0.030444	3.359427	0.000027
C	6	3.406849	-2.845742	-0.000105
C	6	3.406859	2.845736	0.000122
H	1	4.336682	-3.400772	-0.000155
H	1	4.336692	3.400766	0.000171
C	6	3.425621	-1.474055	-0.000086
C	6	3.425627	1.474049	0.000104
H	1	4.379888	-0.968763	-0.000138
H	1	4.379891	0.968752	0.000153
C	6	2.176115	-3.537157	-0.000066
C	6	2.176126	3.537153	0.000080
H	1	2.168475	-4.620660	-0.000070
H	1	2.168492	4.620656	0.000083
C	6	-5.006220	-0.705263	-0.000033
C	6	-5.006218	0.705269	-0.000013
H	1	-5.949530	1.237640	-0.000012

H	1	-3.797942	2.495245	0.000017
H	1	-5.949534	-1.237632	-0.000044

Total electronic energy = -878.825740329

XYZ coordinates of optimized geometry of compound 1_neutral



1	9	-2.055538	-3.439944	1.086234
2	9	-2.056298	3.440085	-1.086572
3	9	-3.930712	-3.400272	-0.000272
4	9	-3.930677	3.400289	0.001304
5	7	-0.240082	-1.397945	-0.000246
6	7	-0.240078	1.397918	0.000020
7	6	-1.399205	0.714796	-0.000004
8	6	0.895198	0.718796	-0.000081
9	6	-2.644931	-1.414541	-0.000397
10	6	0.895207	-0.718832	-0.000130
11	6	-2.644925	1.414545	0.000279
12	6	-2.662520	-2.925504	-0.000453
13	6	3.384585	-0.736326	0.000224
14	6	2.160640	1.447942	-0.000184
15	6	2.160637	-1.447961	0.000054
16	6	3.384590	0.736324	-0.000219
17	6	-2.662495	2.925500	0.000491
18	6	-3.820082	-0.707529	-0.000145
19	1	-4.763875	-1.235236	-0.000575
20	6	-1.399197	-0.714825	-0.000326
21	6	4.576052	1.486179	-0.000738
22	1	5.533587	0.983816	-0.001009
23	6	2.155568	-2.853825	0.000367
24	1	1.199281	-3.359984	0.000210
25	6	2.155518	2.853805	-0.000497
26	1	1.199222	3.359948	-0.000485
27	6	-3.820092	0.707545	0.000283
28	1	-4.763883	1.235258	0.000851
29	6	3.341656	3.562412	-0.000893
30	1	3.328874	4.645950	-0.001097
31	6	3.341722	-3.562409	0.000896
32	1	3.328977	-4.645948	0.001140

33	6	4.576066	-1.486146	0.000930
34	1	5.533585	-0.983754	0.001366
35	6	4.557848	2.870460	-0.001059
36	1	5.493853	3.417492	-0.001537
37	6	4.557893	-2.870434	0.001222
38	1	5.493907	-3.417450	0.001795
39	9	-2.055243	3.440013	1.087172
40	9	-2.056066	-3.440144	-1.087510

Total electronic energy = -1553.37399459

XYZ coordinates of optimized geometry of compound 1_anion

F	9	2.073875	-3.461296	-1.085263
F	9	2.073903	3.461297	1.085261
F	9	3.948977	-3.388469	-0.000253
F	9	3.948976	3.388470	0.000200
N	7	0.239382	-1.413210	-0.000121
N	7	0.239382	1.413210	0.000125
C	6	1.397274	0.724162	0.000057
C	6	-0.910912	0.705006	0.000072
C	6	2.643977	-1.409205	-0.000110
C	6	-0.910912	-0.705006	-0.000061
C	6	2.643976	1.409206	0.000093
C	6	2.669140	-2.903824	-0.000217
C	6	-3.410353	-0.730379	-0.000080
C	6	-2.170738	1.428405	0.000165
C	6	-2.170738	-1.428405	-0.000148
C	6	-3.410353	0.730379	0.000102
C	6	2.669139	2.903824	0.000197
C	6	3.847479	-0.693705	-0.000066
H	1	4.785872	-1.231300	-0.000109
C	6	1.397274	-0.724162	-0.000057
C	6	-4.598306	1.492876	0.000226
H	1	-5.558236	0.991413	0.000204
C	6	-2.167617	-2.841049	-0.000311
H	1	-1.203581	-3.333355	-0.000354
C	6	-2.167617	2.841048	0.000327
H	1	-1.203581	3.333355	0.000366
C	6	3.847479	0.693705	0.000031
H	1	4.785872	1.231301	0.000059
C	6	-3.346981	3.555978	0.000436
H	1	-3.325242	4.641135	0.000562
C	6	-3.346981	-3.555979	-0.000414
H	1	-3.325242	-4.641135	-0.000539
C	6	-4.598306	-1.492877	-0.000198
H	1	-5.558236	-0.991414	-0.000171

C	6	-4.575727	2.875043	0.000389
H	1	-5.508474	3.430153	0.000484
C	6	-4.575727	-2.875043	-0.000361
H	1	-5.508474	-3.430154	-0.000452
F	9	2.073851	3.461448	-1.084759
F	9	2.073880	-3.461449	1.084756

Total electronic energy = -1553.44142964

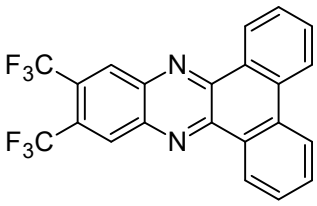
XYZ coordinates of optimized geometry of compound 1_cation

F	9	2.036748	-3.441721	-1.087351
F	9	2.036724	3.441745	1.087339
F	9	3.914367	-3.412438	-0.000172
F	9	3.914326	3.412477	0.000131
N	7	0.242505	-1.406397	-0.000086
N	7	0.242483	1.406401	0.000090
C	6	1.384624	0.729727	0.000038
C	6	-0.907536	0.725724	0.000061
C	6	2.637510	-1.430607	-0.000076
C	6	-0.907526	-0.725729	-0.000048
C	6	2.637488	1.430634	0.000058
C	6	2.653948	-2.947480	-0.000147
C	6	-3.381710	-0.737048	-0.000096
C	6	-2.146711	1.447457	0.000156
C	6	-2.146683	-1.447479	-0.000138
C	6	-3.381717	0.737016	0.000121
C	6	2.653910	2.947507	0.000127
C	6	3.798769	-0.716618	-0.000050
H	1	4.748189	-1.235730	-0.000080
C	6	1.384634	-0.729712	-0.000040
C	6	-4.555209	1.490817	0.000317
H	1	-5.521895	1.006297	0.000354
C	6	-2.130128	-2.868871	-0.000308
H	1	-1.169152	-3.365827	-0.000320
C	6	-2.130180	2.868844	0.000326
H	1	-1.169211	3.365815	0.000334
C	6	3.798757	0.716656	0.000015
H	1	4.748171	1.235782	0.000032
C	6	-3.311183	3.584517	0.000488
H	1	-3.296595	4.666834	0.000618
C	6	-3.311113	-3.584552	-0.000465
H	1	-3.296517	-4.666869	-0.000595
C	6	-4.555187	-1.490866	-0.000286
H	1	-5.521882	-1.006364	-0.000317
C	6	-4.523844	2.892698	0.000493
H	1	-5.459654	3.439031	0.000638

C	6	-4.523793	-2.892741	-0.000463
H	1	-5.459593	-3.439092	-0.000603
F	9	2.036694	3.441841	-1.087023
F	9	2.036753	-3.441822	1.087011

Total electronic energy = -1553.07758194

XYZ coordinates of optimized geometry of compound 2_neutral



F	9	0.224953	2.848152	-4.000895
F	9	-0.224953	-2.848152	-4.000895
F	9	0.815879	1.135966	-5.184637
F	9	-0.815879	-1.135966	-5.184637
C	6	0.000018	0.736088	4.229436
C	6	-0.000018	-0.736088	4.229436
C	6	-0.000116	1.447510	3.005629
C	6	0.000116	-1.447510	3.005629
N	7	-0.000576	1.406924	0.604140
N	7	0.000576	-1.406924	0.604140
C	6	-0.003573	1.397509	-1.790464
C	6	0.003573	-1.397509	-1.790464
H	1	-0.007141	2.477985	-1.766251
H	1	0.007141	-2.477985	-1.766251
C	6	-0.000507	0.710469	-0.551259
C	6	0.000507	-0.710469	-0.551259
C	6	-0.000187	0.721497	1.736681
C	6	0.000187	-0.721497	1.736681
C	6	-0.000133	2.853369	3.004354
C	6	0.000133	-2.853369	3.004354
H	1	-0.000208	3.361347	2.049342
H	1	0.000208	-3.361347	2.049342
C	6	0.000187	2.868758	5.406183
C	6	-0.000187	-2.868758	5.406183
H	1	0.000336	3.414543	6.342887
H	1	-0.000336	-3.414543	6.342887
C	6	-0.059998	1.551503	-4.251571
C	6	0.059998	-1.551503	-4.251571
C	6	0.000171	1.484689	5.421839

C	6	-0.000171	-1.484689	5.421839
H	1	0.000336	0.981122	6.378678
H	1	-0.000336	-0.981122	6.378678
C	6	0.000018	3.561521	4.190633
C	6	-0.000018	-3.561521	4.190633
H	1	0.000016	4.645137	4.178780
H	1	-0.000016	-4.645137	4.178780
C	6	-0.000822	0.719036	-2.984131
C	6	0.000822	-0.719036	-2.984131
F	9	-1.289254	1.527603	-4.805179
F	9	1.289254	-1.527603	-4.805179

Total electronic energy = -1553.37007067

XYZ coordinates of optimized geometry of compound 2_anion

F	9	0.278314	2.841267	-4.018422
F	9	-0.278314	-2.841267	-4.018422
F	9	0.803338	1.122839	-5.224627
F	9	-0.803338	-1.122839	-5.224627
C	6	0.000786	0.729247	4.258754
C	6	-0.000786	-0.729247	4.258754
C	6	0.001250	1.425687	3.017183
C	6	-0.001250	-1.425687	3.017183
N	7	0.000266	1.426906	0.606261
N	7	-0.000266	-1.426906	0.606261
C	6	-0.000046	1.387211	-1.788854
C	6	0.000046	-1.387211	-1.788854
H	1	0.001745	2.467955	-1.765323
H	1	-0.001745	-2.467955	-1.765323
C	6	0.000046	0.717162	-0.547279
C	6	-0.000046	-0.717162	-0.547279
C	6	0.000252	0.707501	1.754740
C	6	-0.000252	-0.707501	1.754740
C	6	0.002744	2.839403	3.017777
C	6	-0.002744	-2.839403	3.017777
H	1	0.002991	3.332212	2.054352
H	1	-0.002991	-3.332212	2.054352
C	6	0.003536	2.873861	5.425732
C	6	-0.003536	-2.873861	5.425732
H	1	0.004490	3.428660	6.358604
H	1	-0.004490	-3.428660	6.358604
C	6	-0.046053	1.543586	-4.254679
C	6	0.046053	-1.543586	-4.254679
C	6	0.002010	1.491967	5.446762
C	6	-0.002010	-1.491967	5.446762

H	1	0.001861	0.989858	6.406353
H	1	-0.001861	-0.989858	6.406353
C	6	0.003886	3.554641	4.196320
C	6	-0.003886	-3.554641	4.196320
H	1	0.005110	4.639943	4.174729
H	1	-0.005110	-4.639943	4.174729
C	6	0.005563	0.709544	-3.006210
C	6	-0.005563	-0.709544	-3.006210
F	9	-1.282342	1.577333	-4.822954
F	9	1.282342	-1.577333	-4.822954

Total electronic energy = -1553.43765793

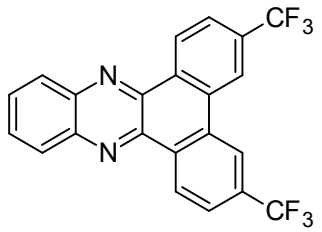
XYZ coordinates of optimized geometry of compound 2_cation

F	9	0.182724	2.852686	-3.988628
F	9	-0.182724	-2.852686	-3.988628
F	9	0.809344	1.144461	-5.160049
F	9	-0.809344	-1.144461	-5.160049
C	6	0.001131	0.736754	4.225999
C	6	-0.001131	-0.736754	4.225999
C	6	0.001816	1.447093	2.991349
C	6	-0.001816	-1.447093	2.991349
N	7	0.000584	1.415900	0.600749
N	7	-0.000584	-1.415900	0.600749
C	6	-0.004873	1.411641	-1.784556
C	6	0.004873	-1.411641	-1.784556
H	1	-0.011447	2.492176	-1.765046
H	1	0.011447	-2.492176	-1.765046
C	6	0.000122	0.724874	-0.537088
C	6	-0.000122	-0.724874	-0.537088
C	6	0.000541	0.728717	1.748371
C	6	-0.000541	-0.728717	1.748371
C	6	0.003848	2.868227	2.979468
C	6	-0.003848	-2.868227	2.979468
H	1	0.004350	3.368045	2.020542
H	1	-0.004350	-3.368045	2.020542
C	6	0.004639	2.890190	5.372844
C	6	-0.004639	-2.890190	5.372844
H	1	0.005770	3.435199	6.309397
H	1	-0.005770	-3.435199	6.309397
C	6	-0.076897	1.558356	-4.247419
C	6	0.076897	-1.558356	-4.247419
C	6	0.002583	1.488841	5.400955
C	6	-0.002583	-1.488841	5.400955
H	1	0.002187	1.002464	6.366593

H	1	-0.002187	-1.002464	6.366593
C	6	0.005250	3.583041	4.160821
C	6	-0.005250	-3.583041	4.160821
H	1	0.006852	4.665384	4.147502
H	1	-0.006852	-4.665384	4.147502
C	6	-0.005250	0.728097	-2.966103
C	6	0.005250	-0.728097	-2.966103
F	9	-1.306110	1.493499	-4.779331
F	9	1.306110	-1.493499	-4.779331

Total electronic energy = -1553.07034589

XYZ coordinates of optimized geometry of compound 3_neutral



C	6	3.133179	3.648074	0.000221
C	6	1.850447	2.861439	-0.000038
C	6	0.633347	3.558589	-0.000348
H	1	0.626348	4.641593	-0.000504
C	6	-0.549158	2.850749	-0.000429
H	1	-1.503484	3.359525	-0.000617
C	6	-0.550054	1.444272	-0.000246
C	6	0.672585	0.735392	-0.000040
C	6	1.868132	1.479255	0.000112
H	1	2.825471	0.980212	0.000387
C	6	-1.820242	0.717413	-0.000186
C	6	-4.111486	0.716566	-0.000229
C	6	-5.350041	1.411930	-0.000472
H	1	-5.324290	2.494782	-0.000831
C	6	-6.527811	0.710521	-0.000241
H	1	-7.473599	1.239946	-0.000426
N	7	-2.952224	1.405201	-0.000412
F	9	4.227493	2.859524	0.000505
F	9	3.220546	4.452421	1.084066
C	6	3.133179	-3.648074	-0.000221
C	6	1.850447	-2.861438	0.000038
C	6	0.633347	-3.558589	0.000348
H	1	0.626348	-4.641593	0.000504
C	6	-0.549158	-2.850749	0.000429
H	1	-1.503484	-3.359525	0.000617
C	6	-0.550054	-1.444272	0.000246

C	6	0.672585	-0.735392	0.000040
C	6	1.868132	-1.479255	-0.000112
H	1	2.825471	-0.980212	-0.000387
C	6	-1.820242	-0.717413	0.000186
C	6	-4.111486	-0.716567	0.000229
C	6	-5.350041	-1.411930	0.000472
H	1	-5.324290	-2.494782	0.000831
C	6	-6.527811	-0.710521	0.000241
H	1	-7.473599	-1.239946	0.000426
N	7	-2.952224	-1.405201	0.000412
F	9	4.227493	-2.859524	-0.000504
F	9	3.220546	-4.452421	-1.084067
F	9	3.221042	4.452312	-1.083684
F	9	3.221042	-4.452312	1.083684

Total electronic energy = -1553.38148209

XYZ coordinates of optimized geometry of compound 3_anion

C	6	-0.000089	-3.657495	-3.123981
C	6	-0.000041	-2.866998	-1.859655
C	6	-0.000016	-3.554978	-0.625663
H	1	-0.000014	-4.638932	-0.610012
C	6	0.000006	-2.839608	0.546243
H	1	0.000022	-3.333358	1.509038
C	6	0.000006	-1.423024	0.551344
C	6	-0.000006	-0.727324	-0.692984
C	6	-0.000037	-1.484372	-1.881118
H	1	-0.000063	-0.986953	-2.840530
C	6	0.000013	-0.712597	1.816191
C	6	0.000021	-0.718091	4.122866
C	6	0.000046	-1.397211	5.358948
H	1	0.000081	-2.481754	5.331860
C	6	0.000024	-0.700782	6.561117
H	1	0.000043	-1.243570	7.501394
N	7	0.000035	-1.426527	2.956135
F	9	-0.000057	-2.889110	-4.239789
F	9	-1.082667	-4.479230	-3.225909
C	6	0.000089	3.657495	-3.123981
C	6	0.000041	2.866998	-1.859655
C	6	0.000016	3.554978	-0.625663
H	1	0.000014	4.638932	-0.610012
C	6	-0.000006	2.839608	0.546243
H	1	-0.000022	3.333358	1.509038
C	6	-0.000006	1.423024	0.551344
C	6	0.000006	0.727324	-0.692984

C	6	0.000037	1.484372	-1.881118
H	1	0.000063	0.986953	-2.840530
C	6	-0.000013	0.712597	1.816191
C	6	-0.000021	0.718091	4.122866
C	6	-0.000046	1.397211	5.358948
H	1	-0.000081	2.481754	5.331860
C	6	-0.000024	0.700782	6.561117
H	1	-0.000043	1.243570	7.501394
N	7	-0.000035	1.426527	2.956135
F	9	0.000057	2.889110	-4.239789
F	9	1.082667	4.479230	-3.225909
F	9	1.082406	-4.479340	-3.225918
F	9	-1.082406	4.479340	-3.225918

Total electronic energy = -1553.44470767

XYZ coordinates of optimized geometry of compound 3_cation

C	6	-0.000343	-3.667961	-3.131291
C	6	-0.000223	-2.878549	-1.836114
C	6	-0.000197	-3.576825	-0.625021
H	1	-0.000245	-4.659285	-0.617340
C	6	-0.000113	-2.865136	0.556786
H	1	-0.000099	-3.370857	1.512452
C	6	-0.000049	-1.447126	0.549967
C	6	-0.000048	-0.736938	-0.681408
C	6	-0.000151	-1.481495	-1.861884
H	1	-0.000184	-0.996405	-2.826753
C	6	-0.000009	-0.730880	1.797283
C	6	0.000004	-0.732870	4.085819
C	6	0.000016	-1.428271	5.327226
H	1	0.000028	-2.510413	5.306927
C	6	0.000009	-0.719739	6.494207
H	1	0.000017	-1.239482	7.444753
N	7	-0.000004	-1.416931	2.940162
F	9	-0.000297	-2.865317	-4.208206
F	9	-1.085896	-4.456344	-3.198896
C	6	0.000343	3.667961	-3.131291
C	6	0.000223	2.878549	-1.836114
C	6	0.000197	3.576825	-0.625021
H	1	0.000245	4.659285	-0.617340
C	6	0.000113	2.865136	0.556786
H	1	0.000099	3.370857	1.512452
C	6	0.000049	1.447126	0.549967
C	6	0.000048	0.736938	-0.681408
C	6	0.000151	1.481495	-1.861884

H	1	0.000184	0.996405	-2.826753
C	6	0.000009	0.730880	1.797283
C	6	-0.000004	0.732870	4.085819
C	6	-0.000016	1.428271	5.327226
H	1	-0.000028	2.510413	5.306927
C	6	-0.000009	0.719739	6.494207
H	1	-0.000017	1.239482	7.444753
N	7	0.000004	1.416931	2.940162
F	9	0.000297	2.865317	-4.208206
F	9	1.085896	4.456344	-3.198896
F	9	1.085048	-4.456562	-3.198965
F	9	-1.085048	4.456562	-3.198965

Total electronic energy = -1553.07921207

References:

1. Y.-C. Chang and I. Chao, *J. Phys. Chem. Lett.*, 2010, **1**, 116-121.