Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Orthogonally Arranged Tripyrrin-BODIPY Conjugates with an "Edge to Plane" Mode

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Outline

1. Supporting Tables and Figures.

Table S1. Crystal data and structure refinement.

Complex	**1** (CCDC: 1889398)	**2** (CCDC: 1889399)	**4** (CCDC: 1889400)	**5** (CCDC: 1896685)
Molecular formula	$C_{34}H_{12}Cl_3F_{10}N_3O_3$	$C_{41}H_{16}BF_{12}N_5O_2$	$C_{46}H_{23}BCl_3F_{12}I_2N_5O_2$	$C_{63}H_{36}BF_{12}N_5O_4$
Formula wt. (g mol^{-1})	806.82	849.40	1276.65	1165.78
Temperature (K)	180 K	180 K	180 K	180 K
Radiation (λ, Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	orthorhombic	orthorhombic	monoclinic	monoclinic
Space group	*Pna*2$_1$	*Pna*2$_1$	*P*2$_1$/*n*	*C2/c*
a (Å)	7.7138(7)	9.9933 (3)	12.2174(3)	19.3974(5)
b (Å)	25.522(2)	18.8319 (7)	25.6864(7)	26.0855(6)
c (Å)	16.1814(16)	21.7044 (7)	15.7955(6)	28.6167(6)
α (º)	90	90	90	90
β (º)	90	90	109.134(3)	101.742(2)
γ (º)	90	90	90	90
Volume (Å^3)	3185.6(5)	4084.6 (2)	4683.1(3)	14176.8(6)
Z	4	4	4	4
ρ_{calcd} (g cm^{-3})	1.682	1.381	1.811	1.092
μ (mm^{-1})	0.390	0.124	1.608	0.090
F(000)	1608.0	1704.0	2480	4752
Crystal size (mm^3)	0.4×0.15×0.12	0.2×0.12×0.07	0.08×0.05×0.02	0.45×0.2×0.18
Theta range	3.8650 to 24.7000º	1.877 to 27.480º	1.843 to 27.483º	2.123 to 27.485º
Reflections collected	18667	27817	34840	91201
Independent reflections	5992 [R(int) = 0.1006]	8602 [R(int) = 0.0452]	10731 [R(int) = 0.0400]	16259 [R(int) = 0.0449]
Completeness	99.40%	99.40%	99.55%	100.01%
Goodness-of-fit on F^2	1.044	1.056	1.027	1.072
Final R indices [R > 2σ (I)]	R1^a = 0.0846 *w*R$_2^b$= 0.2100	R1^a = 0.0621 wR$_2^b$= 0.1483	R1^a = 0.0519 *w*R$_2^b$= 0.1113	R1a = 0.0671 wR2b= 0.1688
R indices (all data)	R1^a=0.1174 *w*R$_2^b$=0.2278	R1^a=0.0835 wR$_2^b$=0.1587	R1^a=0.0964 *w*R$_2^b$=0.1252	R1a=0.0932 wR2b=0.1823
Largest diff. peak and hole (e Å^{-3})	0.882 and -0.519	0.352 and -2.09	1.573 and -0.633	0.375 and -0.300

Table S2. Calculated absorption peak at S_0 optimized structures by TDDFT.

`	UV		
	Exp.	**Comp. (*f*)**	**Contribution**[a]
1	317, 497, 532	479 (0.4664)	H -> L (96.8%)
2	318, 512	479 (0.4167)	H -> L (95.5%)
3	318, 512	521 (0.3606)	H-1 -> L (97.9%)
4	317, 392, 544	519 (0.3703)	H-1 -> L (96.9%)
5	262, 315, 420, 501, 535, 595	597 (0.5345)	H -> L+1 (95.2%)

[a] H and L indicate HOMO and LUMO respectively.

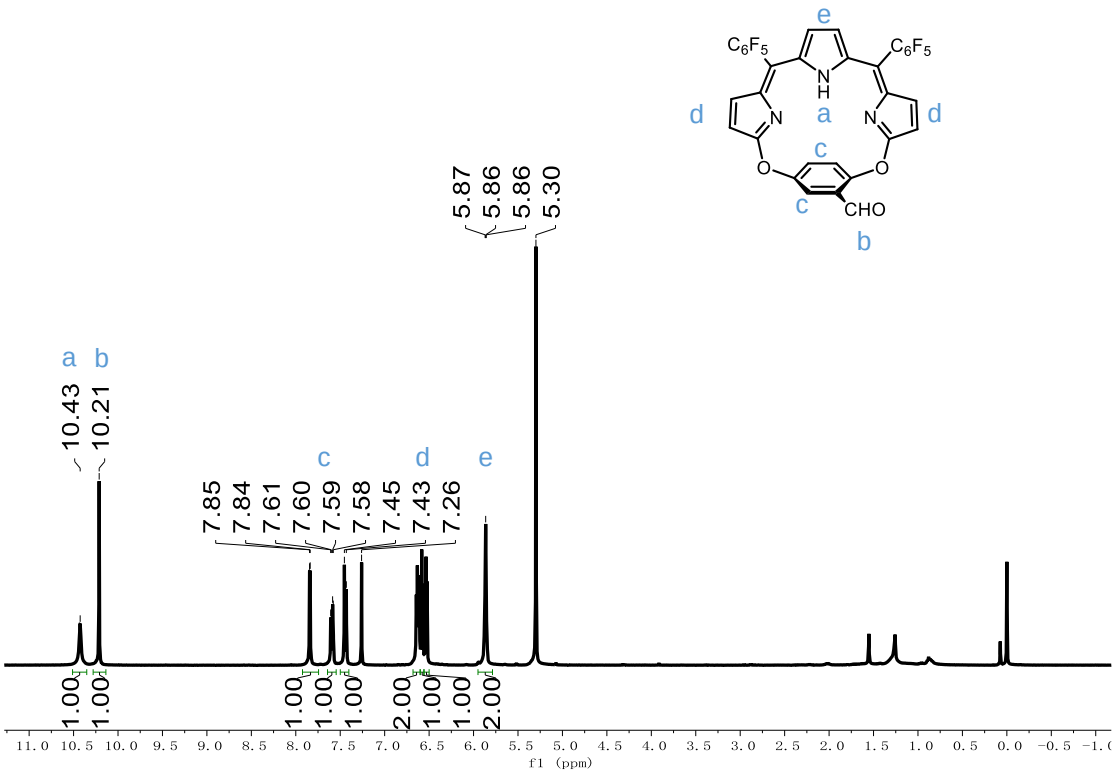


Figure S1. [1]H-NMR spectrum of **1**.

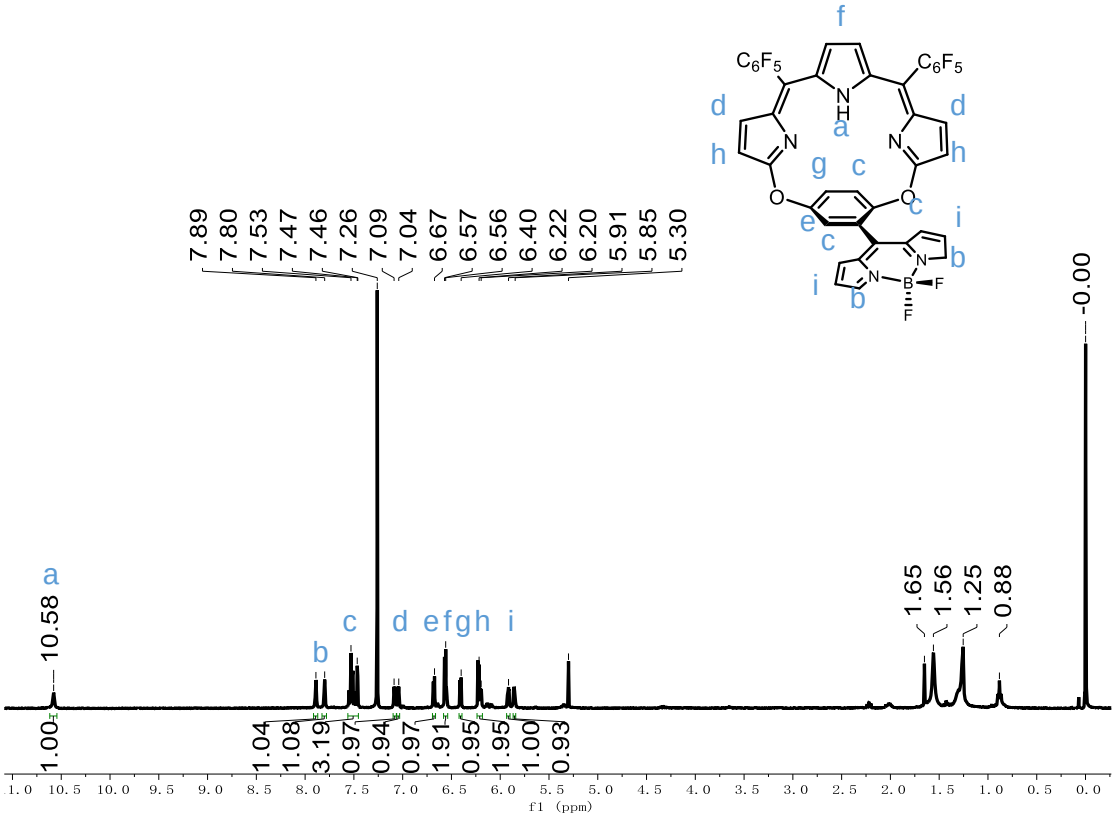


Figure S2. [1]H-NMR spectrum of **2.**

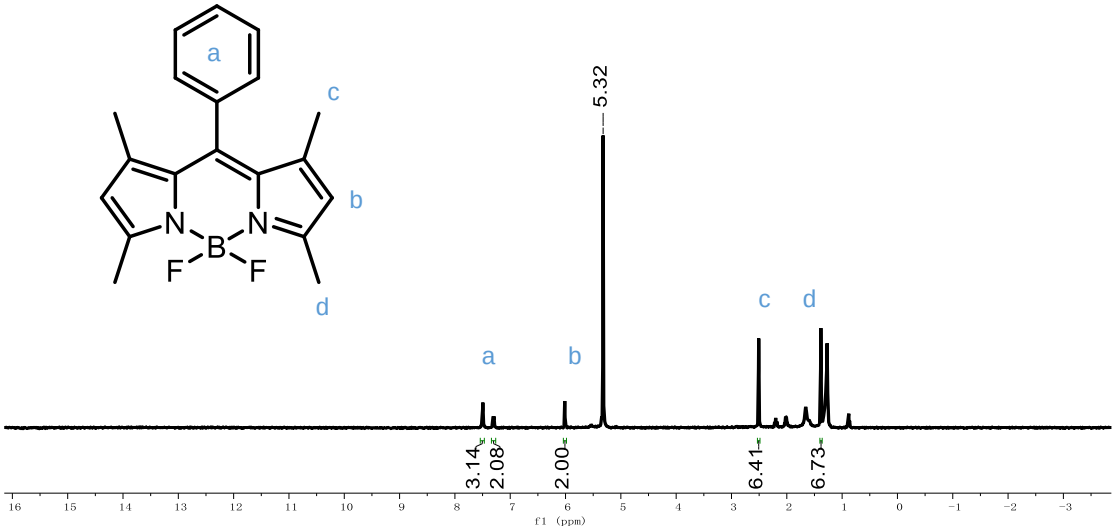


Figure S3. ^{1}H-NMR spectrum of **BODIPY-3.**

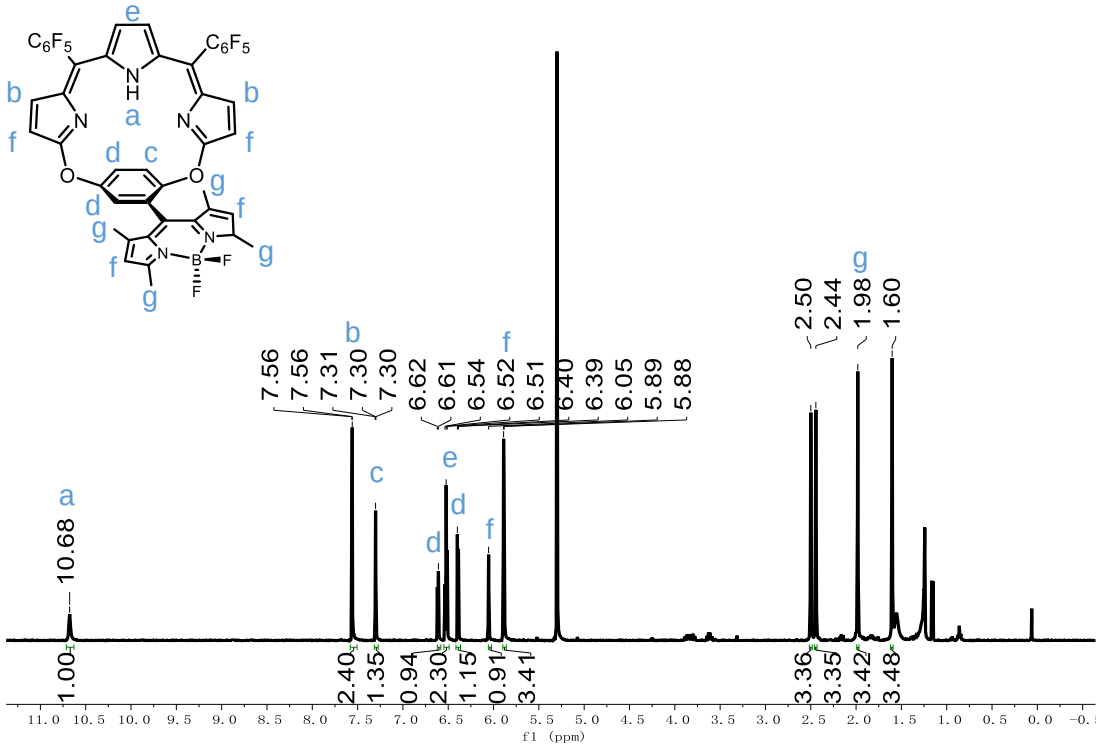


Figure S4. ^{1}H-NMR spectrum of **3.**

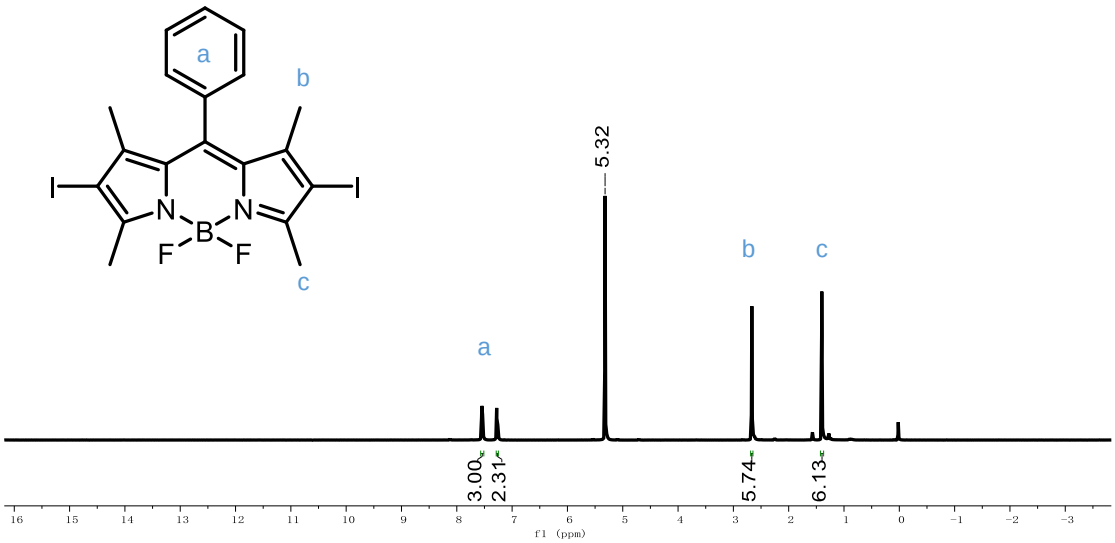


Figure S5. [1]H-NMR spectrum of **BODIPY-4.**

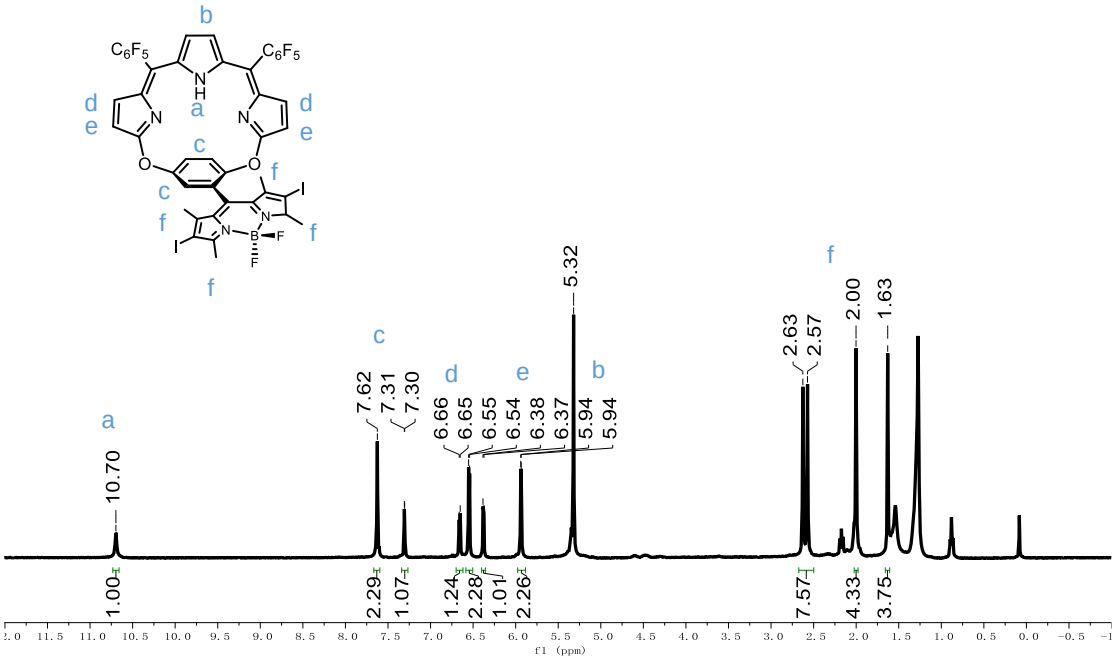


Figure S6. [1]H-NMR spectrum of **4.**

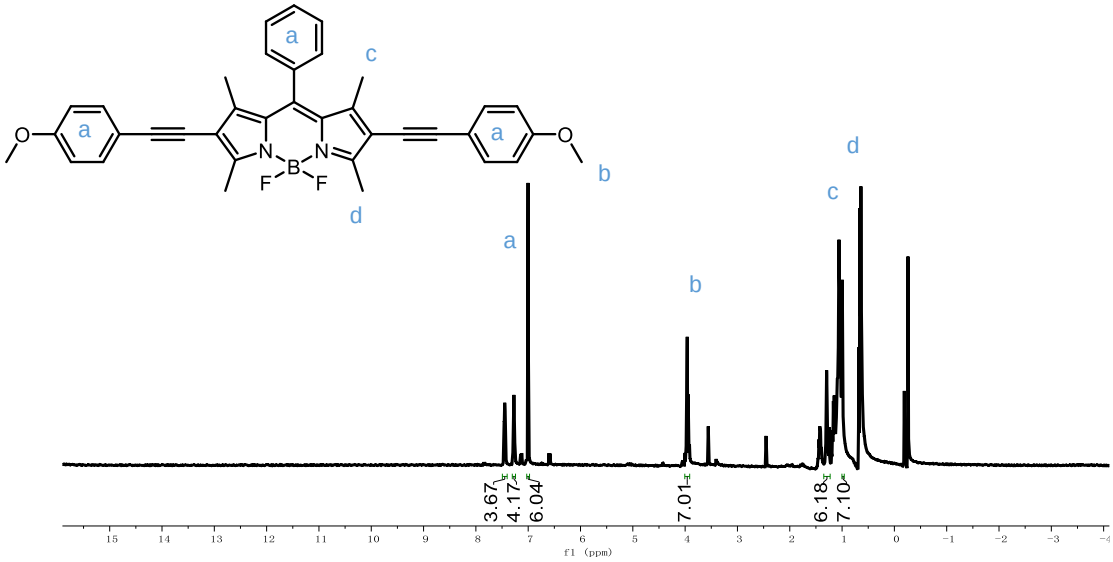


Figure S7. ^{1}H-NMR spectrum of **BODIPY-5.**

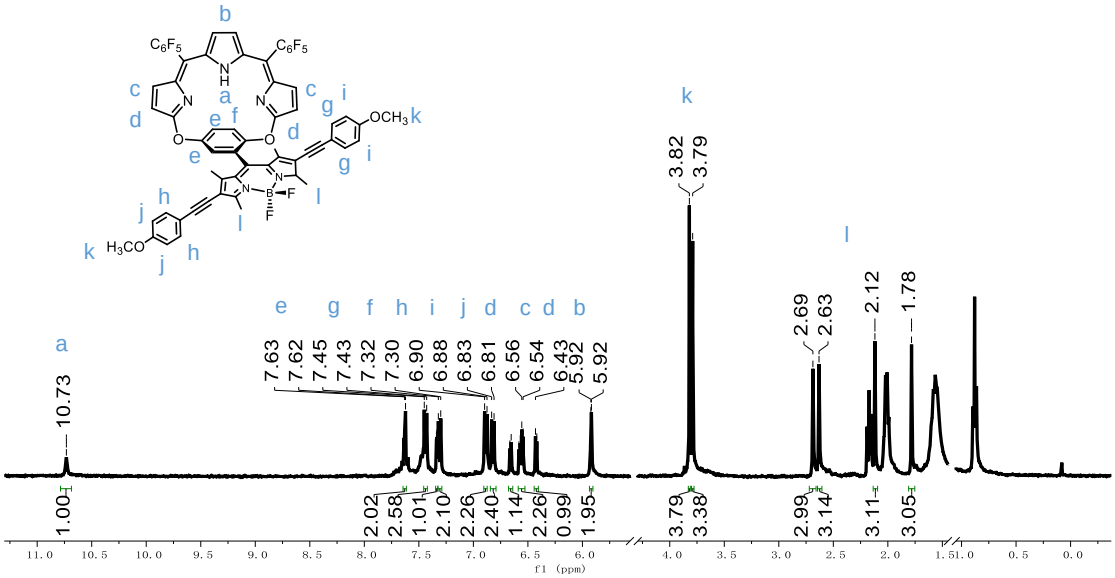


Figure S8. ^{1}H-NMR spectrum of **5.**

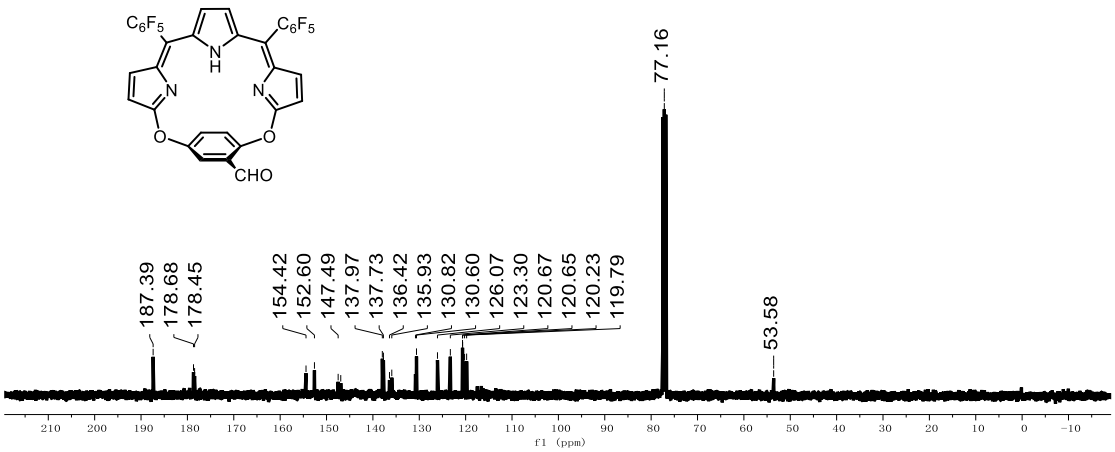


Figure S9. ^{13}C-NMR spectrum of **1**.

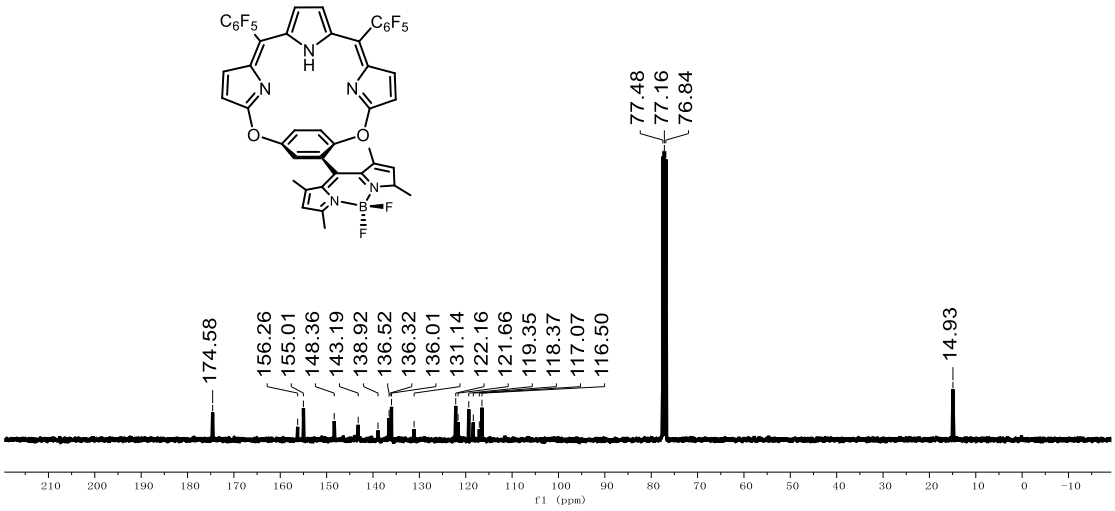


Figure S10. ^{13}C-NMR spectrum of **3.**

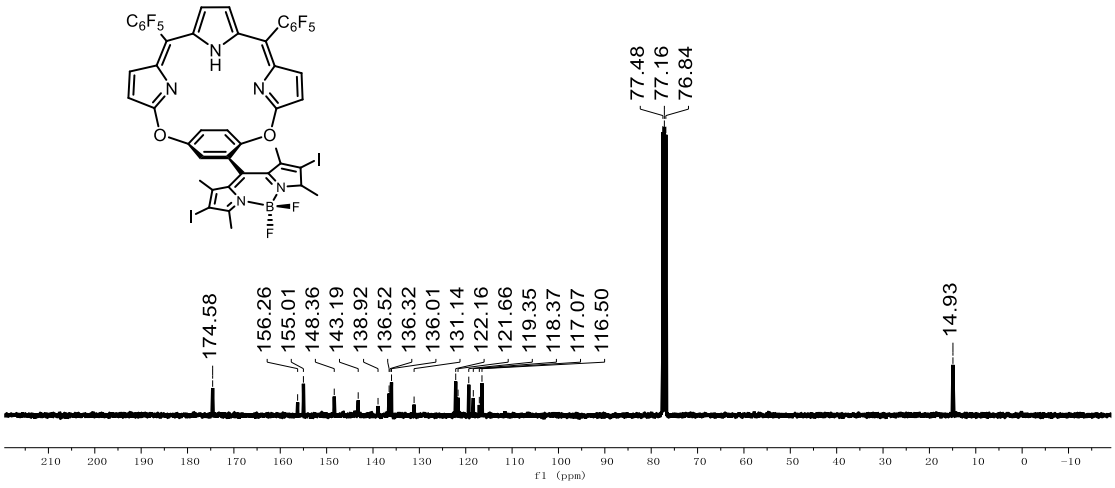


Figure S11. ^{13}C-NMR spectrum of **4.**

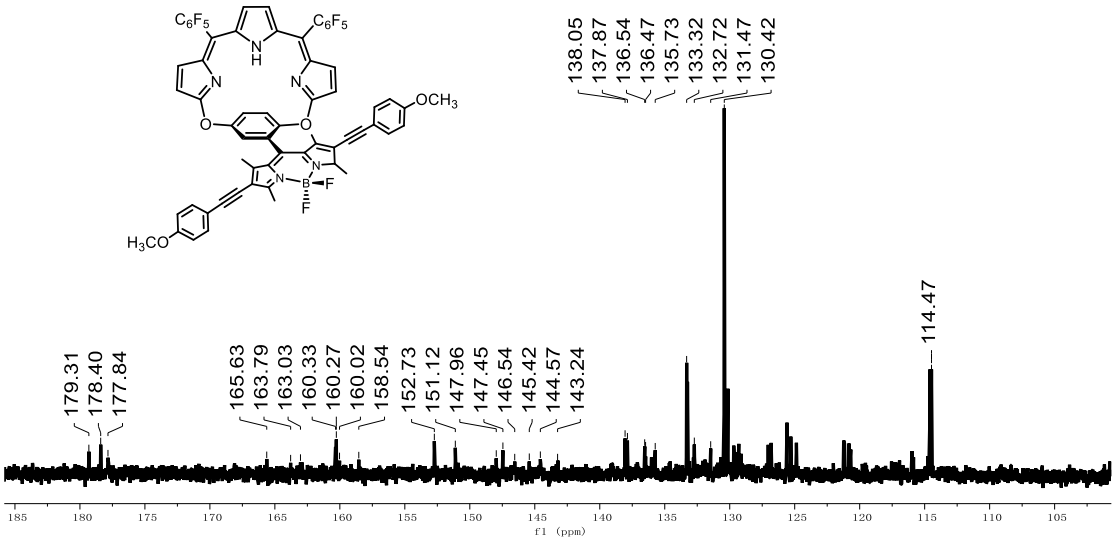


Figure S12. ^{13}C-NMR spectrum of **5.**

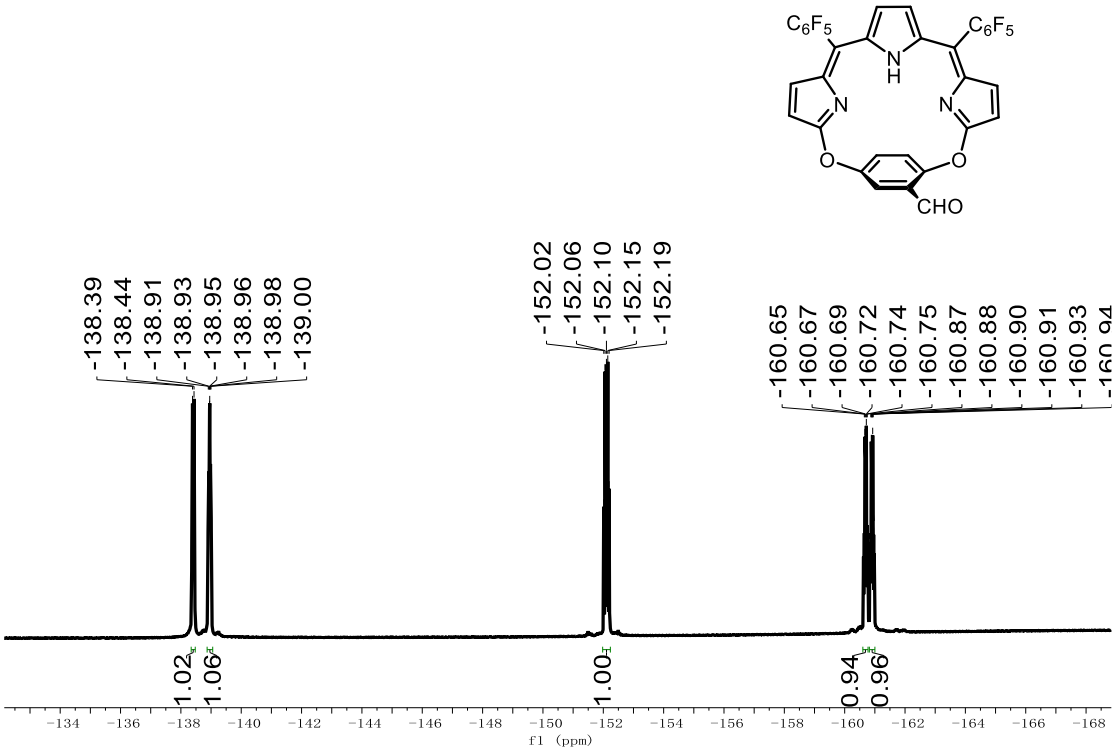


Figure S13. ^{19}F-NMR spectrum of **1**.

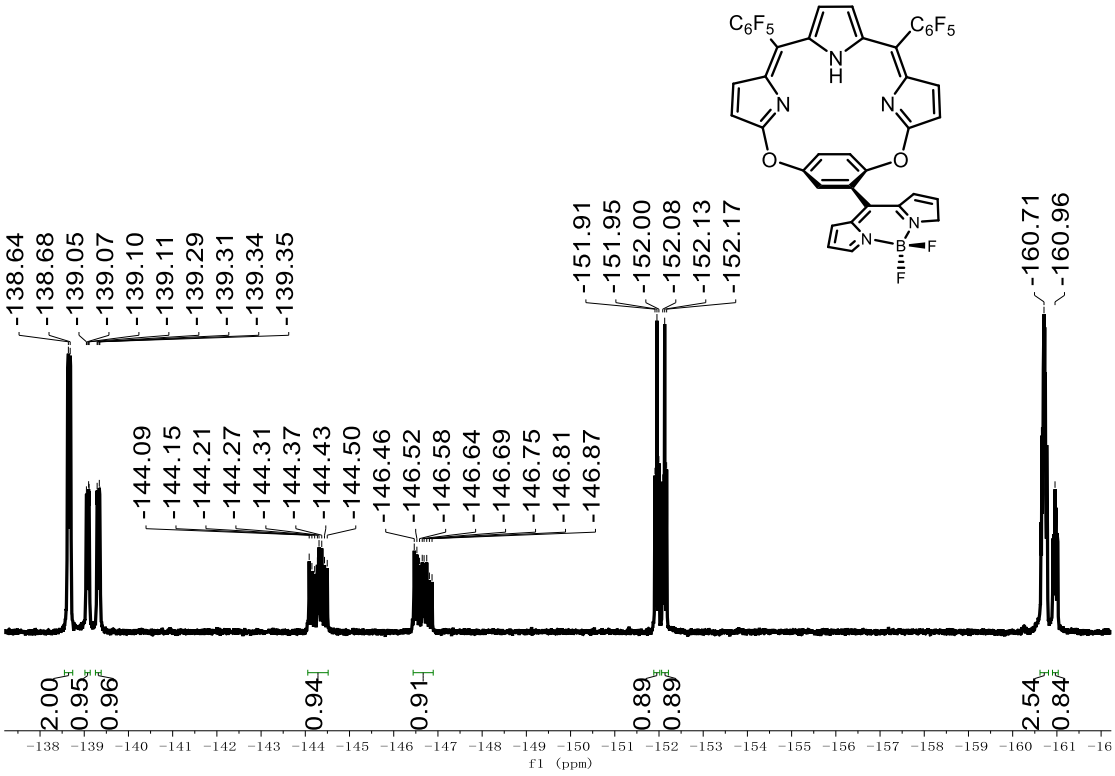


Figure S14. ^{19}F-NMR spectrum of **2.**

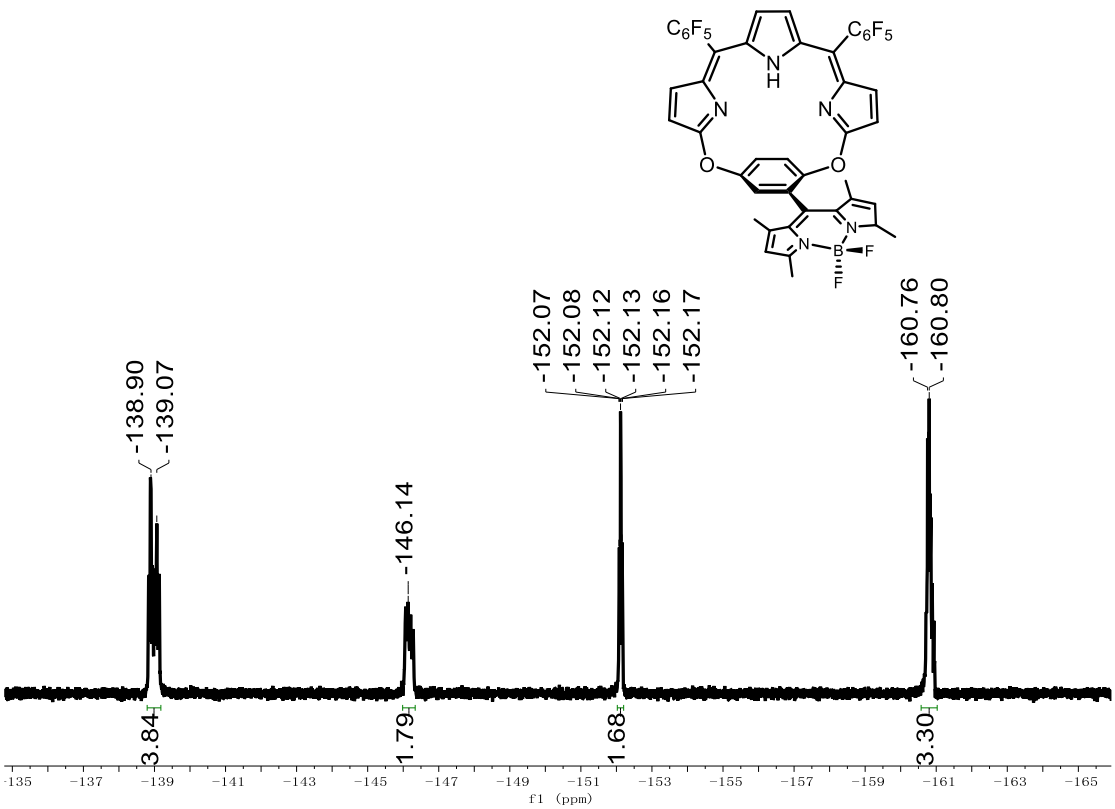


Figure S15. ^{19}F-NMR spectrum of **3.**

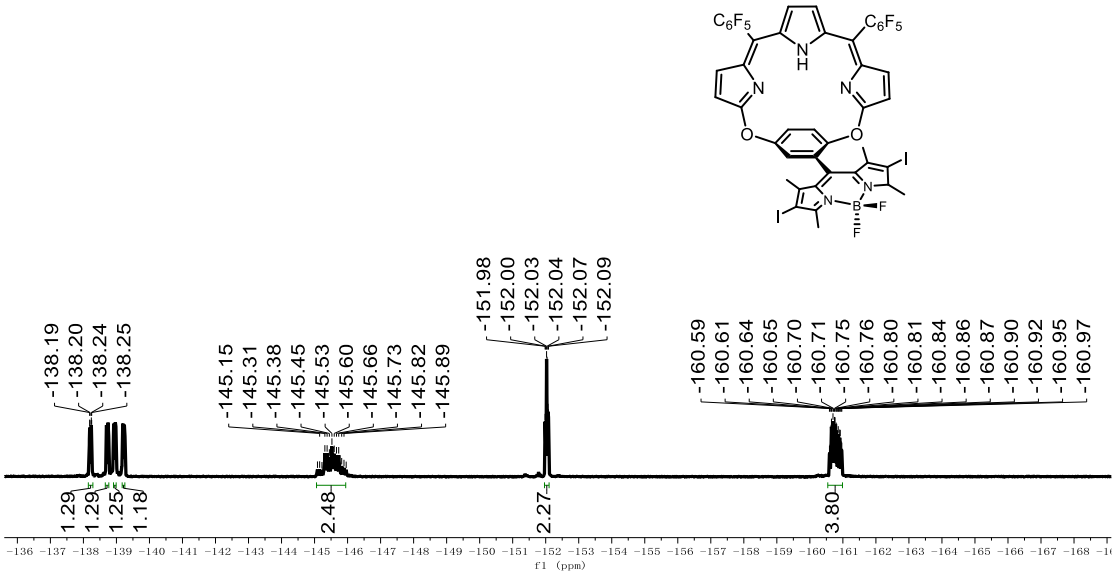


Figure S16. ^{19}F-NMR spectrum of **4.**

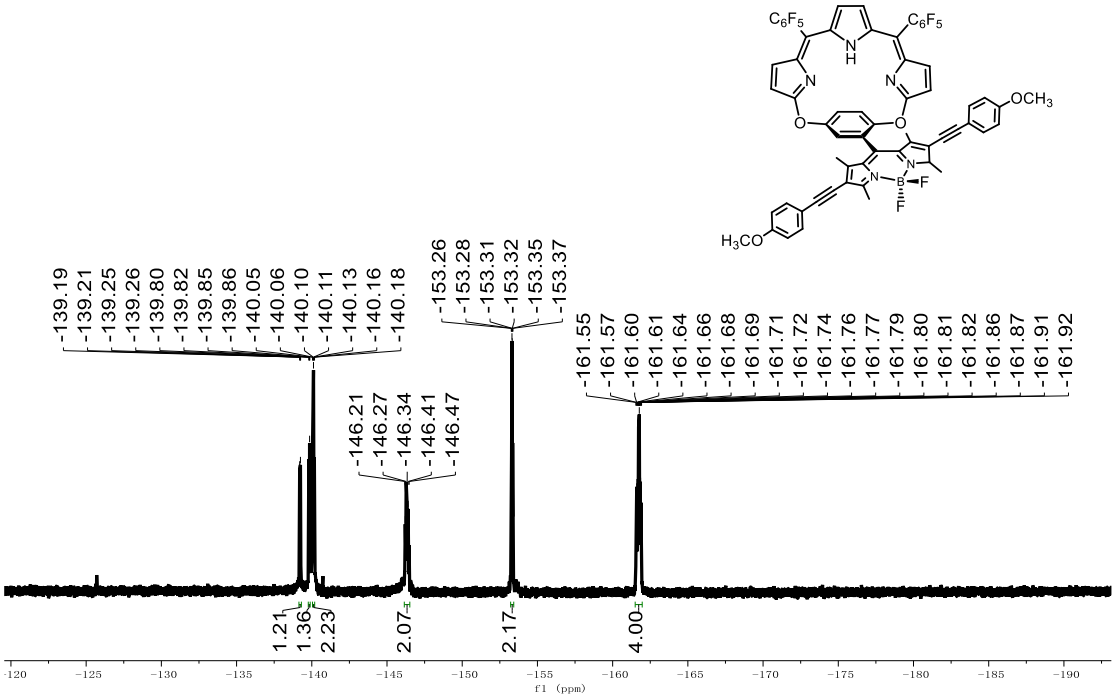
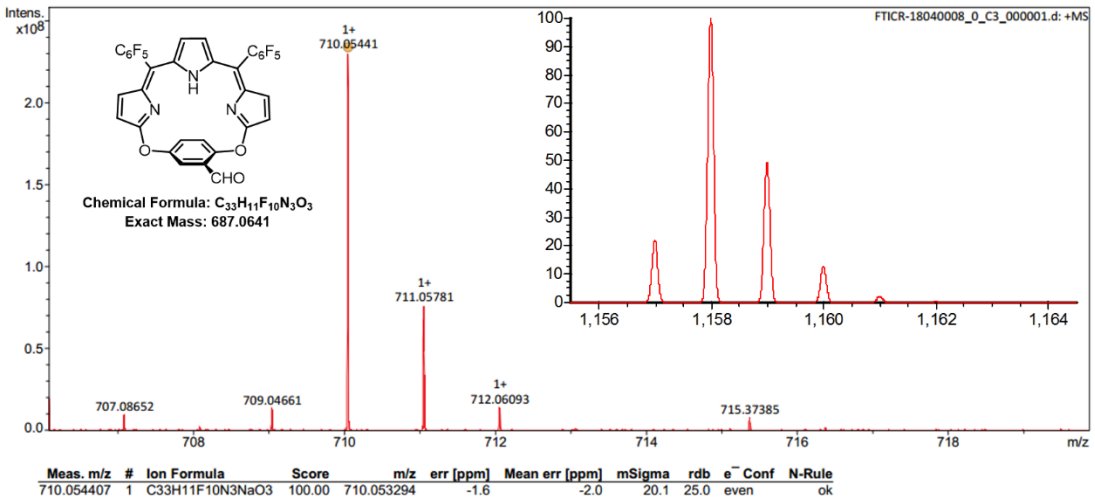
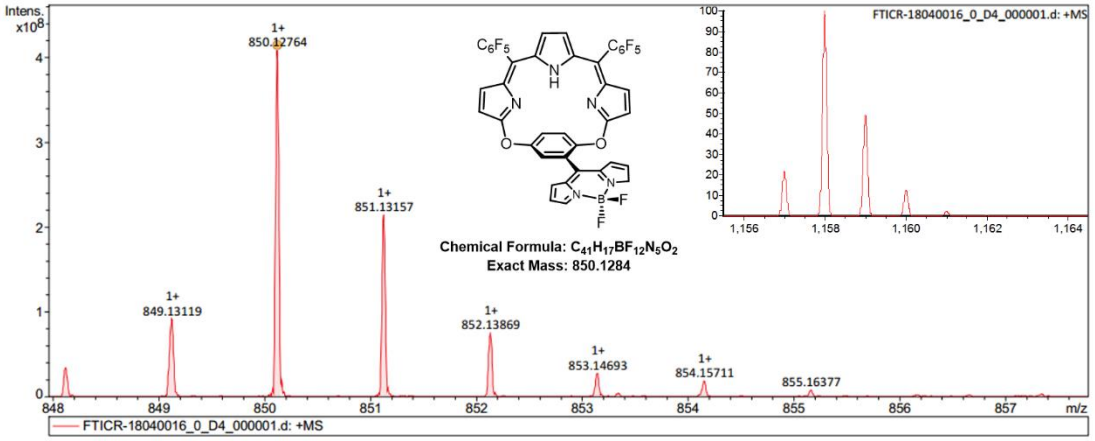


Figure S17. ^{19}F-NMR spectrum of **5.**



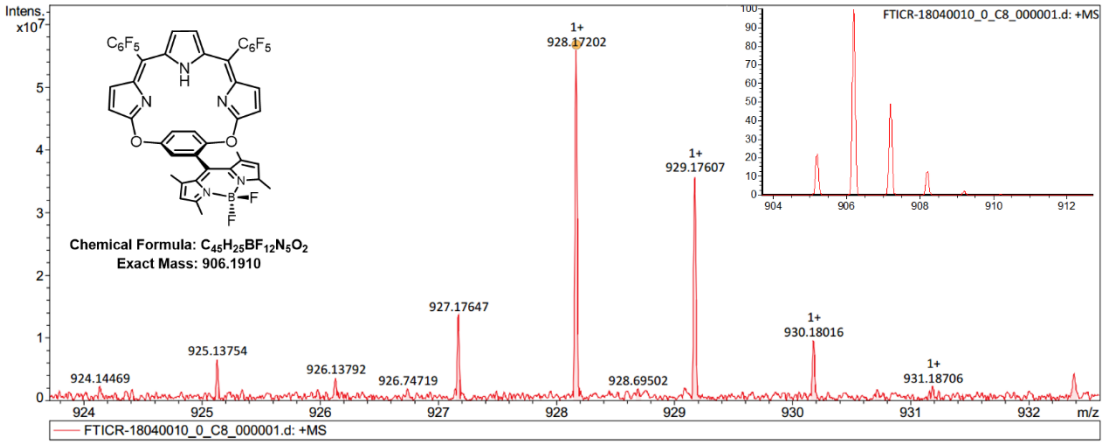
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
710.054407	1	C33H11F10N3NaO3	100.00	710.053294	-1.6	-2.0	20.1	25.0	even	ok

Figure S18. HR-MS (MALDI-TOF) of **1**.



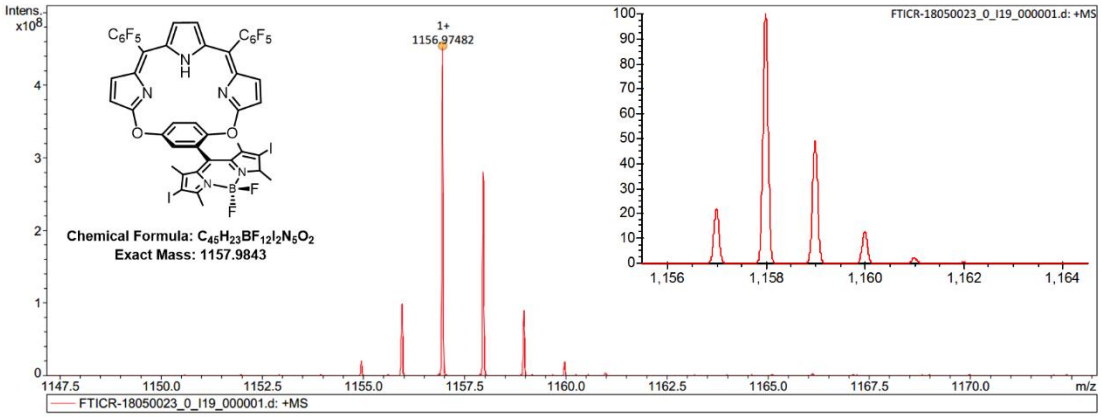
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
850.127638	1	C41H17BF12N5O2	100.00	850.127820	1.0	-0.4	53.0	31.0	even	ok

Figure S19. HR-MS (MALDI-TOF) of **2.**



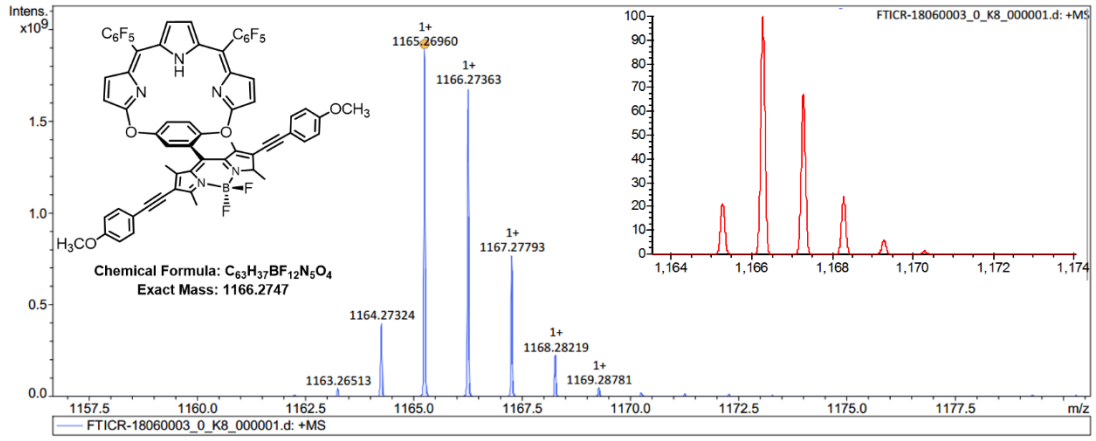
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
928.172017	1	C45H24BF12N5NaO2	100.00	928.172365	1.2	-0.7	76.9	31.0	even	ok

Figure S20. HR-MS (MALDI-TOF) of **3.**



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
1156.974824	1	C45H22BF12I2N5O2	100.00	1156.975891	1.6	0.6	n.a.	31.5	odd	ok

Figure S21. HR-MS (MALDI-TOF) of **4.**



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
1165.269599	1	C63H36BF12N5O4	100.00	1165.266325	-1.9	-3.6	123.2	43.5	odd	ok

Figure S22. HR-MS (MALDI-TOF) of **5.**

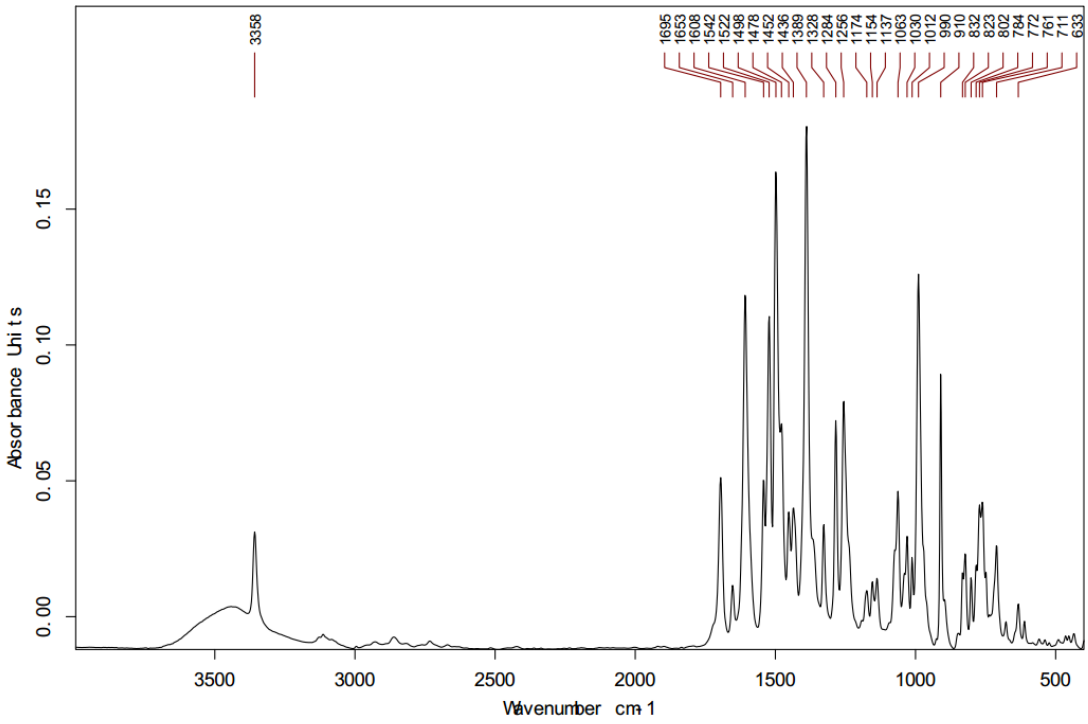


Figure S23. FT-IR spectrum of **1**.

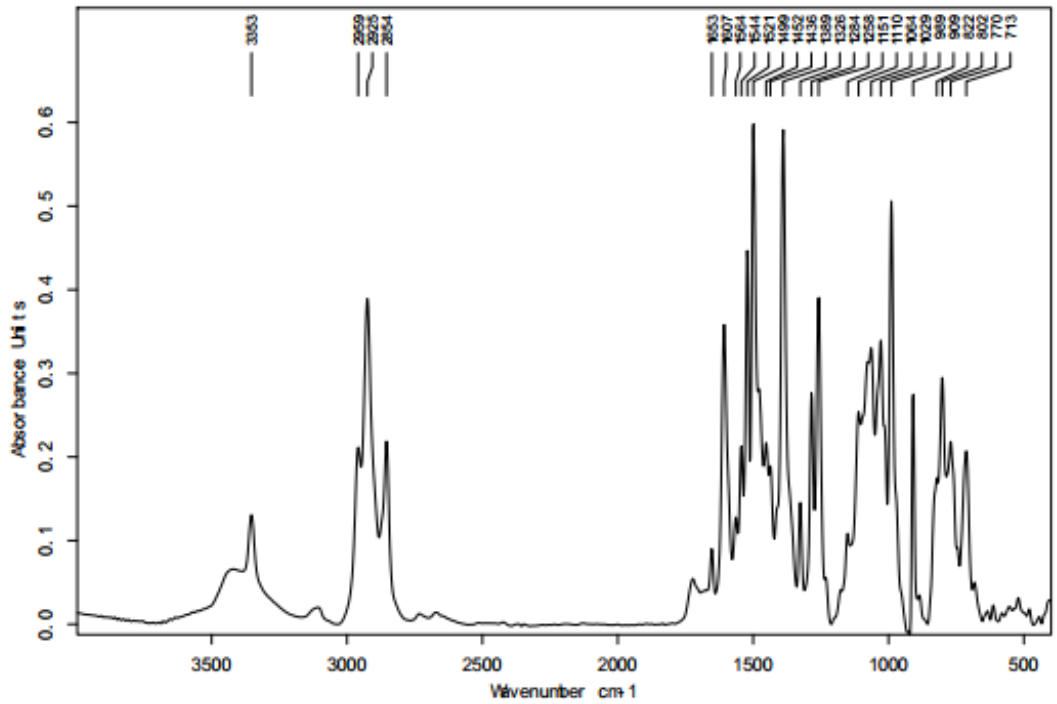


Figure S24. FT-IR spectrum of **2.**

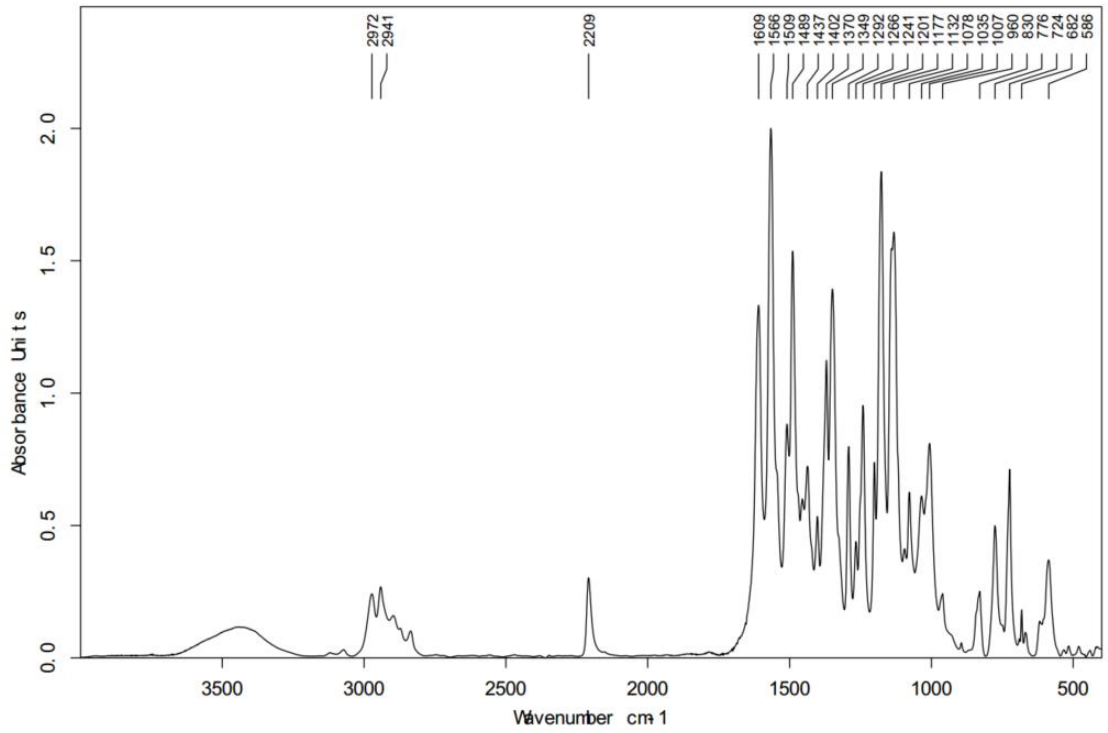


Figure S25. FT-IR spectrum of **3.**

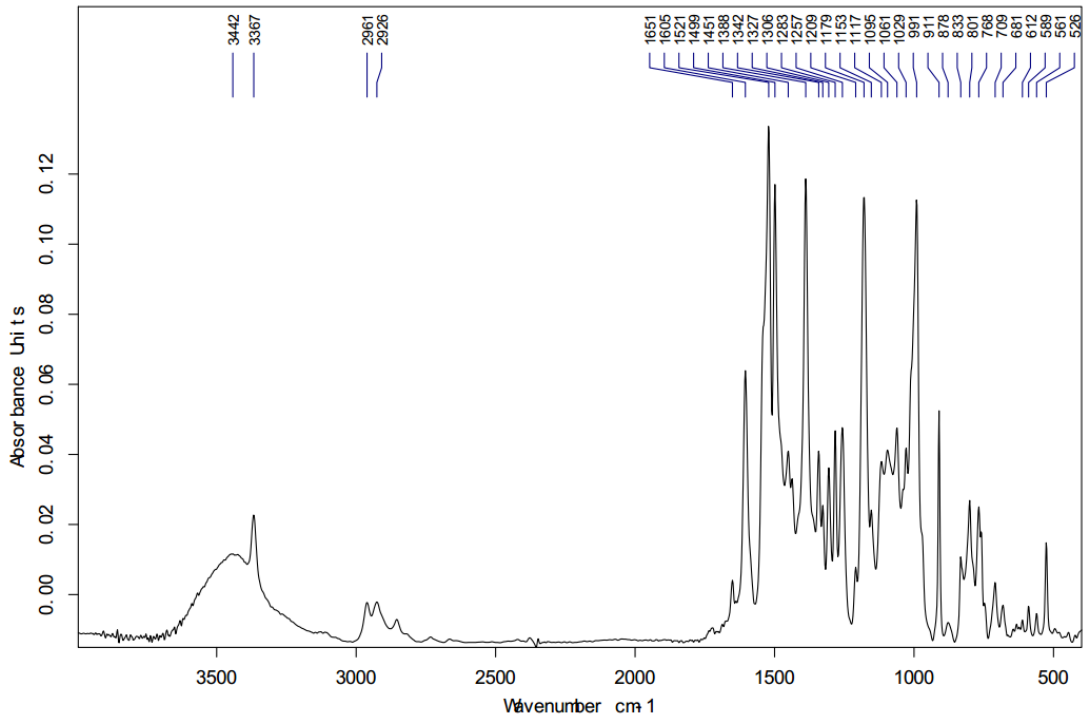


Figure S26. FT-IR spectrum of **4.**

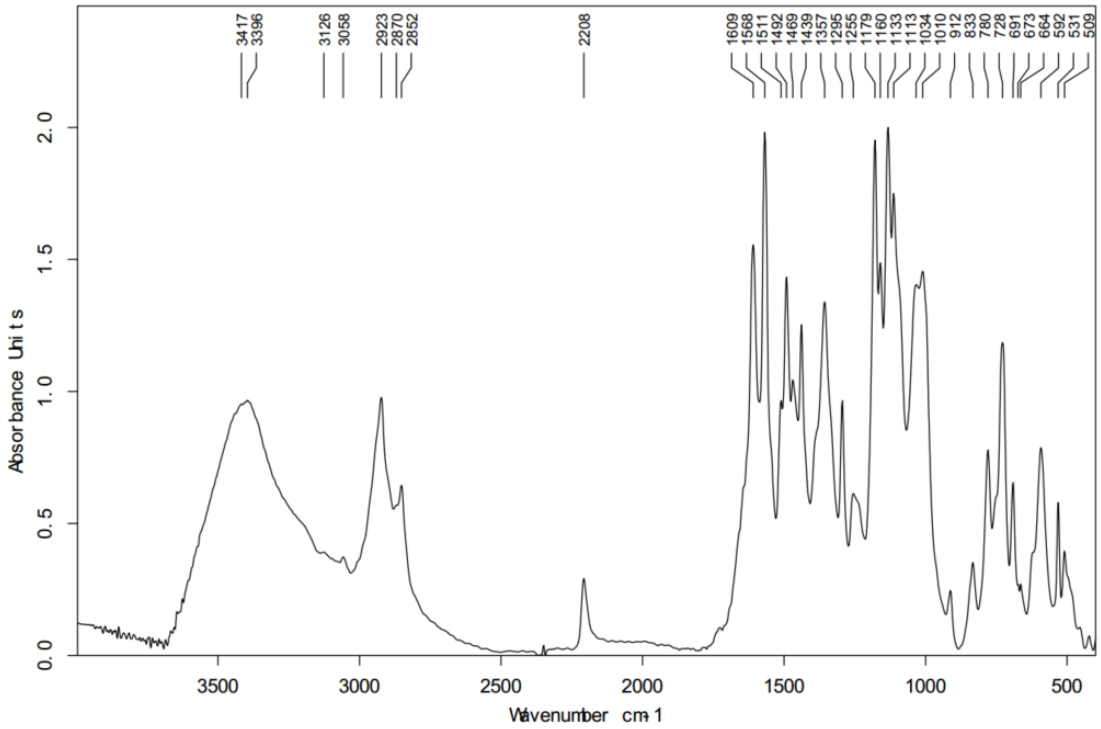


Figure S27. FT-IR spectrum of **5.**

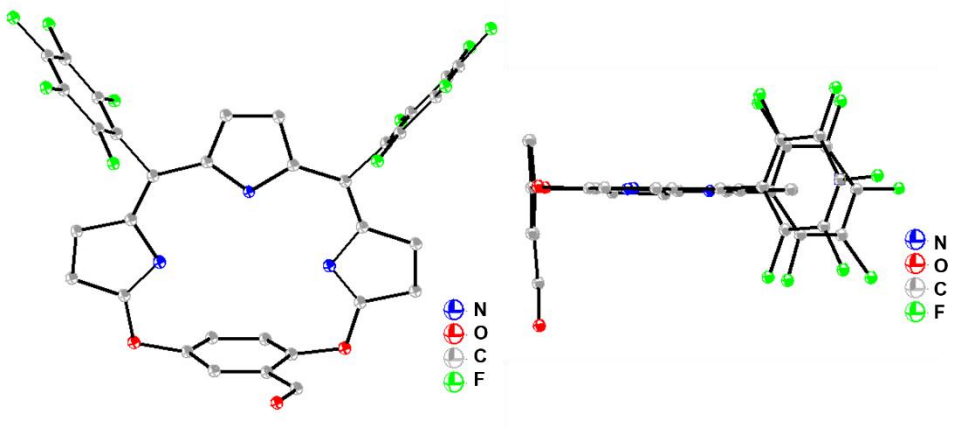


Figure S28. Single crystal structure of **1**. The thermal ellipsoids are scaled to the 50% probability level and solvent molecules are omitted for clarity.

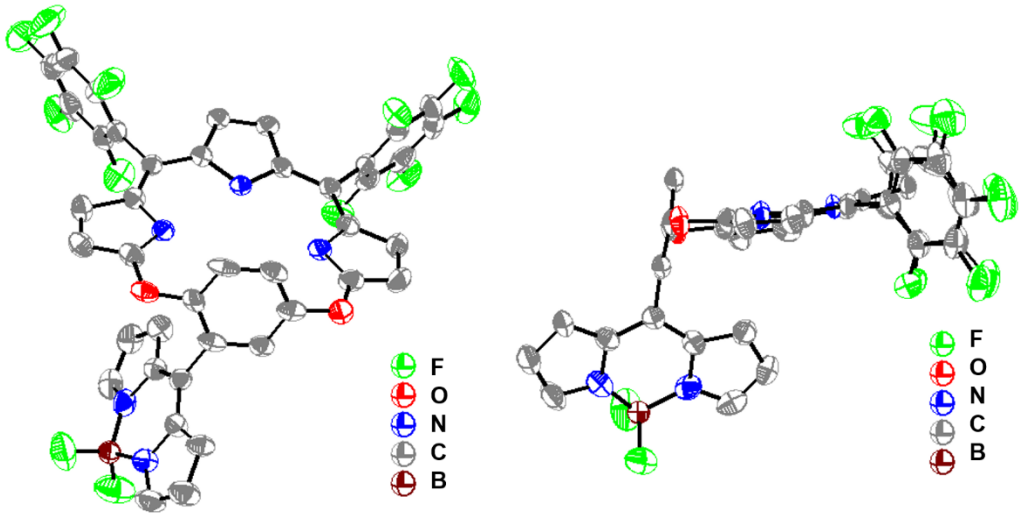


Figure S29. Single crystal structure of **2**. The thermal ellipsoids are scaled to the 50% probability level and solvent molecules are omitted for clarity.

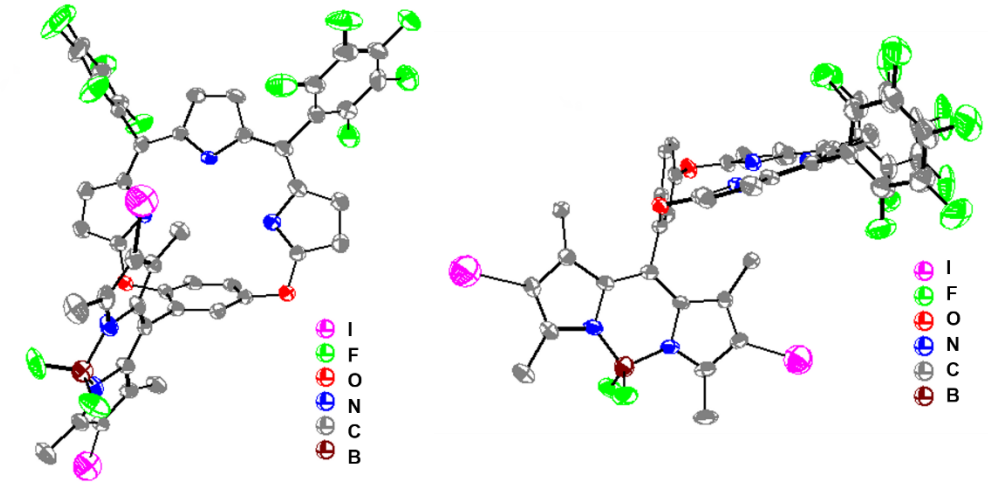


Figure S30. Single crystal structure of **4**. The thermal ellipsoids are scaled to the 50% probability level and solvent molecules are omitted for clarity.

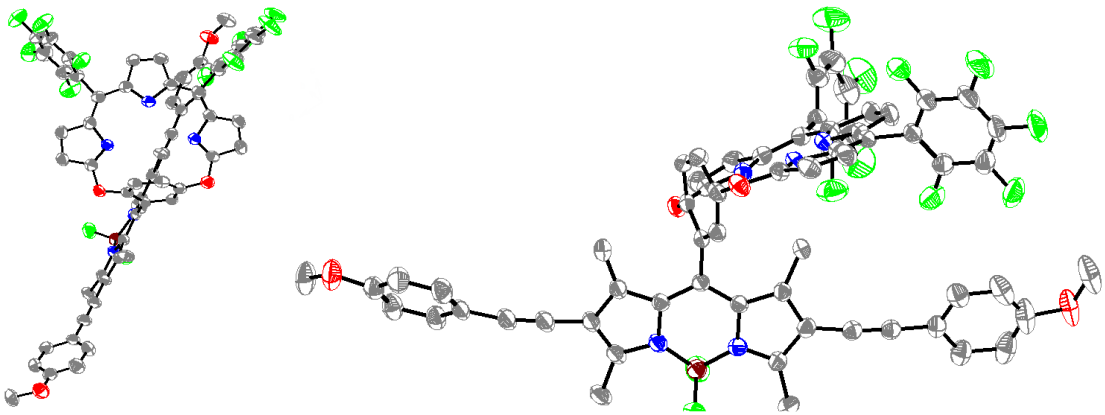


Figure S31. Single crystal structure of **5**. The thermal ellipsoids are scaled to the 50% probability level and solvent molecules are omitted for clarity.

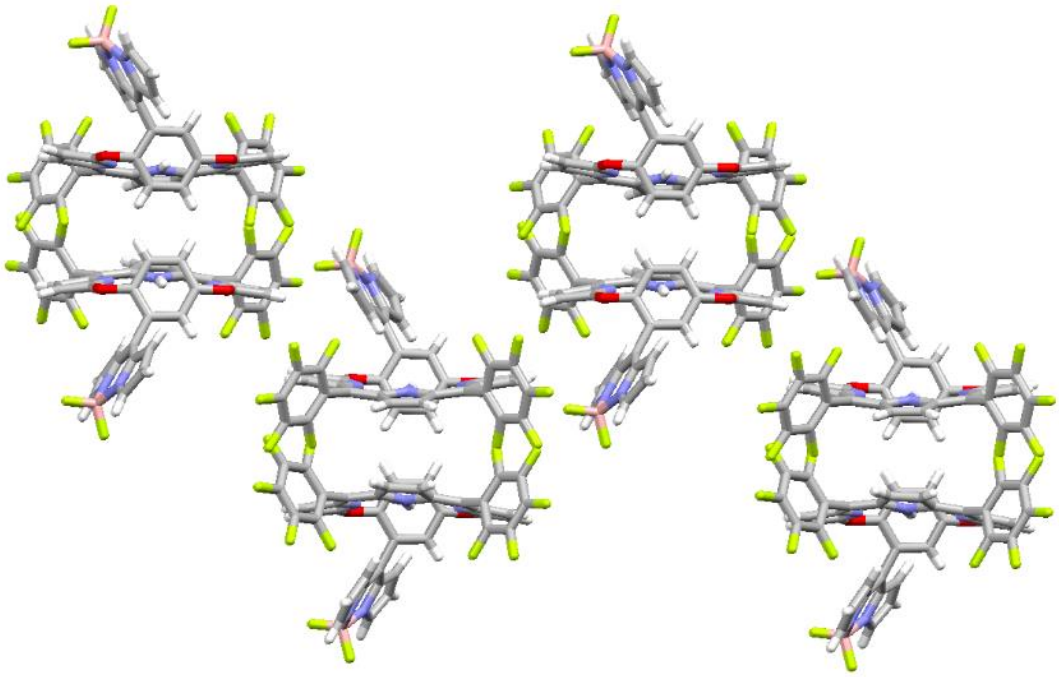


Figure S32. Crystal packing pattern of **2**.

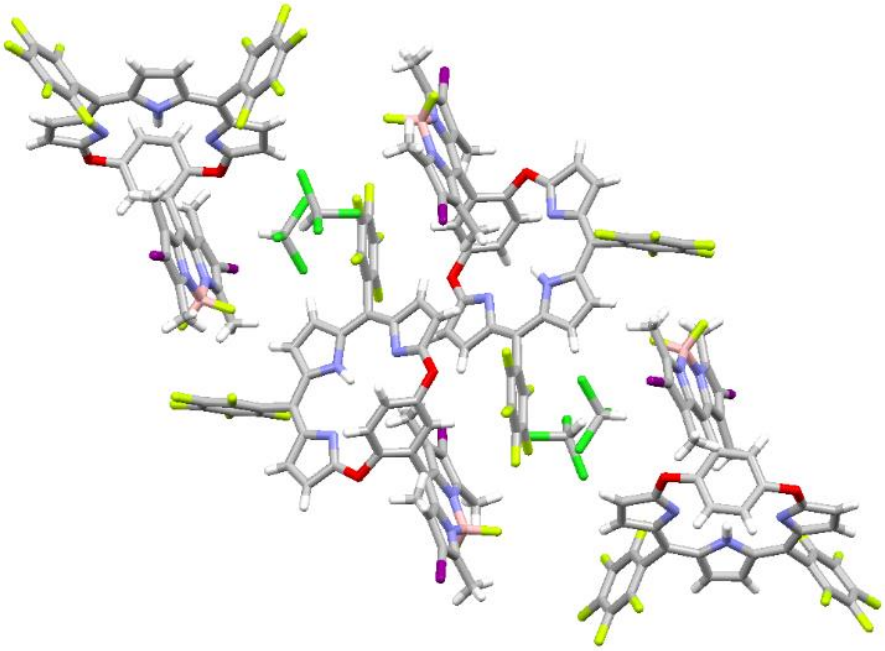


Figure S33. Crystal packing pattern of **4**.

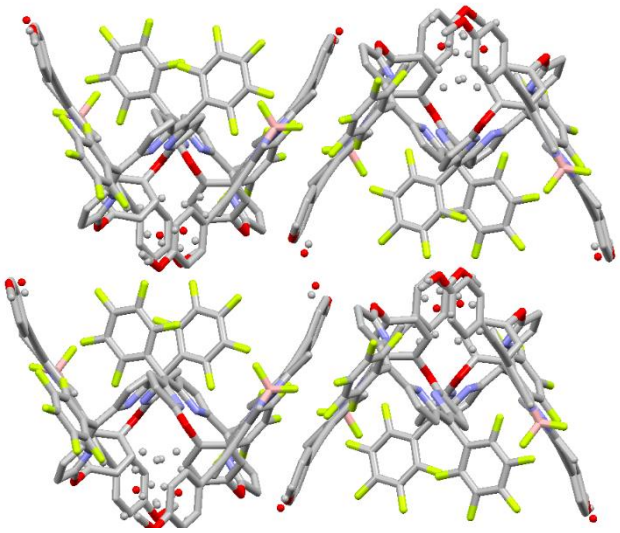


Figure S34. Crystal packing pattern of **5**.

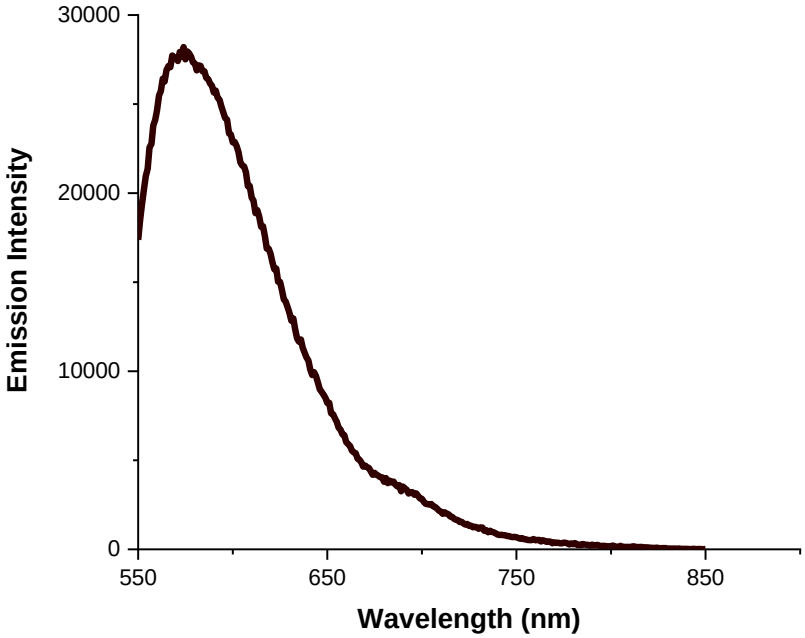


Figure S35. Emission spectra of **2** excited at 530 nm in CH_2Cl_2.

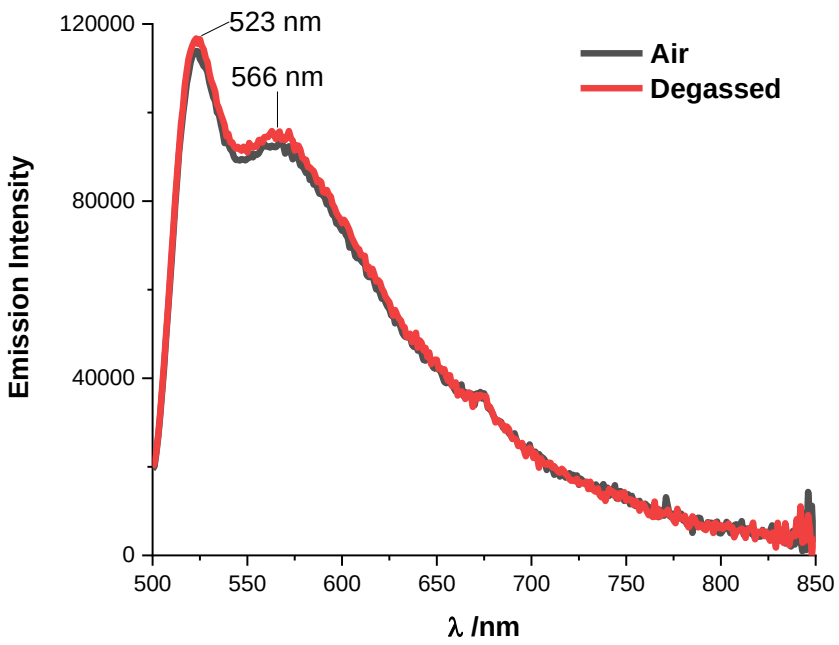


Figure S36. Emission spectra of **3** in air and degassed conditions excited at 500 nm in CH_2Cl_2.

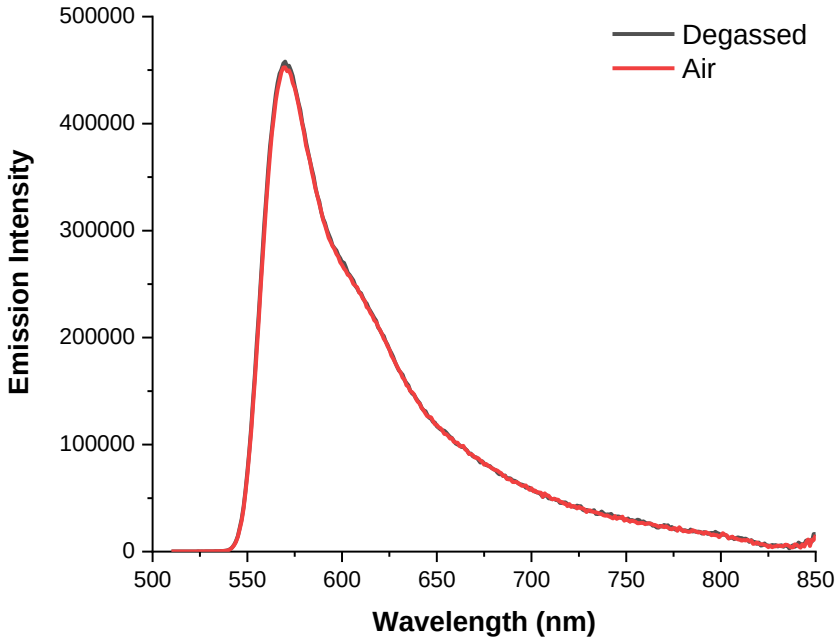


Figure S37. Emission spectra of **4** in air and degassed conditions excited at 500 nm in CH_2Cl_2.

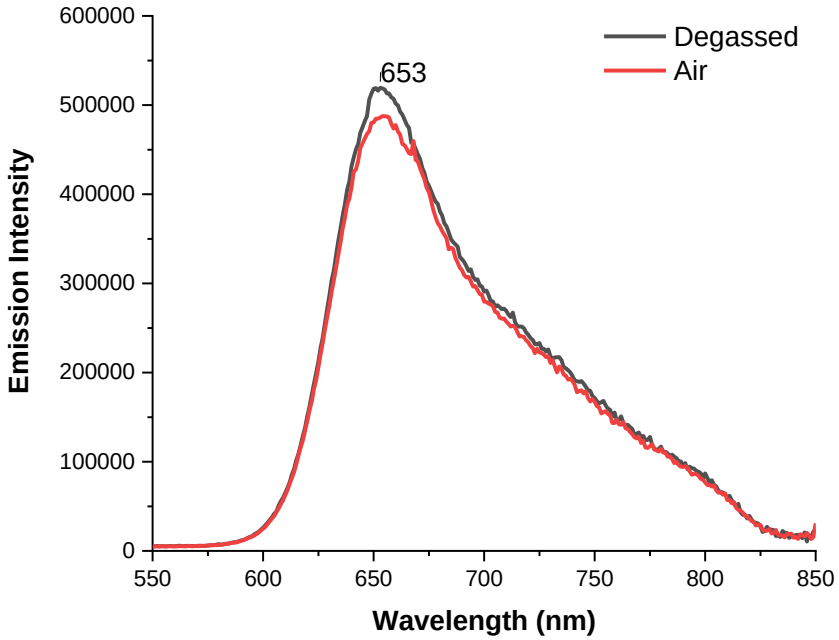


Figure S38. Emission spectra of **5** in air and degassed conditions excited at 500 nm in CH_2Cl_2.

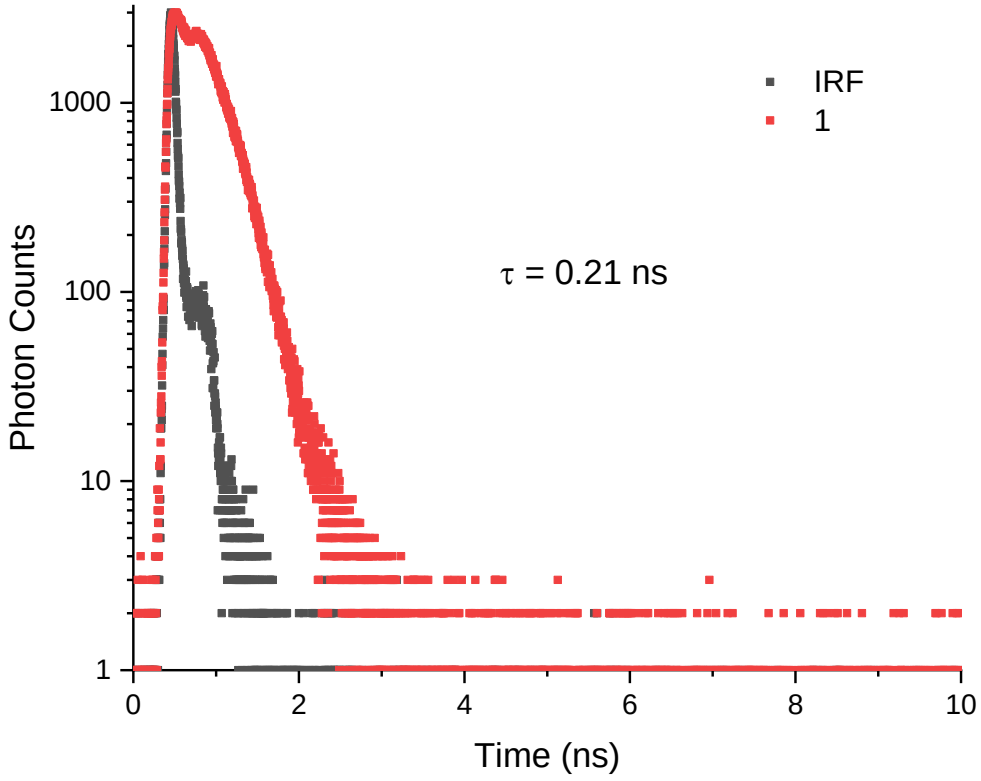


Figure S39. Lifetime measurement of **1** in CH_2Cl_2.

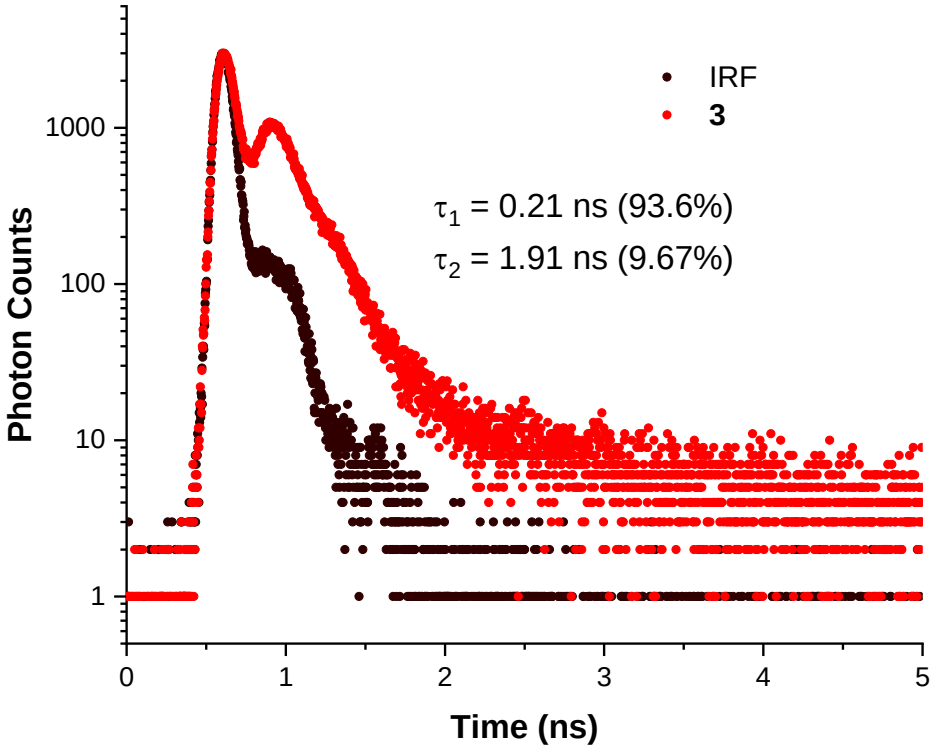


Figure S40. Lifetime measurement of **3** in CH_2Cl_2.

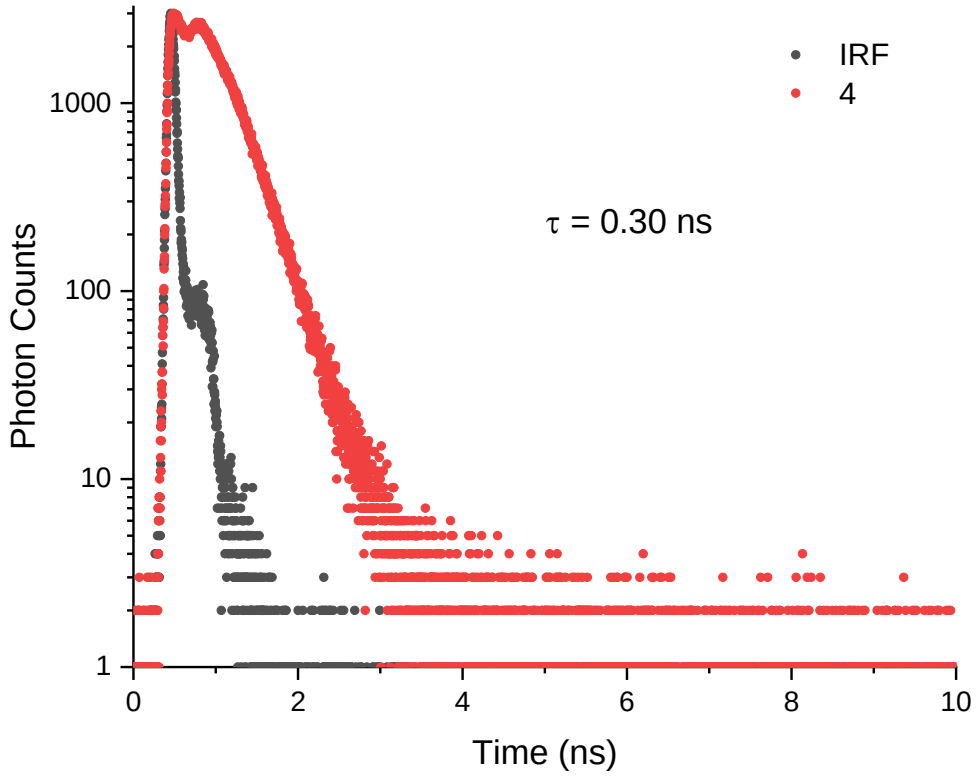


Figure S41. Lifetime measurement of **4** in CH_2Cl_2.

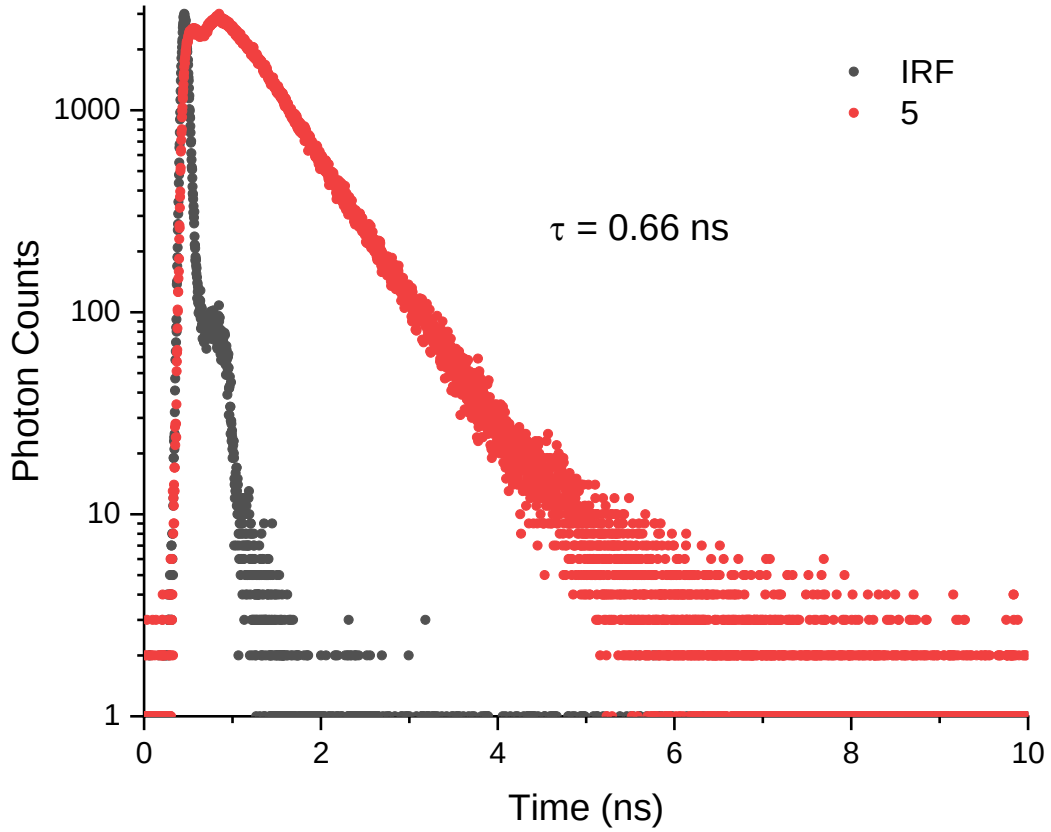


Figure S42. Lifetime measurement of **5** in CH_2Cl_2.

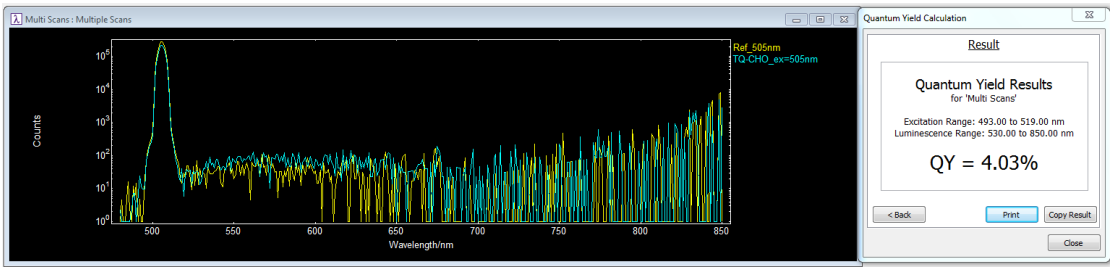


Figure S43. Absolute quantum yield of **1** in CH_2Cl_2.

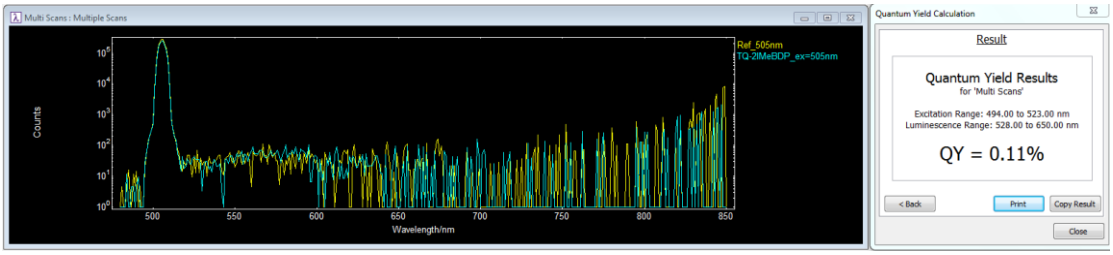


Figure S44. Absolute quantum yield of **3** in CH_2Cl_2.

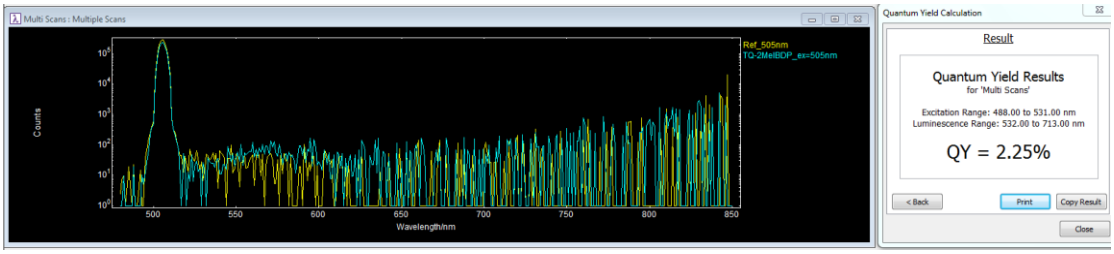


Figure S45. Absolute quantum yield of **4** in CH_2Cl_2.

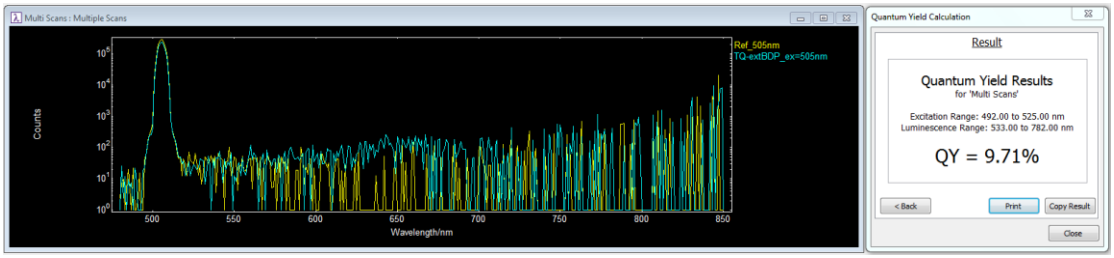


Figure S46. Absolute quantum yield of **5** in CH_2Cl_2.

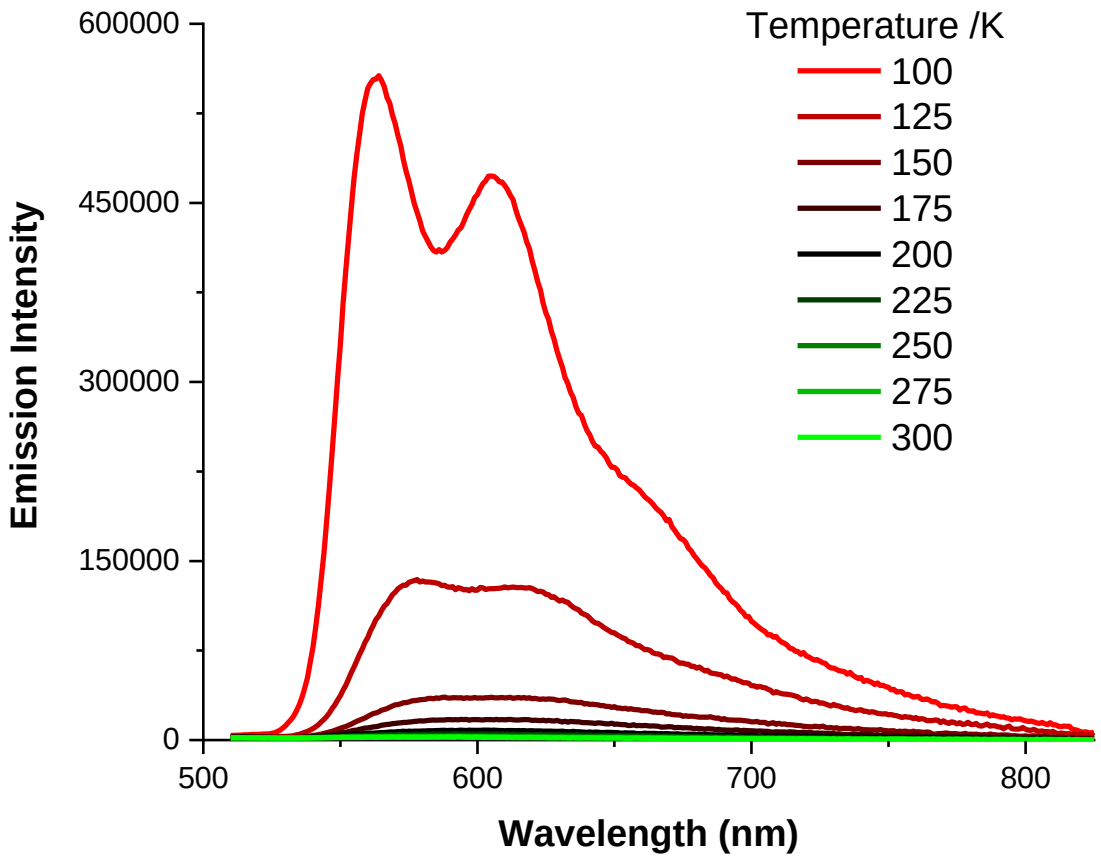


Figure S47. Temperature-dependent emission spectra of **3** in dimethyltetrahydrofuran collected from 78 to 300 K, excited at 500 nm.

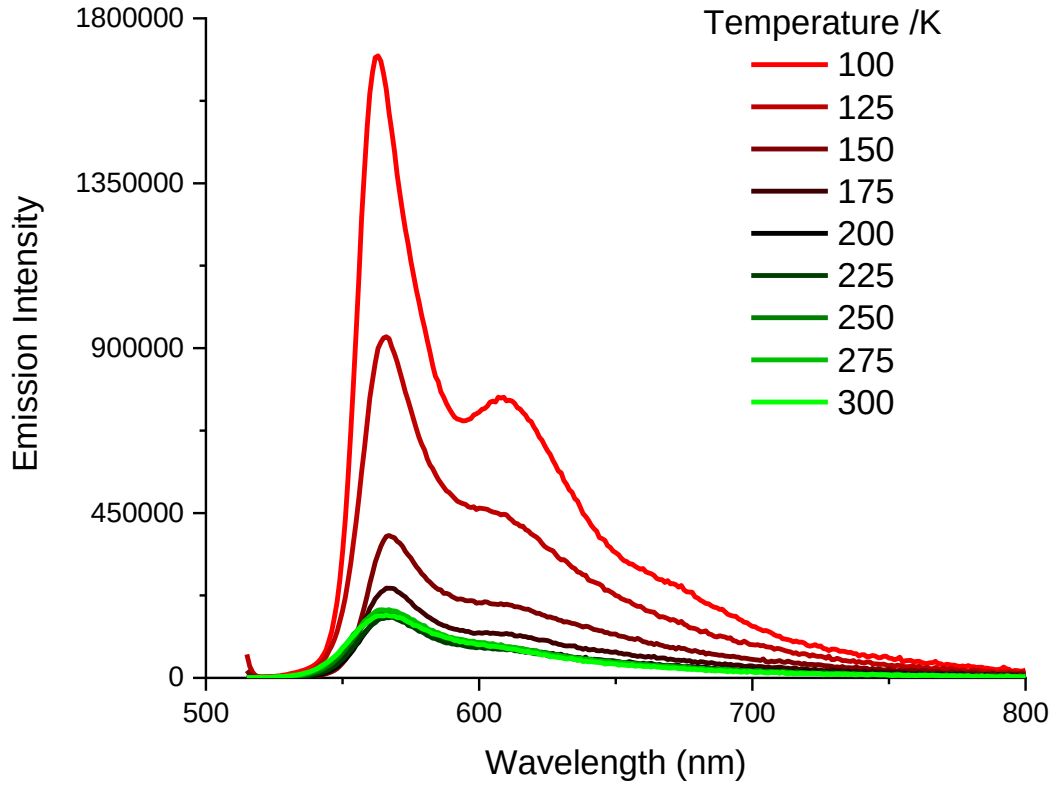


Figure S48. Temperature-dependent emission spectra of **4** in dimethyltetrahydrofuran collected from 78 to 300 K, excited at 500 nm.

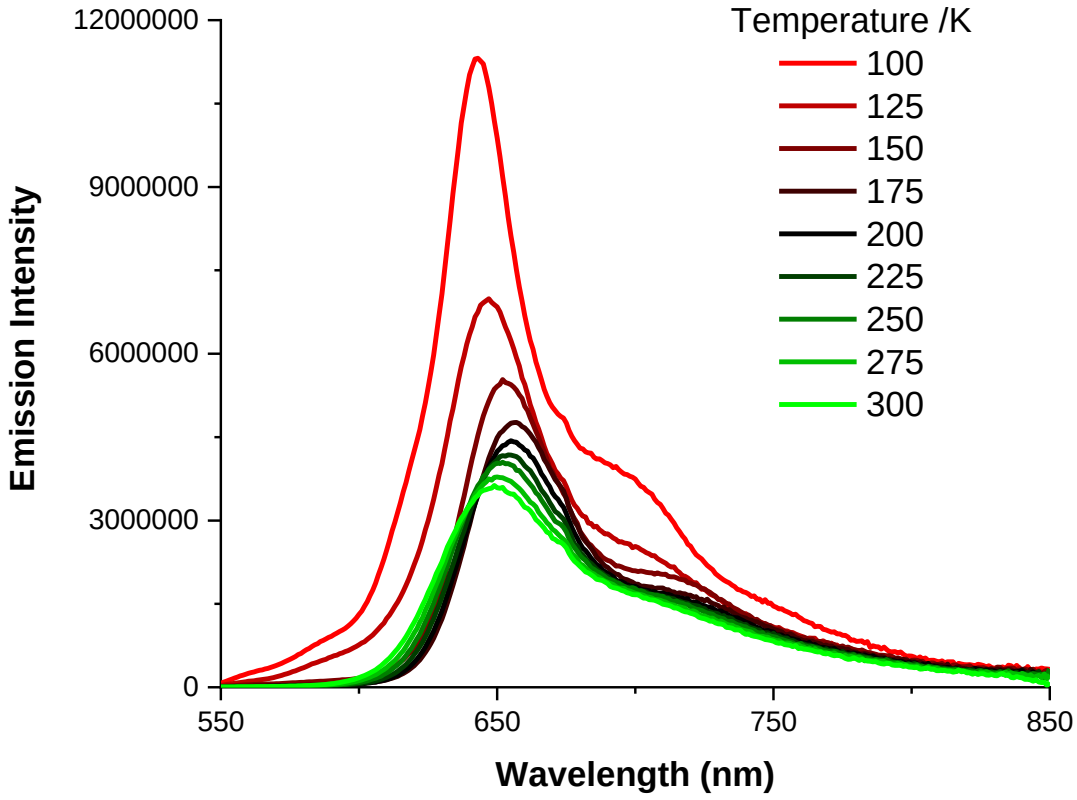


Figure S49. Temperature-dependent emission spectra of **5** in dimethyltetrahydrofuran collected from 78 to 300 K, excited at 500 nm.

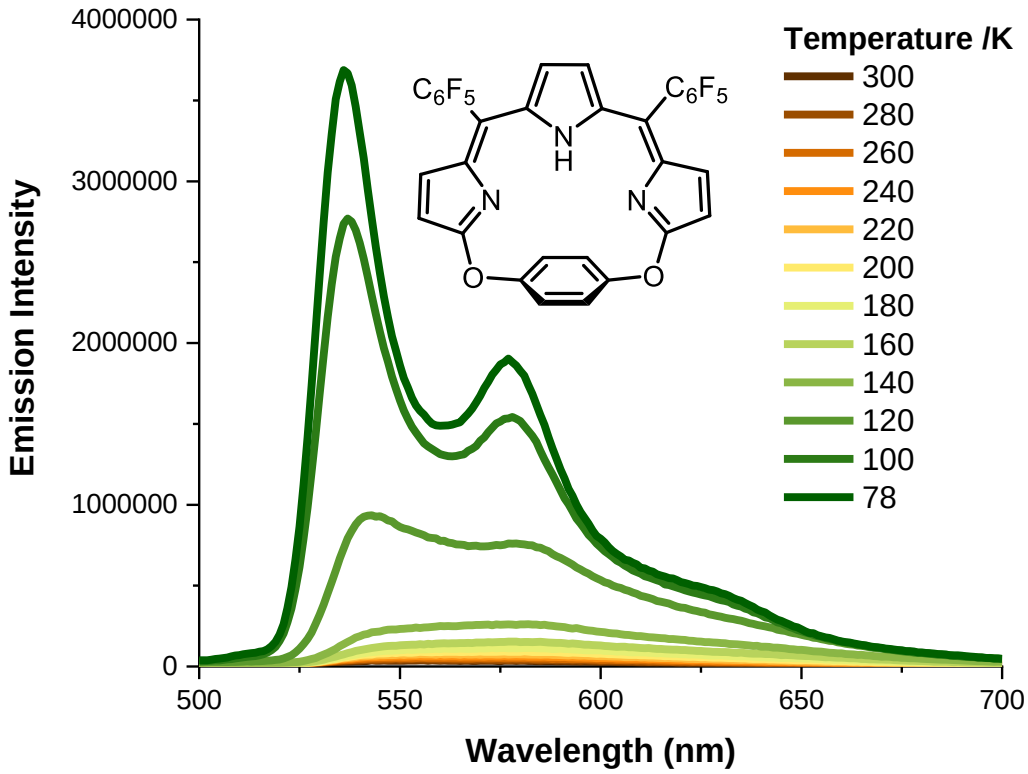


Figure S50. Temperature-dependent emission spectra of the tripyrrins in dimethyltetrahydrofuran collected from 78 to 300 K, excited at 495 nm.

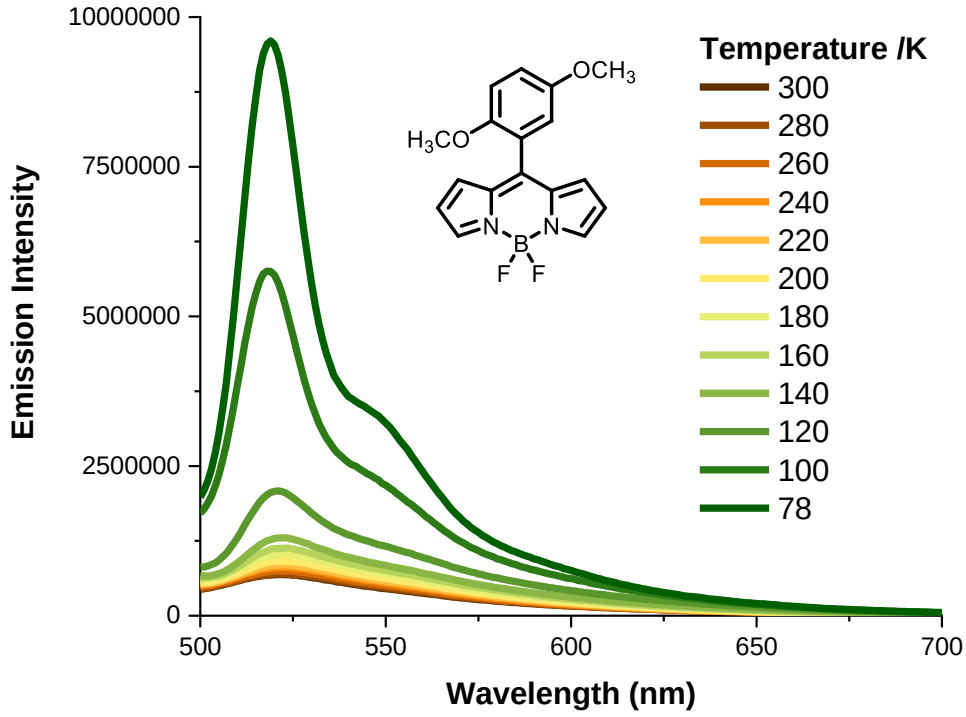


Figure S51. Temperature-dependent emission spectra of the BODIPY in dimethyltetrahydrofuran collected from 78 to 300 K, excited at 495 nm.

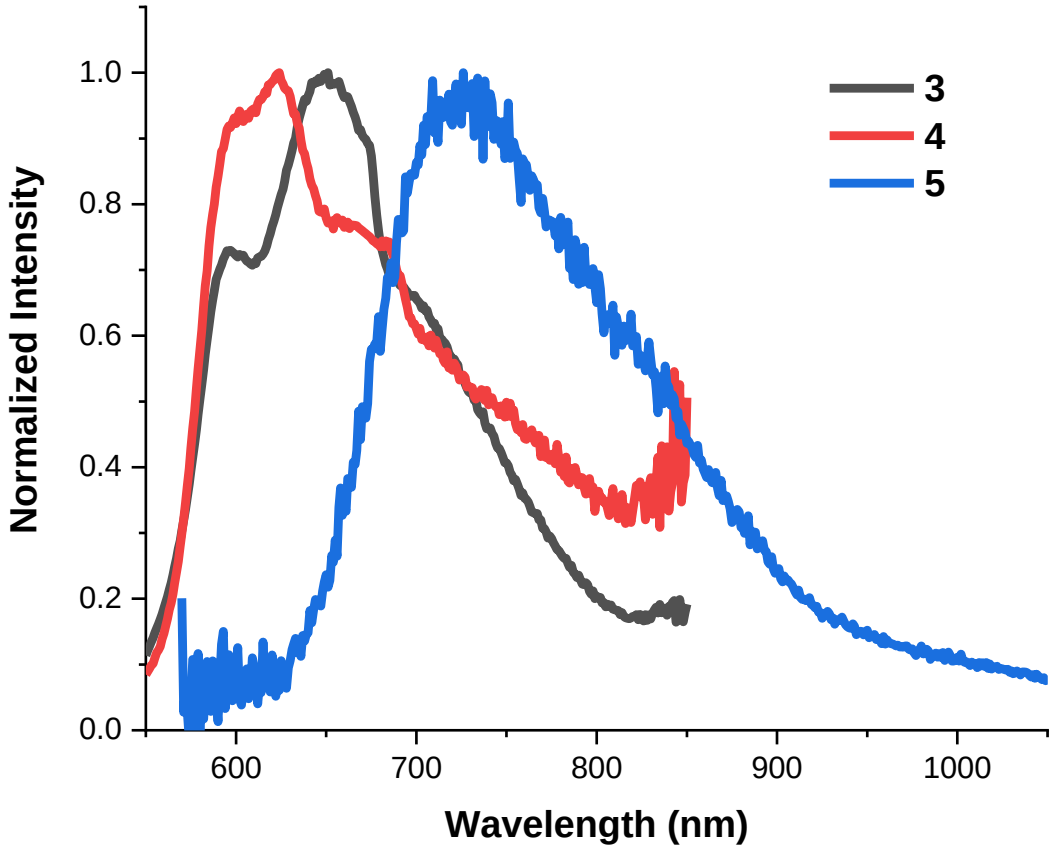


Figure S52. Emission spectra of **3-5** in solid state.

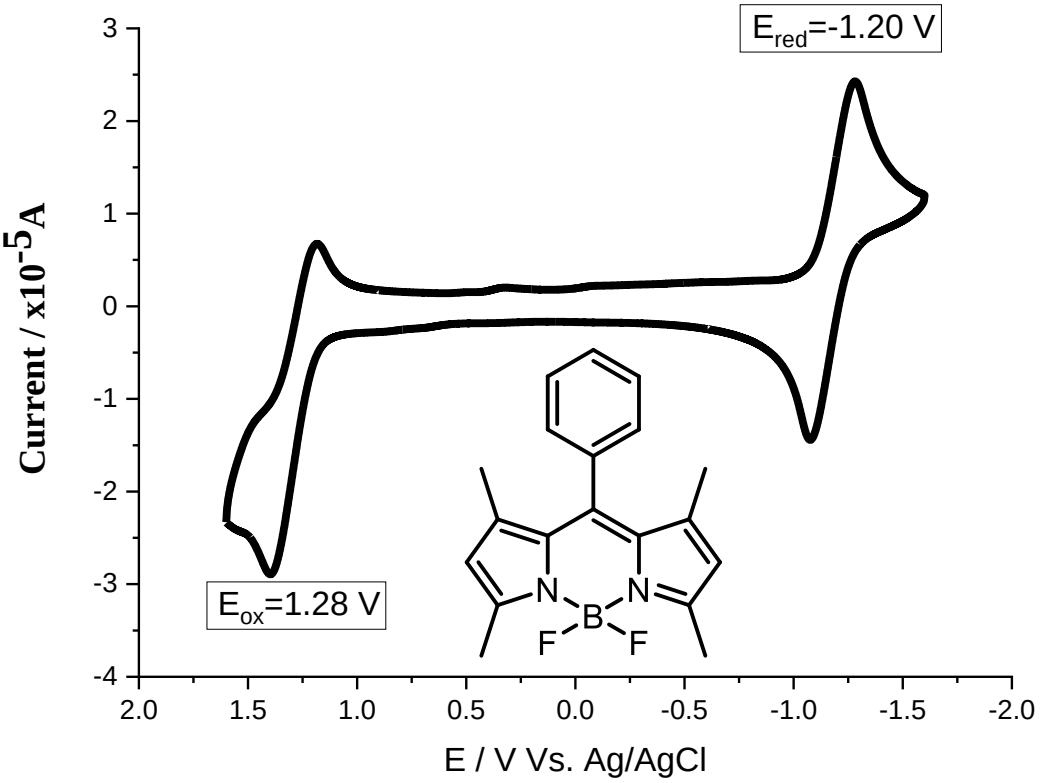


Figure S53. Cyclic voltammetry of **BODIPY-3** in CH_2Cl_2.

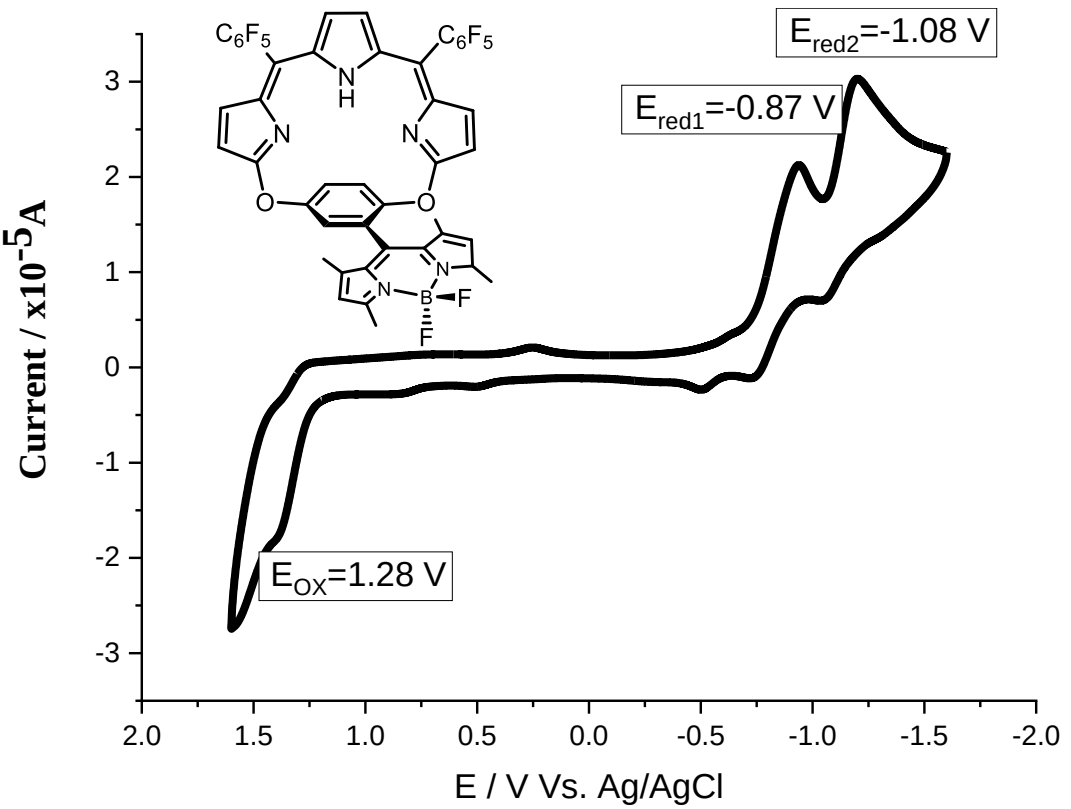


Figure S54. Cyclic voltammetry of **3** in CH_2Cl_2.

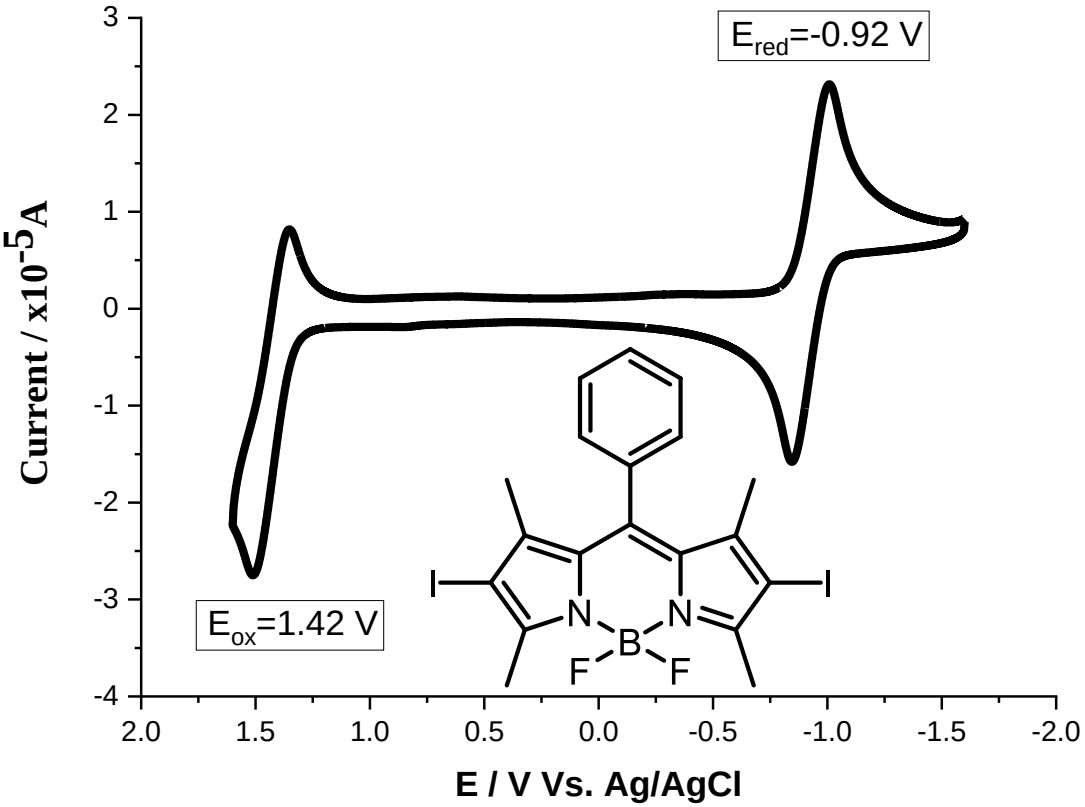


Figure S55. Cyclic voltammetry of **BODIPY-4** in CH_2Cl_2.

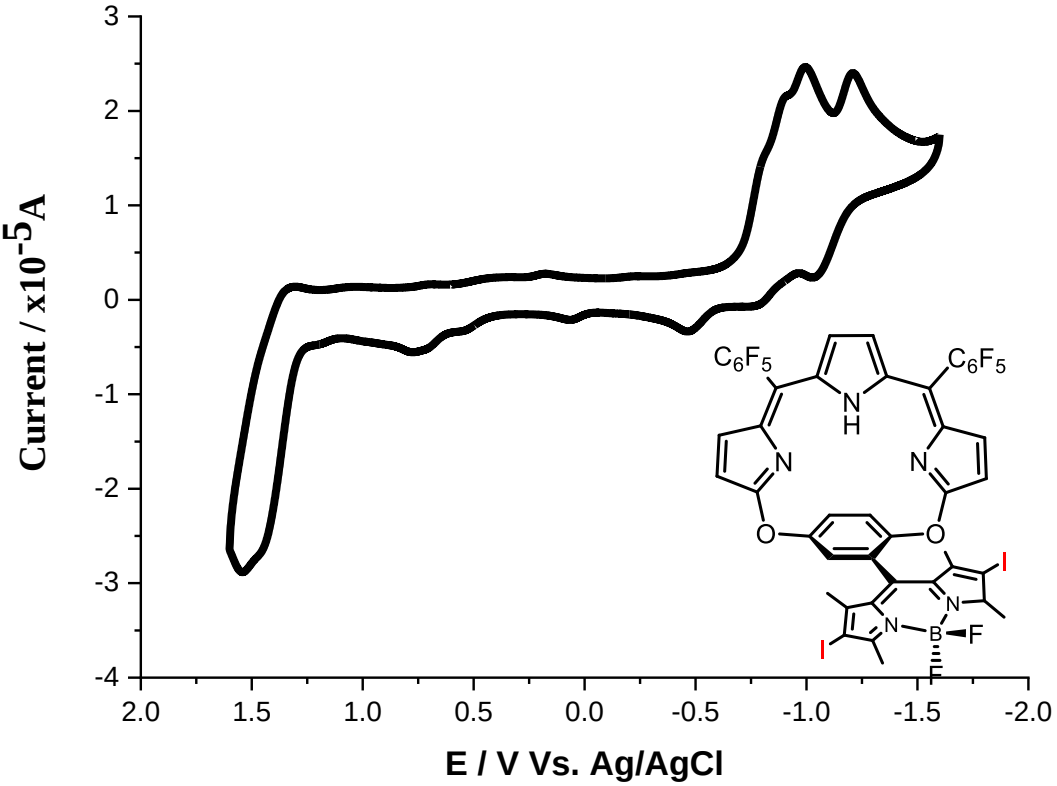


Figure S56. Cyclic voltammetry of **4** in CH_2Cl_2.

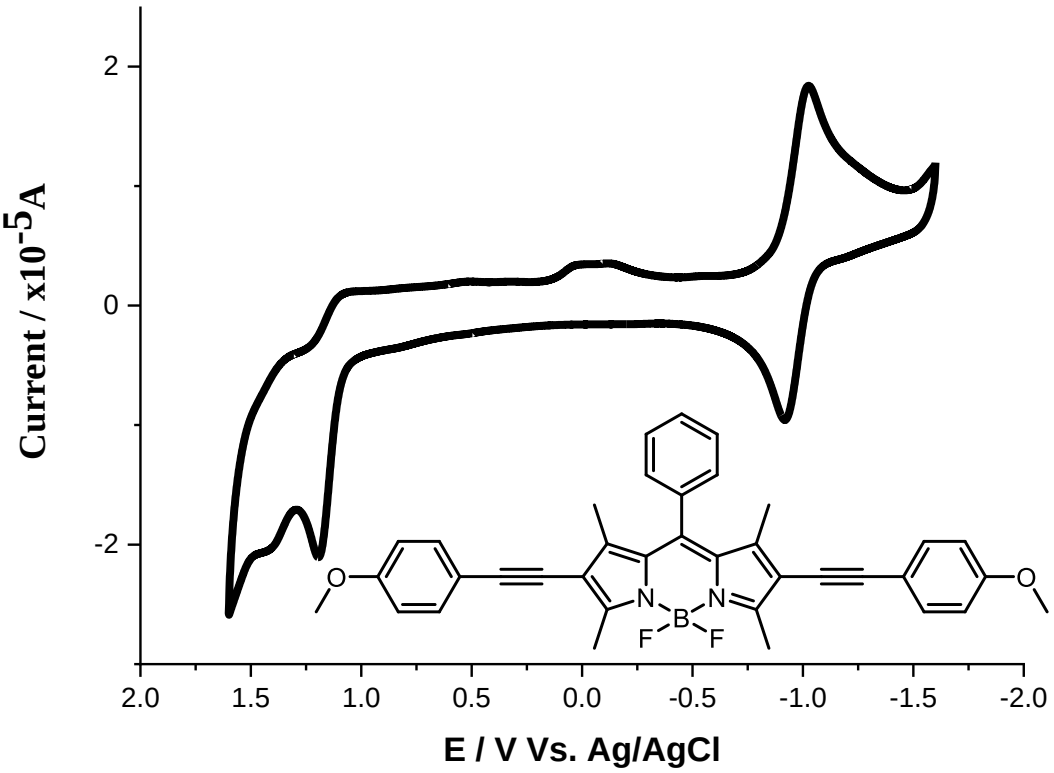


Figure S57. Cyclic voltammetry of **BODIPY-5** in CH_2Cl_2.

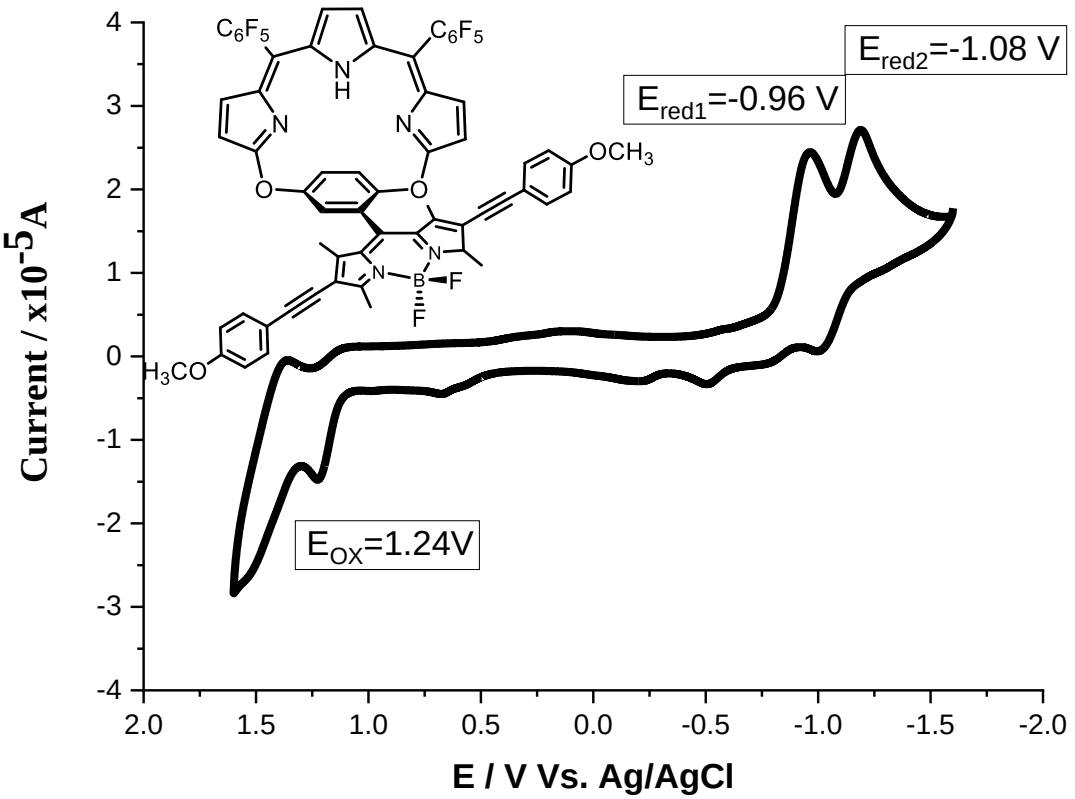


Figure S58. Cyclic voltammetry of **5** in CH_2Cl_2.

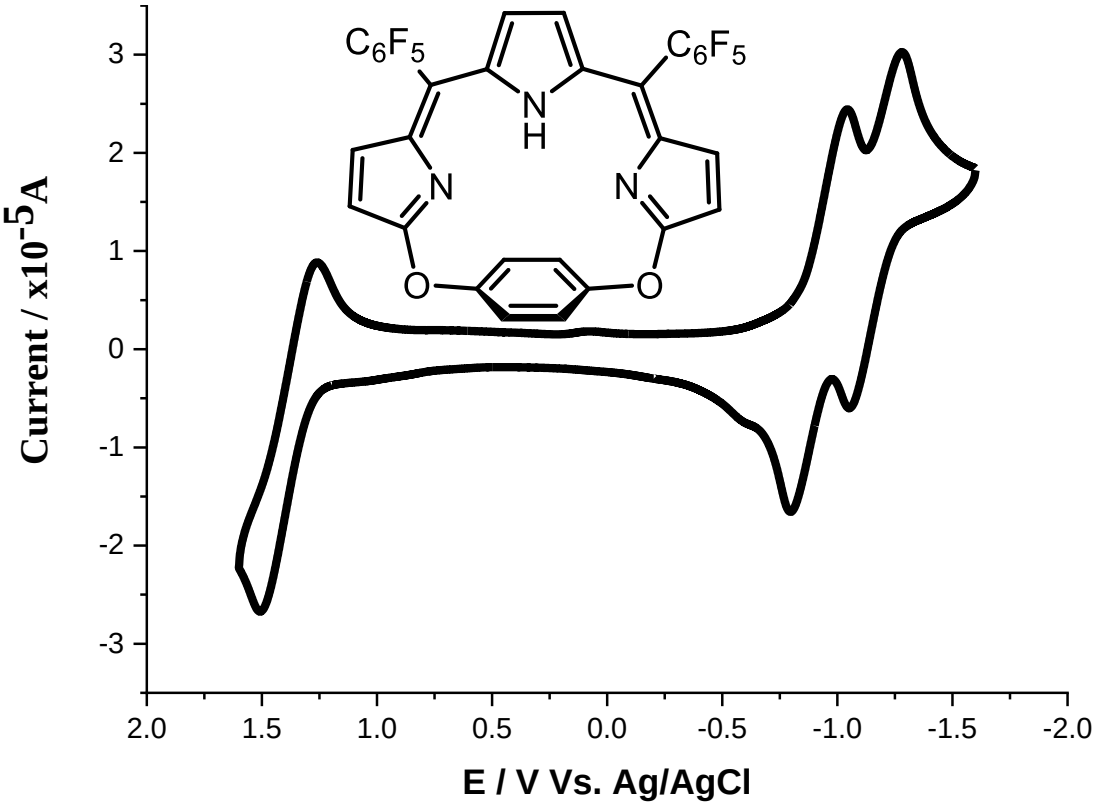


Figure S59. Cyclic voltammetry of tripyrrins in CH_2Cl_2.

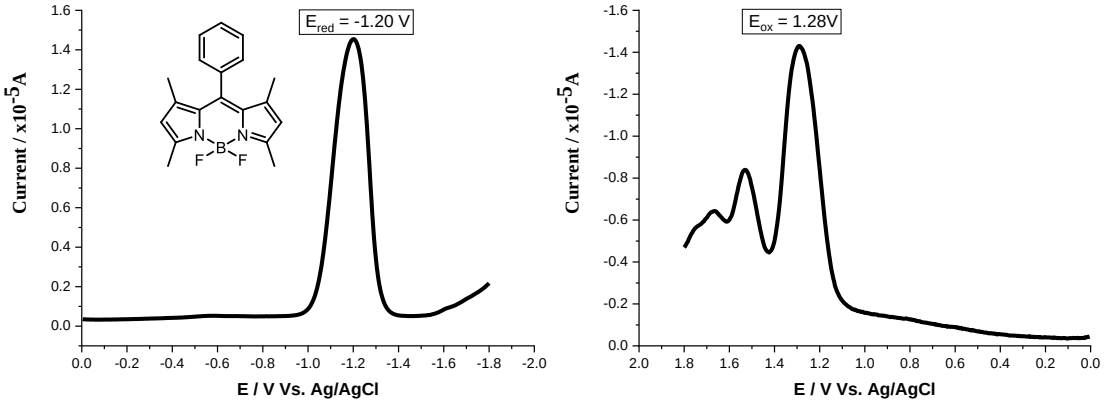


Figure S60. Differential pulse voltammetry of **BODIPY-3** in CH_2Cl_2.

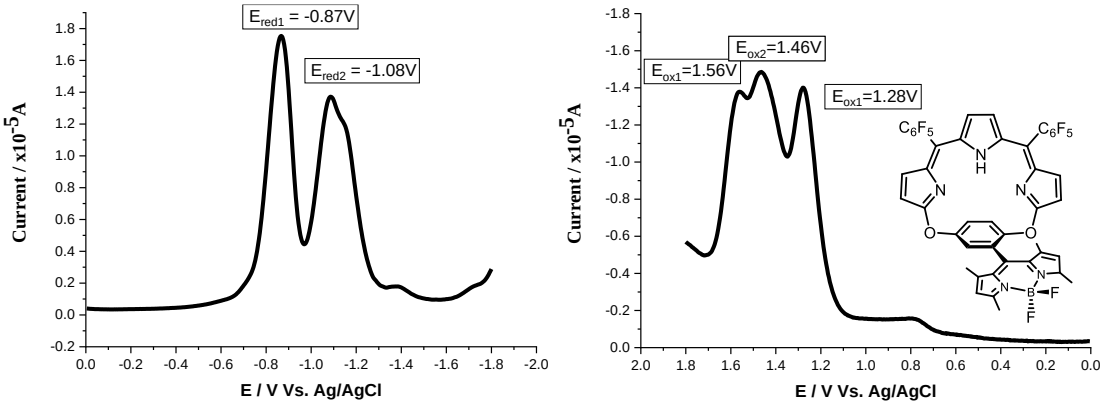


Figure S61. Differential pulse voltammetry of **3** in CH_2Cl_2.

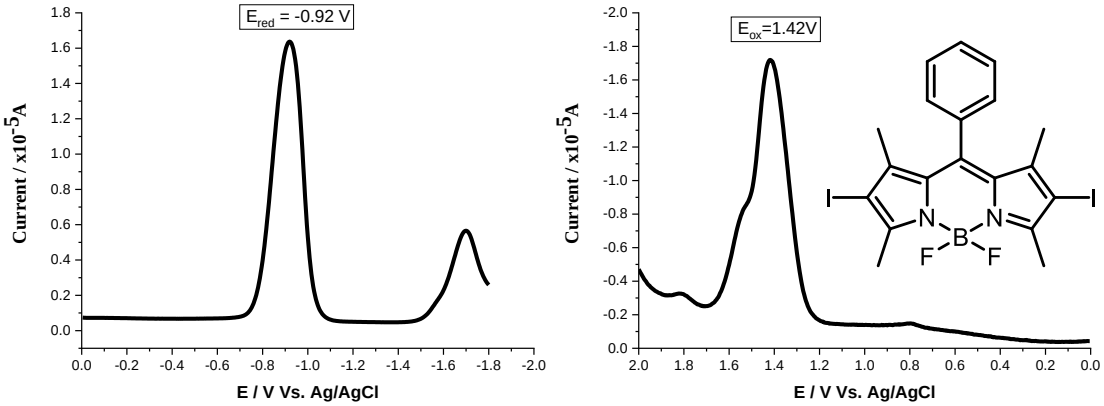


Figure S62. Differential pulse voltammetry of **BODIPY-4** in CH_2Cl_2.

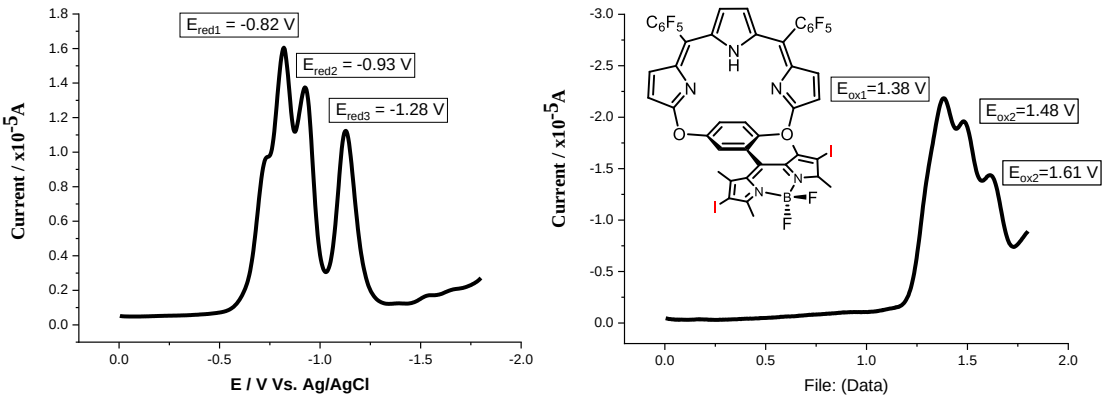


Figure S63. Differential pulse voltammetry of **4** in CH_2Cl_2.

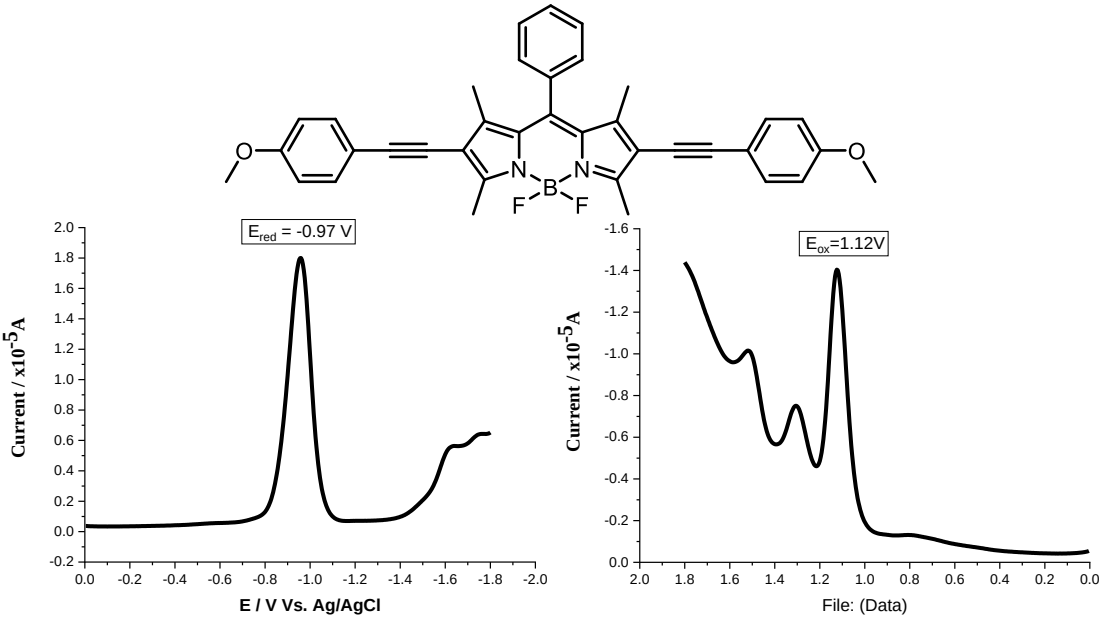


Figure S64. Differential pulse voltammetry of **BODIPY-5** in CH_2Cl_2.

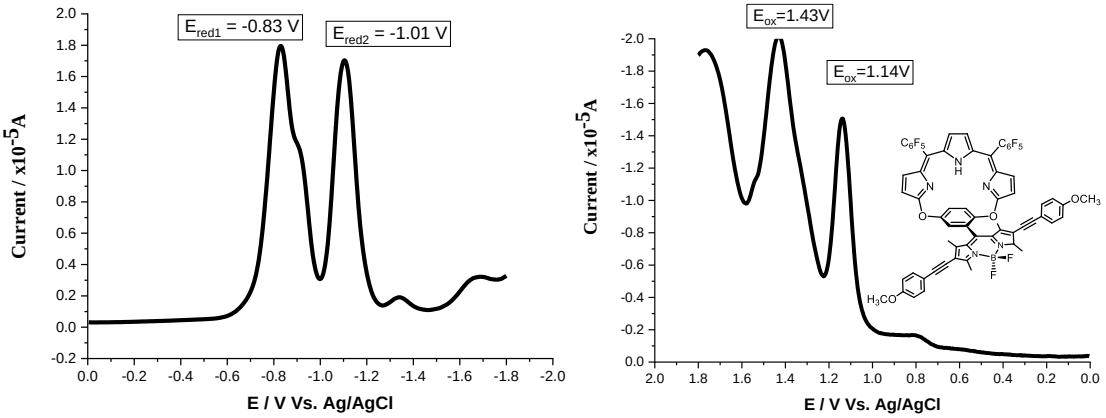


Figure S65. Differential pulse voltammetry of **5** in CH_2Cl_2.

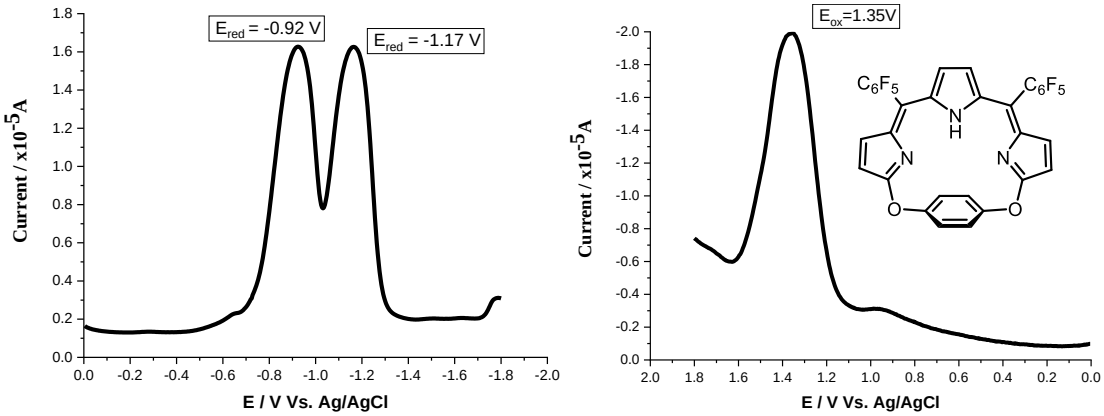


Figure S66. Differential pulse voltammetry of tripyrrins in CH_2Cl_2.

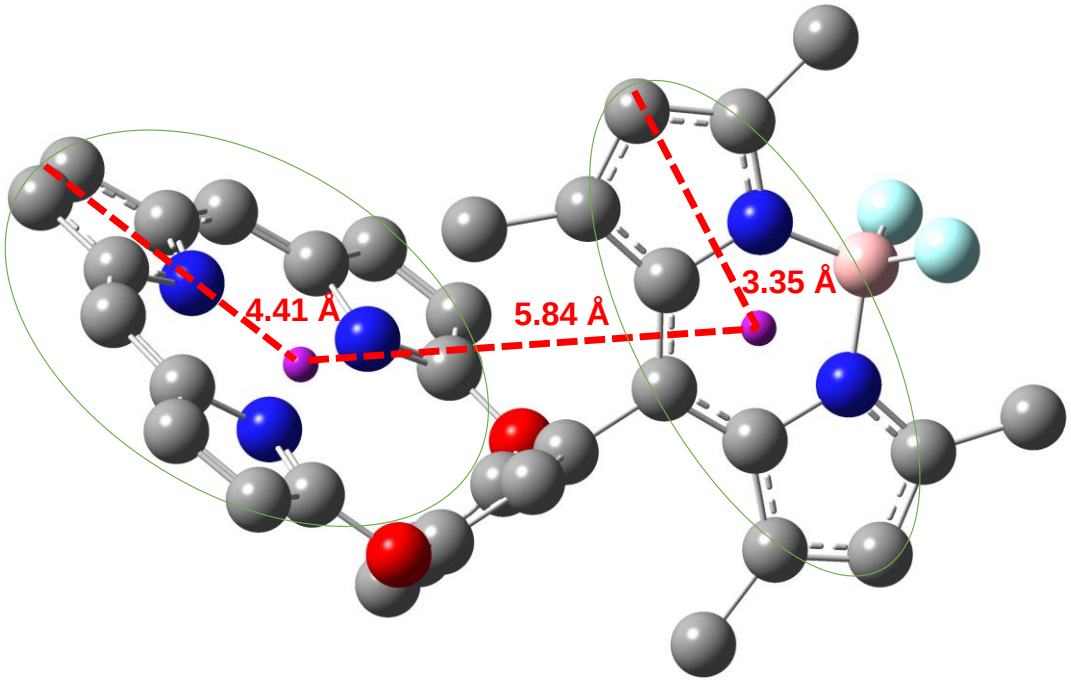


Figure S67. Center-to-center separation distance, the radius of the electron donor and acceptor determined by density functional theory (DFT) optimization of the geometry of **3**. Hydrogen atoms, meso-substituted moieties and solvent molecules are omitted for clarity.

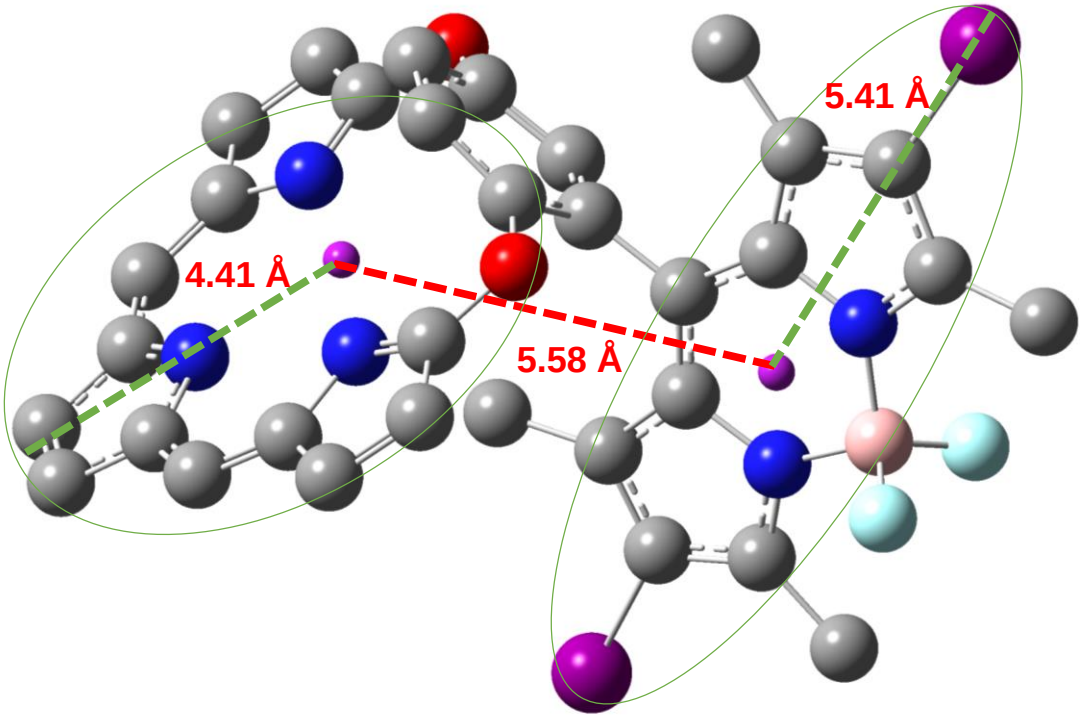


Figure S68. Center-to-center separation distance, the radius of the electron donor and acceptor determined by density functional theory (DFT) optimization of the geometry of **4**. Hydrogen atoms, meso-substituted moieties and solvent molecules are omitted for clarity.

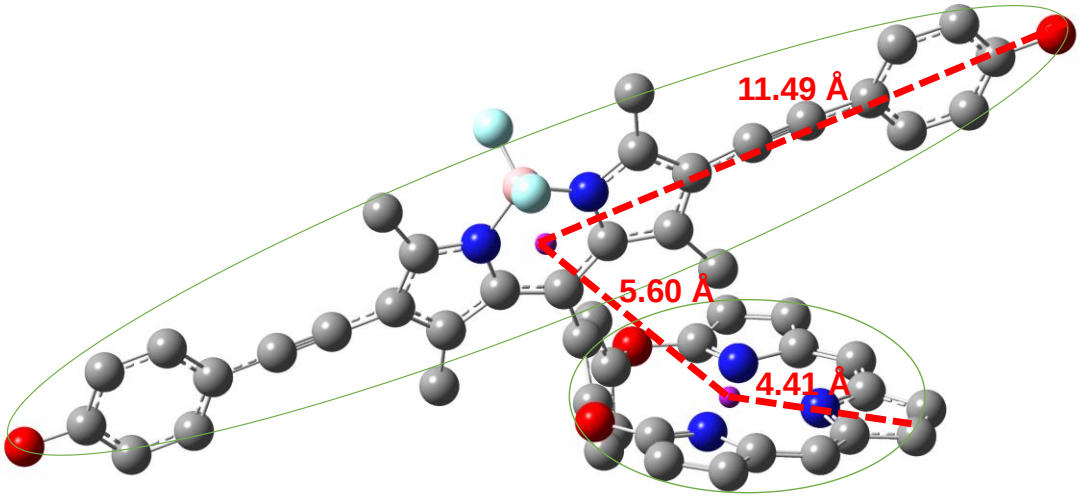


Figure S69. Center-to-center separation distance, the radius of the electron donor and acceptor determined by density functional theory (DFT) optimization of the geometry of **5**. Hydrogen atoms, meso-substituted moieties and solvent molecules are omitted for clarity.

2. Cartesian coordinates of DFT optimized structures in PDB format.

TITLE Compound-**1**
REMARK 1 File created by GaussView 6.0.16

HETATM	1	O	0	2.542	4.607	-0.390	O
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HETATM	3	F	0	4.156	-0.962	-2.317	F
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HETATM	38	C	0	-0.912	4.854	0.820	C
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END

TITLE Compound-**2**
REMARK 1 File created by GaussView 6.0.16

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HETATM	5	F	0	-8.433	-1.671	1.496	F
HETATM	6	F	0	-6.419	-1.476	3.327	F
HETATM	7	N	0	-1.149	-2.694	-1.079	N
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HETATM	9	C	0	1.251	-2.930	-3.237	C
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HETATM	11	C	0	-2.465	-2.592	-0.615	C
HETATM	12	C	0	2.033	-3.372	-0.978	C
HETATM	13	C	0	-2.177	-4.785	-1.087	C
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HETATM   20  C               0       -3.157    1.081    0.158                      C
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HETATM   26  C               0       -7.164   -1.609    1.087                      C
HETATM   27  O               0        3.630   -0.332   -2.262                      O
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HETATM   56  H               0        2.189   -1.245   -4.214                      H
HETATM   57  H               0        0.572   -3.169   -4.048                      H
HETATM   58  C               0        3.822   -1.996    0.097                      C
HETATM   59  C               0        1.879   -1.545    1.721                      C
HETATM   60  C               0        1.872   -1.197    3.064                      C
HETATM   61  H               0        1.029   -1.650    1.062                      H
HETATM   62  C               0        3.220   -1.153    3.480                      C
HETATM   63  H               0        1.012   -0.983    3.683                      H
HETATM   64  H               0        3.628   -0.914    4.453                      H
HETATM   65  C               0        6.038   -2.229   -1.187                      C
HETATM   66  C               0        7.356   -2.091   -0.775                      C
HETATM   67  H               0        5.681   -2.458   -2.181                      H
HETATM   68  C               0        7.320   -1.790    0.603                      C
HETATM   69  H               0        8.249   -2.191   -1.377                      H
HETATM   70  H               0        8.140   -1.623    1.289                      H
HETATM   71  C               0        3.241   -1.713    1.342                      C
HETATM   72  C               0        5.218   -1.997   -0.051                      C
HETATM   73  N               0        4.034   -1.459    2.461                      N
HETATM   74  N               0        6.052   -1.733    1.035                      N
HETATM   75  B               0        5.597   -1.567    2.527                      B
HETATM   76  F               0        6.130   -0.413    3.067                      F
HETATM   77  F               0        5.962   -2.687    3.253                      F
END

TITLE     Compound-3
REMARK    1 File created by GaussView 6.0.16
HETATM    1  O               0        0.548   -4.294   -1.508                      O
HETATM    2  F               0       -4.209   -1.708    2.543                      F
HETATM    3  F               0       -5.329   -2.797   -1.930                      F
HETATM    4  F               0       -7.830   -3.444   -1.141                      F
HETATM    5  F               0       -8.537   -3.225    1.486                      F
HETATM    6  F               0       -6.716   -2.355    3.323                      F
HETATM    7  N               0       -1.129   -2.749   -0.886                      N
HETATM    8  C               0       -0.690   -3.971   -1.063                      C
HETATM    9  C               0        1.094   -2.414   -2.901                      C
HETATM   10  C               0        1.360   -3.189   -1.776                      C
HETATM   11  C               0       -2.444   -2.916   -0.441                      C
HETATM   12  C               0        2.356   -2.855   -0.869                      C
HETATM   13  C               0       -1.653   -5.014   -0.745                      C
HETATM   14  H               0       -1.480   -6.079   -0.820                      H
HETATM   15  C               0       -2.764   -4.343   -0.349                      C
HETATM   16  H               0       -3.705   -4.764   -0.021                      H
HETATM   17  C               0       -3.296   -1.877   -0.151                      C
HETATM   18  C               0       -4.687   -2.234    0.283                      C
HETATM   19  C               0       -3.024   -0.463   -0.216                      C
HETATM   20  C               0       -3.961    0.554    0.059                      C
HETATM   21  H               0       -4.994    0.394    0.329                      H
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HETATM   22  C           0       -5.082   -2.132    1.620                       C
HETATM   23  C           0       -5.643   -2.681   -0.633                       C
HETATM   24  C           0       -6.370   -2.460    2.035                       C
HETATM   25  C           0       -6.937   -3.018   -0.241                       C
HETATM   26  C           0       -7.300   -2.905    1.099                       C
HETATM   27  O           0        3.068    0.543   -2.047                       O
HETATM   28  F           0       -1.400    3.657    1.929                       F
HETATM   29  F           0       -1.581    4.423   -2.743                       F
HETATM   30  F           0       -2.414    6.952   -2.291                       F
HETATM   31  F           0       -2.745    7.849    0.264                       F
HETATM   32  F           0       -2.234    6.191    2.371                       F
HETATM   33  N           0        0.900    1.159   -1.347                       N
HETATM   34  C           0        2.134    1.450   -1.681                       C
HETATM   35  C           0        1.729   -1.187   -3.018                       C
HETATM   36  C           0        2.615   -0.779   -2.026                       C
HETATM   37  C           0        0.317    2.397   -1.060                       C
HETATM   38  C           0        3.019   -1.624   -0.988                       C
HETATM   39  C           0        2.454    2.868   -1.639                       C
HETATM   40  H           0        3.415    3.306   -1.869                       H
HETATM   41  C           0        1.302    3.466   -1.243                       C
HETATM   42  H           0        1.131    4.522   -1.081                       H
HETATM   43  C           0       -0.990    2.556   -0.664                       C
HETATM   44  C           0       -1.461    3.958   -0.420                       C
HETATM   45  C           0       -1.983    1.532   -0.449                       C
HETATM   46  C           0       -3.323    1.776   -0.083                       C
HETATM   47  H           0       -3.764    2.752    0.054                       H
HETATM   48  C           0       -1.643    4.449    0.877                       C
HETATM   49  C           0       -1.733    4.832   -1.477                       C
HETATM   50  C           0       -2.074    5.750    1.119                       C
HETATM   51  C           0       -2.163    6.139   -1.260                       C
HETATM   52  C           0       -2.334    6.598    0.044                       C
HETATM   53  N           0       -1.832    0.162   -0.530                       N
HETATM   54  H           0       -0.982   -0.321   -0.808                       H
HETATM   55  H           0        2.577   -3.517   -0.039                       H
HETATM   56  H           0        1.486   -0.505   -3.826                       H
HETATM   57  H           0        0.338   -2.728   -3.611                       H
HETATM   58  C           0        4.109   -1.242   -0.037                       C
HETATM   59  C           0        2.566   -0.716    1.992                       C
HETATM   60  C           0        2.905   -0.298    3.272                       C
HETATM   61  C           0        4.307   -0.178    3.350                       C
HETATM   62  H           0        2.215   -0.090    4.080                       H
HETATM   63  C           0        6.012   -1.732   -1.741                       C
HETATM   64  C           0        7.388   -1.596   -1.597                       C
HETATM   65  C           0        7.658   -1.109   -0.303                       C
HETATM   66  H           0        8.136   -1.831   -2.344                       H
HETATM   67  C           0        3.808   -0.857    1.280                       C
HETATM   68  C           0        5.440   -1.306   -0.494                       C
HETATM   69  N           0        4.843   -0.513    2.161                       N
HETATM   70  N           0        6.493   -0.943    0.353                       N
HETATM   71  B           0        6.361   -0.462    1.826                       B
HETATM   72  F           0        6.837    0.842    1.952                       F
HETATM   73  F           0        7.064   -1.320    2.671                       F
HETATM   74  C           0        5.135    0.252    4.516                       C
HETATM   75  H           0        5.862   -0.524    4.779                       H
HETATM   76  H           0        5.711    1.150    4.267                       H
HETATM   77  H           0        4.500    0.461    5.381                       H
HETATM   78  C           0        1.161   -0.938    1.522                       C
HETATM   79  H           0        0.934   -1.996    1.353                       H
HETATM   80  H           0        0.460   -0.568    2.278                       H
HETATM   81  H           0        0.959   -0.415    0.584                       H
HETATM   82  C           0        5.349   -2.244   -2.986                       C
HETATM   83  H           0        4.611   -3.025   -2.778                       H
HETATM   84  H           0        4.830   -1.448   -3.534                       H
HETATM   85  H           0        6.106   -2.664   -3.656                       H
HETATM   86  C           0        8.984   -0.804    0.314                       C
HETATM   87  H           0        9.028    0.242    0.636                       H
HETATM   88  H           0        9.142   -1.415    1.209                       H
HETATM   89  H           0        9.790   -0.994   -0.400                       H
END

TITLE     Compound-4
REMARK    1 File created by GaussView 6.0.16
HETATM    1  O           0        0.218   -4.266   -1.248                       O
HETATM    2  F           0       -4.963   -2.457    2.119                       F
HETATM    3  F           0       -5.910   -2.948   -2.487                       F
HETATM    4  F           0       -8.398   -3.813   -1.879                       F
HETATM    5  F           0       -9.177   -4.002    0.723                       F
HETATM    6  F           0       -7.453   -3.324    2.718                       F
HETATM    7  N           0       -1.668   -2.885   -0.955                       N
HETATM    8  C           0       -1.088   -4.055   -0.972                       C
HETATM    9  C           0        0.718   -2.479   -2.771                       C
HETATM   10  C           0        0.931   -3.102   -1.548                       C
HETATM   11  C           0       -3.002   -3.160   -0.642                       C
HETATM   12  C           0        1.770   -2.563   -0.588                       C
HETATM   13  C           0       -1.971   -5.170   -0.669                       C
HETATM   14  H           0       -1.685   -6.211   -0.630                       H
HETATM   15  C           0       -3.182   -4.601   -0.460                       C
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HETATM   16  H                0         -4.106   -5.101   -0.210                          H
HETATM   17  C                0         -3.980   -2.206   -0.536                          C
HETATM   18  C                0         -5.363   -2.682   -0.201                          C
HETATM   19  C                0         -3.855   -0.783   -0.705                          C
HETATM   20  C                0         -4.911    0.139   -0.573                          C
HETATM   21  H                0         -5.933   -0.111   -0.338                          H
HETATM   22  C                0         -5.791   -2.786    1.121                          C
HETATM   23  C                0         -6.268   -3.033   -1.201                          C
HETATM   24  C                0         -7.068   -3.229    1.443                          C
HETATM   25  C                0         -7.551   -3.478   -0.902                          C
HETATM   26  C                0         -7.950   -3.575    0.426                          C
HETATM   27  O                0          2.238    0.762   -2.052                          O
HETATM   28  F                0         -2.480    3.946    1.037                          F
HETATM   29  F                0         -3.178    3.675   -3.631                          F
HETATM   30  F                0         -4.345    6.114   -3.594                          F
HETATM   31  F                0         -4.583    7.474   -1.248                          F
HETATM   32  F                0         -3.647    6.386    1.065                          F
HETATM   33  N                0         -0.039    1.180   -1.632                          N
HETATM   34  C                0          1.176    1.582   -1.895                          C
HETATM   35  C                0          1.222   -1.204   -2.956                          C
HETATM   36  C                0          1.934   -0.595   -1.931                          C
HETATM   37  C                0         -0.793    2.355   -1.571                          C
HETATM   38  C                0          2.304   -1.282   -0.775                          C
HETATM   39  C                0          1.319    3.023   -2.020                          C
HETATM   40  H                0          2.238    3.551   -2.226                          H
HETATM   41  C                0          0.073    3.510   -1.816                          C
HETATM   42  H                0         -0.235    4.545   -1.825                          H
HETATM   43  C                0         -2.139    2.391   -1.318                          C
HETATM   44  C                0         -2.791    3.742   -1.298                          C
HETATM   45  C                0         -3.025    1.287   -1.060                          C
HETATM   46  C                0         -4.402    1.409   -0.791                          C
HETATM   47  H                0         -4.952    2.335   -0.759                          H
HETATM   48  C                0         -2.930    4.461   -0.112                          C
HETATM   49  C                0         -3.282    4.324   -2.465                          C
HETATM   50  C                0         -3.529    5.715   -0.083                          C
HETATM   51  C                0         -3.885    5.576   -2.461                          C
HETATM   52  C                0         -4.008    6.272   -1.264                          C
HETATM   53  N                0         -2.721   -0.057   -1.004                          N
HETATM   54  H                0         -1.805   -0.457   -1.172                          H
HETATM   55  H                0          1.965   -3.110    0.326                          H
HETATM   56  H                0          1.000   -0.642   -3.855                          H
HETATM   57  H                0          0.091   -2.949   -3.518                          H
HETATM   58  C                0          3.236   -0.681    0.227                          C
HETATM   59  C                0          1.441   -0.170    2.032                          C
HETATM   60  C                0          1.609    0.380    3.297                          C
HETATM   61  C                0          2.973    0.691    3.500                          C
HETATM   62  C                0          5.344   -1.119   -1.222                          C
HETATM   63  C                0          6.668   -0.776   -0.966                          C
HETATM   64  C                0          6.753   -0.111    0.276                          C
HETATM   65  C                0          2.758   -0.208    1.460                          C
HETATM   66  C                0          4.607   -0.631   -0.092                          C
HETATM   67  N                0          3.648    0.333    2.395                          N
HETATM   68  N                0          5.514   -0.039    0.791                          N
HETATM   69  B                0          5.170    0.571    2.179                          B
HETATM   70  F                0          5.446    1.942    2.186                          F
HETATM   71  F                0          5.901   -0.075    3.178                          F
HETATM   72  C                0          3.636    1.301    4.685                          C
HETATM   73  H                0          4.298    0.577    5.168                          H
HETATM   74  H                0          4.259    2.144    4.381                          H
HETATM   75  H                0          2.899    1.642    5.410                          H
HETATM   76  C                0          0.141   -0.606    1.437                          C
HETATM   77  H                0         -0.005   -1.686    1.519                          H
HETATM   78  H                0         -0.686   -0.129    1.963                          H
HETATM   79  H                0          0.068   -0.345    0.384                          H
HETATM   80  C                0          4.860   -1.860   -2.429                          C
HETATM   81  H                0          4.110   -2.611   -2.184                          H
HETATM   82  H                0          4.417   -1.184   -3.165                          H
HETATM   83  H                0          5.696   -2.364   -2.915                          H
HETATM   84  C                0          7.951    0.426    0.980                          C
HETATM   85  H                0          7.742    1.414    1.393                          H
HETATM   86  H                0          8.222   -0.219    1.820                          H
HETATM   87  H                0          8.802    0.490    0.304                          H
HETATM   88  I                0          8.327   -1.175   -2.214                          I
HETATM   89  I                0          0.089    0.703    4.728                          I
END

TITLE     Compound-5
REMARK    1 File created by GaussView 6.0.16
HETATM    1  O                0          0.601   -2.247   -3.797                          O
HETATM    2  F                0         -5.134   -1.767   -0.276                          F
HETATM    3  F                0         -5.234   -0.755   -4.906                          F
HETATM    4  F                0         -7.752   -1.711   -5.052                          F
HETATM    5  F                0         -8.976   -2.702   -2.822                          F
HETATM    6  F                0         -7.650   -2.726   -0.433                          F
HETATM    7  N                0         -1.333   -1.157   -2.986                          N
HETATM    8  C                0         -0.737   -2.133   -3.627                          C
HETATM    9  C                0          1.440   -0.001   -3.597                          C
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HETATM   10  C   0      1.344   -1.293   -3.093                       C
HETATM   11  C   0     -2.691   -1.485   -3.041                       C
HETATM   12  C   0      1.888   -1.647   -1.866                       C
HETATM   13  C   0     -1.636   -3.149   -4.153                       C
HETATM   14  H   0     -1.341   -4.029   -4.709                       H
HETATM   15  C   0     -2.873   -2.743   -3.771                       C
HETATM   16  H   0     -3.814   -3.242   -3.957                       H
HETATM   17  C   0     -3.689   -0.721   -2.481                       C
HETATM   18  C   0     -5.093   -1.235   -2.588                       C
HETATM   19  C   0     -3.556    0.525   -1.766                       C
HETATM   20  C   0     -4.633    1.330   -1.342                       C
HETATM   21  H   0     -5.677    1.122   -1.523                       H
HETATM   22  C   0     -5.754   -1.745   -1.465                       C
HETATM   23  C   0     -5.801   -1.234   -3.793                       C
HETATM   24  C   0     -7.052   -2.239   -1.530                       C
HETATM   25  C   0     -7.103   -1.725   -3.883                       C
HETATM   26  C   0     -7.731   -2.229   -2.747                       C
HETATM   27  O   0      2.642    1.709   -0.597                       O
HETATM   28  F   0     -3.146    3.020    2.508                       F
HETATM   29  F   0     -1.861    5.865   -1.055                       F
HETATM   30  F   0     -3.033    7.954    0.195                       F
HETATM   31  F   0     -4.268    7.590    2.601                       F
HETATM   32  F   0     -4.318    5.117    3.752                       F
HETATM   33  N   0      0.323    2.137   -0.535                       N
HETATM   34  C   0      1.559    2.418   -0.202                       C
HETATM   35  C   0      1.950    0.988   -2.770                       C
HETATM   36  C   0      2.350    0.663   -1.476                       C
HETATM   37  C   0     -0.437    3.137    0.079                       C
HETATM   38  C   0      2.414   -0.657   -1.022                       C
HETATM   39  C   0      1.707    3.593    0.641                       C
HETATM   40  H   0      2.640    3.981    1.028                       H
HETATM   41  C   0      0.441    4.050    0.816                       C
HETATM   42  H   0      0.125    4.908    1.393                       H
HETATM   43  C   0     -1.807    3.218   -0.002                       C
HETATM   44  C   0     -2.464    4.376    0.689                       C
HETATM   45  C   0     -2.708    2.309   -0.664                       C
HETATM   46  C   0     -4.113    2.428   -0.673                       C
HETATM   47  H   0     -4.673    3.235   -0.226                       H
HETATM   48  C   0     -3.105    4.223    1.922                       C
HETATM   49  C   0     -2.457    5.655    0.126                       C
HETATM   50  C   0     -3.715    5.293    2.572                       C
HETATM   51  C   0     -3.058    6.741    0.758                       C
HETATM   52  C   0     -3.689    6.557    1.986                       C
HETATM   53  N   0     -2.398    1.151   -1.351                       N
HETATM   54  H   0     -1.457    0.819   -1.542                       H
HETATM   55  H   0      1.842   -2.679   -1.534                       H
HETATM   56  H   0      1.962    2.026   -3.082                       H
HETATM   57  H   0      1.040    0.233   -4.578                       H
HETATM   58  C   0      2.982   -1.026    0.313                       C
HETATM   59  C   0      0.713   -1.636    1.405                       C
HETATM   60  C   0      0.436   -2.191    2.666                       C
HETATM   61  C   0      1.674   -2.344    3.352                       C
HETATM   62  C   0      5.446   -0.623   -0.388                       C
HETATM   63  C   0      6.631   -0.765    0.354                       C
HETATM   64  C   0      6.272   -1.202    1.662                       C
HETATM   65  C   0      2.132   -1.484    1.336                       C
HETATM   66  C   0      4.378   -0.968    0.495                       C
HETATM   67  N   0      2.669   -1.919    2.560                       N
HETATM   68  N   0      4.939   -1.324    1.731                       N
HETATM   69  B   0      4.167   -1.851    2.980                       B
HETATM   70  F   0      4.323   -0.971    4.046                       F
HETATM   71  F   0      4.626   -3.120    3.316                       F
HETATM   72  C   0      1.891   -2.873    4.728                       C
HETATM   73  H   0      2.552   -3.746    4.704                       H
HETATM   74  H   0      2.385   -2.121    5.352                       H
HETATM   75  H   0      0.935   -3.151    5.178                       H
HETATM   76  C   0     -0.344   -1.268    0.416                       C
HETATM   77  H   0     -0.428   -1.991   -0.402                       H
HETATM   78  H   0     -1.313   -1.232    0.922                       H
HETATM   79  H   0     -0.151   -0.292   -0.034                       H
HETATM   80  C   0      5.420   -0.201   -1.826                       C
HETATM   81  H   0      4.780   -0.844   -2.437                       H
HETATM   82  H   0      5.059    0.827   -1.944                       H
HETATM   83  H   0      6.436   -0.242   -2.230                       H
HETATM   84  C   0      7.183   -1.507    2.802                       C
HETATM   85  H   0      6.871   -0.960    3.698                       H
HETATM   86  H   0      7.139   -2.573    3.052                       H
HETATM   87  H   0      8.209   -1.238    2.545                       H
HETATM   88  C   0     -0.849   -2.541    3.138                       C
HETATM   89  C   0      7.953   -0.534   -0.089                       C
HETATM   90  C   0     -1.995   -2.824    3.440                       C
HETATM   91  C   0      9.093   -0.335   -0.470                       C
HETATM   92  C   0     10.426   -0.104   -0.911                       C
HETATM   93  C   0     10.689    0.333   -2.224                       C
HETATM   94  C   0     11.523   -0.304   -0.046                       C
HETATM   95  C   0     11.991    0.560   -2.656                       C
HETATM   96  H   0      9.859    0.493   -2.906                       H
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HETATM   97  C           0       12.824   -0.078   -0.472                       C
HETATM   98  H           0       11.340   -0.640    0.970                       H
HETATM   99  C           0       13.065    0.356   -1.781                       C
HETATM  100  H           0       12.175    0.897   -3.674                       H
HETATM  101  H           0       13.668   -0.232    0.194                       H
HETATM  102  C           0       -3.362   -3.137    3.684                   C
HETATM  103  C           0       -4.302   -2.974    2.647                   C
HETATM  104  C           0       -3.821   -3.609    4.931                   C
HETATM  105  C           0       -5.646   -3.267    2.842                   C
HETATM  106  H           0       -3.967   -2.613    1.681                   H
HETATM  107  C           0       -5.163   -3.906    5.131                   C
HETATM  108  H           0       -3.113   -3.741    5.743                   H
HETATM  109  C           0       -6.082   -3.736    4.087                   C
HETATM  110  H           0       -6.351   -3.129    2.023                   H
HETATM  111  H           0       -5.520   -4.270    6.089                   H
HETATM  112  O           0       -7.389   -4.043    4.344                   O
HETATM  113  H           0       -7.912   -3.881    3.543                   H
HETATM  114  O           0       14.365    0.562   -2.146                       O
HETATM  115  H           0       14.392    0.858   -3.070                       H
END
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3. Reference.

1. (a) Sheldrick, G. M. A short history of SHELX. *Acta. Crystallogr. A* **2008,** *64*, 112-22. (b) Sheldrick, G. M. Crystal structure refinement with SHELXL. *Acta Crystallogr. C* **2015,** *71*, 3-8.
2. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* **2009,** *42*, 339-341.
3. Spek, A. L. Structure validation in chemical crystallography. *Acta Crystallogr. D* **2009,** *65*, 148-155.
4. (a) Lee, C.; Yang, W.; Parr, R. G. Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B* **1988,** *37*, 785. (b) Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993,** *98*, 5648-5652.
5. M. J. Frisch; G. W. Trucks; H. B. Schlegel; G. E. Scuseria; M. A. Robb; J. R. Cheeseman; G. Scalmani; V. Barone; B. Mennucci; G. A. Petersson; H. Nakatsuji; M. Caricato; X. Li; H. P. Hratchian; A. F. Izmaylov; J. Bloino; G. Zheng; J. L. Sonnenberg; M. Hada; M. Ehara; K. Toyota; R. Fukuda; J. Hasegawa; M. Ishida; T. Nakajima; Y. Honda; O. Kitao; H. Nakai; T. Vreven; J. A. Montgomery; Jr., J. E. P.; F. Ogliaro; M. Bearpark; J. J. Heyd; E. Brothers; K. N. Kudin; V. N. Staroverov; R. Kobayashi; J. Normand; K. Raghavachari; A. Rendell; J. C. Burant; S. S. Iyengar; J. Tomasi; M. Cossi; N. Rega; J. M. Millam; M. Klene; J. E. Knox; J. B. Cross; V. Bakken; C. Adamo; J. Jaramillo; R. Gomperts; R. E. Stratmann; O. Yazyev; A. J. Austin; R. Cammi; C. Pomelli; J. W. Ochterski; R. L. Martin; K. Morokuma; V. G. Zakrzewski; G. A. Voth; P. Salvador; J. J. Dannenberg; S. Dapprich; A. D. Daniels; Ö. Farkas; J. B. Foresman; J. V. Ortiz; J. Cioslowski; D. J. Fox, *Gaussian 09 (Revision E.01)*. Gaussian Inc.: Wallingford CT, 2009.
6. (a) Hariharan, P. C.; Pople, J. A. The influence of polarization functions on molecular orbital hydrogenation energies. *Theor. Chim. Acta* **1973,** *28*, 213-222. (b) Francl, M. M.; Pietro, W. J.; Hehre, W. J.; Binkley, J. S.; Gordon, M. S.; DeFrees, D. J.; Pople, J. A. Self-consistent molecular orbital methods. XXIII. A polarization-type basis set for second-row elements. *J. Chem. Phys.* **1982,** *77*, 3654-3665.