Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

The preponderant role of the perfluorobenzene moieties in the electronic properties and the stacking modes of extended benzodifuran-azomethine derivatives.

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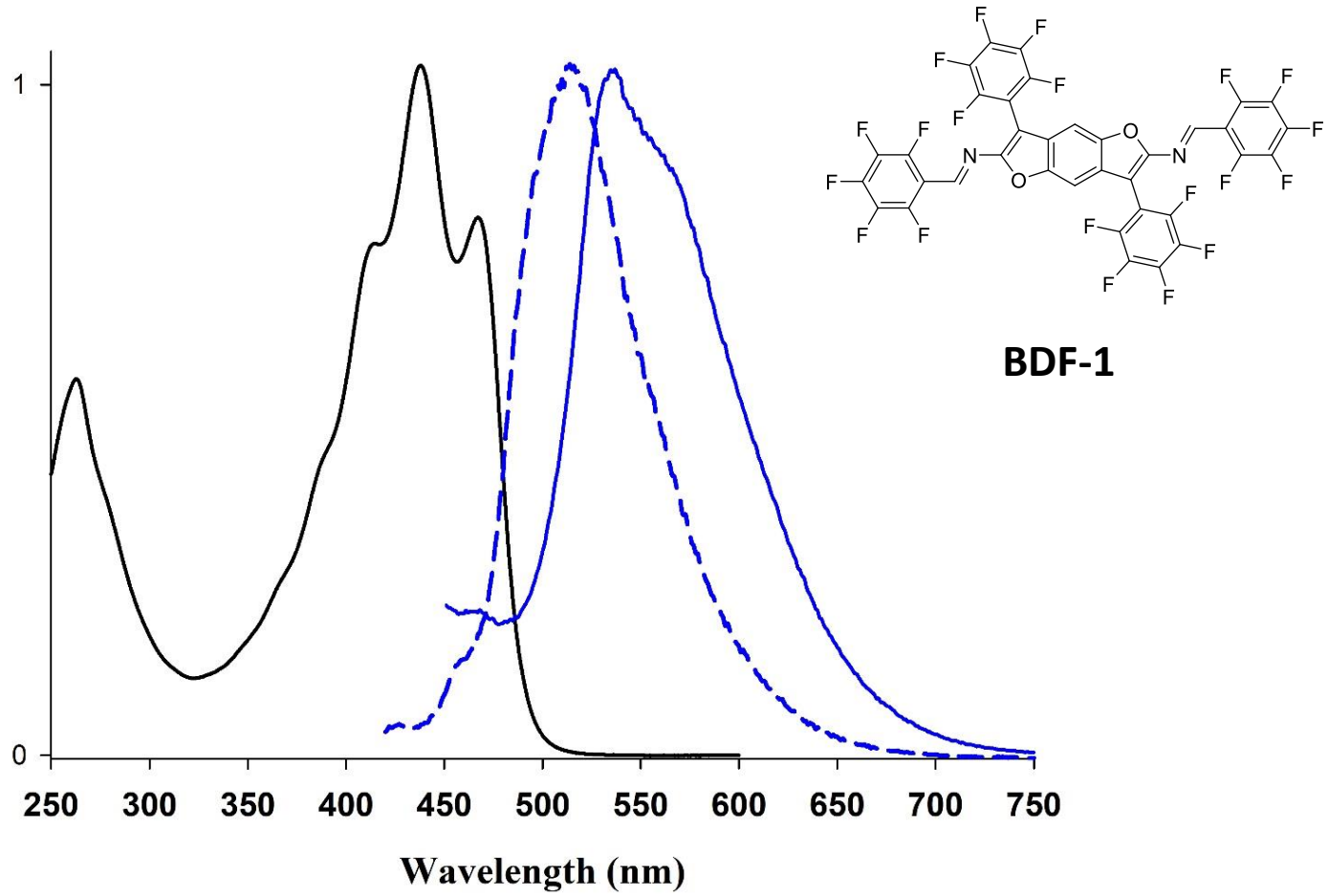


Figure S1: Normalized absorbance spectra 10^{-5} M in $CHCl_3$ (black line), fluorescence spectra 10^{-5} M in $CHCl_3$ (blue dotted line) and fluorescence spectra in the solid state (blue line)

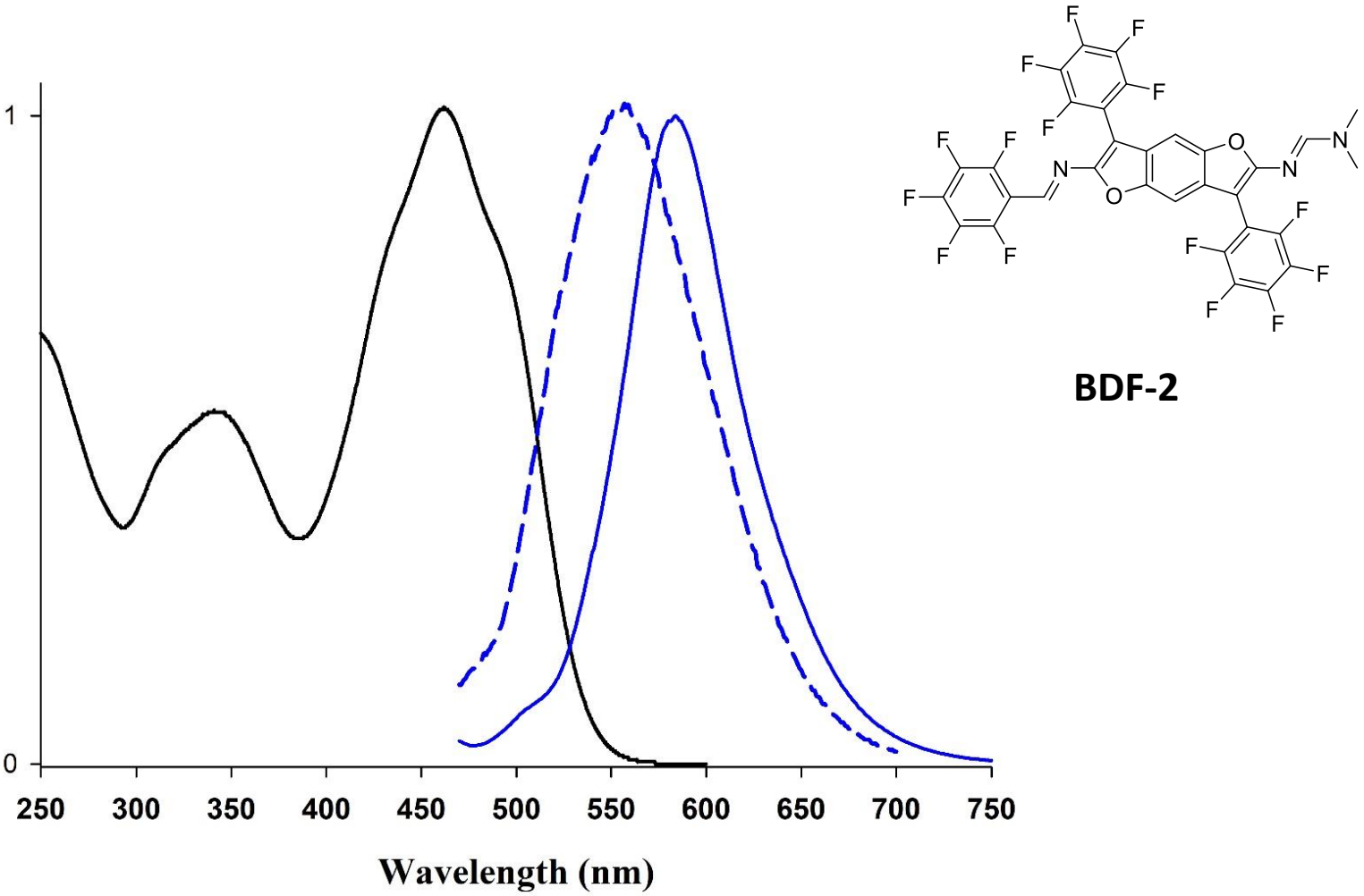


Figure S2: Normalized absorbance spectra 10^{-5} M in $CHCl_3$ (black line), fluorescence spectra 10^{-5} M in $CHCl_3$ (blue dotted line) and fluorescence spectra in the solid state (blue line)

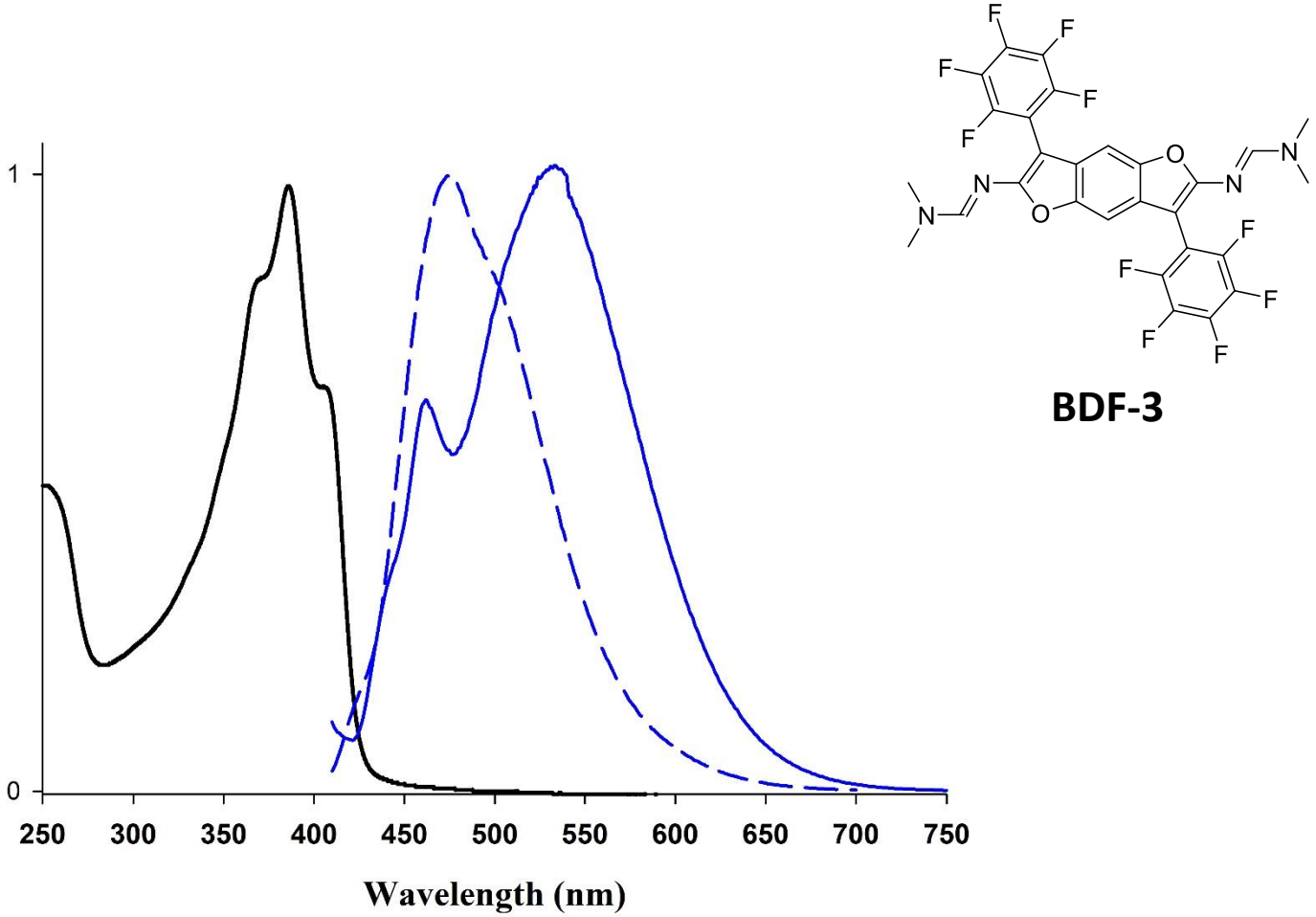
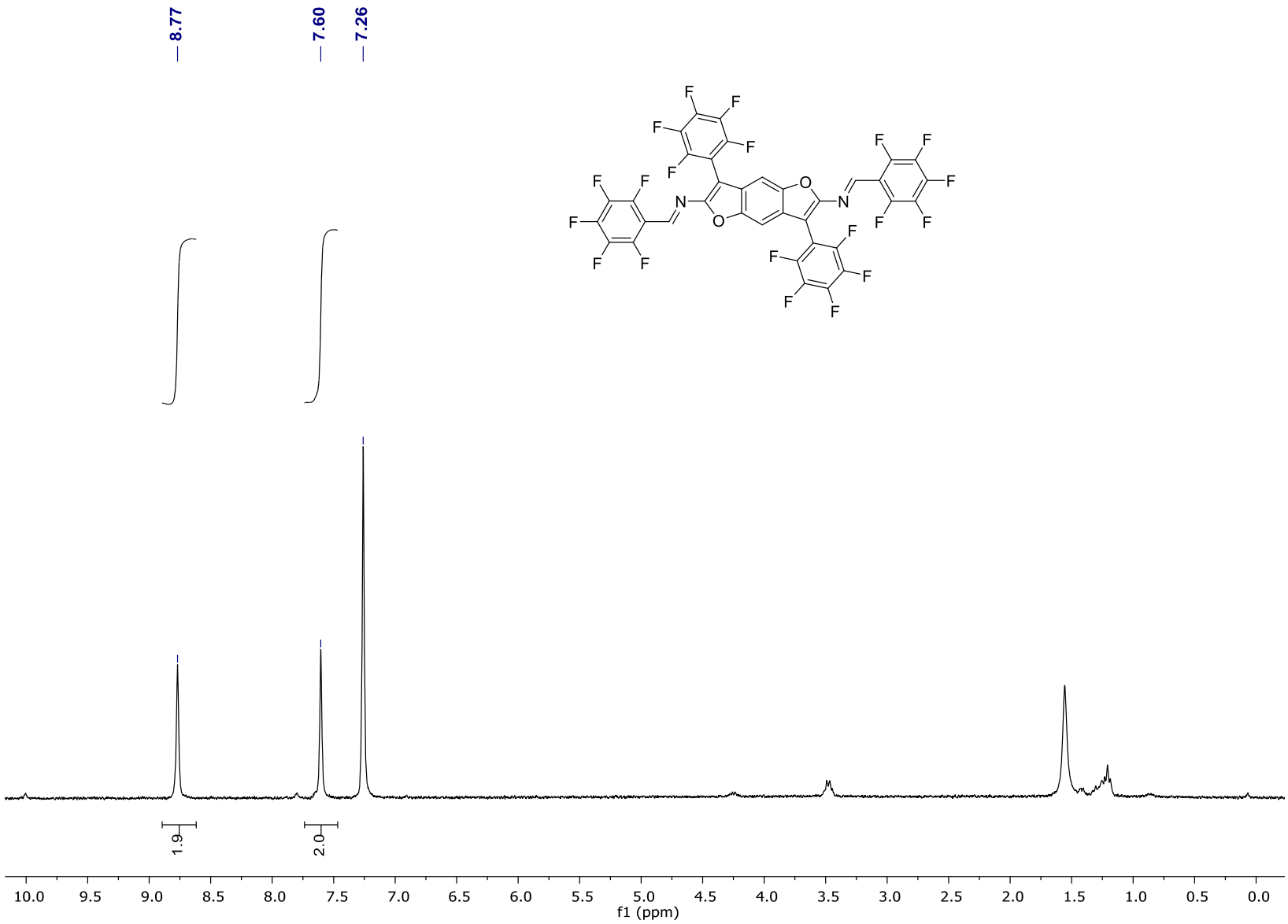


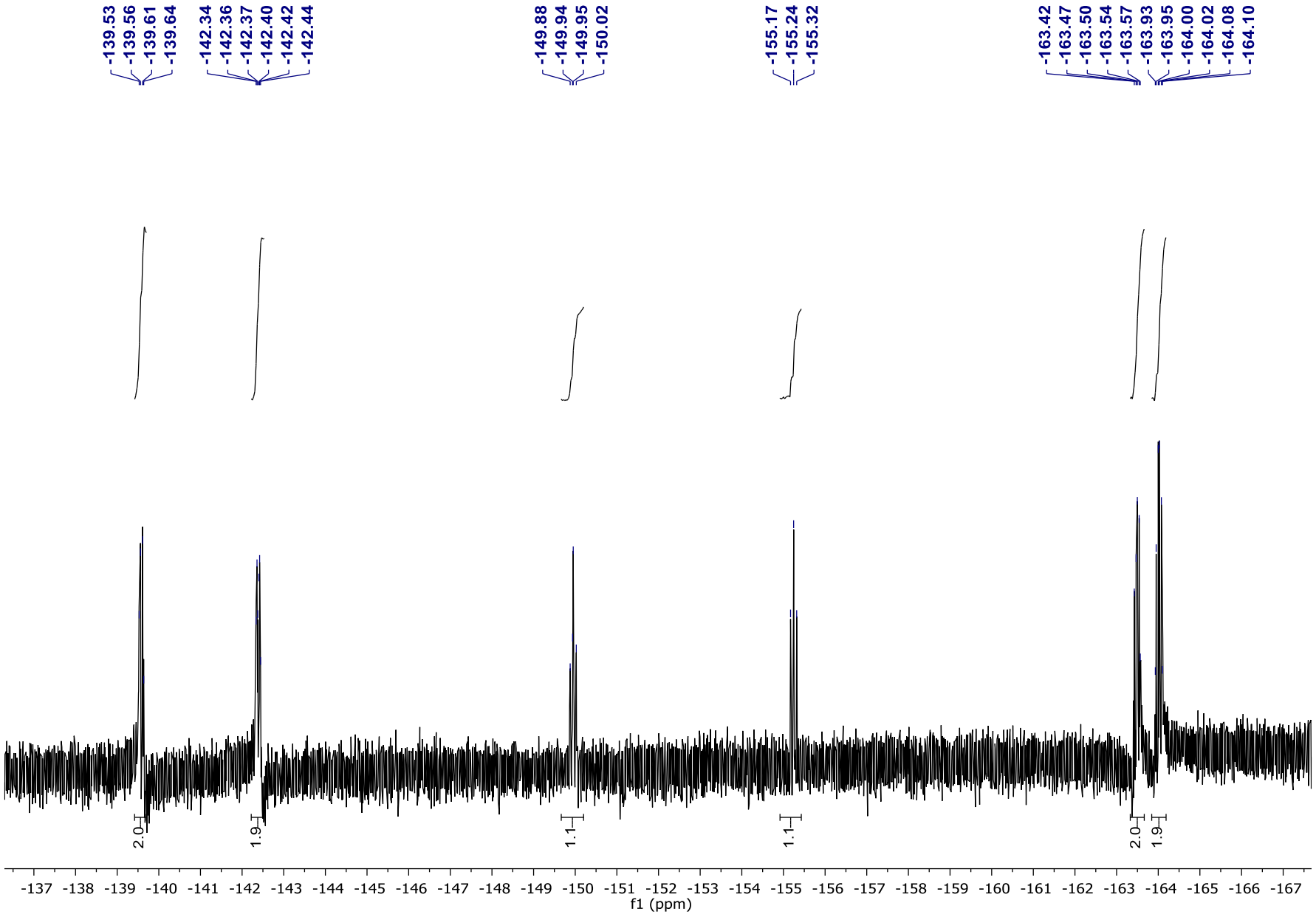
Figure S3: Normalized absorbance spectra 10^{-5} M in $CHCl_3$ (black line), fluorescence spectra 10^{-5} M in $CHCl_3$ (blue dotted line) and fluorescence spectra in the solid state (blue line)

Table S1: Crystallographic data of **BDF-NH2**, **BDF-1** and **DBF-2**

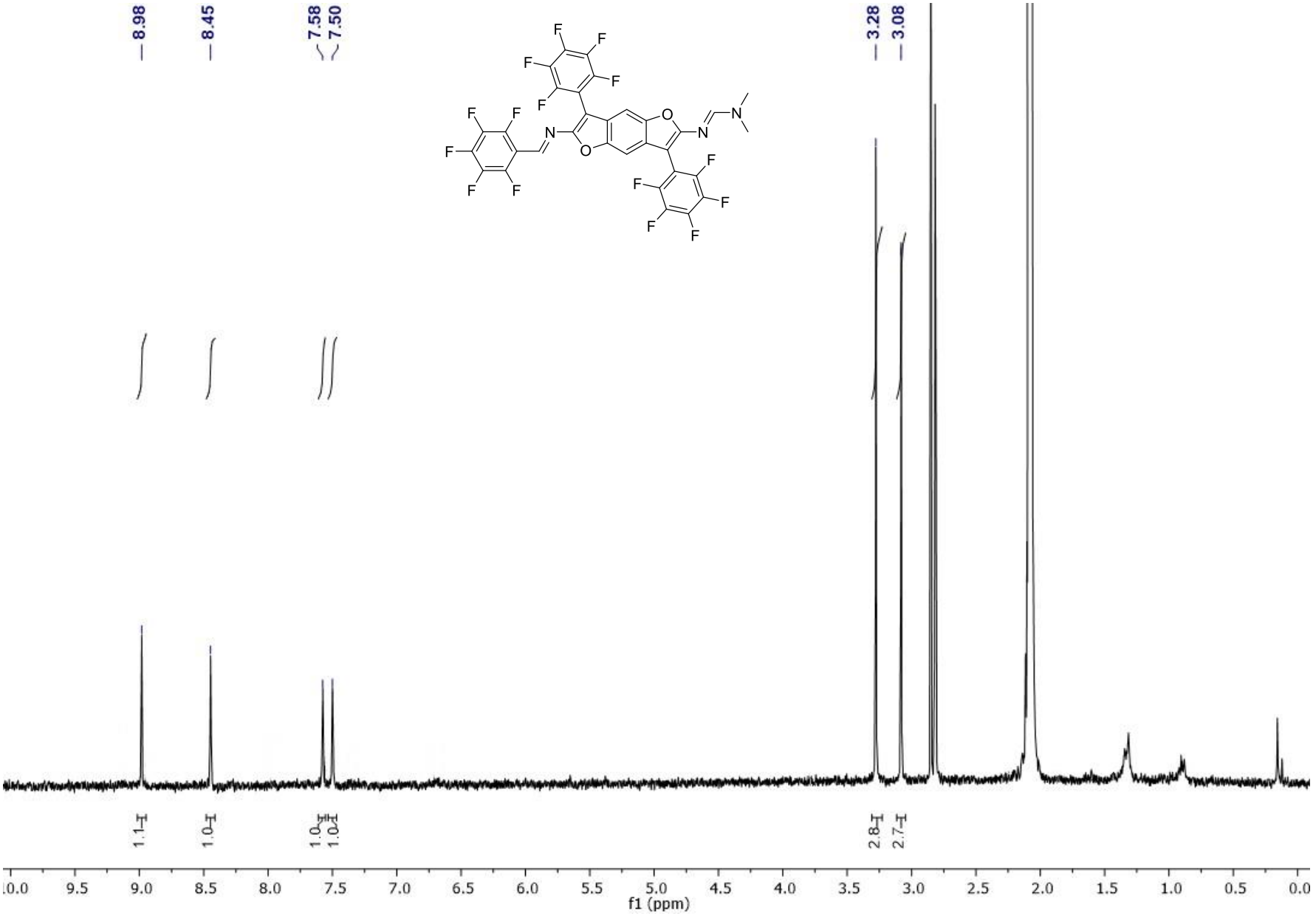
	BDF-NH_2	BDF-1	BDF-2
Formula	$C_{22}H_6F_{10}N_2O_2$	$C_{36}H_4F_{20}N_2O_2$	$C_{32}H_{10}F_{15}N_3O_2$
M	520.29	876.41	753.43
T (K)	293	293	293
Crystal system	Monoclinic	Triclinic	Triclinic
Space group	P 21/n	P -1	P -1
Unit cell.:			
a (Å)	11.3307(7)	6.537(4)	11.334(3)
b (Å)	7.8416(7)	10.866(3)	12.585(1)
c (Å)	11.397(1)	11.701(9)	12.741(3)
a (°)	90	71.27(6)	69.48(1)
b (°)	116.681(5)	89.53(6)	66.48(2)
g (°)	90	78.96(4)	63.37(1)
Volume (Å^3)	904.81(13)	771.3(8)	1456.6(5)
Z	2	1	2
Calculated density (g.cm^{-3})	1.910	1.887	1.718
Absorption coefficient (mm^{-1})	0.194	0.201	0.174
F(000)	516	430	748
q range (°)	4.00 to 30.04	2.25 to 27.25	3.27 to 27.50
Limiting indices	-15<=h<=13 -11<=k<=11 -16<=l<=16	-8<=h<=8 -13<=k<=13 -15<=l<=15	-14<=h<=14 -16<=k<=14 -16<=l<=16
Reflection coll.	18594	12115	48840
Unique	2625	3380	6657
R (int)	0.0344	0.1335	0.14771
Data	2625	3380	6657
Restraints	0	0	0
Parameters	175	271	471
Final R indice [I>2sigma(I)]	[2086]	[1219]	[2905]
R1	0.0391	0.0849	0.0739
wR2	0.1039	0.1539	0.1248
R indices (all data)			
R1	0.0523	0.2570	0.1990
wR2	0.1156	0.2205	0.1699
Goodness of fit on F^2	1.066	1.010	1.074
Largest diff.	0.355	0.323	0.243
Peak and hole (e A^{-3})	-0.245	-0.318	-0.271
CCDC number	2062621	2062622	2062623



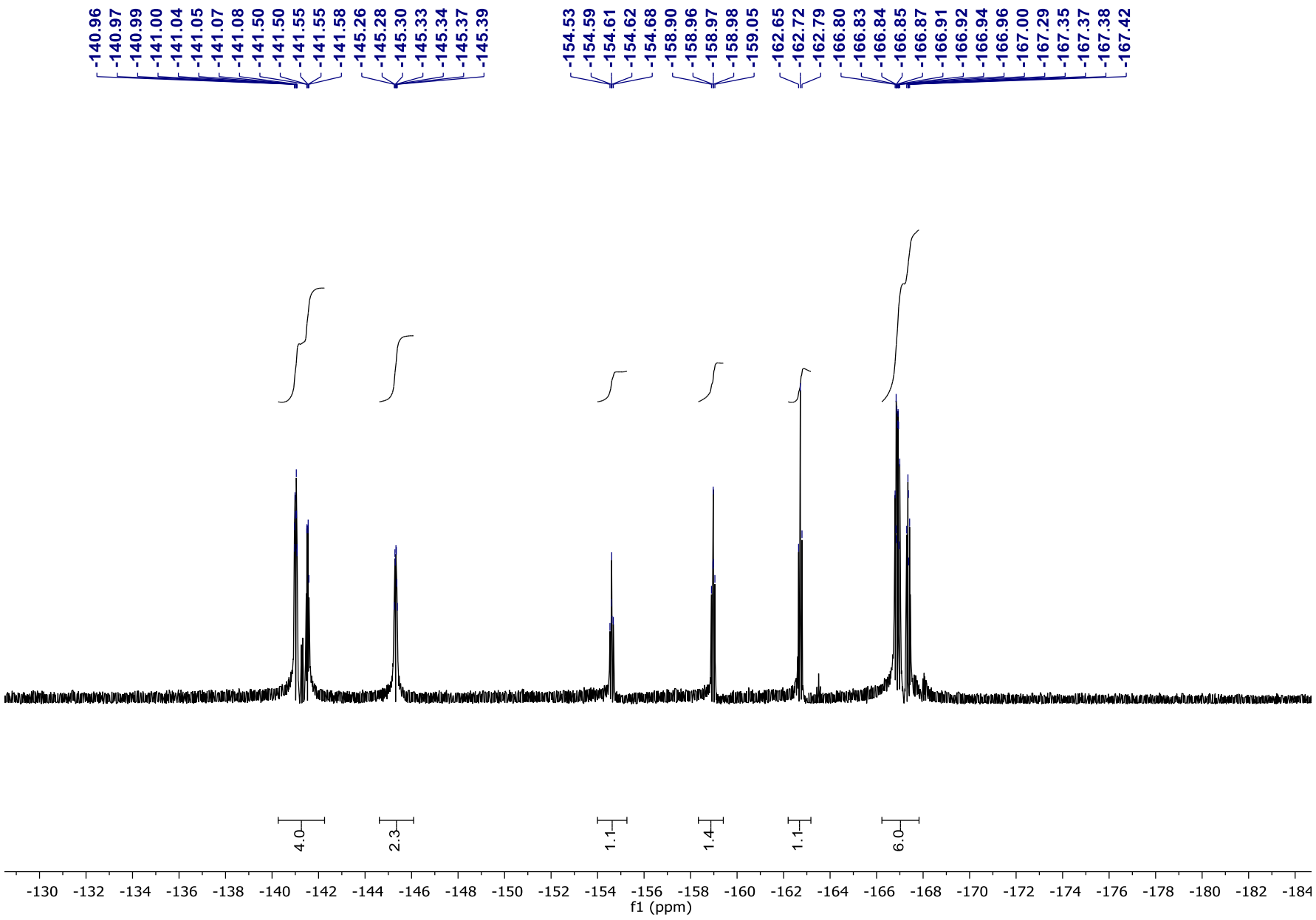
^{1}H NMR of **BDF-1** ($CDCl_3$)



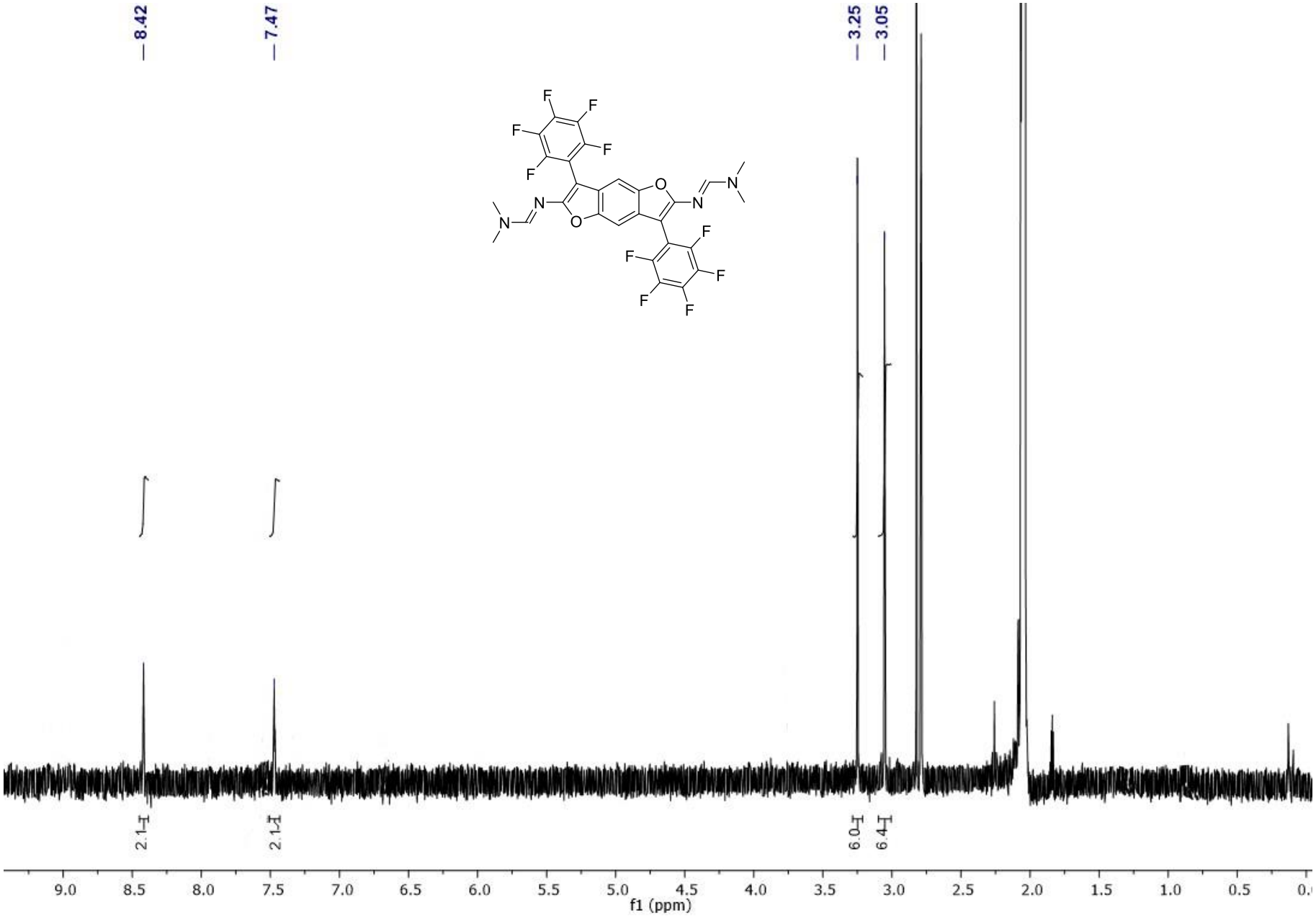
^{19}F NMR of **BDF-1** ($CDCl_3$)



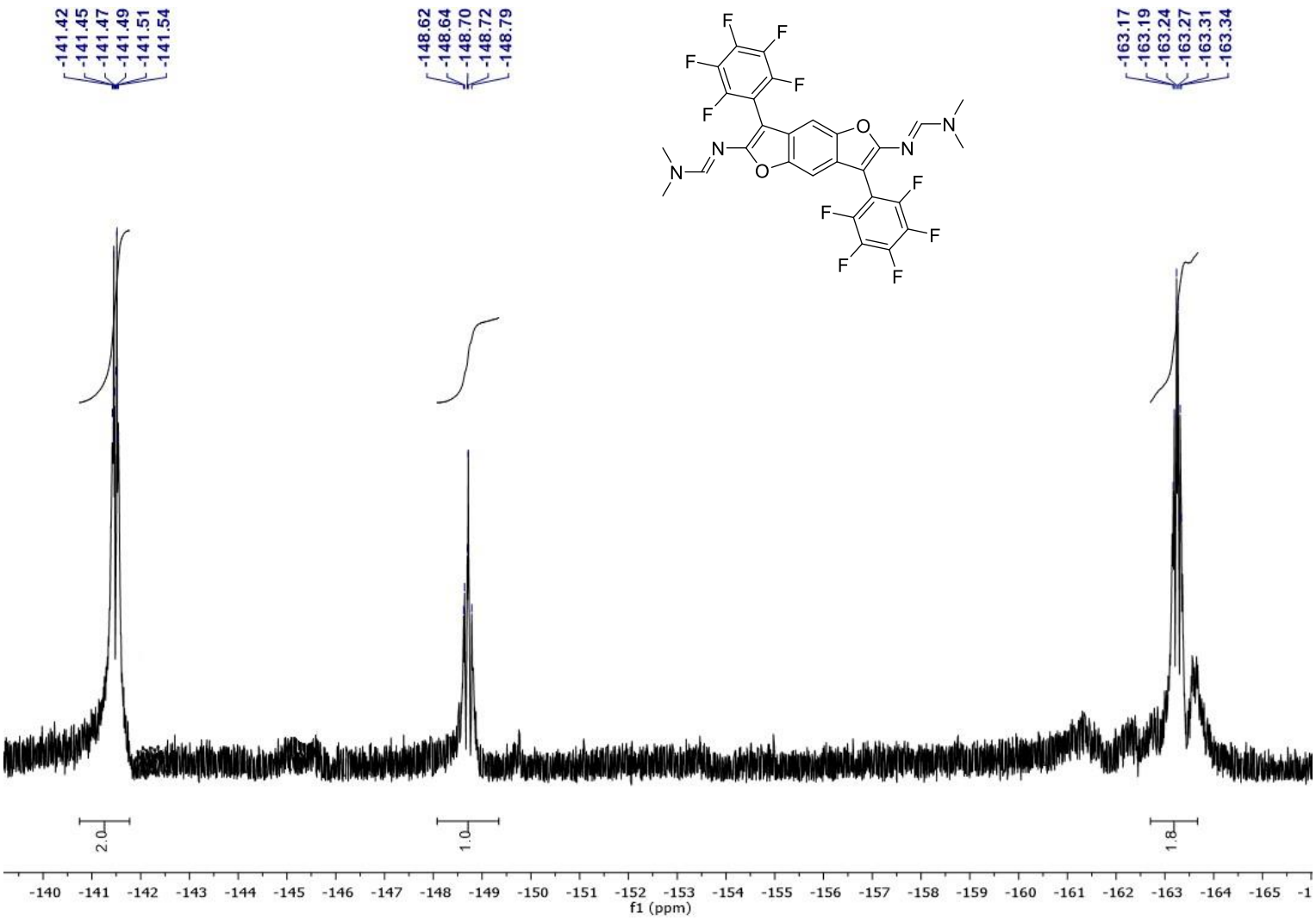
^{1}H NMR of **BDF-2** (CD_3CO)



^{19}F NMR of **BDF-2** (CD_3CO)

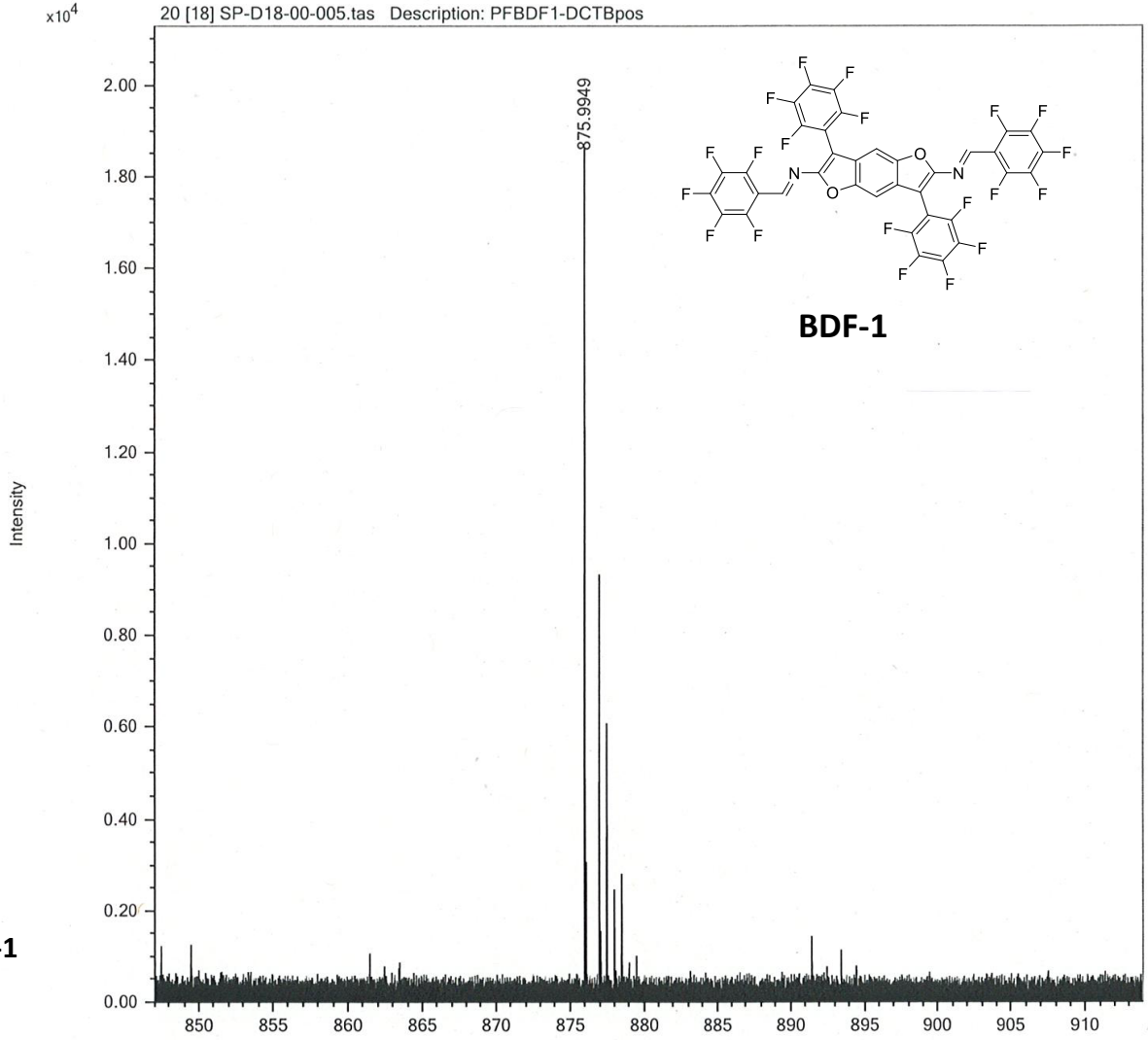


^{1}H NMR of **BDF-3** (CD_3CO)



^{19}F NMR of **BDF-3** (CD_3CO)

HRMS (MALDI TOF) of **BDF-1**



BDF-1

Elemental Composition Estimation

Parameters:

Mass	Tolerance	Electron Mode	Charge	DBE Range	Max Results
875.99494 ± 0.00018	0.2 ppm	Odd/Even	+1	-0.5 - 200.0	100

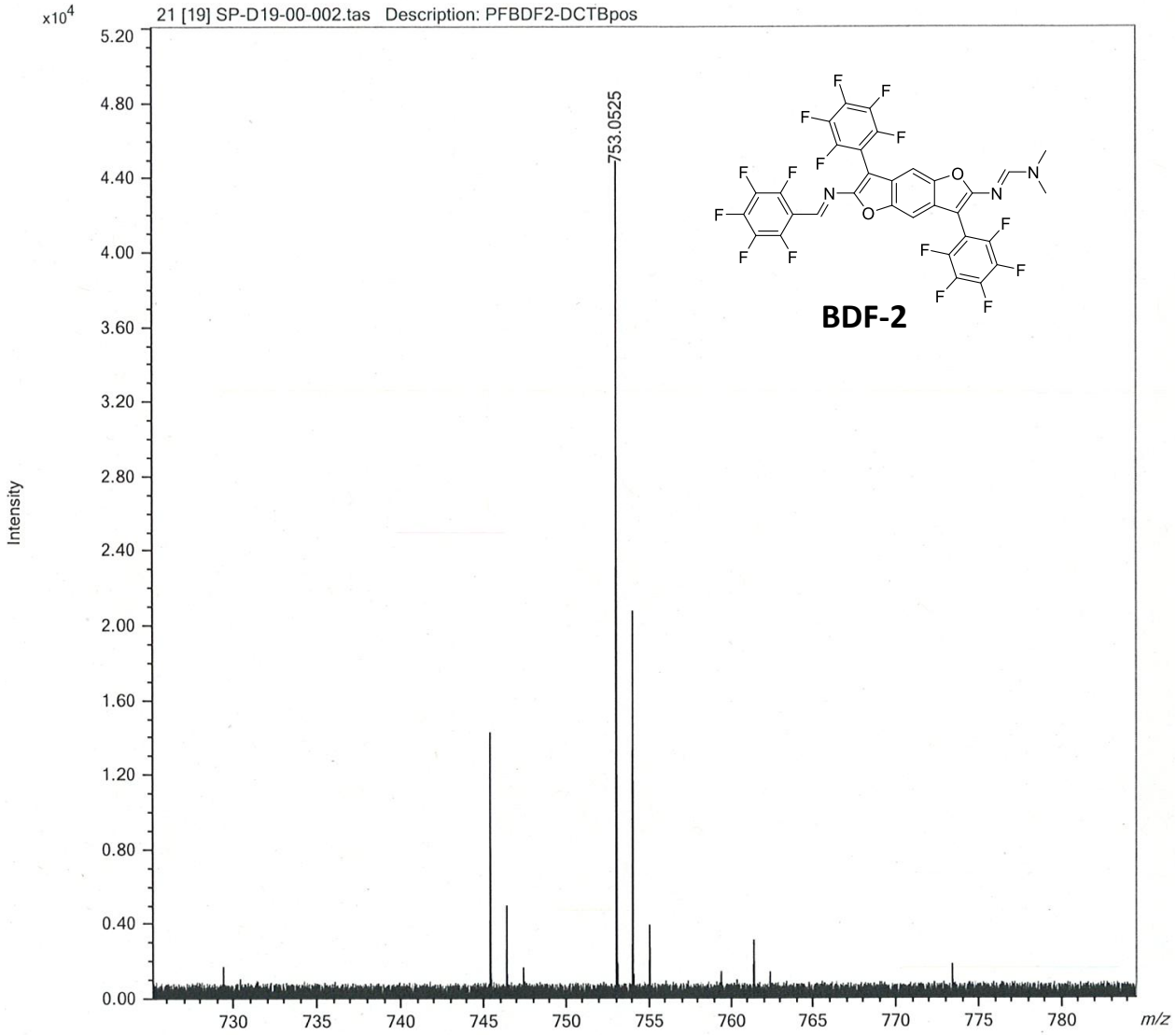
Elements

C 0 - 40 H 0 - 200 N 0 - 5 O 0 - 5 F 0 - 20

Results:

#	Formula	Mass	DBE	Abs. Error (u)	Error (u)	Error (ppm)
1	C36 H4 N2 O2 F20	875.99479	26.0	0.00015	0.00015	0.17

HRMS (MALDI TOF) of **BDF-2**



Elemental Composition Estimation

Parameters:

Mass	Tolerance	Electron Mode	Charge	DBE Range	Max Results
753.05252 ± 0.00030	0.4 ppm	Odd/Even	+1	-0.5 - 200.0	100

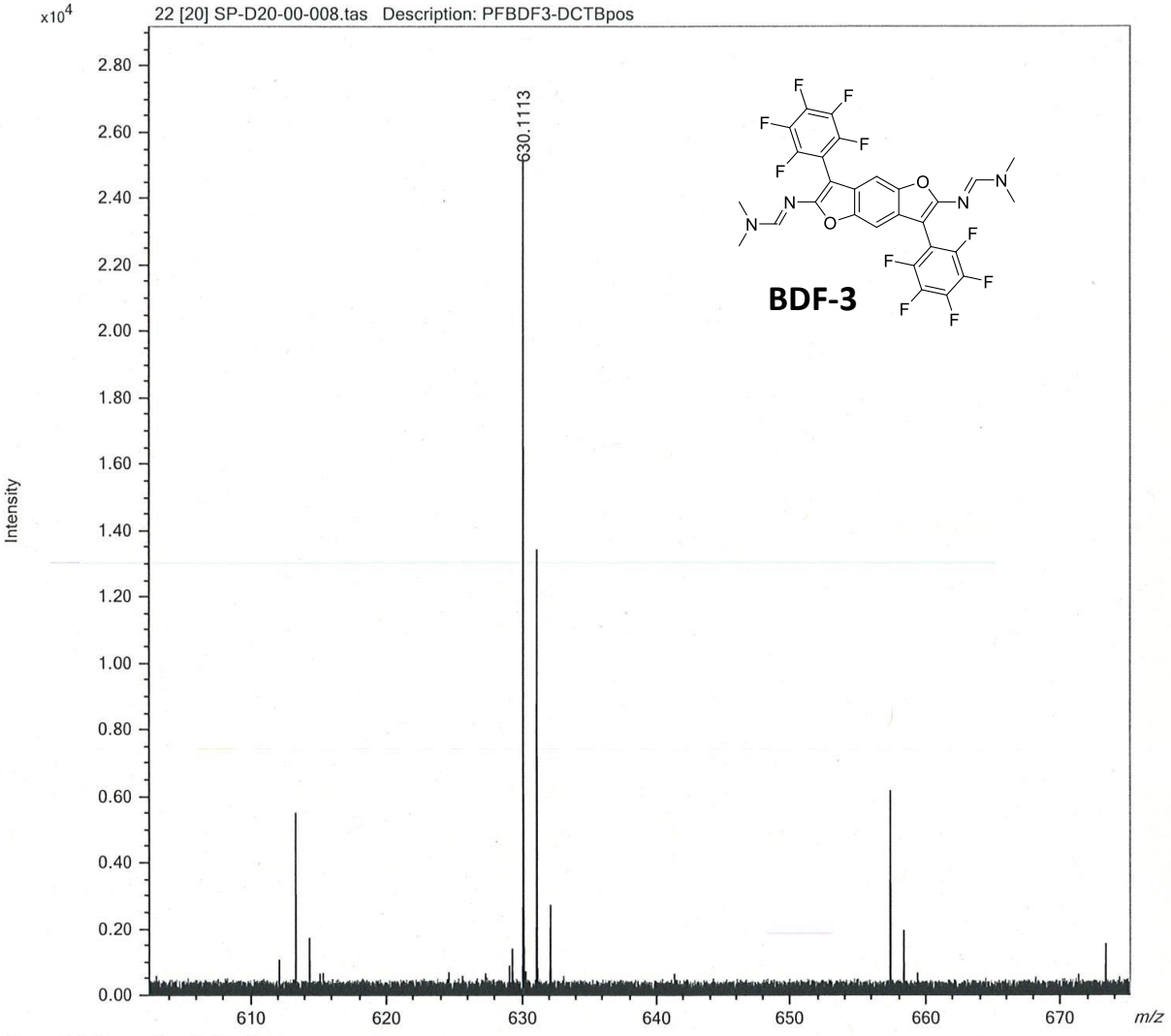
Elements

C 30 - 40 H 0 - 200 N 0 - 5 O 0 - 5 F 0 - 20

Results:

#	Formula	Mass	DBE	Abs. Error (u)	Error (u)	Error (ppm)
1	C32 H10 N3 O2 F15	753.05280	22.0	0.00028	-0.00028	-0.38

HRMS (MALDI TOF) of **BDF-3**



Elemental Composition Estimation

Parameters:

Mass	Tolerance	Electron Mode	Charge	DBE Range	Max Results
630.11134 ± 0.00063	1.0 ppm	Odd/Even	+1	-0.5 - 200.0	100

Elements

C 0 - 30 H 0 - 200 N 0 - 5 O 0 - 5 F 0 - 10

Results:

#	Formula	Mass	DBE	Abs. Error (u)	Error (u)	Error (ppm)
1	C28 H16 N4 O2 F10	630.11081	18.0	0.00053	0.00053	0.85