Branching Effect on Triphenylamine-CF_3 cyanostilbenes: Enhanced Emission and Aggregation in Water

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Supporting Information

Table S1**.** HOMO-LUMO energy gap values and absorption maxima in gaseous and solvent phase obtained through DFT studies

	HOMO (au)	LUMO (au)	Gap (au)	gap (Kcal/mol)	λ_{abs} (nm, gas phase)	λ_{abs} (nm, water)
1	-0.20592	-0.09274	0.11318	71.02079	442	461.5
2	-0.21451	-0.10728	0.10723	67.28715	483	509
3	-0.22082	-0.11389	0.10693	67.09889	485,480	507
4	-0.20983	-0.09823	0.1116	70.02933	447	-
5	-0.2208	-0.11454	0.10626	66.67847	487	-
6	-0.22884	-0.12207	0.10677	66.99849	487,482	-

(The HOMO-LUMO energy gaps were duplicated in the main manuscript for a comparative data with those obtained from Cyclic Voltammetry measurements)

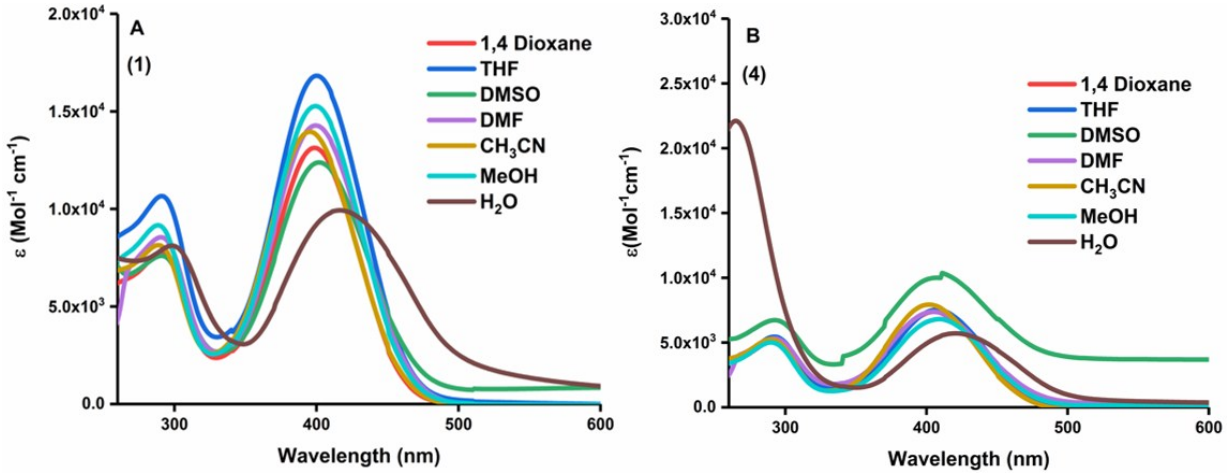


Fig S1. Absorption Spectra of (1) and (4) in solvents of different polarity

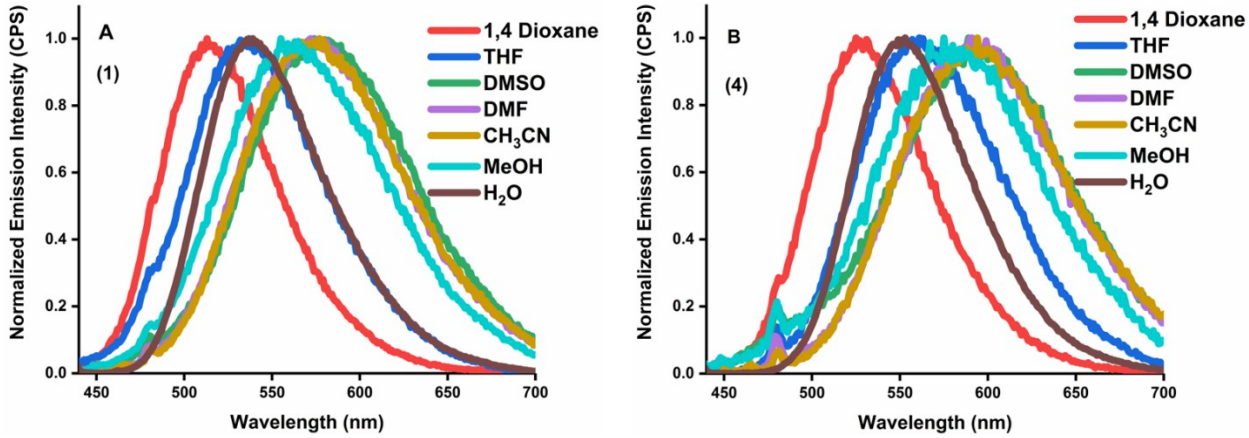
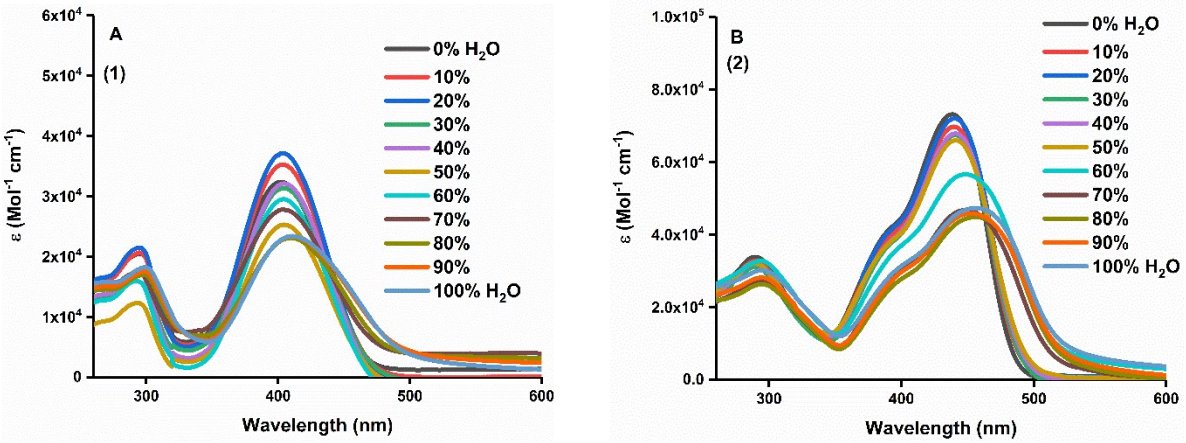


Fig S2. Emission Spectra of **1** and **4** in solvents of different polarity



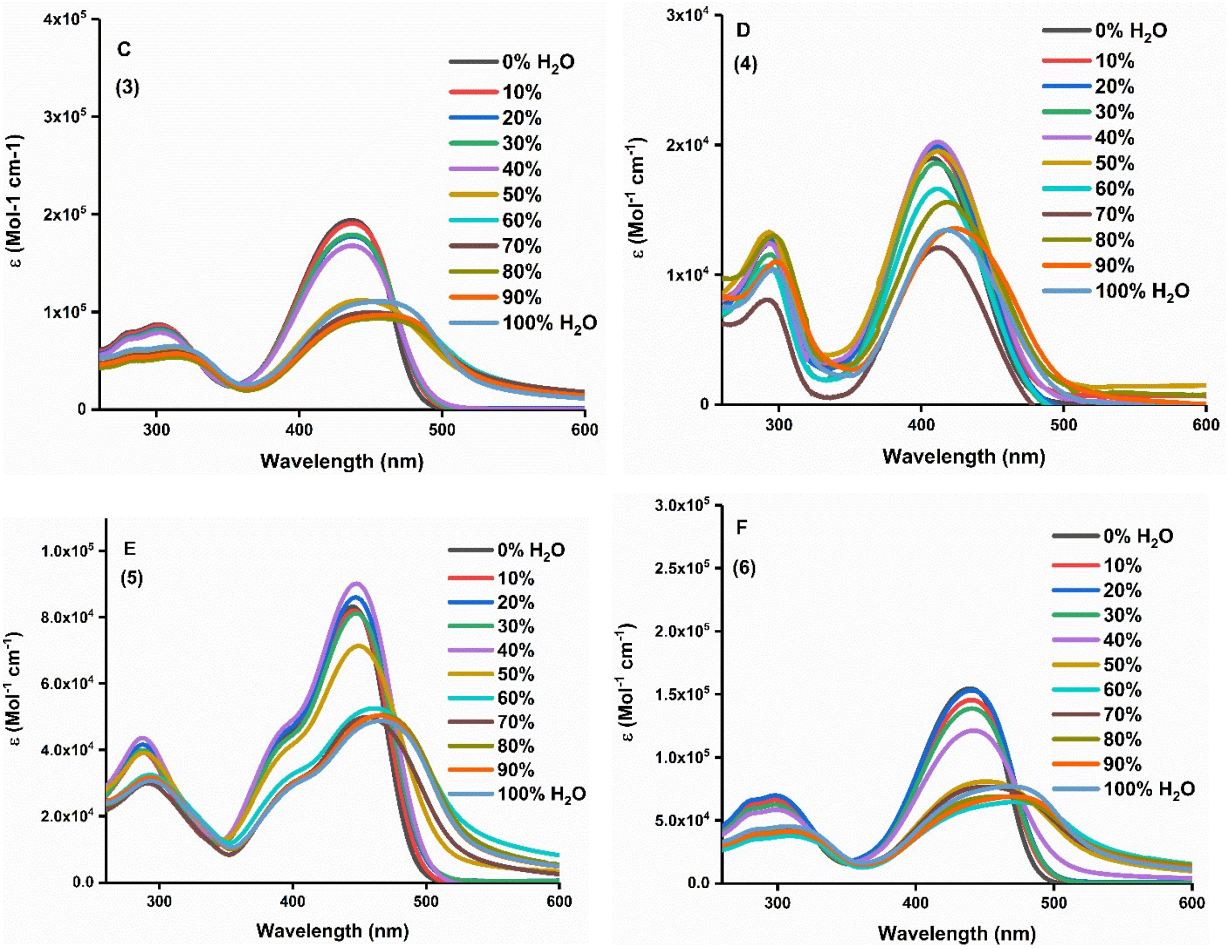


Fig S3. Absorption spectra of **1-6** in the dioxane-water binary mixture.

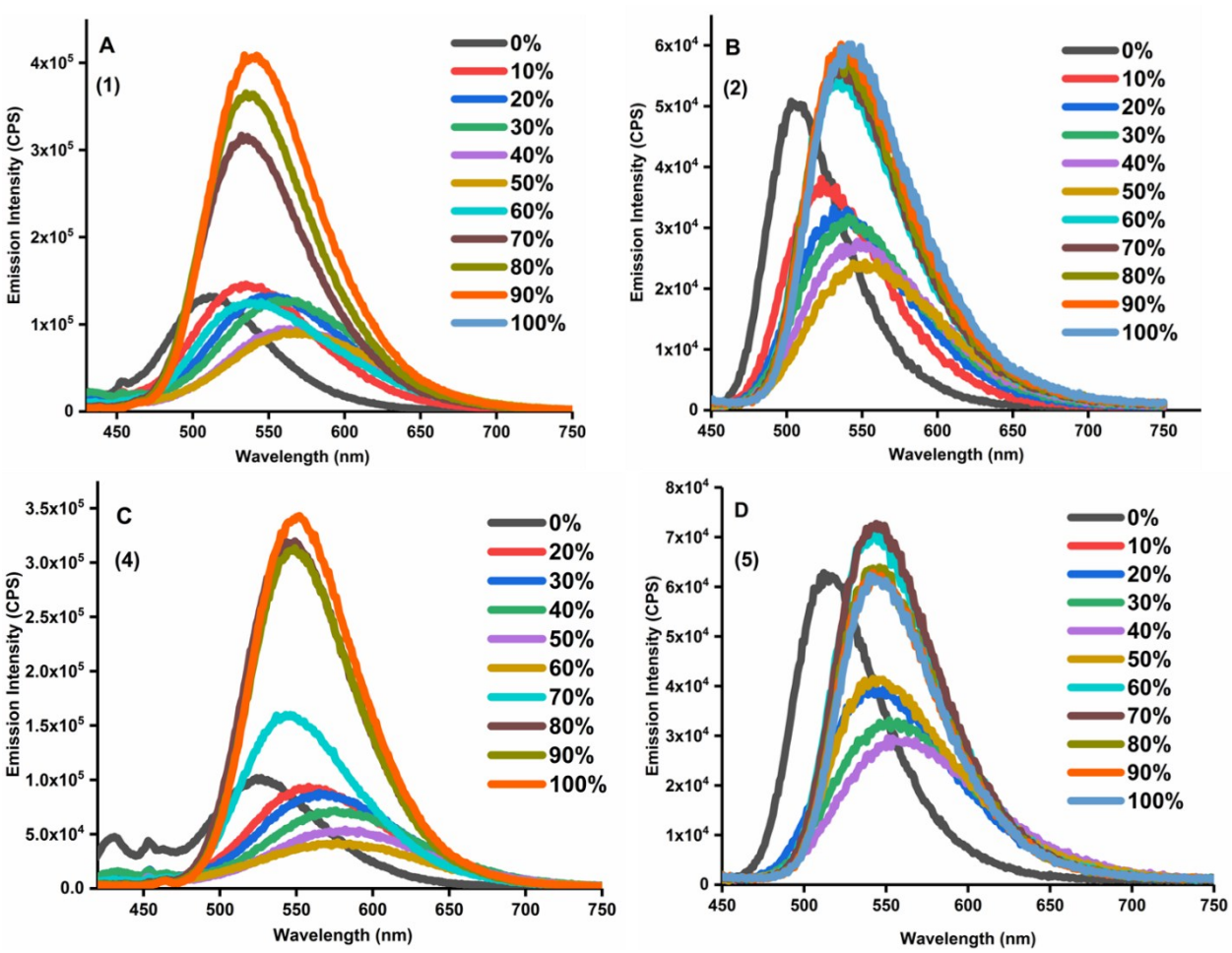


Fig S4. Emission of **1**, **2** & **4**, **5** in the dioxane-water binary mixture.

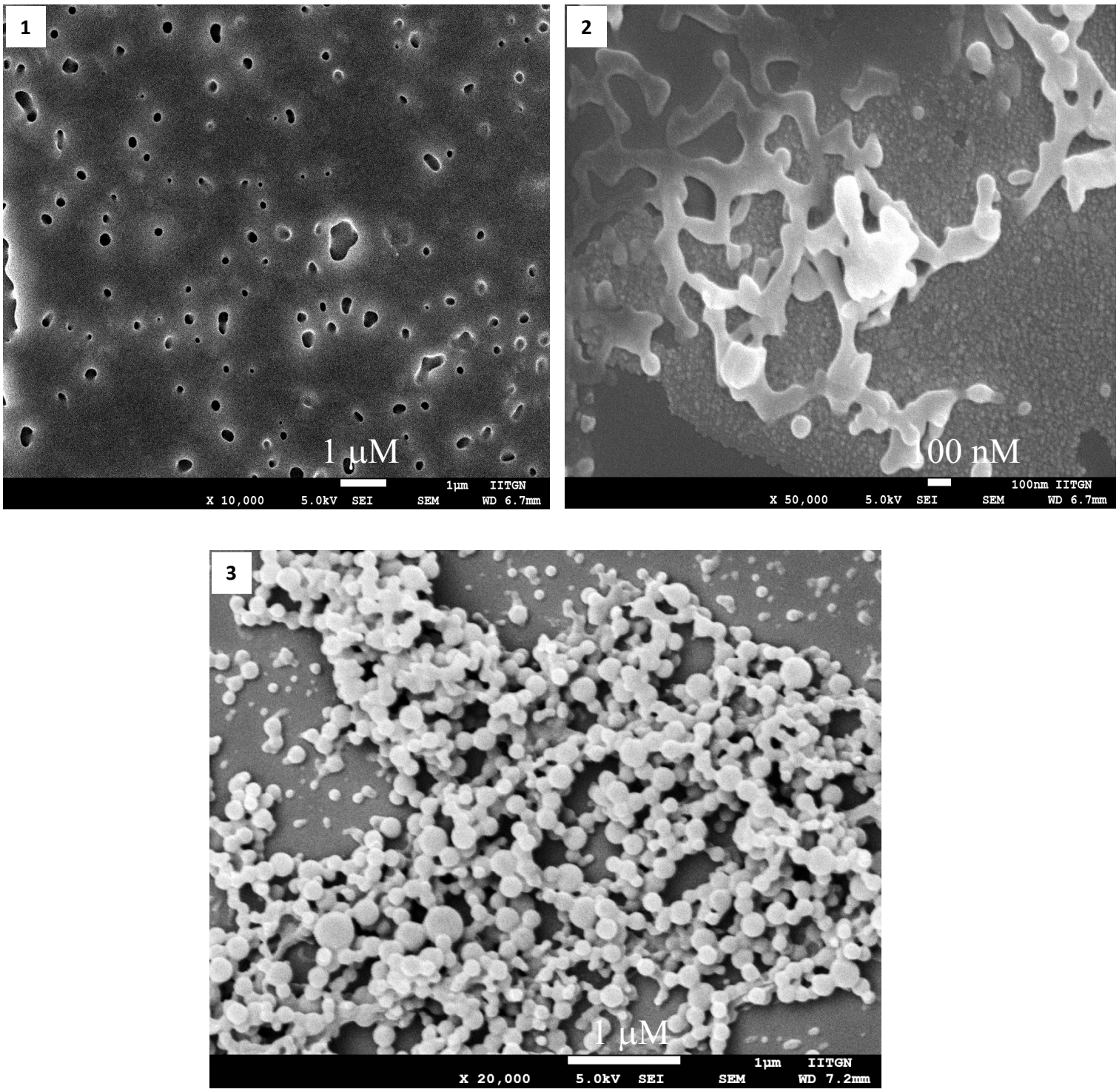


Fig S5. Drop-cast SEM images of molecules **1-3**. The concentrations used are 10μM in water.

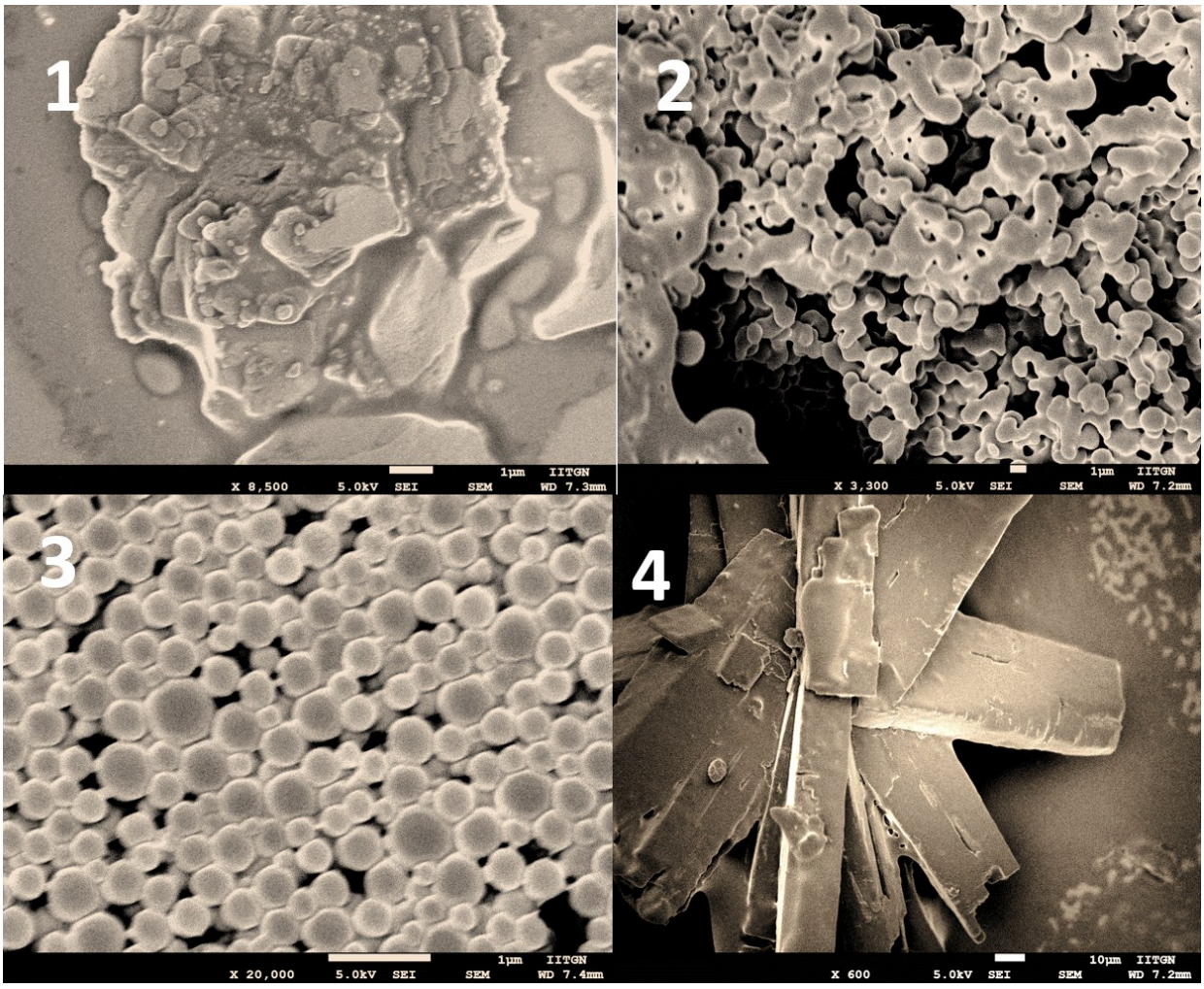
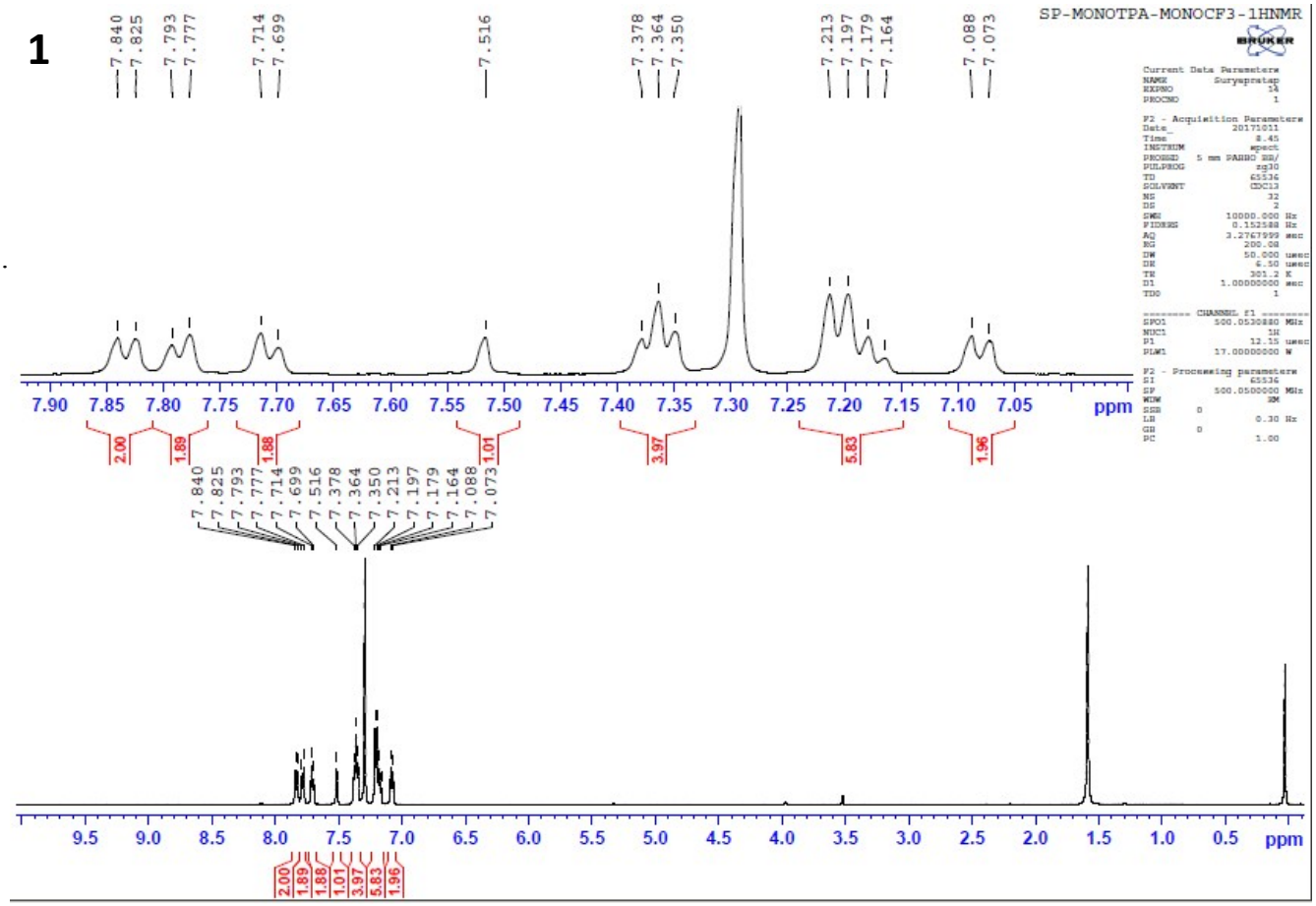


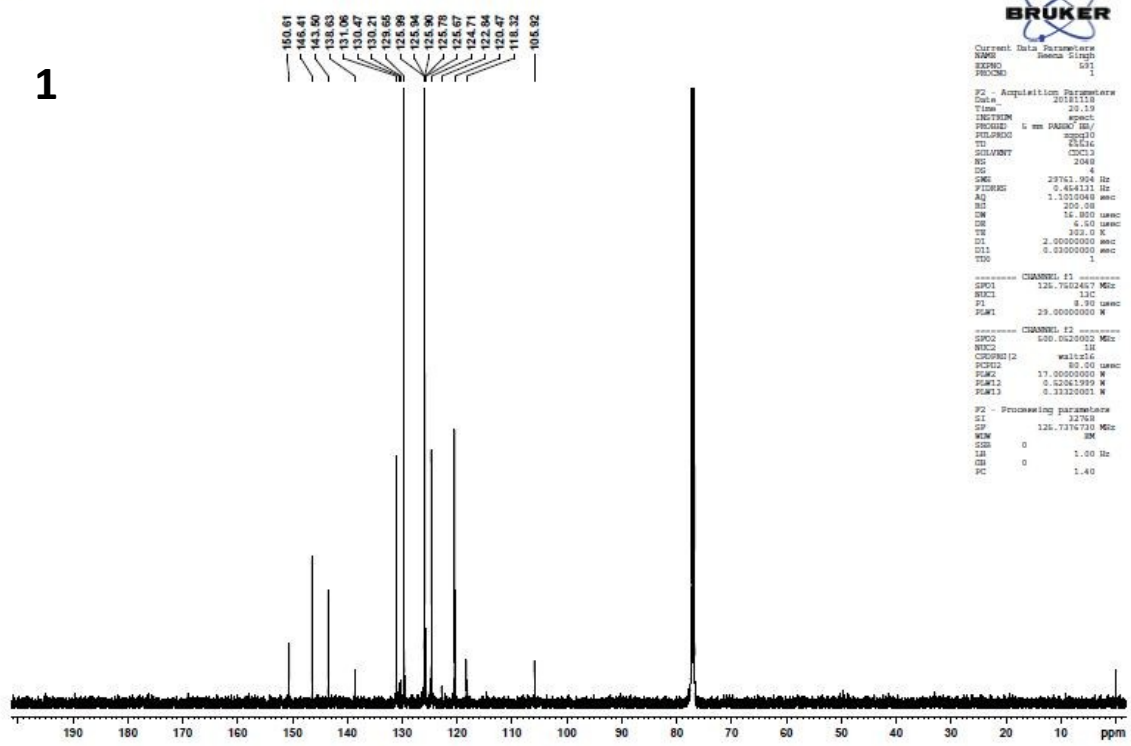
Fig S6. SEM images of the molecules kept in t-BuOH that do not form gel. The sample amounts used are 6 mg/500 µL.

1


SP-MONOTPA-MONOCF3-1HNMR
7.840
7.825
7.793
7.777
7.714
7.699
7.516
7.378
7.364
7.350
7.213
7.197
7.179
7.164
7.088
7.073
ppm
2.00
1.89
1.88
1.01
3.97
5.83
1.96

MM

1



BRUKER

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EXPNO                 591
PROCNO                  1

F2 - Acquisition Parameters
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Time              20.19
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG             200.08
DW               16.800 usec
DE                6.50 usec
TE              323.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
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NUC1              13C
P1               8.90 usec
PLW1       29.00000000 W

======== CHANNEL f2 ========
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NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2       17.00000000 W
PLW12       0.52061999 W
PLW13       0.33320001 W

F2 - Processing parameters
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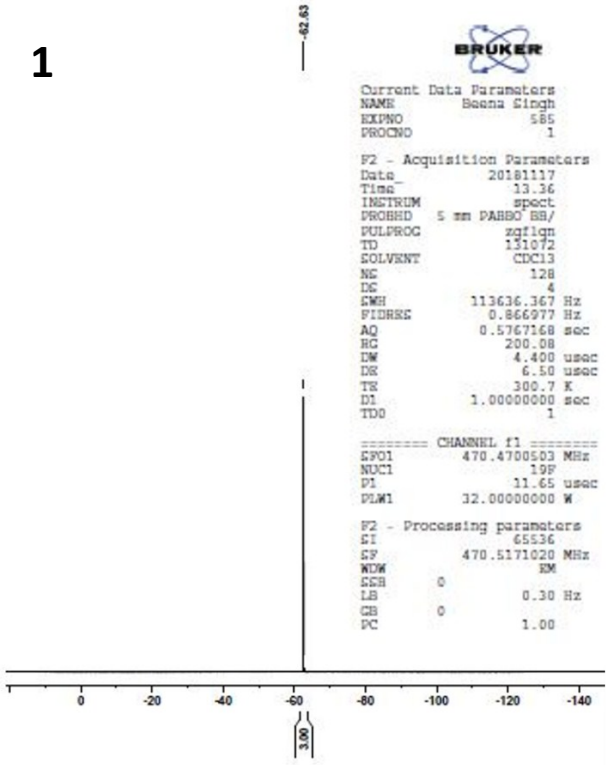
BS_MonoTPA_MONOCF3_1

1



BRUKER

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PROCNO                  1

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PULPROG          zgflqn
TD               131072
SOLVENT           CDCl3
NS                  128
DS                    4
SWH          113636.367 Hz
FIDRES         0.866977 Hz
AQ            0.5767168 sec
RG              200.08
DW               4.400 usec
DE                6.50 usec
TE              300.7 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
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NUC1              19F
P1               11.65 usec
PLW1       32.00000000 W

F2 - Processing parameters
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SF          470.5171020 MHz
WDW                  EM
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LB                0.30 Hz
GB                0
PC                1.00
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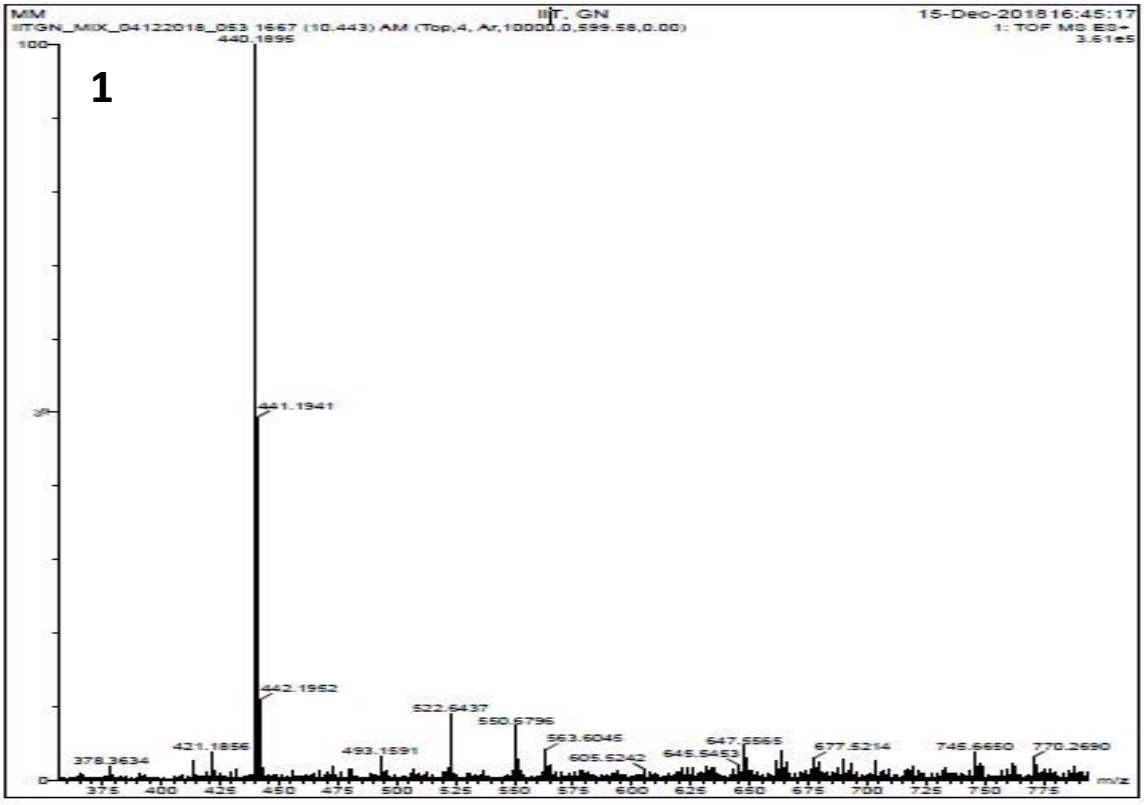
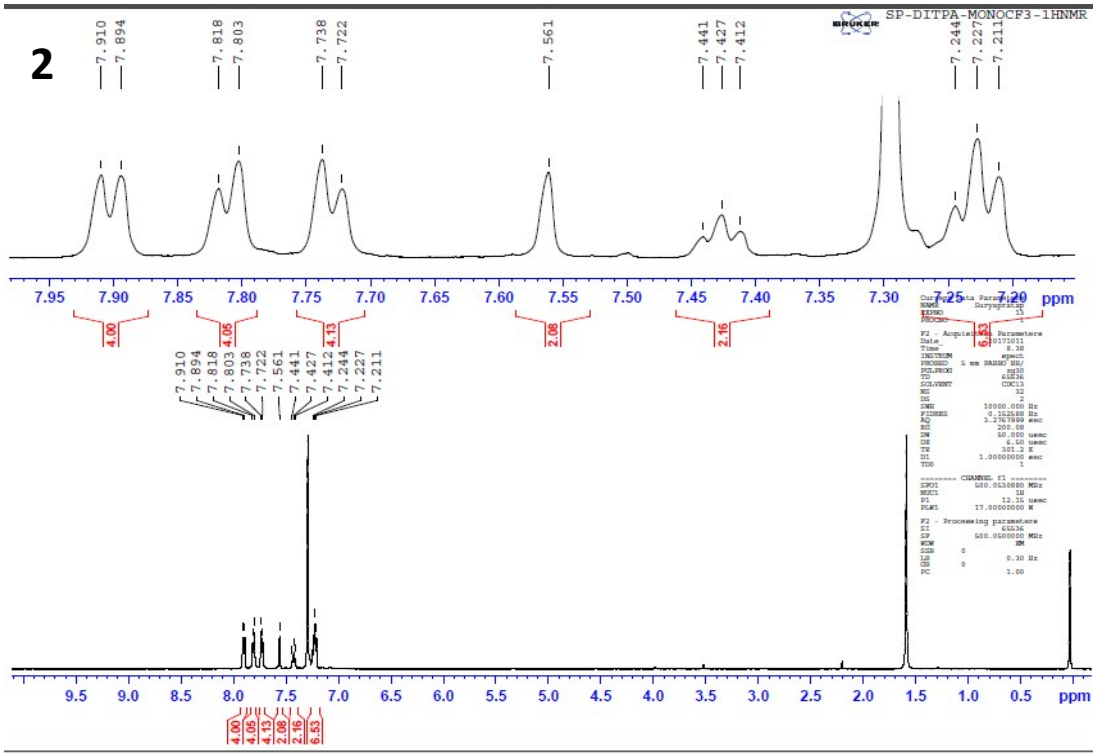
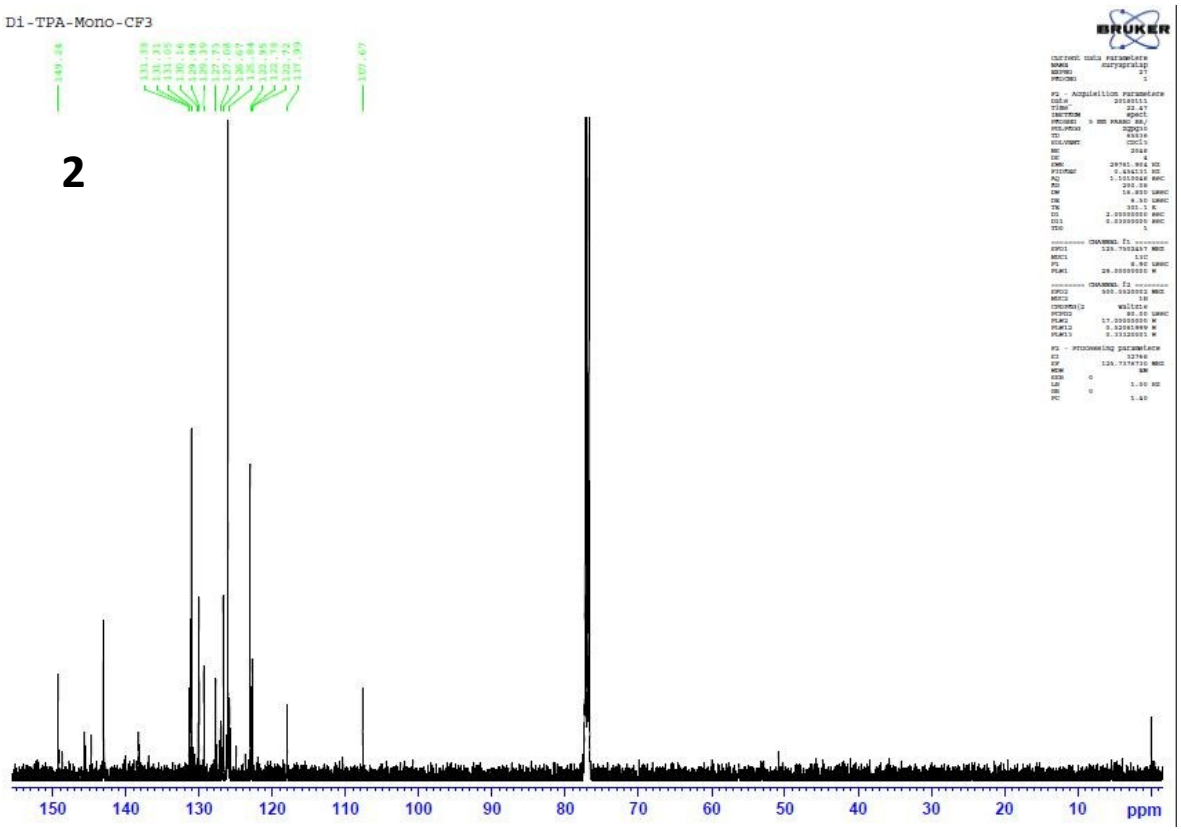


Fig S7. ^{1}H, ^{13}C, ^{19}F NMR and mass spectrometry data of **(1)**

2


SP-DITPA-MONOCF3-1HNMR
7.910
7.894
7.818
7.803
7.738
7.722
7.561
7.441
7.427
7.412
7.244
7.227
7.211
7.95 7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 ppm
4.00
4.05
4.13
2.08
2.16
6.53
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm


Di-TPA-Mono-CF3
2
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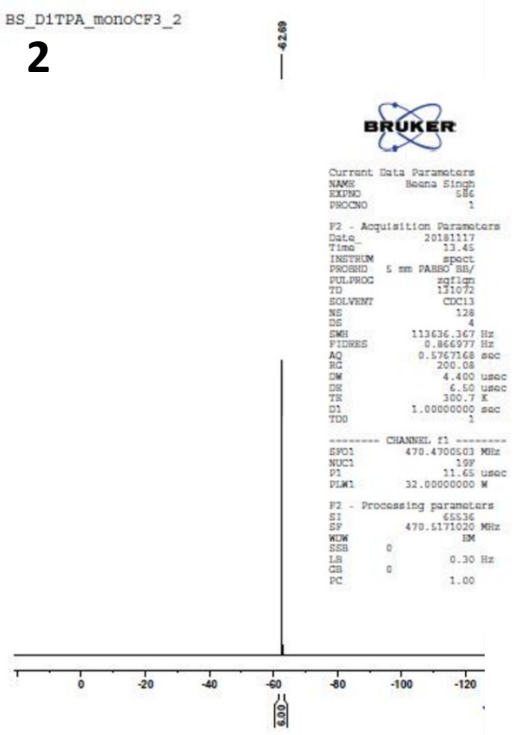
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



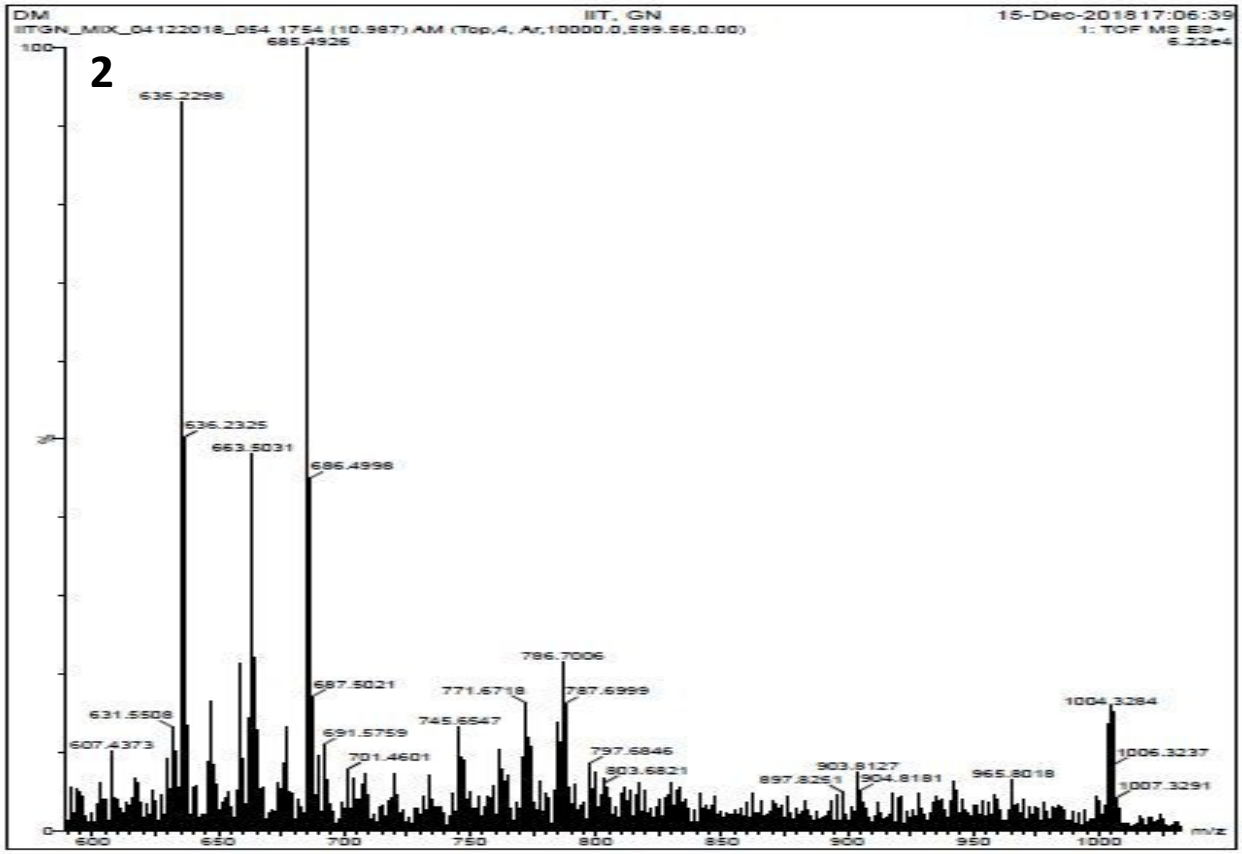
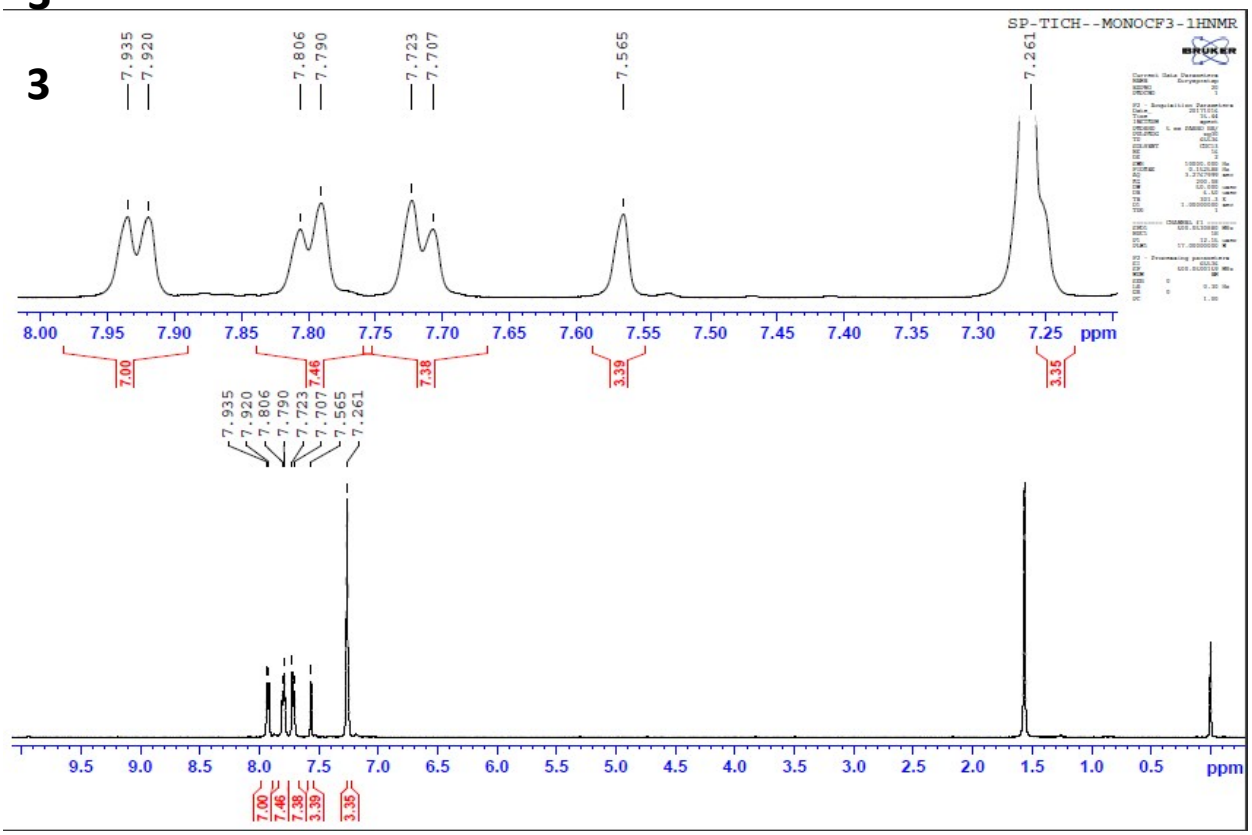


Fig S8. ^{1}H, ^{13}C & ^{19}F NMR and mass spectrometry data of **(2)**

3


SP-TICH--MONOCF3-1HNMR
BRUKER
7.935
7.920
7.806
7.790
7.723
7.707
7.565
7.261
8.00 7.95 7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 ppm
7.00
7.46
7.38
3.39
3.35
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

3

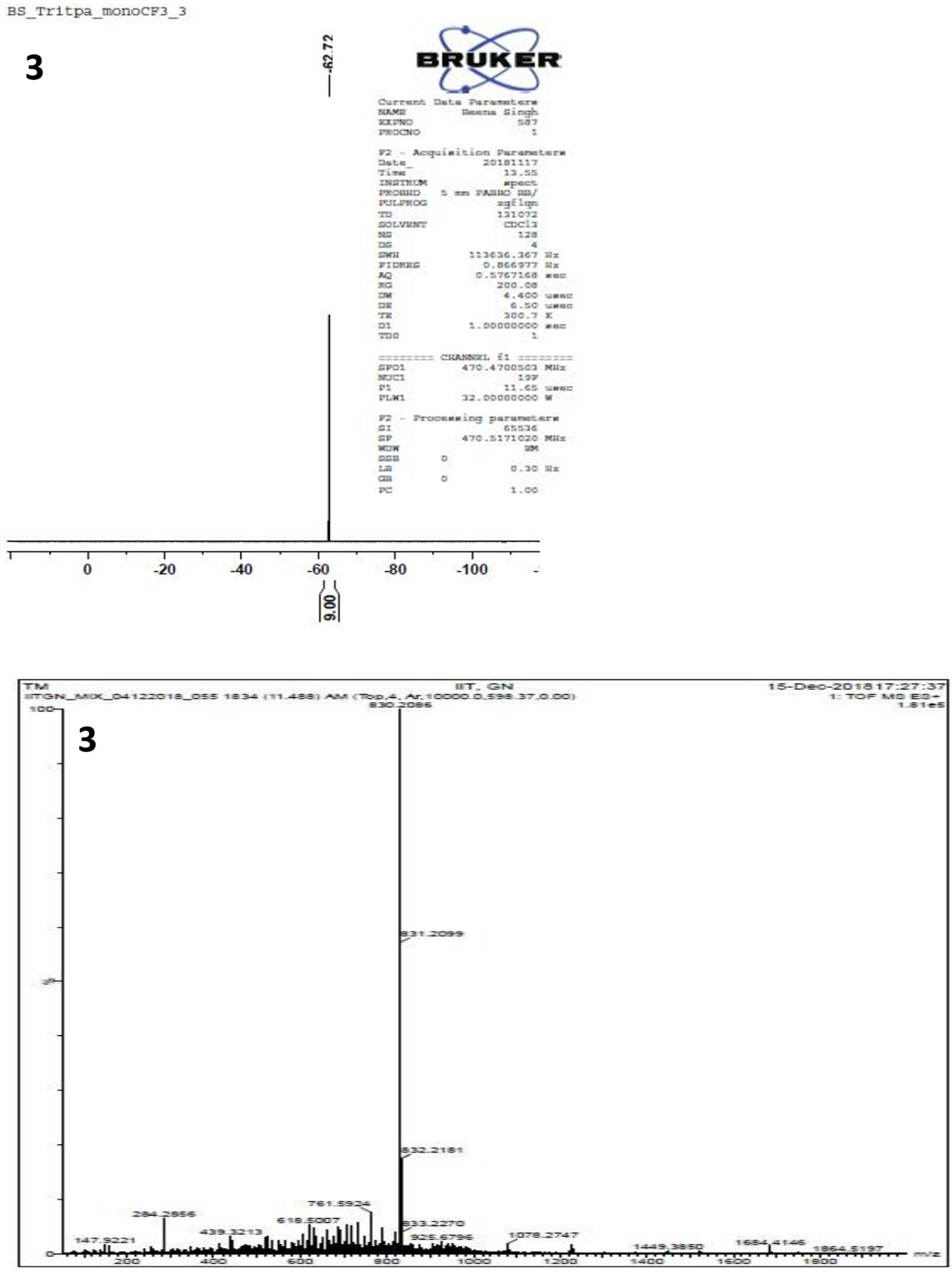
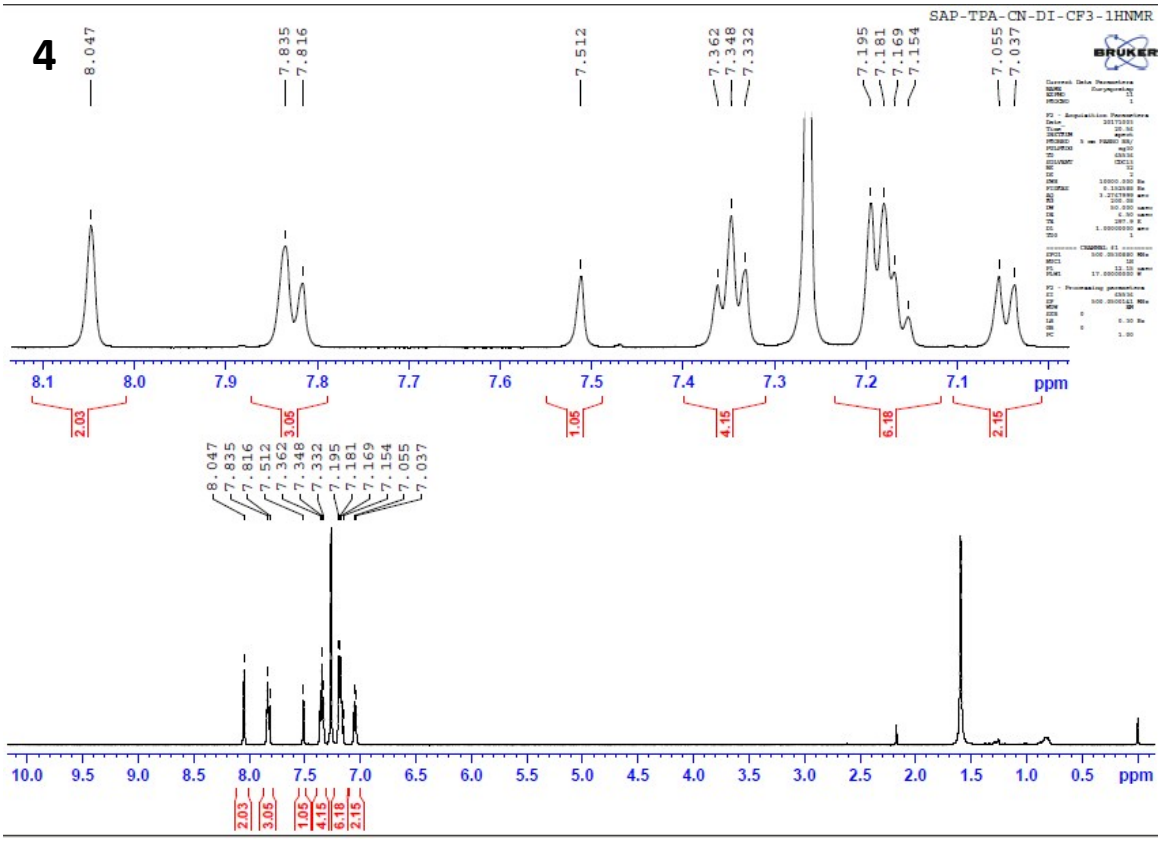
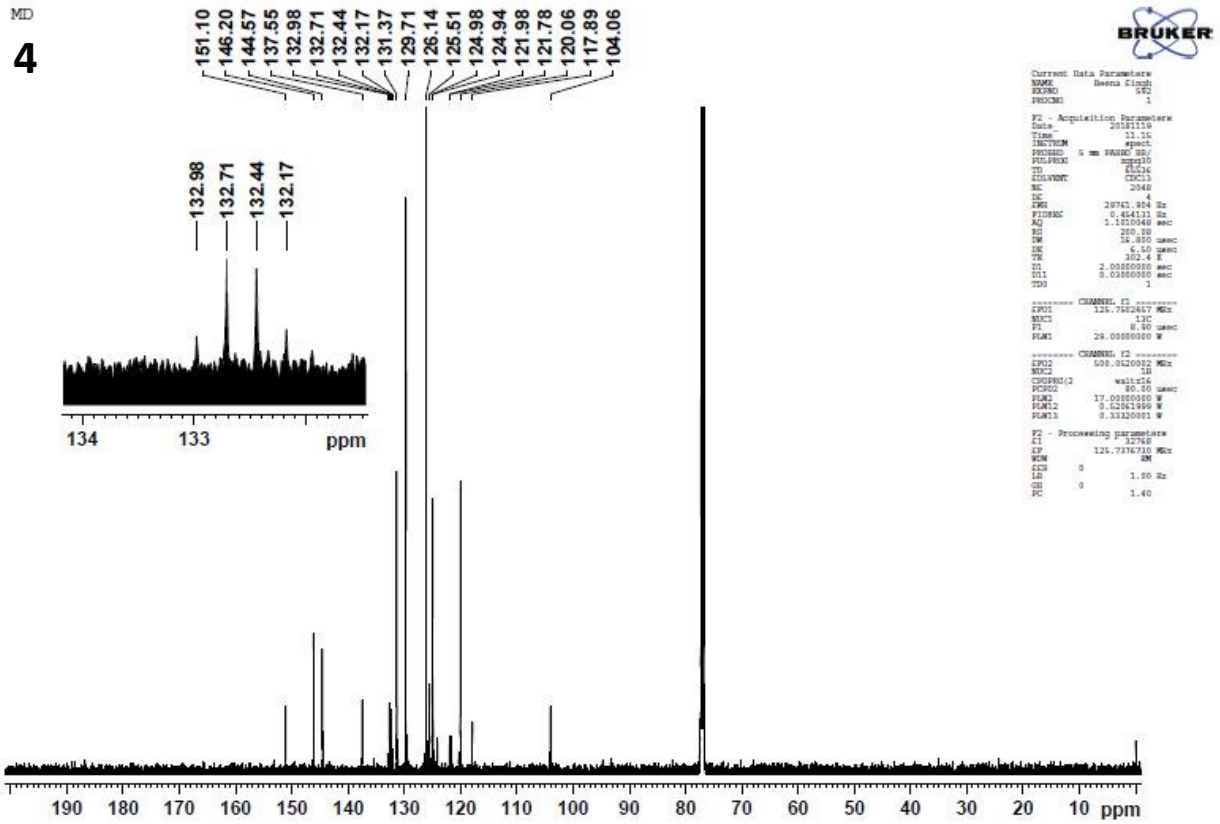


Fig S9. ^{1}H, ^{13}C & ^{19}F NMR and mass spectrometry data of **(3)**


4
SAP-TPA-CN-DI-CF3-1HNMR
8.047
7.835
7.816
7.512
7.362
7.348
7.332
7.195
7.181
7.169
7.154
7.055
7.037
ppm


MD
4
151.10
146.20
144.57
137.55
132.98
132.71
132.44
132.17
131.37
129.71
126.14
125.51
124.98
124.94
121.98
121.78
120.06
117.89
104.06
ppm

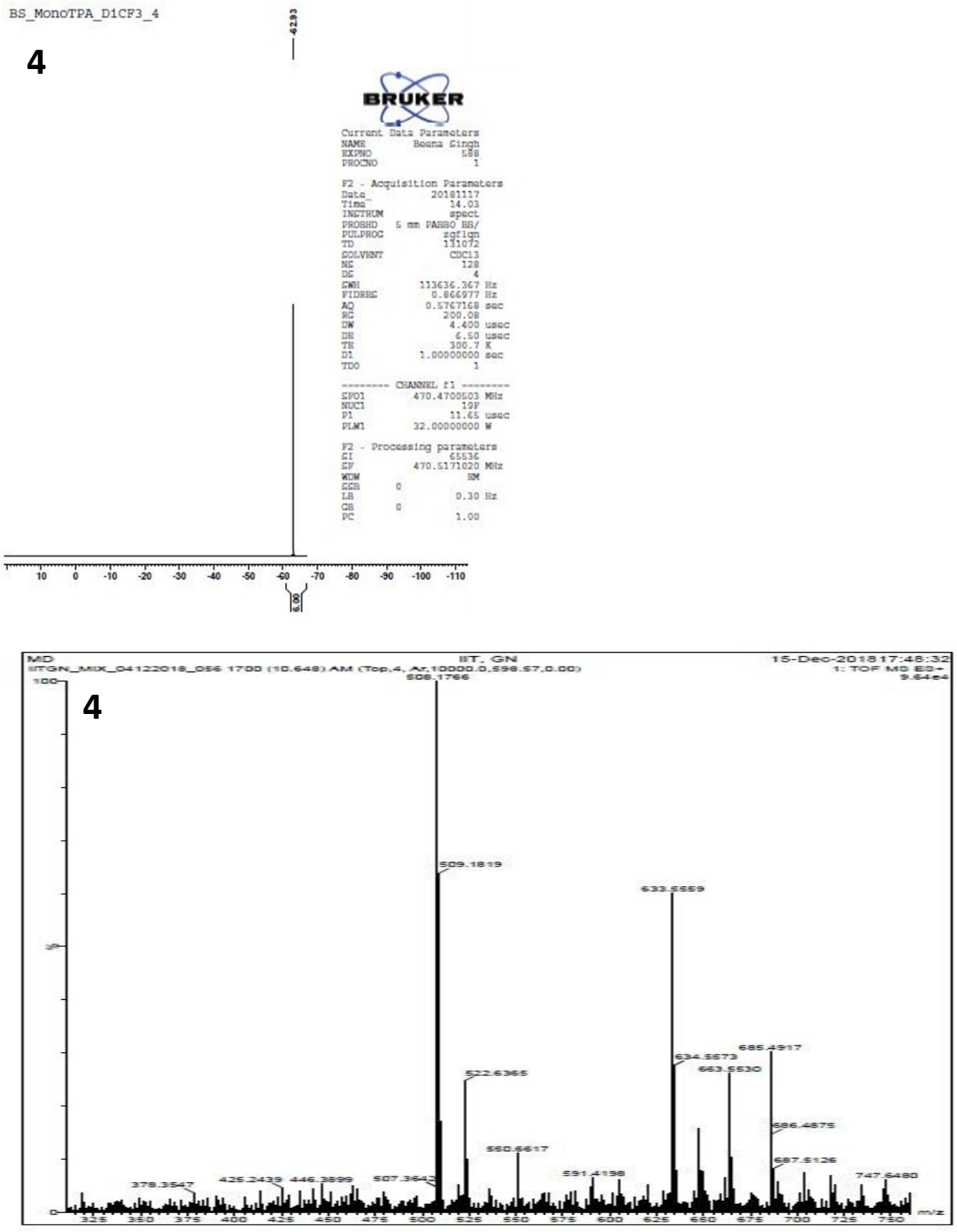
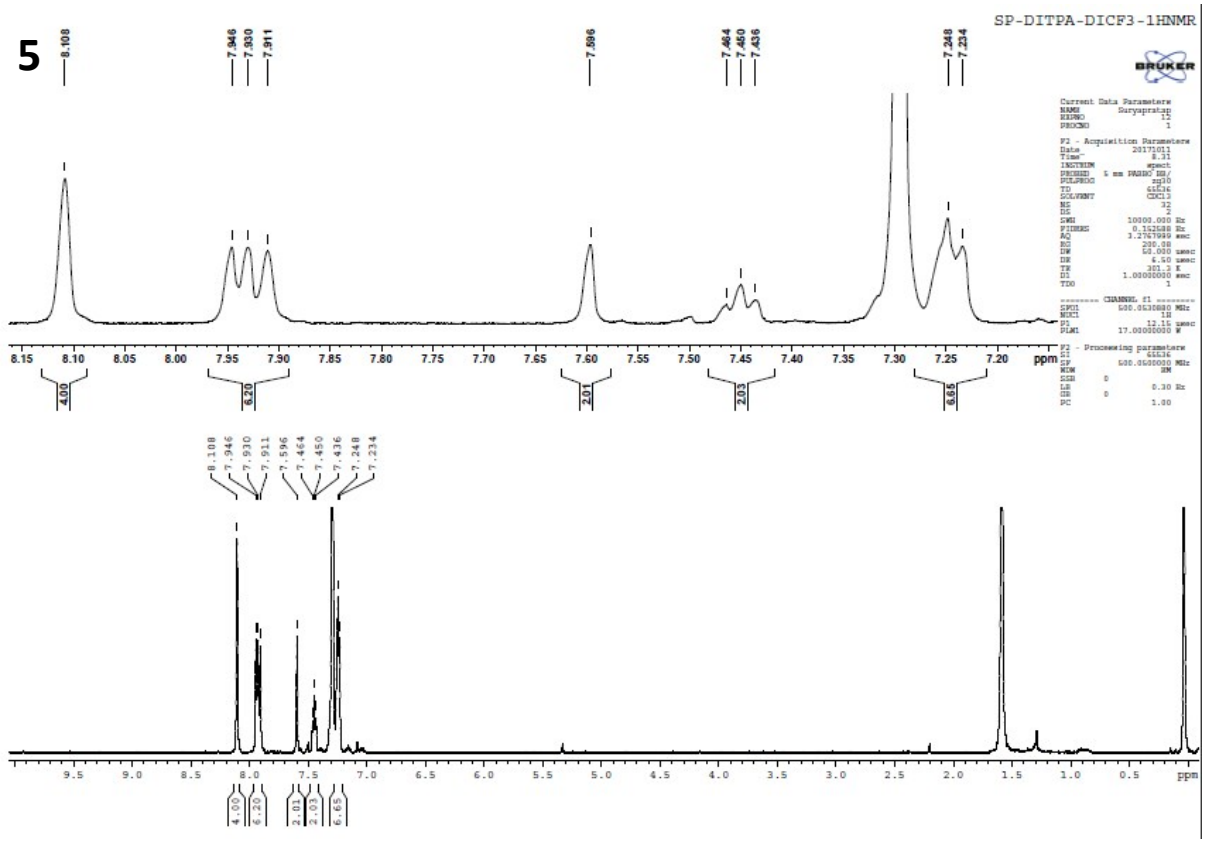
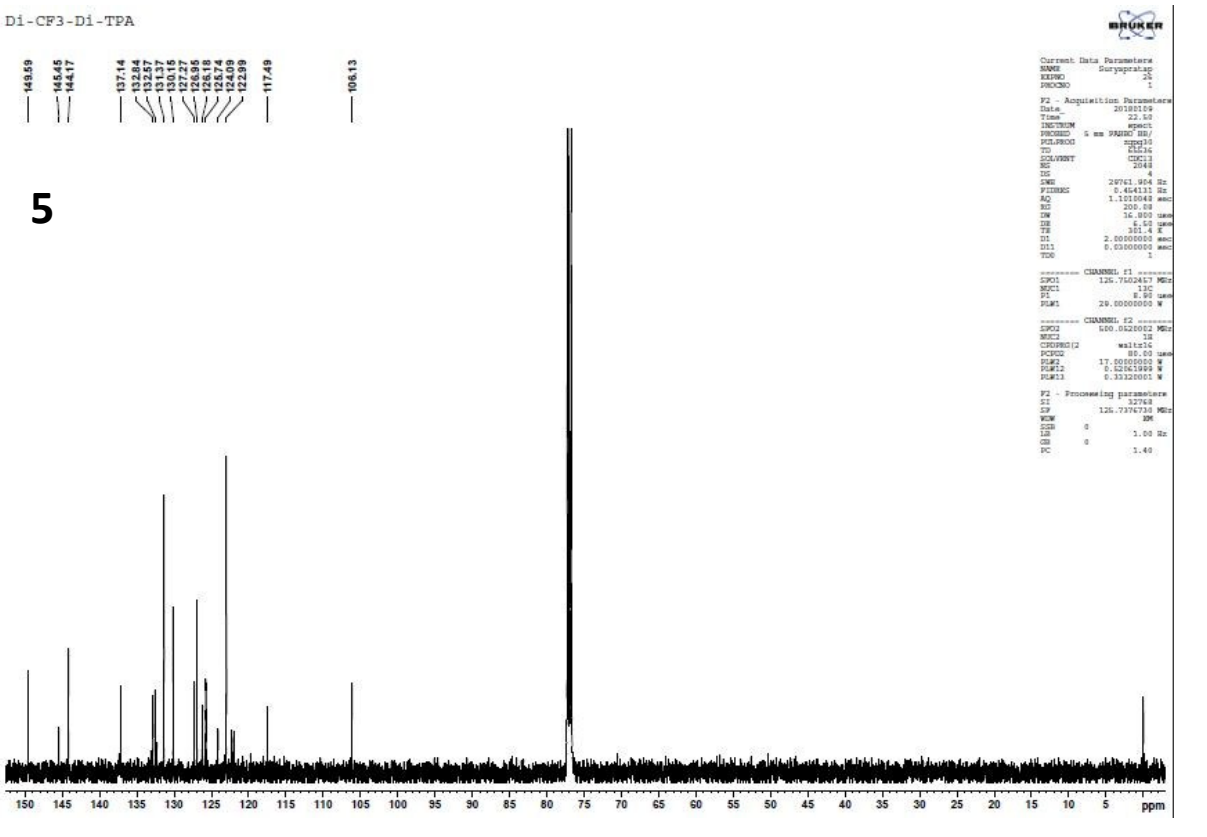


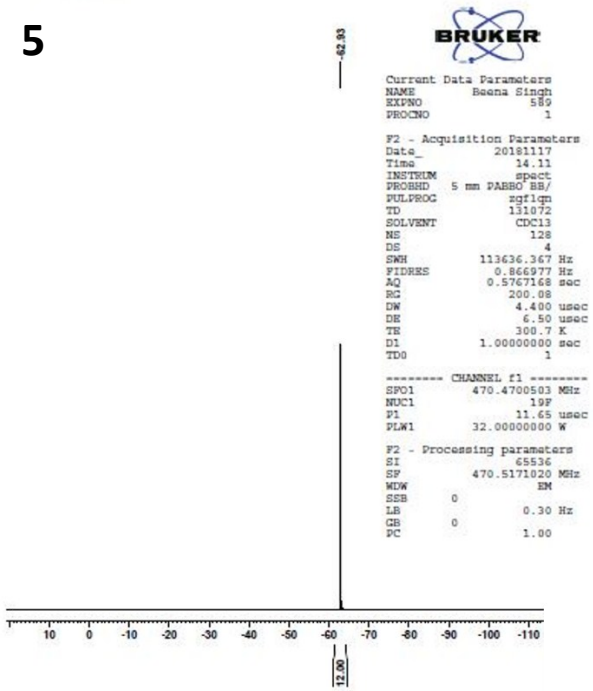
Fig S10. ^{1}H, ^{13}C & ^{19}F NMR and mass spectrometry data of **(4)**


5
SP-DITPA-DICF3-1HNMR
8.108
7.946
7.930
7.911
7.596
7.464
7.450
7.436
7.248
7.234
ppm


Di-CF3-Di-TPA
5
149.59
145.45
144.17
137.14
132.84
132.57
131.17
130.16
127.27
126.95
126.18
125.74
124.09
122.99
117.49
106.13
ppm

BS_DiTPA_diCF3_5

5



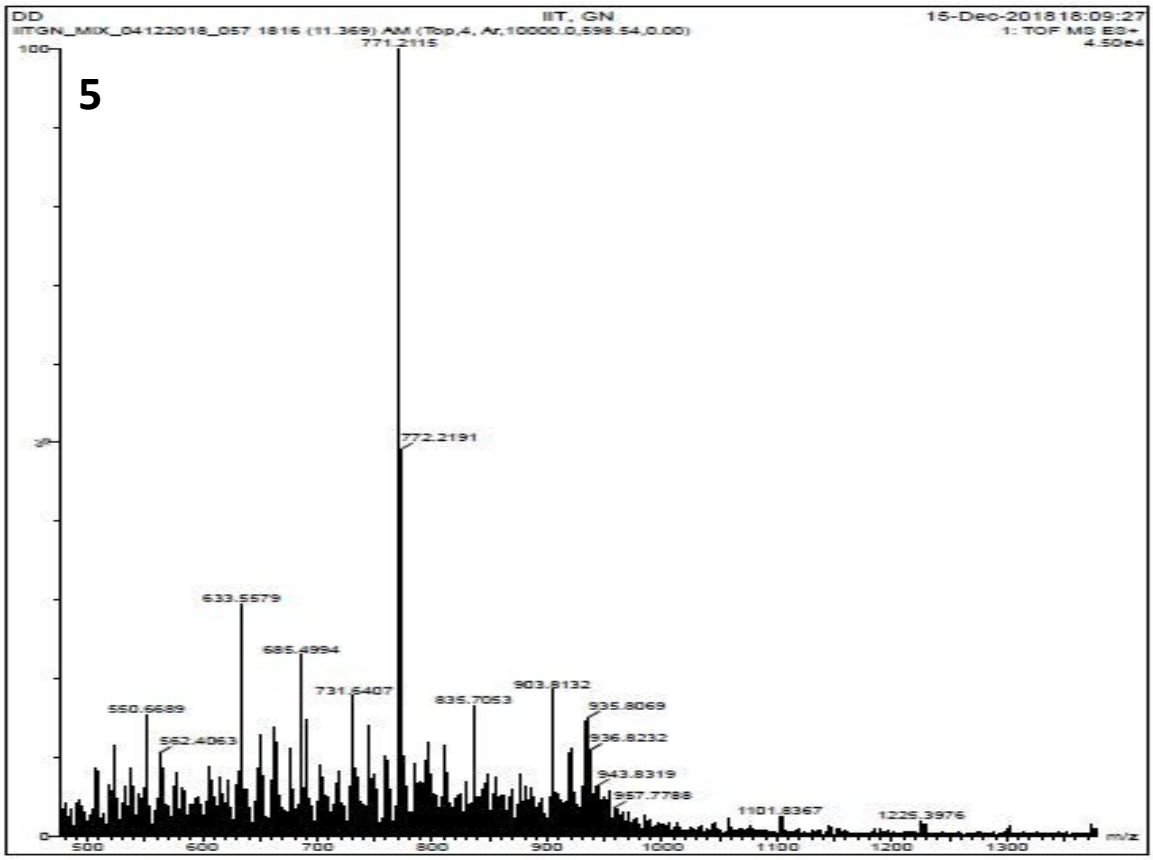
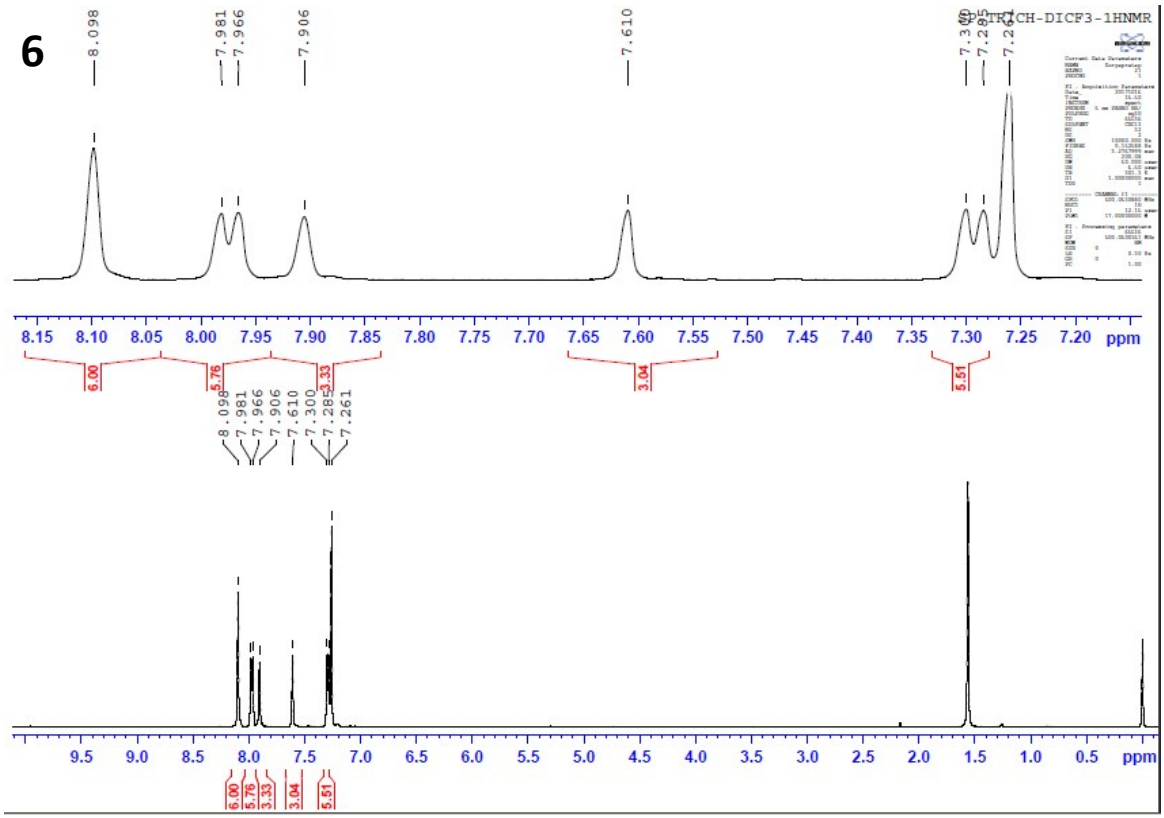
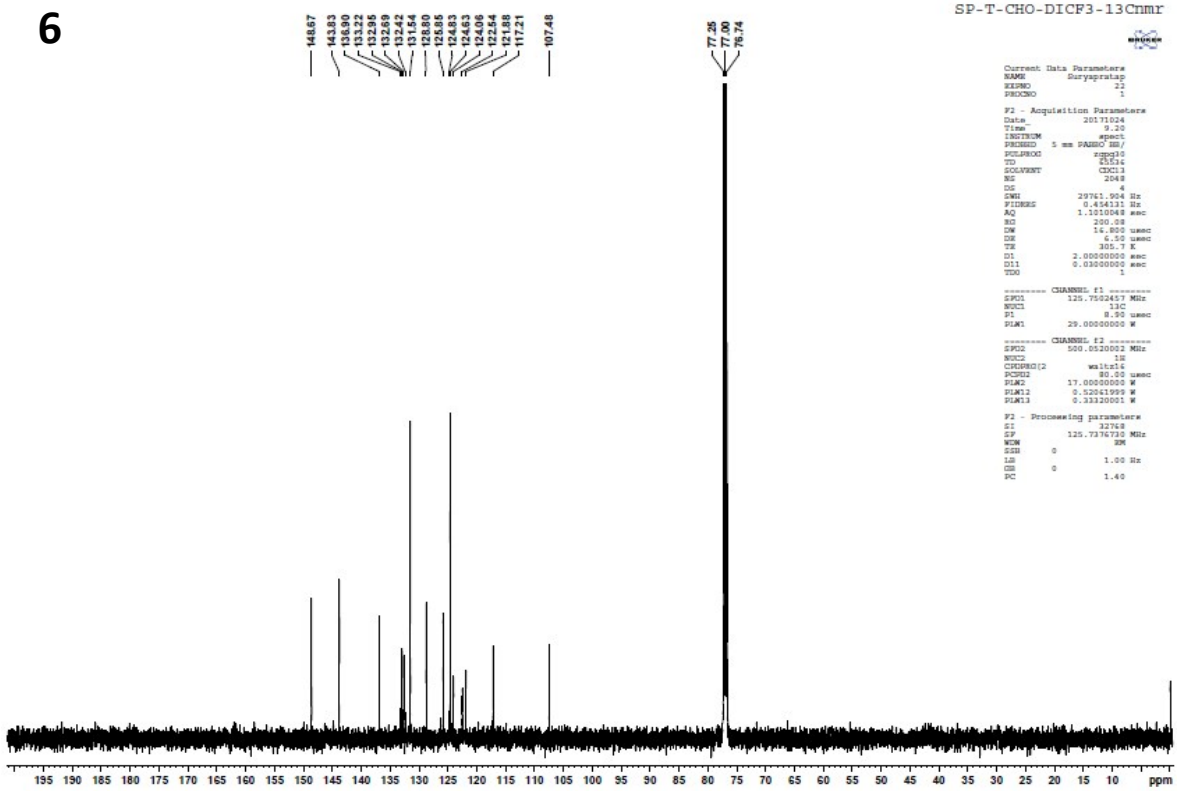


Fig S11. ^{1}H, ^{13}C & ^{19}F NMR and mass spectrometry data of **(5)**

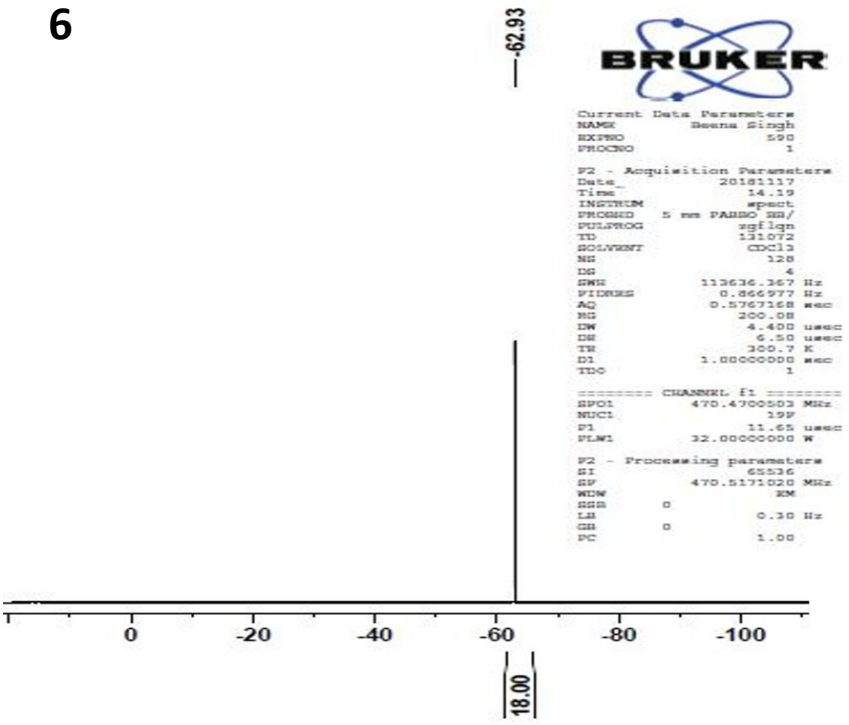
6


SP-T-CH-DICF3-1HNMR
8.098
7.981
7.966
7.906
7.610
7.300
7.285
7.261
ppm

6


SP-T-CHO-DICF3-13Cnmr
148.67
143.83
136.90
133.22
132.95
132.69
132.42
131.54
128.80
125.85
124.83
124.63
124.06
122.54
121.88
117.21
107.48
77.25
77.00
76.74
ppm

BS_Tr1TPA_D1CF3_6



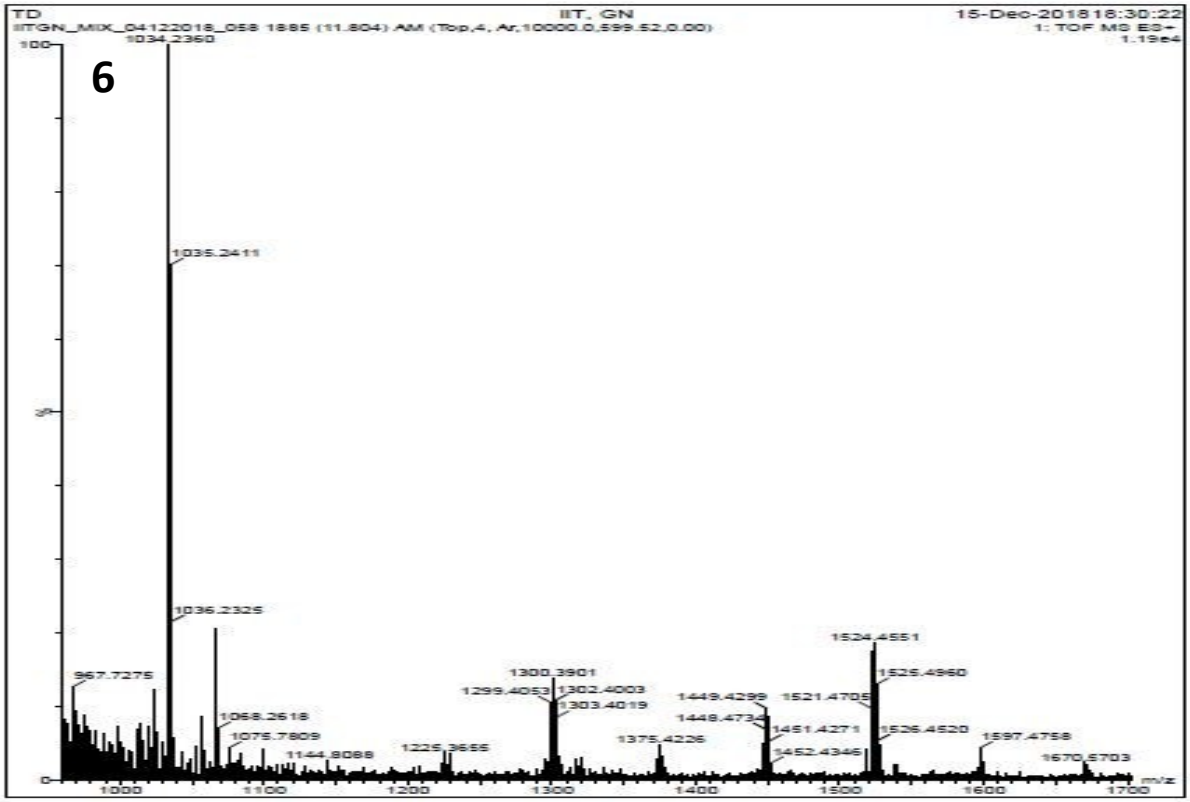
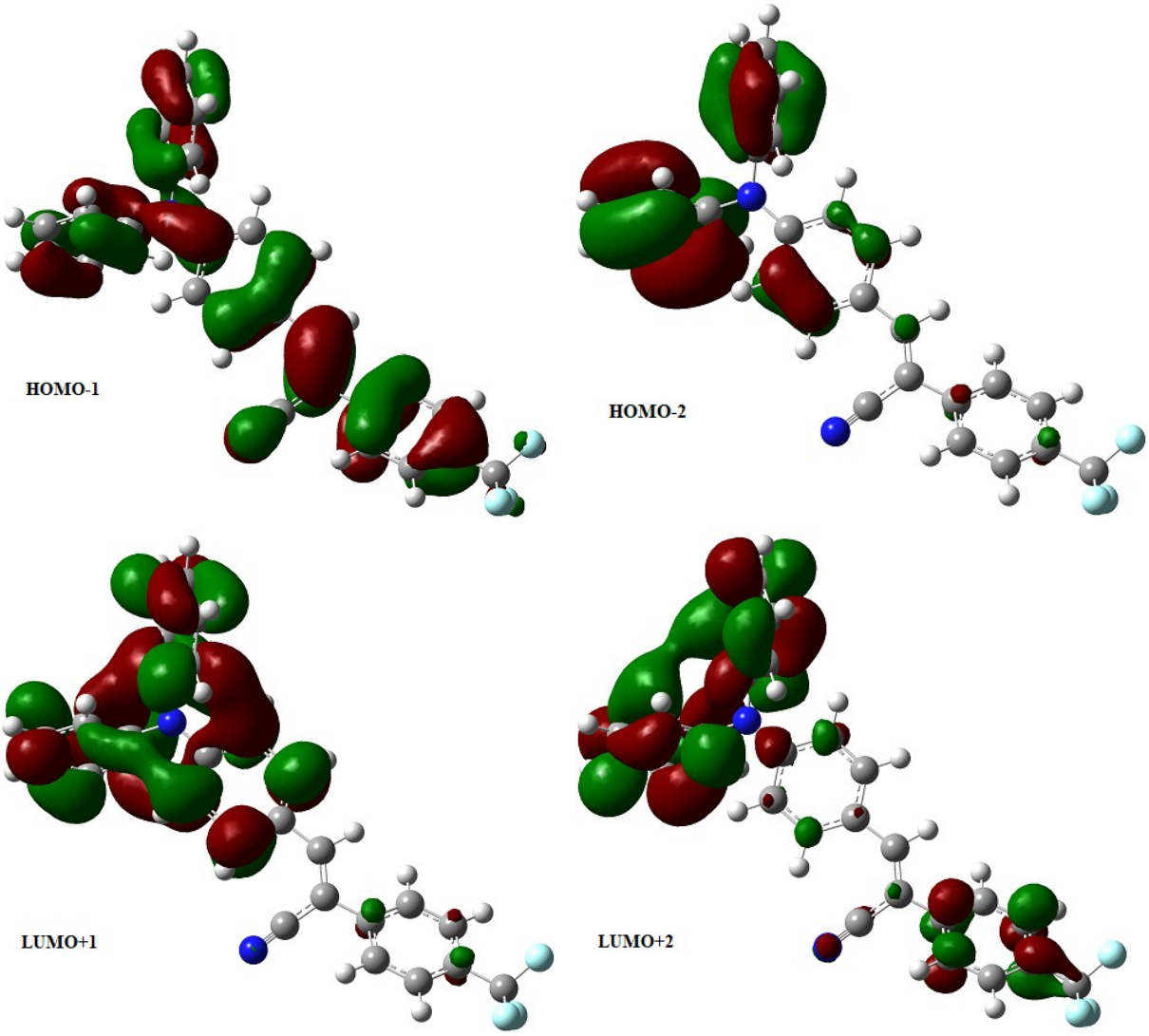


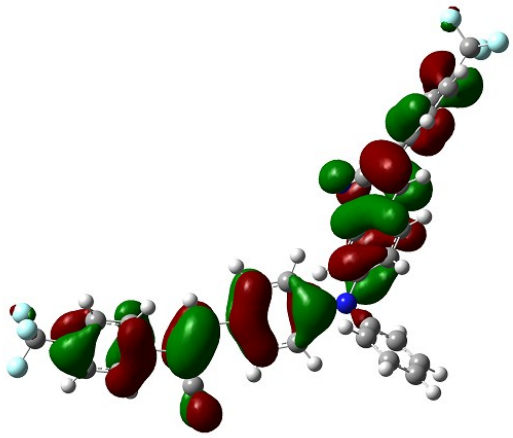
Fig S12. [1] H and 13C NMR and mass spectrometry data of (6)

Fig S13. Molecular Orbitals (HOMO-1, HOMO-2, LUMO+1, LUMO+2) of individual molecules

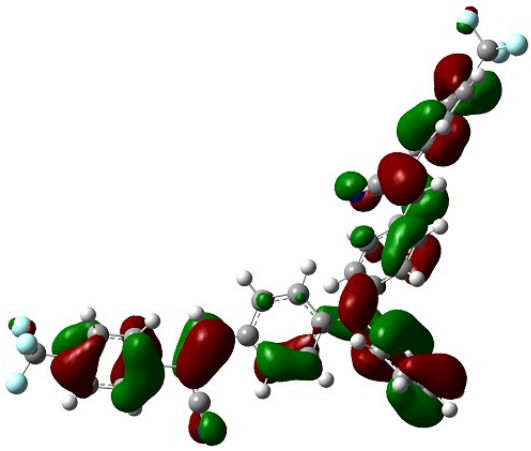
MOLECULE 1



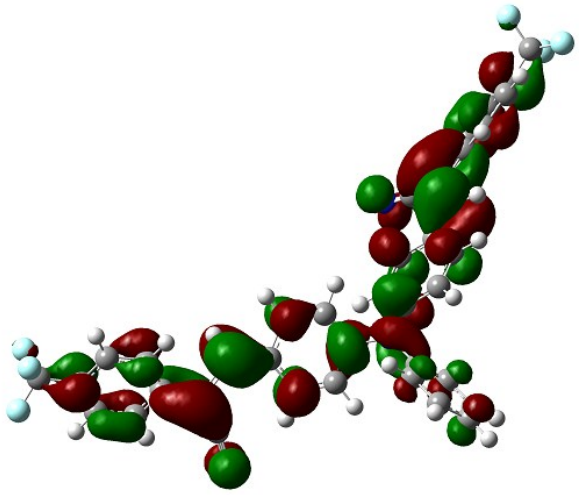
MOLECULE 2



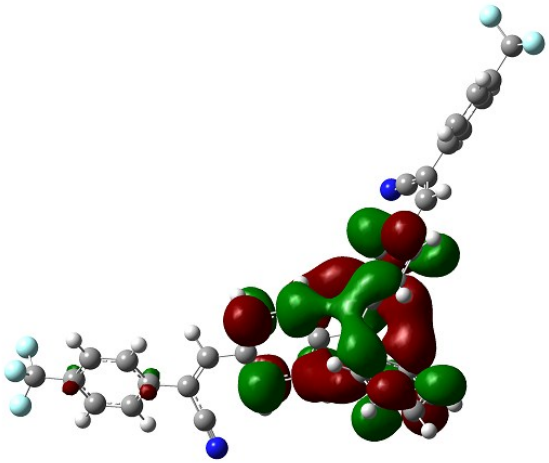
HOMO-1



HOMO-2

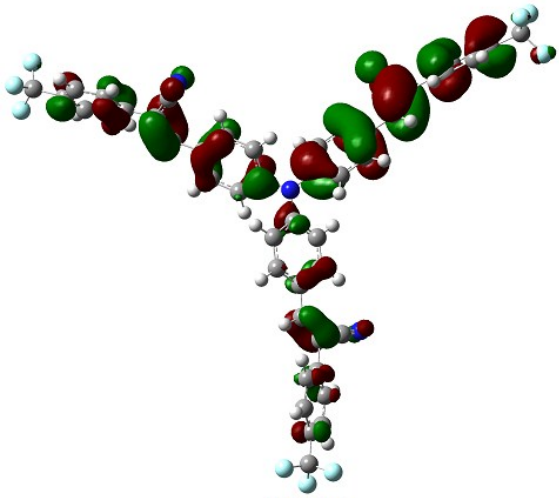


LUMO+1

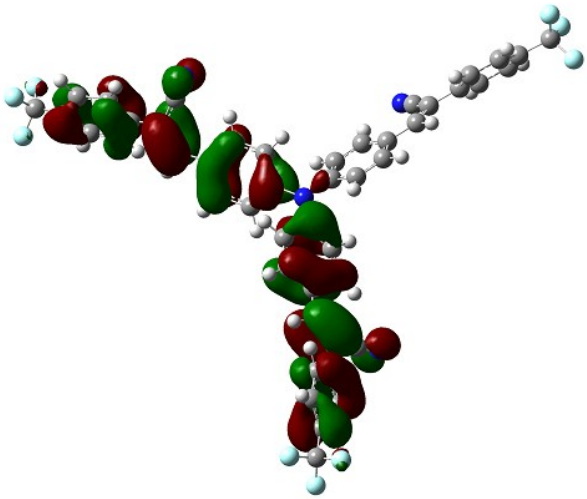


LUMO+2

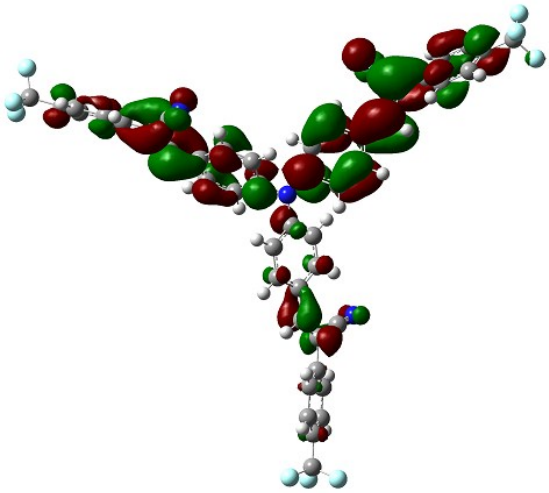
MOLECULE 3



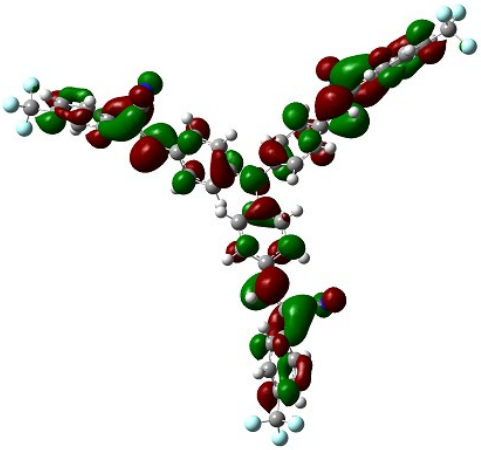
HOMO-1



HOMO-2

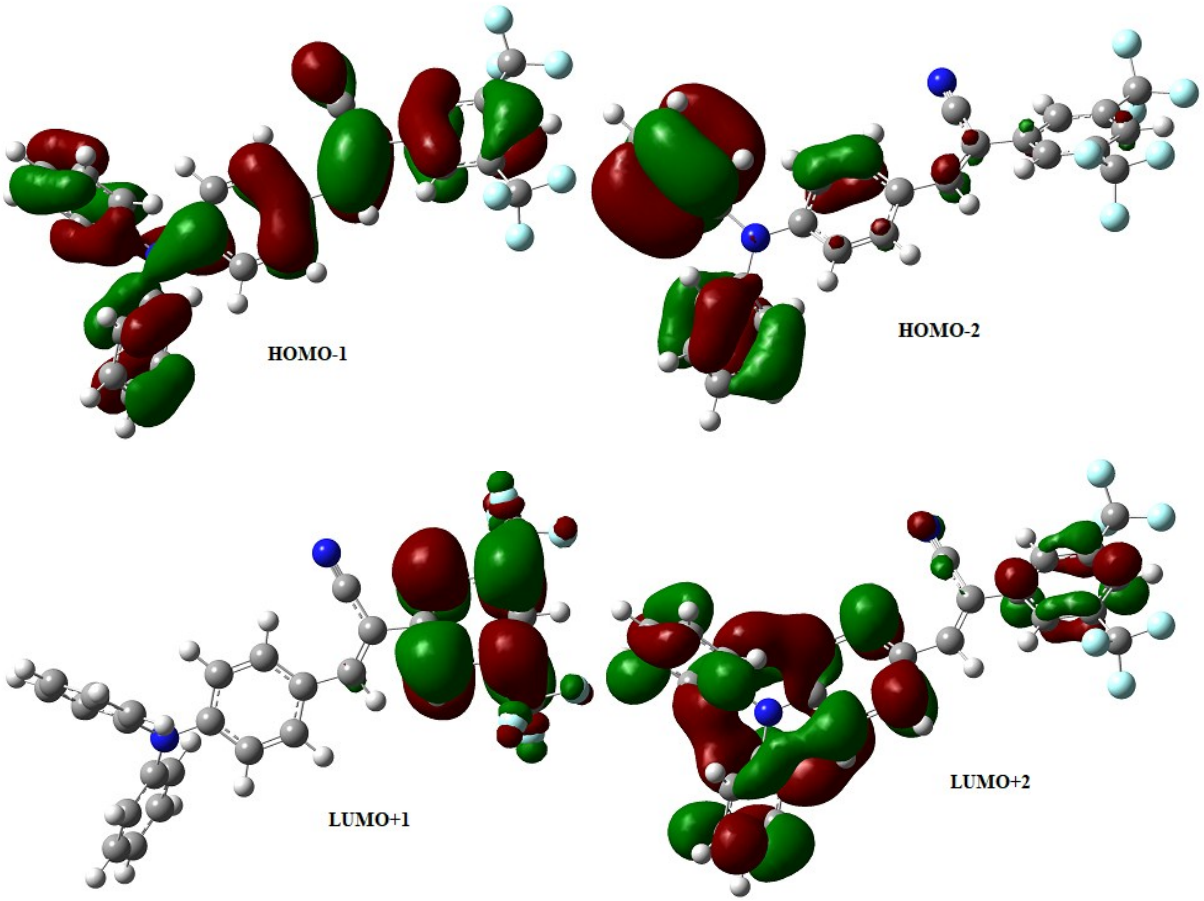


LUMO+1

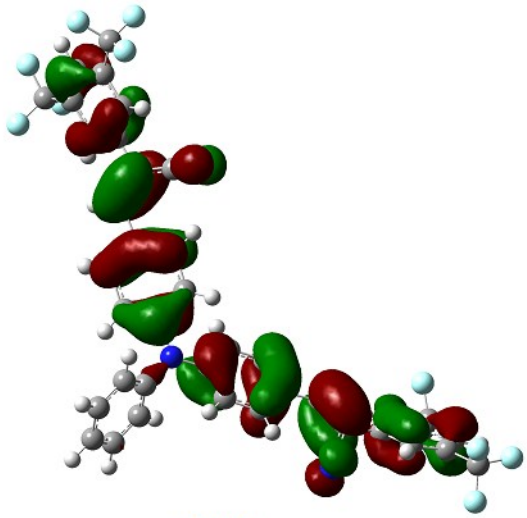


LUMO+2

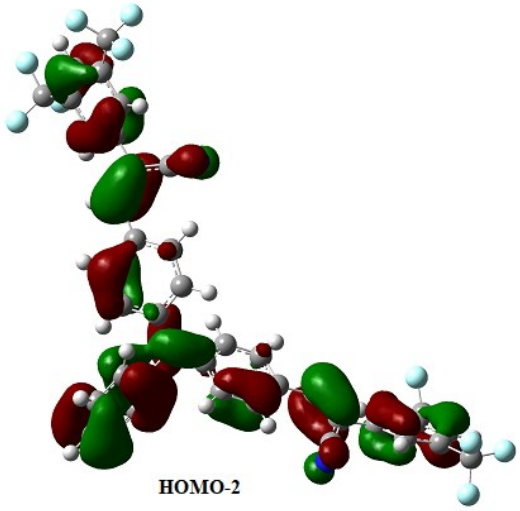
MOLECULE 4



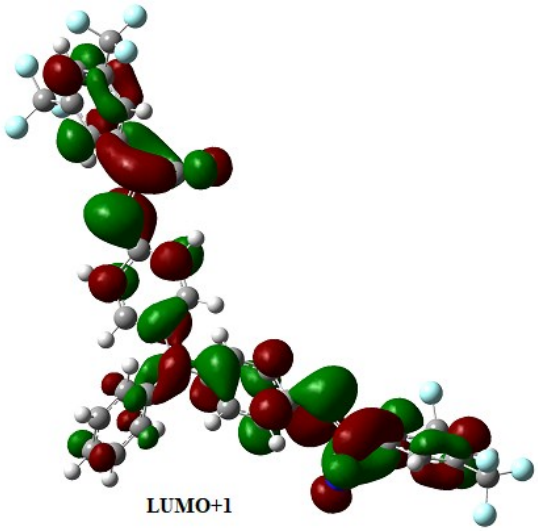
MOLECULE 5



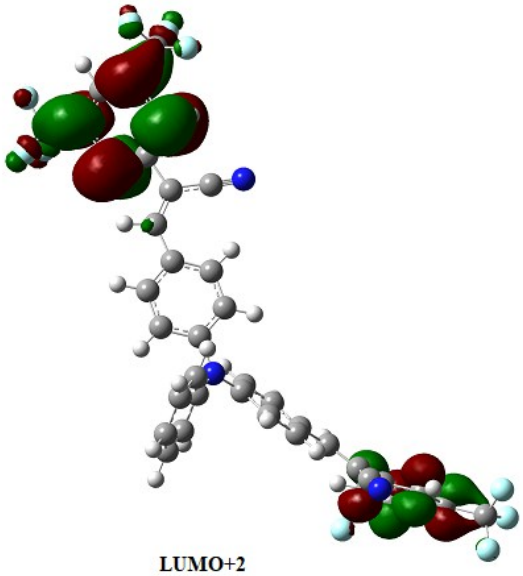
HOMO-1



HOMO-2

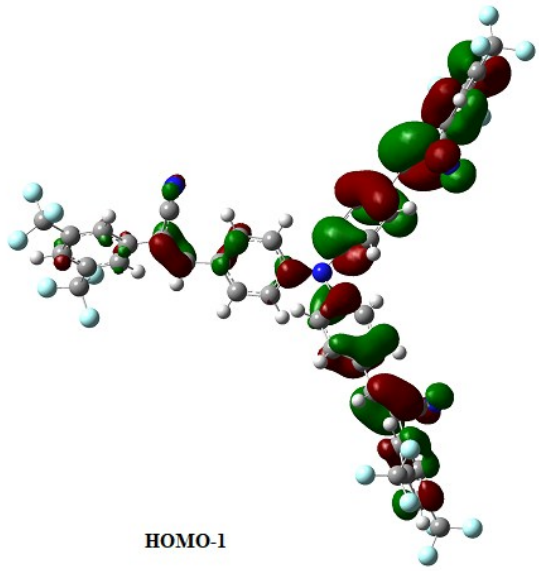


LUMO+1



LUMO+2

MOLECULE 6



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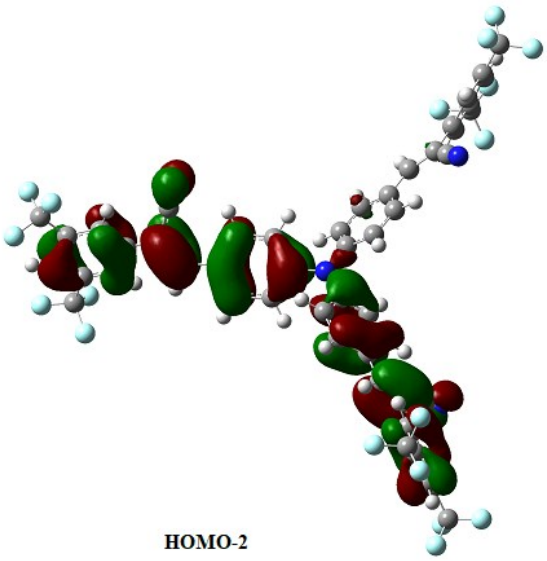

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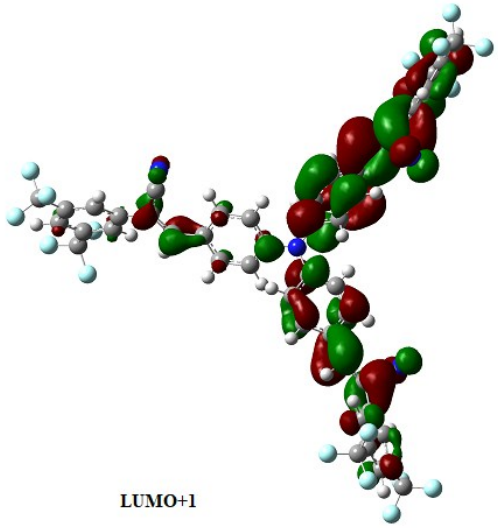

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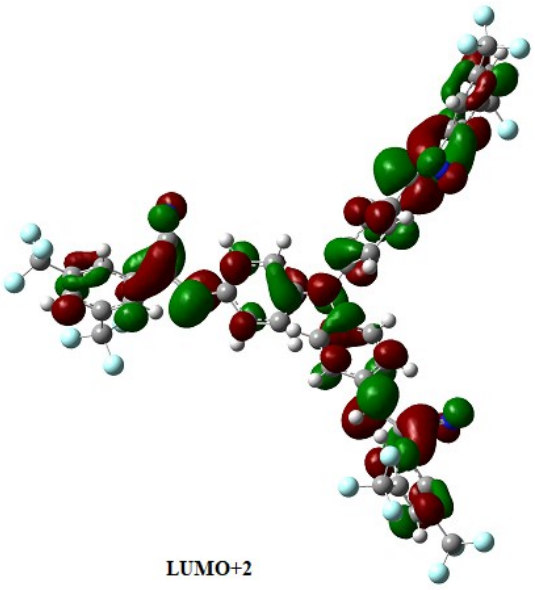

LUMO+2

Table S1. Coordinates for the optimized structures

One (1)

Atom	X	Y	Z
N	-0.34295692	2.00238388	0.06313342
C	-0.35465553	0.57995019	0.20269925
C	0.34166078	-0.02875234	1.25742458
C	-1.07698013	-0.21835604	-0.69741325
C	0.31193090	-1.41580410	1.40831871
H	0.90047379	0.58729643	1.95457599
C	-1.08907373	-1.60582466	-0.54910881
H	-1.62559567	0.25052840	-1.50813005
C	-0.39826141	-2.21165694	0.50479227
H	0.85566696	-1.87504486	2.22876848
H	-1.65126274	-2.21273365	-1.25289867
H	-0.41446984	-3.29097098	0.62088996
C	-0.61463348	2.80157745	1.21579147
C	-1.70493071	2.49573750	2.04397991
C	0.21555597	3.88504867	1.54290636
C	-1.95762483	3.26281724	3.18224105
H	-2.34697780	1.65713193	1.79443842
C	-0.05255732	4.65644892	2.67429055
H	1.06724230	4.11626447	0.91112196
C	-1.13743957	4.34885661	3.50120952
H	-2.80475761	3.01513359	3.81529891
H	0.59856450	5.49126030	2.91710659
H	-1.33868374	4.94655105	4.38493186
C	-0.08821310	2.59973470	-1.18166414
C	0.75540952	1.97574505	-2.12685529
C	-0.66673267	3.83900737	-1.52614270
C	1.01116136	2.55944564	-3.35786312
H	1.21937084	1.02657301	-1.88359344
C	-0.40271826	4.41674672	-2.75802795
H	-1.32818280	4.33806437	-0.82714402
C	0.44135541	3.80476452	-3.71422625
H	1.67355326	2.04266687	-4.04030367
H	-0.87136304	5.36761116	-2.99986326
C	0.64011896	4.50606033	-4.96902527
C	1.42442779	4.24681585	-6.05975627
H	0.06140300	5.42424461	-5.03836527
C	2.32101005	3.13161814	-6.10572838
N	3.06846339	2.24028357	-6.18291327
C	1.43130726	5.12593298	-7.25988640
C	2.57429162	5.21594360	-8.07428066
C	0.30192162	5.88841407	-7.61634665
C	2.60231421	6.05774486	-9.18452802
H	3.45409497	4.62820038	-7.83314353
C	0.32727581	6.73361809	-8.72040719
H	-0.61536512	5.80265862	-7.04367055
C	1.48149894	6.82670836	-9.50723883
H	3.49858941	6.12002088	-9.79167224
H	-0.55434896	7.31158262	-8.97790341

C	1.47549310	7.71064191	-10.72361217
F	0.86547599	8.90167178	-10.48510949
F	0.80292043	7.14200391	-11.76337741
F	2.72325317	7.98597865	-11.17343389

Two (2)	X	Y	Z
N	0.33425501	2.15770650	-0.20200481
C	-0.12790325	0.81446315	-0.01540304
C	0.61889410	-0.08668650	0.75673388
C	-1.32790895	0.39351468	-0.60564320
C	0.16265332	-1.39271233	0.94075041
H	1.55190012	0.23829193	1.20616786
C	-1.77012941	-0.91857058	-0.42962759
H	-1.90635885	1.09327375	-1.20049297
C	-1.03016235	-1.81557991	0.34642241
H	0.74875799	-2.08409832	1.53896938
H	-2.70006449	-1.23574284	-0.89220165
H	-1.37862079	-2.83431785	0.48545580
C	0.69231023	2.93069898	0.92436945
C	-0.00710787	2.79691320	2.13816213
C	1.76858694	3.83915349	0.86827630
C	0.36231629	3.54944545	3.24362972
H	-0.84044941	2.10658616	2.20690341
C	2.12838724	4.59270729	1.97594471
H	2.33335926	3.94425178	-0.05160494
C	1.43473350	4.46989540	3.20251485
H	2.96882219	5.26823303	1.88407620
C	0.40252809	2.68888127	-1.51017900
C	0.78766302	1.87411711	-2.59289783
C	0.06838300	4.03145025	-1.76782235
C	0.84119046	2.37792034	-3.88472626
H	1.05060686	0.83726868	-2.41422035
C	0.12954406	4.52990149	-3.06096339
H	-0.24751070	4.67563437	-0.95470732
C	0.51712671	3.72677684	-4.15822907
H	1.15034739	1.71357698	-4.68112826
H	-0.14247929	5.56782802	-3.23516001
C	0.53818130	4.35976801	-5.46757644
C	0.92630796	3.91447894	-6.69967481
H	0.19359315	5.39096534	-5.44796688
C	1.49181338	2.61350807	-6.89846866
N	1.96068158	1.56643868	-7.10383880
C	0.82304023	4.76251543	-7.91848146
C	1.71638622	4.58613103	-8.98985541
C	-0.16857243	5.75492884	-8.03560807
C	1.64472131	5.39206677	-10.12428845
H	2.47826041	3.81524789	-8.93480944
C	-0.24173496	6.56358116	-9.16516437
H	-0.91025080	5.87797451	-7.25352860
C	0.66765432	6.38681654	-10.21424689
H	-0.20009569	3.43352745	4.16662696
C	1.72445776	5.20534394	4.42311900
H	1.03803517	4.97176833	5.23351799

C	2.69687286	6.10987650	4.74549976
C	3.73579153	6.47235391	3.82826083
N	4.60095382	6.79068975	3.11512049
C	2.76851722	6.75866368	6.08305541
C	4.00351638	7.18428221	6.60417144
C	1.61254863	6.96594585	6.85911427
C	4.08709658	7.76760593	7.86643857
H	4.90890010	7.05050594	6.02106388
C	1.69218215	7.54464647	8.12198763
H	0.63737669	6.69904043	6.46589711
C	2.93232088	7.94259199	8.63373685
H	5.05082207	8.07774772	8.25505893
H	0.78966595	7.69683488	8.70446562
C	3.00567643	8.61588394	9.97714617
F	2.09384447	8.11628707	10.85017649
F	4.22508745	8.48464105	10.55386554
F	2.75963592	9.95281348	9.89009047
H	2.34614977	5.24280613	-10.93763970
H	-1.01969014	7.31595405	-9.24118730
C	0.60465538	7.29486443	-11.41221110
F	1.19720254	6.75522847	-12.50443744
F	1.22771938	8.48393132	-11.17886748
F	-0.67327234	7.59675201	-11.75774537

Three (3)	X	Y	Z
N	-0.04101847	0.05781735	-0.04162095
C	-1.26057400	-0.66755714	-0.04055338
C	-2.33768465	-0.25793886	0.76372814
C	-1.41488994	-1.81099716	-0.84535692
C	-3.52620305	-0.97482366	0.75276427
H	-2.23563760	0.61497697	1.39950664
C	-2.60375345	-2.52820207	-0.84672275
H	-0.59584363	-2.13417617	-1.47899086
C	-3.69757154	-2.12929909	-0.04500557
H	-4.34280791	-0.64532872	1.38979226
H	-2.67844639	-3.39612915	-1.48848781
C	-0.05963345	1.47529944	-0.03998590
C	-0.99412738	2.18115431	-0.81769571
C	0.85749446	2.20492202	0.73920938
C	-1.00447030	3.56891176	-0.80469189
H	-1.70224772	1.63880436	-1.43482994
C	0.84614092	3.59309811	0.74301317
H	1.57959307	1.67567898	1.35166440
C	-0.09084100	4.31817354	-0.02852959
H	1.56576148	4.10992785	1.36428719
C	1.19594503	-0.63771573	-0.04812499
C	1.37252628	-1.79189615	0.73648769
C	2.26704013	-0.18915598	-0.83956780
C	2.57941779	-2.47815605	0.73505209
H	0.55709852	-2.14844651	1.35663454
C	3.47300991	-0.87629583	-0.83245037
H	2.14803099	0.69158833	-1.46132291
C	3.66988582	-2.03523070	-0.04758773

H	2.67040104	-3.35699147	1.35981247
H	4.28533931	-0.51611504	-1.45824112
C	4.97732001	-2.67257794	-0.12350862
C	5.53035422	-3.71580445	0.56203022
H	5.63695137	-2.20974508	-0.85352190
C	4.84073214	-4.37979365	1.62844065
N	4.31861450	-4.94128209	2.50591783
C	6.90487974	-4.21241295	0.27932874
C	7.67360225	-4.80409172	1.29699525
C	7.46744998	-4.10909616	-1.00667172
C	8.97127139	-5.24684673	1.04942730
H	7.25634927	-4.91512060	2.29260068
C	8.76383079	-4.54773178	-1.25733540
H	6.87966651	-3.71296018	-1.82793846
C	9.52240447	-5.11623836	-0.22793182
H	-1.72982150	4.09341636	-1.42125459
C	-0.19505391	5.76869528	-0.10041297
H	-0.95278480	6.10784901	-0.80261567
C	0.45901144	6.77085767	0.55753469
C	1.42572973	6.50768687	1.58194586
N	2.21286622	6.33728560	2.42411939
C	0.18981700	8.20921266	0.28452136
C	0.36572174	9.17198070	1.29378264
C	-0.24417398	8.64315001	-0.98230916
C	0.08865076	10.51706502	1.05777949
H	0.71423104	8.86683514	2.27516984
C	-0.52555094	9.98450850	-1.22074123
H	-0.33793485	7.93442366	-1.79828923
C	-0.36575923	10.92671415	-0.19822397
H	0.21920638	11.24272187	1.85283649
H	-0.85767390	10.30042547	-2.20412000
C	-0.62596003	12.38151798	-0.48282782
F	-1.70285079	12.55709386	-1.29117894
F	-0.85160125	13.09678400	0.64500150
F	0.42661902	12.97043420	-1.11470512
H	9.54987570	-5.69643894	1.84875288
H	9.17684151	-4.46955467	-2.25741674
C	10.93896037	-5.54766927	-0.49687873
F	11.36953078	-6.48559890	0.38046864
F	11.80964814	-4.50366334	-0.40841955
F	11.08829345	-6.06470349	-1.74289539
C	-4.98786500	-2.80060409	0.03121157
H	-5.68884122	-2.30271592	0.69667015
C	-5.46960319	-3.93576083	-0.55500663
C	-4.66034343	-4.76185423	-1.40127883
N	-4.03660551	-5.46338398	-2.09178339
C	-6.86150838	-4.41574662	-0.33389016
C	-7.16198750	-5.78732788	-0.40348608
C	-7.90788003	-3.51745250	-0.05224432
C	-8.45517112	-6.25076544	-0.16965213
H	-6.37695601	-6.50036184	-0.63360079
C	-9.19955010	-3.97637859	0.18492765
H	-7.72115878	-2.44883272	-0.04386641
C	-9.47686321	-5.34719206	0.13287878

H	-8.66432425	-7.31370912	-0.21574288
H	-9.99359342	-3.26870114	0.39902453
C	-10.88805987	-5.82686806	0.34178916
F	-11.64178951	-5.68838539	-0.78388113
F	-11.52454511	-5.12642997	1.31537868
F	-10.94385775	-7.13499496	0.68823149

Four (4)	X	Y	Z
N	-0.38036585	1.99415273	0.05868377
C	-0.31527662	0.57447121	0.21908585
C	0.39248649	0.02070146	1.29578618
C	-0.97474519	-0.27418618	-0.68282320
C	0.43767211	-1.36382737	1.46567054
H	0.90152366	0.67651900	1.99485471
C	-0.91262050	-1.65808893	-0.51479510
H	-1.53281635	0.15273615	-1.51017110
C	-0.20940720	-2.20986571	0.56033491
H	0.98971175	-1.78105372	2.30279219
H	-1.42643789	-2.30498345	-1.21988339
H	-0.16772434	-3.28673186	0.69165958
C	-0.73311421	2.78941424	1.19295795
C	-1.83872740	2.43947341	1.98200311
C	0.03499158	3.91111040	1.54132062
C	-2.16888099	3.20293132	3.10287280
H	-2.43181125	1.57022713	1.71650701
C	-0.31010485	4.67776520	2.65489352
H	0.89928555	4.17586419	0.94054391
C	-1.41110074	4.32733959	3.44244579
H	-3.02728352	2.92167548	3.70594912
H	0.29306028	5.54283481	2.91486741
H	-1.67296401	4.92177702	4.31235691
C	-0.11210641	2.58987404	-1.18146459
C	0.78265543	1.99098940	-2.09683908
C	-0.72656612	3.80451546	-1.55385347
C	1.05407617	2.57570541	-3.32323226
H	1.27446110	1.06191544	-1.83219816
C	-0.44757158	4.38276317	-2.78133968
H	-1.42786328	4.28280480	-0.87981802
C	0.44884072	3.79662521	-3.70630682
H	1.75671046	2.08006725	-3.98073695
H	-0.94505385	5.31286131	-3.04520999
C	0.66123054	4.49668629	-4.95732600
C	1.48712517	4.25769402	-6.02250753
H	0.05484177	5.39511853	-5.04838066
C	2.42320650	3.17603752	-6.03890970
N	3.20485684	2.31277433	-6.09301998
C	1.49867944	5.13426481	-7.22456609
C	2.66224108	5.27041858	-8.00032565
C	0.35372067	5.84624870	-7.61982371
C	2.68372128	6.11559198	-9.11083390
H	3.55674524	4.71858992	-7.72996100
C	0.38744563	6.69387862	-8.72707848
H	-0.57849740	5.72069976	-7.08060855

C	1.55170544	6.84147547	-9.48348068
H	1.57208849	7.49448702	-10.34628286
C	-0.85860798	7.46564506	-9.08246730
C	3.95839122	6.22030504	-9.91238567
F	-0.78300133	8.04216923	-10.30281481
F	-1.09956549	8.46276513	-8.18789512
F	-1.96219927	6.67481353	-9.07814816
F	3.88870345	7.17201064	-10.87197325
F	4.25748461	5.05059496	-10.53327637
F	5.02191647	6.52285208	-9.12523345

Five (5)	X	Y	Z
N	0.56244715	2.15759768	-0.22045677
C	0.19308368	0.78373922	-0.03654340
C	1.02368500	-0.07467978	0.69677720
C	-0.99778124	0.29432592	-0.59031510
C	0.65958386	-1.40975161	0.87845448
H	1.94902742	0.30549630	1.11807086
C	-1.34838624	-1.04556098	-0.41661650
H	-1.64087014	0.96239890	-1.15459415
C	-0.52437132	-1.90132776	0.32039459
H	1.30972309	-2.06879023	1.44612192
H	-2.27204125	-1.41718007	-0.85020209
H	-0.80149321	-2.94199244	0.45736709
C	0.87059940	2.94354328	0.91104896
C	0.18501620	2.74831404	2.12472026
C	1.88386510	3.92263103	0.86297068
C	0.50496804	3.51145333	3.23781228
H	-0.59917926	2.00215559	2.18655855
C	2.19568512	4.68491456	1.97878956
H	2.43867218	4.07508785	-0.05621324
C	1.51411303	4.50132644	3.20468621
H	2.98898184	5.41610782	1.89366816
C	0.59655748	2.69291805	-1.52646930
C	0.99987246	1.89331424	-2.61478282
C	0.20853827	4.02243296	-1.77998521
C	1.01923499	2.39863075	-3.90635919
H	1.30425062	0.86734302	-2.44027174
C	0.23700469	4.52292034	-3.07299008
H	-0.12469733	4.65452149	-0.96449000
C	0.64111994	3.73448043	-4.17529375
H	1.34464750	1.74609794	-4.70598093
H	-0.07637889	5.54976212	-3.24317626
C	0.62181431	4.36686451	-5.48348261
C	0.98670931	3.92574372	-6.72454730
H	0.25982721	5.39196590	-5.45443385
C	1.56639335	2.63460416	-6.93977083
N	2.04635564	1.59580210	-7.16059957
C	0.83669364	4.77019086	-7.94142669
C	1.69667027	4.59908032	-9.03992759
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C	0.59174540	6.39583192	-10.24421843
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C	-1.35568665	7.60878111	-9.19127625
C	2.49501725	5.16649066	-11.34308716
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F	-2.58041135	7.07706926	-8.94193862
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C	3.94206538	7.86815215	7.92669439
H	4.83354435	7.19668702	6.09303141
C	1.56832363	7.57024515	8.13055601
H	0.56997380	6.70627492	6.43935405
C	2.77199917	8.00742906	8.67970753
H	2.79948430	8.44976774	9.66791271
C	0.27433170	7.71450506	8.89245330
C	5.24148774	8.38870413	8.49208218
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F	-0.62674784	8.46875547	8.21119839
F	-0.31788717	6.50825446	9.10215942
F	5.33296153	8.16874922	9.82705620
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C	-2.13573804	-0.87552355	0.78262229
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C	1.82382208	-1.54780890	0.80421657
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C	-2.03409095	9.65158489	1.33531566
H	-1.75440804	7.59707422	1.88715883
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H	5.61627303	-2.56354547	0.82632994
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C	-7.69837838	-7.67729697	-0.34717335

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F	12.14889774	-1.86655135	-1.89122372
F	11.86210744	-4.02048495	-2.02267212
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F	8.84411370	-4.71932441	2.97645741
F	10.96344858	-4.23361250	2.80815994
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F	-8.00127918	-7.51501640	3.27147785
F	-9.75430407	-7.32565043	1.99167291
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F	-5.80772004	-8.16163099	-3.11467969
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