Supporting Information

Aggregation Induced Emitting Cyanostilbenes for Live Cell Imaging of Lipid Droplets

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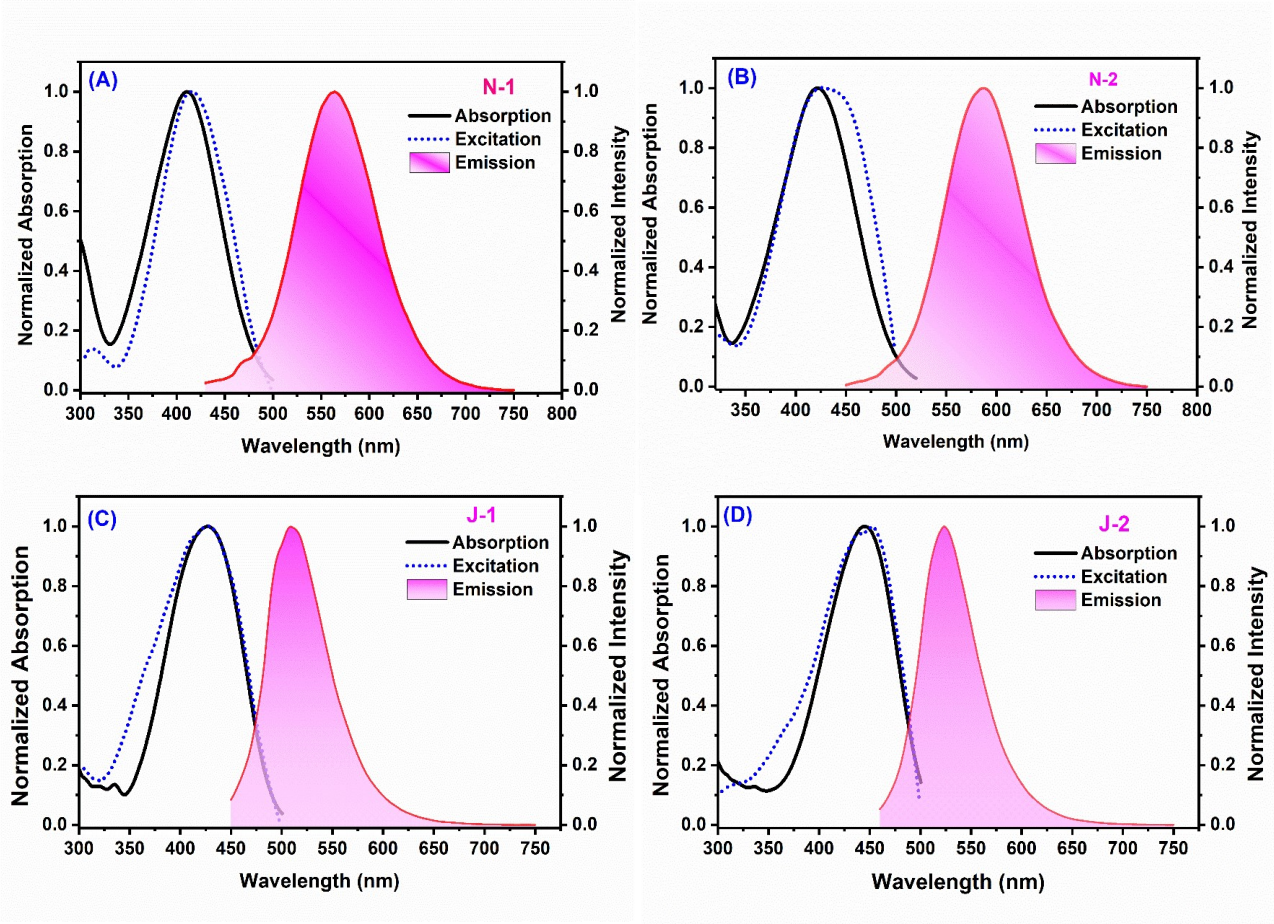


Figure S1: Combined Absorption/Excitation and Emission Spectra of A) **N1**, B) **N2**, C) **J1** & D) **J2** in Ethanol. [Concentration-10 µM]

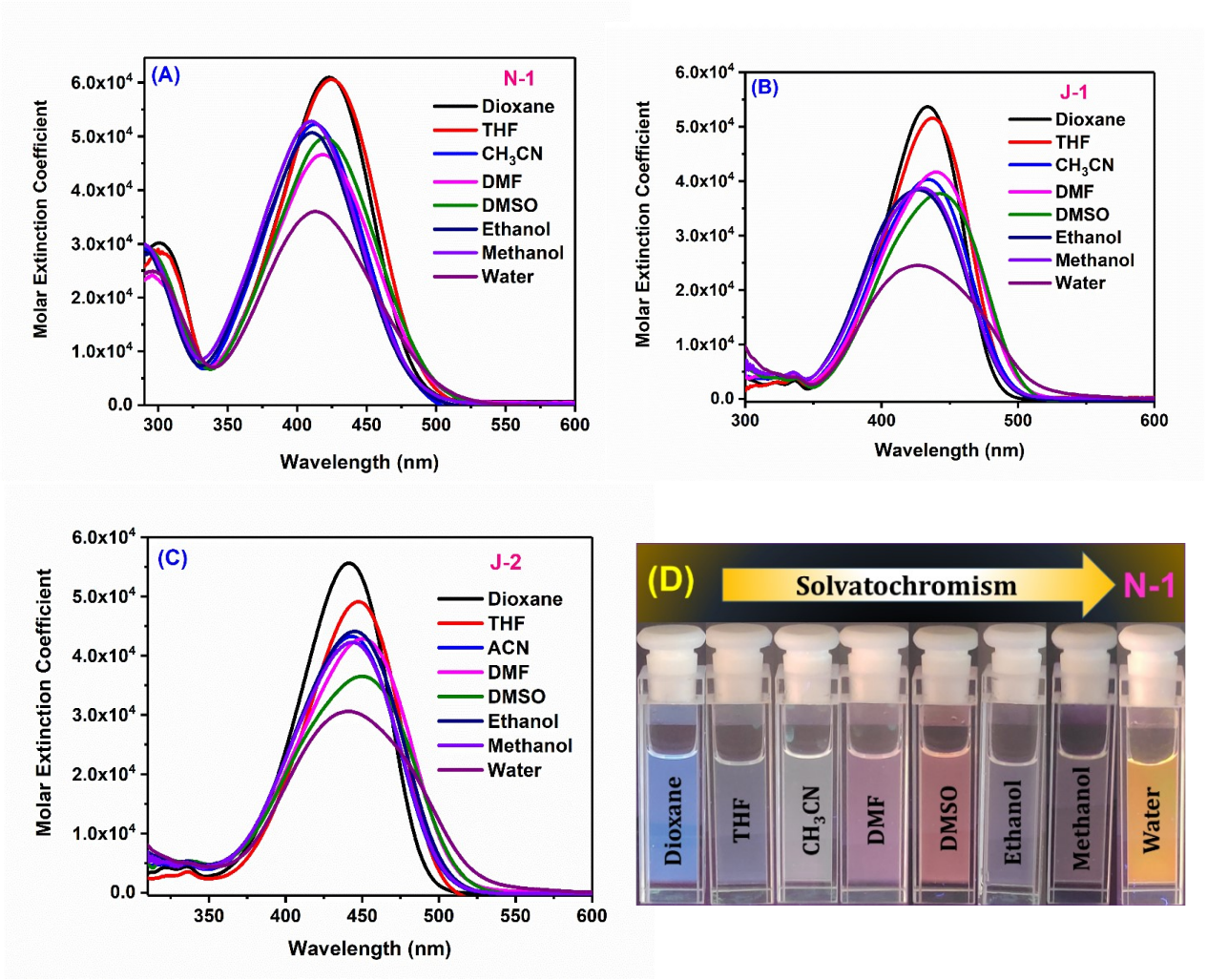


Figure S2: Absorption Spectra of A) **N1**, B) **J1** & C) **J2** in all solvents; D) Cuvette pictures of **N1** solutions in different solvents. [Concentration-10 µM]

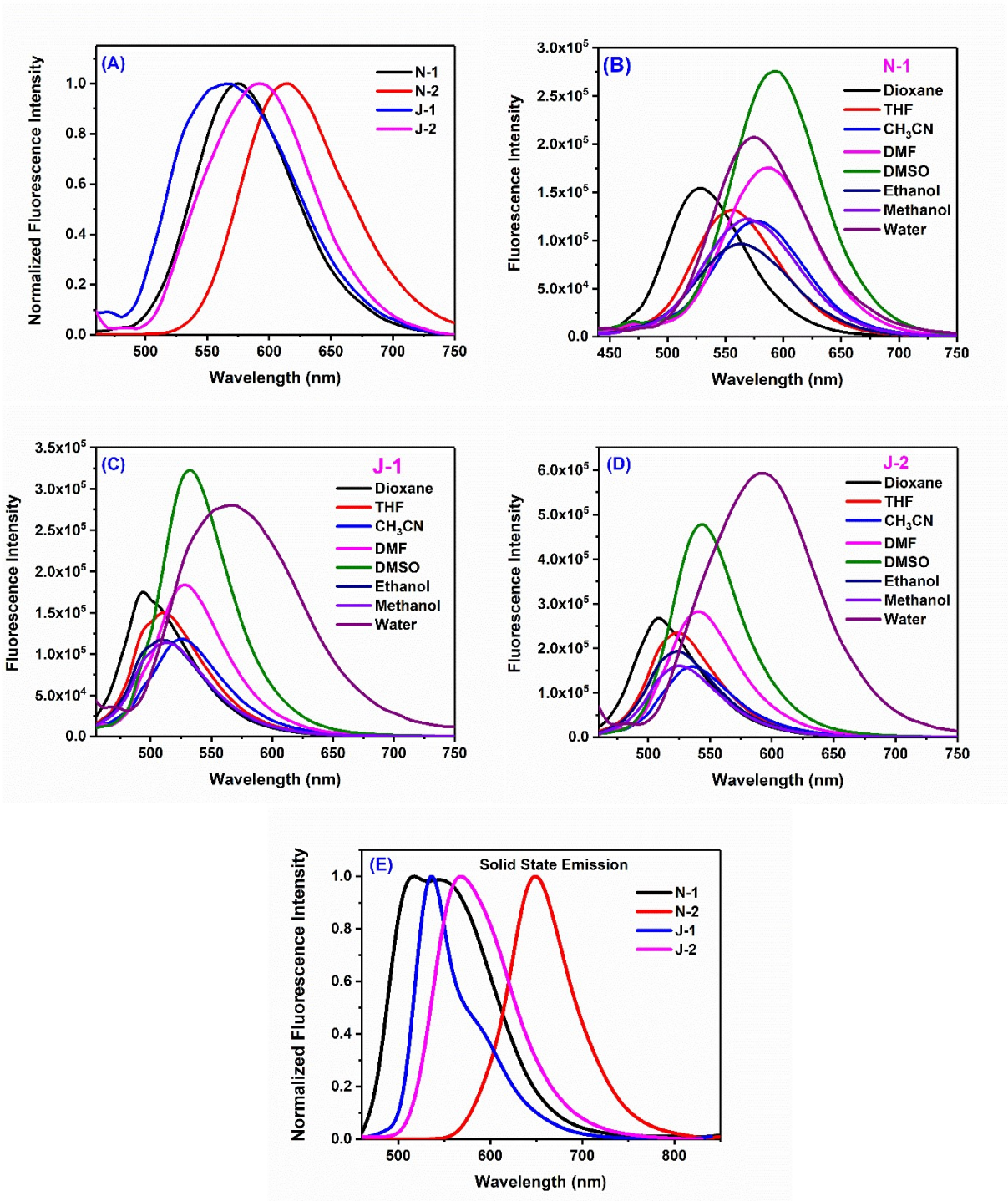

(A)
Normalized Fluorescence Intensity
Wavelength (nm)
N-1
N-2
J-1
J-2
(B)
N-1
Fluorescence Intensity
Wavelength (nm)
Dioxane
THF
CH3CN
DMF
DMSO
Ethanol
Methanol
Water
(C)
J-1
Fluorescence Intensity
Wavelength (nm)
Dioxane
THF
CH3CN
DMF
DMSO
Ethanol
Methanol
Water
(D)
J-2
Fluorescence Intensity
Wavelength (nm)
Dioxane
THF
CH3CN
DMF
DMSO
Ethanol
Methanol
Water
(E)
Solid State Emission
Normalized Fluorescence Intensity
Wavelength (nm)
N-1
N-2
J-1
J-2

Figure S3: A) Emission of all compounds in water; Emission spectra of B) **N1**, C) **J1** & D) **J2** in all solvents. E) Solid state emission [Concentration-10 μM]

S4: Emission Spectra of N-1, J-1 and J-2 in dioxane/water binary solvent system

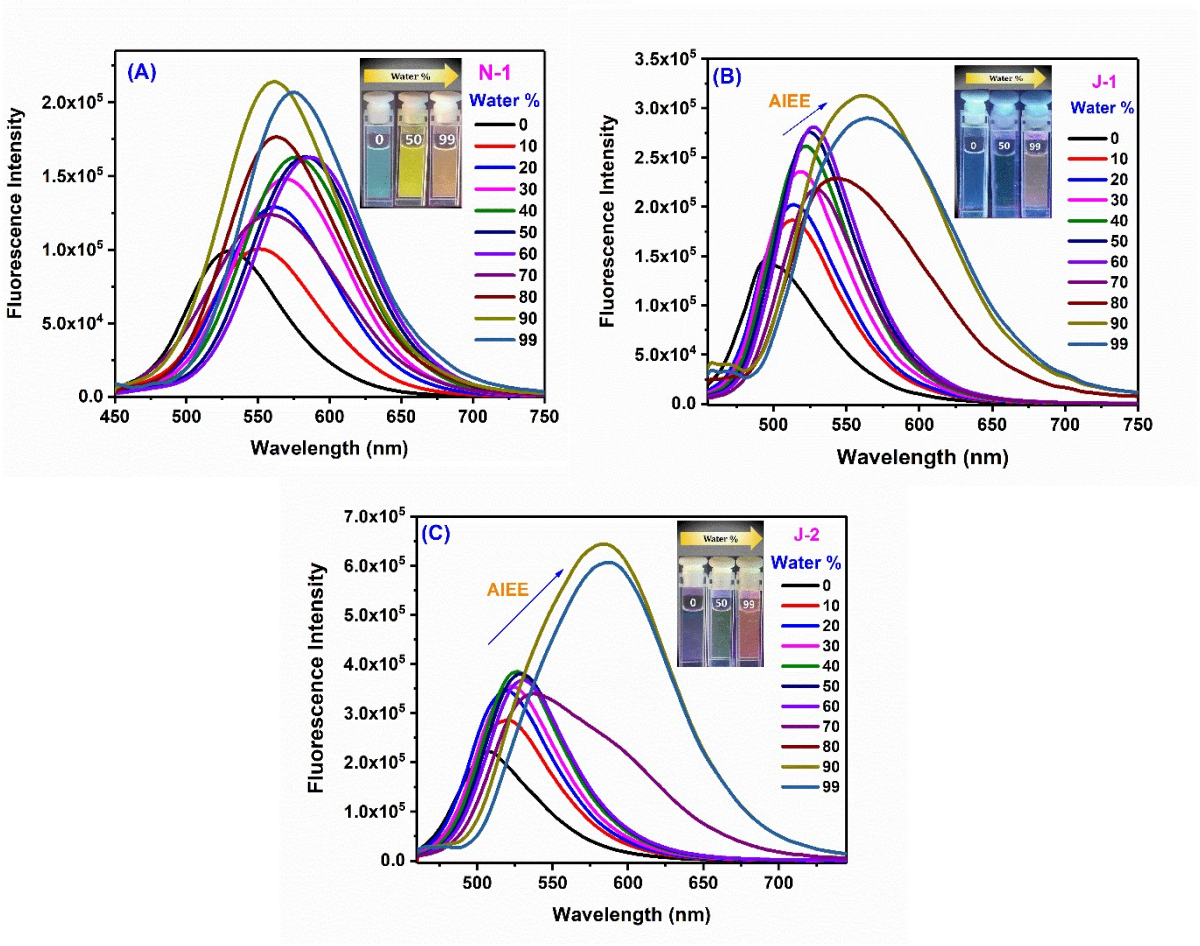
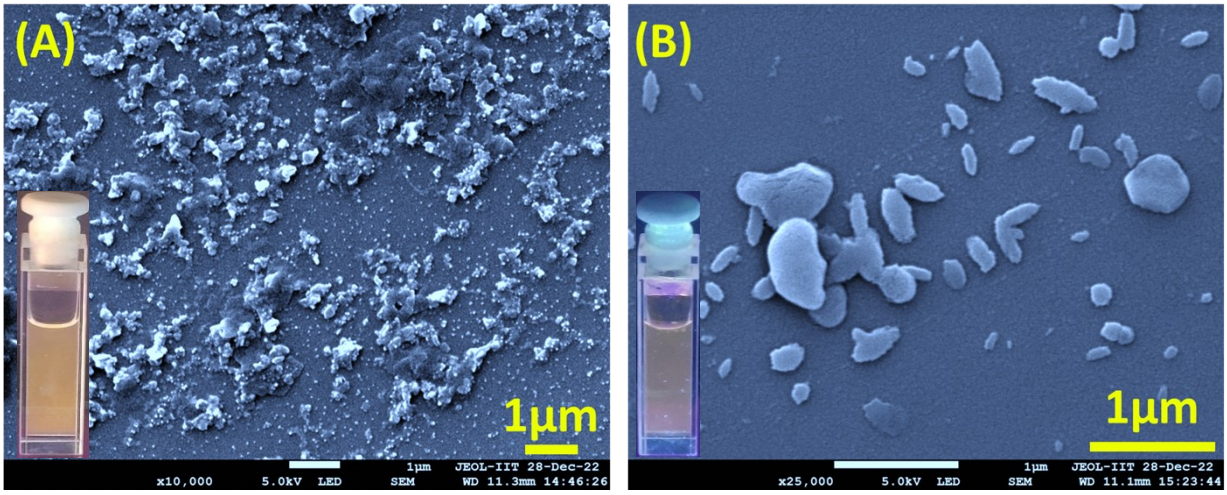
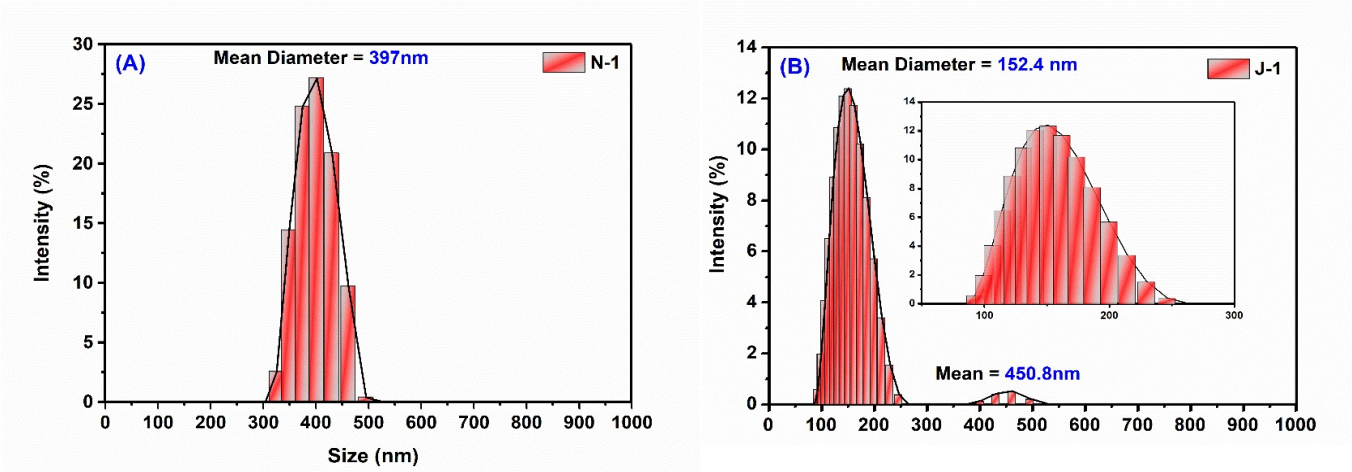


Figure S4: A) Emission spectra of A) **N1**, B) **J1** & C) **J2** in dioxane/water binary solvent system (Inset – Pictures of cuvette with solutions). [Concentration-10 μM]**.**

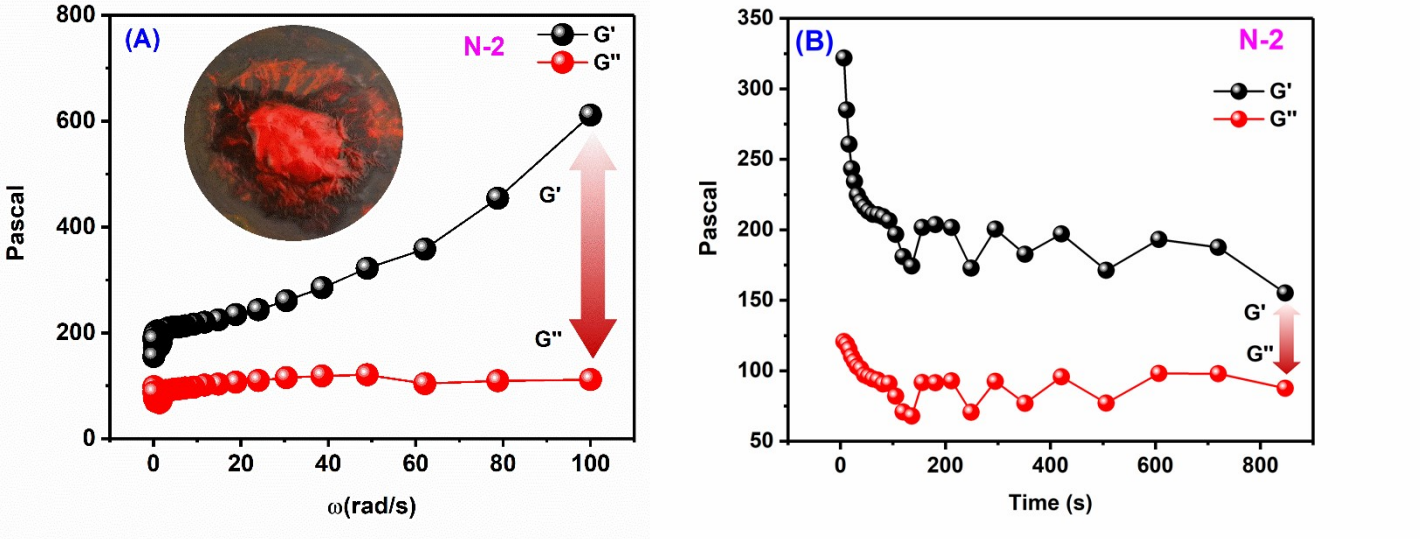
S5a: Field Emission Scanning Electron Microscopic Images of N-1 and J-1





S5b: DLS Spectra of N-1 & J-1

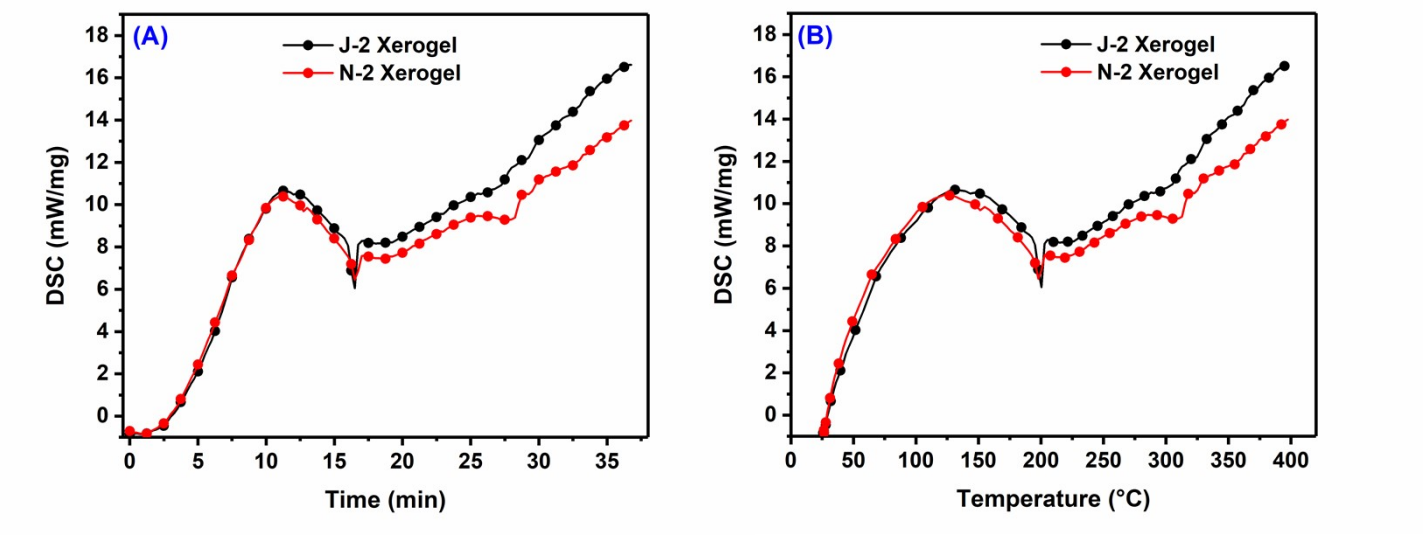
Figure S5a: Field emission scanning electron microscopic images of A) **N1** and B) **J1** drop-casted on Si wafer and dried over vacuum. [Concentration-10µM]**.** Figure S5b: Dynamic Light Scattering Plots of A) N-1 & B) J-1 depicting size of aggregates formed in water. [Concentration-10µm].



S6: Rheology data for N-2:

Figure S6: A) Frequency sweep and B) Time sweep for **N2** (Inset of figure – Gel picture on Rheometer and in cuvette)

Figure S7: TGA-DSC analysis for obtaining degradation temperature and time for **N2** and **J2** Xerogels, respectively



S8: Live Cell Imaging of Lipid Droplets:

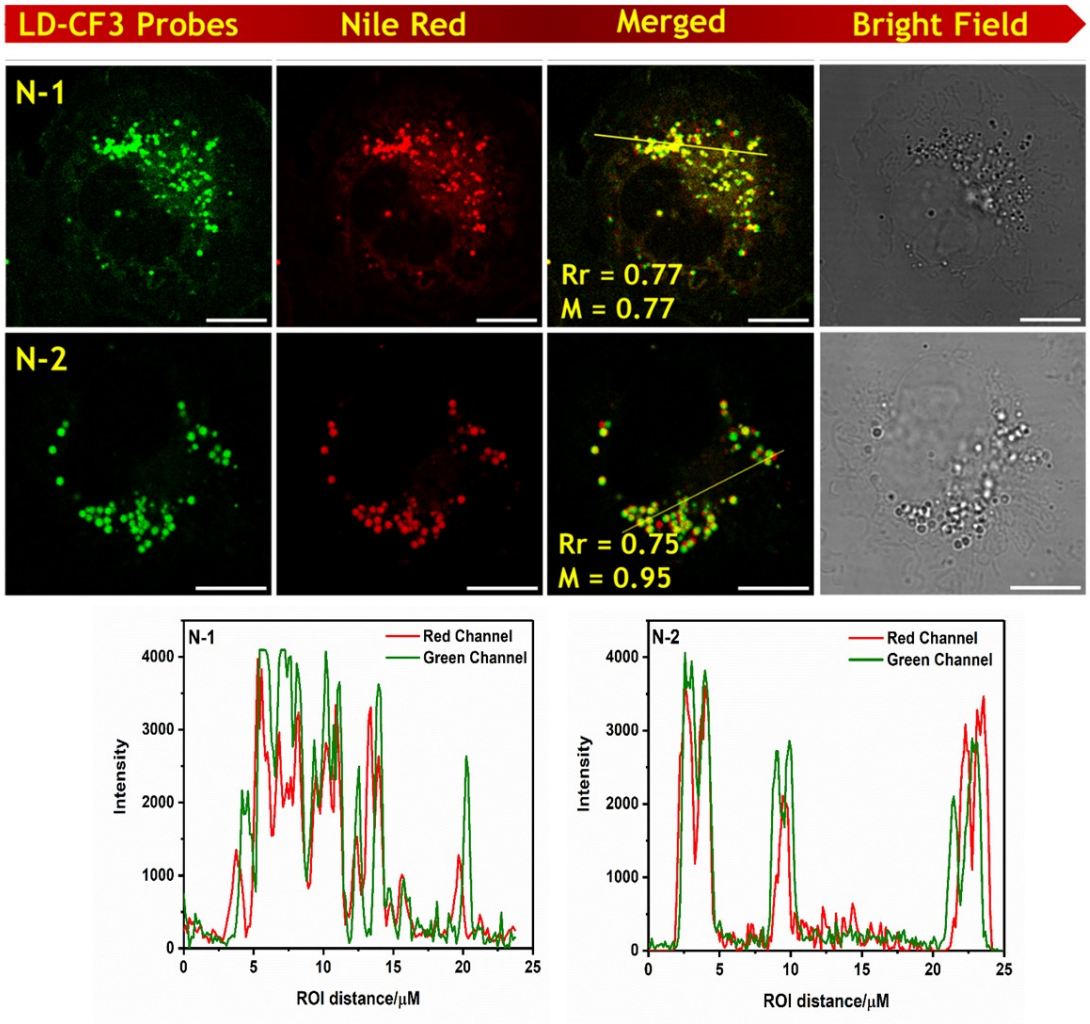


Figure S8: Colocalization of **N1** and **N2** to Lipid Droplets in Cos-7 cells. Nile red was used as a Lipid droplet marker. Scale Bar = 10μm. Intensity Profile plots for **N1** and **N2** were shown in red and green channel showing overlap.

S9: Cytotoxicity Assay (MTT Assay):

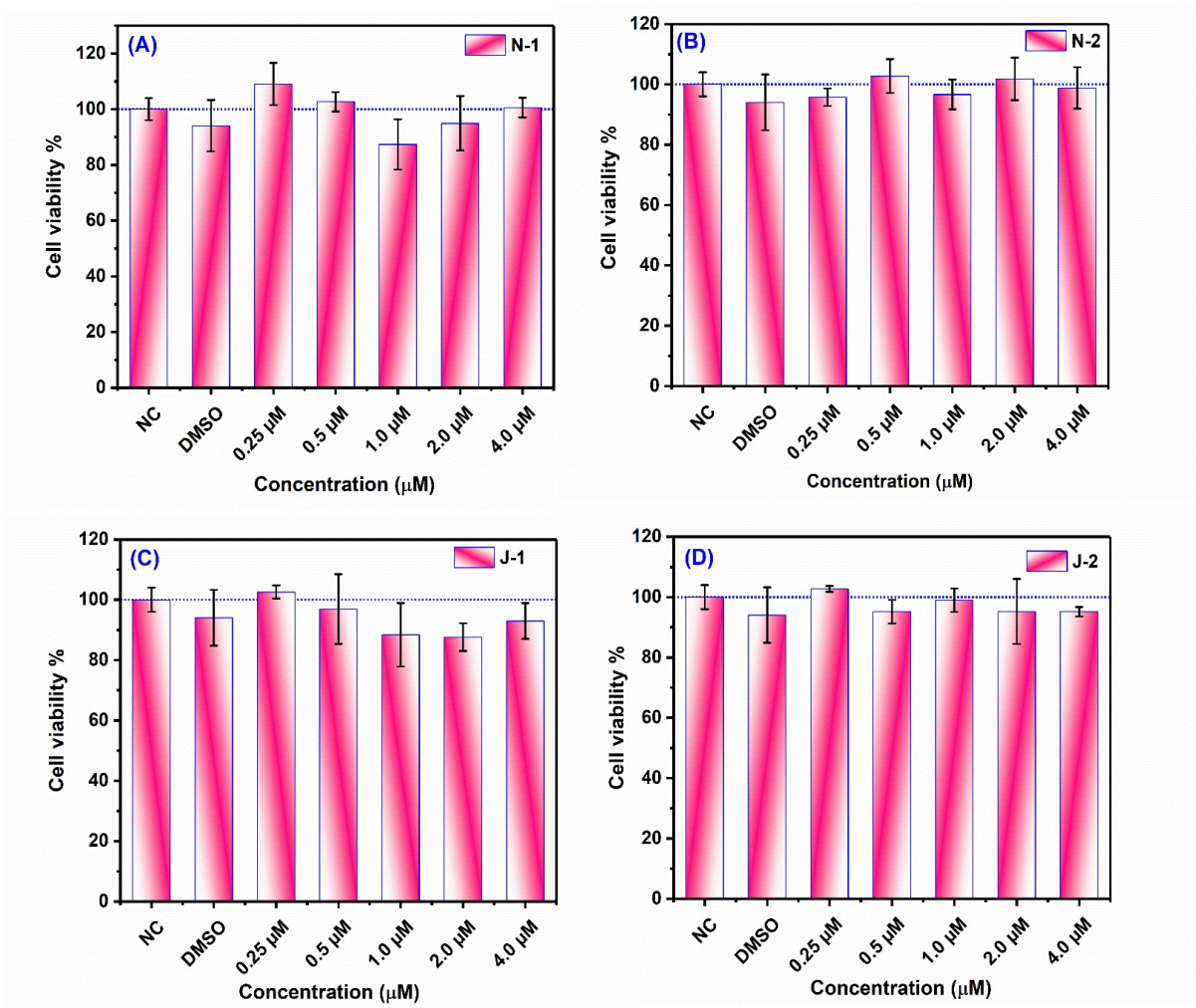


Figure S9: MTT Assay (Cytotoxicity Assay) for all the compounds in cos-7 cells at different concentrations such as 0.25μM, 0.5 μM, 1 μM, 2 μM and 4 μM respectively. Negative control represents only cells in media without any solvent and compound concentration. The compounds were incubated for 4h.

S10: Detailed Synthetic Procedures:

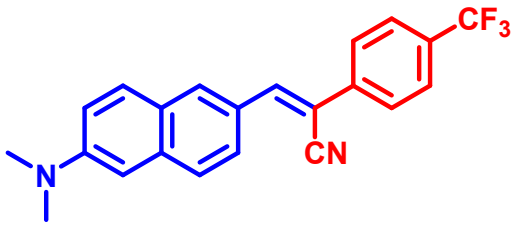
Synthesis of 6-Formyl-2-Dimethylaminonaphthalene: 6-Formyl-2-Dimethylaminonapthalene is synthesized *via* 2 steps (Bucherer reaction and formylation using n-butyl lithium and dimethylformamide) with the procedure mentioned in literature[1] which involves Bucherer reaction and formylation *via* lithiation using n-butyl lithium.

General Procedure for Knoevenagel condensation reaction:

The respective trifluoromethylphenyl acrylonitriles were dissolved in absolute ethanol and 2eq. of potassium tertiary butoxide was added and the reaction mixture was allowed to stir for 10 min. After 10 min, the respective carbaldehyde was added to the reaction and allowed to stir at room temperature for 6-8 h to yield the products in N1 (60%); N2 (65%); J1 (71%) and J2 (63%) yields.

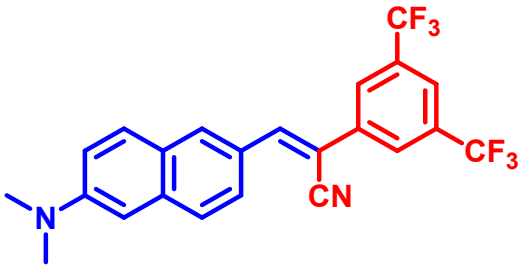
S11: Characterization Details:

Compound N1: ((Z)-3-(6-(dimethylamino) naphthalen-2-yl)-2-(4-(trifluoromethyl)phenyl) acrylonitrile)



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (s, 1H), 8.04 (dd, *J* = 8.7, 1.8 Hz, 1H), 7.76 (t, *J* = 9.1 Hz, 3H), 7.67 (dd, *J* = 8.5, 4.9 Hz, 3H), 7.63 (s, 1H), 7.15 (dd, *J* = 9.1, 2.5 Hz, 1H), 6.86 (d, *J* = 2.4 Hz, 1H), 3.11 (s, 6H).; ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.55; ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.04, 144.69, 138.73, 136.57, 131.69, 130.40, 130.16, 126.81, 126.65, 125.97 (d, *J* = 3.9 Hz), 125.71, 118.48, 116.43, 106.35, 105.50, 40.44; (ESI-MS) m/z: ($[M + H]^+$), calculated mass 367.1456; found, 367.1622.

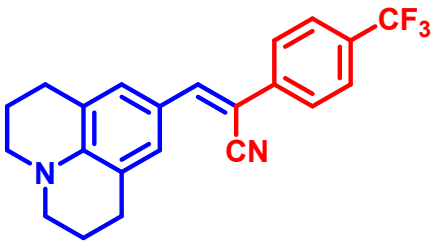
Compound N2: ((Z)-2-(3,5-bis(trifluoromethyl)phenyl)-3-(6-(dimethylamino) naphthalen-2-yl) acrylonitrile)



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.18 (d, *J* = 1.3 Hz, 1H), 8.11 – 8.05 (m, 3H), 7.85 (s, 1H), 7.77 (d, *J* = 9.1 Hz, 1H), 7.68 (d, *J* = 6.7 Hz, 2H), 7.16 (dd, *J* = 9.1, 2.6 Hz, 1H), 6.86 (d, *J* = 2.4 Hz, 1H), 3.12 (s, 6H).; ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.87; ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.25, 145.79, 137.64, 136.86, 132.66, 132.40, 132.13, 130.33, 126.93, 126.13, 125.57 (d, *J* = 7.3 Hz), 124.18, 122.01, 121.82,

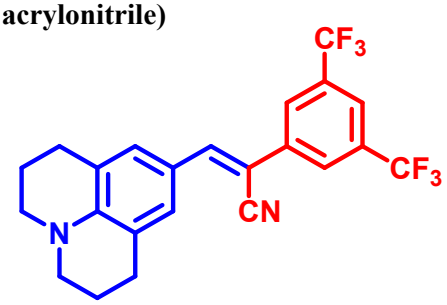
118.00, 116.46, 105.44, 104.61, 40.41; (ESI-MS) m/z: ([M + H]$^+$), calculated mass 435.1251; found, 435.1298.

Compound J1: ((Z)-3-(2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij] quinolin-9-yl)-2-(4-(trifluoromethyl)phenyl) acrylonitrile)



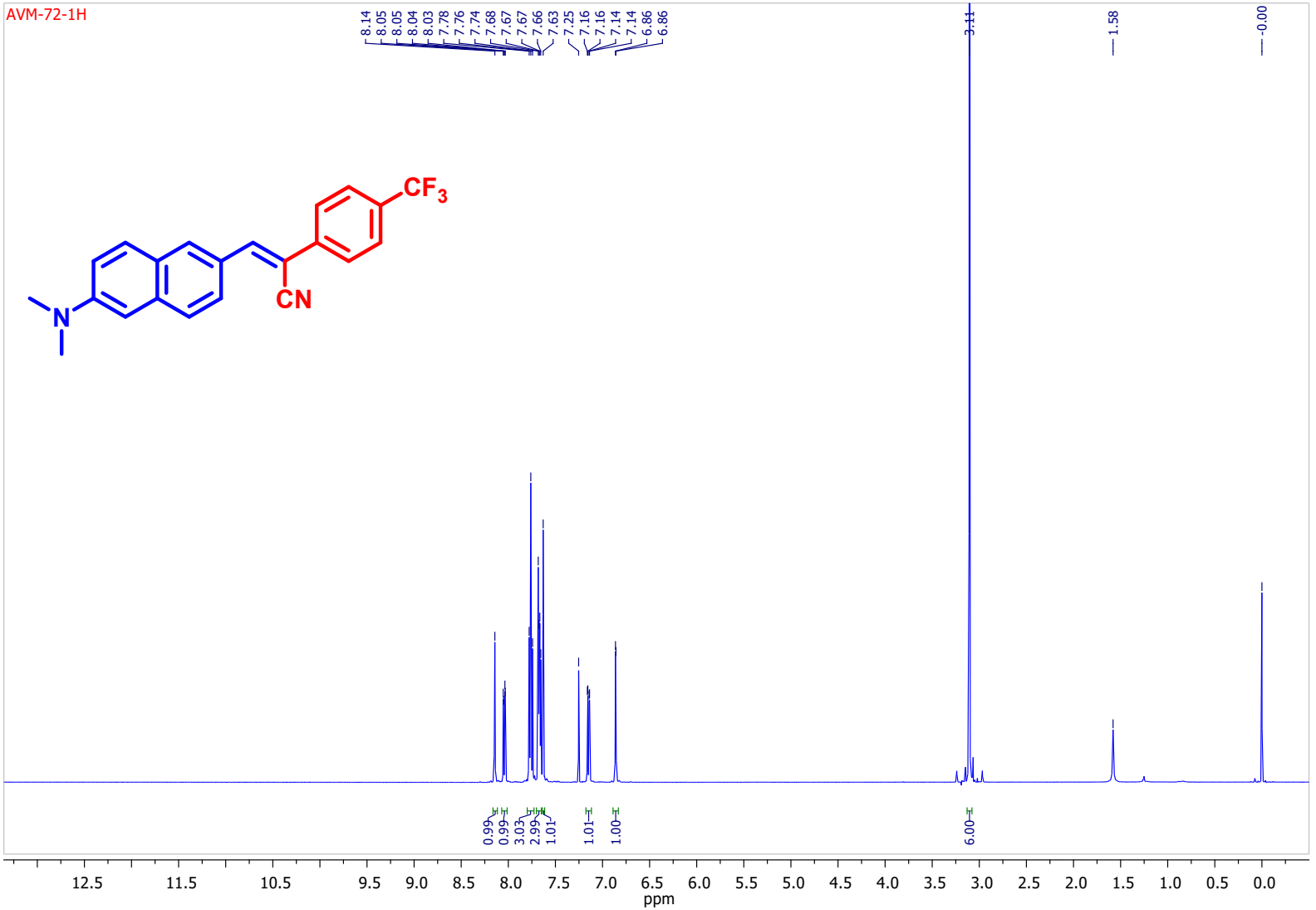
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.3 Hz, 2H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.45 (s, 2H), 7.34 (s, 1H), 3.31 – 3.24 (m, 4H), 2.76 (t, *J* = 6.3 Hz, 4H), 1.96 (td, *J* = 11.7, 6.1 Hz, 4H); ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.40; ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.59, 144.36, 139.57, 129.48, 129.29, 129.03, 125.79 (q, *J* = 3.7 Hz), 125.26 (d, *J* = 13.2 Hz), 123.04, 120.83, 120.00, 119.42, 100.63, 49.98, 27.71, 21.41; (ESI-MS) m/z: ([M + H] $^+$), calculated mass 369.1579; found, 369.1671.

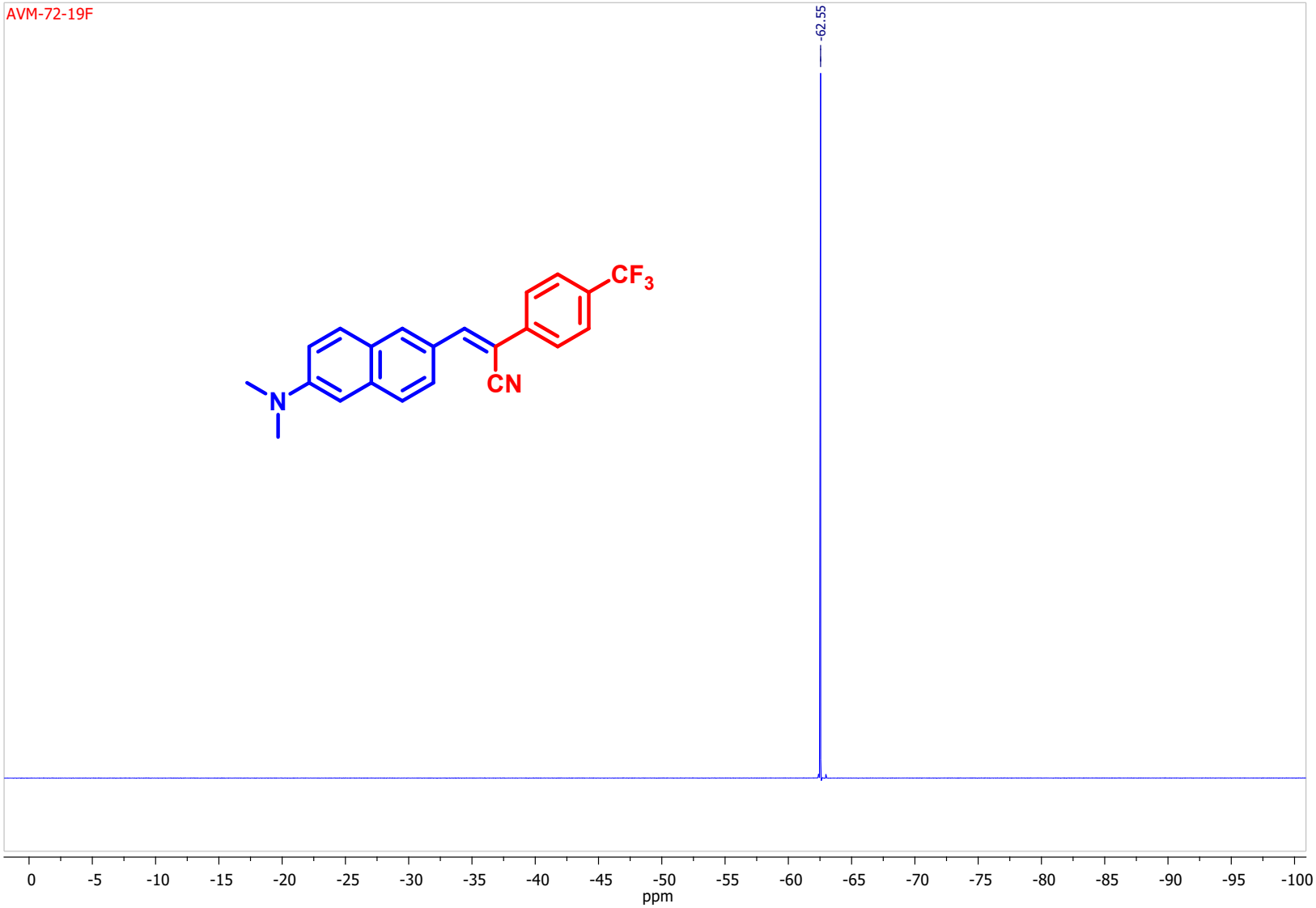
Compound J2: ((Z)-2-(3,5-bis(trifluoromethyl)phenyl)-3-(2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij] quinolin-9-yl) acrylonitrile)



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 (s, 2H), 7.75 (s, 1H), 7.49 (s, 2H), 7.37 (s, 1H), 3.35 – 3.26 (m, 4H), 2.78 (t, *J* = 6.3 Hz, 4H), 2.04 – 1.92 (m, 4H).; ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.89; ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.07, 145.20, 138.48, 132.40, 132.13, 129.80, 124.89, 124.31, 122.14, 120.88, 120.62, 119.53, 118.96, 98.74, 50.03, 27.69, 21.33; (ESI-MS) m/z: ([M + H] $^+$), calculated mass 437.1408; found, 437.1449.

NMR and HRMS Spectral Copies of all the compounds

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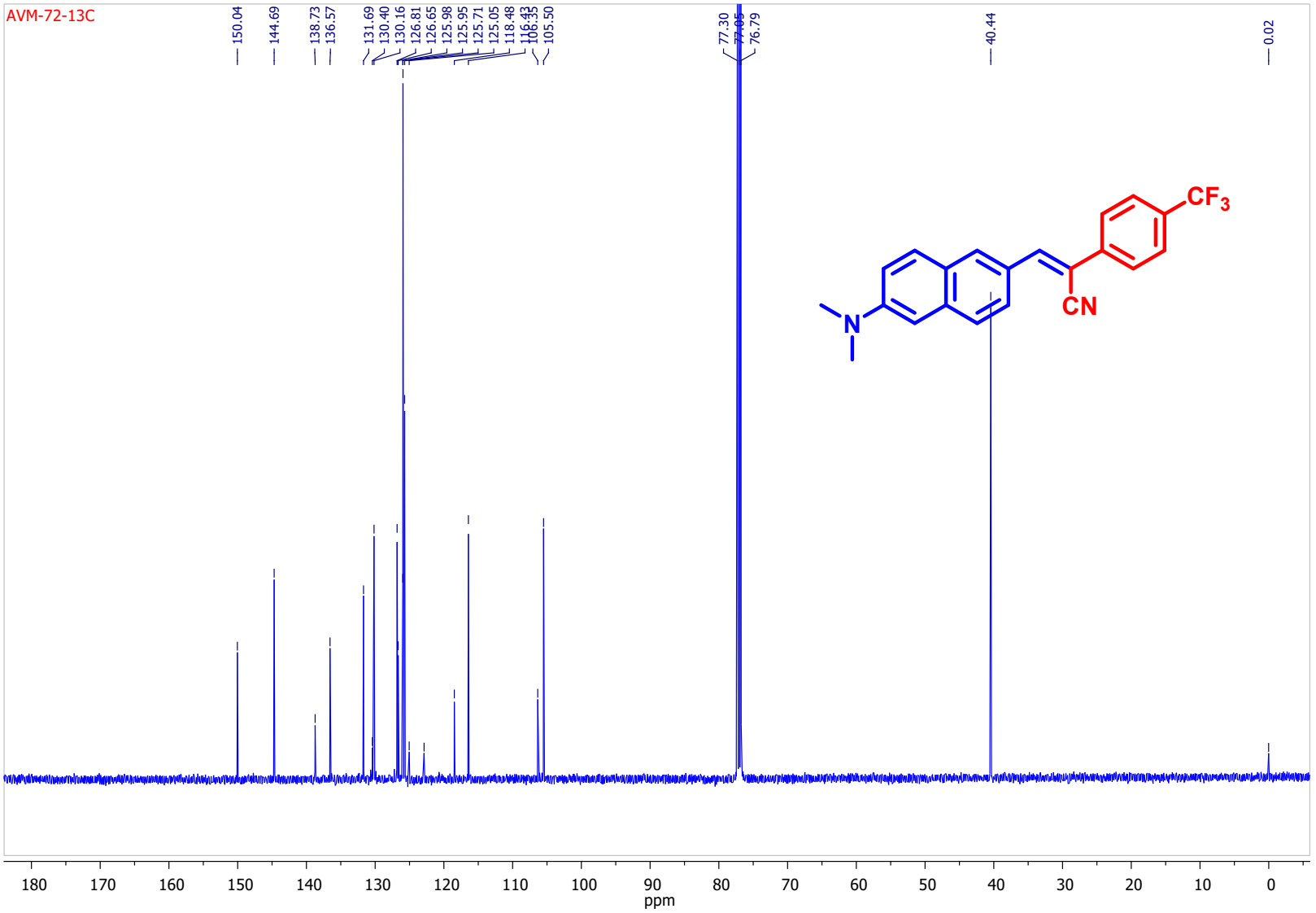
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116.43
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77.05
76.79
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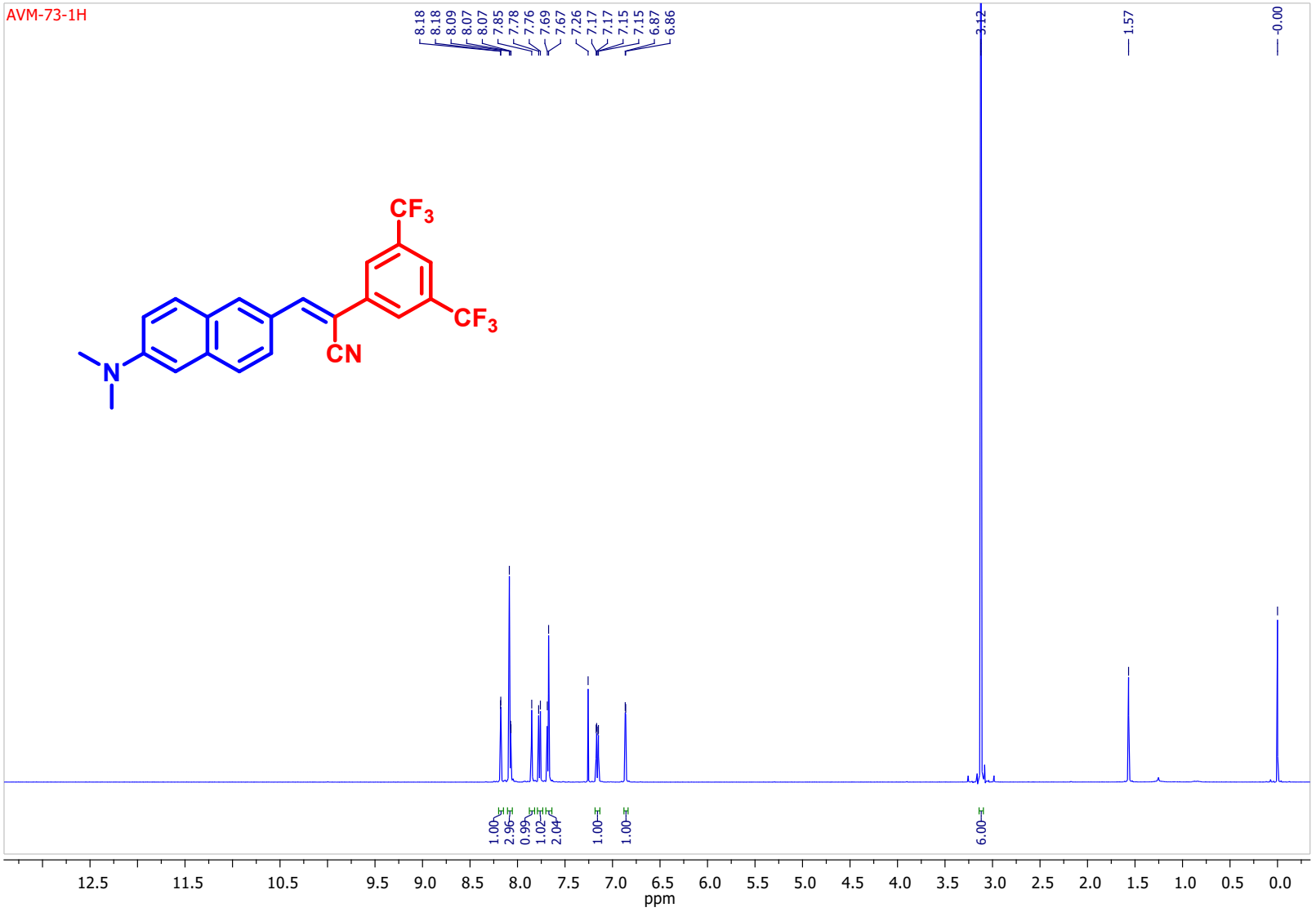
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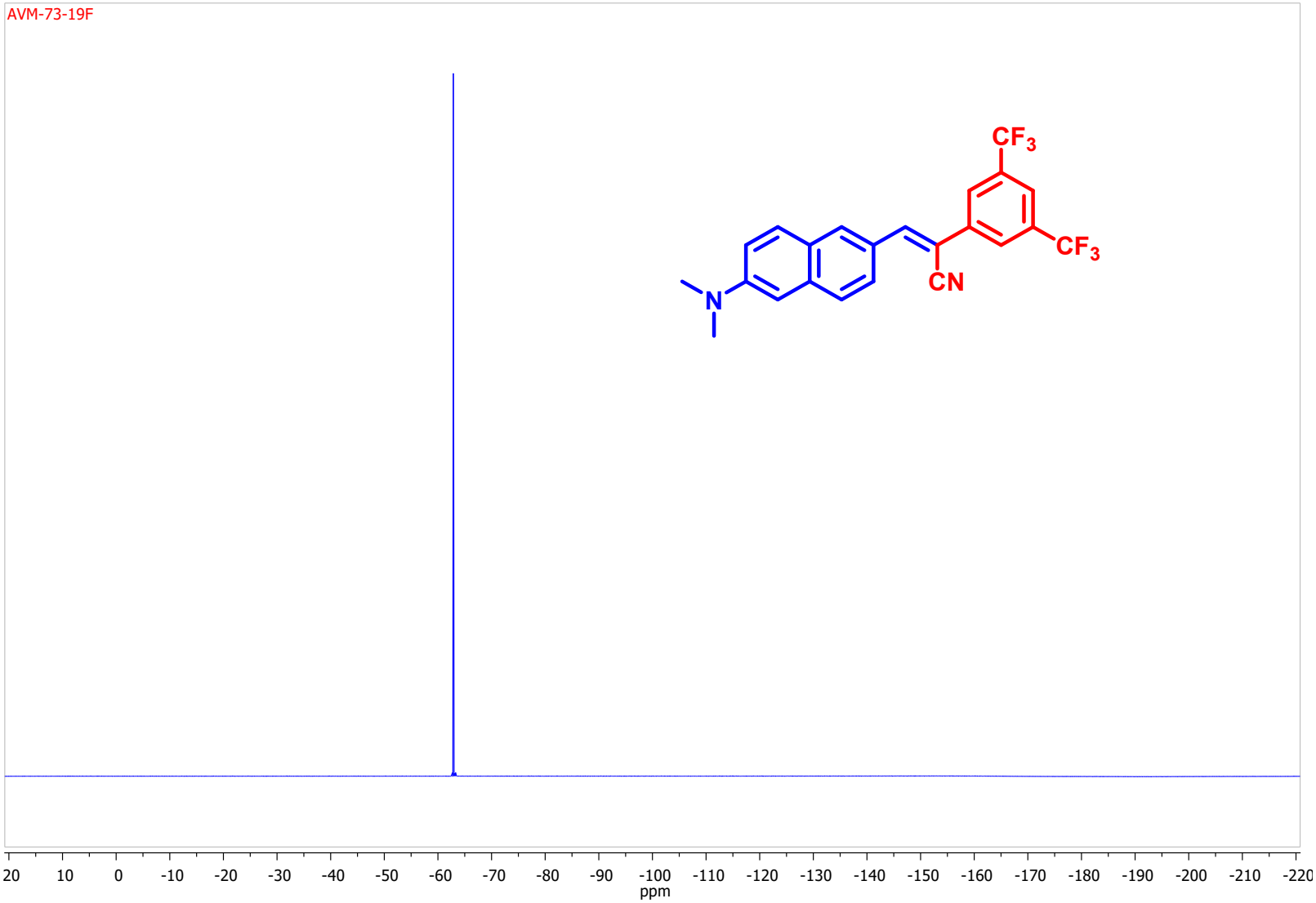
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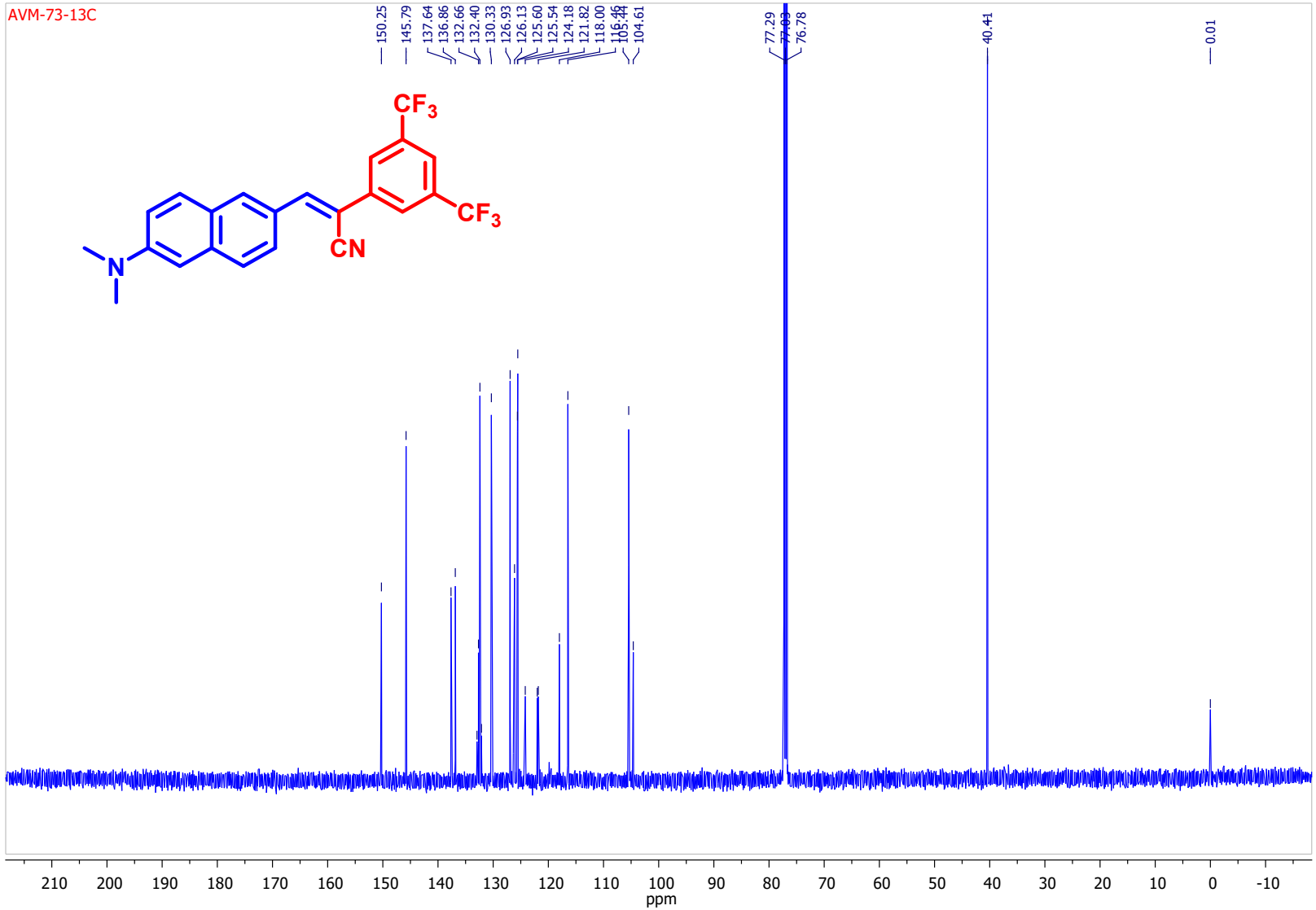
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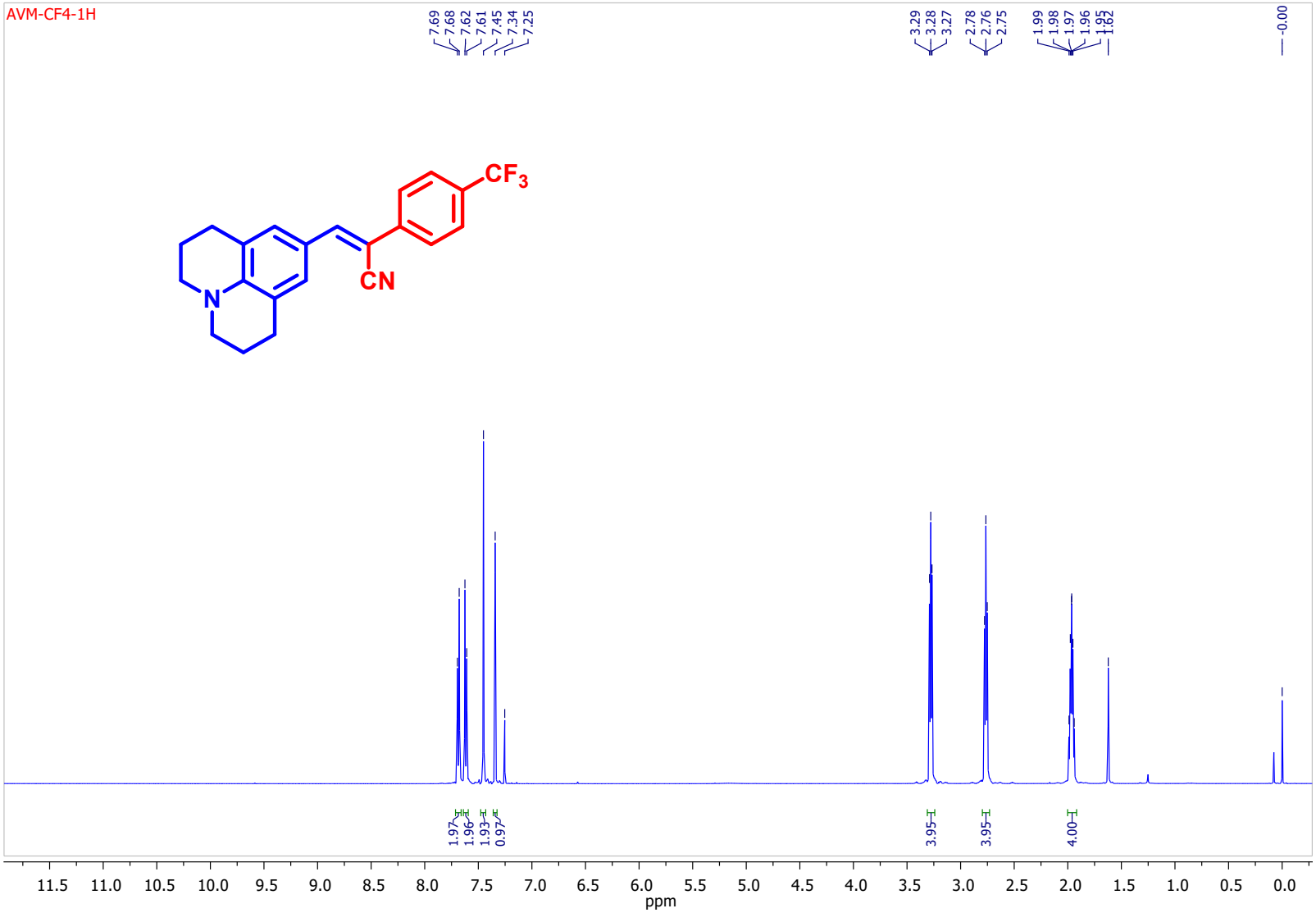
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2.78
2.76
2.75
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1.98
1.97
1.96
1.95
1.62
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CN
N
1.97
1.96
1.93
0.97
3.95
3.95
4.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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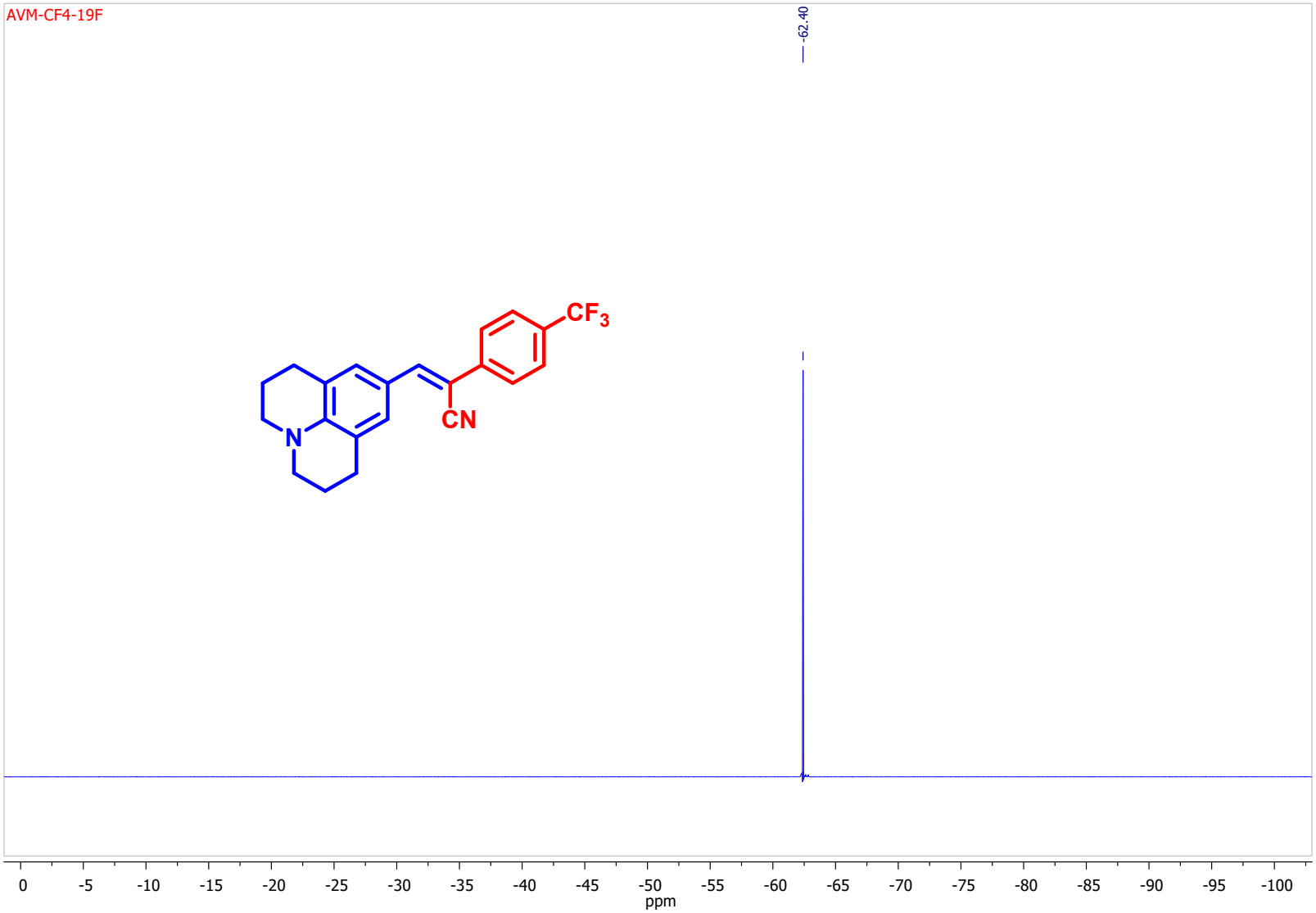
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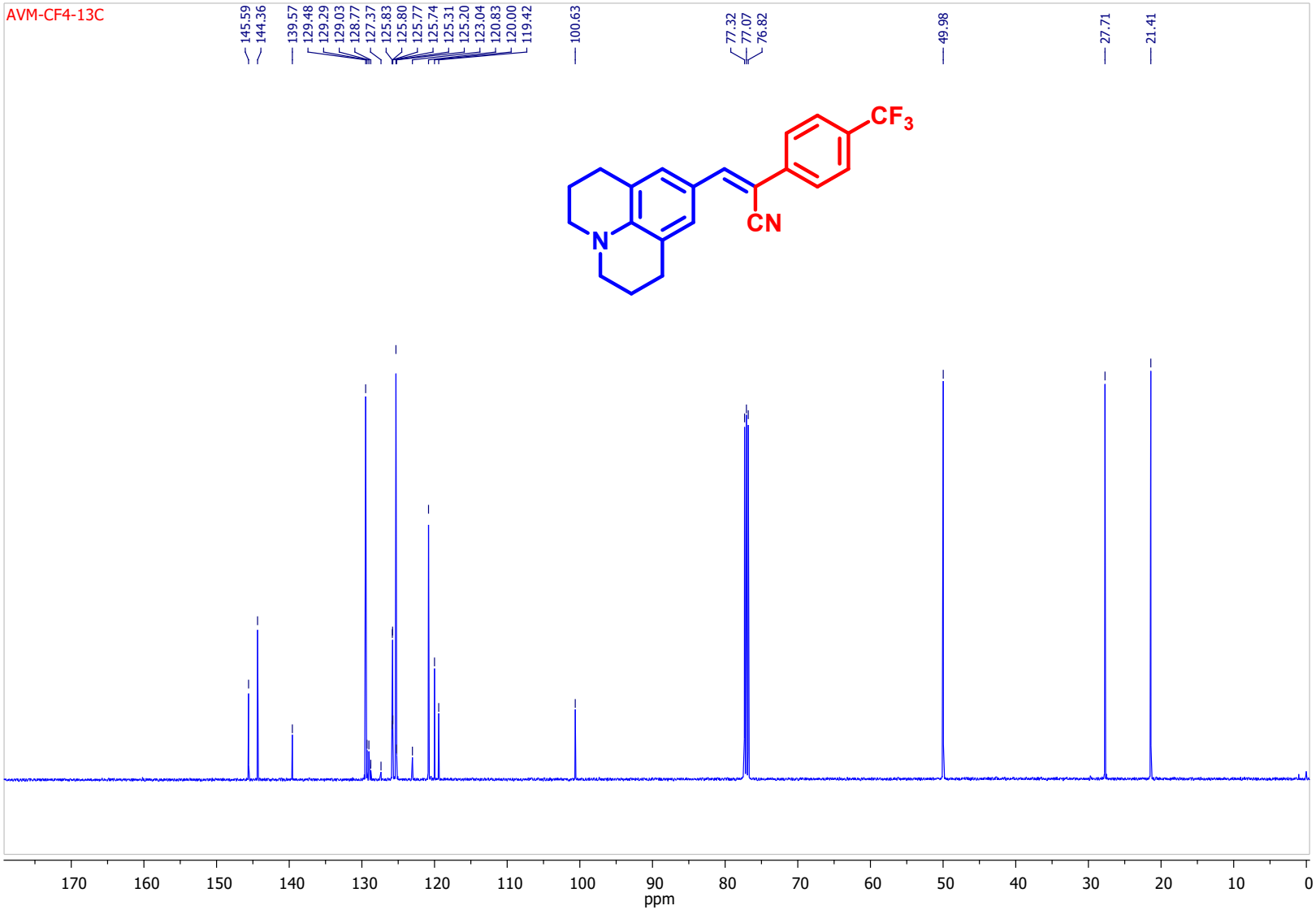
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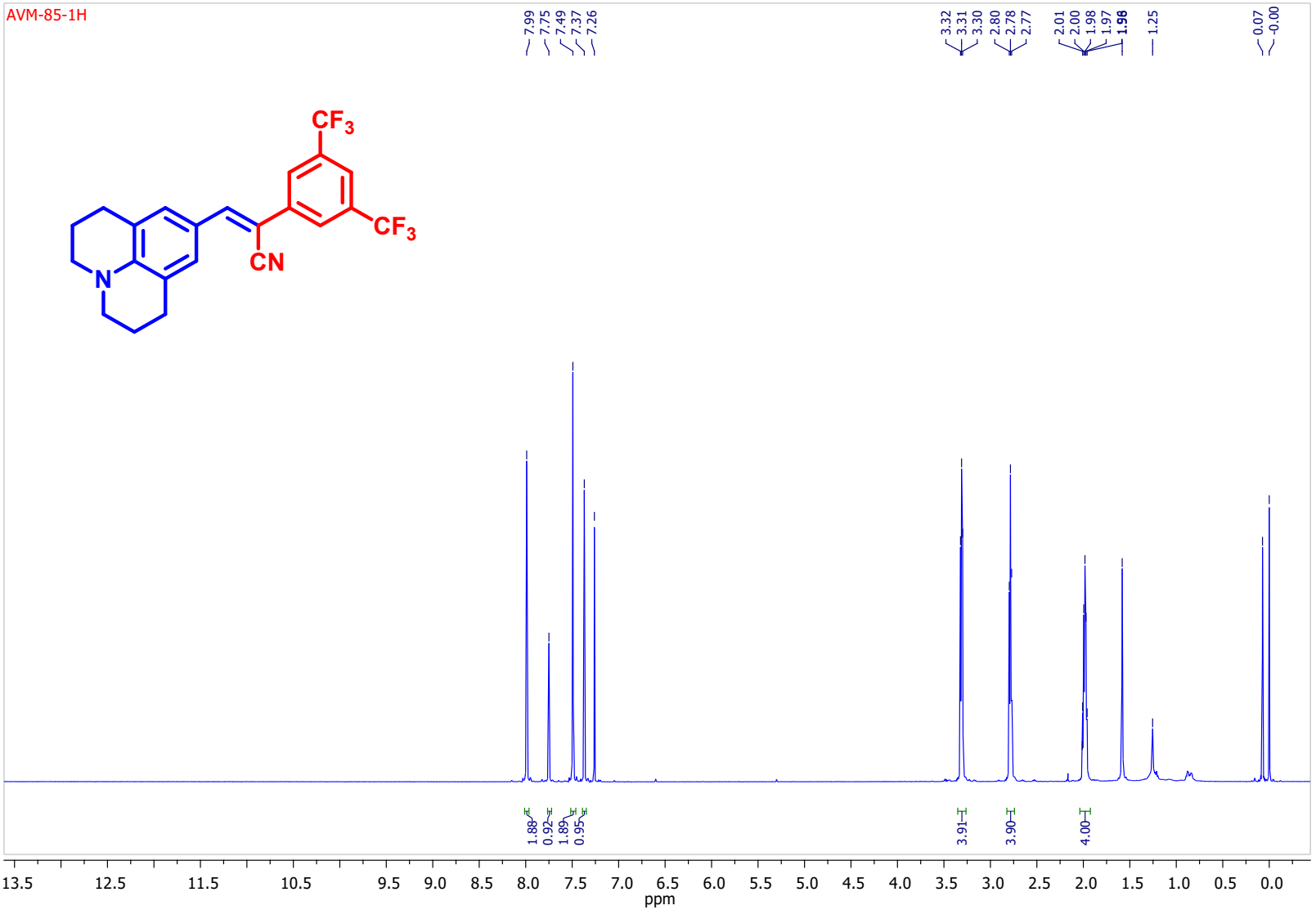
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2.00
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1.96
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CF3
CN
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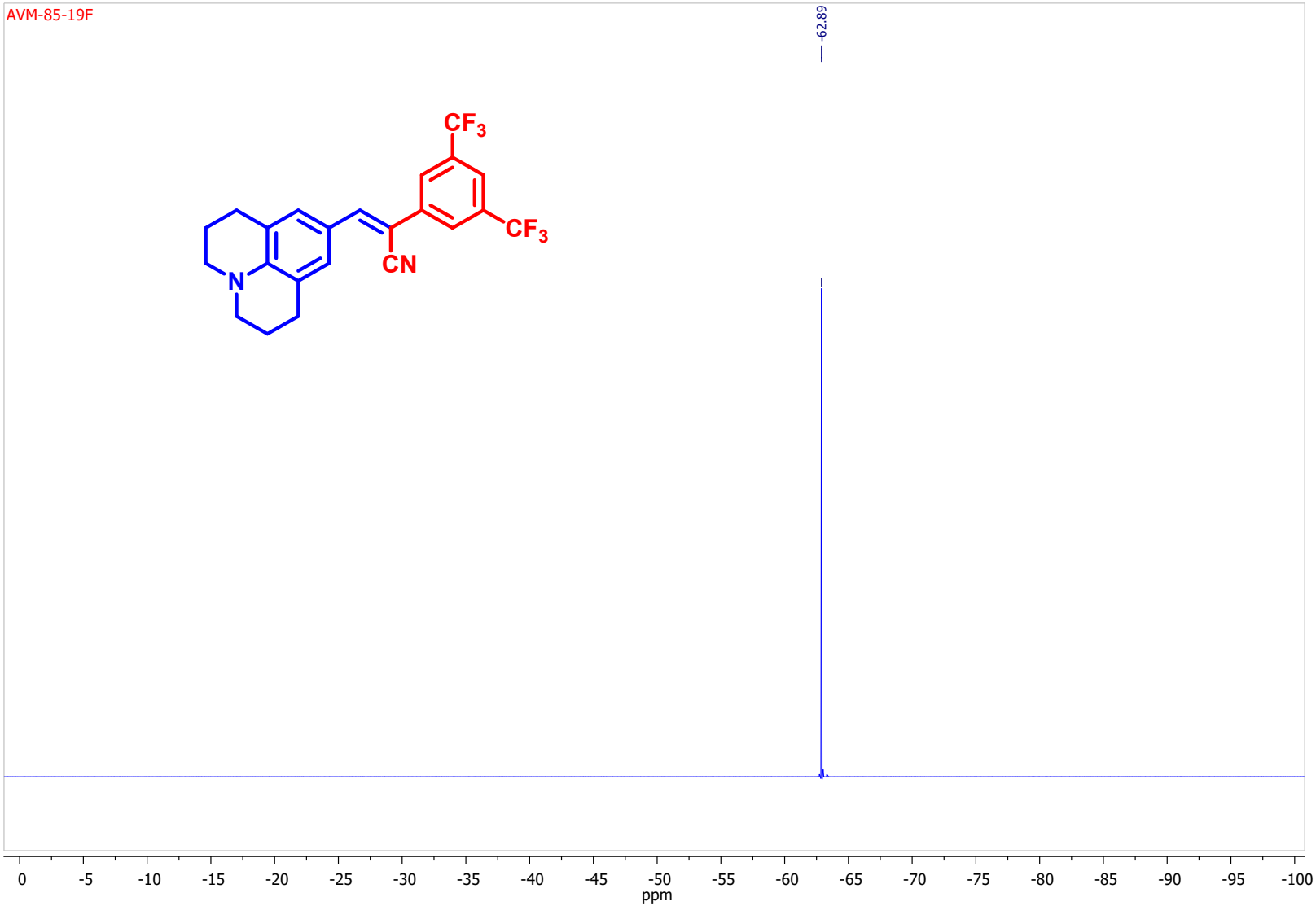
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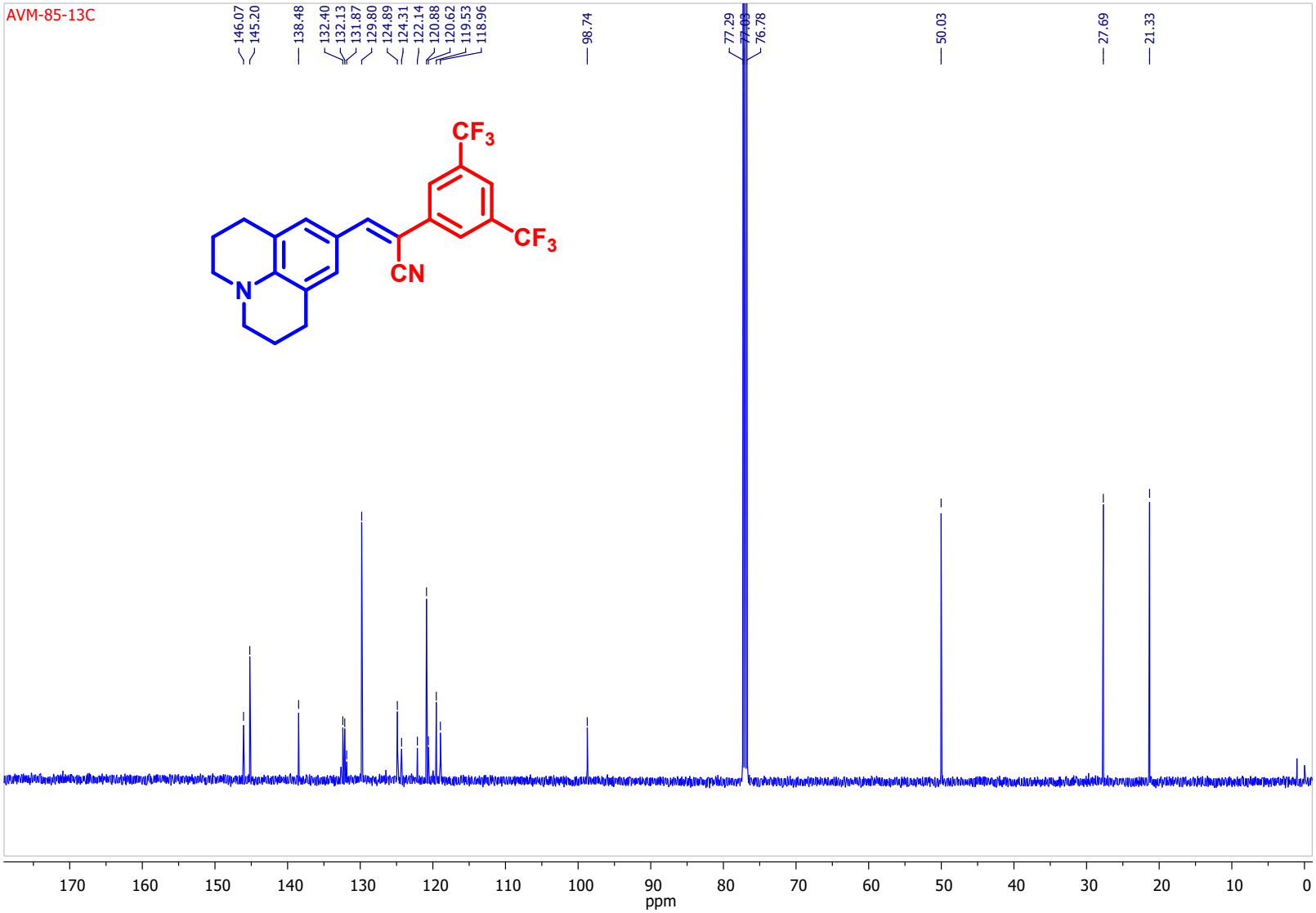
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120.62
119.53
118.96
98.74
77.29
77.03
76.78
50.03
27.69
21.33
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CF3
CN
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140
130
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100
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60
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30
20
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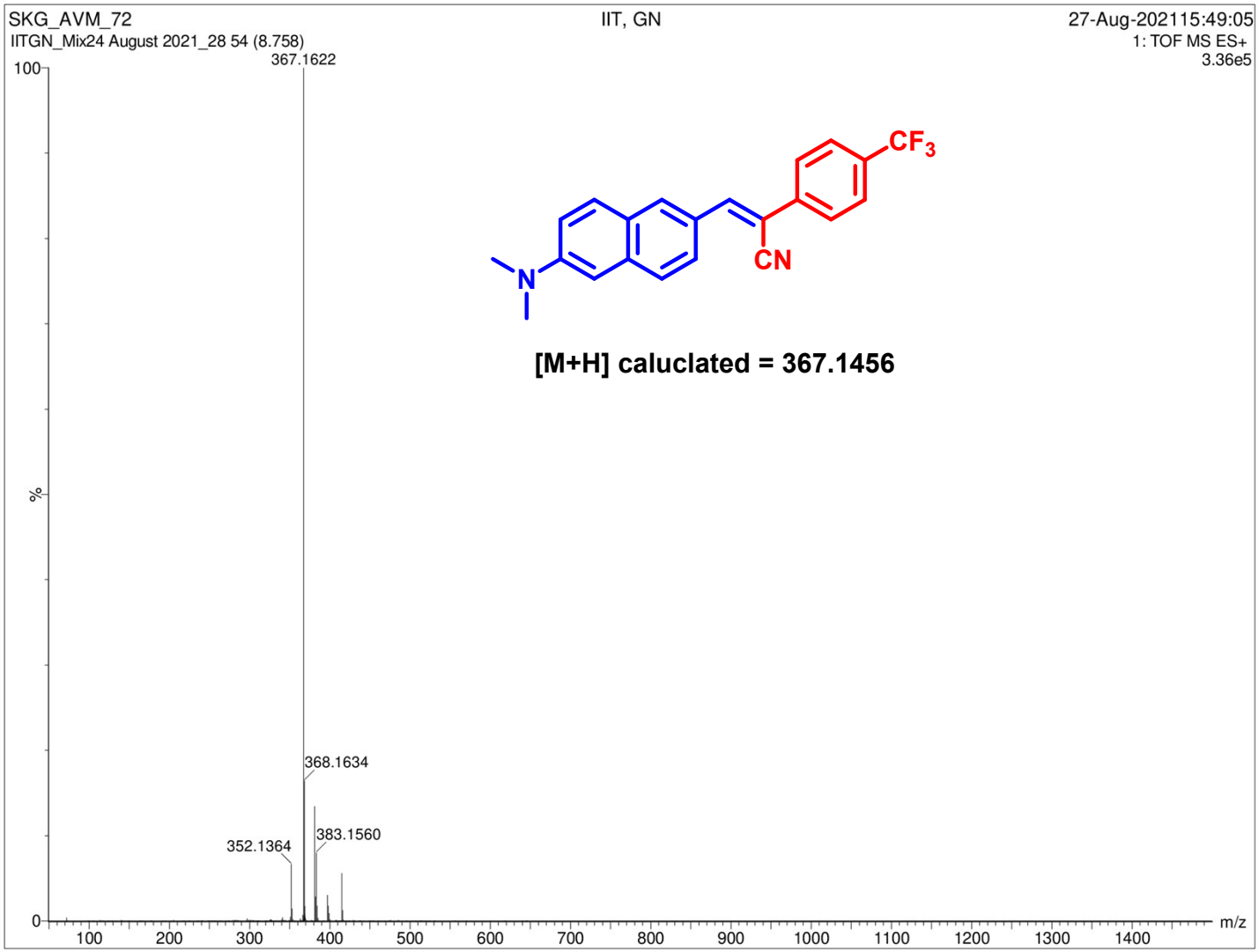
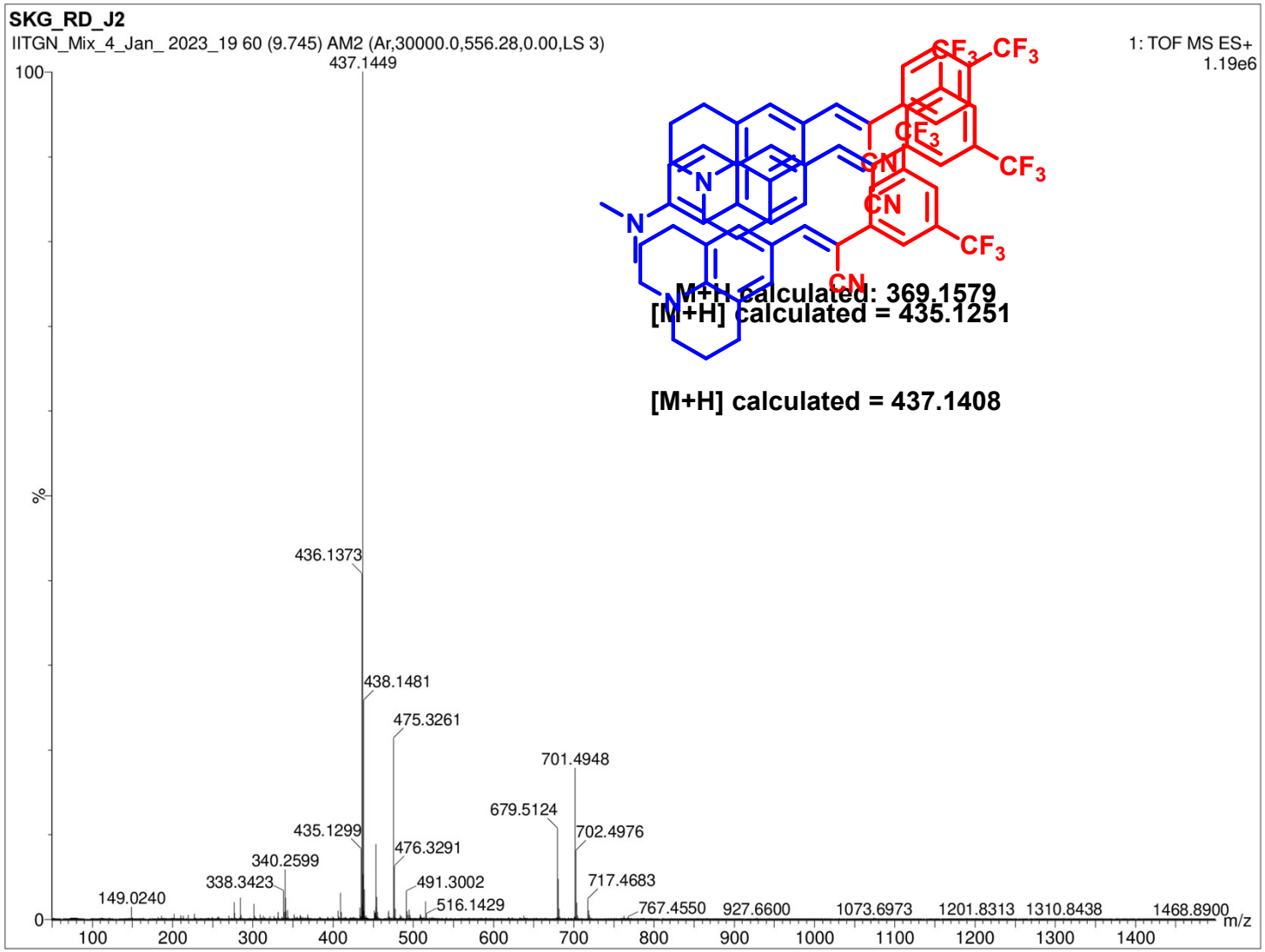
ppm



[M+H] caluclated = 367.1456


SKG_RD_J2
IITGN_Mix_4_Jan_ 2023_19 60 (9.745) AM2 (Ar,30000.0,556.28,0.00,LS 3)
1: TOF MS ES+
1.19e6
437.1449
100
%
0
436.1373
438.1481
475.3261
701.4948
679.5124
435.1299
702.4976
476.3291
340.2599
338.3423
491.3002
717.4683
149.0240
516.1429
767.4550
927.6600
1073.6973
1201.8313
1310.8438
1468.8900
m/z
100
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
CF3
CF3
CF3
CF3
CN
CN
CN
N
N
N
M+H calculated: 369.1579
[M+H] calculated = 435.1251
[M+H] calculated = 437.1408