Electronic Supplementary Information (ESI)

Mechanistic investigation on cellular internalization triggering structure-induced conformational modulation of boron-nitrogen luminogens

Retwik Parui,[a] Hirakjyoti Roy,[b] Niranjan Meher,[a] Siddhartha Sankar Ghosh [b,c] and Parameswar Krishnan Iyer*[a,b]

[a]Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati-781039. Assam. India.

[b]Centre for Nanotechnology, Indian Institute of Technology Guwahati, Guwahati-781039. Assam. India

[c]Department of Bioscience and Bioengineering, Indian Institute of Technology Guwahati, Guwahati-781039, Assam, India

1.1 Experimental Section

1.1.1 Materials and Instrumentation

All the precursor materials and other reagents [(1,8-Diaminonaphthalene, (4-(dimethylamino)phenyl)boronic acid, (4-methoxyphenyl)boronic acid, (4-fluorophenyl)boronic acid, (4-chlorophenyl)boronic acid, (4-bromophenyl)boronic acid, pyridin-4-ylboronic acid, and (4-cyanophenyl)boronic acid] were procured from Sigma Aldrich (INDIA) and TCI Chemicals. HPLC-grade solvents and Milli-Q water were used for the photophysical experiments. NMR (^{1}H, ^{13}C) spectra were recorded with a Varian-AS400 NMR spectrometer, Bruker Advance III 400 MHz, and 600 MHz spectrometer. All ^{1}H and ^{13}C spectra solutions were acquired using the residual solvent signal as the internal reference. Electrospray ionization mass (ESI-MS) spectra were recorded on a Waters (Micro mass MS-Technologies) Q-Tof MS Analyzer spectrometer. Microbalance (± 0.1mg) and volumetric glassware were used for the preparation of solutions. UV-vis and photoluminescence experiments were carried out on a Perkin-Elmer Model Lambda-750 spectrophotometer and a Horiba Fluoromax-4 spectrofluorometer, respectively, using quartz cuvettes at 298 K. Nano-ZS90 Zeta sizer Nano series instrument was used for DLS experiment to determine the average hydrodynamic sizes of the nanoparticles. FESEM and TEM images were recorded using a Zeiss SIGMA 300 and JEOL JEM-2100F transmission electron microscope. SCXRD data was collected from BRUKER D8 QUEST, and structure refinement was executed using instrument-integrated Apex4 software.

1.1.2 Synthesis of Compounds

All the boron-doped congeners (NBNMe2, NBOMe, NBF, NBCl, NBBr, NBPy, NBCN) were synthesized following a similar catalyst-free room temperature procedure. Naphthalene-1,8-diamine (100 mg, 0.633 mmol) and an equivalent amount of (4-fluorophenyl) boronic acid (Corresponding boronic acid was selected according to the functional group anchored in the final product) were placed in a 50 mL round bottom flask, and solubilized in 10 mL THF at room temperature. Then the mixture was kept for stirring up to 15 hours at room temperature. After completion of the reaction, the reaction mixture was extracted from the solvent under low pressure using a rotatory evaporator. The mixture was washed with water and extracted with ethyl acetate. The

organic phase was dried over anhydrous sodium sulphate. The residue was purified by column chromatography over silica gel.

Characterization Data of NBNMe2: Light brown solid (125 mg, 68% yield), ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.6 Hz, 2H), 7.17 (t, *J* = 7.8 Hz, 2H), 7.07 (d, *J* = 8.2 Hz, 2H), 6.81 (d, *J* = 8.5 Hz, 2H), 6.44 (d, *J* = 7.2 Hz, 2H), 6.03 (brs, 2H), 3.04 (s, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 152.0, 141.6, 136.5, 132.8, 127.7, 119.7, 117.5, 111.9, 105.8, 40.3. HRMS (+ESI): Calculated for $C_{18}H_{18}BN_3$, Found 288.1668 $[M+H]^+$.

Characterization Data of NBOMe: Light grey colored solid (130 mg, 74% yield), ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.4 Hz, 2H), 7.14 (t, *J* = 7.8 Hz, 2H), 7.05 (d, *J* = 8.2 Hz, 2H), 6.98 (d, *J* = 8.4 Hz, 2H), 6.41 (d, *J* = 7.3 Hz, 2H), 6.00 (brs, 2H), 3.86 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.6, 141.3, 136.5, 133.1, 127.7, 119.8, 117.8, 114.0, 106.1, 55.3, 29.8. HRMS (+ESI): Calculated for $C_{17}H_{15}BN_2O$, Found 275.1359 $[M+H]^+$.

Characterization Data of NBF: Grey colored solid (108 mg, 65 % yield), ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.54 (dd, *J* = 7.8, 6.3 Hz, 2H), 7.12 – 7.01 (m, 2H), 6.99 (d, *J* = 8.2 Hz, 2H), 6.33 (d, *J* = 7.2 Hz, 2H), 5.89 (brs, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 164.4 (d, *J* = 248.0 Hz), 141.0, 136.4, 133.5 (d, *J* = 7.9 Hz), 127.7, 119.9, 118.1, 115.4 (d, *J* = 20.0 Hz), 106.2. HRMS (+ESI): Calculated for $C_{16}H_{12}BFN_2$, Found 263.1164 $[M+H]^+$.

Characterization Data of NBCl: Dark grey powder (110 mg, 62 % yield), ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.2 Hz, 2H), 7.41 (d, *J* = 8.2 Hz, 2H), 7.14 (t, *J* = 7.8 Hz, 2H), 7.06 (d, *J* = 8.2 Hz, 2H), 6.41 (d, *J* = 7.3 Hz, 2H), 5.97 (brs, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 140.9, 136.6, 136.5, 132.9, 128.7, 128.4, 127.8, 120.0, 118.2, 106.3. HRMS (+ESI): Calculated for $C_{16}H_{12}BClN_2$, Found 279.0853 $[M+H]^+$.

Characterization Data of NBBr: : Gray powder (106mg, 52 % yield), ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.2 Hz, 2H), 7.41 (d, *J* = 8.2 Hz, 2H), 7.06 (t, *J* = 7.6 Hz, 2H), 6.99 (d, *J* = 8.3 Hz, 2H), 6.33 (d, *J* = 7.3 Hz, 2H), 5.89 (brs, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 140.9, 136.4, 133.1, 131.6, 127.7, 125.0, 119.9, 118.2, 106.3. HRMS (+ESI): Calculated for $C_{16}H_{12}BBrN_2$, Found 323.0370 $[M+H]^+$.

Characterization Data of NBPy: : Light brown powder (63 mg, 40 % yield), ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.65 (d, *J* = 5.7 Hz, 2H), 8.45 (s, 2H), 7.84 (d, *J* = 5.7 Hz, 2H), 7.09 (t, *J* = 7.8 Hz, 2H), 6.93 (d, *J* = 8.1 Hz, 2H), 6.58 (d, *J* = 7.3 Hz, 2H). ^{13}C NMR

(150 MHz, DMSO) δ 149.4, 142.4, 136.4, 128.1, 127.6, 120.5, 117.2, 106.4. HRMS (+ESI): Calculated for $C_{15}H_{12}BN_3$, Found 246.1195 $[M+H]^+$.

Characterization Data of NBCN: : Pale yellow powder 95 mg, 55 % yield, ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (q, *J* = 7.8 Hz, 4H), 7.15 (t, *J* = 7.8 Hz, 2H), 7.09 (d, *J* = 8.2 Hz, 2H), 6.43 (d, *J* = 7.2 Hz, 2H), 6.00 (brs, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 140.6, 136.4, 132.1, 131.8, 127.8, 120.1, 118.9, 118.6, 113.8, 106.5. HRMS (+ESI): Calculated for $C_{17}H_{12}BN_3$, Found 270.1197 $[M+H]^+$.

1.1.3 Fluorescence Quantum Yield Calculation

Fluorescence quantum yield of the congeners was recorded in solution (Methanol) and aggregate phase (water) using a standard material, Quinine sulphate (Φ_r = 0.52 in 0.1N H_2SO_4). Quantum yield values were determined using the equation mentioned below.

$$\Phi_s = \Phi_r (A_r E_s / A_s E_r)(\eta_s^2 / \eta_r^2)$$

Here, ‘s’ and ‘r’ mentioned in the subscript, denote the sample and reference fluorophore respectively. A and E represent absorbance and integrated fluorescence emission intensity. η signifies the refractive index of the corresponding solvent.

1.1.4 Sample Preparation and Photophysical Study in Aggregate Phase

Initially Methanol was selected as a good solvent to prepare the Stock solutions of all the probes with a concentration of 10 mM. For Self-assembly formation, a binary solvent mixture was chosen where a certain quantity of stock solution was dispersed in different methanol-water fractions and 50 μM concentration of the probes were served for the photophysical studies. With increasing water fraction, all the probes formed a dispersion which was properly mixed with a micropipette and measured their luminescence at room temperature. From the distinctive fluorescence emission, the 99.9% water containing dispersed solutions were considered for the analysis of the self-assembly in the next step.

1.1.5 Sample Preparation for Morphological Experiment

The morphology of the spontaneously grown nano assemblies was captured through FESEM and TEM experiments. For that, 5 µL mixture of nanoaggregate solution prepared by dispersing 50 µM probe in maximum water fraction was drop casted on a silicon wafer or carbon coated copper grid for the FESEM and TEM analysis respectively. Then the nanoaggregates placed on top of the respective substrate were dried under vacuum at room temperature instantly. For analyzing time-dependant change in the morphology, the prepared dispersion was kept in ambient temperature up to a particular time to observe the propagation phenomena of self-assemblies and then processed for the similar vacuum dry process.

1.1.6 Theoretical Studies

To investigate the effect of donor and acceptor functional groups on the electronic distribution and HOMO-LUMO band gap variation, electronic properties of all the congeners (NBNMe2, NBOMe, NBF, NBCl, NBBr, NBPy, NBCN) were calculated theoretically with density functional theory (DFT). Ground state geometry was optimized by DFT method using the B3LYP/6-31G basis set in Gaussian 09 software. Along with the HOLO-LUMO band gap calculations, the electrostatic potential diagram was evaluated using the optimized structure.

1.1.7 Cellular Uptake Study

To investigate how NBCN, NBF, NBNMe2, and NBOMe are taken up by cells, the HeLa cells (procured from NCCS Pune, India) were cultured on coverslips in 6-well plates at a density of 1.5×10^5 cells/well and allowed to adhere for 24 hours. Subsequently, the cells were exposed to a concentration of 50 µM of each compound and incubated for an additional 4 hours at 37 °C. After the incubation period, the cells were rinsed with PBS and fixed with a 4% formaldehyde solution for 10 minutes. After fixation, the cells were washed again with PBS and examined using confocal microscopy (ZEISS LSM-880).

1.1.8 Mechanism of Uptake

To explore how the four compounds are internalized within the HeLa cells, cells were initially seeded in a 96-well plate at a density of 5000 cells/well in triplicate. To assess uptake at a low temperature (4 °C), cells were incubated at 4 °C for 1 hour before being exposed to 50 µM of NBCN, NBF, NBNMe2, and NBOMe for 4 hours. For the inhibition of energy-dependent endocytosis, HeLa cells were treated with 0.2% sodium azide in serum-free DMEM for 1 h, followed by incubation with four compounds for 4 h at 37 °C in CO_2. For methyl β-cyclodextrin (MβCD), cells were pre-incubated in serum-free DMEM containing 5 mM MβCD for 30 min at 37 °C/5% CO_2. The media were then replenished with fresh media containing the inhibitor with the compound and further incubated for 4 h at 37 °C/5% CO_2. Following incubation, cells were washed with cold PBS to remove any free compound. Following treatment, the fluorescence intensities of the compounds were measured in Promega multiplate reader. For Clathrin-mediated endocytosis, cells were treated with dynasore in serum-free DMEM media for 2 hours prior to the compound treatment. Next, the cells were incubated for another 4 hours. After treatments, cells were washed with PBS to remove any unbound molecules, and the fluorescence intensities of the compounds were measured using a Thermo Fisher Scientific multiplate reader.

1.1.9 Cell Viability Assay

Cell viability was carried out in 96 well plates in triplicate. HeLa cells were treated with NBCN, NBF, NBNMe2, and NBOMe in the concentration range of 10 to 100 µM for 48 h. After the treatment, 3-(4,5-Dimethylthiazol-2-yl)-2,5-Diphenyltetrazolium Bromide (MTT) was added to each well and incubated for about 1.5 h. Following the incubation period, the media was carefully removed and DMSO was added to dissolve the purple color formazan crystals produced as a result of cellular respiration. Colorimetric analysis was conducted using a multi-well plate reader (ThermoFisher Scientific) by measuring the absorbance at 570 nm for the sample and 630 nm for background subtraction. Cell viability was calculated using the provided equation.

$$\% \text{ of cell viability} = \frac{(A570-A630)Sample}{(A570-A630)Control} X100$$

1.1.10 Colocalization study

For the colocalization study, HeLa cells were cultured on coverslips in 6-well plates at a density of 1.5 × 10^5 cells/well and allowed to adhere for 24 h. After 24 h, cells were treated with compounds for 3 h and stained with LysoTracker Deep Red (Invitrogen) for 1 h. After treatment, the cells were washed with PBS and fixed with a 4% formaldehyde solution for 10 min. Following fixation, cells were examined using confocal microscopy (ZEISS LSM-880).

1.2 Theoretical Data

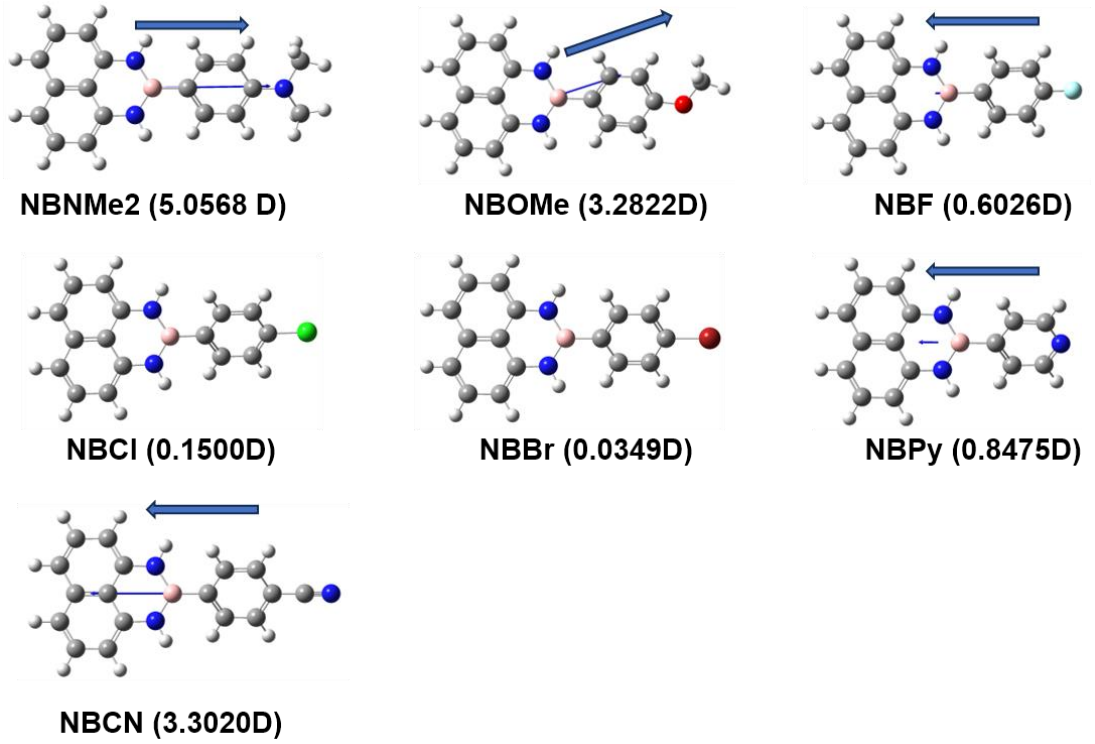


Fig. S1: Dipole Moment magnitude and direction of all the congeners calculated from DFT optimized structure.

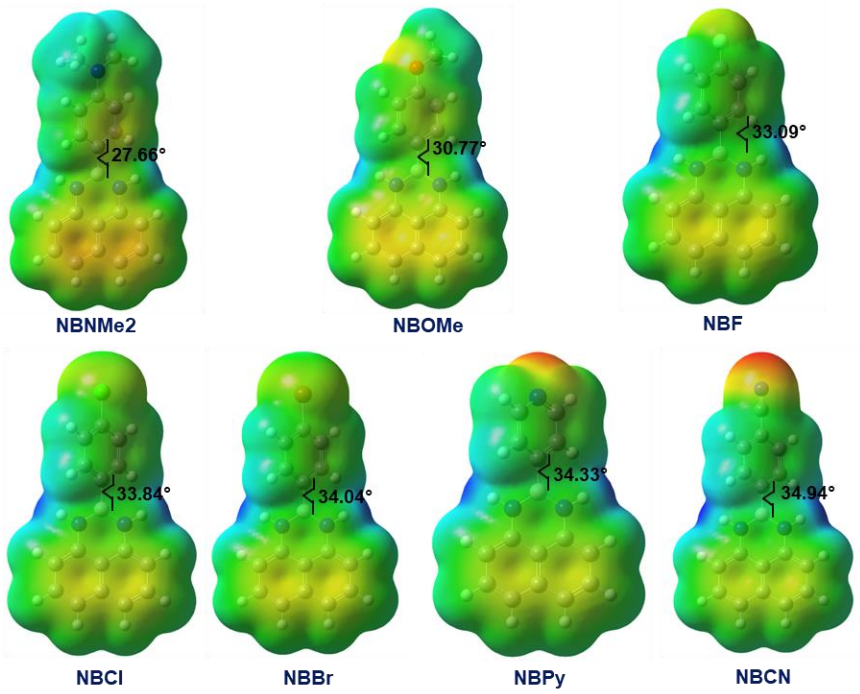


Fig. S2: Electrostatic potential diagram of all the congeners reflecting enhancement in the dihedral angle and variation in the electronic distribution, calculated at B3LYP/6-31G.

1.3 Experimental data

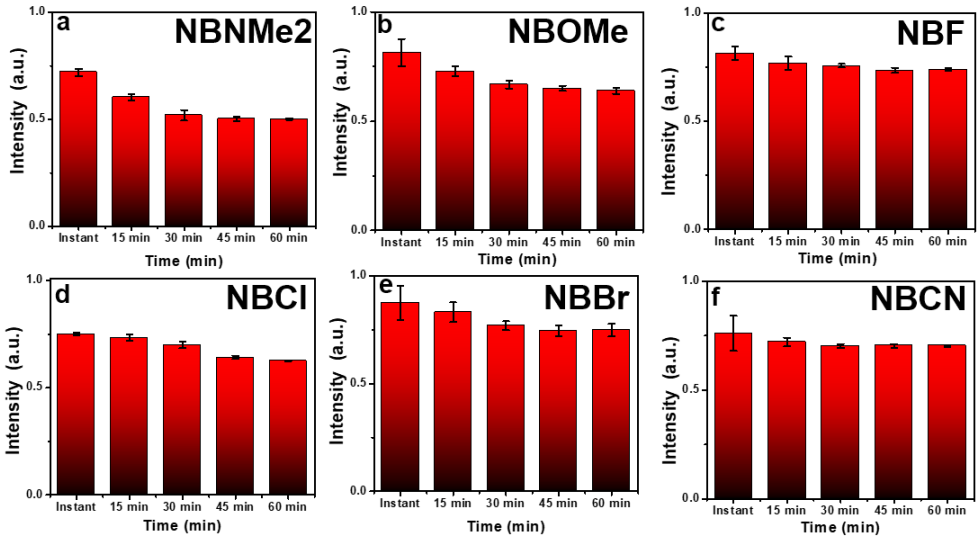


Fig. S3: The bar diagram represents the variation in the fluorescence intensity maxima with time for the respective compounds at 50 μM concentration.

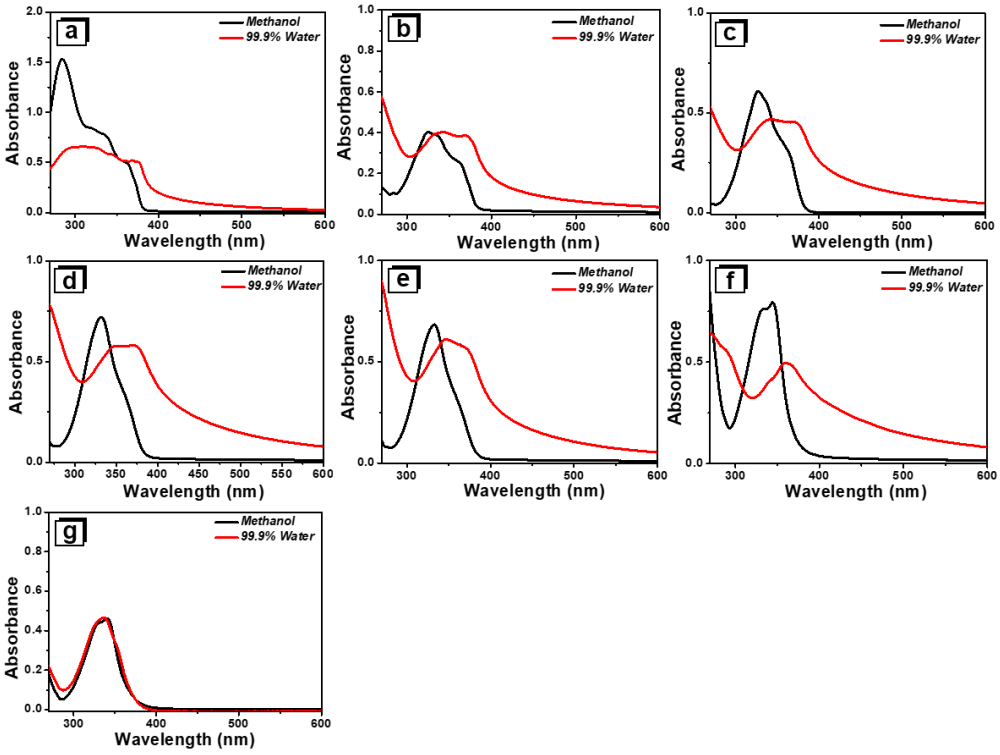


Fig. S4: Absorbance spectra of (a) **NBNMe2**, (b) **NBOMe**, (c) **NBF**, (d) **NBCl**, (e) **NBBr**, (f) **NBCN**, (g) **NBPy** at 50 μM concentration in MeOH and 99.9% water fractions.

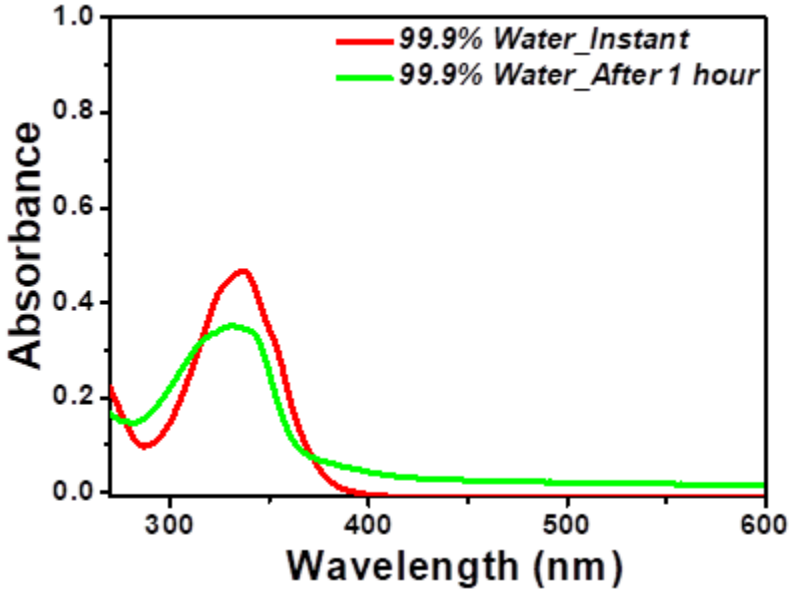


Fig. S5: UV-Vis spectra of NBPy at 50 μM concentration in 99.9% water fractions instant and after 1 hour.

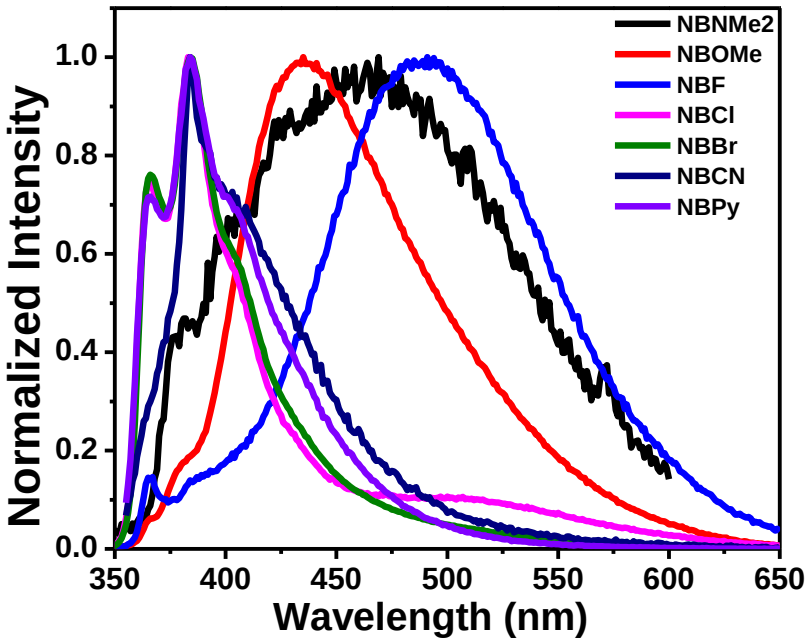


Fig. S6: Normalized PL spectra of all the boron-embedded derivatives in MeOH solution (50 μM).

Table S1: Summarization of optical properties measured using 1 cm × 1 cm dimension of quartz cuvettes at mentioned excitation wavelength slit 3 at 50 μM concentration of the probe.

Name	Excitation (λ_{ex}) (nm)	Emission in solution (λ_{em1}) (nm)	Emission in Aggregate(λ_{em2}) (nm)	QY (solution) (%)	QY (aggregate) (%)	Properties
NBNMe2	285	465	427	0.160	3.344	AIE
NBOMe	330	434	425	0.770	0.768	DSE
NBF	330	490	443	0.195	2.967	AIE
NBCl	330	385	460	0.074	2.109	AIE
NBBr	330	385	455	0.337	0.379	DSE
NBCN	345	385	515	0.038	0.254	AIE
NBPy	345	385	424	0.440	0.986 (instant), 6.321(after1 hr)	AIE

Table S2: Summarized CIE coordinates for emission of the corresponding luminogens in solid powder form.

Name of the Solvent	X Coordinate	Y coordinate
NBNMe2	0.149079	0.0945645
NBOMe	0.167332	0.168058
NBF	0.149662	0.129281
NBCl	0.18823	0.244953
NBBr	0.169465	0.210294
NBCN	0.321383	0.604505
NBPy	0.258184	0.461923

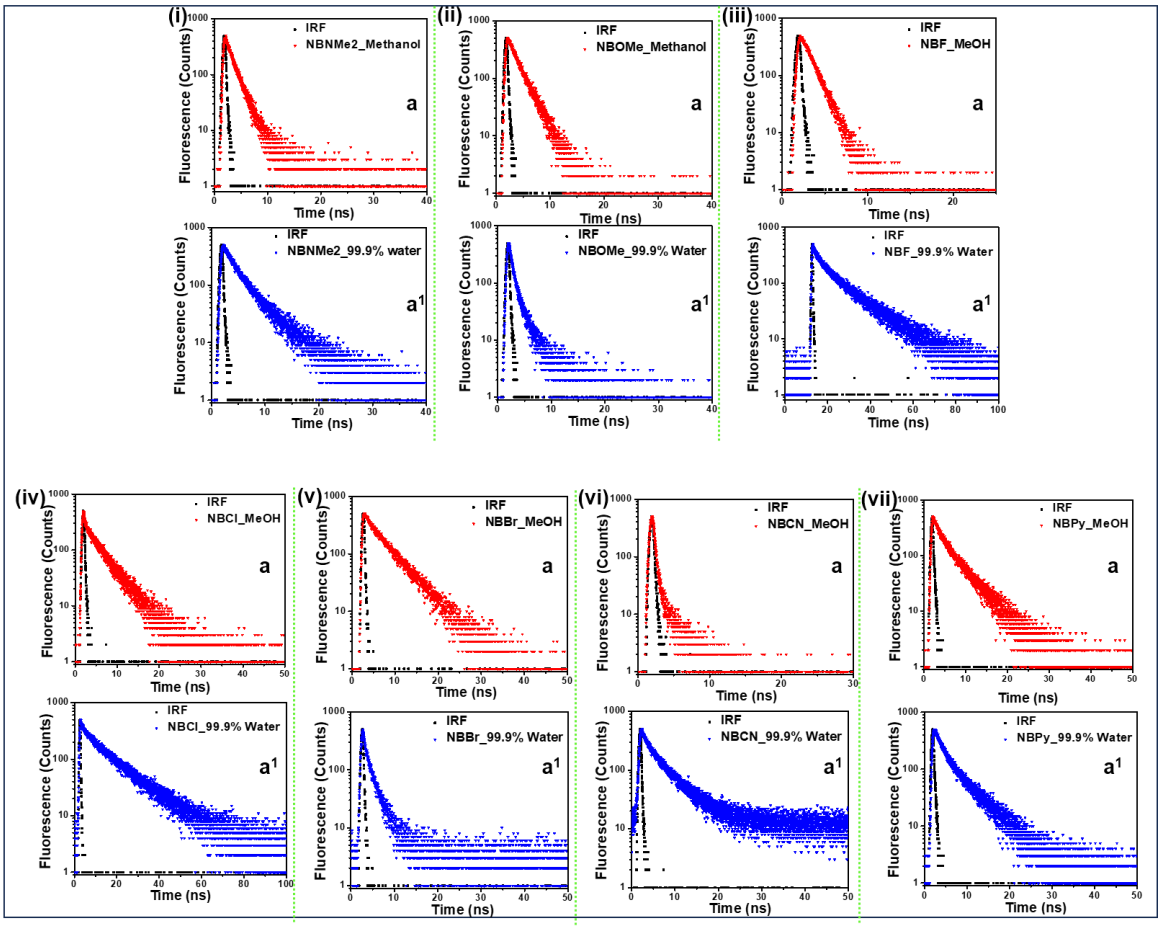


Fig. S7: Variation in the luminescence lifetime decay of (i) NBNMe2, (ii) NBOMe, (iii) NBF, (iv) NBCl, (v) NBBr, (vi) NBCN, (vii) NBPy, recorded at 50 μM concentration in (a) MeOH and (a^1) in 99.9% water fraction using excitation of 336 nm LED source.

Table S3: Contained details of fluorescence lifetime spectra represented in Fig. S7.

Name	Average τ_i (ns)		Chi-square (χ^2)		Exponential fitting	
	Methanol	Water	Methanol	Water	Methanol	Water
NBNMe2	1.68	3.71	1.01	1.02	Bi	Bi
NBOMe	2.14	0.96	1.02	1.01	Mono	Bi
NBF	1.28	12.02	1.01	1.06	Mono	Bi
NBCl	3.20	12.74	1.01	1.23	Bi	Bi
NBBr	4.74	3.25	1.01	1.25	Mono	Bi
NBCN	0.48	4.48	1.01	1.23	Bi	Bi
NBPy	4.08	4.34	1.02	1.00	Bi	Bi

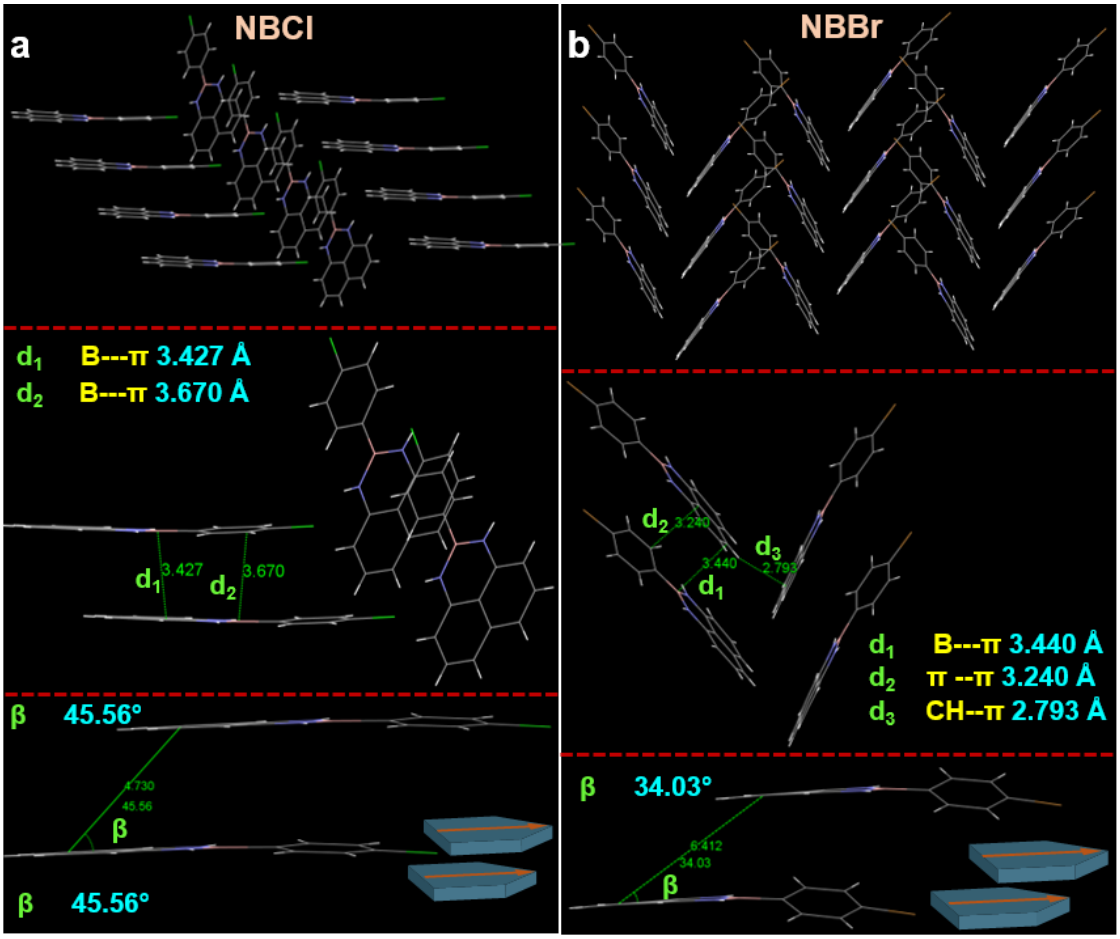


Fig. S8: Molecular packing orientation, intermolecular interaction, molecular structural conformation, and slip angle for (a) NBCl, (b) NBBr obtained from SCXRD experiment.

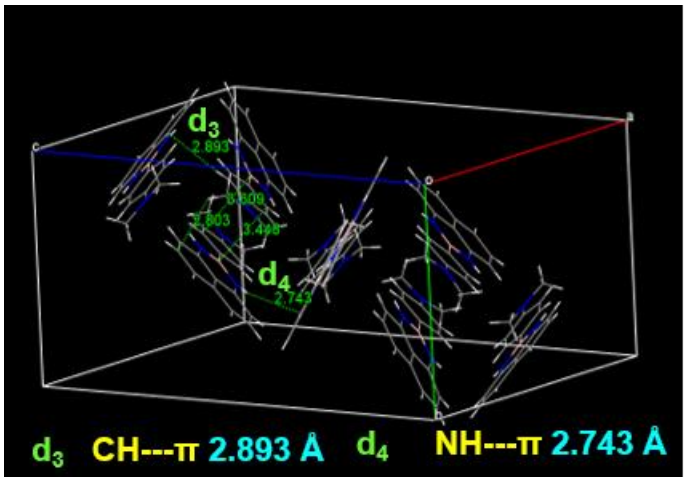


Fig. S9: Additional intermolecular interaction between the monomeric and dimeric unit of NBNMe2 probe inside a unit cell.

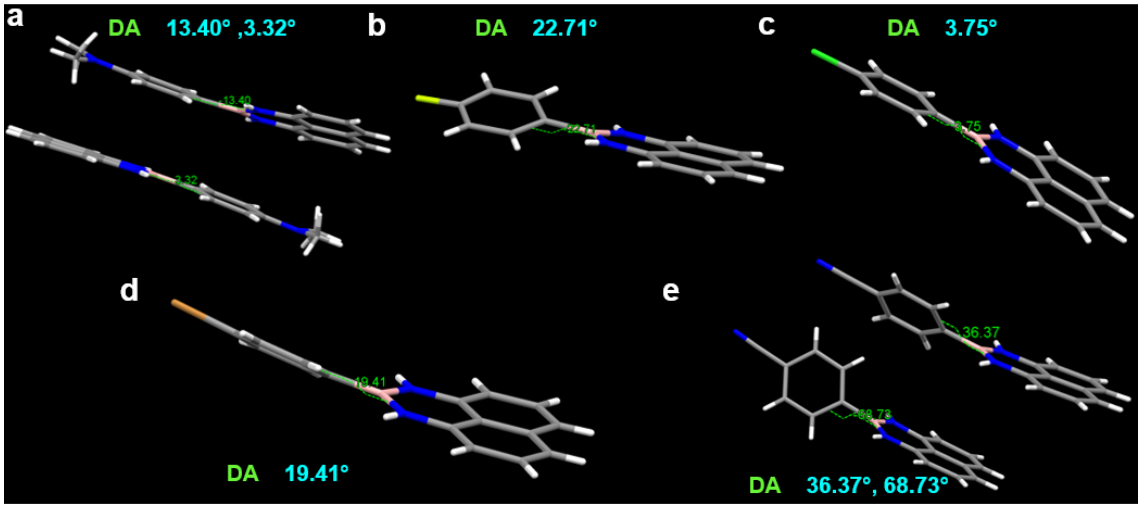


Fig. S10: Regulation in Torsional angle in (a) **NBNMe2**, (b) **NBF**, (c) **NBCl**, (d) **NBBr**, (f) **NBCN** skeleton along with the variation in the functional group, obtained from the SCXRD analysis.

Table S4: Single Crystal data and parameters of all the obtained crystals.

Compound code	**NBNMe2**	**NBF**	**NBCN**
CCDC	2336090	2336105	2336104
Empirical Formula	C18 H18 B N3	C16 H12 B F N2	C17 H12 B N3
Formula Weight	287.16	262.09	269.11
Temperature	297 K	273 K	273 K
Wavelength	0.71073	0.71073	0.71073
Crystal System	monoclinic	tetragonal	monoclinic
Space Group	P 21/n	I -4	P 1 21/n 1
Unit Cell Dimension	a=13.9391(9) b=11.2303(7) c=20.3661(13) alpha=90 beta=104.938(2) gamma=90	a=22.7941(12) b=22.7941(12) c=5.0803(4 alpha=90 beta=90 gamma=90	a=8.2259(7) b=26.151(2) c=19.2586(17) alpha=90 beta=95.282 (2) gamma=90
Volume	3080.4(3)	2639.6(3)	4125.2(6)
Z	8	8	12

Absorption coefficient	0.074	0.088	0.078
F (000)	1216.0	1088.0	1680.0
Theta range for data collection	2.041-24.995	1.263- 24.998	1.317-25.000
Index Range	-16<=h<=16, -13<=k<=13, -24<=l<=24	-27<=h<=27, -27<=k<=27, -6<=l<=6	-9<=h<=9, -31<=k<=31, -22<=l<=22
Reflections Collected/unique	73129/5403 (R_{int} = 0.0488)	43785/2326 (R_{int} = 0.0678)	82066/7172 (R_{int} = 0.0600)
Goodness-of-fit on F2	1.243	1.177	1.154
Final R indices [I>2σ(I)]	R1 = 0.0543, ωR2 = 0.1597	R1 = 0.0604, ωR2 = 0.1401	R1 = 0.0849, ωR2 = 0.1557
R indices (all data)	R1 = 0.0777, ωR2 = 0.2005	R1 = 0.1079, ωR2 = 0.1786	R1 = 0.1229, ωR2 = 0.1811
Largest difference peak and hole (e $Å^{-3}$)	0.182, -0.150	0.124, -0.192	0.189, -0.191

Table S5: Single Crystal data and parameters of all the obtained crystals.

Compound code	**NBCl**	**NBBr**
CCDC	2336103	2336092
Empirical Formula	C16 H12 B Cl N2	C16 H12 B Br N2
Formula Weight	278.54	323.00
Temperature	300 K	297K
Wavelength	0.71073	0.71073
Crystal System	monoclinic	monoclinic
Space Group	P 21	P 21/n

Unit Cell Dimension	a=4.7299(7) b=10.3015(15) c=13.5889(19) alpha=90 beta=96.928 (4) gamma=90	a=12.963(9) b=6.412(4) c=16.767(11) alpha=90 beta=92.356 (19) gamma=90
Volume	657.69(16)	1392.6(16)
Z	2	4
Absorption coefficient	0.278	2.941
F (000)	288.0	648.0
Theta range for data collection	1.509-24.996	1.947- 26.316
Index Range	-5<=h<=5, -12<=k<=12, -16<=l<=16	-16<=h<=16, -7<=k<=7, -20<=l<=20
Reflections Collected/unique	12533/2295 (R_{int} = 0.0415)	34504/2791 (R_{int} = 0.0444)
Goodness-of-fit on F2	1.070	1.061
Final R indices [I>2σ(I)]	R1 = 0.0289, ωR2 = 0.0760	R1 = 0.0428, ωR2 = 0.1296
R indices (all data)	R1 = 0.0306, ωR2 = 0.0824	R1 = 0.0521, ωR2 = 0.1379
Largest difference peak and hole (e $Å^{-3}$)	0.149, -0.157	0.391, -0.866

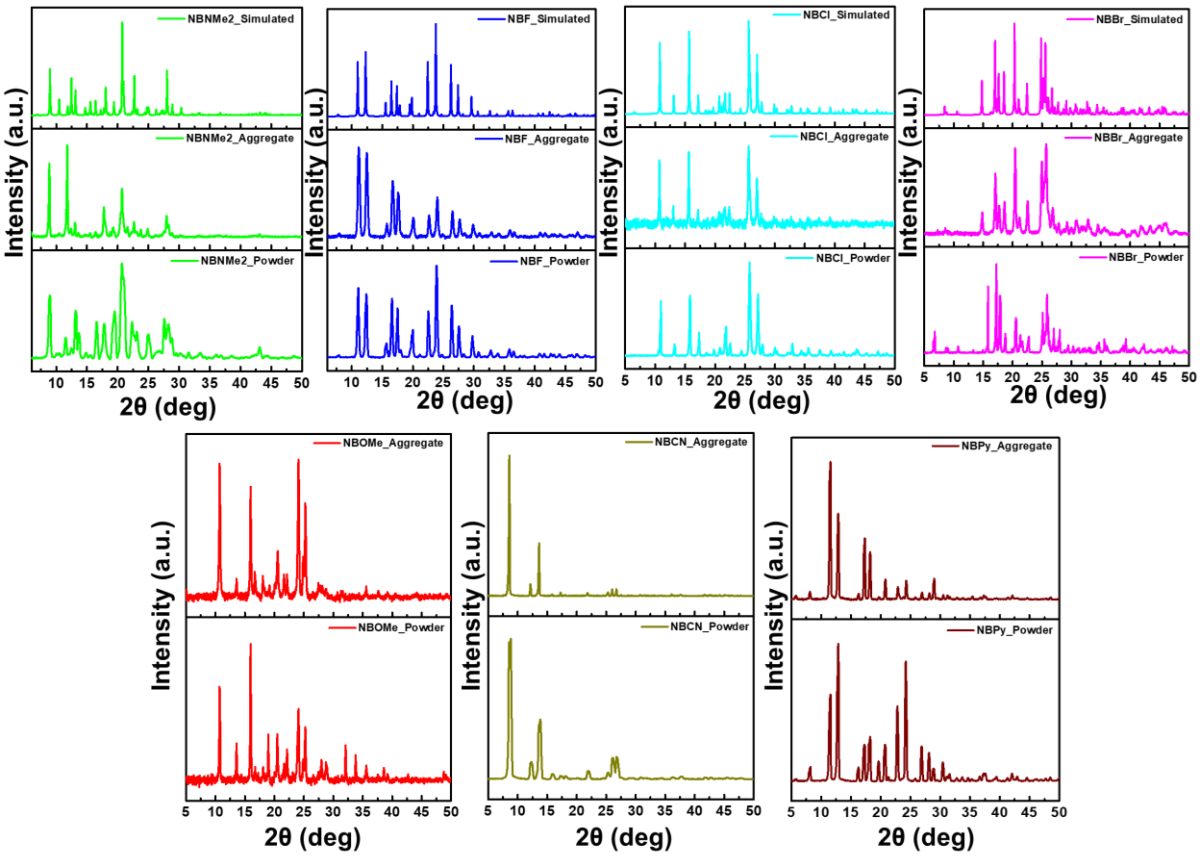


Fig. S11: PXRD patterns of all the boron congeners in solid powder, aggregate (generated in water) compared with crystal's simulated spectra scanned 2θ from 5° to 50°.

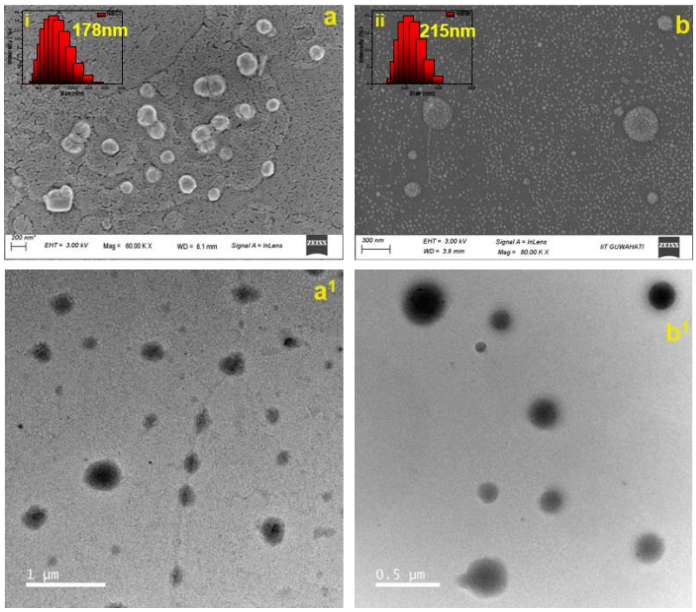


Fig. S12: Morphology pattern of (a, a[1]) NBCl and (b, b[1]) NBBr nano-assemblies captured in FESEM (above) and FETEM (below) respectively. Inset (i, ii) represents the corresponding DLS spectra with their average hydrodynamic diameter.

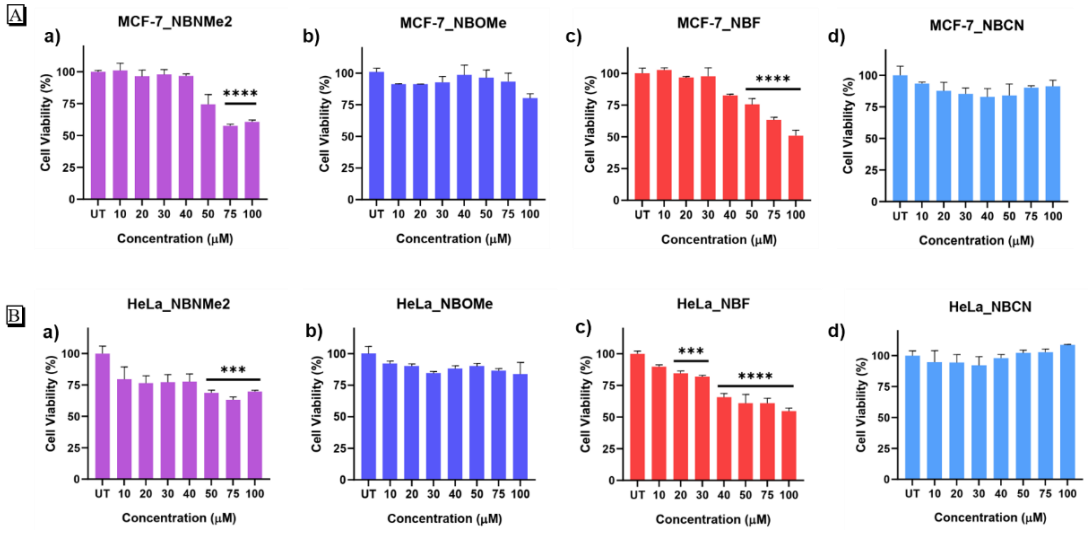


Fig. S13: Cell viability of the boron congeners at different self-assembly constructions in two cancerous cell lines (A) MCF-7 and (B) HeLa. (n = 3, mean ± SD).

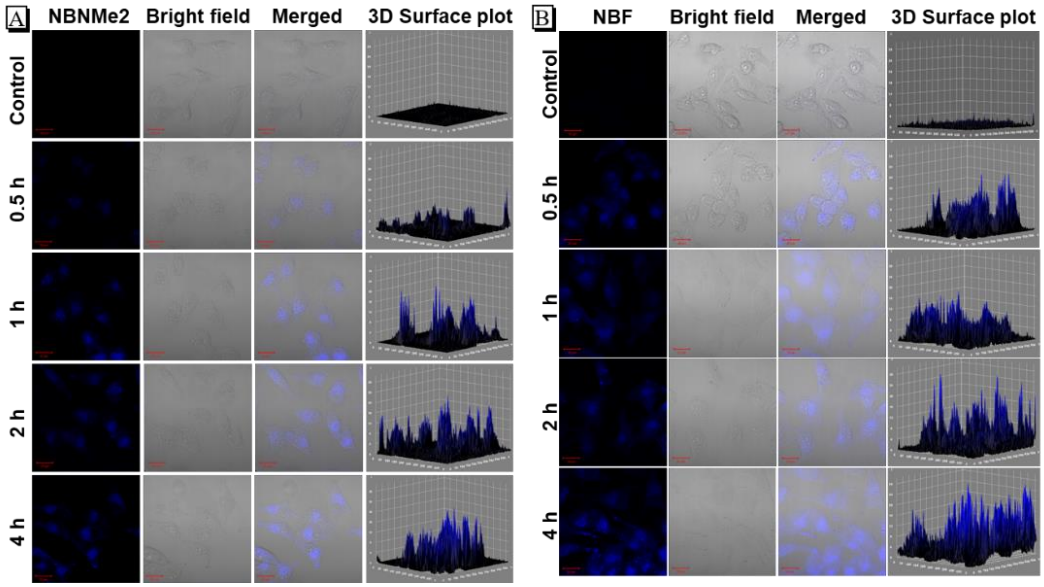


Fig. S14: Time-dependent CLSM images of (A) nanosheet assemblies of NBNMe2 and (B) nanowire conformation of NBF incubated in a HeLa cell for up to 4 hours. The 3D surface plot depicts the regular increment in the fluorescence intensity as a function of more population fluorescence moieties with time.

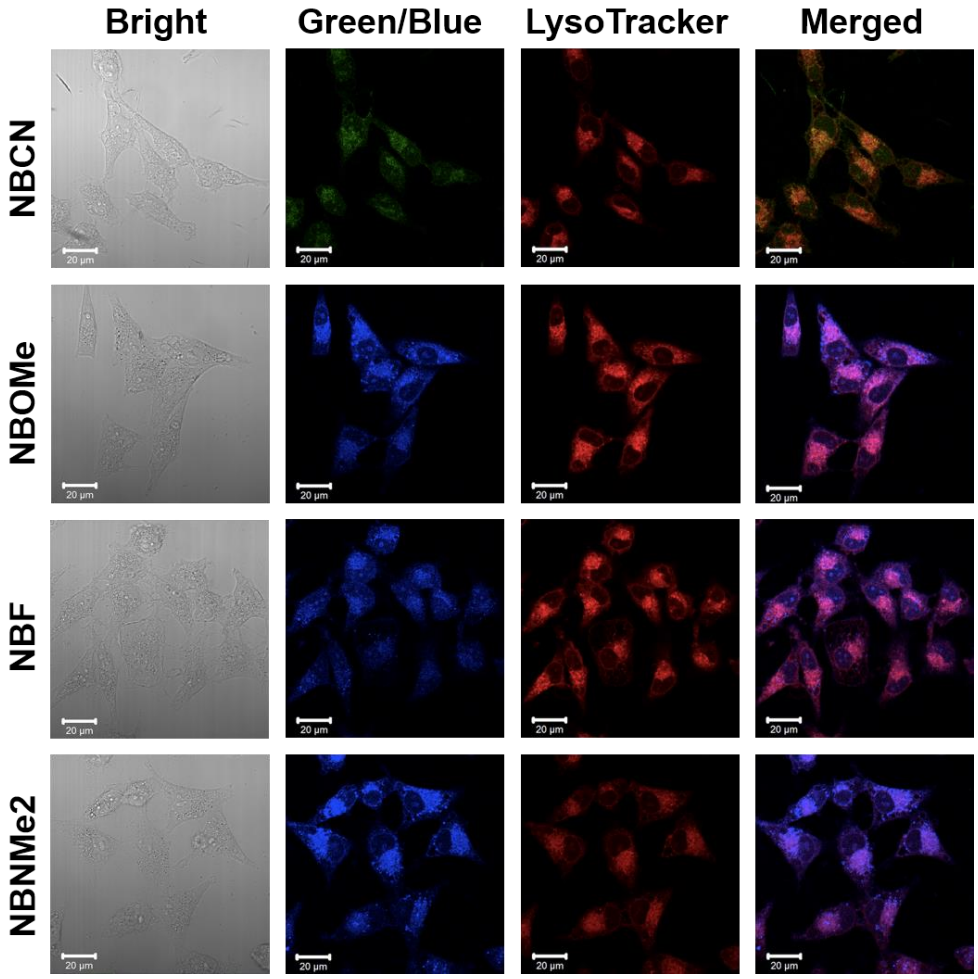


Fig. S15: CLSM images of cellular colocalization in HeLa cells using LysoTracker Deep Red.

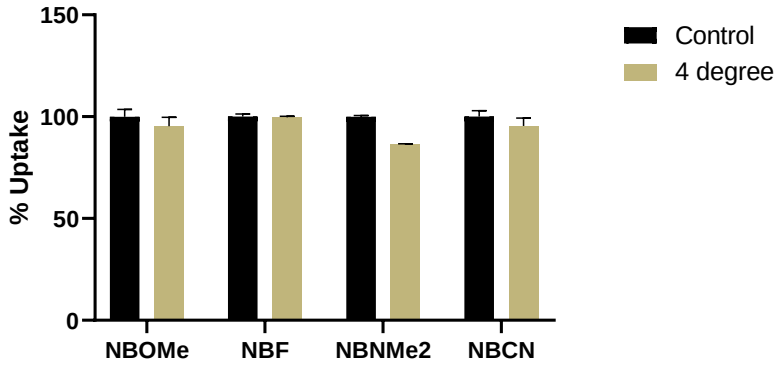
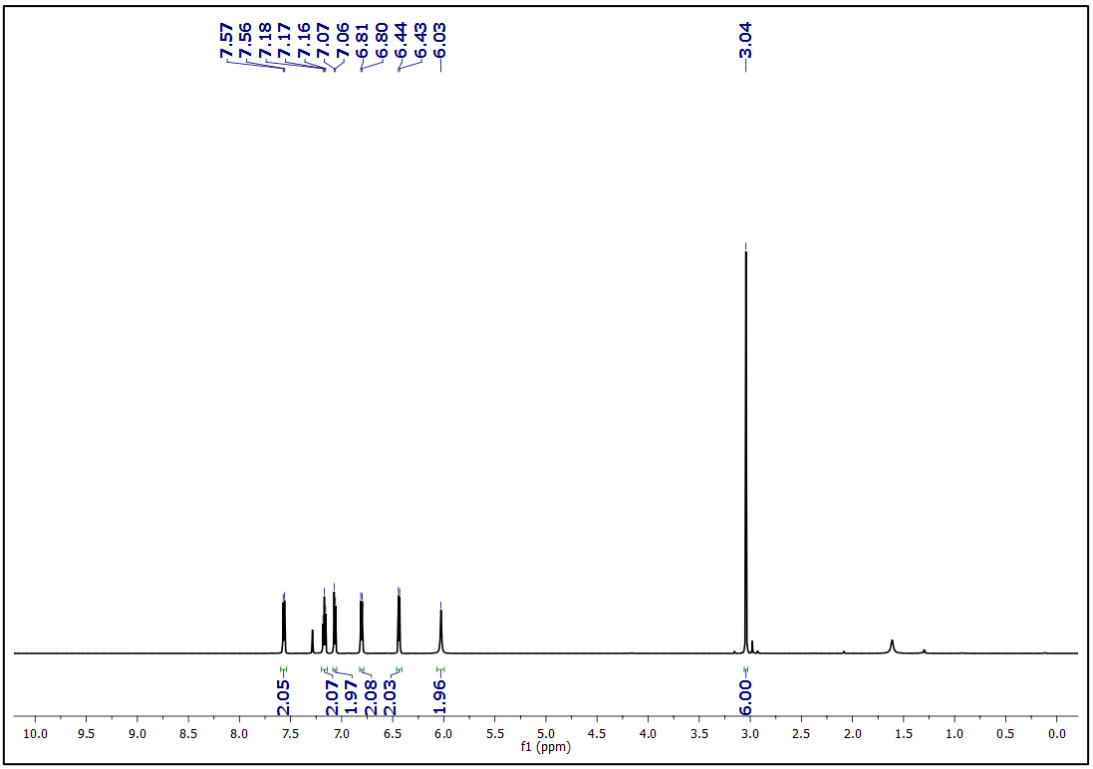
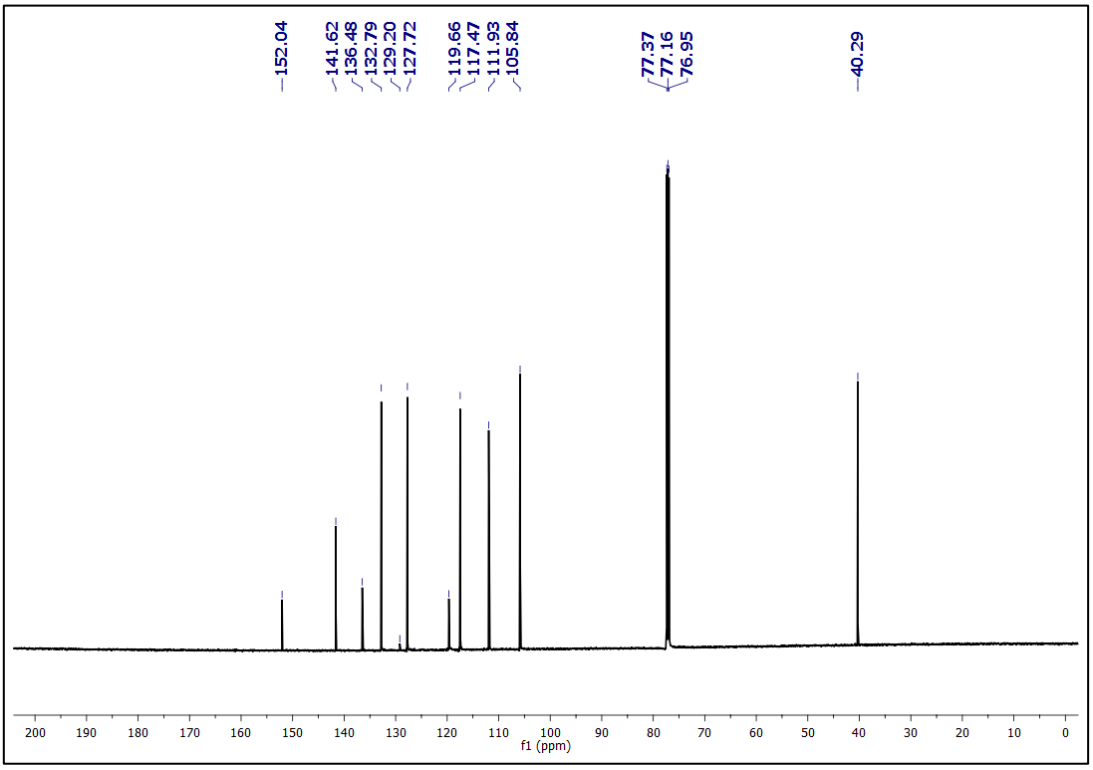


Fig. S16: Percentage of uptake at 4 °C.

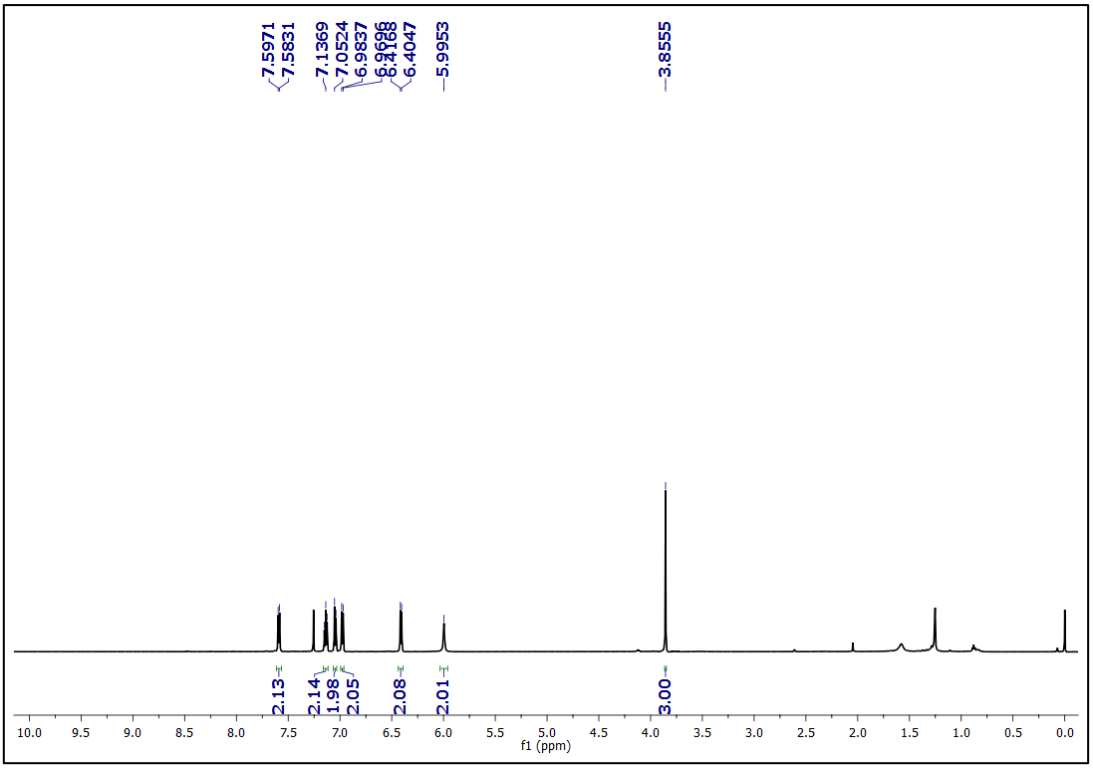
- **^{1}H-NMR, ^{13}C-NMR, and Mass Spectra**



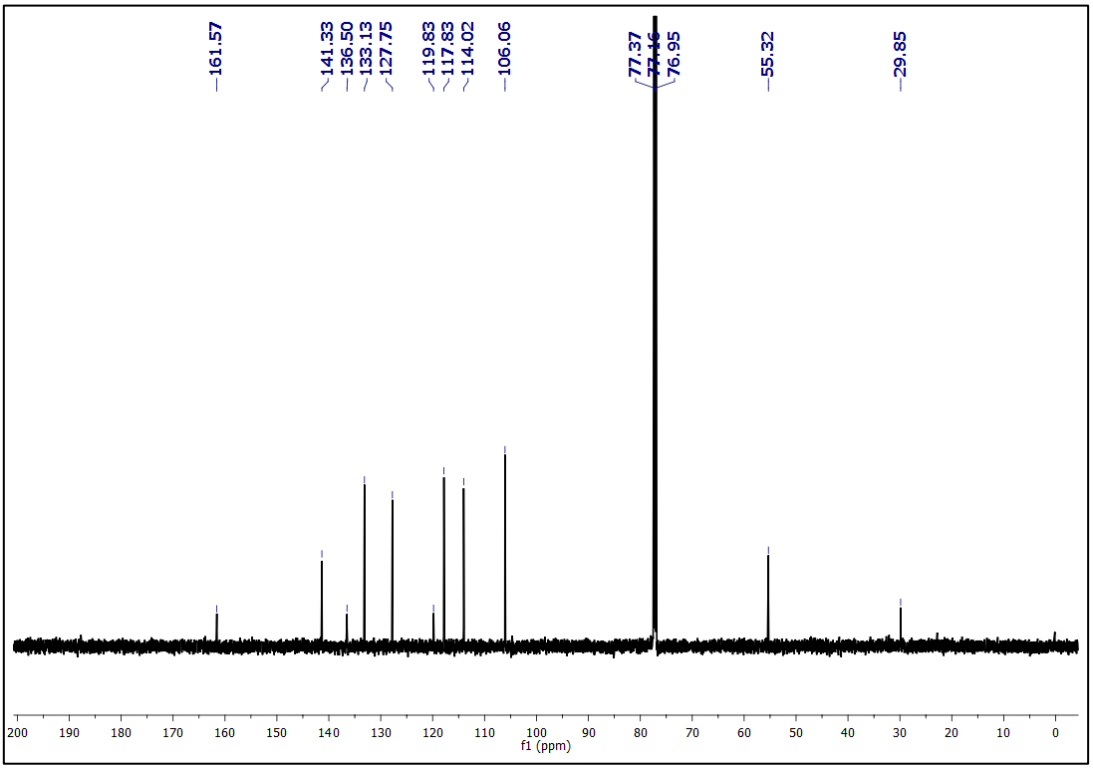
^{1}H-NMR of NBNMe2



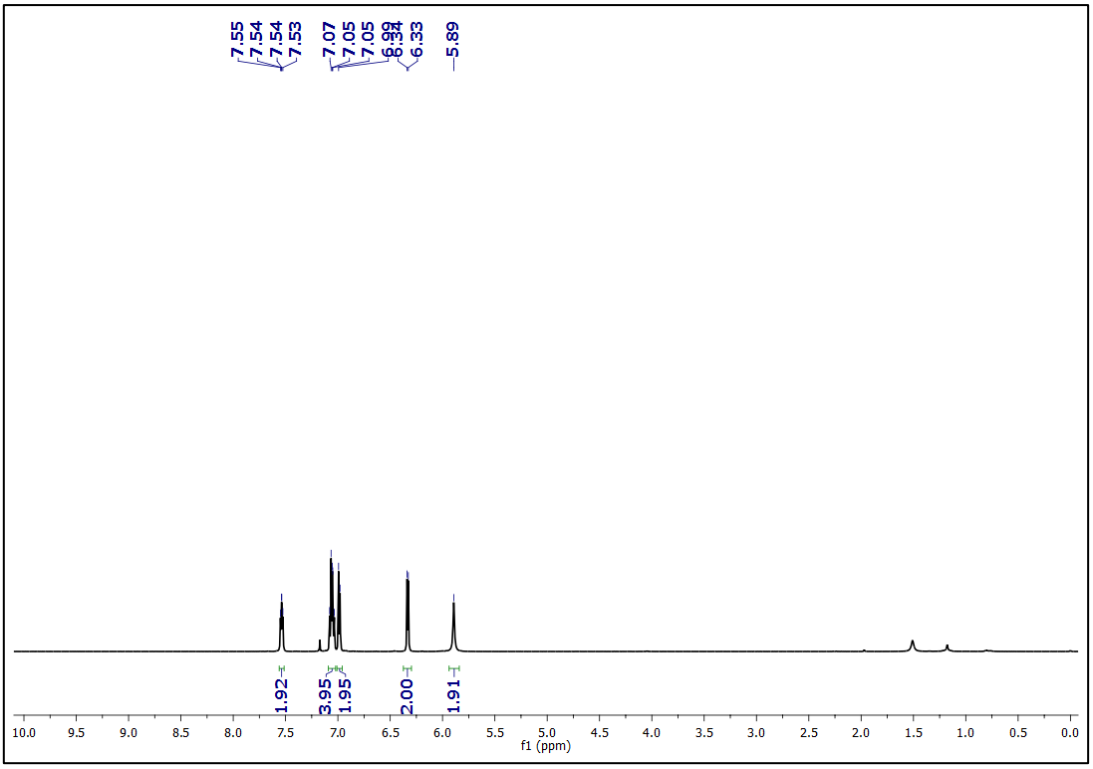
^{13}C-NMR of NBNMe2



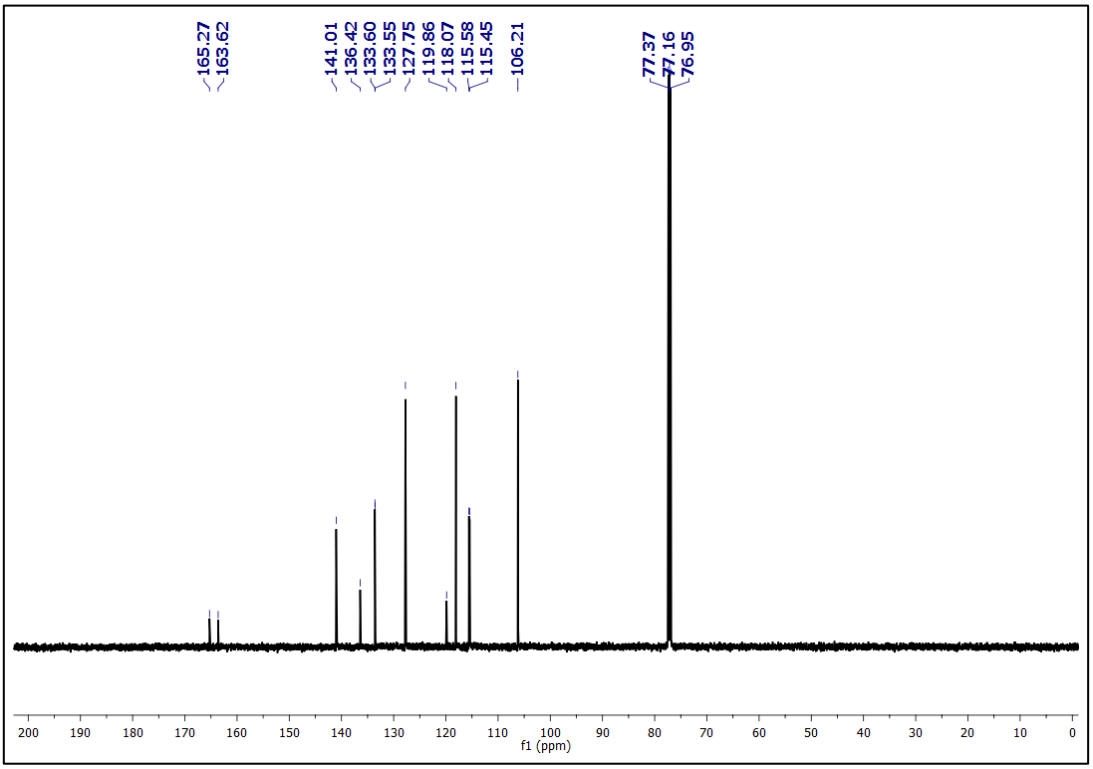
^{1}H-NMR of NBOMe



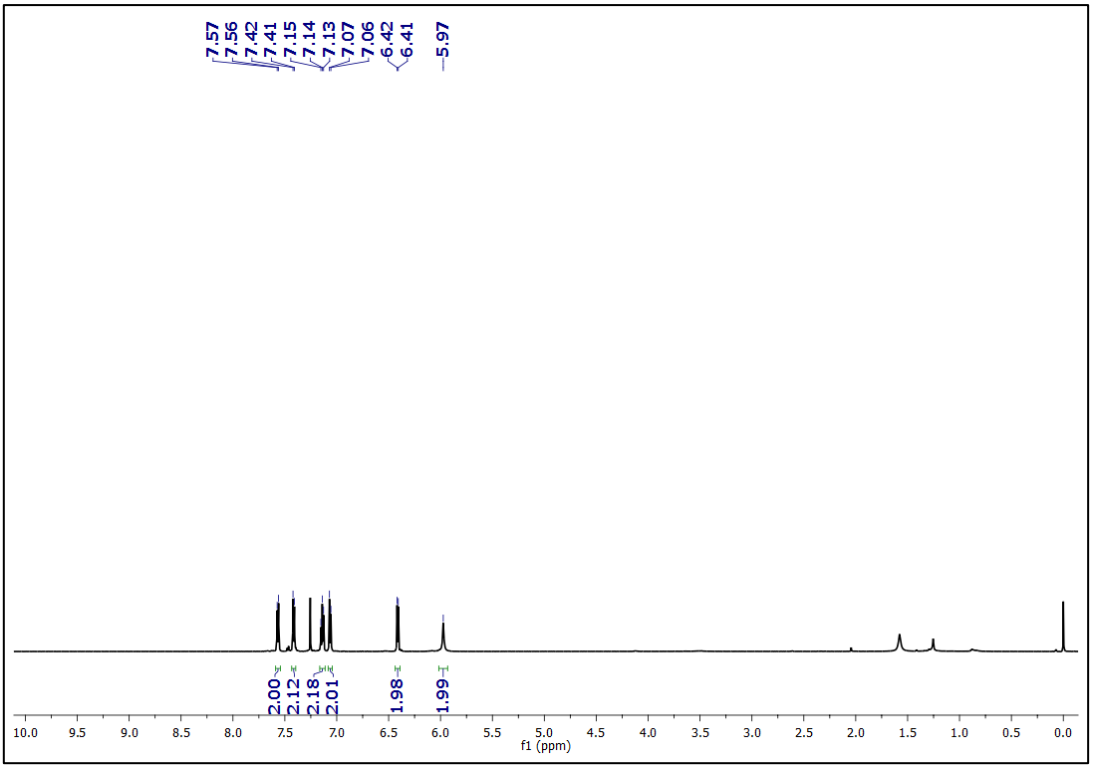
^{13}C-NMR of NBOMe



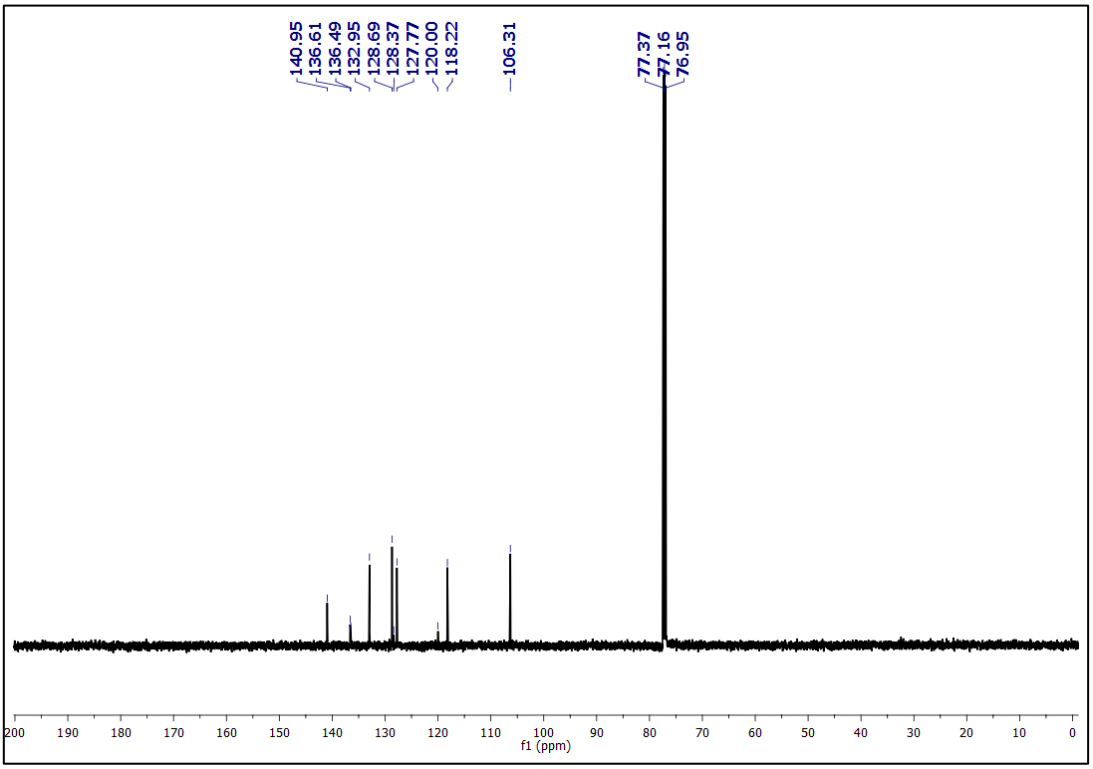
^{1}H-NMR of NBF



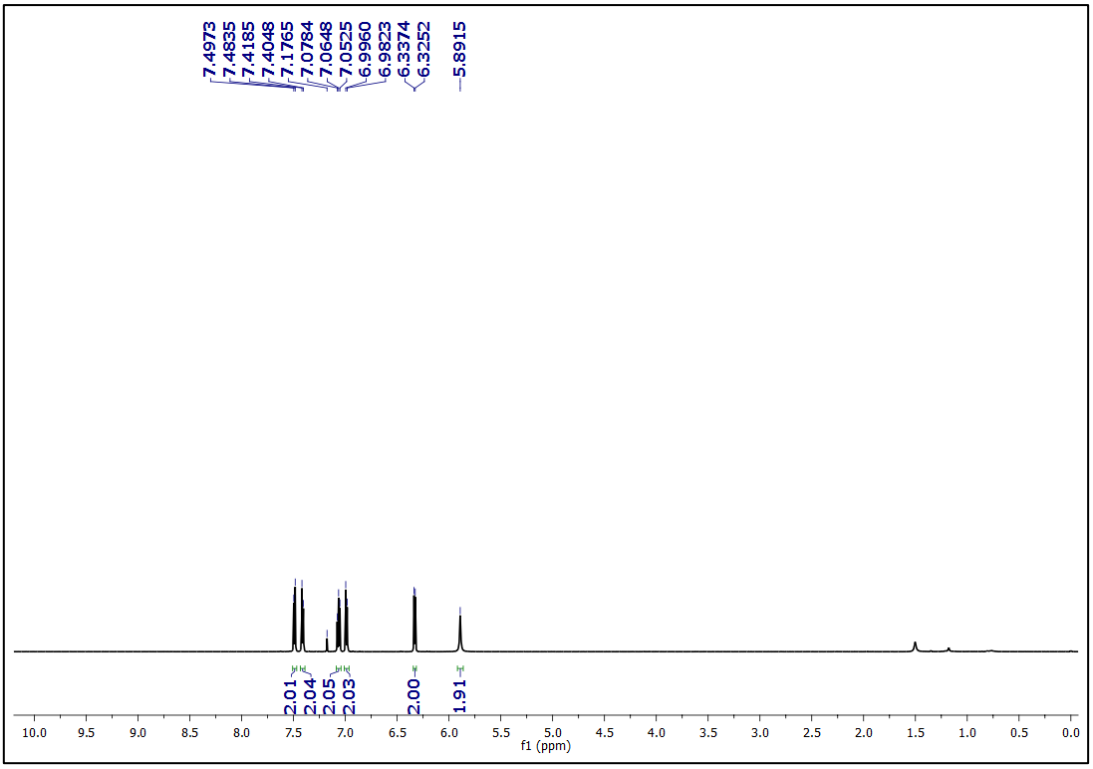
^{13}C-NMR of NBF



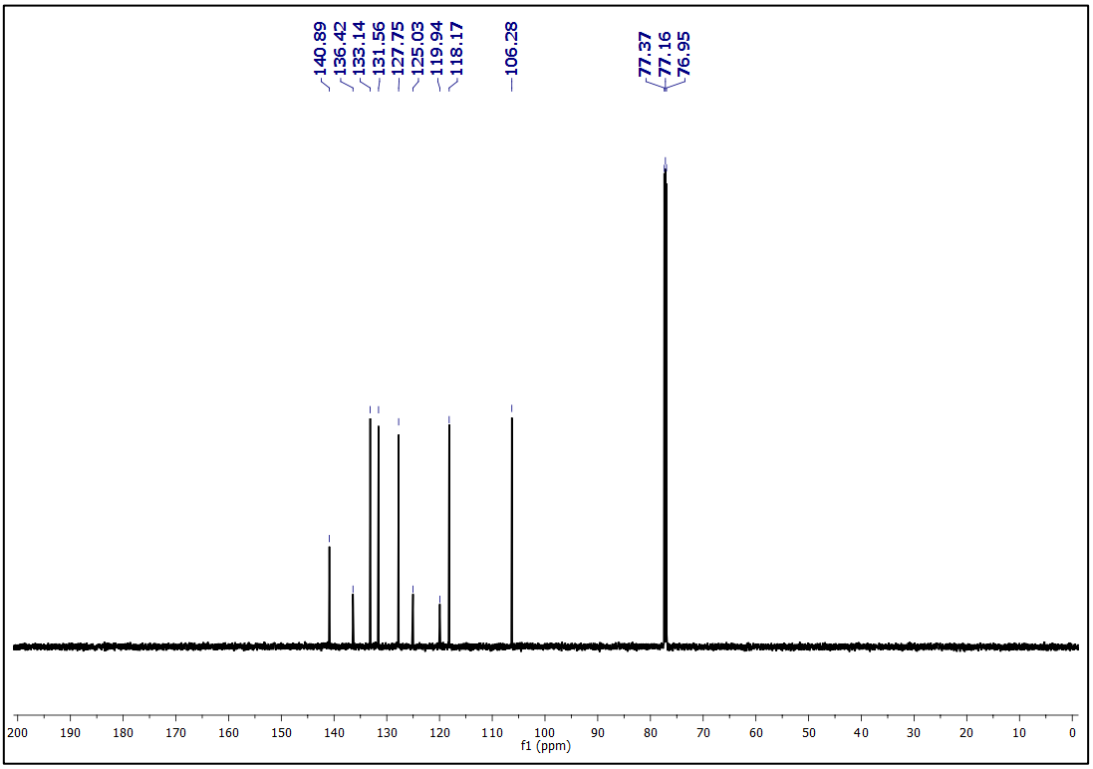
^{1}H-NMR of NBCl



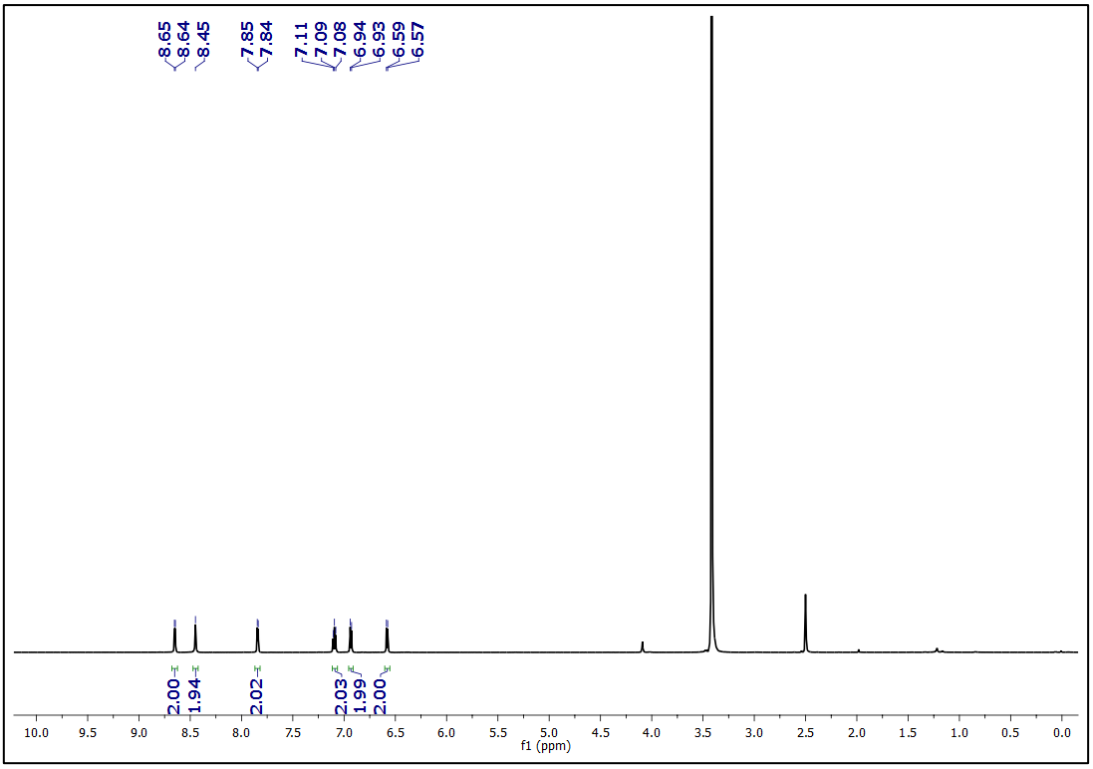
^{13}C-NMR of NBCl



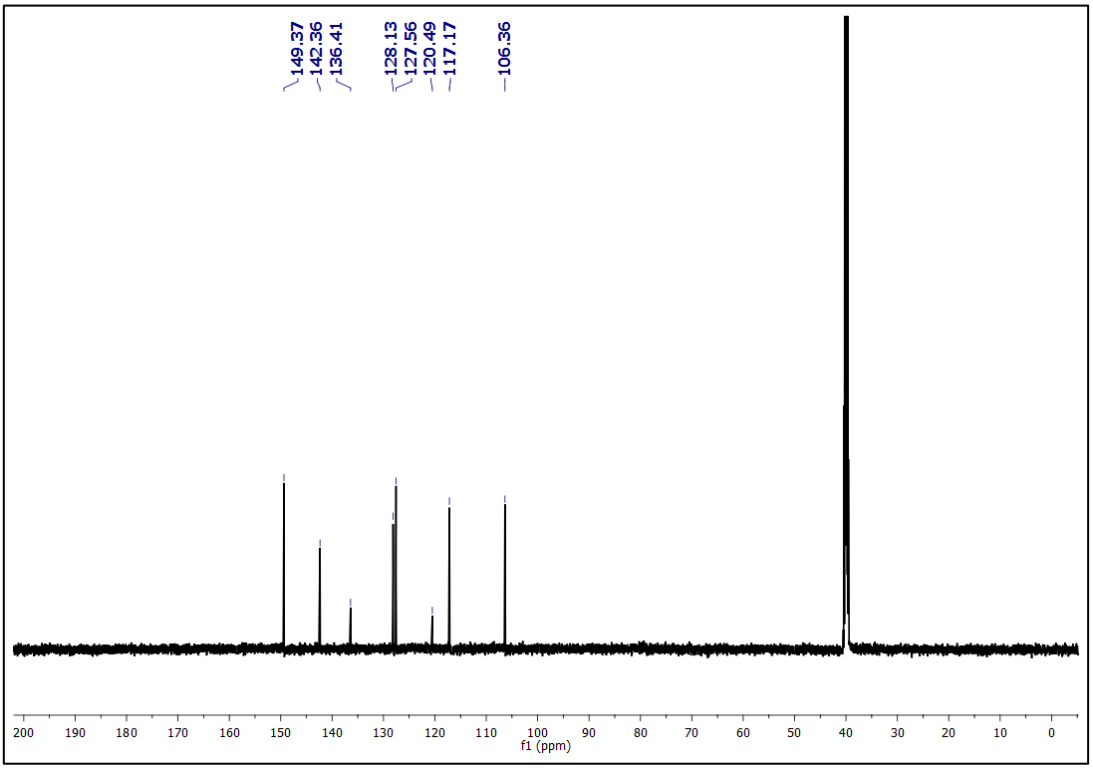
^{1}H-NMR of NBBr



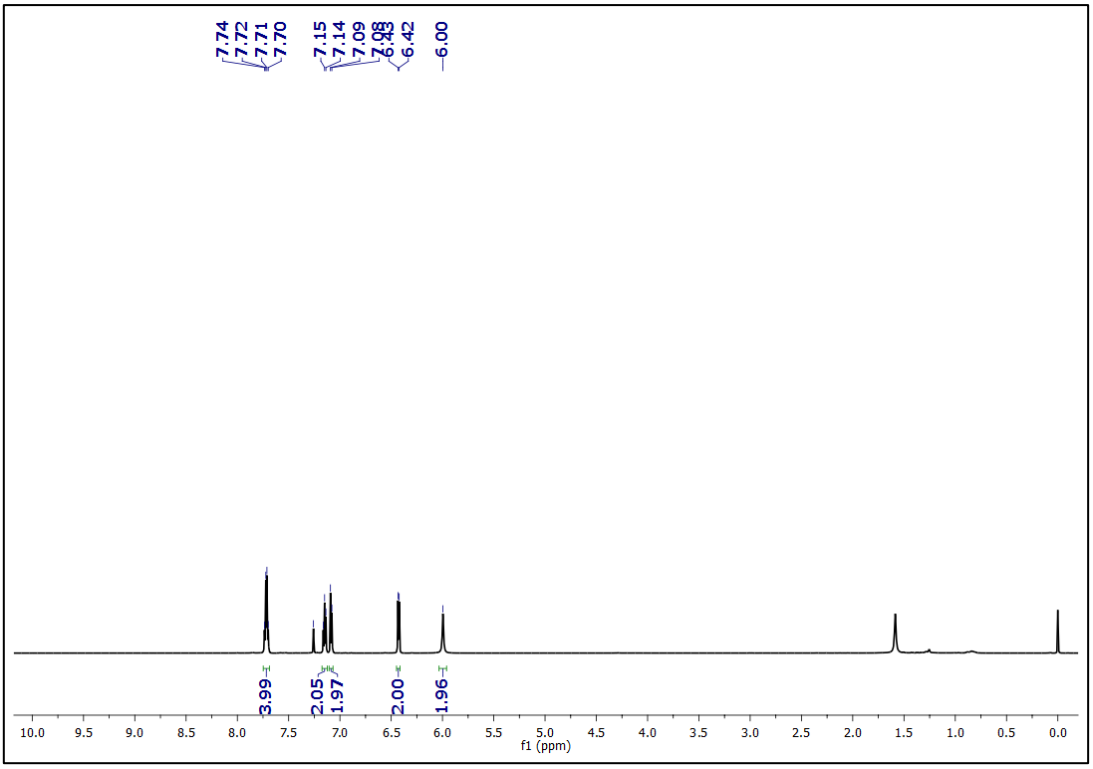
^{13}C-NMR of NBBr



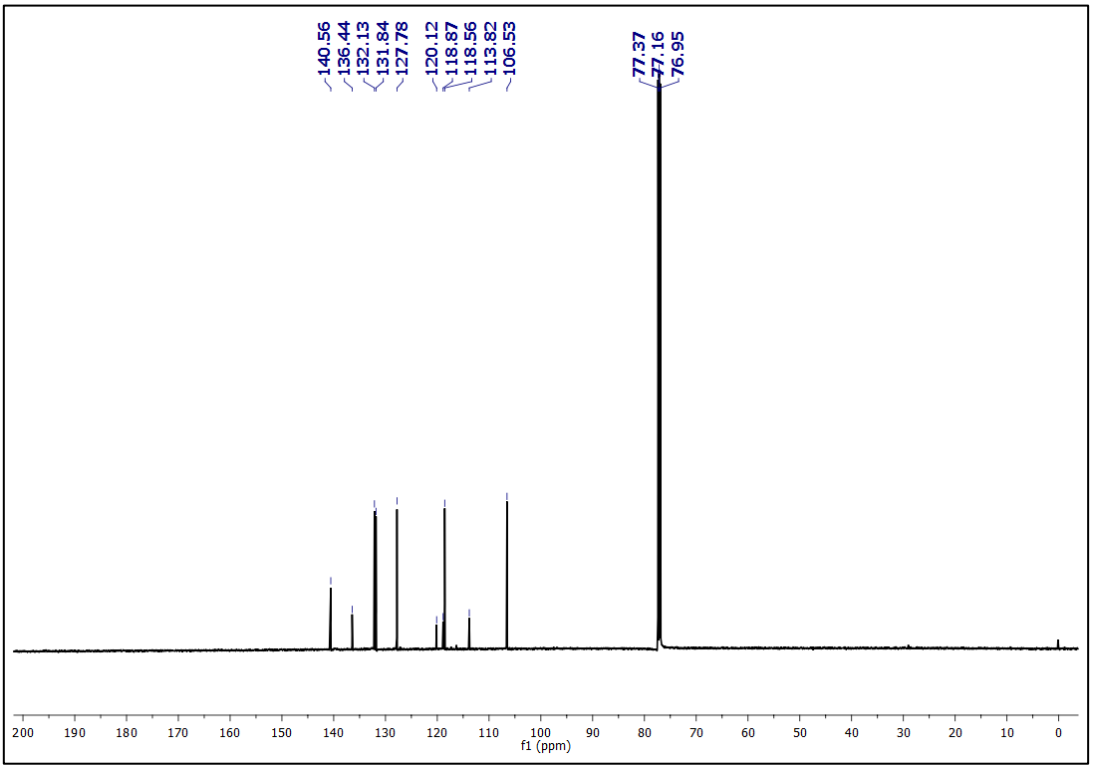
^{1}H-NMR of NBPy



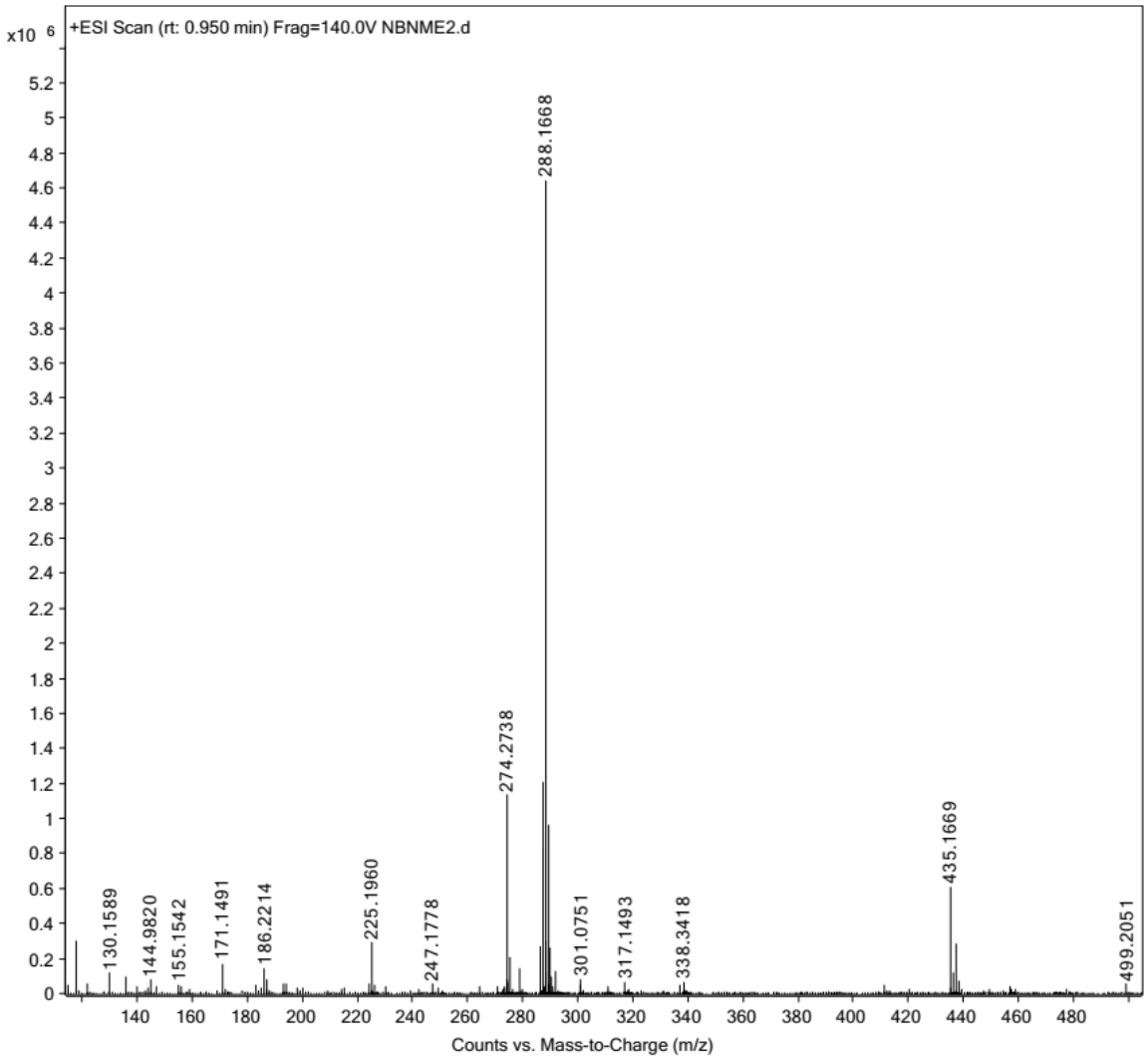
^{13}C-NMR of NBPy



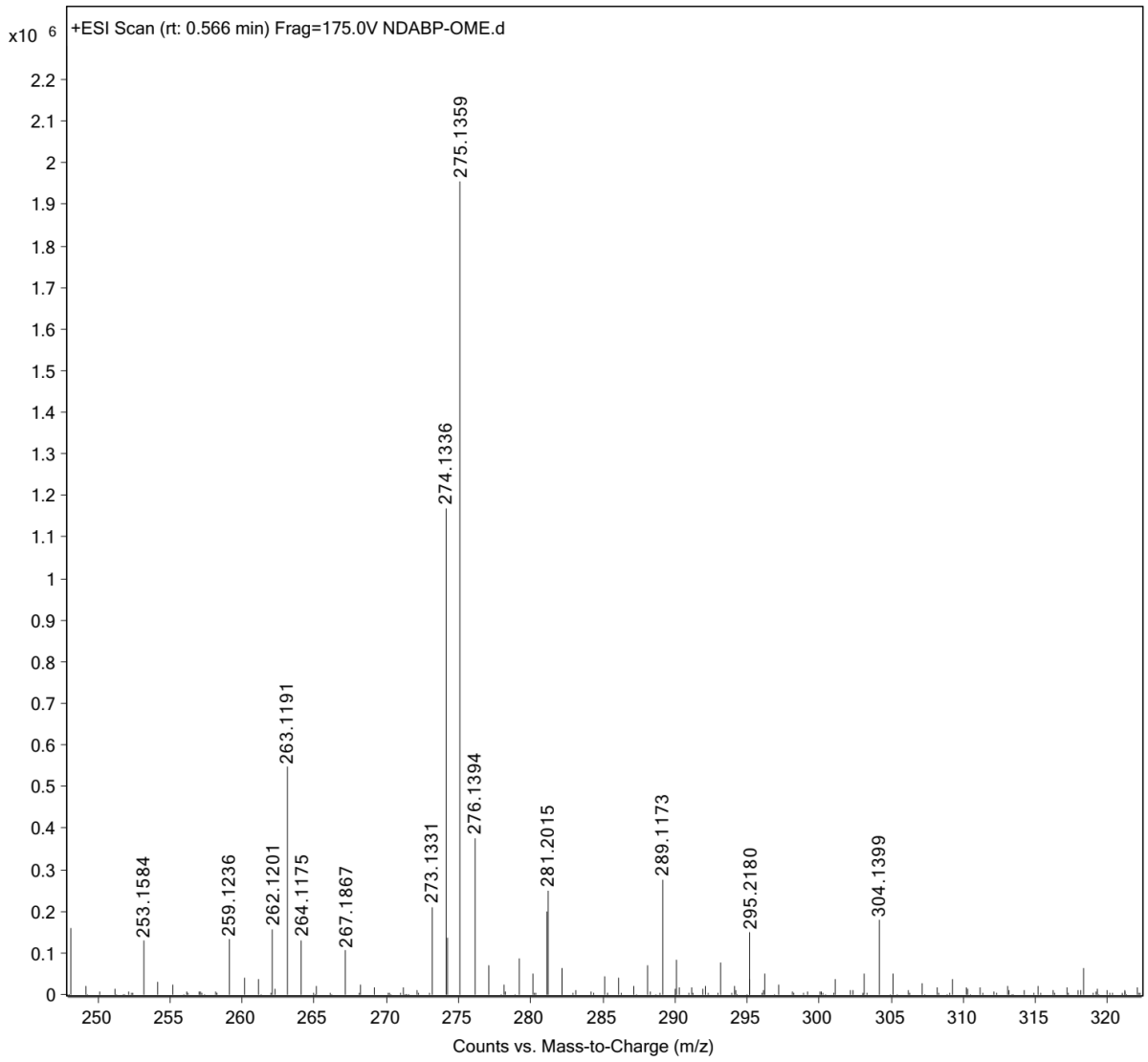
^{1}H-NMR of NBCN



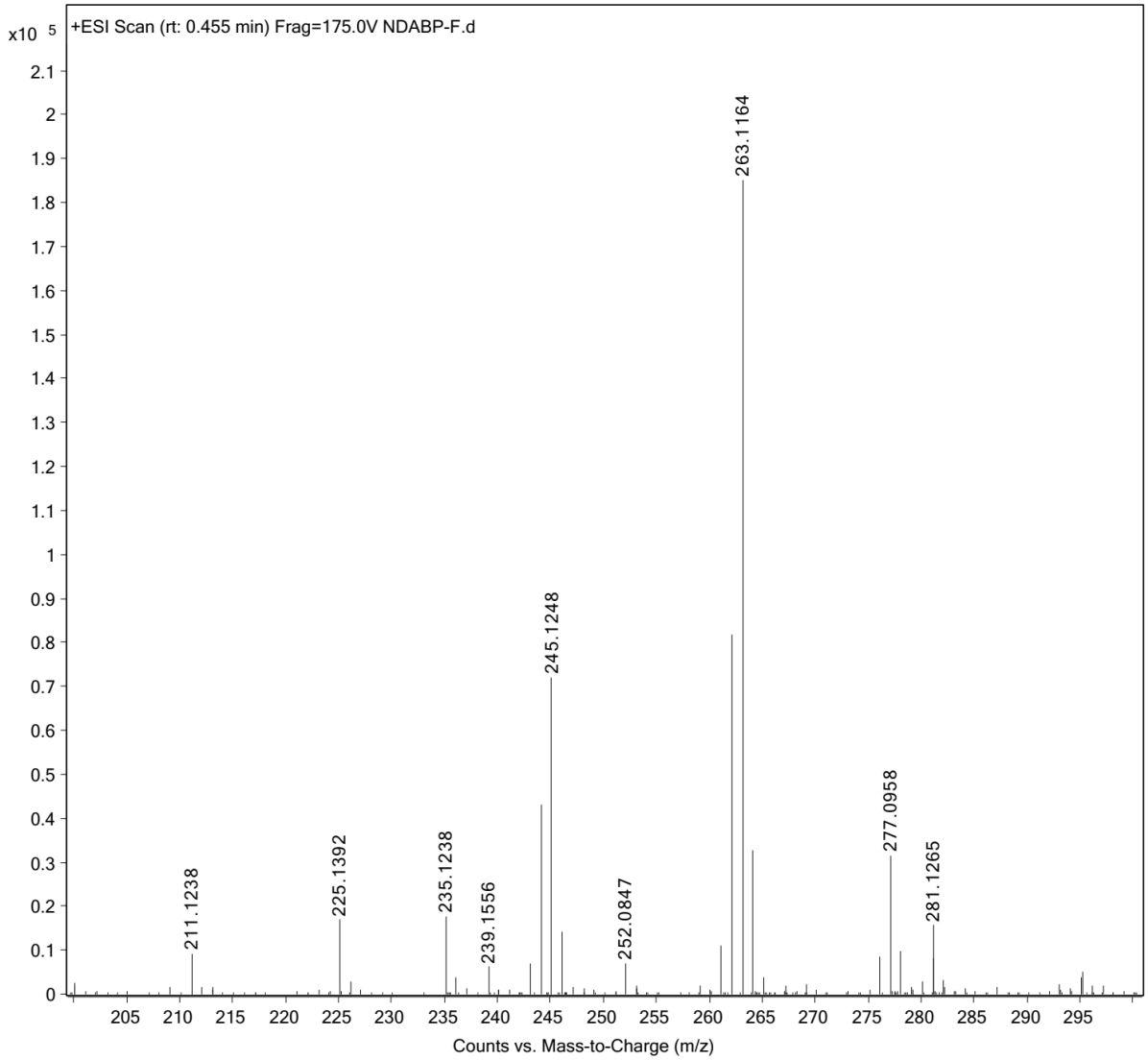
^{13}C-NMR of NBCN



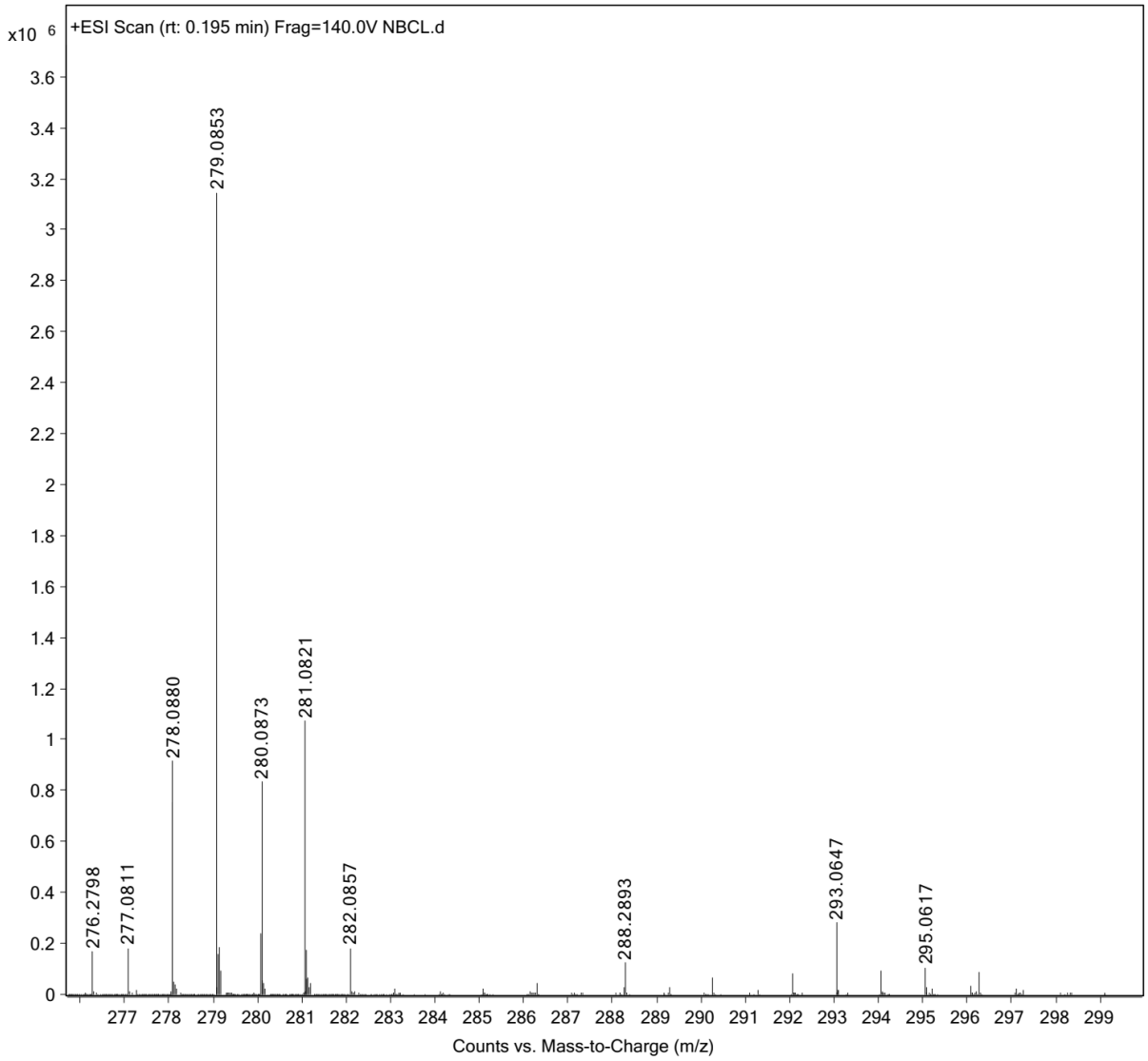
Mass spectrum of NBNMe2



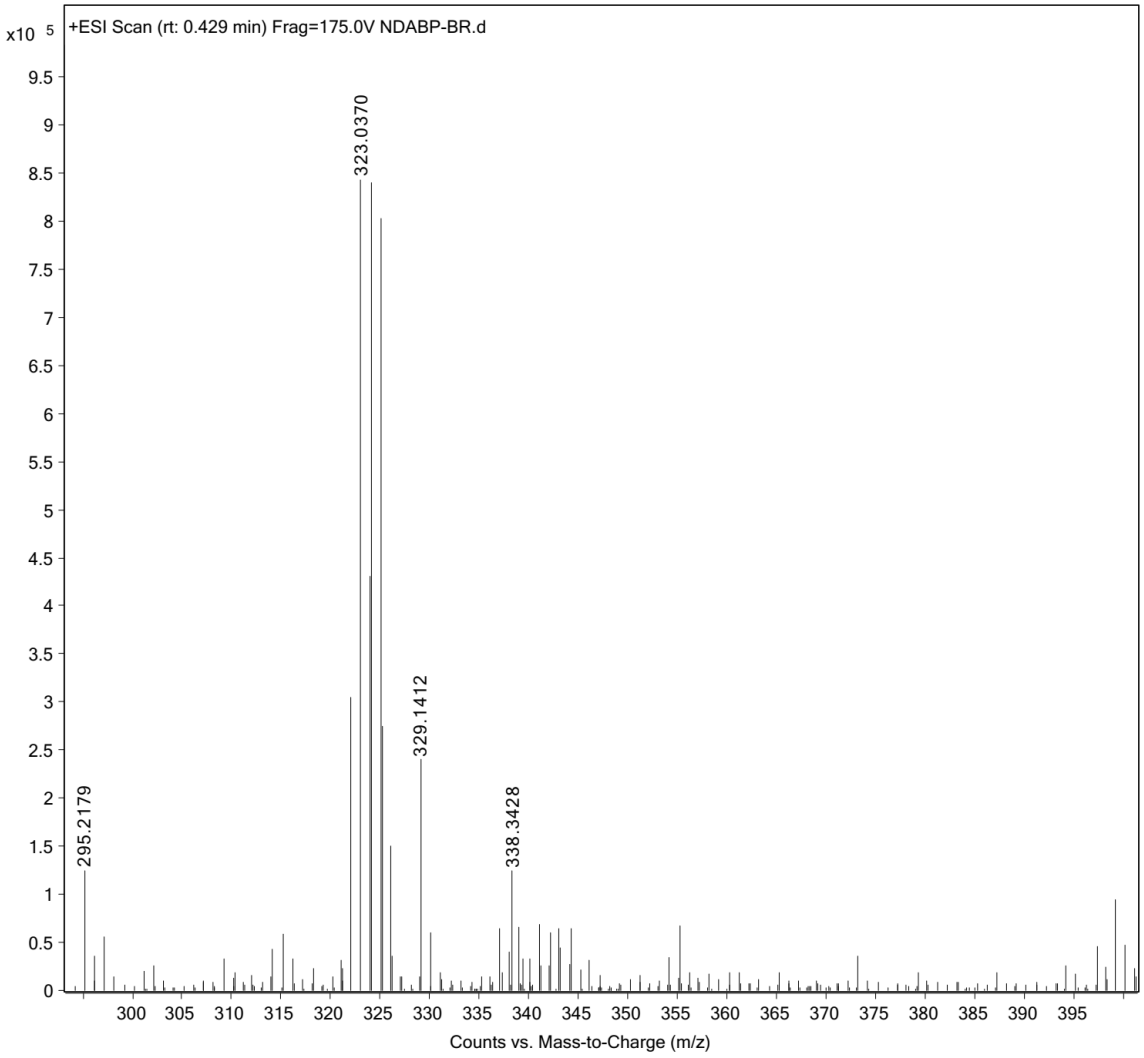
Mass spectrum of NBOMe



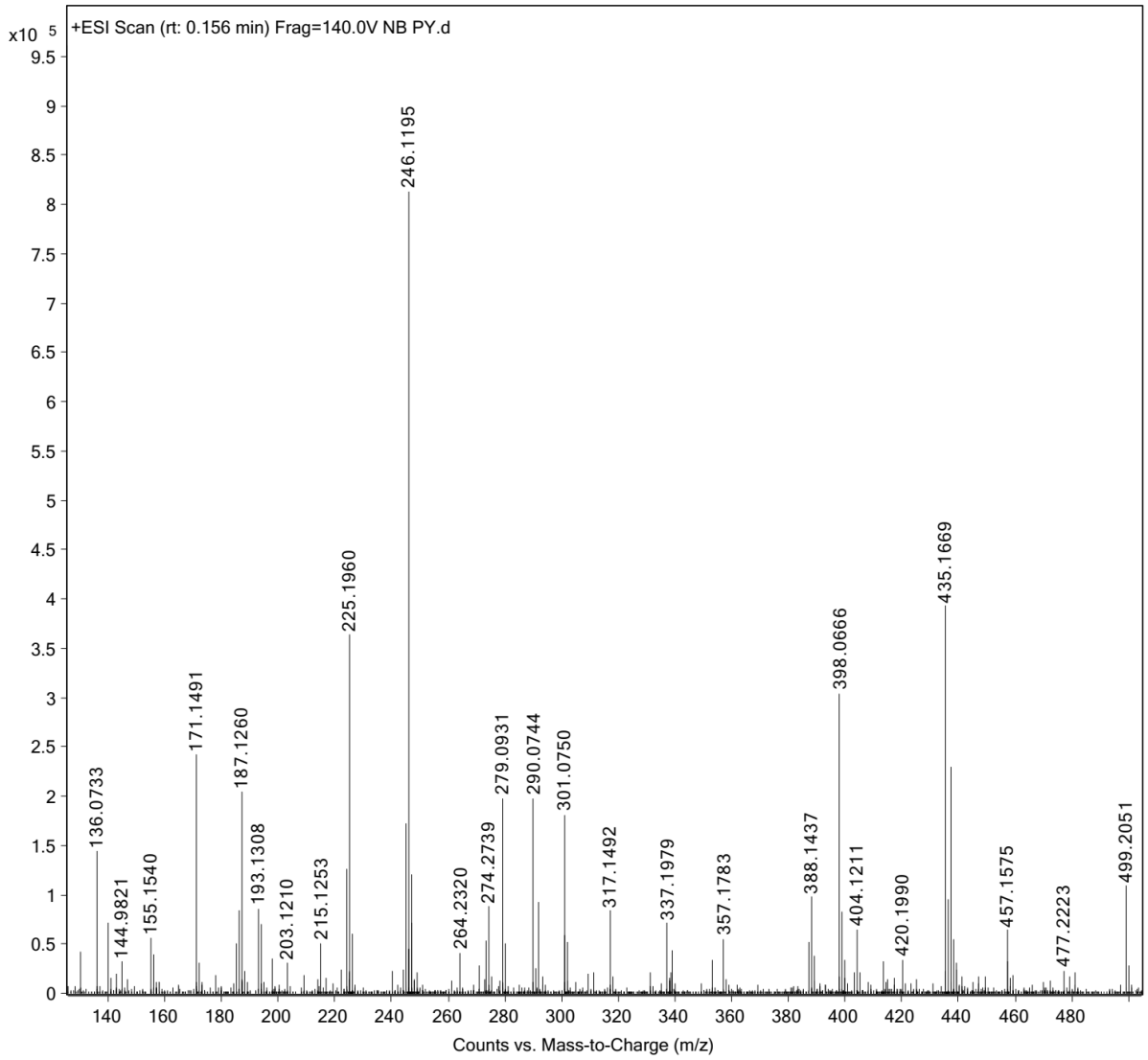
Mass spectrum of NBF



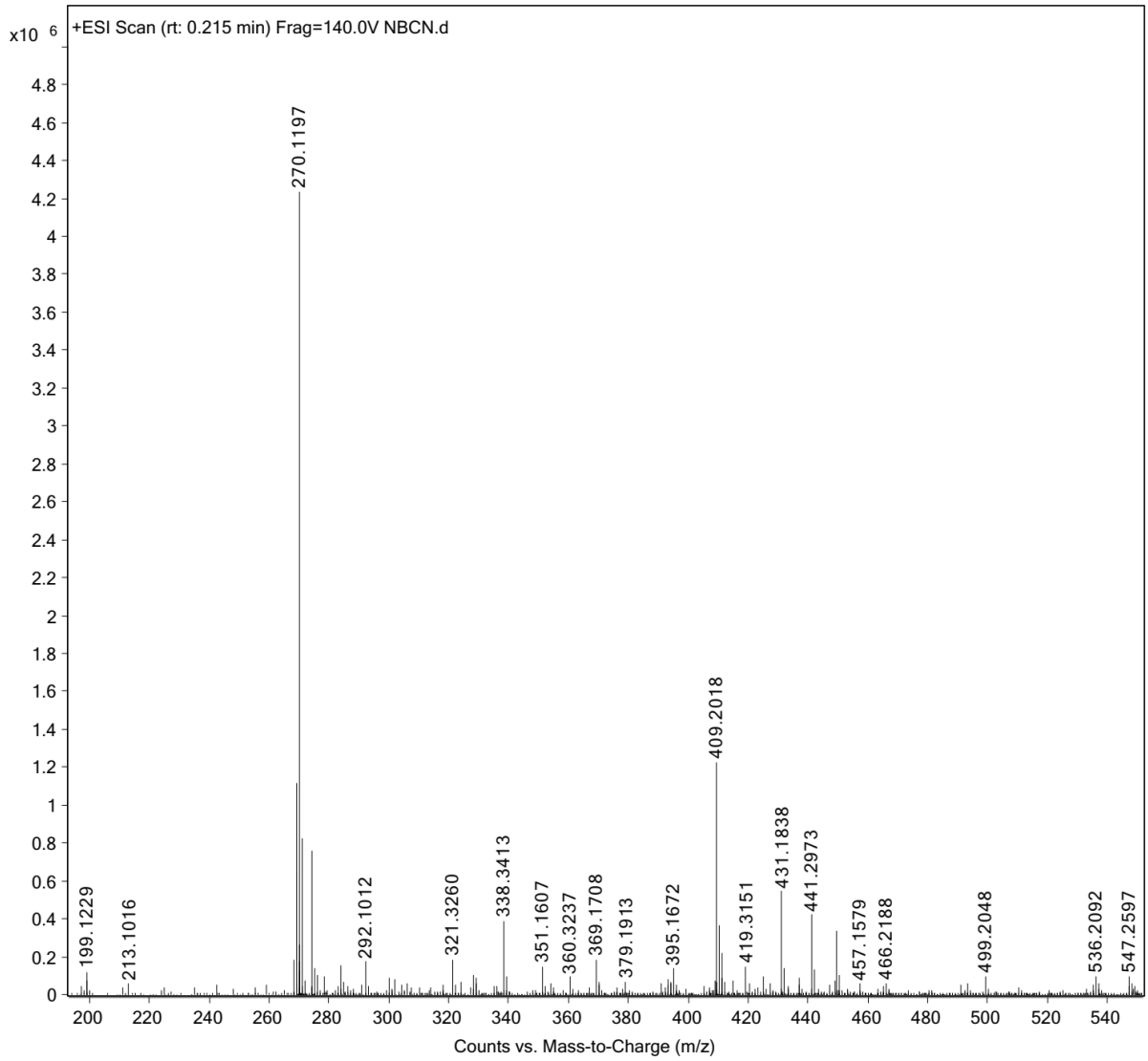
Mass spectrum of NBCl



Mass spectrum of NBBr



Mass spectrum of NBPy



Mass spectrum of NBCN