Supporting Information

for

Unveiling the reactivity of N-heterocyclic methylene hydrazines

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Table of Contents

1. General procedures and instrumentation

All manipulations and experiments were performed in an inert argon atmosphere using standard Schlenk techniques and in an argon-filled MBRAUN glove box. The solvents, especially toluene and THF, were purified by the MBRAUN solvent purification system MB SPS-800 and stored over activated 4 Å molecular sieves before use. All chemicals were purchased from Sigma Aldrich and TCI. $B(C_6F_5)_3$ was freshly sublimized before use. The starting materials **1** and **2** were synthesized using a literature procedure recently reported by our group.[1] Deuterated NMR solvents, benzene-d_6 and $CDCl_3$ were stored over 4 Å molecular sieves at least 48 h before use. The ^{1}H, ^{13}C, and ^{11}B NMR spectra were recorded in a Bruker Avance DPX 400 and Bruker Avance DPX 500 spectrometer. Chemical shifts (δ) are given in ppm. NMR spectra were referenced to external $SiMe_4$ (^{1}H and ^{13}C) and $BF_3{\cdot}OEt_2$ (^{11}B). High-resolution mass spectra (HRMS) were obtained using a Q Exactive Thermo Scientific.

2. Experimental section with spectroscopic evidences

Synthesis of 3: 1 (0.100 g, 0.45 mmol) was dissolved in 10 mL toluene or THF in a Schlenk flask. After that, 4 M HCl in dioxane (0.12 mL, 0.50 mmol) was added to it at room temperature. The reaction was run for 12 hours. Completely removed all volatiles to give a white solid, followed by a hexane wash. Decanted the hexane part and completely dried the residue to obtain pure product, **3** in 95% yield. Suitable crystals for XRD analysis were grown by slow evaporation of a DCM-hexane mixture at room temperature.

^{1}H NMR (400 MHz, 298 K, $CDCl_3$): δ = 1.68 (singlet, 18 H, $C(C\boldsymbol{H}_3)_3$), 6.38 (d, 1 H, $NNC\boldsymbol{H}_2$), 7.16 (singlet, 2 H, $NC\boldsymbol{H}C\boldsymbol{H}N$), 7.58 (d, 1 H, $NNC\boldsymbol{H}_2$), 11.83 ($N^{+}\boldsymbol{H}$) ppm.

$^{13}C\{^{1}H\}$ NMR (125.7 MHz, 298 K, $CDCl_3$): δ= 30.4 ($C(\boldsymbol{C}H_3)_3$, 62.7 ($\boldsymbol{C}(CH_3)_3$, 117.3 ($N\boldsymbol{C}H\boldsymbol{C}HN$),133.6 ($CNN\boldsymbol{C}H_2$), 141.5 ($\boldsymbol{C}NNCH_2$) ppm.

HRMS: m/z calcd for $[M]^{+}[Cl]^{-}$ $C_{12}H_{23}ClN_4$, 258.1611; found **223.1917** for $C_{12}H_{23}N_4^{+}$.

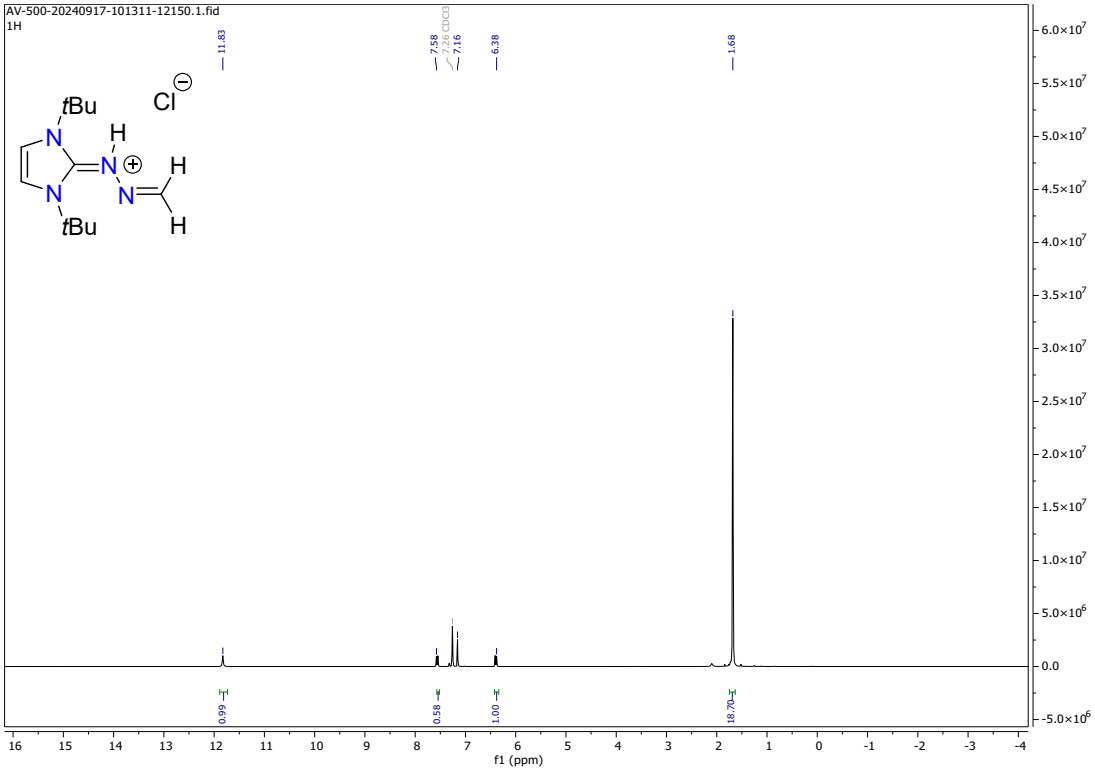

Figure S1: ^{1}H NMR spectrum of **3**

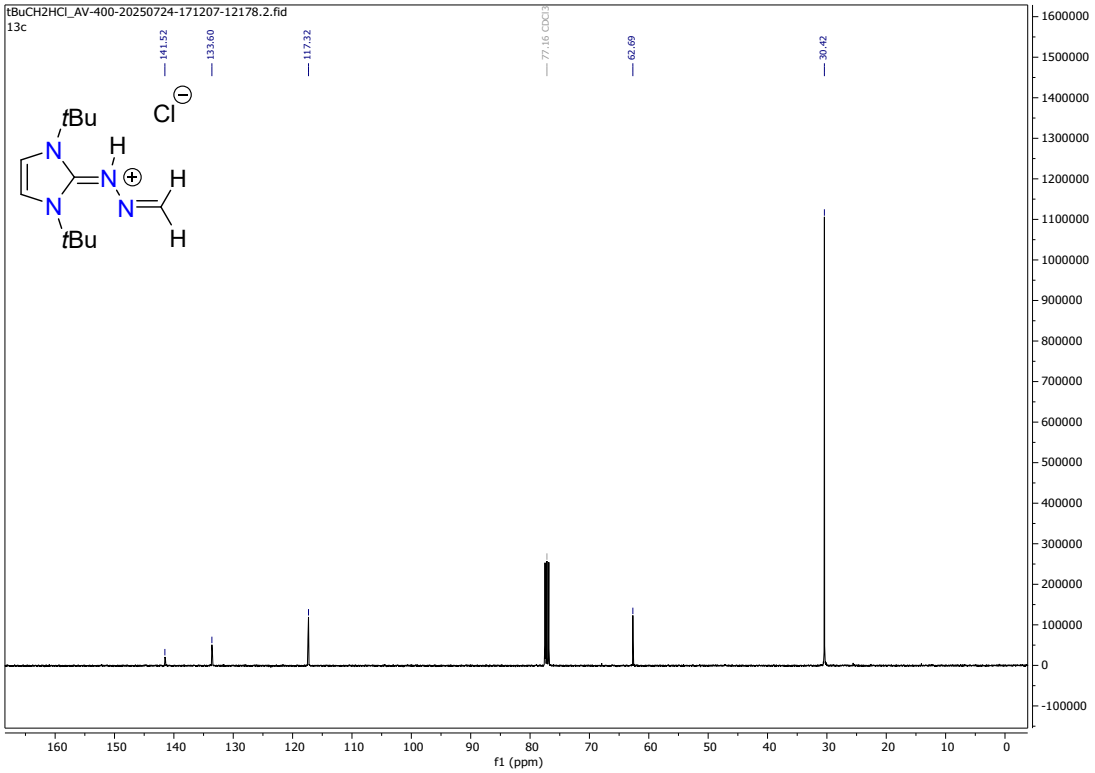

Figure S2: ^{13}C{^{1}H} NMR spectrum of **3**

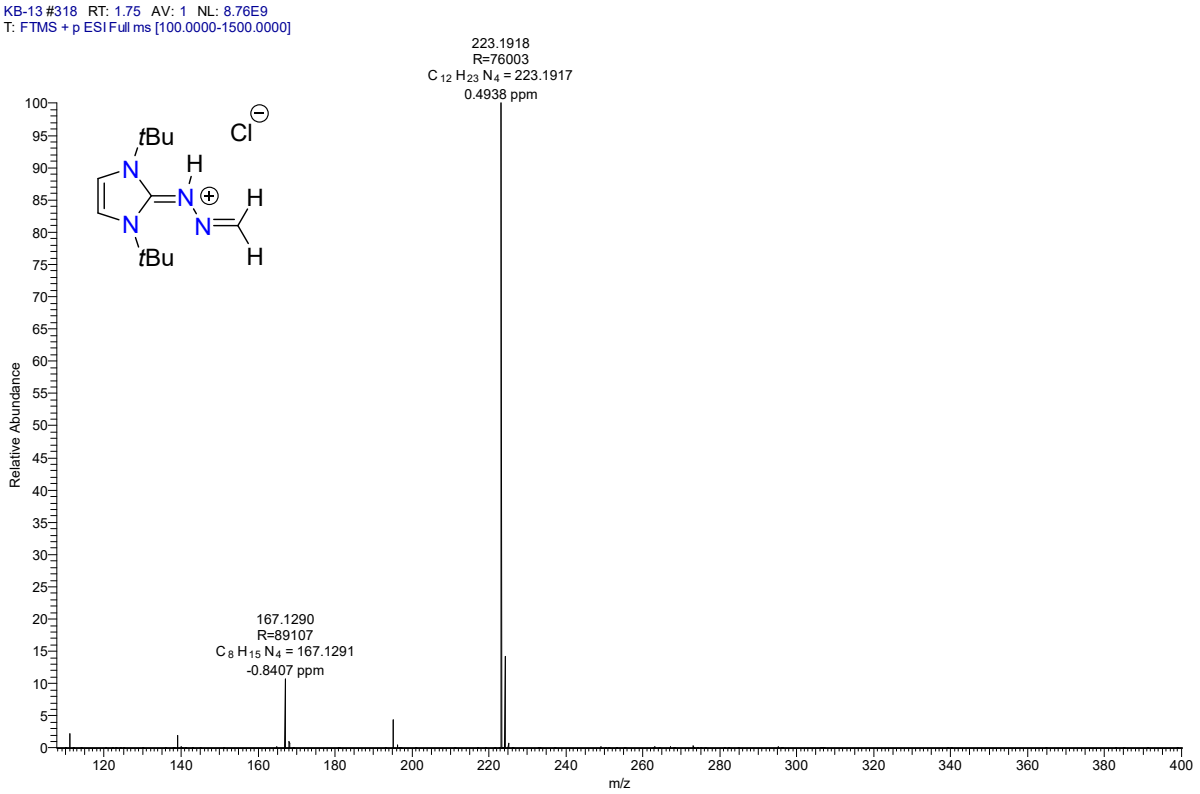

Figure S3: HRMS spectrum of **3**

Synthesis of 4: 1 (0.100 g, 0.45 mmol) and $B(C_6F_5)_3$ (0.241 g, 0.47 mmol) were taken together in a Schlenk flask and dissolved in 15 mL of toluene at room temperature and stirred for 24 hours with no change in color. After that, all the volatiles were completely removed and dissolved again in 10 mL of toluene, and the solution was filtered using a cannula. Concentrated the solution to supersaturation yielded the green-colored needle-shaped crystals after a week in 28% yield.

^{1}H NMR (400 MHz, 298 K, C_6D_6): δ = 1.01 (singlet, 18 H, C(C***H***$_3$)$_3$), 4.86 (d, 1 H, NNC***H***$_2$), 6.13 (d, 1 H, NNC***H***$_2$), 6.32 (d, 1 H, NNC***H***$_2$) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, C_6D_6): δ= 28.0 (C(***C***H$_3$)$_3$, 59.9 (***C***(CH$_3$)$_3$, 114.9 (N***C***H***C***HN),122.7 (CNN***C***H$_2$), 136.5 (Ar-C), 139.0 (Ar-C), 147.7(Ar-C), 148.3 (Ar-C), 150.0 (***C***NNCH$_2$) ppm.

^{11}B{^{1}H} NMR (400 MHz, 298 K, C_6D_6): -3.57 ppm.

HRMS: m/z calcd $C_{30}H_{23}BF_{15}N_4$, 735.1776; found **735.1776**.

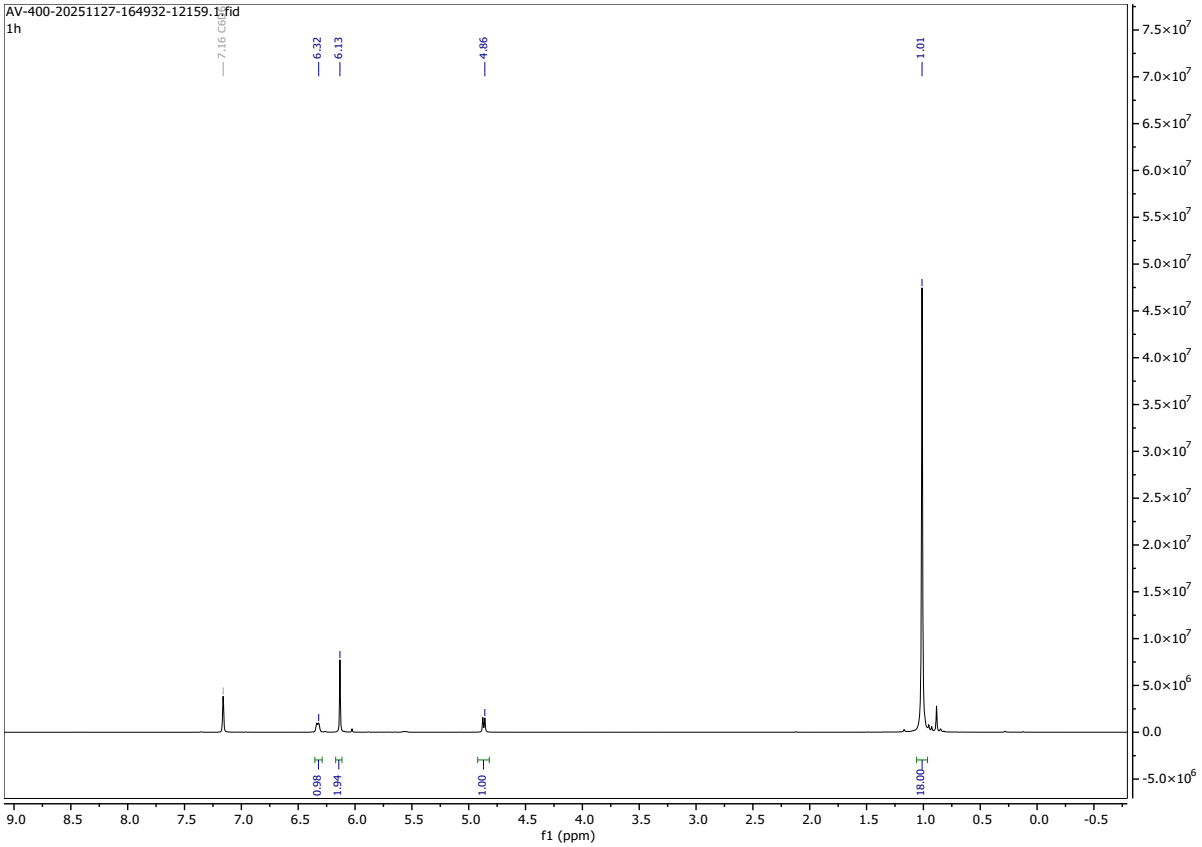

Figure S4: ^{1}H NMR spectrum of **4**

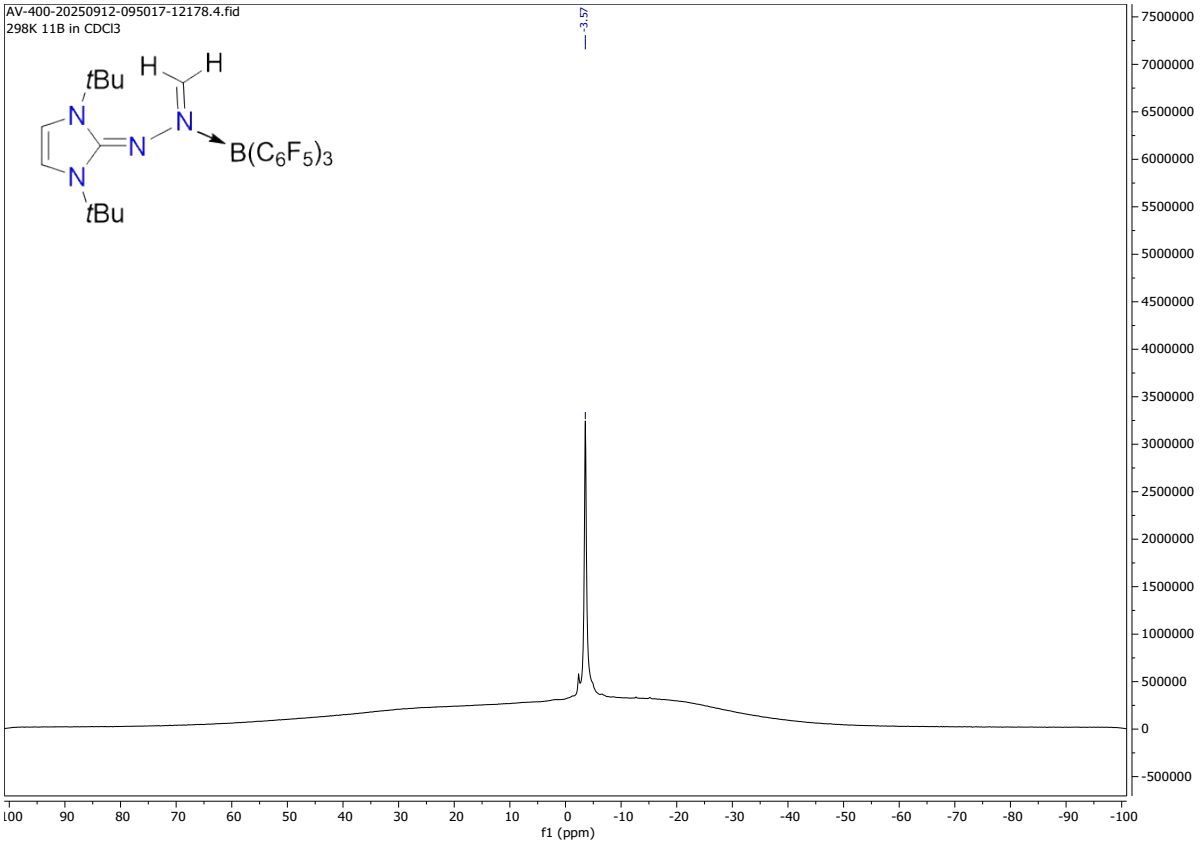

Figure S5: $^{11}B\{^{1}H\}$ NMR spectrum of **4**

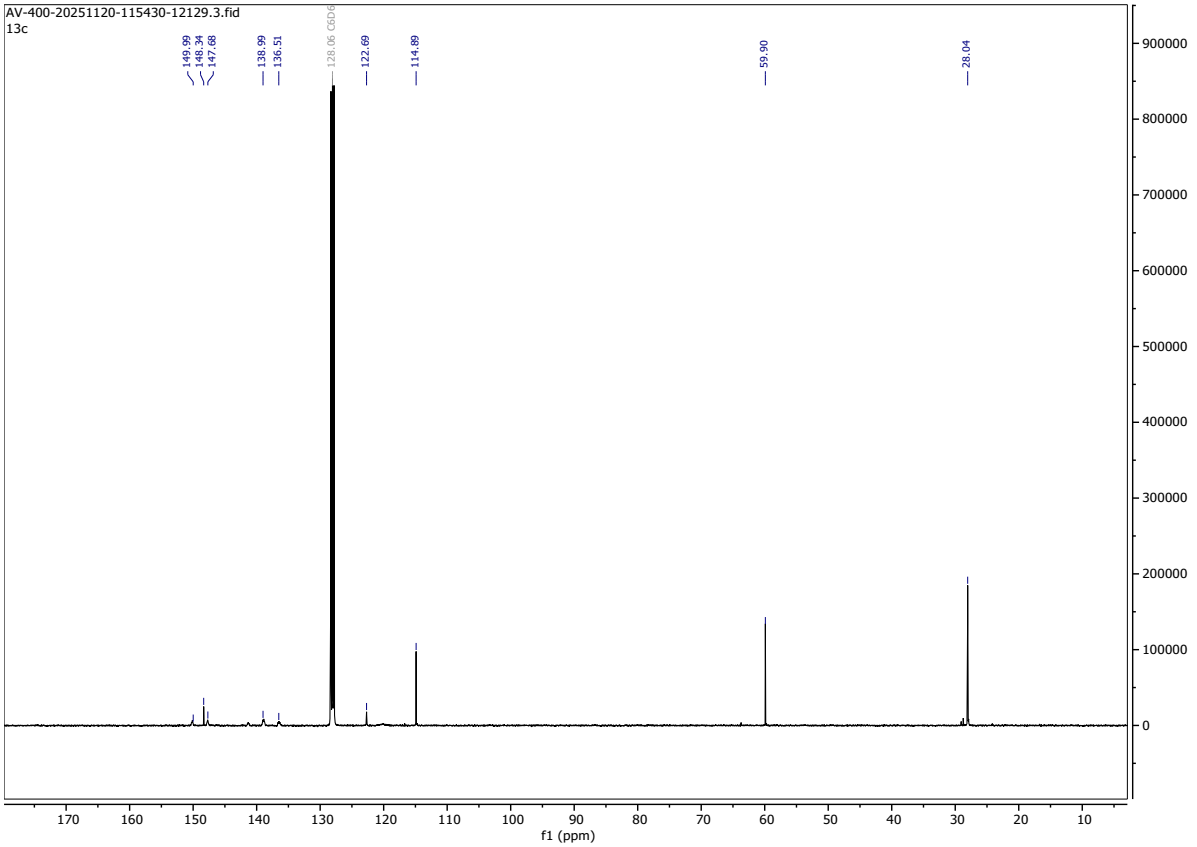

Figure S6: $^{13}C\{^{1}H\}$ NMR spectrum of **4**

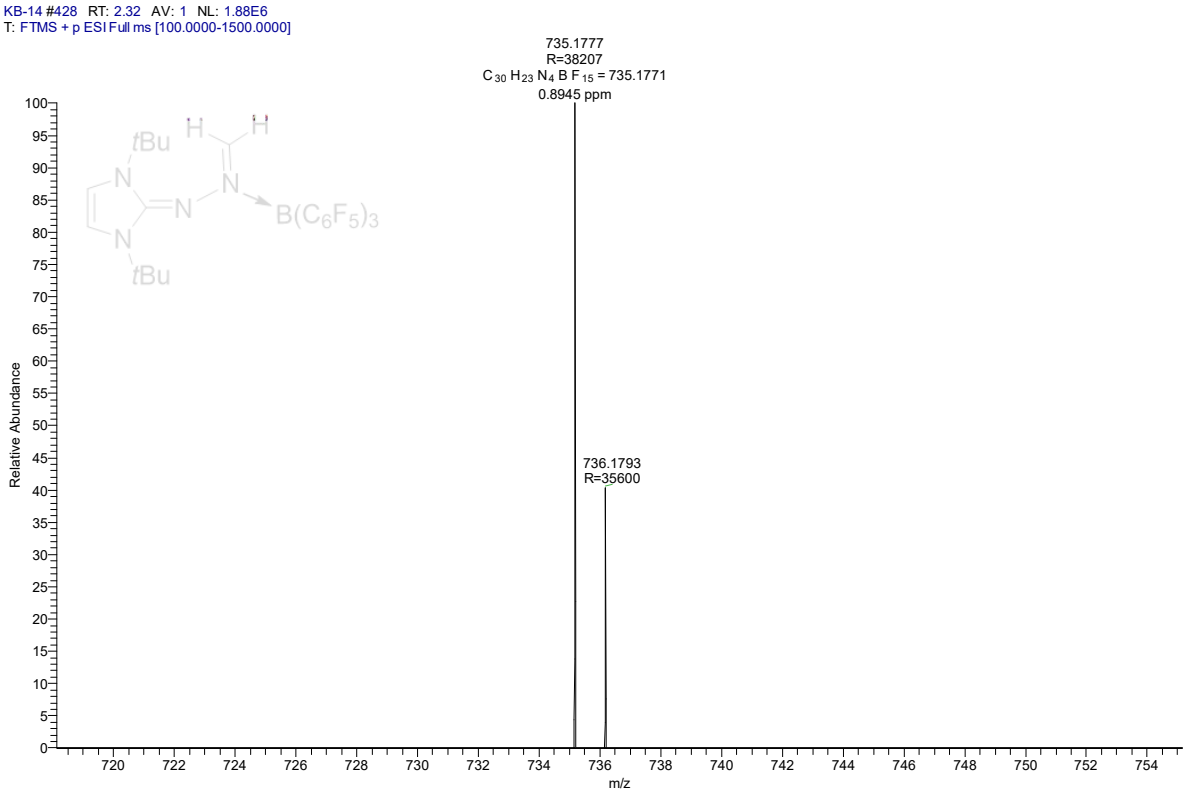

Figure S7: HRMS spectrum of **4**

Synthesis of 5: 1 (0.100 g, 0.45 mmol) and TCNE (0.060 g, 0.47 mmol) were taken together in a Schlenk flask, and then dissolved in 15 mL of THF at room temperature, resulting in the color change from green to deep-red, and stirred for 6 hours. After that, all the volatiles were completely removed and dissolved again in 10 mL of THF. The solution was filtered using a cannula. Completely removed all volatiles to get pure, **5** in 75% yield. Suitable crystals for XRD analysis were grown in THF at -4 ˚C, affording plate-shaped red crystals.

^{1}H NMR (500 MHz, 298 K, $CDCl_3$): δ = 1.65 (singlet, 18 H, C(C***H***$_3$)$_3$), 7.09 (singlet, 2 H, NC***H***C***H***N), 8.03 (C***H***(CN)CC(CN)$_2$) ppm.

^{13}C{^{1}H} NMR (125.7 MHz, 298 K, $CDCl_3$): δ= 30.1 (C(***C***H$_3$)$_3$, 61.7 (***C***(CH$_3$)$_3$, 114.0 (NNCH(CN)C***C***(CN)$_2$), 114.6 (NNCH(CN)CC(***C***N)$_2$), 115.5 (N***C***H***C***HN), 116.8 (NNCH(***C***N)CC(CN)$_2$), 136.2 (NNCH(CN)***C***C(CN)$_2$), 138.6 (N***C***N), 150.6 ((NN***C***H(CN)CC(CN)$_2$) ppm.

HRMS: m/z calcd for [M+H]$^+$ $C_{17}H_{21}N_7$, 324.1858; found **324.1931**.

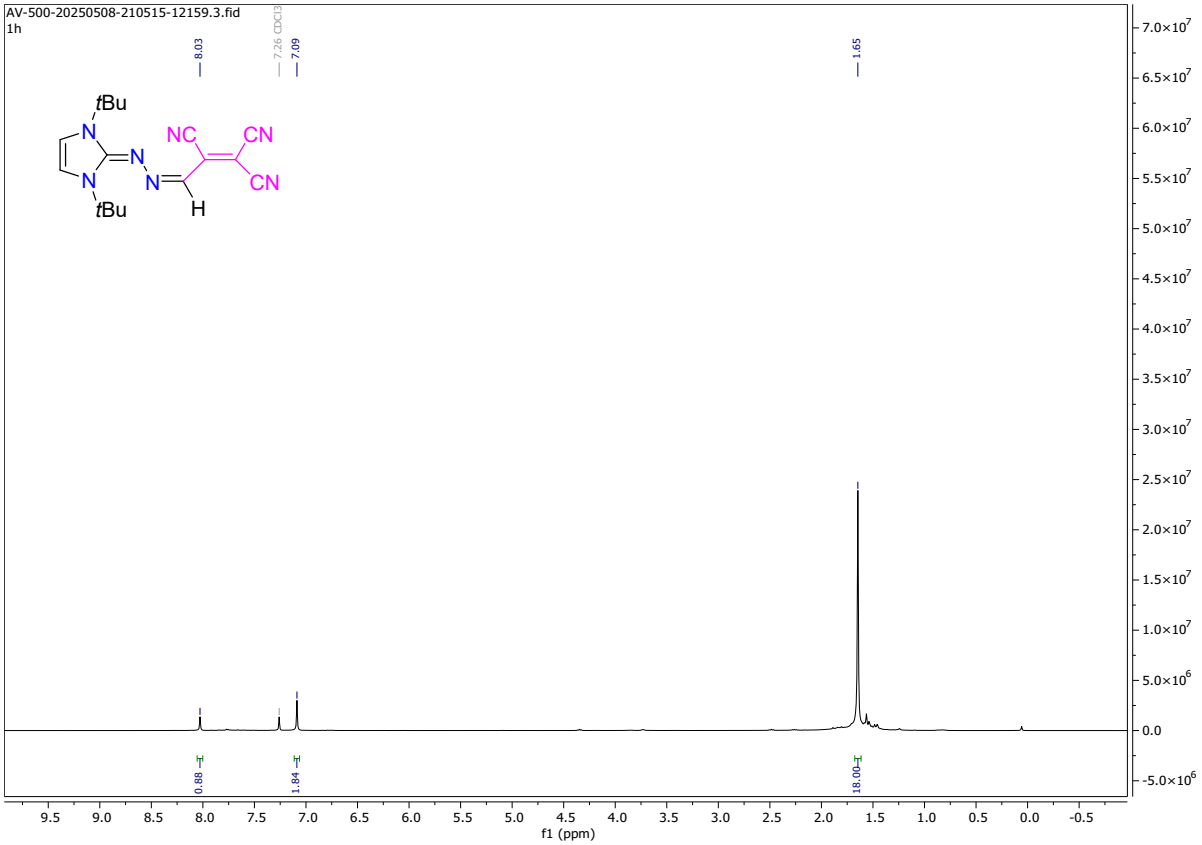

Figure S8: ^{1}H NMR spectrum of **5**

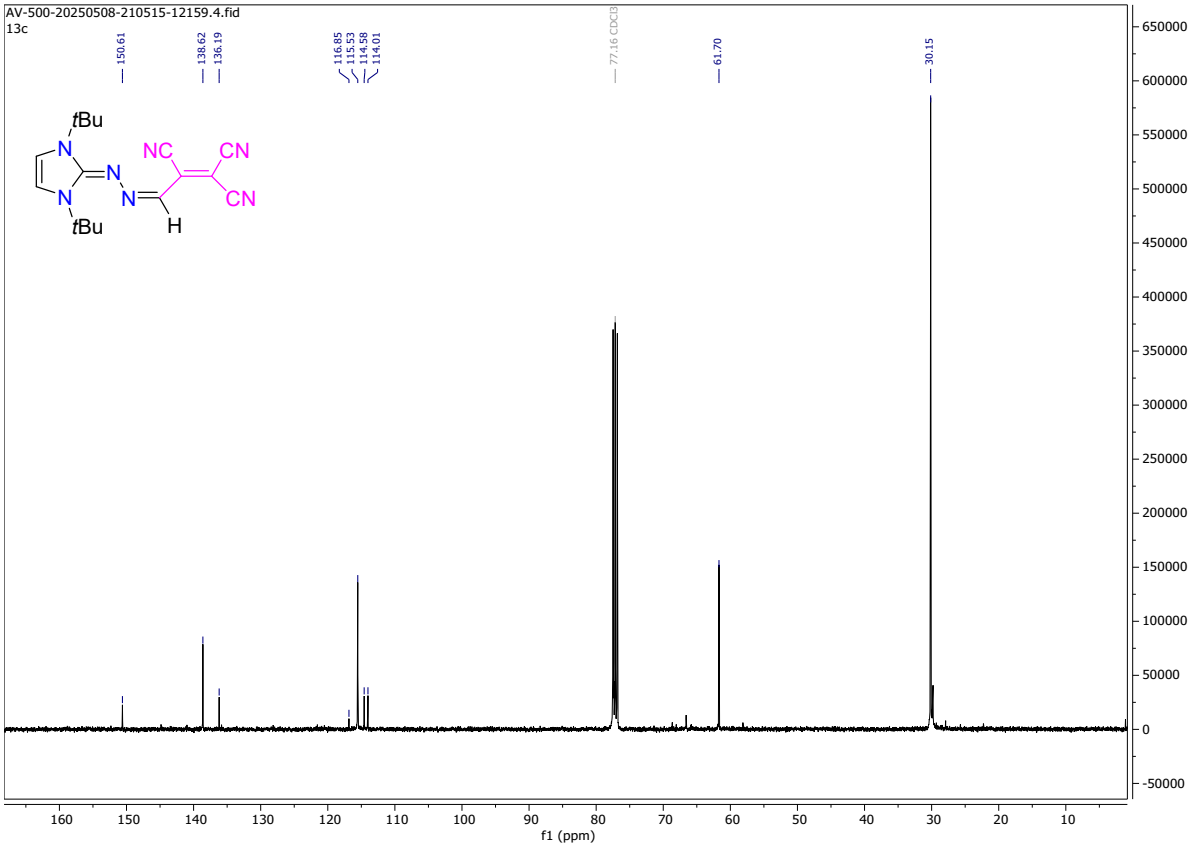

Figure S9: ^{13}C{^{1}H} NMR spectrum of **5**

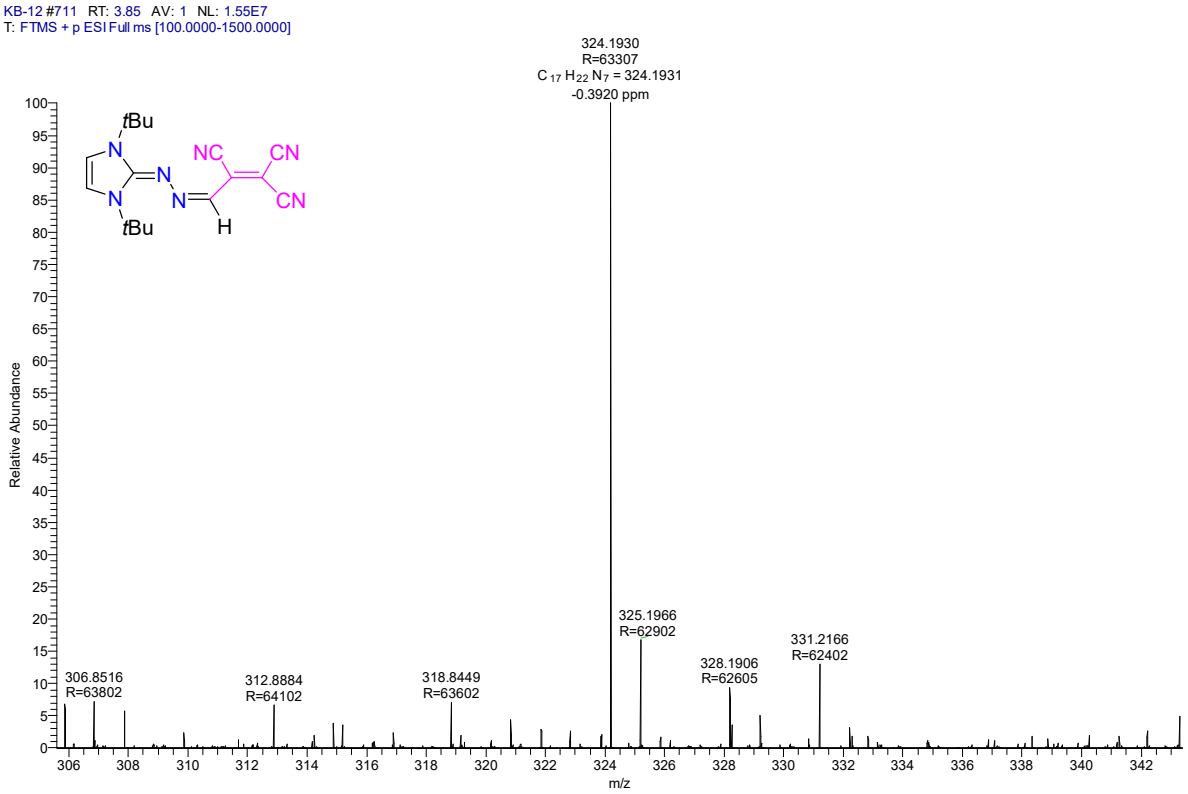

Figure S10: HRMS spectrum of **5**

Synthesis of 6: 2 (0.100 g, 0.23 mmol) and TCNE (0.031 g, 0.24 mmol) were taken together in a Schlenk flask, and then dissolved in 15 mL of THF at room temperature resulting in the color change from green to deep-violet, and stirred for 6 hours. After that, all the volatiles were completely removed and dissolved again in 10 mL of THF. The solution was filtered using a cannula. Completely removed all volatiles to get pure, **6** in 80% yield. Suitable crystals for XRD analysis were grown in THF at -4 ˚C, affording plate-shaped red crystals.

^{1}H NMR (500 MHz, 298 K, $CDCl_3$): δ = 1.13 (d, 12H, CH(C***H***$_3$)$_2$), 1.25 (d, 12H, CH(C***H***$_3$)$_2$), 2.63 (sept, 4H, C***H***(CH$_3$)$_2$), 6.89 (singlet, 2H, NC***H***C***H***N), 7.32 (d, 4H, Ar-H), 7.51 (t, 2H, Ar-H), 7.71 (C***H***(CN)CC(CN)$_2$) ppm.

^{13}C{^{1}H} NMR (101 MHz, 298 K, $CDCl_3$): δ= 23.4, 23.9 (CH(***C***H$_3$)$_2$), 29.3 (***C***H(CH$_3$)$_2$, 111.6 (NNCH(CN)C=***C***(CN)$_2$), 113.1 (NNCH(CN)C=C(***C***N)$_2$), 114.0 (NNCH(***C***N)C=C(CN)$_2$), 120.4 (N***C***H***C***HN), 124.7 (Ar-***C***), 131.0 (Ar-***C***), 132.0 (NNCH(CN)***C***=C(CN)$_2$), 137.0 (Ar-***C***), 140.5 (N***C***N), 144.8 (Ar-***C***), 150.3 (NN***C***H(CN)C=C(CN)$_2$) ppm.

HRMS: m/z calcd for [M+H]$^+$ $C_{33}H_{38}N_7$, 532.3110; found **532.3183**.

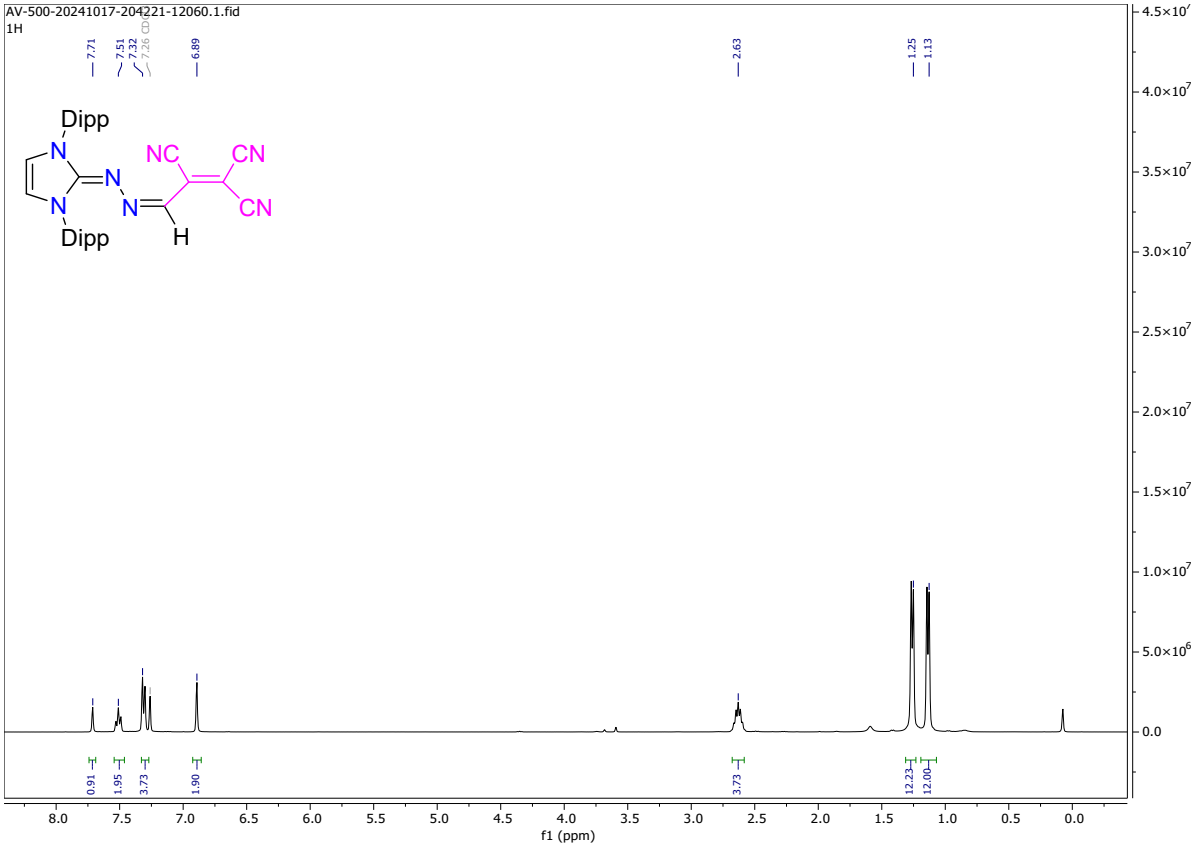

Figure S11: ^{1}H NMR spectrum of **6**

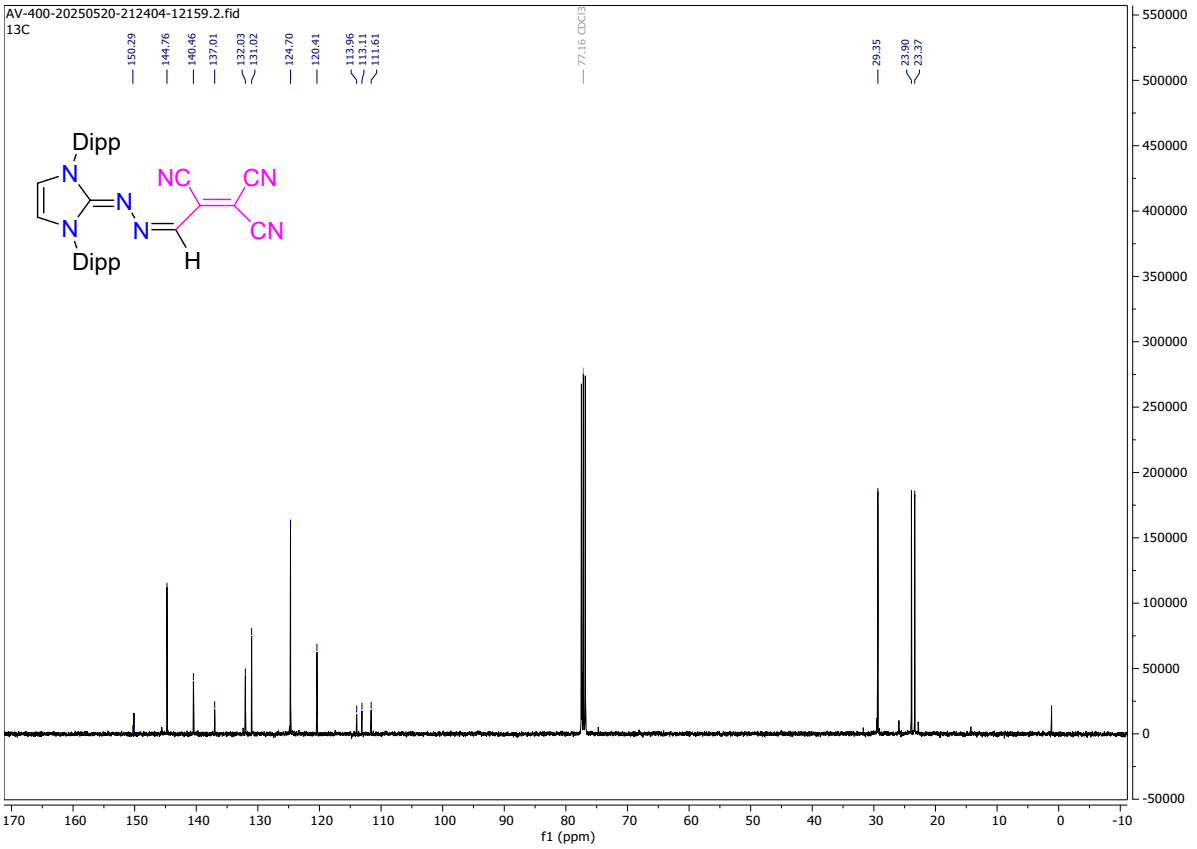

Figure S12: ^{13}C{^{1}H} NMR spectrum of **6**

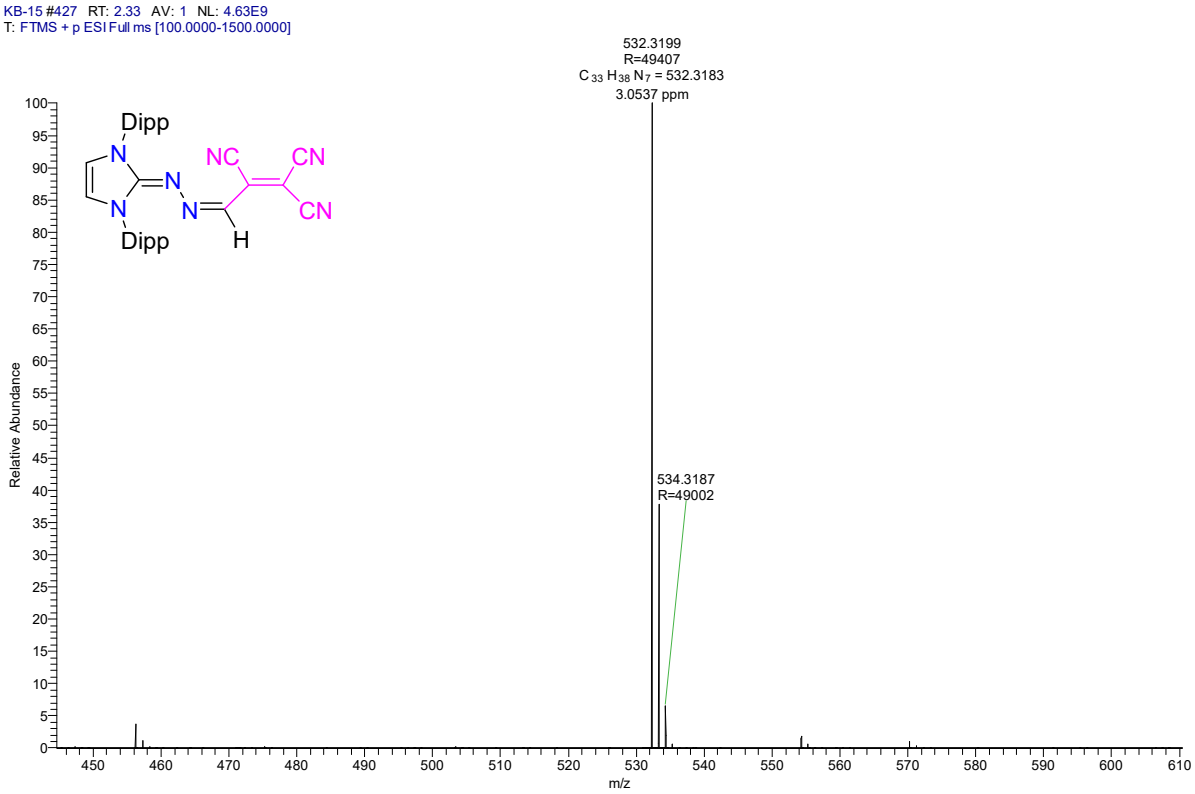

Figure S13: HRMS spectrum of **6**

3. Crystallographic data for the structural analysis

X-ray intensity data measurements were carried out on a Bruker SMART APEX II single crystal X-ray CCD diffractometer with graphite-monochromatized (Mo-Kα = 0.71073 Å) radiation. The X-ray generator was operated at 50 kV and 30 mA. A preliminary set of cell constants and an orientation matrix were calculated from three sets of 36 frames. Data were collected with ω scan width of 0.5 ° at different settings of ϕ and 2θ keeping the sample-to-detector distance fixed at 5.00 cm. The X-ray data collection was monitored by the APEX3 program (Bruker, 2006).[2] All the data were corrected for Lorentzian, polarization, and absorption effects using SAINT and SADABS programs (Bruker, 2006). SHELX-97 was used for structure solution and full-matrix least-squares refinement on F2.[3] All the hydrogen atoms were placed in geometrically idealized position and constrained to ride on their parent atoms. An ORTEPIII [4] view was drawn with 50% probability displacement ellipsoids and H atoms omitted for clarity.

Identification code	**Compound 3**	**Compound 4**
CCDC Number	2529673	2529674
Empirical formula	$C_{24}H_{47.5}Cl_2N_8O_{0.75}$	$C_{30}H_{22}BF_{15}N_4$
Formula weight	531.10	734.32
Temperature/K	201(2)	298(2)
Crystal system	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$
a/Å	12.5515(12)	10.473(5)
b/Å	11.5612(13)	12.522(7)
c/Å	21.090(2)	23.783(12)
α/°	90	90
β/°	91.906(3)	97.234(15)
γ/°	90	90
Volume/Å^3	3058.7(6)	3094(3)
Z	4	4
ρ_{calc}g/cm^3	1.153	1.576
μ/mm^{-1}	0.241	0.157
F(000)	1150.0	1480.0
Crystal size/mm^3	0.19 × 0.11 × 0.05	0.16 × 0.09 × 0.04
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.722 to 51	4.08 to 60.186
Index ranges	-15 ≤ h ≤ 15, -14 ≤ k ≤ 14, -25 ≤ l ≤ 25	-14 ≤ h ≤ 14, -17 ≤ k ≤ 17, -33 ≤ l ≤ 33
Reflections collected	87615	148157
Independent reflections	5672 [R_{int} = 0.0707, R_{sigma} = 0.0286]	9027 [R_{int} = 0.0666, R_{sigma} = 0.0271]
Data/restraints/parameters	5672/0/337	9027/0/466
Goodness-of-fit on F^2	1.102	1.028
Final R indexes [I>=2σ (I)]	R_1 = 0.0701, wR_2 = 0.1901	R_1 = 0.0529, wR_2 = 0.1456
Final R indexes [all data]	R_1 = 0.0796, wR_2 = 0.1991	R_1 = 0.0814, wR_2 = 0.1701
Largest diff. peak/hole / e Å^{-3}	0.79/-0.36	0.26/-0.24

Identification code	**Compound 5**	**Compound 6**
CCDC Number	2529672	2529671
Empirical formula	$C_{17}H_{21}N_7$	$C_{33}H_{37}N_7$
Formula weight	323.41	531.69
Temperature/K	100(2)	100(2)
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$
a/Å	14.6450(6)	10.5216(3)
b/Å	11.6884(4)	19.1906(7)
c/Å	10.8720(4)	16.0936(6)
α/°	90	90
β/°	111.1540(10)	106.3710(10)
γ/°	90	90
Volume/Å^3	1735.62(11)	3117.81(19)
Z	4	4
ρ_{calc}g/cm^3	1.238	1.133
μ/mm^{-1}	0.080	0.069
F(000)	688.0	1136.0
Crystal size/mm^3	0.37 × 0.23 × 0.11	0.23 × 0.16 × 0.09
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.318 to 60.208	5.276 to 51
Index ranges	-20 ≤ h ≤ 20, -16 ≤ k ≤ 16, -15 ≤ l ≤ 15	-12 ≤ h ≤ 12, -23 ≤ k ≤ 23, -19 ≤ l ≤ 19
Reflections collected	94288	66935
Independent reflections	5101 [R_{int} = 0.0950, R_{sigma} = 0.0331]	5782 [R_{int} = 0.0747, R_{sigma} = 0.0355]
Data/restraints/parameters	5101/0/223	5782/0/369
Goodness-of-fit on F^2	1.060	1.104
Final R indexes [I>=2σ (I)]	R_1 = 0.0456, wR_2 = 0.0999	R_1 = 0.0545, wR_2 = 0.1421
Final R indexes [all data]	R_1 = 0.0585, wR_2 = 0.1057	R_1 = 0.0604, wR_2 = 0.1487
Largest diff. peak/hole / e Å^{-3}	0.32/-0.24	0.70/-0.50

4. Computational Details

The geometries of complexes **1**, **2**, **5**, and **6** were fully optimized using *Gaussian 09*[5] at the PBE0-D3[6,7]/def2-TZVP[8] level of theory for all atoms. Solvent effects were included in all calculations using the PCM model[9] with a dielectric constant (ε) of 2.38 to simulate toluene, consistent with the experimental conditions. Natural charge analyses were carried out using NBO 7.0[10] at the same level of theory.

Natural Bond Orbital (NBO)

The energetic estimate of the donor(i) – acceptor(j) orbital interactions can be obtained by the second-order perturbation theory analysis of the Fock matrix in the NBO basis. The donor-acceptor interaction energy E(2) is given by,

$$E(2) = \Delta E(i,j) = [q(i,j)F(i,j)^2]/\varepsilon(i)-\varepsilon(j)$$

where q(i) is the donor orbital occupancy, ε(i) and ε(j) are the diagonal elements (orbital energies), and F(i,j) is the off-diagonal NBO Fock matrix element.

Optimized XYZ Coordinates:

Comp 1

N	-1.22080200	-0.66021600	-0.00874100	H	-4.59177100	-0.94926200	0.00210000
N	0.98565400	-0.76427500	-0.03915600	H	-3.45133500	-1.98566900	0.85665400
N	-0.22364000	1.42602300	0.03287000	H	-3.46295600	-1.93655500	-0.92337800
N	0.86703200	2.20447100	-0.10260000	C	2.44729000	-0.48818700	0.01675900
C	-0.08261600	0.11989300	-0.00794800	C	3.20850100	-1.81106400	0.09214500
C	0.47557300	-2.05548200	-0.07075400	H	4.27196500	-1.57687200	0.15266400
H	1.09965400	-2.92634500	-0.10605800	H	3.06039400	-2.42587900	-0.79807400
C	-0.86085500	-1.98995200	-0.04909200	H	2.94714900	-2.39056100	0.98018700
H	-1.57558200	-2.79034700	-0.06260100	C	2.89300300	0.23004800	-1.25440100
C	-2.61364600	-0.15569200	0.01068400	H	3.97376000	0.38787900	-1.22184400
C	-2.85682300	0.63668100	1.29411100	H	2.39973000	1.19501500	-1.34287800
H	-3.88964900	0.99211300	1.31047900	H	2.66310900	-0.38225900	-2.12999800
H	-2.18420700	1.49005000	1.35039700	C	2.77608000	0.30133000	1.28168800
H	-2.69970000	-0.00032400	2.16821400	H	3.85572500	0.45828500	1.33628400
C	-2.86935900	0.70152400	-1.22813500	H	2.46624500	-0.26049300	2.16638700
H	-3.90457900	1.05023700	-1.21939600	H	2.28804800	1.27217500	1.27920900
H	-2.71380600	0.11256400	-2.13555000	C	0.65946500	3.46071800	-0.01042300
H	-2.20354000	1.56184700	-1.24486500	H	-0.33382000	3.87548000	0.17634300
C	-3.57349000	-1.33951900	-0.01549600	H	1.50873500	4.12511800	-0.12570100

Comp 2

N	1.03901900	0.13223800	-0.68915200	H	-1.39778100	0.36505500	-2.85981900
N	-1.14305900	0.19683300	-0.72982600	C	-2.50073000	0.09165600	-0.31713400
N	-0.24475500	-0.00295500	1.40954300	C	-3.07588700	-1.18011800	-0.23976400
N	0.91476600	-0.04885000	2.12006700	C	-4.40554900	-1.26243000	0.15940700
C	-0.07225000	0.10168600	0.12005300	H	-4.88153200	-2.23329300	0.23694100
C	0.63479700	0.24960700	-2.01716000	C	-5.12606000	-0.12172700	0.46996100
H	1.35731500	0.29015300	-2.81365100	H	-6.16137000	-0.20566400	0.78156900
C	-0.70528900	0.28671000	-2.04014700	C	-4.52933400	1.12511600	0.39191800

H	-5.10214600	2.00833700	0.65047500	H	6.14896700	-0.40452100	0.42699100
C	-3.20174000	1.25809600	-0.00150100	C	4.57961400	0.95817700	-0.08743100
C	-2.53135500	2.61223300	-0.02240900	H	5.24348700	1.81351300	-0.10371500
H	-1.58788700	2.50750700	-0.56439100	C	3.22606100	1.12868200	-0.36121700
C	-3.35934800	3.66826800	-0.74581000	C	2.63343500	2.49831400	-0.61589600
H	-2.80162900	4.60629200	-0.80328300	H	1.83111400	2.38233400	-1.35100100
H	-4.29532000	3.87778200	-0.22189600	C	3.62720900	3.49807800	-1.19064400
H	-3.60604200	3.35475100	-1.76295600	H	3.10772300	4.41881800	-1.46579100
C	-2.19358800	3.04933700	1.40290000	H	4.12468000	3.10814300	-2.08187400
H	-1.65032400	3.99816200	1.39332800	H	4.39666200	3.76790700	-0.46263500
H	-1.57689600	2.29790900	1.90001500	C	2.00108300	3.04416600	0.66553000
H	-3.10645600	3.18654400	1.98982100	H	1.51009200	4.00155900	0.47058500
C	-2.27762700	-2.43301400	-0.52069100	H	2.76841000	3.20264900	1.42842200
H	-1.33887000	-2.13564400	-0.99463700	H	1.26502600	2.35419400	1.07956500
C	-2.98816800	-3.37668700	-1.48512000	C	1.98094200	-2.47944000	0.01017900
H	-2.34451500	-4.22897100	-1.71712200	H	0.99807100	-2.12612600	0.33074800
H	-3.23920300	-2.87408900	-2.42212600	C	1.82715900	-3.08780500	-1.38380400
H	-3.91276600	-3.77202600	-1.05701800	H	1.11845700	-3.92049200	-1.36064800
C	-1.92667000	-3.13819300	0.78904200	H	2.78666200	-3.46854600	-1.74512900
H	-1.29416300	-4.00928100	0.59606900	H	1.46130900	-2.35409300	-2.10475600
H	-2.83253300	-3.48312300	1.29564800	C	2.40717600	-3.54060600	1.01574100
H	-1.39536600	-2.46151500	1.46129400	H	1.63176000	-4.30650500	1.09329800
C	2.41336600	-0.00774300	-0.32766500	H	2.55769100	-3.10769600	2.00674100
C	2.90233500	-1.28087600	-0.02095800	H	3.33015200	-4.04334800	0.71472200
C	4.25930100	-1.39860000	0.25197900	C	0.77435200	-0.20918200	3.37500200
H	4.67412800	-2.36728800	0.50209700	H	-0.20802100	-0.30987000	3.84257100
C	5.09157500	-0.29186300	0.21431900	H	1.67045700	-0.24143200	3.98503900

Comp 5

N	-2.82566800	-0.68330800	-0.00014300	C	-4.41674900	-2.55211800	0.00000900
N	-2.02033900	1.36522700	-0.00016500	H	-4.48105600	-3.64043800	0.00014100
N	-0.51317000	-0.64709100	0.00012300	H	-4.93515600	-2.19264000	-0.89138600
N	0.60715200	-0.00365300	0.00013200	H	-4.93526600	-2.19241800	0.89125100
N	6.43011100	0.33407600	-0.00047900	C	-1.15495600	2.59189800	0.00000400
N	4.14214500	-3.41823400	-0.00038300	C	-2.04608000	3.83100300	0.00002400
N	3.06418600	2.42267800	0.00017000	H	-1.38904400	4.70082600	0.00027800
C	-1.66854100	0.04023200	-0.00000200	H	-2.67233200	3.89428100	0.89230400
C	-3.39384000	1.43392200	-0.00040000	H	-2.67196800	3.89454600	-0.89248700
H	-3.92860900	2.36344500	-0.00057200	C	-0.32062200	2.61851400	-1.27591000
C	-3.88620600	0.18038100	-0.00038700	H	0.29908600	3.51634400	-1.27689600
H	-4.90889300	-0.14375300	-0.00054700	H	-0.97449300	2.64770700	-2.15066200
C	-2.94049000	-2.17411200	0.00005300	H	0.34002300	1.75986300	-1.34420000
C	-2.29285600	-2.73284900	-1.26399400	C	-0.32088000	2.61832400	1.27607400
H	-2.42772200	-3.81585300	-1.28111500	H	0.29891800	3.51609500	1.27724300
H	-1.22847100	-2.51189300	-1.29178400	H	0.33969200	1.75962000	1.34444000
H	-2.76874800	-2.31549000	-2.15434500	H	-0.97492800	2.64752100	2.15069200
C	-2.29304000	-2.73249300	1.26436300	C	1.68245800	-0.76565100	0.00020900
H	-2.42788200	-3.81549500	1.28176200	H	1.60132800	-1.85133600	0.00025900
H	-2.76908800	-2.31490800	2.15452600	C	2.94713500	-0.15609200	0.00016900
H	-1.22866600	-2.51150900	1.29226900	C	4.15171200	-0.84946400	0.00011600

C	5.40250800	-0.19186800	0.00020500	C	3.00002500	1.27388600	0.00015500
C	4.15915000	-2.26390900	-0.00001500				

Comp 6

N	2.16137200	-0.81342500	-0.05901400	H	2.35152200	2.11879000	-3.60905500
N	0.23656100	-1.80791700	0.10400500	H	1.07804700	1.58849500	-2.50319200
N	0.35908300	0.66025000	0.03070900	C	-1.15395700	-2.10897600	0.27896800
N	-0.92963800	0.77604100	-0.12499900	C	-1.69440600	-2.01834700	1.56193400
N	-1.90520300	5.53338500	0.58182000	C	-3.03302300	-2.36466100	1.71216800
N	-5.85235000	3.90461800	-0.40719800	H	-3.49276600	-2.29862300	2.69175200
N	-4.32933600	0.31790300	-0.86332400	C	-3.78451700	-2.78671100	0.63086700
C	0.82739200	-0.59070000	0.00905800	H	-4.82933600	-3.04077800	0.76596000
C	1.21511000	-2.78381000	0.09597200	C	-3.21398100	-2.87202800	-0.62745200
H	0.95796300	-3.82613800	0.16999100	H	-3.82260500	-3.18542300	-1.46645700
C	2.40891100	-2.16640600	-0.01026400	C	-1.88277400	-2.53411900	-0.83423000
H	3.40988700	-2.55786600	-0.05754400	C	-1.28022600	-2.56334200	-2.22176800
C	3.14815300	0.21235300	-0.20010100	H	-0.19147800	-2.57001000	-2.11943700
C	3.43592800	0.68197100	-1.48255100	C	-1.66253500	-3.81389900	-3.00509600
C	4.39907000	1.67944900	-1.59241700	H	-1.12509400	-3.83613400	-3.95601000
H	4.64634100	2.07583900	-2.57035300	H	-2.72995700	-3.83578400	-3.23603800
C	5.03765500	2.17767000	-0.47057200	H	-1.41822400	-4.72391200	-2.45222500
H	5.78302600	2.95771200	-0.57680600	C	-1.66141500	-1.29678300	-2.98819700
C	4.72598000	1.69175300	0.78827200	H	-1.19157300	-1.29349100	-3.97529900
H	5.22713500	2.10146700	1.65692100	H	-1.35078800	-0.39960400	-2.45016200
C	3.76952700	0.69634700	0.95357300	H	-2.74454100	-1.24088600	-3.12190800
C	3.37537600	0.21808600	2.33285200	C	-0.88969000	-1.55882100	2.75682900
H	2.84044600	-0.72944300	2.22339400	H	0.12729300	-1.33501600	2.42467700
C	2.41272700	1.21763100	2.97541300	C	-0.78504100	-2.65845800	3.81084600
H	2.07307200	0.85017600	3.94730500	H	-0.16500900	-2.32461100	4.64663000
H	1.53997100	1.38688200	2.34164200	H	-0.34063400	-3.56573700	3.39500100
H	2.90834600	2.17982400	3.13007500	H	-1.76875300	-2.91944900	4.20871100
C	4.57694200	-0.04665900	3.23304500	C	-1.46651100	-0.27631400	3.35147500
H	4.24428100	-0.47544600	4.18113900	H	-0.84127400	0.07347400	4.17652000
H	5.11854300	0.87309900	3.46565600	H	-2.47395100	-0.44211800	3.74091700
H	5.27891400	-0.74374600	2.76986600	H	-1.52175300	0.51637100	2.60344200
C	2.71594400	0.17533500	-2.71148500	C	-1.38262100	2.00163500	-0.00926600
H	2.09693000	-0.67720900	-2.42002100	H	-0.71165200	2.82608300	0.22728200
C	3.68721400	-0.31828800	-3.77980900	C	-2.75678100	2.24921100	-0.19166600
H	3.13438200	-0.72746400	-4.62878200	C	-3.34069500	3.49960800	-0.05582400
H	4.34502700	-1.09897700	-3.39103200	C	-2.55645600	4.62510200	0.29447300
H	4.31449600	0.49333000	-4.15609700	C	-4.72493100	3.71381200	-0.25198300
C	1.78265300	1.25090600	-3.26534600	C	-3.60809600	1.15894800	-0.55382300
H	1.21478300	0.86137300	-4.11382400				

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