Supplementary information

C-H functionalization of aromatic amines for azidation catalyzed by Betti base coordinated copper(II) complexes under ultrasonication

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Table S1 Crystallographic data of complex **C4**

Parameters	**Complex C4**
Empirical formula	$C_{46}H_{48}CuN_2O_2$
Formula weight	724.40
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.5553(6)
b/Å	9.9379(6)
c/Å	16.2405(11)
α/°	90
β/°	91.878(5)
γ/°	90
Volume/Å^3	1863.98(19)
Z	2
ρ_{calc}g/cm^3	1.291
μ/mm^{-1}	0.627
F(000)	766.0
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	7.302 to 60.58
Index ranges	-15 ≤ h ≤ 13, -14 ≤ k ≤ 13, -21 ≤ l ≤ 20
Reflections collected	19542
Independent reflections	4572 [R_{int} = 0.1143, R_{sigma} = 0.0718]
Data/restraints/parameters	4572/0/232
Goodness-of-fit on F^2	1.073
Final R indexes [I > =2σ (I)]	R_1 = 0.0863, wR_2 = 0.2150
Final R indexes [all data]	R_1= 0.1000, wR_2 =

	0.2239
Largest diffraction peak/hole/e $Å^{-3}$	1.81/-0.88
CCDC number	2241114

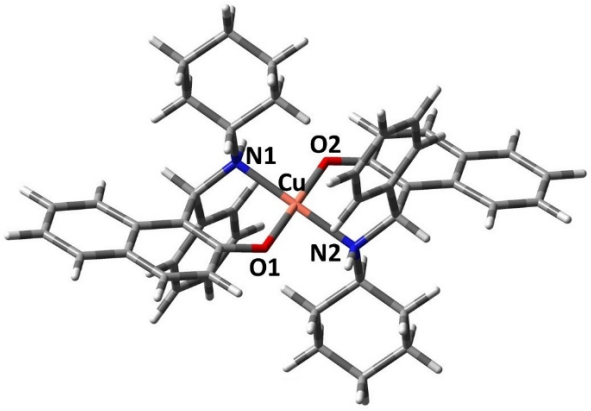


Fig S1. DFT optimized geometry of complex **C4** using B3LYP functional and basis set 6-31G(d,p) for C, H, N and O, LANL2DZ for Cu atom.

Table S2 Selected bond lengths [Å] of the optimized structures **C1, C2, C3 and C5** obtained from DFT calculations

C1		**C2**		**C3**		**C5**	
Cu-O(1)	1.907	Cu-O(1)	1.912	Cu-O(1)	1.907	Cu-O(1)	1.908
Cu-N(1)	2.070	Cu-N(1)	2.074	Cu-N(1)	2.070	Cu-N(1)	2.176
Cu-O(2)	1.907	Cu-O(2)	1.912	Cu-O(2)	1.907	Cu-O(2)	1.908
Cu-N(2)	2.069	Cu-N(2)	2.073	Cu-N(2)	2.070	Cu-N(2)	2.176

Table S3 Selected bond angles [°] of the optimized structures **C1, C2, C3 and C5** obtained from DFT calculations

C1		**C2**		**C3**		**C5**	
O(1)-Cu-N(1)	92.49	O(1)-Cu-N(1)	92.75	O(1)-Cu-N(1)	92.39	O(1)-Cu-N(1)	90.53
O(2)-Cu-N(2)	92.48	O(2)-Cu-N(2)	92.75	O(2)-Cu-N(2)	92.39	O(2)-Cu-N(2)	90.54
N(1)-Cu-O(2)	87.51	N(1)-Cu-O(2)	87.24	N(1)-Cu-O(2)	87.60	N(1)-Cu-O(2)	89.47
O(1)-Cu-N(2)	87.51	O(1)-Cu-N(2)	87.24	O(1)-Cu-N(2)	87.60	O(1)-Cu-N(2)	89.45
O(1)-Cu-O(2)	179.99	O(1)-Cu-O(2)	179.99	O(1)-Cu-O(2)	179.99	O(1)-Cu-O(2)	179.96
N(1)-Cu-N(2)	179.99	N(1)-Cu-N(2)	179.99	N(1)-Cu-N(2)	179.99	N(1)-Cu-N(2)	179.96

Characterization data for the Ligands and complexes:

Ligand L1:

Reaction of benzaldehyde (1 equiv) and aniline (1.2 equiv), 2-naphthol (1mmol) and N,N-dimethylethanolamine (DMEA) (7.5 mol%) afforded ligand **L1** as white solid. Yield, 90%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.54 (s, 1H), 7.84 – 7.79 (m, 2H), 7.78 (d, J = 8.9 Hz, 1H), 7.50 (d, 2H), 7.44 – 7.29 (m, 5H), 7.21 – 7.13 (m, 3H), 6.95 (t, J = 7.4 Hz, 1H), 6.80 (d, J = 7.6 Hz, 2H), 6.21 (s, 1H), 4.19 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.31, 146.85, 141.12, 131.62, 130.14, 129.60, 129.54, 129.25, 129.15, 128.71, 128.15, 126.92, 122.98, 121.99, 121.55, 120.16, 116.44, 113.89, 62.89. Selected FT-IR frequencies (KBr, cm^{-1}): 3348 (N-H stretching), 2886 (O-H stretching). UV (nm): 236, 280, 335 nm. Anal. calcd for $C_{23}H_{19}NO$: C 84.89, H 5.89, N 4.30, found: C 84.53, H 5.33, N 4.95. ESI-MS: for $C_{23}H_{19}NO$ $[M + H]^+$ calculated m/z = 326.1539; found m/z = 326.1529.

Ligand L2:

Reaction of benzaldehyde (1 equiv) and o-toluidine (1.2 equiv), 2-naphthol (1mmol) and N,N-dimethylethanolamine (DMEA) (7.5 mol%) afforded ligand **L2** as white solid. Yield, 88%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.41 (s, 1H), 7.83 (t, 2H), 7.77 (d, J = 8.9 Hz, 1H), 7.52 (d, J = 6.9 Hz, 2H), 7.46 – 7.30 (m, 5H), 7.16 (d, J = 8.8 Hz, 2H), 6.99 (t, J = 7.7 Hz, 1H), 6.89 (t, J = 7.4 Hz, 1H), 6.73 (d, J = 8.0 Hz, 1H), 6.26 (s, 1H), 4.08 (s, 1H), 2.26 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.34, 144.90, 141.27, 131.67, 130.45, 130.11, 129.59, 129.25, 129.17, 128.71, 128.13, 127.70, 126.96, 125.07, 122.99, 121.63, 121.50, 120.11, 114.50, 113.85, 62.32, 17.97. Selected FT-IR frequencies (KBr, cm^{-1}): 3364 (N-H stretching), 2935 (O-H stretching). UV (nm): 236, 280, 333 nm. Anal. calcd for $C_{24}H_{21}NO$: C 84.92, H 6.24, N 4.13, found: C 84.73, H 5.83, N 4.34. ESI-MS: for $C_{24}H_{21}NO$ $[M + H]^+$ calculated m/z = 340.1696; found m/z = 340.1690.

Ligand L3:

Reaction of benzaldehyde (1 equiv), 4-tert-butylaniline (1.2 equiv), 2-naphthol (1mmol) and N,N-dimethylethanolamine (DMEA) (7.5 mol%) afforded ligand **L3** as white solid. Yield, 90%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.70 (s, 1H), 7.80 – 7.71 (m, 3H), 7.47 (d, J = 6.9 Hz, 2H), 7.40 – 7.25 (m, 5H), 7.16 (t, J = 9.3 Hz, 3H), 6.72 (d, J = 8.6 Hz, 2H), 6.17 (s, 1H), 4.09 (s, 1H), 1.23 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.44, 144.92, 144.39, 141.28, 131.70,

130.09, 129.52, 129.25, 129.15, 128.65, 128.16, 126.89, 126.42, 122.93, 121.54, 120.19, 116.25, 114.08, 63.12, 34.24, 31.52. Selected FT-IR frequencies (KBr, cm^{-1}): 3354 (N-H stretching), 2961 (O-H stretching). UV (nm): 236, 280, 334 nm. Anal. calcd for $C_{27}H_{27}NO$: C 85.00, H 7.13, N 3.67, found: C 85.41, H 6.74, N 4.08. ESI-MS: for $C_{27}H_{27}NO$ $[M + H]^+$ calculated m/z = 382.2165; found m/z = 382.2160.

Ligand L4:

Reaction of benzaldehyde (1 equiv), cyclohexylamine (1.2 equiv), 2-naphthol (1mmol) and N,N-dimethylethanolamine (DMEA) (7.5 mol%) afforded ligand **L4** as white solid. Yield, 92%. ^1H NMR (400 MHz, $CDCl_3$) δ 7.70 (t, J = 7.8 Hz, 1H), 7.40 (d, J = 7.6 Hz, 0H), 7.35 – 7.27 (m, 0H), 7.24 – 7.18 (m, 0H), 7.15 (d, J = 8.9 Hz, 0H), 5.85 (s, 0H), 2.75 – 2.63 (m, 0H), 2.27 – 2.19 (m, 0H), 1.98 – 1.90 (m, 0H), 1.77 – 1.52 (m, 0H), 1.23 – 1.08 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.64, 142.31, 132.49, 129.68, 129.29, 128.98, 128.09, 127.91, 126.55, 122.43, 121.26, 120.52, 114.04, 60.72, 55.89, 33.56, 25.95, 25.17, 25.02. Selected FT-IR frequencies (KBr, cm^{-1}): 3305 (N-H stretching), 2663 (O-H stretching). UV (nm): 235, 281, 335 nm. Anal. calcd for $C_{23}H_{25}NO$: C 83.34, H 7.60, N 4.23, found: C 83.43, H 7.25, N 4.41. ESI-MS: for $C_{23}H_{25}NO$ $[M + Na]^+$ calculated m/z = 354.1828; found m/z = 354.1828.

Ligand L5:

Reaction of benzaldehyde (1 equiv), morpholine (1.2 equiv), 2-naphthol (1mmol) and N,N-dimethylethanolamine (DMEA) (7.5 mol%) afforded ligand **L5** as white solid. Yield, 92%. ^1H NMR (400 MHz, $CDCl_3$) δ 13.12 (s, 1H), 7.85 (d, J = 8.6 Hz, 1H), 7.69 (t, 2H), 7.57 (d, J = 7.8 Hz, 2H), 7.38 (t, J = 1.4 Hz, 1H), 7.31 – 7.20 (m, 4H), 7.15 (d, J = 8.8 Hz, 1H), 5.12 (s, 1H), 3.90 – 3.58 (m, 4H), 2.52 – 2.14 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.85, 138.74, 132.44, 129.89, 129.07, 129.03, 128.99, 128.92, 128.32, 126.68, 122.74, 121.14, 119.89, 115.22, 72.11, 66.99. Selected FT-IR frequencies (KBr, cm^{-1}): 2762 (O-H stretching). UV (nm): 236, 282, 338 nm. Anal. calcd for $C_{21}H_{21}NO_2$: C 78.97, H 6.63, N 4.39, found: C 78.50, H 6.24, N 4.50. ESI-MS: for $C_{21}H_{21}NO_2$ $[M + H]^+$ calculated m/z = 320.1645; found m/z = 320.1648.

Complex C1:

The reaction of $Cu(OAc)_2.H_2O$ (0.5 mmol) and Ligand **L1** (2 equiv) afforded complex **C1**. Brown solid. Yield, 76%. M.P. 200 °C. Anal. calcd for $C_{46}H_{36}CuN_2O_2$: C 77.56, H 5.09, N 3.93, found: C 76.74, H 5.11, N 4.05. Selected FT-IR frequencies (KBr, cm^{-1}): 3274 (N-H stretching), No peak found for O-H stretching. UV (nm): 242, 322, 474, 692 nm. ESI-MS: for $C_{46}H_{36}CuN_2O_2$ $[M]^+$ calculated m/z = 711.2073; found m/z = 711.1823.

Complex C2:

The reaction of $Cu(OAc)_2.H_2O$ (0.5 mmol) and Ligand **L2** (2 equiv) afforded complex **C2**. Brown solid. Yield, 70%. M.P. 210 °C. Anal. calcd for $C_{48}H_{40}CuN_2O_2$: C 77.87, H 5.45, N 3.78, found: C 78.61, H 6.20, N 3.71. Selected FT-IR frequencies (KBr, cm^{-1}): 3294 (N-H stretching), No peak found for O-H stretching. UV (nm): 236, 278, 331, 473, 680 nm. ESI-MS: for $C_{48}H_{40}CuN_2O_2$ $[M + Na]^+$ calculated m/z = 762.2278; found m/z = 762.2279.

Complex C3:

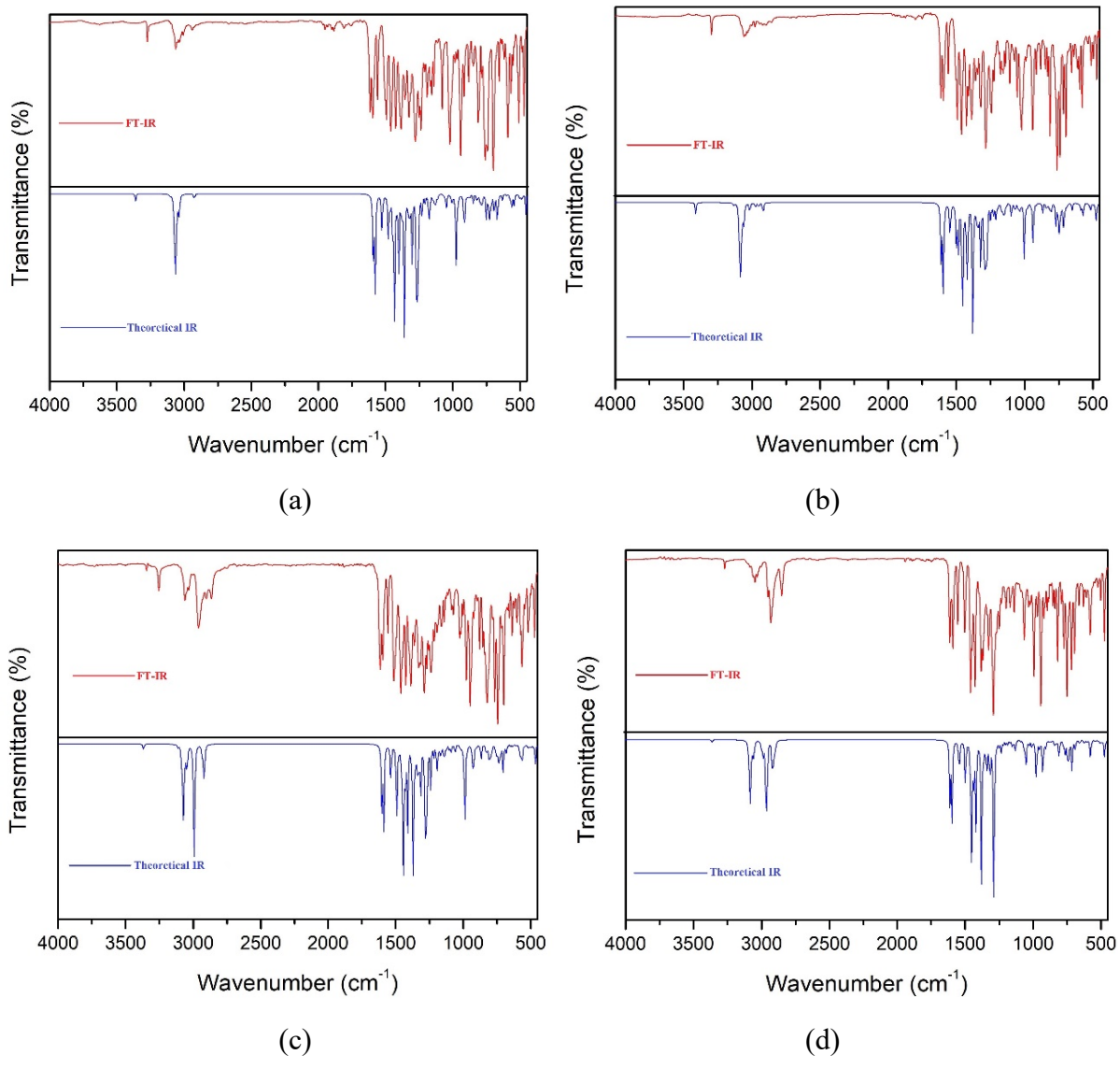
The reaction of $Cu(OAc)_2.H_2O$ (0.5 mmol) and Ligand **L3** (2 equiv) afforded complex **C3**. Light brown solid. Yield, 82%. M.P. 227 °C. Anal. calcd for $C_{54}H_{52}CuN_2O_2$: C 78.66, H 6.36, N 3.40, found: C 78.57, H 6.47, N 3.66. Selected FT-IR frequencies (KBr, cm^{-1}): 3253 (N-H stretching), No peak found for O-H stretching. UV (nm): 237, 278, 324, 476, 697 nm. ESI-MS: for $C_{54}H_{52}CuN_2O_2$ $[M + Na]^+$ calculated m/z = 846.3217; found m/z = 846.3219.

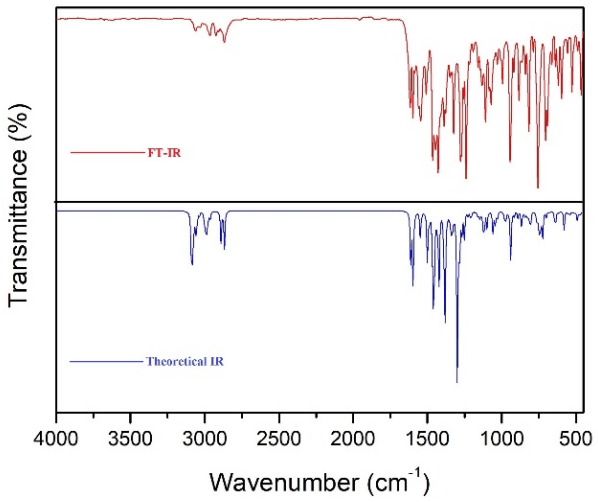
Complex C4:

The reaction of $Cu(OAc)_2.H_2O$ (0.5 mmol) and Ligand **L4** (2 equiv) afforded complex **C4**. Brown solid. Yield, 95%. M.P. 254 °C. Anal. calcd for $C_{46}H_{48}CuN_2O_2$: C 76.27, H 6.68, N 3.87, found: C 76.27, H 6.57, N 3.83. Selected FT-IR frequencies (KBr, cm^{-1}): 3269 (N-H stretching), No peak found for O-H stretching. UV (nm): 241, 290, 341, 463, 646 nm. ESI-MS: for $C_{46}H_{48}CuN_2O_2$ $[M + Na]^+$ calculated m/z = 746.2904; found m/z = 746.2881. CCDC number: 2241114.

Complex C5:

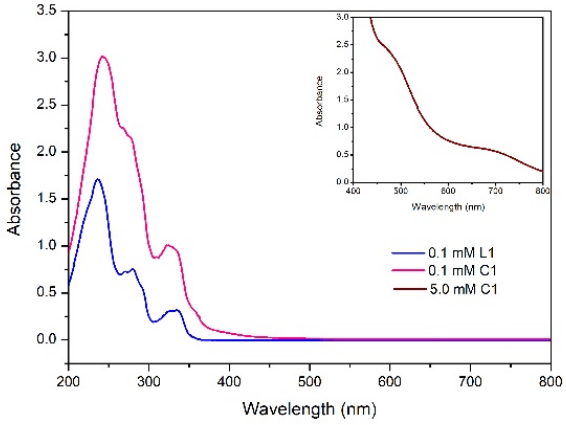
The reaction of $Cu(OAc)_2.H_2O$ (0.5 mmol) and Ligand **L5** (2 equiv) afforded complex **C5**. Green solid. Yield, 65%. M.P. 220 °C. Anal. calcd for $C_{42}H_{40}CuN_2O_4$: C 72.03, H 5.76, N 4.00, found: C 71.00, H 5.99, N 4.51. Selected FT-IR frequencies (KBr, cm^{-1}): 2964 cm^{-1} (C-H stretching), No peak found for O-H stretching. UV (nm): 238, 280, 327, 667 nm. ESI-MS: for $C_{42}H_{40}CuN_2O_4$ $[M + H]^+$ calculated m/z = 700.2357; found m/z = 700.2351.



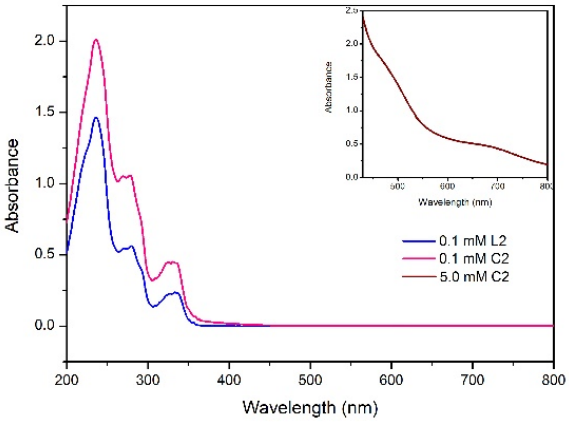


(e)

Fig S2. Comparison of experimental and theoretical IR spectrum of complexes (a) **C1**, (b) **C2**, (c) **C3**, (d) **C4**, (e) **C5**



(a)



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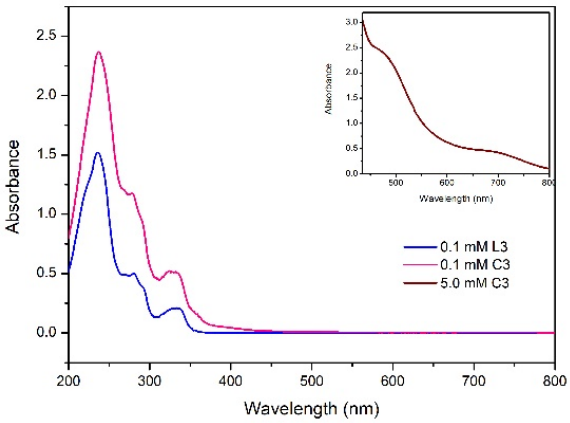

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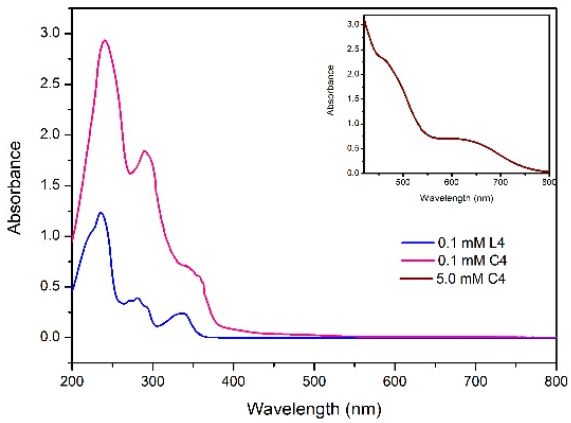

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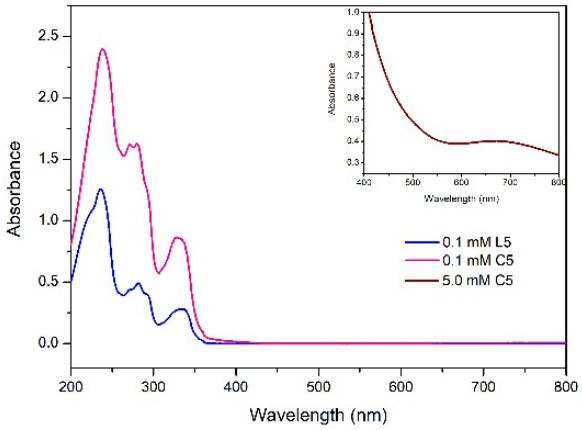
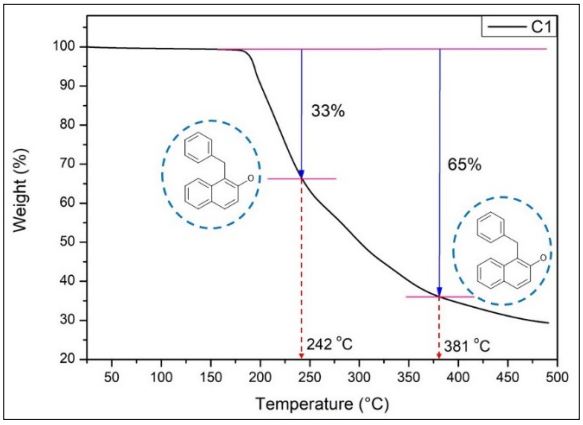
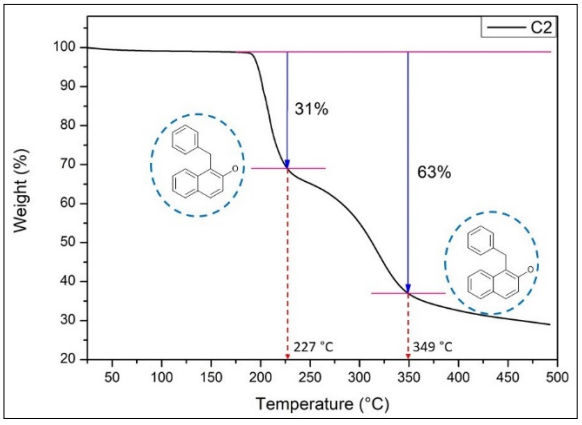


(e)

Fig S3. UV-Visible spectrum of ligands and complexes (a) **L1**, **C1**, (b) **L2**, **C2**, (c) **L3**, **C3**, (d) **L4**, **C4**, (e) **L5**, **C5** inset represents the corresponding complexes in 5mM concentration



(a)



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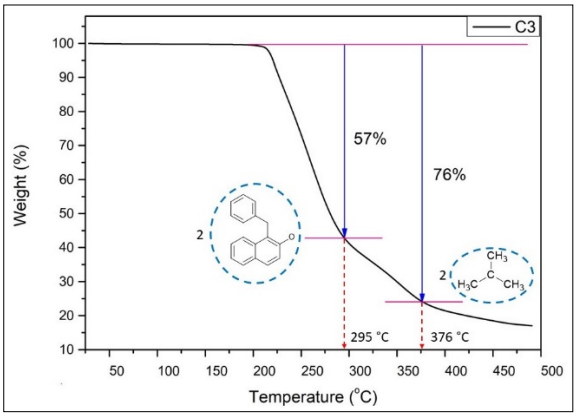

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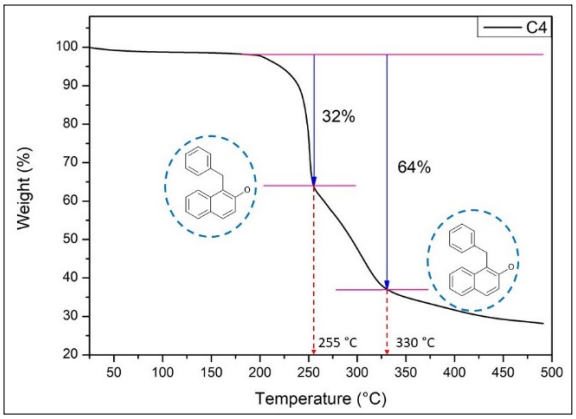

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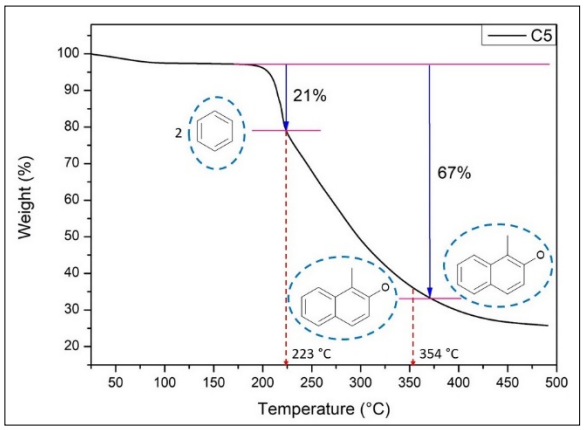


(e)

Fig S4. TGA plot of complexes (a) **C1**, (b) **C2**, (c) **C3**, (d) **C4**, (e) **C5**

Table S4 Calculated and experimental weight loss percentage for complexes **C1-C5**

Complex	Temperature (°C)	Calculated (%)	Experimental (%)
C1	242	33	33
	381	66	65
C2	227	31	31
	349	62	63
C3	295	56	57
	376	71	76
C4	255	32	32
	330	64	64
C5	223	22	21
	354	67	67

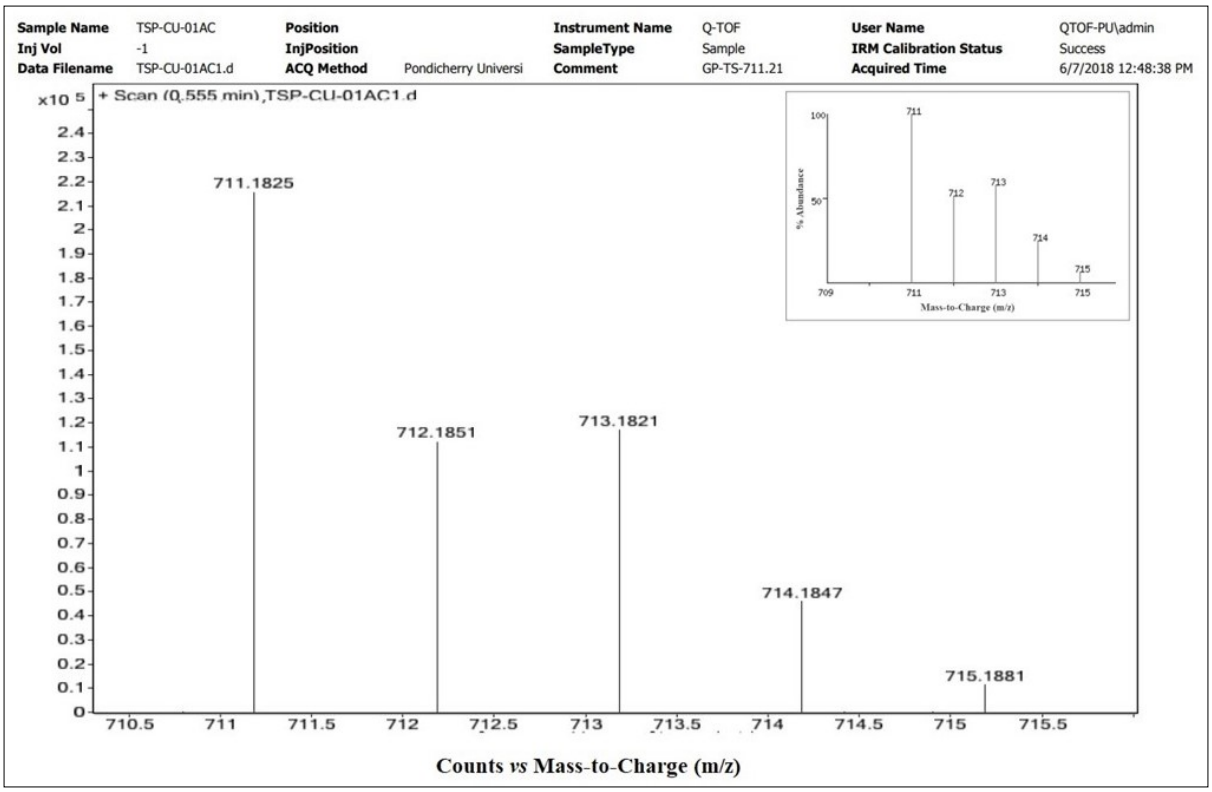


Fig S5. ESI-MS spectrum of complex **C1** in dichloromethane. Inset represents the theoretical isotopic distribution

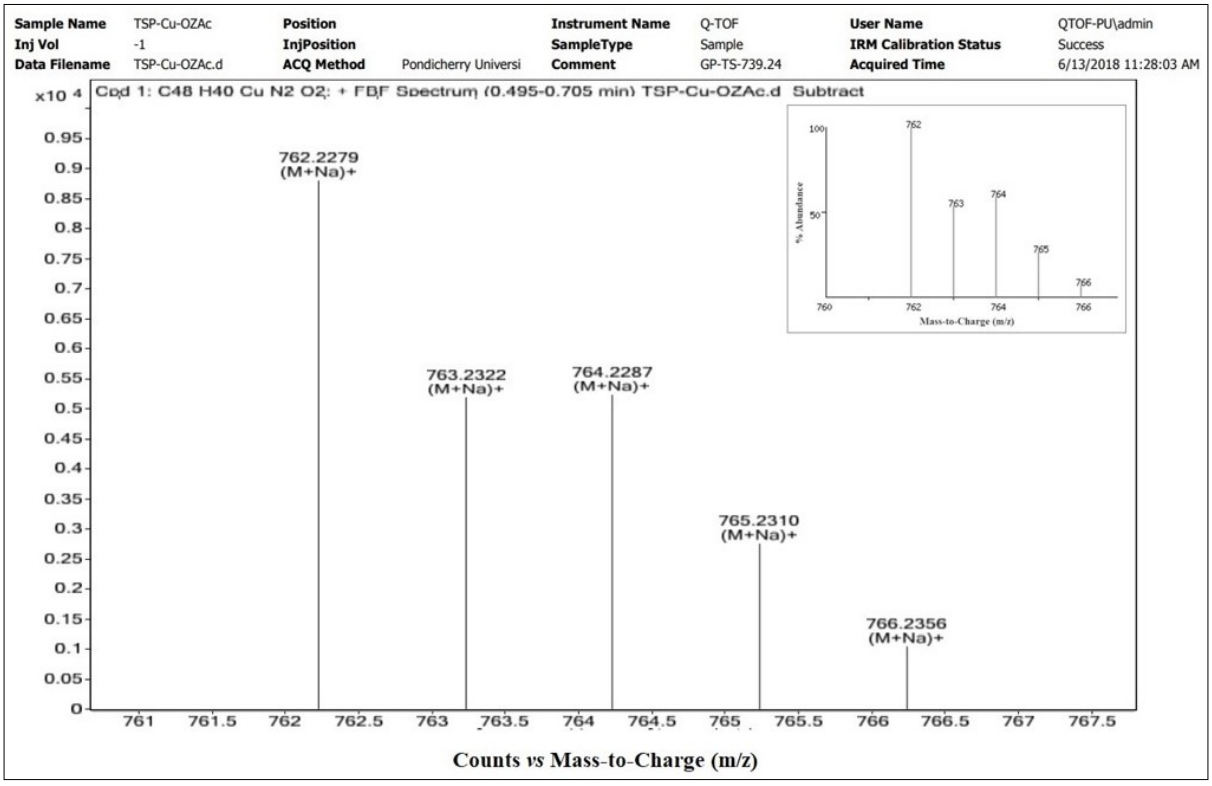


Fig S6. ESI-MS spectrum of complex **C2** in dichloromethane. Inset represents the theoretical isotopic distribution

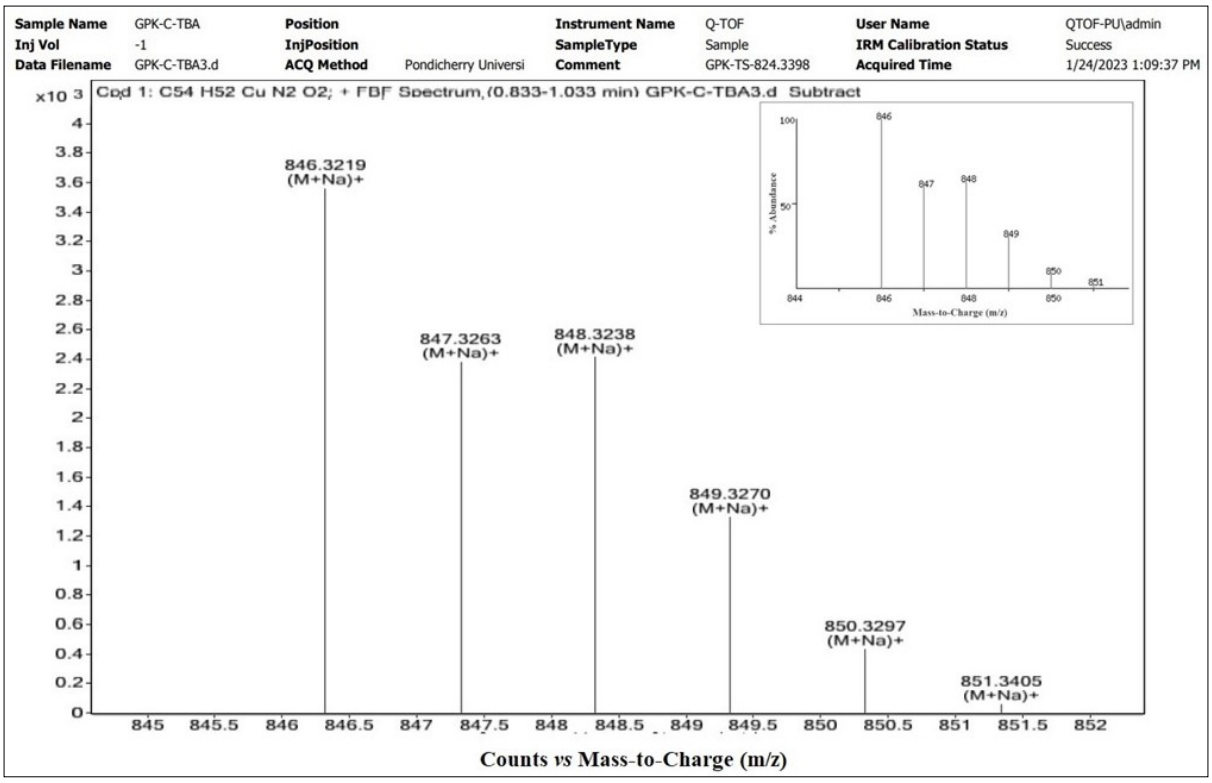


Fig S7. ESI-MS spectrum of complex **C3** in dichloromethane. Inset represents the theoretical isotopic distribution

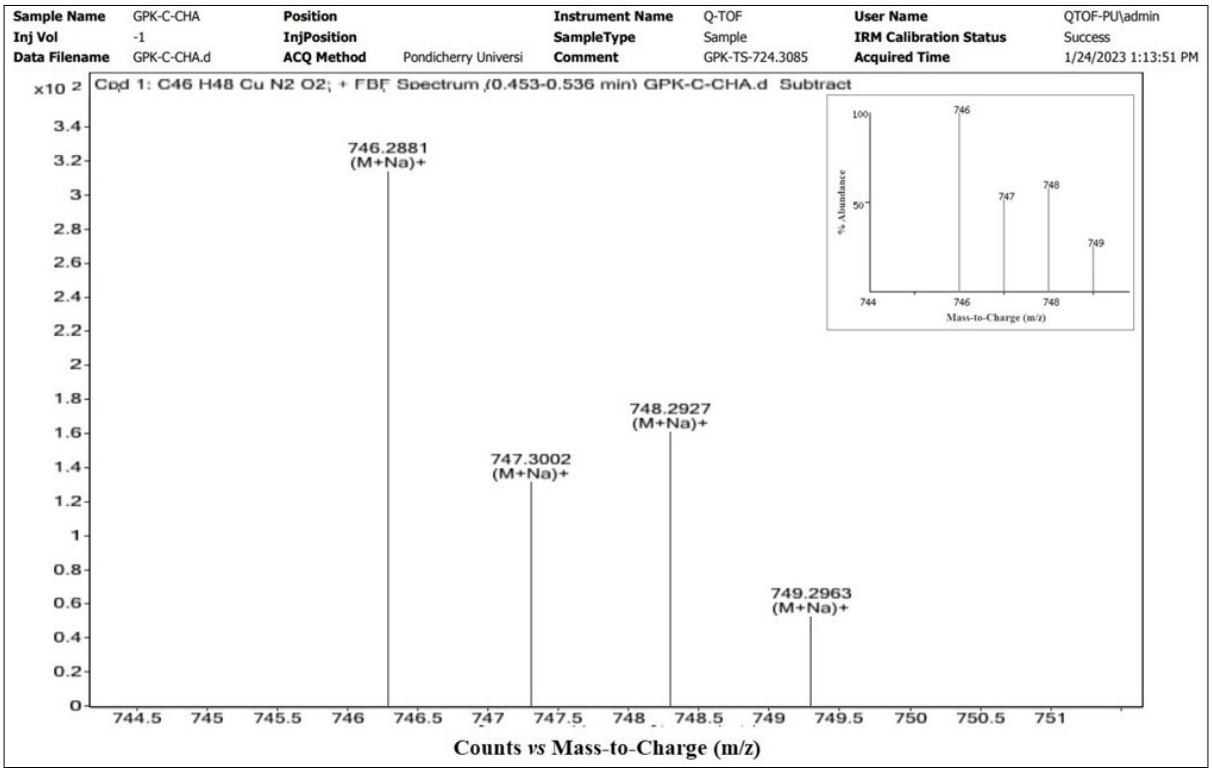


Fig S8. ESI-MS spectrum of complex **C4** in dichloromethane. Inset represents the theoretical isotopic distribution

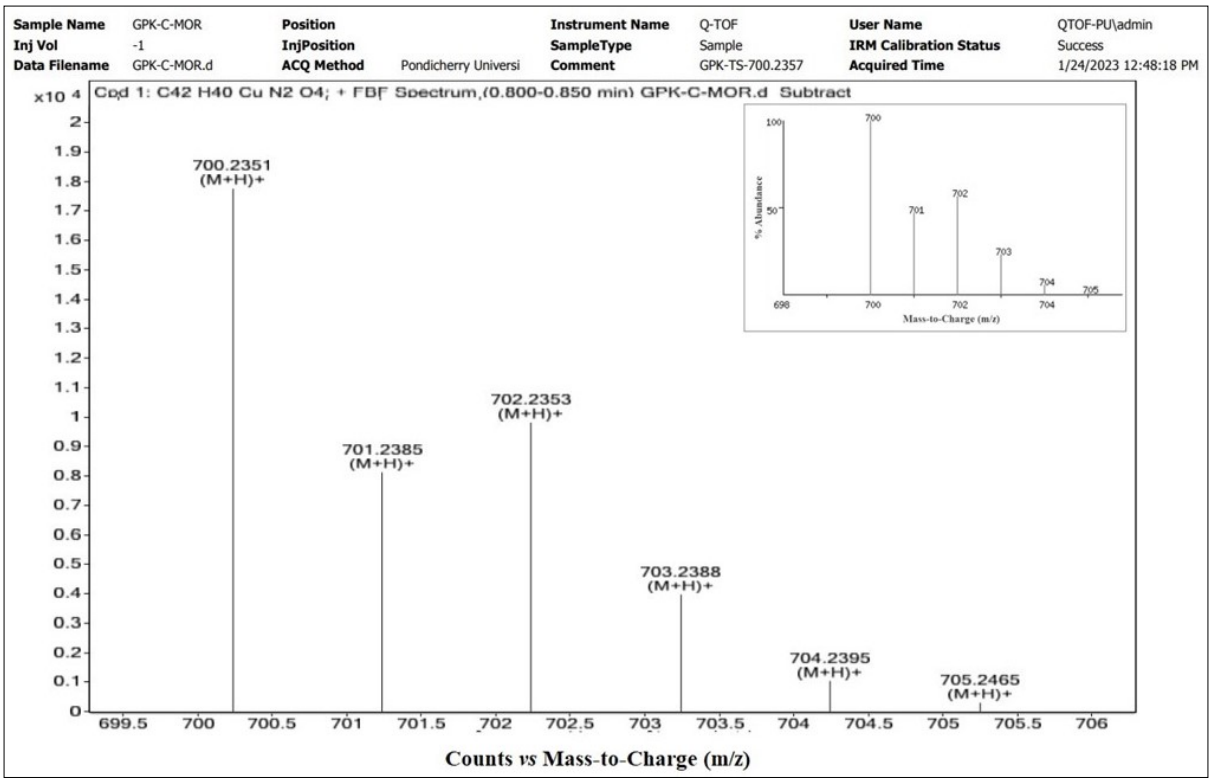


Fig S9. ESI-MS spectrum of complex **C5** in dichloromethane. Inset represents the theoretical isotopic distribution

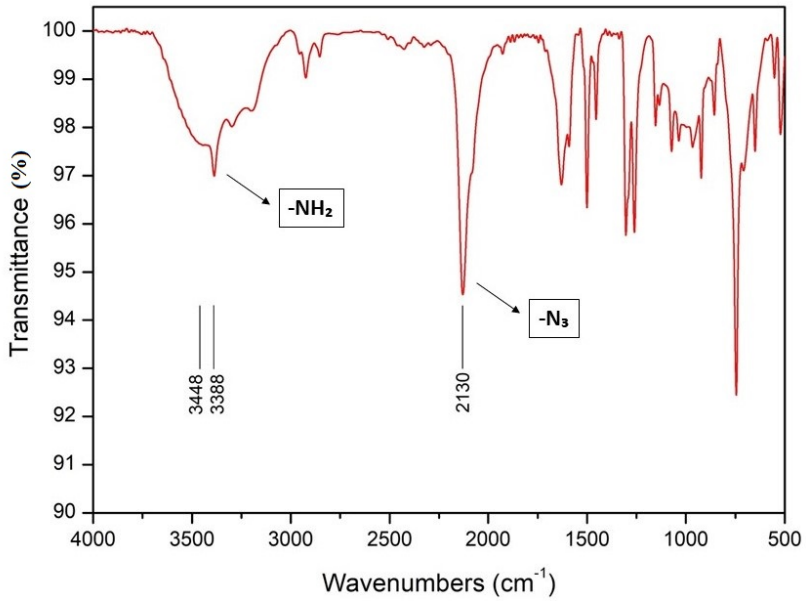
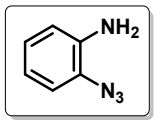


Fig S10. FT-IR spectrum of 2-azidoaniline (**2a**)

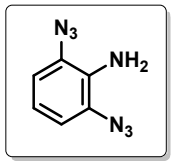
Characterization data for the products:

2-azidoaniline (2a)[1]:



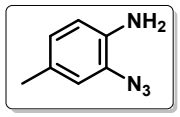
Brown solid, Yield = 85% (0.113 g, 0.85 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.04 (dd, J = 7.9, 1.3 Hz, 1H), 6.97 (td, J = 7.8, 1.4 Hz, 1H), 6.80 (td, J = 7.7, 1.4 Hz, 1H), 6.70 (dd, J = 7.9, 1.3 Hz, 1H), 3.79 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.22, 125.71, 125.33, 119.21, 118.48, 116.00; Selected FT-IR frequencies (KBr, cm^{-1}): 3448, 3388, 2130; ESI-MS: for $C_6H_6N_4$ $[M + Na]^+$ calculated m/z = 157.0485; found m/z = 157.0473.

2,6-diazidoaniline (2a')[1]:



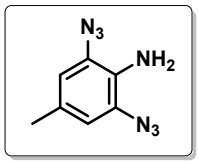
Light brown solid, Yield = 8% (0.014 g, 0.08 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.84 (d, J = 6.1 Hz, 2H), 6.81 (d, J = 5.7 Hz, 1H), 3.94 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 126.18, 118.55, 114.61, 111.61; ESI-MS: for $C_6H_5N_7$ $[M + H]^+$ calculated m/z = 176.0679; found m/z = 176.0677.

2-azido-4-methylaniline (2b)[2]:



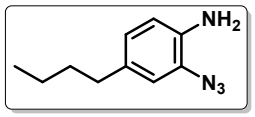
Brown liquid, Yield = 66% (0.097 g, 0.654 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.84 (s, 1H), 6.76 (ddd, J = 8.0, 1.7, 0.6 Hz, 1H), 6.61 (d, J = 8.0 Hz, 1H), 3.66 (s, 1H), 2.26 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.67, 128.95, 126.32, 125.21, 118.91, 116.18, 77.48, 77.16, 76.84, 20.66; ESI-MS: for $C_7H_8N_4$ $[M + H]^+$ calculated m/z = 149.0822; found m/z = 149.0816.

2,6-diazido-4-methylaniline (2b')[3]:



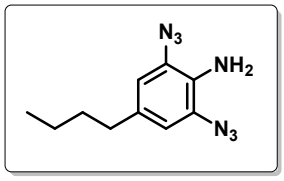
Light brown solid, Yield = 14% (0.026 g, 0.137 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.64 (s, 2H), 3.78 (s, 2H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 128.59, 127.75, 126.07, 115.20, 20.84; ESI-MS: for $C_7H_7N_7$ $[M + Na]^+$ calculated m/z = 212.0655; found m/z = 212.0661.

2-azido-4-butylaniline (2c):



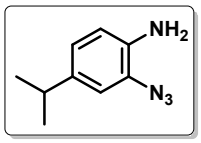
Brown liquid, Yield = 82% (0.155 g, 0.814 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.84 (s, 1H), 6.78 (dd, J = 8.0, 1.8 Hz, 1H), 6.62 (d, J = 8.0 Hz, 1H), 3.68 (s, 2H), 2.53 (t, 3H), 1.61 – 1.52 (m, 2H), 1.35 (dq, J = 14.5, 7.3 Hz, 2H), 0.93 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.85, 134.22, 125.68, 125.09, 118.23, 116.12, 77.48, 77.16, 76.84, 34.95, 33.96, 22.40, 14.06; ESI-MS: for $C_{10}H_{14}N_4$ $[M + H]^+$ calculated m/z = 191.1291; found m/z = 191.1293.

2,6-diazido-4-butylaniline (2c'):



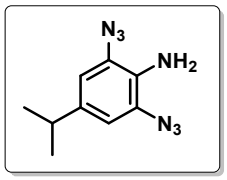
Brown solid, Yield = 7% (0.016 g, 0.069 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.64 (s, 2H), 3.79 (s, 2H), 2.53 (t, J = 7.7 Hz, 2H), 1.61 – 1.52 (m, 2H), 1.35 (dq, J = 14.5, 7.3 Hz, 2H), 0.94 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.89, 127.93, 125.98, 114.54, 35.15, 33.87, 22.42, 14.06; ESI-MS: for $C_{10}H_{13}N_7$ $[M + H]^+$ calculated m/z = 232.1305; found m/z = 232.1304.

2-azido-4-isopropylaniline (2d):



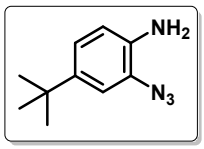
Brown liquid, Yield = 72% (0.126 g, 0.715 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.90 (s, 1H), 6.85 (d, J = 8.0 Hz, 1H), 6.65 (d, J = 8.0 Hz, 1H), 3.69 (s, 1H), 2.85 (dq, J = 13.5, 6.6 Hz, 1H), 1.25 (d, J = 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.29, 135.96, 124.99, 123.62, 116.31, 116.15, 77.48, 77.16, 76.84, 33.51, 24.20; ESI-MS: for $C_9H_{12}N_4$ $[M + H]^+$ calculated m/z = 177.1135; found m/z = 177.1134.

2,6-diazido-4-isopropylaniline (2d'):



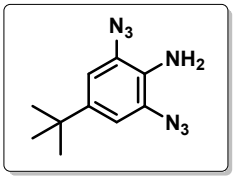
Brown solid, Yield = 13% (0.028 g, 0.128 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.69 (s, 2H), 3.80 (s, 2H), 2.90 – 2.77 (m, 1H), 1.24 (d, J = 6.9 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.00, 128.08, 125.96, 112.62, 33.84, 24.16; ESI-MS: for $C_9H_{11}N_7$ $[M + H]^+$ calculated m/z = 218.1149; found m/z = 218.1147.

2-azido-4-(tert-butyl)aniline (2e)[1]:



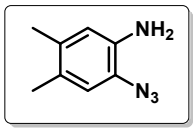
Brown liquid, Yield = 68% (0.129 g, 0.678 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.02 (s, 1H), 6.98 (dd, J = 8.3, 2.1 Hz, 1H), 6.65 (d, J = 8.3 Hz, 1H), 3.69 (s, 1H), 1.29 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.71, 135.71, 124.72, 122.75, 115.90, 115.40, 34.40, 31.57; ESI-MS: for $C_{10}H_{14}N_4$ $[M + H]^+$ calculated m/z = 191.1291; found m/z = 191.1286.

2,6-diazido-4-(tert-butyl)aniline (2e')[1]:



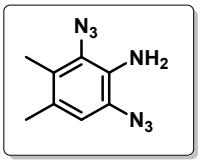
Brown solid, Yield = 18% (0.041 g, 0.177 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.83 (s, 2H), 3.81 (s, 2H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.39, 127.85, 125.63, 111.77, 34.72, 31.47; ESI-MS: for $C_{10}H_{13}N_7$ $[M + H]^+$ calculated m/z = 232.1305; found m/z = 232.1301.

2-azido-4,5-dimethylaniline (2f)[4]:



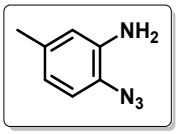
Brown solid, Yield = 70% (0.113 g, 0.696 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.79 (s, 1H), 6.51 (s, 1H), 3.60 (s, 2H), 2.17 (s, 3H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.74, 134.03, 127.53, 122.60, 119.45, 117.77, 77.48, 77.16, 76.84, 19.42, 19.03; ESI-MS: for $C_8H_{10}N_4$ $[M + H]^+$ calculated m/z = 163.0978; found m/z = 163.0978.

2,6-diazido-3,4-dimethylaniline (2f'):



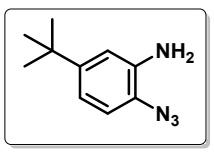
Brown solid, Yield = 10% (0.020 g, 0.098 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.71 (s, 1H), 3.88 (s, 2H), 2.24 (s, 3H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 130.48, 127.94, 127.33, 125.69, 123.23, 117.12, 19.84, 14.02; ESI-MS: for $C_8H_9N_7$ $[M + H]^+$ calculated m/z = 204.0992; found m/z = 204.0987.

2-azido-5-methylaniline (2g)[4]:



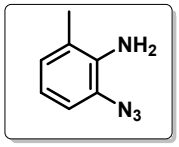
Brown liquid, Yield = 68% (0.100 g, 0.676 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.91 (d, J = 8.0 Hz, 1H), 6.60 (dd, J = 8.0, 0.6 Hz, 1H), 6.52 (s, 1H), 3.73 (s, 1H), 2.24 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.93, 135.64, 122.66, 119.98, 118.33, 116.73, 21.12; ESI-MS: for $C_7H_8N_4$ $[M + H]^+$ calculated m/z = 149.0822; found m/z = 149.0813.

2-azido-5-(tert-butyl)aniline (2h):



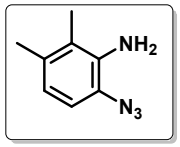
Brown liquid, Yield = 57% (0.108 g, 0.567 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, J = 8.3 Hz, 0H), 6.83 (dd, J = 8.3, 2.2 Hz, 0H), 6.74 (s, 0H), 3.76 (s, 0H), 1.28 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.18, 137.64, 122.70, 118.13, 116.47, 113.46, 34.50, 31.43; ESI-MS: for $C_{10}H_{14}N_4$ $[M + H]^+$ calculated m/z = 191.1291; found m/z = 191.1289.

2-azido-6-methylaniline (2i)[2]:



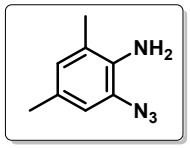
Brown liquid, Yield = 63% (0.093 g, 0.627 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.93 (dd, J = 7.9, 0.7 Hz, 1H), 6.86 (dd, J = 7.5, 0.6 Hz, 1H), 6.73 (t, J = 7.7 Hz, 1H), 3.76 (s, 1H), 2.16 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.46, 126.88, 124.97, 123.61, 118.51, 116.10, 77.48, 17.47; ESI-MS: for $C_7H_8N_4$ $[M + H]^+$ calculated m/z = 149.0822; found m/z = 149.0817.

6-azido-2,3-dimethylaniline (2j)[4]:



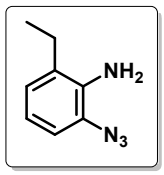
Brown liquid, Yield = 58% (0.094 g, 0.579 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.82 (d, J = 8.1 Hz, 1H), 6.65 (d, J = 8.1 Hz, 1H), 3.75 (s, 1H), 2.25 (s, 1H), 2.06 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.28, 133.67, 123.04, 122.01, 120.34, 115.19, 20.40, 13.20; ESI-MS: for $C_8H_{10}N_4$ $[M + H]^+$ calculated m/z = 163.0978; found m/z = 163.0965.

2-azido-4,6-dimethylaniline (2k)[1]:



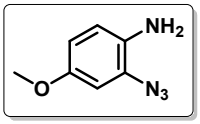
Brown solid, Yield = 71% (0.115 g, 0.709 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.74 (s, 1H), 6.69 (s, 1H), 3.62 (s, 1H), 2.25 (s, 1H), 2.13 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.89, 128.12, 127.68, 124.86, 123.75, 116.45, 20.64, 17.42; ESI-MS: for $C_8H_{10}N_4$ $[M]^+$ calculated m/z = 162.0905; found m/z = 162.0900.

2-azido-6-ethylaniline (2l)[2]:



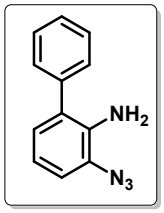
Brown liquid, Yield = 61% (0.098 g, 0.604 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (dd, J = 7.9, 1.1 Hz, 1H), 6.91 (d, 1H), 6.79 (t, J = 7.7 Hz, 1H), 3.82 (s, 1H), 2.52 (q, J = 7.5 Hz, 2H), 1.26 (t, J = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.84, 129.27, 125.08, 124.78, 118.63, 115.93, 24.10, 12.87; ESI-MS: for $C_8H_{10}N_4$ $[M + H]^+$ calculated m/z = 163.0978; found m/z = 163.0936.

2-azido-4-methoxyaniline (2m)[1]:



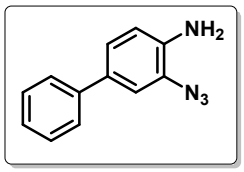
Brown solid, Yield = 60% (0.098 g, 0.596 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.65 (d, J = 8.6 Hz, 1H), 6.62 (s, 1H), 6.55 (dd, J = 8.6, 2.6 Hz, 1H), 3.76 (s, 3H), 3.52 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.32, 131.93, 126.27, 117.15, 111.35, 104.72, 56.00; ESI-MS: for $C_7H_8N_4O$ $[M + H]^+$ calculated m/z = 165.0771; found m/z = 165.0780.

3-azido-[1,1'-biphenyl]-2-amine (2n):[1]



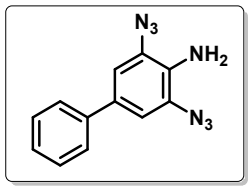
Brown solid, Yield = 66% (0.138 g, 0.656 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.42 (m, J = 5.5 Hz, 2H), 7.42 – 7.34 (m, 1H), 7.07 (d, J = 7.8 Hz, 1H), 6.96 (d, J = 7.5 Hz, 1H), 6.86 (t, J = 7.7 Hz, 1H), 3.96 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.81, 135.64, 129.02, 128.99, 128.51, 127.59, 126.86, 125.32, 118.44, 117.41; ESI-MS: for $C_{12}H_{10}N_4$ $[M + H]^+$ calculated m/z = 211.0978; found m/z = 211.0979.

3-azido-[1,1'-biphenyl]-4-amine (2o)[2]:



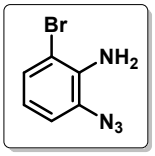
Brown solid, Yield = 81% (0.170 g, 0.808 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (dd, J = 8.3, 1.2 Hz, 1H), 7.42 (t, J = 7.7 Hz, 1H), 7.32 (d, J = 7.4 Hz, 1H), 7.25 (s, 1H), 7.21 (dd, J = 8.2, 2.0 Hz, 1H), 6.77 (d, J = 8.2 Hz, 1H), 3.87 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.54, 137.62, 132.63, 128.93, 126.91, 126.61, 125.61, 124.57, 117.02, 116.25; ESI-MS: for $C_{12}H_{10}N_4$ $[M + H]^+$ calculated m/z = 211.0978; found m/z = 211.0977.

3,5-diazido-[1,1'-biphenyl]-4-amine (2o'):



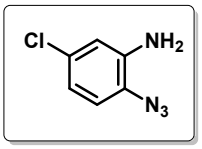
Brown solid, Yield = 11% (0.027 g, 0.107 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, J = 7.7 Hz, 2H), 7.44 (t, J = 7.4 Hz, 2H), 7.34 (t, J = 7.2 Hz, 1H), 7.04 (s, 2H), 4.00 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.92, 132.23, 129.56, 129.04, 127.38, 126.65, 126.37, 113.33; ESI-MS: for $C_{12}H_9N_7$ $[M + H]^+$ calculated m/z = 252.0992; found m/z = 252.0992.

2-azido-6-bromoaniline (2p)[5]:



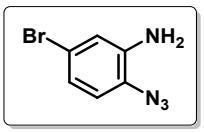
Brown solid, Yield = 58% (0.123 g, 0.577 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 (dd, J = 8.1, 1.2 Hz, 1H), 6.98 (dd, J = 7.9, 1.2 Hz, 1H), 6.65 (t, J = 8.0 Hz, 1H), 4.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.52, 128.74, 126.01, 118.92, 117.32, 109.57; ESI-MS: for $C_6H_5BrN_4$ $[M + H]^+$ calculated m/z = 212.9770; found m/z = 212.9774.

2-azido-5-chloroaniline (2q)[5]:



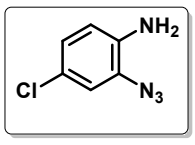
Orange liquid, Yield = 53% (0.089 g, 0.527 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.92 (d, J = 8.4 Hz, 1H), 6.74 (dd, J = 8.4, 2.3 Hz, 1H), 6.67 (s, 1H), 3.88 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.20, 130.84, 123.88, 119.31, 118.78, 115.50; ESI-MS: for $C_6H_5ClN_4$ $[M + H]^+$ calculated m/z = 169.0276; found m/z = 169.0289.

2-azido-5-bromoaniline (2r)[5]:



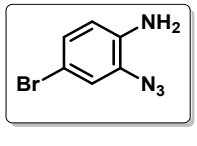
Brown liquid, Yield = 56% (0.119 g, 0.558 mmol); ^{1}H NMR (400 MHz, MeOD) δ 6.91 (d, J = 8.3 Hz, 1H), 6.87 (s, 1H), 6.80 (d, J = 8.4 Hz, 1H), 4.88 (s, 1H); ^{13}C NMR (100 MHz, MeOD) δ 142.26, 125.30, 121.48, 120.64, 119.38, 118.97; ESI-MS: for $C_6H_5BrN_4$ $[M + H]^+$ calculated m/z = 212.9770; found m/z = 212.9772.

2-azido-4-chloroaniline (2s)[2]:



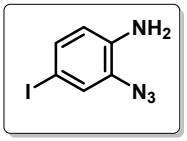
Brown solid, Yield =63% (0.105 g, 0.626 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00 (s, 1H), 6.91 (dd, J = 8.5, 2.2 Hz, 1H), 6.61 (d, J = 8.5 Hz, 1H), 3.80 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.89, 126.34, 125.66, 123.36, 118.41, 116.65; ESI-MS: for $C_6H_5ClN_4$ $[M + H]^+$ calculated m/z = 169.0276; found m/z = 169.0287.

2-azido-4-bromoaniline (2t)[2]:



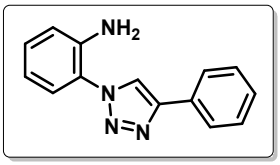
Brown solid, Yield = 70% (0.149 g, 0.699 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 (s, 1H), 7.04 (dd, J = 8.5, 2.1 Hz, 1H), 6.56 (d, J = 8.5 Hz, 1H), 3.81 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.36, 128.52, 126.62, 121.18, 117.03, 109.92; ESI-MS: for $C_6H_5BrN_4$ $[M + H]^+$ calculated m/z = 212.9770; found m/z = 212.9767.

2-azido-4-iodoaniline (2u)[6]:



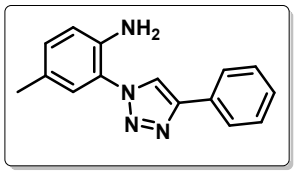
Brown solid, Yield = 61% (0.158 g, 0.607 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (s, 1H), 7.21 (d, J = 8.3 Hz, 1H), 6.45 (d, J = 8.3 Hz, 1H), 3.83 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.04, 134.42, 126.86, 126.78, 117.50, 78.51; ESI-MS: for $C_6H_5IN_4$ $[M + H]^+$ calculated m/z = 260.9632; found m/z = 260.9629.

2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3a)[7]:



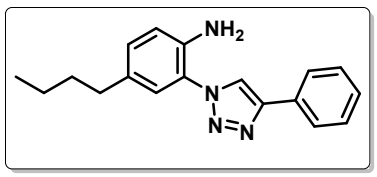
Light yellow solid, Yield = 81% (0.047 g, 0.202 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.90 (d, J = 7.1 Hz, 1H), 7.46 (t, J = 8.1, 6.9 Hz, 1H), 7.37 (t, 1H), 7.29 – 7.20 (m, 1H), 6.89 (dd, J = 8.0, 1.1 Hz, 1H), 6.84 (td, J = 7.7, 1.3 Hz, 1H), 4.60 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.74, 141.04, 130.26, 129.06, 128.56, 125.94, 124.43, 123.17, 120.40, 118.39, 117.77; ESI-MS: for $C_{14}H_{12}N_4$ $[M + H]^+$ calculated m/z = 237.1135; found m/z = 237.1128.

4-methyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3b)[7]:



Yellow solid, Yield = 83% (0.052 g, 0.207 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.90 (d, J = 7.4 Hz, 2H), 7.46 (t, J = 7.4 Hz, 2H), 7.38 (d, J = 7.4 Hz, 1H), 7.07 (d, J = 12.2 Hz, 2H), 6.81 (d, J = 8.0 Hz, 1H), 4.42 (s, 2H), 2.30 (s,3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.68, 138.47, 130.96, 130.35, 129.06, 128.52, 128.14, 125.93, 124.74, 123.18, 120.39, 117.91, 20.35; ESI-MS: for $C_{15}H_{14}N_4$ $[M + Na]^+$ calculated m/z = 273.1111; found m/z = 273.1112.

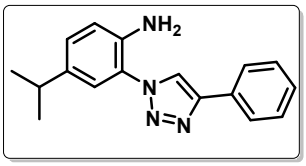
4-butyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3c):



Yellow solid, Yield = 78% (0.056 g, 0.195 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.91 (d, J = 7.3 Hz, 2H), 7.46 (t, J = 7.2 Hz, 2H), 7.38 (d, J = 7.1 Hz, 1H), 7.08 (d, J = 6.1 Hz, 2H), 6.83 (d, J = 7.5 Hz, 1H), 4.42 (s, 2H), 2.57 (t, J = 7.4 Hz, 2H), 1.64 – 1.52 (m, 2H), 1.43 – 1.30 (m, 2H), 0.93 (t, J

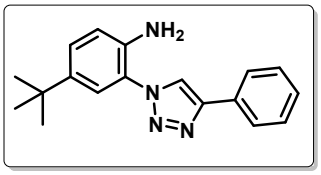
= 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.72, 138.67, 135.16, 133.46, 130.36, 129.08, 128.54, 125.98, 124.16, 123.23, 120.43, 117.89, 34.61, 33.83, 22.38, 14.09; ESI-MS: for $C_{18}H_{20}N_4$ $[M + H]^+$ calculated m/z = 293.1761; found m/z = 293.1759.

4-isopropyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3d):



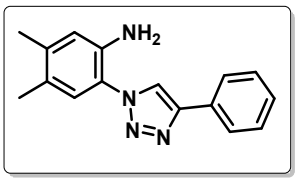
Yellow solid, Yield = 85% (0.059 g, 0.212 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.91 (d, J = 7.2 Hz, 2H), 7.46 (t, J = 10.4, 4.7 Hz, 2H), 7.37 (d, 1H), 7.14 (d, J = 2.0 Hz, 1H), 7.12 (s, 1H), 6.84 (d, J = 8.0 Hz, 1H), 4.40 (s, 2H), 2.87 (hept, J = 6.9 Hz, 1H), 1.25 (d, J = 6.9 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.65, 139.45, 138.78, 130.34, 129.01, 128.46, 128.42, 125.91, 123.13, 122.32, 120.49, 117.86, 33.16, 24.15; ESI-MS: for $C_{17}H_{18}N_4$ $[M + H]^+$ calculated m/z = 279.1604; found m/z = 279.1600.

4-(tert-butyl)-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3e):



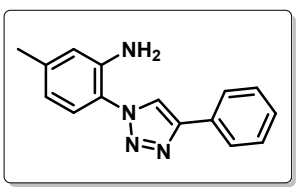
Yellow solid, Yield = 78% (0.056 g, 0.195 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.92 (d, J = 7.5 Hz, 2H), 7.47 (t, J = 7.4 Hz, 2H), 7.38 (d, J = 7.3 Hz, 1H), 7.30 (d, J = 8.5 Hz, 1H), 7.24 (s, 1H), 6.86 (d, J = 8.4 Hz, 1H), 4.37 (s, 2H), 1.32 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.77, 142.02, 138.54, 130.40, 129.08, 128.54, 127.56, 125.98, 122.97, 121.49, 120.58, 117.63, 34.20, 31.52; ESI-MS: for $C_{18}H_{20}N_4$ $[M + H]^+$ calculated m/z = 293.1761; found m/z = 293.1751.

4,5-dimethyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3f):



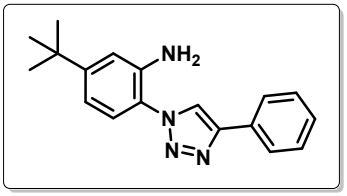
Light yellow solid, Yield = 87% (0.057 g, 0.217 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.89 (d, J = 7.8 Hz, 2H), 7.45 (t, J = 7.5 Hz, 2H), 7.37 (d, 1H), 7.02 (s, 1H), 6.69 (s, 1H), 4.36 (s, 2H), 2.23 (s, 3H), 2.20 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.51, 139.03, 138.47, 130.40, 128.99, 128.41, 126.85, 125.87, 125.03, 121.08, 120.37, 119.04, 19.70, 18.75; ESI-MS: for $C_{16}H_{16}N_4$ $[M + H]^+$ calculated m/z = 265.1448; found m/z = 265.1453.

5-methyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3g):



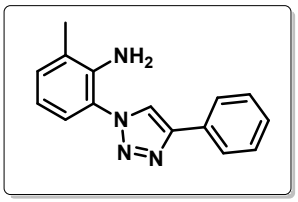
Light yellow solid, Yield = 76% (0.047 g, 0.188 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.90 (d, J = 7.1 Hz, 2H), 7.46 (t, J = 8.1, 6.9 Hz, 2H), 7.37 (t, 1H), 7.15 (d, J = 8.0 Hz, 1H), 6.71 (s, 1H), 6.66 (dd, 1H), 4.51 (s, 2H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.66, 140.77, 140.57, 130.38, 129.06, 128.51, 125.94, 124.26, 121.09, 120.42, 119.39, 118.15, 21.37; ESI-MS: for $C_{15}H_{14}N_4$ $[M + H]^+$ calculated m/z = 251.1291; found m/z = 251.1287.

5-(tert-butyl)-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3h):



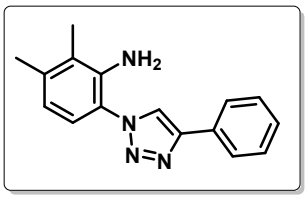
Yellow solid, Yield = 83% (0.06 g, 0.207 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.82 (dd, J = 8.0, 1.0 Hz, 2H), 7.37 (t, J = 7.6 Hz, 2H), 7.28 (d, J = 7.6 Hz, 1H), 7.11 (d, J = 8.4 Hz, 1H), 6.83 (d, J = 2.0 Hz, 1H), 6.79 (dd, J = 8.3, 1.9 Hz, 1H), 4.48 (s, 2H), 1.24 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.75, 147.56, 140.44, 130.34, 129.00, 128.44, 125.88, 123.97, 120.88, 120.33, 115.83, 114.80, 34.77, 31.24; ESI-MS: for $C_{18}H_{20}N_4$ $[M + H]^+$ calculated m/z = 293.1761; found m/z = 293.1756.

2-methyl-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3i):



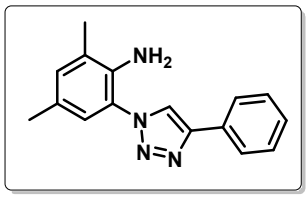
Light yellow solid, Yield = 80% (0.049 g, 0.198 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.90 (d, J = 7.1 Hz, 2H), 7.45 (t, J = 8.1, 6.9 Hz, 2H), 7.37 (d, J = 7.4 Hz, 1H), 7.16 (d, J = 7.5 Hz, 1H), 7.13 (d, J = 8.2 Hz, 1H), 6.77 (t, J = 7.7 Hz, 1H), 4.51 (s, 2H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.68, 139.46, 131.27, 130.28, 129.02, 128.49, 125.88, 124.74, 122.88, 122.50, 120.78, 117.61, 17.82; ESI-MS: for $C_{15}H_{14}N_4$ $[M + K]^+$ calculated m/z = 289.0850; found m/z = 289.0847.

2,3-dimethyl-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3j):



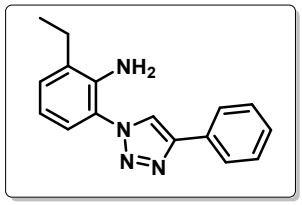
Yellow solid, Yield = 81% (0.053 g, 0.202 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.90 (d, J = 7.1 Hz, 2H), 7.45 (t, J = 8.1, 6.9 Hz, 2H), 7.37 (d, J = 7.4 Hz, 1H), 7.03 (d, J = 8.1 Hz, 1H), 6.69 (d, J = 8.1 Hz, 1H), 4.44 (s, 2H), 2.34 (s, 3H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.68, 139.36, 138.52, 130.39, 129.04, 128.47, 125.91, 122.80, 121.75, 121.53, 120.95, 119.78, 20.87, 13.41; ESI-MS: for $C_{16}H_{16}N_4$ $[M + H]^+$ calculated m/z = 265.1448; found m/z = 265.1452.

2,4-dimethyl-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3k)[1]:



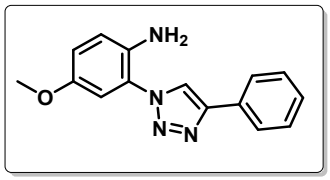
Yellow solid, Yield = 85% (0.056 g, 0.212 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.90 (d, J = 7.1 Hz, 2H), 7.45 (t, J = 8.1, 6.9 Hz, 2H), 7.37 (d, J = 7.4 Hz, 1H), 6.99 (s, 1H), 6.95 (s, 1H), 4.33 (s, 2H), 2.28 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.63, 136.90, 132.18, 130.35, 129.02, 128.46, 127.22, 125.88, 124.85, 122.91, 122.75, 120.76, 20.29, 17.81; ESI-MS: for $C_{16}H_{16}N_4$ $[M + Na]^+$ calculated m/z = 287.1267; found m/z = 287.1267.

2-ethyl-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3l):



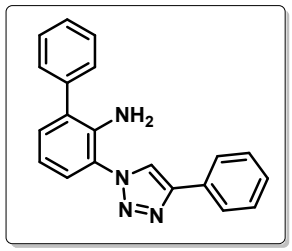
Light yellow solid, Yield = 82% (0.054 g, 0.205 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.91 (d, J = 7.5 Hz, 2H), 7.46 (t, J = 7.4 Hz, 2H), 7.38 (d, J = 7.4 Hz, 1H), 7.20 (d, J = 7.5 Hz, 1H), 7.14 (d, J = 7.9 Hz, 1H), 6.83 (t, J = 7.7 Hz, 1H), 4.51 (s, 2H), 2.61 (q, J = 7.5 Hz, 2H), 1.31 (t, J = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.77, 141.98, 139.07, 130.38, 129.35, 129.08, 128.54, 125.95, 123.24, 122.61, 120.98, 117.90, 24.41, 12.88; ESI-MS: for $C_{16}H_{16}N_4$ $[M + Na]^+$ calculated m/z = 287.1267; found m/z = 287.1264.

4-methoxy-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3m):



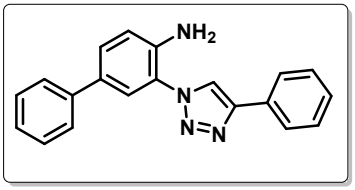
Light yellow solid, Yield = 75% (0.05 g, 0.187 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.90 (d, J = 7.2 Hz, 2H), 7.46 (t, J = 7.5 Hz, 2H), 7.37 (d, J = 7.4 Hz, 1H), 6.88 (dd, J = 9.2, 2.1 Hz, 1H), 6.86 (s, 1H), 6.84 (d, J = 6.3 Hz, 1H), 4.23 (s, 2H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.53, 147.79, 134.62, 130.24, 129.06, 128.57, 125.95, 123.68, 120.45, 119.06, 116.77, 109.96, 56.11; ESI-MS: for $C_{15}H_{14}N_4O$ $[M + H]^+$ calculated m/z = 267.1240; found m/z = 267.1239.

3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)-[1,1'-biphenyl]-2-amine (3n):



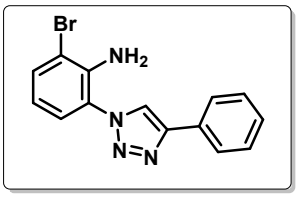
Yellow solid, Yield = 88% (0.068 g, 0.219 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.92 (d, J = 7.6 Hz, 2H), 7.53 – 7.44 (m, J = 8.5 Hz, 6H), 7.44 – 7.35 (m, J = 16.9, 9.6 Hz, 2H), 7.30 – 7.20 (m, J = 14.8, 7.8 Hz, 2H), 6.91 (t, J = 7.7 Hz, 1H), 4.61 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.83, 138.91, 138.36, 131.53, 130.29, 130.22, 129.26, 129.10, 128.59, 128.06, 125.96, 124.18, 123.44, 120.93, 117.83; ESI-MS: for $C_{20}H_{16}N_4$ $[M + H]^+$ calculated m/z = 313.1448; found m/z = 313.1444.

3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)-[1,1'-biphenyl]-4-amine (3o):



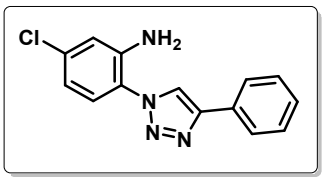
Yellow solid, Yield = 87% (0.067 g, 0.217 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.92 (dd, J = 8.3, 1.3 Hz, 2H), 7.55 (dd, J = 8.3, 1.2 Hz, 2H), 7.52 – 7.48 (m, 2H), 7.48 – 7.42 (m, 3H), 7.40 (d, J = 4.5 Hz, 1H), 7.37 (d, J = 7.3 Hz, 1H), 7.32 (t, J = 7.3 Hz, 1H), 6.97 (d, J = 8.9 Hz, 1H), 4.69 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.83, 140.25, 139.77, 131.81, 130.23, 129.09, 129.02, 128.83, 128.61, 127.14, 126.52, 125.97, 123.42, 122.87, 120.41, 118.19; ESI-MS: for $C_{20}H_{16}N_4$ $[M + H]^+$ calculated m/z = 313.1448; found m/z = 313.1446.

2-bromo-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3p):



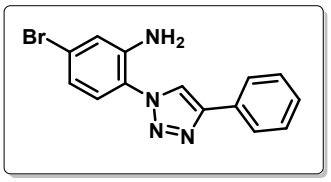
Orange solid, Yield = 79% (0.061 g, 0.196 mmol); 1H NMR (400 MHz, CDCl3) δ 8.05 (s, 1H), 7.91 (d, J = 7.2 Hz, 2H), 7.55 (d, J = 7.9 Hz, 1H), 7.47 (t, J = 7.4 Hz, 2H), 7.40 (d, J = 7.2 Hz, 1H), 7.25 (d, J = 9.3 Hz, 1H), 6.73 (t, J = 7.9 Hz, 1H), 5.13 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.98, 139.49, 133.62, 130.04, 129.14, 128.76, 125.99, 123.76, 123.43, 120.55, 118.22, 111.34; ESI-MS: for $C_{14}H_{11}BrN_4$ $[M + H]^+$ calculated m/z = 315.0240; found m/z = 315.0238.

5-chloro-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3q):



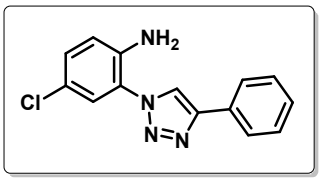
Yellow solid, Yield = 73% (0.049 g, 0.181 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.89 (d, J = 7.1 Hz, 2H), 7.46 (t, J = 10.6, 4.3 Hz, 2H), 7.39 (d, J = 7.4 Hz, 1H), 7.20 (d, J = 8.5 Hz, 1H), 6.90 (s, 1H), 6.81 (dd, J = 8.5, 2.2 Hz, 1H), 4.74 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.94, 142.08, 135.80, 130.07, 129.13, 128.73, 125.99, 125.33, 121.65, 120.26, 118.33, 117.28; ESI-MS: for $C_{14}H_{11}ClN_4$ $[M + H]^+$ calculated m/z = 271.0745; found m/z = 271.0738.

5-bromo-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3r)[8]:



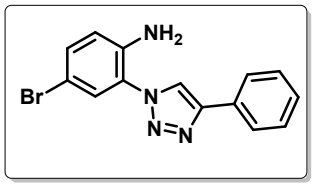
Orange solid, Yield = 80% (0.063 g, 0.199 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.89 (d, J = 8.1 Hz, 2H), 7.46 (t, 2H), 7.39 (dd, J = 7.3, 1.5 Hz, 1H), 7.13 (dd, J = 8.5, 1.3 Hz, 1H), 7.06 (s, 1H), 6.96 (d, J = 8.4 Hz, 1H), 4.75 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.94, 142.22, 130.04, 129.13, 128.74, 125.98, 125.45, 123.74, 122.05, 121.21, 120.25, 120.19; ESI-MS: for $C_{14}H_{11}BrN_4$ $[M + H]^+$ calculated m/z = 315.0240; found m/z = 315.0232.

4-chloro-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3s):



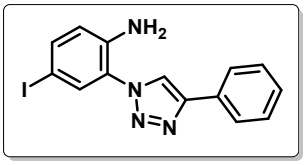
Yellow solid, Yield = 75% (0.051 g, 0.188 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.89 (d, J = 7.5 Hz, 2H), 7.46 (t, J = 7.3 Hz, 2H), 7.39 (d, J = 7.5 Hz, 1H), 7.28 (s, 1H), 7.20 (d, J = 8.7 Hz, 1H), 6.84 (d, J = 8.6 Hz, 1H), 4.70 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.94, 139.67, 130.07, 129.98, 129.12, 128.75, 125.98, 123.99, 123.39, 122.66, 120.16, 118.80; ESI-MS: for $C_{14}H_{11}ClN_4$ $[M + H]^+$ calculated m/z = 271.0745; found m/z = 271.0750.

4-bromo-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3t):



Orange solid, Yield = 78% (0.061 g, 0.193 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.89 (d, J = 7.5 Hz, 2H), 7.46 (t, J = 7.3 Hz, 2H), 7.41 (d, J = 6.8 Hz, 1H), 7.38 (s, 1H), 7.33 (d, J = 8.6 Hz, 1H), 6.79 (d, J = 8.6 Hz, 1H), 4.72 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.94, 140.14, 132.89, 129.97, 129.13, 128.76, 126.76, 125.99, 123.77, 120.17, 119.14, 109.13; ESI-MS: for $C_{14}H_{11}BrN_4$ $[M + H]^+$ calculated m/z = 315.0240; found m/z = 315.0232.

4-iodo-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (3u):



Yellow solid, Yield = 88% (0.079 g, 0.219 mmol); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.89 (d, 2H), 7.56 (s, 1H), 7.52 – 7.42 (m, 3H), 7.38 (d, J = 6.6 Hz, 1H), 6.67 (d, J = 8.5 Hz, 1H), 4.74 (s, 2H); ^{13}C NMR (100 MHz, MeOD) δ 148.93, 143.47, 139.98, 134.26, 131.36, 129.99, 129.54, 126.87, 125.02, 123.00, 120.28, 76.62; ESI-MS: for $C_{14}H_{11}IN_4$ $[M + H]^+$ calculated m/z = 363.0101; found m/z = 363.0095.

Copies of ^{1}H and ^{13}C NMR Spectra of the Products

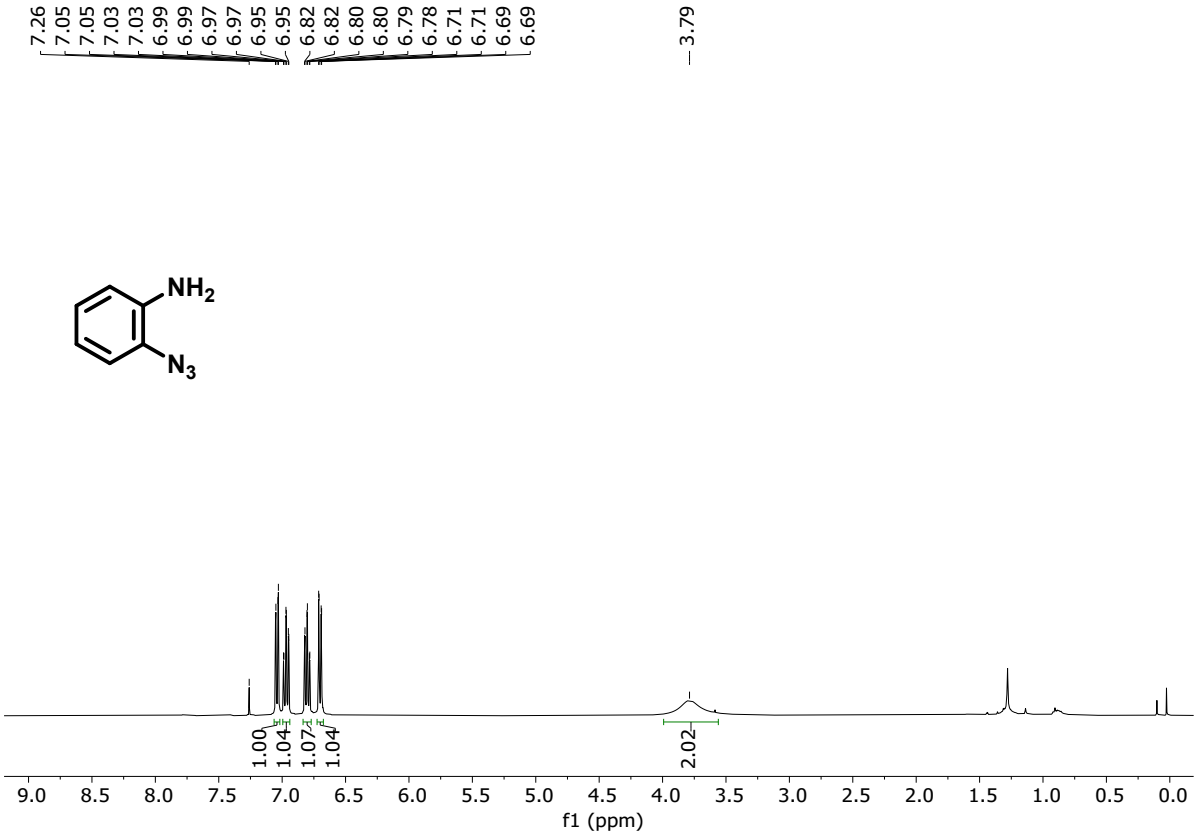


Fig S11. ^{1}H NMR spectrum of 2-azidoaniline (**2a**)

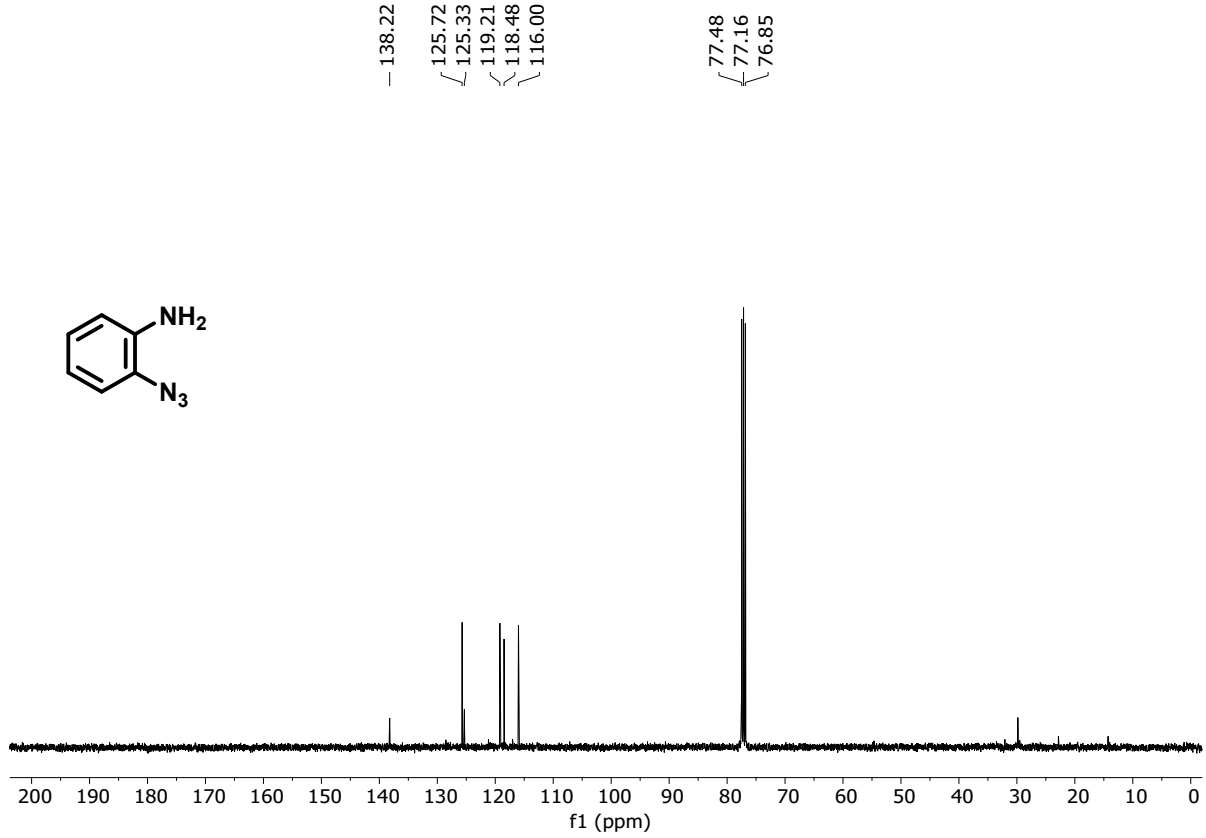


Fig S12. ^{13}C NMR spectrum of 2-azidoaniline (**2a**)

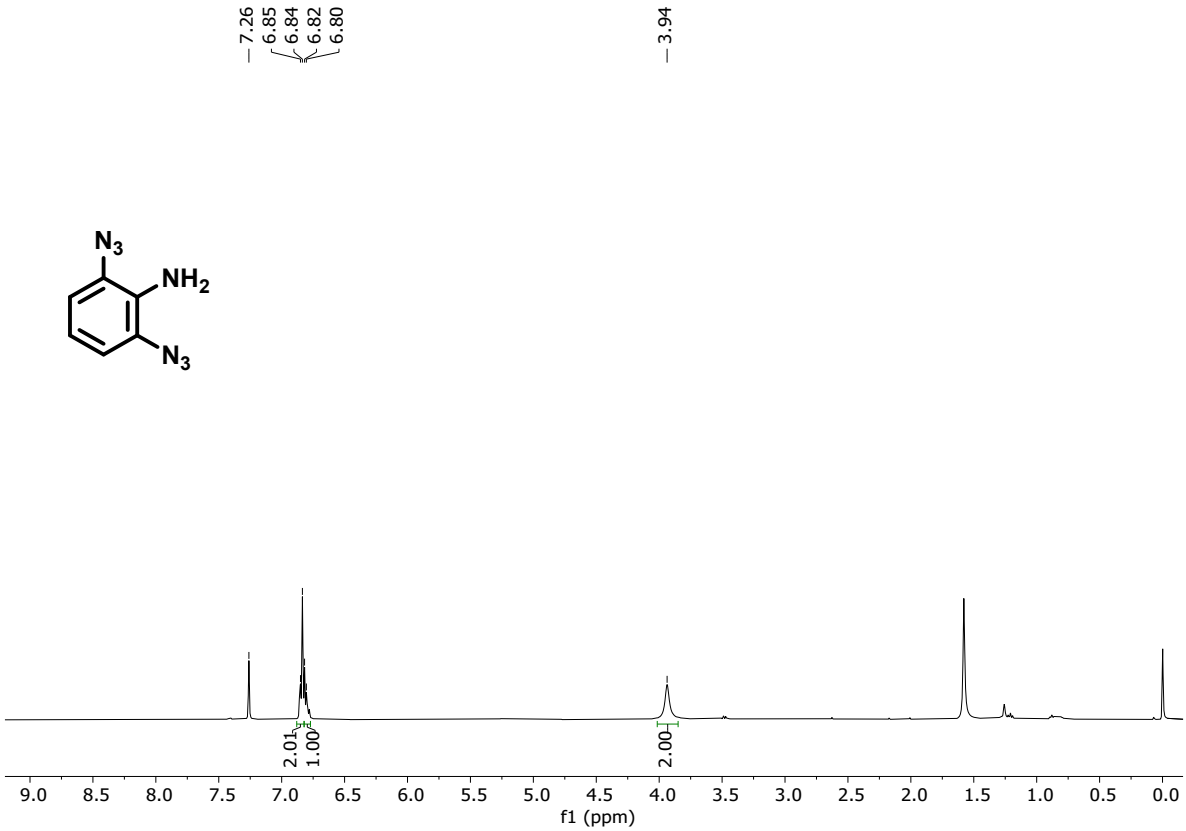


Fig S13. ^{1}H NMR spectrum of 2,6-diazidoaniline (**2a'**)

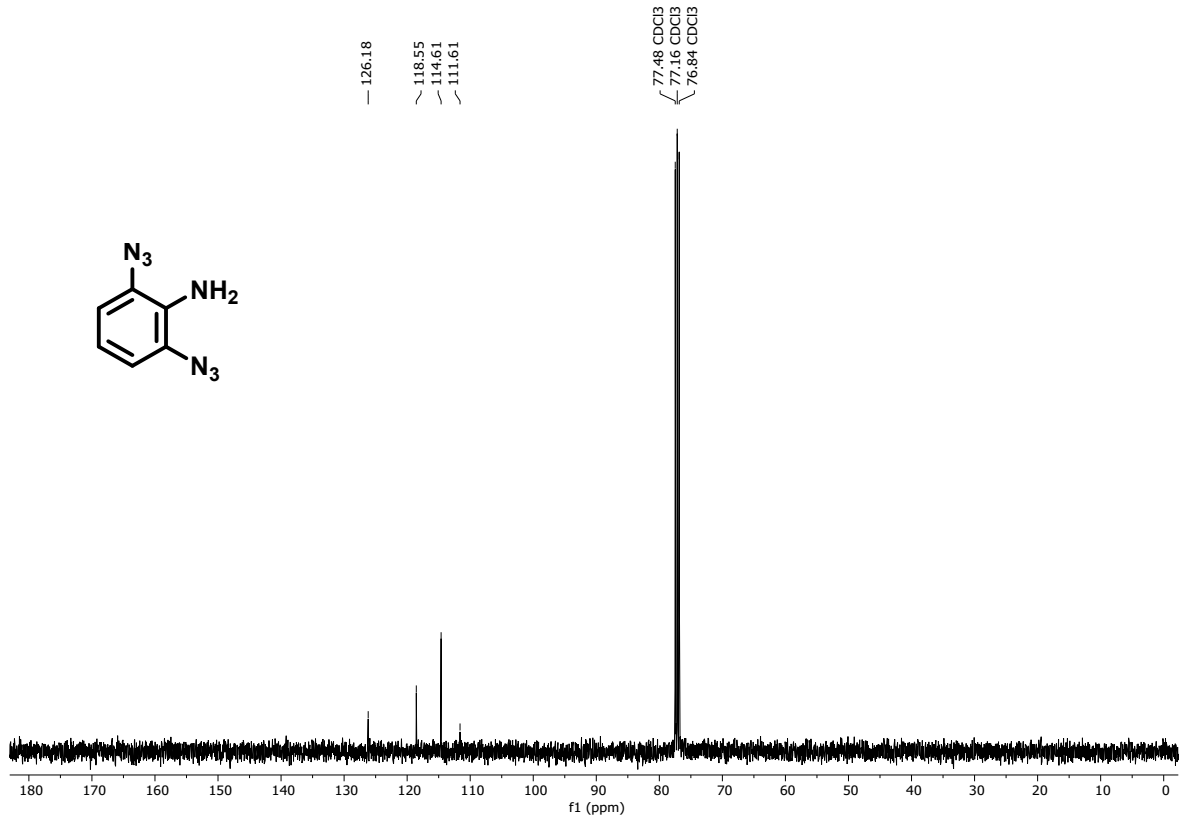


Fig S14. ^{13}C NMR spectrum of 2,6-diazidoaniline (**2a'**)

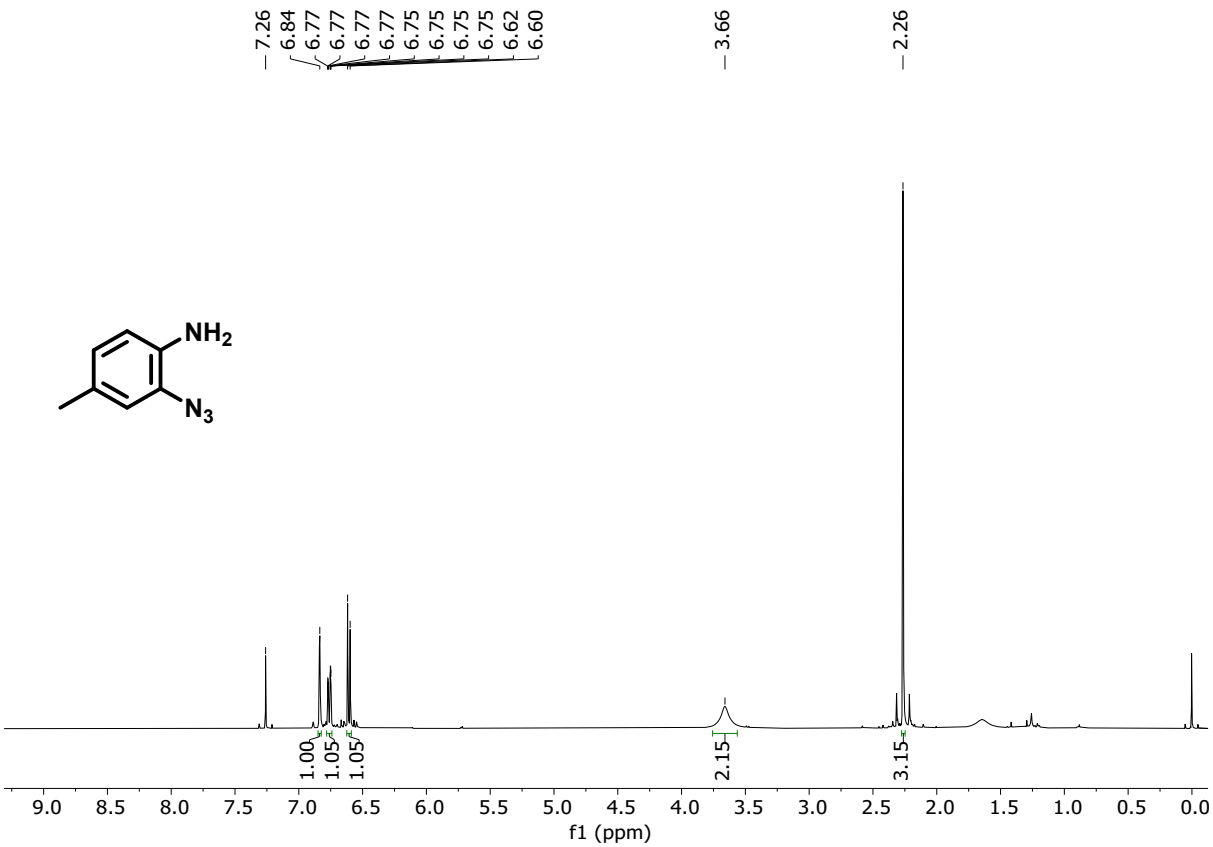


Fig S15. ^{1}H NMR spectrum of 2-azido-4-methylaniline (**2b**)

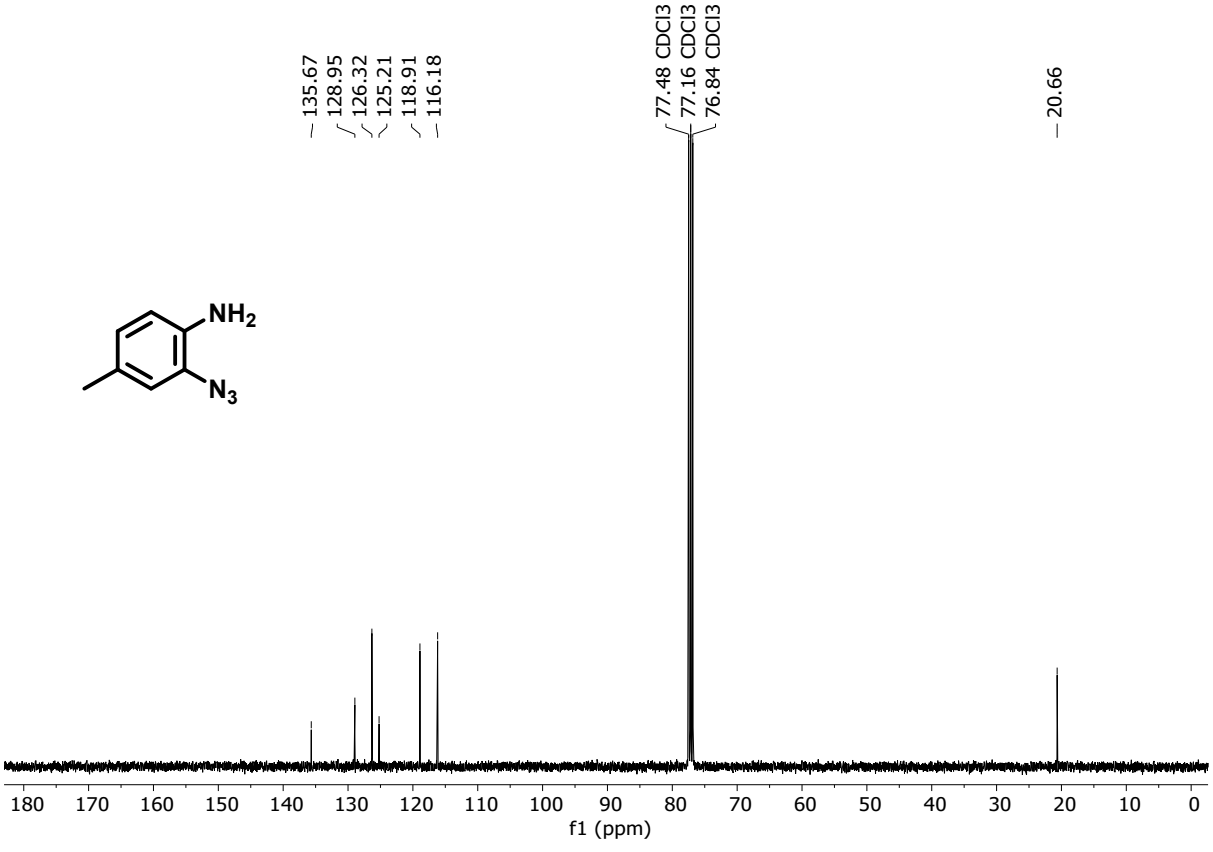


Fig S16. ^{13}C NMR spectrum of 2-azido-4-methylaniline (**2b**)

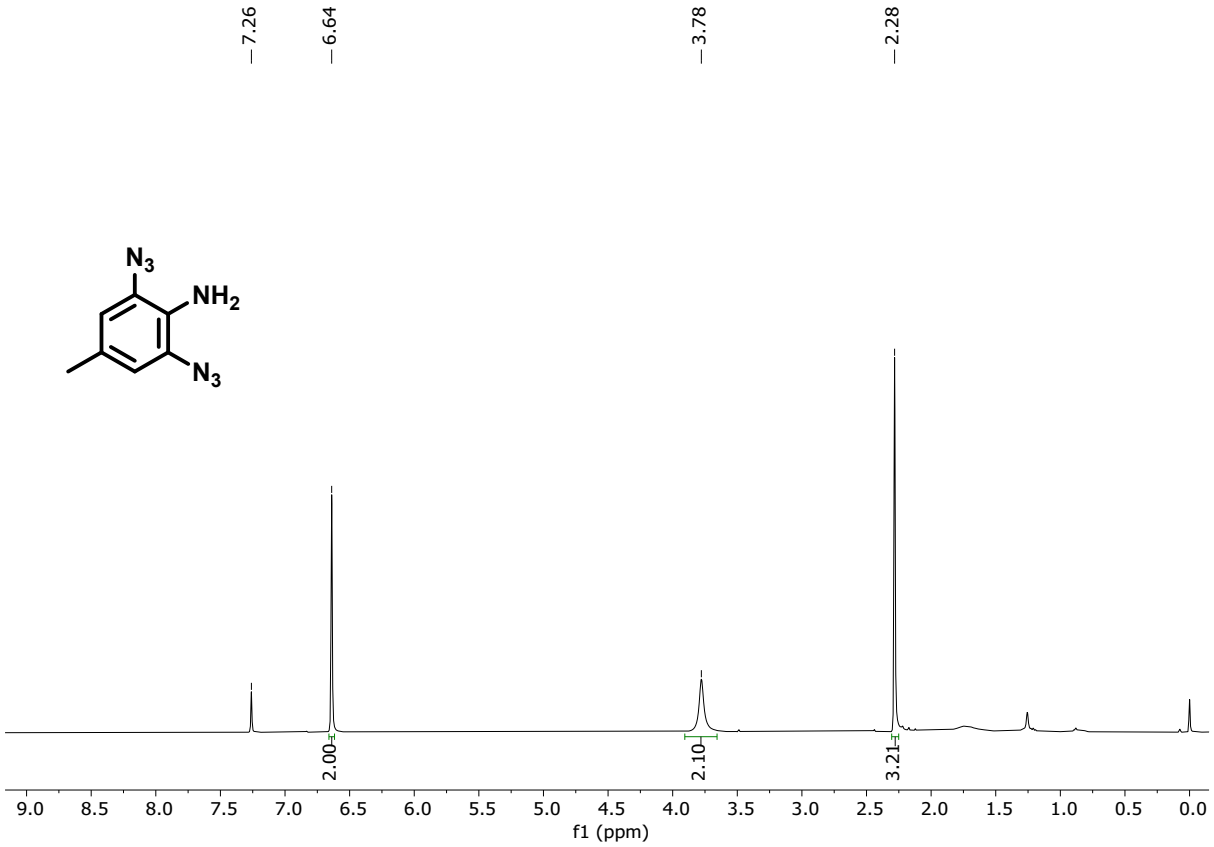


Fig S17. ^{1}H NMR spectrum of 2,6-diazido-4-methylaniline (**2b'**)

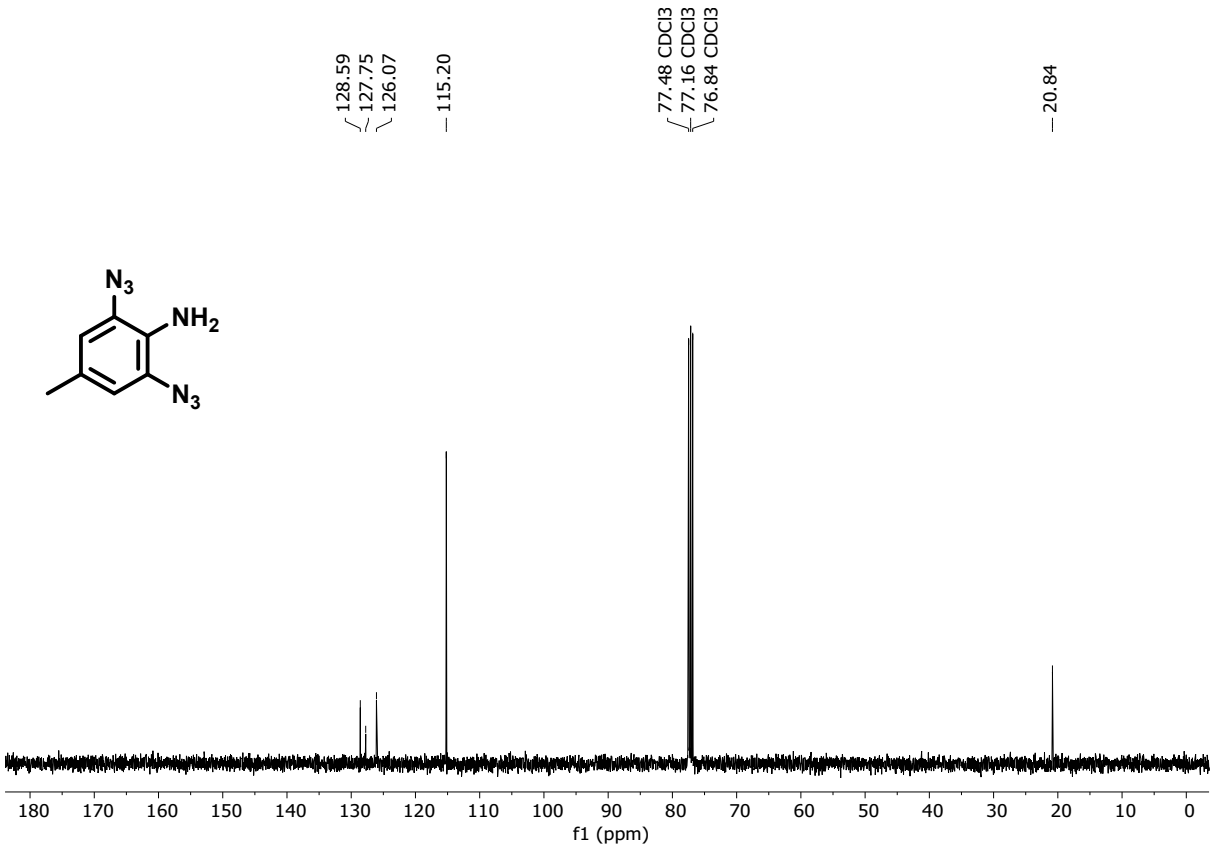


Fig S18. ^{13}C NMR spectrum of 2,6-diazido-4-methylaniline (**2b'**)

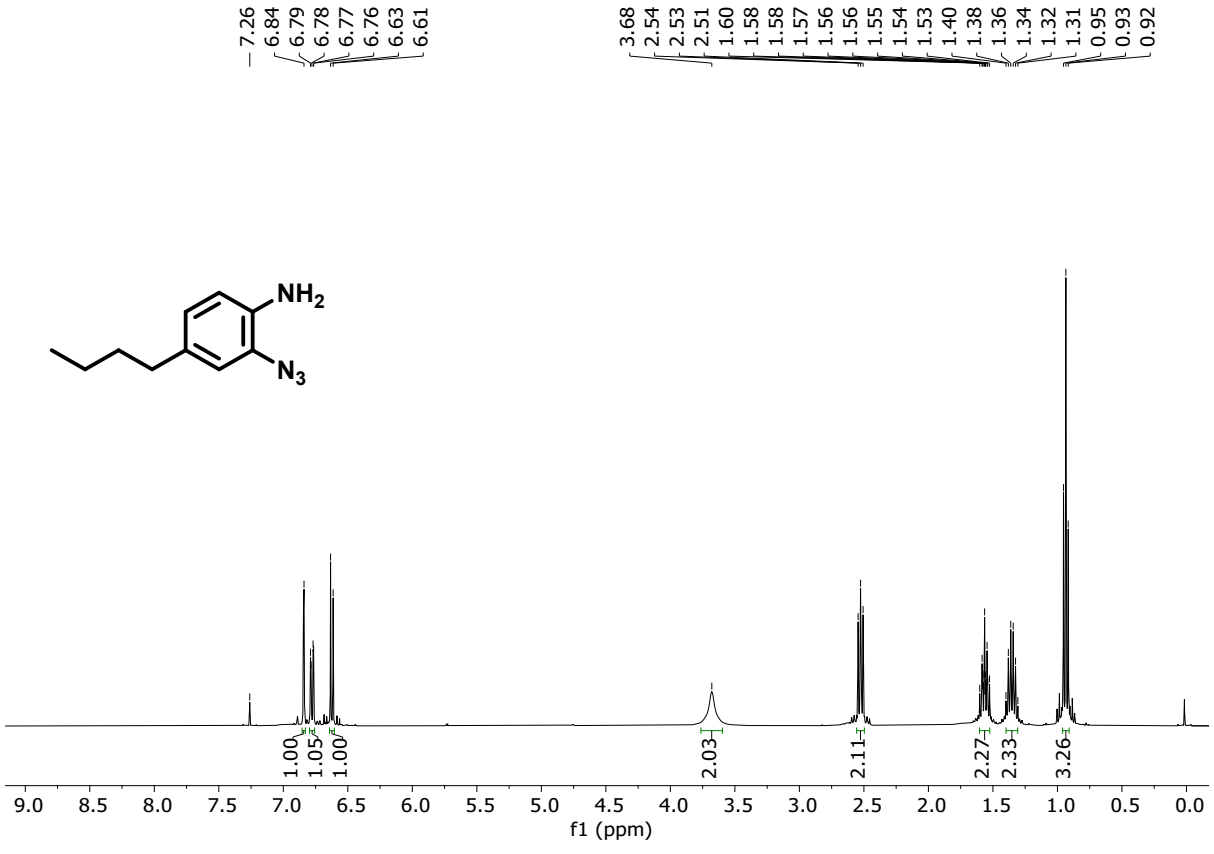


Fig S19. ^{1}H NMR spectrum of 2-azido-4-butylaniline (**2c**)

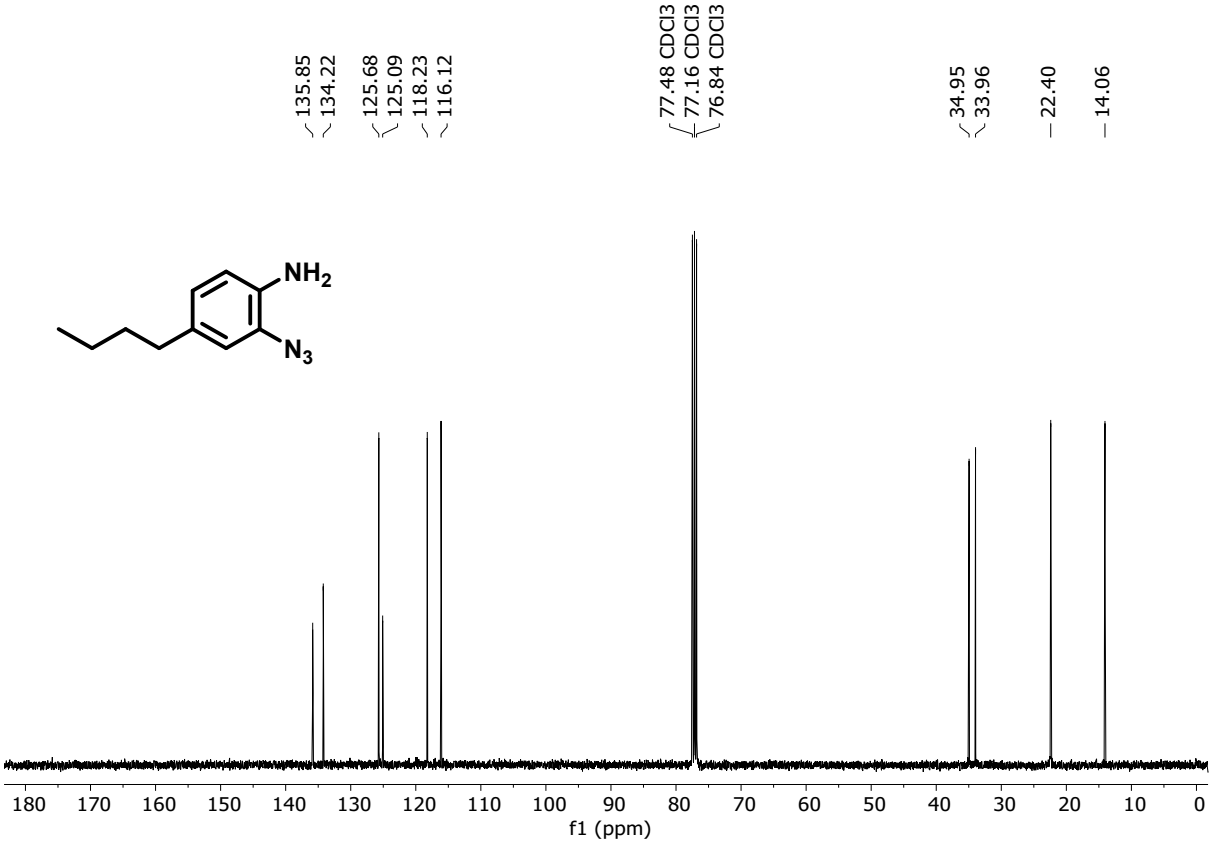


Fig S20. ^{13}C NMR spectrum of 2-azido-4-butylaniline (**2c**)

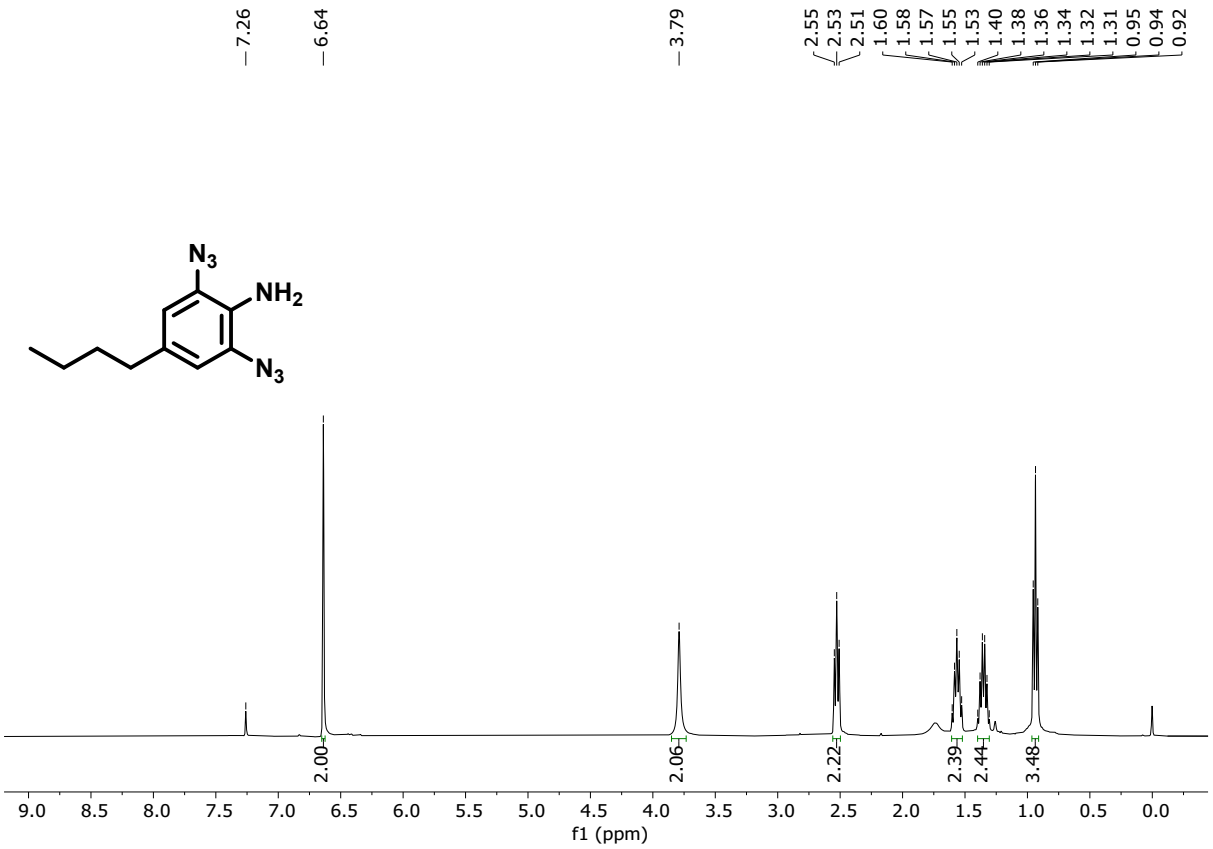


Fig S21. ^{1}H NMR spectrum of 2,6-diazido-4-butylaniline (**2c'**)

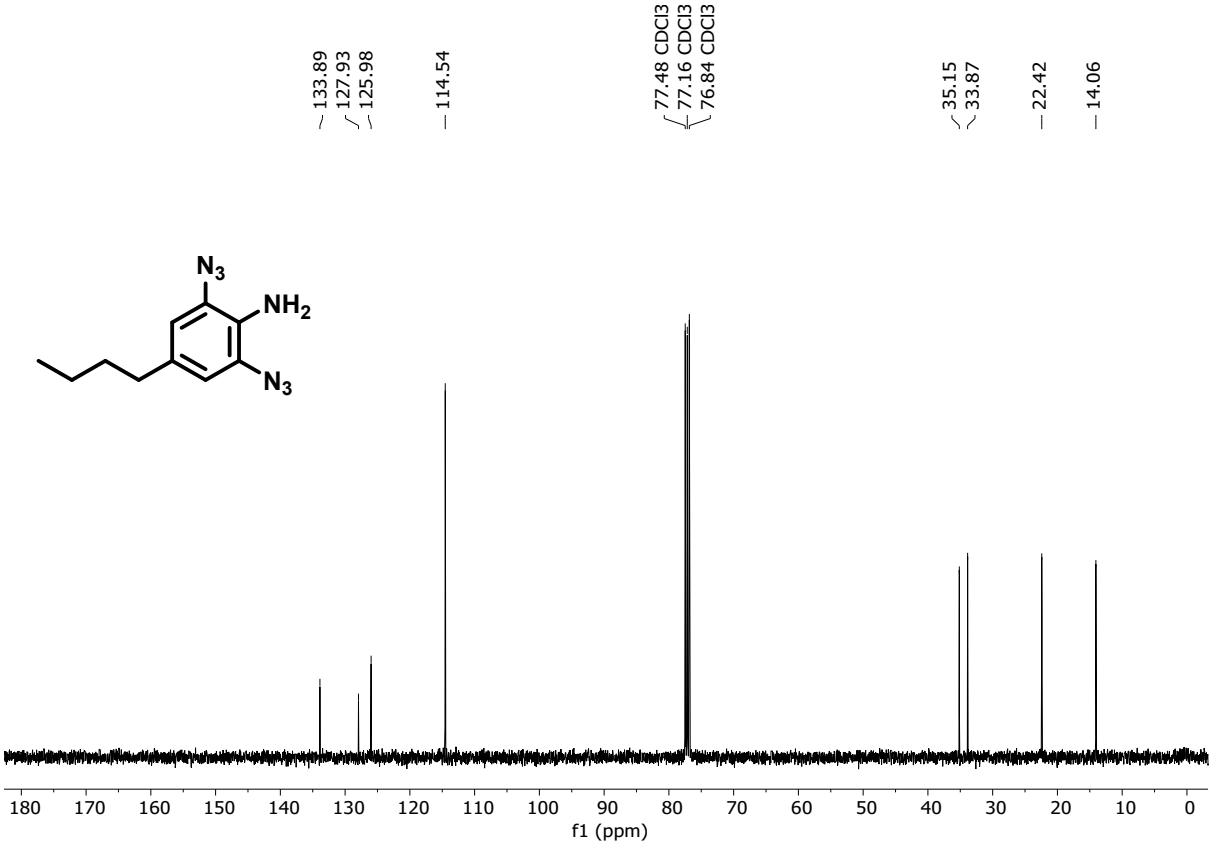


Fig S22. [1]H NMR spectrum of 2,6-diazido-4-butylaniline (**2c'**)

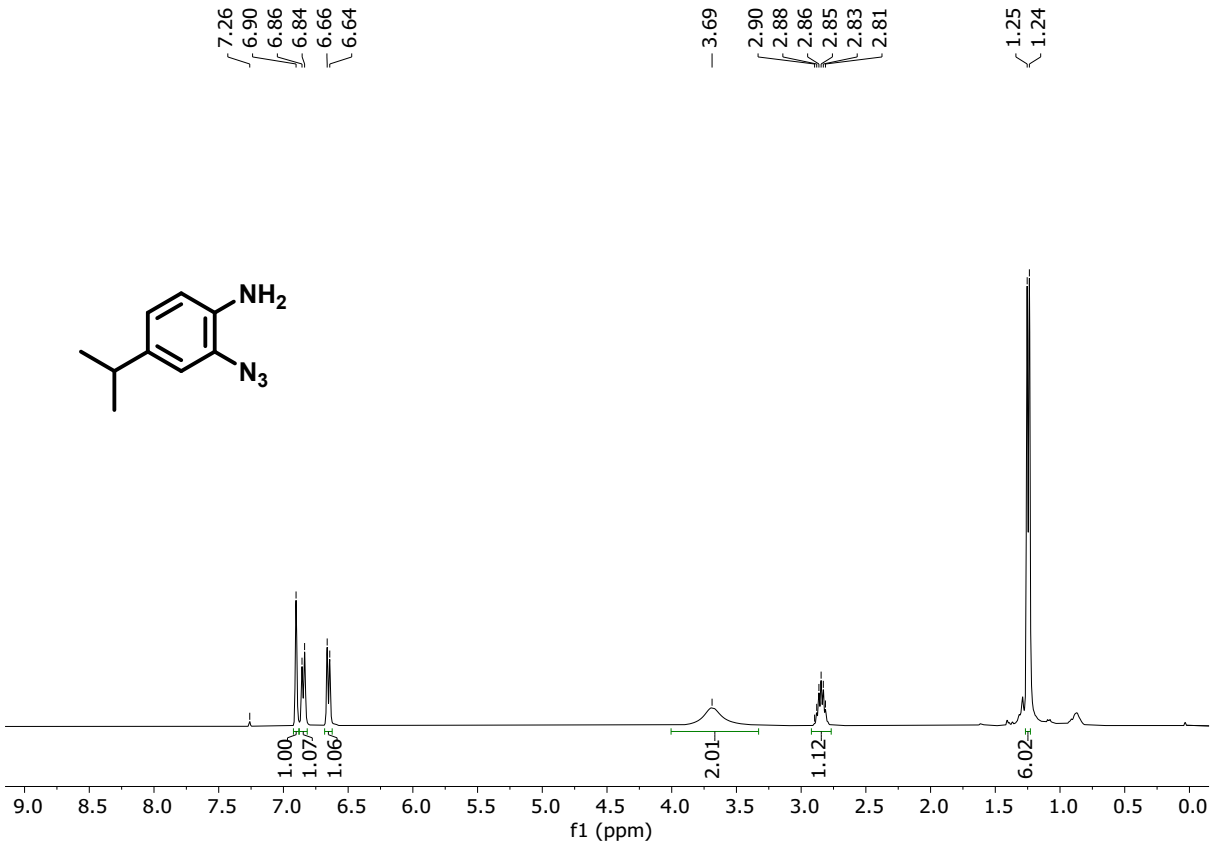


Fig S23. [1]H NMR spectrum of 2-azido-4-isopropylaniline (**2d**)

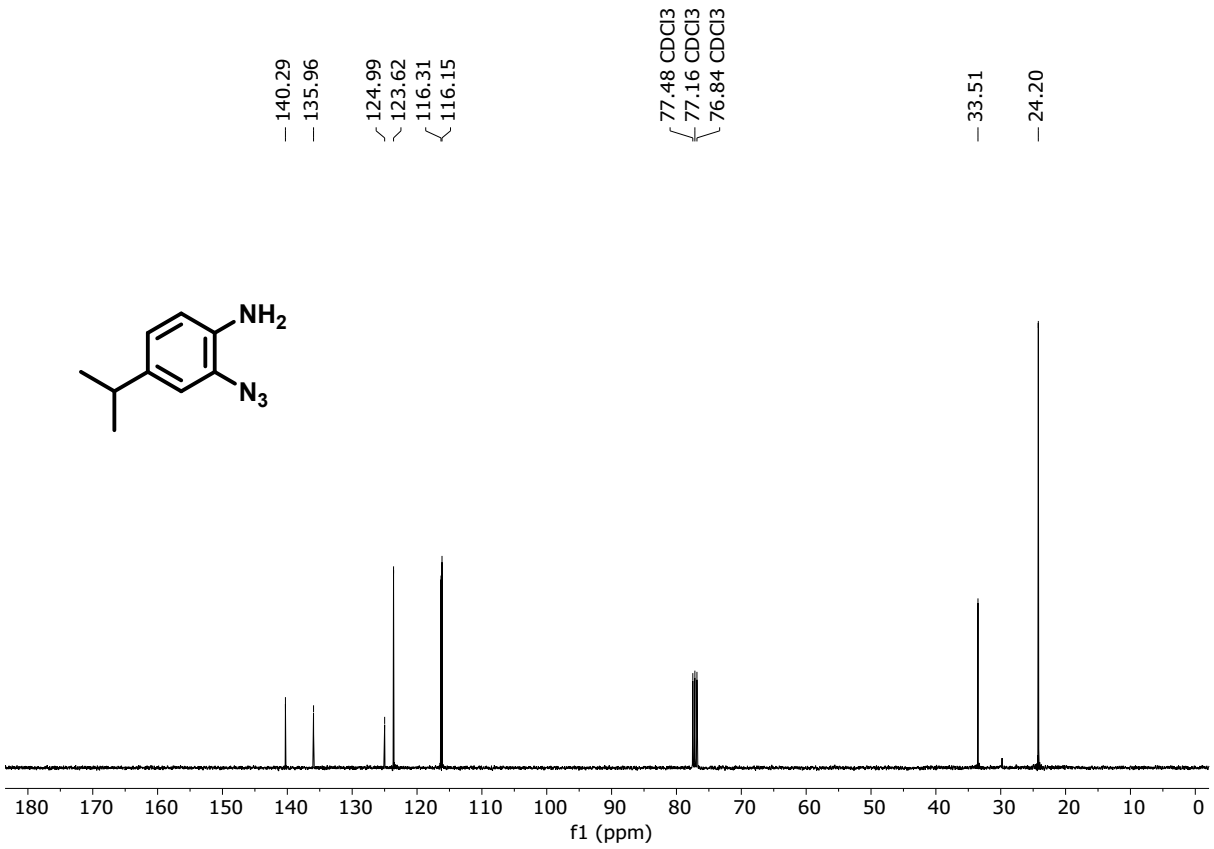


Fig S24. ^{13}C NMR spectrum of 2-azido-4-isopropylaniline (**2d**)

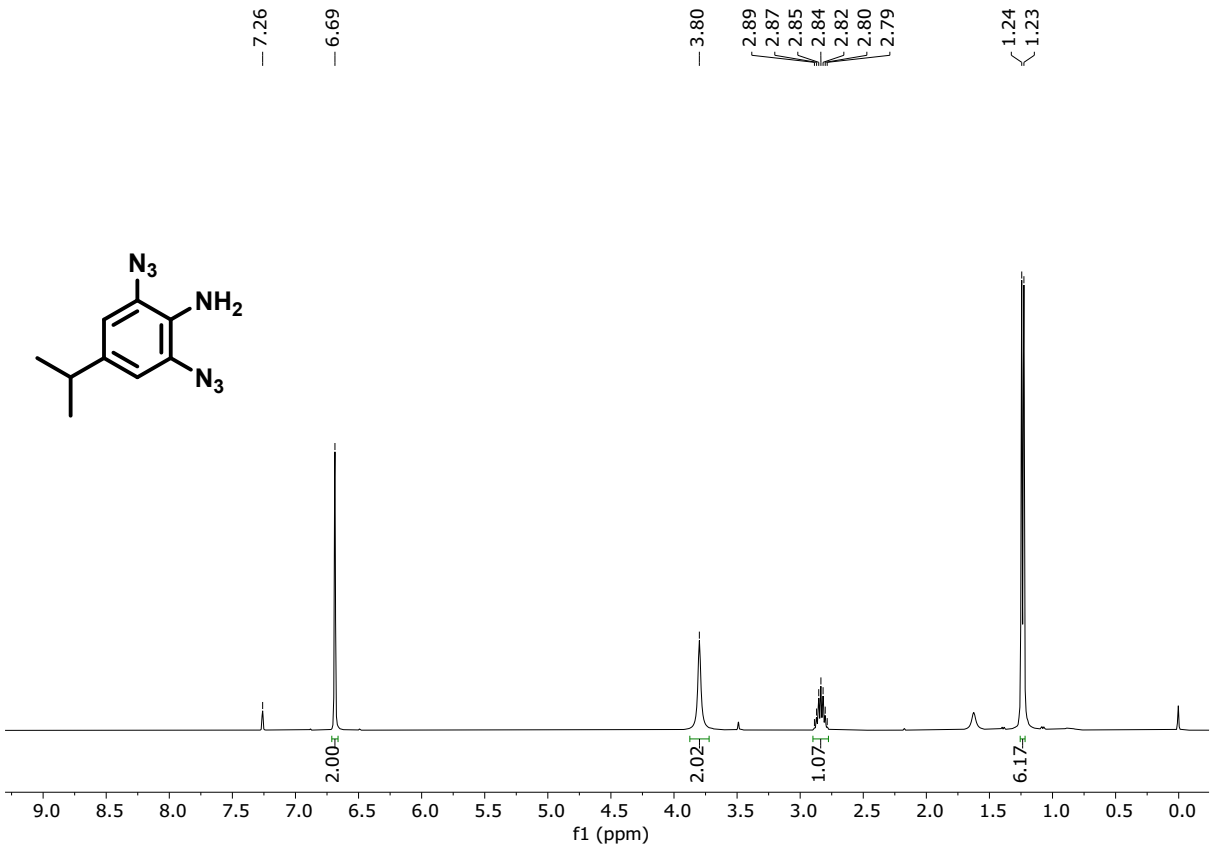


Fig S25. ^{1}H NMR spectrum of 2,6-diazido-4-isopropylaniline (**2d'**)

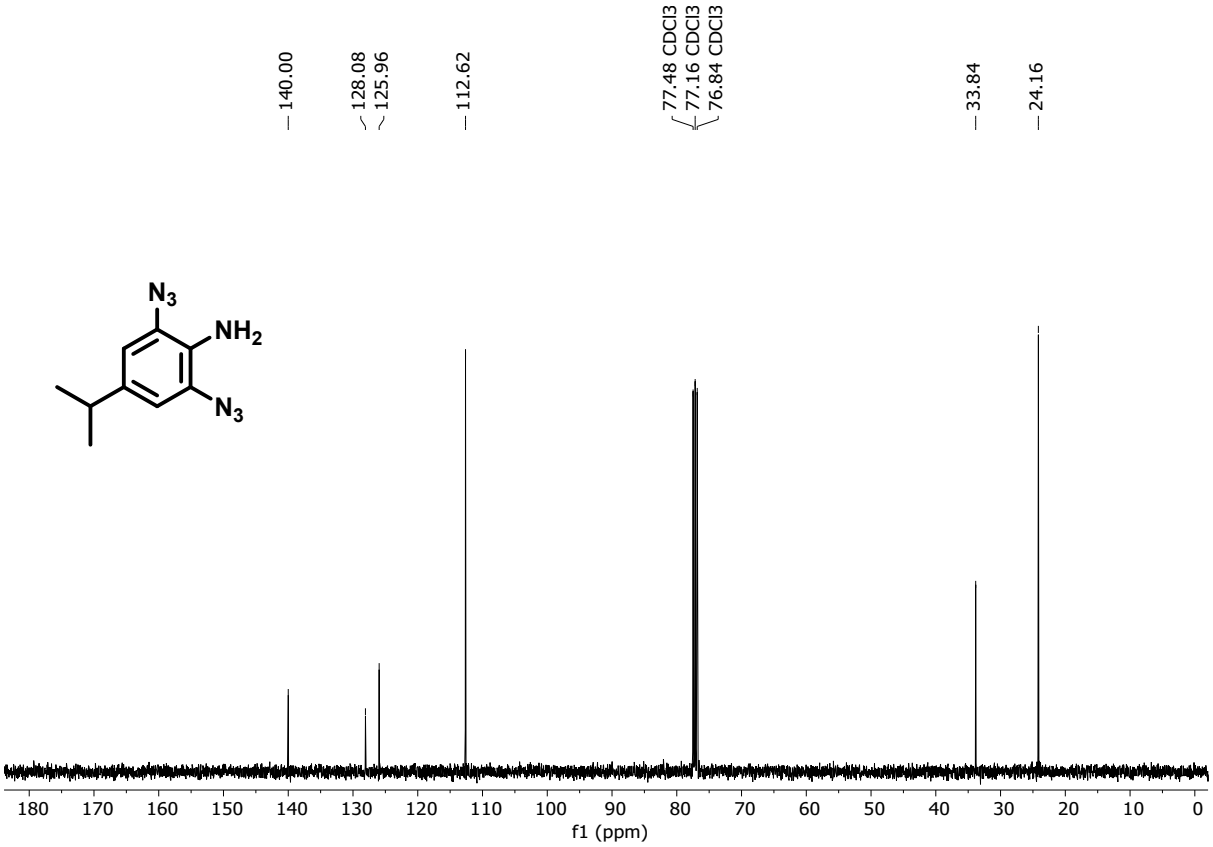


Fig S26. ^{13}C NMR spectrum of 2,6-diazido-4-isopropylaniline (**2d'**)

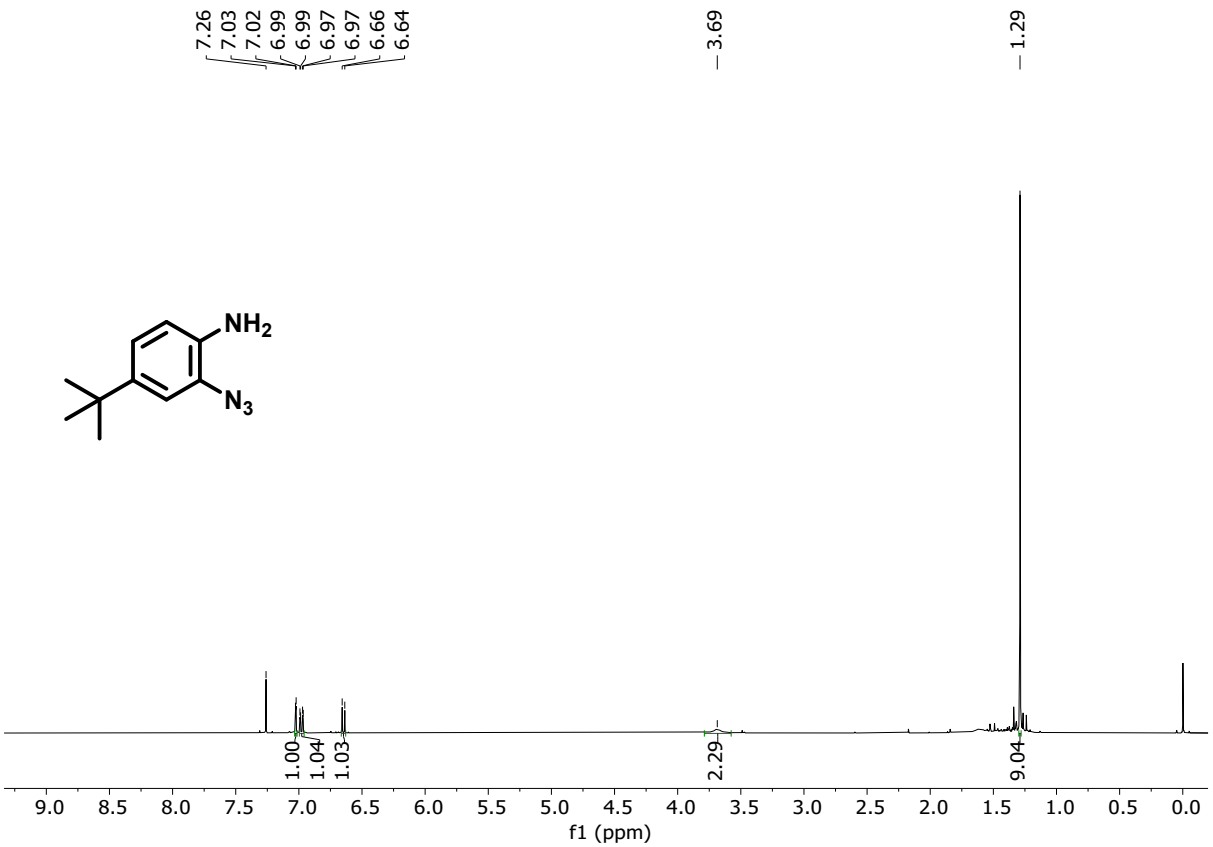


Fig S27. [1]H NMR spectrum of 2-azido-4-(tert-butyl)aniline (**2e**)

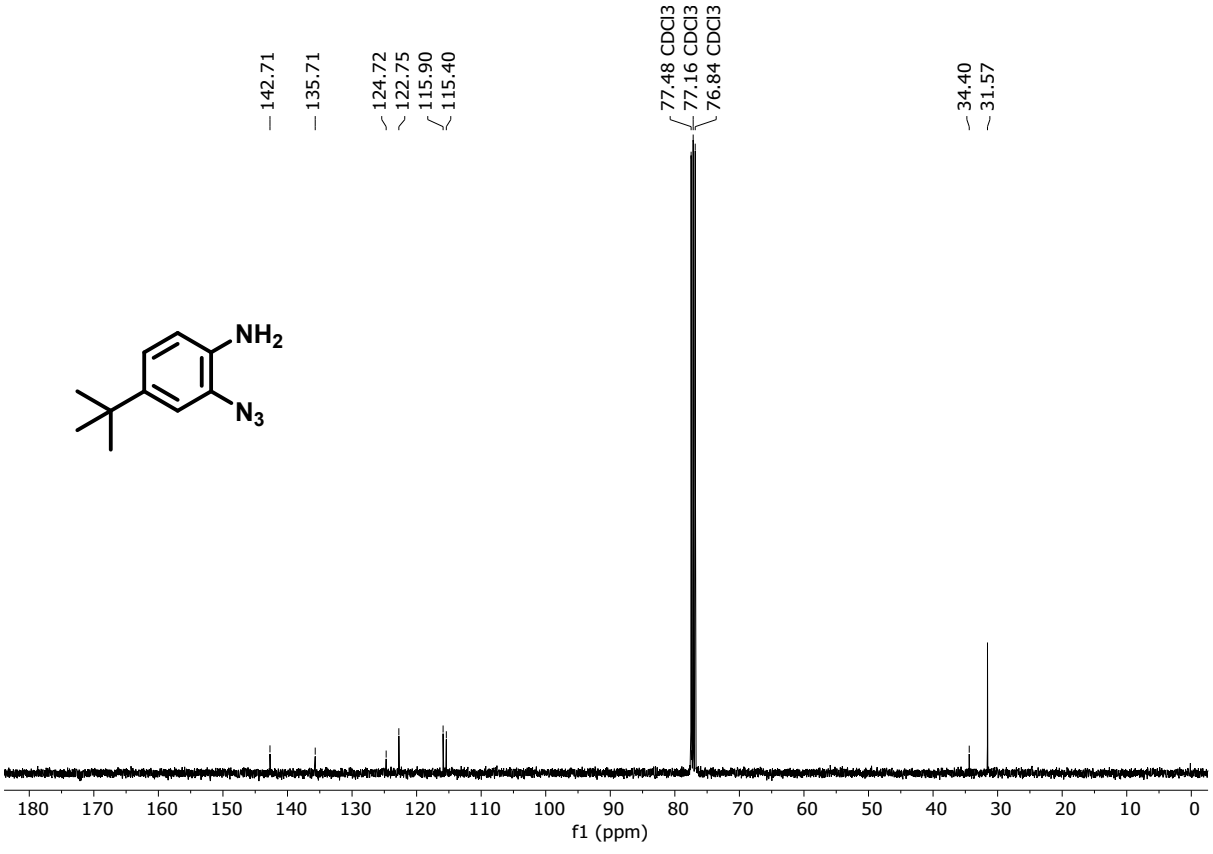


Fig S28. ^{13}C NMR spectrum of 2-azido-4-(tert-butyl)aniline (**2e**)

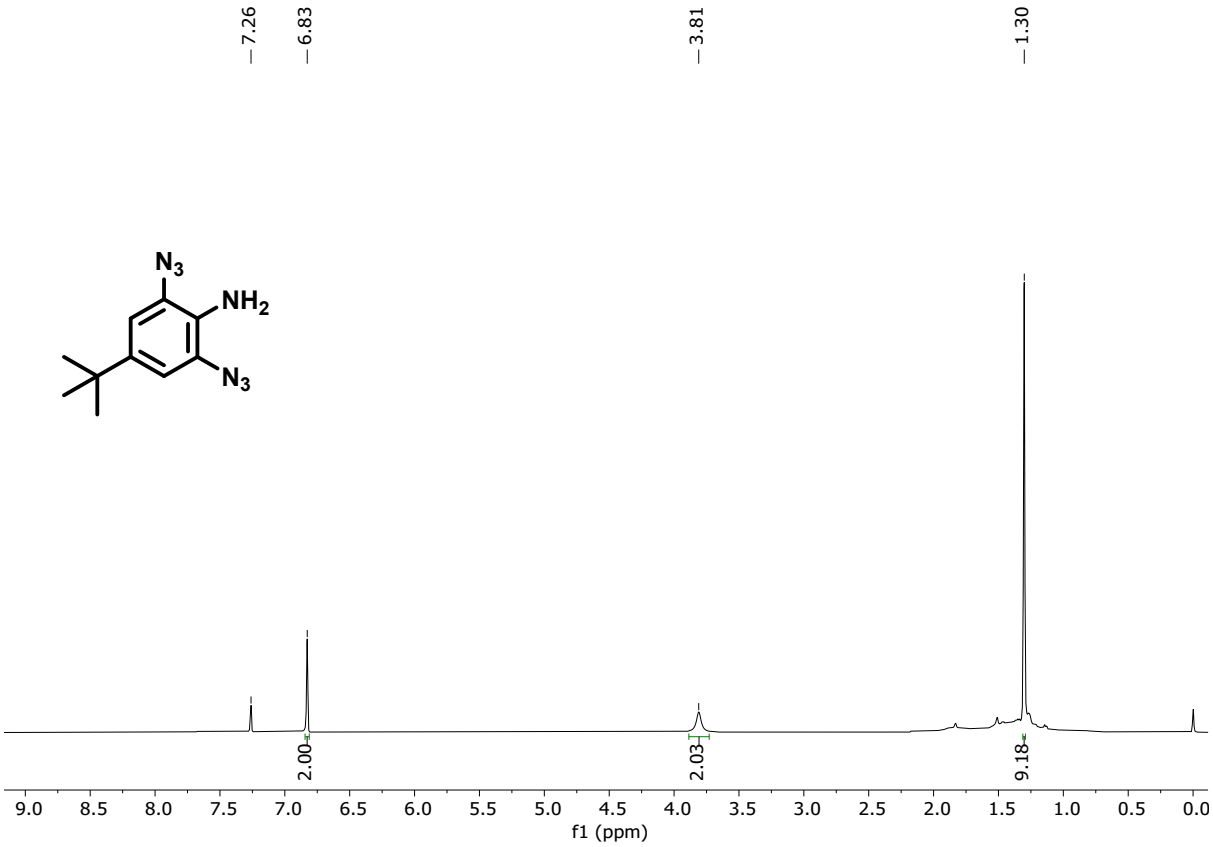


Fig S29. ^{1}H NMR spectrum of 2,6-diazido-4-(tert-butyl)aniline (**2e'**)

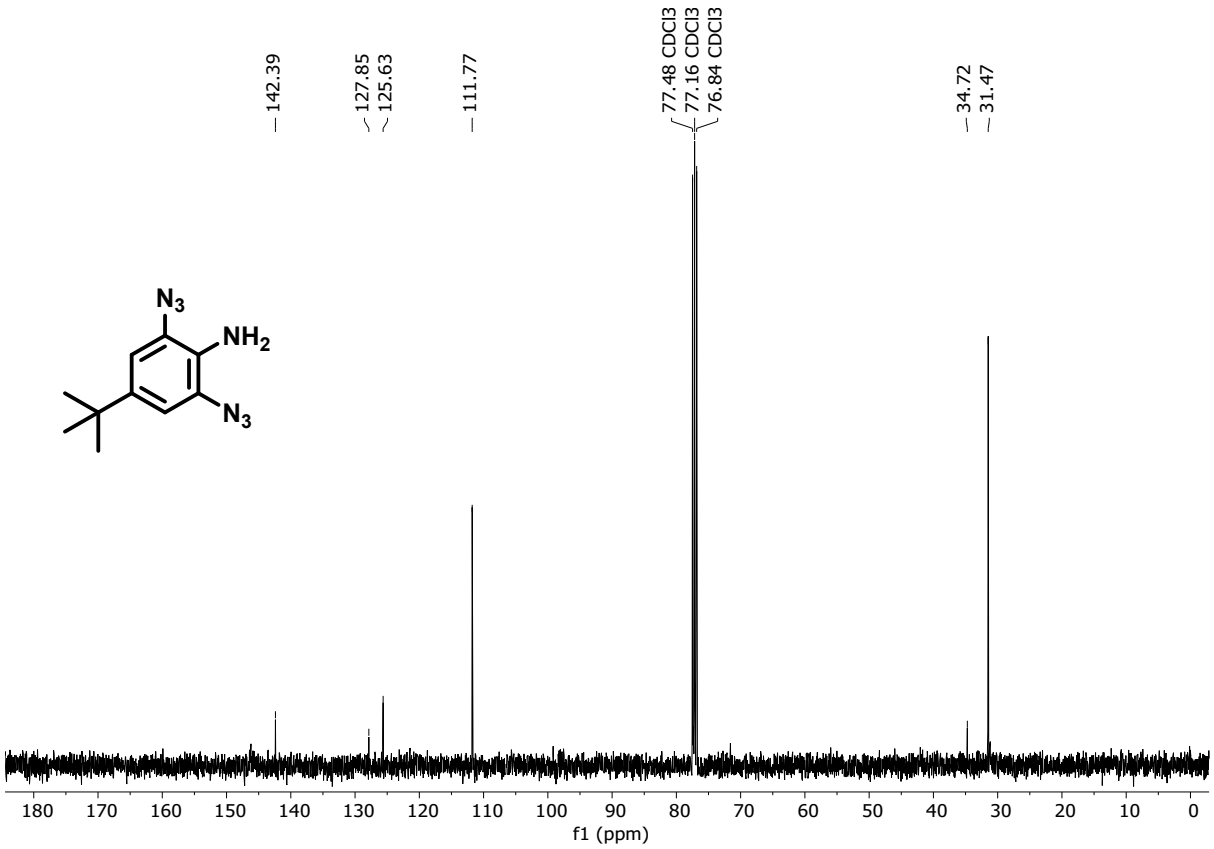


Fig S30. ^{13}C NMR spectrum of 2,6-diazido-4-(tert-butyl)aniline (**2e'**)

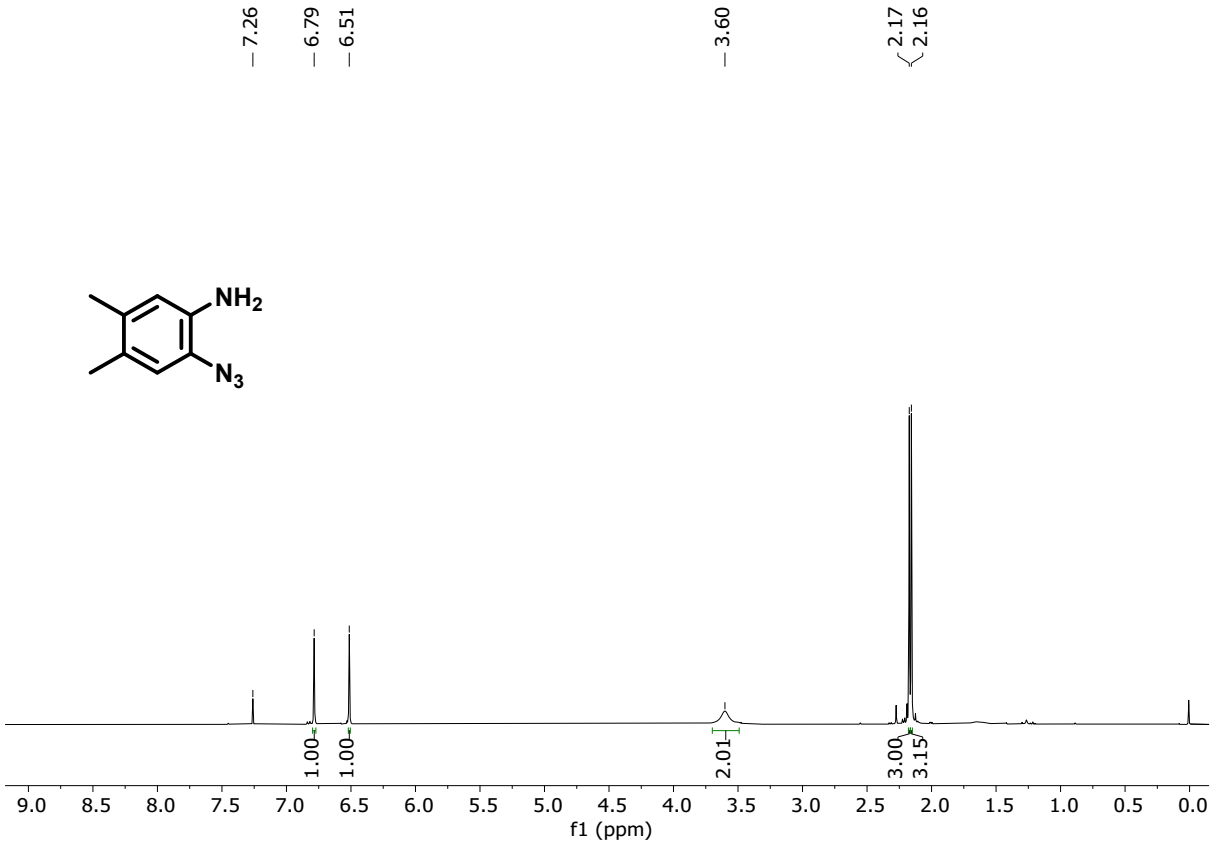


Fig S31. ^{1}H NMR spectrum of 2-azido-4,5-dimethylaniline (**2f**)

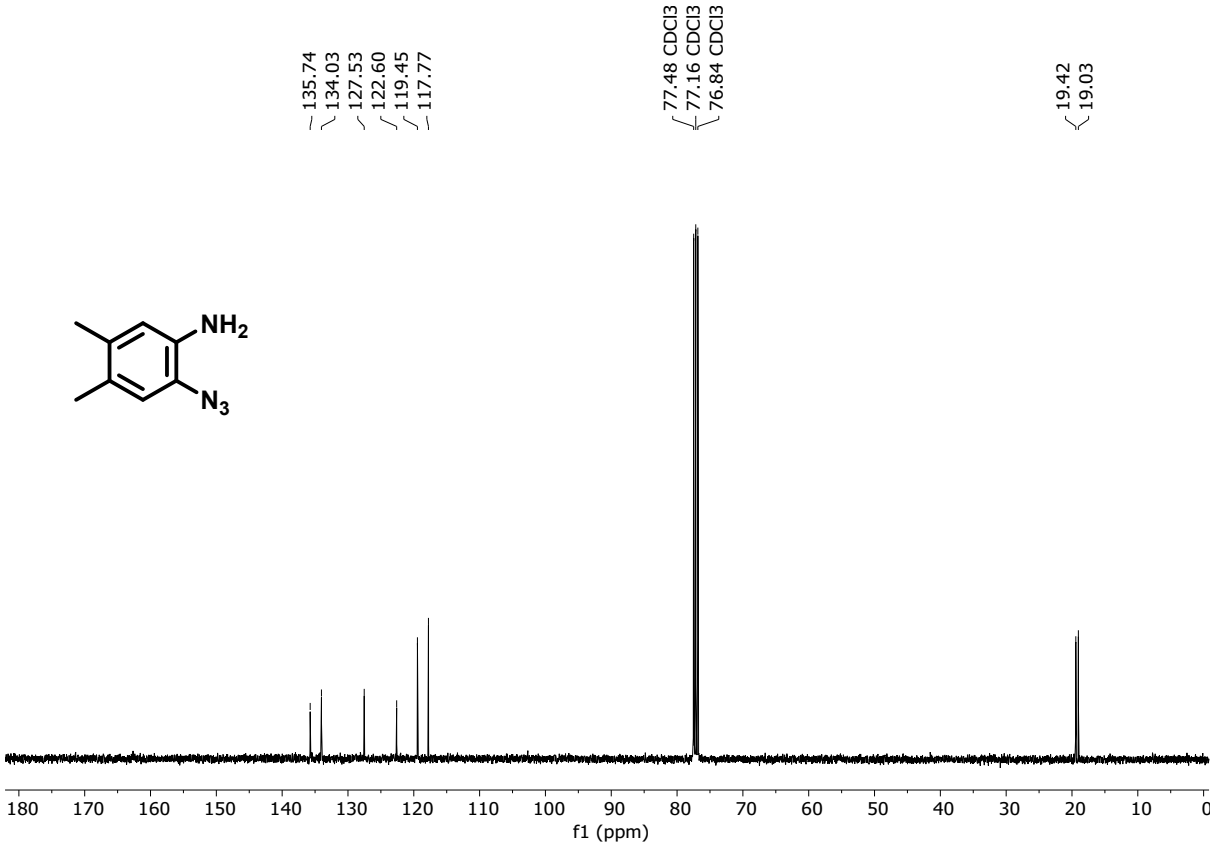


Fig S32. ^{13}C NMR spectrum of 2-azido-4,5-dimethylaniline (**2f**)

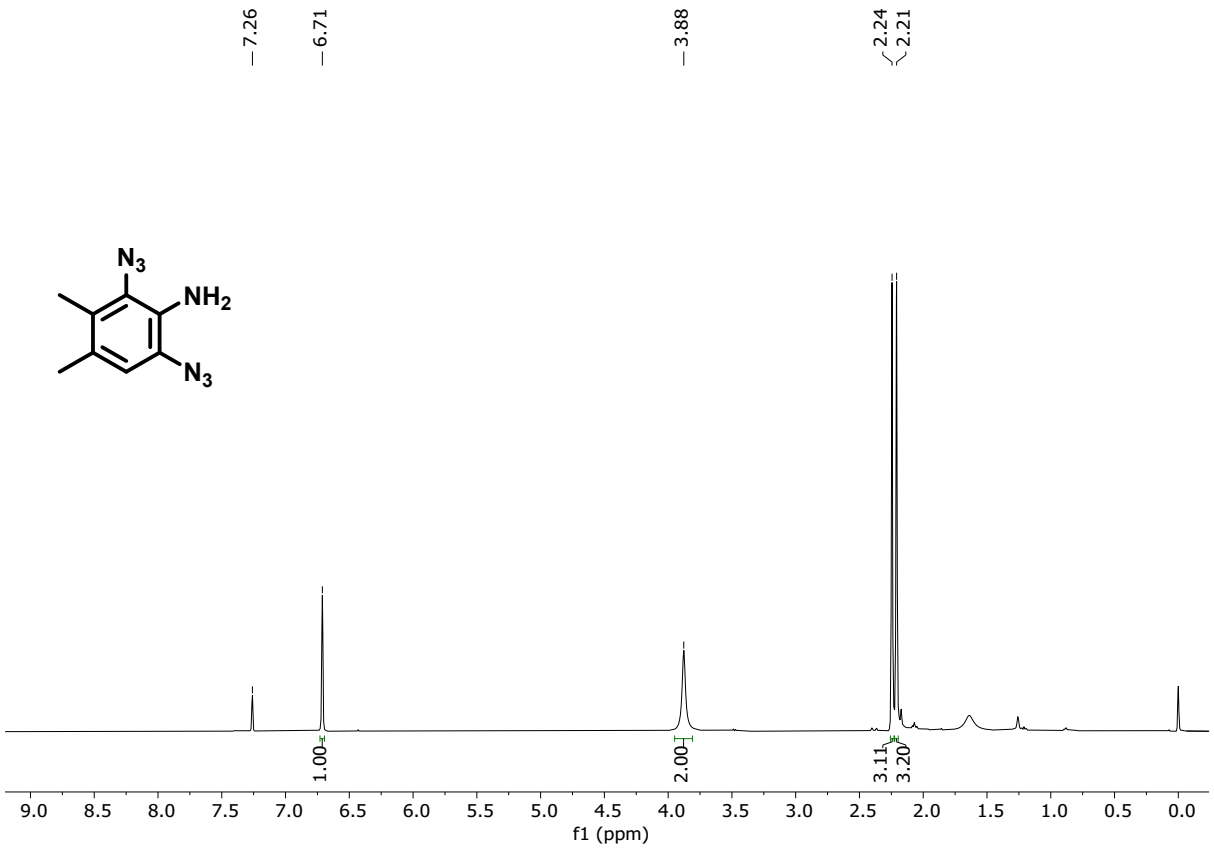


Fig S33. ^{1}H NMR spectrum of 2,6-diazido-3,4-dimethylaniline (**2f'**)

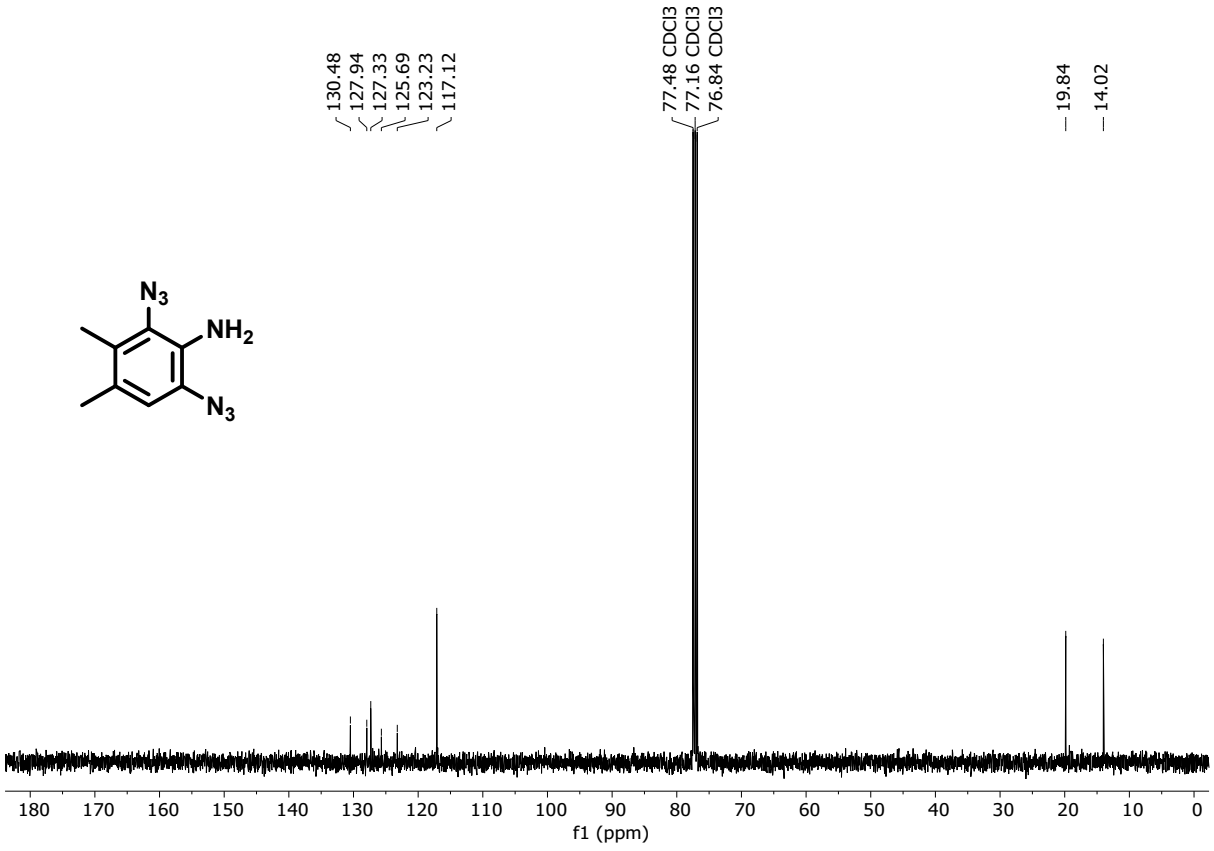


Fig S34. ^{13}C NMR spectrum of 2,6-diazido-3,4-dimethylaniline (**2f'**)

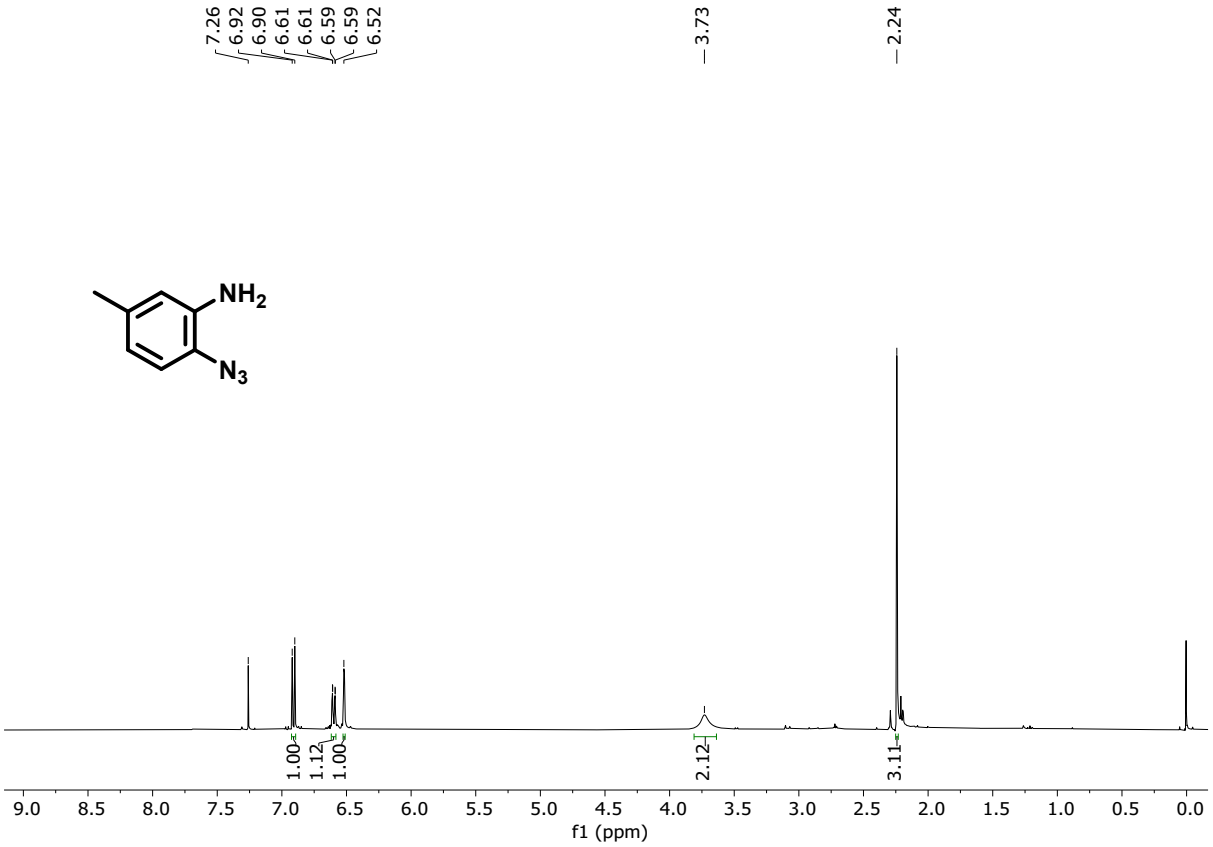


Fig S35. ^{1}H NMR spectrum of 2-azido-5-methylaniline (**2g**)

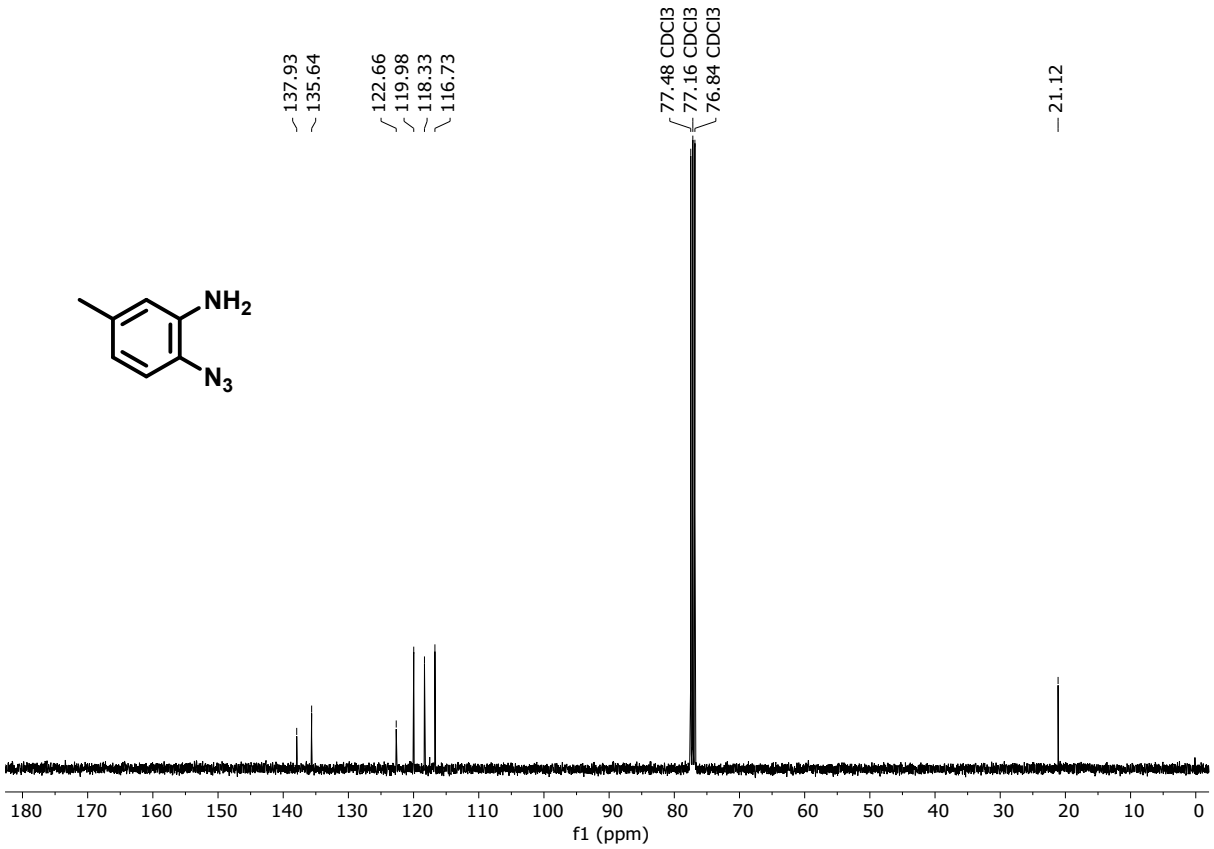


Fig S36. ^{13}C NMR spectrum of 2-azido-5-methylaniline (**2g**)

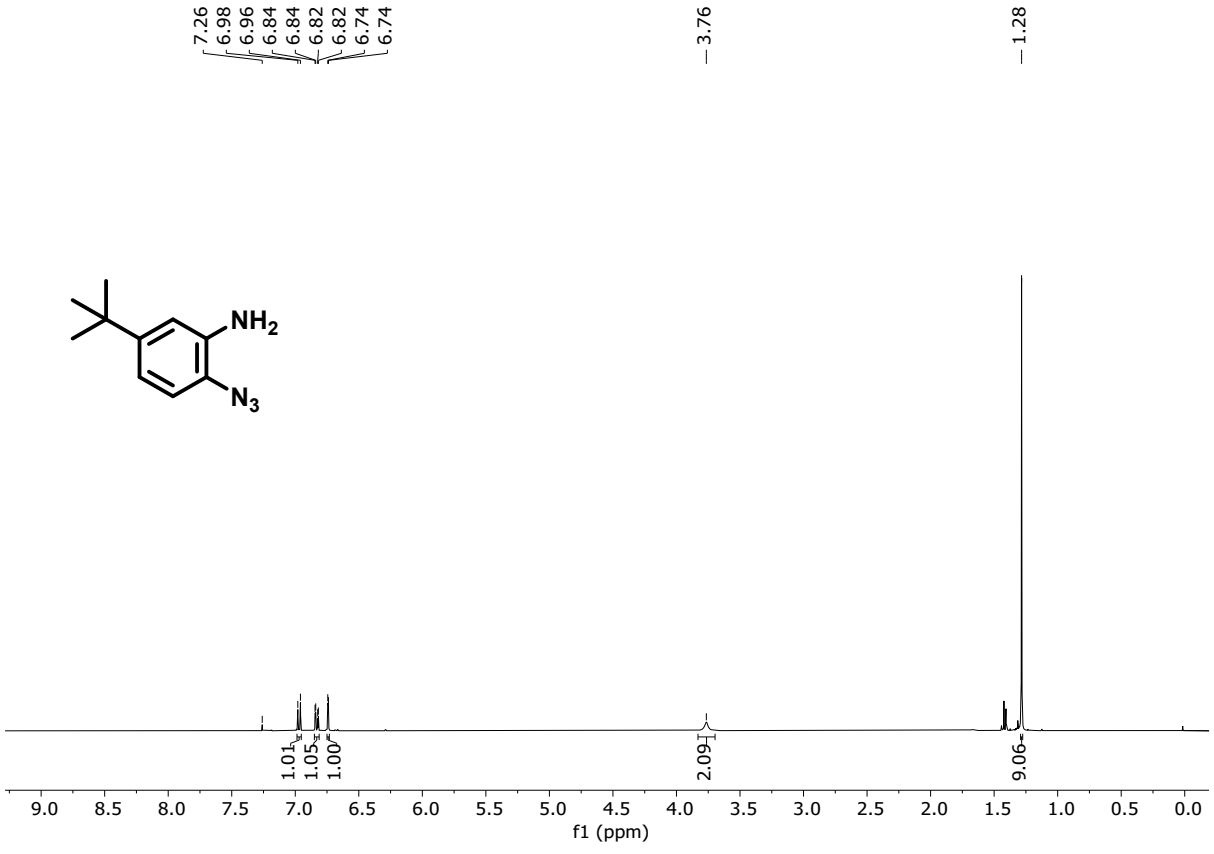


Fig S37. ^{1}H NMR spectrum of 2-azido-5-(tert-butyl)aniline (**2h**)

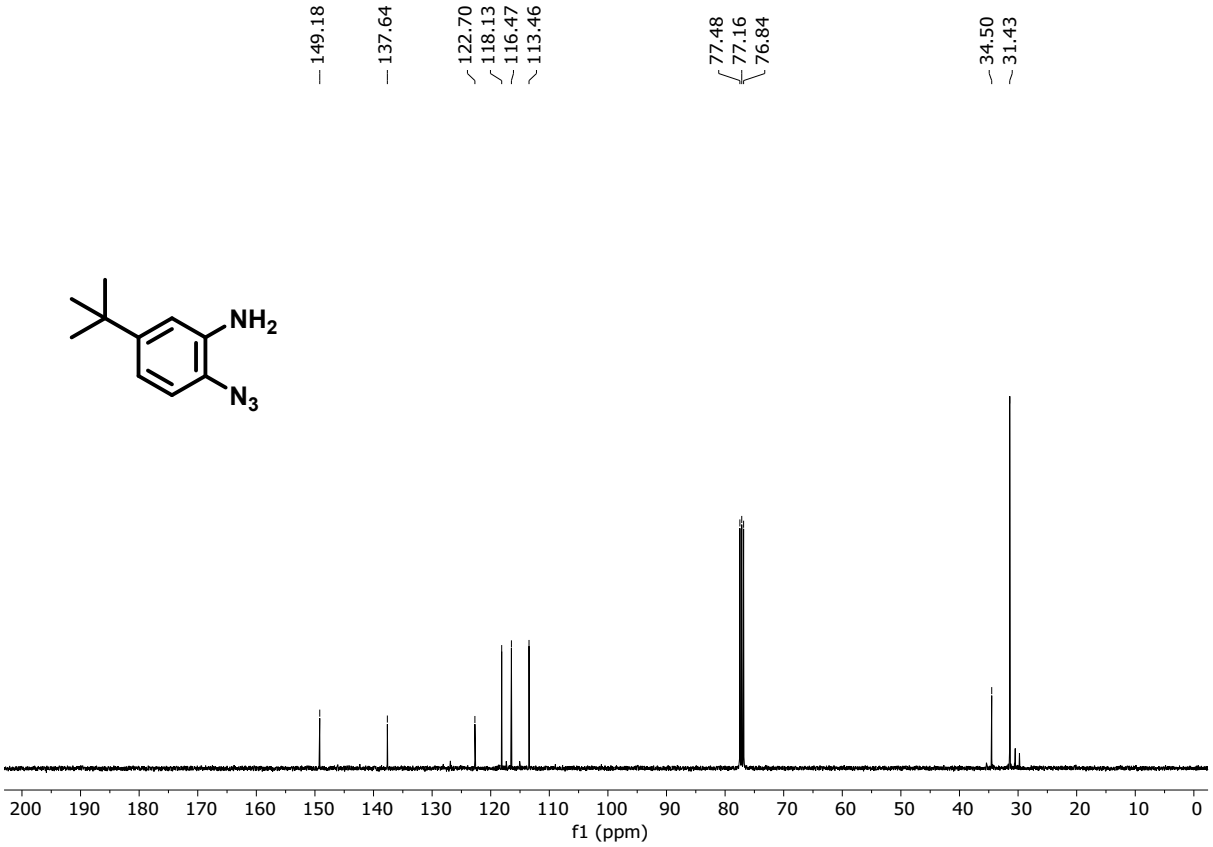


Fig S38. ^{13}C NMR spectrum of 2-azido-5-(tert-butyl)aniline (**2h**)

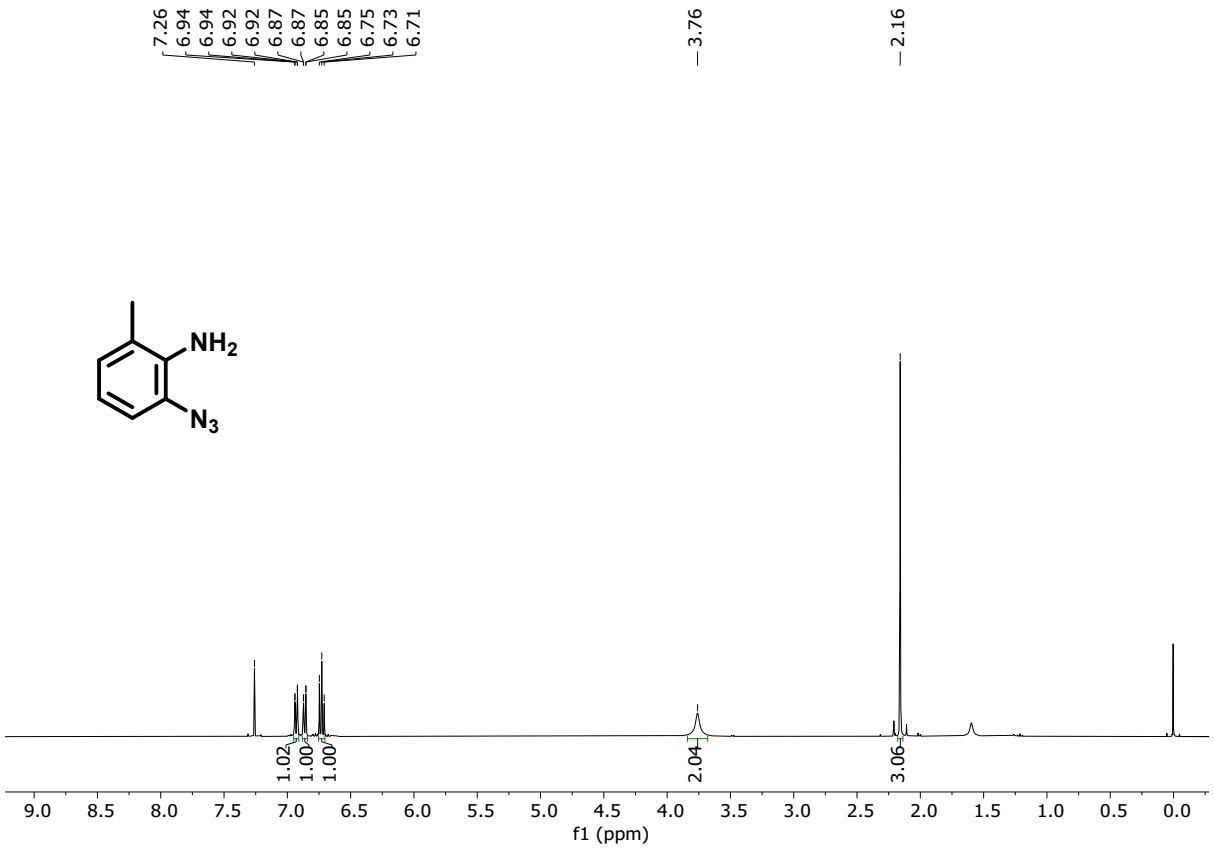


Fig S39. ^{1}H NMR spectrum of 2-azido-6-methylaniline (**2i**)

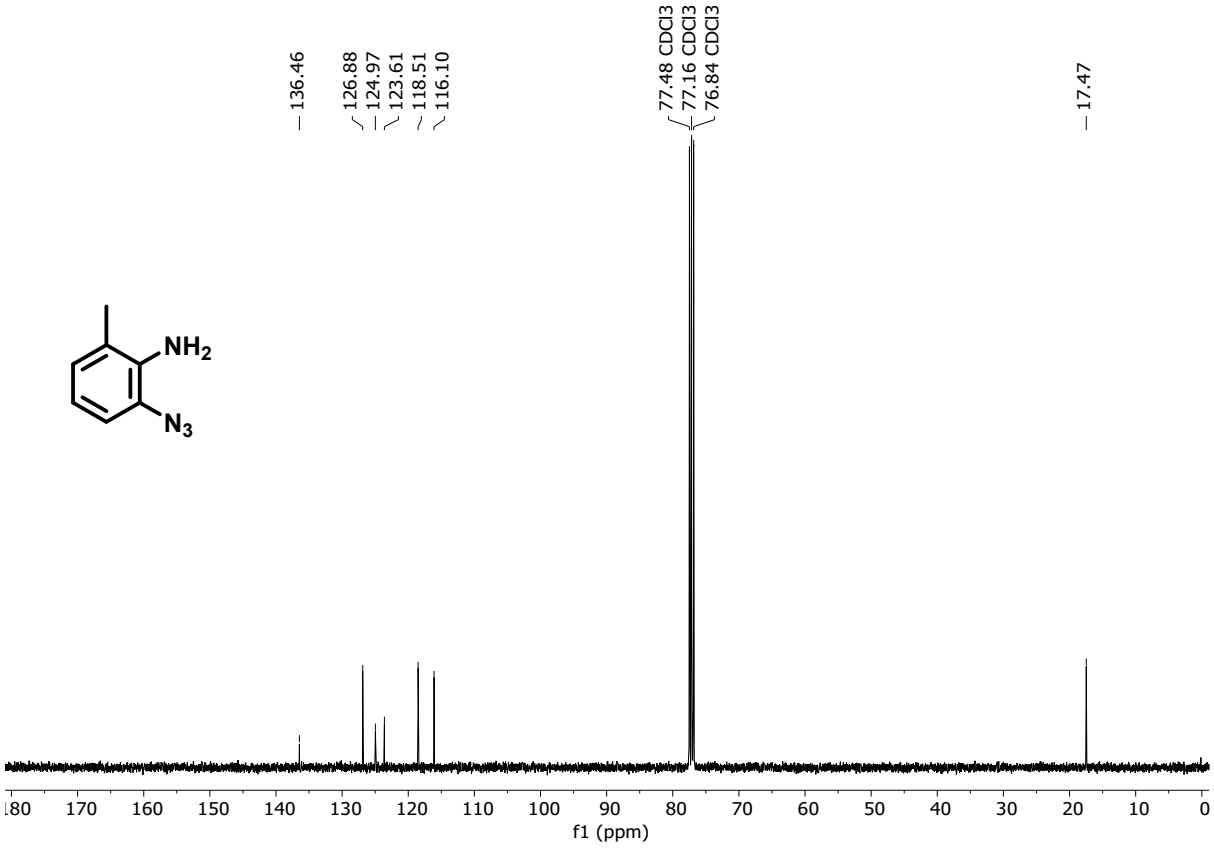


Fig S40. ^{13}C NMR spectrum of 2-azido-6-methylaniline (**2i**)

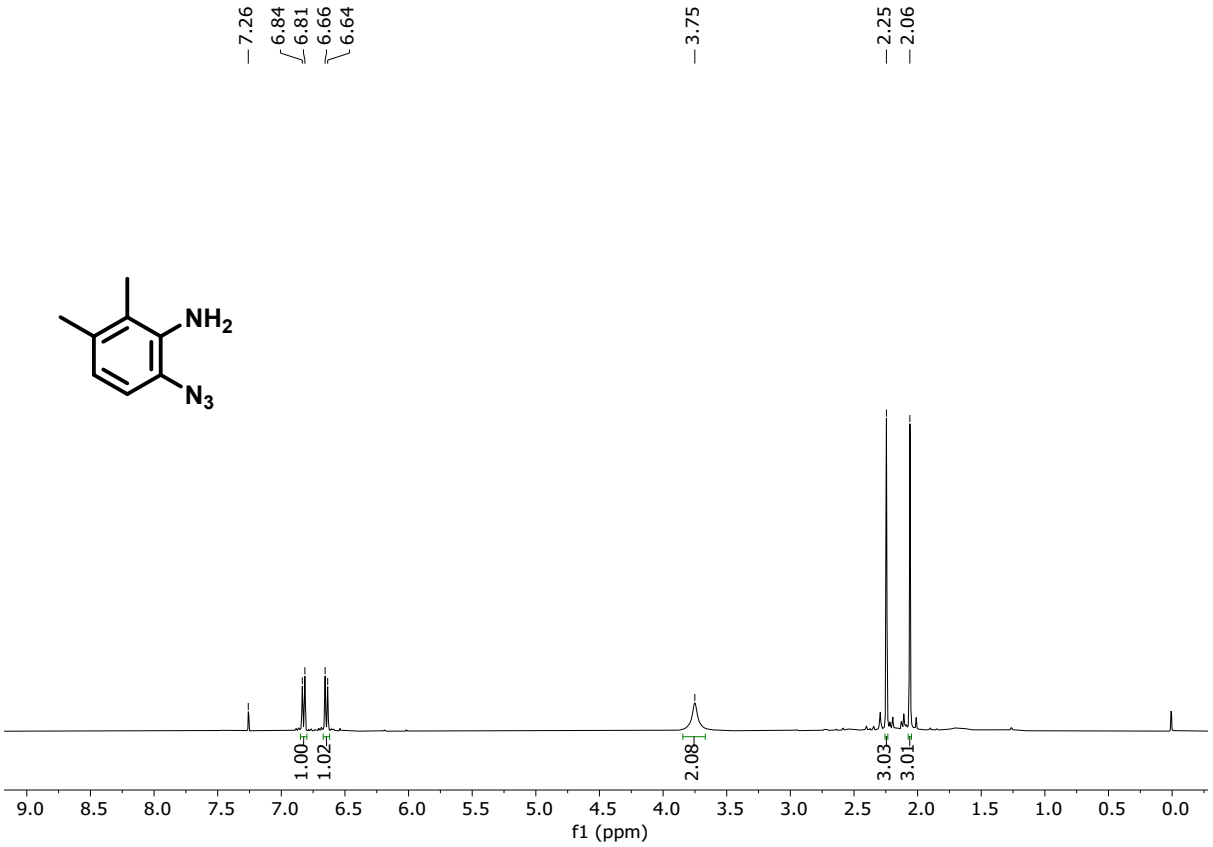


Fig S41. ^{1}H NMR spectrum of 6-azido-2,3-dimethylaniline (**2j**)

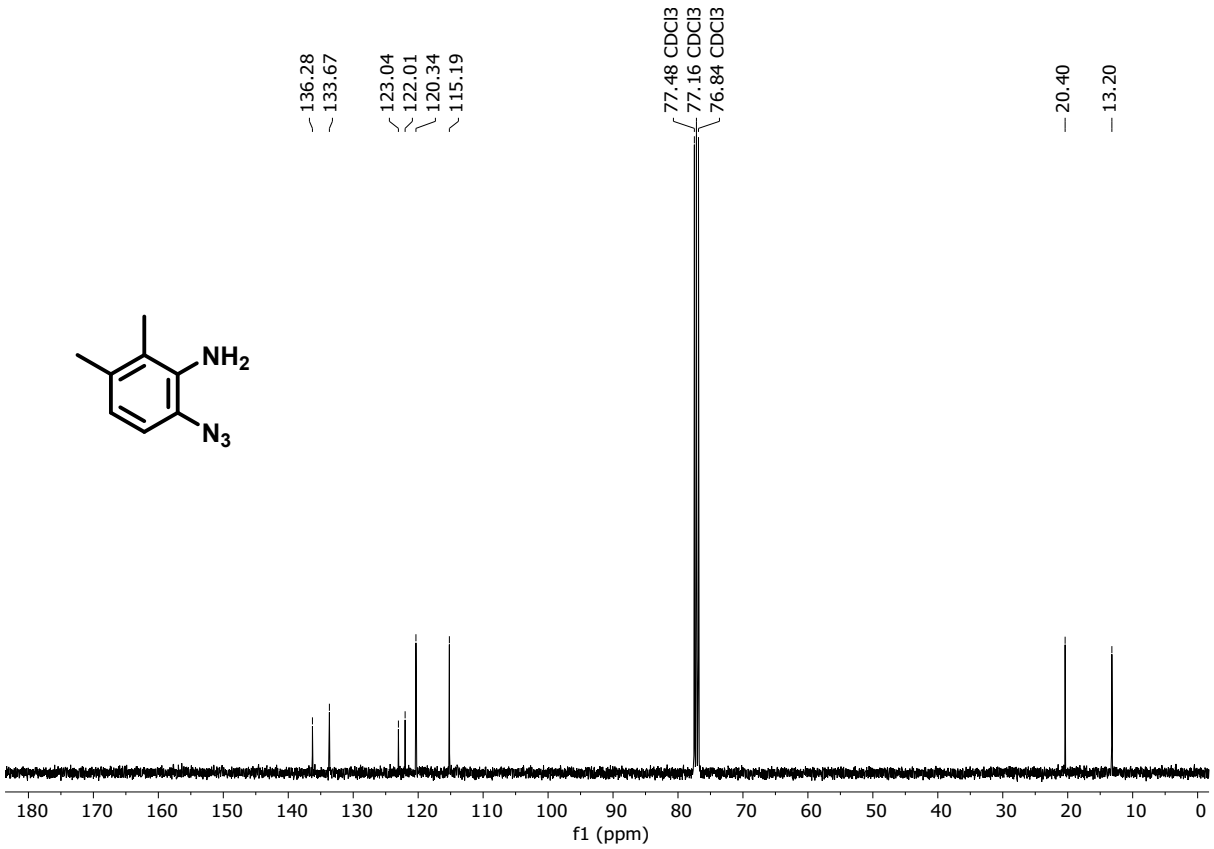


Fig S42. ^{13}C NMR spectrum of 6-azido-2,3-dimethylaniline (**2j**)

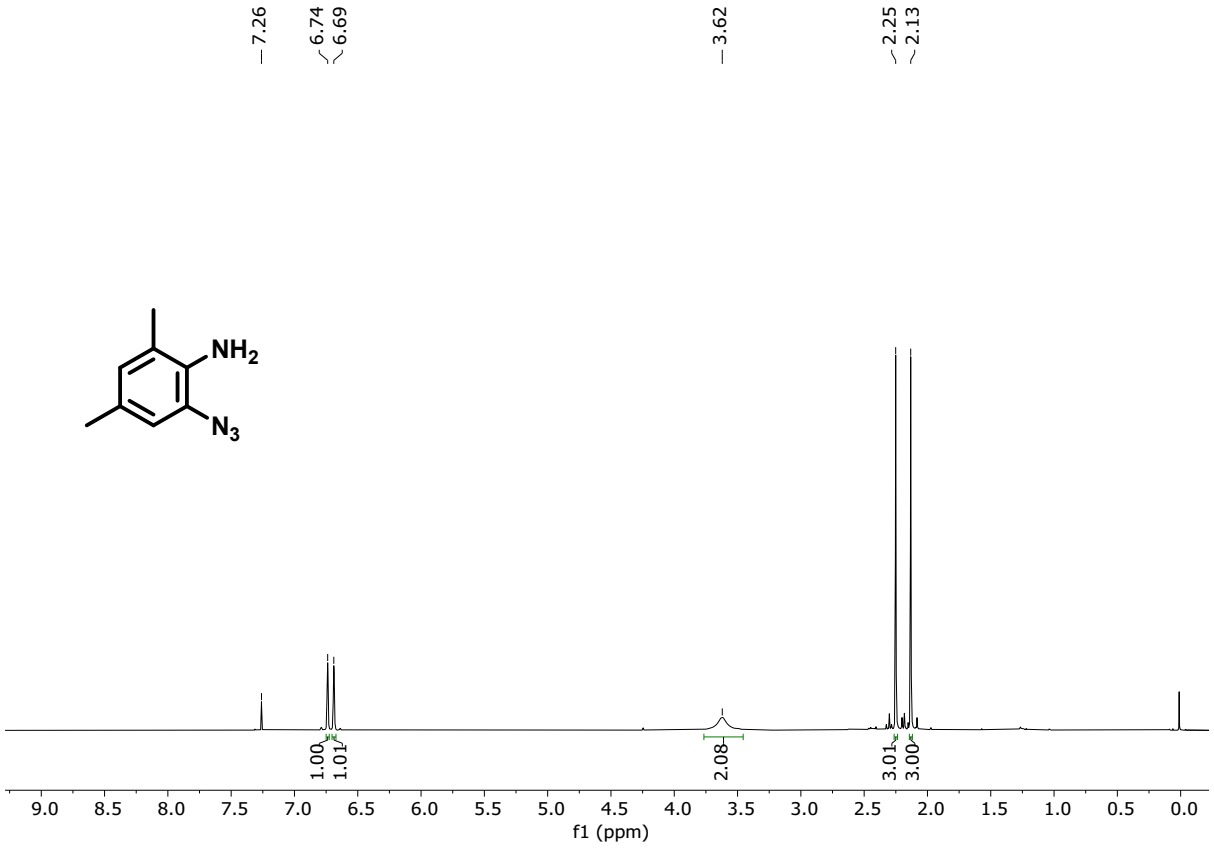


Fig S43. [1]H NMR spectrum of 2-azido-4,6-dimethylaniline (**2k**)

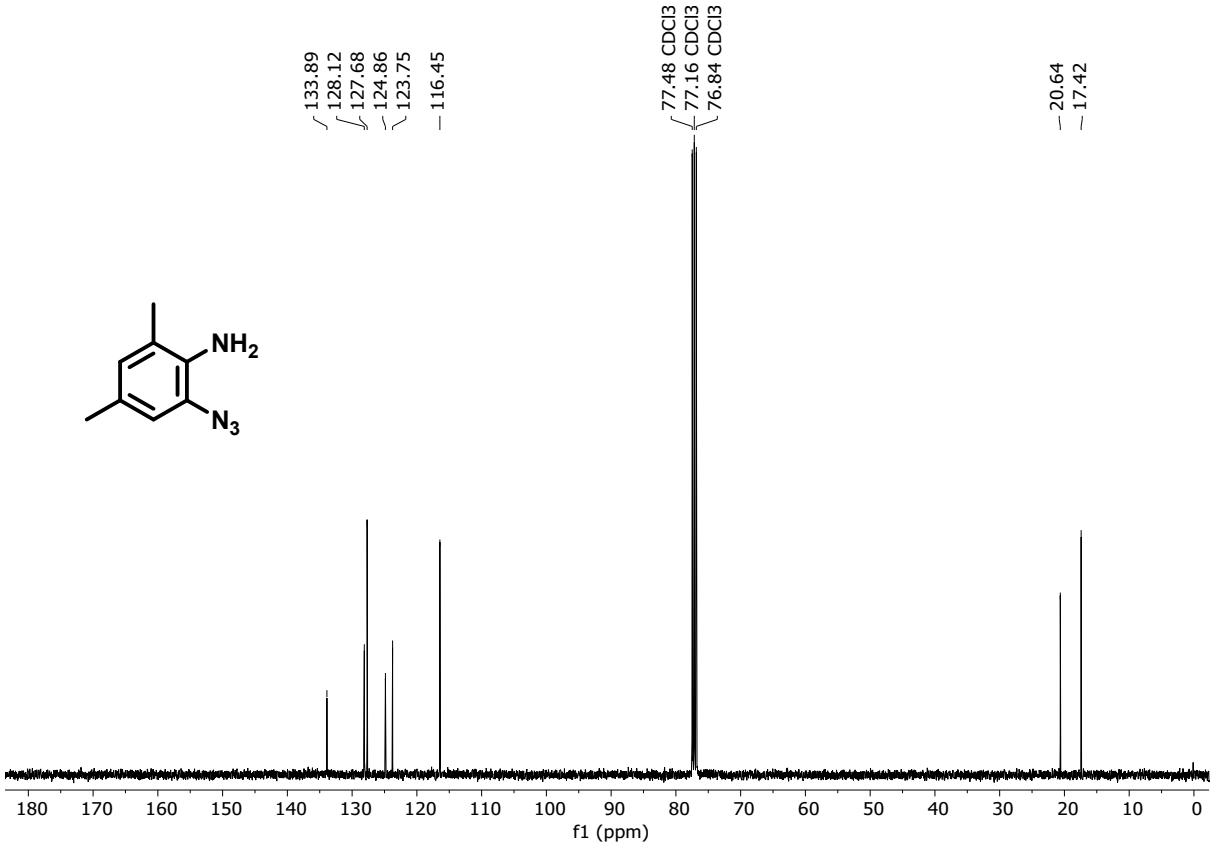


Fig S44. [13]C NMR spectrum of 2-azido-4,6-dimethylaniline (**2k**)

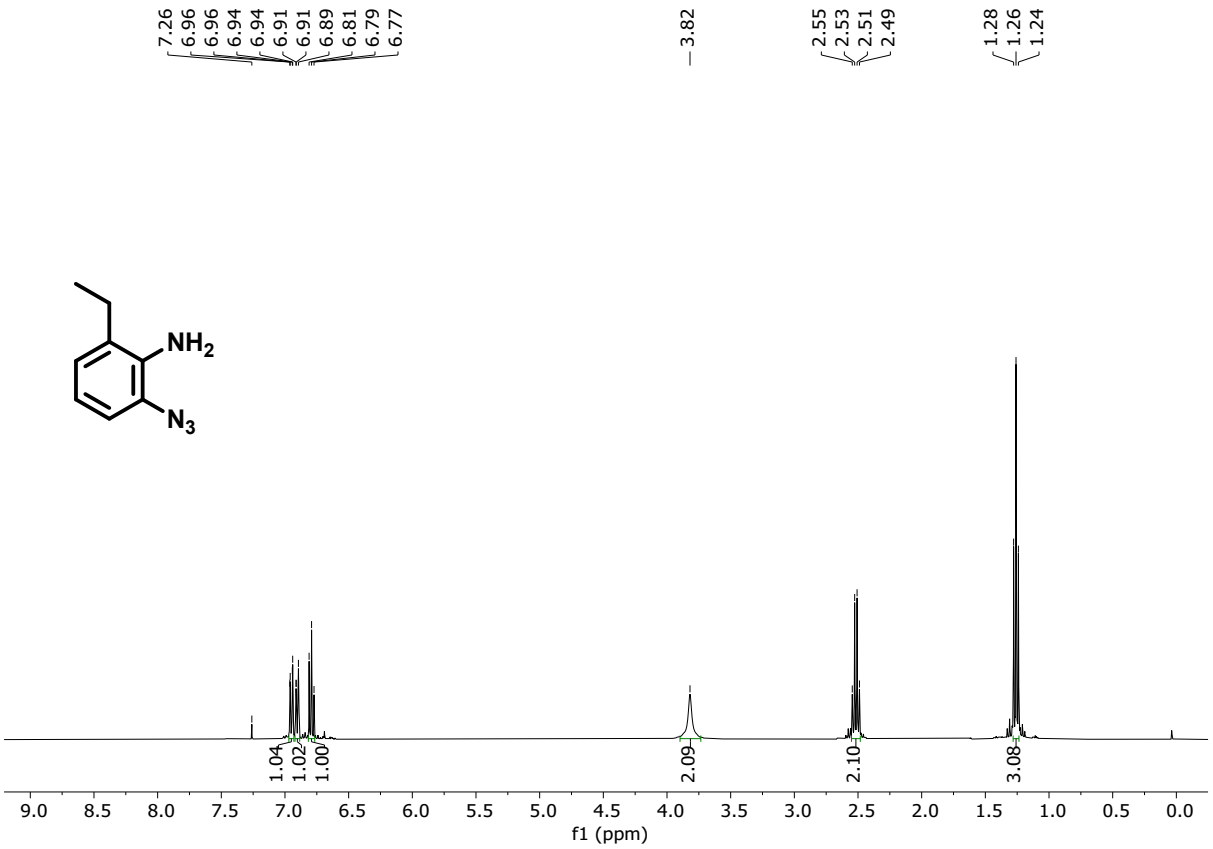


Fig S45. ^{1}H NMR spectrum of 2-azido-6-ethylaniline (**2l**)

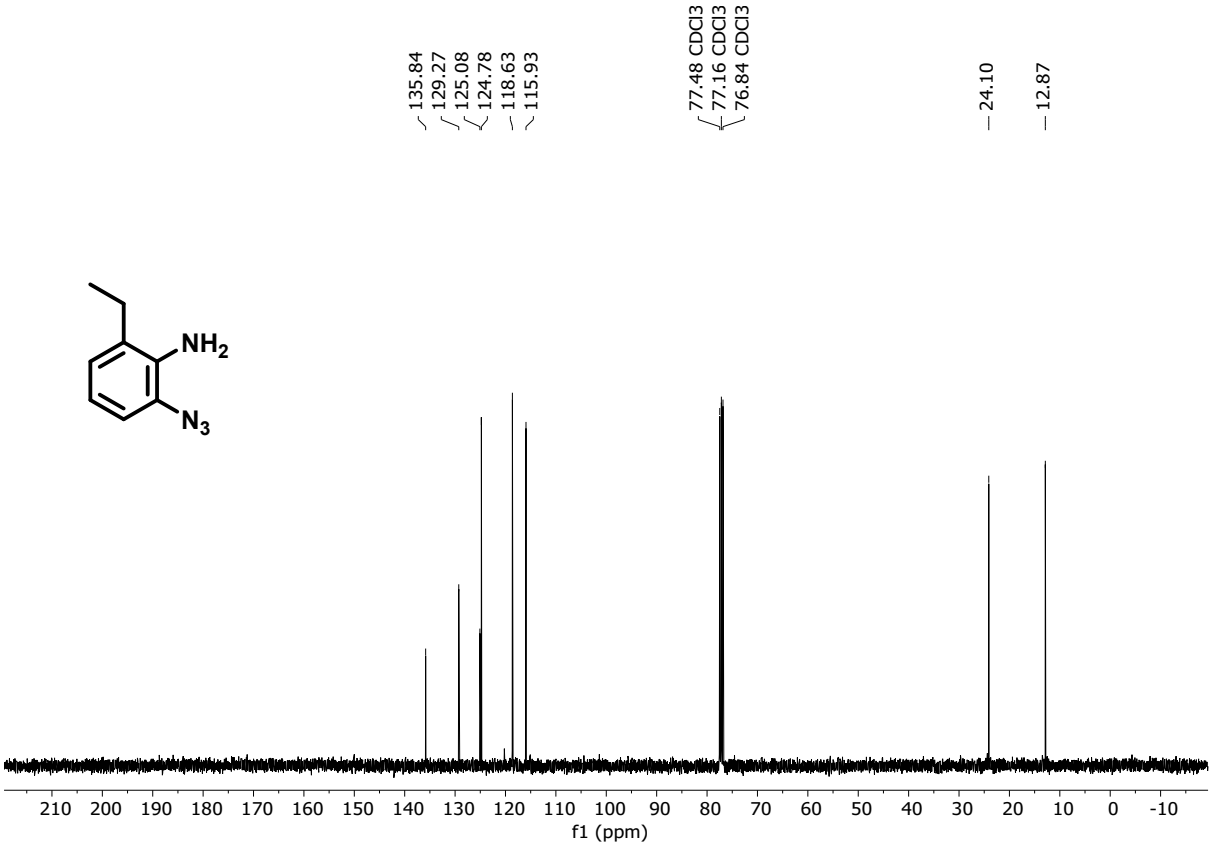


Fig S46. ^{13}C NMR spectrum of 2-azido-6-ethylaniline (**2l**)

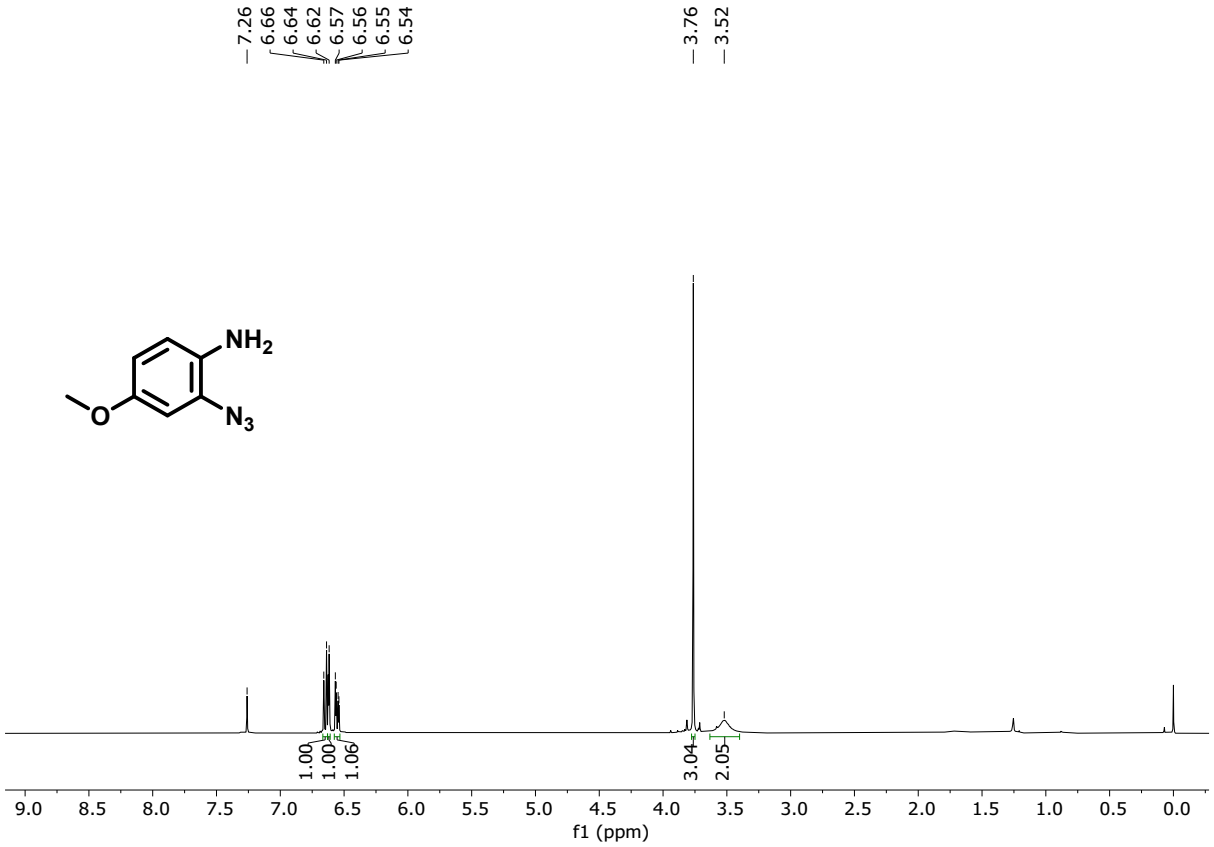


Fig S47. ^{1}H NMR spectrum of 2-azido-4-methoxyaniline (**2m**)

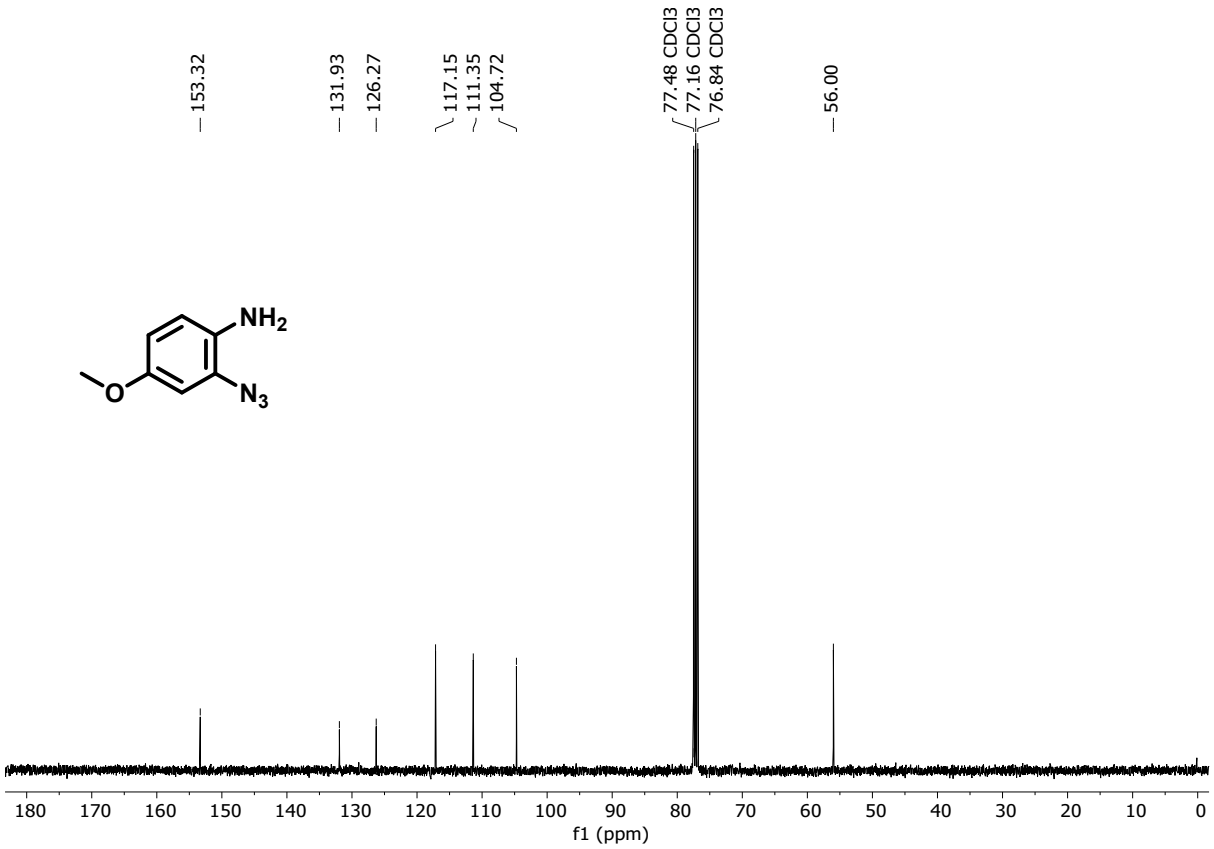


Fig S48. ^{13}C NMR spectrum of 2-azido-4-methoxyaniline (**2m**)

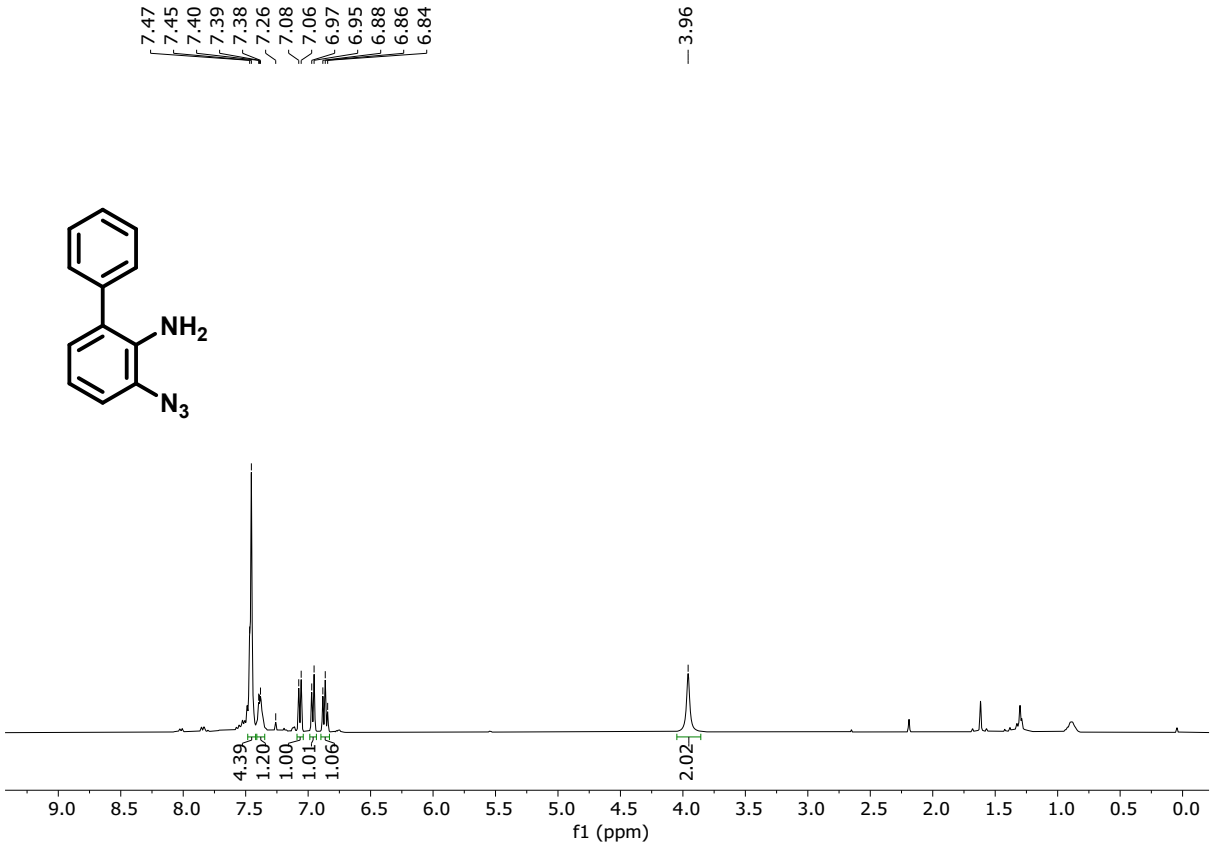


Fig S49. ^{1}H NMR spectrum of 3-azido-[1,1'-biphenyl]-2-amine (**2n**)

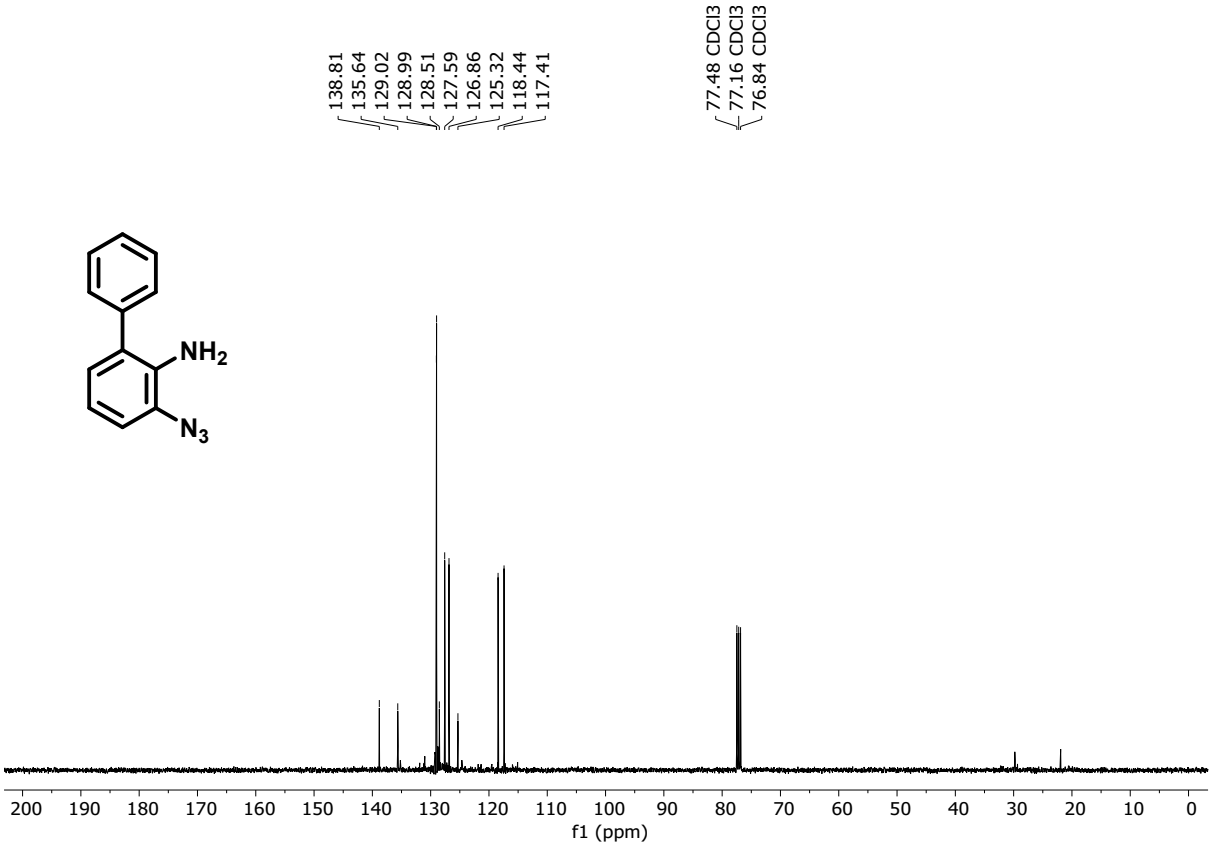


Fig S50. ^{13}C NMR spectrum of 3-azido-[1,1'-biphenyl]-2-amine (**2n**)

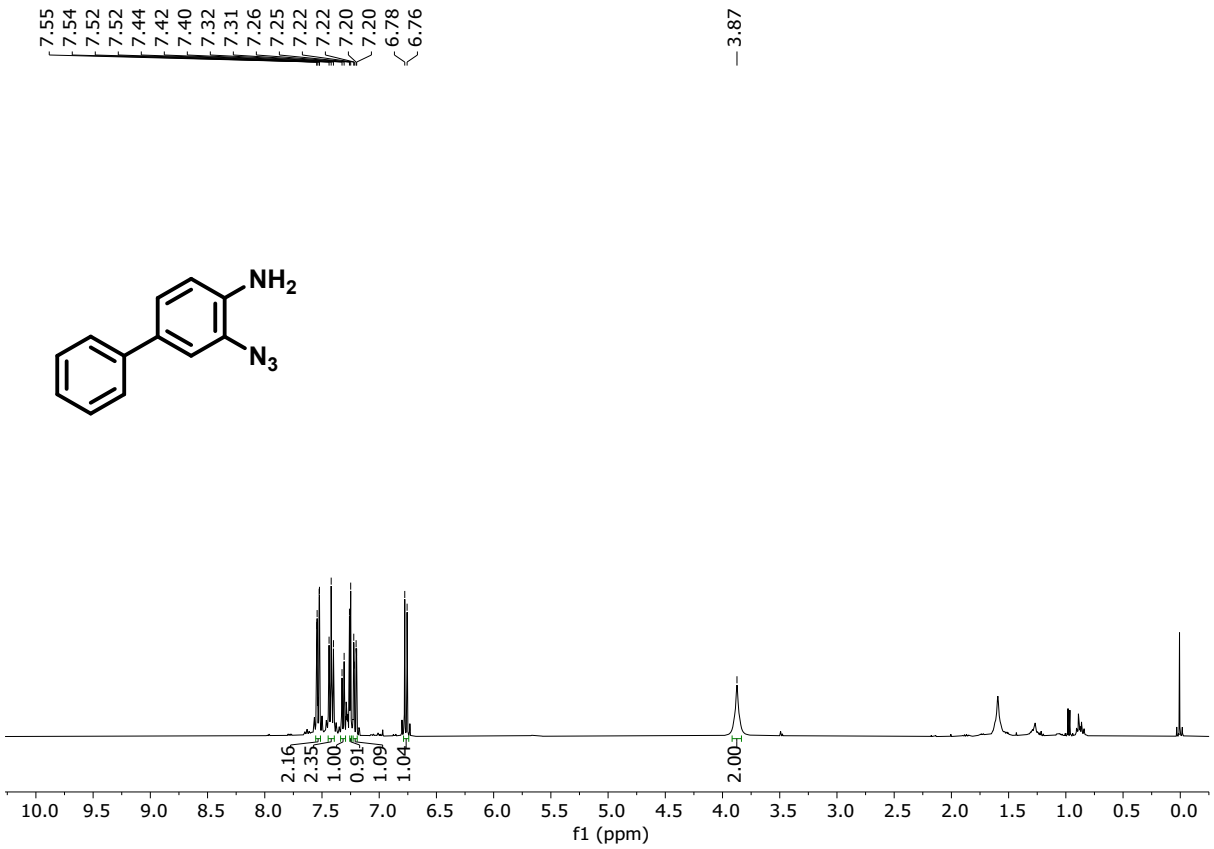


Fig S51. ^{1}H NMR spectrum of 3-azido-[1,1'-biphenyl]-4-amine (**2o**)

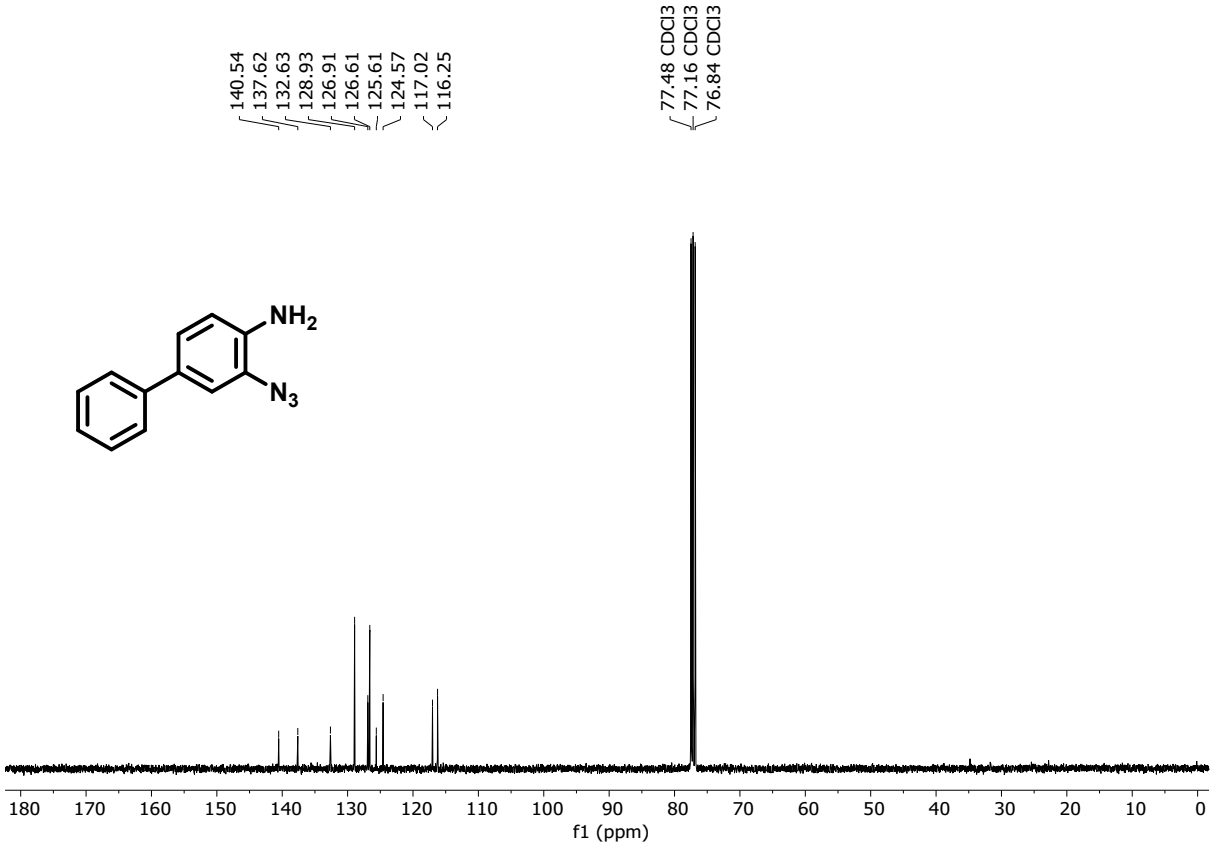


Fig S52. ^{13}C NMR spectrum of 3-azido-[1,1'-biphenyl]-4-amine (**2o**)

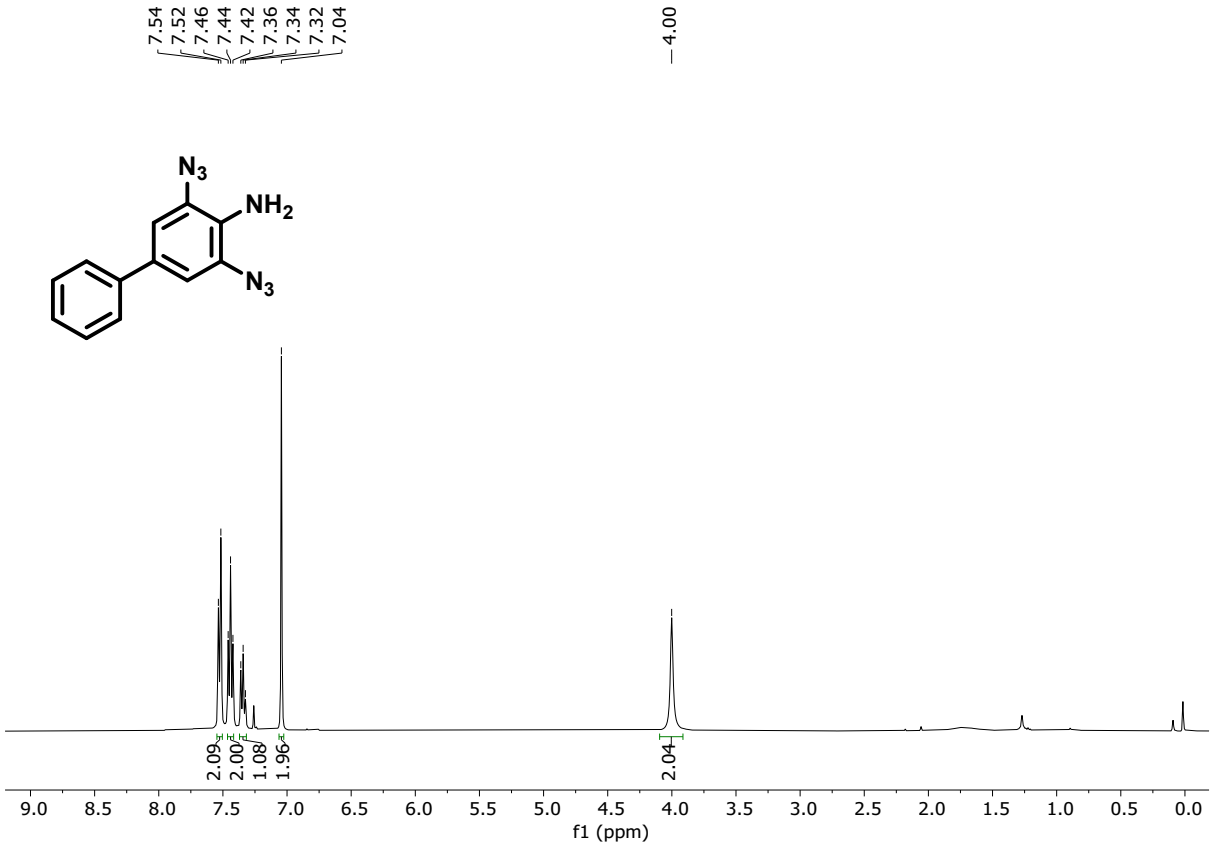


Fig S53. ^{1}H NMR spectrum of 3,5-diazido-[1,1'-biphenyl]-4-amine (**2o'**)

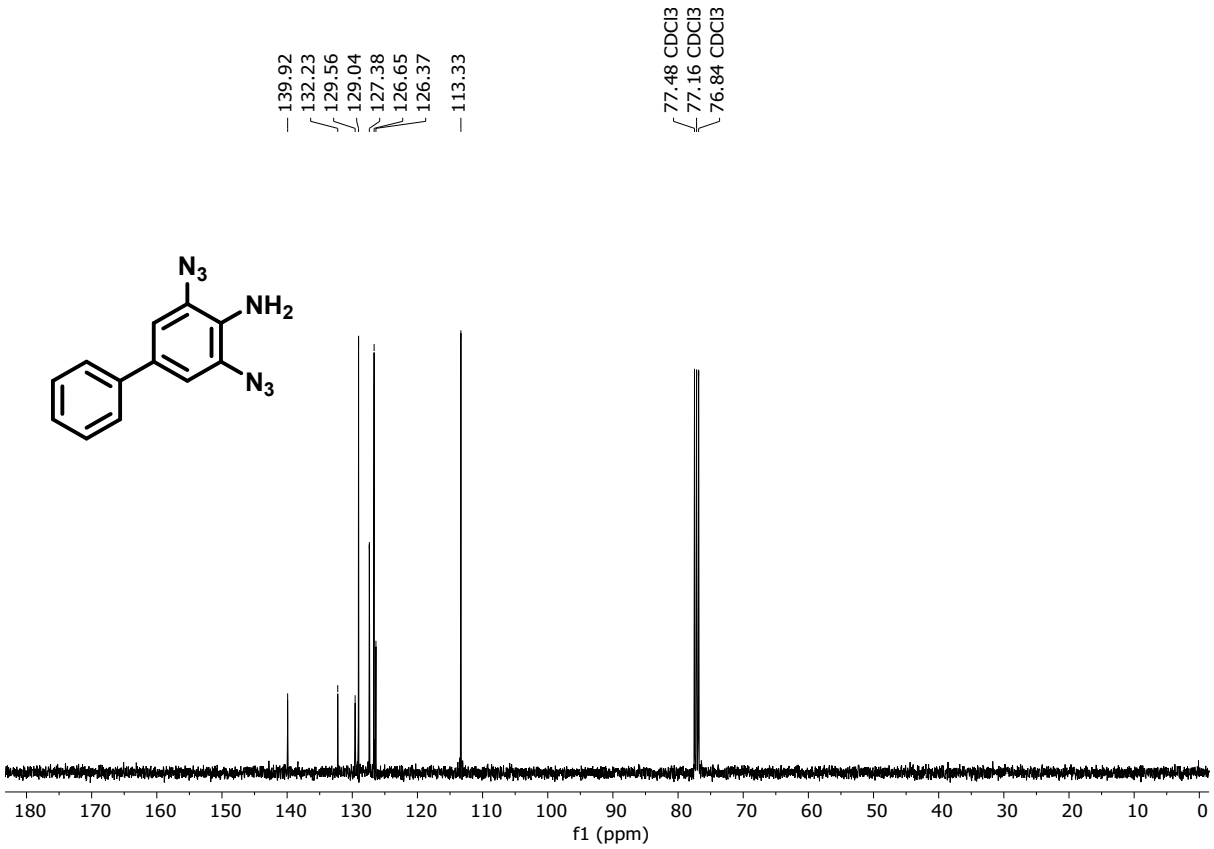


Fig S54. ^{13}C NMR spectrum of 3,5-diazido-[1,1'-biphenyl]-4-amine (**2o'**)

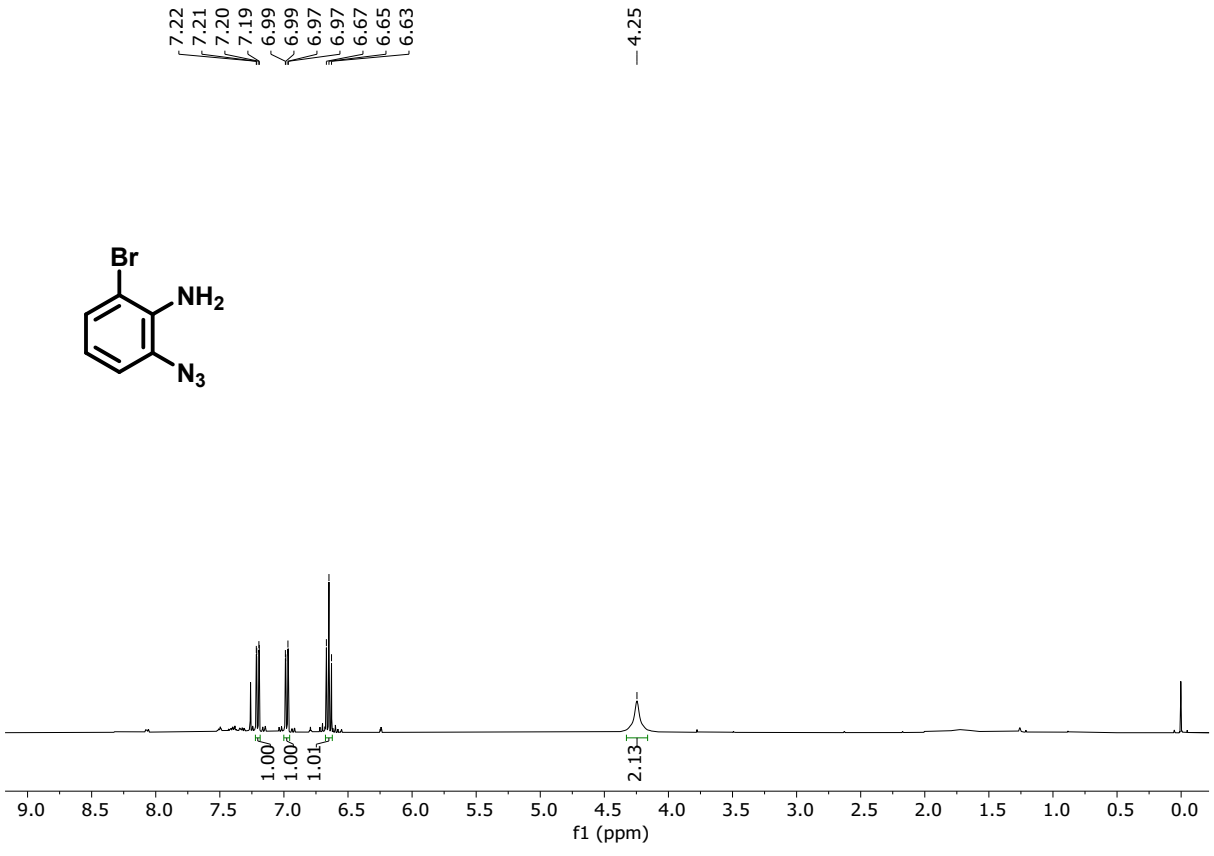


Fig S55. ^{1}H NMR spectrum of 2-azido-6-bromoaniline (**2p**)

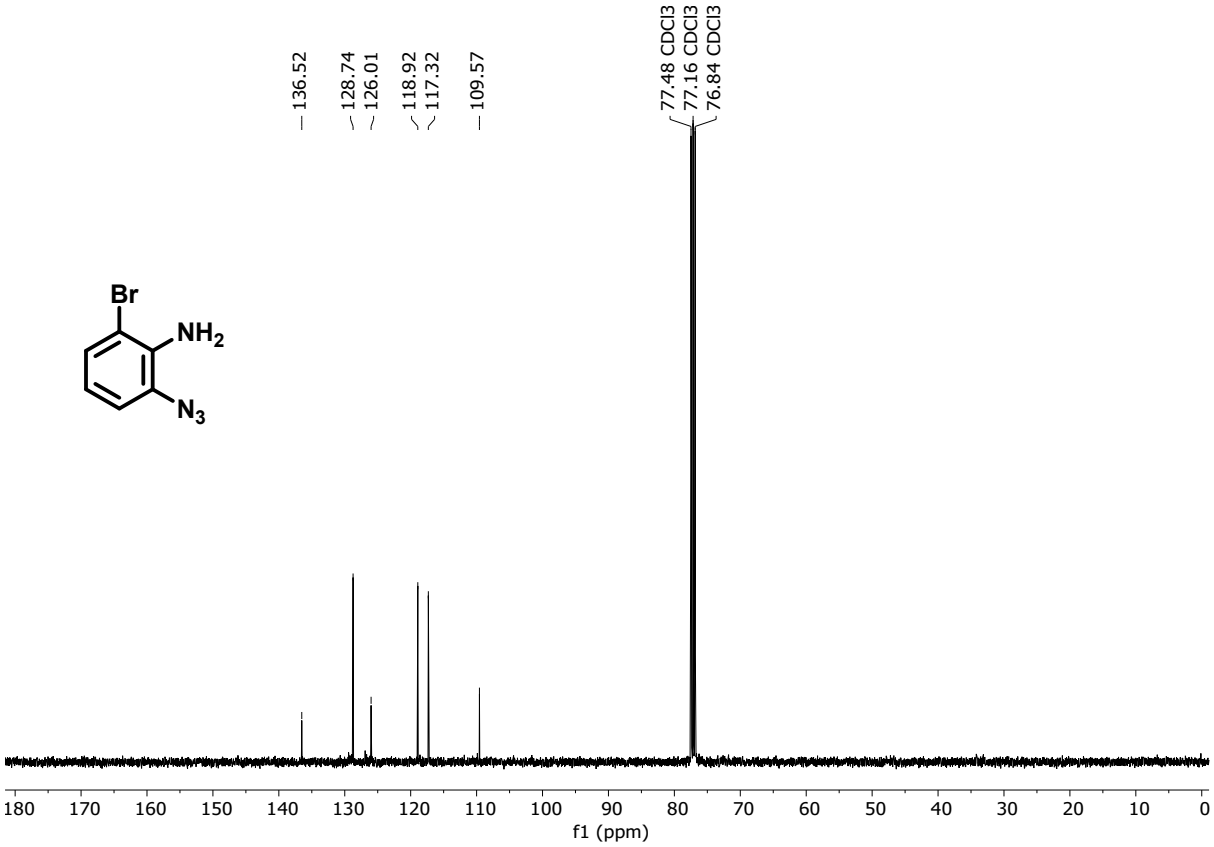


Fig S56. ^{13}C NMR spectrum of 2-azido-6-bromoaniline (**2p**)

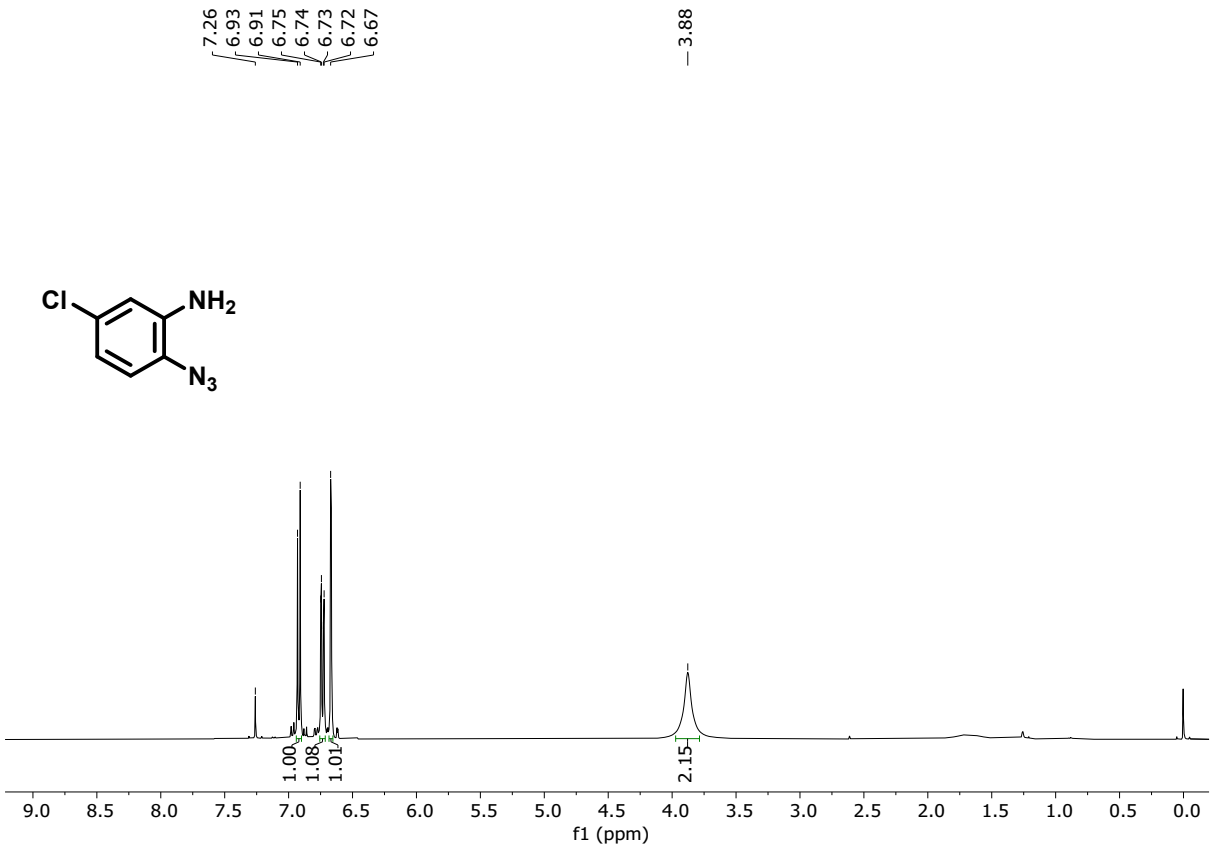


Fig S57. [1]H NMR spectrum of 2-azido-5-chloroaniline (**2q**)

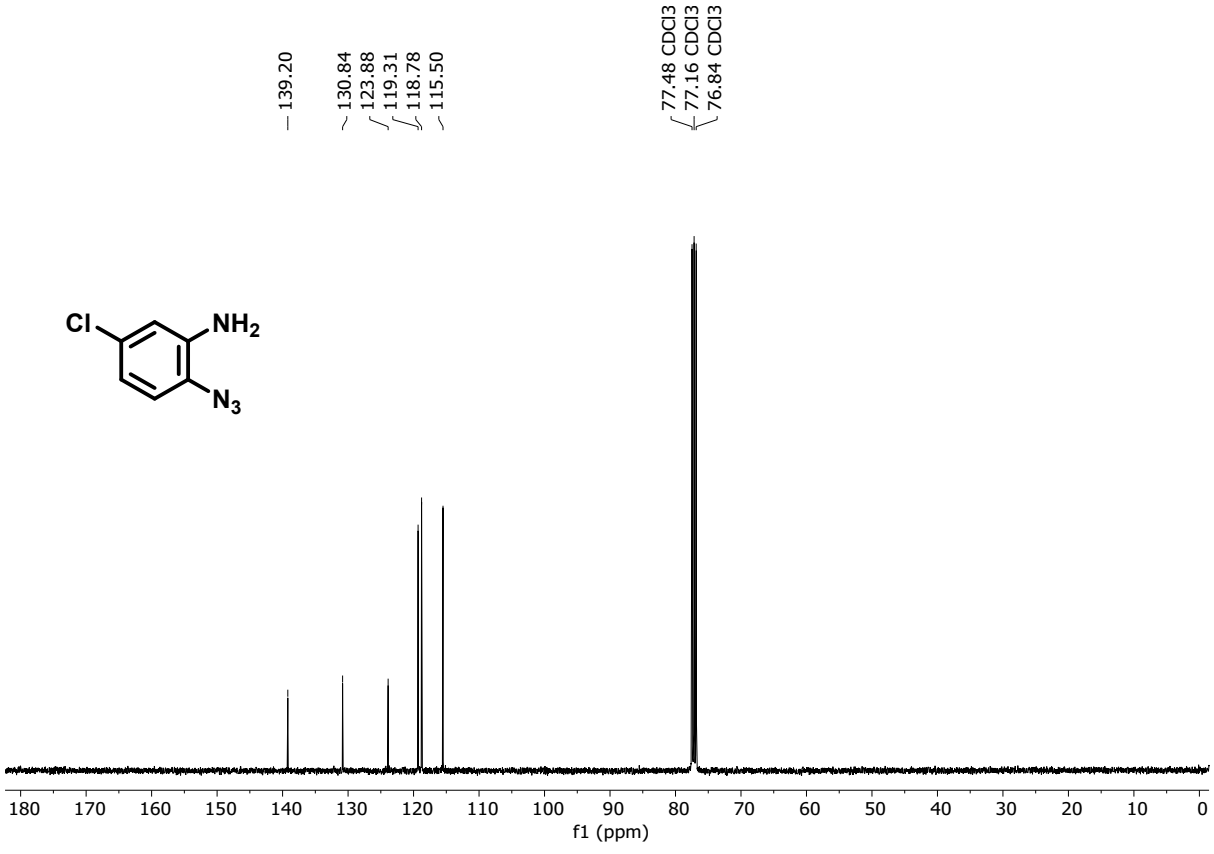


Fig S58. ^{13}C NMR spectrum of 2-azido-5-chloroaniline (**2q**)

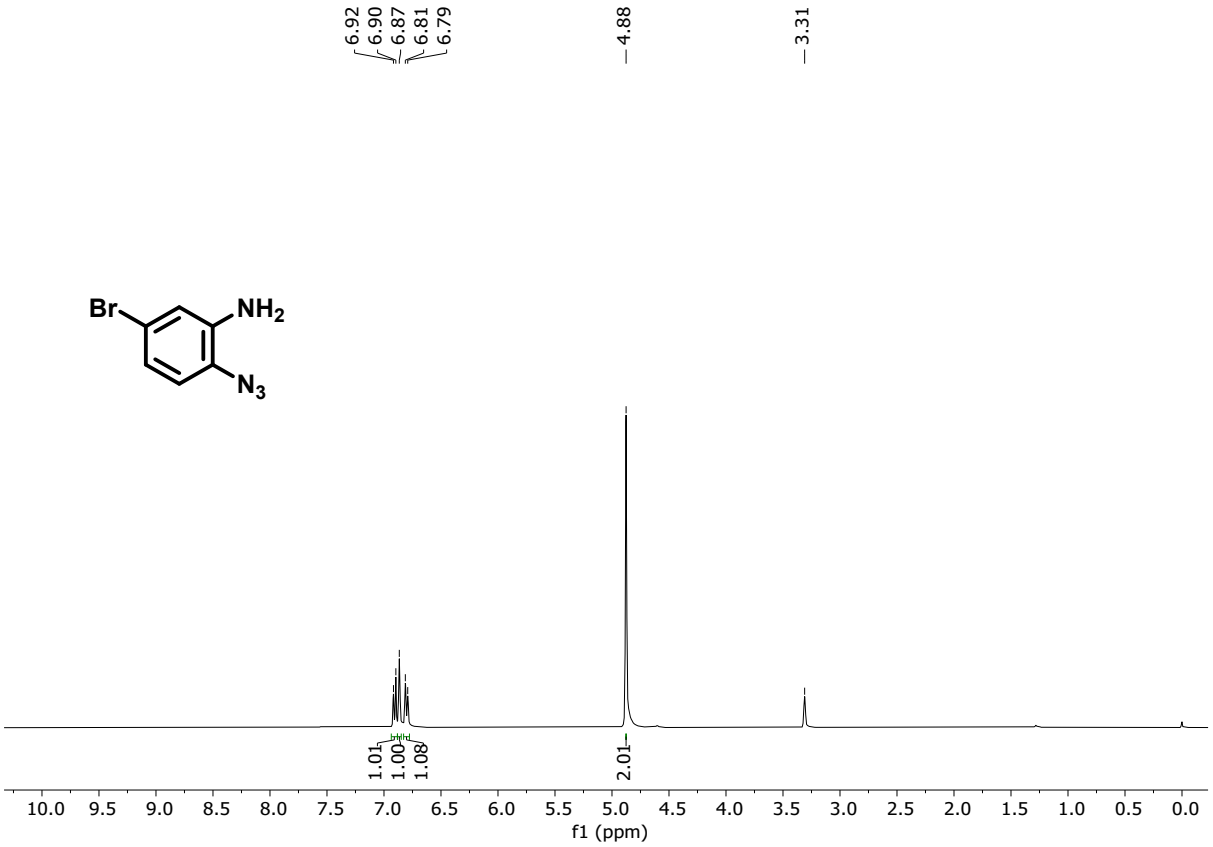


Fig S59. ^{1}H NMR spectrum of 2-azido-5-bromoaniline (**2r**)

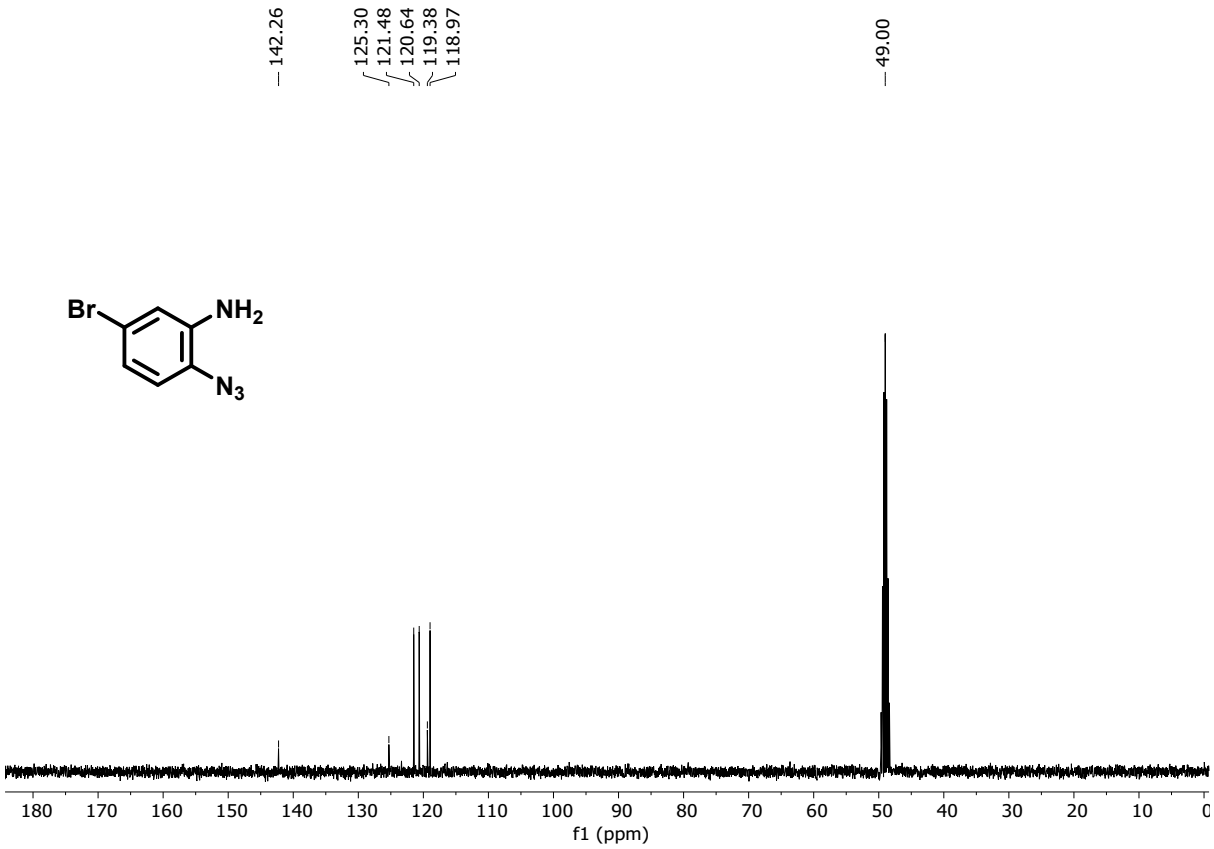


Fig S60. ^{13}C NMR spectrum of 2-azido-5-bromoaniline (**2r**)

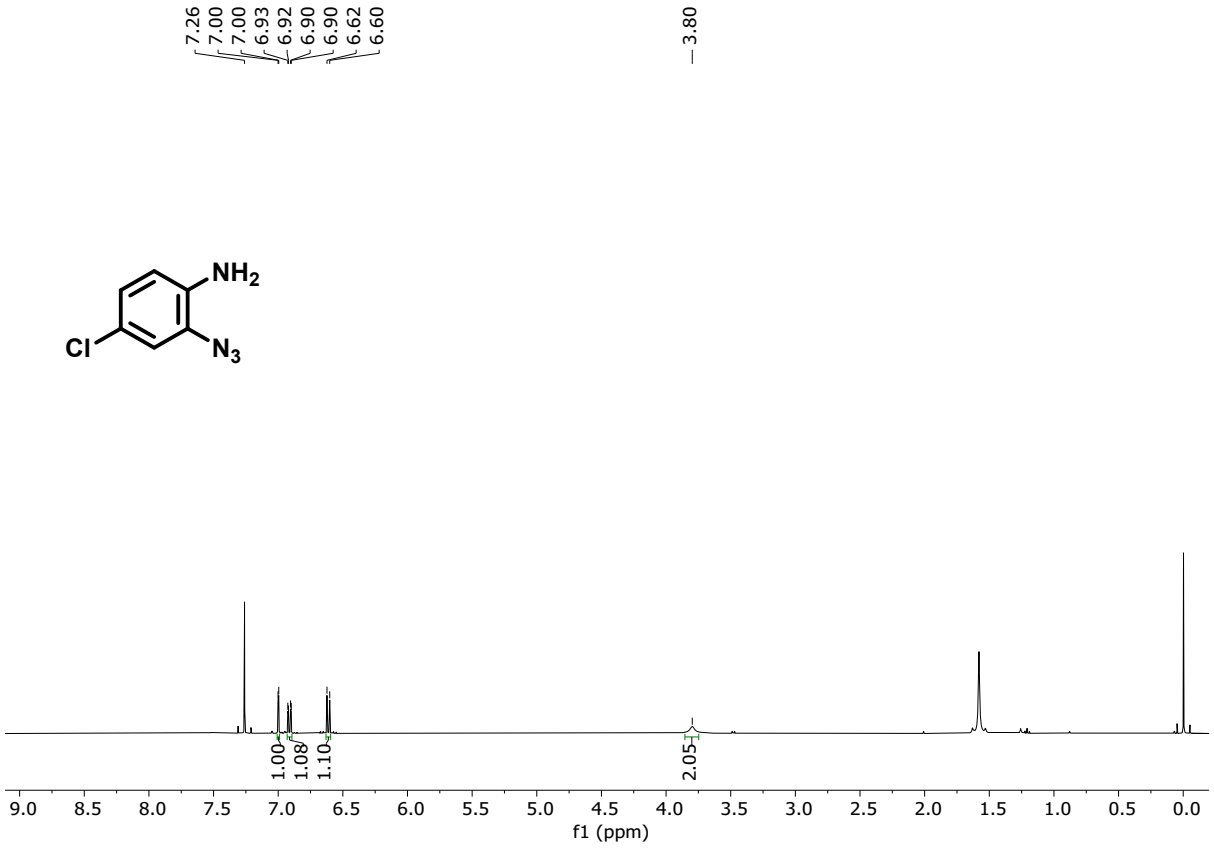


Fig S61. ^{1}H NMR spectrum of 2-azido-4-chloroaniline (**2s**)

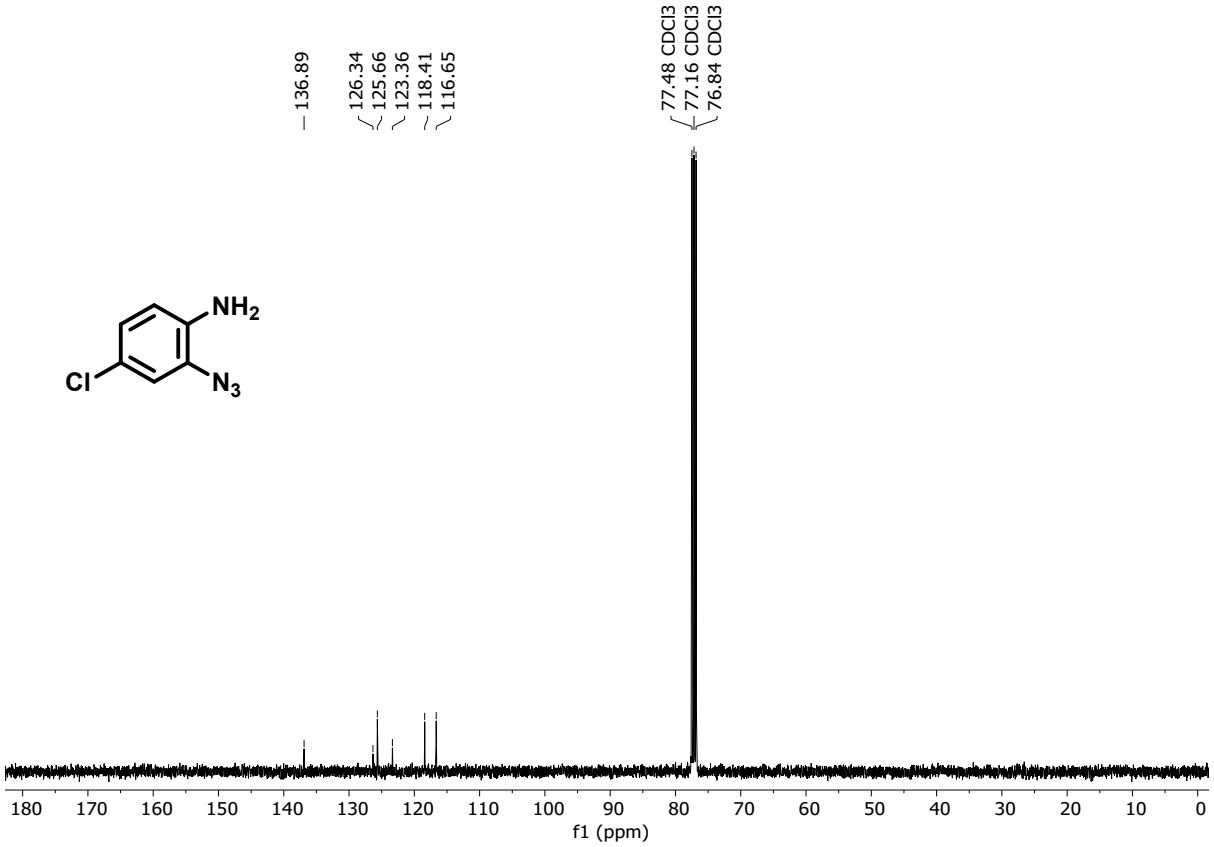


Fig S62. ^{13}C NMR spectrum of 2-azido-4-chloroaniline (**2s**)

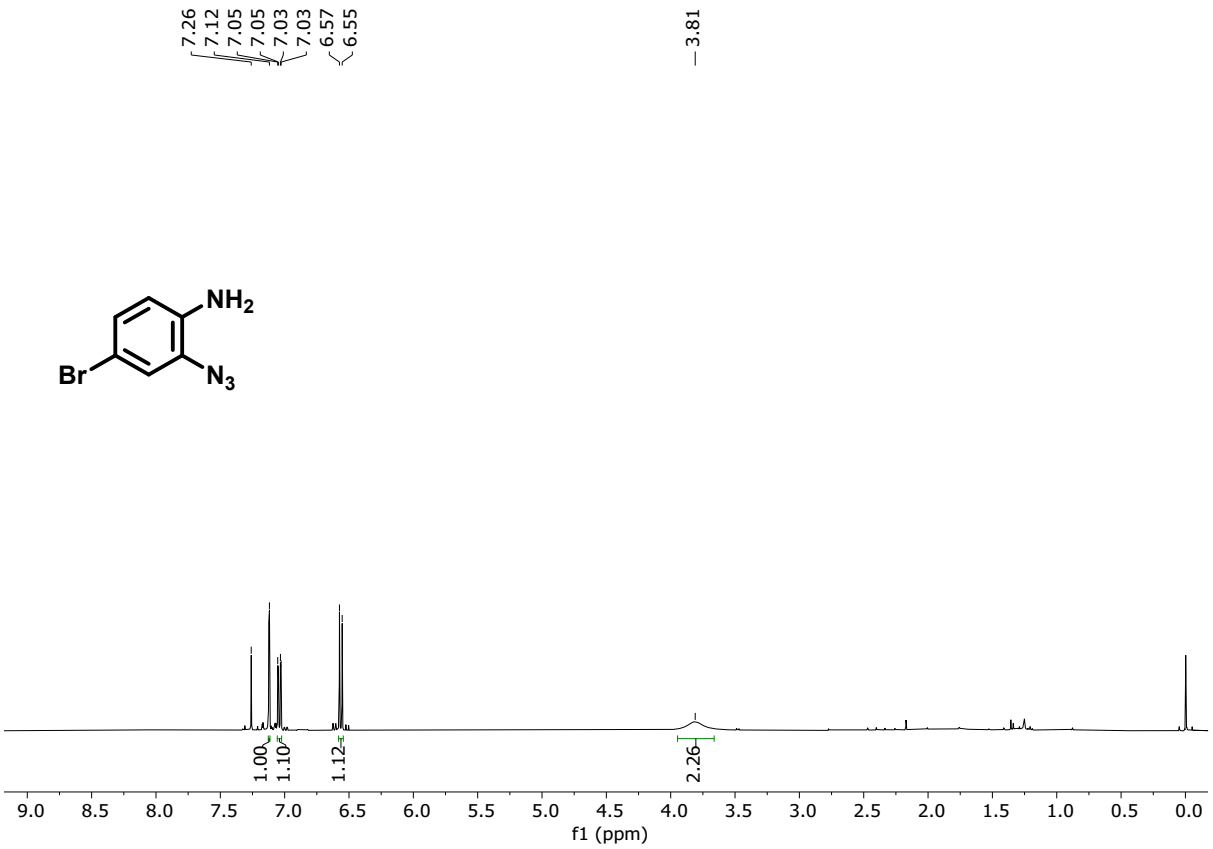


Fig S63. ^{1}H NMR spectrum of 2-azido-4-bromoaniline (**2t**)

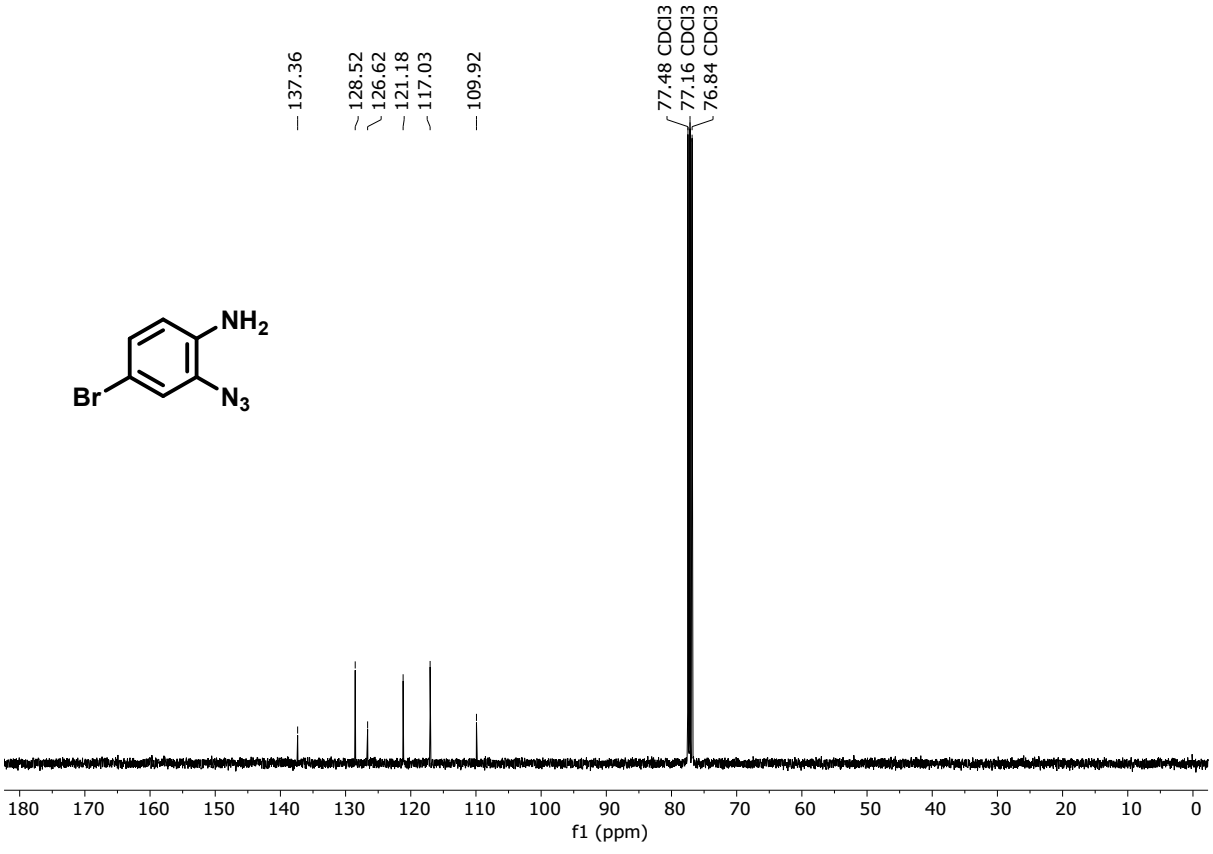


Fig S64. ^{13}C NMR spectrum of 2-azido-4-bromoaniline (**2t**)

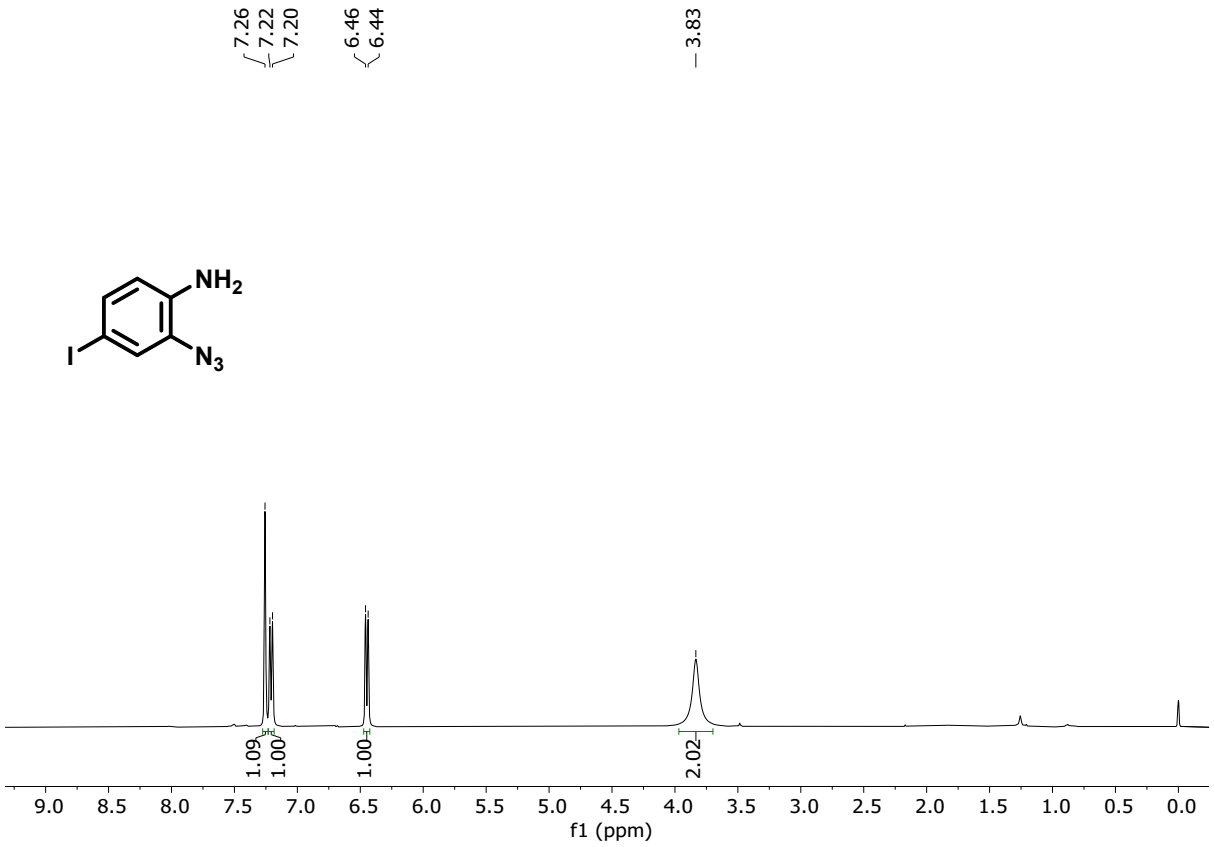


Fig S65. ^{1}H NMR spectrum of 2-azido-4-iodoaniline (**2u**)

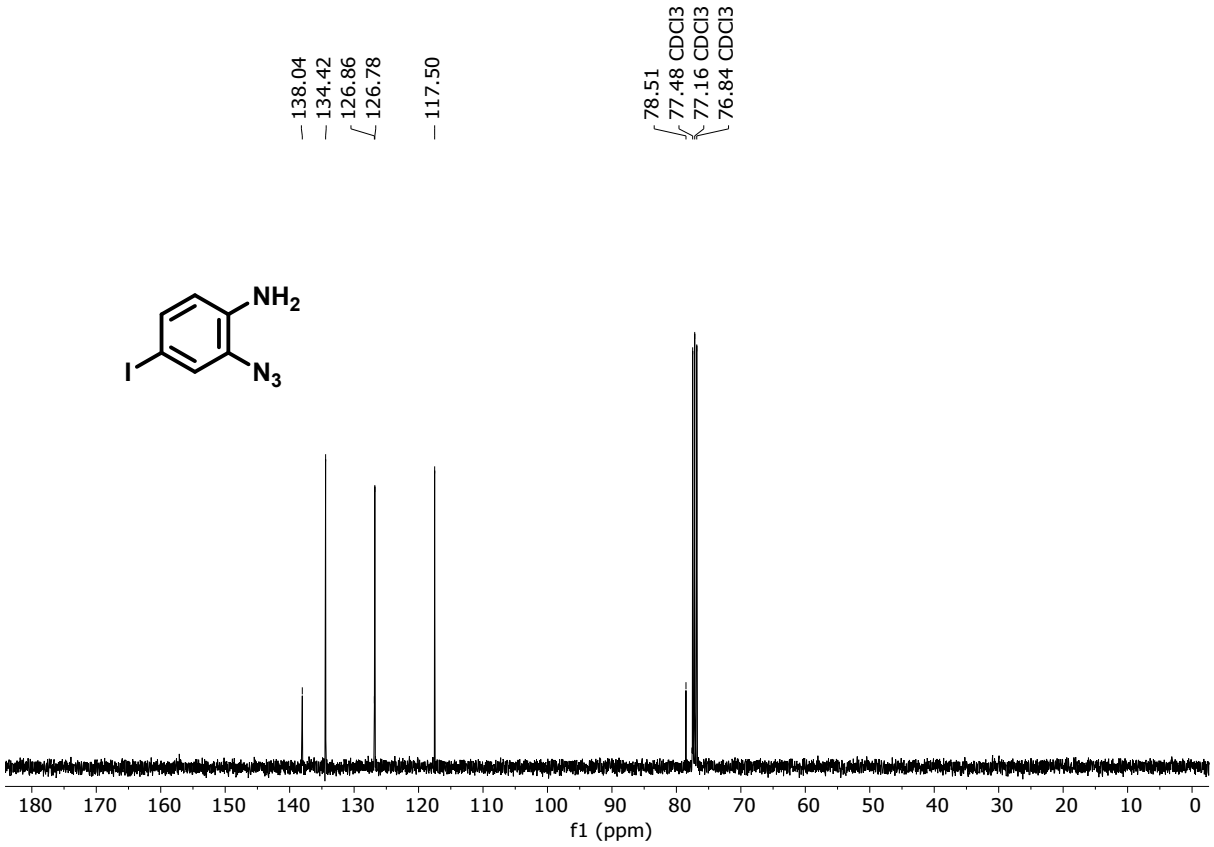


Fig S66. ^{13}C NMR spectrum of 2-azido-4-iodoaniline (**2u**)

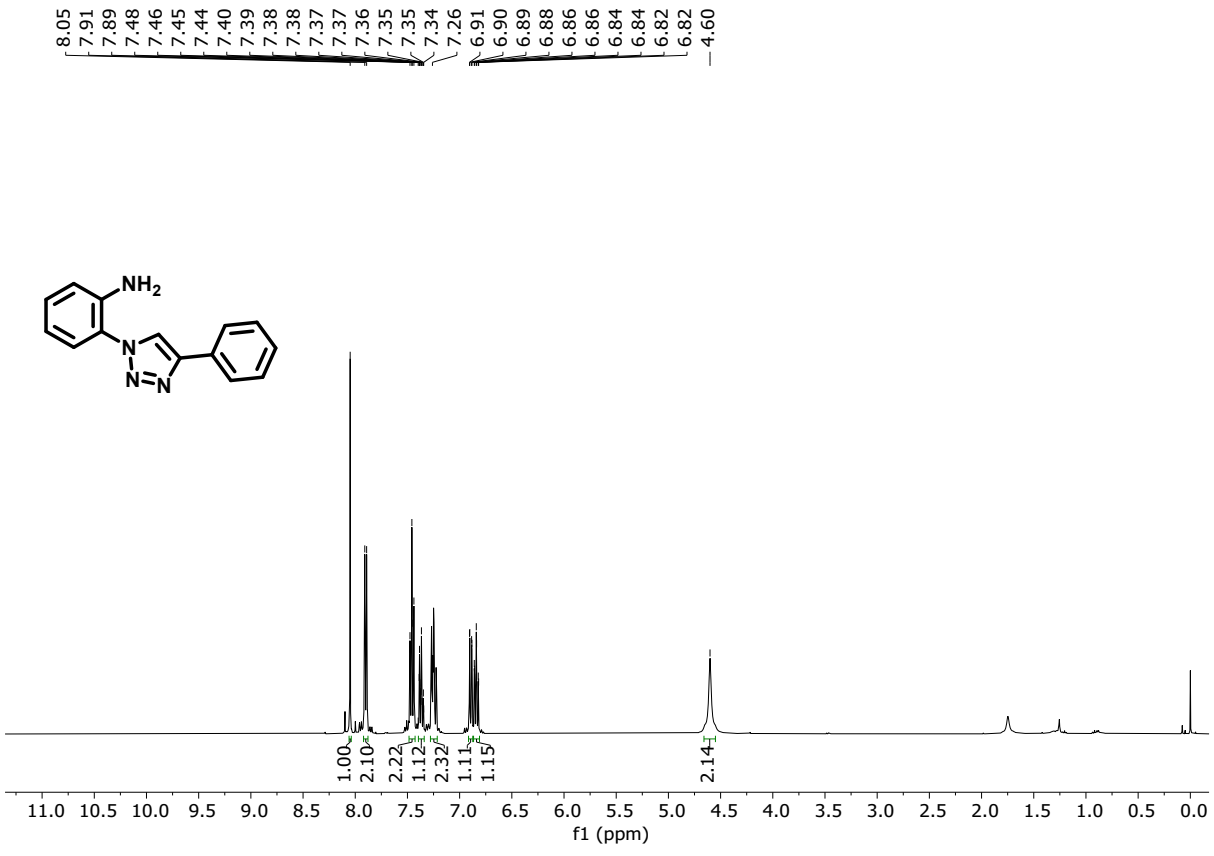


Fig S67. [1]H NMR spectrum of 2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3a**)

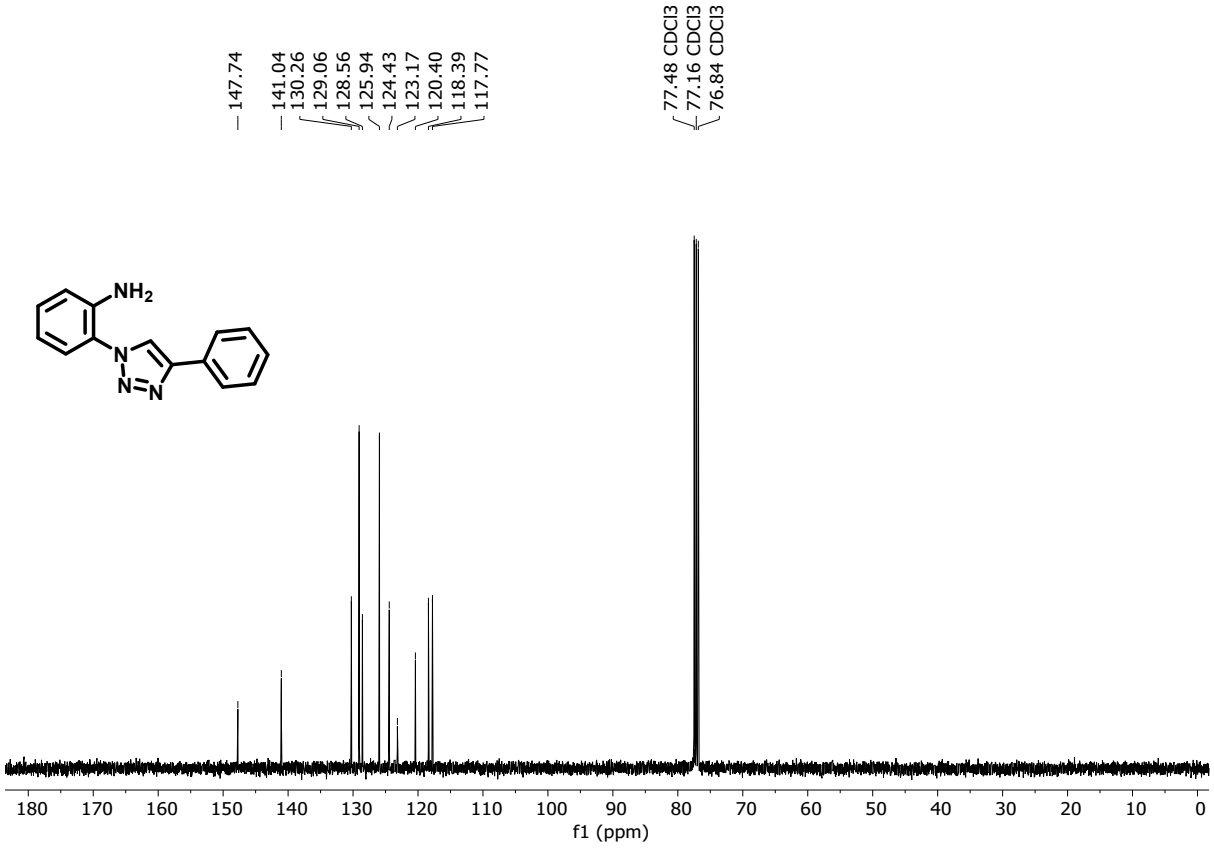


Fig S68. [13]C NMR spectrum of 2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3a**)

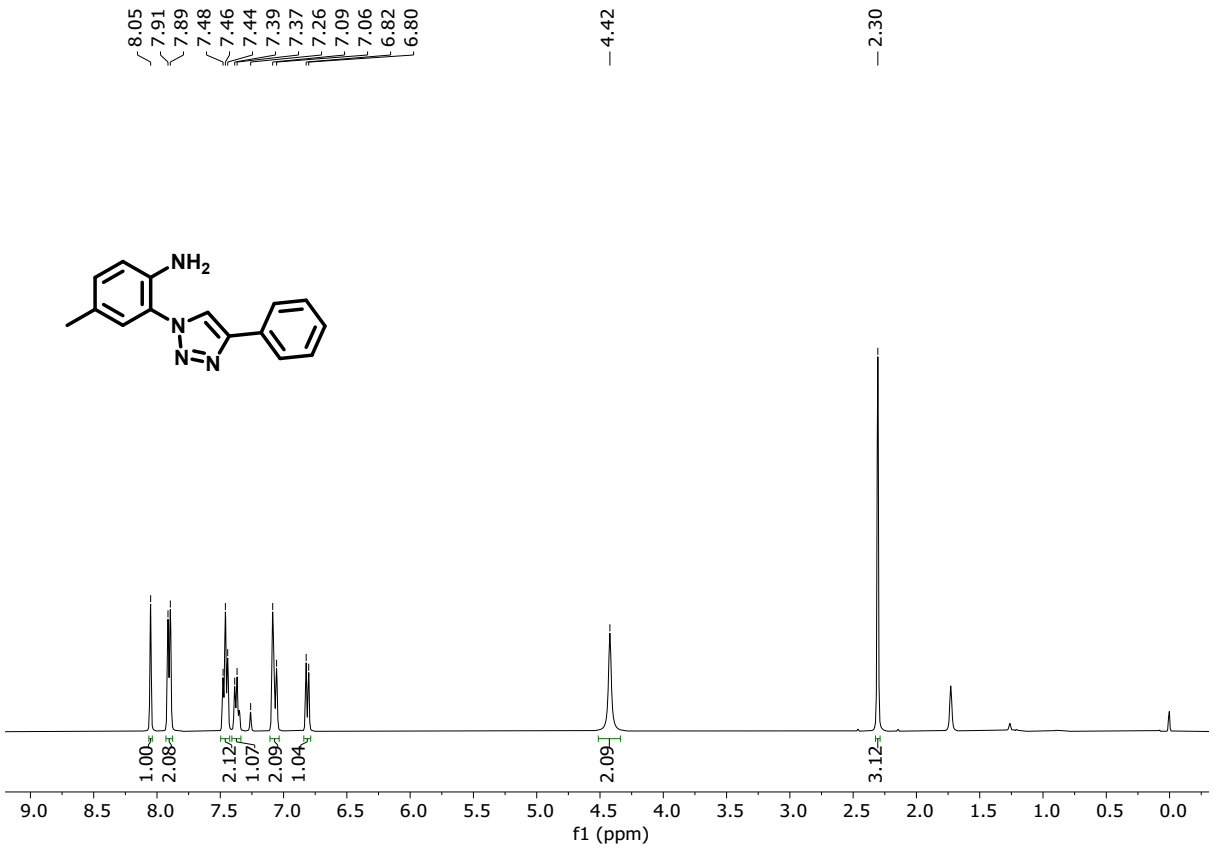


Fig S69. ^{1}H NMR spectrum of 4-methyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3b**)

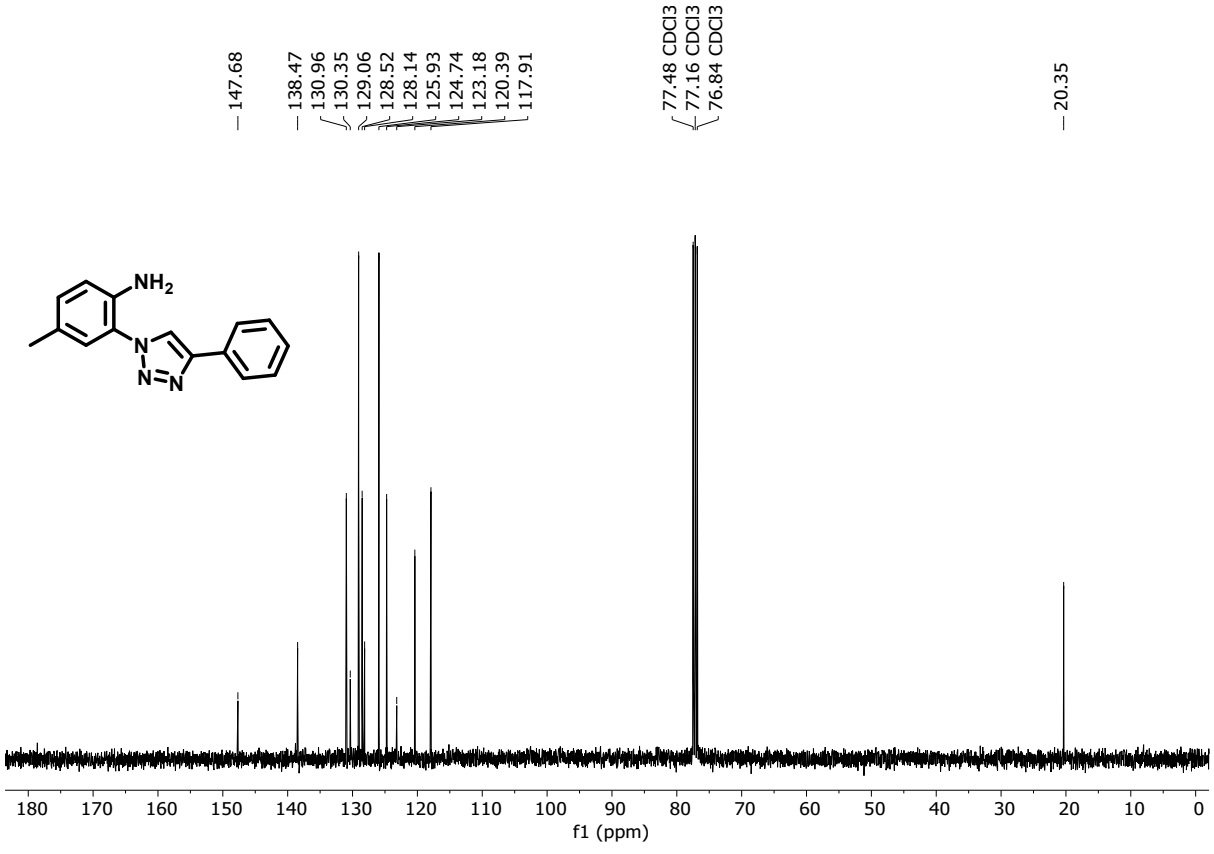


Fig S70. ^{13}C NMR spectrum of 4-methyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3b**)

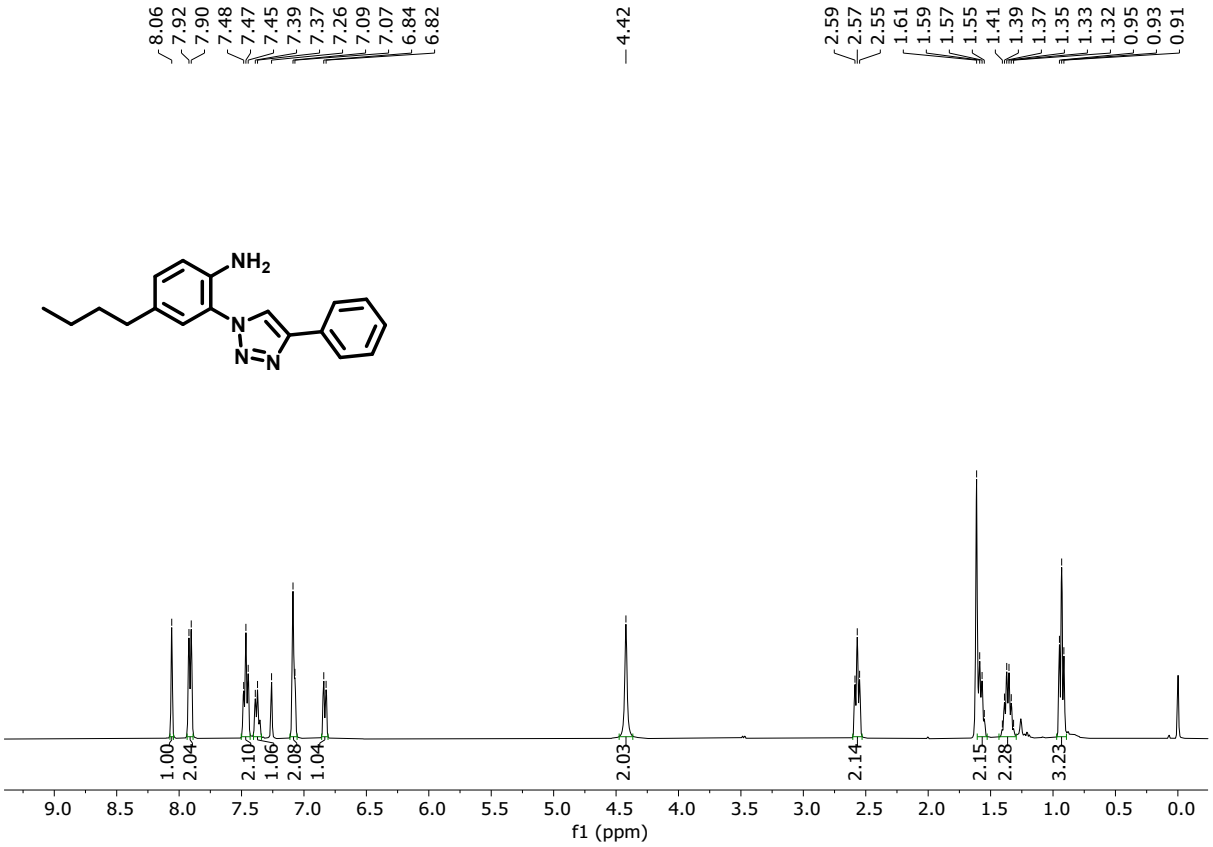


Fig S71. ^{1}H NMR spectrum of 4-butyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3c**)

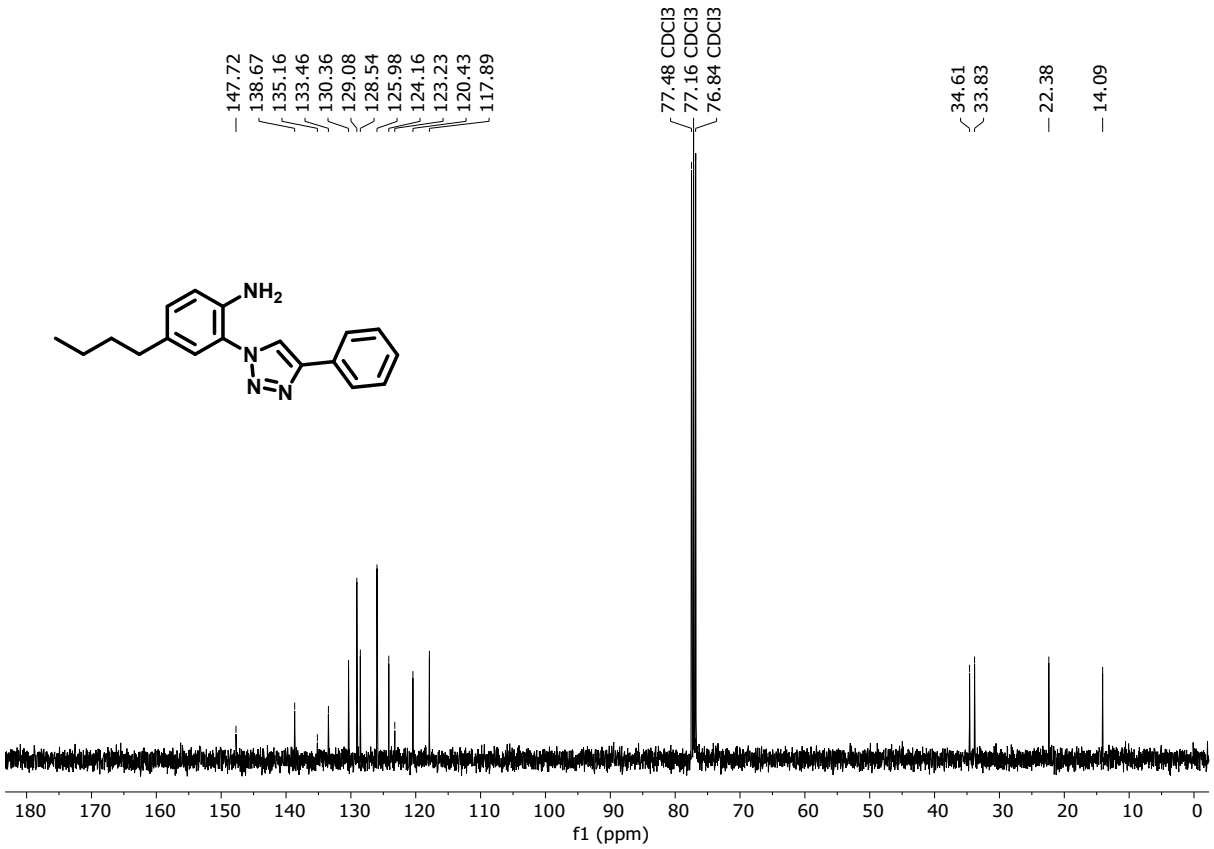


Fig S72. ^{13}C NMR spectrum of 4-butyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3c**)

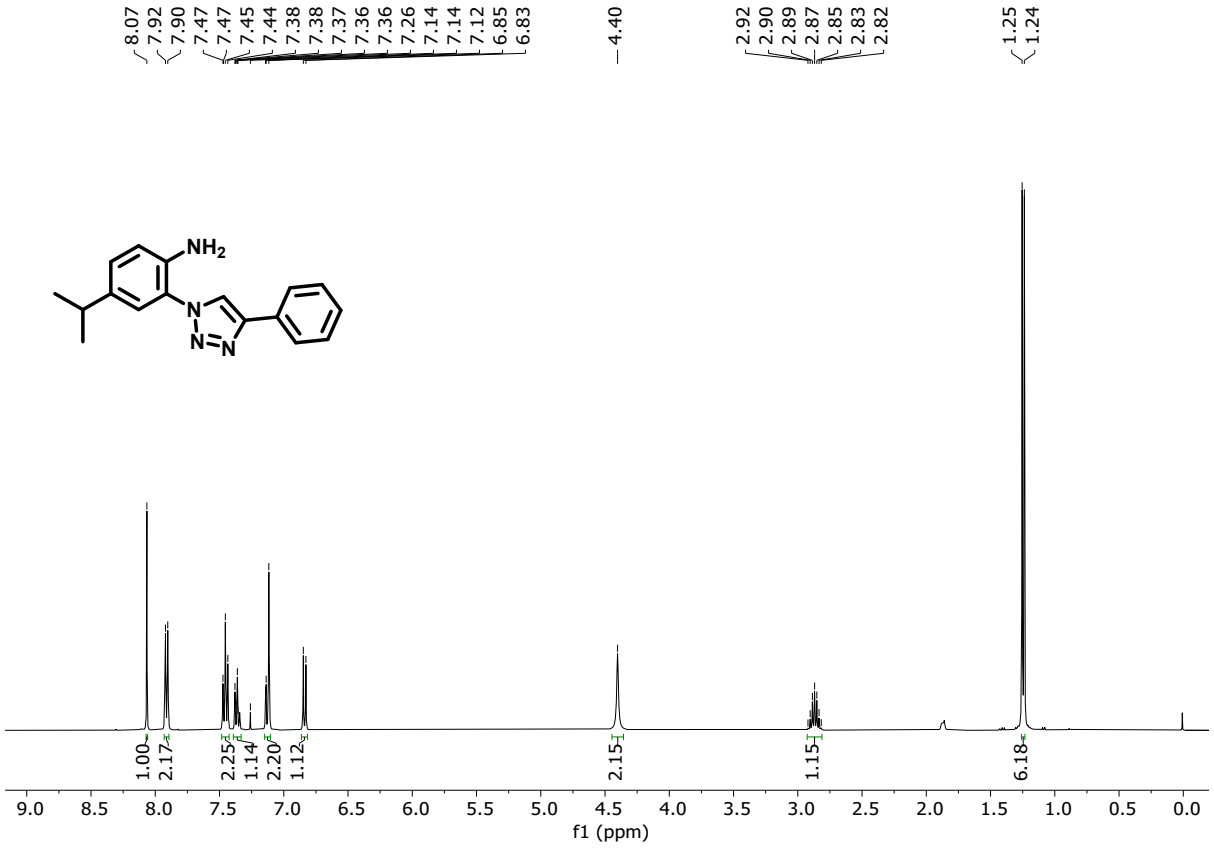


Fig S73. ^{1}H NMR spectrum of 4-isopropyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3d**)

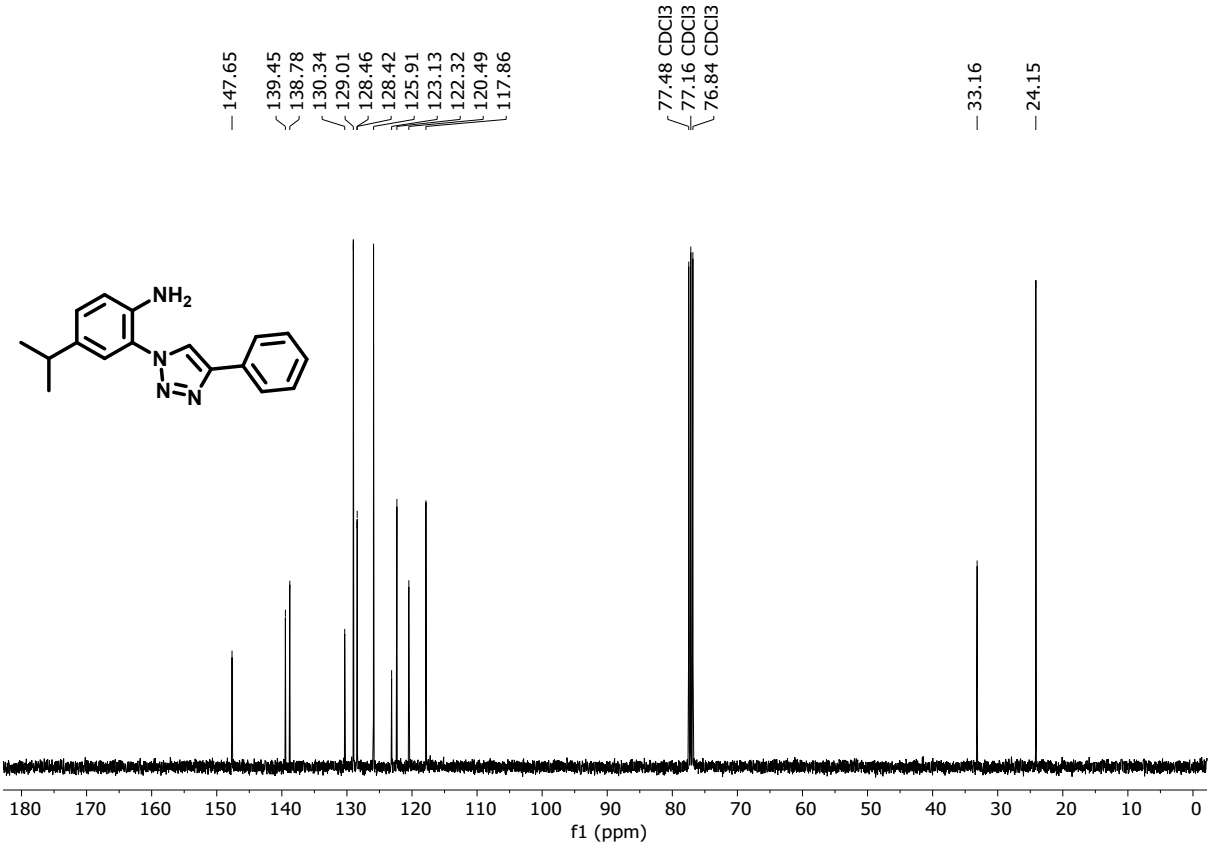


Fig S74. ^{13}C NMR spectrum of 4-isopropyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3d**)

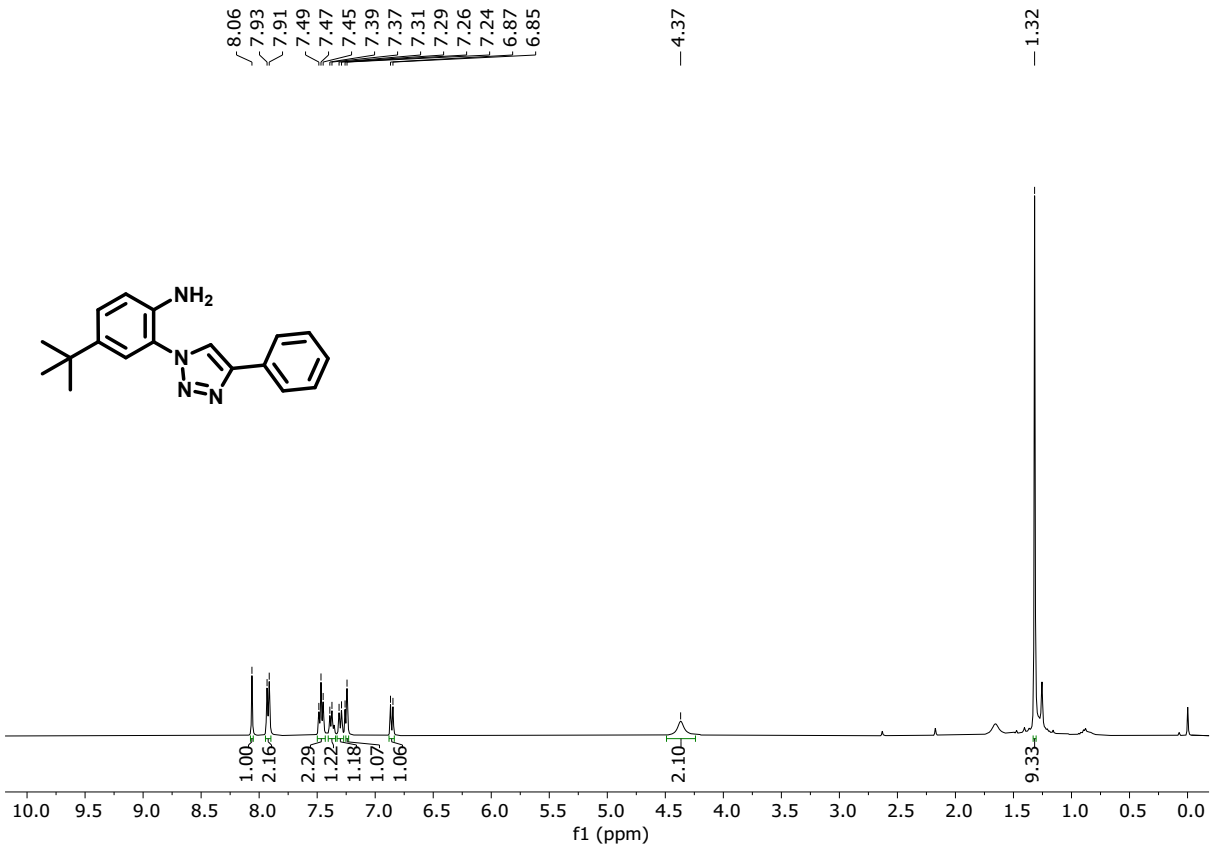


Fig S75. ^{1}H NMR spectrum of 4-(tert-butyl)-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3e**)

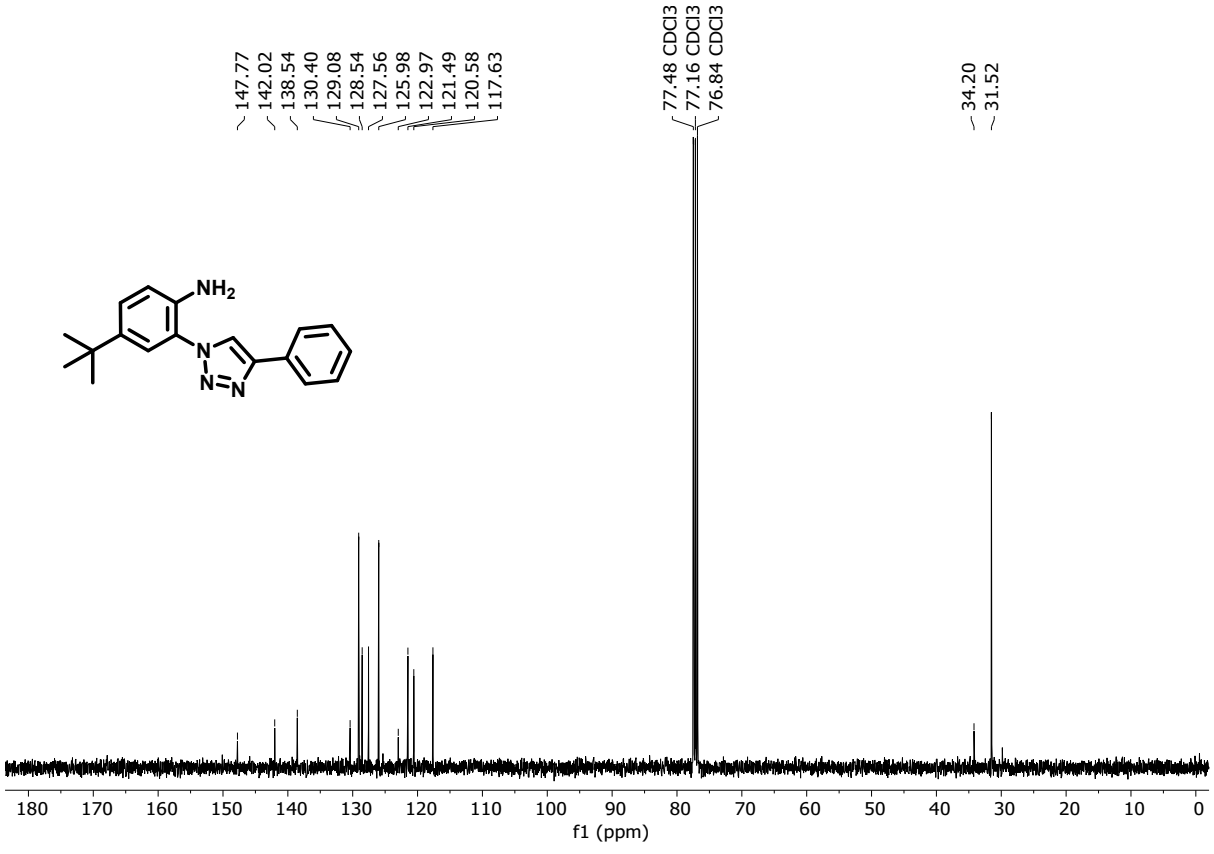


Fig S76. ^{13}C NMR spectrum of 4-(tert-butyl)-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3e**)

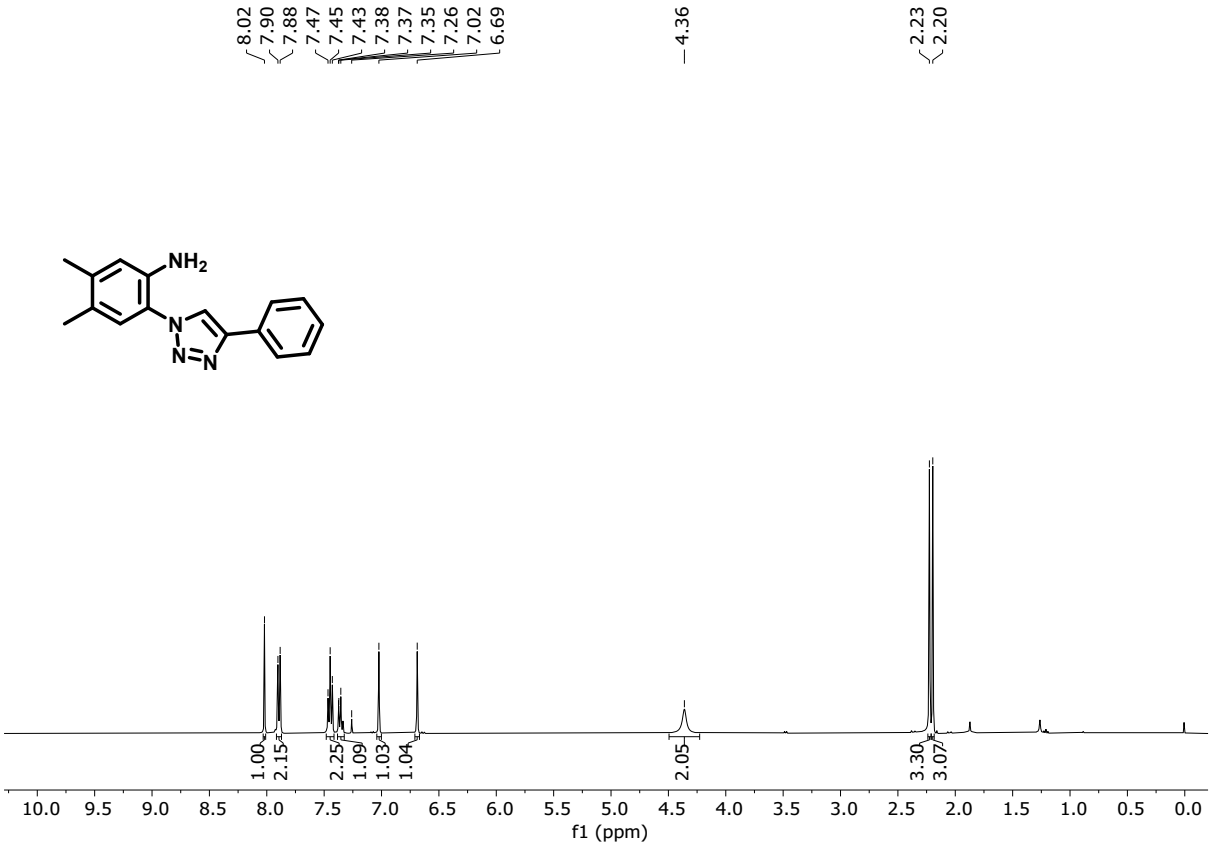


Fig S77. ^{1}H NMR spectrum of 4,5-dimethyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3f**)

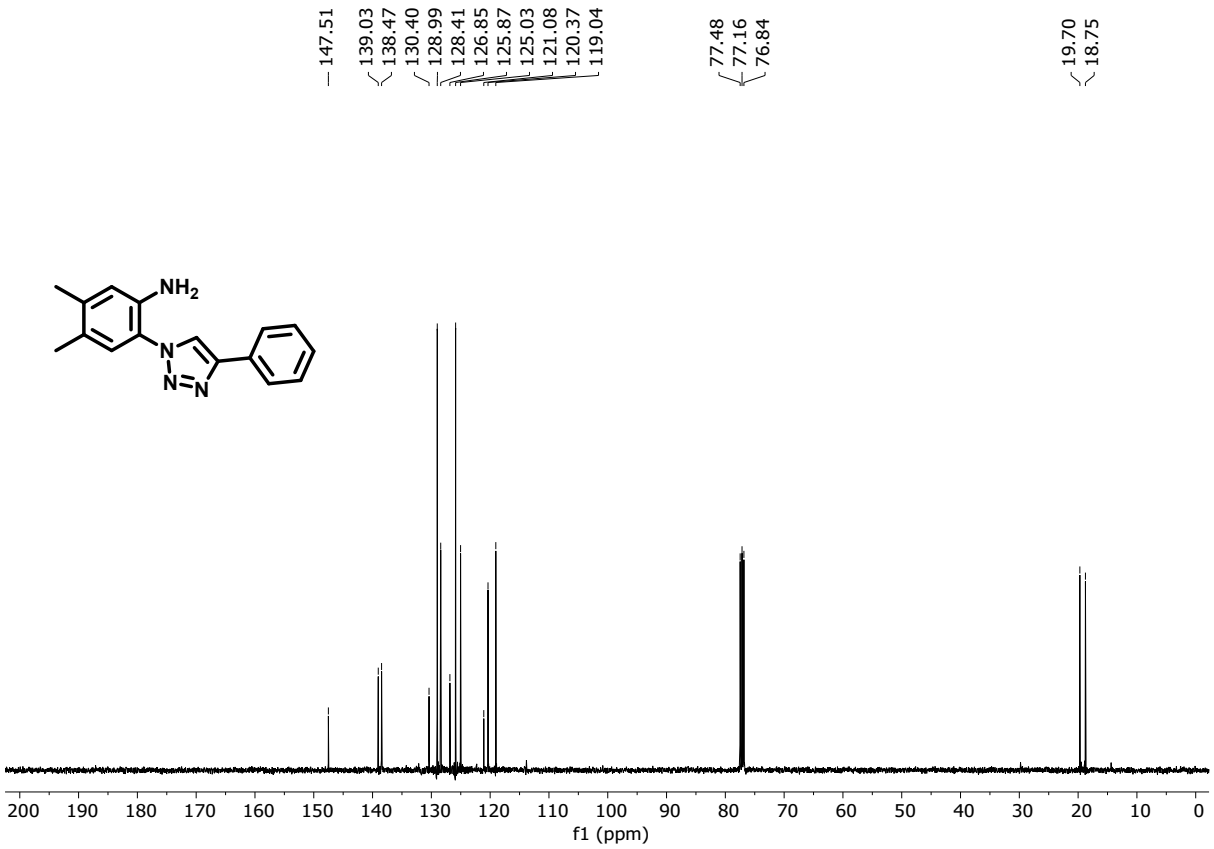


Fig S78. ^{13}C NMR spectrum of 4,5-dimethyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3f**)

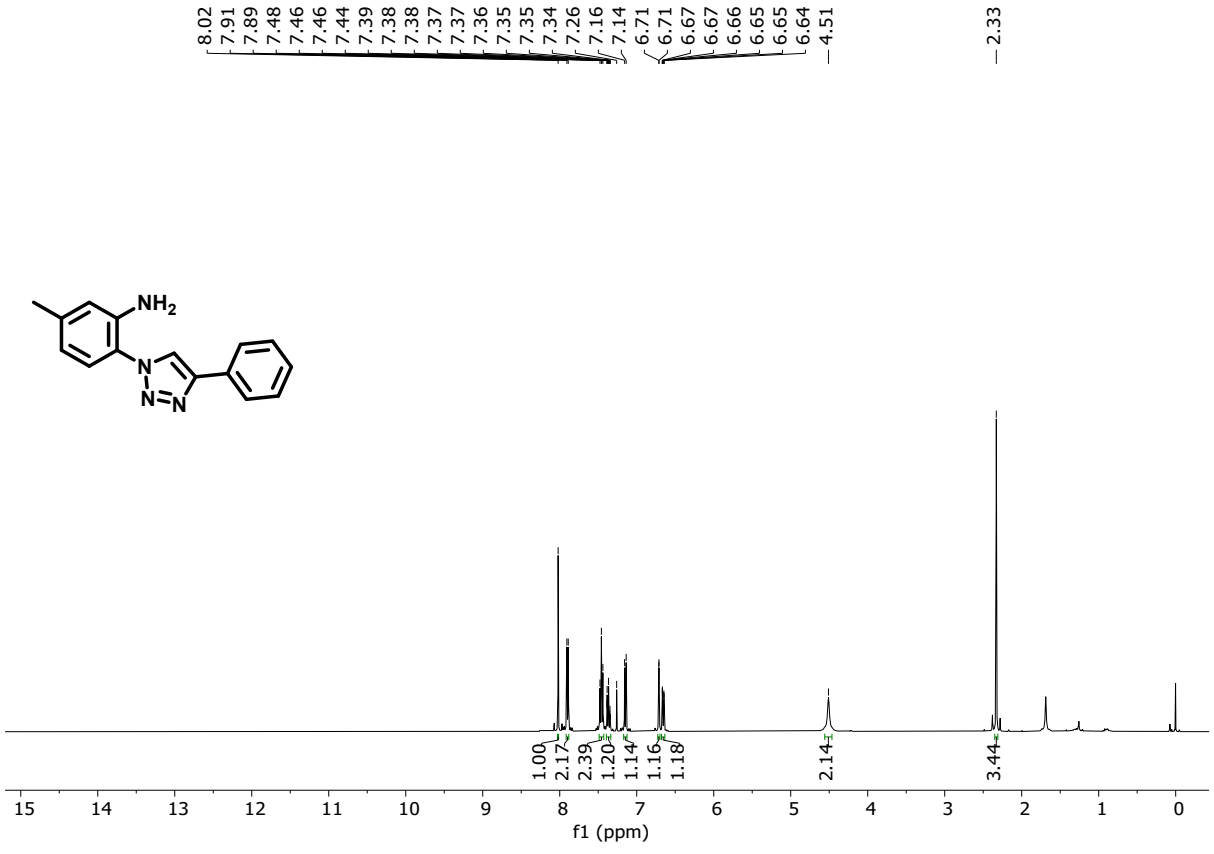


Fig S79. ^{1}H NMR spectrum of 5-methyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3g**)

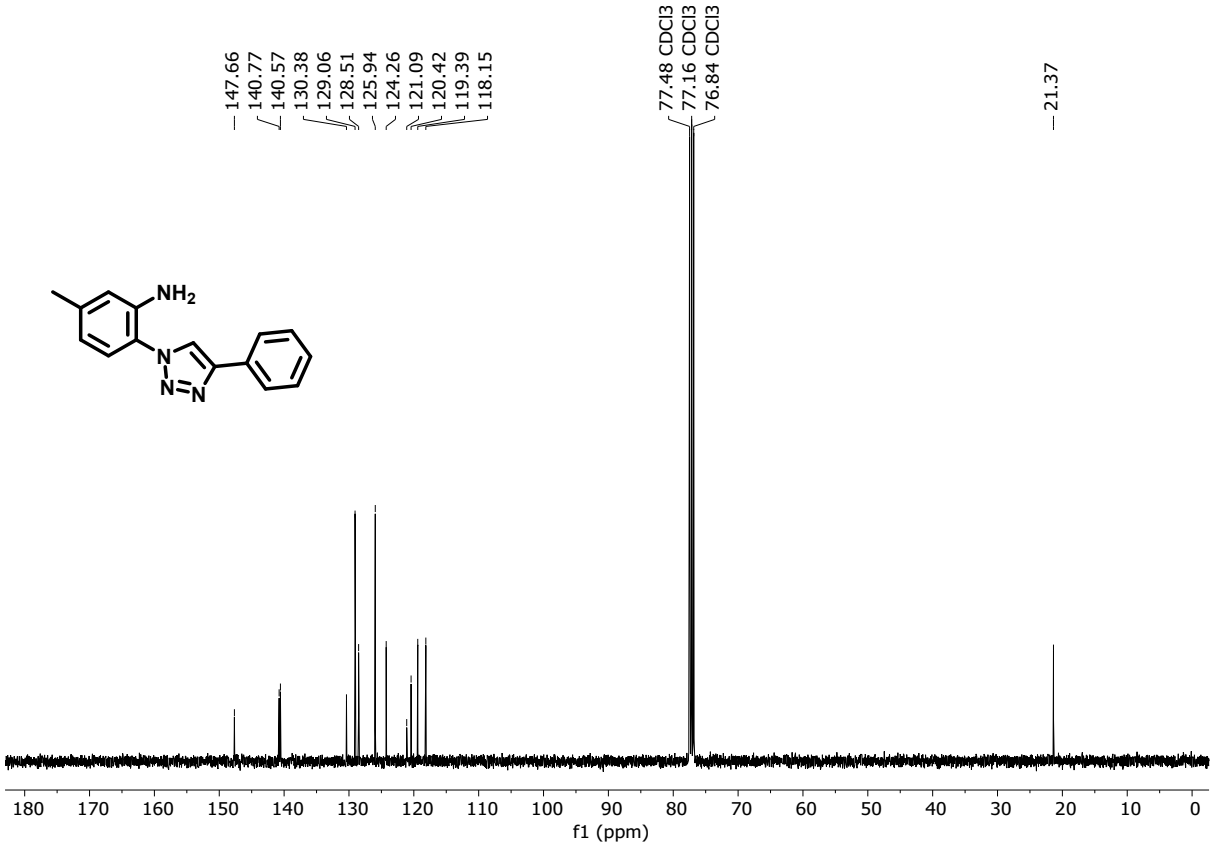


Fig S80. ^{13}C NMR spectrum of 5-methyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3g**)

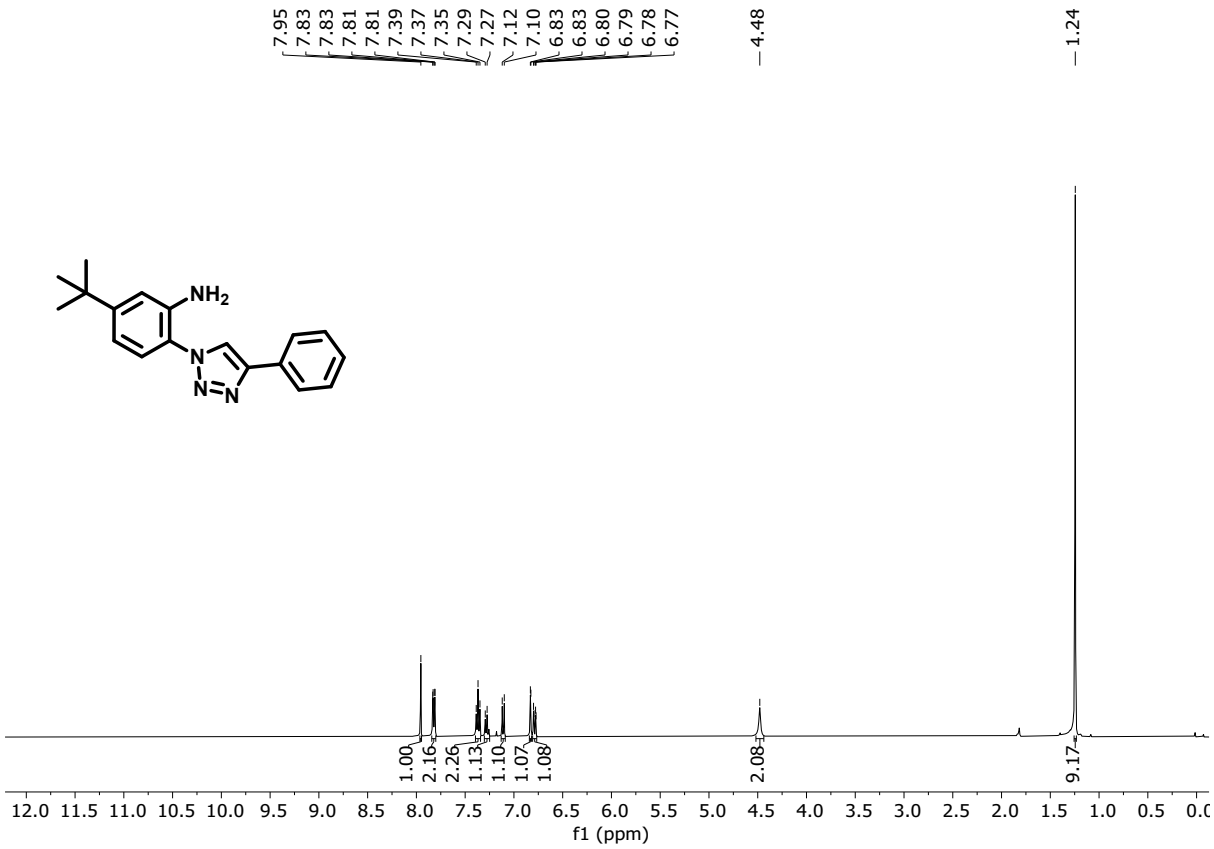


Fig S81. ^{1}H NMR spectrum of 5-(tert-butyl)-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3h**)

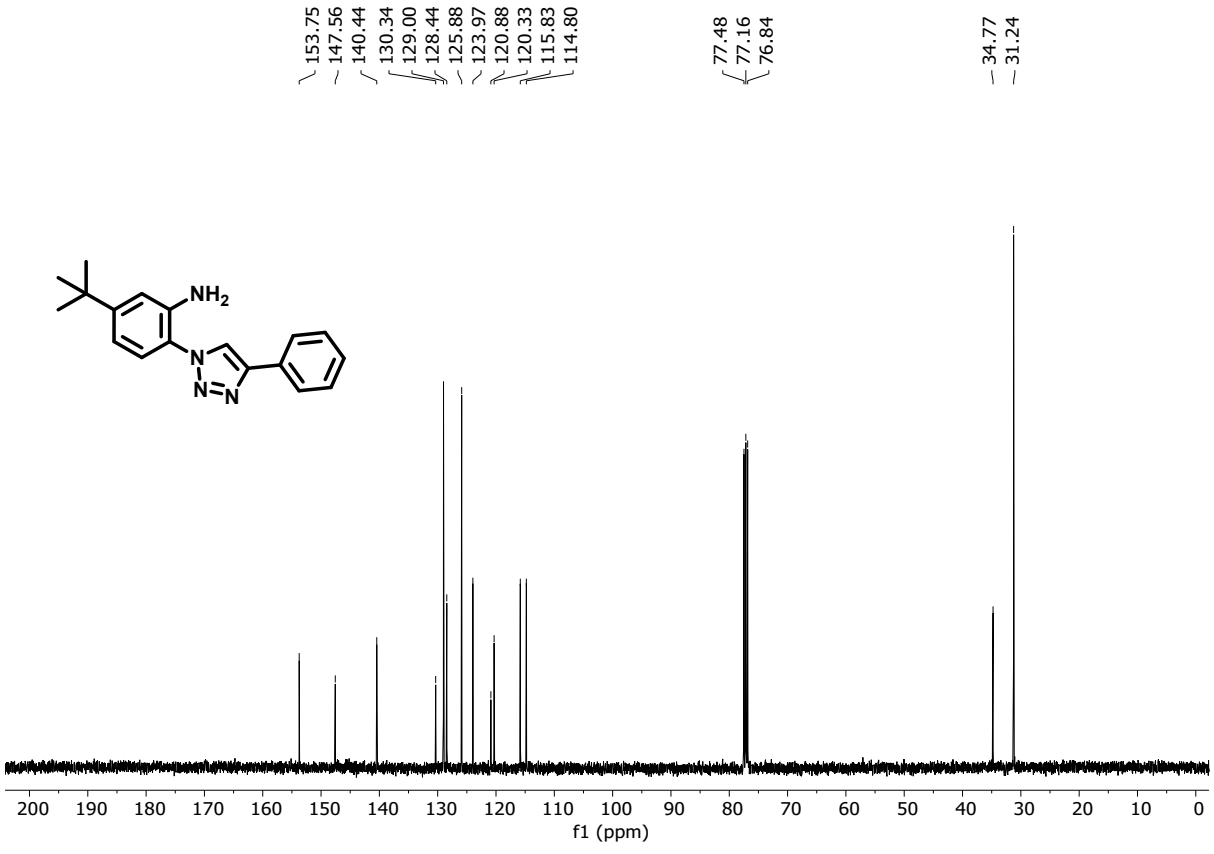


Fig S82. ^{13}C NMR spectrum of 5-(tert-butyl)-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3h**)

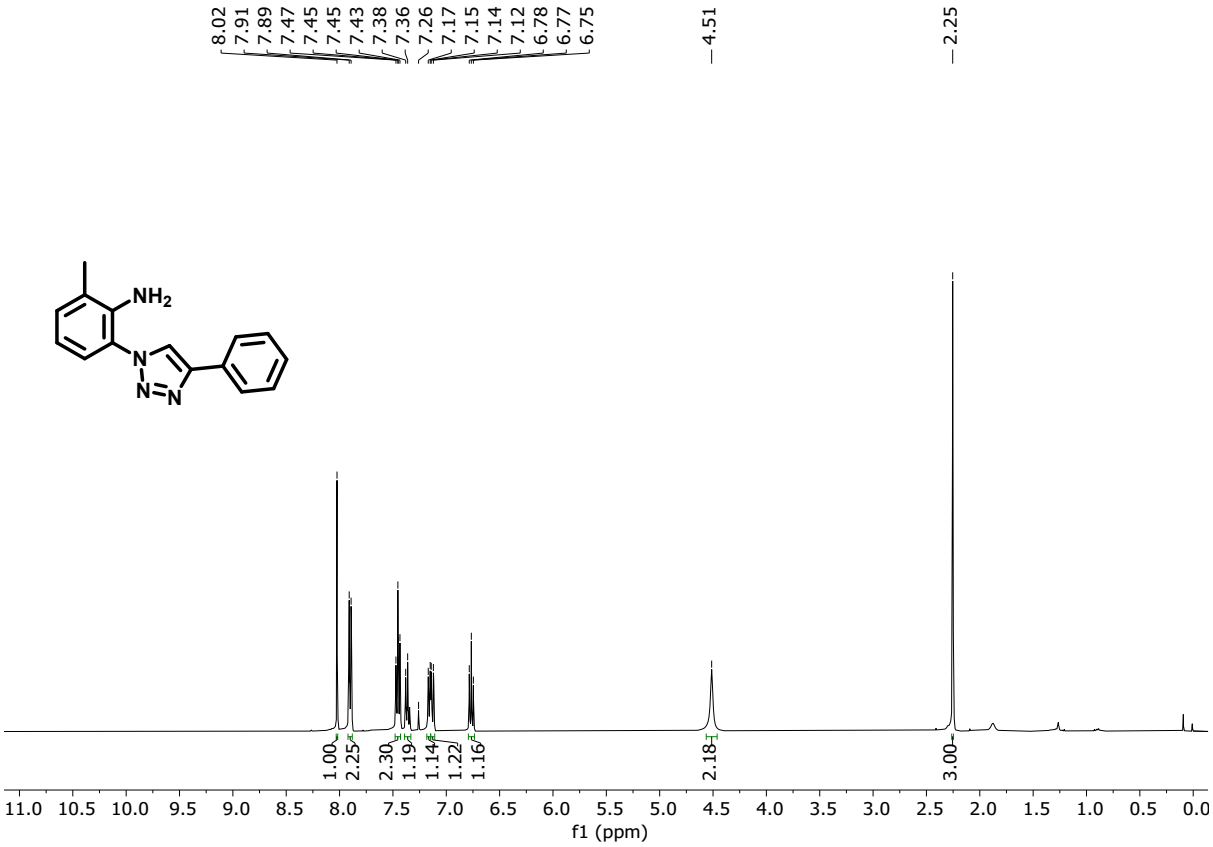


Fig S83. ^{1}H NMR spectrum of 2-methyl-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3i**)

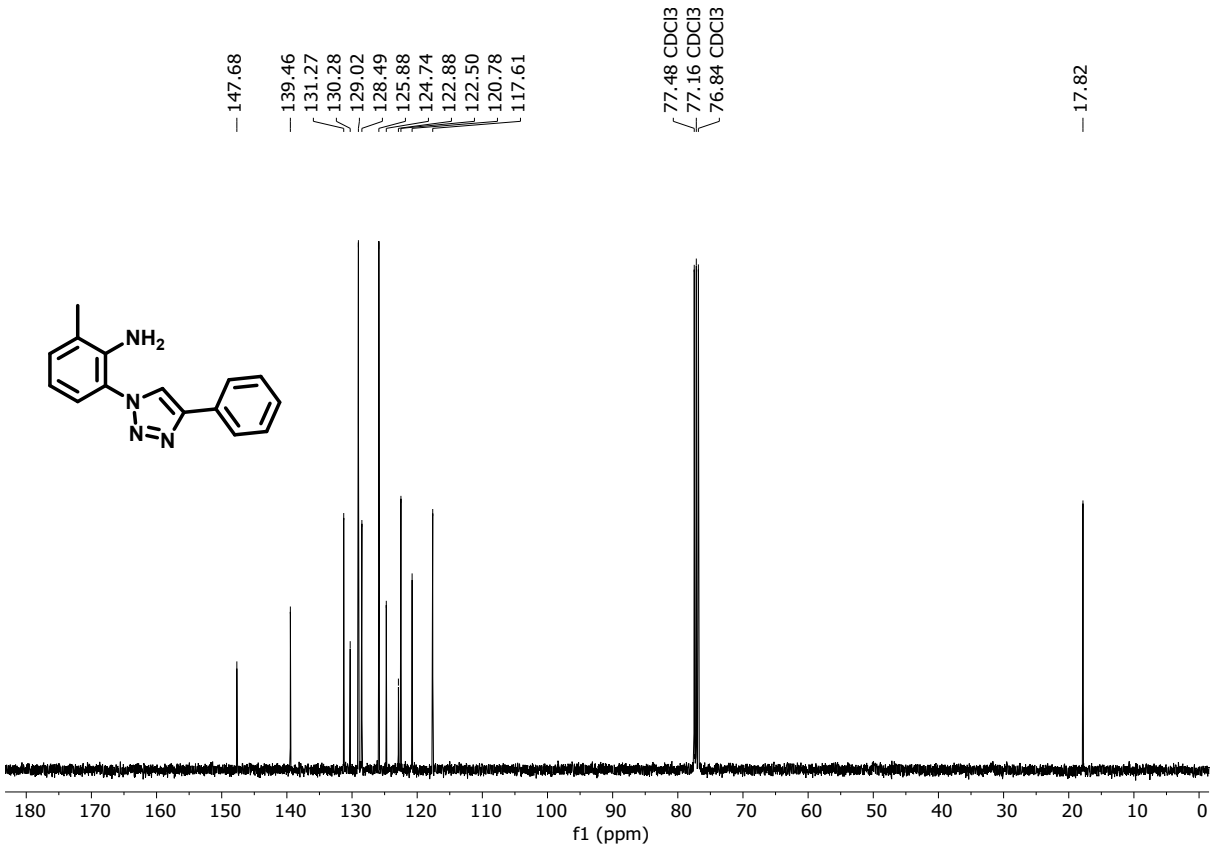


Fig S84. ^{13}C NMR spectrum of 2-methyl-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3i**)

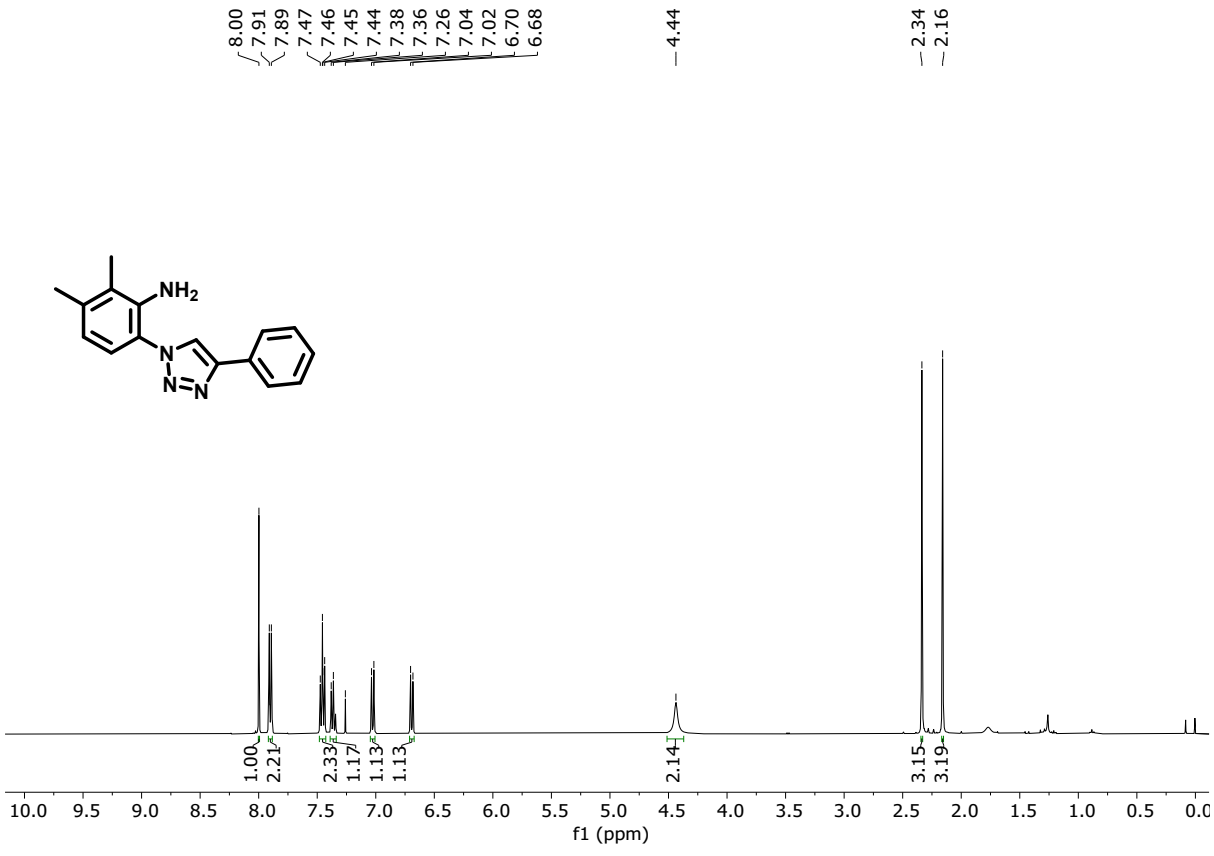


Fig S85. [1]H NMR spectrum of 2,3-dimethyl-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3j**)

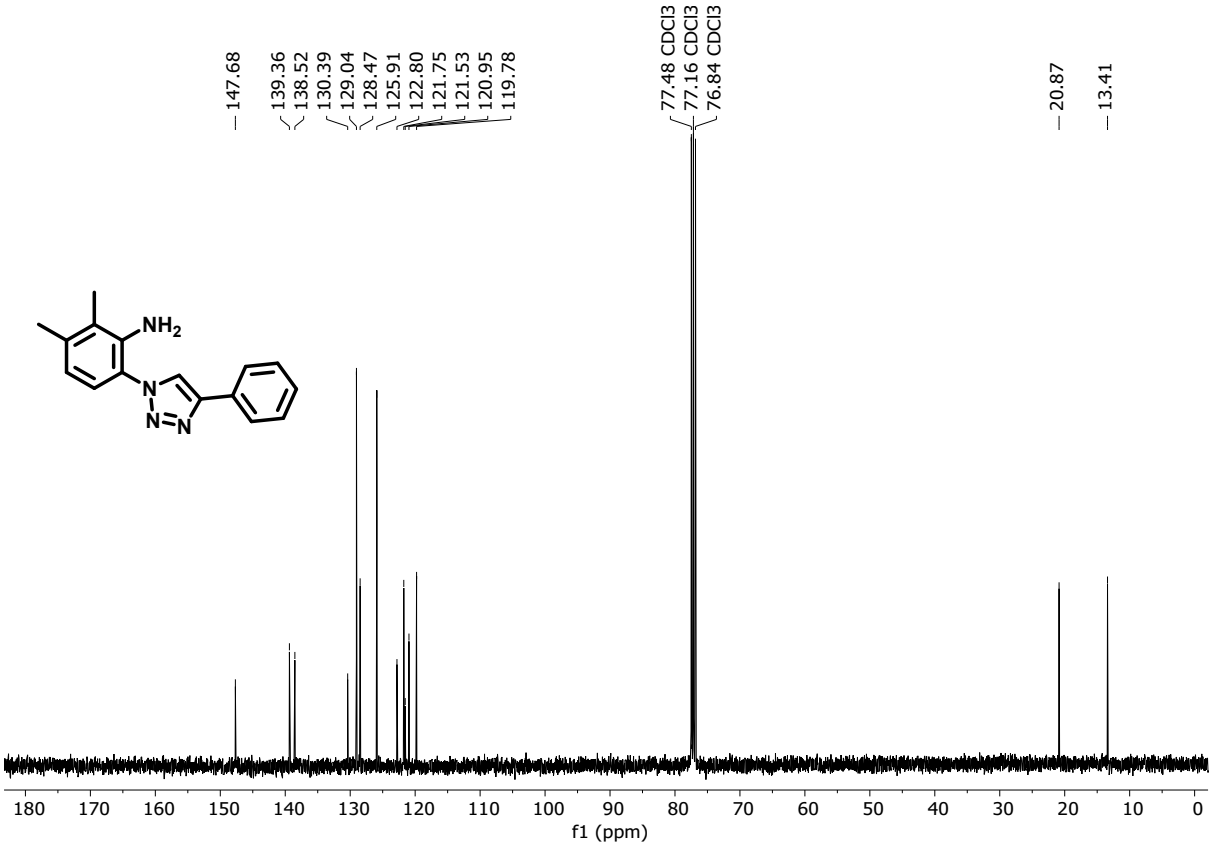


Fig S86. [13]C NMR spectrum of 2,3-dimethyl-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3j**)

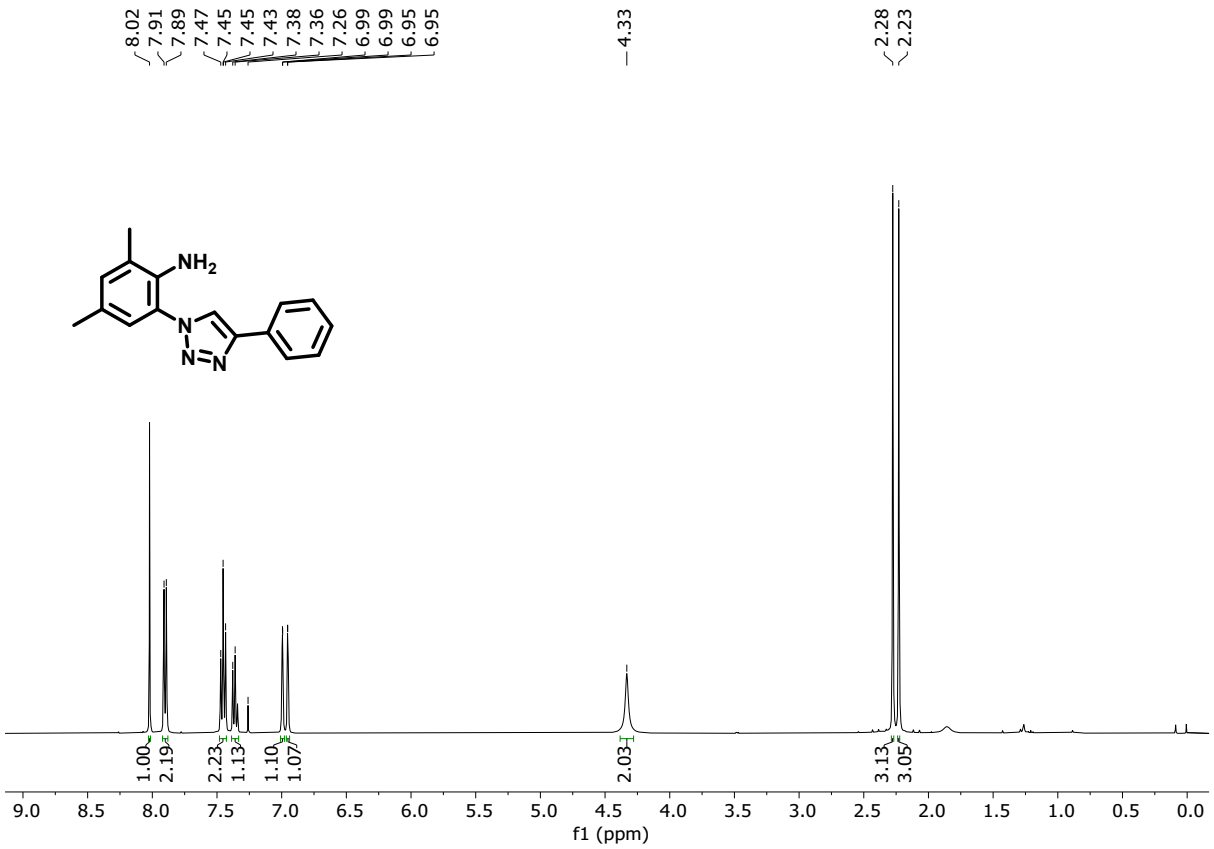


Fig S87. ^{1}H NMR spectrum of 2,4-dimethyl-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3k**)

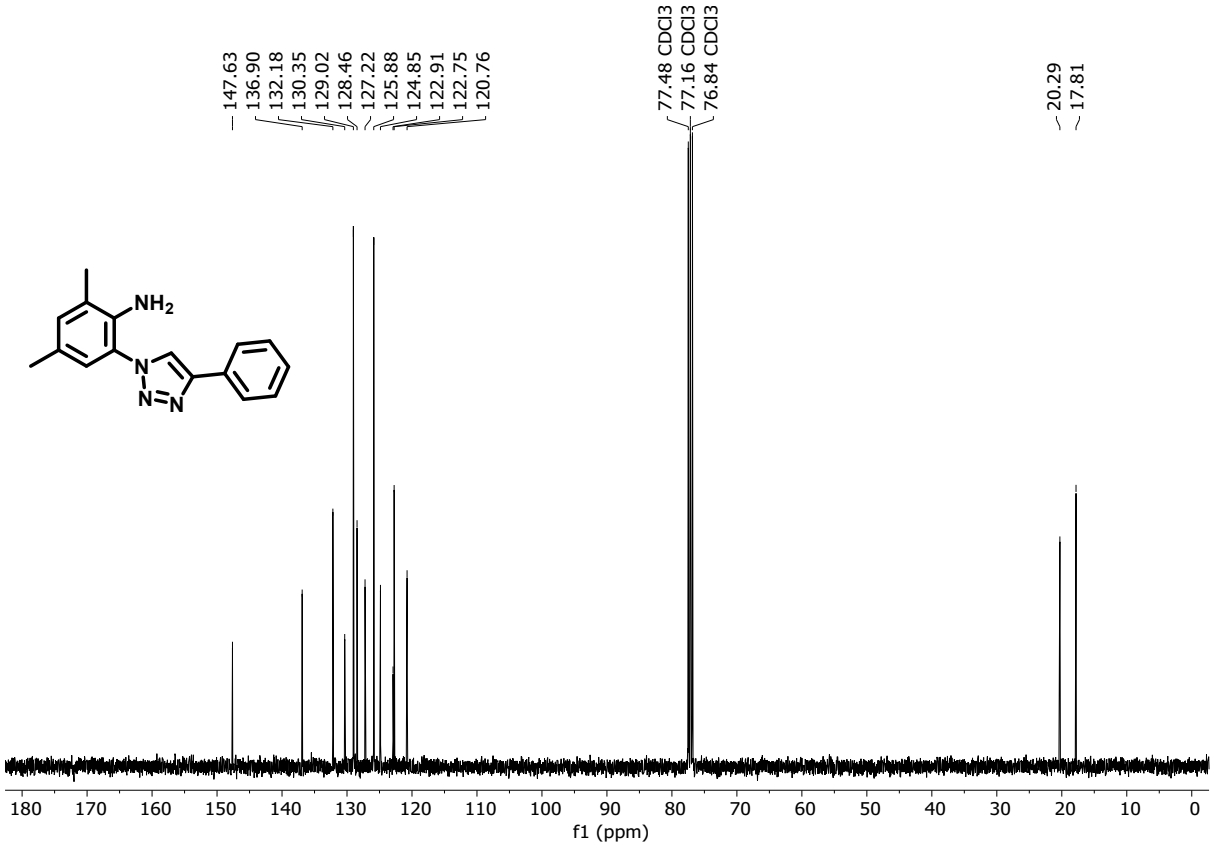


Fig S88. ^{13}C NMR spectrum of 2,4-dimethyl-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3k**)

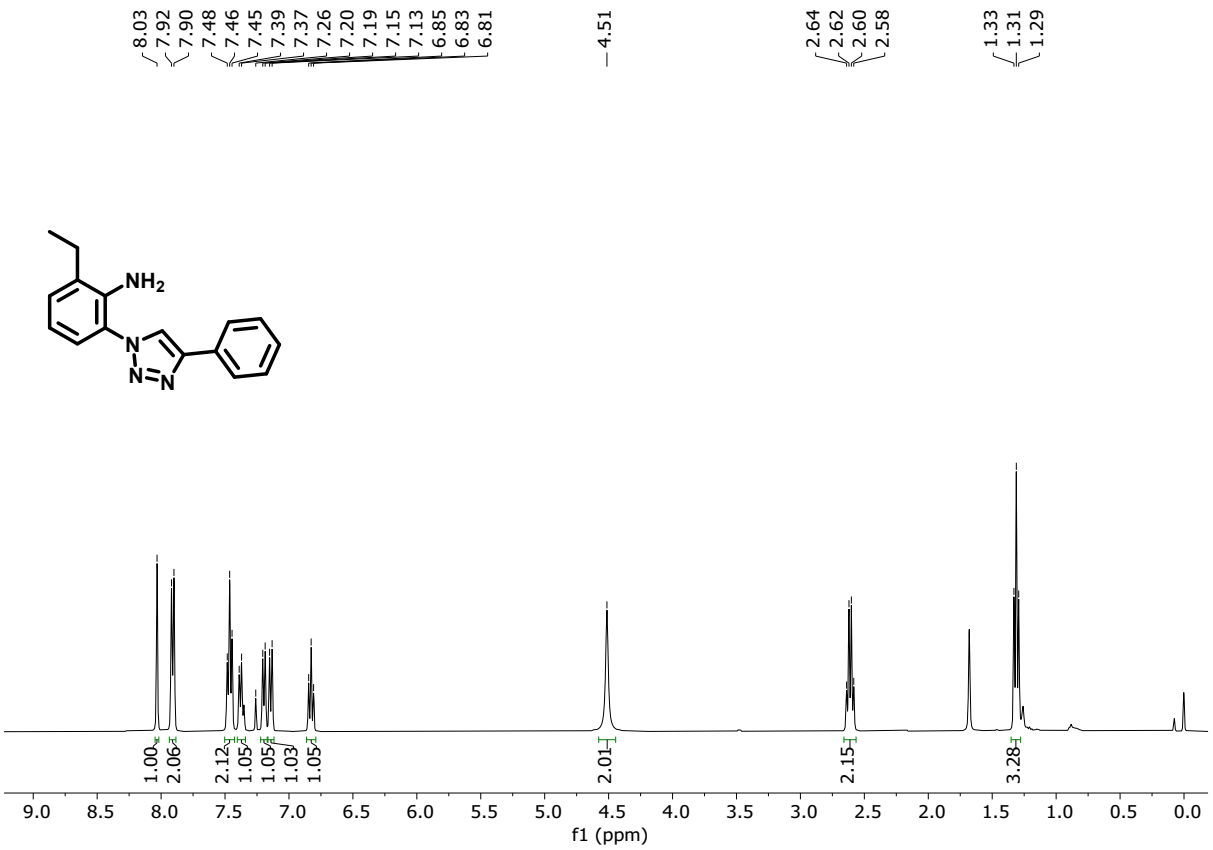


Fig S89. ^{1}H NMR spectrum of 2-ethyl-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3l**)

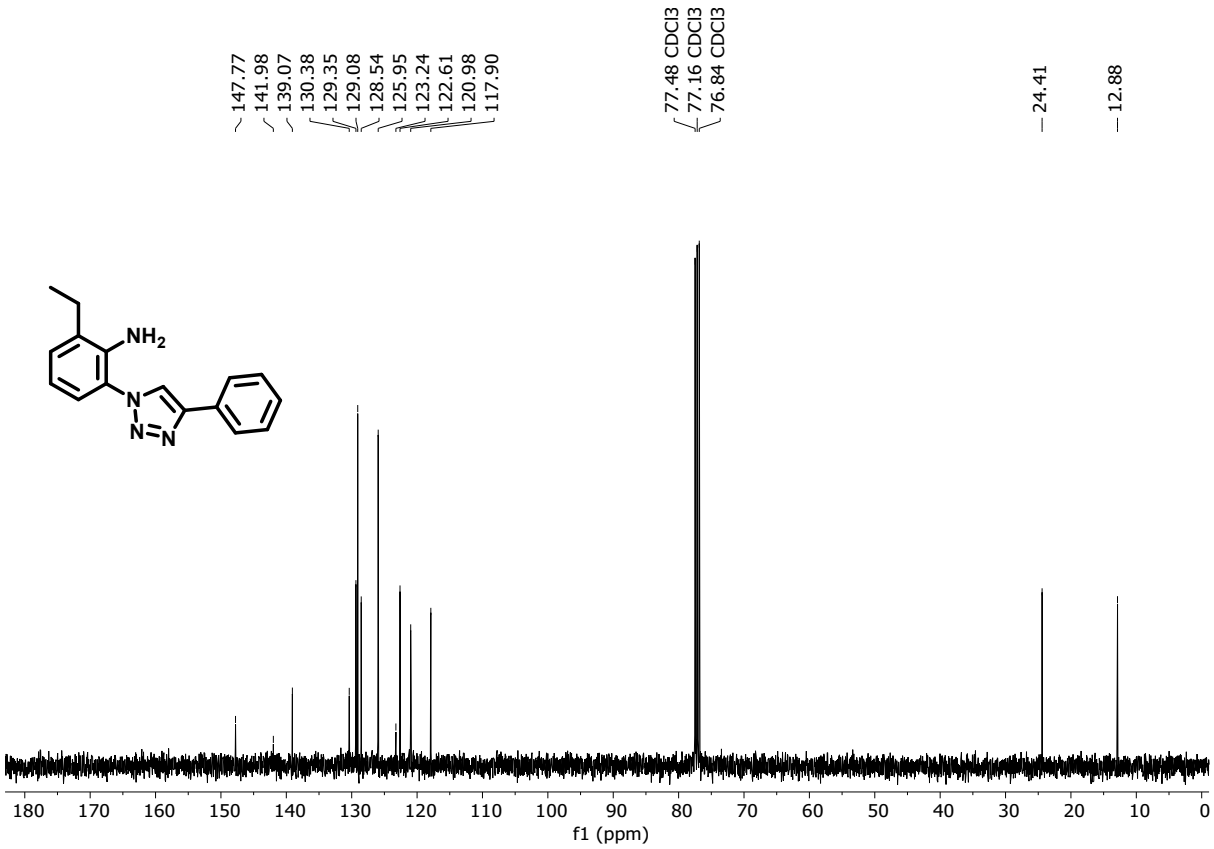


Fig S90. ^{13}C NMR spectrum of 2-ethyl-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3l**)

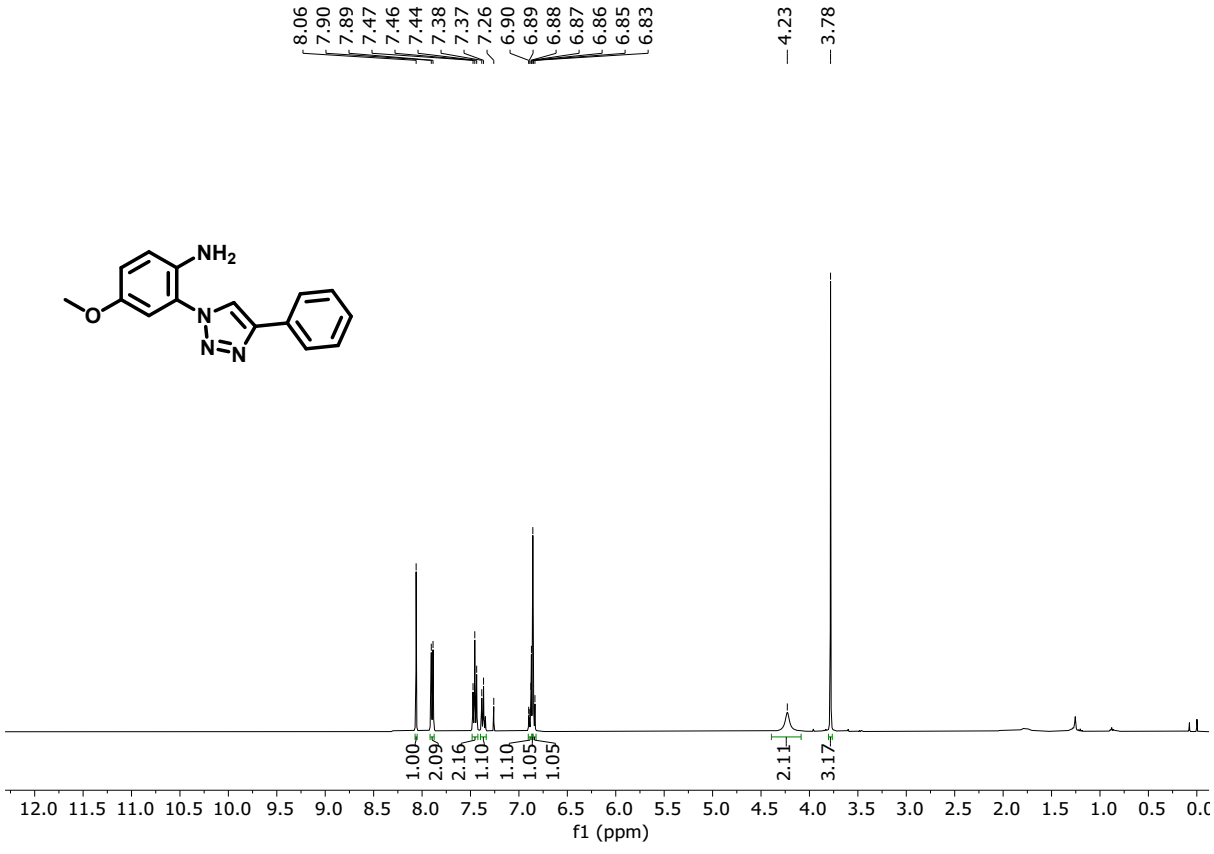


Fig S91. ^{1}H NMR spectrum of 4-methoxy-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3m**)

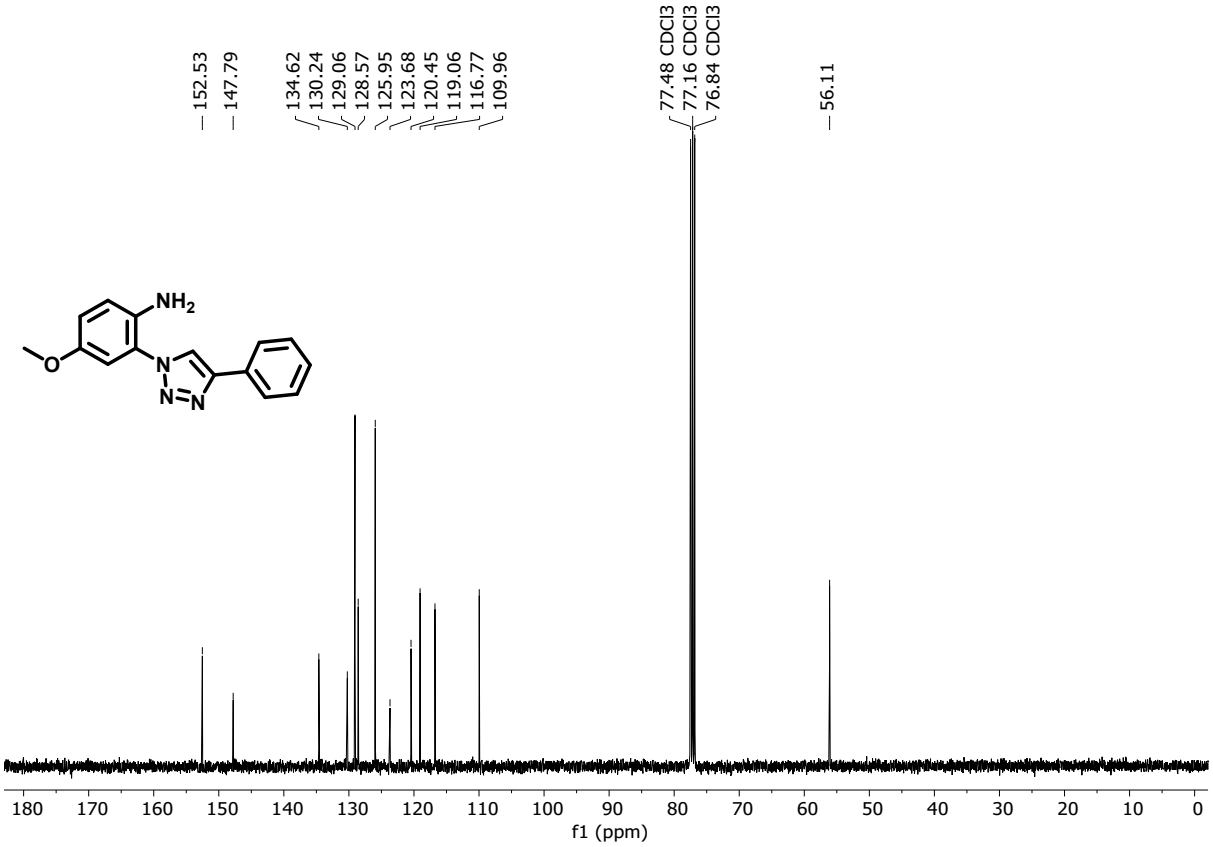


Fig S92. ^{13}C NMR spectrum of 4-methoxy-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3m**)

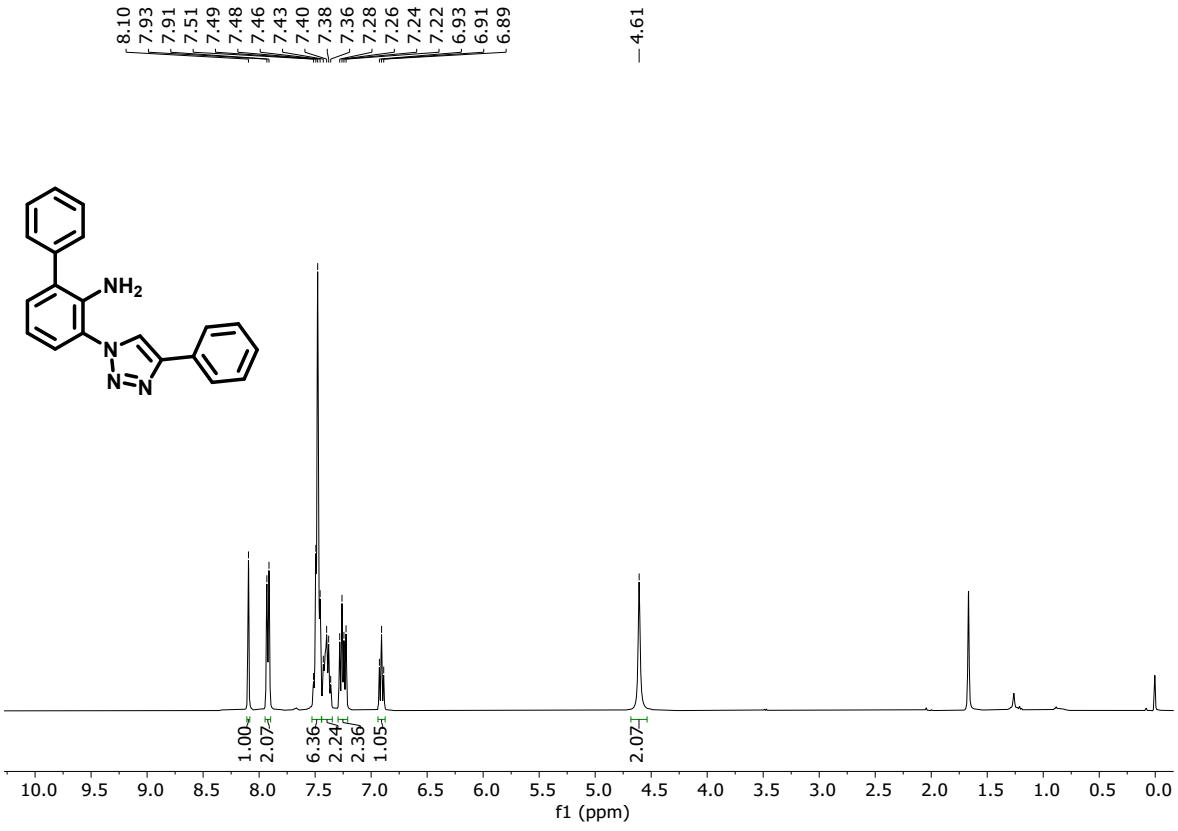


Fig S93. ^{1}H NMR spectrum of 3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)-[1,1'-biphenyl]-2-amine (**3n**)

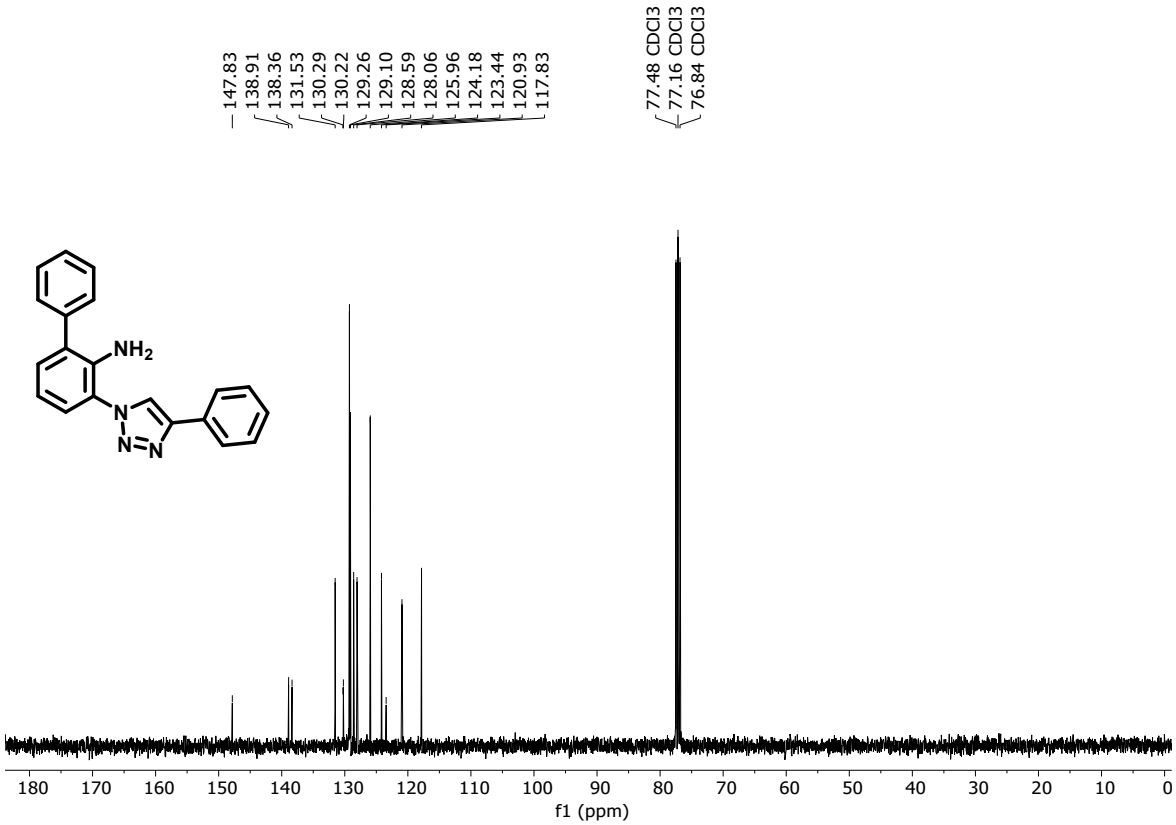


Fig S94. ^{13}C NMR spectrum of 3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)-[1,1'-biphenyl]-2-amine (**3n**)

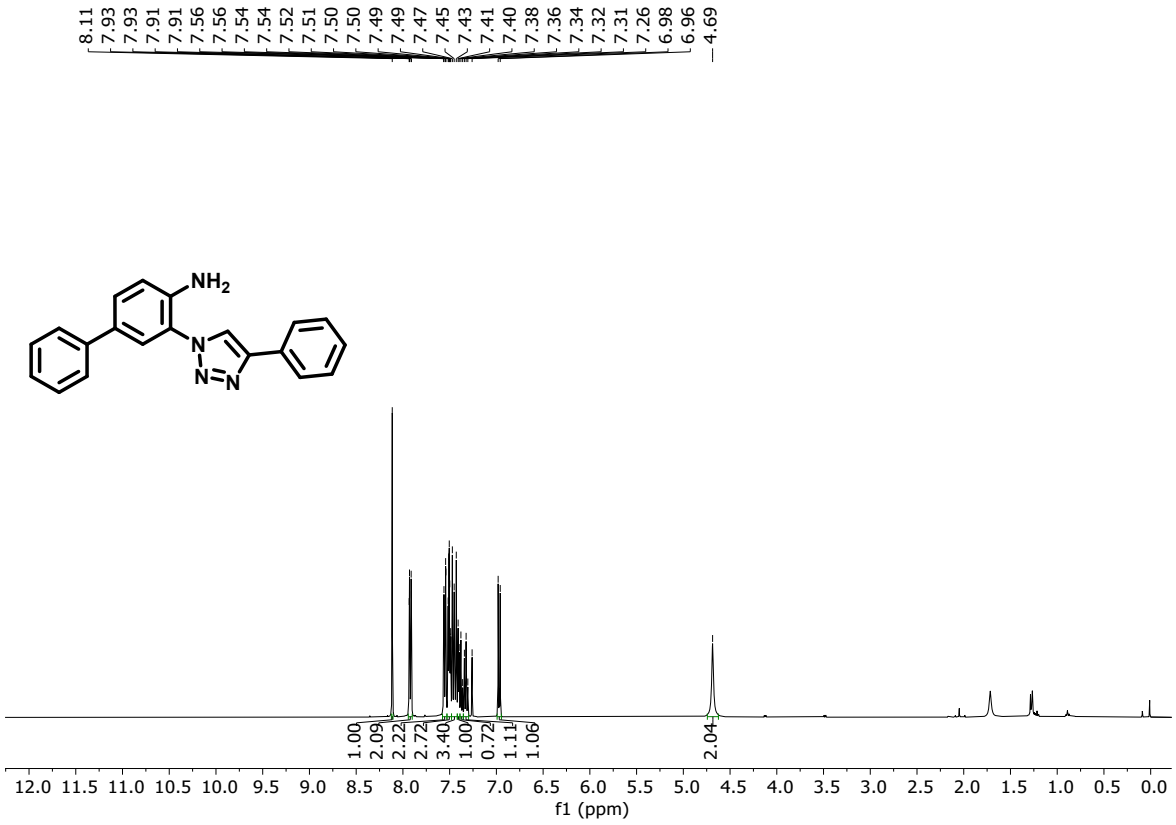


Fig S95. ^{1}H NMR spectrum of 3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)-[1,1'-biphenyl]-4-amine (**3o**)

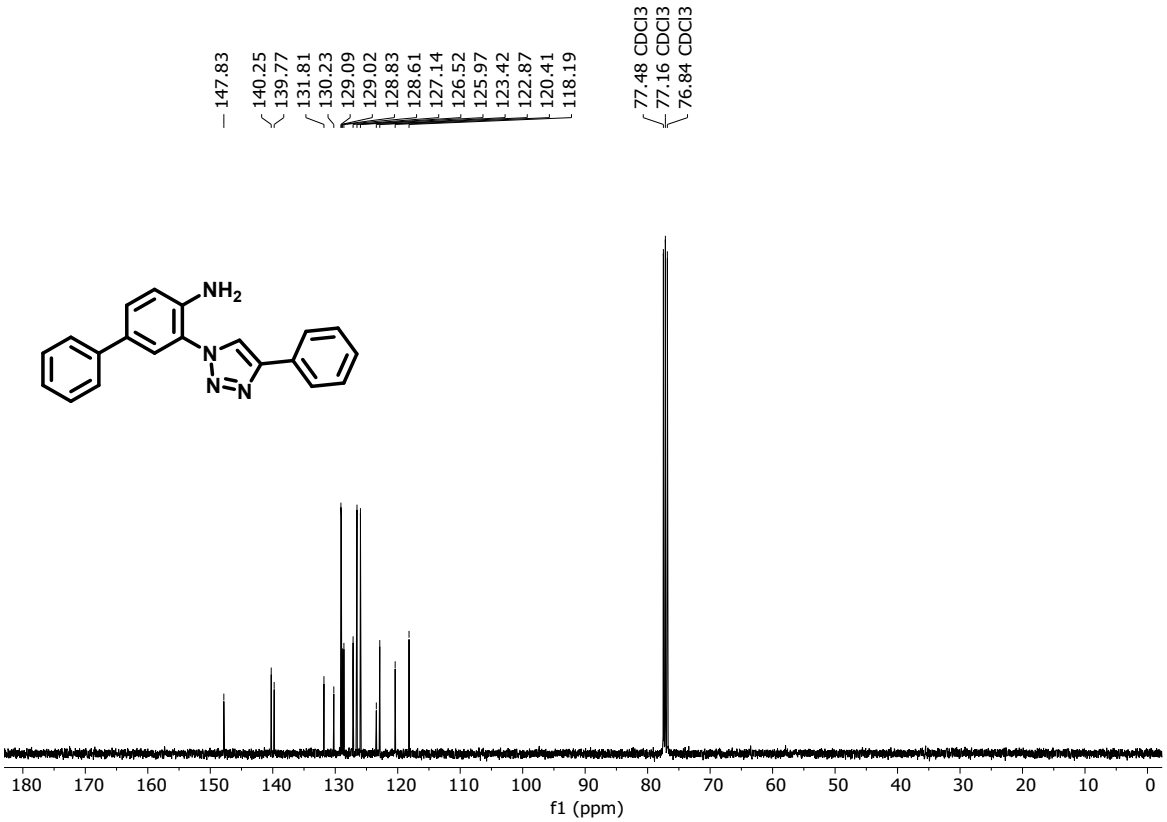


Fig S96. ^{13}C NMR spectrum of 3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)-[1,1'-biphenyl]-4-amine (**3o**)

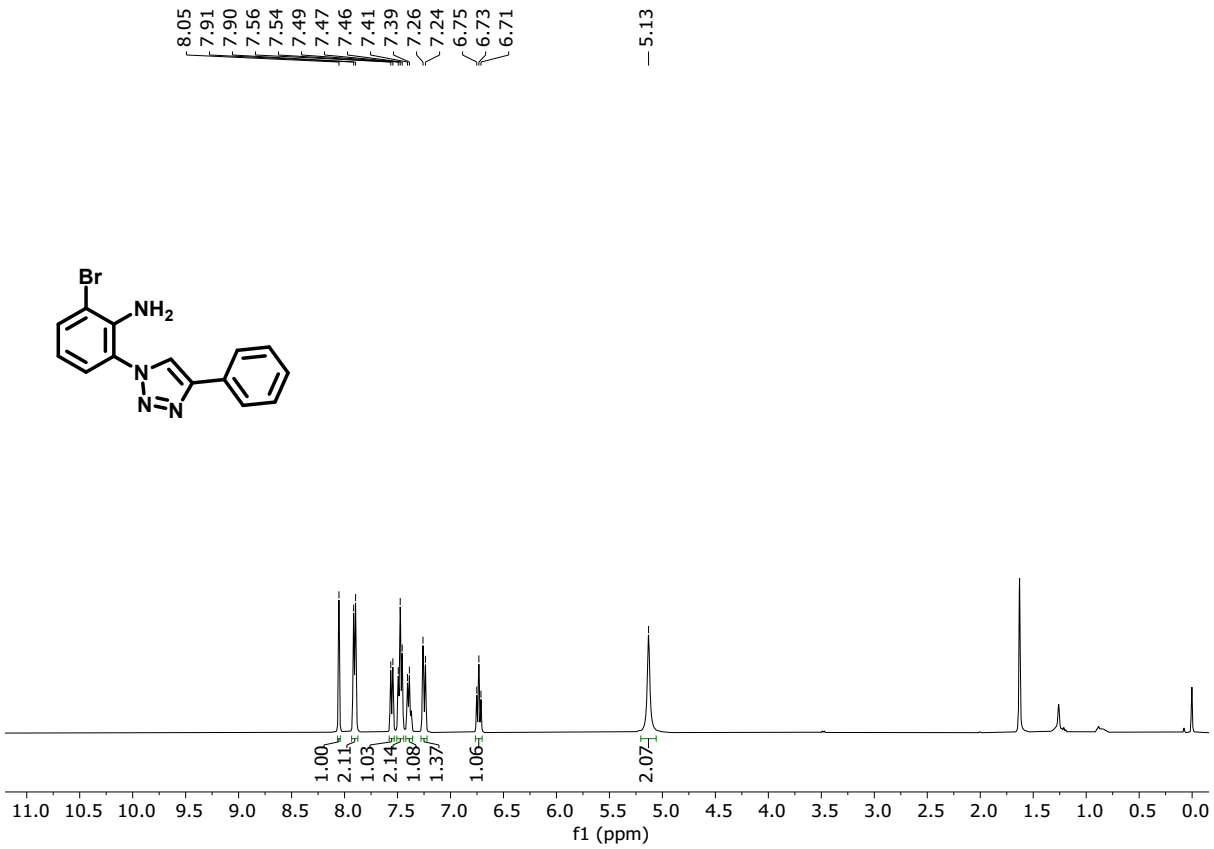


Fig S97. ^{1}H NMR spectrum of 2-bromo-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3p**)

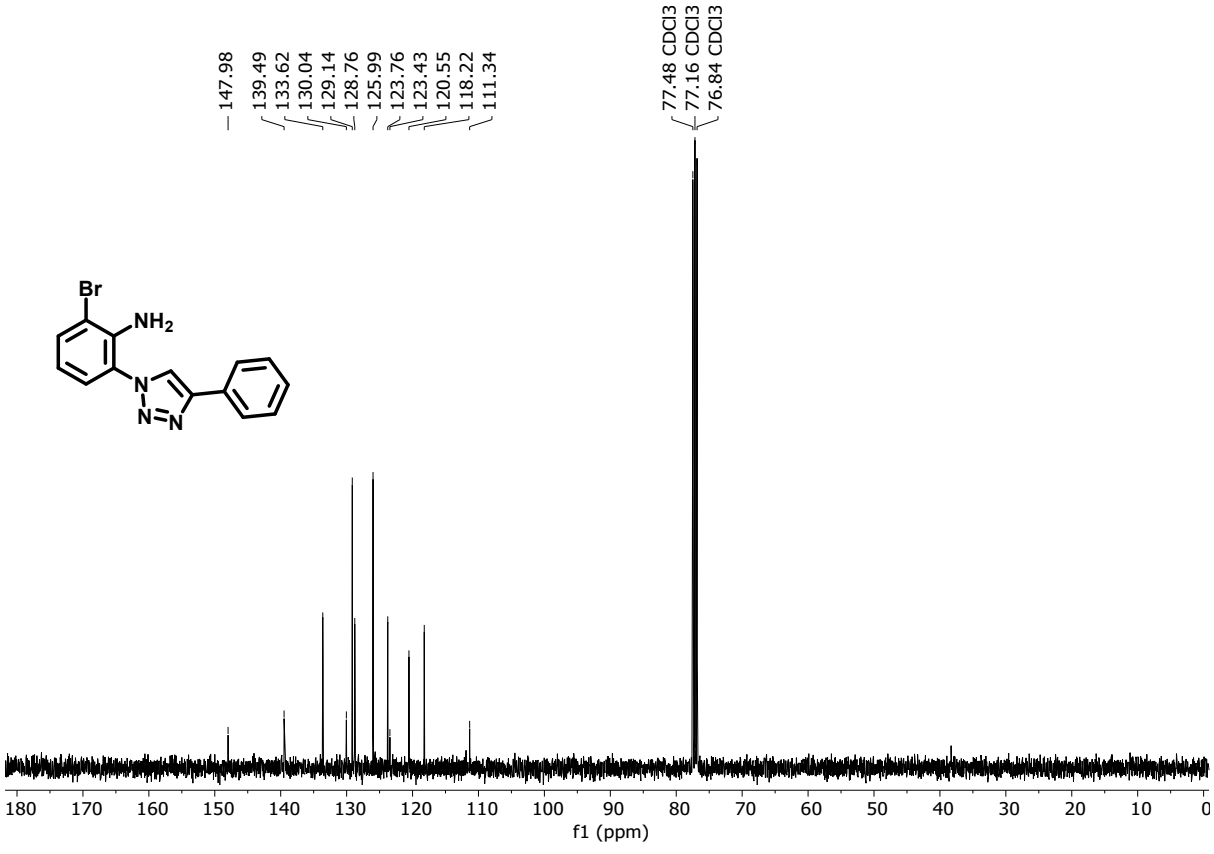


Fig S98. ^{13}C NMR spectrum of 2-bromo-6-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3p**)

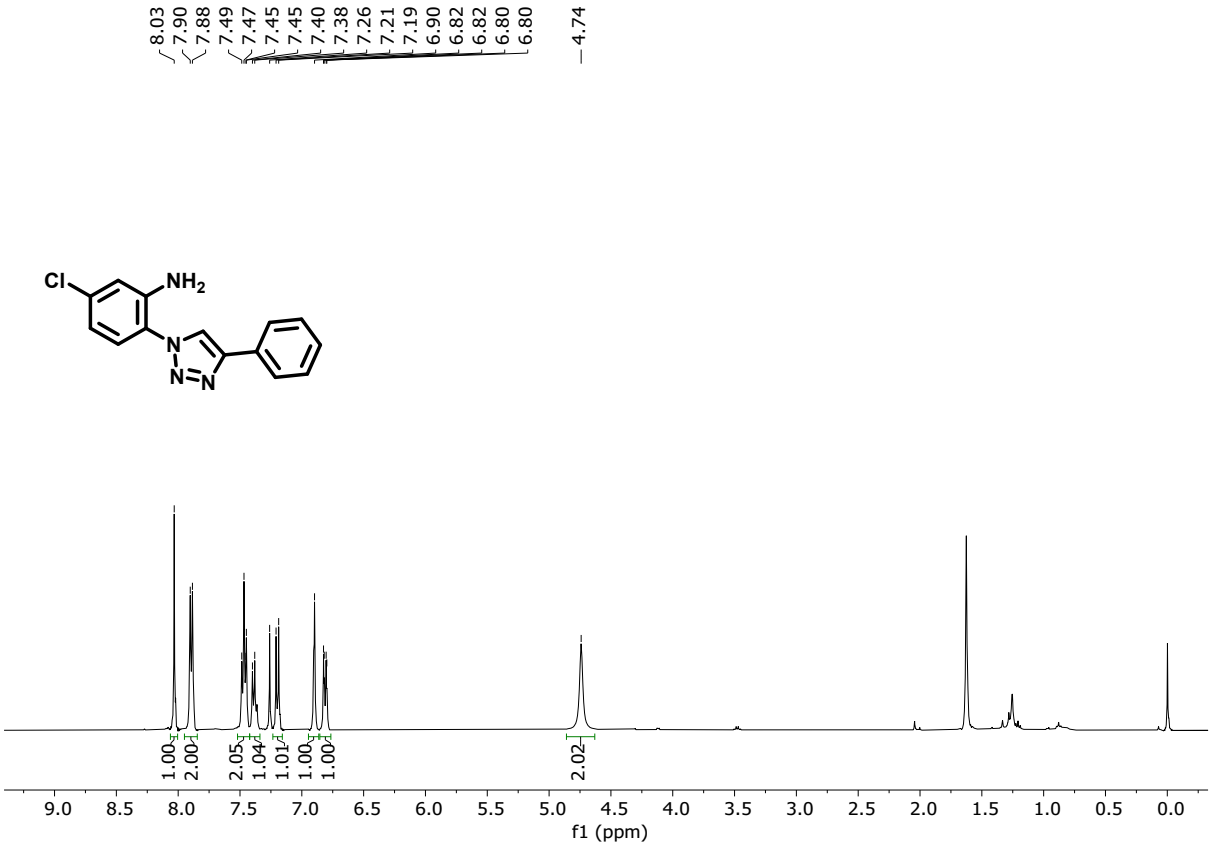


Fig S99. ^{1}H NMR spectrum of 5-chloro-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3q**)

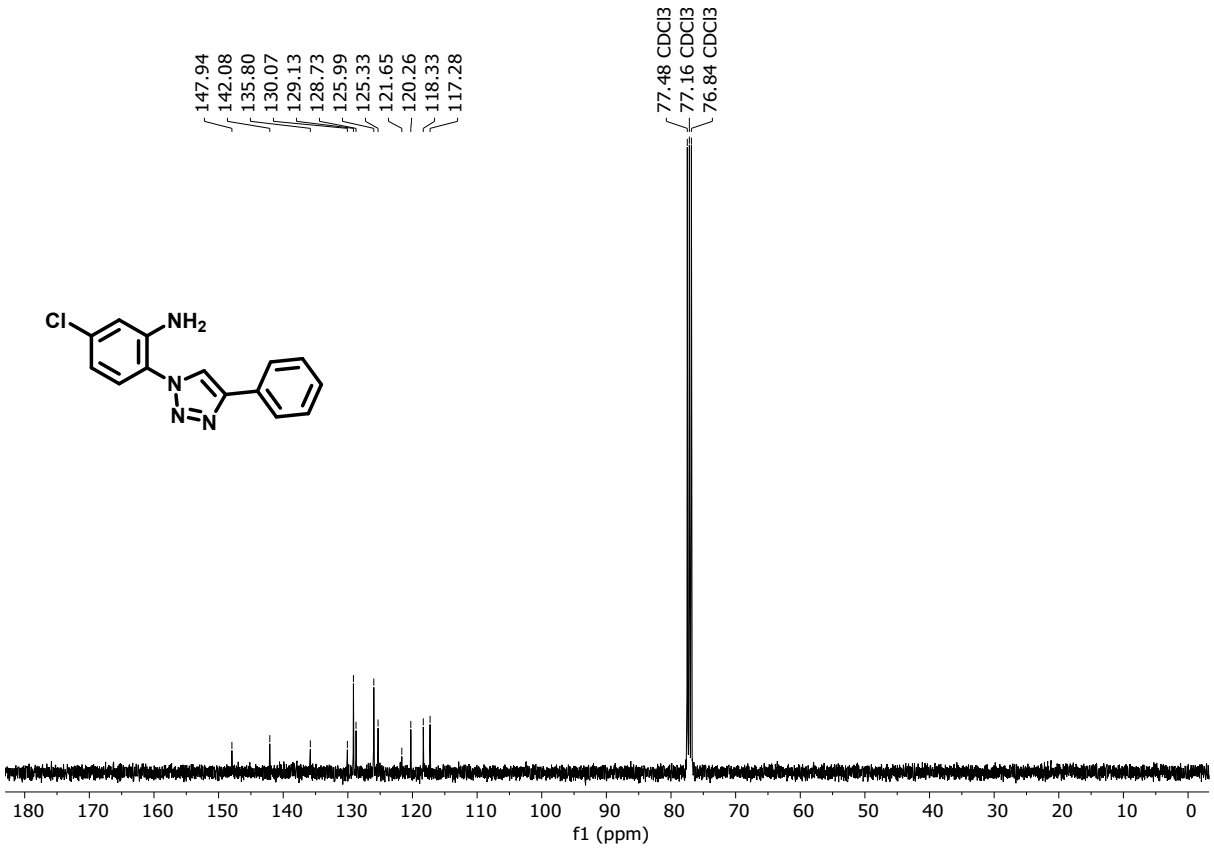


Fig S100. ^{13}C NMR spectrum of 5-chloro-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3q**)

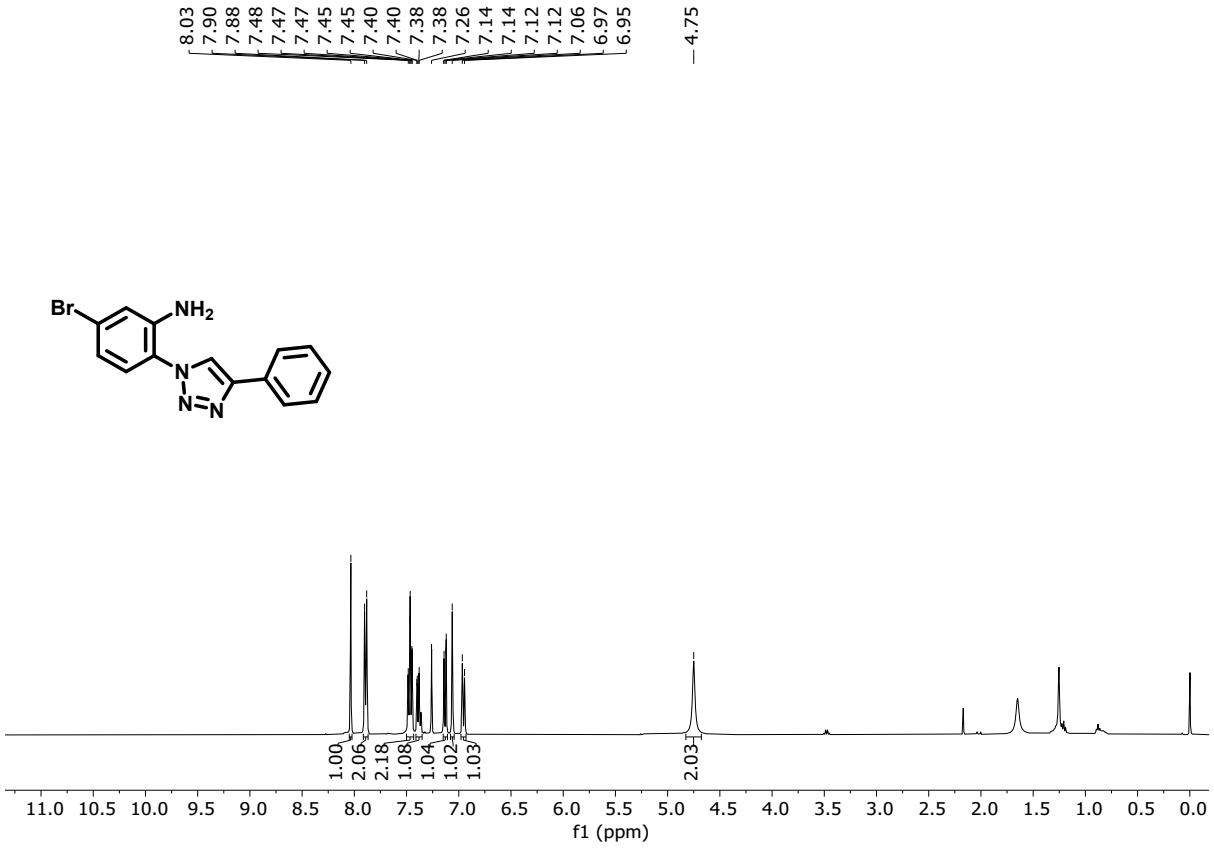


Fig S101. ^{1}H NMR spectrum of 5-bromo-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3r**)

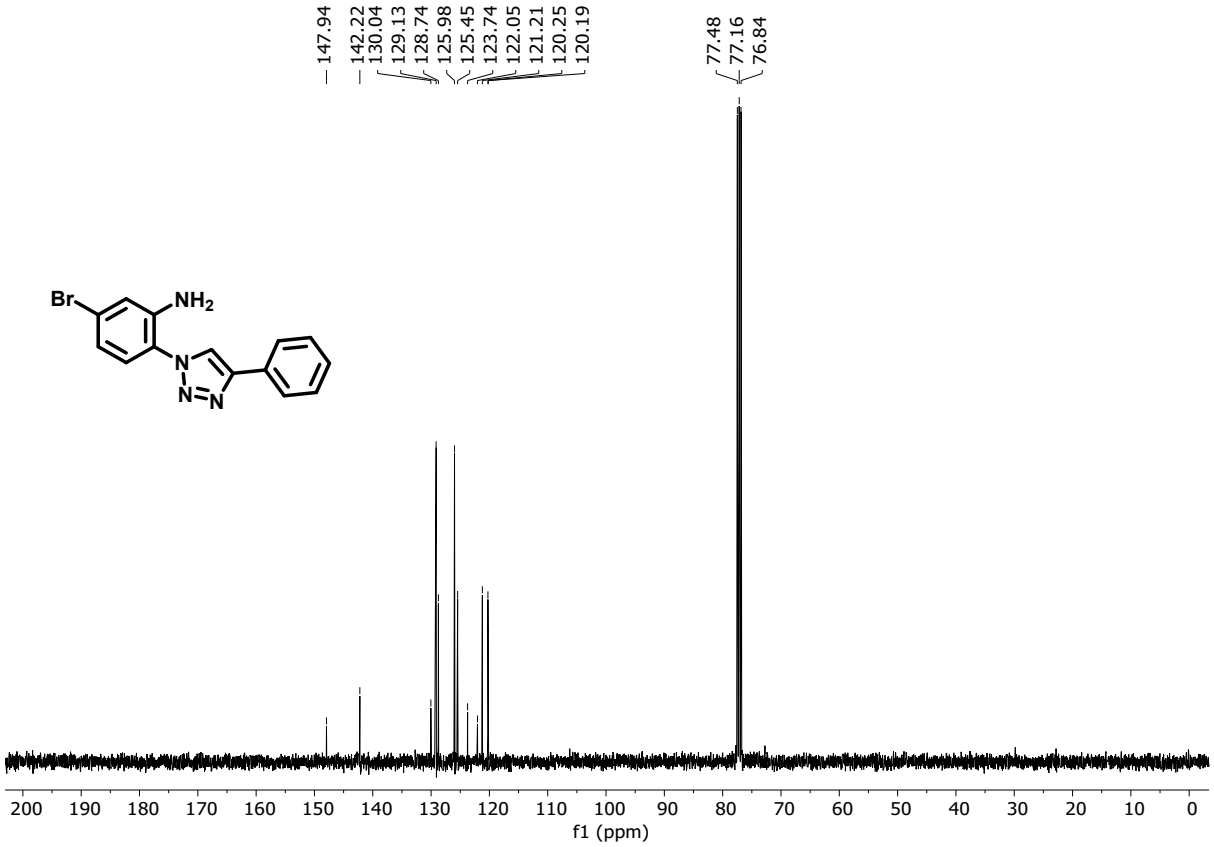


Fig S102. ^{13}C NMR spectrum of 5-bromo-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3r**)

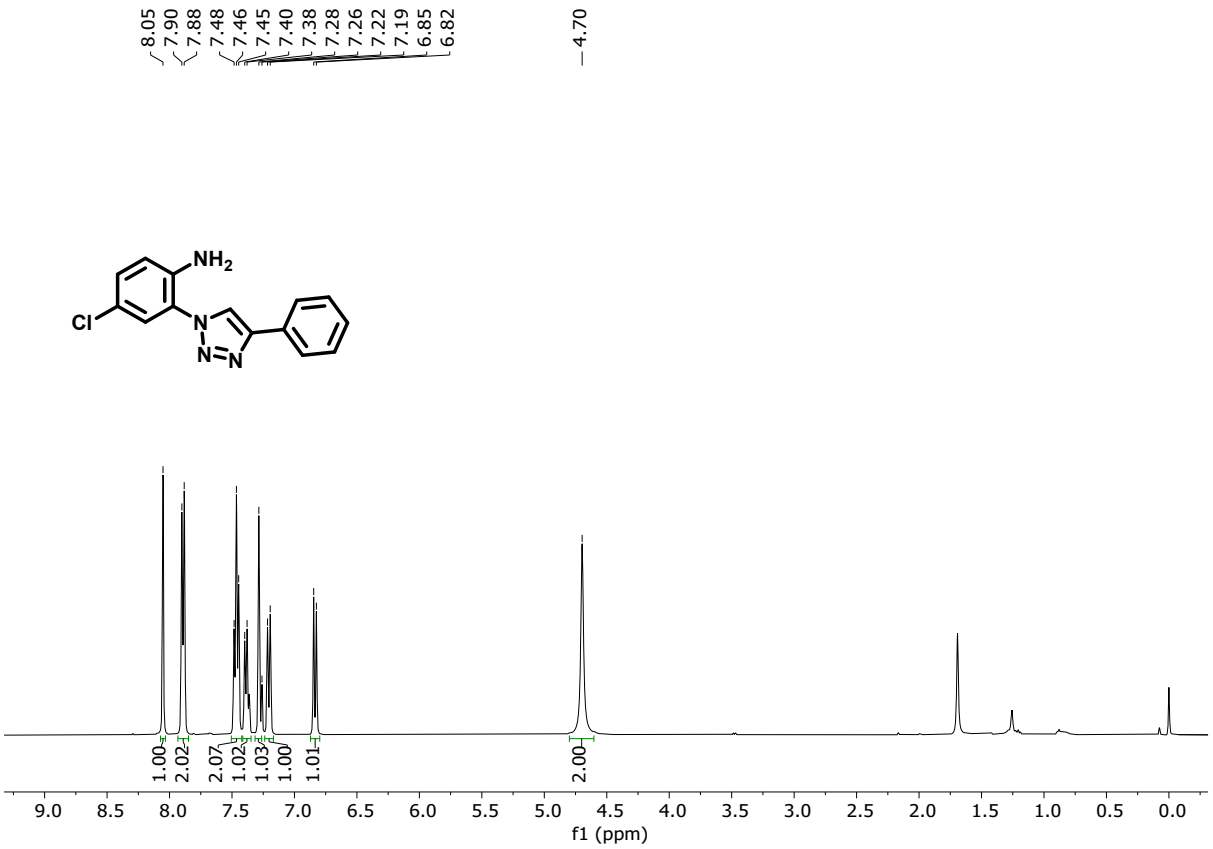


Fig S103. ^{1}H NMR spectrum of 4-chloro-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3s**)

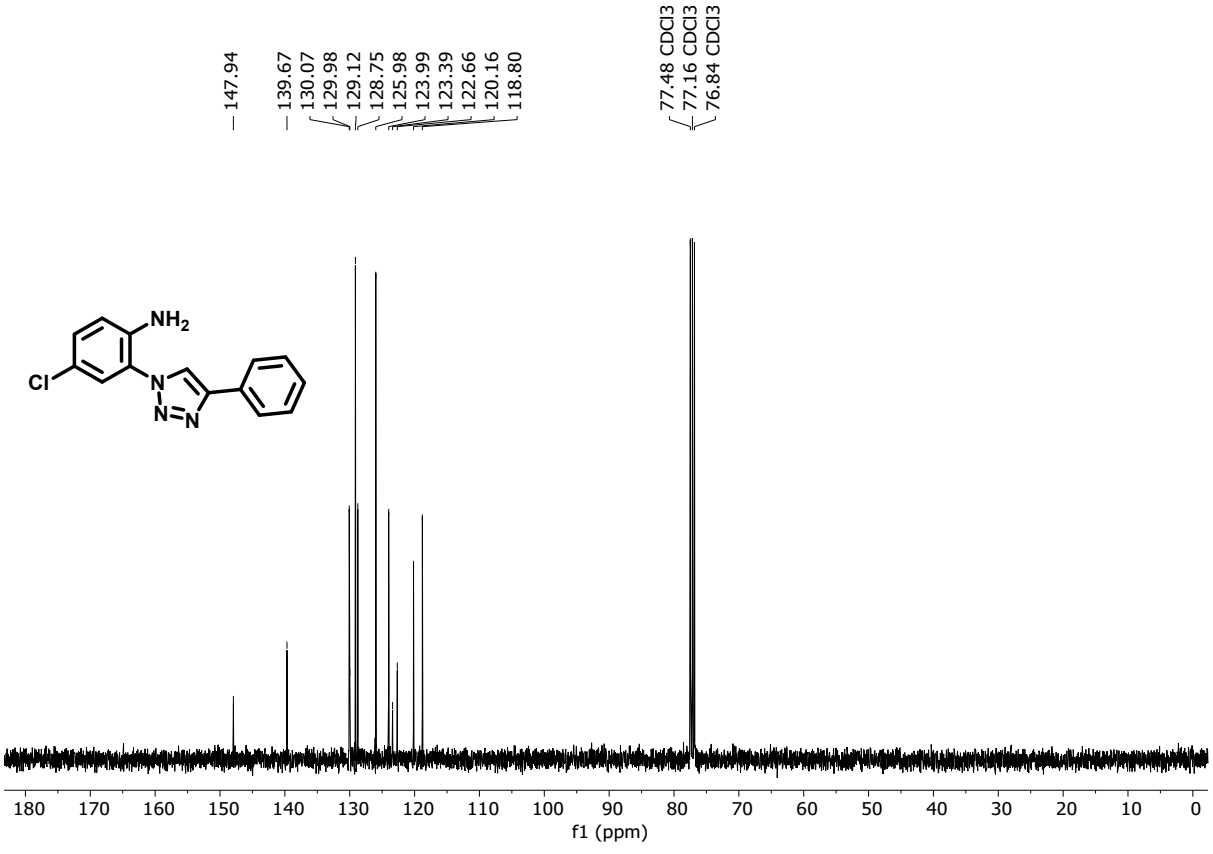


Fig S104. ^{13}C NMR spectrum of 4-chloro-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3s**)

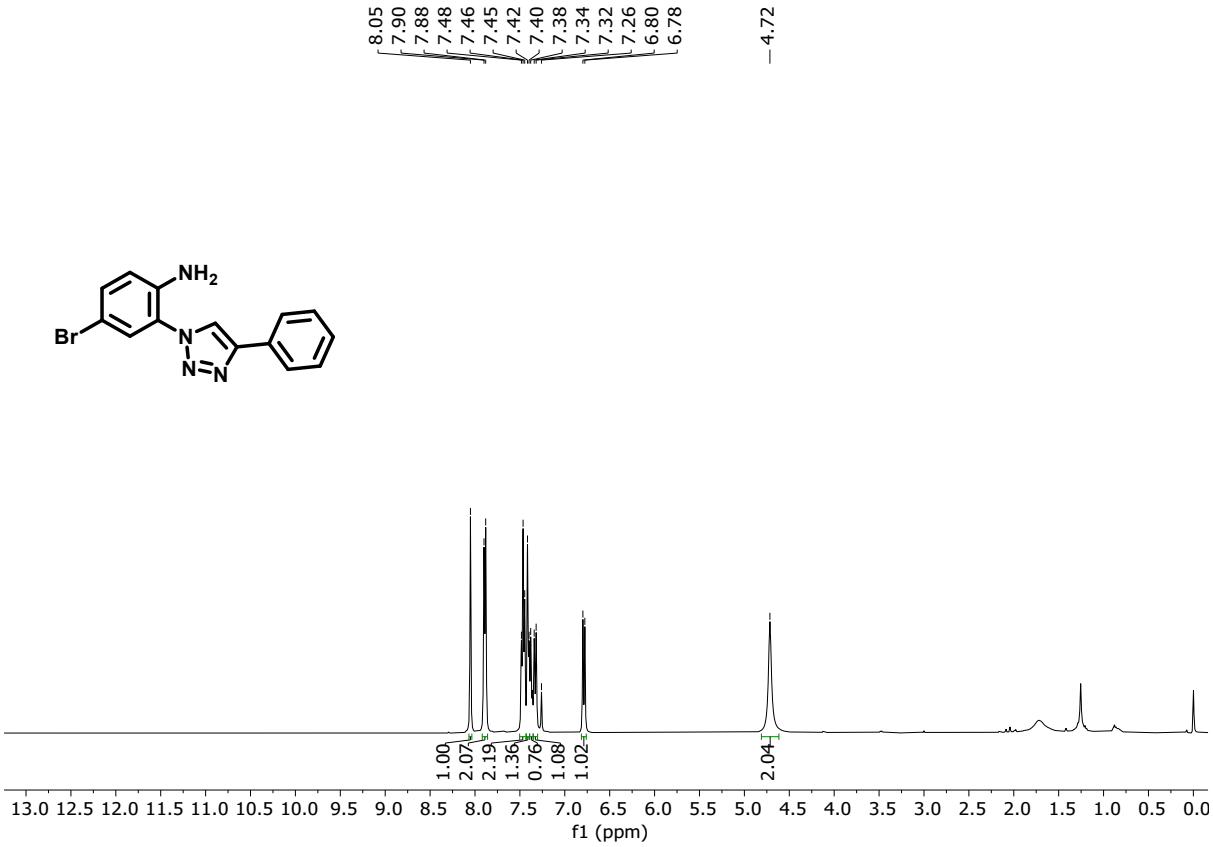


Fig S105. ^{1}H NMR spectrum of 4-bromo-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3t**)

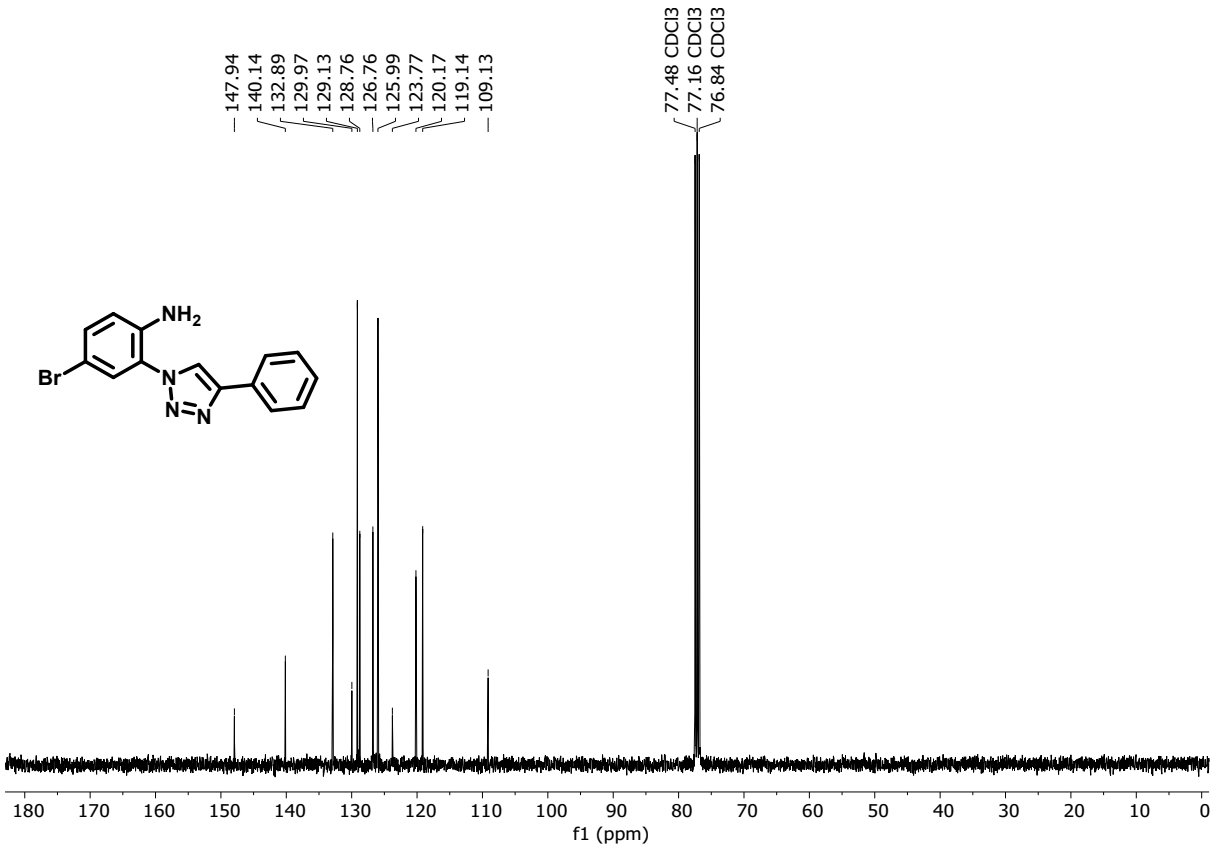


Fig S106. ^{13}C NMR spectrum of 4-bromo-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3t**)

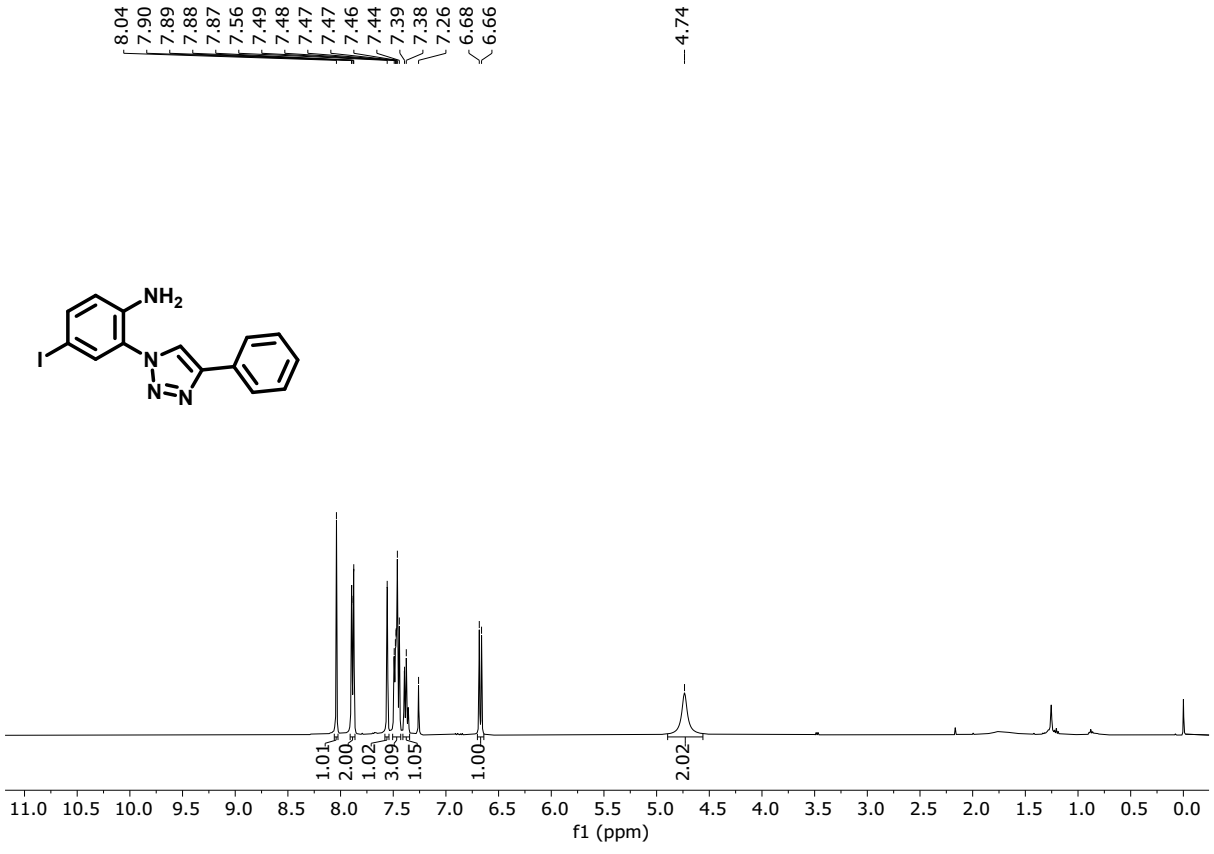


Fig S107. ^{1}H NMR spectrum of 4-iodo-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3u**)

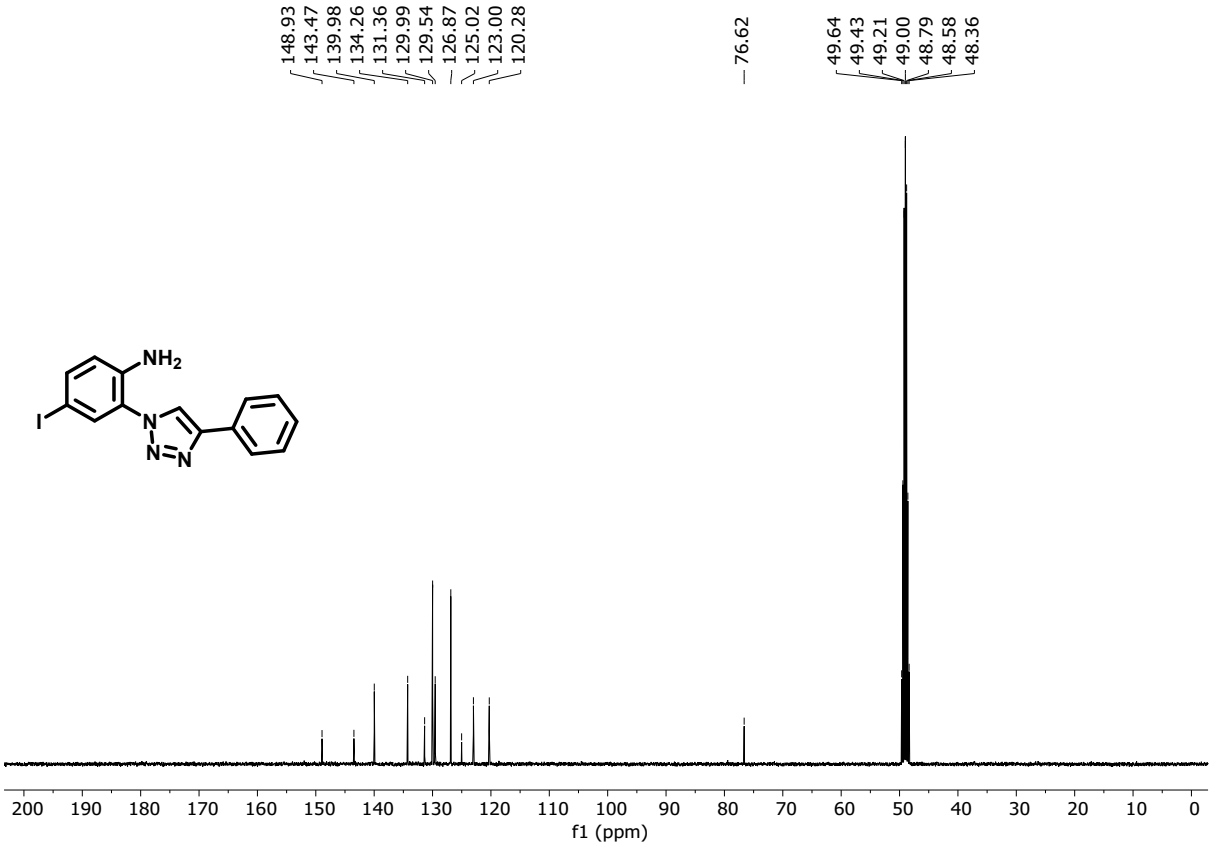


Fig S108. ^{13}C NMR spectrum of 4-iodo-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)aniline (**3u**)

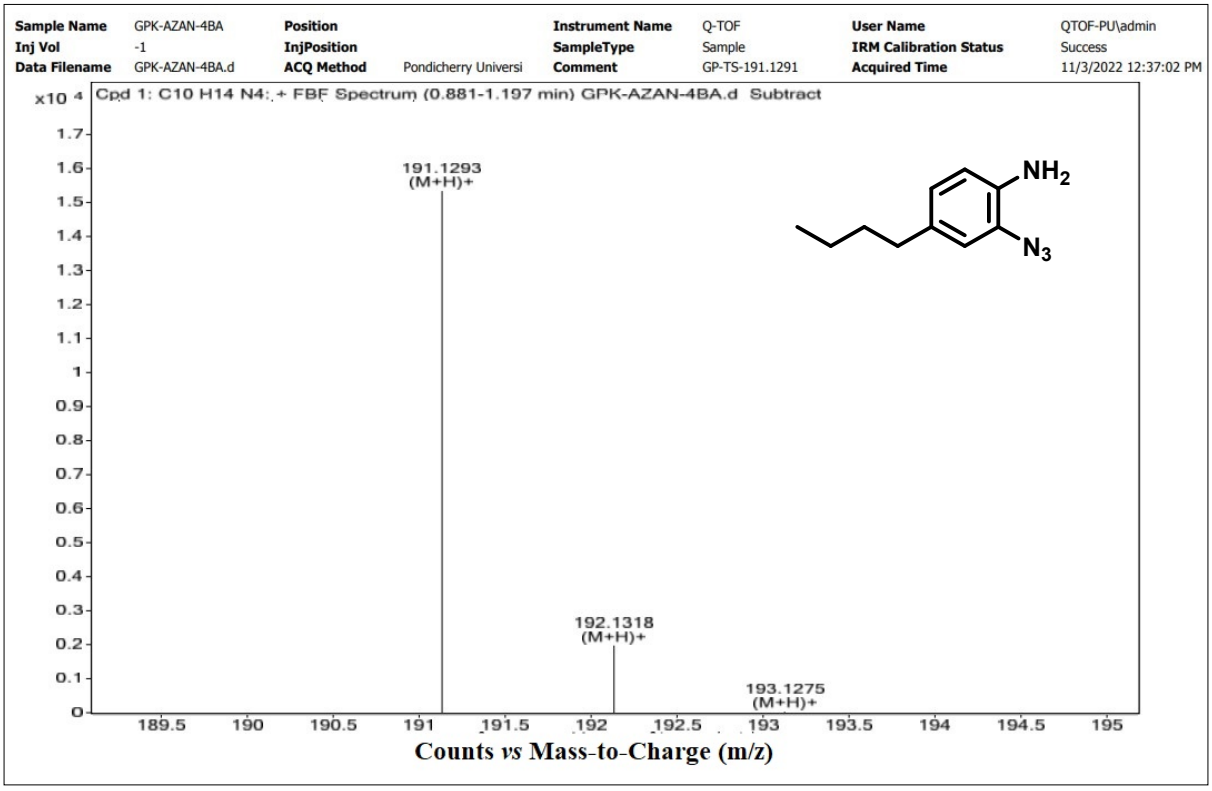


Fig S109. ESI-MS spectrum of the compound **2c**

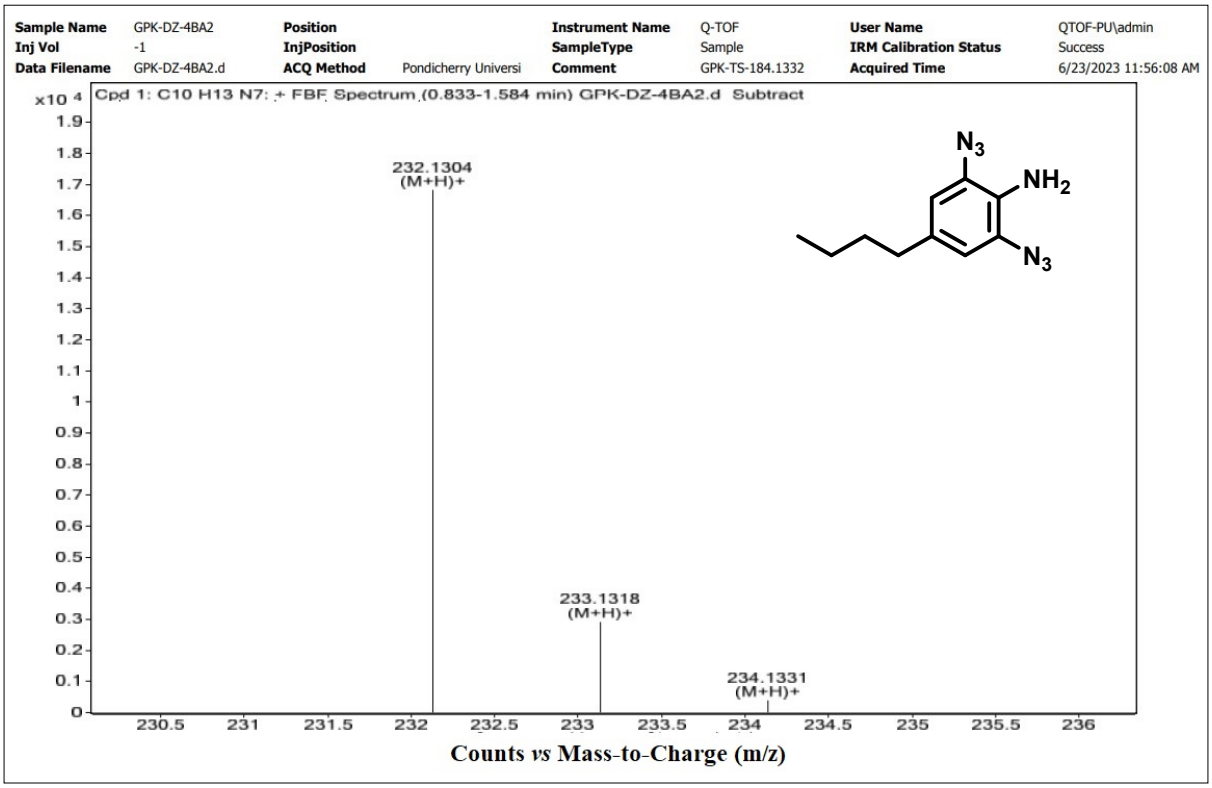


Fig S110. ESI-MS spectrum of the compound **2c'**

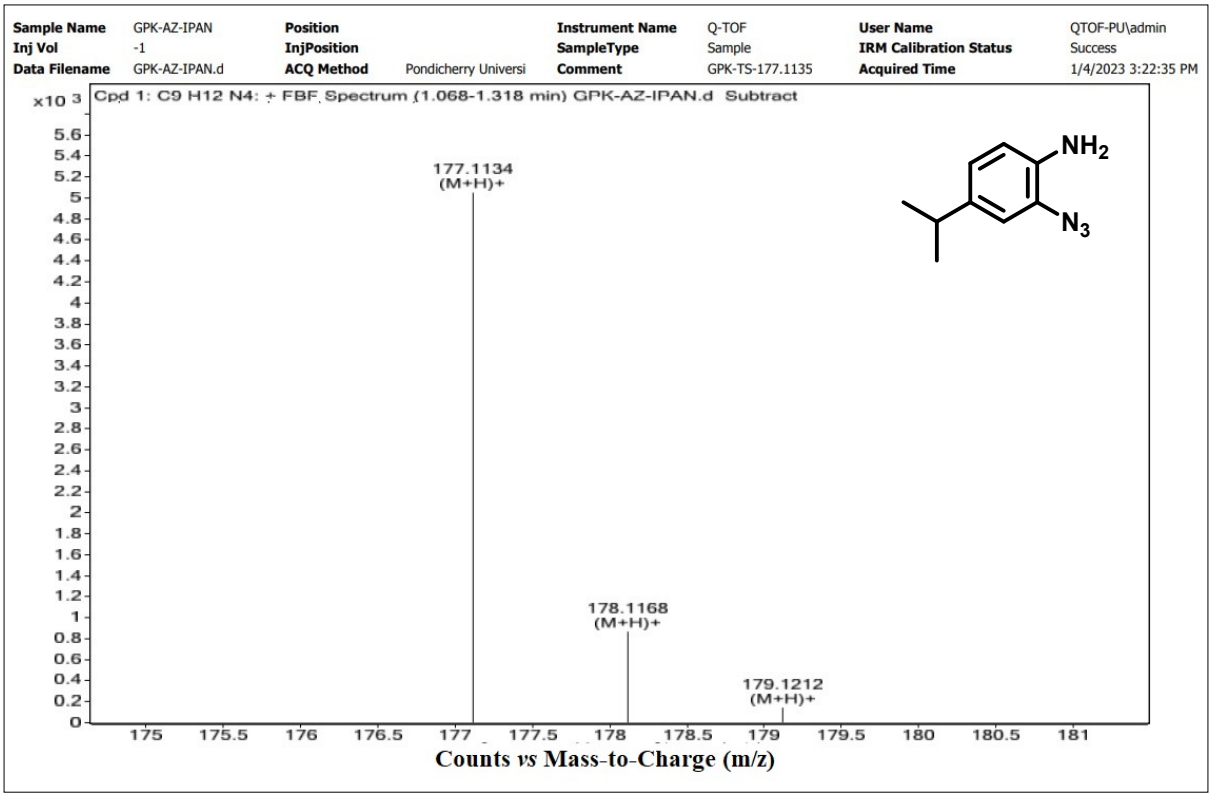


Fig S111. ESI-MS spectrum of the compound **2d**

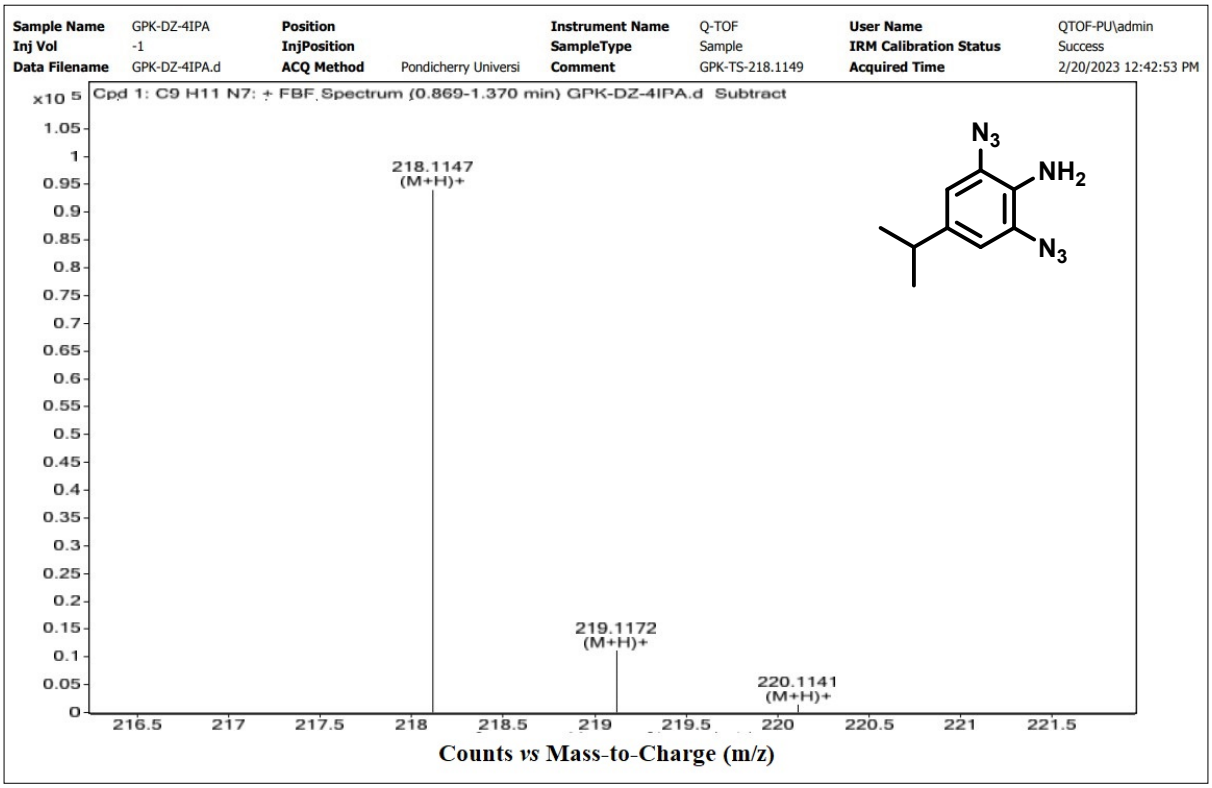


Fig S112. ESI-MS spectrum of the compound **2d'**

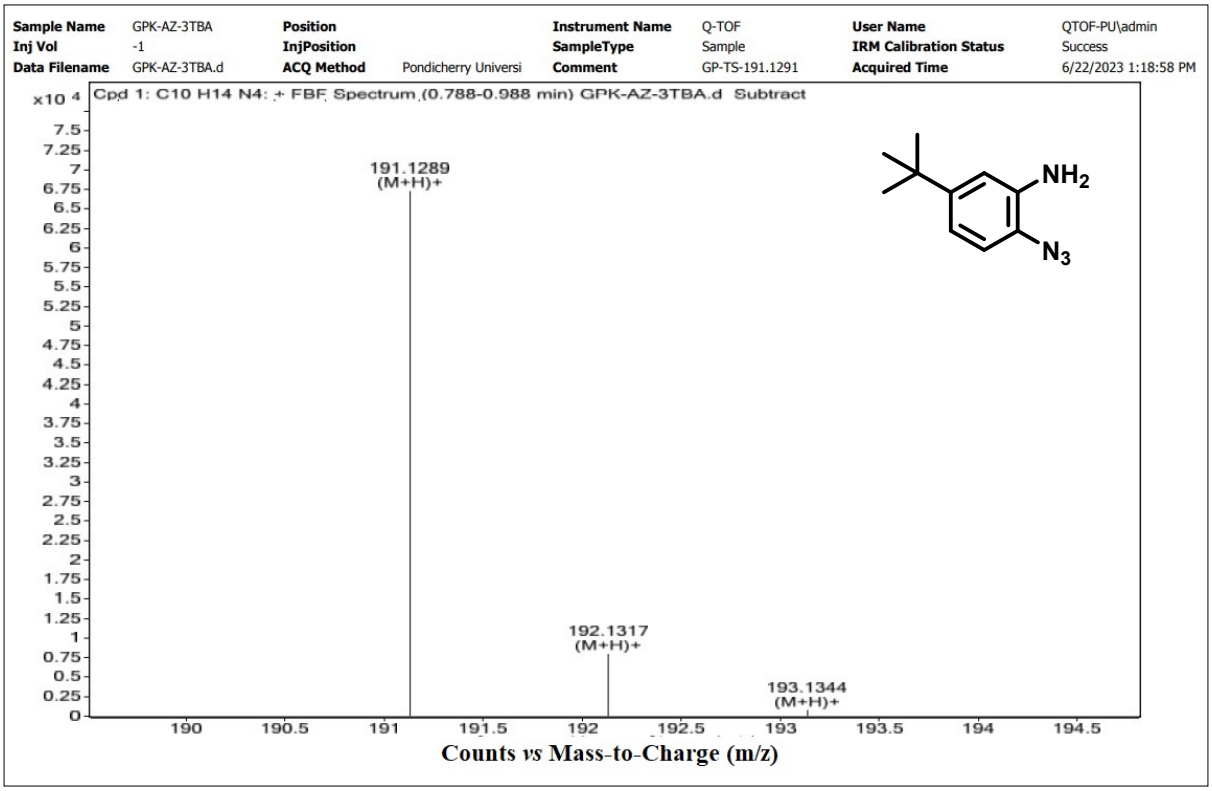


Fig S113. ESI-MS spectrum of the compound **2h**

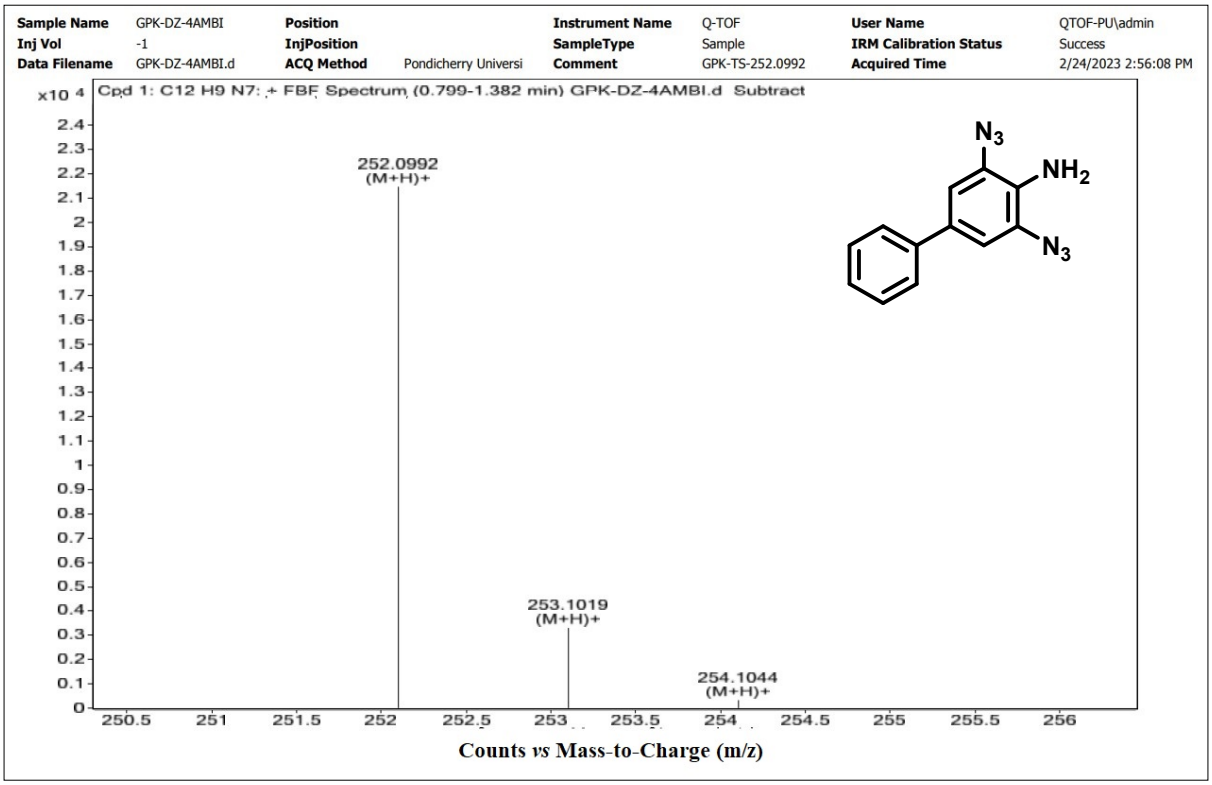


Fig S114. ESI-MS spectrum of the compound **2o'**

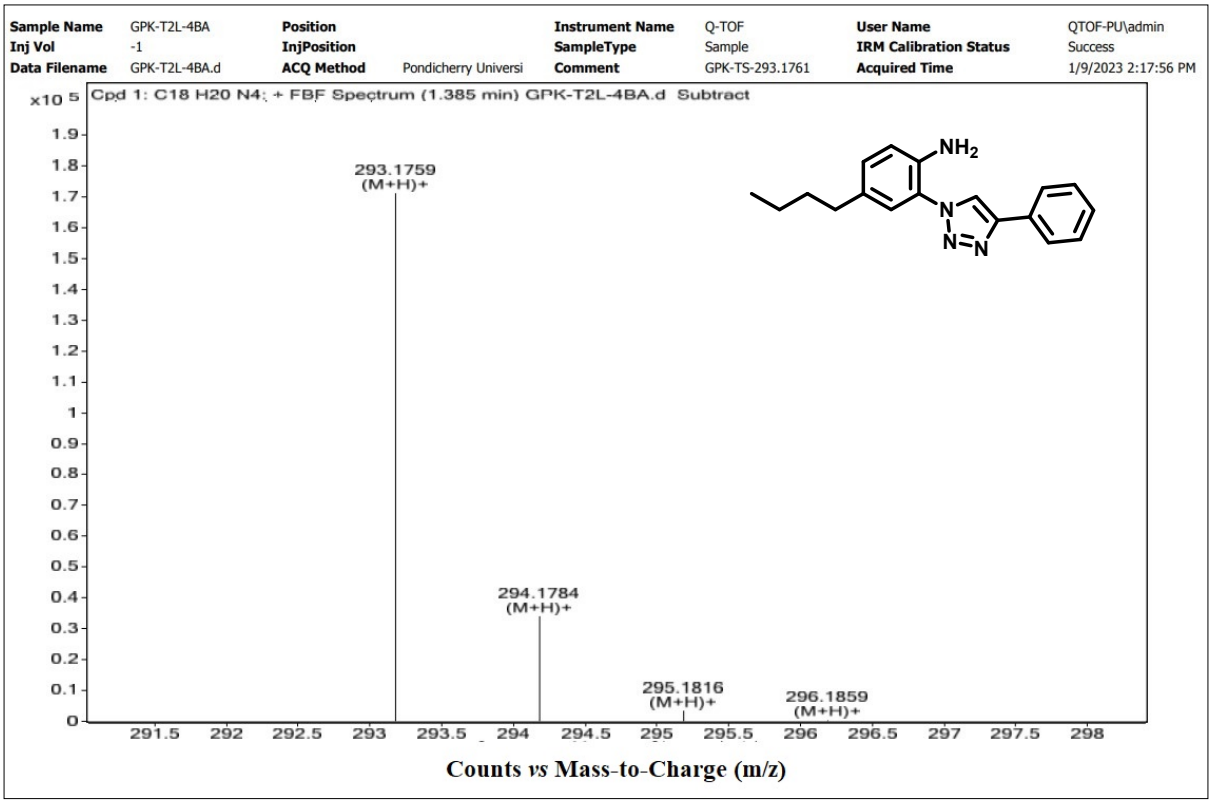


Fig S115. ESI-MS spectrum of the compound **3c**

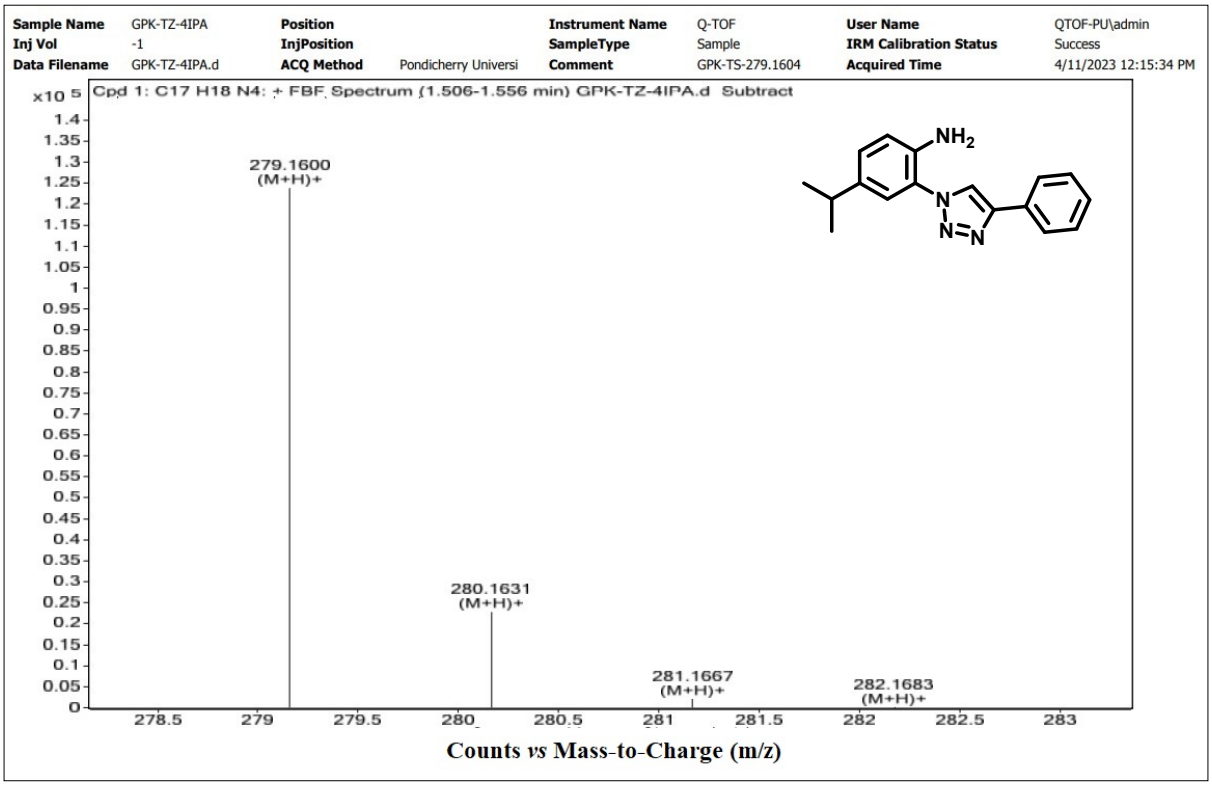


Fig S116. ESI-MS spectrum of the compound **3d**

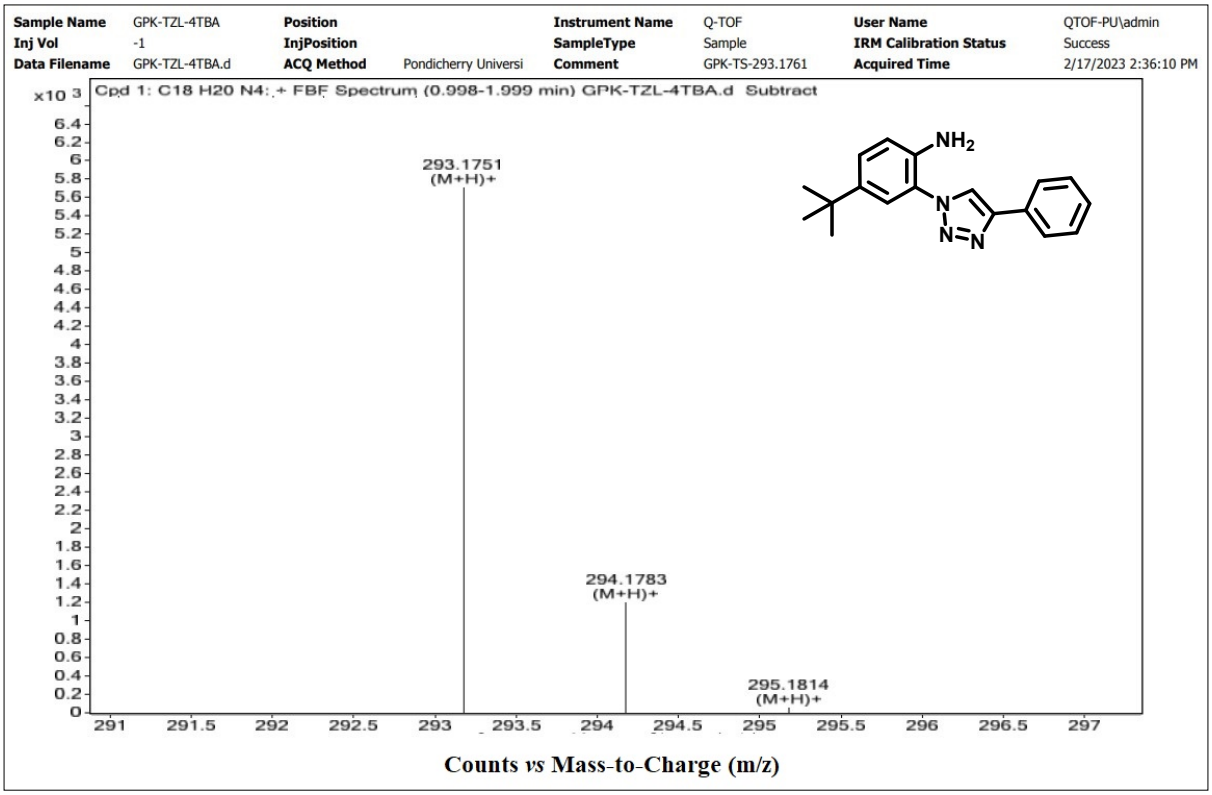


Fig S117. ESI-MS spectrum of the compound **3e**

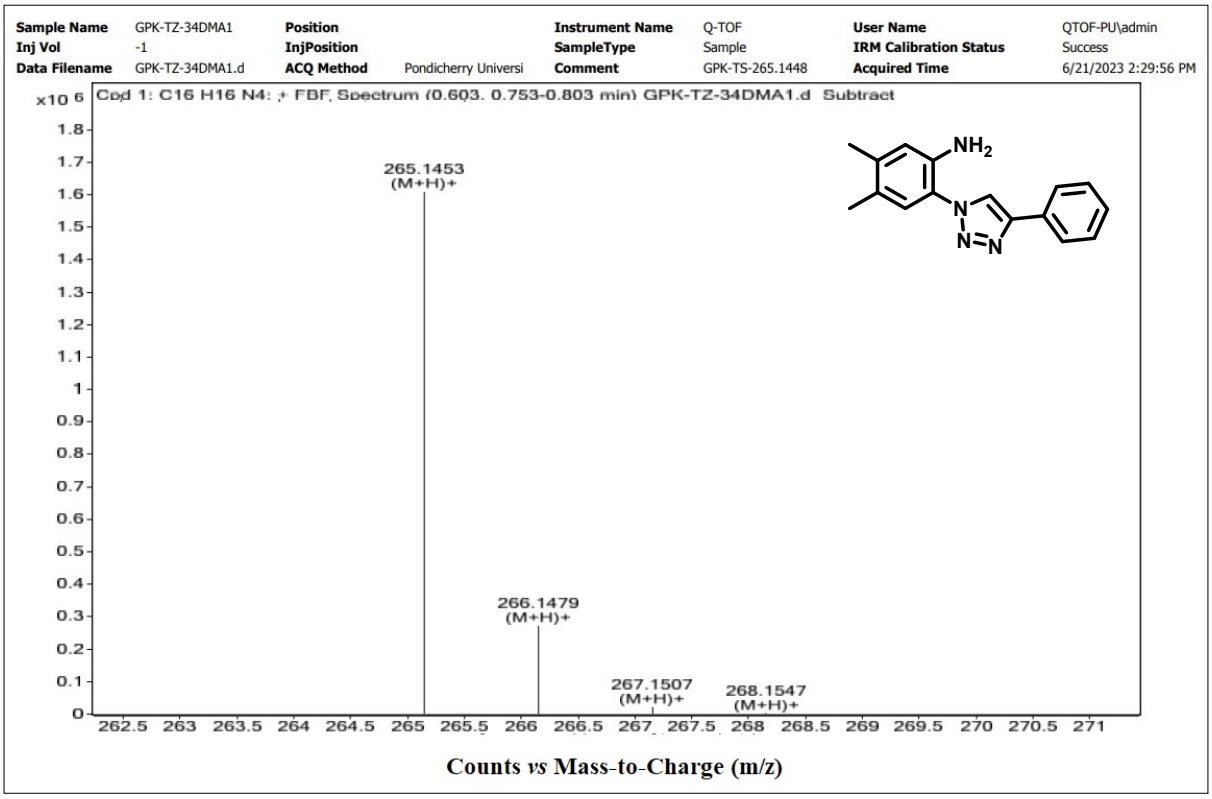


Fig S118. ESI-MS spectrum of the compound **3f**

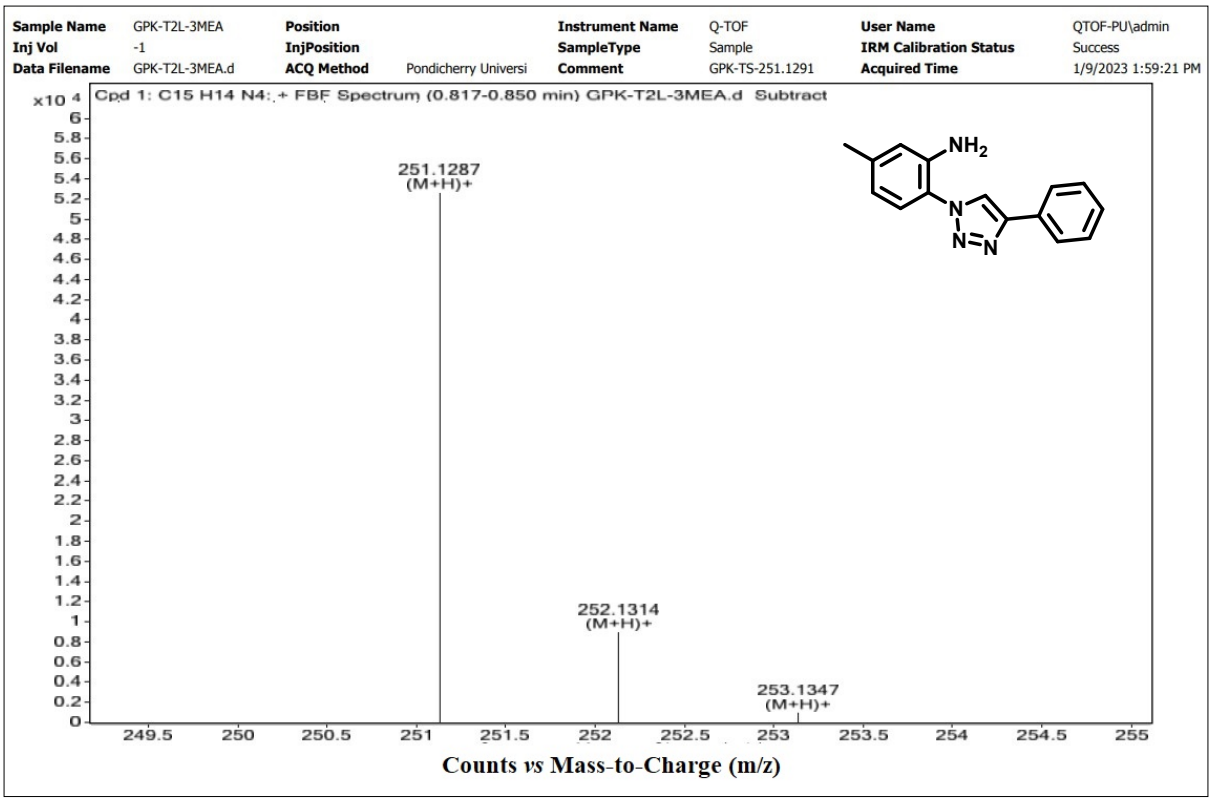


Fig S119. ESI-MS spectrum of the compound **3g**

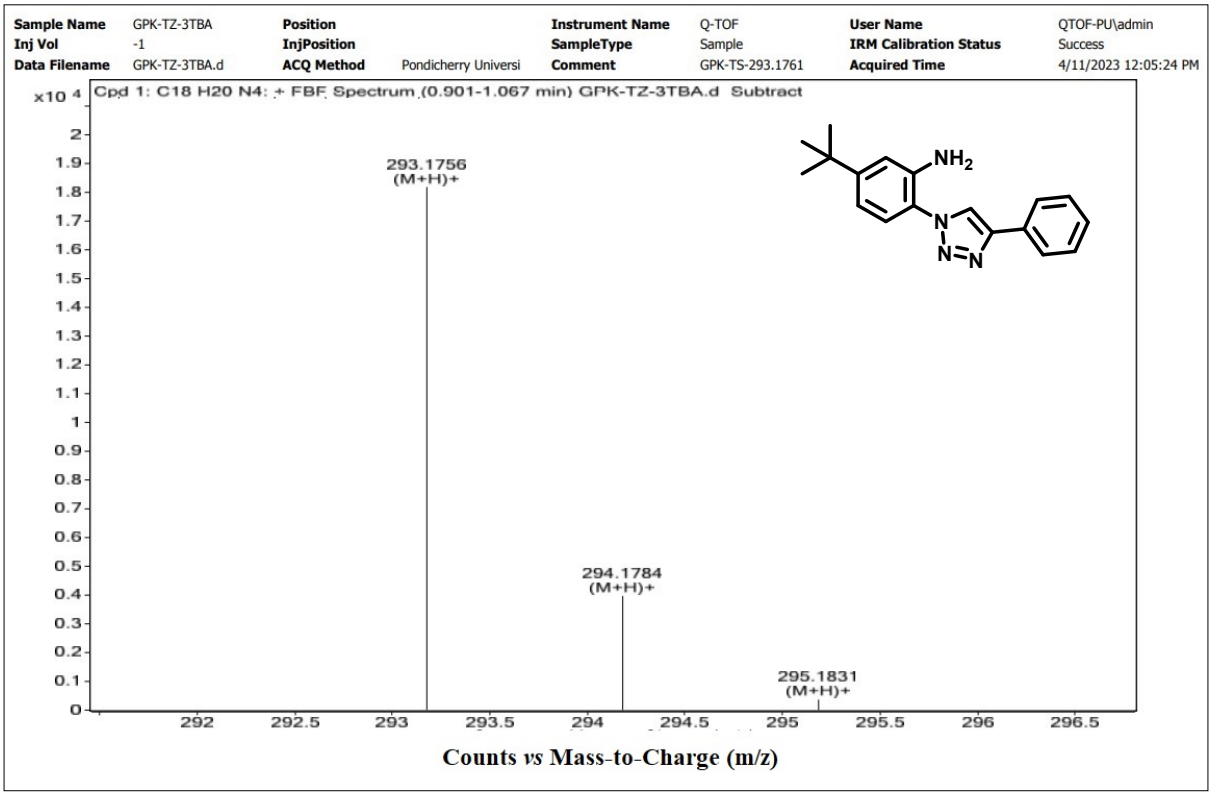


Fig S120. ESI-MS spectrum of the compound **3h**

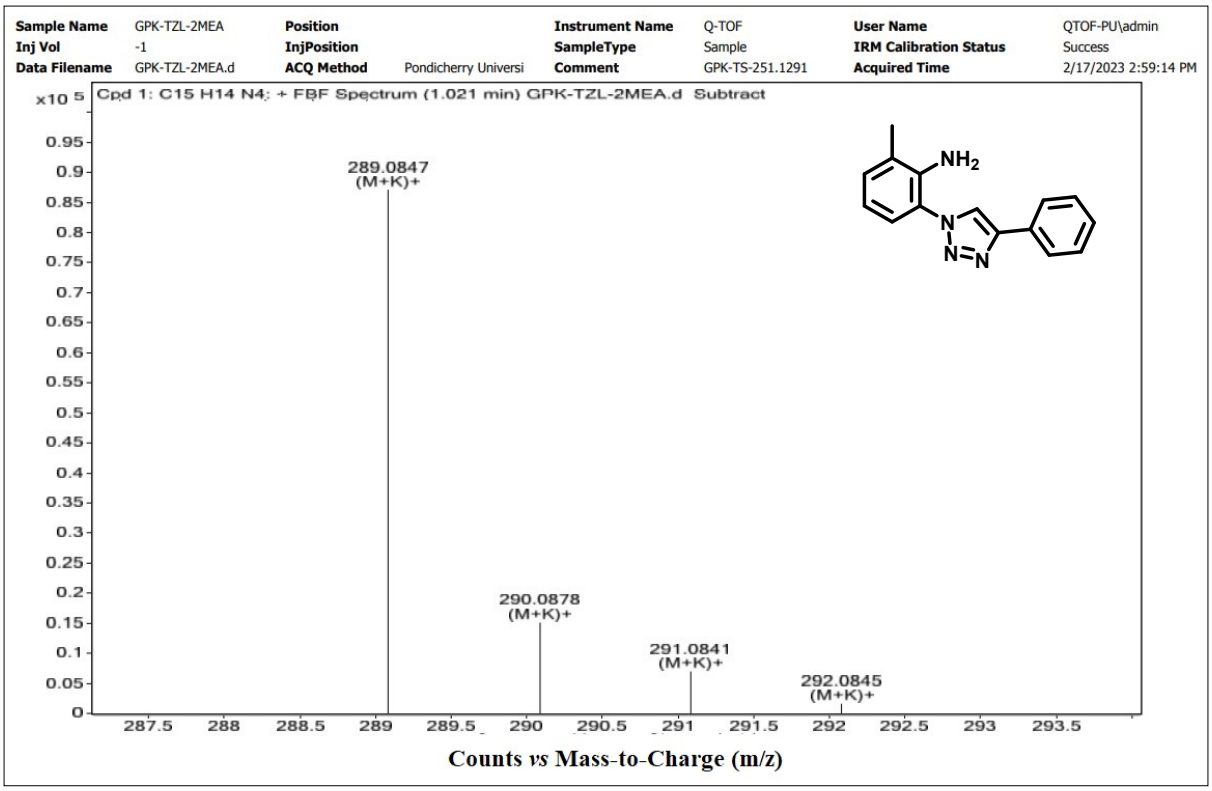


Fig S121. ESI-MS spectrum of the compound **3i**

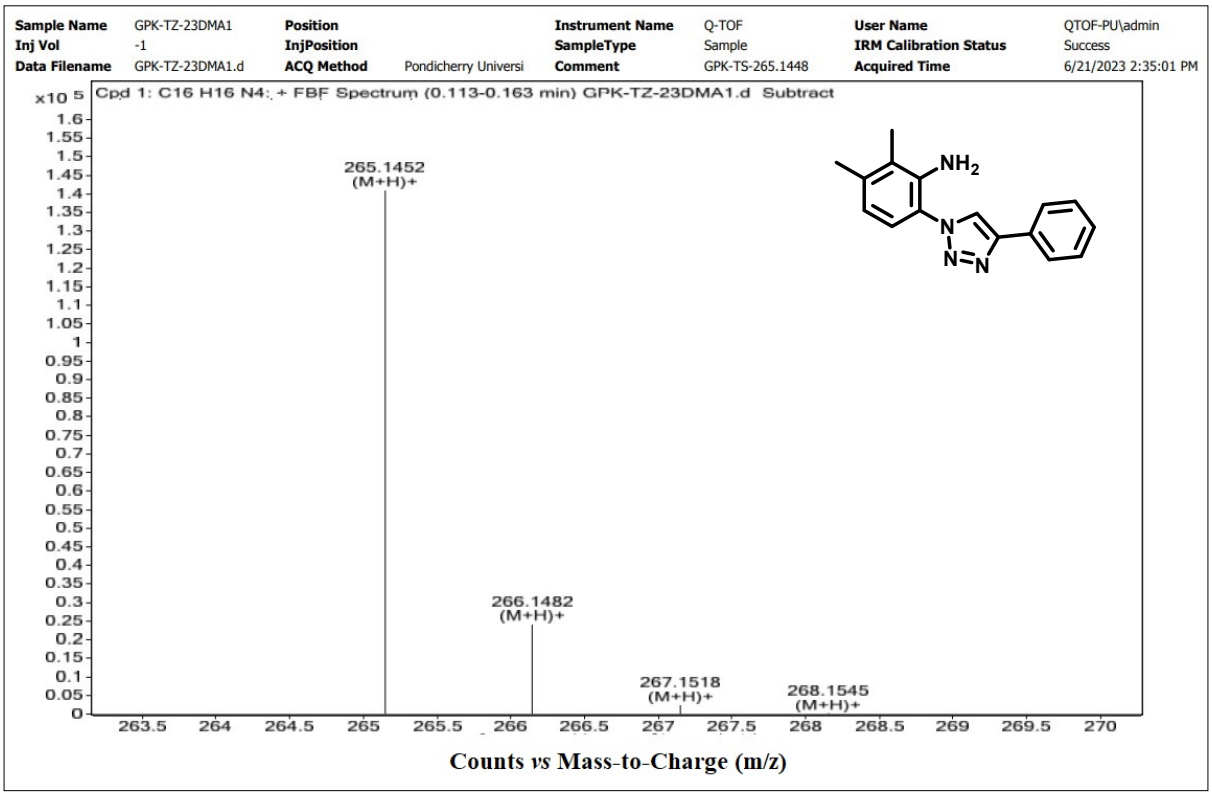


Fig S122. ESI-MS spectrum of the compound **3j**

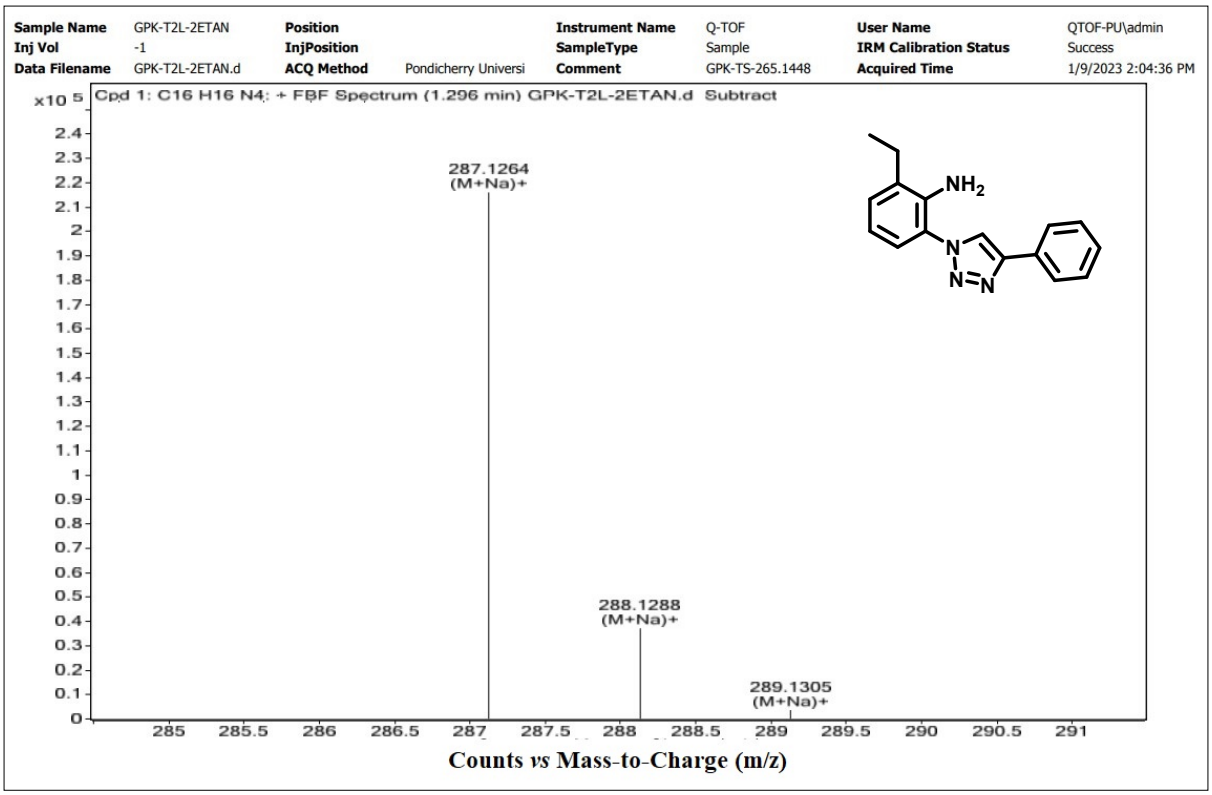


Fig S123. ESI-MS spectrum of the compound **3l**

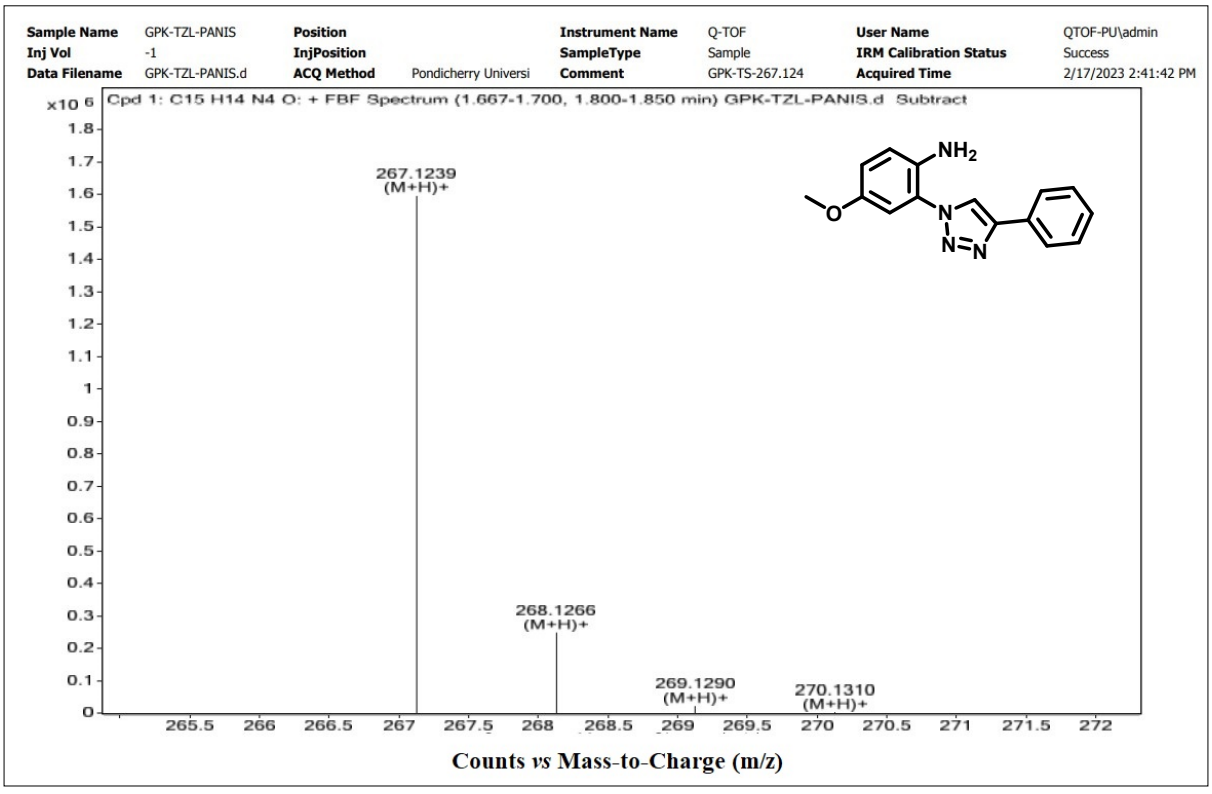


Fig S124. ESI-MS spectrum of the compound **3m**

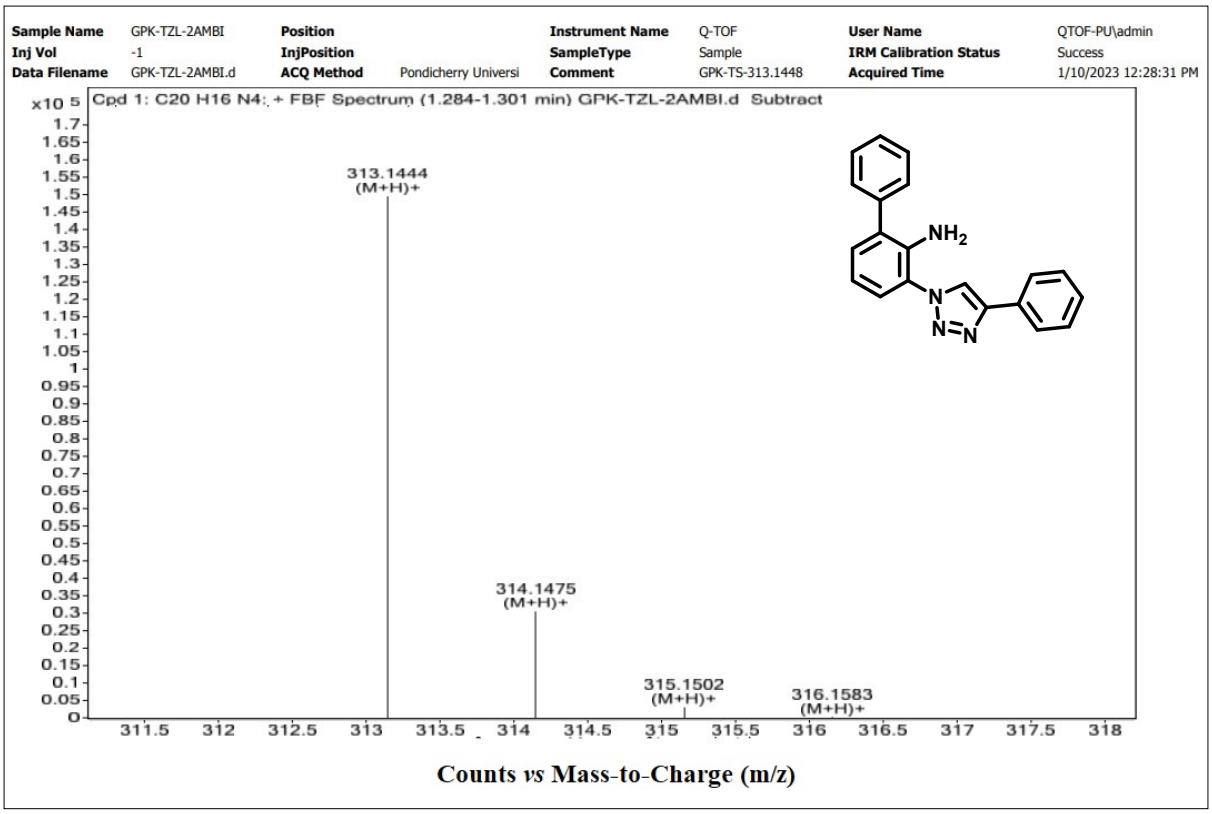


Fig S125. ESI-MS spectrum of the compound **3n**

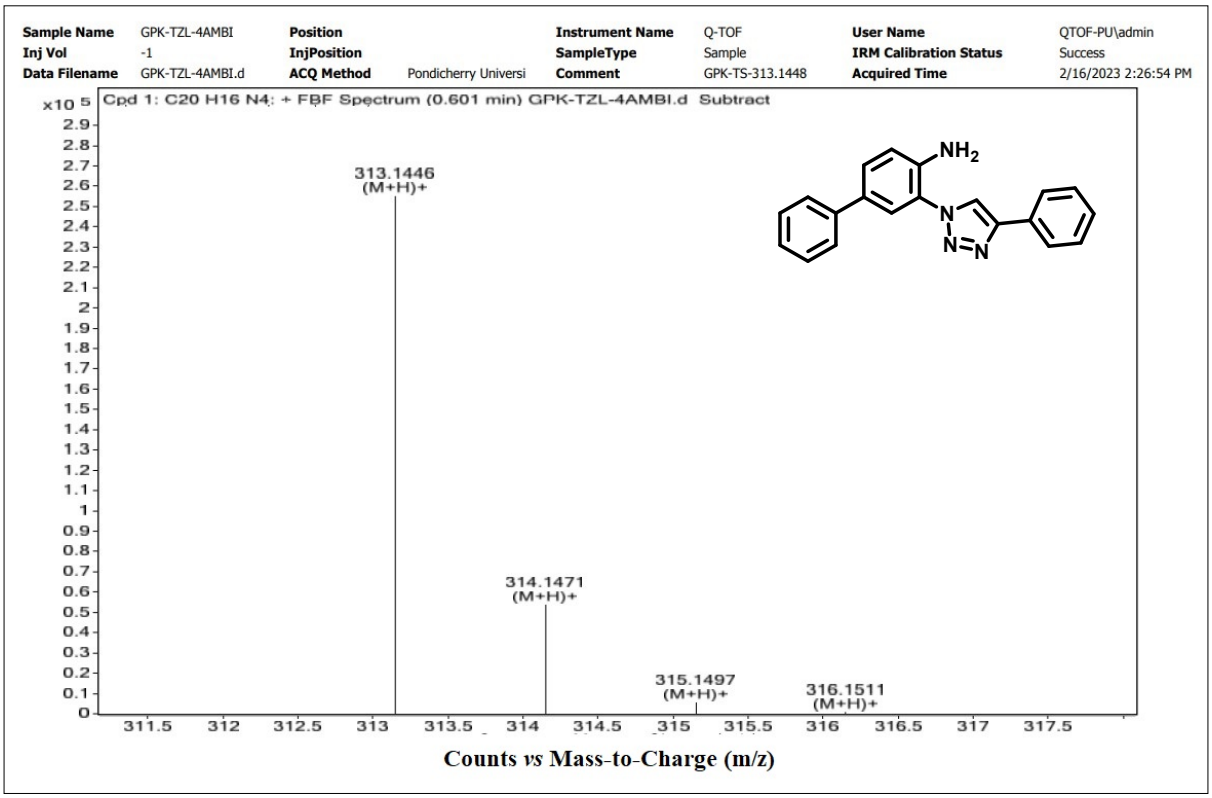


Fig S126. ESI-MS spectrum of the compound **3o**

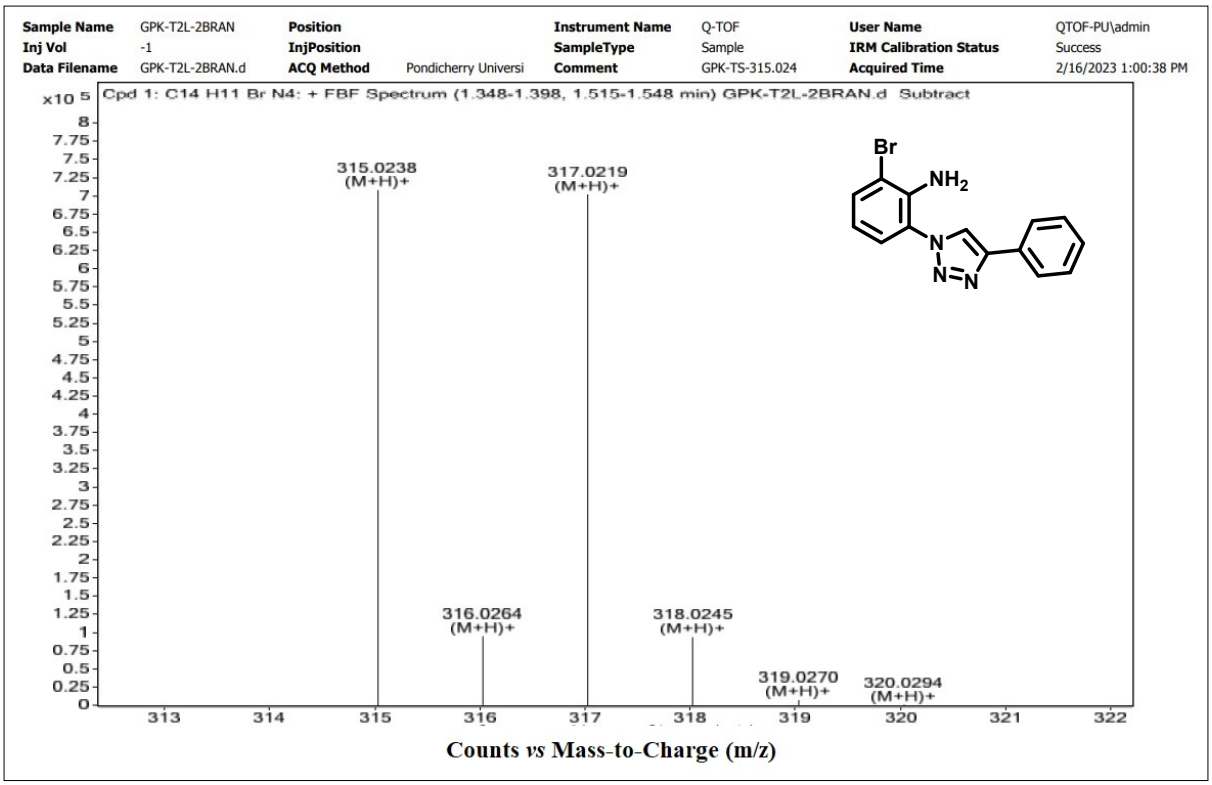


Fig S127. ESI-MS spectrum of the compound **3p**

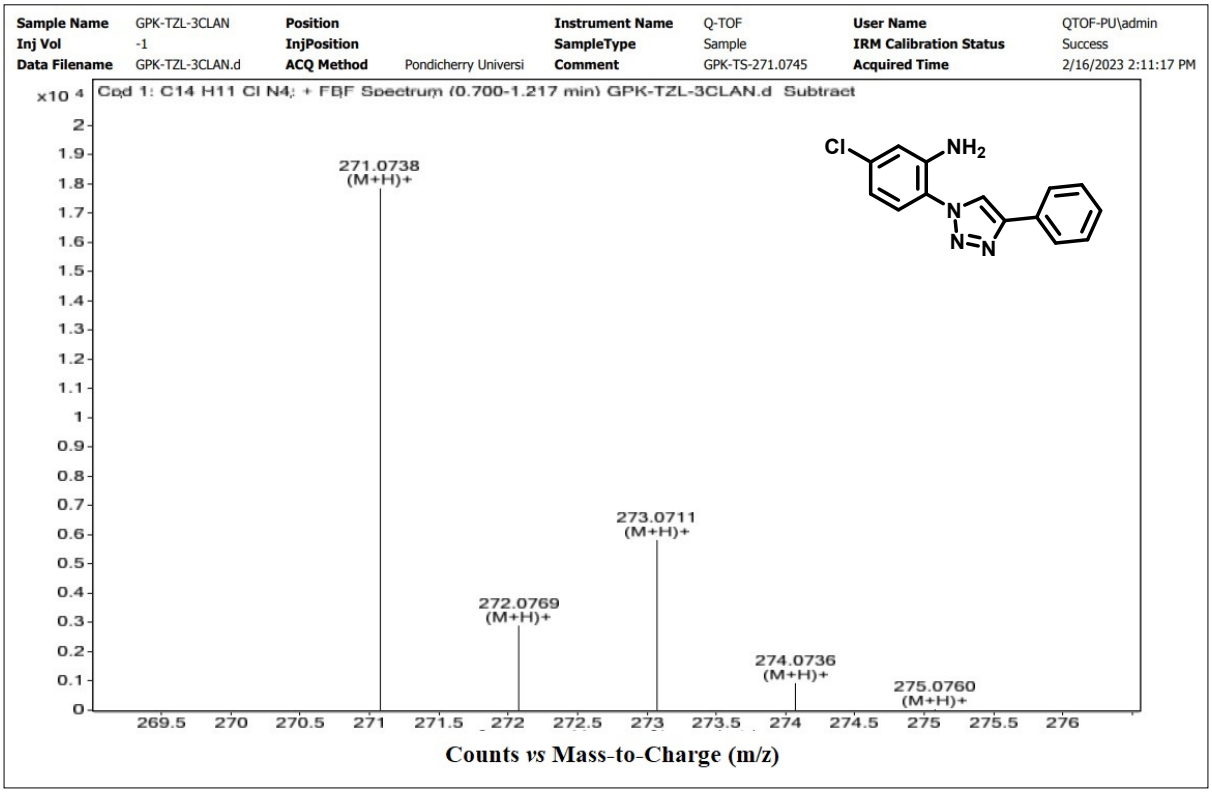


Fig S128. ESI-MS spectrum of the compound **3q**

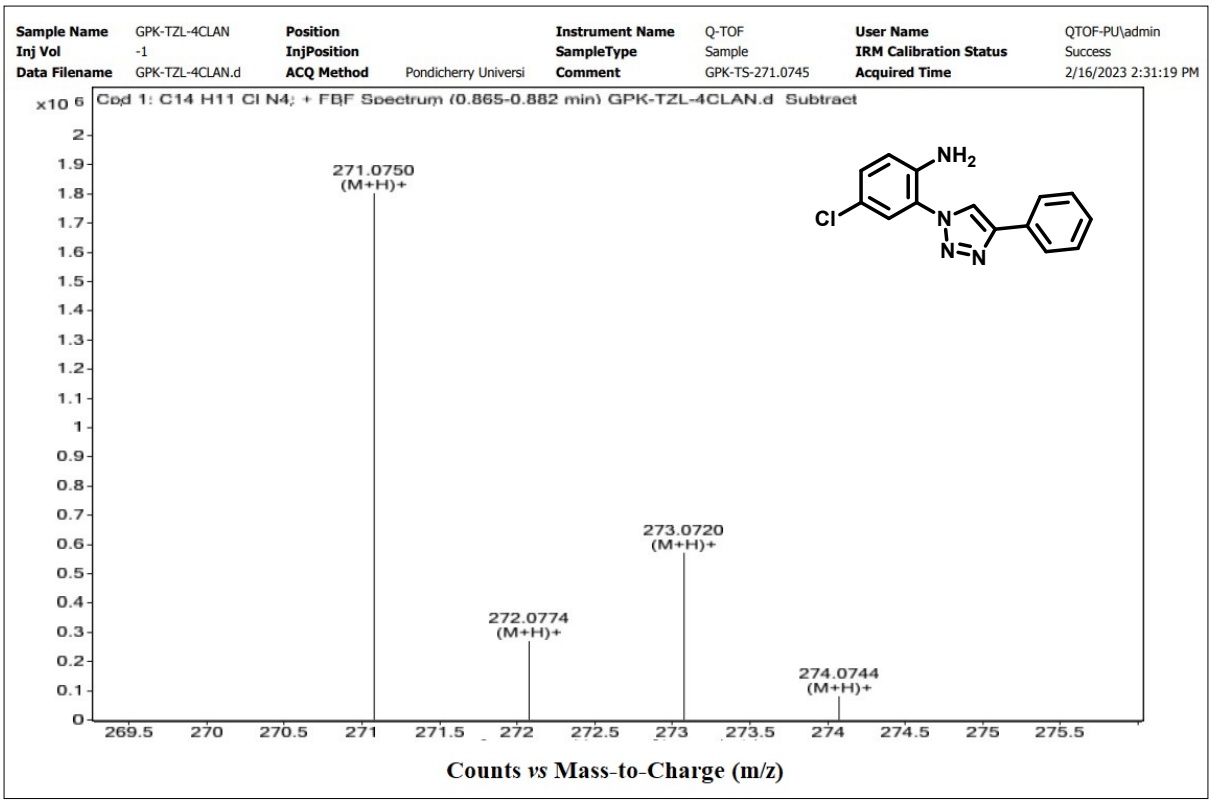


Fig S129. ESI-MS spectrum of the compound **3s**

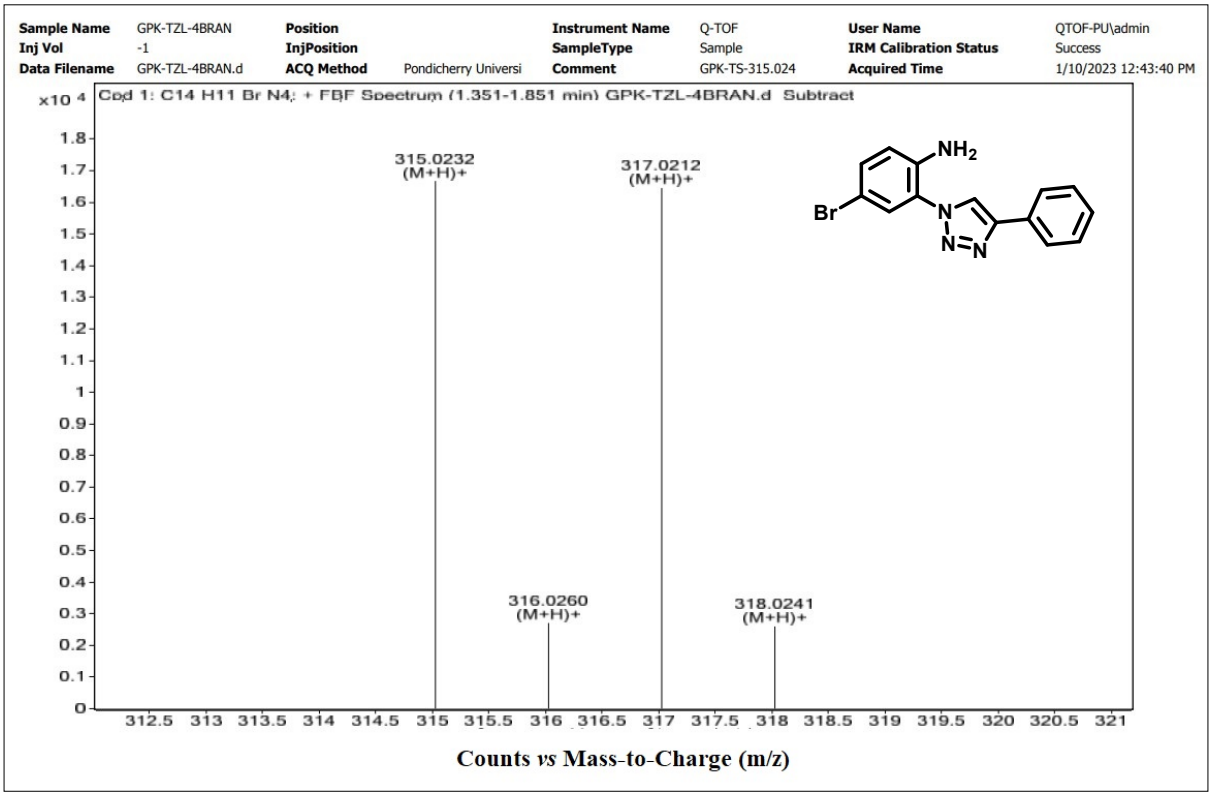


Fig S130. ESI-MS spectrum of the compound **3t**

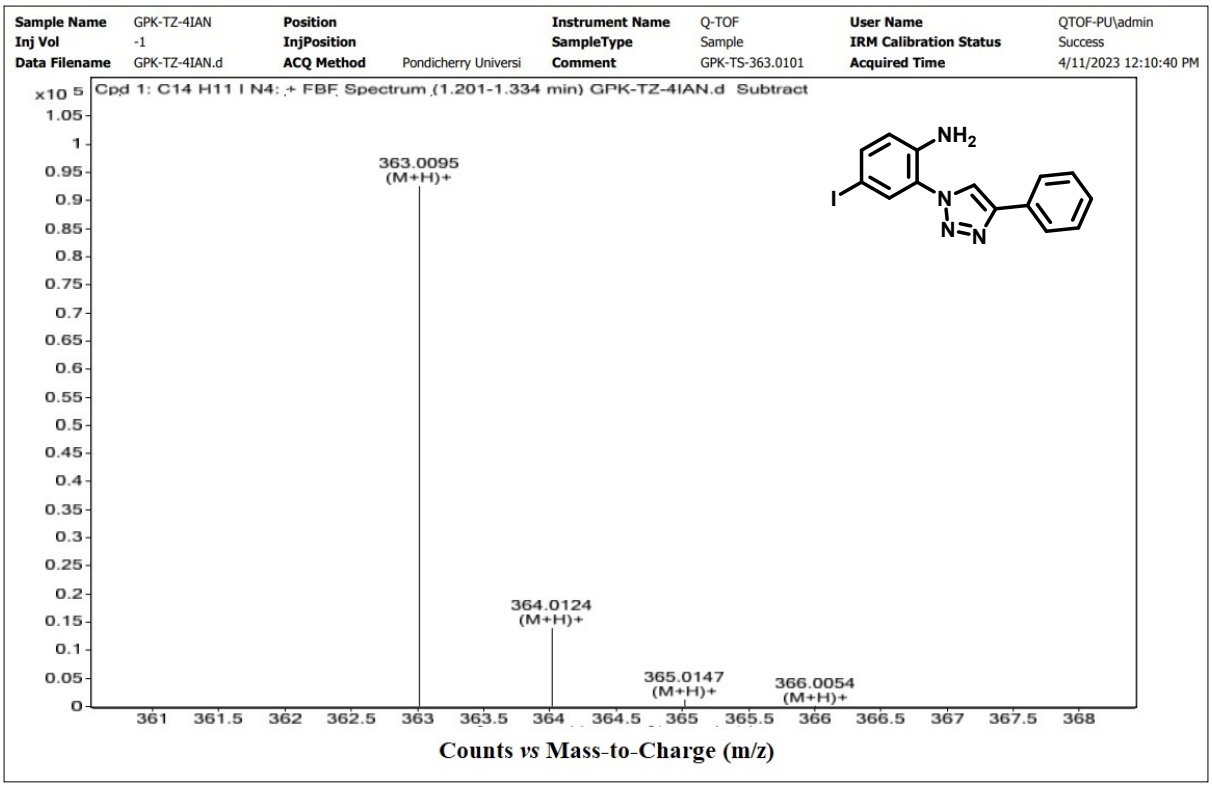


Fig S131. ESI-MS spectrum of the compound **3u**

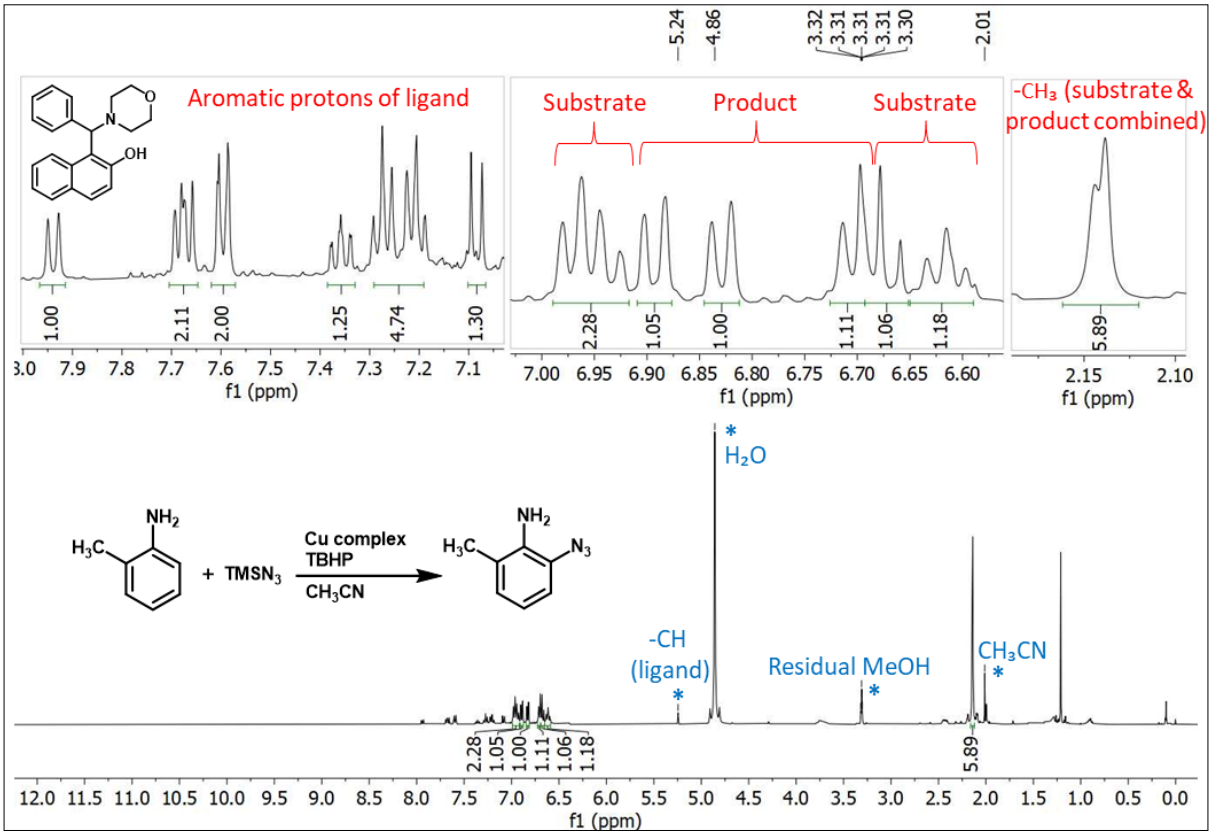


Fig S132. NMR spectrum of the crude mixture after 1h of reaction time

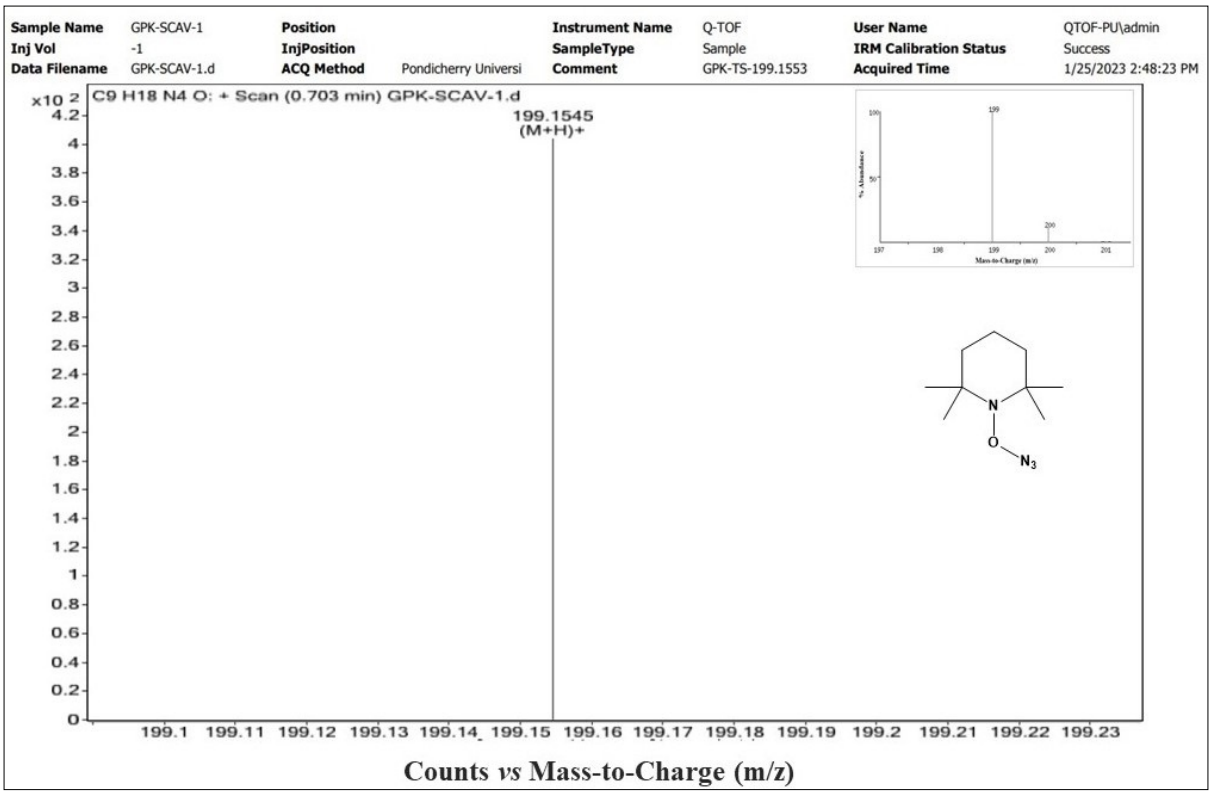


Fig S133. ESI-MS spectrum of the TEMPO-azide adduct

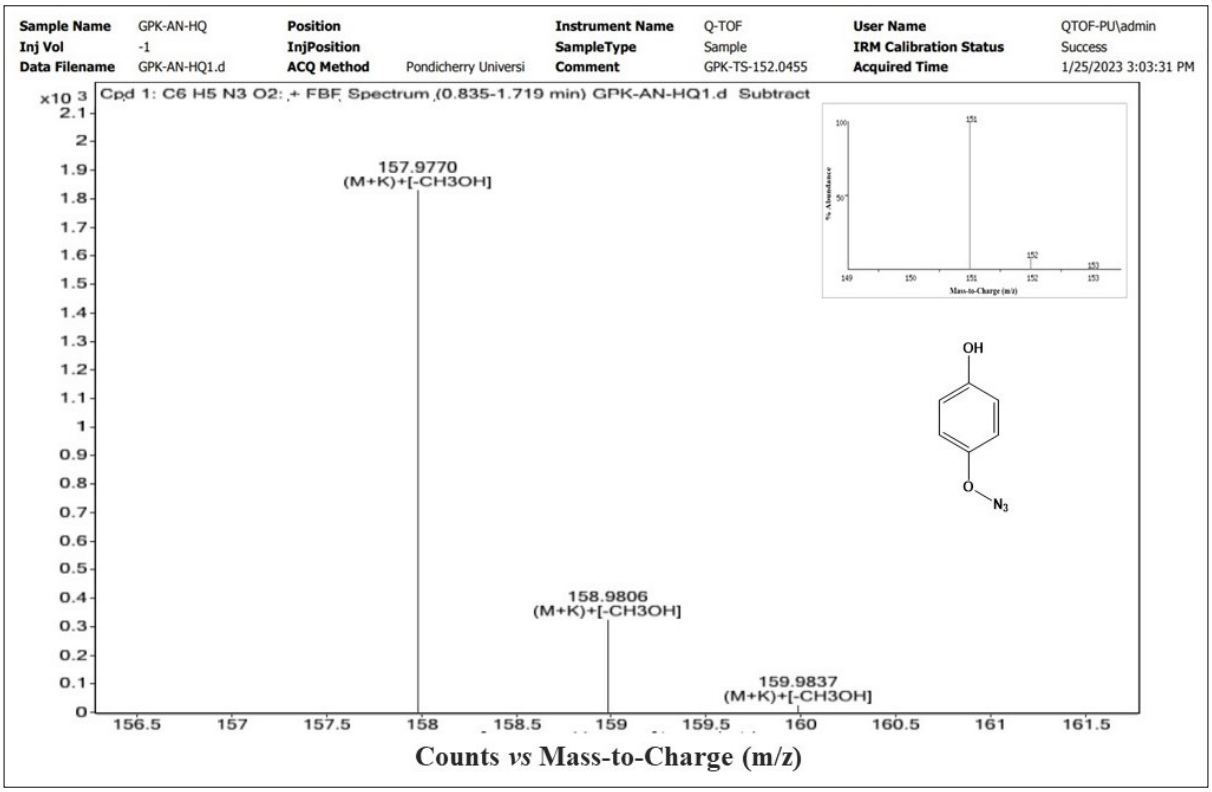


Fig S134. ESI-MS spectrum of the hydroquinone-azide adduct

NMR time-course experiment:

The aliquots of the crude reaction mixture at different time points were filtered through a small pad of silica, and their NMR spectra were recorded and are presented in Fig S135. The signals present in the aromatic region are briefly discussed in the manuscript. At 2.1 ppm, the methyl group of the substrate and product get combined in the spectra that are recorded after 20 min of the reaction due to their similar chemical environment. As a result, they appear as a slightly broad peak with splitting at the top of the signal indicating that it corresponds to two methyl units. This is further justified by the corresponding number of protons i.e., six, for the broad peak, as seen in Fig S137 – S139.

The signals corresponding to the ligand of the copper complex that is present in the crude mixture are also seen in the spectra at different time points in the range 7.1 - 8.0 ppm. This region is individually measured to see the number of protons and found that it is in agreement with the number of aromatic protons present in the ligand. The proton of the -CH unit of the ligand is also observed at 5.24 ppm at all the time points. Weak signals are observed around 2.4 and 3.7 ppm for the methylene protons present in the morpholine unit of the ligand. The signals at 3.31 ppm and 4.86 ppm correspond to the residual solvent and water from MeOD, respectively. The signal at 2.01 ppm corresponds to the reaction solvent, i.e., CH_3CN.

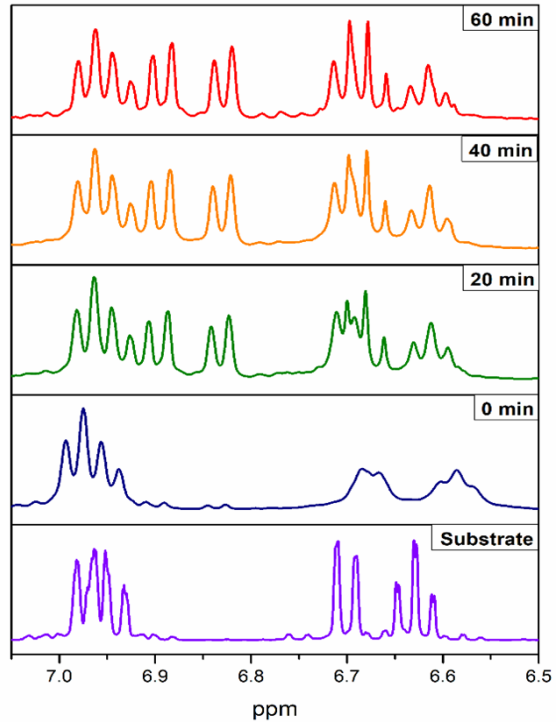


Fig S135. NMR spectrum of the crude mixture at different time points (Only the aromatic region is displayed to clearly visualise the progress of the reaction)

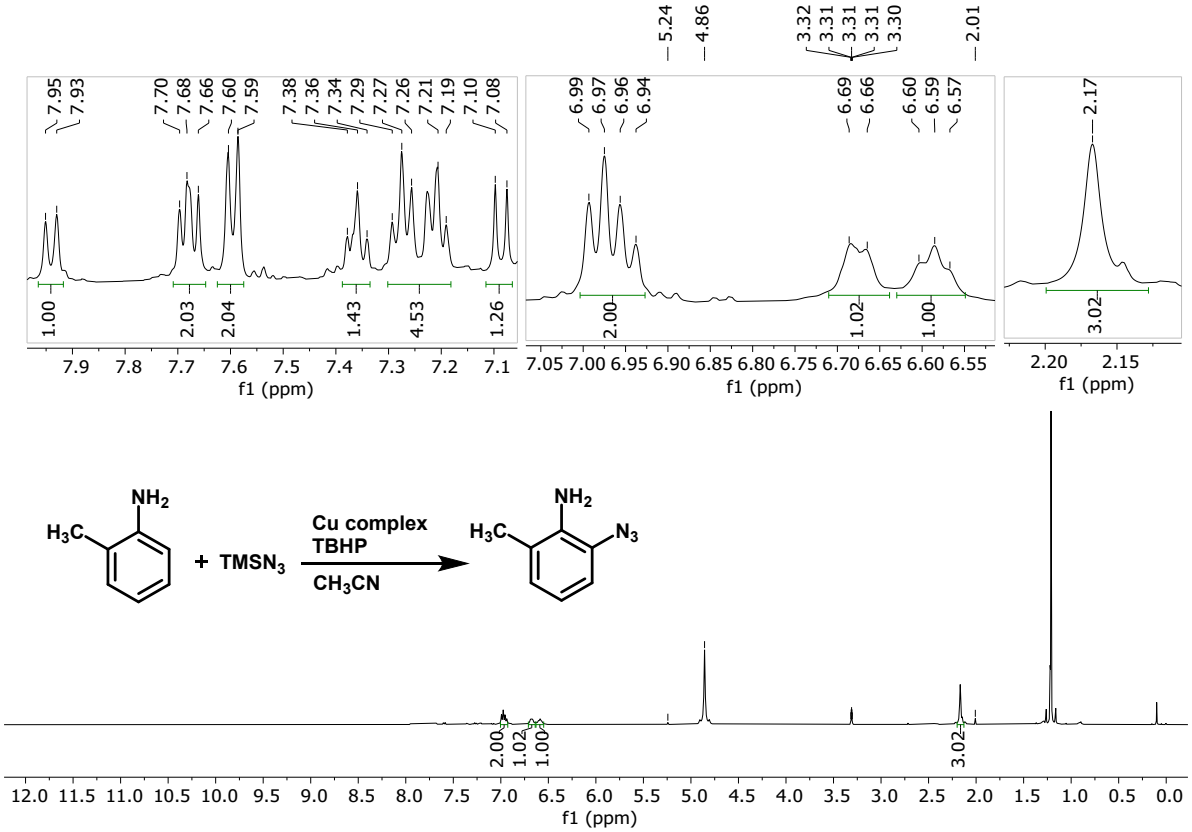


Fig S136. NMR spectrum of the crude mixture at 0 min

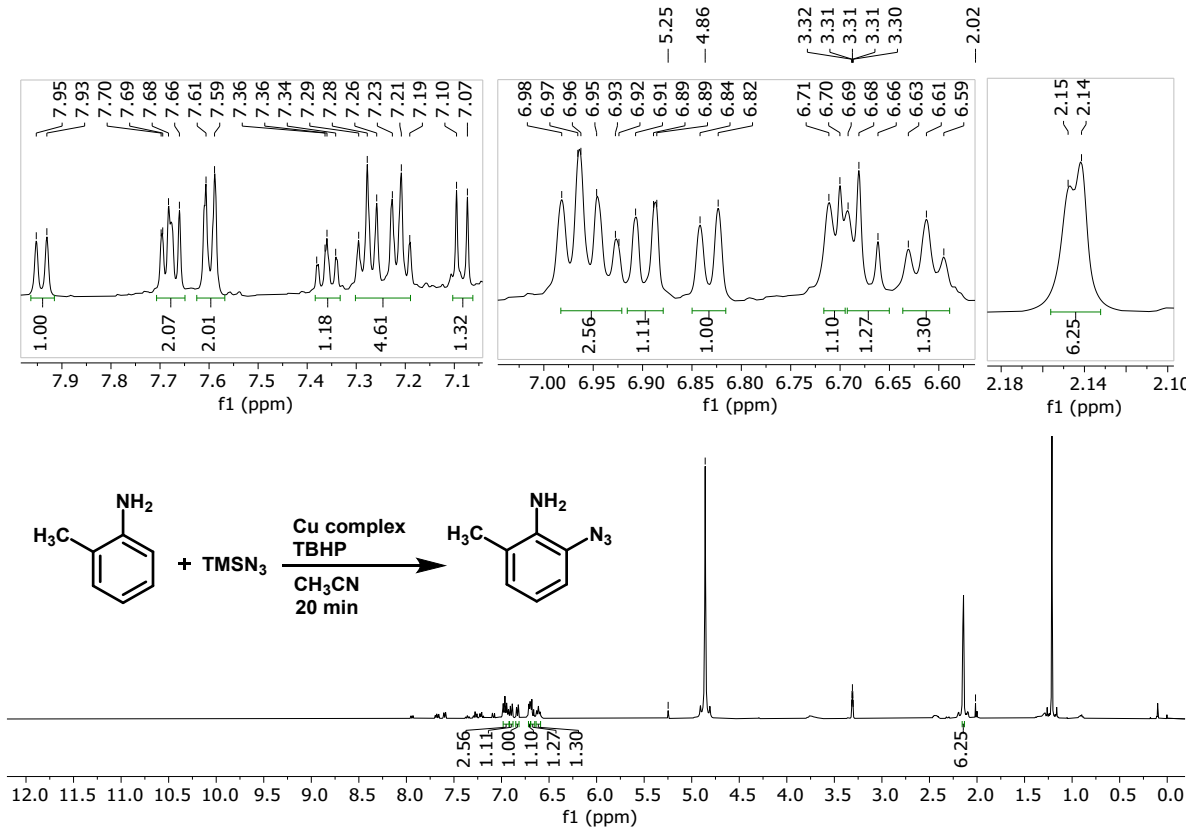


Fig S137. NMR spectrum of the crude mixture at 20 min

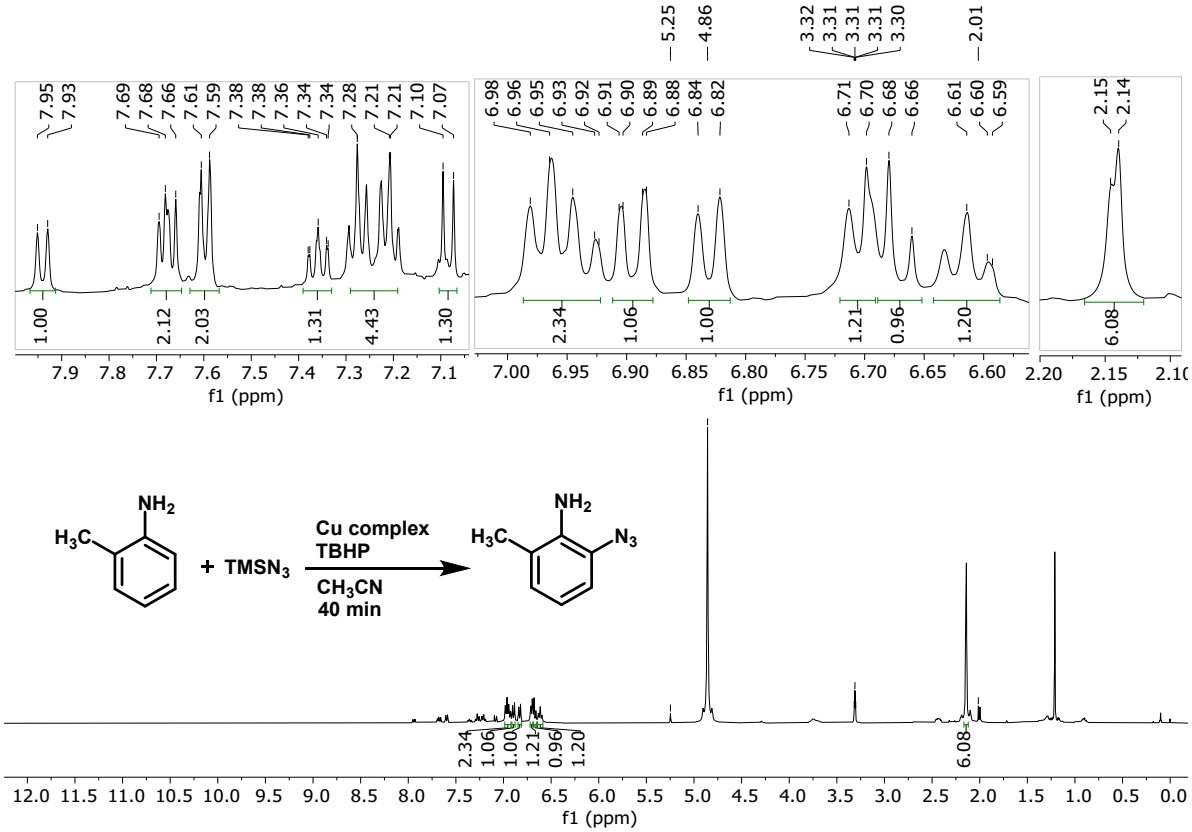


Fig S138. NMR spectrum of the crude mixture at 40 min

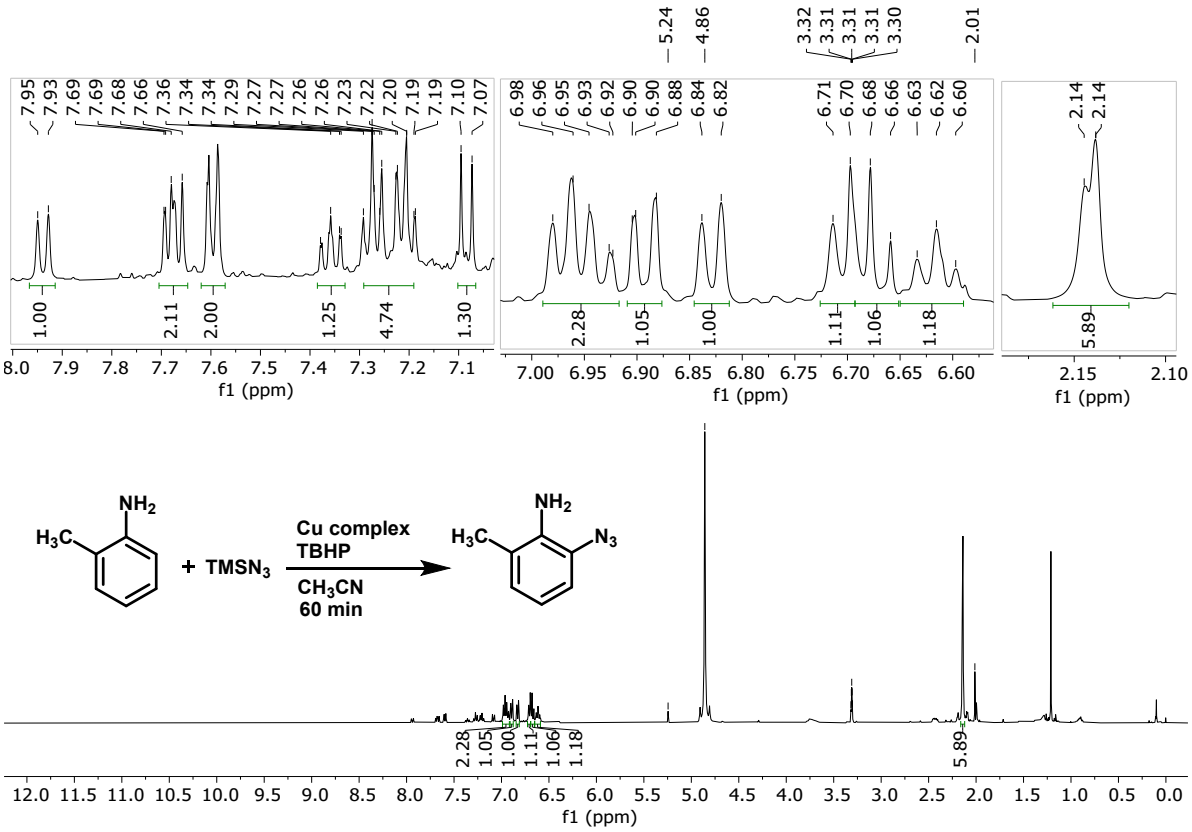


Fig S139. NMR spectrum of the crude mixture at 60 min

Table S5 Grid box parameters for the docking study

Parameters	Values
receptor	7tll.pdbqt
exhaustiveness	8
center_x	14.4847
center_y	-0.2238
center_z	15.2147
size_x	62.6546332169
size_y	65.171065979
size_z	39.70264884

Table S6 Results of molecular docking of triazoles against SARS-CoV-2 Omicron P132H

Compound	Binding energy (kcal/mol)	Interacting amino acids
3a	-7.0	HIS41, MET165, LEU167, GLU166, PRO168, THR190, GLN192, GLN189, ARG188, ASP187, HIS164
3b	-7.2	THR190, GLN189, GLN192, ARG188, ASP187, HIS164, HIS41, MET165, LEU167, GLU166, PRO168
3c	-6.9	ASP164, THR190, GLN192, LEU167, GLU166, PRO168, ARG188, MET165, GLN189, HIS41
3d	-7.2	HIS41, MET165, LEU167, GLU166, PRO168, GLN192, THR190, ARG188, GLN189, ASP187, HIS164
3e	-7.4	HIS41, MET165, ASP187, GLU166, LEU167, PRO168, GLN192, THR190, ARG188, GLN189, HIS 164
3f	-7.4	HIS41, MET165, GLU166, LEU167, PRO168, ALA191, THR190, GLN192, ARG188, GLN189, ASP187, HIS164
3g	-7.2	HIS41, MET165, GLN189, PRO168, GLU166, LEU167, THR190, GLN192, ARG188, ASP187, HIS164
3h	-7.4	GLY109, GLN110, ASN151, ASP295, THR292, ILE249, PRO293, VAL202, HIS246
3i	-7.1	HIS41, ASP187, HIS164, GLU166, LEU167, PRO168, THR190, GLN192, GLN189, ARG188, MET165
3j	-7.2	HIS41, MET165, GLN189, PRO168, GLU166, THR190, LEU167, ARG188, GLN192, ASP187, HIS164
3k	-7.2	HIS41, GLU166, GLN189, MET49, MET165, LEU167, ALA191, PRO168, THR190, ARG188, GLN192
3l	-6.9	HIS 41, THR190, GLN192, GLN189, ARG188, MET165, ASP187, HIS164, GLU166, LEU167, PRO168
3m	-6.9	HIS41, MET165, MET49, CYS145, HIS172, HIS163, LEU141, SER144, PHE140, HIS164, GLU166, GLN189
3n	-7.5	GLN189, MET165, LEU27, THR25, GLY143, SER144, CYS145, HIS163, HIS164, HIS41, ARG188
3o	-7.6	HIS41, MET165, LEU167, GLU166, PRO168, ALA191, THR190, GLN189, GLN192, ARG188, ASP187, HIS164
3p	-6.9	THR292, PRO293, ILE249, VAL202, GLY109, HIS246, ILE200, GLU240, PRO108
3q	-7.1	HIS41, MET165, ASP187, GLN189, ARG188, GLN192, THR190, HIS164, GLU166, LEU167, PRO168
3r	-7.1	HIS41, ASP187, MET165, ARG188, GLN189, GLN192, THR190,

		PRO168, GLU166, LEU167, HIS164
3s	-7.1	HIS41, MET165, GLN189, PRO168, HIS164, ASP187, ARG188, GLN192, THR190, LEU167
3t	-7.2	HIS41, HIS164, ASP187, ARG188, MET165, THR190, GLN192, GLN189, PRO168, GLU166, LEU167
3u	-7.4	HIS41, MET165, GLN189, PRO168, HIS164, ASP187, ARG188, GLN192, THR190, GLU166, LEU167

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