Supporting Information

Regioselective One-pot Synthesis of 1,4-Disubstituted 1,2,3-Triazoles Over Ag-Zn-based Nanoheterostructured Catalysts

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1. Single Crystal XRD Studies:

We have developed single crystals for **4af** (**Table 3**, main manuscript) and analyses clearly suggests discrete formation of the molecules.

The single crystal data collections were carried out using a Bruker D-8 Quest diffractometer with a photon detector (Mo Kα: 0.71073 Å, monochromator: graphite). Frames were collected at room temperature by ω, φ, and 2θ rotation at 3 s per frame. The SAINT software was used to integrate the measured intensities. Structure solution, refinement, and data output were carried out using the inbuilt SHELXTL-2018 program. Non-hydrogen atoms were refined anisotropically. C–H hydrogen atoms were placed in geometrically calculated positions by using a riding model. Images were created by using the ORTEP program.

The thin needle like crystals of **4af** crystallized in the monoclinic system with the space group *P21*. The crystals contain one molecule in each of its asymmetric unit (**Figure S1**). All crystallographic details are listed in **Table S1**.

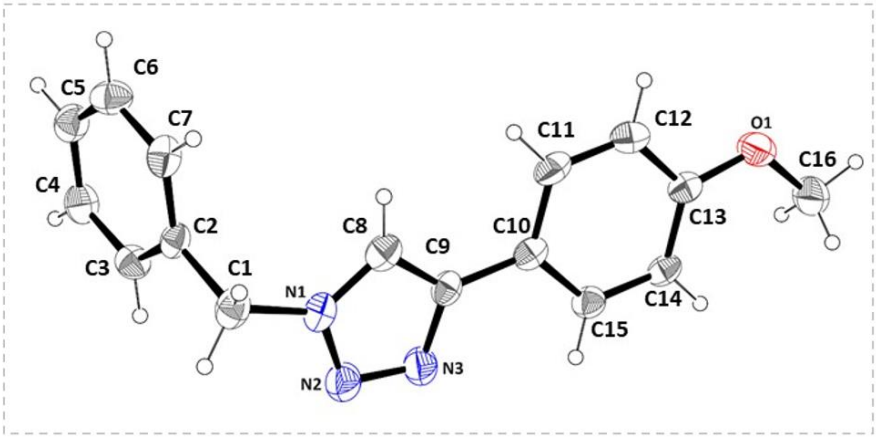

Fig. S1: X-ray structure (ORTEP view) of 1,2,3-triazole compound **4af** (**Table 3**, main manuscript).

Table S1: Crystallographic parameters

CCDC	2308691
Molecular formula	$C_{16}H_{15}N_3O$
Molecular weight	265.32
Crystal system	Monoclinic
Space group	$P2_1$
Temperature (K)	296 (2)

a (Å)	8.1513(8)
b (Å)	5.6813(6)
c (Å)	14.7970(15)
α (°)	90
β (°)	93.787(3)
γ (°)	90
V ($Å^3$)	683.75(12)
Z	2
D_{calc} (g cm^{-3})	1.289
μ (mm^{-1})	0.083
Total collected reflections	11528
Unique reflections	1275
Observed reflections	1539
R_{int}	0.0435
R_1(obs)	0.0492
wR_1(obs)	0.1057
R_2(all)	0.0666
wR_2(all)	0.1202

Table S2: Ag and Zn content of Ag_2O-ZnO before and after reaction

Metal	**Measured loading before reaction (mol%)[a]**	**Measured loading after 8th cycle of reaction (mol%)[a]**
Ag	2.162	2.154
Zn	12.88	12.82

[a]mol% of metal present in 20 mg of the catalyst

Table S3: Comparison of the current work with some earlier nanomaterials catalysed AAC reactions.

Catalyst	Solvent	Temperature	Yield (%)	No. of substrates	*Ref.*
Cu NPs/C	H_2O	100 °C	89	20	**A**
Cu NPs/C	H_2O	70 °C	99	13	**B**
Cu_2O/CPG	H_2O	100 °C	98	17	**C**
Ag_2O NPs	Toluene	20 °C	90	8	**D**
Ag NPs-Al_2O_3@Fe_2O_3	H_2O	RT	96	6	**E**
Ag NPs-graphene	H_2O	RT	96	13	**F**
Au NPs/TiO_2	MeCN:H_2O (1:1)	150 °C MW 30W	79	10	**G**
Ni-rGO-zeolite NCs	H_2O	90 °C	94	17	**H**
$ZnC_2O_4.2H_2O$ NCs	H_2O:EG (10:1)	60 °C	99	25	**I**
Ag_2O-ZnO	**H_2O:EG (1:1)**	**RT**	**98**	**48**	**This work**

CPG; Controlled Pore Glass, rGO; reduced graphene oxide, NCs; Nanocrystals, NPs; nanoparticles.

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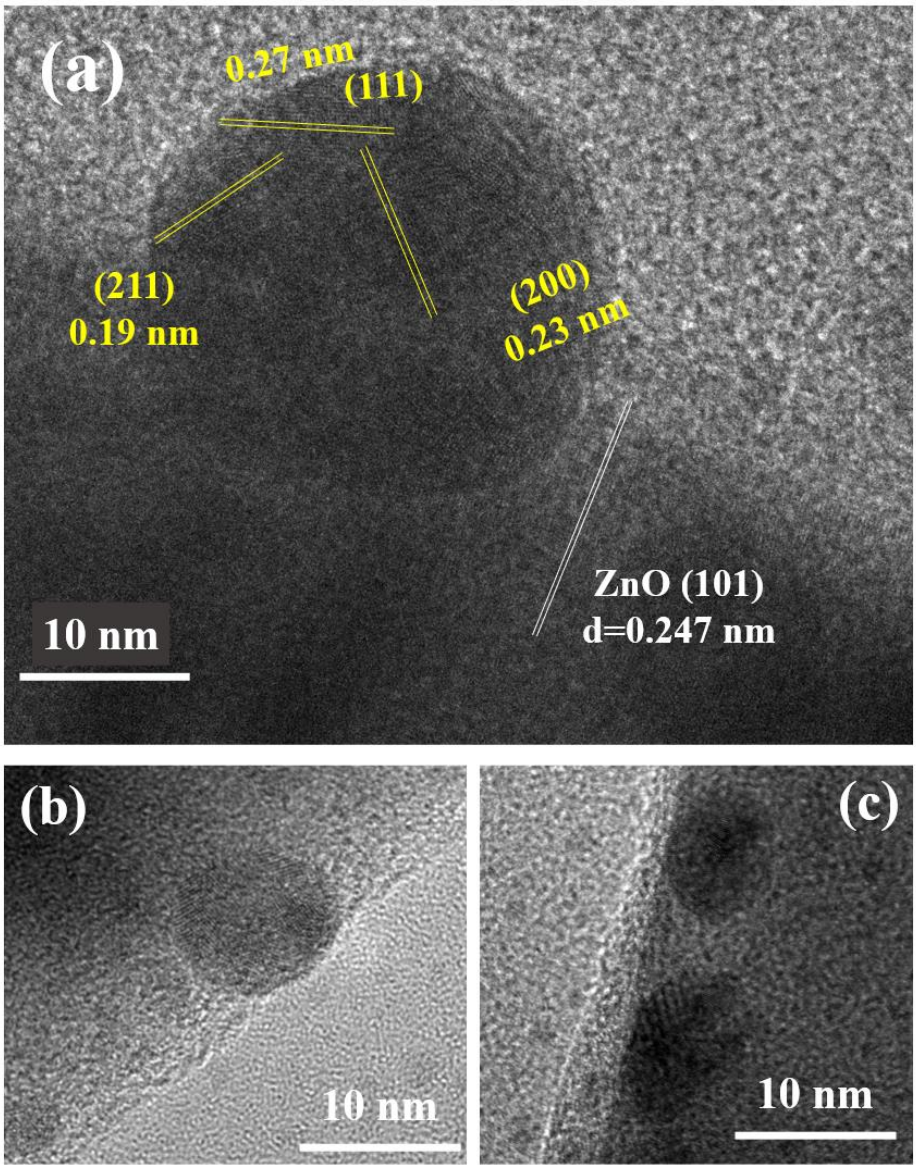
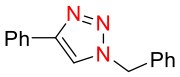


Fig. S2: (a-c) High resolution transmission electron microscope (HRTEM) image of as-synthesized Ag_2O-ZnO nanocomposites.

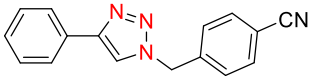
Analytical data of 1,2,3-triazole derivatives:

1-Benzyl-4-phenyl-1H-1,2,3-triazole (4aa)



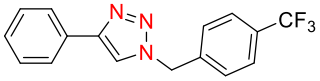
95% yield; white solid; mp 129-130 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.1 Hz, 2H), 7.69 (s, 1H), 7.42 (dt, *J* = 11.2, 8.1 Hz, 5H), 7.35 (t, *J* = 6.5 Hz, 3H), 5.61 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.9, 135.3, 131.2, 129.8, 129.4, 128.81, 128.7, 126.3, 120.1, 54.9; LCMS (ESI) m/z calcd for $C_{15}H_{14}N_3$ ($[M+H]^+$) 236.11, found 236.11.

4-((4-phenyl-1H-1,2,3-triazol-1-yl)methyl)benzonitrile (4ba)



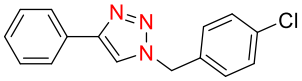
94% yield; colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.7 Hz, 2H), 7.66 (s, 1H), 7.60 (d, *J* = 8.1 Hz, 2H), 7.30 (ddt, *J* = 23.0, 14.8, 7.4 Hz, 5H), 5.57 (s, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.6, 142.9, 135.9, 133.1, 131.9, 131.5, 131.4, 128.8, 122.7, 121.1, 115.8, 56.5; LCMS (ESI) m/z calcd for $C_{16}H_{13}N_4$ ($[M+H]^+$) 261.11, found 261.14.

4-phenyl-1-(4-(trifluoromethyl)benzyl)-1H-1,2,3-triazole (4ca)



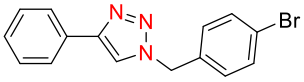
93% yield; white solid; mp 118-120 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.7 Hz, 2H), 7.63 (s, 1H), 7.58 (d, *J* = 7.9 Hz, 2H), 7.39 – 7.30 (m, 4H), 7.26 (t, *J* = 7.3 Hz, 1H), 5.58 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.6, 138.7, 131.5-130.7 (q, J=32.5 Hz), 130.3, 128.9, 128.4, 128.2, 126.1 (q, J=3.75 Hz), 125.8, 124.8, 122.7, 119.5, 53.6; ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.91; LCMS (ESI) m/z calcd for $C_{16}H_{13}F_3N_3$ ($[M+H]^+$) 304.10, found 304.12.

1-(4-chlorobenzyl)-4-phenyl-1H-1,2,3-triazole (4da)



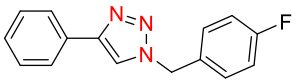
87% yield; white solid; mp 150-152 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.8 Hz, 2H), 7.74 (s, 1H), 7.47 – 7.37 (m, 5H), 7.01 (d, *J* = 8.3 Hz, 2H), 5.51 (s, 2H); LCMS (ESI) m/z calcd for $C_{15}H_{12}ClN_3Na$ ($[M+Na]^+$) 292.07, found 292.10.

1-(4-bromobenzyl)-4-phenyl-1H-1,2,3-triazole (4ea)



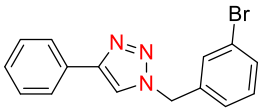
88% yield; pale yellow solid; mp 149-151 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (d, *J* = 9.4 Hz, 2H), 7.75 (s, 1H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.43 (dd, *J* = 14.2, 7.9 Hz, 5H), 5.54 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 132.2, 131.9, 130.2, 129.5, 128.9, 128.7, 128.2, 126.6, 125.6, 122.8, 122.2, 119.3, 66.5; LCMS (ESI) m/z calcd for $C_{15}H_{12}BrN_3Na$ ($[M+Na]^+$) 336.02, found 336.02.

1-(4-fluorobenzyl)-4-phenyl-1H-1,2,3-triazole (4fa)



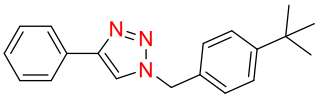
86% yield; yellow solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (d, 2H), 7.73 (s, 1H), 7.30 – 7.44 (m, 5H), 7.10 (t, 2H), 5.55 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.9 (d, *J* = 248.3 Hz), 130.5 (d, *J* = 3.1 Hz), 130.4, 130.0 (d, *J* = 8.3 Hz), 128.9, 128.3, 125.7, 116.3, 116.1, 53.5; ^{19}F NMR (471 MHz, $CDCl_3$) δ -112.57; LCMS (ESI) m/z calcd for $C_{15}H_{12}FN_3Na$ ($[M+Na]^+$) 276.01, found 276.03.

1-(3-bromobenzyl)-4-phenyl-1H-1,2,3-triazole (4ha)



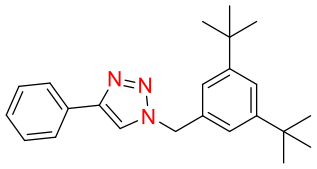
72% yield; yellow solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (t, 3H), 7.53 – 7.45 (m, 2H), 7.42 (s, 1H), 7.43 (s, 1H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.22 (d, *J* = 8.9 Hz, 2H), 5.54 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 136.9, 131.9, 131.1, 130.7, 130.4, 129.0, 128.4, 126.6, 125.7, 123.1, 53.6; LCMS (ESI) m/z calcd for $C_{15}H_{13}BrN_3$ ($[M+H]^+$) 314.02, found 314.03.

1-(4-(tert-butyl)benzyl)-4-phenyl-1H-1,2,3-triazole (**4ia**)



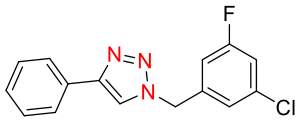
80% yield; white solid; mp 114-115 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.1 Hz, 2H), 7.64 (s, 1H), 7.37 (t, *J* = 7.7 Hz, 3H), 7.29 (d, *J* = 7.6 Hz, 2H), 7.24 (d, 2H), 5.51 (s, 2H), 1.30 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.0, 148.2, 131.7, 130.7, 128.9, 128.2, 128.0, 127.5, 126.2, 125.8, 125.6, 119.6, 54.03; LCMS (ESI) m/z calcd for $C_{19}H_{22}N_3$ ($[M+H]^+$) 292.17, found 292.13.

1-(3,5-di-tert-butylbenzyl)-4-phenyl-1H-1,2,3-triazole (**4ja**)



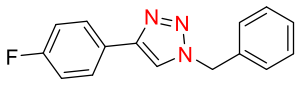
71% yield; white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (d, *J* = 7.6 Hz, 2H), 7.58 (s, 1H), 7.32 (t, *J* = 8.0 Hz, 4H), 7.23 (t, *J* = 7.1 Hz, 1H), 7.17 (s, 1H), 5.47 (s, 2H), 1.24 (s, 10H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.9, 148.2, 131.7, 130.6, 128.8, 128.1, 127.9, 126.1, 125.7, 119.5, 53.9, 34.7, 31.3; LCMS (ESI) m/z calcd for $C_{23}H_{30}N_3$ ($[M+H]^+$) 348.24, found 348.28.

1-(3-chloro-5-fluorobenzyl)-4-phenyl-1H-1,2,3-triazole (**4ka**)



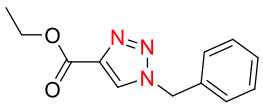
50% yield; light brown solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.6 Hz, 2H), 7.77 (s, 1H), 7.44 (t, *J* = 7.4 Hz, 2H), 7.36 (t, *J* = 7.3 Hz, 1H), 7.11 (s, 2H), 6.92 (d, *J* = 8.3 Hz, 1H), 5.56 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.8 (d, *J* =251.7 Hz), 148.6, 138.3 (d, *J* = 8.2 Hz), 135.9 (d, *J* = 10.6 Hz), 130.2, 128.9, 128.5, 125.8, 123.9, 123.8, 119.7, 116.7 (d, *J* = 24.5 Hz), 113.5 (d, *J* = 22.4 Hz), 53.0; ^{19}F NMR (470 MHz, $CDCl_3$) δ -109.06; LCMS (ESI) m/z calcd for $C_{15}H_{11}ClFN_3Na$ ($[M+Na]^+$) 310.06, found 310.08.

1-benzyl-4-(4-fluorophenyl)-1H-1,2,3-triazole (**4ab**)



98% yield; white solid; mp 110-111 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (dd, *J* = 8.6, 5.4 Hz, 2H), 7.66 (s, 1H), 7.40 (q, *J* = 5.8 Hz, 3H), 7.36 – 7.29 (m, 2H), 7.09 (d, *J* = 8.6 Hz, 2H), 5.58 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.7 (d, *J* = 247.2 Hz), 134.6, 129.2, 128.9, 128.1, 127.4 (d, *J* = 8.2 Hz), 126.8 (d, *J* = 3.3 Hz), 119.3,115.8 (d, *J* = 21.8 Hz), 54.3; LCMS (ESI) m/z calcd for $C_{15}H_{13}FN_3$ ($[M+H]^+$) 254.10, found 254.19.

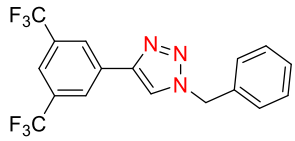
Ethyl 1-benzyl-1H-1,2,3-triazole-4-carboxylate (**4ac**)



88% yield; Pale white solid; mp 64-65 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.35 (dd, *J* = 5.1, 1.9 Hz, 3H), 7.30 – 7.21 (m, 2H), 5.54 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.6, 140.5, 133.6, 129.2,

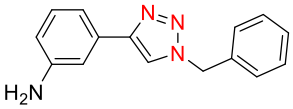
129.1, 128.2, 127.2, 61.2, 54.4, 14.2; LCMS (ESI) m/z calcd for $C_{12}H_{13}N_3O_2Na$ ($[M+Na]^+$) 254.10, found 254.10.

1-benzyl-4-(3,5-bis(trifluoromethyl)phenyl)-1H-1,2,3-triazole (**4ad**)



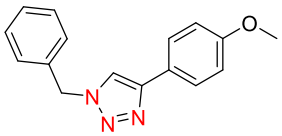
86% yield; White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.17 (s, 2H), 7.73 (d, *J* = 11.1 Hz, 2H), 7.36 – 7.29 (m, 3H), 7.25 (dd, *J* = 7.4, 1.9 Hz, 2H), 5.53 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.5, 134.1, 132.7, 132.6-132.8 (q, *J* = 33.5 Hz), 131.8, 129.3 (q, *J* = 270 Hz) , 129.1, 128.2, 125.6, 125.6, 124.3, 122.1, 121.6-121.5 (dt, *J* = 7.4, 3.7 Hz), 120.5, 54.5; ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.80; LCMS (ESI) m/z calcd for $C_{17}H_{12}F_6N_3$ ($[M+H]^+$) 372.09, found 372.11.

3-(1-benzyl-1H-1,2,3-triazol-4-yl)aniline (**4ae**)



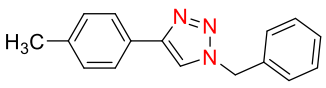
92% yield; Pale brown solid; mp 146-148 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (s, 1H), 7.40 (d, *J* = 6.8 Hz, 3H), 7.35 – 7.29 (m, 4H), 7.24 (d, *J* = 7.2 Hz, 1H), 7.19 (t, *J* = 7.7 Hz, 1H), 7.15 (d, *J* = 7.6 Hz, 1H), 5.57 (s, 2H), 4.55 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 135.5, 132.2, 132.1, 132.0, 130.5, 129.8, 129.4, 128.7, 120.6, 116.5, 115.7, 115.3, 112.9, 112.2, 54.8; LCMS (ESI) m/z calcd for $C_{15}H_{14}N_4Na$ ($[M+Na]^+$) 273.12, found 273.11.

1-benzyl-4-(4-methoxyphenyl)-1H-1,2,3-triazole (**4af**)



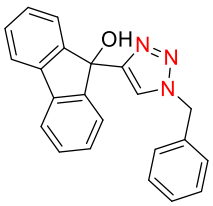
95% yield; White solid; mp 141-143 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 – 7.75 (m, 2H), 7.64 (s, 1H), 7.46 – 7.38 (m, 3H), 7.35 (dd, *J* = 7.6, 1.7 Hz, 2H), 7.01 – 6.94 (m, 2H), 5.60 (s, 2H), 3.87 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.7, 148.2, 134.9, 129.3, 128.9, 128.2, 127.1, 123.4, 118.9, 114.3, 55.4, 54.3; LCMS (ESI) m/z calcd for $C_{16}H_{16}N_3O$ ($[M+H]^+$) 265.12, found 265.14.

1-benzyl-4-(p-tolyl)-1H-1,2,3-triazole (**4ag**)



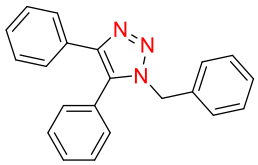
95% yield; Pale yellow solid; mp 151-153 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.1 Hz, 2H), 7.66 (s, 1H), 7.45 – 7.29 (m, 5H), 7.23 (d, *J* = 8.1 Hz, 2H), 5.59 (s, 2H), 2.39 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.3, 139.3, 138.1, 134.7, 129.5, 129.2, 128.9, 128.8, 128.1, 127.6, 127.2, 125.6, 119.2, 54.2, 21.3; LCMS (ESI) m/z calcd for $C_{16}H_{16}N_3$ ($[M+H]^+$) 250.13, found 250.11.

9-(1-benzyl-1H-1,2,3-triazol-4-yl)-9H-fluoren-9-ol (**4ak**)



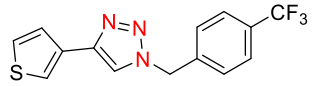
76% yield; Light orange solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.56 (s, 1H), 8.36 (s, 1H), 7.82 (d, *J* = 7.1 Hz, 2H), 7.59 (d, *J* = 6.9 Hz, 3H), 7.37 (dt, *J* = 43.4, 6.7 Hz, 5H), 7.10 (d, *J* = 7.8 Hz, 1H), 6.97 (t, *J* = 7.0 Hz, 1H), 6.47 (s, 1H), 3.37 (s, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 149.8, 149.6, 149.5, 139.6, 130.4, 129.3, 128.4, 125.6, 125.4, 120.6, 120.0, 117.5, 115.1, 78.6; LCMS (ESI) m/z calcd for $C_{22}H_{17}N_3ONa$ ($[M+Na]^+$) 362.14, found 362.13.

1-benzyl-4,5-diphenyl-1H-1,2,3-triazole (**4al**)



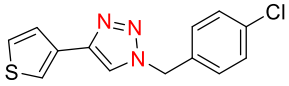
45% yield; Dark brown solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.3 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.27 (dd, *J* = 8.7, 4.5 Hz, 6H), 7.16 (d, *J* = 7.4 Hz, 2H), 7.08 – 7.00 (m, 2H), 5.42 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.5, 134.4, 134.2, 132.9, 130.6, 129.9, 129.1, 128.7, 128.2, 127.7, 127.6, 127.5, 127.4, 127.2, 126.8, 126.7, 126.7, 126.5, 126.2, 125.7, 51.0; LCMS (ESI) m/z calcd for $C_{21}H_{18}N_3$ ($[M+Na]^+$) 312.14, found 312.19.

4-(thiophen-3-yl)-1-(4-(trifluoromethyl)benzyl)-1H-1,2,3-triazole (**4ci**)



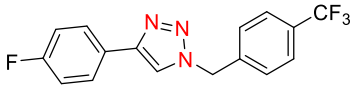
98% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 – 7.55 (m, 3H), 7.53 (s, 1H), 7.39 – 7.27 (m, 4H), 5.57 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.7, 138.6, 131.5–131.2 (q, *J* = 32.8 Hz), 131.0, 128.2, 126.5, 126.2–126.1 (q, *J* = 3.8 Hz), 125.7, 121.4, 119.3, 53.5; LCMS (ESI) m/z calcd for $C_{14}H_{11}F_3N_3S$ ($[M+H]^+$) 310.05, found 310.05.

1-(4-chlorobenzyl)-4-(thiophen-3-yl)-1H-1,2,3-triazole (**4di**)



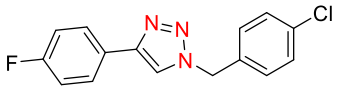
83% yield; Brown solid; mp 179-181 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 2.9, 1.1 Hz, 1H), 7.62 (s, 1H), 7.44 (dd, *J* = 5.0, 1.1 Hz, 1H), 7.40 – 7.35 (m, 3H), 7.25 (d, *J* = 8.4 Hz, 2H), 5.54 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.8, 135.0, 133.4, 131.9, 129.6, 126.7, 126.0, 121.5, 119.6, 53.7; LCMS (ESI) m/z calcd for $C_{13}H_{11}ClN_3S$ ($[M+H]^+$) 276.03, found 276.04.

4-(4-fluorophenyl)-1-(4-(trifluoromethyl)benzyl)-1H-1,2,3-triazole (**4cb**)



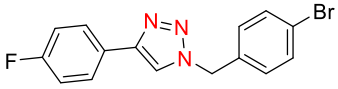
90% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (dd, *J* = 8.3, 5.5 Hz, 2H), 7.68 (d, *J* = 8.1 Hz, 3H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.13 (t, *J* = 8.6 Hz, 2H), 5.67 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.6 – 162.0 (d, *J* = 247.7 Hz), 147.7, 138.5, 131.3– 131.0 (d, *J* = 32.7 Hz), 128.2, 127.5 – 127.5 (d, *J* = 8.1 Hz), 126.5, 126.5, 126.2 –126.1 (q, *J* = 3.6 Hz), 124.6 –122.9 (q, *J* = 272.1 Hz), 119.3, 115.9 –115.8 (d, *J* = 21.8 Hz), 53.6; LCMS (ESI) m/z calcd for $C_{16}H_{12}F_4N_3$ ($[M+H]^+$) 322.09, found 322.10.

1-(4-chlorobenzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (**4db**)



81% yield; White solid; mp 106-108 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (dd, *J* = 8.6, 5.3 Hz, 2H), 7.66 (s, 1H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.28 (t, *J* = 8.3 Hz, 2H), 7.11 (t, *J* = 8.6 Hz, 2H), 5.56 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.6 (d, *J* = 247.8 Hz), 147.6, 135.0, 133.2, 129.5, 127.6 (d, *J* = 7.9 Hz), 126.7 (d, *J* = 2.7 Hz), 119.3, 116.0 (d, *J* = 21.7 Hz), 53.6; LCMS (ESI) m/z calcd for $C_{15}H_{12}ClFN_3$ ($[M+H]^+$) 288.06, found 288.07.

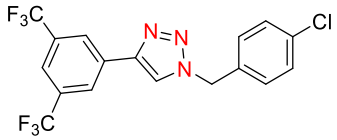
1-(4-bromobenzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (**4eb**)



85% yield; Pale yellow solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (dd, *J* = 7.9, 5.6 Hz, 2H), 7.61 (s, 1H), 7.49 (d, *J* = 8.2 Hz, 2H),

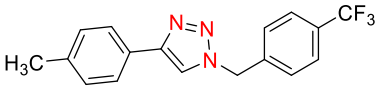
7.16 (d, *J* = 8.1 Hz, 2H), 7.07 (t, *J* = 8.3 Hz, 2H), 5.50 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.8 (d, *J* = 247.2 Hz), 147.6, 135.3, 133.7, 132.4, 129.8, 127.6 (d, *J* = 8.4 Hz), 126.7 (d, *J* = 3.3 Hz), 125.1, 123.1, 119.3, 115.9 (d, *J* = 21.7 Hz), 53.6; LCMS (ESI) m/z calcd for $C_{15}H_{12}BrFN_3$ ($[M+H]^+$) 332.01, found 332.10; ([M+2]) 333.01, found 333.07.

4-(3,5-bis(trifluoromethyl)phenyl)-1-(4-chlorobenzyl)-1H-1,2,3-triazole (**4dd**)



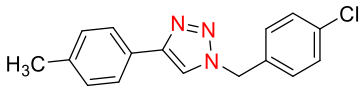
78% yield; colourless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 (s, 2H), 7.98 (s, 1H), 7.79 (s, 1H), 7.36 – 7.22 (m, 4H), 5.58 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.9, 135.5, 133.2, 133.0, 132.99–132.2 (q, *J* = 33.5 Hz), 129.9, 129.8, [(126.86,124.69,122.52,120.35) (q, *J* = 271.25)], 126.0, 125.9, 122.0 –121.9 (dt, *J* = 7.4, 3.7 Hz), 121.3, 54.1; ^{19}F NMR (470 MHz, $CDCl_3$) δ -63.10; LCMS (ESI) m/z calcd for $C_{17}H_{11}ClF_6N_3$ ($[M+H]^+$) 406.05, found 406.05.

4-(p-tolyl)-1-(4-(trifluoromethyl)benzyl)-1H-1,2,3-triazole (**4cg**)



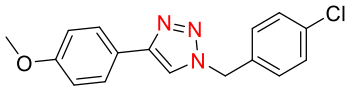
90% yield; Pale yellow solid; mp 151-153 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 – 7.64 (m, 5H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 5.66 (s, 2H), 2.40 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.7, 138.8, 138.3, 131.4 – 130.8 (q, *J* = 32.6, 32.1 Hz), 129.6, 128.3, 127.5, 126.2 –126.2 (q, *J* = 3.6 Hz), 125.7, 124.8 –122.9 (q, *J* = 271.7 Hz), 119.3, 53.6, 21.4; LCMS (ESI) m/z calcd for $C_{17}H_{15}F_3N_3$ ($[M+H]^+$) 318.11, found 318.12.

1-(4-chlorobenzyl)-4-(p-tolyl)-1H-1,2,3-triazole (**4dg**)



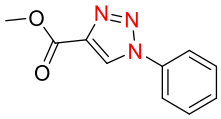
95% yield; Off white solid; mp 140-142 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.5 Hz, 2H), 7.65 (s, 1H), 7.39 (d, *J* = 7.6 Hz, 2H), 7.26 (dd, *J* = 18.1, 7.7 Hz, 4H), 5.56 (s, 2H), 2.39 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.5, 138.2, 134.9, 133.2, 129.6, 129.4, 127.5, 125.7, 119.2, 53.5, 21.3; LCMS (ESI) m/z calcd for $C_{16}H_{15}ClN_3$ ($[M+H]^+$) 284.09, found 284.11.

1-(4-chlorobenzyl)-4-(4-methoxyphenyl)-1H-1,2,3-triazole (**4df**)



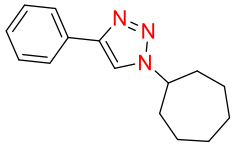
98% yield; White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.7 Hz, 2H), 7.61 (s, 1H), 7.39 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 6.97 (d, *J* = 8.7 Hz, 2H), 5.56 (s, 2H), 3.86 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.7, 134.8, 133.3, 129.4, 127.0, 126.9, 123.1, 120.1, 118.6, 114.2, 55.3; LCMS (ESI) m/z calcd for $C_{16}H_{15}ClN_3O$ ($[M+H]^+$) 300.08, found 300.07.

methyl 1-phenyl-1H-1,2,3-triazole-4-carboxylate (**7ac**)



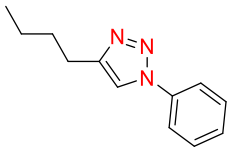
85% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.57 (s, 1H), 7.76 (d, *J* = 8.0 Hz, 2H), 7.54 (dt, *J* = 28.6, 7.4 Hz, 3H), 3.99 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.0, 140.3, 136.2, 130.0, 129.8, 126.1, 125.7, 120.8, 52.5; LCMS (ESI) m/z calcd for $C_{10}H_{10}N_3O_2$ ($[M+H]^+$) 203.07, found 203.08.

1-cycloheptyl-4-phenyl-1H-1,2,3-triazole (**7ce**)



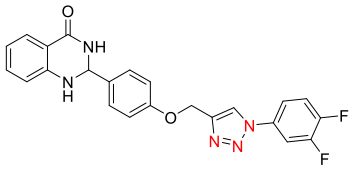
45% yield; Light green liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (s, 1H), 7.56 (d, *J* = 6.8 Hz, 2H), 7.43 – 7.33 (m, 3H), 2.64 (s, 1H), 1.28 (s, 10H), 0.94 – 0.87 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 132.5, 129.22, 128.5, 121.8, 63.7, 31.9, 29.7, 29.4, 22.7, 14.1; LCMS (ESI) m/z calcd for $C_{15}H_{20}N_3$ ($[M+H]^+$) 242.16, found 242.16.

4-butyl-1-phenyl-1H-1,2,3-triazole (**7af**)



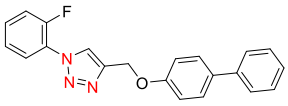
39% yield; Colourless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, *J* = 5.9 Hz, 3H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.35 (t, *J* = 7.9 Hz, 1H), 2.77 – 2.70 (m, 2H), 1.65 (d, *J* = 7.4 Hz, 2H), 1.36 (h, *J* = 7.4 Hz, 2H), 0.89 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.1, 137.2, 129.6, 128.3, 120.3, 118.7, 31.4, 25.2, 22.2, 13.7.

2-(4-((1-(3,4-difluorophenyl)-1H-1,2,3-triazol-4-yl)methoxy)phenyl)-2,3-dihydroquinazolin-4(1H)-one (**10b**)



49% yield; Dark brown solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.25 (d, *J* = 36.1 Hz, 1H), 8.13 (d, *J* = 34.8 Hz, 1H), 7.76 (d, *J* = 49.7 Hz, 2H), 7.55 (s, 4H), 7.12 – 6.81 (m, 5H), 6.78 – 6.60 (m, 2H), 5.88 (s, 2H); LCMS (ESI) m/z calcd for $C_{23}H_{18}F_2N_5O_2$ ($[M+H]^+$) 434.14, found 434.33 (Spectra given, **Figure S68**).

4-(([1,1'-biphenyl]-4-yloxy)methyl)-1-(2-fluorophenyl)-1H-1,2,3-triazole (**10c**)



31% yield; Off white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 (d, *J* = 2.2 Hz, 1H), 8.00 (t, *J* = 7.5 Hz, 1H), 7.65 – 7.54 (m, 4H), 7.45 (q, *J* = 7.8, 6.9 Hz, 3H), 7.34 (dq, *J* = 13.9, 8.1 Hz, 3H), 7.14 (d, *J* = 8.6 Hz, 2H), 5.38 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.7, 153.36 (d, *J* = 251.0 Hz), 144.6, 140.6, 134.4, 130.38 (d, *J* = 7.9 Hz), 128.8, 128.3, 127.2, 126.8, 126.8, 125.3, 125.3, 125.2, 125.2, 124.9, 124.16 (d, *J* = 8.3 Hz), 117.10 (d, *J* = 19.9 Hz), 115.1, 61.9; ^{19}F NMR (470 MHz, $CDCl_3$) δ -123.55; LCMS (ESI) m/z calcd for $C_{21}H_{17}FN_3O$ ($[M+H]^+$) 346.13, found 346.34. (Spectra given, **Figure S72**).

NMR spectra

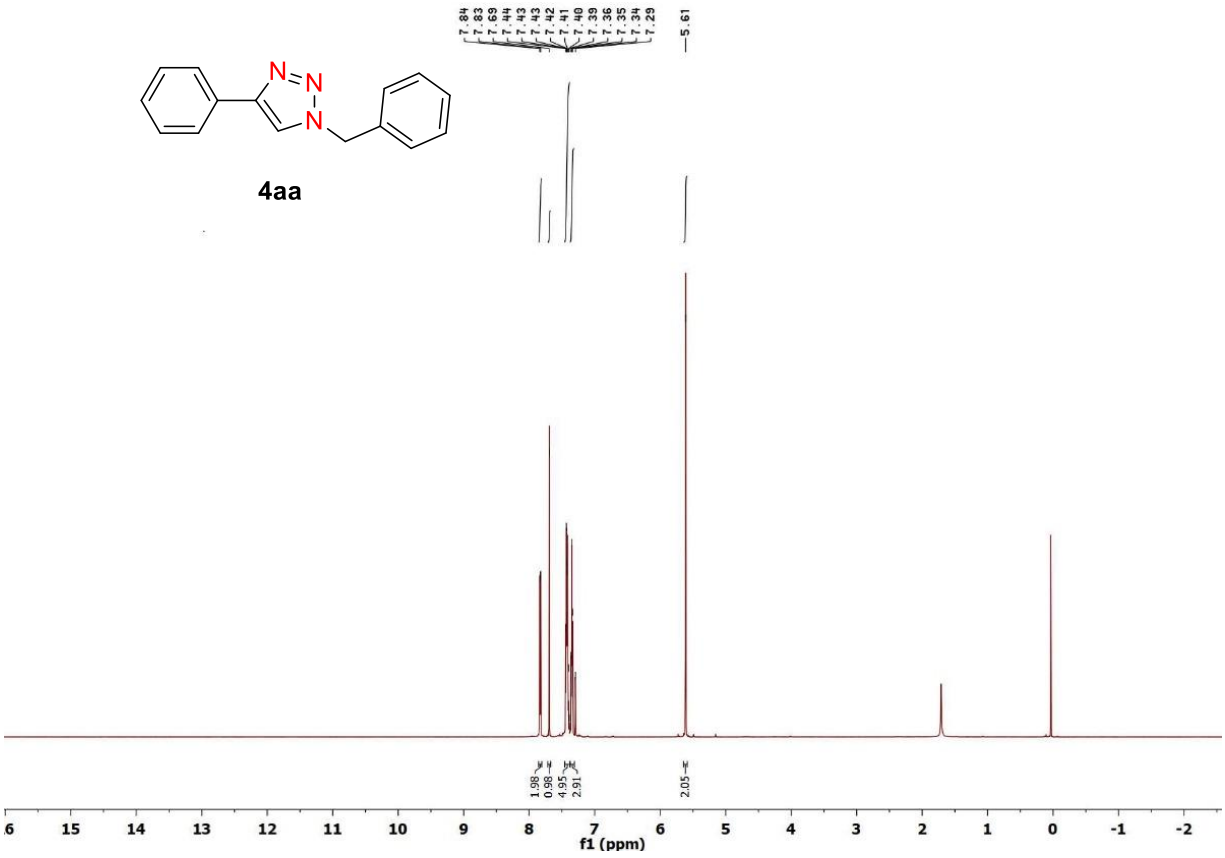


Fig. S3: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4aa**.

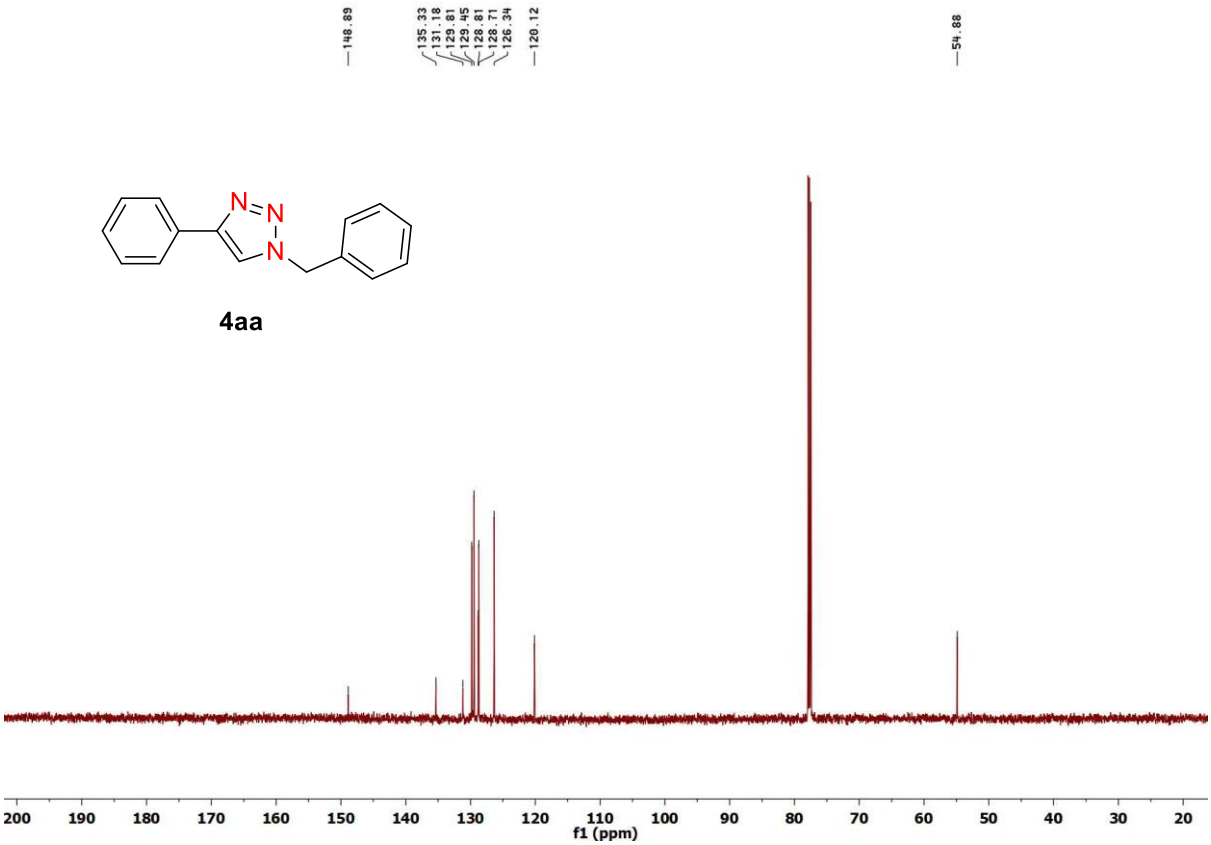


Fig. S4: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4aa**.

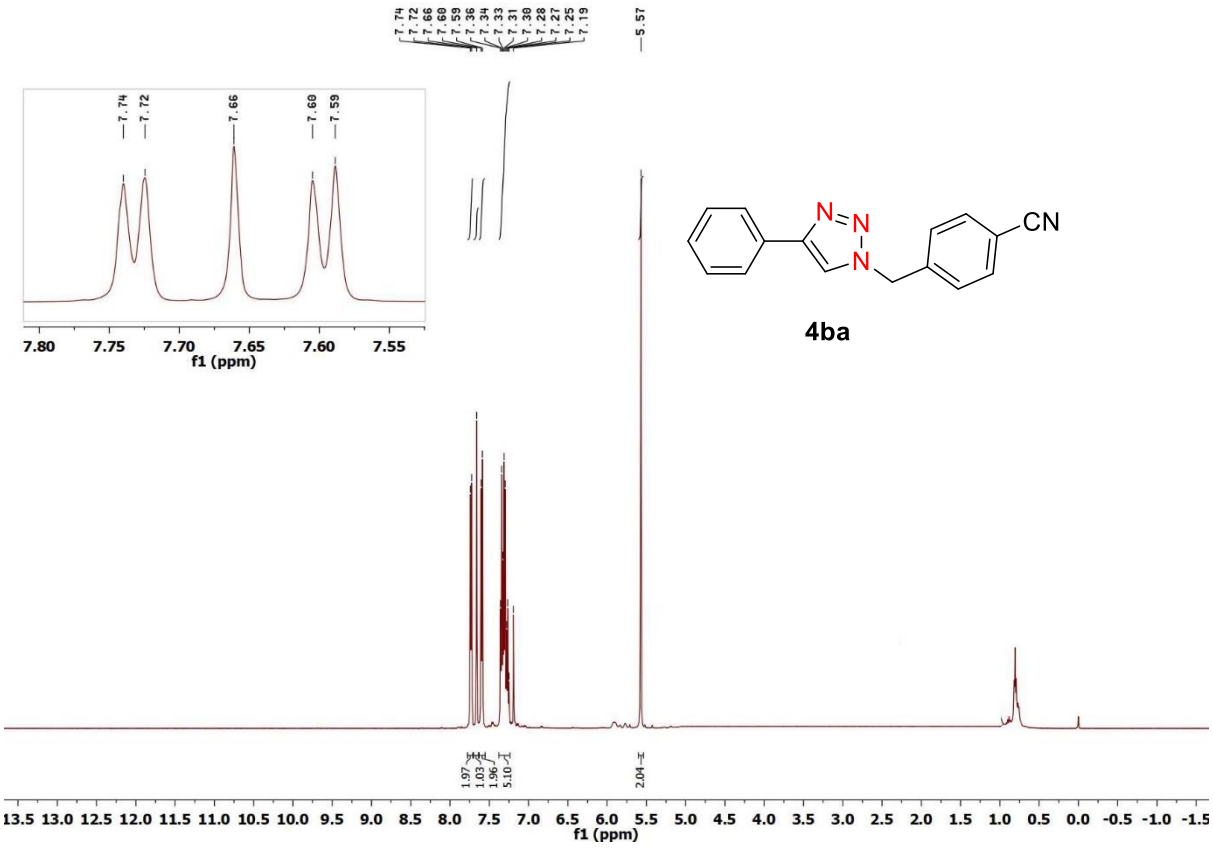


Fig. S5: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4ba**.

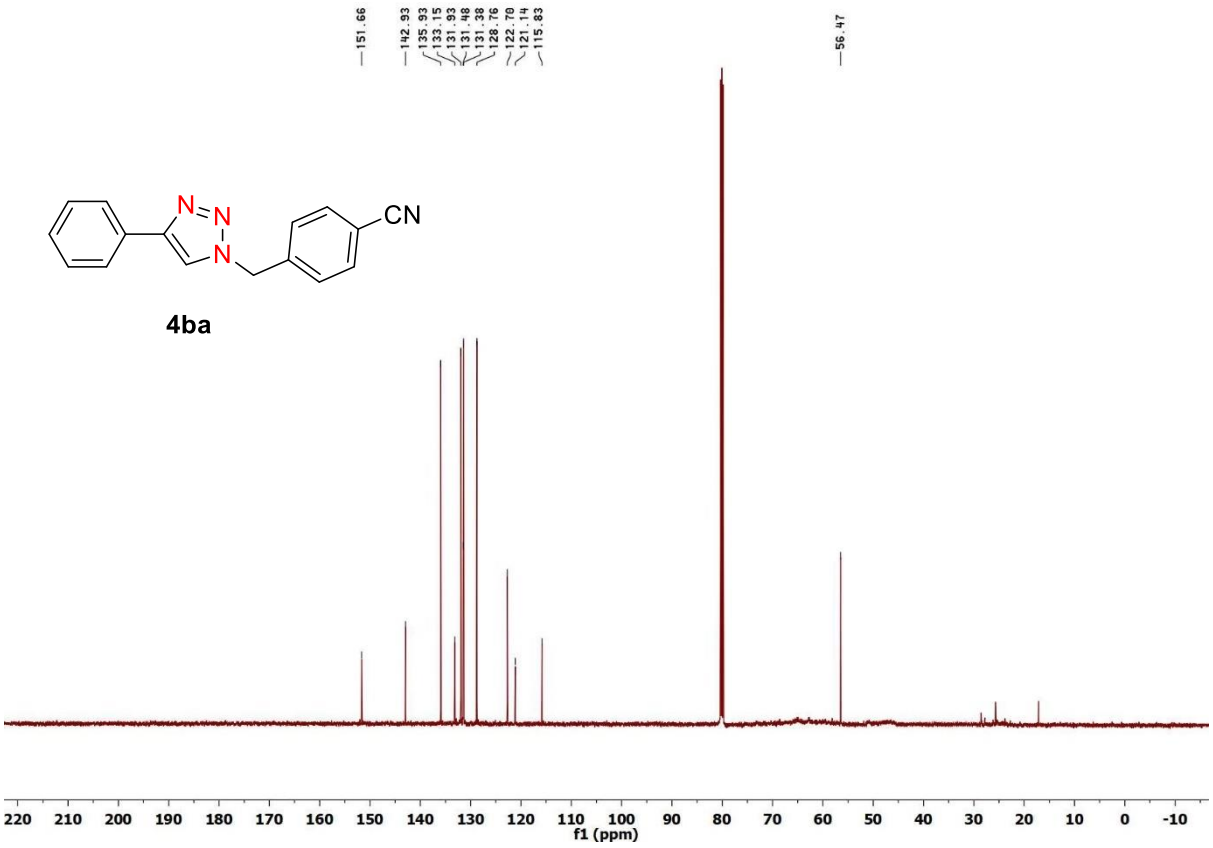


Fig. S6: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4ba**.

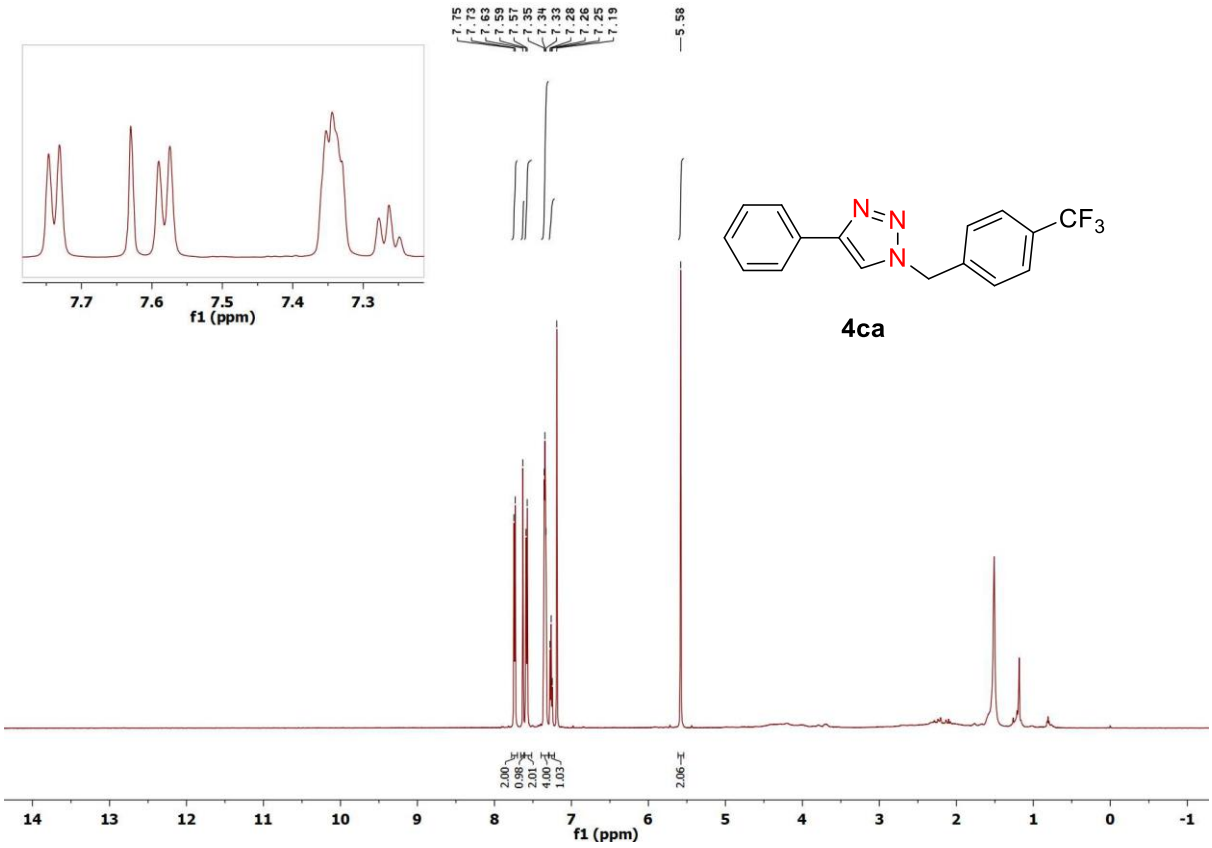


Fig. S7: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4ca**.

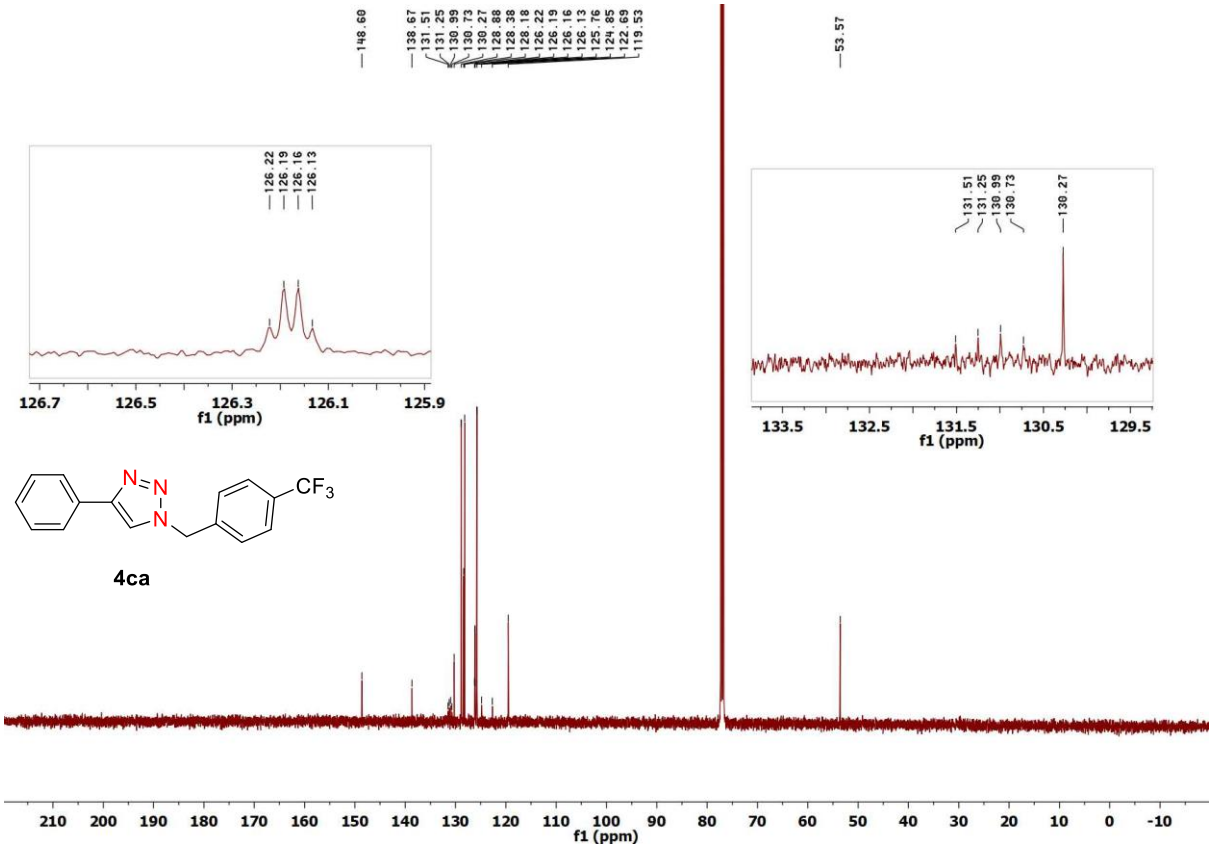


Fig. S8: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4ca**.

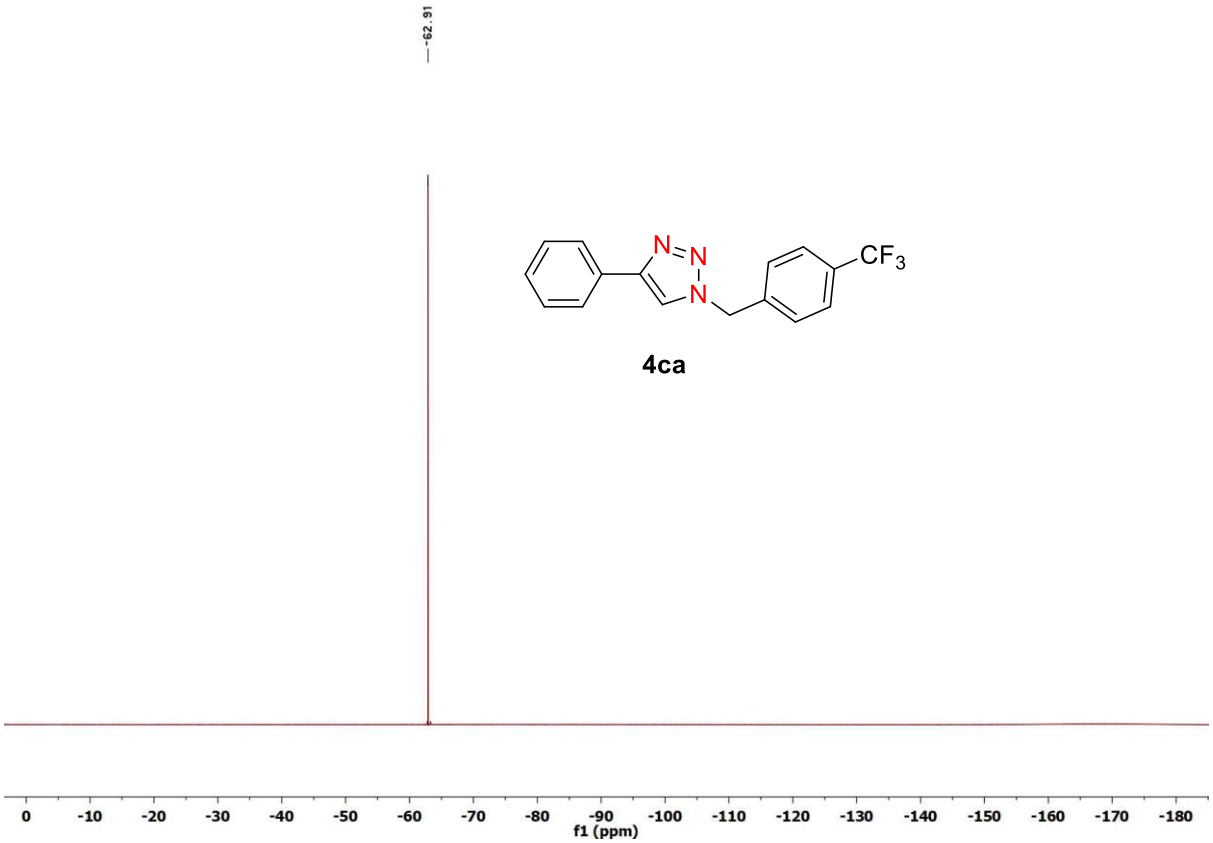


Fig. S9: ^{19}F NMR (470 MHz, $CDCl_3$) of the compound **4ca**.

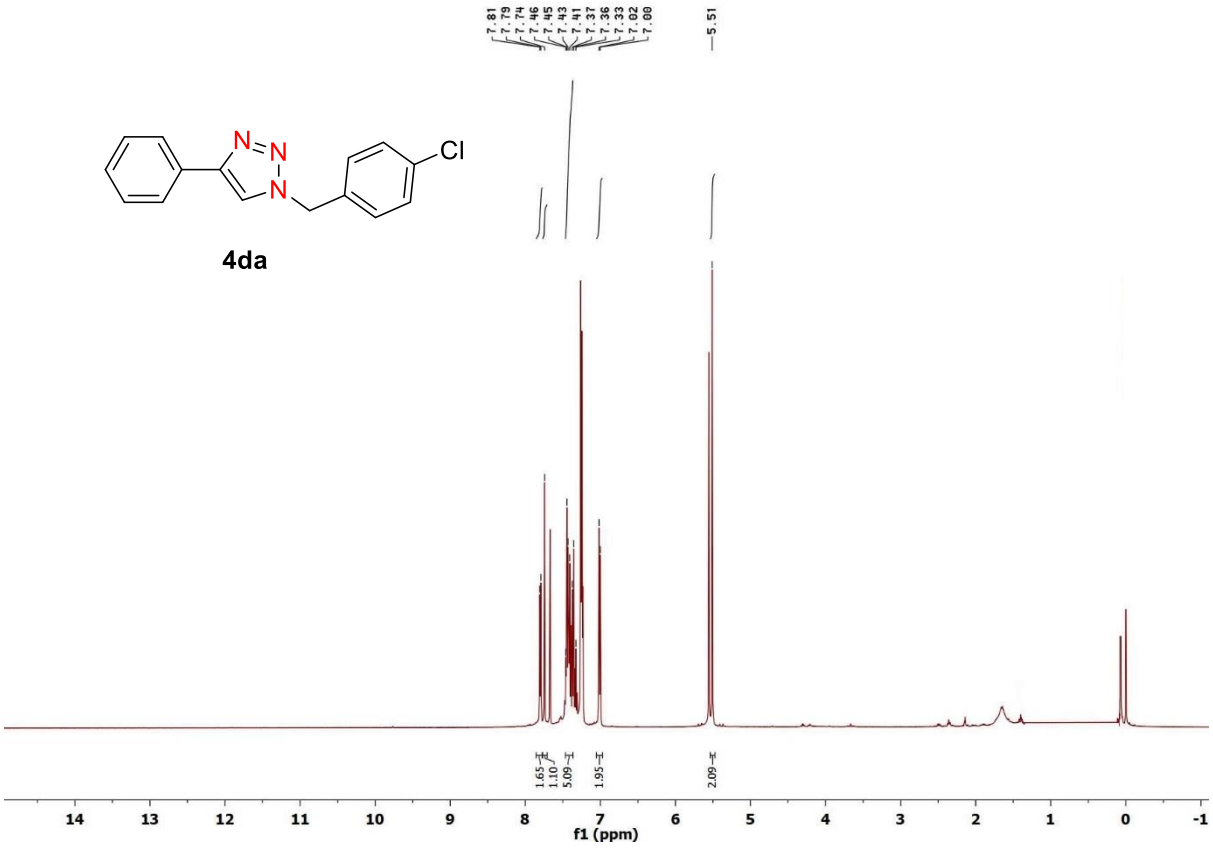


Fig. S10: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4da**.

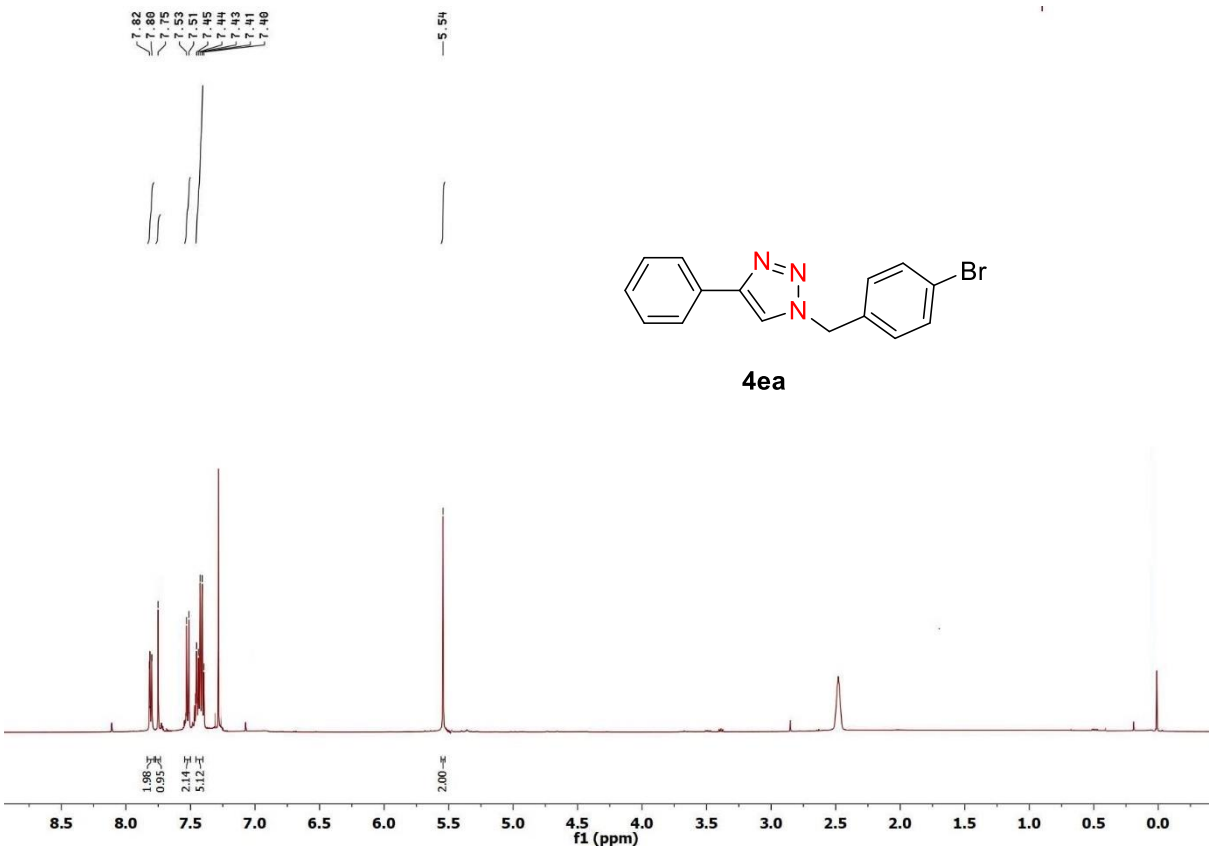


Fig. S11: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4ea**.

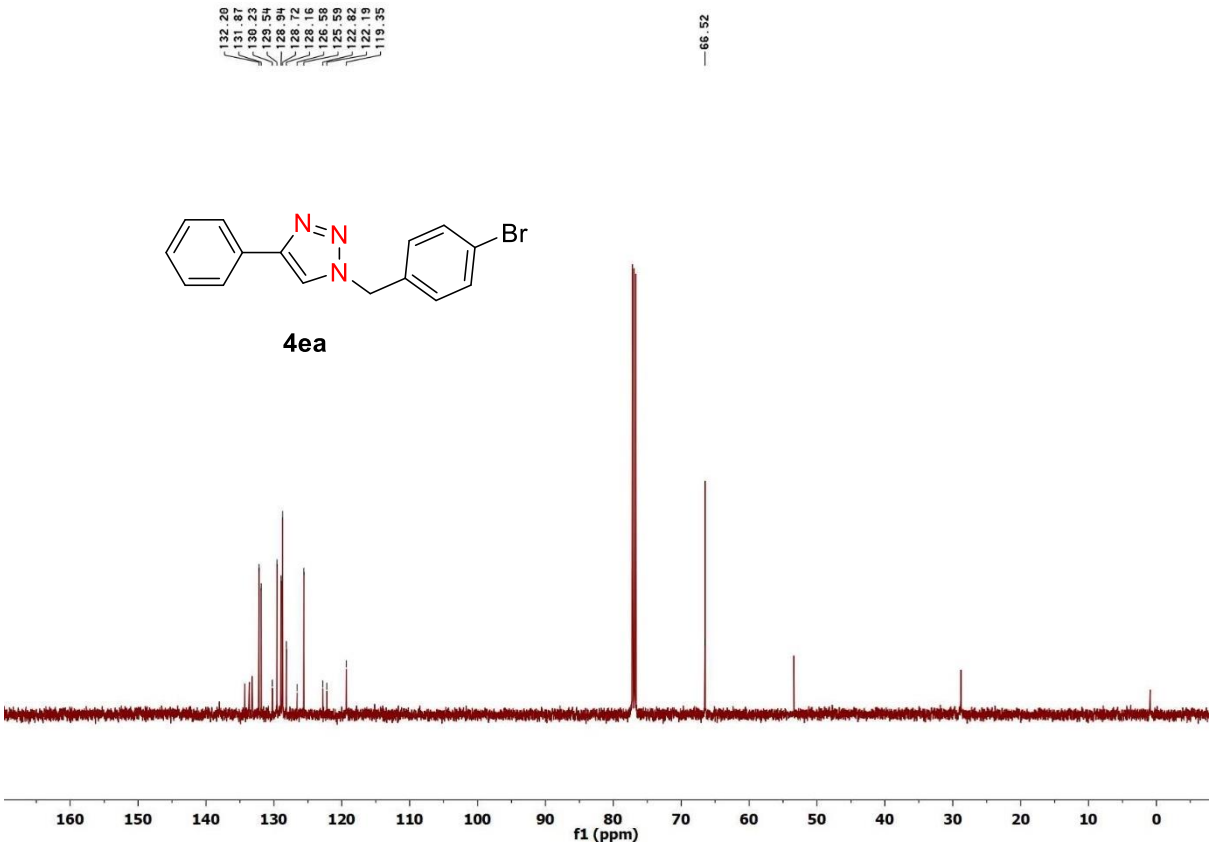


Fig. S12: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4ea**.

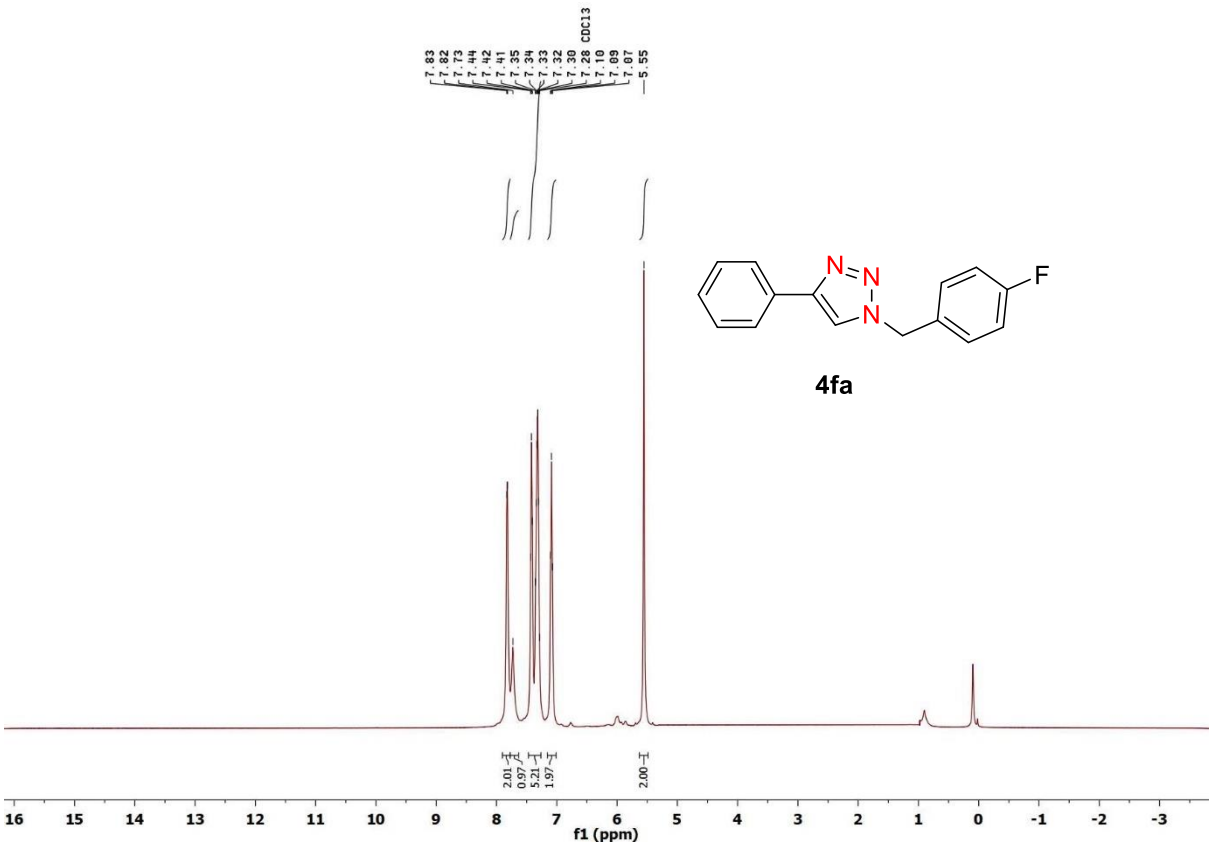


Fig. S13: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4fa**.

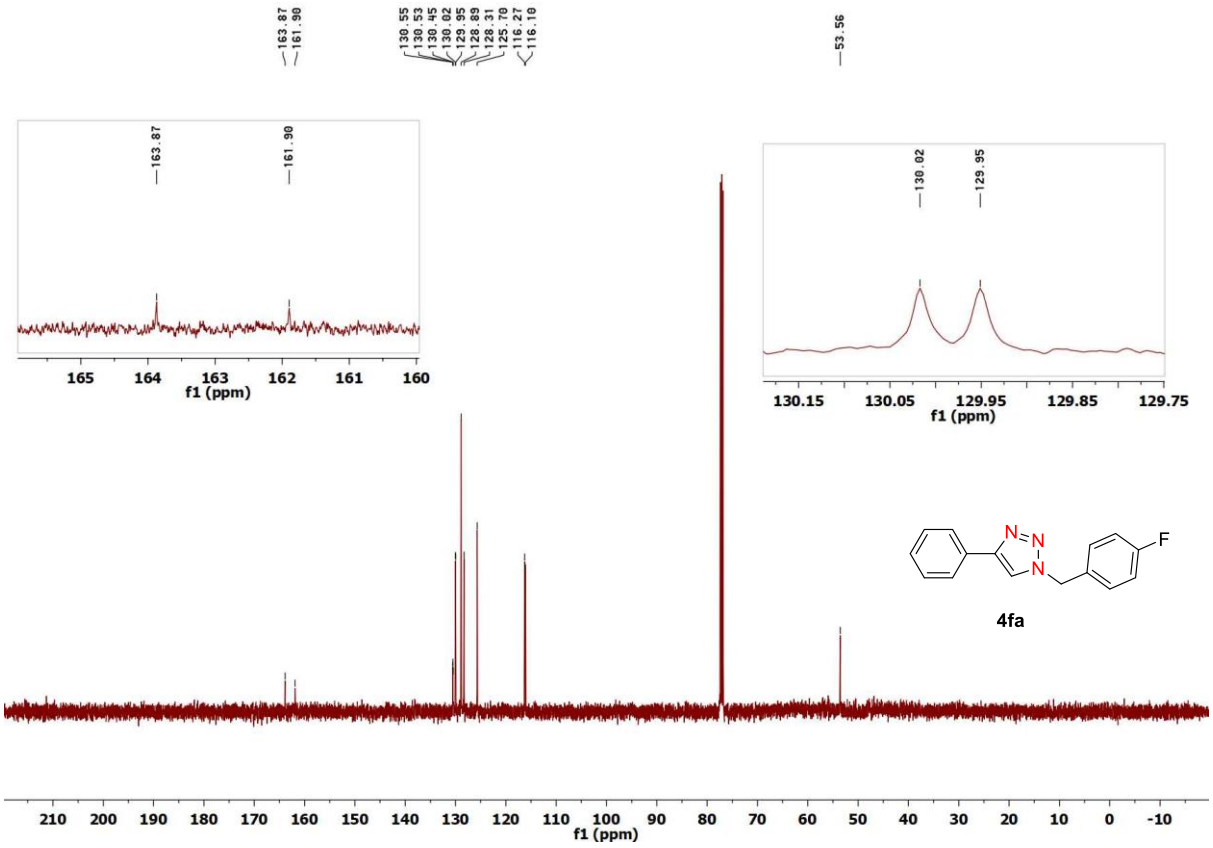


Fig. S14: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4fa**.

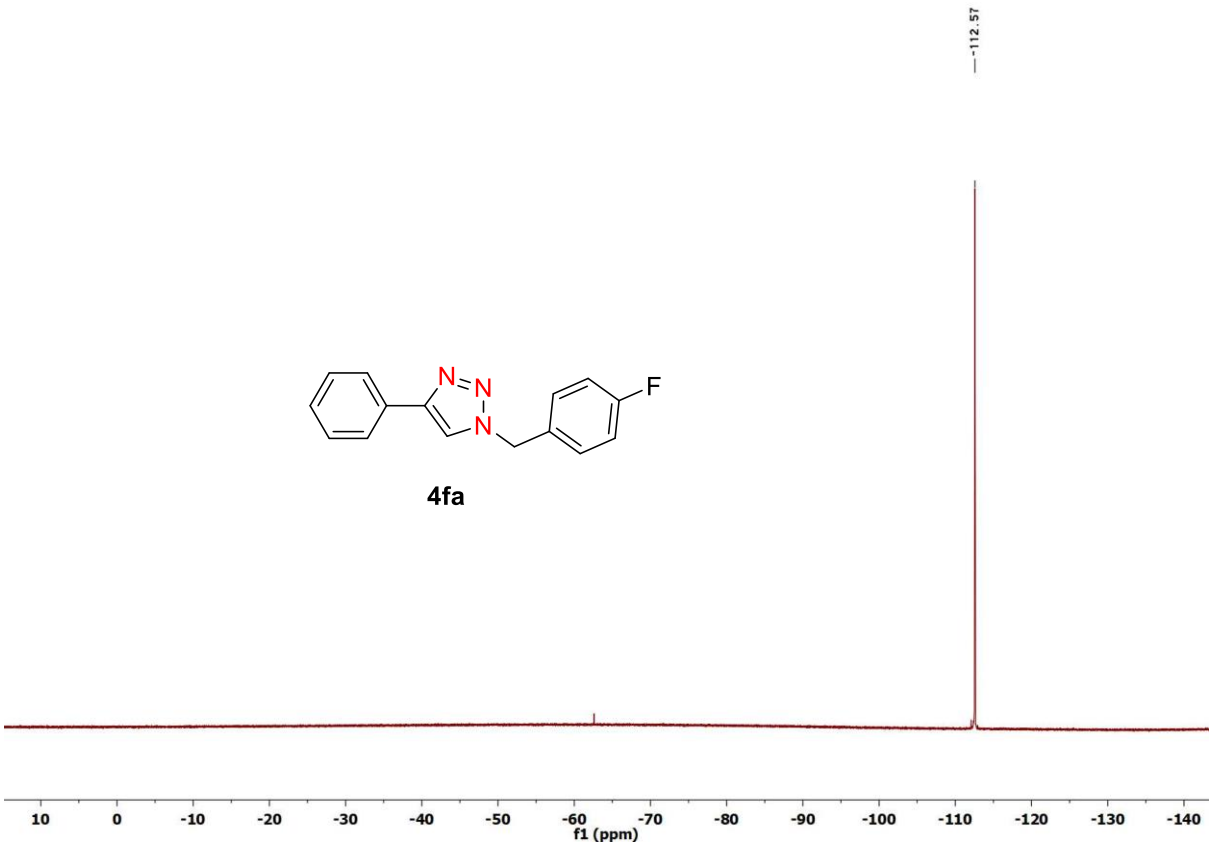


Fig. S15: ^{19}F NMR (470 MHz, $CDCl_3$) of the compound **4fa**.

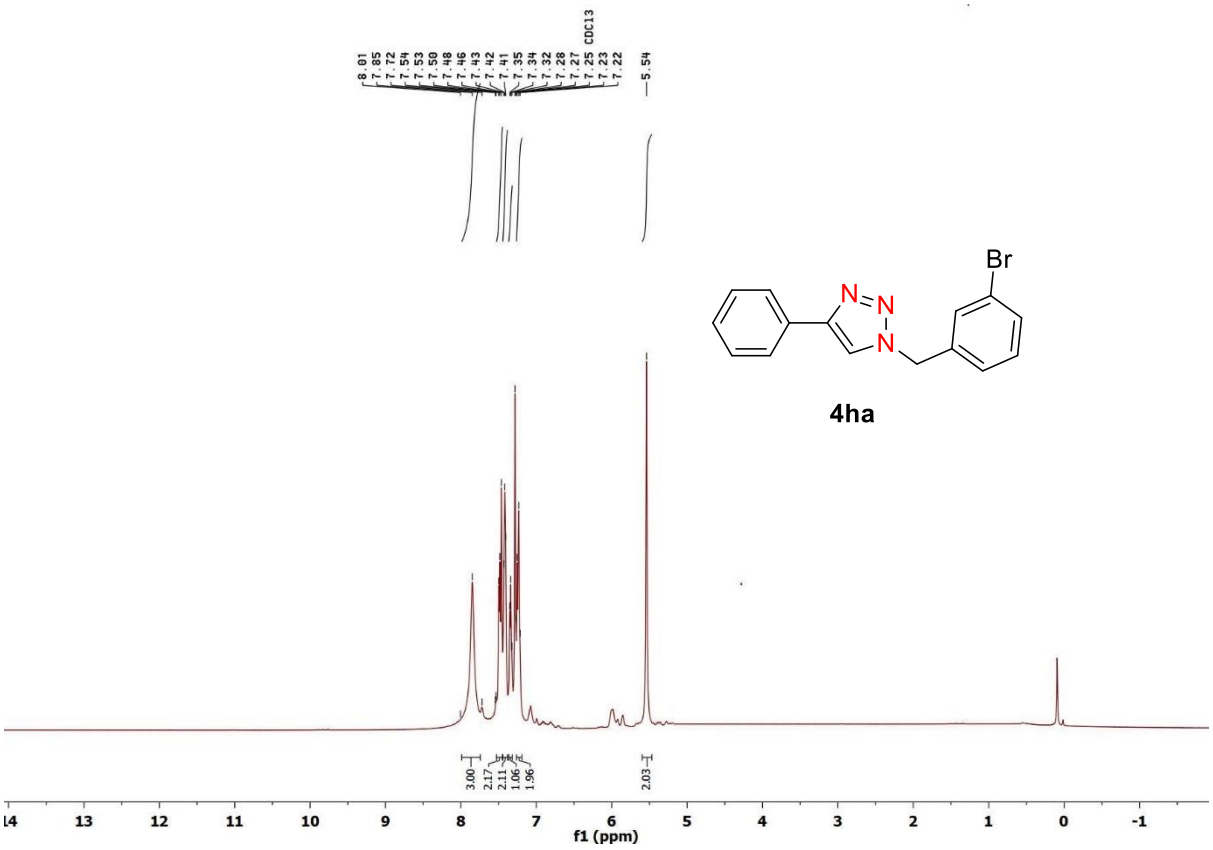


Fig. S16: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4ha**.

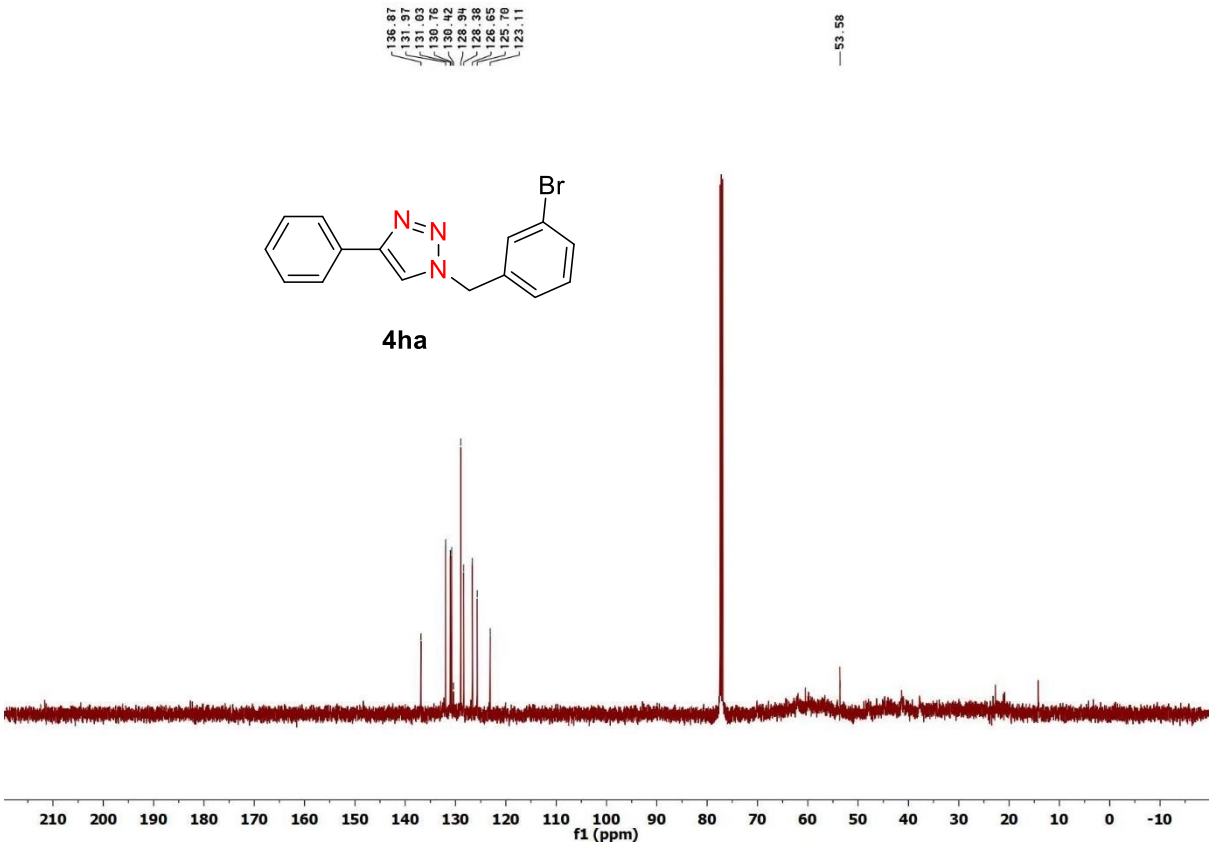


Fig. S17: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4ha**.

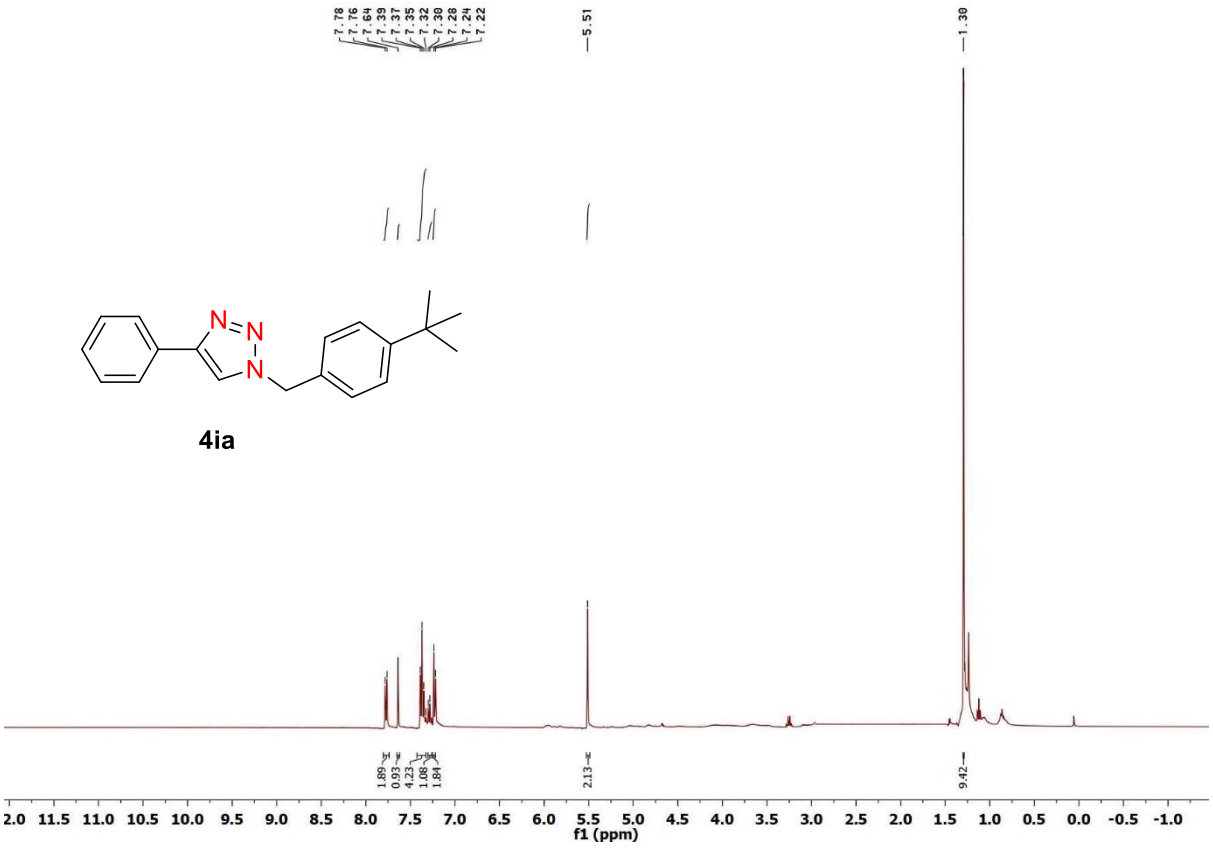


Fig. S18: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4ia**.

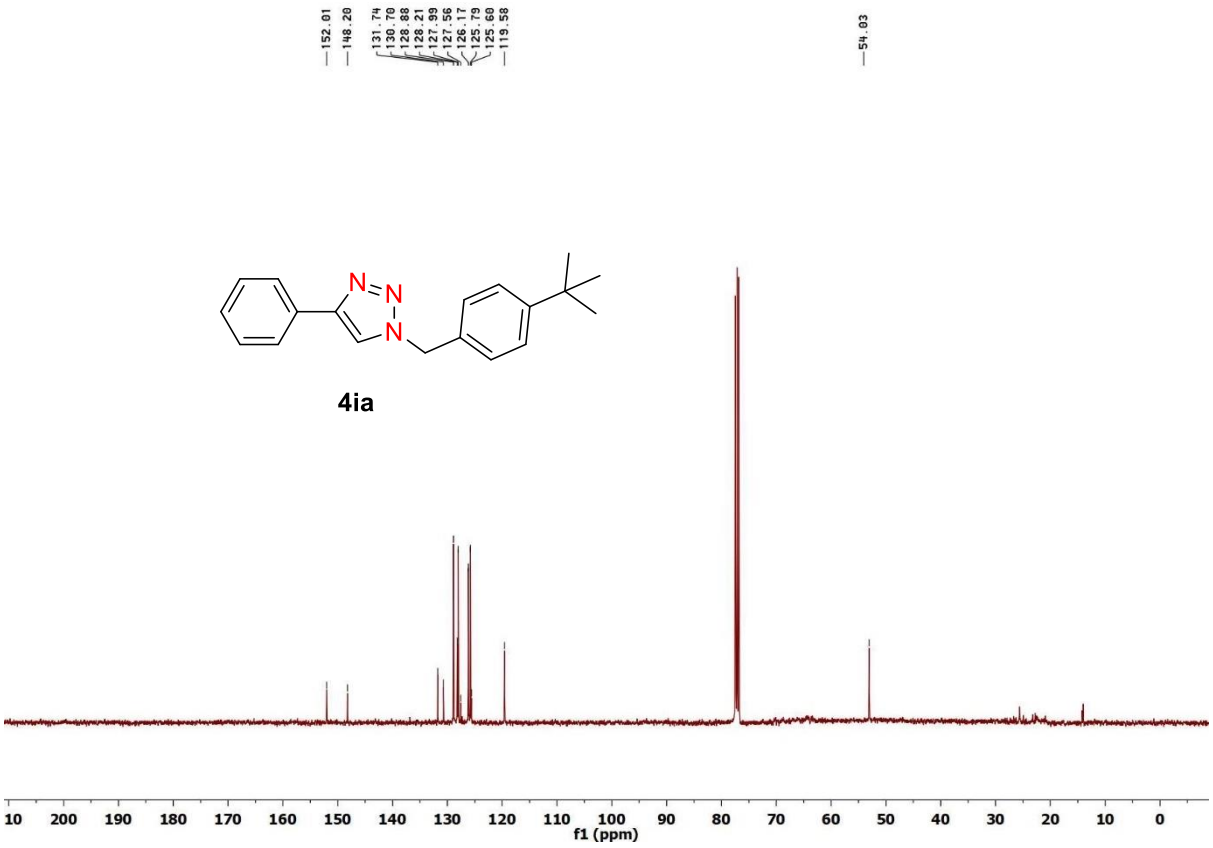


Fig. S19: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4ia**.

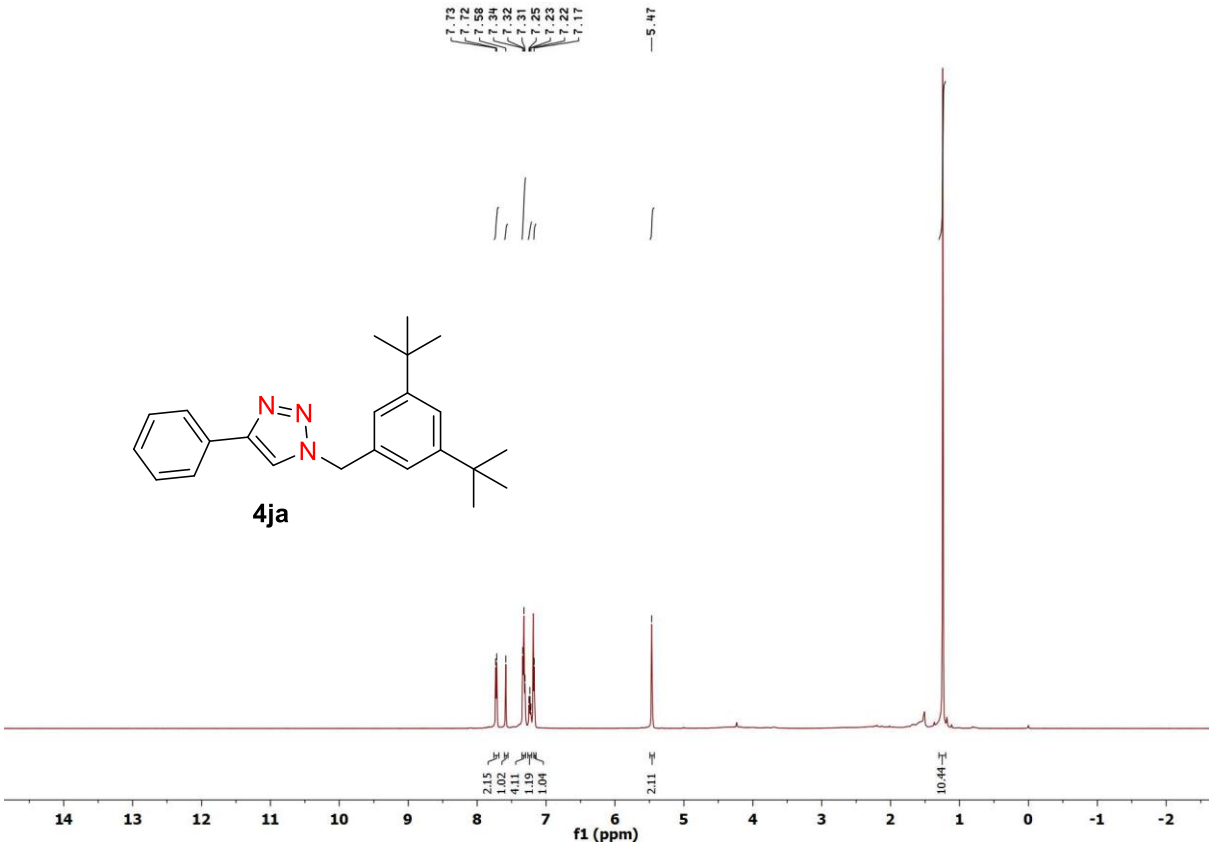


Fig. S20: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4ja**.

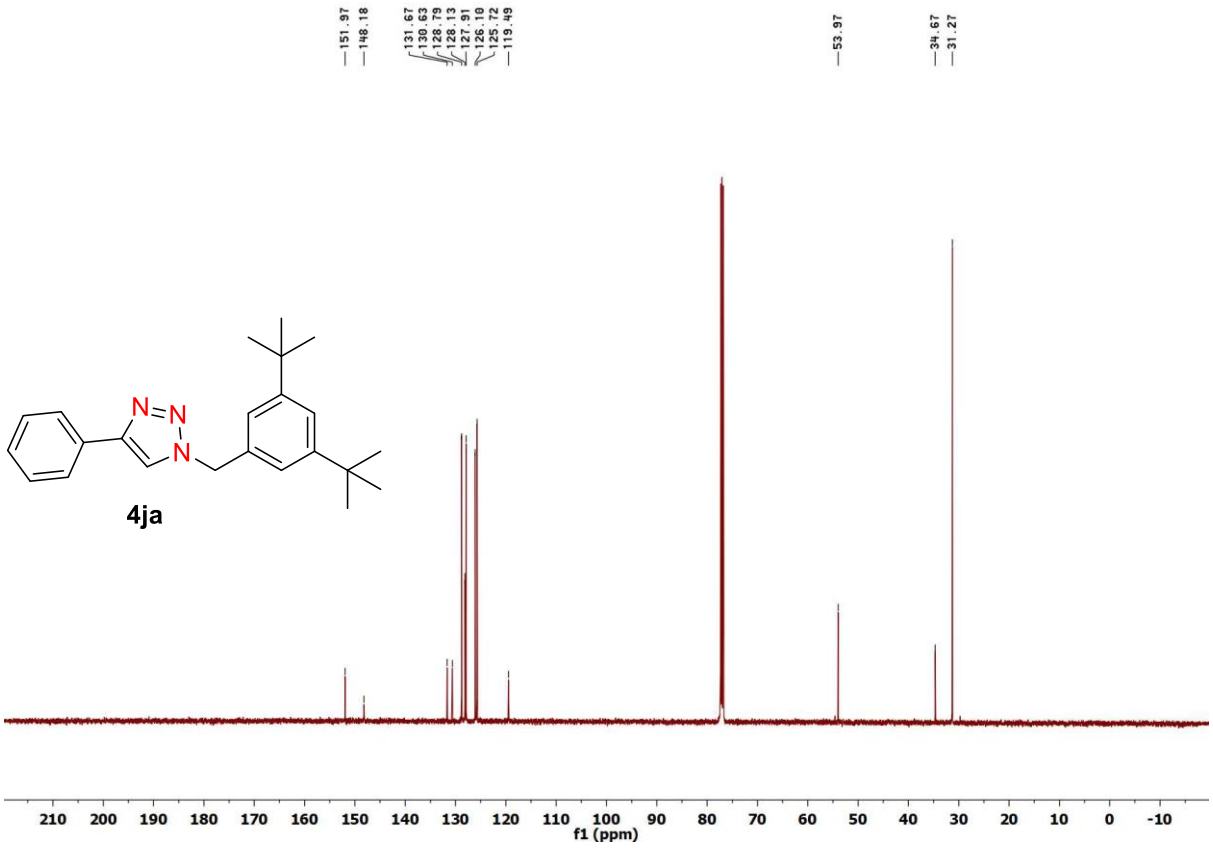


Fig. S21: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4ja**.

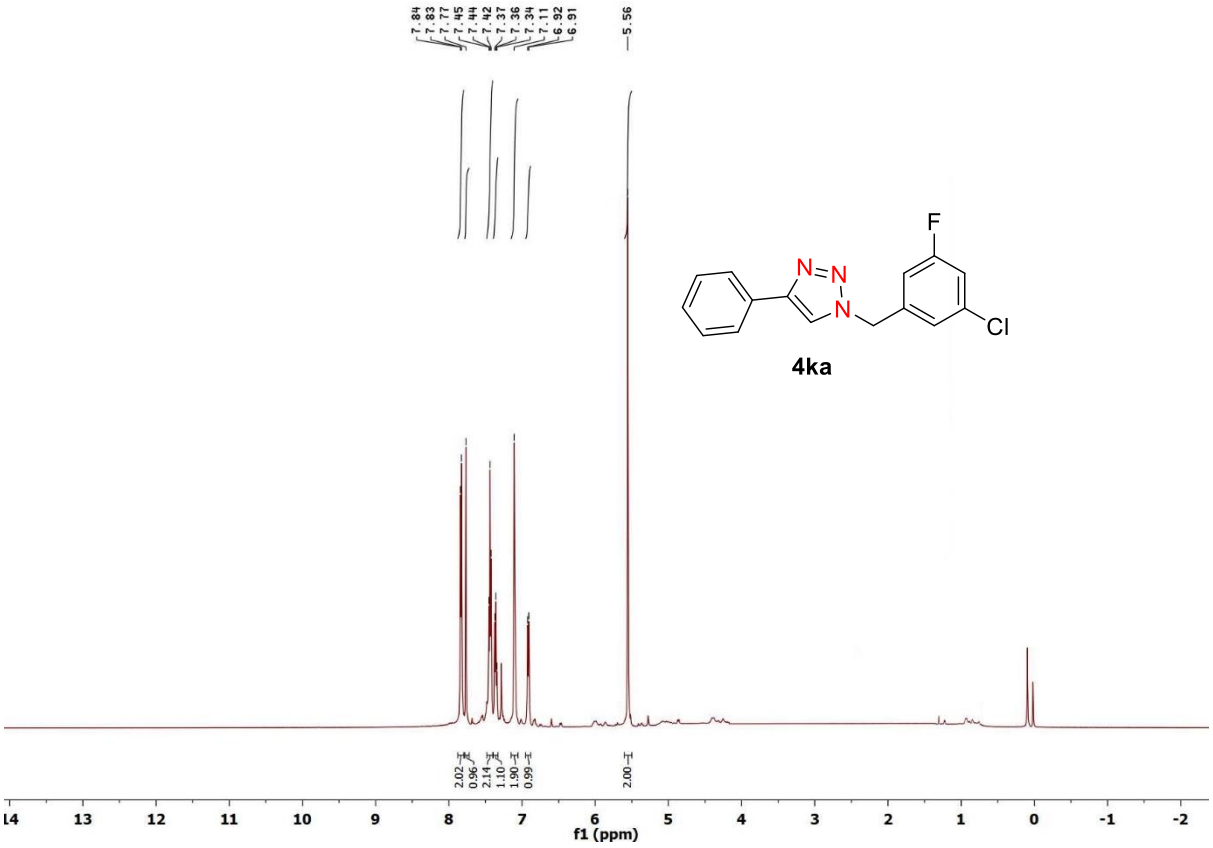


Fig. S22: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4ka**.

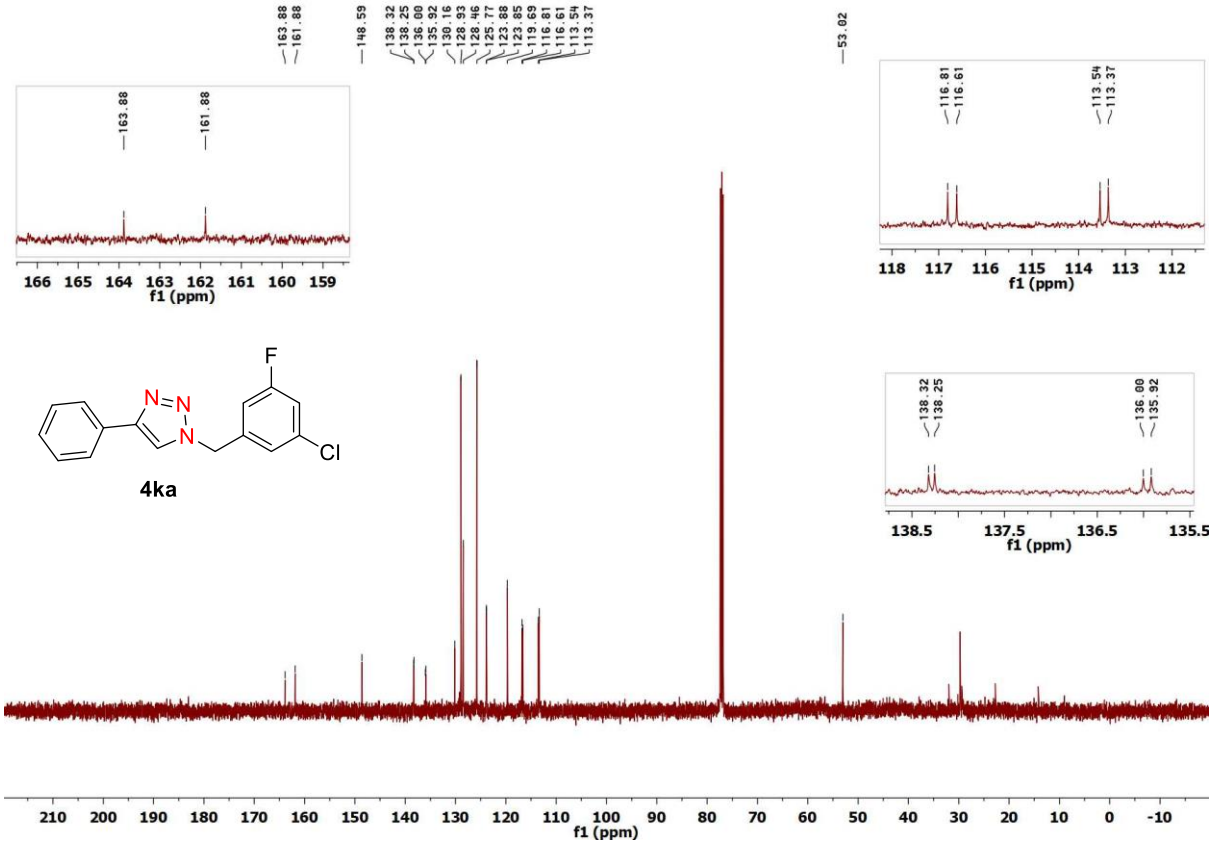


Fig. S23: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4ka**.

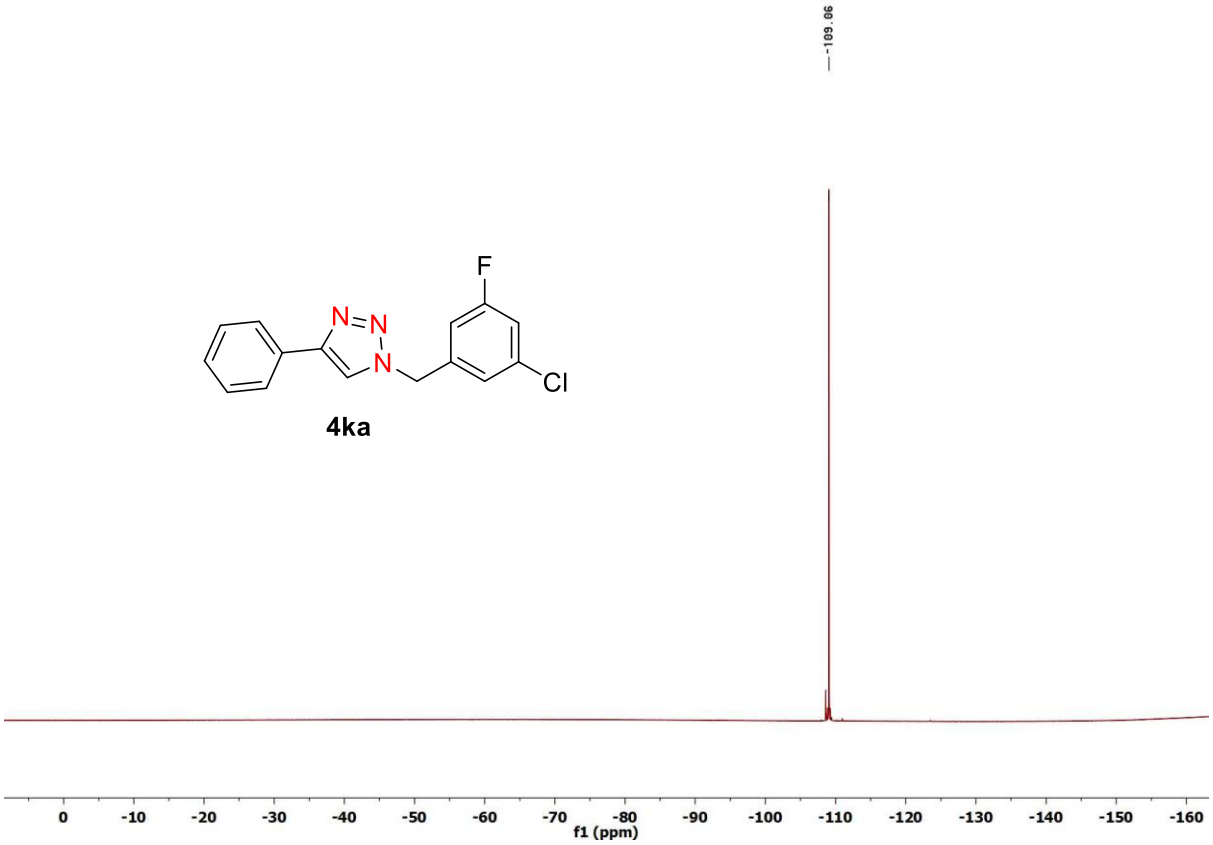


Fig. S24: ^{19}F NMR (470 MHz, $CDCl_3$) of the compound **4ka**.

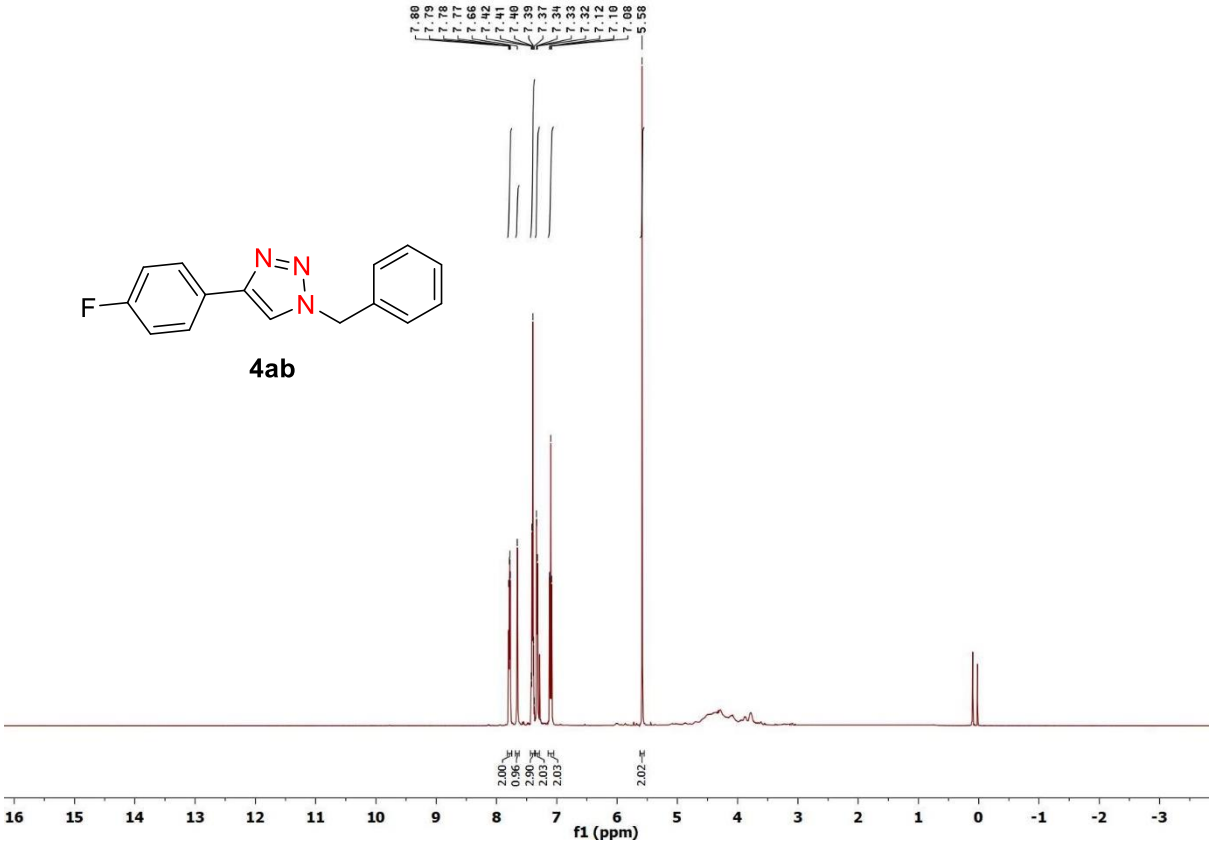


Fig. S25: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4ab**.

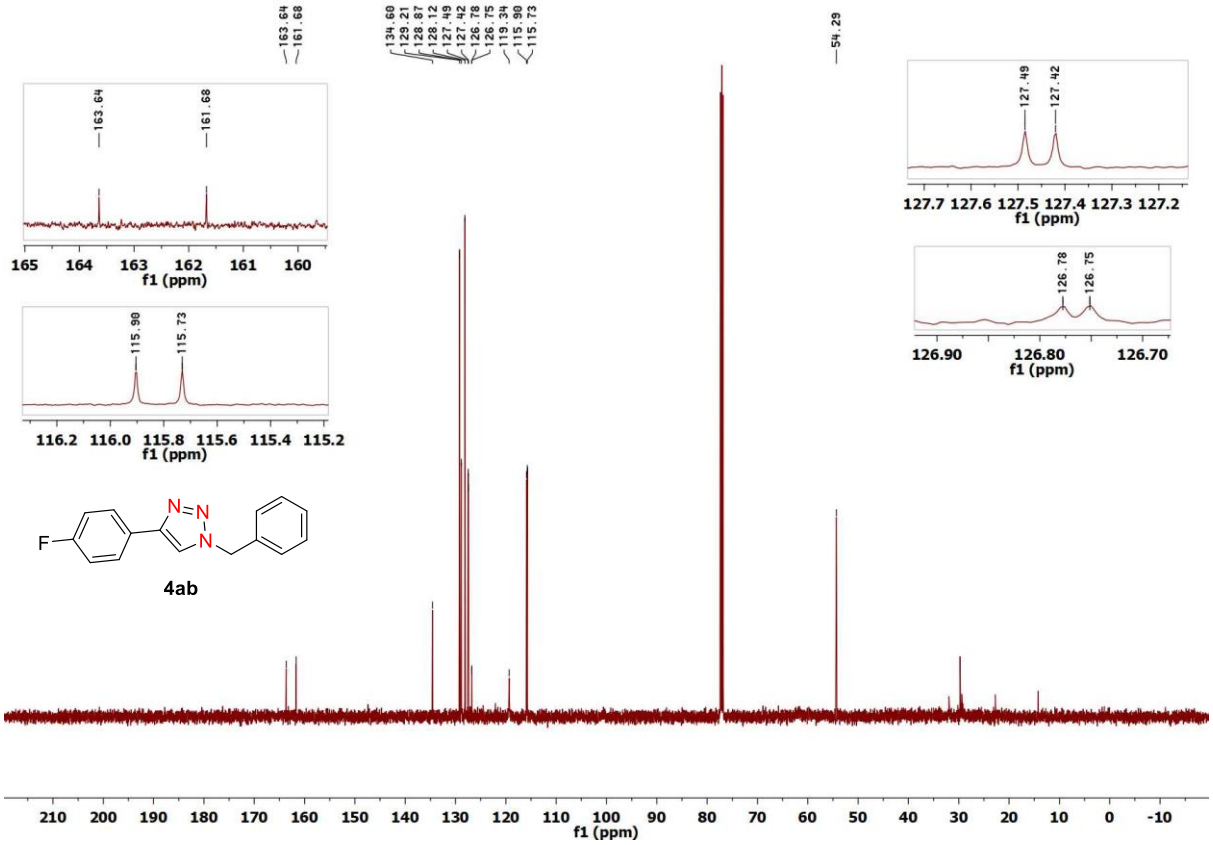


Fig. S26: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4ab**.

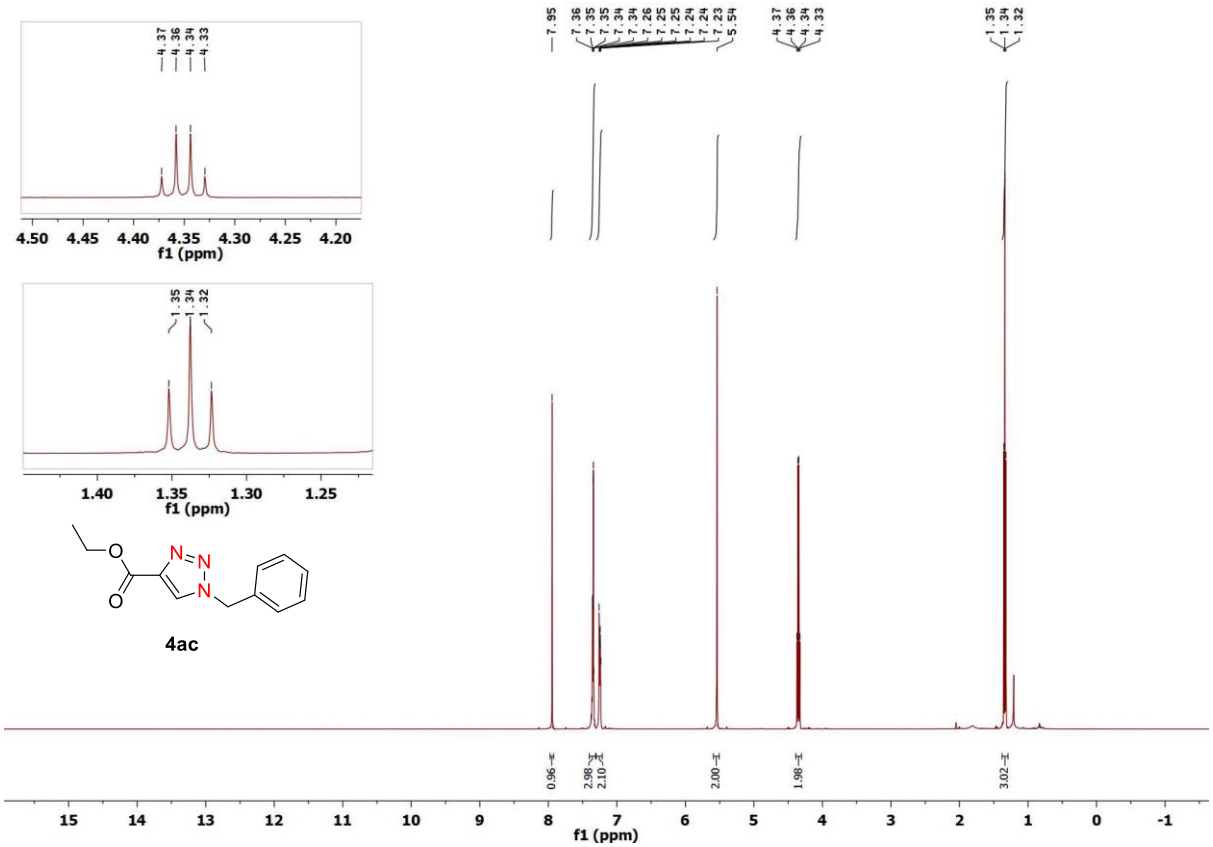


Fig. S27: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4ac**.

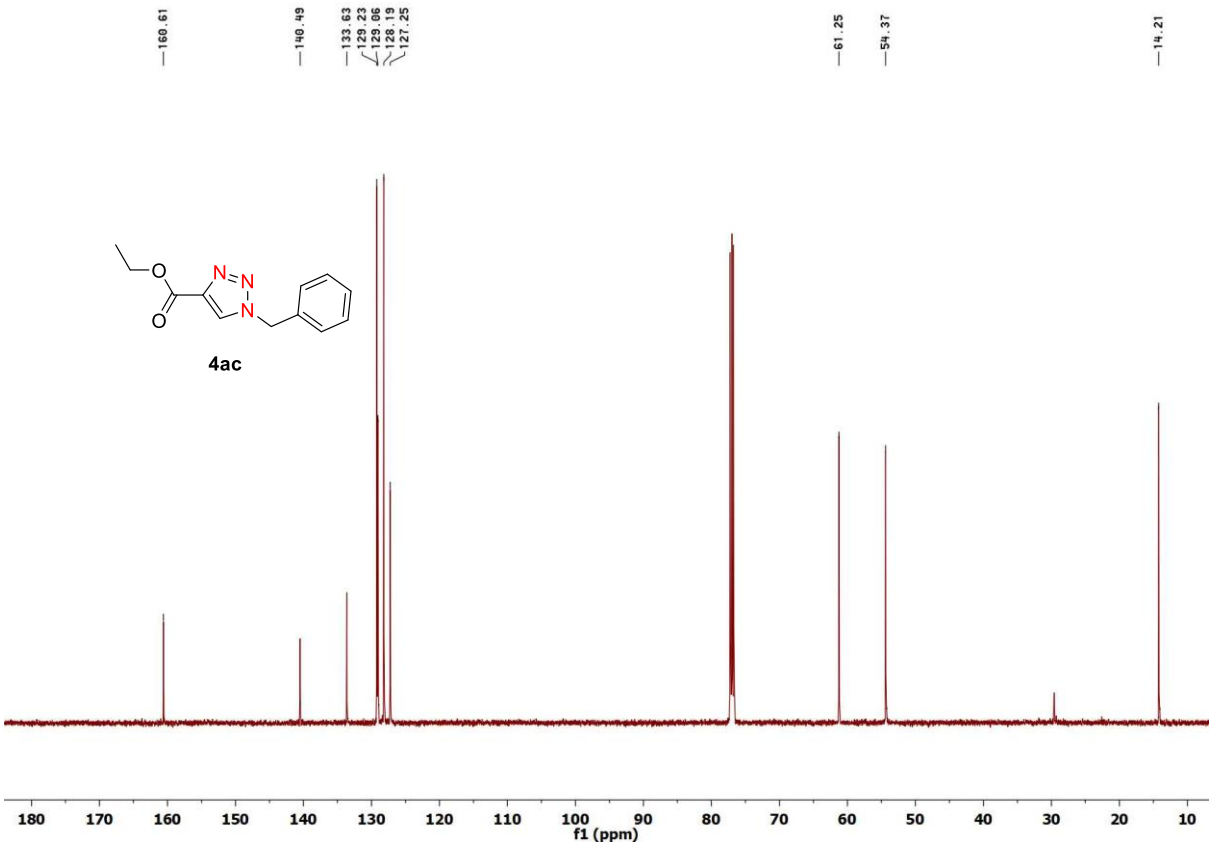


Fig. S28: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4ac**.

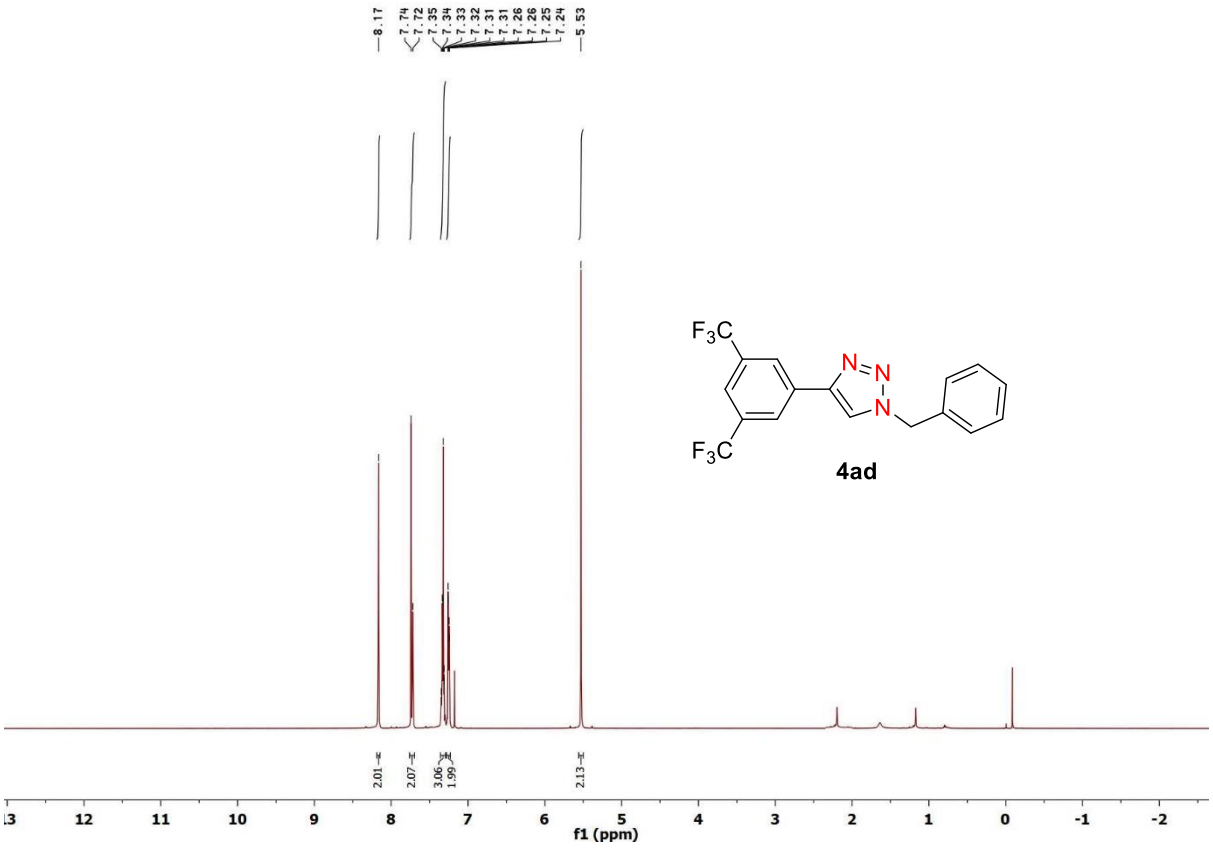


Fig. S29: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4ad**.

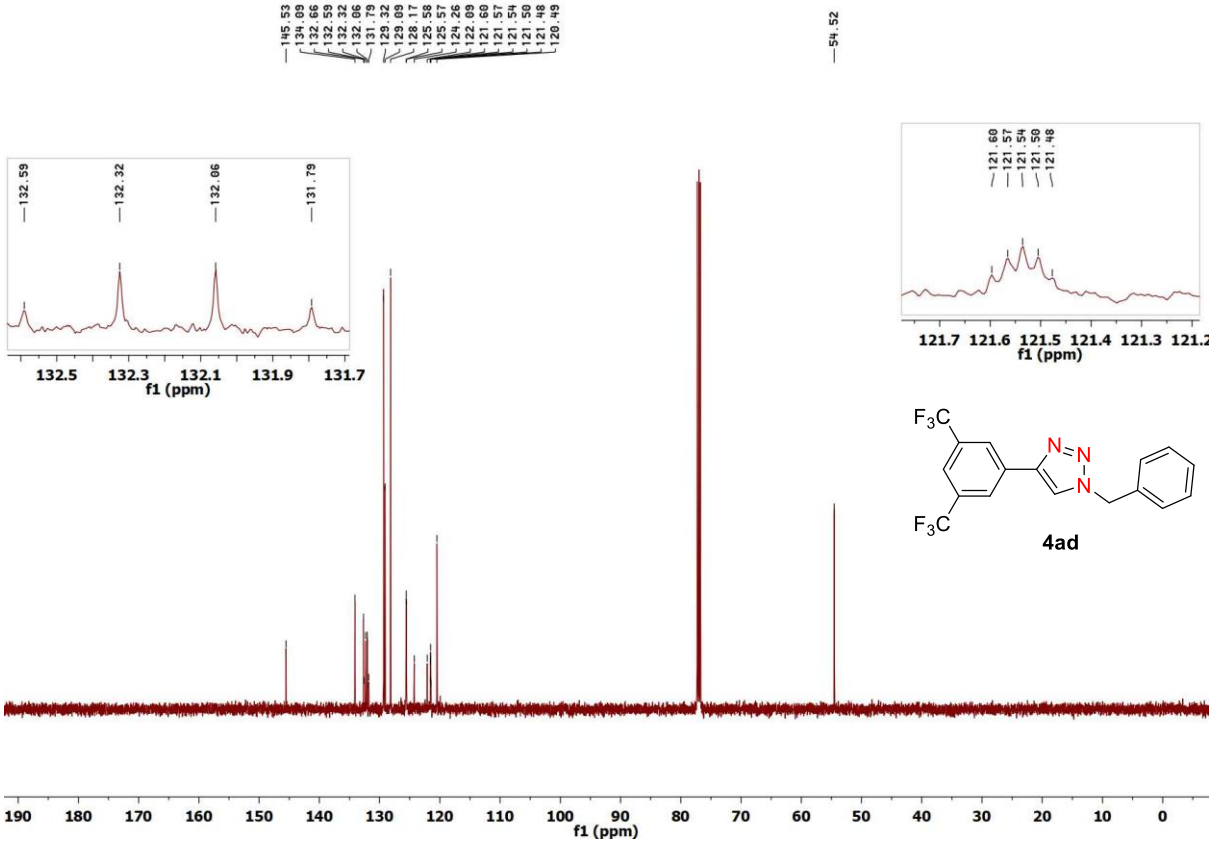


Fig. S30: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4ad**.

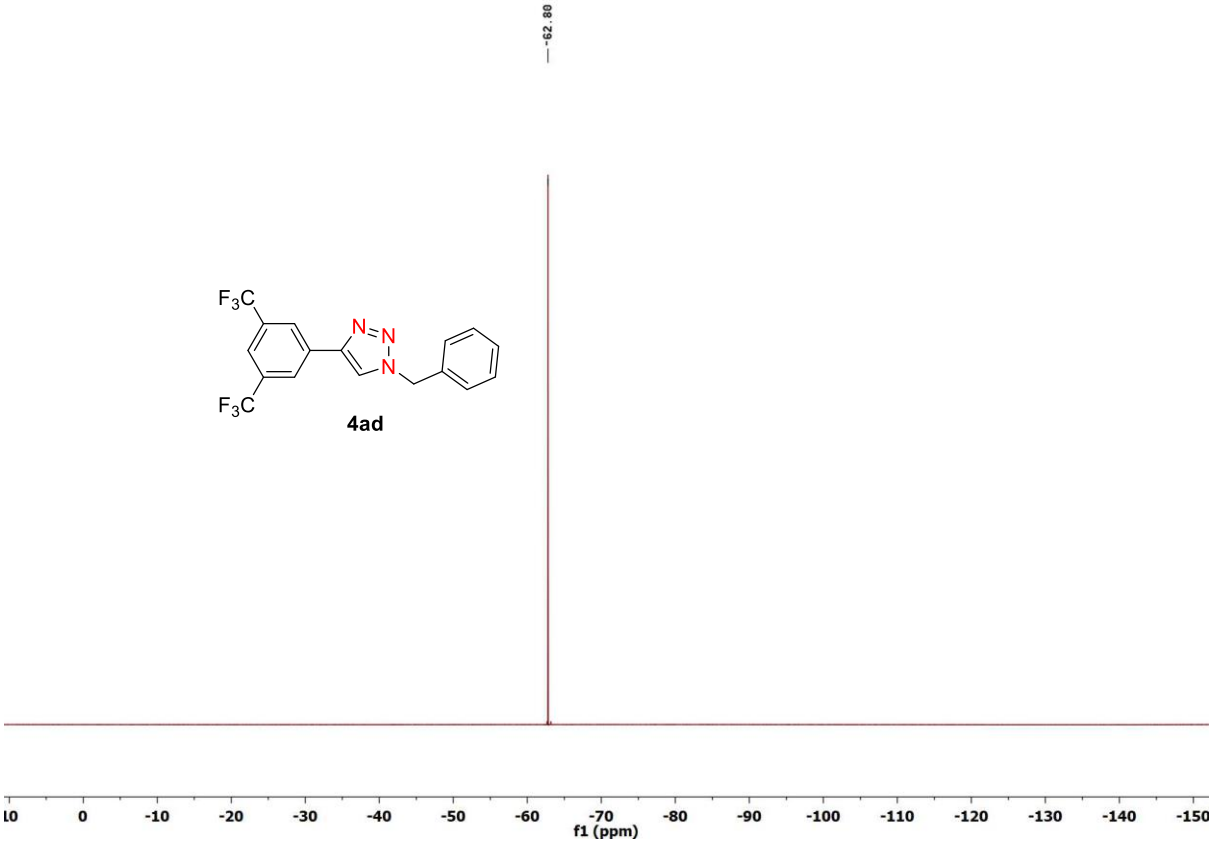


Fig. S31: ^{19}F NMR (470 MHz, $CDCl_3$) of the compound **4ad**.

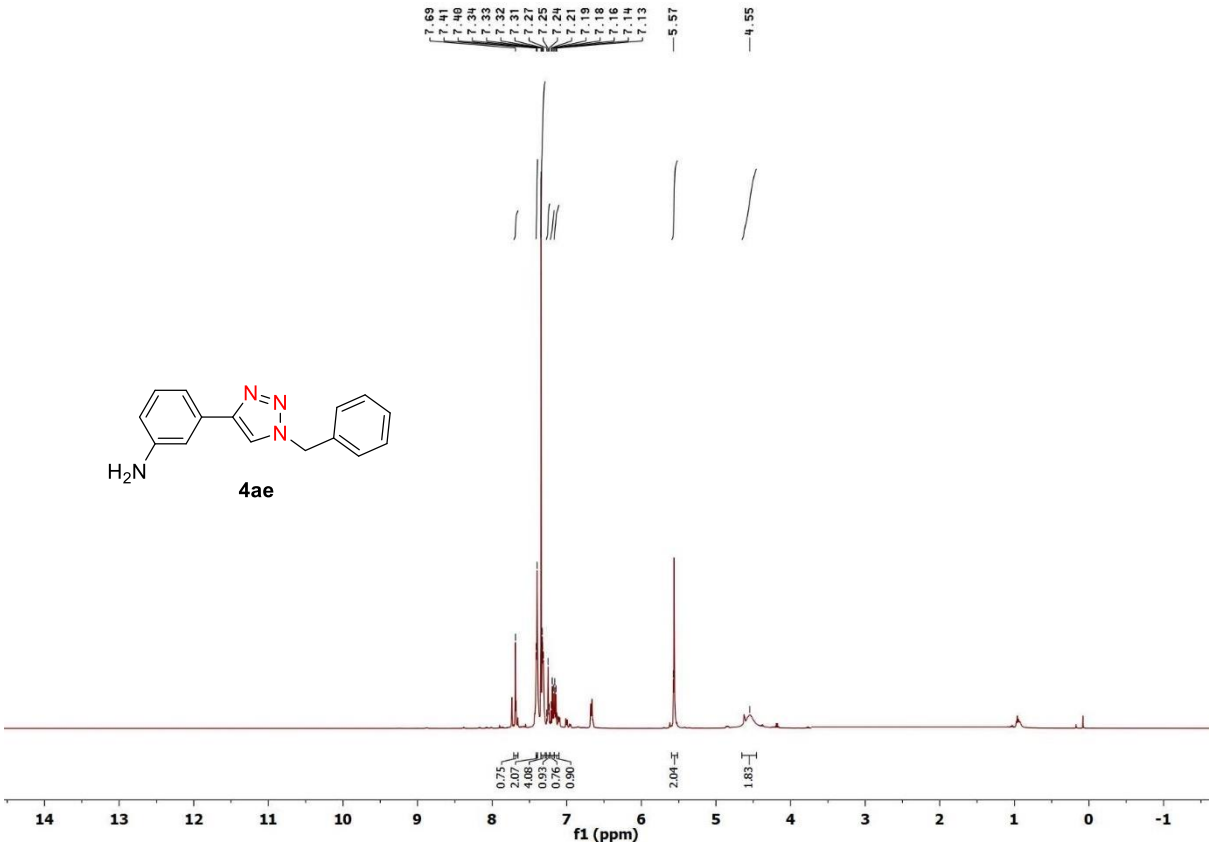


Fig. S32: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4ae**.

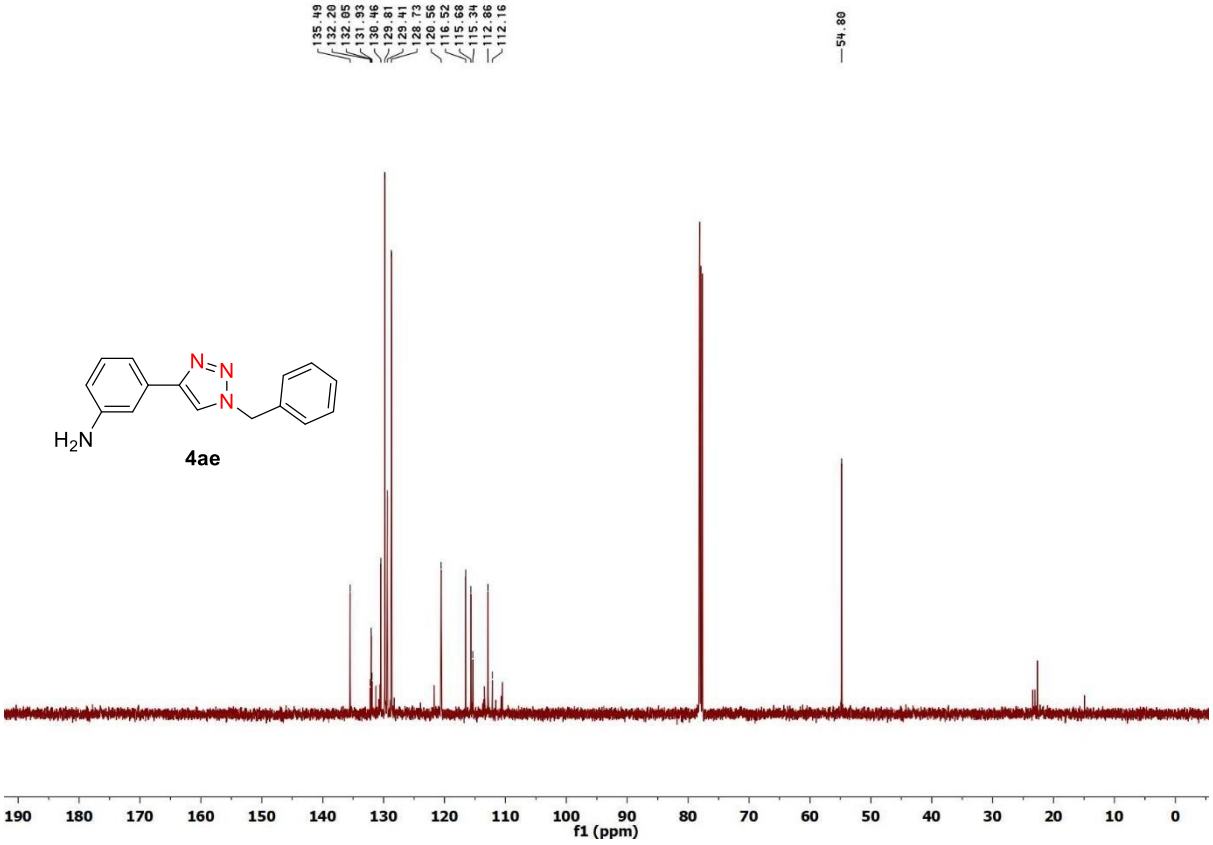


Fig. S33: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4ae**.

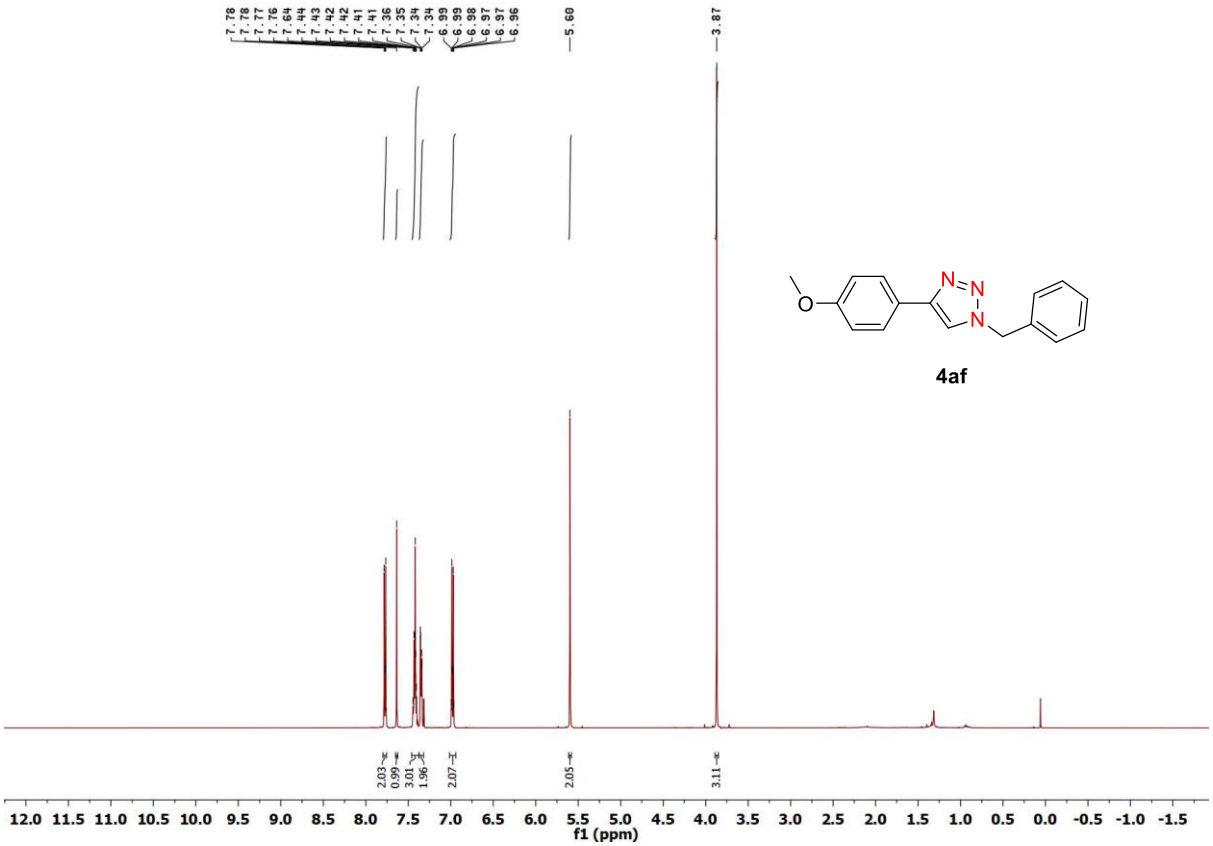


Fig. S34: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4af**.

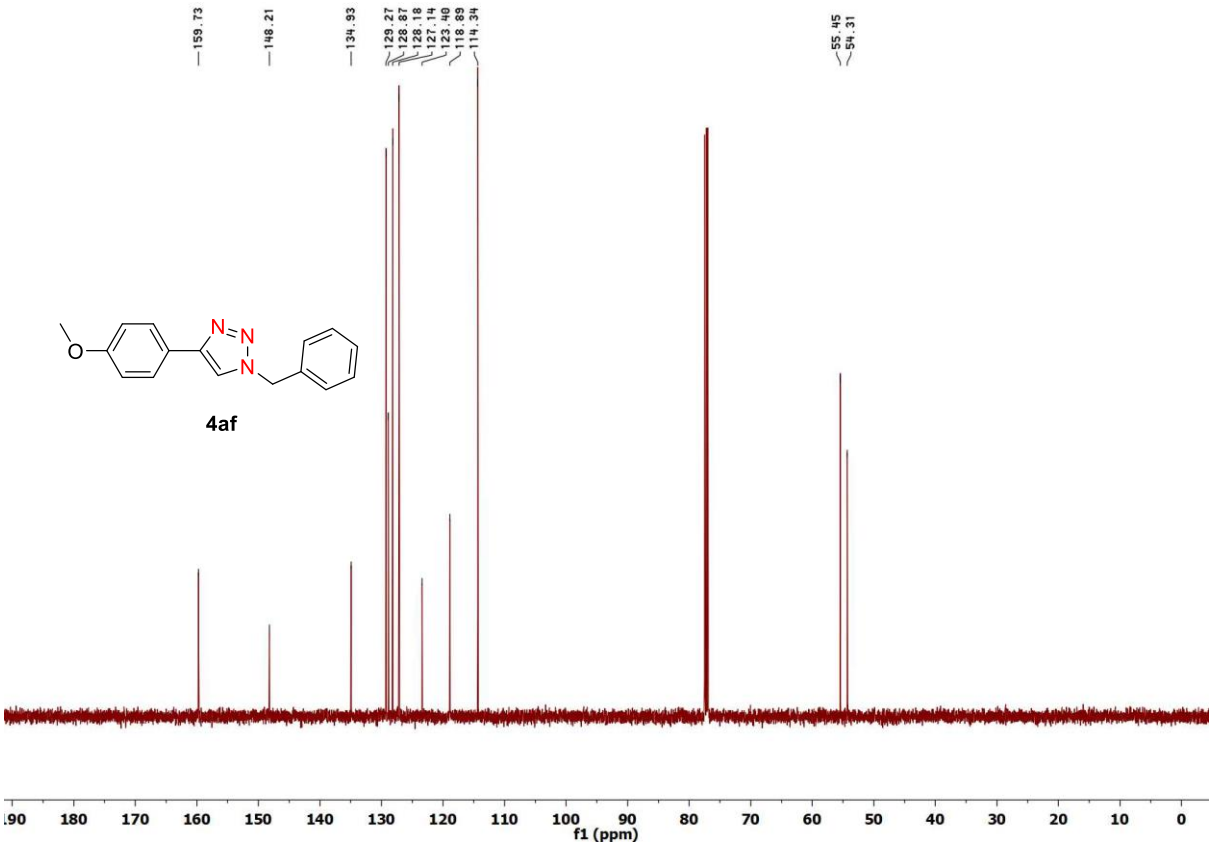


Fig. S35: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4af**.

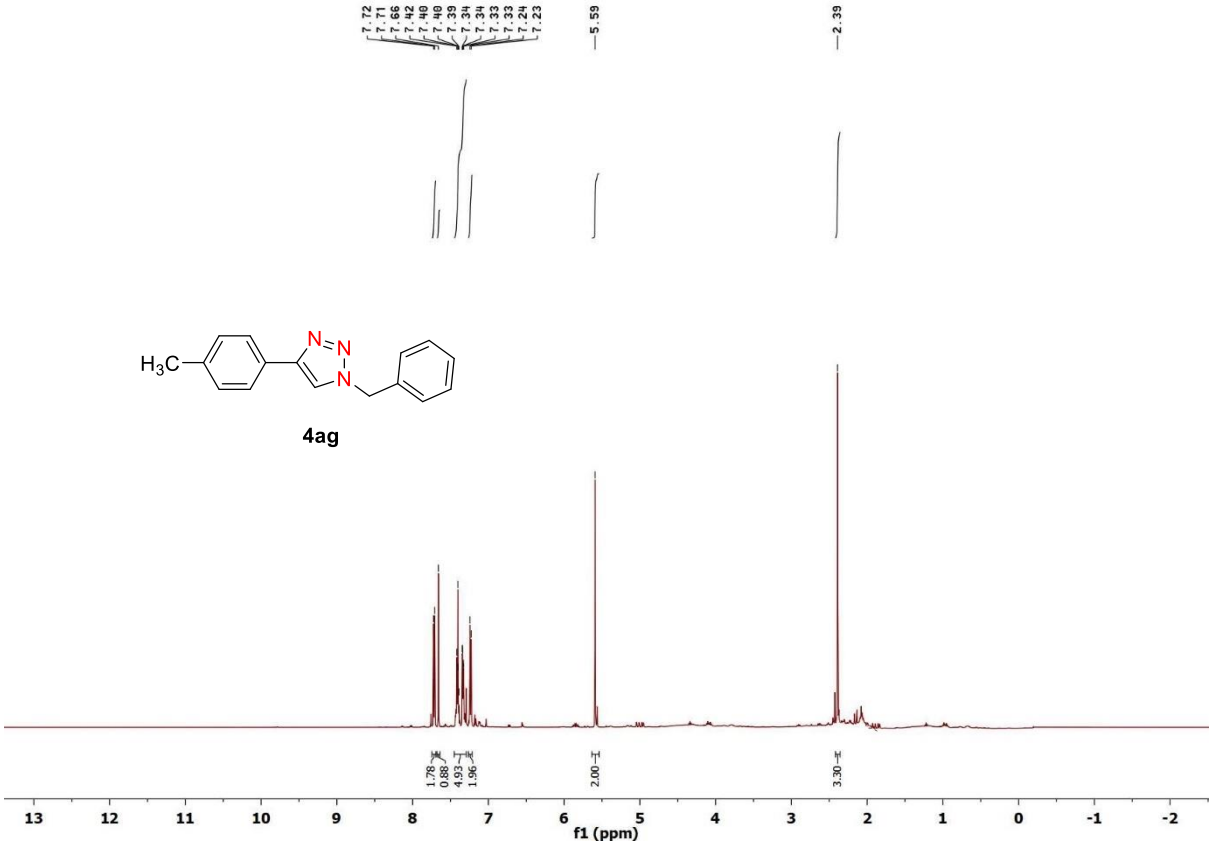


Fig. S36: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4ag**.

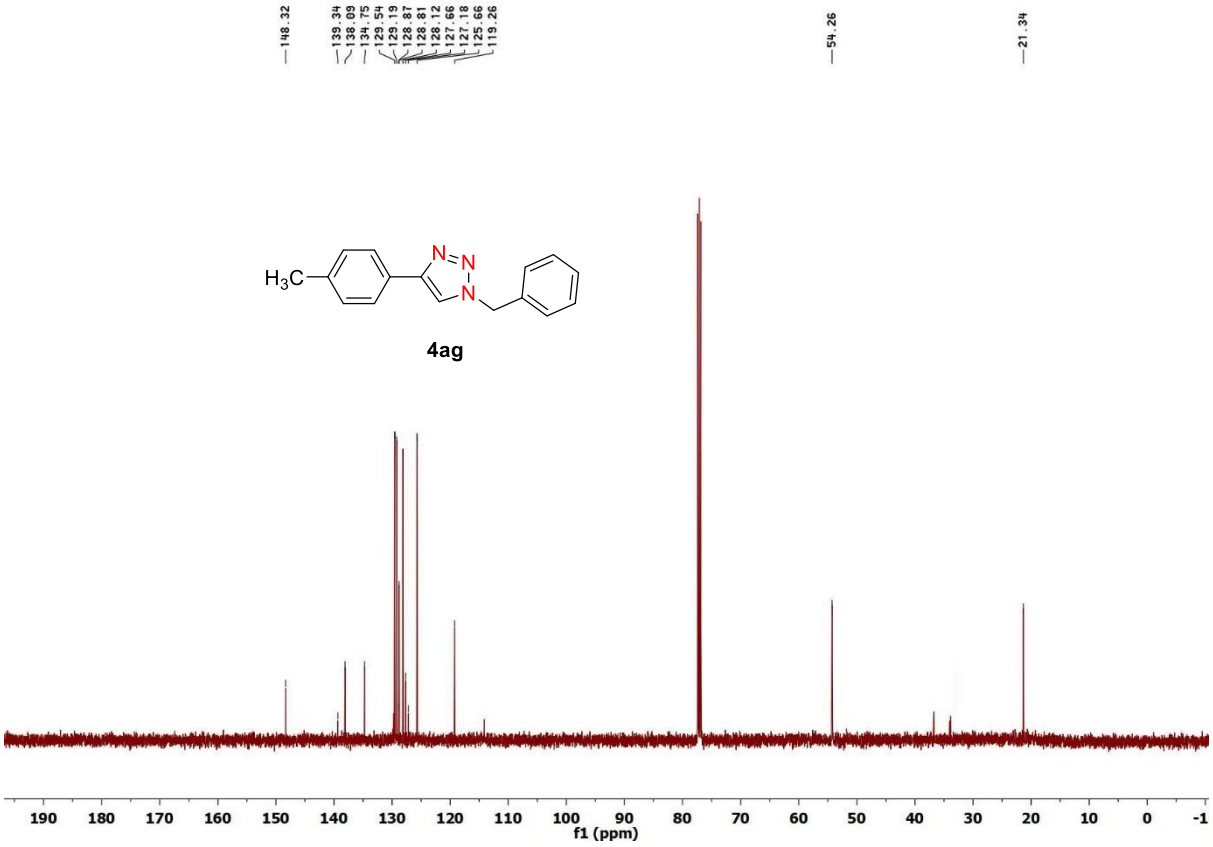


Fig. S37: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4ag**.

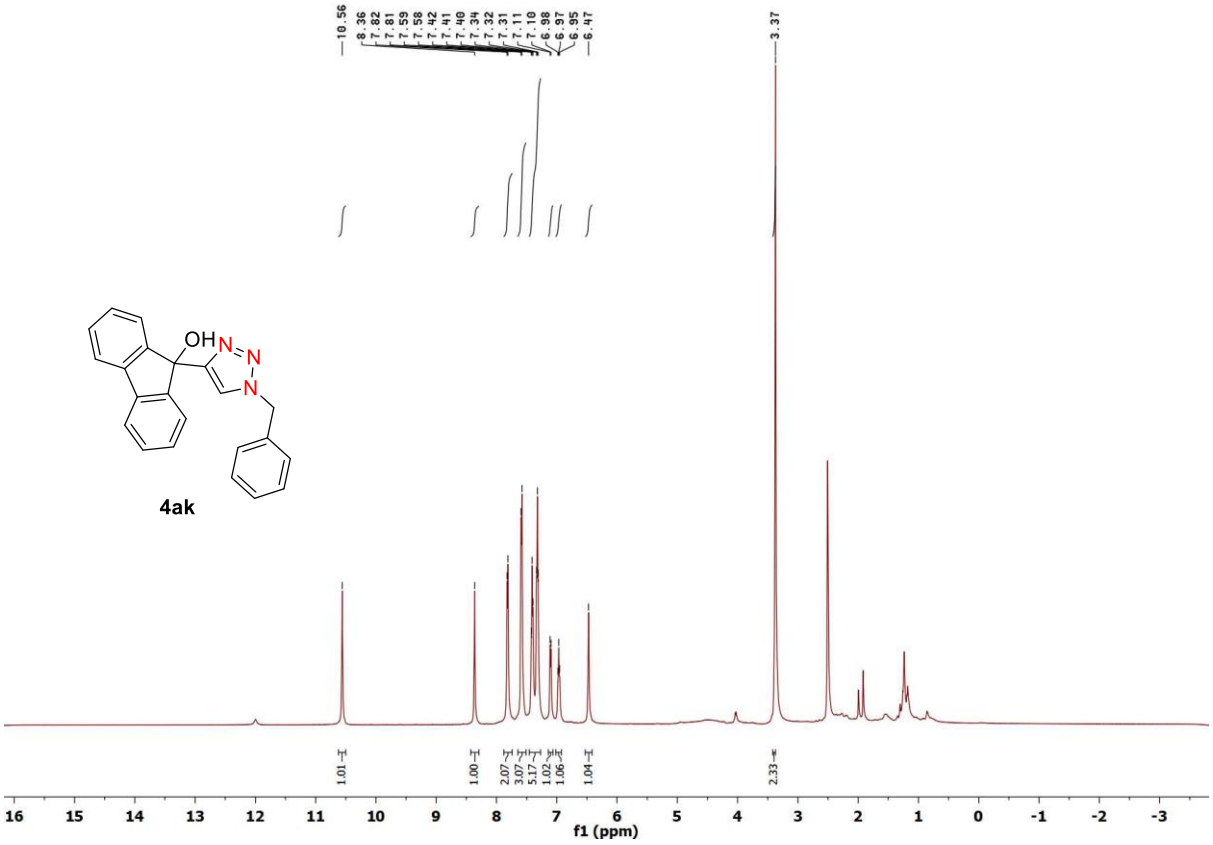


Fig. S38: ^{1}H NMR (500 MHz, DMSO-*d6*) of the compound **4ak**.

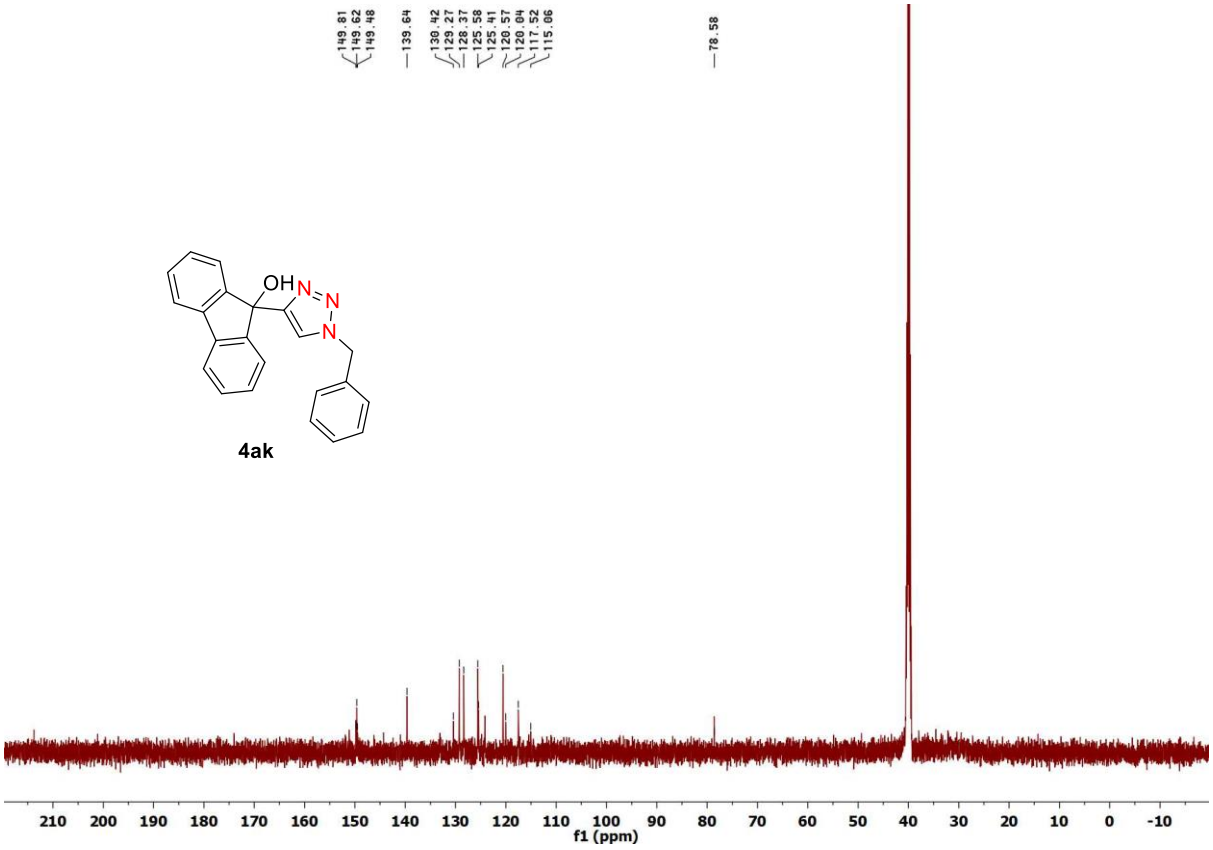


Fig. S39: ^{13}C NMR (125 MHz, DMSO-*d6*) of the compound **4ak**.

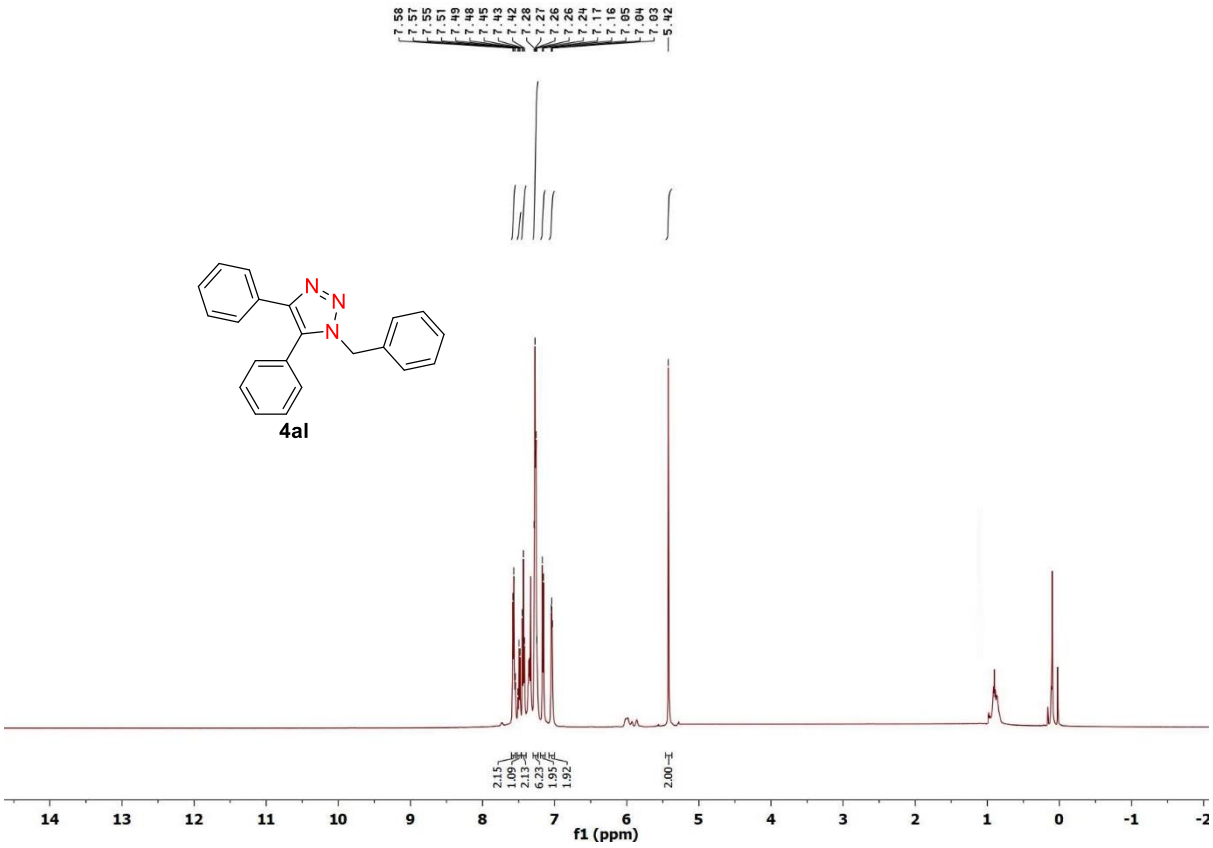


Fig. S40: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4al**.

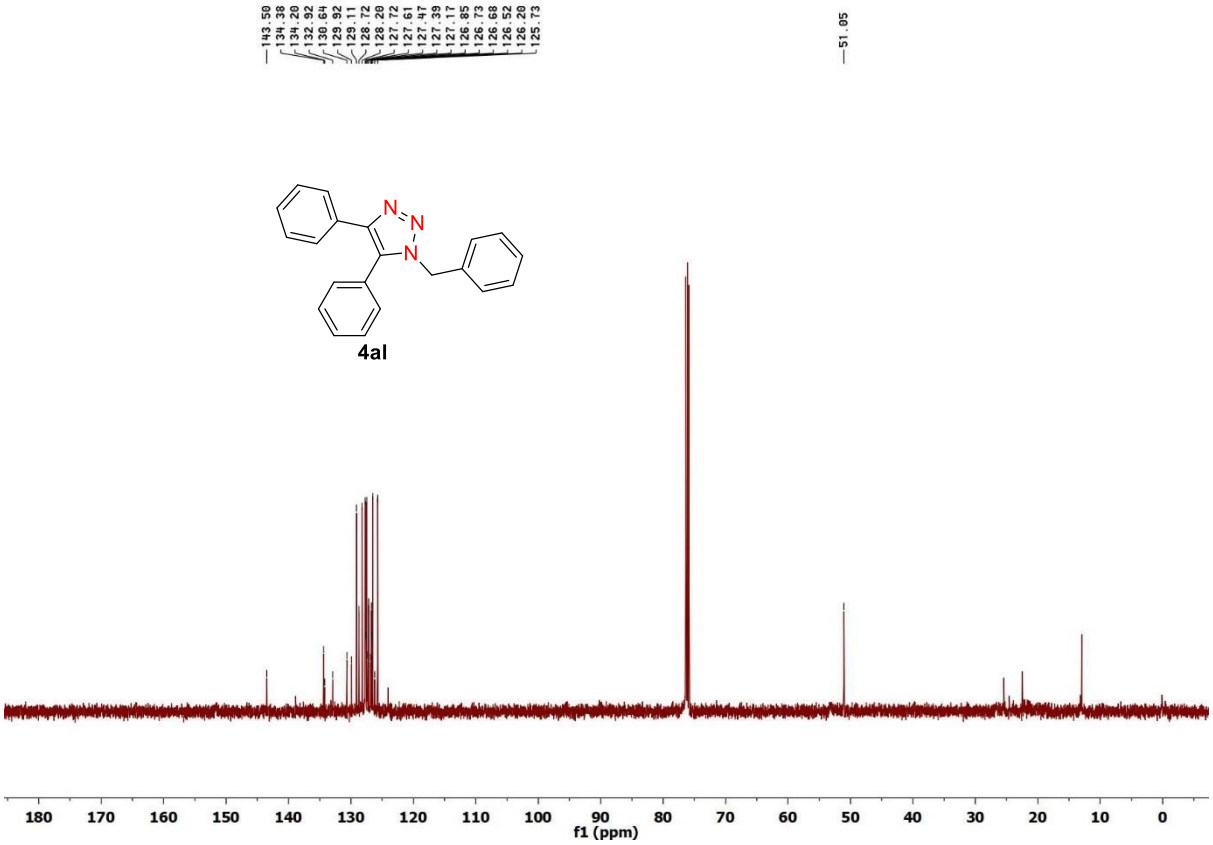


Fig. S41: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4al**.

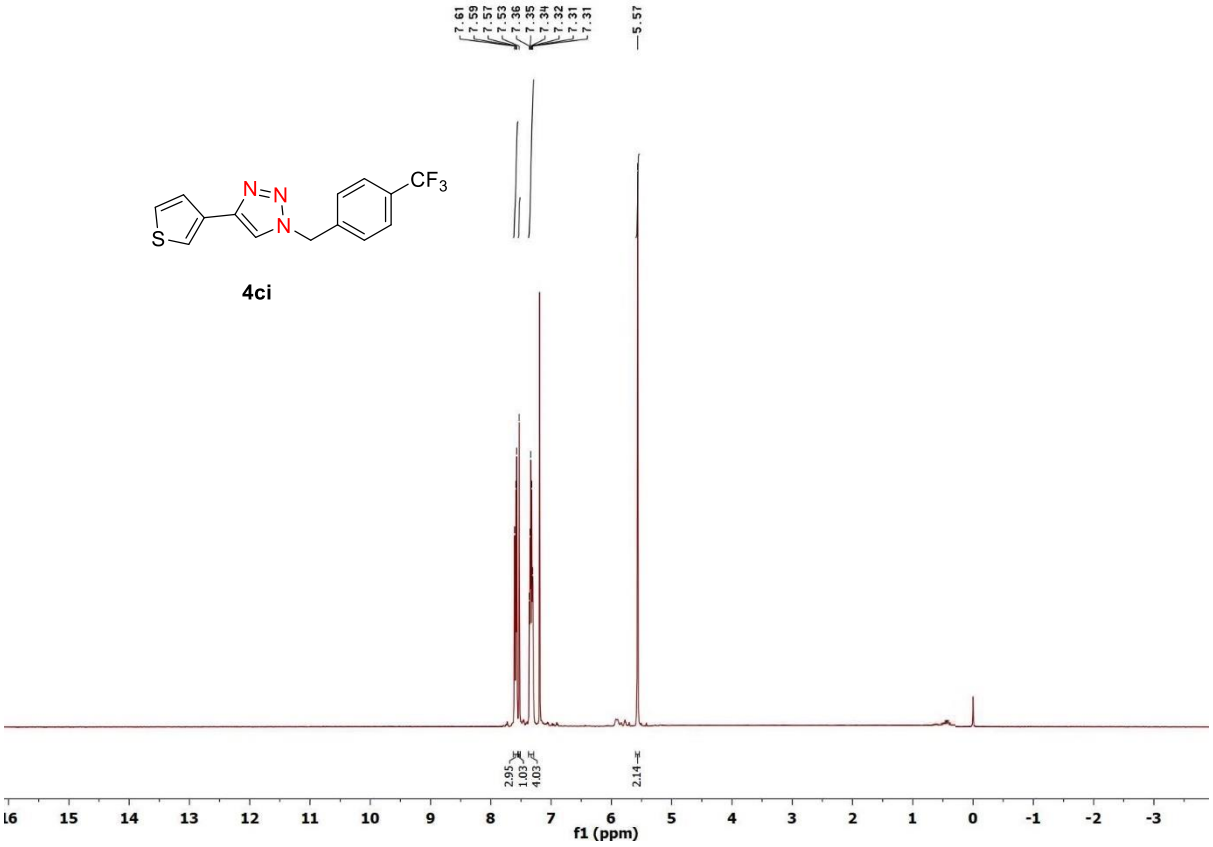


Fig. S42: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4ci**.

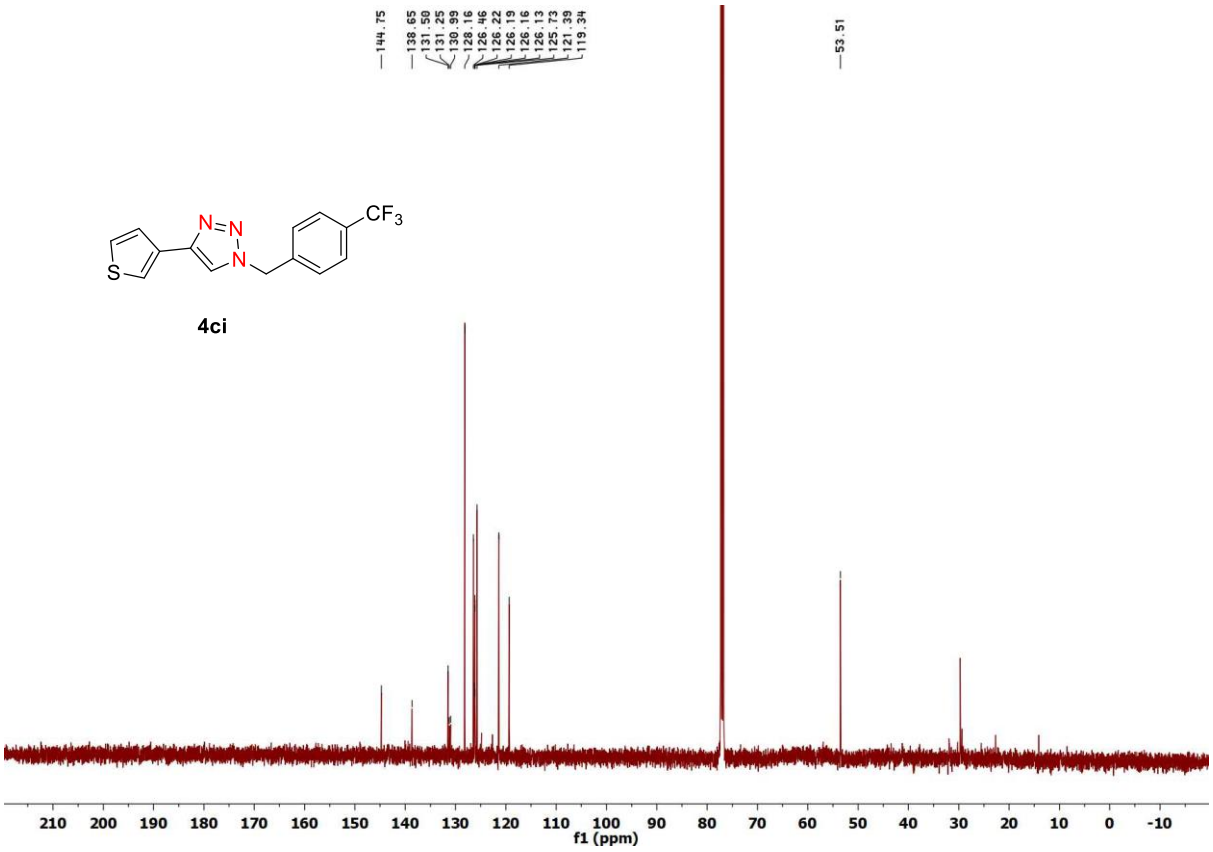


Fig. S43: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4ci**.

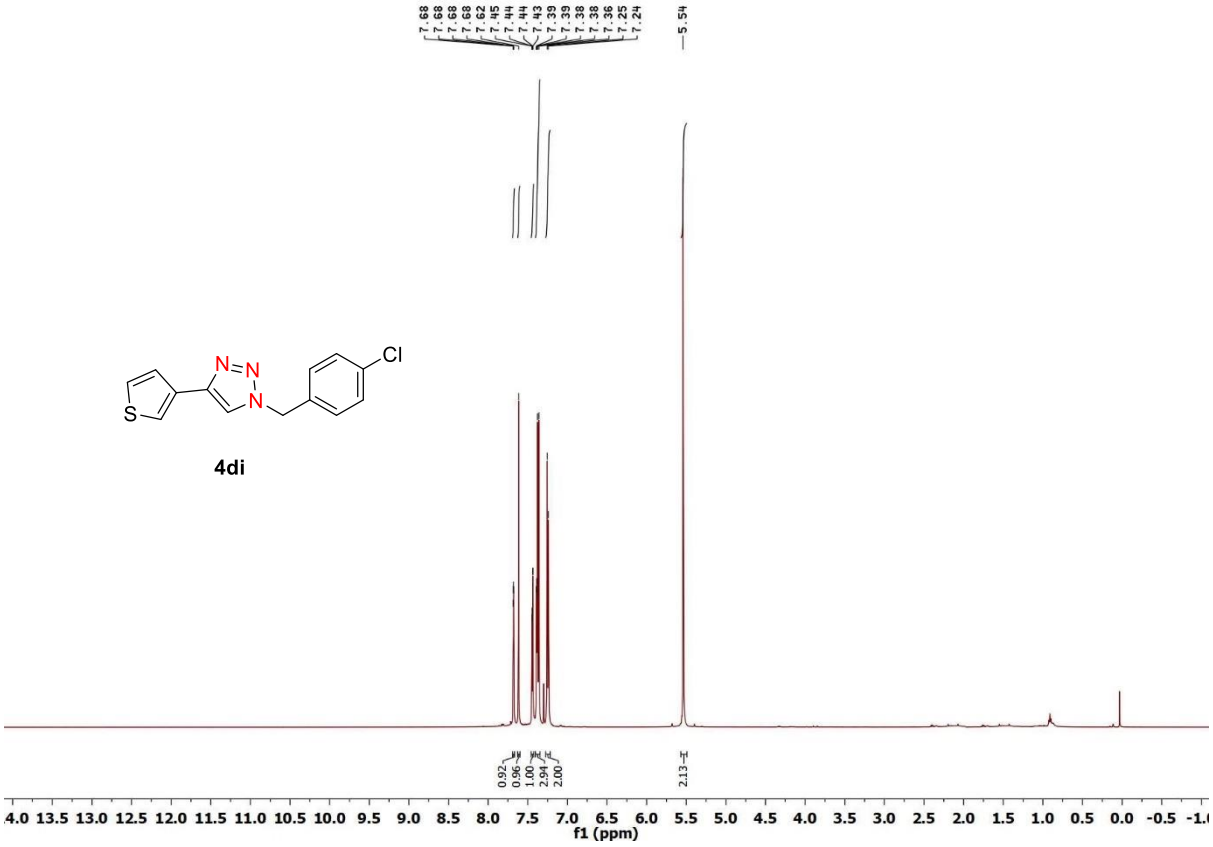


Fig. S44: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4di**.

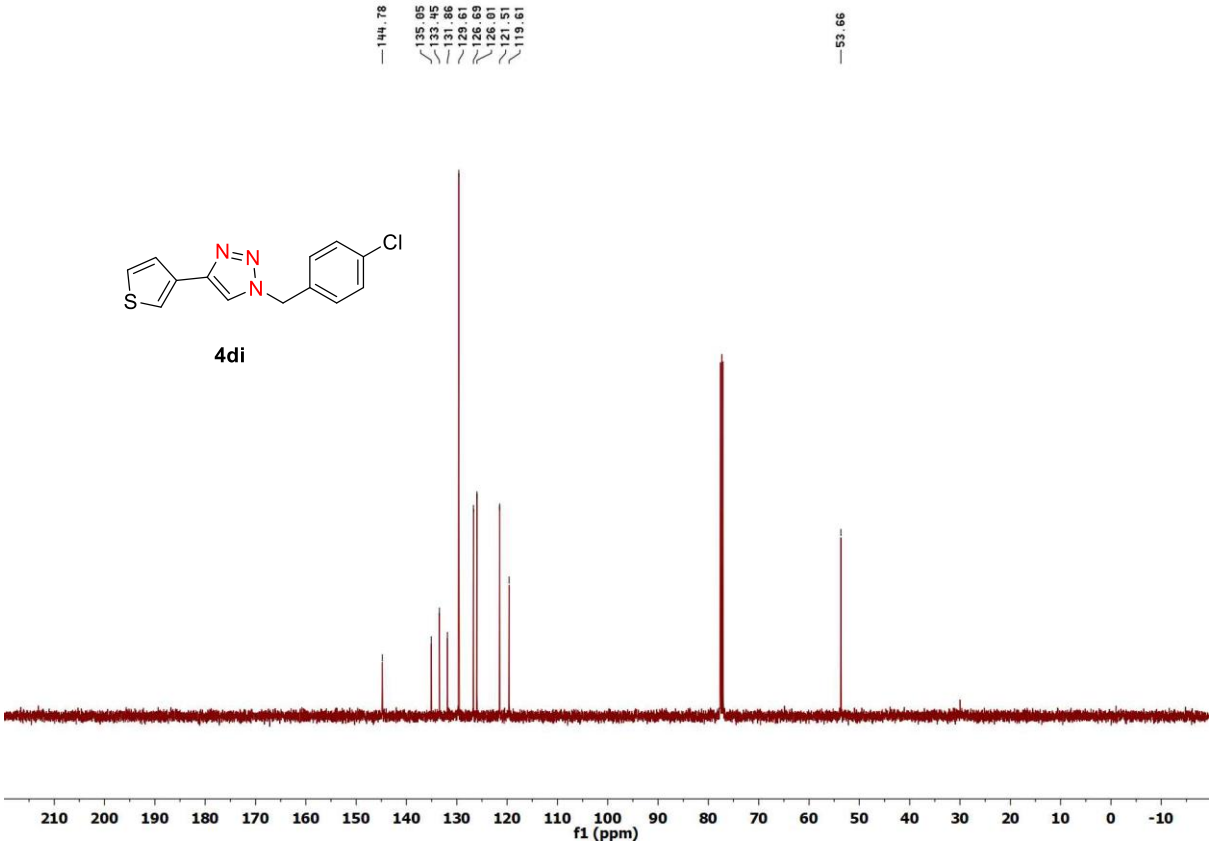


Fig. S45: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4di**.

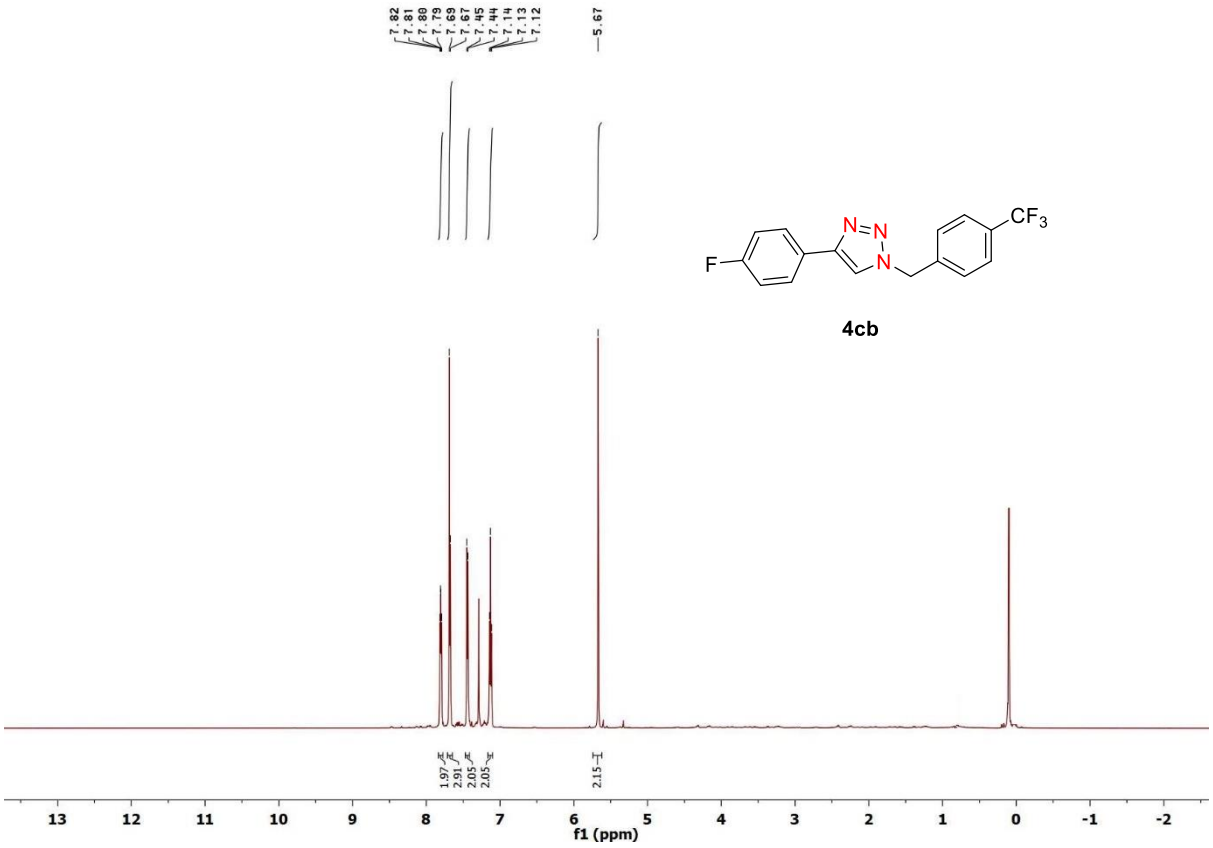


Fig. S46: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4cb**.

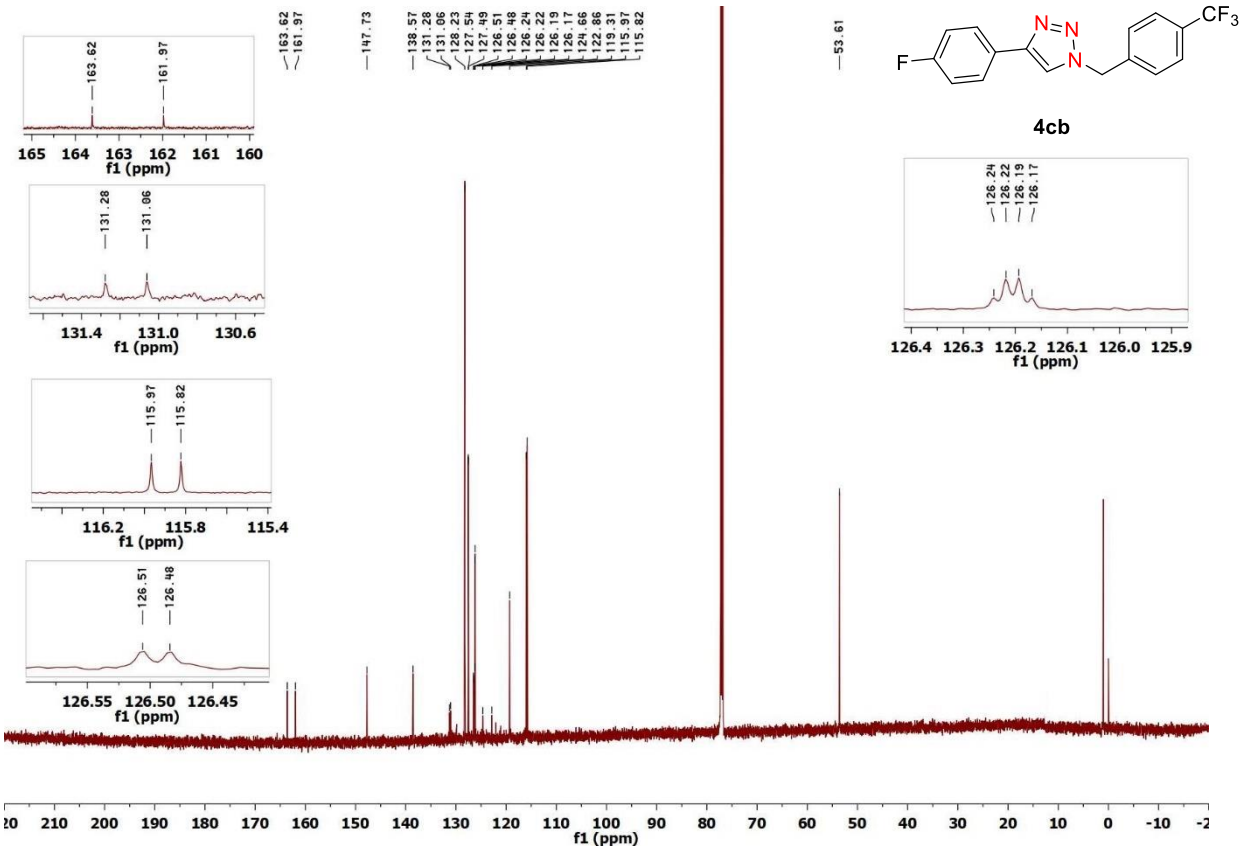


Fig. S47: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4cb**.

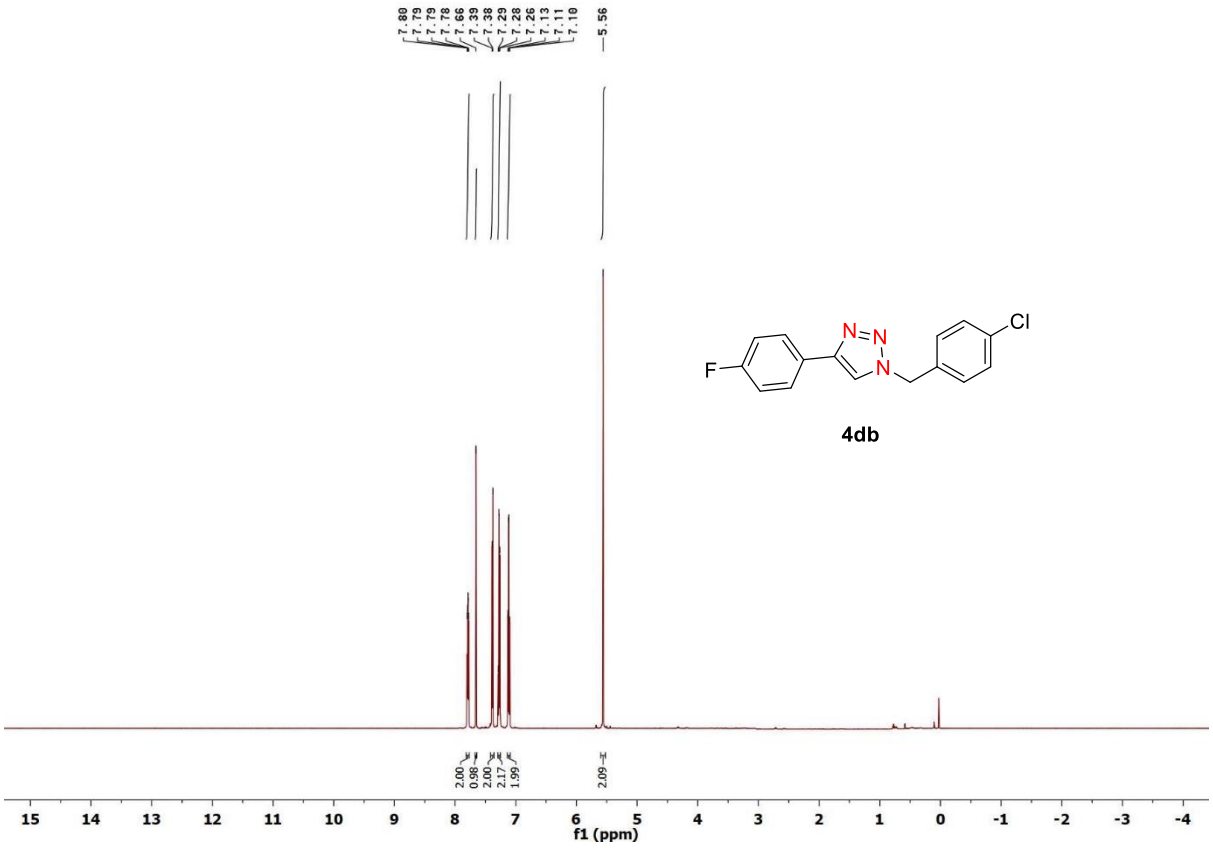


Fig. S48: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4db**.

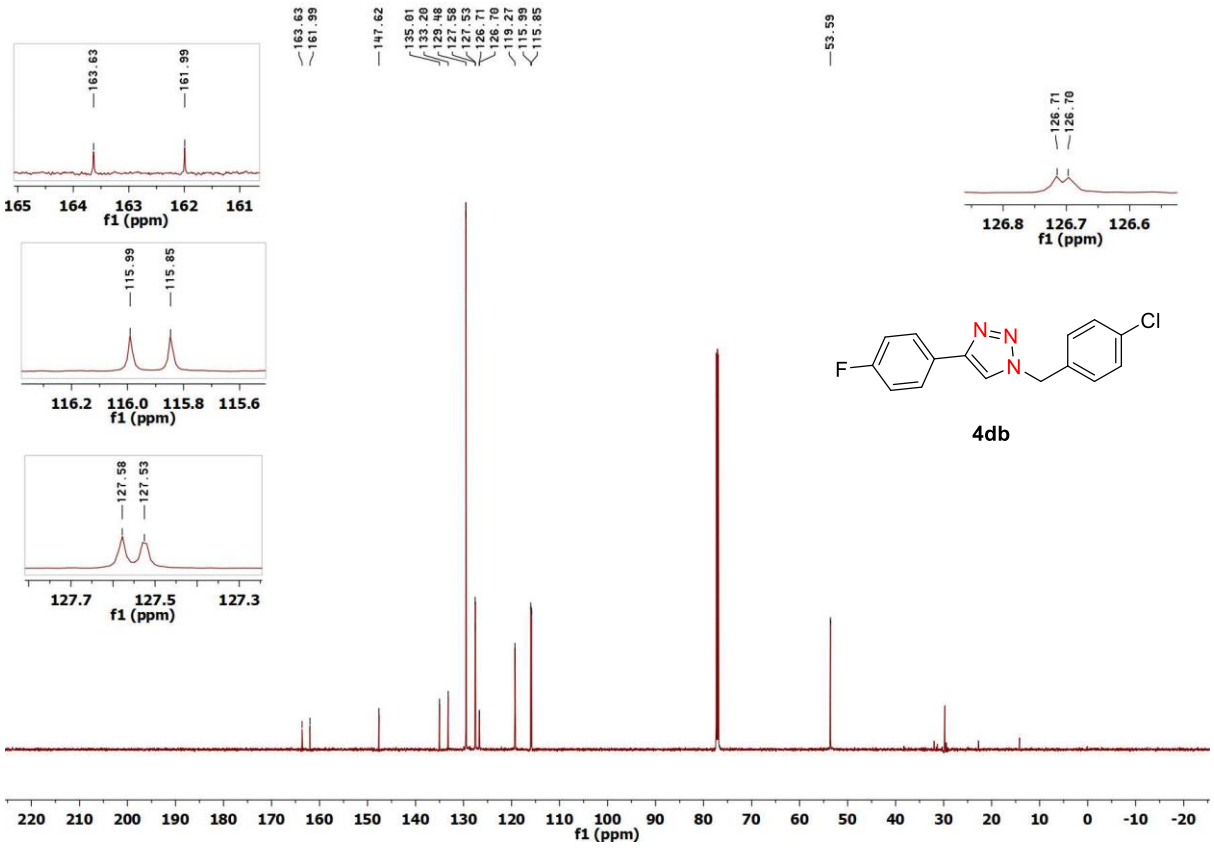


Fig. S49: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4db**.

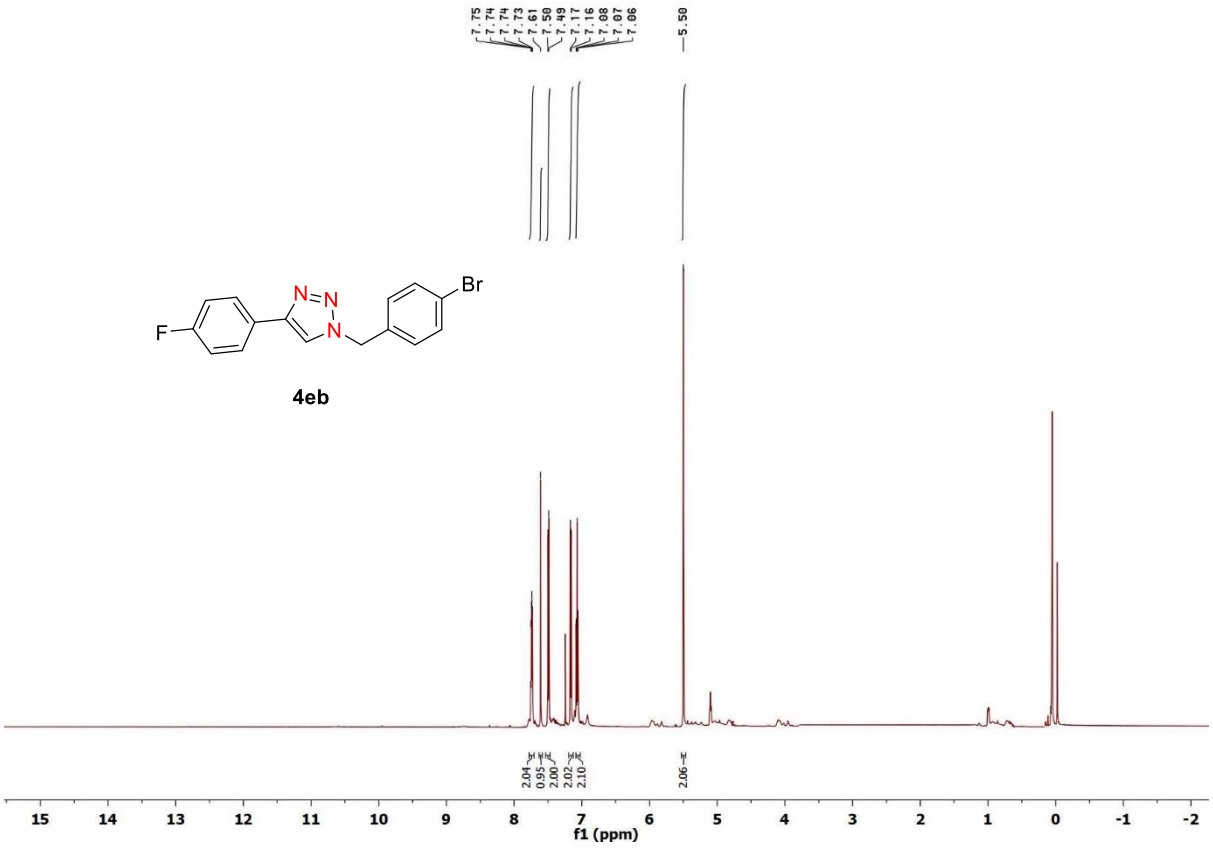


Fig. S50: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4eb**.

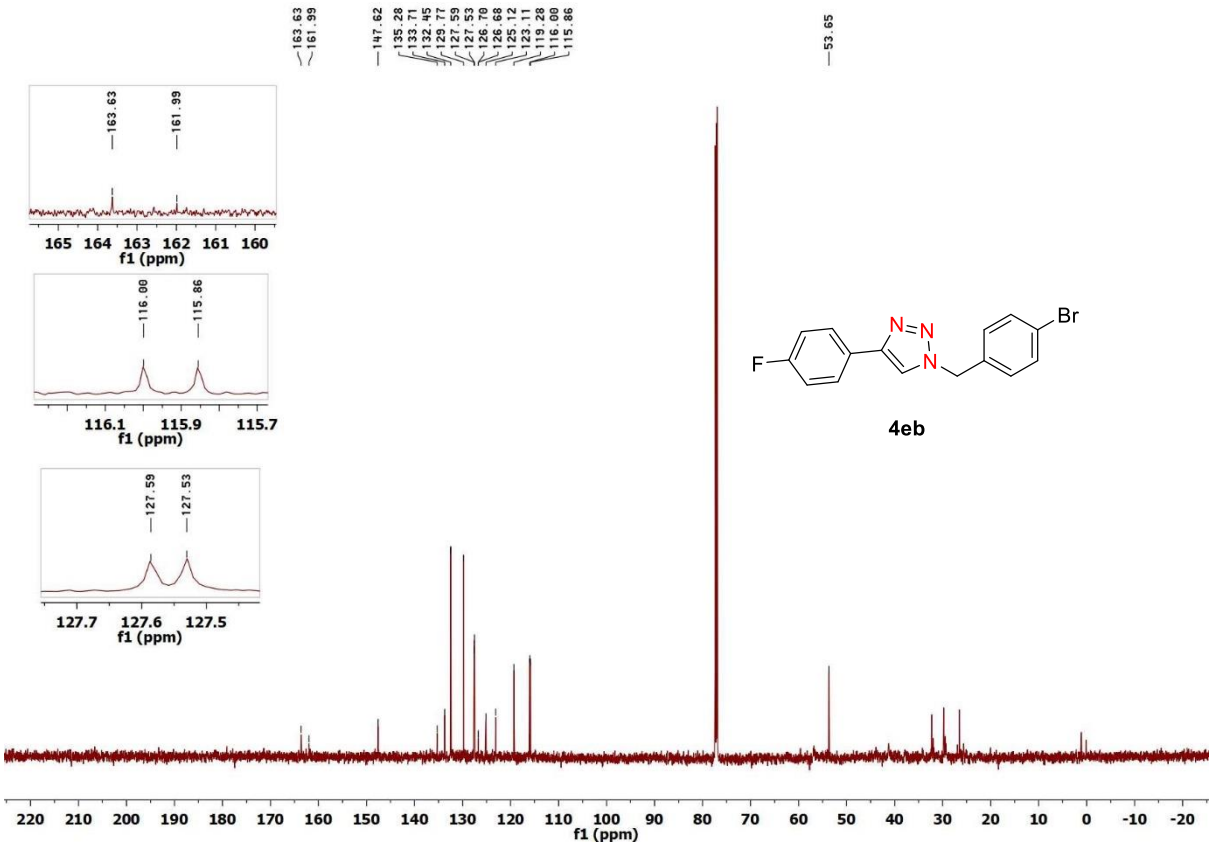


Fig. S51: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4eb**.

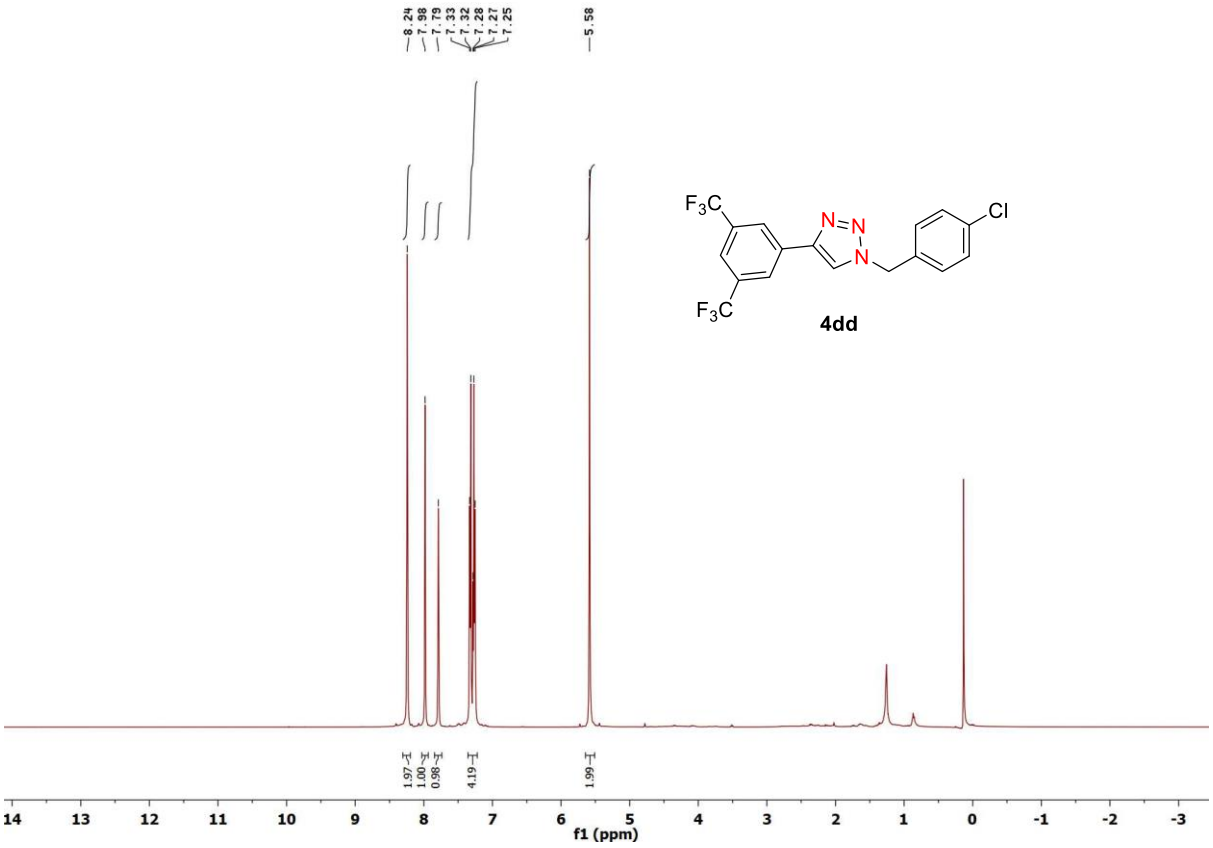


Fig. S52: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4dd**.

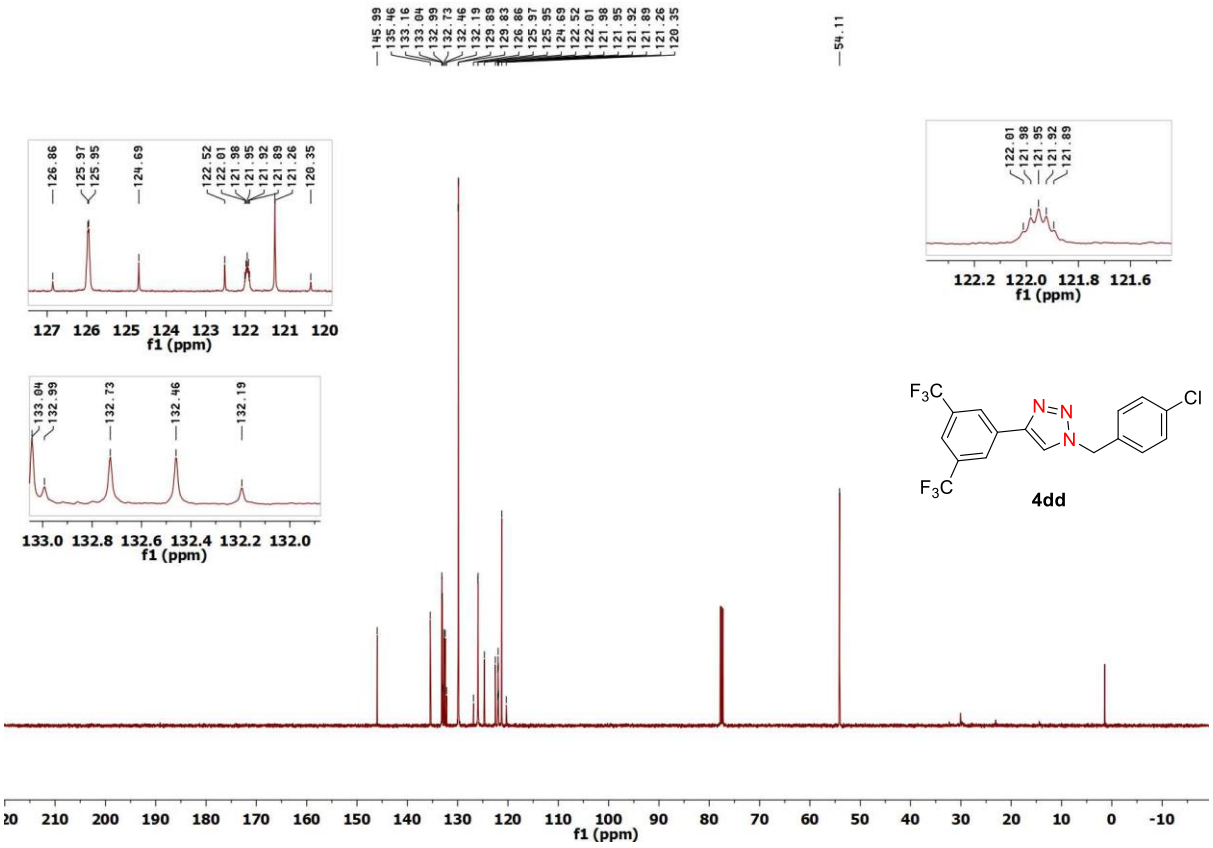


Fig. S53: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4dd**.

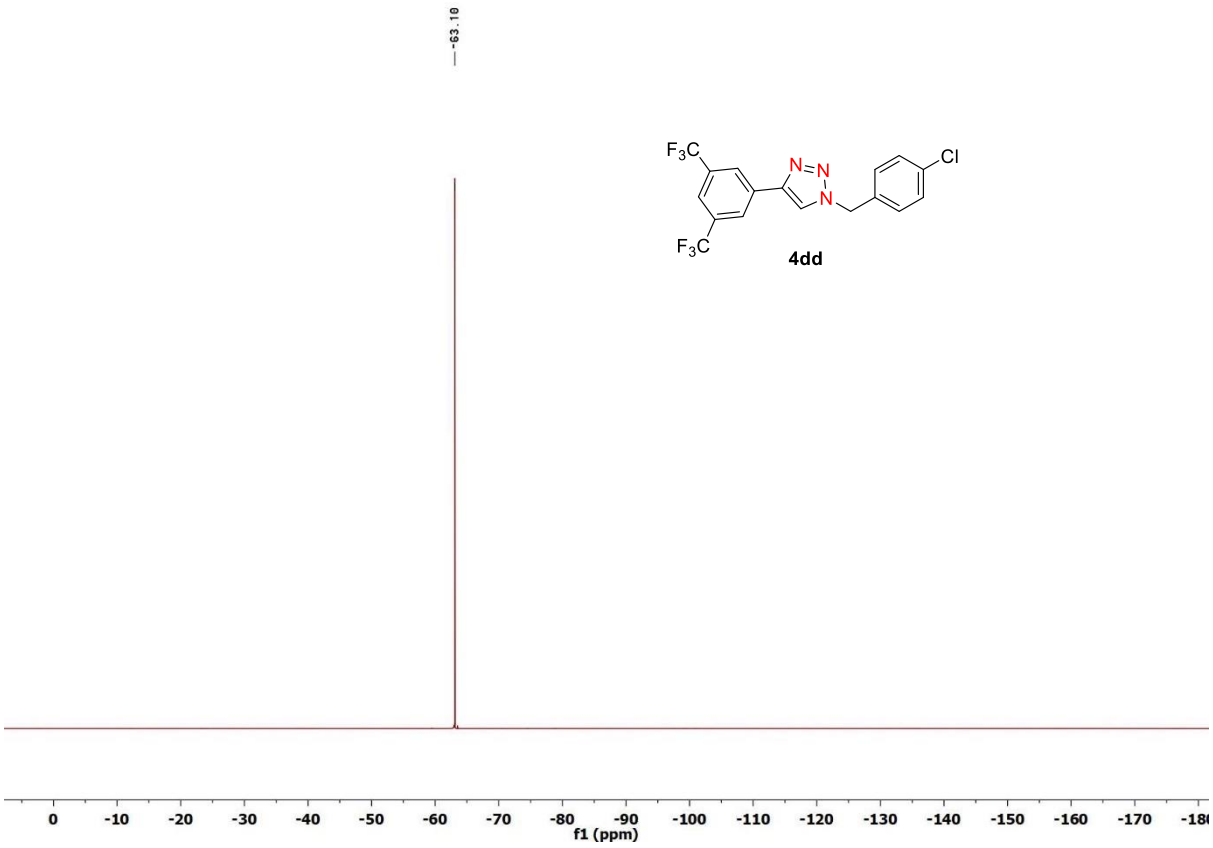


Fig. S54: ^{19}F NMR (470 MHz, $CDCl_3$) of the compound **4dd**.

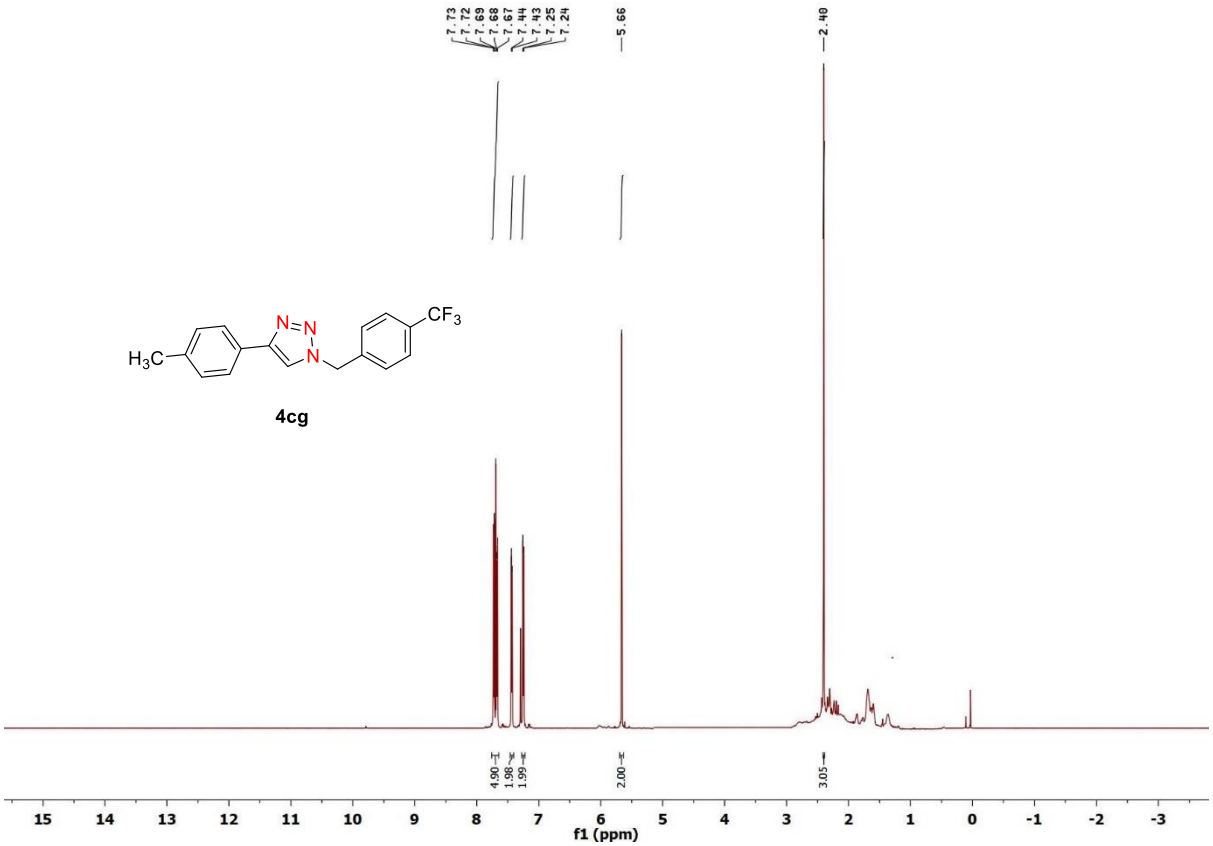


Fig. S55: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4cg**.

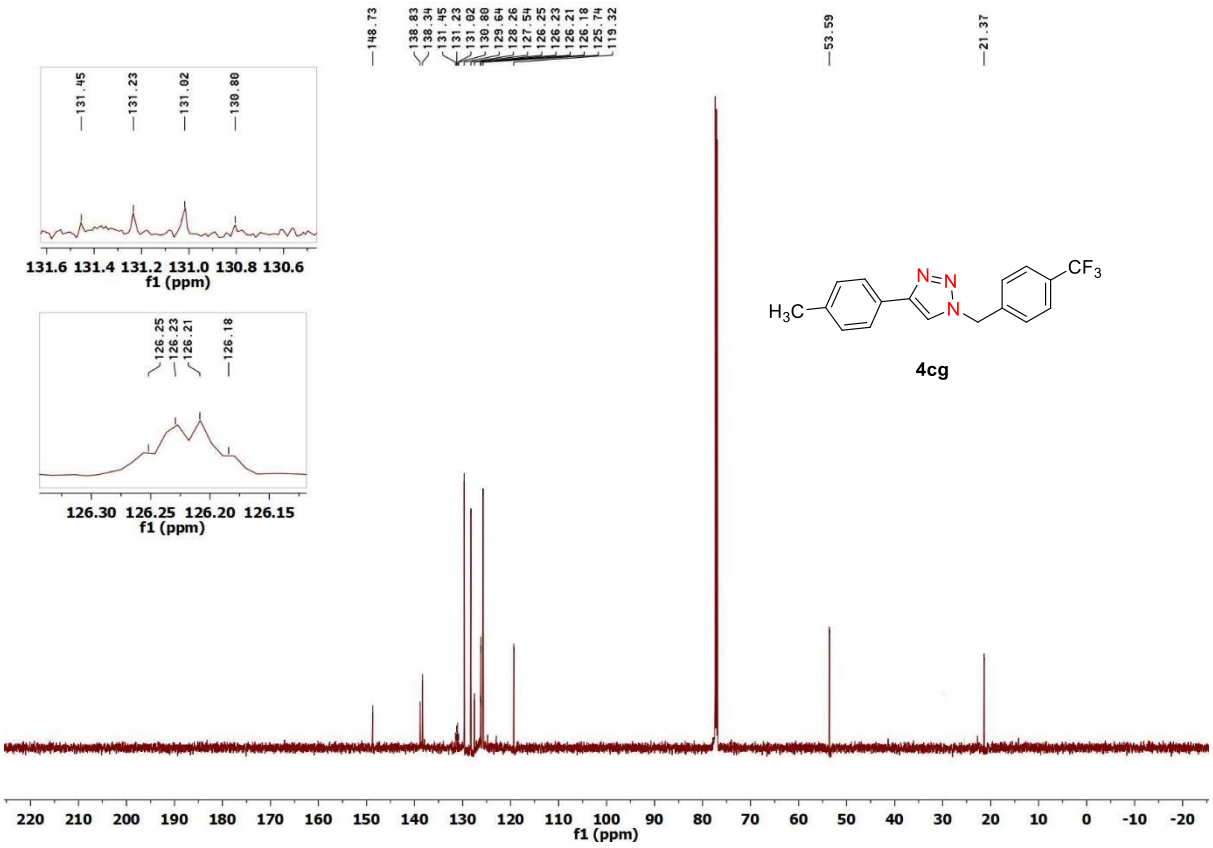


Fig. S56: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4cg**.

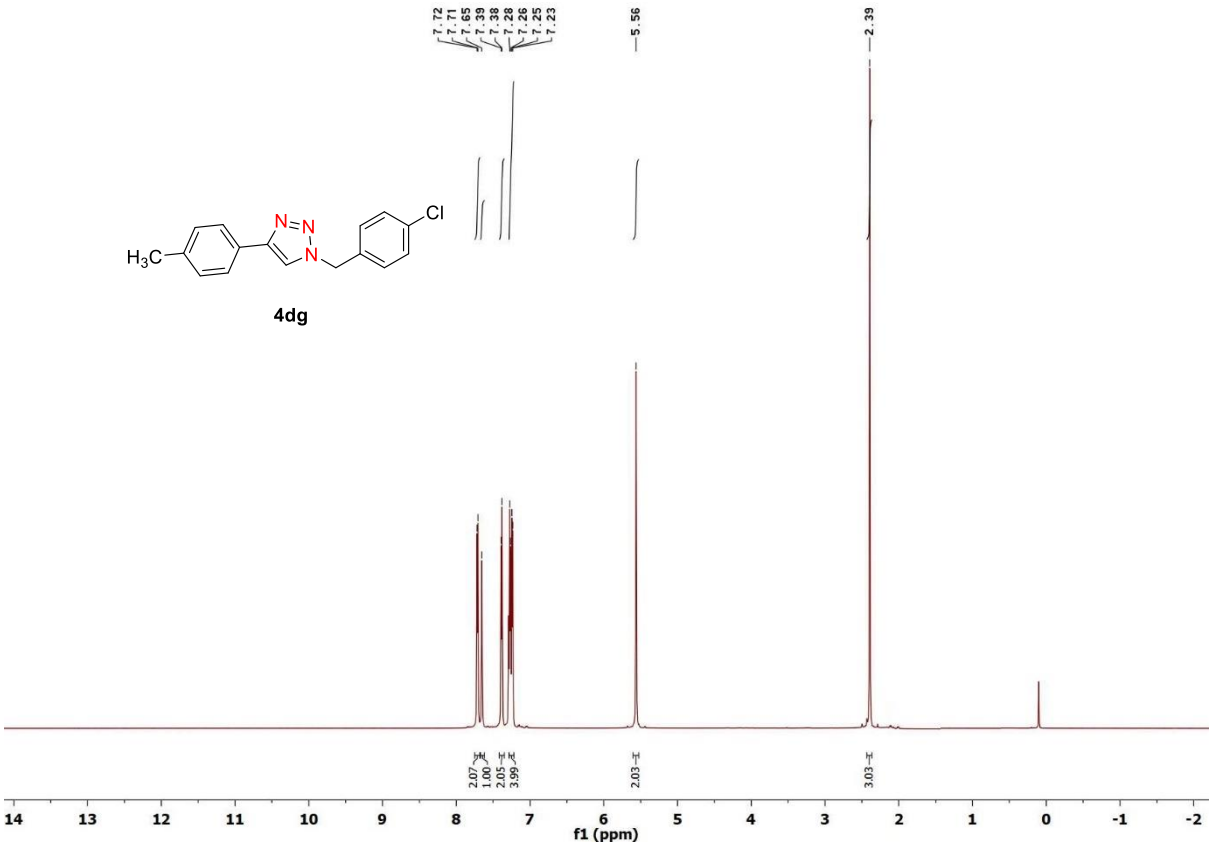


Fig. S57: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4dg**.

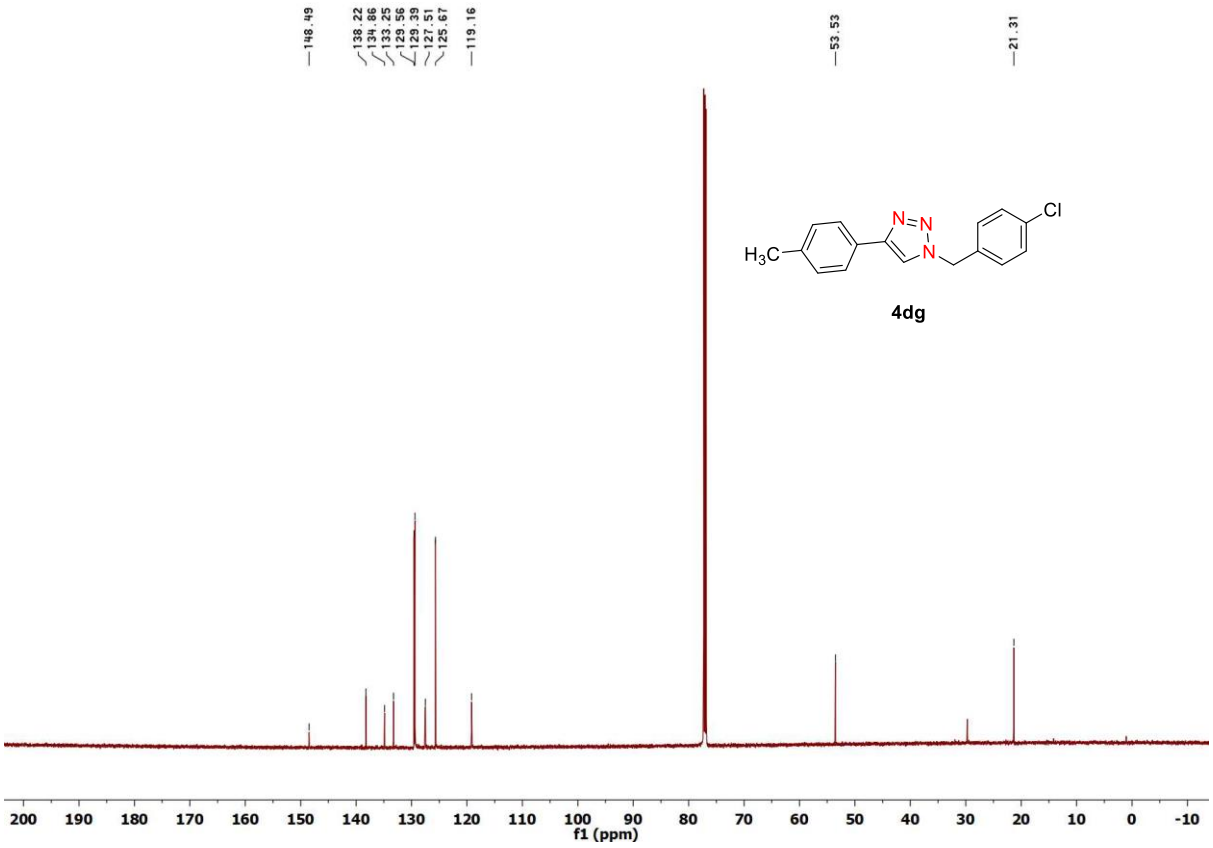


Fig. S58: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4dg**.

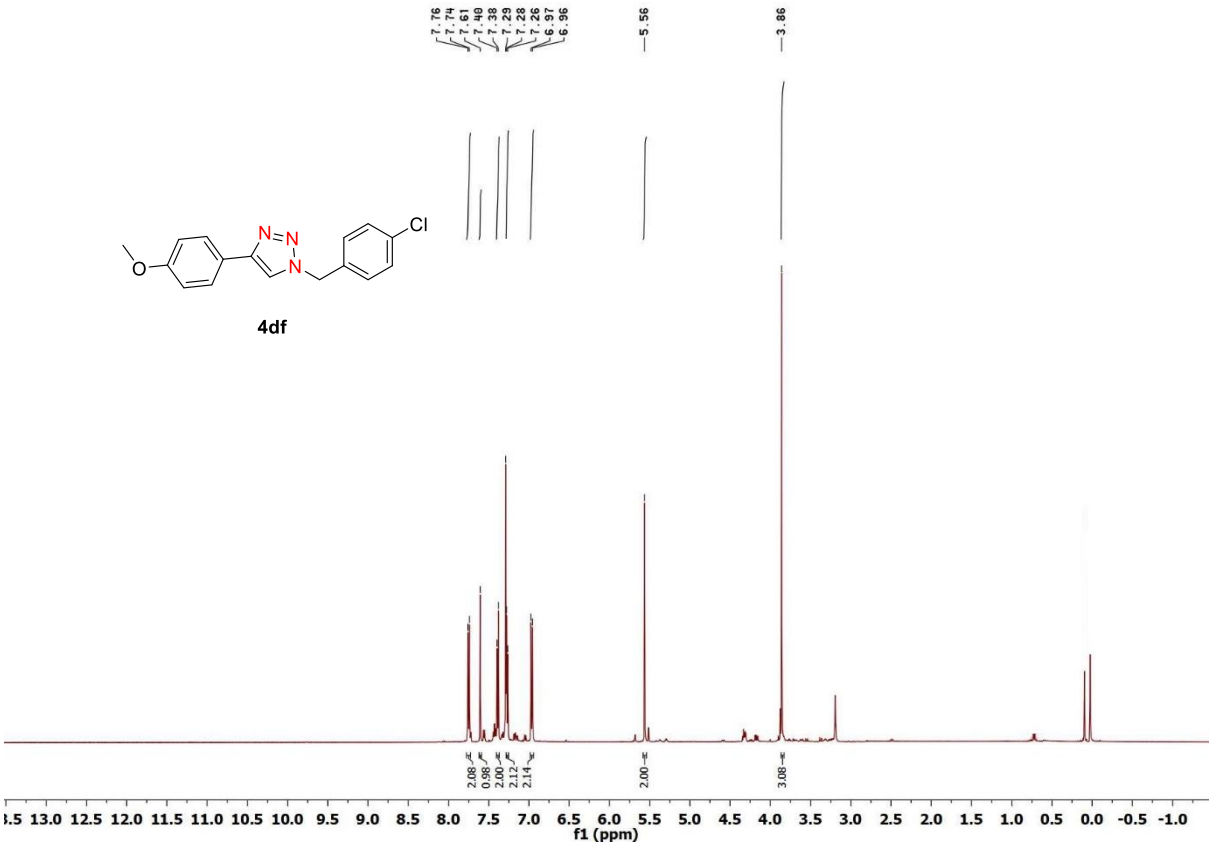


Fig. S59: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **4df**.

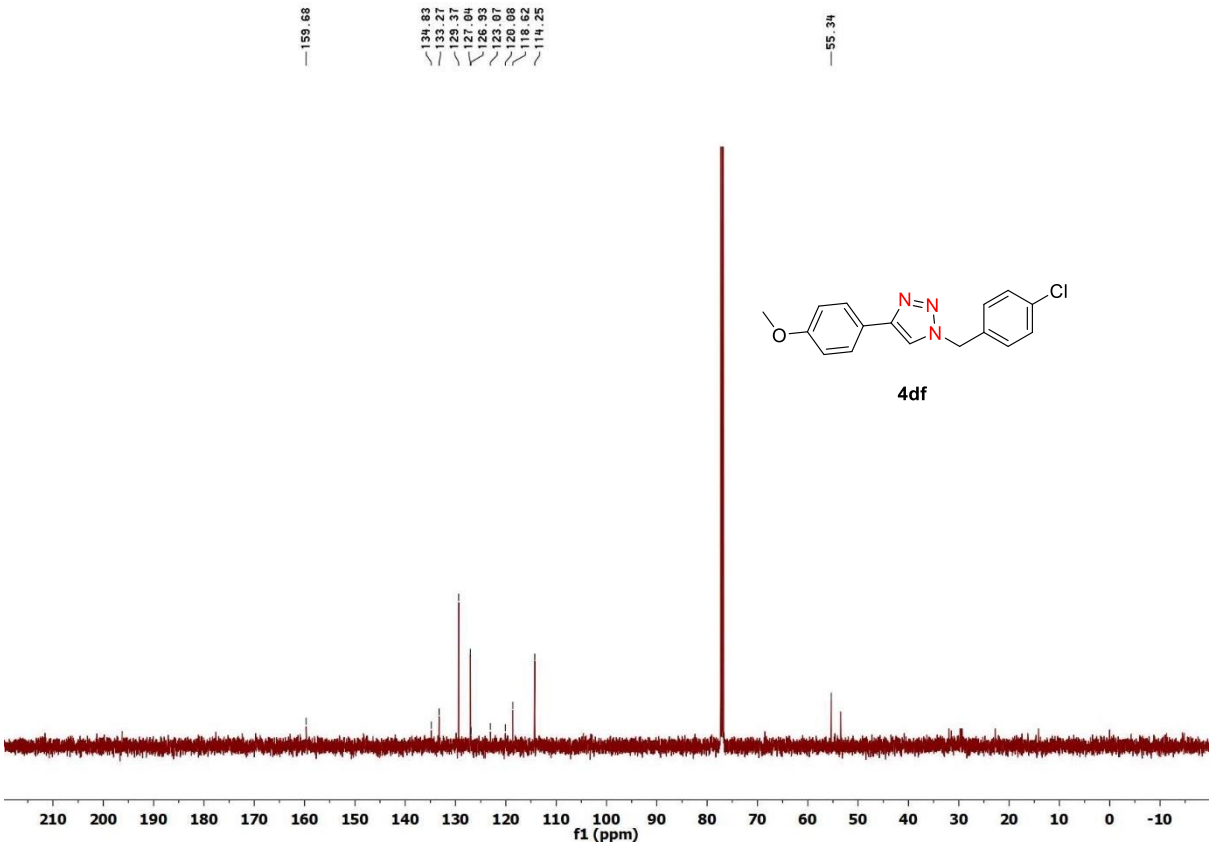


Fig. S60: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **4df**.

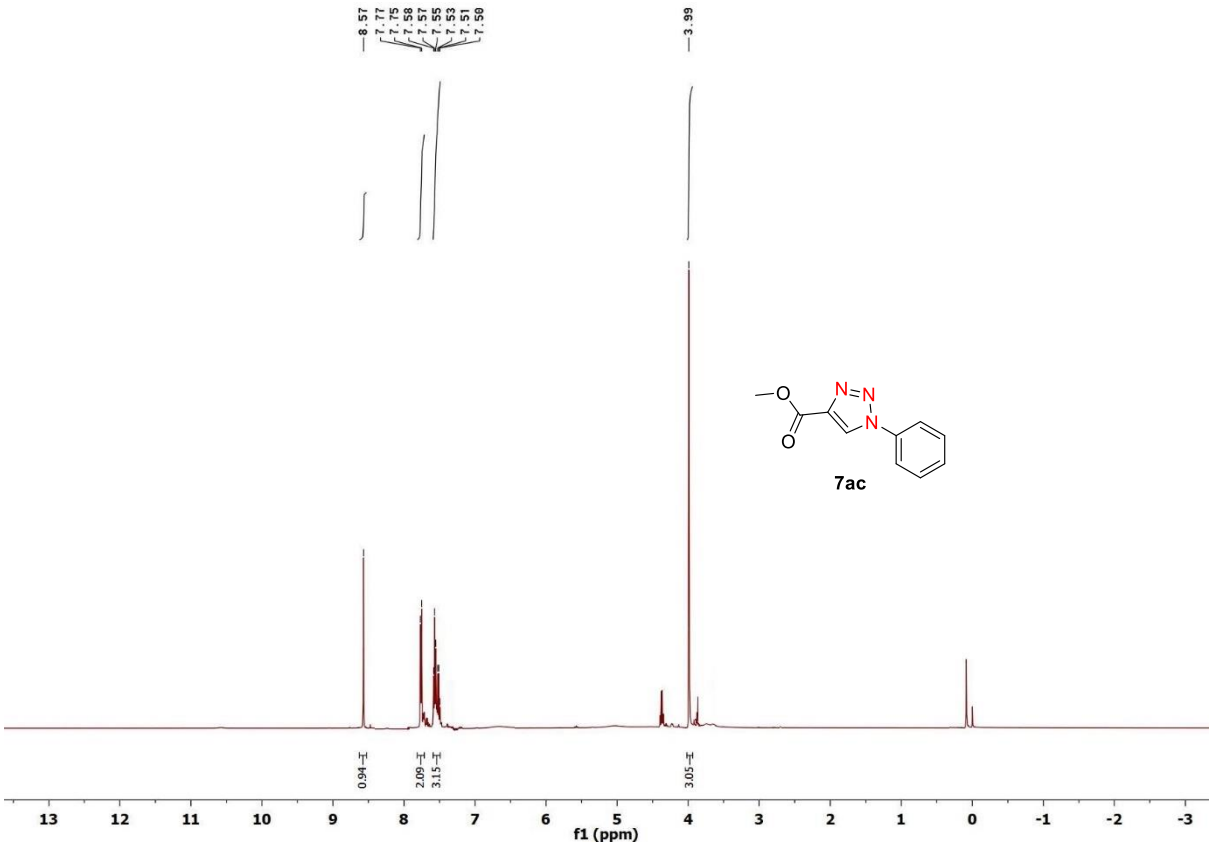


Fig. S61: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **7ac**.

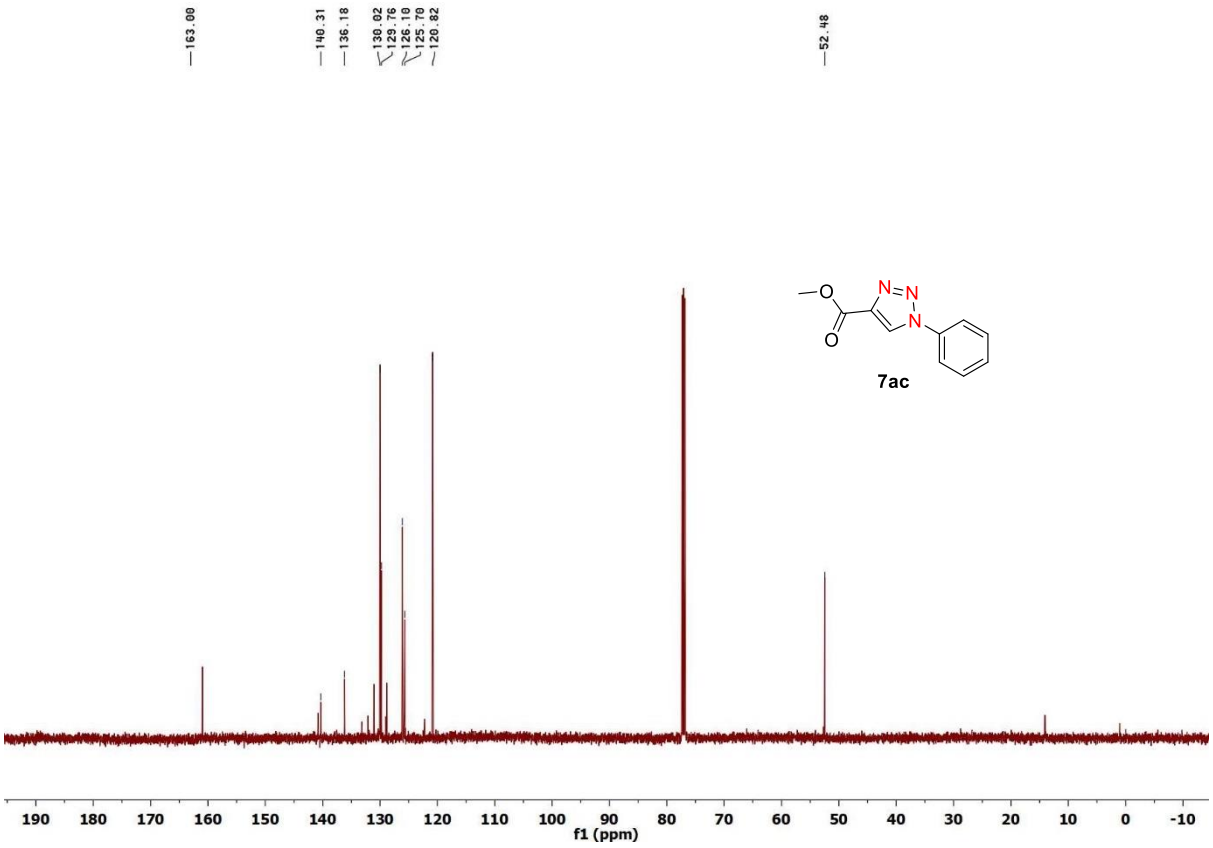


Fig. S62: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **7ac**.

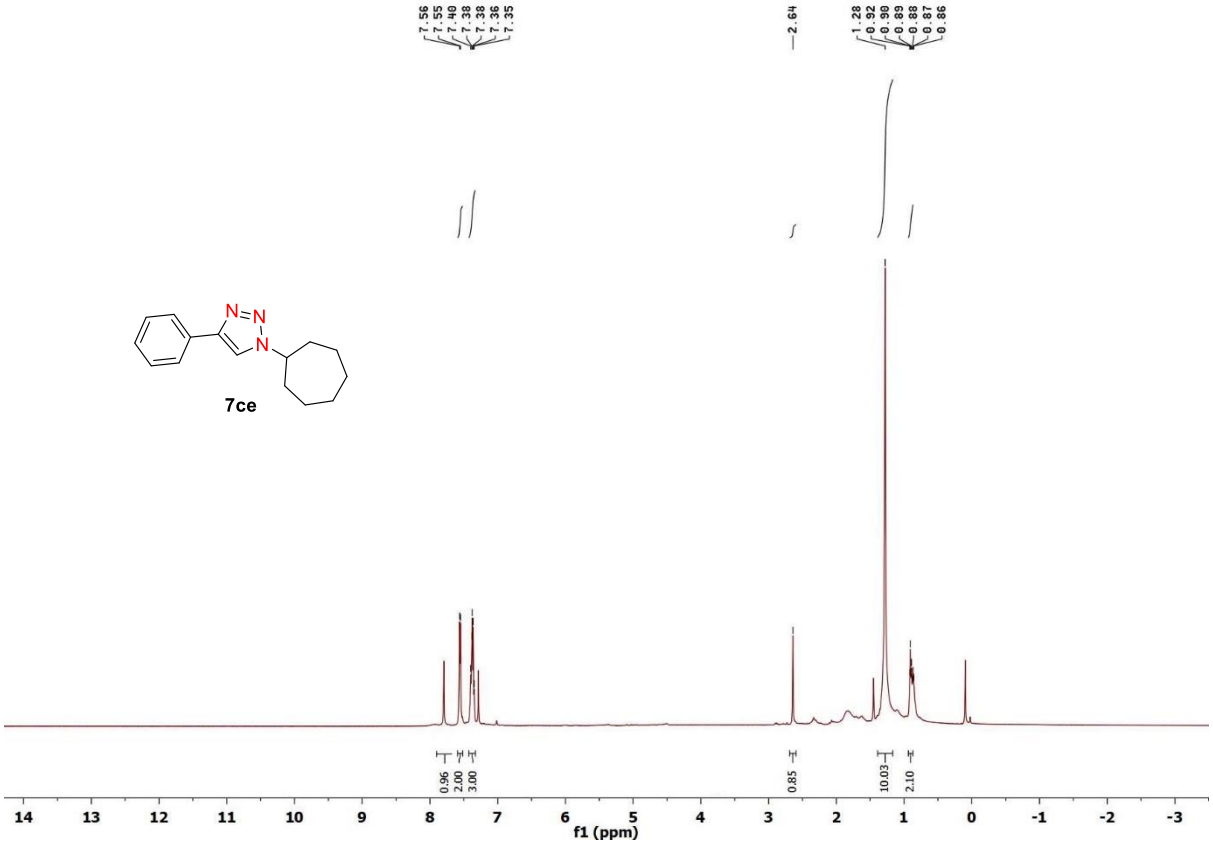


Fig. S63: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **7ce**.

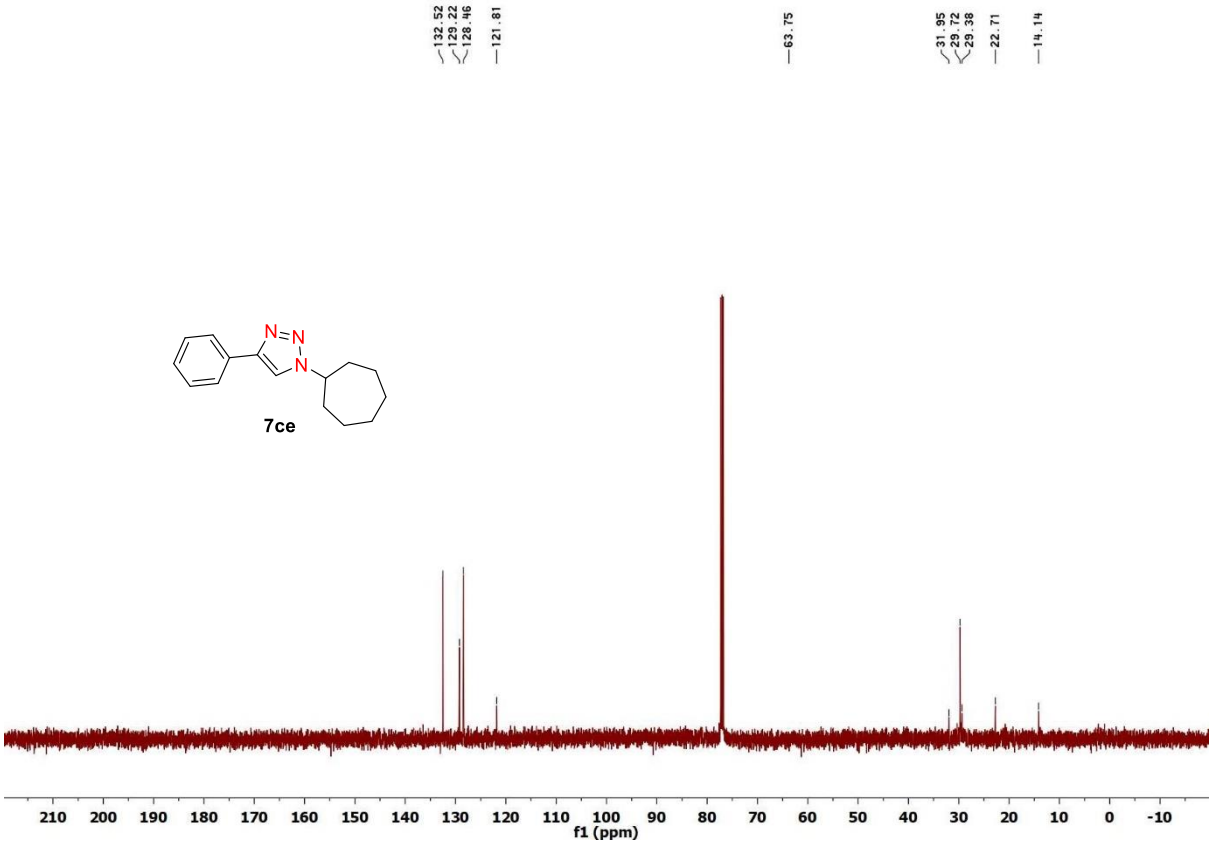


Fig. S64: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **7ce**.

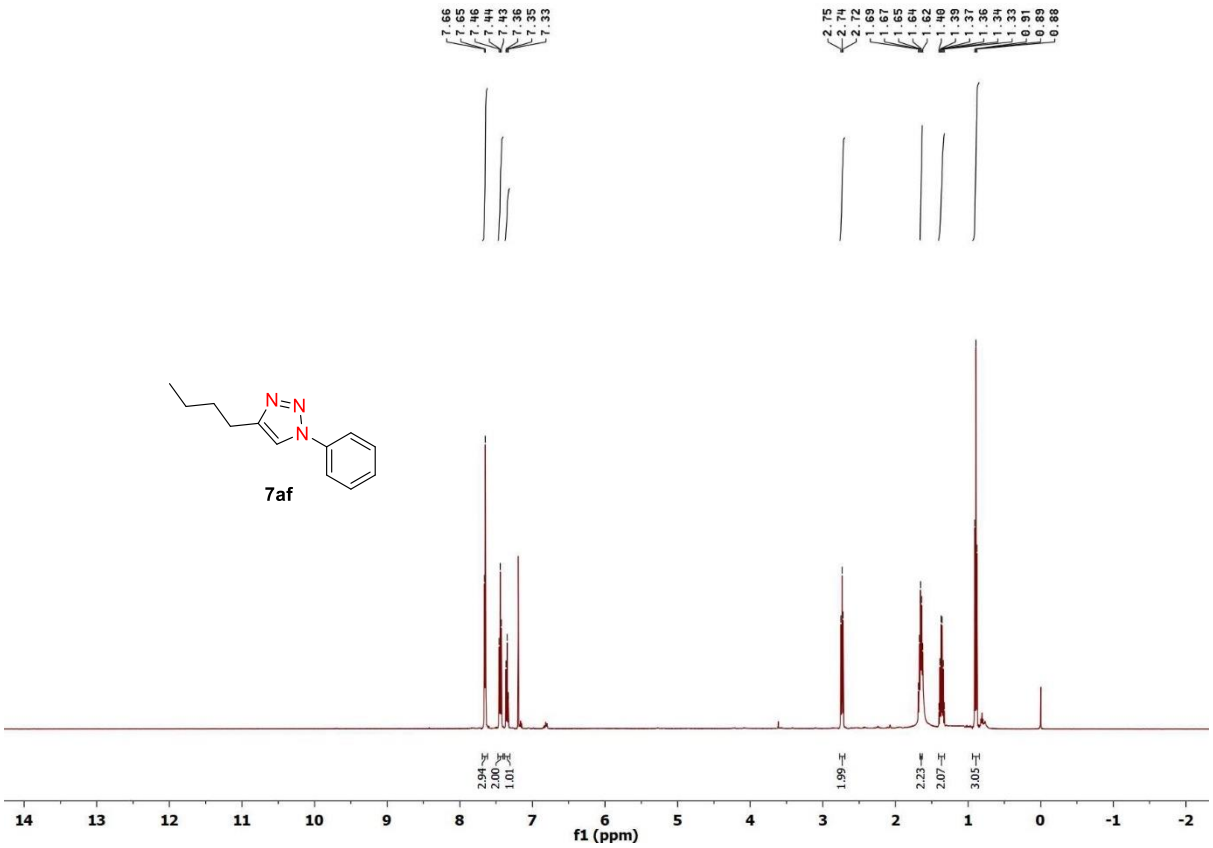


Fig. S65: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **7af**.

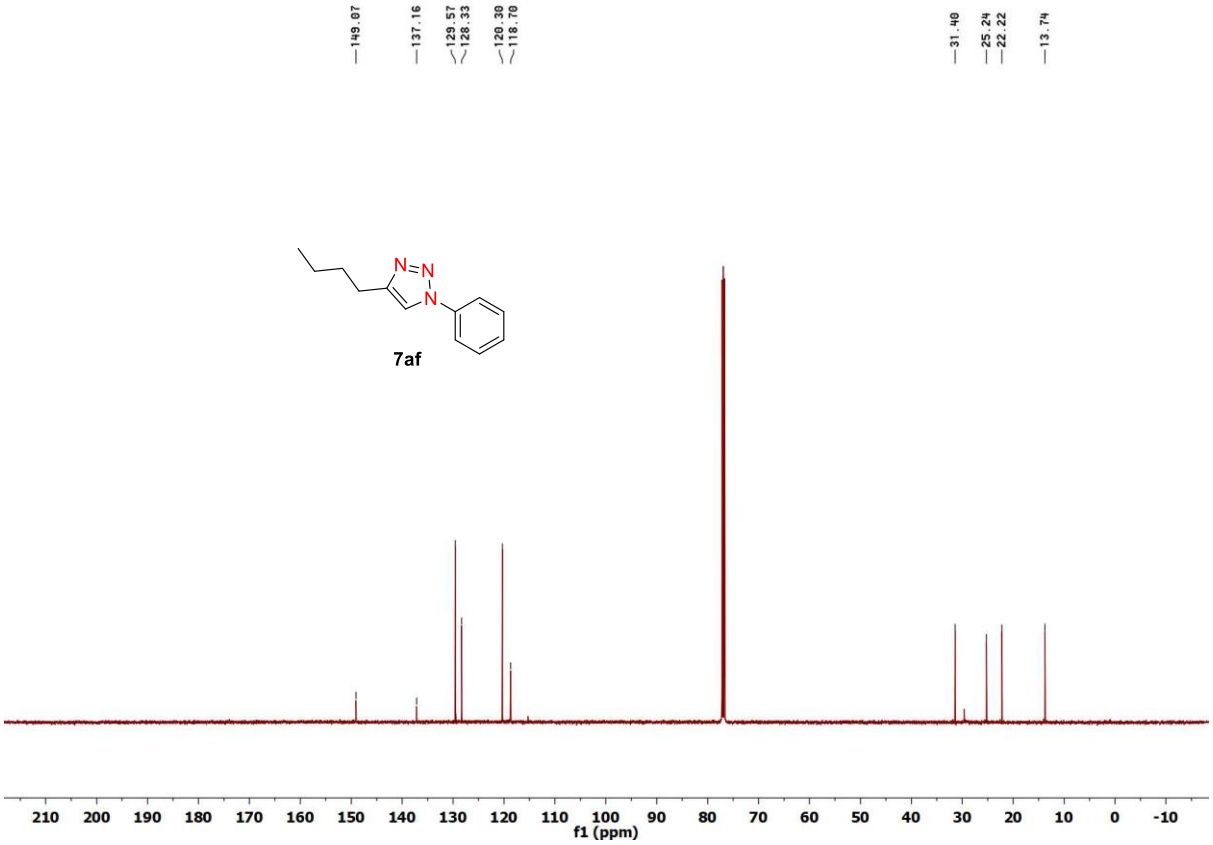


Fig. S66: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **7af**.

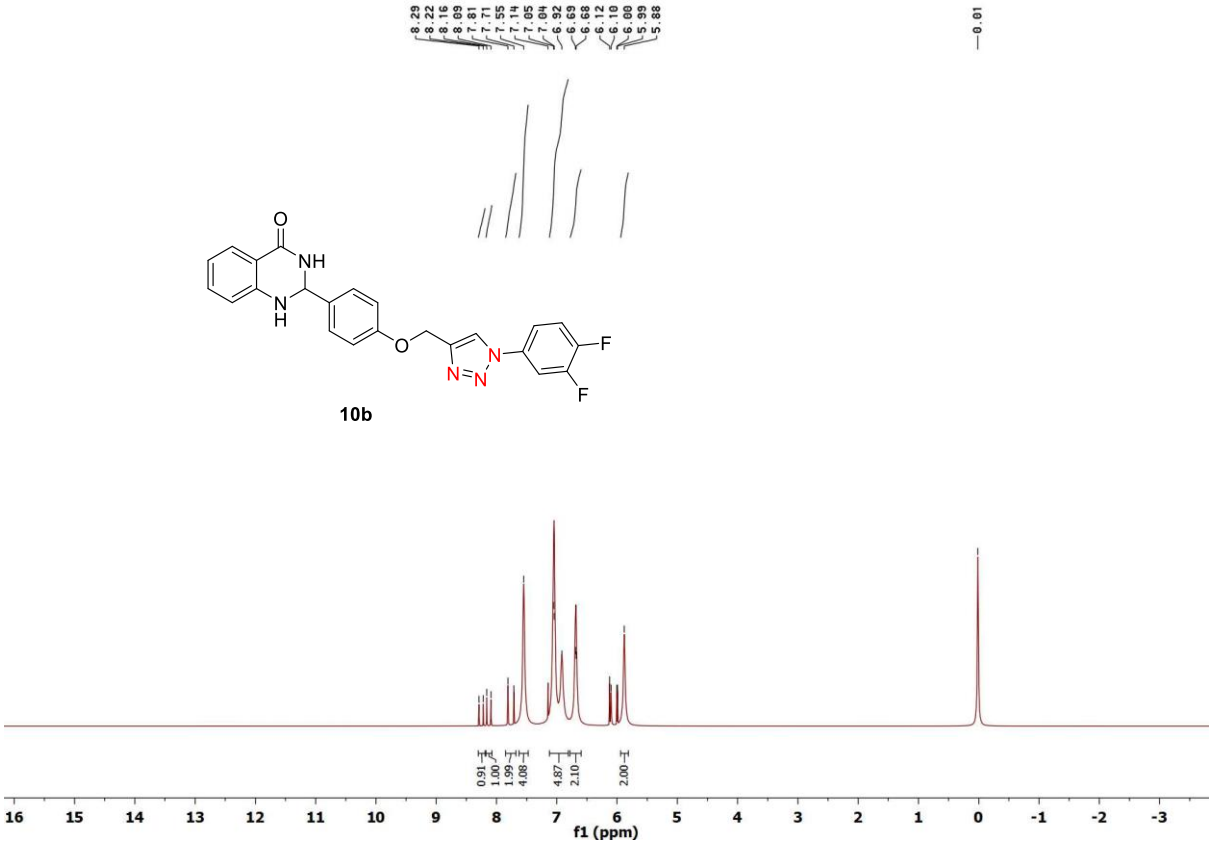


Fig. S67: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **10b**.

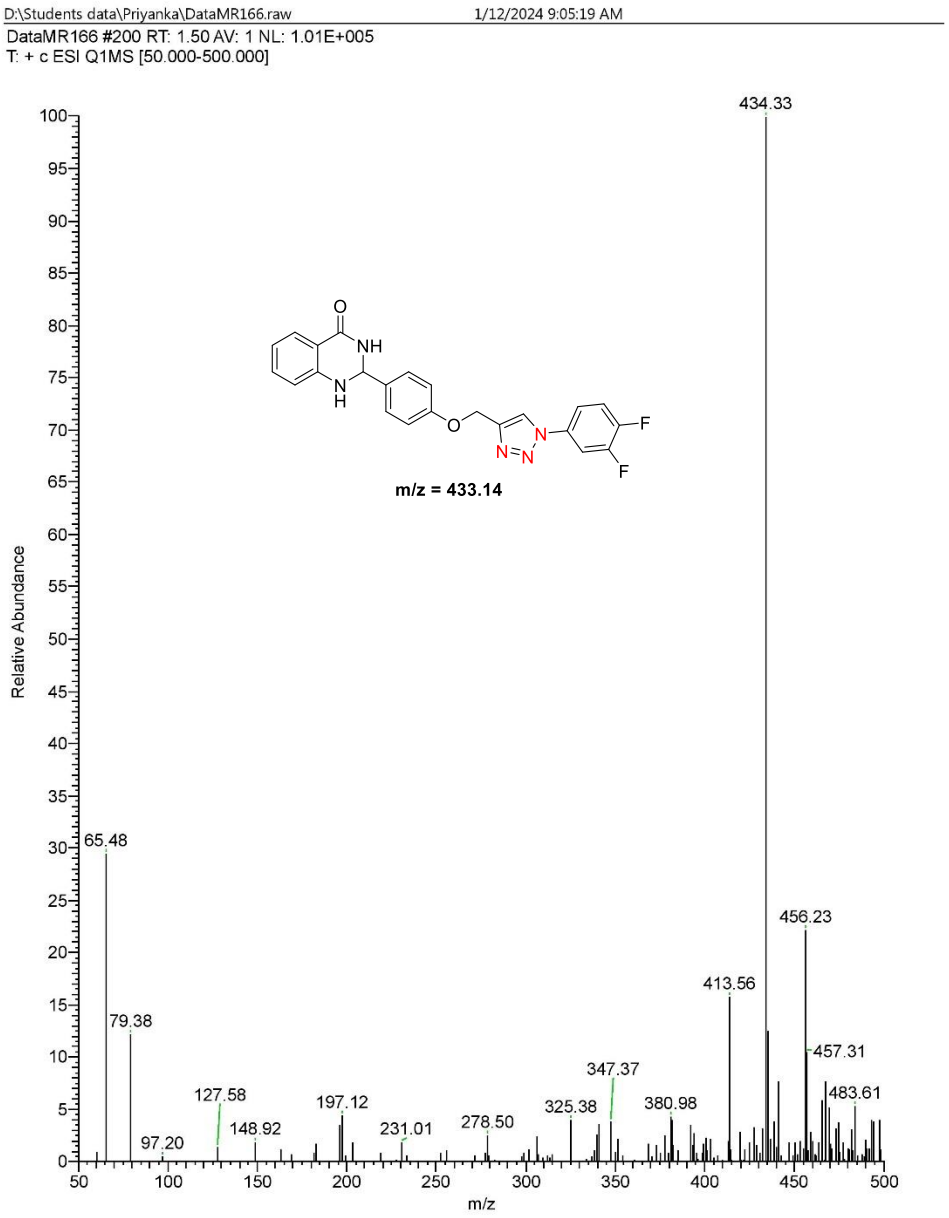


Fig. S68: LC-MS spectra of the compound **10b**.

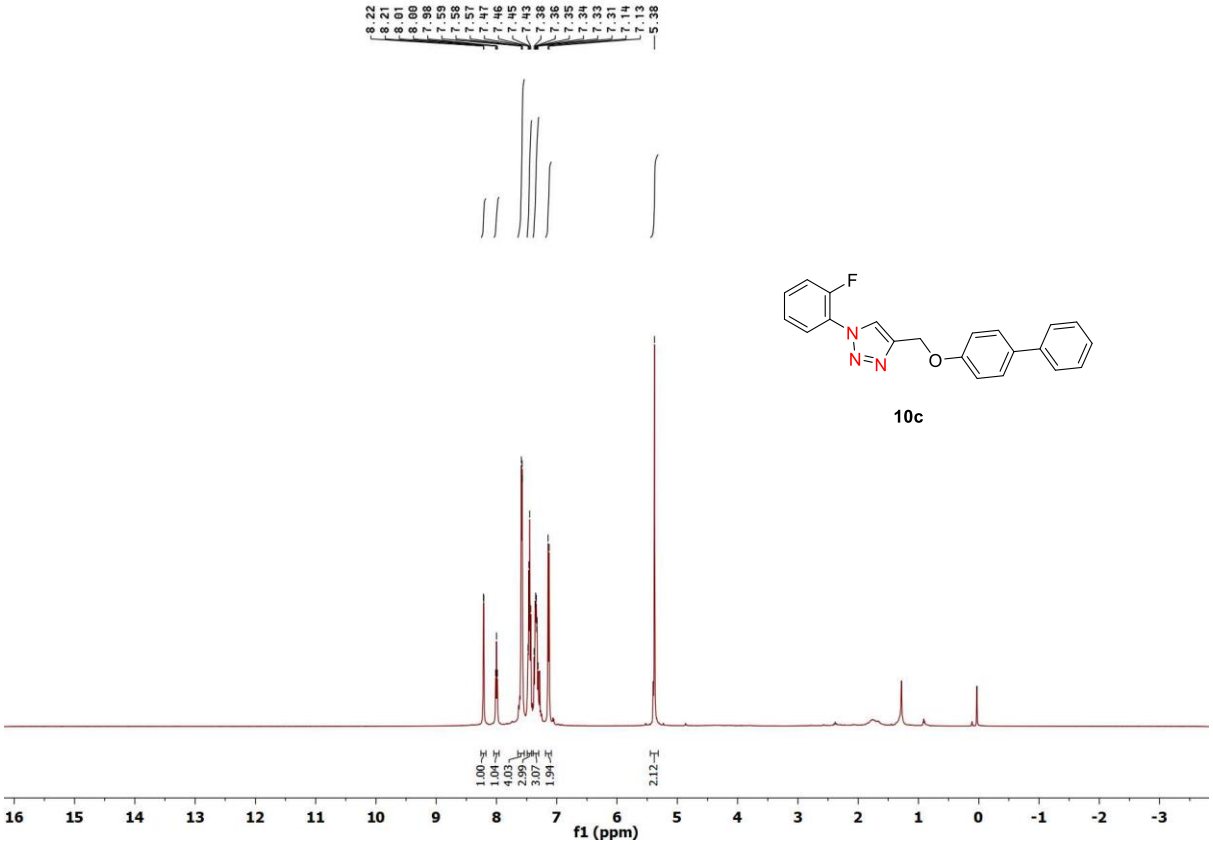


Fig. S69: ^{1}H NMR (500 MHz, $CDCl_3$) of the compound **10c**.

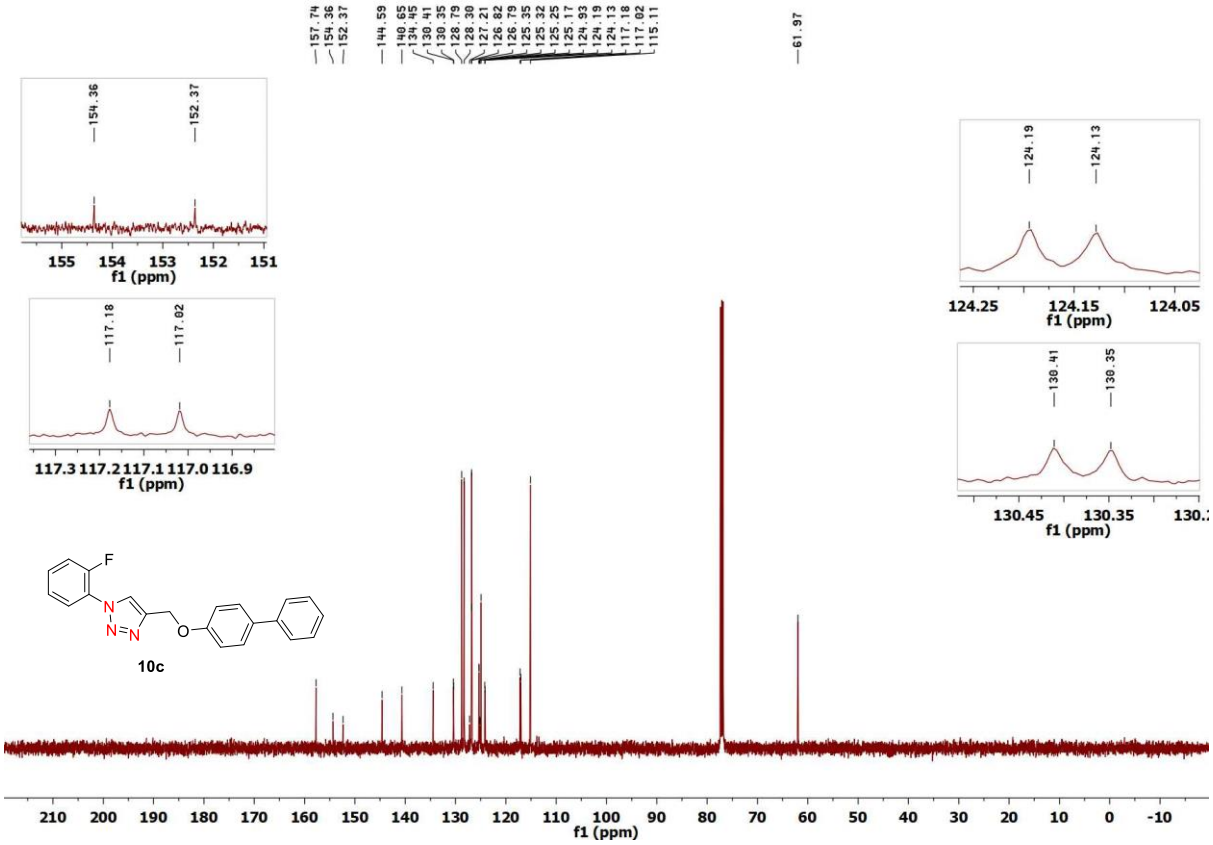


Fig. S70: ^{13}C NMR (125 MHz, $CDCl_3$) of the compound **10c**.

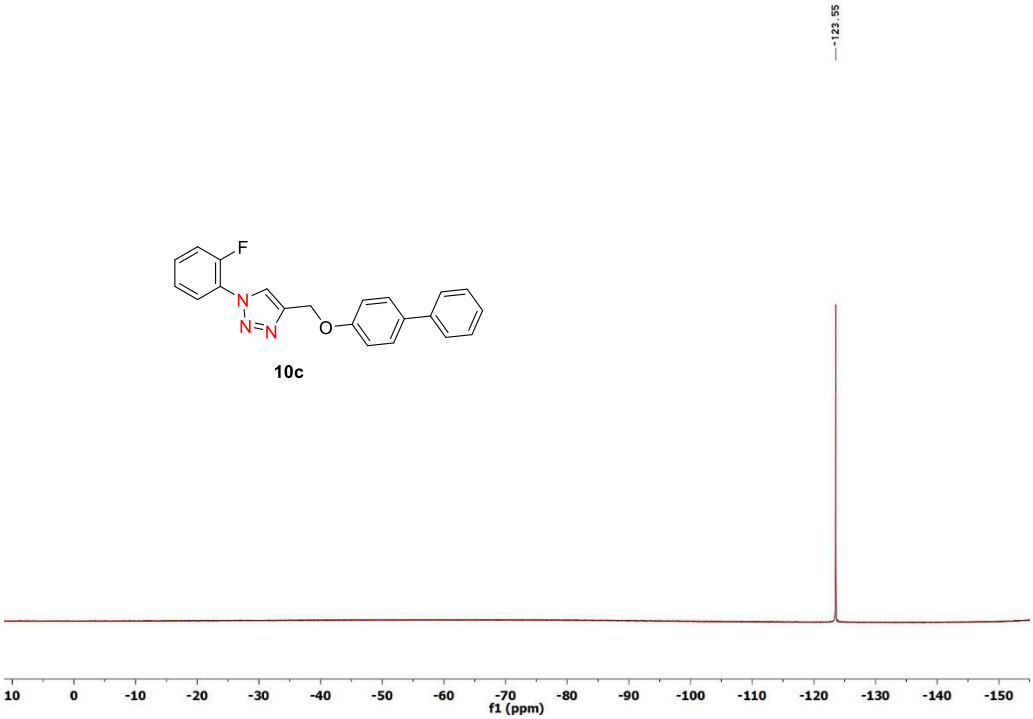


Fig. S71: ^{19}F NMR (470 MHz, $CDCl_3$) of the compound **10c**.

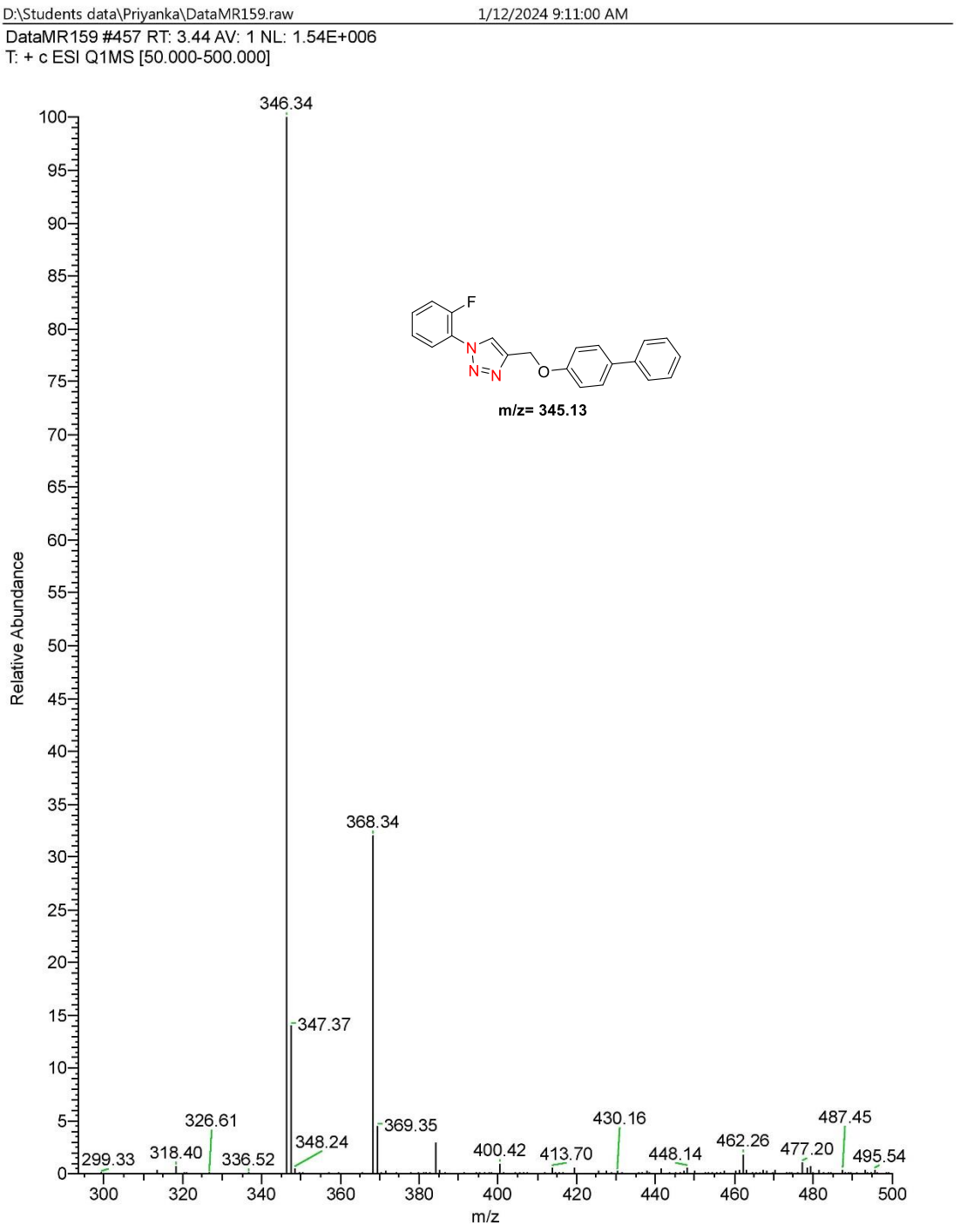


Fig. S72: LC-MS spectra of the compound **10c**.

Check CIF Report-Datablock: P-380

```
Bond precision:      C-C = 0.0089 A              Wavelength=0.71073
Cell:         a=8.1513(8)     b=5.6813(6)     c=14.7970(15)
              alpha=90        beta=93.787(3)  gamma=90
Temperature: 298 K
                    Calculated                      Reported
Volume              683.75(12)                      683.75(12)
Space group         P 21                            P 21
Hall group          P 2yb                           P 2yb
Moiety formula      C16 H15 N3 O                    ?
Sum formula         C16 H15 N3 O                    C32 H30 N6 O2
Mr                  265.31                          530.62
Dx,g cm-3           1.289                           1.289
Z                   2                               1
Mu (mm-1)           0.083                           0.083
F000                280.0                           280.0
F000'               280.10
h,k,lmax            8,5,15                          8,5,15
Nref                1547[ 873]                      1539
Tmin,Tmax           0.986,0.993
Tmin'               0.980
Correction method= Not given
Data completeness= 1.76/0.99    Theta(max)= 21.398
R(reflections)= 0.0492( 1275)                wR2(reflections)=
                                             0.1202( 1539)
S = 1.076              Npar= 182
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5133

Alert level B

PLAT089_ALERT_3_B Poor Data / Parameter Ratio (Zmax < 18) ..... 4.79 Note

Alert level C

STRVA01_ALERT_2_C Chirality of atom sites is inverted?
From the CIF: _refine_ls_abs_structure_Flack 1.000
From the CIF: _refine_ls_abs_structure_Flack_su 1.000
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00893 Ang.
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? . 1.00 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.513 2 Report
7 1 7, -1 4 11,

Alert level G

PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 1.000 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 2 Check

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 34 Note
N002 N003 N004 C005 C006 C007 C008 H008
C009 H009 C00A H00A C00B C00C H00C C00D
H00D C00E H00B H00E C00F H00F C00G H00G
C00H H00H C00I H00I C00J H00J C00K H00K
H00L H00M
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 58% Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 0.60 Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.93 Note
Predicted wR2: Based on SigI**2 4.10 or SHELX Weight 11.90
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
11 **ALERT level G** = General information/check it is not something unexpected

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PLATON version of 06/01/2024; check.def file version of 05/01/2024

Datablock 4af - ellipsoid plot