Supporting Information

Electrochemical desulfurative formation of C−N bonds through selective activation of inert C(sp^3)-S bonds activation

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General Information

Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. Reactions were monitored by thin layer chromatography (TLC) using silica gel 60 F-254 plates. The instrument for electrolysis was dual display potentiostat (M8801) (made in China). Cyclic voltammograms were obtained on a CHI 600E potentiostat. GC/MS analysis was conducted on an PerKinElmer Clarus 690 gas chromatography instrument with PerKinElmer Clarus SQ 8T Mass Spectrometer.The anode electrode was graphite rod (ϕ 6 mm) and cathodic electrode was platinum plate (15 mm×10 mm×0.1 mm). Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum (bp. 60-90 ℃). NMR spectras were measured on a Bruker avanceIIIHD400 (^{1}H at 400 MHz, ^{13}C at 101 MHz) magnetic resonance spectrometer. 19F NMR spectra were recorded on the same Spectrometer. Chemical shifts (δ) are reported in ppm using tetramethylsilane as internal standard (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet (denotes complex pattern), dd = doublet of doublets, dt = doublet of triplets, td = triplet of doublets), and coupling constants (*J*) were reported in Hertz (Hz). ESI-HRMS spectra were recorded on a UPLC of Thermo Q Exactive Focus.

Abbreviations used: GR = graphite rod; RVC = Reticulated Vitreous Carbon; HFIP = 1,1,1,3,3,3-Hexafluoro-2-propanol.

Standard Reaction Setup

Electrode material

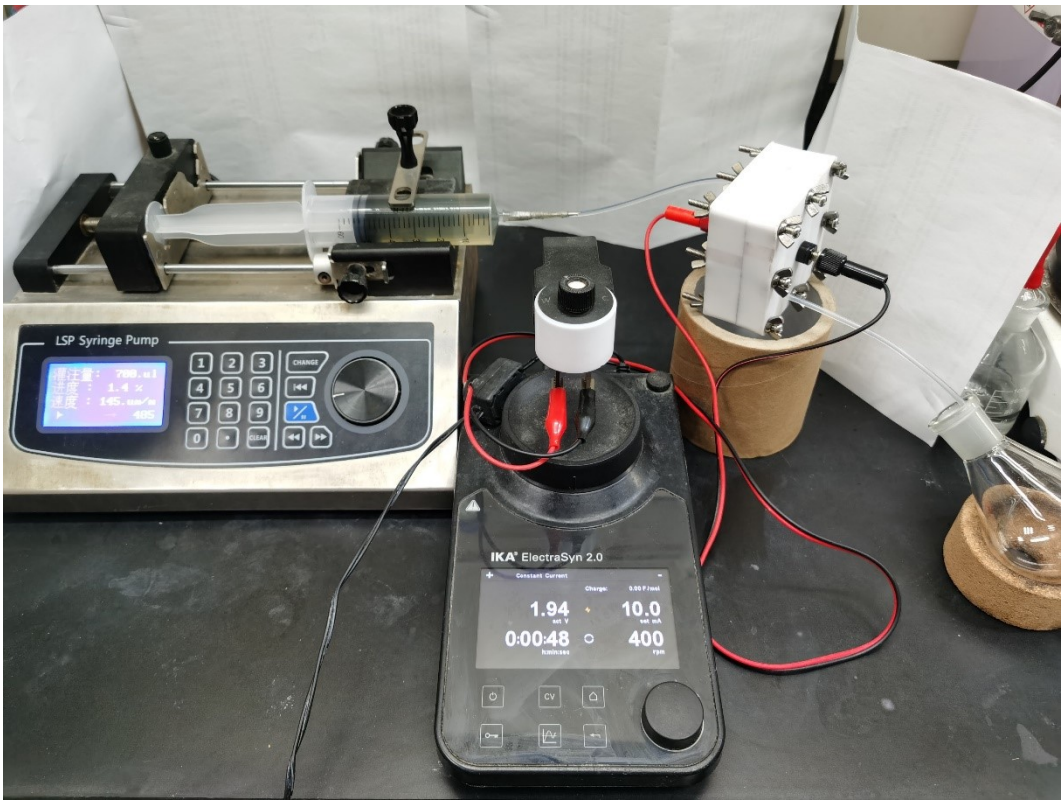
electrolytic cell

Figure S1 Electrodes and electrolytic cell

Potentiostat

ElectraSyn 2.0

Figure S2 Potentiostat

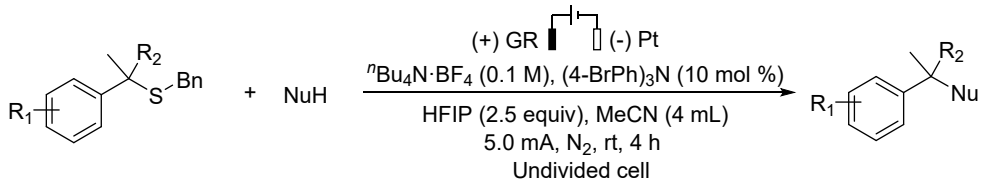


continuous flow electric reactor

Figure S3 Continuous flow electric reactor

General Procedure and Reaction Optimization

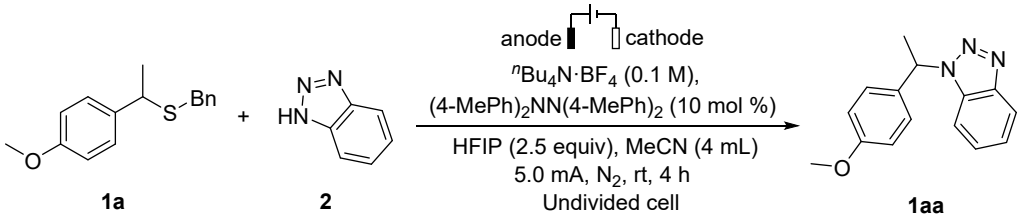
General Procedure:



In an oven-dried three-necked round-bottomed flask (10 mL) equipped with a graphite rod (ϕ 6 mm) anode and a platinum plate (15 mm×10 mm×0.1 mm) cathode (Figure S1 left). Thioether (1 equiv, 0.2 mmol), NuH (1.5 equiv, 0.3 mmol), ^{n}Bu$_4$N·BF$_4$ (0.1 M, 131.7 mg), (4-BrPh)$_3$N (0.1 equiv, 9.6 mg), HFIP (2.5 equiv, 50 μL) were dissolved in MeCN (4 mL). The resulting mixture was electrolyzed at a constant current mode with a constant current density of 5.0 mA/cm^2 under ambient temperature and N_2 atmosphere for corresponding time. When the reaction was finished, the solvent was concentrated in vacuum, the residue was purified by column chromatography on silica gel (petroleum: ethyl ether = 10:1) to afford the desired product.

Reaction Optimization:

Table S1 Investigation of electrode materials

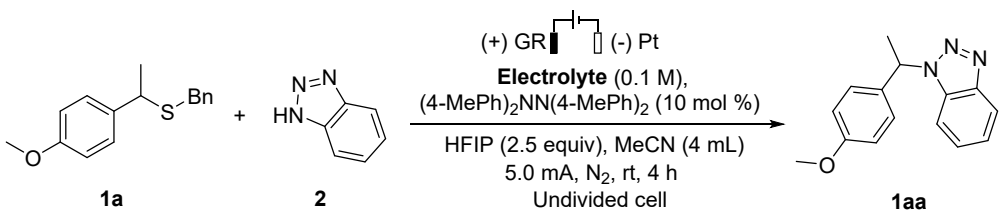


1a **2** **1aa**

Entry	Electrode	Yield (%)
1	RVC (+)/Pt (-)	55
2	Pt (+)/Pt (-)	50
3	Ni (+)/Pt (-)	trace
4	Ni (+)/RVC (-)	trace
5	RVC (+)/Ni (-)	trace
6	GR (+)/GR (-)	60
7	GR (+)/Pt (-)	70

Reaction conditions: **1a** (0.2 mmol), **2** (1.5 equiv, 0.3 mmol), ^{n}Bu$_4$N·BF$_4$ (0.1 M), [(4-MePh)$_2$N]$_2$ (10 mol %), HFIP (2.5 equiv, 50 μL), MeCN = 4 mL, undivided cell, graphite rod anode (ϕ 6 mm), platinum plate cathode (15 mm×10 mm×0.1 mm), constant current (5 mA), under N_2, r.t., 4 h. Isolated yield.

Table S2 Investigation of electrolytes

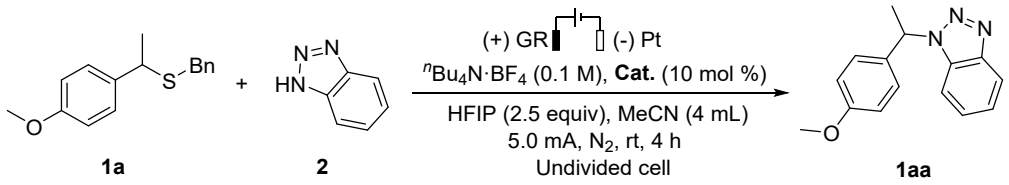


1a **2** **1aa**

Entry	Electrolyte	Yield (%)
1	$LiClO_4$	14
2	KPF_6	trace
3	$^nBu_4N{\cdot}ClO_4$	45
4	KCl	trace
5	LiF	trace
6	$^nBu_4N{\cdot}F$	trace
7	$^nBu_4N{\cdot}Cl$	trace
8	$^nBu_4N{\cdot}Br$	trace
9	$^nBu_4N{\cdot}I$	trace
10	$Et_4N{\cdot}PF_6$	66
11	$Et_4N{\cdot}BF_4$	70
12	$^nBu_4N{\cdot}BF_4$	72

Reaction conditions: **1a** (0.2 mmol), **2** (1.5 equiv, 0.3 mmol), $^nBu_4N{\cdot}BF_4$ (0.1 M), $[(4\text{-MePh})_2N]_2$ (10 mol %), HFIP (2.5 equiv, 50 μL), MeCN = 4 mL, undivided cell, graphite rod anode (ϕ 6 mm), platinum plate cathode (15 mm×10 mm×0.1 mm), constant current (5 mA), under N_2, r.t., 4 h. Isolated yield.

Table S3 Investigation of electrocatalyst

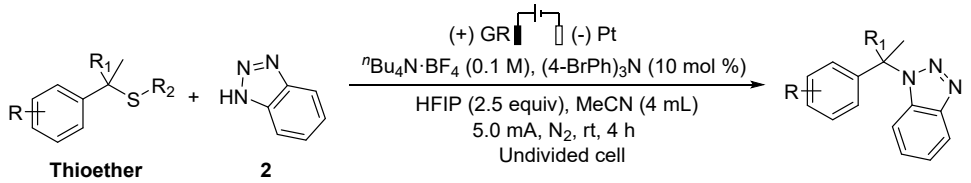


1a **2** **1aa**

Entry	Electrocatalyst	Yield (%)
1	Ph_3N	62
2	4-$MePhNPh_2$	68
3	$(4\text{-MePh})_3N$	66
4	$(4\text{-MePh})_2NN(4\text{-MePh})_2$	72
5	$(Bn)_3N$	45
6	TEMPO	N.R.
7	Iron phthalocyanine	N.R.
8	$(4\text{-BrPh})_3N$	74

Reaction conditions: **1a** (0.2 mmol), **2** (1.5 equiv, 0.3 mmol), $^nBu_4N{\cdot}BF_4$ (0.1 M), Cat (10 mol %), HFIP (2.5 equiv, 50 μL), MeCN = 4 mL, undivided cell, graphite rod anode (ϕ 6 mm), platinum plate cathode (15 mm×10 mm×0.1 mm), constant current (5 mA), under N_2, r.t., 4 h. Isolated yield.

Table S4 The effect of Substituents and NuH on the model reaction



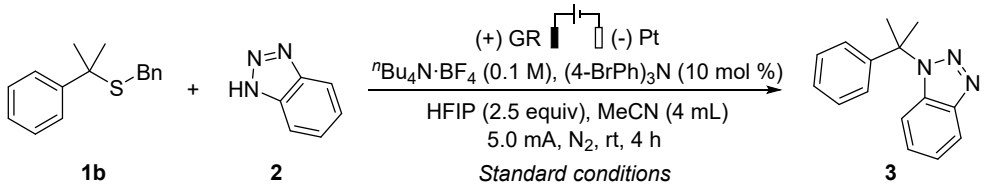
Thioether **2**

Entry	R	R_1	R_2	Yield (%)
1	4-MeO	H	Cy	69
2	4-MeO	H	Ph	70
3	4-MeO	H	Bn	74
4	H	Me	Bn	80

Reaction conditions: **Thioether** (0.2 mmol), **2** (1.5 equiv, 0.3 mmol), $^nBu_4N{\cdot}BF_4$ (0.1 M), $(4\text{-BrPh})_3N$ (10 mol %), HFIP (2.5 equiv, 50 μL), MeCN = 4 mL, undivided cell, graphite rod anode

(ϕ 6 mm), platinum plate cathode (15 mm×10 mm×0.1 mm), constant current (5 mA), under N_2, r.t., 4 h. Isolated yield.

Table S5 Deviation from standard conditions



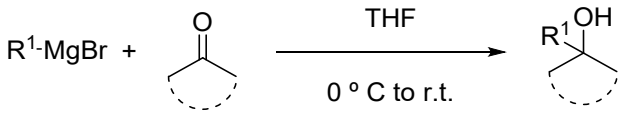
1b **2** **3**

Entry	Deviation from 'standard' conditions	Yield (%)
1	None	80
2	Air	55
3	50 mg 5Å MS	79
4	MeCN (dry)	80
5	DCM	30
6	Acetone	N.R.[c]
7	DMF	N.R.[c]
8	Without current	N.R.[c]
9	Without $(4\text{-BrPh})_3N$	60
10	5.0 mol% of $(4\text{-BrPh})_3N$	65
11	20.0 mol% of $(4\text{-BrPh})_3N$	69
12	$(4\text{-MePh})_2NN(4\text{-MePh})_2$	78
13	$(4\text{-MePh})_3N$	72
14	$(Bn)_3N$	48
15	TEMPO	N.R.[c]
16	DCA	70
17	Without HFIP	55
18	5.0 equiv. HFIP	62
19	10.0 equiv. HFIP	76
20	2.5 equiv. *t*BuOH	60
21	10.0 equiv. *t*BuOH	68
22	$Et_4N\cdot PF_6$	79
23	$^nBu_4N\cdot ClO_4$	58
24	Pyridine instead of HFIP	N.R.
25	2,4,6-Collidine instead of HFIP	N.R.
26	Et_3N instead of HFIP	N.R.
27	3.0 h	67
28	4.5 h	73
29	5.0 h	62
30	6.0 h	34
31	2.5 mA	45
32	10.0 mA	58
33	Divided cell	35

Reaction conditions: **1b** (0.2 mmol), **2** (1.5 equiv, 0.3 mmol), $^nBu_4N\cdot BF_4$ (0.1 M), $(4\text{-BrPh})_3N$ (10 mol %), HFIP (2.5 equiv, 50 μL), MeCN = 4 mL, undivided cell, graphite rod anode (ϕ 6 mm), platinum plate cathode (15 mm×10 mm×0.1 mm), constant current (5 mA), under N_2, r.t., 4 h. Isolated yield.

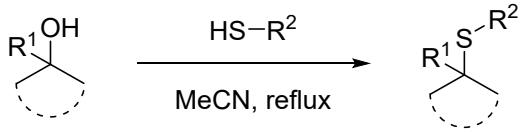
Synthesis of the Substrates

General procedure for the synthesis of Corresponding alcohol:



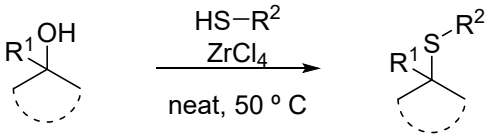
Corresponding ketone (10 mmol) was added to a 150 mL round-bottom flask and dry THF (0.1 M) was then added. After cooling the solution to 0 ℃, R^1-MgBr (1.5 equiv, 3.0 M in THF) was added dropwise. After complete addition, the resulting mixture was left to warm to room temperature and stirred for 5 h. After completion of the reaction as indicated by TLC, the mixture was poured slowly into sat. NH_4Cl (aq.) and extracted with EtOAc. The organic phase was concentrated in vacuum, the mixture was directly used in the next step without purification.

General procedure A for the synthesis of corresponding thioether[1]:



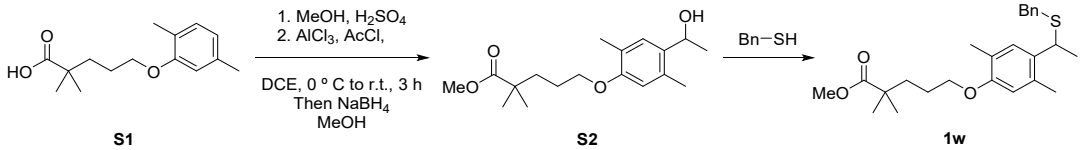
Corresponding alcohol (1 equiv), $TsOH{\cdot}H_2O$ (5 mol%) and thiol (1.05 equiv) were dissolved in MeCN (0.2 M). Otherwise specifically mentioned, the solution was heated at reflux over until complete conversion (monitored by TLC). Volatiles were then removed under reduced pressure and the residue was purified by silica gel flash chromatography (petroleum ether).

General procedure B for the synthesis of corresponding thioether[2]:



A round-bottom flask with stirring bar was equipped with alcohol (1 eq.), $ZrCl_4$ (0.5 equiv) and thiol (1.05 equiv). Then the mixture was transferred to 50 ℃ oil bath until complete conversion (monitored by TLC). CH_2Cl_2 was added to extract the product. Then filtered through a pad of silica gel, the filtrate was concentrated and purified by silica gel flash chromatography (petroleum ether).

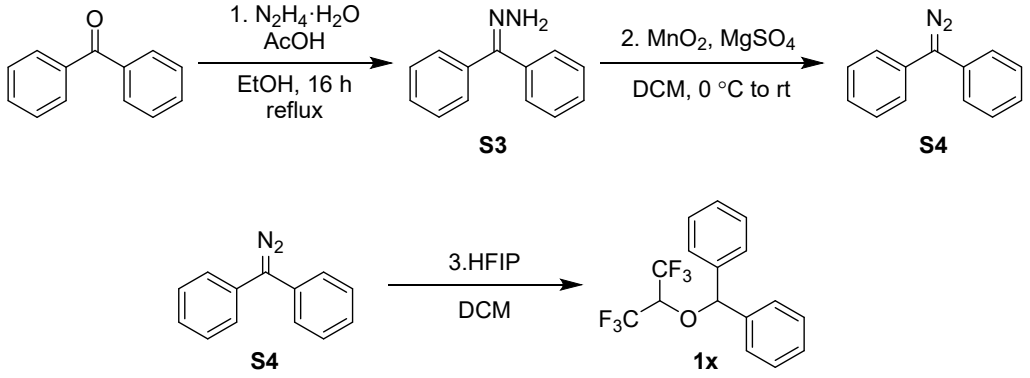
General procedure for the synthesis of methyl 5-(4-(1-(benzylthio)ethyl)-2,5-dimethylphenoxy)-2,2-dimethylpentanoate[3]:



Gemfibrozil (750 mg, 3.0 mmol) was dissolved in 10 mL of dry methanol, 4 drops of concentrated sulfuric acid was added to the mixture and the reaction was allowed to stir at reflux overnight. The reaction mixture was cooled to room temperature and quenched with sat. $NaHCO_3$ (aq.) until a basic pH was reached. The organic layer was extracted using EtOAc (3 x 20 mL) and the organic layer was washed with brine (1 x 40 mL) and dried using $MgSO_4$. The organic layer was concentrated to give pure product as a colorless oil. To the suspension of aluminium (III) chloride ($AlCl_3$) (1.2 g, 9.0 mmol) in 1,2-dichloroethane (15 mL), was added acetyl chloride (AcCl) (642 μL, 9.0 mmol) at

0 ℃. The reaction mixture was stirred at 0 ℃ for 45 min. The above colorless oil was then added and stirred at 0 ℃ for 4 h. After the reaction mixture was quenched with H_2O (30 mL), extracted with CH_2Cl_2 (120 mL). The combined organic phases were concentrated, then $NaBH_4$ (136 mg, 3.6 mmol) was added and stirred in MeOH (15 mL) for 5 h. Volatiles were then removed under reduced pressure and the residue without further purification. Then follow **general procedure B** to give the thioether. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.24 – 7.09 (m, 6H), 6.43 (s, 1H), 3.90 – 3.77 (m, 3H), 3.58 (s, 3H), 3.48 (dd, *J* = 31.5, 13.5 Hz, 2H), 2.12 (s, 3H), 1.98 (s, 3H), 1.63 (d, *J* = 2.9 Hz, 4H), 1.41 (d, *J* = 7.0 Hz, 3H), 1.14 (s, 6H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 177.28, 154.53, 137.56, 132.74, 131.24, 127.81, 127.31, 125.73, 123.45, 111.78, 66.90, 50.71, 41.06, 37.30, 36.08, 34.69, 24.15, 20.85, 17.96, 14.85.

General procedure for the synthesis of (((1,1,1,3,3,3-hexafluoropropan-2-yl)oxy)methylene)dibenzene[4]:



The Diaryldiazo compounds were prepared in accordance to a modified procedure by Zhou et al[5]. In a first step, the corresponding benzophenone (5 mmol) was dissolved in 30 mL EtOH, followed by the addition of hydrazine monohydrate (50 mmol) and 0.5 mL concentrated acetic acid. The resulting mixture was refluxed for 16 h overnight. After cooling to room temperature, the corresponding hydrazone participated as crystals and was filtered. (ps: If crystals cannot be obtained, the product is obtained by extracting and evaporating the solvent.) The above products are used directly in the next step without purification.

A two-necked flask was taken and the crude product zeolite and anhydrous $MgSO_4$ (2.5 equiv) were measured and the flask was replaced three times with N_2. The mixture was dissolved in DCM (0.24 M) and stirred at 0 °C. The mixture was then dissolved in MnO_2 (3.5 equiv). MnO_2 (3.5 equiv) was added immediately to the stirred solution. Bring the mixture to room temperature and continue stirring for 5h. (work up: After filtration, the solvent was removed under reduced pressure and the product was purified by silica column chromatography using petroleum ether: EtOAc:Et_3N as eluent.)

In an oven-dried test tube diazo compound S4 (1.0 equiv) was evaporated and flushed with argon for three times. Then dry, degassed DCM was added, followed by addition of the 1,1,1,3,3,3-Hexafluoro-2-propanol (3.0 equiv). The reaction mixture was stirred in the dark until the color of the diazo compound disappeared. The product was purified by silica columns chromatography using petroleum ether: EtOAc as eluent. (Reactions in the dark were performed in test tubes wrapped with aluminum foil.)

(((1,1,1,3,3,3-hexafluoropropan-2-yl)oxy)methylene)dibenzene: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.32 (m, 1H), 5.86 (s, 1H), 4.35 – 4.01 (m, 1H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 138.85,

128.67, 128.60, 127.60, 121.67 (d, J = 284.8 Hz), 85.56, 72.48 (dt, J = 64.5, 32.2 Hz). **^{19}F NMR (376 MHz, $CDCl_3$)** δ -72.76.

Thioether substrate:

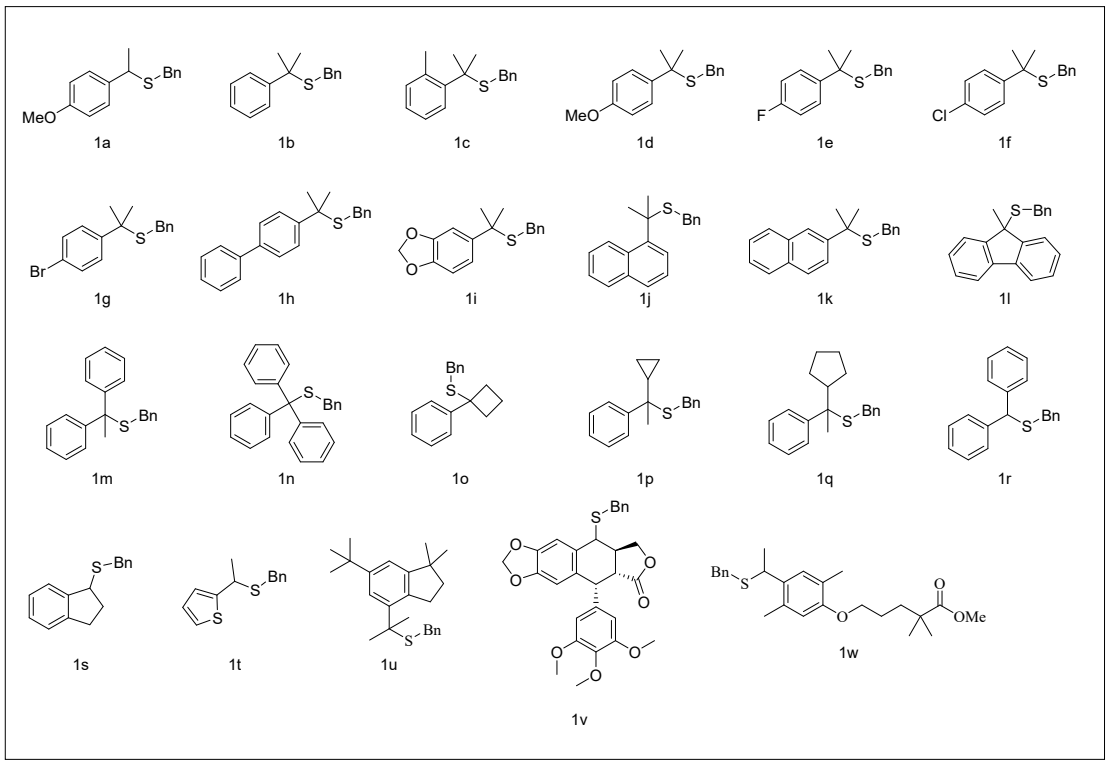


Figure S4 Thioether substrates

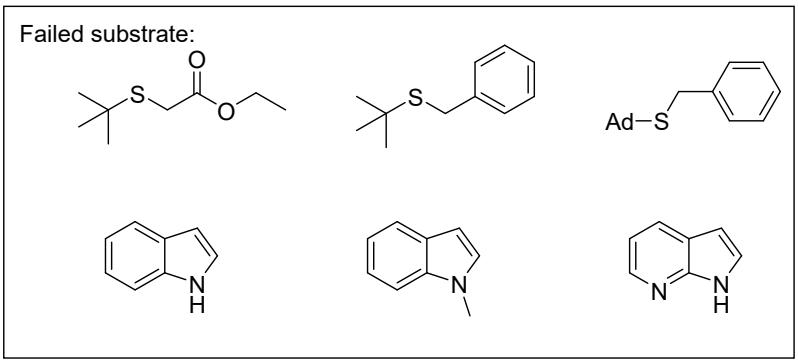
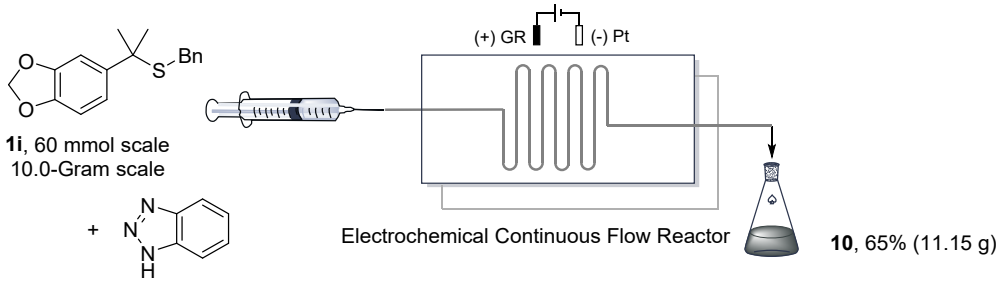


Figure S5 Failed substrate

The Application of the Reaction

Procedure for gram scale synthesis:



Flow chemistry:

FEP (fluorinated ethylene propylene) with channel 3 mm width; thickness: 0.5 mm; total length of the pipeline of 30.1 cm; volume: 450 µL; exposed electrode surface: 9.57 cm^2. The device comprises a micro-flow electrochemical reactor made out of two bodies (75x75x25 mm, Figure S3), which can be polymer. The main body has a square space (50x50mm^2) in the center where carbon (3.0 mm thickness) and platinum (0.1 mm thickness) electrodes are placed and the FEP is sandwiched between the two electrodes. The housing of the reactor has a hole in the middle that allows an easy connection of the electrodes to the power supply by a copper wire. This plate also has 2 holes, one for the inlet and one for the outlet of the reaction solution.

General procedure for continuous flow photoreactions:

A well-dried round-bottomed flask equipped with a stirring bar was weighed for **1i** (60 mmol, 17.166 g), benzotriazole (1.5 equiv, 90 mmol, 10.17 mg), $^{n}Bu_4NBF_4$ (0.1 M, 10 mmol, 3.293 g), $[(4\text{-}MePh)_2N]_2$ (0.1 equiv, 6 mmol, 2.3532 g). The above solid mixture was washed three times with nitrogen and dissolved in MeCN (120 mL). HFIP (2.5 equiv, 15.79 mL) was added to the above mixture. The solution was dissolved by shaking well, then withdrawn with a 60 mL syringe and placed in a syringe pump. The solution was passed through the electrode at a rate of 0.1 mL/min at a constant current of 35 mA.

Mechanistic Studies

Cyclic Voltammetry Study

Cyclic voltammetry was performed in a three-electrode cell connected to a schlenk line at room temperature (air). The working electrode was a carbon rod electrode, the counter electrode a platinum wire. The reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution, and separated from reaction by a salt bridge. 5 mL of MeCN containing 0.1 M $^{n}Bu_4NPF_6$ were poured into the electrochemical cell in all experiments. Concentration of a sample: 0.05 M. The scan rate is 0.1 V/s, ranging from 0 V to 2.5 V. The peak potentials vs. Ag/AgCl for used.

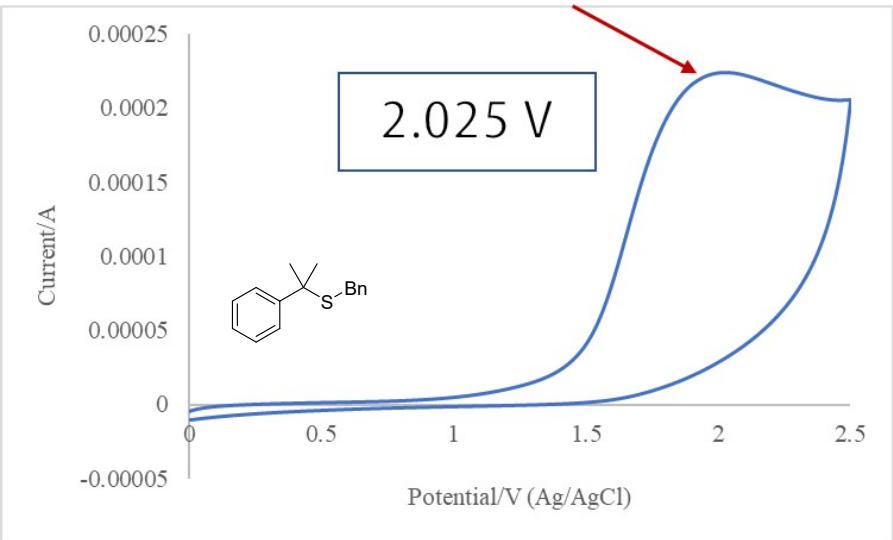


Figure S6 Cyclic voltammogram for oxazolone **1b** (0.05 M) in (0.1 M) $TBAPF_6$ in MeCN

The scan rate is 0.1 V/s, ranging from 0 V to 3.0 V. The peak potentials vs. Ag/AgCl for used.

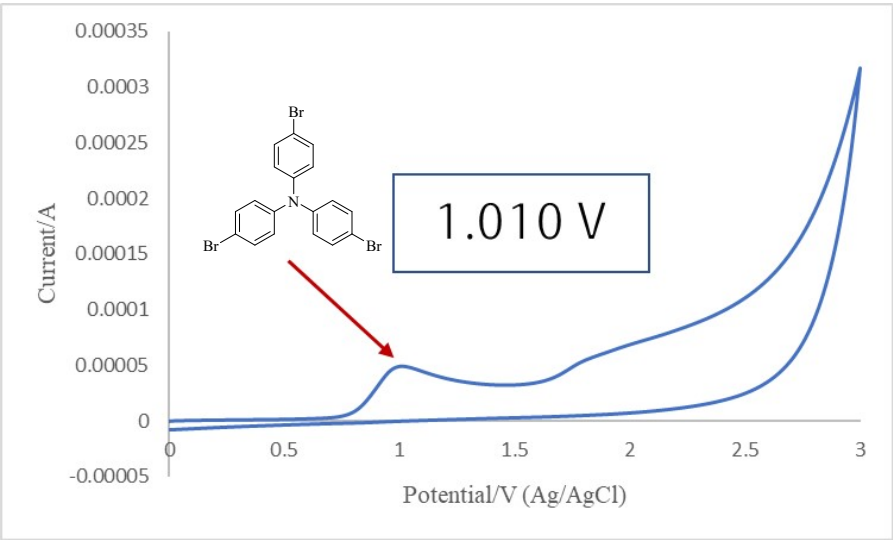


Figure S7 Cyclic voltammogram for oxazolone **$(4\text{-BrPh})_3N$** (0.05 M) in (0.1 M) $TBAPF_6$ in MeCN

Open circuit potential-time

Anode potential measured by OCPT (CHI 600E potentiostat). According to the general procedure), the electrode potential was monitored under standard conditions using Ag/AgCl as a reference electrode. The electrodes (graphite rod anode/ Platinum sheet cathode) and reference electrode were inserted into the reaction mixture together during the electrolysis. (*ps*: keep anode or cathode with reference electrode as close as possible when testing. When taking multiple measurements, keep the electrodes mounted at the same height as much as possible.)

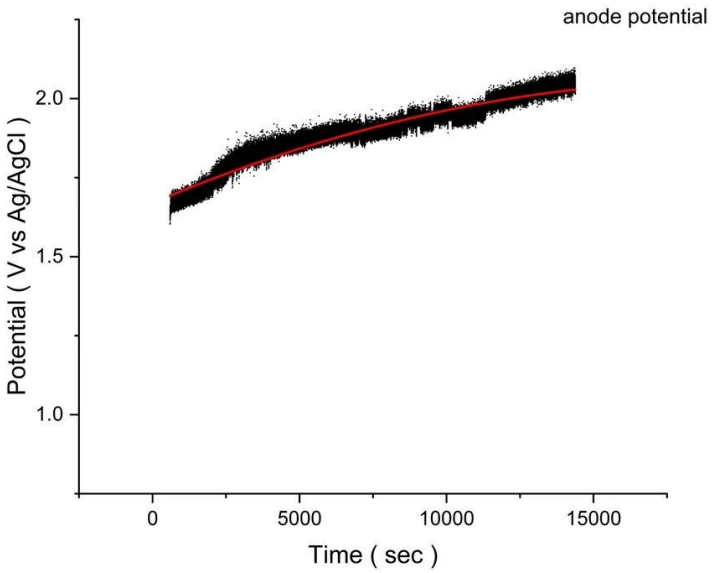


Figure S8 Electrode voltage over the course of electrolysis.

Intermediate validation experiments

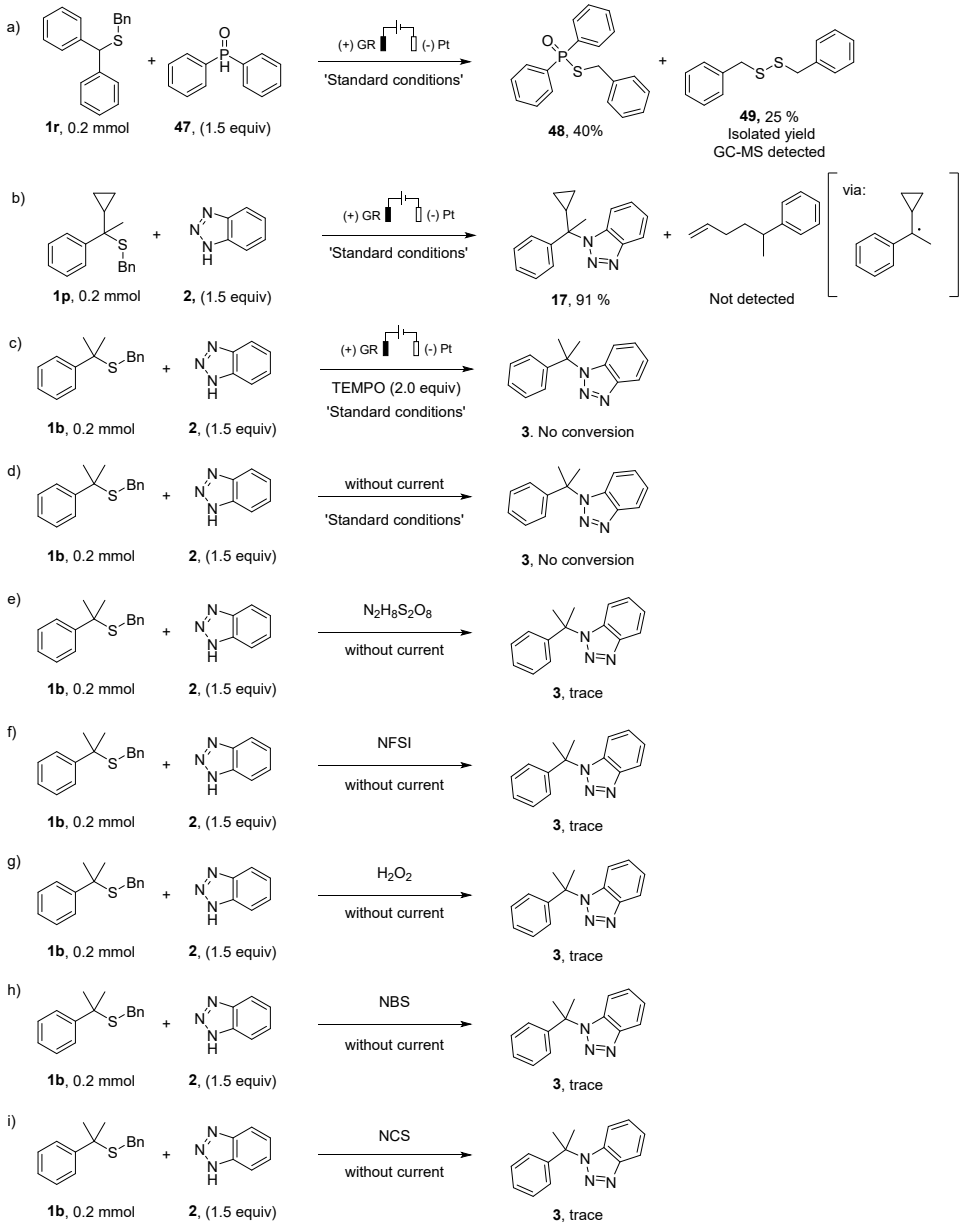
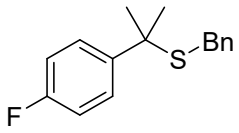


Figure S9 Intermediate validation control experiments

To shine light on the mechanism of this electrochemical dehydrogenative cross-coupling reaction, several control experiments were conducted. There is no corresponding conversion when adding 2.0 equivalent TEMPO under standard conditions. When the corresponding thioether **1p** was used as the substrate, the *N*-alkylation product **17** was obtained in 91% yield, and no discernible radical ring-opening product was observed (Fig. S8-b). These results collectively indicated a sulfur radical cation was produced at the anode, leading to the decomposition into a carbocation and a thiyl radical. The capture of the carbocation by the nucleophilic reagent benzotriazole **2**, resulting in the formation of addition product **17**. And no reaction occurred in the absence of an electric current. No desired product was obtained, when the chemical oxidants such as NBS/NCS, NFSI, H_2O_2, $N_2H_8S_2O_6$, were adding to the reaction without electricity.

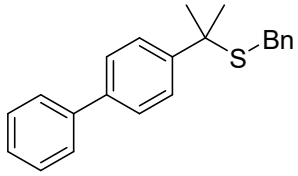
Characterization Data



benzyl(2-(4-fluorophenyl)propan-2-yl)sulfane(1e)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.39 (m, 2H), 7.17 – 7.00 (m, 5H), 6.96 – 6.87 (m, 2H), 3.30 (s, 2H), 1.60 (s, 6H).

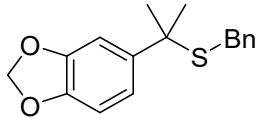
^{13}C NMR (101 MHz, $CDCl_3$) δ 161.4 (d, *J* = 245.6 Hz), 142.2 (d, *J* = 3.4 Hz), 138.0, 128.9, 128.4, 128.3, 126.8, 114.8 (d, *J* = 21.1 Hz), 48.1, 34.6, 30.4.



(2-([1,1'-biphenyl]-4-yl)propan-2-yl)(benzyl)sulfane(1h)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.46 (m, 6H), 7.39 – 7.32 (m, 2H), 7.29 – 7.24 (m, 1H), 7.15 – 7.02 (m, 5H), 3.36 (s, 2H), 1.66 (s, 6H).

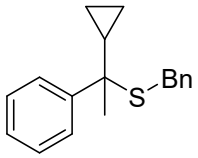
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.4, 140.7, 139.3, 138.1, 129.0, 128.8, 128.4, 127.3, 127.1, 127.0, 126.8, 126.7, 48.4, 34.6, 30.2.



5-(2-(benzylthio)propan-2-yl)benzo[d][1,3]dioxole(1i)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 – 7.05 (m, 6H), 6.91 – 6.87 (m, 1H), 6.71 – 6.65 (m, 1H), 5.89 (s, 2H), 3.35 (s, 2H), 1.59 (s, 6H).

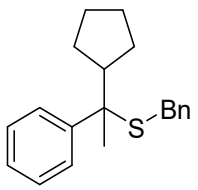
^{13}C NMR (101 MHz, $CDCl_3$) δ 147.7, 146.0, 140.5, 138.1, 128.9, 128.3, 126.7, 119.5, 107.7, 107.3, 101.0, 48.6, 34.5, 30.5.



benzyl(1-cyclopropyl-1-phenylethyl)sulfane(1p)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.58 (m, 2H), 7.31 – 7.23 (m, 2H), 7.20 – 7.04 (m, 6H), 3.35 (s, 2H), 1.46 (s, 3H), 1.38 – 1.27 (m, 1H), 0.56 – 0.34 (m, 4H).

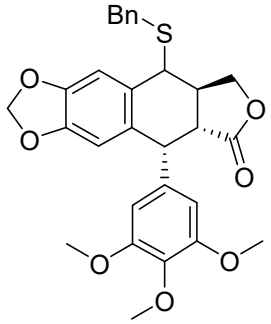
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.3, 138.1, 128.9, 128.3, 128.0, 127.6, 126.7, 126.6, 52.8, 34.4, 24.9, 21.9, 2.8, 2.7.



benzyl(1-cyclopentyl-1-phenylethyl)sulfane(1q)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.7 Hz, 2H), 7.27 (t, *J* = 7.7 Hz, 2H), 7.18 – 7.03 (m, 6H), 3.38 (d, *J* = 11.8 Hz, 1H), 3.11 (d, *J* = 11.8 Hz, 1H), 2.44 – 2.34 (m, 1H), 1.73 – 1.09 (m, 12H).

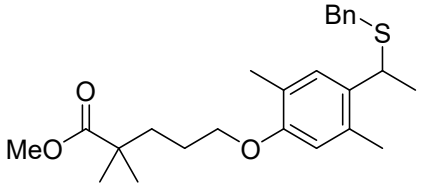
^{13}C NMR (151 MHz, $CDCl_3$) δ 144.3, 137.1, 127.9, 127.3, 126.9, 126.6, 125.6, 125.1, 54.6, 50.1, 32.7, 27.0, 26.8, 24.7, 24.2, 21.0.



(5R,5aR,8aR,9R)-9-(benzylthio)-5-(3,4,5-trimethoxyphenyl)-5,8,8a,9-tetrahydrofuro[3',4':6,7]naphtho[2,3-d][1,3]dioxol-6(5aH)-one(1v)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.30 (m, 5H), 6.52 (s, 1H), 6.38 (s, 1H), 6.24 (s, 2H), 5.92 (dd, *J* = 4.9, 1.2 Hz, 2H), 4.50 (d, *J* = 5.3 Hz, 1H), 4.36 (dd, *J* = 10.5, 8.3 Hz, 1H), 4.26 (t, *J* = 7.7 Hz, 1H), 4.01 (d, *J* = 4.4 Hz, 1H), 3.83 (dd, *J* = 12.9, 10.4 Hz, 1H), 3.78 (s, 3H), 3.72 (s, 6H), 3.63 (d, *J* = 13.6 Hz, 1H), 3.18 (dd, *J* = 13.7, 5.3 Hz, 1H), 3.10 – 2.98 (m, 1H).

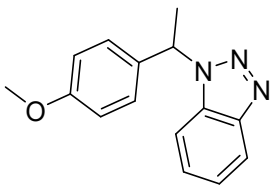
^{13}C NMR (101 MHz, $CDCl_3$) δ 174.5, 152.5, 147.6, 147.1, 137.6, 137.2, 135.7, 131.2, 130.0, 129.1, 128.9, 127.7, 109.7 (d, *J* = 3.5 Hz), 108.3, 101.4, 69.5, 60.7, 56.3, 45.9, 43.6, 42.3, 38.5, 37.5.



methyl 5-(4-(1-(benzylthio)ethyl)-2,5-dimethylphenoxy)-2,2-dimethylpentanoate(1w)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 – 7.09 (m, 6H), 6.43 (s, 1H), 3.90 – 3.77 (m, 3H), 3.58 (s, 3H), 3.48 (q, *J* = 31.5, 13.5 Hz, 2H), 2.12 (s, 3H), 1.98 (s, 3H), 1.63 (d, *J* = 2.9 Hz, 4H), 1.41 (d, *J* = 7.0 Hz, 3H), 1.14 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 177.2, 154.5, 137.5, 132.7, 131.2, 127.8, 127.3, 125.7, 123.4, 111.7, 66.9, 50.7, 41.0, 37.3, 36.0, 34.6, 24.1, 20.8, 17.9, 14.8.

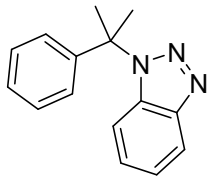


1-(1-(4-methoxyphenyl)ethyl)-1H-benzo[d][1,2,3]triazole (1aa)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, 1H), 7.76 (dd, *J* = 8.8, 0.8 Hz, 1H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.32 – 7.24 (m, 3H), 7.10 – 7.04 (m, 1H), 6.89 (d, *J* = 8.8 Hz, 2H), 5.81 (q, *J* = 7.0 Hz, 1H), 3.81 (s, 3H), 2.04 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.3, 147.4, 131.9, 126.9, 124.7, 120.5 (d, *J* = 9.2 Hz), 120.1, 119.1, 116.5, 113.0, 61.1, 54.2, 20.6.

HRMS (ESI) calcd for $C_{15}H_{15}N_3O$ ($M+Na^+$): 276.1107, found: 276.1109.

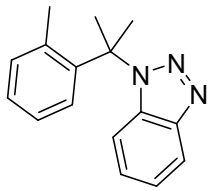


1-(2-phenylpropan-2-yl)-1H-benzo[d][1,2,3]triazole (3)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.4 Hz, 1H), 7.34 – 7.26 (m, 2H), 7.26 – 7.17 (m, 2H), 7.16 – 7.06 (m, 3H), 6.66 (d, *J* = 8.4 Hz, 1H), 2.13 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.0, 144.1, 132.0, 128.8, 127.8, 126.4, 125.3, 123.5, 119.9, 112.1, 64.7, 29.6.

HRMS (ESI) calcd for $C_{15}H_{15}N_3$ ($M+H^+$): 238.1339, found: 238.1339.

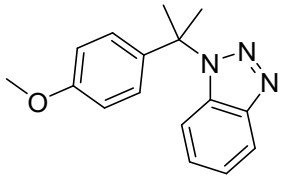


1-(2-(o-tolyl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (4)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.4 Hz, 1H), 7.67 (dd, *J* = 7.9, 0.8 Hz, 1H), 7.35 (dd, *J* = 11.1, 4.1 Hz, 1H), 7.27 (dd, *J* = 5.9, 1.5 Hz, 1H), 7.25 – 7.22 (m, 1H), 7.11 (ddd, *J* = 8.0, 6.9, 0.9 Hz, 1H), 7.02 (d, *J* = 7.4 Hz, 1H), 6.57 (d, *J* = 8.4 Hz, 1H), 2.21 (s, 6H), 1.44 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.9, 139.6, 135.6, 132.2, 131.0, 127.2, 125.4, 125.4, 124.4, 122.5, 118.8, 110.2, 63.7, 27.9, 18.5.

HRMS (ESI) calcd for $C_{16}H_{17}N_3$ ($M+H^+$): 252.1495, found: 252.1492.

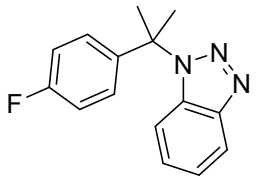


1-(2-(4-methoxyphenyl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (5)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.3 Hz, 1H), 7.21 – 7.13 (m, 1H), 7.11 – 7.02 (m, 3H), 6.81 – 6.73 (m, 2H), 6.64 (d, *J* = 8.4 Hz, 1H), 3.71 (s, 3H), 2.07 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.9, 145.9, 135.1, 131.0, 125.6, 125.3, 122.4, 118.8, 113.0, 111.1, 63.3, 54.2, 28.6.

HRMS (ESI) calcd for $C_{16}H_{17}N_3O$ ($M+H^+$): 290.1264, found: 290.1262.



1-(2-(4-fluorophenyl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (6)

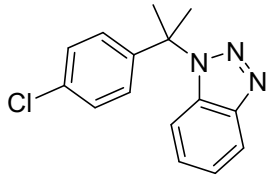
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.3 Hz, 1H), 7.29 – 7.24 (m, 1H), 7.22 – 7.13 (m, 3H), 7.06 – 6.96 (m, 2H), 6.78 – 6.66 (m, 1H), 2.17 (s, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 161.0 (d, *J* = 247.4 Hz), 146.0, 139.0 (d, *J* = 3.2 Hz), 130.8, 126.1 (d, *J*

= 8.2 Hz), 125.6, 122.6, 119.0, 114.7 (d, *J* = 21.3 Hz), 110.8, 63.2, 28.6.

^{19}F NMR (377 MHz, $CDCl_3$) δ -114.17 – -114.34 (m).

HRMS (ESI) calcd for $C_{15}H_{14}FN_3$ ($M+H^+$): 256.1245, found: 256.1242.

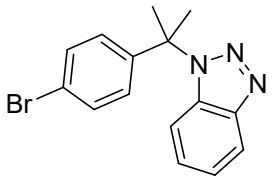


1-(2-(4-chlorophenyl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (7)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.3 Hz, 1H), 7.32 – 7.27 (m, 3H), 7.20 (M, 1H), 7.14 – 7.07 (m, 2H), 6.75 (d, *J* = 8.4 Hz, 1H), 2.17 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 146.0, 141.7, 132.7, 130.8, 128.0, 127.2, 125.7 (d, *J* = 12.3 Hz), 124.9, 122.6, 119.0, 110.8, 63.3, 28.5.

HRMS (ESI) calcd for $C_{15}H_{14}ClN_3$ ($M+H^+$): 272.0949, found: 272.0948.



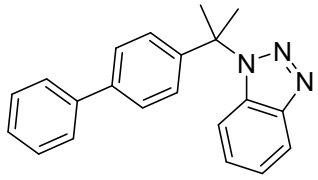
1-(2-(4-bromophenyl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (8)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 – 7.91 (m, 1H), 7.38 (d, *J* = 8.7 Hz, 2H), 7.24 – 7.09 (m, 2H), 7.02 – 6.94 (m, 2H), 6.71 – 6.64 (m, 1H), 2.09 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 146.0, 142.3, 131.0, 130.8, 126.1, 125.7, 122.6, 120.9, 119.0, 110.8, 63.3, 28.4.

HRMS (ESI) calcd for $C_{15}H_{14}BrN_3$ ($M+H^+$): 316.0444, found: 316.0440.

HRMS (ESI) calcd for $C_{15}H_{14}BrN_3$ ($M+H^+$): 318.0423, found: 318.0419.

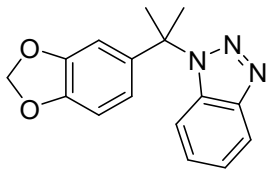


1-(2-([1,1'-biphenyl]-4-yl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (9)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.3 Hz, 1H), 7.53 – 7.44 (m, 4H), 7.38 – 7.31 (m, 2H), 7.29 – 7.23 (m, 1H), 7.20 – 7.14 (m, 3H), 7.09 (ddd, *J* = 8.1, 6.9, 1.0 Hz, 1H), 6.77 – 6.67 (m, 1H), 2.14 (s, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 147.0, 143.1, 140.6, 140.1, 132.0, 128.8, 127.6, 127.4, 127.0, 126.5, 125.8, 123.6, 119.9, 112.2, 64.6, 29.6.

HRMS (ESI) calcd for $C_{21}H_{19}N_3$ ($M+H^+$): 314.1652, found: 314.1649.

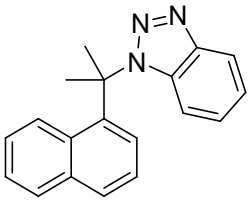


1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (10)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.93 (m, 1H), 7.16 (dddd, 2H), 6.79 – 6.73 (m, 1H), 6.71 – 6.65 (m, 2H), 6.52 (d, *J* = 1.4, 0.7 Hz, 1H), 5.87 (s, 2H), 2.06 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.2, 147.1, 147.0, 138.2, 132.0, 126.5, 123.5, 119.9, 118.6, 112.1, 108.1, 106.4, 101.3, 64.5, 29.7.

HRMS (ESI) calcd for $C_{16}H_{15}N_3O_2$ ($M+H^+$): 282.1237, found: 282.1234.

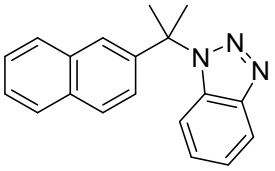


1-(2-(naphthalen-1-yl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (11)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.4 Hz, 1H), 7.94 – 7.87 (m, 2H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.59 (dd, *J* = 8.1, 7.5 Hz, 1H), 7.31 – 7.21 (m, 2H), 7.16 – 7.01 (m, 2H), 6.96 – 6.88 (m, 1H), 6.49 (d, *J* = 8.5 Hz, 1H), 2.39 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.9, 137.1, 133.5, 131.3, 129.6, 129.1, 128.2, 125.4, 125.3, 124.5, 123.7, 122.8, 122.6, 122.4, 118.7, 110.1, 64.0, 28.8.

HRMS (ESI) calcd for $C_{19}H_{17}N_3$ ($M+H^+$): 288.1495, found: 288.1493.

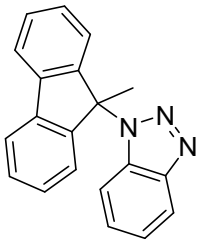


1-(2-(naphthalen-2-yl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (12)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.4 Hz, 1H), 7.82 – 7.61 (m, 4H), 7.50 – 7.38 (m, 2H), 7.19 – 7.11 (m, 1H), 7.05 – 6.95 (m, 2H), 6.63 (d, *J* = 8.5 Hz, 1H), 2.20 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 146.0, 140.5, 131.9, 131.6, 131.0, 127.9, 127.2, 126.6, 125.5, 125.5, 122.7, 122.6, 122.5, 118.8, 111.0, 63.8, 28.4.

HRMS (ESI) calcd for $C_{19}H_{17}N_3$ ($M+H^+$): 288.1493, found: 288.1492.

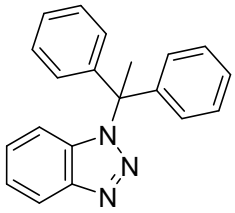


1-(9-methyl-9H-fluoren-9-yl)-1H-benzo[d][1,2,3]triazole (13)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.4 Hz, 1H), 7.74 (d, *J* = 7.6 Hz, 2H), 7.36 (ddd, *J* = 7.6, 6.6, 2.0 Hz, 2H), 7.18 – 7.11 (m, 4H), 7.04 (ddd, *J* = 8.2, 7.0, 0.8 Hz, 1H), 6.84 (ddd, *J* = 8.1, 7.0, 0.9 Hz, 1H), 5.95 (d, *J* = 8.5 Hz, 1H), 2.41 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 146.7, 146.4, 139.1, 131.7, 129.6, 128.6, 126.7, 123.8, 123.5, 120.6, 119.6, 111.2, 70.7, 26.3.

HRMS (ESI) calcd for $C_{20}H_{15}N_3$ ($M+H^+$): 298.1339, found: 298.1337.

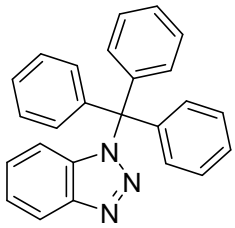


1-(1,1-diphenylethyl)-1H-benzo[d][1,2,3]triazole (14)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.4 Hz, 1H), 7.29 – 7.20 (m, 6H), 7.20 – 7.14 (m, 1H), 7.04 – 6.94 (m, 5H), 6.15 (d, *J* = 8.5 Hz, 1H), 2.66 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.4, 141.6, 132.9, 127.5, 127.0, 126.3, 125.7, 122.4, 118.9, 111.5, 70.2, 30.9.

HRMS (ESI) calcd for $C_{20}H_{17}N_3$ ($M+Na^+$): 322.1315, found: 322.1314.

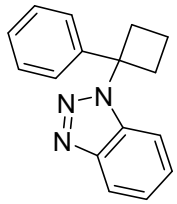


1-trityl-1H-benzo[d][1,2,3]triazole (15)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.4 Hz, 1H), 7.23 – 7.16 (m, 10H), 7.12 – 7.07 (m, 6H), 7.01 (ddd, *J* = 8.2, 7.0, 1.0 Hz, 1H), 6.34 (d, *J* = 8.5 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 146.4, 141.4, 134.3, 130.1, 127.9, 127.8, 126.7, 123.6, 120.0, 113.7, 79.0.

HRMS (ESI) calcd for $C_{25}H_{19}N_3$ ($M+Na^+$): 384.1471, found: 384.1471.

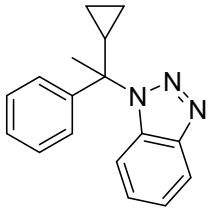


1-(1-phenylcyclobutyl)-1H-benzo[d][1,2,3]triazole (16)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.93 (m, 1H), 7.28 – 7.15 (m, 7H), 7.05 (ddd, *J* = 8.3, 2.9, 1.5 Hz, 1H), 3.32 (ddd, *J* = 12.7, 11.3, 8.7 Hz, 2H), 3.05 – 2.93 (m, 2H), 2.16 – 2.04 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.7, 141.1, 130.6, 127.7, 126.7, 125.7, 124.3, 122.6, 118.9, 110.0, 65.5, 32.9, 14.7.

HRMS (ESI) calcd for $C_{16}H_{15}N_3$ ($M+H^+$): 250.1339, found: 250.1336.



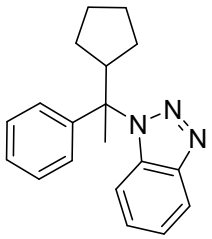
1-(1-cyclopropyl-1-phenylethyl)-1H-benzo[d][1,2,3]triazole (17)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 7.86 (m, 1H), 7.28 – 7.14 (m, 7H), 7.05 (ddd, *J* = 8.0, 6.9, 1.0 Hz, 1H), 6.58 (d, *J* = 8.4 Hz, 1H), 1.96 (ddd, *J* = 8.4, 5.5, 2.9 Hz, 1H), 1.92 (s, 2H), 0.82 – 0.72 (m, 1H), 0.56

– 0.46 (m, 1H), 0.39 (ddt, *J* = 11.1, 9.2, 5.5 Hz, 1H), 0.26 (dq, *J* = 9.7, 5.5 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.2, 141.9, 130.8, 127.0, 126.3, 124.8, 124.7, 121.8, 118.3, 110.8, 66.6, 24.1, 18.9, 2.2.

HRMS (ESI) calcd for $C_{17}H_{17}N_3$ ($M+H^+$): 264.1495, found: 264.1493.

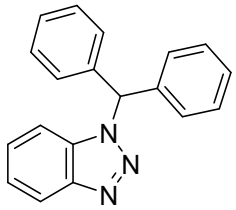


1-(1-cyclopentyl-1-phenylethyl)-1H-benzo[d][1,2,3]triazole (18)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.4 Hz, 1H), 7.34 – 7.26 (m, 3H), 7.25 – 7.20 (m, 1H), 7.20 – 7.15 (m, 2H), 7.14 – 7.07 (m, 1H), 6.66 (d, *J* = 8.4 Hz, 1H), 3.50 – 3.36 (m, 1H), 2.08 (s, 3H), 1.87 – 1.72 (m, 2H), 1.63 – 1.39 (m, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.71, 141.8, 131.4, 127.3, 126.6, 125.6, 125.1, 122.3, 118.7, 111.4, 69.2, 47.1, 27.8, 27.3, 24.5, 24.3, 22.7.

HRMS (ESI) calcd for $C_{19}H_{21}N_3$ ($M+H^+$): 292.1808, found: 292.1803.

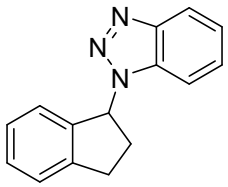


1-benzhydryl-1H-benzo[d][1,2,3]triazole (19)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 7.96 (m, 1H), 7.34 – 7.26 (m, 6H), 7.26 – 7.21 (m, 3H), 7.18 – 7.10 (m, 4H), 7.06 – 6.99 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.2, 136.6, 131.9, 127.7, 127.4, 127.2, 126.3, 125.5, 122.8, 119.1, 109.5, 66.1.

HRMS (ESI) calcd for $C_{19}H_{15}N_3$ ($M+H^+$): 286.1339, found: 286.1336.

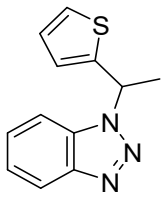


1-(2,3-dihydro-1H-inden-1-yl)-1H-benzo[d][1,2,3]triazole (20)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 6.9, 1.4 Hz, 1H), 7.44 – 7.27 (m, 4H), 7.17 (t, *J* = 7.4 Hz, 1H), 7.00 (d, *J* = 7.6 Hz, 1H), 6.91 (dd, *J* = 6.9, 1.3 Hz, 1H), 6.66 (t, *J* = 7.7 Hz, 1H), 3.33 (ddd, *J* = 16.0, 9.1, 4.1 Hz, 1H), 3.15 (dt, *J* = 16.2, 8.0 Hz, 1H), 2.88 (dtd, *J* = 12.7, 8.5, 4.2 Hz, 1H), 2.54 (ddt, *J* = 14.4, 9.0, 7.3 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.6, 142.4, 138.2, 130.6, 128.0, 126.1, 125.9, 124.2, 123.7, 122.7, 119.1, 109.4, 63.8, 31.5, 29.7.

HRMS (ESI) calcd for $C_{15}H_{13}N_3$ ($M+H^+$): 236.1182, found: 236.1181.

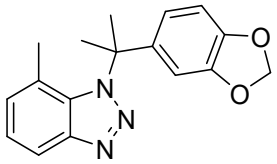


1-(1-(thiophen-2-yl)ethyl)-3a,7a-dihydro-1H-benzo[d][1,2,3]triazole (21)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.1 Hz, 1H), 7.35 – 7.23 (m, 3H), 7.18 (dd, *J* = 5.1, 1.1 Hz, 1H), 6.96 (d, *J* = 3.5 Hz, 1H), 6.88 (dd, *J* = 5.0, 3.6 Hz, 1H), 6.34 (q, *J* = 7.0 Hz, 1H), 2.12 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.0, 141.7, 130.8, 126.2, 125.9, 124.8, 124.6, 123.1, 118.9, 109.2, 53.9, 20.4.

HRMS (ESI) calcd for $C_{12}H_{11}N_3S$ ($M+H^+$): 230.0746, found: 230.0746.

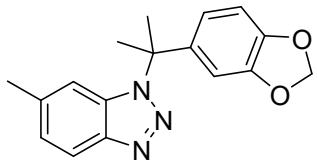


1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-4-methyl-1H-benzo[d][1,2,3]triazole (22)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 – 6.93 (m, 2H), 6.72 – 6.63 (m, 2H), 6.58 (d, *J* = 8.2 Hz, 1H), 6.51 (d, *J* = 1.2 Hz, 1H), 5.86 (s, 2H), 2.72 (s, 3H), 2.05 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.1, 146.0, 145.6, 137.2, 130.8, 129.6, 125.5, 122.4, 117.5, 108.4, 107.0, 105.3, 100.2, 63.4, 28.6, 15.7.

HRMS (ESI) calcd for $C_{17}H_{17}N_3O_2$ ($M+H^+$): 296.1394, found: 296.1394.

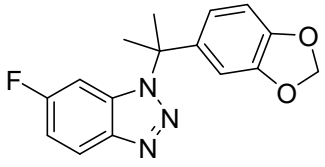


1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-5-methyl-1H-benzo[d][1,2,3]triazole (23)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 – 7.76 (m, 1H), 7.12 – 6.99 (m, 1H), 6.80 – 6.54 (m, 4H), 5.94 (d, *J* = 3.4 Hz, 2H), 2.38 (d, *J* = 40.4 Hz, 3H), 2.11 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.1, 146.5, 146.0, 146.0, 144.6, 137.3, 137.3, 135.9, 132.4, 131.4, 129.4, 127.7, 124.8, 118.3, 117.7, 117.5, 117.4, 110.5, 110.2, 110.2, 107.0, 105.3, 105.3, 100.2, 100.2, 63.4, 63.3, 28.7, 28.6, 21.0, 20.9, 20.3, 20.3.

HRMS (ESI) calcd for $C_{17}H_{17}N_3O_2$ ($M+H^+$): 296.1394, found: 296.1390.



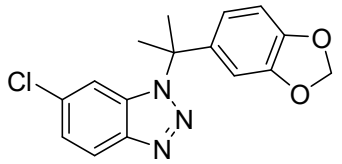
1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-5-fluoro-1H-benzo[d][1,2,3]triazole (24)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (dd, *J* = 9.1, 4.8 Hz, 1H), 7.59 (dd, *J* = 8.4, 2.2 Hz, 1H), 7.02 – 6.88 (m, 1H), 6.77 – 6.31 (m, 4H), 5.89 (d, *J* = 3.8 Hz, 2H), 2.05 (d, *J* = 3.2 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.2 (d, *J* = 246.7 Hz), 158.3 (d, *J* = 243.0 Hz), 147.3 (d, *J* = 3.5 Hz), 146.3 (d, *J* = 3.6 Hz), 146.1, 145.9, 142.7, 136.7, 136.4, 131.2 (d, *J* = 13.8 Hz), 127.9, 120.2, 120.1, 117.5, 117.5, 115.5 (d, *J* = 27.5 Hz), 112.7, 112.5, 112.0, 111.9, 107.2, 107.1, 105.2, 105.2, 103.3, 103.0, 100.4, 96.8, 96.6, 63.9, 63.7, 28.6, 28.5.

^{19}F NMR (376 MHz, $CDCl_3$) δ -112.61, -118.46.

HRMS (ESI) calcd for $C_{16}H_{14}FN_3O_2$ ($M+H^+$): 300.1143, found: 300.1143.

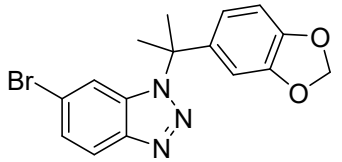


1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-5-chloro-1H-benzo[d][1,2,3]triazole (25)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.93 (m, 1H), 7.25 – 7.12 (m, 1H), 6.82 – 6.70 (m, 3H), 6.58 – 6.54 (m, 1H), 5.95 (d, *J* = 5.3 Hz, 2H), 2.11 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.3, 147.2, 146.6, 146.3, 146.3, 144.5, 136.6, 136.5, 131.8, 131.5, 129.6, 128.4, 126.4, 123.8, 119.8, 118.2, 117.5, 117.4, 111.9, 110.6, 107.2, 107.1, 105.2, 105.2, 100.4, 63.8, 63.8, 28.6.

HRMS (ESI) calcd for $C_{16}H_{14}ClN_3O_2$ ($M+H^+$): 316.0847, found: 316.0845.



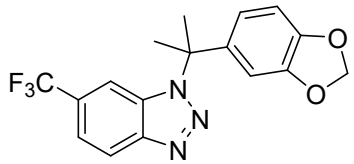
1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-5-bromo-1H-benzo[d][1,2,3]triazole (26)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 – 7.80 (m, 1H), 7.32 – 7.18 (m, 1H), 6.95 – 6.58 (m, 3H), 6.52 – 6.46 (m, 1H), 5.89 (d, *J* = 6.0 Hz, 2H), 2.05 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.3, 148.3, 148.0, 147.4, 147.3, 145.7, 137.6, 137.5, 133.0, 130.9, 129.9, 127.4, 122.4, 121.0, 121.0, 118.5, 118.5, 117.0, 114.8, 113.3, 108.2, 108.2, 106.3, 106.2, 101.4, 65.0, 64.9, 29.7, 29.7.

HRMS (ESI) calcd for $C_{16}H_{14}Br^{79}N_3O_2$ ($M+H^+$): 360.0342, found: 360.0342.

HRMS (ESI) calcd for $C_{16}H_{14}Br^{81}N_3O_2$ ($M+H^+$): 362.0322, found: 362.0320.



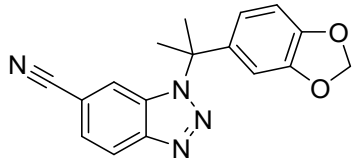
1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-5-(trifluoromethyl)-1H-benzo[d][1,2,3]triazole (27)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 – 8.05 (m, 1H), 7.48 – 7.30 (m, 1H), 7.04 – 6.81 (m, 1H), 6.76 – 6.69 (m, 2H), 6.56 – 6.47 (m, 1H), 5.89 (s, 2H), 2.11 – 2.06 (m, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.4, 148.4, 147.5, 147.4, 146.1, 137.5, 137.2, 133.4, 131.3, 128.8, 126.4, 126.0, 125.4, 123.2, 123.2, 120.9, 120.4, 118.6, 118.5, 118.1, 118.1, 113.0, 110.1 (d, *J* = 4.8 Hz), 108.2, 106.3, 101.4, 65.3, 65.1, 29.8, 29.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ -61.51, -61.69.

HRMS (ESI) calcd for $C_{17}H_{14}F_3N_3O_2$ ($M+K^+$): 390.0737, found: 390.0736.

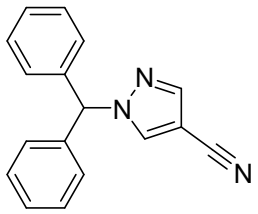


1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-1H-benzo[d][1,2,3]triazole-5-carbonitrile(28)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 – 8.10 (m, 1H), 7.53 – 7.37 (m, 1H), 7.20 – 6.85 (m, 1H), 6.82 – 6.72 (m, 2H), 6.60 – 6.54 (m, 1H), 6.01 – 5.96 (m, 2H), 2.14 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.5, 147.4, 146.6, 135.8, 130.2, 127.7, 125.0, 120.4, 117.5, 117.5, 116.8, 112.4, 109.0, 107.4, 107.3, 106.4, 105.2, 105.0, 100.5, 100.5, 64.6, 64.4, 28.7, 28.7.

HRMS (ESI) calcd for $C_{17}H_{14}N_4O_2$ ($M+Na^+$): 329.1009, found: 329.1007.

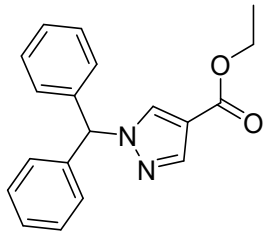


1-benzhydryl-1H-pyrrole-3-carbonitrile (29)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.56 (s, 1H), 7.33 – 7.28 (m, 6H), 7.05 – 6.97 (m, 4H), 6.71 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 141.6, 136.7, 133.7, 128.0, 127.7, 127.0, 112.3, 91.2, 69.3.

HRMS (ESI) calcd for $C_{18}H_{14}N_2$ ($M+H^+$): 260.1182, found: 260.1179.

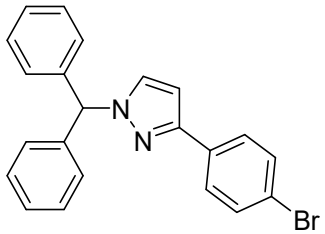


ethyl 1-benzhydryl-1H-pyrazole-4-carboxylate (30)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.67 (s, 1H), 7.30 – 7.25 (m, 6H), 7.06 – 6.97 (m, 4H), 6.69 (s, 1H), 4.19 (q, *J* = 7.1 Hz, 2H), 1.24 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.0, 140.4, 137.4, 131.9, 127.8, 127.4, 127.1, 113.9, 68.9, 59.2, 13.3.

HRMS (ESI) calcd for $C_{19}H_{18}N_2O_2$ ($M+H^+$): 307.1441, found: 307.1438.



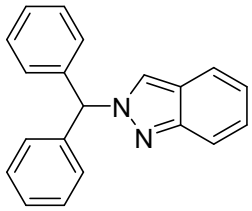
1-benzhydryl-3-(4-bromophenyl)-1H-pyrazole (31)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 1.7 Hz, 1H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.27 – 7.17 (m, 6H), 7.12 (d, *J* = 8.5 Hz, 2H), 7.08 – 7.04 (m, 4H), 6.47 (s, 1H), 6.26 (d, *J* = 1.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.3, 139.1, 138.5, 130.9, 129.7, 128.7, 127.4, 127.3, 126.7, 122.1, 105.2, 64.5.

HRMS (ESI) calcd for $C_{22}H_{17}BrN_2$ ($M+H^+$): 389.0648, found: 389.0644.

HRMS (ESI) calcd for $C_{22}H_{17}BrN_2$ ($M+H^+$): 391.0622, found: 391.0627.

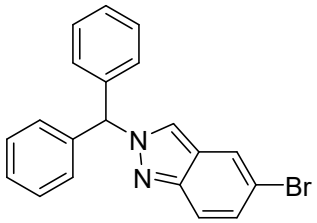


2-benzhydryl-2H-indazole (32)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.63 (m, 2H), 7.55 – 7.51 (m, 1H), 7.30 – 7.24 (m, 6H), 7.20 (ddd, *J* = 8.6, 6.5, 0.9 Hz, 1H), 7.06 – 7.02 (m, 5H), 7.01 – 6.97 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.8, 137.9, 127.7, 127.3, 125.0, 122.2, 120.7, 120.4, 119.3, 116.7, 70.0.

HRMS (ESI) calcd for $C_{20}H_{16}N_2$ ($M+H^+$): 285.1386, found: 285.1384.



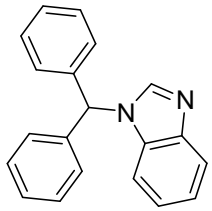
2-benzhydryl-5-bromo-2H-indazole (33)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 1.2 Hz, 1H), 7.69 (s, 1H), 7.61 (d, *J* = 9.2 Hz, 1H), 7.40 – 7.30 (m, 7H), 7.11 (dd, *J* = 6.6, 2.7 Hz, 4H), 7.07 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 146.2, 137.5, 128.7, 127.8, 127.4, 127.2, 121.7, 121.6, 121.4, 118.5, 114.2, 70.1.

HRMS (ESI) calcd for $C_{20}H_{15}BrN_2$ ($M+Na^+$): 385.0311, found: 385.0308.

HRMS (ESI) calcd for $C_{20}H_{15}BrN_2$ ($M+Na^+$): 387.0290, found: 387.0286.

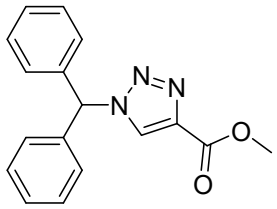


1-benzhydryl-1H-benzo[d]imidazole (34)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.1 Hz, 1H), 7.53 (s, 1H), 7.28 (dd, *J* = 5.1, 1.9 Hz, 6H), 7.19 (M, 1H), 7.14 – 7.03 (m, 6H), 6.67 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.0, 141.5, 137.0, 133.0, 128.0, 127.5, 127.1, 121.9, 121.3, 119.3, 109.7, 62.5.

HRMS (ESI) calcd for $C_{20}H_{16}N_2$ ($M+H^+$): 285.1386, found: 285.1385.

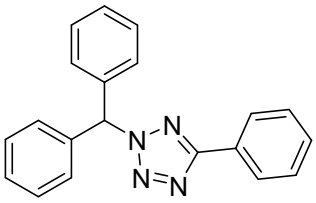


methyl 1-benzhydryl-1H-1,2,3-triazole-4-carboxylate (35)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.77 (s, 1H), 7.32 – 7.14 (m, 10H), 3.84 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.0, 137.0, 136.9, 127.6, 127.5, 127.3, 126.9, 65.7, 51.4.

HRMS (ESI) calcd for $C_{17}H_{15}N_3O_2$ ($M+H^+$): 294.1237, found: 294.1237.

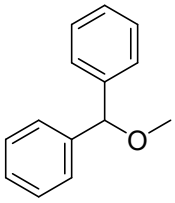


2-benzhydryl-5-phenyl-2H-tetrazole (36)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (M, 2H), 7.49 – 7.45 (m, 3H), 7.39 – 7.35 (m, 6H), 7.35 – 7.32 (m, 5H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.2, 136.1, 129.2, 127.7, 127.7, 127.6, 127.2, 126.3, 125.9, 70.1.

HRMS (ESI) calcd for $C_{20}H_{16}N_4$ ($M+H^+$): 313.1448, found: 313.1445.

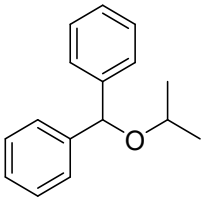


(methoxymethylene)dibenzene (37)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.20 (m, 8H), 7.19 – 7.13 (m, 2H), 5.16 (s, 1H), 3.30 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 141.0, 127.3, 126.4, 125.8, 84.3, 55.9.

HRMS (ESI) calcd for $C_{14}H_{14}O$ ($M+Na^+$): 221.0937, found: 221.0936.

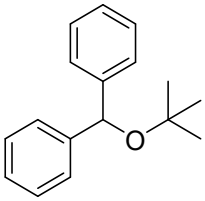


(isopropoxymethylene)dibenzene (38)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.20 (m, 8H), 7.17 – 7.12 (m, 2H), 5.41 (s, 1H), 3.59 (dt, *J* = 12.2, 6.1 Hz, 1H), 1.14 (d, *J* = 6.1 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 141.9, 127.2, 126.2, 126.0, 79.4, 68.0, 21.2.

HRMS (ESI) calcd for $C_{16}H_{18}O$ ($M+Na^+$): 249.1250, found: 249.1248.

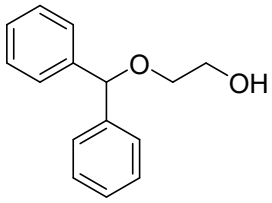


(tert-butoxymethylene)dibenzene (39)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.24 (m, 4H), 7.20 (t, *J* = 7.5 Hz, 4H), 7.14 – 7.08 (m, 2H), 5.51 (s, 1H), 1.15 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.0, 127.0, 125.8, 125.7, 74.6, 73.9, 27.7.

HRMS (ESI) calcd for $C_{17}H_{20}O$ ($M+Na^+$): 263.1406, found: 263.1404.

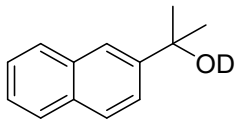


2-(benzhydryloxy)ethan-1-ol (40)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.14 (m, 10H), 5.32 (s, 1H), 3.69 (s, 2H), 3.52 – 3.48 (m, 2H), 2.11 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 140.8, 127.4, 126.5, 125.9, 83.0, 69.3, 60.9.

HRMS (ESI) calcd for $C_{15}H_{16}O_2$ ($M+Na^+$): 251.1043, found: 251.1040.

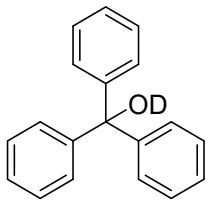


2-(naphthalen-2-yl)propan-2-ol-d(41)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.75 (t, *J* = 8.3 Hz, 3H), 7.53 (d, *J* = 8.5 Hz, 1H), 7.42 – 7.36 (m, 2H), 1.60 (s, 7H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 145.3, 132.1, 131.2, 127.0, 126.9, 126.4, 125.0, 124.6, 122.4, 121.3, 71.6, 30.6.

HRMS (ESI) calcd for $C_{13}H_{13}DO$ ($M+H^+$): 188.1180, found: 188.1180.

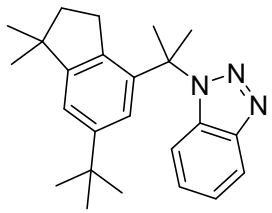


triphenylmethanol-d(42)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.24 – 7.16 (m, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 145.7, 126.8, 126.2, 80.9.

HRMS (ESI) calcd for $C_{19}H_{15}DO$ ($M+H^+$): 262.1337, found: 262.1337.

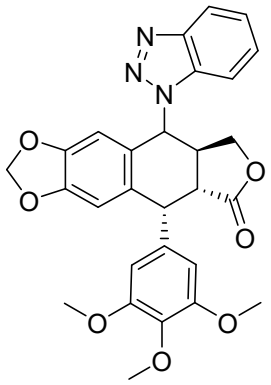


1-(2-(6-(tert-butyl)-1,1-dimethyl-2,3-dihydro-1H-inden-4-yl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (43)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.4 Hz, 1H), 7.43 (d, *J* = 1.7 Hz, 1H), 7.26 – 7.21 (m, 1H), 7.14 (d, *J* = 1.6 Hz, 1H), 7.09 (ddd, *J* = 8.0, 6.9, 0.9 Hz, 1H), 6.47 (d, *J* = 8.4 Hz, 1H), 2.18 (s, 6H), 1.62 (t, *J* = 7.0 Hz, 2H), 1.47 (t, *J* = 7.0 Hz, 2H), 1.41 (s, 9H), 1.01 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.5, 149.4, 145.8, 137.5, 136.4, 131.2, 125.1, 122.4, 118.7, 117.5, 110.2, 63.9, 41.8, 40.0, 33.9, 30.6, 27.6, 27.1, 26.8.

HRMS (ESI) calcd for $C_{24}H_{31}N_3$ ($M+H^+$): 362.2591, found: 362.2572.

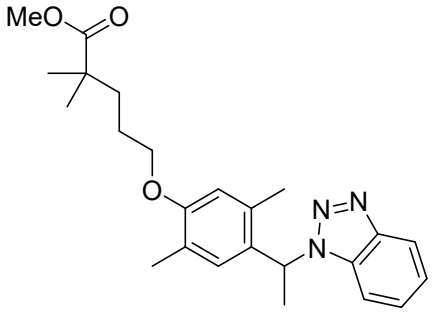


(5R,5aR,8aS)-9-(1H-benzo[d][1,2,3]triazol-1-yl)-5-(3,4,5-trimethoxyphenyl)-5,8,8a,9-tetrahydrofuro[3',4':6,7]naphtho[2,3-d][1,3]dioxol-6(5aH)-one (44)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dd, *J* = 6.7, 1.8 Hz, 1H), 7.42 – 7.33 (m, 2H), 6.71 (s, 1H), 6.57 (s, 1H), 6.39 (s, 2H), 6.35 (d, *J* = 4.9 Hz, 1H), 5.98 (d, *J* = 1.1 Hz, 1H), 5.94 (d, *J* = 1.1 Hz, 1H), 4.85 (d, *J* = 4.8 Hz, 1H), 4.33 (dd, *J* = 8.8, 7.5 Hz, 1H), 3.85 (d, *J* = 7.2 Hz, 1H), 3.81 (s, 3H), 3.76 (s, 6H), 3.46 (dd, *J* = 14.2, 4.3 Hz, 1H), 3.40 – 3.27 (m, 1H), 3.04 (t, *J* = 9.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.3, 151.7, 148.2, 147.0, 145.0, 136.4, 133.5, 132.5, 132.1, 127.4, 123.9, 123.4, 119.5, 109.4, 108.3, 107.9, 107.2, 100.9, 66.3, 59.7, 56.6, 55.3, 42.7, 41.4, 37.0.

HRMS (ESI) calcd for $C_{28}H_{25}N_3O_7$ ($M+Na^+$): 538.1585, found: 538.1589.

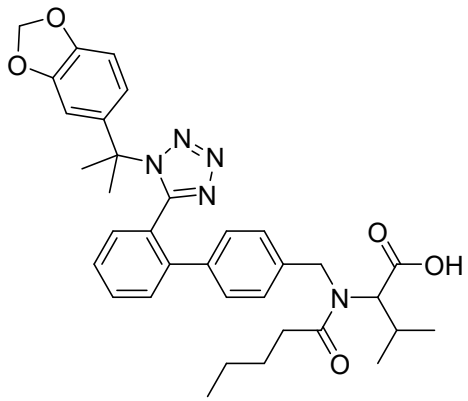


Methyl 5-(4-(1-(1H-benzo[d][1,2,3]triazol-1-yl)ethyl)-2,5-dimethylphenoxy)-2,2-dimethylpentanoate (45)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 – 7.98 (m, 1H), 7.30 – 7.24 (m, 2H), 7.09 (dd, *J* = 5.0, 2.3 Hz, 1H), 7.05 (s, 1H), 6.56 (s, 1H), 6.16 (q, *J* = 7.0 Hz, 1H), 3.88 (d, *J* = 5.4 Hz, 2H), 3.63 (s, 3H), 2.23 (s, 3H), 2.13 (s, 3H), 2.08 (d, *J* = 7.0 Hz, 3H), 1.75 – 1.64 (m, 4H), 1.20 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 177.2, 155.6, 145.3, 133.0, 131.2, 127.8, 127.2, 125.8, 123.7, 122.6, 118.8, 112.1, 109.1, 66.8, 54.8, 50.7, 41.0, 35.9, 24.1, 24.0, 19.7, 18.1, 14.8.

HRMS (ESI) calcd for $C_{24}H_{31}N_3O_3$ ($M+H^+$): 410.2438, found: 410.2433.

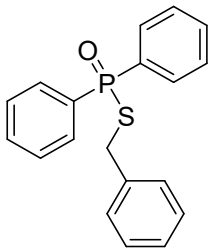


N-((2'-(1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-1H-tetrazol-5-yl)-[1,1'-biphenyl]-4-yl)methyl)-N-pentanoylvaline (46)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.74 (m, 1H), 7.53 – 7.40 (m, 2H), 7.38 (dd, *J* = 7.4, 1.2 Hz, 1H), 7.17 – 7.06 (m, 4H), 6.70 (d, *J* = 8.2 Hz, 1H), 6.61 (dd, *J* = 8.2, 1.9 Hz, 1H), 6.40 (d, *J* = 1.9 Hz, 1H), 5.93 (d, *J* = 0.5 Hz, 2H), 4.73 (d, *J* = 16.9 Hz, 1H), 4.43 (d, *J* = 16.9 Hz, 1H), 3.87 (d, *J* = 10.5 Hz, 1H), 2.69 – 2.55 (m, 1H), 2.48 – 2.29 (m, 2H), 1.98 (s, 6H), 1.68 – 1.54 (m, 2H), 1.42 – 1.28 (m, 2H), 1.01 – 0.83 (m, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 176.0, 170.8, 163.5, 146.7, 146.0, 140.2, 139.7, 136.6, 133.2, 129.6, 129.3, 128.9, 128.8, 127.8, 126.6, 125.3, 125.2, 117.0, 106.8, 104.8, 100.2, 66.8, 59.4, 52.9, 33.0, 28.0, 27.9, 26.2, 26.1, 21.3, 20.0, 18.7, 18.4, 13.1, 12.8.

HRMS (ESI) calcd for $C_{34}H_{39}N_5O_5$ ($M+Na^+$): 620.2843, found: 620.2843.



S-benzyl diphenylphosphinothioate (48)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.74 (m, 4H), 7.49 – 7.34 (m, 6H), 7.15 – 7.08 (m, 5H), 3.95 (d, *J* = 9.2 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 135.7 (d, *J* = 5.7 Hz), 131.3 (d, *J* = 2.9 Hz), 130.5, 130.4, 127.9, 127.7, 127.5 (d, *J* = 3.4 Hz), 126.4, 32.1 (d, *J* = 2.1 Hz).

HRMS (ESI) calcd for $C_{19}H_{17}OPS$ ($M+H^+$): 325.0810, found: 325.0807.

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3. Liu, J.; Qiu, X.; Huang, X.; Luo, X.; Zhang, C.; Wei, J.; Pan, J.; Liang, Y.; Zhu, Y.; Qin, Q.; Song, S.; Jiao, N., From alkylarenes to anilines via site-directed carbon–carbon amination. *Nat. Chem.* **2019,** *11*, 71-77.
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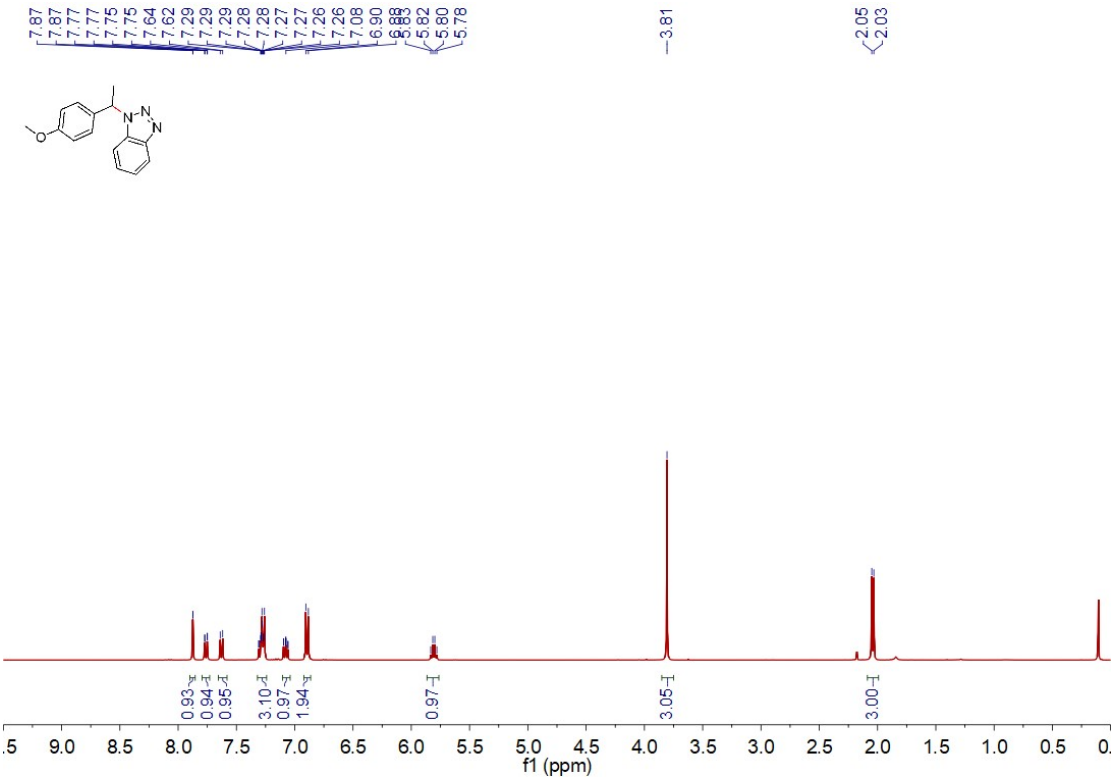
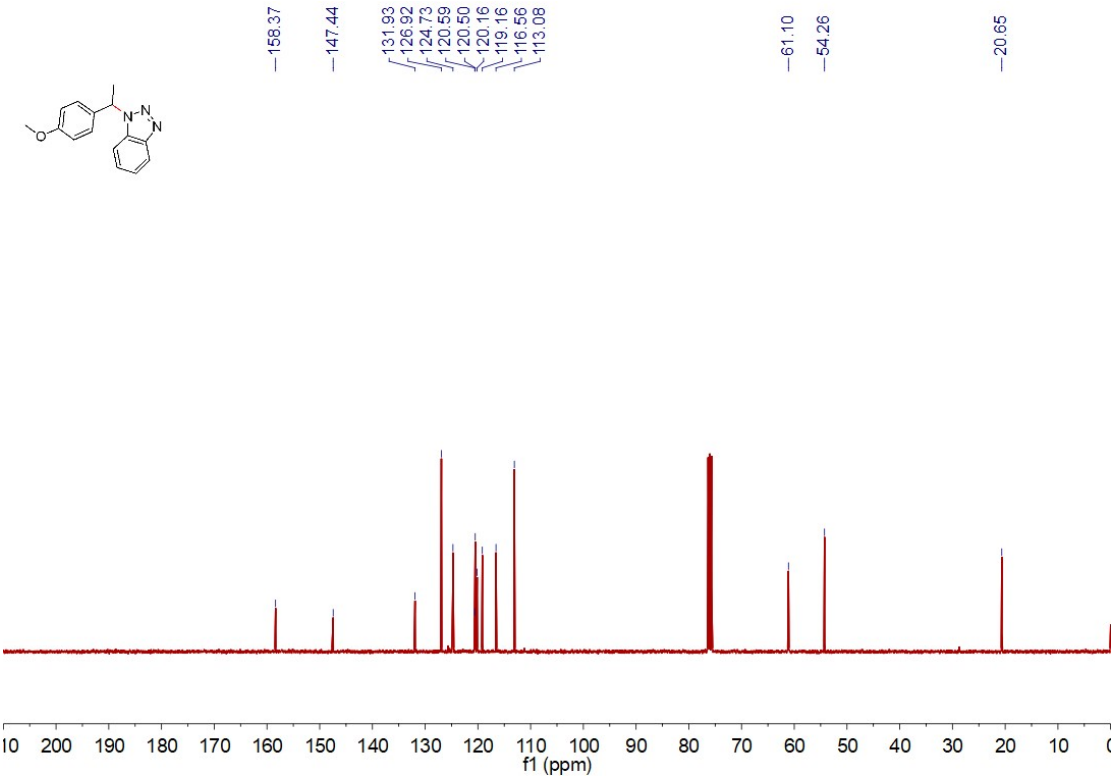
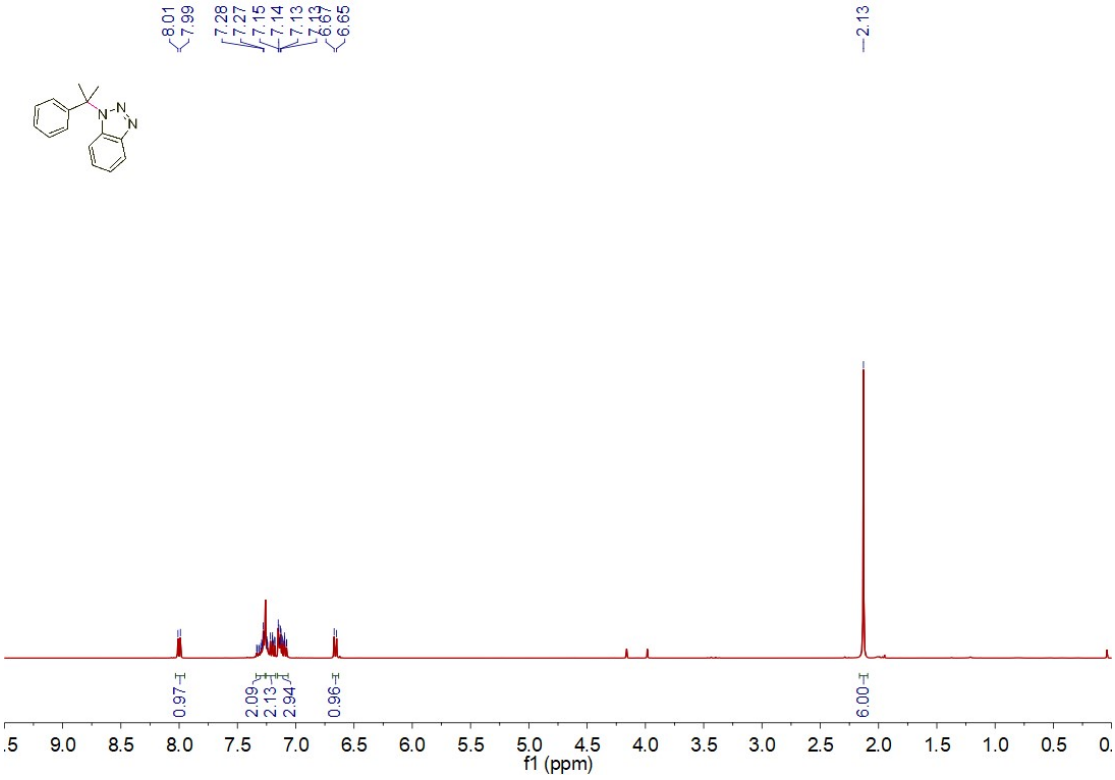
NMR Spectra

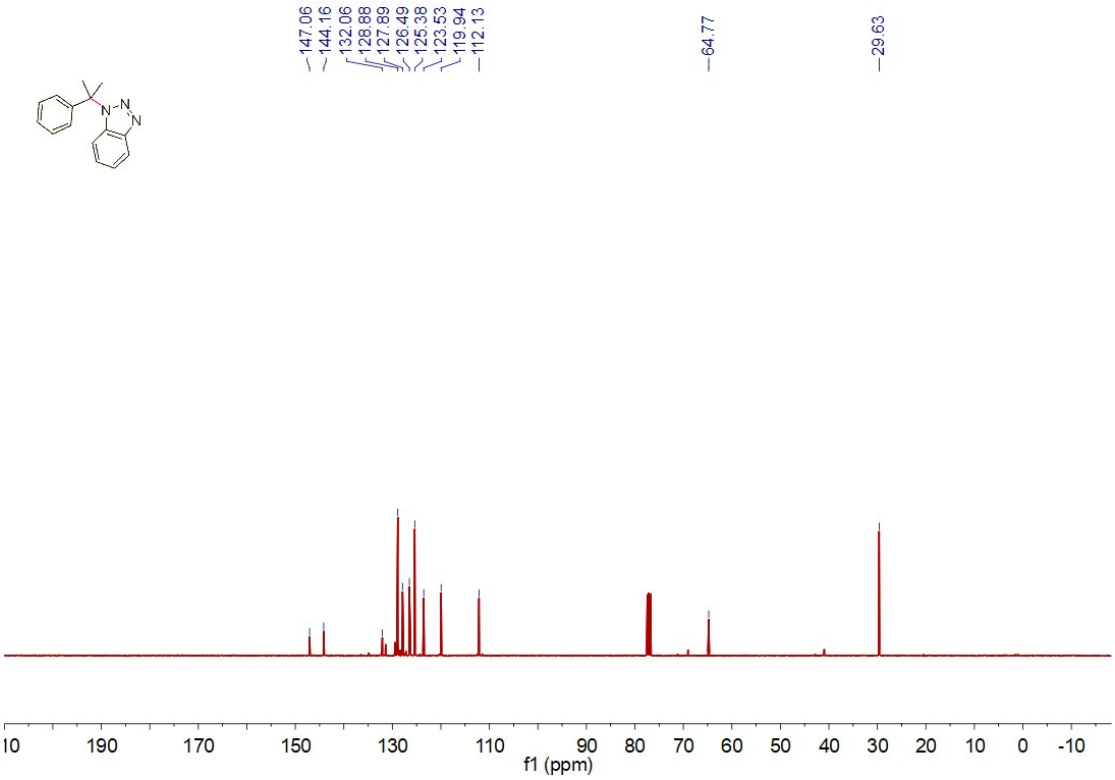
1-(1-(4-methoxyphenyl)ethyl)-1H-benzo[d][1,2,3]triazole (1aa)



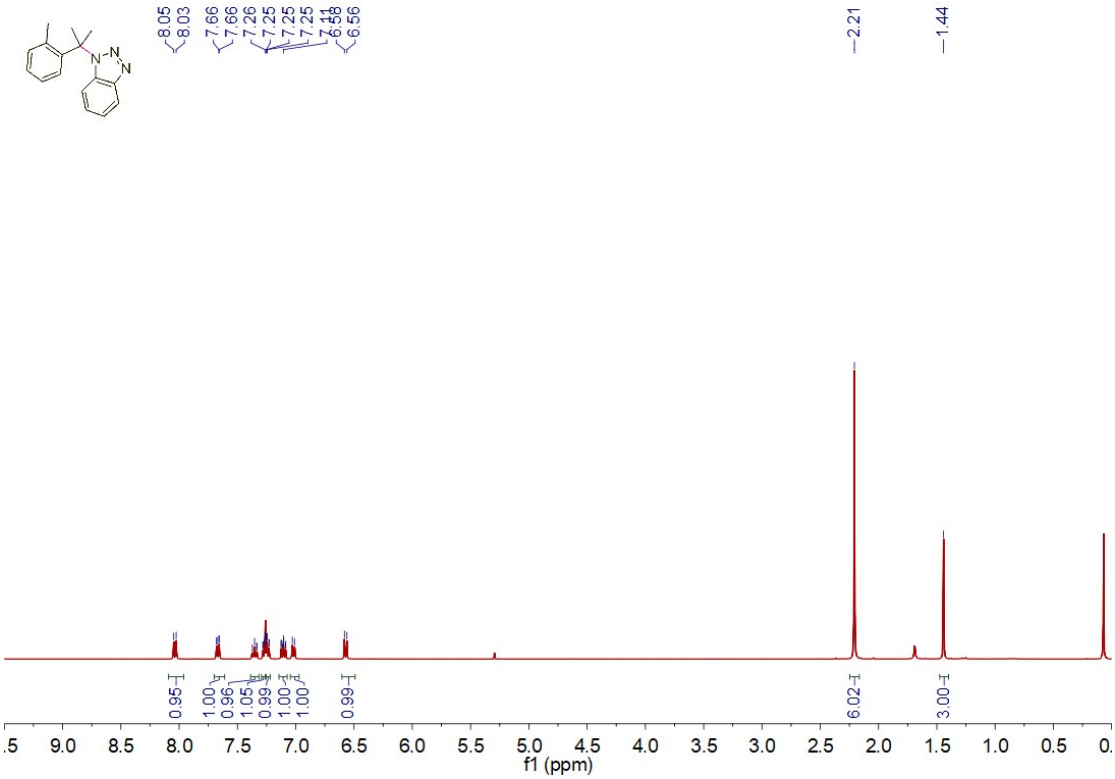


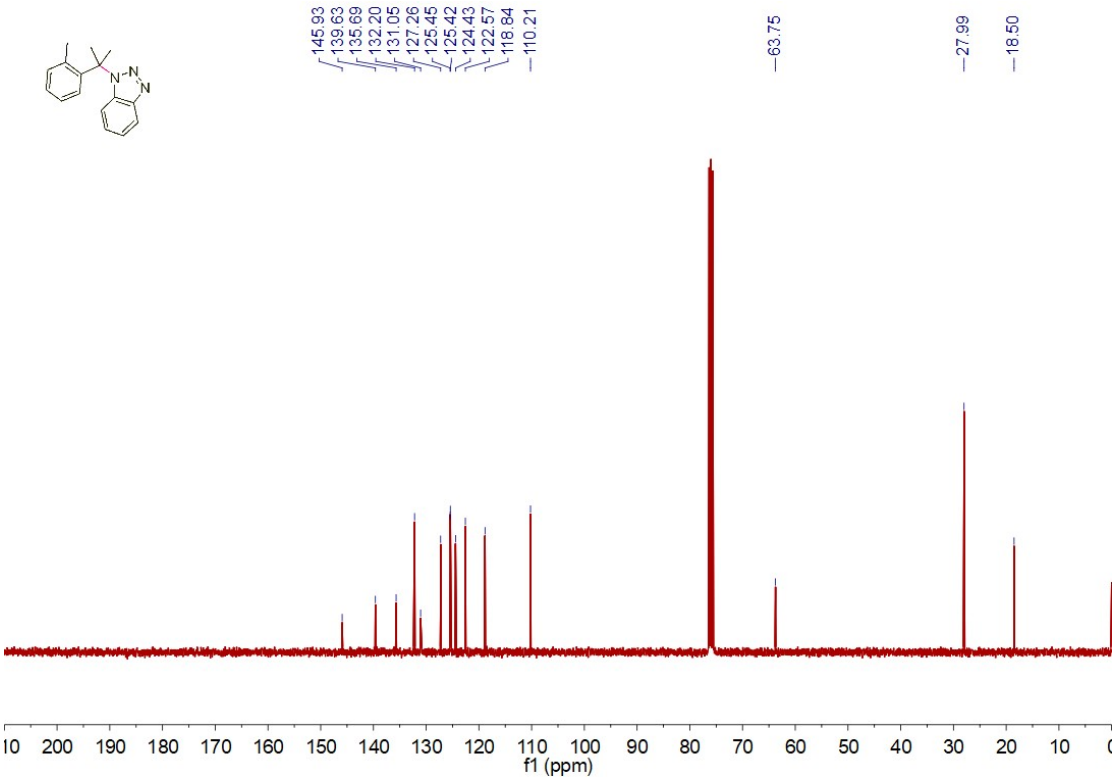
1-(2-phenylpropan-2-yl)-1H-benzo[d][1,2,3]triazole (3)



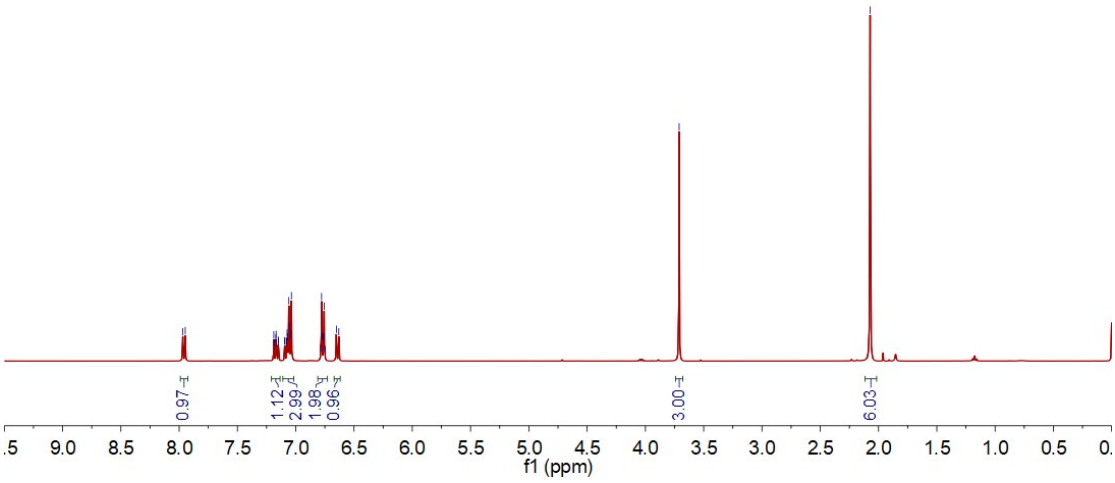


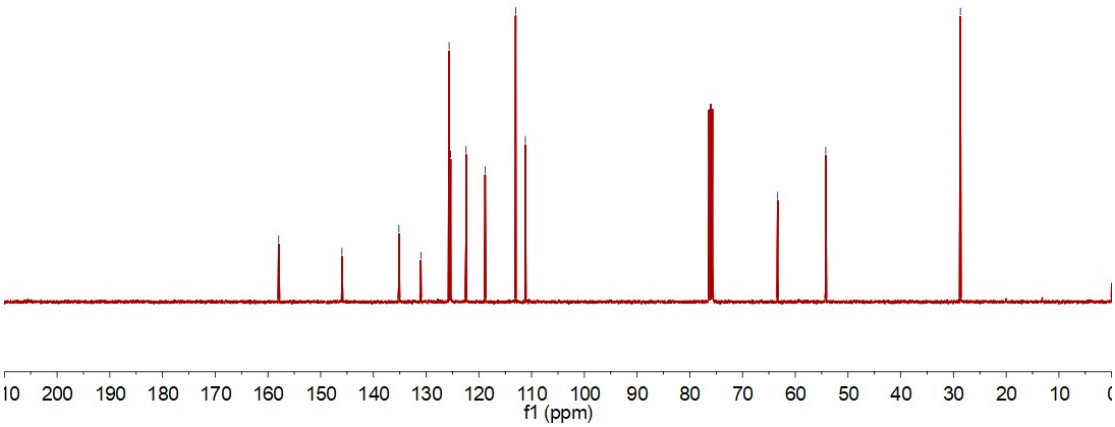
1-(2-(o-tolyl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (4)



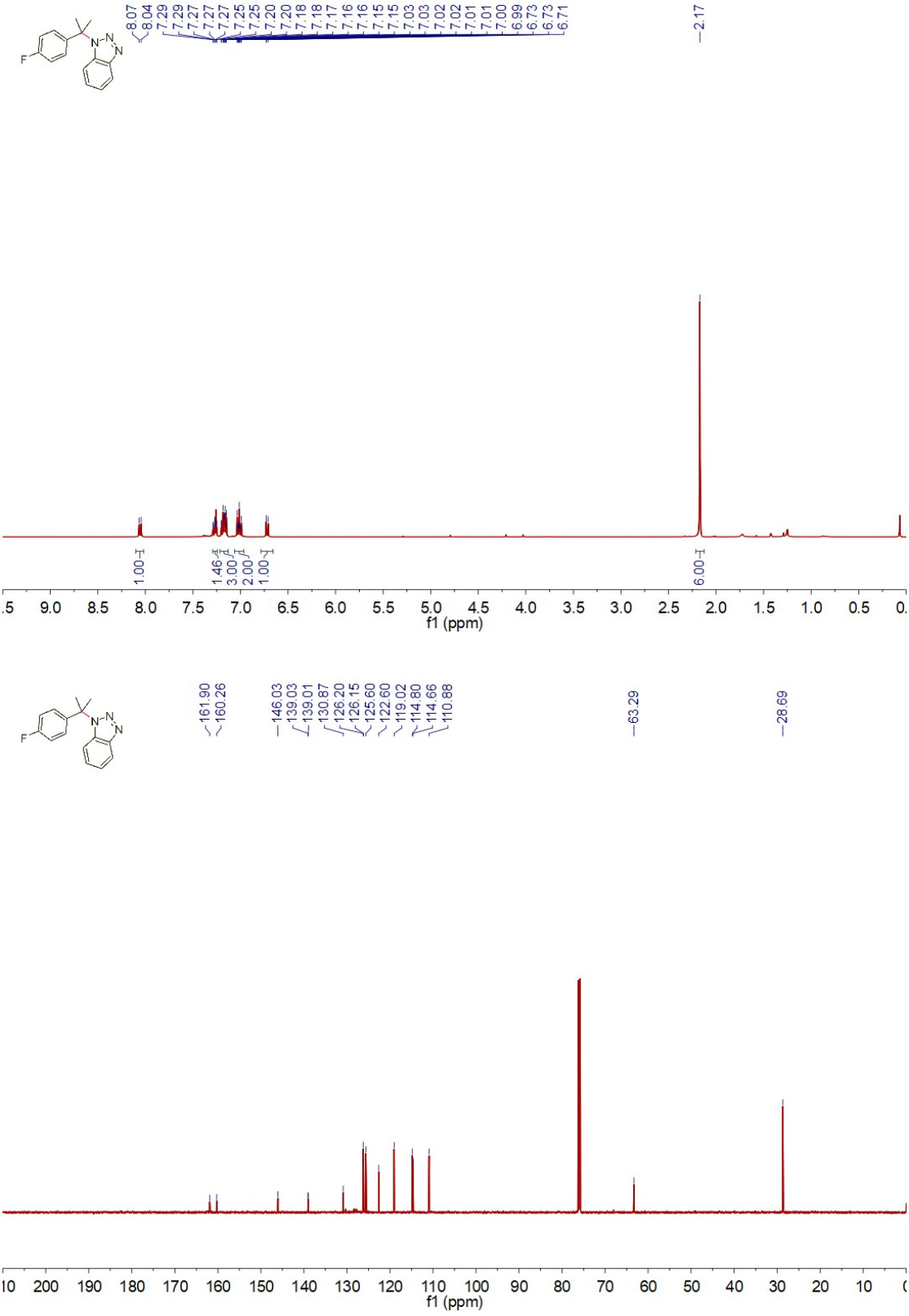


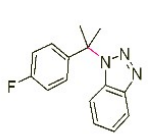
1-(2-(4-methoxyphenyl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (5)





1-(2-(4-fluorophenyl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (6)

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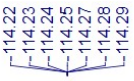
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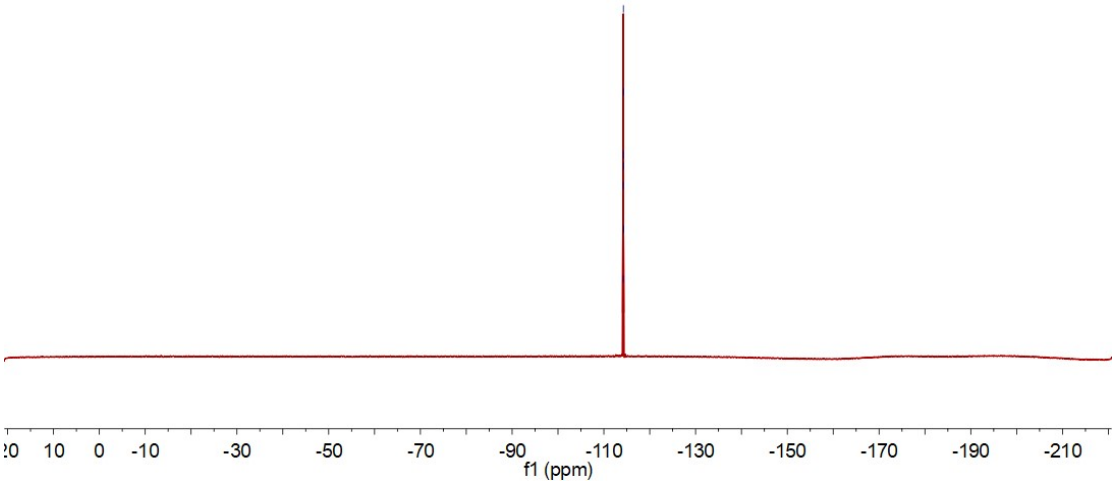
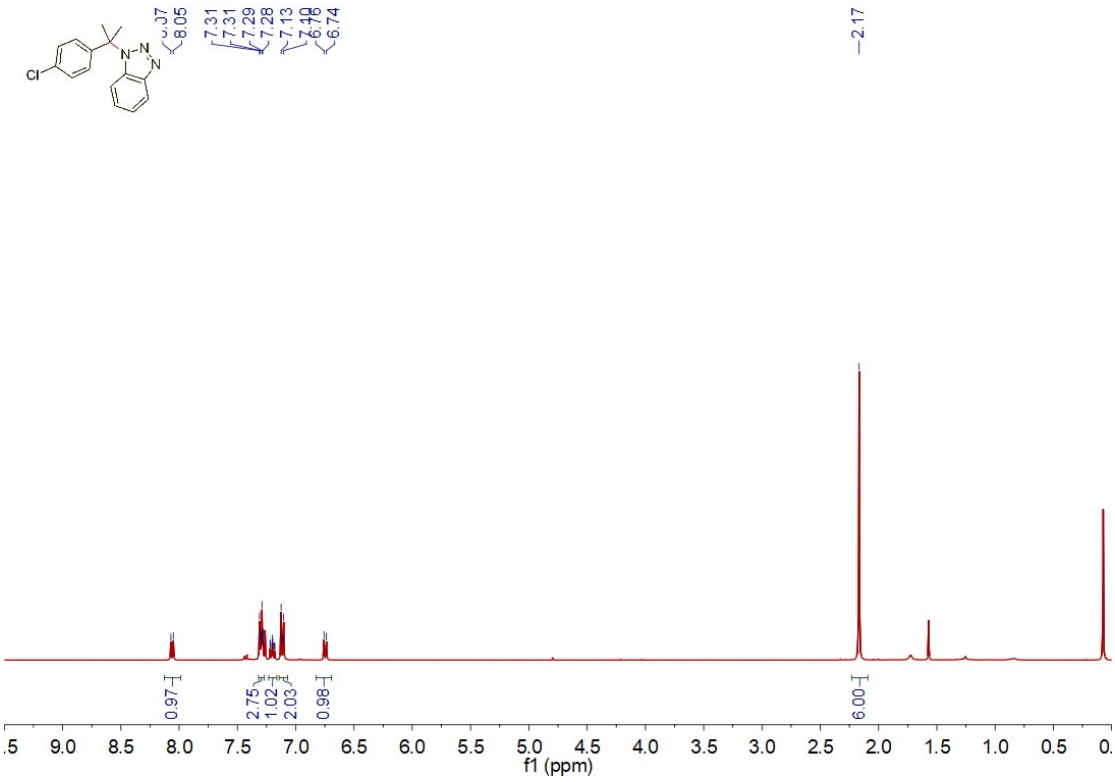
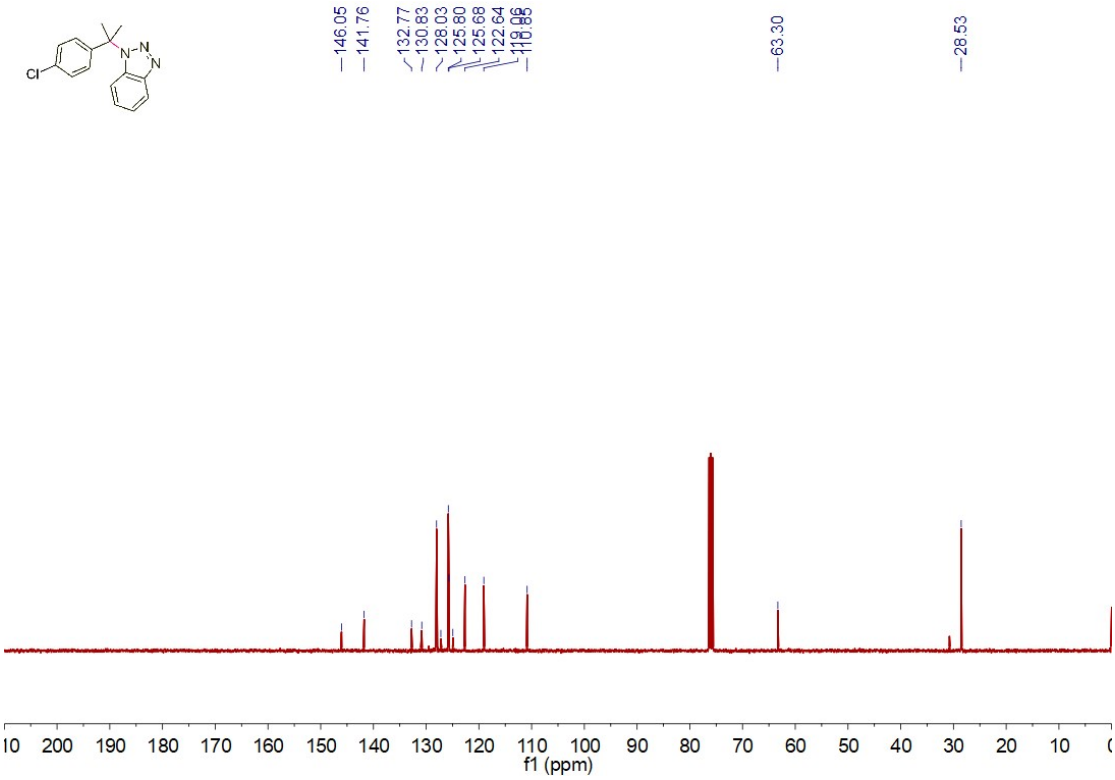
114.28
114.29

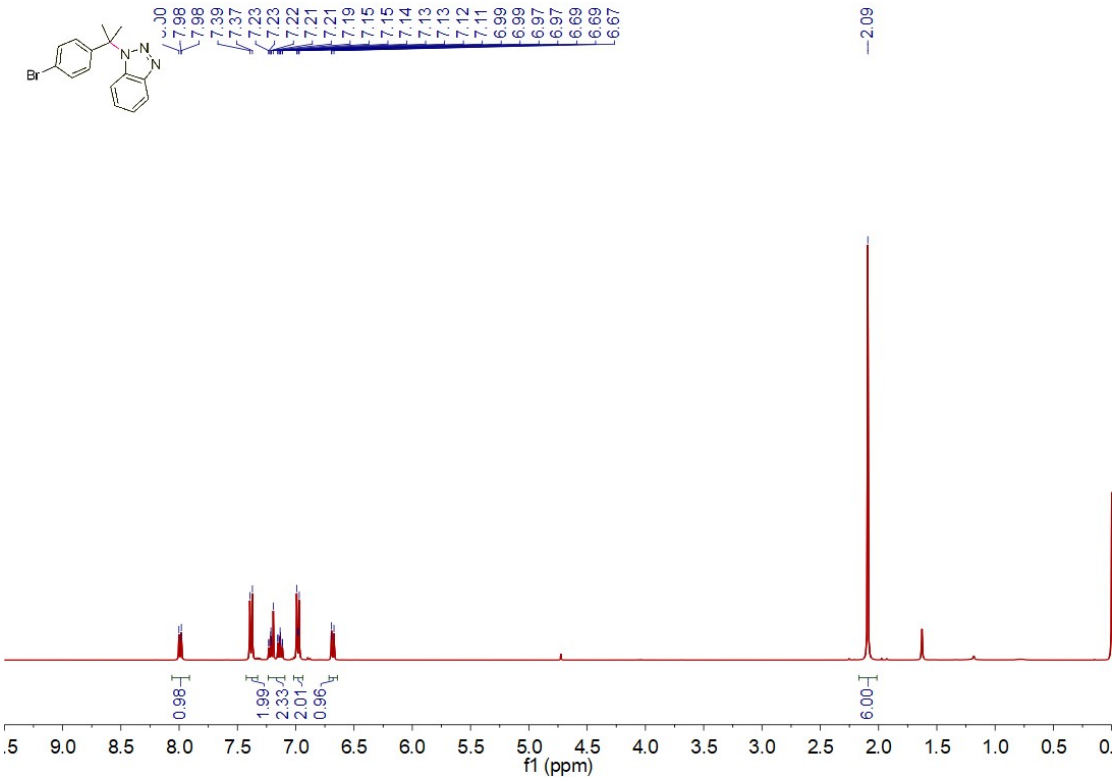

10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)

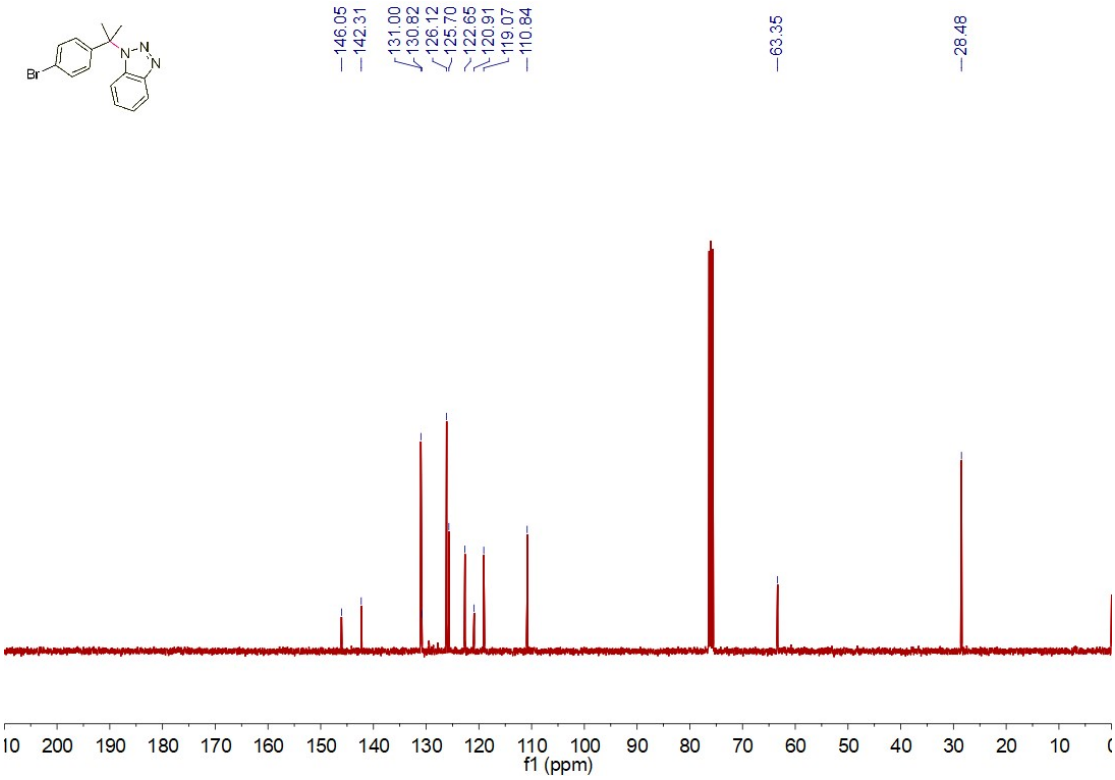
1-(2-(4-chlorophenyl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (7)



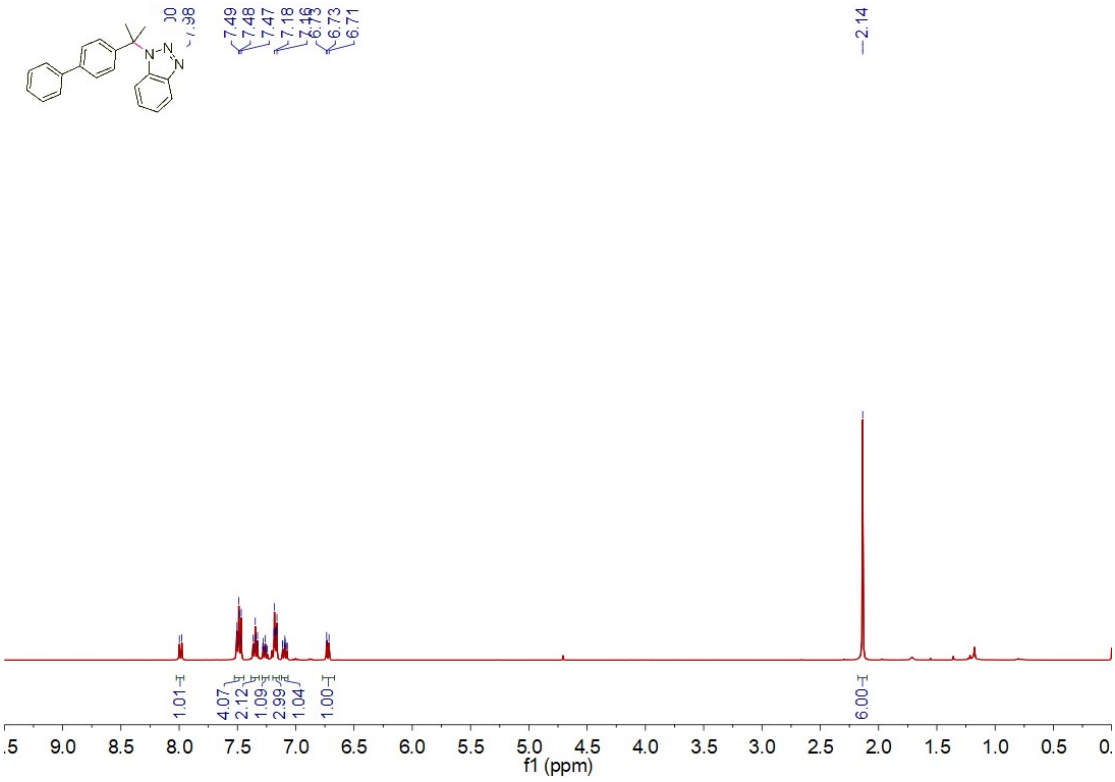


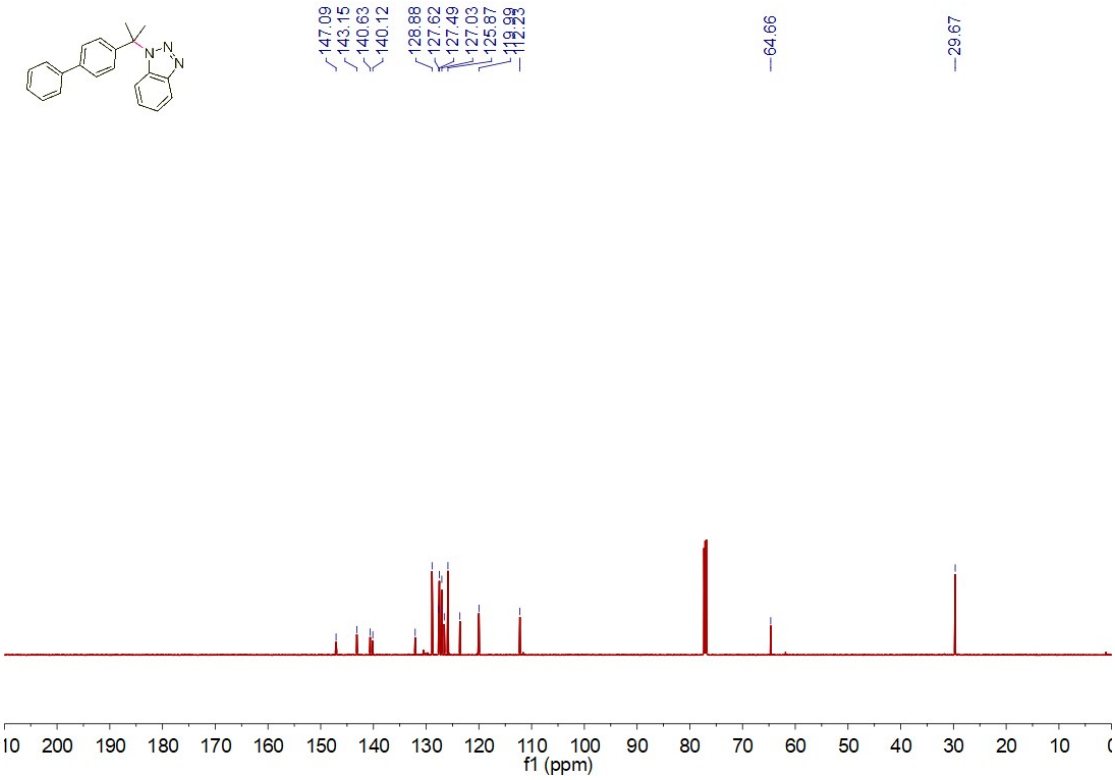
1-(2-(4-bromophenyl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (8)



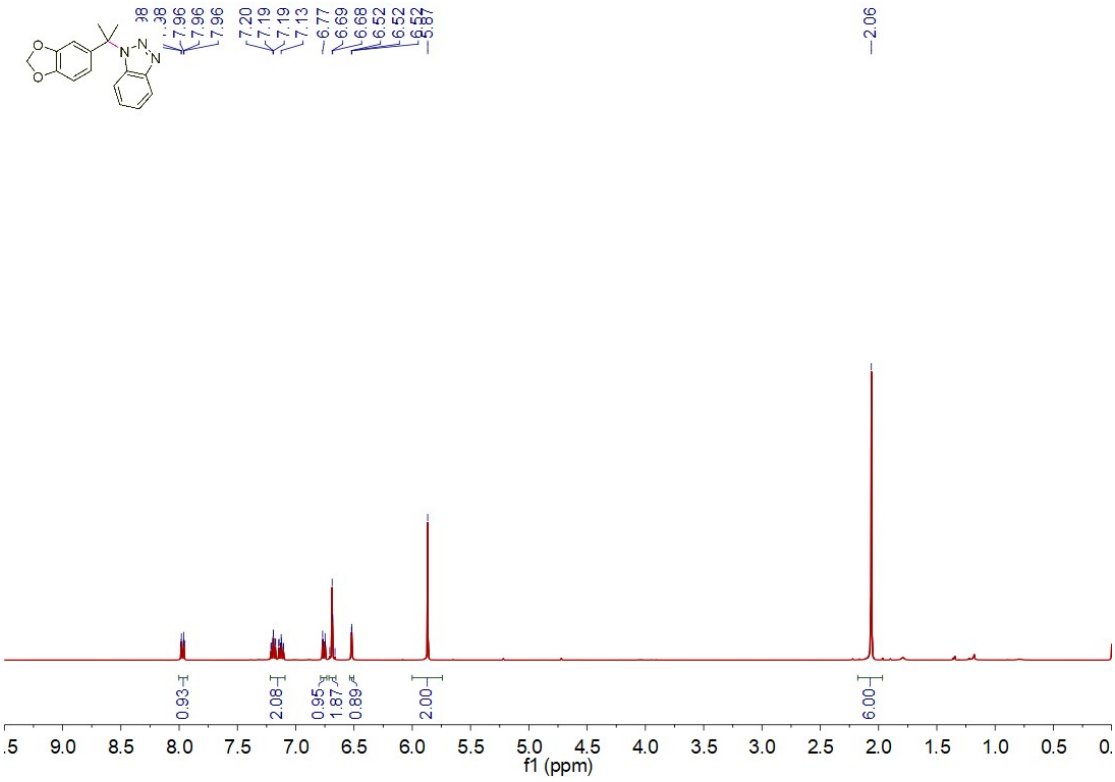


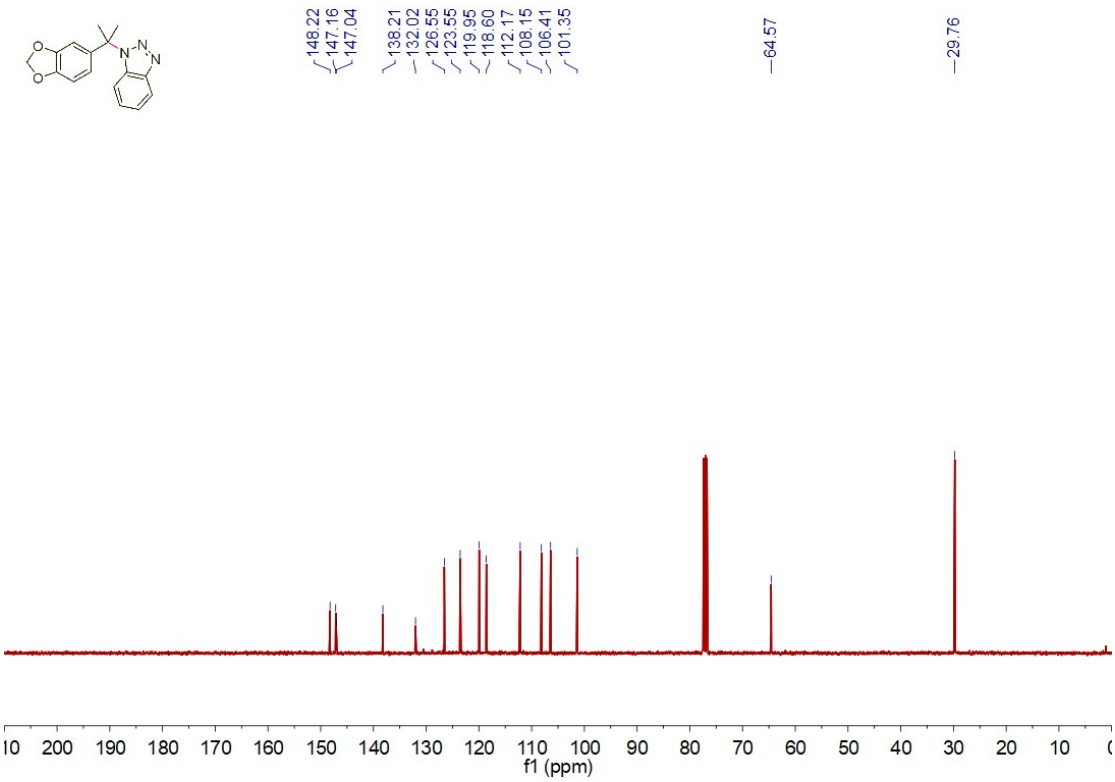
1-(2-([1,1'-biphenyl]-4-yl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (9)



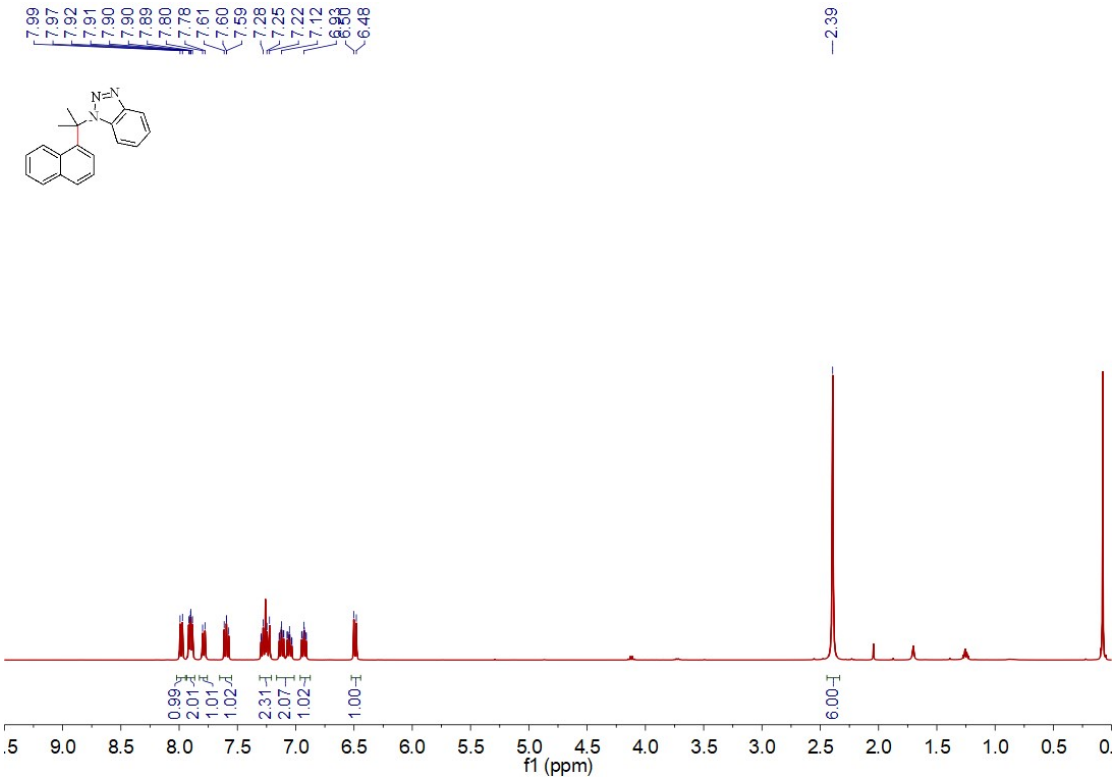


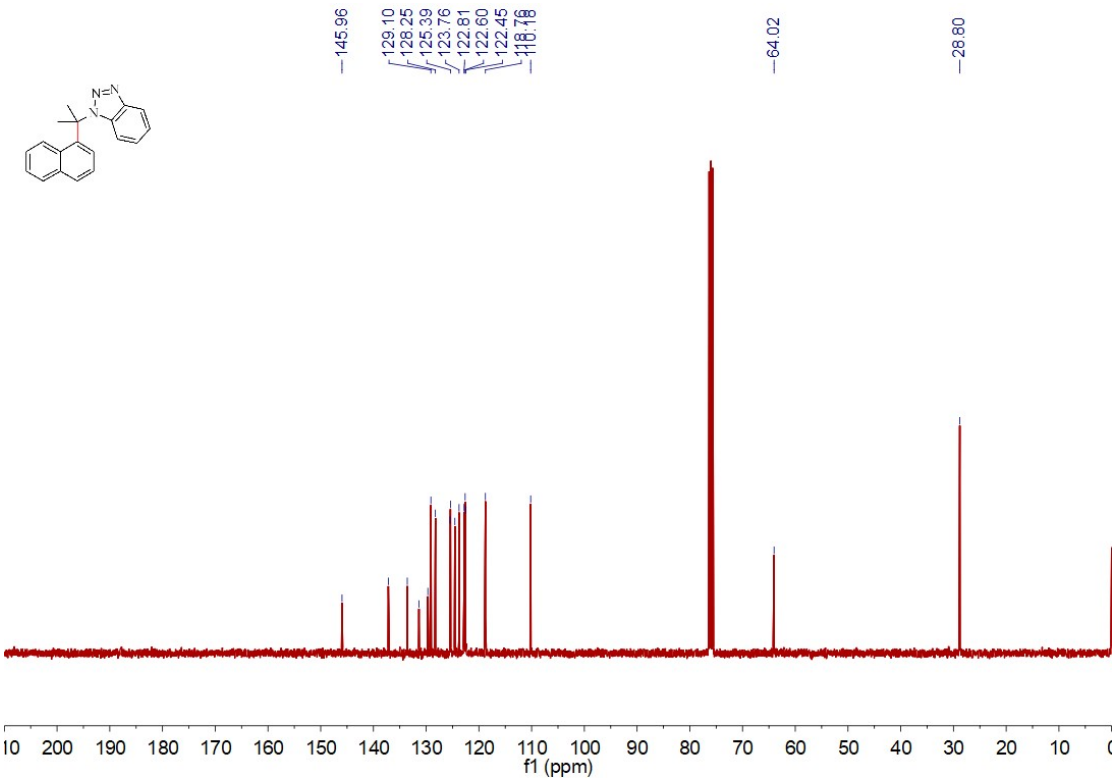
1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (10)



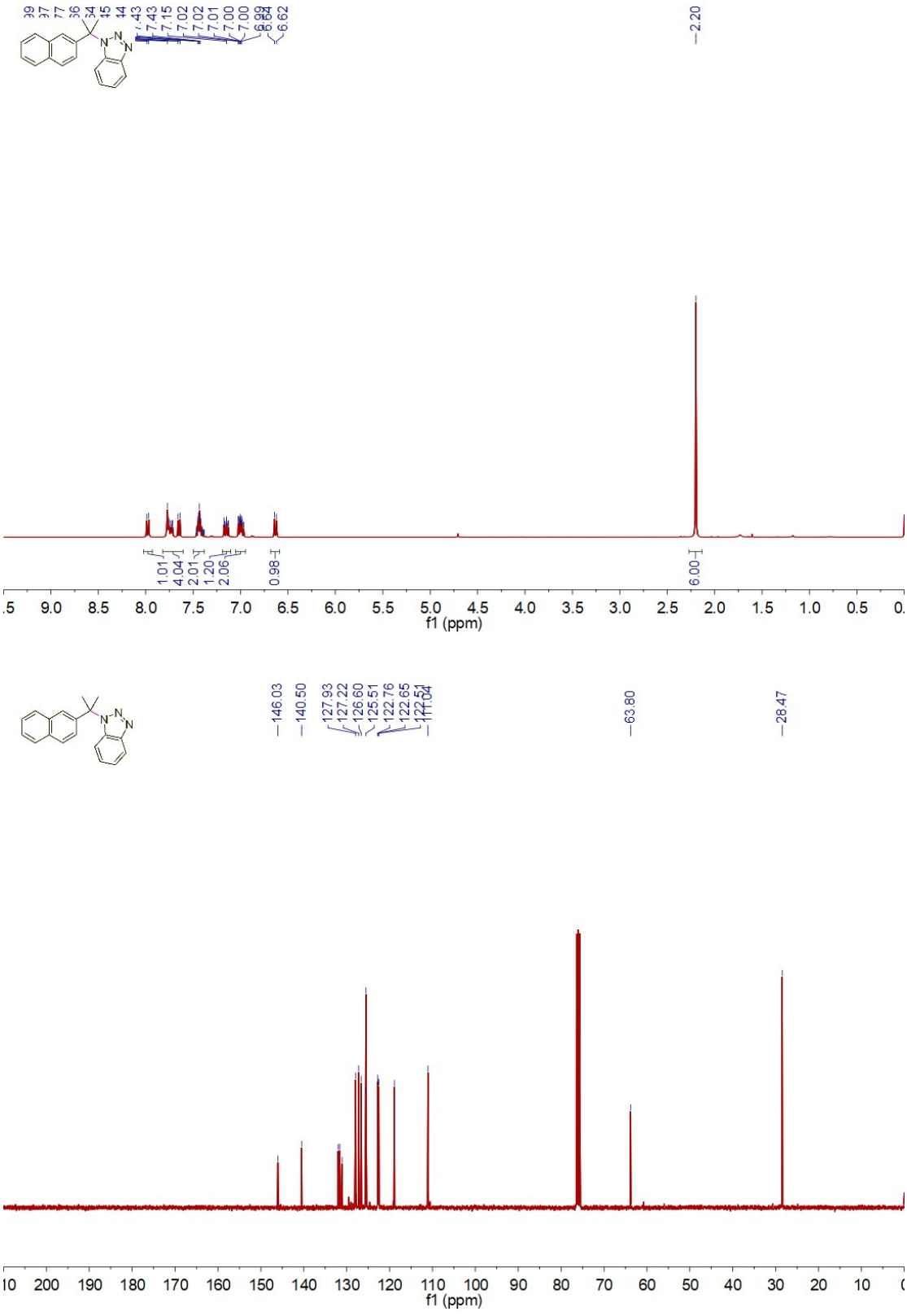


1-(2-(naphthalen-1-yl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (11)

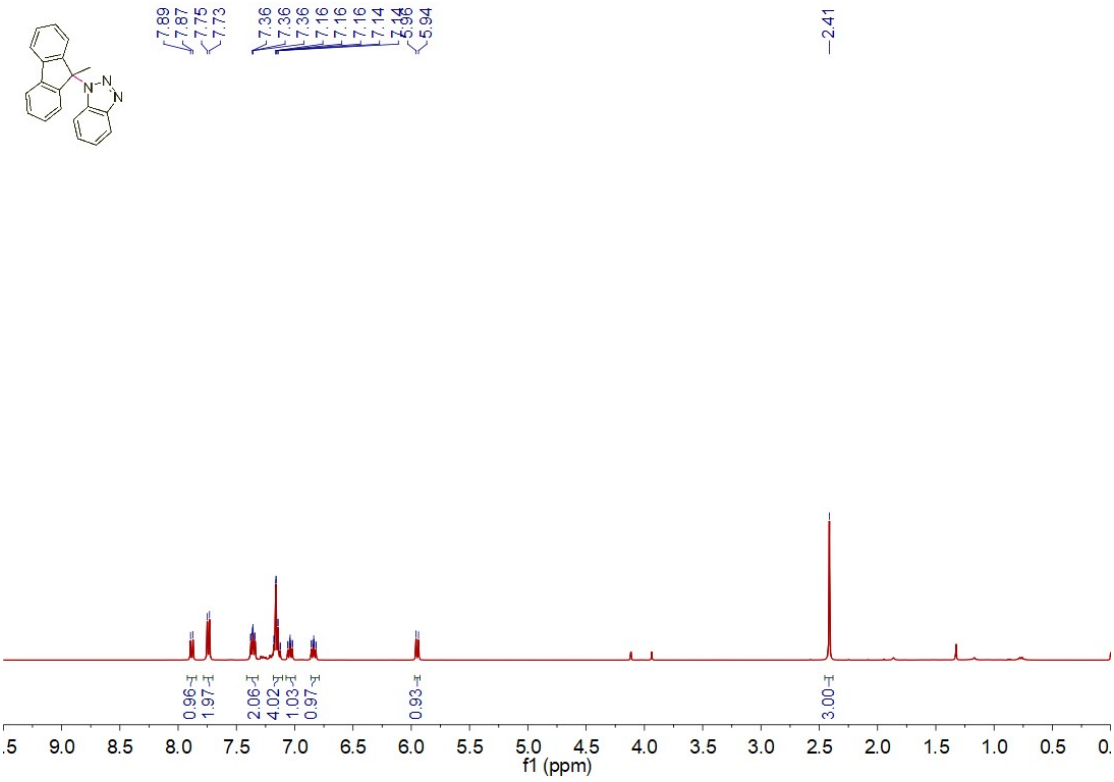


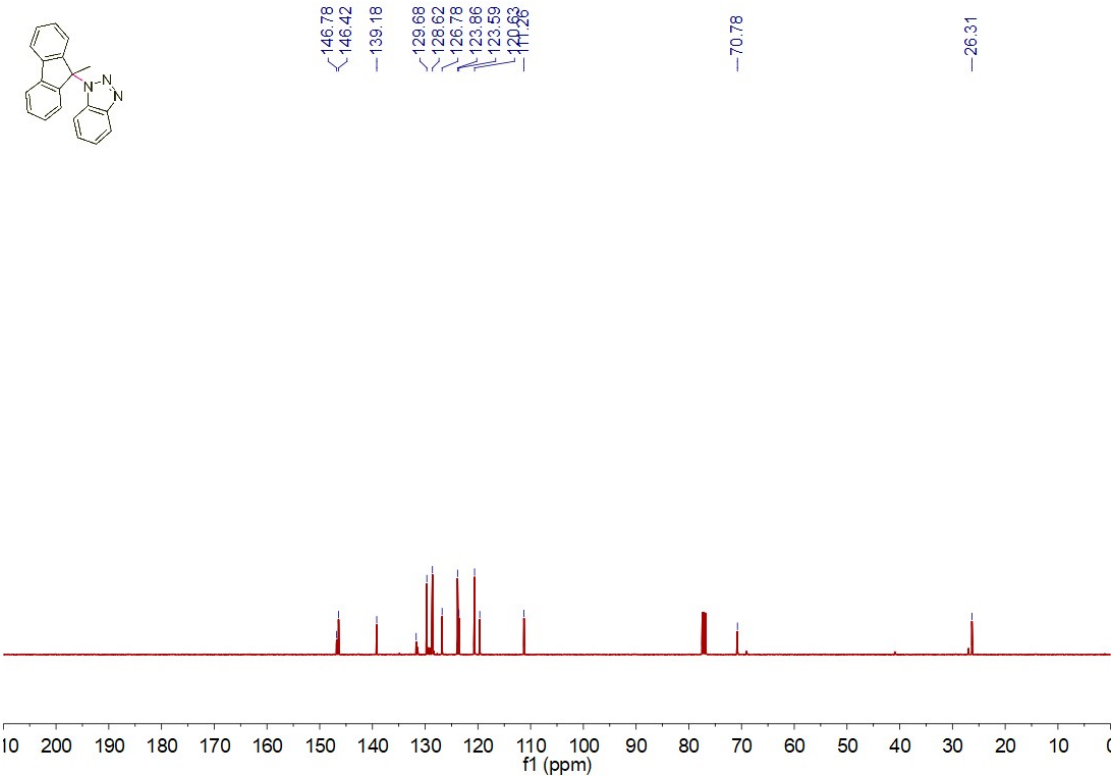


1-(2-(naphthalen-2-yl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (12)

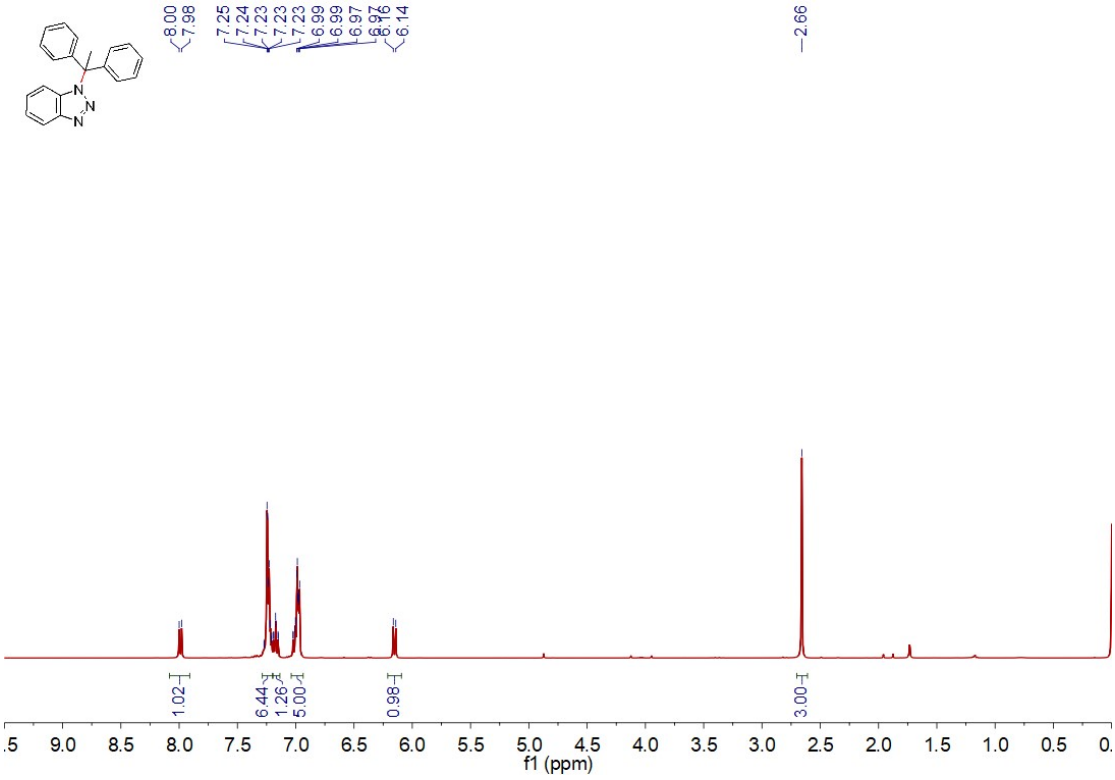


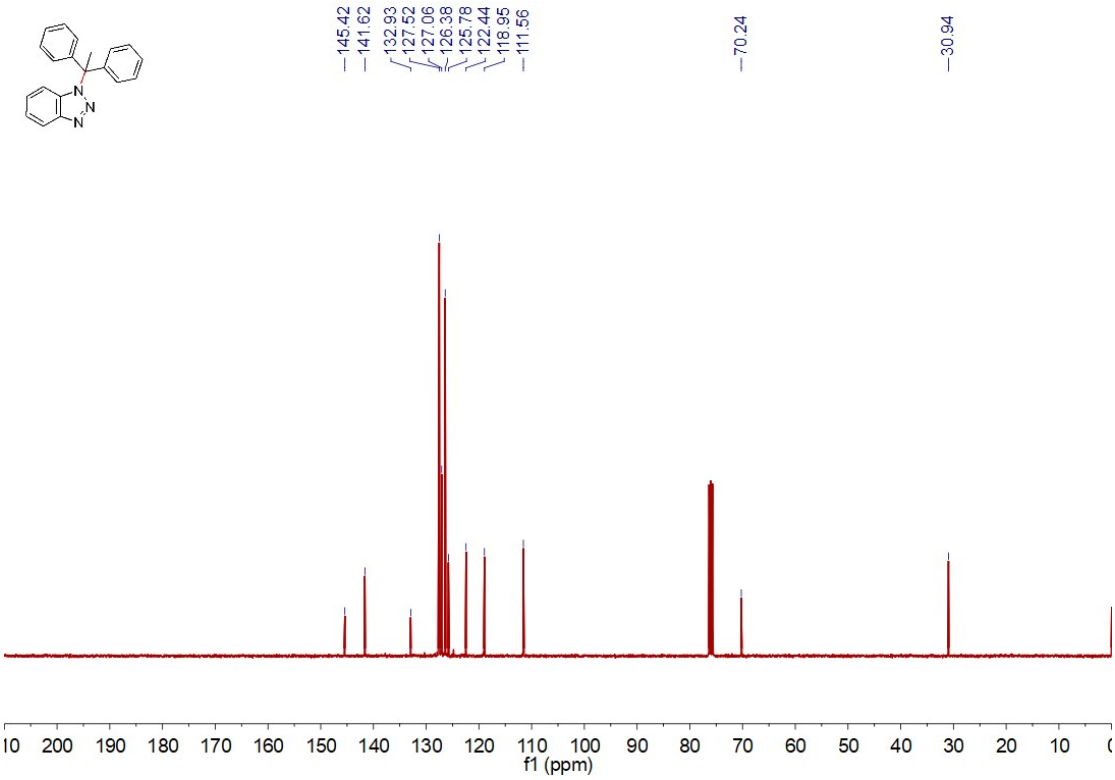
1-(9-methyl-9H-fluoren-9-yl)-1H-benzo[d][1,2,3]triazole (13)



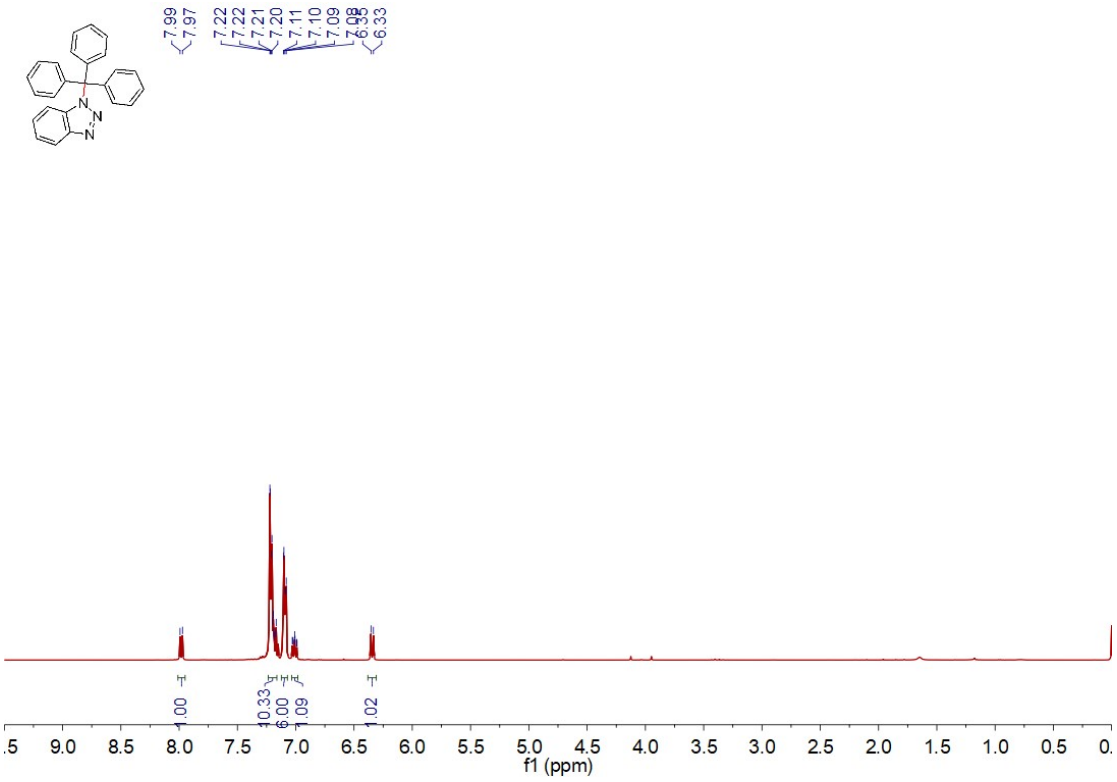


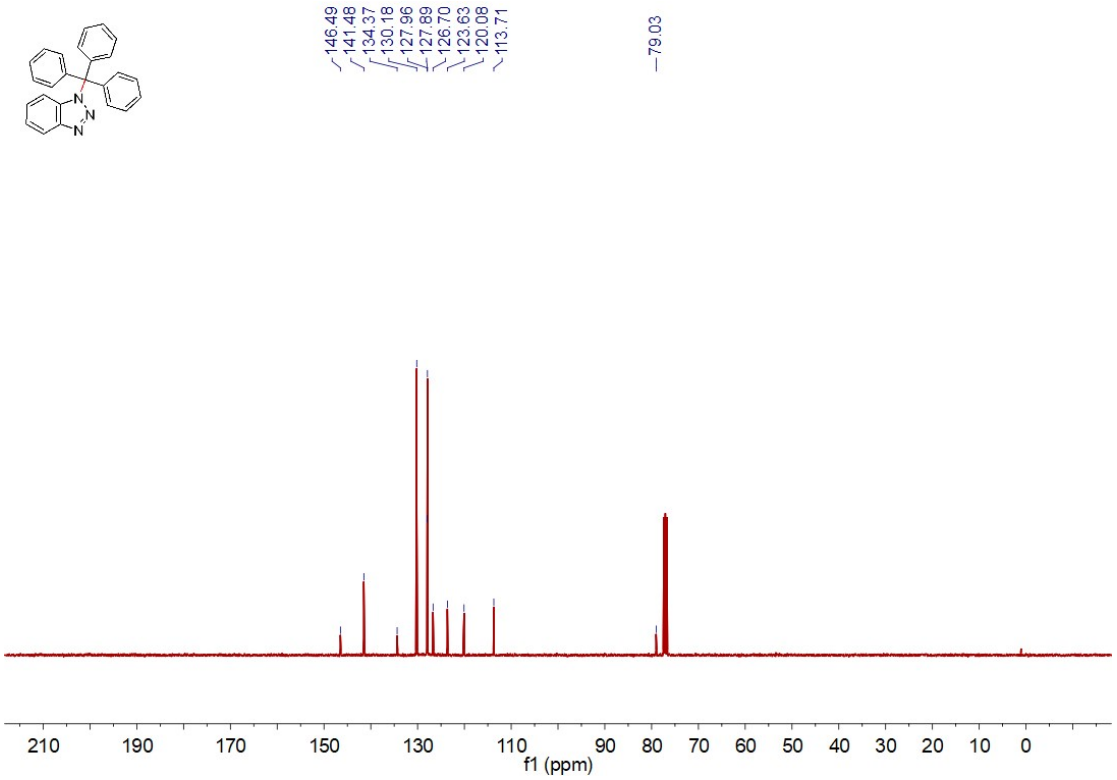
1-(1,1-diphenylethyl)-1H-benzo[d][1,2,3]triazole (14)



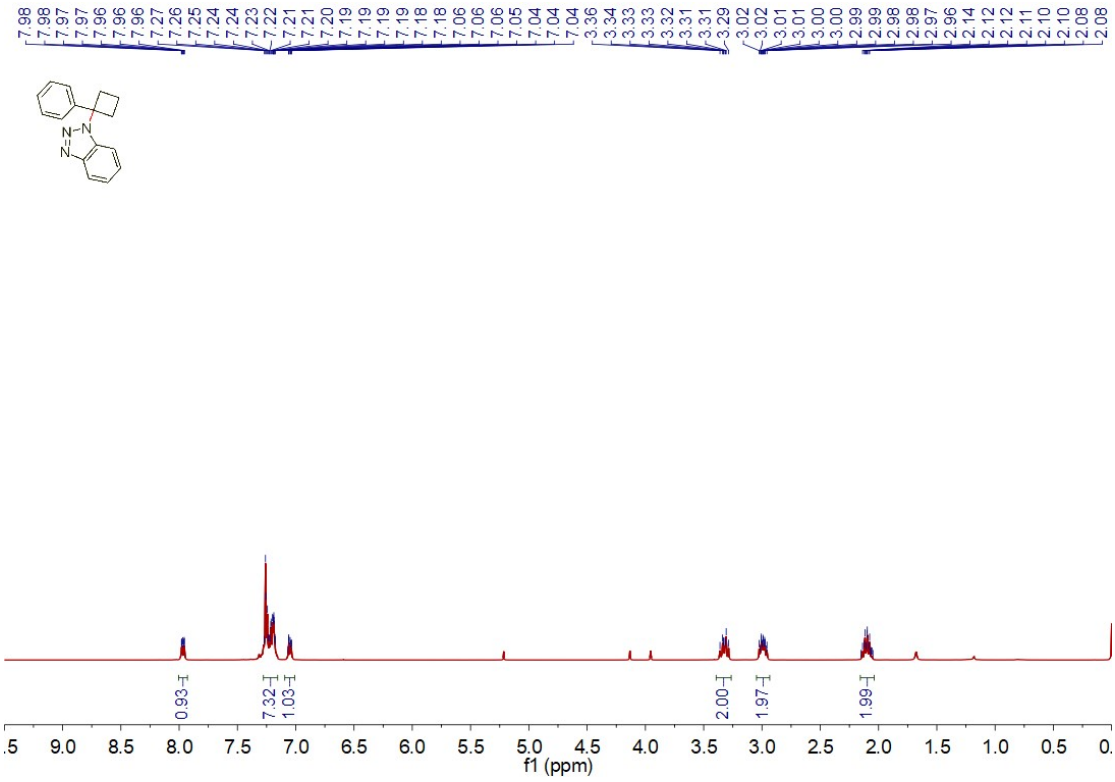


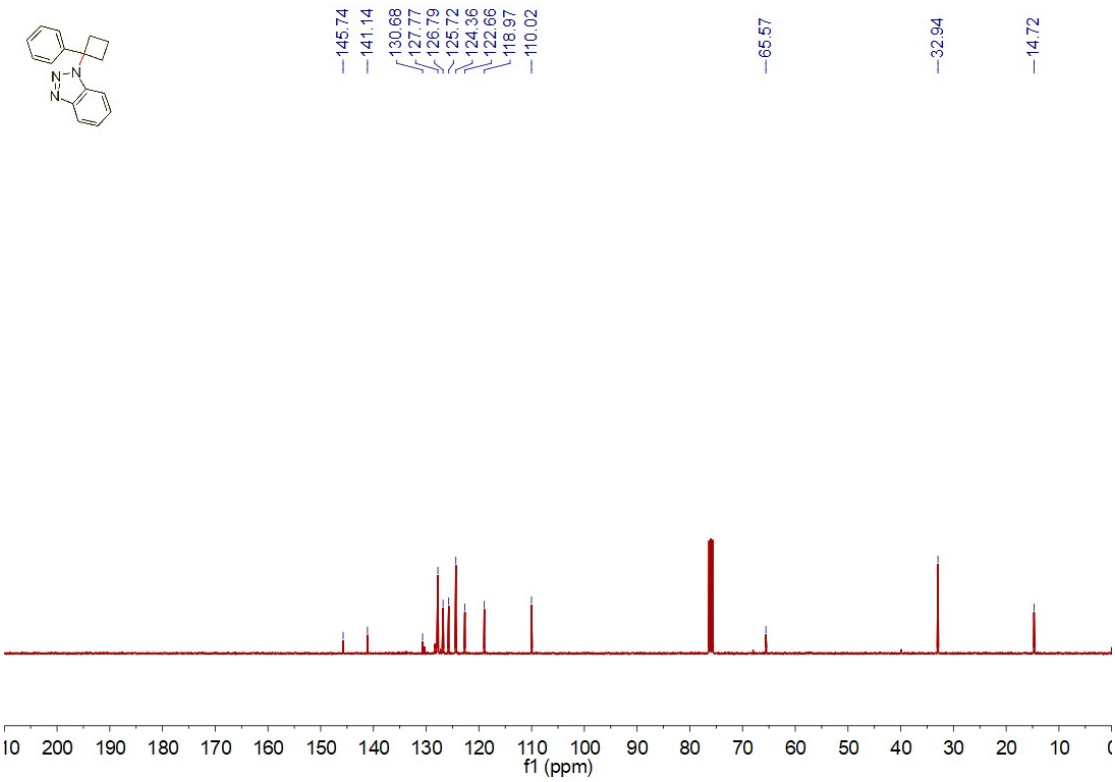
1-trityl-1H-benzo[d][1,2,3]triazole (15)



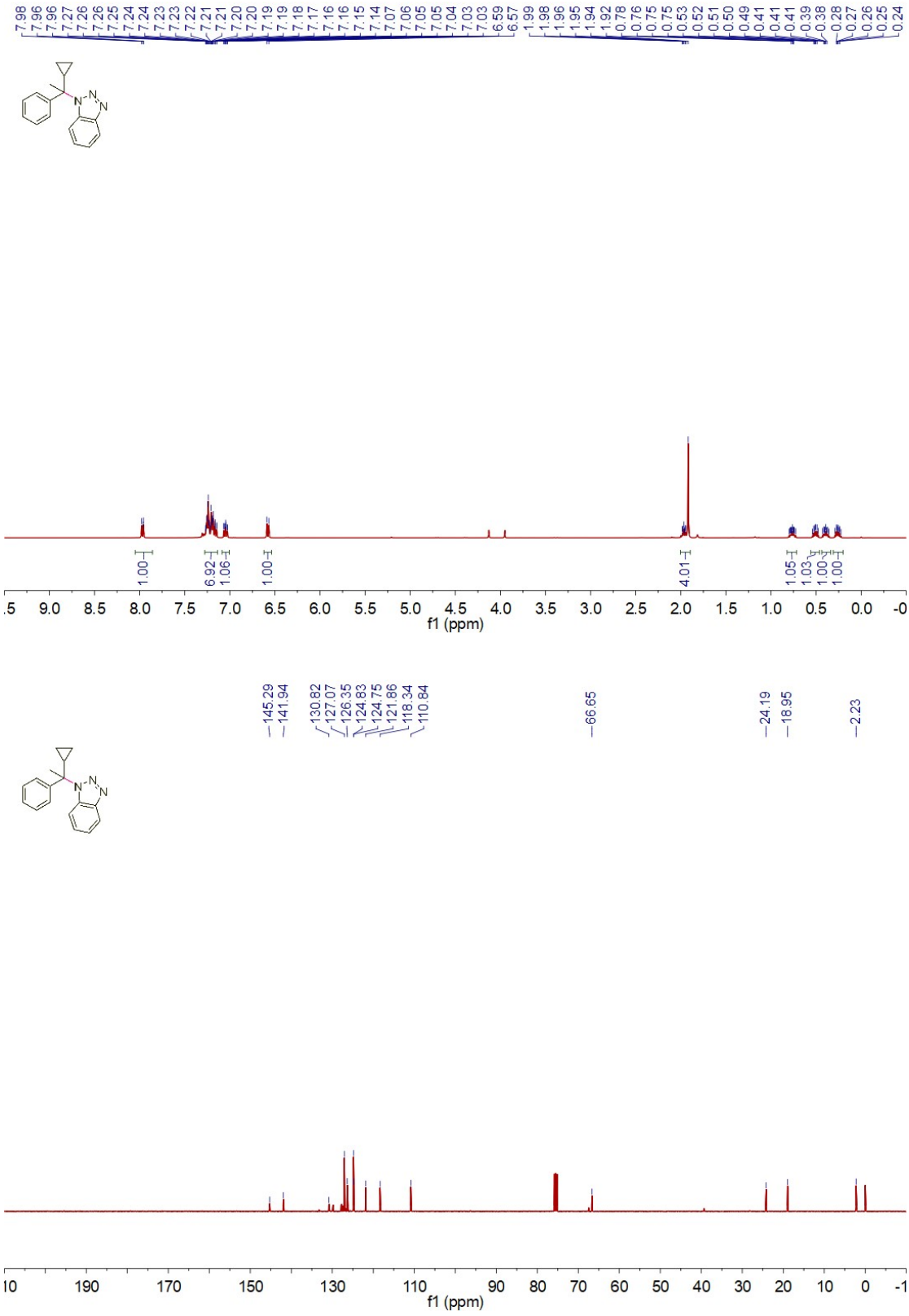


1-(1-phenylcyclobutyl)-1H-benzo[d][1,2,3]triazole (16)

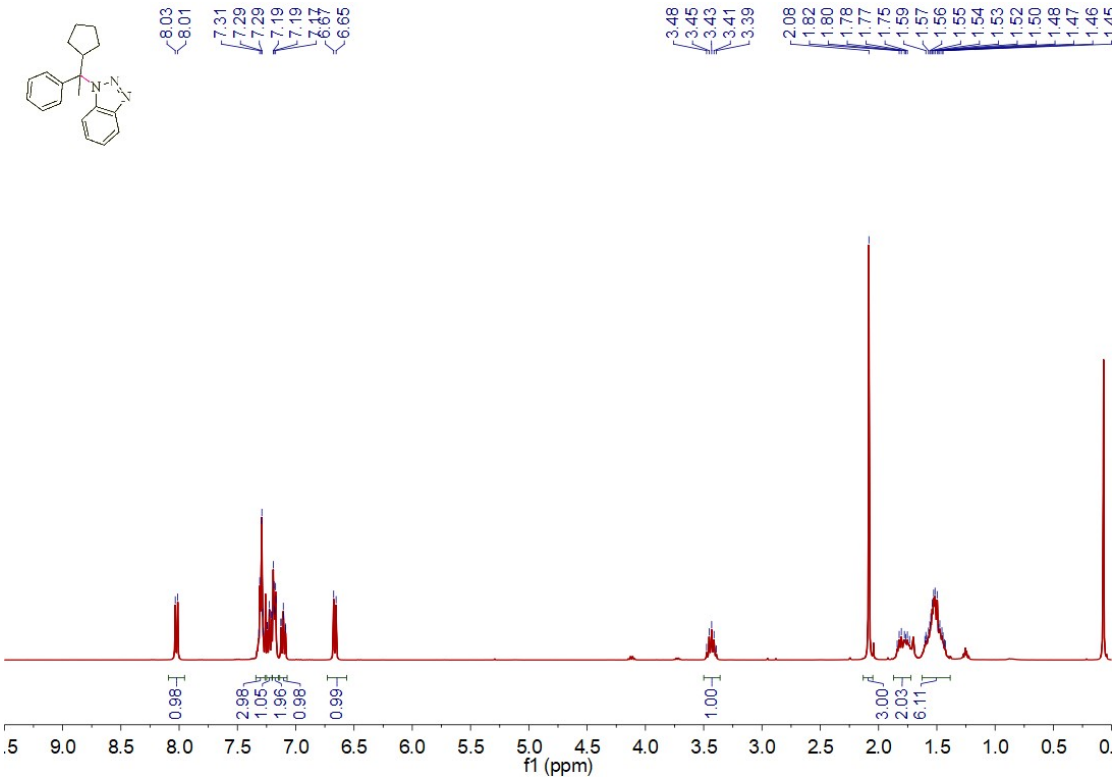


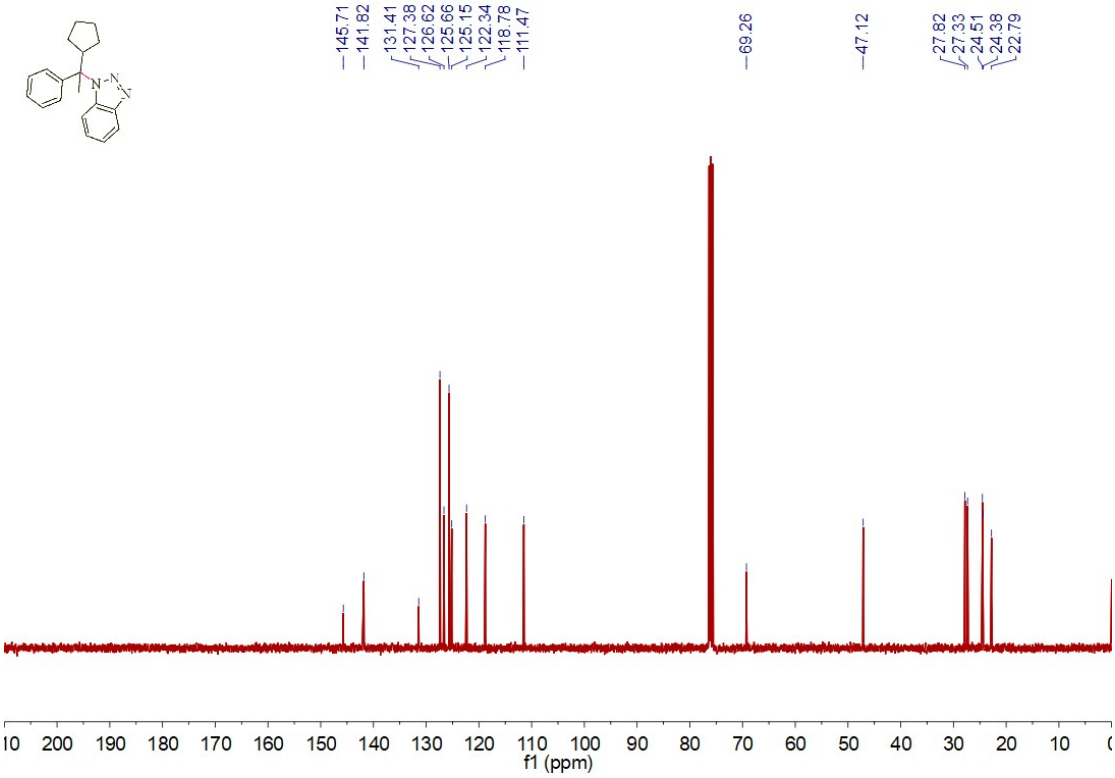


1-(1-cyclopropyl-1-phenylethyl)-1H-benzo[d][1,2,3]triazole (17)

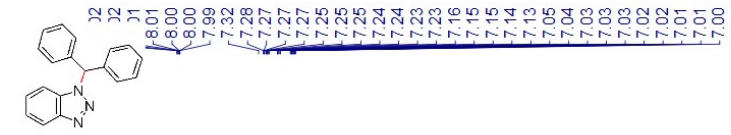


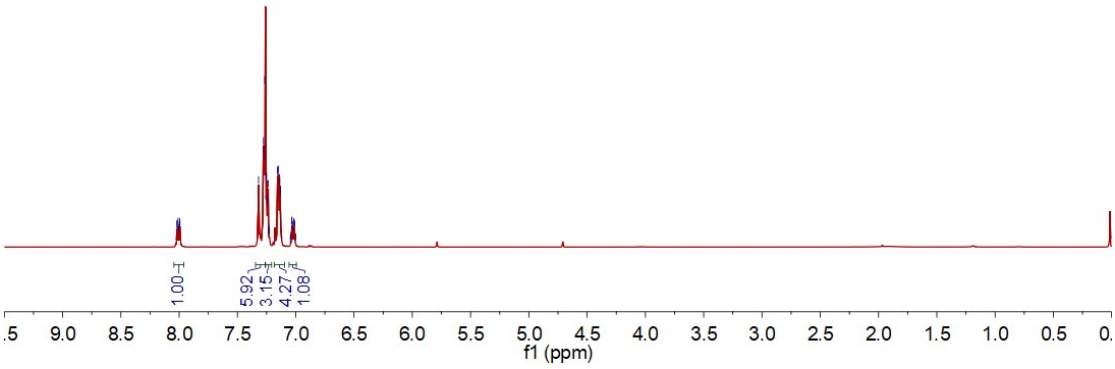
1-(1-cyclopentyl-1-phenylethyl)-1H-benzo[d][1,2,3]triazole (18)

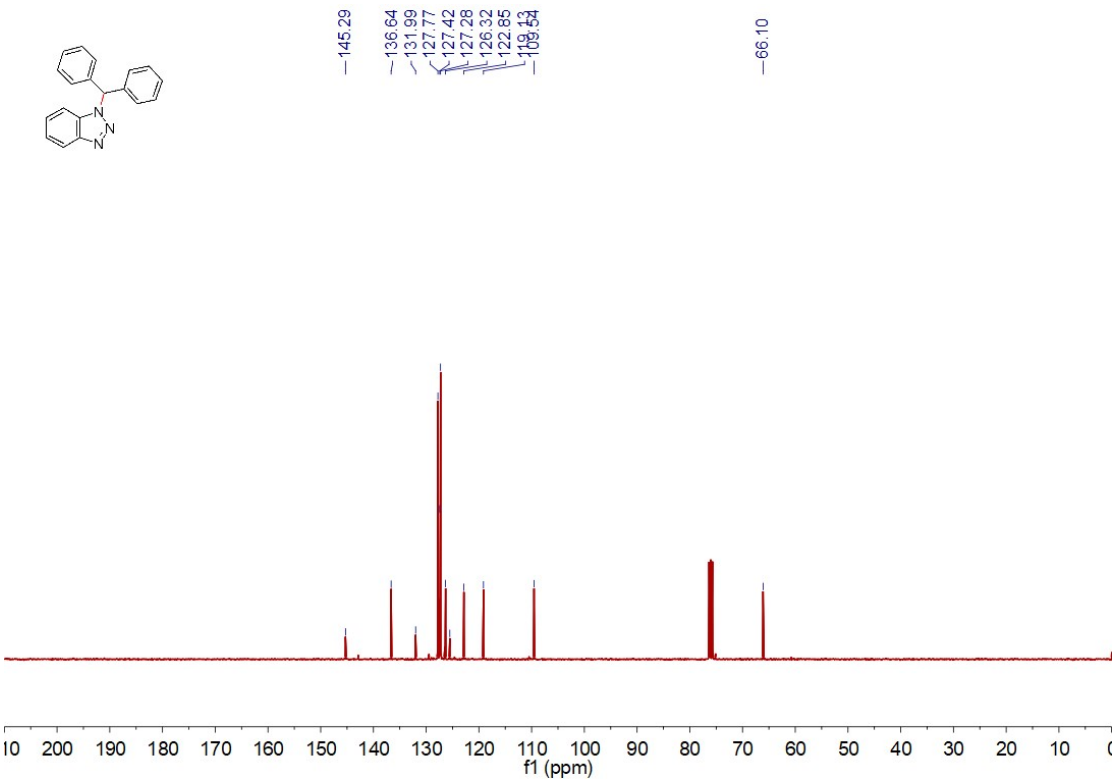




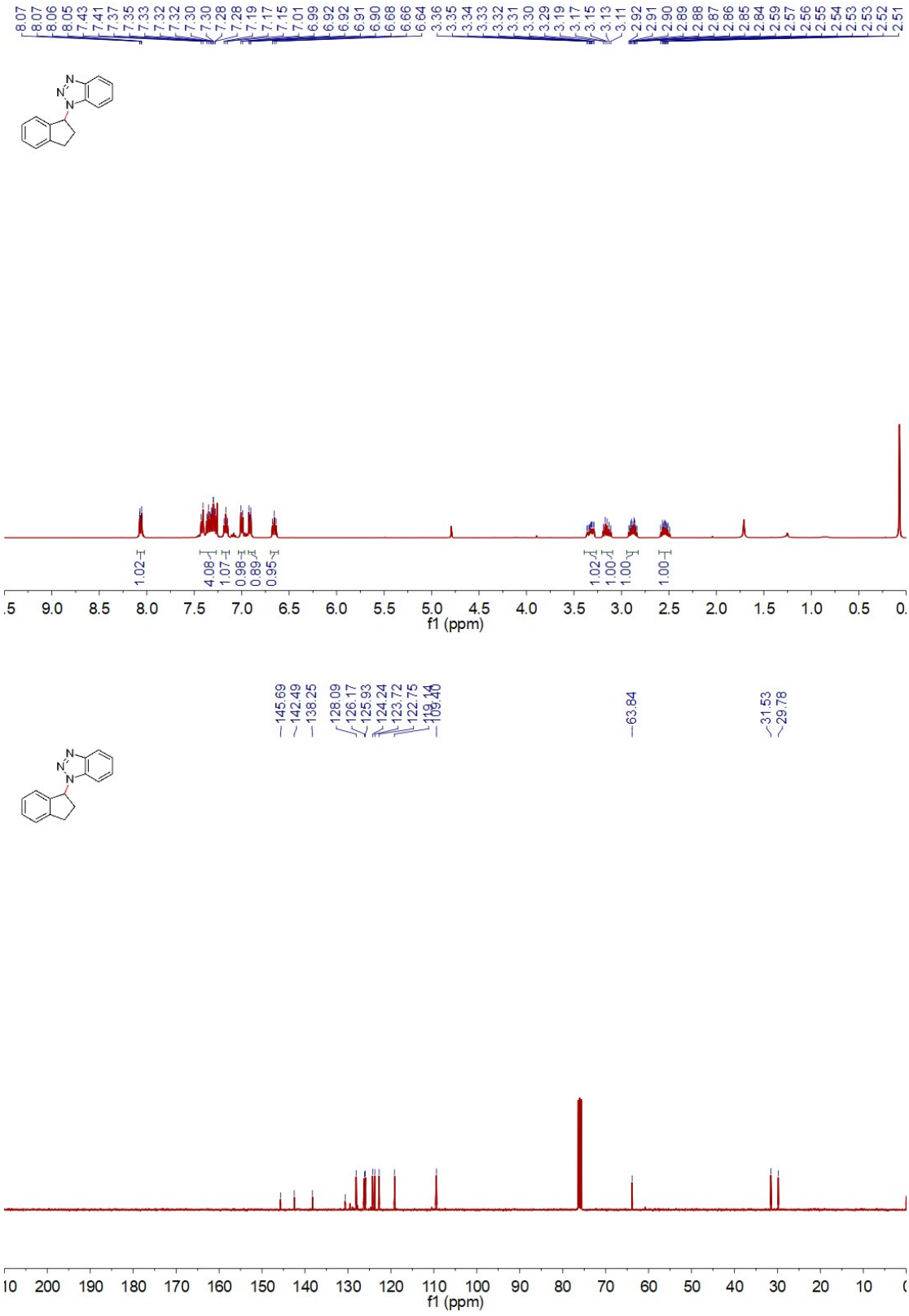
1-benzhydryl-1H-benzo[d][1,2,3]triazole (19)



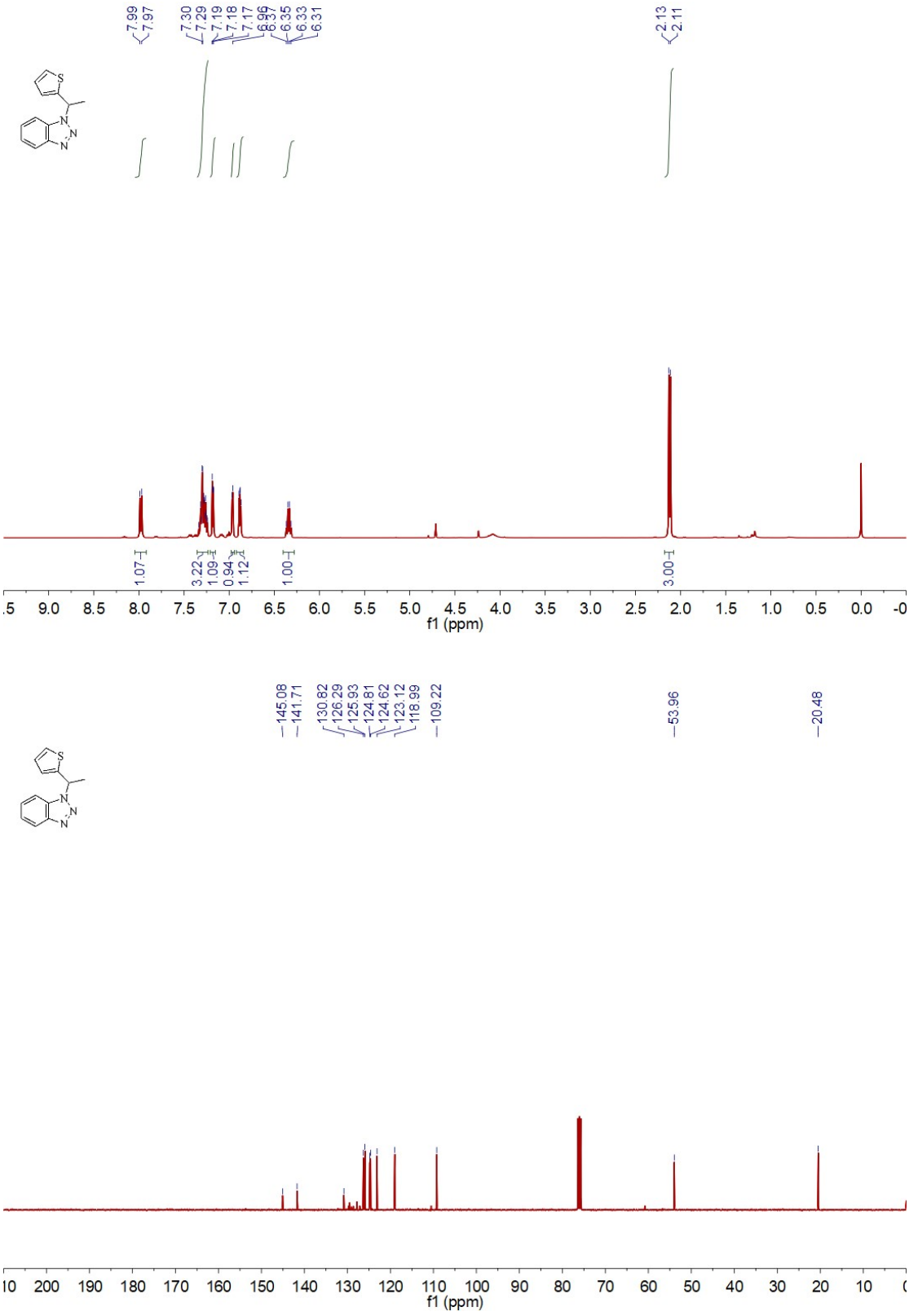




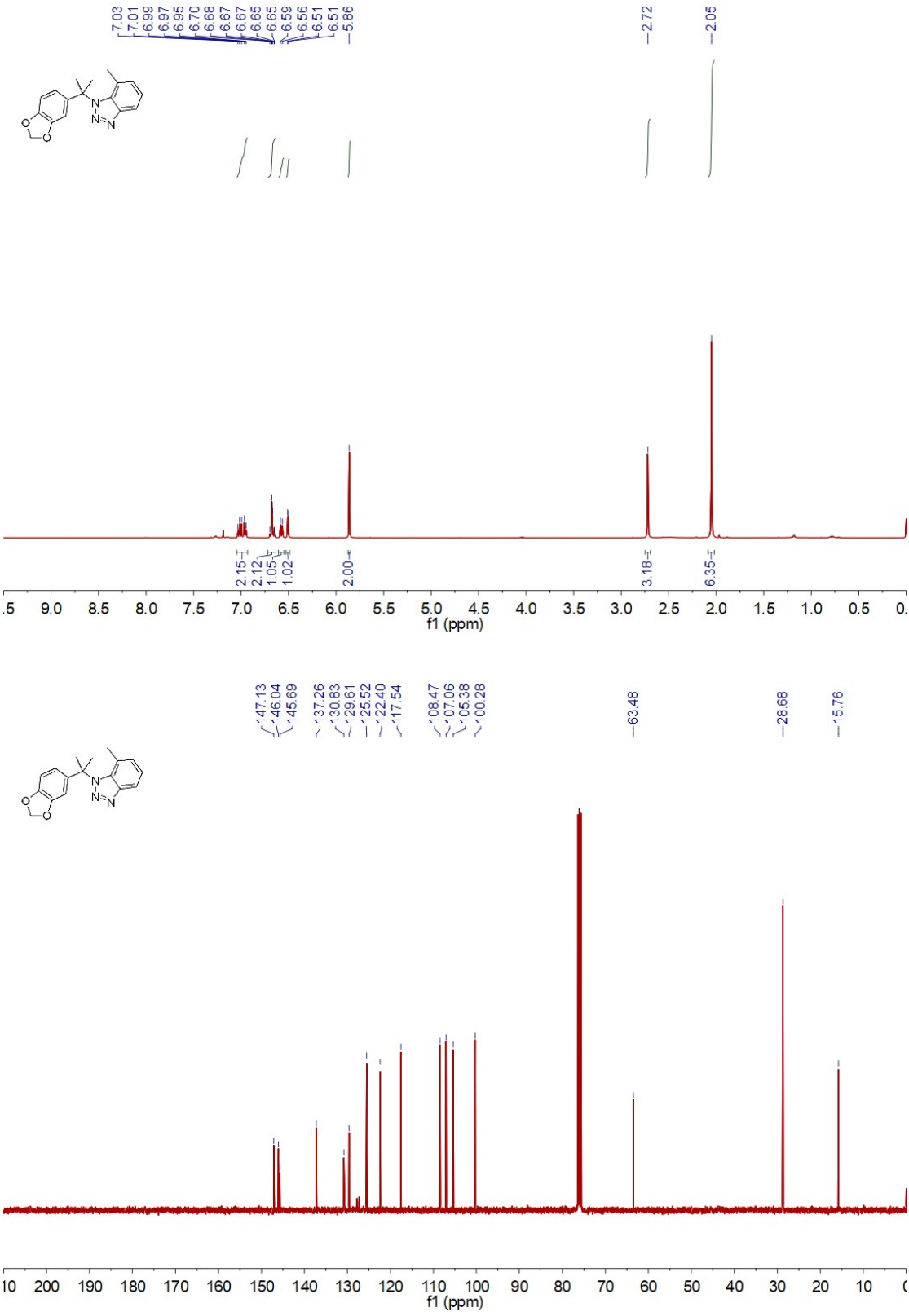
1-(2,3-dihydro-1H-inden-1-yl)-1H-benzo[d][1,2,3]triazole (20)



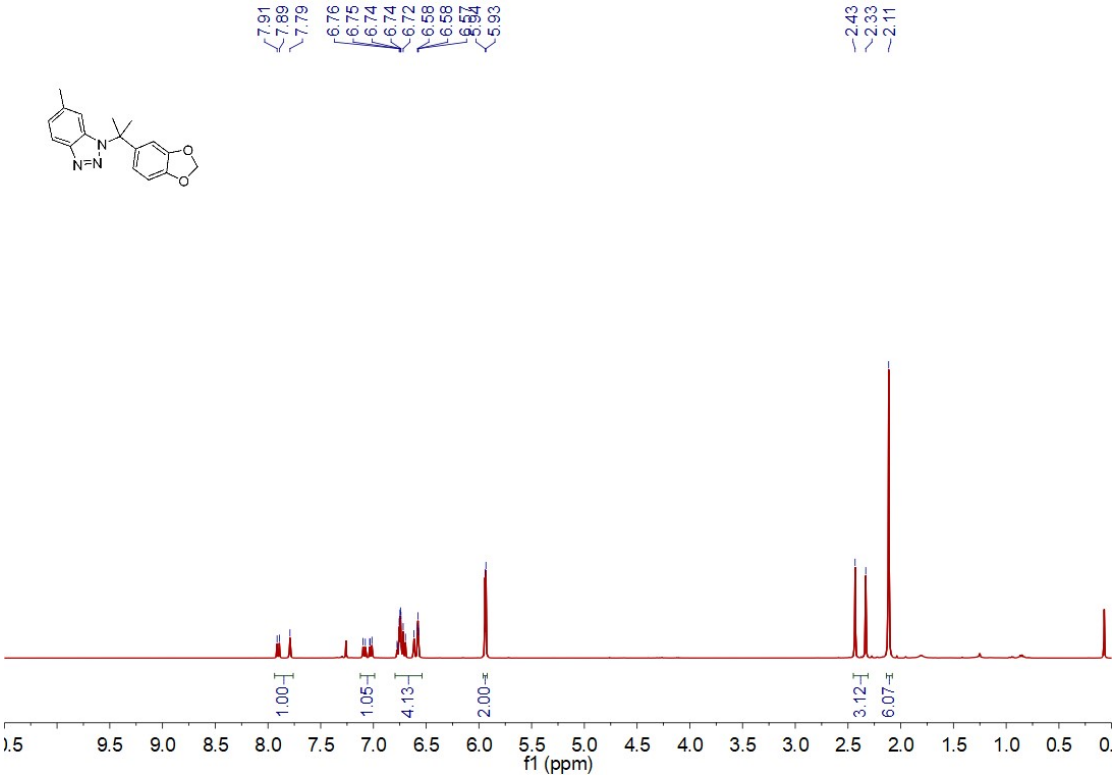
1-(1-(thiophen-2-yl)ethyl)-3a,7a-dihydro-1H-benzo[d][1,2,3]triazole (21)

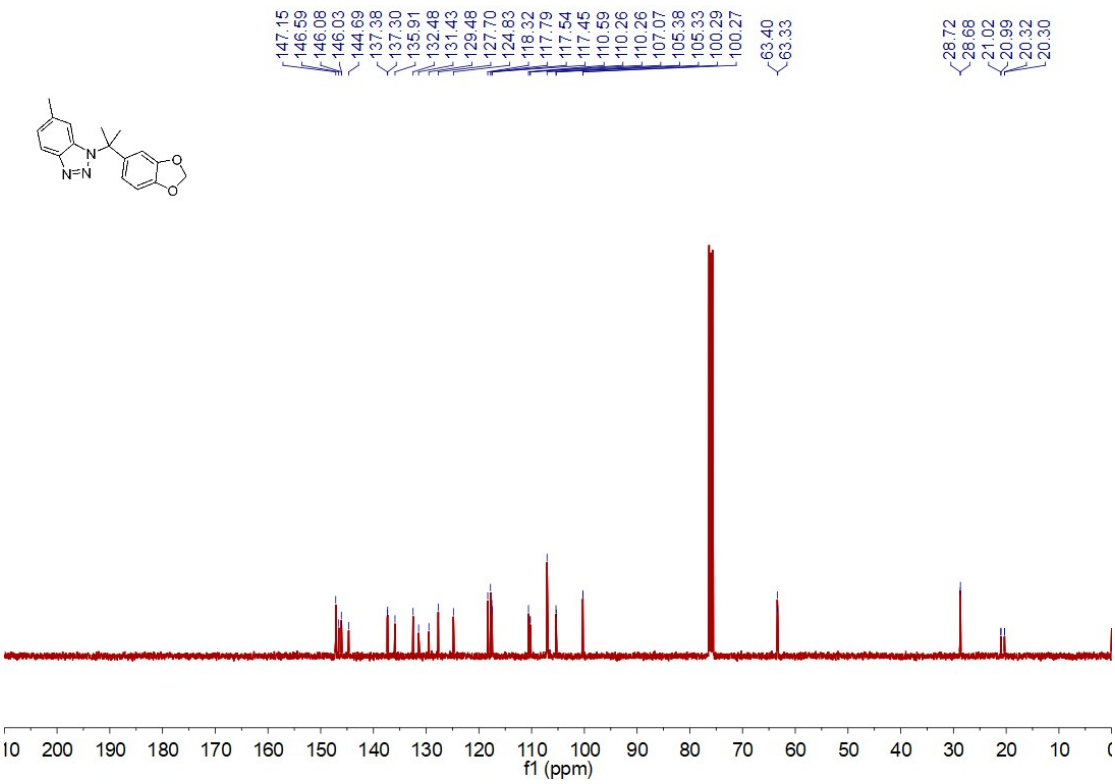


1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-4-methyl-1H-benzo[d][1,2,3]triazole(22)

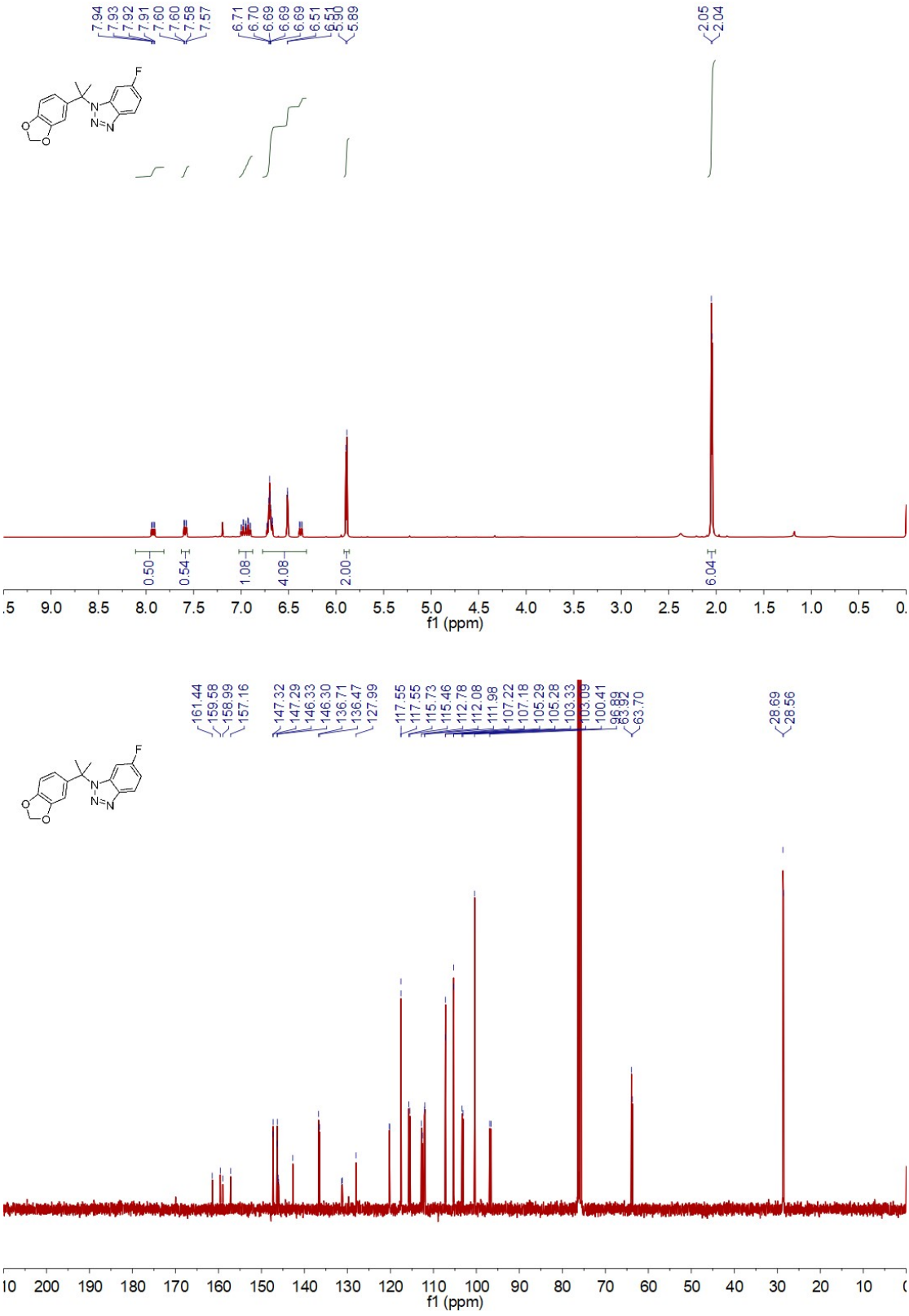


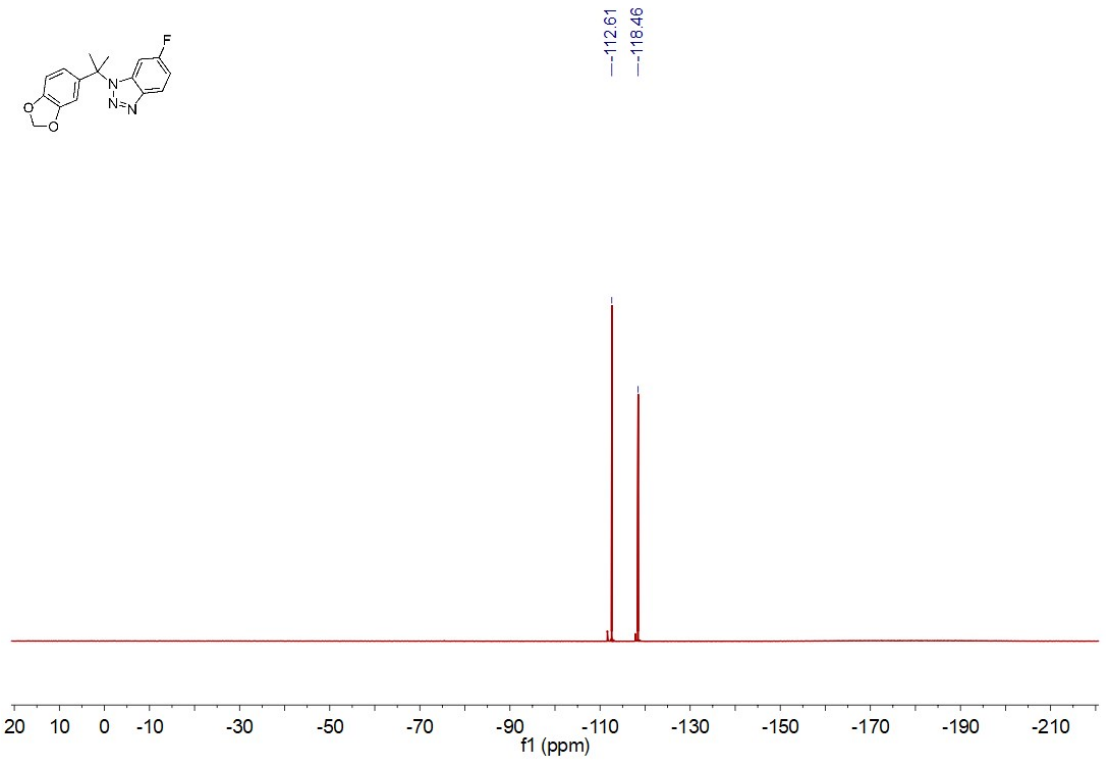
1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-5-methyl-1H-benzo[d][1,2,3]triazole (23)



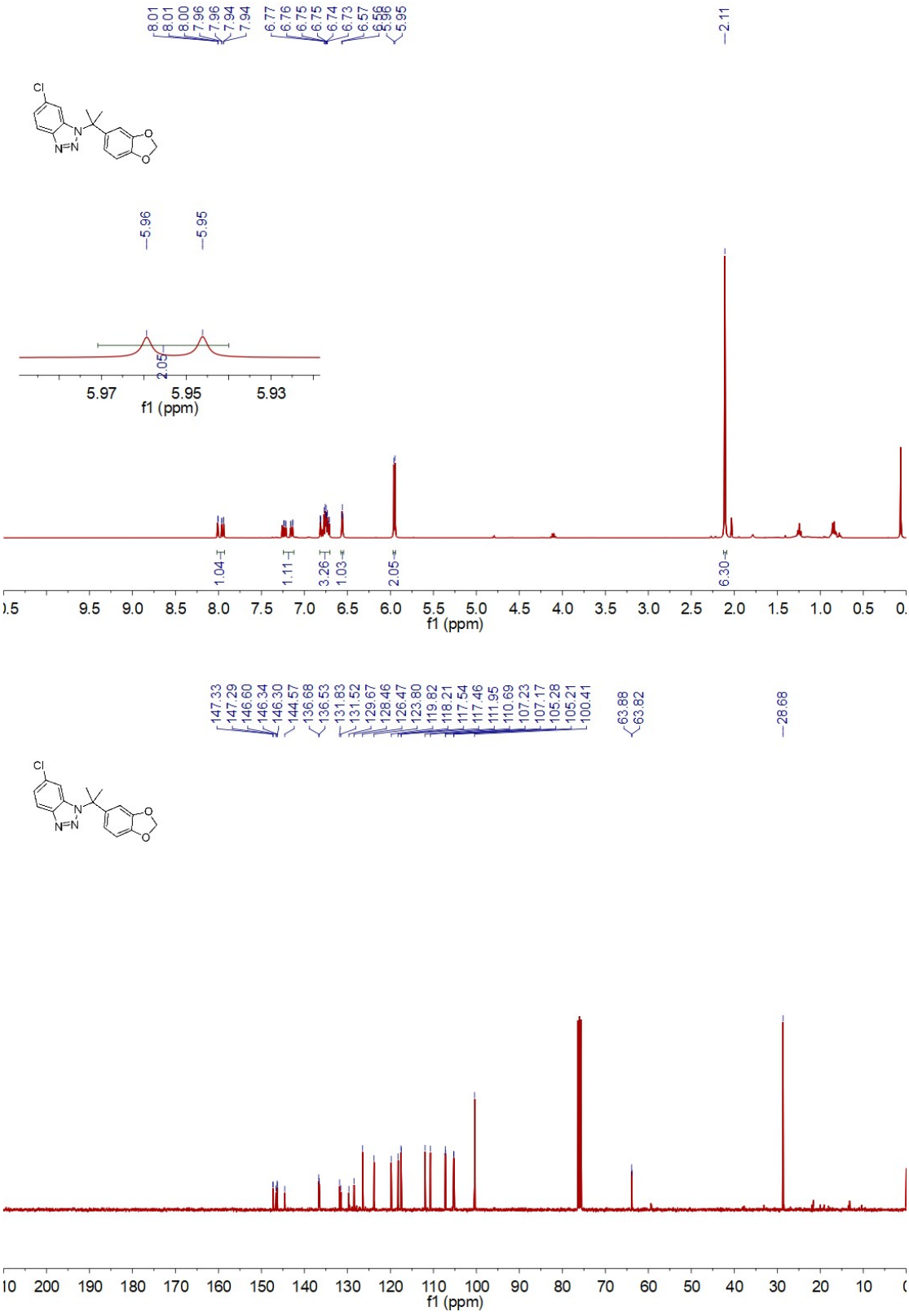


1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-5-fluoro-1H-benzo[d][1,2,3]triazole(24)

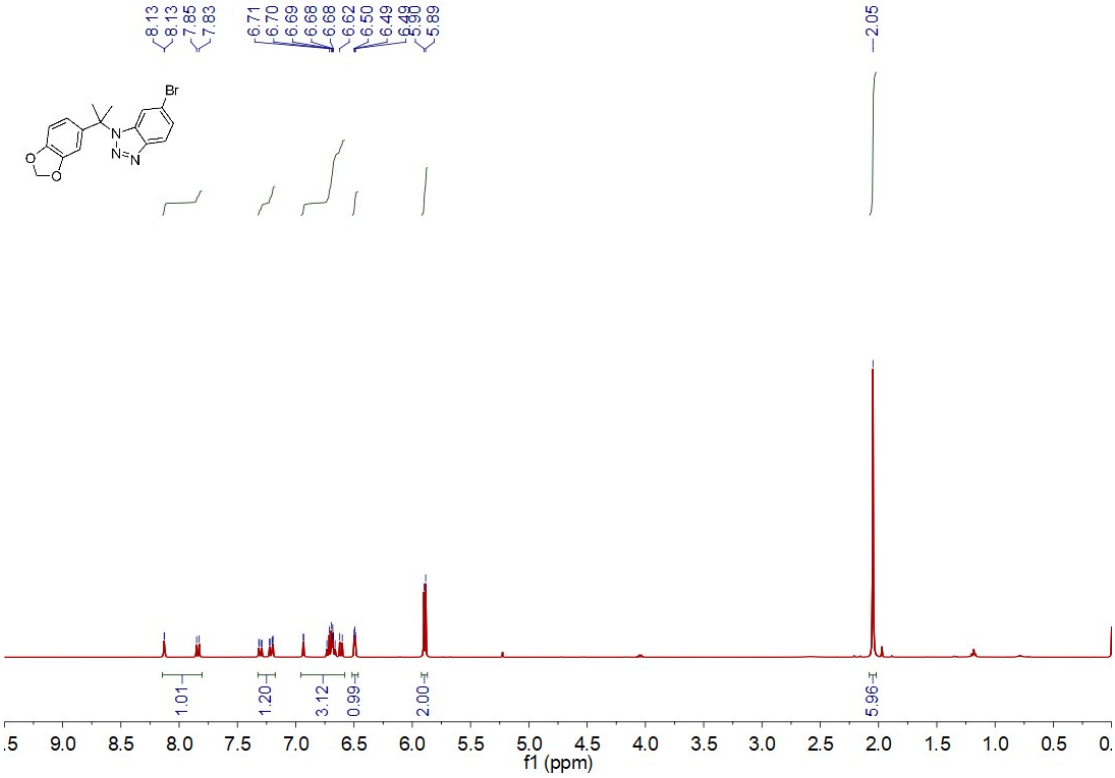


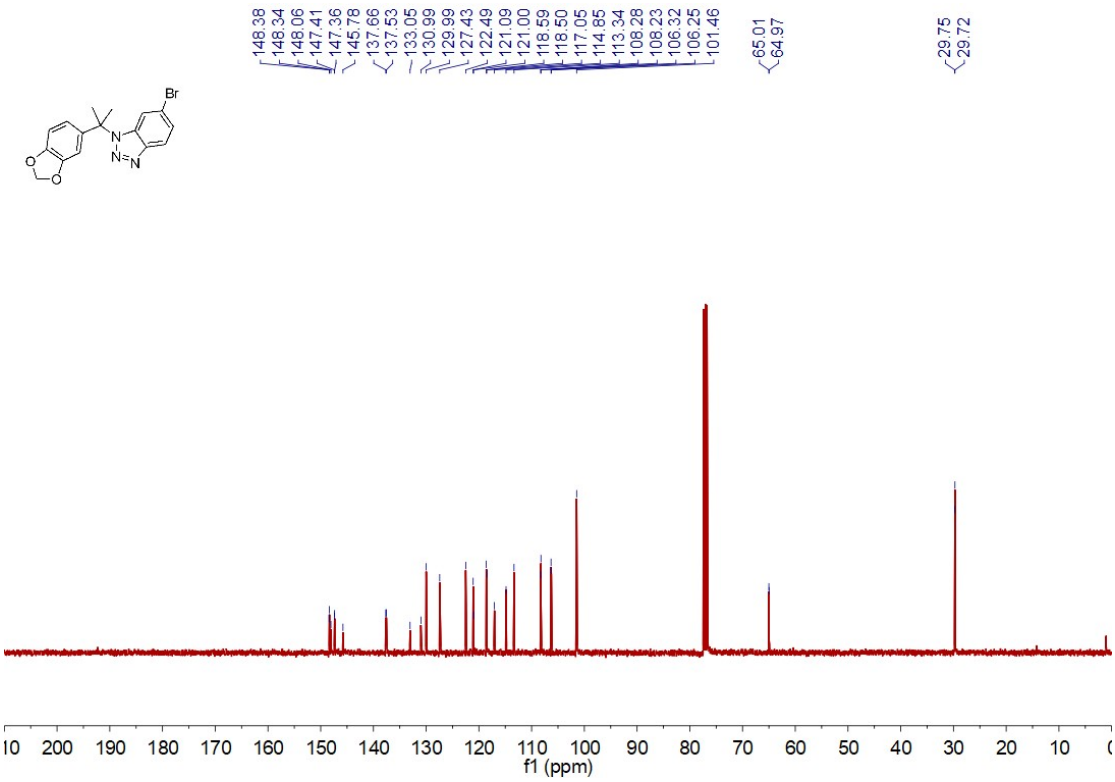

F
O
O
N
N
N
-112.61
-118.46
20
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)

1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-5-chloro-1H-benzo[d][1,2,3]triazole(25)

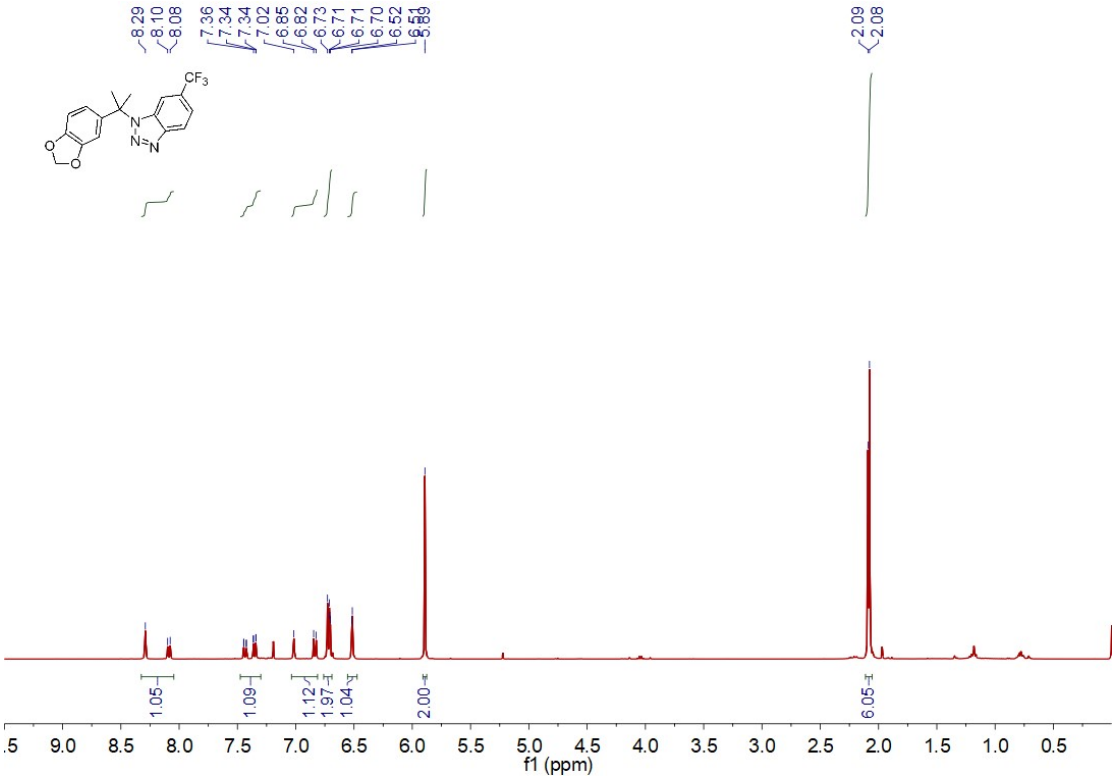


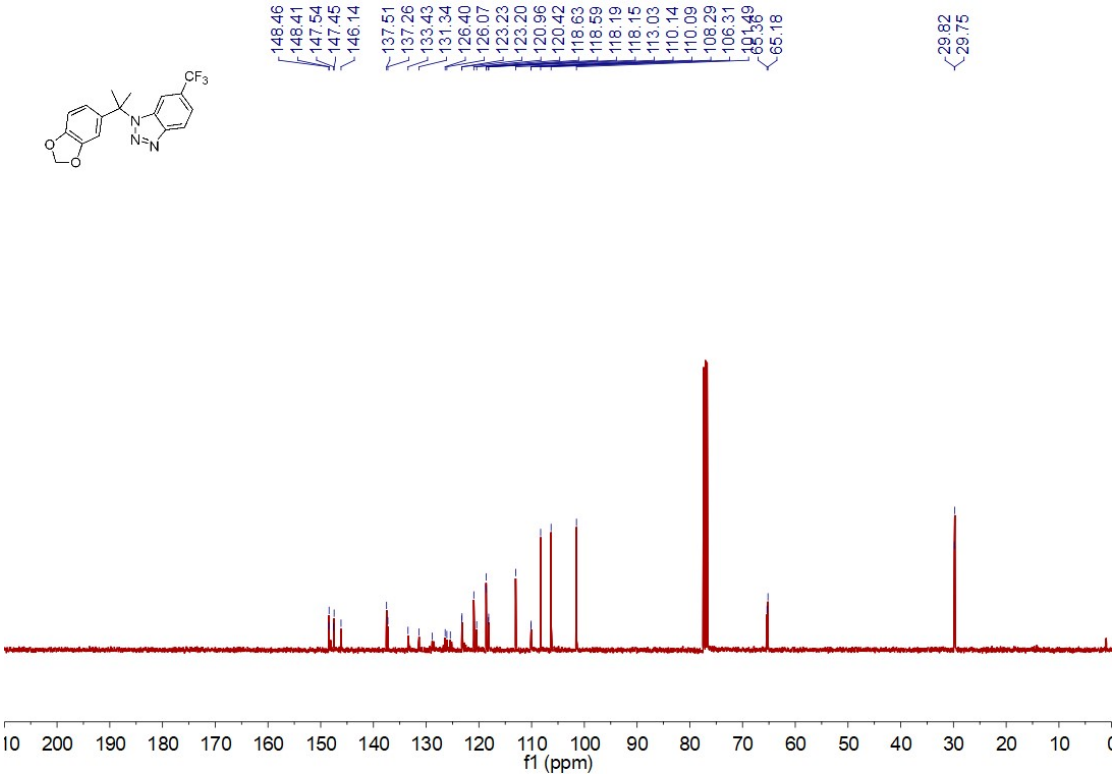
1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-5-bromo-1H-benzo[d][1,2,3]triazole(26)

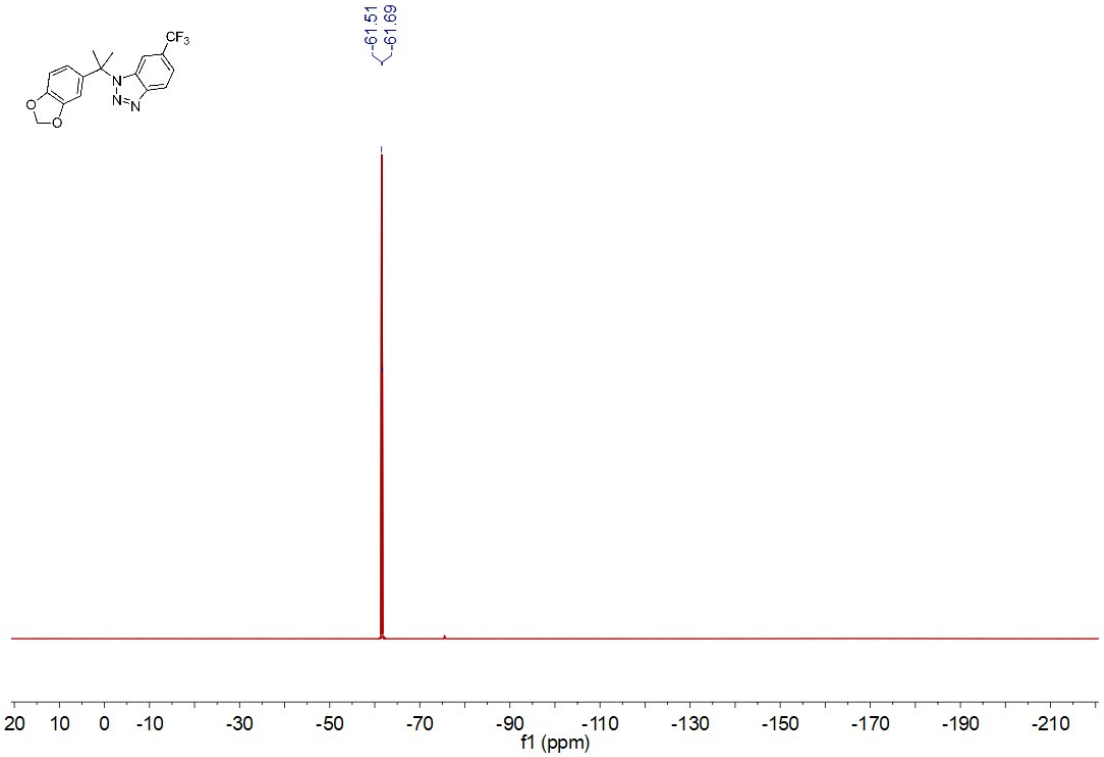




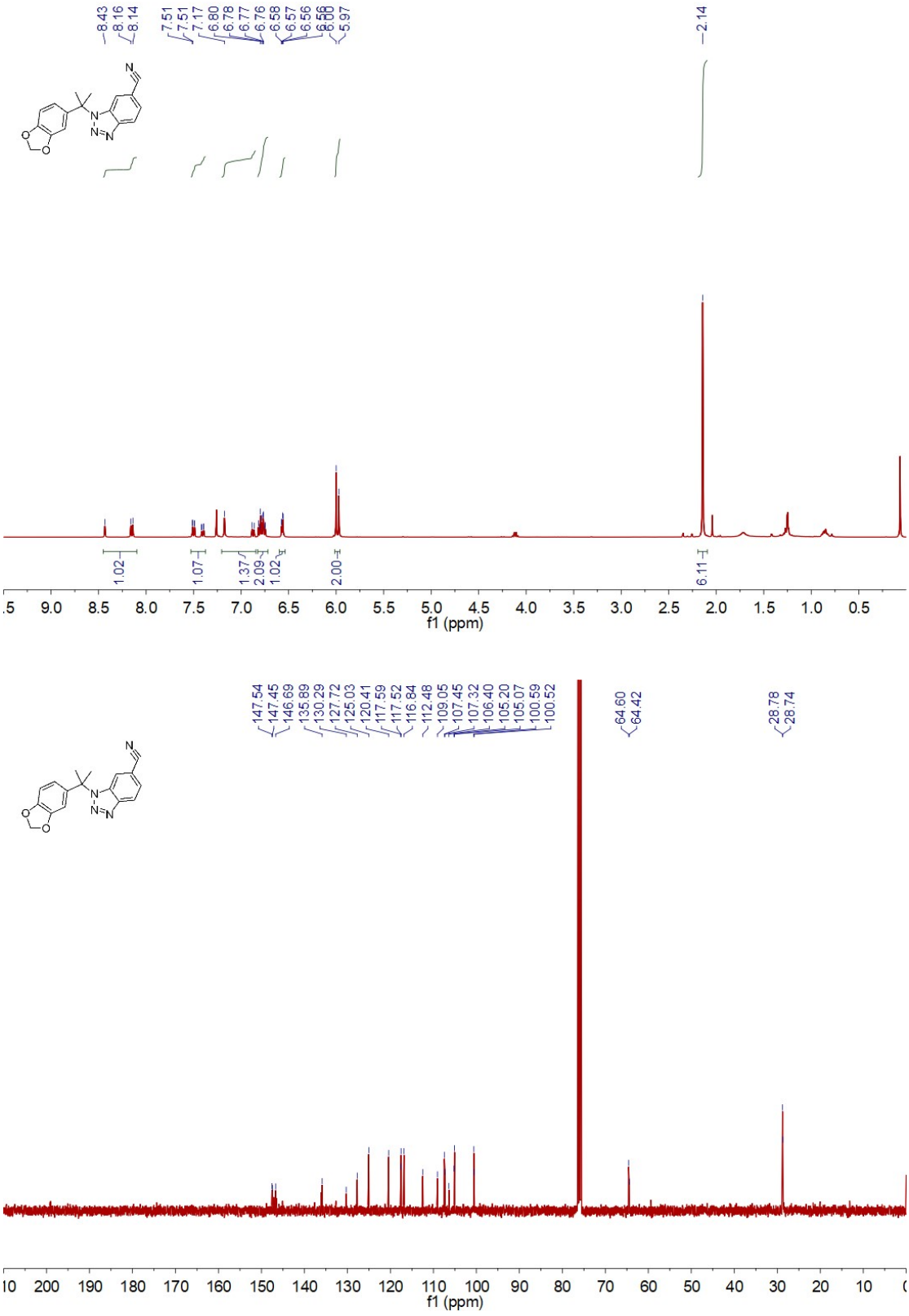
1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-5-(trifluoromethyl)-1H-benzo[d][1,2,3]triazole(27)



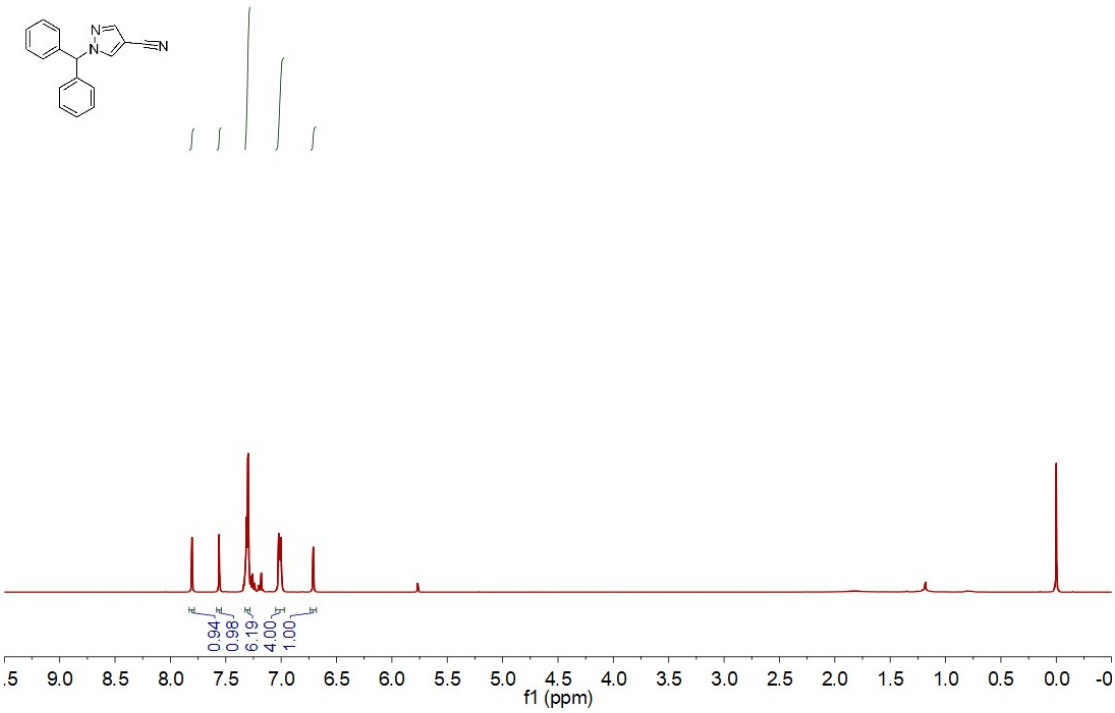


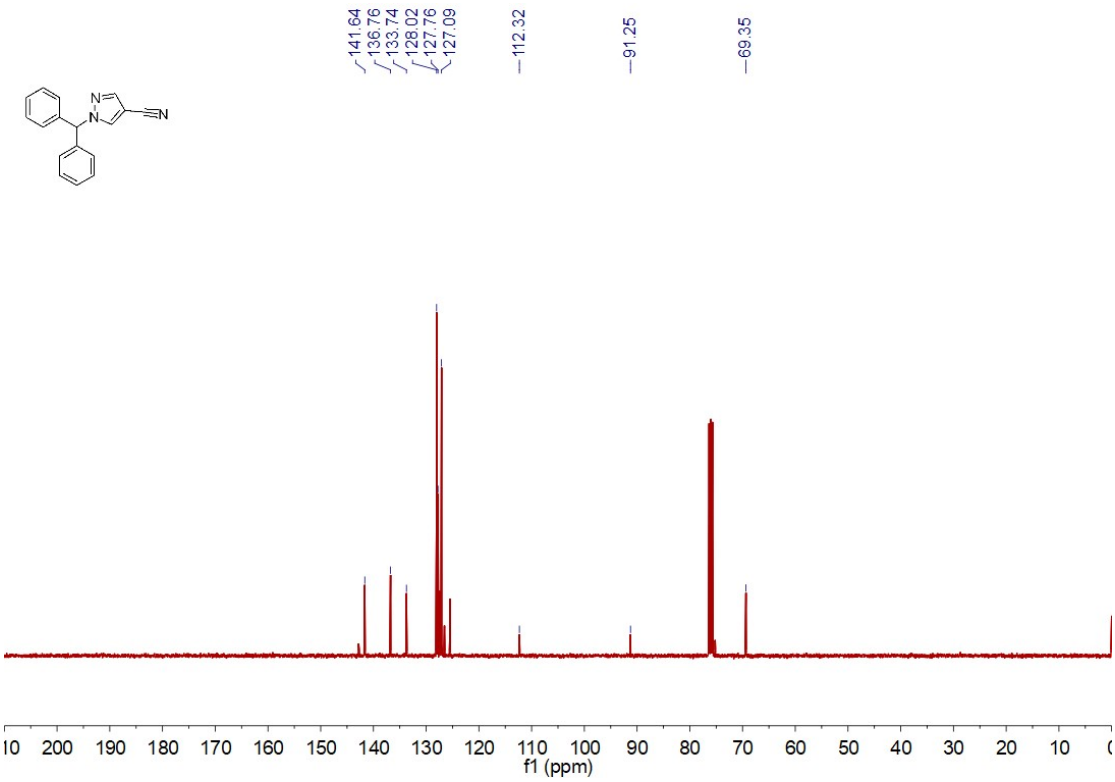

CF3
N
N
N
O
O
-61.51
-61.69
20
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)

1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-1H-benzo[d][1,2,3]triazole-5-carbonitrile(28)

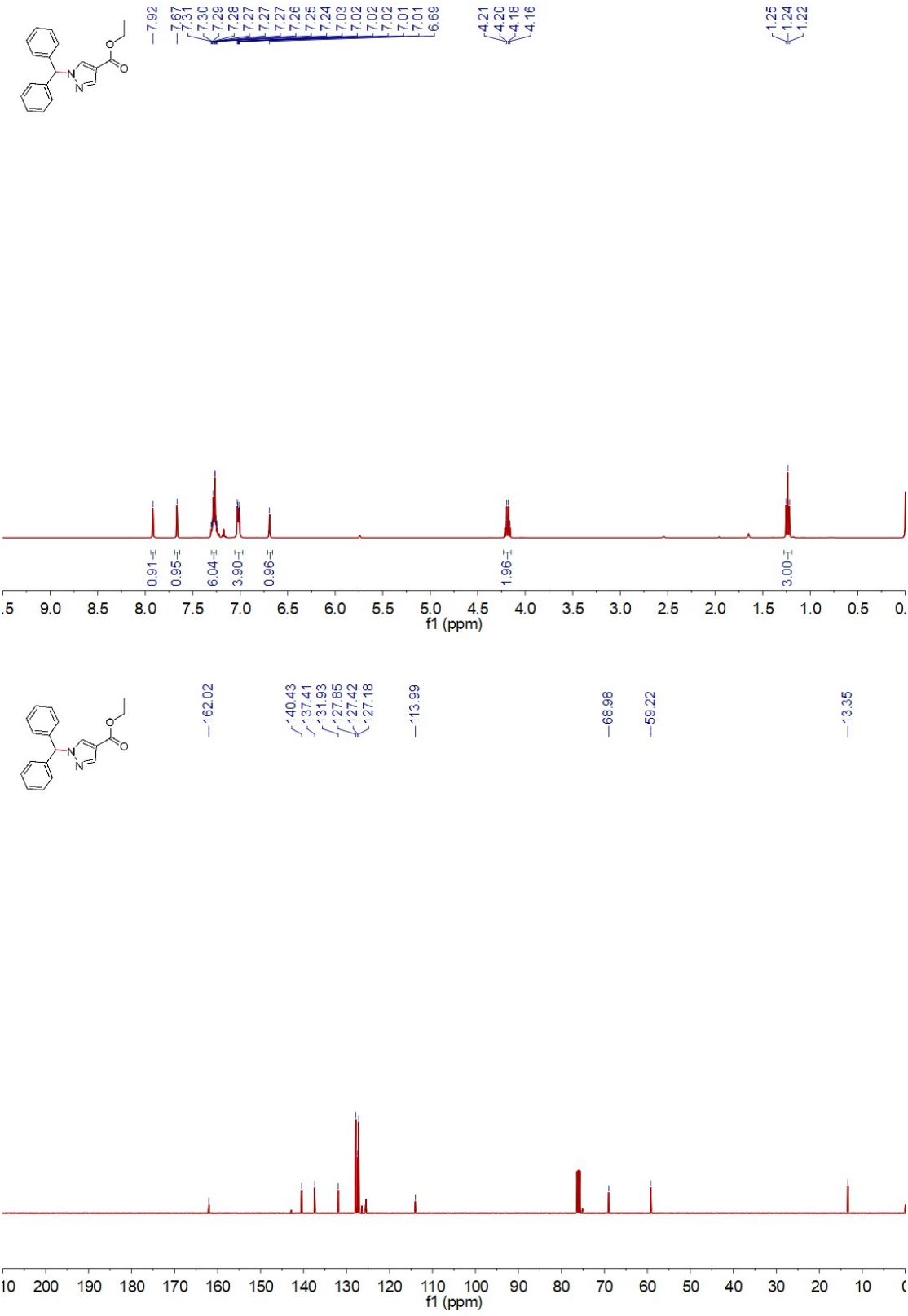


1-benzhydryl-1H-pyrrole-3-carbonitrile(29)

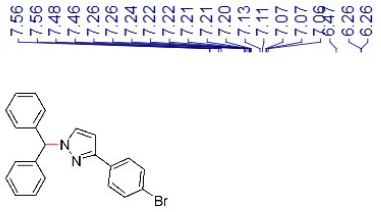


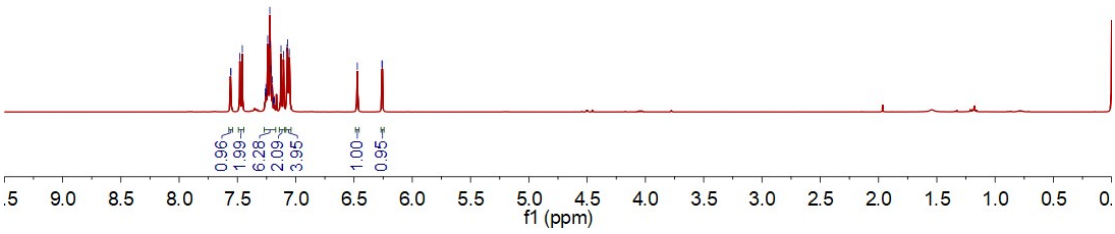


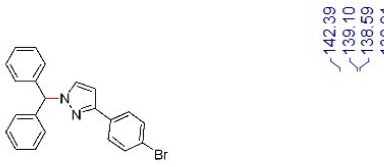
ethyl 1-benzhydryl-1H-pyrazole-4-carboxylate(30)

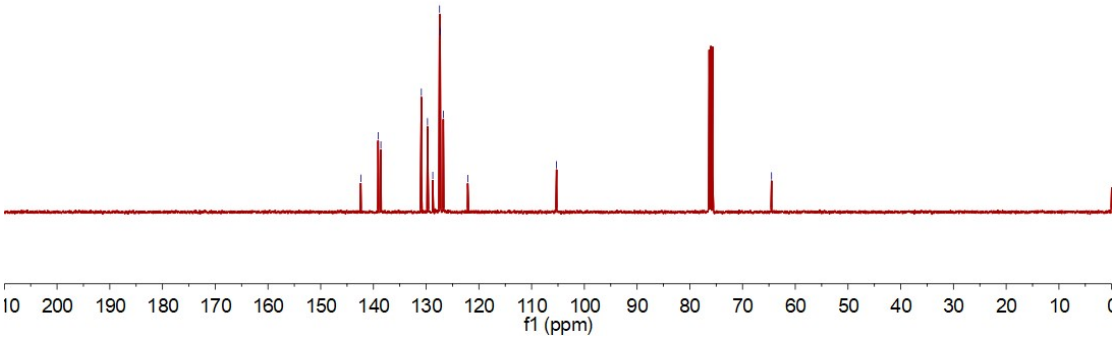


1-benzhydryl-3-(4-bromophenyl)-1H-pyrazole(31)

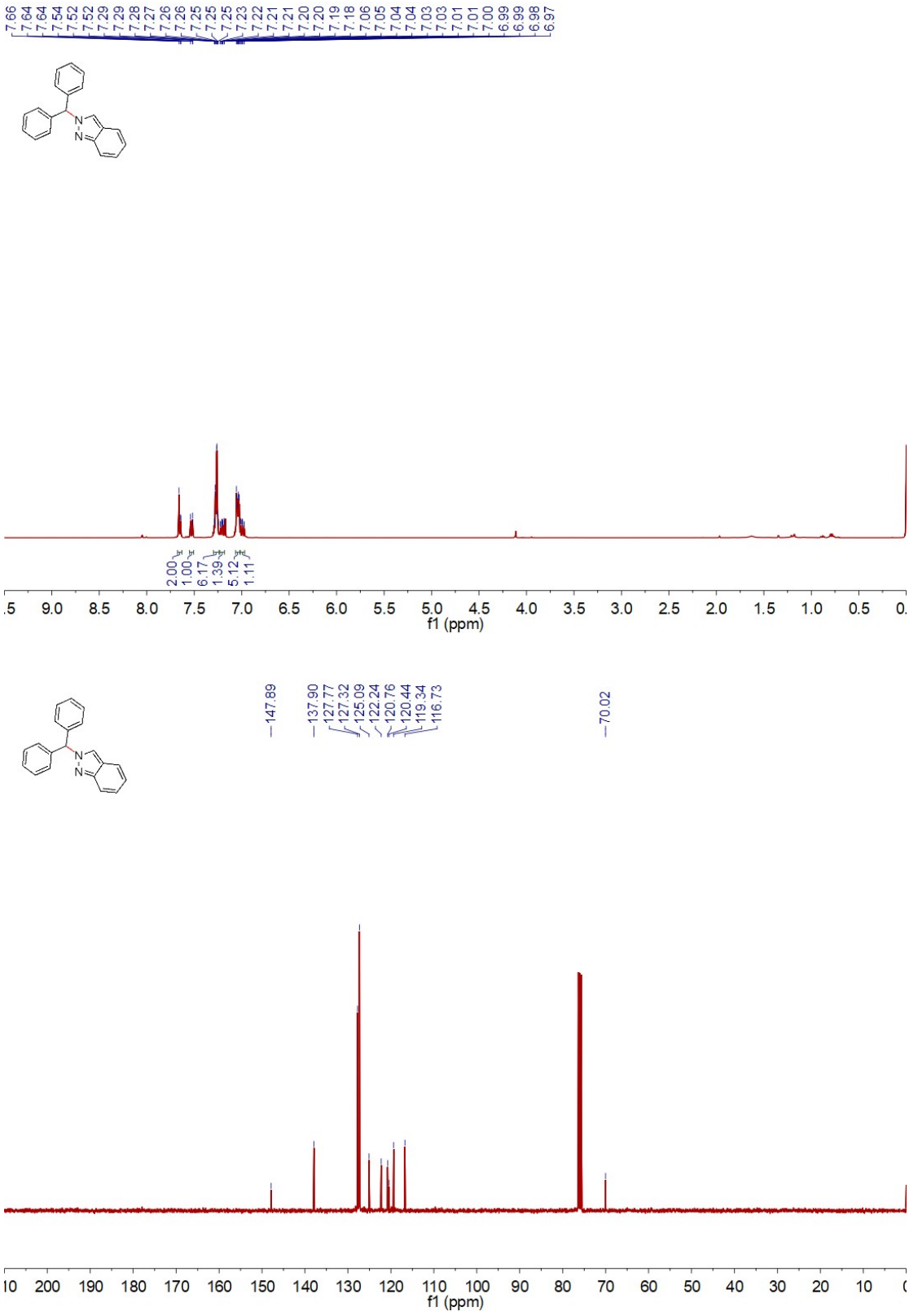




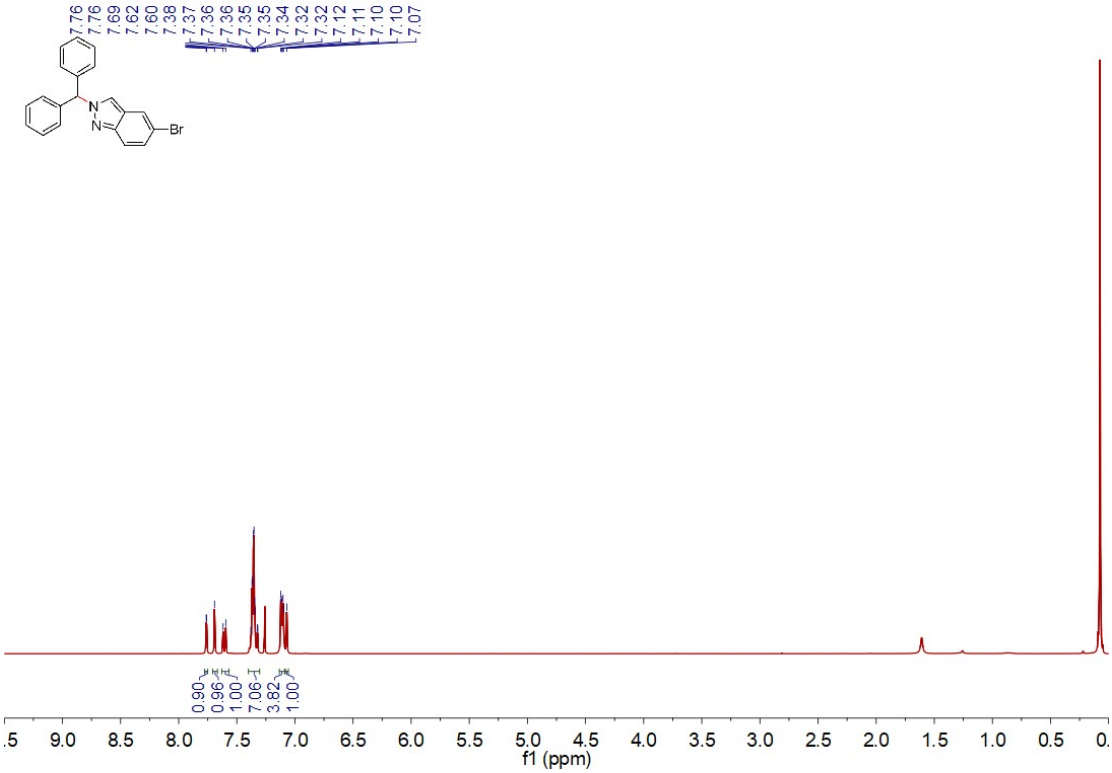


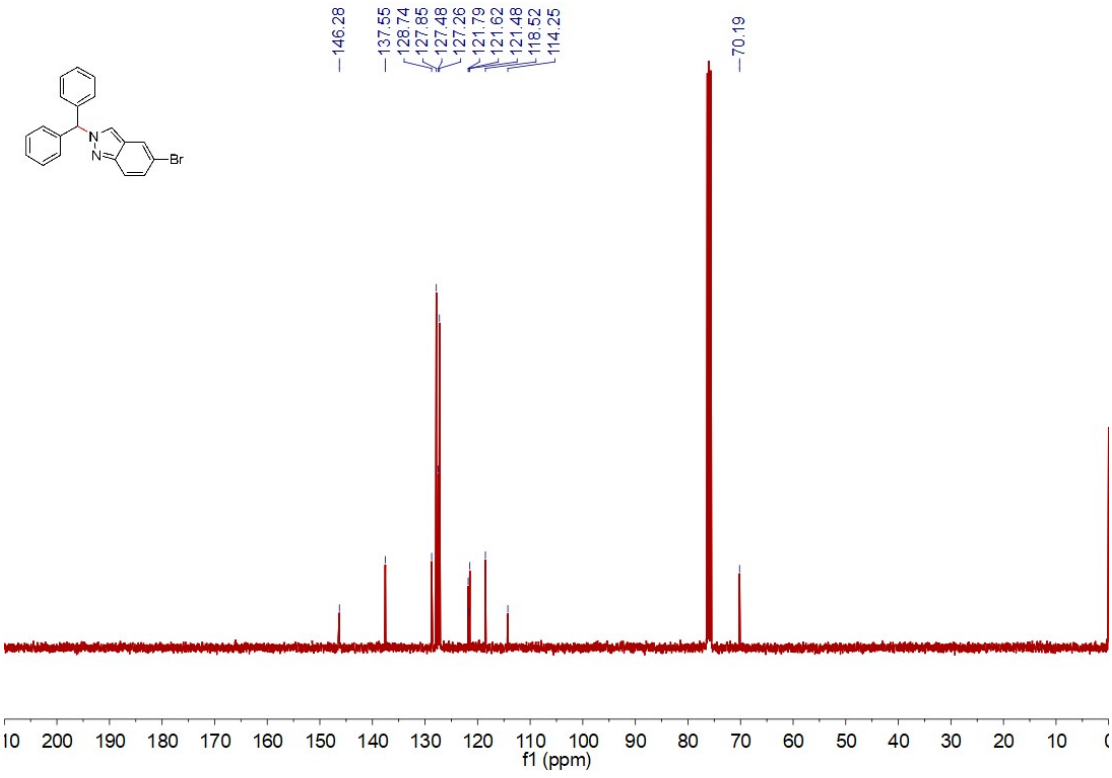


2-benzhydryl-2H-indazole(32)

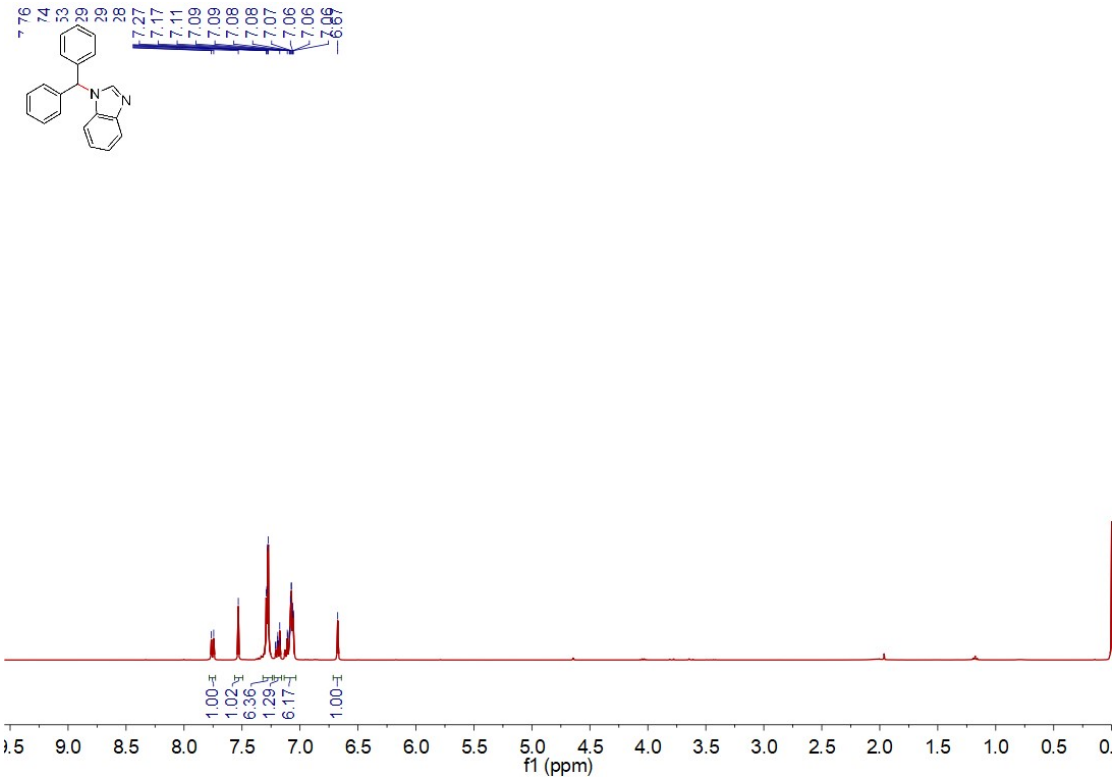


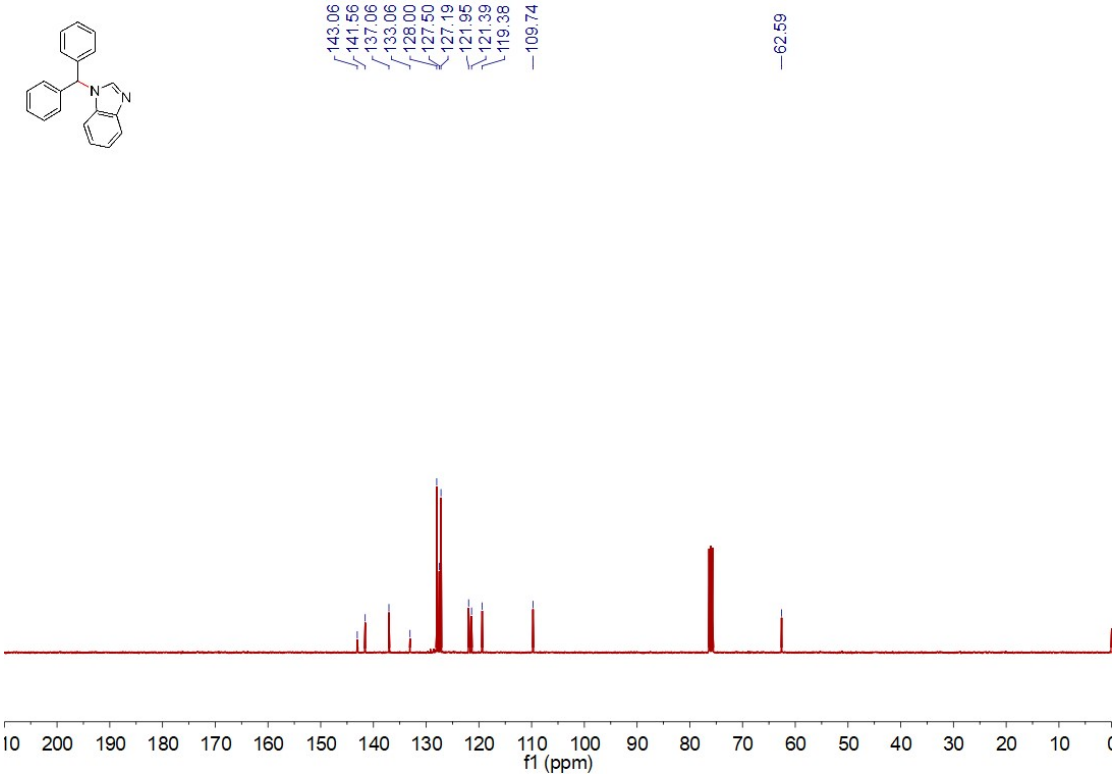
2-benzhydryl-5-bromo-2H-indazole(33)



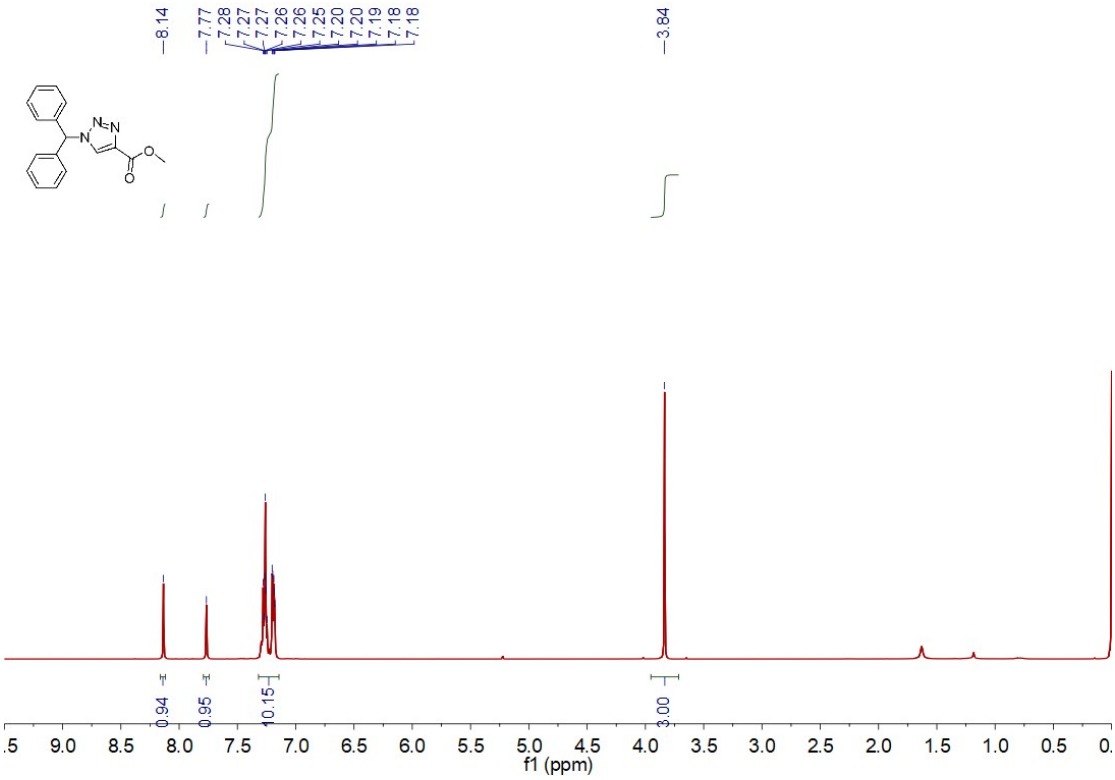


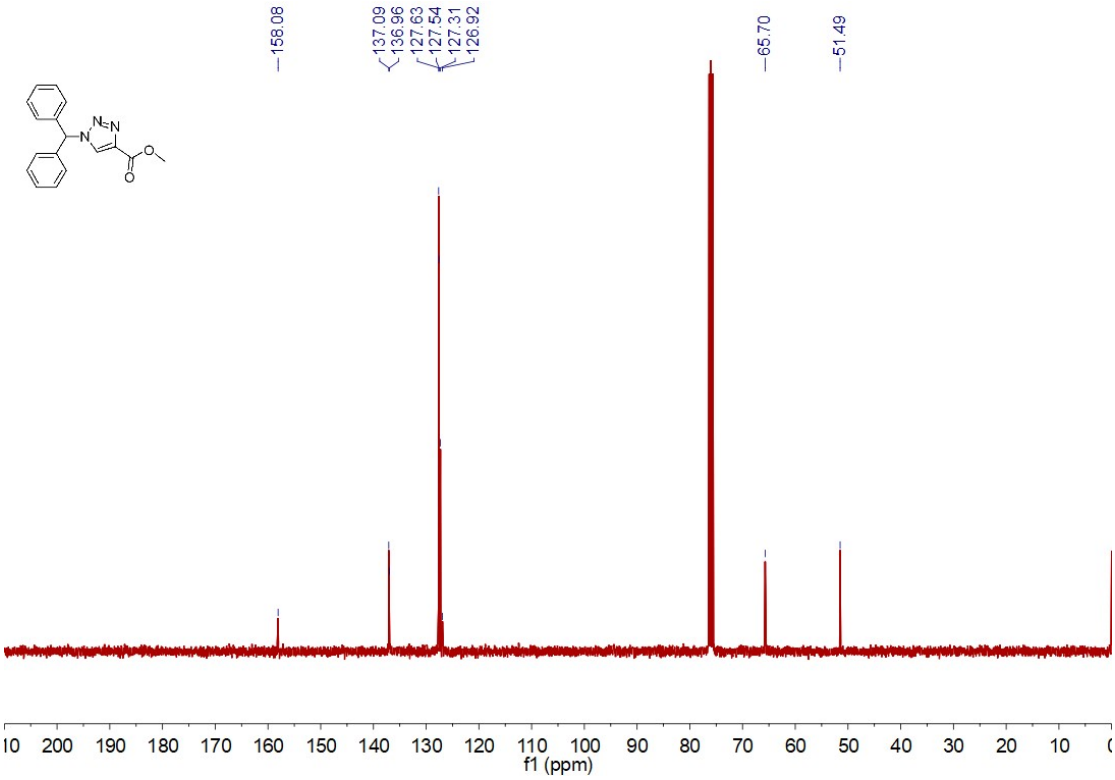
1-benzhydryl-1H-benzo[d]imidazole(34)



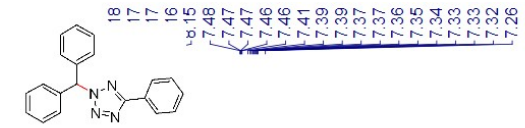


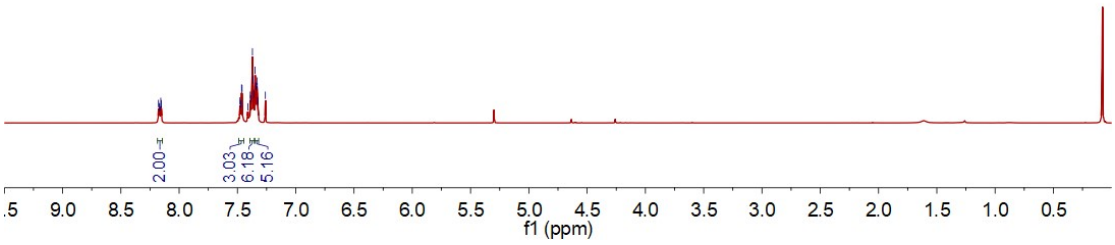
methyl 1-benzhydryl-1H-1,2,3-triazole-4-carboxylate(35)

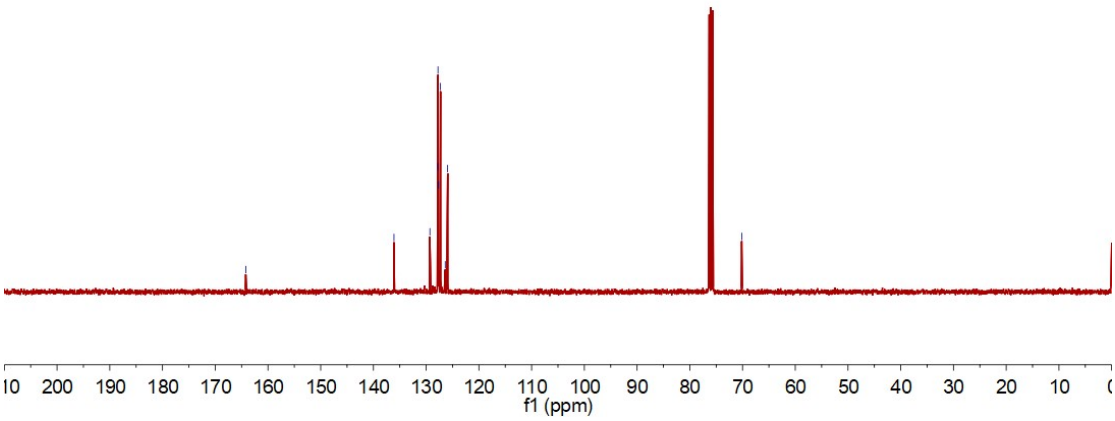




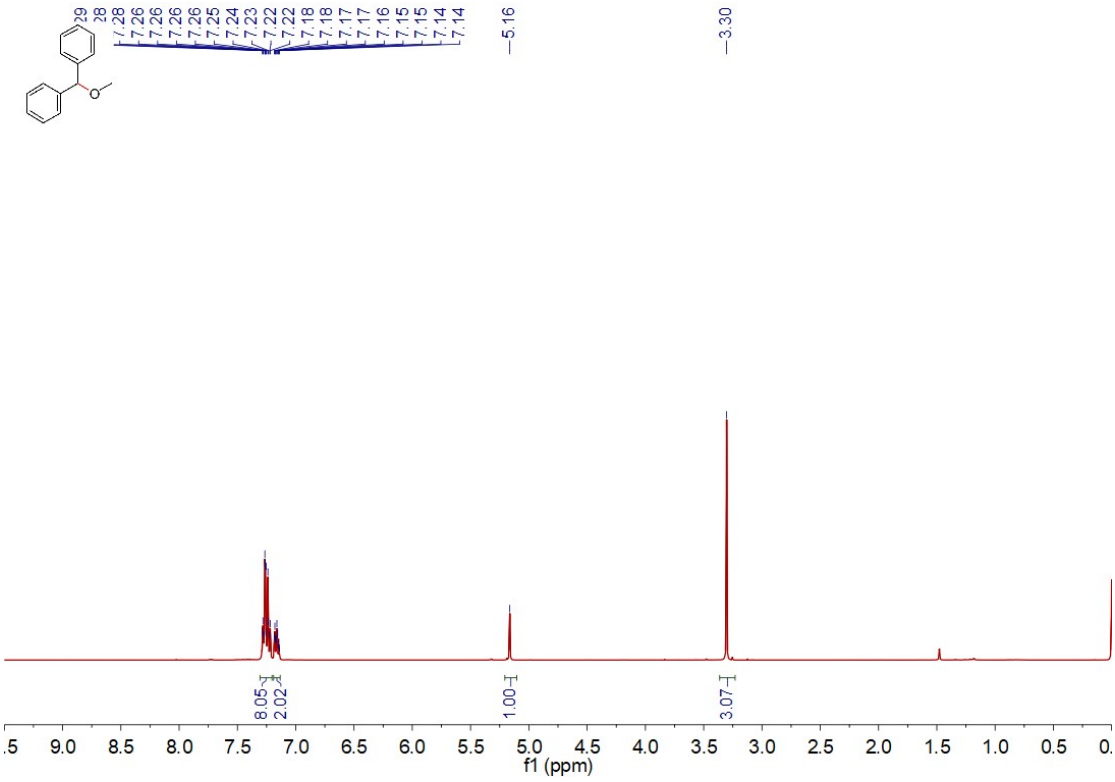
2-benzhydryl-5-phenyl-2H-tetrazole(36)

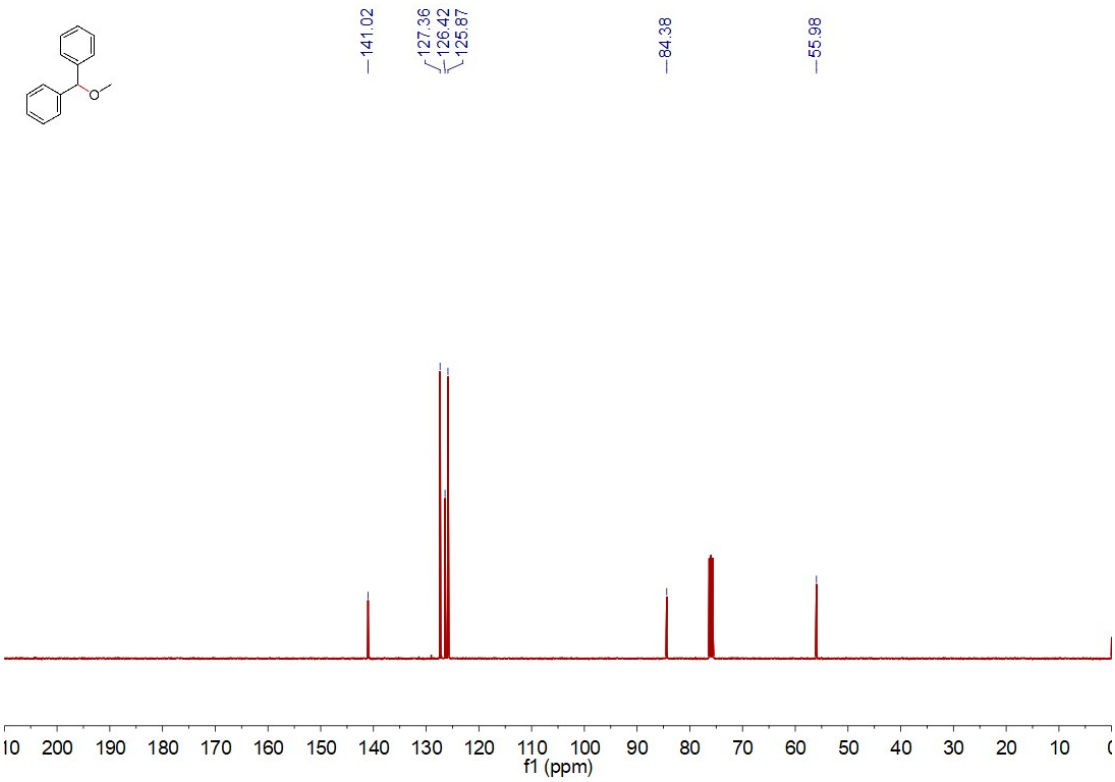




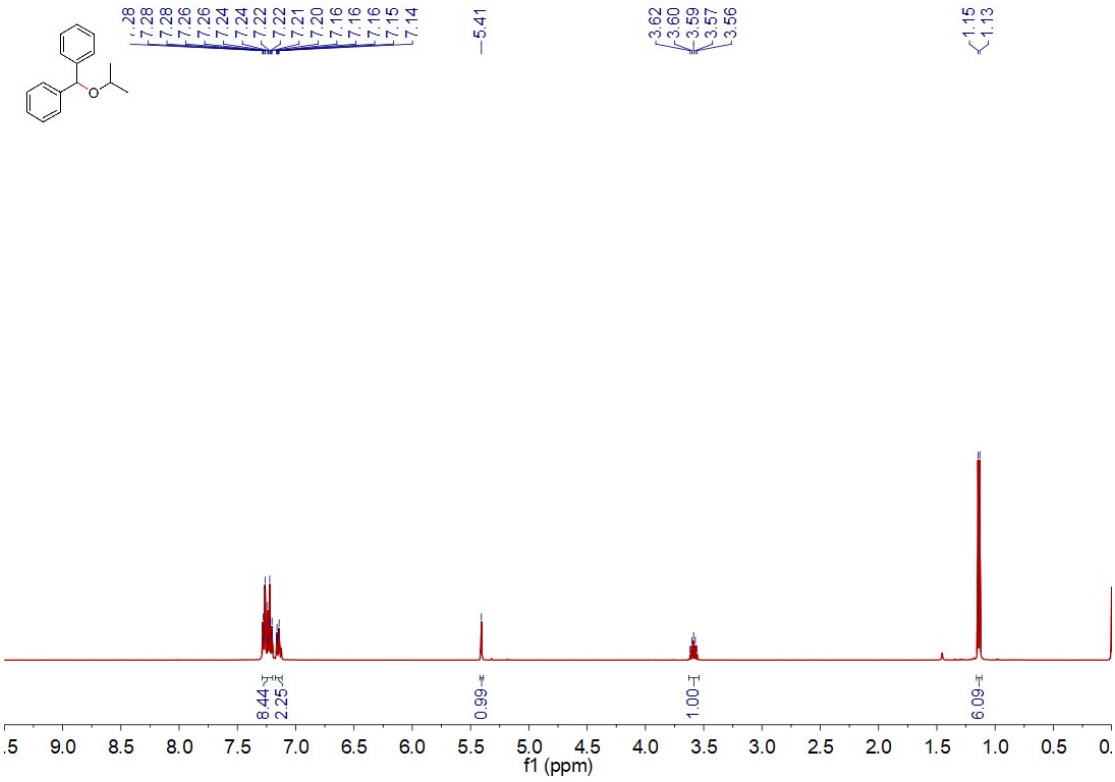


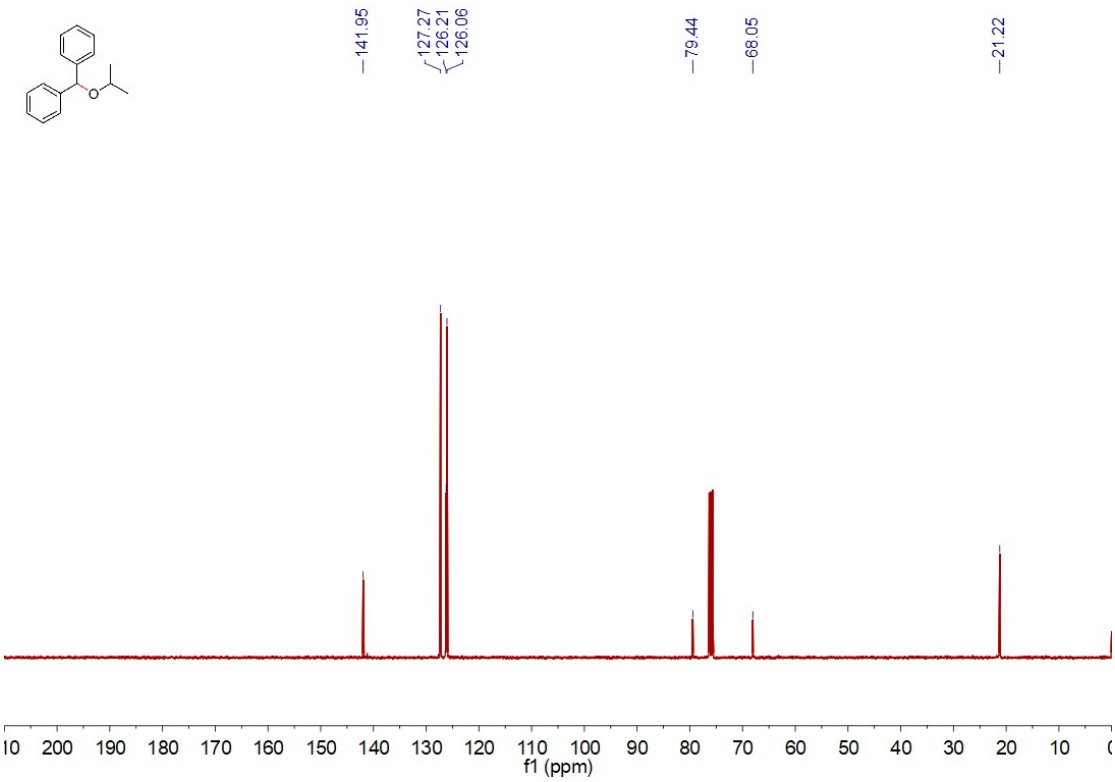
(methoxymethylene)dibenzene(37)



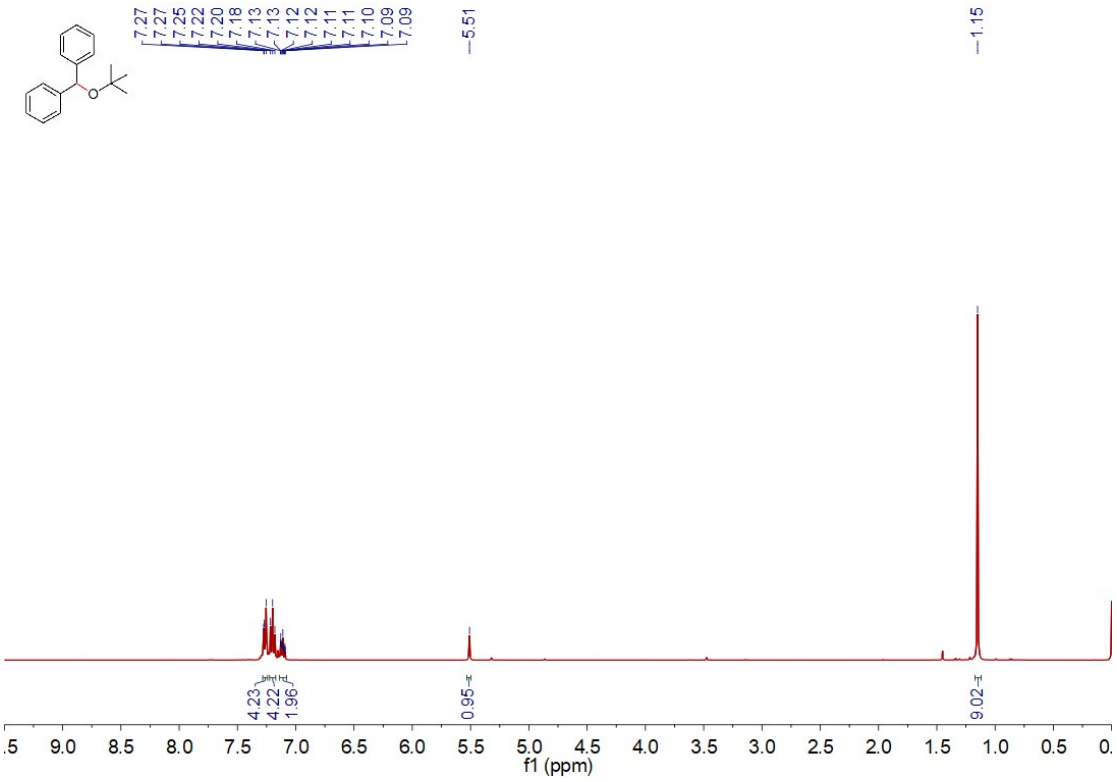


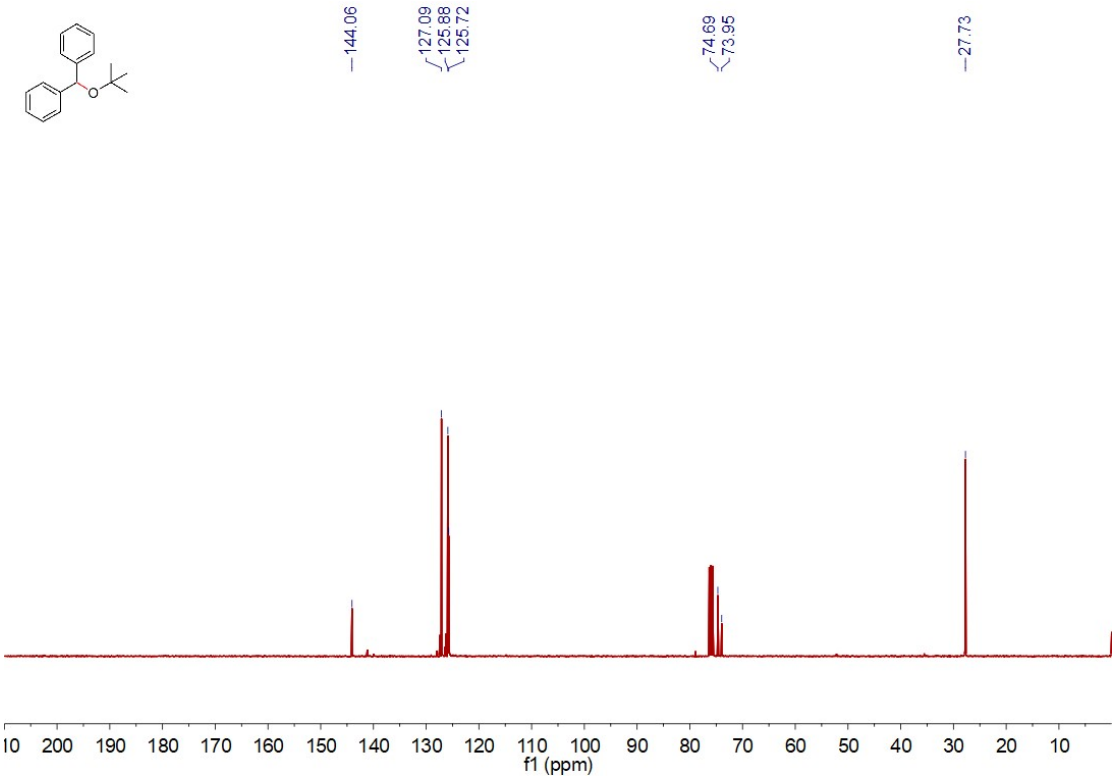
(isopropoxymethylene)dibenzene(38)



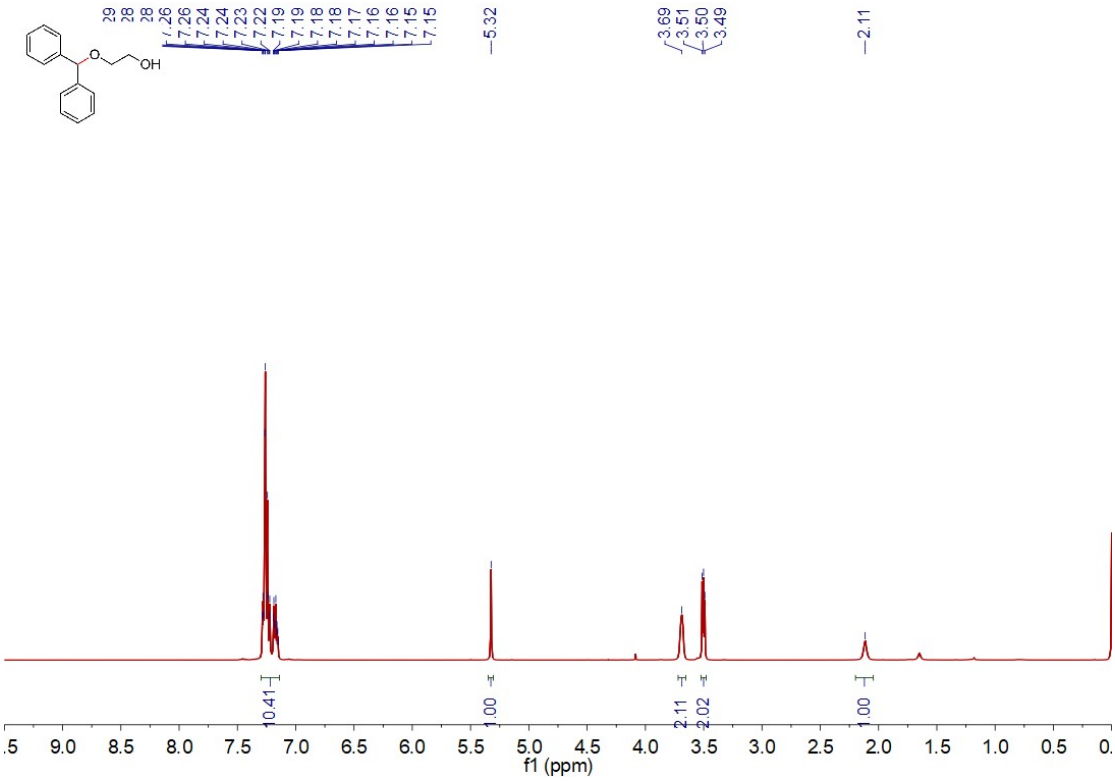


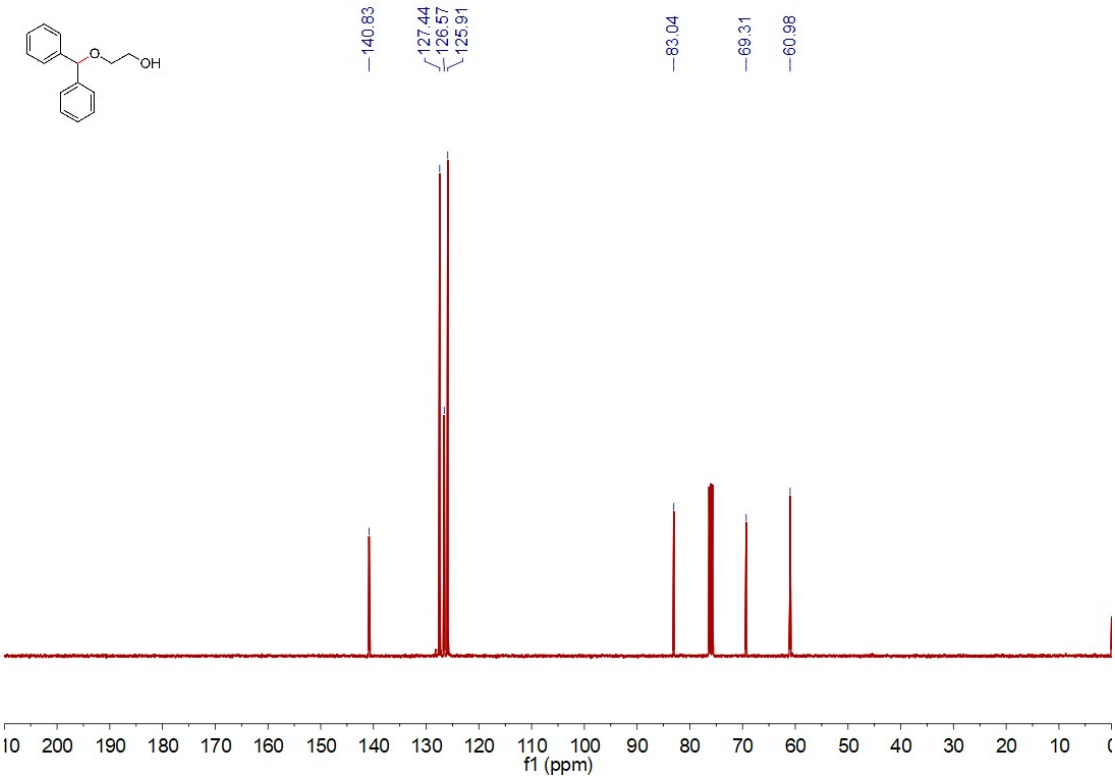
(tert-butoxymethylene)dibenzene(39)



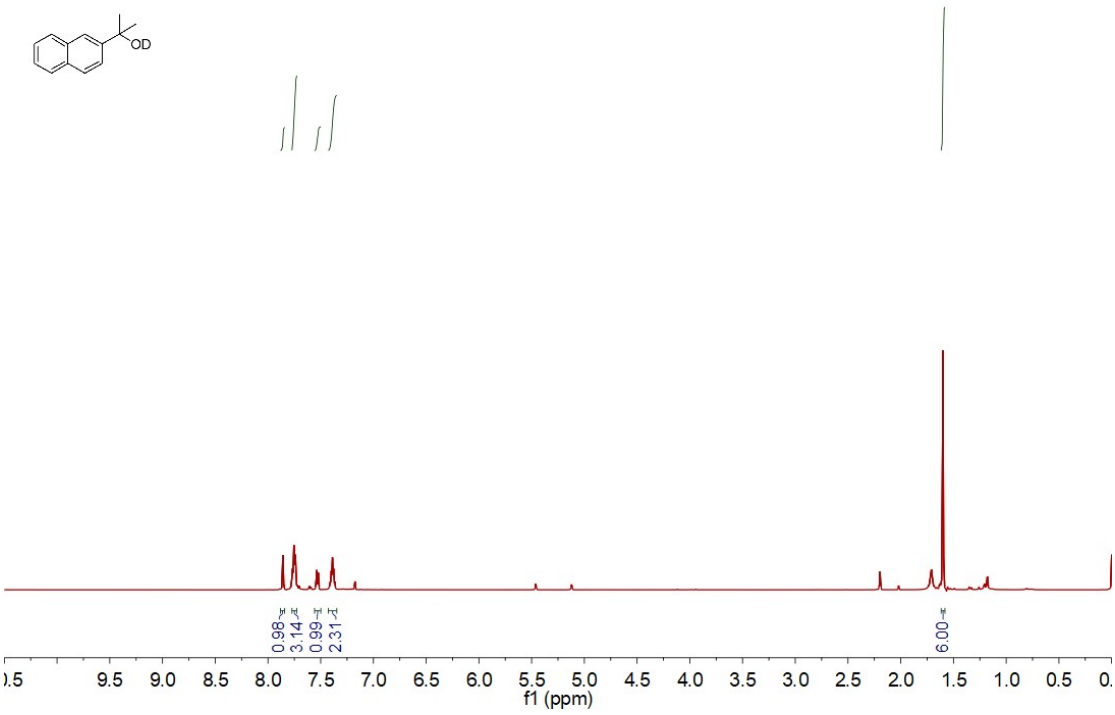


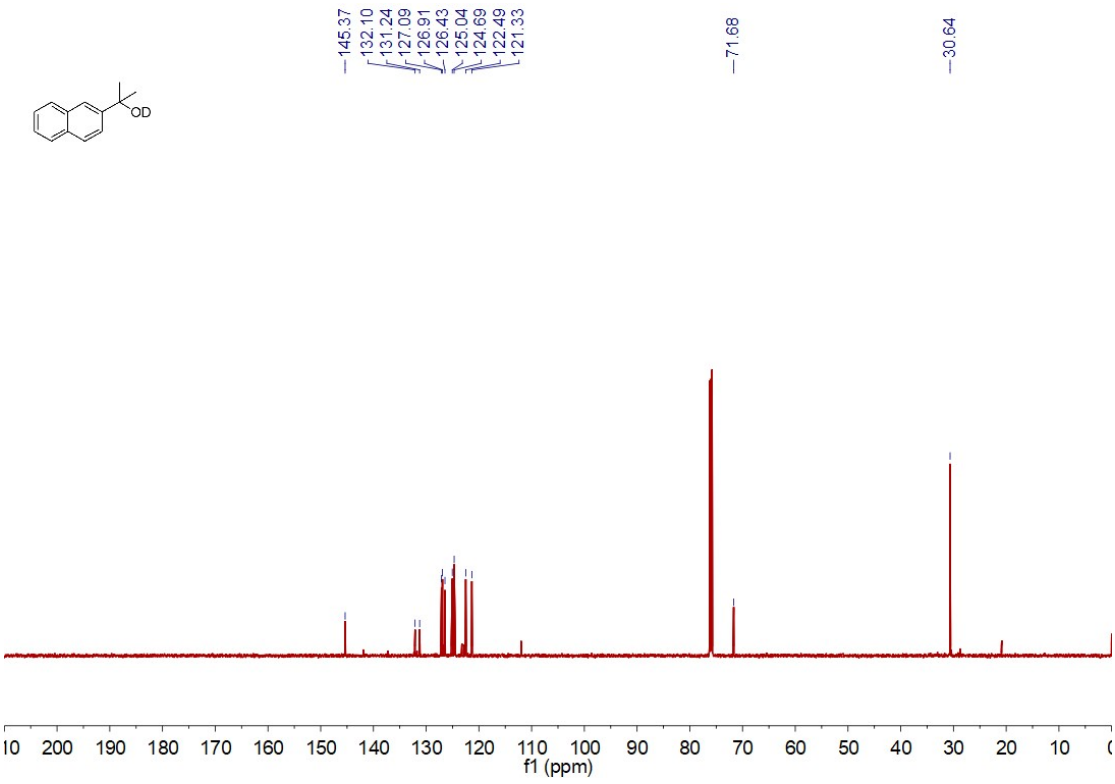
2-(benzhydryloxy)ethan-1-ol(40)



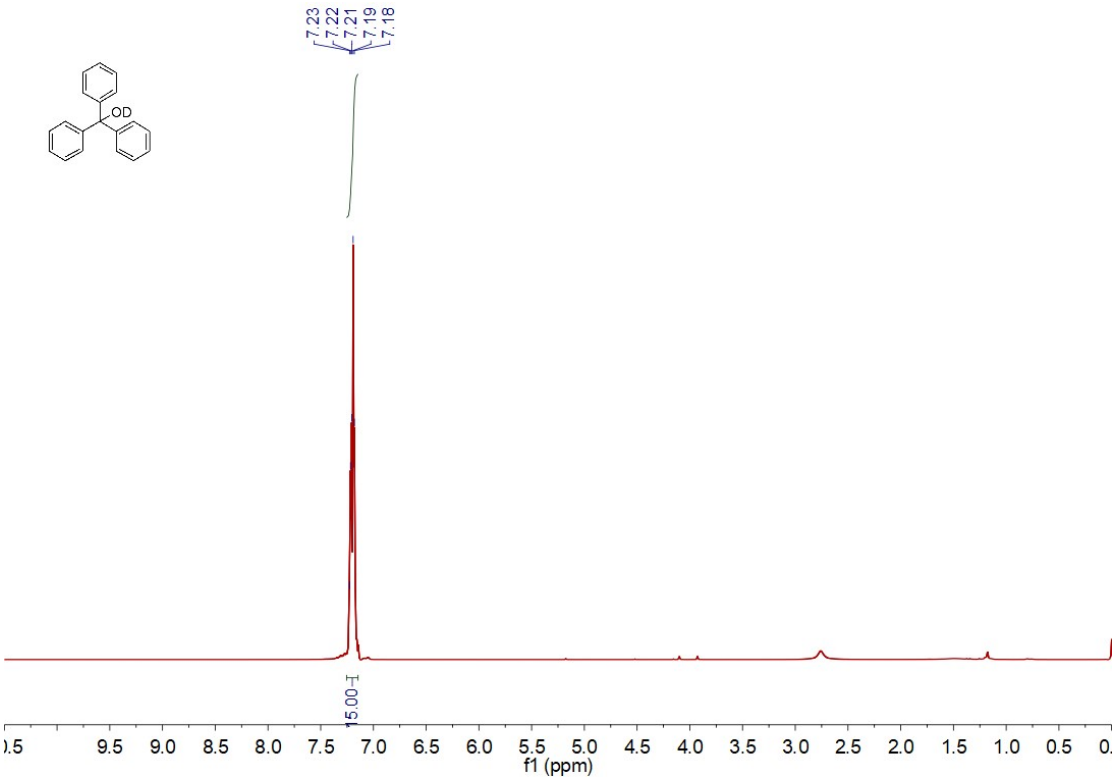


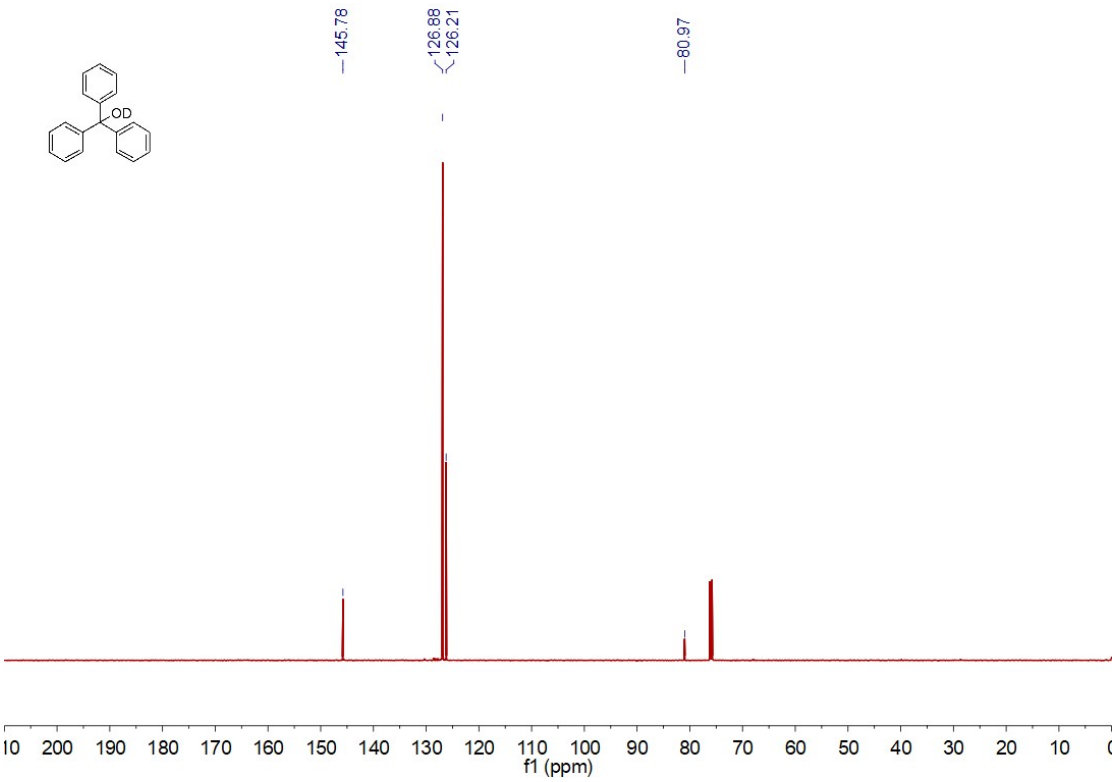
2-(naphthalen-2-yl)propan-2-ol-d(41)



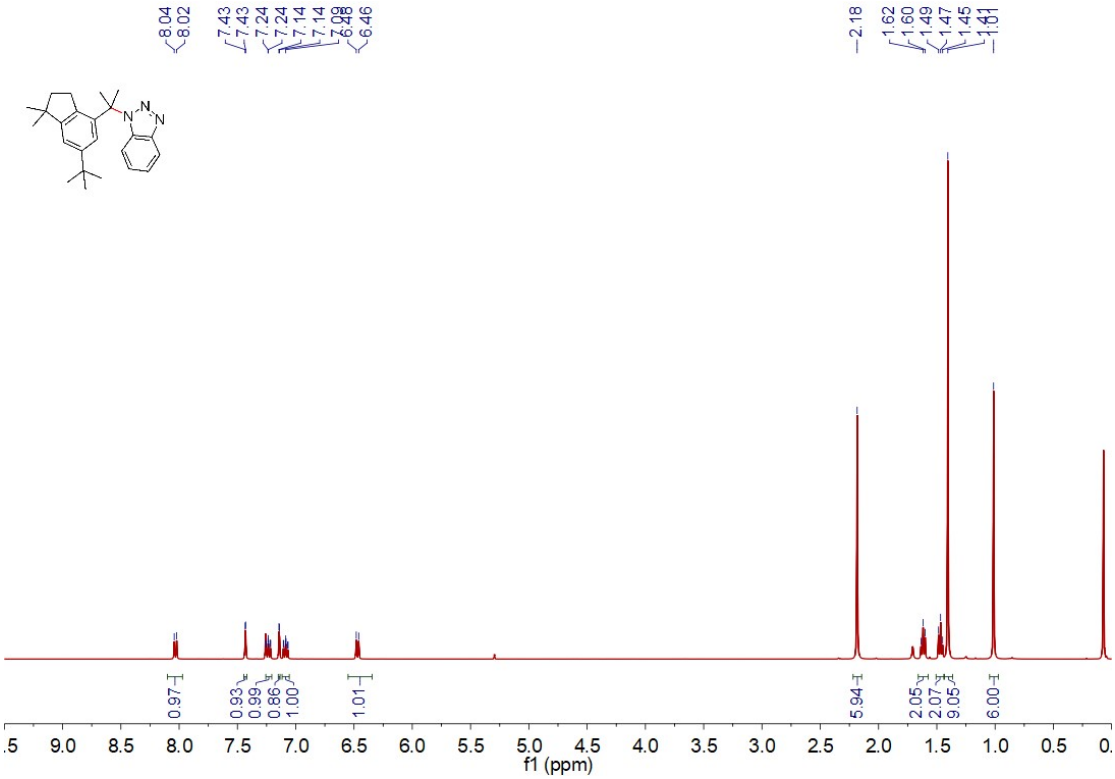


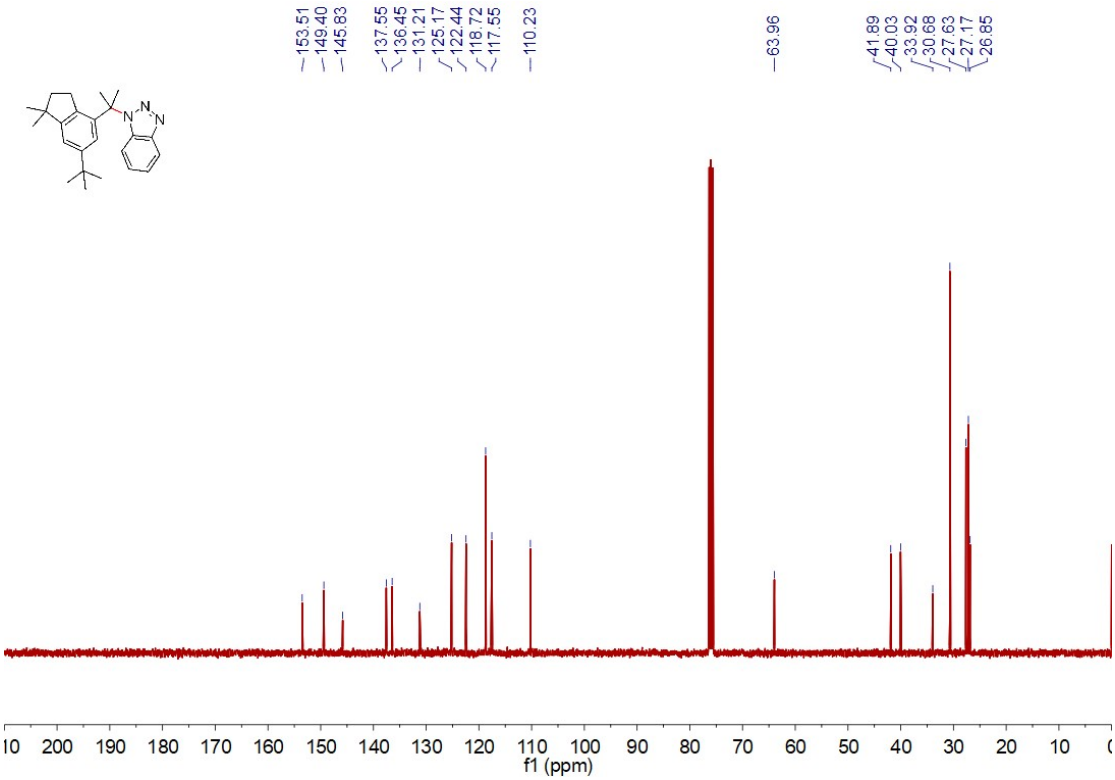
triphenylmethanol-d(42)



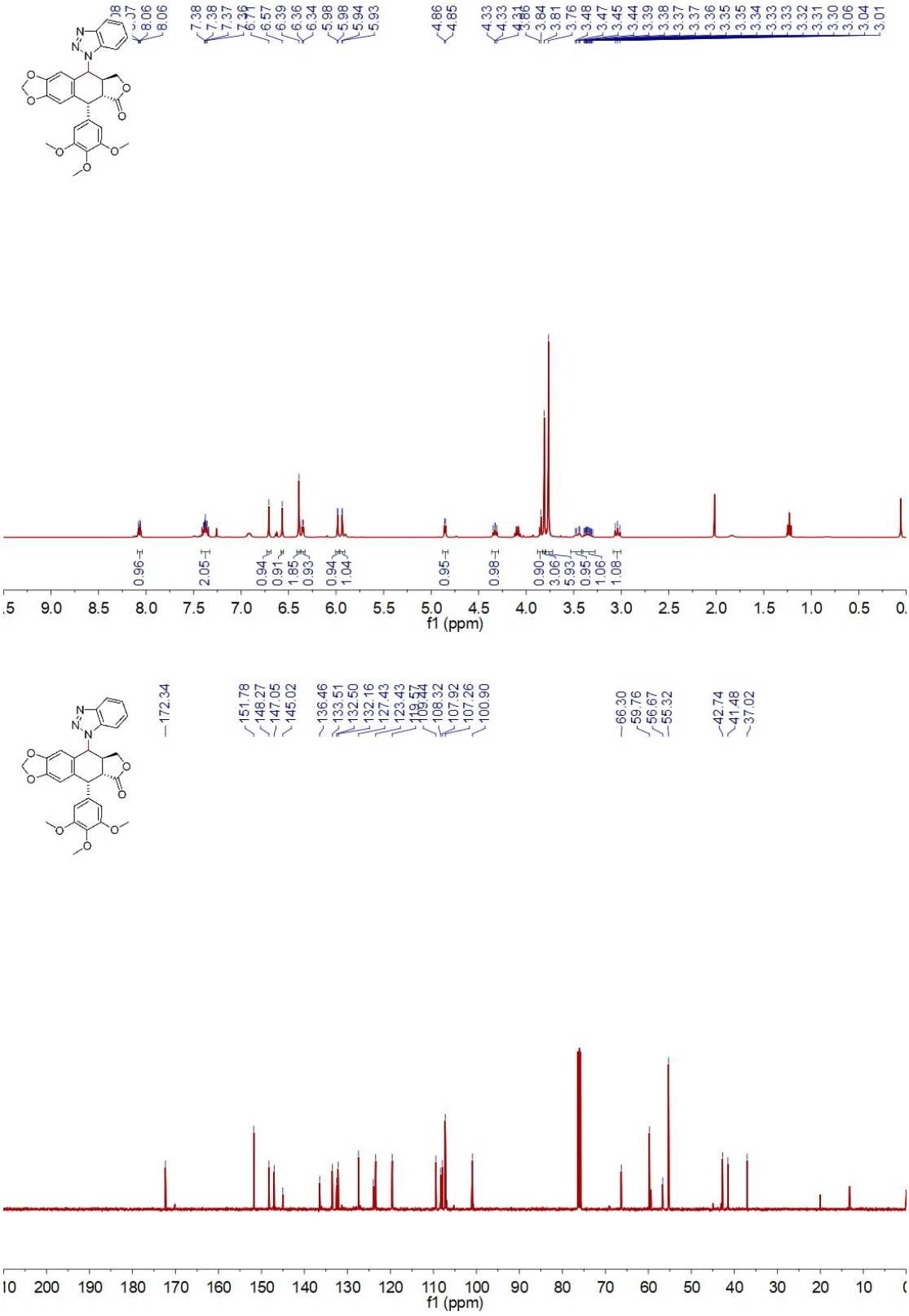


1-(2-(6-(tert-butyl)-1,1-dimethyl-2,3-dihydro-1H-inden-4-yl)propan-2-yl)-1H-benzo[d][1,2,3]triazole (43)

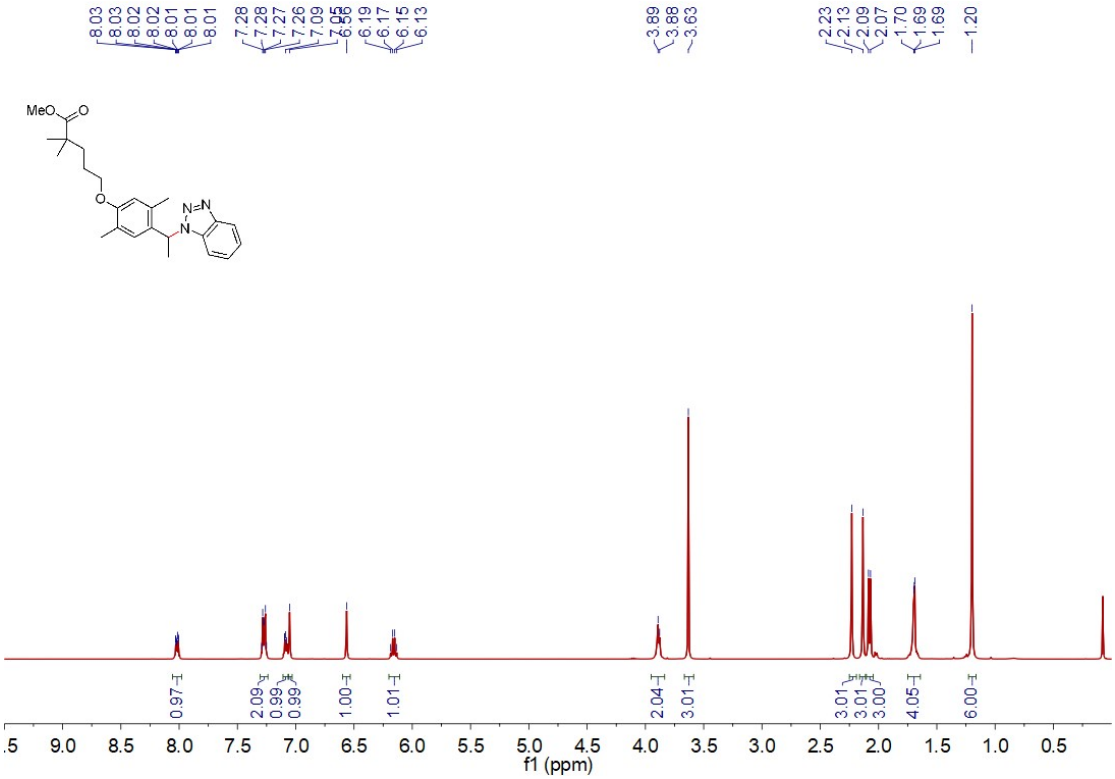


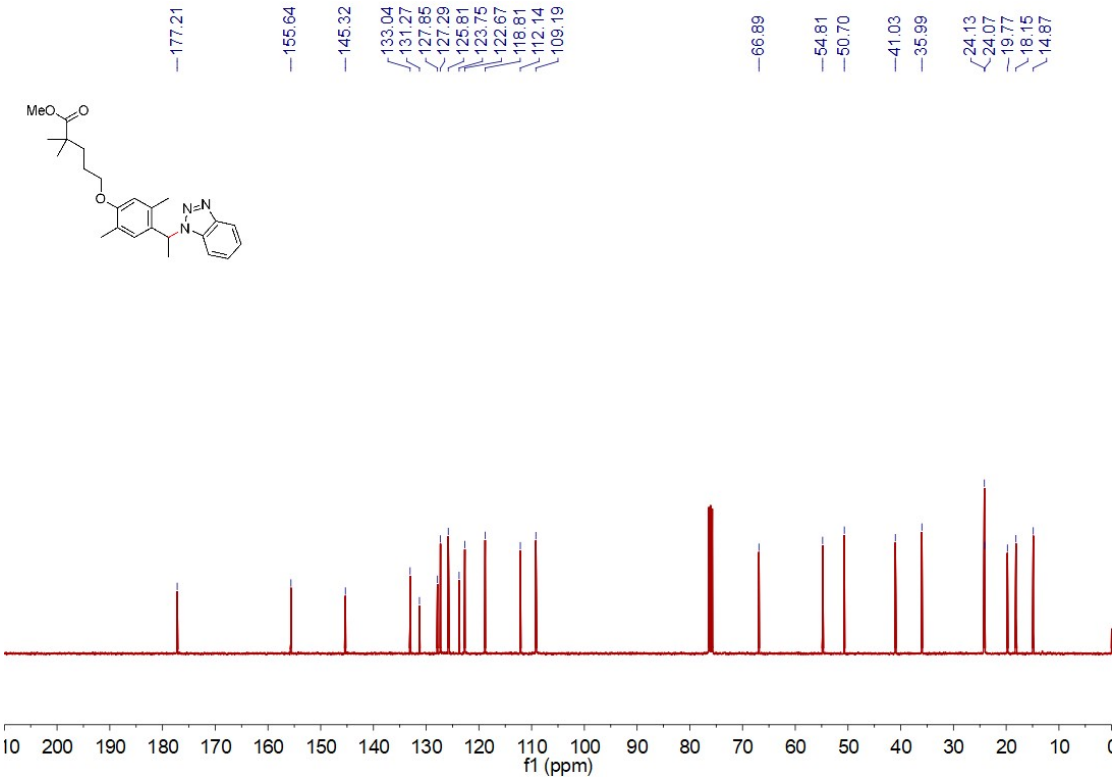


(5R,5aR,8aS)-9-(1H-benzo[d][1,2,3]triazol-1-yl)-5-(3,4,5-trimethoxyphenyl)-5,8,8a,9-tetrahydrofuro[3',4':6,7]naphtho[2,3-d][1,3]dioxol-6(5aH)-one (44)

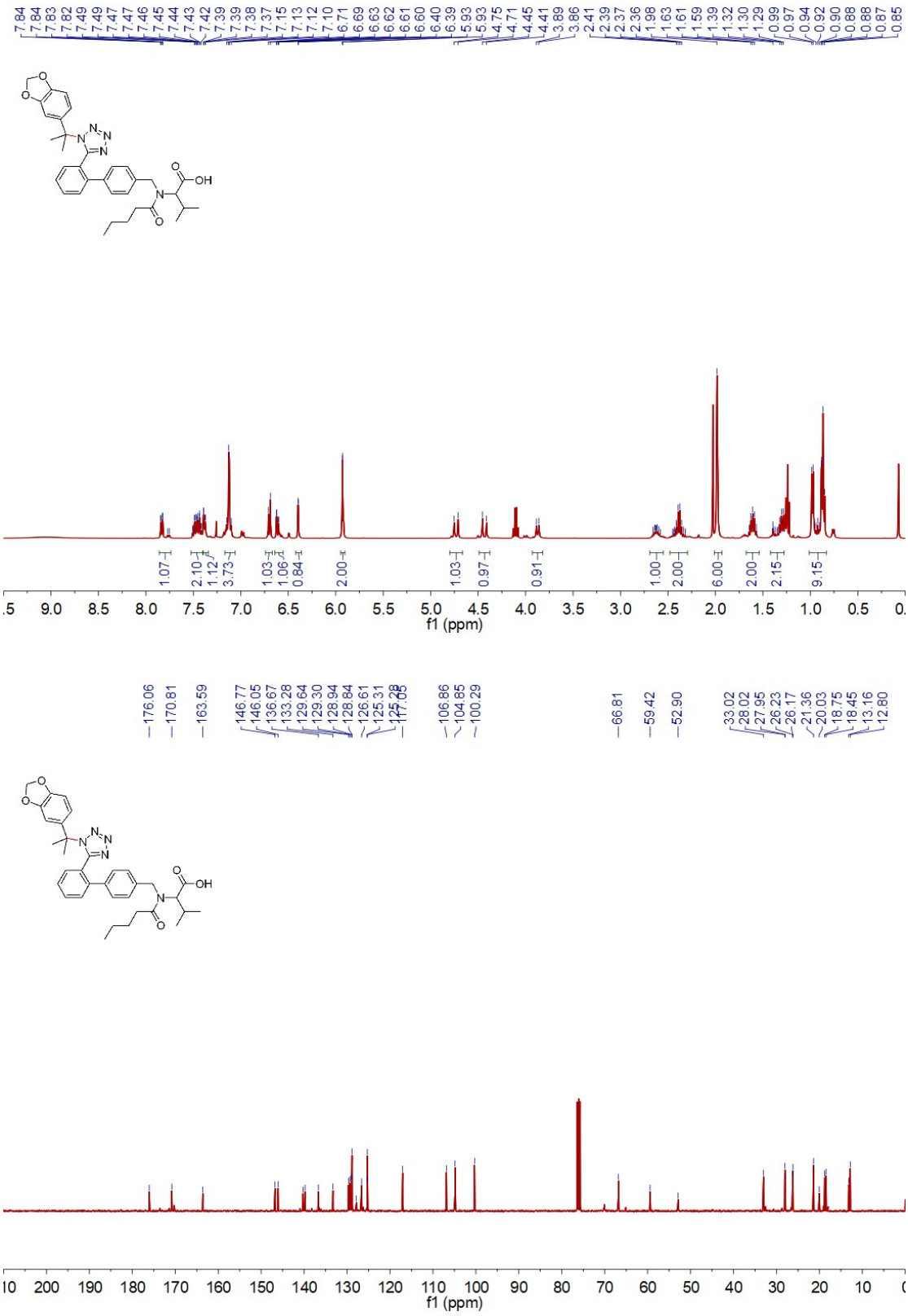


Methyl 5-(4-(1-(1H-benzo[d][1,2,3]triazol-1-yl)ethyl)-2,5-dimethylphenoxy)-2,2-dimethylpentanoate (45)

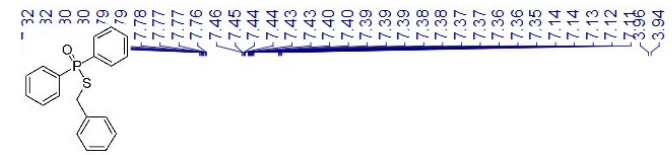


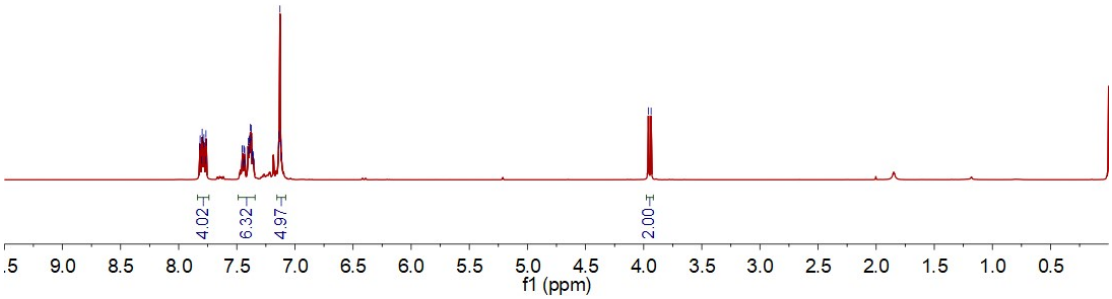


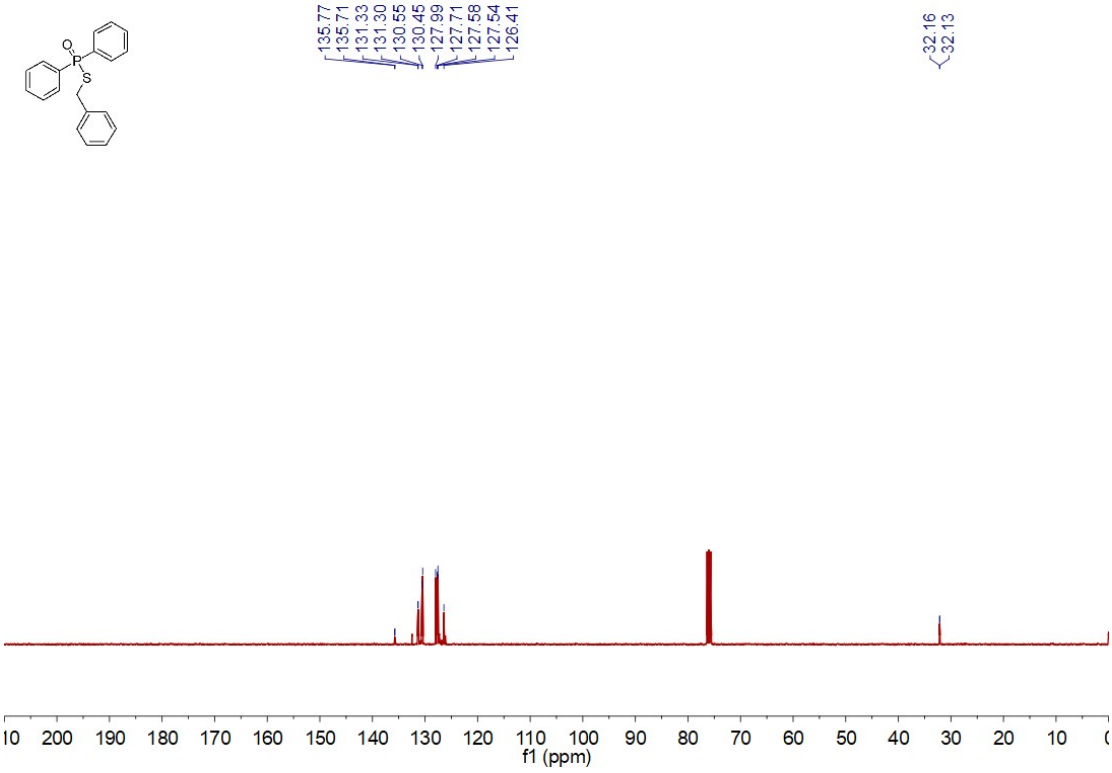
N-((2'-(1-(2-(benzo[d][1,3]dioxol-5-yl)propan-2-yl)-1H-tetrazol-5-yl)-[1,1'-biphenyl]-4-yl)methyl)-N-pentanoylvaline(46)



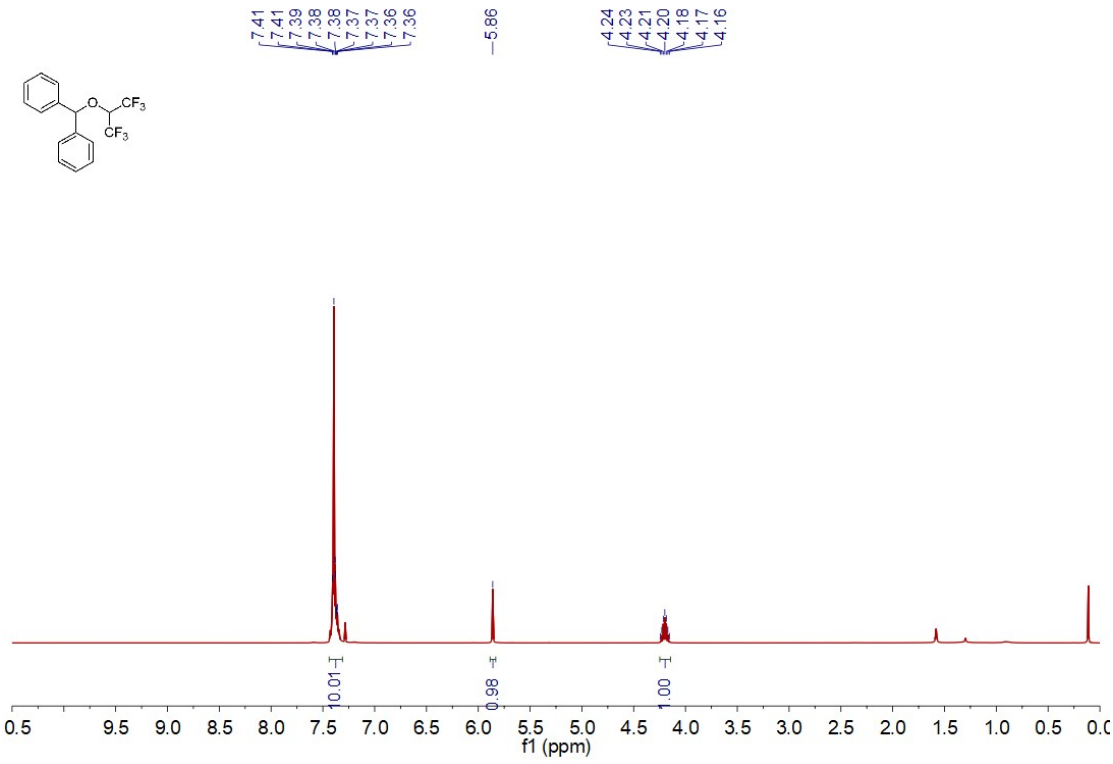
S-benzyl diphenylphosphinothioate(48)

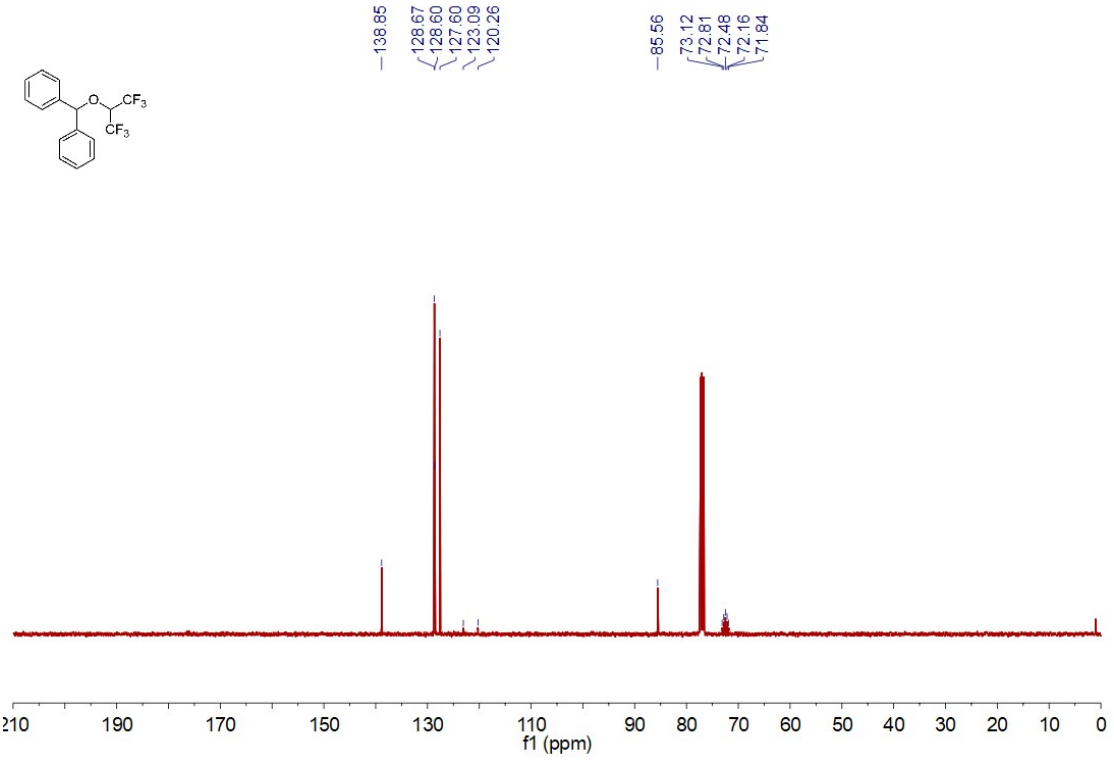


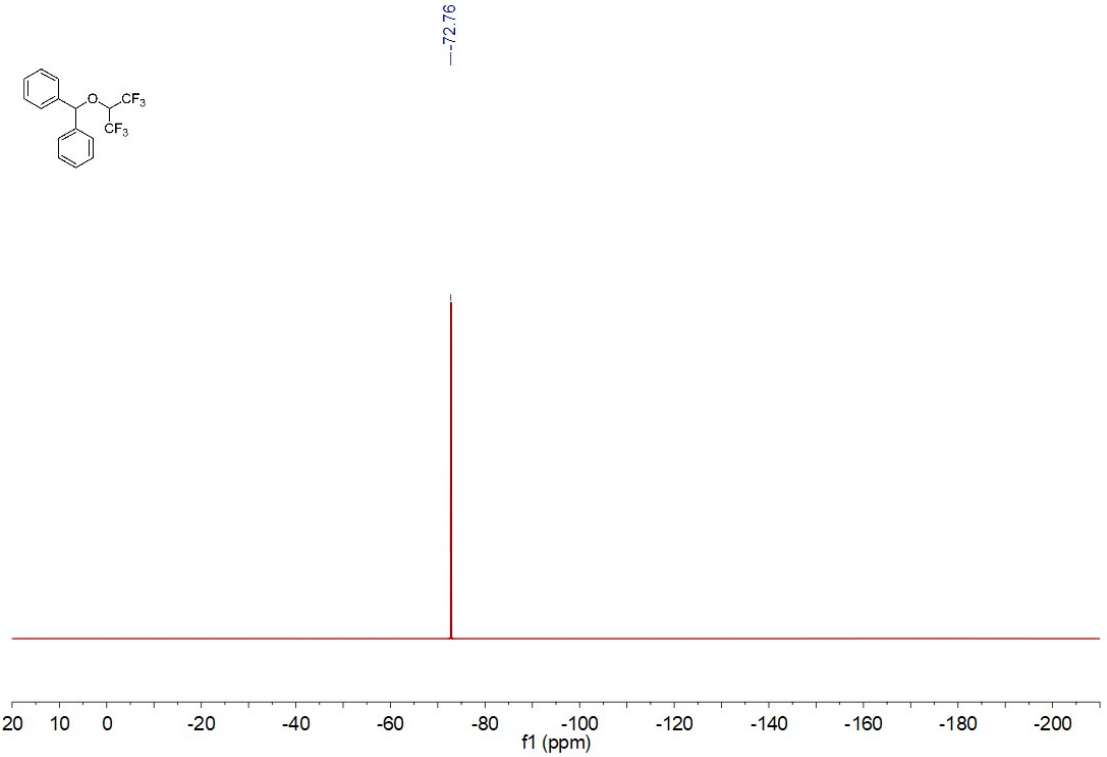




(((1,1,1,3,3,3-hexafluoropropan-2-yl)oxy)methylene)dibenzene(1x)



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CF3
CF3
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-140
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f1 (ppm)