Electronic Supplementary Material (ESI) for Green Chemistry.

Continuous flow synthesis of 1,4-disubstituted 1,2,3-triazoles *via* consecutive β-azidation of α,β-unsaturated carbonyl compounds and CuAAC reaction.

Giulia Brufani, [a†] Federica Valentini,[a†] Gabriele Rossini,[a] Luigi Carpisassi,[a] Daniela Lanari,*[b] Luigi Vaccaro*[a]

[a]*Laboratory of Green S.O.C. – Dipartimento di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia, Via Elce di Sotto 8, 06123 – Perugia – Italy;*
E-mail: luigi.vaccaro@unipg.it; Web: http://greensoc.chm.unipg.it/

[b]*Dipartimento di Scienze Farmaceutiche, Università degli Studi di Perugia, Via del Liceo 1, 06123 – Perugia – Italy;*

[†] *These authors contributed equally.*

e-mail: luigi.vaccaro@unipg.it

daniela.lanari@unipg.it

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1. General Remarks

Unless otherwise stated, all chemicals were purchased and used without any further purification. GLC analyses were performed by using Hewlett-Packard HP 5890 SERIES II equipped with a capillary column DB-5MS (30 m, 0.32 mm), a FID detector, and helium as gas carrier. GC-EIMS analyses were carried out by using a Hewlett-Packard HP 6890N Network GC system/5975 mass selective detector equipped with an electron impact ionizer at 70 eV. Melting points were measured on a Büchi 510 apparatus. NMR spectra were recorded on a Bruker DRX-ADVANCE 400 MHz (^{1}H at 400 MHz, ^{13}C at 100.6 MHz and ^{19}F at 376.4 MHz) in $CDCl_3$. Chemical shifts are reported in ppm (δ), coupling constant (J) in hertz and multiplicity are reported as follows: *s* = singlet, *bs* = broad singlet, *d* = doublet, *dd* = double doublet, *td* = double triplet, *t* = triplet, *m* = multiplet. Elemental Analysis (EA) were conducted on Elementar UNICUBE® elemental analyzer. Metal contamination in the final products was measured using MP-AES 4210 instrument.

Pyncer-type ligand 3,3-di(1H-imidazol-1-yl)propan-1-ol (**L**),[1] and **POLITAG-F** organocatalyst[2] were prepared as described in literature.

The aqueous acetonitrile azeotrope consists of 83.7 wt% of acetonitrile and 16.3 wt% of water.

Characterization data, ^{1}H, ^{13}C and ^{19}F NMR spectra are reported below.

2. General procedures

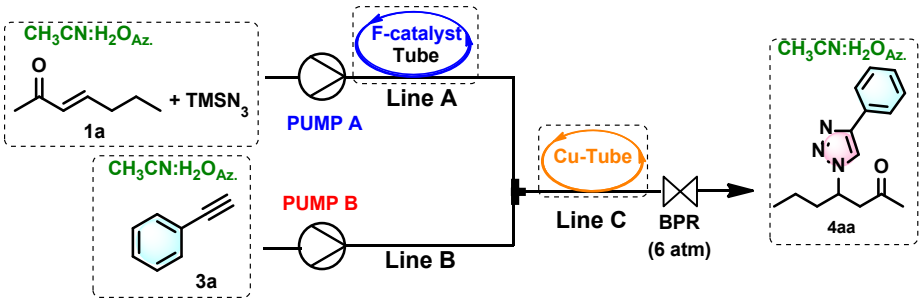
Loading calculation of POLITAG-F.[2]

Loading of fluoride anions supported on polymer were determined by elemental analysis calculated on the *bis*-imidazolium units (C: 54.31; H: 6.02; N: 3.54; loading F^-: 1.26 mmol/g).

Continuous flow protocol for the synthesis of triazoles (4)

The mixture of **1** (5 mmol) and trimethylsilylazide (1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, packed with **POLITAG-F** (2.0 g) and quartz powder, thermostated at 60 °C (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate **2** formed was mixed, through a T joint, with a 1.2 M solution of terminal alkyne **3** (1.2 eq) in CH_3CN:H_2O azeotrope pumped at 0.1 mL/min. The obtained mixture was passed in a CTFR (10 m, 1/32'' ID, 2 mL) heated at 100 °C with a BPR of 10 atm. The reactors were finally washed with 15 mL of aqueous azeotrope. The azeotrope was recovered by distillation affording in pure product **4**.

Table ESI-1. Optimization of the consecutive flow protocol.[a]



entry	Conc A (M)[b]	Conc B (M)[c]	mL/min A	mL/min B	$TMSN_3$ (eq)	3a (eq)	4aa (%)[d]
1	5	1.0	0.05	0.10	1.05	1.0	-
2	5	1.0	0.10	0.25	1.05	1.0	-
3	5	1.0	0.25	0.25	1.05	1.0	-
4	5	1.0	0.10	0.10	1.05	1.0	<5
5	5	0.1	0.10	0.10	1.05	2.0	<5
6	5	1.2	0.10	0.10	1.05	2.0	<5
7[e]	5	1.2	0.10	0.10	1.02	1.2	25
8[f]	5	1.2	0.10	0.10	1.02	1.2	30
9[g]	5	1.2	0.10	0.10	1.02	1.2	27
10[h,i]	5	1.2	0.10	0.10	1.02	1.2	56
11[h,j]	5	1.2	0.10	0.10	1.02	1.2	70
12[i]	5	1.2	0.10	0.10	1.02	1.2	>99
13[e,i]	5	1.2	0.10	0.10	1.02	1.2	75
14[f,i]	5	1.2	0.10	0.10	1.02	1.2	84
15[g,i]	5	1.2	0.10	0.10	1.02	1.2	82

[a]Reaction conditions: **1a** (5 mmol), 1st reactor (POLITAG-F, 0.2 g) thermostated at 60 °C; Cu-tube thermostated at 100 °C. BPR (6 atm). [b]Referred to **1a**. [c]Referred to **3a**. [d]Determined by GC analysis. [e]*PS-DABCOF$_2$ catalyst*[3] *(0.346 g; loading: 7.4 mmol$_F$/g).* [f]*IRA900-F catalyst*[4] *(0.983 g; loading: 2.6 mmol$_F$/g).* [g]*POLITAG-M-F catalyst*[2] *(0.947 g; loading: 2.7 mmol$_F$/g).* [h]Cu-tube (5 m). [i]BPR (10 atm). [j]BPR (17 atm).

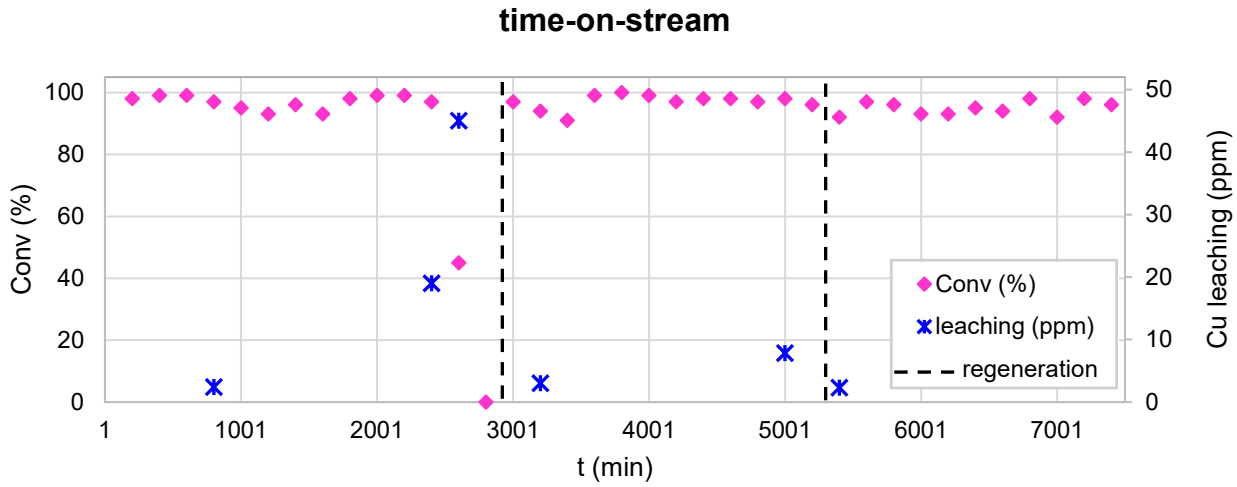


Figure ESI-1. Time on stream of the consecutive flow protocol for the synthesis of 1,4-disubstituted 1,2,3-triazoles.

3. Green Metrics Calculation[5]

Batch	Flow
Reactants: **1a** = 112.17 mg (1 mmol) $TMSN_3$ = 120.97 (1.05 eq) H_2O = 18.01 mg (1 eq) **3a** = 102.13 mg (1 eq) **Solvent:** $CH_3CN/H_2O_{Az.}$ = 1 mL **Work-up:** $CH_3CN/H_2O_{Az.}$ = 2 mL **Purification:** $CH_3CN/H_2O_{Az.}$ = 0.5mL **Recovered materials:** $CH_3CN/H_2O_{Az.\ [solvent+work-up]}$ = 2.67 mL (89 %) **Product:** **4aa** = 241.9 mg (94 % yield)	**Reactants:** **1a** = 560.85 mg (5 mmol) $TMSN_3$ = 587.57 mg (1.02 eq) H_2O = 90.05 mg (1 eq) **3a** = 612.78 mg (1.2 eq) **Solvent:** $CH_3CN/H_2O_{Az.}$ = 6 mL **Work-up:** $CH_3CN/H_2O_{Az.}$ = 15 mL **Purification:** Not performed **Recovered materials:** $CH_3CN/H_2O_{Az.\ [solvent+work-up]}$ = 19.74 mL (94 %) **Product:** **4aa** = 1.248 g (97 % yield)
E-factor = 3.25	**E-factor** = 1.27
AE = 0.741	**AE** = 0.741
Rxn Yield = 0.940	**Rxn Yield** = 0.970
1/SF = 0.984	**1/SF** = 0.939
MRP = 0.343	**MRP** = 0.654
RME = 0.235	**RME** = 0.441
VMR = 0.717327917	**VMR** = 0.773582143

Atom Economy (AE)

$$AE = \frac{MW_{product}}{\sum_{jv_j} MW_{reactant}}$$

Reaction Mass Efficiency (RME)

$$RME = \frac{1}{1 + E\ factor}$$

Stoichiometric Factor (SF)

$$SF = 1 + \frac{m_{excess\ reagents}}{m_{stoichiometric\ reagents}}$$

Mass Recovery Parameter (MRP)

$$MRP = \frac{RME \cdot SF}{AE \cdot (\frac{yield}{100})}$$

References

1. V. Kozell, F. Rahmani, O. Piermatti, D. Lanari, L. Vaccaro, *Mol. Catal*. **2018**, *455*, 188−191

2. F. Ferlin, F. Valentini, G. Brufani, D. Lanari, L. Vaccaro *ACS Sustainable Chem. Eng*. **2021**, *9*, 5740−5749

3. T. Angelini, D. Lanari, R. Maggi, F. Pizzo, G. Sartori, L. Vaccaro, *Adv. Synth. Catal*., **2012**, *354*, 908-916

4. L. Castrica, F. Fringuelli, L. Gregoli, F. Pizzo, L. Vaccaro, *J. Org. Chem*. **2006**, *71*, 9536–9539

5. J. Andraos, A. Hent, *J. Chem. Educ*. **2015**, *92*, 1820–1830

4. E-factor calculation (continuous flow protocol)

β-Azidation of **1a** and consecutive CuAAC with **3a**:

E-factor = [560.85 mg (**1a**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 612.78 mg (**3a**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1248.00 mg (**4aa**)] / 1248.00 mg (**4aa**) = 1.3

β-Azidation of **1b** and consecutive CuAAC with **3a**:

E-factor = [701.10 mg (**1b**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 612.78 mg (**3a**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1384.12 mg (**4ba**)] / 1384.12 mg (**4ba**) = 1.2

β-Azidation of **1a** and consecutive CuAAC with **3b**:

E-factor = [560.85 mg (**1a**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 792.96 mg (**3b**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1408.06mg (**4ab**)] / 1408.06mg (**4ab**) = 1.1

β-Azidation of **1b** and consecutive CuAAC with **3b**:

E-factor = [701.10 mg (**1b**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 792.96 mg (**3b**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1545.55 mg (**4bb**)] / 1545.55 mg (**4bb**) = 1.0

β-Azidation of **1a** and consecutive CuAAC with **3c**:

E-factor = [560.85 mg (**1a**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 1086.18 mg (**3c**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1646.82 mg (**4ac**)] / 1646.82 mg (**4ac**) = 1.0

β-Azidation of **1b** and consecutive CuAAC with **3c**:

E-factor = [701.10 mg (**1b**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 1086.18 mg (**3c**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1784.49 mg (**4bc**)] / 1784.49 mg (**4bc**) = 0.9

β-Azidation of **1a** and consecutive CuAAC with **3d**:

E-factor = [560.85 mg (**1a**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 1020.78 mg (**3d**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1495.67 mg (**4ad**)] / 1495.67 mg (**4ad**) = 1.2

β-Azidation of **1b** and consecutive CuAAC with **3d**:

E-factor = [701.10 mg (**1b**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 1020.78 mg (**3d**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1730.6 mg (**4bd**)] / 1730.6 mg (**4bd**) = 1.0

β-Azidation of **1a** and consecutive CuAAC with **3e**:

E-factor = [560.85 mg (**1a**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 696.96 mg (**3e**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1248.59 mg (**4ae**)] / 1248.59 mg (**4ae**) = 1.3

β-Azidation of **1b** and consecutive CuAAC with **3e**:

E-factor = [701.10 mg (**1b**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 696.96 mg (**3e**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1481.85 mg (**4be**)] / 1481.85 mg (**4be**) = 1.1

β-Azidation of **1a** and consecutive CuAAC with **3f**:

E-factor = [560.85 mg (**1a**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 1482.78 mg (**3a**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1908.55 mg (**4af**)] / 1908.55 mg (**4af**) = 0.9

β-Azidation of **1b** and consecutive CuAAC with **3f**:

E-factor = [701.10 mg (**1b**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 1482.78 mg (**3a**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 2021.88 mg (**4bf**)] / 2021.88 mg (**4bf**) = 0.9

β-Azidation of **1a** and consecutive CuAAC with **3g**:

E-factor = [560.85 mg (**1a**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 648.96 mg (**3g**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1211.69 mg (**4ag**)] / 1211.69 mg (**4ag**) = 1.4

β-Azidation of **1b** and consecutive CuAAC with **3g**:

E-factor = [701.10 mg (**1b**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 648.96 mg (**3g**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1413.91 mg (**4bg**)] / 1413.91 mg (**4bg**) = 1.1

β-Azidation of **1a** and consecutive CuAAC with **3h**:

E-factor = [560.85 mg (**1a**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 492.84 mg (**3h**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1101.49 mg (**4ah**)] / 1101.49 mg (**4ah**) = 1.5

β-Azidation of **1b** and consecutive CuAAC with **3h**:

E-factor = [701.10 mg (**1b**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 492.84 mg (**3h**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1235.13 mg (**4bh**)] / 1235.13 mg (**4bh**) = 1.3

β-Azidation of **1a** and consecutive CuAAC with **3i**:

E-factor = [560.85 mg (**1a**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 661.20 mg (**3i**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1166.45 mg (**4ai**)] / 1166.45 mg (**4ai**) = 1.5

β-Azidation of **1b** and consecutive CuAAC with **3i**:

E-factor = [701.10 mg (**1b**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 661.20 mg (**3i**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1290.39 mg (**4ai**)] / 1290.39 mg (**4ai**) = 1.3

β-Azidation of **1a** and consecutive CuAAC with **3j**:

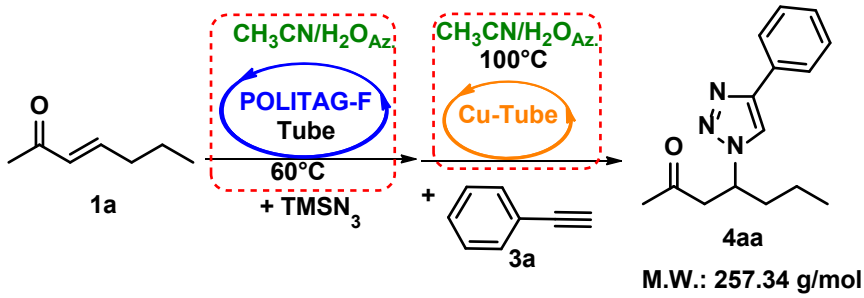
E-factor = [560.85 mg (**1a**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 649.08 mg (**3j**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1092.83 mg (**4aj**)] / 1092.83 mg (**4aj**) = 1.6

β-Azidation of **1b** and consecutive CuAAC with **3j**:

E-factor = [701.10 mg (**1b**) + 90.05 mg (H_2O) + 587.57 mg ($TMSN_3$) + 649.08 mg (**3j**) + 980.00 mg ($CH_3CN/H2O_{Az.}$ not recovered) – 1354.97 mg (**4bj**)] / 1354.97 mg (**4bj**) = 1.2

5. Characterization data

Chem. Name	4-(4-phenyl-1H-1,2,3-triazol-1-yl)heptan-2-one (4aa)



METHOD:

The mixture of **1a** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of phenylacetylene **3a** (1.2 eq) in CH_3CN:H_2O azeotrope continuously pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

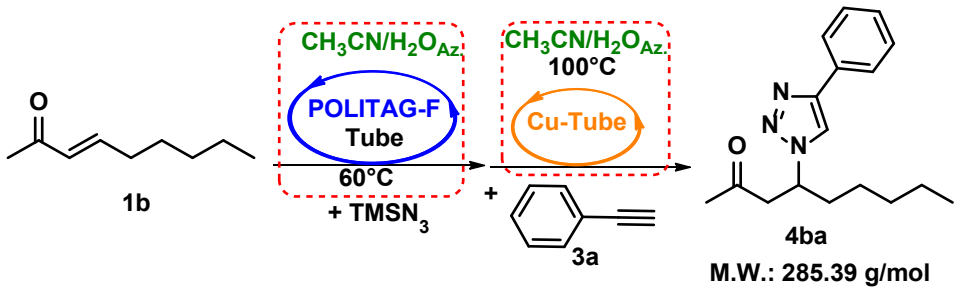
The azeotrope was recovered by distillation affording in **4aa** pure product as white solid (1.248 g, 97 % yield, >98% NMR purity).

Mol Formula		$C_{15}H_{19}N_3O$		m. p.	68-71 °C
^{1}H NMR (400 MHz, DMSO-d_6)	δ Value	No. H	Mult.	j Value/Hz	
	8.65	1	*s*		
	7.83	2	*d*	7.6	
	7.44	2	*t*	7.6	
	7.32	1	*t*	7.5	
	4.97-4.95	2	*m*		
	3.32-3.35	1	*m*		
	3.13	1	*dd*	17.8-5.4	
	2.09	3	*s*		
	1.85-1.74	1	*m*		
	1-17-1.13	1	*m*		
	1.10-1.05	1	*m*		
	0.83	3	*t*	7.4	

^{13}C NMR (100.6 MHz, DMSO-d_6) δ : 205.4, 145.9, 130.8, 128.9, 127.8, 125.0, 120.7, 56.3, 47.4, 36.9, 29.9, 18.4, 13.3

GC-EIMS (m/z, %): 257 (M^+, 40); 186 (27); 145 (70); 118 (23); 117 (100); 116 (80); 113 (24); 91 (21); 90 (21); 89 (32).

Chem. Name	4-(4-phenyl-1H-1,2,3-triazol-1-yl)nonan-2-one (4ba)



METHOD:

The mixture of **1b** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of phenylacetylene **3a** (1.2 eq) in CH_3CN:H_2O azeotrope continuously pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

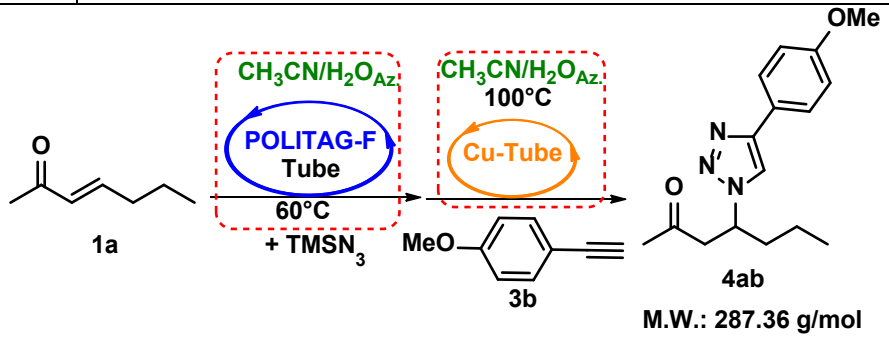
The azeotrope was recovered by distillation affording in **4ba** pure product as white solid (1.384 g, 97 % yield).

Mol Formula		$C_{17}H_{23}N_3O$		**m. p.**	64-67 °C
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**	
	7.83	2	*d*	7.5	
	7.79	1	*s*		
	7.41	2	*t*	7.4	
	7.33-7.30	1	*m*		
	4.96-4.89	1	*m*		
	3.42	1	*dd*	18.4-8.6	
	2.95	1	*dd*	18.0-4.4	
	2.12	3	*s*		
	2.09-2.04	1	*m*		
	1.88-1.82	1	*m*		
	1.30-1.20	5	*m*		
	1.13-1.11	1	*m*		
	0.86-0.84	3	*m*		

^{13}C NMR (100.6 MHz, $CDCl_3$) δ : 205.4, 147.0, 130.8, 128.9, 128.2, 125.8, 120.7, 57.3, 48.4, 35.3, 31.3, 30.6, 25.7, 22.5, 14.1

GC-EIMS (m/z, %): 285 (M^+, 43); 242 (28); 186 (36); 144 (22), 123 (27); 118 (100); 116 (76); 102 (28); 91 (19); 90 (22); 43 (89).

Chem. Name	4-(4-(4-methoxyphenyl)-1H-1,2,3-triazol-1-yl)heptan-2-one



M.W.: 287.36 g/mol

METHOD:

The mixture of **1a** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of 1-ethynyl-4-methoxybenzene **3b** (1.2 eq) in CH_3CN:H_2O azeotrope continuously pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

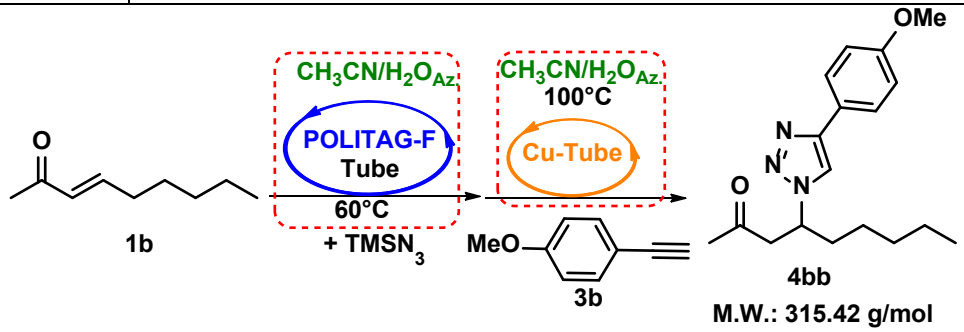
The azeotrope was recovered by distillation affording in **4ba** pure product as white solid (1.408 g, 98 % yield).

Mol Formula	$C_{16}H_{21}N_3O_2$		m. p.	104-107 °C
^{1}H NMR (400 MHz, DMSO-d_6)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**
	8.52	1	*s*	
	7.75	2	*d*	8.7
	7.70	2	*d*	8.7
	4.97-4.90	1	*m*	
	3.78	3	*s*	
	3.27	1	*dd*	17.9-8.3
	3.12	1	*dd*	17.7-5.3
	2.08	3	*s*	.
	1.87-1.71	2	*m*	
	1.18-1.09	1	*m*	
	1.08-1.01	1	*m*	
	1.83	3	*t*	7.3

^{13}C NMR (100.6 MHz, DMSO-d_6) δ : 205.5, 158.9, 145.9, 126.4, 123.5, 119.7, 114.3, 56.2, 55.1, 47.4, 36.9, 30.0, 18.4, 13.3

GC-EIMS (m/z, %): 287 (M^+,75); 244 (97); 216 (98); 202 (25); 189 (33); 188 (28); 175 (22); 174 (20); 173 (27); 158 (23); 147 (100); 146 (78); 133 (32); 132 (80); 121 (23); 119 (23); 117 (20); 89 (22).

Chem. Name	4-(4-(4-methoxyphenyl)-1H-1,2,3-triazol-1-yl)nonan-2-one



METHOD:

The mixture of **1b** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of 1-ethynyl-4-methoxybenzene **3b** (1.2 eq) in CH_3CN:H_2O azeotrope continuously pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

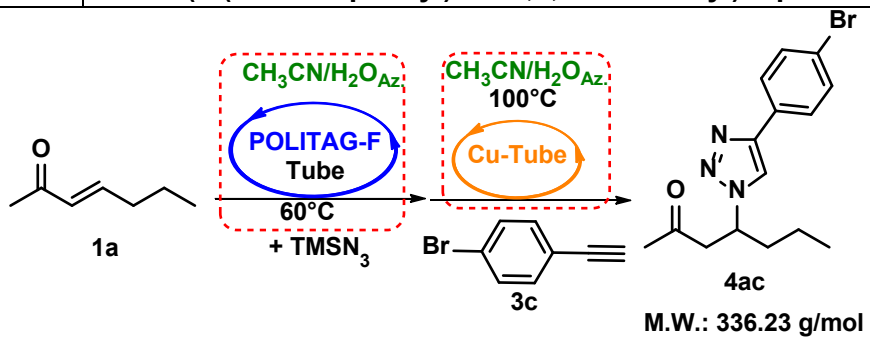
The azeotrope was recovered by distillation affording in **4ba** pure product as white solid (1.546 g, 98 % yield, 95% NMR purity).

Mol Formula	$C_{18}H_{25}N_3O_2$		**m. p.**	99-103 °C
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**
	7.75	2	*d*	8.6
	7.70	1	*s*	
	6.95	2	*d*	8.7
	4.94-4.88	1	*m*	
	3.84	3	*s*	
	3.41	1	*dd*	17.9-8.3
	2.94	1	*dd*	17.8-4.7
	2.12	3	*s*	
	2.08-2.01	1	*m*	
	1.88-1.80	1	*m*	
	1.27-1.20	5	*m*	
	1.17-1.04	1	*m*	
	0.84	3	*t*	6.3

^{13}C NMR (100.6 MHz, $CDCl_3$) δ: 205.5; 159.7; 146.9; 127.1; 123.5; 119.9; 114.3; 57.3; 55.5; 48.4; 35.3; 31.3; 30.6; 25.7; 22.5; 14.1.

GC-EIMS (m/z, %): 315 (M^+, 72); 272 (67); 244 (33); 231 (20); 230 (23); 229 (33); 216 (51); 207 (27); 189 (23); 188 (48); 176 (25); 175 (100); 174 (29); 160 (37); 159 (20); 148 (28); 147 (90); 146 (42); 133 (48); 132 (94); 125 (28); 121 (23); 119 (23); 104 (27); 97 (29); 89 (20); 83 (21); 77 (25), 69 (27); 68 (24); 55 (47).

Chem. Name	4-(4-(4-bromophenyl)-1H-1,2,3-triazol-1-yl)heptan-2-one (4ac)



METHOD:

The mixture of **1a** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of 1-bromol-4-ethynylbenzene **3c** (1.2 eq) in CH_3CN:H_2O azeotrope continuously pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

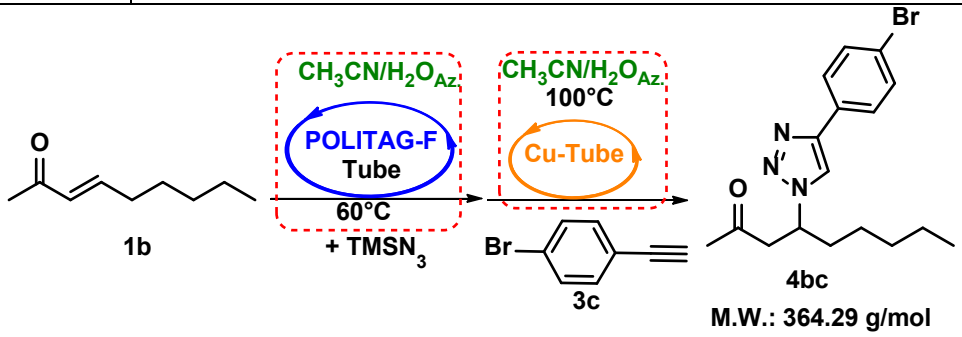
The azeotrope was recovered by distillation affording in **4ac** pure product as white solid (1.648 g, 98 % yield).

Mol Formula		$C_{15}H_{18}BrN_3O$		**m. p.**	118-122 °C
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**	
	7.80	1	*s*		
	7.70	2	*d*	8.4	
	7.53	2	*d*	8.4	
	4.97-4.90	1	*m*		
	3.43	1	*dd*	18.0-8.6	
	2.95	1	*dd*	18.0-4.7	
	2.12	3	*s*		
	2.09-2.02	1	*m*		
	1.87-1.78	1	*m*		
	1.31-1.10	2	*m*		
	0.90	3	*t*	7.3	

^{13}C NMR (100.6 MHz, $CDCl_3$) δ : 205.3; 146.0; 132.1; 129.8; 127.3; 122.0; 120.9; 57.1; 48.3; 37.3; 30.5; 19.3; 13.6

GC-EIMS (m/z, %): 336 (M^+, <1); 335 (71); 294 (41); 292 (37); 266 (54); 264 (53); 237 (20); 224 (21); 223 (25); 197 (94); 196 (99); 195 (100); 194 (85); 182 (31); 180 (26); 169 (38); 167 (27); 143 (27); 116 (40); 115 (44); 114 (25); 113 (52); 102 (20); 101 (36); 89 (37); 88 (26).

Chem. Name	4-(4-(4-bromophenyl)-1H-1,2,3-triazol-1-yl)nonan-2-one (4bc)



METHOD:

The mixture of **1b** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of 1-bromol-4-ethynylbenzene **3c** (1.2 eq) in CH_3CN:H_2O azeotrope continuously pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

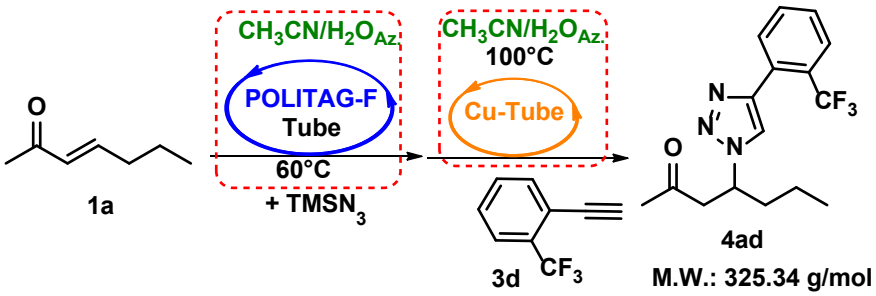
The azeotrope was recovered by distillation affording in **4bc** pure product as white solid (1.784 g, 98 % yield, 96% NMR purity).

Mol Formula	$C_{17}H_{22}BrN_3O$		**m. p.**	118-122 °C
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**
	7.80	1	*s*	
	7.70	2	*d*	8.1
	7.53	2	*d*	8.2
	4.95-4.88	1	*m*	
	3.41	1	*dd*	18.4-8.6
	2.95	1	*dd*	18.1-4.3
	2.12	3	*s*	
	2.08-2.03	1	*m*	
	1.87-1.81	1	*m*	
	1.29-1.17	5	*m*	
	1.15-1.10	1	*m*	
	0.85-0.83	3	*m*	

^{13}C NMR (100.6 MHz, CD) δ: 205.3; 146.0; 132.0; 129.8; 127.3; 122.0; 120.8; 57.4; 48.3; 35.2; 31.3; 30.5; 25.7; 22.5; 14.0

GC-EIMS (m/z, %): 366 (M+2, 25); 365 (M+1, 58); 364 (M^+, < 1); 363 (75); 322 (33); 320 (63); 291 (27); 281 (30); 278 (24); 266 (42); 264 (54); 239 (26); 238 (56); 237 (26); 236 (31); 226 (20); 225 (57); 224 (21); 223 (58); 221 (25); 209 (21); 208 (20); 207 (40); 198 (26); 197 (64); 196 (100); 195 (85); 194 (56); 182 (27); 181 (24); 180 (29); 171 (20); 169 (47); 168 (24); 166 (23); 143 (22); 128 (25); 123 (77); 117 (20); 116 (35); 115 (41); 114 (21); 101 (25); 88 (25); 81 (23); 55 (25)

Chem. Name	4-(4-(2-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-1-yl)heptan-2-one



METHOD:

The mixture of **1a** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of 1-ethynyl-2-(trifluoromethyl)benzene **3d** (1.2 eq) in CH_3CN:H_2O azeotrope pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

The azeotrope was recovered by distillation affording in **4ad** pure product as oil (1.496 g, 92 % yield).

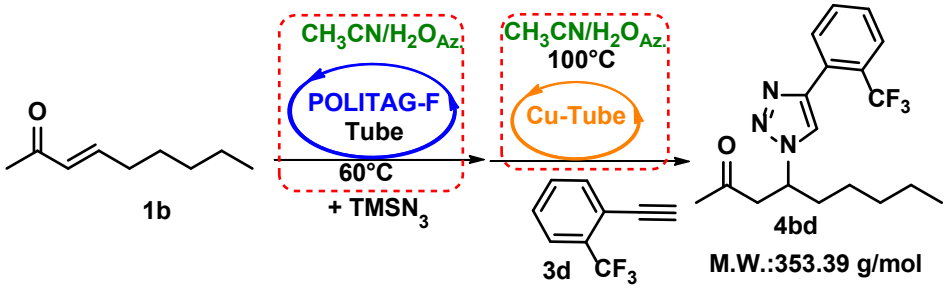
Mol Formula		$C_{16}H_{18}F_3N_3O$		**m. p.**	Oil
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**	
	7.94	1	*d*	7.8	
	7.78	1	*s*		
	7.74	1	*d*	7.9	
	7.61	1	*t*	7.4	
	7.46	1	*t*	7.9	
	4.99-4.92	1	*m*		
	3.43	1	*dd*	17.9-8.2	
	2.98	1	*dd*	17.9-4.9	
	2.13	3	*s*		
	2.08-2.03	1	*m*		
	1.87-1.78	1	*m*		
	1.26-1.10	2	*m*		
	0.90	3	*t*	7.3	

^{13}C NMR (100.6 MHz, CD) δ : 205.1; 143.5; 132.0; 131.7; 129.7; 128.2; 127.4 (*q*, J_{C-F}= 30.3); 126.1(*q*, J_{C-F}= 5.6); 124.2 (*q*, J_{C-F}= 273.3), 123.8 (*q*, J_{C-F}= 5.6); 57.0; 48.2; 37.2; 30.4; 19.0; 13.4

^{19}F NMR (100.6 MHz, CD) δ: -58.74

GC-EIMS (m/z, %): 325 (M^+, 50); 282 (40); 255 (27); 254 (62); 240 (27); 194 (27); 185 (69); 184 (94); 172 (20); 169 (45); 166 (40); 165 (100); 164 (72); 151 (54); 134 (31); 113 (62).

Chem. Name	4-(4-(2-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-1-yl)nonan-2-one



METHOD:

The mixture of **1b** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of 1-ethynyl-2-(trifluoromethyl)benzene **3d** (1.2 eq) in CH_3CN:H_2O azeotrope pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

The azeotrope was recovered by distillation affording in **4bd** pure product as oil (1.730 g, 98 % yield).

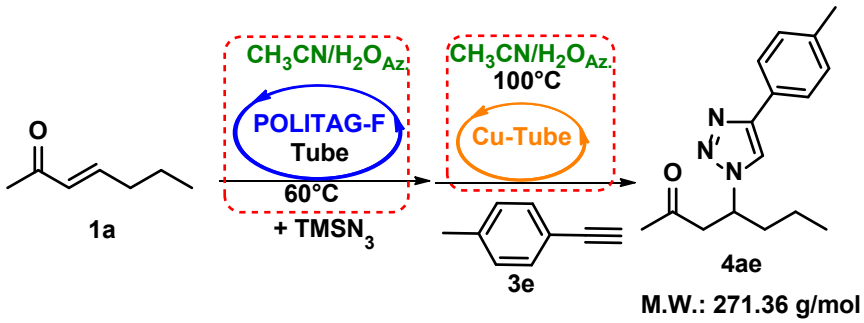
Mol Formula	$C_{18}H_{22}F_3N_3O$		m. p.	Oil
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**
	7.91	1	*d*	7.8
	7.77	1	*s*	
	7.71	1	*d*	7.7
	7.59	1	*t*	7.5
	7.44	1	*t*	7.7
	4.95-4.90	1	*m*	
	3.40	1	*dd*	18.0-8.4
	2.96	1	*dd*	18.1-4.7
	2.10	3	*s*	
	2.07-2.04	1	*m*	
	1.88-1.82	1	*m*	
	1.25-1.20	5	*m*	
	1.11-1.08	1	*m*	
	0.84-0.80	3	*m*	

^{13}C NMR (100.6 MHz, CD) δ: 205.2; 143.5; 132.0, 131.8, 129.7, 127.7 (*q*, J_{C-F}= 30.3), 128.3, 126.3 (q, J_{C-F}= 272.9), 126.2, 124.0, 57.4, 48.3, 35.3, 31.2, 30.5, 25.5, 22.4, 13.9

^{19}F NMR (100.6 MHz, CD) δ: -58.73

GC-EIMS (m/z, %): 353 (M^+, < 1); 325 (38); 282 (41); 255 (26); 254 (62); 240 (29); 214 (21); 213 (29); 194 (34); 185 (69); 184 (91); 172 (20); 169 (40); 167 (20); 166 (42); 165 (100); 164 (72); 151 (55); 138 (20); 134 (34); 113 (74); 55 (22).

Chem. Name	4-(4-(p-tolyl)-1H-1,2,3-triazol-1-yl)heptan-2-one



METHOD:

The mixture of **1a** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of 1-ethynyl-4-methylbenzene **3e** (1.2 eq) in CH_3CN:H_2O azeotrope pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

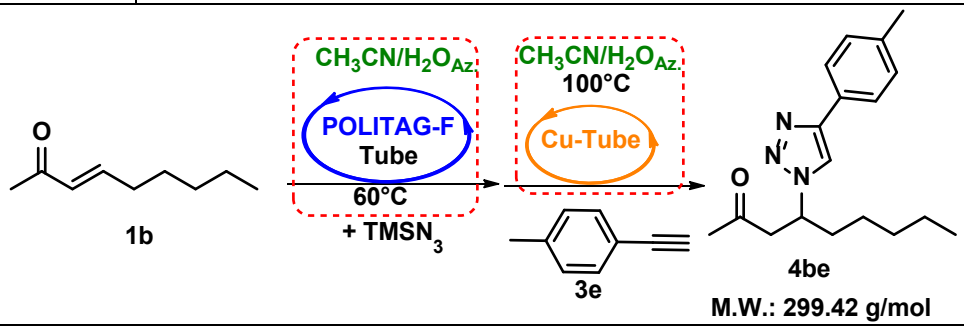
The azeotrope was recovered by distillation affording in **4ae** pure product as white solid (1.249 g, 92 % yield, 95% NMR purity)

Mol Formula		$C_{16}H_{21}N_3O$		**m. p.**	129-131 °C
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**	
	7.75	1	*s*		
	7.71	1	*d*	7.4	
	7.22	2	*d*	7.5	
	4.95-4.93	1	*m*		
	3.42	1	*dd*	18.0-8.5	
	2.94	1	*dd*	18.1-4.1	
	2.37	3	*s*		
	2.12	3	*s*		
	2.07-2.01	1	*m*		
	1.84-1.79	1	*m*		
	1.25-1.18	2	*m*		
	0.90	3	*t*	7.2	

^{13}C NMR (100.6 MHz, $CDCl_3$) δ: 205.4; 147.1; 138.0; 129.6; 128.0; 125.7; 120.3; 57.0; 48.4; 37.3; 30.6; 21.4; 19.3; 13.6

GC-EIMS (m/z, %): 271 (M^+, 52); 228 (28); 200 (39); 131 (100); 130 (55); 115 (31); 103 (25).

Chem. Name	4-(4-(p-tolyl)-1H-1,2,3-triazol-1-yl)nonan-2-one



METHOD:

The mixture of **1b** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of 1-ethynyl-4-methylbenzene **3e** (1.2 eq) in CH_3CN:H_2O azeotrope pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

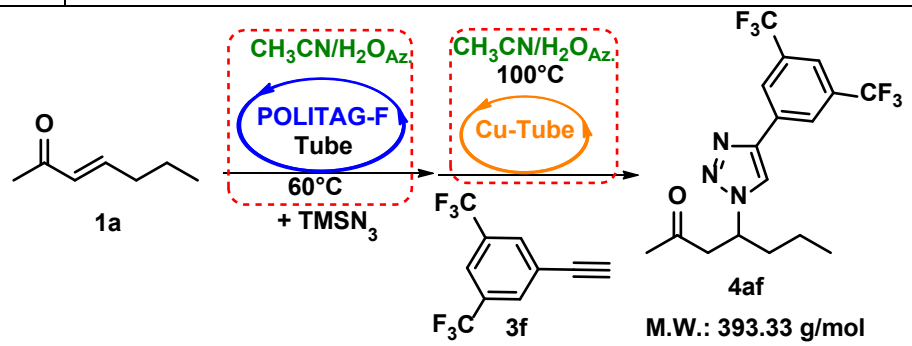
The azeotrope was recovered by distillation affording in **4be** pure product as white solid (1.482 g, 99 % yield)

Mol Formula	$C_{18}H_{25}N_3O$		**m. p.**	90-93 °C
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**
	7.75	1	*s*	
	7.71	2	*d*	8.0
	7.22	2	*d*	7.8
	4.95-4.88	1	*m*	
	3.42	1	*dd*	17.9-8.5
	2.95	1	*dd*	17.9-4.6
	2.37	3	*s*	
	2.12	3	*s*	
	2.08-2.04	1	*m*	
	1.89-1.80	1	*m*	
	1.26-1.20	5	*m*	
	1.16-1.11	1	*m*	
	0.86-0.84	3	*m*	

^{13}C NMR (100.6 MHz, $CDCl_3$) δ: 205.4; 147.1; 138.0; 129.6; 128.0; 125.7; 120.3; 57.3; 48.4; 35.3; 31.3; 30.6; 25.7; 22.5; 21.4; 14.1.

GC-EIMS (m/z, %): 299 (M^+, 47); 256 (36); 200 (32); 131 (100); 130 (48); 115 (28).

Chem. Name	4-(4-(3,5-bis(trifluoromethyl)phenyl)-1H-1,2,3-triazol-1-yl)heptan-2-one



METHOD:

The mixture of **1a** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of 1-ethynyl-3,5-bis(trifluoromethyl)benzene **3f** (1.2 eq) in CH_3CN:H_2O azeotrope pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

The azeotrope was recovered by distillation affording in **4af** pure product as white solid (1.908 g, 97 % yield)

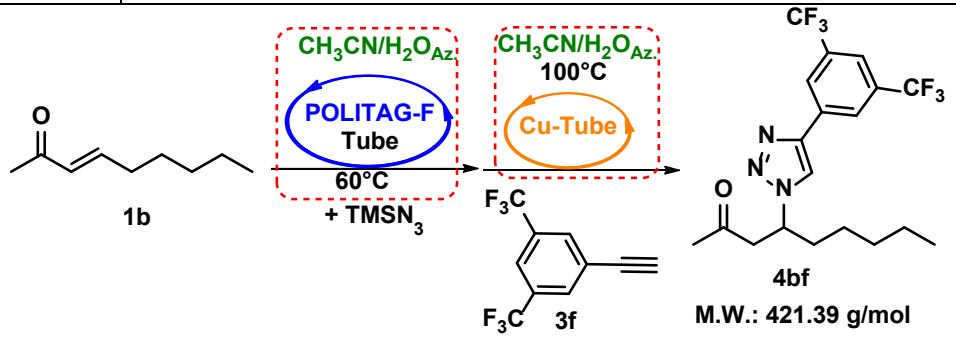
Mol Formula	$C_{17}H_{17}F_6N_3O$		**m. p.**	80-82 °C
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**
	8.27	2	*s*	
	7.98	1	*s*	
	7.80	1	*s*	
	5.00-4.95	1	*m*	
	3.46	1	*dd*	18.4-9.1
	2.97	1	*dd*	18.3-4.2
	2.13	3	*s*	
	2.12-2.06	1	*m*	
	1.89-1.80	1	*m*	
	1.30-1.18	2	*m*	
	0.91	3	*t*	7.5

^{13}C NMR (100.6 MHz, $CDCl_3$) δ: 205.2; 144.3; 133.0; 132.3 (*q*, J_{C-F}= 33.4), 125.7, 123.4 (*q*, J_{C-F}= 272.9), 122.0; 121.5 (q, J_{C-F}= 3.8); 57.4; 48.2; 37.1; 30.4; 19.3; 13.5.

^{19}F NMR (100.6 MHz, CD) δ: -63.04

GC-EIMS (m/z, %): 394 (M+1, 21); 393 (M^+, 83); 374 (87); 350 (76); 323 (22); 322 (88); 308 (40); 295 (24); 294 (31); 282 (30); 253 (51); 252 (100); 233 (20); 169 (21); 113 (22).

Chem. Name	4-(4-(3,5-bis(trifluoromethyl)phenyl)-1H-1,2,3-triazol-1-yl)nonan-2-one



METHOD:

The mixture of **1b** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of 1-ethynyl-3,5-bis(trifluoromethyl)benzene **3f** (1.2 eq) in CH_3CN:H_2O azeotrope pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm. The azeotrope was recovered by distillation affording in **4bf** pure product as white solid (2.021 g, 96 % yield).

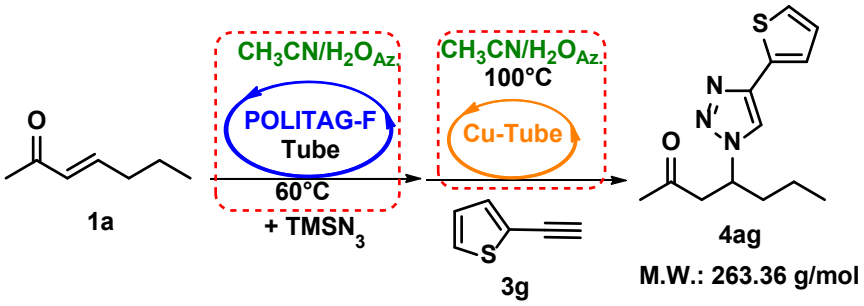
Mol Formula	$C_{19}H_{21}F_6N_3O$		**m. p.**	95-97 °C
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**
	8.28	2	*s*	
	7.98	1	*s*	
	7.81	1	*s*	
	5.01-4.90	1	*m*	
	3.45	1	*dd*	18.6-8.8
	2.97	1	*dd*	18.2-4.1
	2.18-2.03	4	*m*	
	1.94-1.82	1	*m*	
	1.38-1.19	5	*m*	
	1.18-1.03	1	*m*	
	0.89-0.79	3	*m*	

^{13}C NMR (100.6 MHz, $CDCl_3$) δ: 205.2; 144.3; 133.0, 132.3 (*q*, J_{C-F}= 33.5), 125.7, 123.4 (*q*, J_{C-F}= 272.9) 122.0, 121.5 (*q*, J_{C-F}= 3.8), 57.7, 48.3, 35.1, 31.3, 30.4, 25.7, 22.5, 14.0.

^{19}F NMR (100.6 MHz, CD) δ: -63.00

GC-EIMS (m/z, %): 422 (M+1, 24); 421 (M^+, 13); 402 (59); 401 (47); 392 (50); 378 (71); 365 (30); 364 (52); 349 (56); 336 (37); 333 (23); 324 (22); 322 (66); 321 (33); 308 (54); 307 (43); 306 (41); 294 (44); 293 (21); 292 (31); 282 (56); 281 (37); 280 (79); 279 (38); 264 (20); 254 (32); 253 (54); 252 (89); 240 (45); 238 (24); 234 (32); 233 (32); 225 (29); 202 (24); 170 (26); 169 (40); 168 (100);); 123 (31).

Chem. Name	4-(4-(thiophen-3-yl)-1H-1,2,3-triazol-1-yl)heptan-2-one



METHOD:

The mixture of **1a** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of 3-ethynyltiophene **3g** (1.2 eq) in CH_3CN:H_2O azeotrope pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

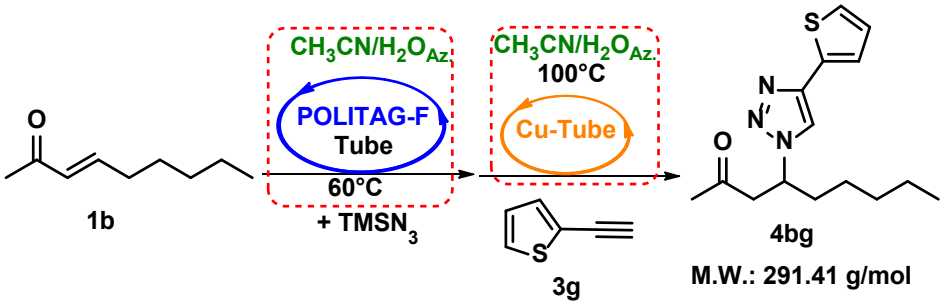
The azeotrope was recovered by distillation affording in **4ag** pure product as white solid (1.212 g, 92 % yield)

Mol Formula	$C_{13}H_{17}N_3OS$		**m. p.**	87-89 °C
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**
	7.69	1	*s*	
	7.67-7.65	1	*m*	
	7.45	1	*d*	4.8
	7.38	1	*d*	4.9
	4.96-4.89	1	*m*	
	3.42	1	*dd*	17.9-8.6
	2.94	1	*dd*	18.0-4.6
	2.12	3	*s*	
	2.09-2.02	1	*m*	
	1.87-1.76	1	*m*	
	1.30-1.10	2	*m*	
	0.90	3	*t*	7.1

^{13}C NMR (100.6 MHz, CD) δ: 205.4; 143.3; 132.0; 126.4; 125.9; 121.1; 120.5; 57.0; 48.4; 37.3; 30.6; 19.3; 13.6.

GC-EIMS (m/z, %): 263 (M^+, 96); 220 (51); 192 (60); 150 (20); 149 (20); 124 (21); 123 (100); 122 (79); 113 (21); 108 (21); 97 (21); 95 (22).

Chem. Name	4-(4-(thiophen-3-yl)-1H-1,2,3-triazol-1-yl)nonan-2-one



METHOD:

The mixture of **1b** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of 3-ethynyltiophene **3g** (1.2 eq) in CH_3CN:H_2O azeotrope pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

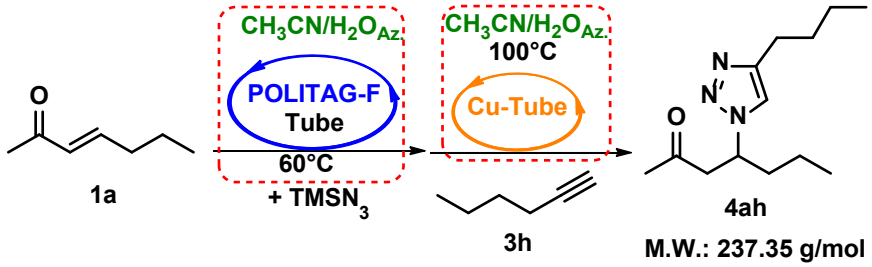
The azeotrope was recovered by distillation affording in **4bg** pure product as white solid (1.411 g, 97 % yield, 95% NMR purity).

Mol Formula	$C_{15}H_{21}N_3OS$		**m. p.**	60-62 °C
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**
	7.70	1	*s*	
	7.64	1	*s*	
	7.43	1	*d*	4.8
	7.34	1	*d*	4.8
	4.91-4.86	1	*m*	
	3.36	1	*dd*	17.9-8.5
	2.91	1	*dd*	17.9-4.6
	2.08	3	*s*	
	2.03-1.99	1	*m*	
	1.83-1.77	1	*m*	
	1.23-1.12	5	*m*	
	1.09-1.07	1	*m*	
	0.81-0.79	3	*m*	

^{13}C NMR (100.6 MHz, $CDCl_3$) δ: 205.4, 143.2, 132.0, 126.3, 125.9, 121.0, 120.5, 57.2, 48.4, 35.2, 31.3, 30.5, 25.6, 22.5, 14.0.

GC-EIMS (m/z, %): 291 (M^+, 52); 248 (46); 192 (65); 165 (26); 164 (23); 152 (25); 151 (85); 150 (21); 149 (20); 125 (31); 124 (24); 123 (100); 122 (66); 109 (23); 108 (20); 97 (44); 96 (28); 95 (32); 81 (23); 69 (22); 55 (31).

Chem. Name	4-(4-butyl-1H-1,2,3-triazol-1-yl)heptan-2-one



METHOD:

The mixture of **1a** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of hex-1-yne **3h** (1.2 eq) in CH_3CN:H_2O azeotrope pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

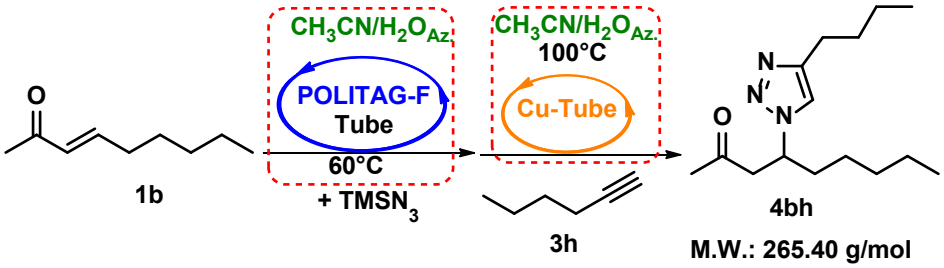
The azeotrope was recovered by distillation affording in **4ah** pure product as oil (1.101 g, 93 % yield, 95% NMR purity)

Mol Formula		$C_{13}H_{23}N_3O$		**m. p.**	Oil
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**	
	7.26	1	*s*		
	4.86-4.79	1	*m*		
	3.33	1	*dd*	17.8-8.3	
	2.88	1	*dd*	17.7-4.9	
	2.66	2	*t*	7.7	
	2.08	3	*s*		
	2.00-0.91	1	*m*		
	1.79-1.70	1	*m*		
	1.61	2	*t*	7.7	
	1.37-1.31	2	*m*		
	1.19-1.05	2	*m*		
	0.92-0.84	6	*m*		

^{13}C NMR (100.6 MHz, $CDCl_3$) δ : 205.4; 147.7; 121.5; 56.7; 48.4; 37.4; 31.6; 30.5; 25.4, 22.4, 19.2, 13.9, 13.6.

GC-EIMS (m/z, %): 238 (M^+, 46); 224 (24); 210 (39); 180 (29); 168 (28); 154 (23); 141 (36); 140 (28); 126 (28); 124 (23); 123 (61); 115 (23); 113 (28); 98 (100); 97 (27); 83 (53); 81 (25); 75 (27); 73 (72); 59 (25); 55 (32).

Chem. Name	4-(4-butyl-1H-1,2,3-triazol-1-yl)nonan-2-one



METHOD:

The mixture of **1b** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of hex-1-yne **3h** (1.2 eq) in CH_3CN:H_2O azeotrope pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

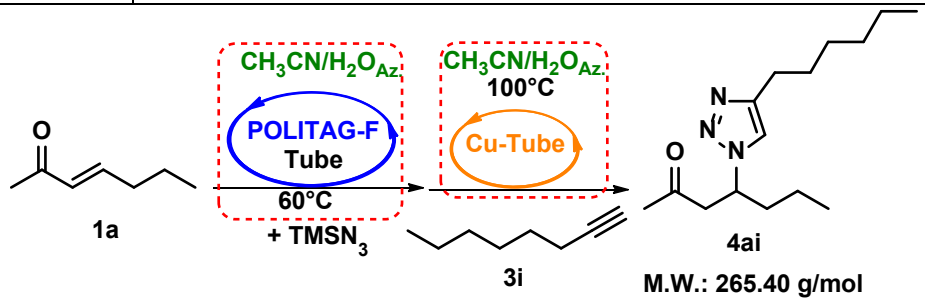
The azeotrope was recovered by distillation affording in **4bh** pure product as oil (1.235 g, 93 % yield).

Mol Formula	$C_{15}H_{27}N_3O$		m. p.	Oil
^{1}H NMR (400 MHz, $CDCl_3$)	δ Value	No. H	Mult.	j Value/Hz
	7.26	1	*s*	
	4.85-4.78	1	*m*	
	3.31	1	*dd*	17.7-8.2
	2.87	1	*dd*	17.7-4.7
	2.62	2	*t*	7.7
	2.06	3	*s*	
	2.05-1.90	1	*m*	
	1.77-1.69	1	*m*	
	1.62-1.57	2	*m*	
	1.34-1.20	6	*m*	
	1.12-1.02	2	*m*	
	0.86-0.81	6	*m*	

^{13}C NMR (100.6 MHz, CD) δ: 205.4; 147.7; 121.4; 56.6; 48.3; 37.3; 31.6; 30.4; 29.4; 28.9; 25.7; 22.6; 19.2; 14.1; 13.5.

GC-EIMS (m/z, %): 265 (M^+, 59); 222 (27); 208 (25); 194 (100); 180 (53); 167 (51); 166 (39); 152 (91); 136 (26); 124 (44); 113 (32); 110 (30); 97 (29); 96 (39); 95 (29); 94 (24); 83 (25); 82 (54); 80 (32); 67 (24); 55 (45); 54 (26).

Chem. Name	4-(4-hexyl-1H-1,2,3-triazol-1-yl)heptan-2-one



METHOD:

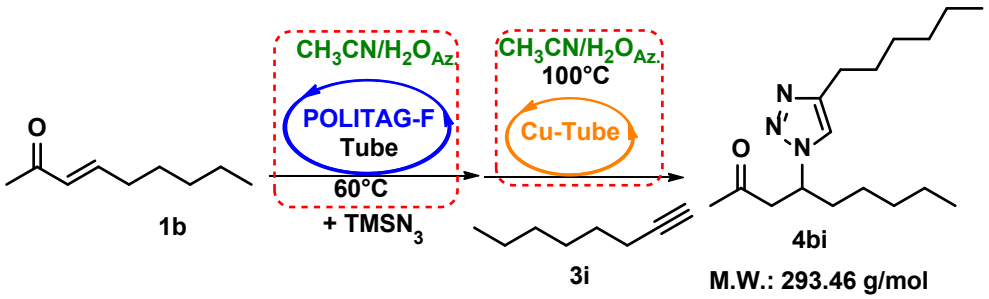
The mixture of **1a** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of oct-1-yne **3i** (1.2 eq) in CH_3CN:H_2O azeotrope pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.
The azeotrope was recovered by distillation affording in **4ai** pure product as oil (1.166 g, 88 % yield, 97% NMR purity).

Mol Formula		$C_{15}H_{27}N_3O$		**m. p.**	Oil
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**	
	7.26	1	*s*		
	4.86-4.79	1	*m*		
	3.32	1	*dd*	17.9-8.3	
	2.88	1	*dd*	18.1-4.7	
	2.66-2.63	2	*m*		
	2.07	3	*s*		
	1.99-1.91	1	*m*		
	1.78-1.70	1	*m*		
	1.65-1.58	2	*m*		
	1.30-1.21	6	*m*		
	1.18-1.07	2	*m*		
	0.87-0.83	6	*m*		

^{13}C NMR (100.6 MHz, $CDCl_3$) δ: 205.4, 128.8, 121.5, 56.6, 48.4, 37.4, 31.6, 30.5, 29.4, 29.0, 25.7, 22.6, 19.2, 14.1, 13.5.

GC-EIMS (m/z, %): 265 (M^+, 58); 222 (25); 208 (25); 195 (81); 180 (55); 166 (39), 152 (94); 136 (29); 124 (43); 113 (30); 110 (27); 97 (26); 96 (37); 95 (26); 94 (22); 83 (21); 82 (50); 80 (31); 67 (21); 55 (39); 54 (22).

Chem. Name	4-(4-hexyl-1H-1,2,3-triazol-1-yl)nonan-2-one



METHOD:

The mixture of **1b** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of oct-1-yne **3i** (1.2 eq) in CH_3CN:H_2O azeotrope pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

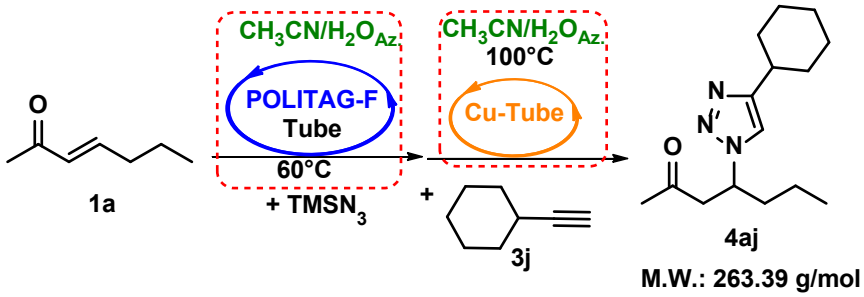
The azeotrope was recovered by distillation affording in **4bi** pure product as oil (1.290 g, 88 % yield, 95% NMR purity).

Mol Formula	$C_{17}H_{31}N_3O$		**m. p.**	Oil
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**
	7.29	1	*s*	
	4.86-4.82	1	*m*	
	3.36	1	*dd*	18.1-8.4
	2.92	1	*dd*	18.1-4.6
	2.70-2.67	3	*m*	
	2.11	3	*s*	
	2.03-1.97	1	*m*	
	184-1.80	1	*m*	
	1.67-1.63	2	*m*	
	1.39-1.30	7	*m*	
	1.27-1.23	5	*m*	
	0.88-0.84	6	*m*	

^{13}C NMR (100.6 MHz, CD) δ: 205.5, 147.7, 121.5, 56.9, 48.4, 35.3, 31.6, 31.2, 30.5, 29.4, 29.0, 25.7, 25.6, 22.6, 22.5, 14.1, 14.0

GC-EIMS (m/z, %): 293 (M^+, 57); 250 (37); 236 (59); 223 (67); 222 (100); 208 (52); 194 (55); 168 (20); 166 (25); 152 (76); 124 (29); 123 (50); 110 (20); 97 (28); 96 (27); 83 (47); 82 (46); 81 (35); 80 (27); 71 (22); 67 (24); 55 (58); 54 (25).

Chem. Name	4-(4-cyclohexyl-1H-1,2,3-triazol-1-yl)heptan-2-one
Lit. Ref.	



METHOD:

The mixture of **1a** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of ethynylcyclohexane **3j** (1.2 eq) in CH_3CN:H_2O azeotrope pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

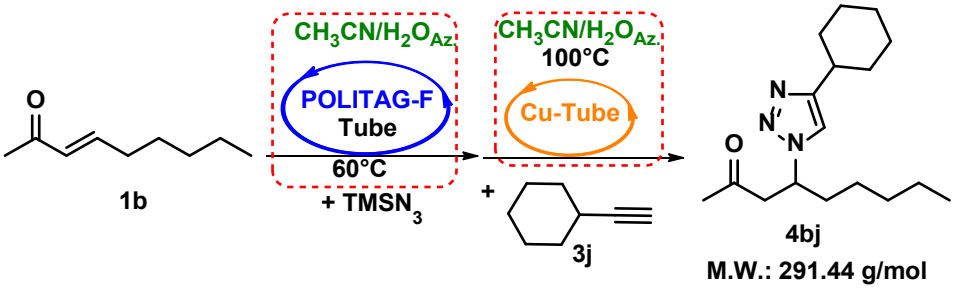
The azeotrope was recovered by distillation affording in **4aj** pure product as white solid (1.093 g, 83 % yield, 98% NMR purity).

Mol Formula	$C_{15}H_{25}N_3O$		m. p.	59-61 °C
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**
	7.24	1	*s*	
	4.86-4.81	1	*m*	
	3.35	1	*dd*	18.0-8.1
	2.90	1	*dd*	17.8-4.9
	2.72-2.65	1	*m*	
	2.10	3	*s*	
	2.08-2.05	2	*m*	
	2.04-1.93	1	*m*	
	1.83-1.79	3	*m*	
	1.79-1.69	1	*m*	
	1.40-1.35	4	*m*	
	1.22-1.16	2	*m*	
	1.15-1.09	1	*m*	
	0.89-0.84	3	*m*	

^{13}C NMR (100.6 MHz, CD) δ: 205.3; 153.0; 120.1; 56.7; 48.5; 37.5; 35.4; 33.1; 26.3; 26.2; 19.3; 13.6

GC-EIMS (m/z, %): 263 (M^+, 72); 207 (30); 192 (100); 178 (77); 164 (21); 150 (79); 148 (22); 134 (29); 122 (36); 113 (34); 106 (23); 95 (24); 94 (23); 67 (24); 55 (22).

Chem. Name	4-(4-cyclohexyl-1H-1,2,3-triazol-1-yl)nonan-2-one



METHOD:

The mixture of **1b** (5 mmol) and trimethylsilylazide (0.67 mL, 1.02 eq) in azeotrope CH_3CN:H_2O (1 mL, 5 M) was pumped through the PTFE reactor, thermostated at 60 °C, packed with **POLITAG-F** (2.0 g) and quartz powder (0.018 mL/min flow rate measured at the outlet of the first reactor). After a residence time of 3.8 h the resulting azide intermediate formed was mixed, through a T joint, with a 1.2 M solution of ethynylcyclohexane **3j** (1.2 eq) in CH_3CN:H_2O azeotrope pumped at 0.1 mL/min. This mixture was passed in a CTFR heated at 100 °C with a BPR of 10 atm.

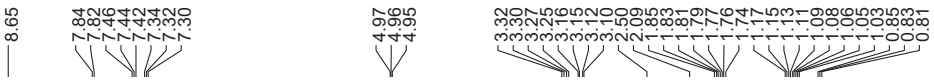
The azeotrope was recovered by distillation affording in **4bj** pure product as white solid (1.355 g, 93 % yield, 95% NMR purity).

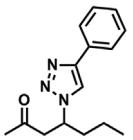
Mol Formula		$C_{17}H_{29}N_3O$		**m. p.**	Oil
^{1}H NMR (400 MHz, $CDCl_3$)	**δ Value**	**No. H**	**Mult.**	**j Value/Hz**	
	7.28	1	*s*		
	4.87-4.80	1	*m*		
	1.36	1	*dd*	18.4-8.2	
	2.92	1	*dd*	17.8-4.8	
	2.76-7.72	1	*m*		
	2.11	3	*s*		
	2.06-2.02	2	*m*		
	2.01-1.94	1	*m*		
	1.83-1.80	3	*m*		
	1.74-1.71	1	*m*		
	1.42-1.37	4	*m*		
	1.22-1.17	6	*m*		
	1.08-1.05	1	*m*		
	0.85-0.82	3	*m*		

^{13}C NMR (100.6 MHz, $CDCl_3$) δ: 205.6, 153.0, 120.1, 56.9, 48.4, 35.3, 35.1, 31.2, 30.5, 26.2, 26.2, 25.6, 22.5, 14.0

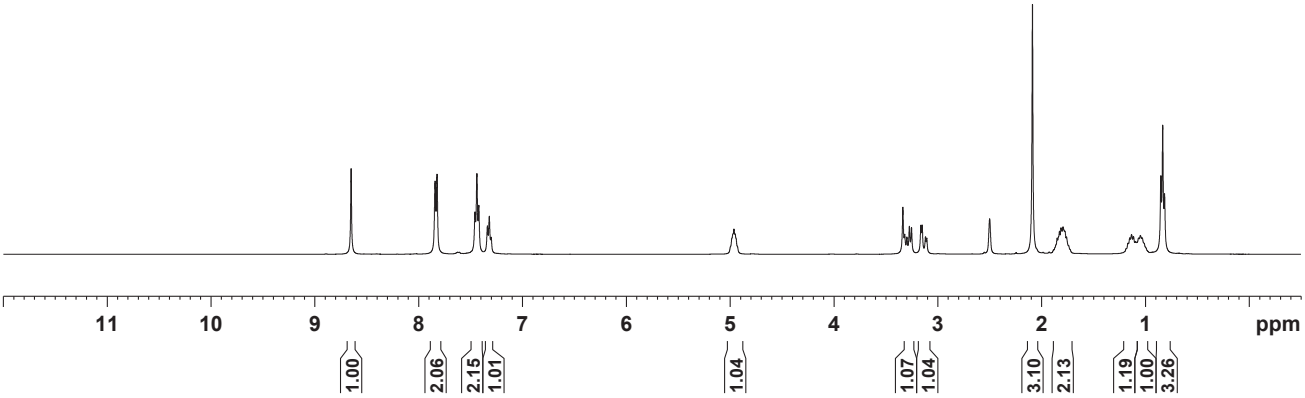
GC-EIMS (m/z, %): 285 (43); 242 (28); 186 (36); 144 (22); 116 (76); 102 (28); 90 (22); 89 (43).

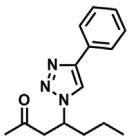
6. NMR copies



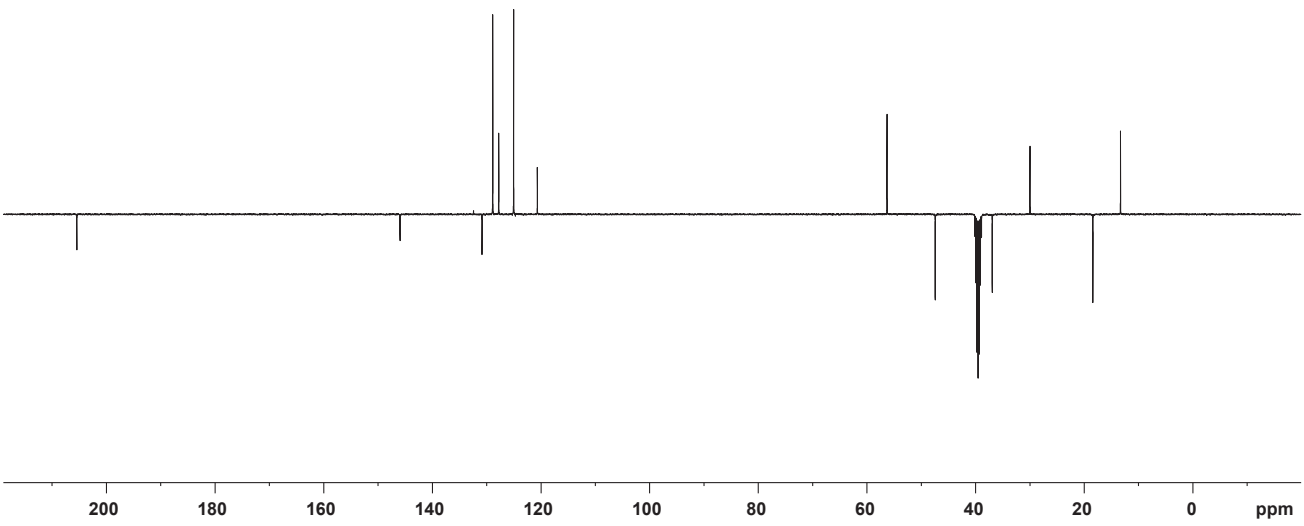


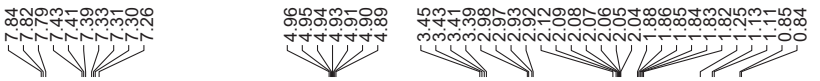
4-(4-phenyl-1*H*-1,2,3-triazol-1-yl)heptan-2-one
4aa

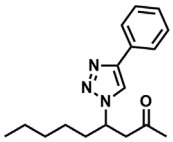




4-(4-phenyl-1*H*-1,2,3-triazol-1-yl)heptan-2-one
4aa

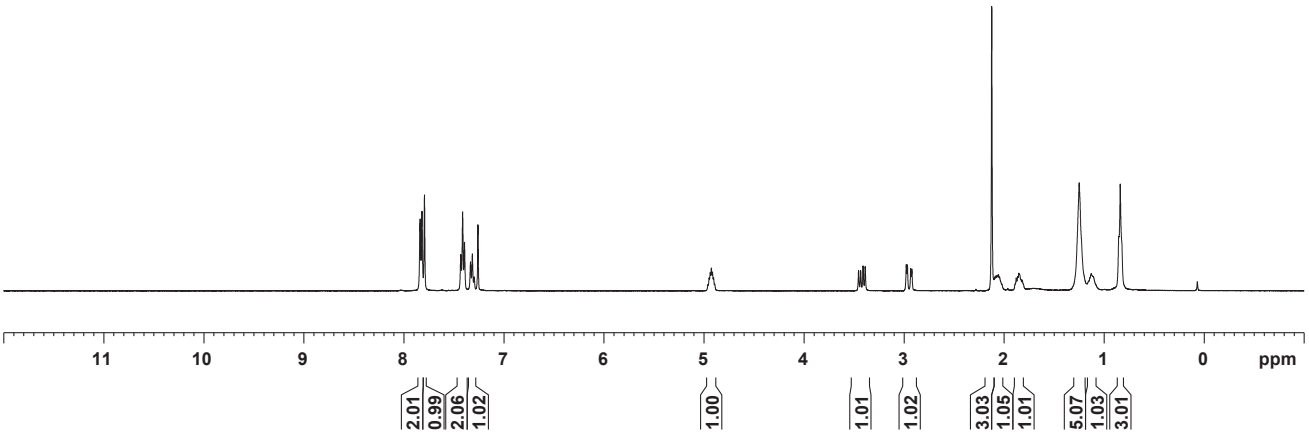


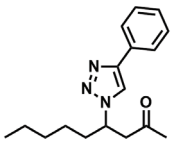




4-(4-phenyl-1*H*-1,2,3-triazol-1-yl)nonan-2-one

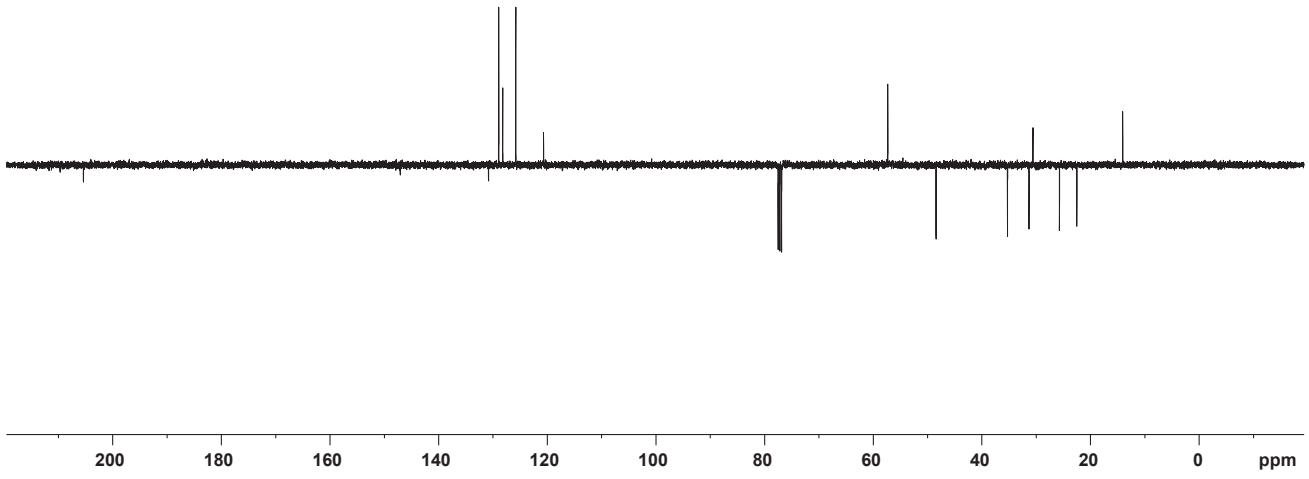
4ba

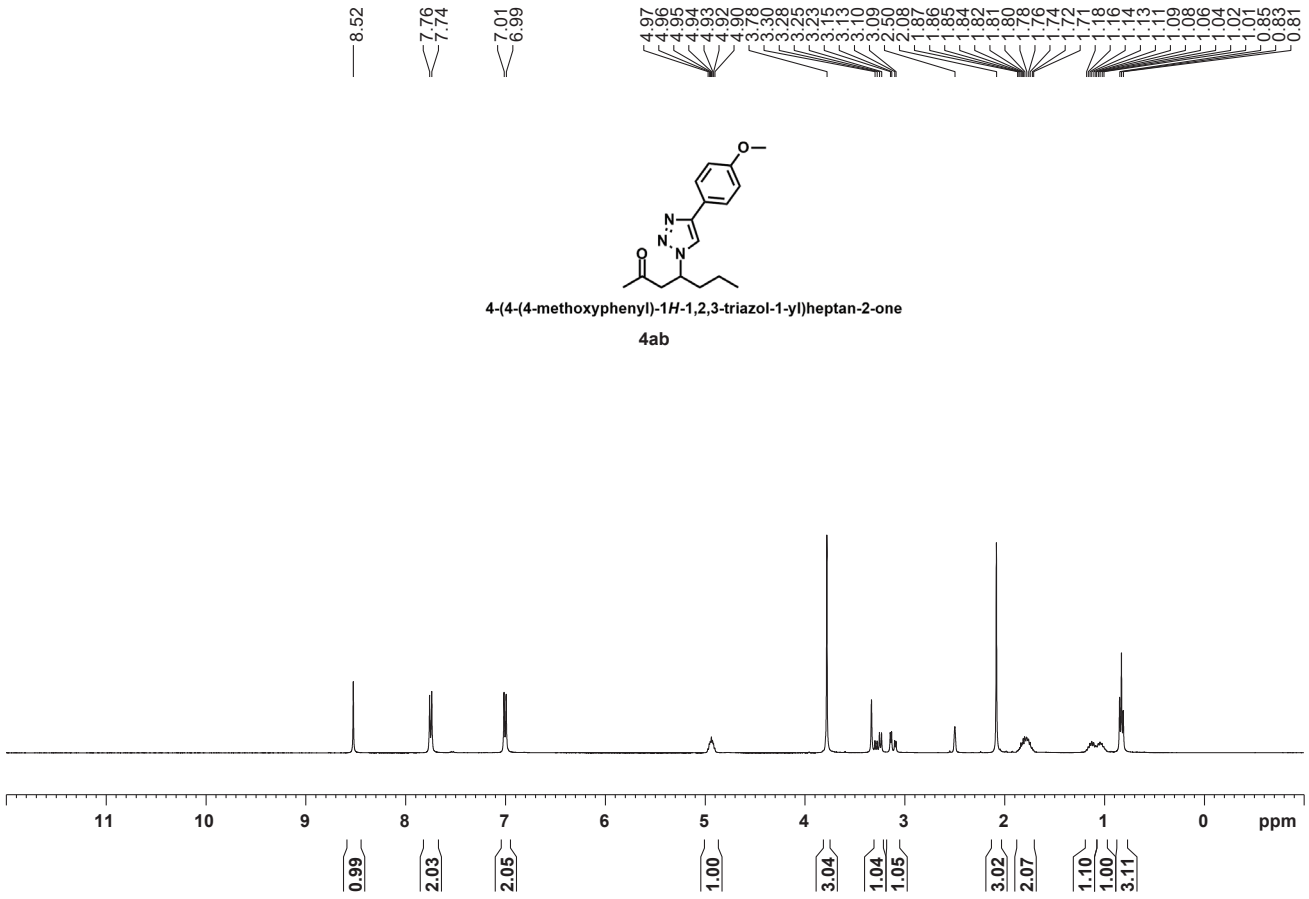




4-(4-phenyl-1*H*-1,2,3-triazol-1-yl)nonan-2-one

4ba

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4.95
4.94
4.93
4.92
4.90
3.78
3.30
3.28
3.25
3.23
3.15
3.13
3.10
3.09
2.50
2.08
1.87
1.86
1.85
1.84
1.82
1.81
1.80
1.78
1.76
1.74
1.72
1.71
1.18
1.16
1.14
1.13
1.11
1.09
1.08
1.06
1.04
1.02
1.01
0.85
0.83
0.81
O
N
N
N
O
4-(4-(4-methoxyphenyl)-1H-1,2,3-triazol-1-yl)heptan-2-one
4ab
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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1.05
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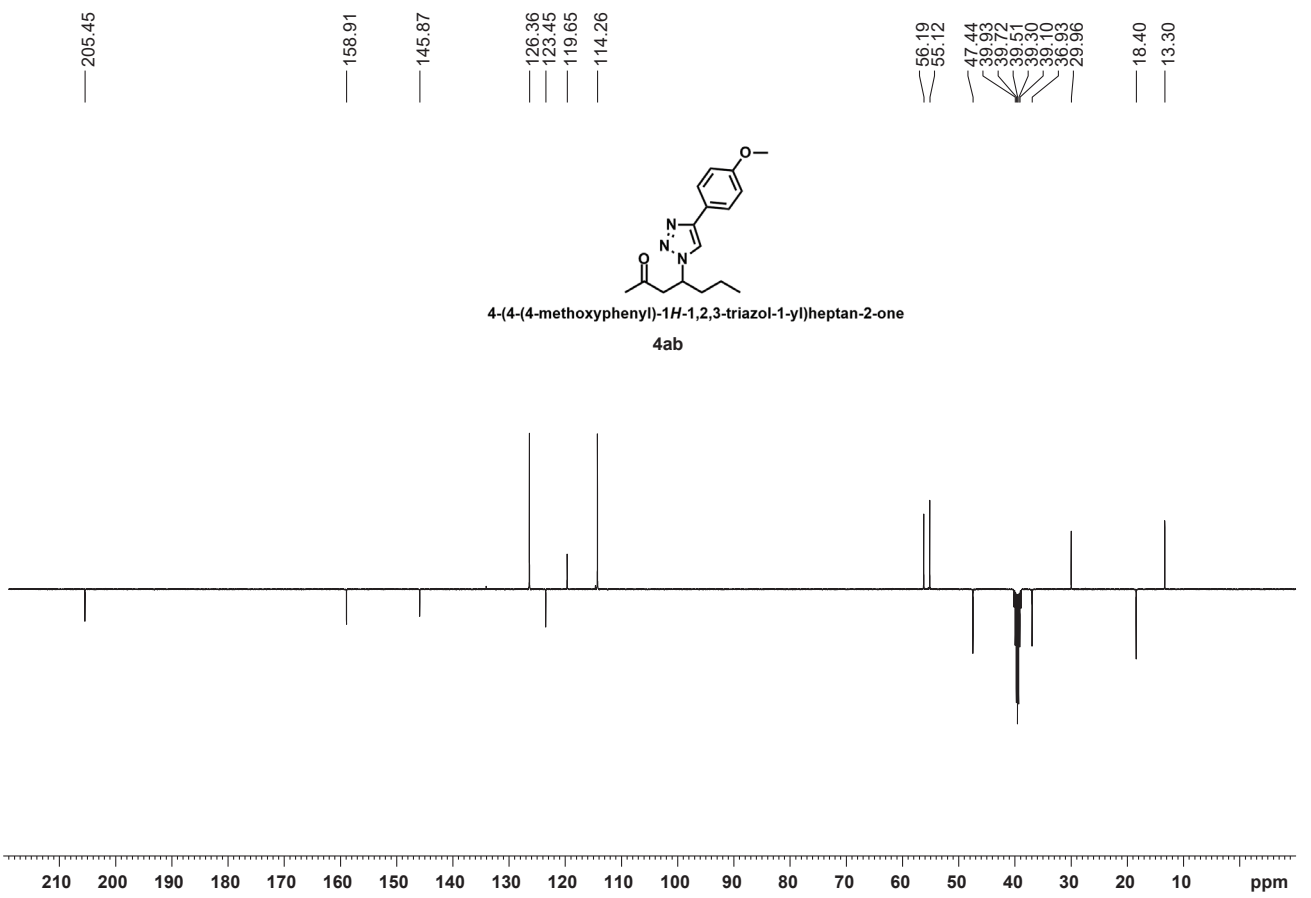
1.00
3.11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56.19
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39.93
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39.51
39.30
39.10
36.93
29.96
18.40
13.30
O
N
N
N
O
4-(4-(4-methoxyphenyl)-1H-1,2,3-triazol-1-yl)heptan-2-one
4ab
210
200
190
180
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150
140
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120
110
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90
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30
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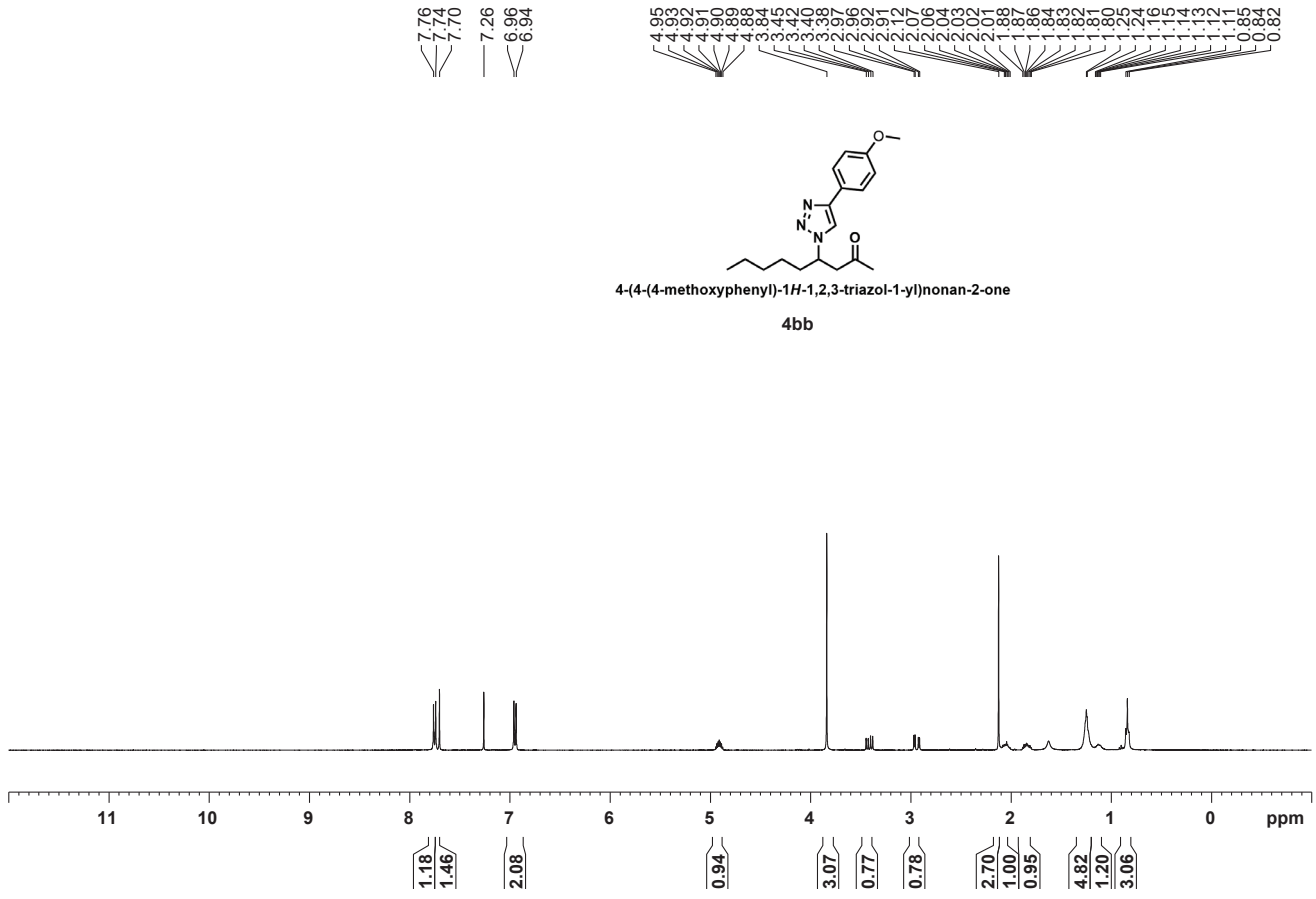
10
ppm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4.89
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3.84
3.45
3.42
3.40
3.38
2.97
2.96
2.92
2.91
2.12
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2.06
2.04
2.03
2.02
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1.83
1.82
1.81
1.80
1.25
1.24
1.16
1.15
1.14
1.13
1.12
1.11
0.85
0.84
0.82
O
N
N
N
O
4-(4-(4-methoxyphenyl)-1H-1,2,3-triazol-1-yl)nonan-2-one
4bb
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.18
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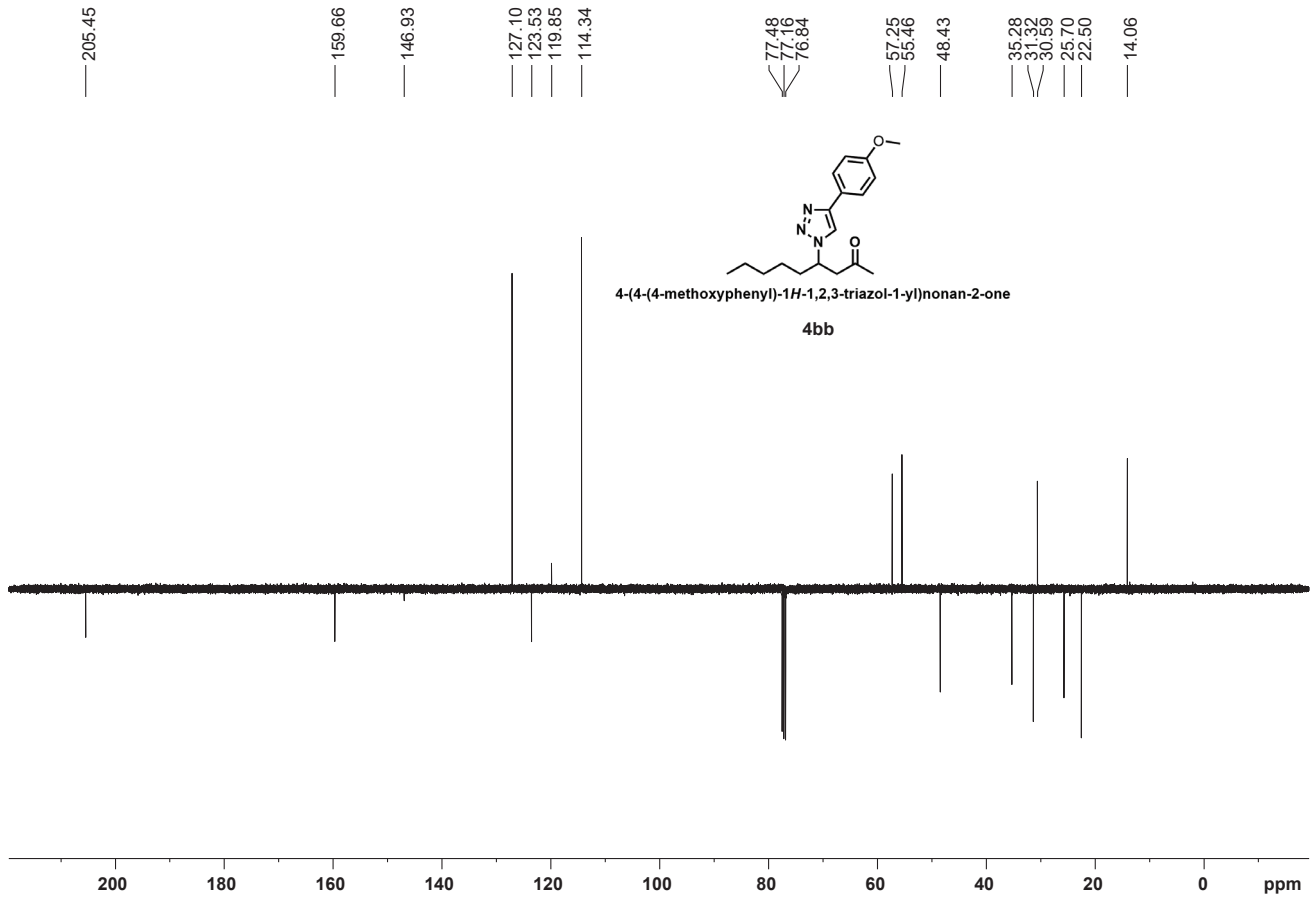
1.20
3.06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114.34
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76.84
57.25
55.46
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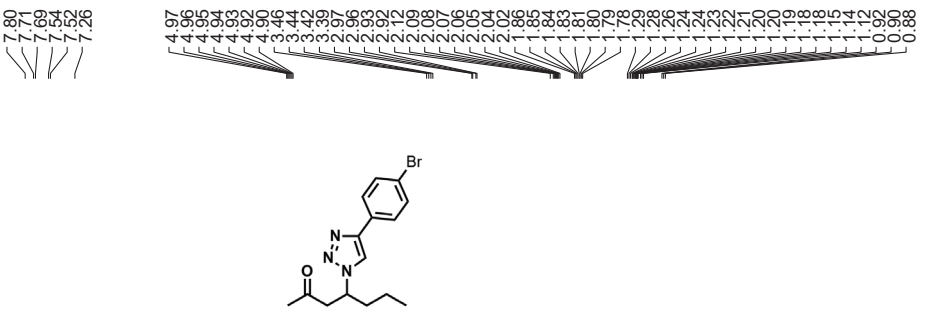
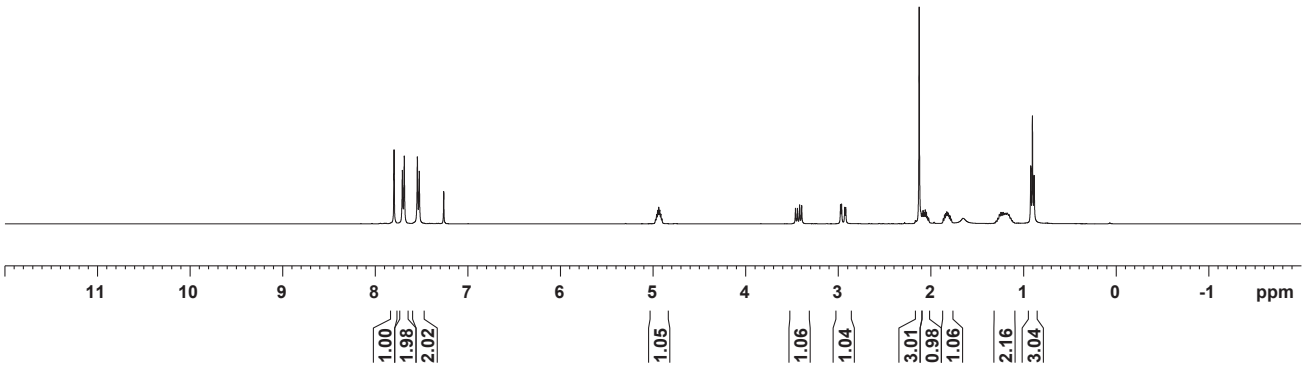
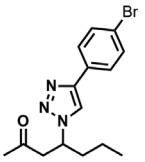
31.32
30.59
25.70
22.50
14.06
O
N
N
N
O
4-(4-(4-methoxyphenyl)-1H-1,2,3-triazol-1-yl)nonan-2-one
4bb
200
180
160
140
120
100
80
60
40
20
0
ppm



4-(4-(4-bromophenyl)-1*H*-1,2,3-triazol-1-yl)heptan-2-one

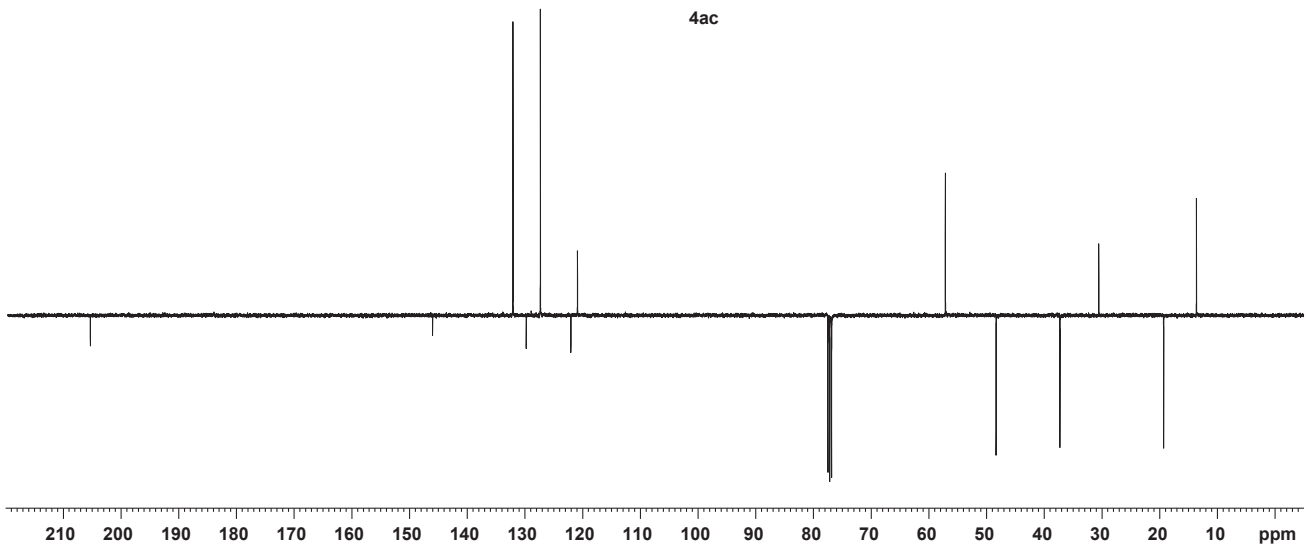
4ac

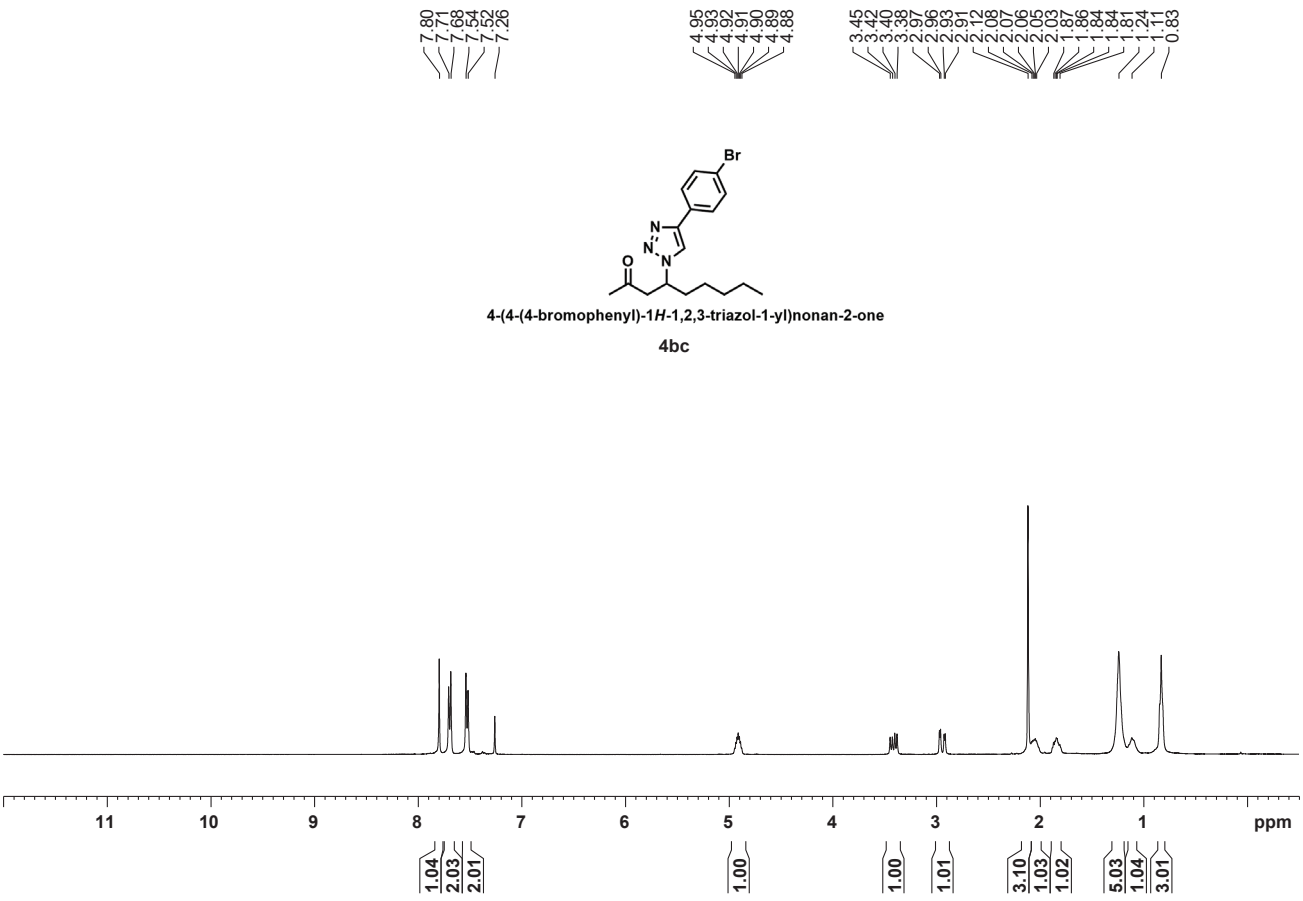




4-(4-(4-bromophenyl)-1*H*-1,2,3-triazol-1-yl)heptan-2-one

4ac

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4.90
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3.38
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2.91
2.12
2.08
2.07
2.06
2.05
2.03
1.87
1.86
1.84
1.84
1.81
1.24
1.11
0.83
Br
N
N
N
O
4-(4-(4-bromophenyl)-1H-1,2,3-triazol-1-yl)nonan-2-one
4bc
11
10
9
8
7
6
5
4
3
2
1
ppm
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2.01
1.00
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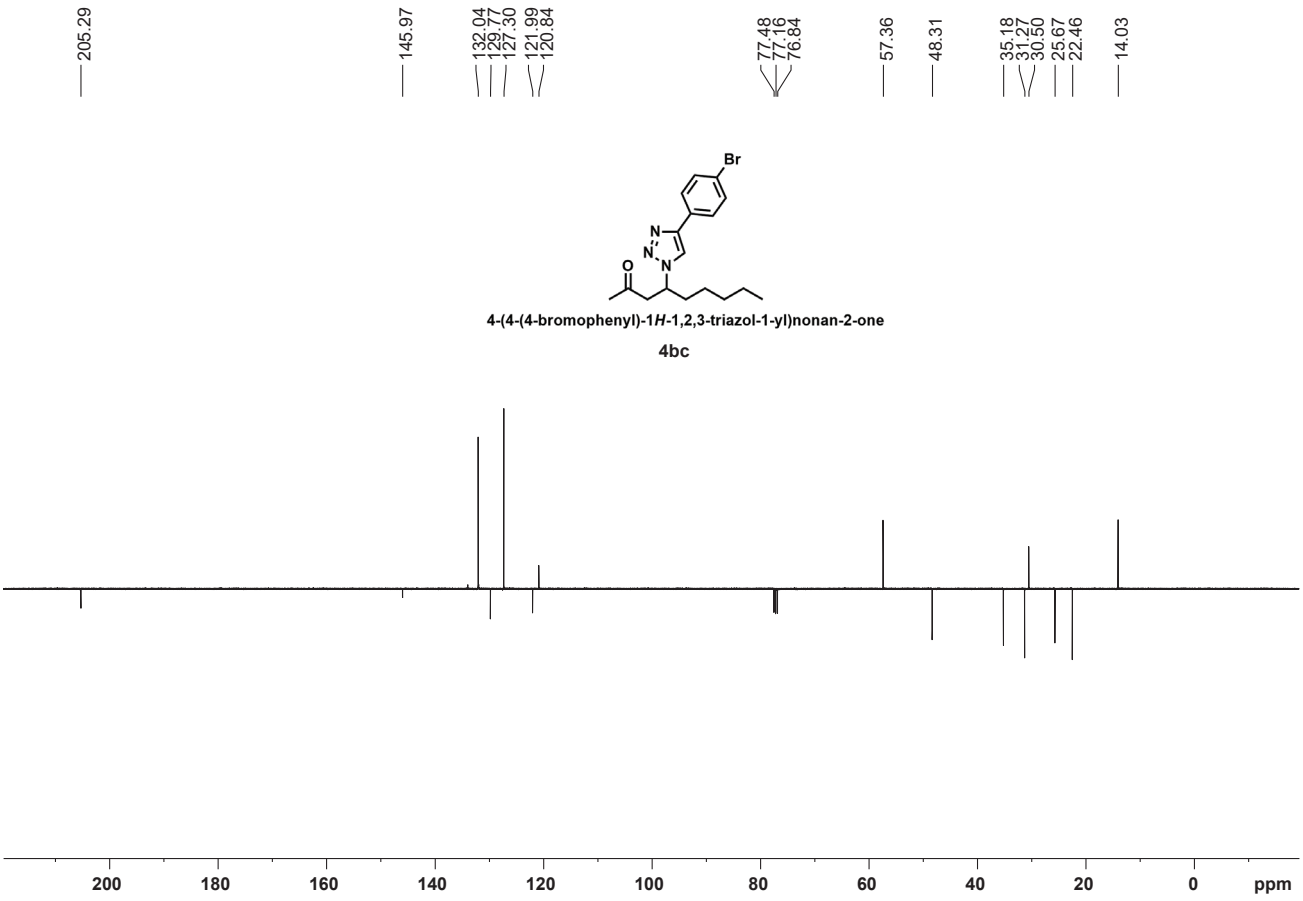
5.03
1.04
3.01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31.27
30.50
25.67
22.46
14.03
Br
N
N
N
O
4-(4-(4-bromophenyl)-1H-1,2,3-triazol-1-yl)nonan-2-one
4bc
200
180
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140
120
100
80
60
40
20
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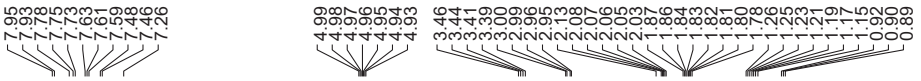
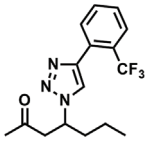
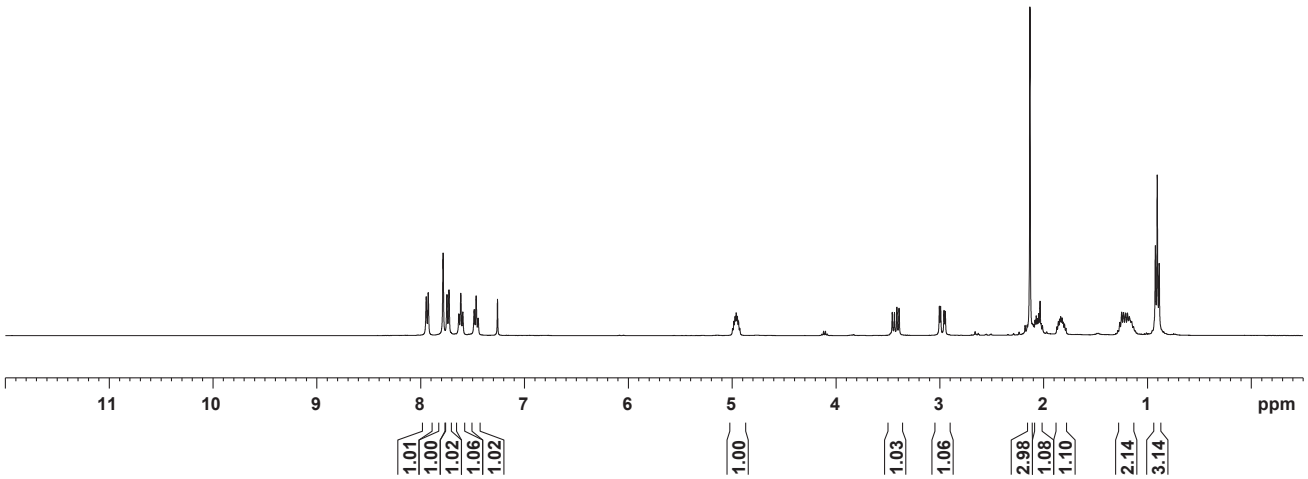
ppm

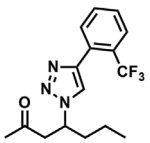




4-(4-(2-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)heptan-2-one

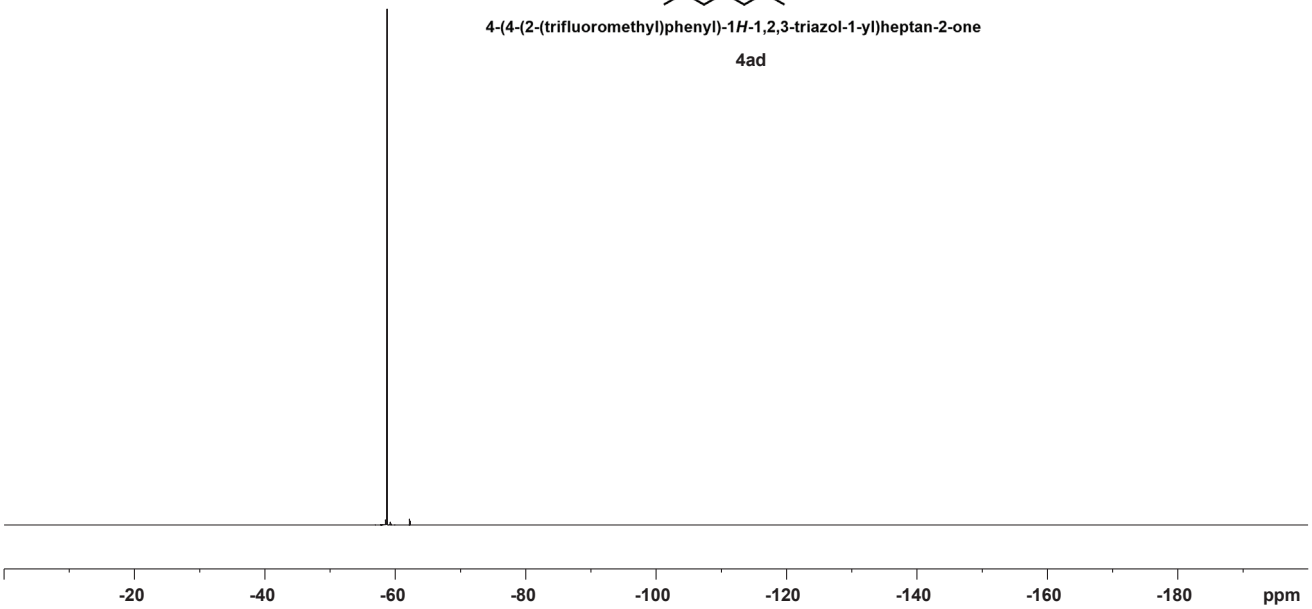
4ad

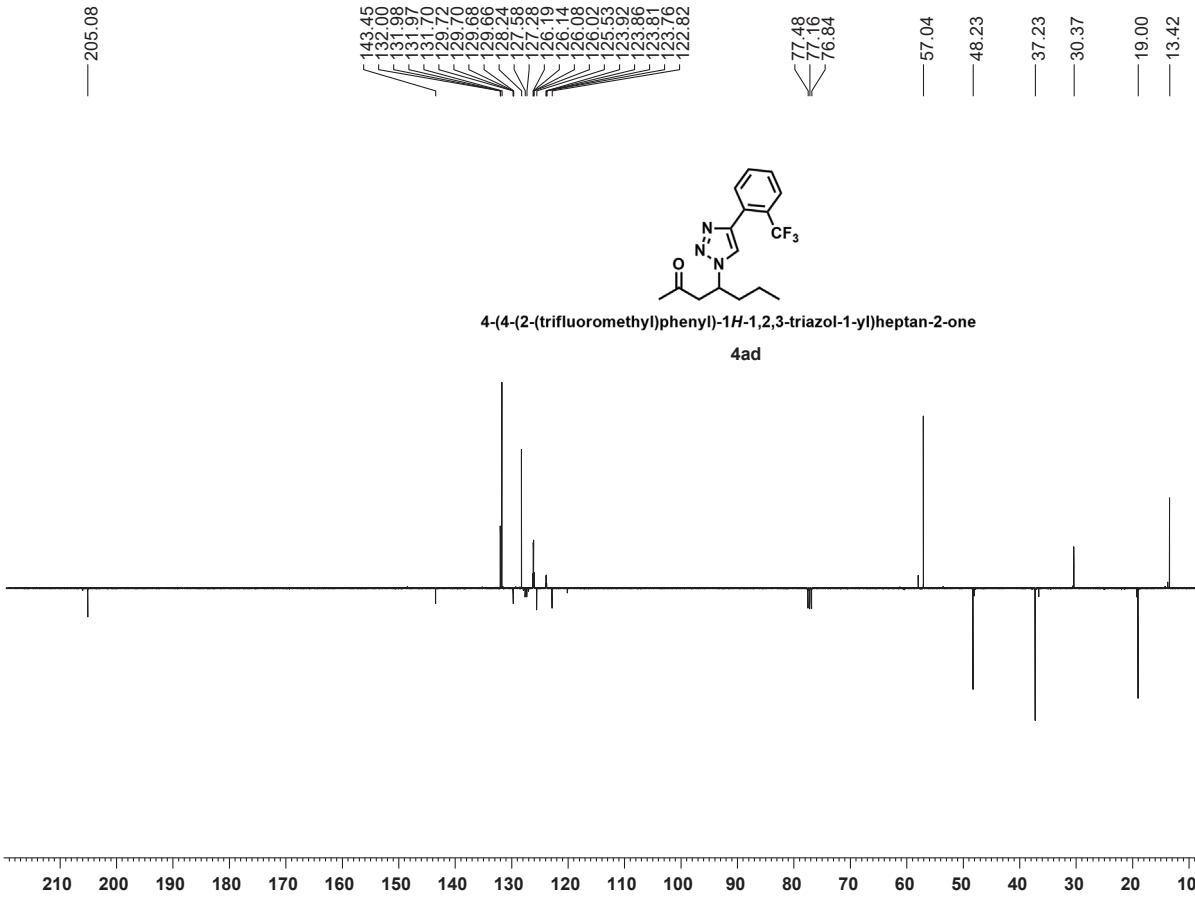




4-(4-(2-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)heptan-2-one

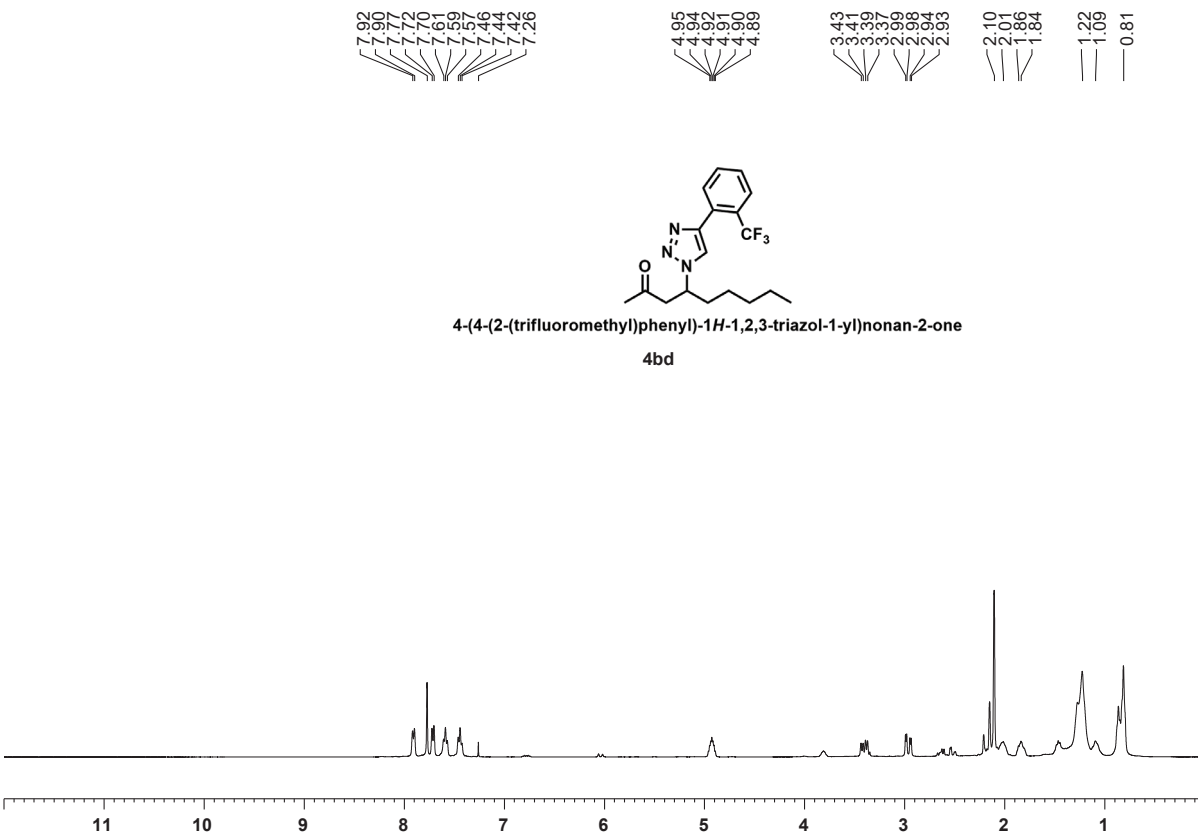
4ad





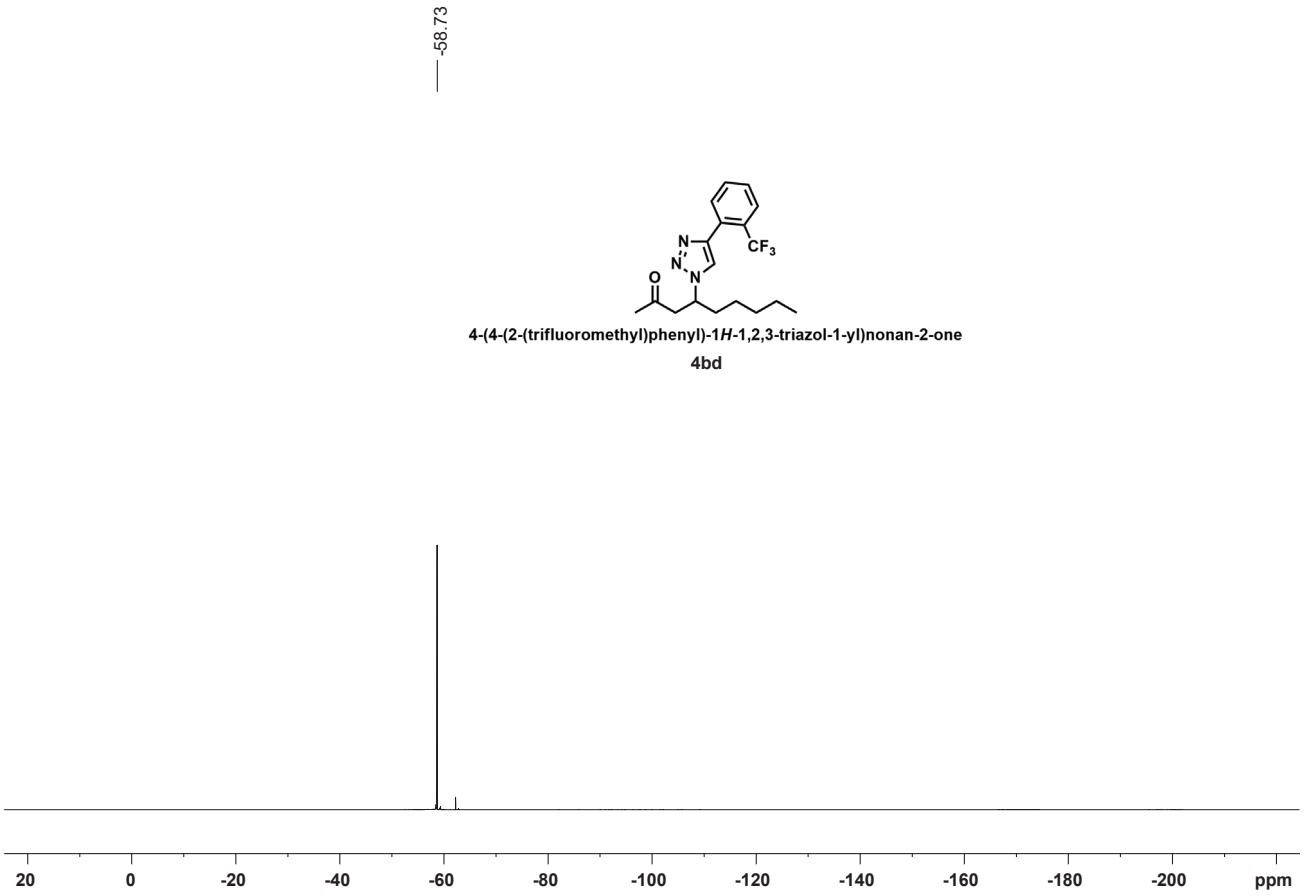
4-(4-(2-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)heptan-2-one

4ad



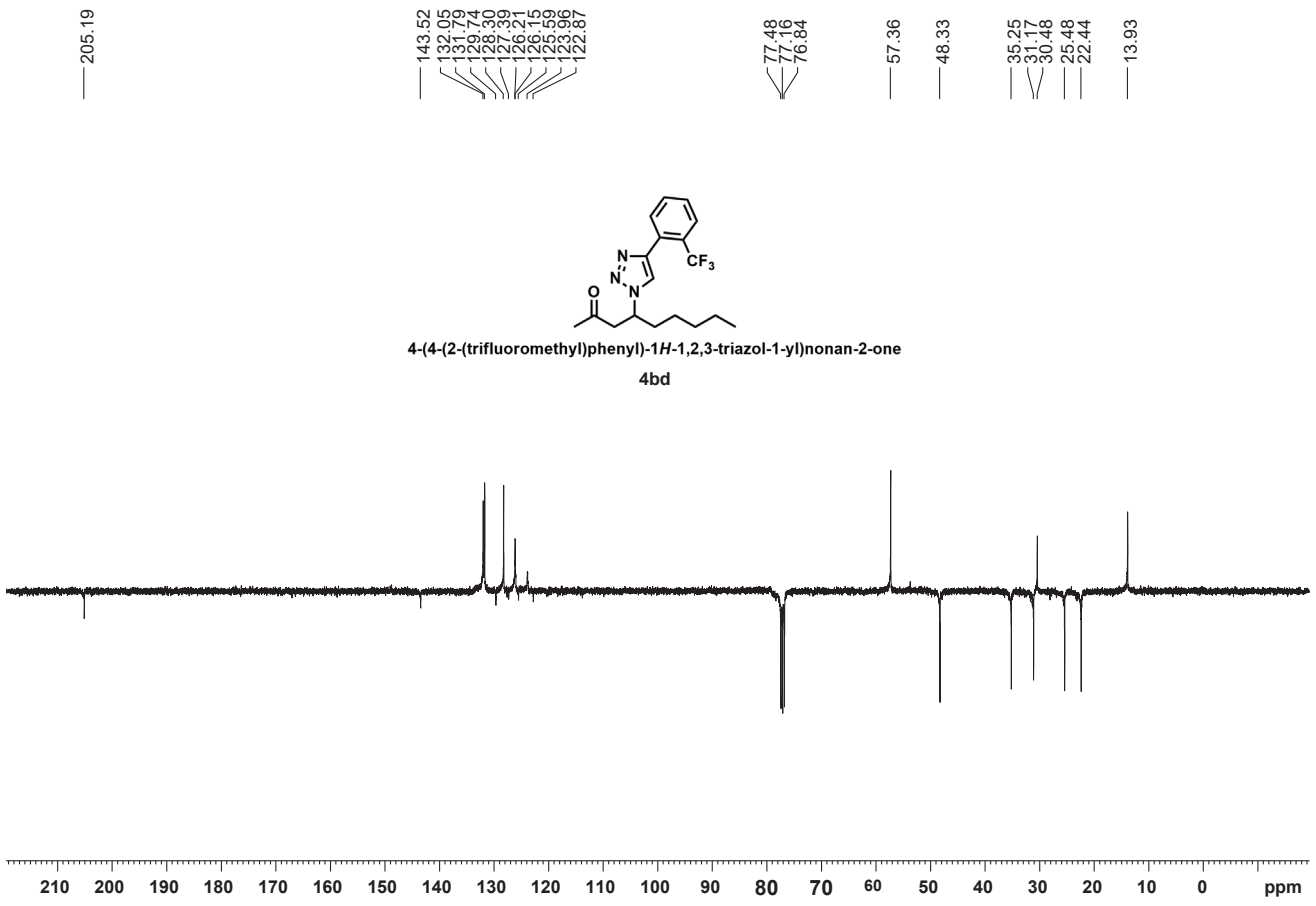
4-(4-(2-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)nonan-2-one

4bd



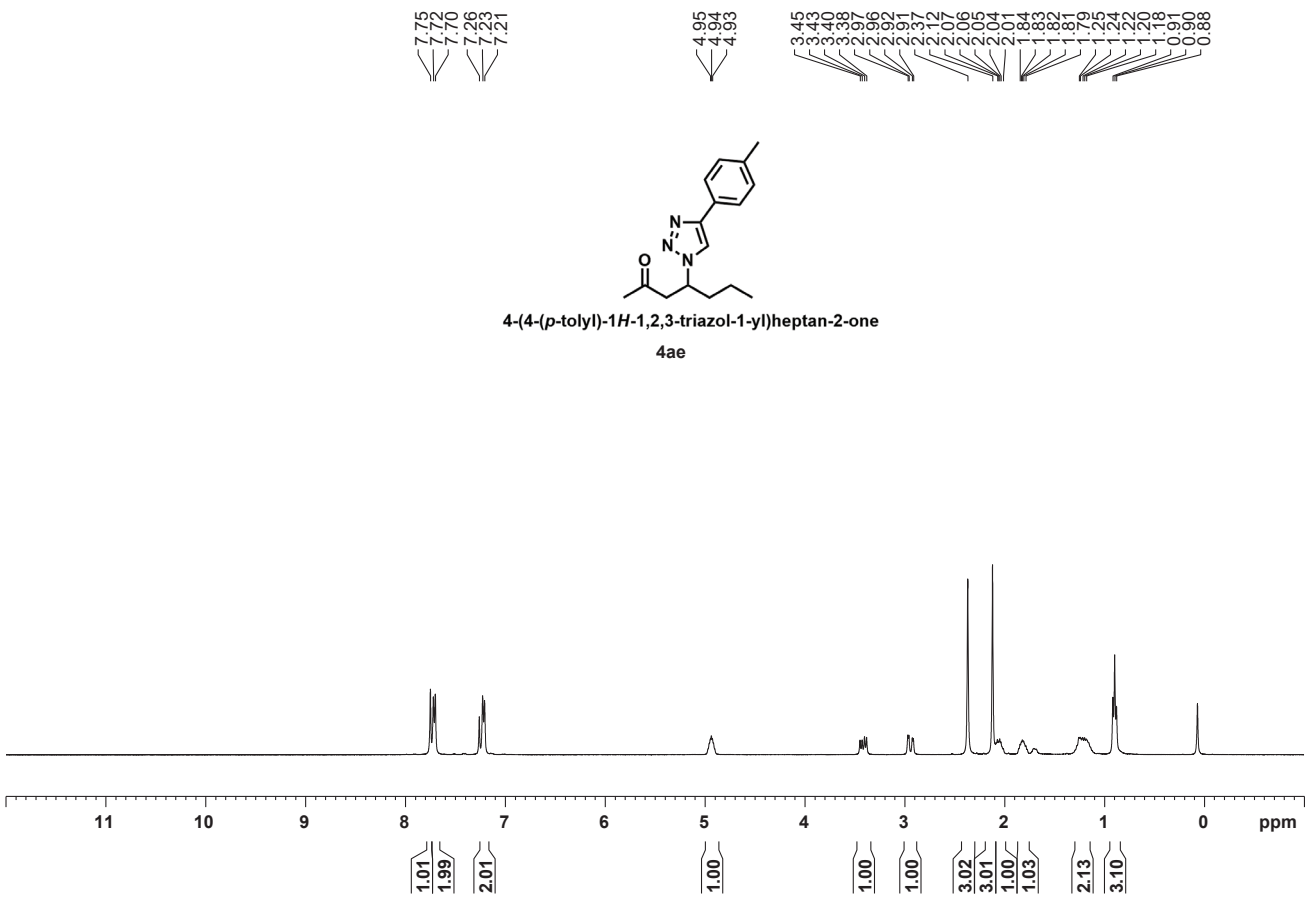
4-(4-(2-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)nonan-2-one

4bd



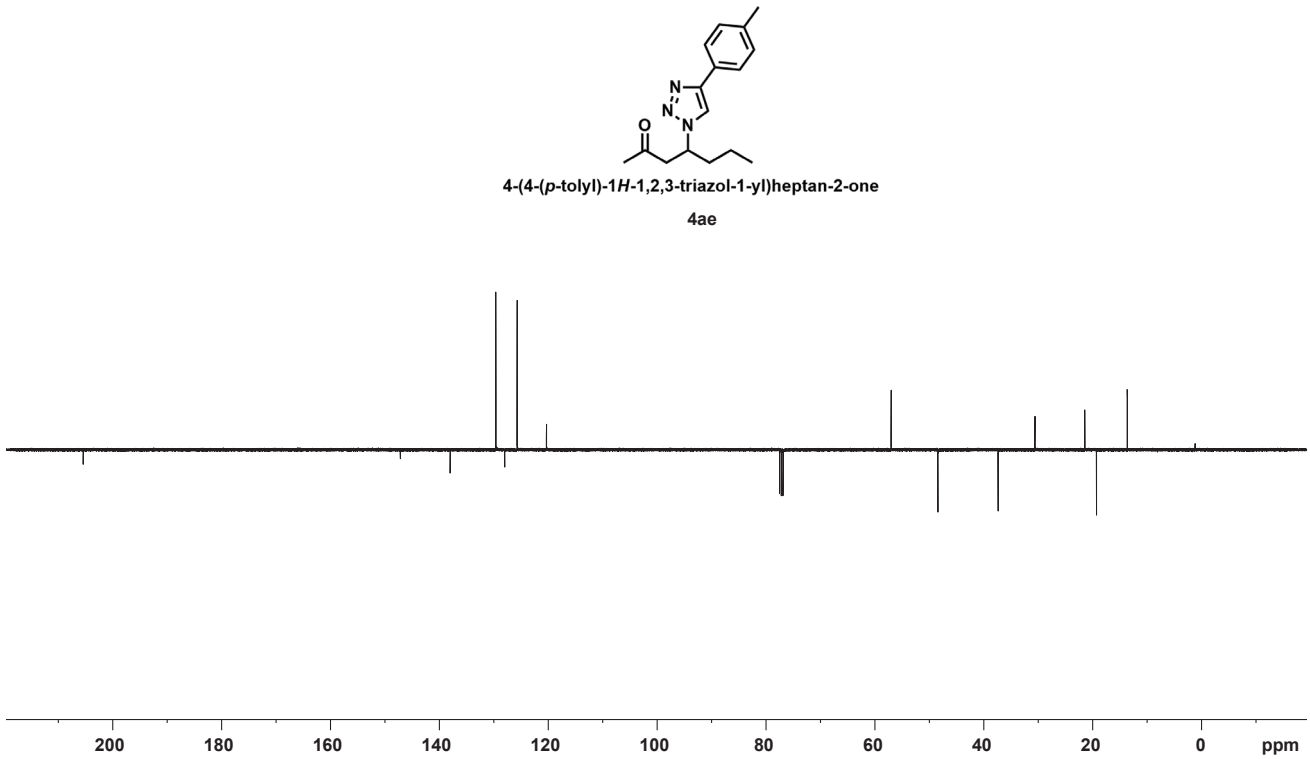
4-(4-(2-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)nonan-2-one

4bd



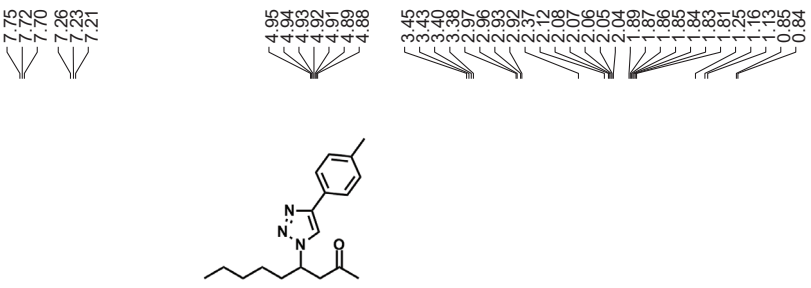
4-(4-(*p*-tolyl)-1*H*-1,2,3-triazol-1-yl)heptan-2-one

4ae



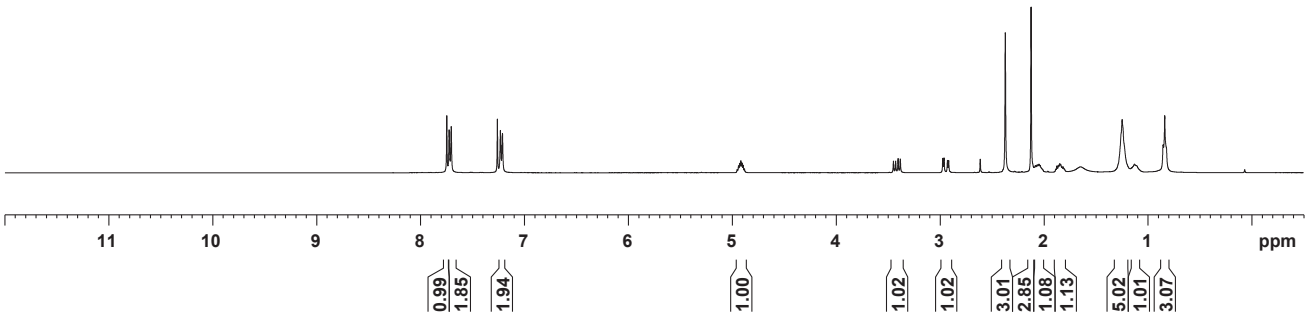
4-(4-(*p*-tolyl)-1*H*-1,2,3-triazol-1-yl)heptan-2-one

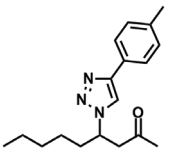
4ae



4-(4-(*p*-tolyl)-1*H*-1,2,3-triazol-1-yl)nonan-2-one

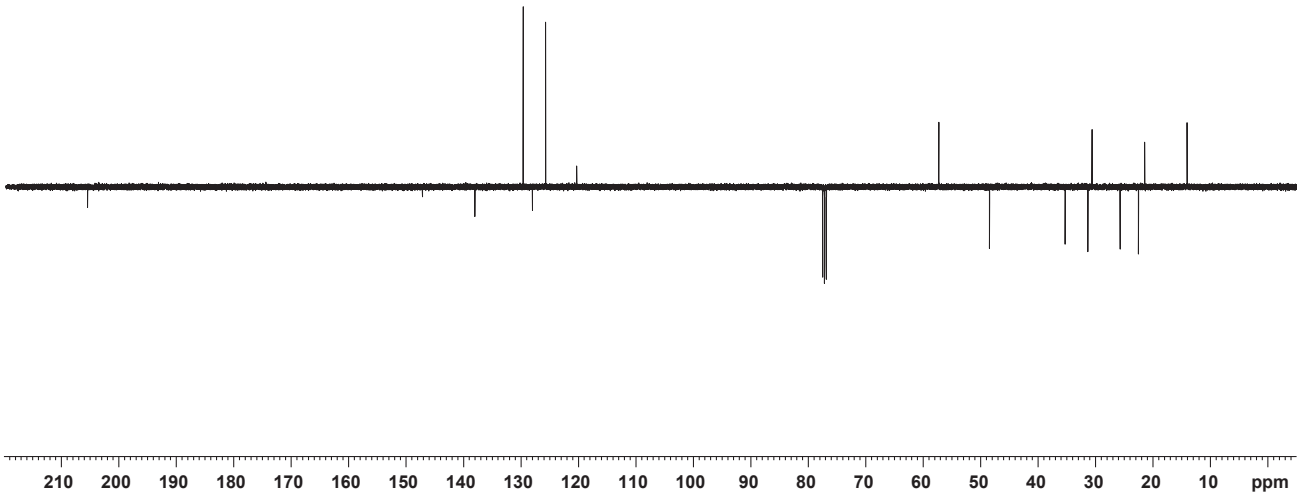
4be

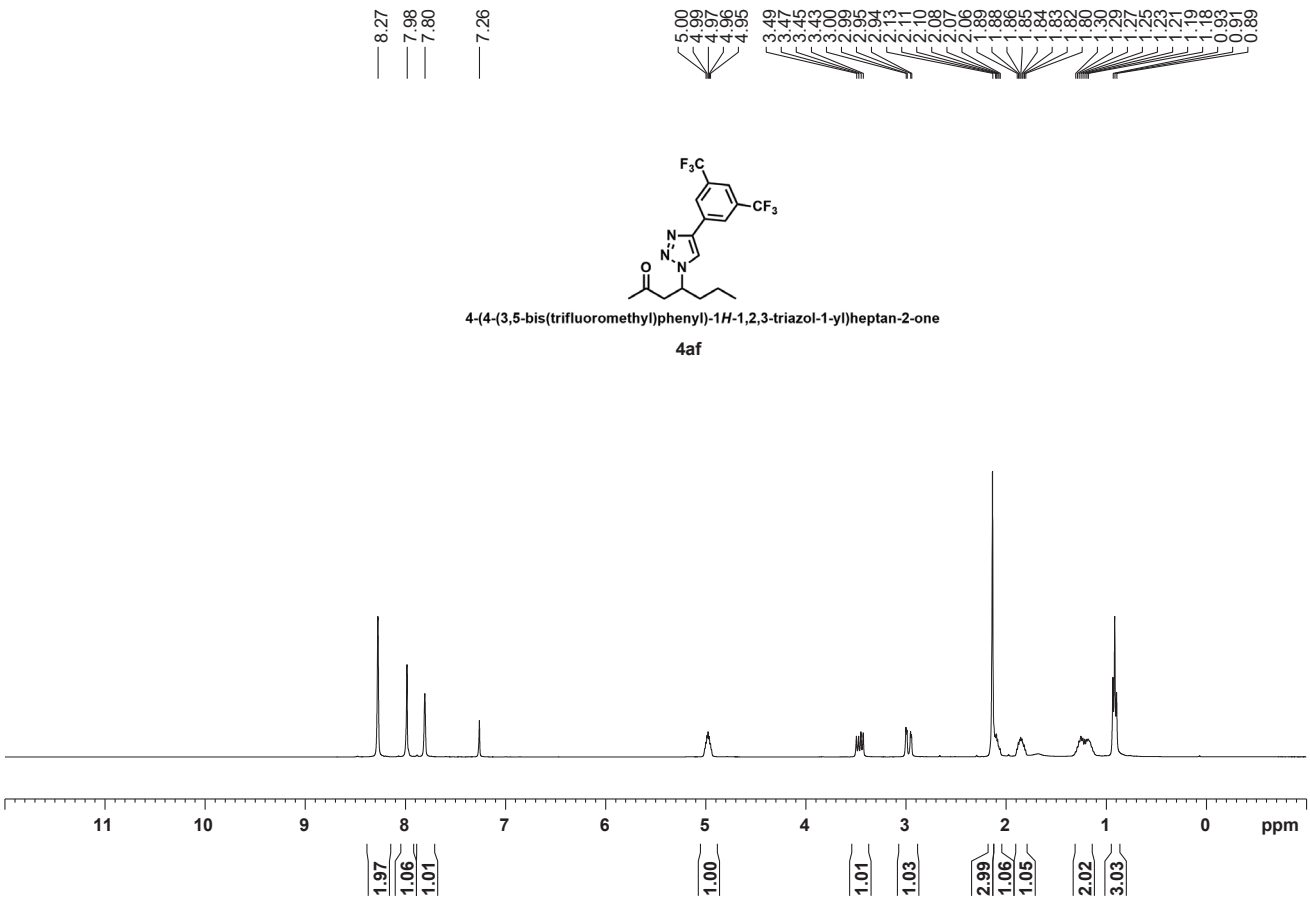




4-(4-(*p*-tolyl)-1*H*-1,2,3-triazol-1-yl)nonan-2-one

4be

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1.80
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1.29
1.27
1.25
1.23
1.21
1.19
1.18
0.93
0.91
0.89
F3C
CF3
N
N
N
O
4-(4-(3,5-bis(trifluoromethyl)phenyl)-1H-1,2,3-triazol-1-yl)heptan-2-one
4af
11
10
9
8
7
6
5
4
3
2
1
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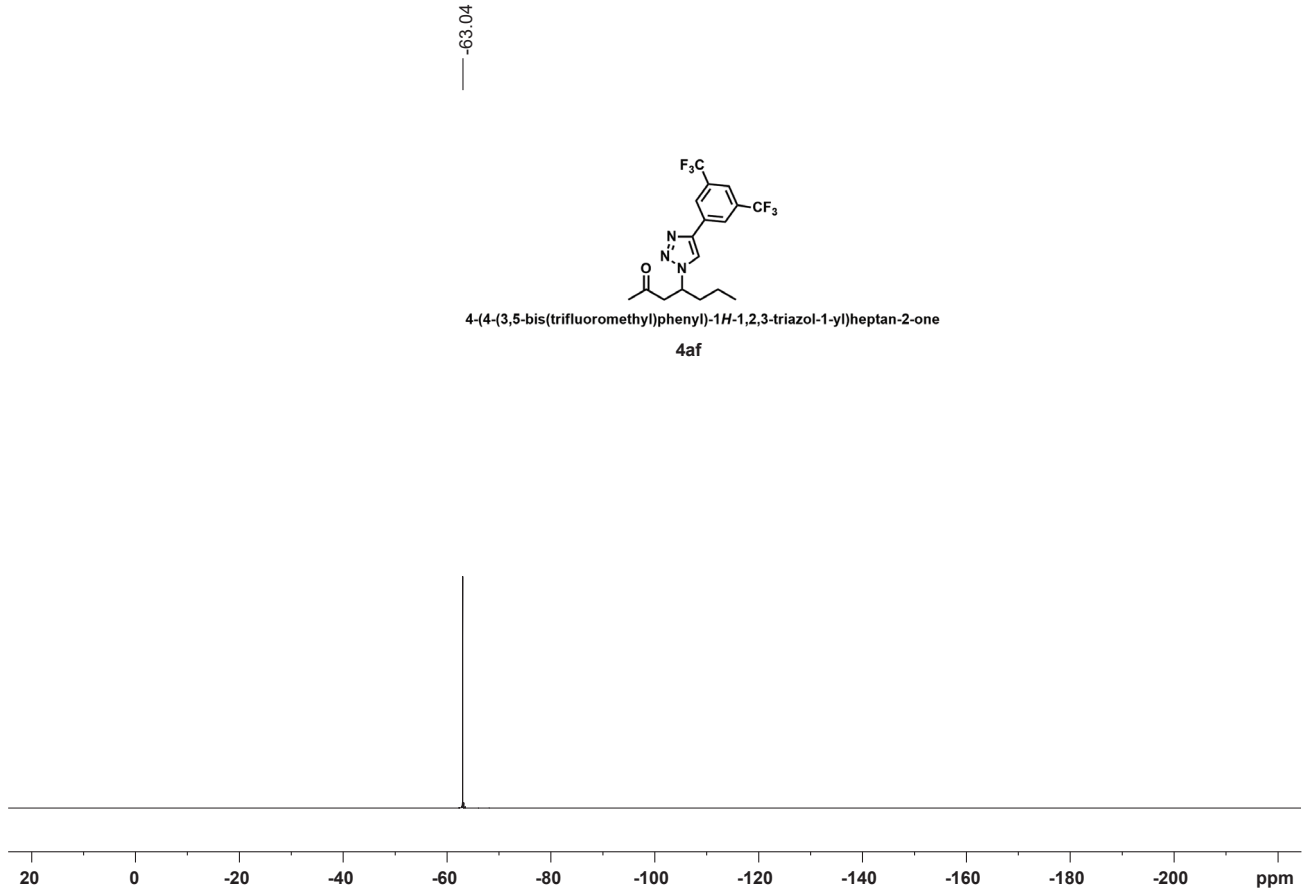
1.05
2.02
3.03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F3C
CF3
N
N
N
O
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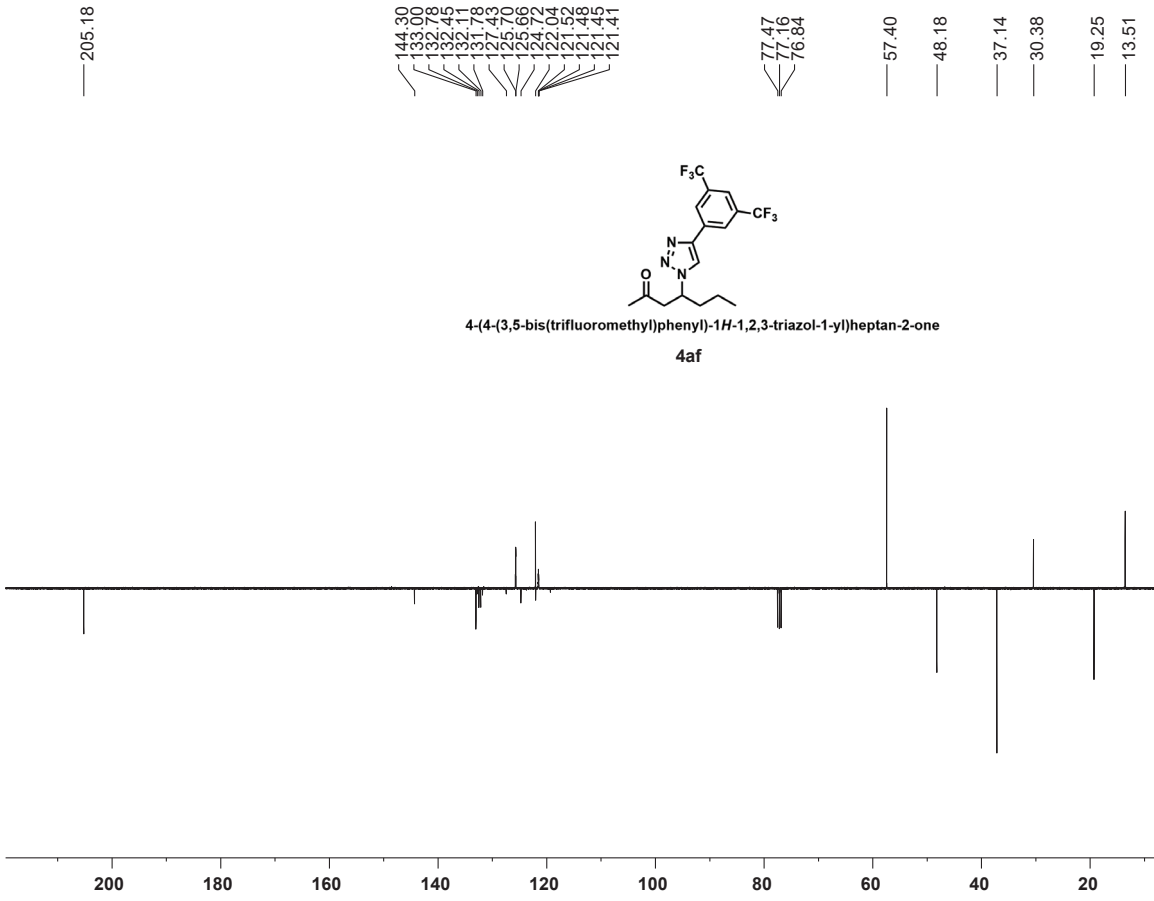
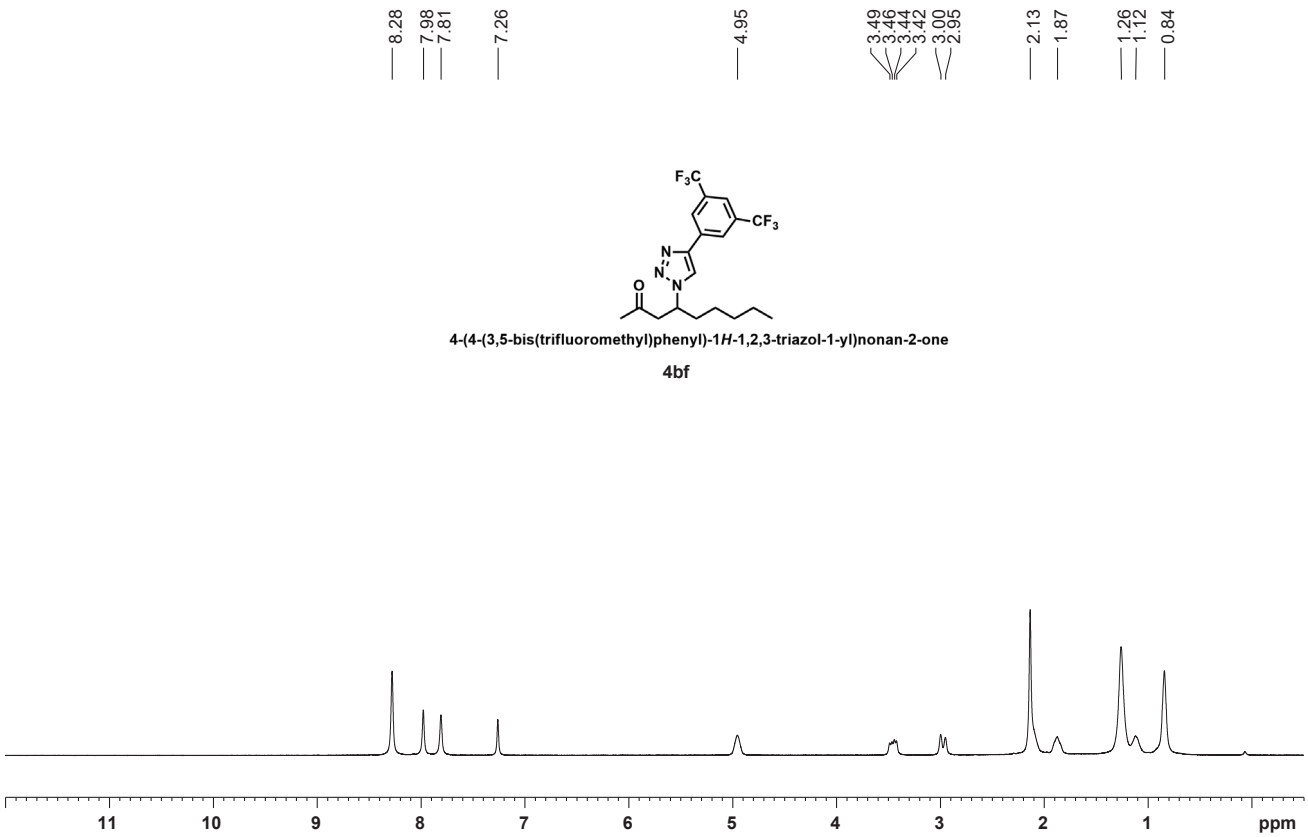
-200
ppm



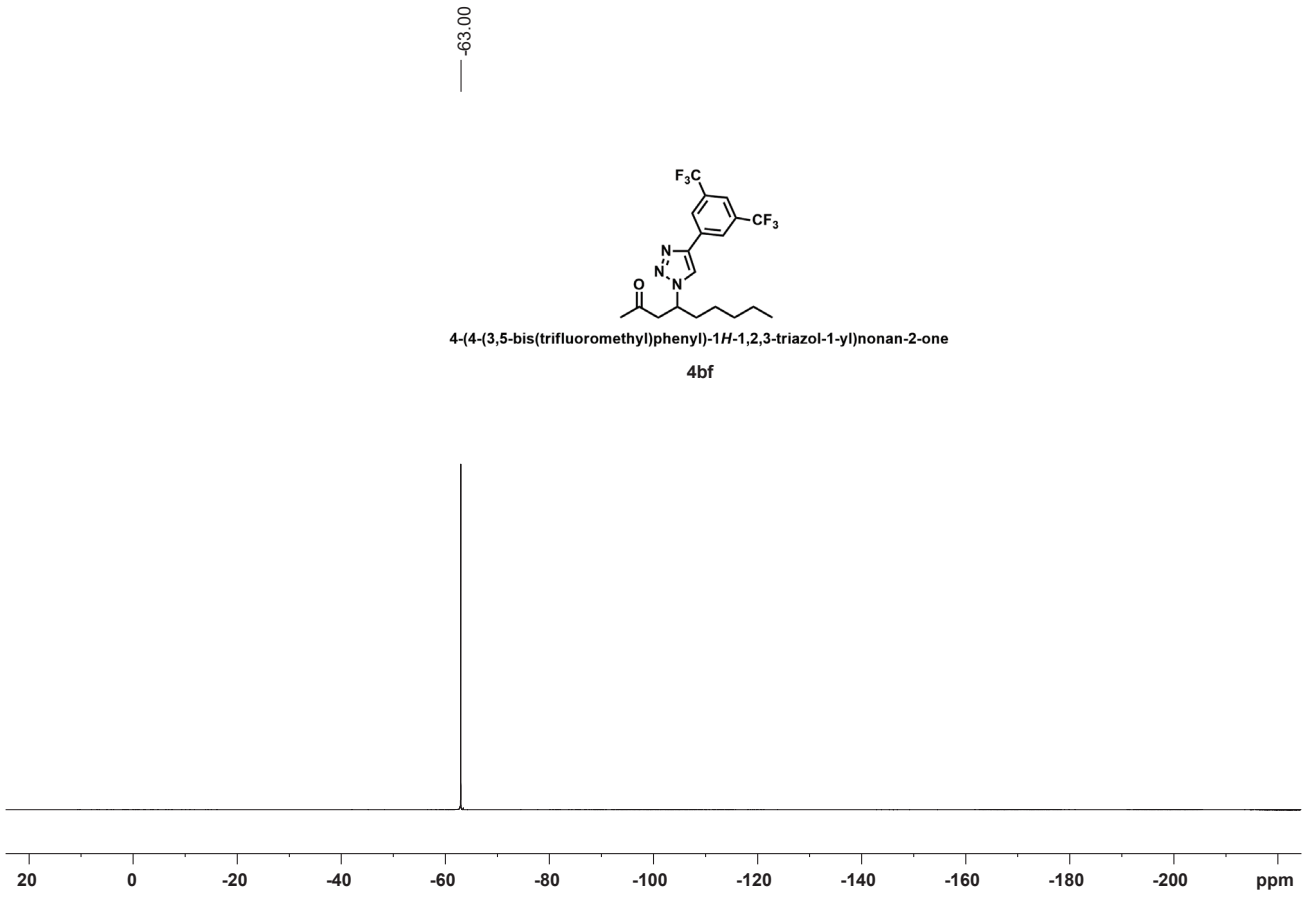
4-(4-(3,5-bis(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)heptan-2-one

4af



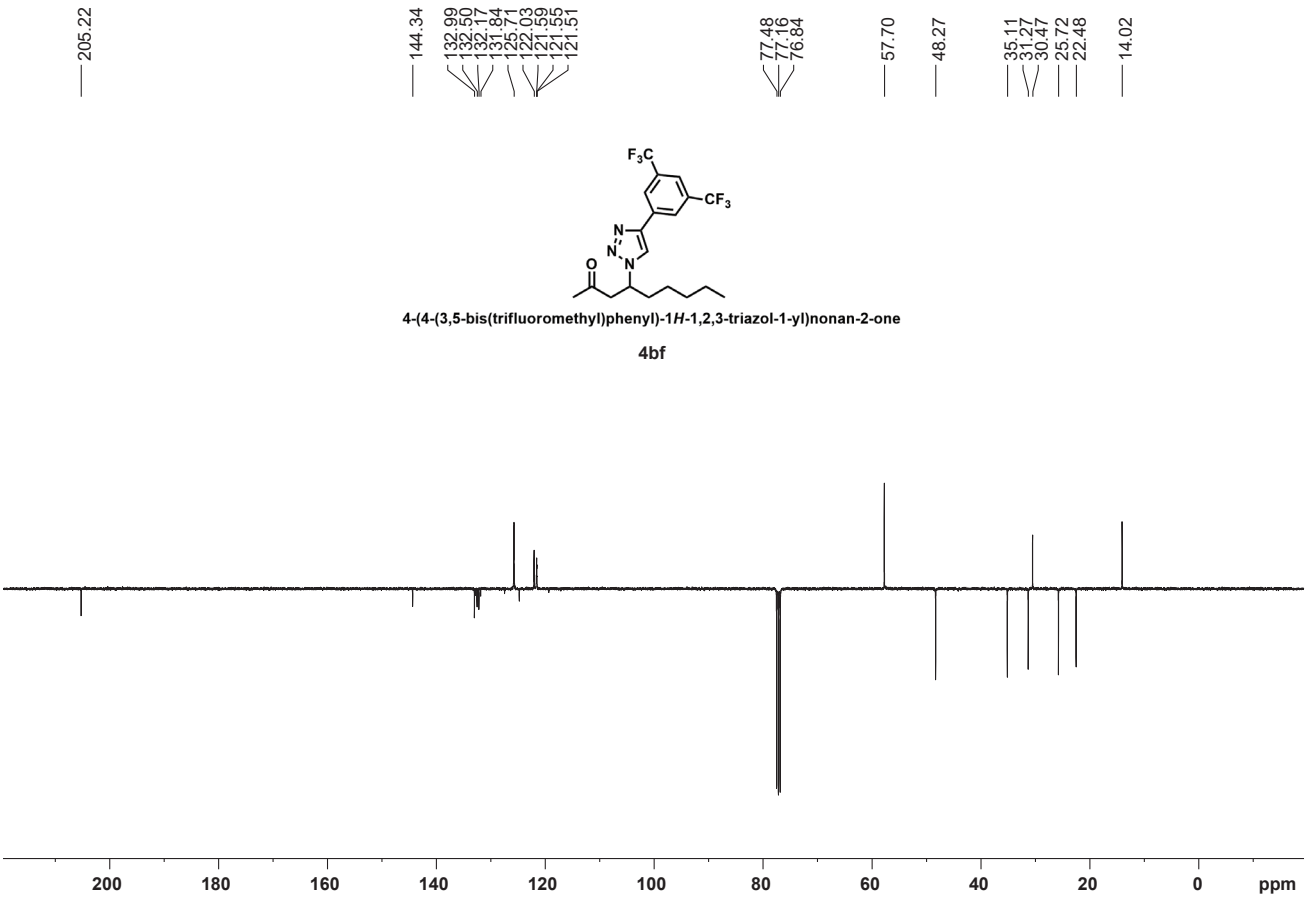
4-(4-(3,5-bis(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)nonan-2-one

4bf



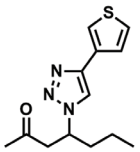
4-(4-(3,5-bis(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)nonan-2-one

4bf



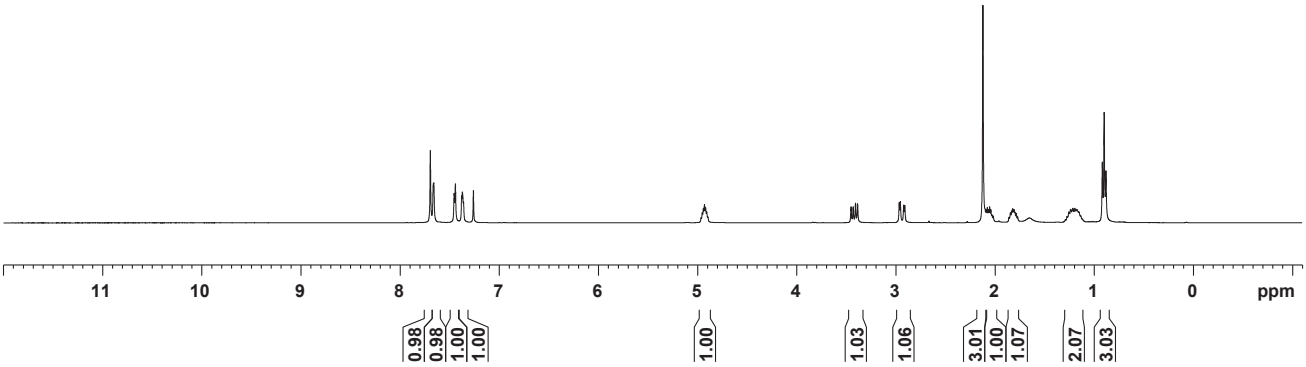
4-(4-(3,5-bis(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)nonan-2-one

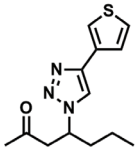
4bf



4-(4-(thiophen-3-yl)-1*H*-1,2,3-triazol-1-yl)heptan-2-one

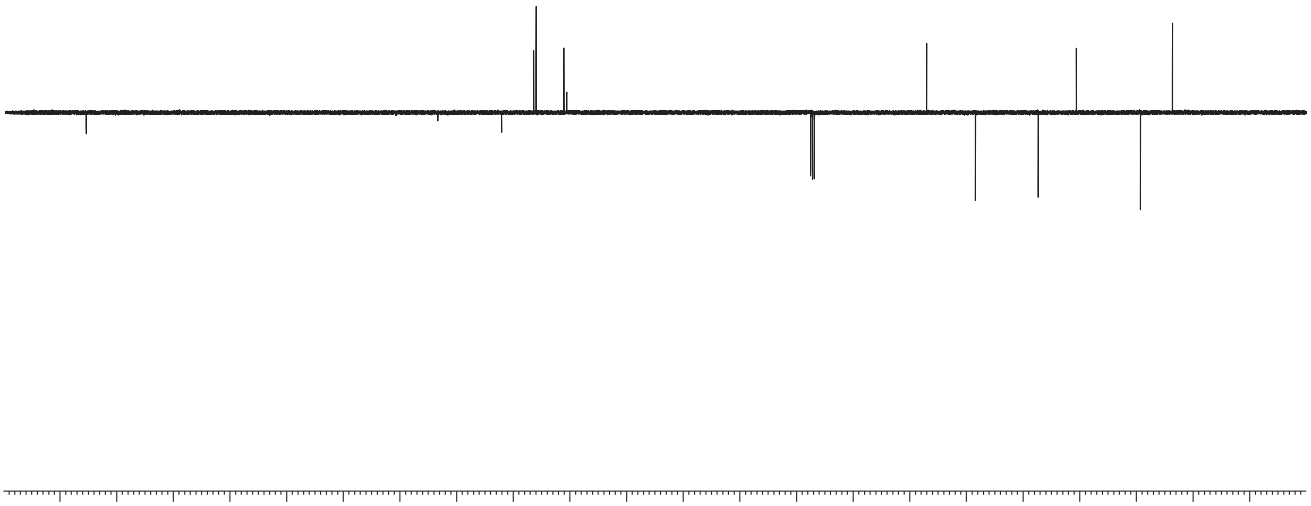
4ag

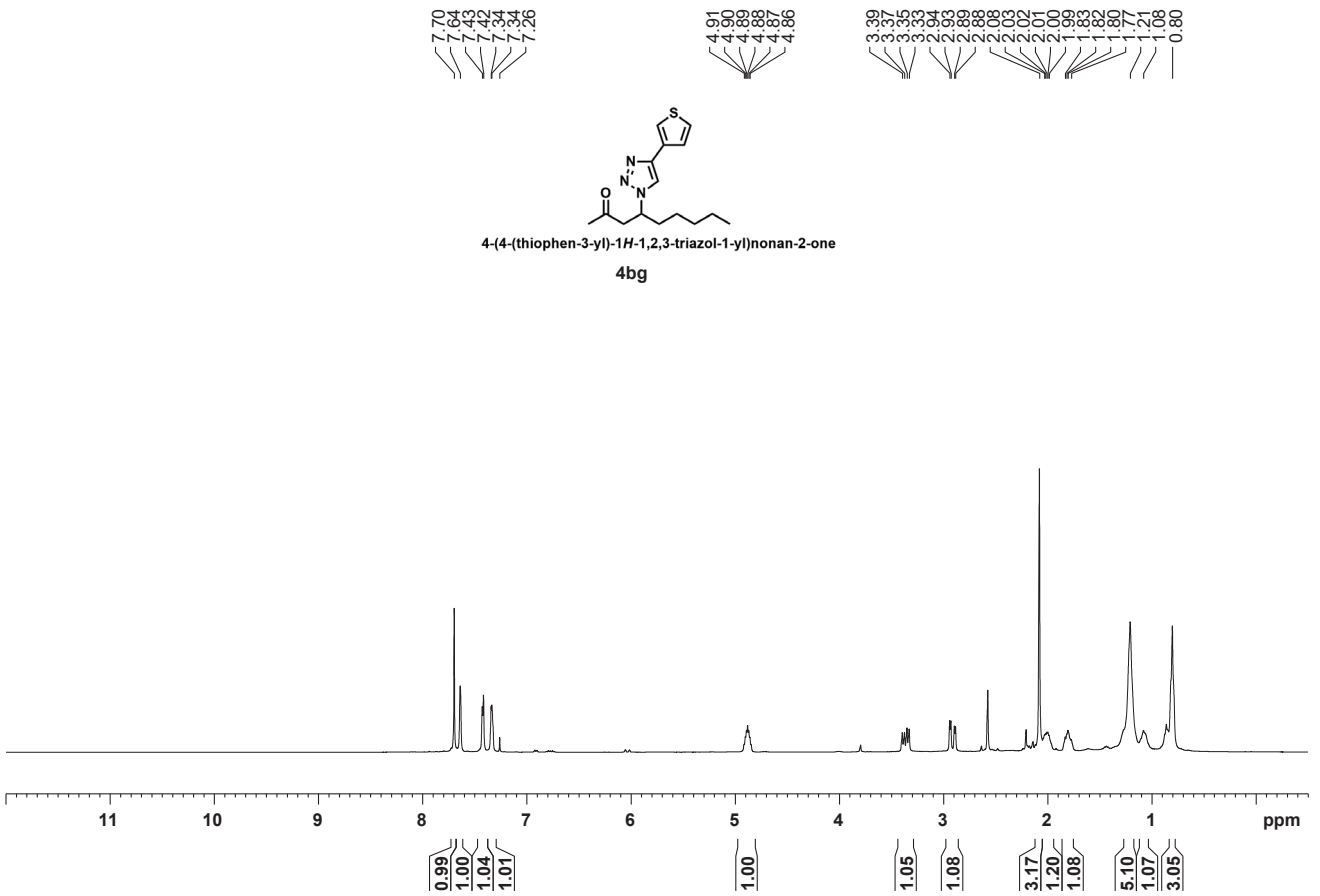




4-(4-(thiophen-3-yl)-1*H*-1,2,3-triazol-1-yl)heptan-2-one

4ag

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1.08
0.80
4-(4-(thiophen-3-yl)-1H-1,2,3-triazol-1-yl)nonan-2-one
4bg
11
10
9
8
7
6
5
4
3
2
1
ppm
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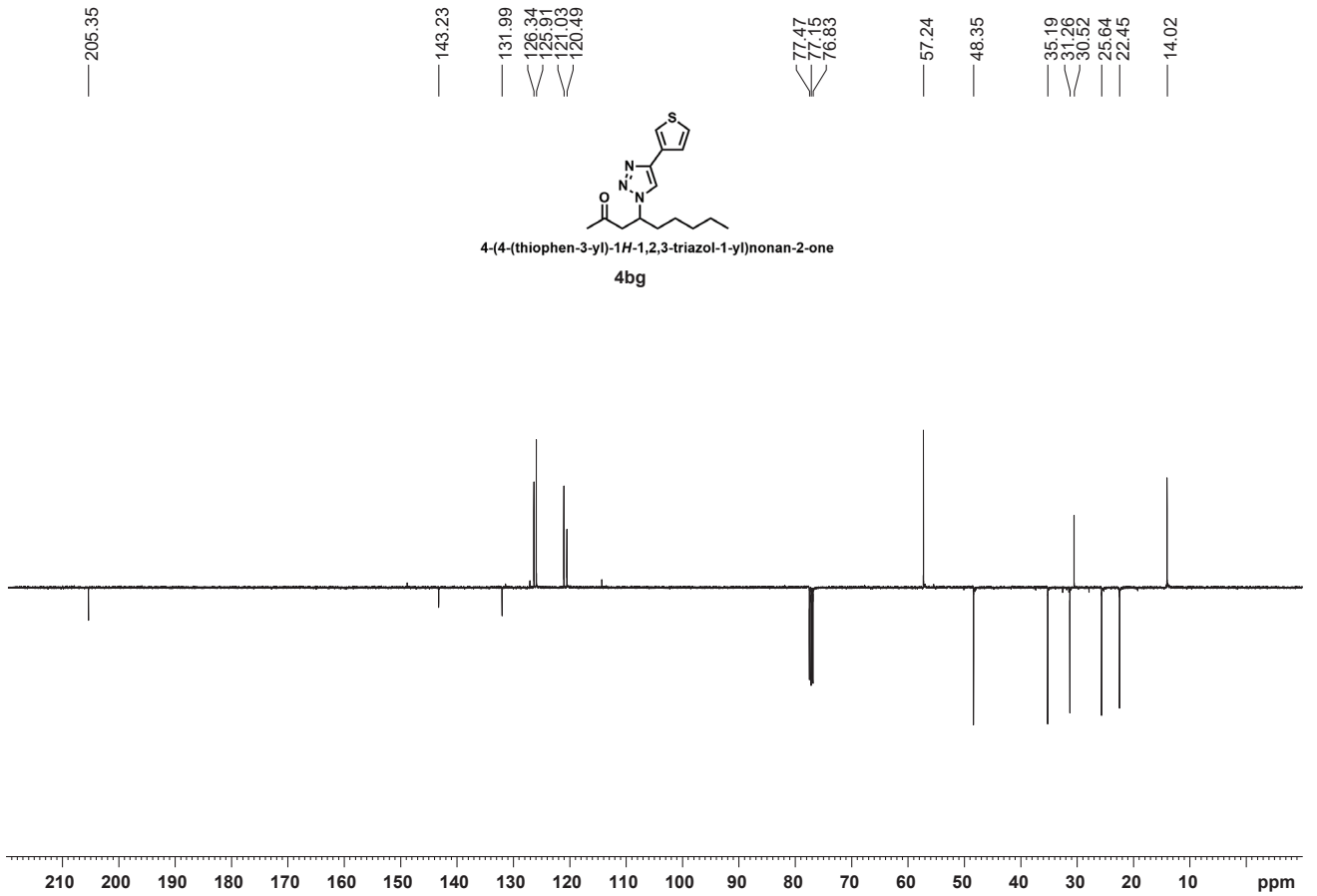
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14.02
4-(4-(thiophen-3-yl)-1H-1,2,3-triazol-1-yl)nonan-2-one
4bg
210
200
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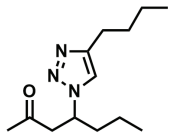
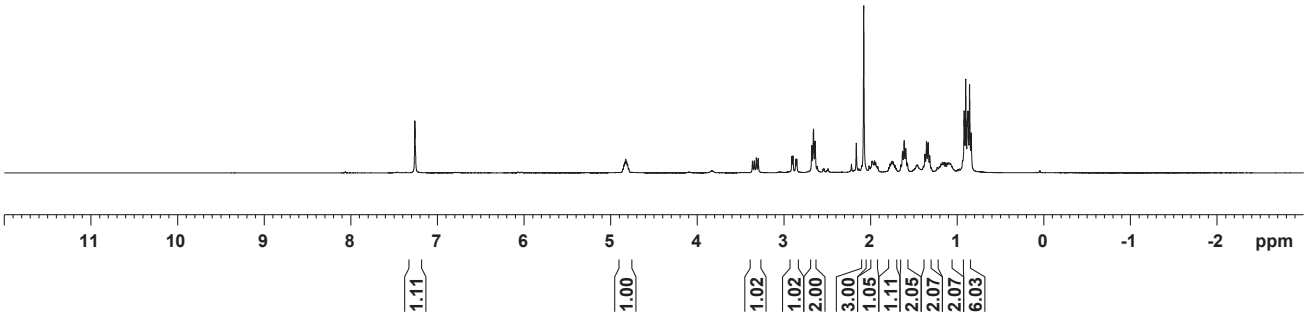
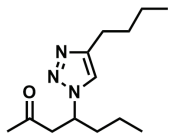


4-(4-butyl-1*H*-1,2,3-triazol-1-yl)heptan-2-one

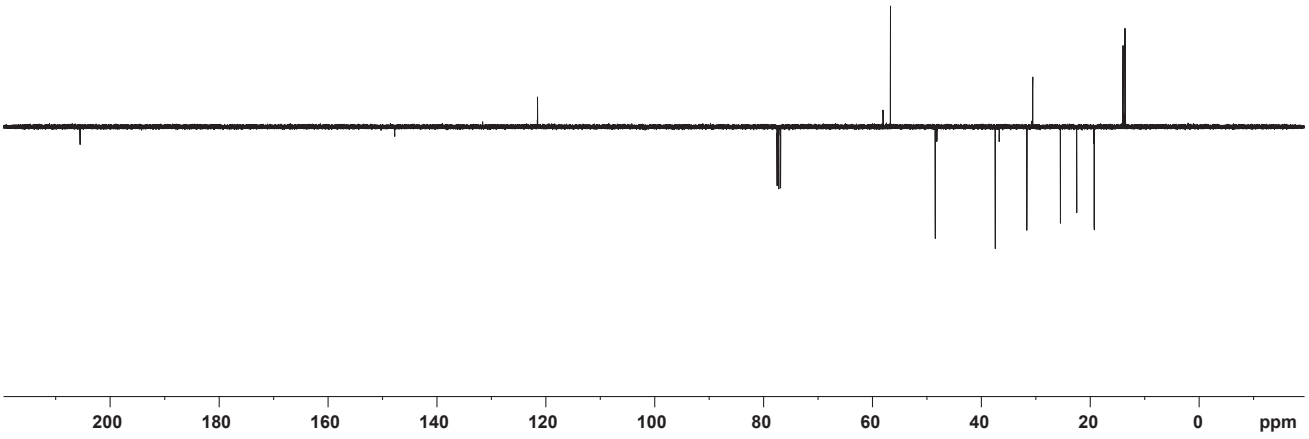
4ah

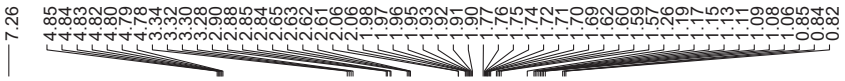


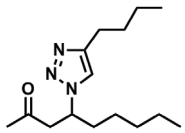


4-(4-butyl-1*H*-1,2,3-triazol-1-yl)heptan-2-one

4ah

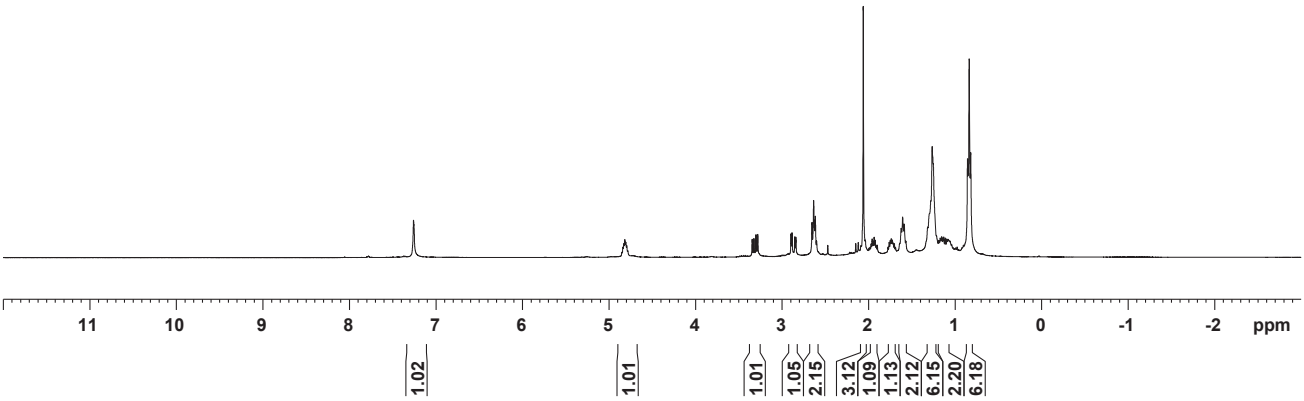


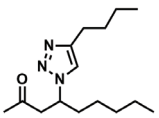




4-(4-butyl-1*H*-1,2,3-triazol-1-yl)nonan-2-one

4bh





4-(4-butyl-1*H*-1,2,3-triazol-1-yl)nonan-2-one

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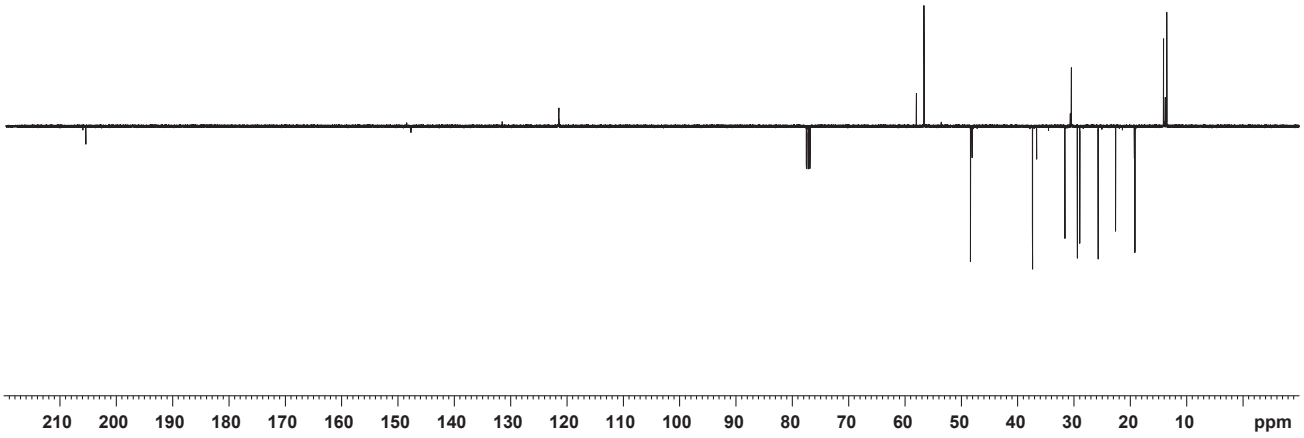

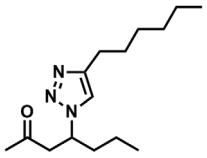

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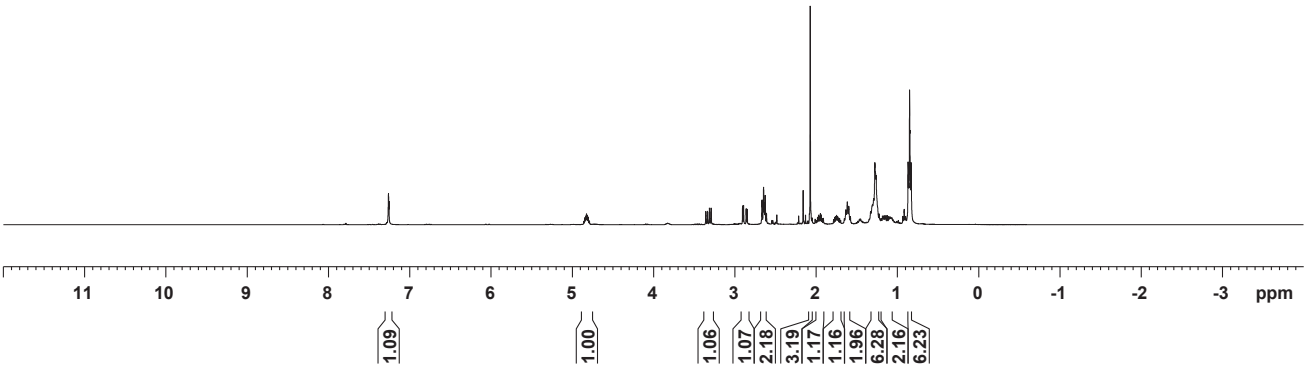
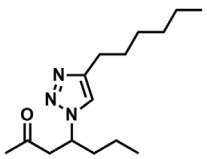
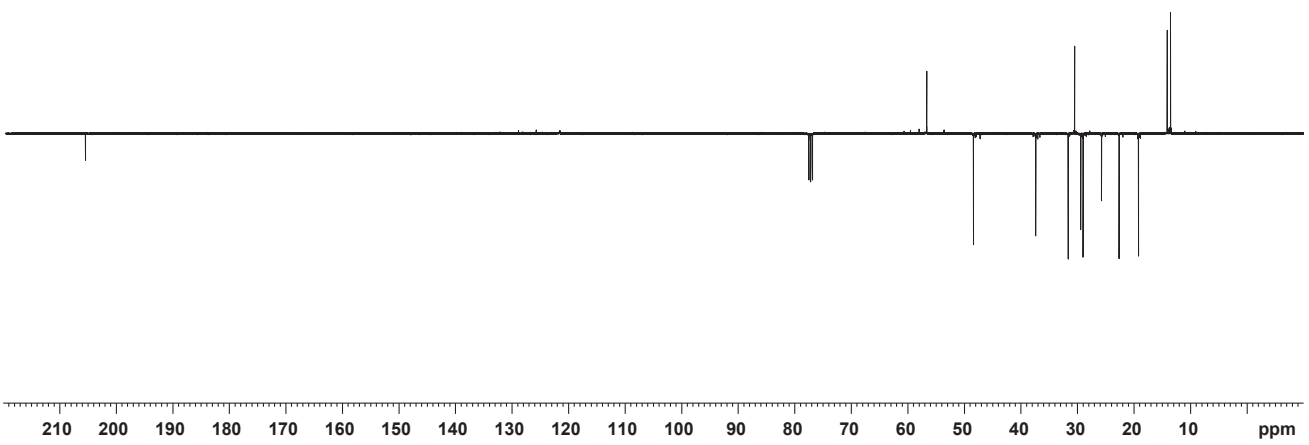
4ai

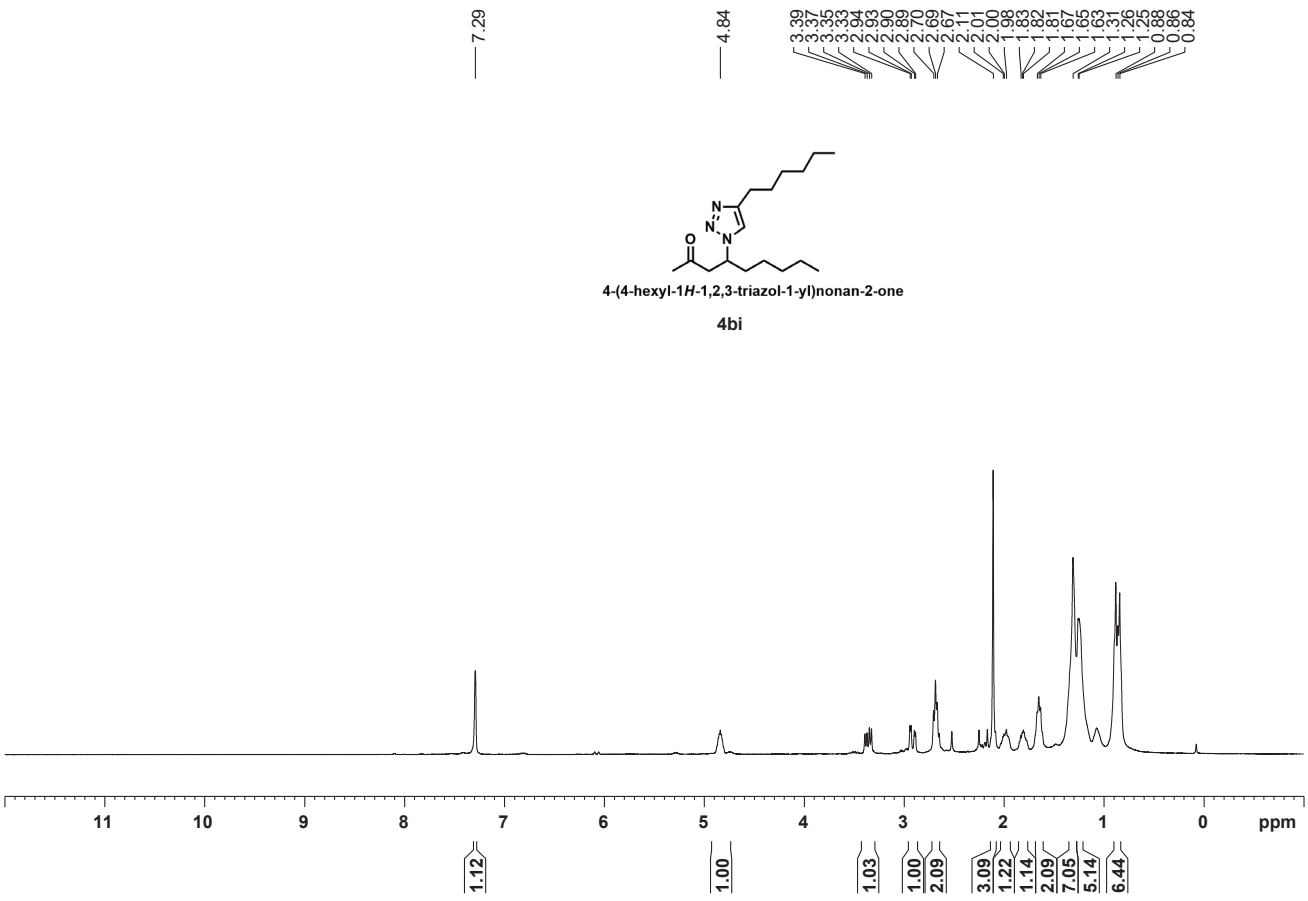




4-(4-hexyl-1*H*-1,2,3-triazol-1-yl)heptan-2-one

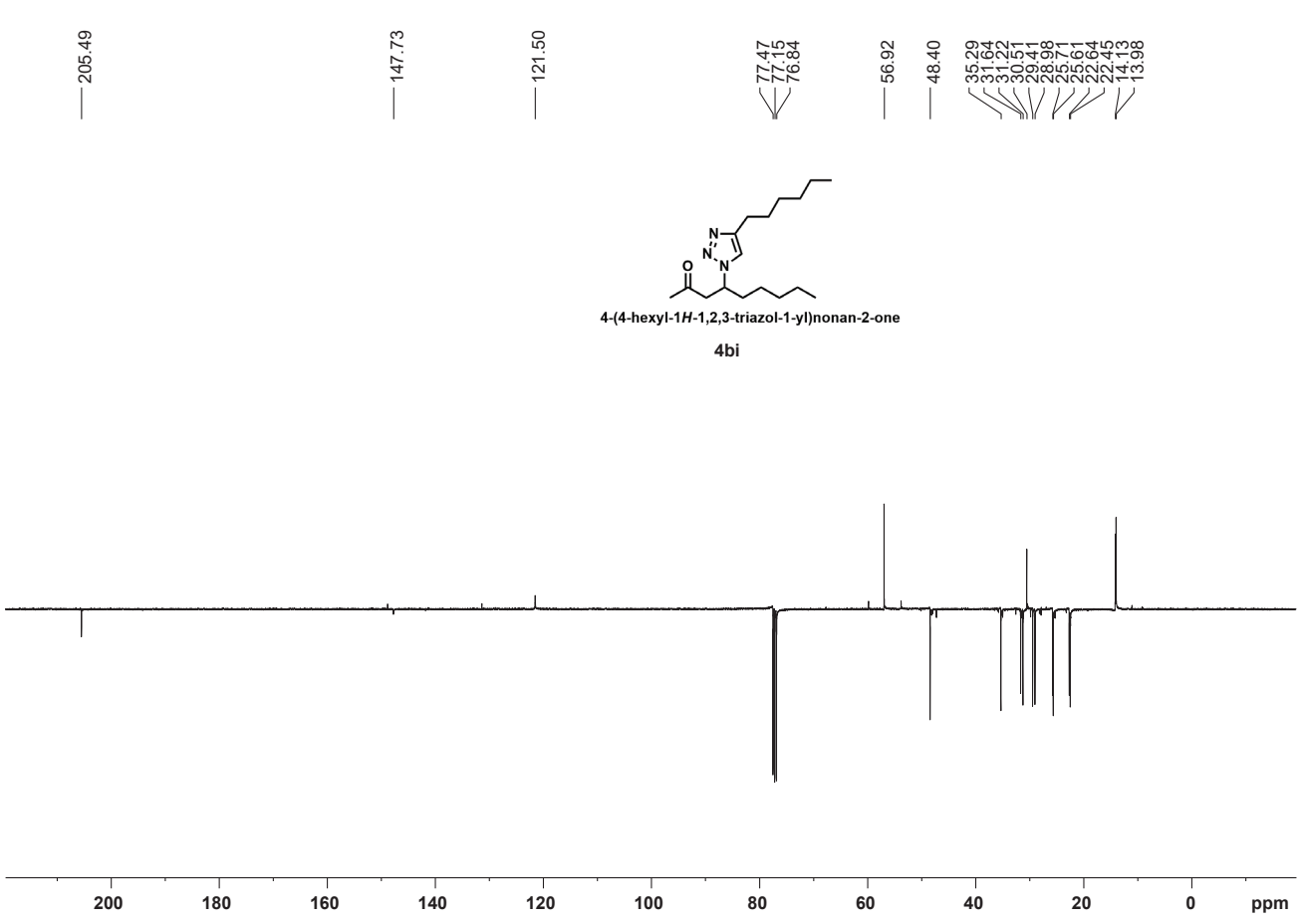
4ai





4-(4-hexyl-1*H*-1,2,3-triazol-1-yl)nonan-2-one

4bi



4-(4-hexyl-1*H*-1,2,3-triazol-1-yl)nonan-2-one

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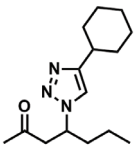
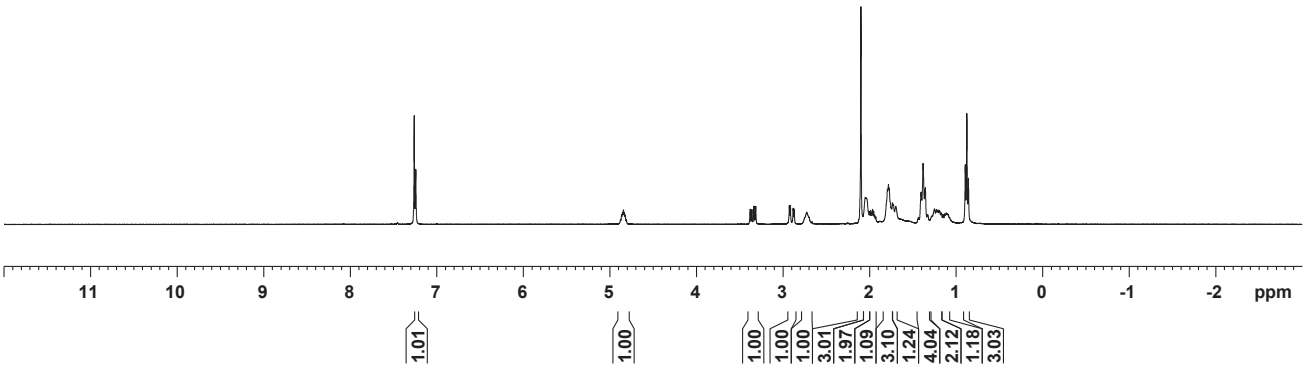
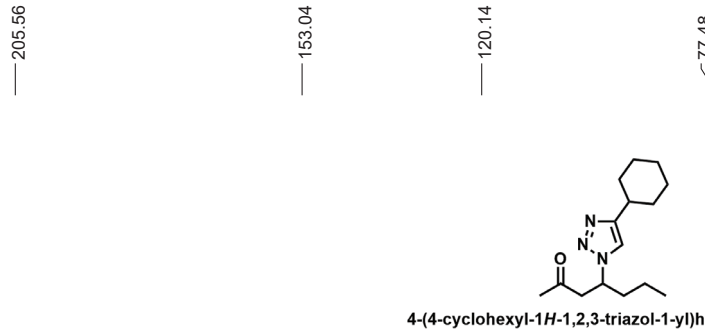


4-(4-cyclohexyl-1*H*-1,2,3-triazol-1-yl)heptan-2-one

4aj





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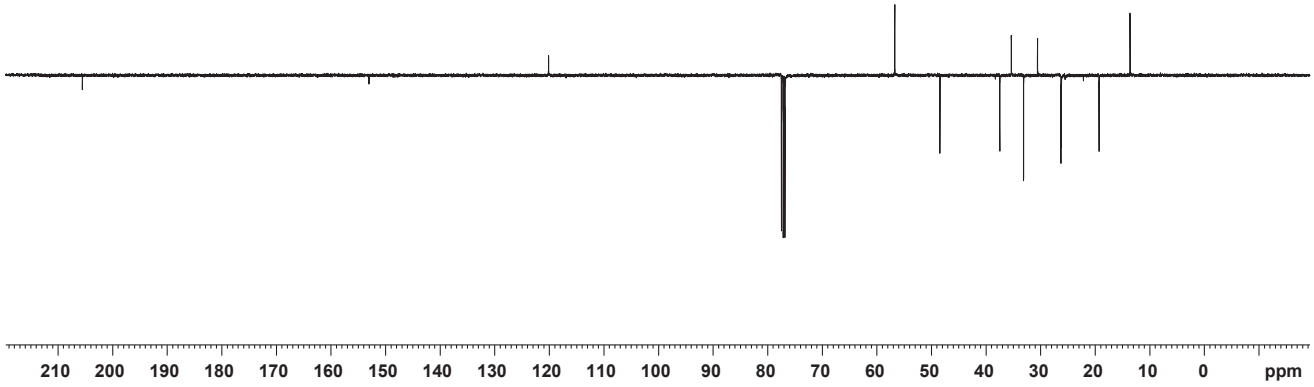

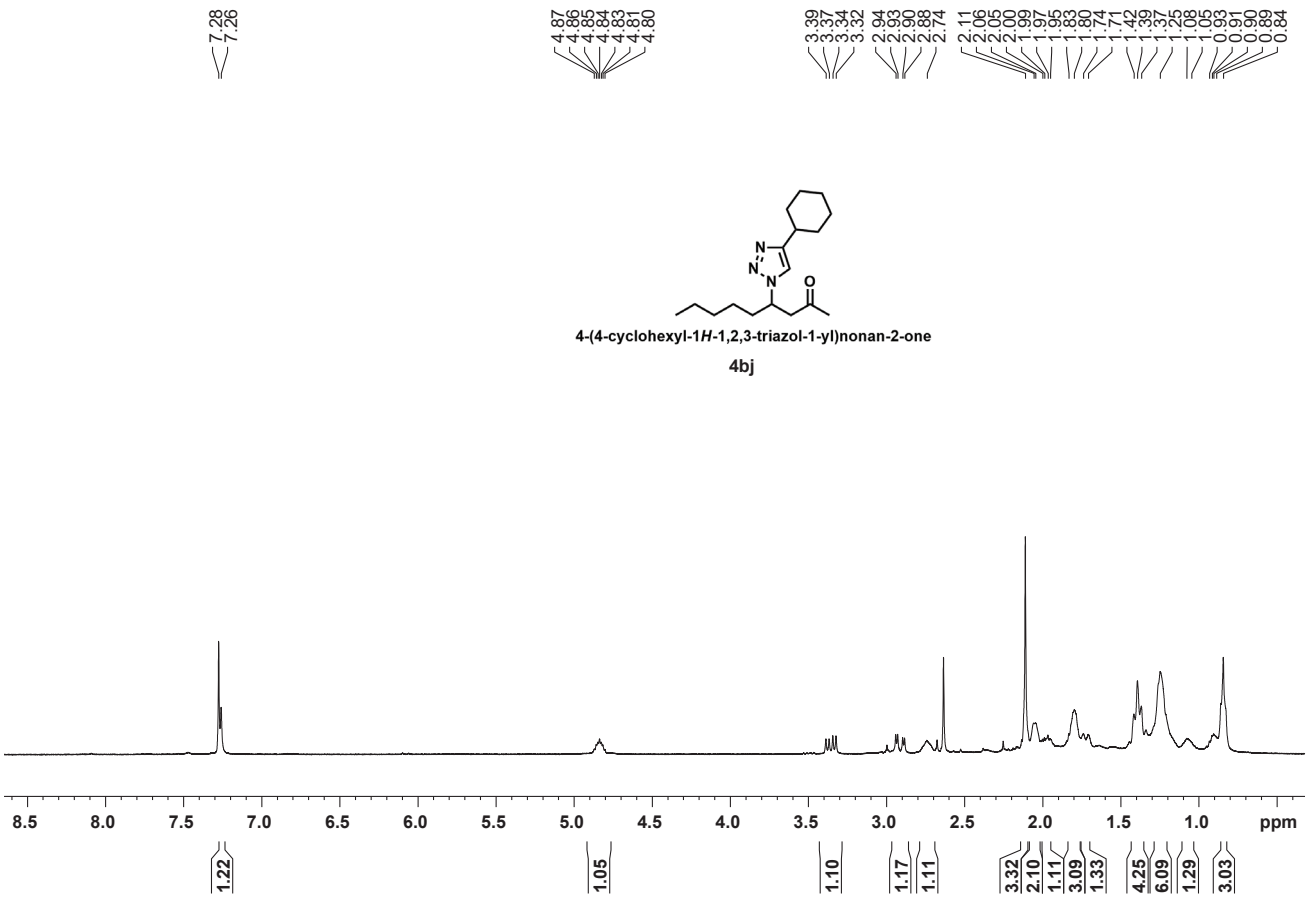
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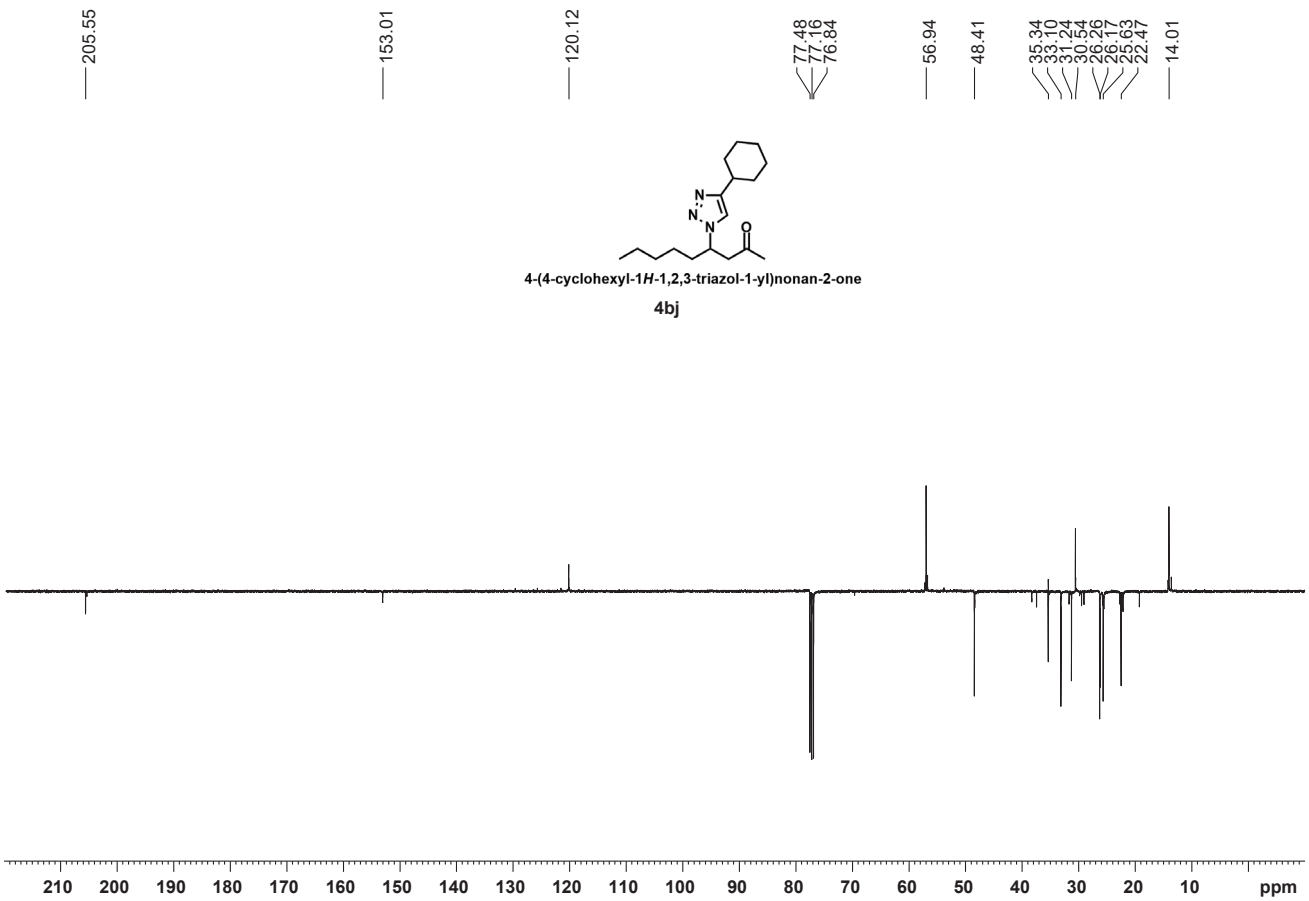
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4-(4-cyclohexyl-1H-1,2,3-triazol-1-yl)nonan-2-one
4bj
210
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ppm