Supporting Information for

Expanding the scope of novel 1,2,3-triazole derivatives as new antiparasitic drug candidates

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[,≠] equal contribution

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Table of Contents

General Information.

All reactions progress was monitored on GP TLC plates. Column chromatography was performed with silica gel 60 (230-400 mesh) under a low pressure of nitrogen, using increasing EtOAc-hexane gradients as a solvent. All the solvents (hexane, ethyl acetate) were distilled before use. Chemical reagents were purchased from commercial suppliers and used without further purification, unless otherwise noted. Solvents were analytical grade or were purified by standard procedures prior to use. ^{1}H and ^{13}C NMR spectra were measured on a 300 MHz Bruker Avance II using $CDCl_3$ as a solvent. Chemical shifts were reported in ppm downfield from tetramethylsilane (δ) as the internal standards and coupling constants are in hertz (Hz). Assignments of proton resonances were confirmed by correlated spectroscopy (Heteronuclear Single Quantum Coherence, HSQC). The following abbreviations are used to indicate NMR signal multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, m = multiplet. High-resolution mass spectra (HRMS) were recorded on a Bruker MicroTOF II spray source. All the melting points were determined in open Pyrex capillaries with an Electrothermal 9000 melting point apparatus.

Table S1. SMILES of compounds tested on this work.

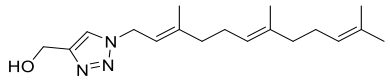
Compound	Smile
1a	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(C(OC)=O)=C1
1b	C/C(CC/C=C(C)/C)=C\CC/C(C)=C\CN1N=NC(C(OC)=O)=C1
1c	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(C2=CC=CC=C2)=C1
1d	C/C(CC\C=C(C)/C)=C\CC/C(C)=C\CN1N=NC(C2=CC=CC=C2)=C1
1e	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CCC)=C1
1f	C/C(CC\C=C(C)/C)=C\CC/C(C)=C\CN1N=NC(CCC)=C1
1g	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CCCCC)=C1
1h	C/C(CC\C=C(C)/C)=C\CC/C(C)=C\CN1N=NC(CCCCC)=C1
1i	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CCCCCCCC)=C1
1j	C/C(CC\C=C(C)/C)=C\CC/C(C)=C\CN1N=NC(CCCCCCCC)=C1
1k	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CO)=C1
1l	C/C(C)=C\CC/C(C)=C/CC/C(C)=C\Cn1nnc(CO)c1
1m	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(C(C)O)=C1
1n	CC(c1nnn(C/C=C(CC/C=C(CC/C=C(C)\C)\C)/C)c1)O
1o	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(C(C)(C)O)=C1
1p	C/C(C)=C\CC/C(C)=C/CC/C(C)=C\Cn1nnc(C(C)(O)C)c1
1q	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CCO)=C1
1r	C/C(C)=C\CC/C(C)=C/CC/C(C)=C\Cn1nnc(CCO)c1
2a	C/C(C)=C/CC/C(C)=C/CN1N=NC(C(OC)=O)=C1
2b	C/C(C)=C/CC/C(C)=C\CN1N=NC(C(OC)=O)=C1
2c	C/C(C)=C/CC/C(C)=C/CN1N=NC(C2=CC=CC=C2)=C1
2d	C/C(C)=C/CC/C(C)=C\CN1N=NC(C2=CC=CC=C2)=C1
2e	C/C(C)=C/CC/C(C)=C/CN1N=NC(CCC)=C1
2f	C/C(C)=C/CC/C(C)=C\CN1N=NC(CCC)=C1
2g	C/C(C)=C/CC/C(C)=C/CN1N=NC(CCCCC)=C1
2h	C/C(C)=C/CC/C(C)=C\CN1N=NC(CCCCC)=C1
2i	C/C(C)=C/CC/C(C)=C/CN1N=NC(CCCCCCCC)=C1
2j	C/C(C)=C/CC/C(C)=C\CN1N=NC(CCCCCCCC)=C1
3a	C/C(C)=C/CN1N=NC(C(OC)=O)=C1
3b	C/C(C)=C/CN1N=NC(C2=CC=CC=C2)=C1
3c	C/C(C)=C/CN1N=NC(CCC)=C1
3d	C/C(C)=C/CN1N=NC(CCCCC)=C1

Table S1 (cont´). SMILES of compounds tested on this work.

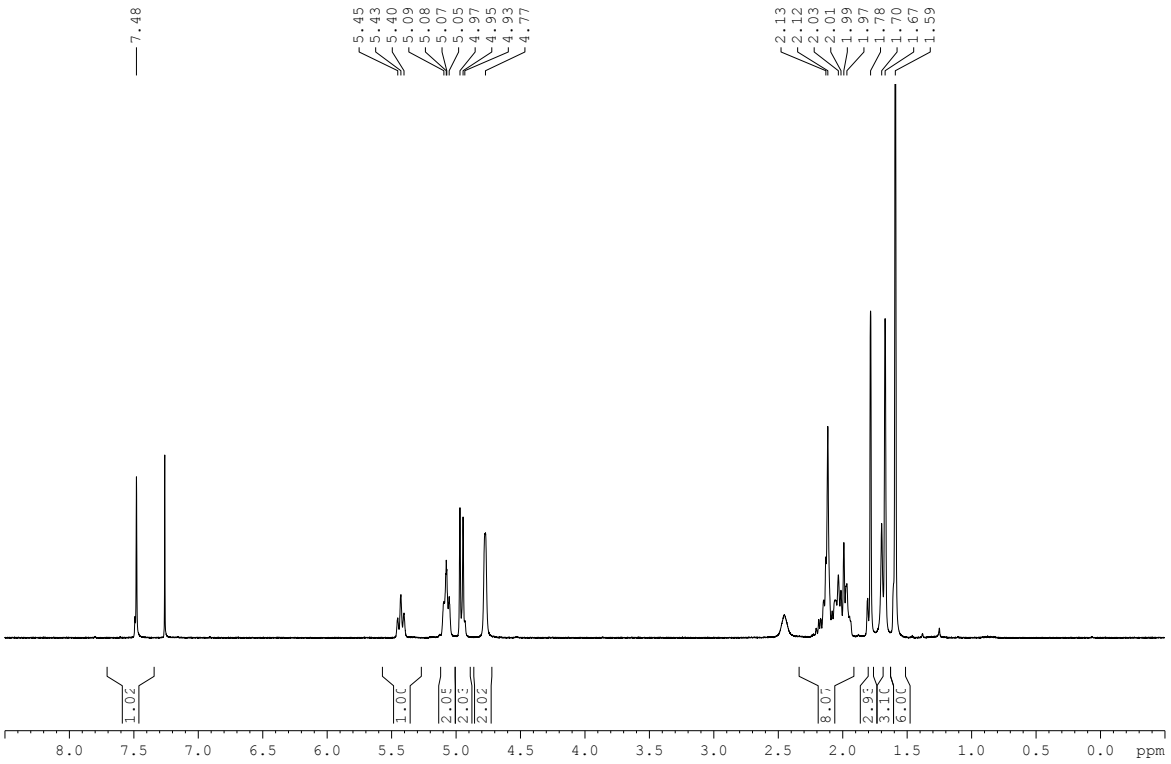
Compound	Smile
3e	C/C(C)=C/CN1N=NC(CCCCCCCC)=C1
4a	C1(C3=CN(N=N3)C/C=C/C2=CC=CC=C2)=CC=CC=C1
4b	CCCC2=CN(N=N2)C/C=C/C1=CC=CC=C1
4c	CCCCCC2=CN(N=N2)C/C=C/C1=CC=CC=C1
4d	CCCCCCCCC2=CN(N=N2)C/C=C/C1=CC=CC=C1
4e	CCCCCCCCCCC2=CN(N=N2)C/C=C/C1=CC=CC=C1
5a	O=C(C2=CN(N=N2)CC1=CC=CC=C1)OC
5b	C1(CN2N=NC(C3=CC=CC=C3)=C2)=CC=CC=C1
5c	CCCC2=CN(N=N2)CC1=CC=CC=C1
5d	CCCCCC2=CN(N=N2)CC1=CC=CC=C1
5e	CCCCCCCCC2=CN(N=N2)CC1=CC=CC=C1
5f	O=C(C2=CN(N=N2)CC1=CC=CC=C1)O
5g	OCC2=CN(N=N2)CC1=CC=CC=C1
5h	CCCCCCCCCCC2=CN(N=N2)CC1=CC=CC=C1
6a	CCOC(CCN(N=N1)C=C1C(OC)=O)=O
6b	CCOC(CN1N=NC(CCC)=C1)=O
6c	O=C(CN1N=NC(CCCCC)=C1)OCC
6d	CCOC(CN1N=NC(CCCCCCCC)=C1)=O
7a	O=C(C2=CN(N=N2)CCCC1=CC=CC=C1)OC
7b	C(Cc1ccccc1)Cn3cc(c2ccccc2)nn3
7c	CCCC2=CN(N=N2)CCCC1=CC=CC=C1
7d	CCCCCC2=CN(N=N2)CCCC1=CC=CC=C1
7e	CCCCCCCCC2=CN(N=N2)CCCC1=CC=CC=C1
7f	OCC2=CN(N=N2)CCCC1=CC=CC=C1
7g	CCCCCCCCCCC2=CN(N=N2)CCCC1=CC=CC=C1
7h	CC(O)c2cn(CCCc1ccccc1)nn2
8a	O=C(OC)C1=CN(N=N1)CCCCCCCC
8b	OCC1=CN(N=N1)CCCCCCCC
9a	O=C(OC)C1=CN(N=N1)CCCCCCCCCC
9b	OCC1=CN(N=N1)CCCCCCCCCC
10a	O=C(OC)C1=CN(N=N1)CCCCCCCCCCCCC
10b	OCC1=CN(N=N1)CCCCCCCCCCCCC

Copies of Spectra

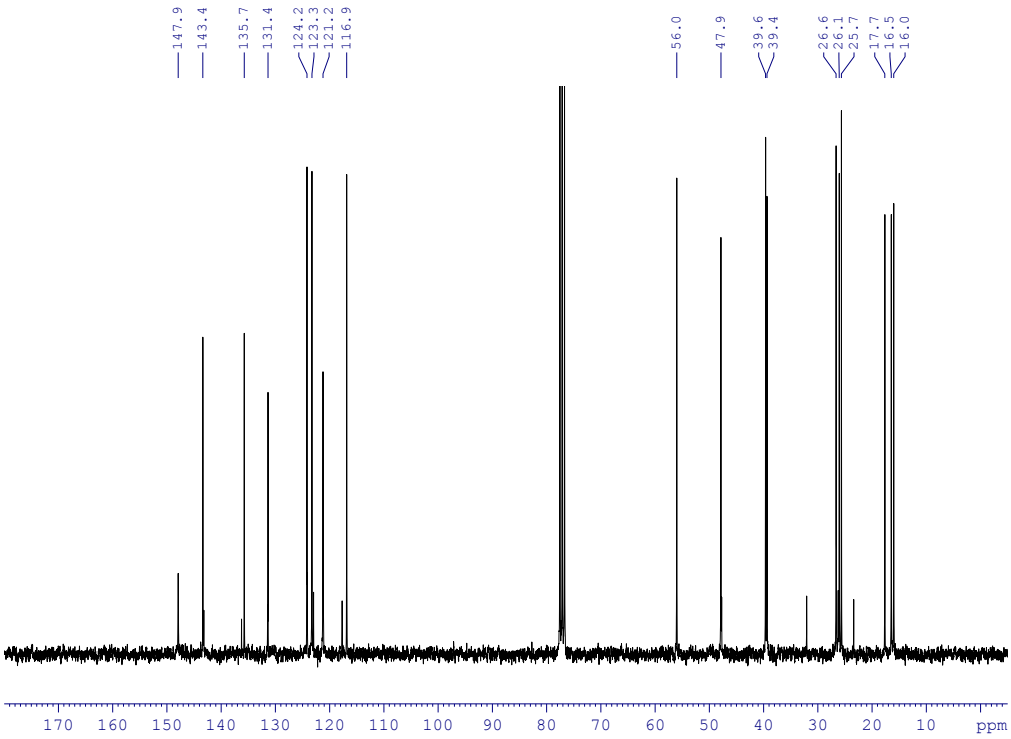
Compound **1k**



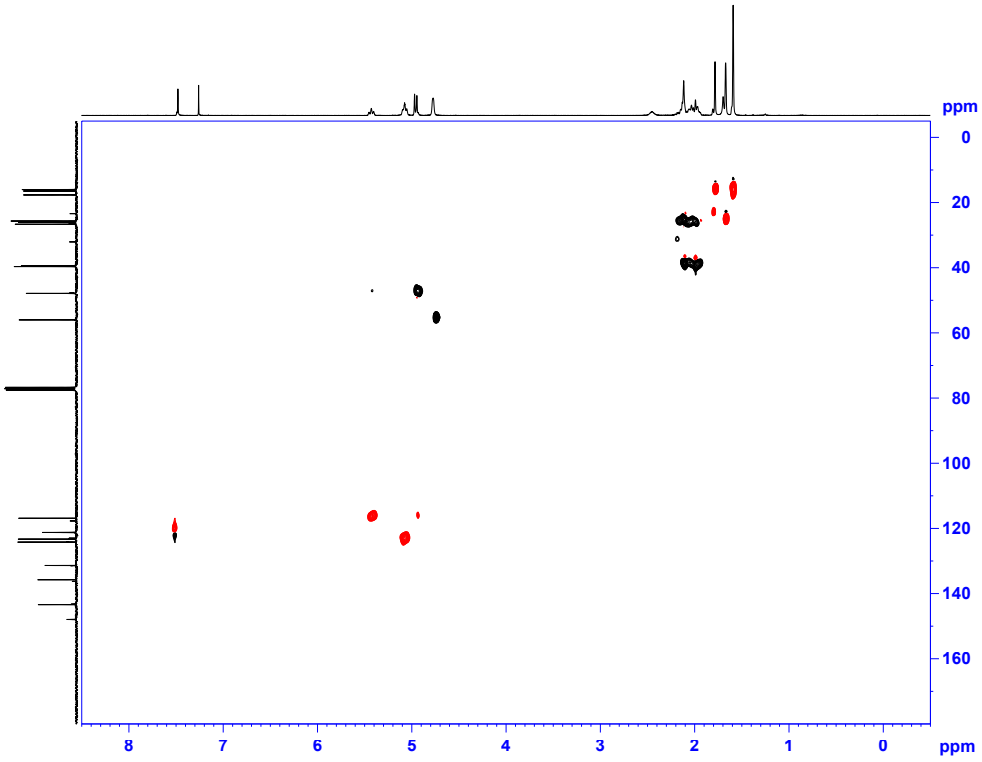
^{1}H NMR (300 MHz, $CDCl_3$)



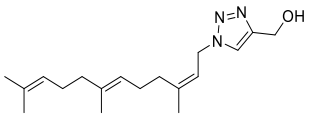
^{13}C NMR (75 MHz, $CDCl_3$)



HSQC ($CDCl_3$)



Compound **1l**



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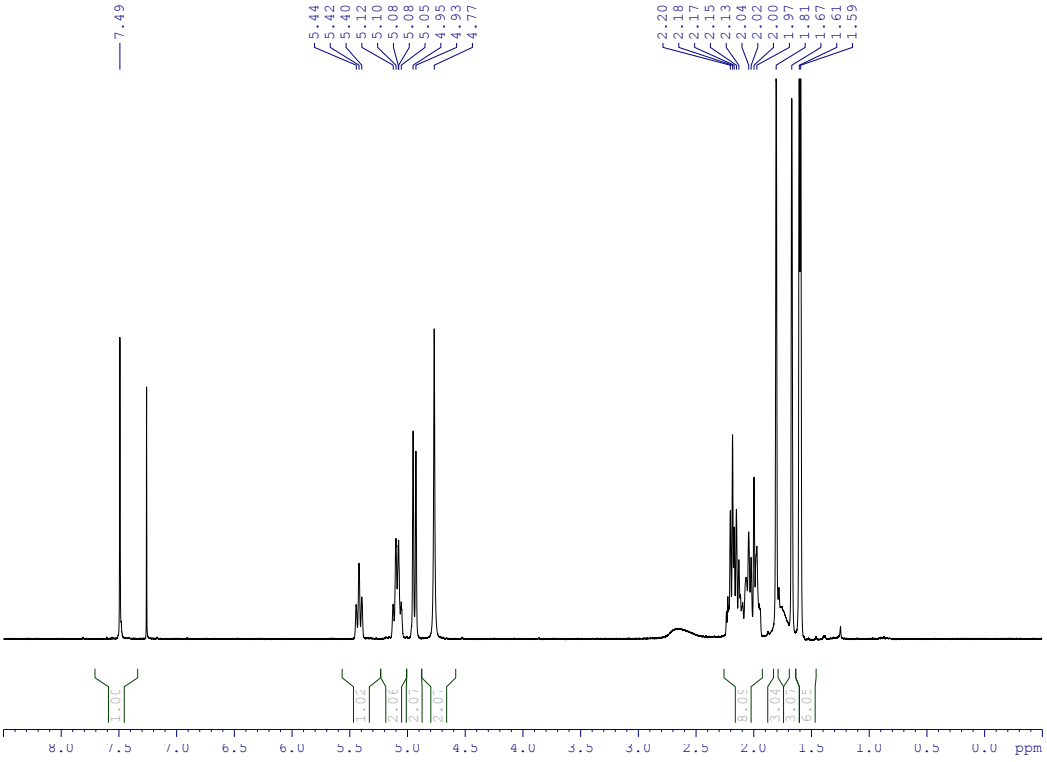
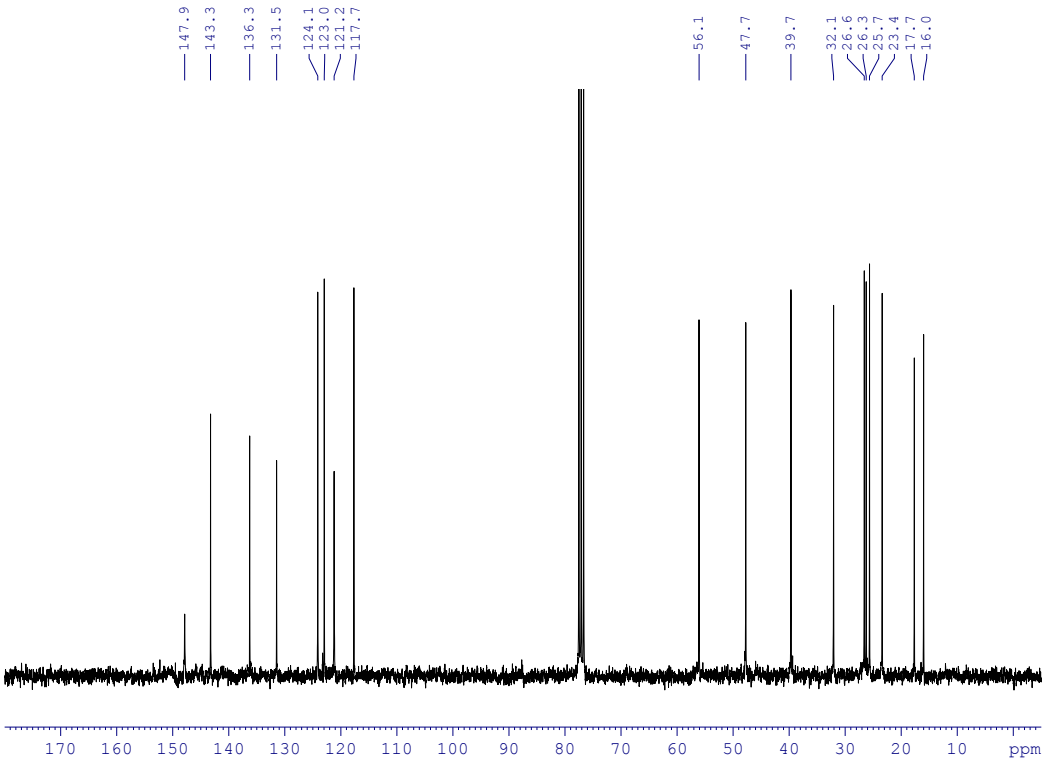
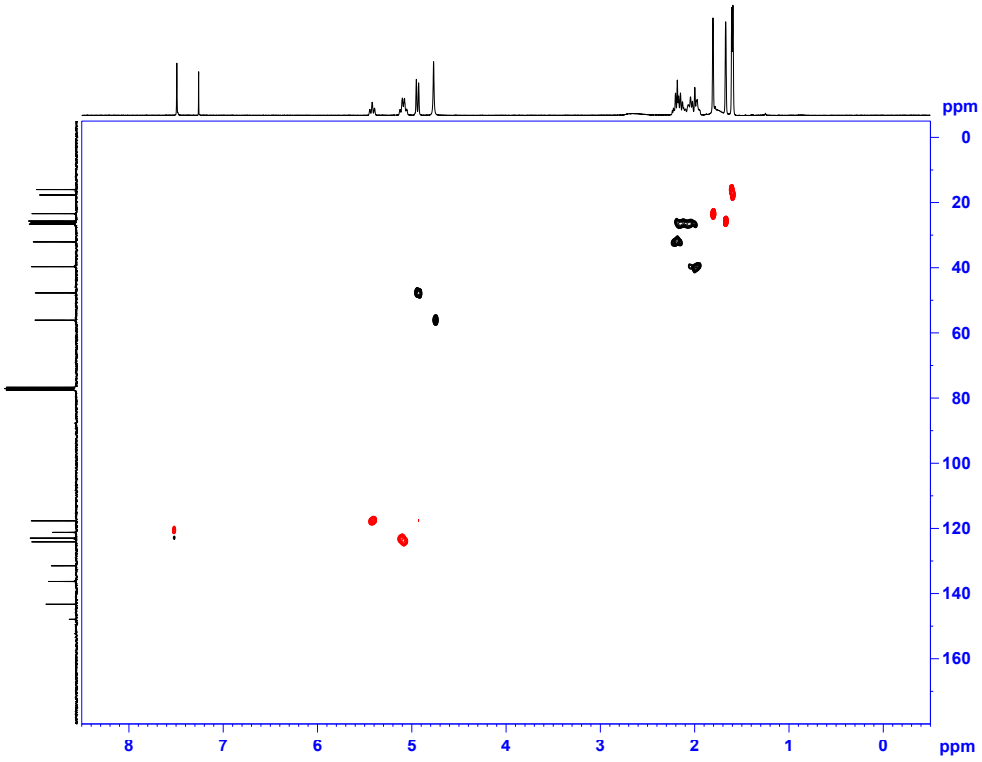


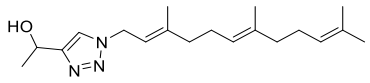
^{13}C NMR (75 MHz, $CDCl_3$)



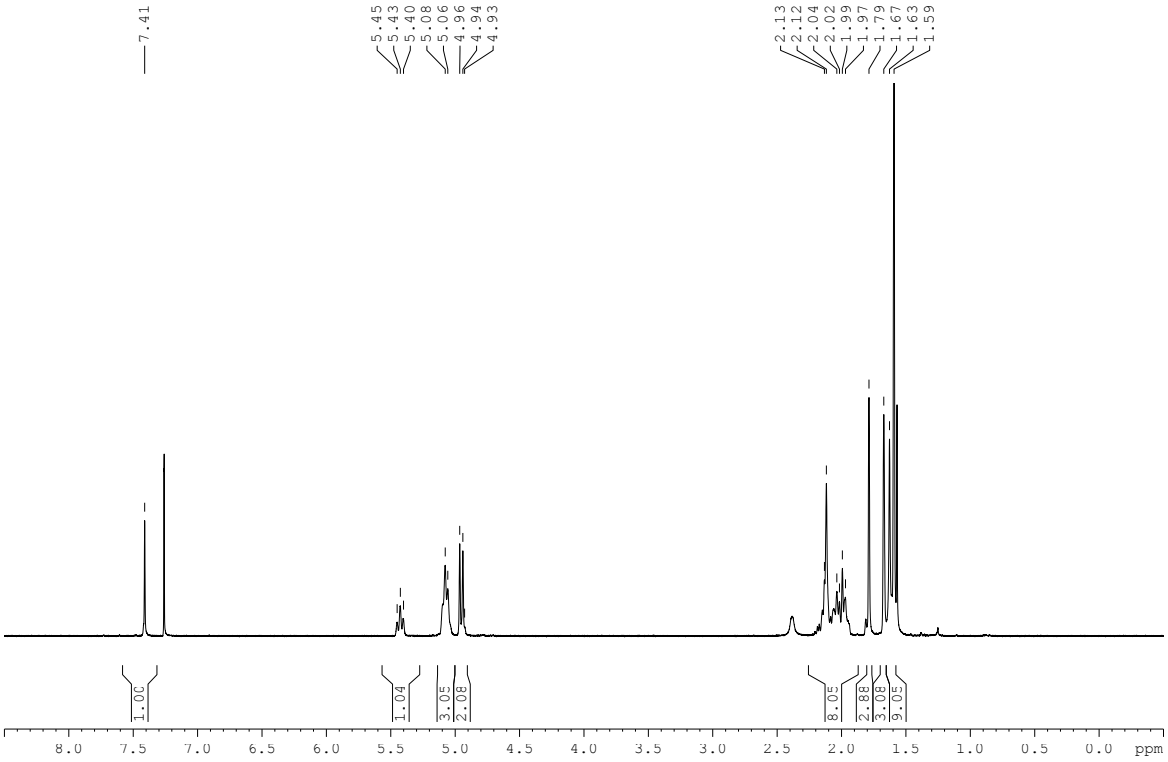
HSQC ($CDCl_3$)



Compound **1m**



^{1}H NMR (300 MHz, $CDCl_3$)



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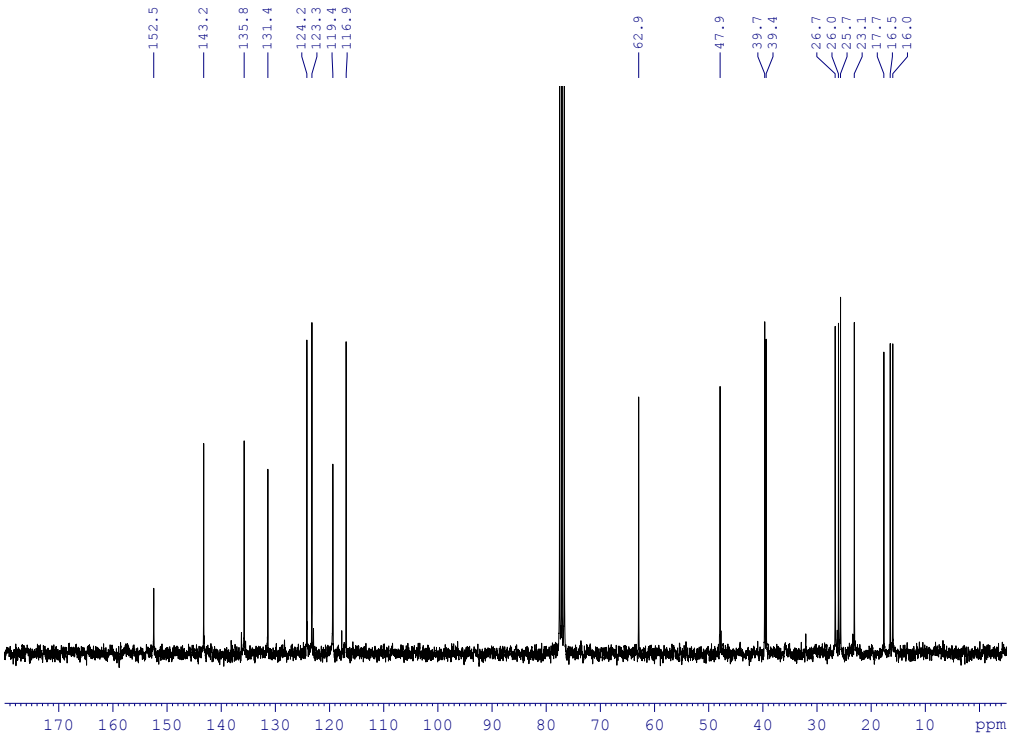

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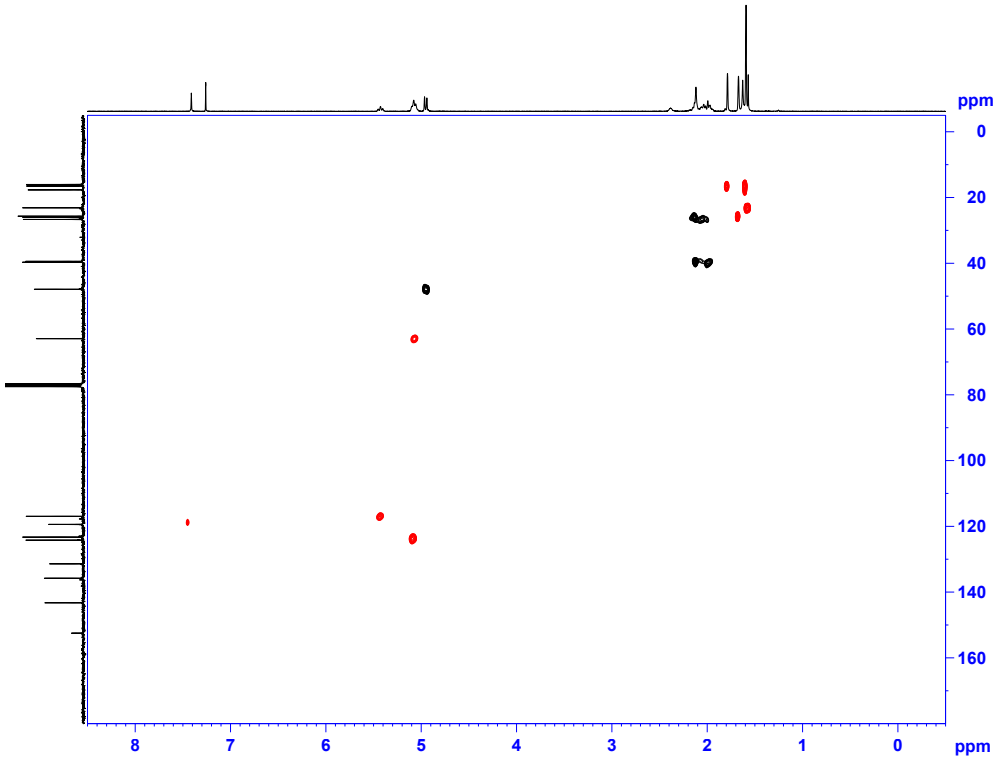
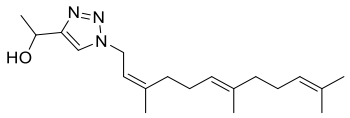
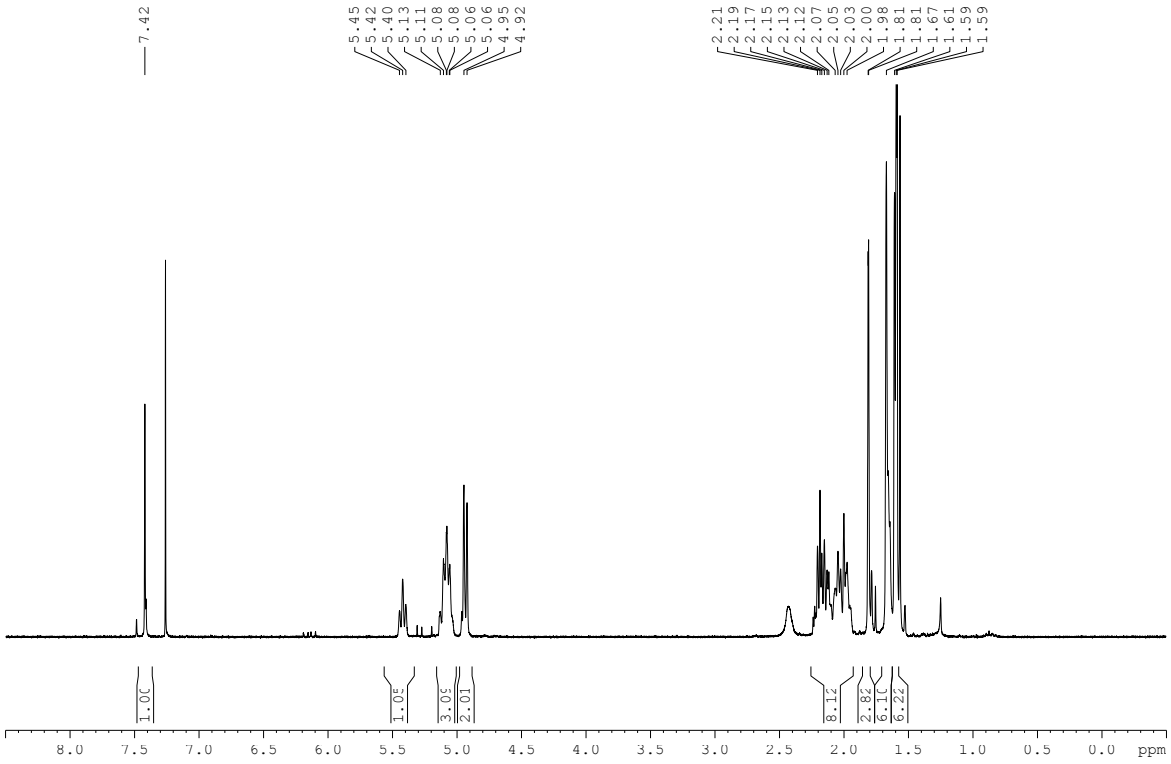


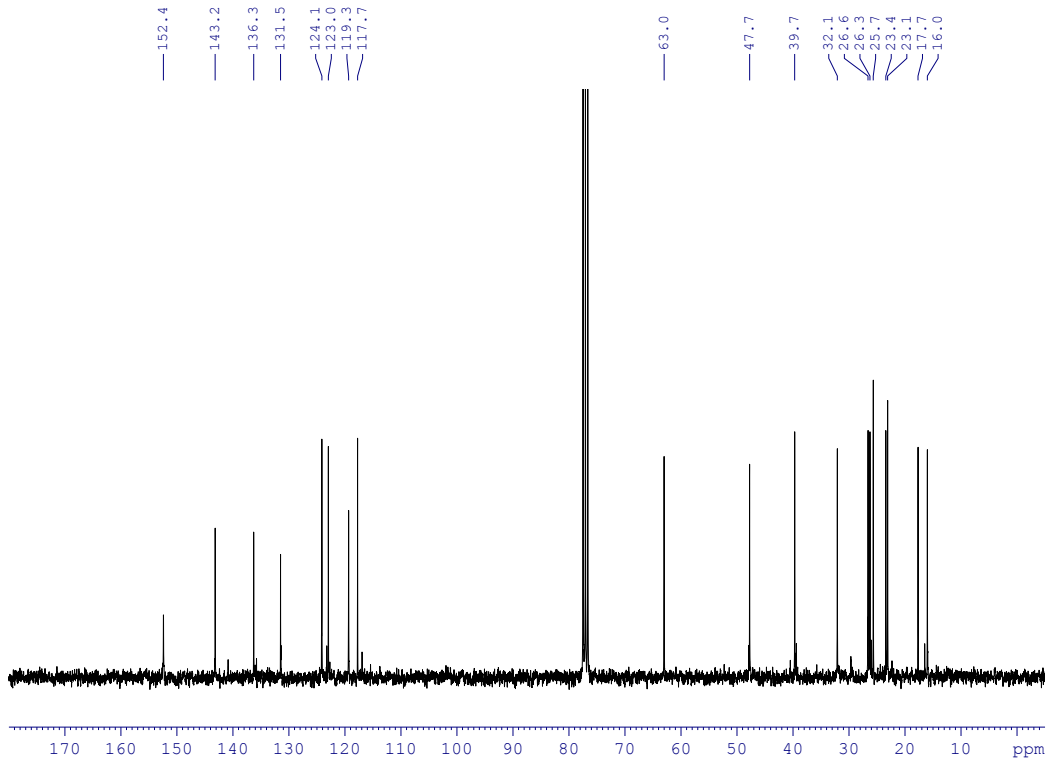
Compound **1n**



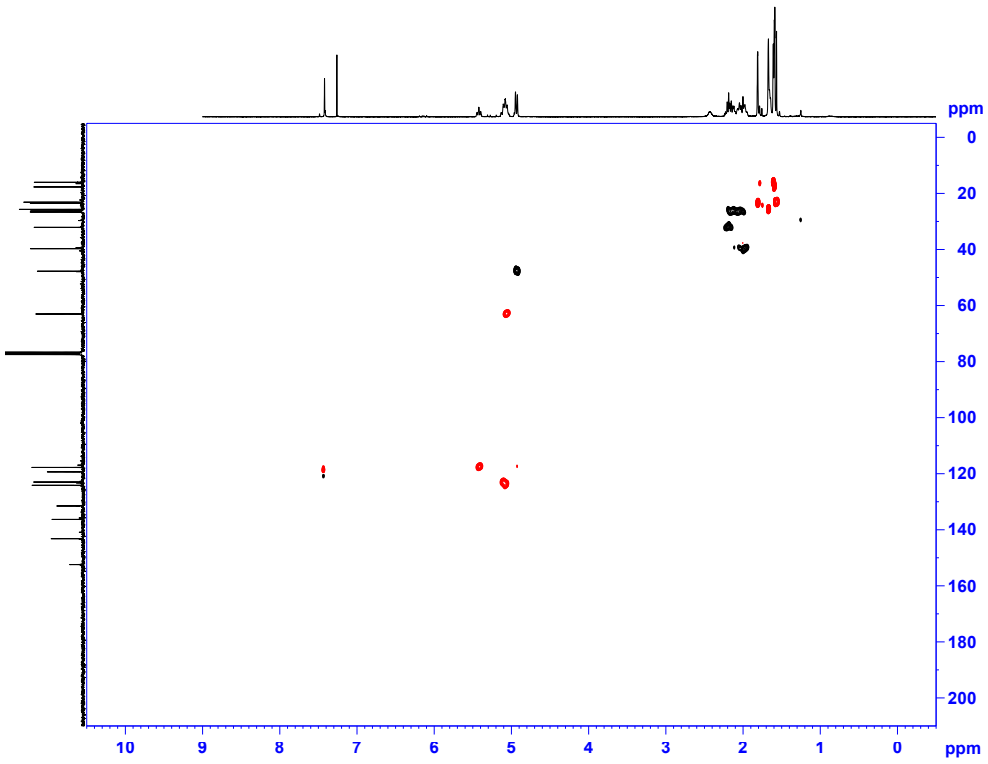
^{1}H NMR (300 MHz, $CDCl_3$)



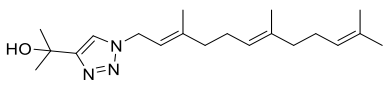
^{13}C NMR (75 MHz, $CDCl_3$)



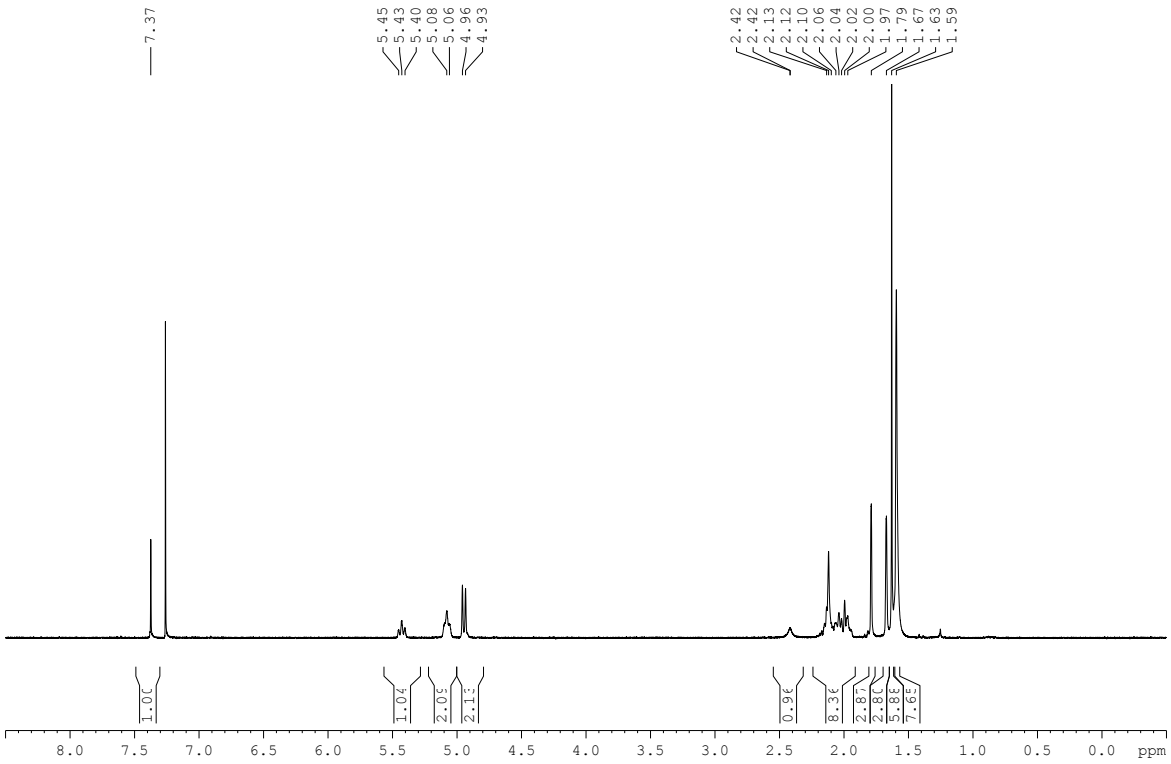
HSQC ($CDCl_3$)



Compound **1o**



^{1}H NMR (300 MHz, $CDCl_3$)



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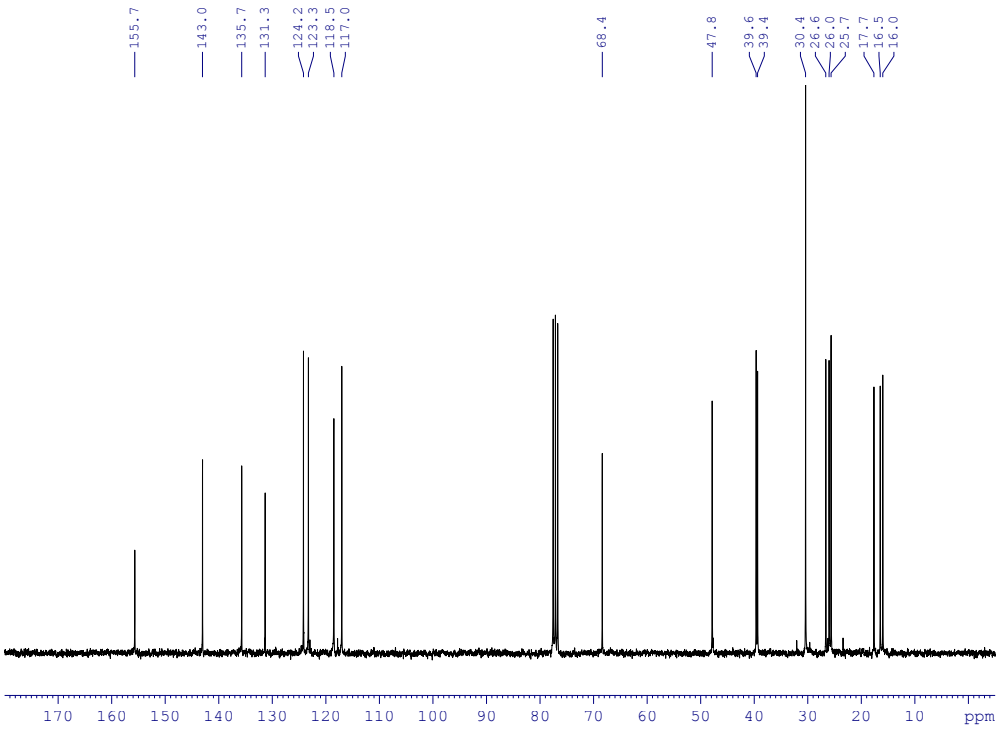
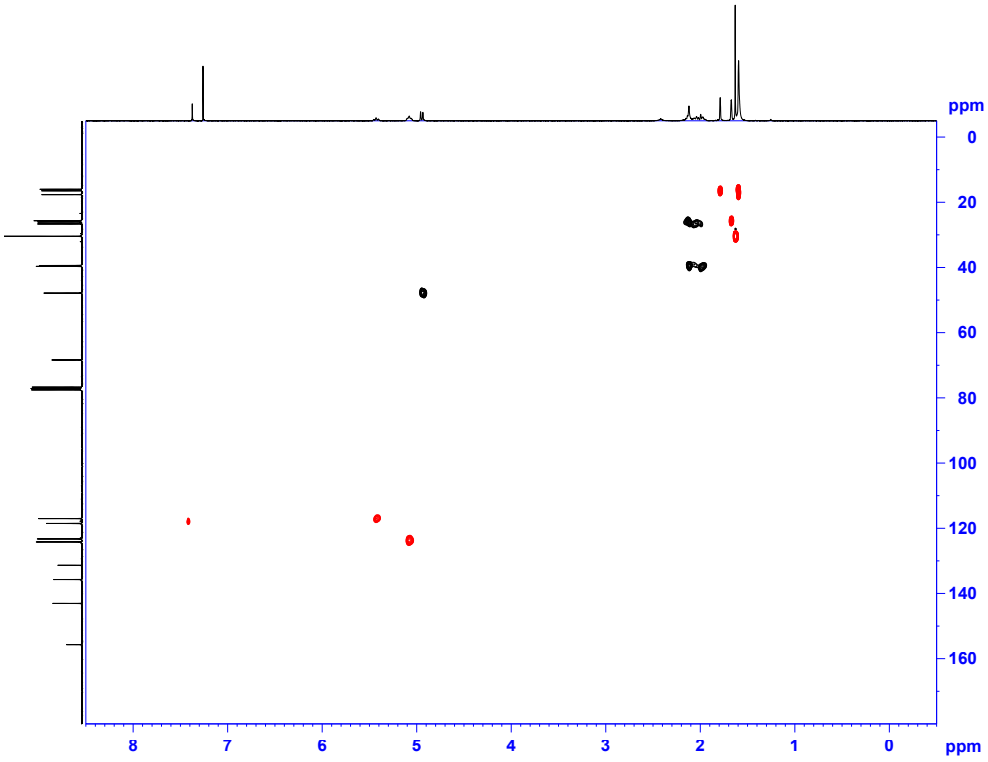
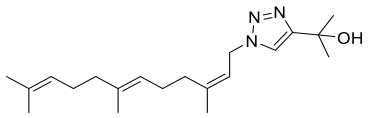


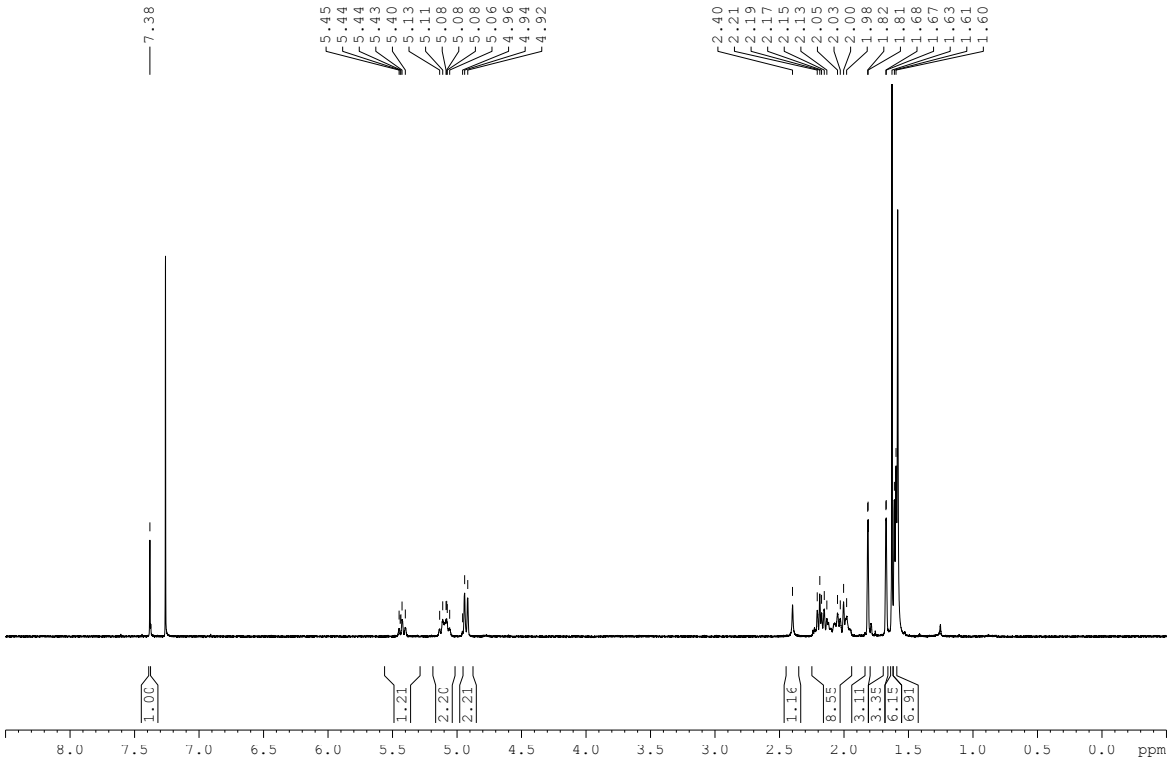
HSQC ($CDCl_3$)



Compound **1p**



^{1}H NMR (300 MHz, $CDCl_3$)



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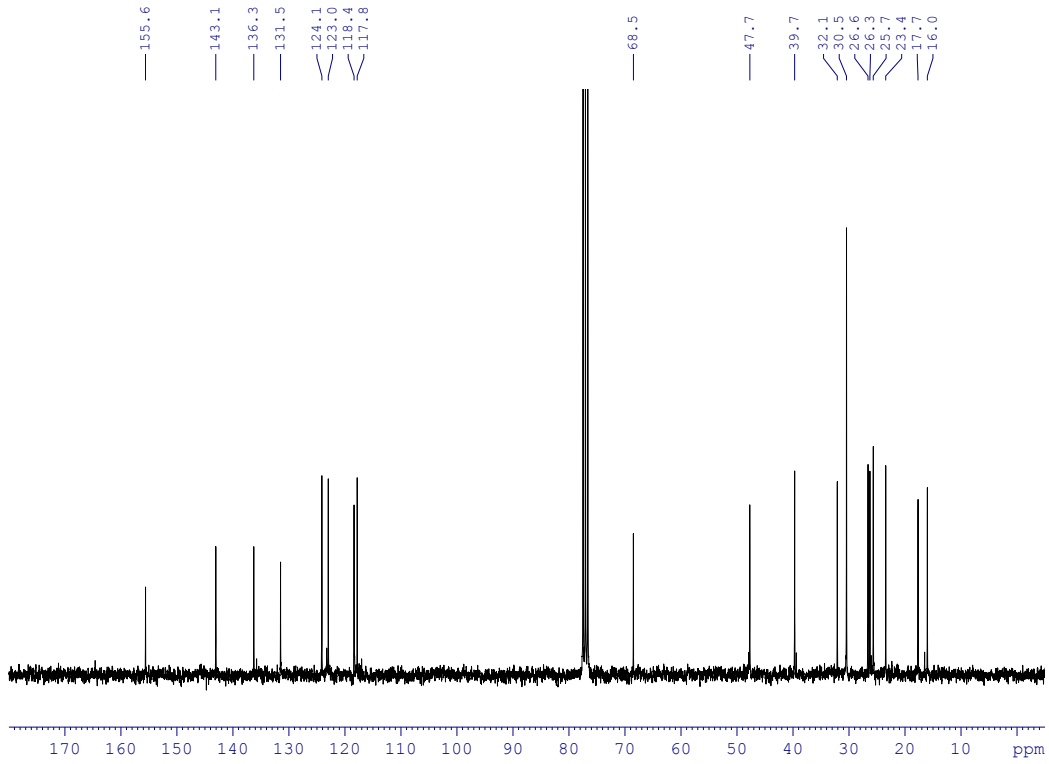

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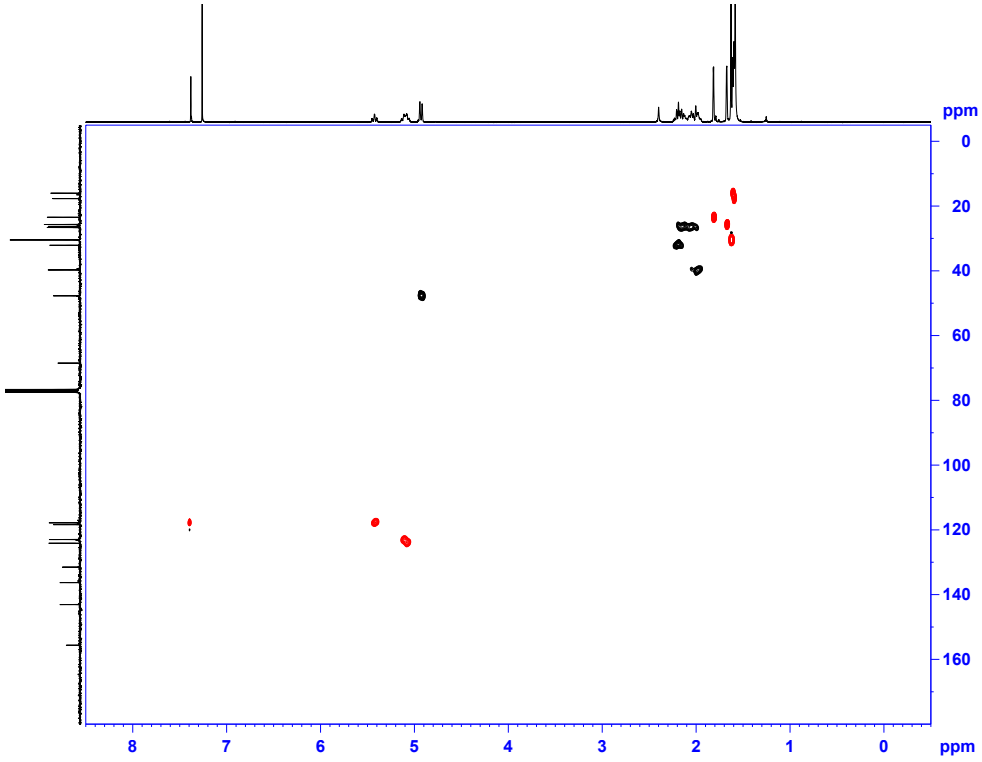
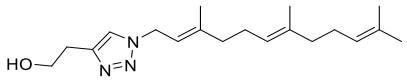
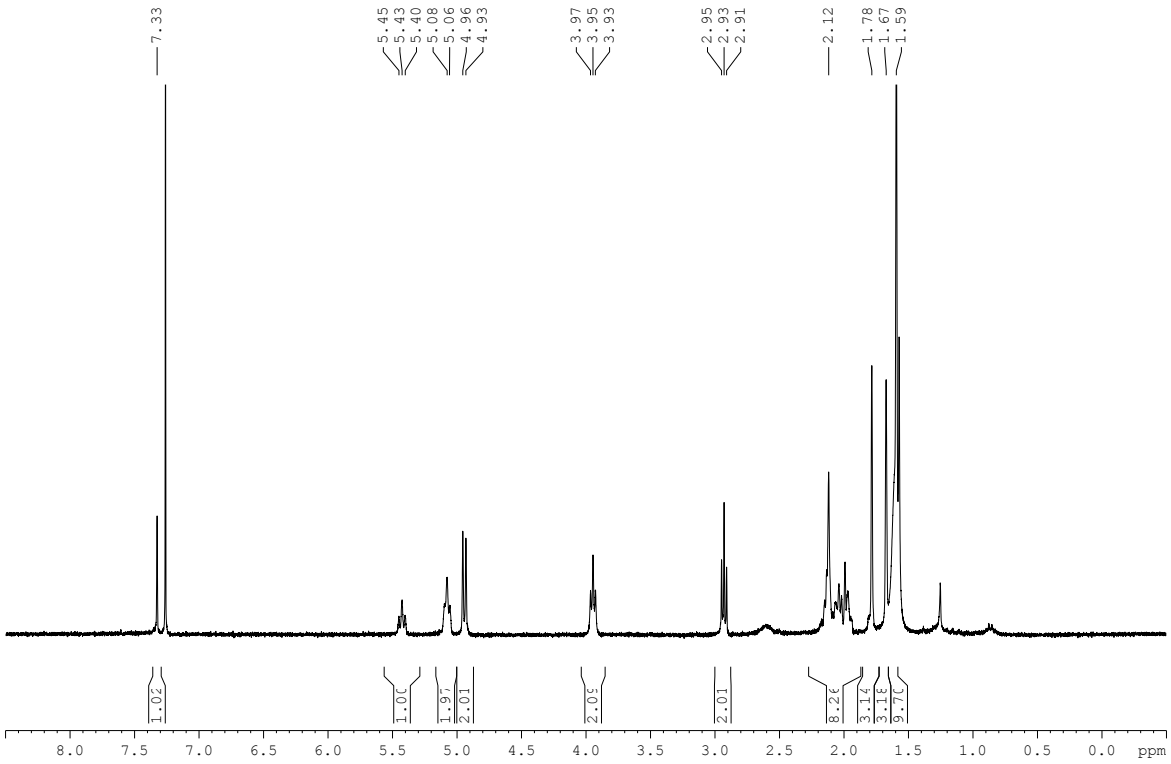


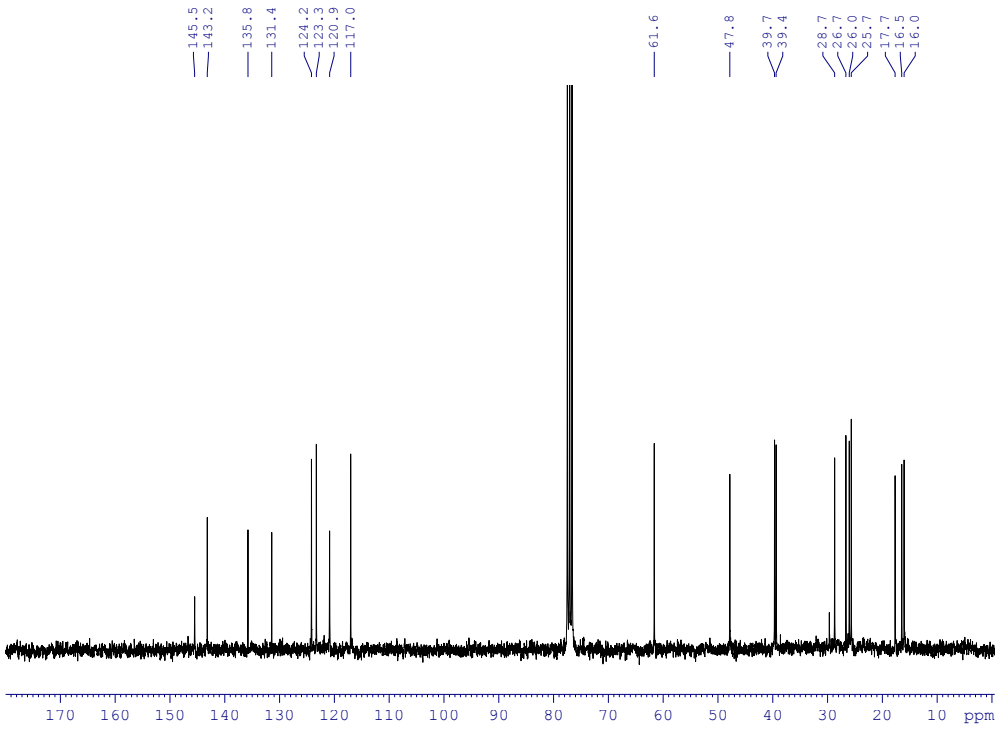
Compound **1q**



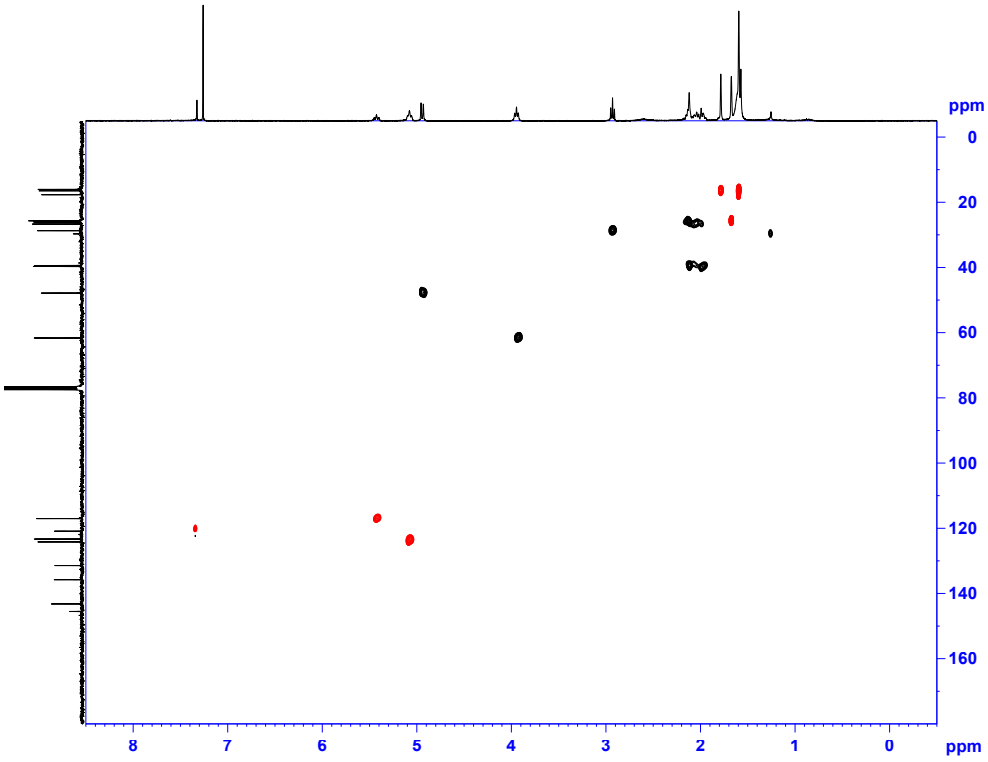
^{1}H NMR (300 MHz, $CDCl_3$)



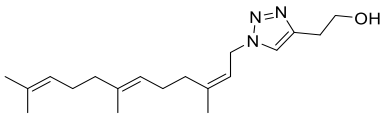
^{13}C NMR (75 MHz, $CDCl_3$)



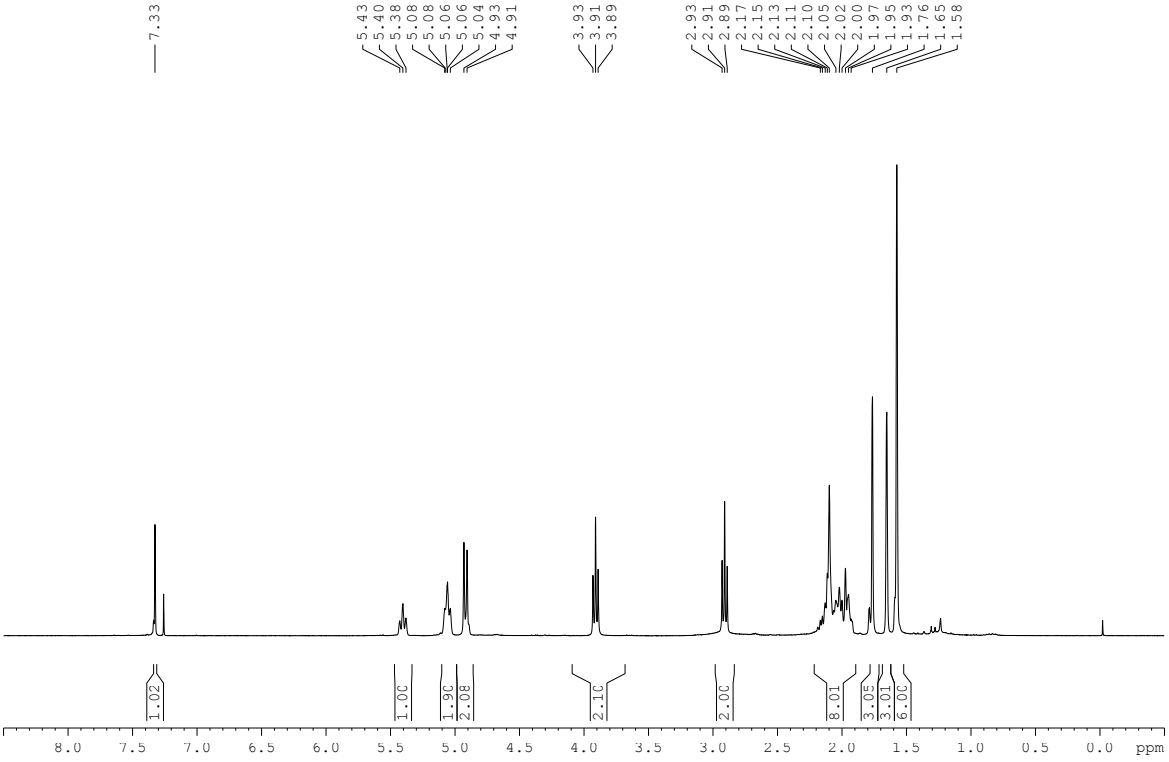
HSQC ($CDCl_3$)



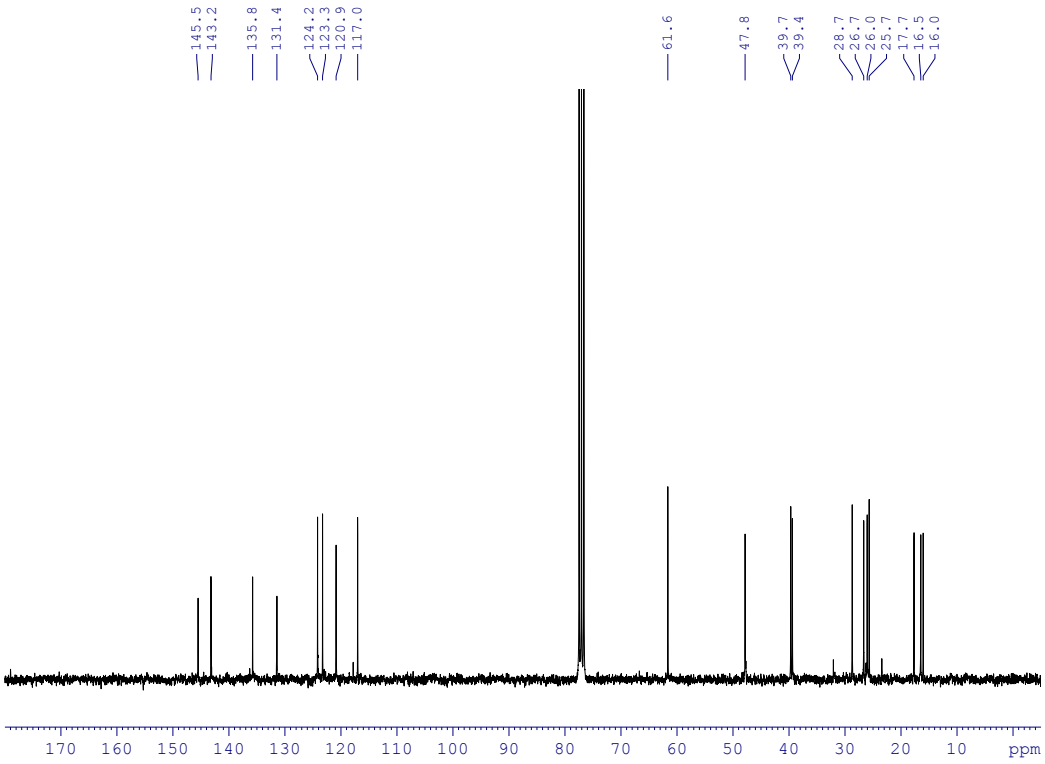
Compound **1r**



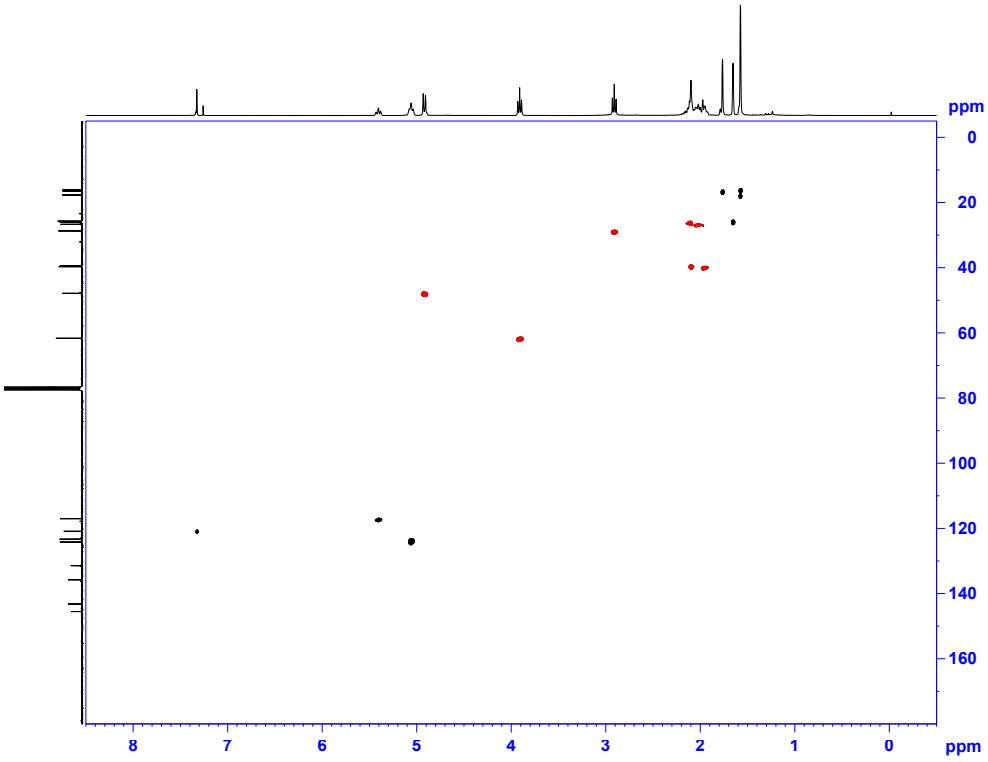
^{1}H NMR (300 MHz, $CDCl_3$)



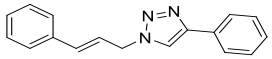
^{13}C NMR (75 MHz, $CDCl_3$)



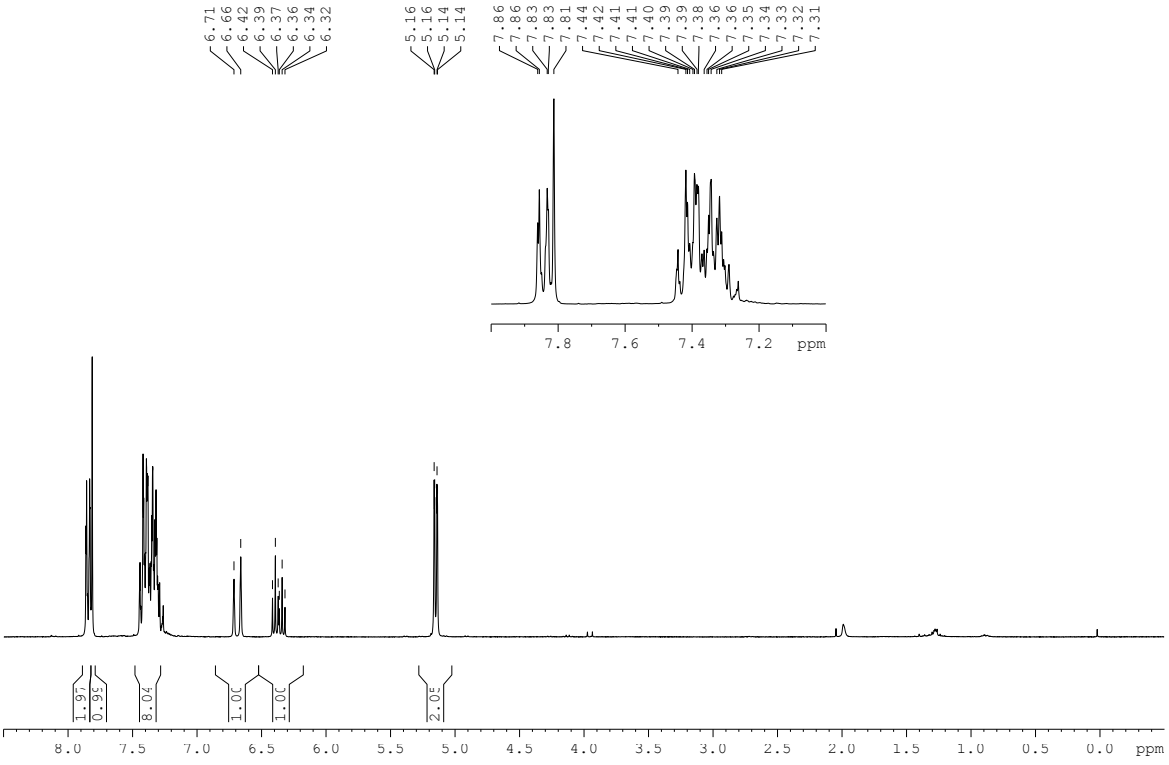
HSQC ($CDCl_3$)



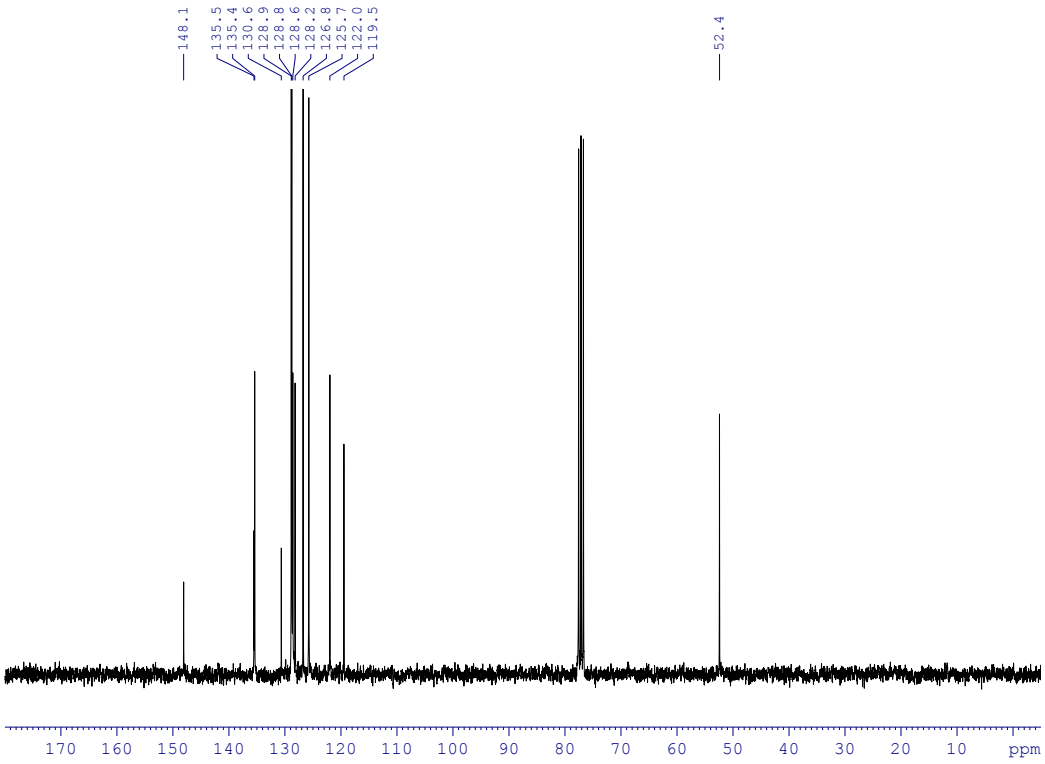
Compound **4a**



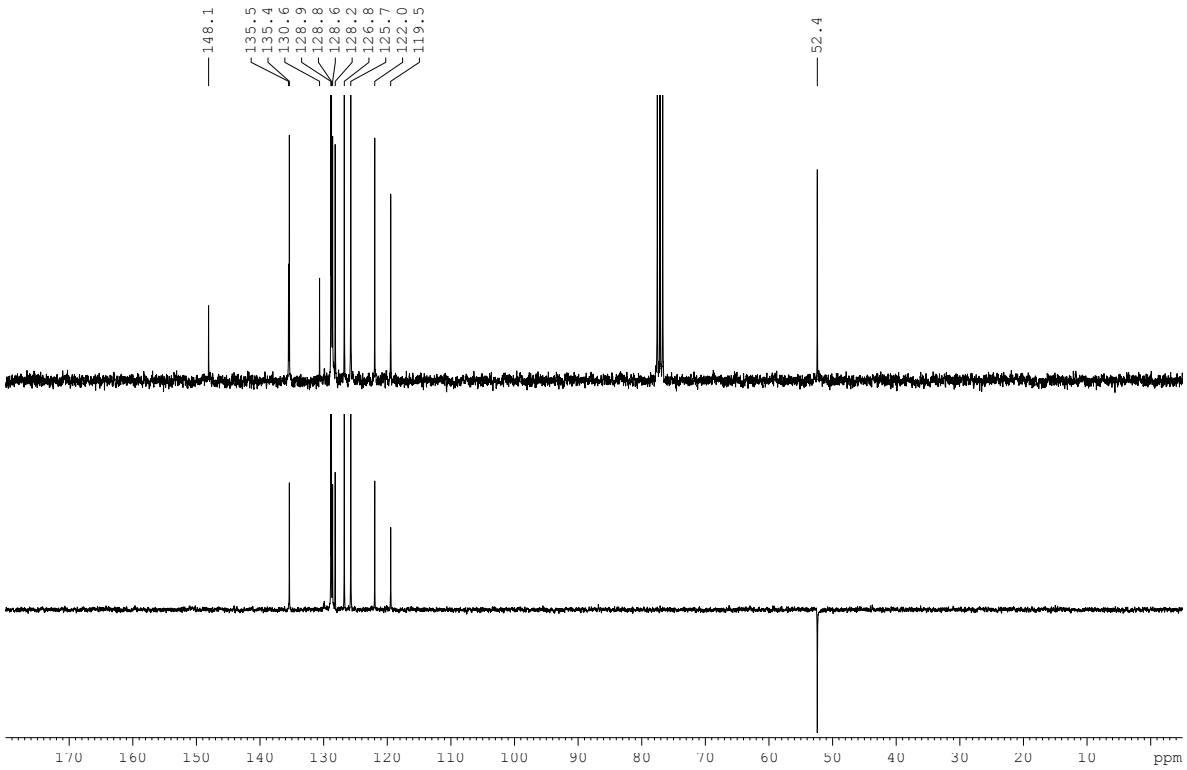
^{1}H NMR (300 MHz, $CDCl_3$)



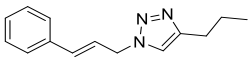
^{13}C NMR (75 MHz, $CDCl_3$)



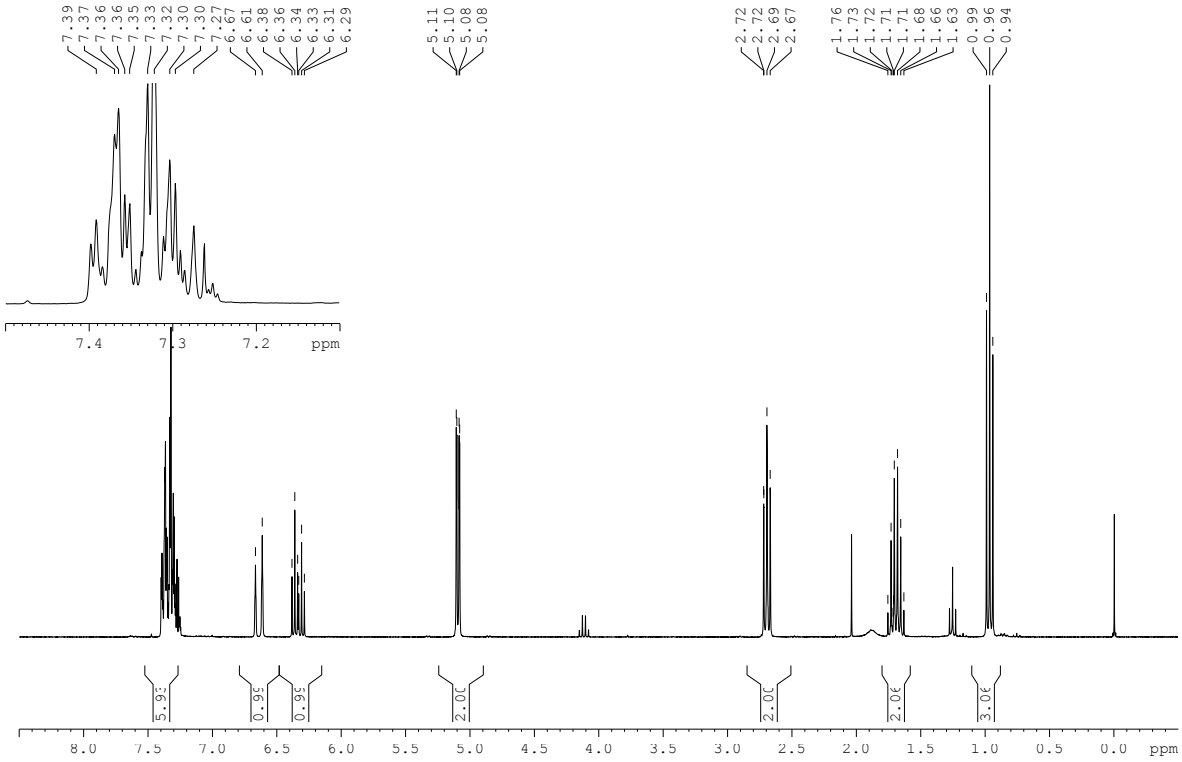
DEPT ($CDCl_3$)


148.1
135.5
135.4
130.6
128.9
128.8
128.6
128.2
126.8
125.7
122.0
119.5
52.4
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

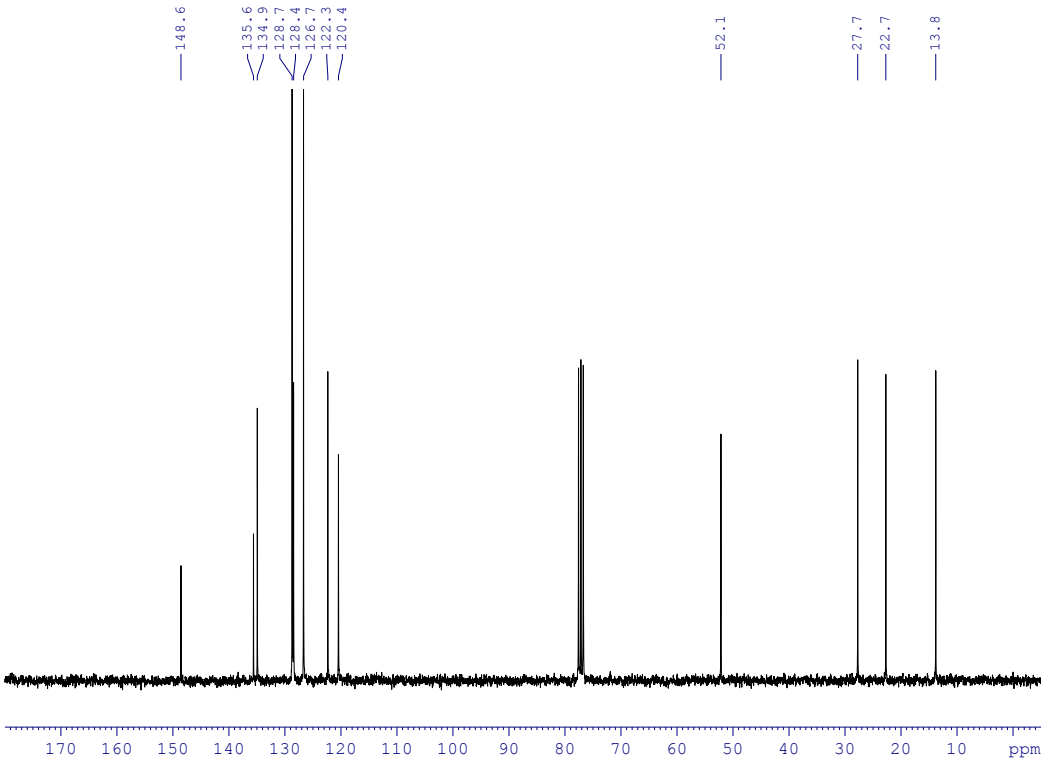
Compound **4b**



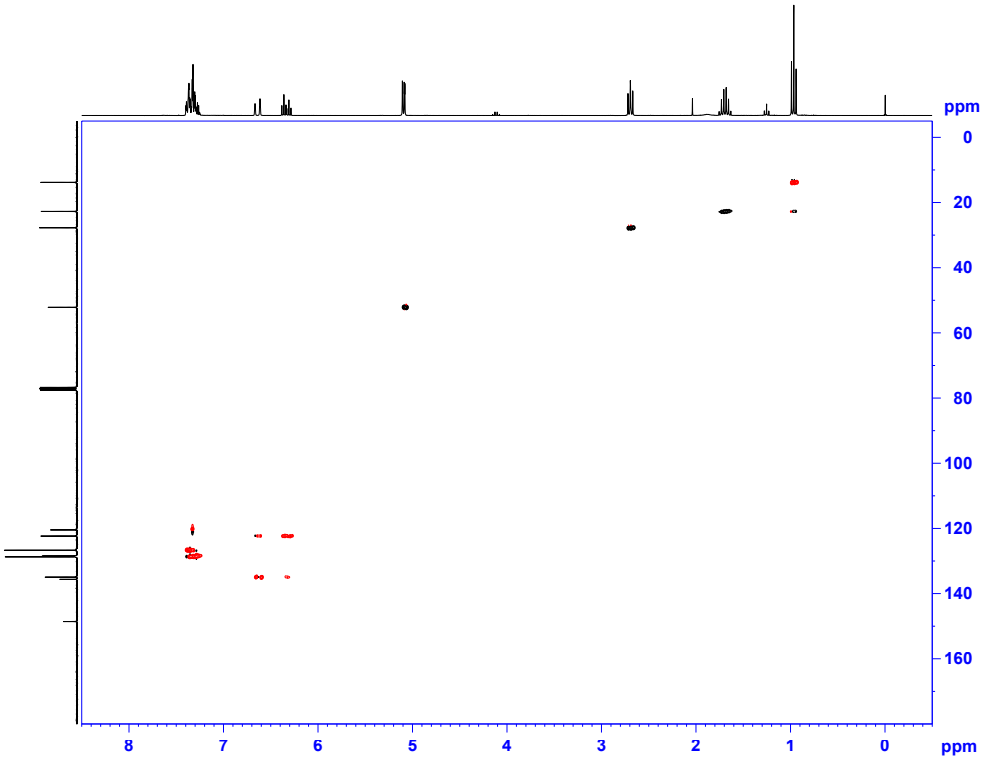
^{1}H NMR (300 MHz, $CDCl_3$)



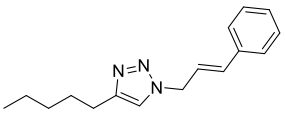
^{13}C NMR (75 MHz, $CDCl_3$)



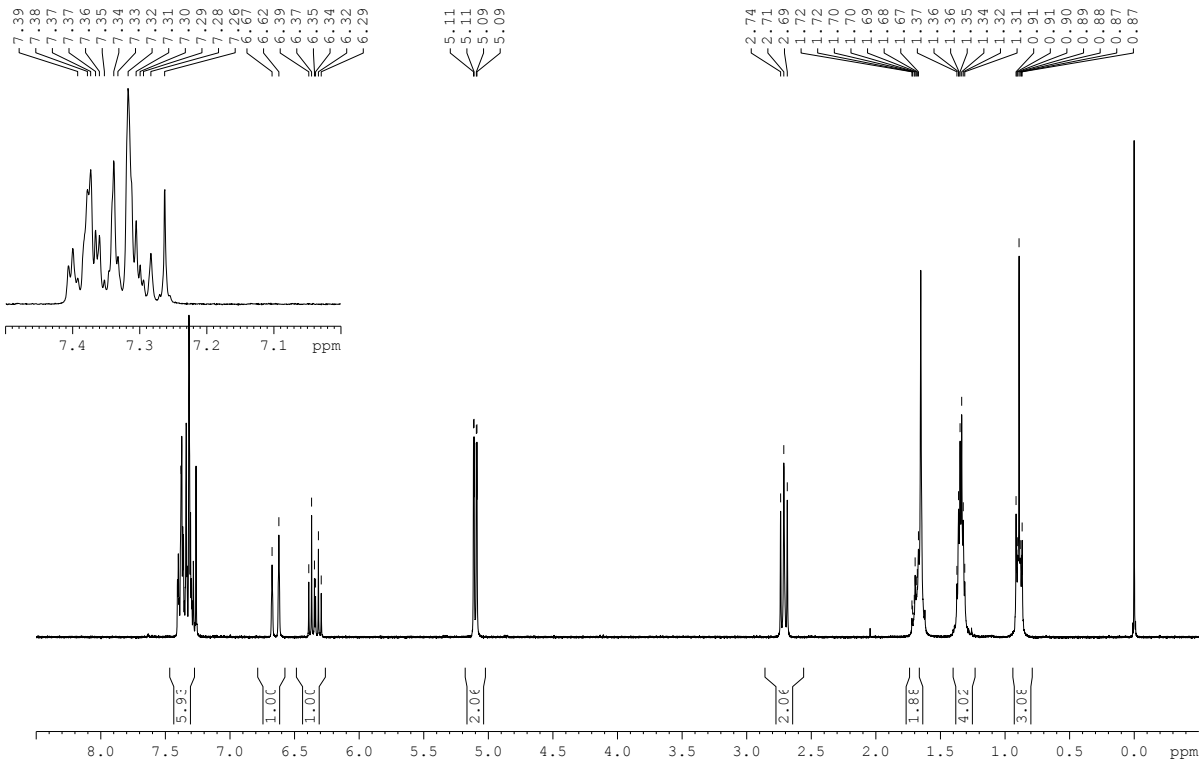
HSQC ($CDCl_3$)



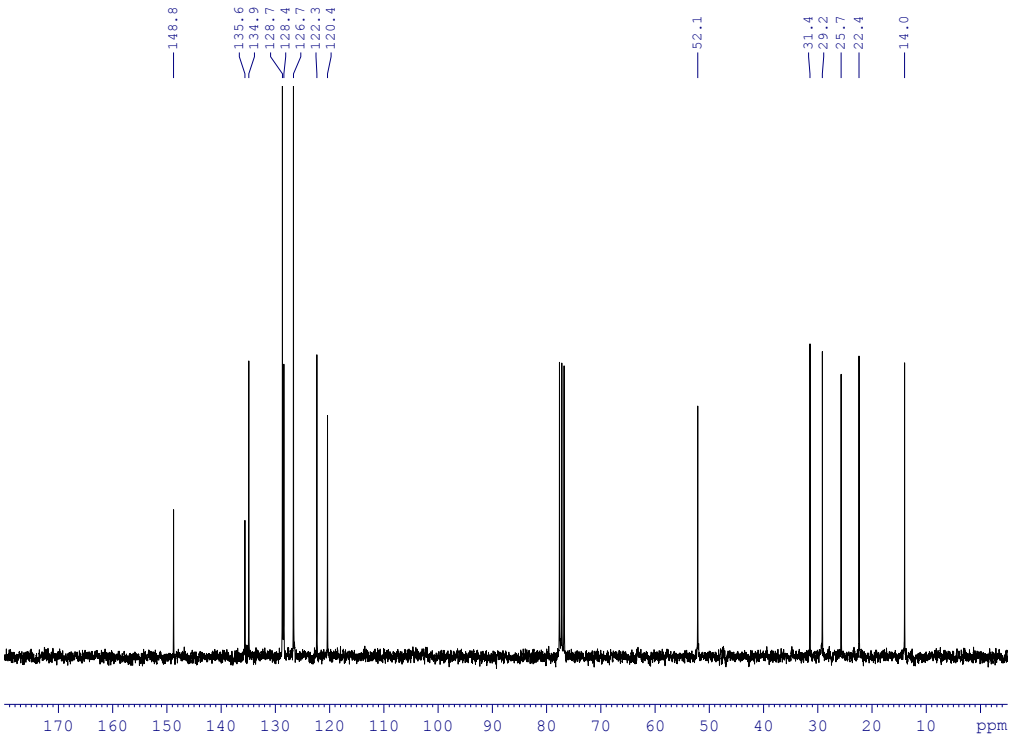
Compound **4c**



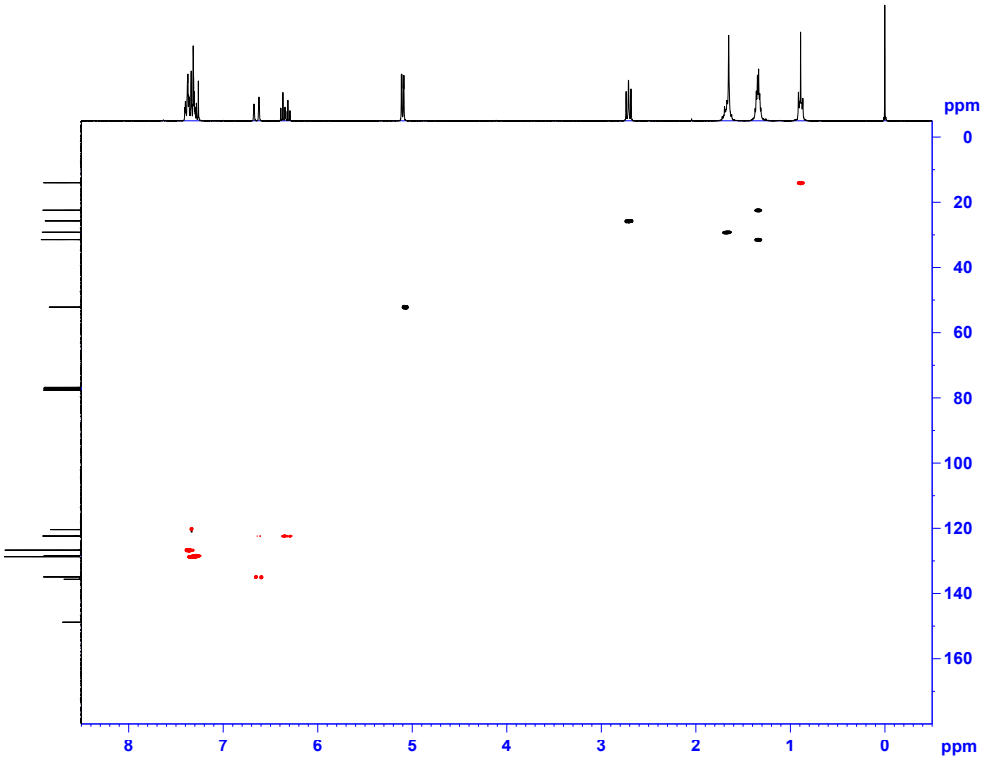
^{1}H NMR (300 MHz, $CDCl_3$)



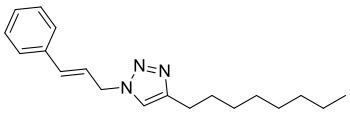
^{13}C NMR (75 MHz, $CDCl_3$)



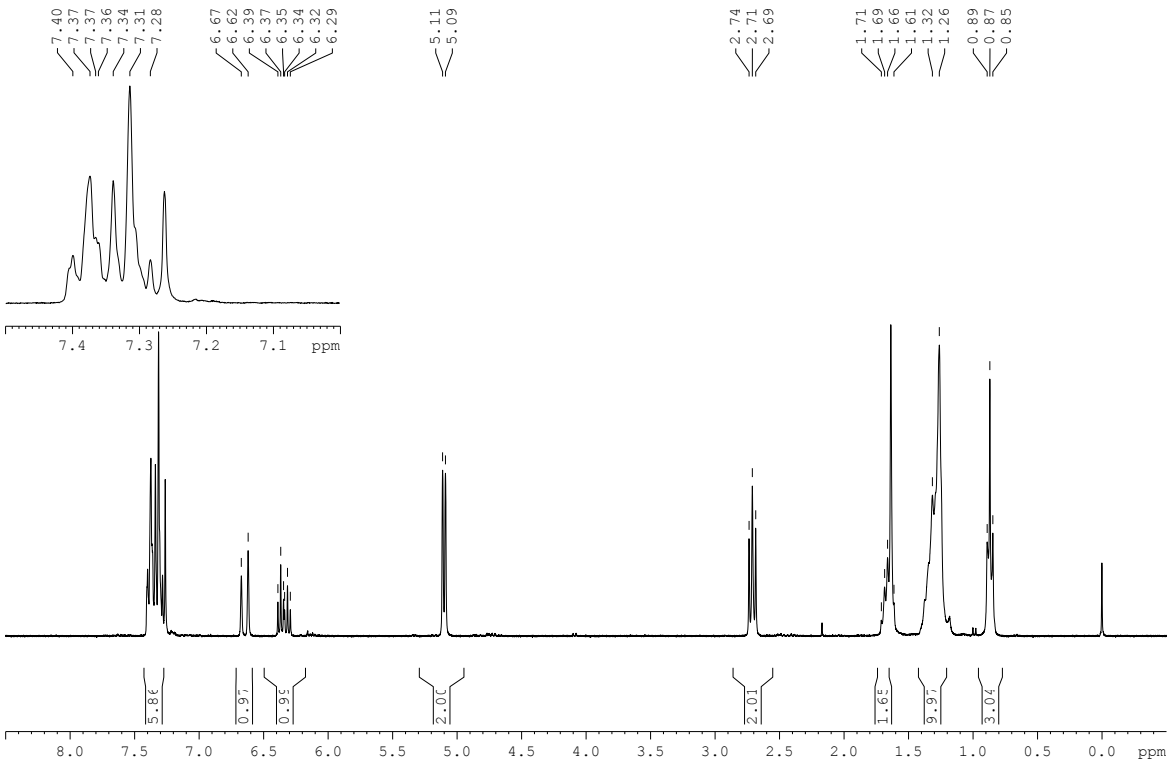
HSQC ($CDCl_3$)



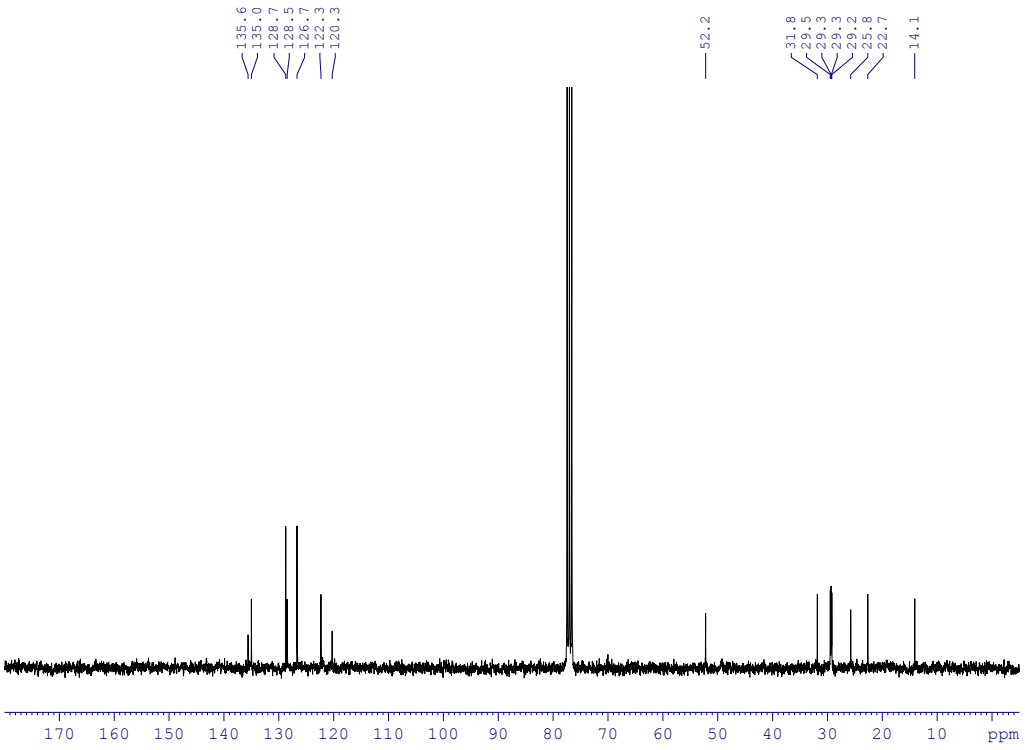
Compound **4d**



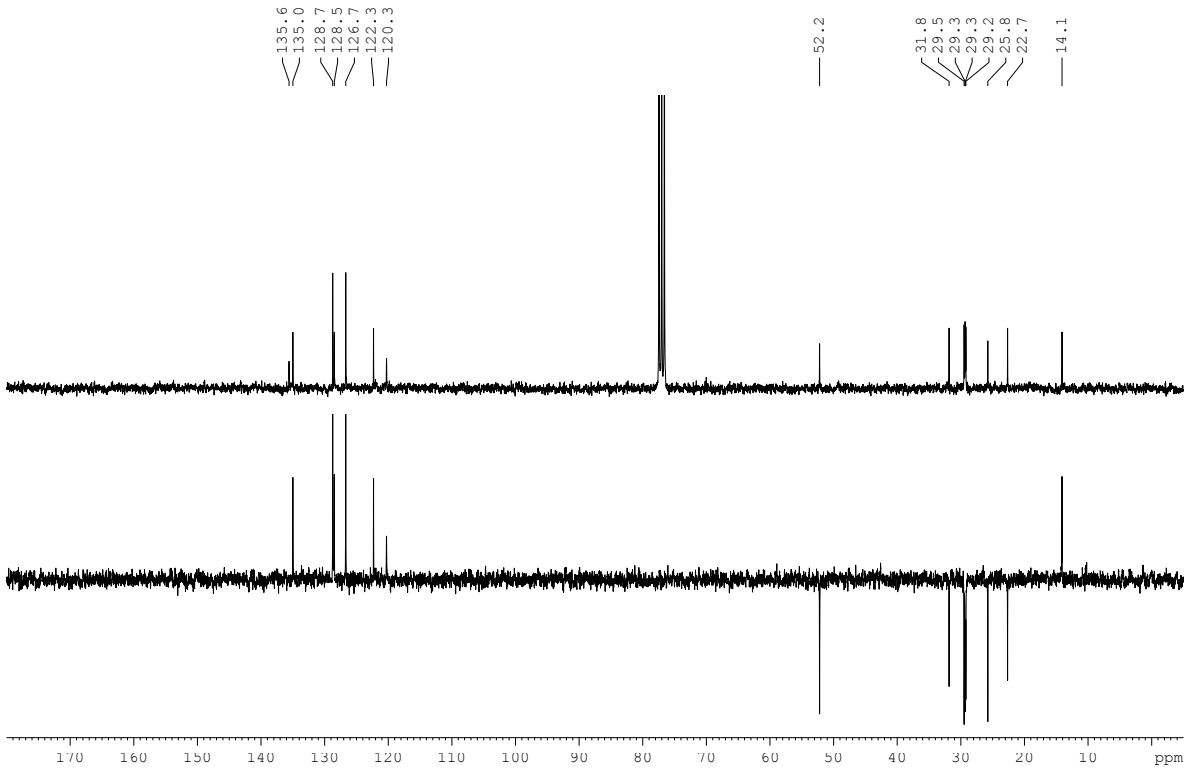
^{1}H NMR (300 MHz, $CDCl_3$)



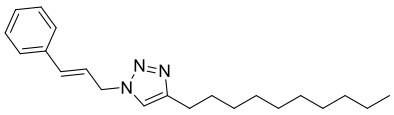
^{13}C NMR (75 MHz, $CDCl_3$)



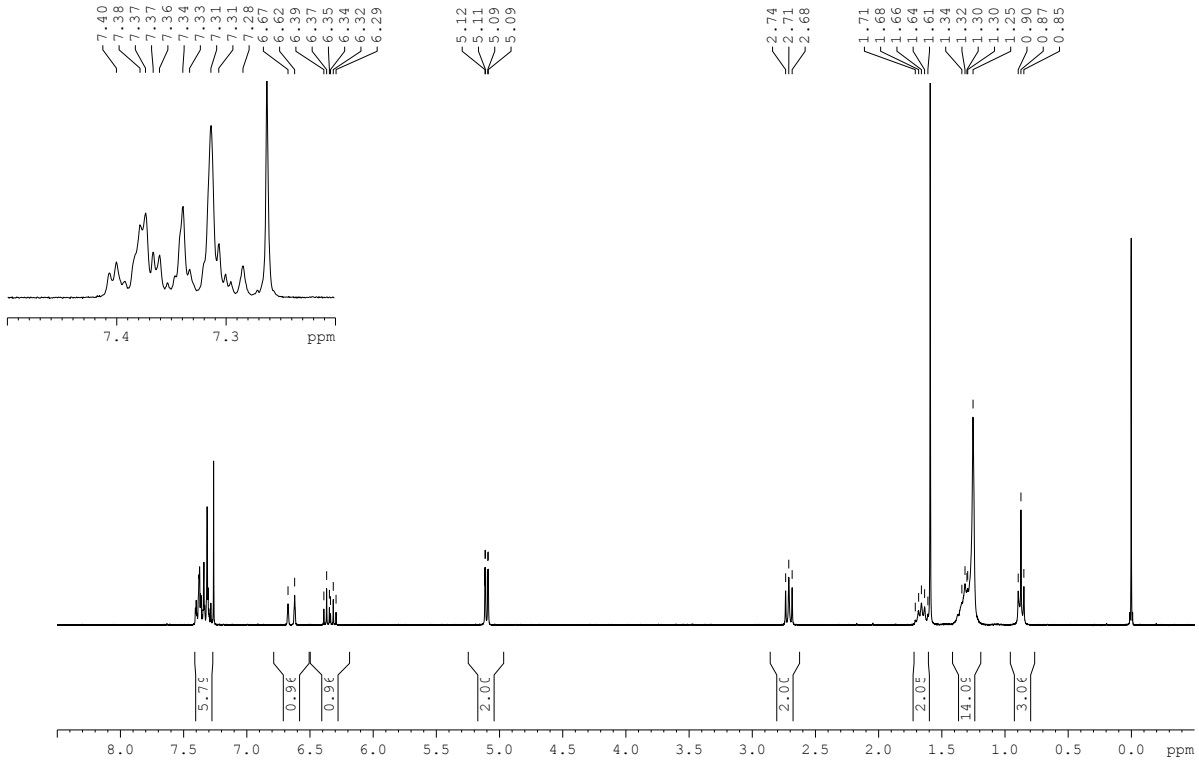
DEPT ($CDCl_3$)


135.6
135.0
128.7
128.5
126.7
122.3
120.3
52.2
31.8
29.5
29.3
29.3
29.2
25.8
22.7
14.1
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

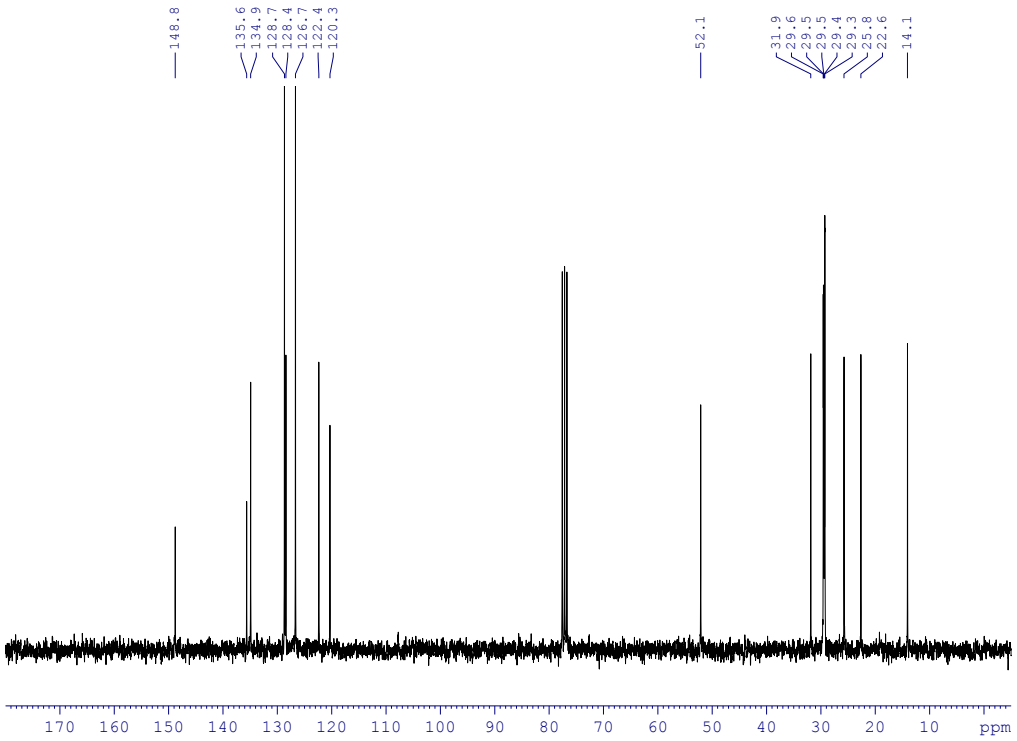
Compound **4e**



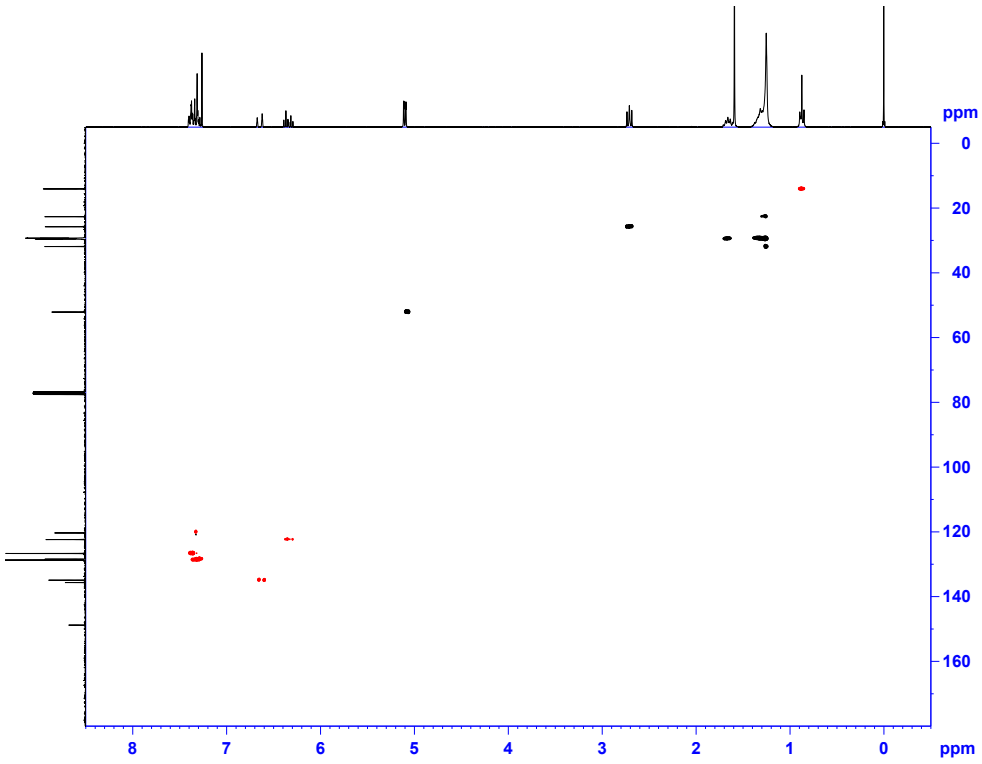
^{1}H NMR (300 MHz, $CDCl_3$)



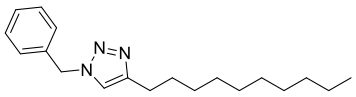
^{13}C NMR (75 MHz, $CDCl_3$)



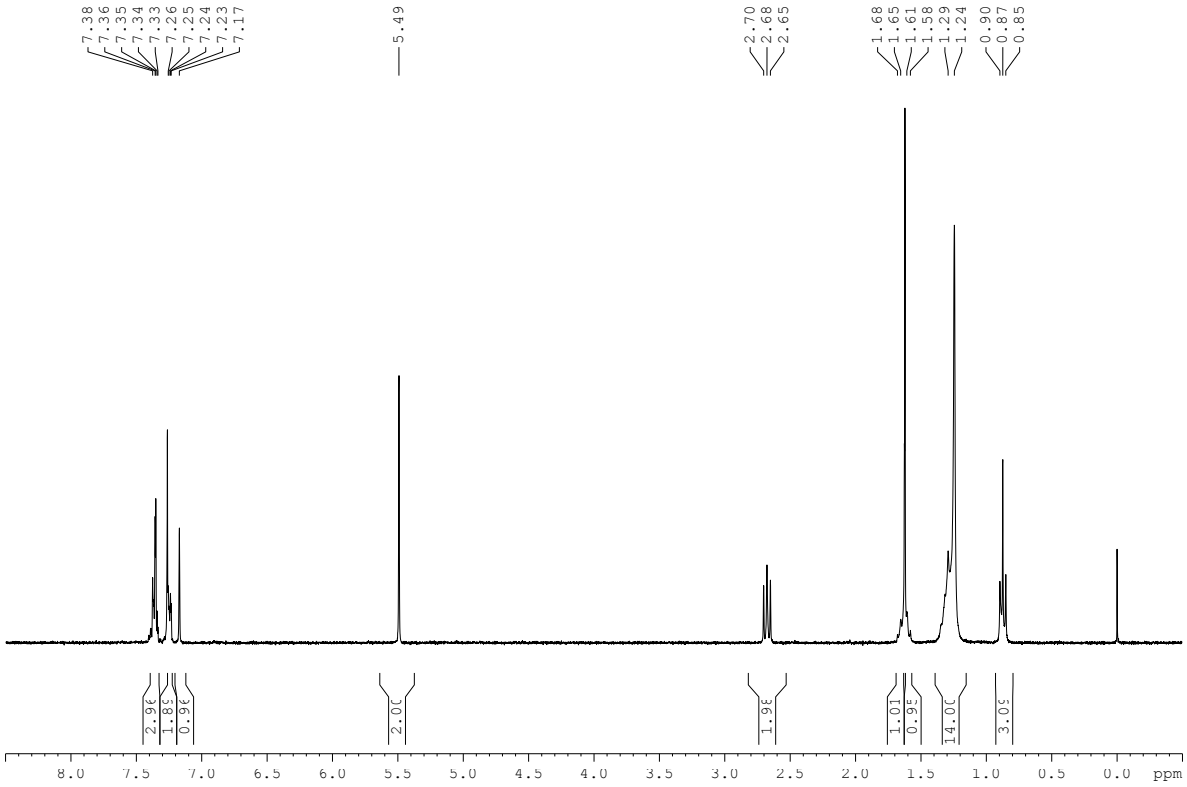
HSQC ($CDCl_3$)



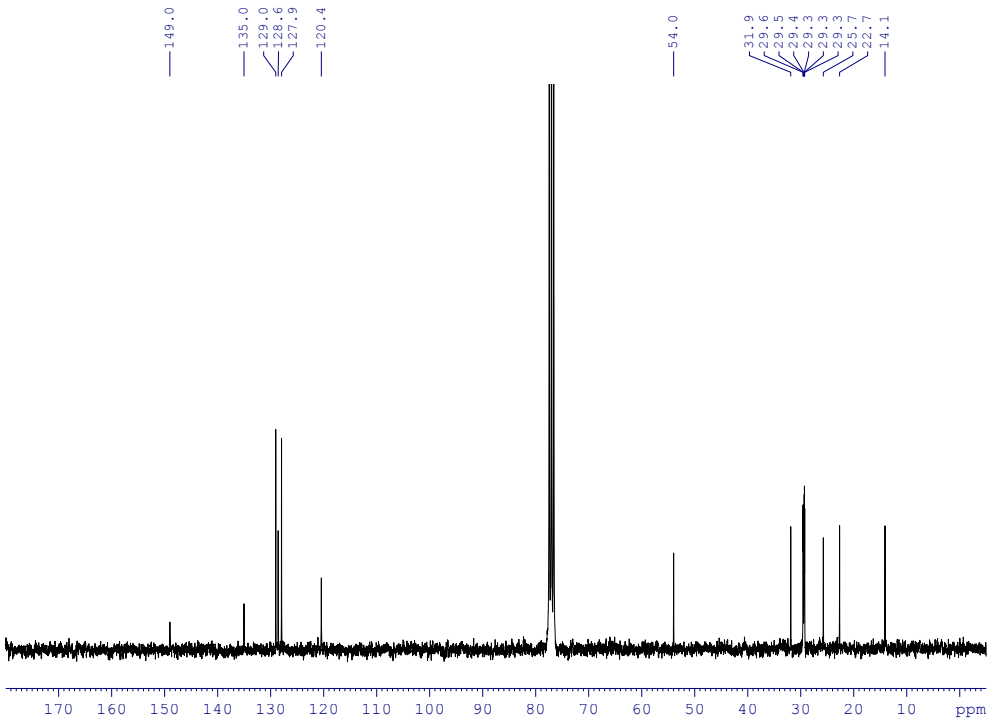
Compound **5h**



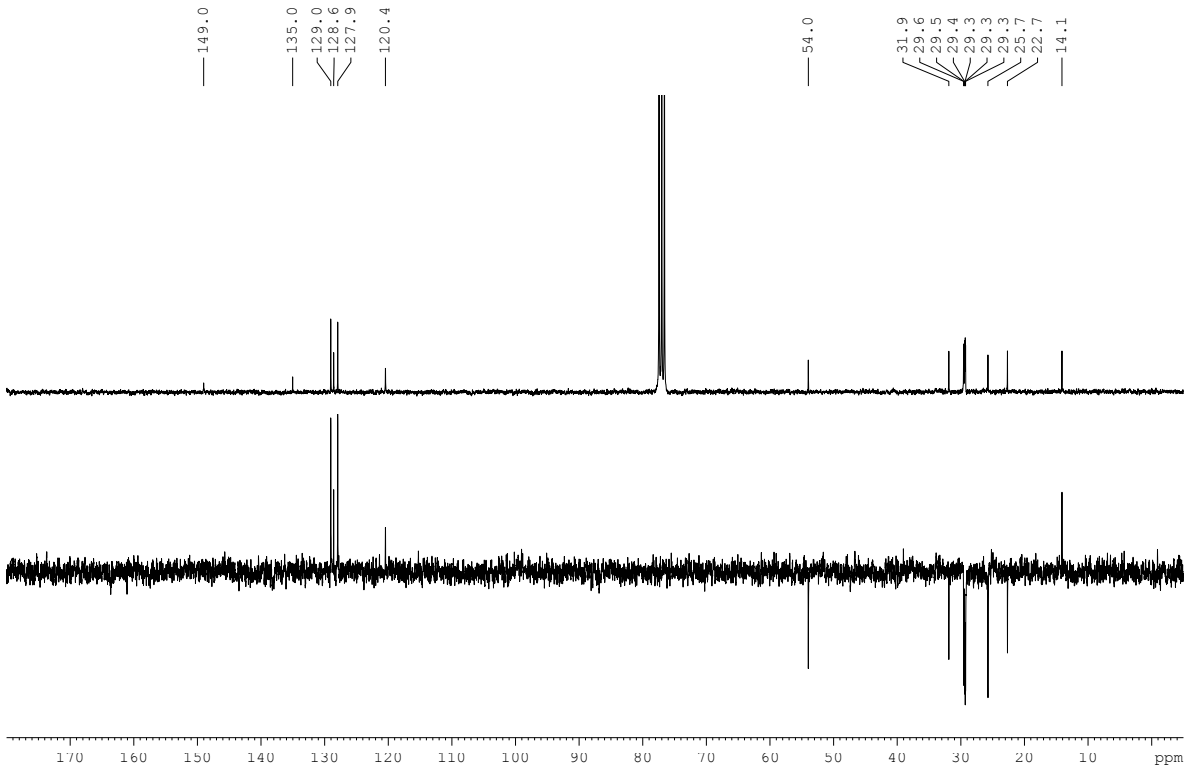
^{1}H NMR (300 MHz, $CDCl_3$)



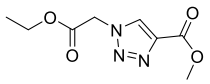
^{13}C NMR (75 MHz, $CDCl_3$)



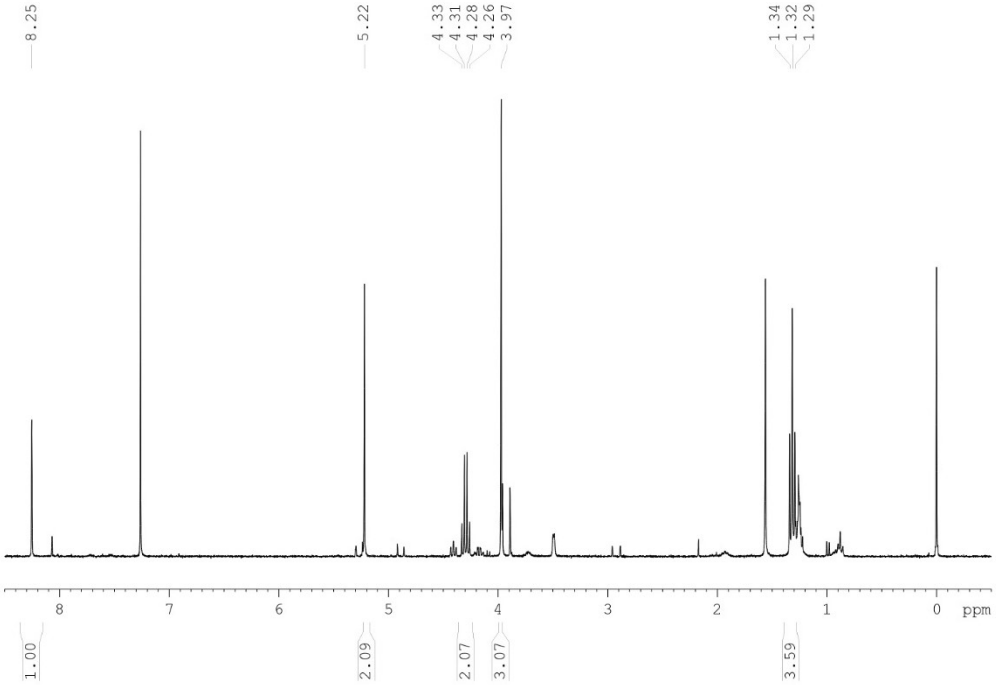
DEPT ($CDCl_3$)


149.0
135.0
129.0
128.6
127.9
120.4
54.0
31.9
29.6
29.5
29.4
29.3
29.3
29.3
25.7
22.7
14.1
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

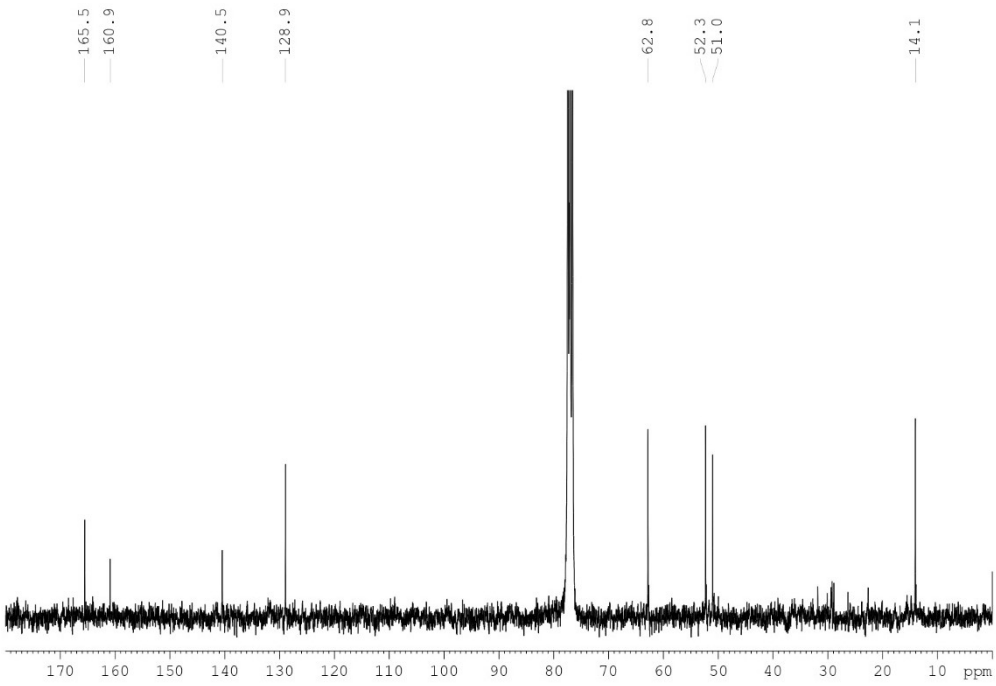
Compound **6a**



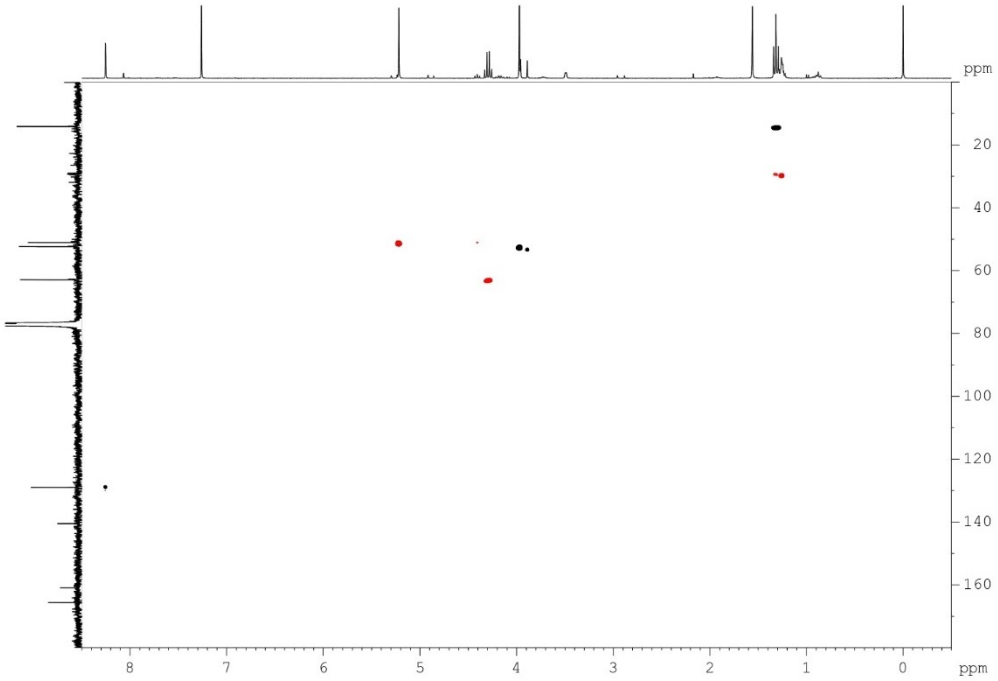
^{1}H NMR (300 MHz, $CDCl_3$)



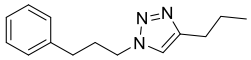
^{13}C NMR (75 MHz, $CDCl_3$)



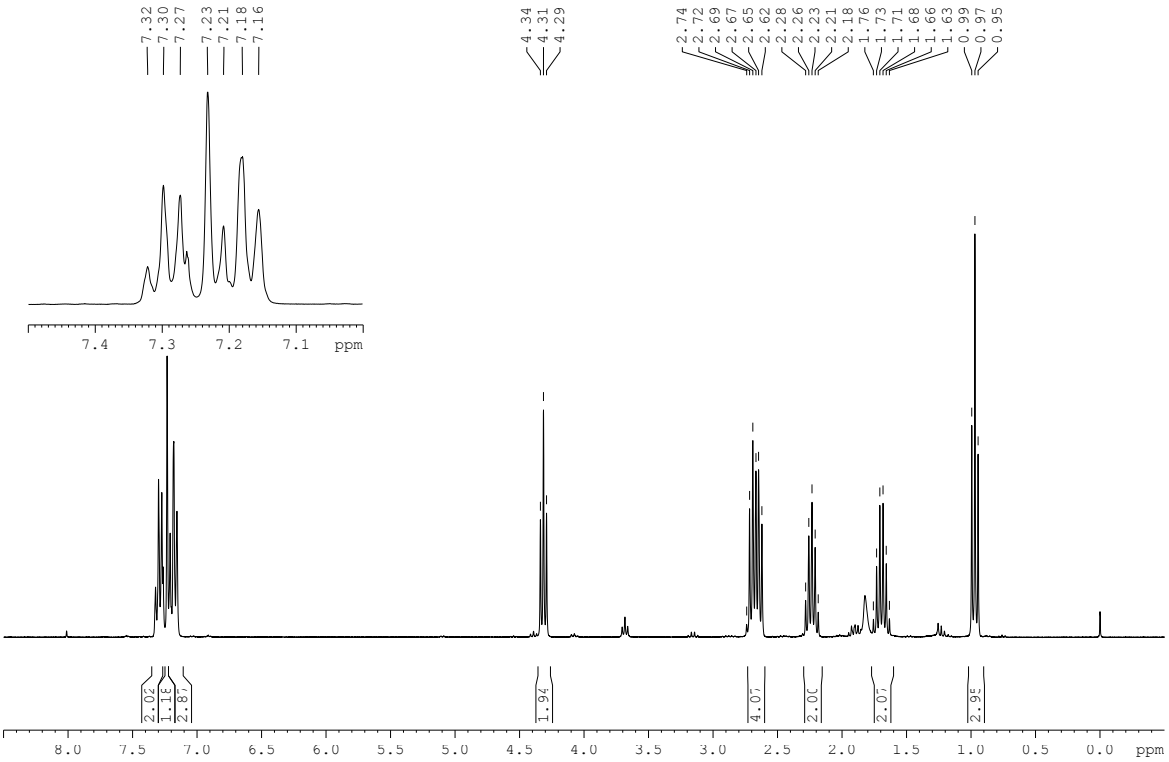
HSQC ($CDCl_3$)



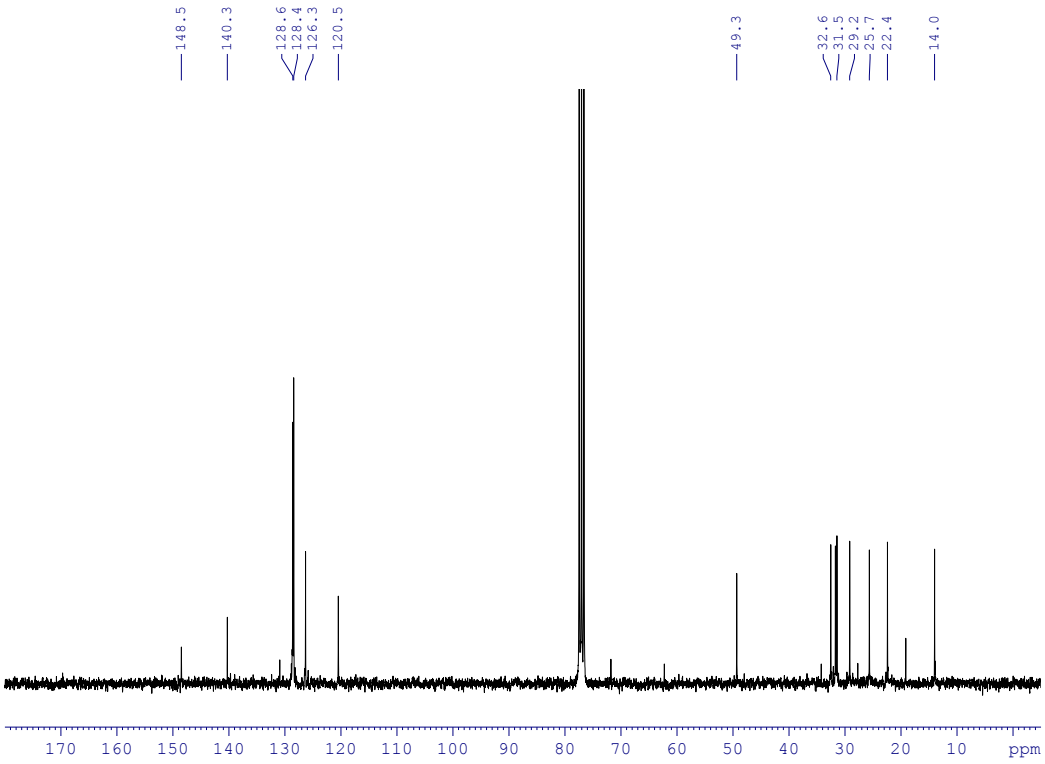
Compound **7c**



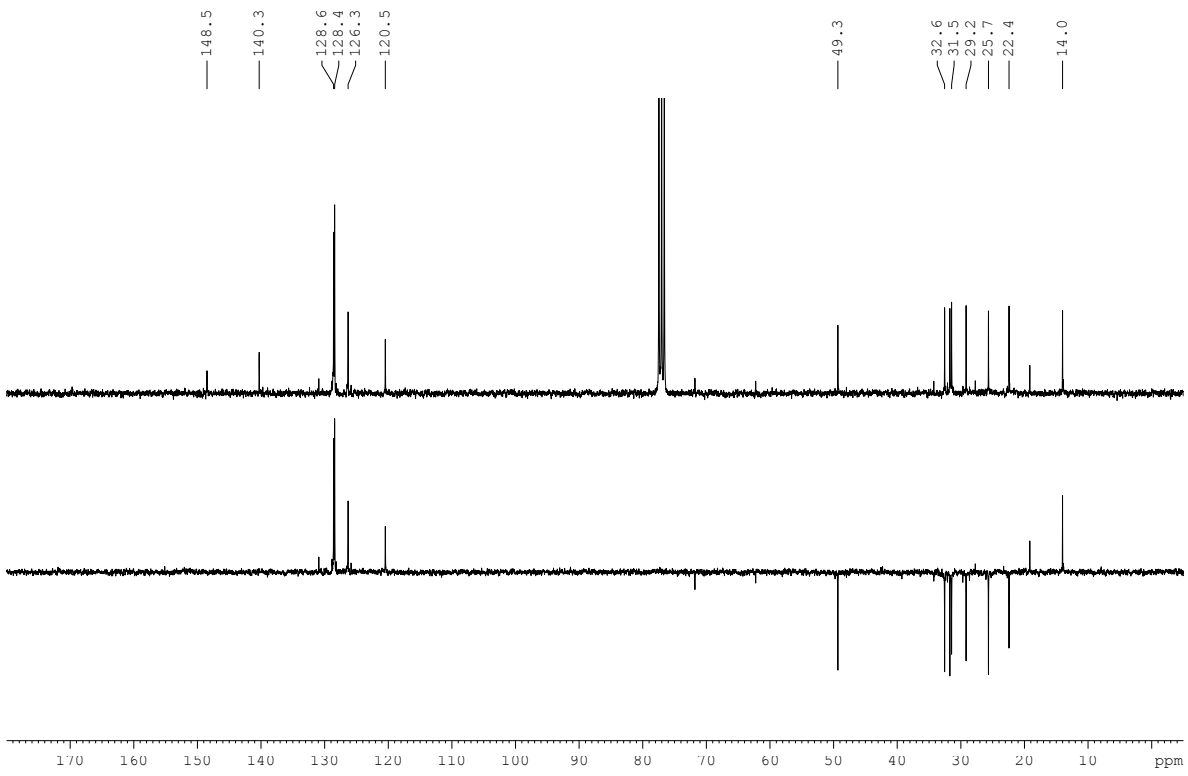
^{1}H NMR (300 MHz, $CDCl_3$)



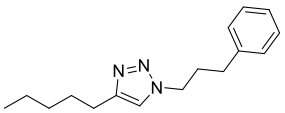
^{13}C NMR (75 MHz, $CDCl_3$)



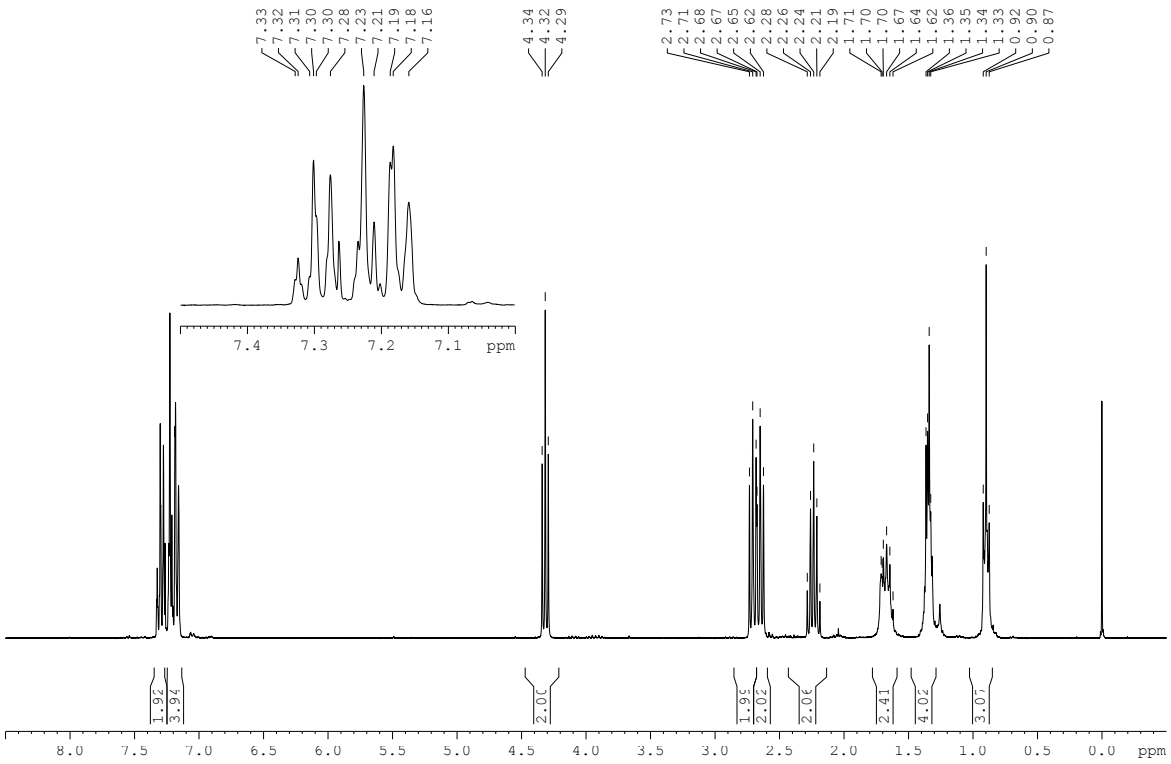
DEPT ($CDCl_3$)


148.5
140.3
128.6
128.4
126.3
120.5
49.3
32.6
31.5
29.2
25.7
22.4
14.0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

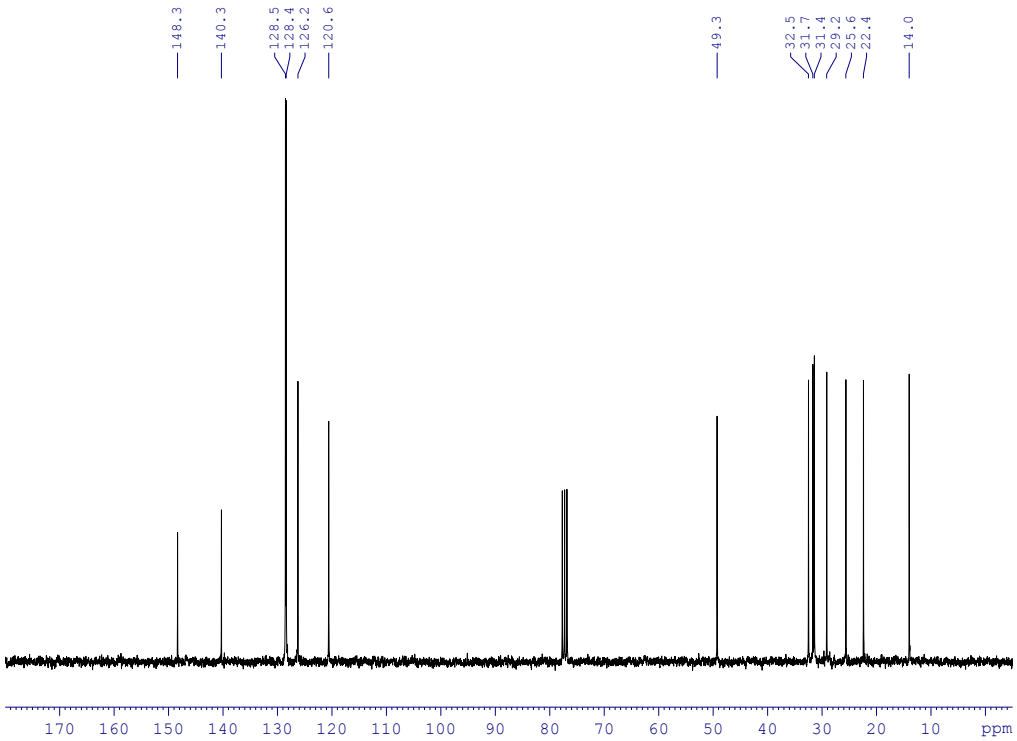
Compound **7d**



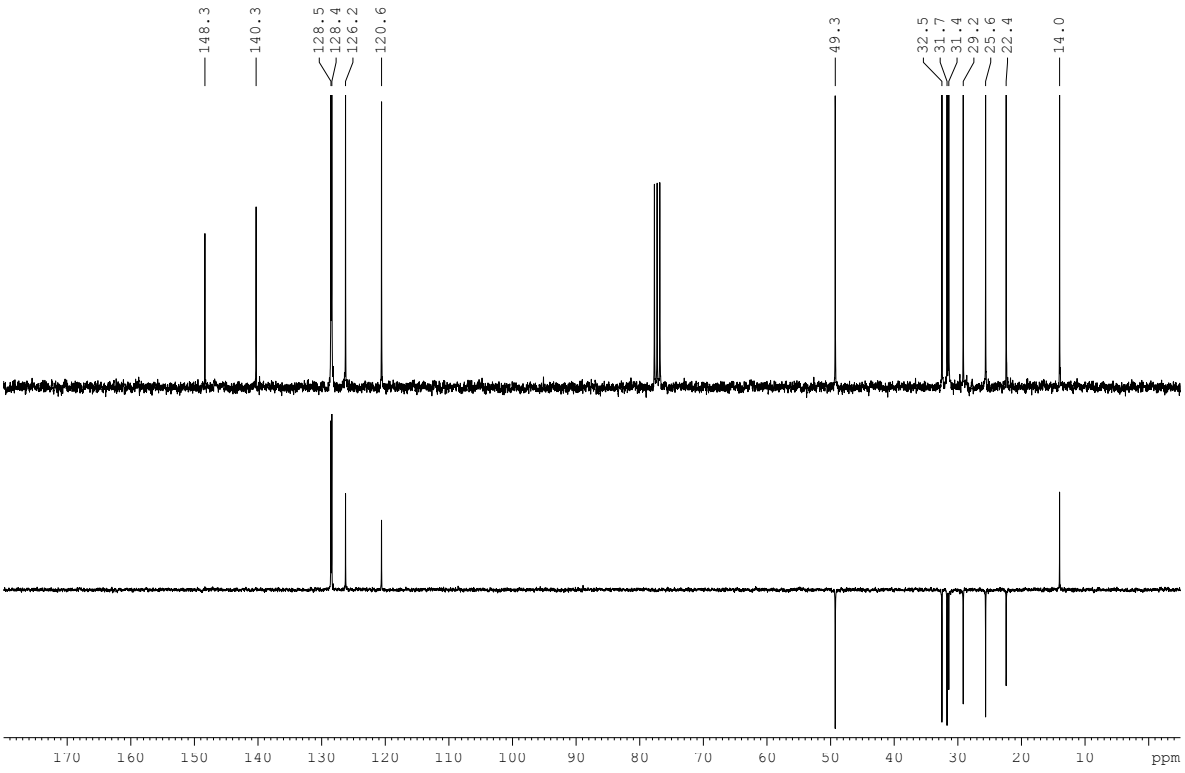
^{1}H NMR (300 MHz, $CDCl_3$)



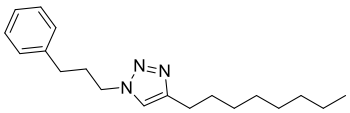
^{13}C NMR (75 MHz, $CDCl_3$)



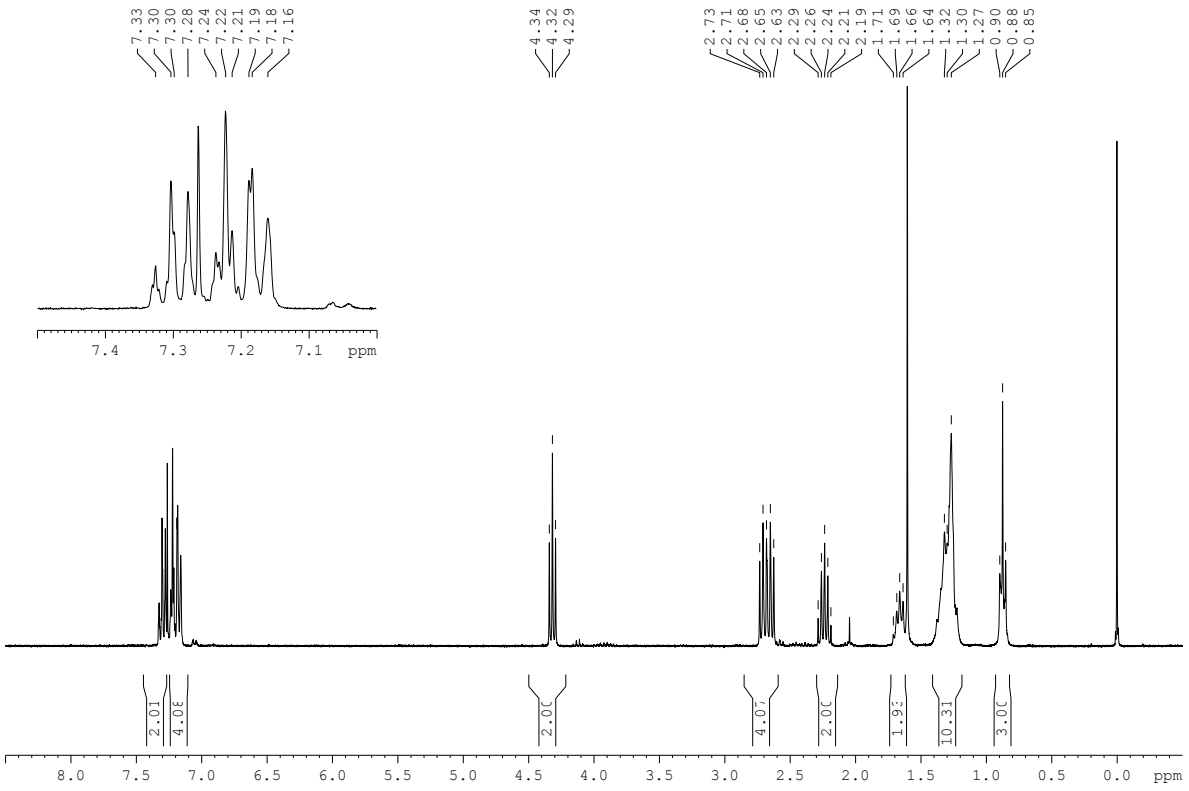
DEPT ($CDCl_3$)


148.3
140.3
128.5
128.4
126.2
120.6
49.3
32.5
31.7
31.4
29.2
25.6
22.4
14.0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

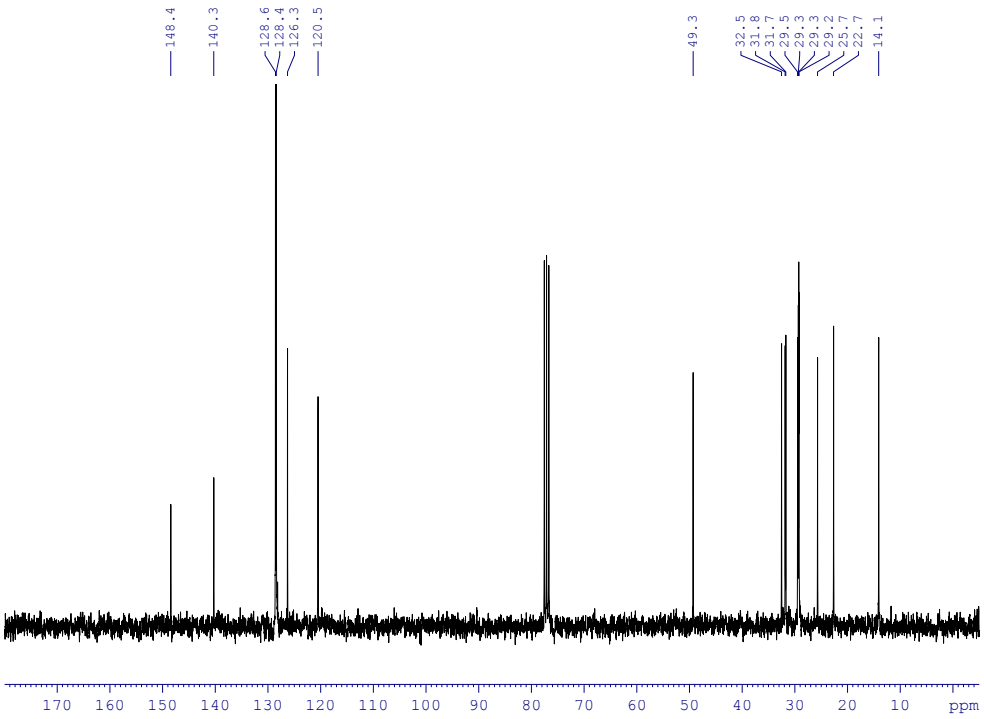
Compound **7e**



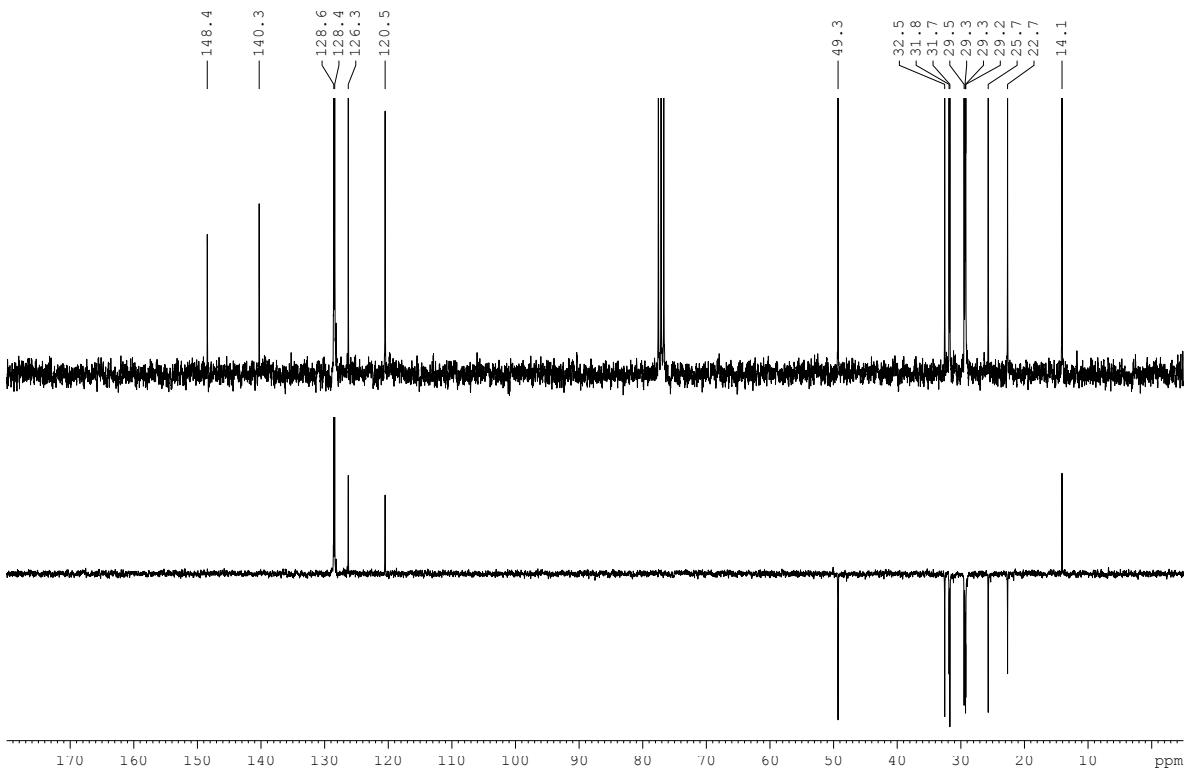
^{1}H NMR (300 MHz, $CDCl_3$)



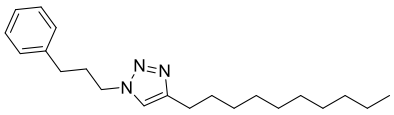
^{13}C NMR (75 MHz, $CDCl_3$)



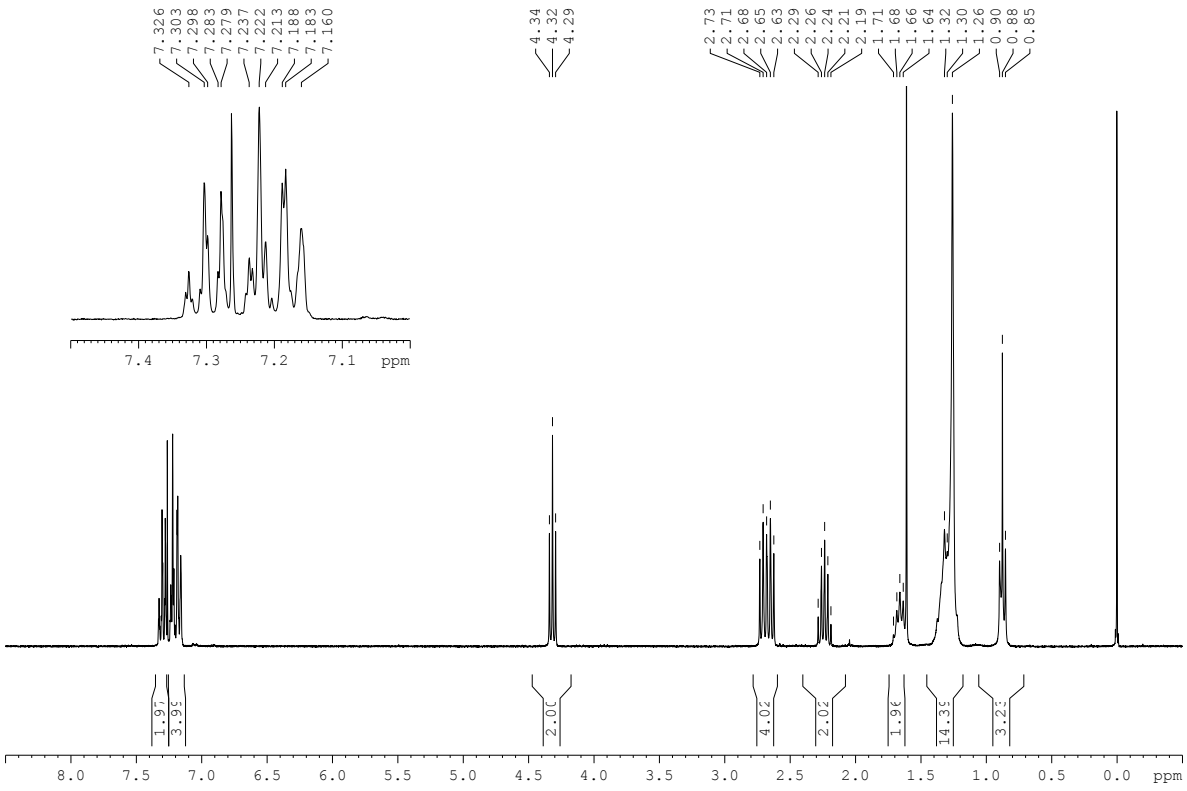
DEPT ($CDCl_3$)


148.4
140.3
128.6
128.4
126.3
120.5
49.3
32.5
31.8
31.7
29.5
29.3
29.3
29.2
25.7
22.7
14.1
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

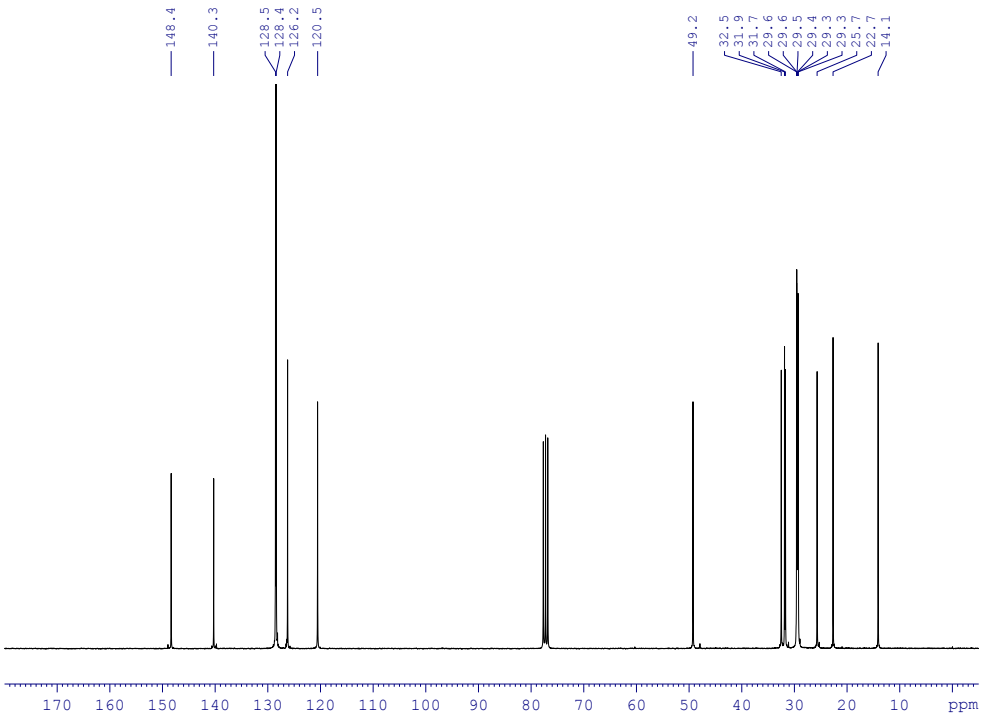
Compound **7g**



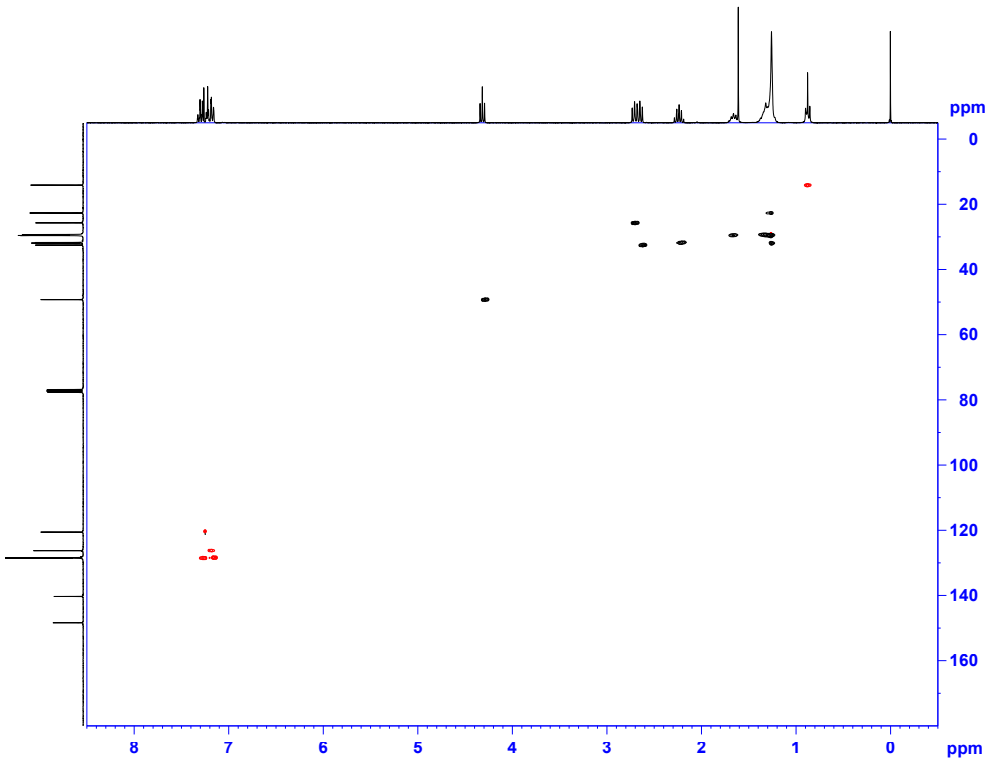
^{1}H NMR (300 MHz, $CDCl_3$)



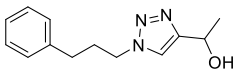
^{13}C NMR (75 MHz, $CDCl_3$)



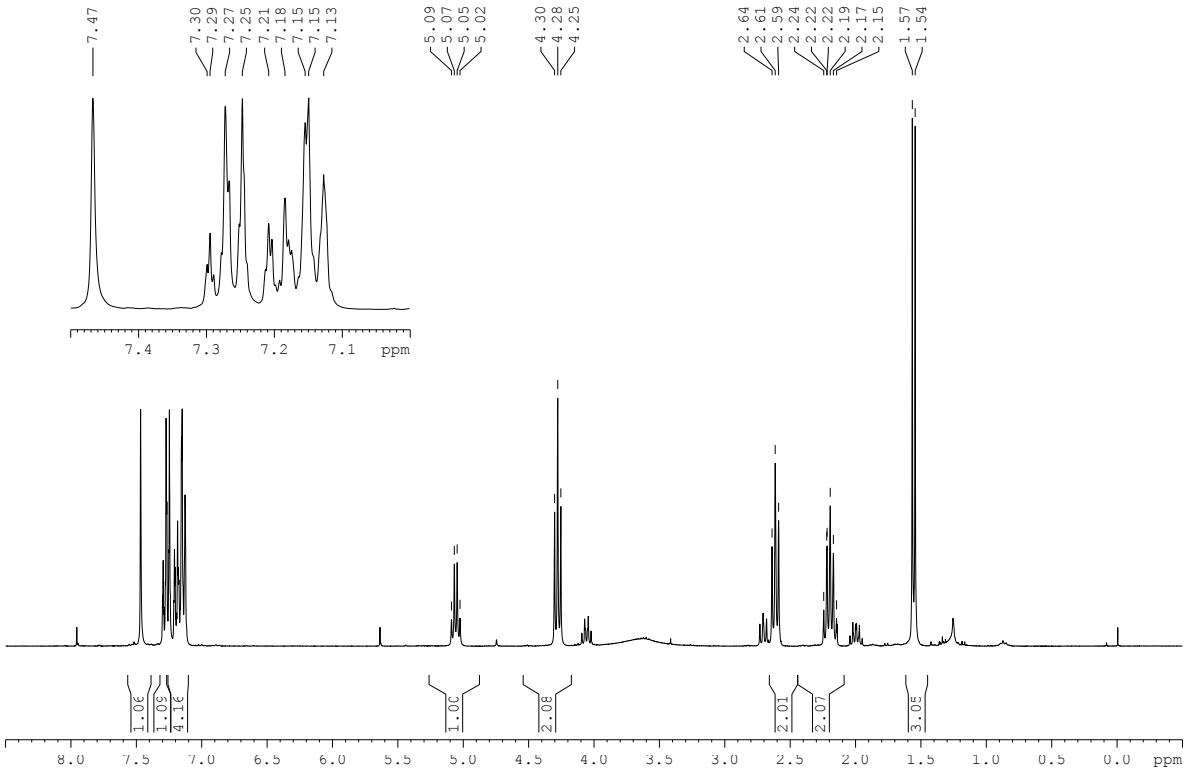
HSQC ($CDCl_3$)



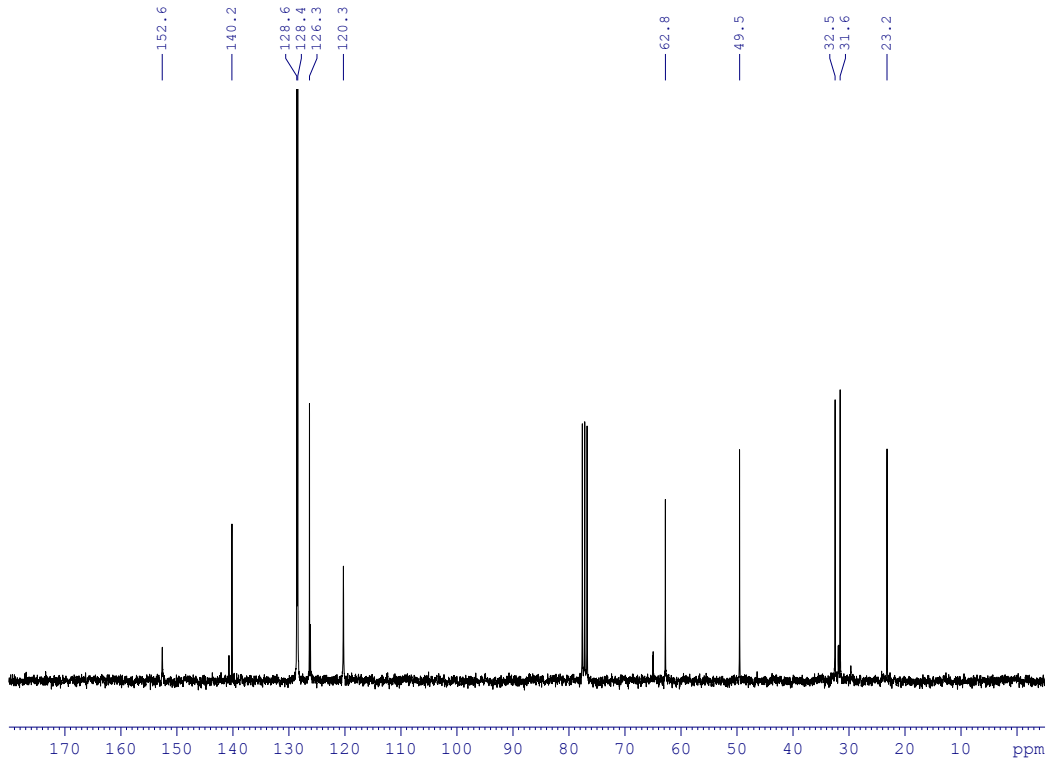
Compound **7h**



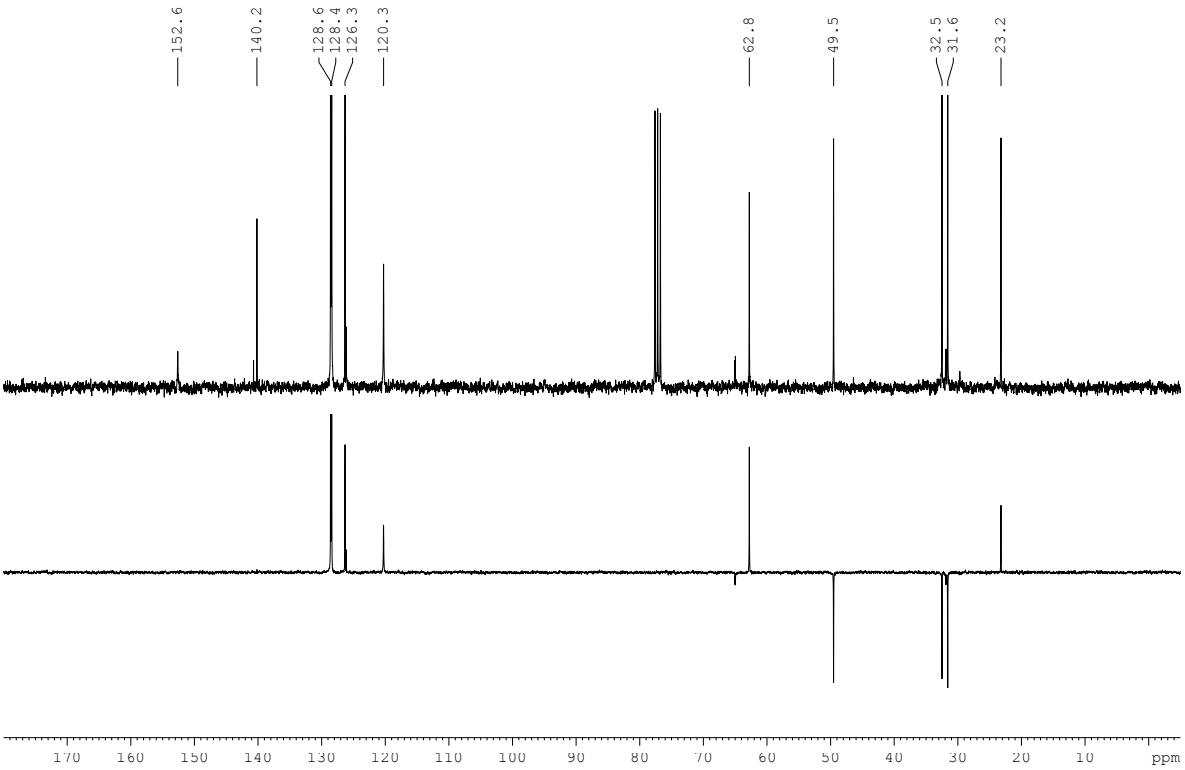
^{1}H NMR (300 MHz, $CDCl_3$)



^{13}C NMR (75 MHz, $CDCl_3$)



DEPT ($CDCl_3$)


152.6
140.2
128.6
128.4
126.3
120.3
62.8
49.5
32.5
31.6
23.2
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

Physicochemical properties calculated in DATAWARRIOR												
ID	SMILE	MW	cLogP	cLogS	HA	HD	TSA	Relative PSA	PSA	Mutagenic	Tumorigenic	Irritant
1a	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CO)=C1	303.45	4.69	-2.67	4	1	272.06	0.15	50.94	none	none	none
1b	C/C(C)=C\CC/C(C)=C/CC/C(C)=C\Cn1nnc(CO)c1	303.45	4.69	-2.67	4	1	272.06	0.15	50.94	none	none	none
1c	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(C(C)O)=C1	317.48	4.97	-2.74	4	1	283.06	0.15	50.94	none	none	none
1d	CC(c1nnn(C/C=C(CC/C=C(CC/C=C(C)\C)\C)/C)c1)O	317.48	4.97	-2.74	4	1	283.06	0.15	50.94	none	none	none
1e	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(C(C)(C)O)=C1	331.50	5.56	-3.16	4	1	293.23	0.14	50.94	none	none	none
1f	C/C(C)=C\CC/C(C)=C/CC/C(C)=C\Cn1nnc(C(C)(O)C)c1	331.50	5.56	-3.16	4	1	293.23	0.14	50.94	none	none	none
1g	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CCO)=C1	317.48	5.12	-2.79	4	1	285.82	0.15	50.94	none	none	none
1h	C/C(C)=C\CC/C(C)=C/CC/C(C)=C\Cn1nnc(CCO)c1	317.48	5.12	-2.79	4	1	285.82	0.15	50.94	none	none	none
1i	C/C(CC\C=C(C)/C)=C\CC/C(C)=C\CN1N=NC(CCCCCCCC)=C1	385.64	8.77	-4.91	3	0	360.53	0.08	30.71	none	none	none
1j	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CCCCCCCC)=C1	385.64	8.77	-4.91	3	0	360.53	0.08	30.71	none	none	none
1k	C/C(CC\C=C(C)/C)=C\CC/C(C)=C\CN1N=NC(CCCCC)=C1	343.56	7.41	-4.10	3	0	319.25	0.09	30.71	none	none	none
1l	C/C(CC\C=C(C)/C)=C\CC/C(C)=C\CN1N=NC(CCC)=C1	315.50	6.50	-3.56	3	0	291.73	0.10	30.71	none	none	none
1m	C/C(CC\C=C(C)/C)=C\CC/C(C)=C\CN1N=NC(C2=CC=CC=C2)=C1	349.52	6.98	-4.54	3	0	311.71	0.09	30.71	none	none	none
1n	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(C2=CC=CC=C2)=C1	349.52	6.98	-4.54	3	0	311.71	0.09	30.71	none	none	none
1o	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CCCCC)=C1	343.56	7.41	-4.10	3	0	319.25	0.09	30.71	none	none	none
1p	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CCC)=C1	315.50	6.50	-3.56	3	0	291.73	0.10	30.71	none	none	none
1q	C/C(CC/C=C(C)/C)=C\CC/C(C)=C\CN1N=NC(C(OC)=O)=C1	331.46	5.20	-2.93	5	0	291.96	0.18	57.01	none	none	none
1r	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(C(OC)=O)=C1	331.46	5.20	-2.93	5	0	291.96	0.18	57.01	none	none	none
2a	C/C(C)=C/CC/C(C)=C\CN1N=NC(CCCCCCCC)=C1	317.52	6.60	-3.94	3	0	296.04	0.10	30.71	none	none	none
2b	C/C(C)=C/CC/C(C)=C/CN1N=NC(CCCCCCCC)=C1	317.52	6.60	-3.94	3	0	296.04	0.10	30.71	none	none	none
2c	C/C(C)=C/CC/C(C)=C\CN1N=NC(CCCCC)=C1	275.44	5.24	-3.13	3	0	254.76	0.11	30.71	none	none	none
2d	C/C(C)=C/CC/C(C)=C/CN1N=NC(CCCCC)=C1	275.44	5.24	-3.13	3	0	254.76	0.11	30.71	none	none	none
2e	C/C(C)=C/CC/C(C)=C\CN1N=NC(CCC)=C1	247.39	4.33	-2.59	3	0	227.24	0.13	30.71	none	none	none
2f	C/C(C)=C/CC/C(C)=C/CN1N=NC(CCC)=C1	247.39	4.33	-2.59	3	0	227.24	0.13	30.71	none	none	none
2g	C/C(C)=C/CC/C(C)=C/CN1N=NC(C(OC)=O)=C1	263.34	3.03	-1.95	5	0	227.47	0.23	57.01	none	none	none
2h	C/C(C)=C/CC/C(C)=C\CN1N=NC(C(OC)=O)=C1	263.34	3.03	-1.95	5	0	227.47	0.23	57.01	none	none	none
2i	C/C(C)=C/CC/C(C)=C/CN1N=NC(C2=CC=CC=C2)=C1	281.40	4.81	-3.57	3	0	247.22	0.12	30.71	none	none	none
2j	C/C(C)=C/CC/C(C)=C\CN1N=NC(C2=CC=CC=C2)=C1	281.40	4.81	-3.57	3	0	247.22	0.12	30.71	none	none	none
3a	C/C(C)=C/CN1N=NC(C(OC)=O)=C1	195.22	0.85	-0.98	5	0	162.98	0.32	57.01	none	none	none
3b	C/C(C)=C/CN1N=NC(C2=CC=CC=C2)=C1	213.28	2.64	-2.59	3	0	182.73	0.16	30.71	none	none	none
3c	C/C(C)=C/CN1N=NC(CCC)=C1	179.27	2.15	-1.61	3	0	162.75	0.18	30.71	none	none	none
3d	C/C(C)=C/CN1N=NC(CCCCC)=C1	207.32	3.06	-2.15	3	0	190.27	0.15	30.71	none	none	none
3e	C/C(C)=C/CN1N=NC(CCCCCCCC)=C1	249.40	4.43	-2.96	3	0	231.55	0.12	30.71	none	none	none

Physicochemical properties calculated in DATAWARRIOR												
ID	SMILE	MW	cLogP	cLogS	HA	HD	TSA	Relative PSA	PSA	Mutagenic	Tumorigenic	Irritant
4a	CCCCCCCCCCC2=CN(N=N2)CC1=CC=CC=C1	299.46	5.17	-3.85	3	0	269.60	0.11	30.71	none	none	none
4b	CCCCCCCCC2=CN(N=N2)CC1=CC=CC=C1	271.41	4.26	-3.31	3	0	242.08	0.12	30.71	none	none	none
4c	CCCCCC2=CN(N=N2)CC1=CC=CC=C1	229.33	2.90	-2.50	3	0	200.80	0.14	30.71	none	none	none
4d	CCCC2=CN(N=N2)CC1=CC=CC=C1	201.27	1.99	-1.96	3	0	173.28	0.17	30.71	none	none	none
4e	O=C(C2=CN(N=N2)CC1=CC=CC=C1)O	203.20	0.26	-1.20	5	1	157.60	0.35	68.01	none	none	none
4f	O=C(C2=CN(N=N2)CC1=CC=CC=C1)OC	217.23	0.69	-1.33	5	0	173.51	0.30	57.01	none	none	none
4g	C1(CN2N=NC(C3=CC=CC=C3)=C2)=CC=CC=C1	235.29	2.48	-2.94	3	0	193.26	0.15	30.71	none	none	none
4h	OCC2=CN(N=N2)CC1=CC=CC=C1	189.22	0.18	-1.07	4	1	153.61	0.27	50.94	none	none	none
5a	CCOC(CN1N=NC(CCCCCCCC)=C1)=O	267.37	2.72	-2.43	5	0	236.09	0.22	57.01	none	none	none
5b	O=C(CN1N=NC(CCCCC)=C1)OCC	225.29	1.36	-1.62	5	0	194.81	0.27	57.01	none	none	none
5c	CCOC(CN1N=NC(CCC)=C1)=O	197.24	0.45	-1.08	5	0	167.29	0.31	57.01	none	none	none
5d	CCOC(CCN(N=N1)C=C1C(OC)=O)=O	227.22	-0.40	-0.72	7	0	181.28	0.41	83.31	none	none	none
6a	CC(O)c2cn(CCCc1ccccc1)nn2	231.30	1.26	-1.76	4	1	192.13	0.22	50.94	none	none	none
6b	CCCCCCCCCCC2=CN(N=N2)CCCC1=CC=CC=C1	327.51	5.97	-4.47	3	0	297.12	0.10	30.71	none	none	none
6c	CCCC2=CN(N=N2)CCCC1=CC=CC=C1	229.33	2.79	-2.58	3	0	200.80	0.14	30.71	none	none	none
6d	CCCCCC2=CN(N=N2)CCCC1=CC=CC=C1	257.38	3.70	-3.12	3	0	228.32	0.13	30.71	none	none	none
6e	CCCCCCCCC2=CN(N=N2)CCCC1=CC=CC=C1	299.46	5.06	-3.93	3	0	269.60	0.11	30.71	none	none	none
6f	O=C(C2=CN(N=N2)CCCC1=CC=CC=C1)OC	245.28	1.49	-1.95	5	0	201.03	0.26	57.01	none	none	none
6g	C(Cc1ccccc1)Cn3cc(c2ccccc2)nn3	263.34	3.27	-3.56	3	0	220.78	0.13	30.71	none	none	none
6h	OCC2=CN(N=N2)CCCC1=CC=CC=C1	217.27	0.98	-1.69	4	1	181.13	0.23	50.94	none	none	none
7a	OCC1=CN(N=N1)CCCCCCCC	211.31	1.81	-1.91	4	1	188.67	0.22	50.94	none	none	none
7b	O=C(OC)C1=CN(N=N1)CCCCCCCC	239.32	2.32	-2.16	5	0	208.57	0.25	57.01	none	none	none
8a	OCC1=CN(N=N1)CCCCCCCCCC	239.36	2.72	-2.45	4	1	216.19	0.19	50.94	none	none	none
8b	O=C(OC)C1=CN(N=N1)CCCCCCCCCC	267.37	3.23	-2.70	5	0	236.09	0.22	57.01	none	none	none
9a	OCC1=CN(N=N1)CCCCCCCCCCCC	281.44	4.08	-3.26	4	1	257.47	0.16	50.94	none	none	none
9b	O=C(OC)C1=CN(N=N1)CCCCCCCCCCCC	309.45	4.59	-3.51	5	0	277.37	0.19	57.01	none	none	none
10a	CCCCCCCCC2=CN(N=N2)C/C=C/C1=CC=CC=C1	297.44	4.94	-4.06	3	0	268.58	0.11	30.71	none	none	none
10b	C1(C3=CN(N=N3)C/C=C/C2=CC=CC=C2)=CC=CC=C1	261.33	3.15	-3.70	3	0	219.76	0.13	30.71	none	none	none
10c	CCCC2=CN(N=N2)C/C=C/C1=CC=CC=C1	227.31	2.66	-2.71	3	0	199.78	0.14	30.71	none	none	none
10d	CCCCCC2=CN(N=N2)C/C=C/C1=CC=CC=C1	255.36	3.57	-3.25	3	0	227.30	0.13	30.71	none	none	none
10e	CCCCCCCCCCC2=CN(N=N2)C/C=C/C1=CC=CC=C1	325.50	5.85	-4.60	3	0	296.10	0.10	30.71	none	none	none
	Max	385.64	8.77	-0.72	7	1	360.53	0.41	83.31	none	none	none
	Min	179.27	-0.40	-4.91	3	0	153.61	0.08	30.71	none	none	none

Physicochemical properties calculated in Osiris and Molinpiration		OSIRIS		MOLINSPIRATION								
ID	SMILE	Drug likeness	Drug Score	miLogP	TPSA	natoms	MW	nON	nONH	n violations	n rotb	volume
1a	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CO)=C1	-4.63	0.36	4.8	50.95	22	303.45	4	1	0	9	318.4
1b	C/C(C)=C\CC/C(C)=C/CC/C(C)=C\Cn1nnc(CO)c1	-4.63	0.36	4.8	50.95	22	303.45	4	1	0	9	318.4
1c	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(C(C)O)=C1	-5.39	0.34	5.02	50.95	23	317.48	4	1	1	9	335
1d	CC(c1nnn(C/C=C(CC/C=C(CC/C=C(C)\C)\C)/C)c1)O	-5.39	0.34	5.02	50.95	23	317.48	4	1	1	9	335
1e	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(C(C)(C)O)=C1	-5.35	0.3	5.61	50.95	24	331.5	4	1	1	9	351.3
1f	C/C(C)=C\CC/C(C)=C/CC/C(C)=C\Cn1nnc(C(C)(O)C)c1	-5.35	0.3	5.61	50.95	24	331.5	4	1	1	9	351.3
1g	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CCO)=C1	-6.39	0.33	5.01	50.95	23	317.48	4	1	1	10	335.2
1h	C/C(C)=C\CC/C(C)=C/CC/C(C)=C\Cn1nnc(CCO)c1	-6.39	0.33	5.01	50.95	23	317.48	4	1	1	10	335.2
1i	C/C(CC\C=C(C)/C)=C\CC/C(C)=C\CN1N=NC(CCCCCCCC)=C1	-21.35	0.17	8.74	30.72	28	385.64	3	0	1	15	427.8
1j	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CCCCCCCC)=C1	-21.35	0.17	8.74	30.72	28	385.64	3	0	1	15	427.8
1k	C/C(CC\C=C(C)/C)=C\CC/C(C)=C\CN1N=NC(CCCCC)=C1	-13.34	0.22	7.58	30.72	25	343.56	3	0	1	12	377.4
1l	C/C(CC\C=C(C)/C)=C\CC/C(C)=C\CN1N=NC(CCC)=C1	-6.7	0.25	6.52	30.72	23	315.5	3	0	1	10	343.8
1m	C/C(CC\C=C(C)/C)=C\CC/C(C)=C\CN1N=NC(C2=CC=CC=C2)=C1	-4.48	0.21	6.89	30.72	26	349.52	3	0	1	9	365
1n	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(C2=CC=CC=C2)=C1	-4.48	0.21	6.89	30.72	26	349.52	3	0	1	9	365
1o	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CCCCC)=C1	-13.34	0.22	7.58	30.72	25	343.56	3	0	1	12	377.4
1p	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CCC)=C1	-6.7	0.25	6.52	30.72	23	315.5	3	0	1	10	343.8
1q	C/C(CC/C=C(C)/C)=C\CC/C(C)=C\CN1N=NC(C(OC)=O)=C1	-6.32	0.32	5.29	57.02	24	331.46	5	0	1	10	338.1
1r	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(C(OC)=O)=C1	-6.32	0.32	5.29	57.02	24	331.46	5	0	1	10	338.1
2a	C/C(C)=C/CC/C(C)=C\CN1N=NC(CCCCCCCC)=C1	-21.49	0.24	7.25	30.72	23	317.52	3	0	1	12	350.2
2b	C/C(C)=C/CC/C(C)=C/CN1N=NC(CCCCCCCC)=C1	-21.5	0.24	7.25	30.72	23	317.52	3	0	1	12	350.2
2c	C/C(C)=C/CC/C(C)=C\CN1N=NC(CCCCC)=C1	-13.49	0.33	5.74	30.72	20	275.44	3	0	1	9	299.8
2d	C/C(C)=C/CC/C(C)=C/CN1N=NC(CCCCC)=C1	-13.49	0.33	5.74	30.72	20	275.44	3	0	1	9	299.8
2e	C/C(C)=C/CC/C(C)=C\CN1N=NC(CCC)=C1	-6.85	0.39	4.67	30.72	18	247.39	3	0	0	7	266.2
2f	C/C(C)=C/CC/C(C)=C/CN1N=NC(CCC)=C1	-6.85	0.39	4.67	30.72	18	247.39	3	0	0	7	266.2
2g	C/C(C)=C/CC/C(C)=C/CN1N=NC(C(OC)=O)=C1	-6.46	0.45	3.45	57.02	19	263.34	5	0	0	7	260.6
2h	C/C(C)=C/CC/C(C)=C\CN1N=NC(C(OC)=O)=C1	-6.46	0.45	3.45	57.02	19	263.34	5	0	0	7	260.6
2i	C/C(C)=C/CC/C(C)=C/CN1N=NC(C2=CC=CC=C2)=C1	-4.62	0.34	5.05	30.72	21	281.4	3	0	1	6	287.4
2j	C/C(C)=C/CC/C(C)=C\CN1N=NC(C2=CC=CC=C2)=C1	-4.62	0.34	5.05	30.72	21	281.4	3	0	1	6	287.4
3a	C/C(C)=C/CN1N=NC(C(OC)=O)=C1	-4.44	0.49	1.6	57.02	14	195.22	5	0	0	4	183
3b	C/C(C)=C/CN1N=NC(C2=CC=CC=C2)=C1	-2.36	0.49	3.2	30.72	16	213.28	3	0	0	3	209.9
3c	C/C(C)=C/CN1N=NC(CCC)=C1	-4.64	0.48	2.83	30.72	13	179.27	3	0	0	4	188.6
3d	C/C(C)=C/CN1N=NC(CCCCC)=C1	-12.33	0.45	3.89	30.72	15	207.32	3	0	0	6	222.2
3e	C/C(C)=C/CN1N=NC(CCCCCCCC)=C1	-20.34	0.48	5.41	30.72	18	249.4	3	0	1	9	272.6

Physicochemical properties calculated in Osiris and Molinpiration		OSIRIS		MOLINSPIRATION								
ID	SMILE	Drug likeness	Drug Score	miLogP	TPSA	natoms	MW	nON	nONH	n violations	n rotb	volume
4a	CCCCCCCCCCC2=CN(N=N2)CC1=CC=CC=C1	-19.85	0.31	6.33	30.72	22	299.46	3	0	1	11	317.1
4b	CCCCCCCCC2=CN(N=N2)CC1=CC=CC=C1	-19.85	0.37	5.33	30.72	20	271.41	3	0	1	9	283.5
4c	CCCCCC2=CN(N=N2)CC1=CC=CC=C1	-11.84	0.45	3.81	30.72	17	229.33	3	0	0	6	233.1
4d	CCCC2=CN(N=N2)CC1=CC=CC=C1	-4.15	0.48	2.74	30.72	15	201.27	3	0	0	4	199.5
4e	O=C(C2=CN(N=N2)CC1=CC=CC=C1)O	-0.83	0.63	1.26	68.02	15	203.2	5	1	0	3	176.3
4f	O=C(C2=CN(N=N2)CC1=CC=CC=C1)OC	-4.08	0.49	1.52	57.02	16	217.23	5	0	0	4	193.8
4g	C1(CN2N=NC(C3=CC=CC=C3)=C2)=CC=CC=C1	-1.77	0.51	3.12	30.72	18	235.29	3	0	0	3	220.7
4h	OCC2=CN(N=N2)CC1=CC=CC=C1	-2.02	0.54	1.02	50.95	14	189.22	4	1	0	3	174.1
5a	CCOC(CN1N=NC(CCCCCCCC)=C1)=O	-25.4	0.45	3.97	57.02	19	267.37	5	0	0	11	273.4
5b	O=C(CN1N=NC(CCCCC)=C1)OCC	-17.39	0.38	2.45	57.02	16	225.29	5	0	0	8	223
5c	CCOC(CN1N=NC(CCC)=C1)=O	-9.7	0.49	1.39	57.02	14	197.24	5	0	0	6	189.4
5d	CCOC(CCN(N=N1)C=C1C(OC)=O)=O	14.35	0.49	0.12	83.33	16	227.22	7	0	0	7	200.6
6a	CC(O)c2cn(CCCc1ccccc1)nn2	-3.48	0.49	1.98	50.95	17	231.3	4	1	0	5	224.3
6b	CCCCCCCCCCC2=CN(N=N2)CCCC1=CC=CC=C1	-19.41	0.25	7.06	30.72	24	327.52	3	0	1	13	350.7
6c	CCCC2=CN(N=N2)CCCC1=CC=CC=C1	-4.76	0.45	3.47	30.72	17	229.33	3	0	0	6	233.1
6d	CCCCCC2=CN(N=N2)CCCC1=CC=CC=C1	-11.4	0.41	4.54	30.72	19	257.38	3	0	0	8	266.7
6e	CCCCCCCCC2=CN(N=N2)CCCC1=CC=CC=C1	-19.41	0.31	6.05	30.72	22	299.46	3	0	1	11	317.1
6f	O=C(C2=CN(N=N2)CCCC1=CC=CC=C1)OC	-4.77	0.47	2.25	57.02	18	245.28	5	0	0	6	227.4
6g	C(Cc1ccccc1)Cn3cc(c2ccccc2)nn3	-2.52	0.44	3.85	30.72	20	263.34	3	0	0	5	254.3
6h	OCC2=CN(N=N2)CCCC1=CC=CC=C1	-2.73	0.51	1.75	50.95	16	217.27	4	1	0	5	207.7
7a	OCC1=CN(N=N1)CCCCCCCC	-19.85	0.47	2.89	50.95	15	211.31	4	1	0	8	220.1
7b	O=C(OC)C1=CN(N=N1)CCCCCCCC	-21.86	0.46	3.38	57.02	17	239.32	5	0	0	9	239.8
8a	OCC1=CN(N=N1)CCCCCCCCCC	-19.85	0.45	3.9	50.95	17	239.36	4	1	0	10	253.7
8b	O=C(OC)C1=CN(N=N1)CCCCCCCCCC	-21.86	0.43	4.39	57.02	19	267.37	5	0	0	11	273.4
9a	OCC1=CN(N=N1)CCCCCCCCCCCC	-19.85	0.38	5.42	50.95	20	281.44	4	1	1	13	304.1
9b	O=C(OC)C1=CN(N=N1)CCCCCCCCCCCC	-21.86	0.35	5.91	57.02	22	309.45	5	0	1	14	323.8
10a	CCCCCCCCC2=CN(N=N2)C/C=C/C1=CC=CC=C1	-20.31	0.31	6.08	30.72	22	297.45	3	0	1	10	310.9
10b	C1(C3=CN(N=N3)C/C=C/C2=CC=CC=C2)=CC=CC=C1	-3.28	0.42	3.88	30.72	20	261.33	3	0	0	4	248.1
10c	CCCC2=CN(N=N2)C/C=C/C1=CC=CC=C1	-5.61	0.45	3.5	30.72	17	227.31	3	0	0	5	226.9
10d	CCCCCC2=CN(N=N2)C/C=C/C1=CC=CC=C1	-13.3	0.41	4.57	30.72	19	255.37	3	0	0	7	260.5
10e	CCCCCCCCCCC2=CN(N=N2)C/C=C/C1=CC=CC=C1	-20.31	0.25	7.09	30.72	24	325.5	3	0	1	12	344.5
	Max	14.35	0.63	8.74	83.33	28	385.64	7	1	1	15	427.8
	Min	-25.4	0.17	0.12	30.72	13	179.27	3	0	0	3	174.1

Physicochemical properties of active compounds

		DATAWARRIOR										
ID	SMILE	MW	cLogP	cLogS	HA	HD	TSA	Relative PSA	PSA	Mutagenic	Tumorigenic	Irritant
1f	C/C(C)=C\CC/C(C)=C/CC/C(C)=C\Cn1nnc(C(C)(O)C)c1	331.502	5.56	-3.158	4	1	293.23	0.14293	50.94	none	none	none
1g	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CCO)=C1	317.475	5.117	-2.785	4	1	285.82	0.14663	50.94	none	none	none
1o	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CCCCC)=C1	343.557	7.407	-4.102	3	0	319.25	0.090243	30.71	none	none	none
3a	C/C(C)=C/CN1N=NC(C(OC)=O)=C1	195.221	0.854	-0.978	5	0	162.98	0.31814	57.01	none	none	none
4a	CCCCCCCCCCC2=CN(N=N2)CC1=CC=CC=C1	299.46	5.174	-3.849	3	0	269.6	0.10686	30.71	none	none	none
5d	CCOC(CCN(N=N1)C=C1C(OC)=O)=O	227.219	-0.397	-0.715	7	0	181.28	0.41312	83.31	none	none	none
6c	CCCC2=CN(N=N2)CCCC1=CC=CC=C1	229.326	2.788	-2.579	3	0	200.8	0.14348	30.71	none	none	none
6d	CCCCCC2=CN(N=N2)CCCC1=CC=CC=C1	257.38	3.697	-3.119	3	0	228.32	0.12618	30.71	none	none	none
7a	OCC1=CN(N=N1)CCCCCCCC	211.308	1.807	-1.905	4	1	188.67	0.22213	50.94	none	none	none
8b	O=C(OC)C1=CN(N=N1)CCCCCCCCCC	267.372	3.226	-2.702	5	0	236.09	0.21962	57.01	none	none	none
10a	CCCCCCCCC2=CN(N=N2)C/C=C/C1=CC=CC=C1	297.444	4.936	-4.064	3	0	268.58	0.10727	30.71	none	none	none
10b	C1(C3=CN(N=N3)C/C=C/C2=CC=CC=C2)=CC=CC=C1	261.327	3.147	-3.695	3	0	219.76	0.1311	30.71	none	none	none
10c	CCCC2=CN(N=N2)C/C=C/C1=CC=CC=C1	227.31	2.664	-2.714	3	0	199.78	0.14421	30.71	none	none	none
	Max	343.557	7.407	-0.715	7	1	319.25	0.41312	83.31	none	none	none
	Min	195.221	-0.397	-4.102	3	0	162.98	0.090243	30.71	none	none	none

		OSIRIS		MOLINSPIRATION								
ID	SMILE	Drug likeness	Drug Score	miLogP	TPSA	natoms	MW	nON	nONH	n violations	n rotb	volume
1f	C/C(C)=C\CC/C(C)=C/CC/C(C)=C\Cn1nnc(C(C)(O)C)c1	-5.35	0.3	5.61	50.95	24	331.5	4	1	1	9	351.3
1g	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CCO)=C1	-6.39	0.33	5.01	50.95	23	317.48	4	1	1	10	335.2
1o	C/C(CC\C=C(C)/C)=C\CC/C(C)=C/CN1N=NC(CCCCC)=C1	-13.34	0.22	7.58	30.72	25	343.56	3	0	1	12	377.4
3a	C/C(C)=C/CN1N=NC(C(OC)=O)=C1	-4.44	0.49	1.6	57.02	14	195.22	5	0	0	4	183
4a	CCCCCCCCCCC2=CN(N=N2)CC1=CC=CC=C1	-19.85	0.31	6.33	30.72	22	299.46	3	0	1	11	317.1
5d	CCOC(CCN(N=N1)C=C1C(OC)=O)=O	14.35	0.49	0.12	83.33	16	227.22	7	0	0	7	200.6
6c	CCCC2=CN(N=N2)CCCC1=CC=CC=C1	-4.76	0.45	3.47	30.72	17	229.33	3	0	0	6	233.1
6d	CCCCCC2=CN(N=N2)CCCC1=CC=CC=C1	-11.4	0.41	4.54	30.72	19	257.38	3	0	0	8	266.7
7a	OCC1=CN(N=N1)CCCCCCCC	-19.85	0.47	2.89	50.95	15	211.31	4	1	0	8	220.1
8b	O=C(OC)C1=CN(N=N1)CCCCCCCCCC	-21.86	0.43	4.39	57.02	19	267.37	5	0	0	11	273.4
10a	CCCCCCCCC2=CN(N=N2)C/C=C/C1=CC=CC=C1	-20.31	0.31	6.08	30.72	22	297.45	3	0	1	10	310.9
10b	C1(C3=CN(N=N3)C/C=C/C2=CC=CC=C2)=CC=CC=C1	-3.28	0.42	3.88	30.72	20	261.33	3	0	0	4	248.1
10c	CCCC2=CN(N=N2)C/C=C/C1=CC=CC=C1	-5.61	0.45	3.5	30.72	17	227.31	3	0	0	5	226.9
	Max	14.35	0.49	7.58	83.33	25	343.56	7	1	1	12	377.4
	Min	-21.86	0.22	0.12	30.72	14	195.22	3	0	0	4	183