

Supporting information for

The Synthesis of macrocyclic peptidomimetics via Ugi/click-strategy

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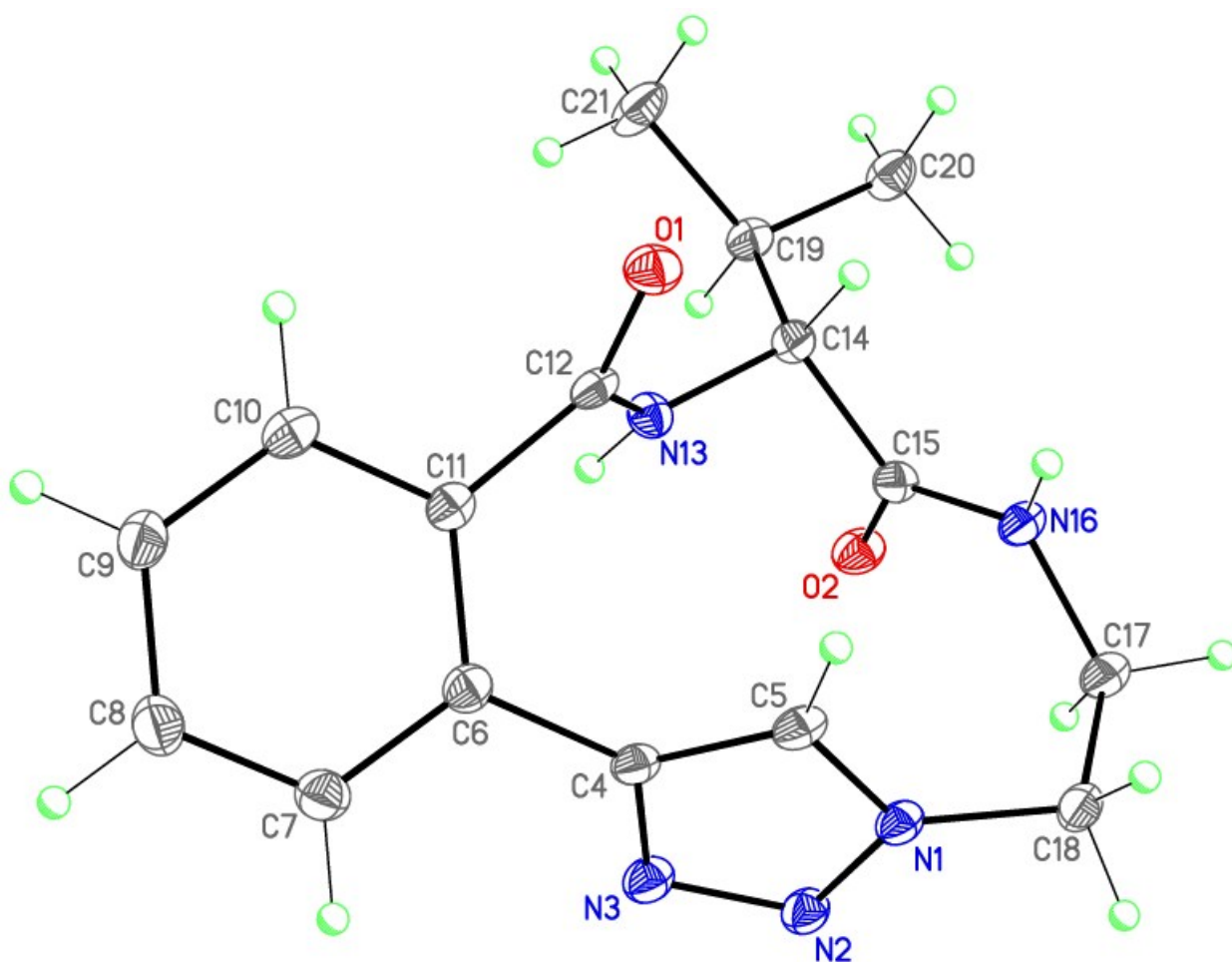


Figure S1. Structure of compound 5o. Anisotropic displacement ellipsoids show 50% probability levels. Hydrogen atoms are drawn as circles with small radii.

Identification code	5o	
Empirical formula	C ₁₆ H ₁₉ N ₅ O ₂	
Formula weight	313.36	
Temperature	100(2) K	
Wavelength	0.96990 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 8.9287(18) Å	∠ = 90°.
	b = 19.324(4) Å	∠ = 110.58(3)°.
	c = 9.833(2) Å	∠ = 90°.
Volume	1588.3(6) Å ³	
Z	4	
Density (calculated)	1.311 Mg/m ³	
Absorption coefficient	0.189 mm ⁻¹	
F(000)	664	
Crystal size	0.20 x 0.03 x 0.02 mm ³	
Theta range for data collection	3.345 to 38.446°.	

Index ranges	-11<=h<=7, -22<=k<=22, -11<=l<=12
Reflections collected	10660
Independent reflections	3285 [R(int) = 0.0886]
Completeness to theta = 35.587°	98.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.987 and 0.960
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3285 / 0 / 211
Goodness-of-fit on F ²	0.959
Final R indices [for 2152 rflns with I>2σ(I)]	R1 = 0.0825, wR2 = 0.1707
R indices (all data)	R1 = 0.1099, wR2 = 0.1881
Extinction coefficient	0.042(4)
Largest diff. peak and hole	0.342 and -0.367 e.Å ⁻³

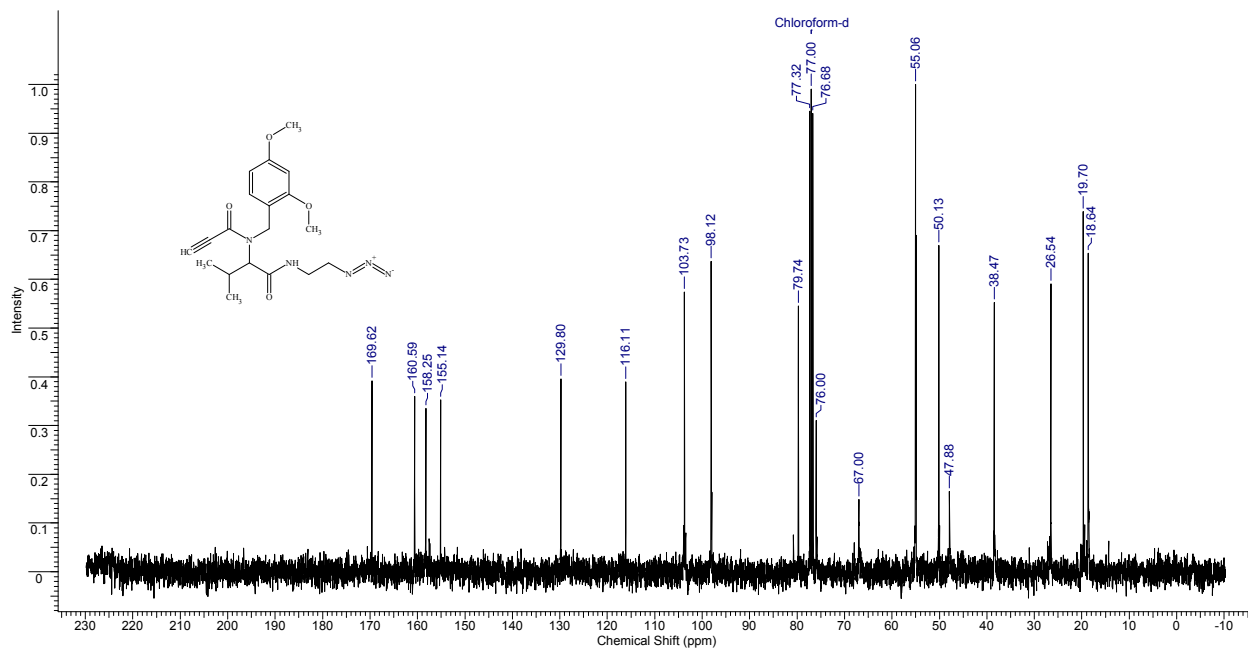
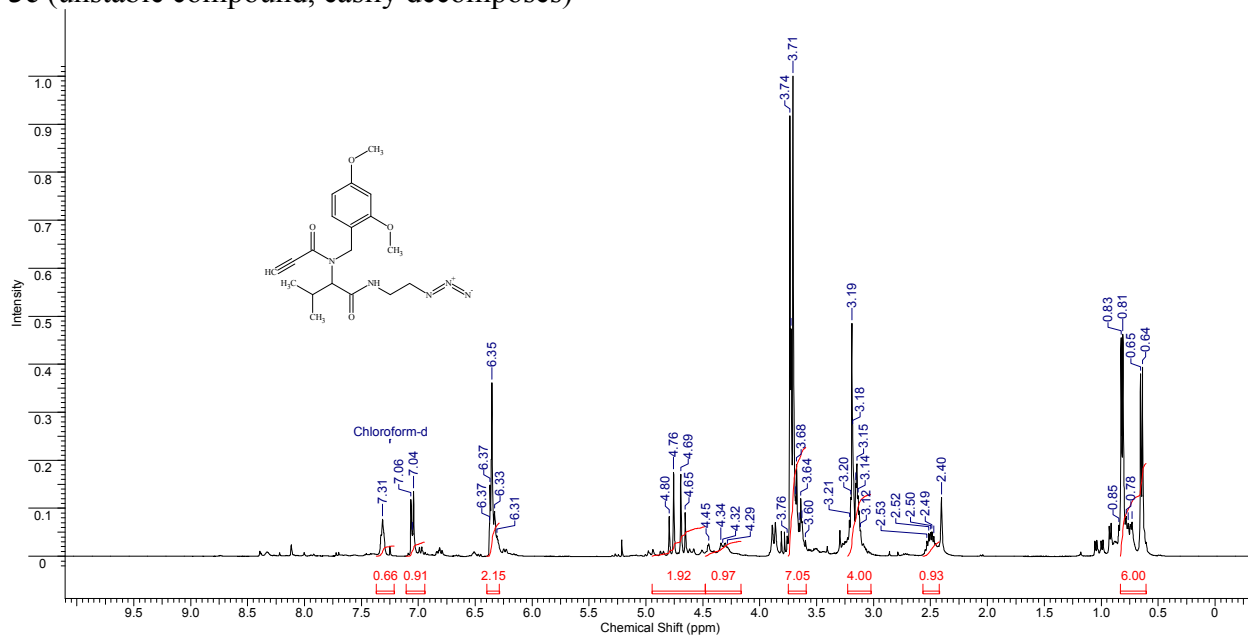
Table S1. Hydrogen bonds for **5o** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(5)-H(5)...O(2)#1	0.95	2.42	3.150(2)	134
N(13)-H(13)...O(1)#2	0.91	1.94	2.846(2)	176
N(16)-H(16)...N(3)#1	0.91	2.09	2.982(3)	165
C(18)-H(18A)...O(1)#3	0.99	2.50	3.483(2)	170
C(18)-H(18B)...N(2)#1	0.99	2.52	3.362(3)	143

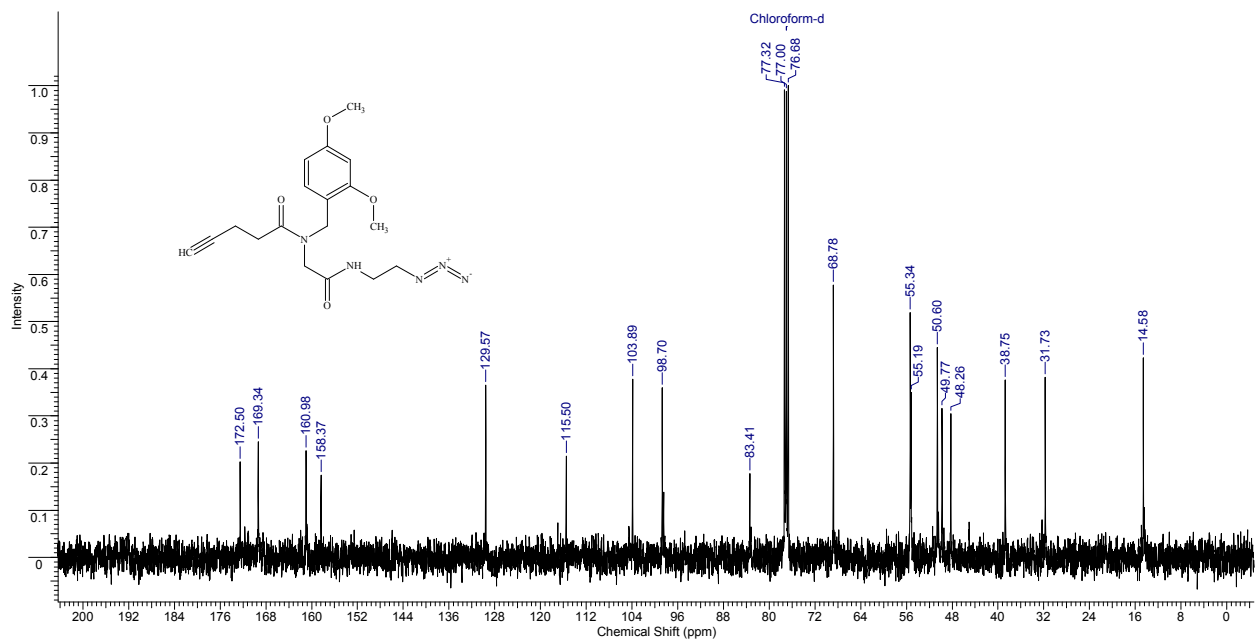
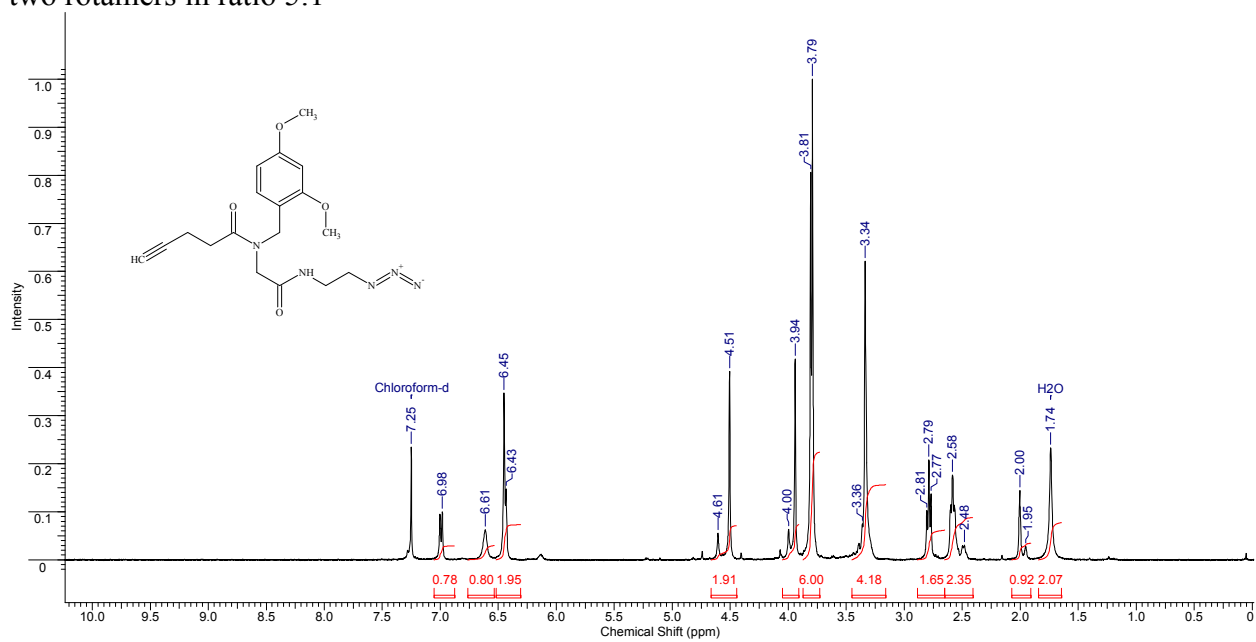
Symmetry transformations used to generate equivalent atoms:

#1 x, -y+3/2, z-1/2 #2 x, -y+3/2, z+1/2 #3 x-1, y, z

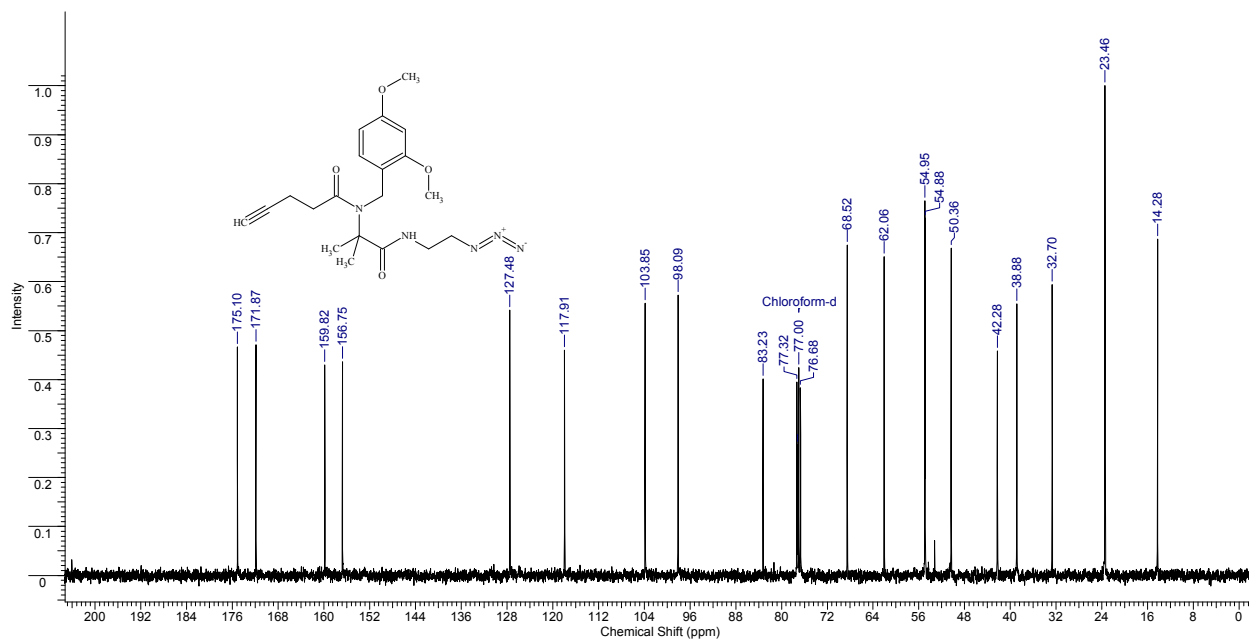
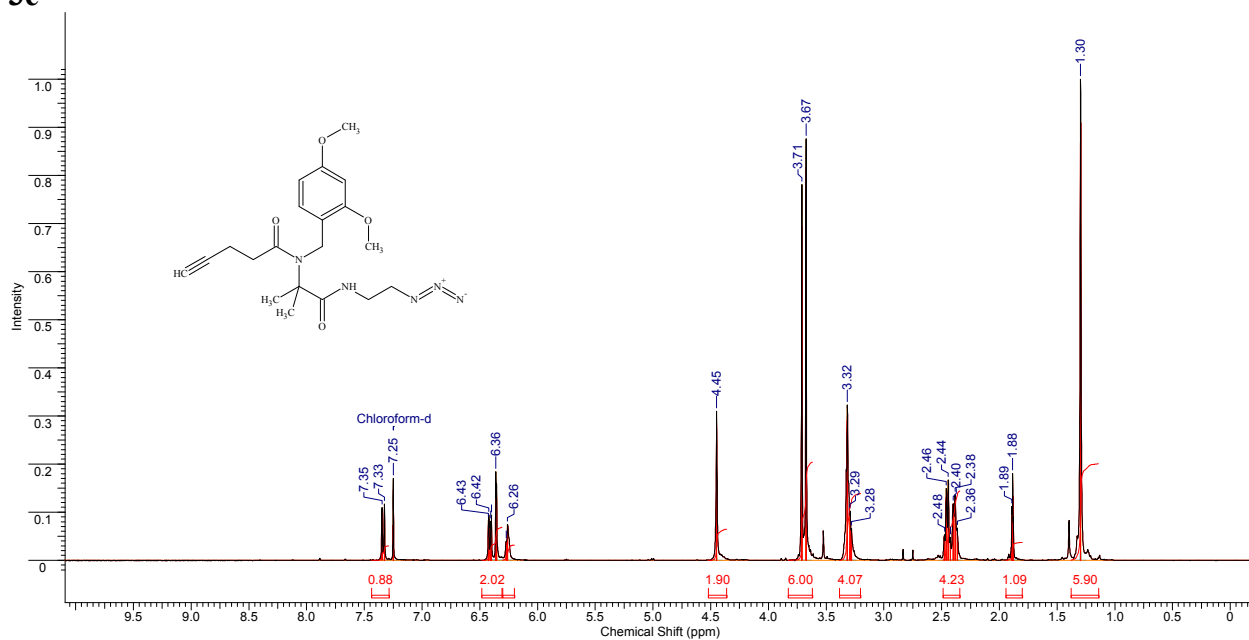
3c (unstable compound, easily decomposes)



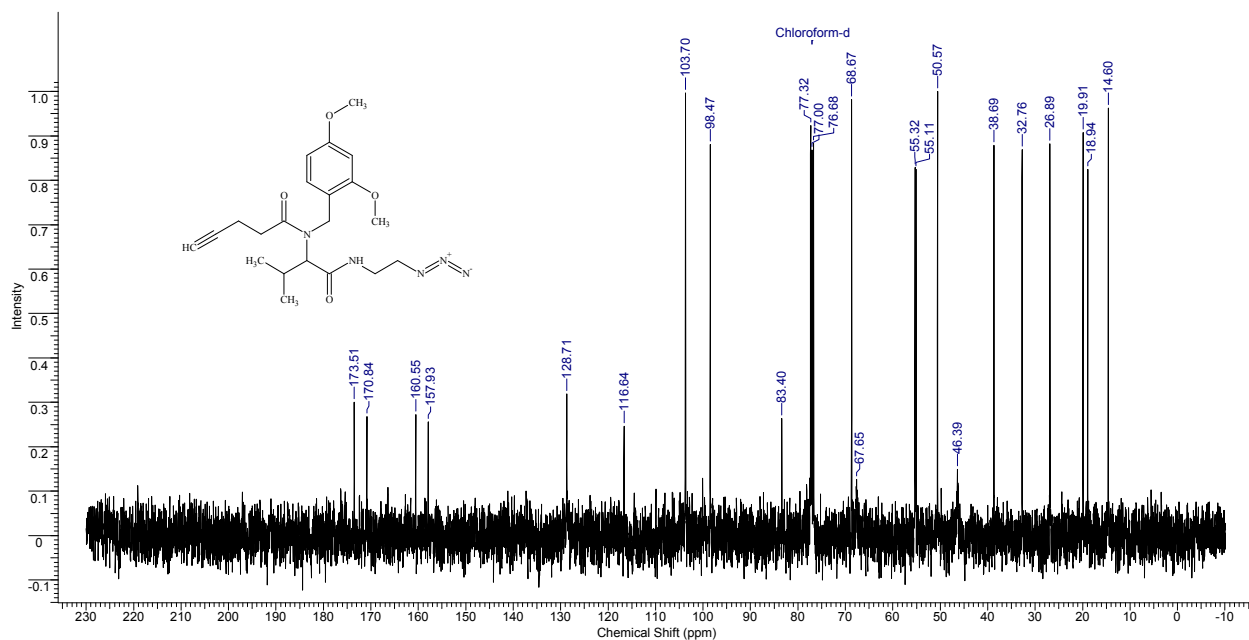
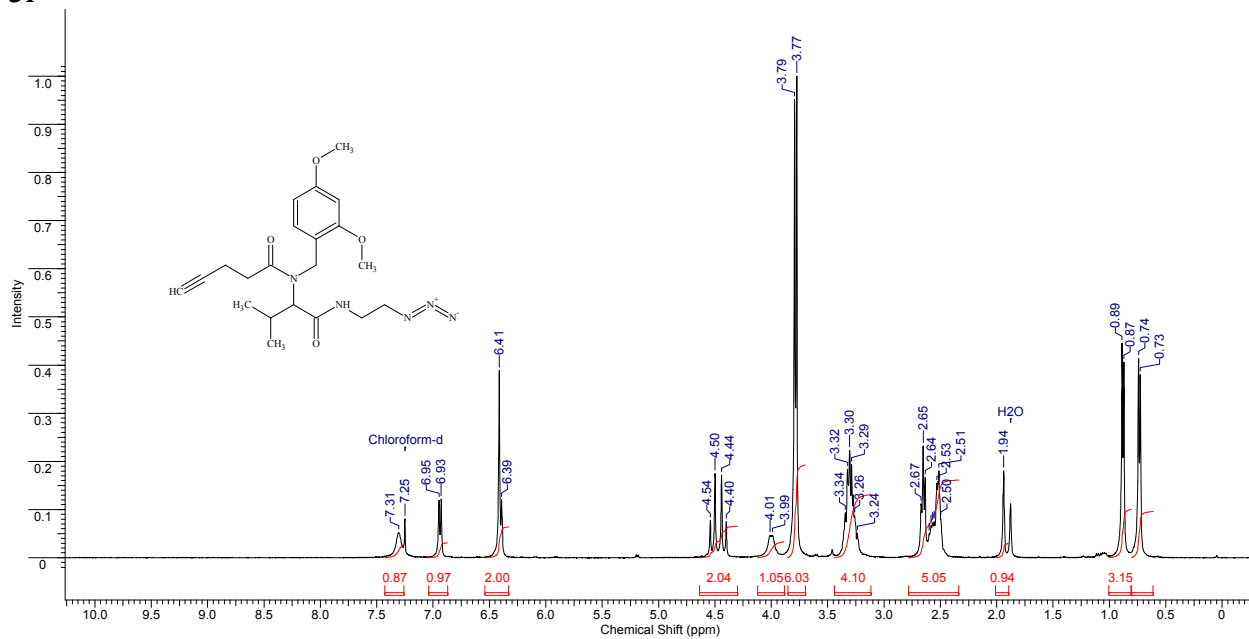
two rotamers in ratio 5:1



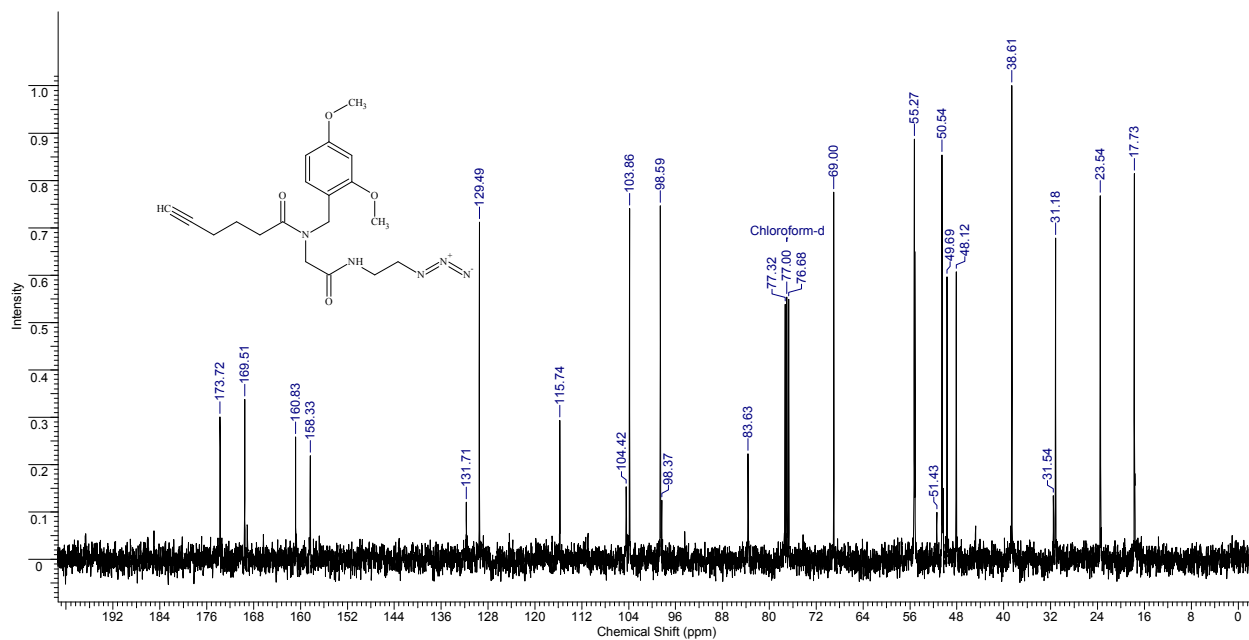
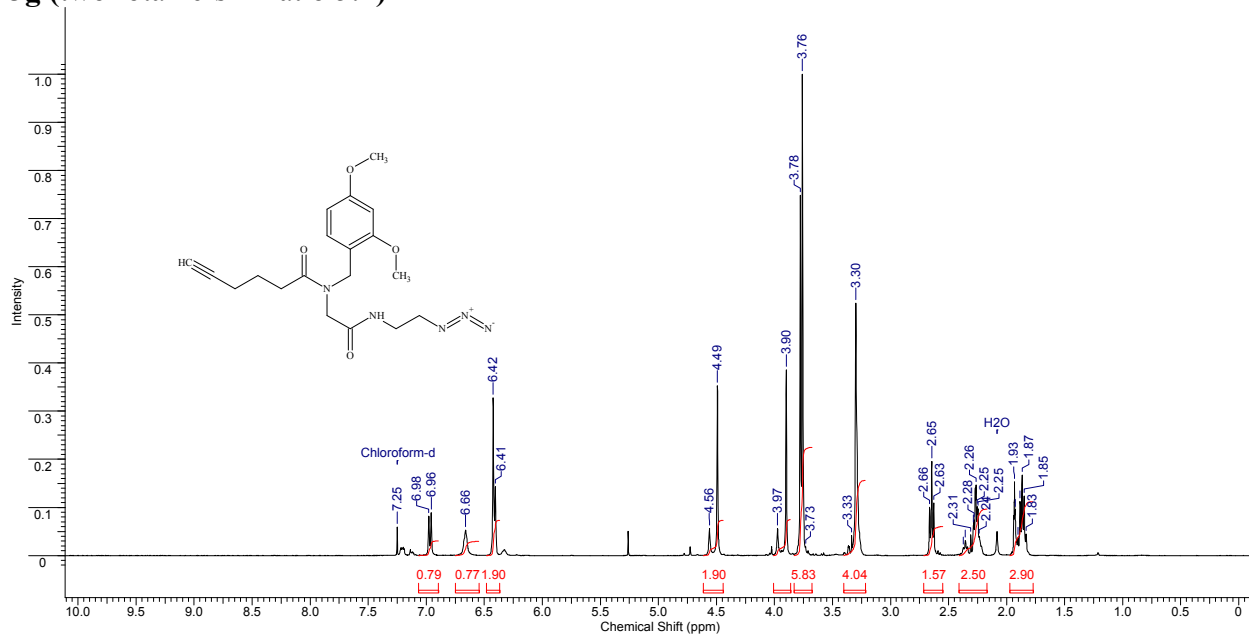
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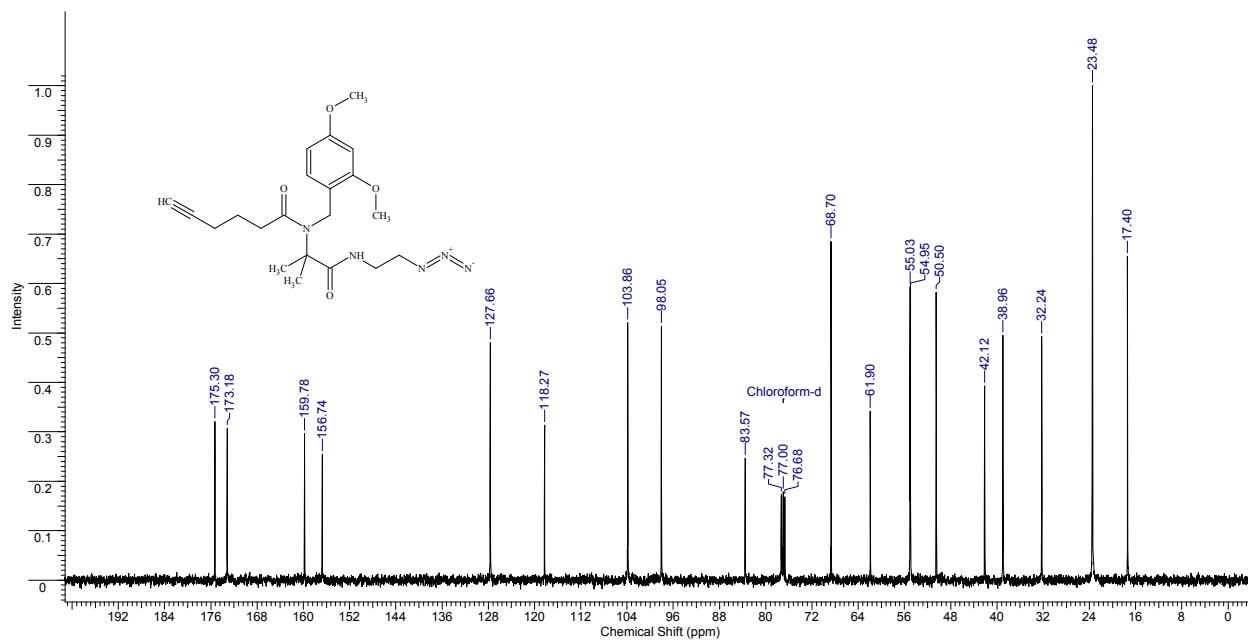
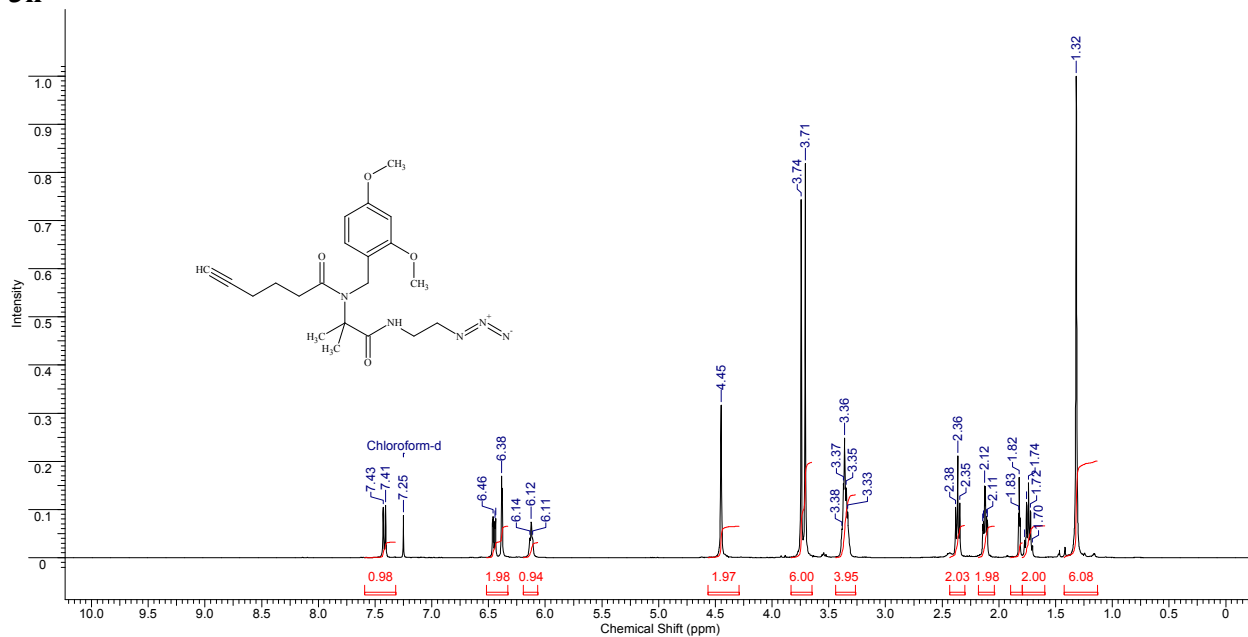
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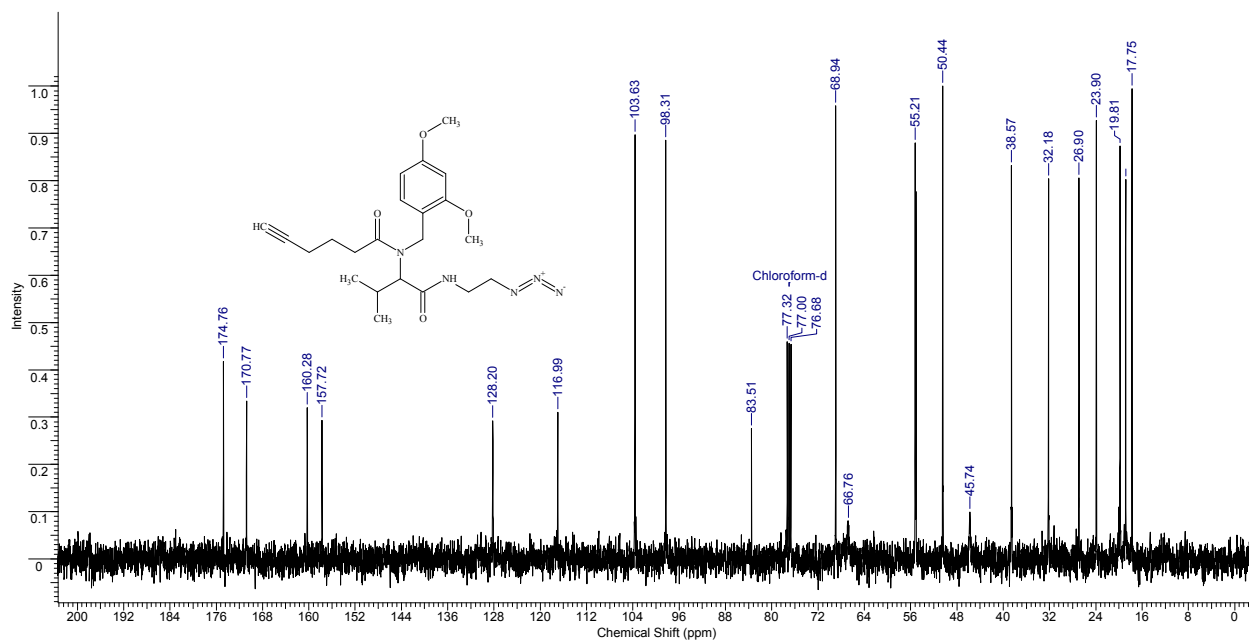
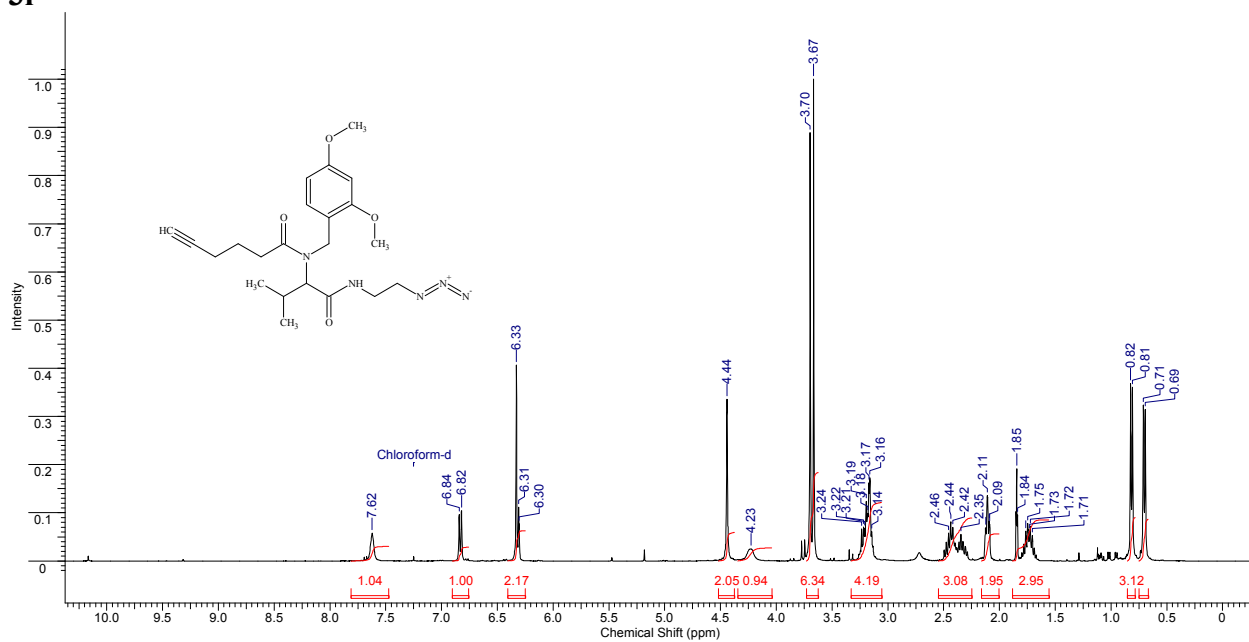
3g (two rotamers in ratio 5:1)



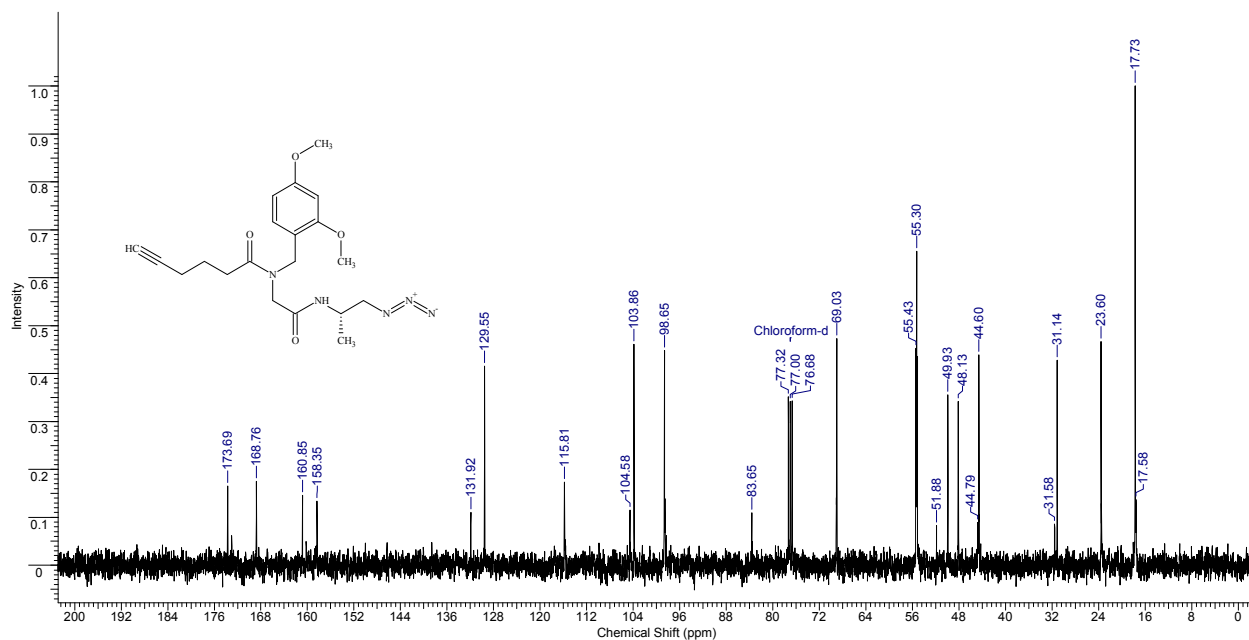
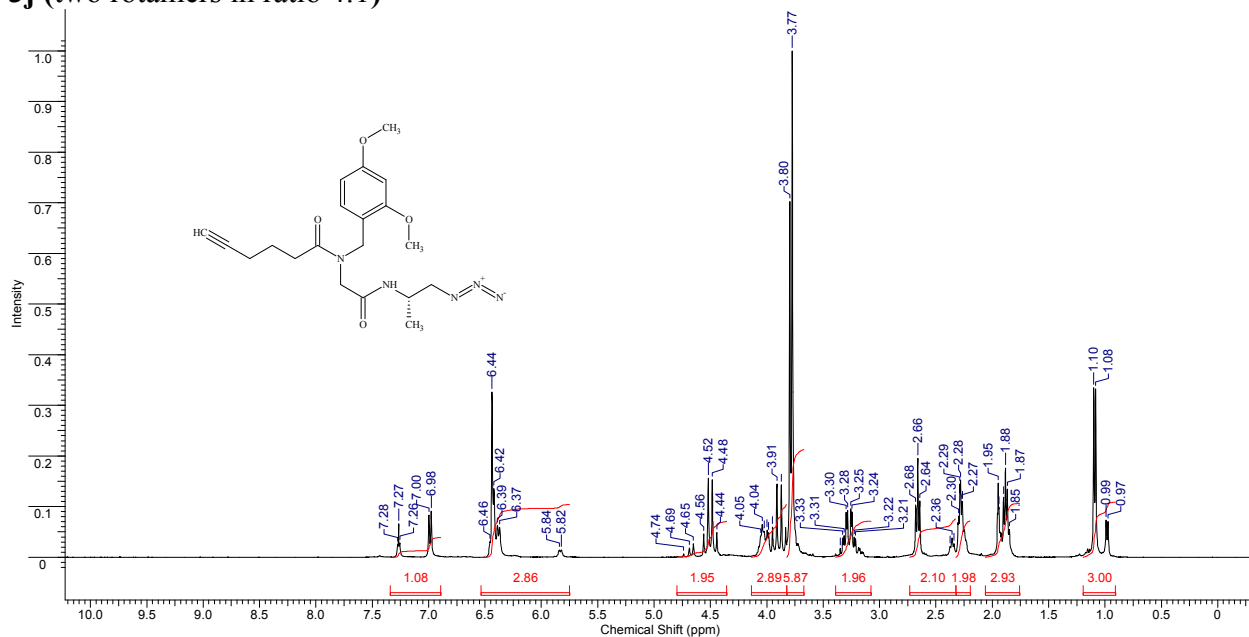
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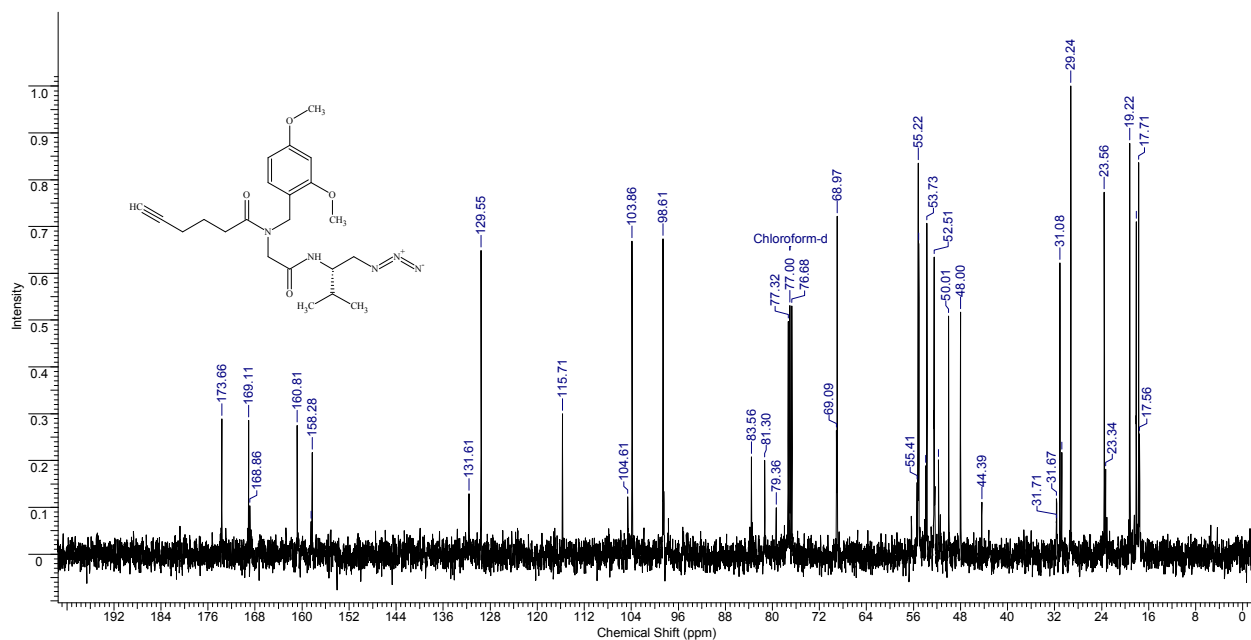
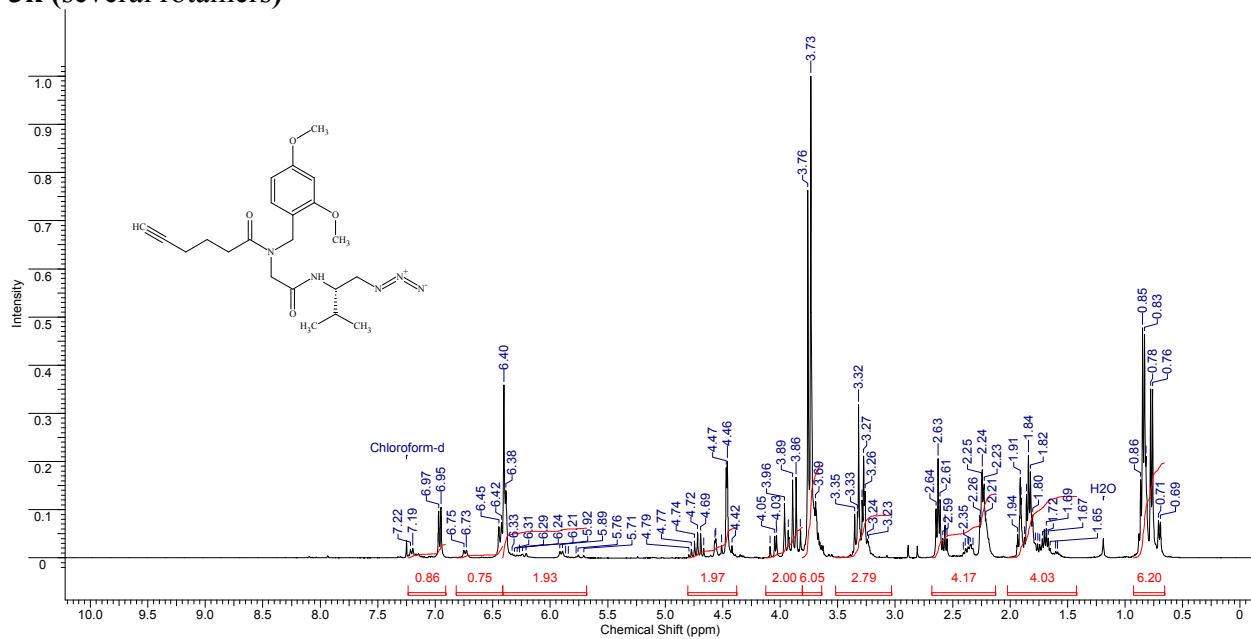
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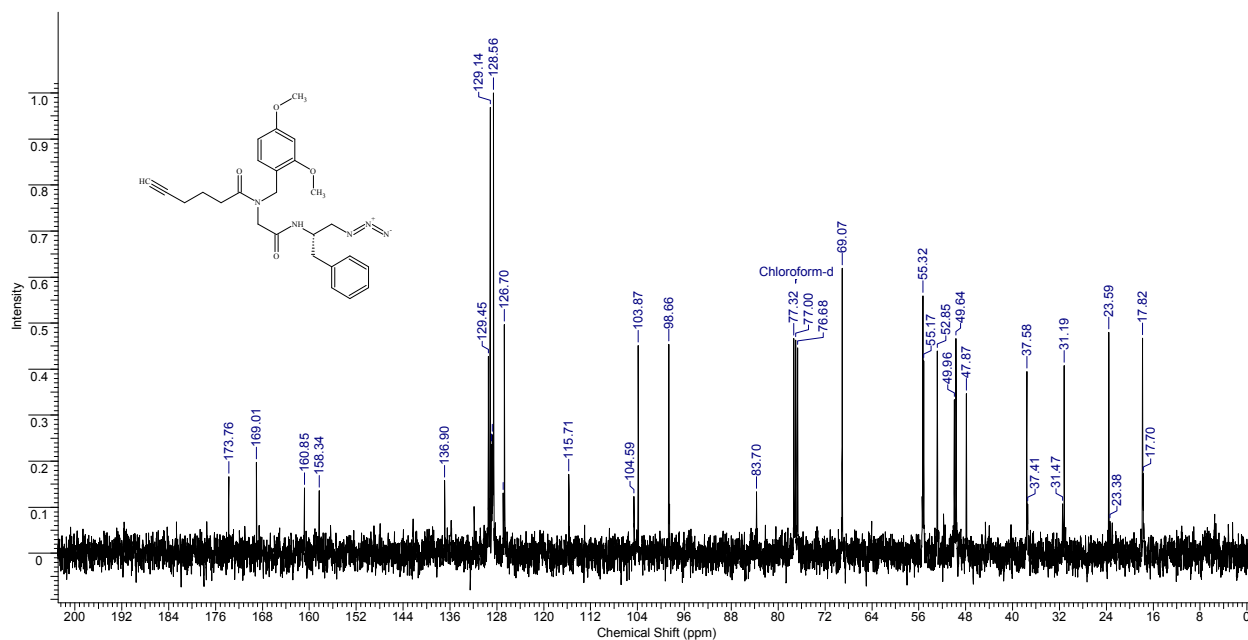
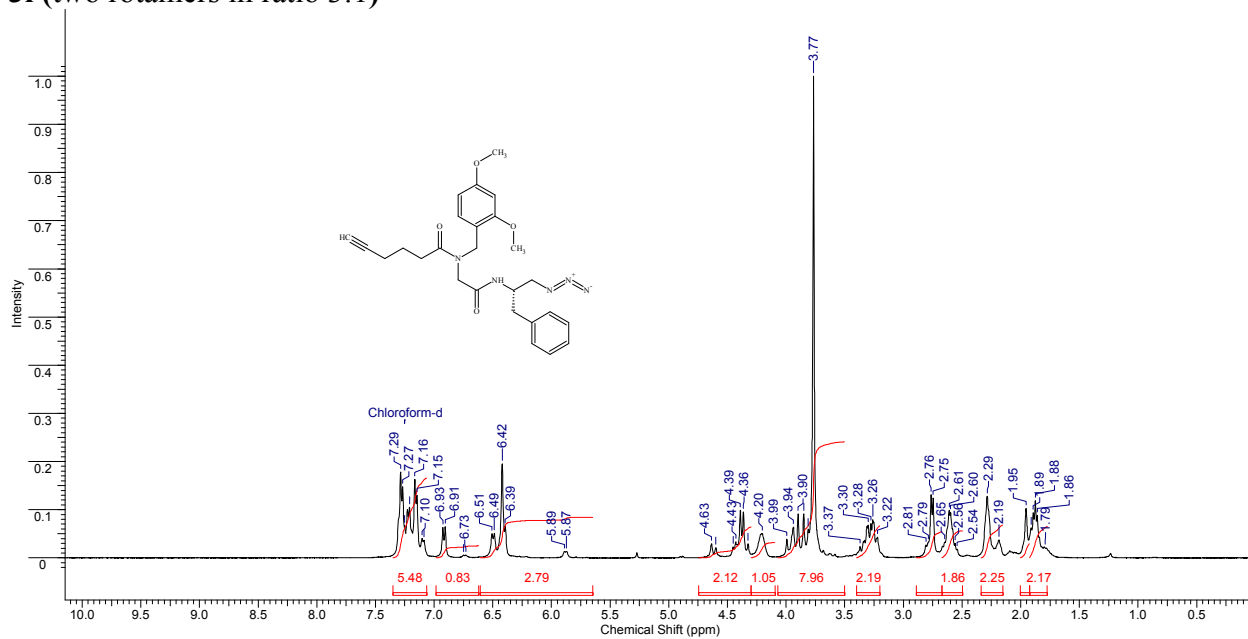
3j (two rotamers in ratio 4:1)



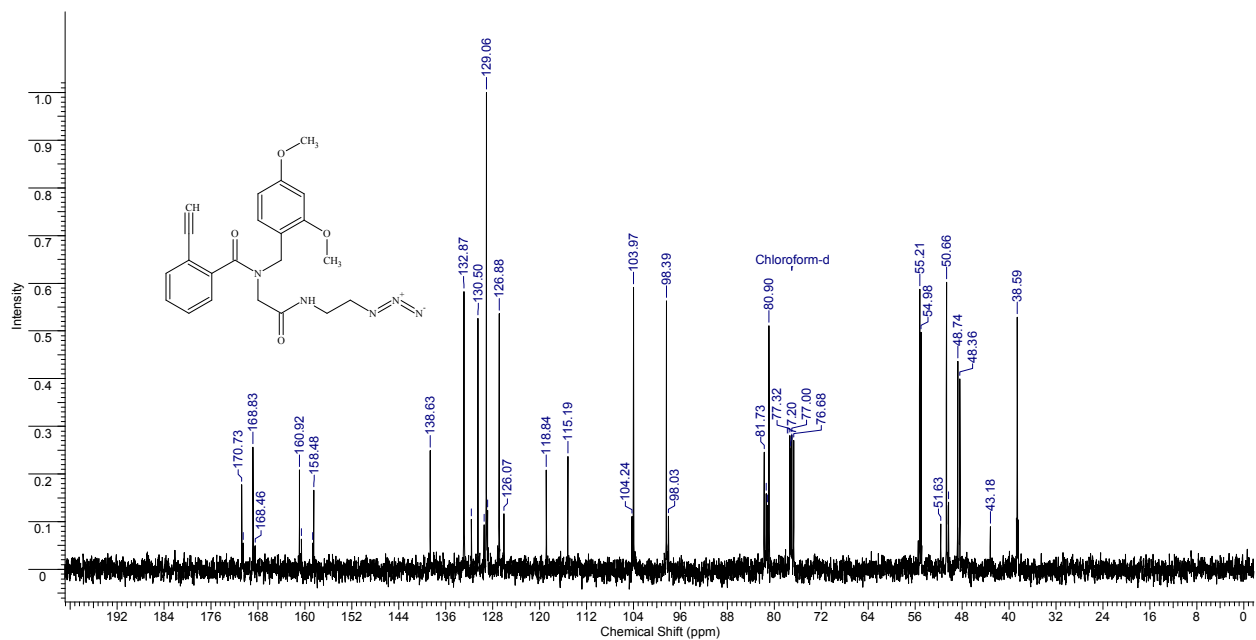
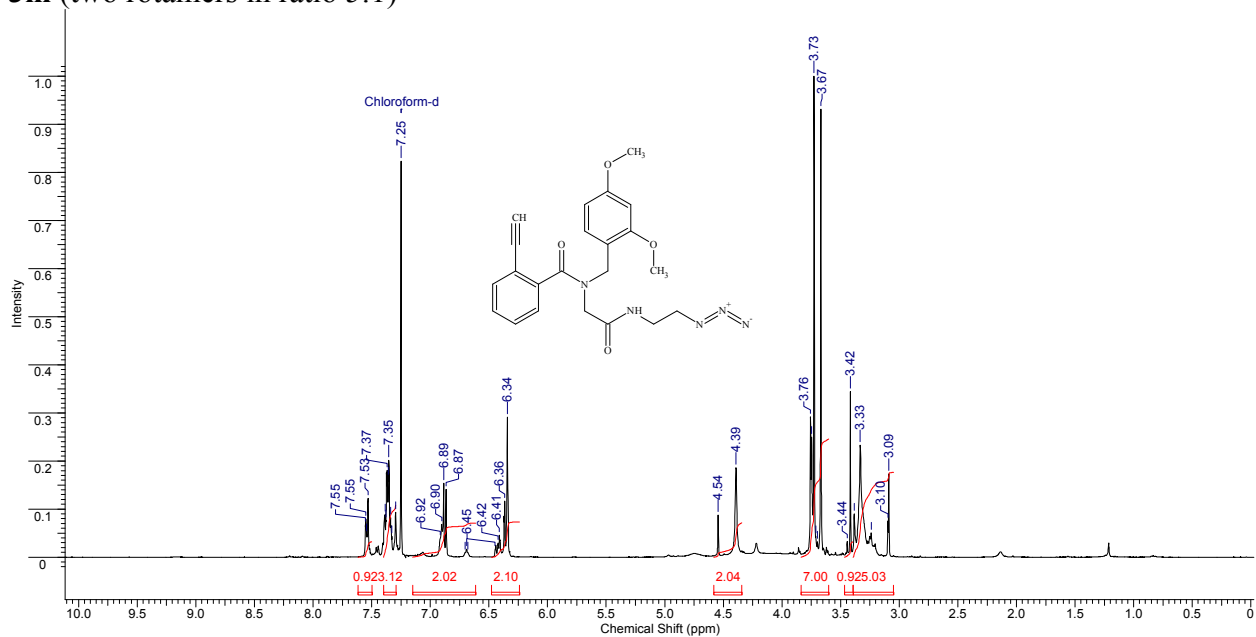
3k (several rotamers)

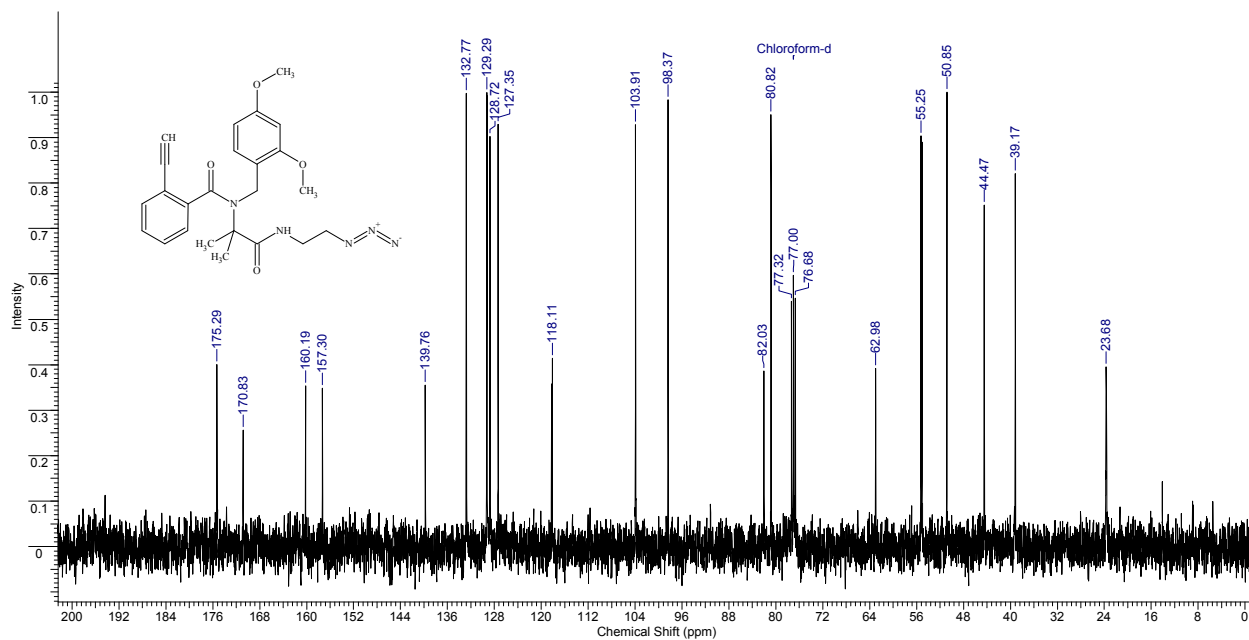
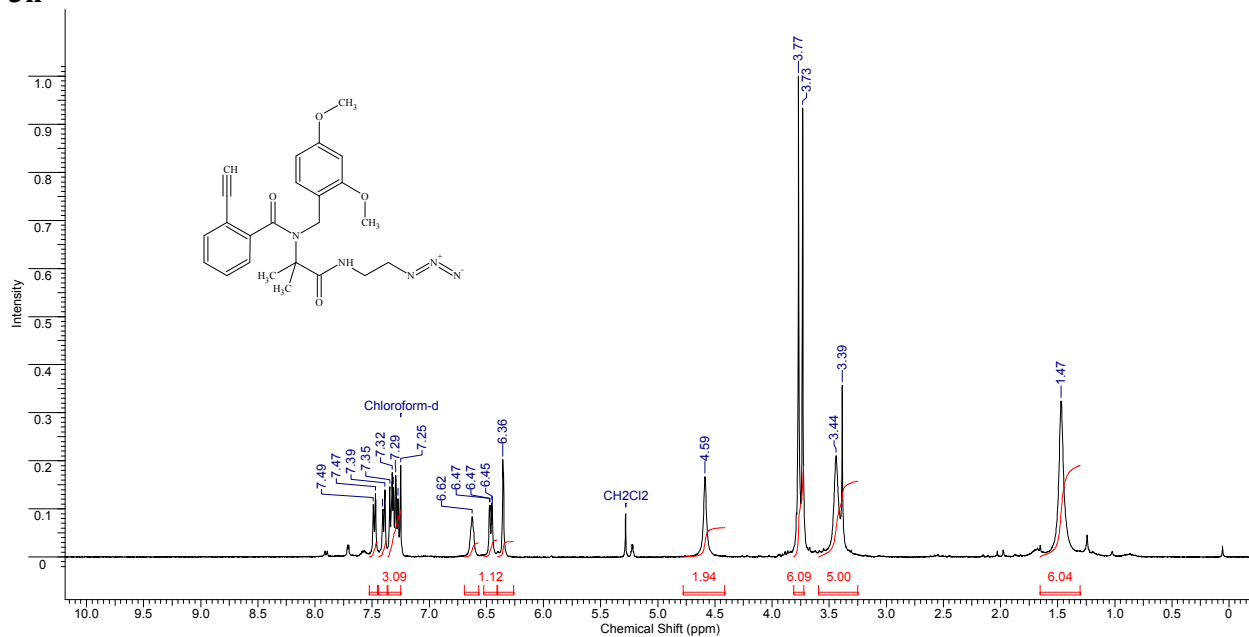


3l (two rotamers in ratio 3:1)

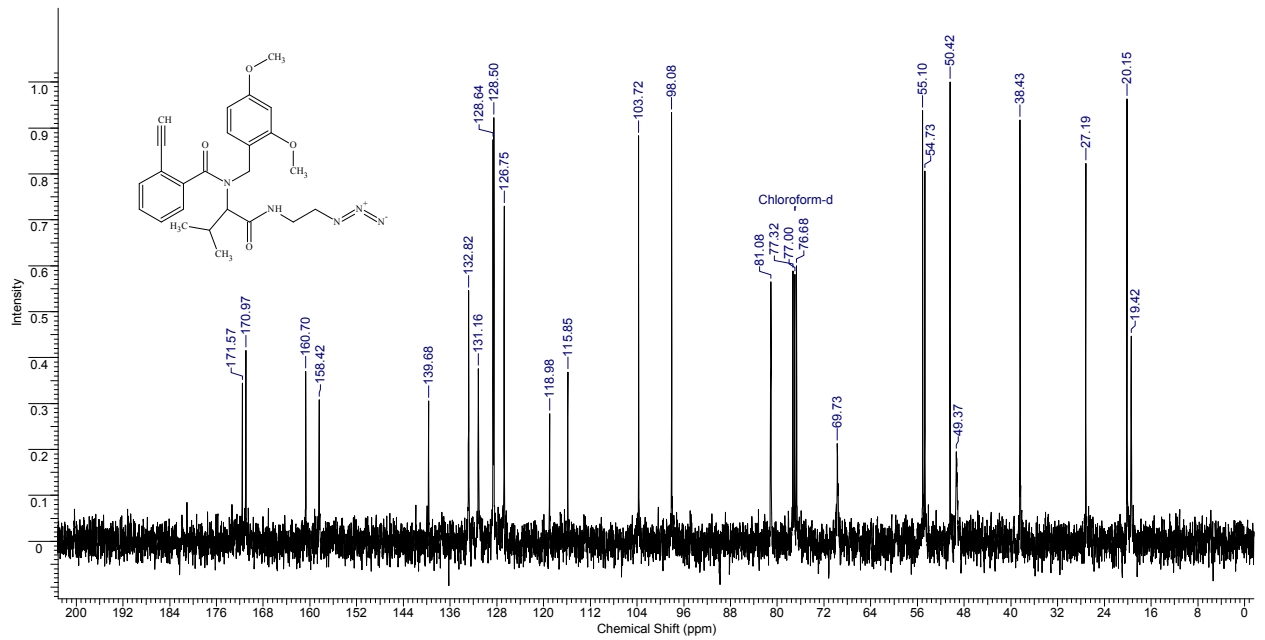
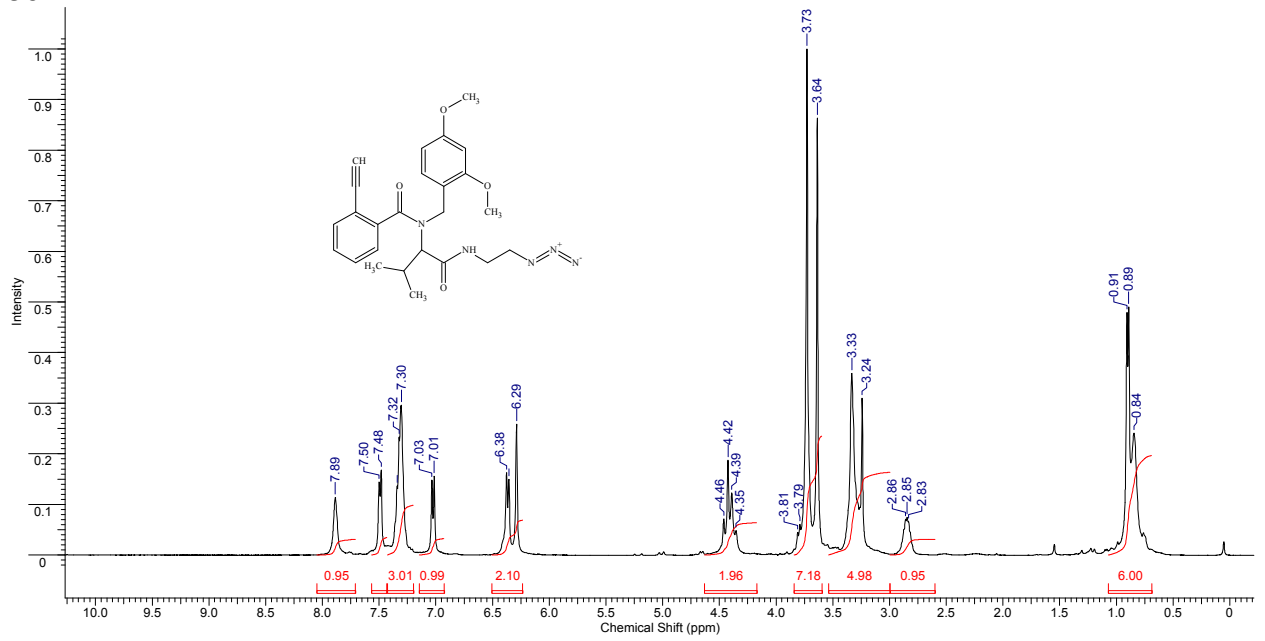


3m (two rotamers in ratio 5:1)

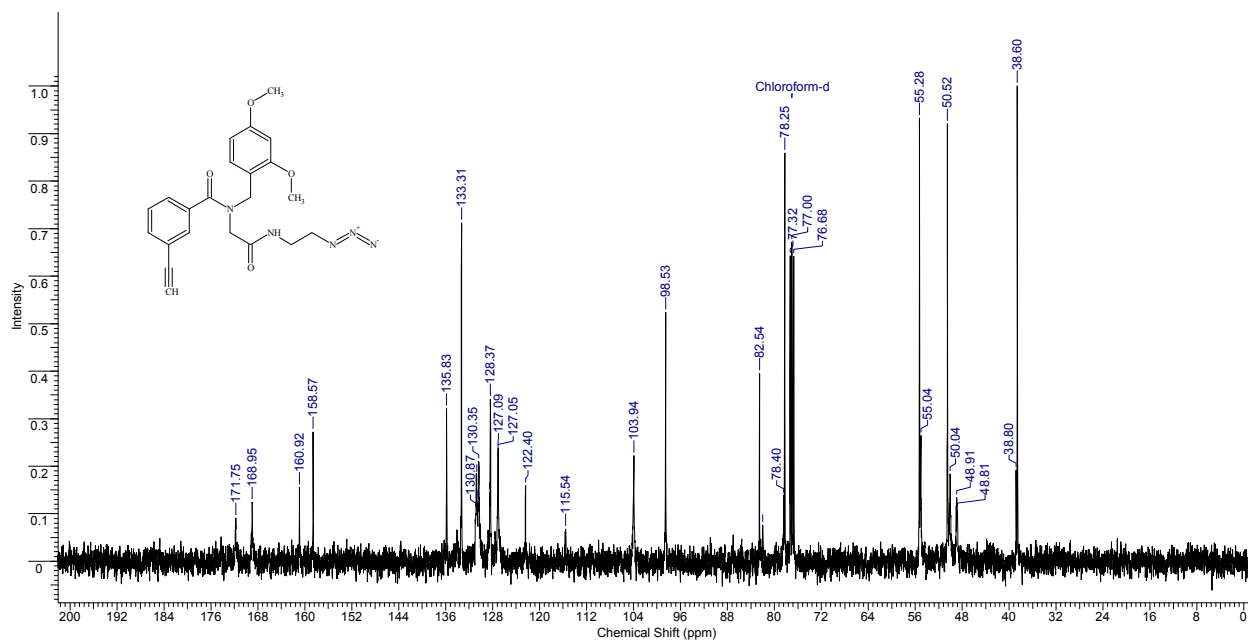
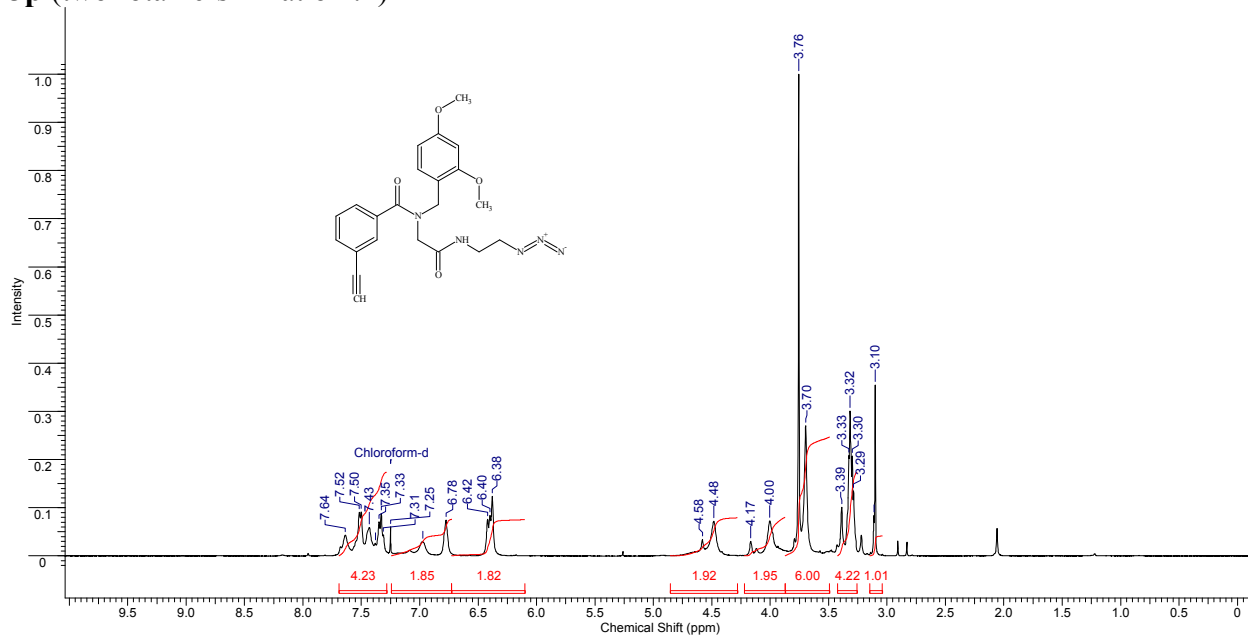


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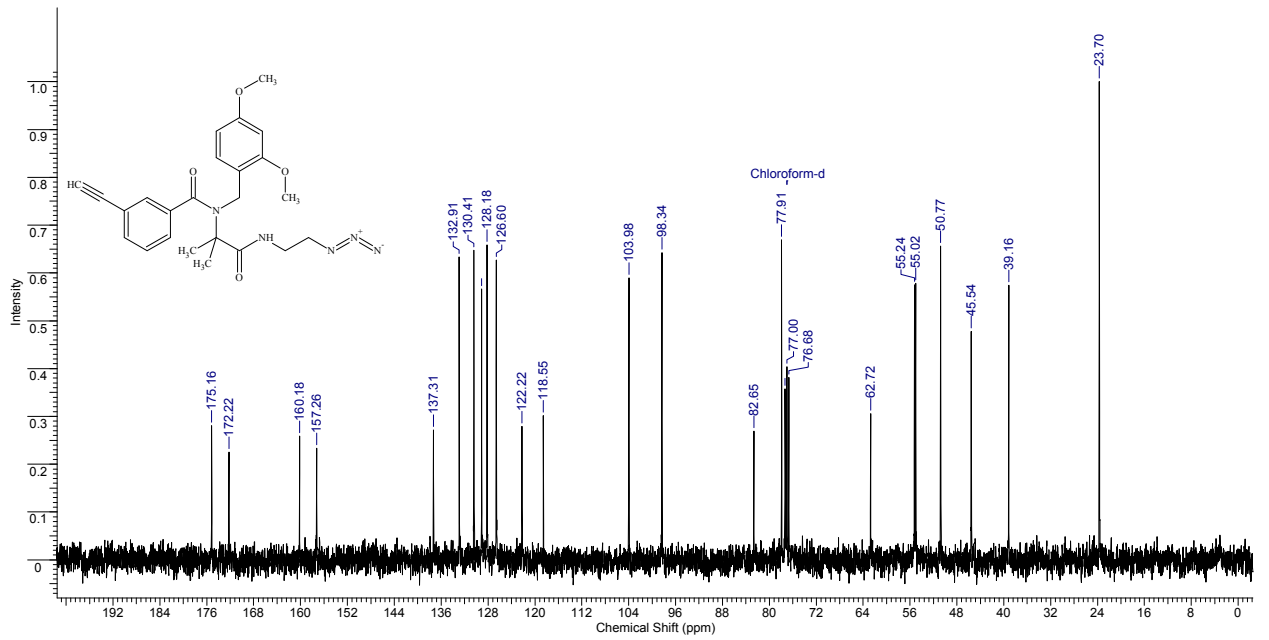
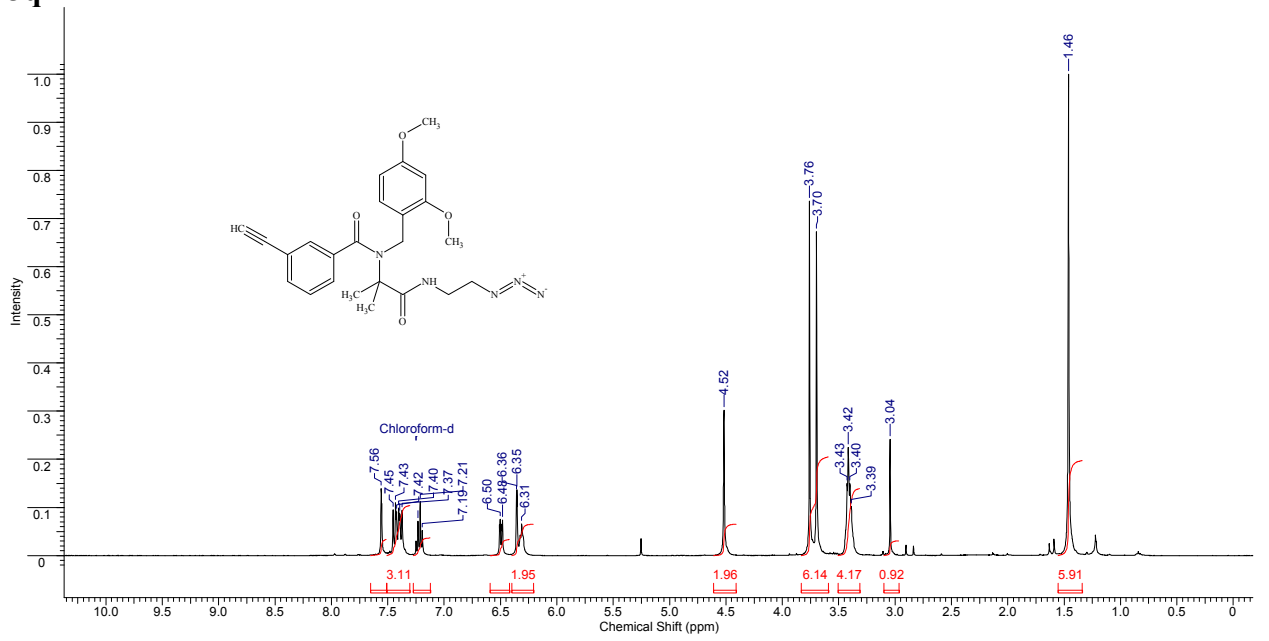
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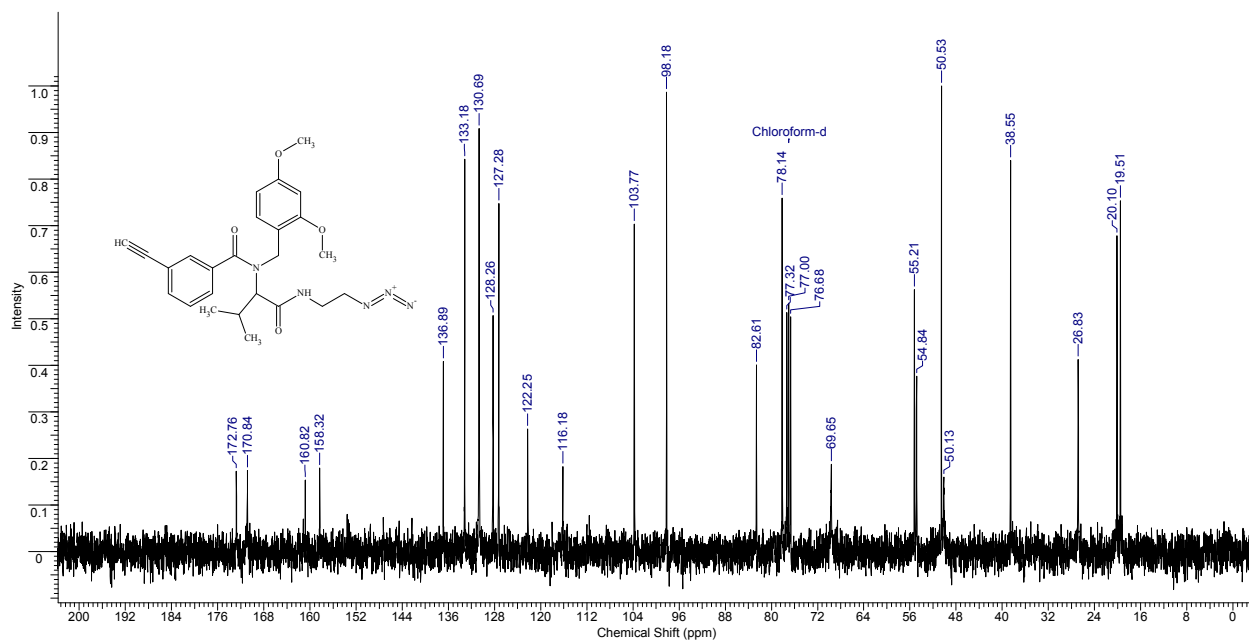
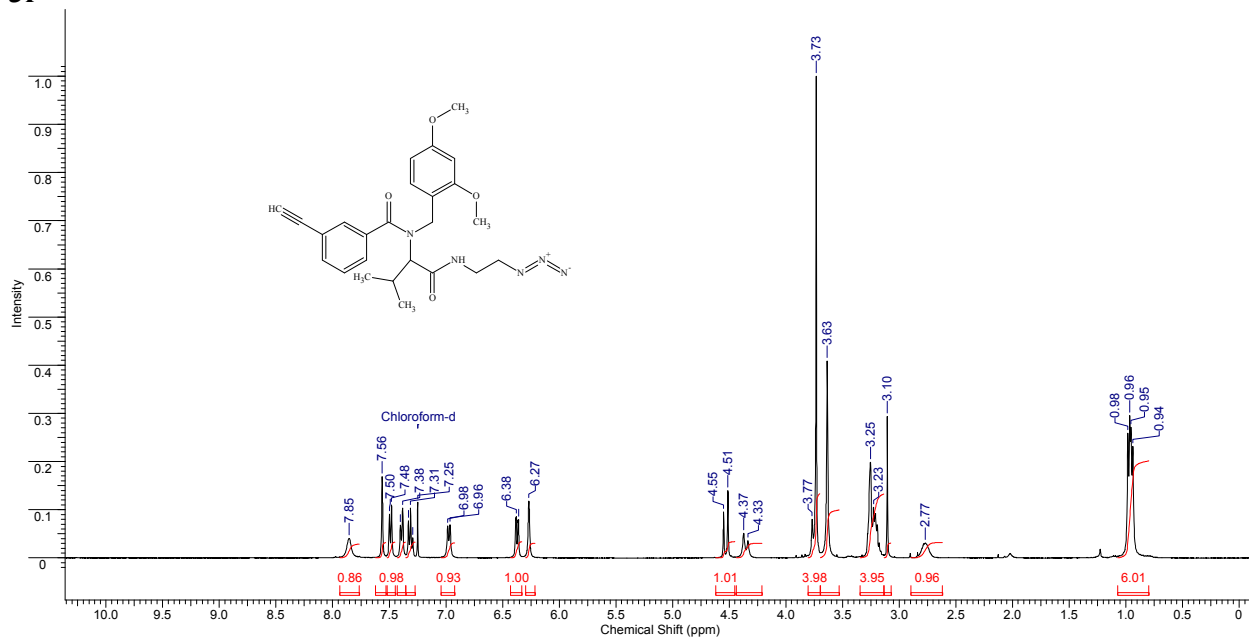
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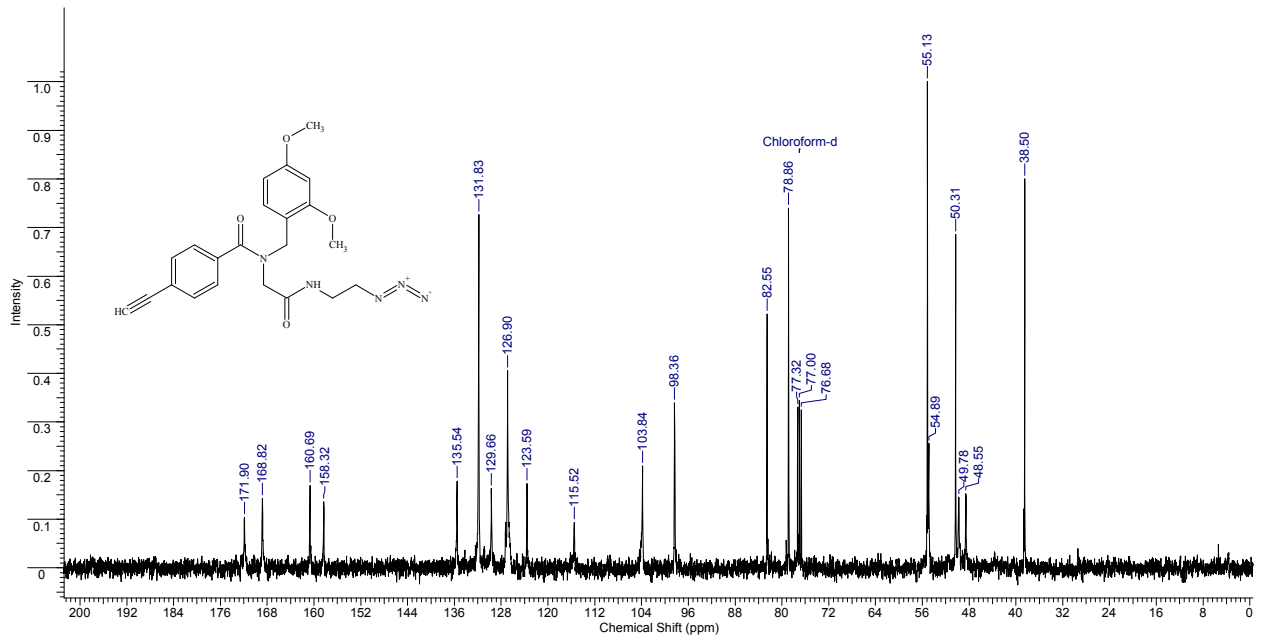
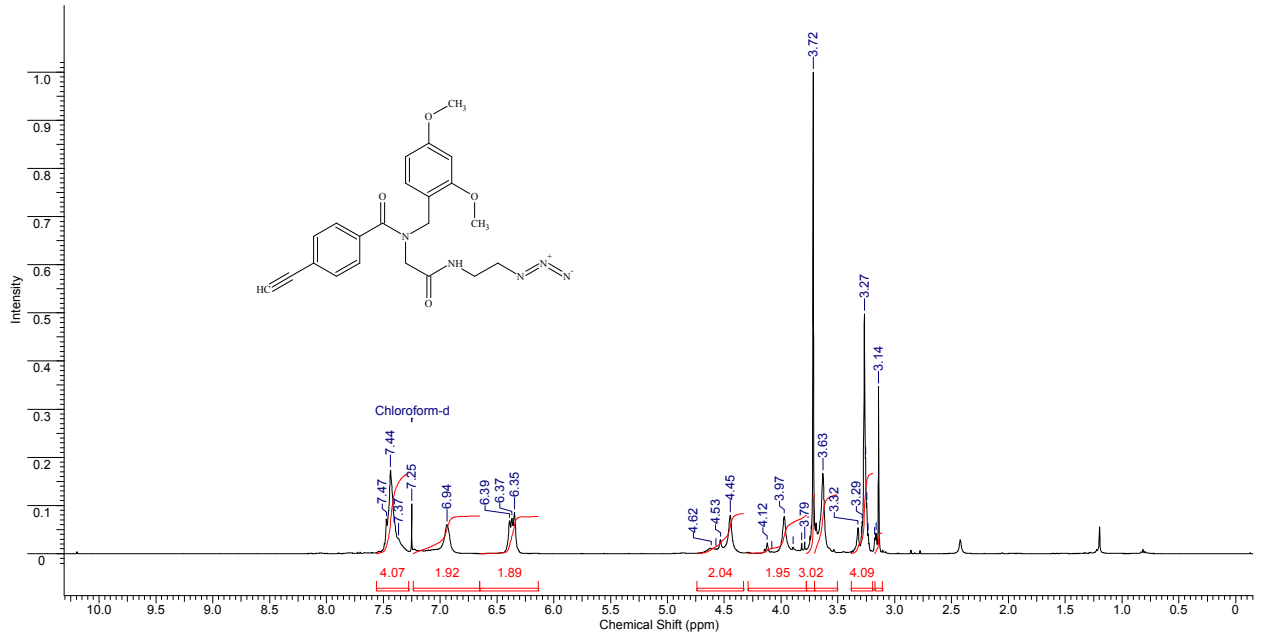
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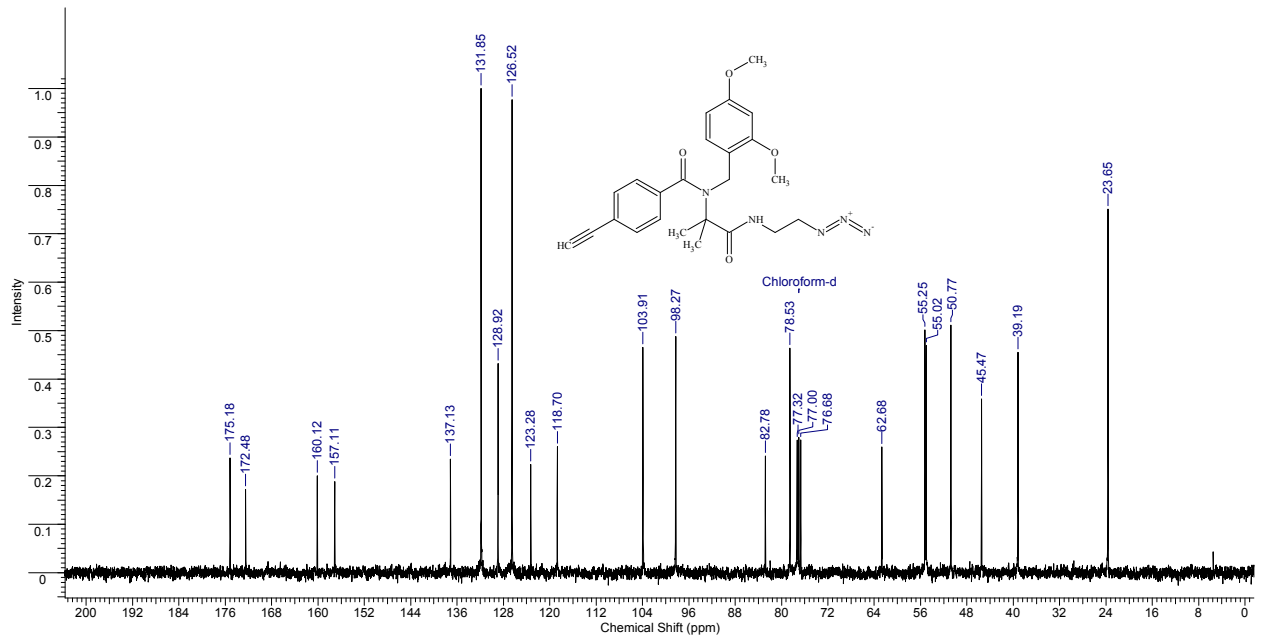
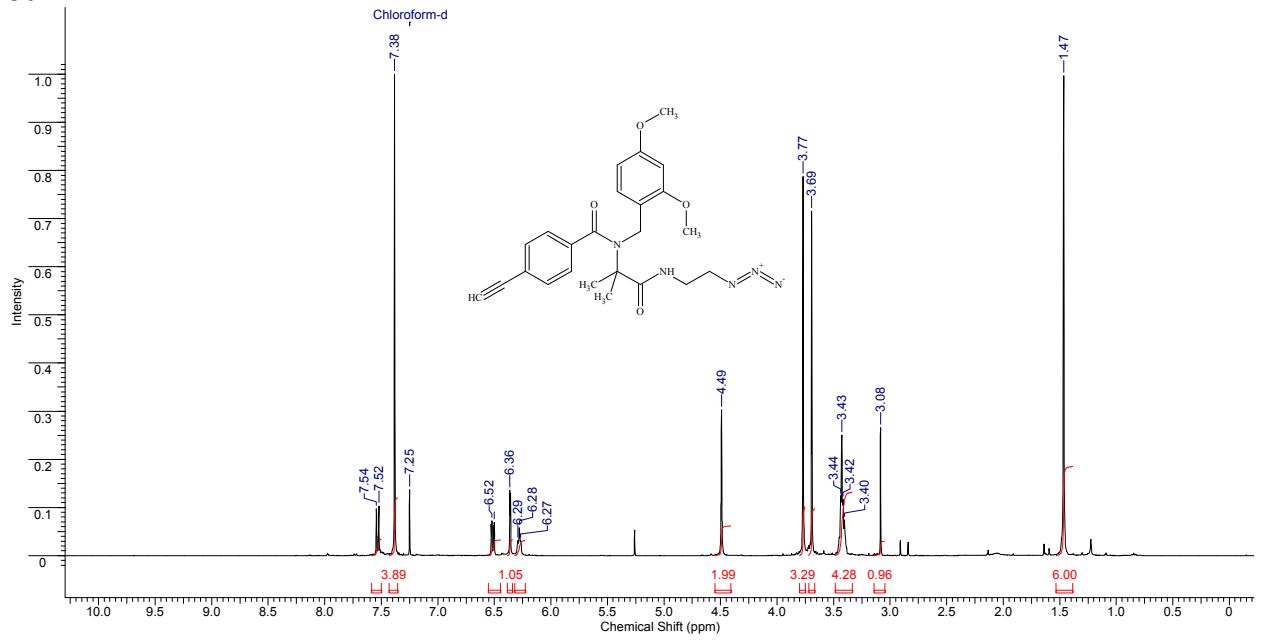
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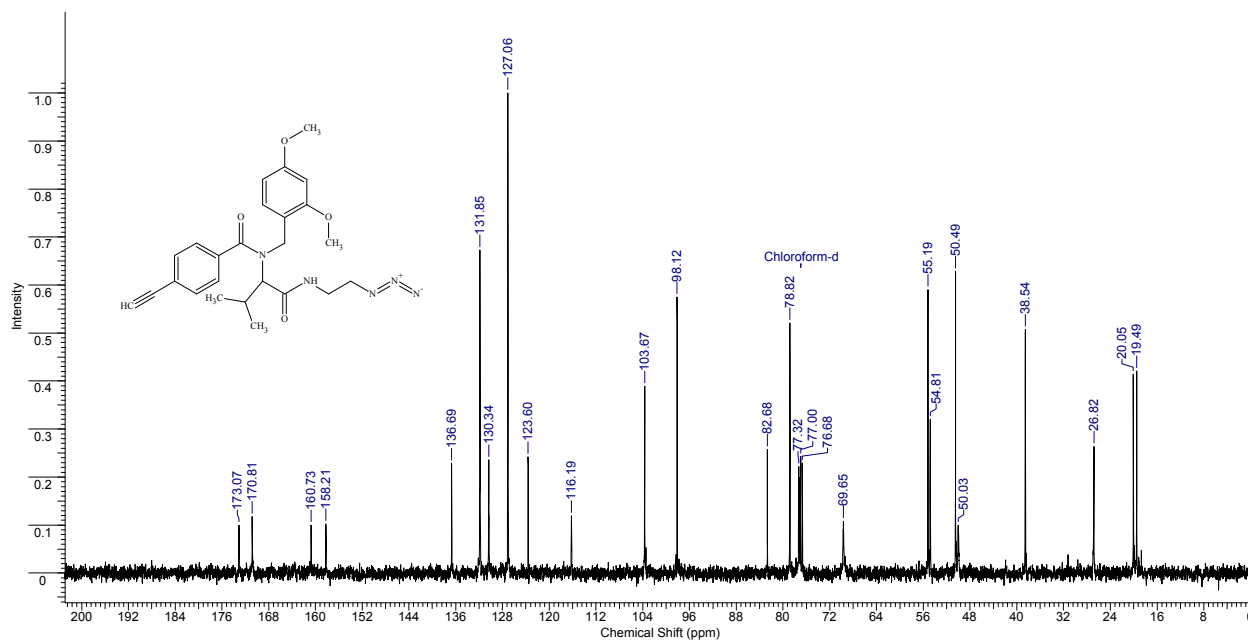
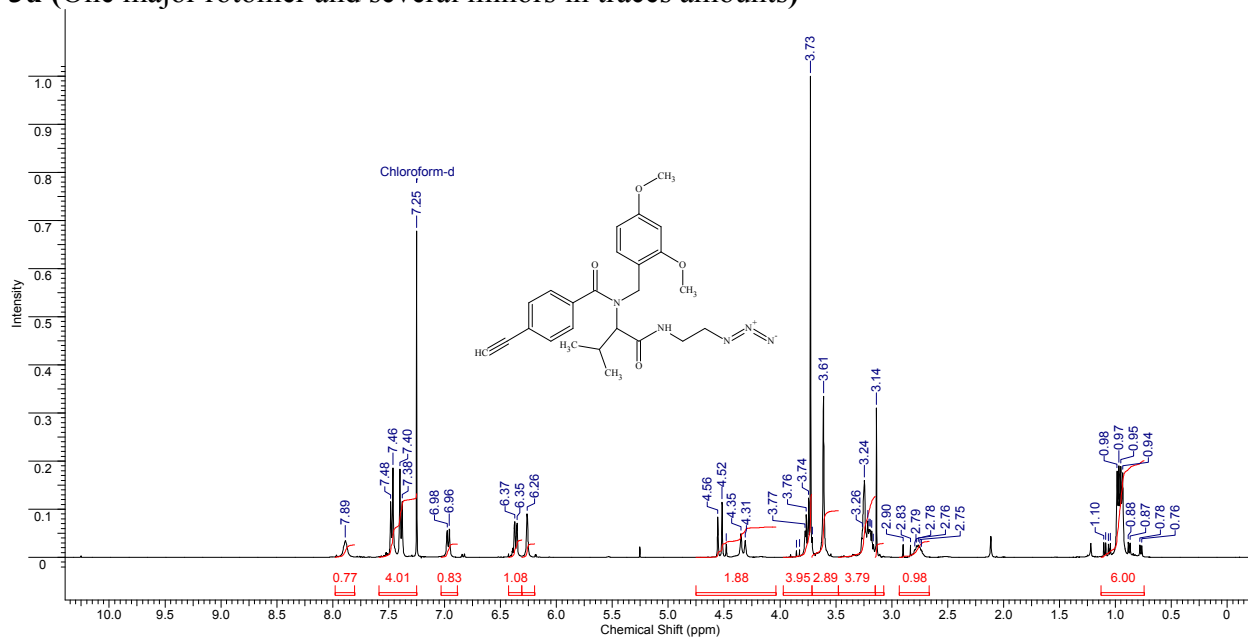
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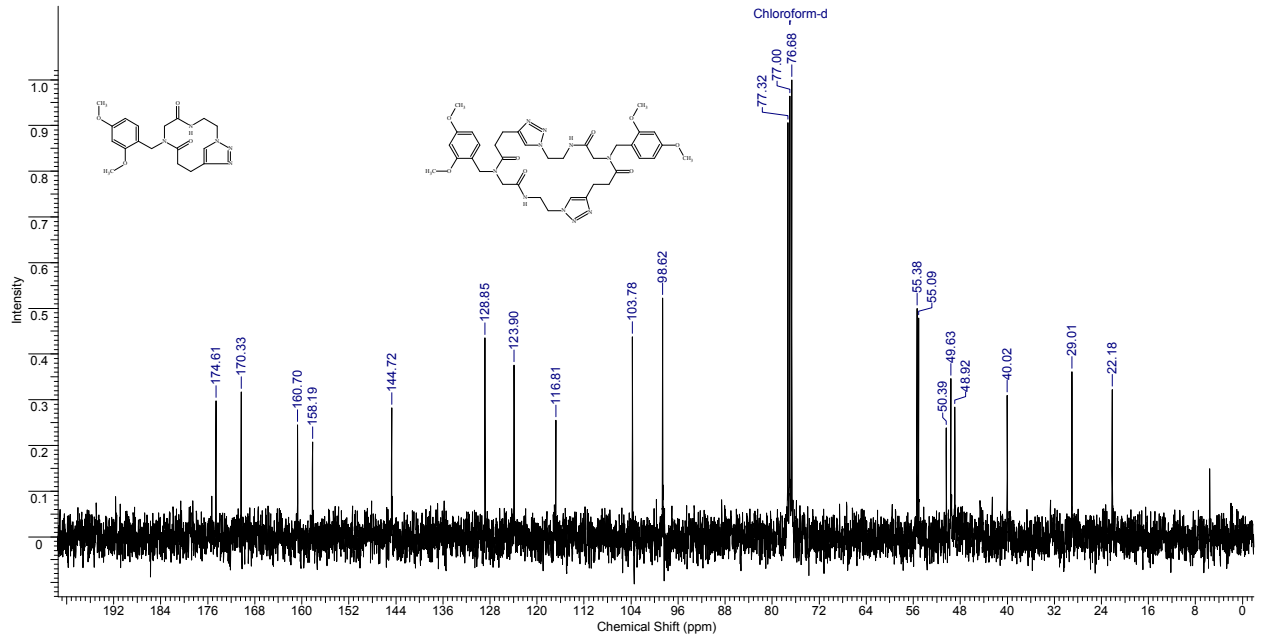
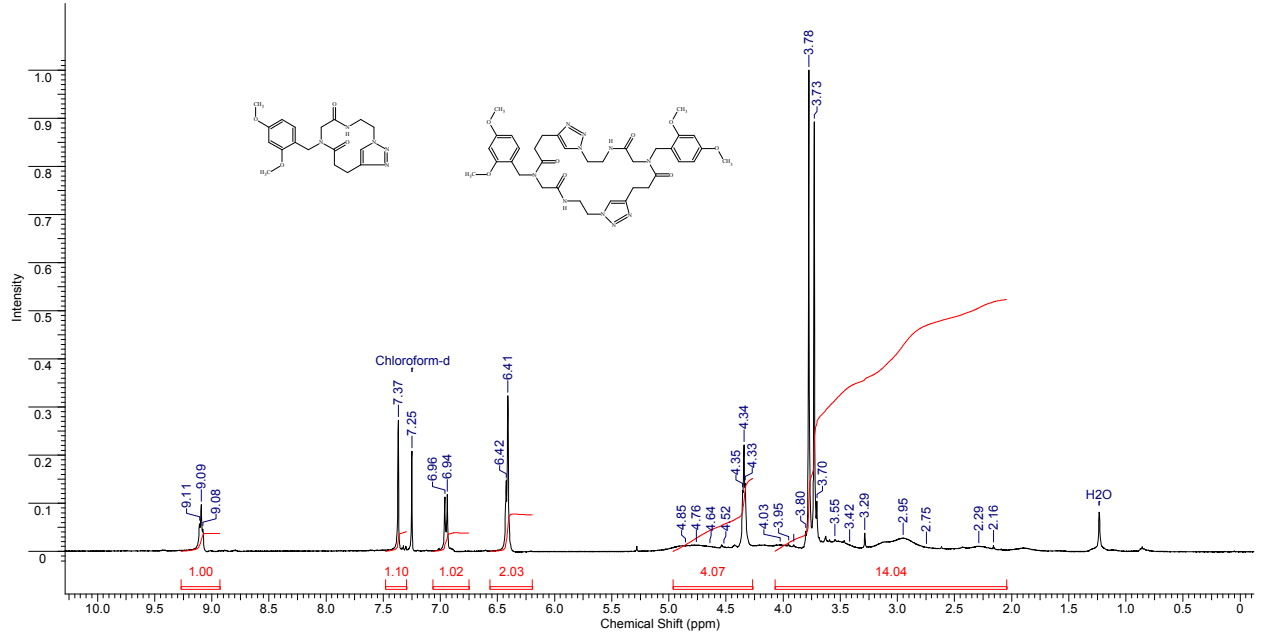
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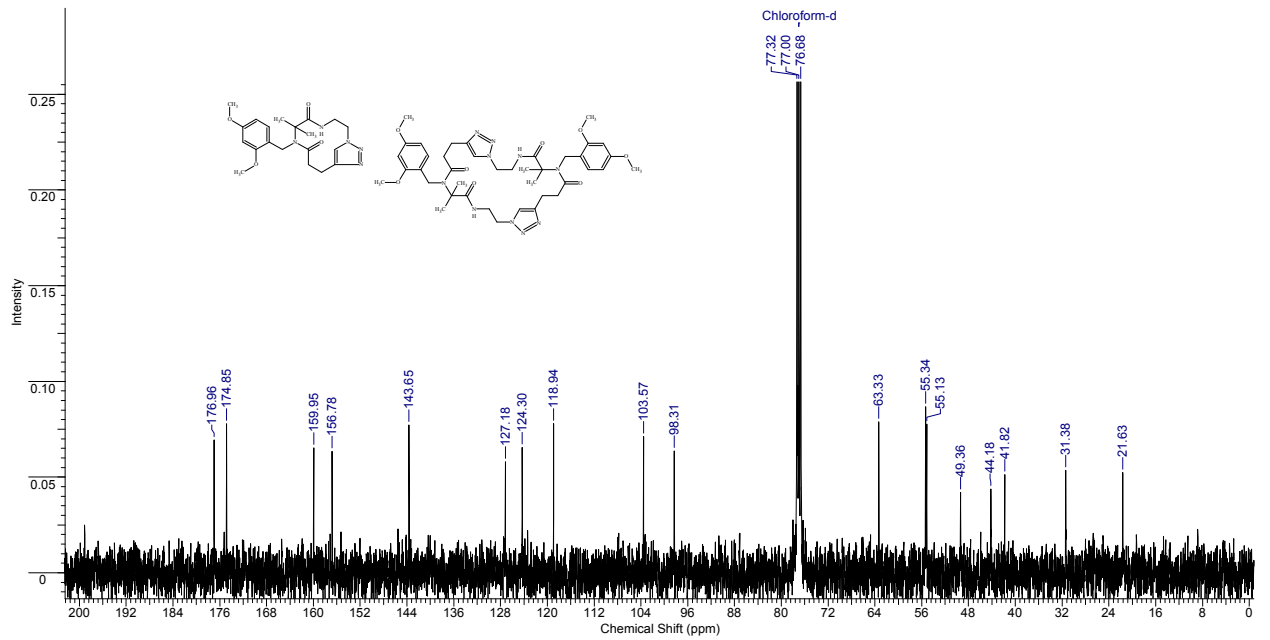
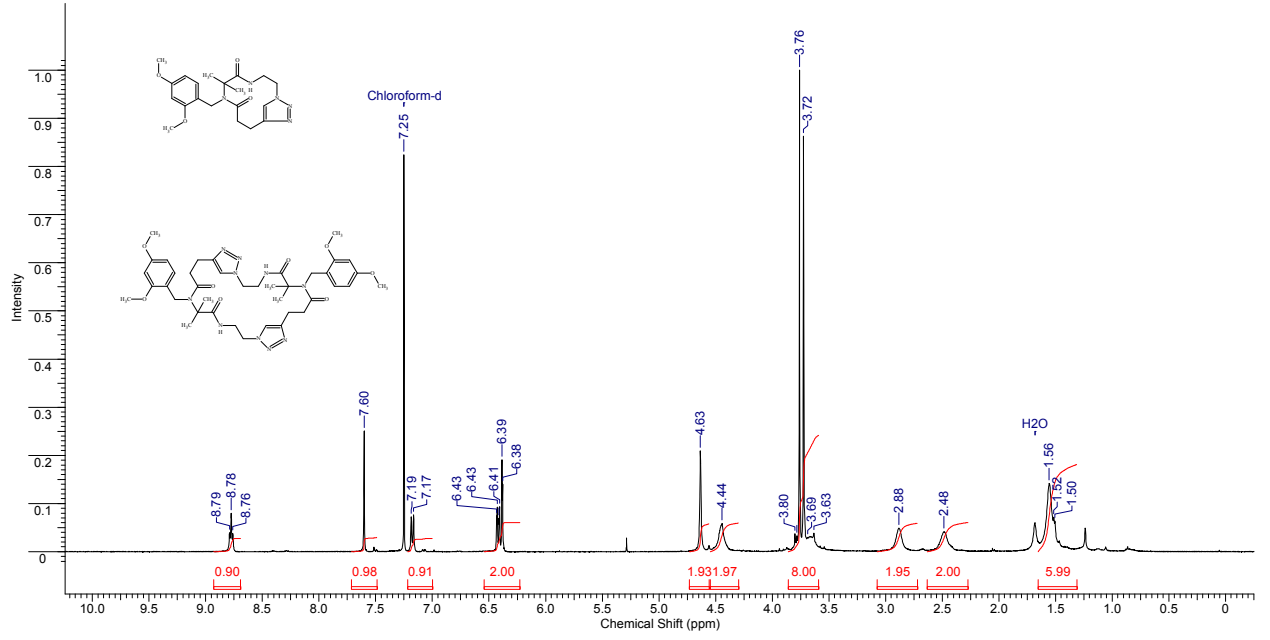
3u (One major rotamer and several minors in traces amounts)



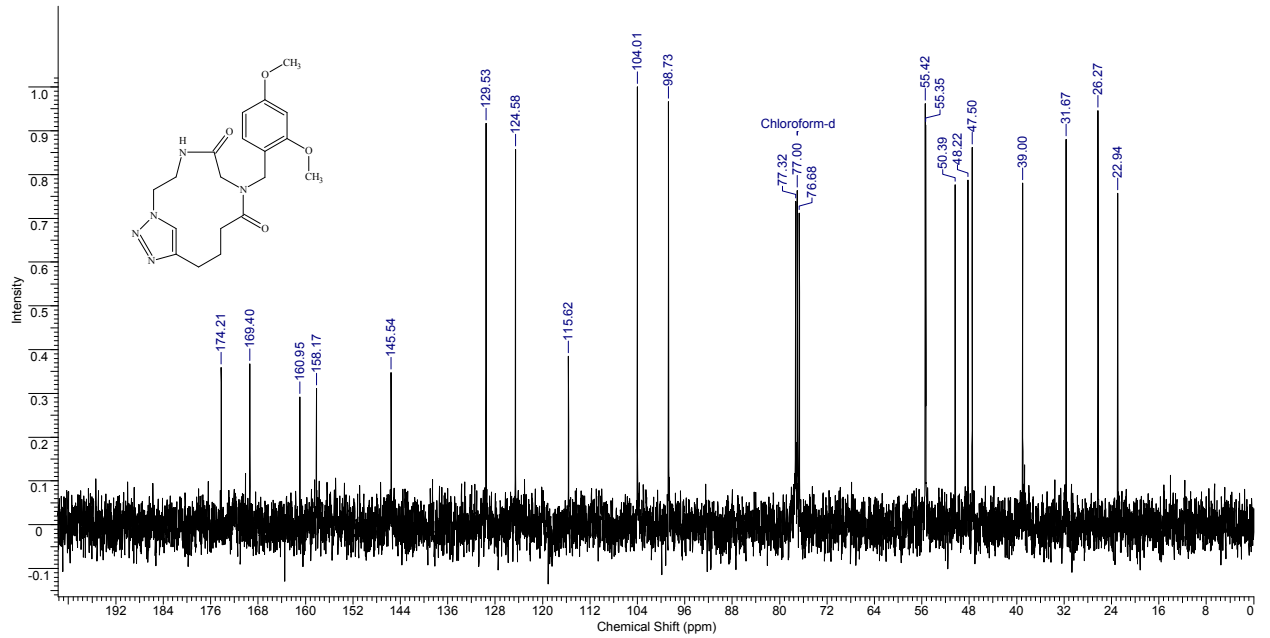
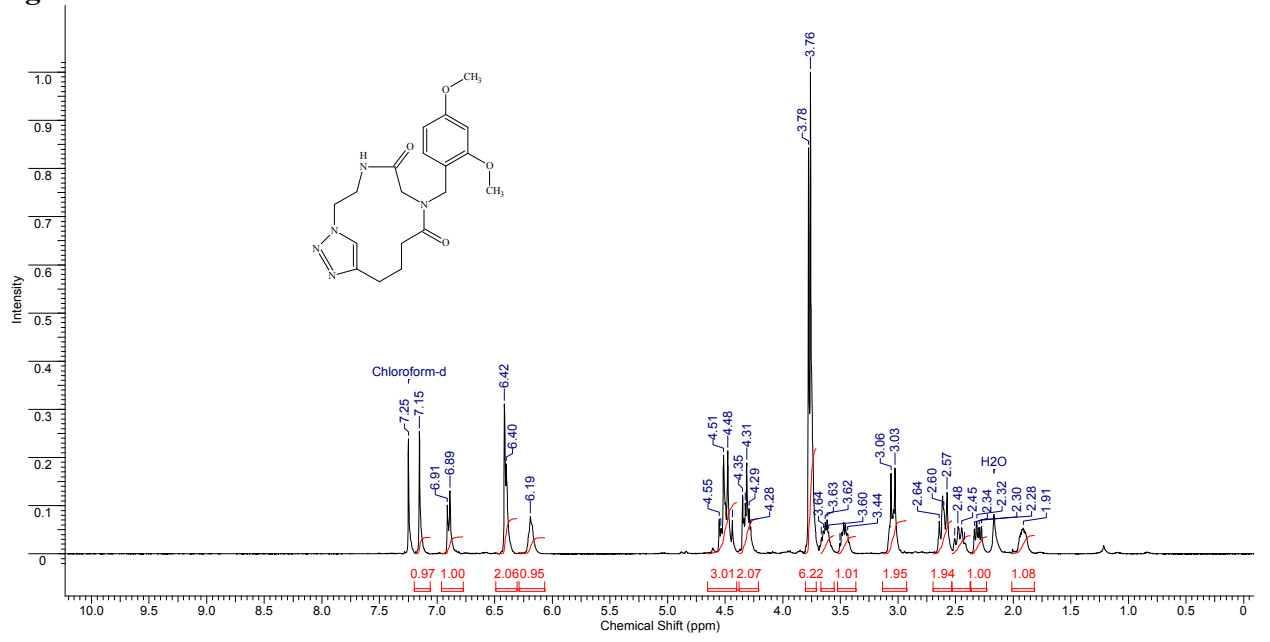
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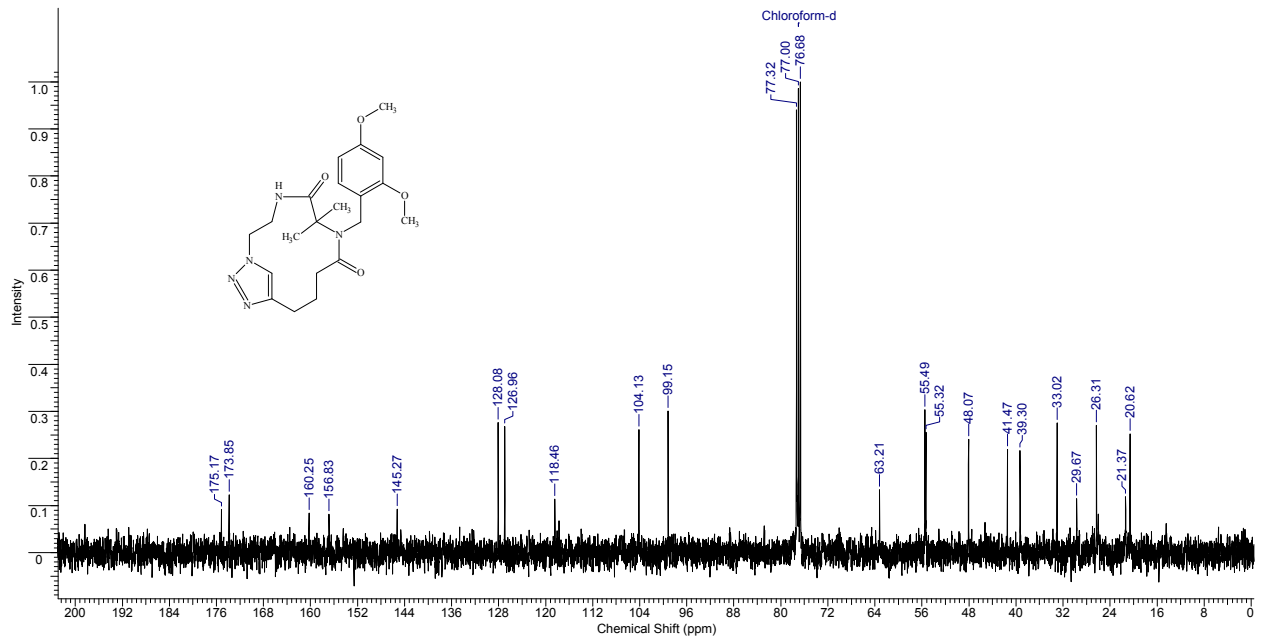
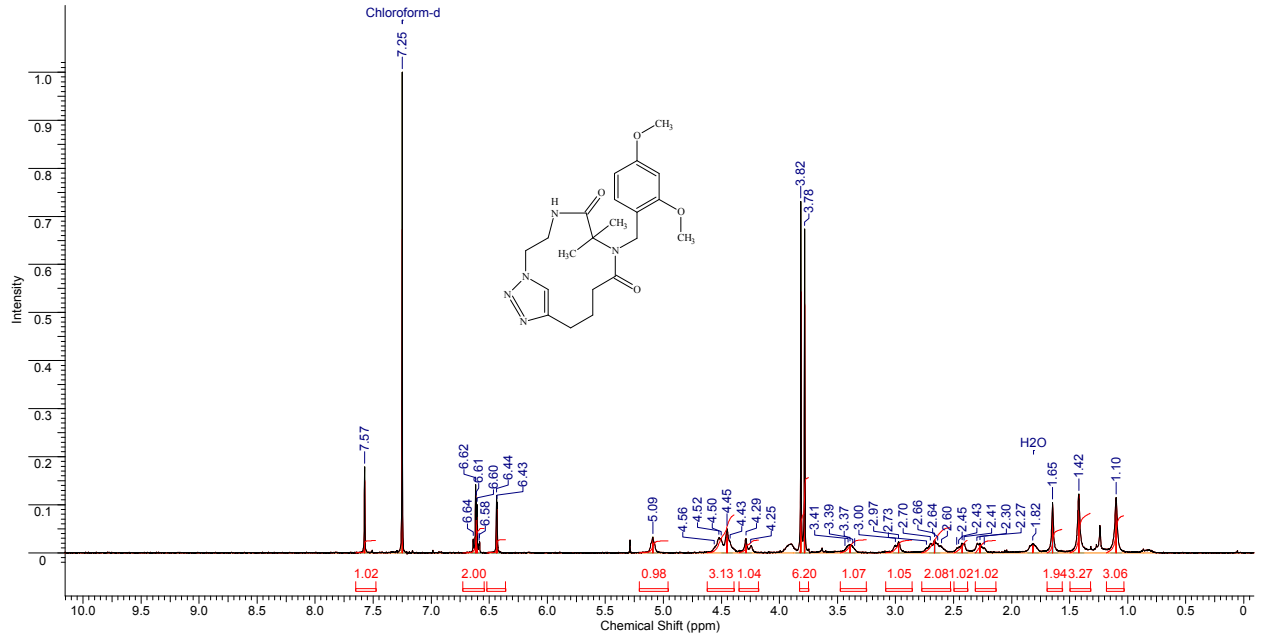
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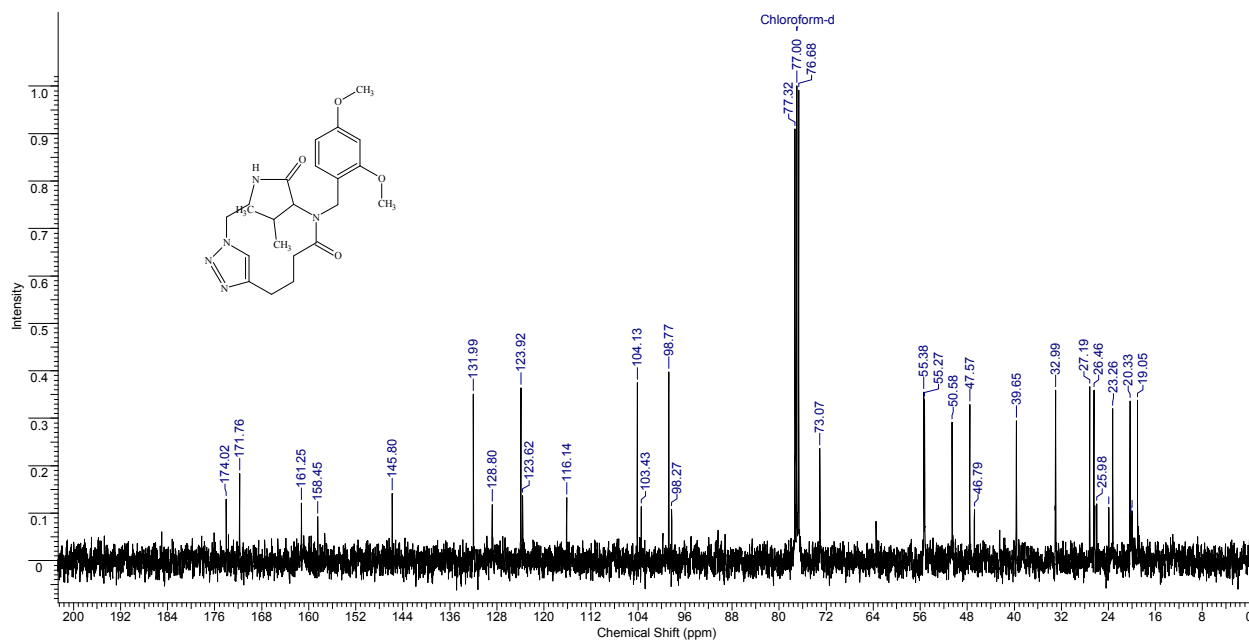
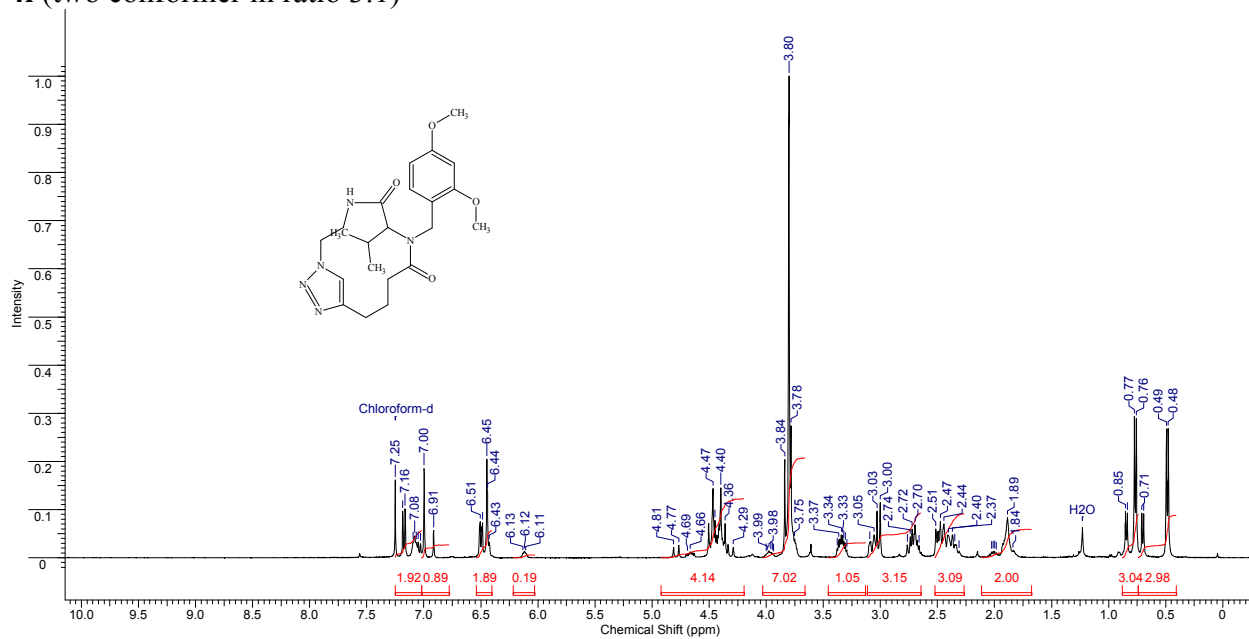
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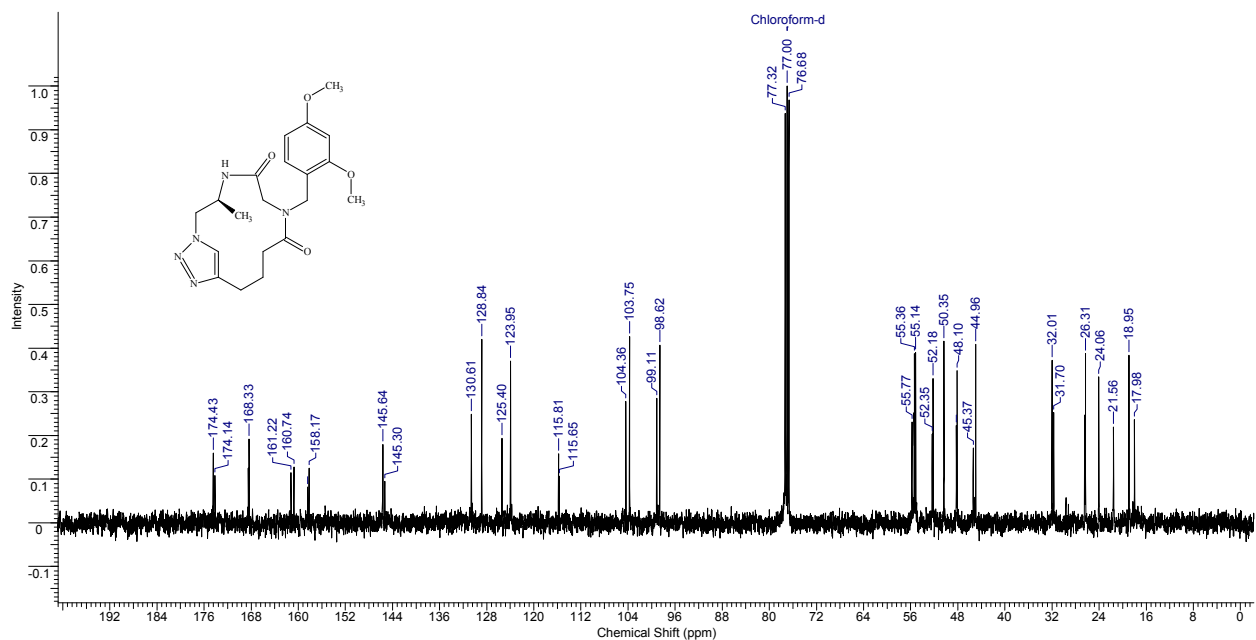
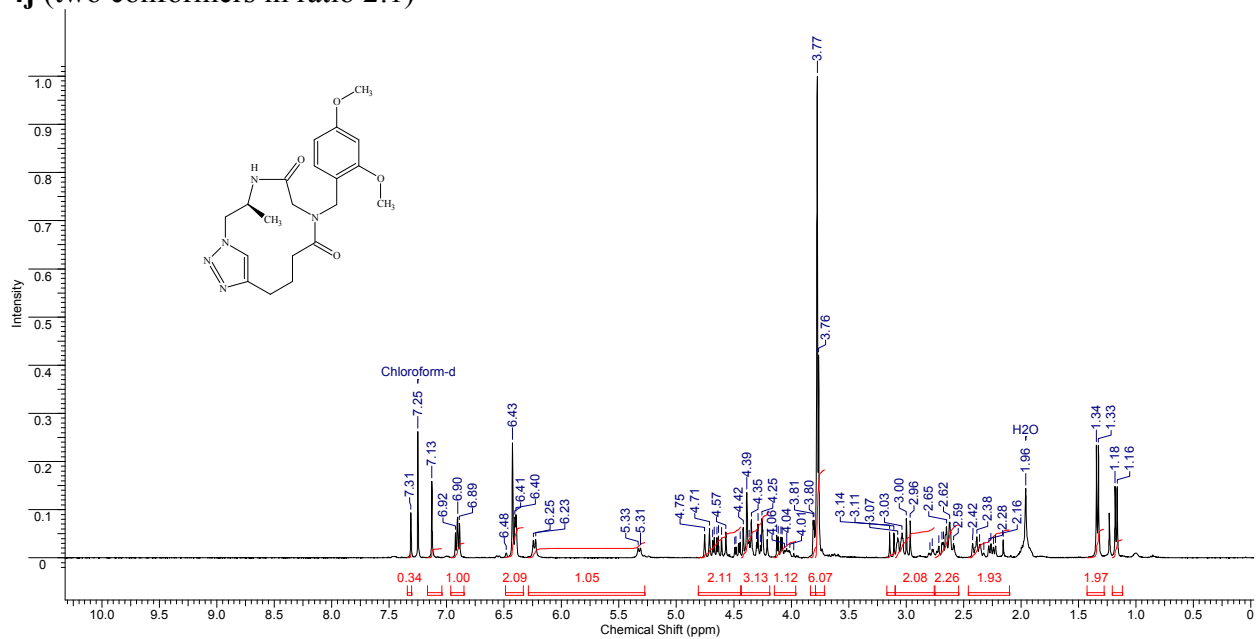
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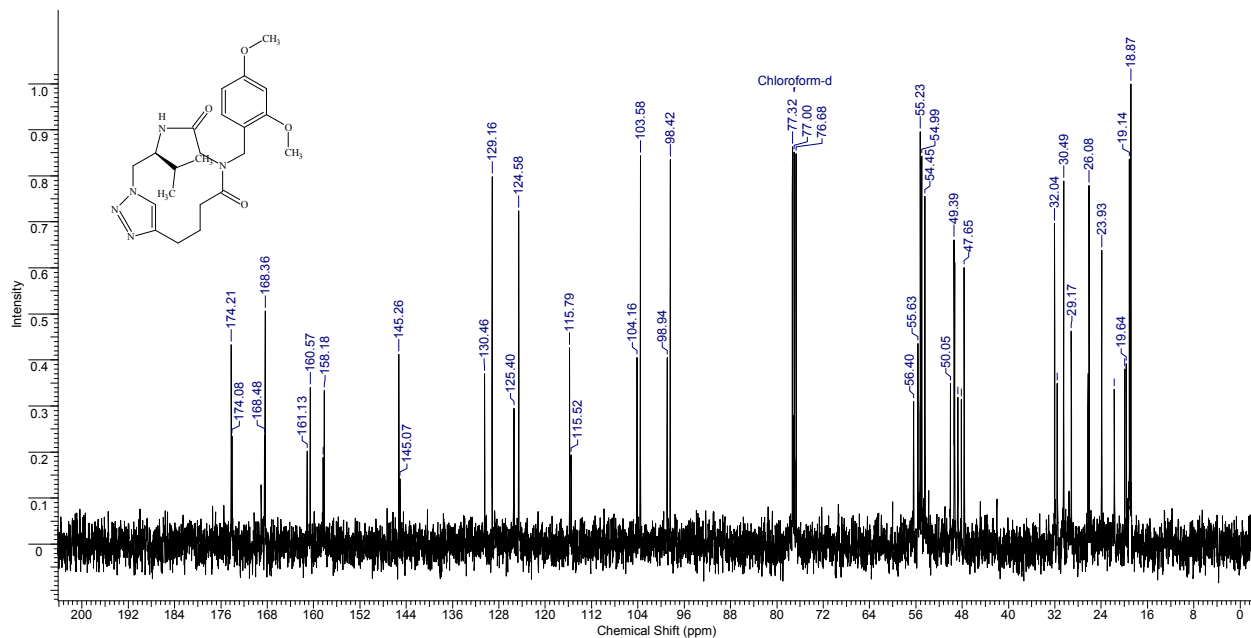
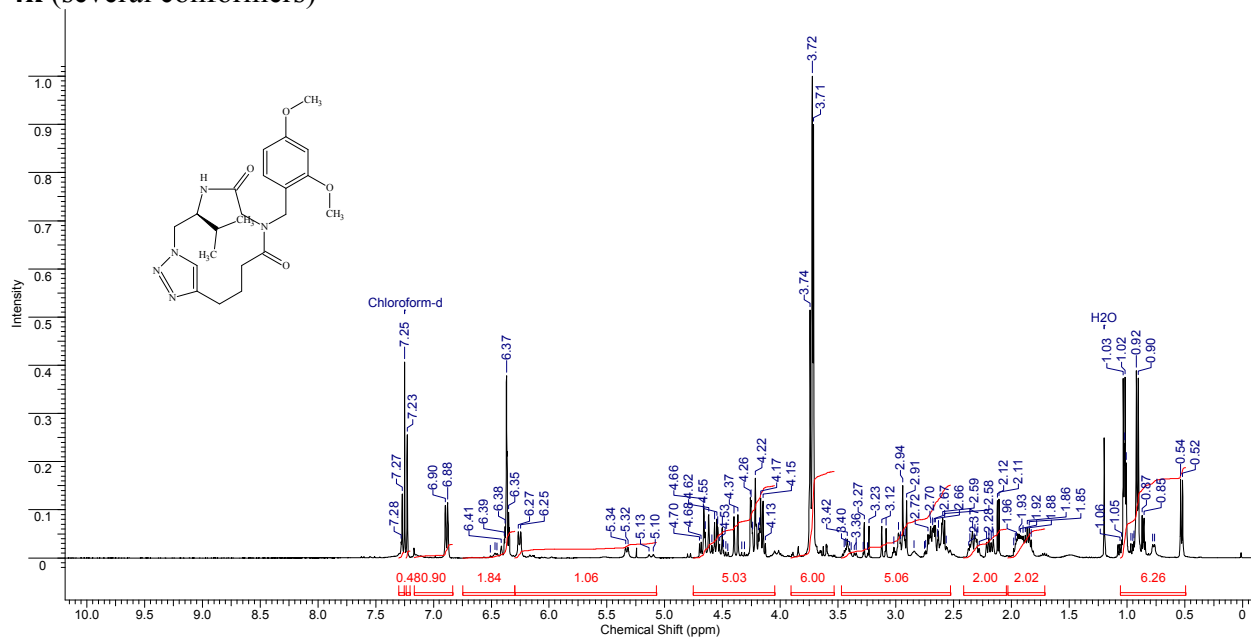
4i (two conformer in ratio 3:1)



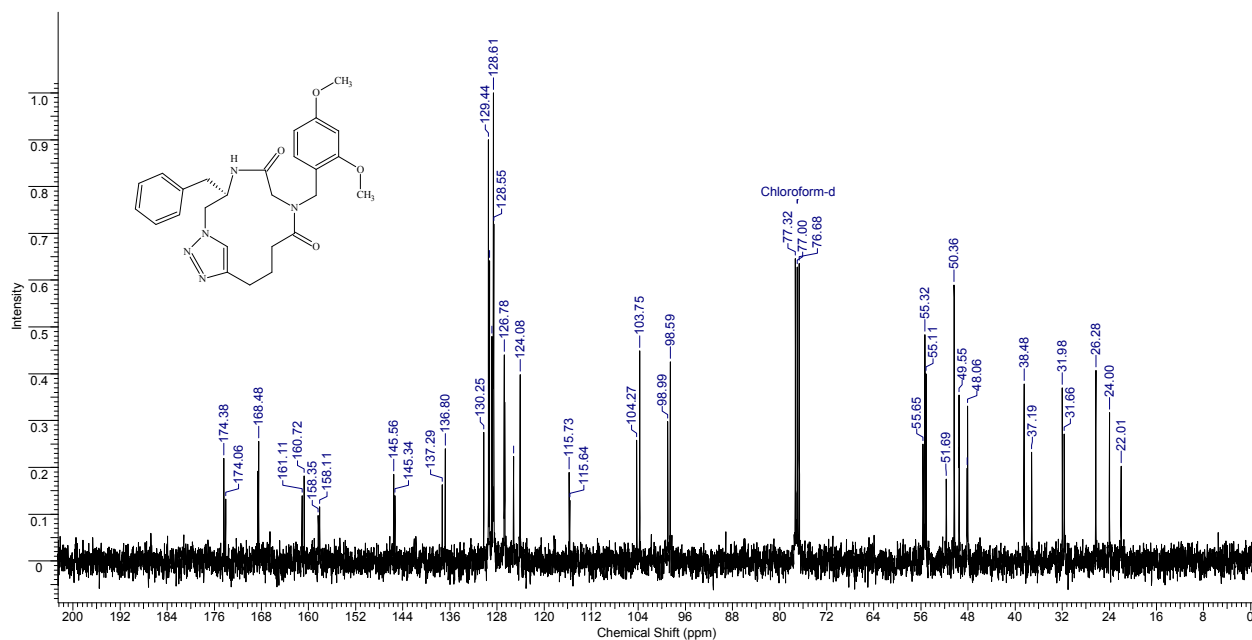
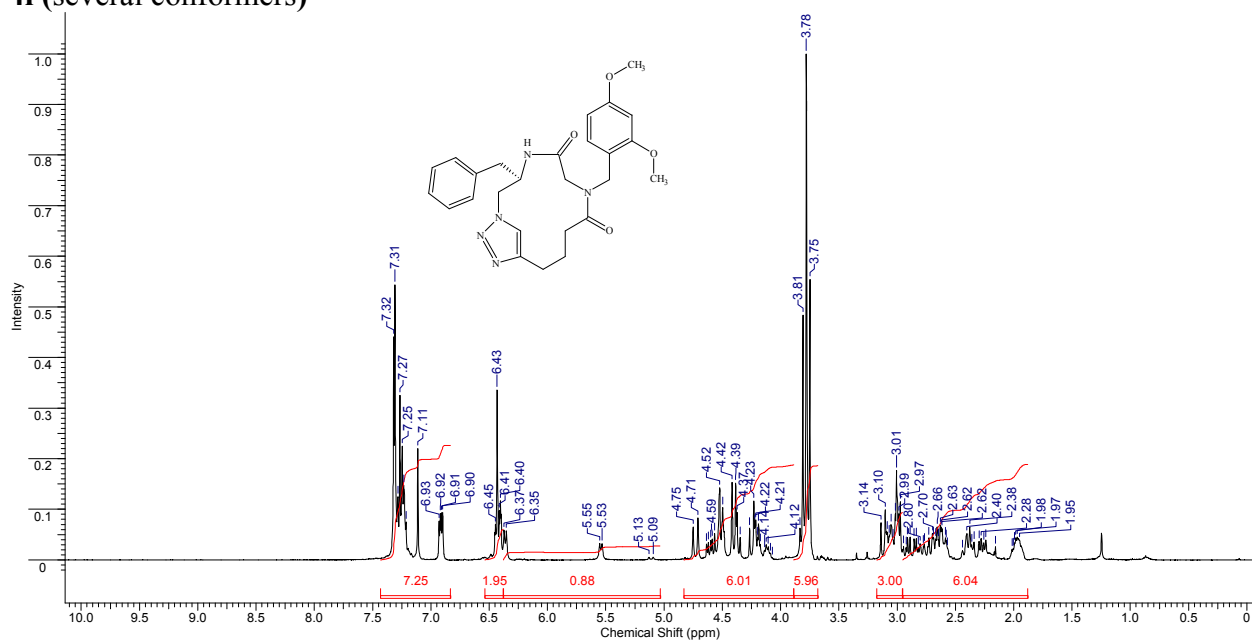
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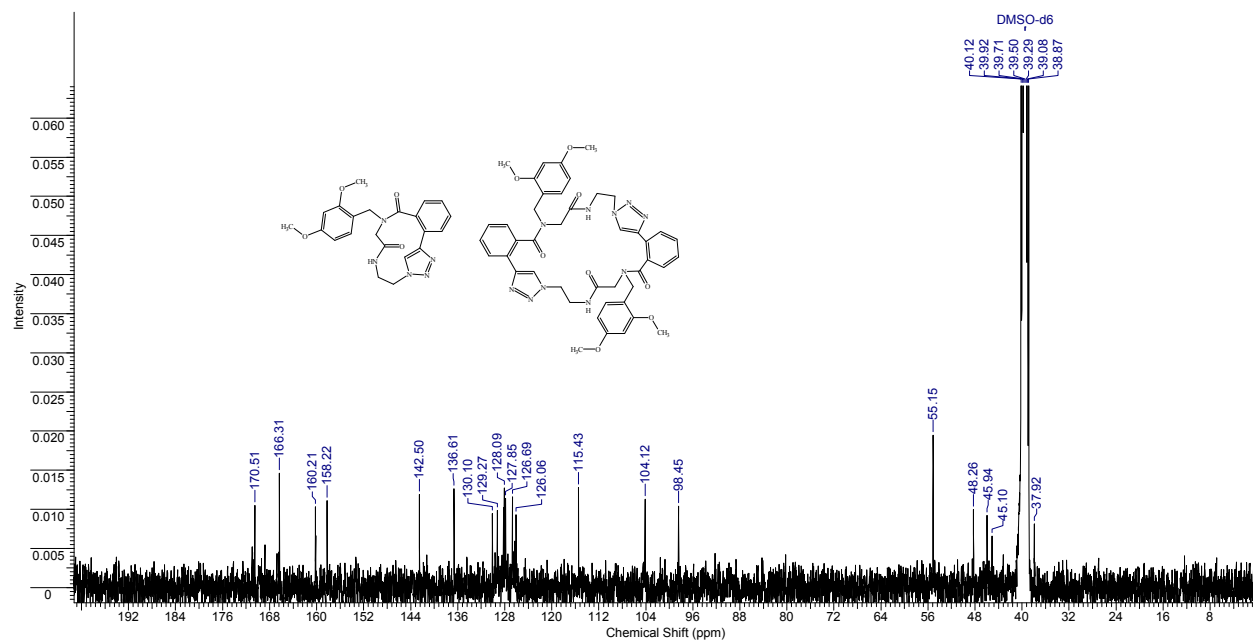
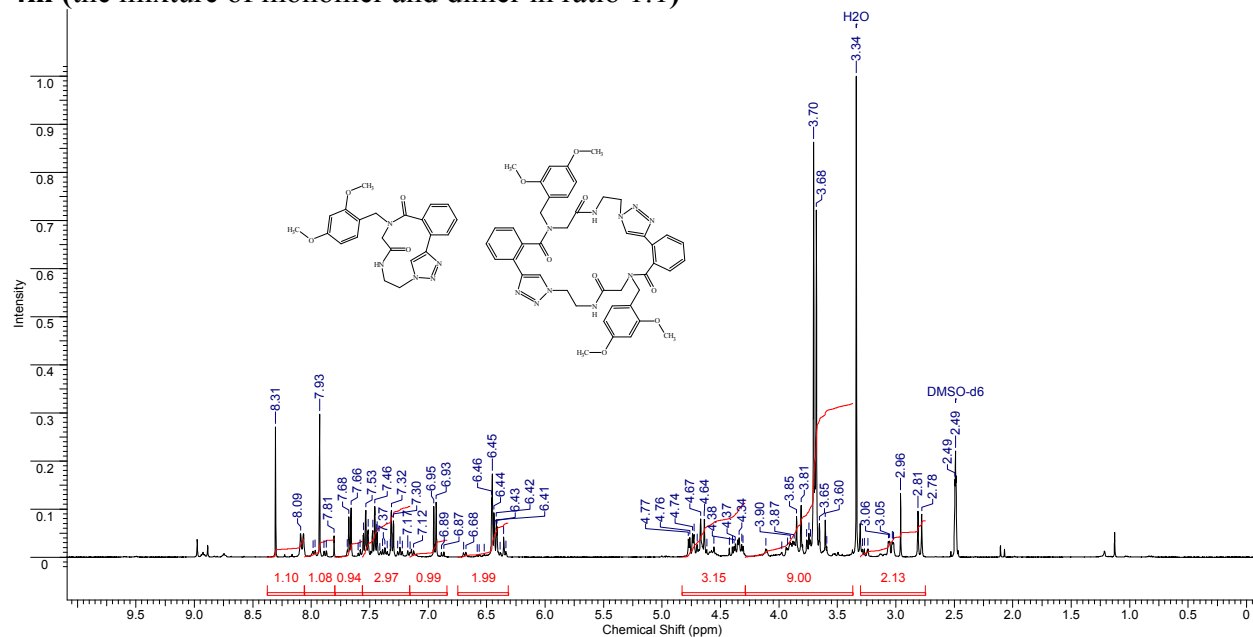
4k (several conformers)



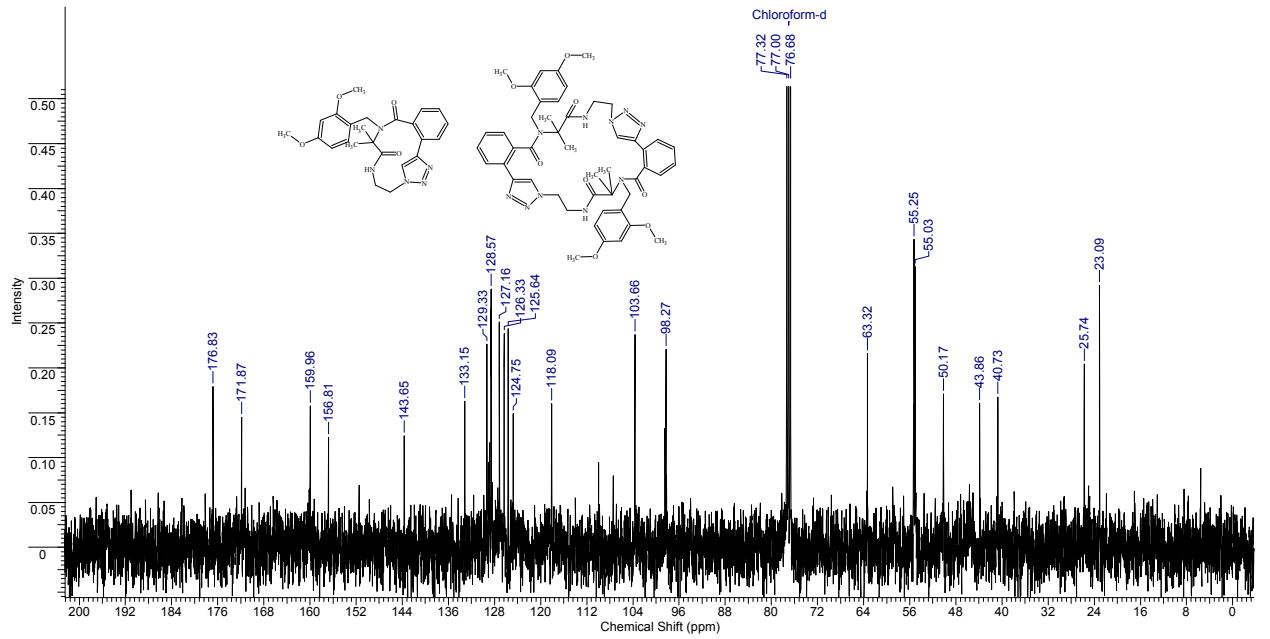
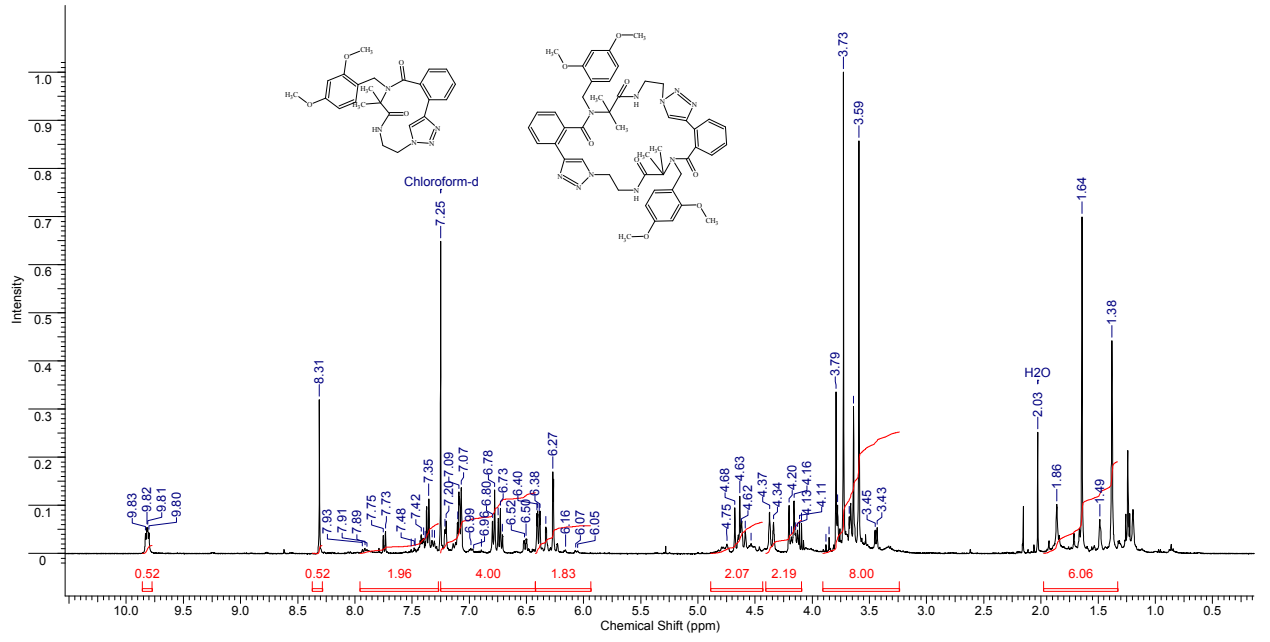
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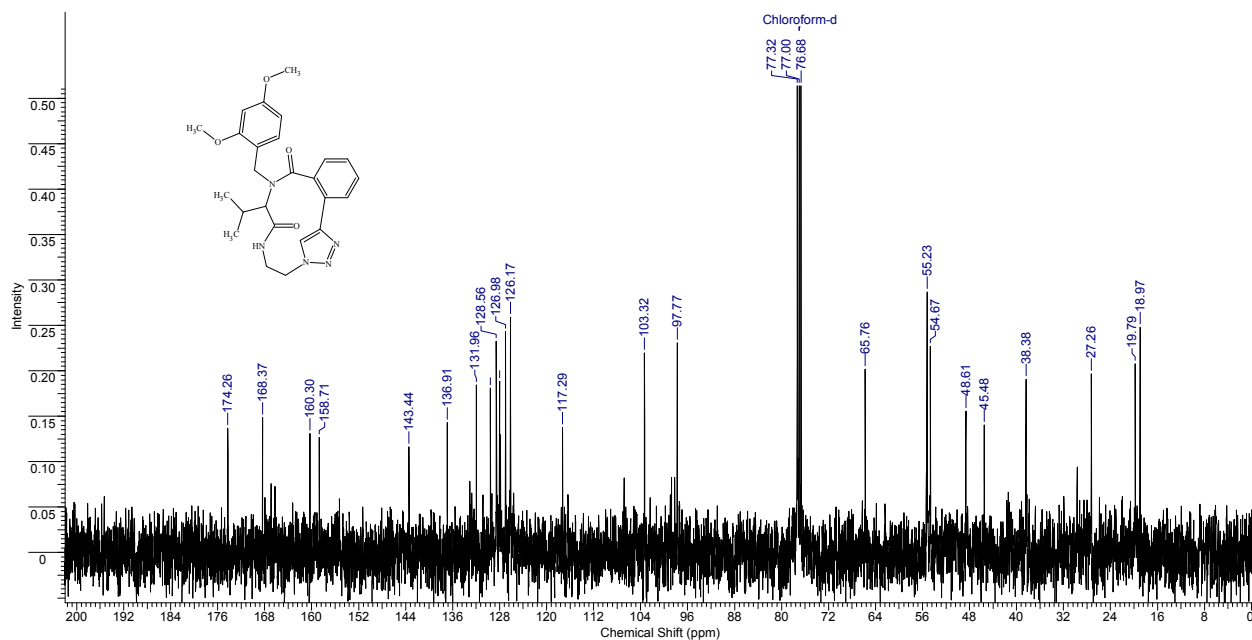
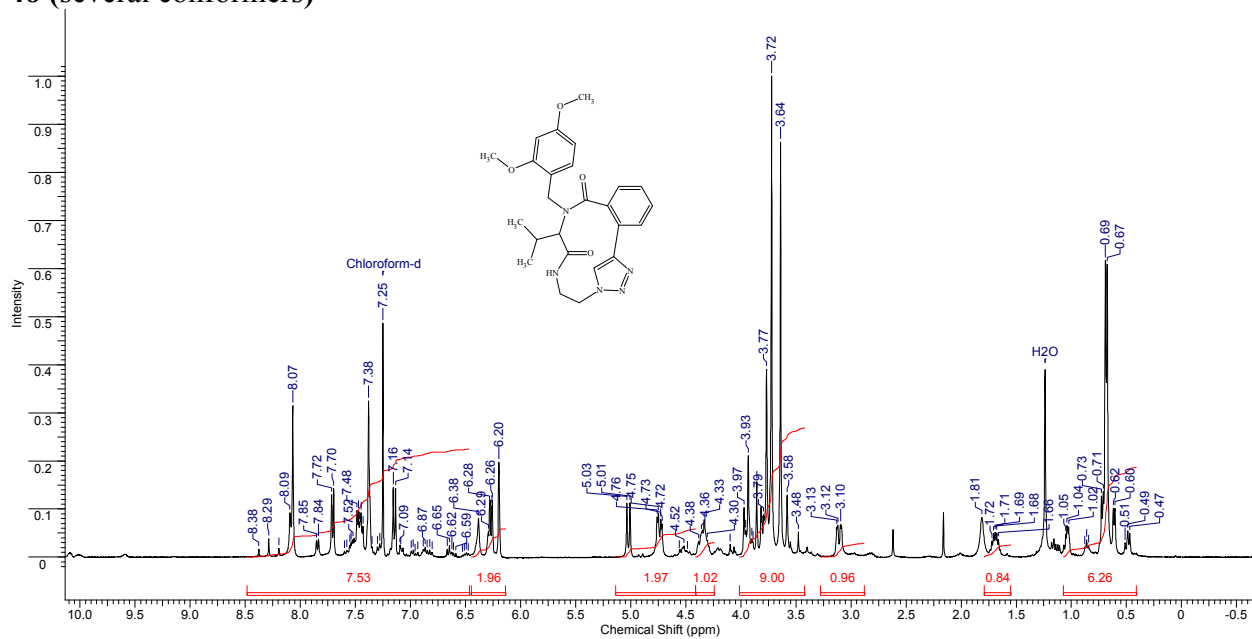
4m (the mixture of monomer and dimer in ratio 1:1)



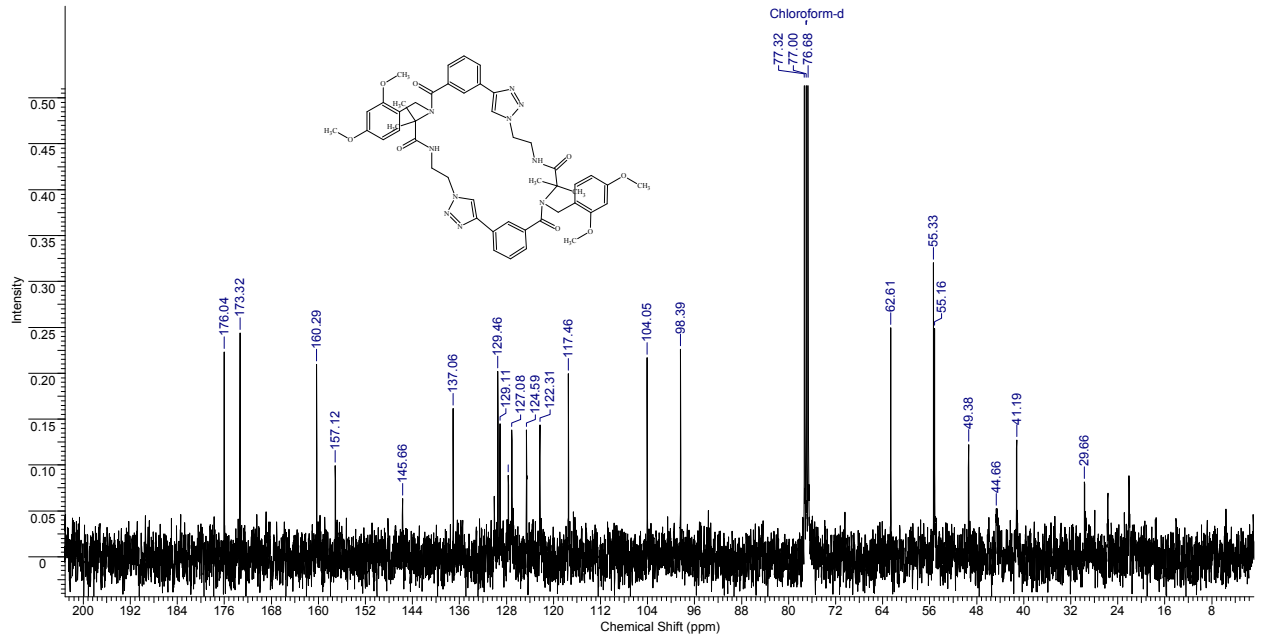
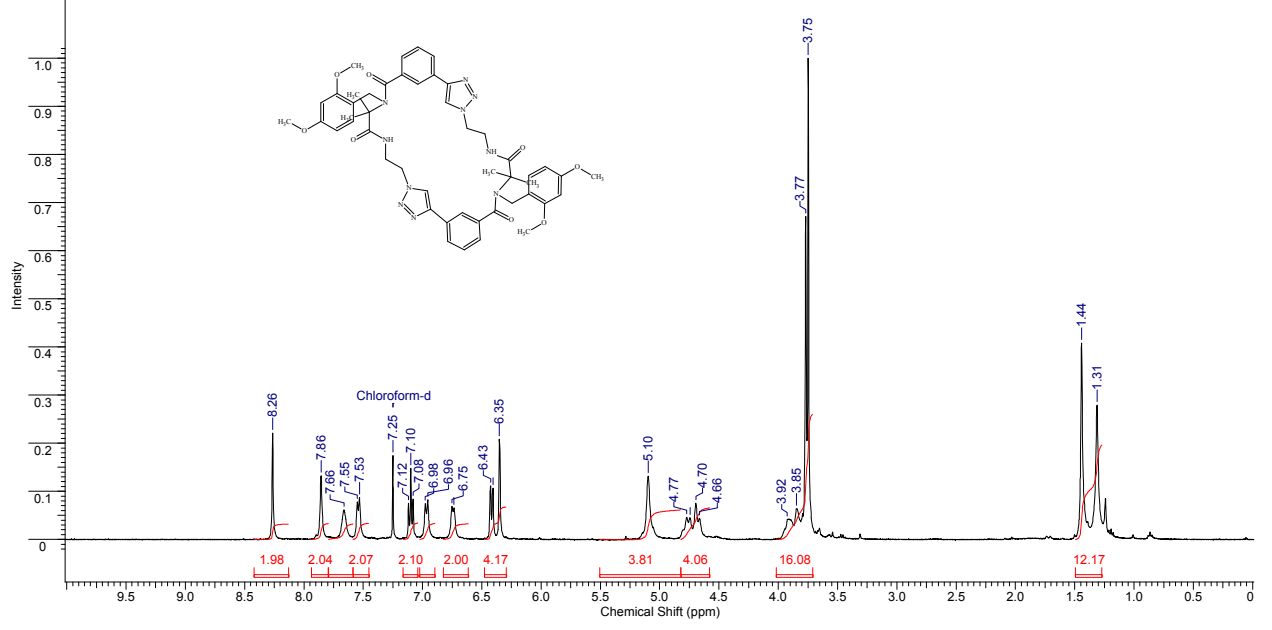
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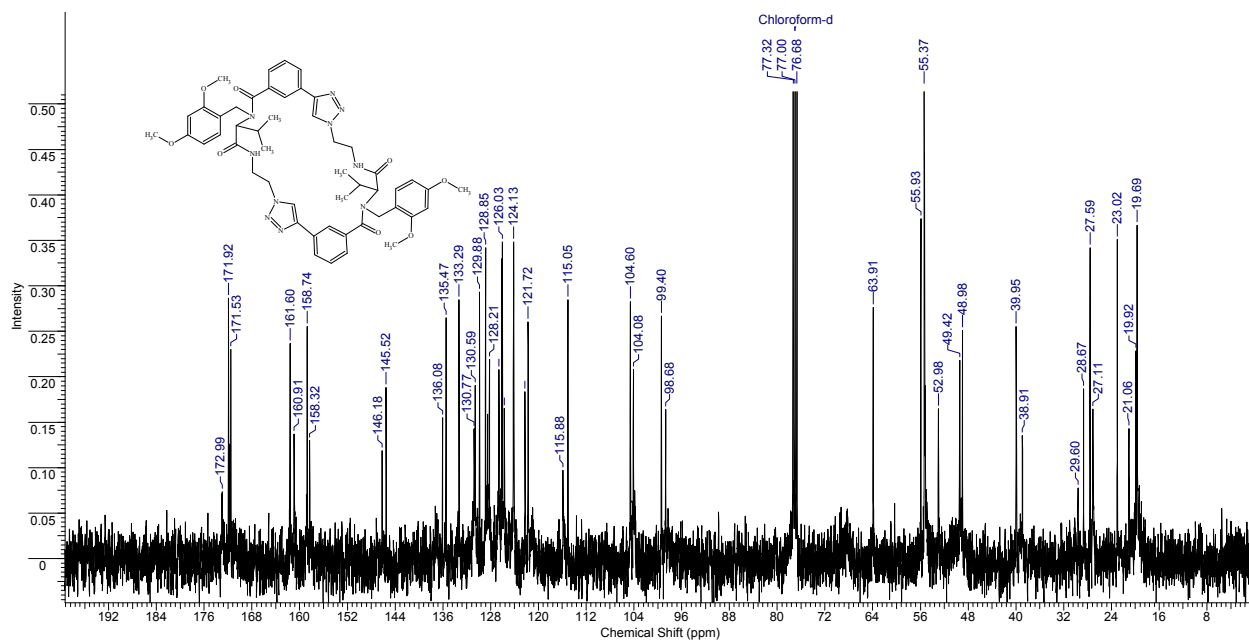
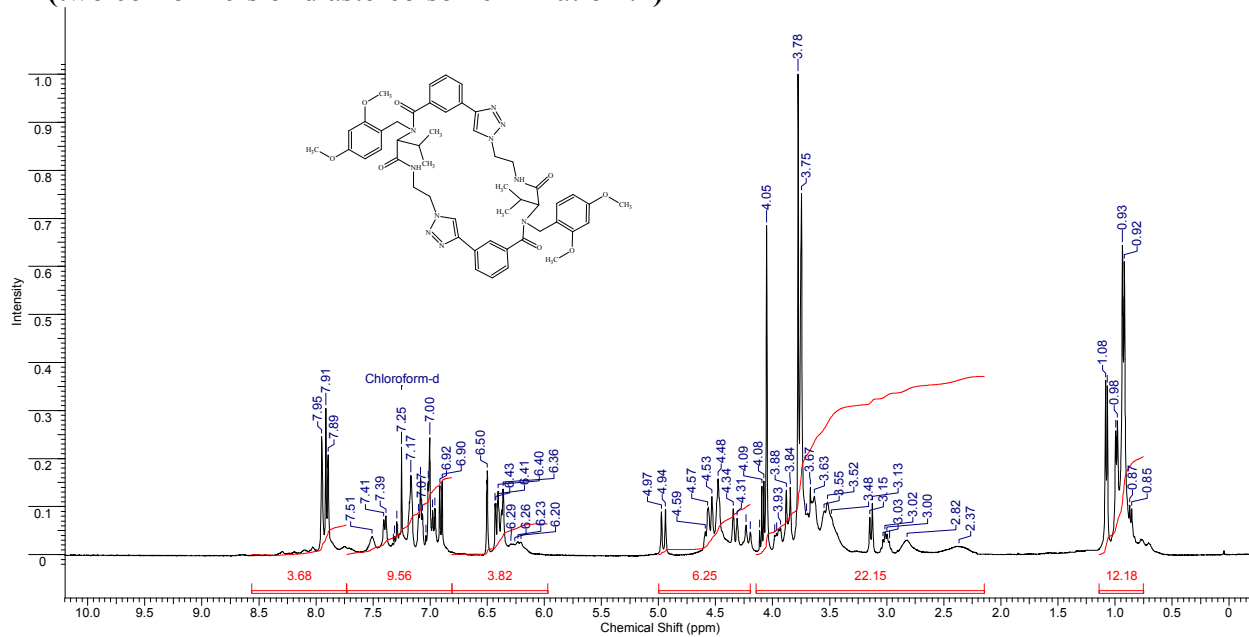
4o (several conformers)



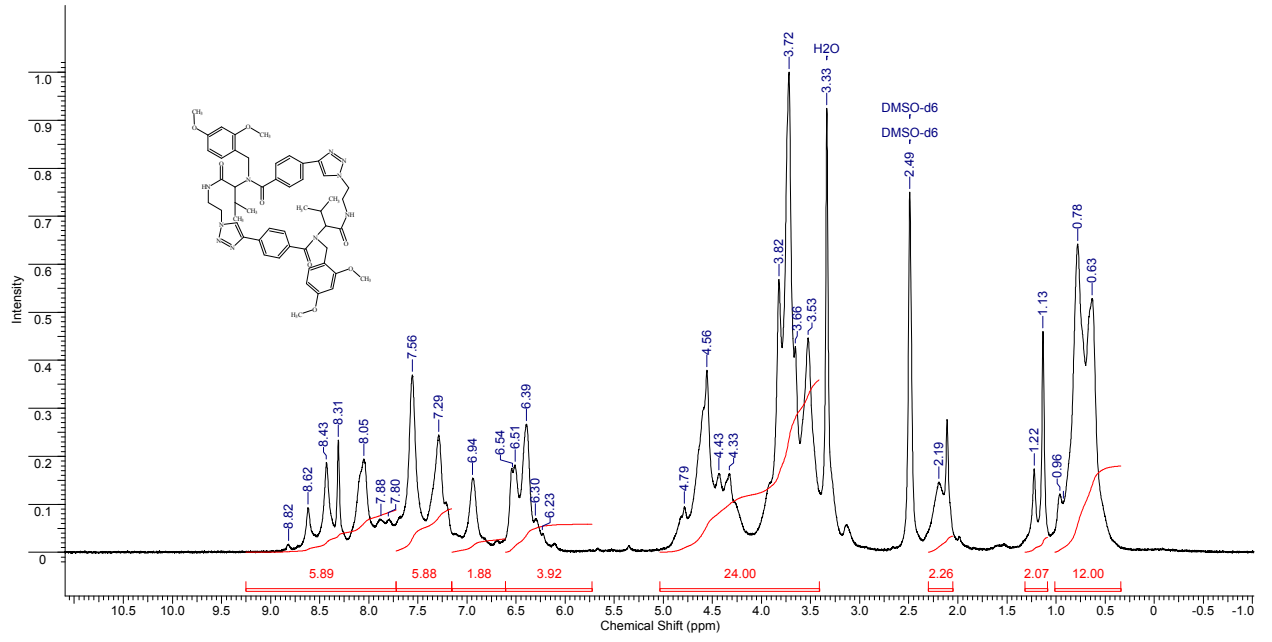
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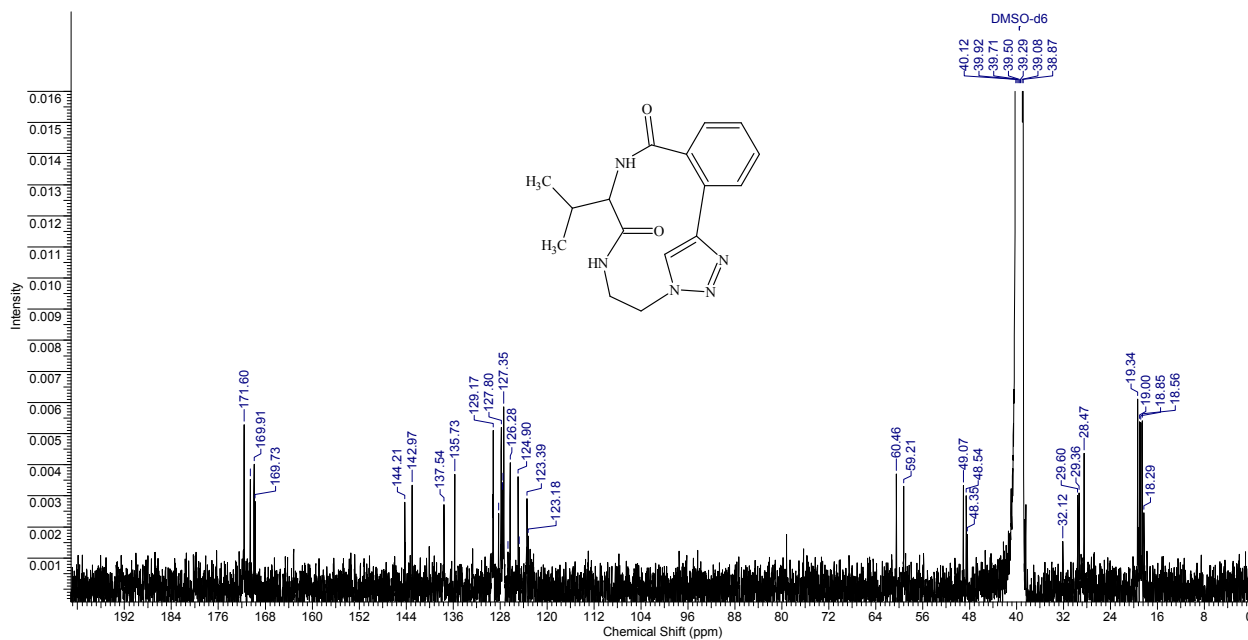
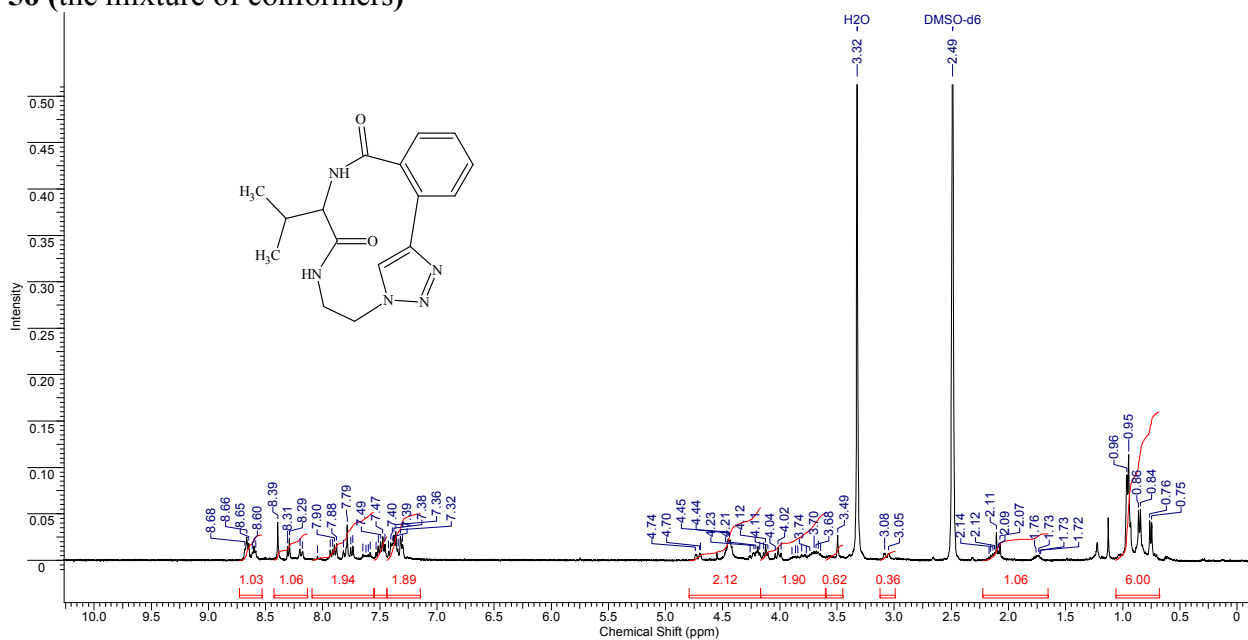
4r (two conformers or diastereoisomer in ratio 2:1)



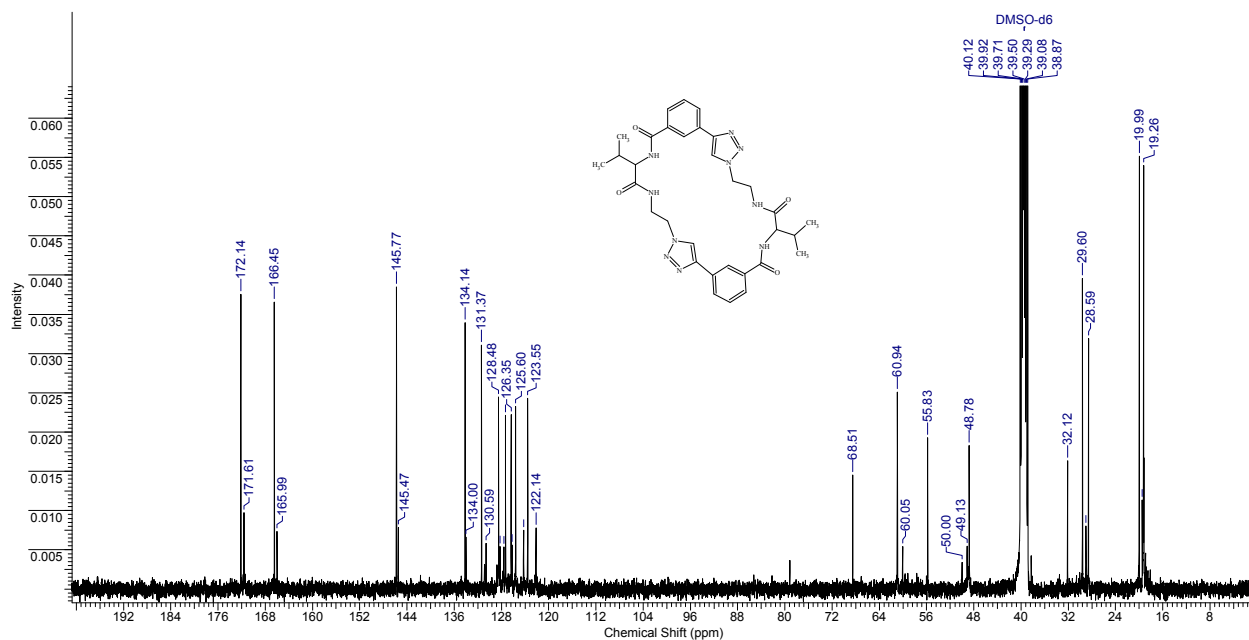
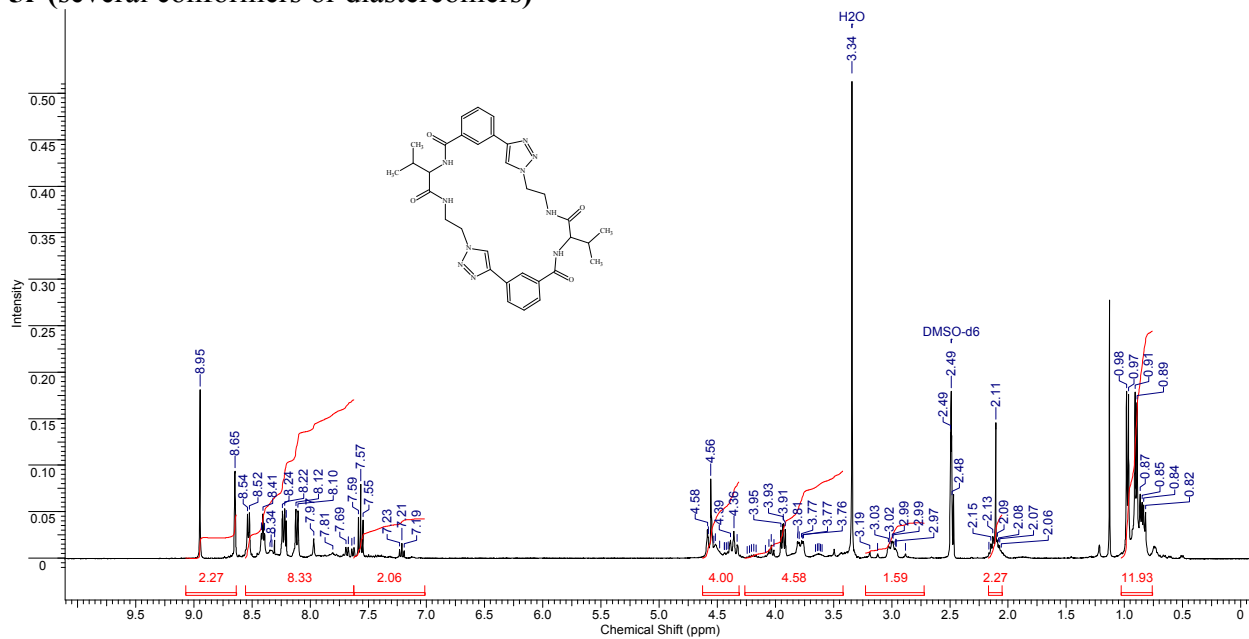
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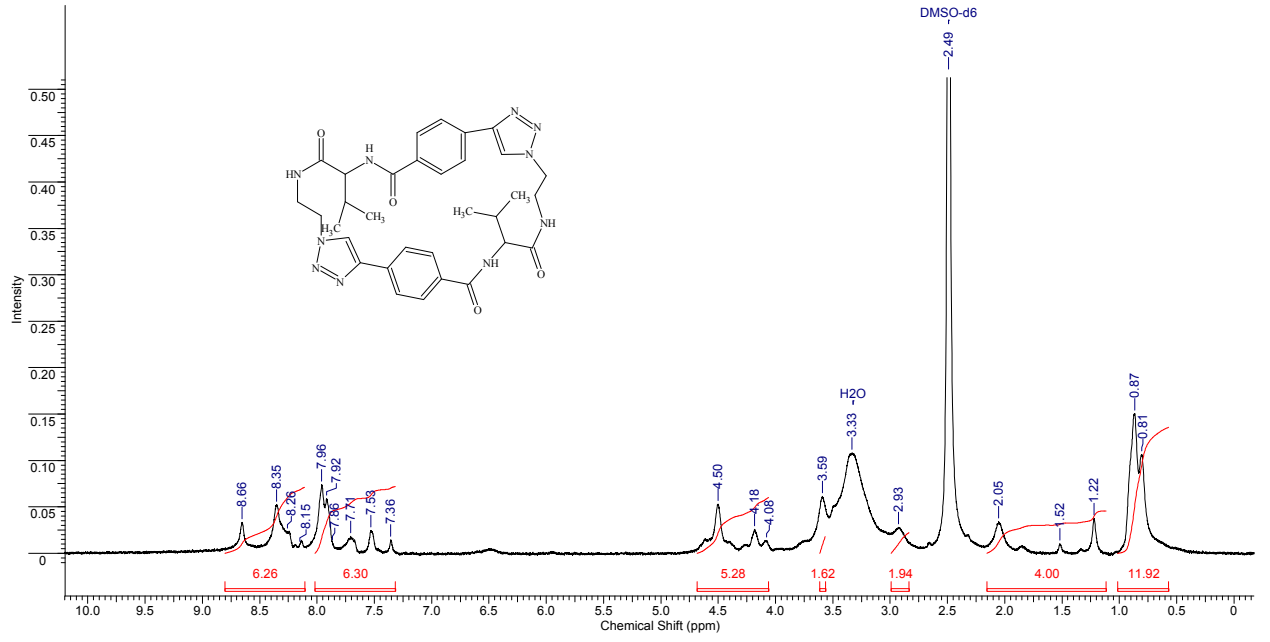
50 (the mixture of conformers)



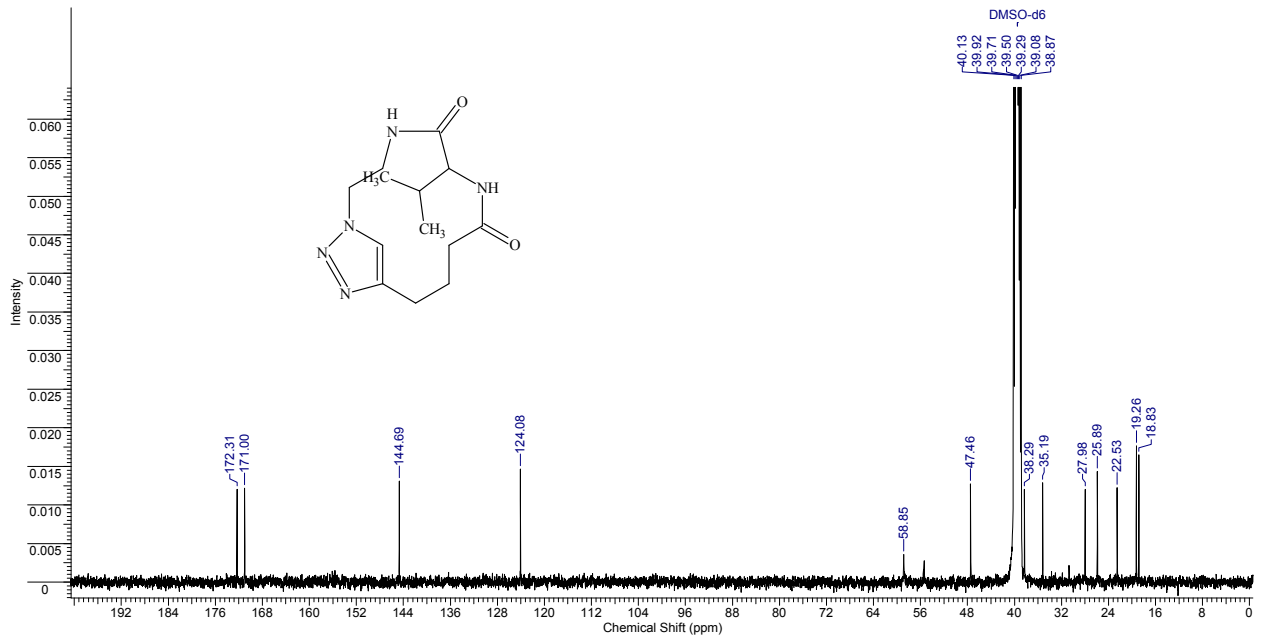
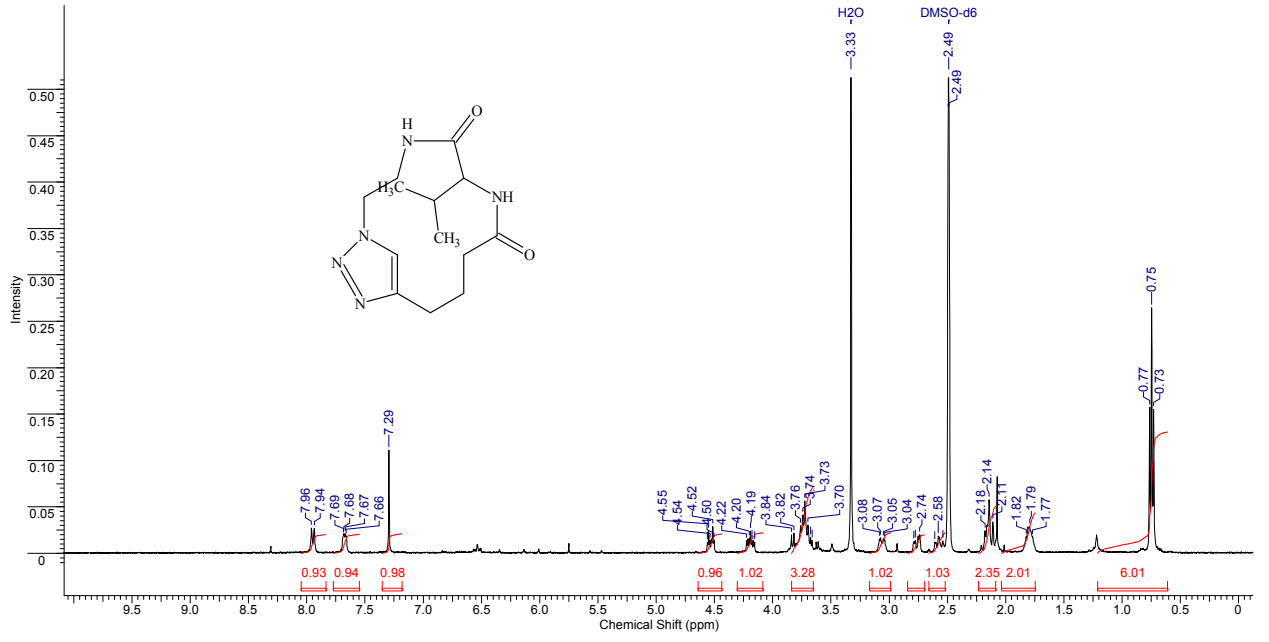
5r (several conformers or diastereomers)



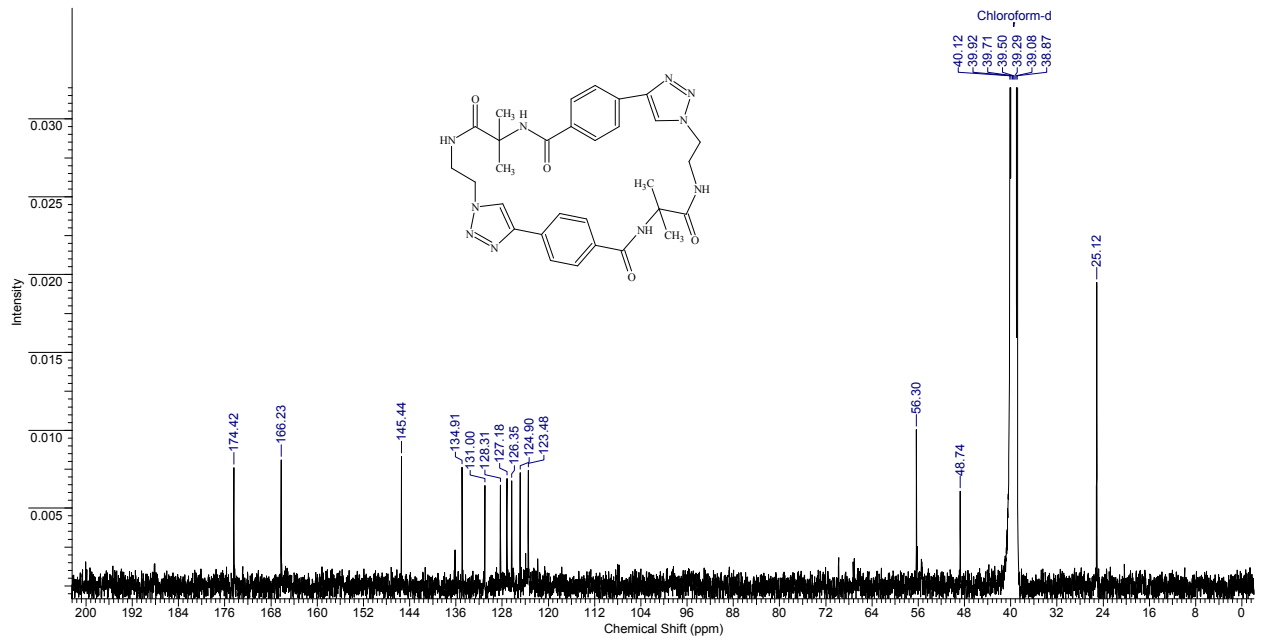
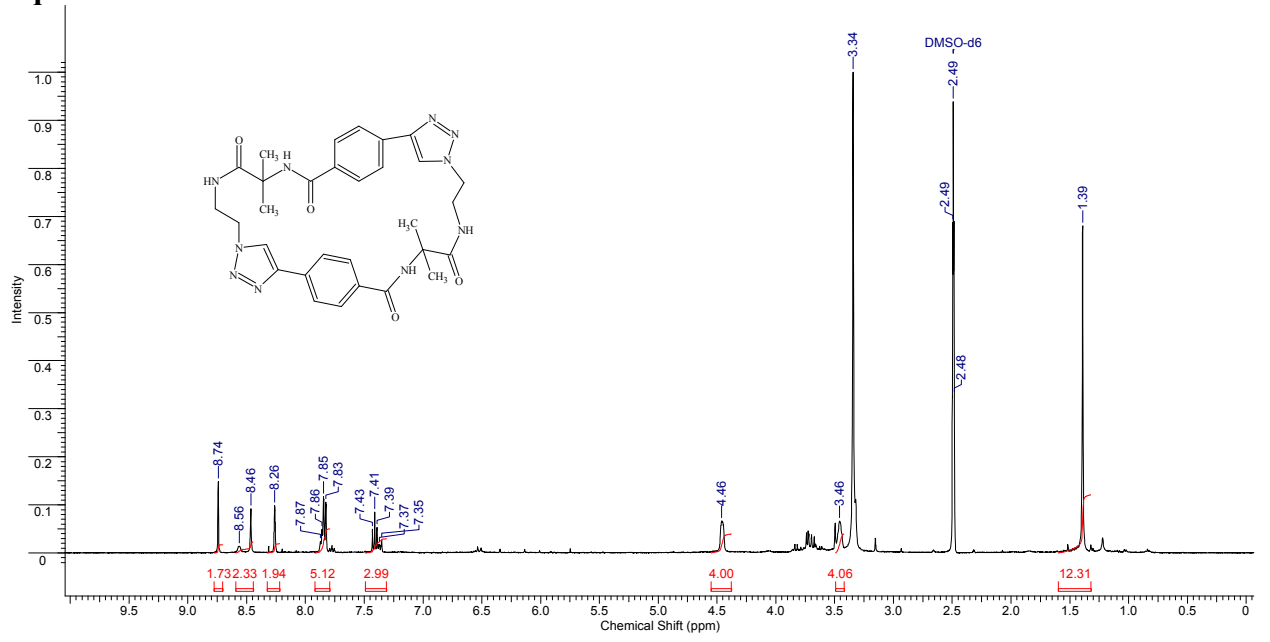
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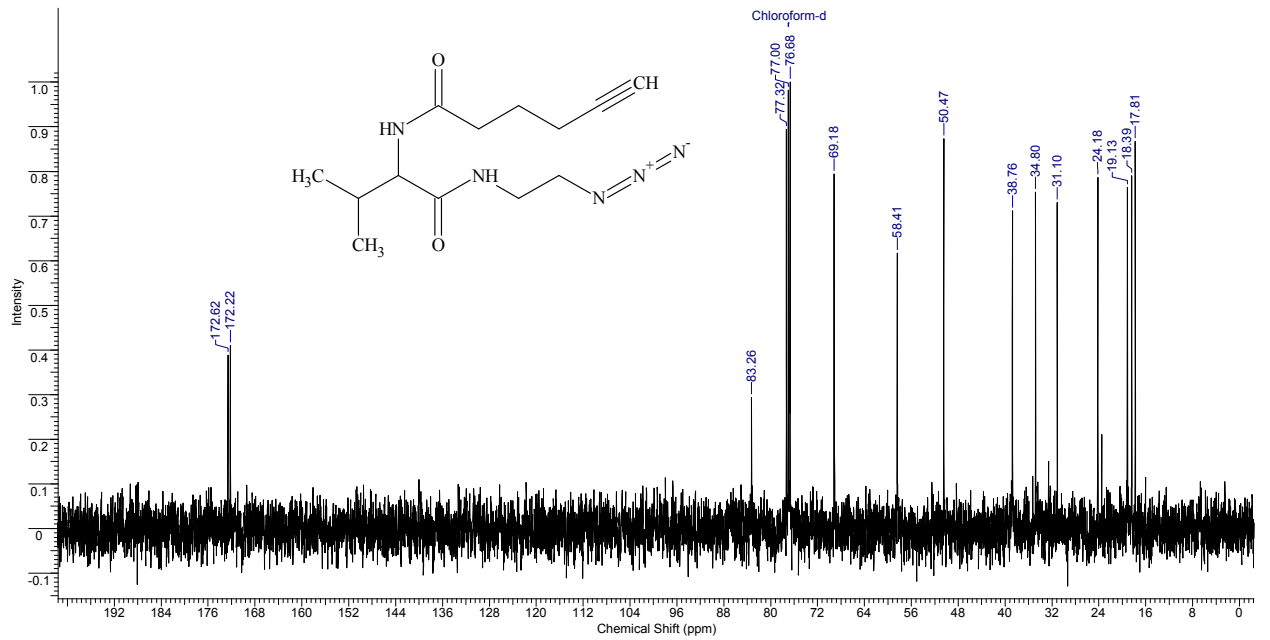
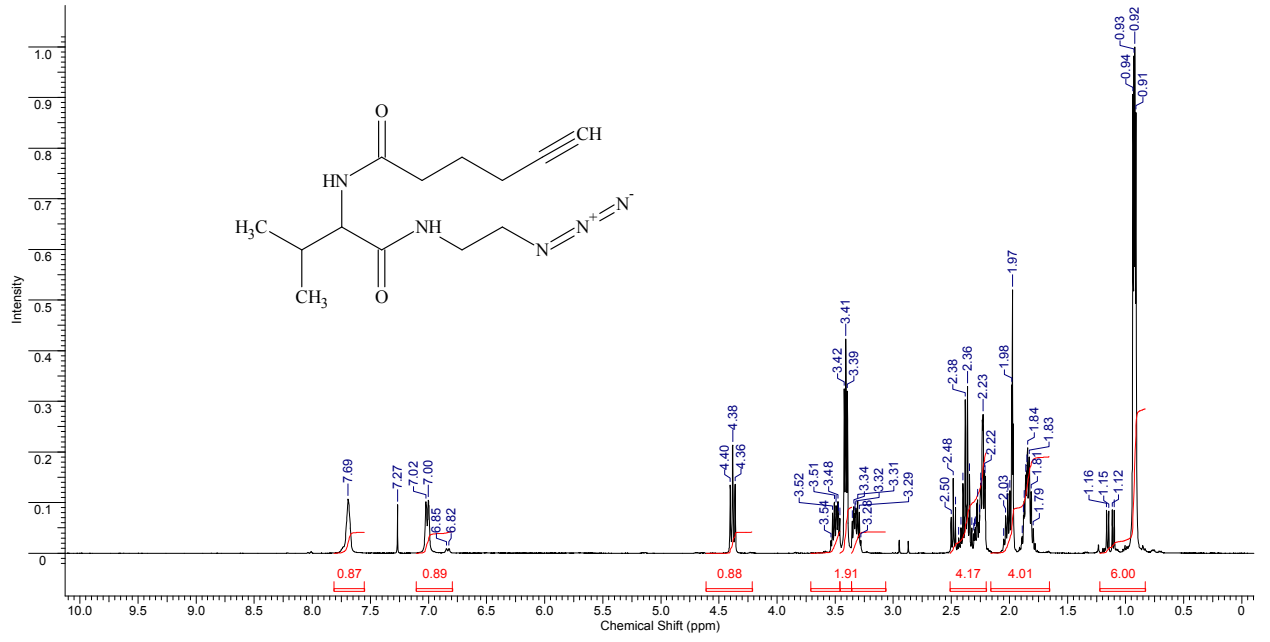
5i



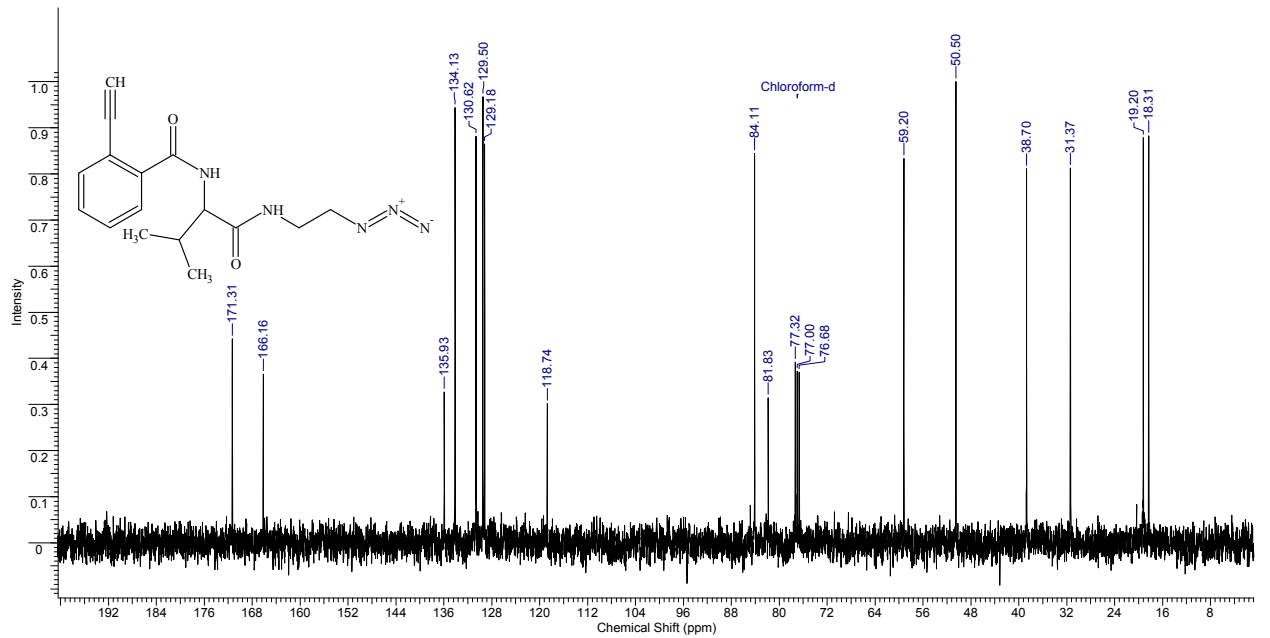
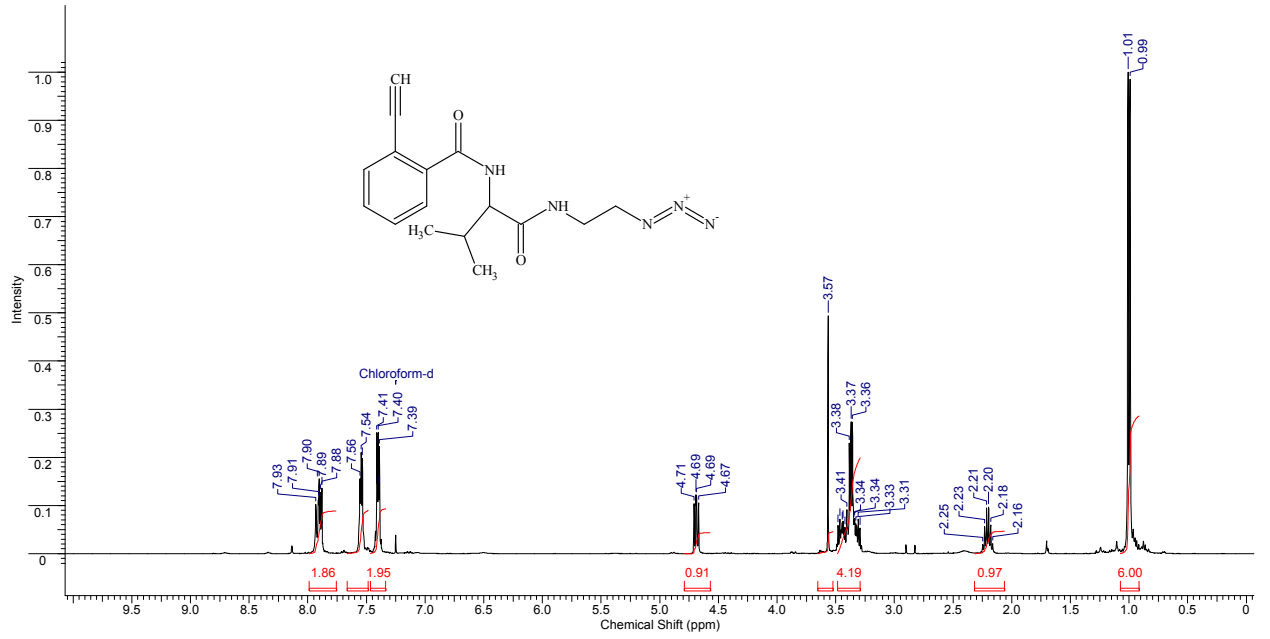
5q



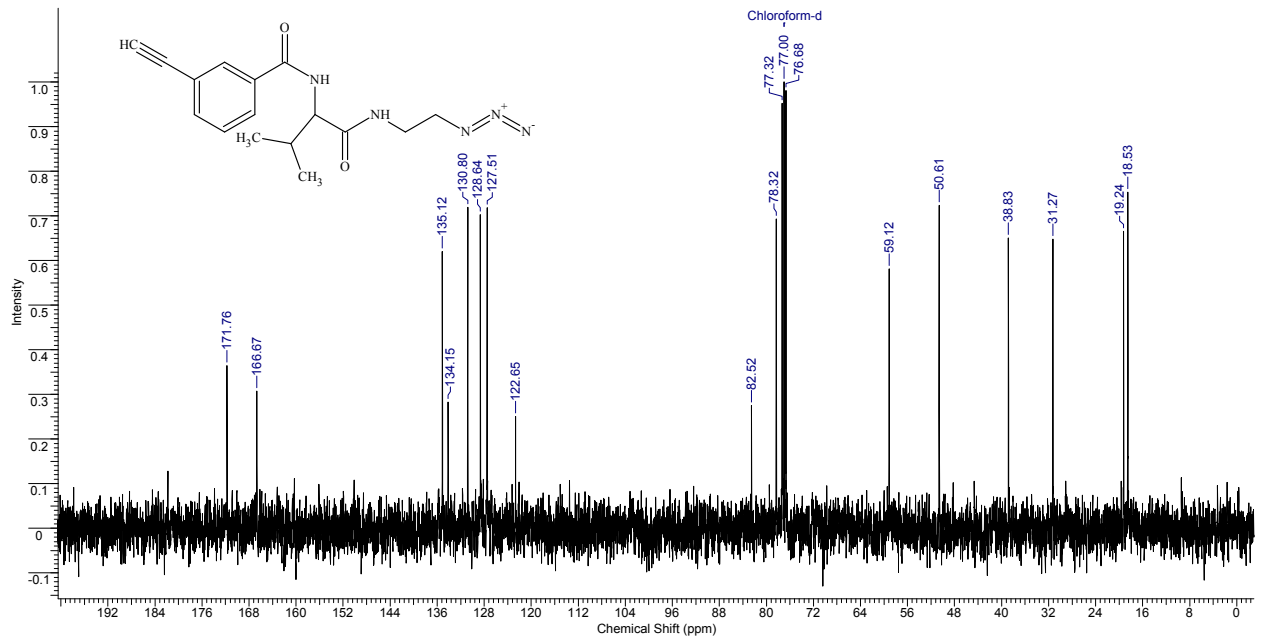
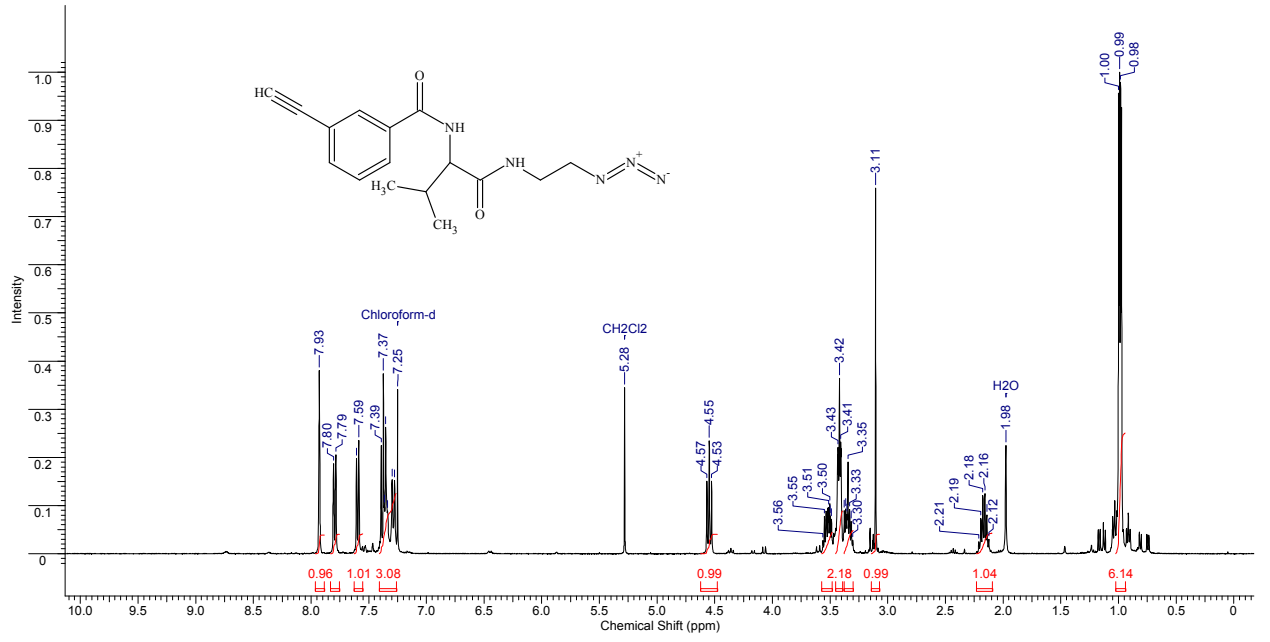
6i



60



6r



6u

