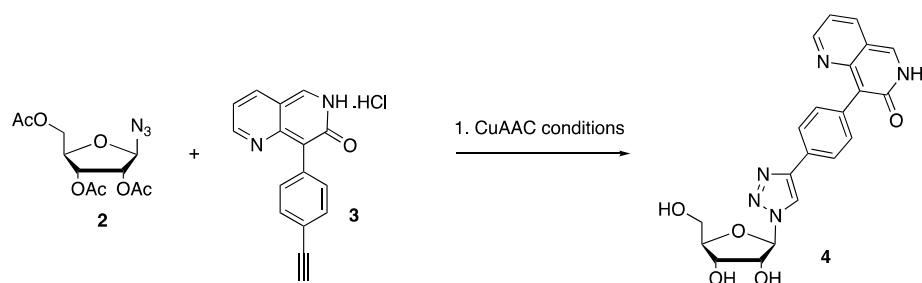


Supporting information

1H-1,2,3-triazolyl-1,6-naphthyridin-7(6*H*)-ones as potential fluorescent nucleoside analogues : Synthesis and optical properties

Anissa Beghennou, Océane Rondot, Vincent Corcé and Candice Botuha

I. Table S1. CuAAC reaction attempts to get Compound 4



a. Tris(benzyltriazolylmethyl)amine. b. Diisopropylethylamine. c. Solubility issues

Conditions	Solvent	Temp	Time	Product/outcome
5% mol. CuSO ₄ ·5H ₂ O, 10% mol. NaAsc	<i>t</i> -BuOH/ Phosphate buffer	20 °C	24h	No reaction
10% mol. CuSO ₄ ·5H ₂ O, 30% mol. NaAsc, 10% mol. TBTA ^a	<i>t</i> -BuOH/ H ₂ O	75 °C	24h	No reaction
10% mol. CuSO ₄ ·5H ₂ O, 30% mol. NaAsc	DMF	150 °C (MW)	30min.	Degradation
10% mol. CuSO ₄ ·5H ₂ O, 30% mol. NaAsc, 1 equiv. DIPEA	CH ₃ CN	60 °C	24h	No reaction
2 equiv.. CuSO ₄ ·5H ₂ O, 4 equiv. NaAsc, 1 equiv. DIPEA	CH ₃ CN/ H ₂ O	20 °C	24h	No reaction ^c
10% mol. CuI, 1 equiv. DIPEA	CH ₃ CN	20 °C	24h	No reaction
10% mol. Cu(IMes)Cl, 1 equiv. DIPEA	CH ₃ CN	20 °C	24h	No reaction
10% mol. Cu(IMes)Cl, 1 equiv. DIPEA	MeOH	20 °C	24h	No reaction
2 equiv. CuI, 1 equiv. DIPEA	THF	60 °C	24h	No reaction ^c

II. Absorption spectra in various solvent of TzNat A-C

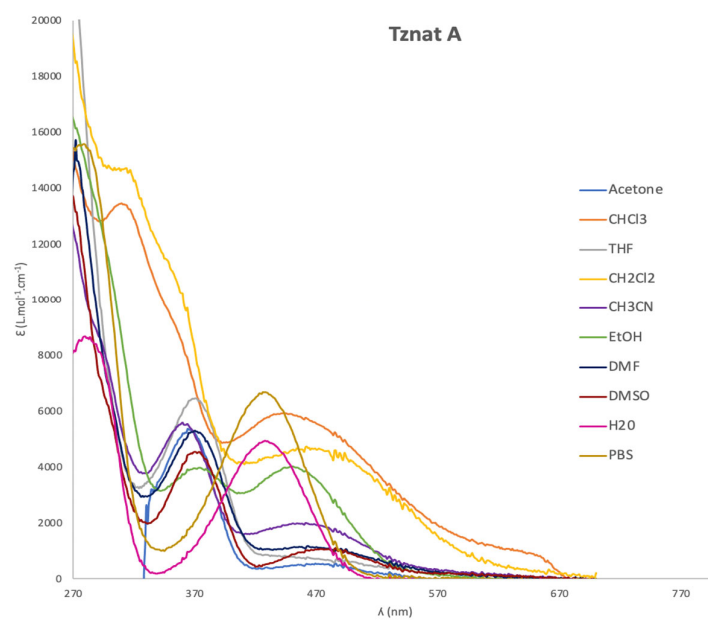


Figure S1

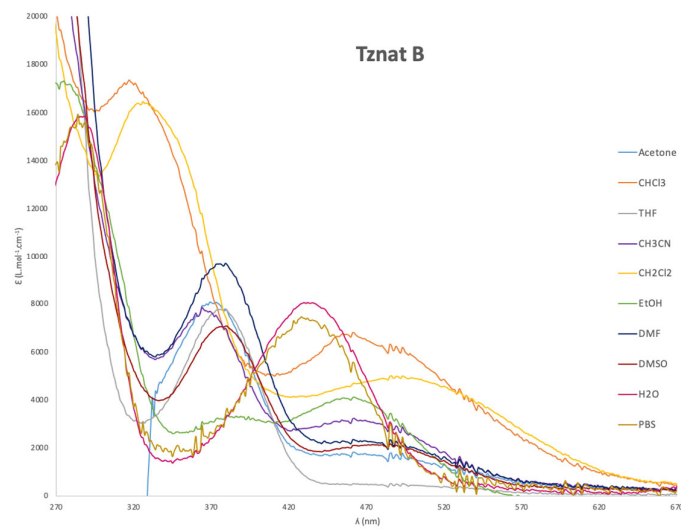


Figure S2

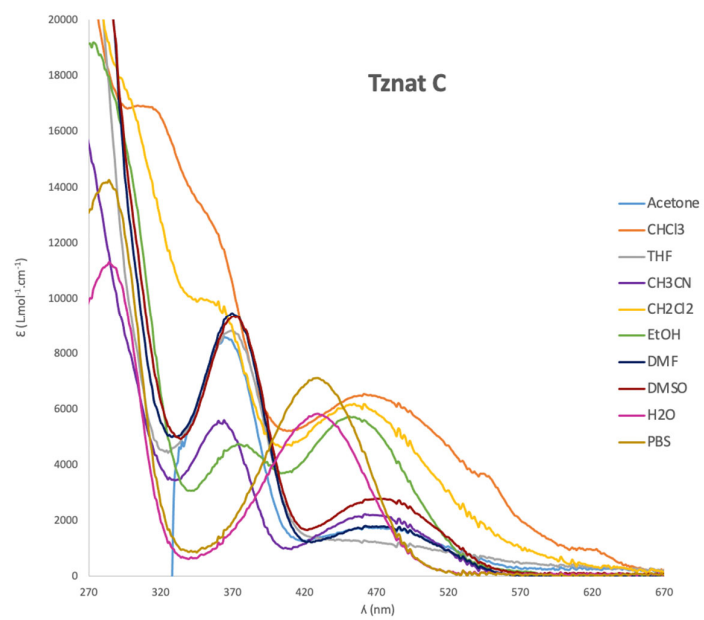
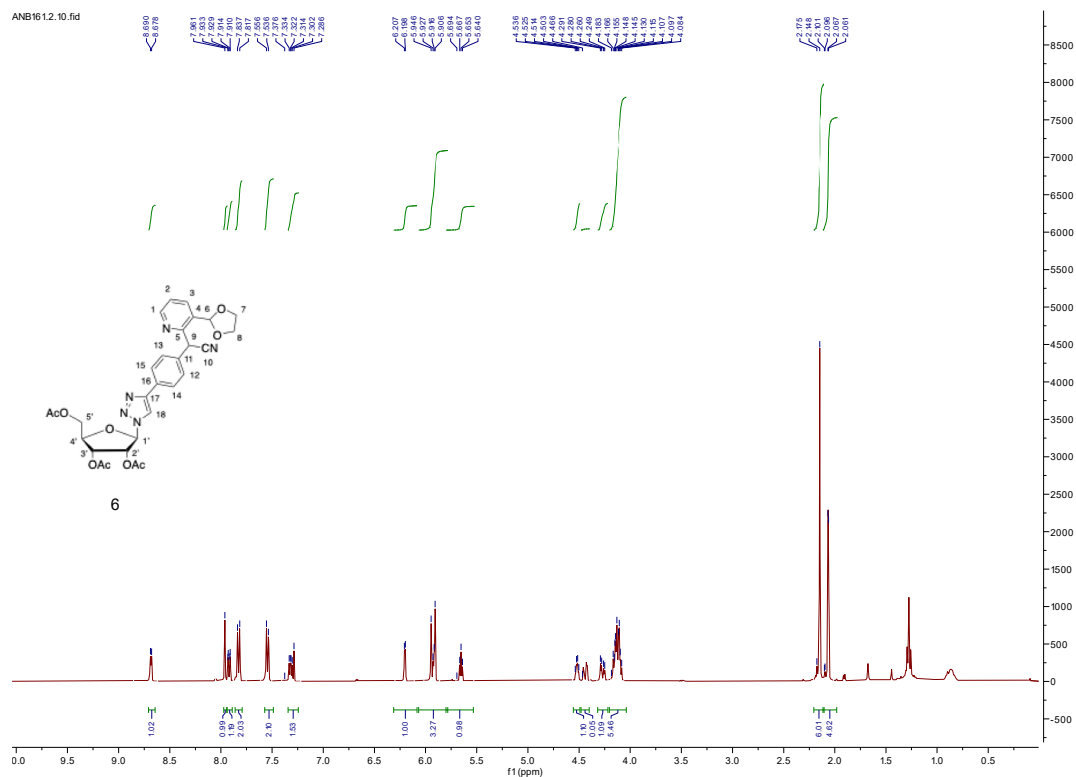
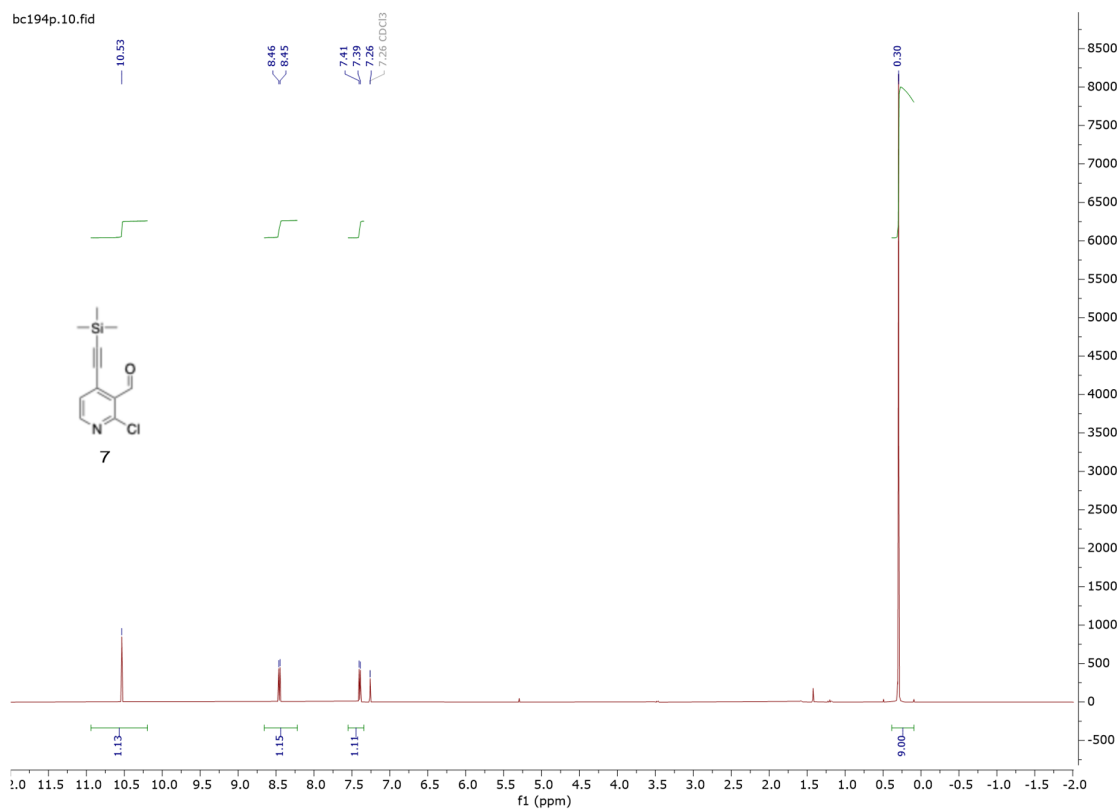


Figure S3

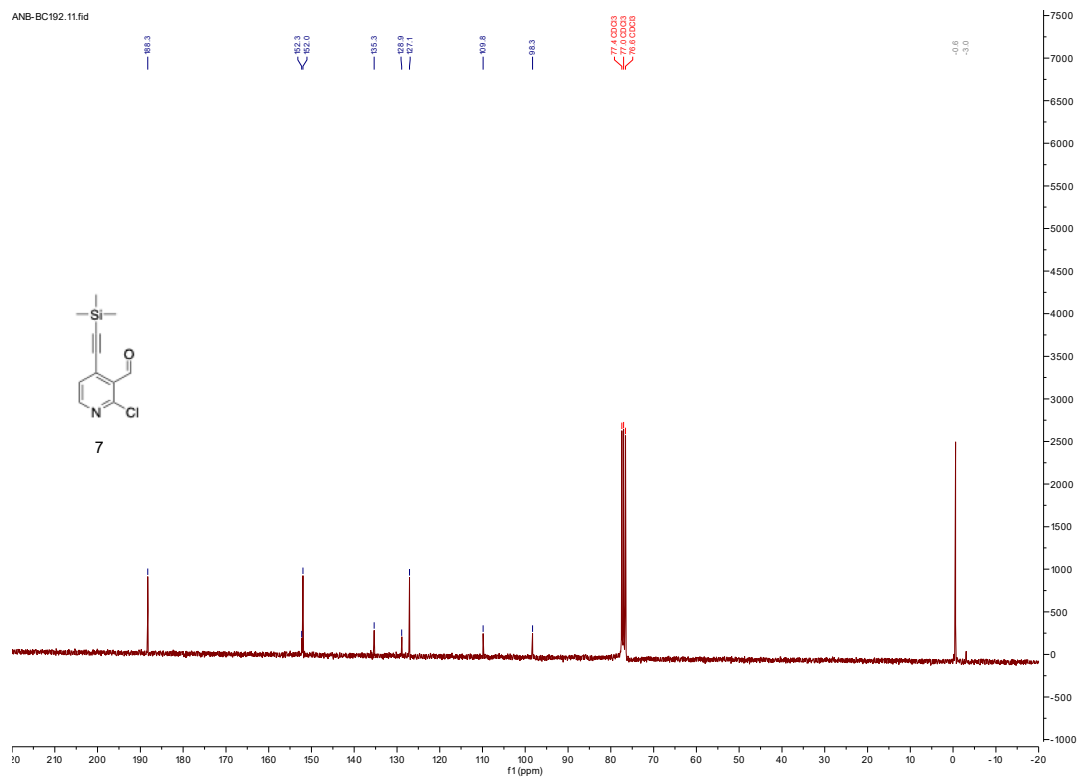
III. ^1H and ^{13}C NMR spectra



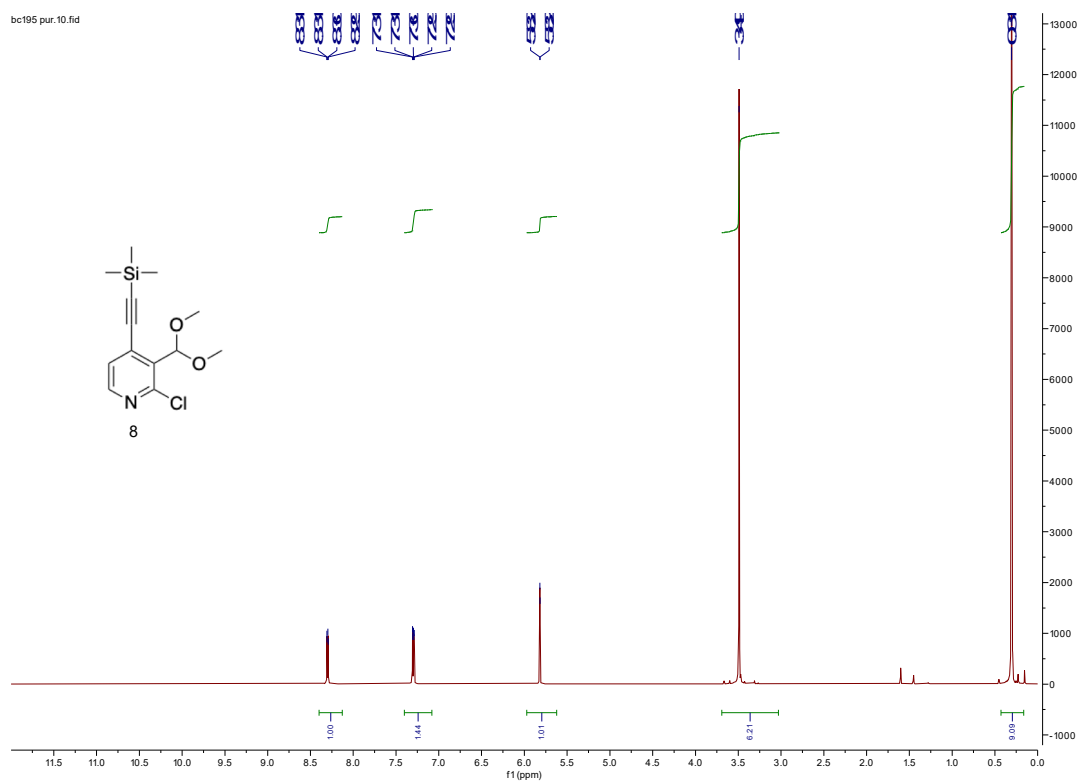
bc194p.10.fid



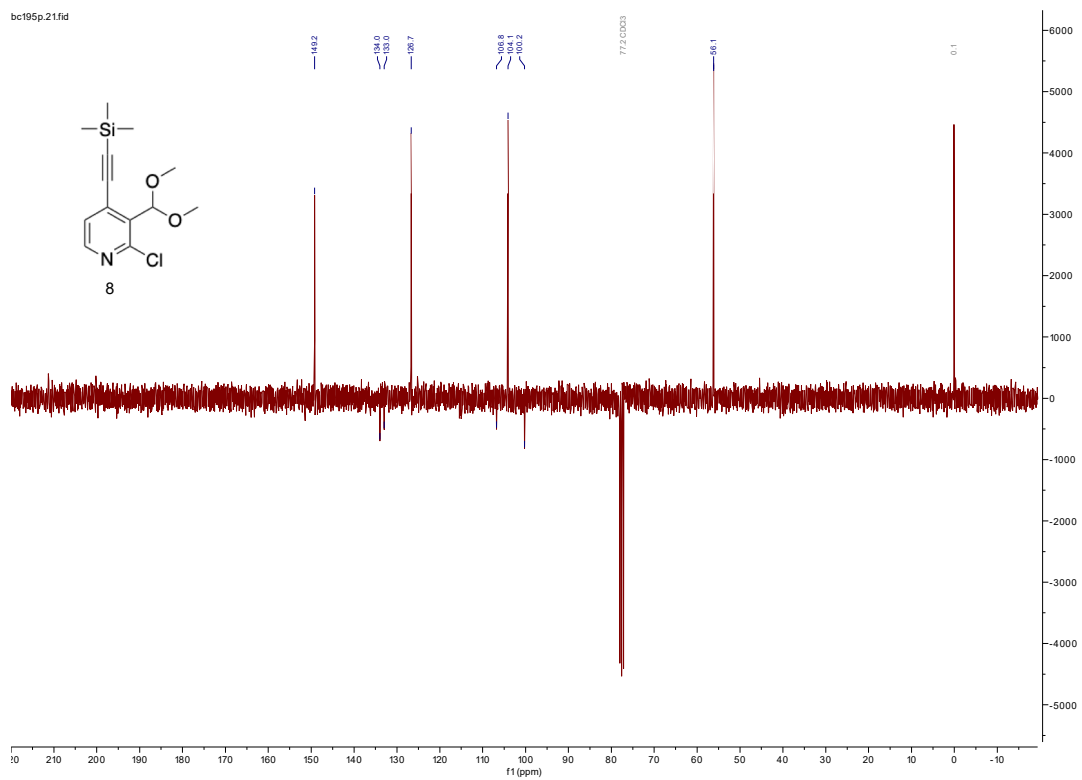
ANB-BC192.11.fid



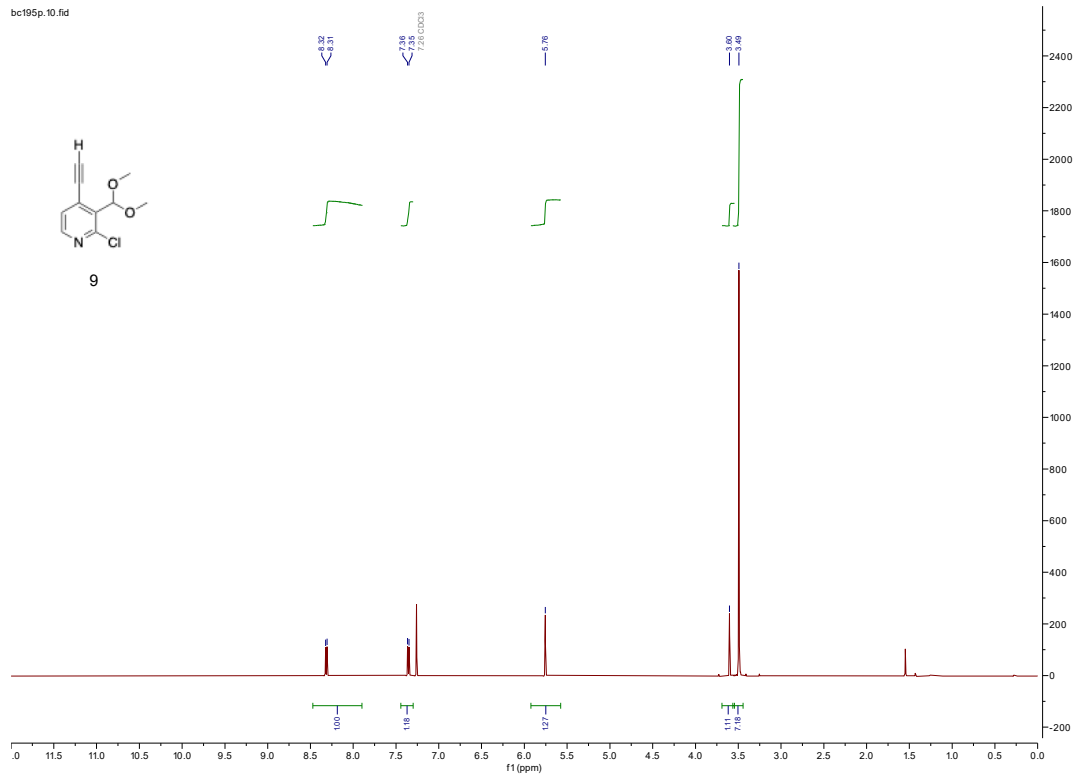
bc195 pur.10.fid



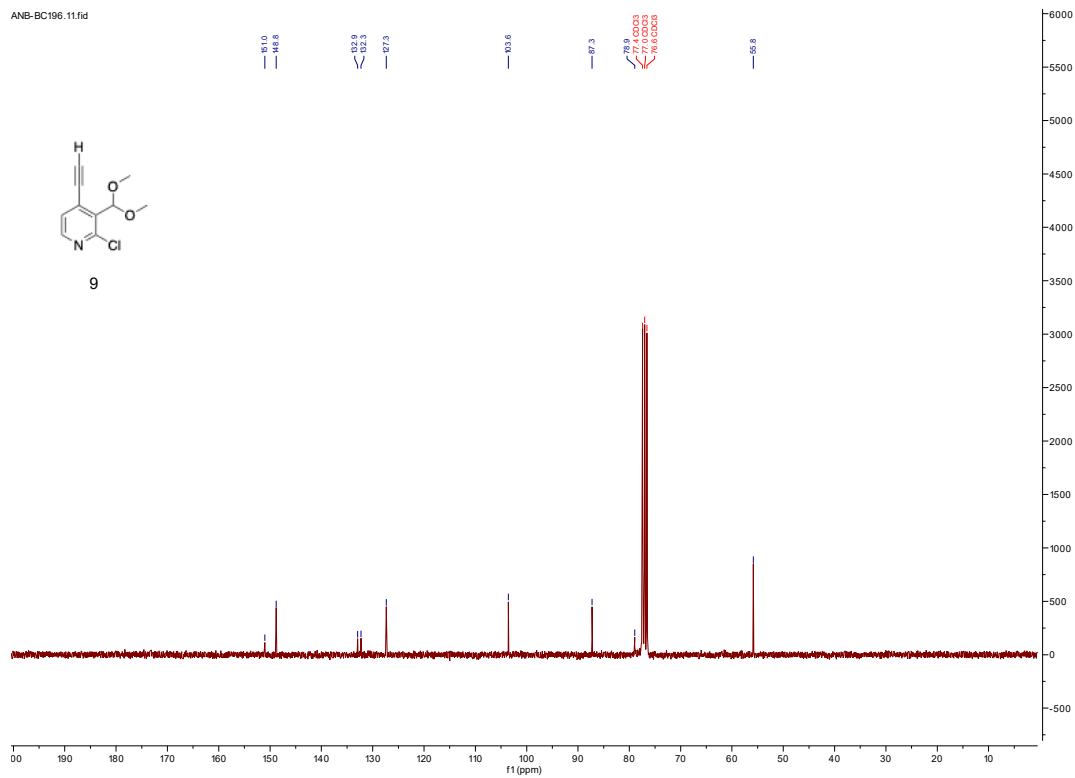
bc195p.21.fid

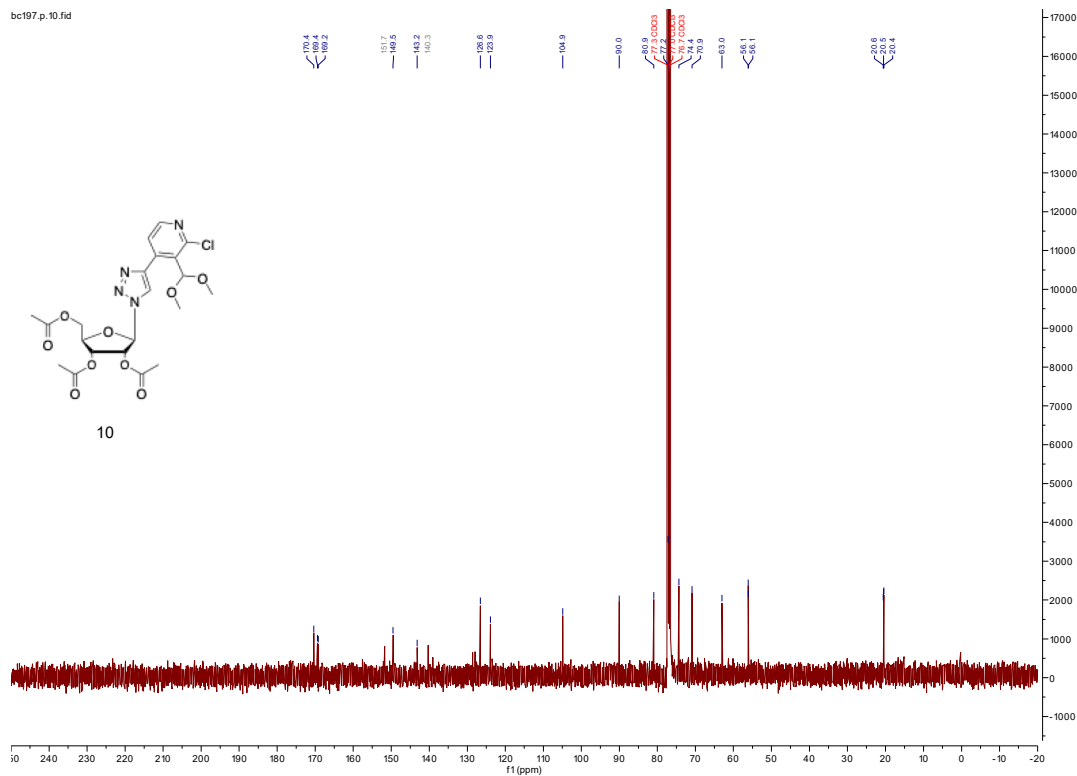
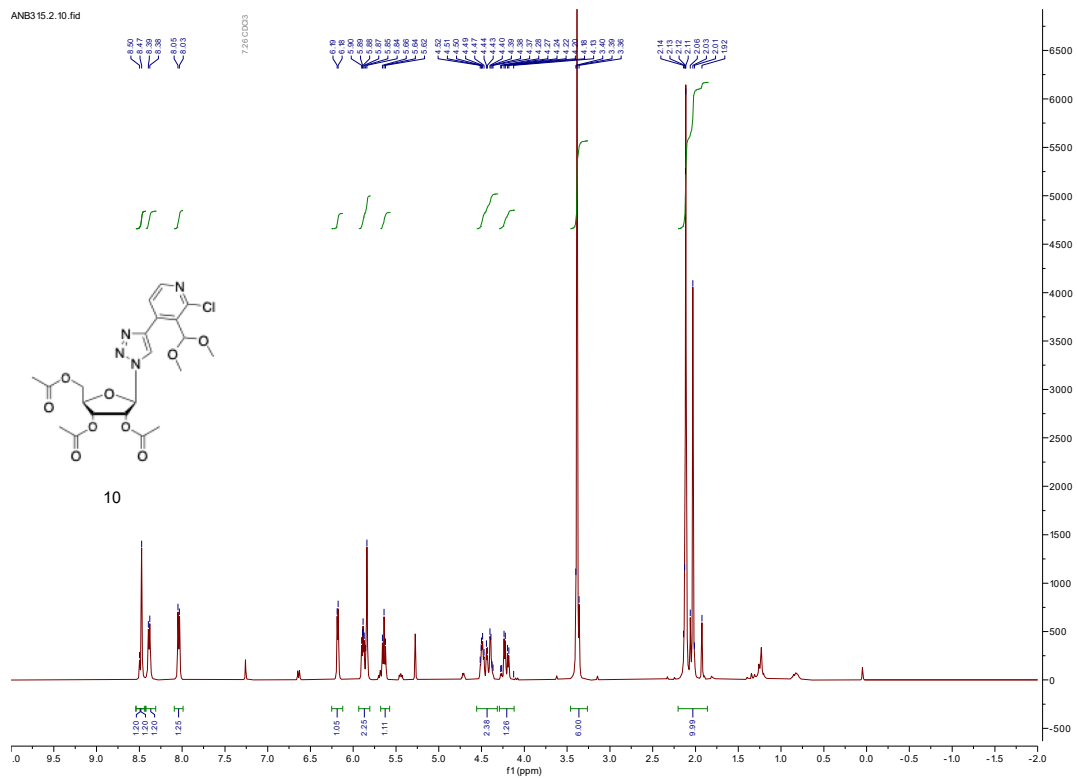


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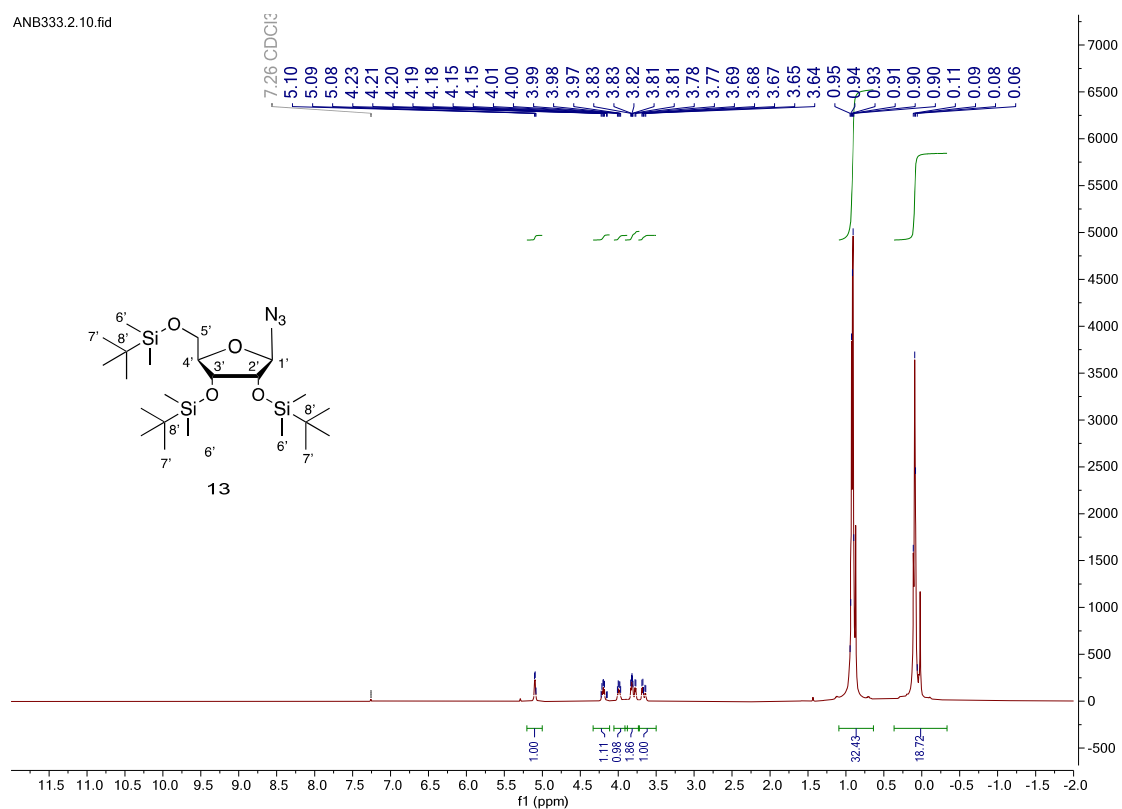


ANB-BC196.11.fid

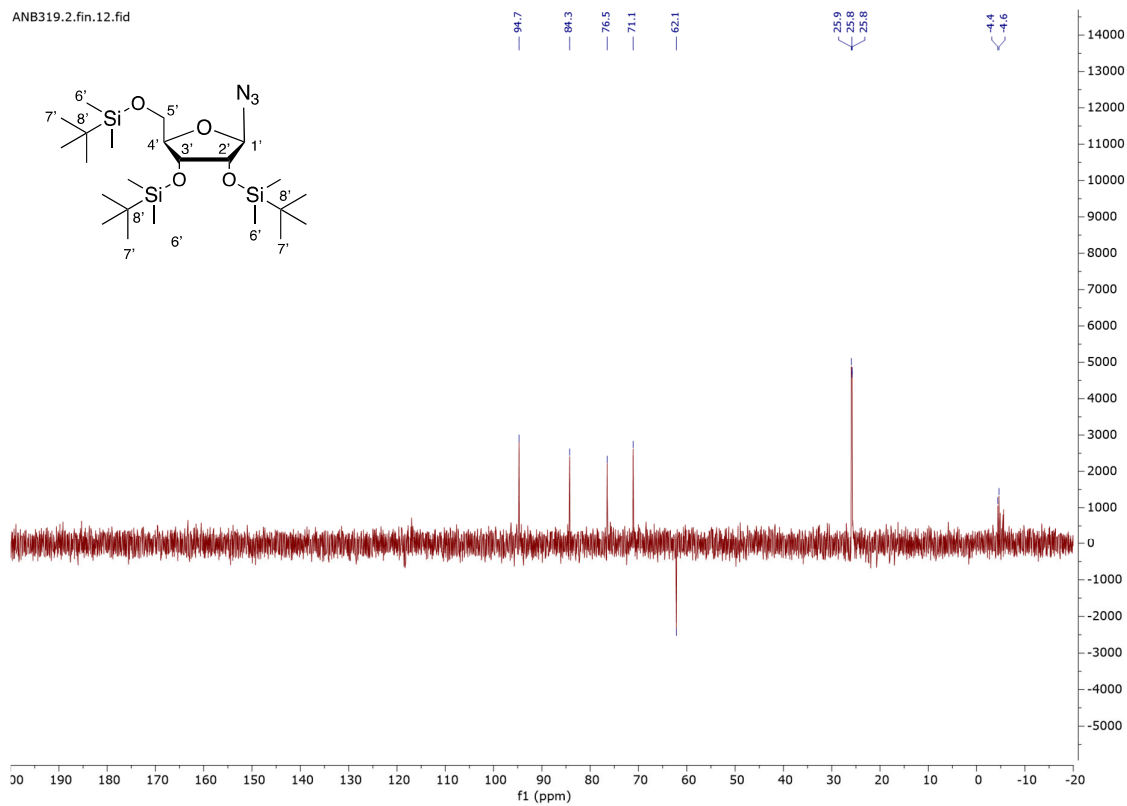




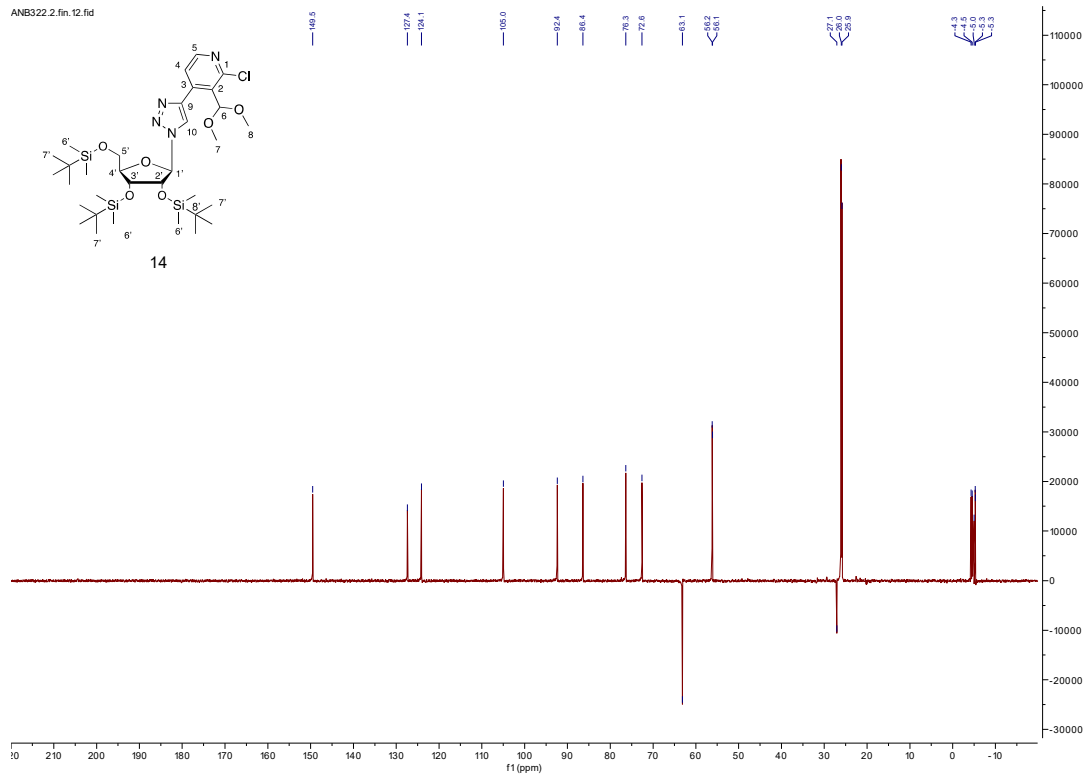
ANB333.2.10.fid



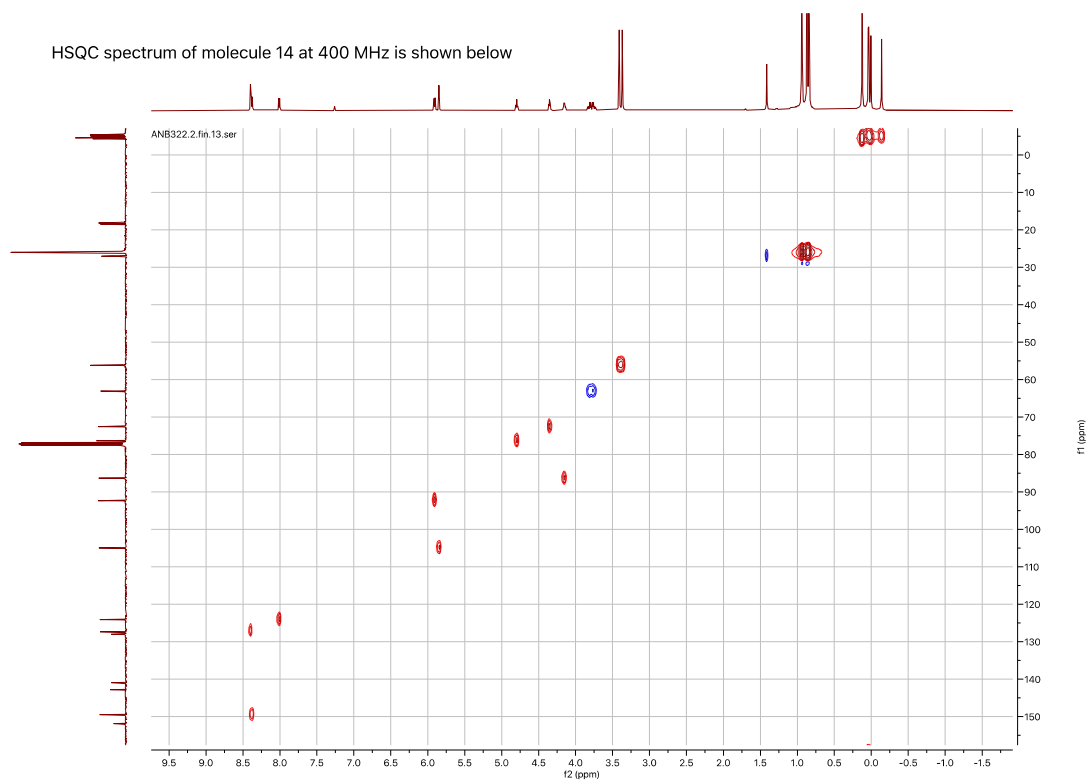
ANB319.2.fin.12.fid



ANB322.2.f1n.12.fid



HSQC spectrum of molecule 14 at 400 MHz is shown below



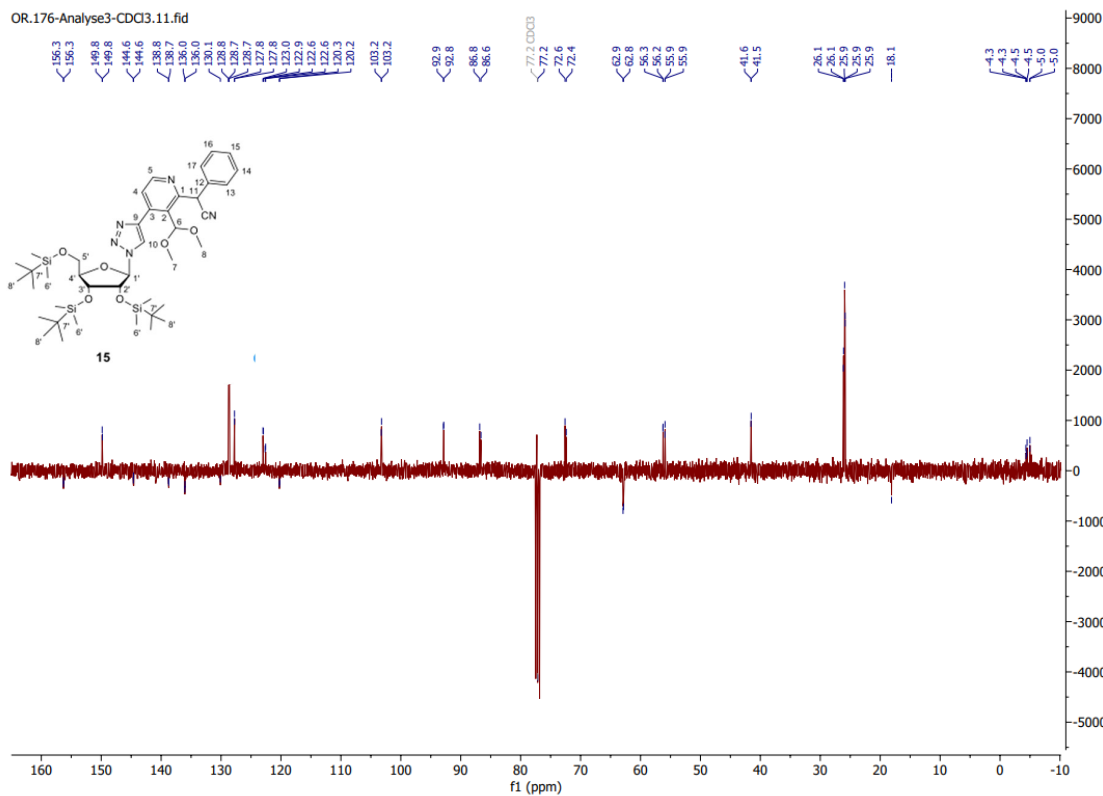
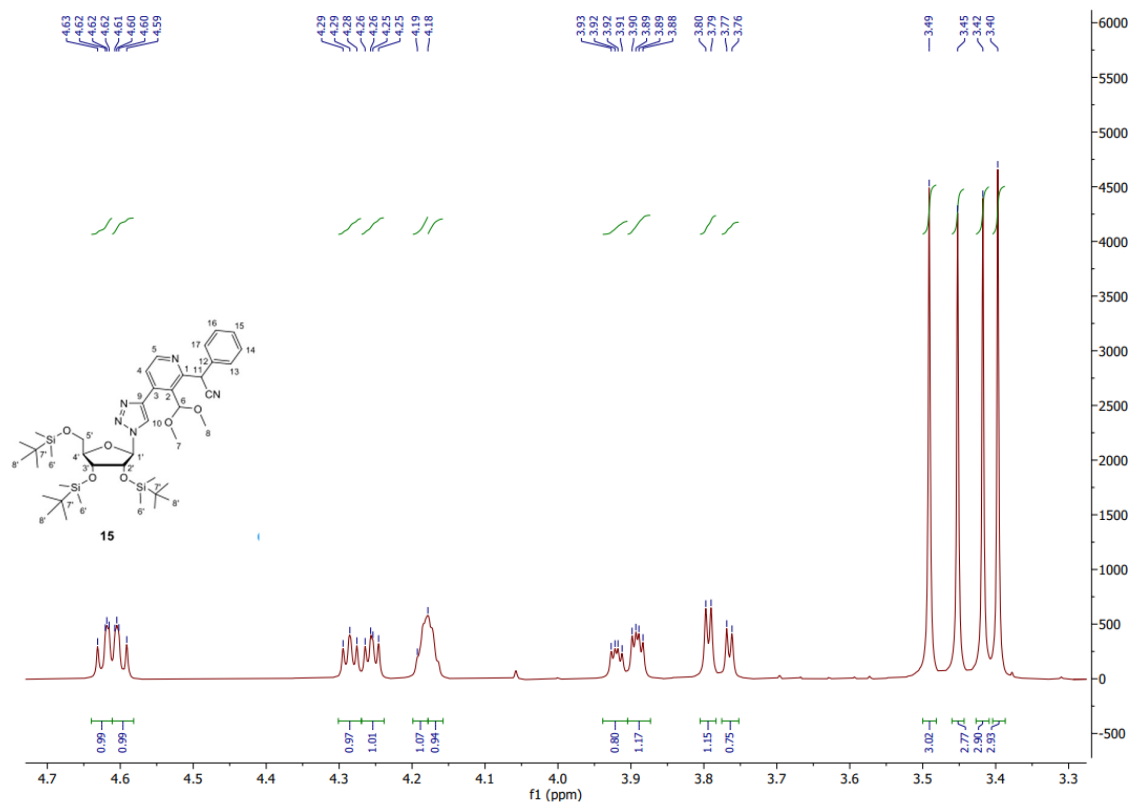
[illegible]

OR-176-Analyse3-CDCl3.10.fid

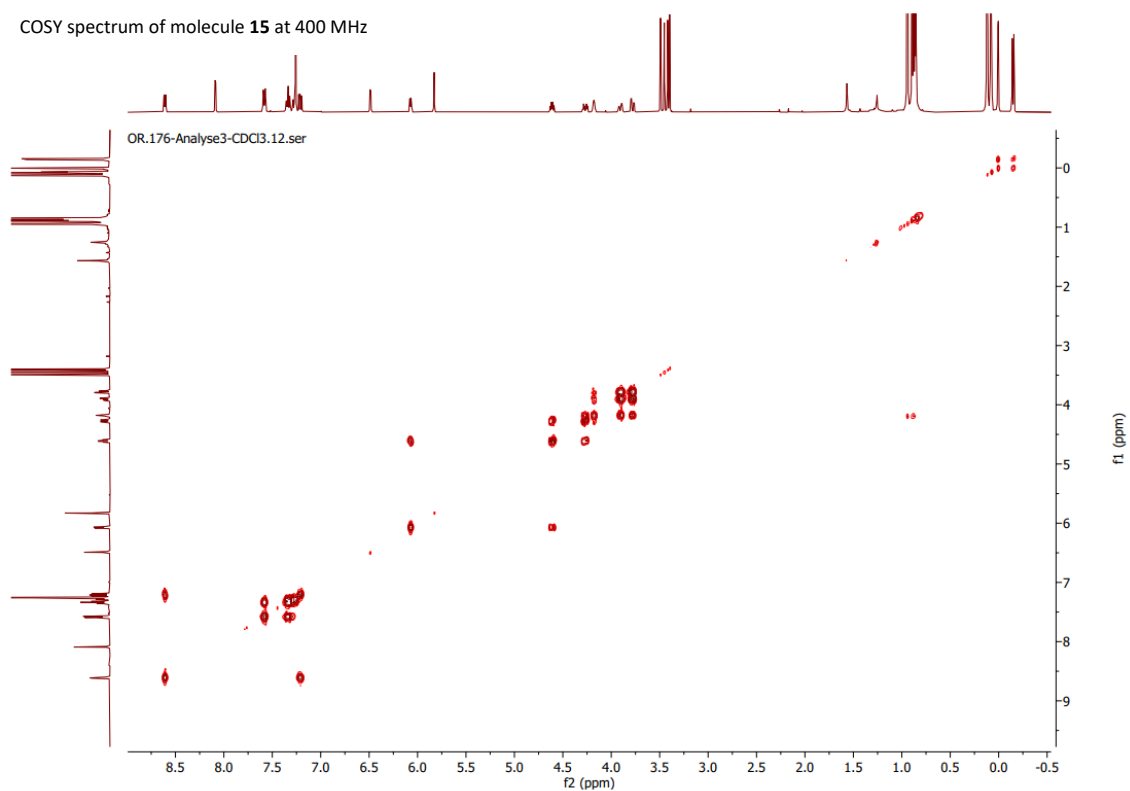
Chemical structure of compound 15 is shown. The structure is a complex molecule with a central benzene ring substituted with a nitrile group and a 1,2,4-triazole ring. The triazole ring is further substituted with a 1,3-bis(trimethylsilyloxy)propyl group. The peaks are labeled with their chemical shifts and integrations.

Chemical Shift (ppm)	Integration
8.62, 8.61, 8.61, 8.60	0.97, 0.97
8.09, 8.08	0.98, 0.93
7.60, 7.59, 7.59, 7.58, 7.57, 7.57, 7.36, 7.35, 7.35, 7.35, 7.34, 7.34, 7.32, 7.32, 7.32, 7.31, 7.31, 7.29, 7.29, 7.28, 7.28, 7.26, 7.26, 7.23, 7.23, 7.22, 7.21, 7.20, 7.19	1.87, 2.13, 1.87, 2.31, 0.98, 1.27, 1.05
6.49, 6.48	1.00, 0.94
6.08, 6.07, 6.06	0.99, 0.95
5.83, 5.83	0.96, 1.00

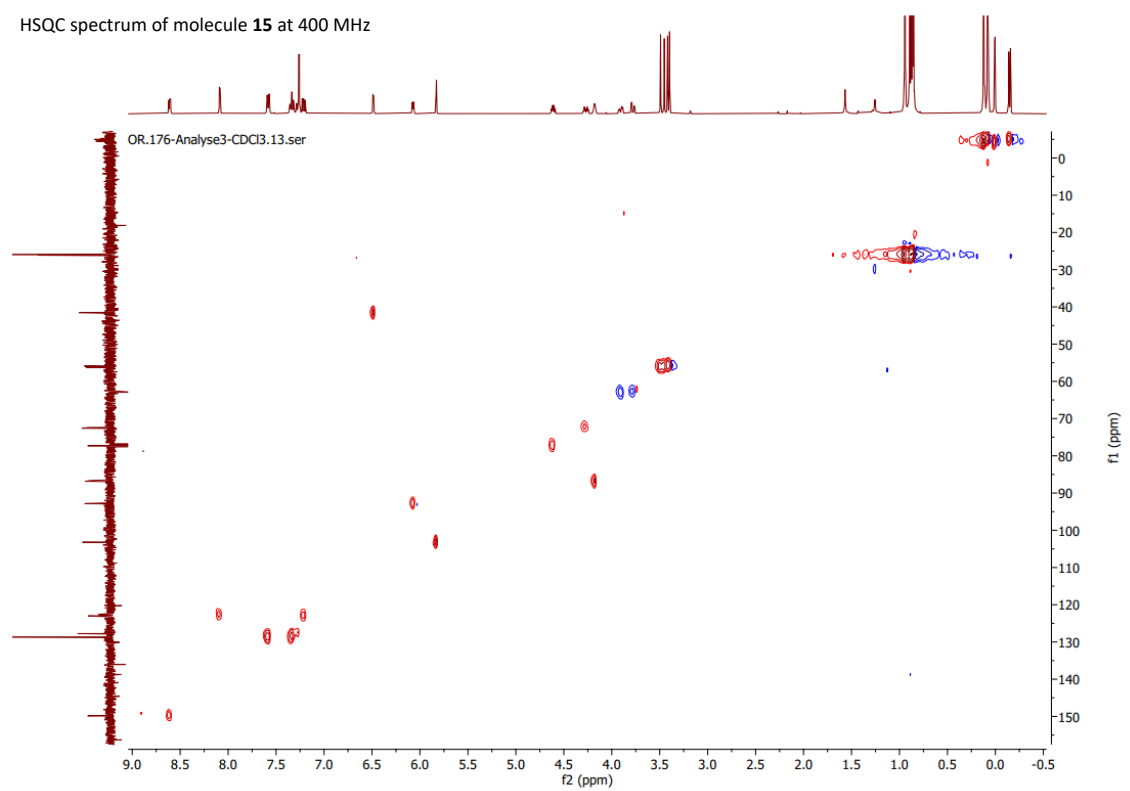
Zoom area 3 – 5 ppm



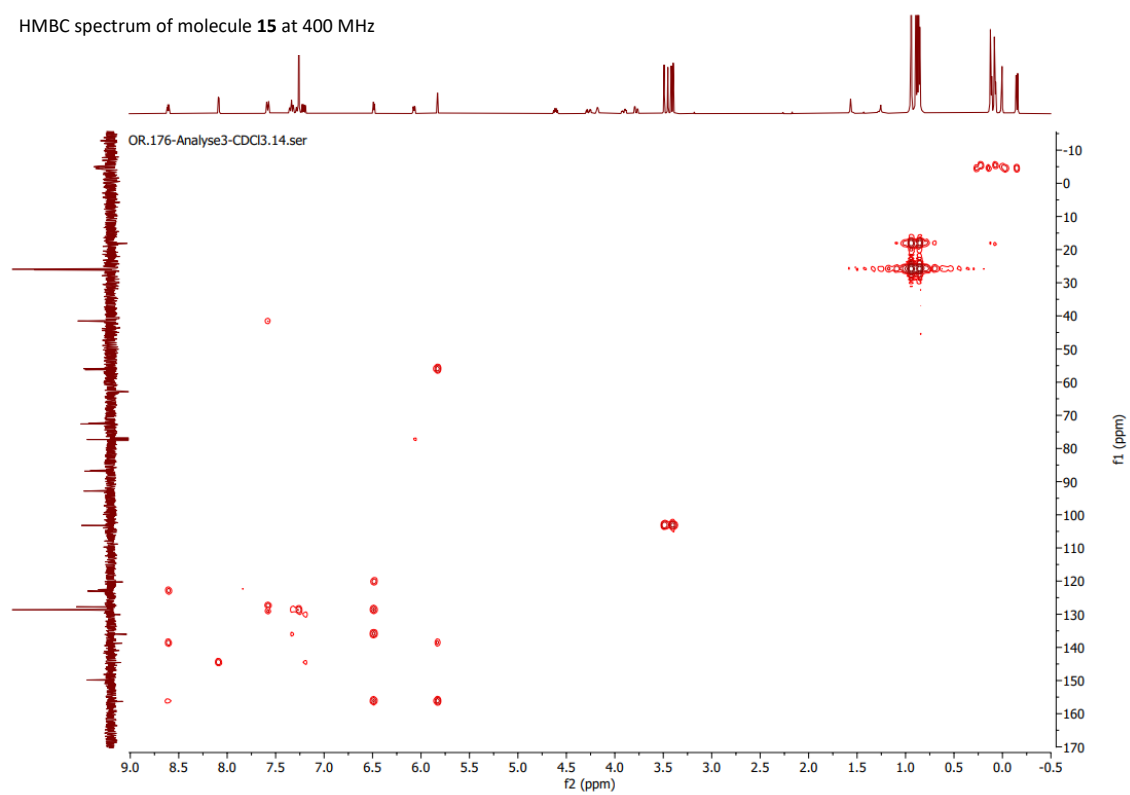
COSY spectrum of molecule **15** at 400 MHz

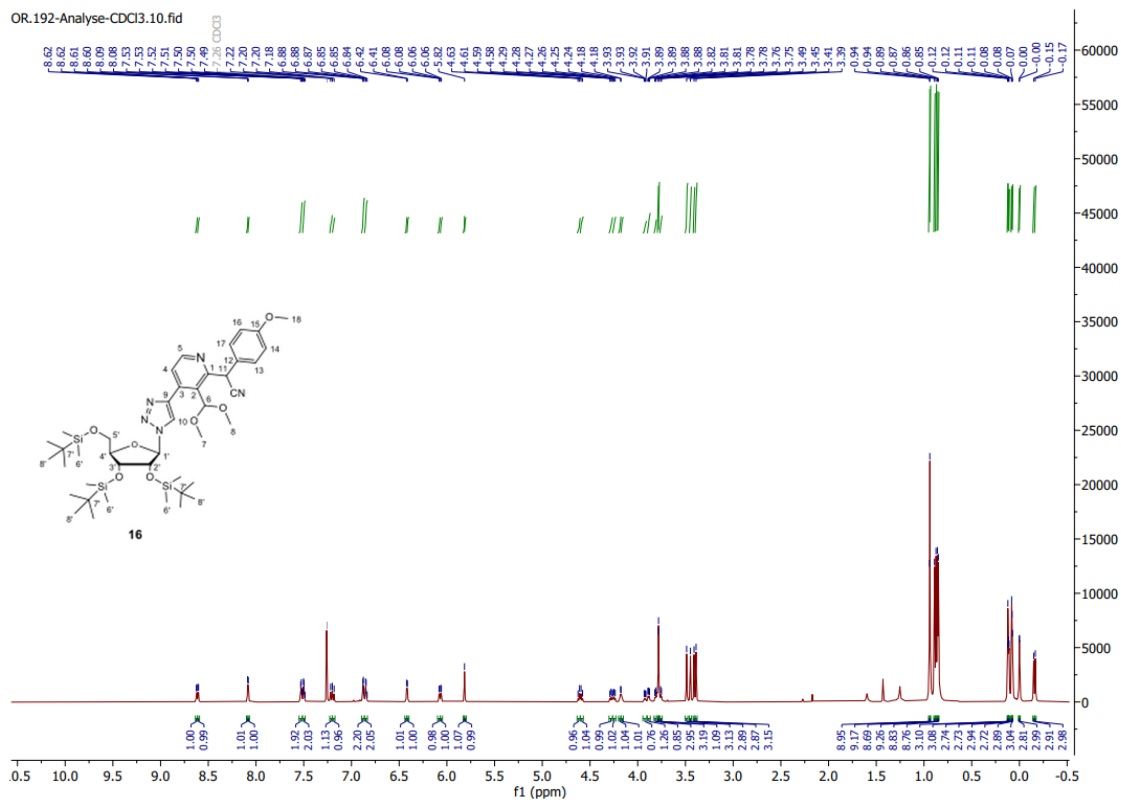


HSQC spectrum of molecule **15** at 400 MHz



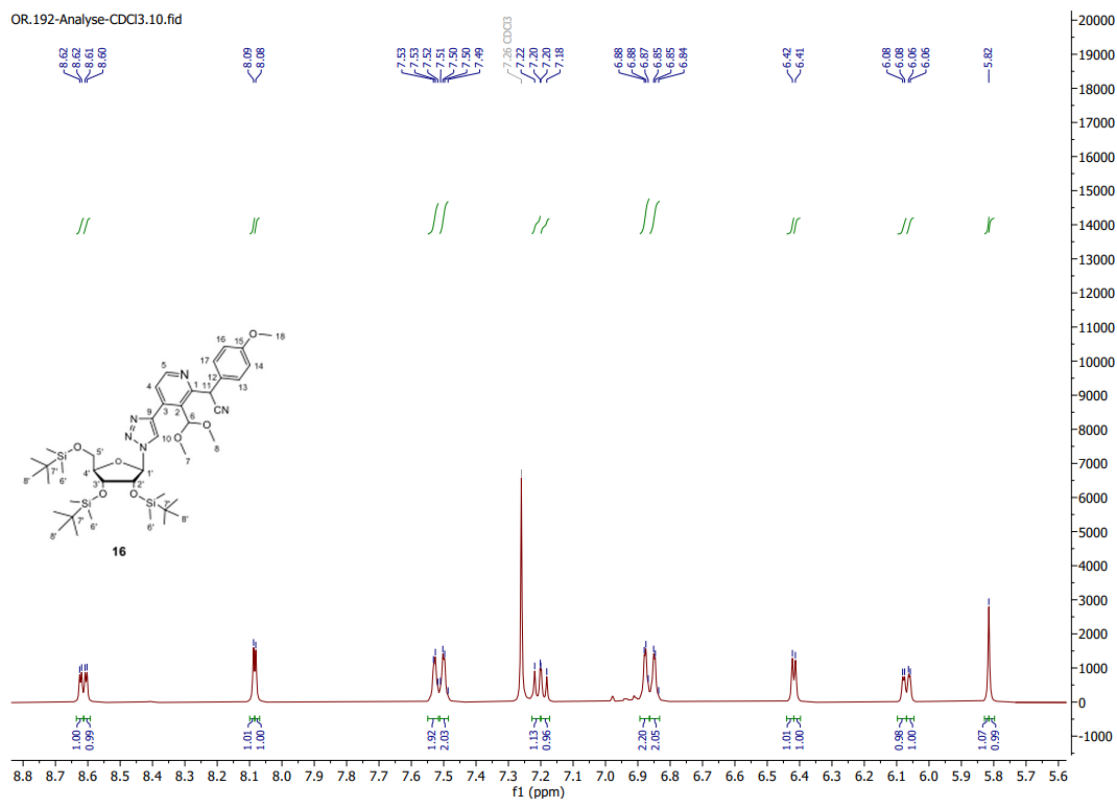
HMBC spectrum of molecule **15** at 400 MHz





Zoom area 5 -9 ppm

OR.192-Analyse-CDCl3.10.fid



Zoom area 3 – 5 ppm

OR_192-Analyse_C003_3.10.fid

Chemical structure of compound **16** is shown on the left. The structure is a complex molecule featuring a central pyridine ring substituted with a cyano group (CN), a methoxy group (OMe), and a 1,2,3-trisubstituted benzene ring. The pyridine ring is also substituted with a 1,2,3-trisubstituted benzene ring. The molecule is labeled **16**.

¹H NMR spectrum (CDCl₃) of compound **16**. The x-axis represents the chemical shift in ppm (f1), ranging from 3.3 to 4.7. The y-axis represents the intensity, ranging from -500 to 9000. The spectrum shows several peaks, with integration values provided below the baseline.

Integration values (from left to right): 0.96, 1.04, 0.99, 1.02, 1.04, 1.01, 0.76, 1.26, 0.85, 2.95, 3.19, 1.09, 3.13, 2.89, 2.87, 3.15.

Chemical shift values (ppm) are listed above the peaks: 4.29, 4.28, 4.27, 4.26, 4.25, 4.24, 4.18, 4.18, 3.93, 3.92, 3.91, 3.91, 3.89, 3.88, 3.88, 3.82, 3.81, 3.81, 3.78, 3.76, 3.75, 3.49, 3.45, 3.41, 3.39.

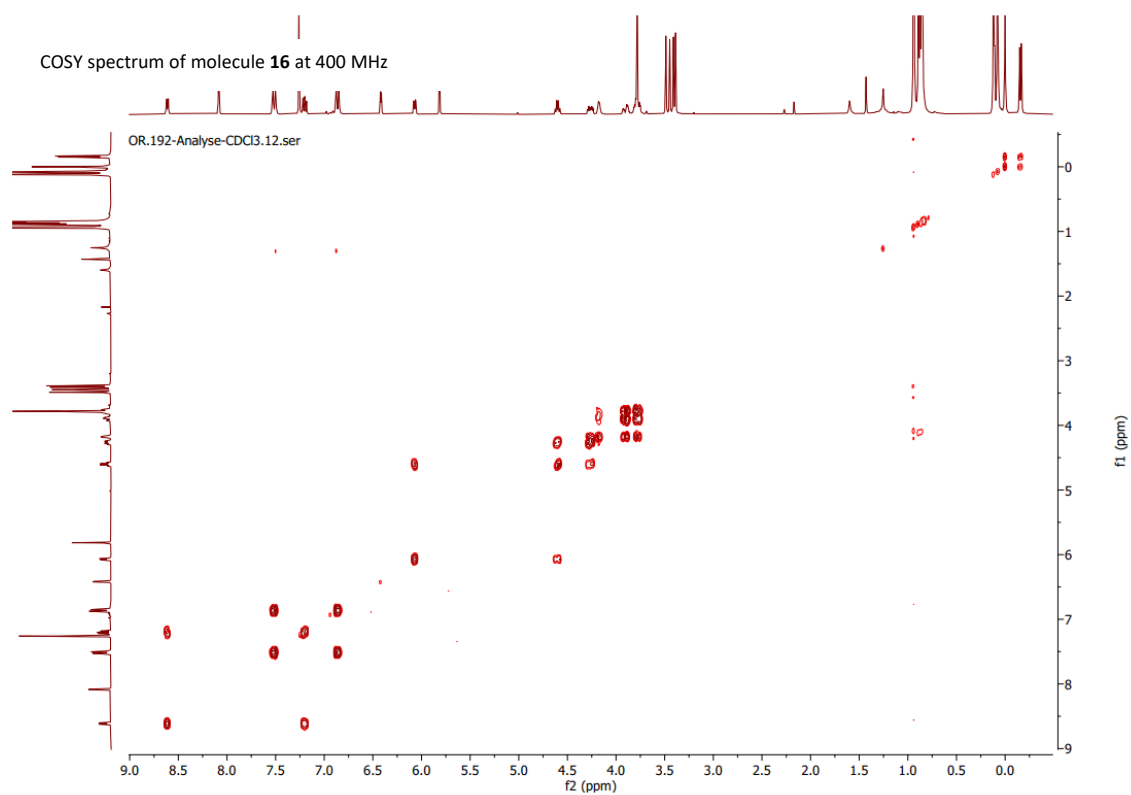
OR.192-Analyse-CDCI3.11.fid

Chemical structure of compound **16** is shown in the top left corner. The structure is a complex molecule with a central pyrazole ring, a nitrile group, and a phenyl ring. It is substituted with a 1,3-bis(trimethylsilyloxy)propyl group.

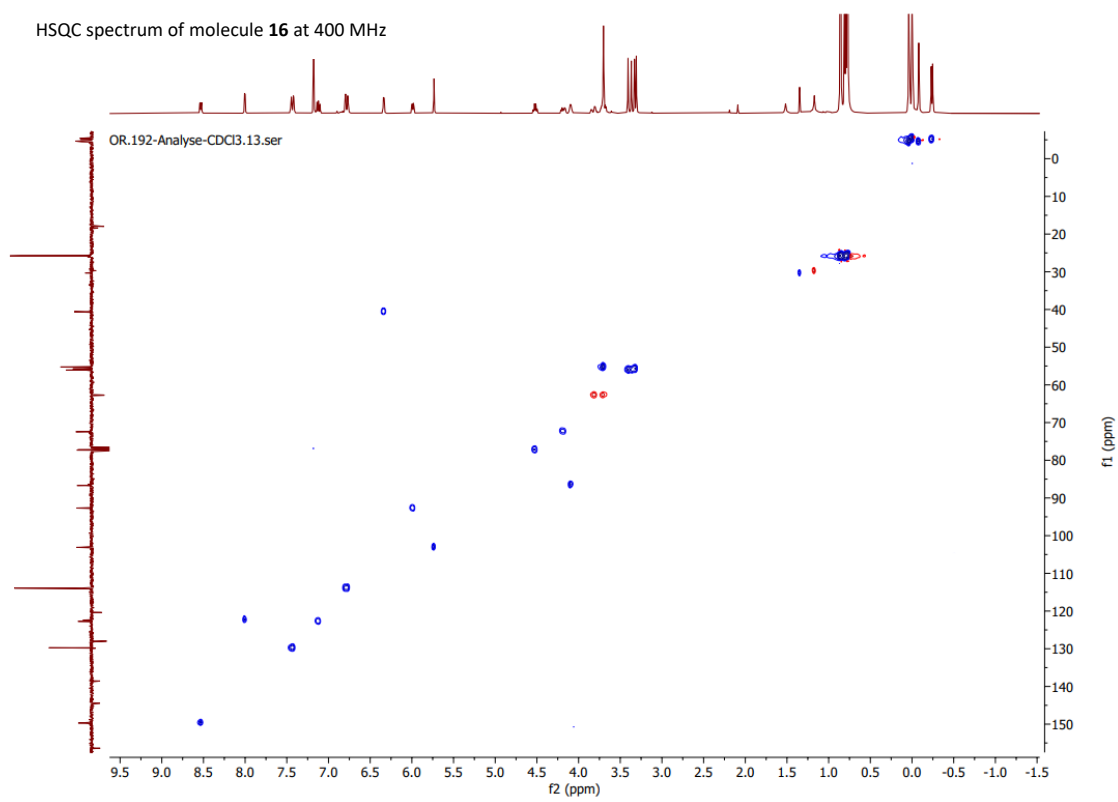
The ¹³C NMR spectrum (CDCl₃) shows the following chemical shifts (ppm):

Chemical Shift (ppm)
159.2
159.1
158.5
156.5
149.8
146.8
144.7
144.6
138.7
138.7
130.0
129.9
129.9
128.1
128.1
127.5
127.5
122.9
122.6
122.5
120.5
120.5
114.0
103.2
103.2
92.9
92.8
86.8
86.6
77.4
77.3
77.2
72.6
72.4
62.9
62.8
56.2
55.9
55.9
55.4
40.7
40.7
26.1
26.1
25.9
25.8
25.8
18.2
18.1
-4.3
-4.3
-4.5
-4.5
-4.5
-4.5
-5.0
-5.0
-5.2
-5.2
-5.3
-5.3

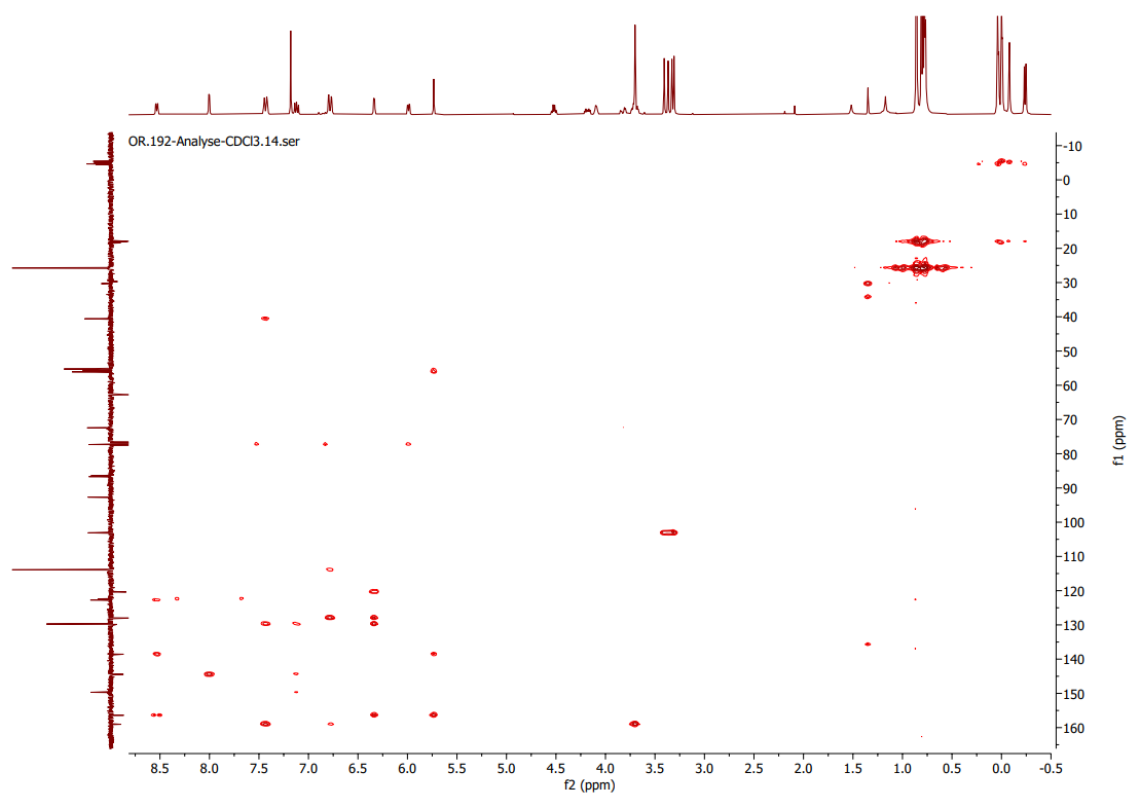
COSY spectrum of molecule **16** at 400 MHz



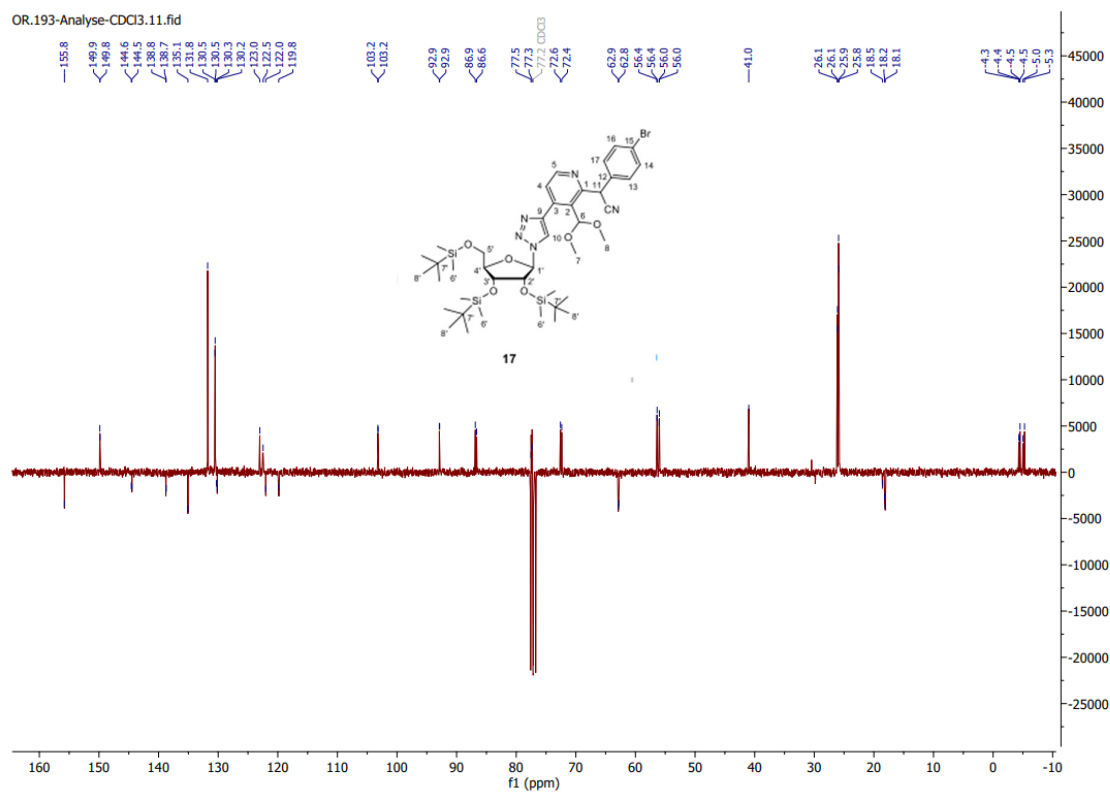
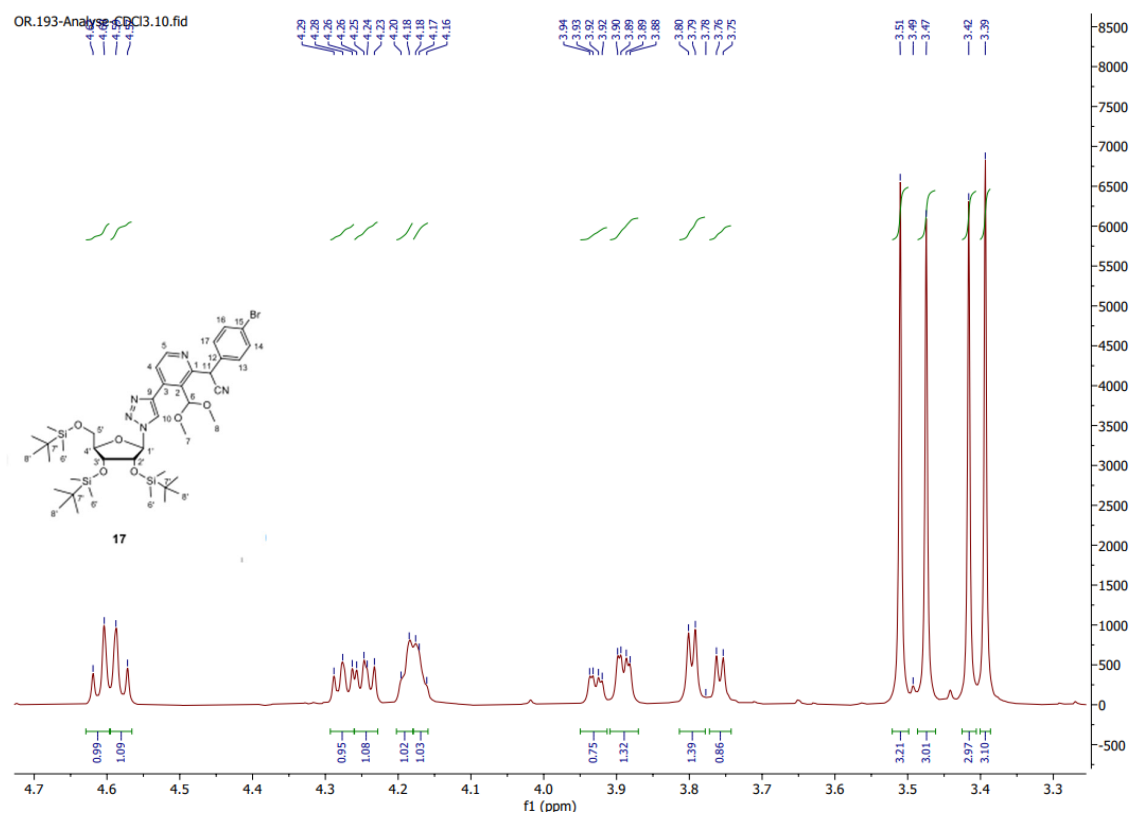
HSQC spectrum of molecule **16** at 400 MHz



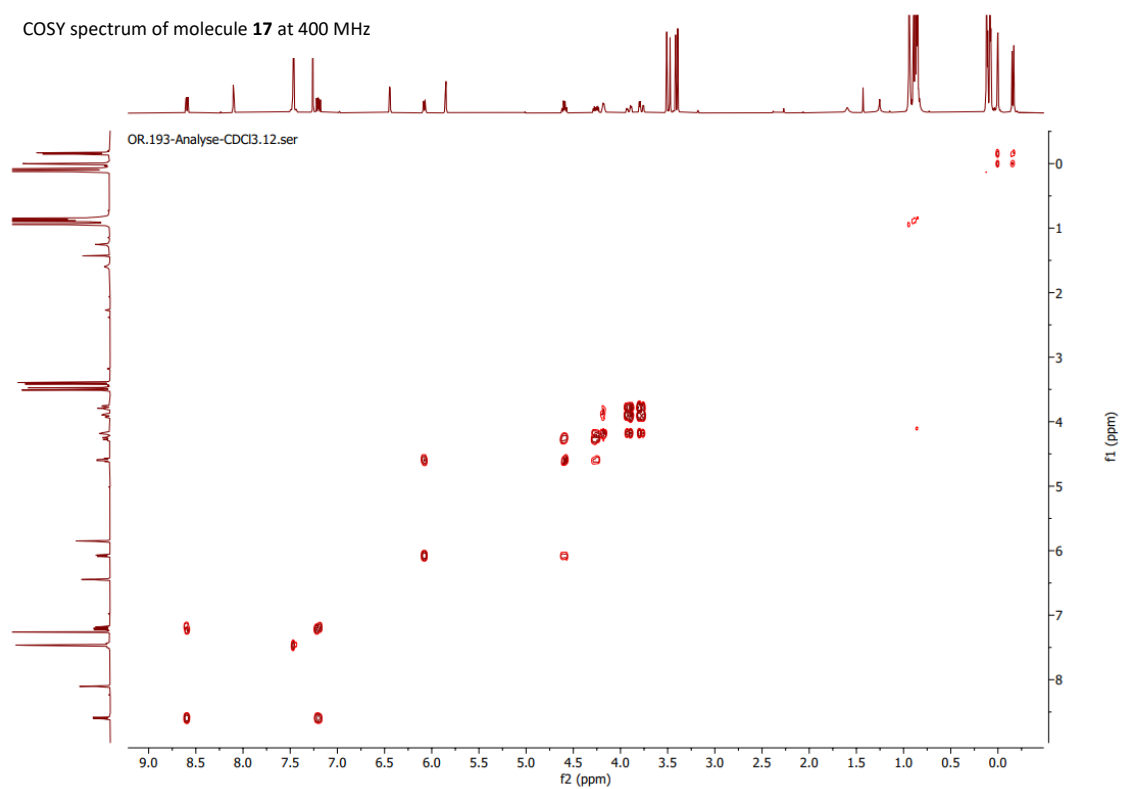
HMBC spectrum of molecule **16** at 400 MHz



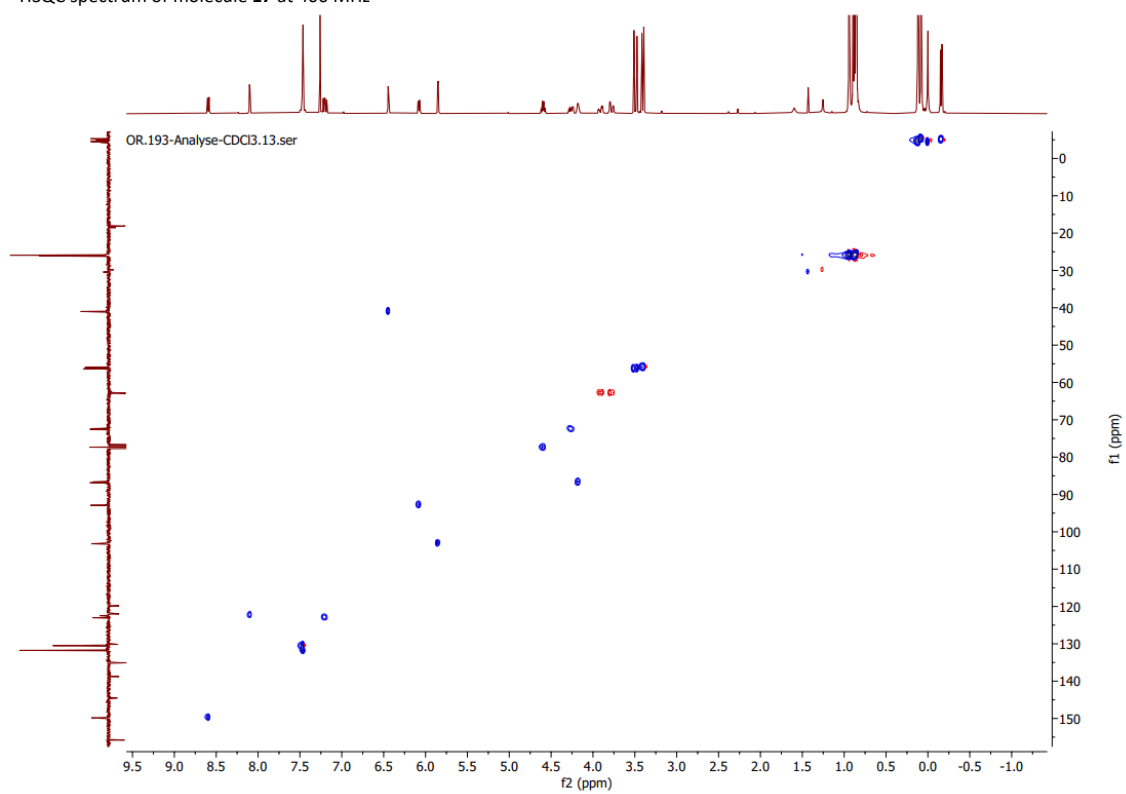
Zoom area 3 – 5 ppm



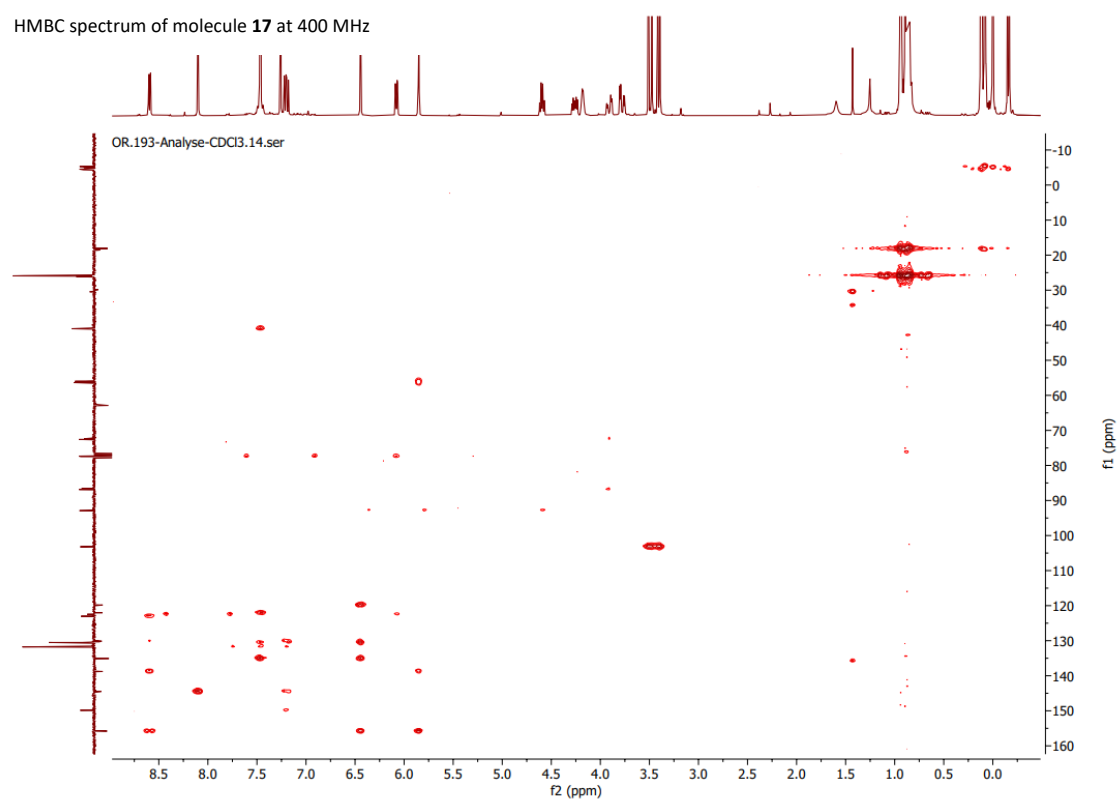
COSY spectrum of molecule **17** at 400 MHz



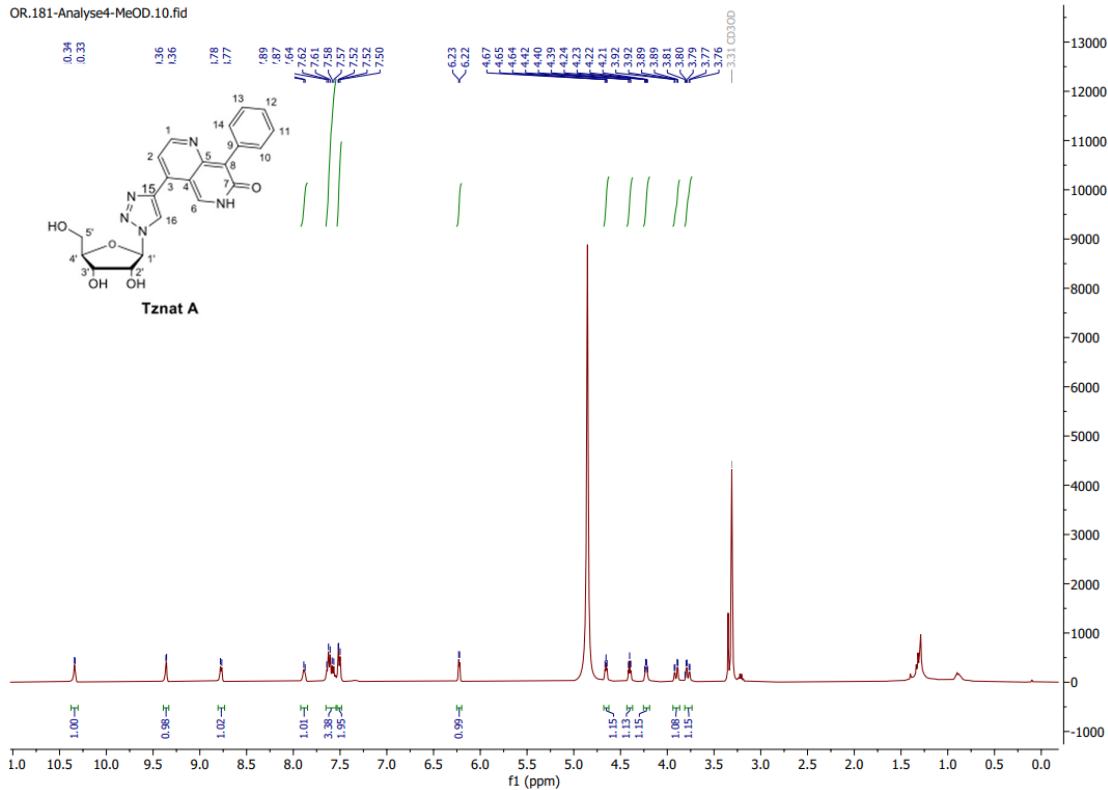
HSQC spectrum of molecule **17** at 400 MHz



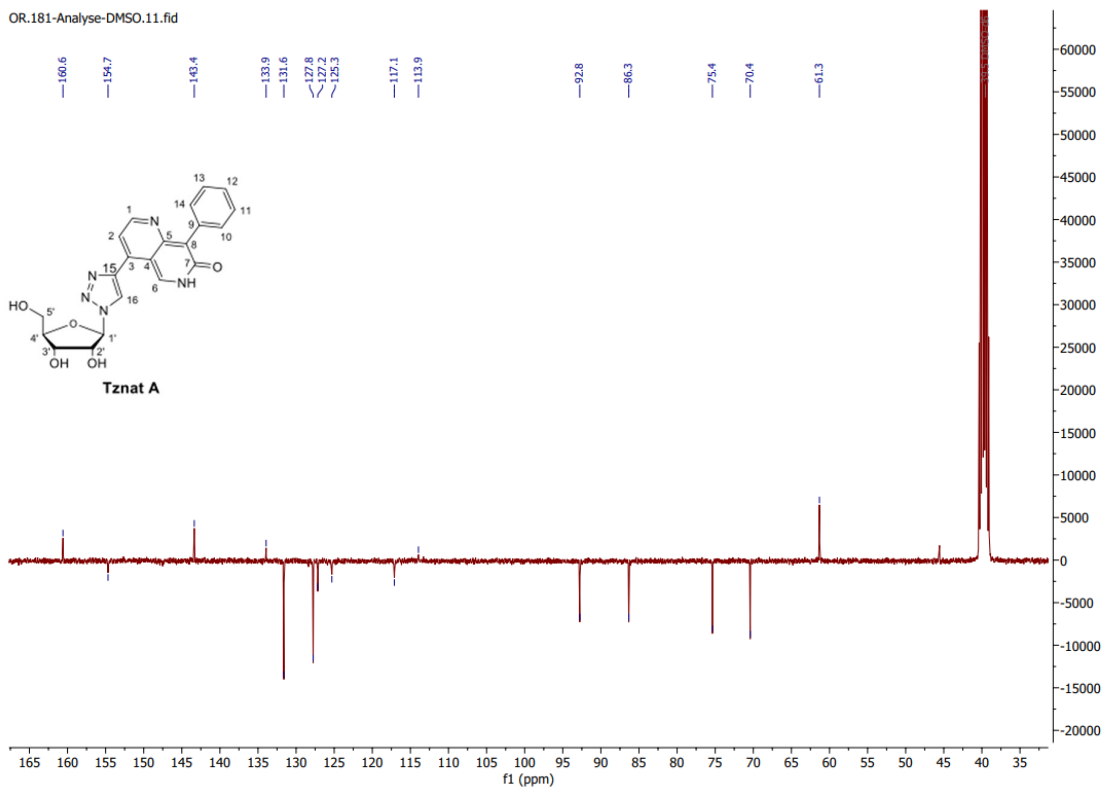
HMBC spectrum of molecule **17** at 400 MHz



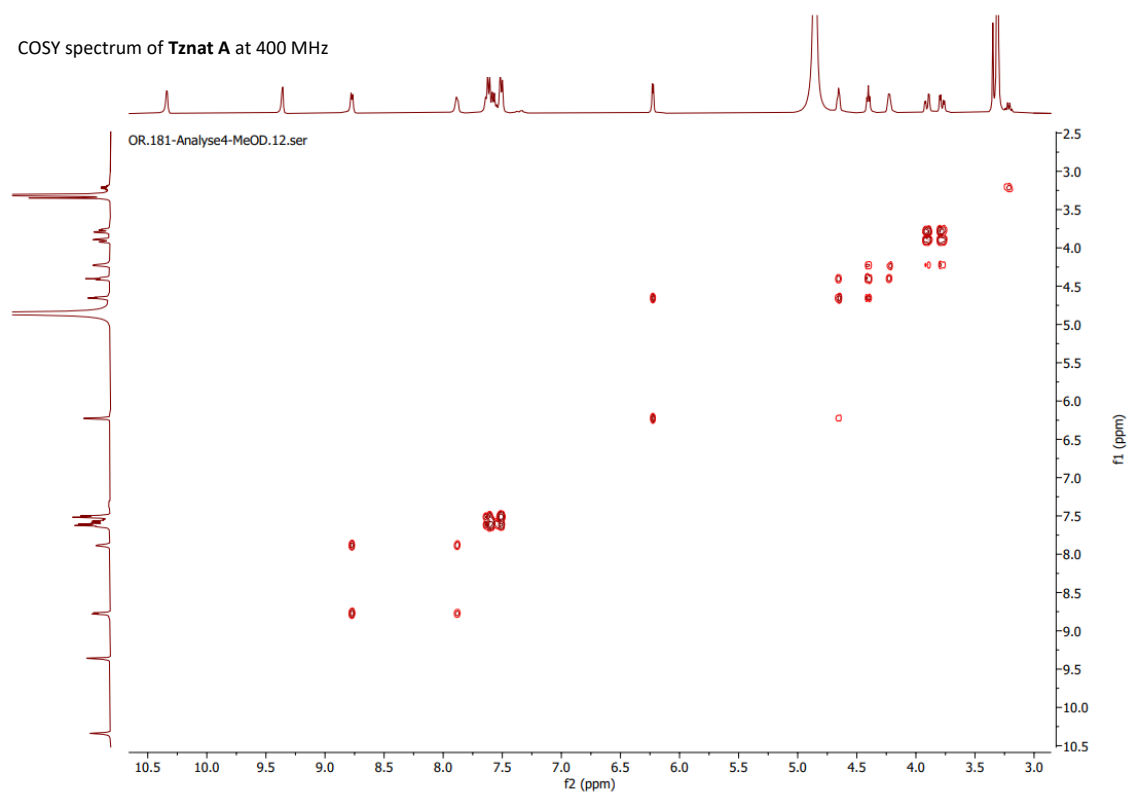
OR.181-Analyse4-MeOD.10.fid



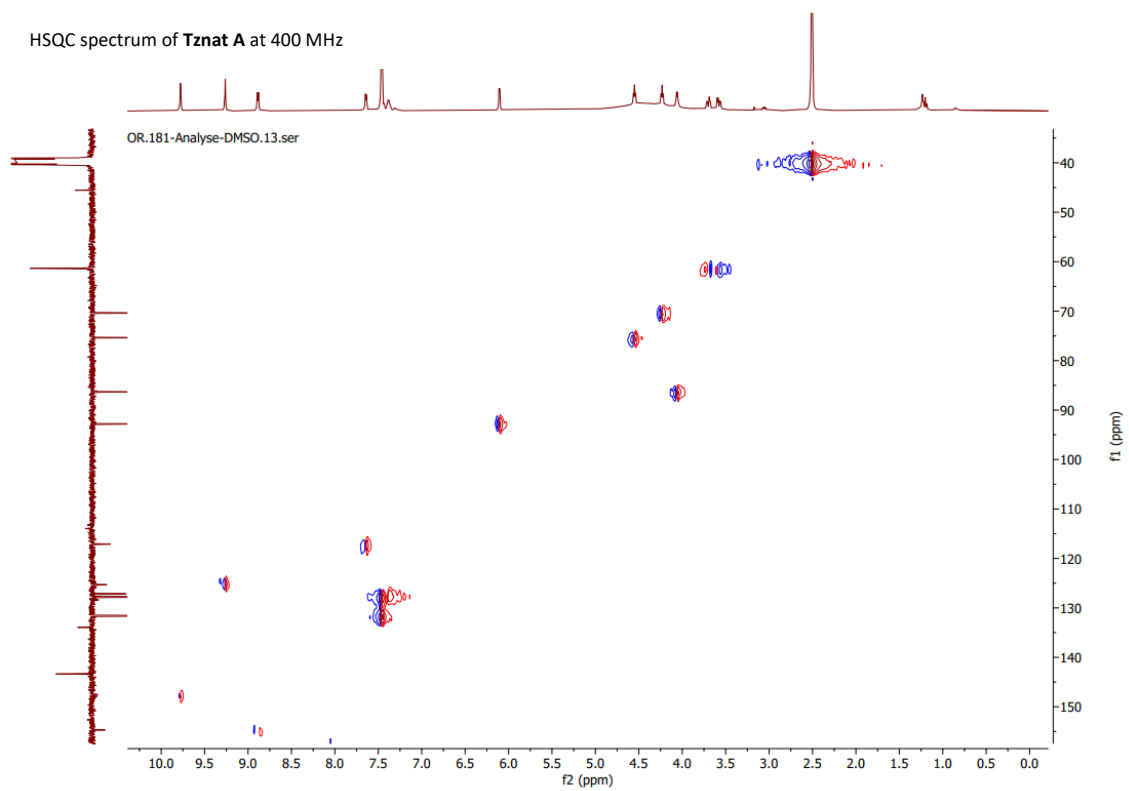
OR.181-Analyse-DMSO.11.fid



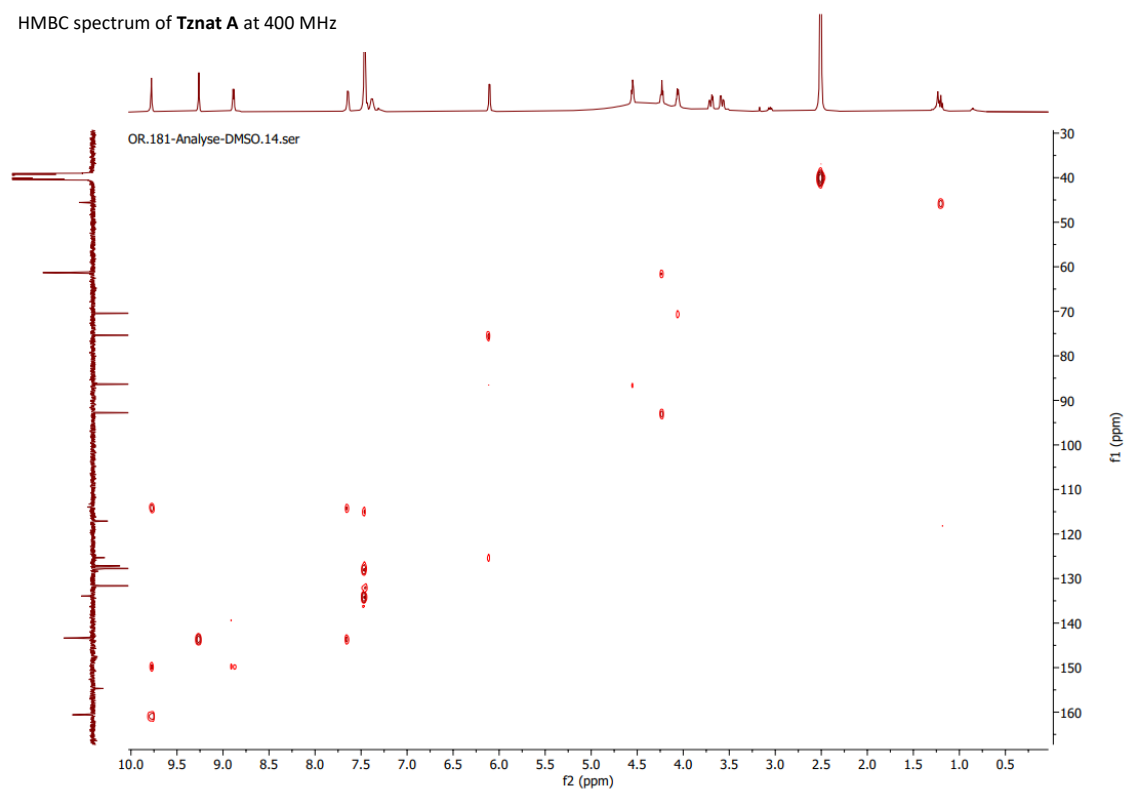
COSY spectrum of **Tznat A** at 400 MHz



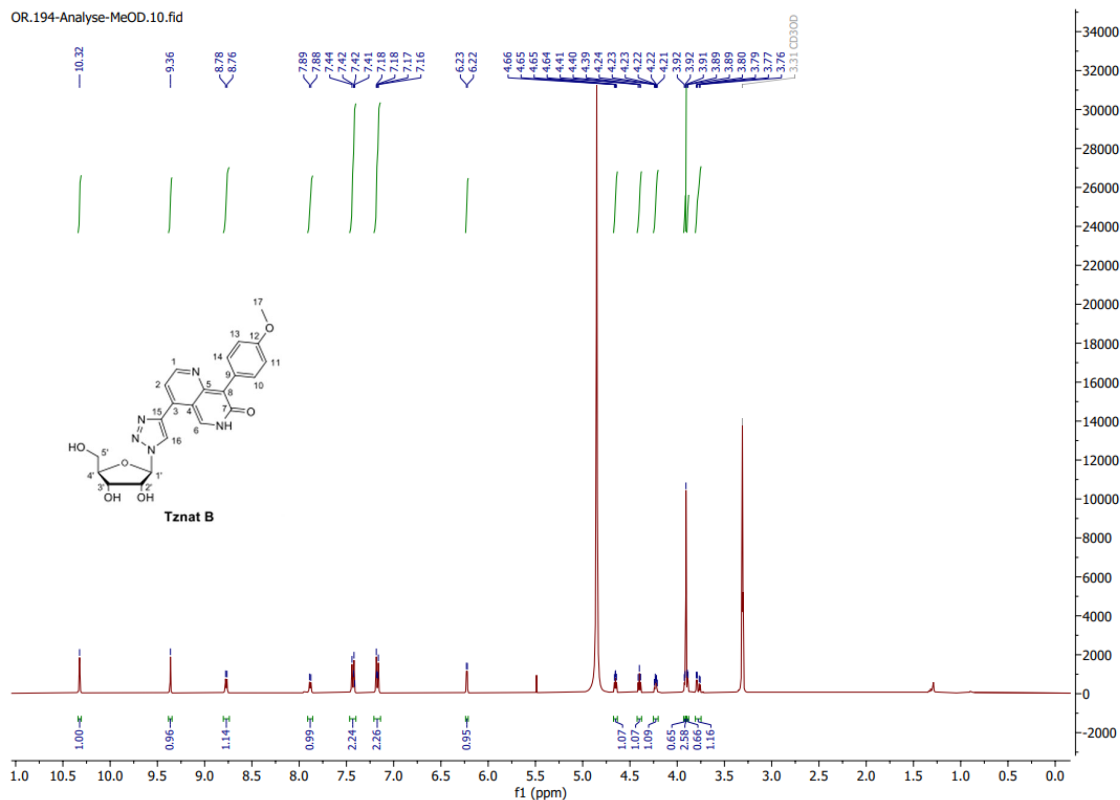
HSQC spectrum of **Tznat A** at 400 MHz



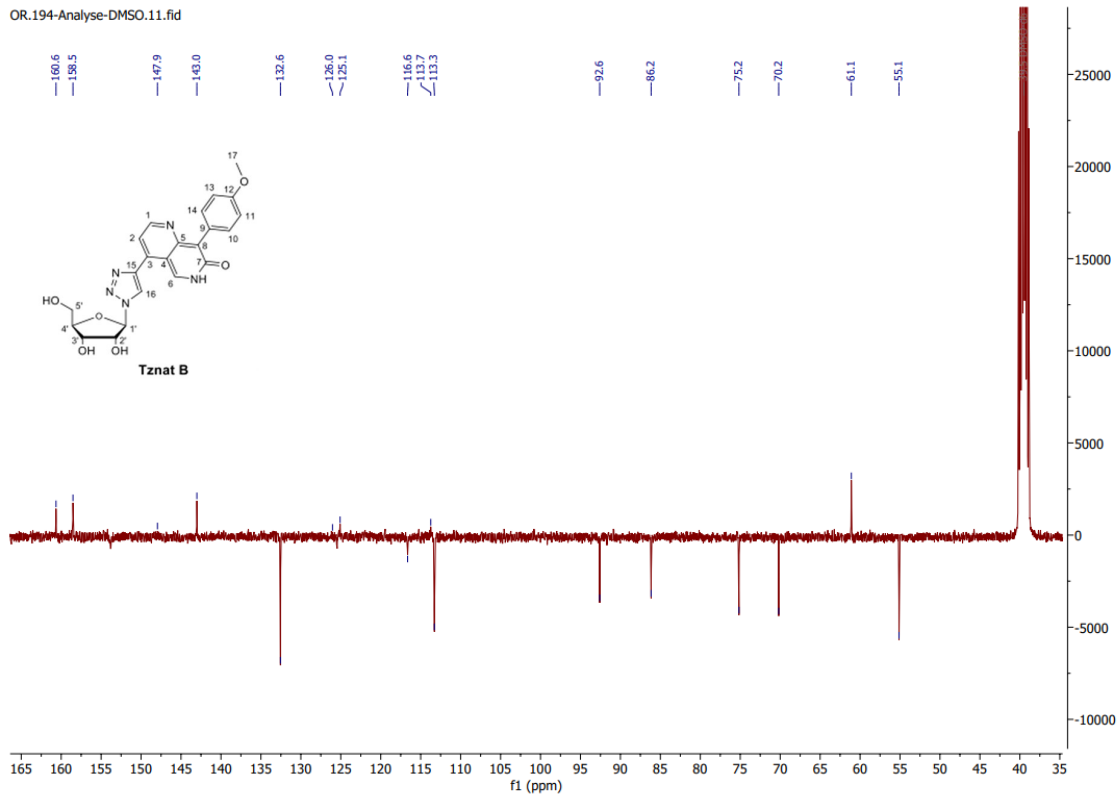
HMBC spectrum of **Tznat A** at 400 MHz



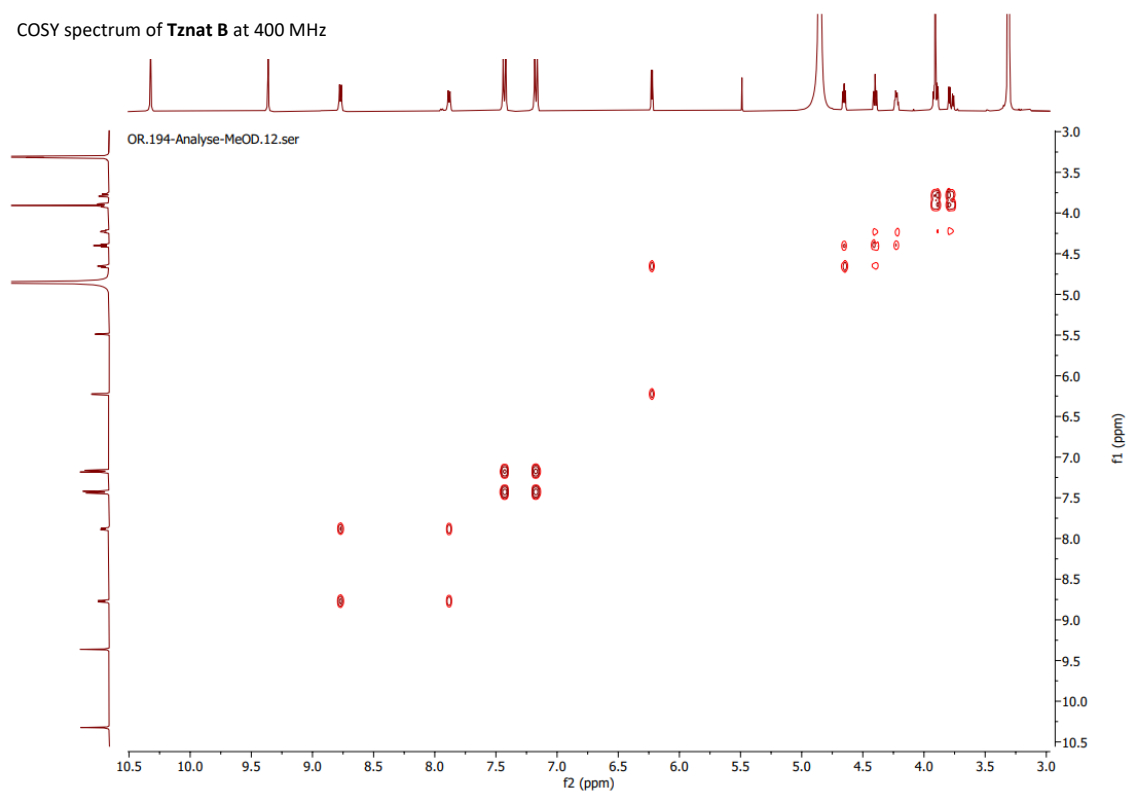
OR.194-Analyse-MeOD.10.fid



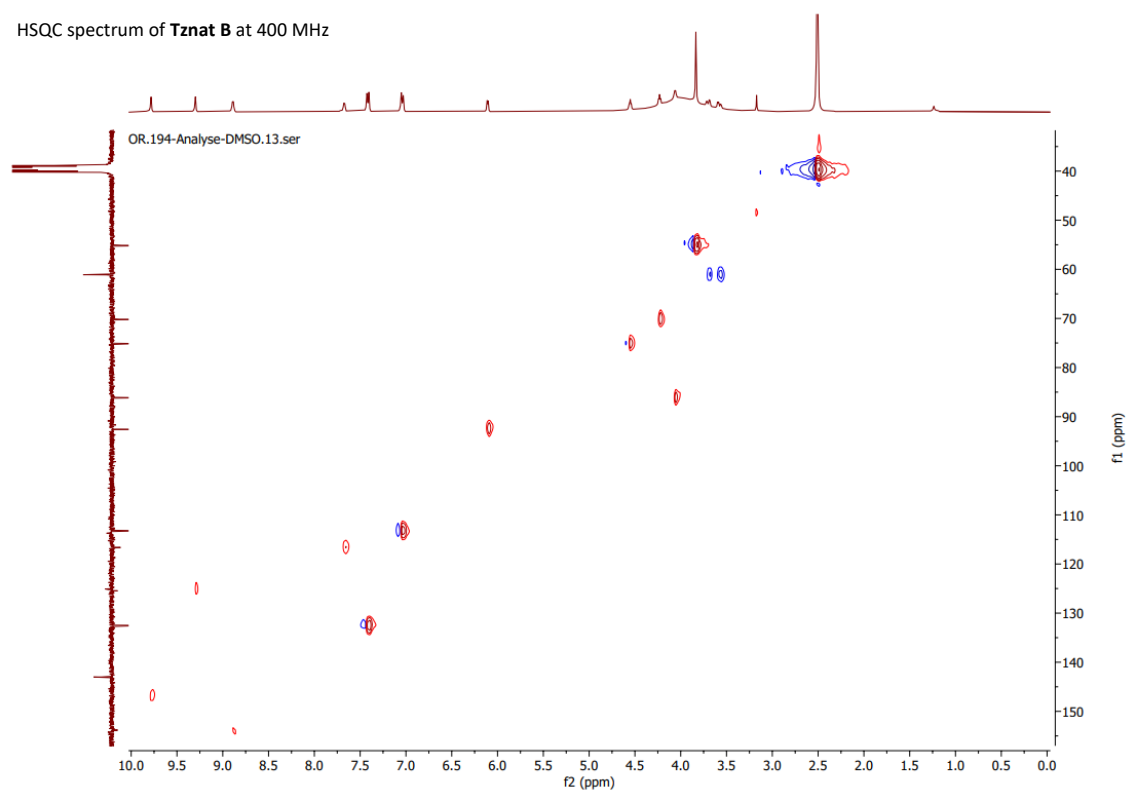
OR.194-Analyse-DMSO.11.fid



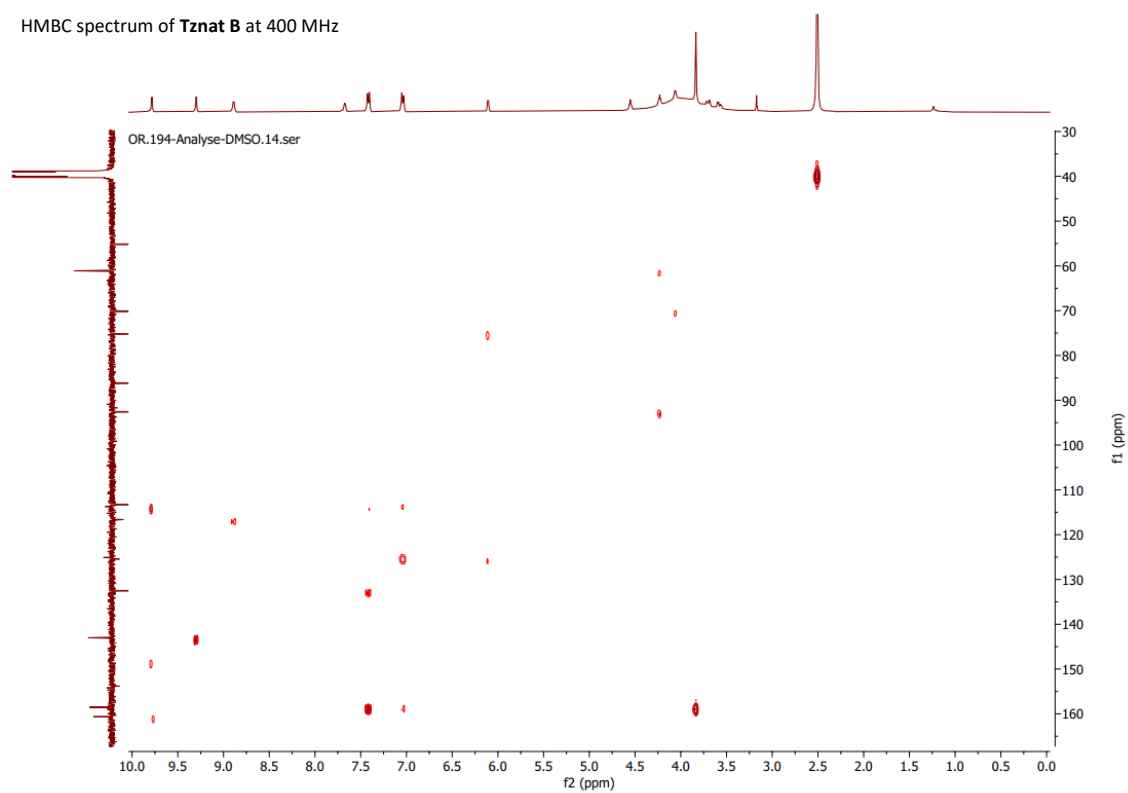
COSY spectrum of **Tznat B** at 400 MHz



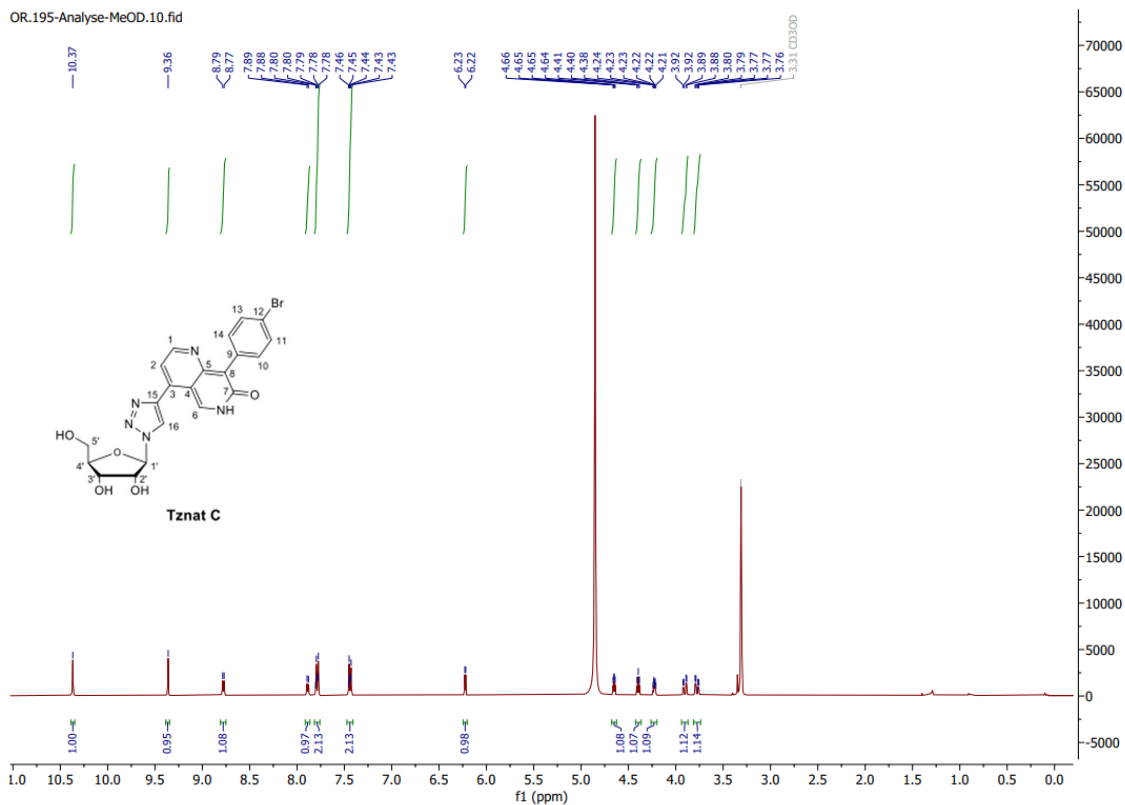
HSQC spectrum of **Tznat B** at 400 MHz



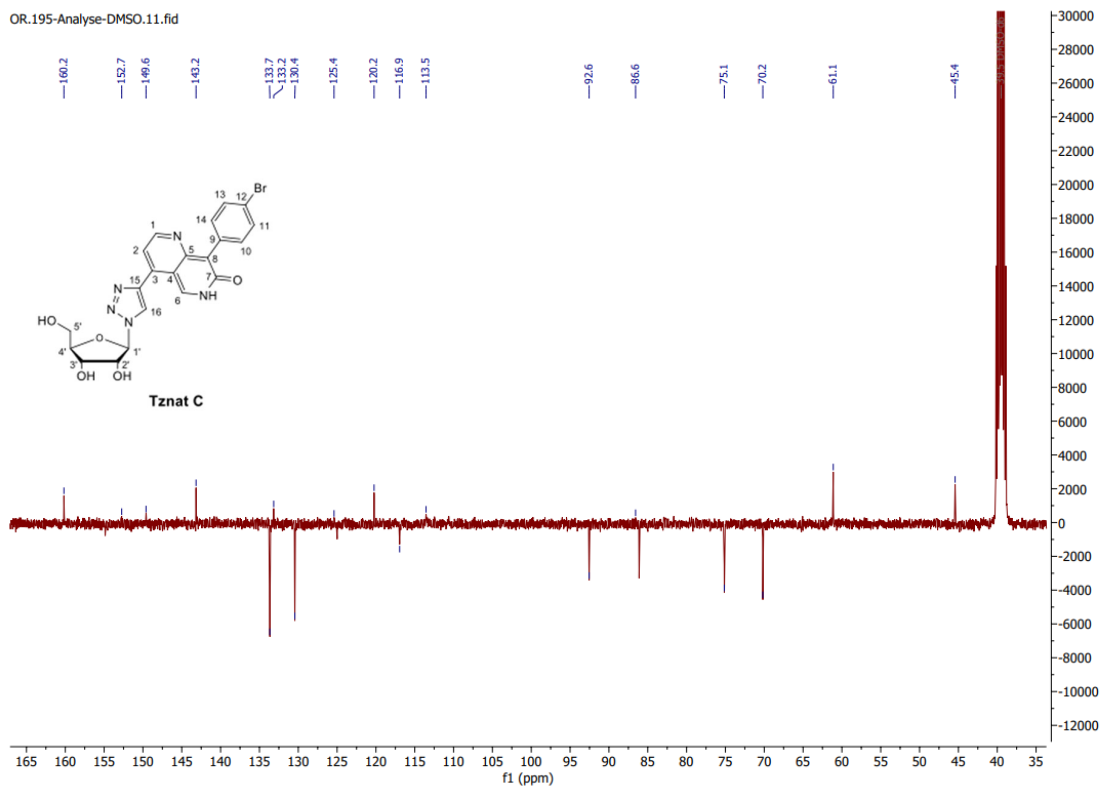
HMBC spectrum of **Tznat B** at 400 MHz



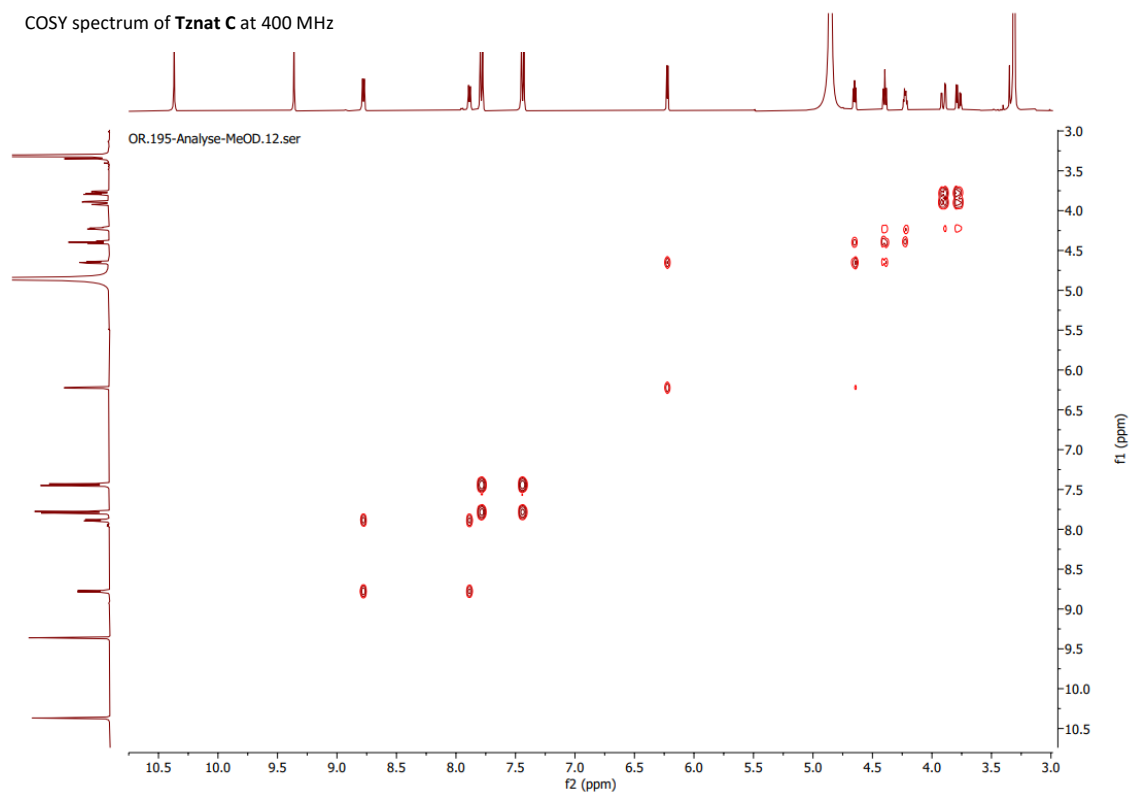
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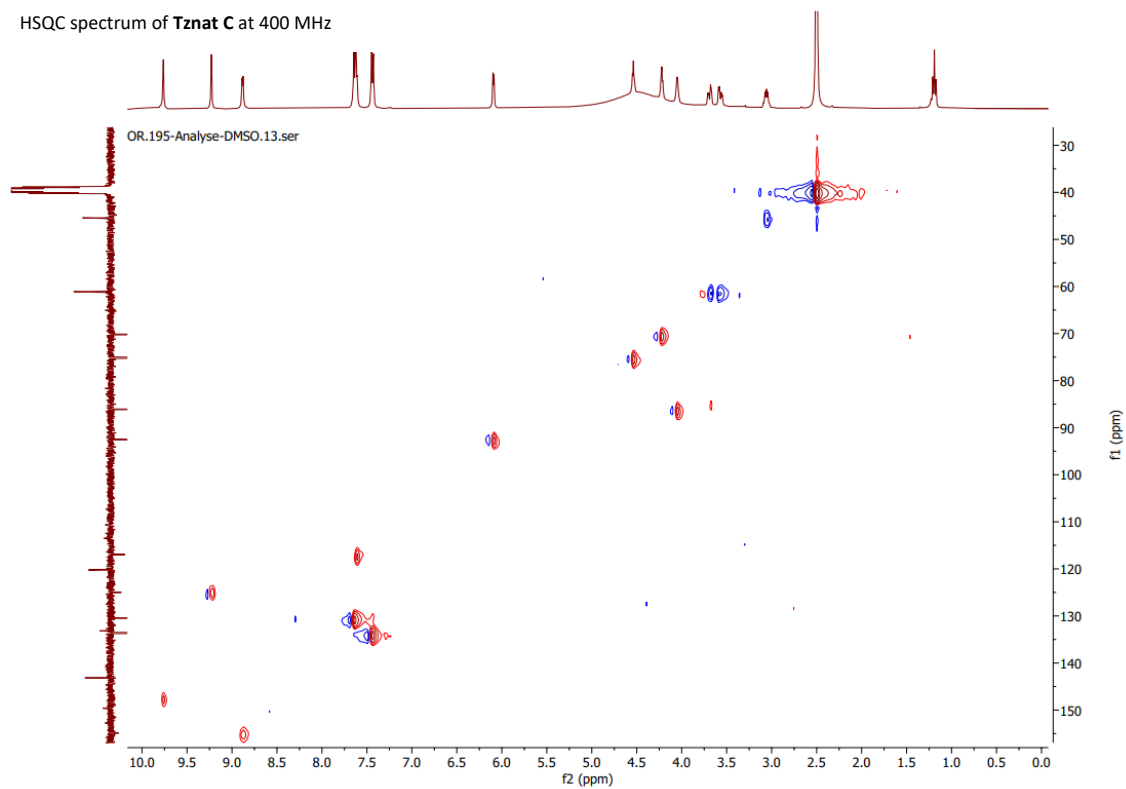
OR.195-Analyse-DMSO.11.fid



COSY spectrum of **Tznat C** at 400 MHz



HSQC spectrum of **Tznat C** at 400 MHz



HMBC spectrum of **Tznat C** at 400 MHz

