Supporting Information

1,6-Naphthyridin-7(6*H*)-ones: Synthesis and optical properties

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I - General information

All reagents and solvents were purchased from commercial suppliers, Sigma-Aldrich, TCI, Alfa-Aesar or fluorochem. All reactions were monitored by TLC on silica gel 60 F254 plates and revealed using UV lamp (l 254nm). Flash chromatography was carried out on a Merck silica gel 60 F 254. Reactions involving air or moisture sensitive reagents were carried out under an inert atmosphere (argon) with oven-dried glassware. THF was distillated over sodium/benzophenone. All final compounds were analyzed by high-resolution ESI mass spectrometry (HRMS) in MeOH using a LTQ-Orbitrap XL mass spectrometer (Thermo Scientific, San Jose, CA, USA) equipped with an electrospray ion source. NMR spectra were recorded on a Bruker Avance spectrometer at 300 or 400 MHz for ^{1}H and 100 MHz for ^{13}C. 2D NMR experiments such as ^{1}H-^{1}H COSY and ^{1}H-^{13}C HSQC experiments were performed to enable signal attributions. Chemical shifts (δ) are given in ppm, referenced to the residual solvent, coupling constant (*J*) are measured in hertz (Hz). Multiplicity is indicated as follows: s, singlet; d, doublet; t, triplet; q, quadruplet; dd, doublet of doublet; m, multiplet. The melting point were performed on electrothermal IA 91000. UV/Vis absorption spectra were measured using a Cary 50 (Varian) spectrophotometer at 20°C.Emission spectra were performed on JASCO J-815 CD spectrofluorometer at 20°C.

II - Absorption and emission spectra

The absorption and emission spectra of compound 4a-4g were recorded in solution at a concentration of $c = 10^{-4}$ mol.L^{-1} for the absorption and at a concentration of $c = 10^{-5}$ mol.L^{-1} for the emission. The excitation was performed at the maximum absorption wavelength for each compound.

1. Normalized absorption and emission spectra of compound 4a-4g in PBS solution.

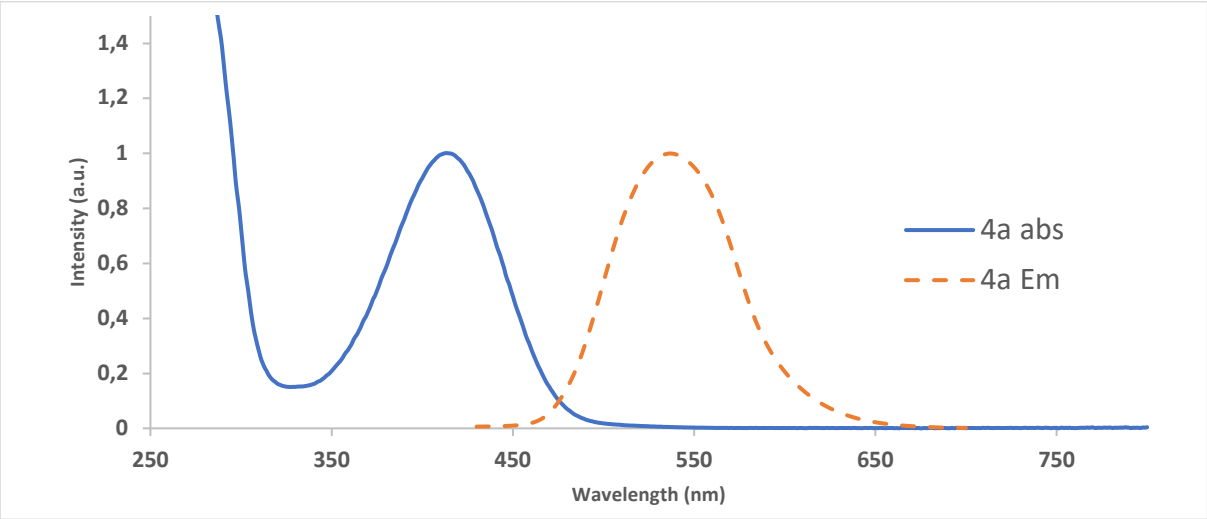


Figure S1: normalized absorption et emission spectra of **4a** in PBS solution.

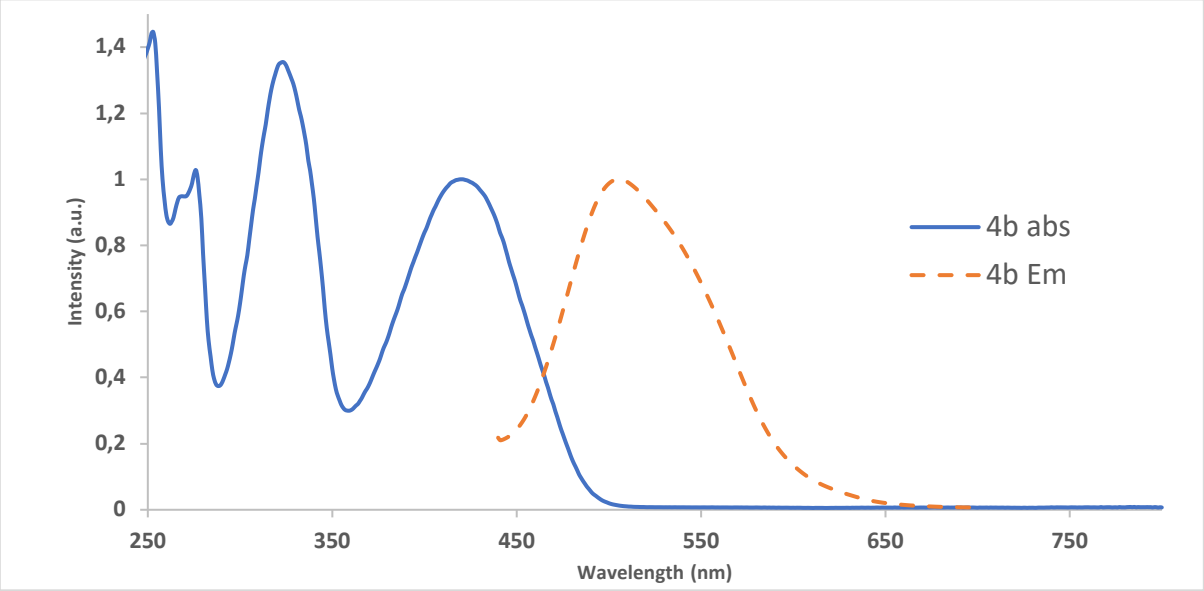


Figure S2: normalized absorption et emission spectra of **4b** in PBS solution.

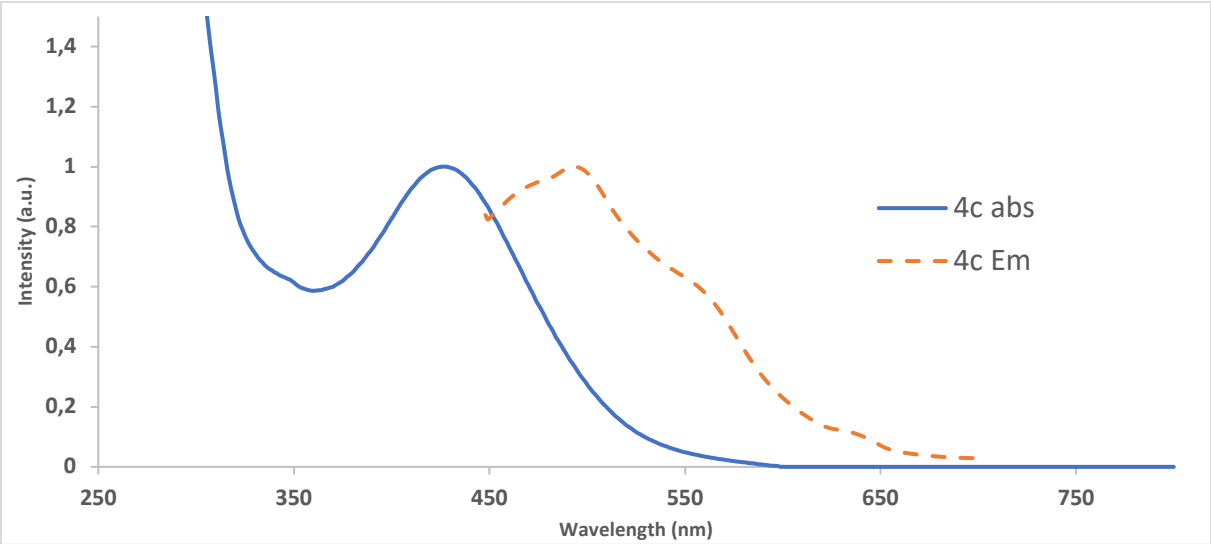


Figure S3: normalized absorption et emission spectra of **4c** in PBS solution.

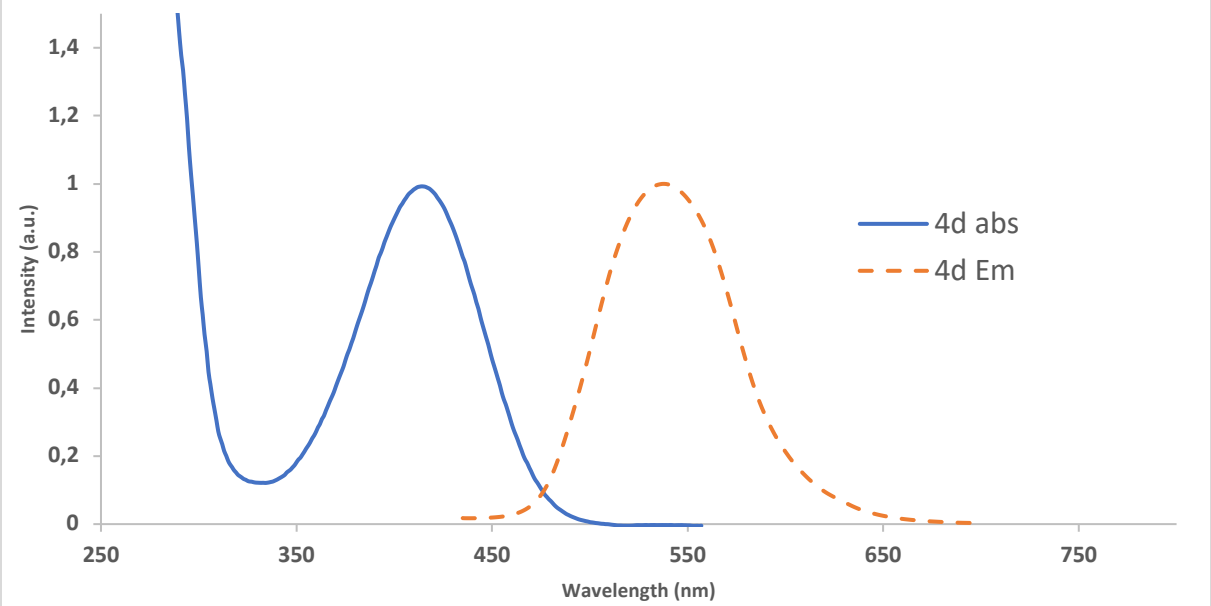


Figure S4: normalized absorption et emission spectra of **4d** in PBS solution.

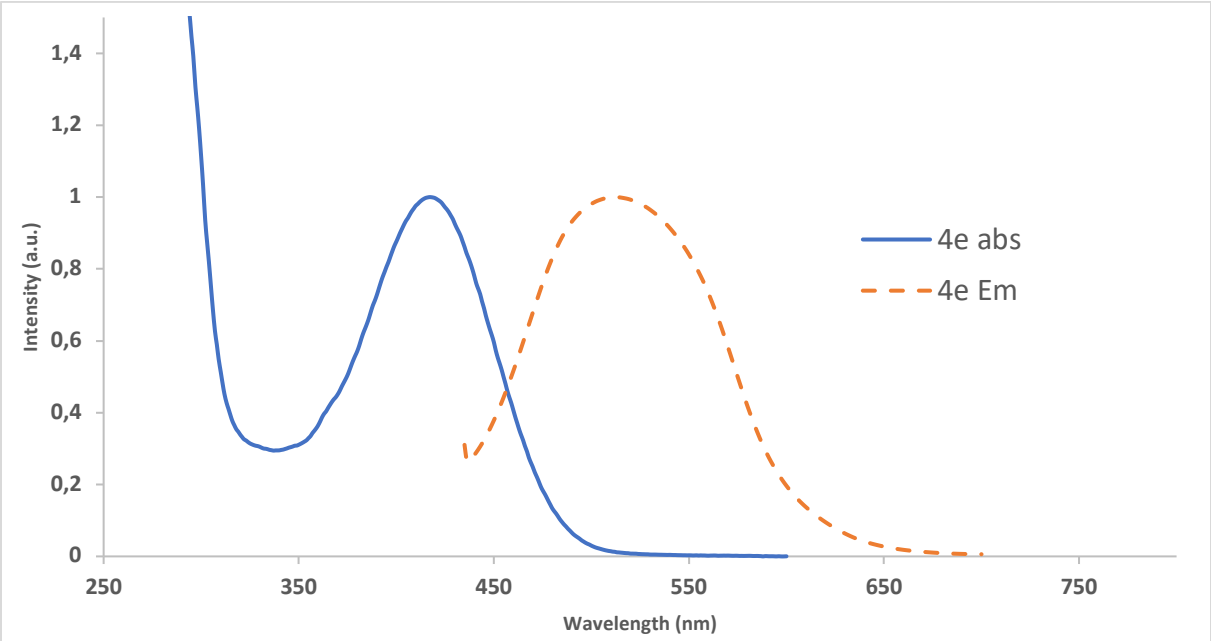


Figure S5: normalized absorption et emission spectra of **4e** in PBS solution.

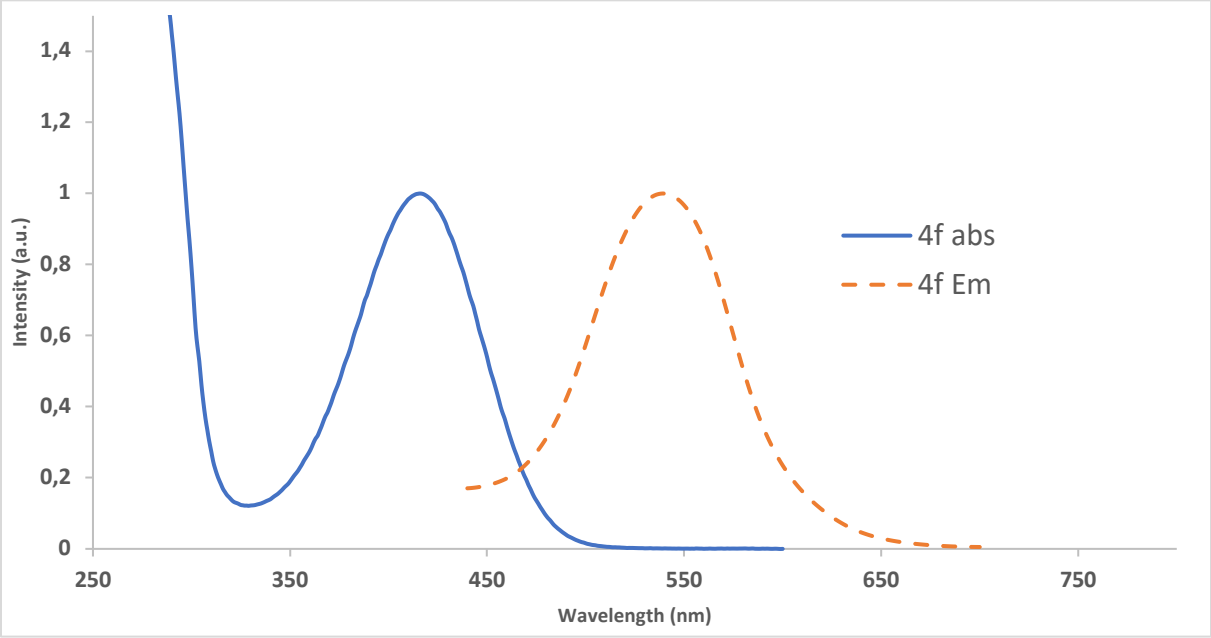


Figure S6: normalized absorption et emission spectra of **4f** in PBS solution.

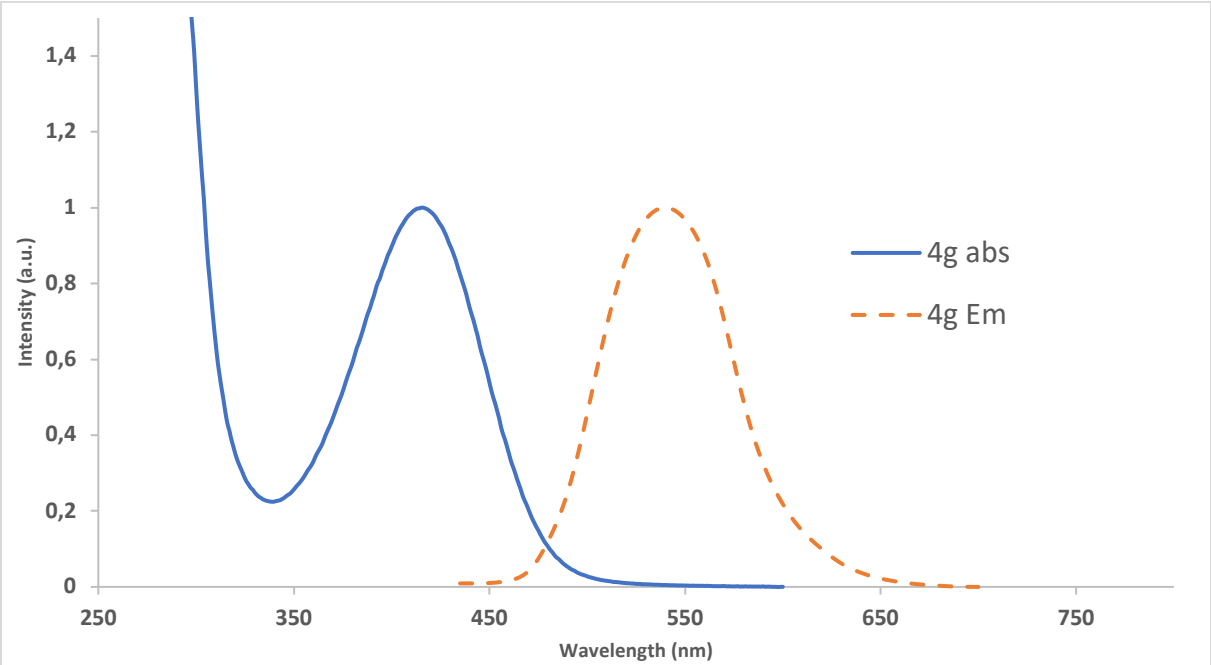


Figure S7: normalized absorption et emission spectra of **4f** in PBS solution.

2. Absorption spectra of compound 4a in various solvents.

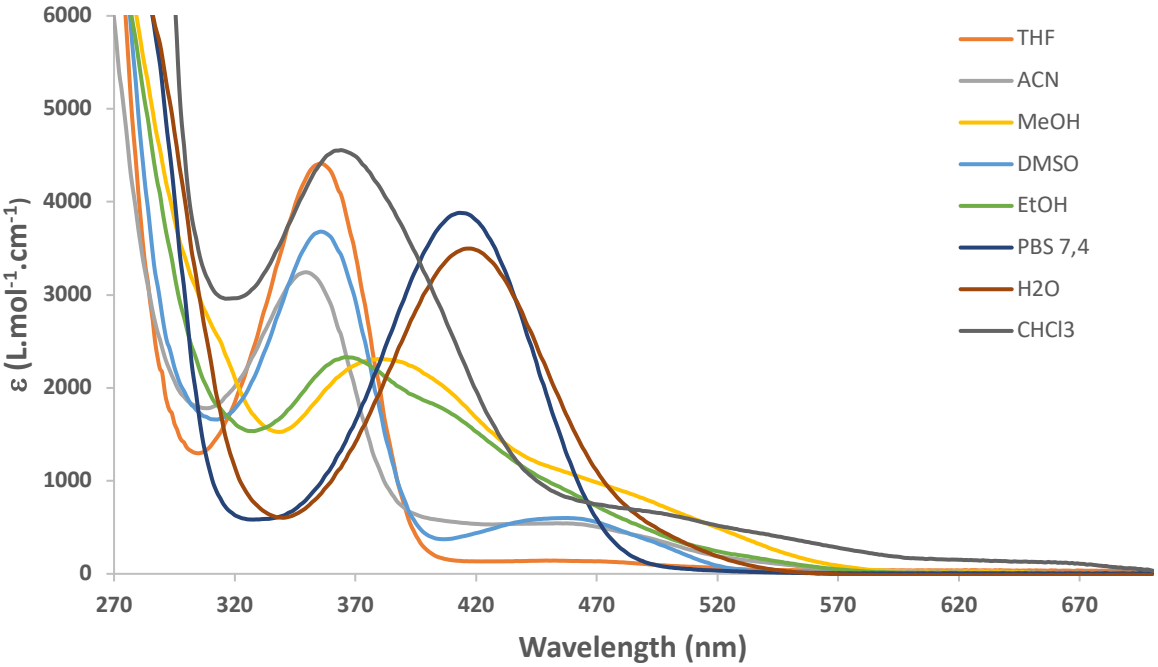


Figure S8: absorption spectra of **4a** in various solvents.

3. Normalized emission spectra of compound 4a in various solvents.

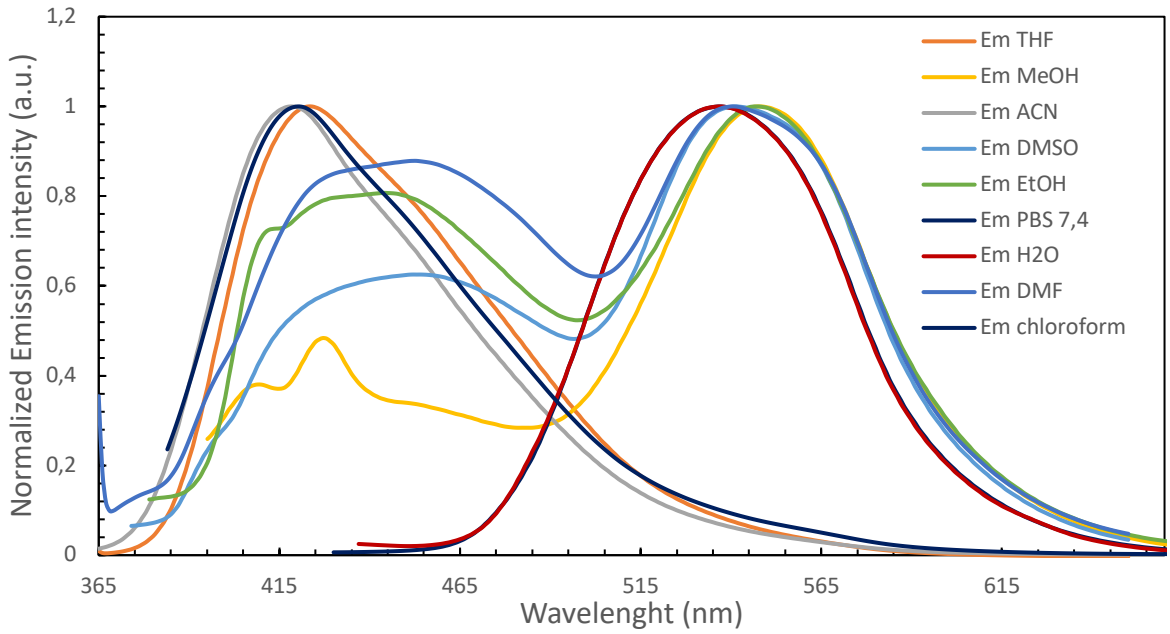


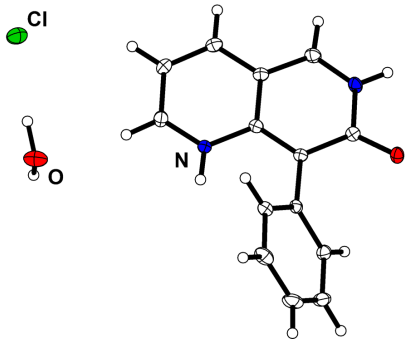
Figure S9: normalized emission spectra of **4a** in various solvents.

III - X-Ray crystal structure determination.

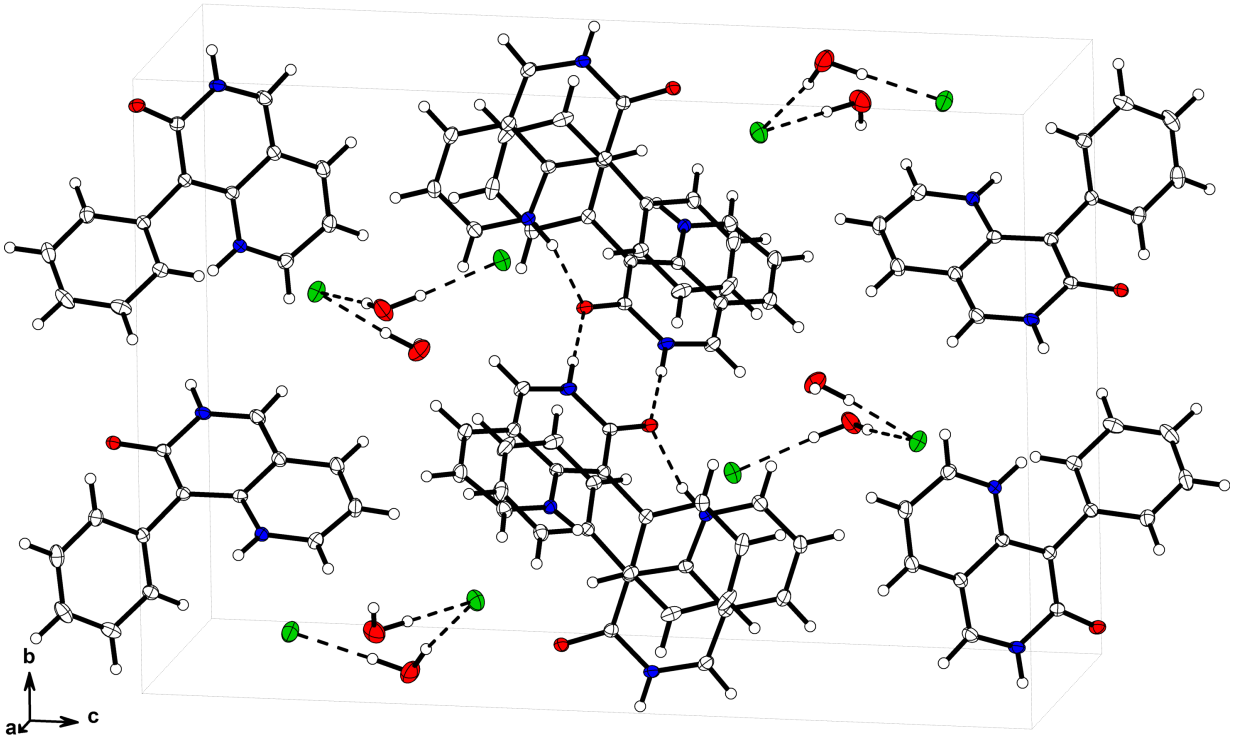
A single crystal was selected, mounted and transferred into a cold nitrogen gas stream. Intensity data was collected with a Bruker Kappa-APEX2 system using micro-source Cu-Kα radiation. Unit-cell parameters determination, data collection strategy, integration and absorption correction were carried out with the Bruker APEX2 suite of programs. The structure was solved with SHELXT and refined anisotropically by full-matrix least-squares methods with SHELXL using WinGX. The structure was deposited at the Cambridge Crystallographic Data Centre with number CCDC 2193379 and can be obtained free of charge via www.ccdc.cam.ac.uk.

Crystal data for 4a. $C_{14}H_{13}ClN_2O_2$, orthorhombic P b c a, a = 7.6114(4) Å, b = 15.1521(7) Å, c = 21.9238(11) Å, α = β = γ = 90°, V = 2528.4(2) Å^3, Z = 8, reddish orange needle 0.35 × 0.05 × 0.05 mm^3, μ = 2.677 mm^{-1}, min / max transmission = 0.50 / 0.95, T= 200(1) K, λ = 1.54178 Å, θ range = 4.04° to 66.59°, 16493 reflections measured, 2218 independent, R_{int} = 0.0351, completeness = 0.997, 175 parameters, 0 restraints, final R indices R1 [I>2σ(I)] = 0.0311 and wR2 (all data) = 0.0881, GOF on F^2 = 1.049, largest difference peak / hole = 0.19 / -0.29 e·Å^{-3}.

Asymmetric unit of 4a. Thermal ellipsoids drawn at 30% probability.



Crystal packing of 4a. Hydrogen bonds represented as dashed lines.

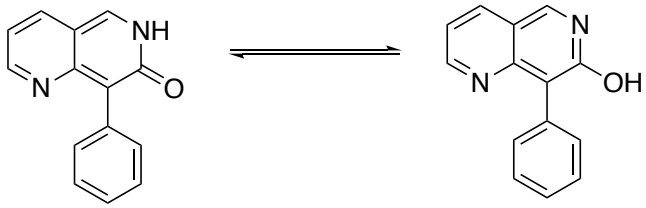


Bond lengths for 4a.		Bond angles for 4a.		Hydrogen bond lengths for 4a.	
O(1)-C(1)	1.262(2) Å	C(5)-N(1)-C(1)	125.33(12)°	N(1)···O(1)	2.742(2) Å
N(1)-C(5)	1.325(2) Å	C(8)-N(2)-C(3)	123.18(12)°	N(2)···O(1)	2.796(2) Å
N(1)-C(1)	1.393(2) Å	O(1)-C(1)-N(1)	117.56(12)°	O(2)···Cl(1)	3.088(2) Å
N(2)-C(8)	1.320(2) Å	O(1)-C(1)-C(2)	125.59(13)°	O(2)···Cl(1)	3.230(2) Å
N(2)-C(3)	1.382(2) Å	N(1)-C(1)-C(2)	116.84(12)°		
C(1)-C(2)	1.418(2) Å	C(3)-C(2)-C(1)	117.97(12)°		
C(2)-C(3)	1.389(2) Å	C(3)-C(2)-C(9)	123.26(12)°		
C(2)-C(9)	1.489(2) Å	C(1)-C(2)-C(9)	118.73(12)°		
C(3)-C(4)	1.424(2) Å	N(2)-C(3)-C(2)	121.05(12)°		
C(4)-C(5)	1.391(2) Å	N(2)-C(3)-C(4)	116.17(12)°		
C(4)-C(6)	1.415(2) Å	C(2)-C(3)-C(4)	122.76(13)°		
C(6)-C(7)	1.366(2) Å	C(5)-C(4)-C(6)	122.92(13)°		
C(7)-C(8)	1.399(2) Å	C(5)-C(4)-C(3)	116.87(13)°		
C(9)-C(10)	1.394(2) Å	C(6)-C(4)-C(3)	120.21(13)°		
C(9)-C(14)	1.397(2) Å	N(1)-C(5)-C(4)	119.98(13)°		
C(10)-C(11)	1.385(2) Å	C(7)-C(6)-C(4)	119.79(14)°		
C(11)-C(12)	1.382(3) Å	C(6)-C(7)-C(8)	118.65(14)°		
C(12)-C(13)	1.380(3) Å	N(2)-C(8)-C(7)	121.64(14)°		
C(13)-C(14)	1.390(2) Å	C(10)-C(9)-C(14)	119.38(13)°		
		C(10)-C(9)-C(2)	120.11(13)°		
		C(14)-C(9)-C(2)	120.48(12)°		
		C(11)-C(10)-C(9)	119.95(15)°		
		C(12)-C(11)-C(10)	120.60(15)°		
		C(13)-C(12)-C(11)	119.74(14)°		
		C(12)-C(13)-C(14)	120.48(15)°		
		C(13)-C(14)-C(9)	119.81(14)°		

IV - Theoretical calculations

(Time-dependent(TD))-Density Functional Theory (DFT) including geometry optimizations, frequency and single-point energy calculations were performed with the Minnesota M06-2X hybrid functional[i] coupled to the correlation consistent augmented aug-cc-pvdz basis set.[ii] The DMF or the THF solvent were mimicked with the Polarizable Continuum Model (PCM) model.[iii] Definitions of the basis sets were obtained from the *Basis Set Exchange* library.[iv] Computed structures and absorption spectra shown in this work have been depicted using the Chemcraft software.[v]

The emission band from the first singlet excited state of lactam and lactim taking into account the solvent effect was computed in several steps using the external iteration approach[vi] to include the solvation effects of the various implied states (ground state, (vertical and relaxed) 1st excited state).



lactam-4a lactim-4a

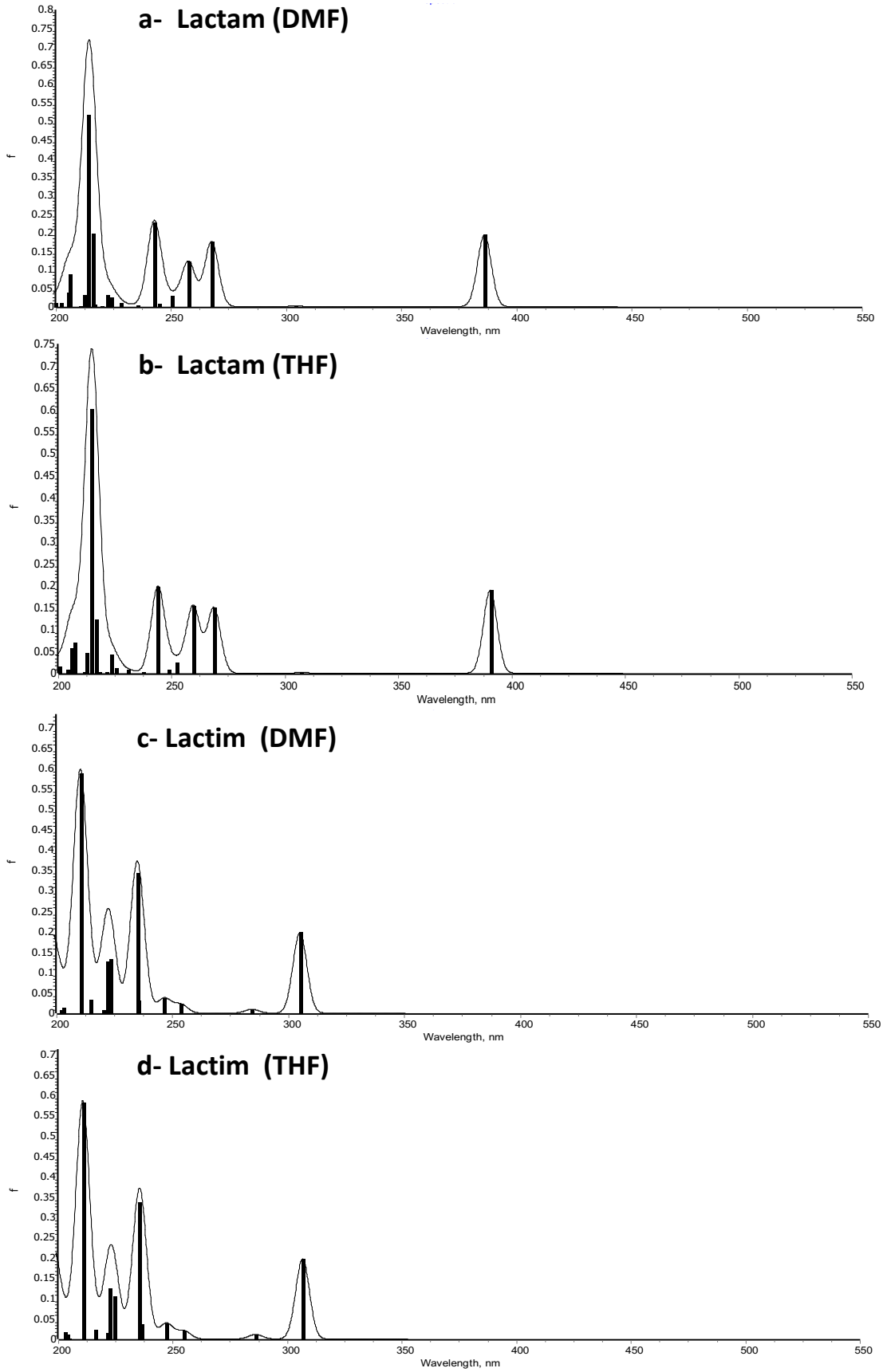


Figure S10: Calculated absorption spectra of **a-** and **b-** lactam (in DMF and THF, resp.) and **c-** and **d-** lactim (in DMF and THF, resp.) isomers in the 200-550 nm wavelength range.

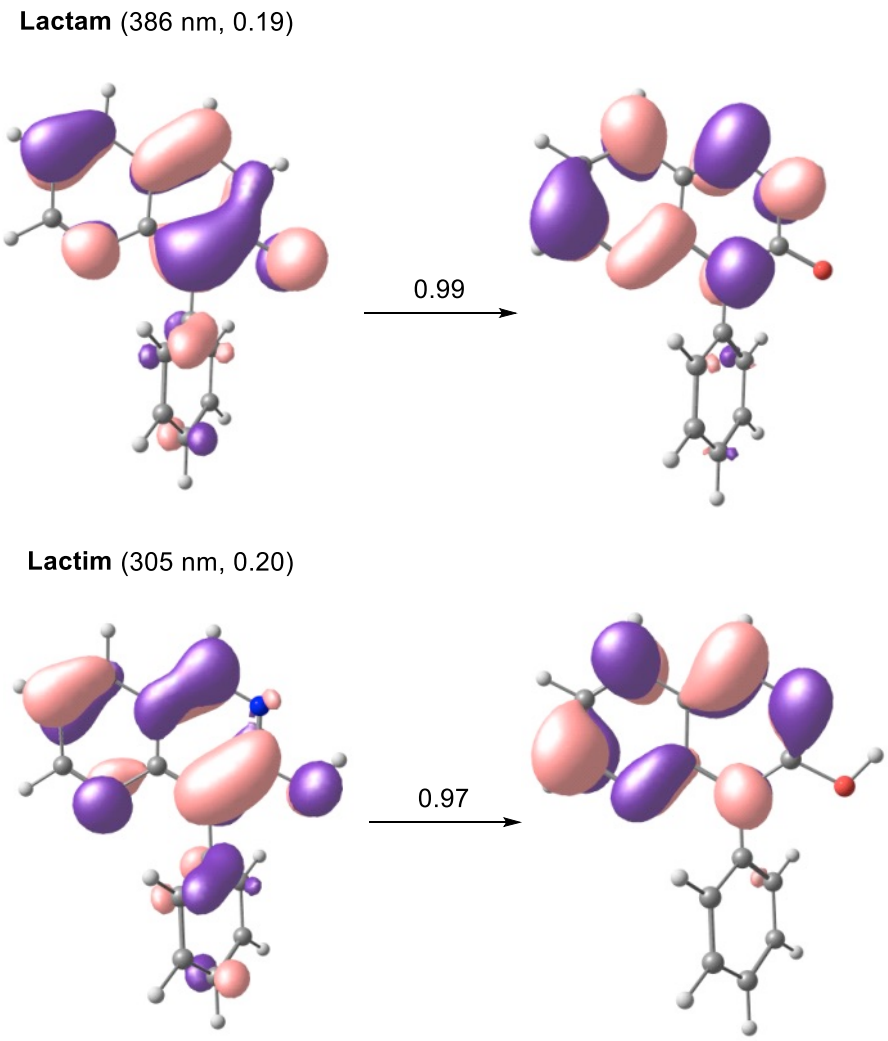


Figure S11: Natural transition orbitals for the first transitions of **4a** lactam and lactim tautomers. The excitation energy and the corresponding oscillator strength are indicated in parentheses and the associated weights above the arrows (isodensity surface 0.04).

Table S1. Calculated absorption and emission maxima (1st singlet excited state) of lactam and lactim isomers in DMF and THF.

	solvent	λ_{abs} (nm)	λ_{em} (nm)
Lactam	DMF	364	474
	THF	372	474
Lactim	DMF	303	409
	THF	306	405

Table S2. Calculated electronic (E_{el}) and zero-point (ZPE) energies (in hartrees, H) of optimized structures of the lactam and lactim in DMF and THF.

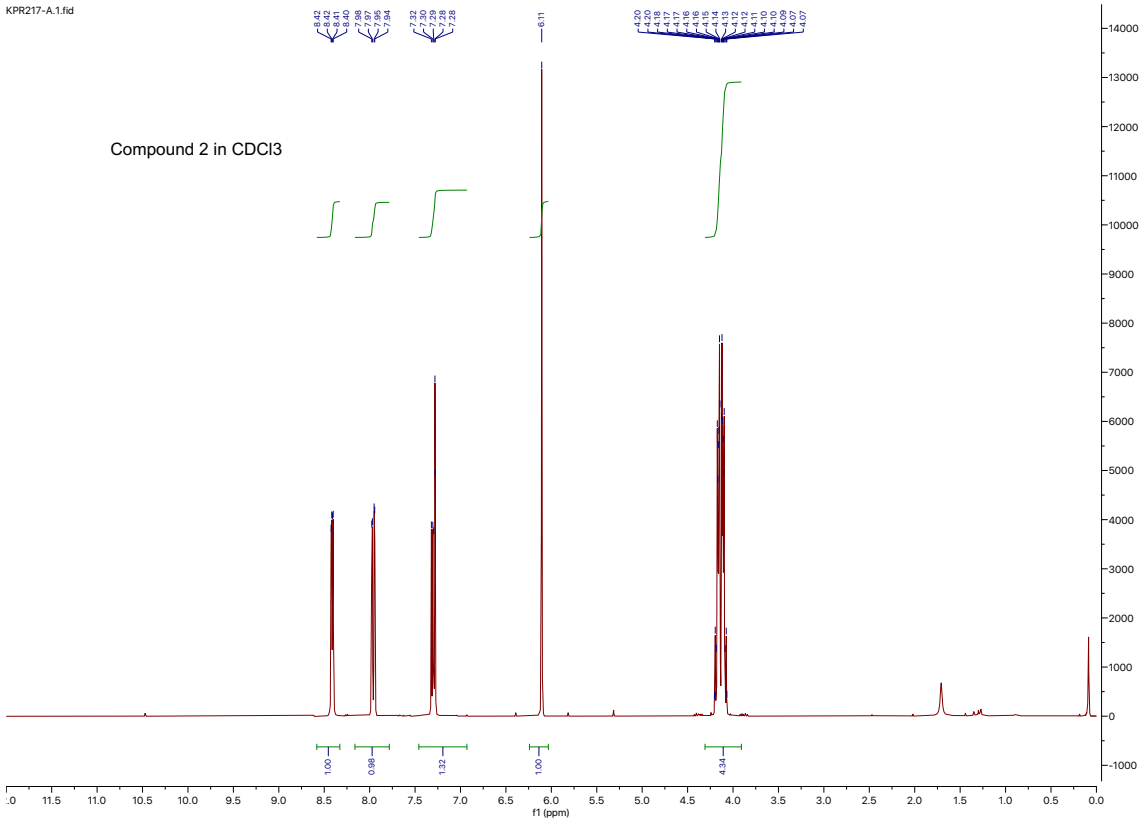
	solvent	E_{el}	ZPE
Lactam	DMF	-724.2323586	0.2112264
	THF	-724.2284362	0.2111945
Lactim	DMF	-724.2354407	0.2107176
	THF	-724.2333085	0.2108523

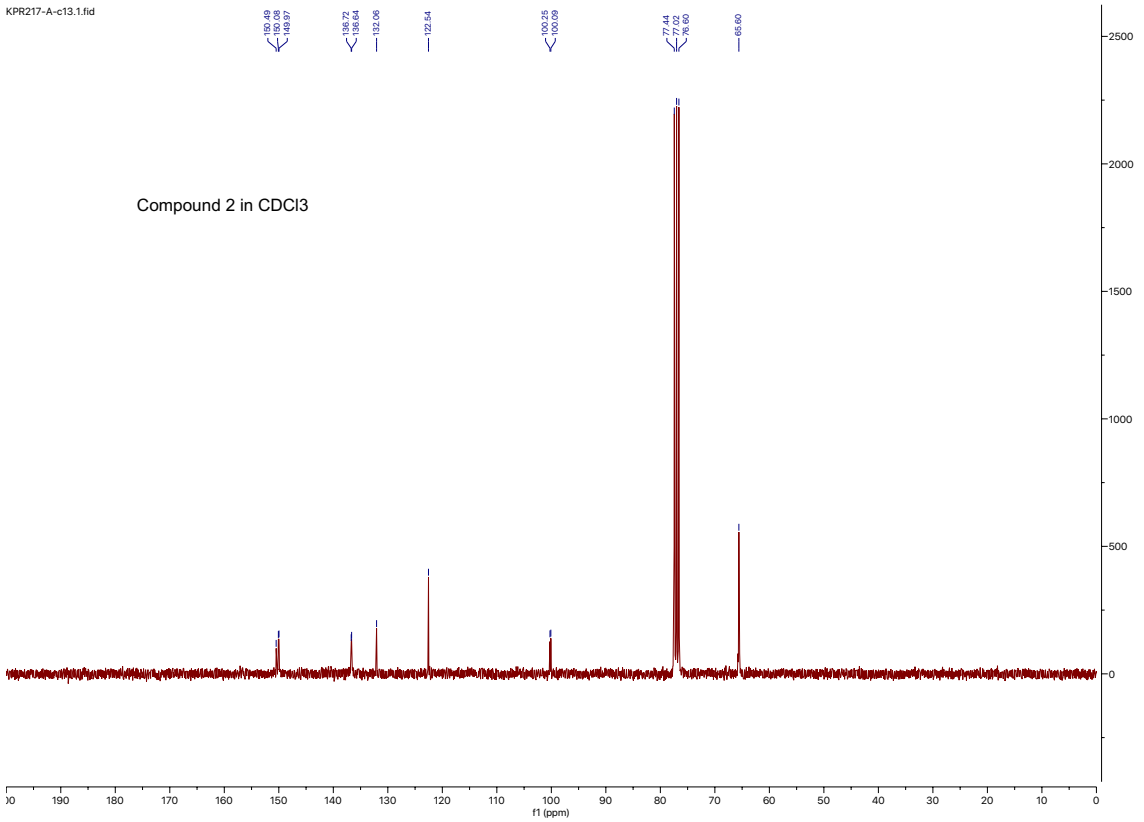
Table S3. Cartesian coordinates of optimized structures of lactam and lactim isomers in DMF and in THF.

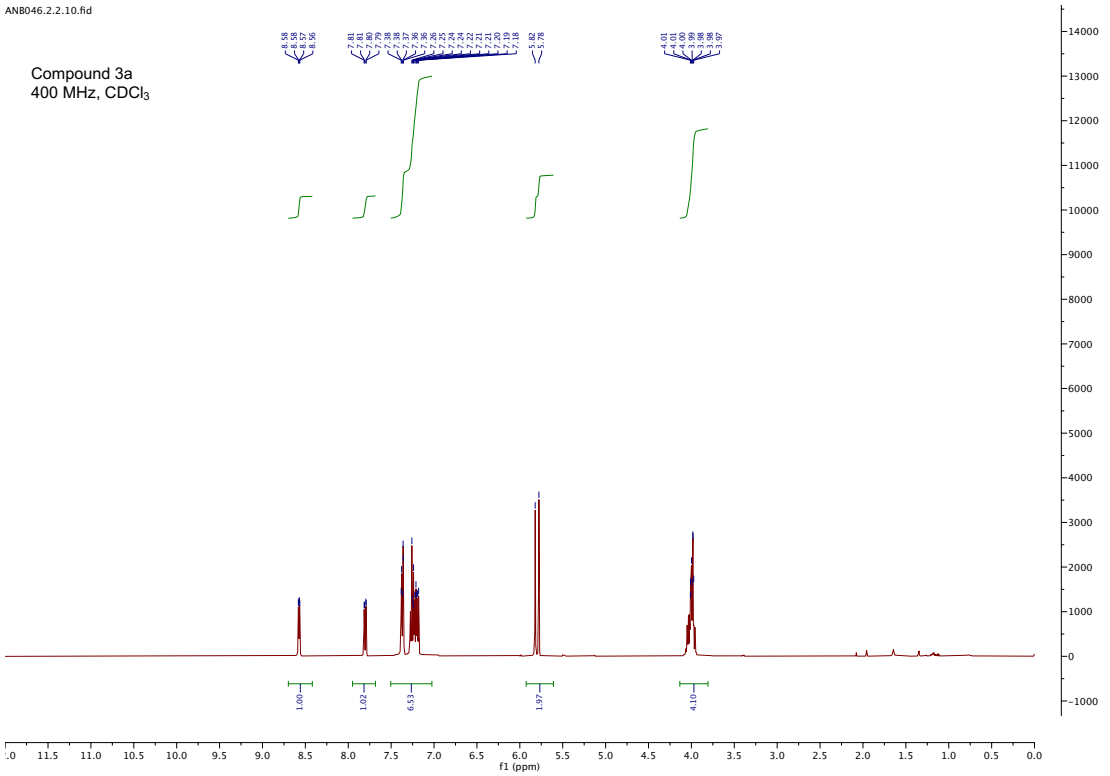
	X	Y	Z
Lactam (DMF)			
O	0.734742	2.805974	0.23758
N	-1.478544	2.363767	0.195324
H	-1.595987	3.36481	0.289894
N	-0.882441	-1.671234	-0.207391
C	-0.140406	1.941004	0.15579
C	0.041691	0.524953	0.037817
C	-1.066843	-0.314841	-0.047427
C	-2.397904	0.218959	0.005392
C	-2.550702	1.580728	0.130358
H	-3.517948	2.060444	0.17924
C	-3.511644	-0.660138	-0.07428
H	-4.51209	-0.249472	-0.027596
C	-3.287185	-1.987746	-0.210114
H	-4.090644	-2.705133	-0.276593
C	-1.932986	-2.432545	-0.281313
H	-1.744985	-3.493364	-0.414605
C	1.430172	0.013039	0.018007
C	2.359765	0.533878	-0.881894
H	2.053375	1.310909	-1.568733
C	3.665466	0.064707	-0.902537
H	4.37159	0.474207	-1.612298
C	4.065871	-0.924385	-0.01327
H	5.084686	-1.287163	-0.025436
C	3.150581	-1.442159	0.894346
H	3.455173	-2.208441	1.594421
C	1.843084	-0.97839	0.90776
H	1.132045	-1.384687	1.613724
Lactam (THF)			
O	0.735611	2.806423	0.232974
N	-1.476633	2.365579	0.198399
H	-1.59012	3.366749	0.293701
N	-0.885239	-1.670542	-0.208565
C	-0.137066	1.942647	0.155837
C	0.043314	0.523206	0.039233
C	-1.066528	-0.313031	-0.046773
C	-2.398372	0.222446	0.006535
C	-2.550173	1.582789	0.13356
H	-3.51749	2.062449	0.184062
C	-3.513101	-0.656342	-0.074955
H	-4.513291	-0.24456	-0.028131
C	-3.290511	-1.983207	-0.213137
H	-4.094963	-2.699428	-0.281505
C	-1.93531	-2.429729	-0.28451
H	-1.748143	-3.490538	-0.420156
C	1.431002	0.010514	0.019353
C	2.37128	0.559581	-0.852248
H	2.07472	1.361112	-1.514238
C	3.675904	0.088675	-0.874223
H	4.390319	0.520888	-1.561856
C	4.065425	-0.929351	-0.013802
H	5.084014	-1.292865	-0.026408
C	3.139841	-1.474589	0.866545
H	3.435844	-2.263309	1.545054
C	1.833114	-1.010057	0.880569
H	1.11442	-1.438458	1.564923
Lactim (DMF)			
O	-0.81291	2.738156	-0.242126
N	1.443775	2.438137	-0.19399
N	0.939472	-1.669784	0.190635
C	0.220935	1.877093	-0.148461
C	-0.030386	0.522917	-0.035774
C	1.104097	-0.325063	0.046194
C	2.39415	0.255829	-0.003893
C	2.488947	1.654861	-0.12617
H	3.466727	2.123014	-0.167937
C	3.526732	-0.581929	0.075776
H	4.51647	-0.144936	0.035122
C	3.340901	-1.92512	0.205819
H	4.169441	-2.614169	0.271556
C	2.014263	-2.412826	0.264331
H	1.851882	-3.478807	0.383028
C	-1.415133	-0.003545	-0.013241
C	-2.33396	0.456983	0.927893
H	-2.026824	1.202593	1.649121
C	-3.632168	-0.033348	0.946482
H	-4.332267	0.329563	1.686739
C	-4.030962	-0.985723	0.017796
H	-5.043249	-1.366208	0.029831
C	-3.123136	-1.446627	-0.927378
H	-3.427008	-2.186211	-1.655773
C	-1.823608	-0.96163	-0.940124
H	-1.116247	-1.325162	-1.672933
H	-0.442398	3.625379	-0.333764
Lactim (THF)			
O	-0.8128	2.738942	-0.244728
N	1.442526	2.438647	-0.196211
N	0.940778	-1.669095	0.188767
C	0.219941	1.877124	-0.150698
C	-0.031416	0.522486	-0.037292
C	1.104128	-0.324163	0.045404

C	2.394089	0.257745	-0.003079
C	2.48797	1.656512	-0.126566
H	3.465272	2.125992	-0.168054
C	3.526873	-0.579394	0.079152
H	4.516484	-0.141631	0.040283
C	3.342042	-1.922479	0.209531
H	4.171197	-2.610699	0.277506
C	2.015183	-2.411104	0.264824
H	1.852594	-3.477227	0.38289
C	-1.415566	-0.004832	-0.013948
C	-2.342386	0.476566	0.90858
H	-2.042077	1.23931	1.614337
C	-3.63986	-0.014603	0.928474
H	-4.346042	0.364925	1.654479
C	-4.030556	-0.988509	0.01928
H	-5.042623	-1.36962	0.032103
C	-3.114863	-1.470425	-0.907188
H	-3.412052	-2.227369	-1.620347
C	-1.815851	-0.985028	-0.920719
H	-1.102334	-1.365893	-1.638242
H	-0.439519	3.624443	-0.339559

V - ^{1}H and ^{13}C NMR spectra



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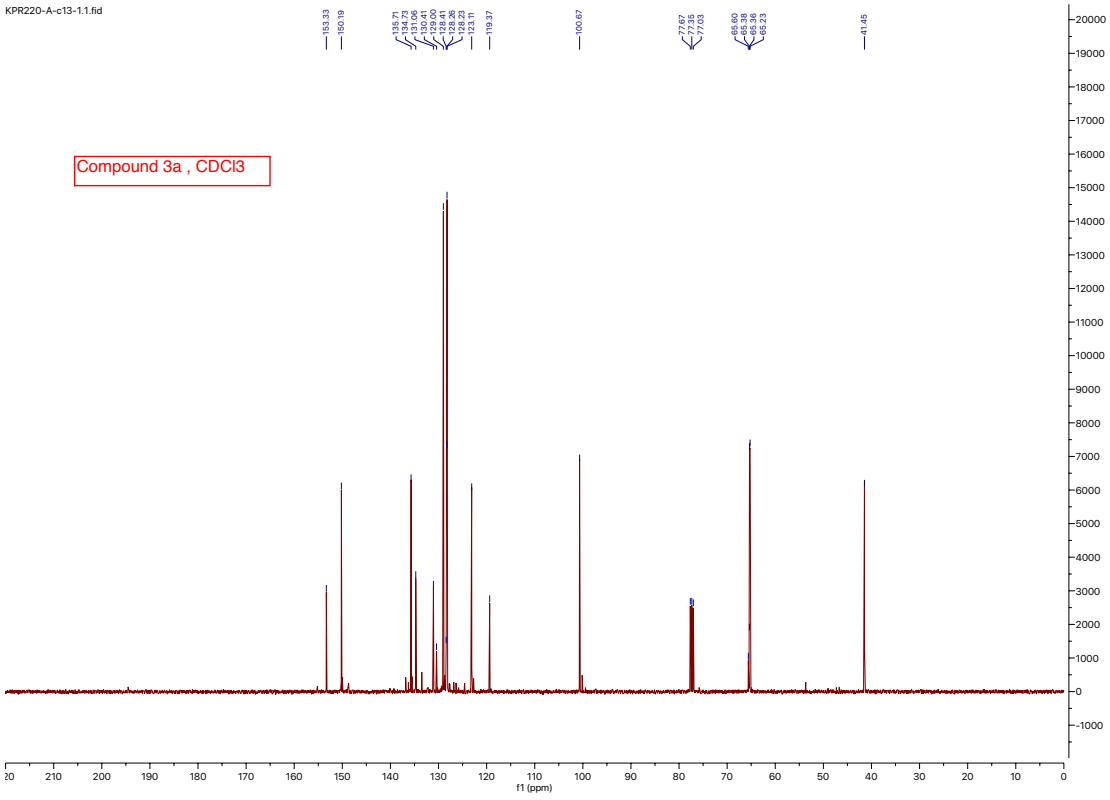
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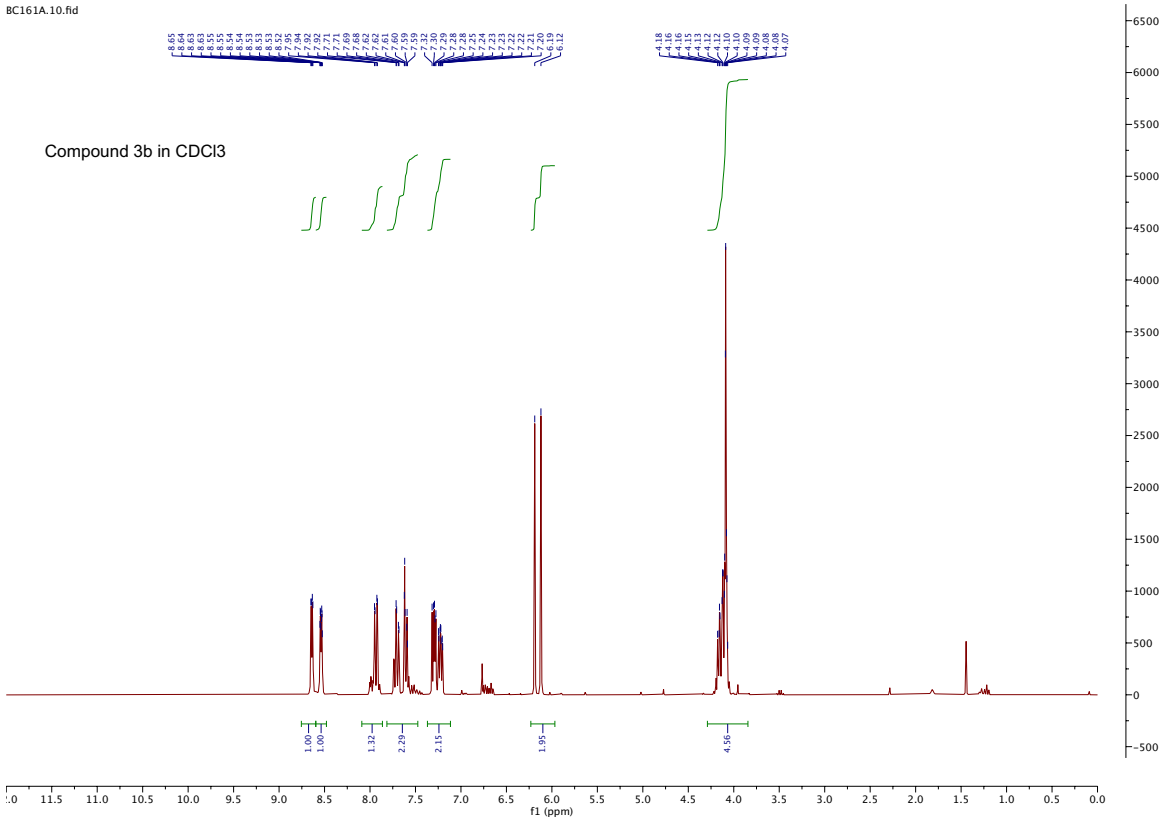
f1 (ppm)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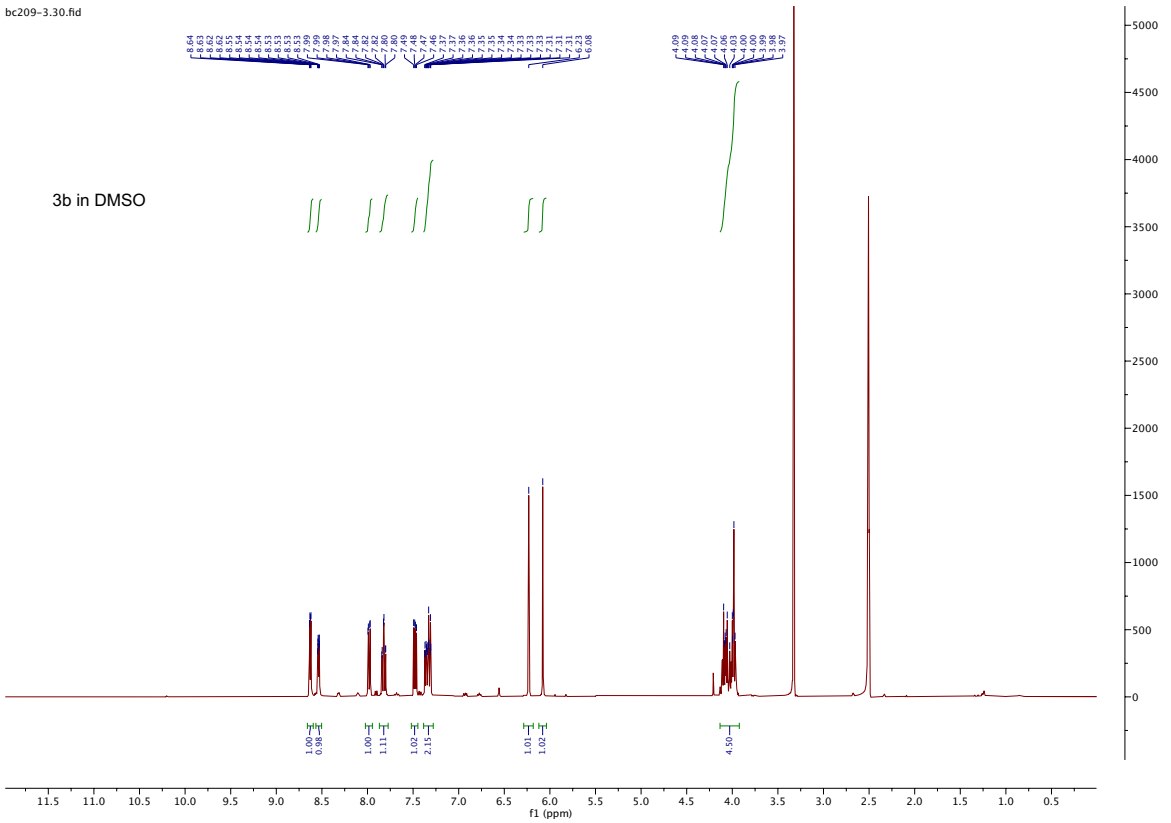
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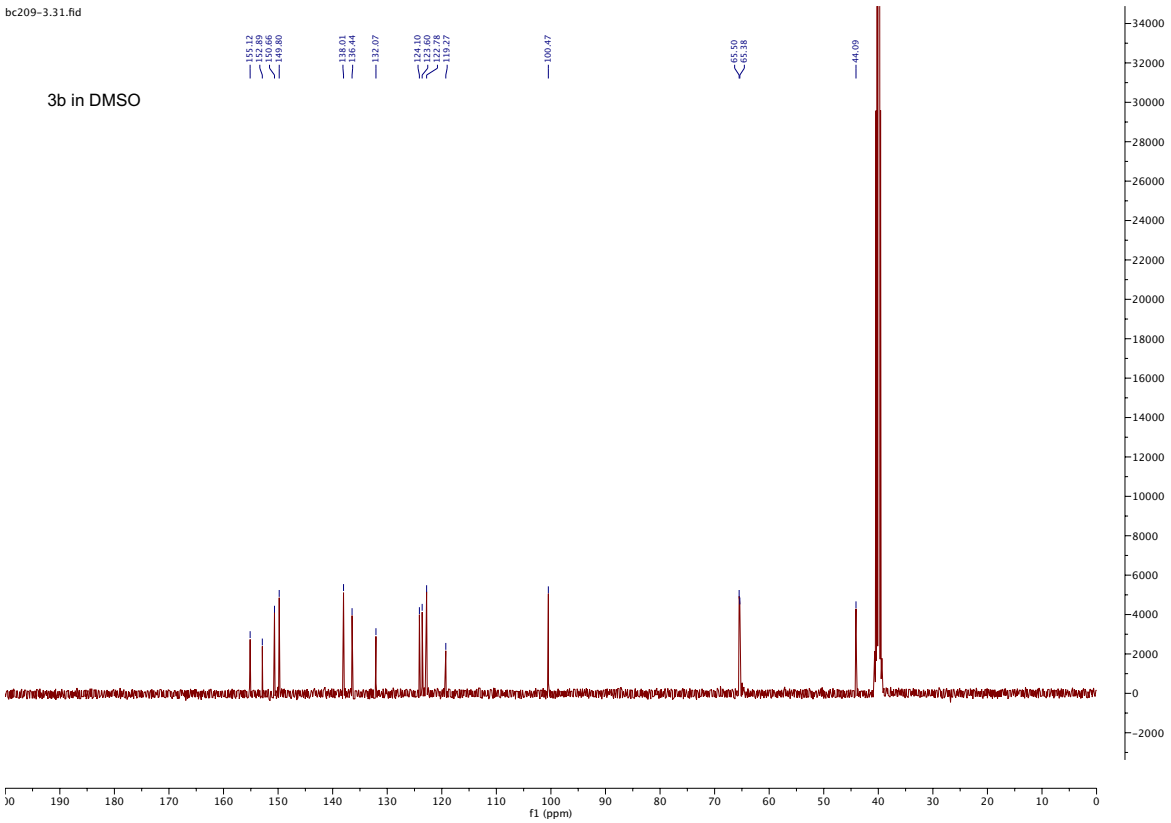
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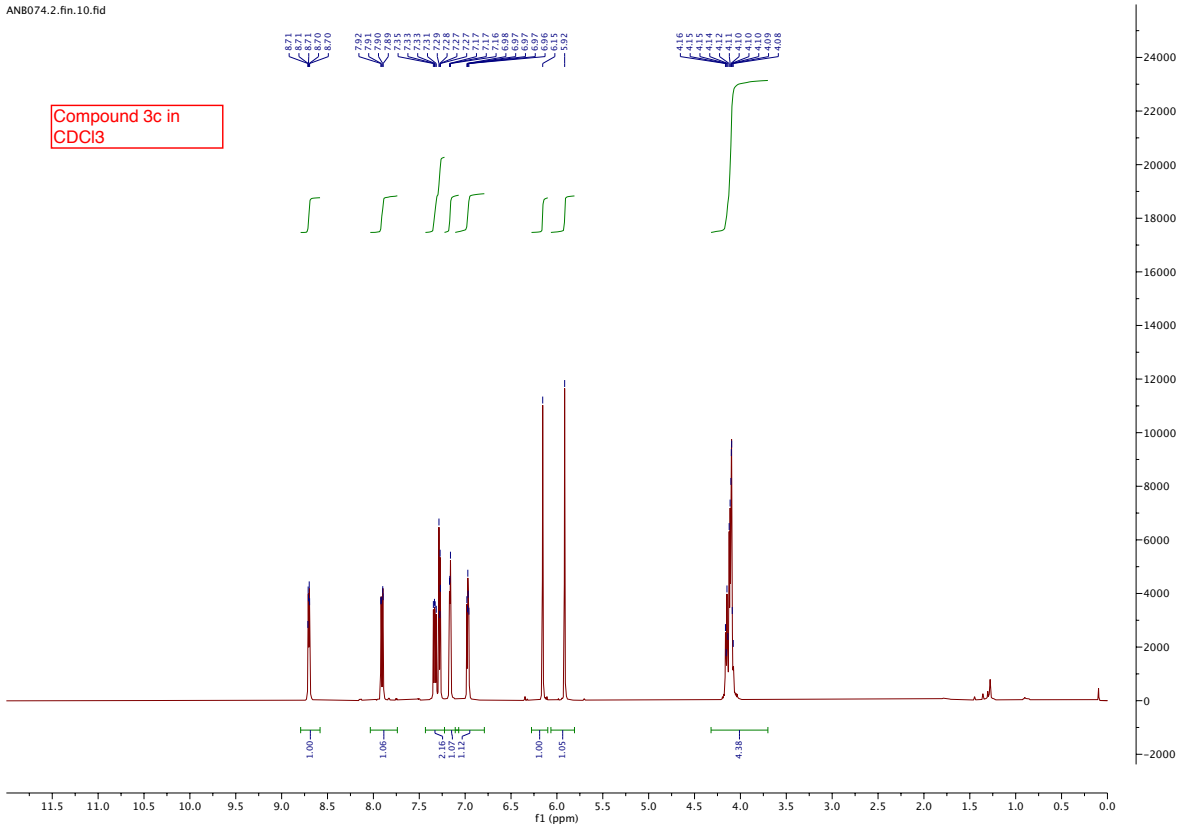
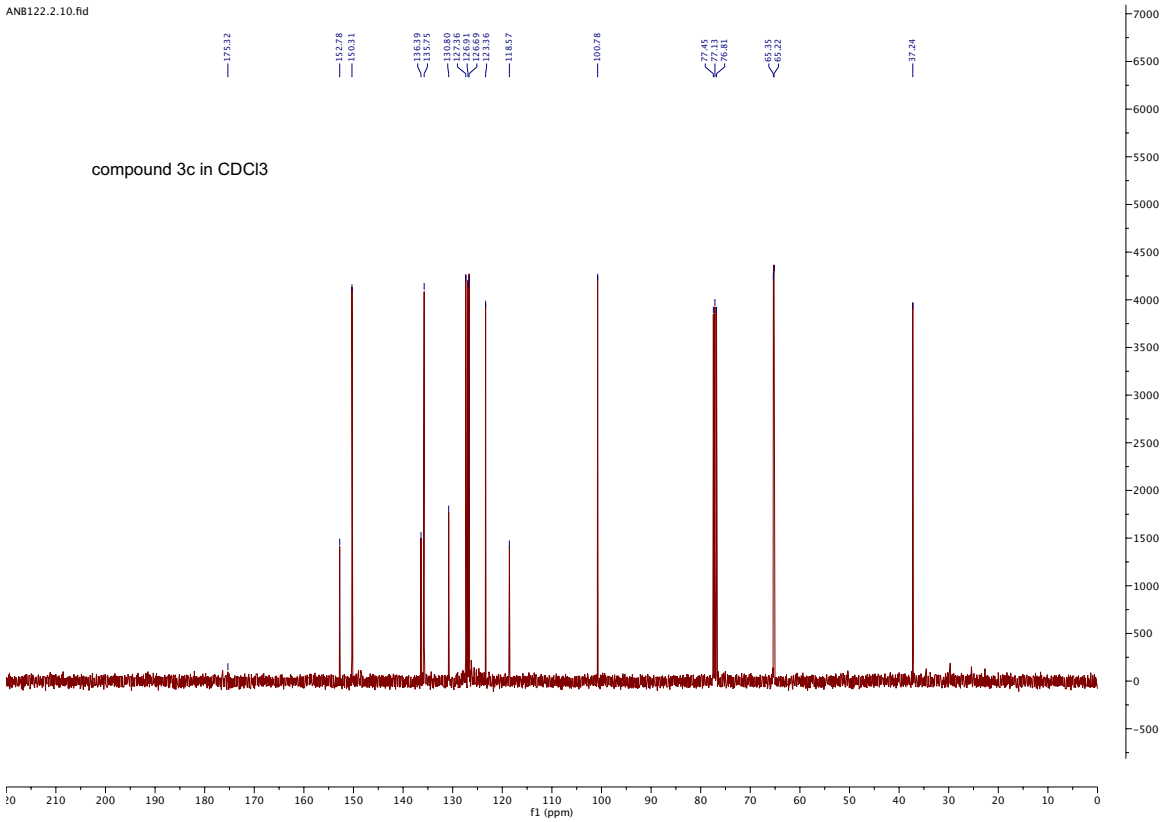
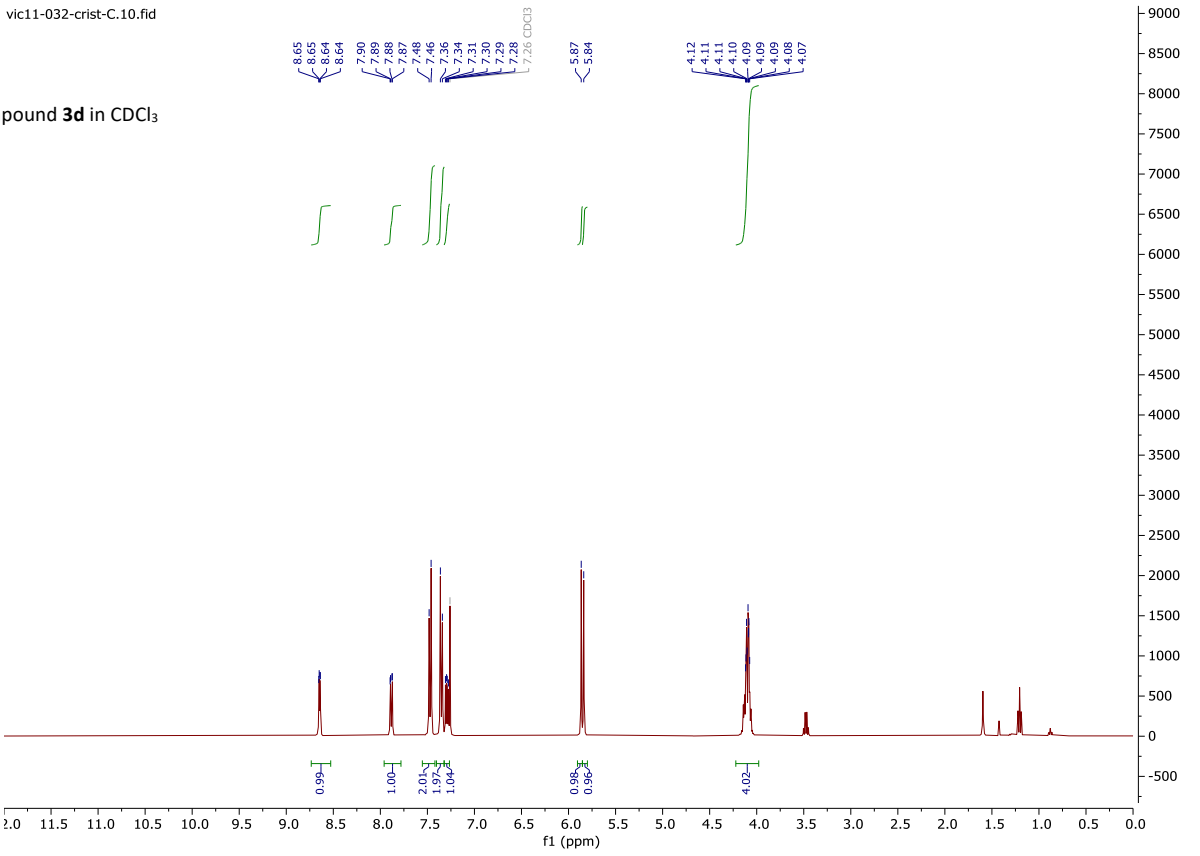
3b in DMSO
f1 (ppm)

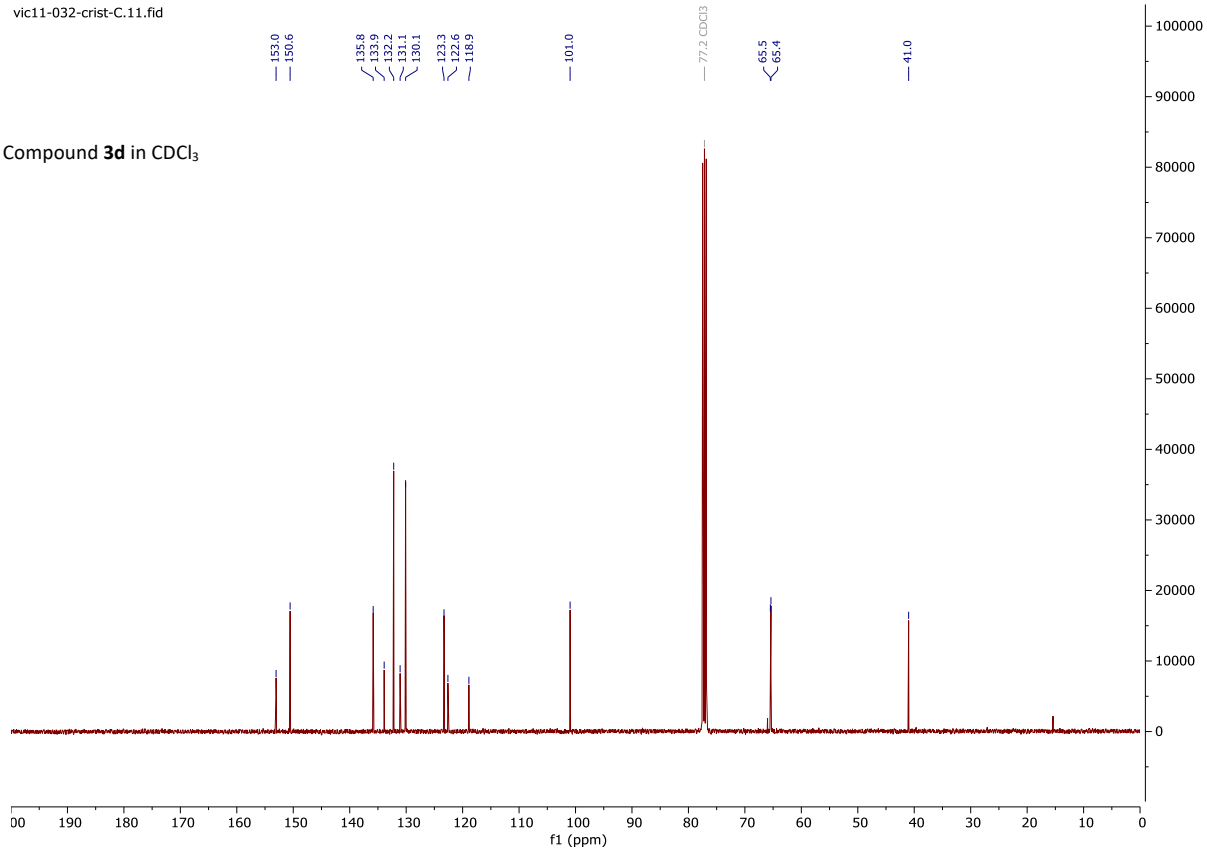

ANB074.2.fin.10.fid
Compound 3c in CDCl3
f1 (ppm)

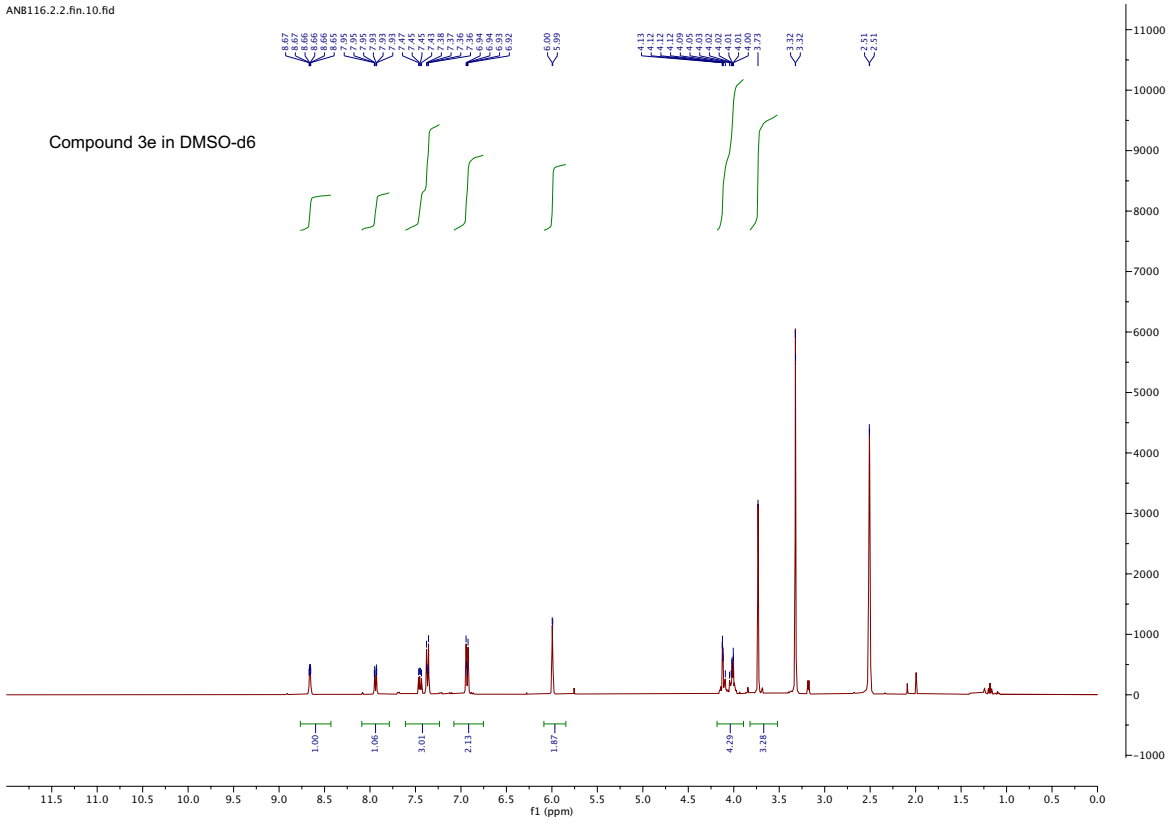

ANB122.2.10.fid
compound 3c in CDCl3
f1 (ppm)

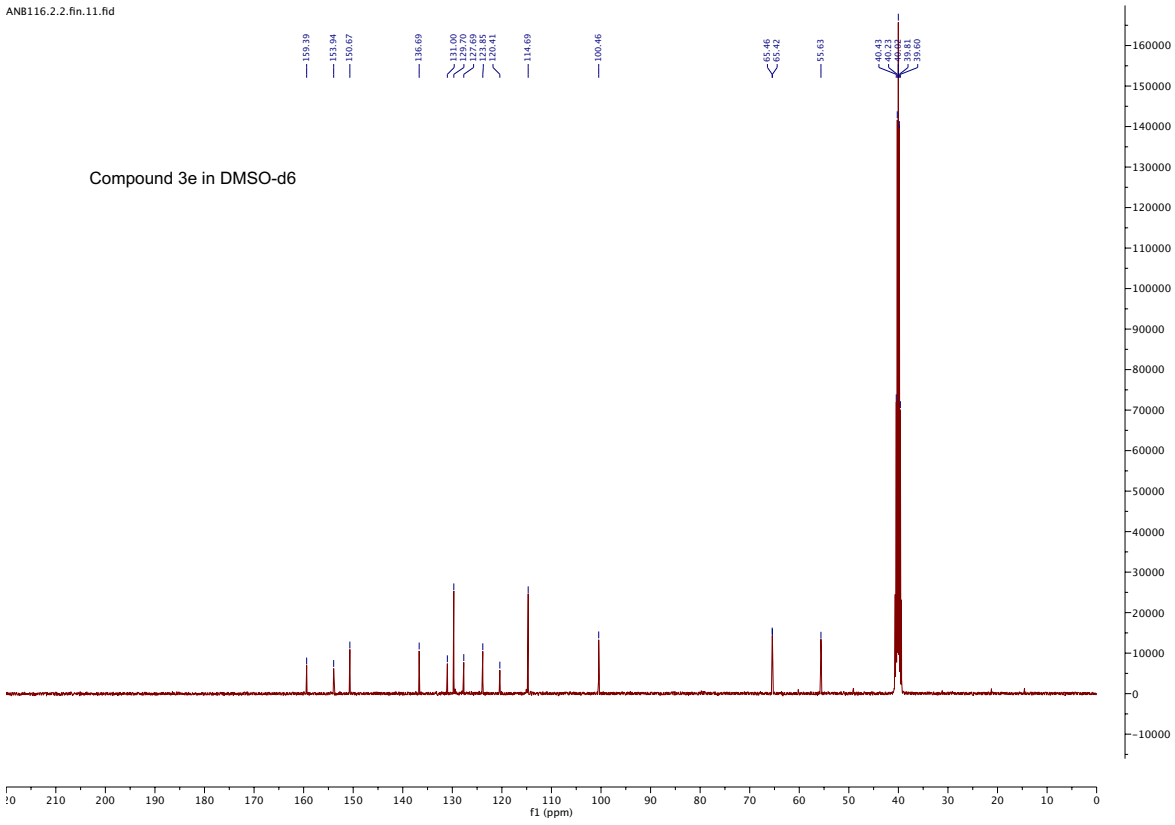
Compound **3d** in $CDCl_3$

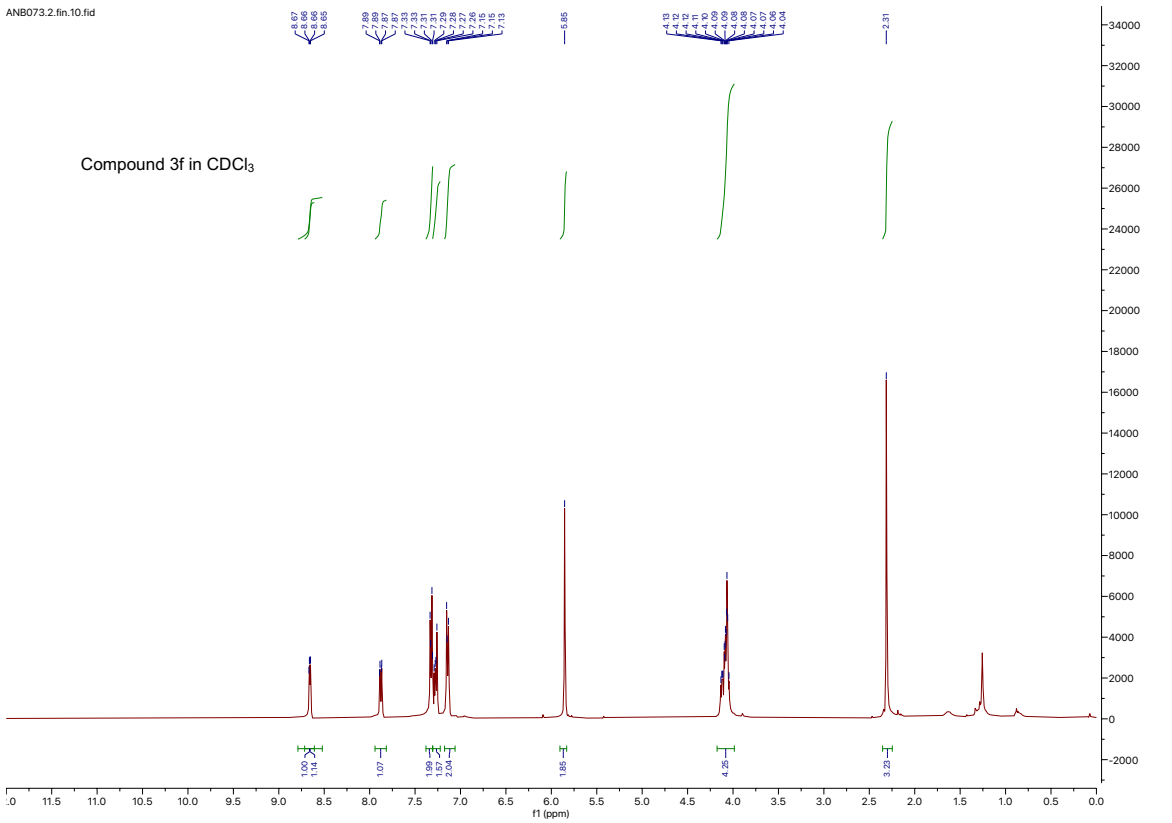


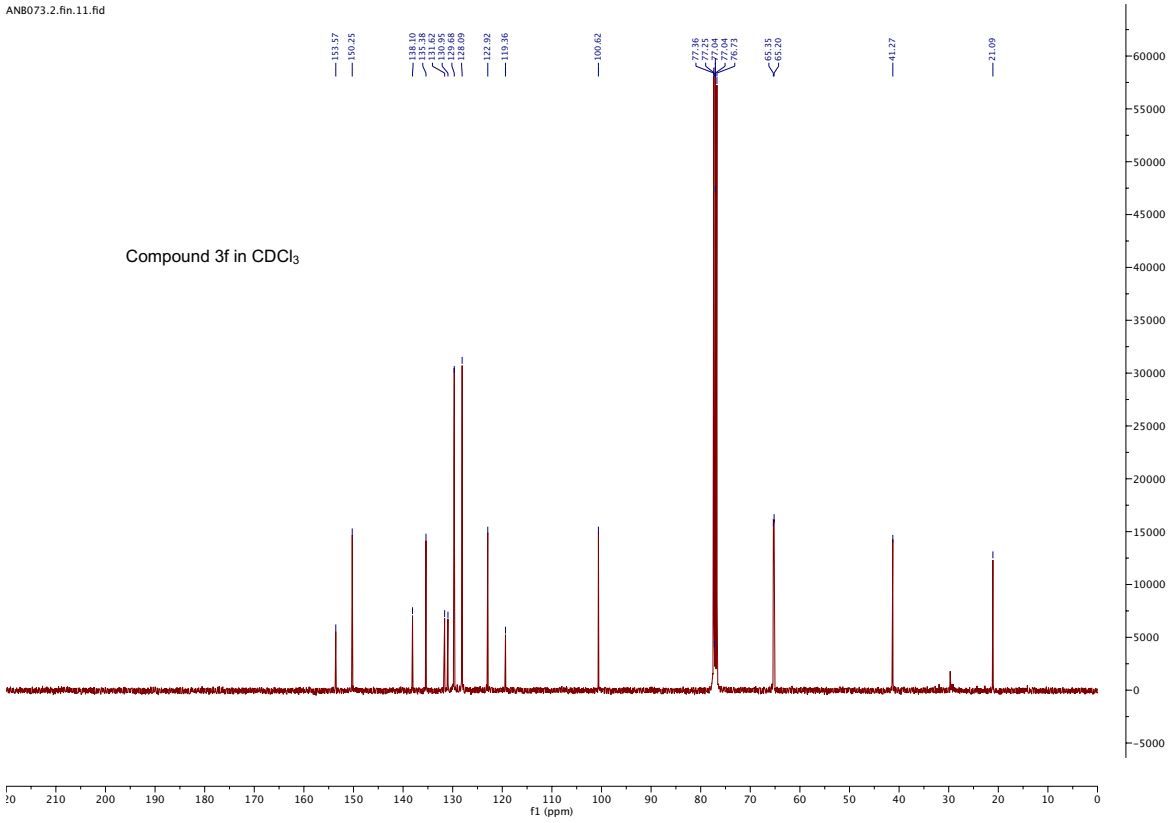
Compound **3d** in $CDCl_3$

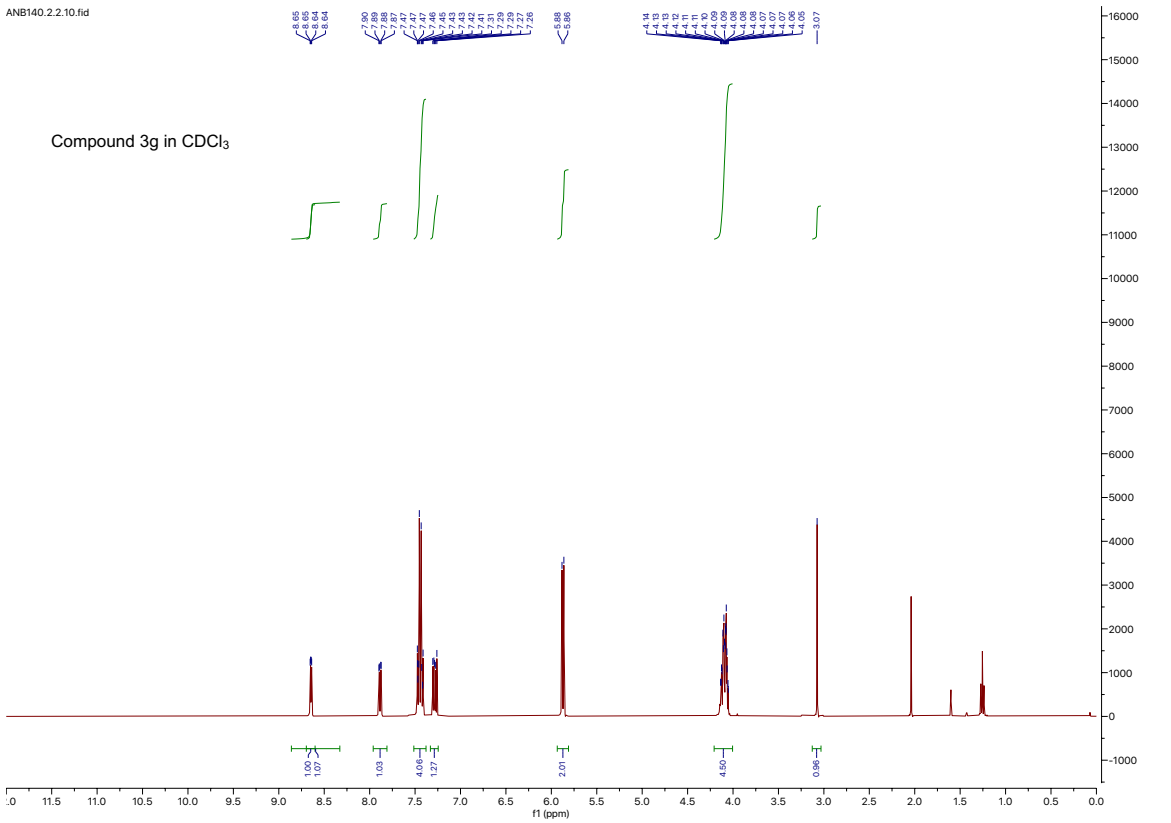


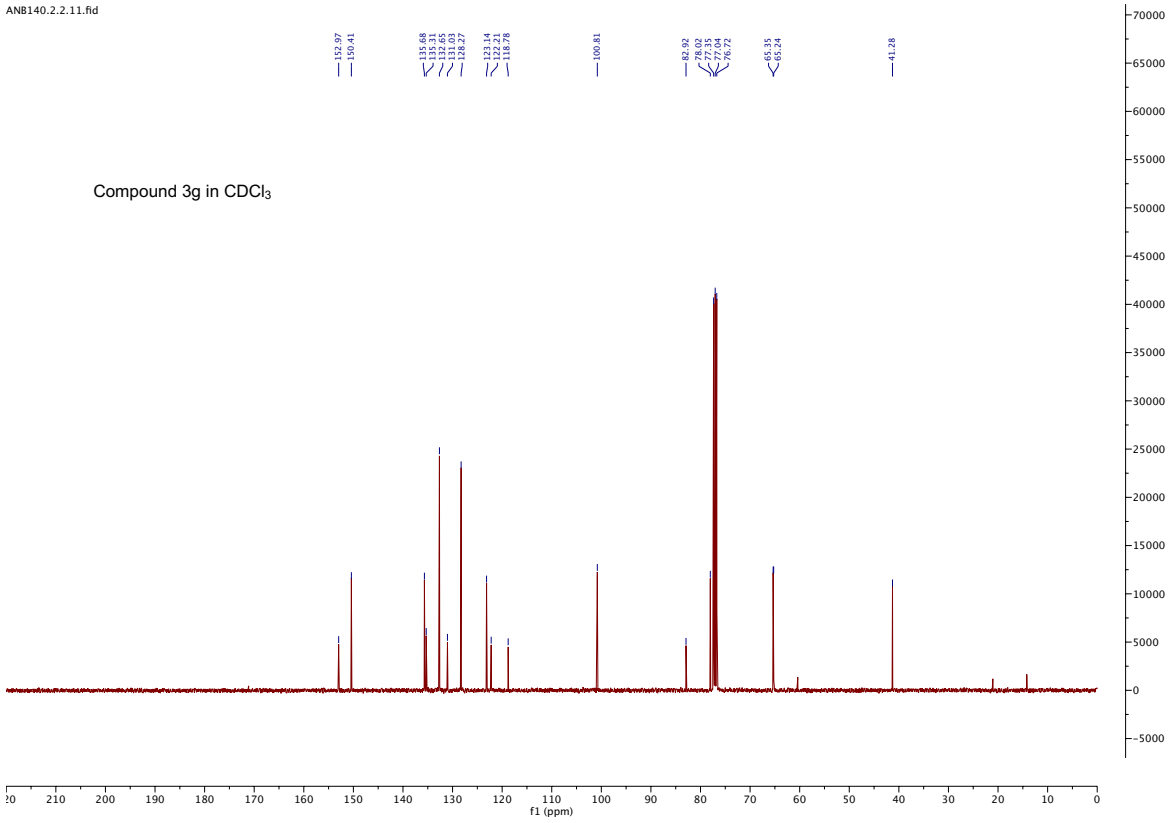

ANB116.2.2.fin.10.fid
Compound 3e in DMSO-d6
f1 (ppm)

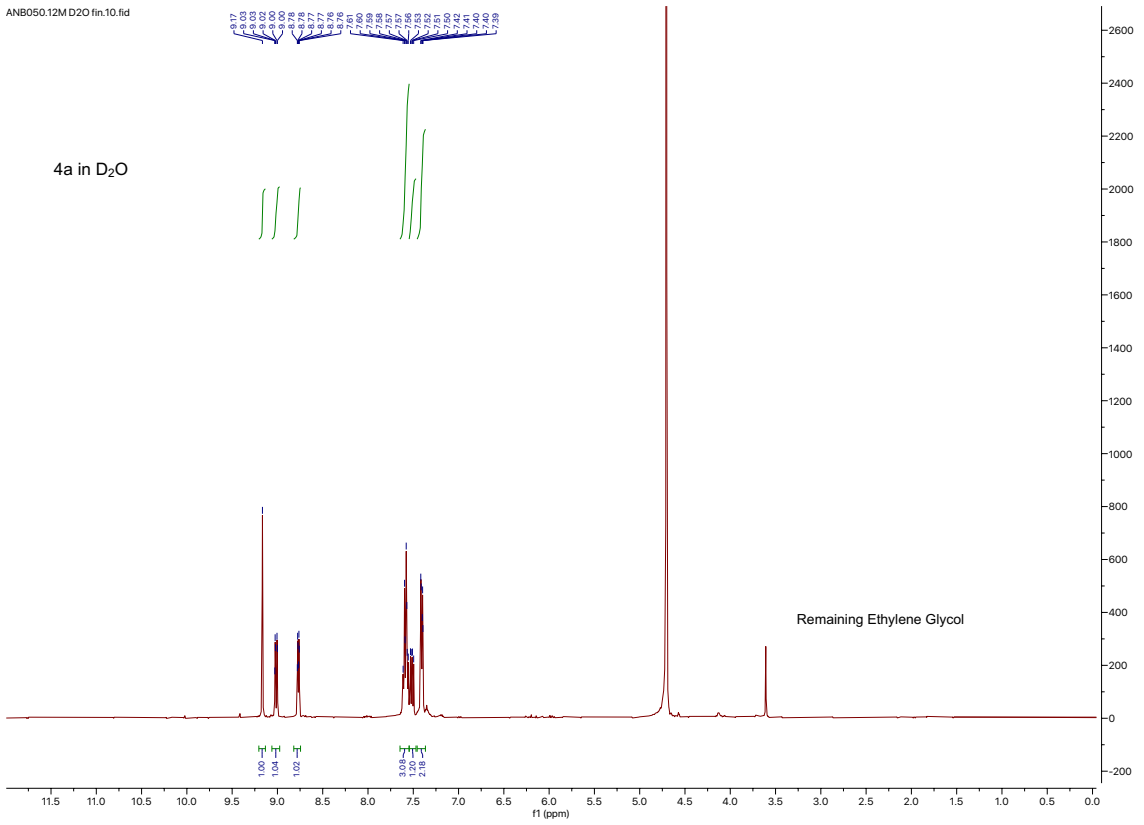

ANB116.2.2.fin.11.fid
Compound 3e in DMSO-d6
f1 (ppm)

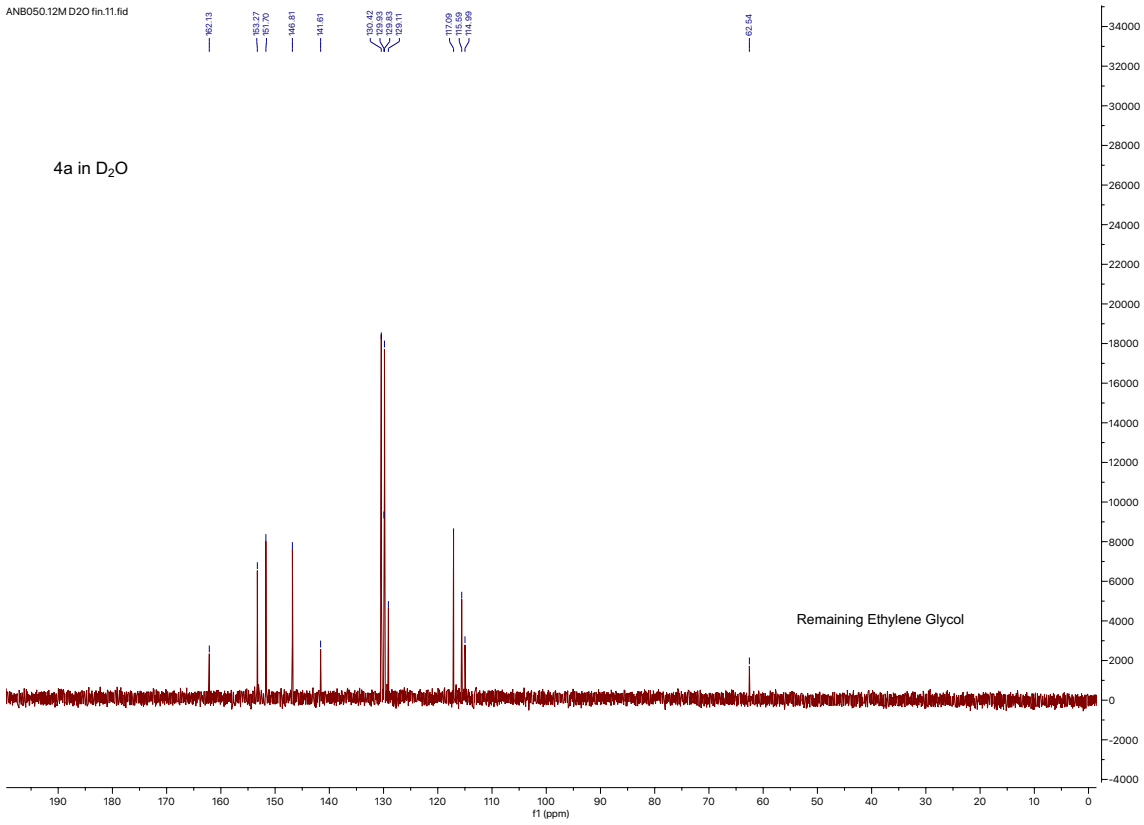

ANB073.2.fin.10.fid
Compound 3f in CDCl3
f1 (ppm)

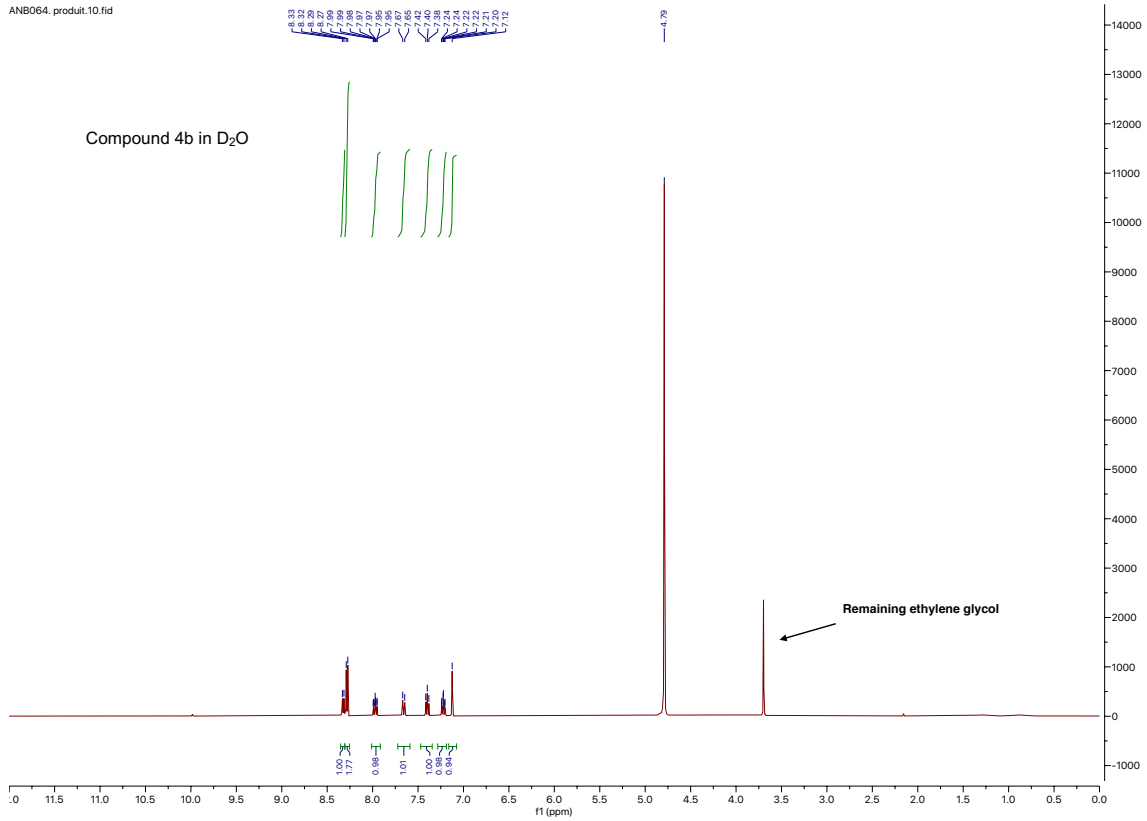

ANB073.2.fin.11.fid
Compound 3f in CDCl3
f1 (ppm)

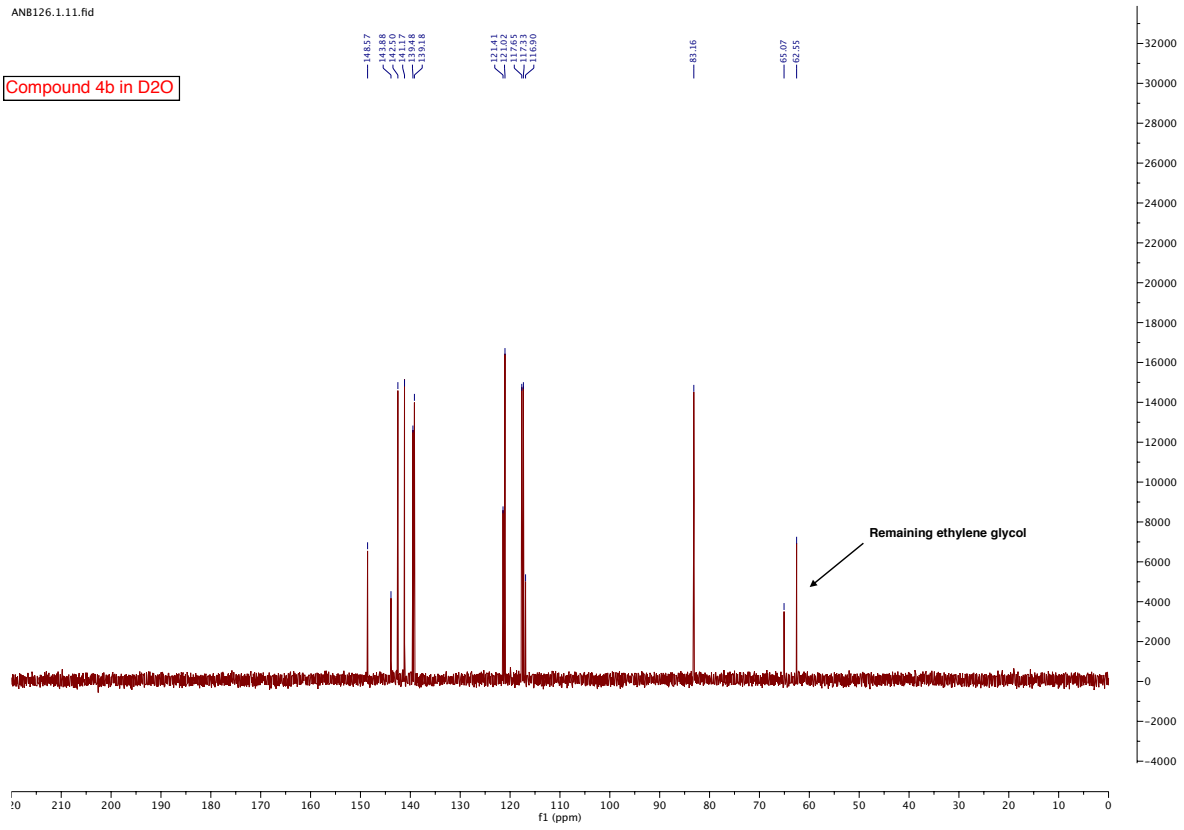

ANB140.2.2.10.fid
Compound 3g in CDCl3
f1 (ppm)

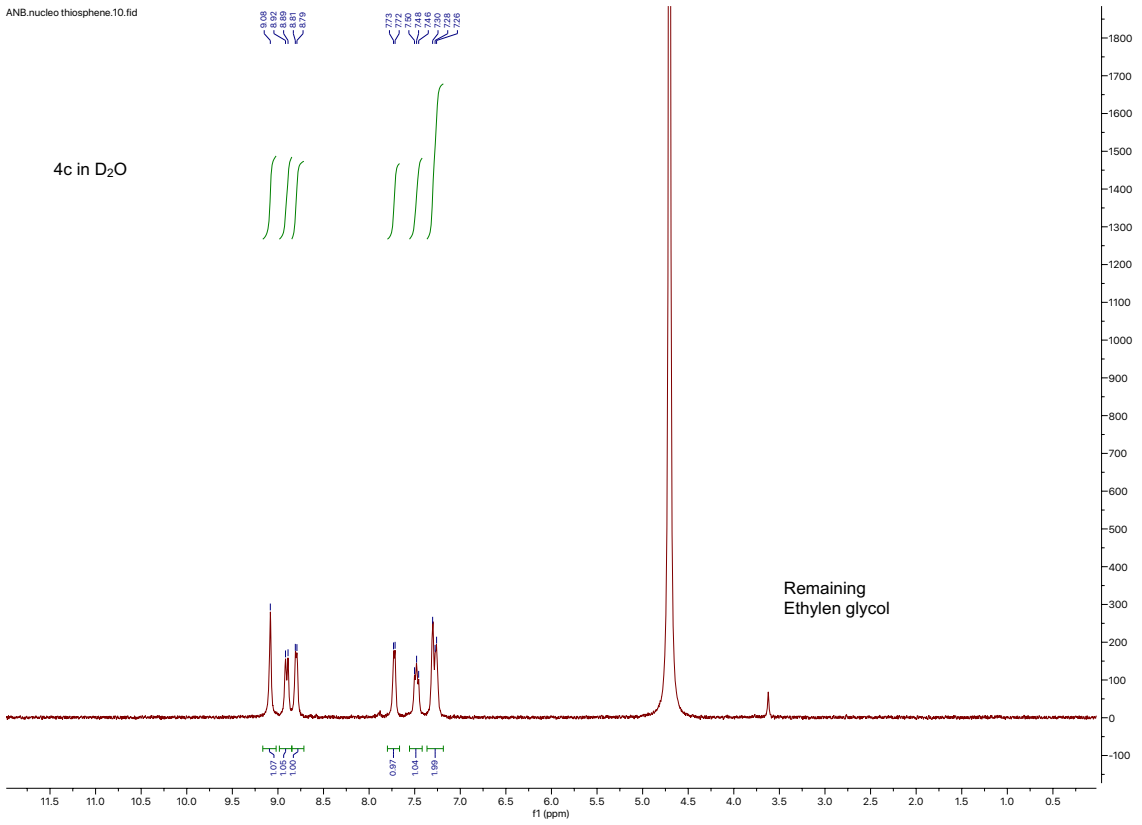

ANB140.2.2.11.fid
Compound 3g in CDCl3
f1 (ppm)

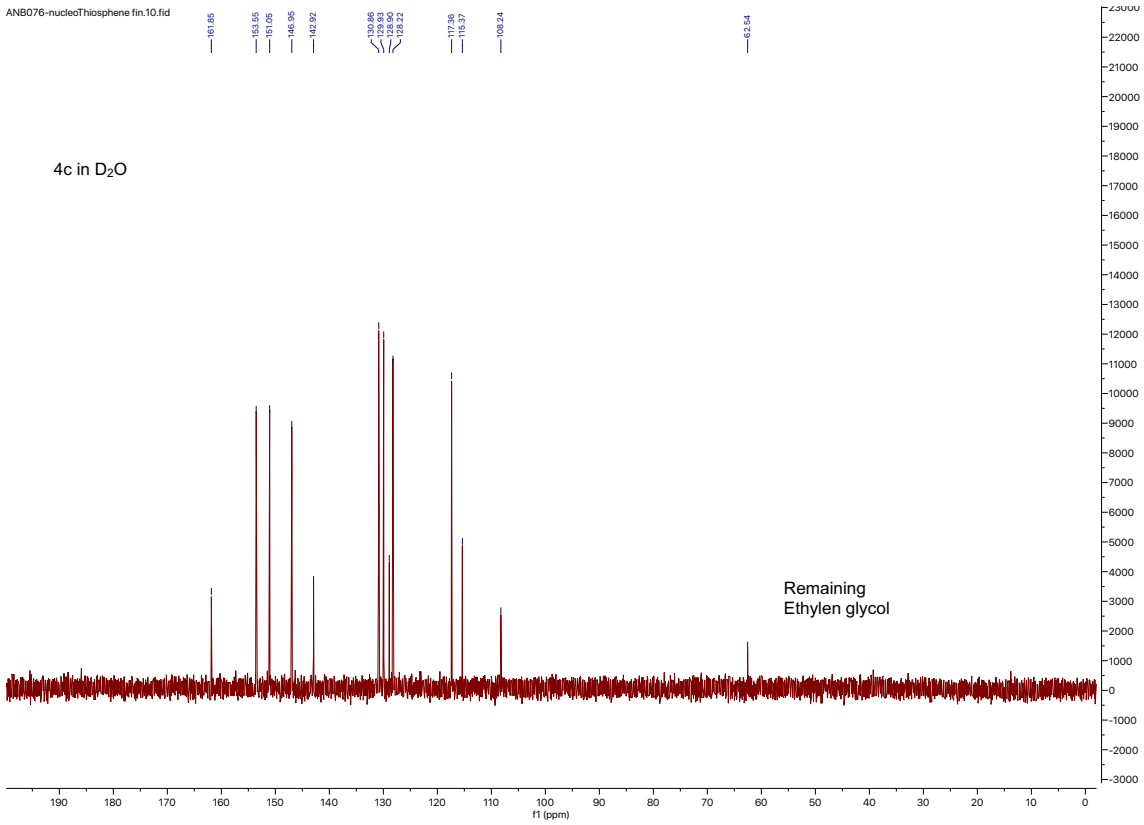

ANB050.12M D2O fin.10.fid
4a in D2O
Remaining Ethylene Glycol
f1 (ppm)

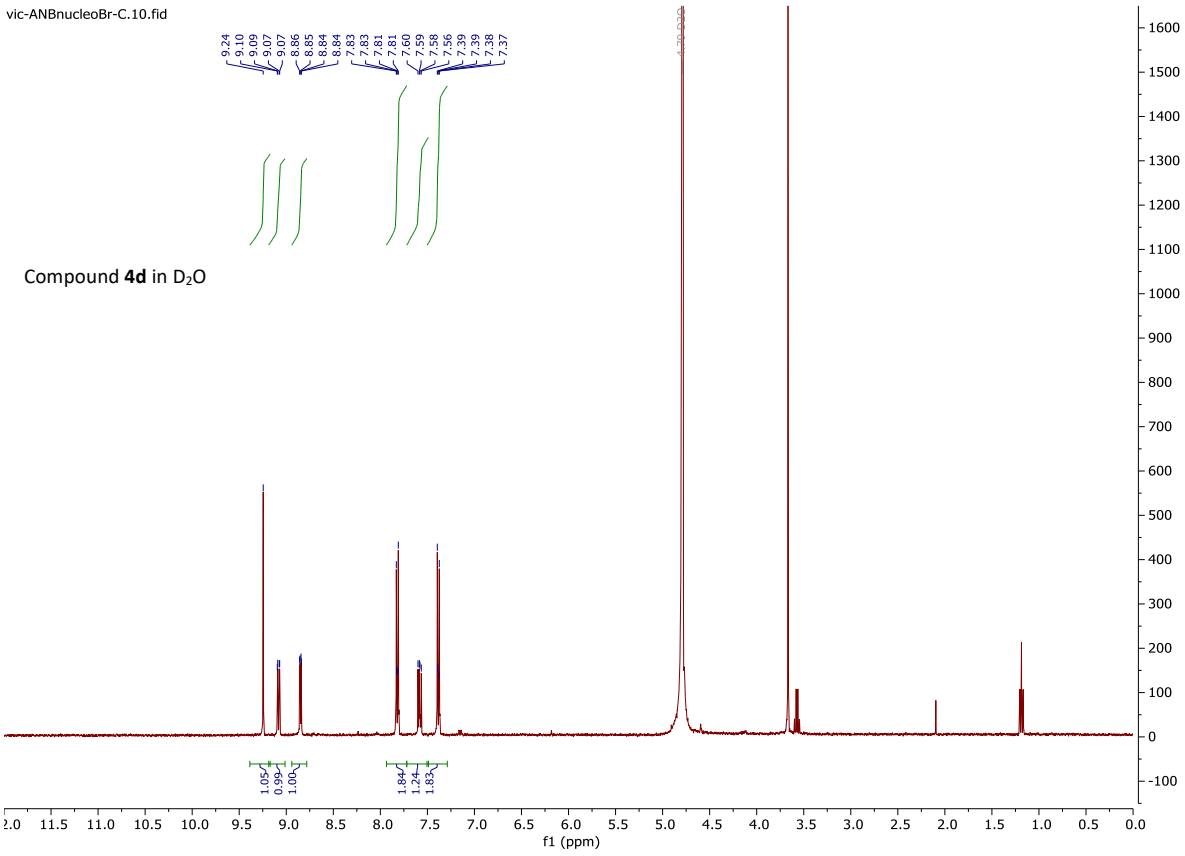

ANB050.12M D2O fin.11.fid
4a in D2O
Remaining Ethylene Glycol
f1 (ppm)

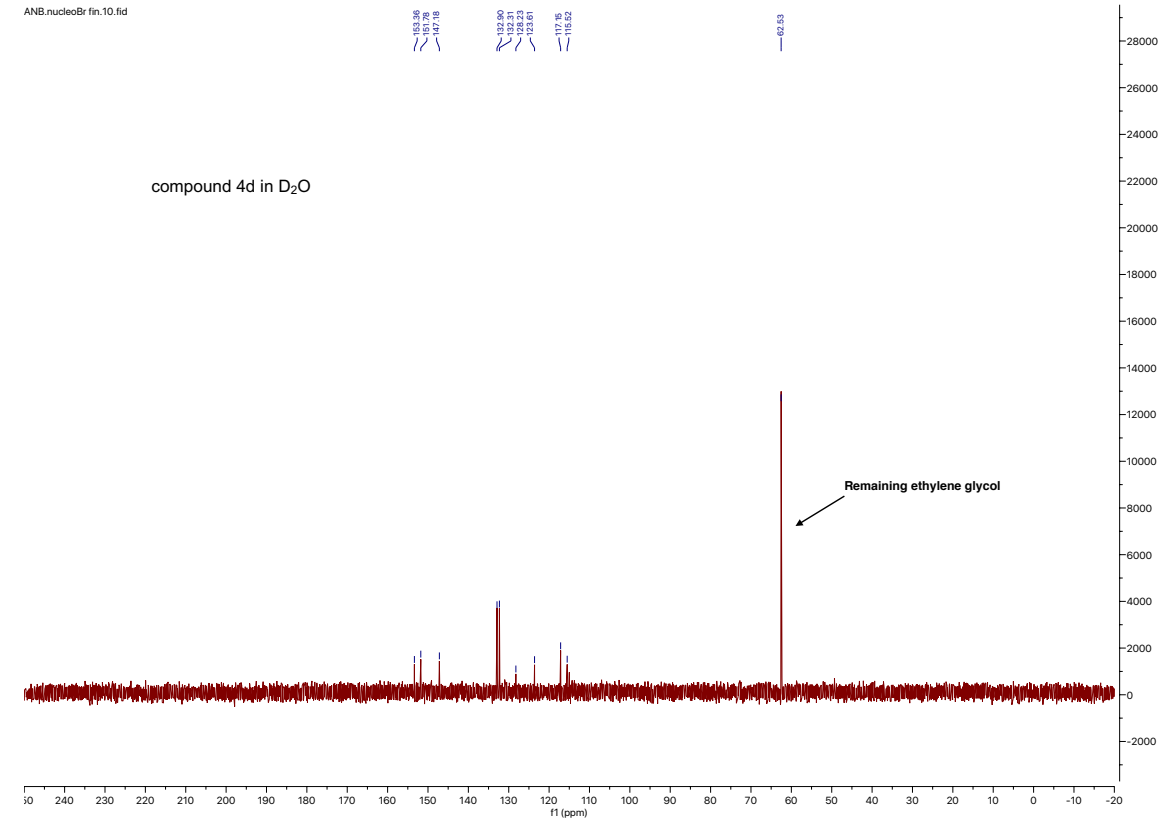

ANB064. produit.10.fid
Compound 4b in D_2O
Remaining ethylene glycol
f1 (ppm)

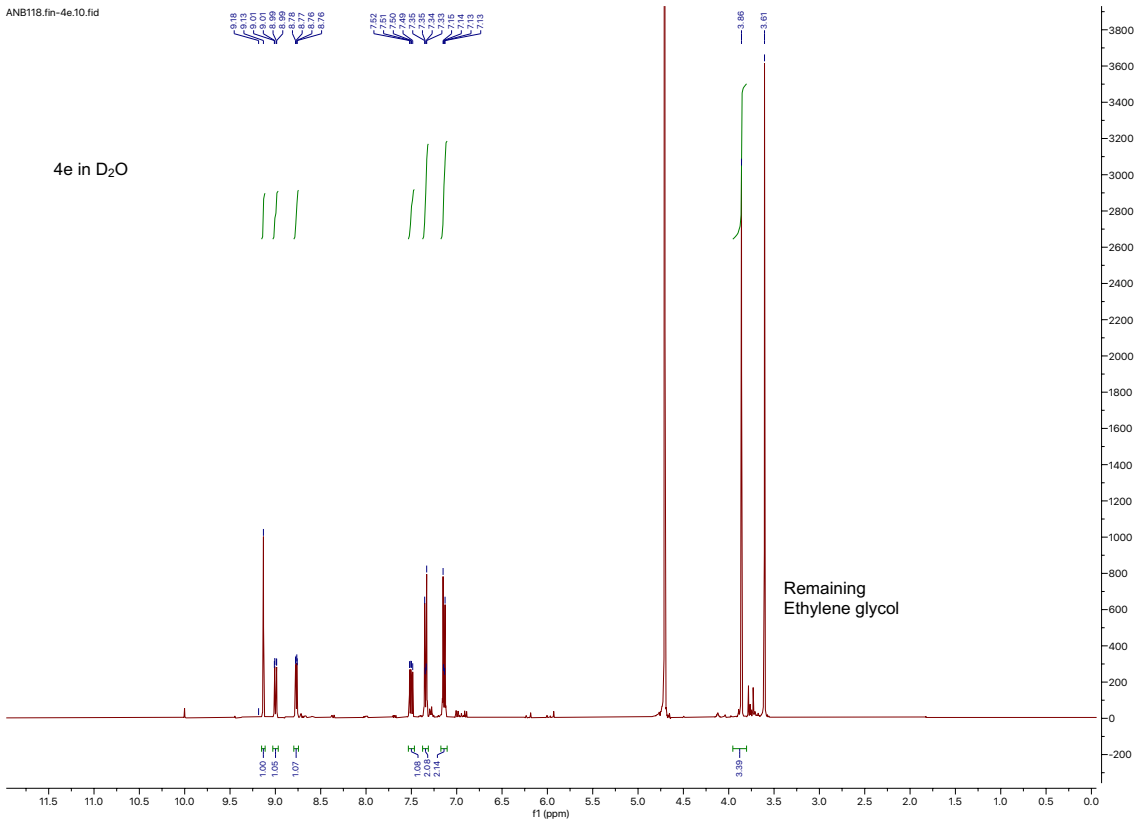

ANB126.1.11.fid
Compound 4b in D2O
Remaining ethylene glycol
f1 (ppm)

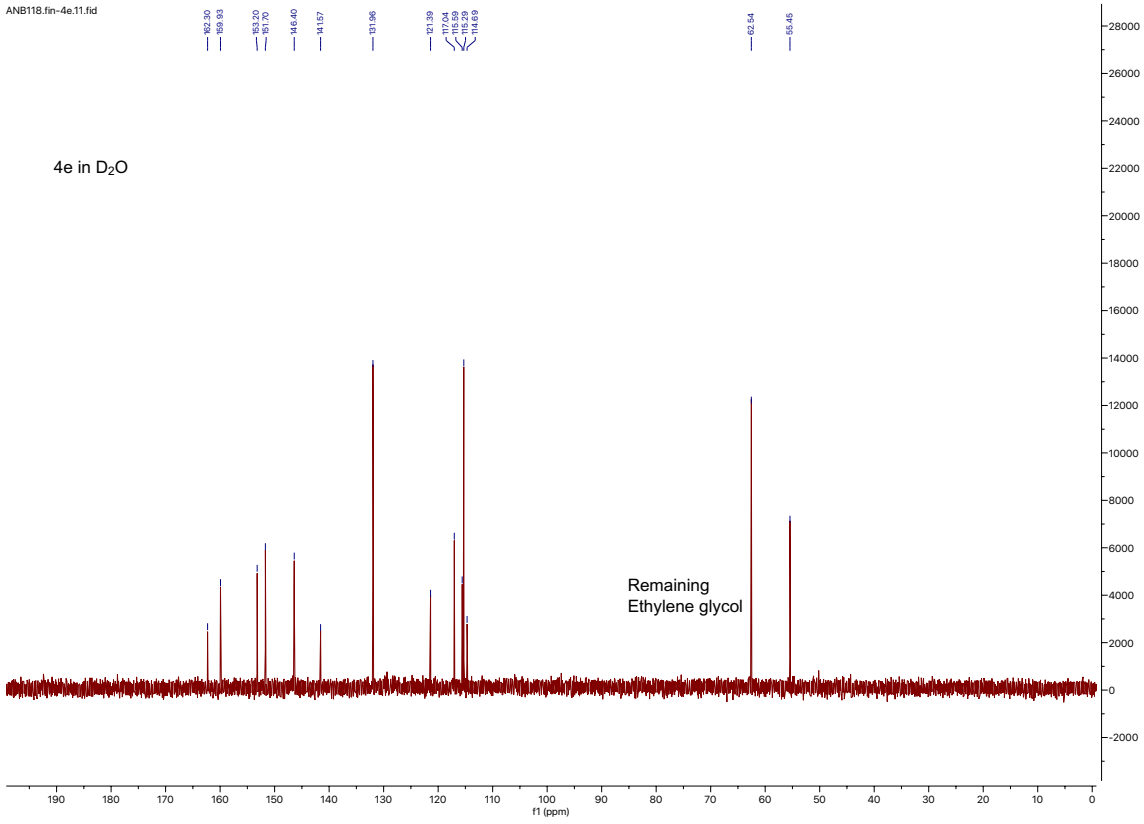

ANB.nucleo thiosphene.10.fid
4c in D2O
Remaining
Ethylen glycol
f1 (ppm)

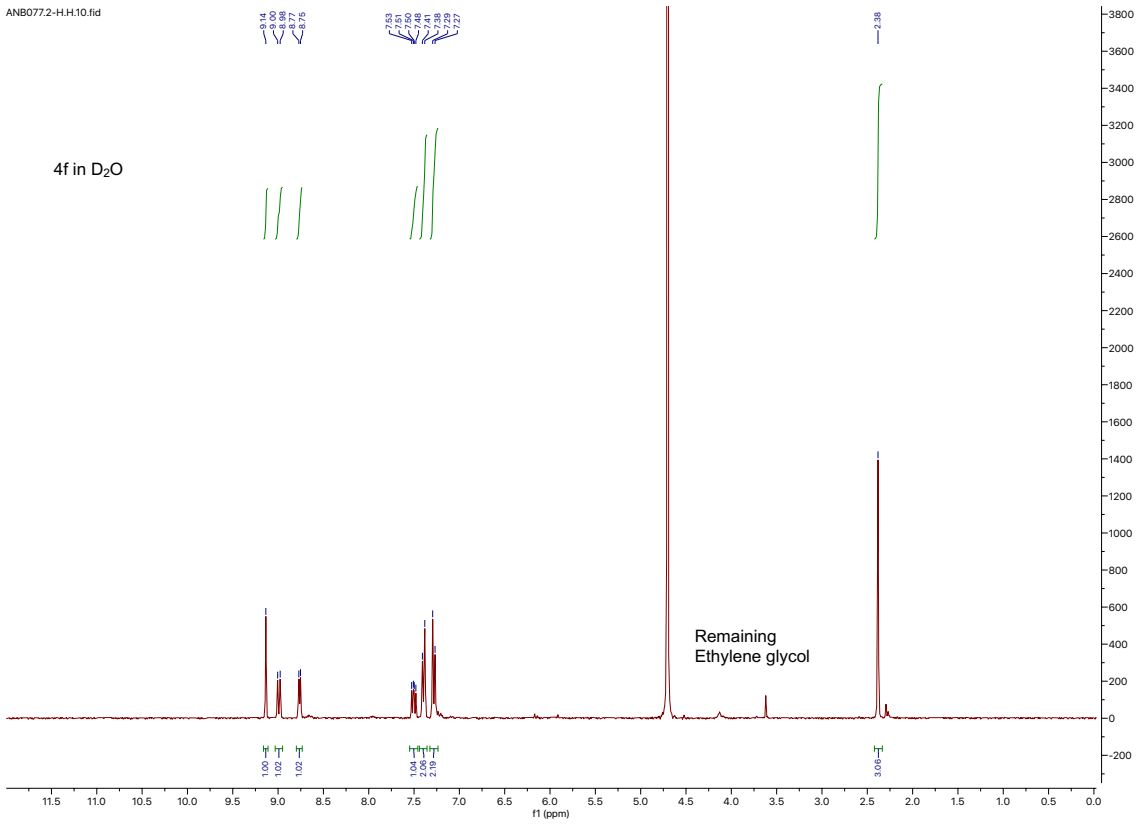

ANB076-nucleoThiosphene fin.10.fid
4c in D2O
Remaining
Ethylen glycol
f1 (ppm)

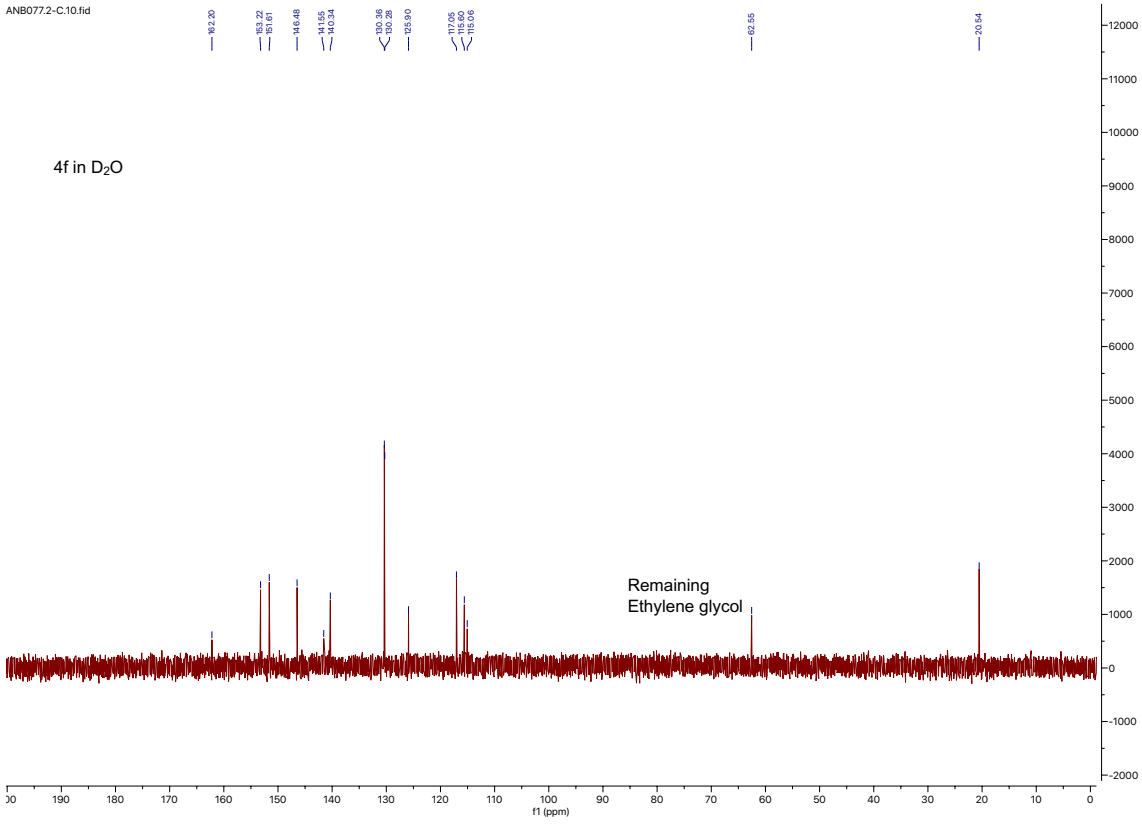

vic-ANBnucleoBr-C.10.fid
9.24
9.10
9.09
9.07
9.07
8.86
8.85
8.84
8.84
7.83
7.83
7.81
7.81
7.60
7.59
7.58
7.56
7.39
7.39
7.38
7.37
Compound 4d in D2O
1.05
0.99
1.00
1.84
1.24
1.83
f1 (ppm)

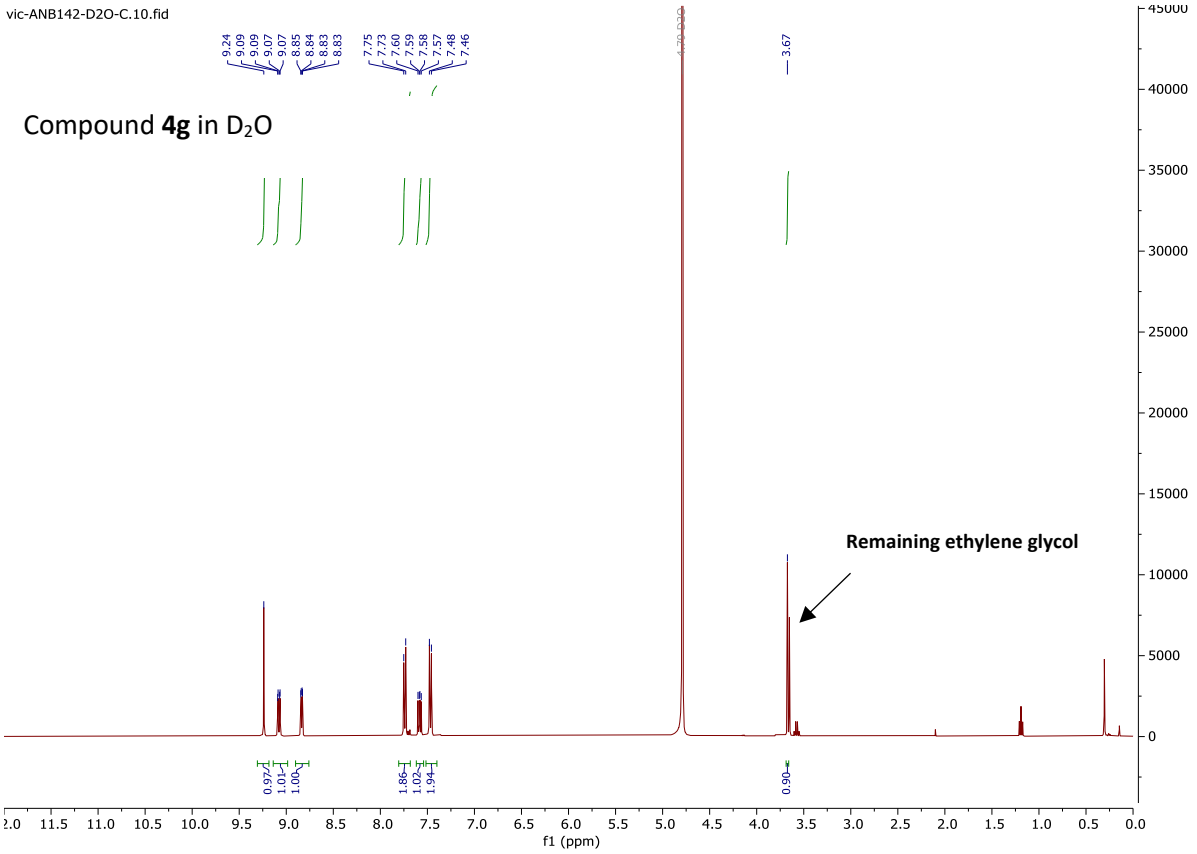

ANB.nucleoBr fin.10.fid
163.36
161.78
147.18
132.90
132.31
128.23
123.61
117.95
115.62
62.53
compound 4d in D2O
Remaining ethylene glycol
f1 (ppm)

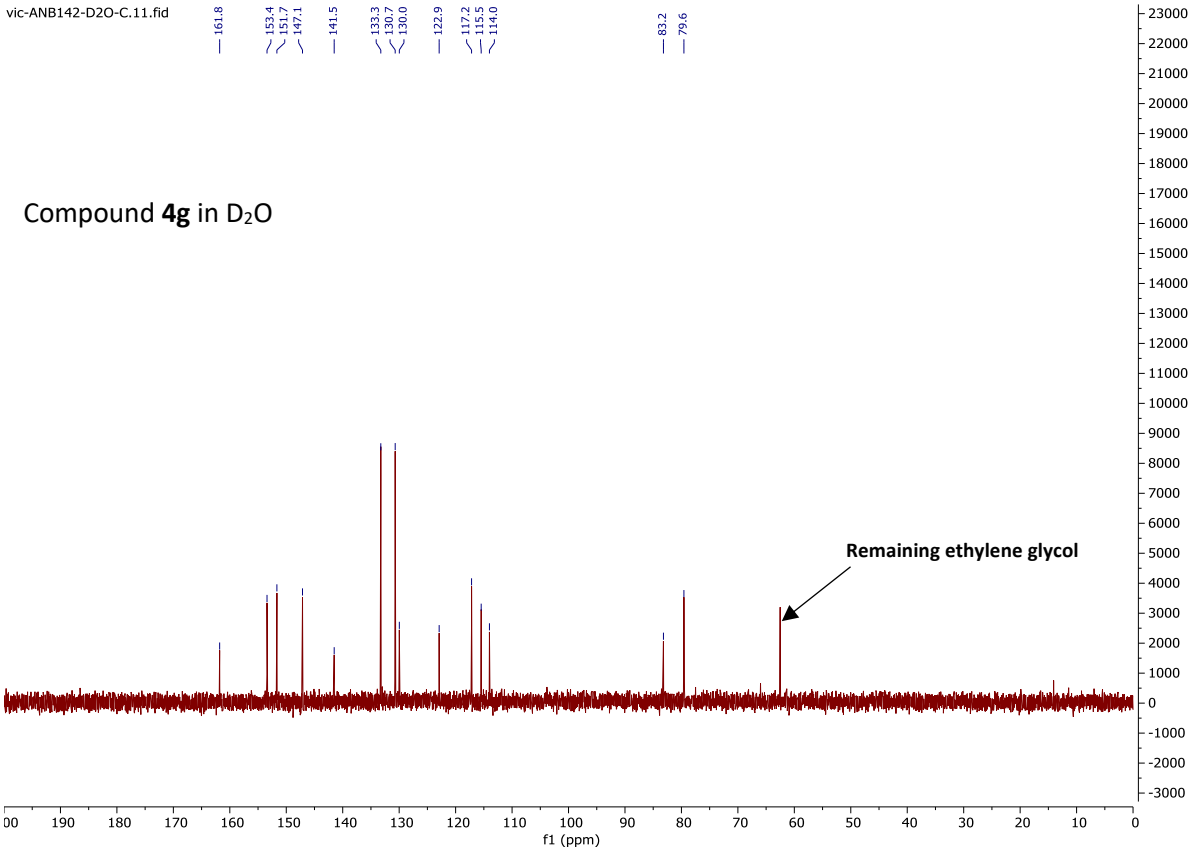

ANB118.fin~4e.10.fid
4e in D2O
Remaining
Ethylene glycol
f1 (ppm)


ANB118.fin~4e.11.fid
4e in D2O
Remaining
Ethylene glycol
f1 (ppm)


ANB077.2-H.H.10.fid
4f in D2O
Remaining
Ethylene glycol
f1 (ppm)


ANB077.2-C.10.fid
4f in D2O
Remaining
Ethylene glycol
f1 (ppm)


vic-ANB142-D2O-C.10.fid
Compound **4g** in D_2O
Remaining ethylene glycol
f1 (ppm)


vic-ANB142-D2O-C.11.fid
Compound **4g** in D_2O
Remaining ethylene glycol
f1 (ppm)

VI - References

[i] Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120,** 215-41.

[ii] a- T. H. Dunning, *J. Chem. Phys.*, 1989, **90**, 1007-1023; b- R. A. Kendall, T. H. Dunning, R. J. Harrison, R, *J. Chem. Phys.*, 1992, **96**, 6796-6806.

[iii] J. Tomasi, B. Mennucci, R. Cammi, *Chem. Rev.*, 2005, **105**, 2999-3094.

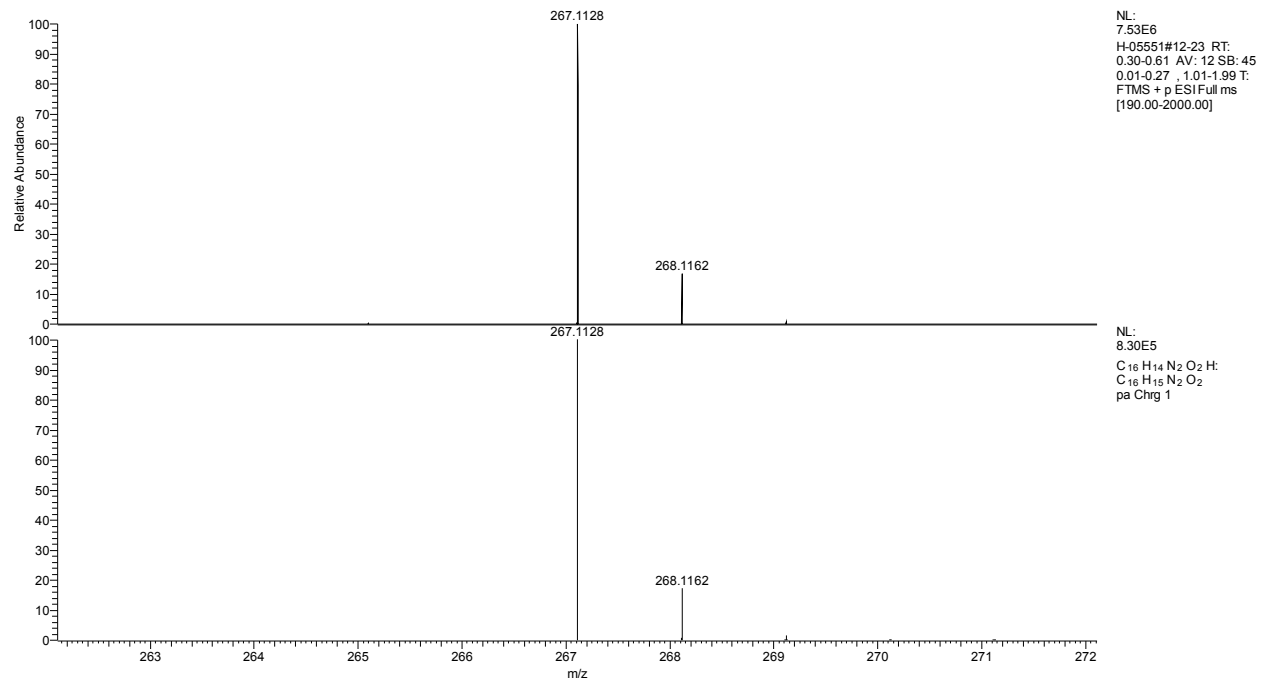
[iv] a) B. P. Pritchard, D. Altarawy, B. Didier, T. D. Gibsom, T. L. Windus, *J. Chem. Inf. Model.*, 2019, **59**, 4814-4820; b) D. J. Feller, *Comput. Chem.*, 1996, **17**, 1571-1586; c) K. L. Schuchardt, B. T. Didier, T. Elsethagen, L. Sun, V. Gurumoorthi, J. Chase, J. Li, T. L. Windus, *J. Chem. Inf. Model.*, 2007, **47**, 1045-1052; d) https://www.basissetexchange.org/.

[v] Chemcraft - graphical software for visualization of quantum chemistry computations. https://www.chemcraftprog.com.

[vi] a) R. Improta, V. Barone, G. Scalmani, M. J. Frisch, *J. Chem. Phys.*, 2006, **125**, 054103; b) R. Improta, G. Scalmani, M. J. Frisch, and V. Barone, *J. Chem. Phys.*, 2007, **127**, 074504.

VI High-Resolution Mass Spectra of 3a-g and 4a-g (HRMS)

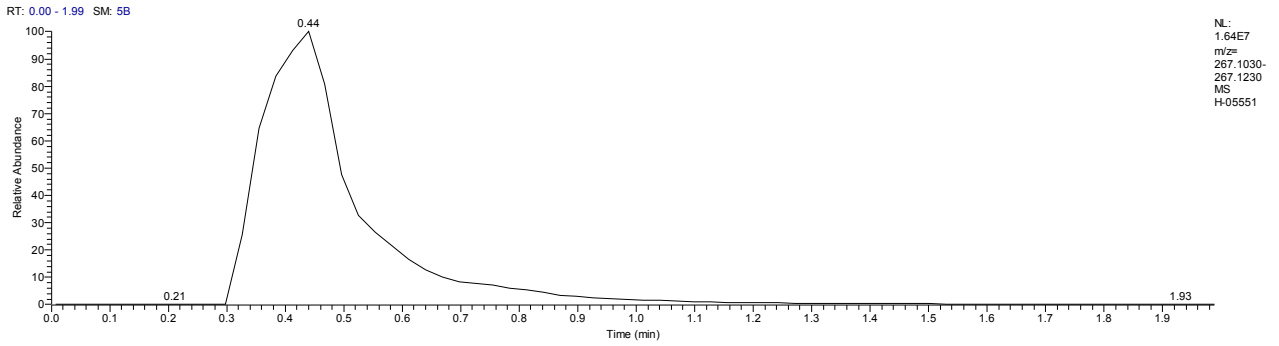
3a



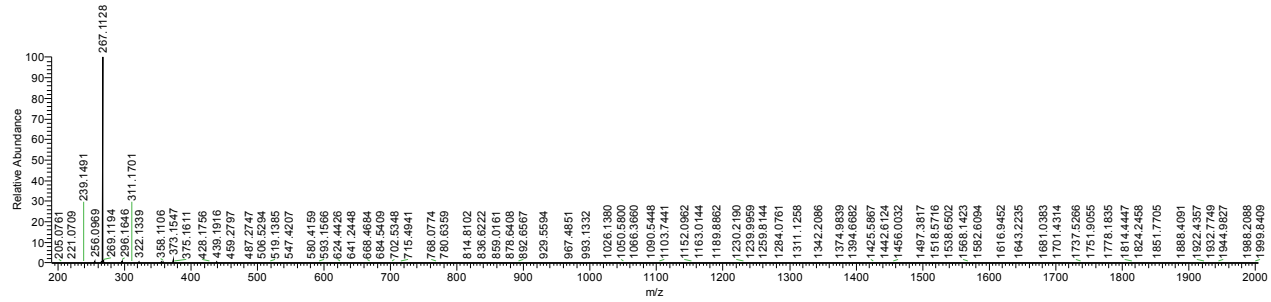
Erreur = 0.0 ppm ; Intensité Relative (%) 100

Calcul des masses monoisotopiques – 1.00728 Th ($-H^+$).
–22.98922 Th ($-Na^+$).
–38.96316 Th ($-K^+$).

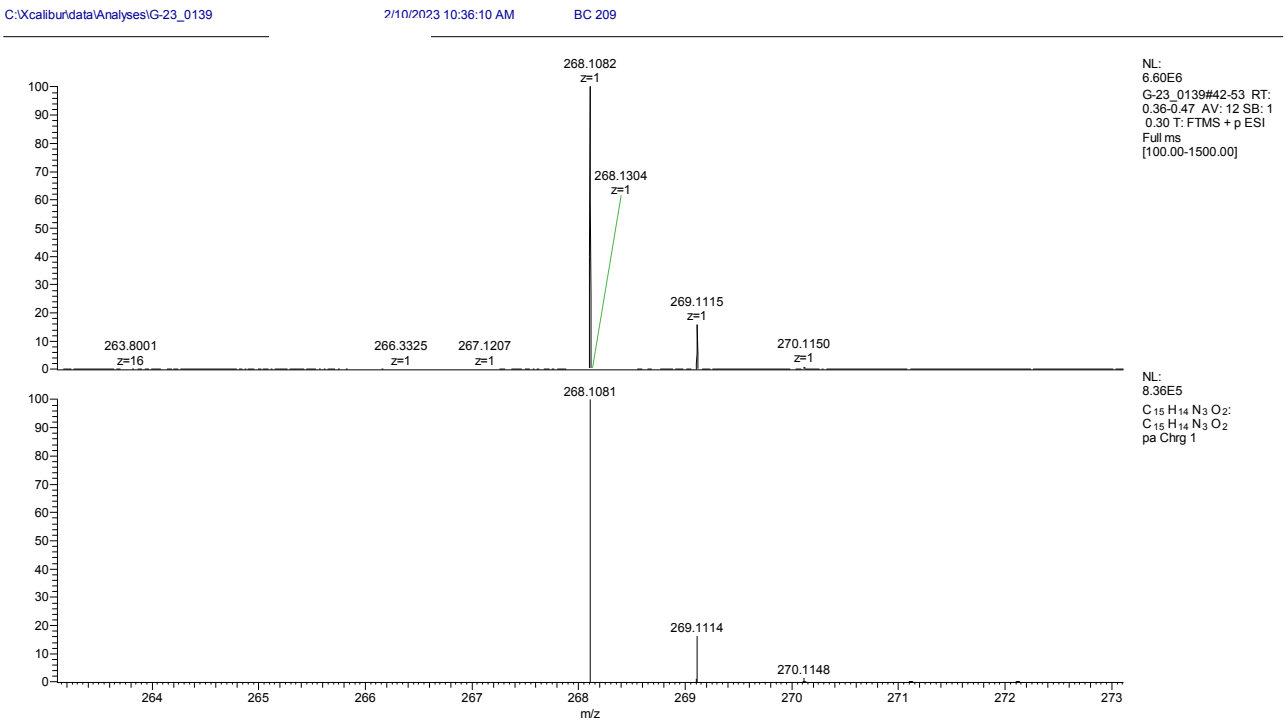
C:\Xcalibur\data\Analyses\H-05551 4/9/2019 3:17:20 PM Anissa Beghennou ANB046
MeOH



H-05551 #12-23 RT: 0.30-0.61 AV: 12 SB: 45 0.01-0.27 , 1.01-1.99 NL: 7.53E6
T: FTMS + p ESI Full ms [190.00-2000.00]



3b



Experimental/theoretical isotopic pattern MS spectrum

Error = 0.5 ppm; Relative Intensity (%) 100

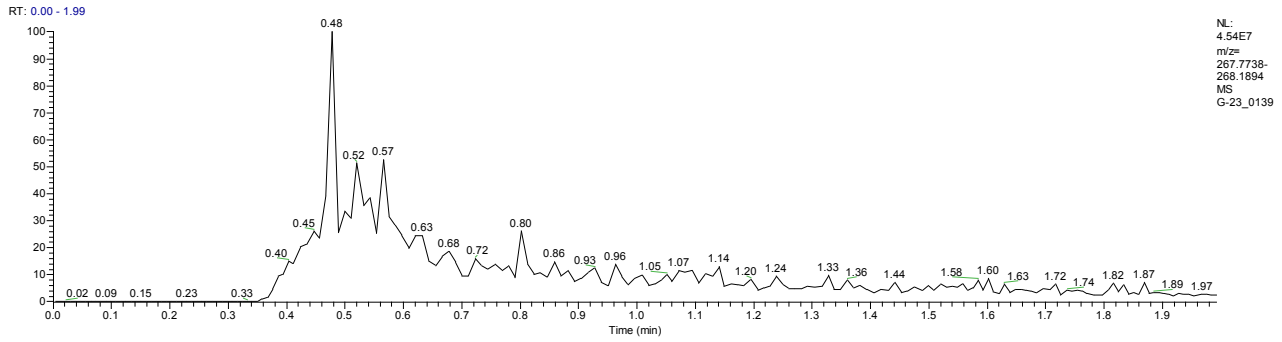
HRMS (ESI) m/z: [M]+ Calcd for C15H14N3O2 268.1081 . Found 268.1082; (Error: 0.5 ppm).

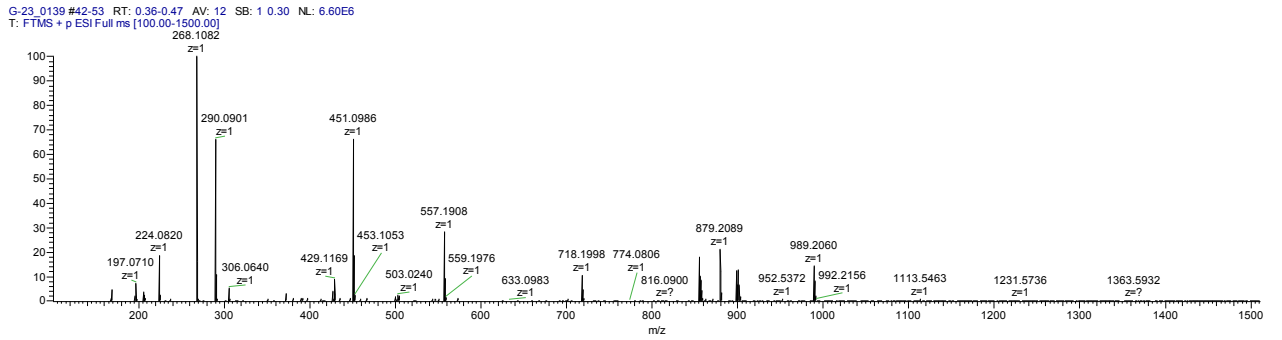
COMPLIANT

Usual adducts for calculation of monoisotopic mass from singly charged ion in positive ionization mode:

– 0.00000 Th (M^+ or $M^{+\bullet}$).
– 1.00728 Th ($M + H^+$).
– 18.0338 Th ($M + NH4^+$).
– 22.98922 Th ($M + Na^+$).
– 38.96316 Th ($M + K^+$).

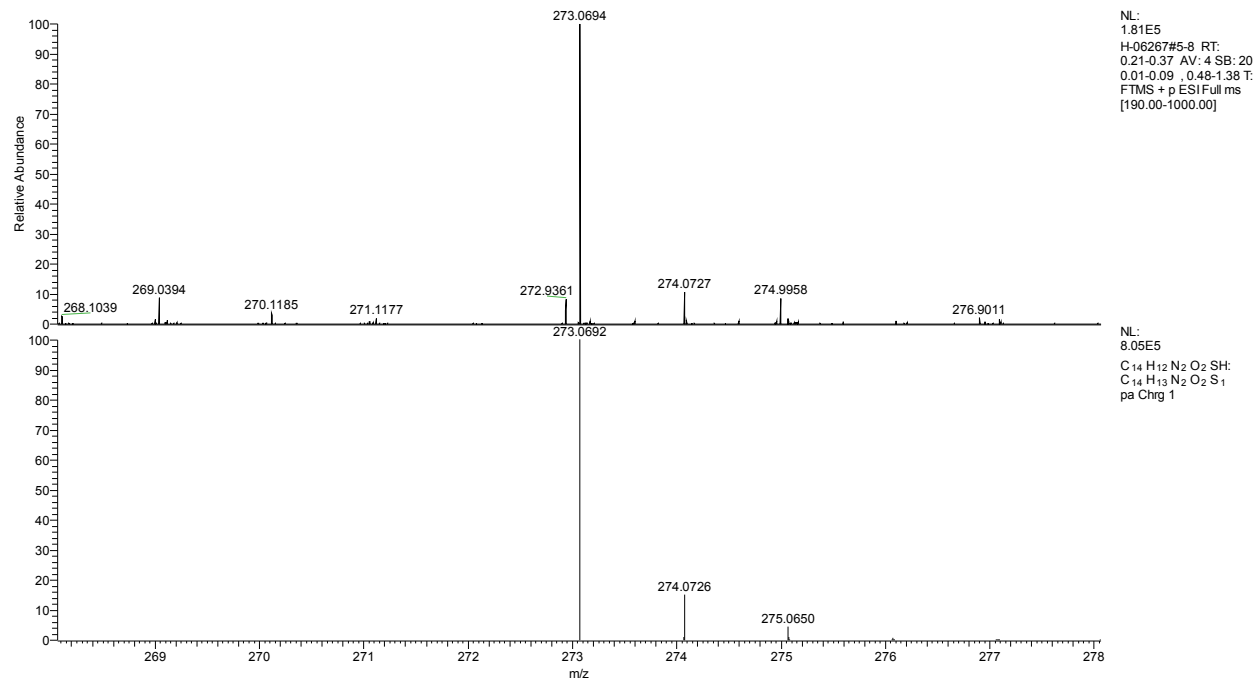
C:\Xcalibur\data\Analyses\G-23_0139 2/10/2023 10:36:10 AM BC 209





Full-MS spectrum

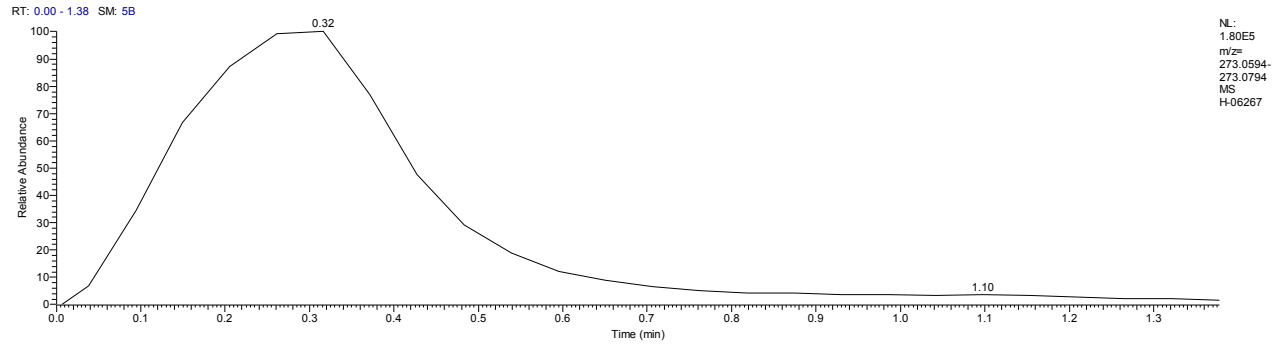
3c



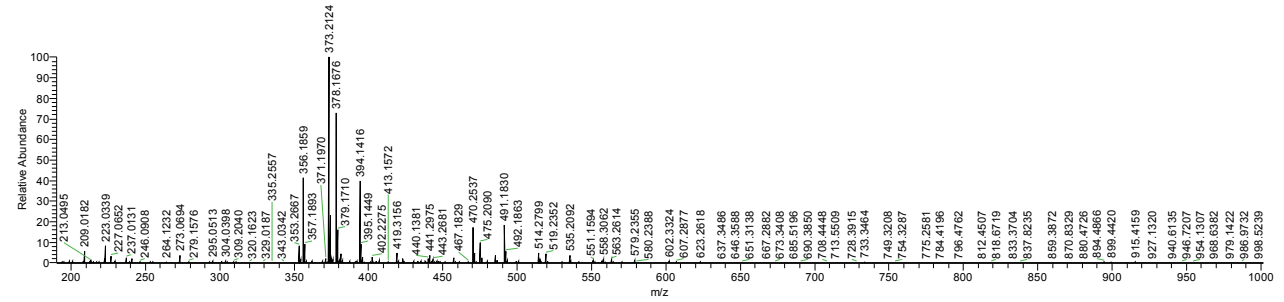
Erreur = 0.6 ppm ; Intensité Relative (%) 100

Calcul des masses monoisotopiques – 1.00728 Th (-H^+).
–18.0338 Th (-$NH4^+$).
–22.98922 Th (-Na^+).
–38.96316 Th (-K^+).

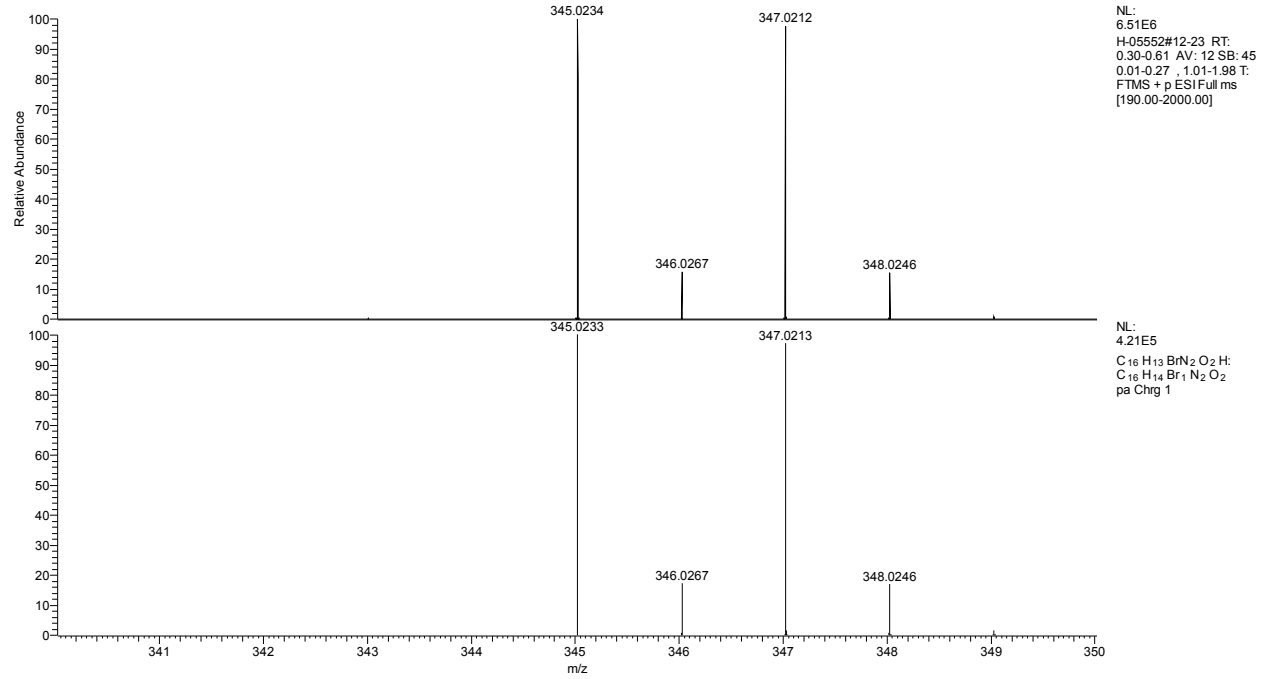
C:\Xcalibur\data\Analyses\H-06267 10/2/2019 10:16:37 AM anissa beghennou ANB122
MeOH



H-06267 #5-9 RT: 0.21-0.43 AV: 5 SB: 20 0.01-0.21 , 0.59-1.38 NL: 3.99E6
T: FTMS + p ESI Full ms [190.00-1000.00]



3d

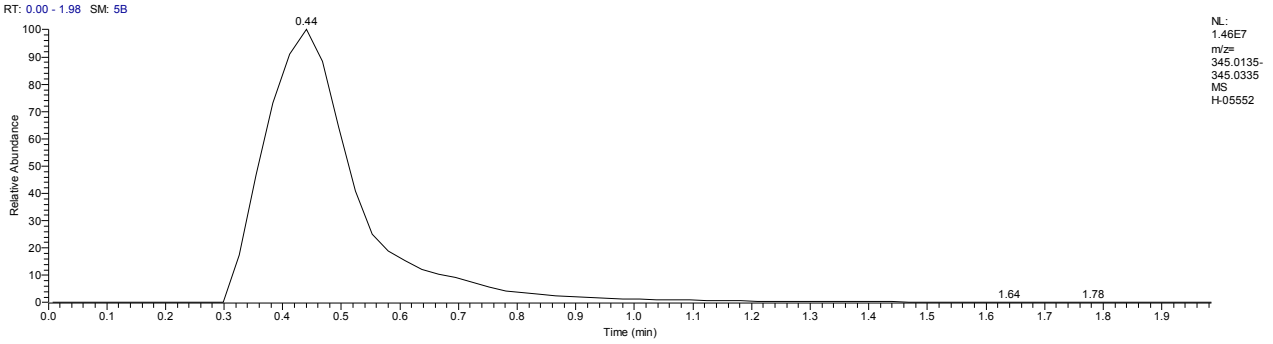


Erreur = 0.2 ppm ; Intensité Relative (%) 100

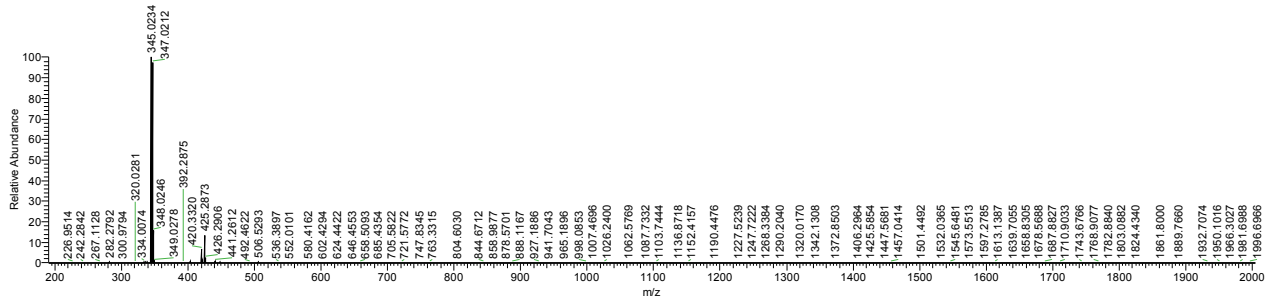
Calcul des masses monoisotopiques – 1.00728 Th (-H^+).
–22.98922 Th (-Na^+).
–38.96316 Th (-K^+).

C:\Xcalibur\data\Analyses\H-05552 4/9/2019 3:33:16 PM Anissa Beghennou ANB061
MeOH

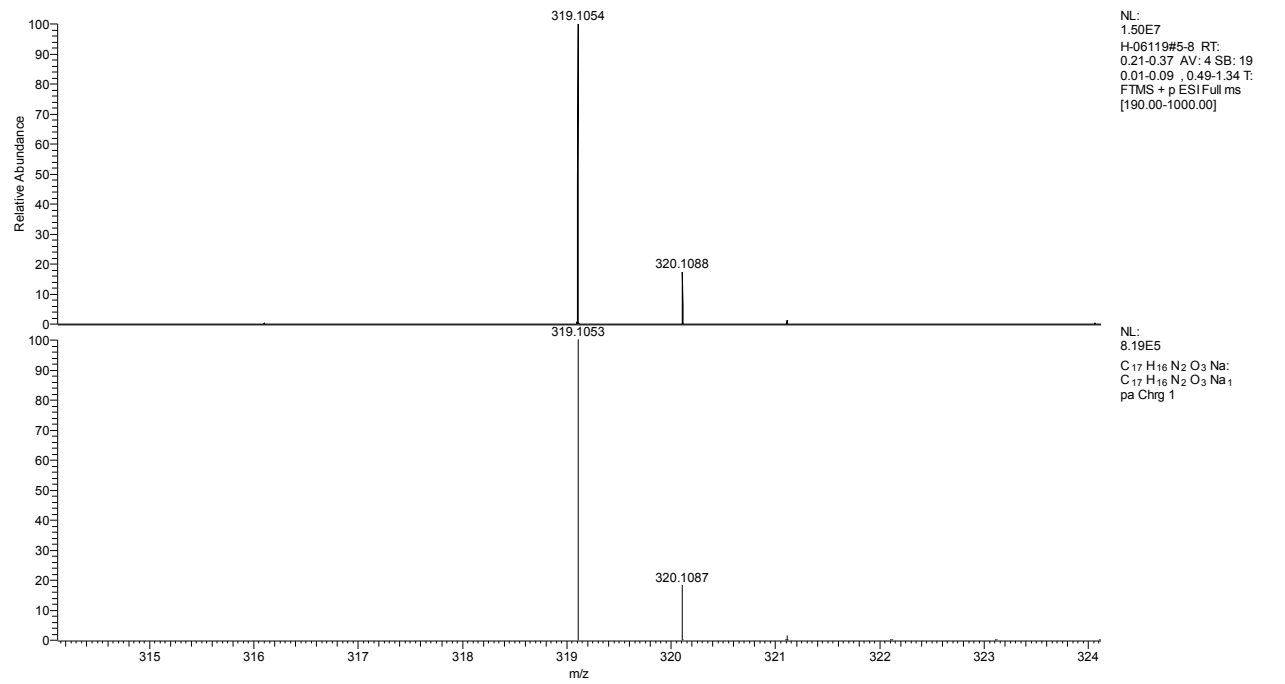
RT: 0.00 - 1.98 SM: 5B



H-05552 #12-23 RT: 0.30-0.61 AV: 12 SB: 45 0.01-0.27 , 1.01-1.98 NL: 6.51E6
T: FTMS + p ESI Full ms [190.00-2000.00]



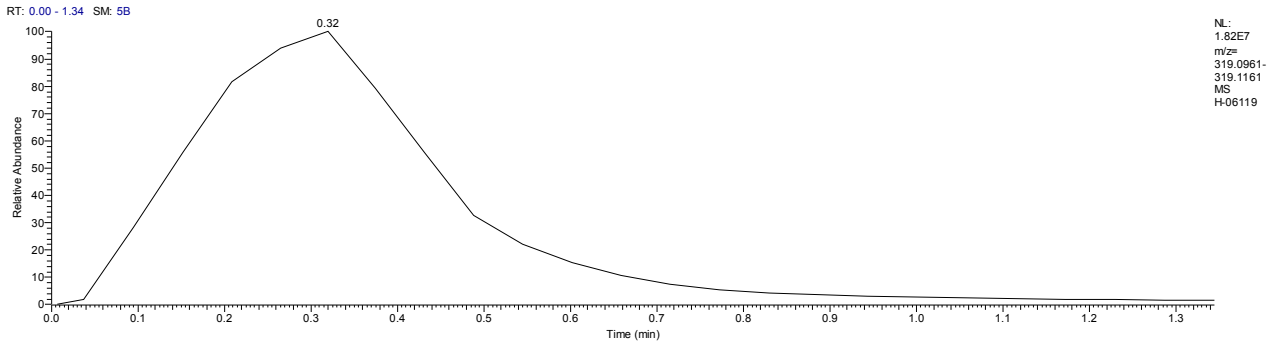
3e



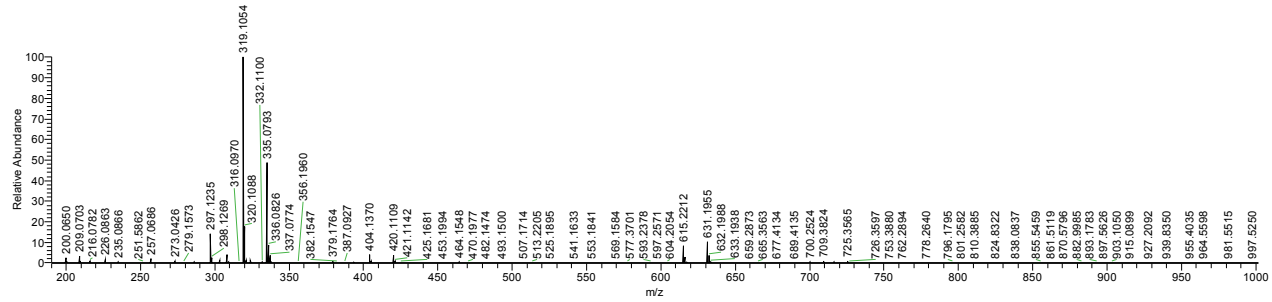
Erreur = 0.3 ppm ; Intensité Relative (%) 100

Calcul des masses monoisotopiques – 1.00728 Th (-H^+).
–18.0338 Th (-$NH4^+$).
–22.98922 Th (-Na^+).
–38.96316 Th (-K^+).

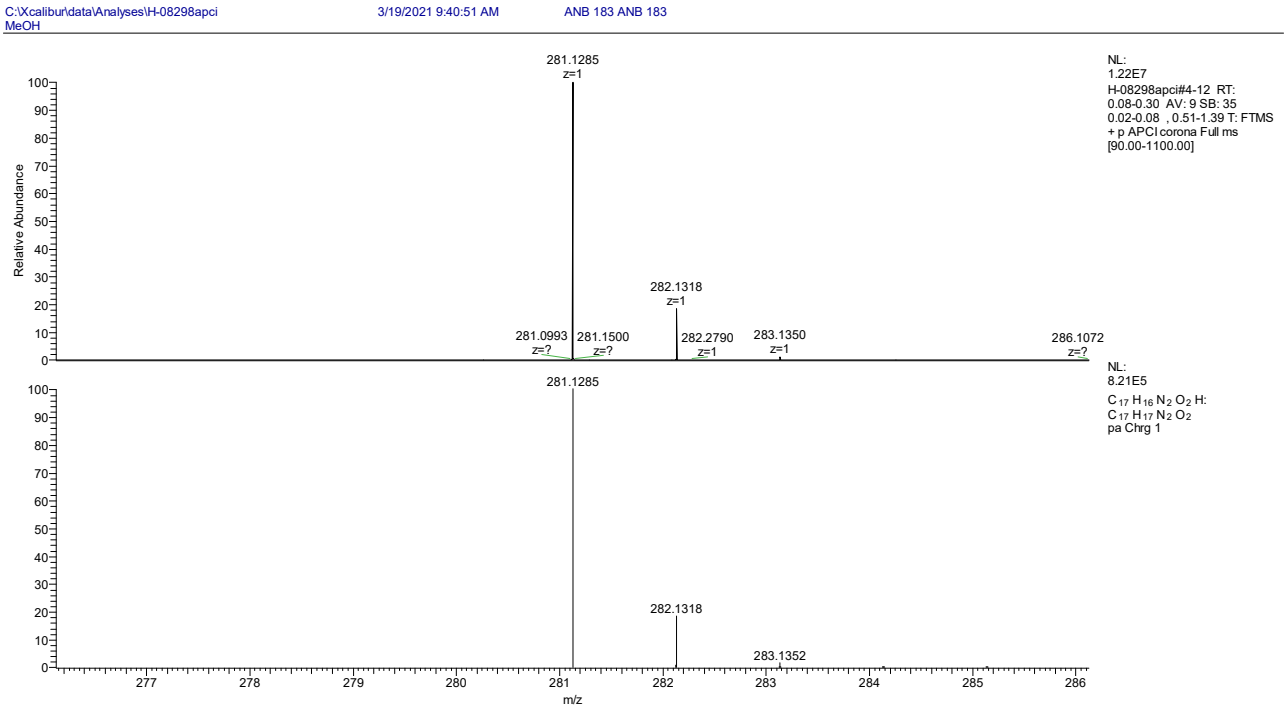
C:\Xcalibur\data\Analyses\H-06119 9/16/2019 8:31:06 AM anissa Beghennou ANB116
MeOH



H-06119 #5-9 RT: 0.21-0.43 AV: 5 SB: 19 0.01-0.21 , 0.60-1.34 NL: 1.30E7
T: FTMS + p ESI Full ms [190.00-1000.00]



3f



Experimental/theoretical isotopic pattern MS spectrum

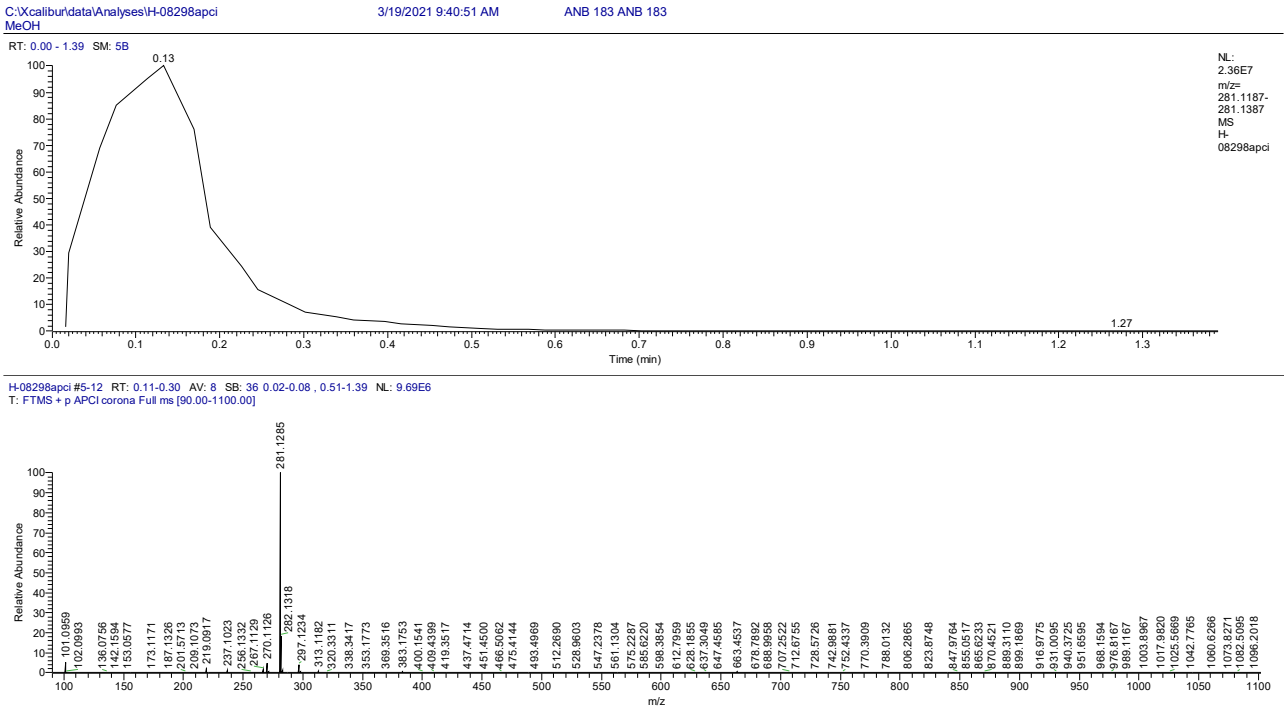
Error = 0.2 ppm; Relative Intensity (%) 100

HRMS (APCI) m/z: [M+H]+ Calcd for C17H16N2O2H 281.1285. Found 281.1285; (Error: 0.2 ppm).

COMPLIANT

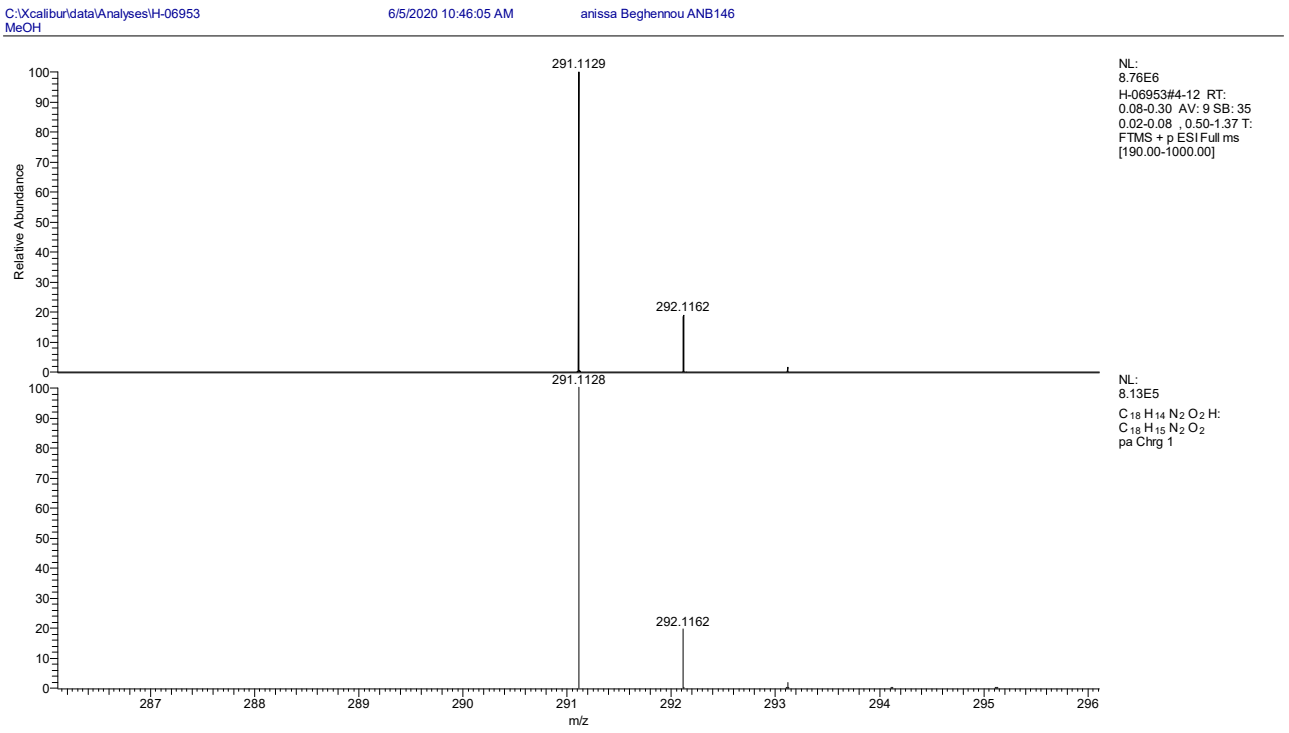
Usual adducts for calculation of monoisotopic mass from singly charged ion in positive ionization mode:

– 0.00000 Th (M^+ or $M^{+\bullet}$).
– 1.00728 Th ($M + H^+$).
– 18.0338 Th ($M + NH4^+$).
– 22.98922 Th ($M + Na^+$).
– 38.96316 Th ($M + K^+$).



Full-MS spectrum

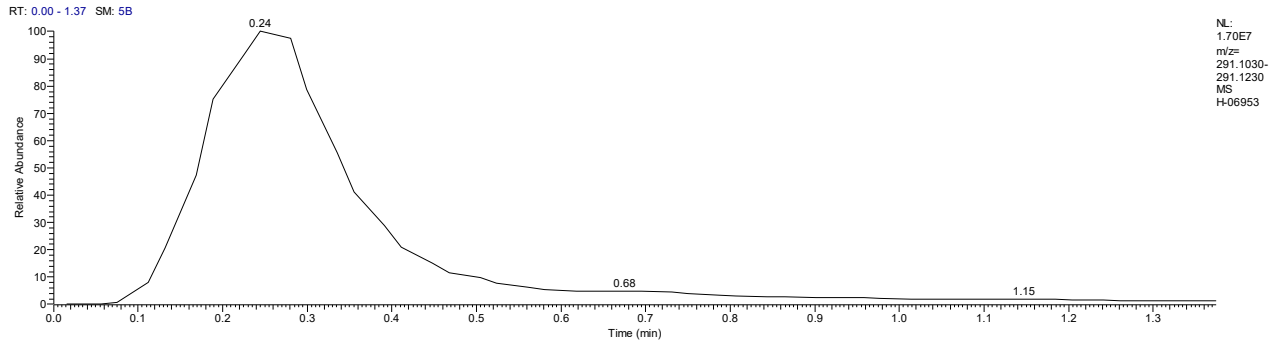
3g



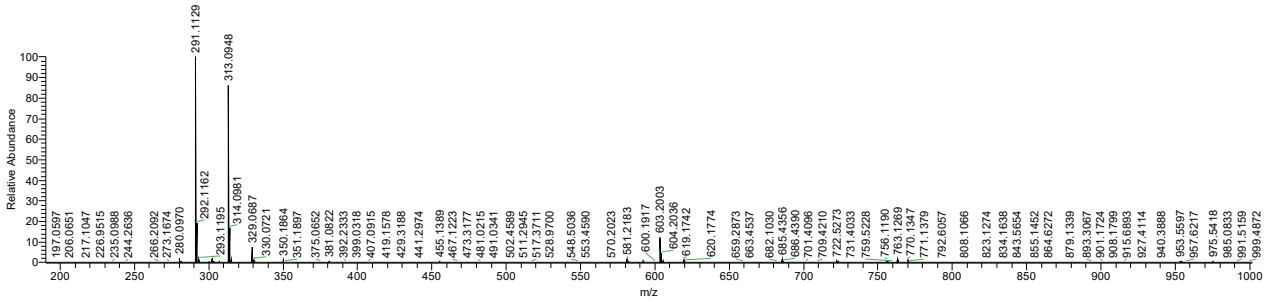
Error = 0.3 ppm; Relative Intensity (%) 100

Calculation of monoisotopic masses – 1.00728 Th (-H^+).
–18.0338 Th (-$NH4^+$).
–22.98922 Th (-Na^+).
–38.96316 Th (-K^+).

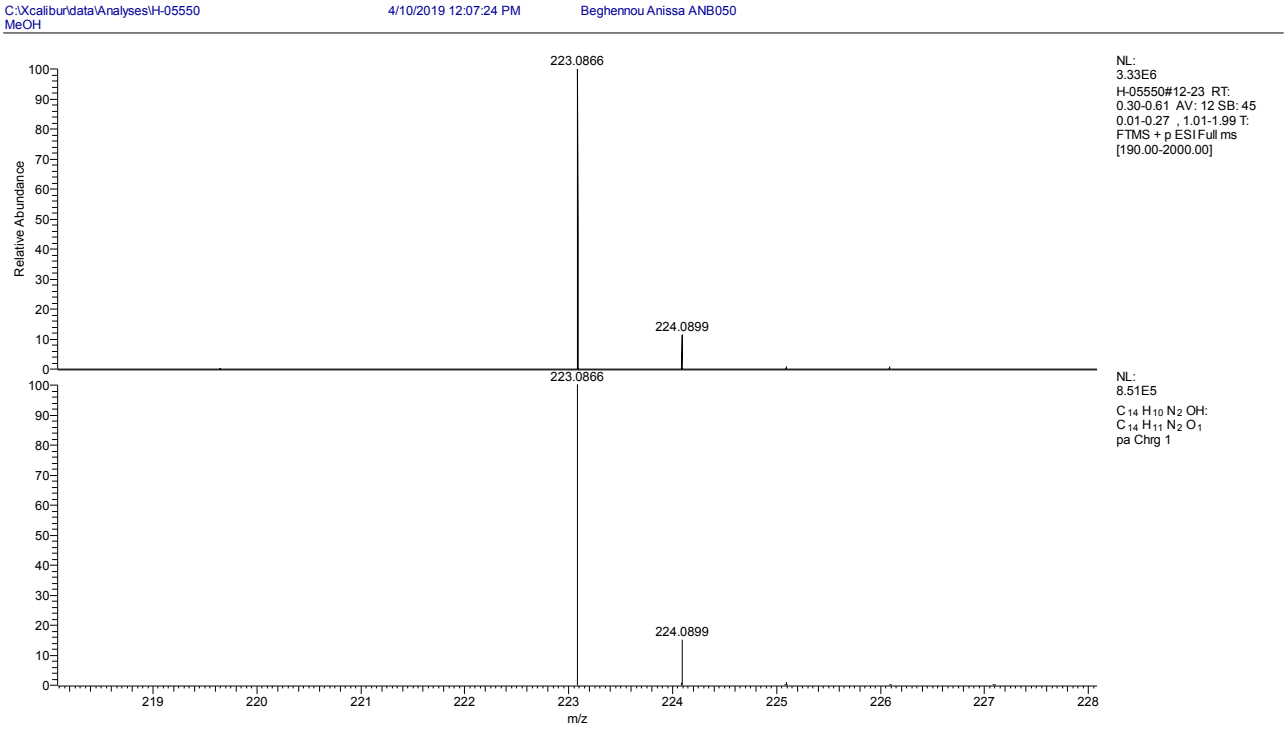
C:\Xcalibur\data\Analyses\H-06953 6/5/2020 10:46:05 AM anissa Beghennou ANB146
MeOH



H-06953 #5-12 RT: 0.11-0.30 AV: 8 SB: 36 0.02-0.08 , 0.50-1.37 NL: 9.92E6
T: FTMS + p ESI Full ms [190.00-1000.00]



4a

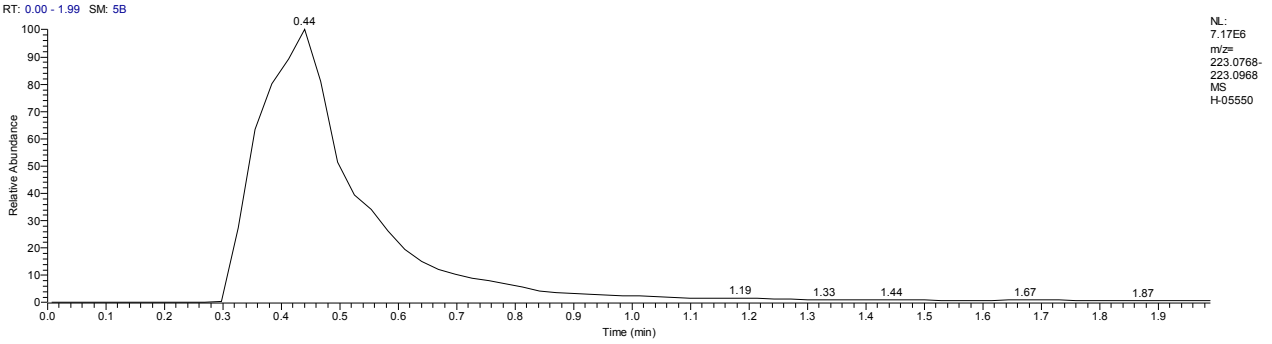


Erreur = 0.0 ppm ; Intensité Relative (%) 100

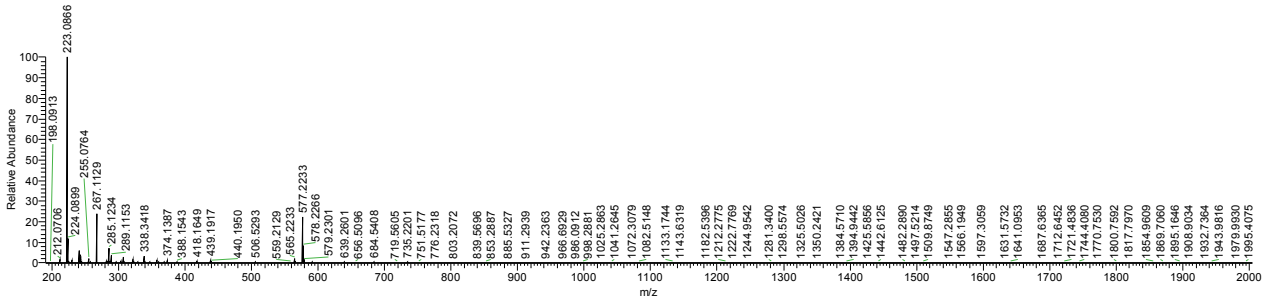
Calcul des masses monoisotopiques – 1.00728 Th ($-H^+$).
–22.98922 Th ($-Na^+$).
–38.96316 Th ($-K^+$).

C:\Xcalibur\data\Analyses\H-05550 4/10/2019 12:07:24 PM Beghennou Anissa ANB050
MeOH

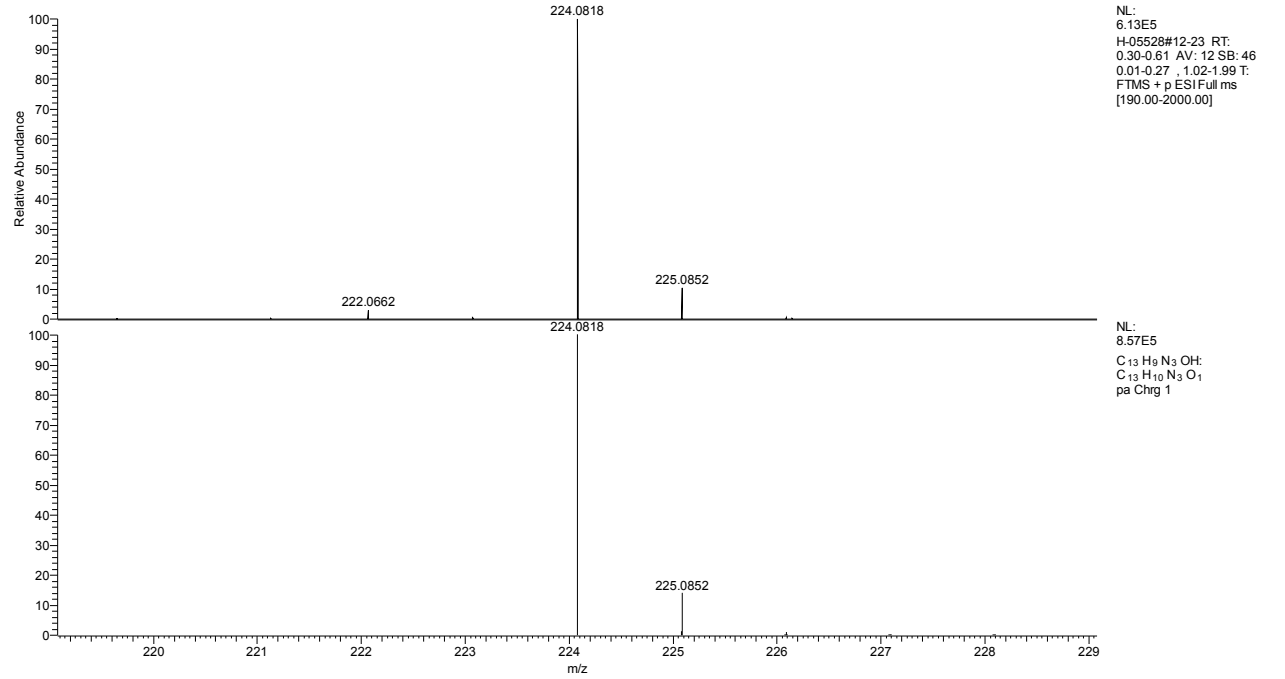
RT: 0.00 - 1.99 SM: 5B



H-05550 #12-23 RT: 0.30-0.61 AV: 12 SB: 45 0.01-0.27 , 1.01-1.99 NL: 3.33E6
T: FTMS + p ESI Full ms [190.00-2000.00]



4b

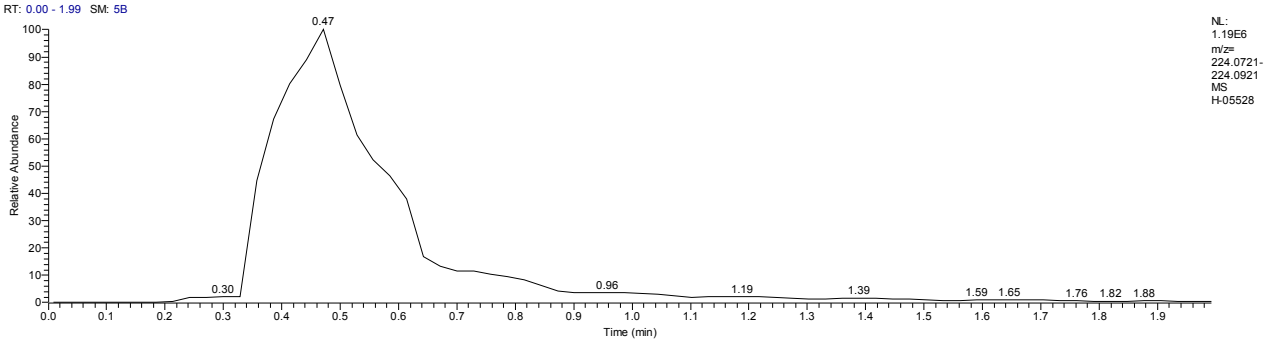


Erreur = -0.2 ppm ; Intensité Relative (%) 100

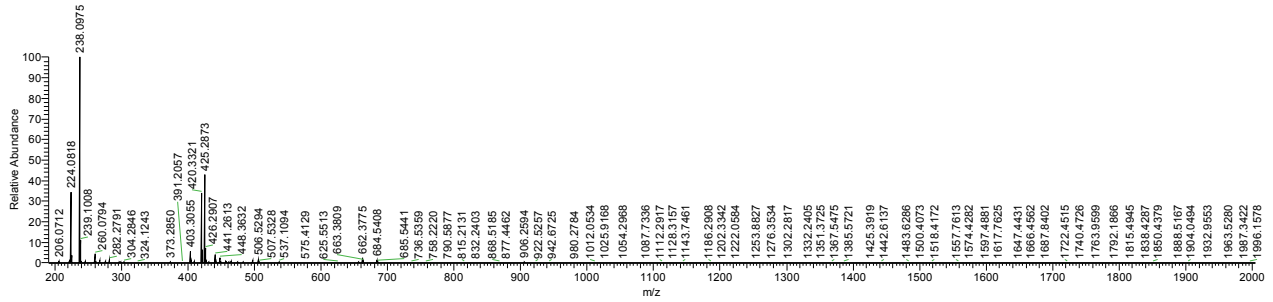
Calcul des masses monoisotopiques – 1.00728 Th (-H^+).
–22.98922 Th (-Na^+).
–38.96316 Th (-K^+).

C:\Xcalibur\data\Analyses\H-05528 4/8/2019 12:34:59 PM Anissa Beghennou ANB064
MeOH

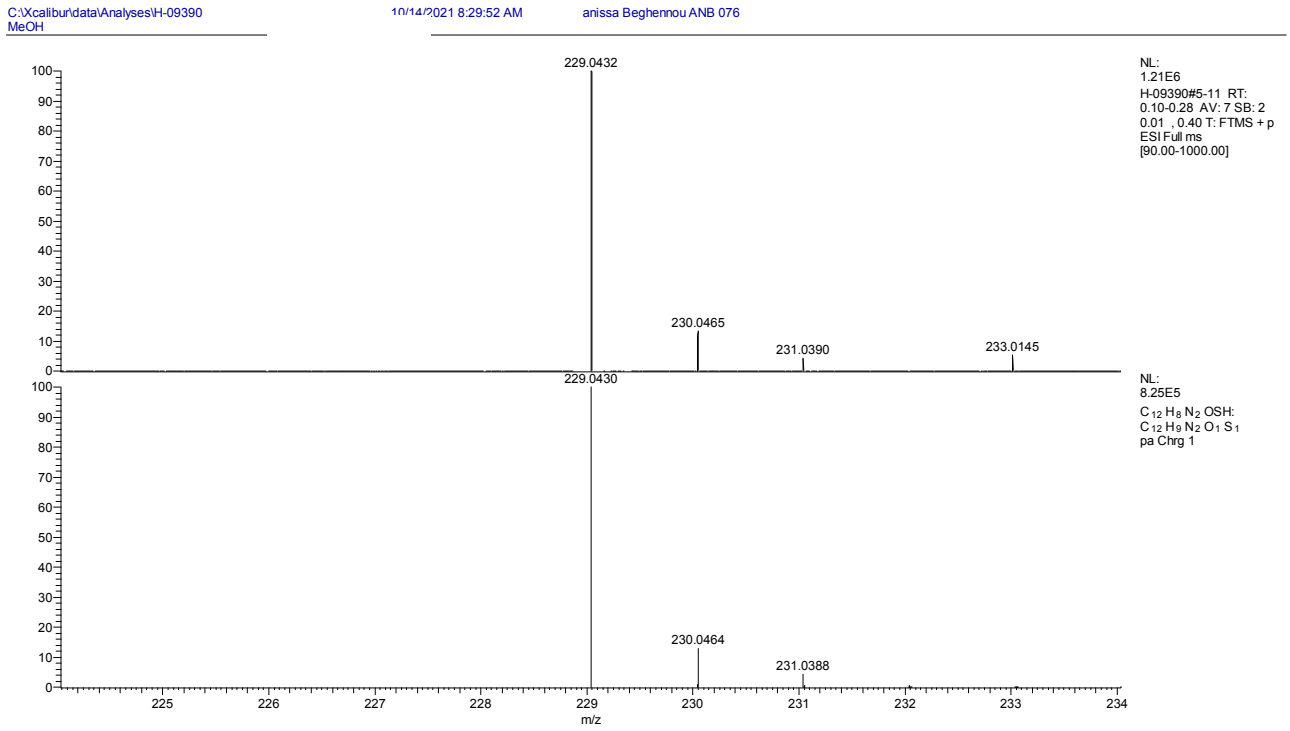
RT: 0.00 - 1.99 SM: 5B



H-05528 #12-23 RT: 0.30-0.61 AV: 12 SB: 46 0.01-0.27 , 1.02-1.99 NL: 1.79E6
T: FTMS + p ESI Full ms [190.00-2000.00]



4c



Experimental/theoretical isotopic pattern MS spectrum

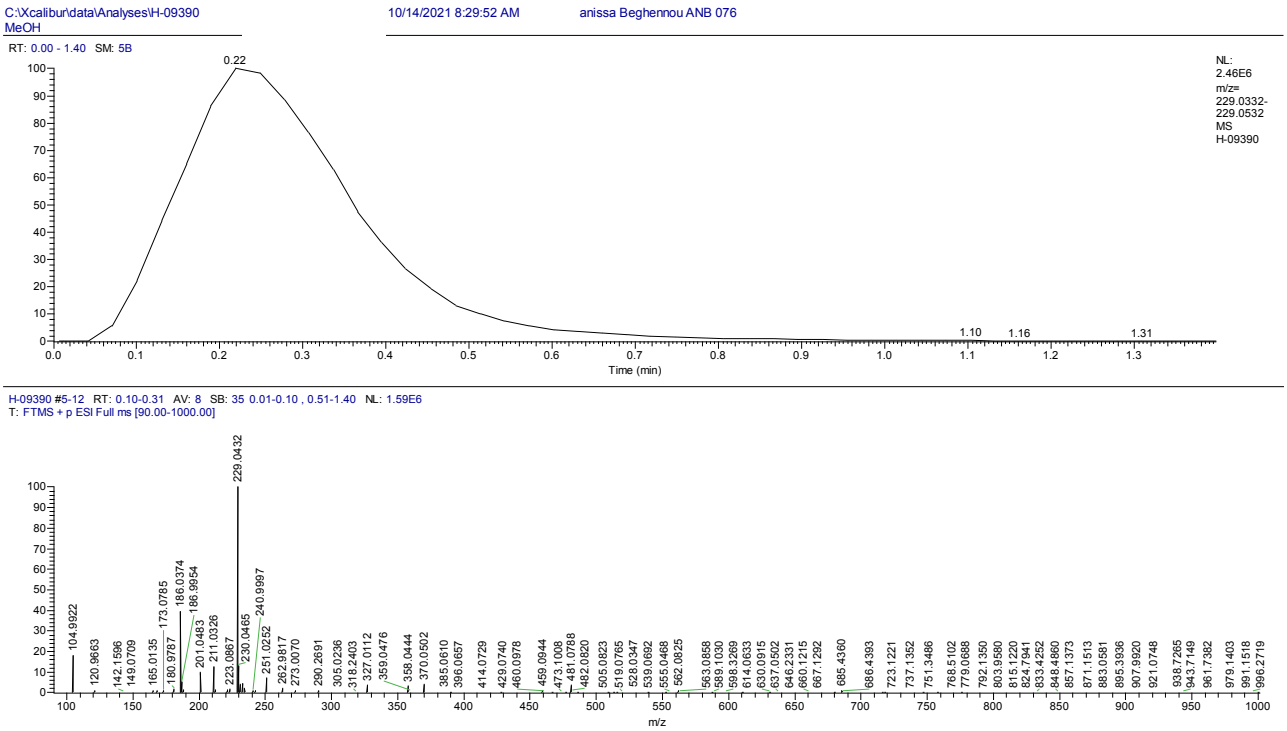
Error = 0.8 ppm; Relative Intensity (%) 100

HRMS (ESI) m/z: [M+H]+ Calcd for C12H8N2OSH 229.0430. Found 229.0432; (Error: 0.8 ppm).

COMPLIANT

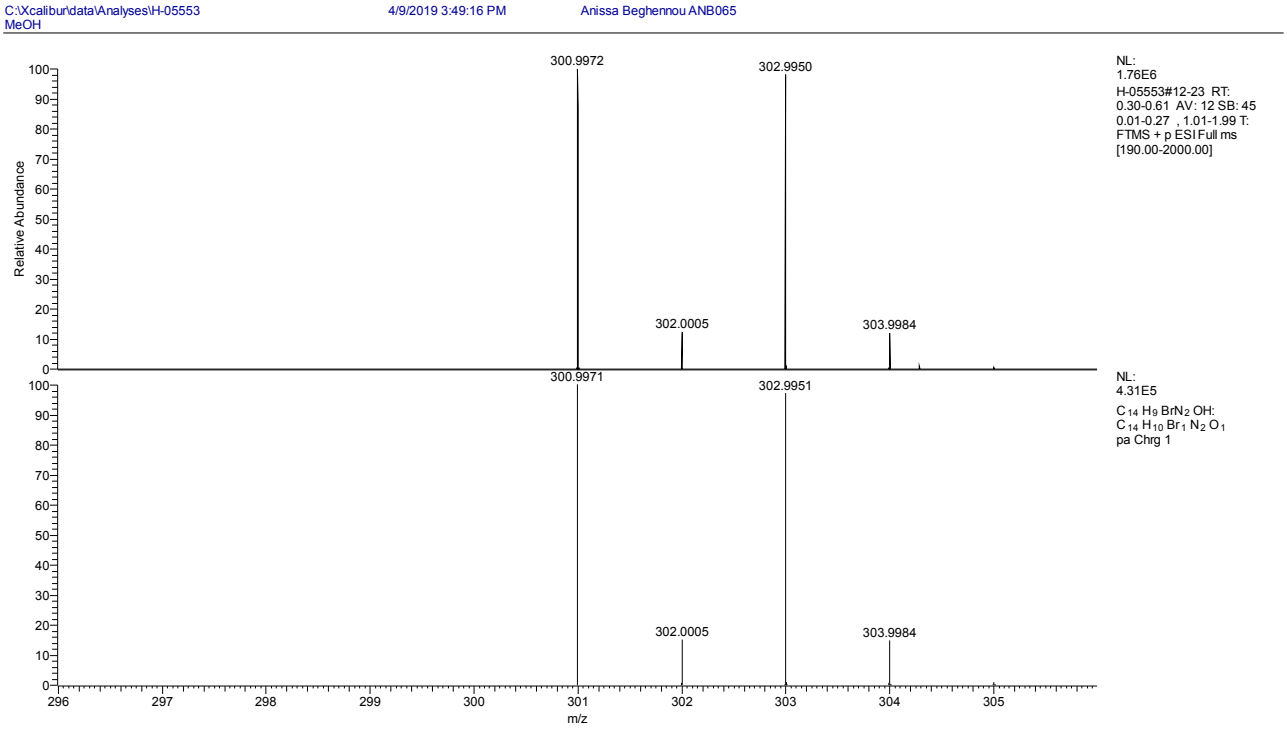
Usual adducts for calculation of monoisotopic mass from singly charged ion in positive ionization mode:

– 0.00000 Th (M^+ or $M^{+\bullet}$).
– 1.00728 Th ($M + H^+$).
– 18.0338 Th ($M + NH4^+$).
– 22.98922 Th ($M + Na^+$).
– 38.96316 Th ($M + K^+$).



Full-MS spectrum

4d



Erreur = 0.3 ppm ; Intensité Relative (%) 100

Calcul des masses monoisotopiques – 1.00728 Th (-H^+).
–22.98922 Th (-Na^+).
–38.96316 Th (-K^+).

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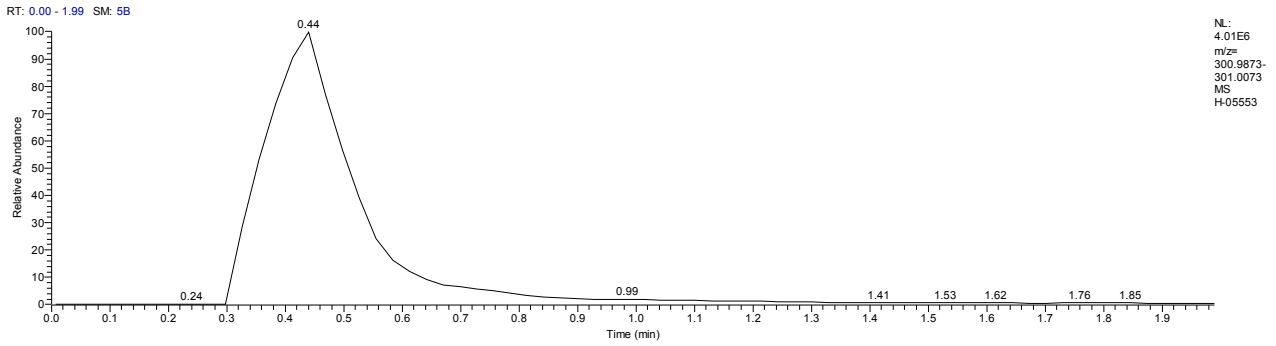
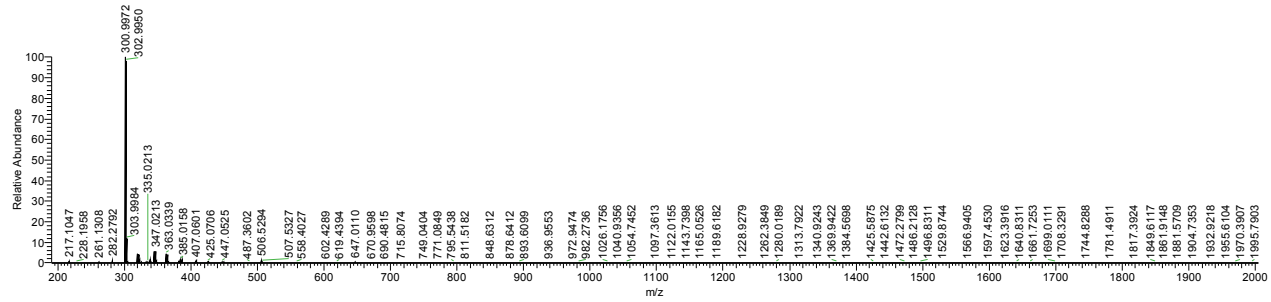
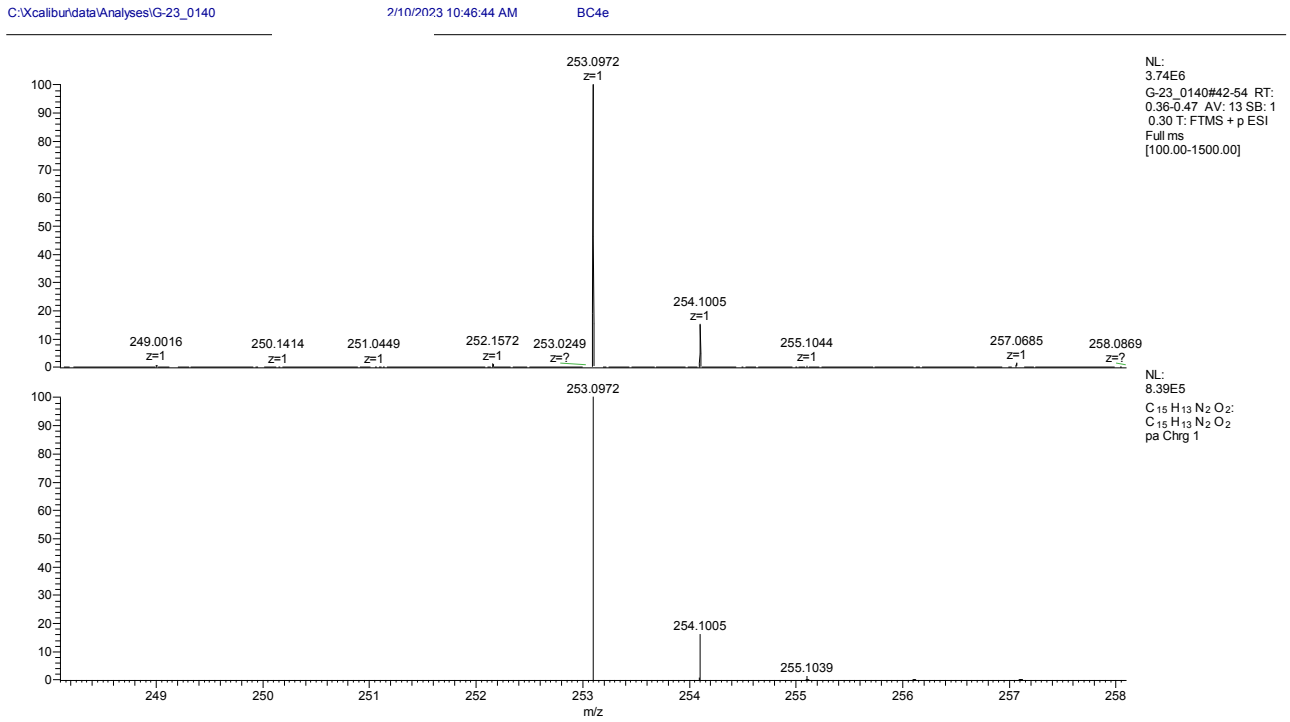
MeOH



H-05553 #12-23 RT: 0.30-0.61 AV: 12 SB: 45 0.01-0.27 , 1.01-1.99 NL: 1.76E6
T: FTMS + p ESI Full ms [190.00-2000.00]



4e



Experimental/theoretical isotopic pattern MS spectrum

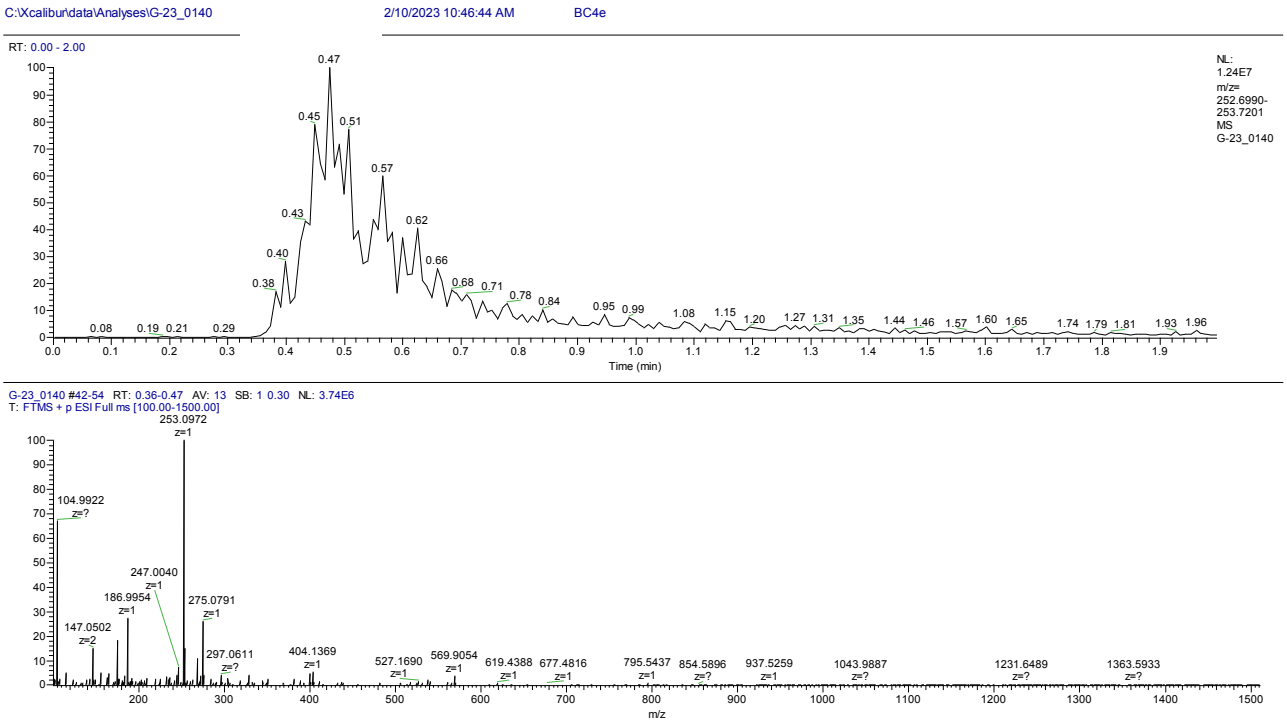
Error = 0.2 ppm; Relative Intensity (%) 100

HRMS (ESI) m/z: [M]+ Calcd for C15H13N2O2 253.0972 . Found 253.0972; (Error: 0.2 ppm).

COMPLIANT

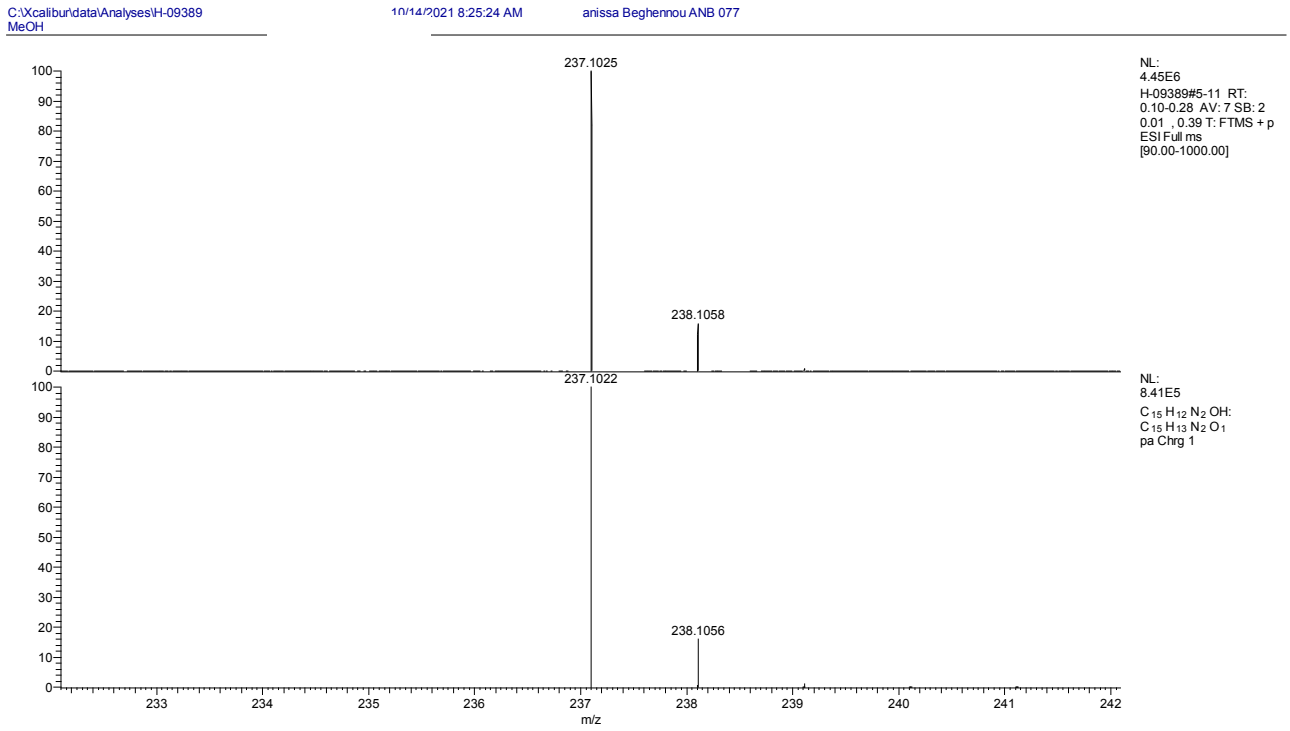
Usual adducts for calculation of monoisotopic mass from singly charged ion in positive ionization mode:

– 0.00000 Th (M^+ or $M^{+\bullet}$).
– 1.00728 Th ($M + H^+$).
– 18.0338 Th ($M + NH4^+$).
– 22.98922 Th ($M + Na^+$).
– 38.96316 Th ($M + K^+$).



Full-MS spectrum

4f



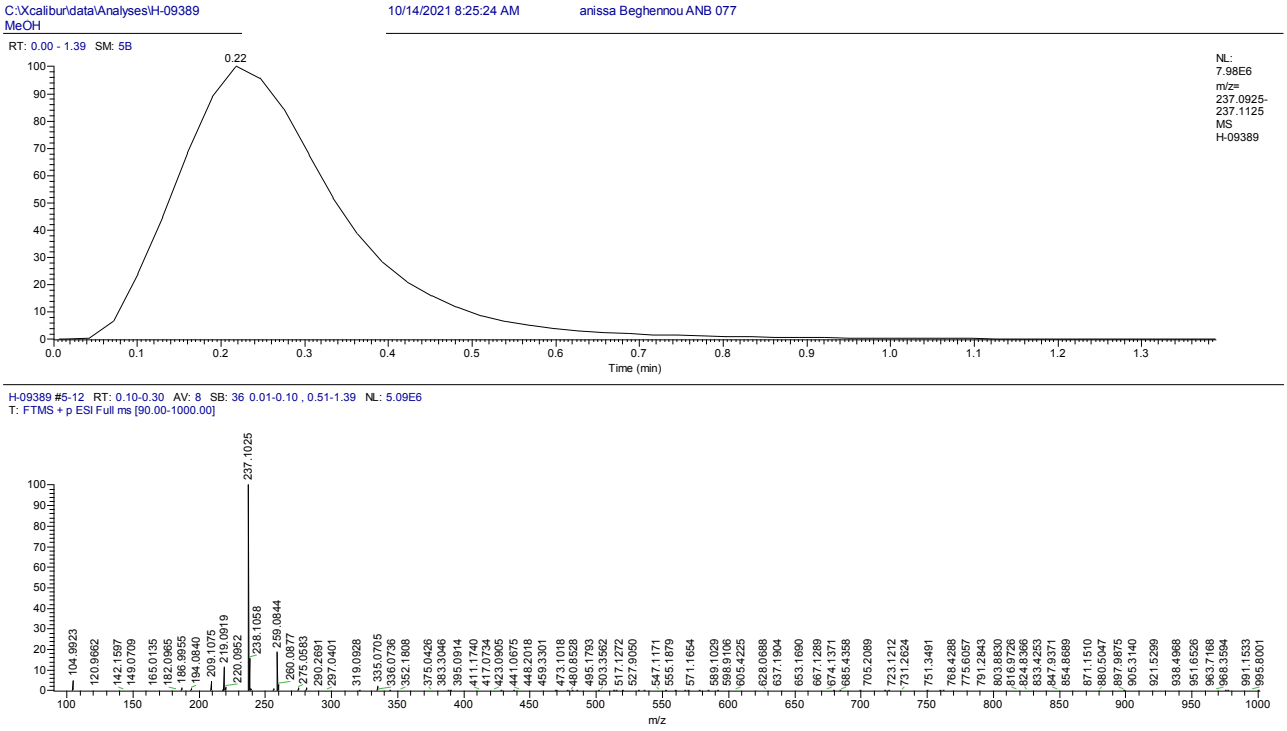
Experimental/theoretical isotopic pattern MS spectrum

Error = 1.1 ppm; Relative Intensity (%) 100

HRMS (ESI) m/z: [M+H]+ Calcd for C15H12N2OH 237.1022. Found 237.1025; (Error: 1.1 ppm).

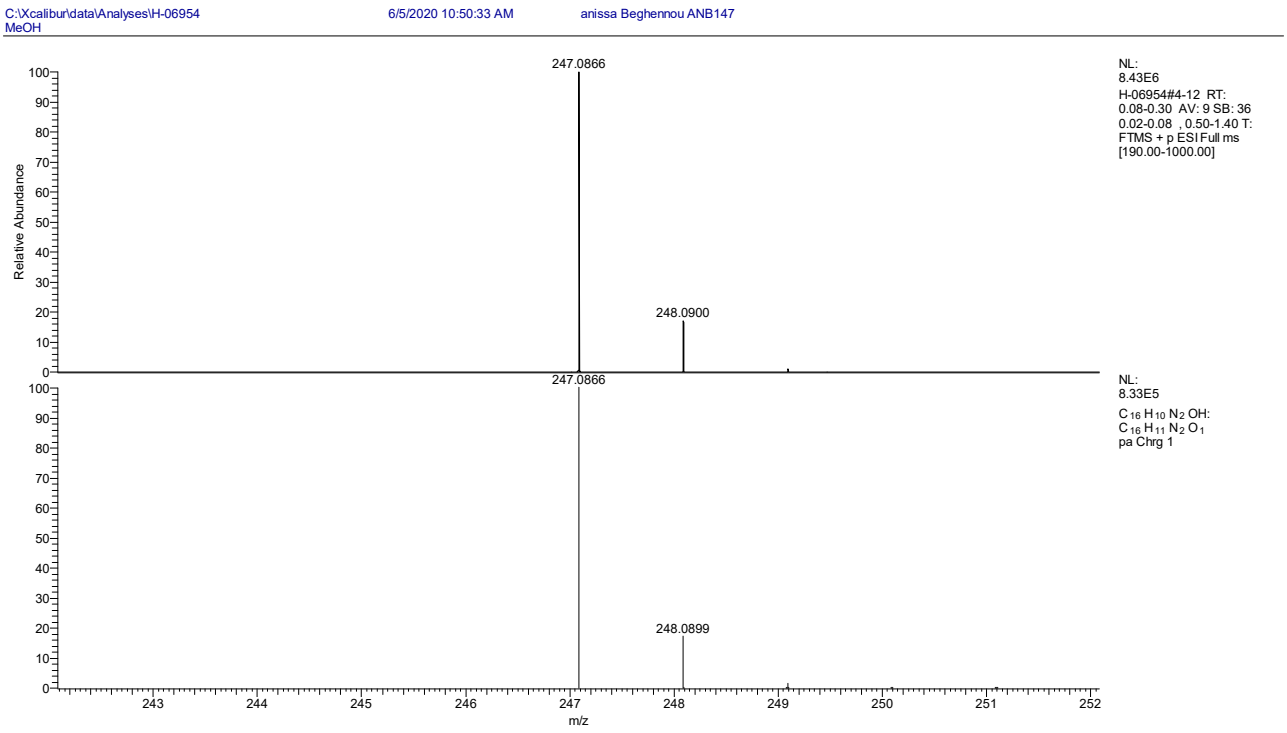
Usual adducts for calculation of monoisotopic mass from singly charged ion in positive ionization mode:

– 0.00000 Th (M^+ or $M^{+\bullet}$).
– 1.00728 Th ($M + H^+$).
– 18.0338 Th ($M + NH4^+$).
– 22.98922 Th ($M + Na^+$).
– 38.96316 Th ($M + K^+$).



Full-MS spectrum

4g



Error = 0.0 ppm; Relative Intensity (%) 100

Calculation of monoisotopic masses – 1.00728 Th (-H^+).
–18.0338 Th (-$NH4^+$).
–22.98922 Th (-Na^+).
–38.96316 Th (-K^+).

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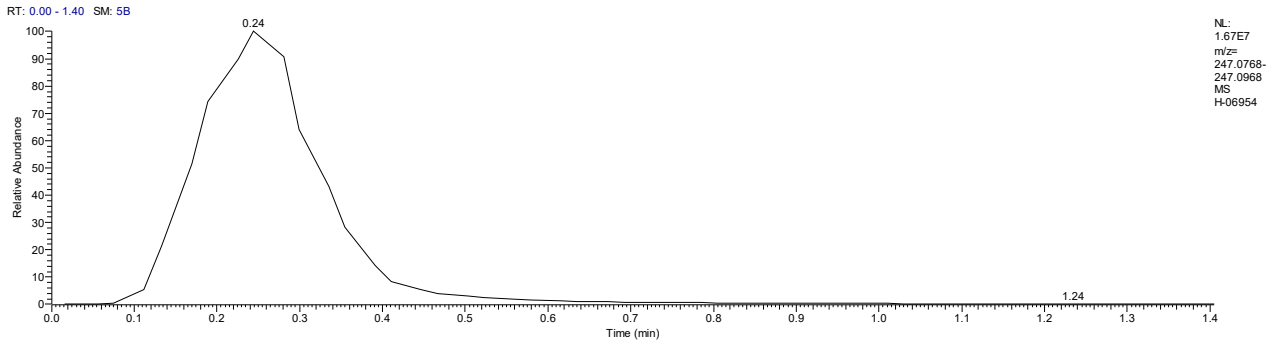
MeOH



H-06954 #5-12 RT: 0.11-0.30 AV: 8 SB: 37 0.02-0.08 , 0.50-1.40 NL: 9.46E6
T: FTMS + p ESI Full ms [190.00-1000.00]