SUPPORTING INFORMATION

Acylpyrazolones possessing heterocyclic moiety in the acyl fragment: intramolecular *vs* intermolecular zwitterionic structure

Stanislava E. Todorova,[a] Rusi I. Rusew,[b] Zhanina S. Petkova,[a] Boris L. Shivachev,[b] Rositsa P. Nikolova,[b] Vanya B. Kurteva[a,*]

[a]*Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Acad. G. Bonchev str., bl. 9, 1113 Sofia, Bulgaria.*
[b]*Institute of Mineralogy and Crystallography "Acad. Ivan Kostov", Bulgarian Academy of Sciences, Acad. G. Bonchev str., bl. 107, 1113 Sofia, Bulgaria.*

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Table S1. The most important crystallographic parameters for the crystal structures of **4a-j** and Cs-complexes.

Compound	B_0124	B_0126	B_0130	B_0144	B_0145	B_0146	B_0147
Compound	**4e solvent**	**4c**	**4e**	**2 compl.**	**4d**	**4d Cs**	**4i compl.**
CCDC	2119868	2119863	2119859	2119866	2119861	2119862	2119864
Empirical formula	$C_{34}H_{41}N_7O_4$	$C_{16}H_{19}N_3O_2S$	$C_{16}H_{19}N_3O_2$	$C_{13}H_{10}ClCsN_2O_5$	$C_{22}H_{24}N_4O_2$	$C_{26}H_{29}CsN_6O_2$	$C_{20}H_{26}CsN_3O_5$
Formula weight	611.74	317.40	285.34	442.59	376.45	590.46	521.35
Temperature	290K	290K	290K	290K	290K	290K	290K
Crystal system	Triclinic	Monoclinic	Monoclinic	Orthorhombic	Monoclinic	Triclinic	Monoclinic
Space group	*P*-1	$P2_1$	$P2_1/n$	*Fdd*2	$P2_1/c$	*P*-1	$P2_1/n$
a/Å	9.9053(5)	9.6424(5)	11.3849(4)	48.4669(10)	13.0544(6)	9.5466(8)	8.1311(3)
b/Å	11.6377(6)	8.0087(3)	9.9562(4)	32.2650(5)	13.0083(6)	11.0591(11)	18.2830(6)
c/Å	15.0249(6)	10.9078(5)	13.2945(5)	4.40930(10)	11.7110(5)	14.5749(14)	14.9298(5)
α/°	86.844(4)	90	90	90	90	72.225(3)	90
β/°	89.823(4)	109.047(2)	101.3400(10)	90	104.3530(10)	80.490(2)	101.0150(10)
γ/°	69.381(5)	90	90	90	90	70.549(2)	90
Volume/Å^3	1618.34(14)	796.22(6)	1477.52(10)	6895.2(2)	1926.64(15)	1378.2(2)	2178.59(13)
Z	2	2	4	16	4	2	4
ρ_{calc}g/cm^3	1.255	1.324	1.283	1.705	1.298	1.423	1.590
μ/mm^{-1}	0.085	0.214	0.087	2.324	0.085	1.376	1.735
F(000)	652.0	336.0	608.0	3424.0	800.0	596.0	1048.0
Crystal size/mm^3	0.35×0.2×0.1	0.1×0.05×0.05	0.5×0.4×0.3	0.3×0.1×0.05	0.2×0.15×0.1	0.3×0.25×0.2	0.3×0.25×0.2
Radiation	Mo*K*α λ = 0.71073	Mo*K*α λ = 0.71073	Mo*K*α λ = 0.71073	Mo*K*α λ = 0.71073	Mo*K*α λ = 0.71073	Mo*K*α λ = 0.71073	Mo*K*α λ = 0.71073
2*Θ* range for data collection/°	3.746–52.742	3.95–61.006	5.482–52.334	3.032–52.028	4.492–54.968	4.536–57.396	4.456–55.296
Reflections collected/ independent	11782/11782	44584/4862	25571/2916	33825/3406	37820/4394	78956/6899	68060/5020
Rint/Rsigma	*twin/0.0906	0.0483/0.0319	0.0531/0.0275	0.0437/0.0185	0.0681/0.0407	0.0410/0.0191	0.0363/0.0146
Data/restraints/ parameters	11782/0/418	4862/1/204	2916/0/195	3406/1/200	4394/0/259	6899/0/319	5020/0/263
Goodness-of-fit on F^2	0.934	1.139	1.065	1.136	1.059	1.083	1.115
Final *R* indexes [I>=2σ (I)]	R_1 = 0.0640 wR_2 = 0.1680	R_1 = 0.0550 wR_2 = 0.1151	R_1 = 0.0475 wR_2 = 0.1218	R_1 = 0.0308 wR_2 = 0.0724	R_1 = 0.0502 wR_2 = 0.1052	R_1 = 0.0287 wR_2 = 0.0630	R_1 = 0.0385 wR_2 = 0.0824
Final *R* indexes [all data]	R_1 = 0.1162 wR_2 = 0.1790	R_1 = 0.0659 wR_2 = 0.1197	R_1 = 0.0556 wR_2 = 0.1294	R_1 = 0.0324 wR_2 = 0.0738	R_1 = 0.0867 wR_2 = 0.1221	R_1 = 0.0379 wR_2 = 0.0701	R_1 = 0.0447 wR_2 = 0.0863
Largest diff. peak/hole / e Å^{-3}	0.49/-0.49	0.24/-0.23	0.37/-0.19	0.61/-0.38	0.18/-0.18	0.62/-0.67	0.94/-0.78

Table S1. Continued.

Compound	B_0161	B_0168	B_0170	B_0175	S_373	A167	B_0178
Compound	**4h**	**4f**	**4j compl.**	**4i**	**4b**	**4a**	**4c compl.**
CCDC	2119867	2119870	2119865	2119869	2119860	2119858	2119871
Empirical formula	$C_{19}H_{25}N_3O_2$	$C_{18}H_{23}N_3O_2$	$C_{22}H_{32}CsN_3O_7$	$C_{20}H_{29}N_3O_6$	$C_{16}H_{19}N_3O_3$	$C_{17}H_{21}N_3O_2$	$C_{17}H_{26}CsN_3O_8S$
Formula weight	327.42	313.39	583.41	407.46	301.34	299.37	565.38
Temperature	290K	290K	290K	290K	290K	290	290
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/n$	$P2_1$	P-1
a/Å	6.7988(8)	6.7130(5)	11.8674(8)	12.097(3)	9.4773(2)	9.6845(4)	7.6127(10)
b/Å	18.792(2)	18.2866(15)	12.8807(8)	14.929(3)	7.8846(2)	7.9709(4)	11.6570(11)
c/Å	13.5975(16)	13.4679(11)	16.3307(11)	11.827(3)	20.2726(5)	10.8995(5)	15.4167(19)
α/°	90	90	90	90	90	90	101.296(4)
β/°	94.066(4)	92.780(3)	92.978(2)	107.816(8)	95.646(2)	108.389(9)	103.003(3)
γ/°	90	90	90	90	90	90	105.412(4)
Volume/Å^3	1732.9(4)	1651.3(2)	2492.9(3)	2033.4(8)	1507.50(7)	798.41(7)	1236.6(3)
Z	4	4	4	4	4	2	2
ρ_{calc}g/cm^3	1.255	1.261	1.554	1.331	1.328	1.245	1.518
μ/mm^{-1}	0.083	0.084	1.531	0.099	0.093	0.083	1.624
F(000)	704.0	672.0	1184.0	872.0	640.0	320.0	568.0
Crystal size/mm^3	0.3×0.3×0.3	0.3×0.25×0.25	0.4×0.3×0.3	0.5×0.3×0.3	0.3×0.25×0.12	0.32 ×0.24×0.22	0.25×0.1×0.1
Radiation	Mo*K*α λ = 0.71073	Mo*K*α λ = 0.71073	Mo*K*α λ = 0.71073	Mo*K*α λ = 0.71073	Mo*K*α λ = 0.71073	Mo*K*α λ = 0.71073	Mo*K*α λ = 0.71073
2Θ range for data collection/°	5.274–54.206	5.388– 54.206	4.03–54.202	4.532–50.536	5.548–87.384	3.938 to 55.95	5.284 to 52.098
Reflections collected/ independent	50776/3786	51749/3619	76373/5427	48896/3601	32182/11468	3905 /3698	62002/4829
Rint/Rsigma	0.0518/0.0216	0.0611/0.0243	0.0429/0.0171	0.0429/0.0175	0.0267/0.0333	0.0381/0.0688	0.0296/0.0130
Data/restraints/ parameters	3786/0/242	3619/0/232	5427/6/329	3601/0/276	11468/0/275	3698/1/204	4829/1/282
Goodness-of-fit on F^2	1.028	1.091	1.064	1.035	1.023	1.000	1.066
Final *R* indexes [I>=2σ (I)]	R_1 = 0.0660 wR_2 = 0.1609	R_1 = 0.0725 wR_2 = 0.1973	R_1 = 0.0383 wR_2 = 0.1034	R_1 = 0.0368 wR_2 = 0.0936	R_1 = 0.0661 wR_2 = 0.1706	R_1 = 0.0568, wR_2 = 0.1202	R_1 = 0.0268, wR_2 = 0.0675
Final *R* indexes [all data]	R_1 = 0.0791 wR_2 = 0.1720	R_1 = 0.0904 wR_2 = 0.2115	R_1 = 0.0458 wR_2 = 0.1106	R_1 = 0.0411 wR_2 = 0.0977	R_1 = 0.1196 wR_2 = 0.2070	R_1 = 0.1150, wR_2 = 0.1419	R_1 = 0.0292, wR_2 = 0.0703
Largest diff. peak/hole / e Å^{-3}	0.57/-0.36	0.29/-0.23	0.61/-0.52	0.17/-0.16	0.35/-0.25	0.14/-0.17	0.56/-0.58

Tables S2. Observed hydrogen bonding and weak interactions:

*Compound **4a***

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13A···O11^{i}	0.97	2.56	3.389 (5)	143
C12—H12B···O11^{i}	0.97	2.60	3.429 (6)	143
C16—H16B···N2^{ii}	0.97	2.65	3.606 (6)	169
C14—H14A···O1^{iii}	0.97	2.48	3.299 (5)	143
C17—H17A···N2^{iv}	0.97	2.62	3.476 (5)	148
C17—H17B···O11^{i}	0.97	2.51	3.351 (5)	145
C10—H10···O1	0.93	2.26	2.886 (5)	124

Symmetry codes: (i) 2−*x*,1/2+*y*,1−*z*; (ii) + *x*,1+ *y*,+ *z*; (iii) 2− *x*,1/2+ *y*,2−*z*; (iv) 1− *x*,1/2+ *y*,1− *z*.

*Compound **4b***

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16A···N2^{i}	0.938 (14)	2.625 (14)	3.4762 (13)	151.1 (11)
C16—H16B···O11^{ii}	1.024 (17)	2.307 (17)	3.2756 (13)	157.4 (13)
C10—H10···O1	0.99 (2)	2.19 (2)	2.8843 (14)	125.8 (15)
C12—H12B···O11^{ii}	1.000 (17)	2.592 (17)	3.4384 (15)	142.3 (13)
N3—H3···O1	1.036 (16)	1.528 (17)	2.5475 (10)	166.8 (15)

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*+1/2; (ii) −*x*+3/2, *y*−1/2, −*z*+1/2.

*Compound **4c***

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13A···O11^{i}	0.97	2.46	3.307 (3)	146
C13—H13B···N2^{ii}	0.97	2.64	3.484 (3)	146
C12—H12A···O11^{i}	0.97	2.60	3.420 (4)	143
C16—H16B···O11^{i}	0.97	2.61	3.421 (4)	141
C15—H15A···S1^{iii}	0.97	3.03	3.688 (4)	126
C15—H15B···O1^{iv}	0.97	2.34	3.223 (4)	151
C14—H14A···N2^{v}	0.97	2.65	3.588 (4)	162
C10—H10···O1	0.93	2.26	2.886 (4)	124

N3—H3···O1	0.86 (4)	1.70 (4)	2.548 (3)	167 (3)
C13—H13A···O11^{i}	0.97	2.46	3.307 (3)	146

Symmetry codes: (i) −*x*, *y* −1/2, − *z* +1; (ii) − *x* +1, *y* −1/2, − *z* +1; (iii) − *x*, *y* +1/2, − *z*; (iv) − *x*, *y* −1/2, −*z*; (v) *x*, *y*−1, *z*.

*Compound **4d***

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15B···N2i	0.97	2.64	3.575 (2)	162
C16—H16B···O11	0.97	2.54	3.077 (2)	115
C14—H14B···O1ii	0.97	2.52	3.218 (2)	128
C22—H22···N2i	0.93	2.53	3.459 (3)	174
C10—H10···O1	0.93	2.44	2.964 (2)	116
N3—H3···O1ii	0.98 (2)	1.76 (2)	2.6944 (19)	159.6 (18)

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+2, −*y*+2, −*z*+1; (iii) *x*−1, *y*, *z*.

*Compound **4e***

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12A···O11^{i}	0.97	2.63	3.3875 (19)	135
C13—H13B···O11^{i}	0.97	2.55	3.424 (2)	151
C16—H16A···N2^{ii}	0.97	2.54	3.458 (2)	158
N3—H3···O1^{iii}	0.90 (2)	1.91 (2)	2.7669 (17)	158.0 (19)

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+3/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+3/2, *y*+1/2, −*z*+3/2.

*Compound **4e** solvate*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C132—H13A···O111	0.97	2.30	3.261 (3)	169
C122—H12B···N2^{i}	0.97	2.64	3.357 (5)	131
C102—H102···O12	0.93	2.51	2.989 (3)	112
C162—H16B···N22^{ii}	0.97	2.56	3.511 (4)	166
C121—H12C···O11	0.97	2.33	2.886 (3)	116
C121—H12D···O112^{iii}	0.97	2.52	3.275 (4)	135
C101—H101···O11	0.93	2.47	2.949 (4)	113

N31—H31···O12	0.91 (3)	1.94 (3)	2.771 (3)	151 (2)
C161—H16C···N2^{i}	0.97	2.58	3.446 (6)	149
N32—H32···O11^{i}	0.89 (3)	1.96 (3)	2.782 (3)	153 (3)

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+2, −*y*+2, −*z*+1; (iii) *x*−1, *y*, *z*.

Compound ***4f***

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O1^{i}	0.93	2.54	3.333 (3)	144
C12—H12B···N2^{ii}	0.97	2.60	3.557 (4)	169
N3—H3···O1	0.99 (3)	1.60 (4)	2.571 (3)	165 (3)

Symmetry code: (i) *x*−1, *y*, *z*; (ii) *x*+1, *y*, *z*.

Compound ***4h***

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O1^{i}	0.93	2.60	3.408 (3)	145
C12—H12A···N2^{ii}	0.97	2.63	3.570 (3)	163
N3—H3···O1	0.93 (3)	1.69 (3)	2.600 (2)	166 (2)

Symmetry code: (i) *x*−1, *y*, *z*; (ii) *x*+1, *y*, *z*.

Compound ***4i***

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20B···O1^{i}	0.97	2.59	3.5193 (17)	161
C10—H10···O1	0.93	2.34	2.8794 (18)	117
C12—H12A···O1*W*^{i}	0.97	2.36	3.294 (2)	160
C12—H12B···O1	0.97	2.30	2.8845 (18)	118
C13—H13A···O11^{ii}	0.97	2.62	3.3145 (18)	128
C13—H13B···O3	0.97	2.63	3.1129 (18)	111
C13—H13B···O4^{ii}	0.97	2.53	3.1244 (19)	119
C19—H19A···O1*W*^{i}	0.97	2.63	3.303 (2)	126
O1W—H1*WA*···O1	0.95 (3)	1.90 (3)	2.8302 (18)	165 (2)
O1W—H1*WB*···O11^{ii}	0.91 (3)	2.17 (3)	2.9858 (17)	150 (2)
O1W—H1*WB*···O2^{ii}	0.91 (3)	2.47 (3)	3.0723 (19)	124 (2)

N3—H3···O11	0.859 (16)	2.168 (15)	2.6650 (15)	116.6 (12)
N3—H3···O3	0.859 (16)	2.428 (15)	2.9904 (15)	123.6 (12)
N3—H3···O4	0.859 (16)	2.461 (15)	2.8885 (16)	111.5 (12)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*, −*y*+1/2, *z*−1/2.

*Compound **4j***

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···O1	0.93	2.28	2.899 (4)	124
C13—H13A···O11	0.97	2.51	3.050 (4)	115
C22—H22B···O11	0.97	2.64	3.105 (4)	110
O1WA—H1WA···O1	0.85	2.19	2.843 (4)	134
O1WA—H1WB···O11^{iv}	0.85	2.33	2.861 (5)	121
O1WB—H1WC···O1	0.90	2.10	2.613 (7)	115
C10—H10···O1	0.93	2.28	2.899 (4)	124

Symmetry code: (iv) −*x*+1, *y*+1/2, −*z*+3/2.

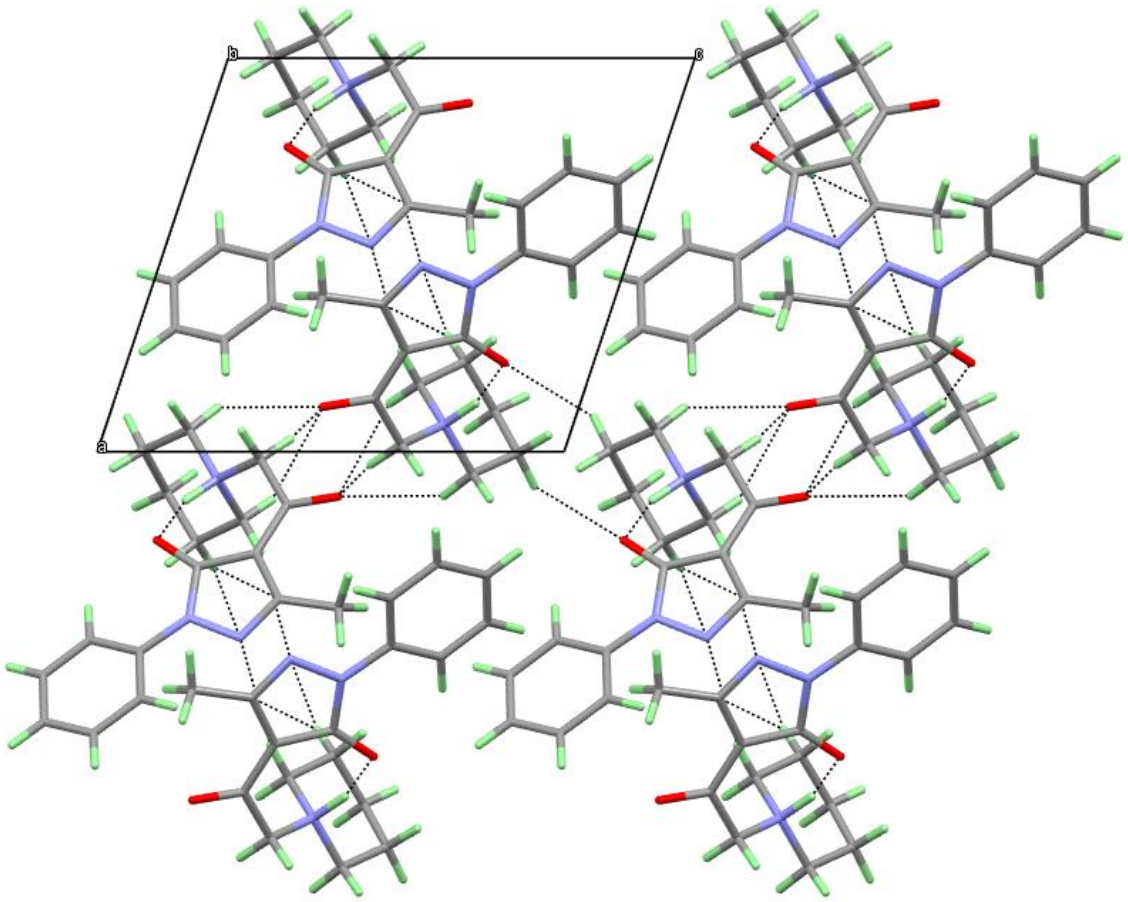
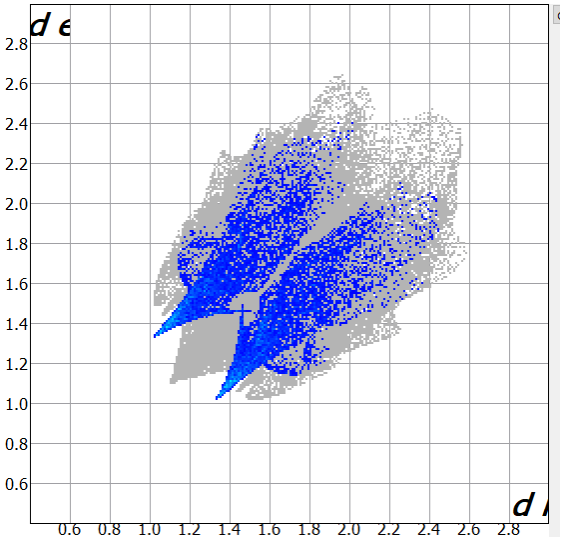


Figure S1. View along *b* of the three-dimensional arrangement of the molecules in the crystal structure of **4a**; hydrogen bonding and weak interactions are shown as dotted lines.

12% O..H conctacts



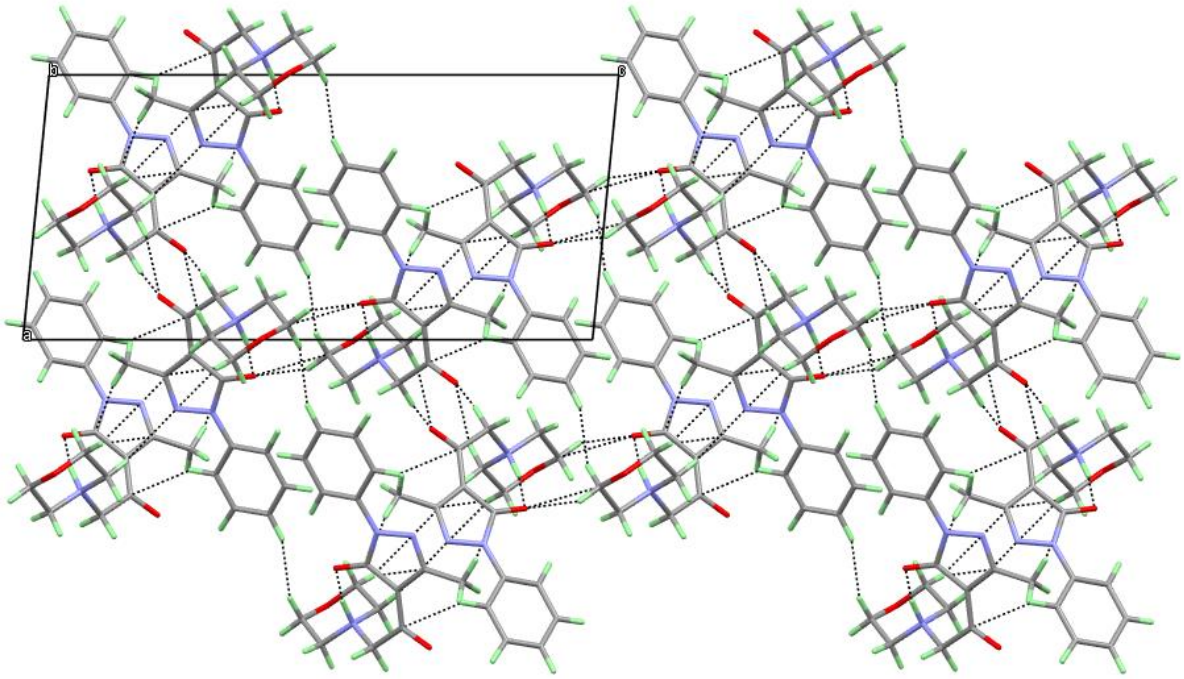


Figure S2. View along *b* of the three-dimensional arrangement of the molecules in the crystal structure of **4b**; hydrogen bonding and weak interactions are shown as dotted lines.

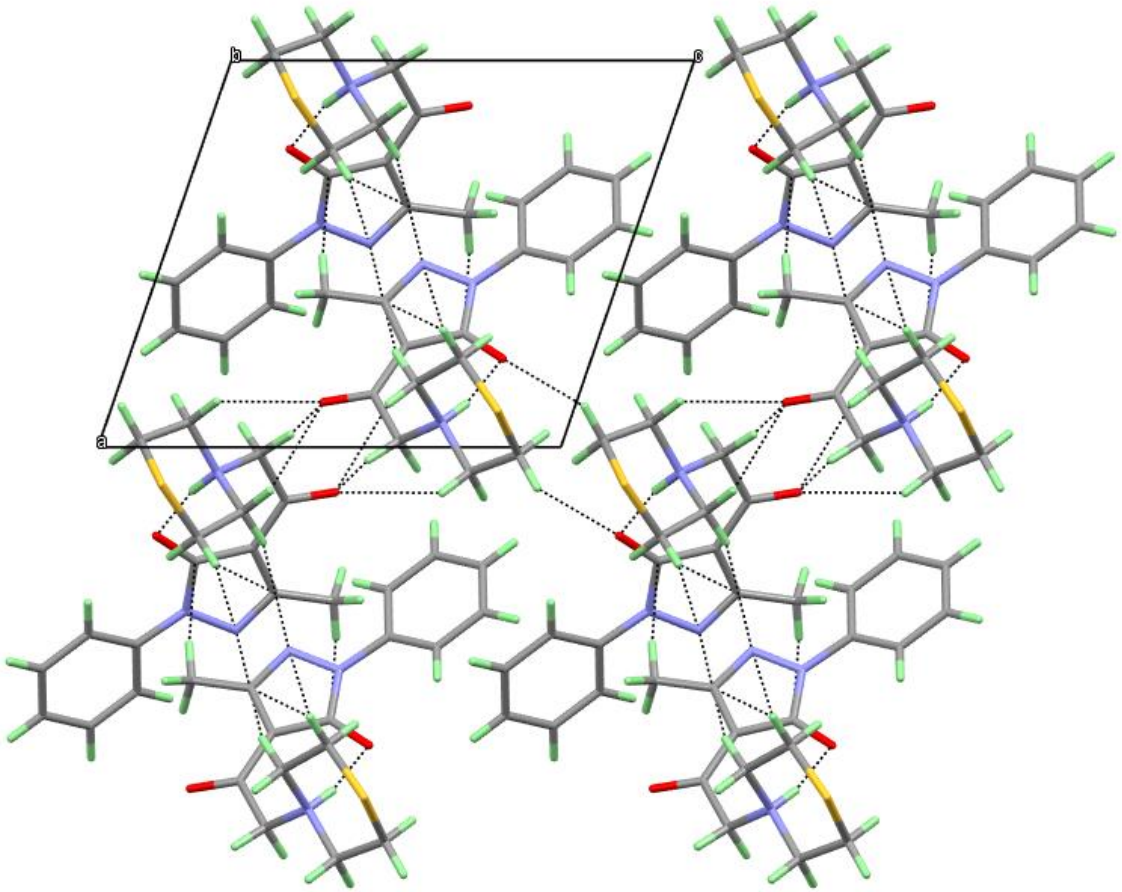


Figure S3. View along *b* of the three-dimensional arrangement of the molecules in the crystal structure of **4c**; hydrogen bonding and weak interactions are shown as dotted lines.

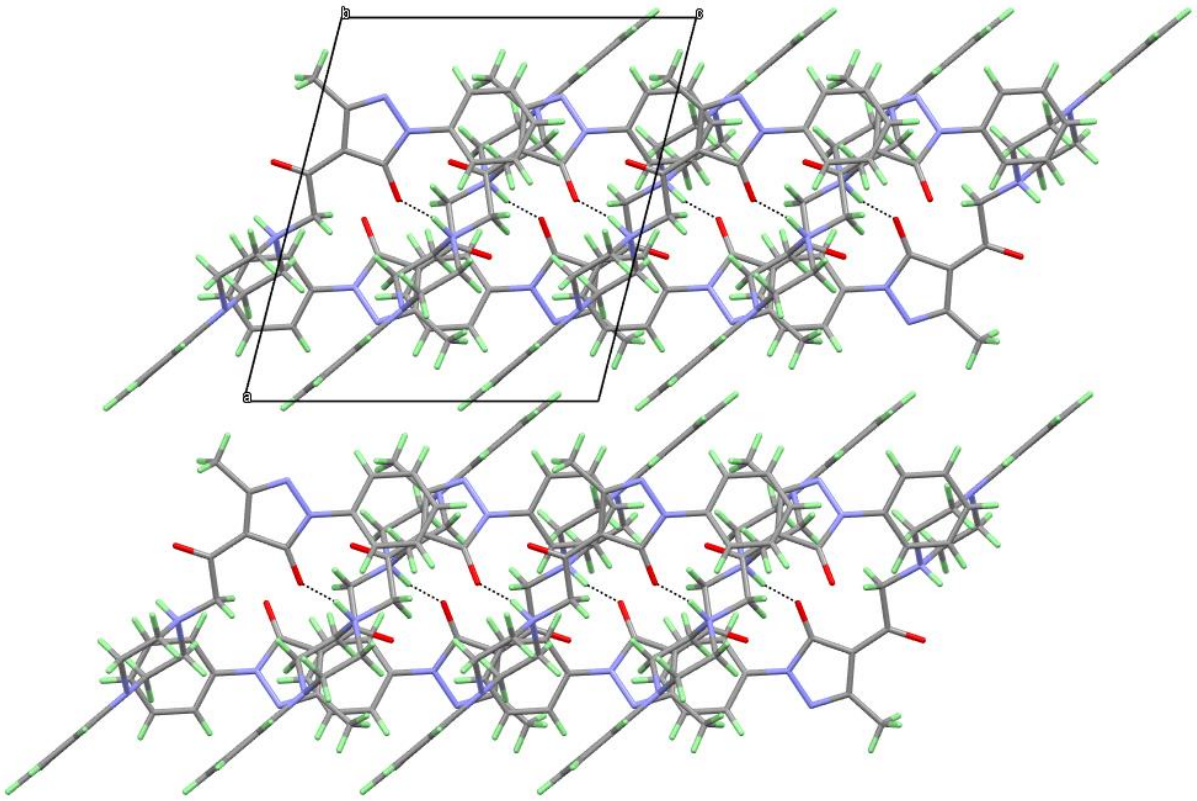


Figure S4. View along *b* of the three-dimensional arrangement of the molecules in the crystal structure of **4d**; hydrogen bonding and weak interactions are shown as dotted lines.

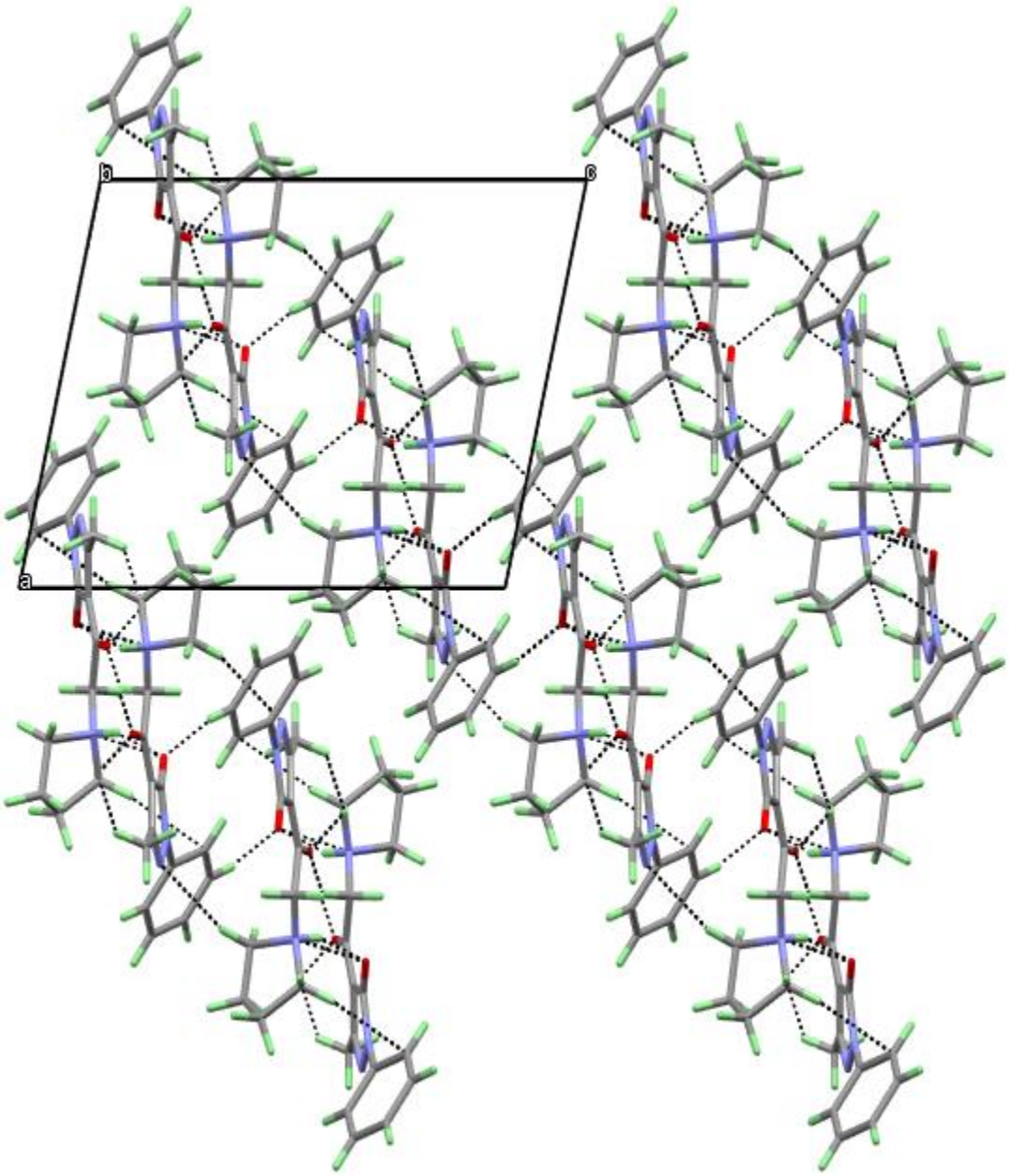


Figure S5. View along *b* of the three-dimensional arrangement of the molecules in the crystal structure of **4e**; hydrogen bonding and weak interactions are shown as dotted lines.

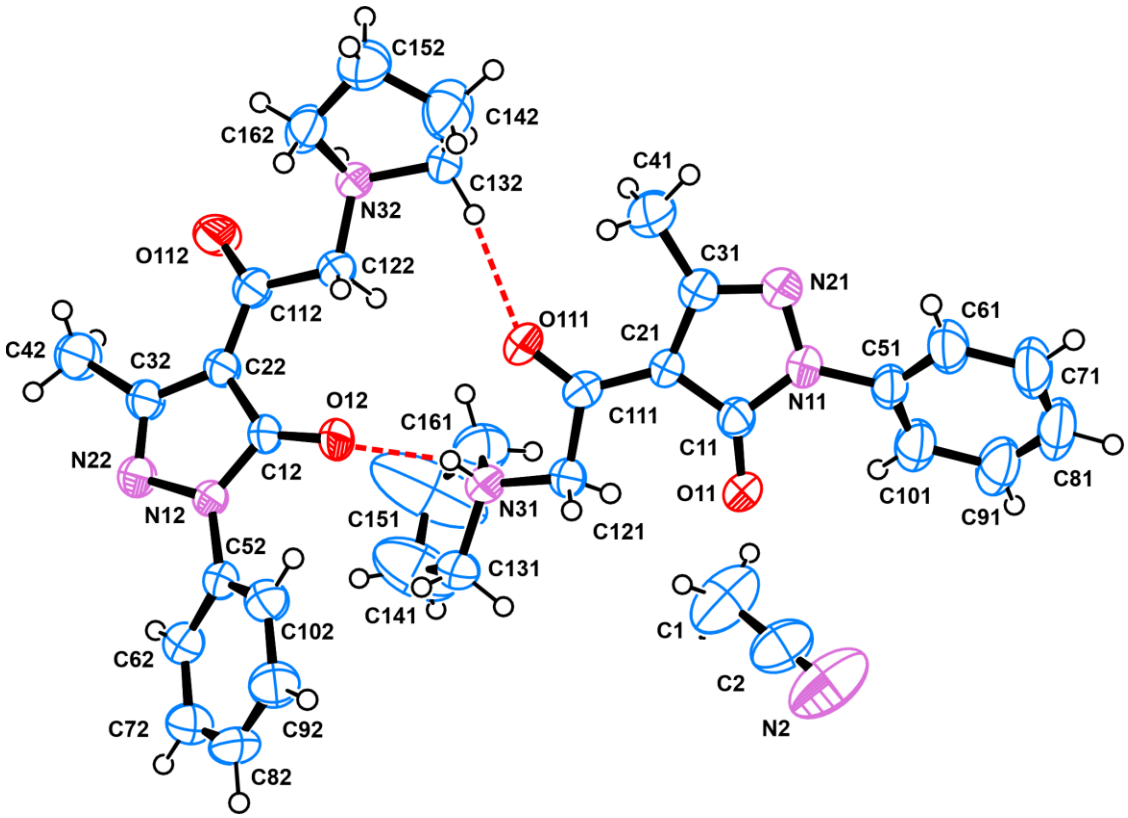


Figure S6. ORTEP view of **4e solvate** (with acetonitrile in the ASU).

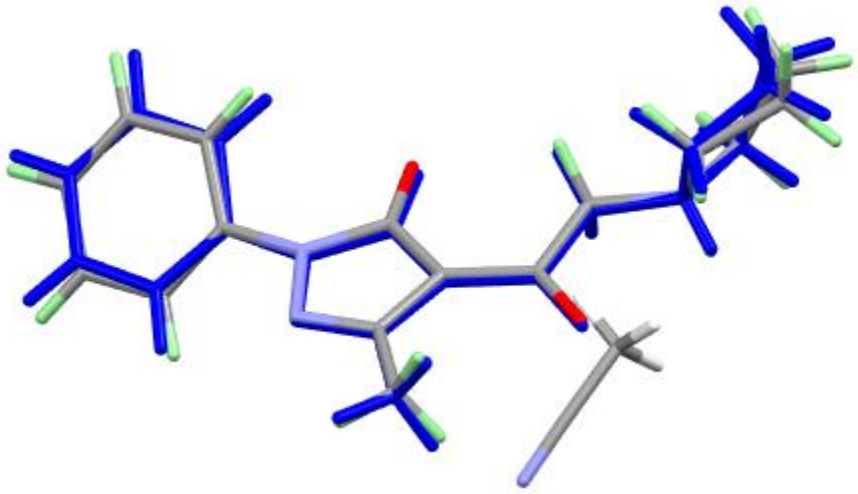


Figure S7. Overlay of the molecules from of compound **4e** with solvent (in blue/dark) and without solvent present in the crystal structure; the *rmsd* is 0.1605 Å (The ACN is not considered).

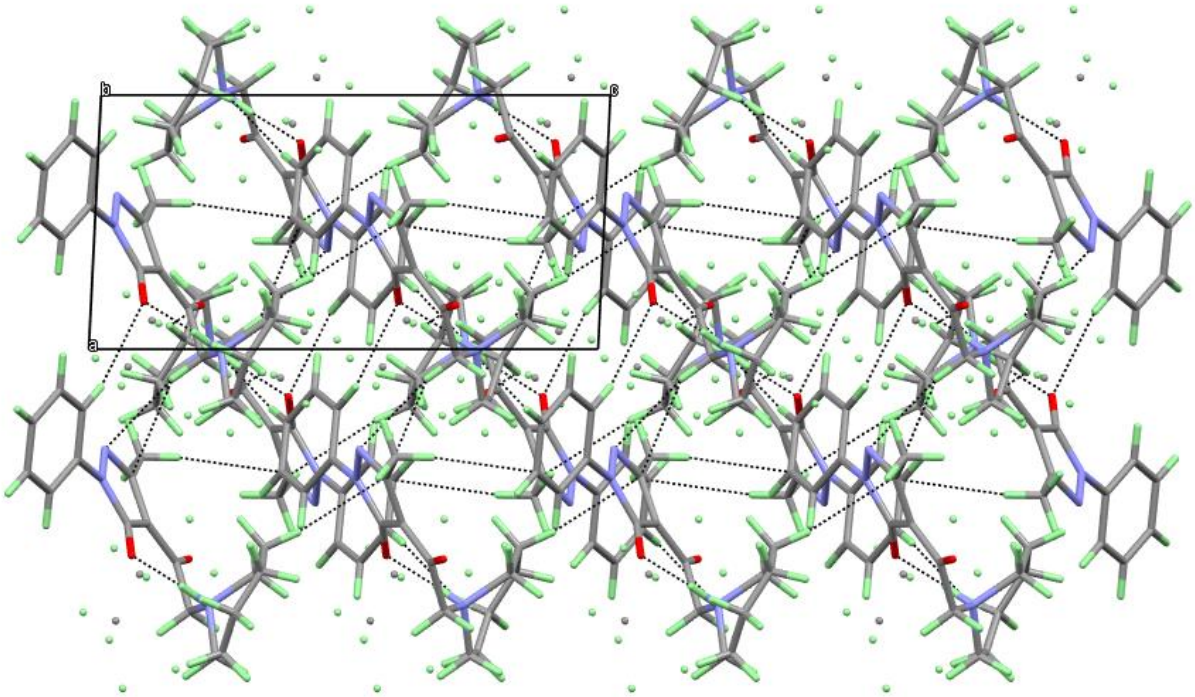


Figure S8. View along *b* of the three-dimensional arrangement of the molecules in the crystal structure of **4f**; hydrogen bonding and weak interactions are shown as dotted lines.

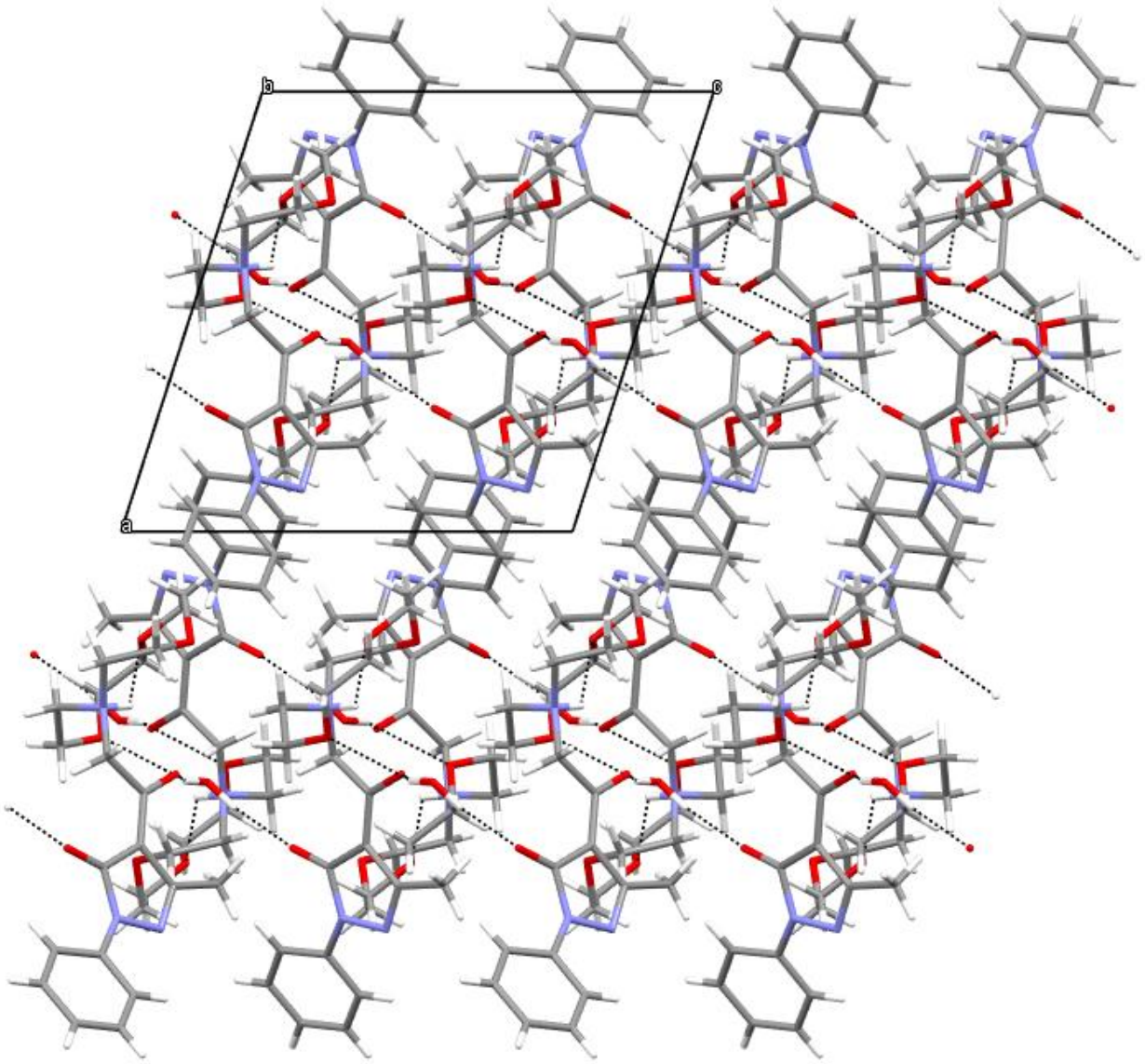


Figure S9. View along *b* of the three-dimensional arrangement of the molecules in the crystal structure of **4i**; hydrogen bonding are shown as dotted lines.

Table S3. Selected signals in the NMR spectra of ligands **4**.

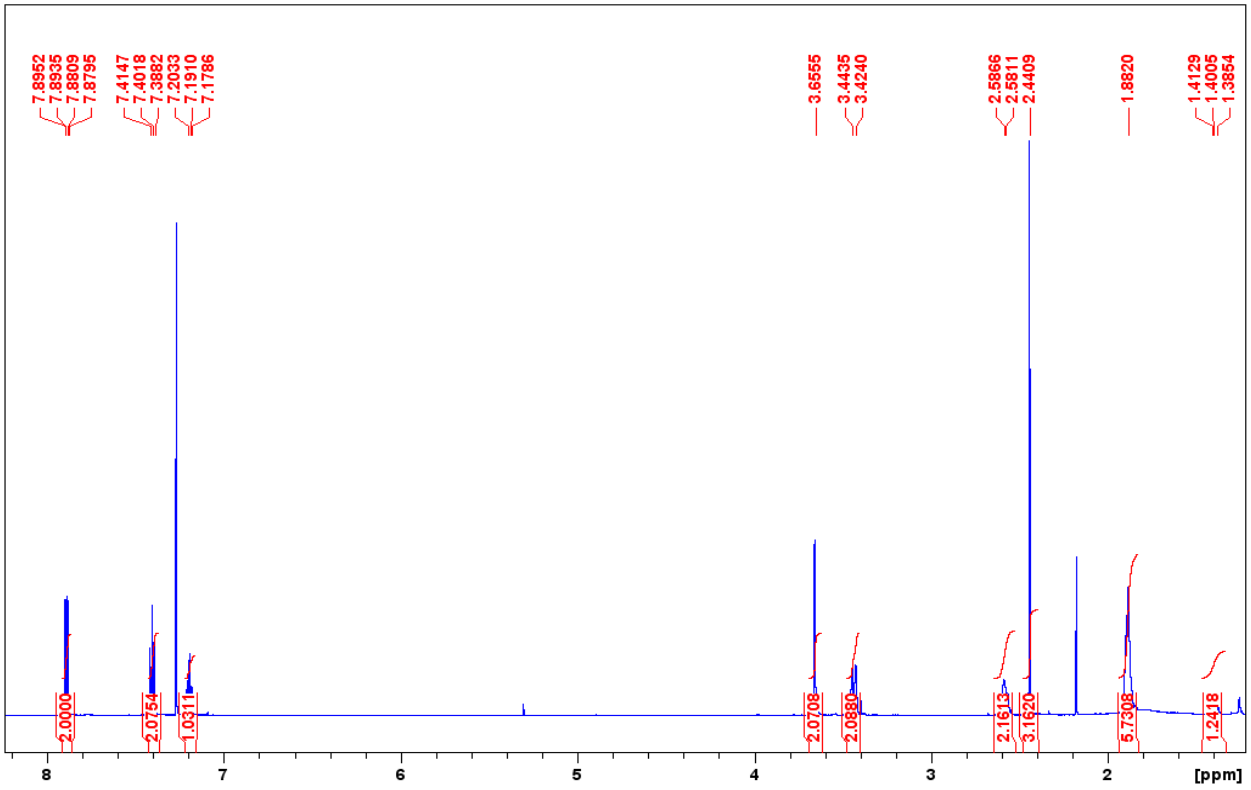
Compd.	*C*=O	*C*q-5	*C*q-4	*C*q-3	CH_2-bridge	
					^{13}C	^{1}H
4a	182.69	163.45	103.97	151.30	66.47	3.659

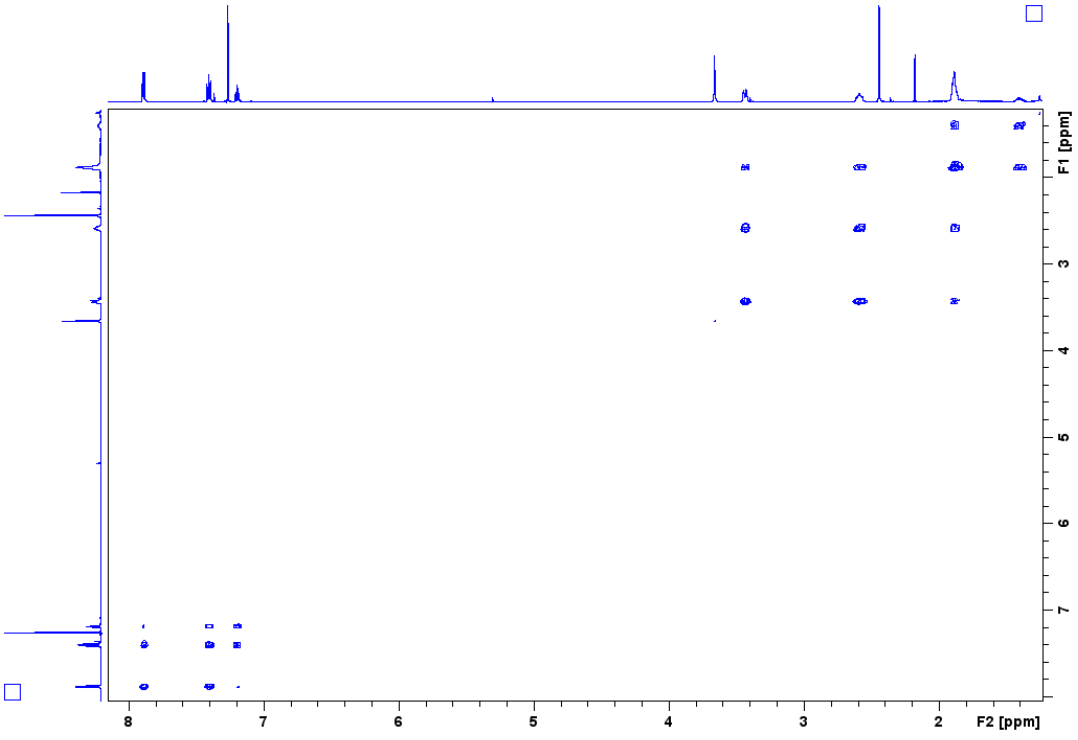
4b	184.39	160.56	104.07	151.47	67.27	3.611
4c	184.28	160.75	104.05	151.47	67.50	3.611
4d	184.23	161.09	104.12	151.49	66.77	3.671
4e	182.65	163.68	103.91	151.24	64.36	3.807
4f	182.17	161.70	104.12	151.36	66.36	3.771
4h	181.59	163.98	104.21	150.98	66.35	3.795
4i	180.53	165.02	103.17	150.52	61.94	4.083
4j	182.29	164.05	103.85	150.90	63.54	3.996

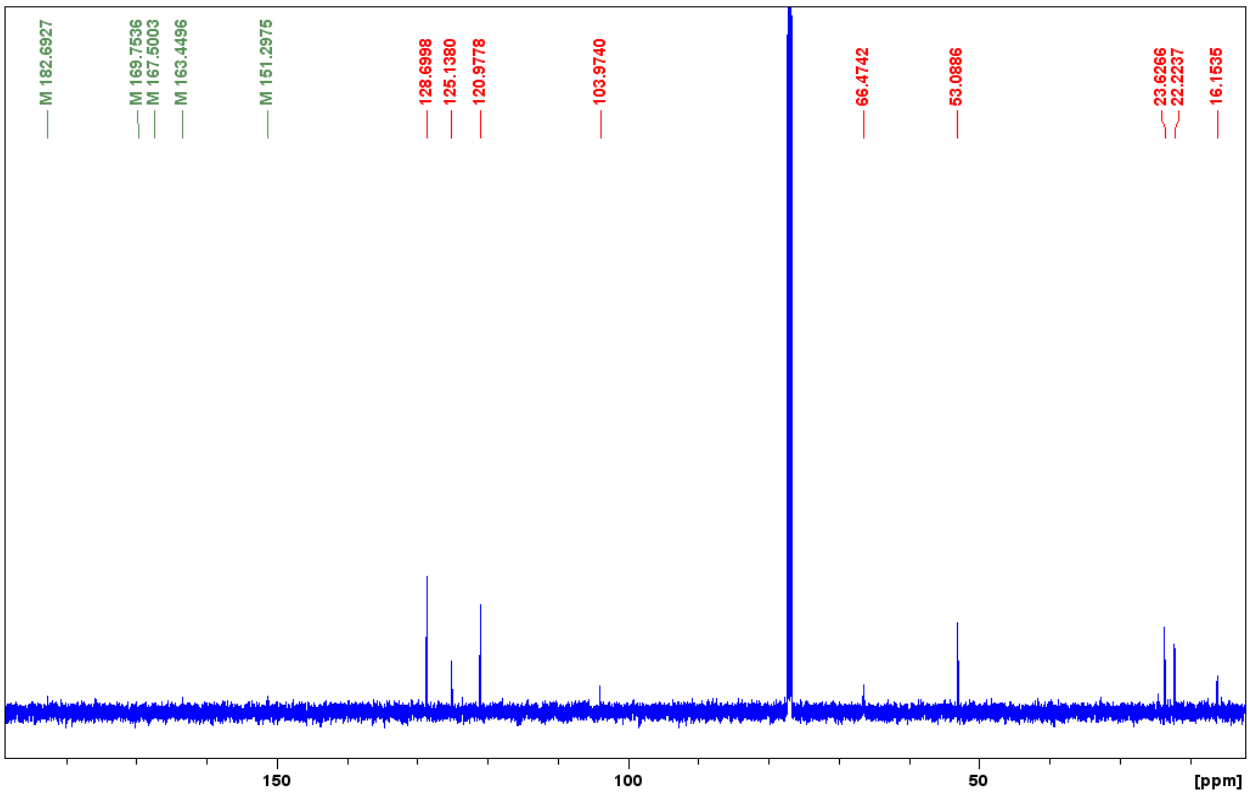
APPENDIX

NMR spectra

Compound **4a**



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M 167.5003
M 163.4496
M 151.2975
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66.4742
53.0886
23.6266
22.2237
16.1535
150
100
50
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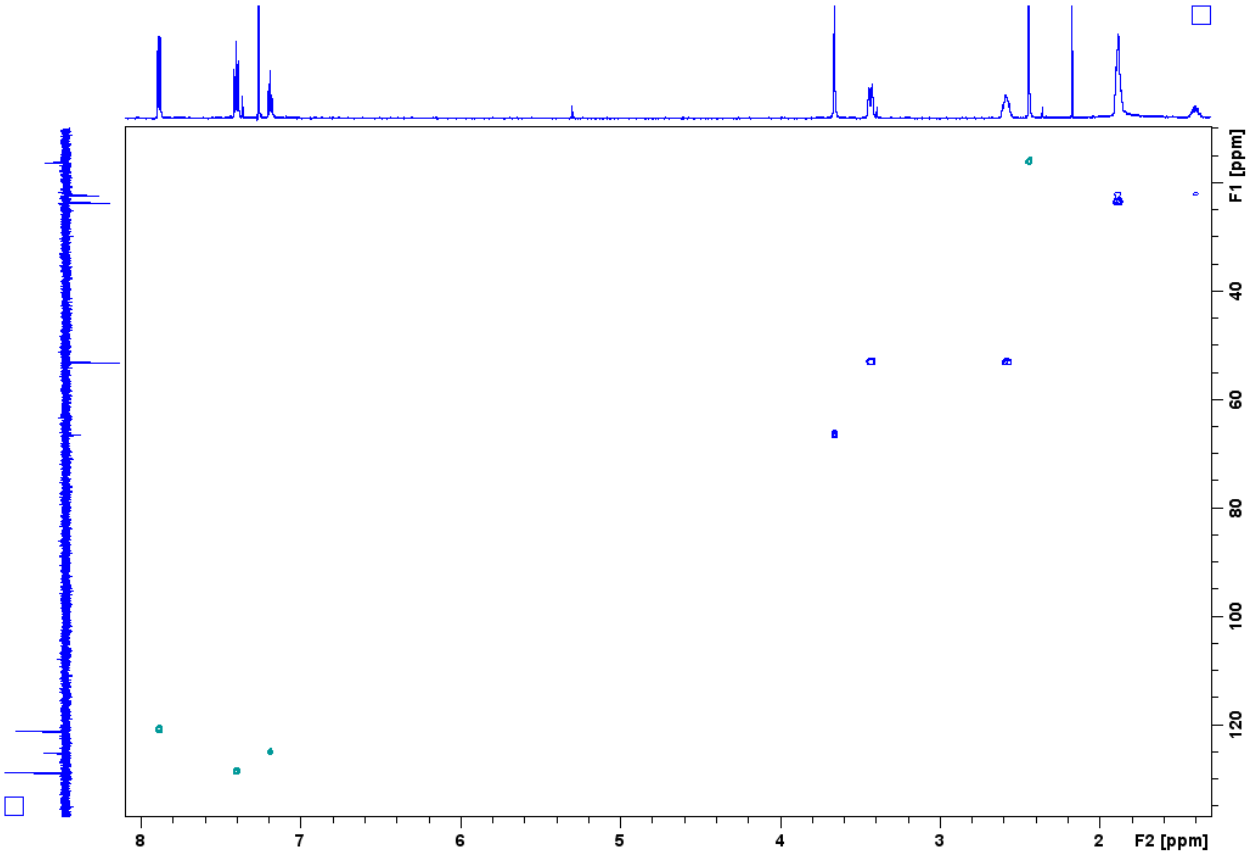
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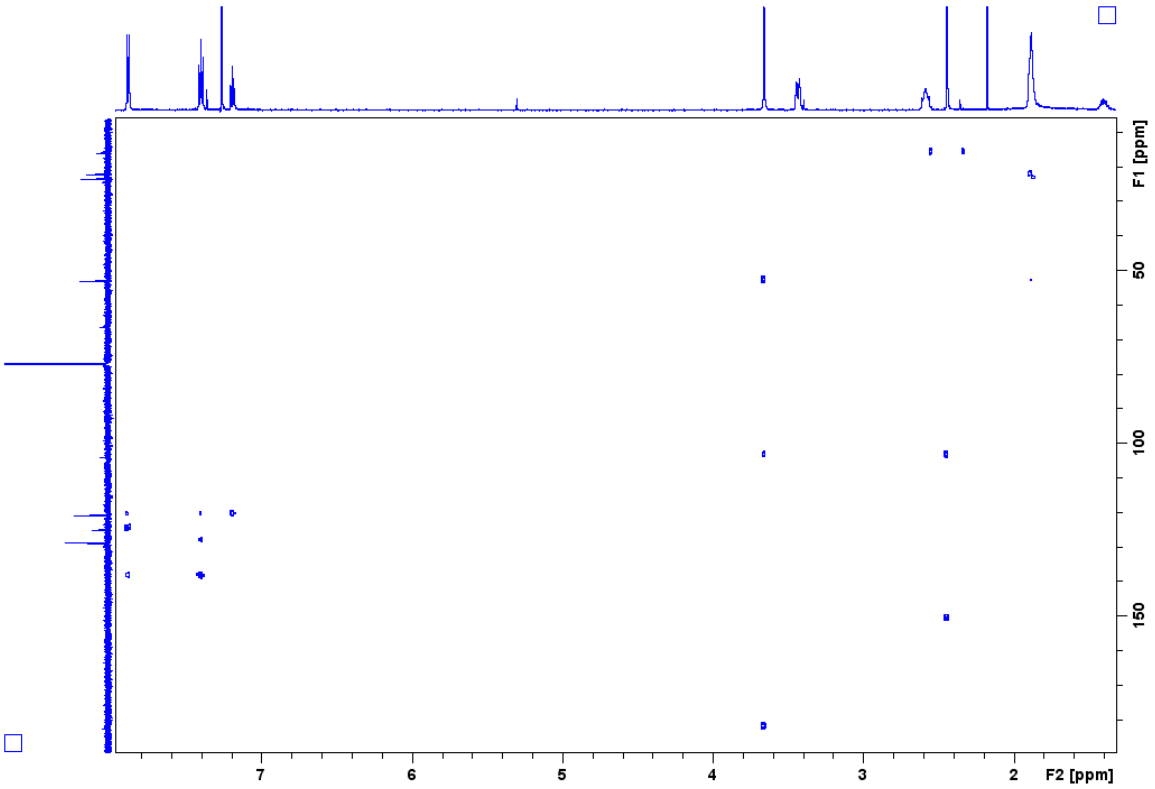
7
6
5
4
3
2
F2 [ppm]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4
3
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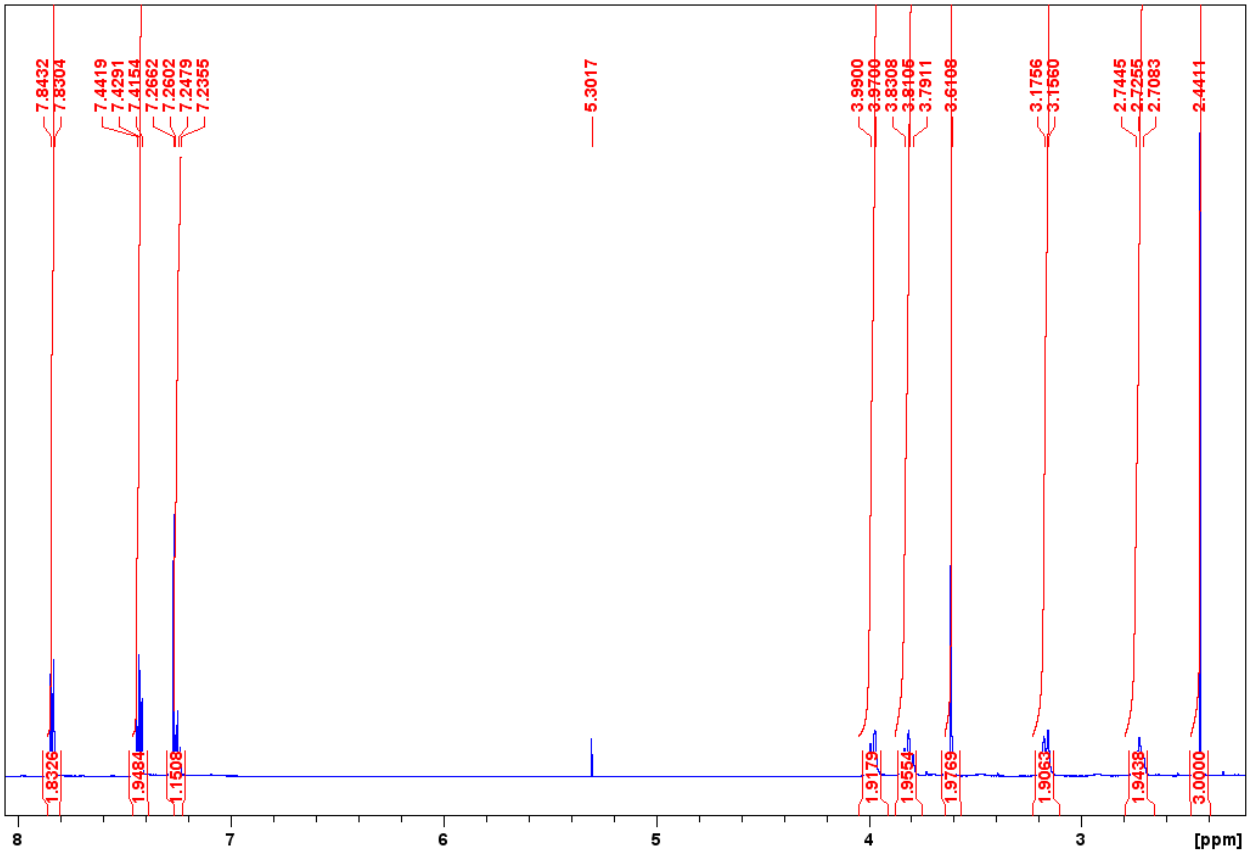
F2 [ppm]

*Compound **4b***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7.4154
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5.3017
3.9900
3.9700
3.8308
3.8106
3.7911
3.6108
3.1756
3.1560
2.7445
2.7255
2.7083
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1.9484
1.1508
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4
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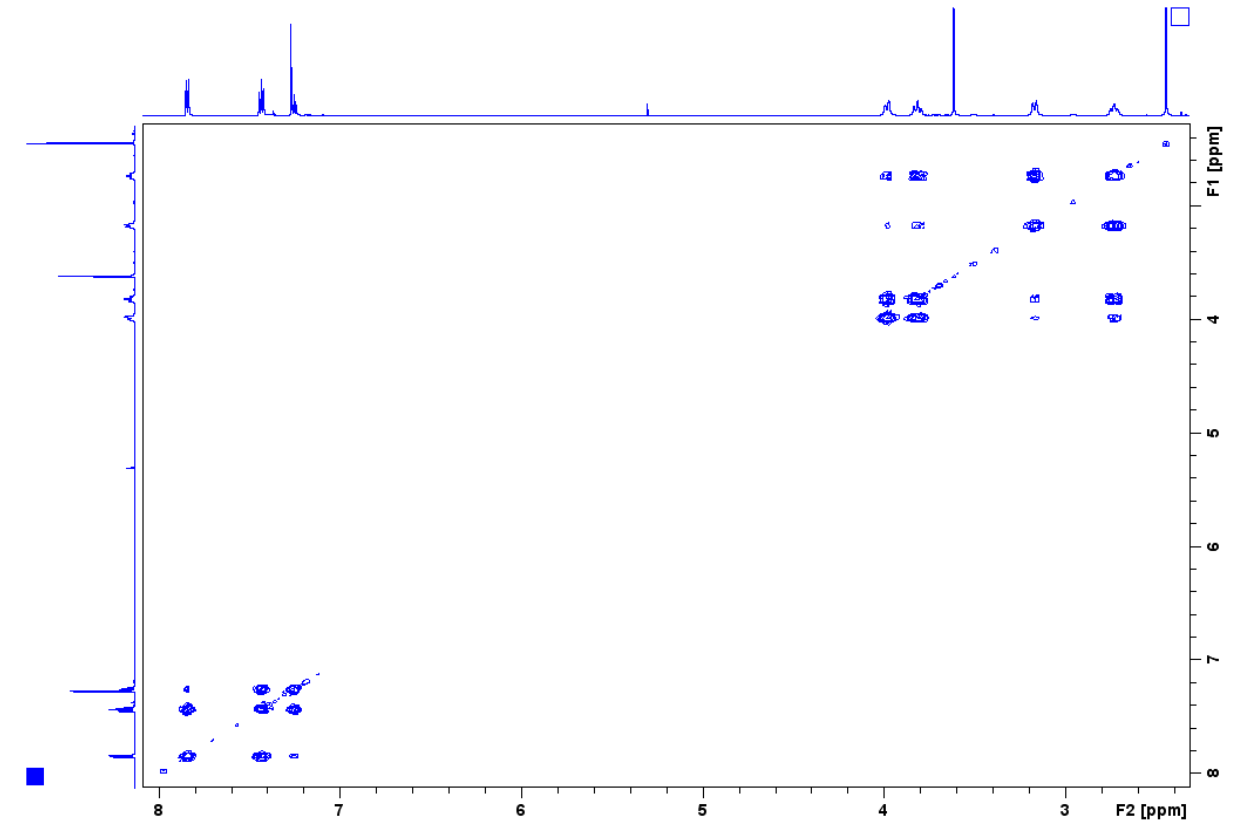
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F2 [ppm]
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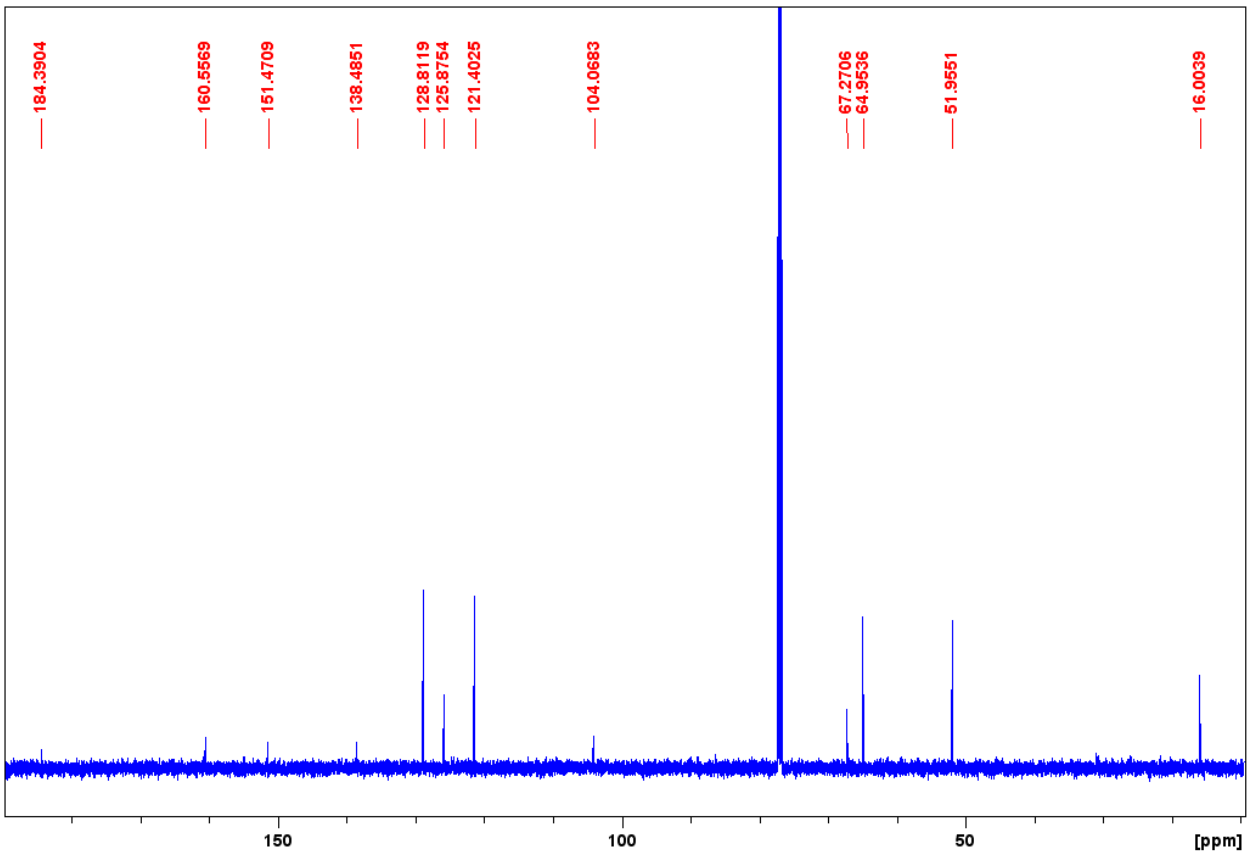
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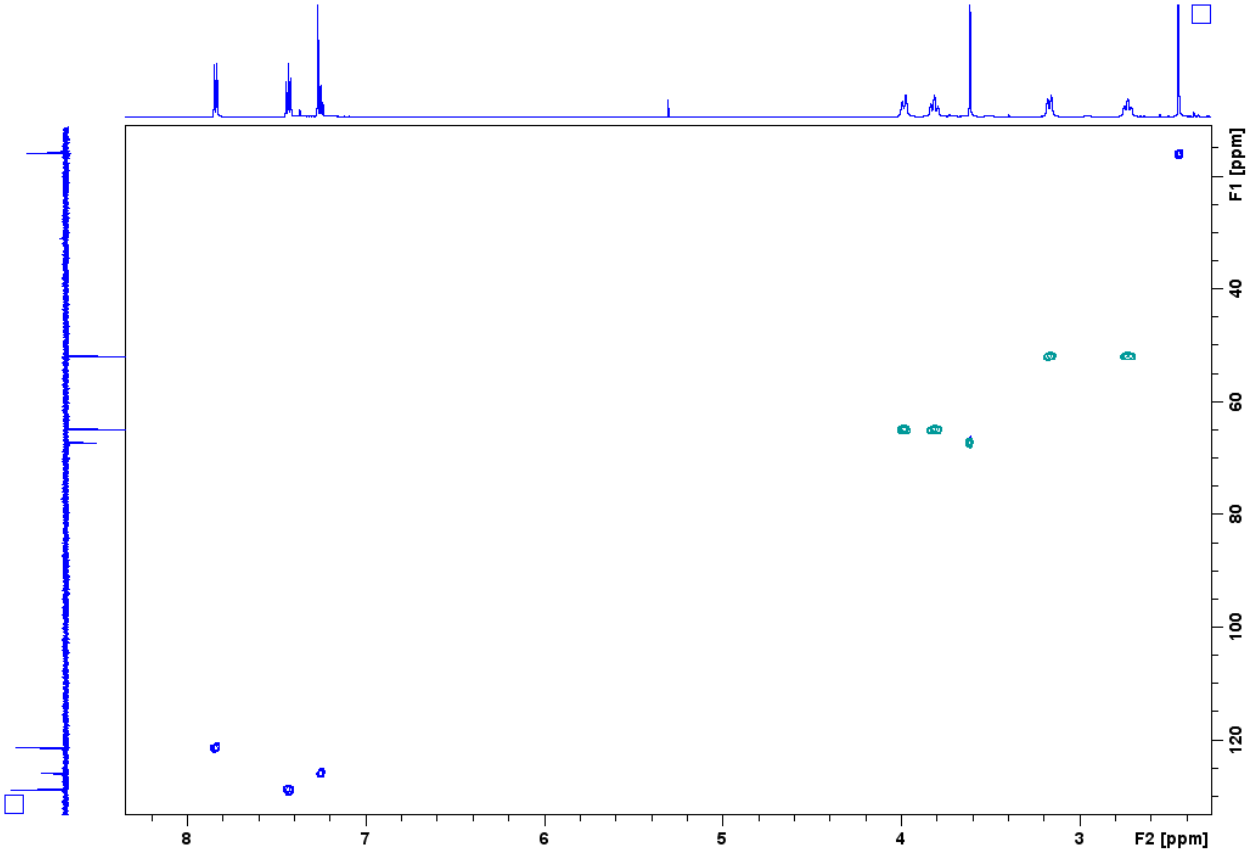
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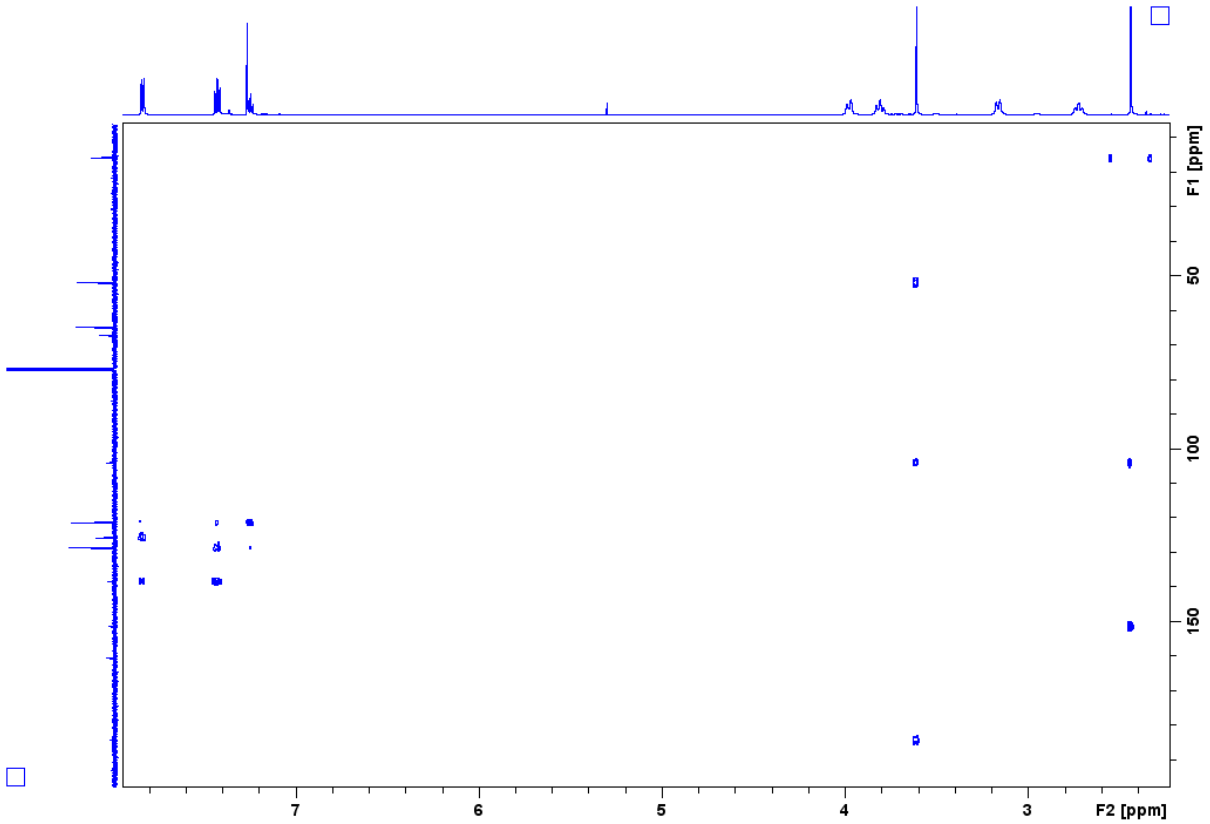
F2 [ppm]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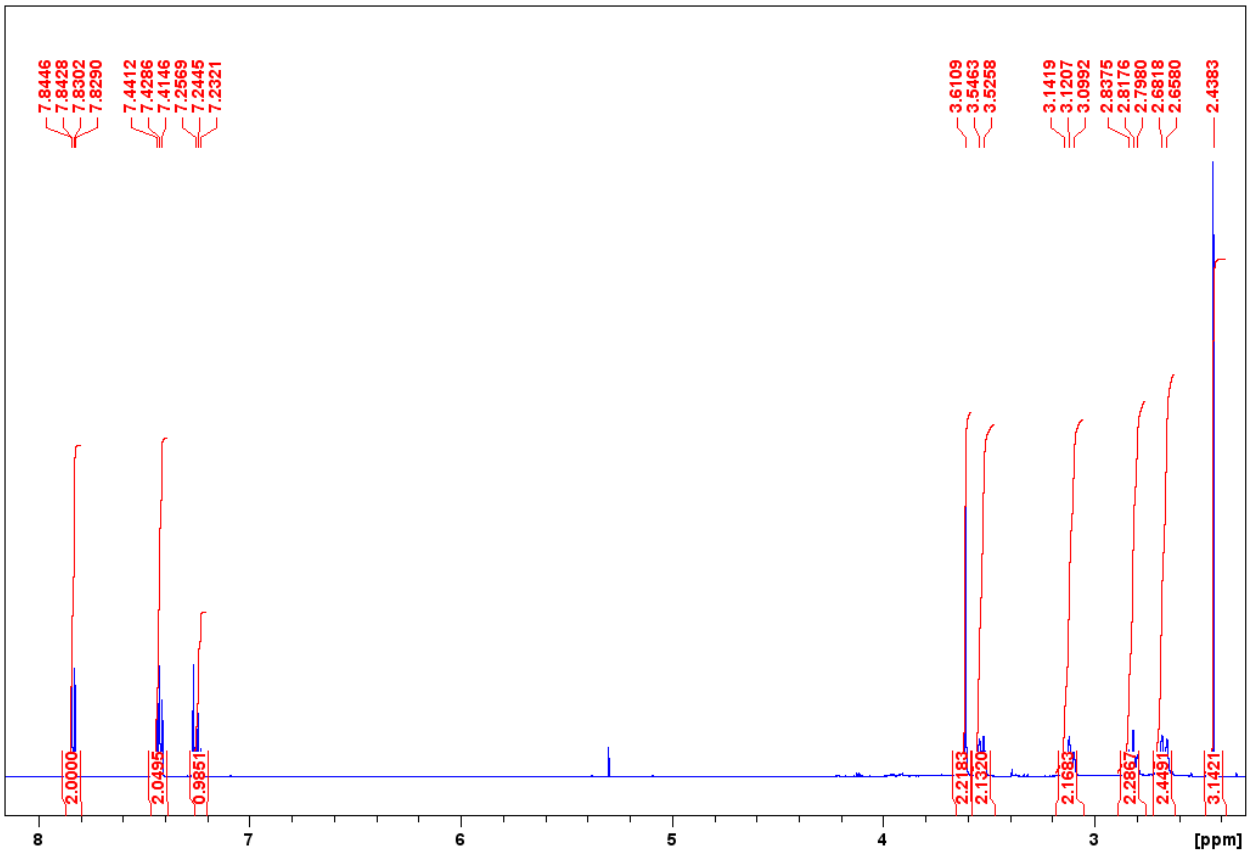
F2 [ppm]

*Compound **4c***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7.8290
7.4412
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7.4146
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7.2445
7.2321
3.6109
3.5463
3.5258
3.1419
3.1207
3.0992
2.8375
2.8176
2.7980
2.6818
2.6580
2.4383
2.0000
2.0495
0.9851
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2.4491
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8
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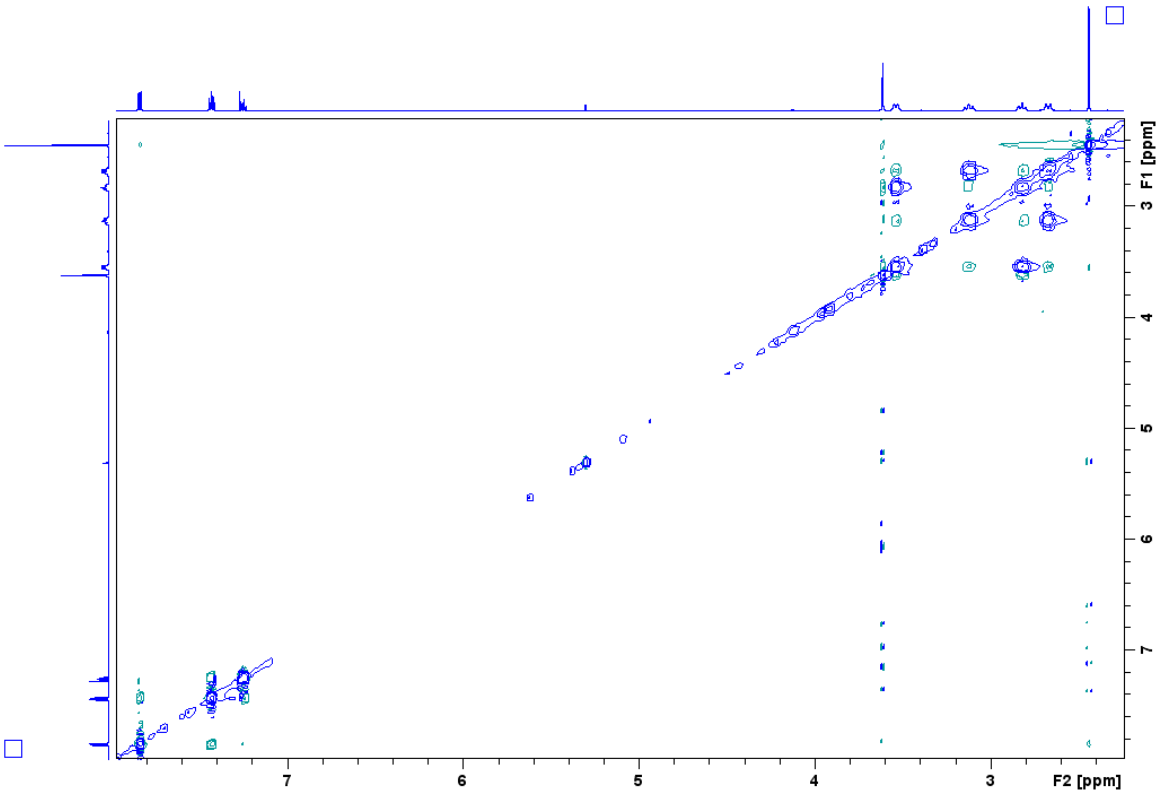
[ppm]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F2 [ppm]
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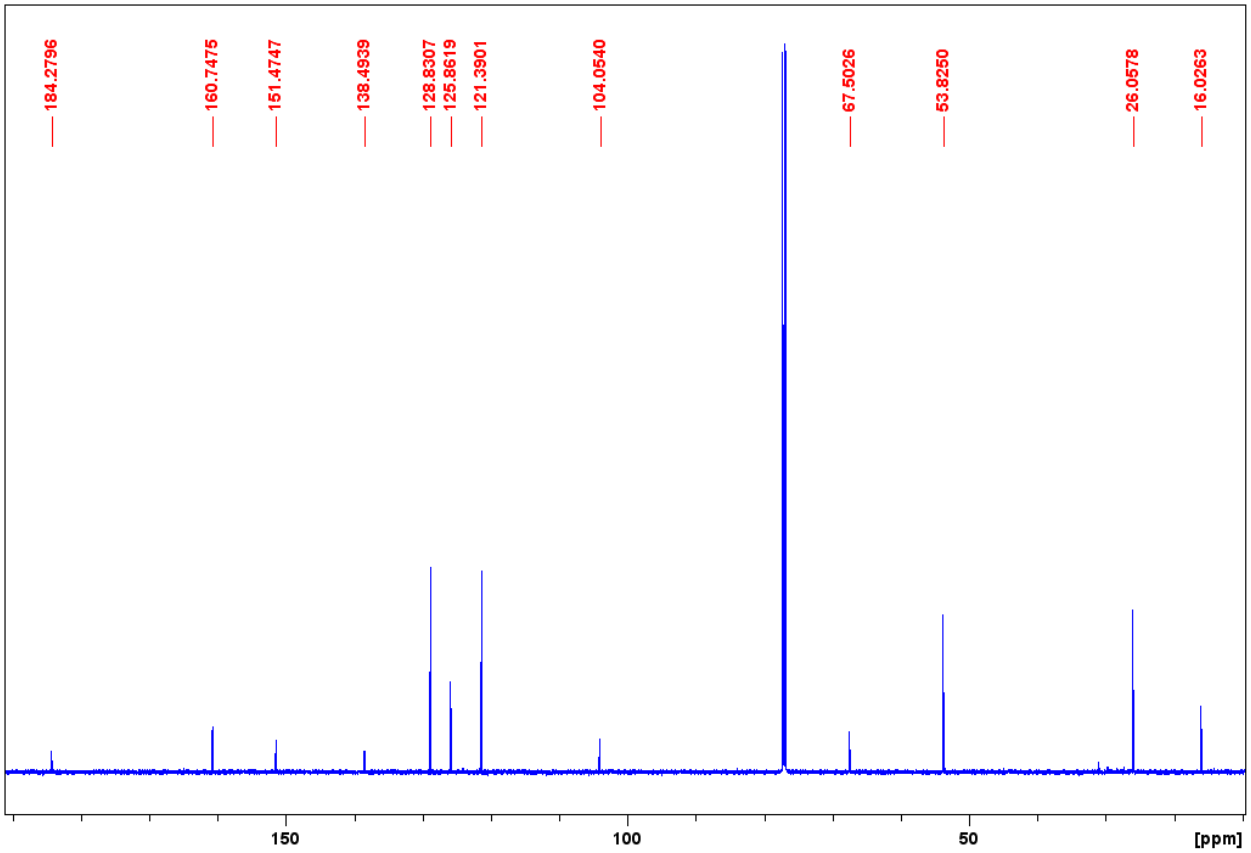
5
4
3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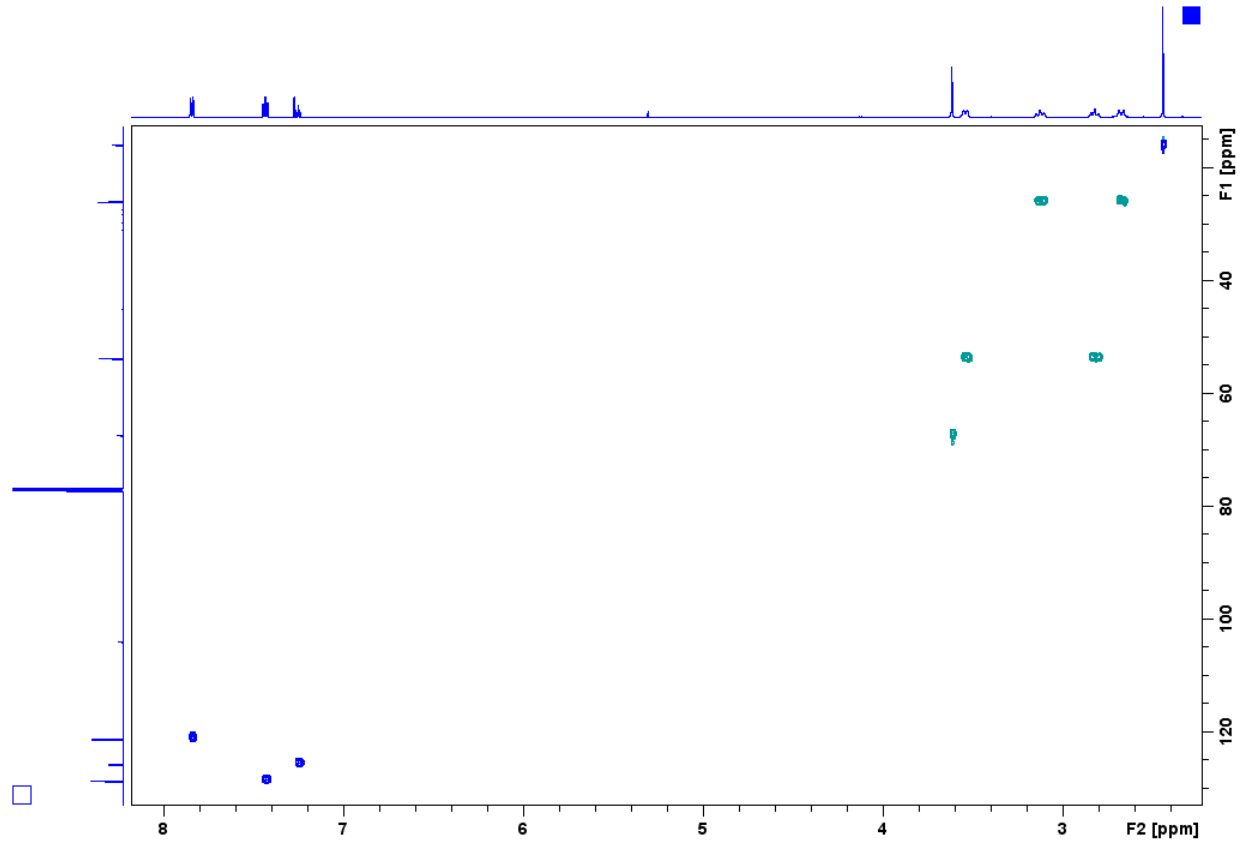
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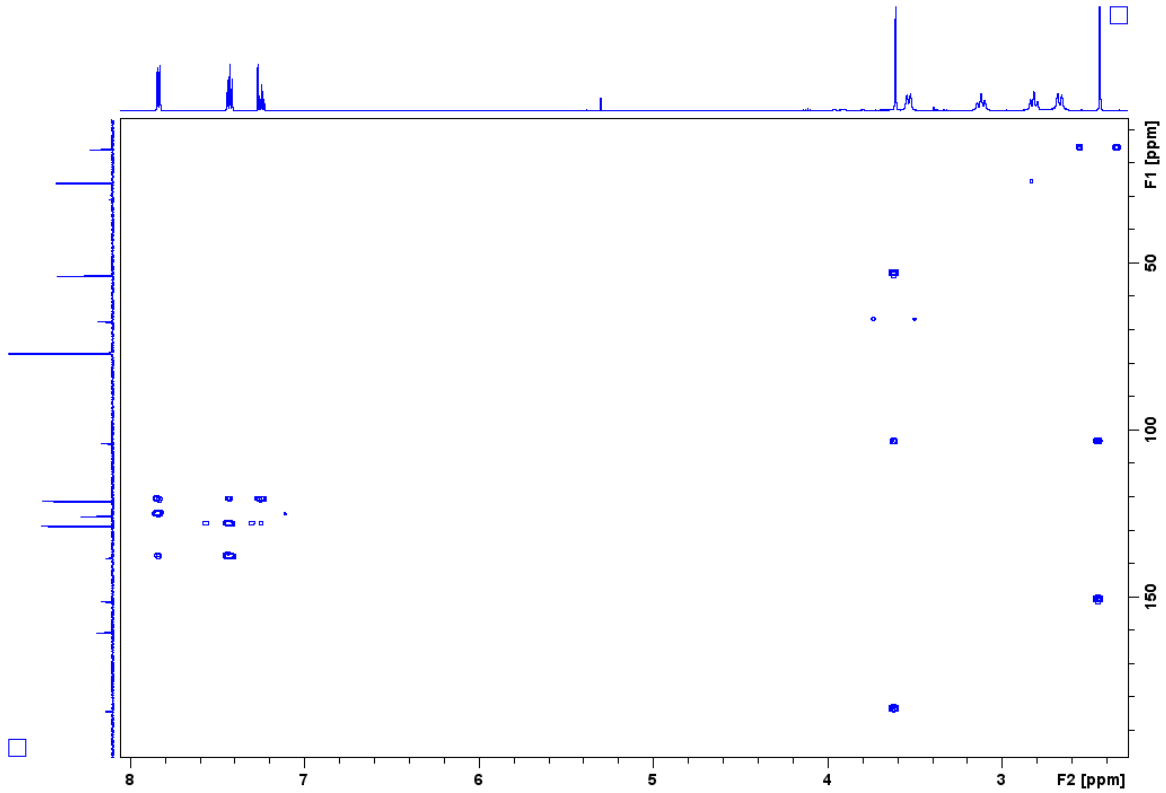
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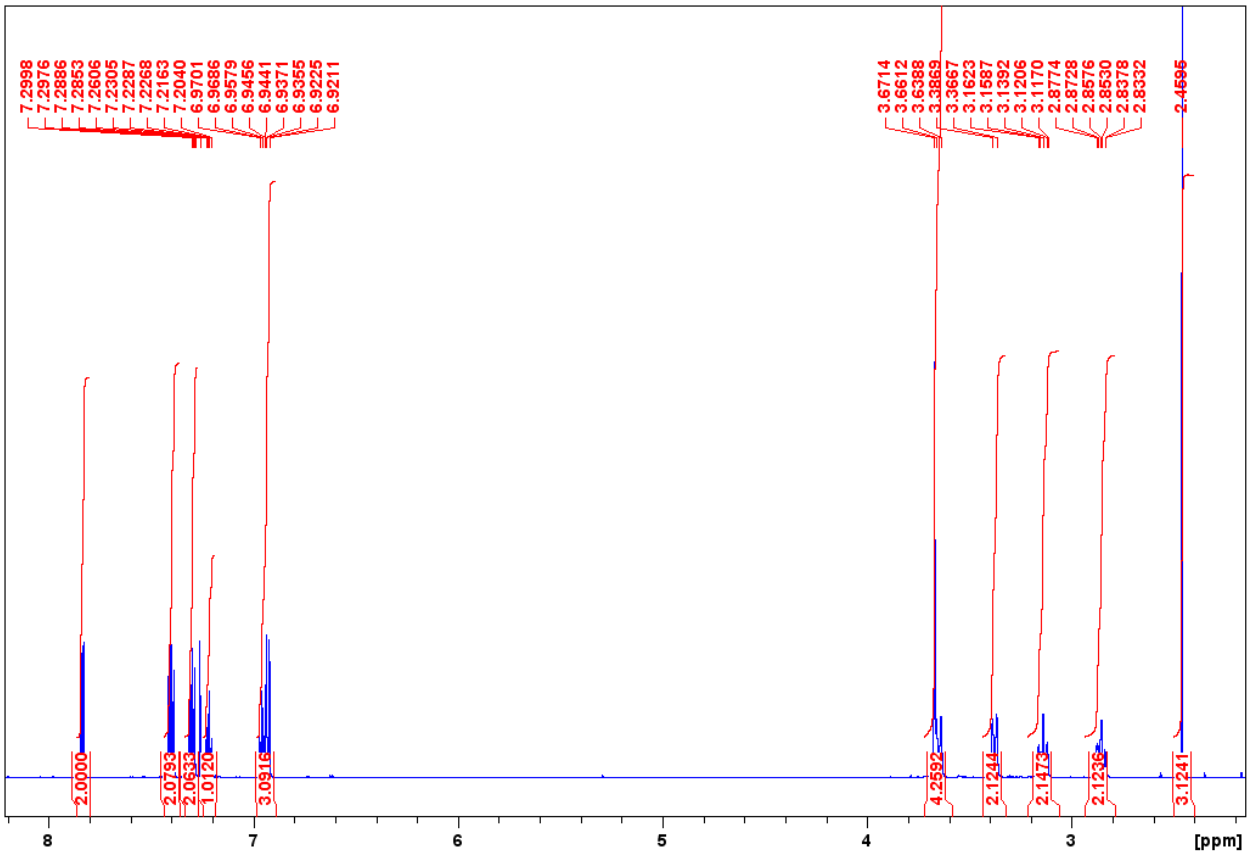
*Compound **4d***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6.9686
6.9579
6.9456
6.9441
6.9371
6.9355
6.9225
6.9211
3.6714
3.6612
3.6388
3.3869
3.3667
3.1623
3.1587
3.1392
3.1206
3.1170
2.8774
2.8728
2.8576
2.8530
2.8378
2.8332
2.4596
2.0000
2.0793
2.0533
1.0120
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2.1473
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8
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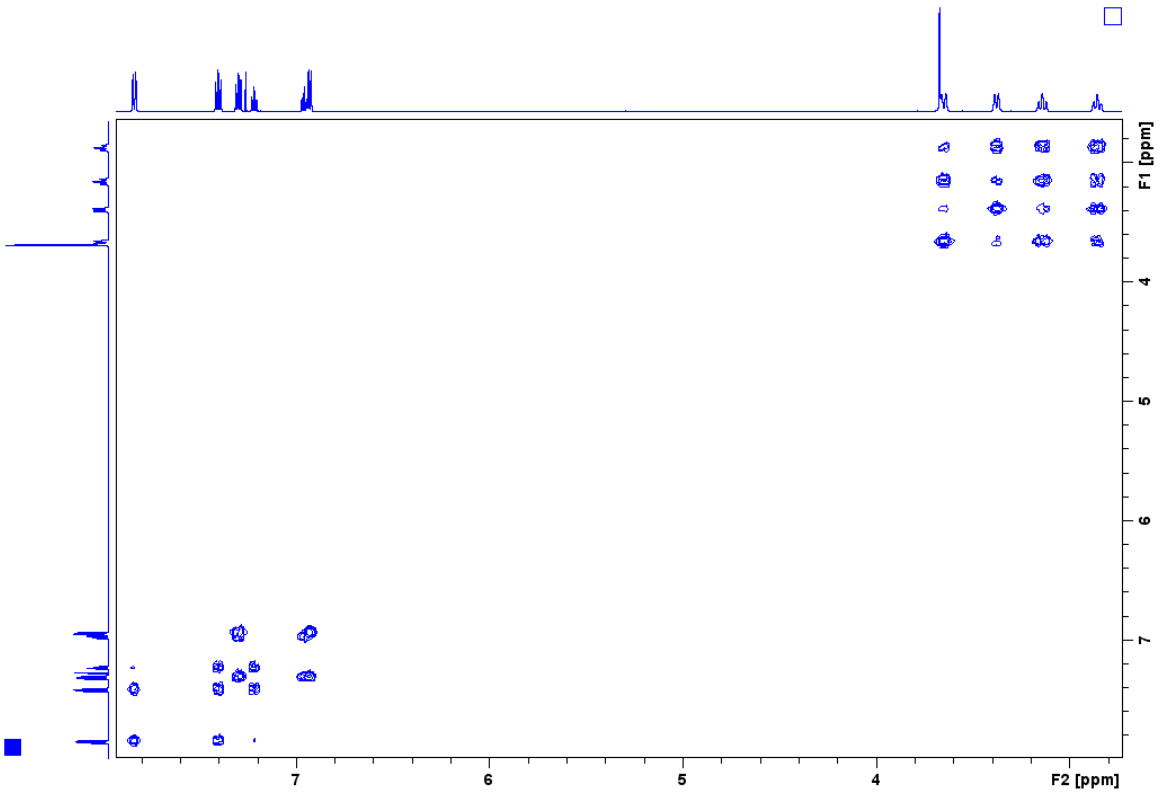
3
[ppm]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F2 [ppm]
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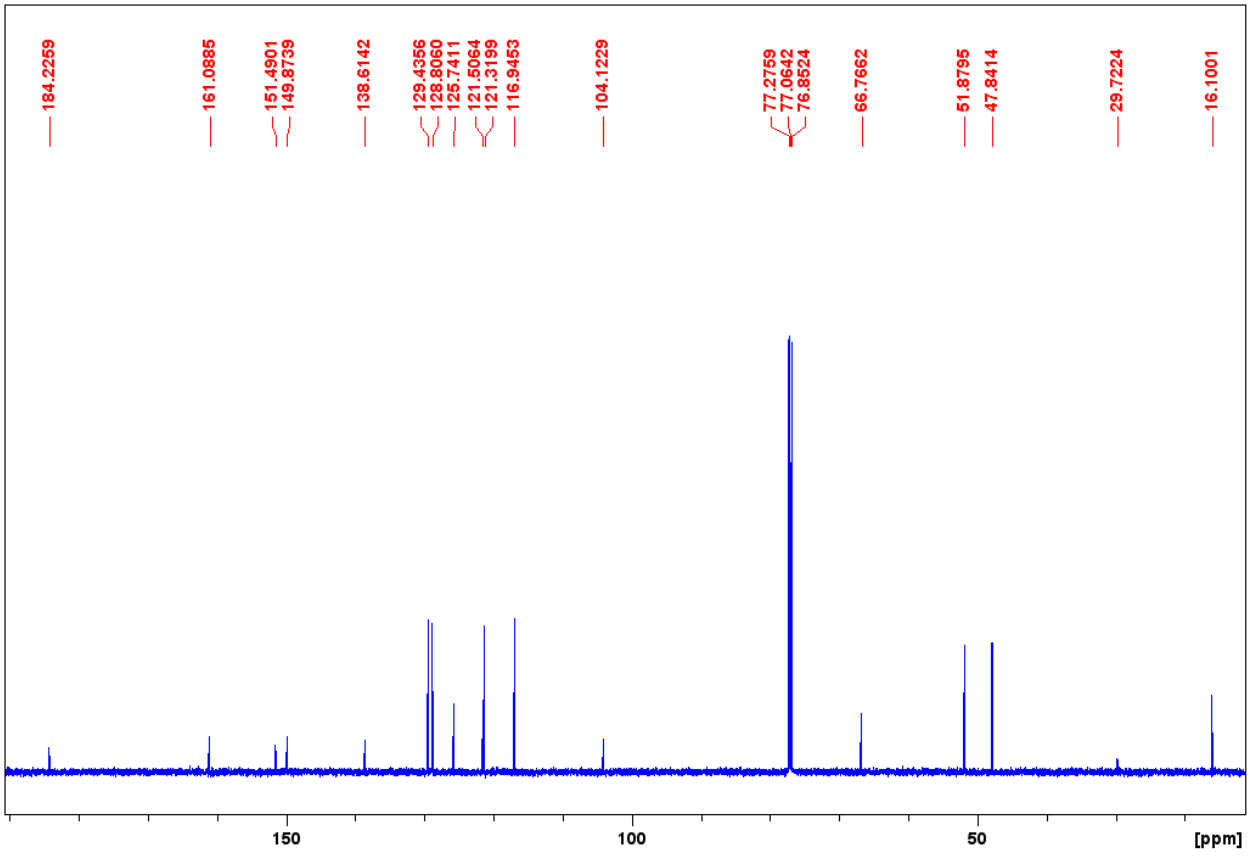
4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104.1229
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50
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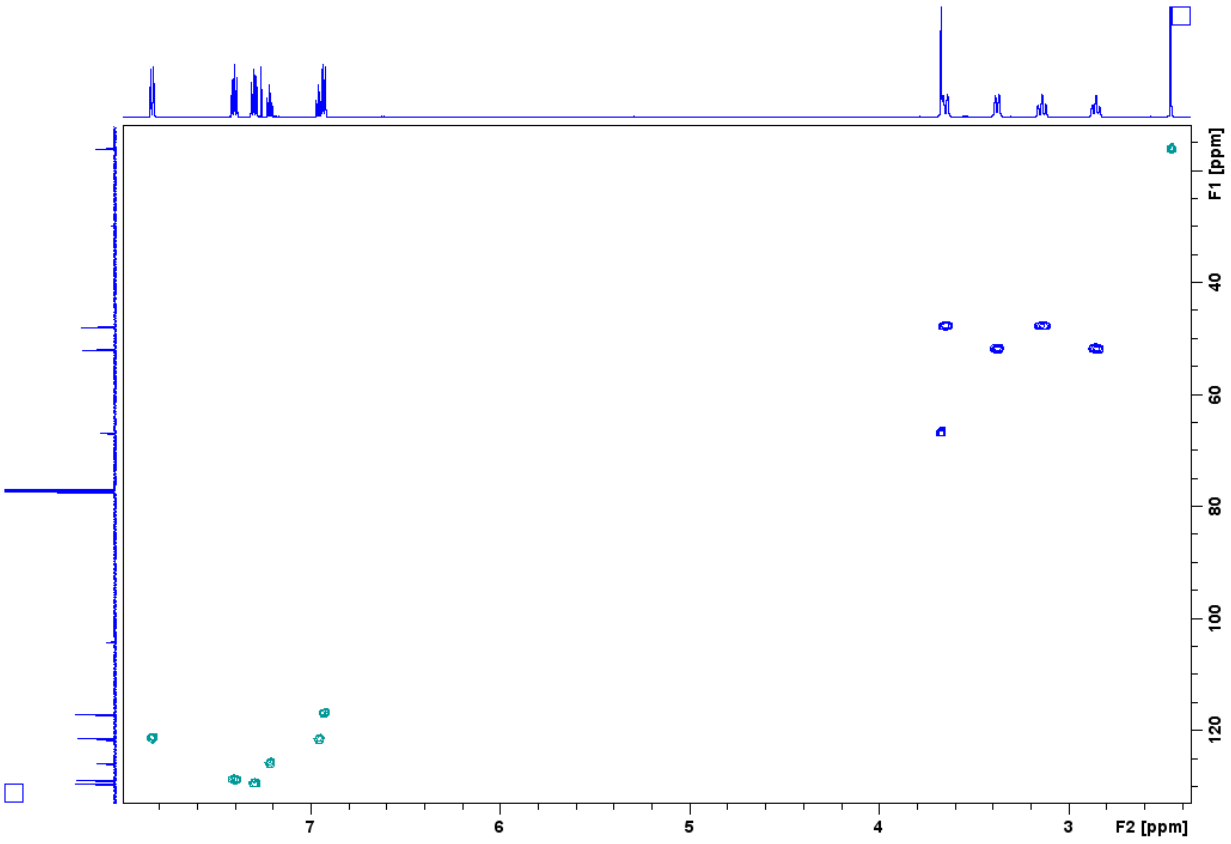
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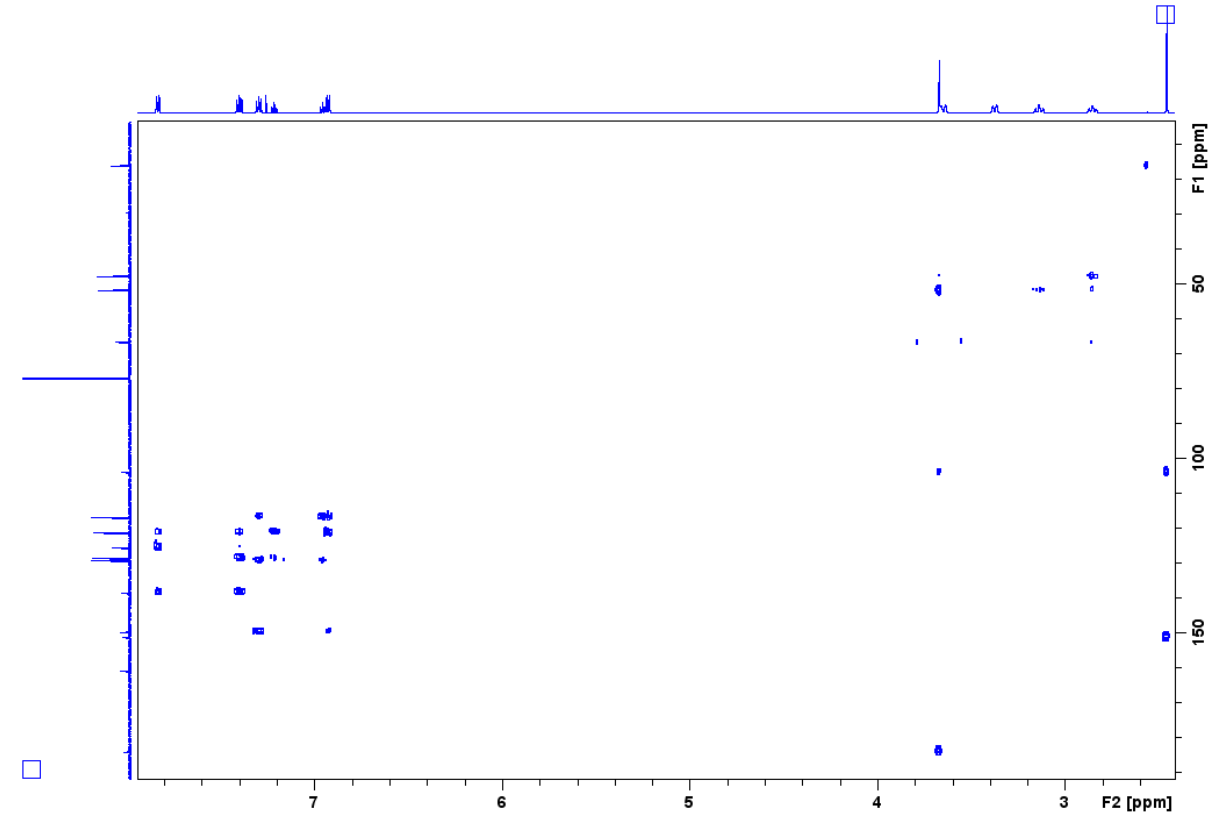
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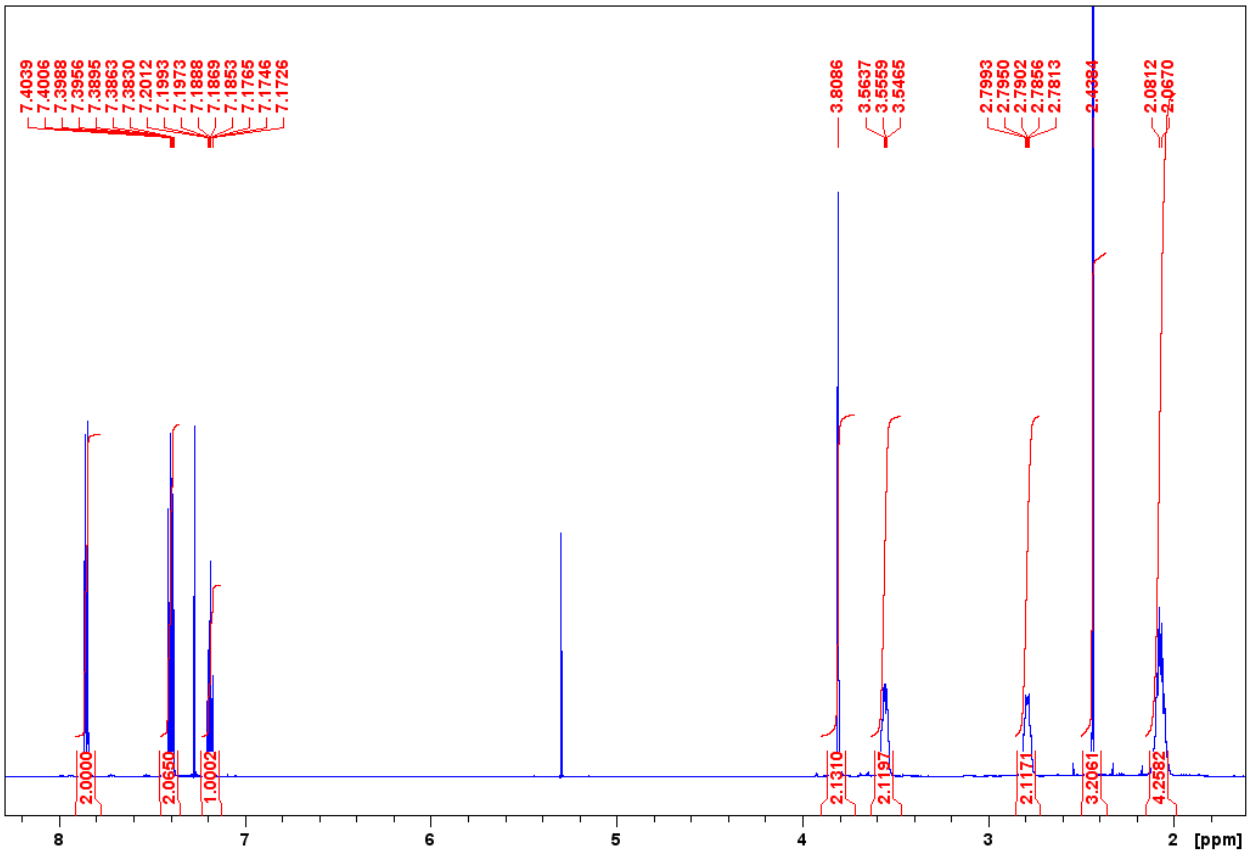
6
5
4
3
F2 [ppm]

*Compound **4e***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7.1853
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7.1726
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3.5465
2.7993
2.7950
2.7902
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2.7813
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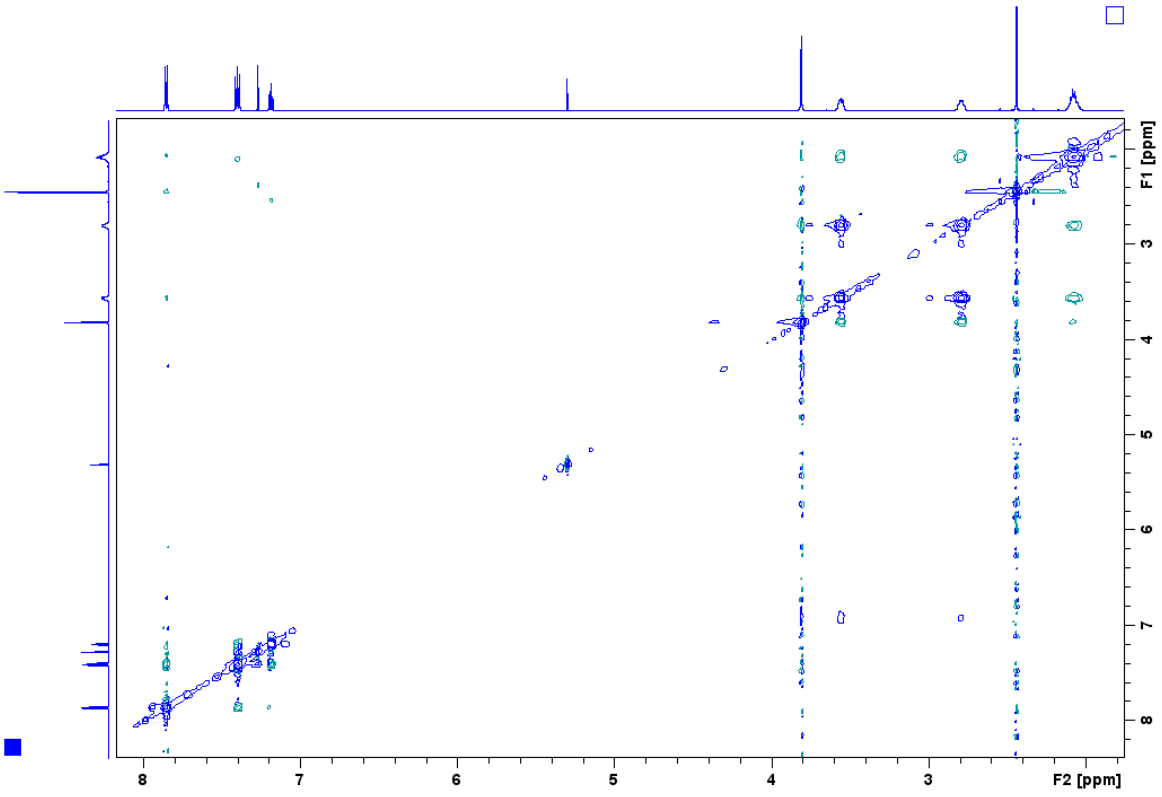
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F2 [ppm]
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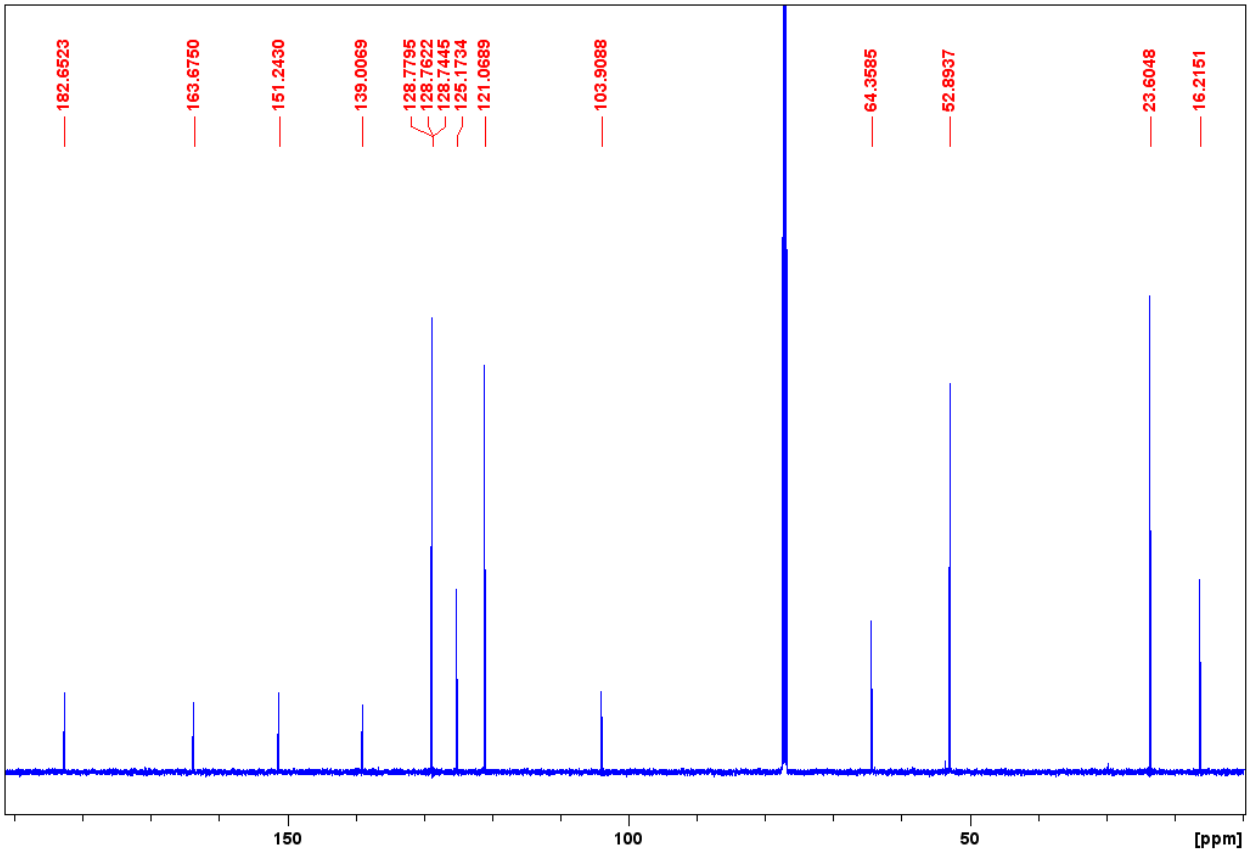
7
6
5
4
3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64.3585
52.8937
23.6048
16.2151
150
100
50
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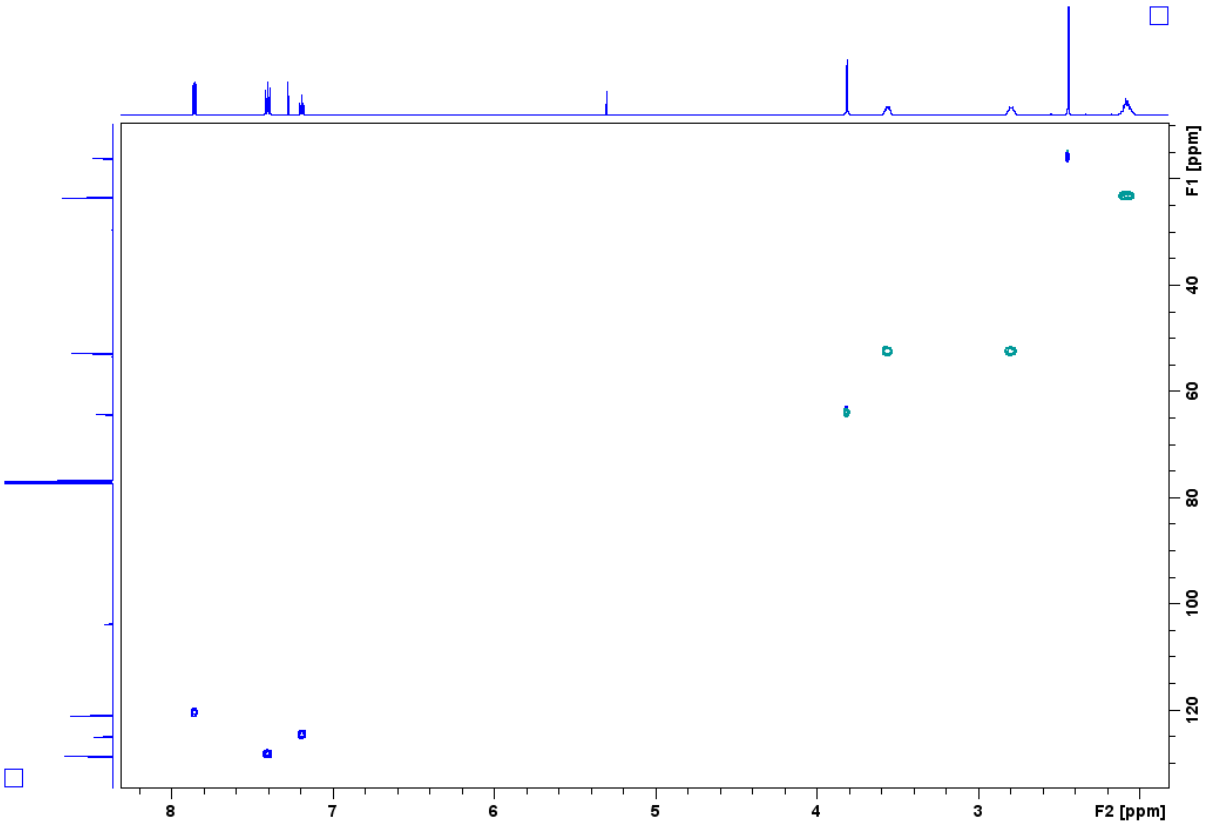
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6
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4
3
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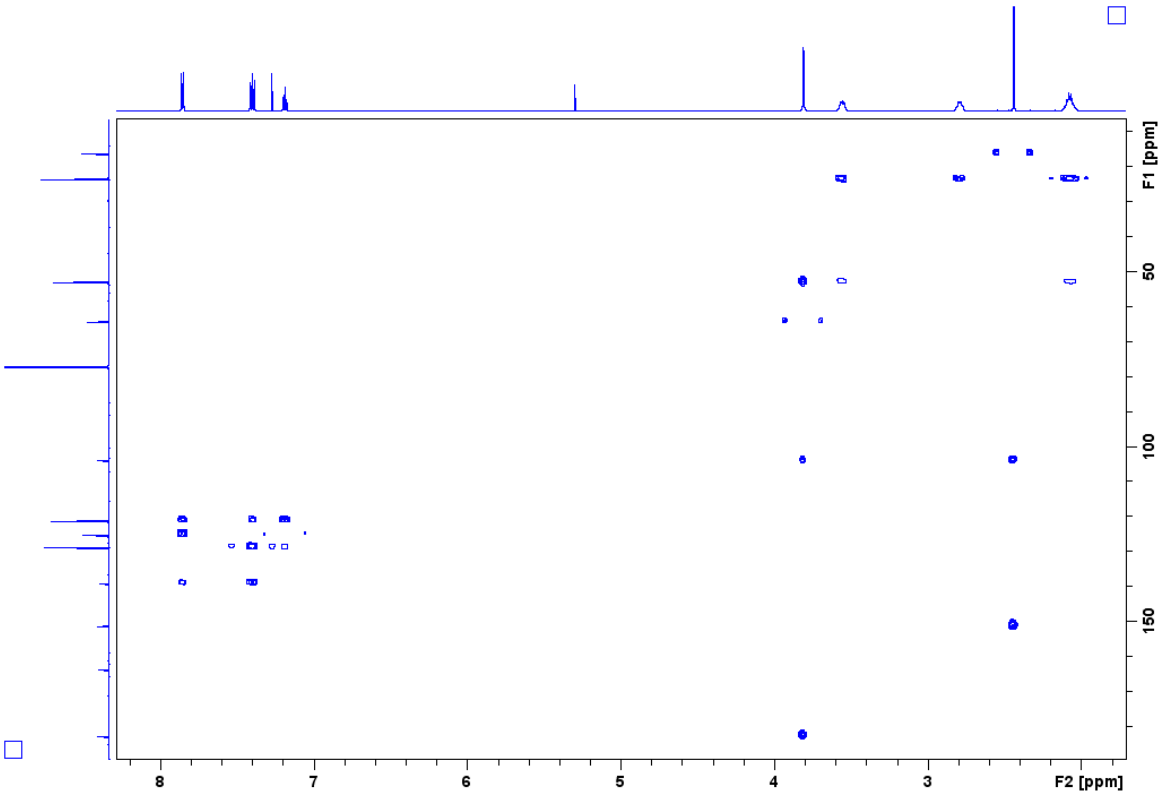
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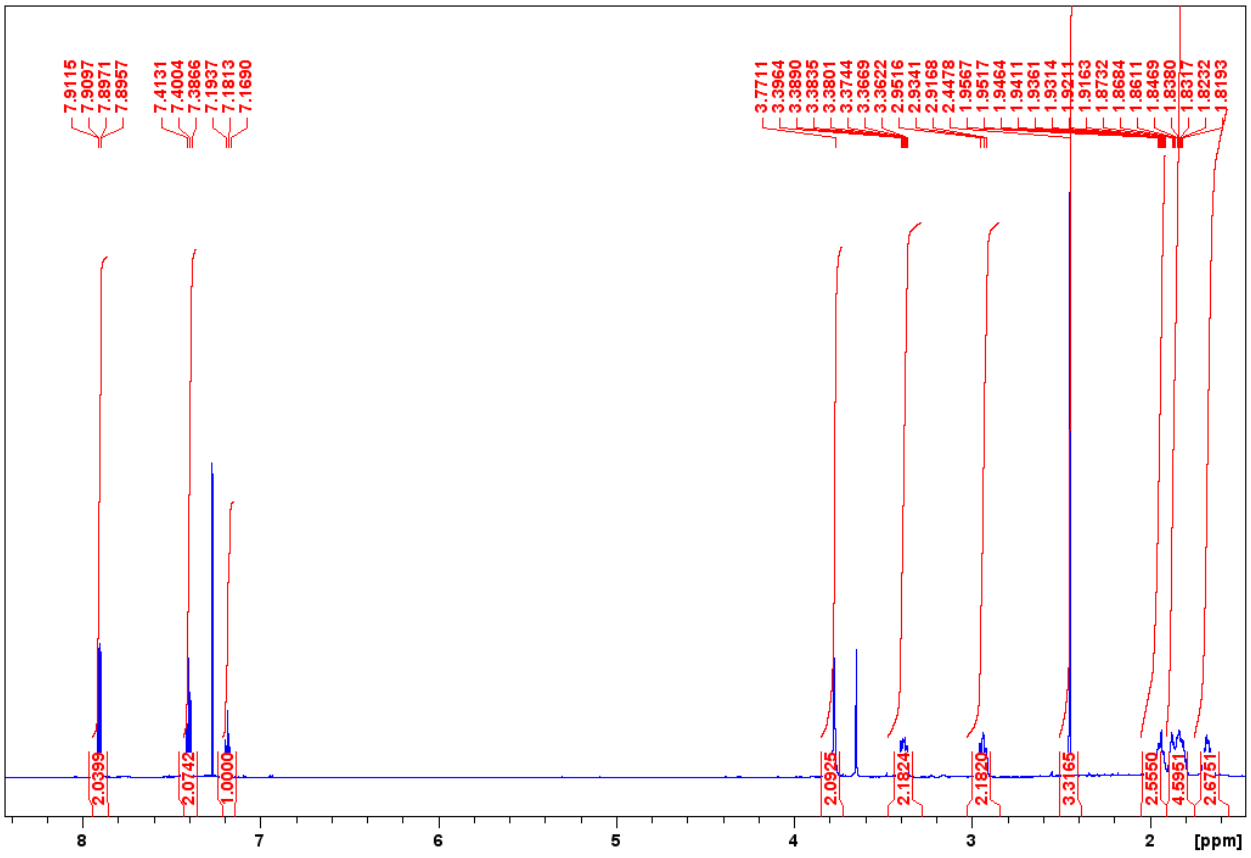
F2 [ppm]

*Compound **4f***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3.3890
3.3835
3.3801
3.3744
3.3669
3.3622
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2.4478
1.9567
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1.9411
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1.9314
1.9211
1.9163
1.8732
1.8684
1.8611
1.8469
1.8380
1.8317
1.8232
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2.0925
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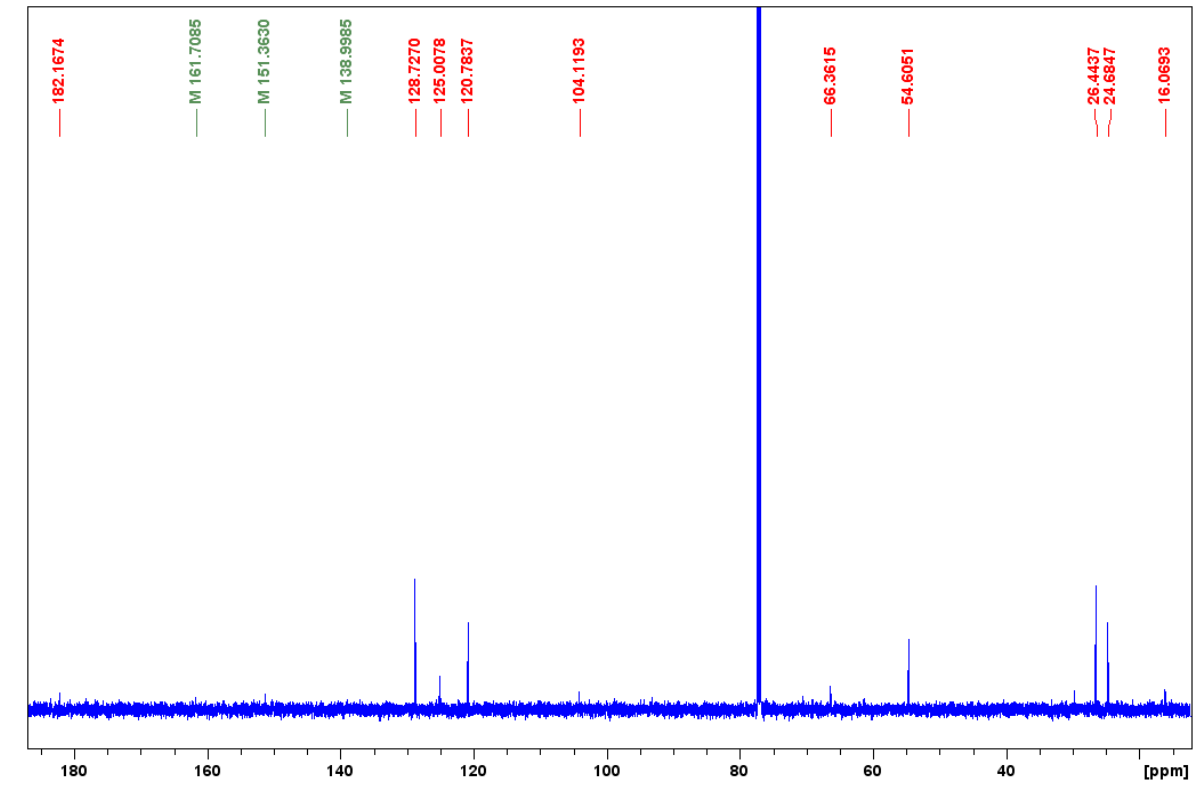
4
3
2
[ppm]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140
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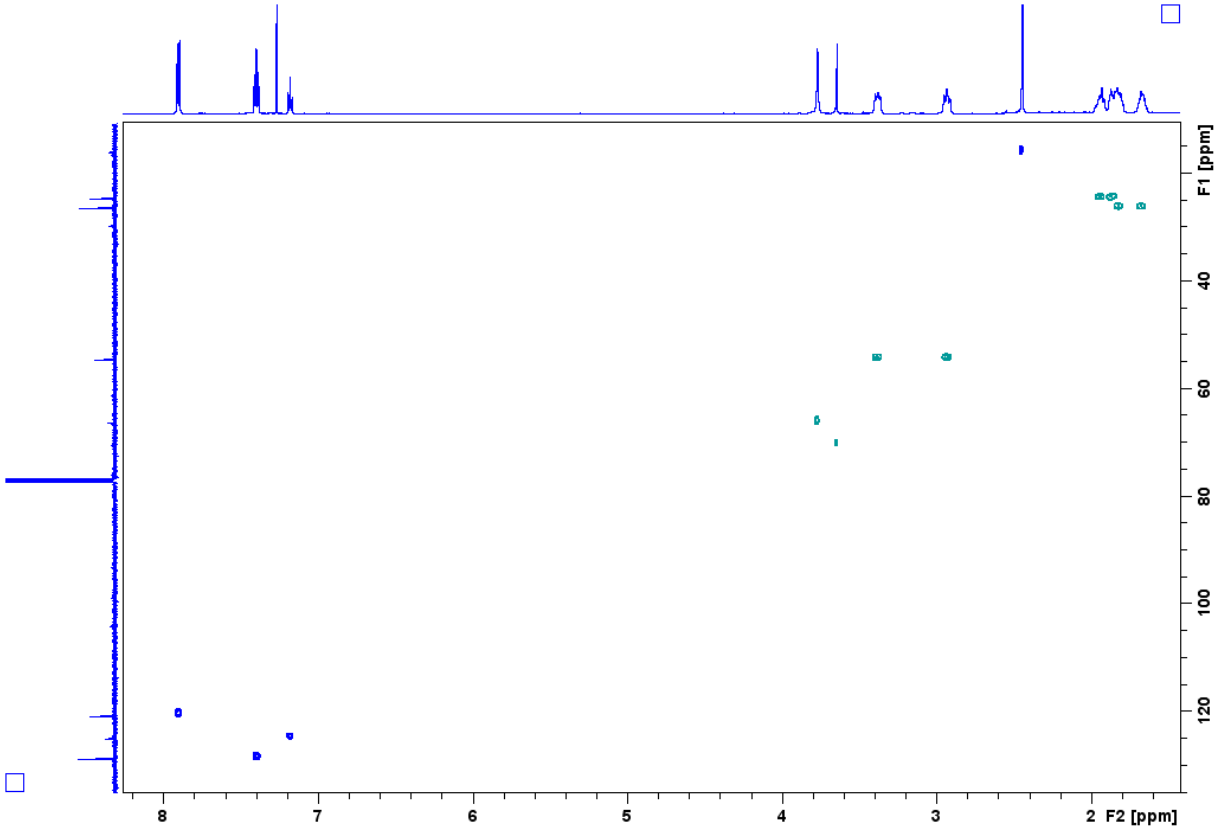
[ppm]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7
6
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4
3
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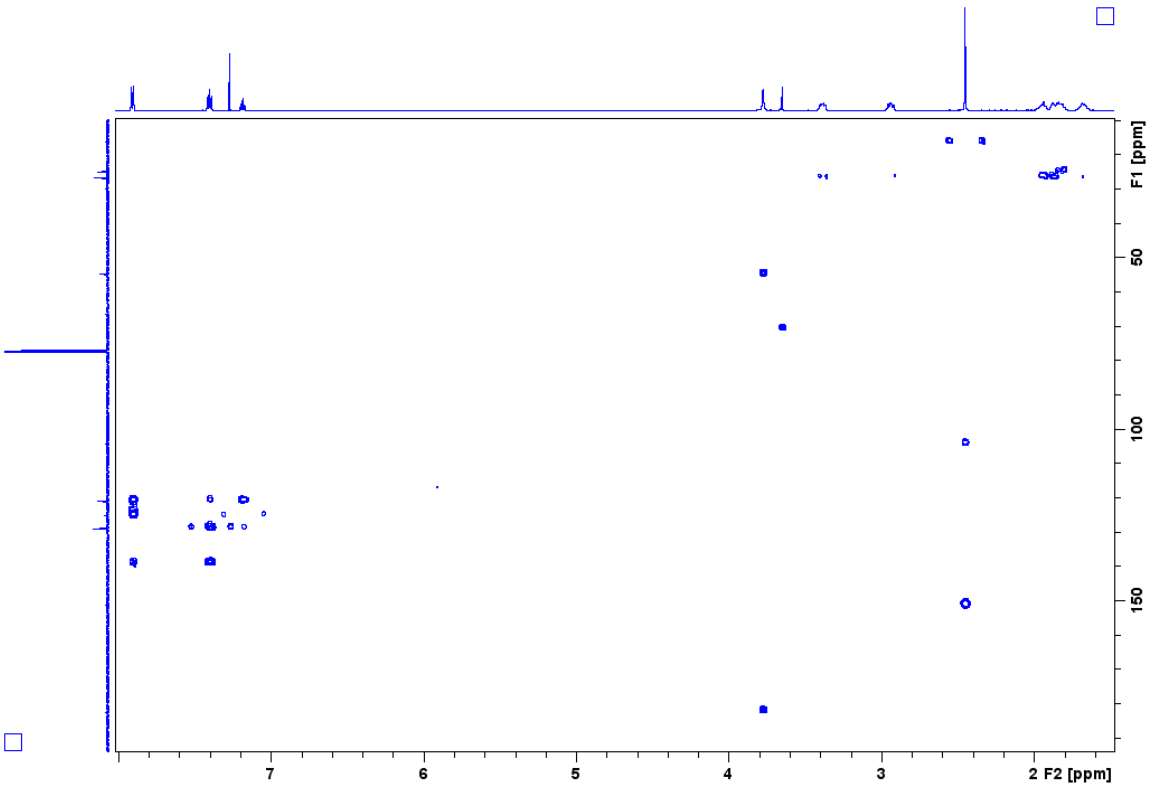
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150
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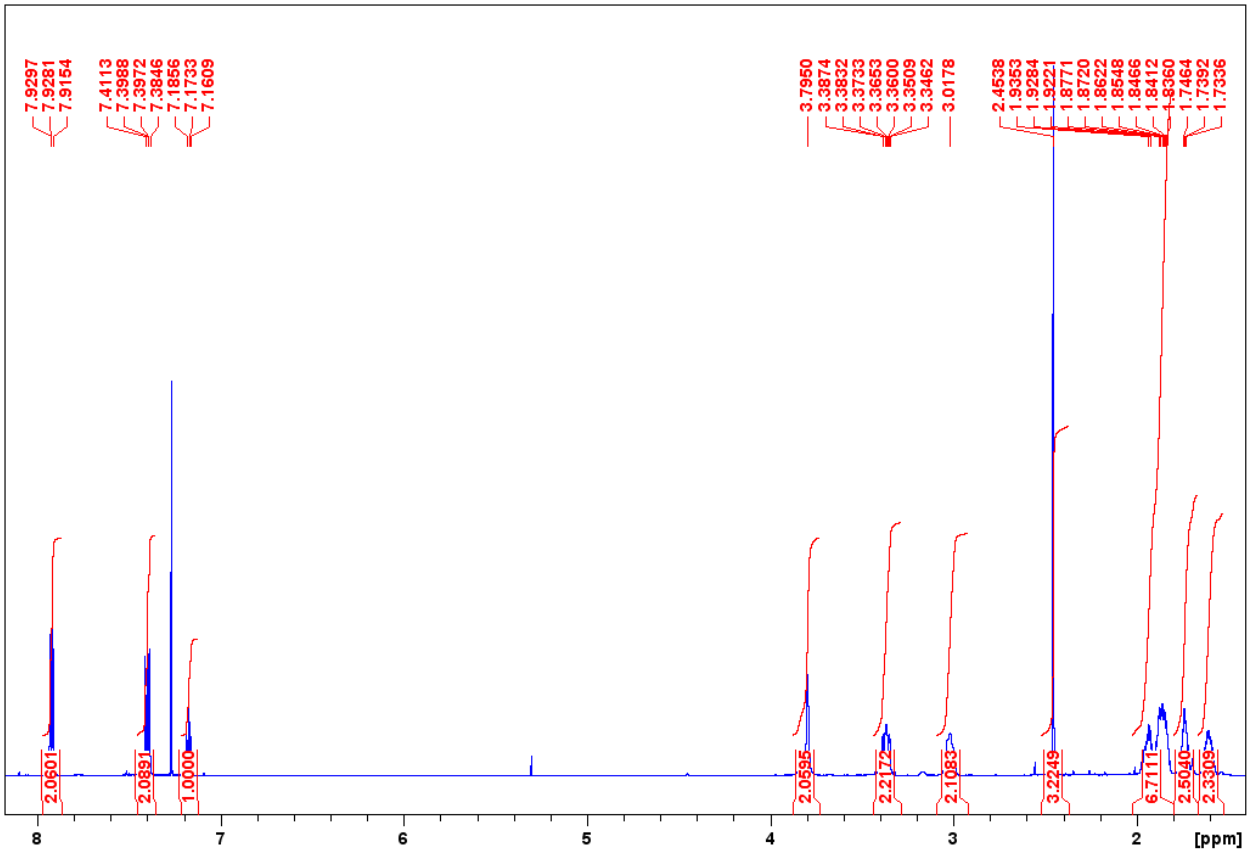
6
5
4
3
2 F2 [ppm]

*Compound **4h***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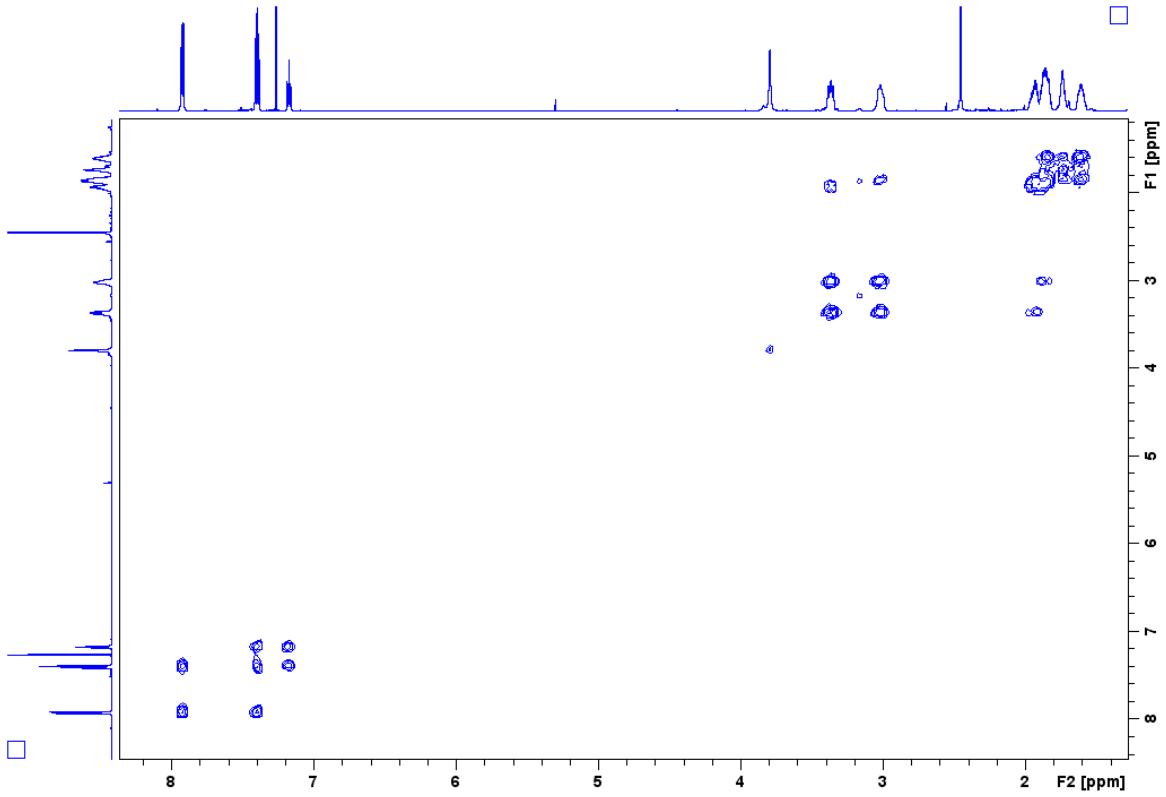
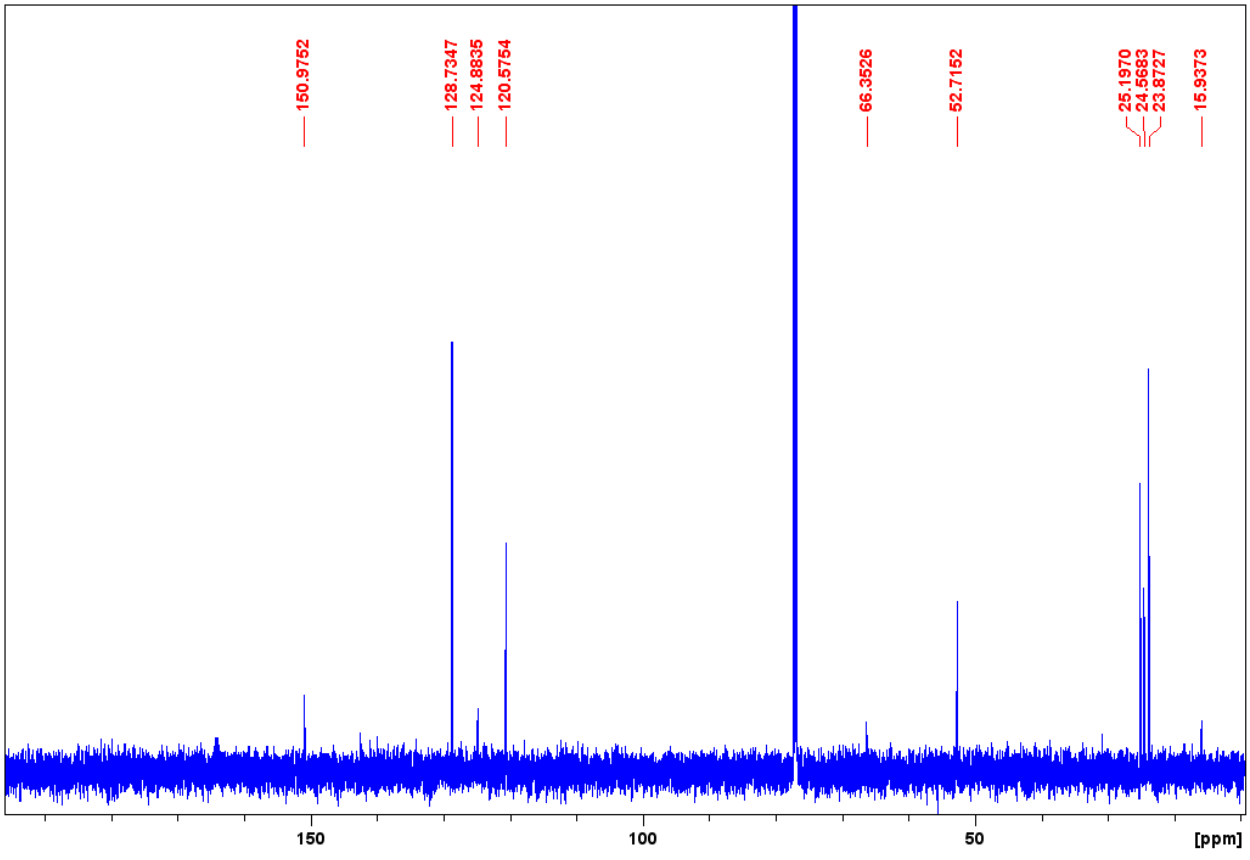
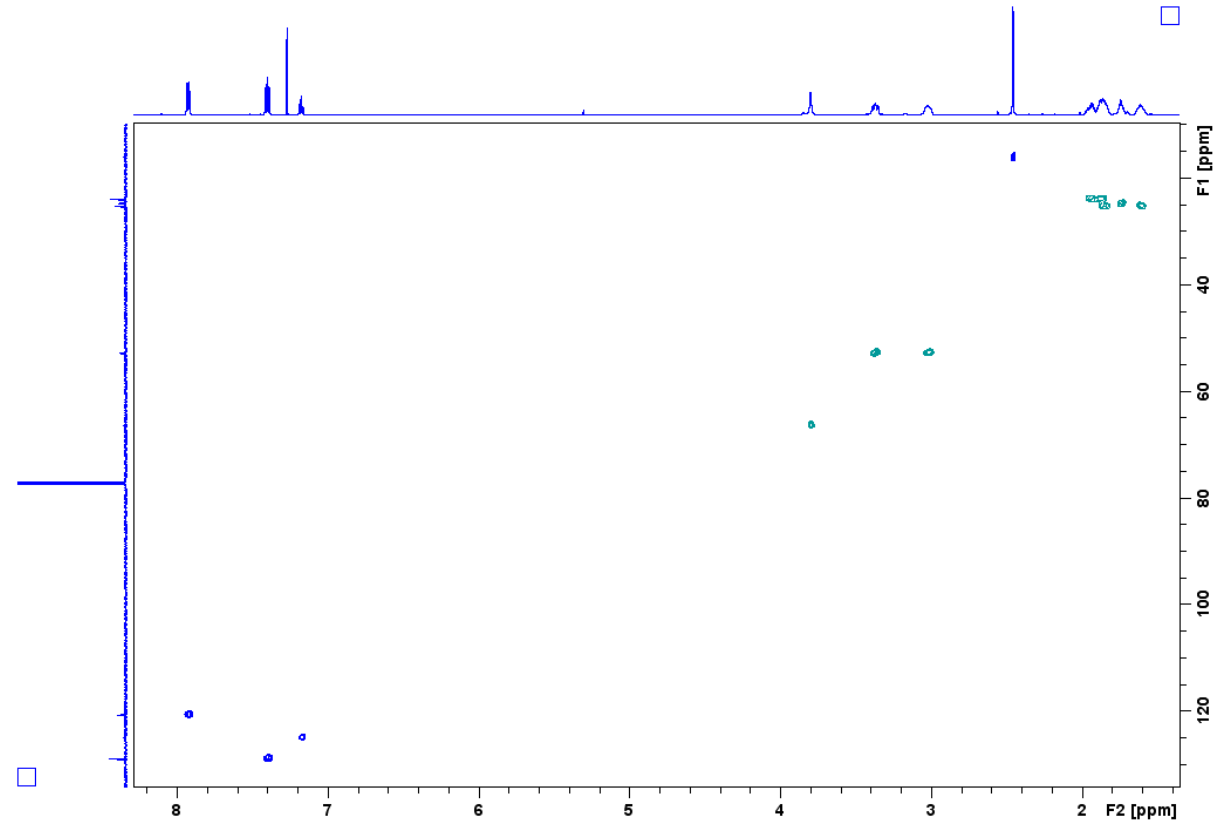
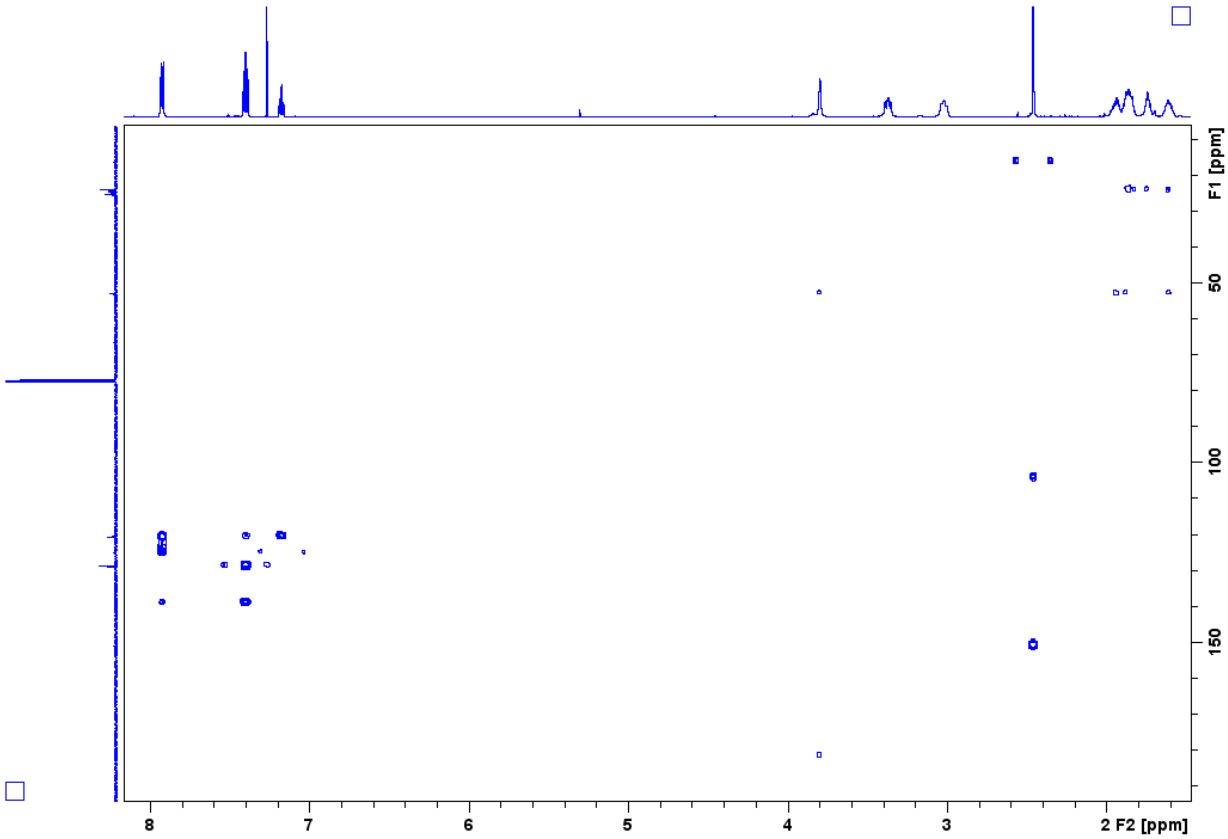
7.1609
3.7950
3.3874
3.3832
3.3733
3.3653
3.3600
3.3509
3.3462
3.0178
2.4538
1.9353
1.9284
1.9221
1.8771
1.8720
1.8622
1.8548
1.8466
1.8412
1.8360
1.7464
1.7392
1.7336
2.0601
2.0891
1.0000
2.0595
2.2172
2.1083
3.2249
6.7111
2.5040
2.3309
8
7
6
5
4
3
2
[ppm]

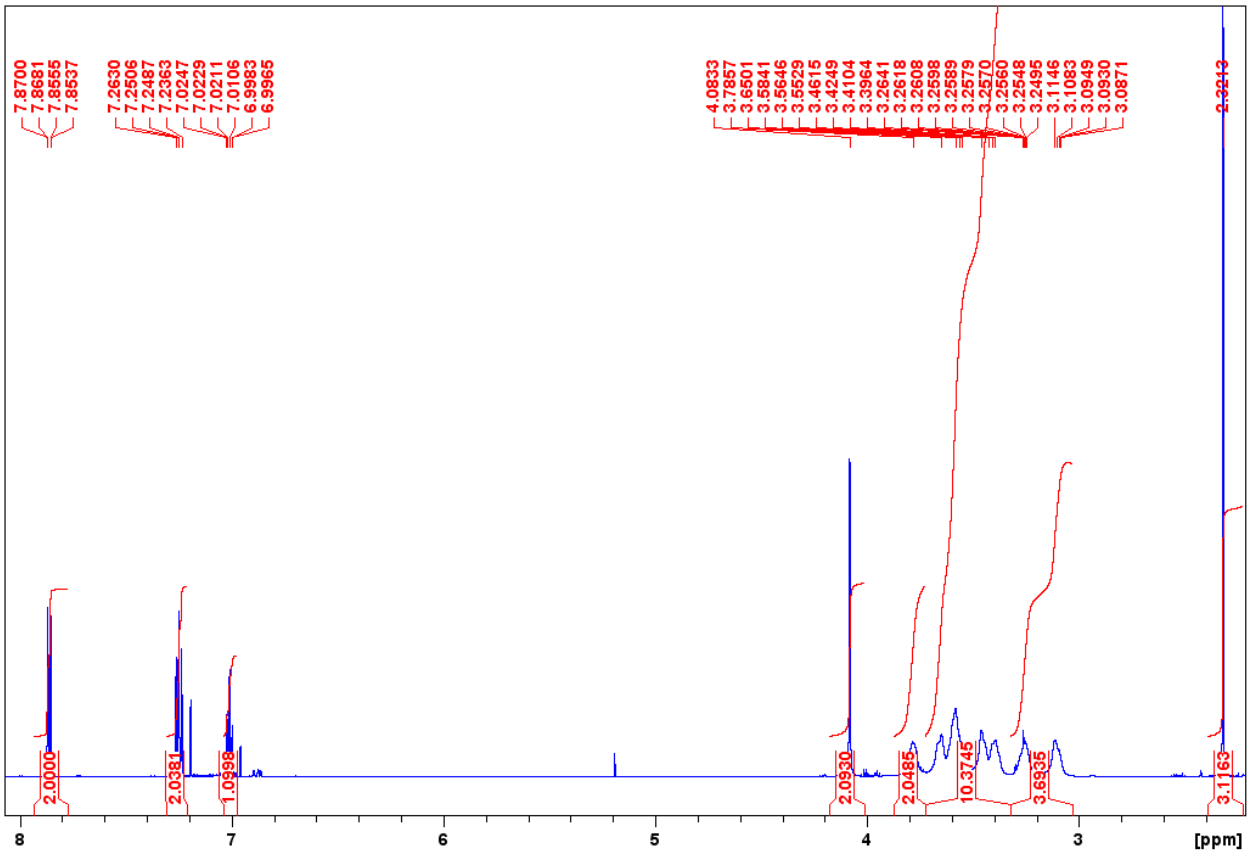

F1 [ppm]
F2 [ppm]
8
7
6
5
4
3
2

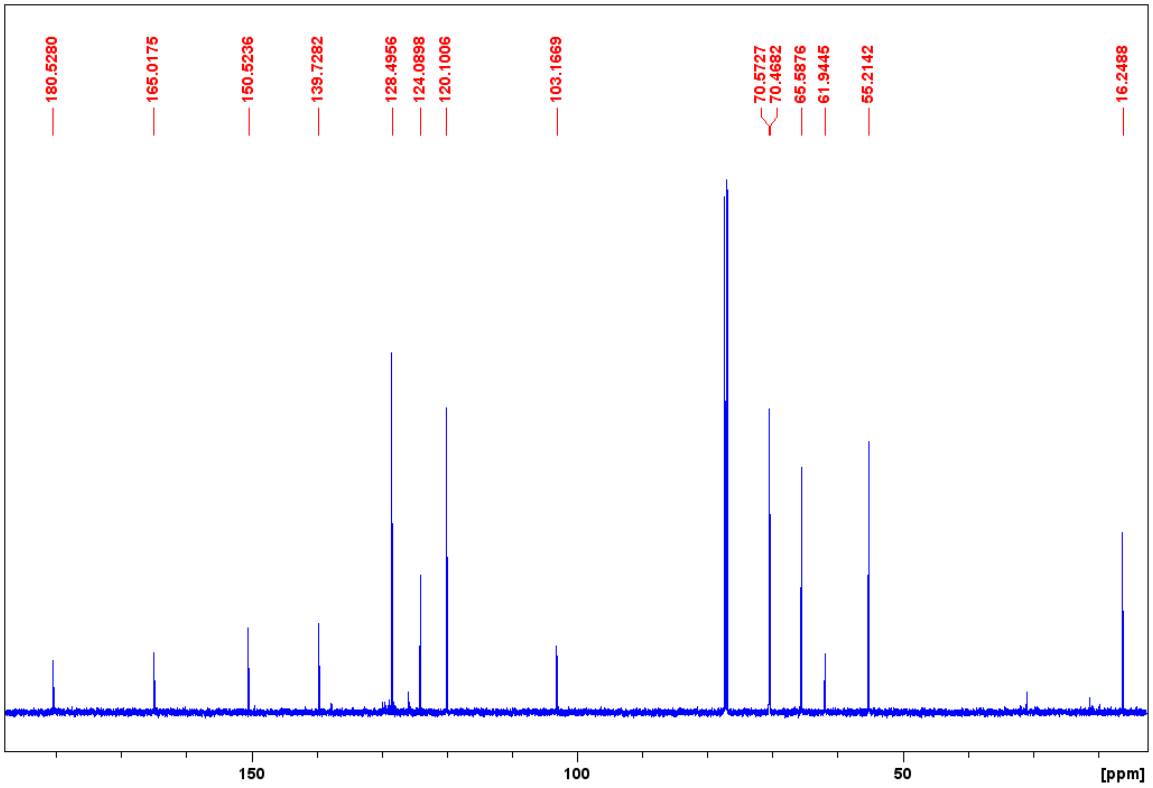

150.9752
128.7347
124.8835
120.5754
66.3526
52.7152
25.1970
24.5683
23.8727
15.9373
150
100
50
[ppm]

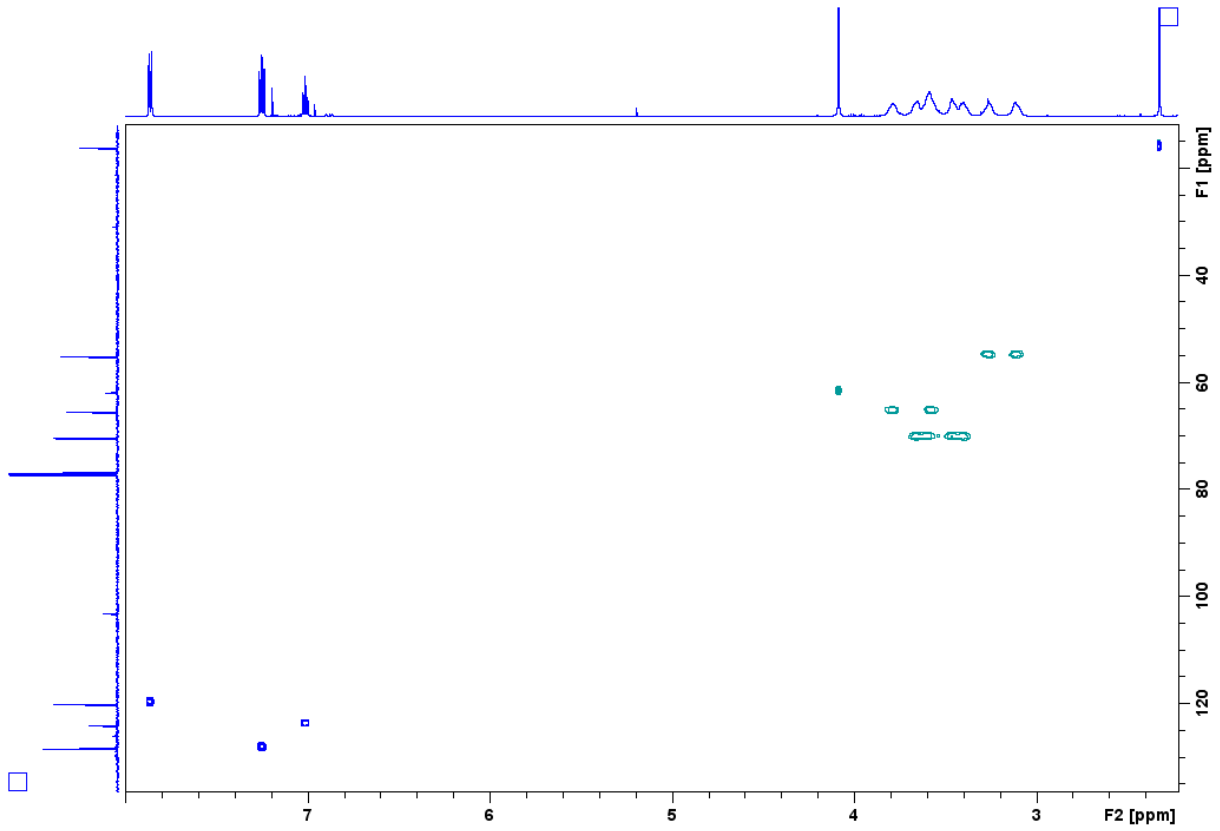

F1 [ppm]
40
60
80
100
120
8
7
6
5
4
3
2
F2 [ppm]

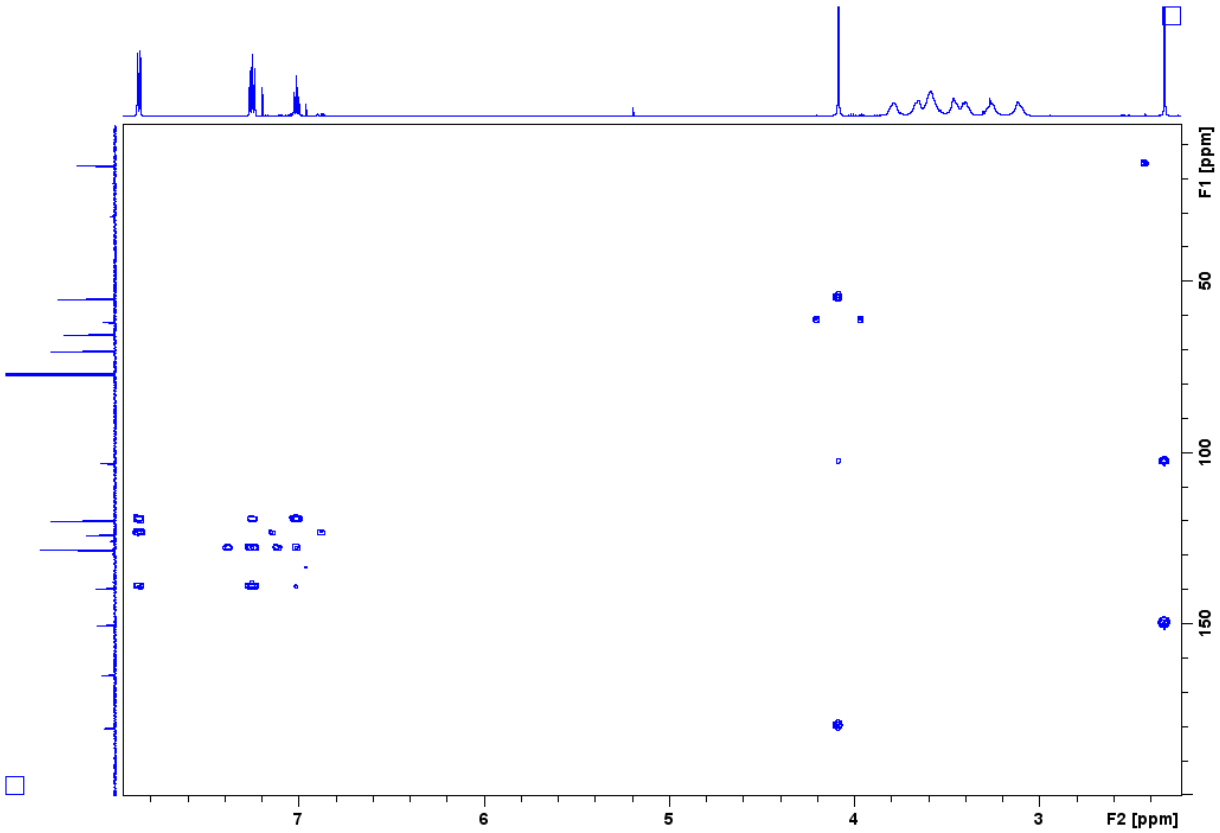

F1 [ppm]
50
100
150
8
7
6
5
4
3
2 F2 [ppm]

*Compound **4i***

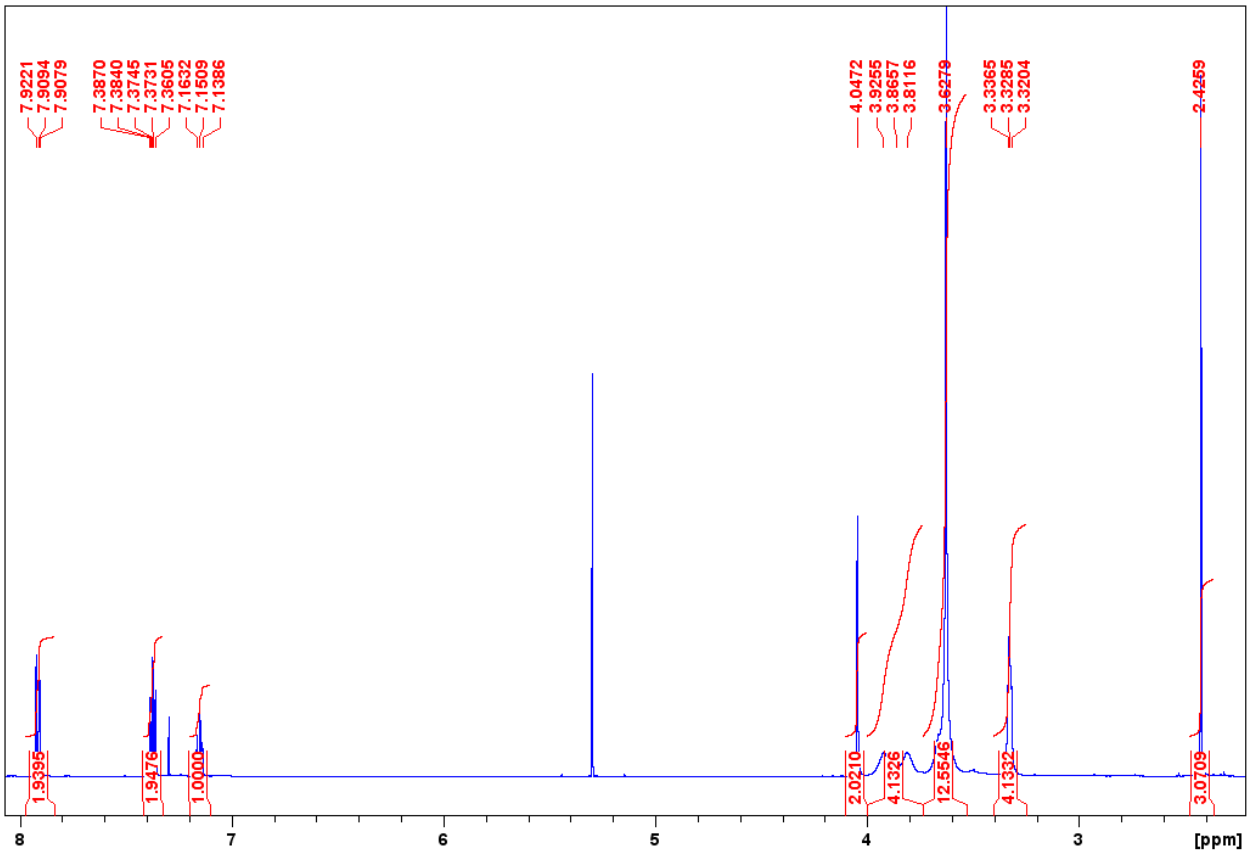

7.8700
7.8681
7.8555
7.8537
7.2630
7.2506
7.2487
7.2363
7.0247
7.0229
7.0211
7.0106
6.9983
6.9965
4.0833
3.7857
3.6501
3.5841
3.5646
3.5529
3.4615
3.4249
3.4104
3.3964
3.2641
3.2618
3.2608
3.2598
3.2589
3.2579
3.2570
3.2560
3.2548
3.2495
3.1146
3.1083
3.0949
3.0930
3.0871
2.3213
2.0000
2.0381
1.0998
2.0930
2.0485
10.3745
3.6835
3.1163
8
7
6
5
4
3
[ppm]

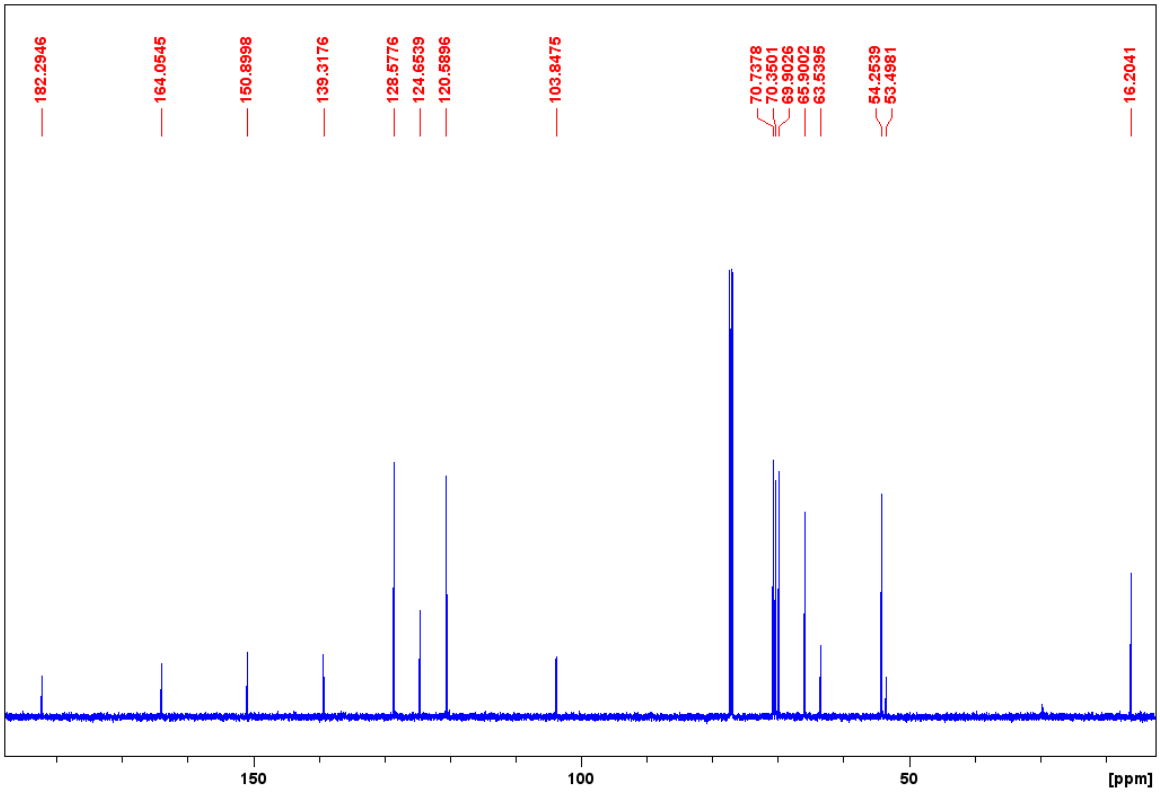

180.5280
165.0175
150.5236
139.7282
128.4956
124.0898
120.1006
103.1669
70.5727
70.4682
65.5876
61.9445
55.2142
16.2488
150
100
50
[ppm]

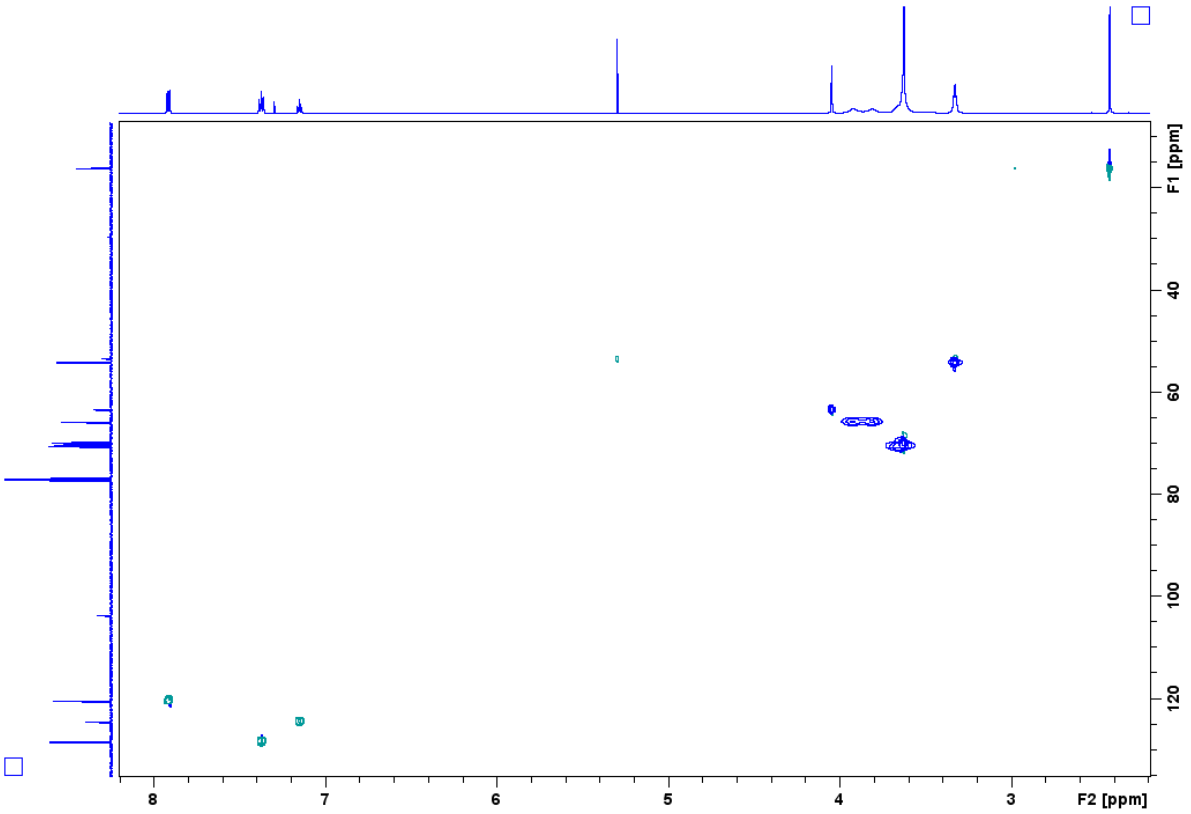

F1 [ppm]
40
60
80
100
120
7
6
5
4
3
F2 [ppm]

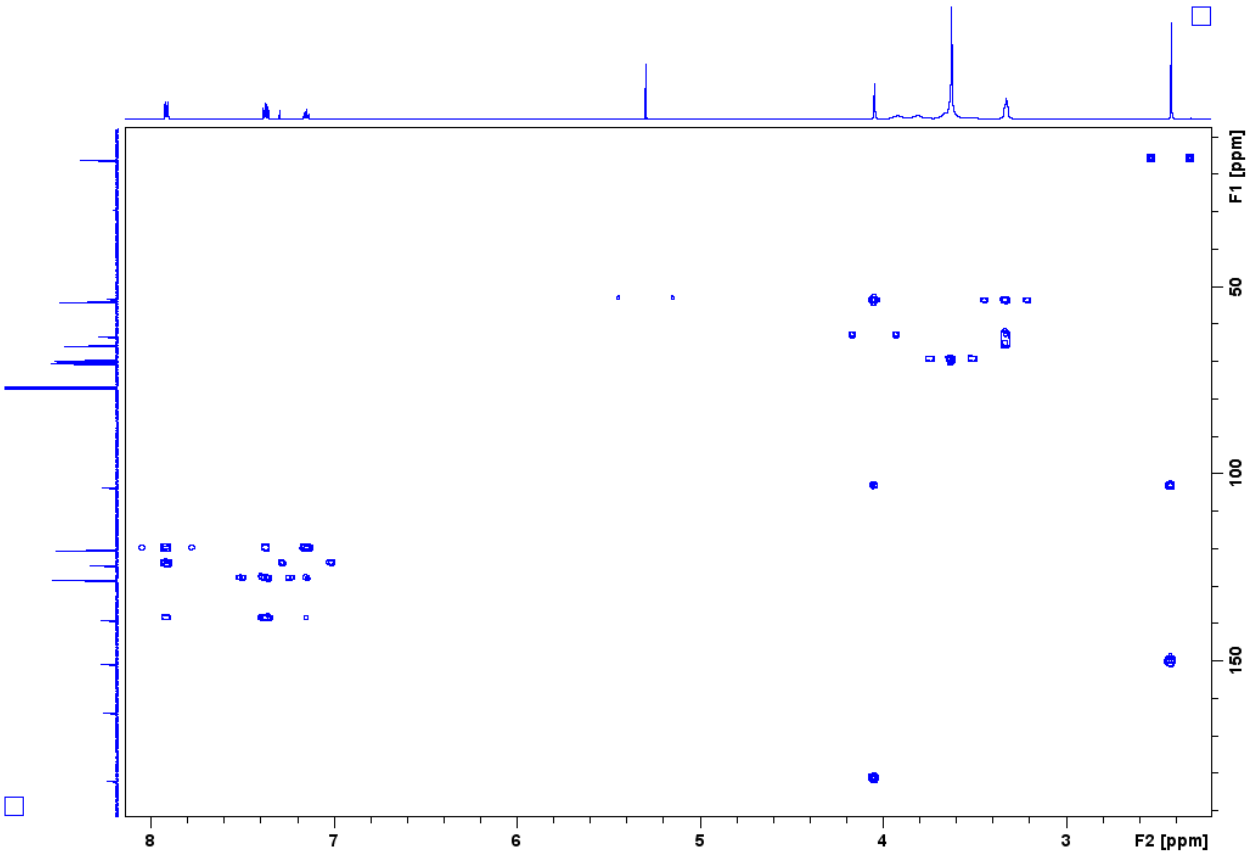

F1 [ppm]
50
100
150
7
6
5
4
3
F2 [ppm]

*Compound **4j***


7.9221
7.9094
7.9079
7.3870
7.3840
7.3745
7.3731
7.3605
7.1632
7.1509
7.1386
4.0472
3.9255
3.8657
3.8116
3.6279
3.3365
3.3285
3.3204
2.4259
1.9395
1.9476
1.0000
2.0210
4.1326
12.5546
4.1332
3.0709
8
7
6
5
4
3
[ppm]

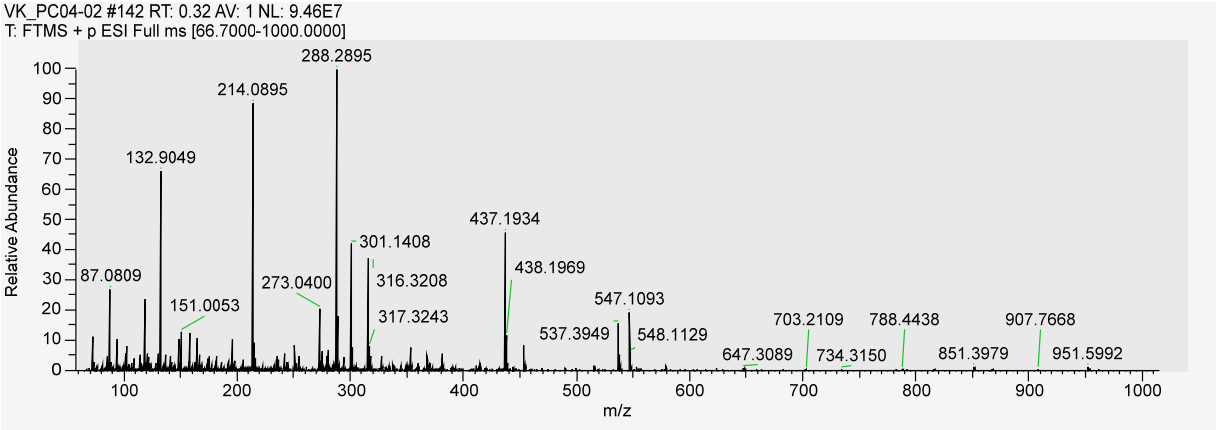

182.2946
164.0545
150.8998
139.3176
128.5776
124.6539
120.5896
103.8475
70.7378
70.3501
69.9026
65.9002
63.5395
54.2539
53.4981
16.2041
150
100
50
[ppm]

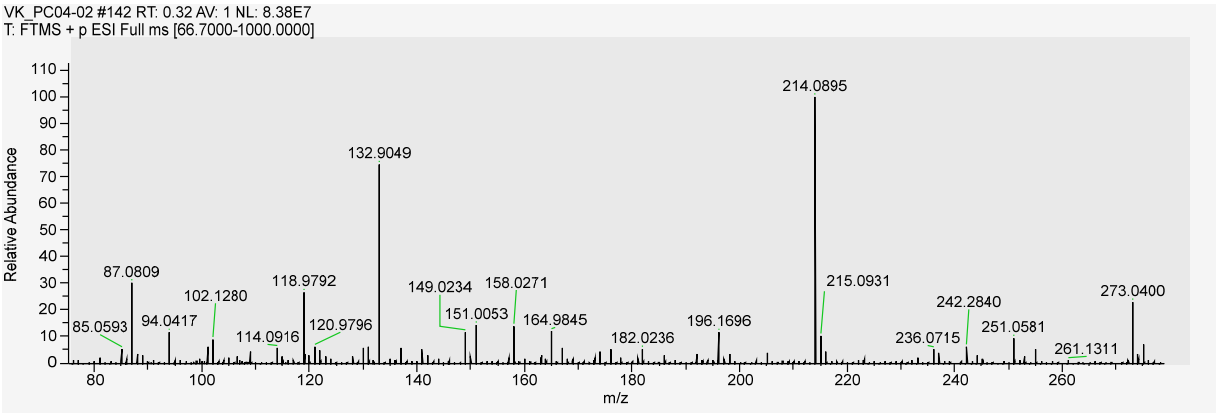

F1 [ppm]
40
60
80
100
120
8
7
6
5
4
3
F2 [ppm]


F1 [ppm]
50
100
150
8
7
6
5
4
3
F2 [ppm]

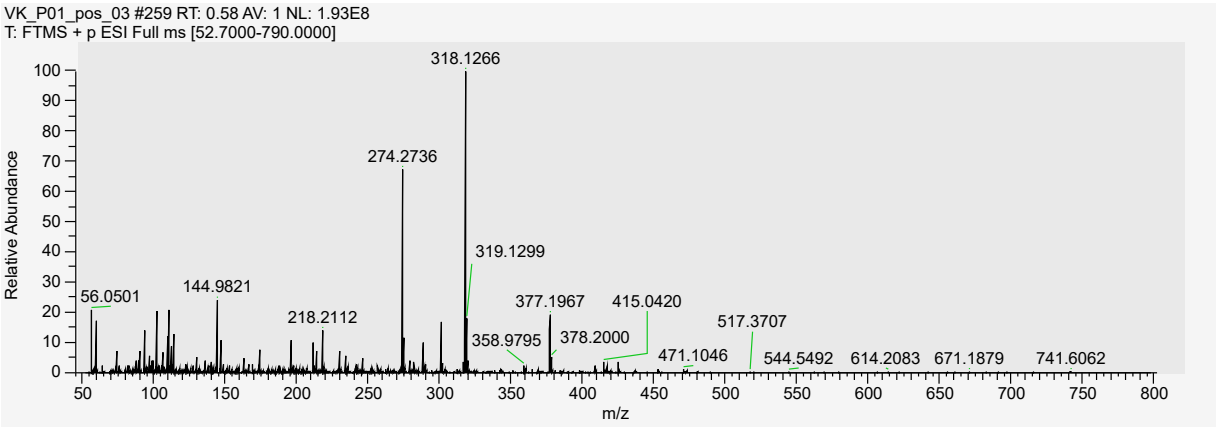
HR-MS spectra:

Compound ***2***-Cs_2CO_3 *complex:*

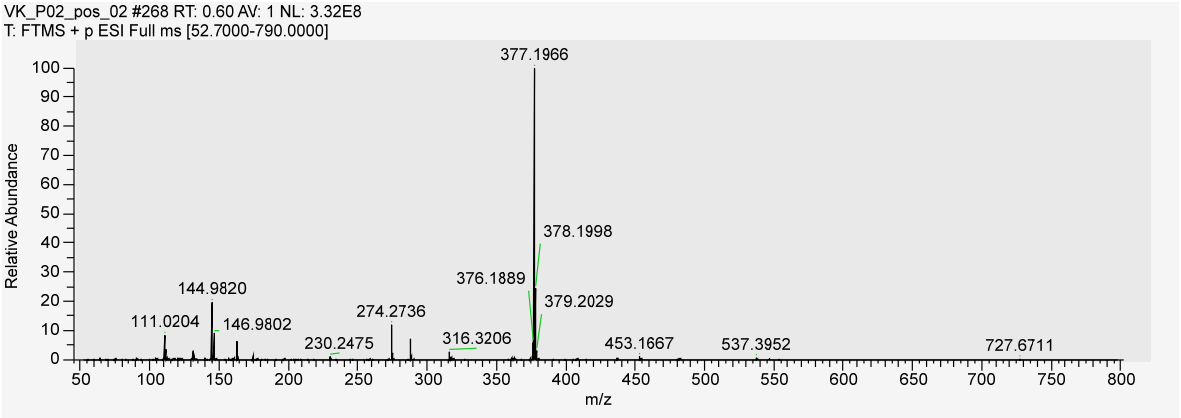




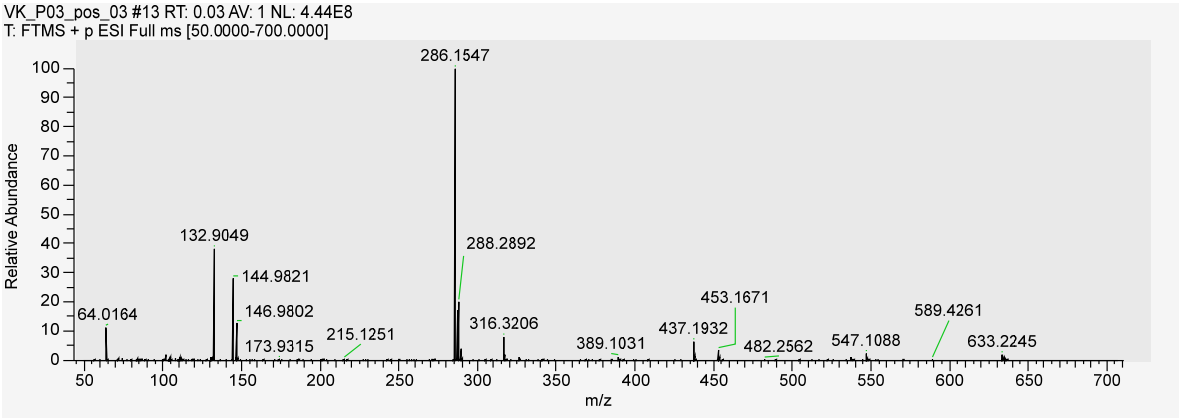
Compound ***4c***



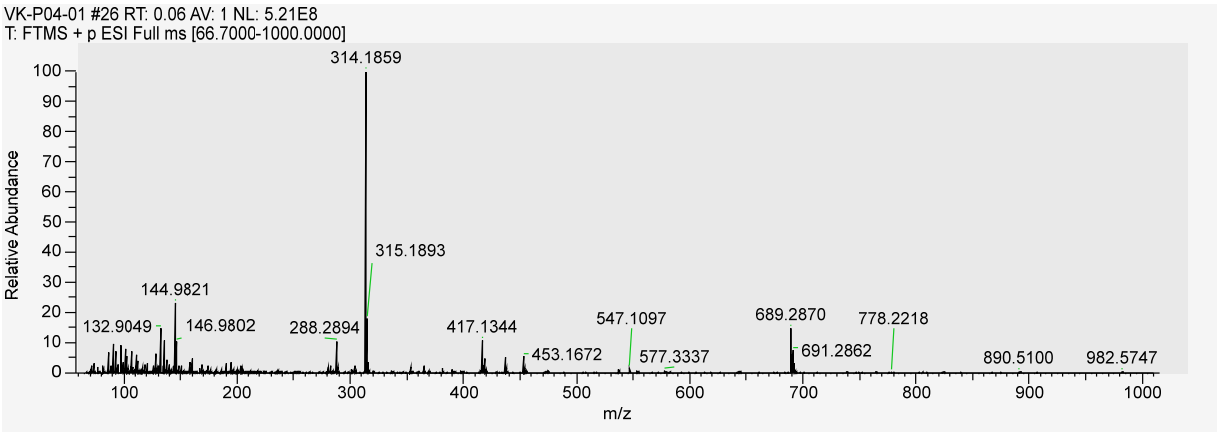
*Compound **4d***



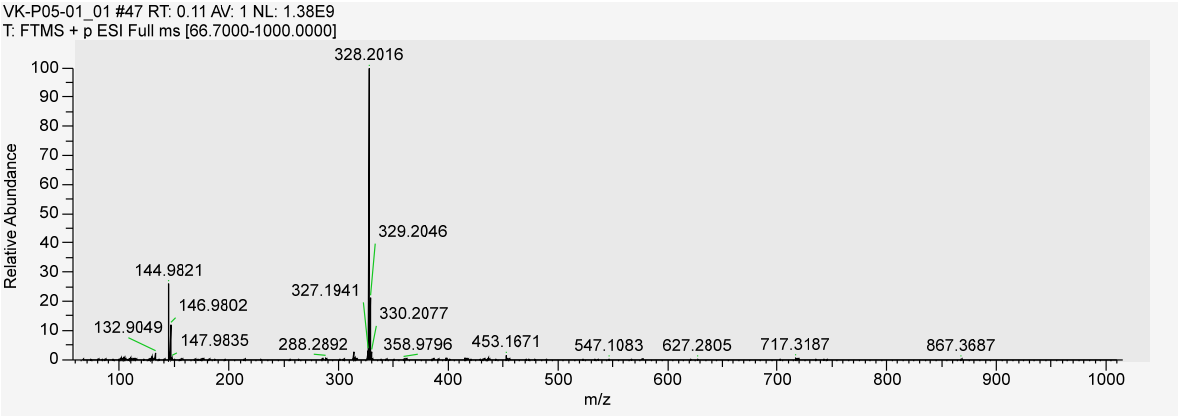
*Compound **4e***



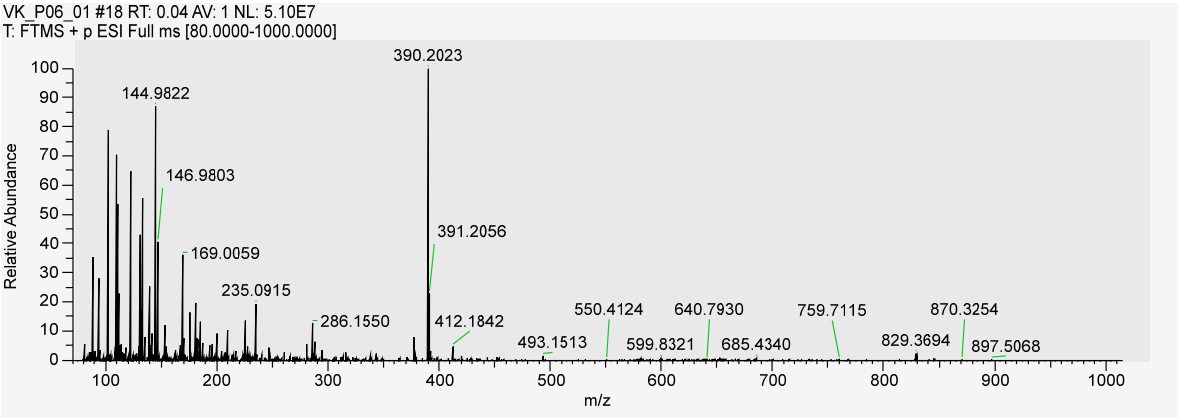
*Compound **4f***



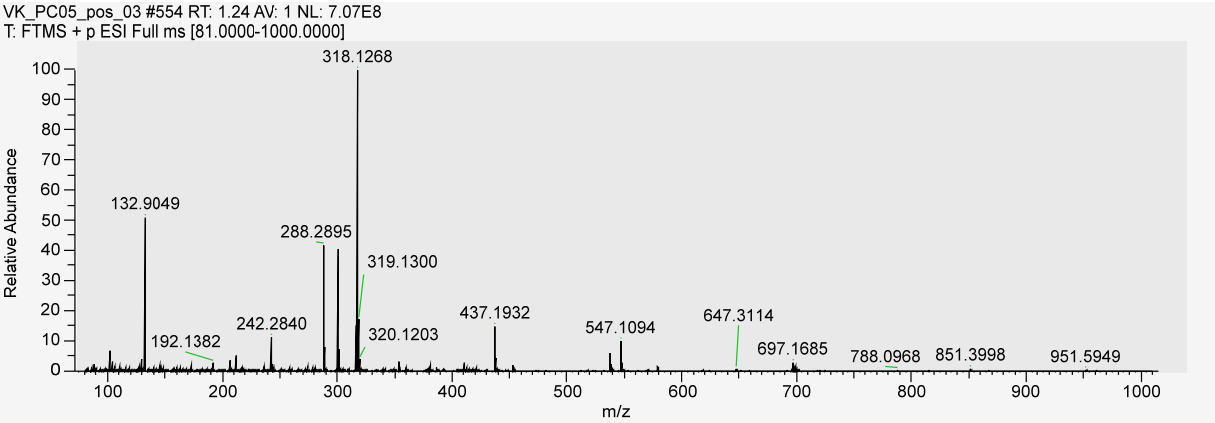
*Compound **4h***

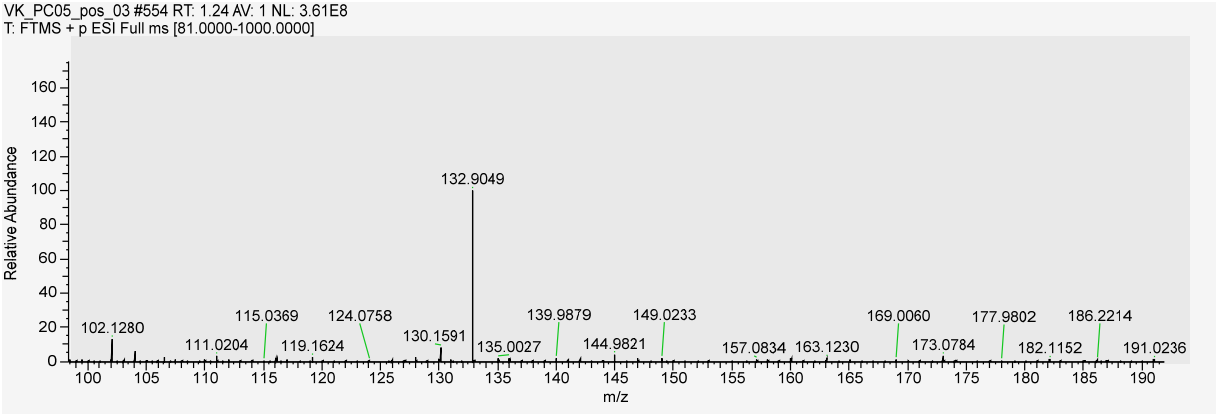


*Compound **4i***

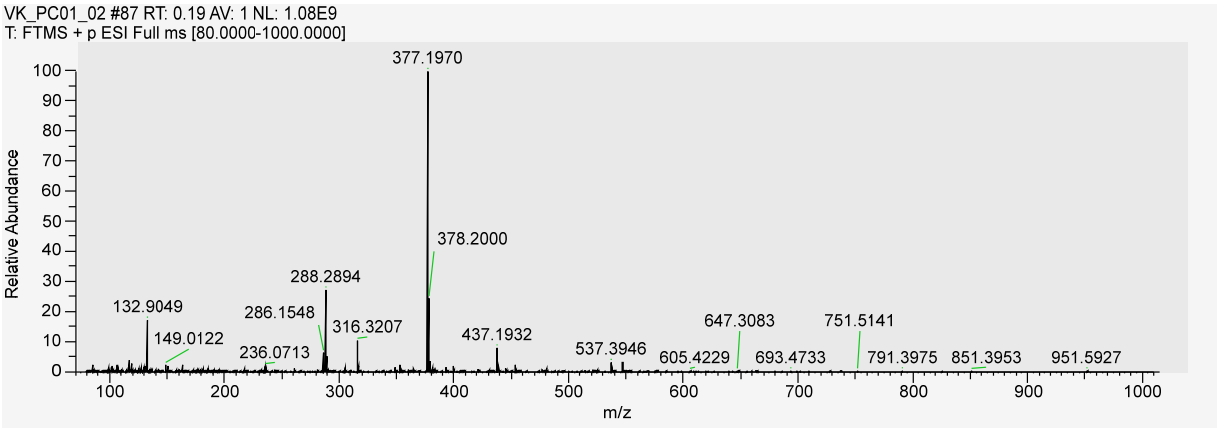


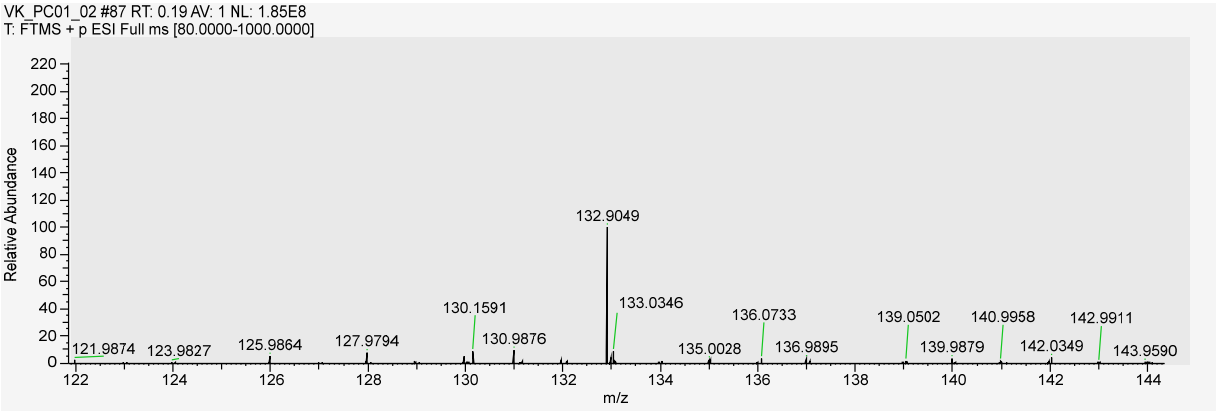
*Compound **4c**-Cs_2CO_3 complex:*



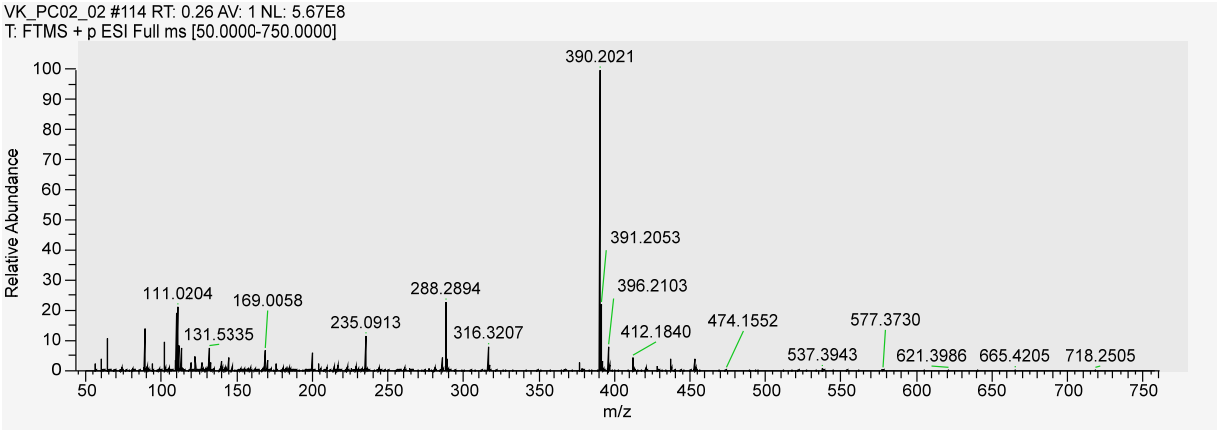


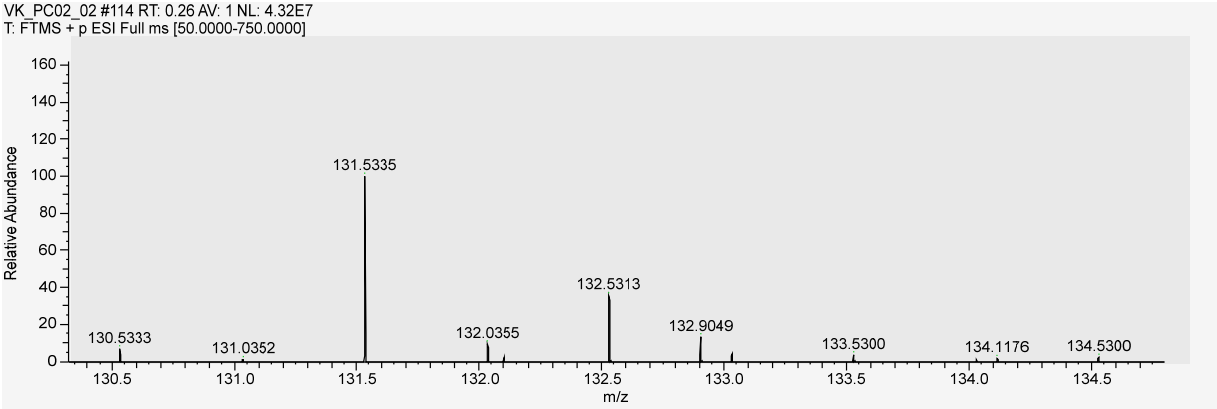
*Compound **4d**-Cs_2CO_3 complex:*



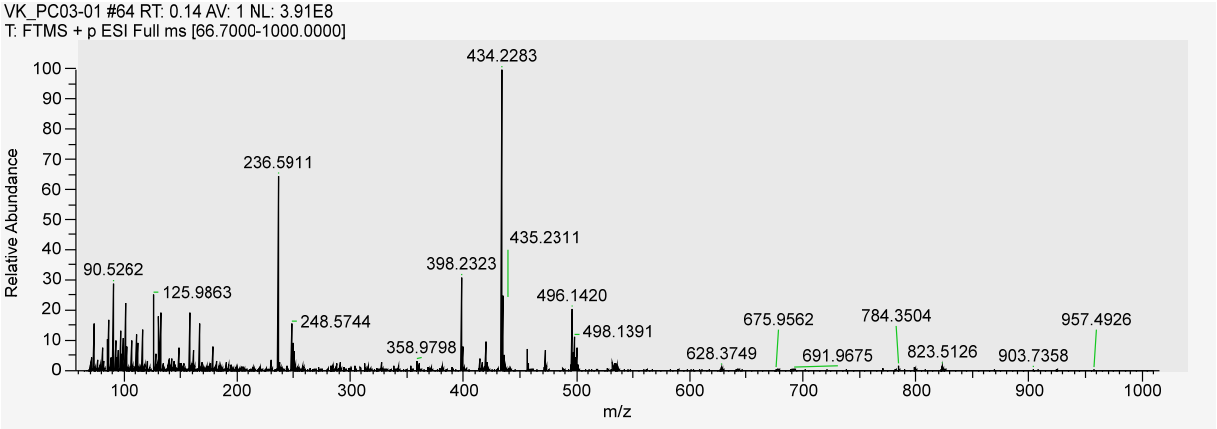


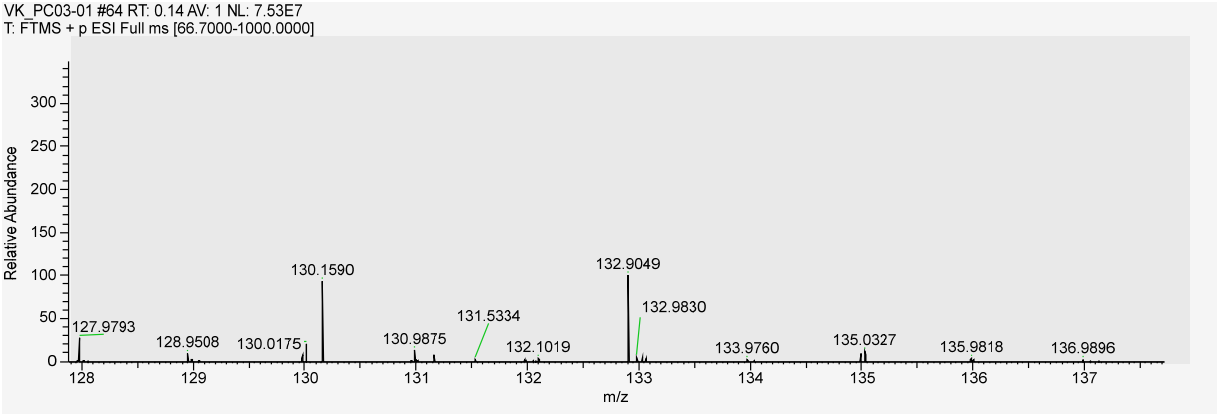
*Compound **4i**-Cs_2CO_3 complex:*





*Compound **4j**-Cs_2CO_3 complex:*




VK_PC03-01 #64 RT: 0.14 AV: 1 NL: 7.53E7
T: FTMS + p ESI Full ms [66.7000-1000.0000]
Relative Abundance
m/z
127.9793
128.9508
130.0175
130.1590
130.9875
131.5334
132.1019
132.9049
132.9830
133.9760
135.0327
135.9818
136.9896