Photoredox functionalization of 3-halogenchromones, 3-formylchromones and chromone-3-carboxylic acids: Routes to 3-acylchromones.

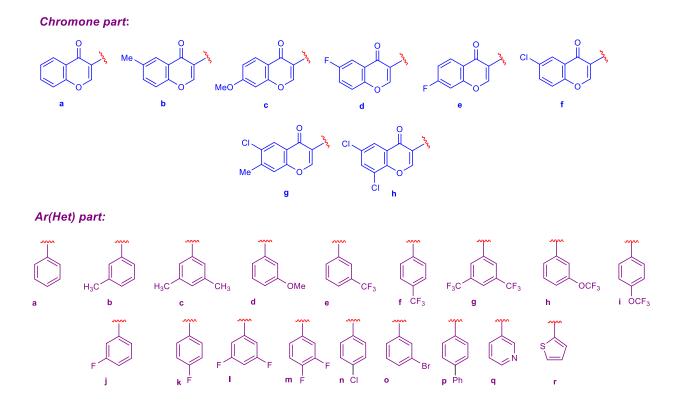
Satenik Mkrtchyan*, Viktor O. Iaroshenko*.

Laboratory of Homogeneous Catalysis and Molecular Design at the Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Sienkiewicza 112, PL-90-363 Łodź, Poland. E-mail: <u>iva108@gmail.com</u>, <u>viktori@cbmm.lodz.pl</u>, <u>sm19860214@gmail.com</u>

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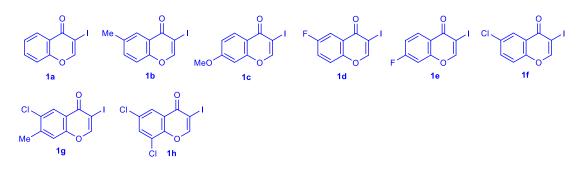
(A) List of used starting materials	S3
(B) Copies ¹ H and ¹³ C NMR spectra	S7

(A) List of used starting materials

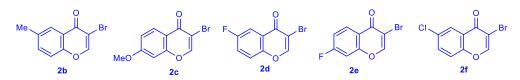


Scheme S1. List of chromone frameworks and aryl substituents.

Scope of 3-iodochromones 1:

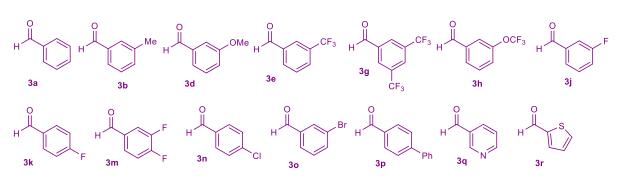


Scope of 3-bromochromones 2:

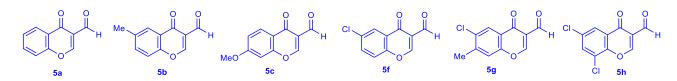


Scheme S2. List of the used 3-iodochromones 1 and 3-bromochromones 2.

Scope of aldehydes 3:

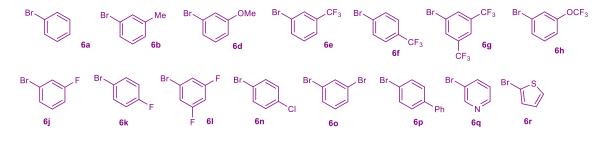


Scheme S3. List of the used aldehydes 3.

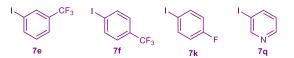


Scheme S4. List of the used 3-formylchromones 5.

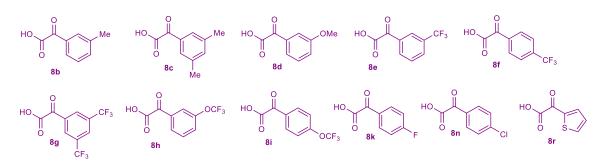




Scope of aryl iodides 7:

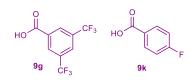


Scheme S5. List of the used aryl bromides 6 and aryl iodides 7.

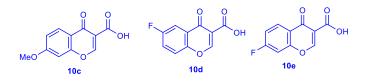


Scheme S6. List of the used α -keto acids 8.





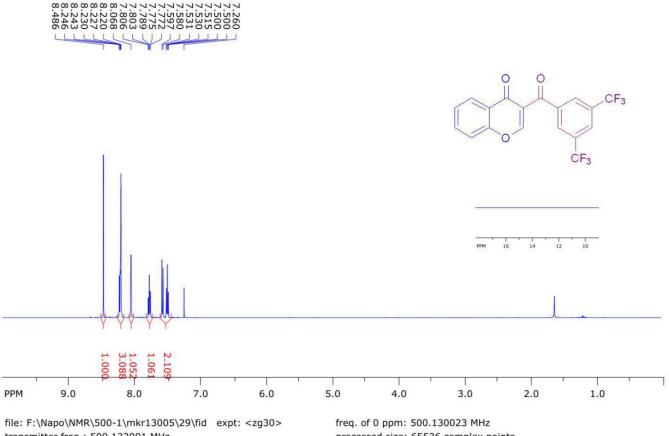
Scope of chromone-3-carboxylic acids 10:



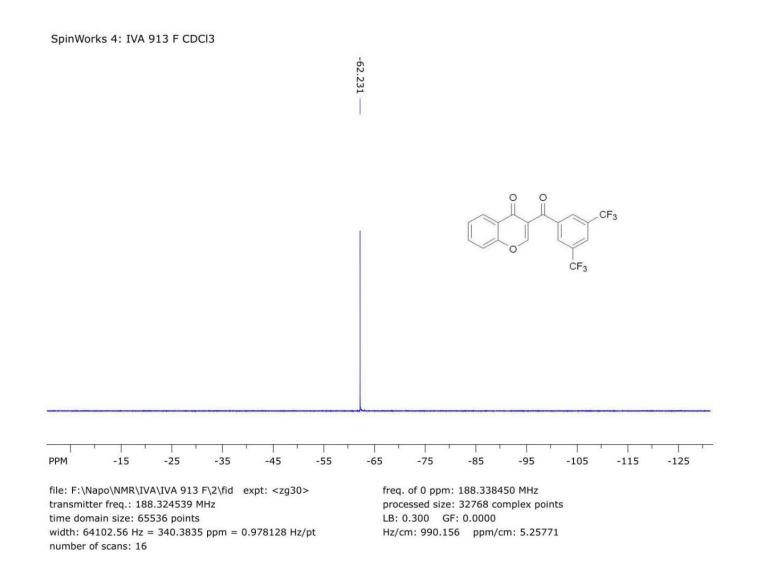
Scheme S7. List of the used reagents carboxylic acids 9 and chromone-3-carboxylic acids 10.

(B) Copies ¹H and ¹³C NMR spectra

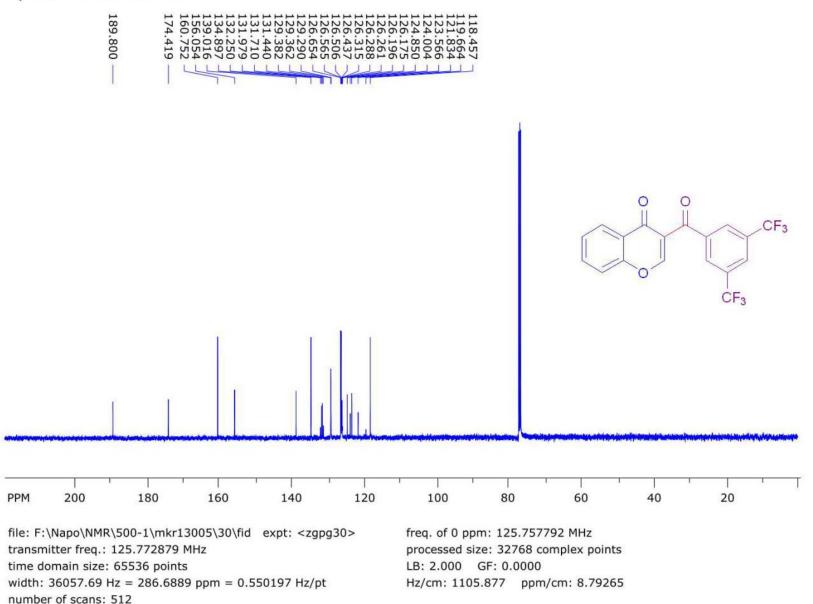
SpinWorks 4: IVA 913 1H



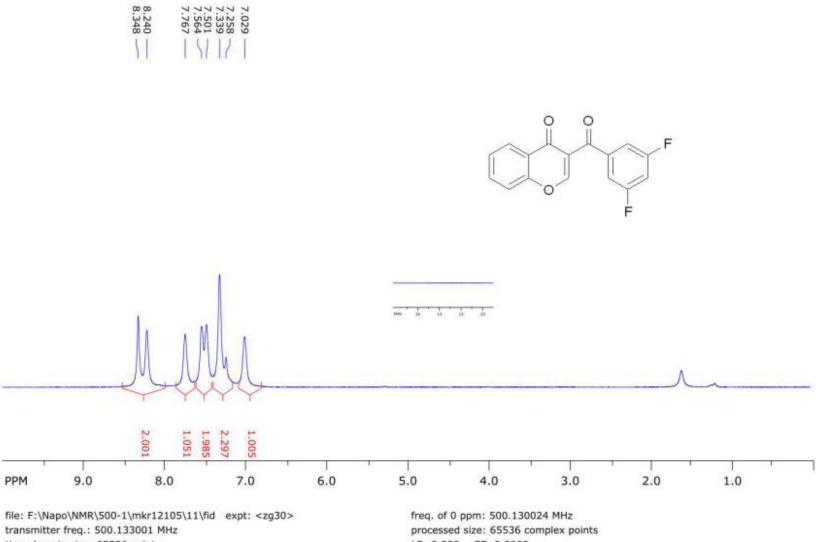
transmitter freq.: 500.133001 MHztime domain size: 65536 pointswidth: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/ptnumber of scans: 24 freq. of 0 ppm: 500.130023 MHz processed size: 65536 complex points LB: 0.300 GF: 0.0000 Hz/cm: 200.452 ppm/cm: 0.40080



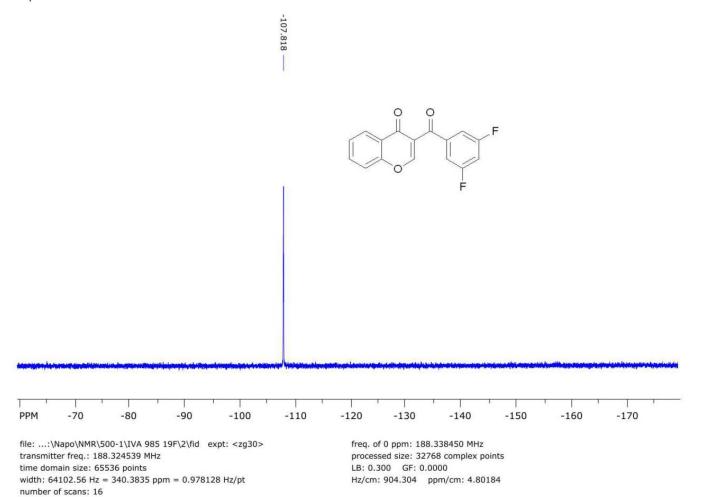
SpinWorks 4: IVA 913 13C



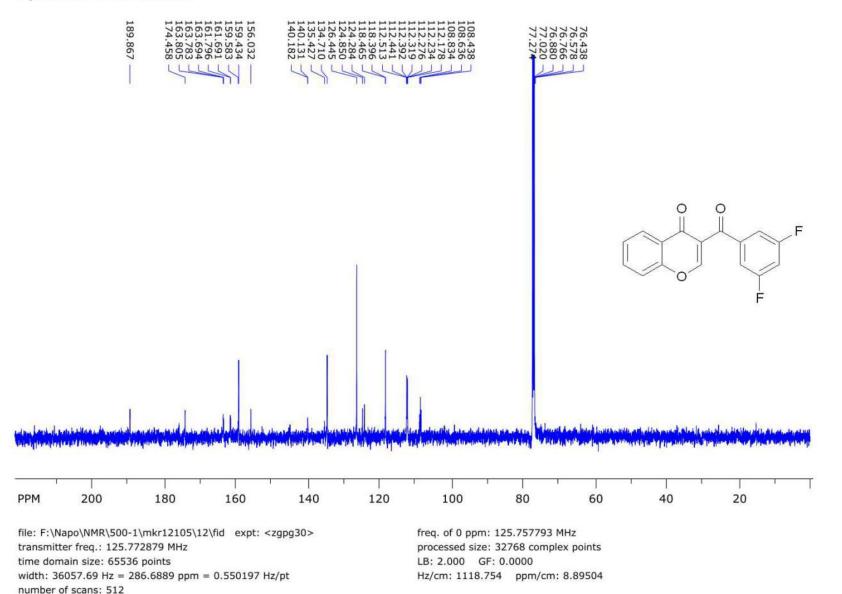
SpinWorks 4: IVA 985 1H



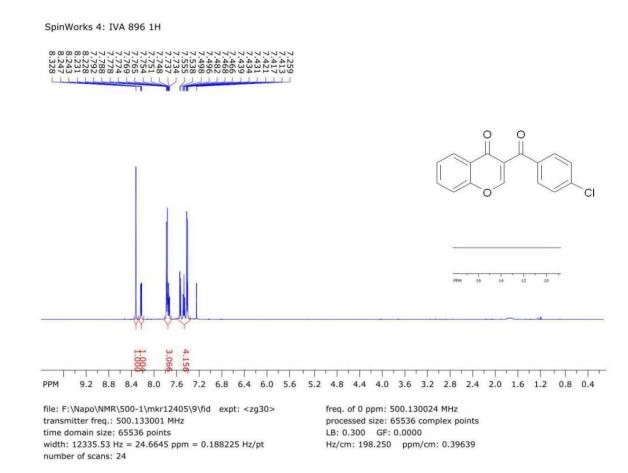
time domain size: 65536 points width: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/pt number of scans: 32 processed size: 65536 complex points LB: 0.300 GF: 0.0000 Hz/cm: 200.452 ppm/cm: 0.40080 SpinWorks 4: IVA 985 19F CDCl3

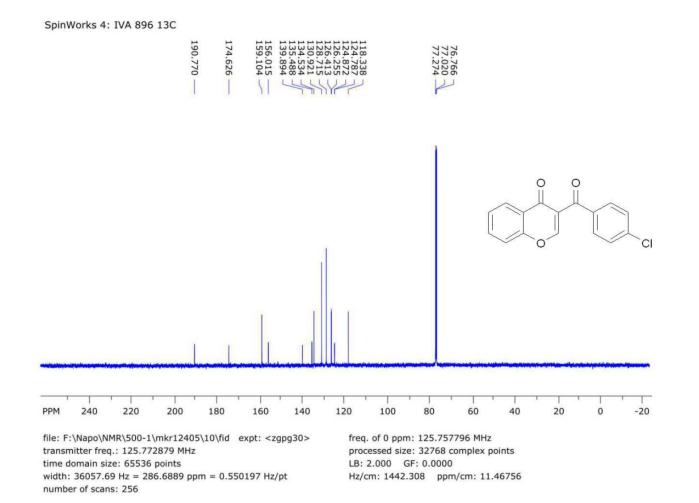


SpinWorks 4: IVA 985 13C



Compound 4an (NMR in CDCl₃)

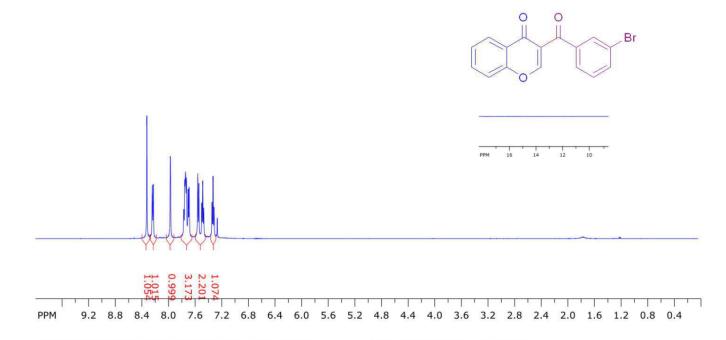




Compound 4ao (NMR in CDCl₃)

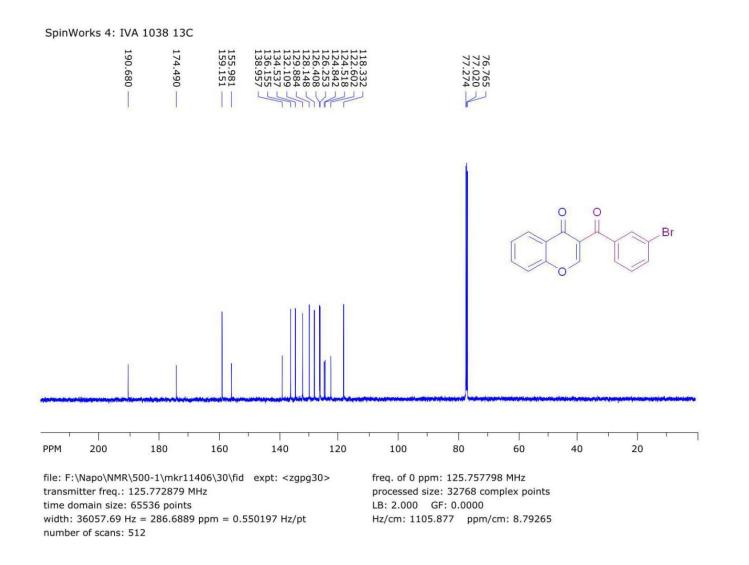
SpinWorks 4: IVA 1038 1H



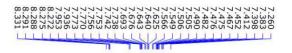


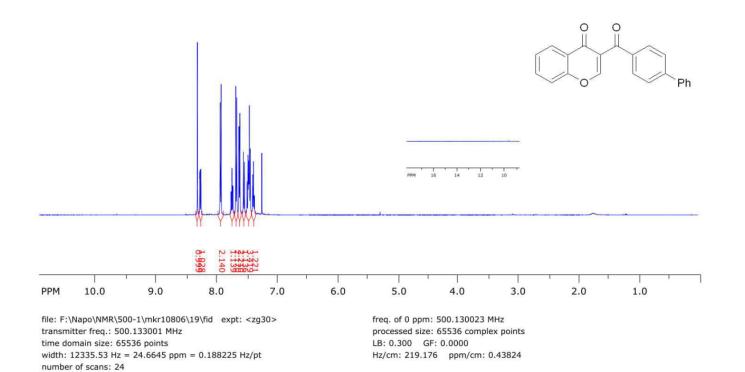
file: F:\Napo\NMR\500-1\mkr11406\29\fid expt: <zg30> transmitter freq.: 500.133001 MHz time domain size: 65536 points width: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/pt number of scans: 24

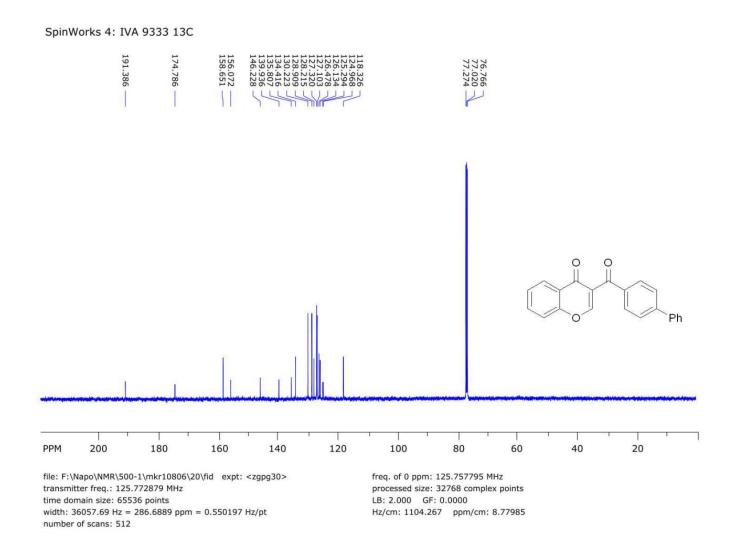
freq. of 0 ppm: 500.130023 MHz processed size: 65536 complex points LB: 0.300 GF: 0.0000 Hz/cm: 199.902 ppm/cm: 0.39970



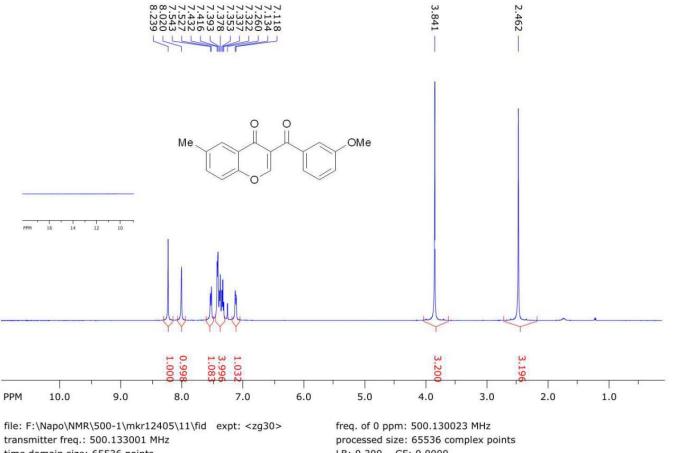
SpinWorks 4: IVA 993-3 1H





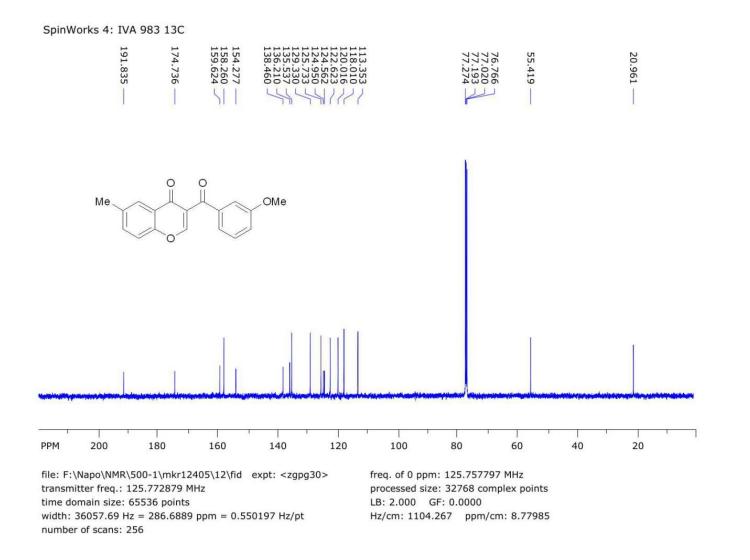


SpinWorks 4: IVA 983 1H

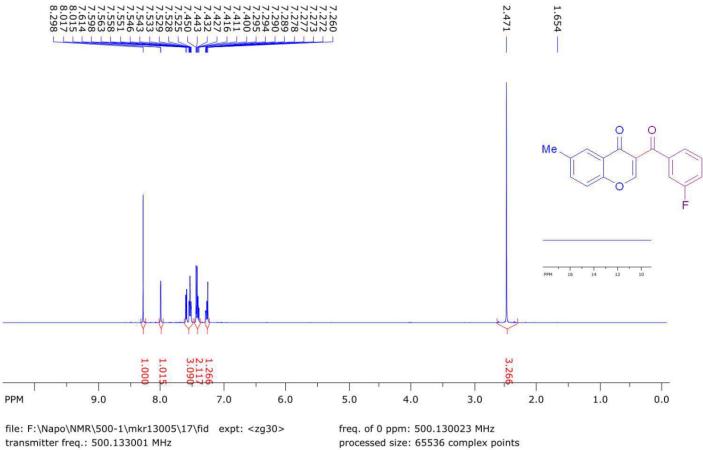


time domain size: 65536 points width: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/pt number of scans: 24

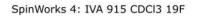
LB: 0.300 GF: 0.0000 Hz/cm: 218.074 ppm/cm: 0.43603

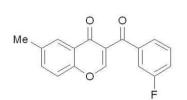


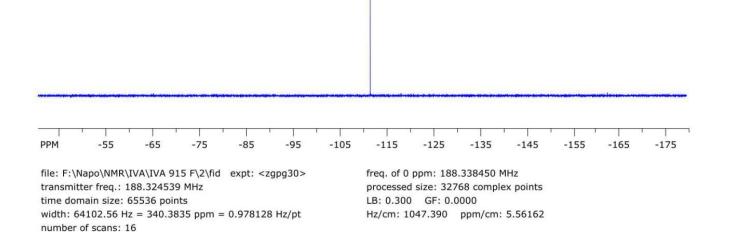
SpinWorks 4: IVA 915 1H

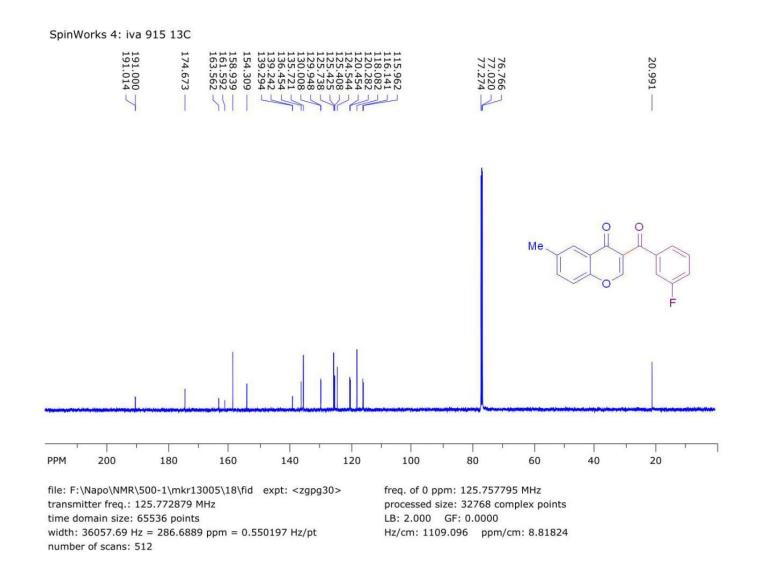


transmitter freq.: 500.133001 MHz time domain size: 65536 points width: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/pt number of scans: 24 Processed size: 65536 complex points LB: 0.300 GF: 0.0000 Hz/cm: 213.118 ppm/cm: 0.42612 -111.621

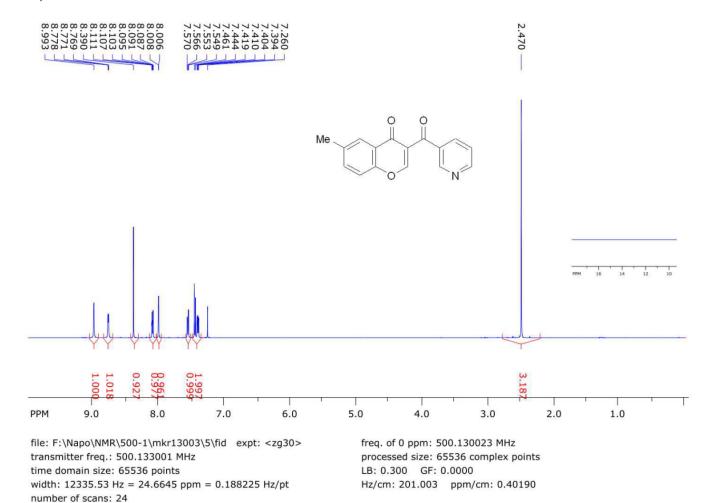


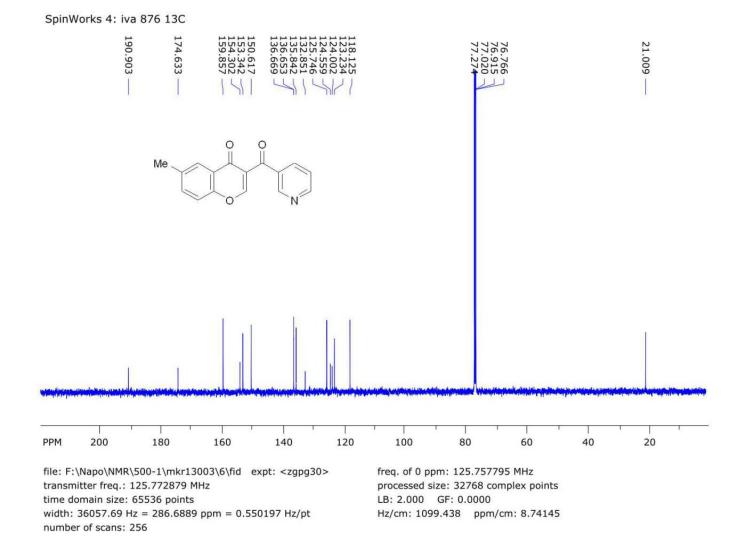






SpinWorks 4: IVA 876 1H

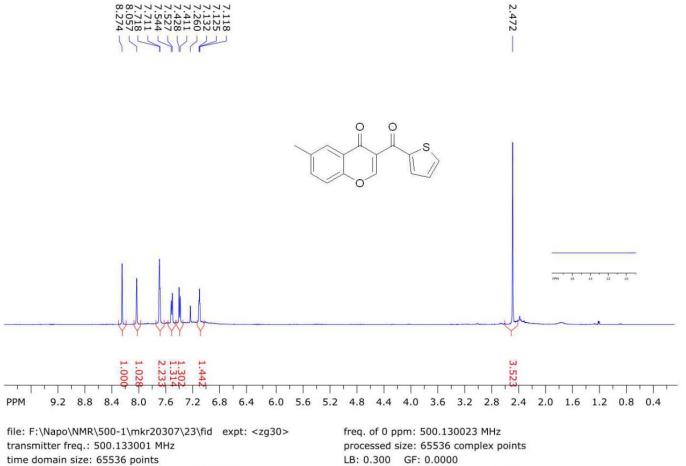




SpinWorks 4: IVA 1002 1H

width: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/pt

number of scans: 32



LB: 0.300 GF: 0.0000 Hz/cm: 199.351 ppm/cm: 0.39860

SpinWorks 4: IVA 1002 13C 174.434 182.939 154.173 158.012 135.137 135.285 135.603 136.262 143.713 118 124 125 125 128 76.766 77.020 77.274 20.973 .019 .029 .764 .198 0 0 185 175 165 155 145 135 125 115 105 85 75 55 25 15 PPM 95 65 45 35 5 file: F:\Napo\NMR\500-1\mkr20307\24\fid expt: <zgpg30> freq. of 0 ppm: 125.757797 MHz transmitter freq.: 125.772879 MHz processed size: 32768 complex points

LB: 2.000 GF: 0.0000

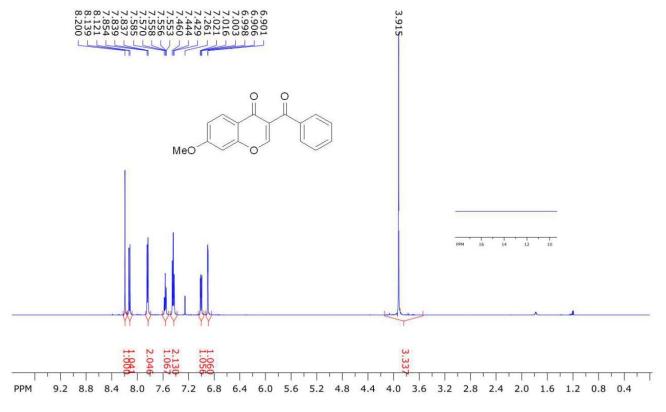
Hz/cm: 1005.851 ppm/cm: 7.99736

time domain size: 65536 points

number of scans: 264

width: 36057.69 Hz = 286.6889 ppm = 0.550197 Hz/pt

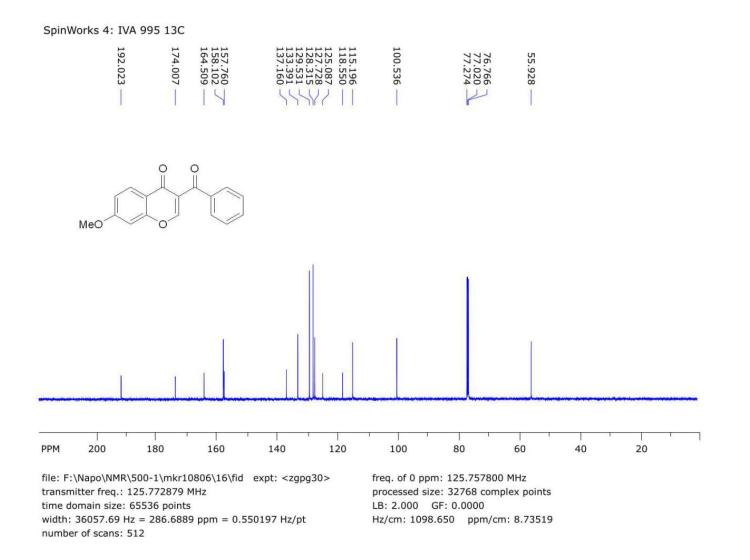
SpinWorks 4: IVA 995 1H



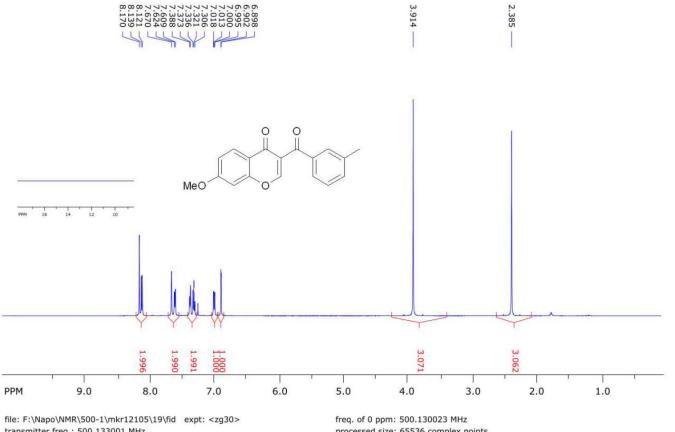
file: F:\Napo\NMR\500-1\mkr10806\15\fid expt: <zg30> transmitter freq.: 500.133001 MHz time domain size: 65536 points width: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/pt number of scans: 24

freq. of 0 ppm: 500.130023 MHz processed size: 65536 complex points LB: 0.300 GF: 0.0000 Hz/cm: 199.902 ppm/cm: 0.39970

Compound 4ca (NMR in CDCl₃)

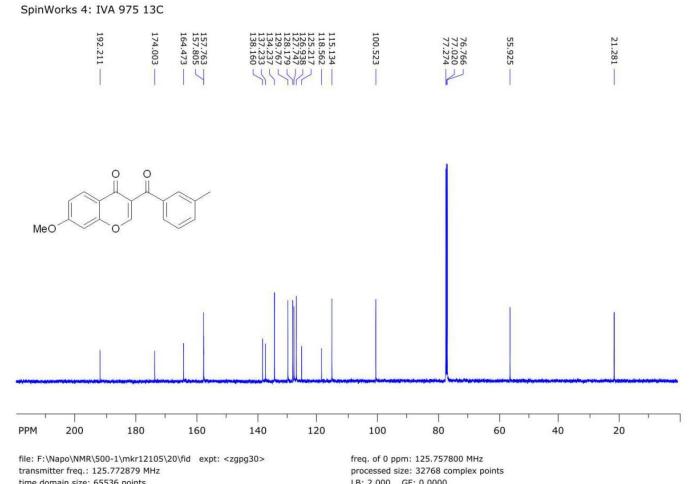


SpinWorks 4: IVA 975 1H



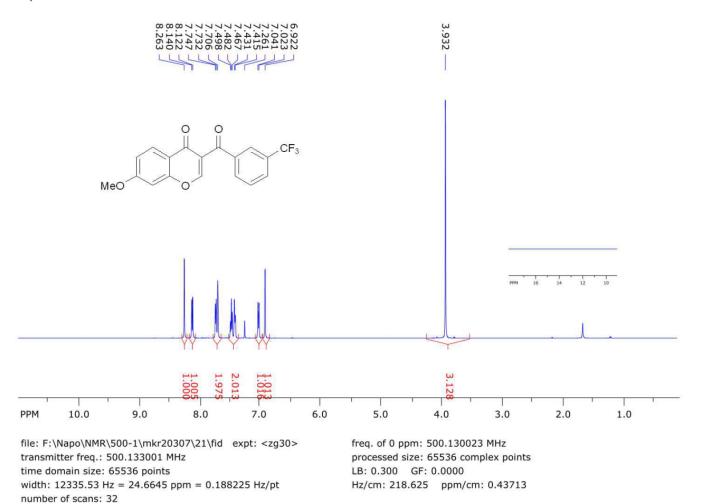
transmitter freq.: 500.133001 MHz time domain size: 65536 points width: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/pt number of scans: 32 freq. of 0 ppm: 500.130023 MHz processed size: 65536 complex points LB: 0.300 GF: 0.0000 Hz/cm: 204.858 ppm/cm: 0.40961

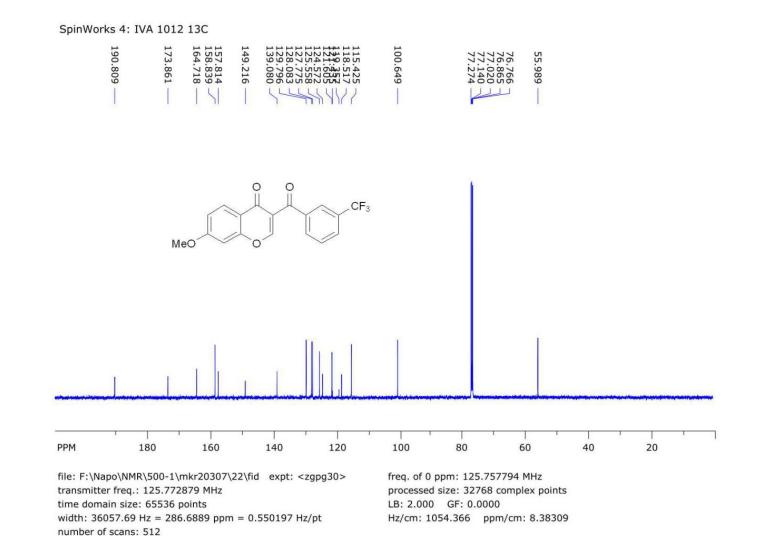
Compound 4cb (NMR in CDCl₃)



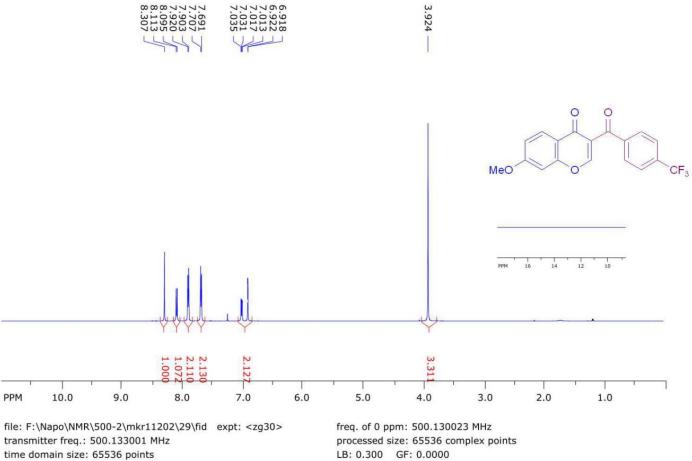
time domain size: 65536 points width: 36057.69 Hz = 286.6889 ppm = 0.550197 Hz/pt number of scans: 512

LB: 2.000 GF: 0.0000 Hz/cm: 1105.877 ppm/cm: 8.79265 SpinWorks 4: IVA 1012 1H





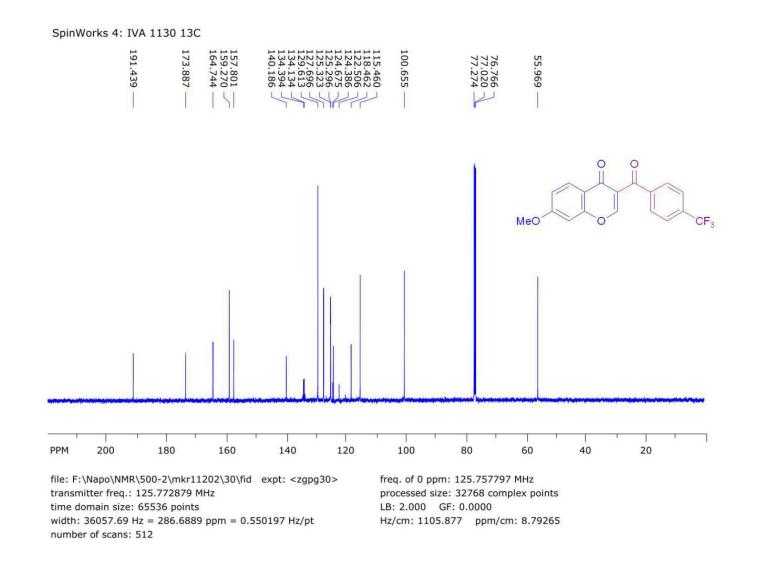
SpinWorks 4: IVA 1130 1H



width: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/pt number of scans: 24

Hz/cm: 220.277 ppm/cm: 0.44044

Compound 4cf (NMR in CDCl₃)

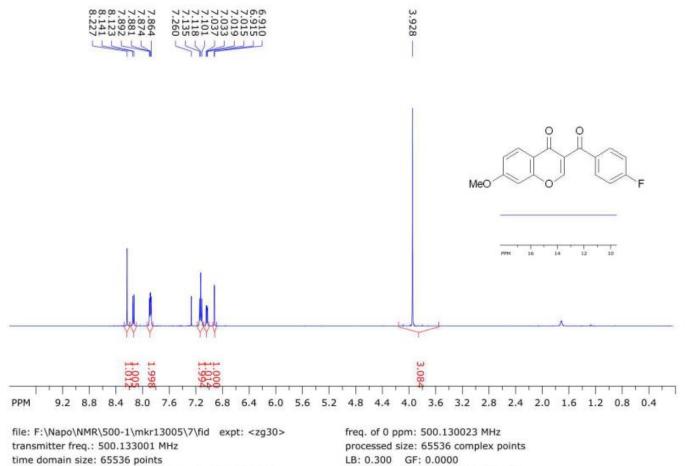


Compound 4ck (NMR in CDCl₃)

SpinWorks 4: IVA 907 1H

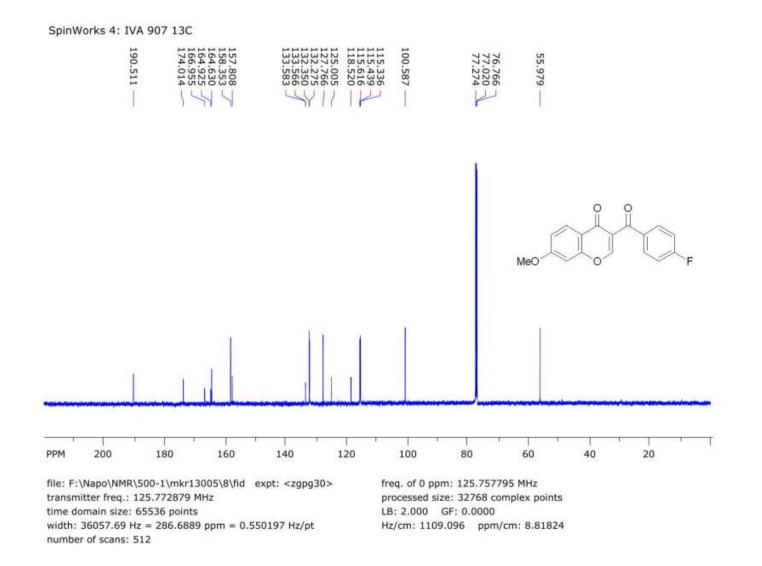
width: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/pt

number of scans: 24



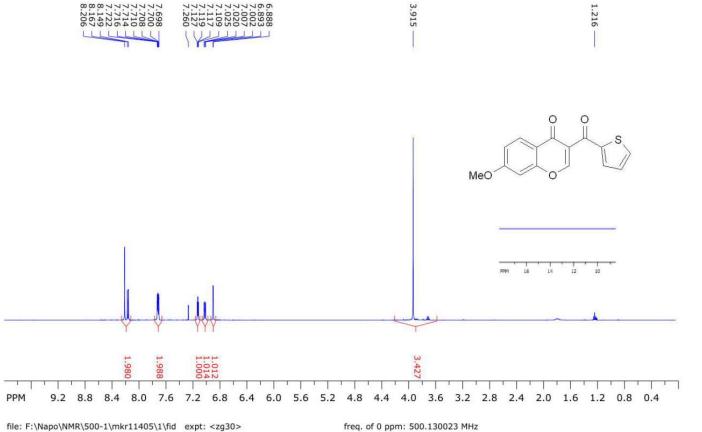
Hz/cm: 199.902 ppm/cm: 0.39970

Compound 4ck (NMR in CDCl₃)



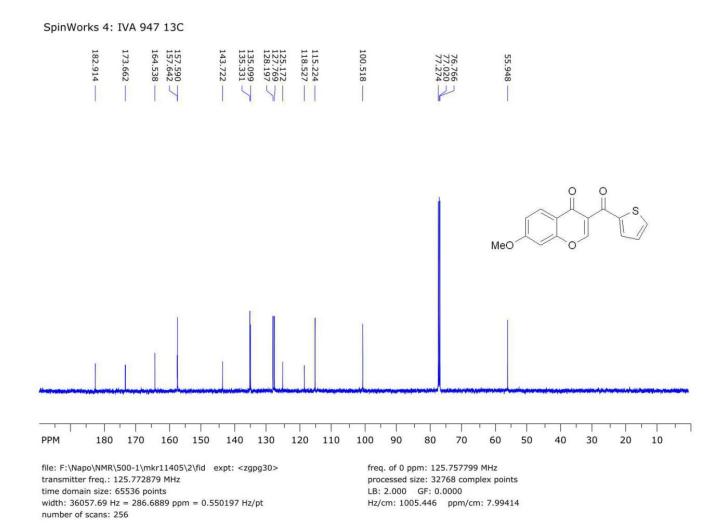
Compound 4cr (NMR in CDCl₃)

SpinWorks 4: IVA 947 1H



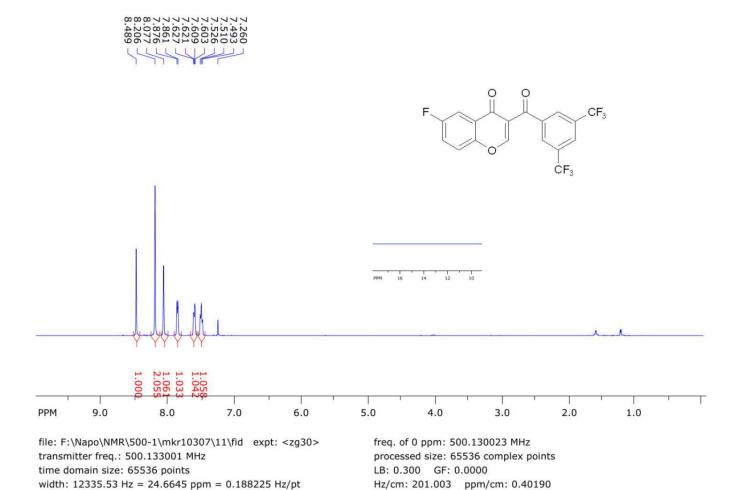
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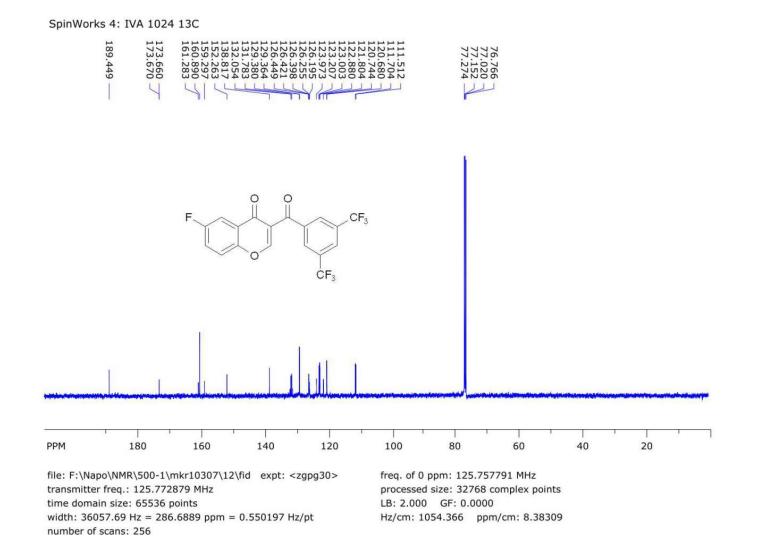
Compound 4cr (NMR in CDCl₃)



SpinWorks 4: IVA 1024 1H

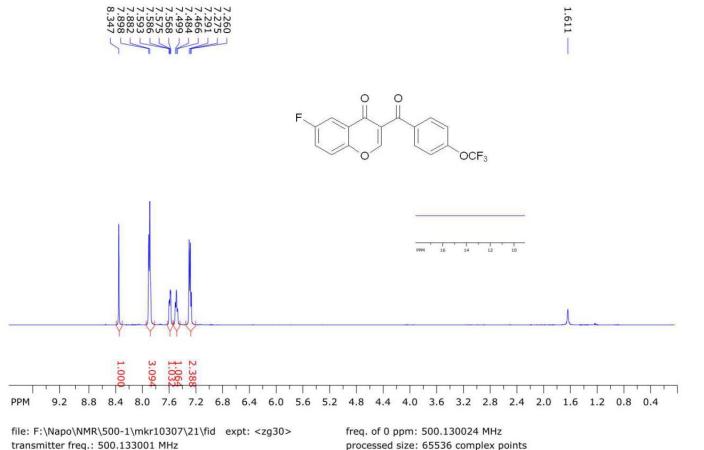
number of scans: 32





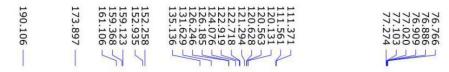
Compound 4di (NMR in CDCl₃)

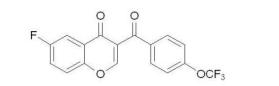
SpinWorks 4: IVA 1024 1H

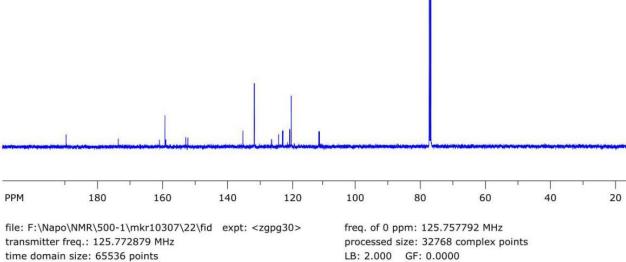


transmitter freq.: 500.133001 MHz time domain size: 65536 points width: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/pt number of scans: 32 rreq. of 0 ppm: 500.130024 MHz processed size: 65536 complex points LB: 0.300 GF: 0.0000 Hz/cm: 199.902 ppm/cm: 0.39970

SpinWorks 4: IVA 1026 13C



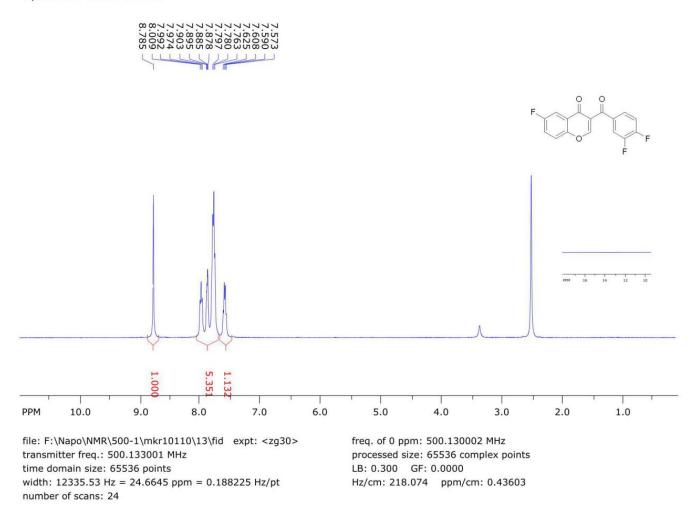


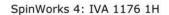


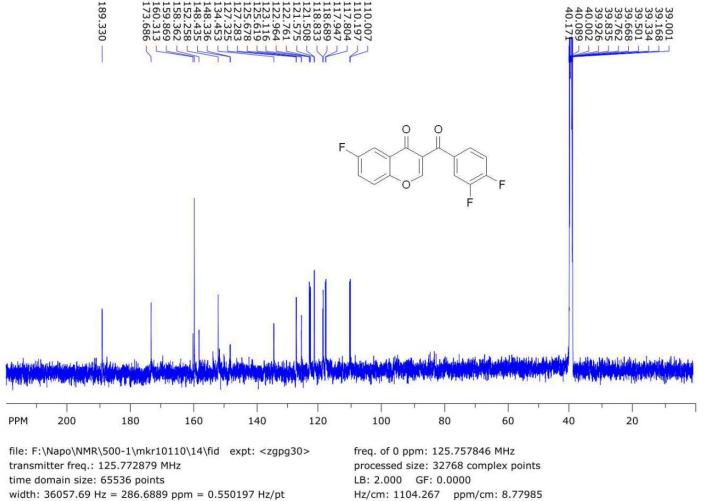
width: 36057.69 Hz = 286.6889 ppm = 0.550197 Hz/pt number of scans: 256

Hz/cm: 1055.975 ppm/cm: 8.39589

SpinWorks 4: IVA 1176 1H



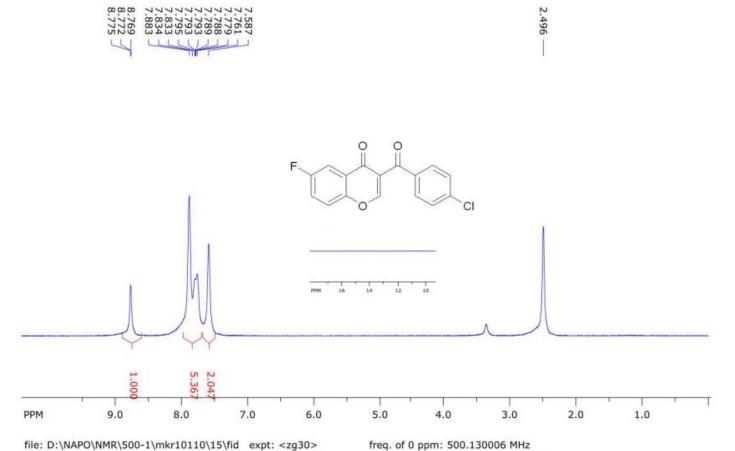




number of scans: 512

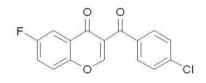
Hz/cm: 1104.267 ppm/cm: 8.77985

SpinWorks 4: IVA 1031 1H



transmitter freq.: 500.133001 MHz time domain size: 65536 points width: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/pt number of scans: 24 freq. of 0 ppm: 500.130006 MHz processed size: 65536 complex points LB: 0.300 GF: 0.0000 Hz/cm: 209.049 ppm/cm: 0.41799 SpinWorks 4: IVA 1031 F DMSO

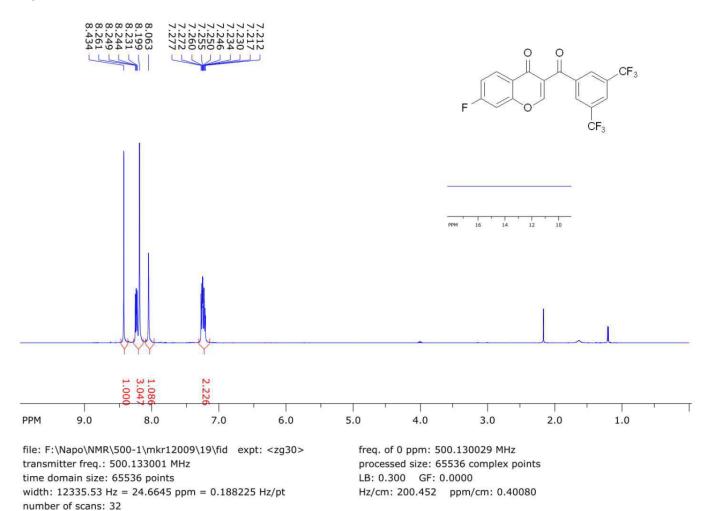
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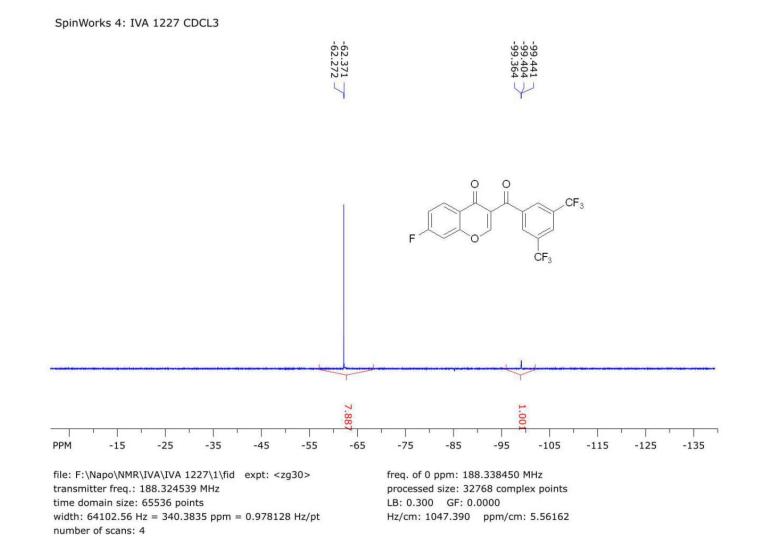


white the second of the second of the second of the second s

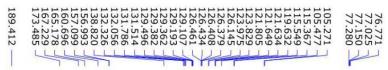
1	1	1	1				1	1	1	1 1	
PPM	-75	-85	-95	-105	-115	-125	-135	-145	-155	-165	-175

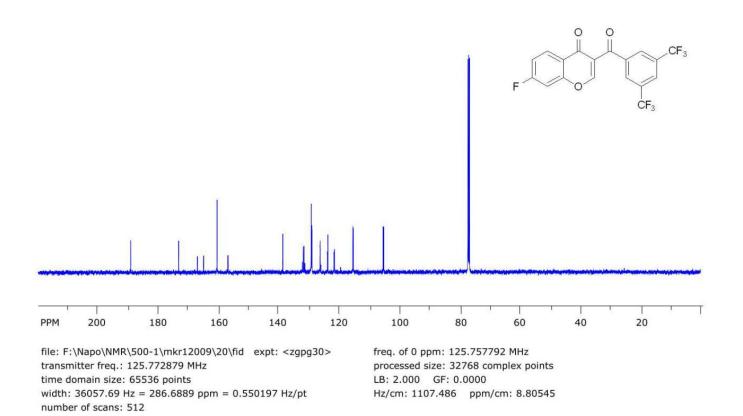
file: F:\Napo\NMR\IVA\IVA 1031 F\1\fid expt: <zg30> transmitter freq.: 188.324539 MHz time domain size: 65536 points width: 64102.56 Hz = 340.3835 ppm = 0.978128 Hz/pt number of scans: 16 freq. of 0 ppm: 188.338450 MHz processed size: 32768 complex points LB: 0.300 GF: 0.0000 Hz/cm: 904.304 ppm/cm: 4.80184 SpinWorks 4: IVA 1227 1H





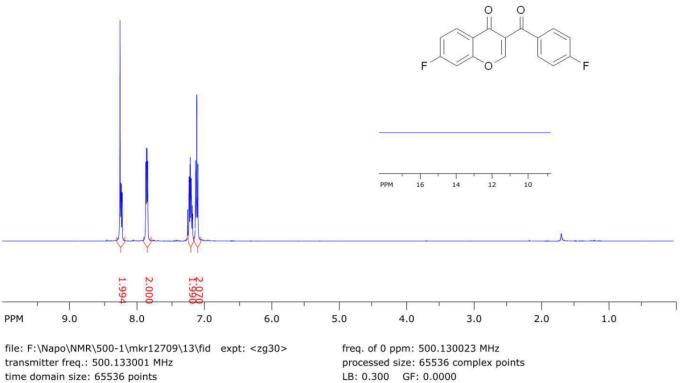
SpinWorks 4: IVA 1227 13C





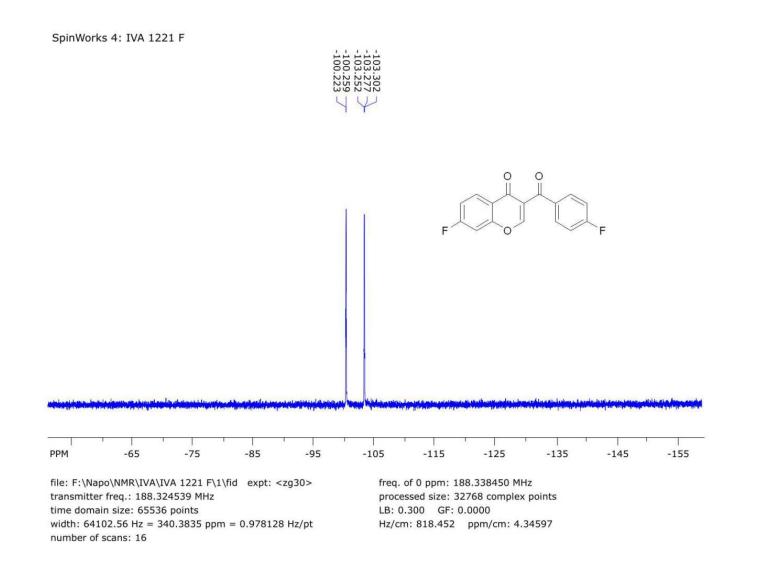
SpinWorks 4: IVA 1221 1H



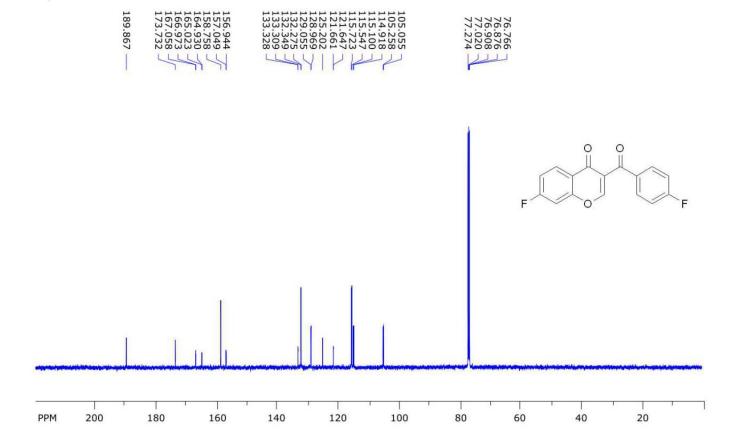


Hz/cm: 200.452 ppm/cm: 0.40080

width: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/pt number of scans: 32

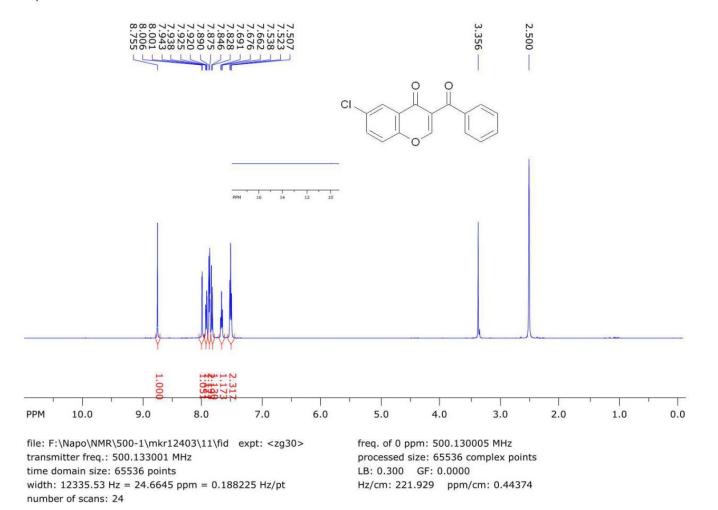


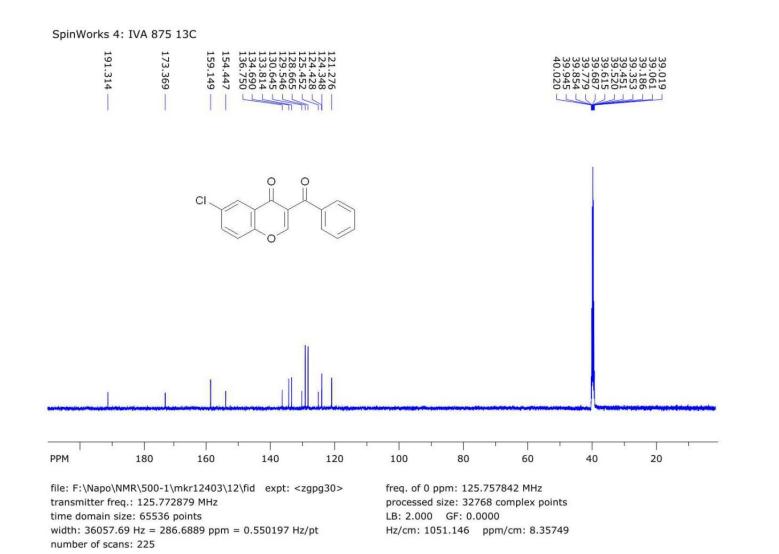
SpinWorks 4: IVA 1221 13C



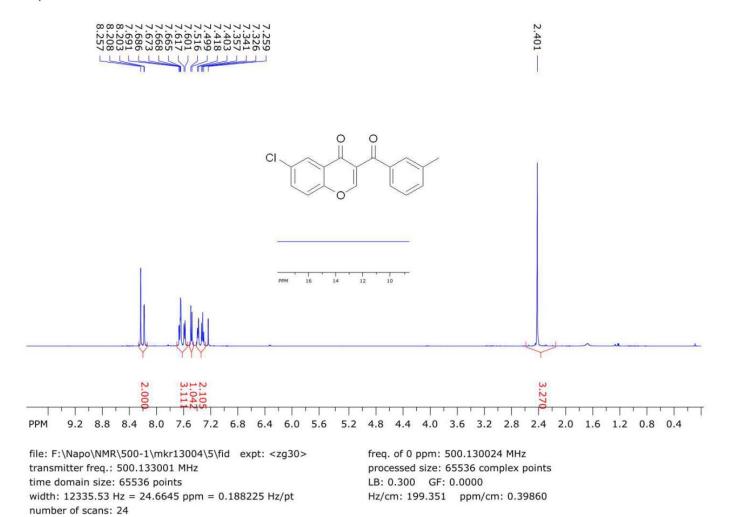
file: F:\Napo\NMR\500-1\mkr12709\14\fid expt: <zgpg30> transmitter freq.: 125.772879 MHz time domain size: 65536 points width: 36057.69 Hz = 286.6889 ppm = 0.550197 Hz/pt number of scans: 332

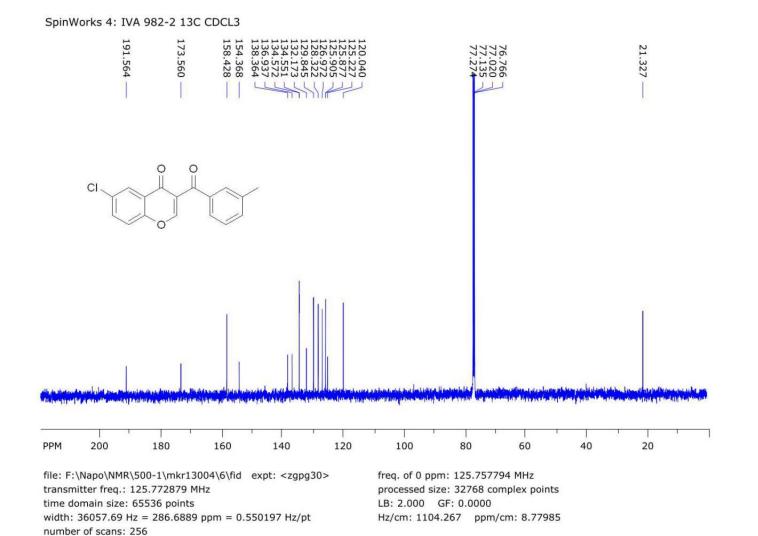
freq. of 0 ppm: 125.757796 MHz processed size: 32768 complex points LB: 2.000 GF: 0.0000 Hz/cm: 1104.267 ppm/cm: 8.77985 SpinWorks 4: IVA 875 1H





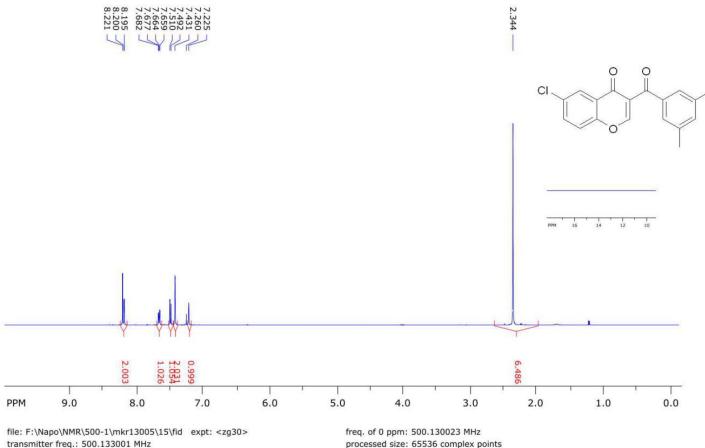
SpinWorks 4: IVA 982-2 CDCl3





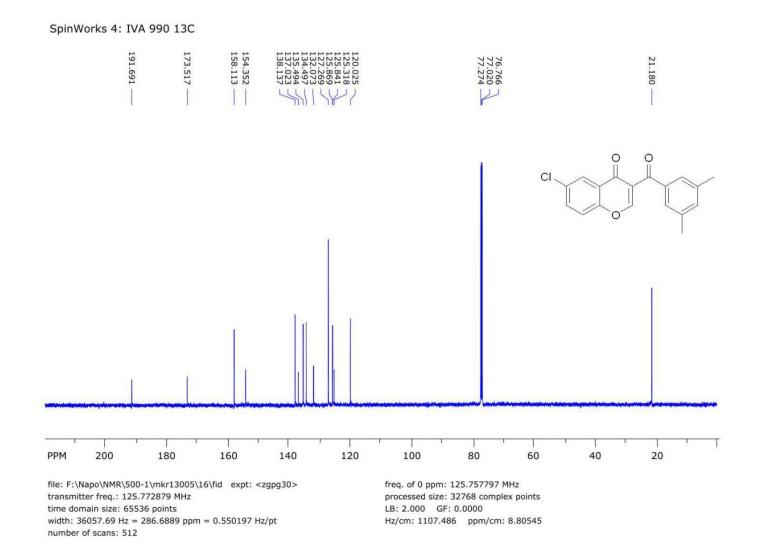
Compound 4fc (NMR in CDCl₃)

SpinWorks 4: IVA 990 1H

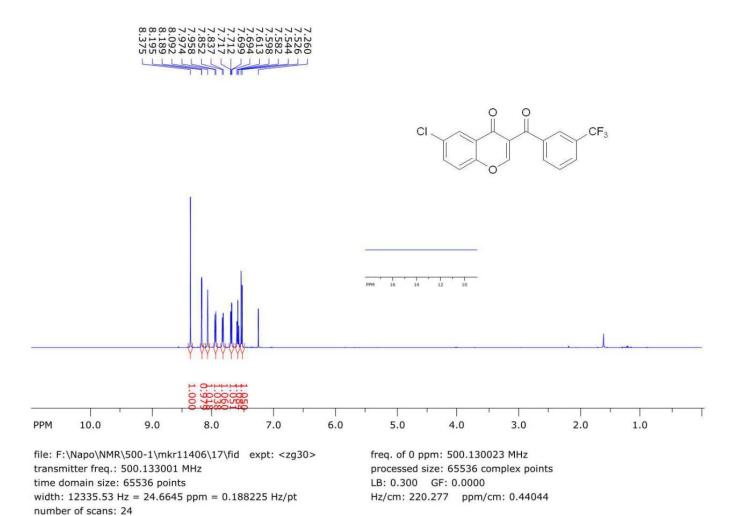


transmitter freq.: 500.133001 MHz time domain size: 65536 points width: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/pt number of scans: 24

freq. of 0 ppm: 500.130023 MHz processed size: 65536 complex points LB: 0.300 GF: 0.0000 Hz/cm: 203.206 ppm/cm: 0.40630

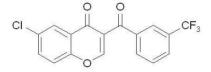


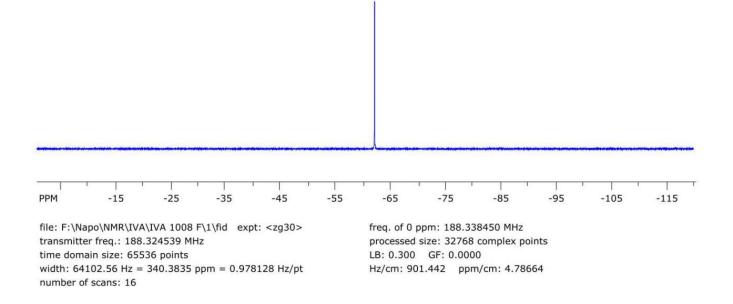
iva 1008



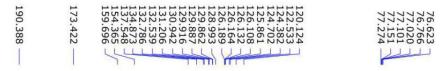
-62.101 -

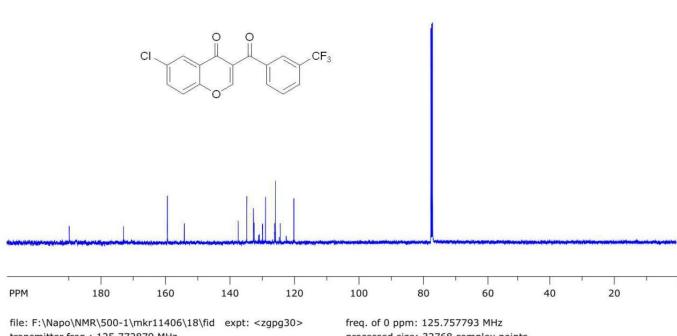






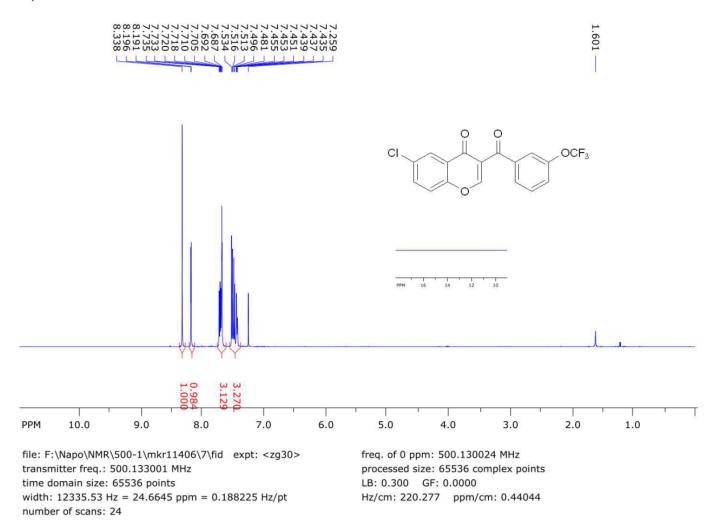
SpinWorks 4: IVA 1008 13C





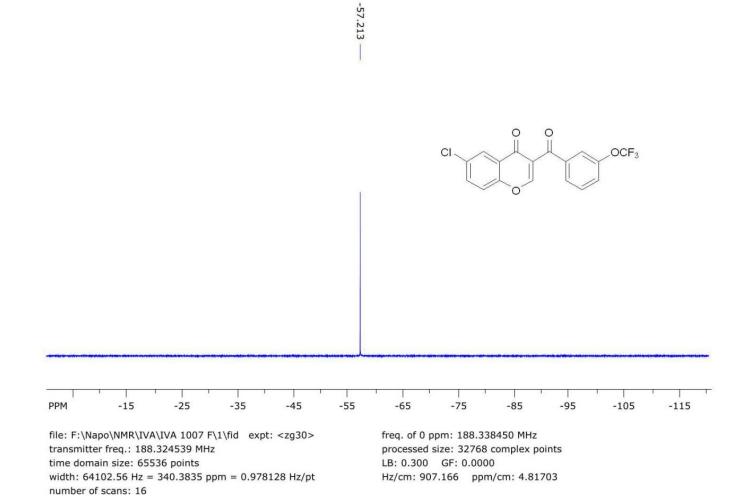
transmitter freq.: 125.772879 MHz time domain size: 65536 points width: 36057.69 Hz = 286.6889 ppm = 0.550197 Hz/pt number of scans: 512

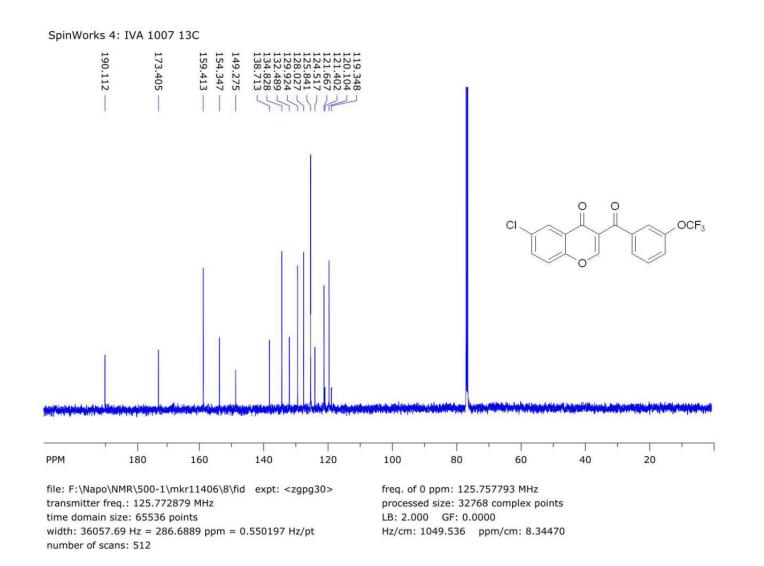
freq. of 0 ppm: 125.757793 MHz processed size: 32768 complex points LB: 2.000 GF: 0.0000 Hz/cm: 1052.756 ppm/cm: 8.37029 SpinWorks 4: IVA 1007 1H



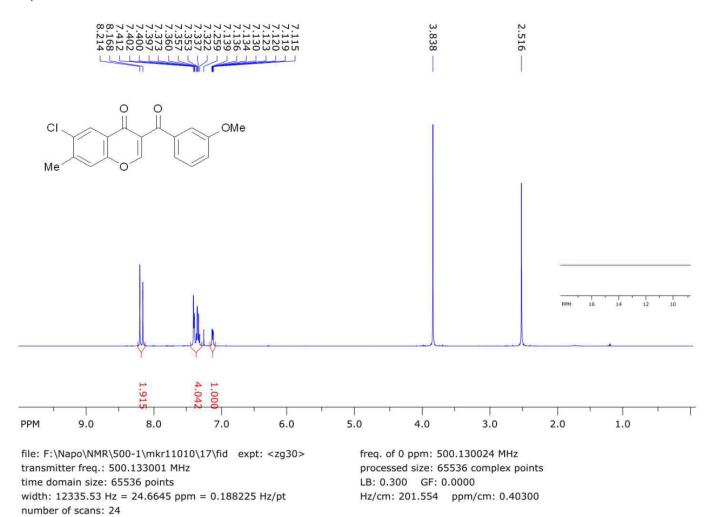
Compound 4fh (NMR in CDCl₃)

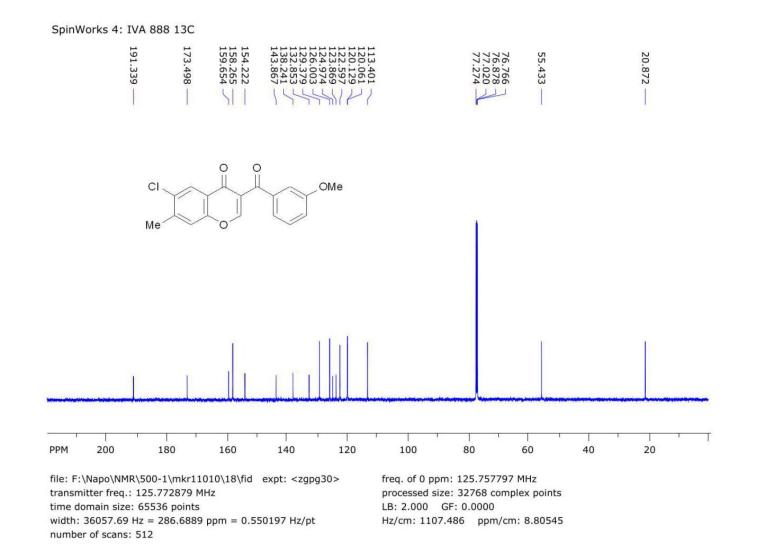
SpinWorks 4: IVA 1007 F CDCl3



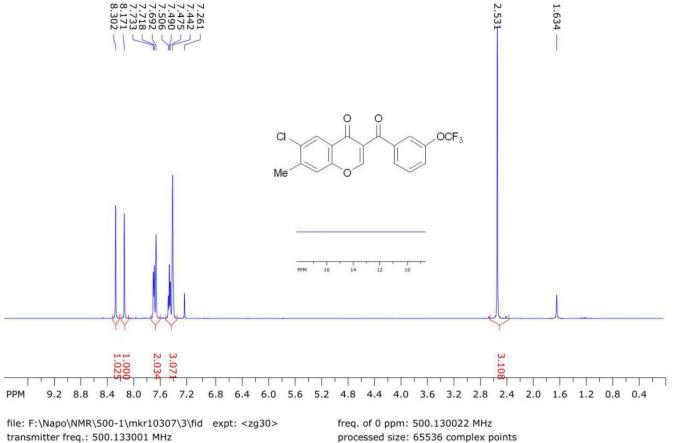


SpinWorks 4: IVA 888 1H

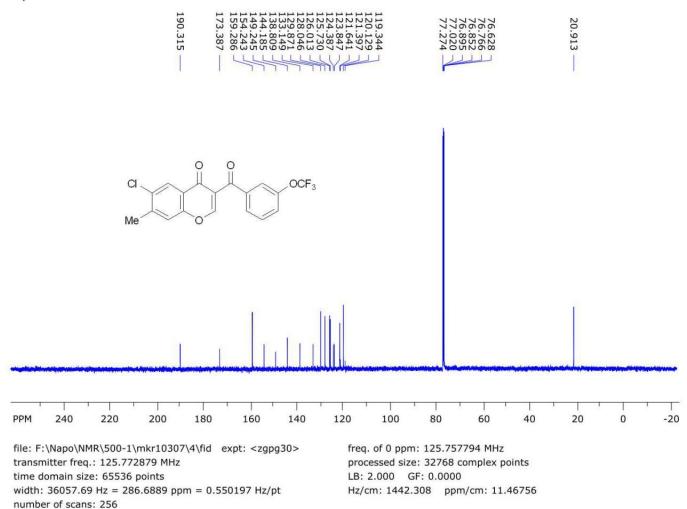




SpinWorks 4: IVA 1063 1H

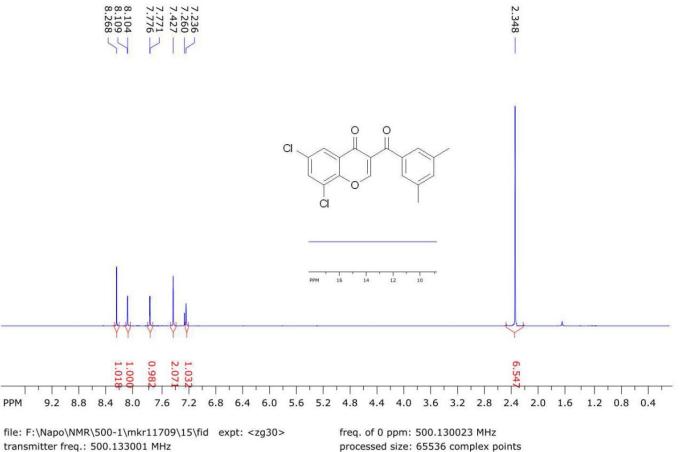


transmitter freq.: 500.133001 MHz time domain size: 65536 points width: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/pt number of scans: 32 freq. of 0 ppm: 500.130022 MHz processed size: 65536 complex points LB: 0.300 GF: 0.0000 Hz/cm: 199.315 ppm/cm: 0.39852

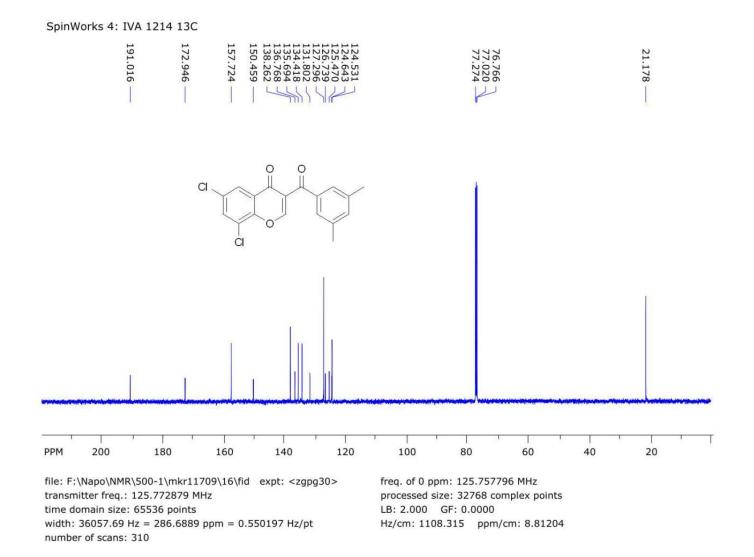


SpinWorks 4: IVA 1063 1H

SpinWorks 4: IVA 1214 1H



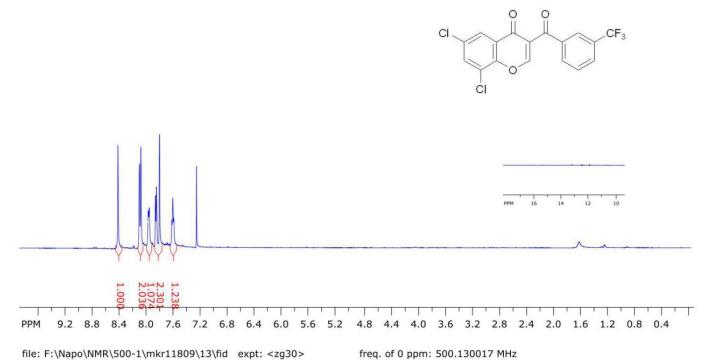
transmitter freq.: 500.133001 MHz time domain size: 65536 points width: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/pt number of scans: 32 freq. of 0 ppm: 500.130023 MHz processed size: 65536 complex points LB: 0.300 GF: 0.0000 Hz/cm: 198.803 ppm/cm: 0.39750



Compound 4he (NMR in CDCl₃)

SpinWorks 4: IVA 1052 1H





transmitter freq.: 500.133001 MHztime domain size: 65536 pointswidth: 12335.53 Hz = 24.6645 ppm = 0.188225 Hz/ptnumber of scans: 32 freq. of 0 ppm: 500.130017 MHz processed size: 65536 complex points LB: 0.300 GF: 0.0000 Hz/cm: 199.351 ppm/cm: 0.39860

