

Supplementary Material

Study of reactions of pentafluorophenylhydrazine with activated enol ethers. Synthesis of *N*-pentafluorophenylpyrazoles

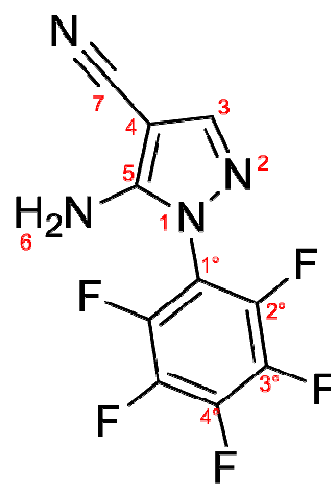
Dušan Bortňák,^a Michal Šoral,^b Martin Breza,^c Silvia Vlčková,^d Daniel Végh,^a
and Viktor Milata*^a

^a *Department of Organic Chemistry, ^b Central Laboratories, and ^c Department of Physical Chemistry, Faculty of Chemical and Food Technology, Slovak University of Technology, Radlinského street 9, SK-812 37 Bratislava, Slovakia*

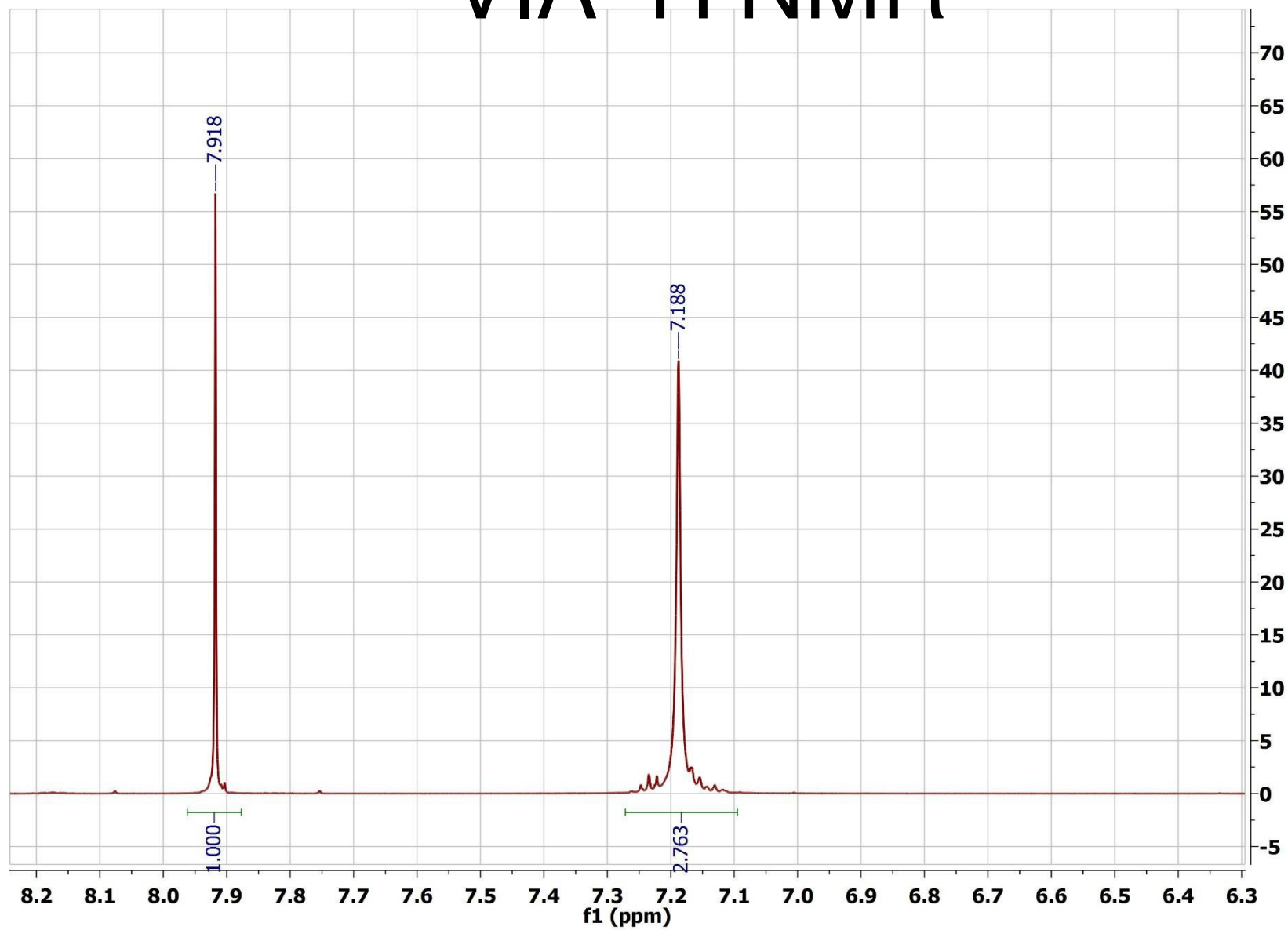
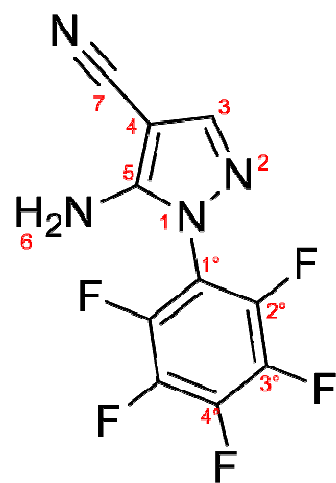
^d *Chemical Institute, Slovak Academy of Sciences, Dúbravská road 9, SK-845 38 Bratislava, Slovakia*

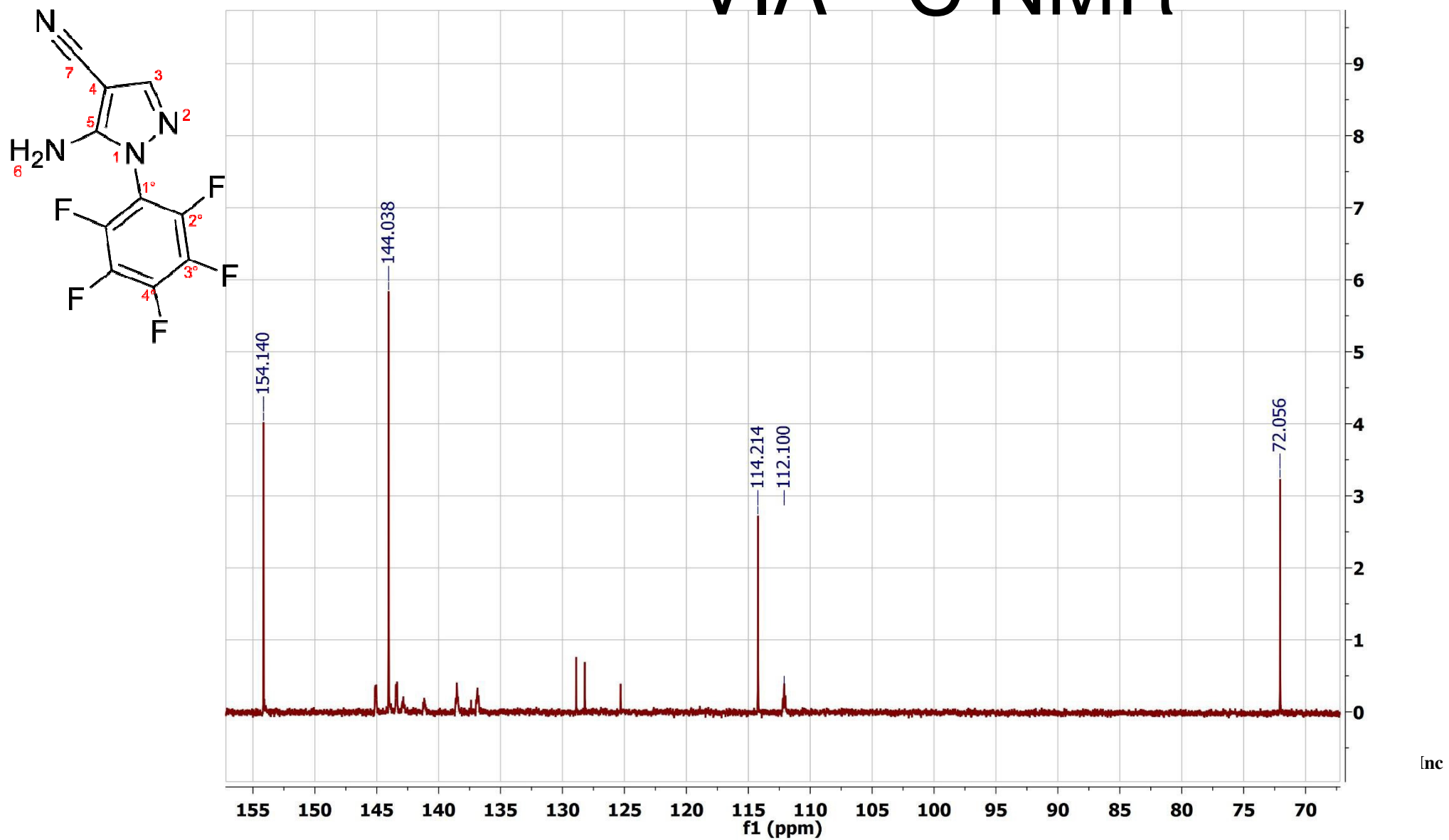
E-mail: viktor.milata@stuba.sk

VIA

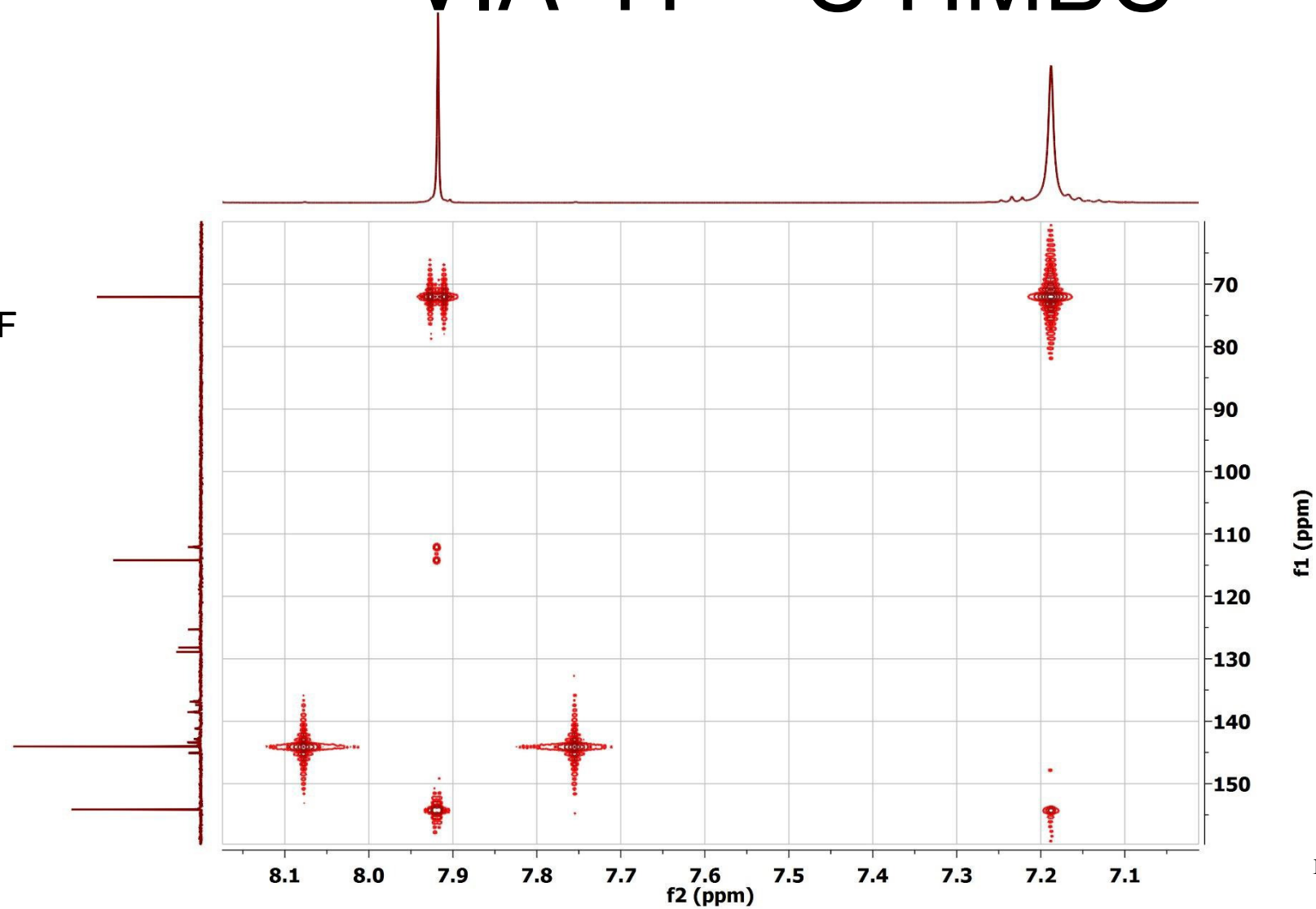
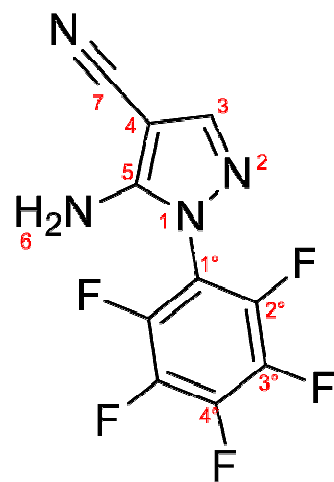


VIA ^1H NMR

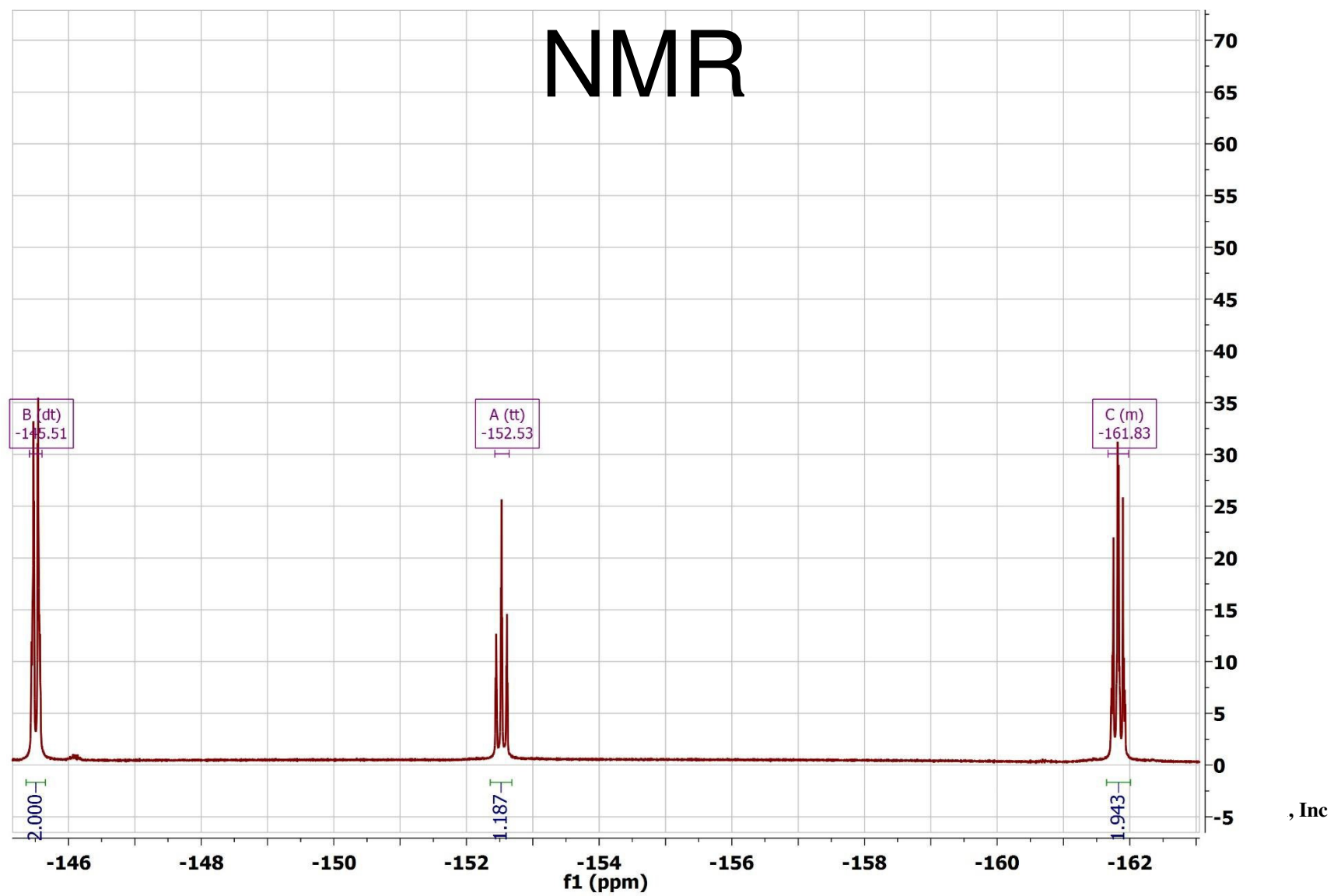
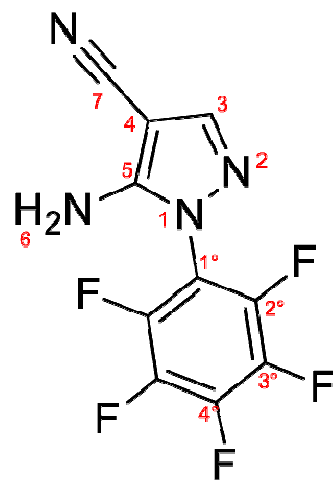


VIA ^{13}C NMR

VIA ^1H - ^{13}C HMBC

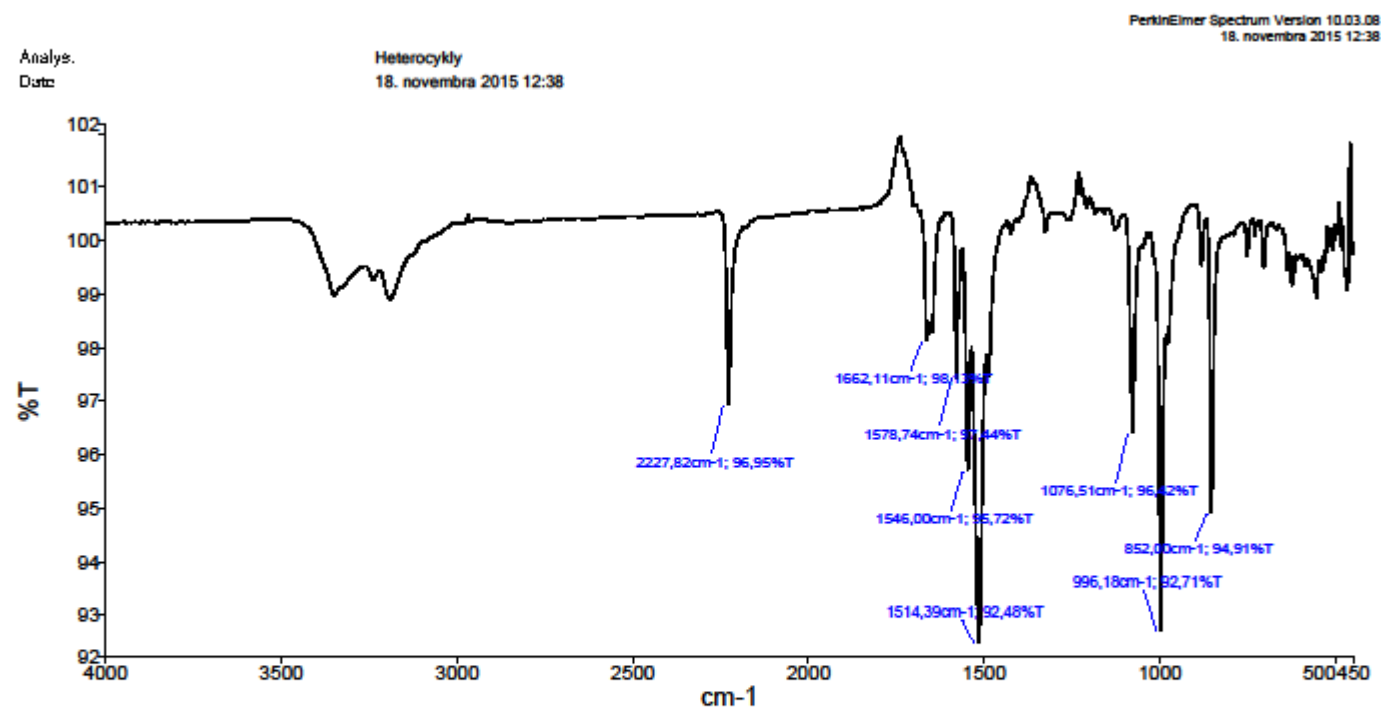
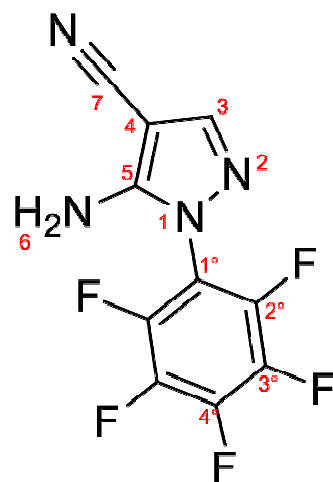


VIA ^{19}F NMR



, Inc

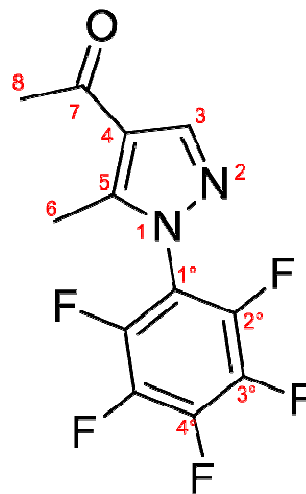
VIA IR



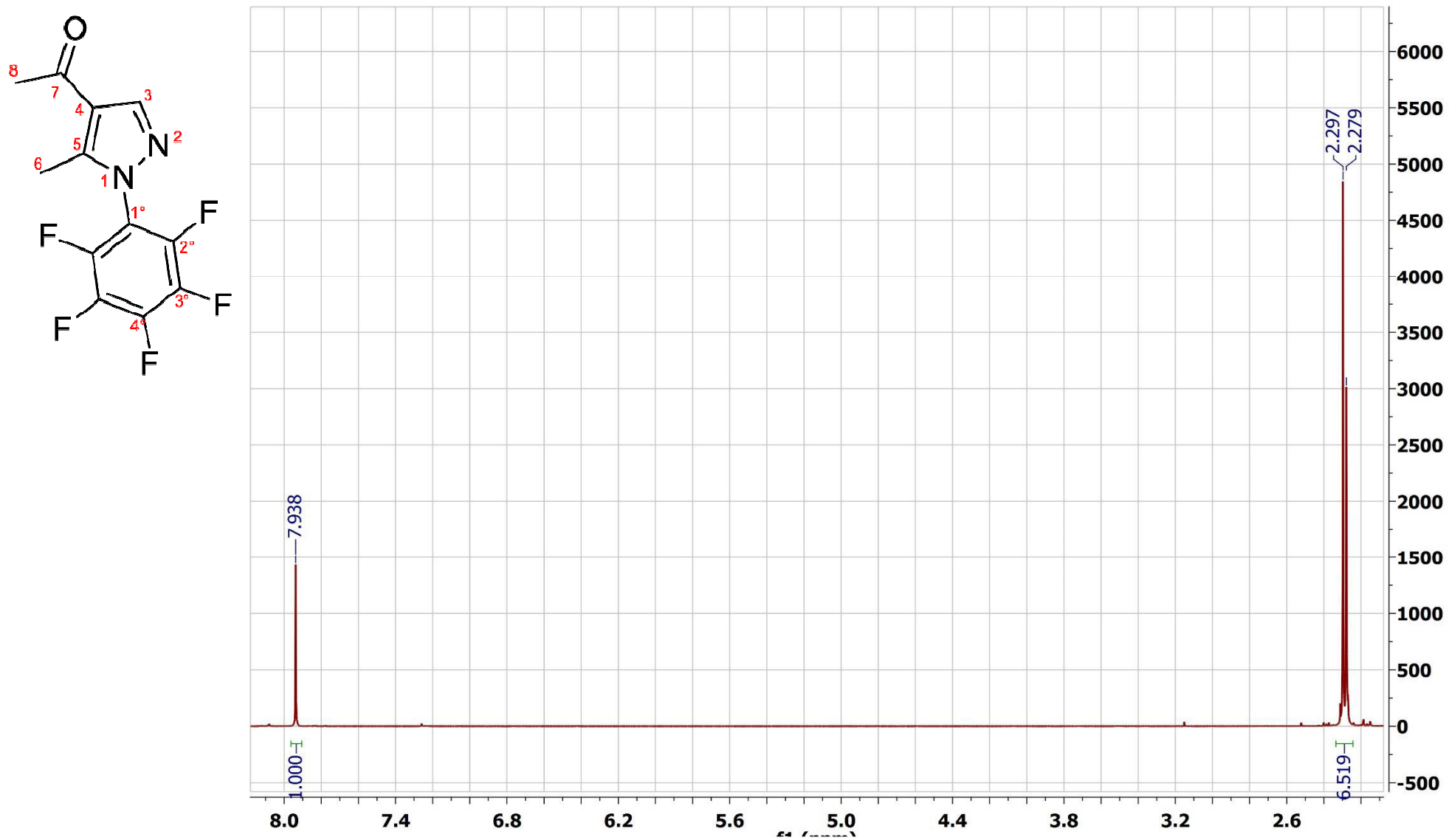
Heter 68 Sample 068 By Heter Date streda, novembra 18 2015

Source: Source Results	
Spectrum Name	Heter 68

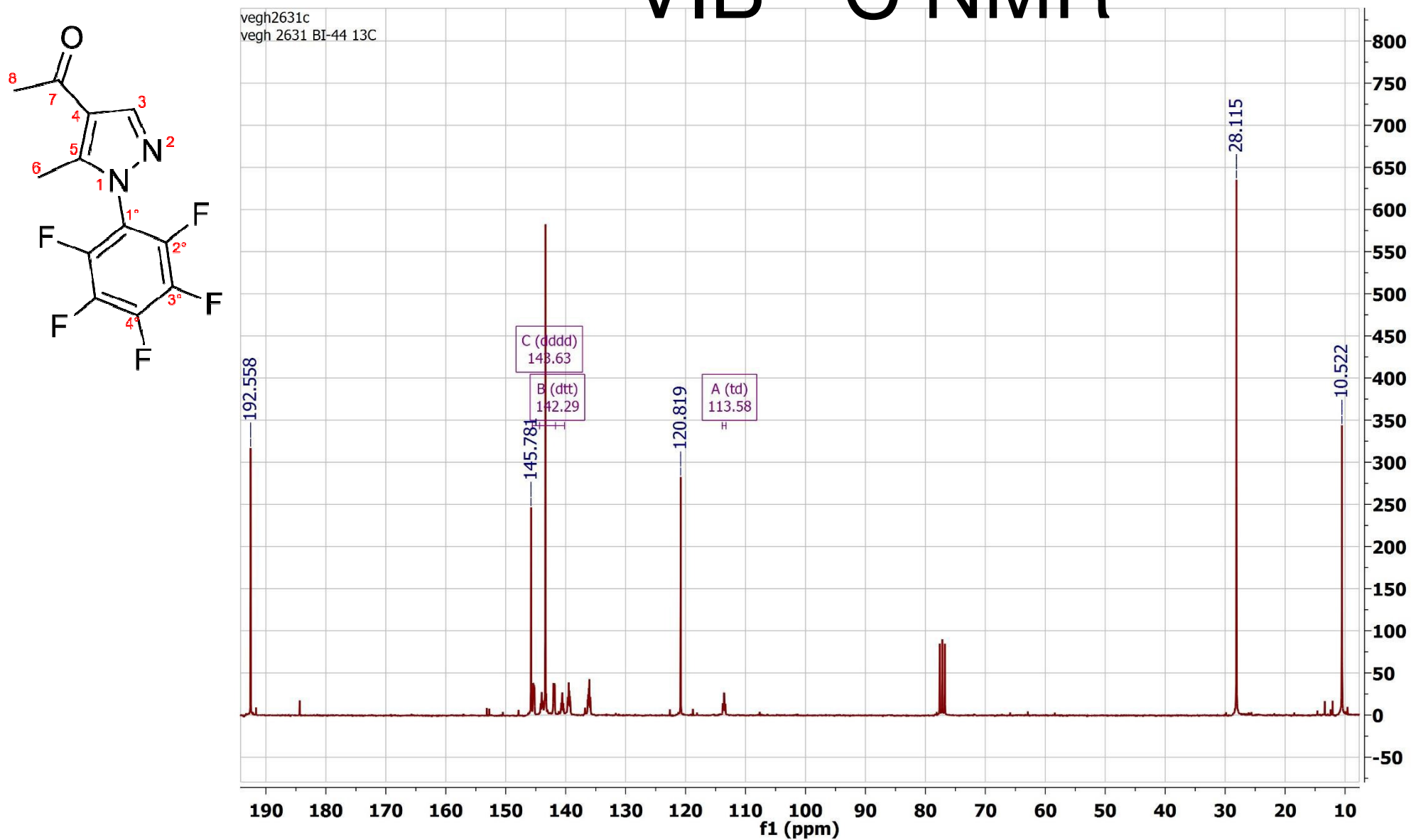
VIB

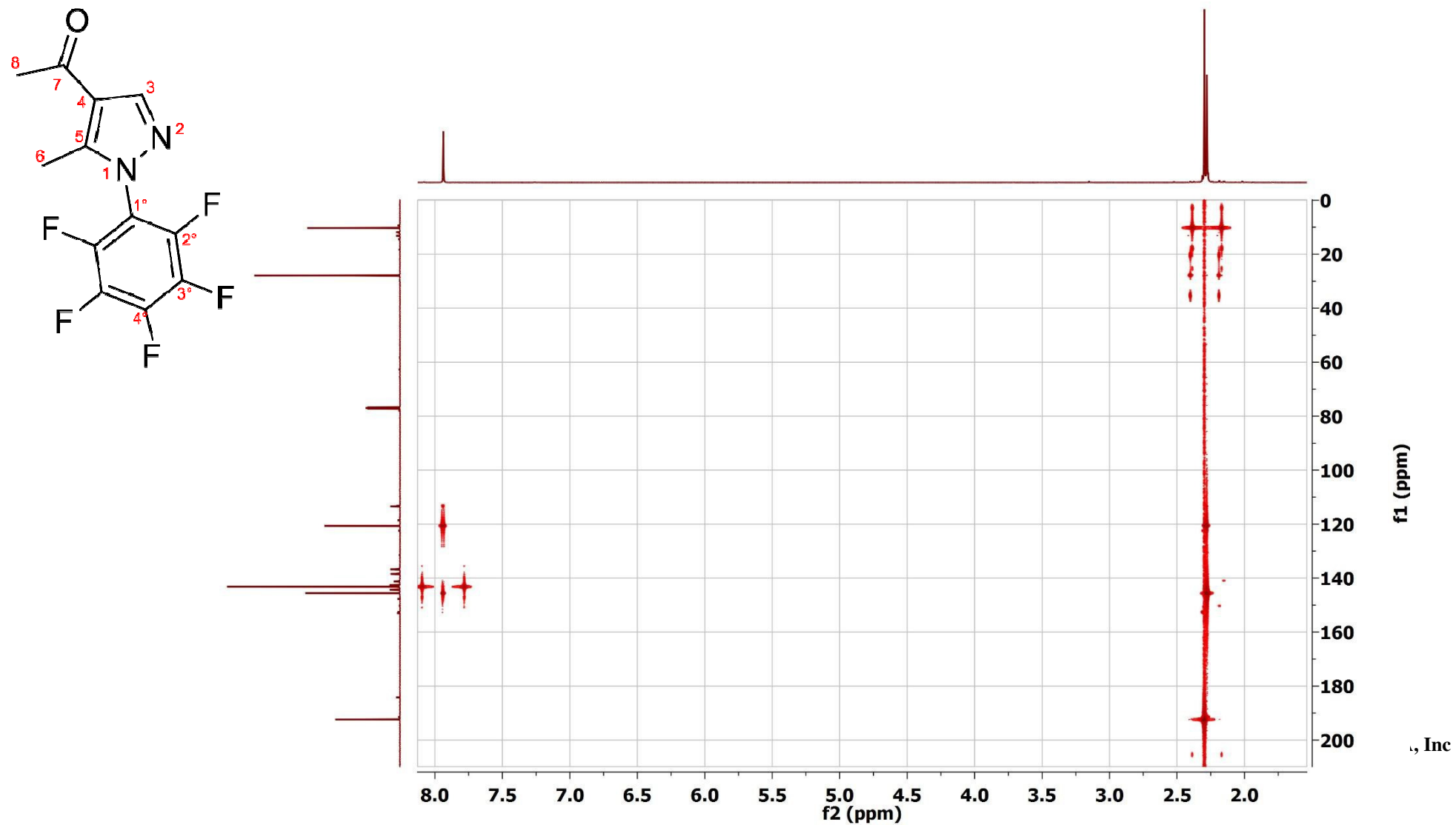


VIB ^1H NMR

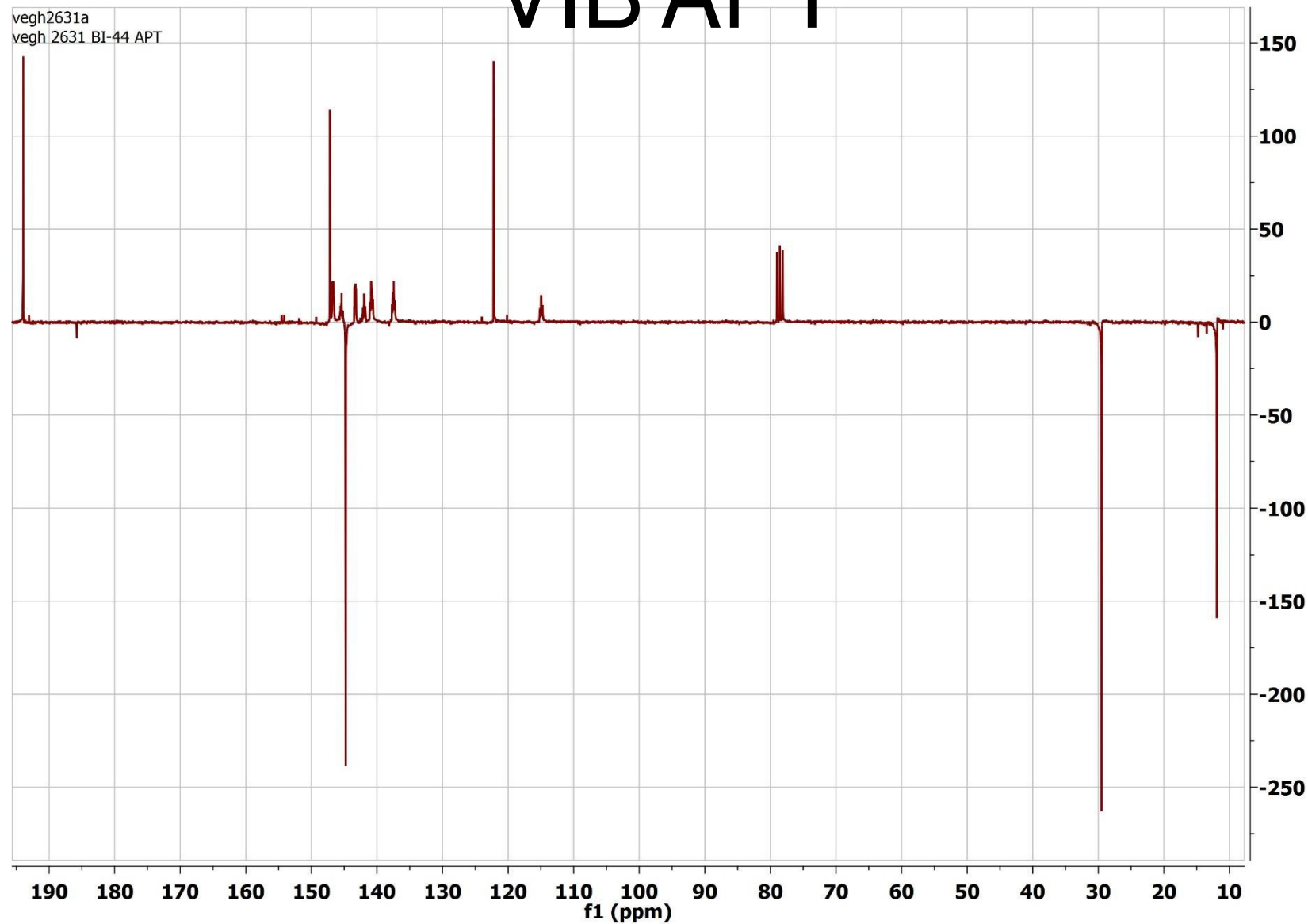
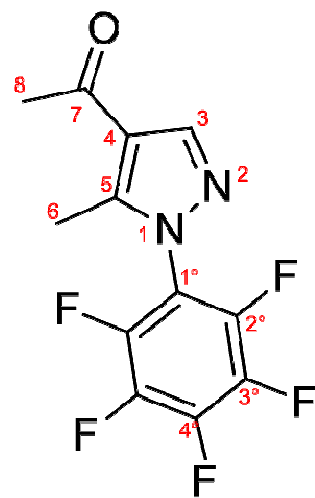


VIB ^{13}C NMR

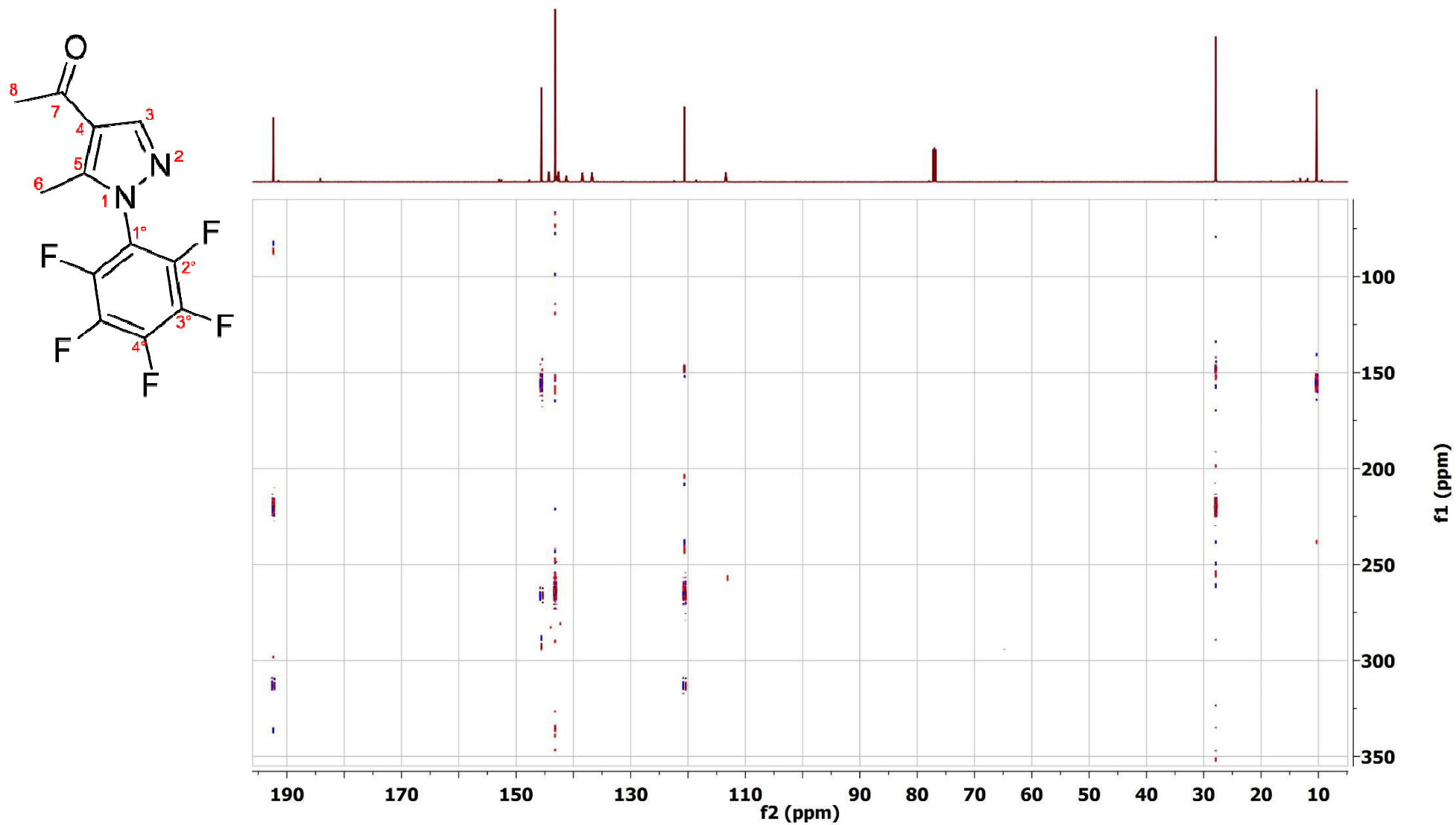


VIB ^1H - ^{13}C HMBC

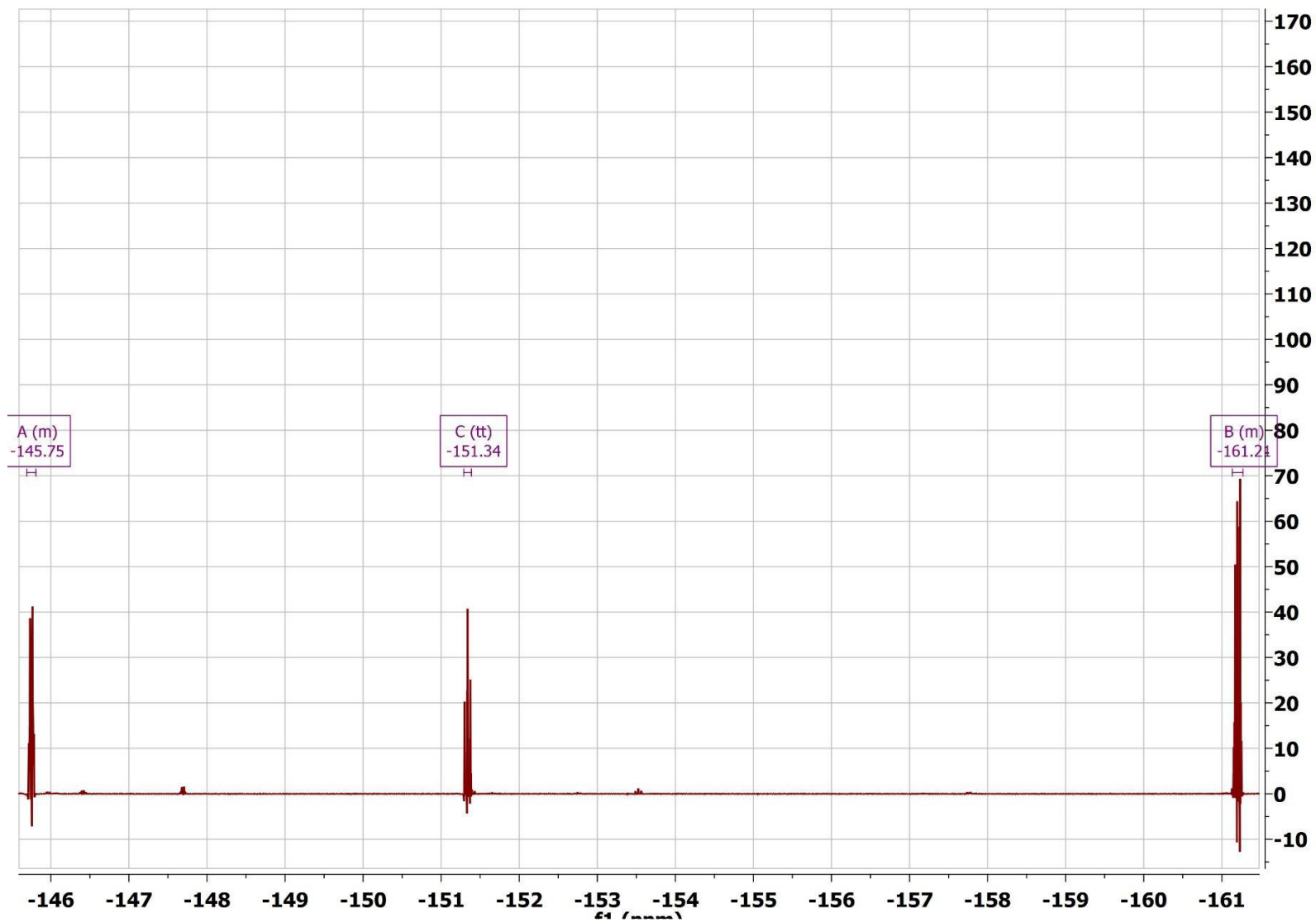
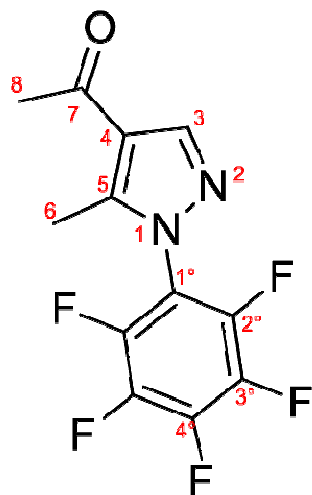
VIB APT

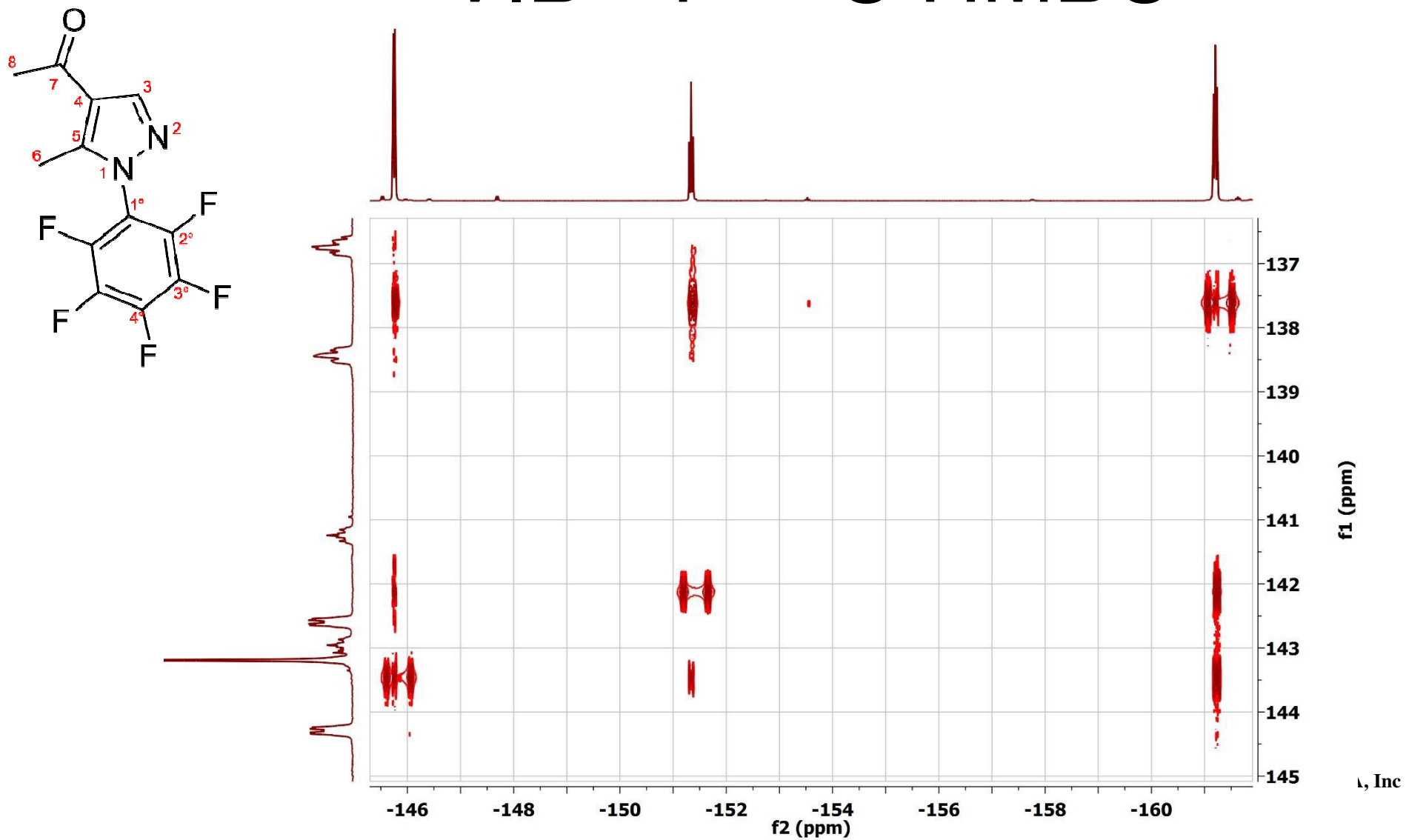


VIB INADEQUATE

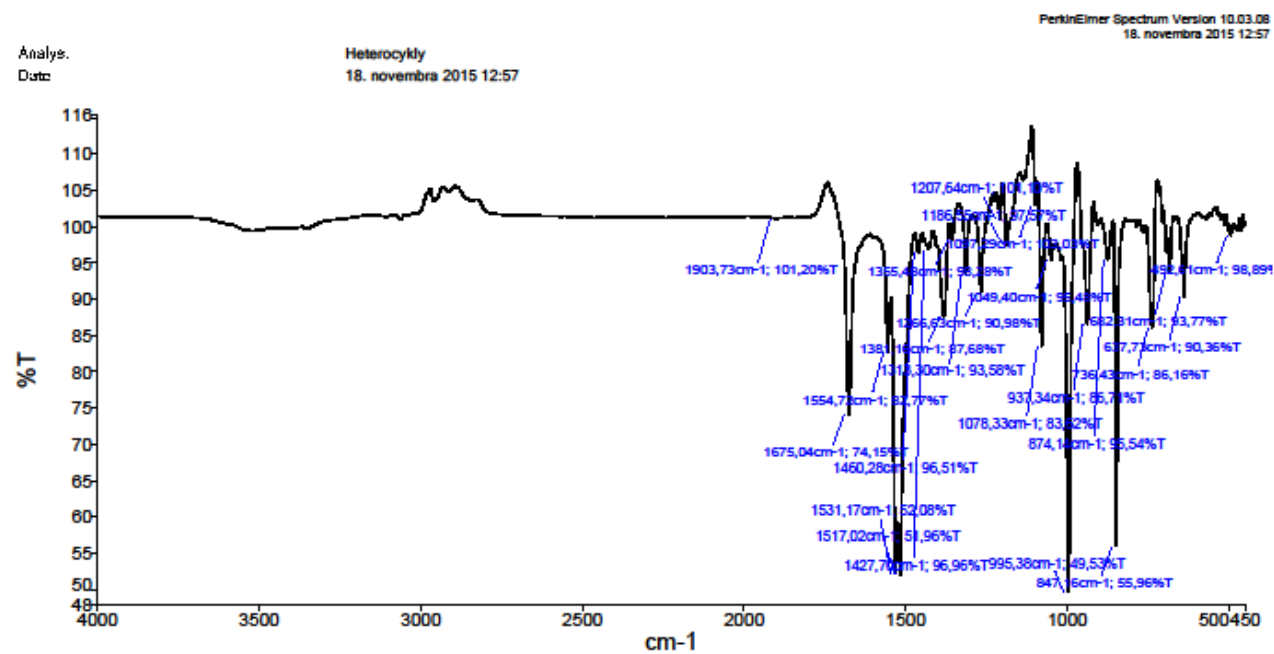
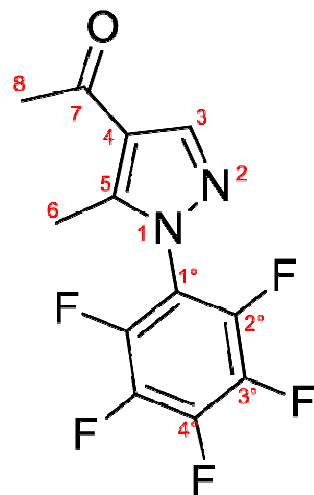


VIB ^{19}F NMR



VIB ^{19}F - ^{13}C HMBC

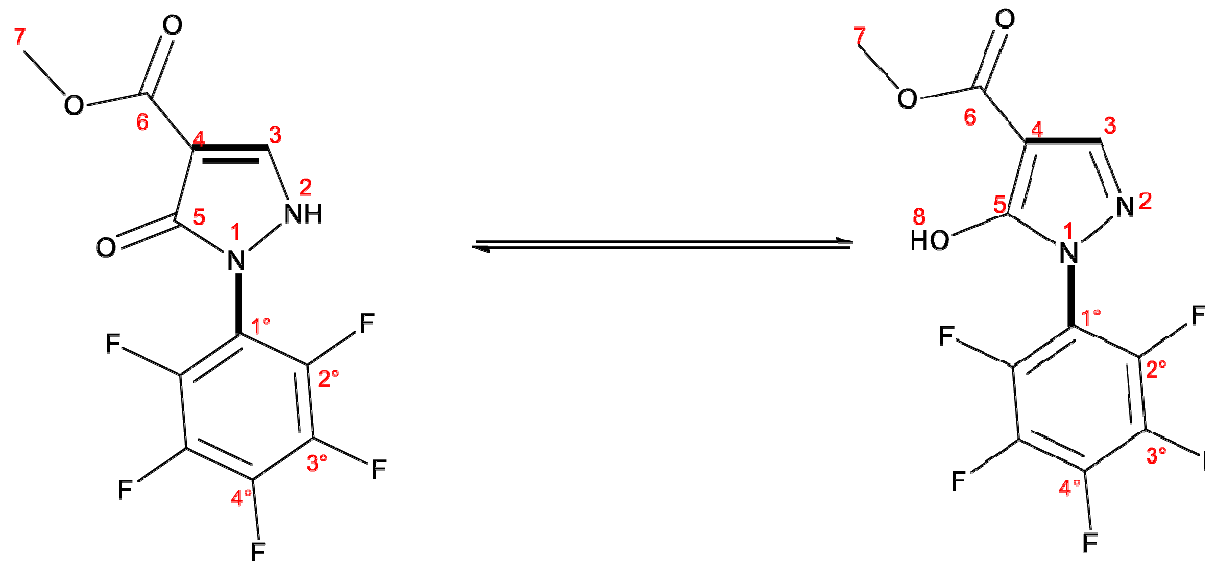
VIB IR



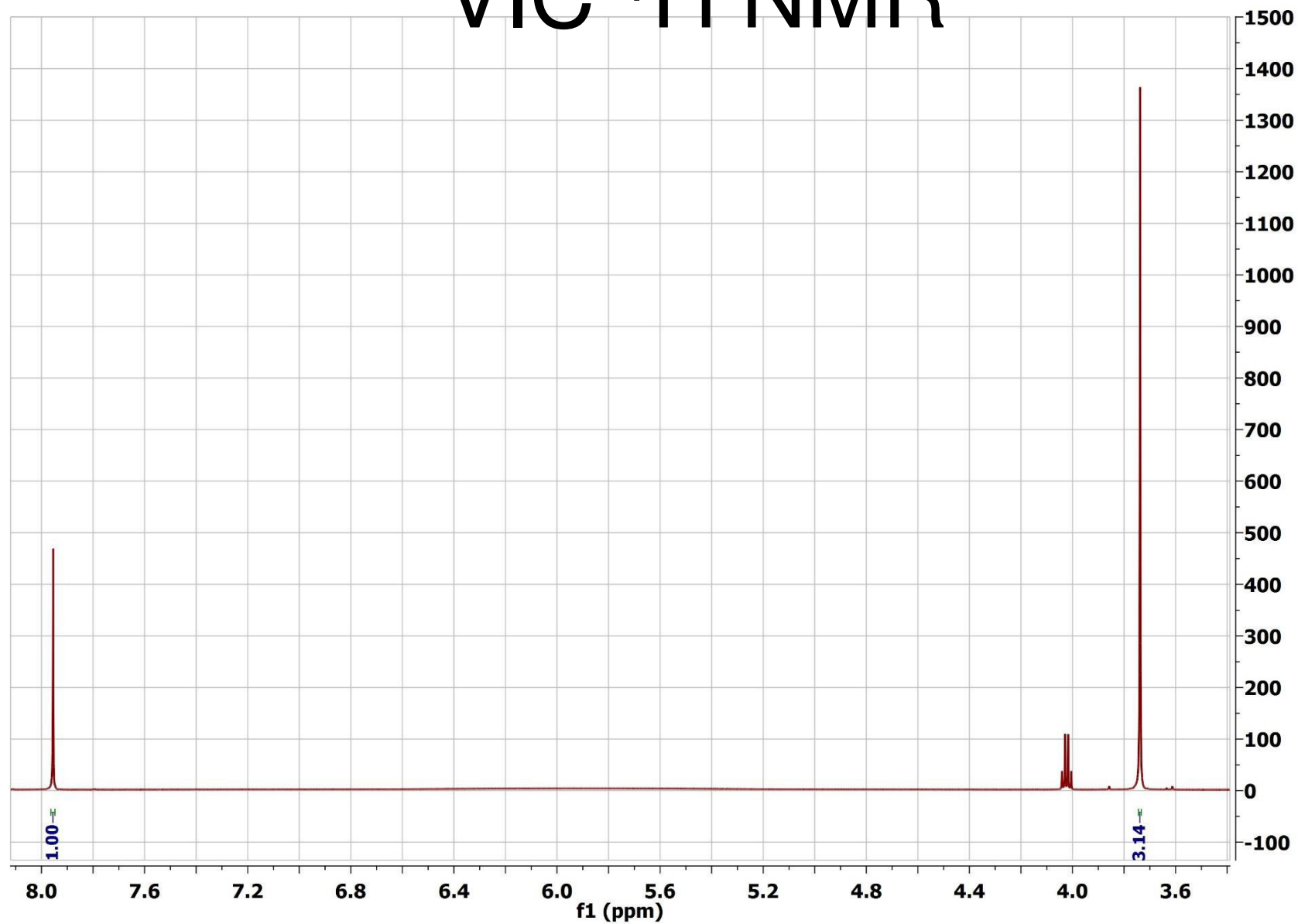
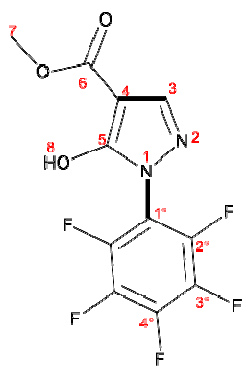
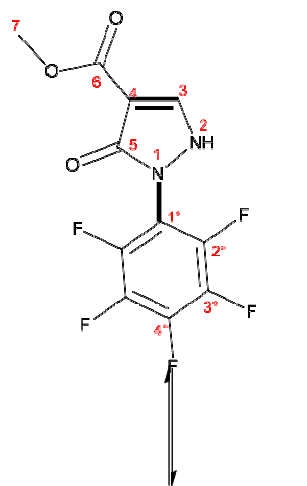
Heter 71 Sample 071 By Heter Date streda, novembra 18 2015

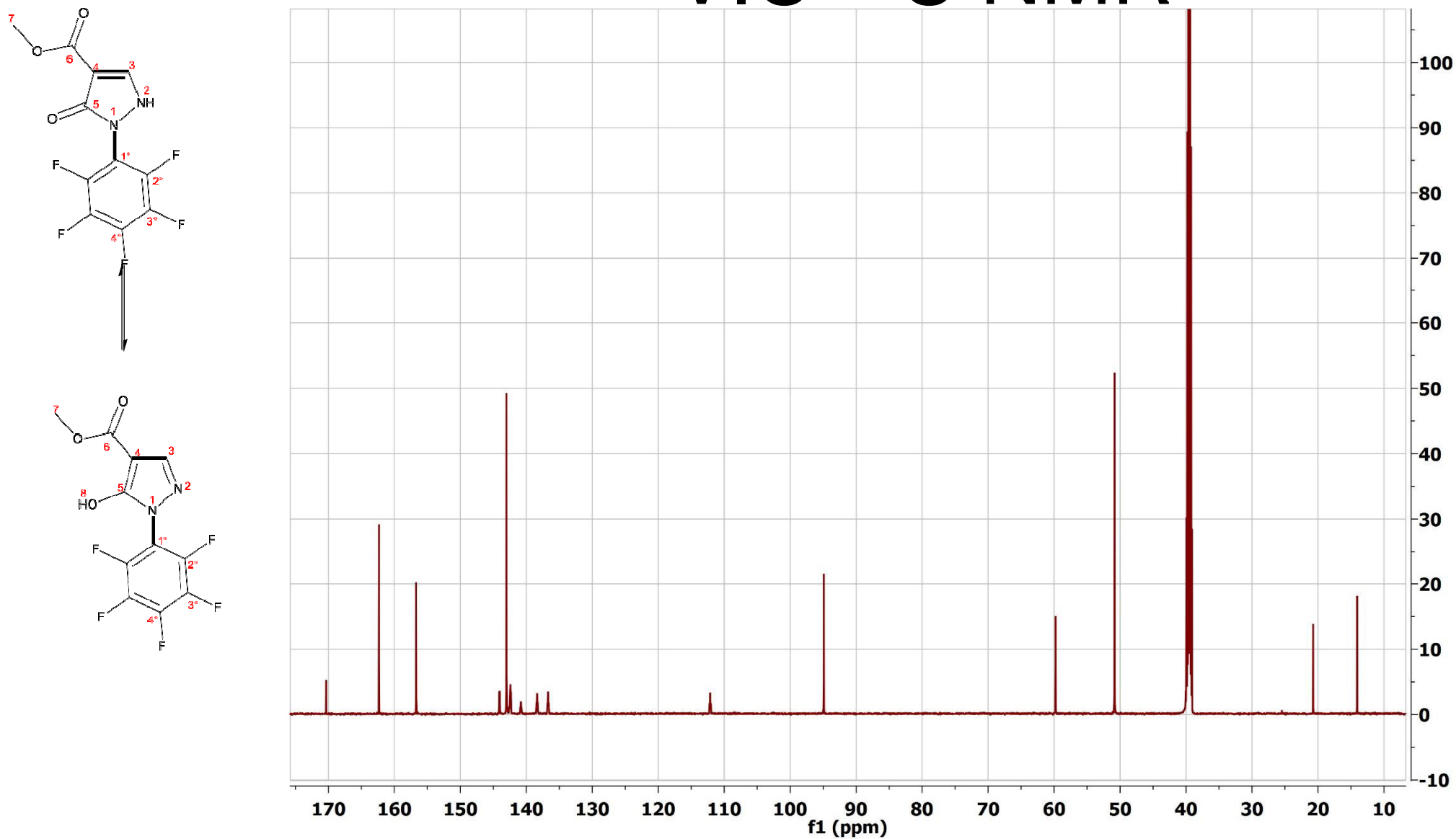
Source: Sacima Results	
Spectrum Name	Heter 71

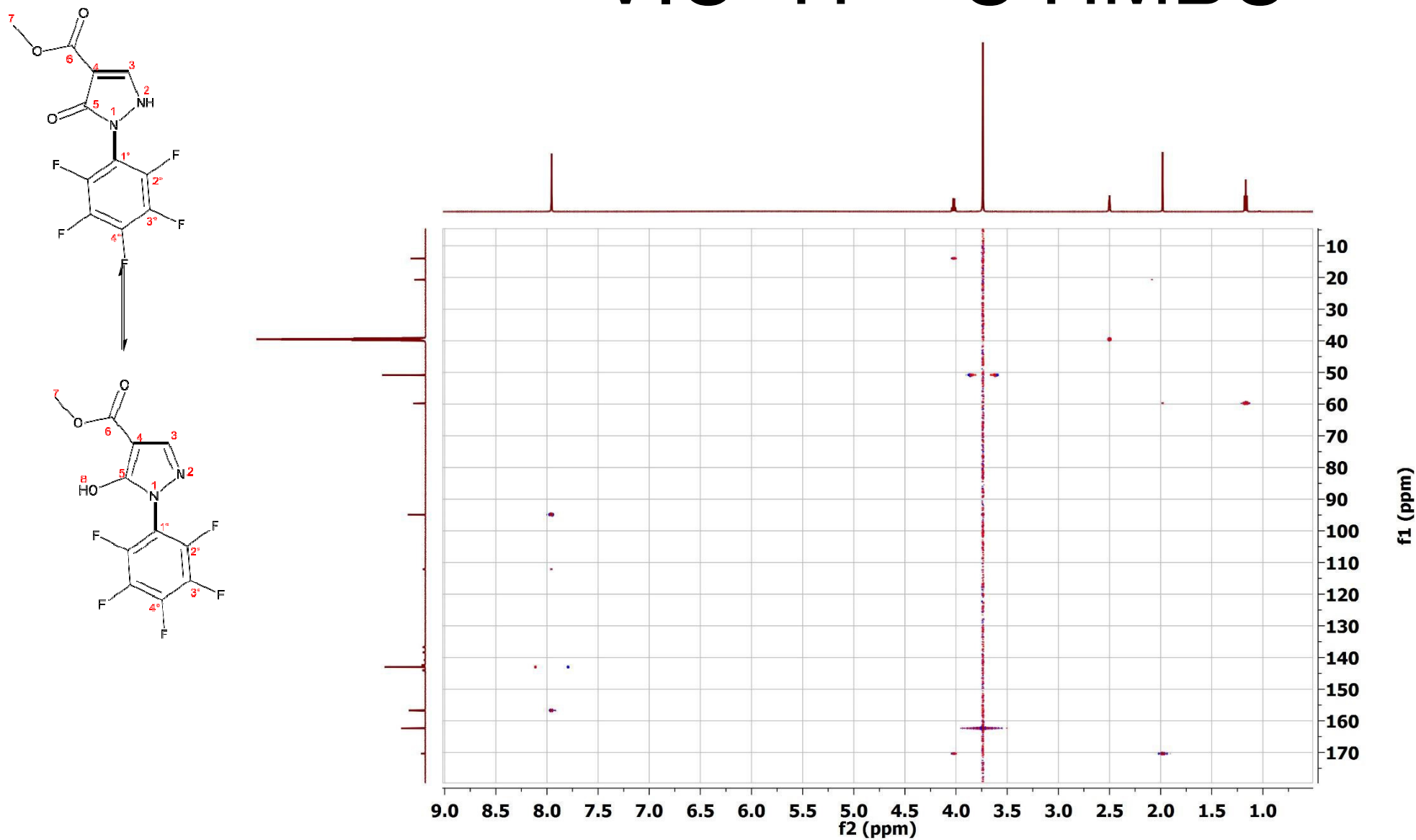
VIC

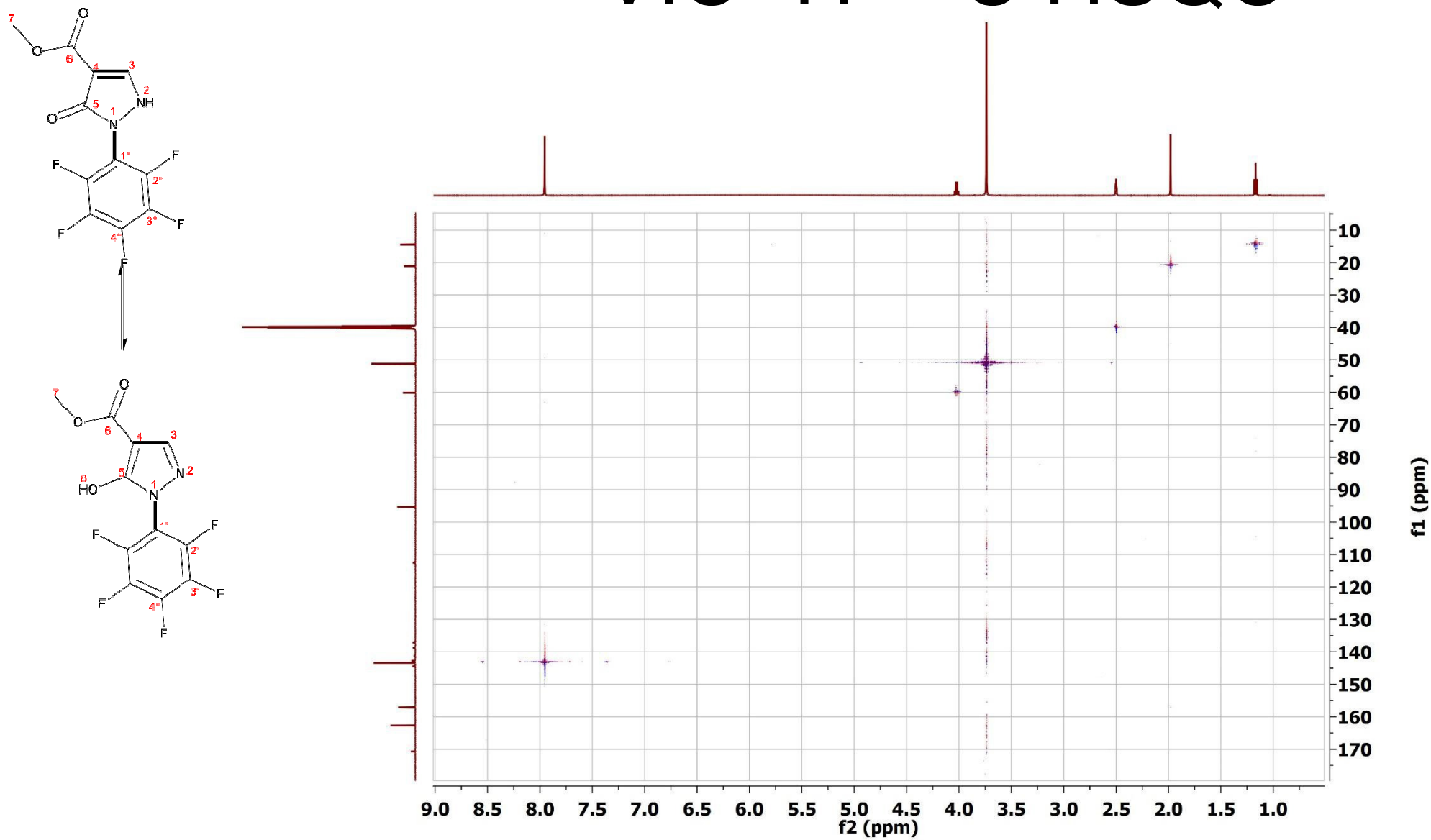


VIC ¹H NMR

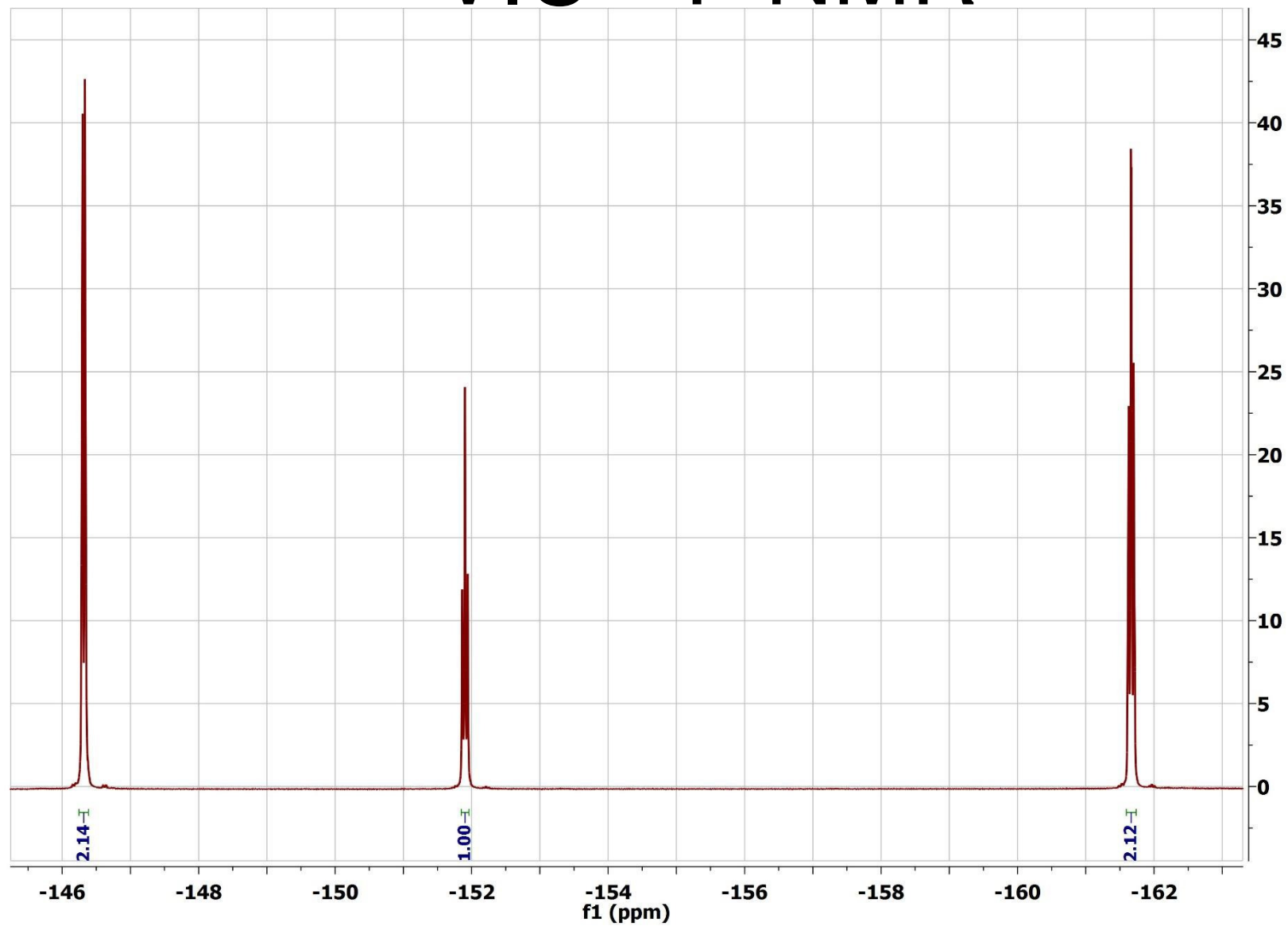
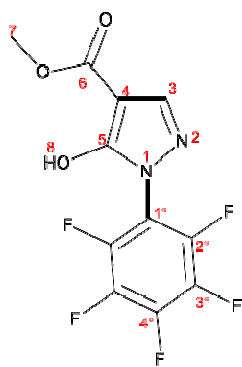
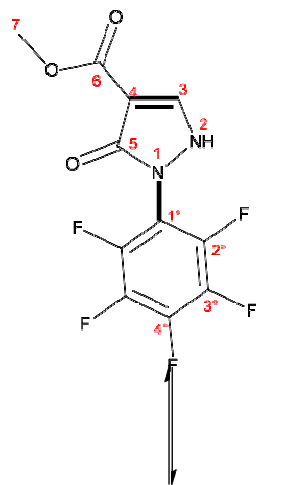


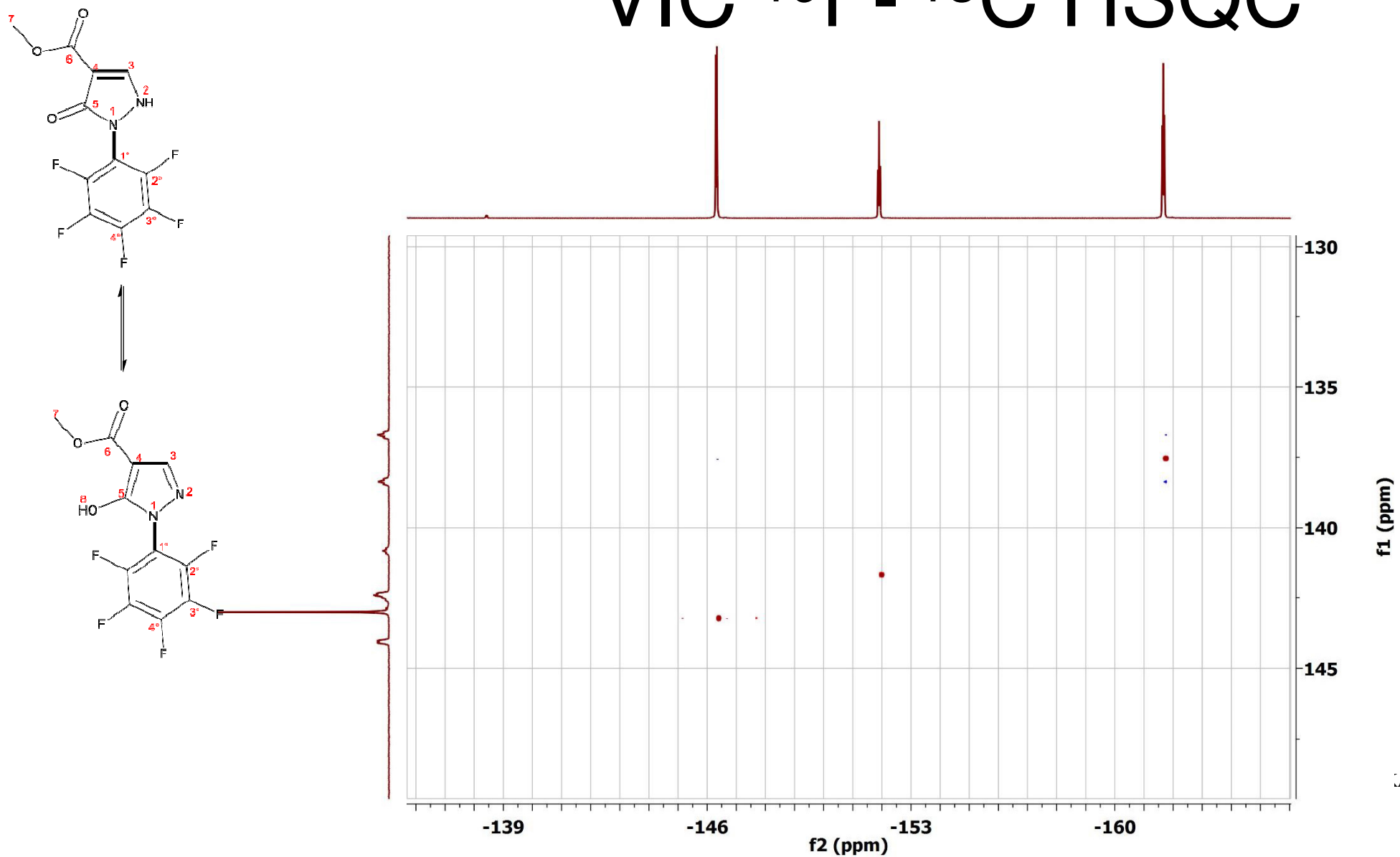
VIC ^{13}C NMR

VIC ^1H - ^{13}C HMBC

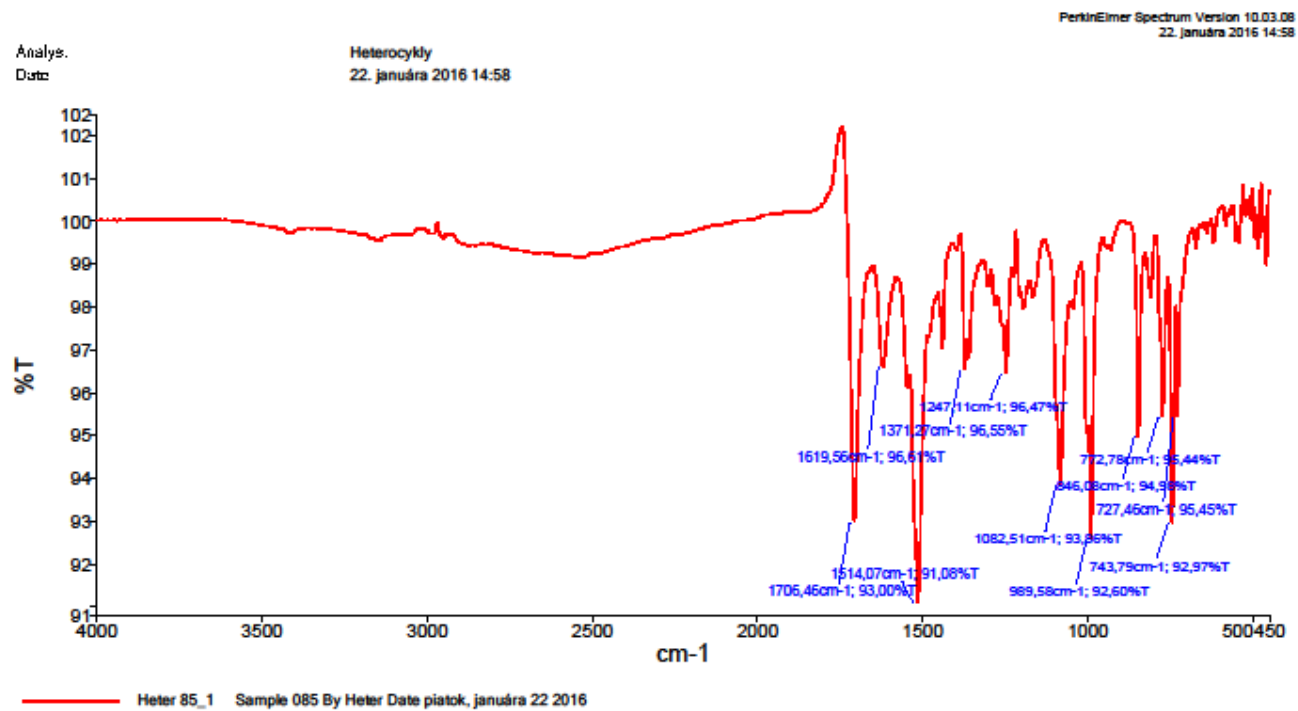
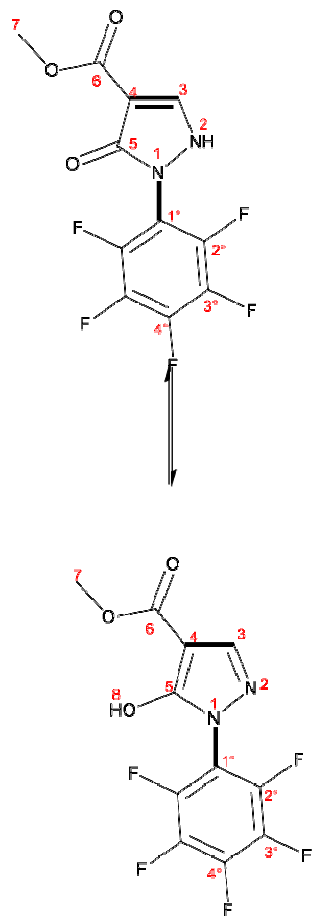
VIC ^1H - ^{13}C HSQC

VIC ^{19}F NMR



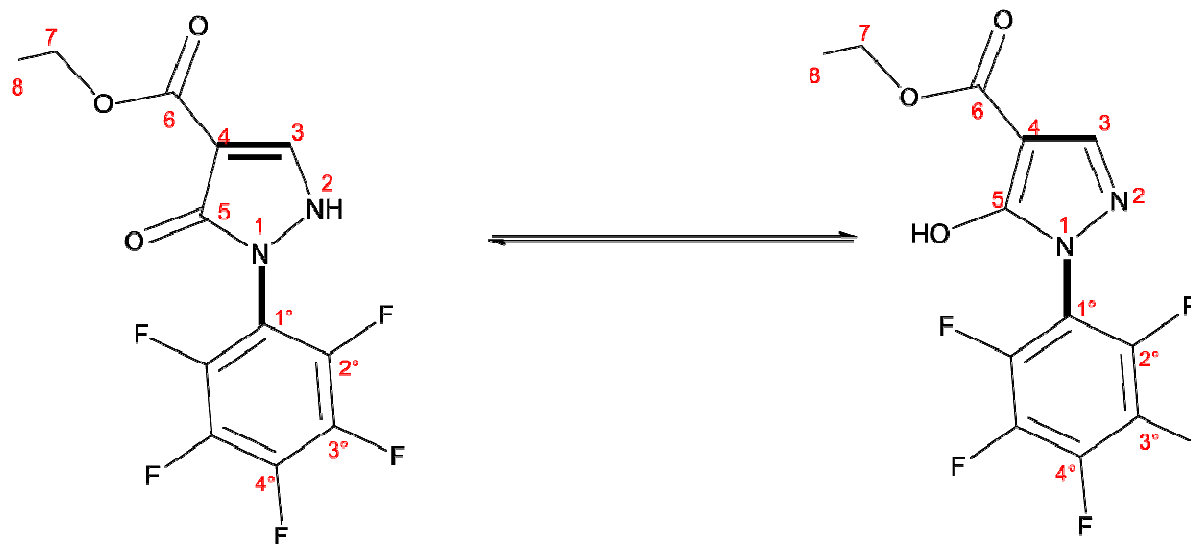
VIC ^{19}F - ^{13}C HSQC

VIC IR

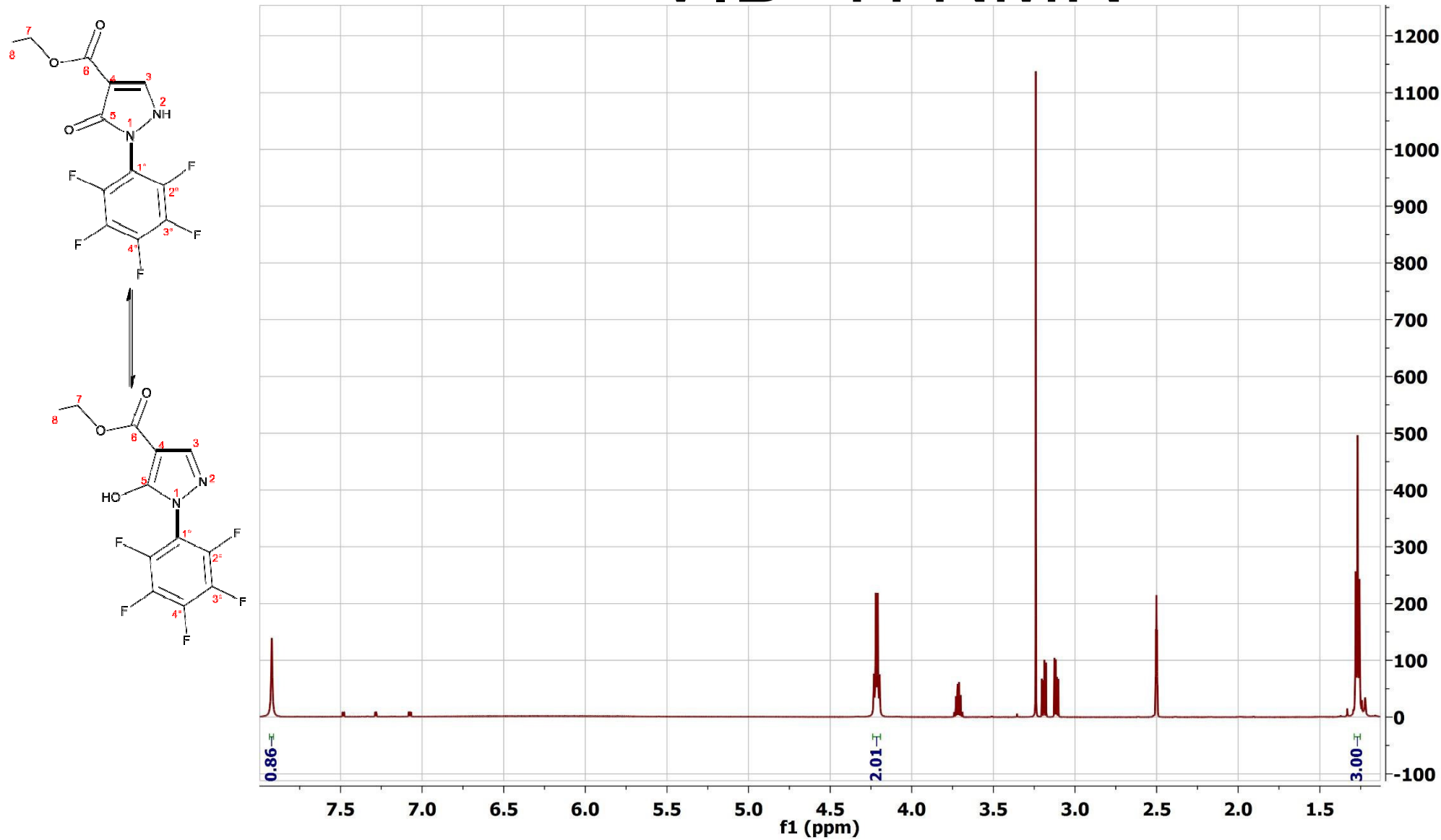


Source: Source Results	
Spectrum Name	Heter 85_1

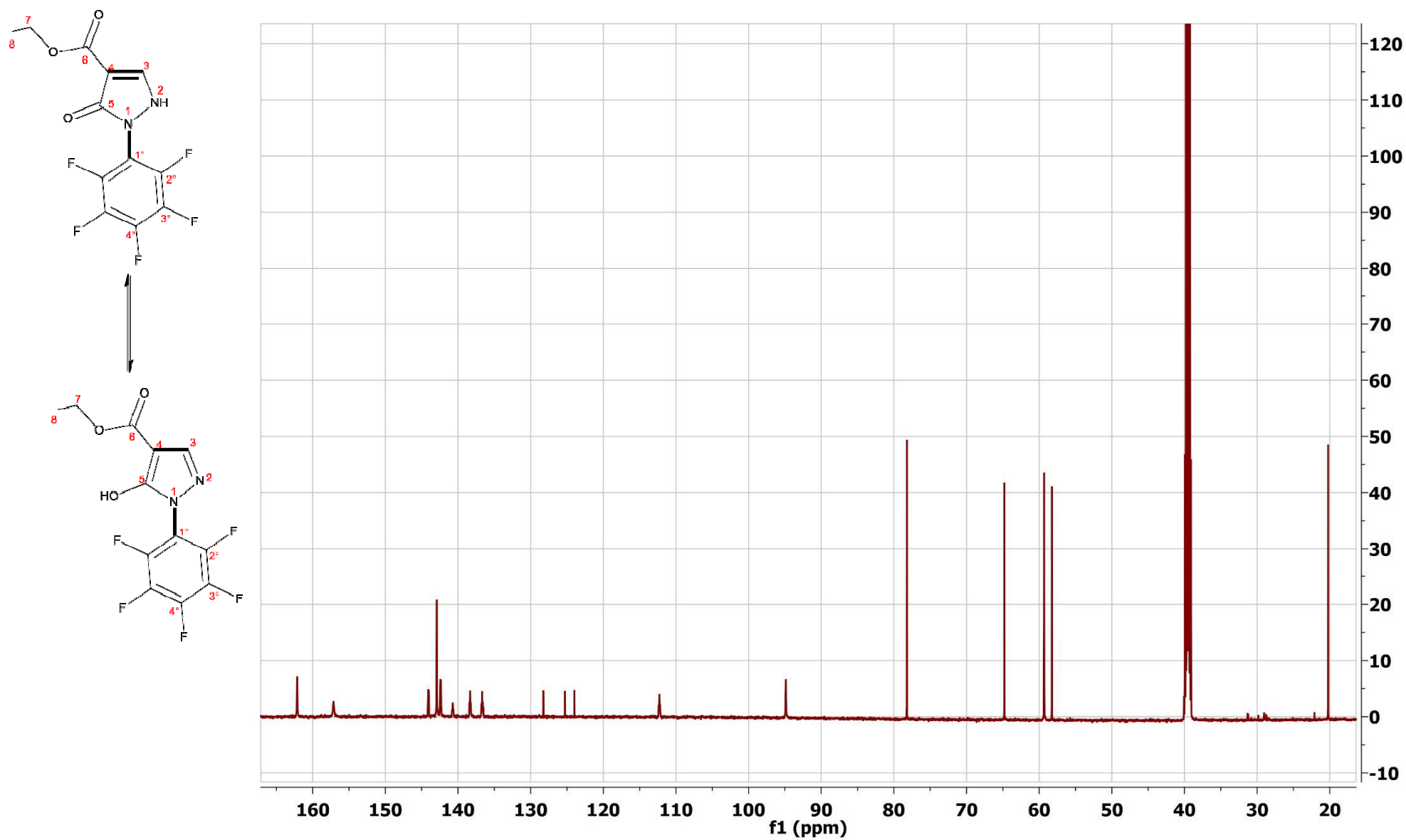
VID



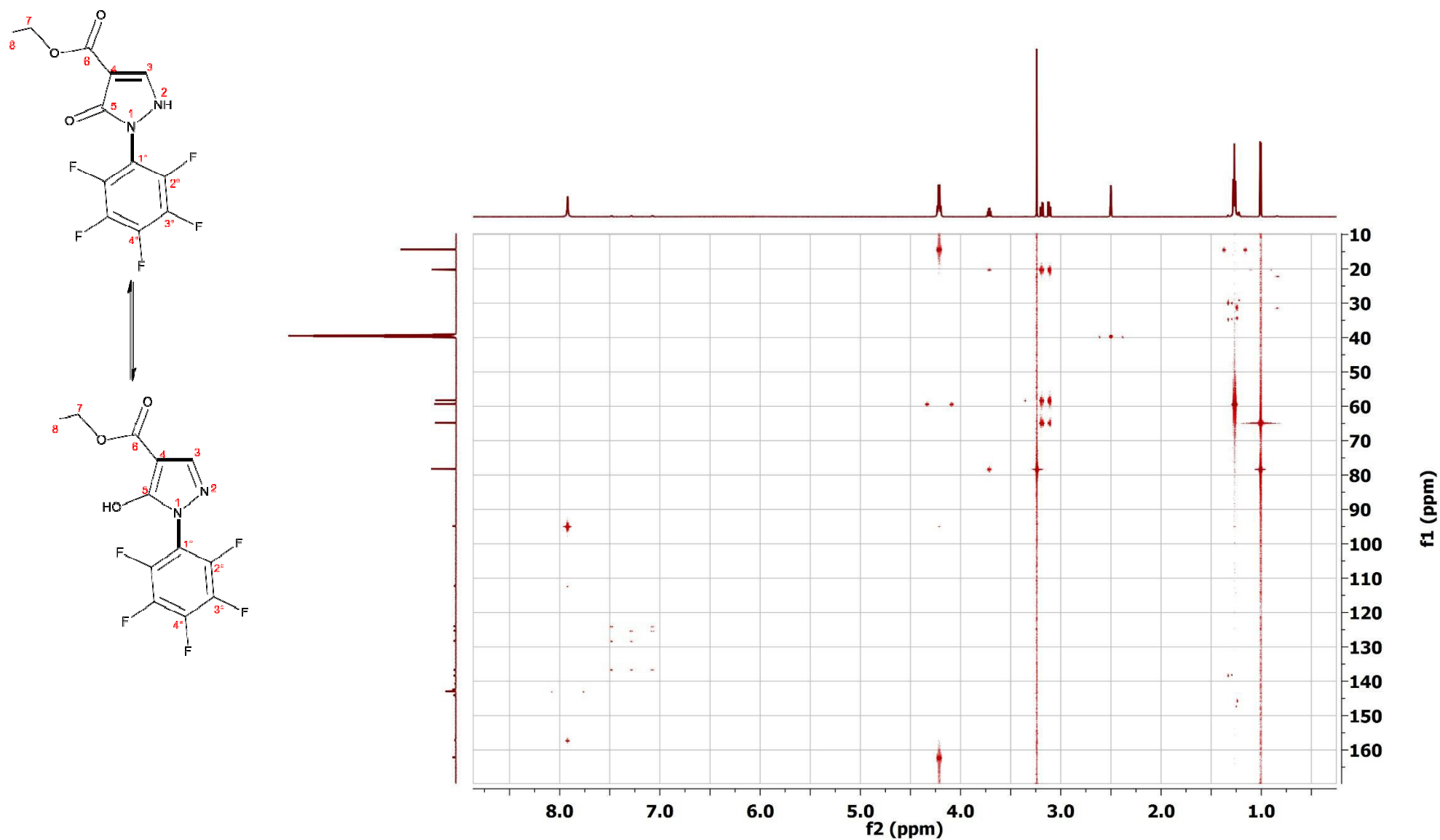
VID ¹H NMR



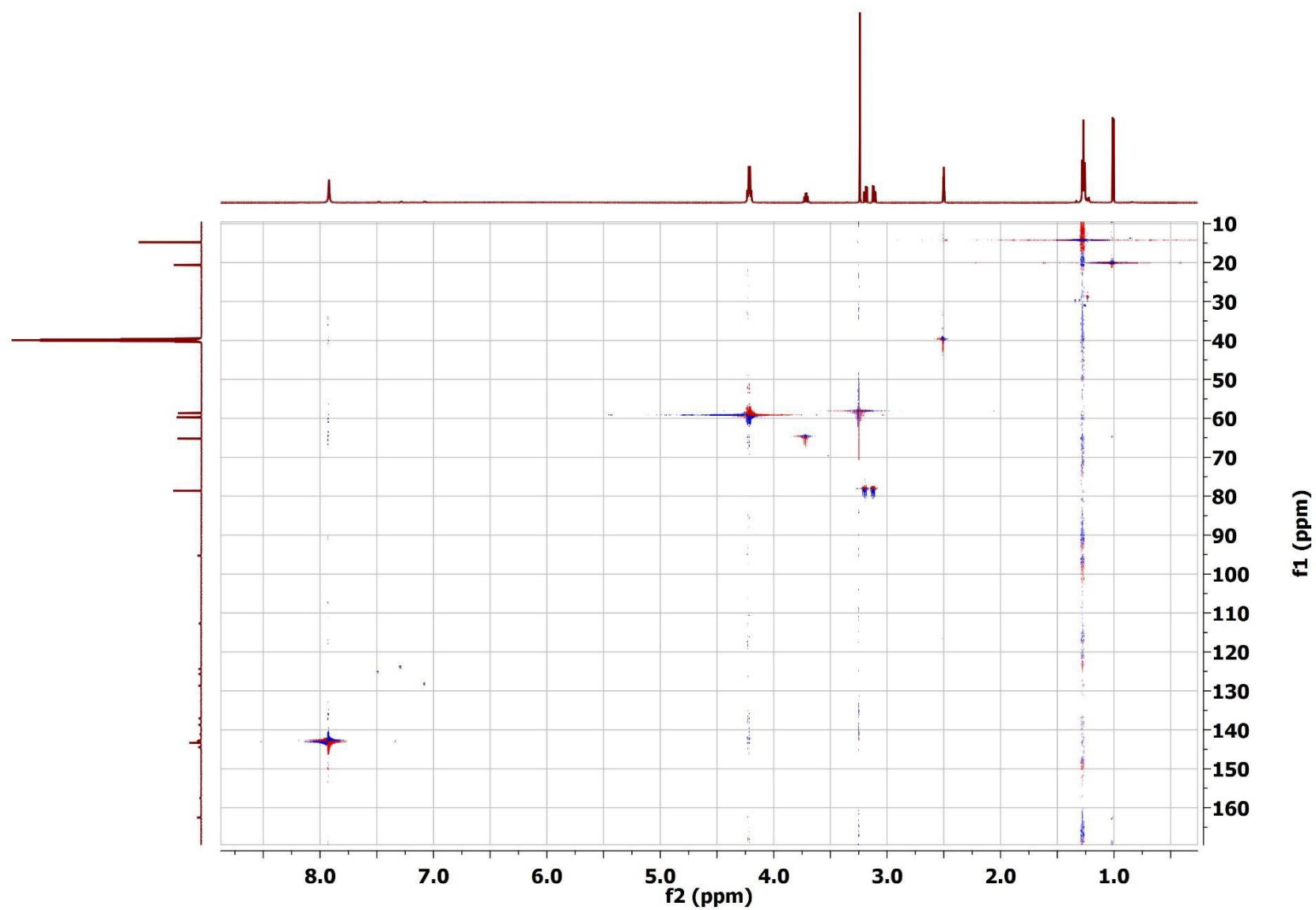
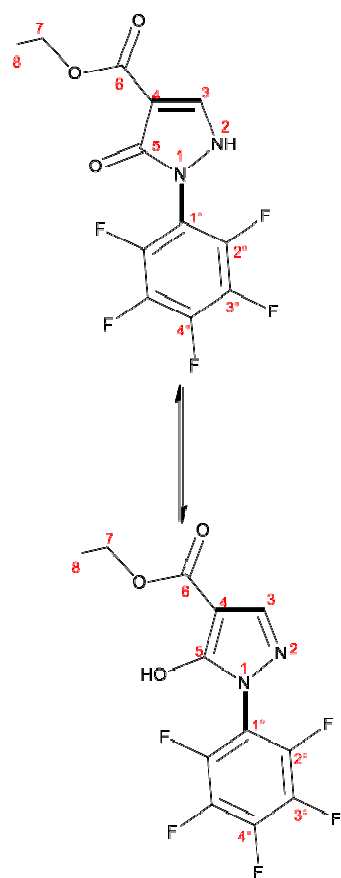
VID ^{13}C NMR



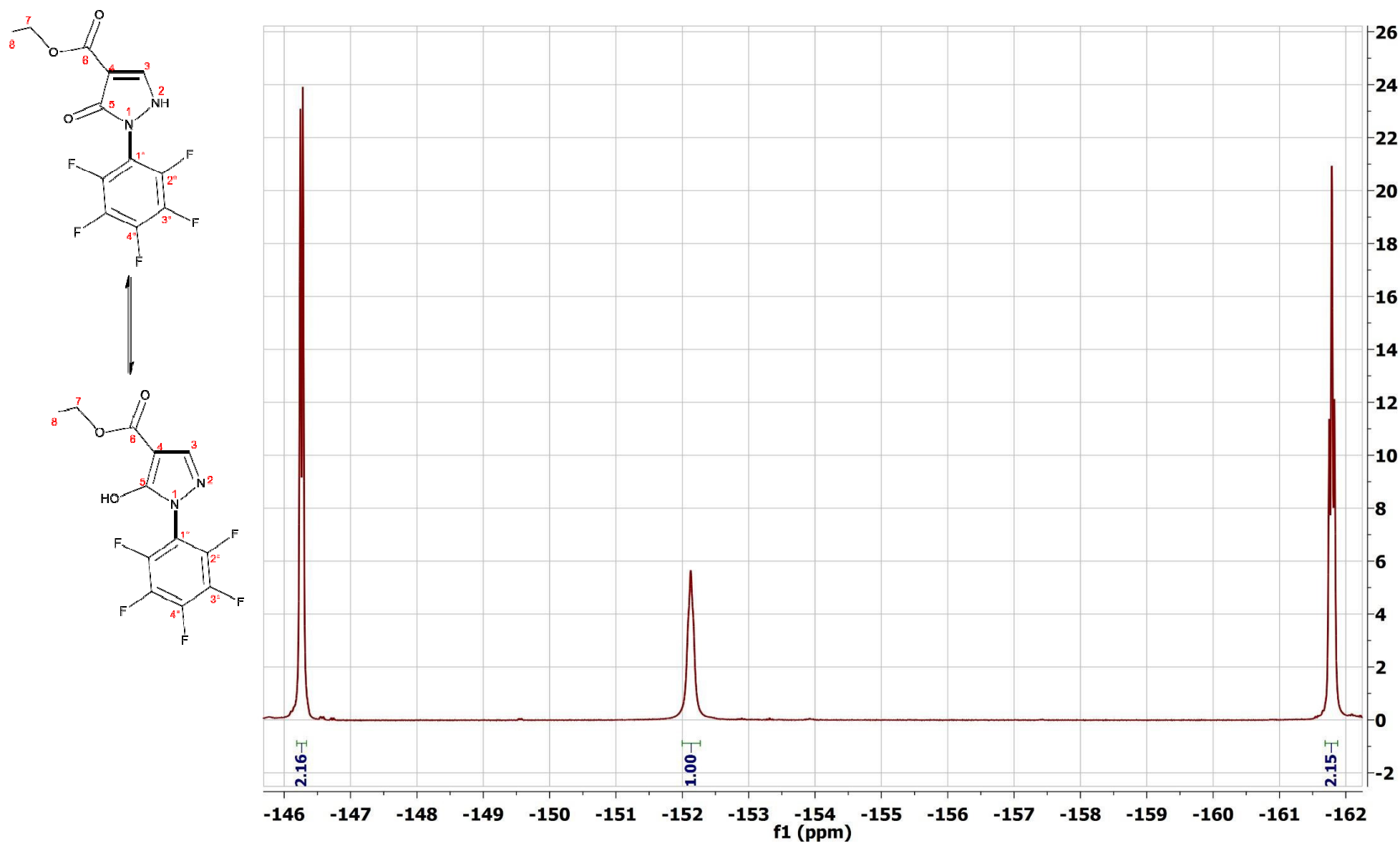
VID ^1H - ^{13}C HMBC



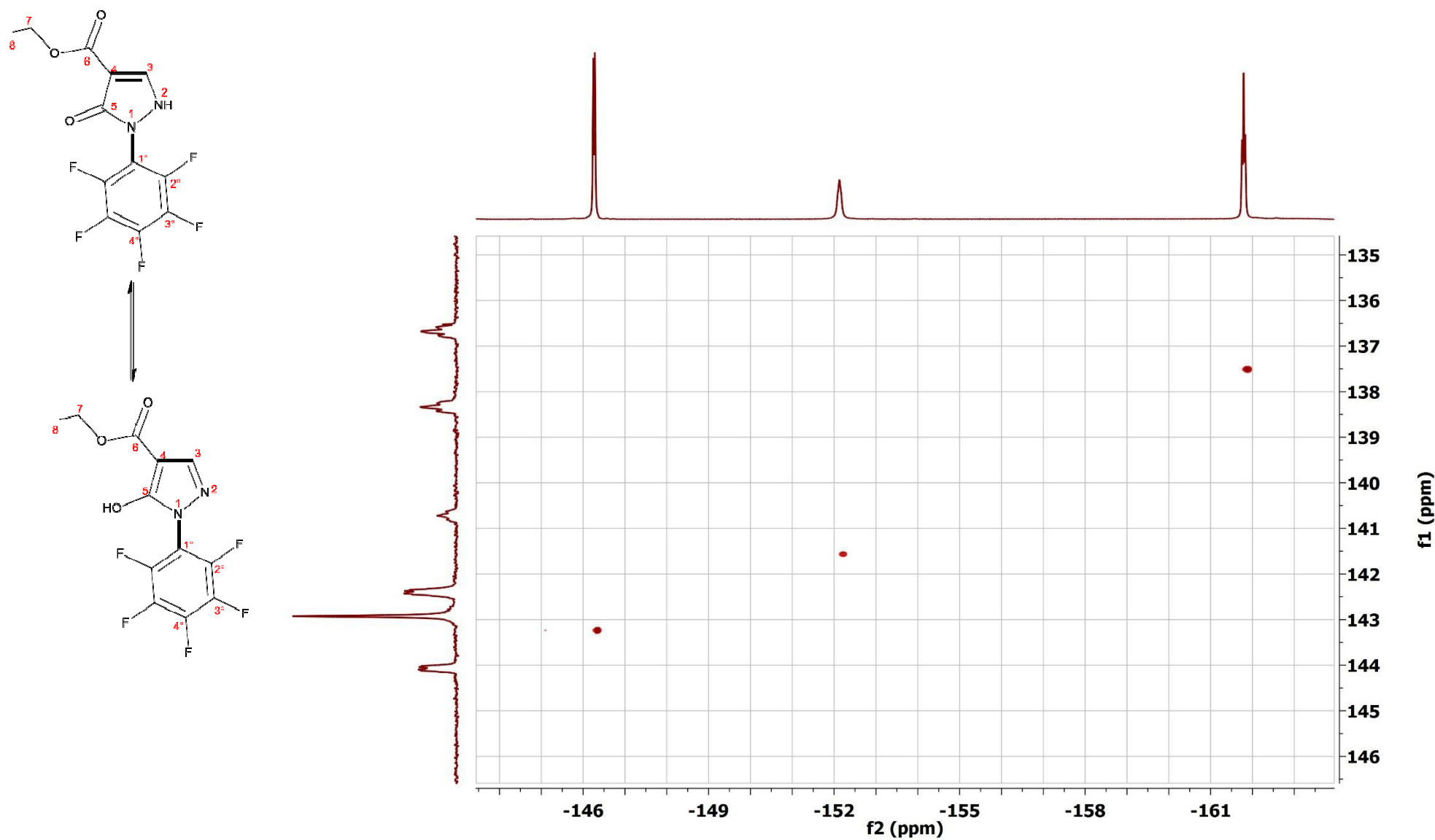
VID ^1H - ^{13}C HSQC



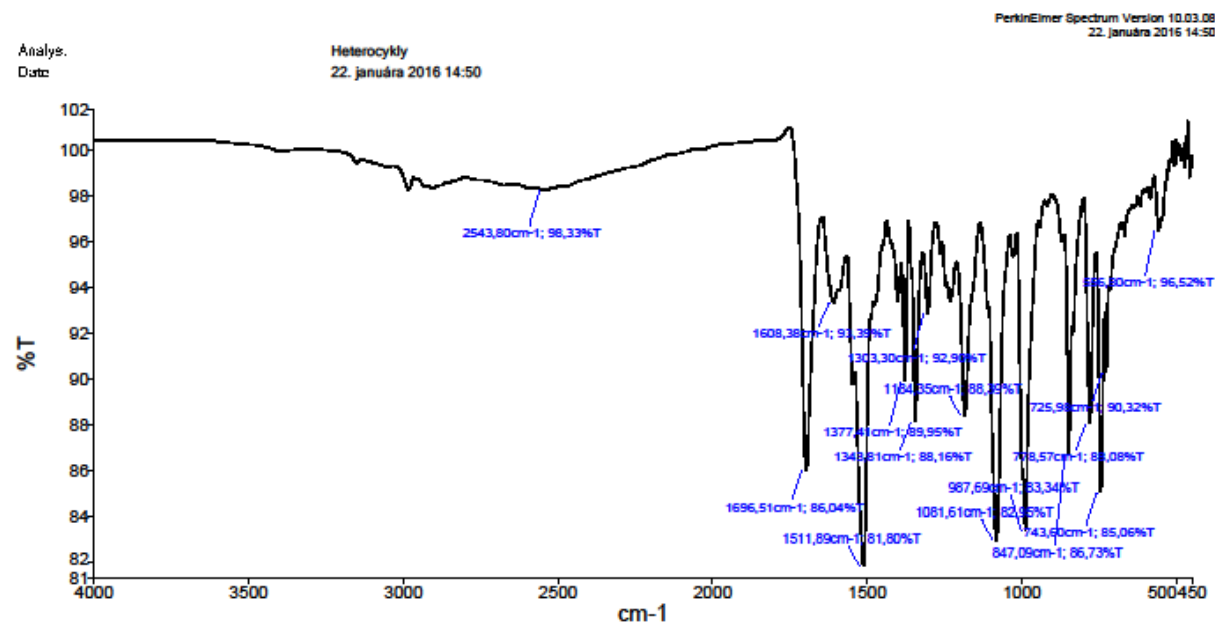
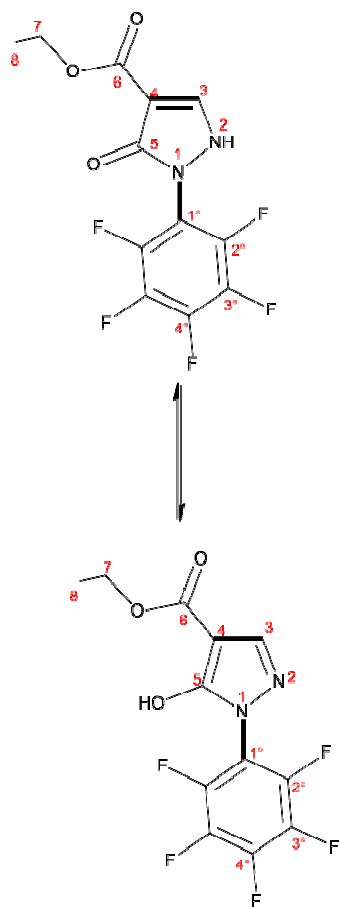
VID ^{19}F NMR



VID ^{19}F - ^{13}C HSQC



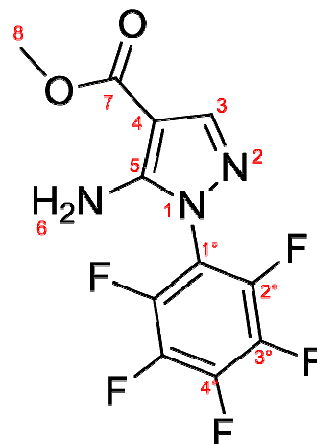
VID IR



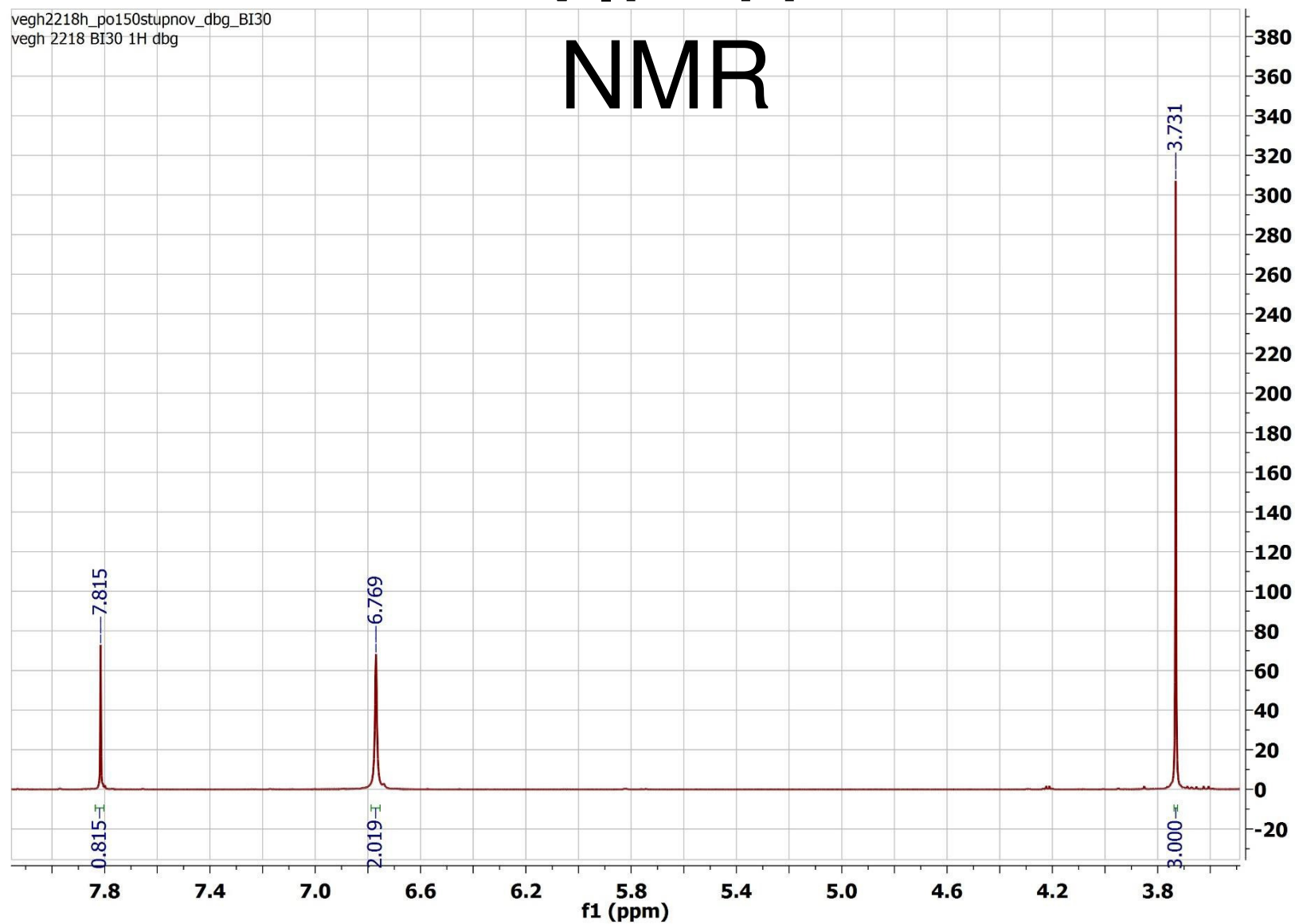
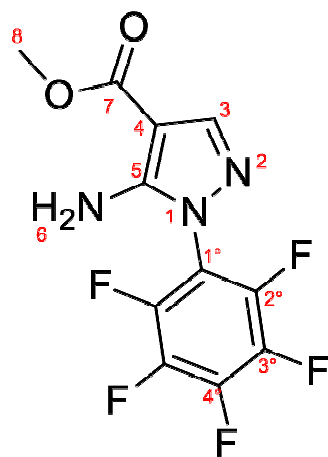
Heter 83 Sample 083 By Heter Date piatok, januára 22 2016

Source: Source Results	
Spectrum Name	Heter 83

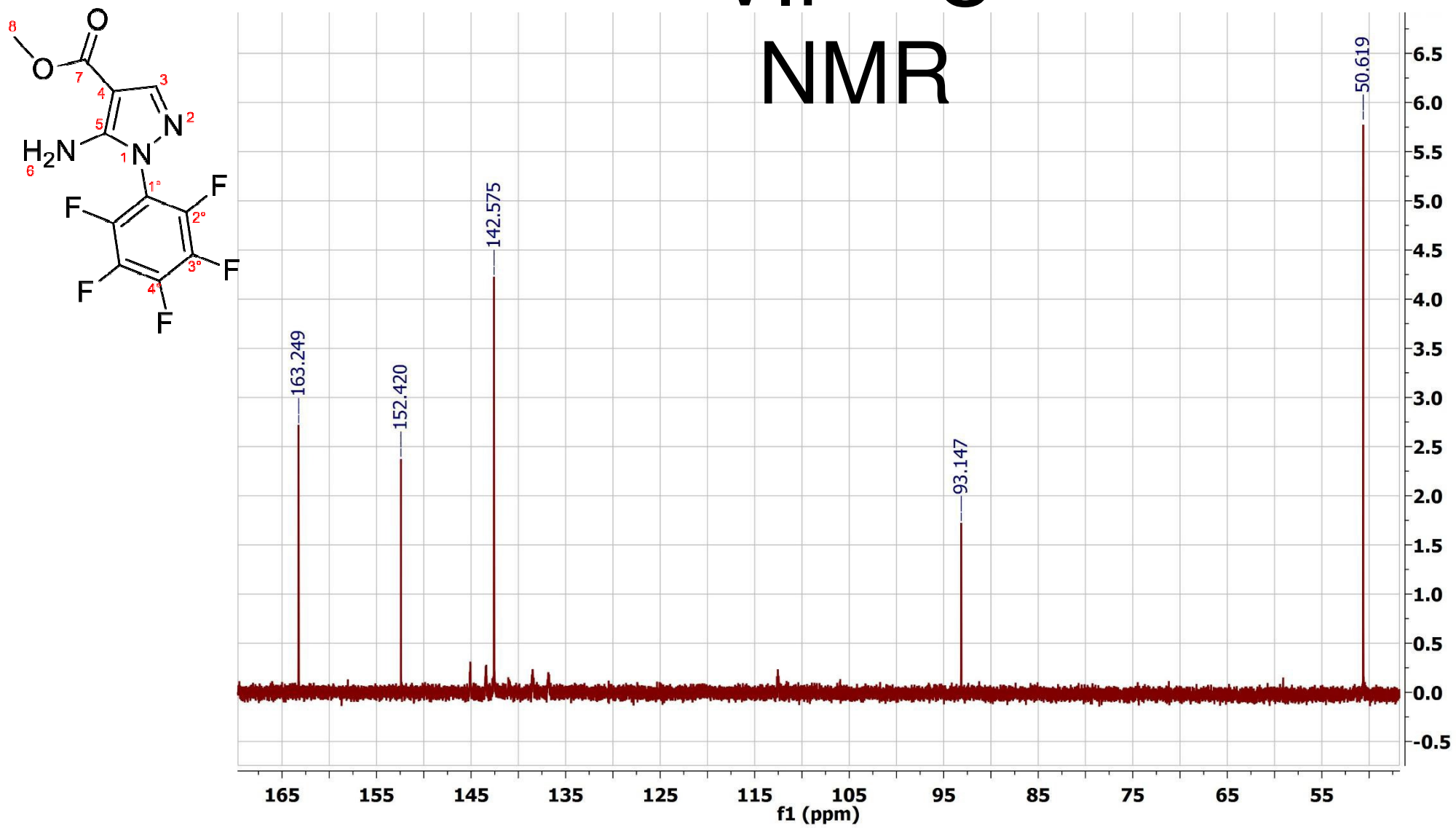
VIF

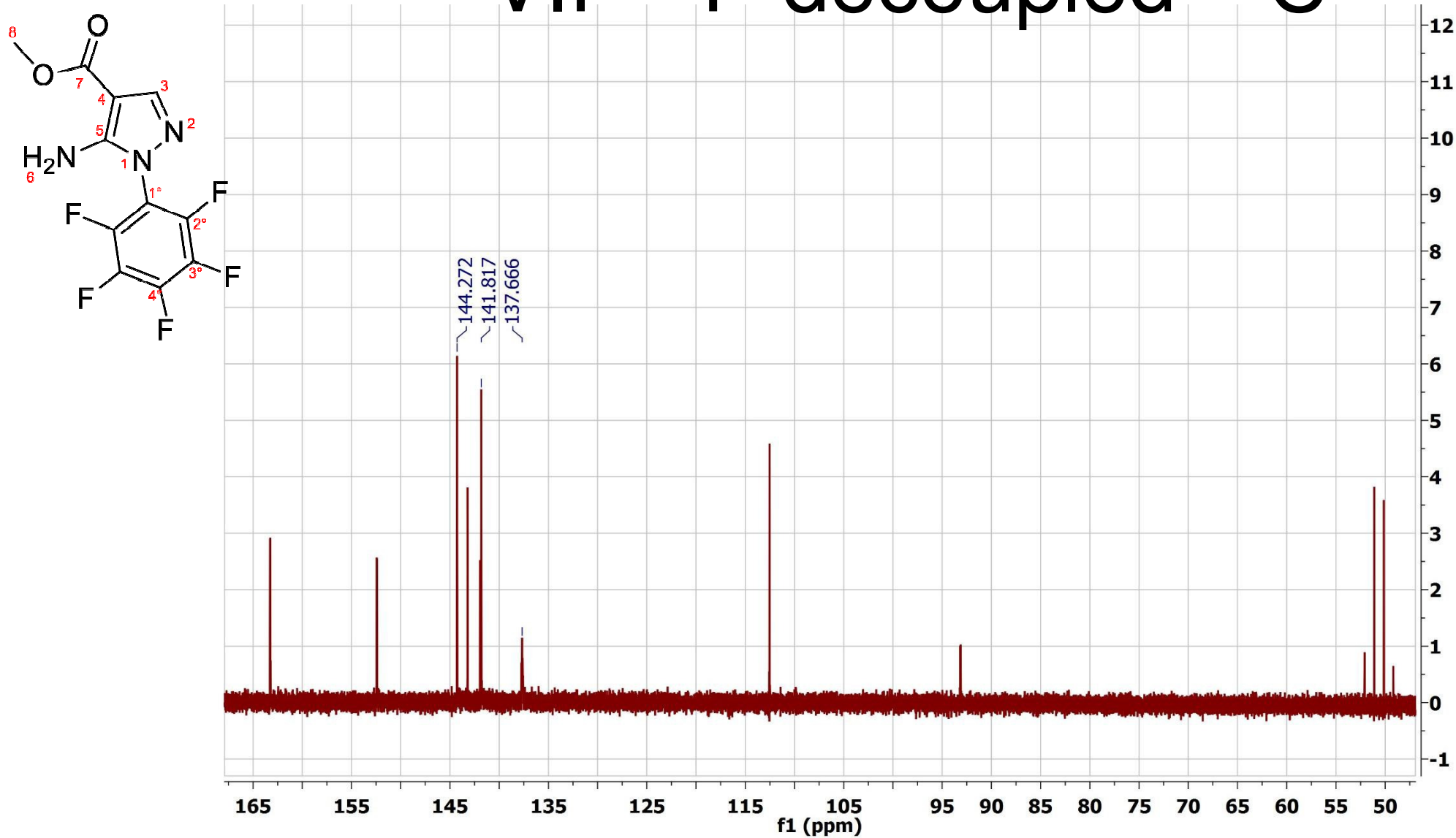


VIF ¹H NMR

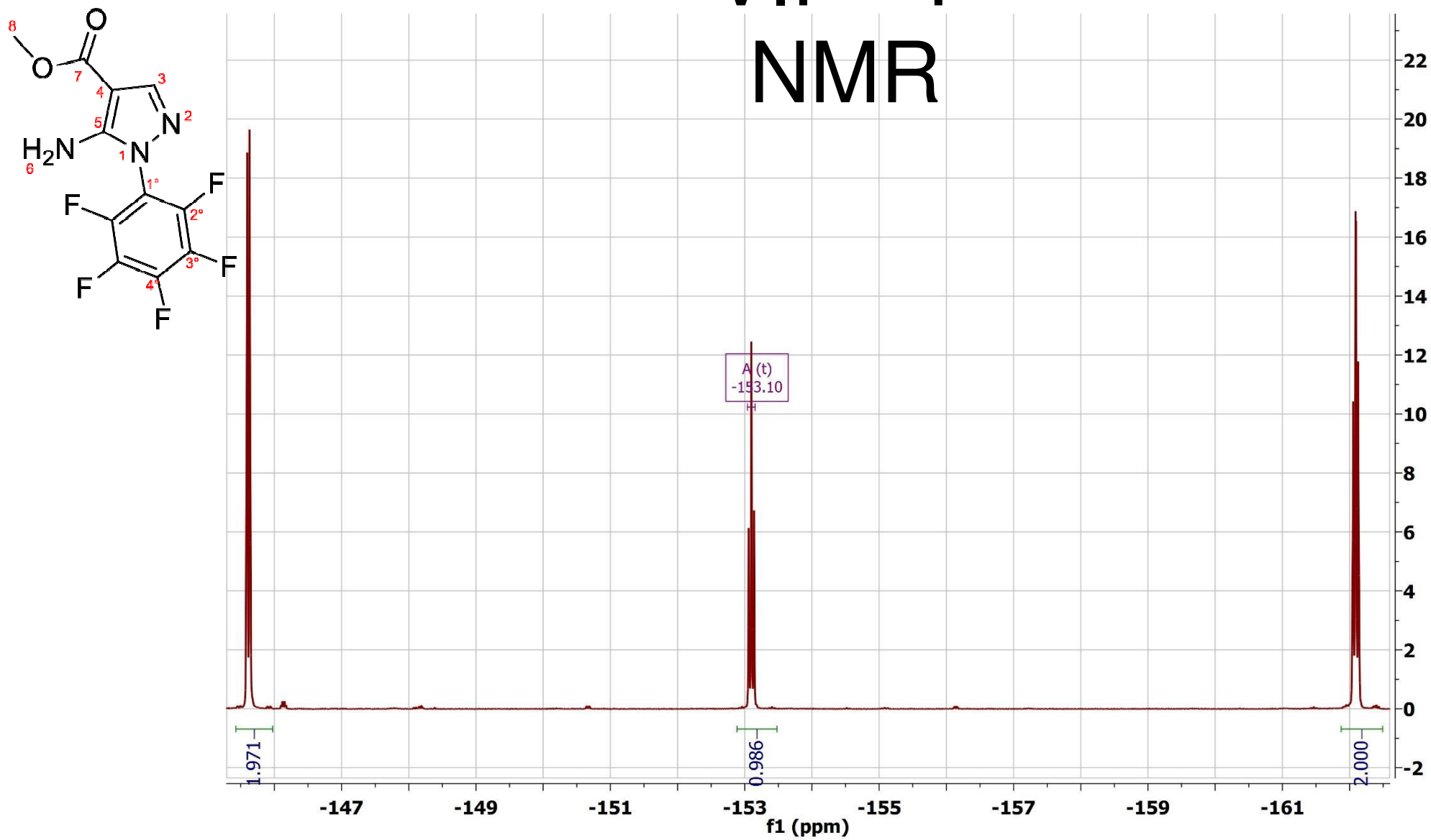


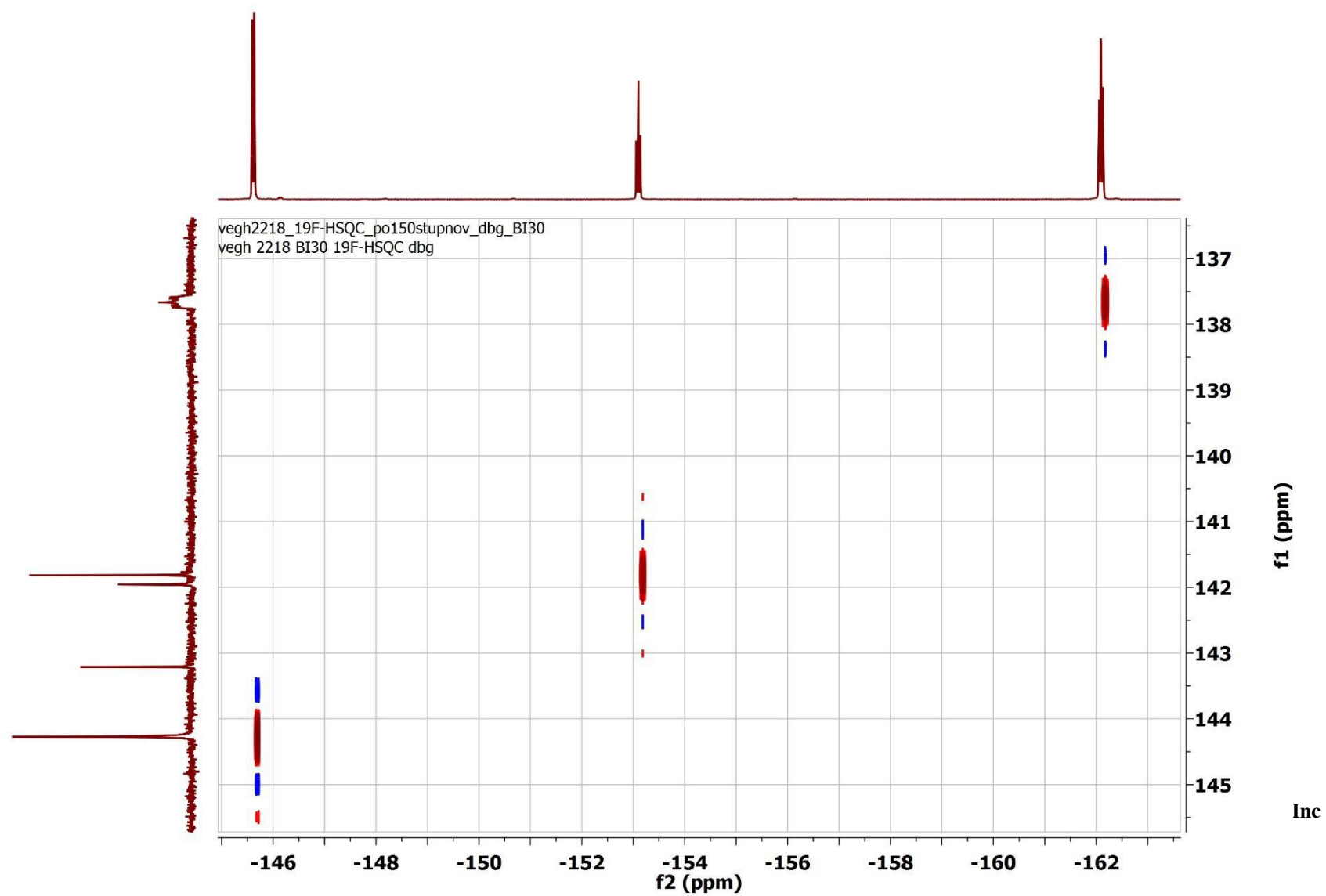
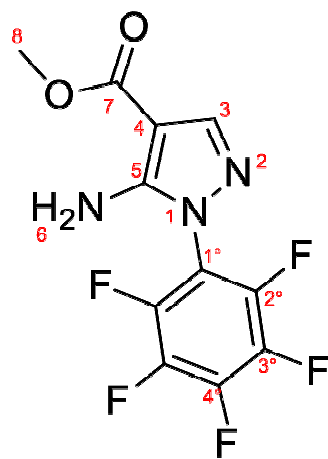
Inc

VIF ^{13}C
NMR

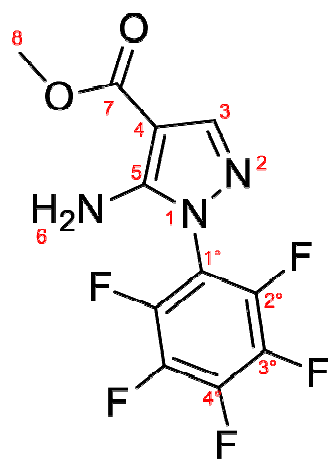
VIF ^{19}F -decoupled- ^{13}C 

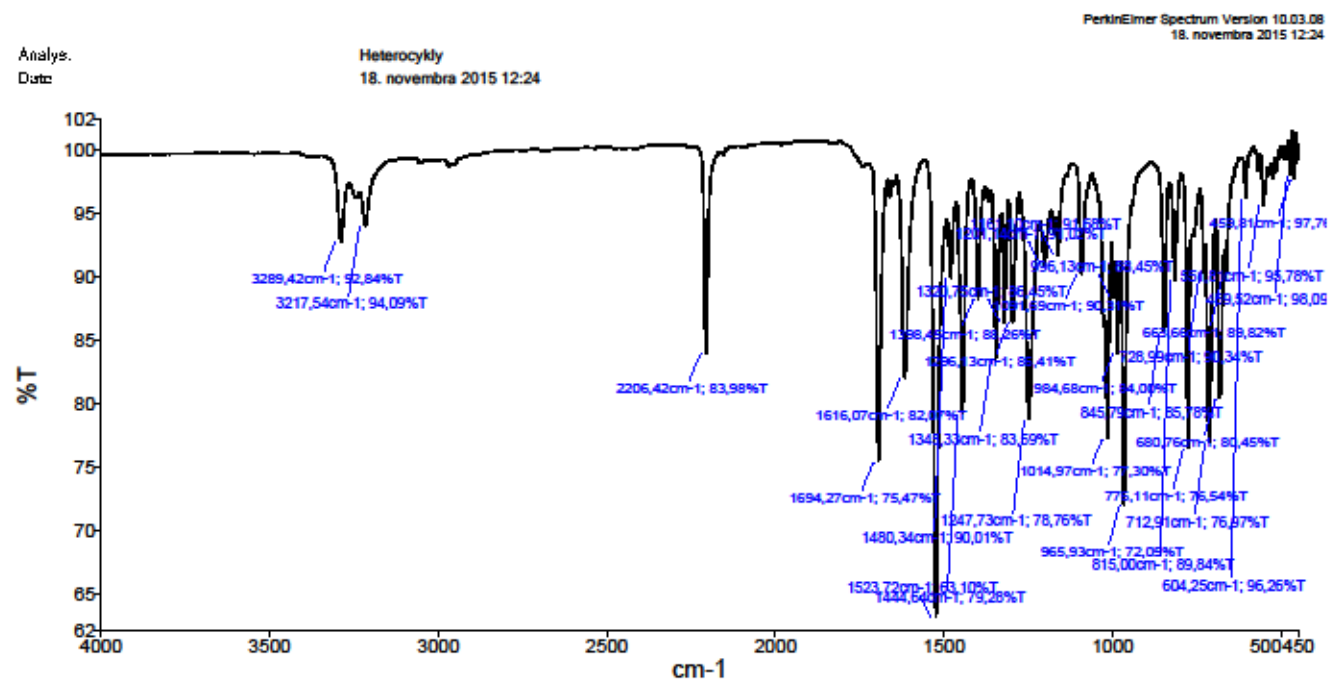
VIF ¹⁹F NMR



VIF ^{19}F - ^{13}C HSQC

VIF IR



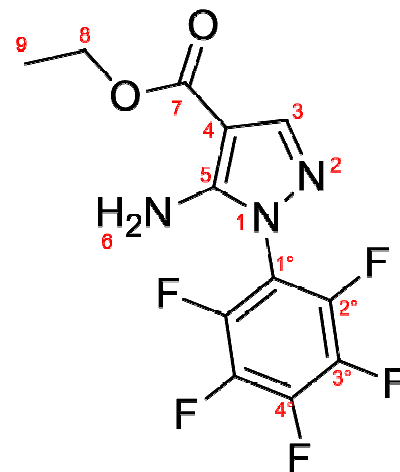


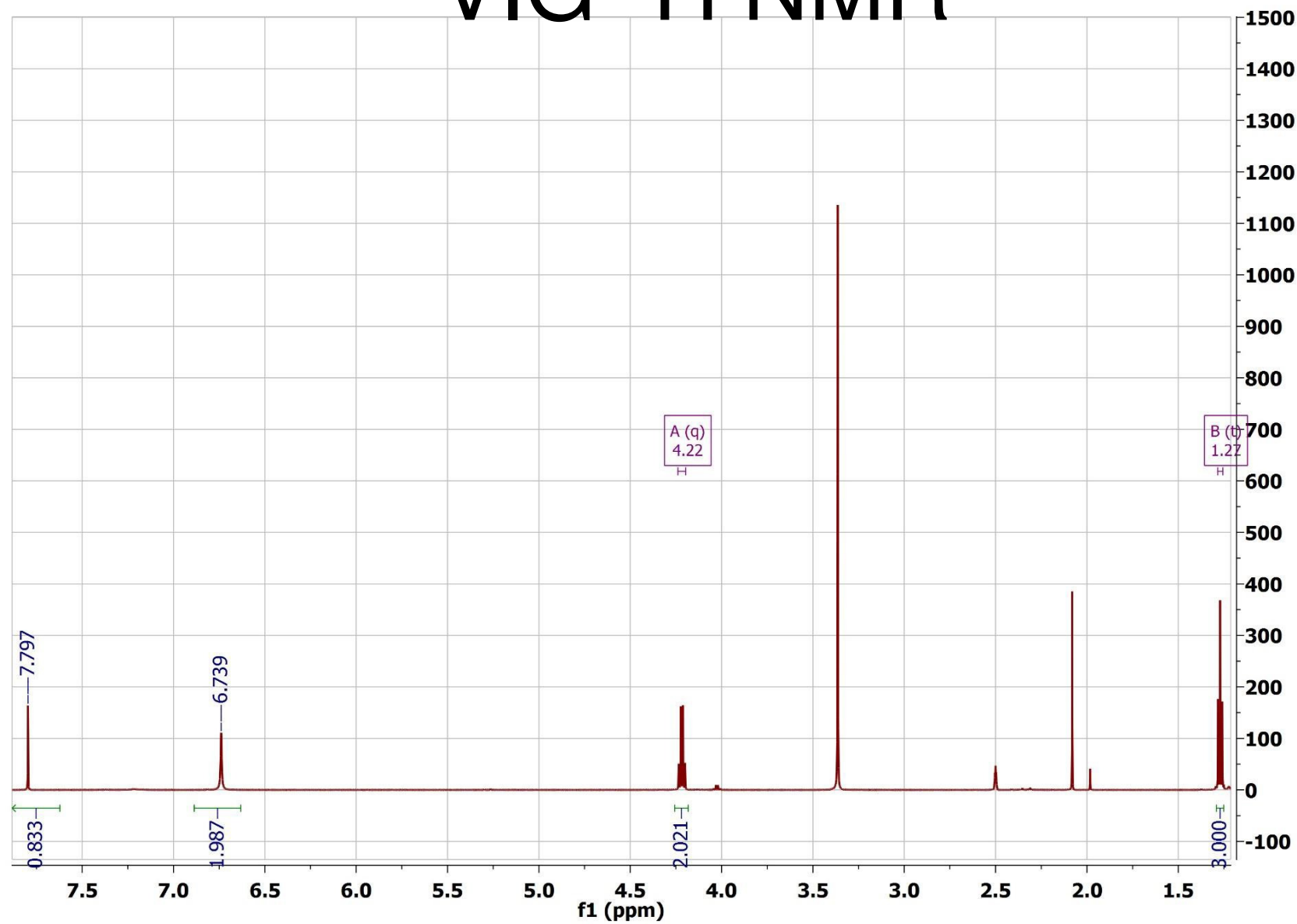
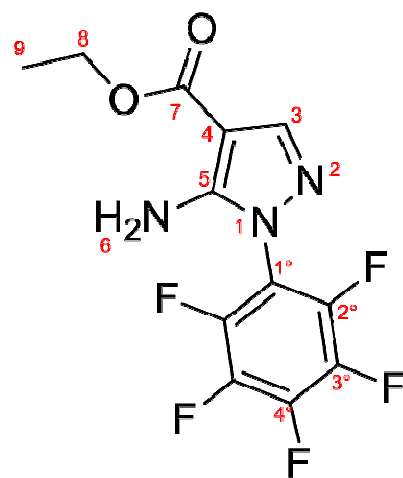
Heter 66 Sample 066 By Heter Date streda, novembra 18 2015

Source: Source Results	
Spectrum Name	Heter 66

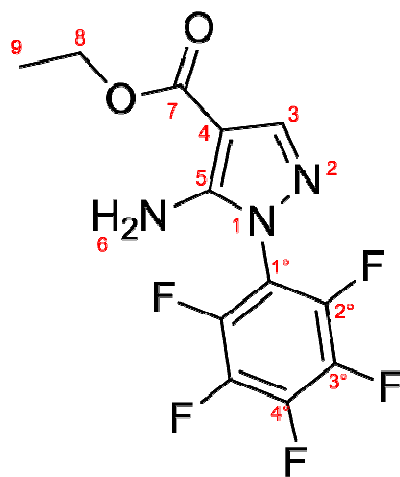
Page 1

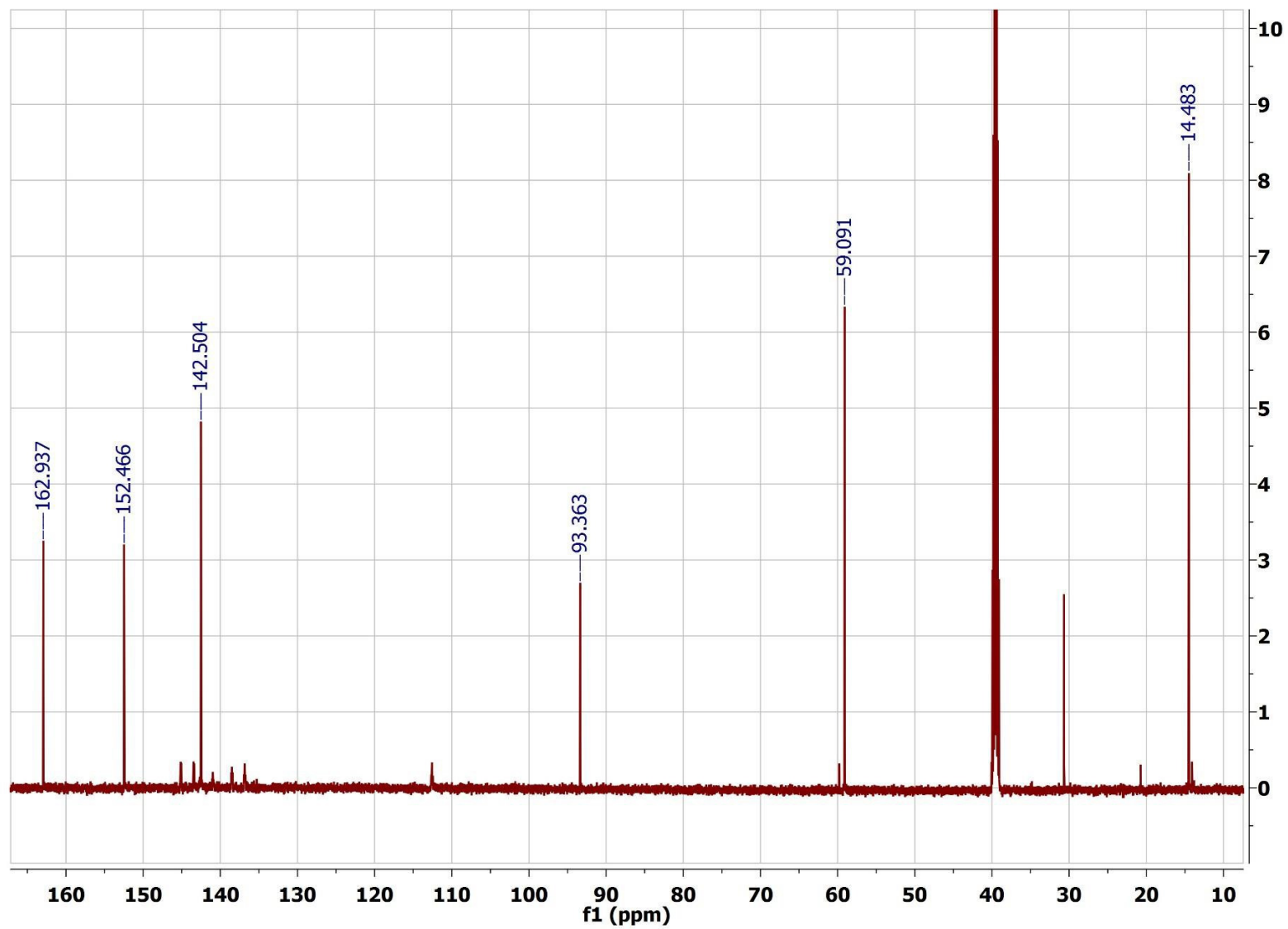
VIG



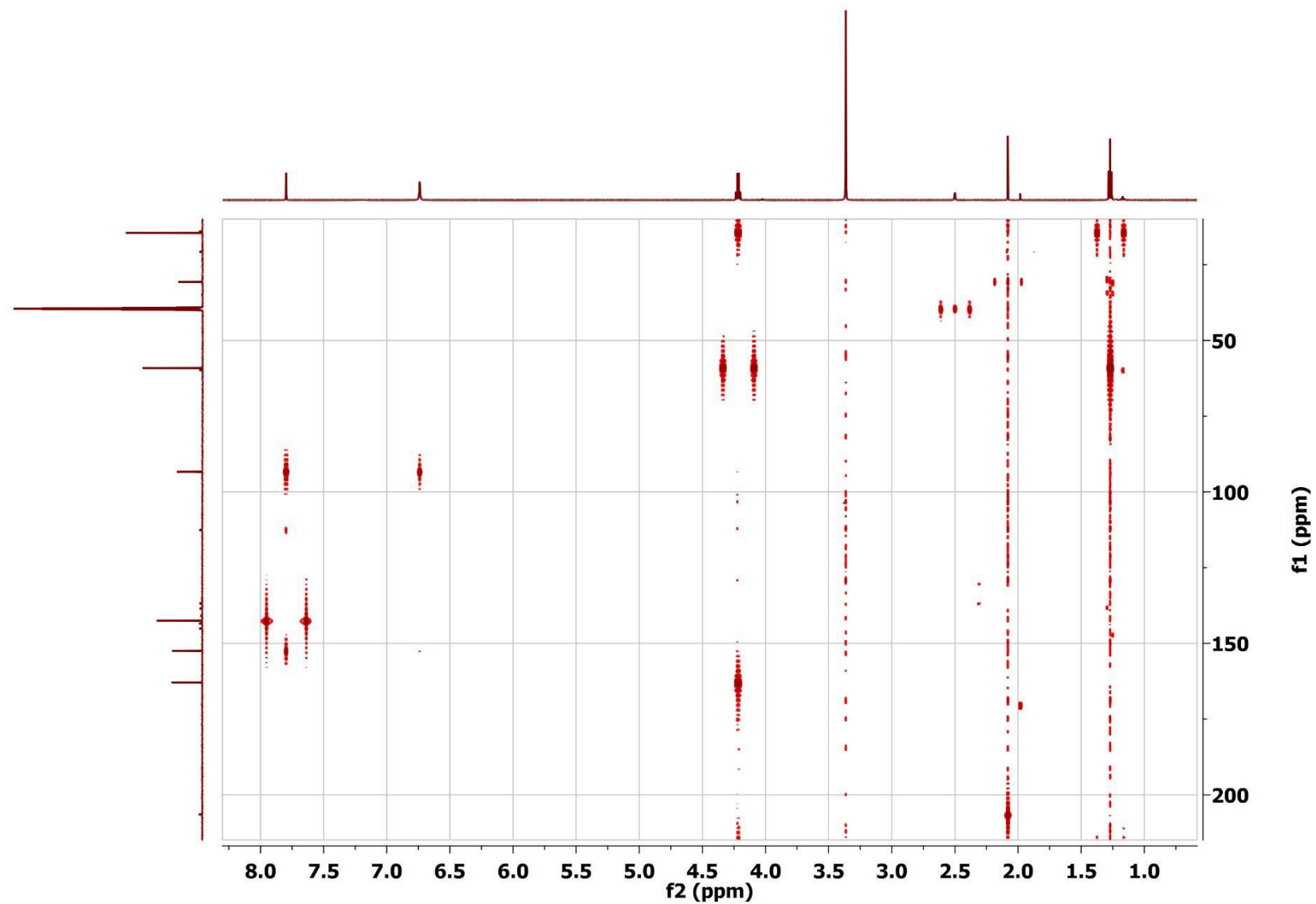
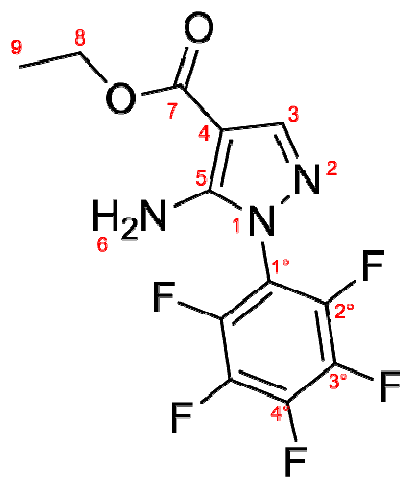
VIG ^1H NMR

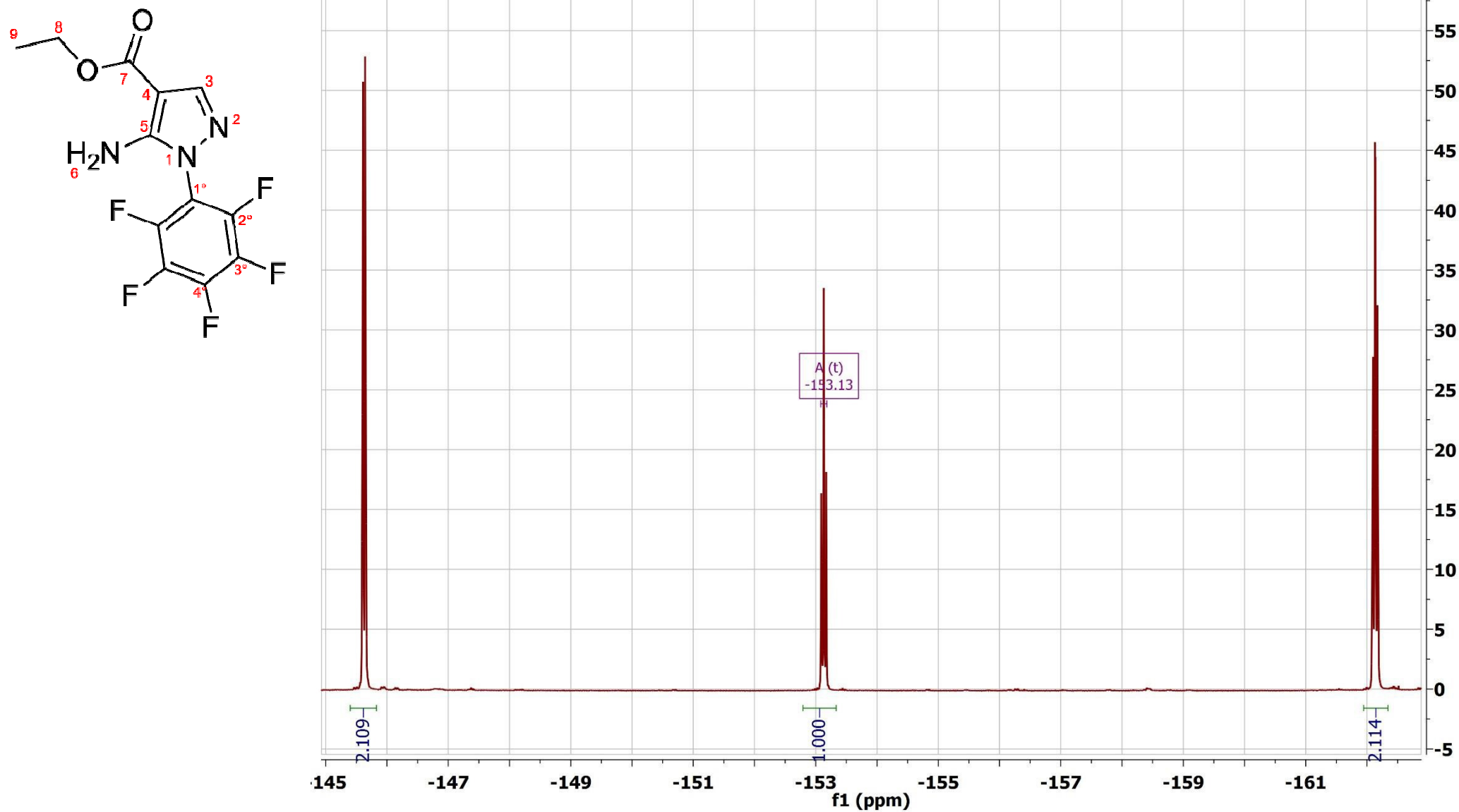
VIG ^{13}C NMR



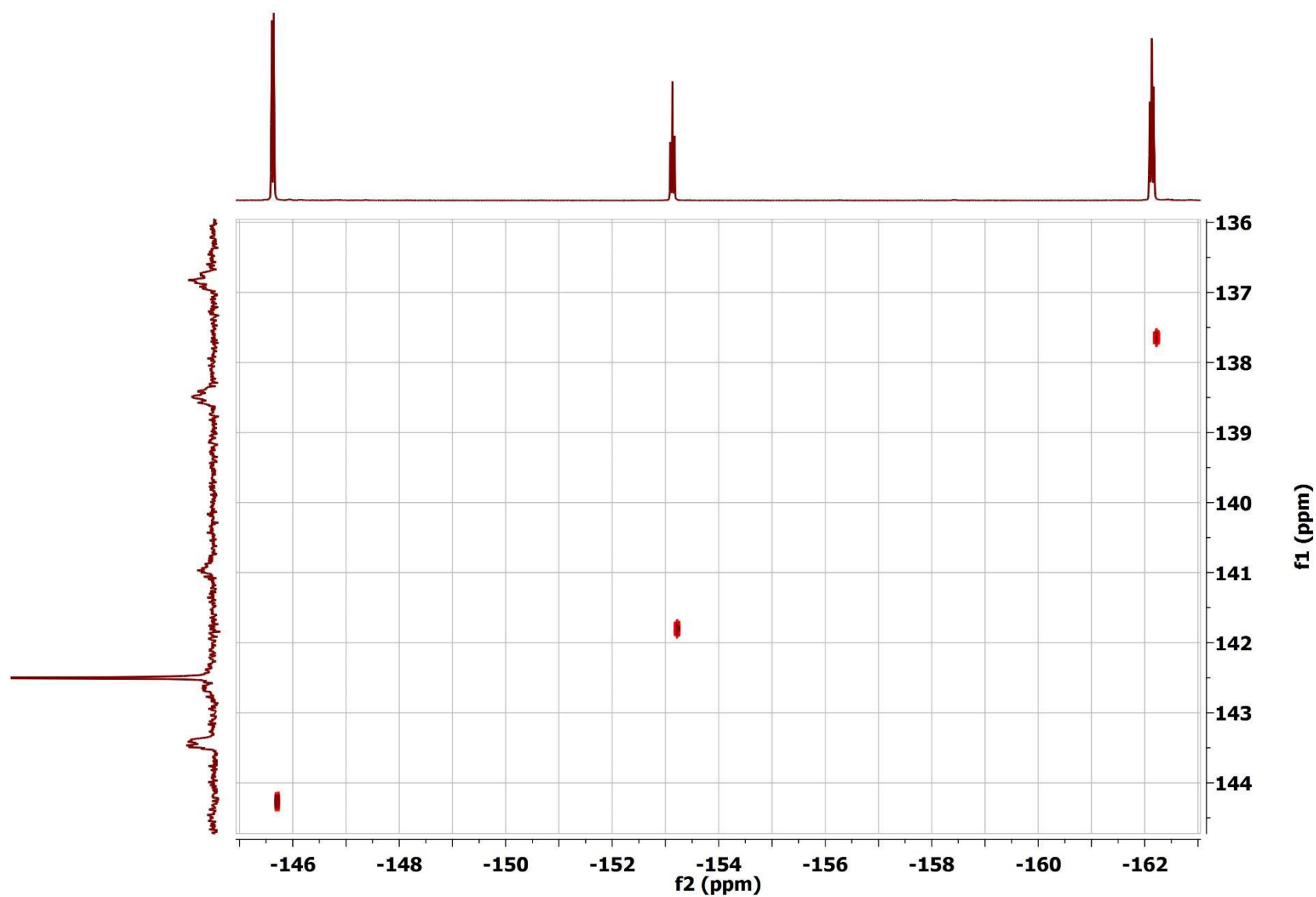
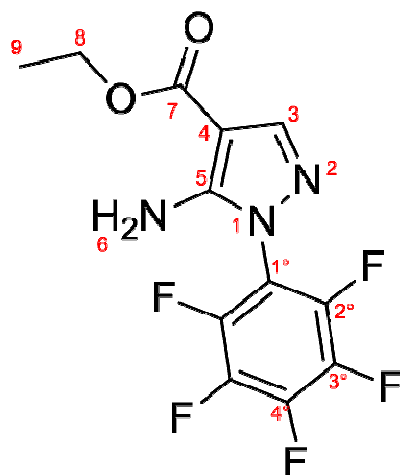


VIG ^1H - ^{13}C HMBC

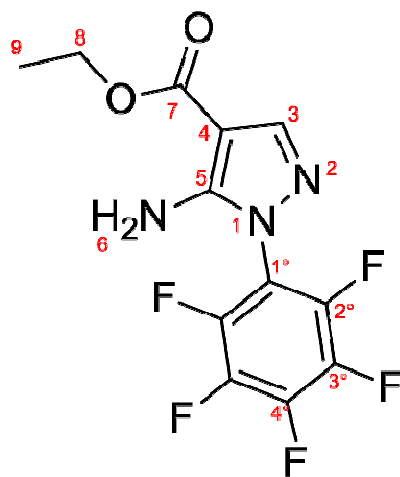


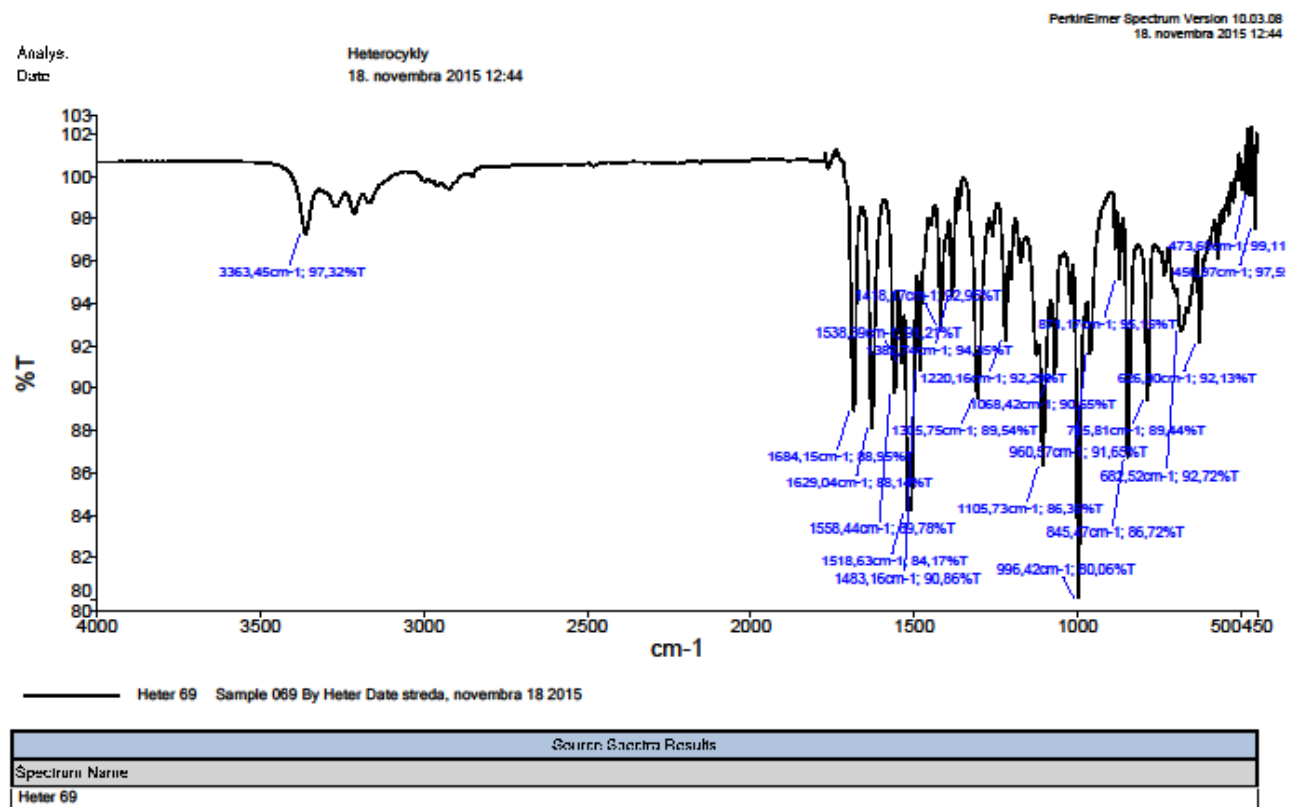
VIG ^{19}F NMR

VIG ^{19}F - ^{13}C HSQC



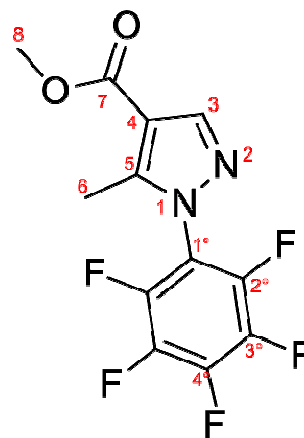
VIG IR

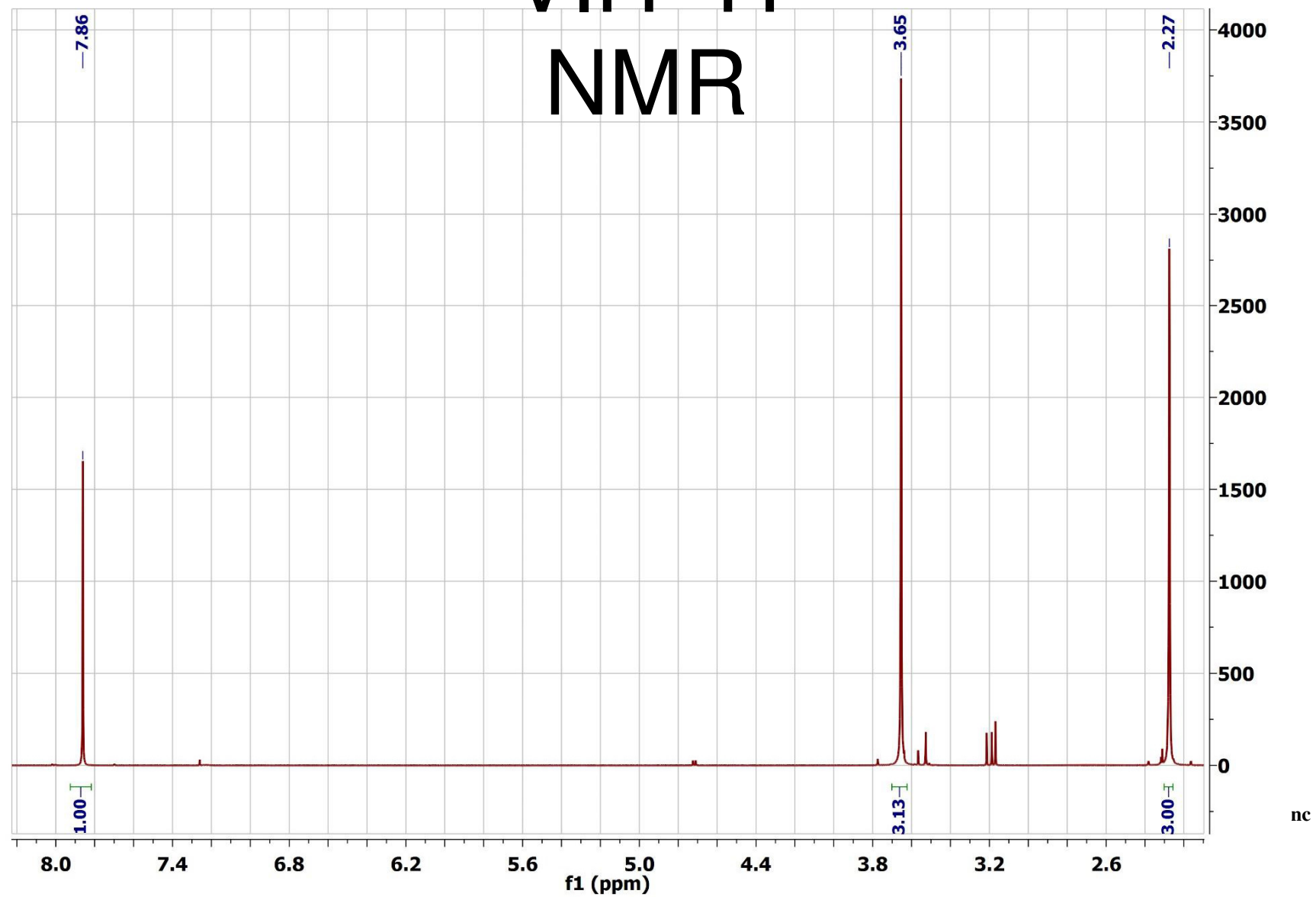
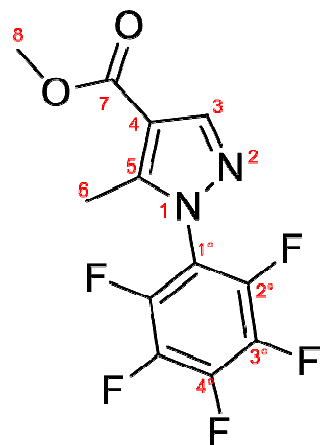


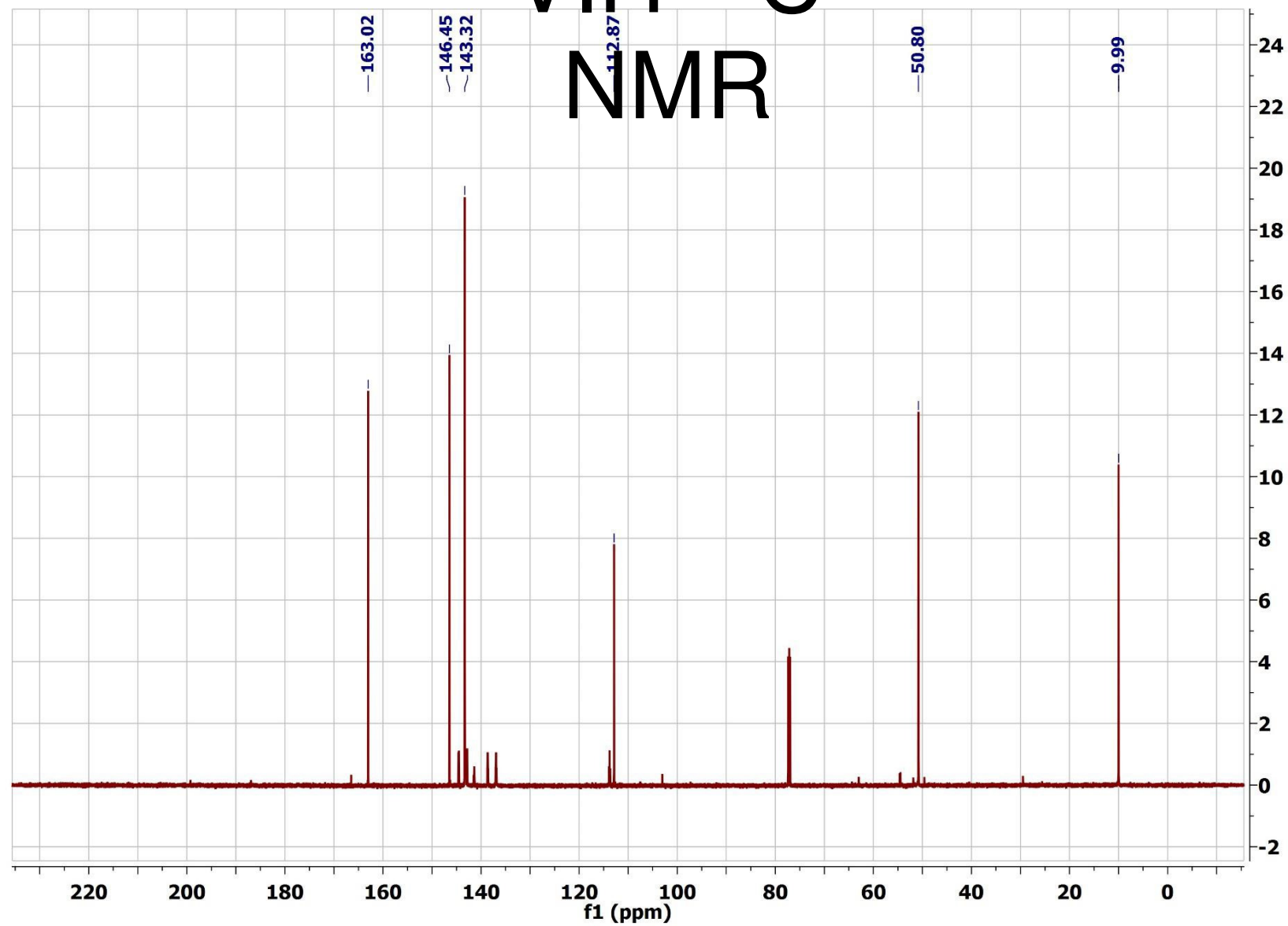
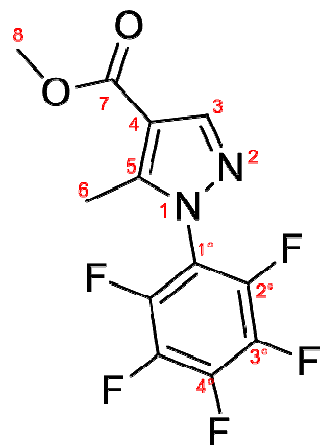


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VIH

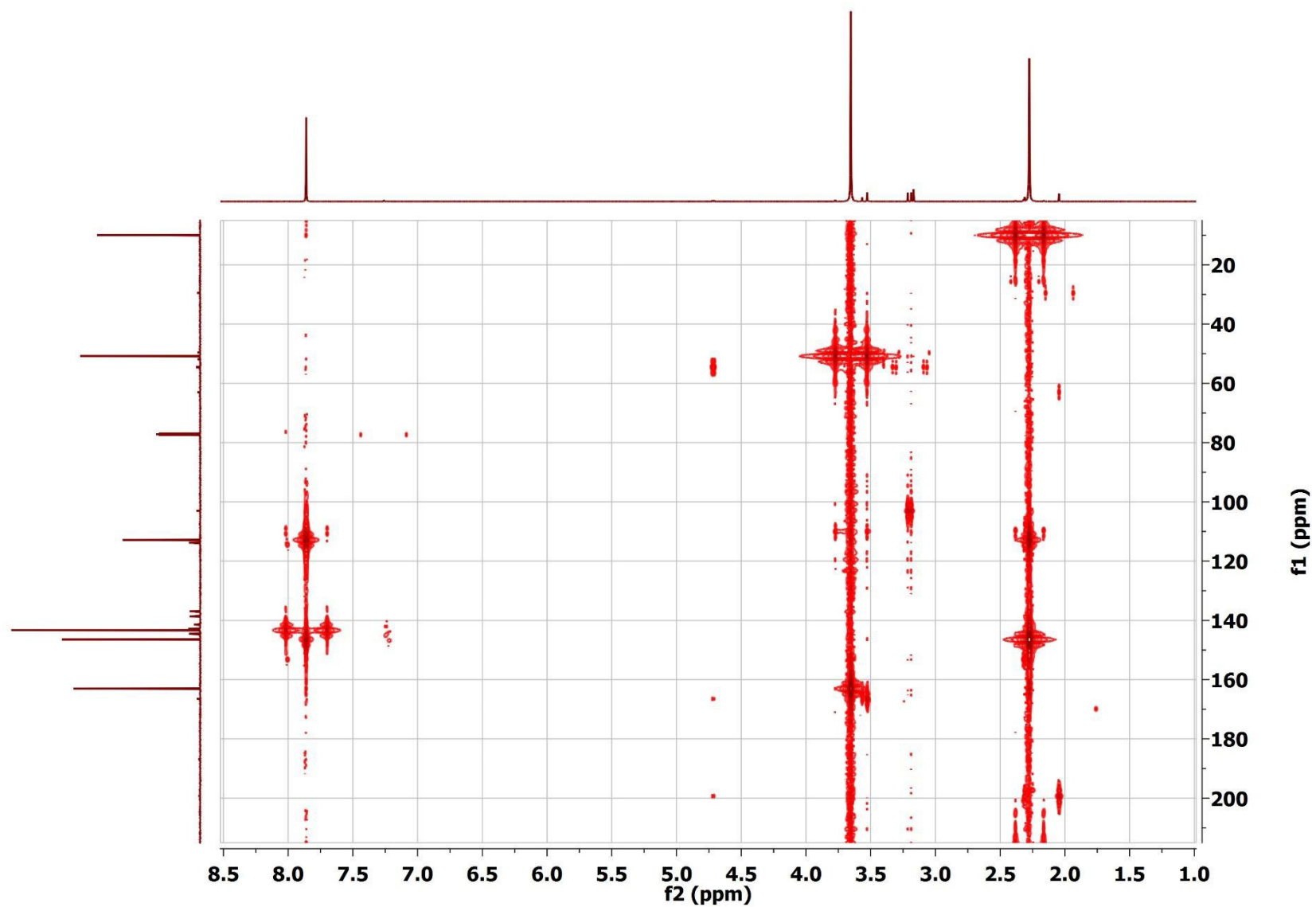
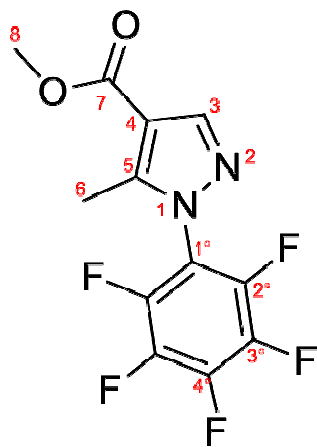


VIH ^1H
NMR

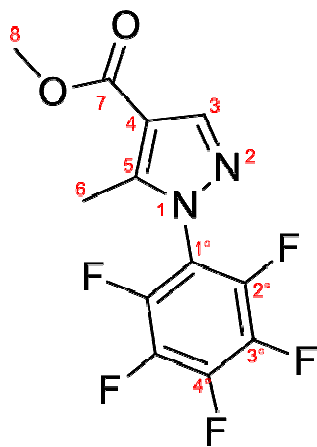
VIH ^{13}C
NMR

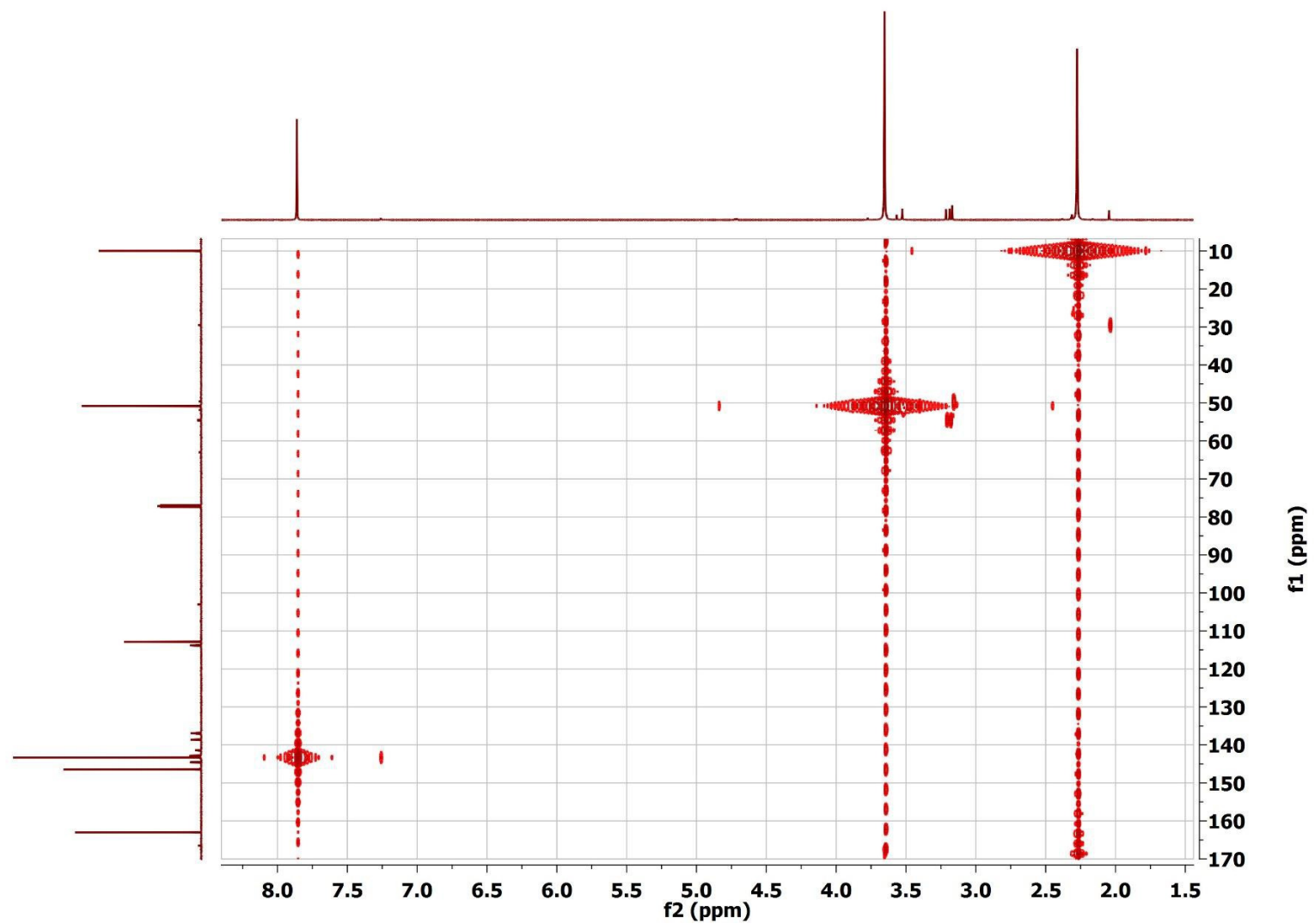
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VIH ^1H - ^{13}C HMBC

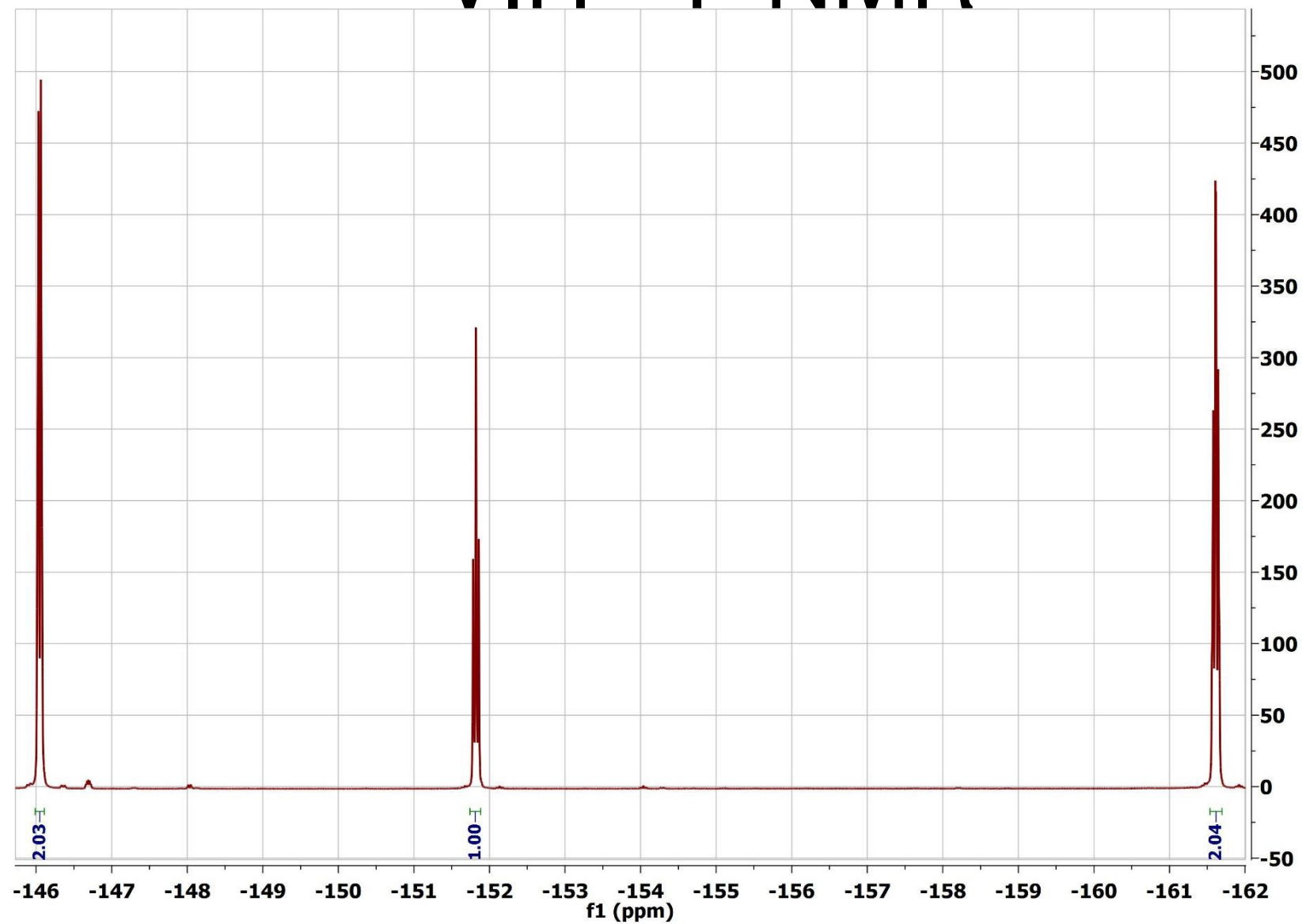
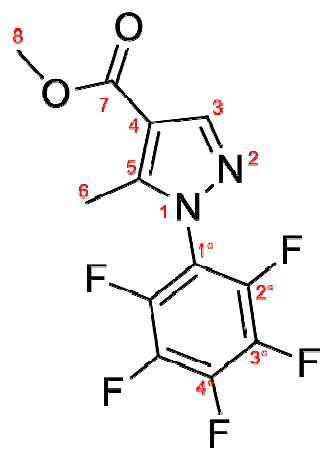


VIH ^1H - ^{13}C HSQC

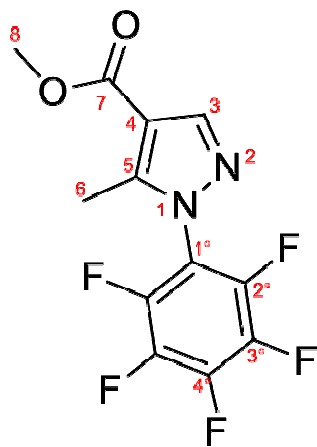


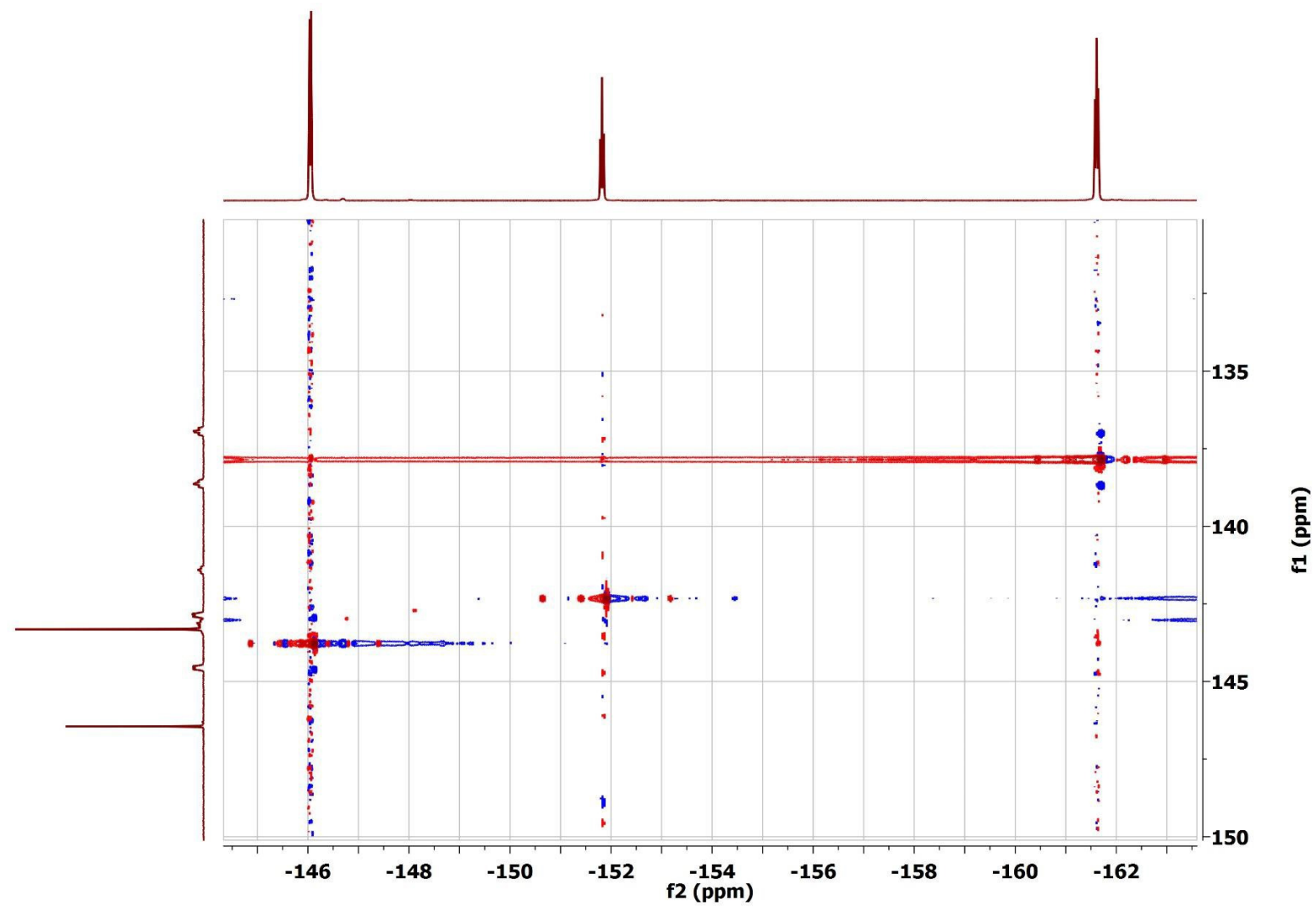


VIH ^{19}F NMR

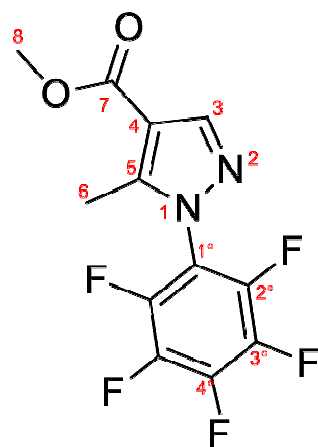


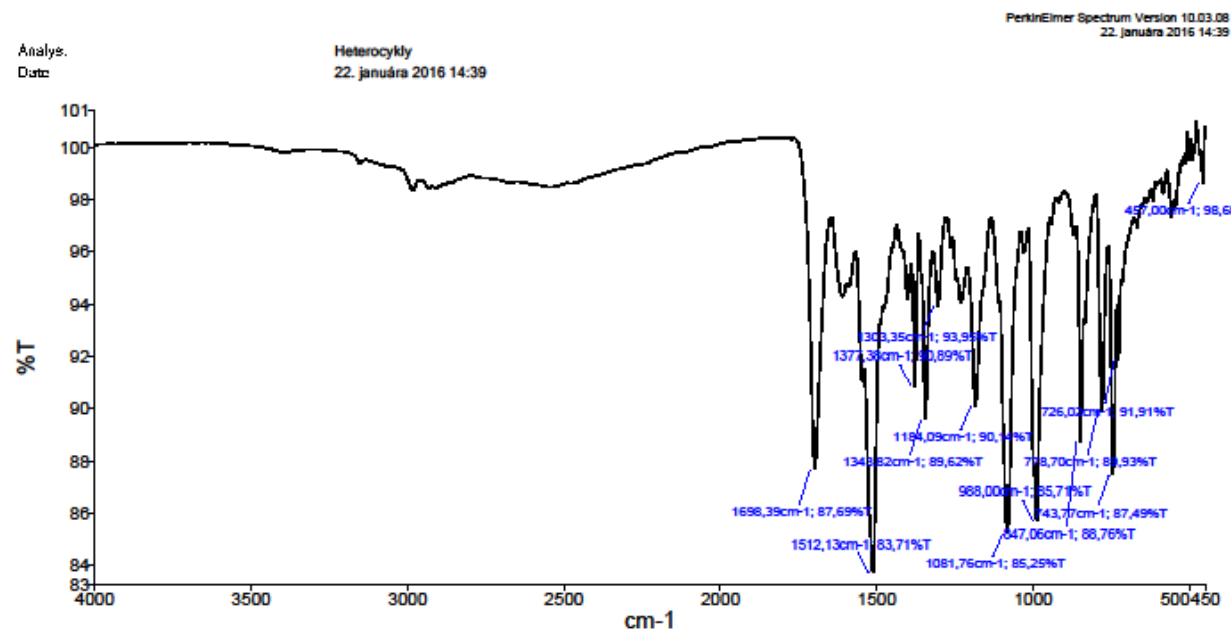
VIH ^{19}F - ^{13}C HSQC





VIH IR



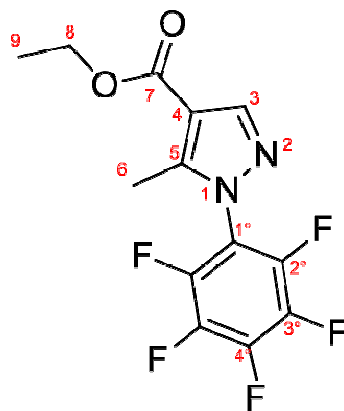


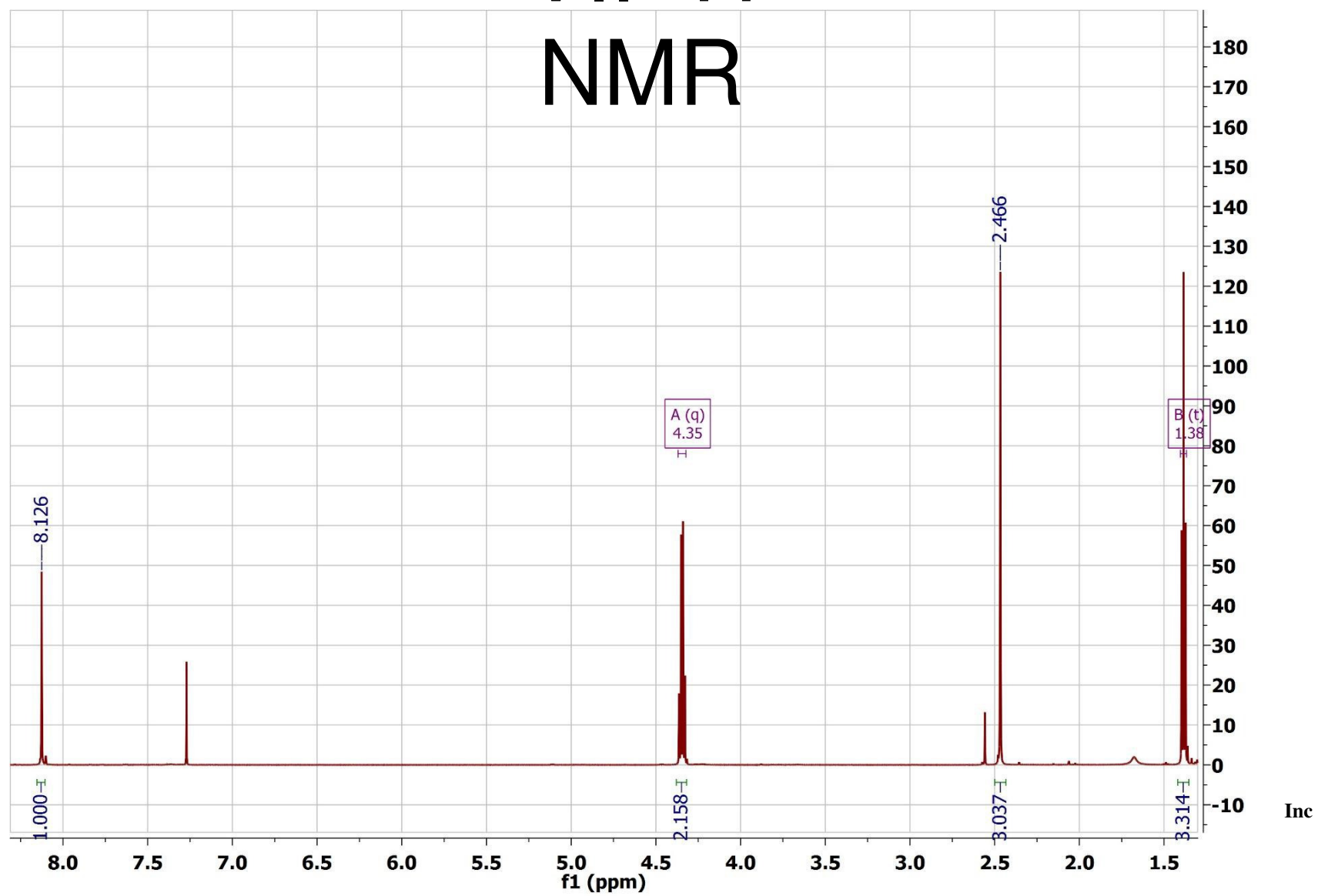
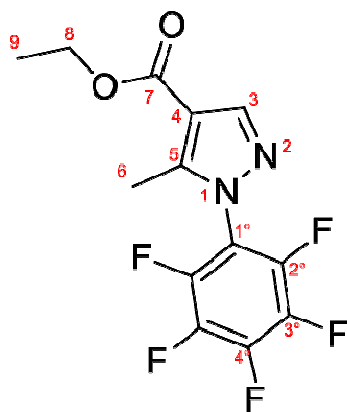
Heter 81 Sample 081 By Heter Date piatok, januára 22 2016

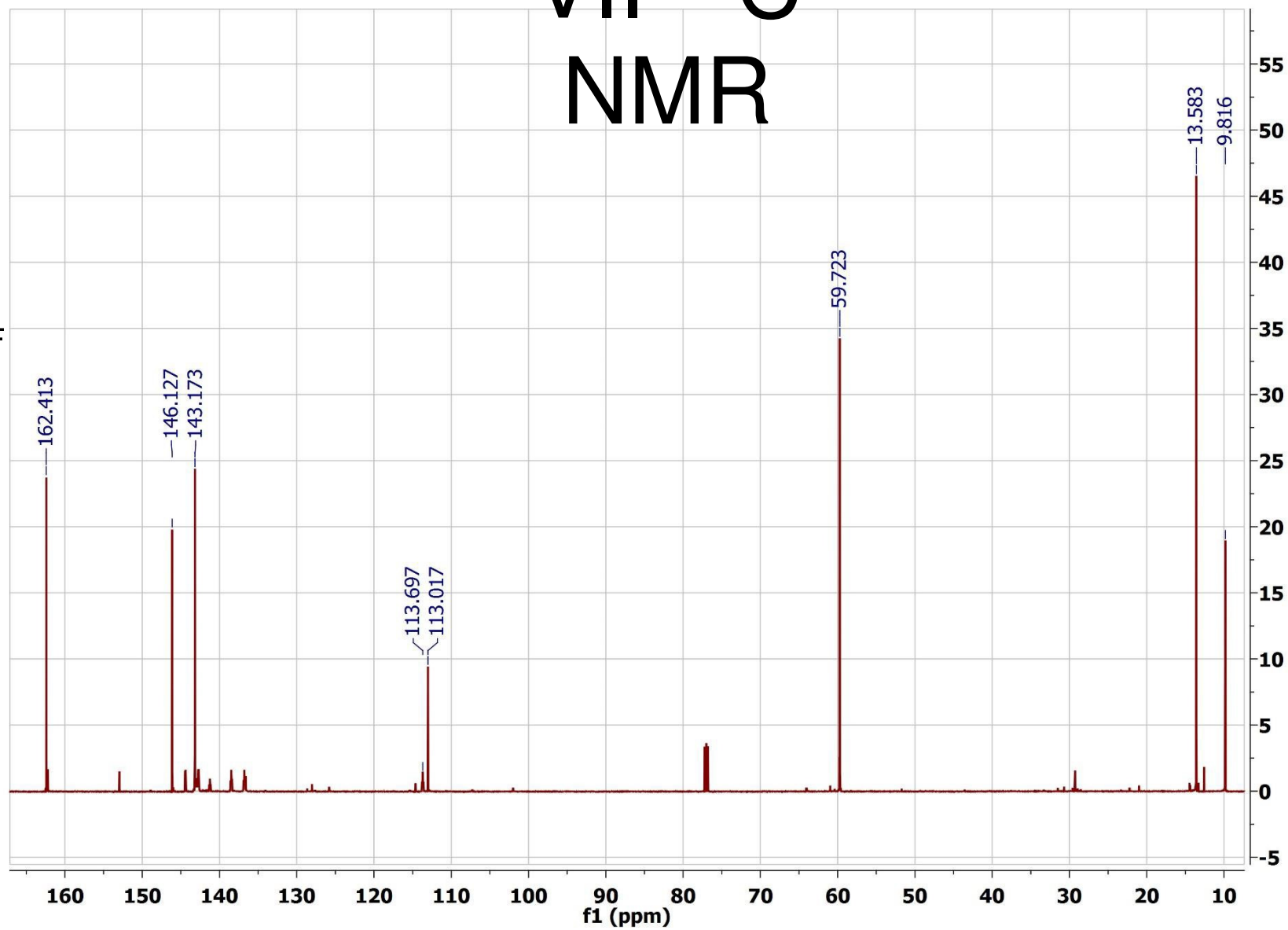
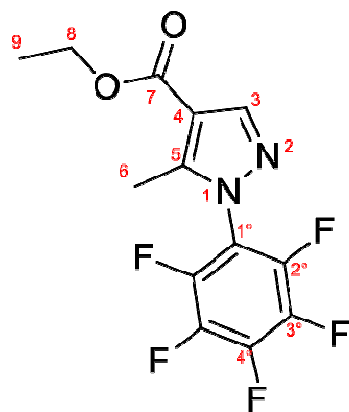
Source: Source Results	
Spectrum Name	Heter 81

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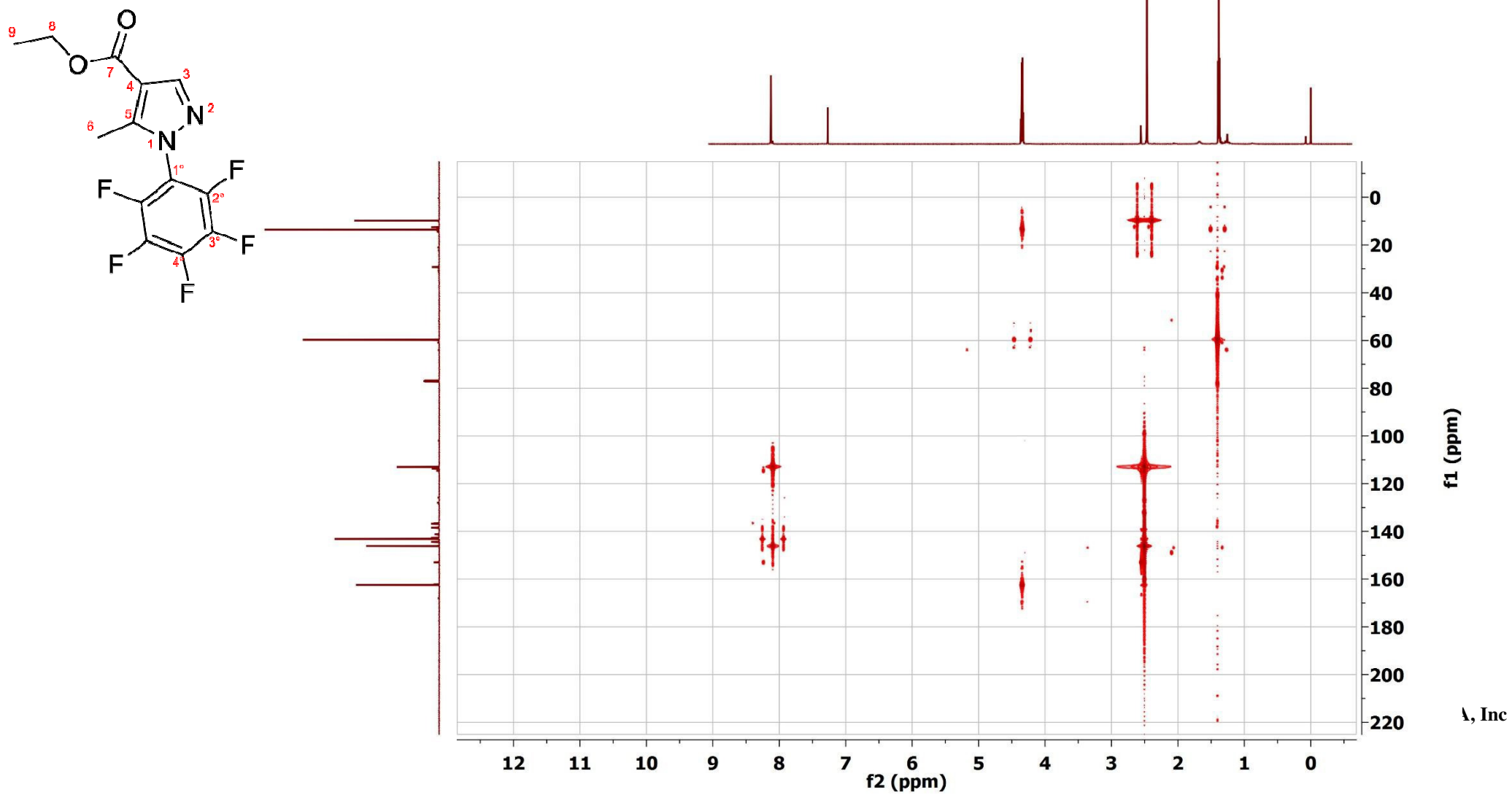
VII



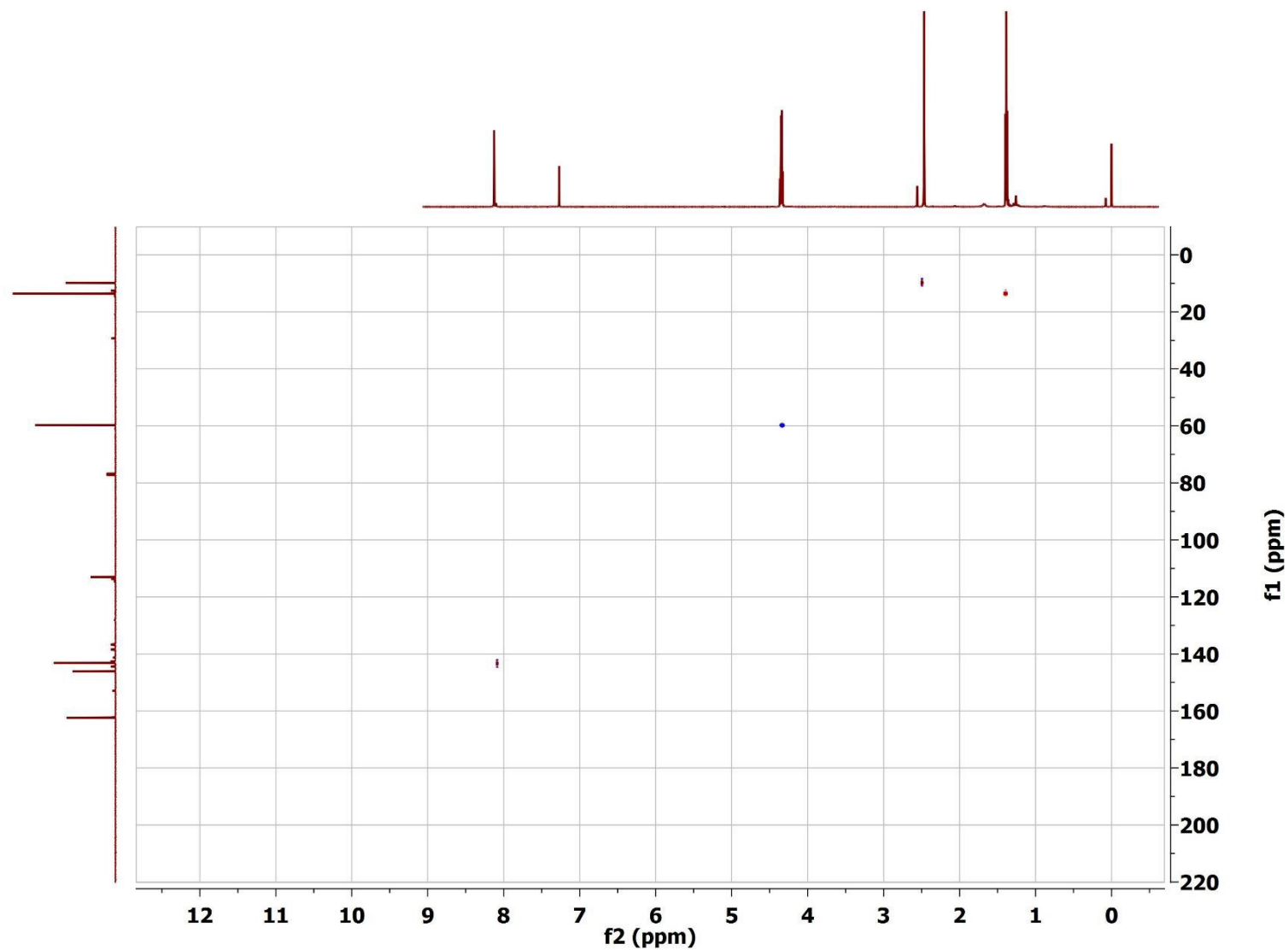
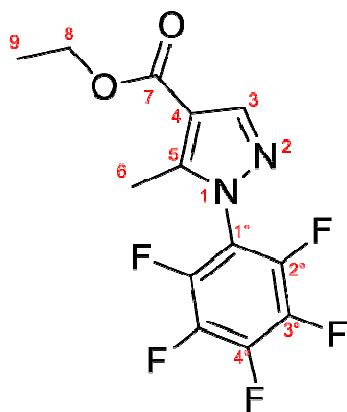
VII ^1H
NMR

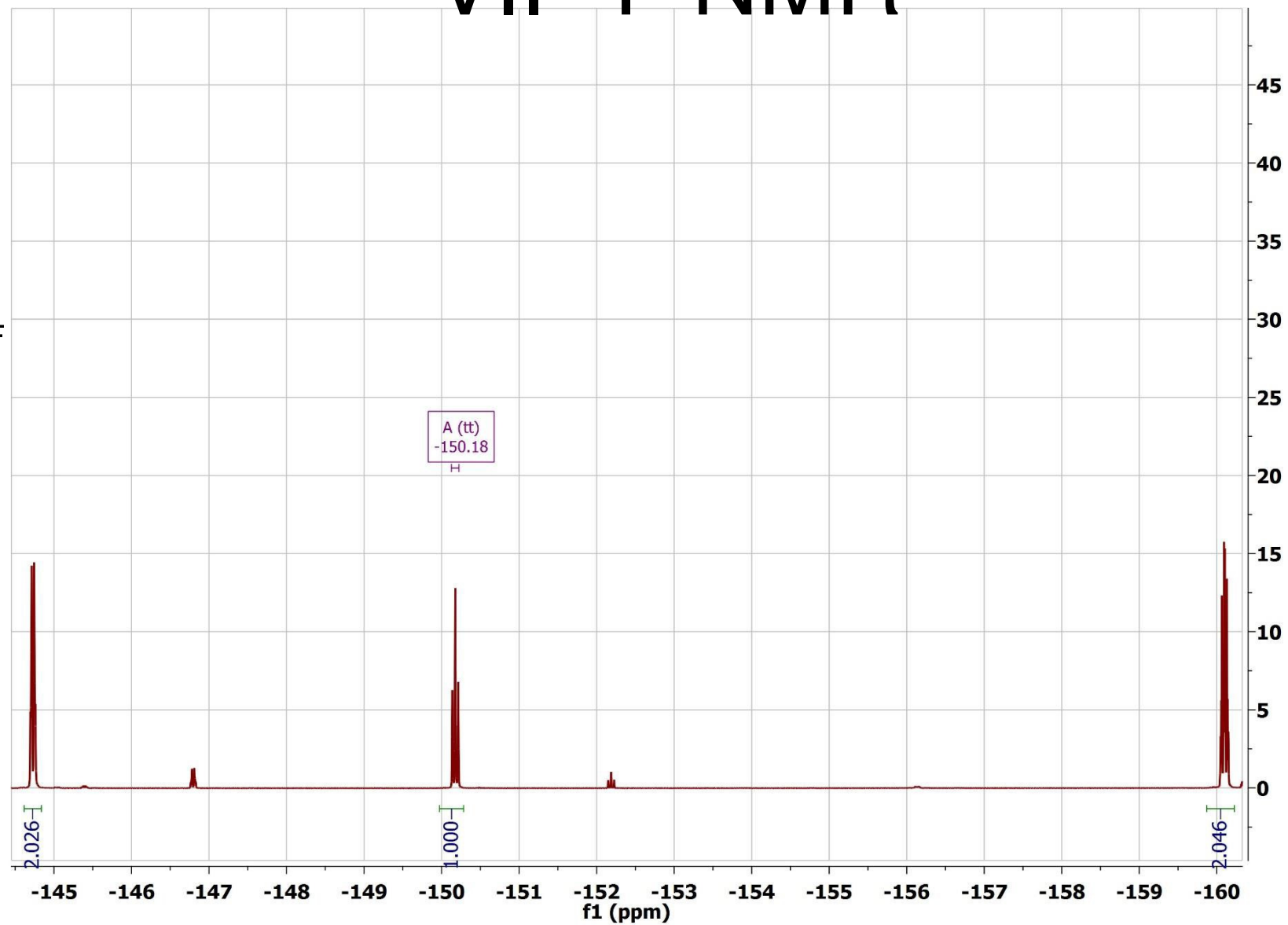
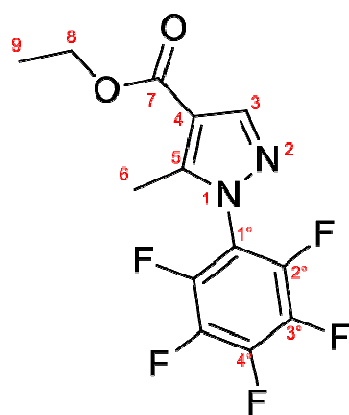
VII ^{13}C
NMR

nc

VII ^1H - ^{13}C HMBC

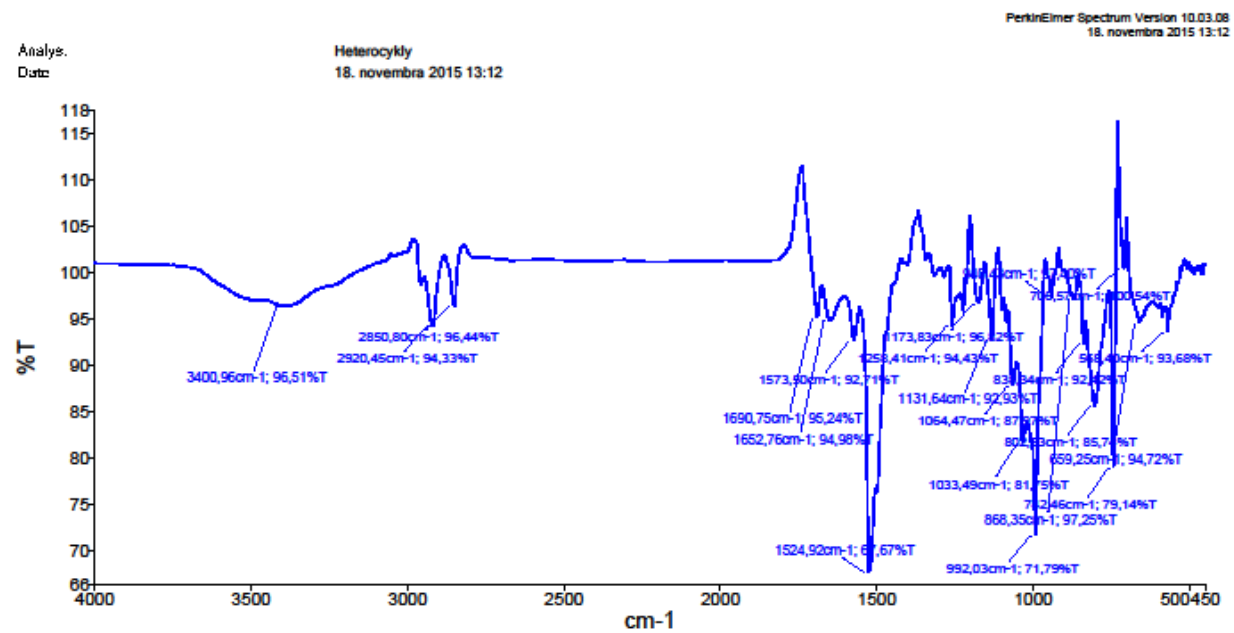
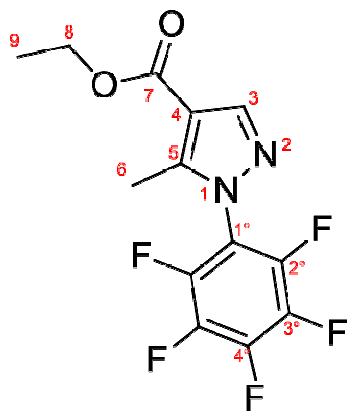
VII ^1H - ^{13}C HSQC



VII ^{19}F NMR

nc

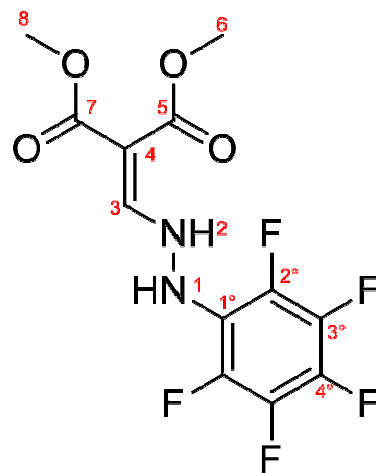
VII IR

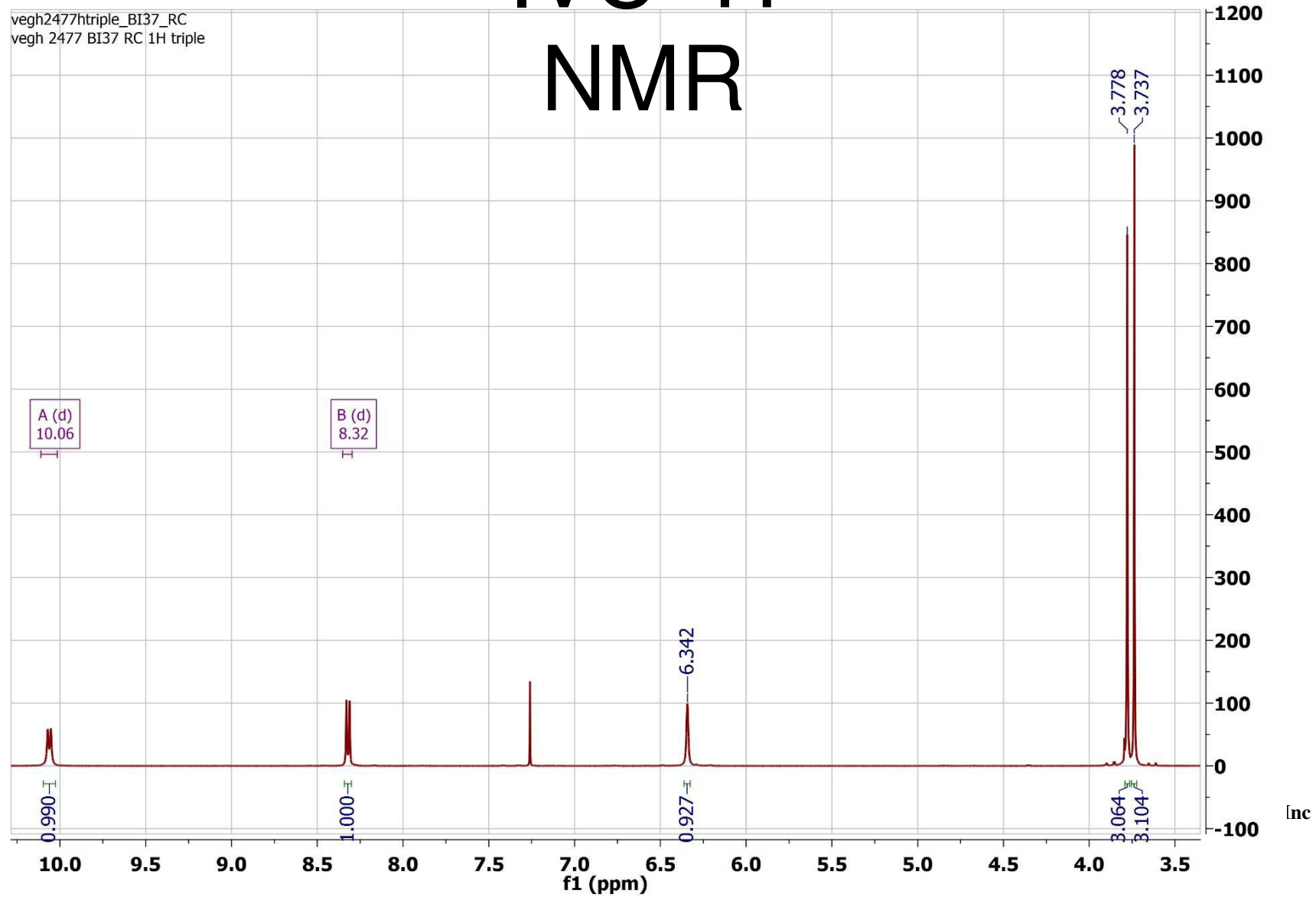
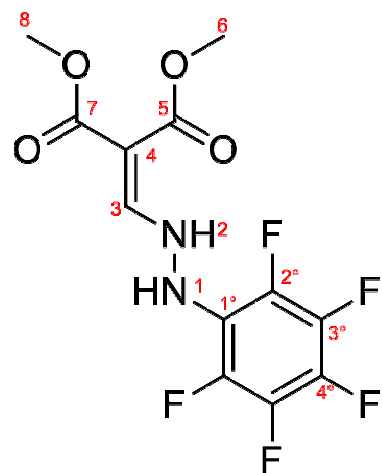


Heter 73 Sample 073 By Heter Date streda, novembra 18 2015

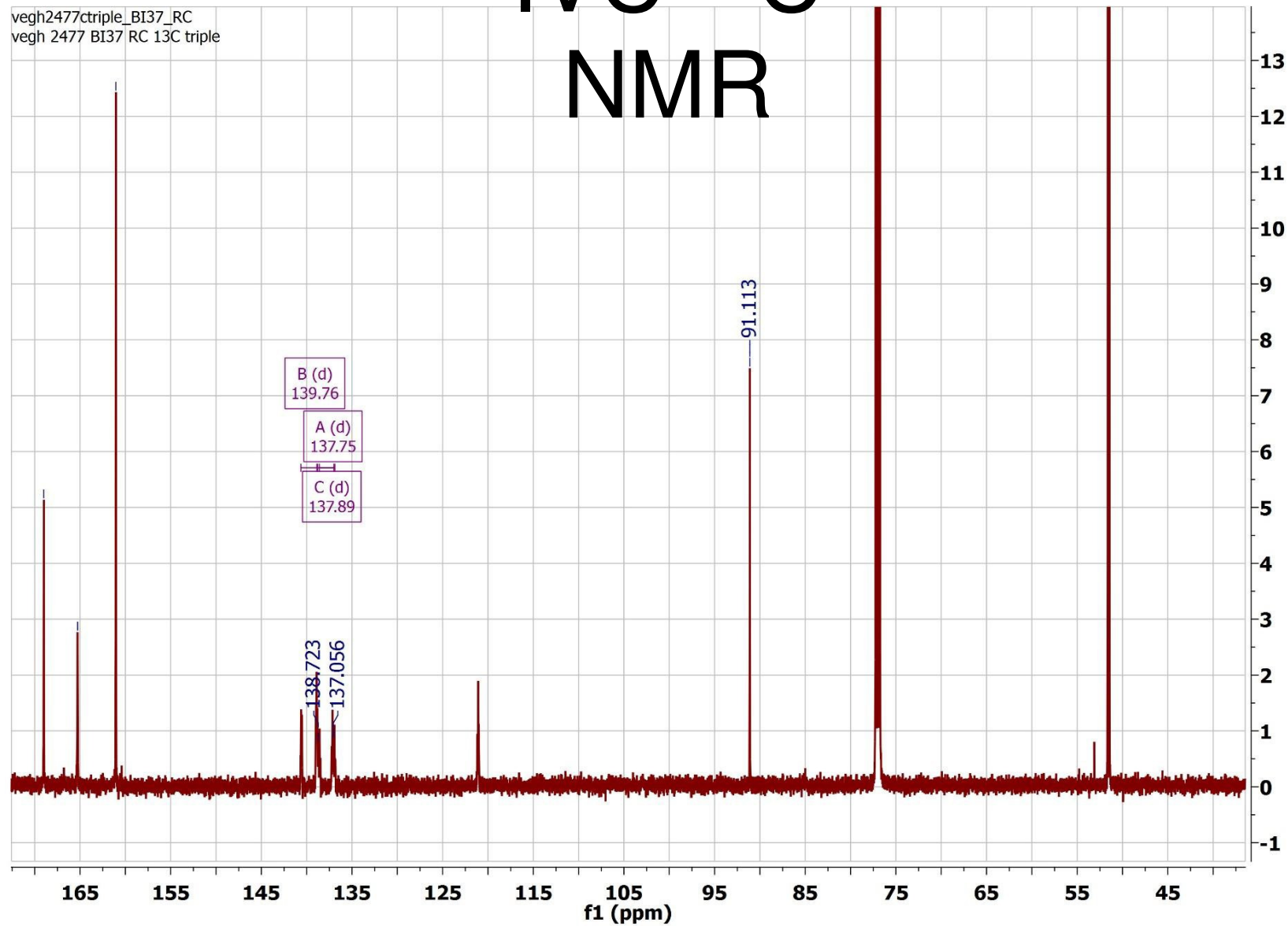
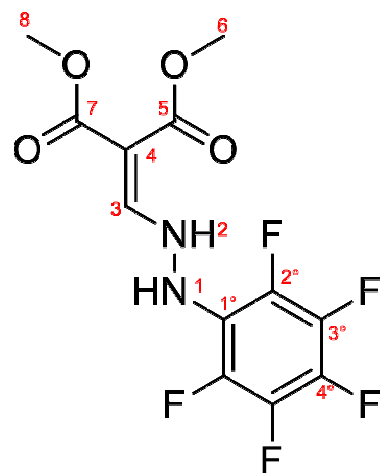
Source: Source Results	
Spectrum Name	
Heter 73	

IVC



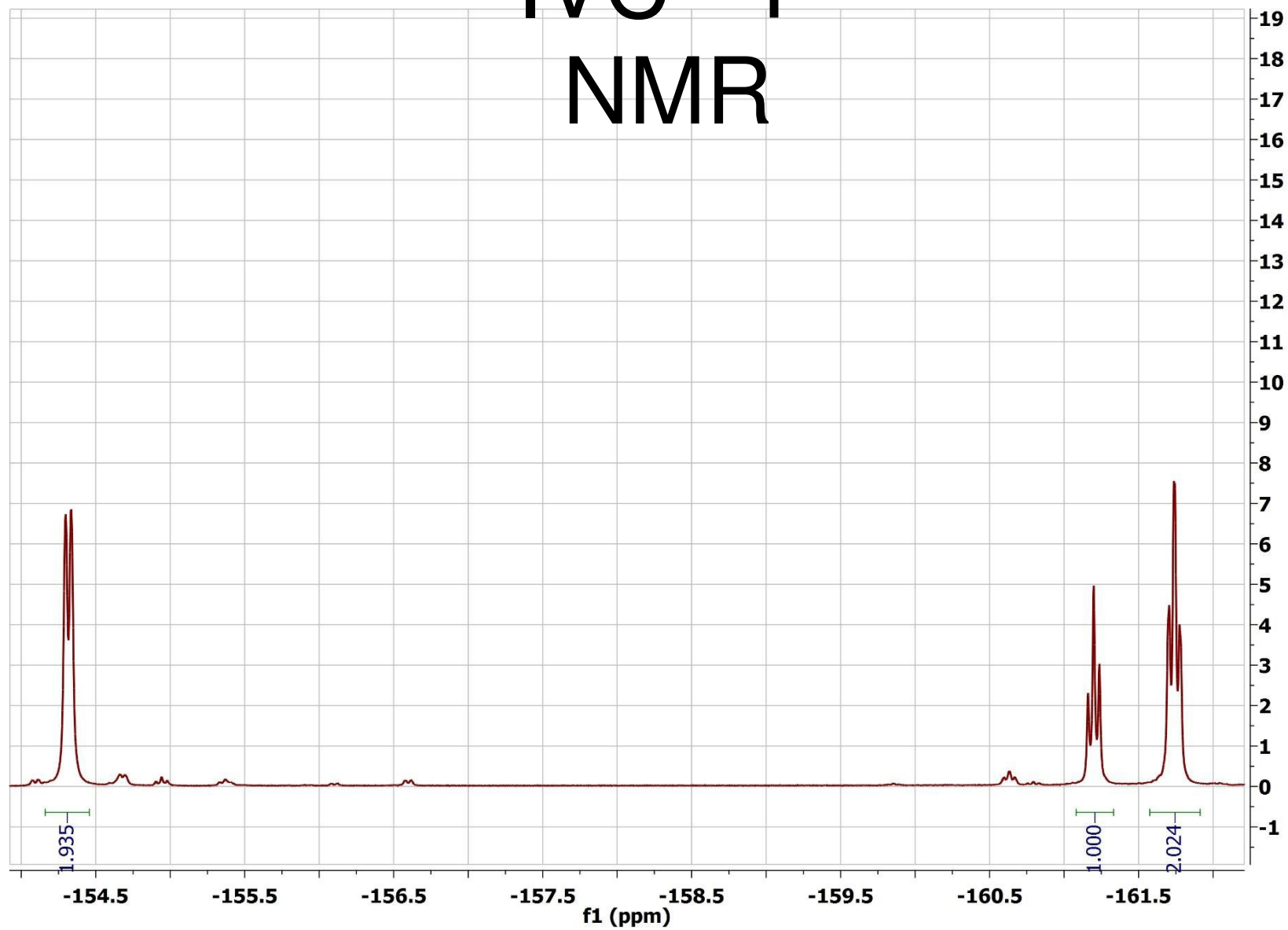
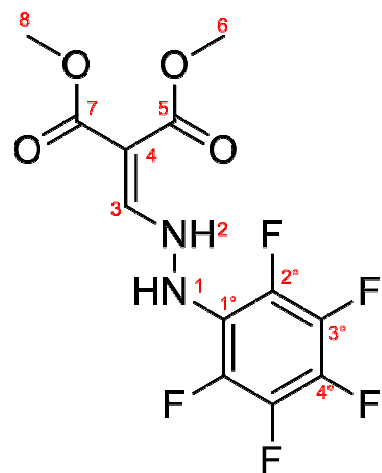
IVC ¹H
NMR

IVC ¹³C NMR

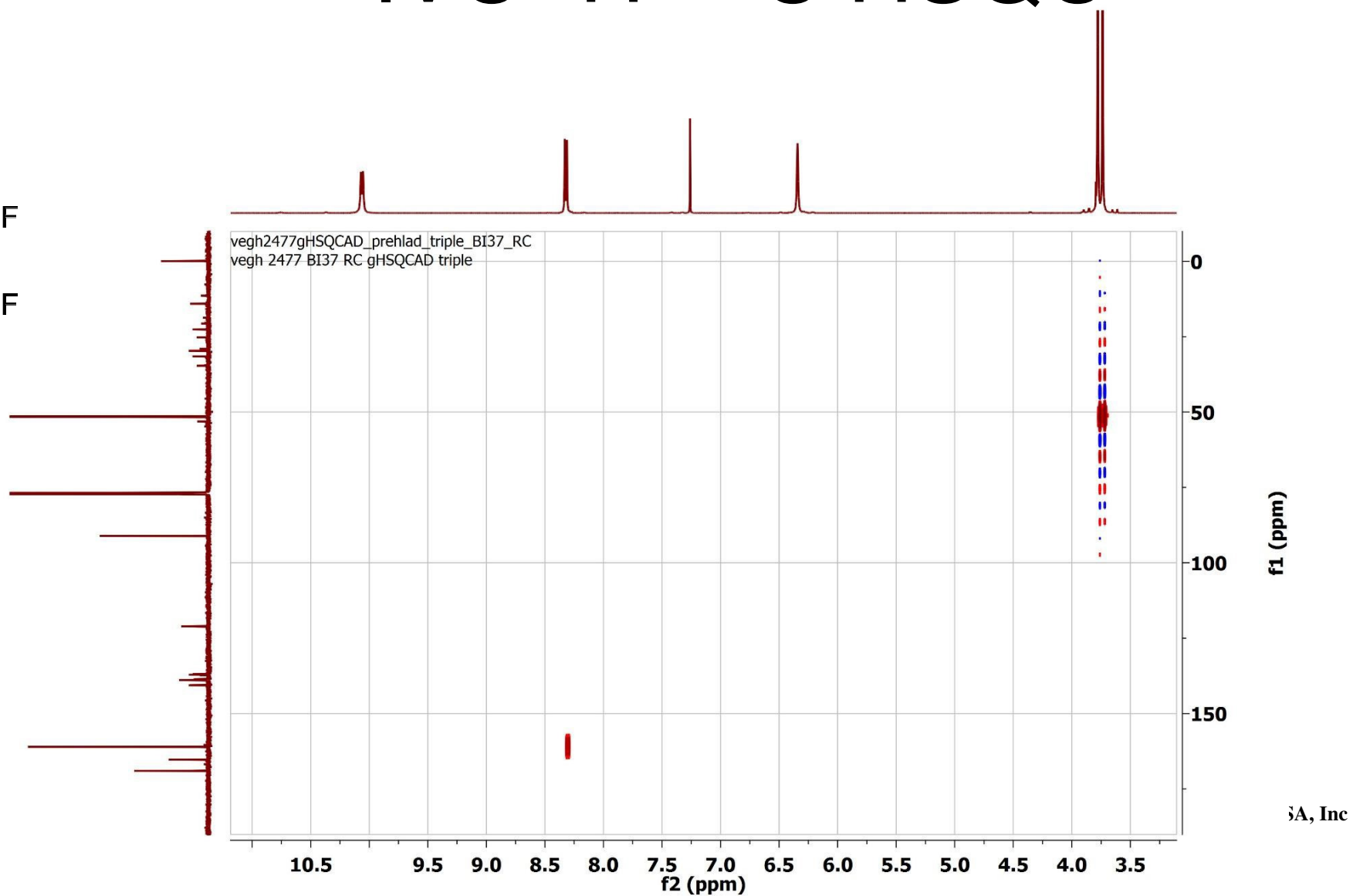
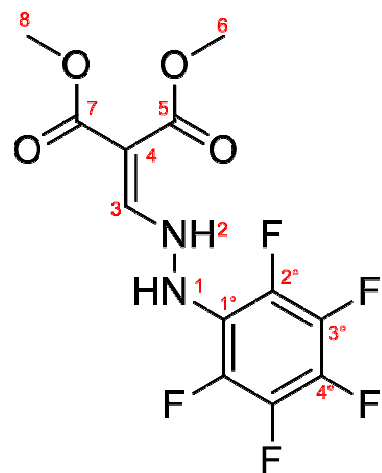


nc

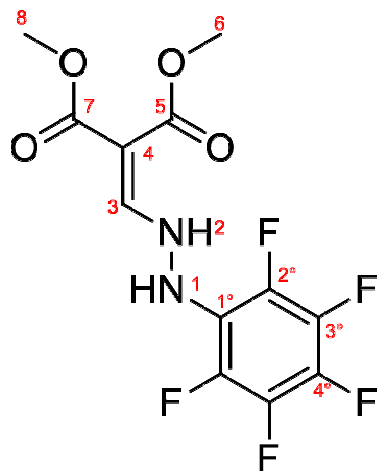
IVC ¹⁹F NMR

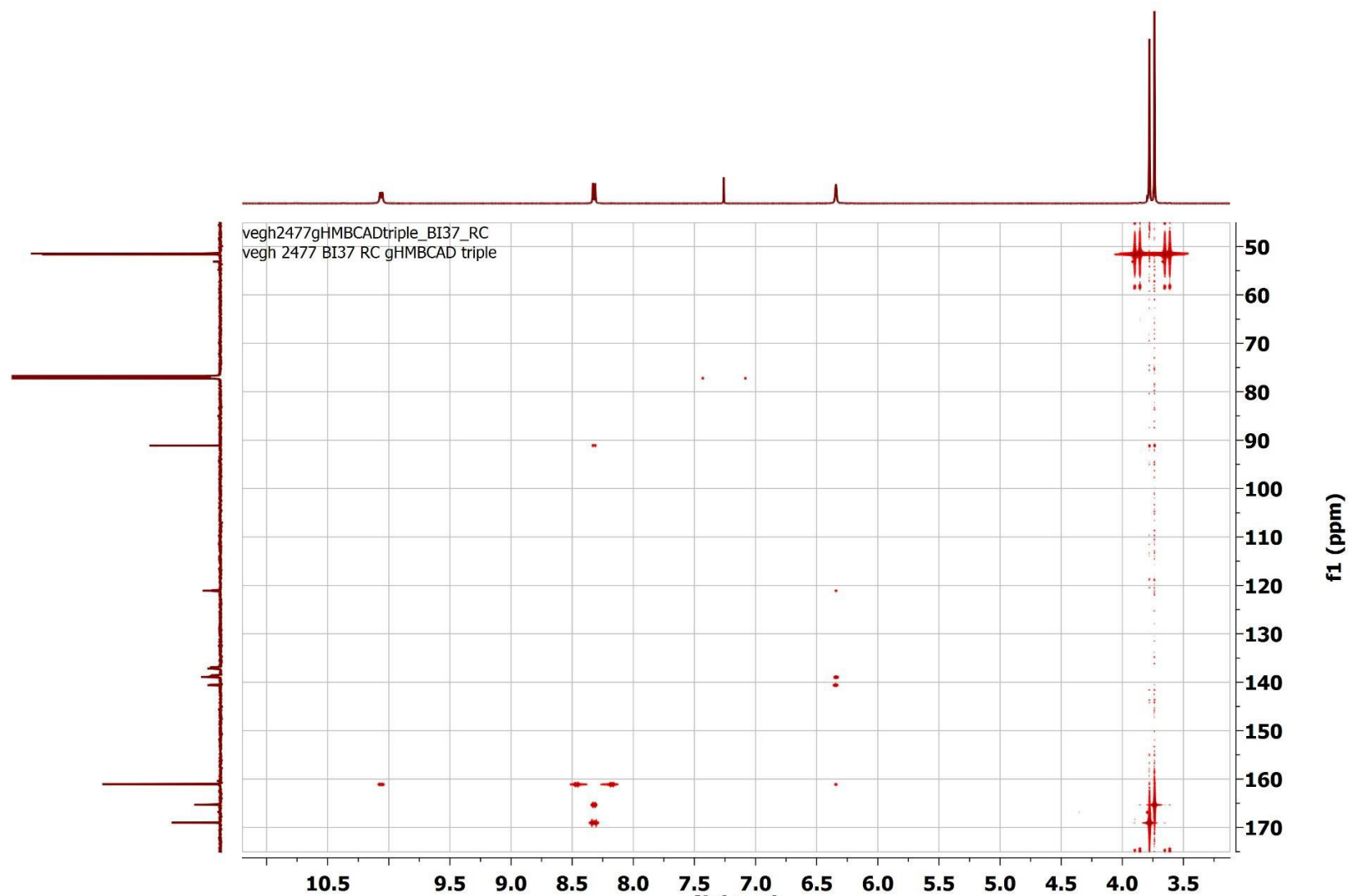


IVC ^1H - ^{13}C HSQC

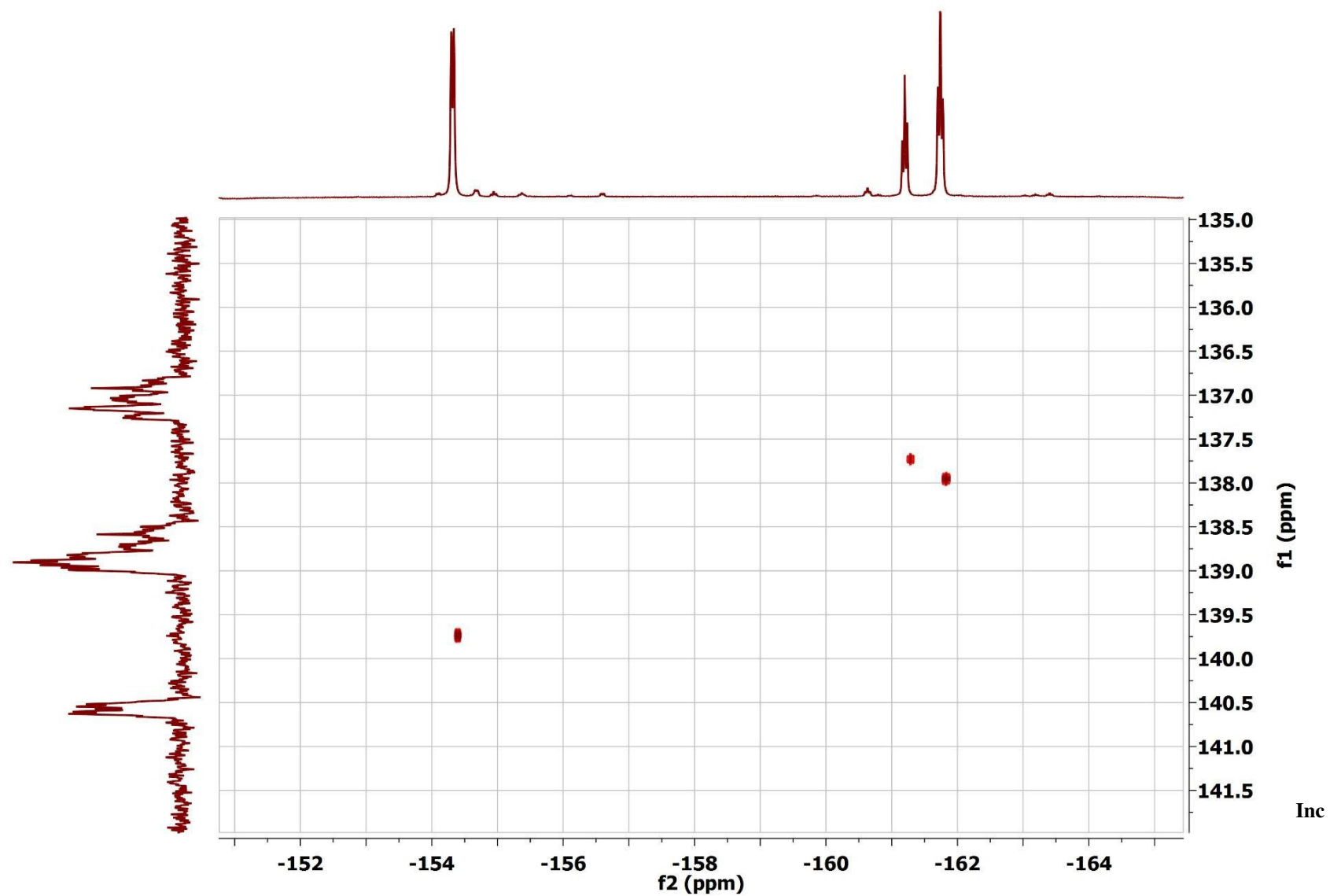
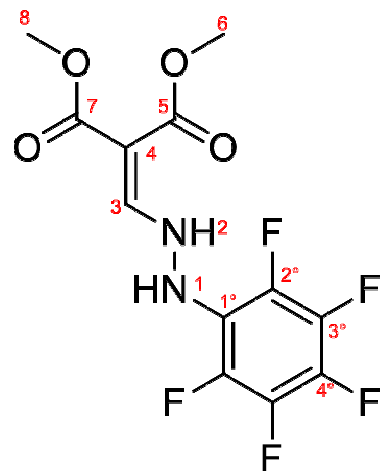


IVC ^1H - ^{13}C HMBC

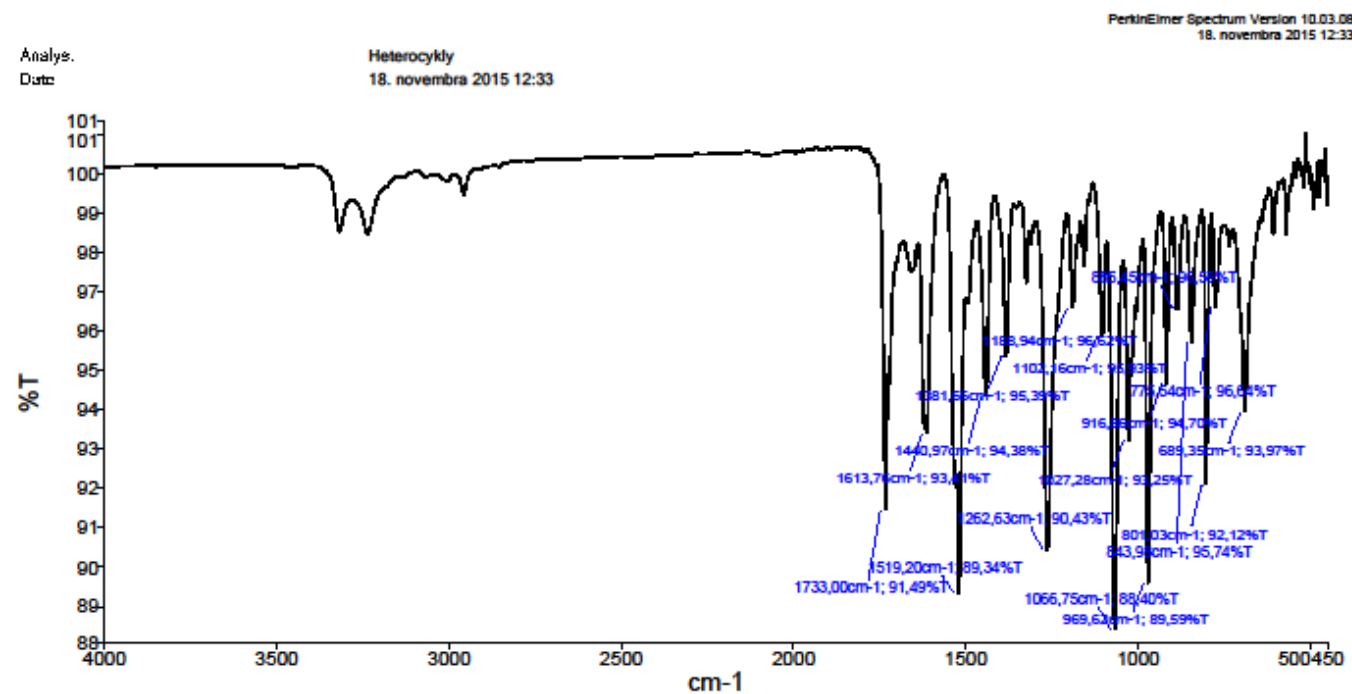
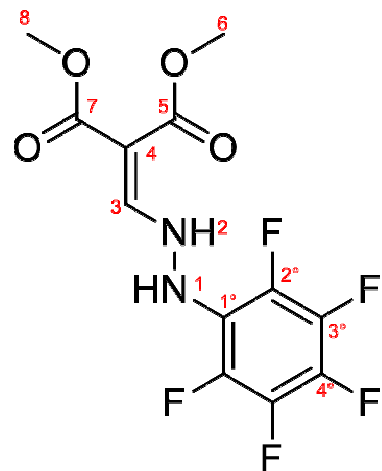




IVC ^{19}F - ^{13}C HSQC



IVC IR



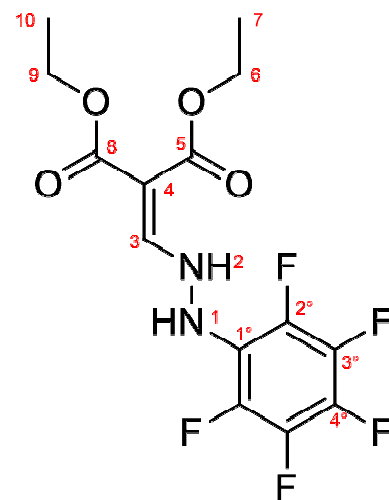
Heter 67 Sample 067 By Heter Date streda, novembra 18 2015

Source	Source Results
Spectrum Name	
Heter 67	

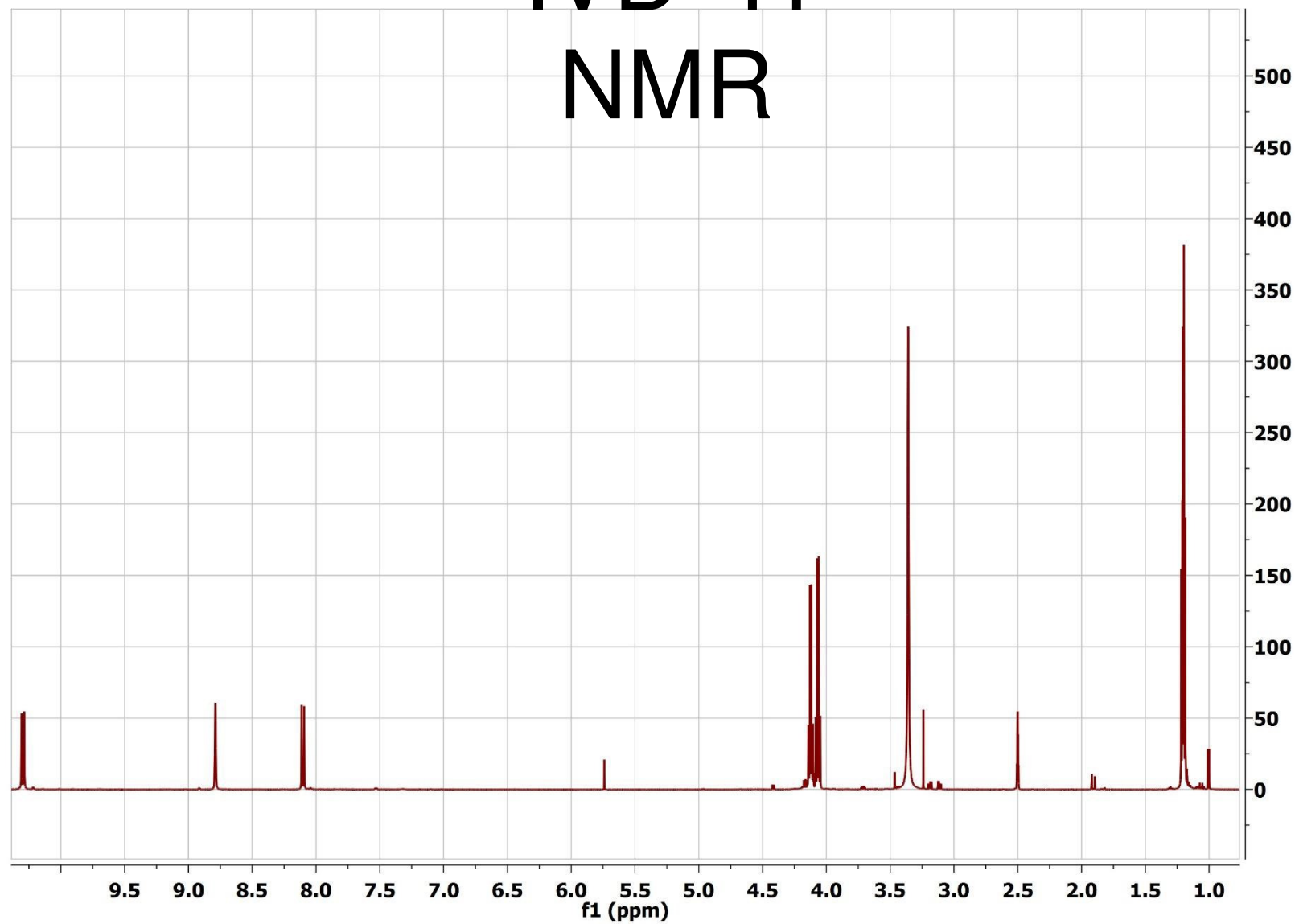
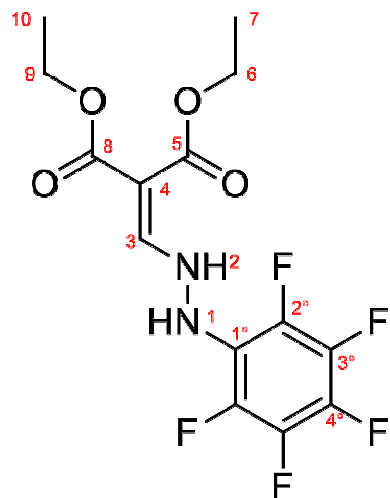
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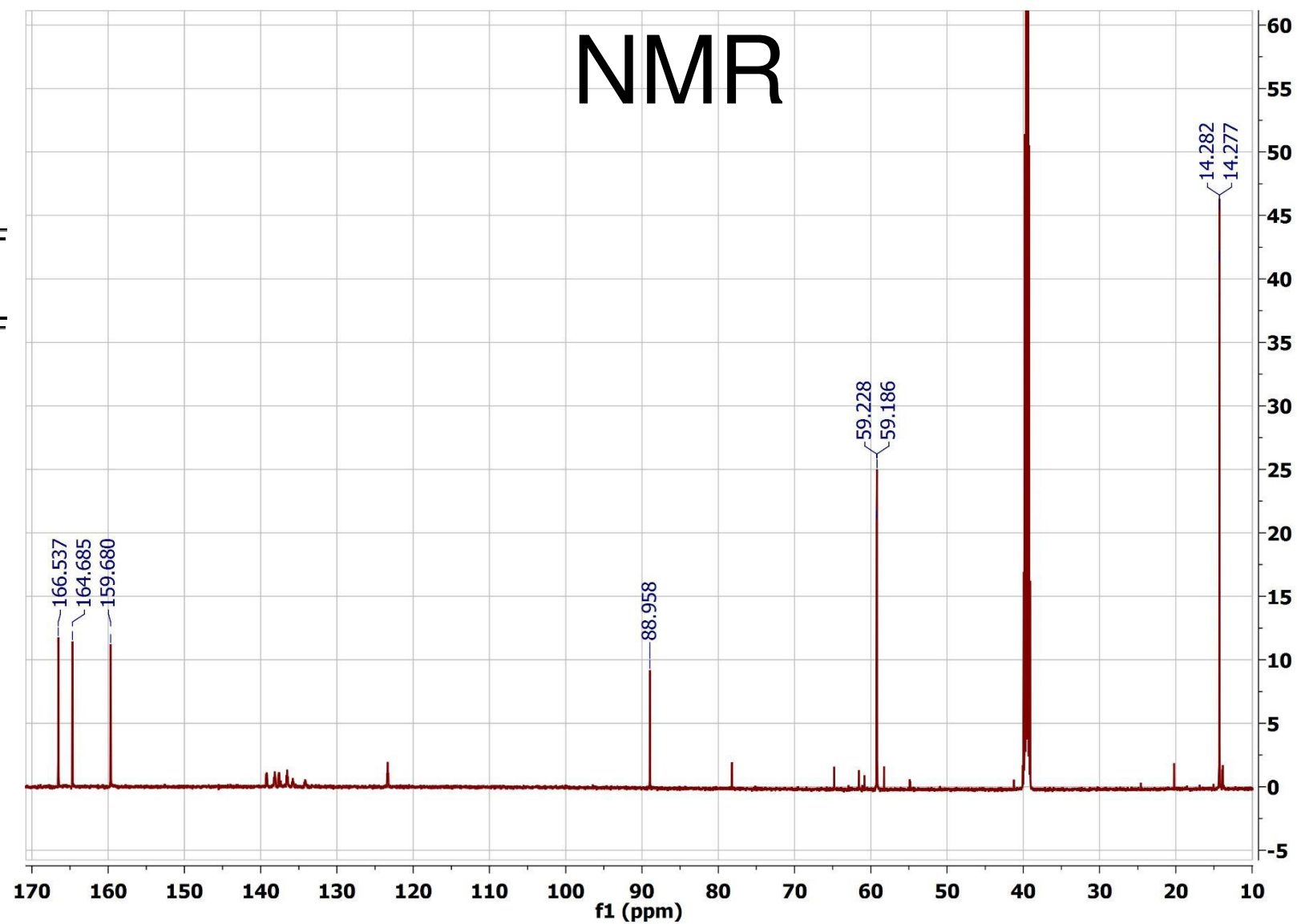
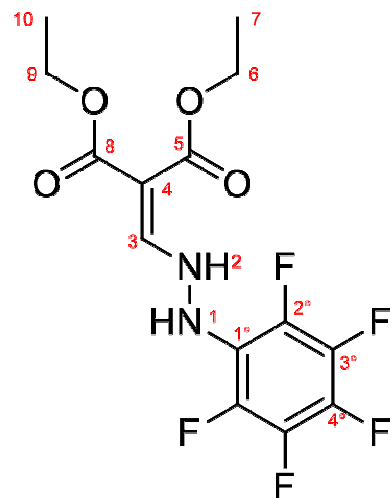
IVD



IVD ¹H NMR

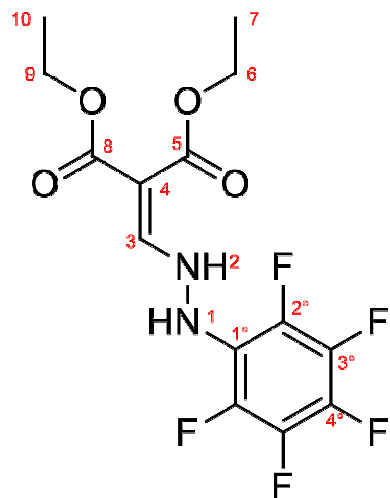


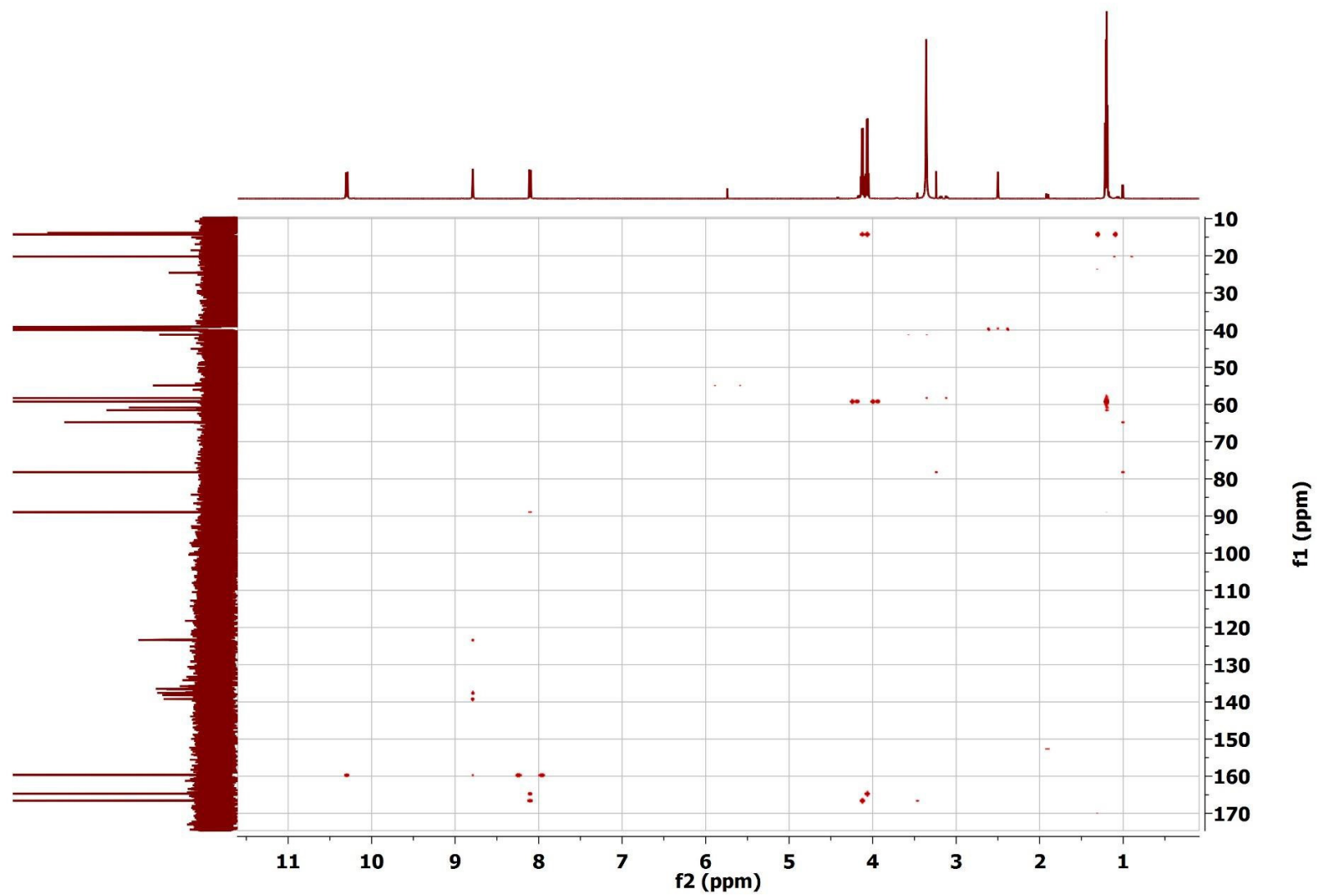
Inc

IVD ^{13}C
NMR

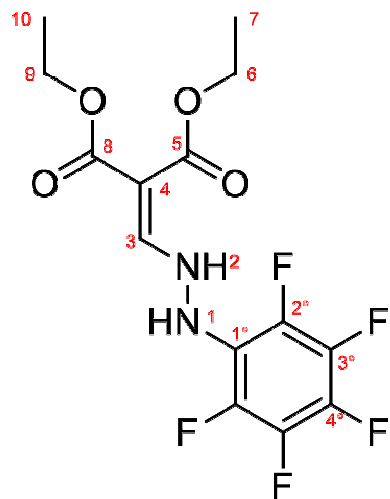
Inc

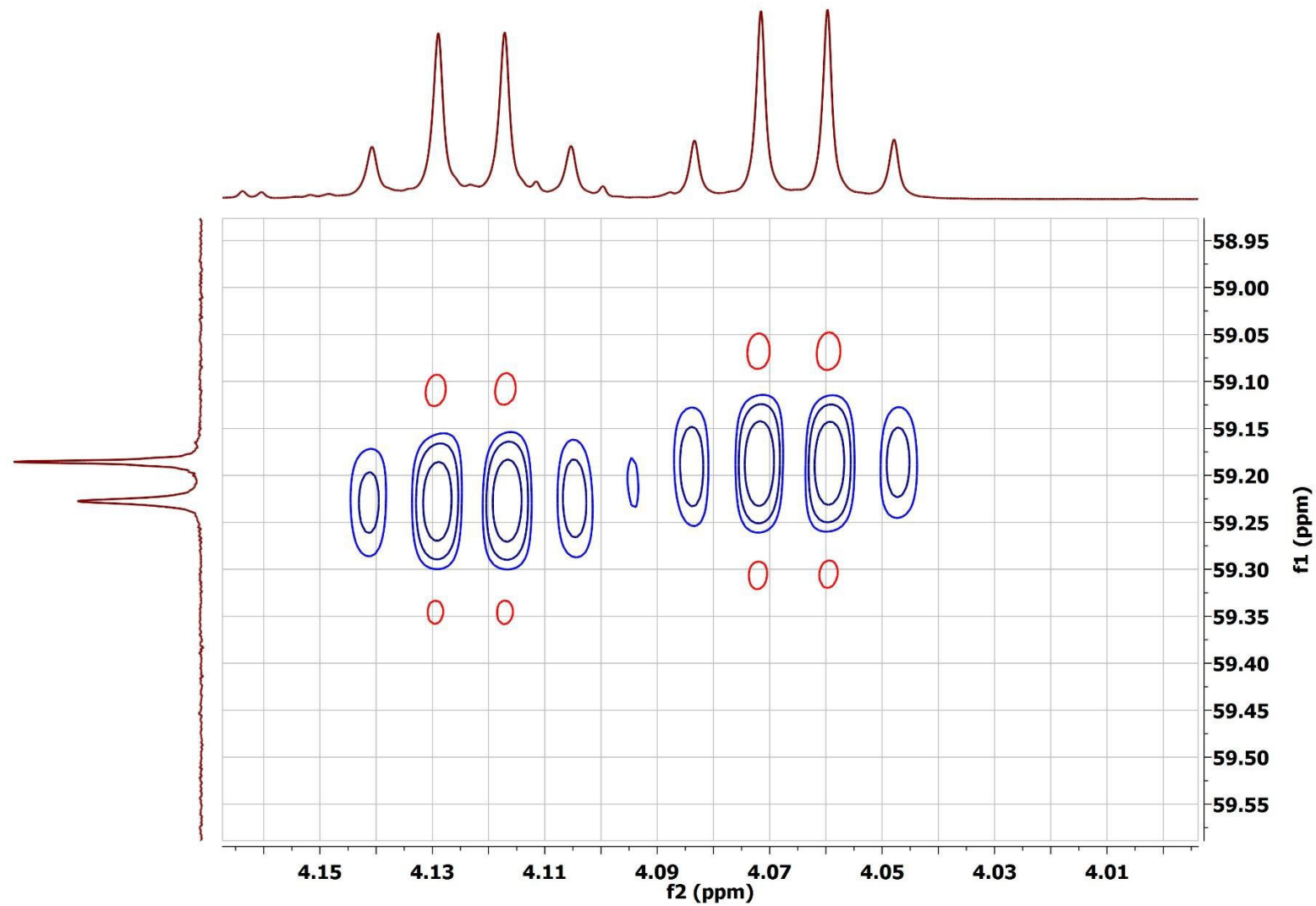
IVD ^1H - ^{13}C HMBC



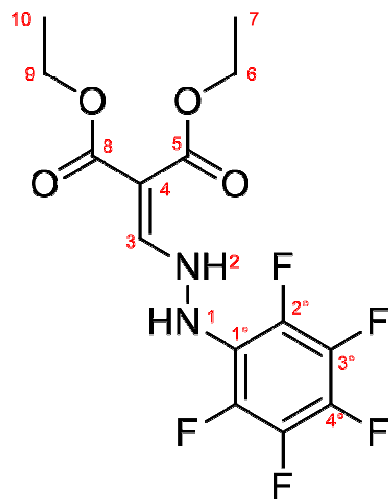


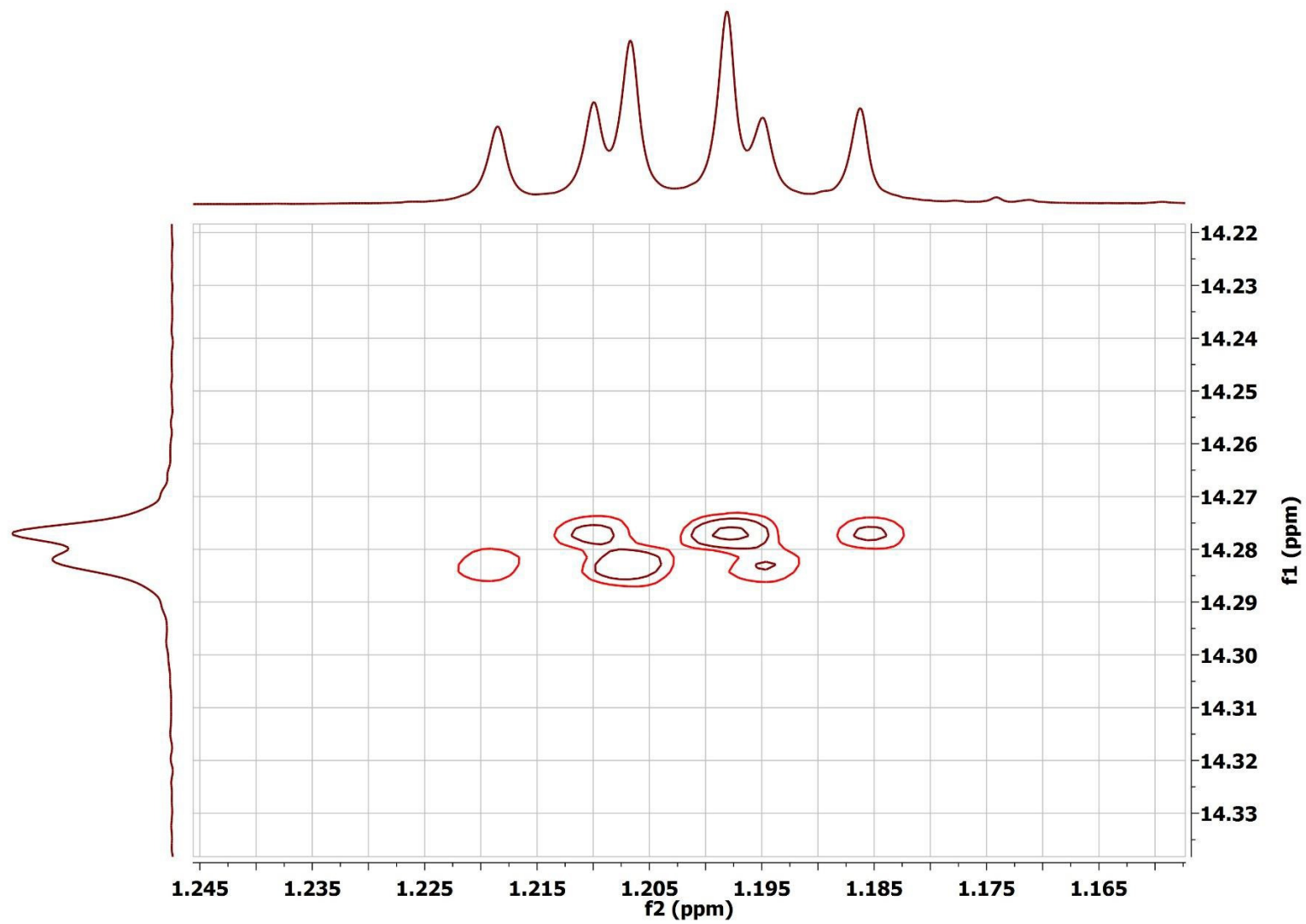
IVD ^1H - ^{13}C HSQC- CH_2

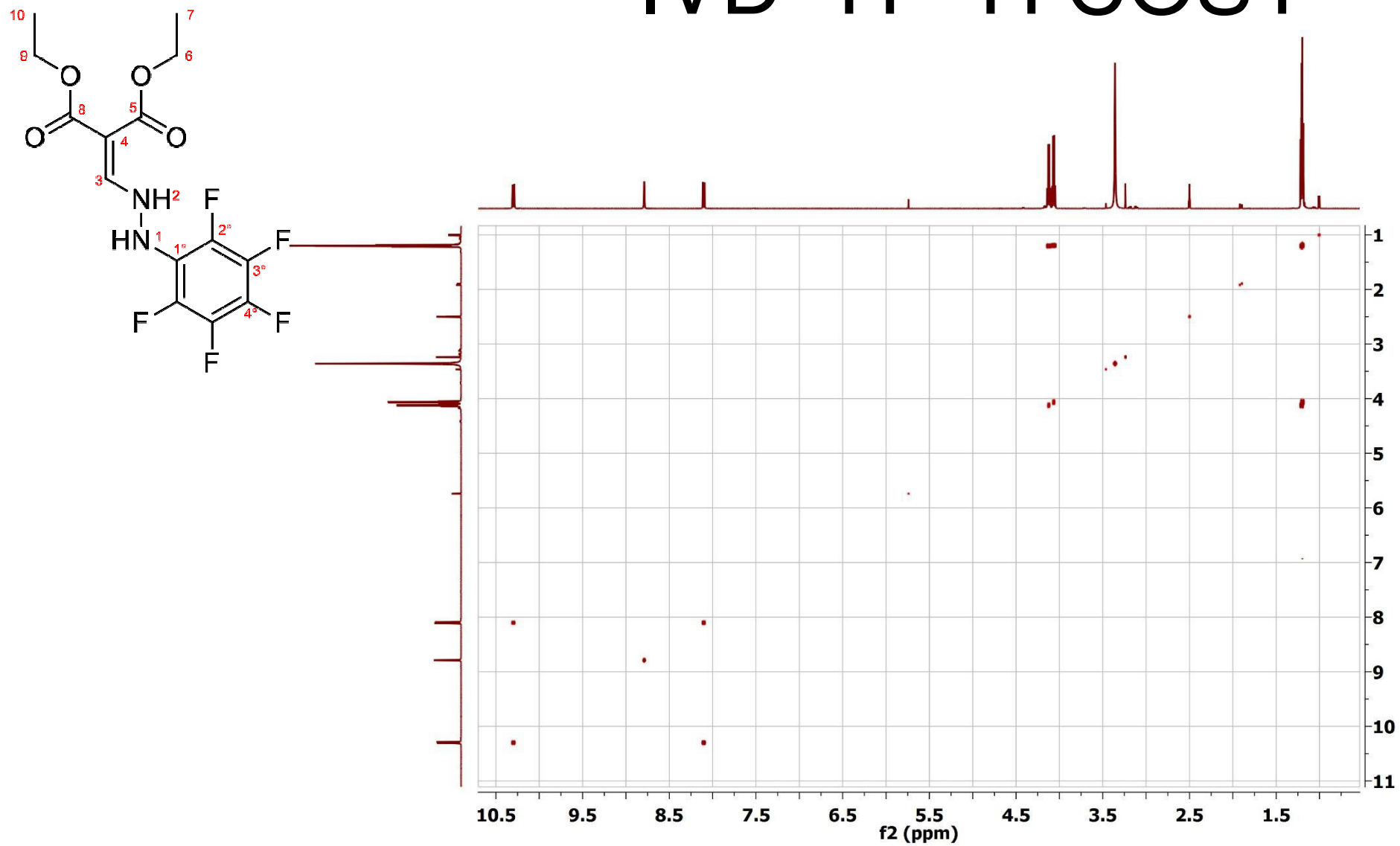




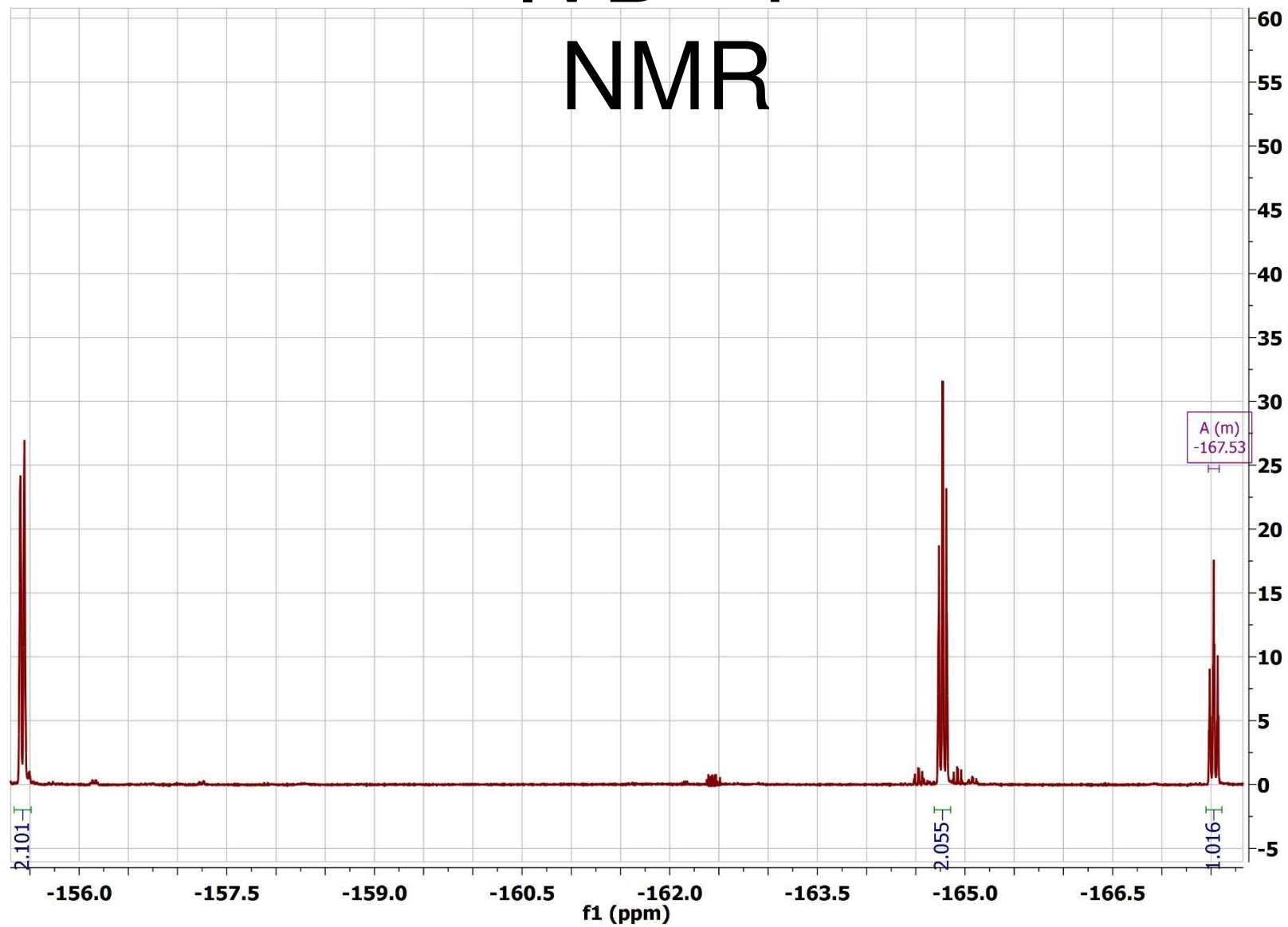
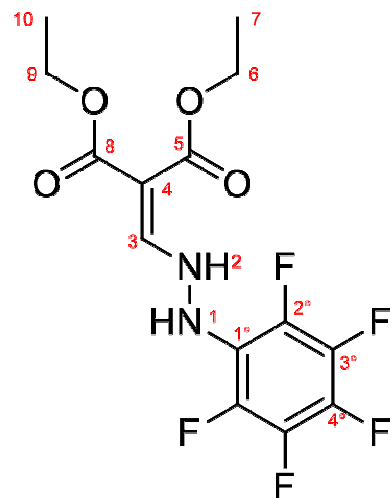
IVD ^1H - ^{13}C HSQC- CH_3





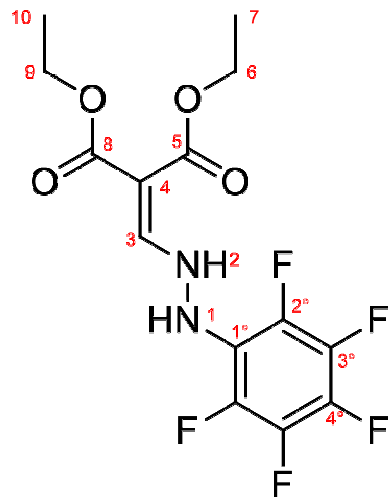
IVD ^1H - ^1H COSY

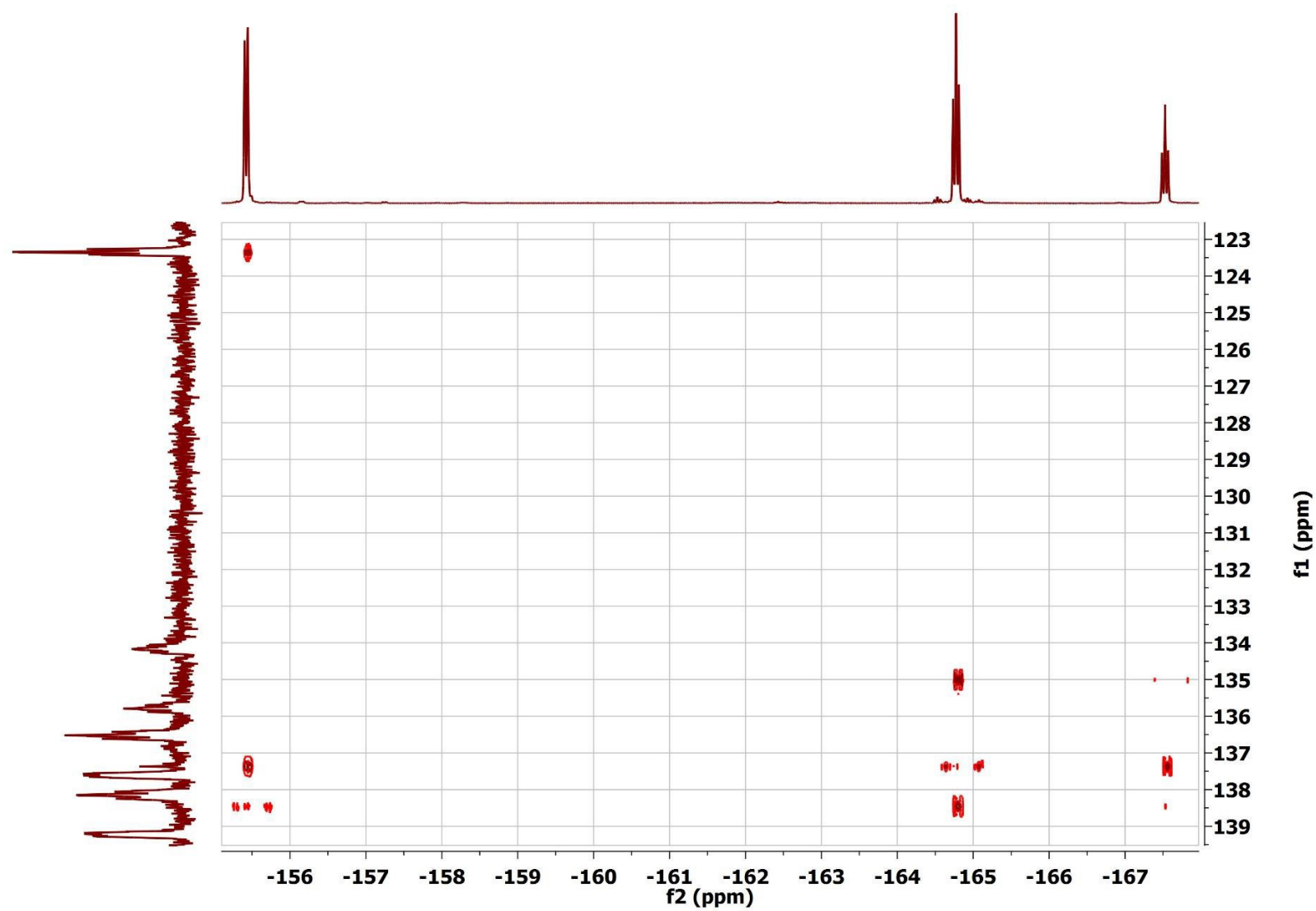
IVD ¹⁹F NMR



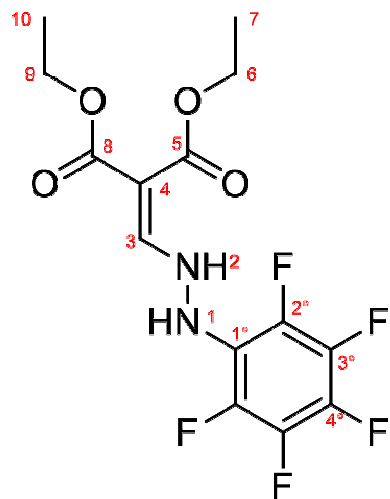
Inc

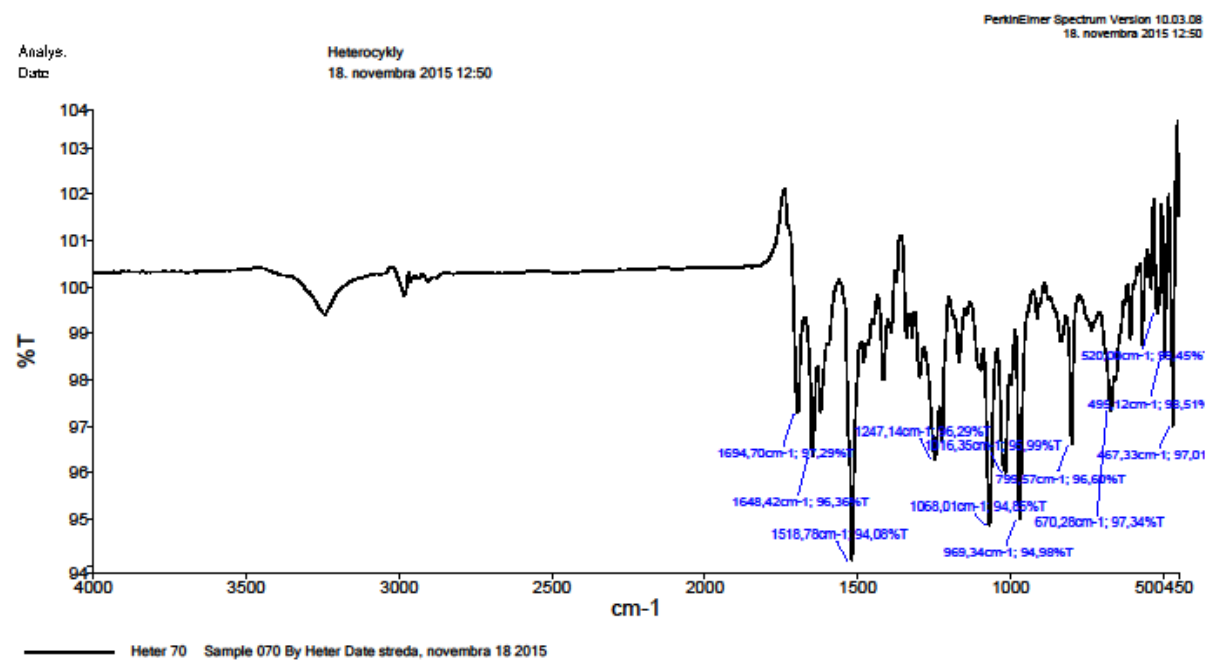
IVD ^{19}F - ^{13}C HMBC





IVD IR





Source: Source Results	
Spectrum Name	Heter 70

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