

Communication

(S)-Ethyl 2-(*tert*-butoxycarbonylamino)-3-(2-iodo-4,5-methylenedioxyphenyl)propanoate

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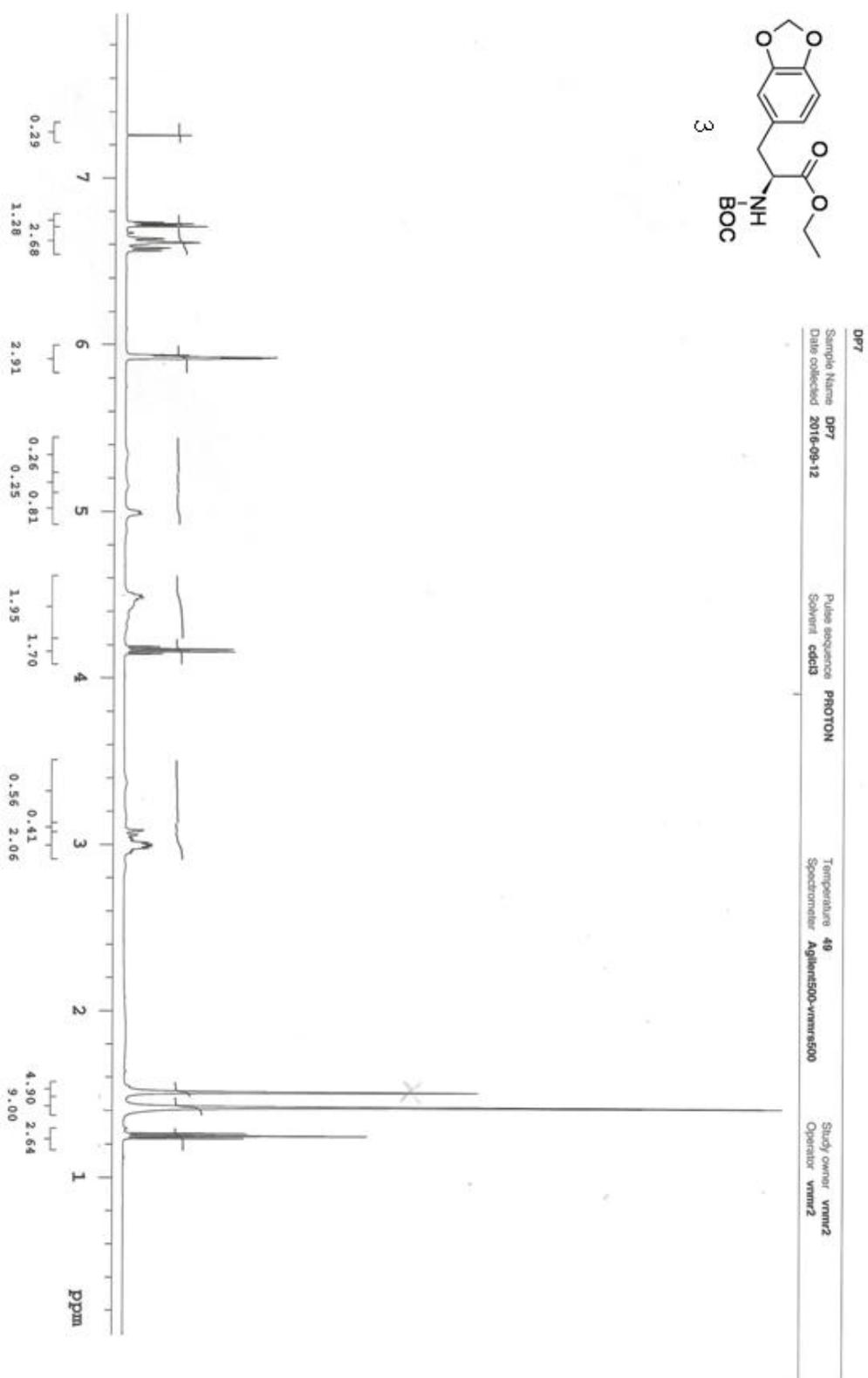
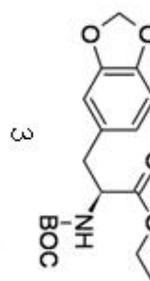
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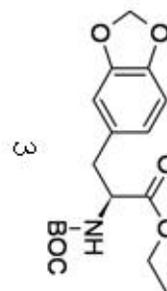
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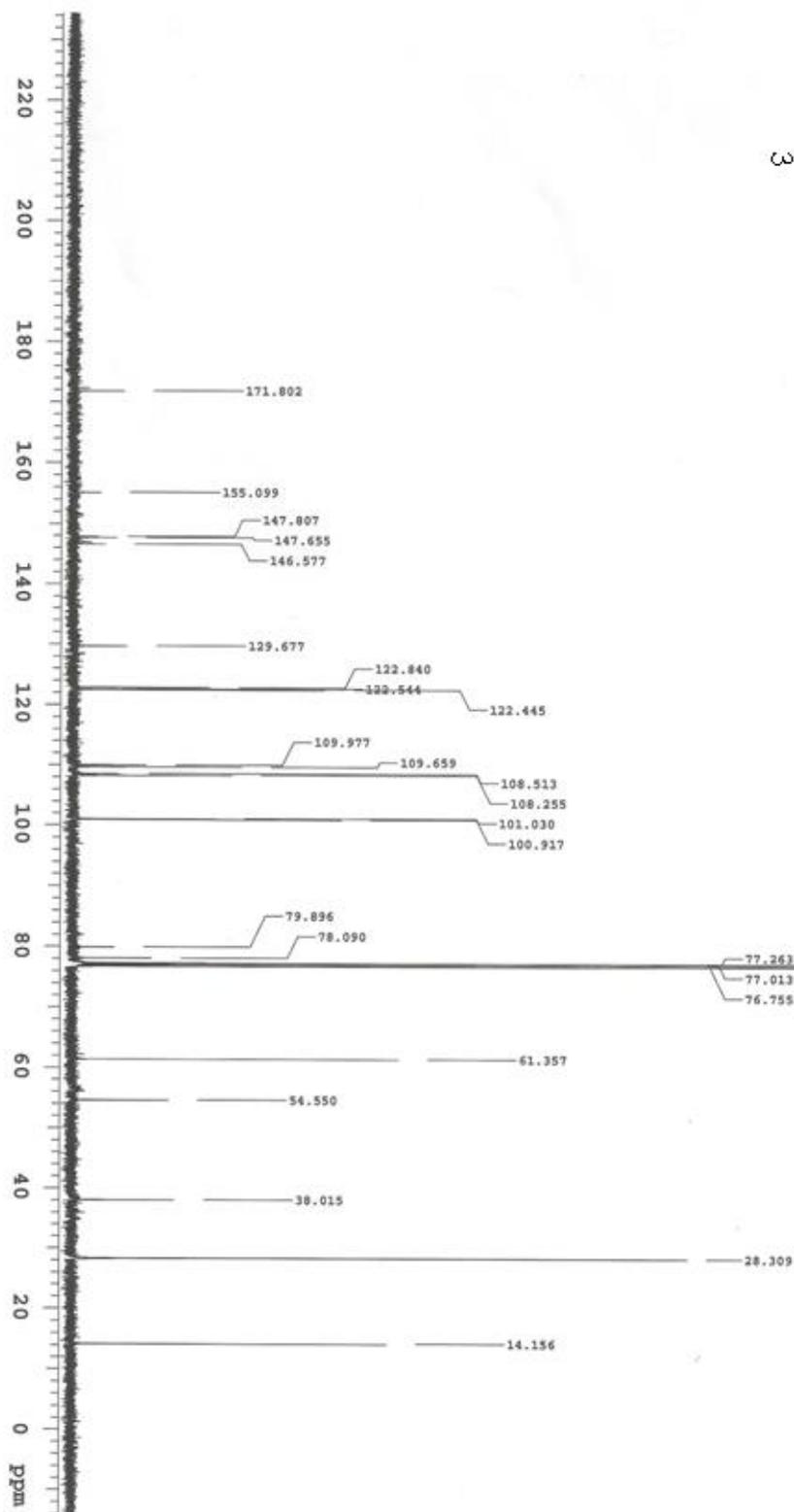
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PDF date: 2016-09-12

Figure S1: ¹H-NMR spectrum of compound 3 (CDCl₃, 500 MHz)



Data file: /home/vmm2/vmm2/Agilent/autosave_20160912_01/160912_01/160912_003/carbon



Plot date: 2016-09-12

DP7
Sample Name: DP7
Date collected: 2016-09-12
Pulse sequence: CARBON
Solvent: cdcl3
Temperature: 49
Spectrometer: Agilent500-vmm2500
Study owner: vmm2
Operator: vmm2

Figure S2: ¹³C-NMR spectrum of compound 3 (CDCl₃, 125 MHz)

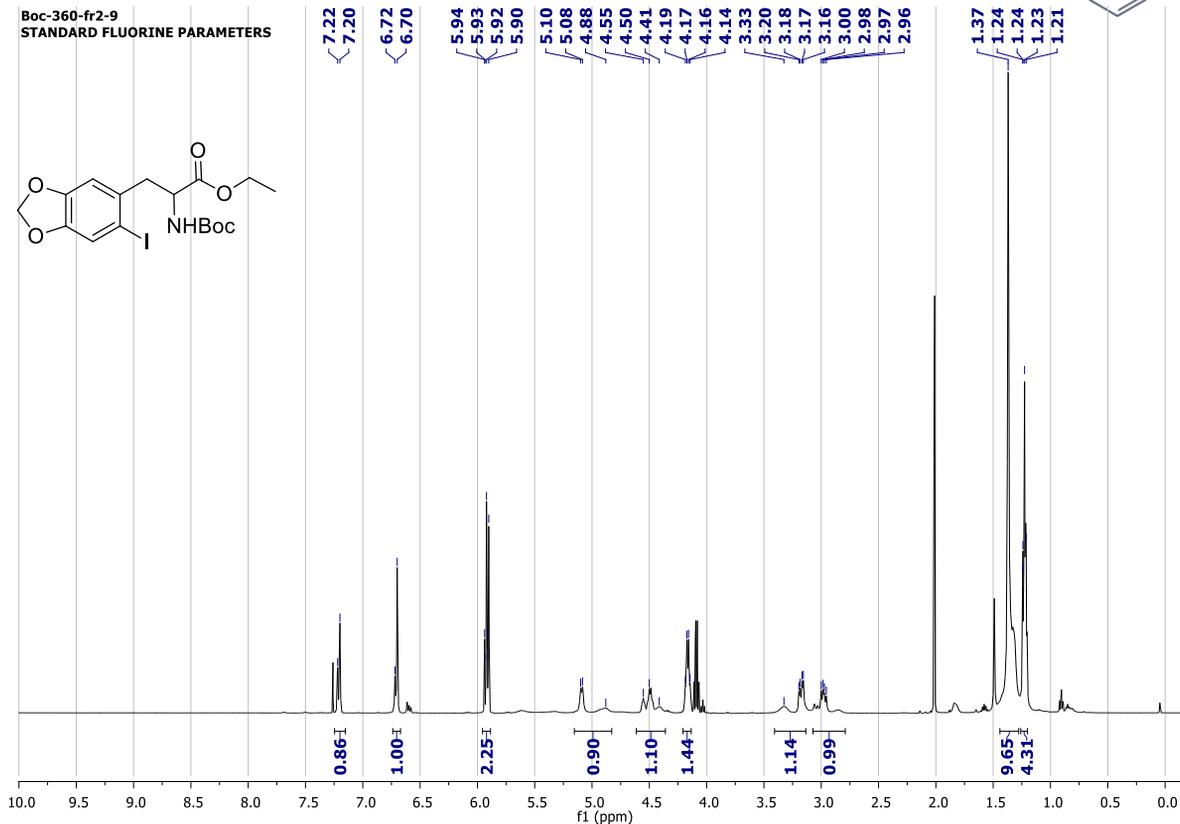


Figure S3: $^1\text{H-NMR}$ spectrum of compound **2** (CDCl_3 , 500 MHz)

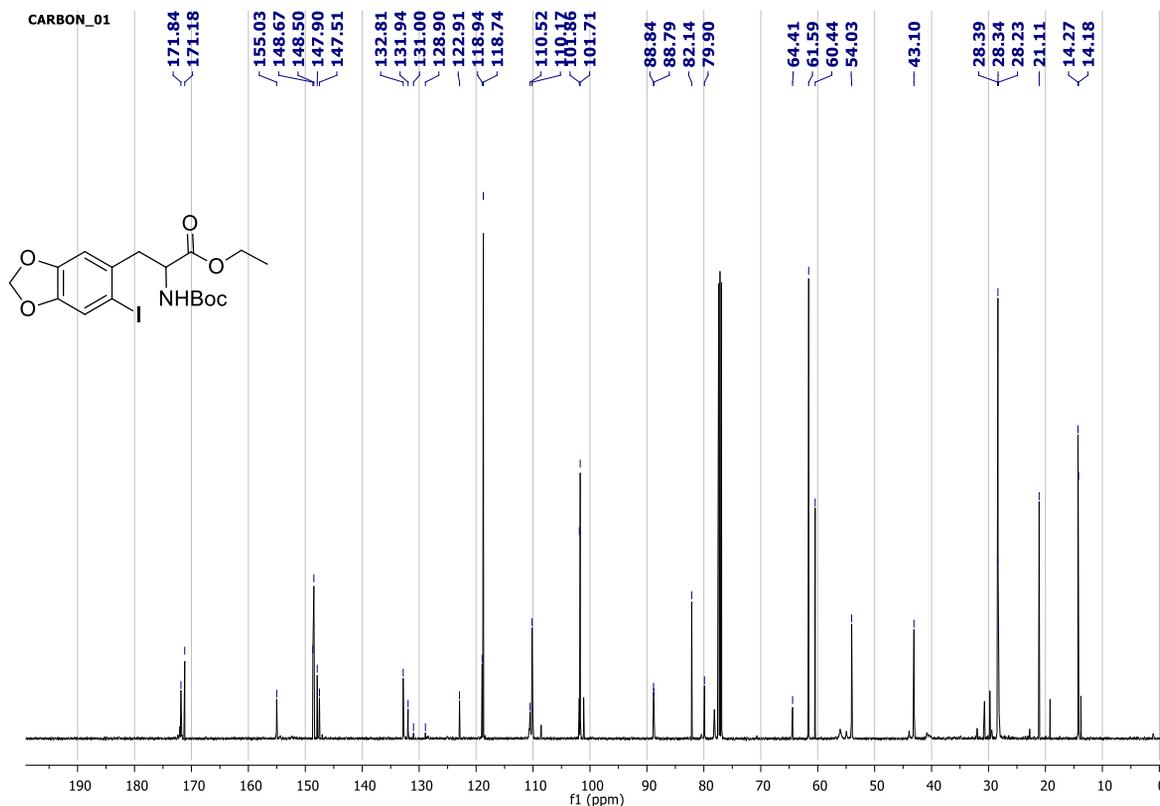


Figure S4: $^{13}\text{C-NMR}$ spectrum of compound **2** (CDCl_3 , 125 MHz)

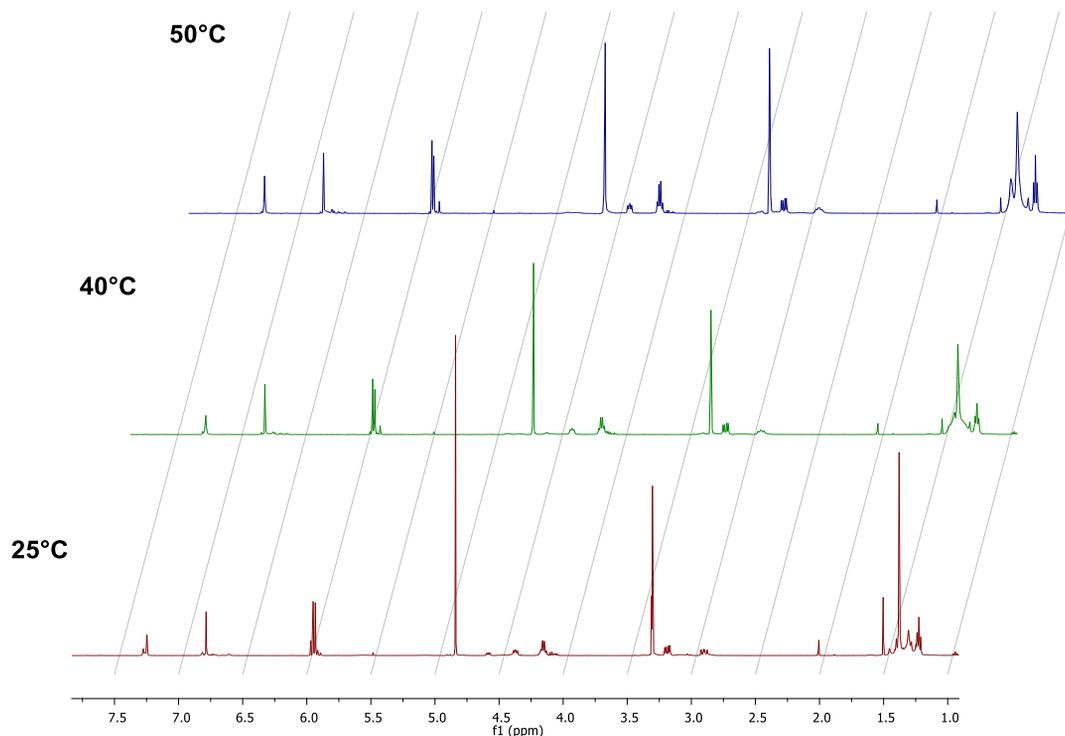


Figure S5: Variable temperature $^1\text{H-NMR}$ spectra of compound **2** (CD_3OD , 500 MHz)

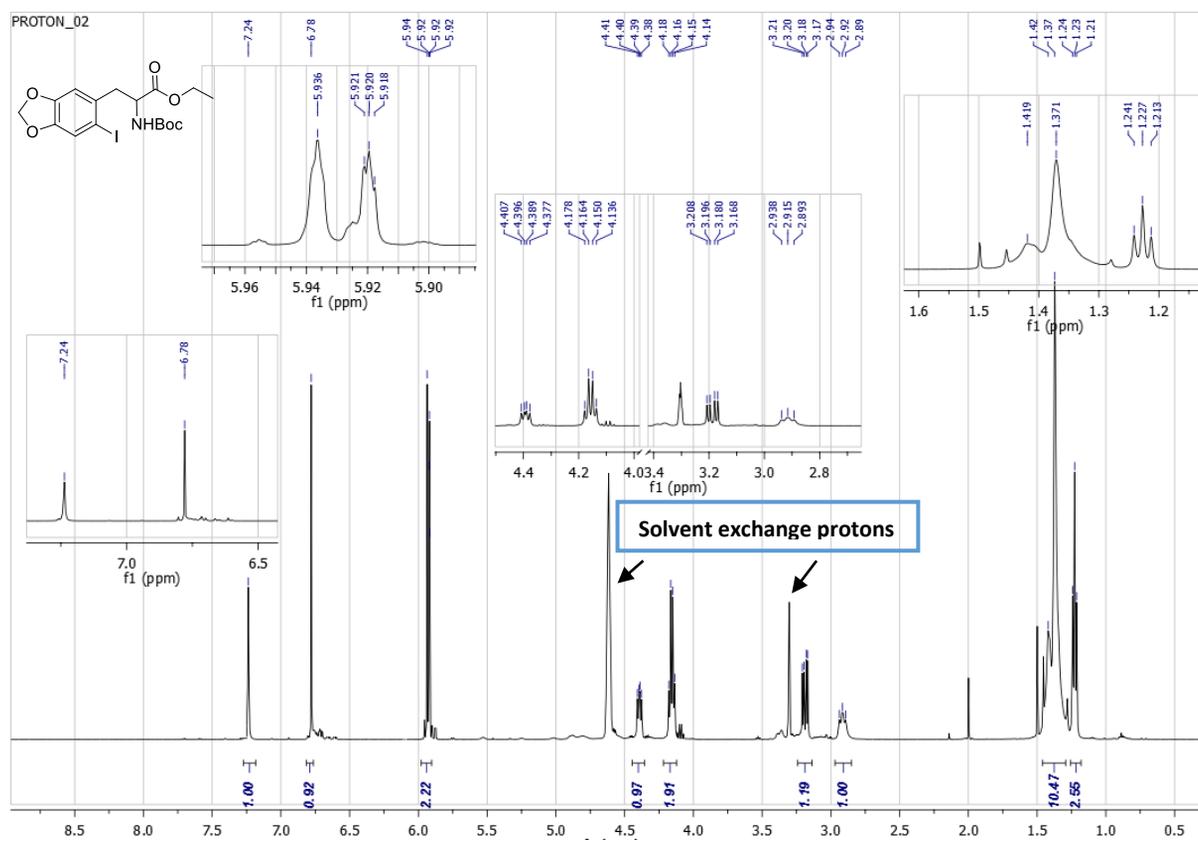


Figure S6: $^1\text{H-NMR}$ spectrum of compound **2** (CD_3OD , 500 MHz, 50 °C)

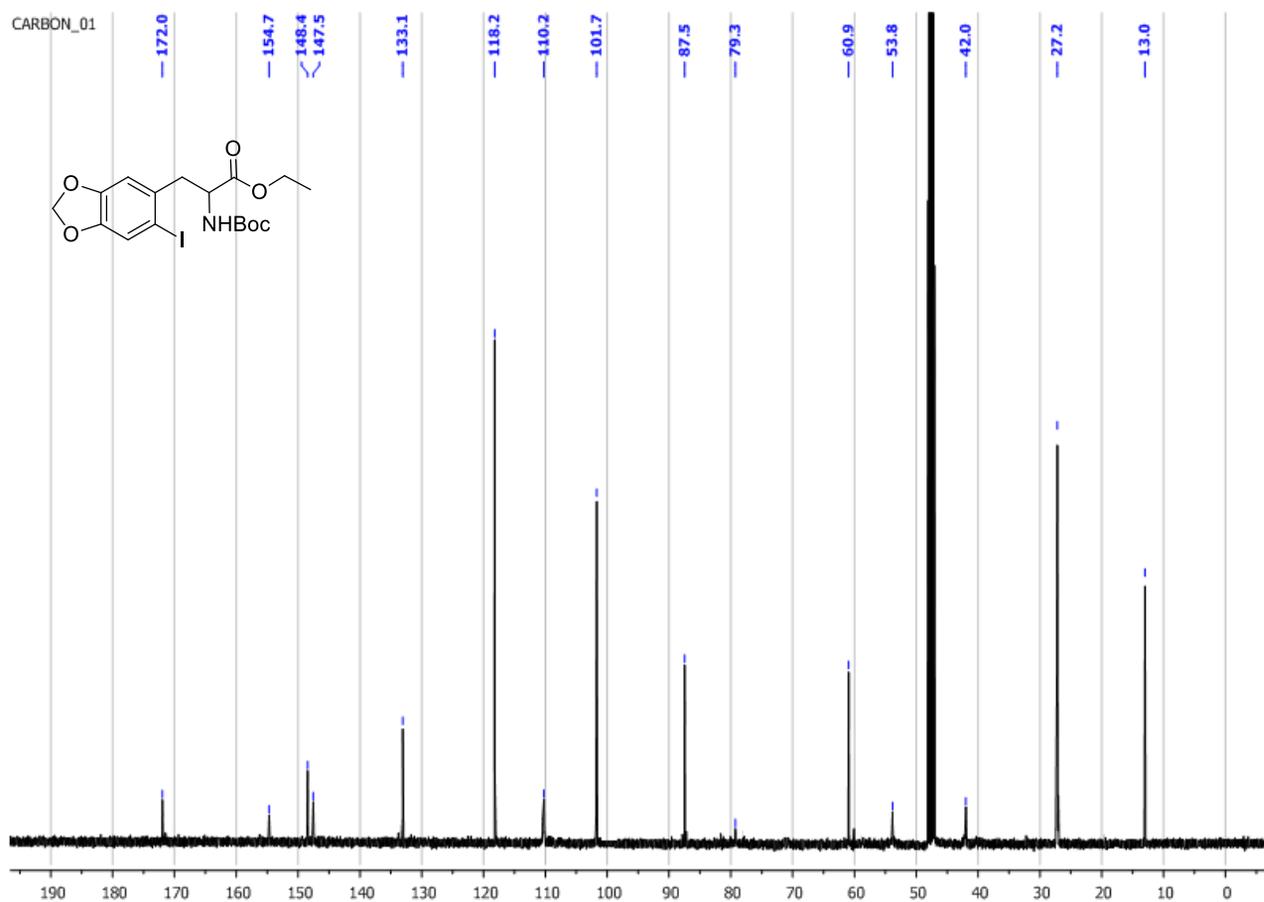


Figure S7: ^{13}C -NMR spectrum of compound **2** (CD_3OD , 500 MHz, 50 °C)

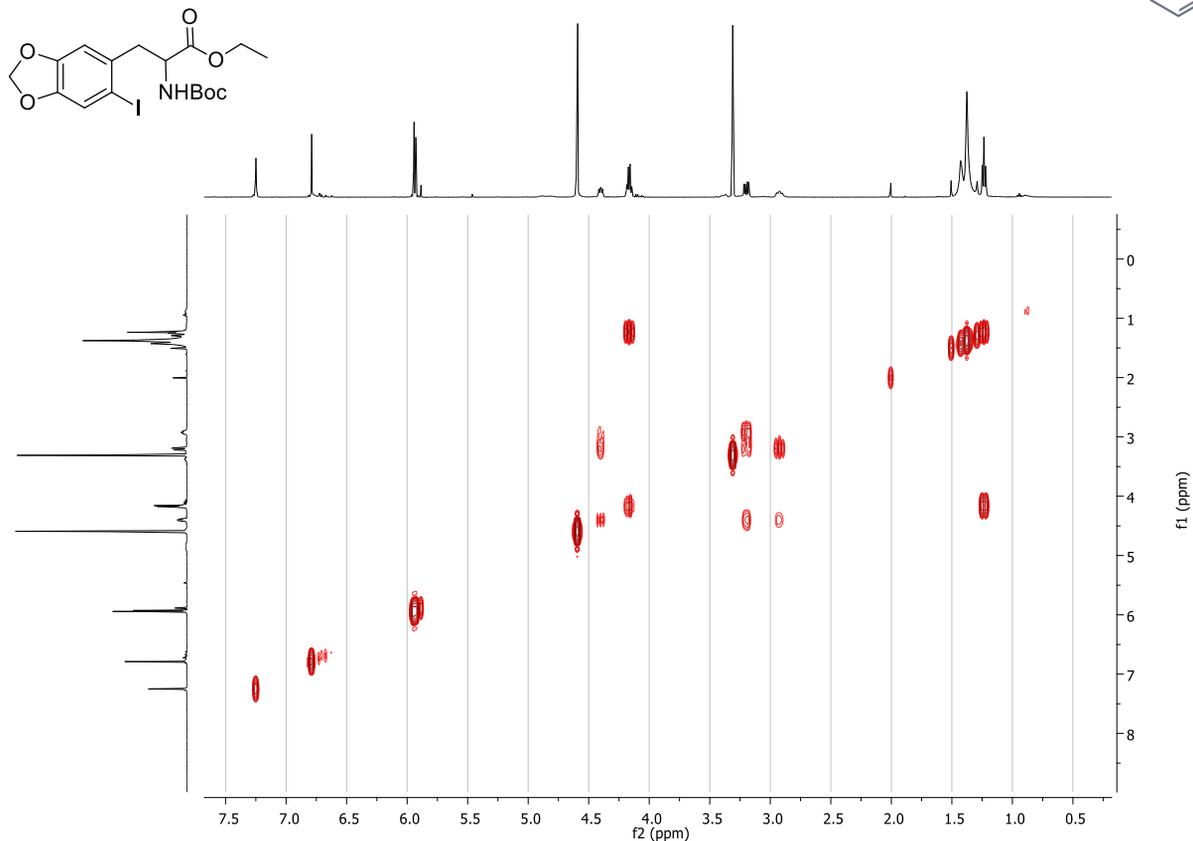


Figure S8: COSY spectrum of compound **2** (CD₃OD, 500 MHz, 50 °C)

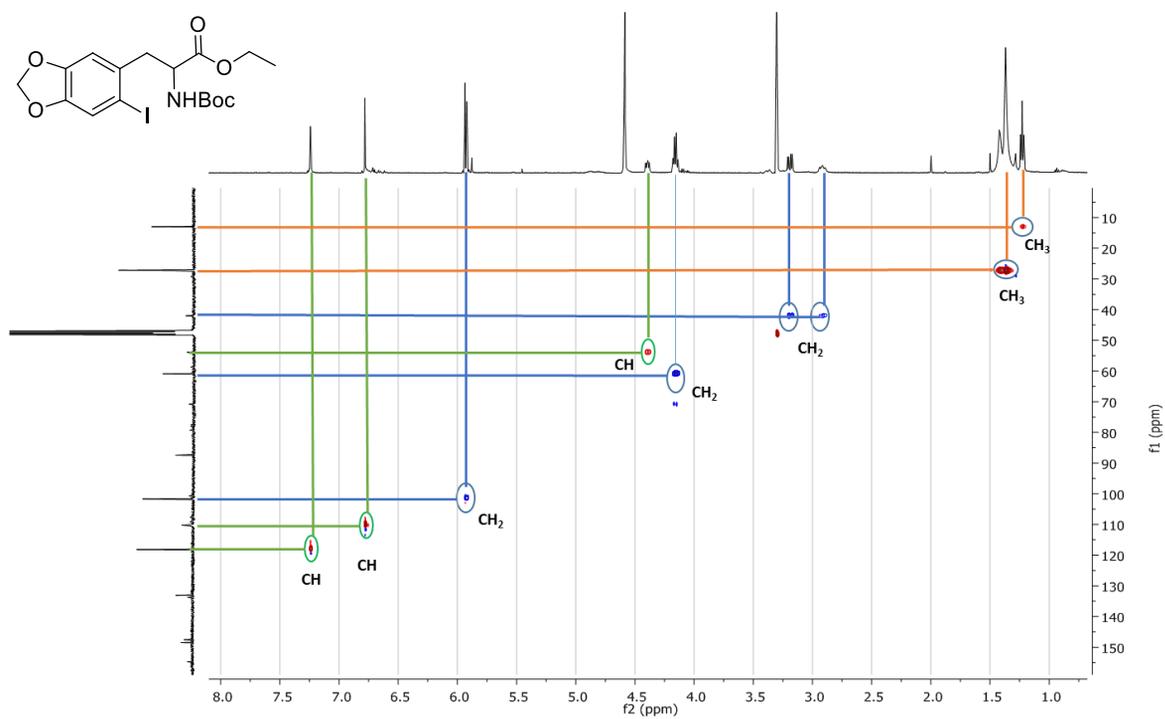
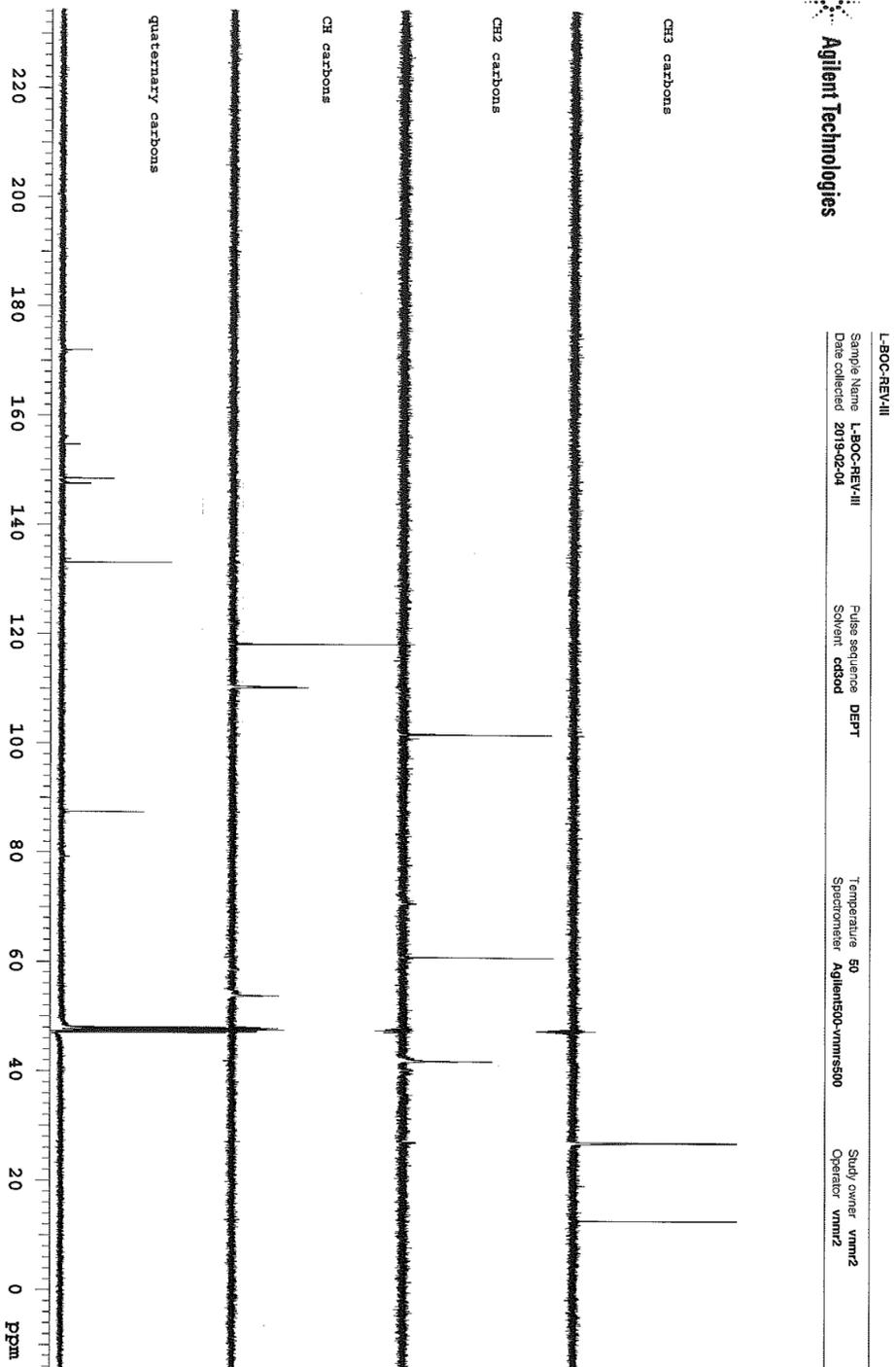


Figure S9: HSQC spectrum of compound **2** (CD₃OD, 500 MHz, 50 °C)



Data file: home/vmr2/FID_NMR500/LUS/L-BOC-REV-III_20190204_01/DEPT_01

Plot date 2019-02-05

Figure S10: DEPT spectrum of compound 2 (CD₃OD, 500 MHz, 50 °C)

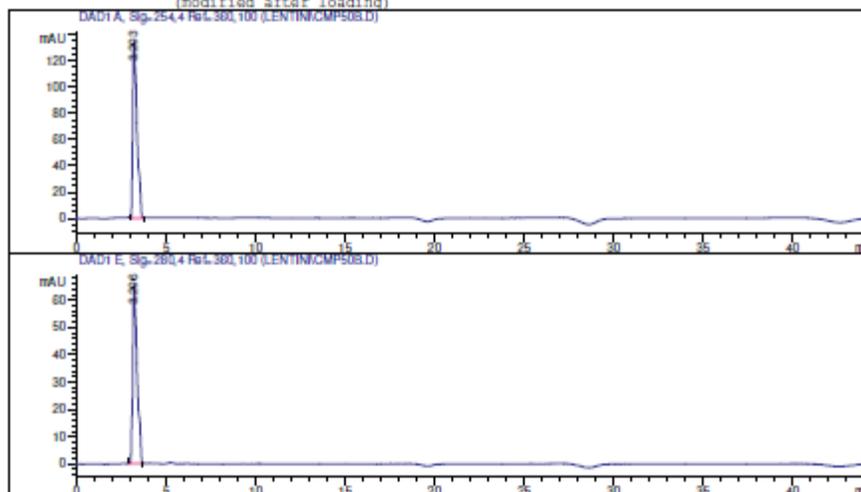


Data File C:\BPCHEM\1\DATA\LENTINI\CMP508.D

Sample Name: 1

Luisi FD 50 Prova b
CH3CN:ETANOL 80/20
0.5 mL/min

Injection Date : 2/6/2019 6:19:00 PM
Sample Name : 1 Location : Vial 1
Acq. Operator : Gualtiero
Acq. Instrument : Instrument 1
Method : C:\BPCHEM\1\METHODS\LENTINI.M
Last changed : 2/6/2019 7:03:34 PM by Gualtiero
(modified after loading)



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig-254,4 Ref-360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.203	VB	0.2175	2224.38525	135.52049	100.0000

Totals : 2224.38525 135.52049

Results obtained with enhanced integrator!

Signal 2: DAD1 E, Sig-280,4 Ref-360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.206	BB	0.2215	1113.25574	65.74659	100.0000

Totals : 1113.25574 65.74659

Results obtained with enhanced integrator!

Figure S11: High-Performance Liquid Chromatography (HPLC) analysis of compound **2** (column Zorbax Eclipse XDB-C18, CH₃CN/EtOH 80:20, 0.5 mL/min)