

Supporting Information

for

A versatile and efficient approach for the synthesis of chiral 1,3-nitroamines and 1,3-diamines via conjugate addition to new (*S,E*)- γ -aminated nitroalkenes derived from *L*- α -amino acids

Vera Lúcia Patrocínio Pereira^{1,§,*}, André Luiz da Silva Moura¹, Daniel Pais Pires Vieira¹, Leandro Lara de Carvalho¹, Eliz Regina Bueno Torres¹ and Jeronimo da Silva Costa²

Address: ¹Núcleo de Pesquisas de Produtos Naturais, Laboratório de Síntese Estereosseletiva de Substâncias Bioativas, Universidade Federal do Rio de Janeiro, 21941-902, Rio de Janeiro, Brazil and ²Instituto Federal de Educação, Ciência e Tecnologia do Rio de Janeiro, 26530-060, Nilópolis, RJ, Brazil

Email: Vera Lúcia Patrocínio Pereira - patrocinio@nppn.ufrj.br

* Corresponding author

[§]Tel.: +55 21 2562 6792; Fax: +55 21 2562 6512

NMR, IR and MS spectra

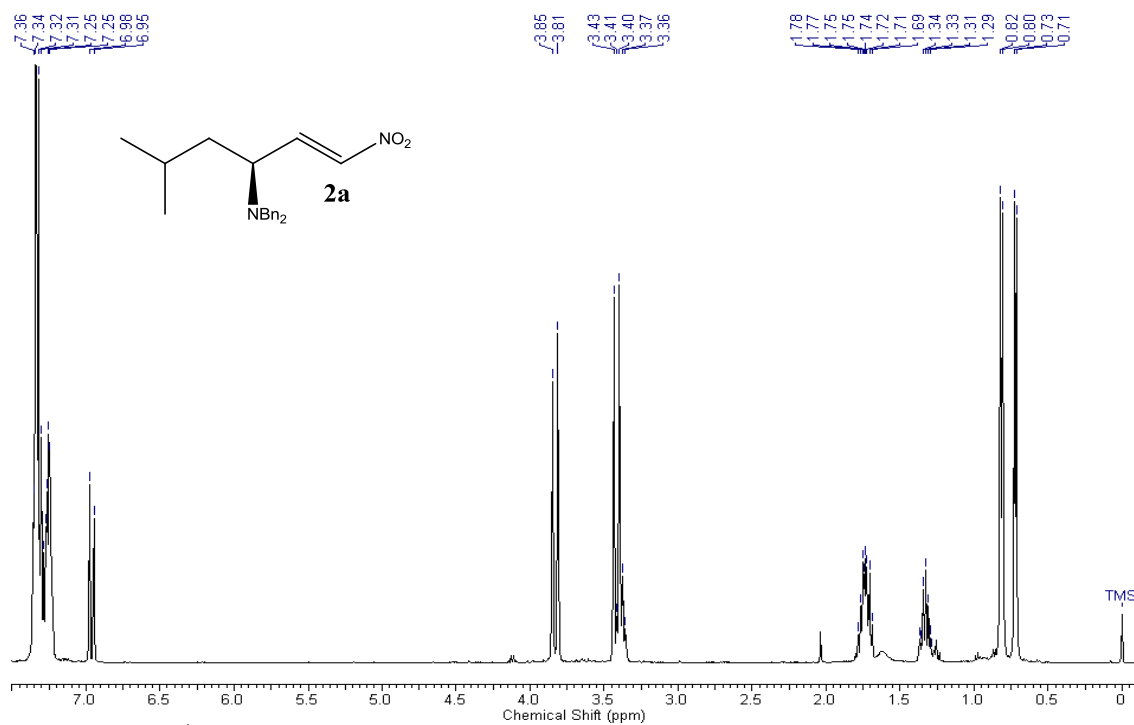
Contents:

Copy of ¹H NMR spectra of **2a–c**, **8a**, **8b**, **7b**, **9b**, **9a**, **10b**, **11a**, **12a**, **14b**.

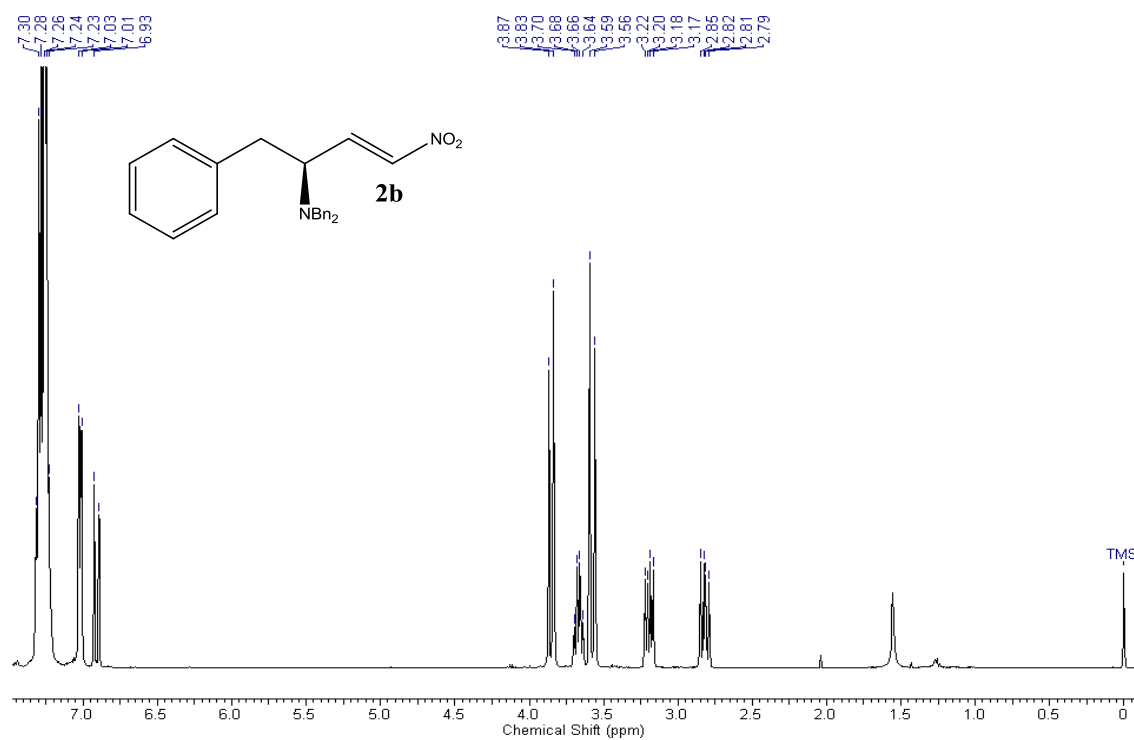
Copy of ¹³C NMR spectra of **11a**, **7b**, **8b**, **9a**, **12a**, **2a**, **2c** and APT of **2b**, **8a**, **9a**, **9b**, **10b**, **14b**.

Copy of IR spectra of **11a**, **12a**, **9a**, **14b**.

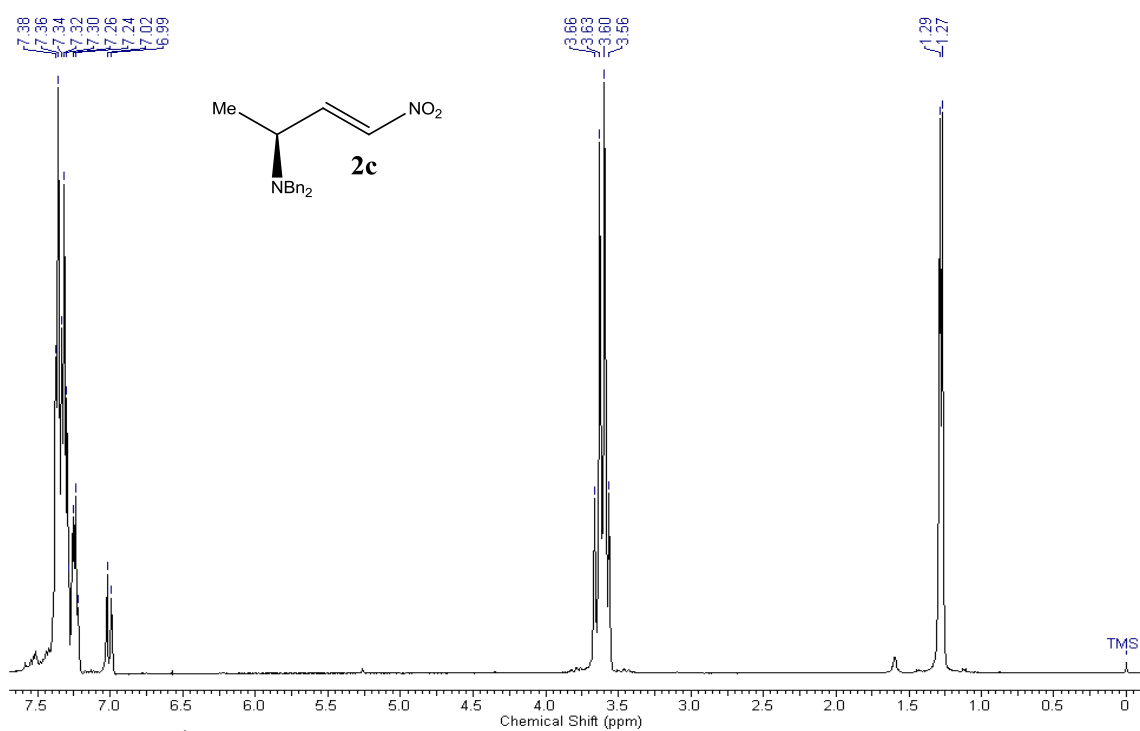
Copy of HRMS spectra of **14a**, **14b**, **9b**, **7b**, **2a**, **2b**.



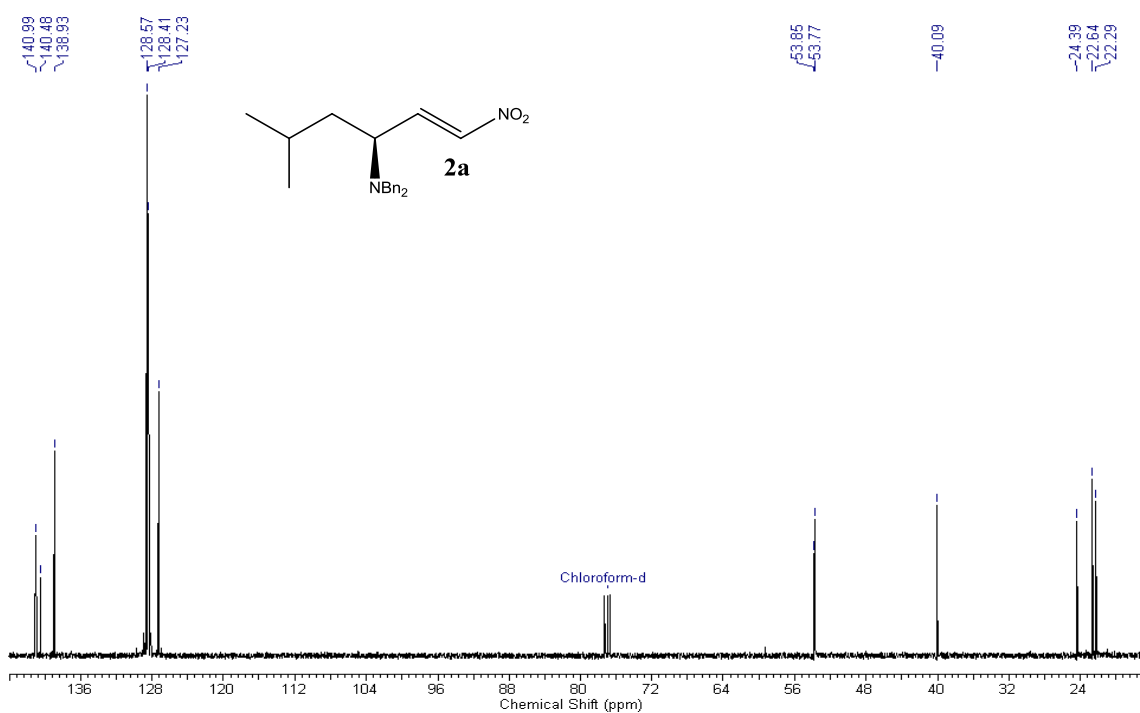
Spectrum 1: ^1H NMR (400 MHz, CDCl_3) of **2a**



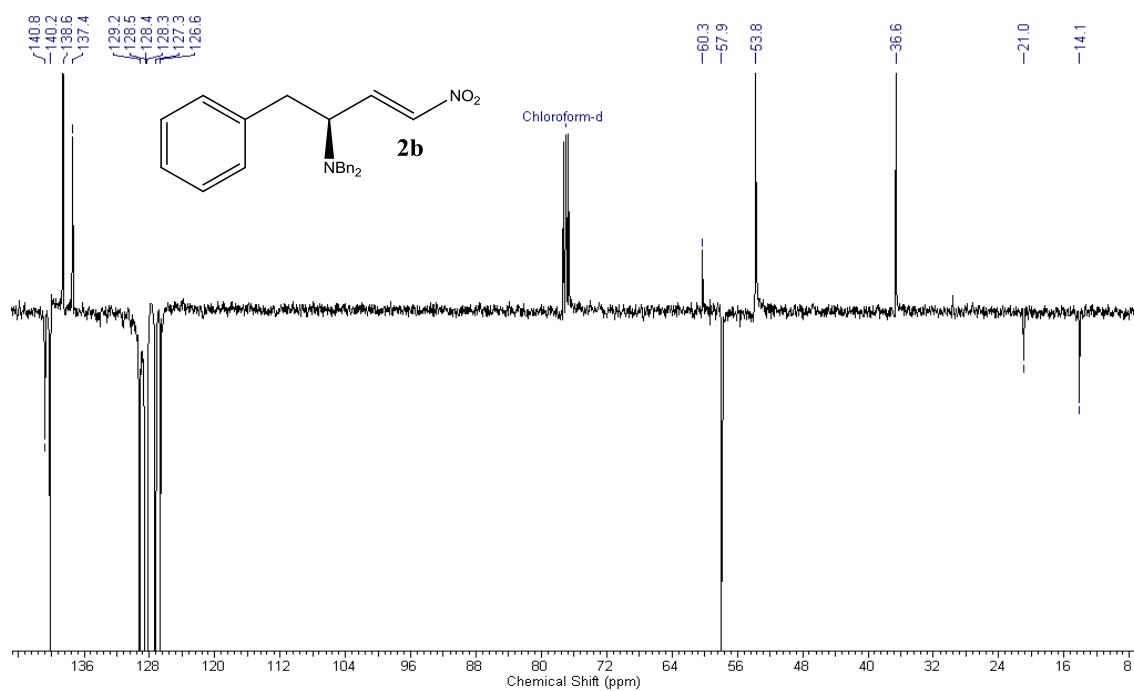
Spectrum 2: ^1H NMR (400 MHz, CDCl_3) of **2b**



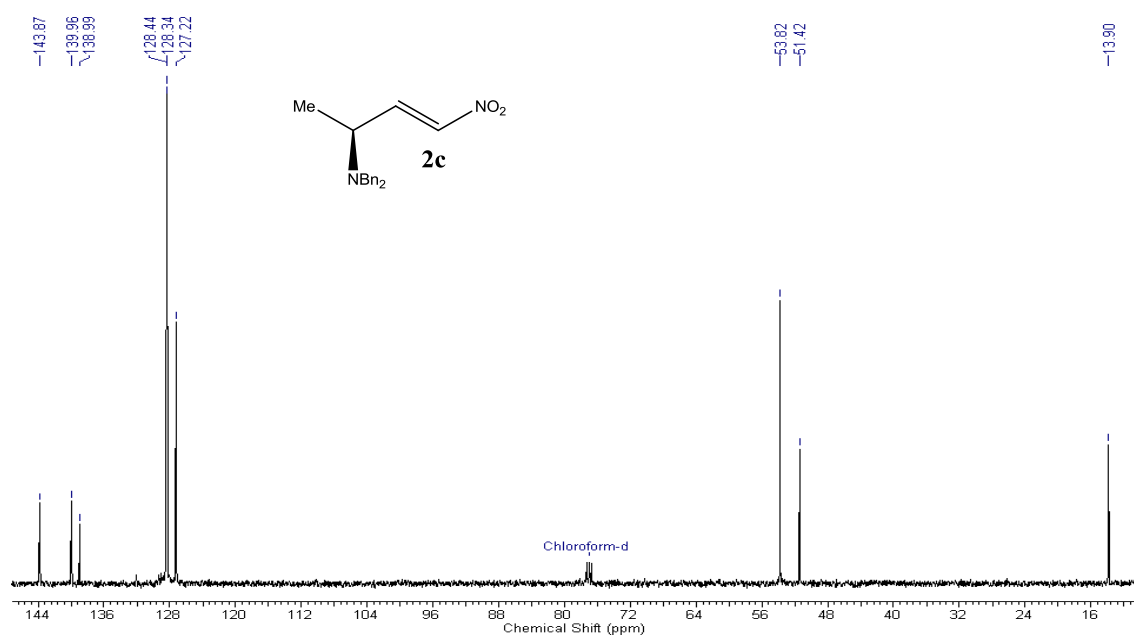
Spectrum 3: ¹H NMR (400 MHz, CDCl₃) of **2c**



Spectrum 4: ¹³C NMR (100 MHz, CDCl₃) of **2a**



Spectrum 5: APT NMR (50 MHz, CDCl₃) of 2b

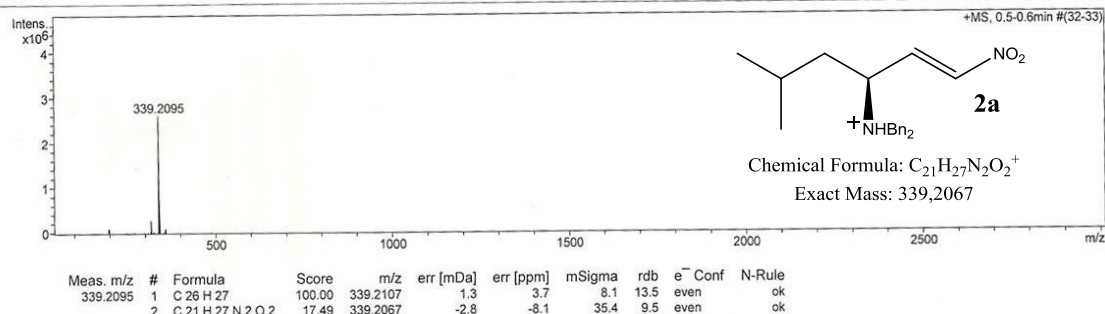


Spectrum 6: ¹³C NMR (100 MHz, CDCl₃) of 2c

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	5/22/2012 4:28:50 PM	
Analysis Name	D:\Data\Usuarios\Vera Patrocinio\ER202_Pos_22-05-12.d	Operator	BDAL@DE	
Method	Tune_pos_50-3000_Lab-Mass.m	Instrument / Ser#	microTOF 10368	
Sample Name	ER202_Pos_22-05-12			
Comment				

Acquisition Parameter		Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Source Type	ESI			Set Dry Heater	180 °C
Focus	Not active	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste
Scan End	3000 m/z				

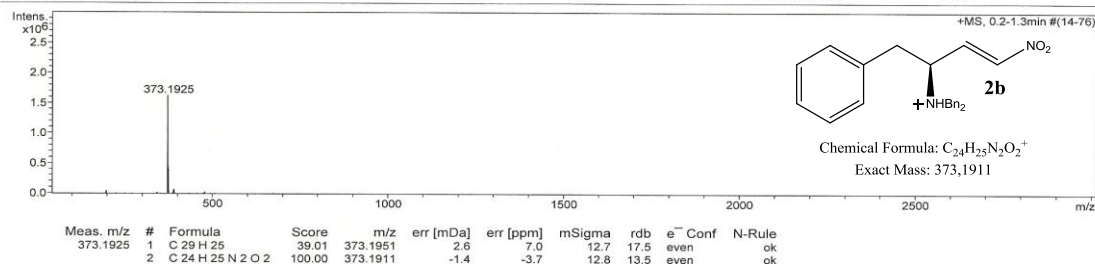


Spectrum 7: HRMS of 2a

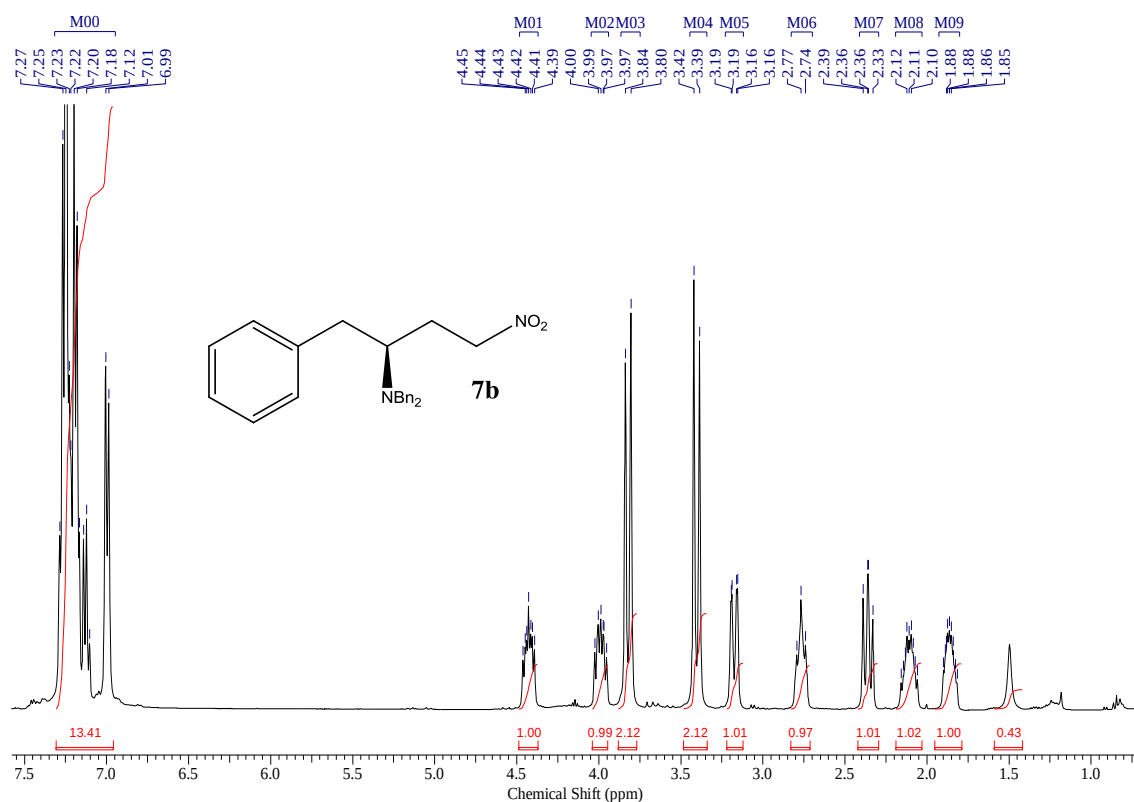
Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	5/22/2012 4:15:39 PM	
Analysis Name	D:\Data\Usuarios\Vera Patrocínio\ER204_Pos_22-05-12.d	Operator	BDAL@DE	
Method	Tune_pos_50-3000_Lab-Mass.m		10368	
Sample Name	ER204_Pos_22-05-12		microTOF	
Comment		Instrument / Ser#		

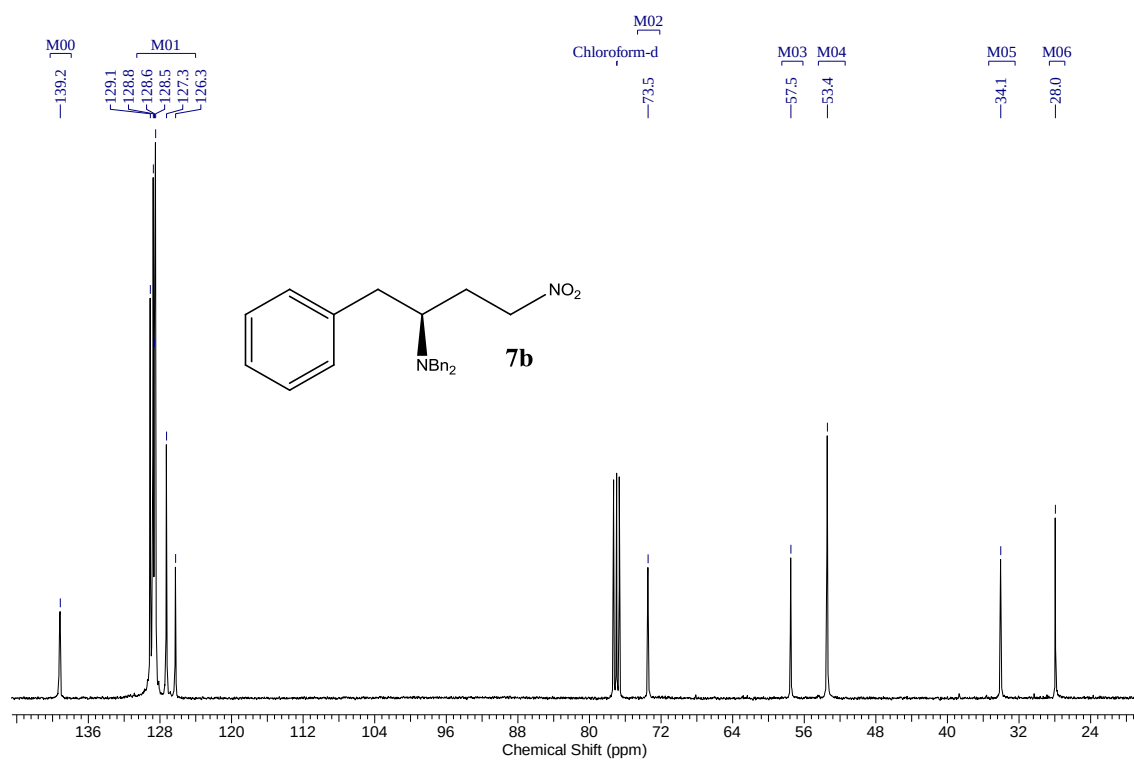
Acquisition Parameter		Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Source Type	ESI			Set Dry Heater	180 °C
Focus	Not active	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste
Scan End	3000 m/z				



Spectrum 8: HRMS of 2b

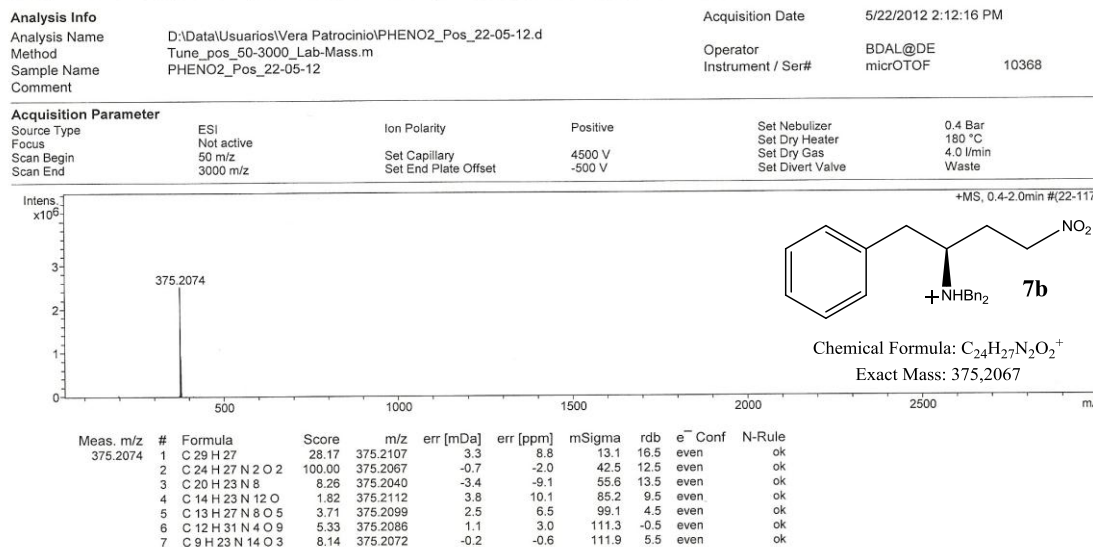


Spectrum 9: ¹H NMR (400 MHz, CDCl₃) of **7b**.



Spectrum 10: ¹³C NMR (100 MHz, CDCl₃) of **7b**

Mass Spectrum SmartFormula Report

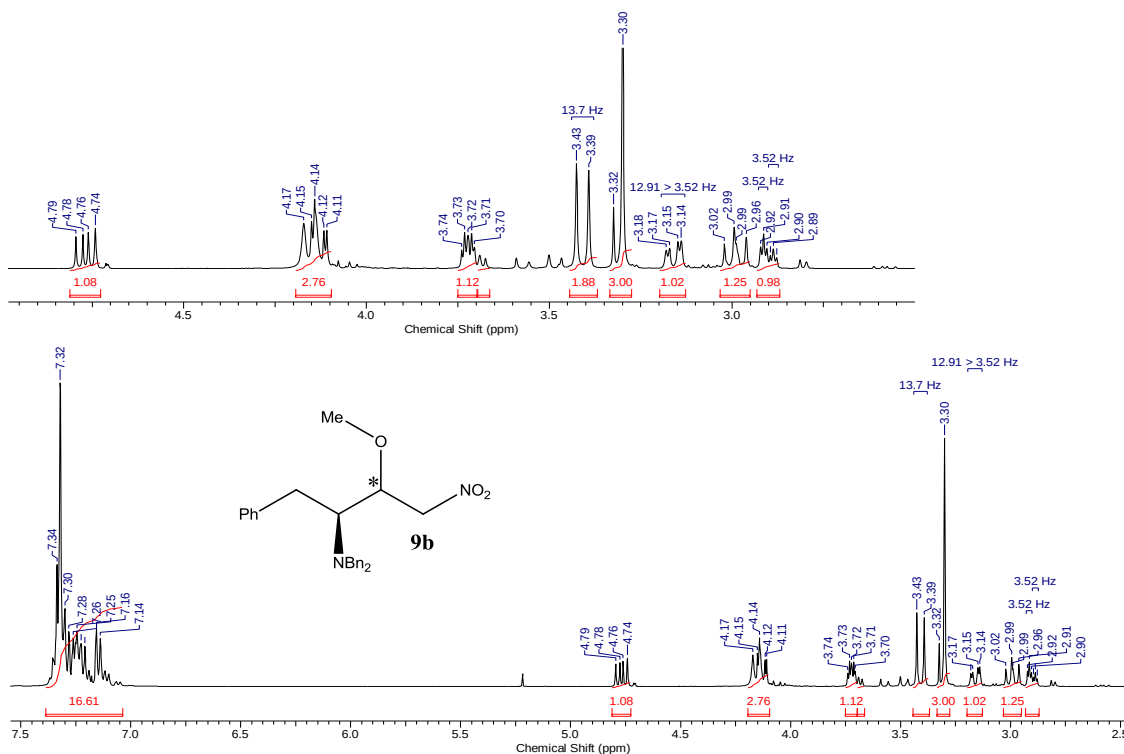


Bruker Compass DataAnalysis 4.0

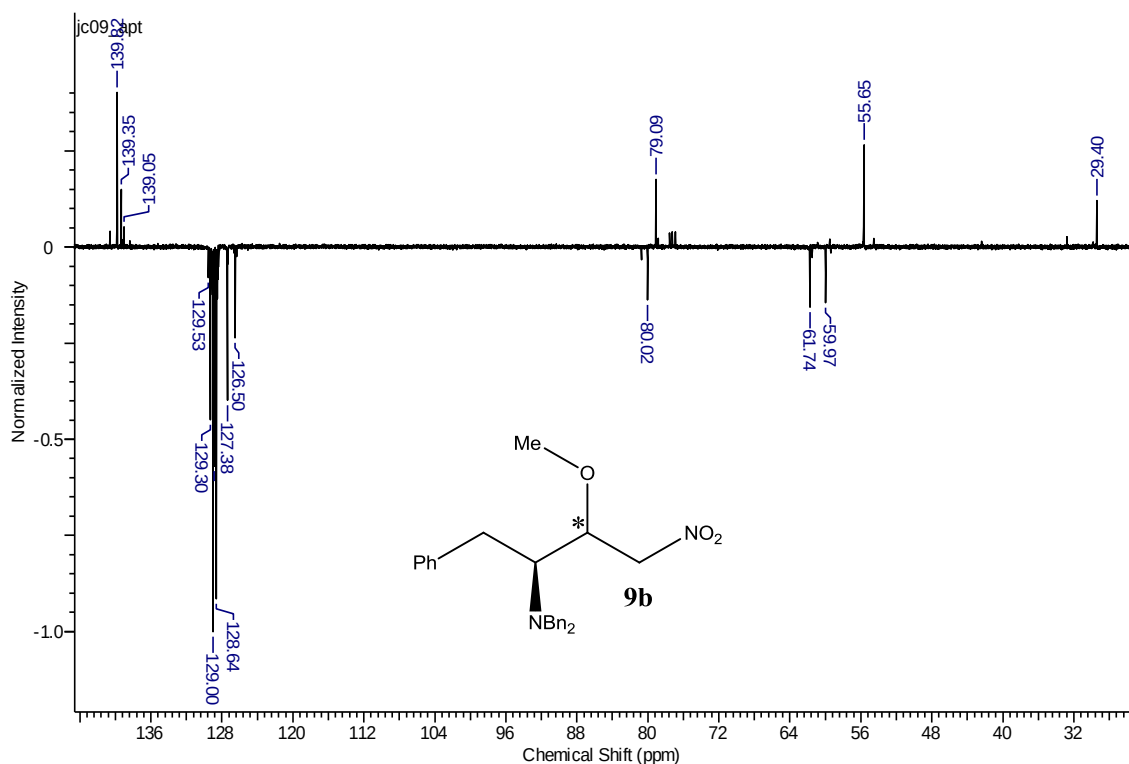
printed: 5/22/2012 2:40:00 PM

Page 1 of 1

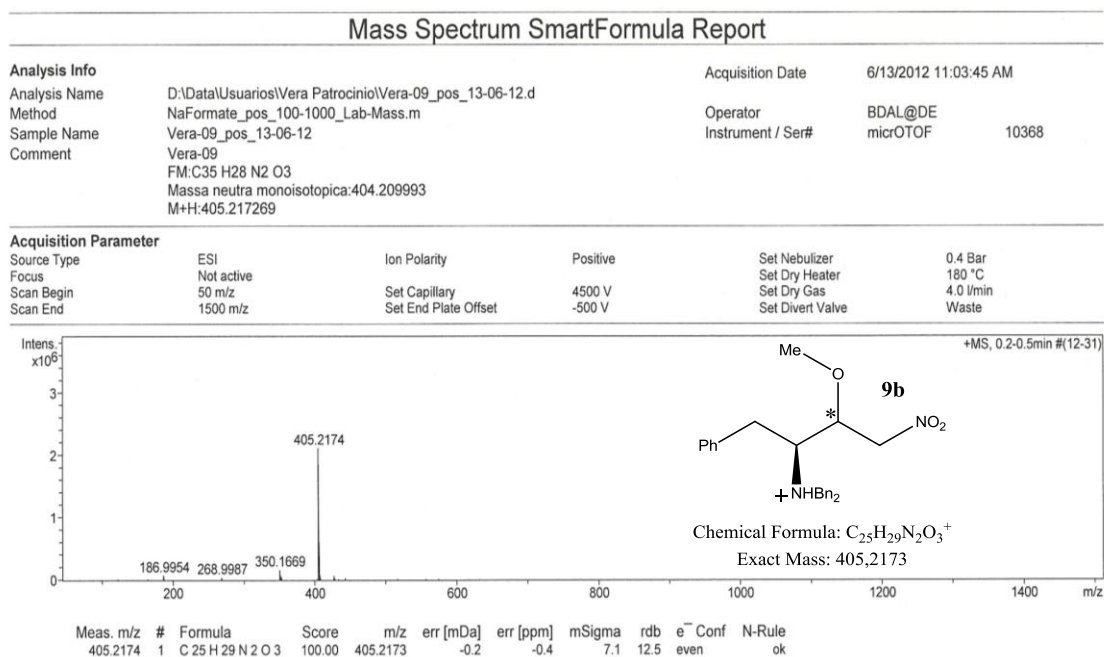
Spectrum 11: HRMS of 7b



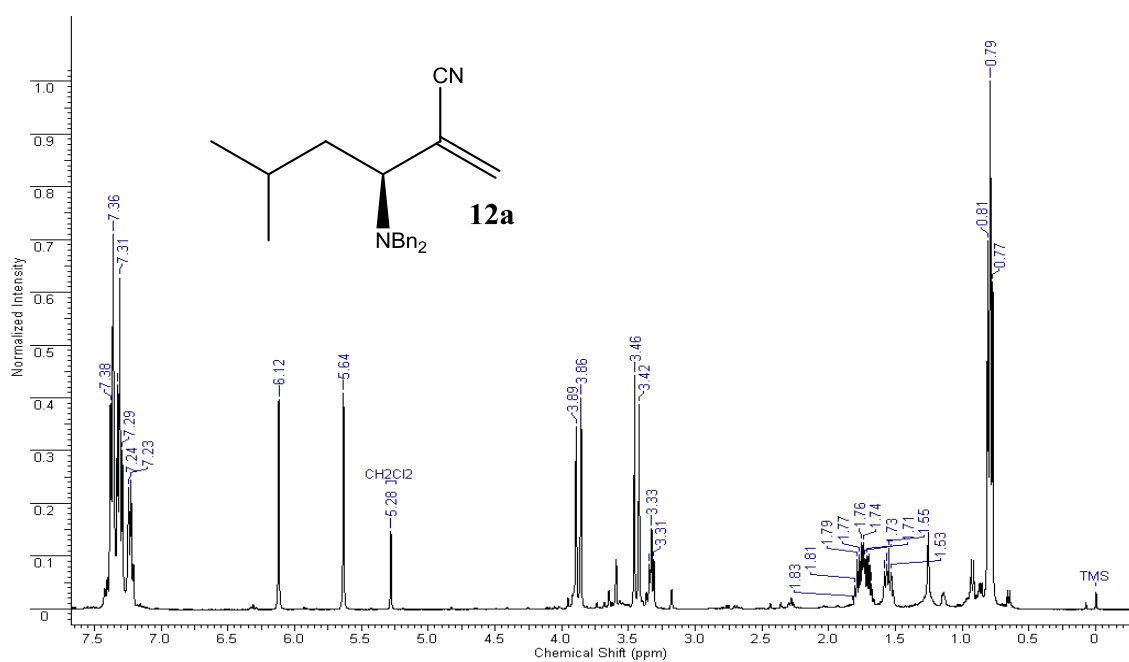
Spectrum 12: ¹H NMR (400 MHz, CDCl₃) of 9b



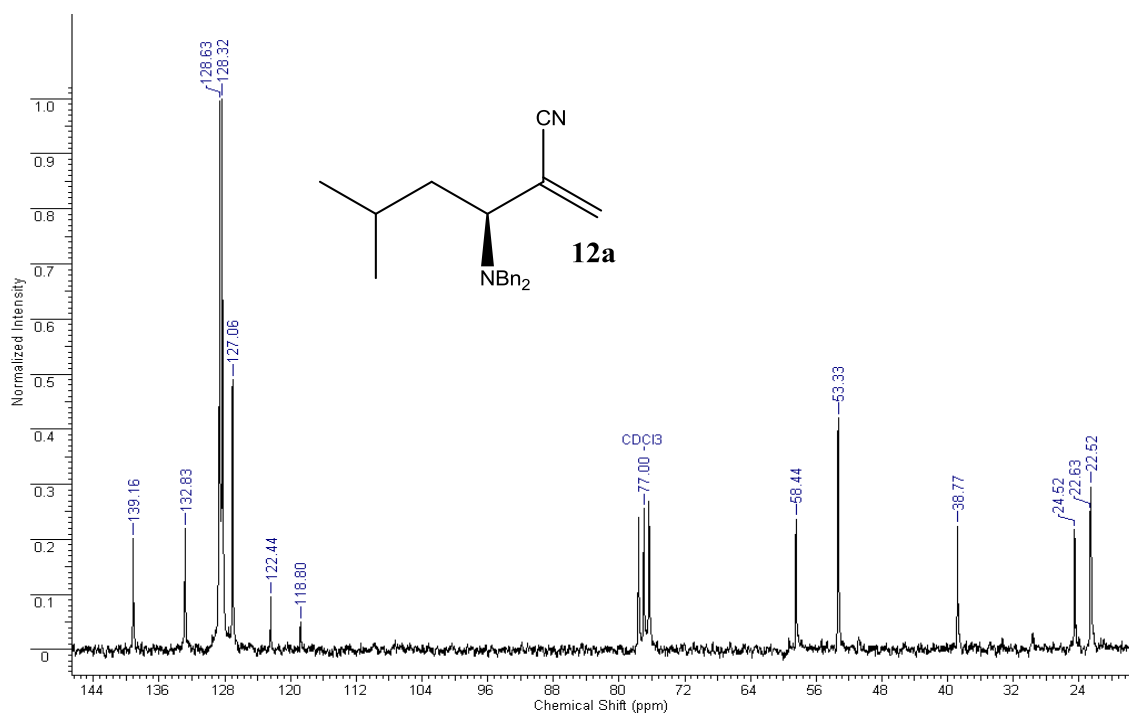
Spectrum 13: ^{13}C NMR (100 MHz, CDCl_3) (APT) of **9b**



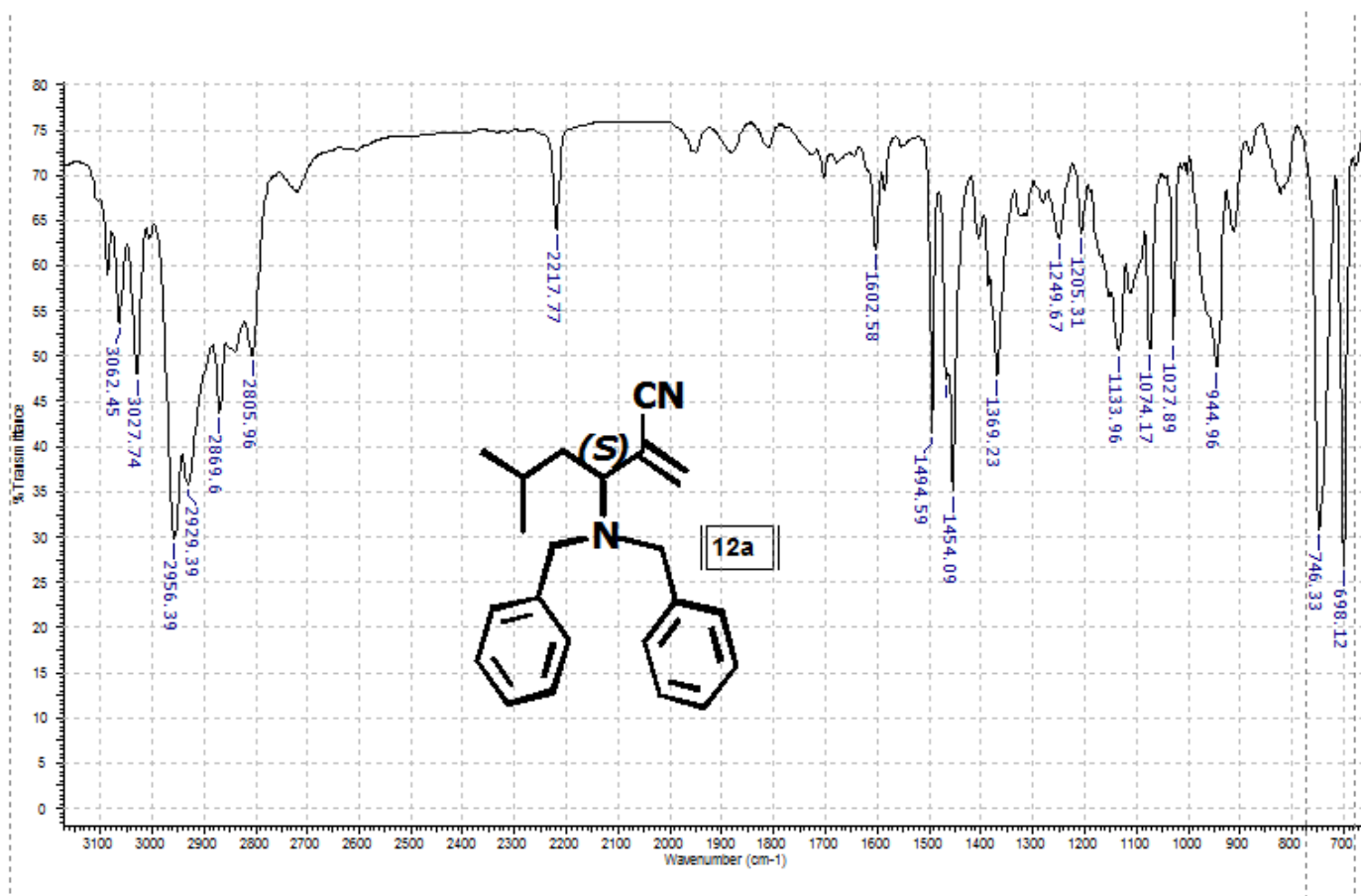
Spectrum 14: HRMS of **9b**



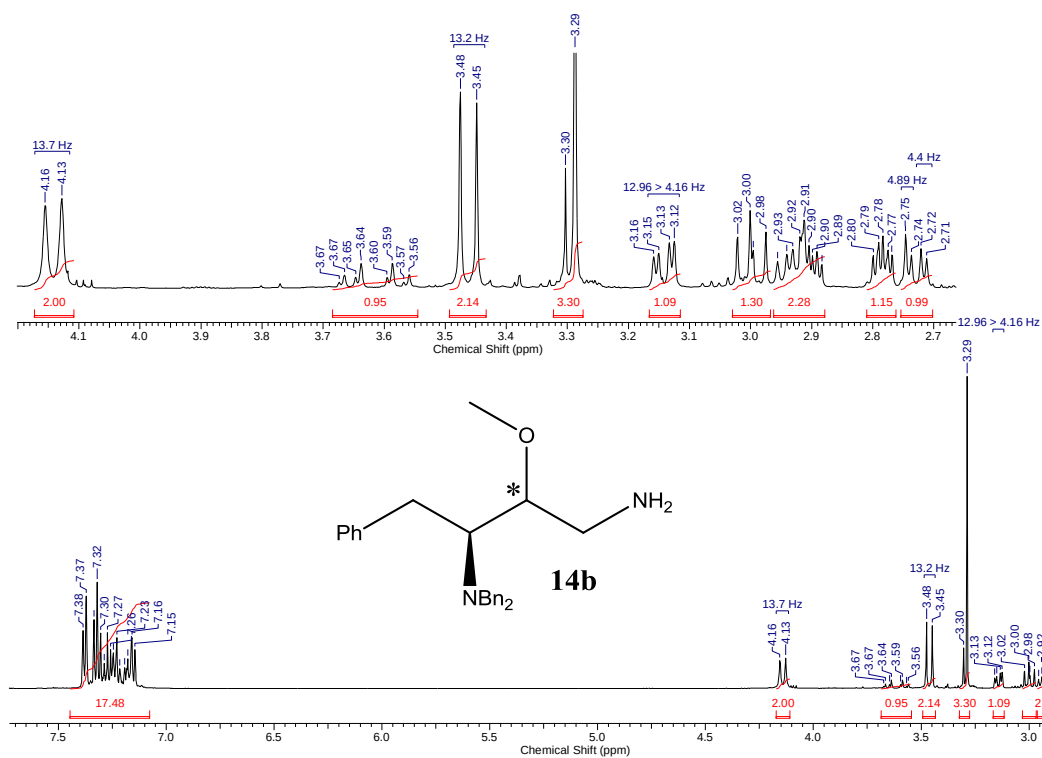
Spectrum 15: ¹H NMR (400 MHz, CDCl₃) of **12a**



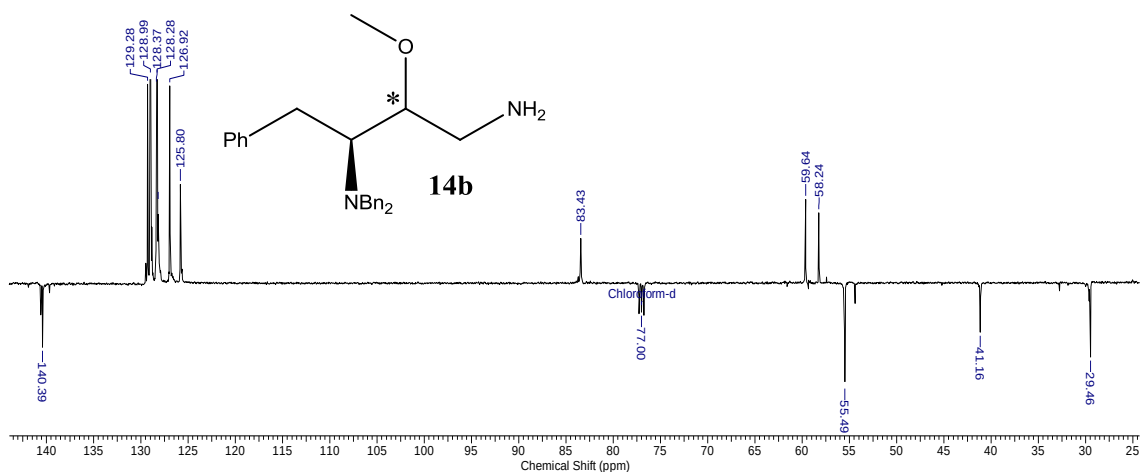
Spectrum 16: ¹³C NMR (100 MHz, CDCl₃) of **12a**



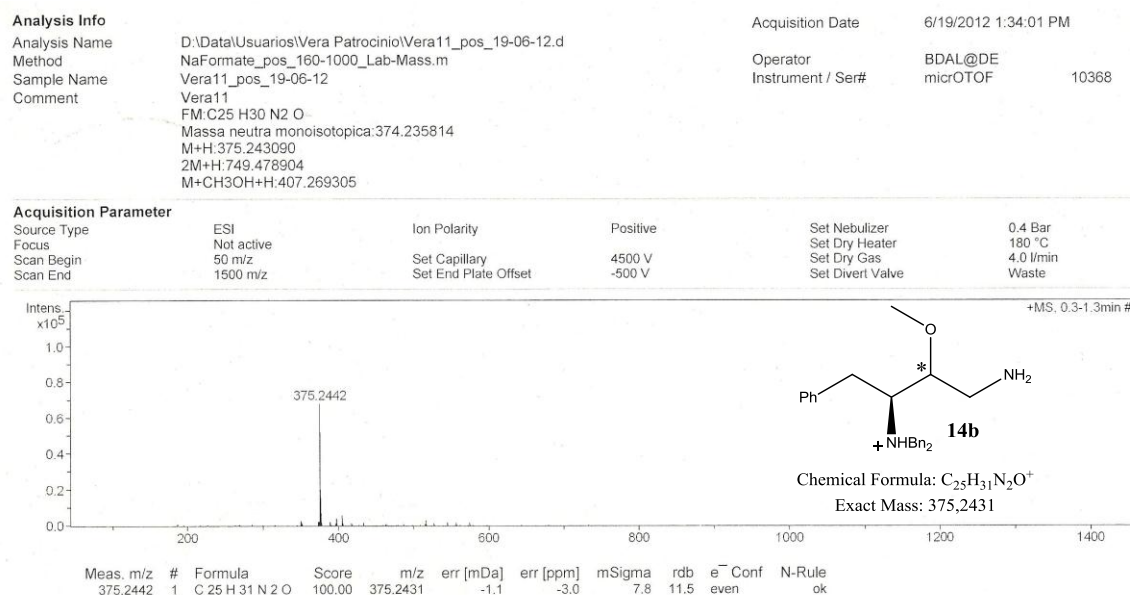
Spectrum 17: IR of 12a



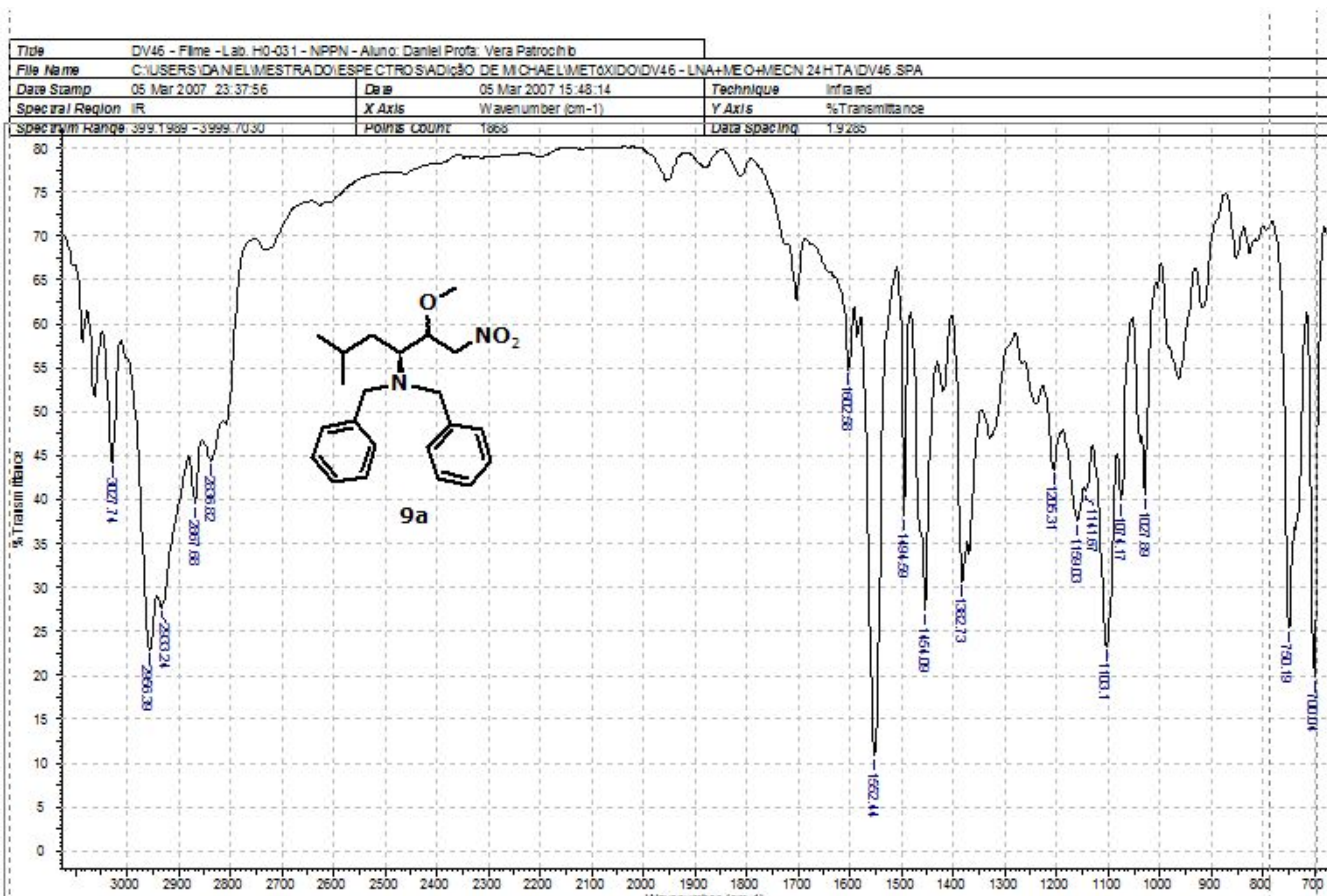
Spectrum 18: ¹H NMR (400 MHz, CDCl₃) of 14b



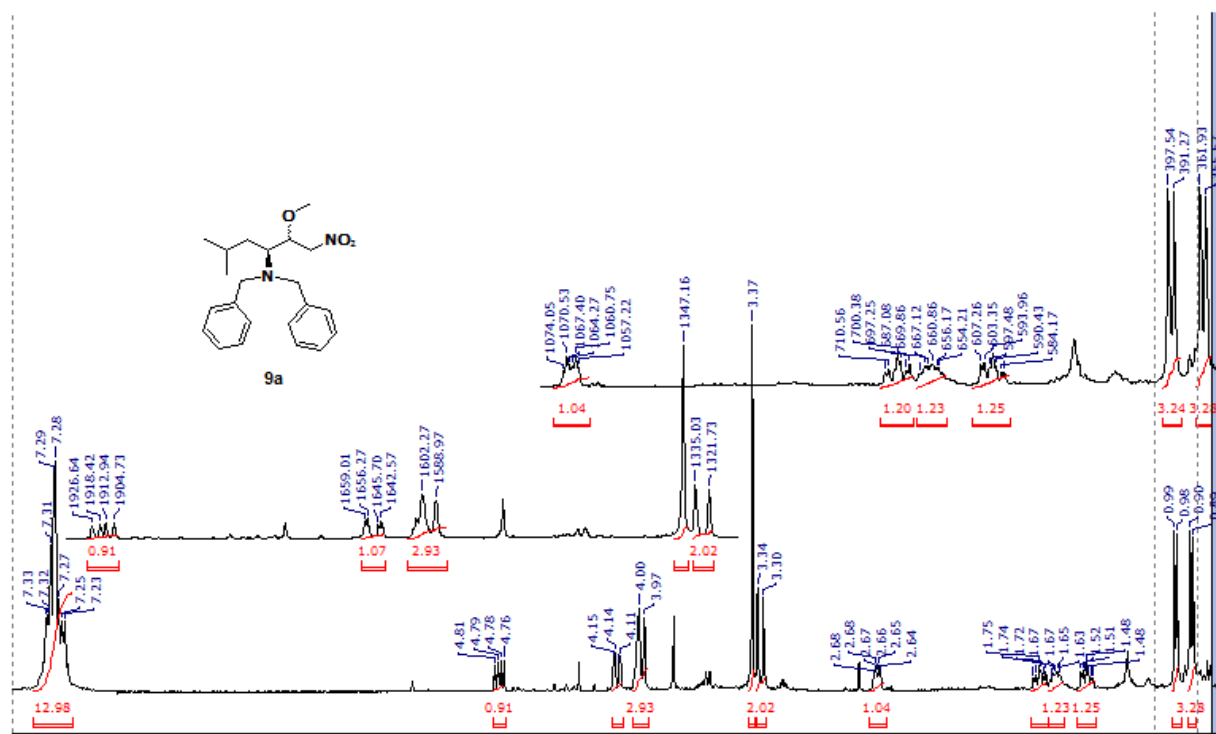
Spectrum 19: ¹³C NMR-APT (100 MHz, CDCl₃) of 14b



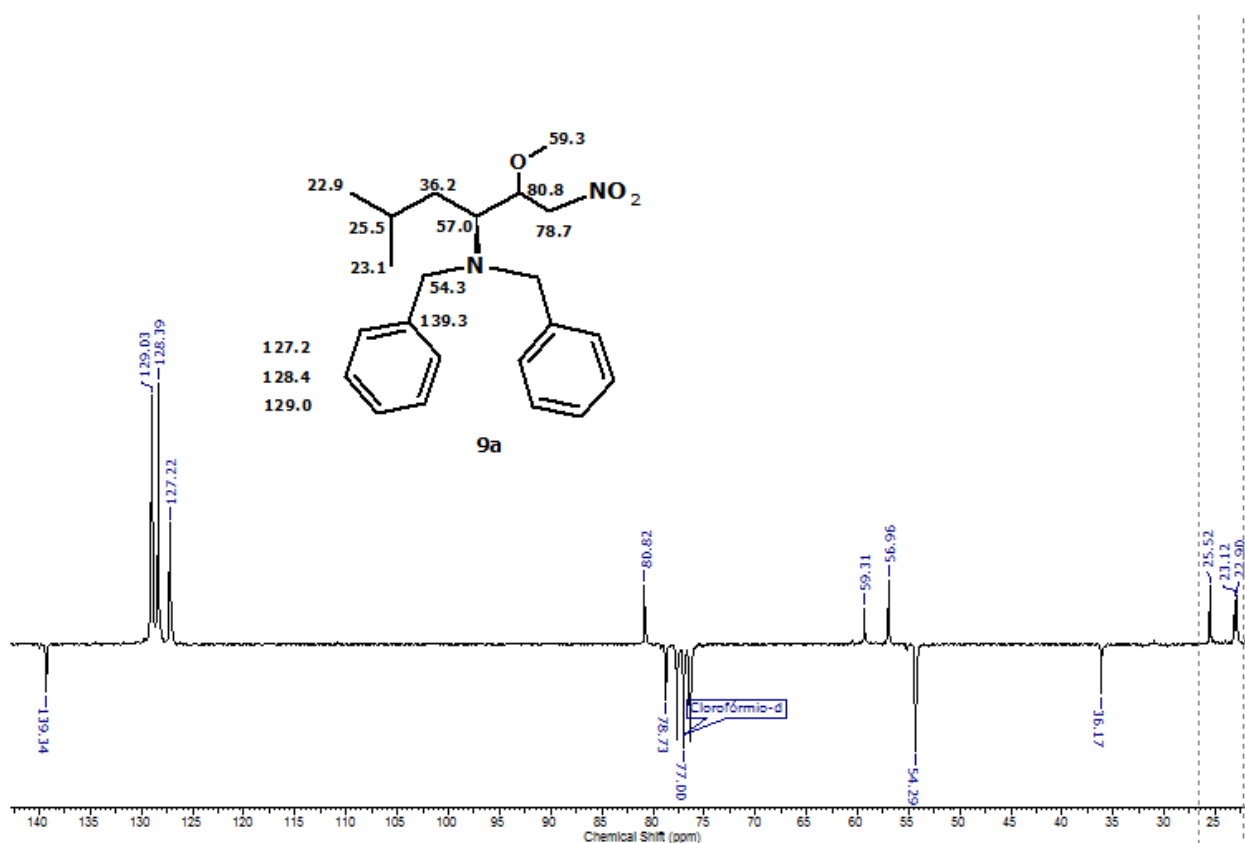
Spectrum 20: HRMS of 14b



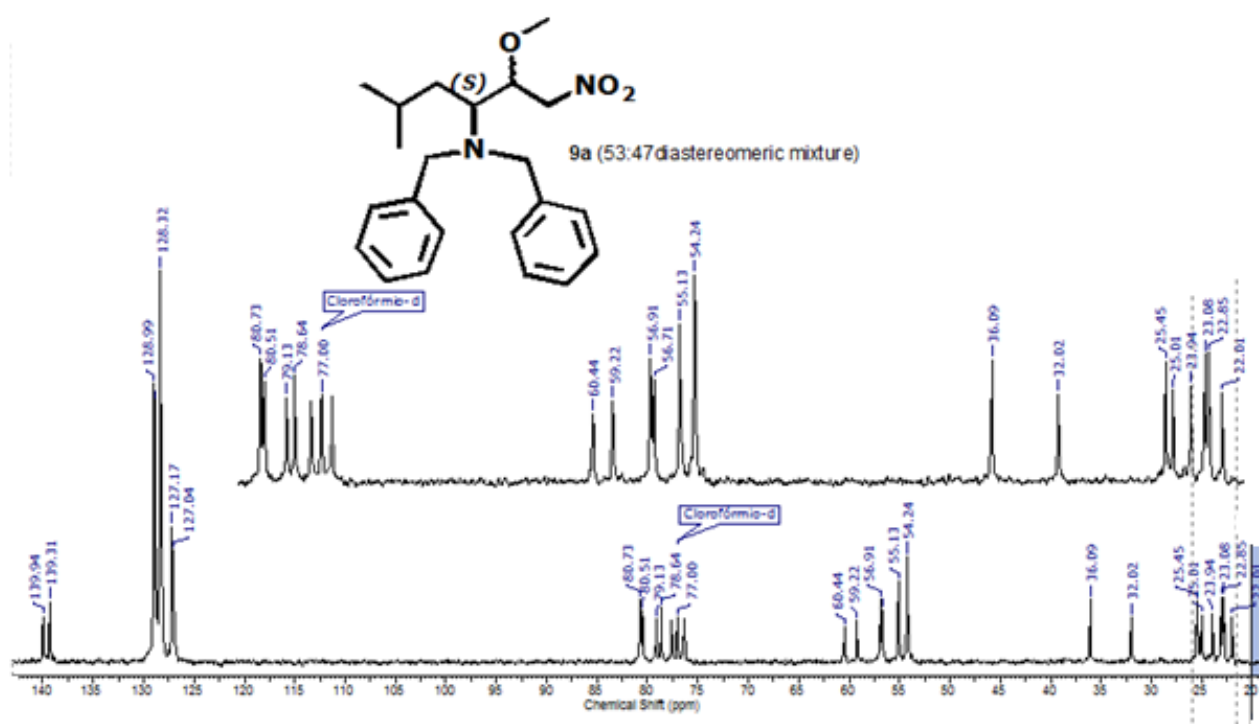
Spectrum 21: IR of 9a



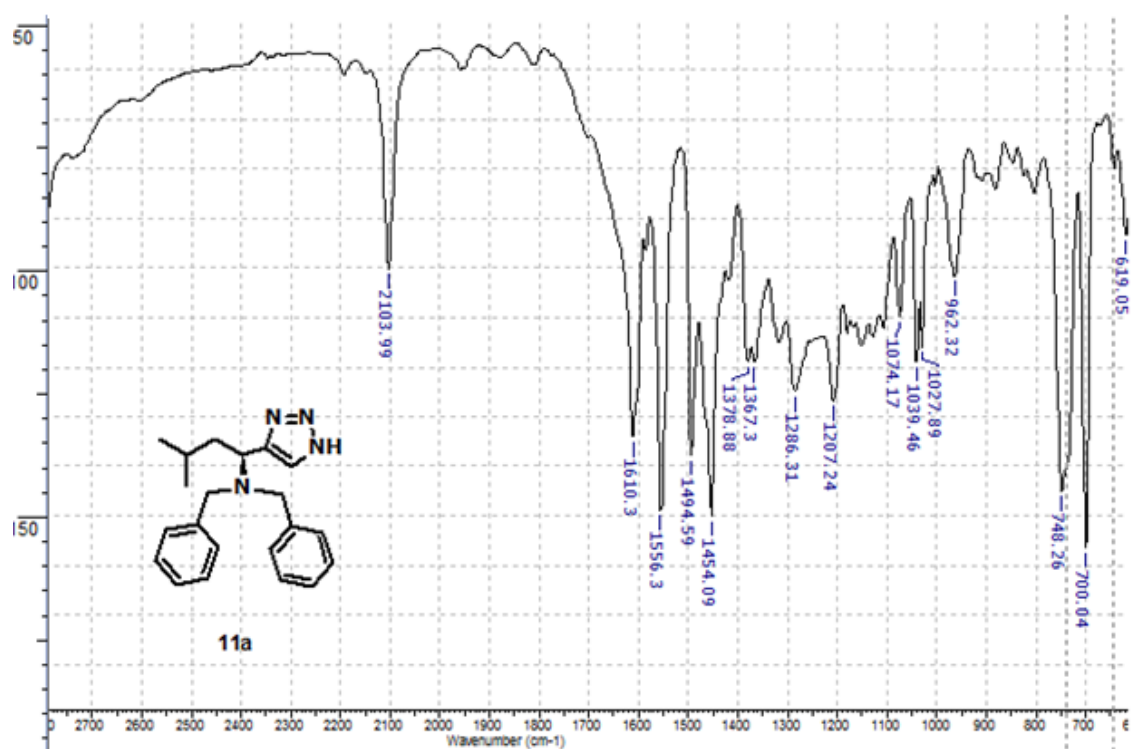
Spectrum 22: ¹H NMR of 9a (400 MHz - CDCl₃) - diastereomeric mixture 53:47



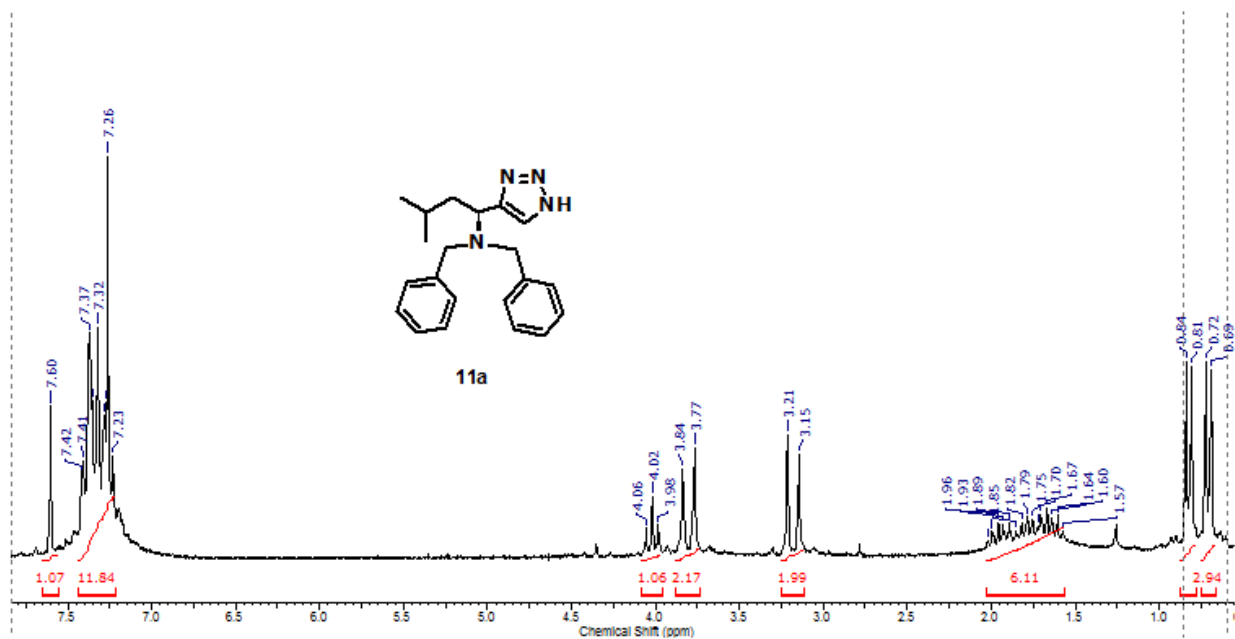
Spectrum 23: ¹³C NMR-APT (400 MHz, CDCl₃) of 9a (d.e. >95%)



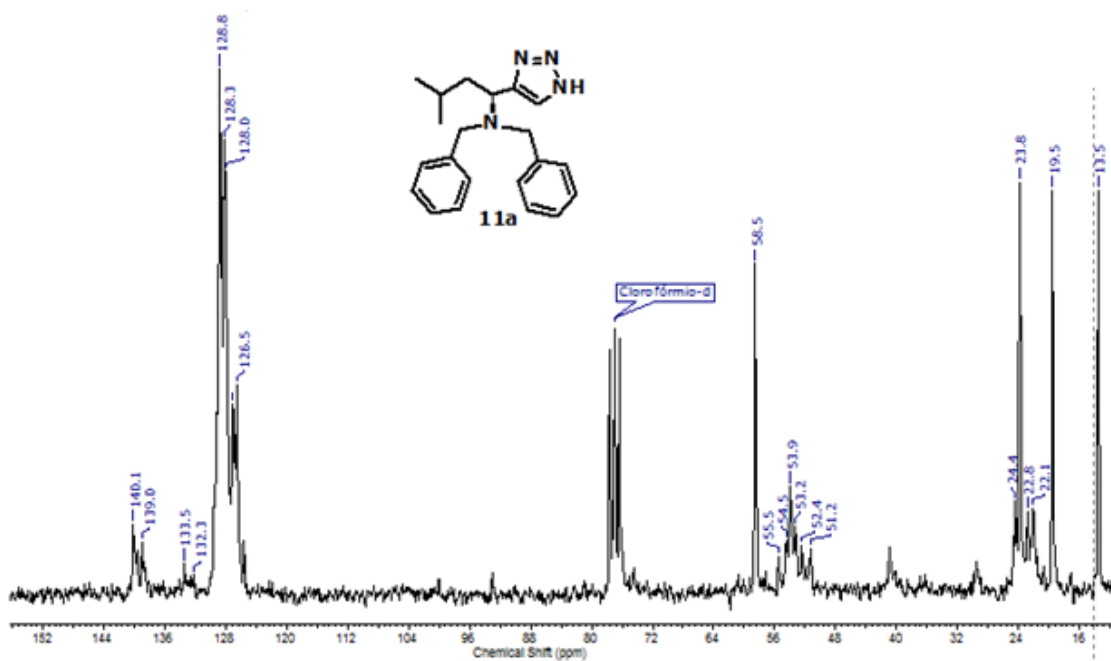
Spectrum 24: ¹³C NMR of 9a (50 MHz, CDCl₃) (53:47 diastereomeric mixture)



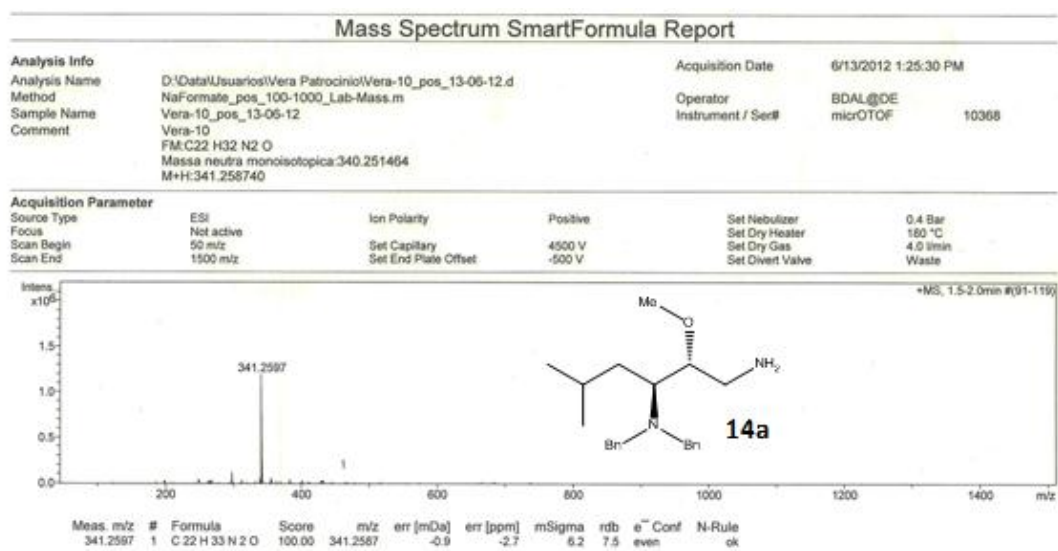
Spectrum 25: IR of 11a



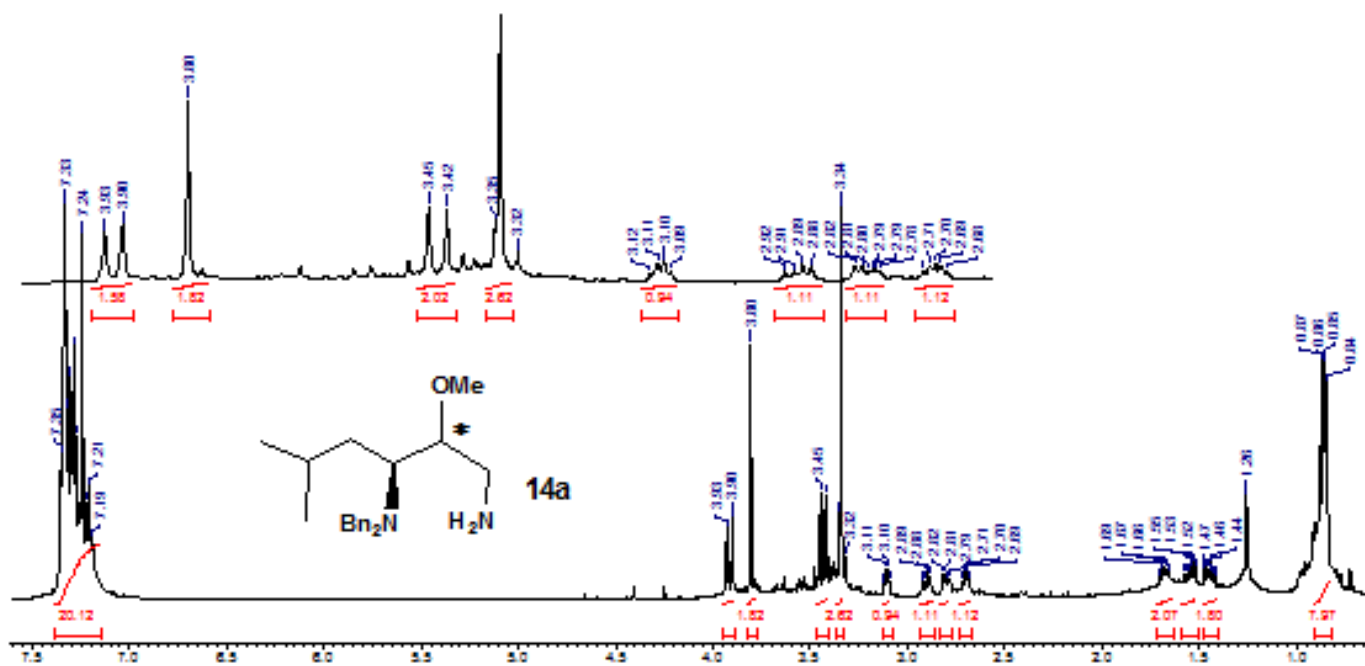
Spectrum 26: ¹H NMR (400 MHz, CDCl₃) of 11a (Mixture of tautomers)



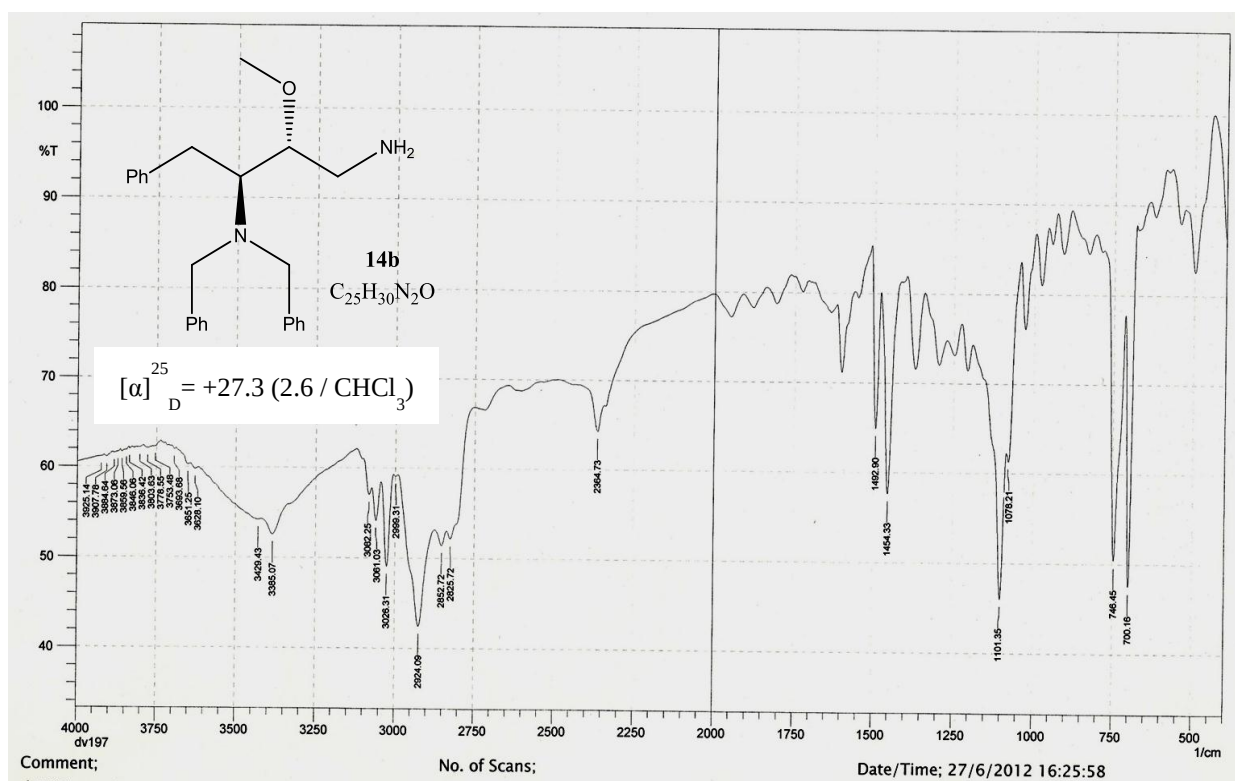
Spectrum 27: ^{13}C NMR (50 MHz, CDCl_3) of 11a (Mixture of tautomers)



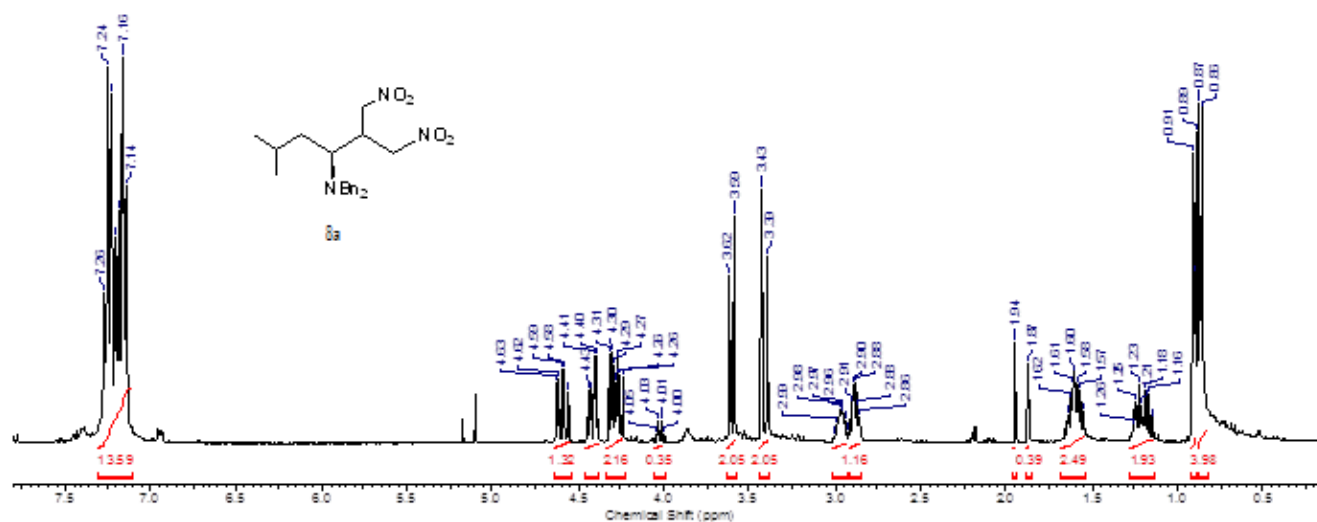
Spectrum 28: HRMS of 14a



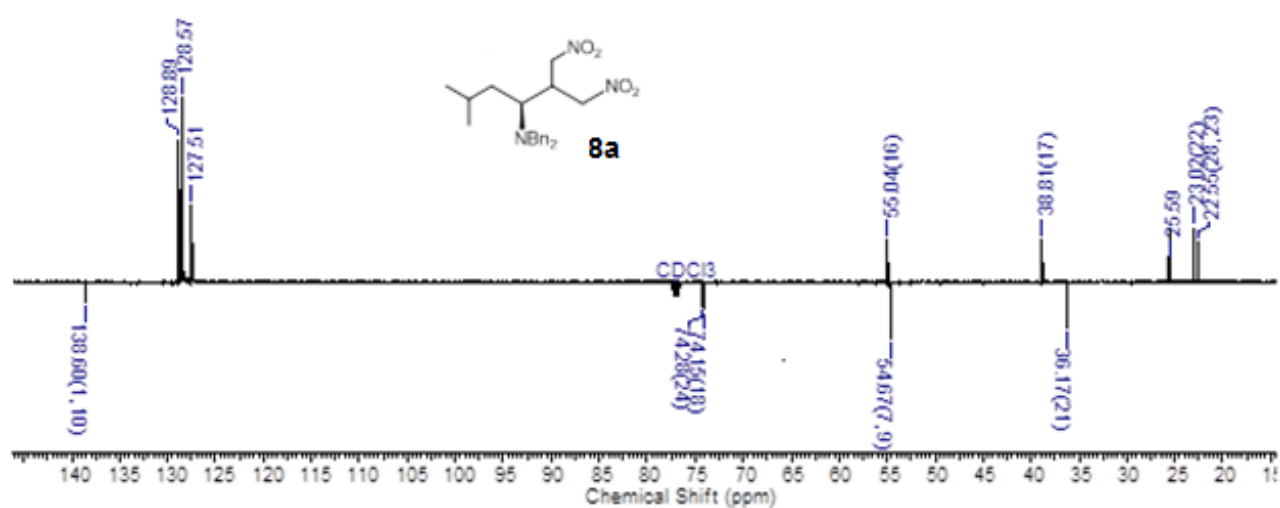
Spectrum 29: ^{13}C NMR of 14a (400 MHz, CD_3OD)



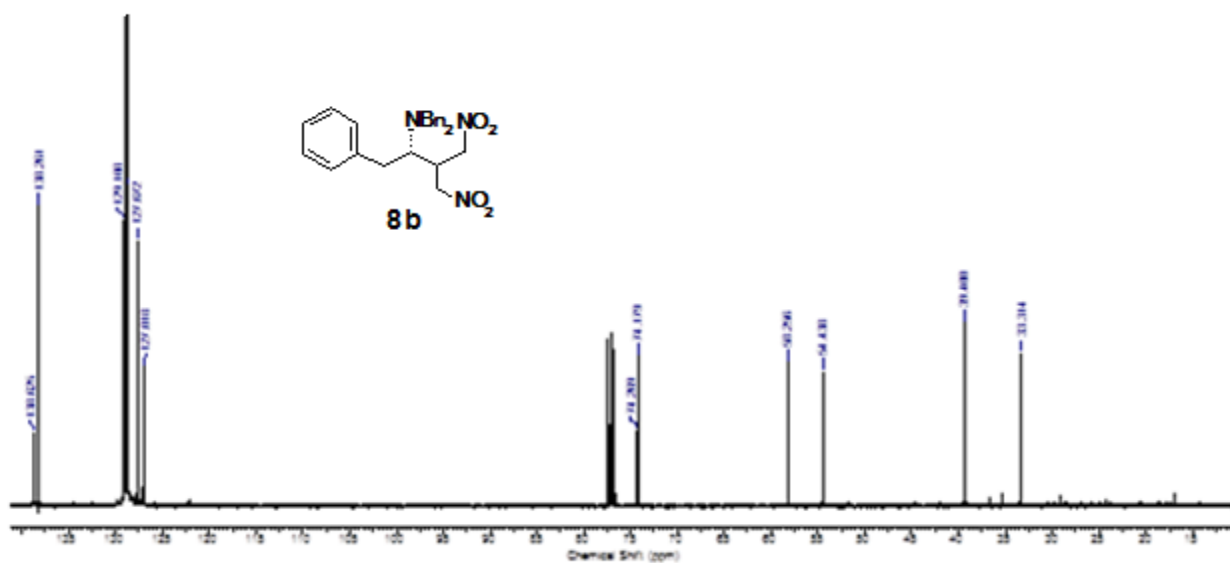
Spectrum 30: IR of 14b



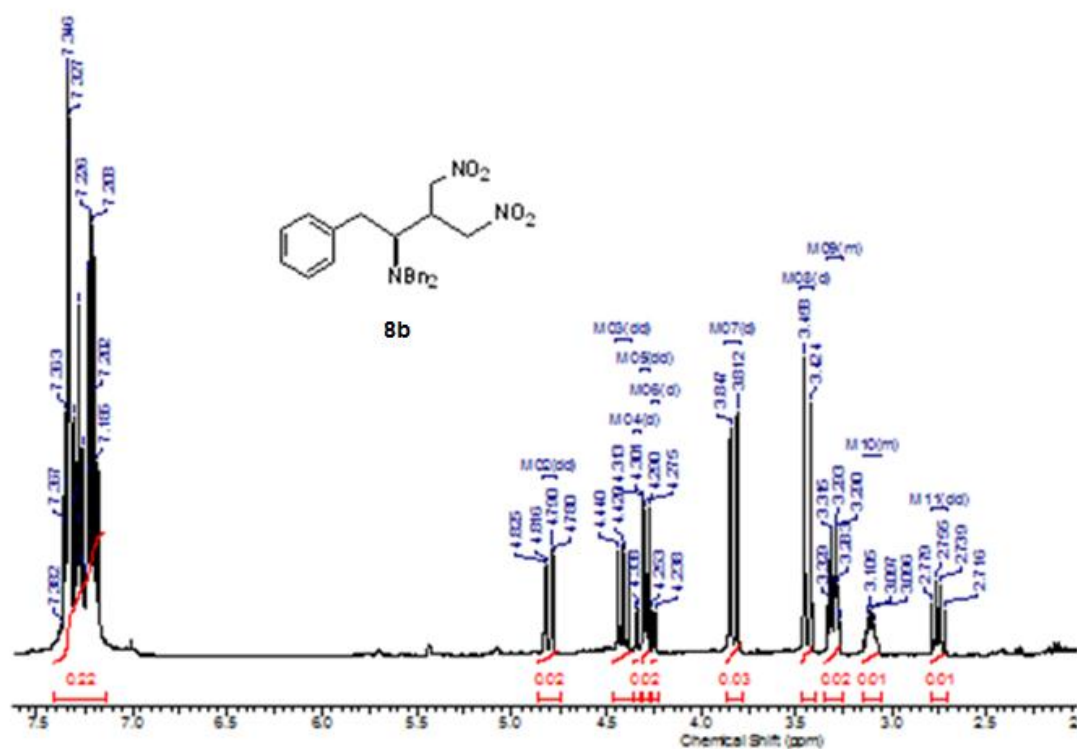
Spectrum 31: ¹H NMR (400 MHz, CDCl₃) of **8a**



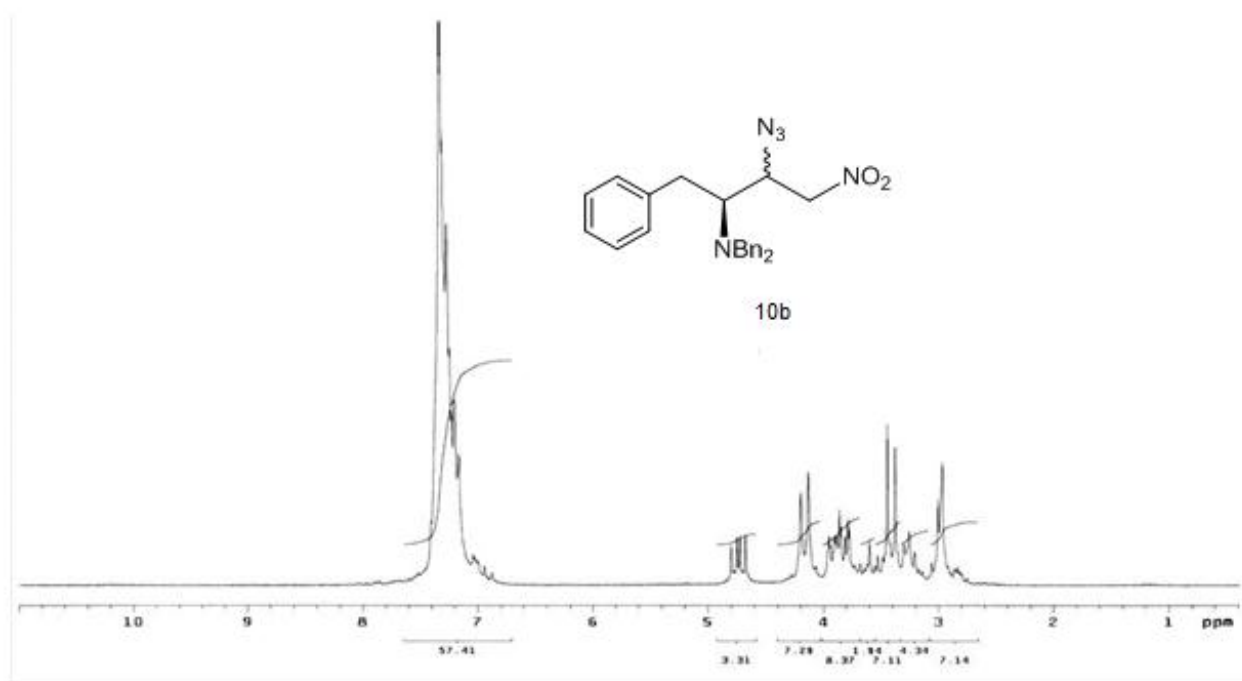
Spectrum 32: ¹³C NMR (50 MHz, CDCl₃) of **8a**



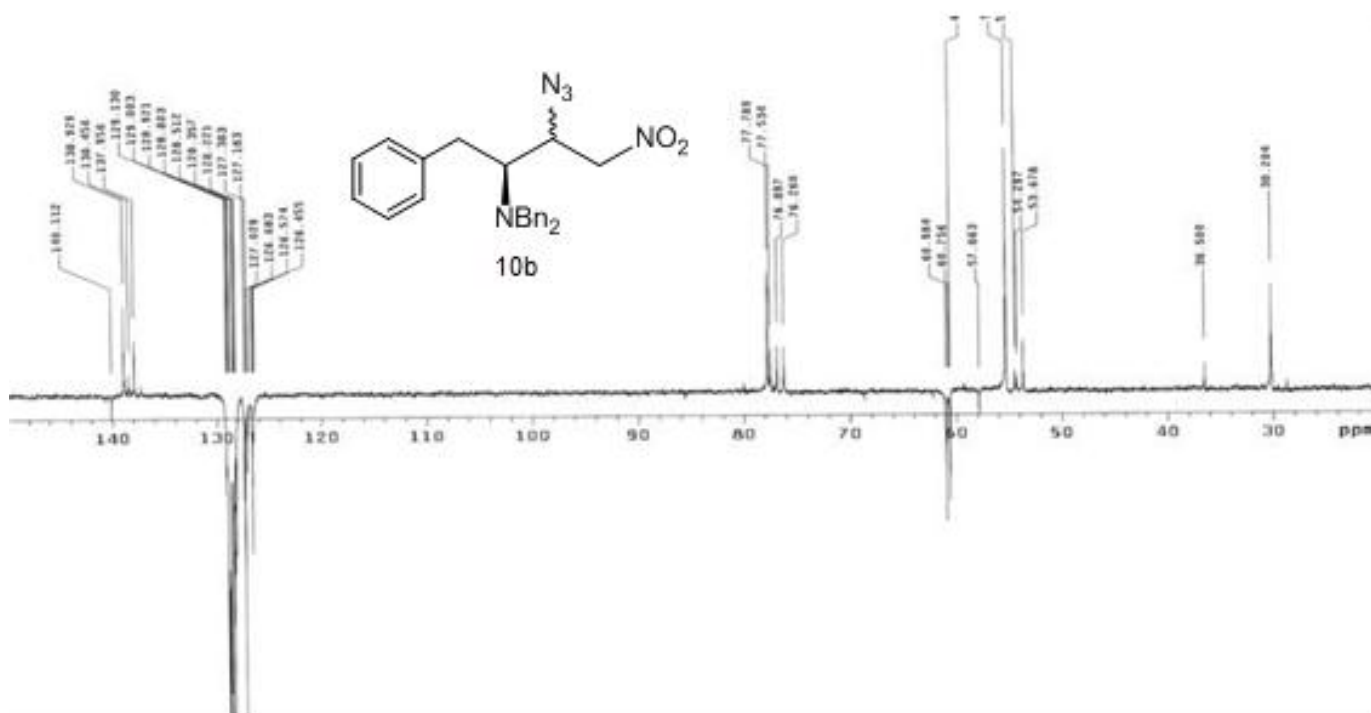
Spectrum 33: ¹³C NMR (50 MHz, CDCl₃) of 8b



Spectrum 34: ¹H NMR (400 MHz, CDCl₃) of 8b.



Spectrum 35: ¹H NMR (200 MHz, CDCl₃) of 10b.



Spectrum 36: ¹³C NMR-APT (200 MHz, CDCl₃) of 10b.