

Electronic Supporting information

Straightforward synthesis of bistetraazacycloalkanes: towards new potential CXCR4 antagonists?

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Franck Denat ^{[b]*}

Table of contents

Figure 1: ¹ H NMR of the mixture compound 2 a-c (300 MHz, CDCl ₃ , 300 K).....	1
Figure 2: ¹³ C NMR of the mixture of compounds 2 a-c (75 MHz, CDCl ₃ , 300 K)	1
Figure 3: Mass spectrum of the mixture of compounds 2 a-c (HRMS-MALDI-TOF)	2
Figure 4: ¹ H NMR of the mixture of compounds 3 a-c (300 MHz, CDCl ₃ , 300 K).....	2
Figure 5: ¹³ C NMR of the mixture of compounds 3 a-c (75 MHz, CDCl ₃ , 300 K)	3
Figure 6: Mass spectrum of the mixture of compounds 3 a-c (HRMS-MALDI-TOF)	3
Figure 7: ¹ H NMR of compound 4 a -c (300 MHz, CDCl ₃ , 300 K)	4
Figure 8: Mass spectrum of compound 4 a - c (ESI-TOF)	4
Figure 9: ¹ H NMR of compound 5 (300 MHz, D ₂ O, 300 K)	5
Figure 10: ¹³ C NMR of compound 5 (75 MHz, D ₂ O, 300 K)	5
Figure 11: Mass spectrum of compound 5 (ESI-TOF).....	6
Figure 12: ¹ H NMR of compound 6 (300 MHz, D ₂ O, 300 K)	6
Figure 13: ¹³ C NMR of compound 6 (75 MHz, D ₂ O, 300 K)	7
Figure 14: Mass spectrum of compound 6 (ESI-TOF)	7
Figure 15: ¹ H NMR of compound 7 (600 MHz, D ₂ O, 300 K)	8
Figure 16: ¹³ C NMR of compound 7 (150 MHz, D ₂ O, 300 K)	8
Figure 17: Mass spectrum of compound 7 (ESI-TOF)	9
Figure 18: ¹ H NMR of compound 8 (300 MHz, CDCl ₃ , 300 K)	9
Figure 19: ¹³ C NMR of compound 8 (150 MHz, CDCl ₃ , 300 K)	10
Figure 20: Mass spectrum of compound 8 (HRMS-MALDI-TOF)	10
Figure 21: ¹ H NMR of compound 9 (150 MHz, CDCl ₃ , 300 K)	11
Figure 22: ¹³ C NMR of compound 9 (150 MHz, CDCl ₃ , 300 K)	11
Figure 23: Mass spectrum of compound 9 (HRMS-MALDI-TOF)	12
Figure 24: ¹ H NMR of compound 11 (300 MHz, CDCl ₃ , 300 K)	12
Figure 25: ¹³ C NMR of compound 11 (75 MHz, CDCl ₃ , 300 K)	13
Figure 26: Mass spectrum of compound 11 (MALDI-TOF)	13
Figure 27: ¹ H NMR of compound 12 (300 MHz, CDCl ₃ , 300 K)	14
Figure 28: ¹³ C NMR of compound 12 (75 MHz, CDCl ₃ , 300 K)	14
Figure 29: Mass spectrum of compound 12 (ESI-TOF)	15

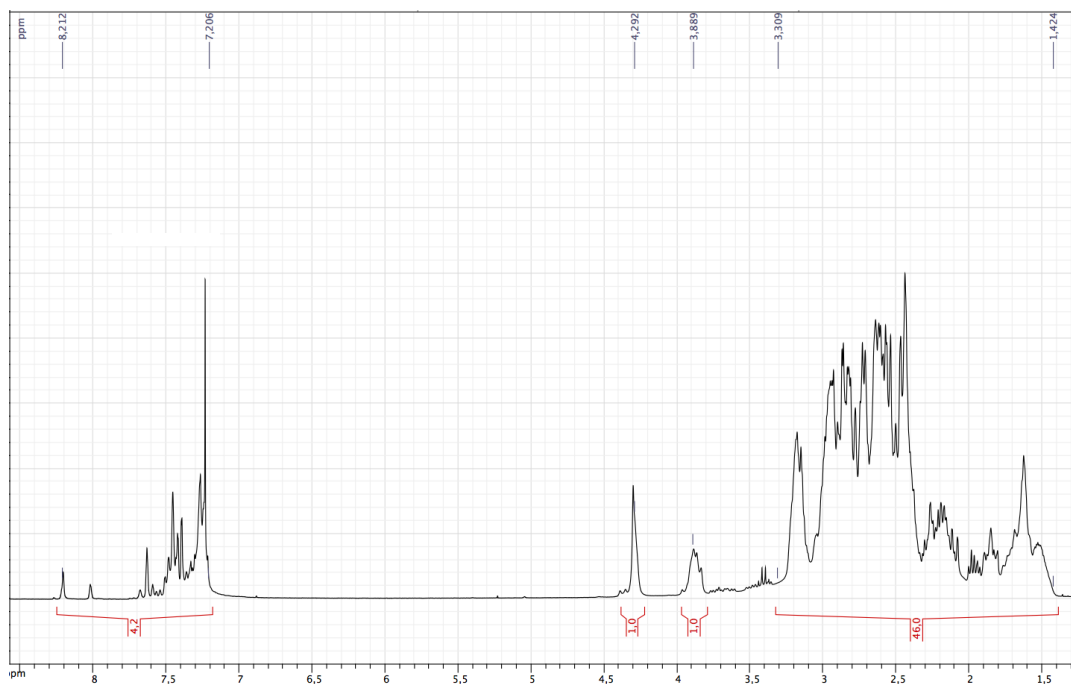


Figure 1: ^1H NMR of the mixture compound 2 a-c (300 MHz, CDCl_3 , 300 K)

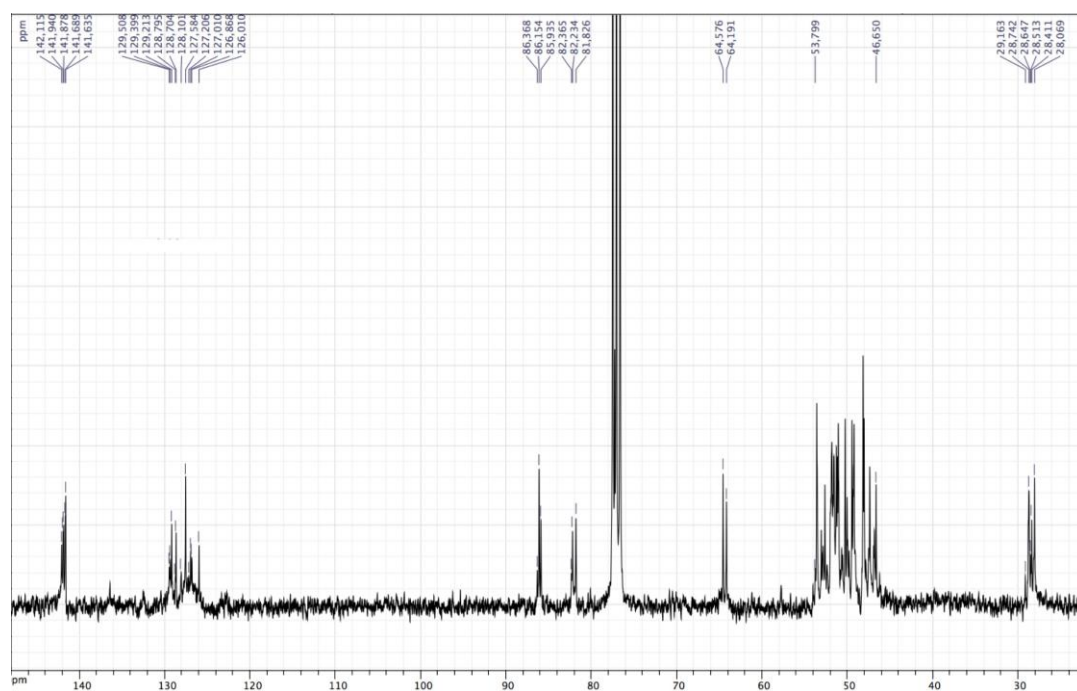


Figure 2: ^{13}C NMR of the mixture of compounds 2 a-c (75 MHz, CDCl_3 , 300 K)

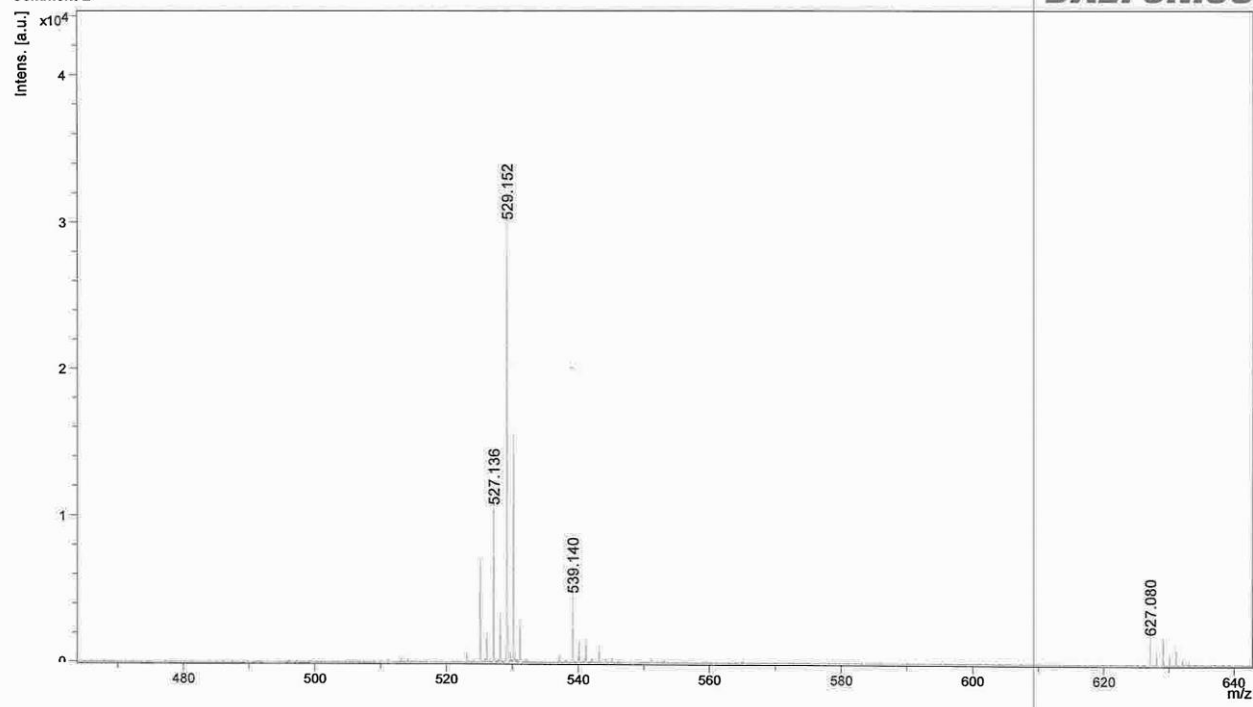


Figure 3: Mass spectrum of the mixture of compounds 2 a-c (HRMS-MALDI-TOF)

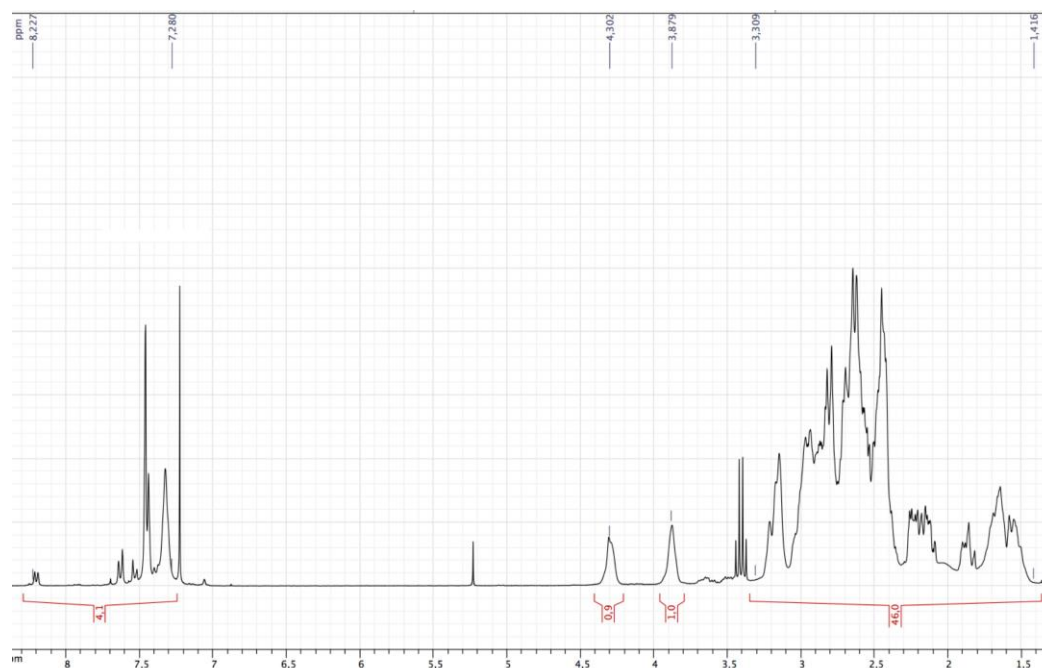


Figure 4: ¹H NMR of the mixture of compounds 3 a-c (300 MHz, CDCl₃, 300 K)

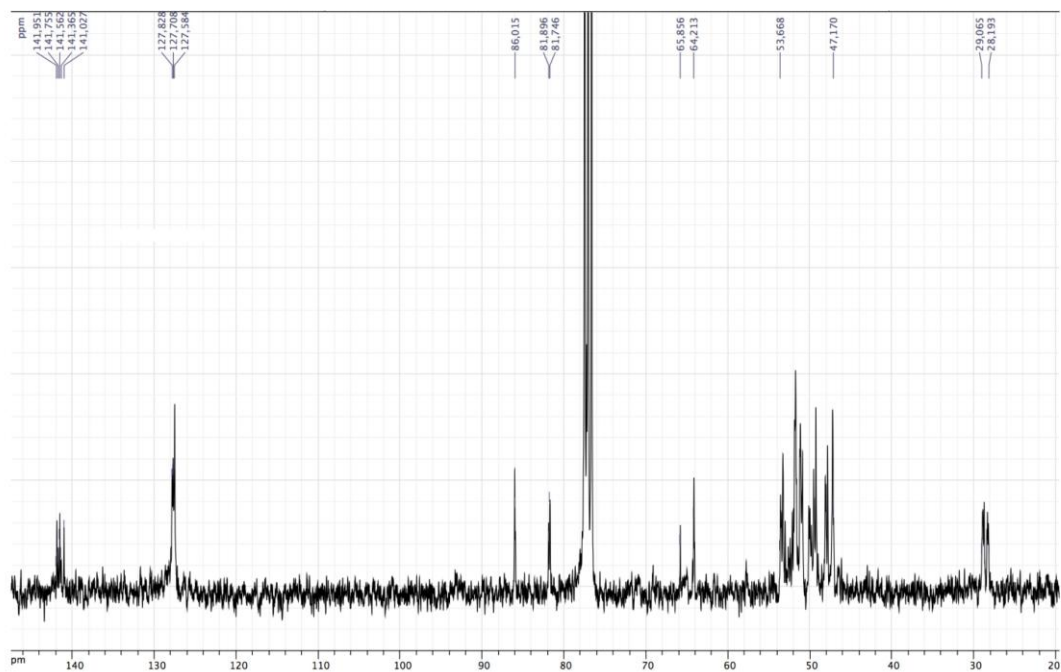


Figure 5: ^{13}C NMR of the mixture of compounds 3 a-c (75 MHz, CDCl_3 , 300 K)

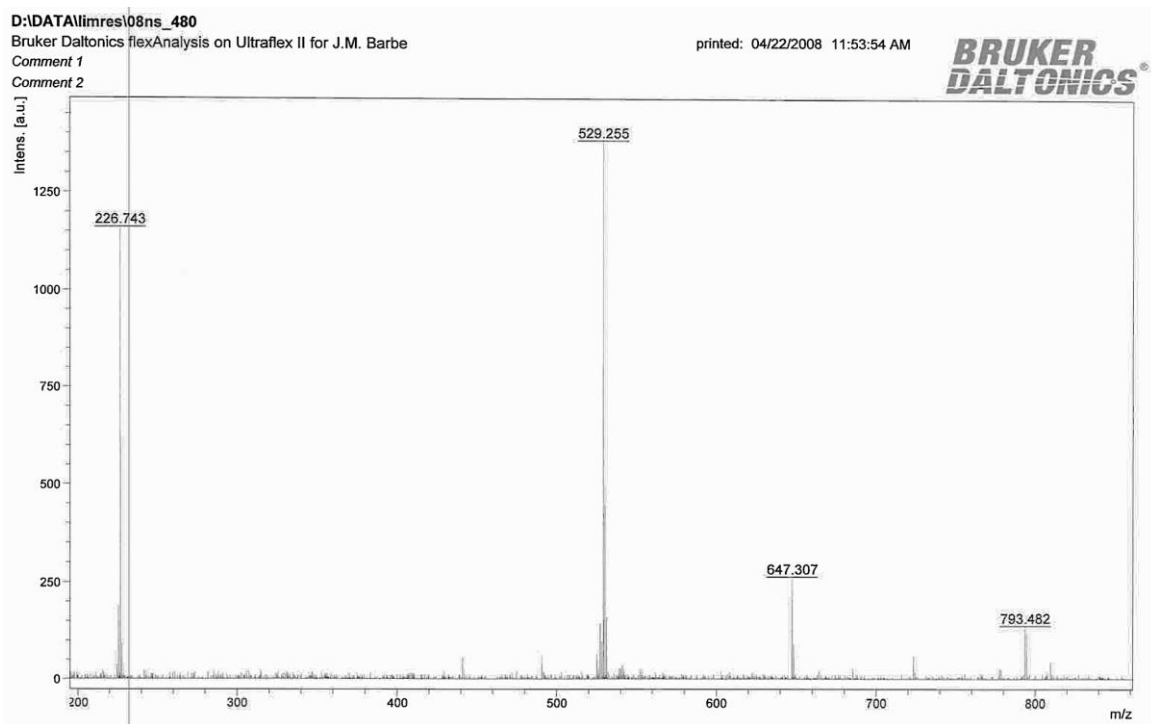


Figure 6: Mass spectrum of the mixture of compounds 3 a-c (HRMS-MALDI-TOF)

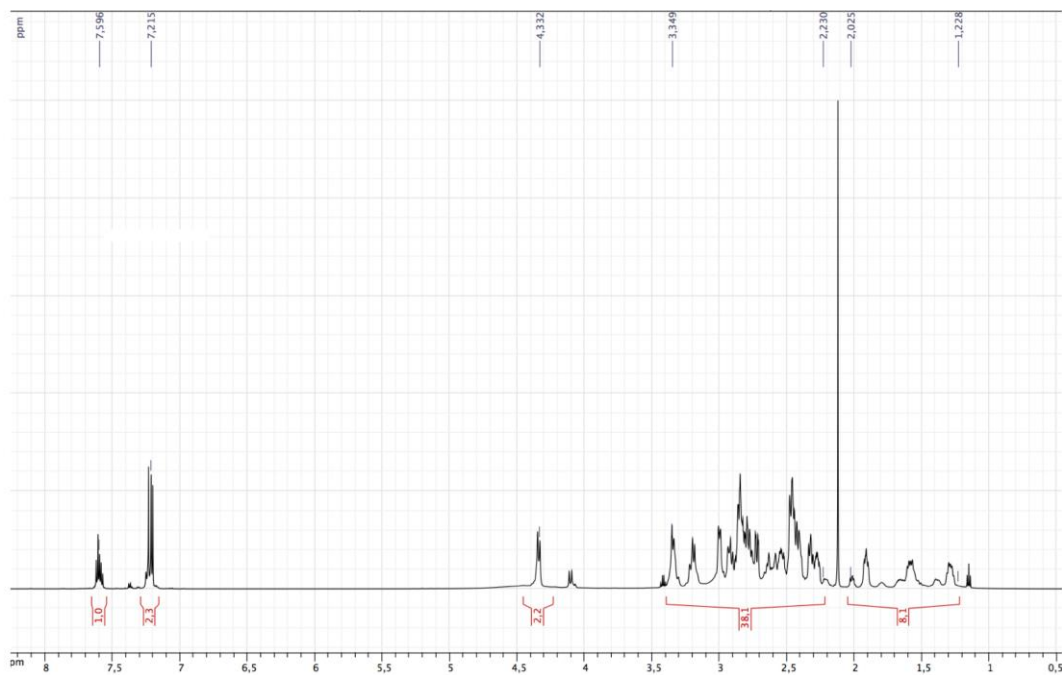


Figure 7: ^1H NMR of compound 4 a - c (300 MHz, CDCl_3 , 300 K)

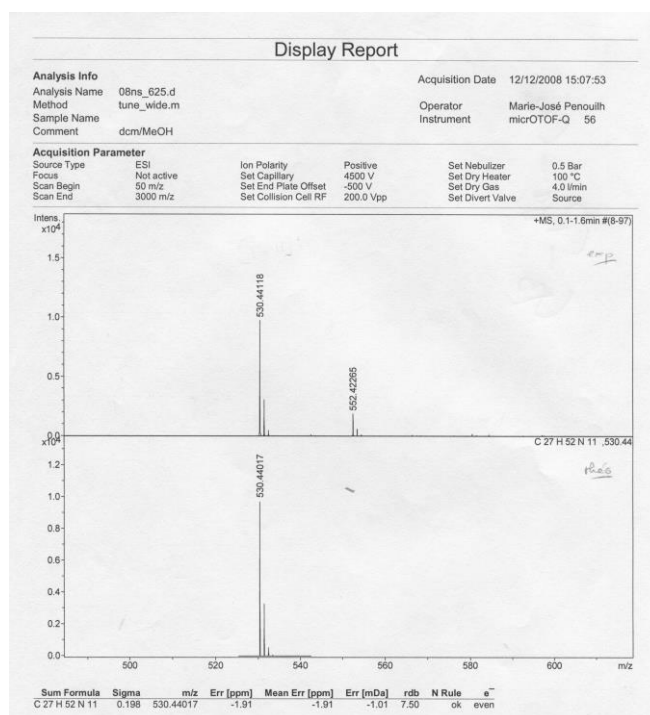


Figure 8: Mass spectrum of compound 4 a - c (ESI-TOF)

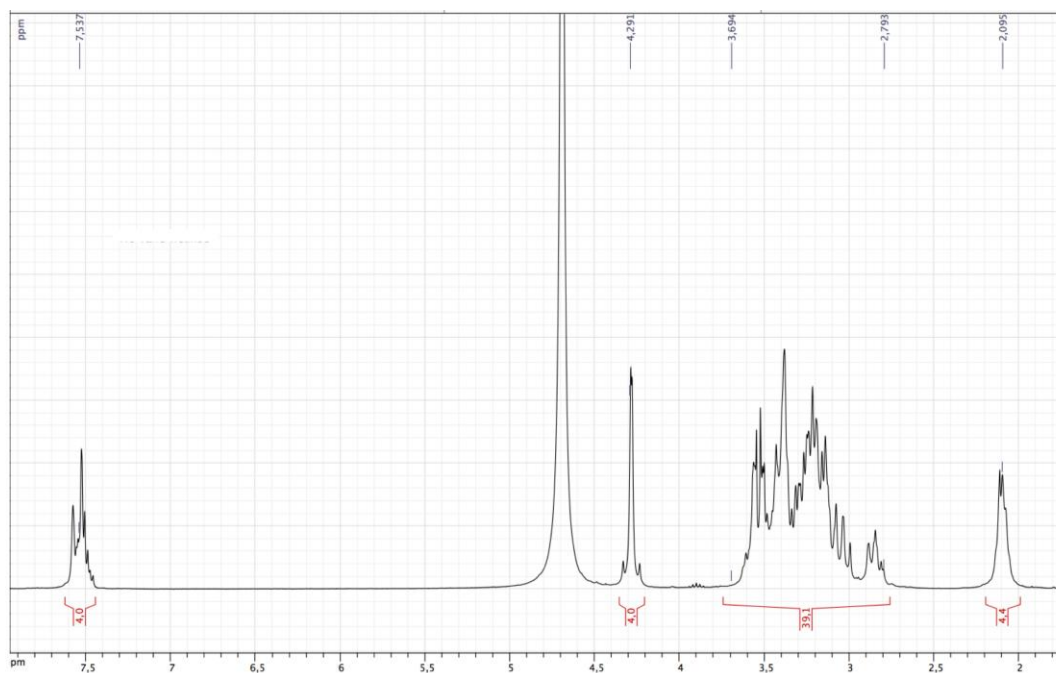


Figure 9: ^1H NMR of compound 5 (300 MHz, D_2O , 300 K)

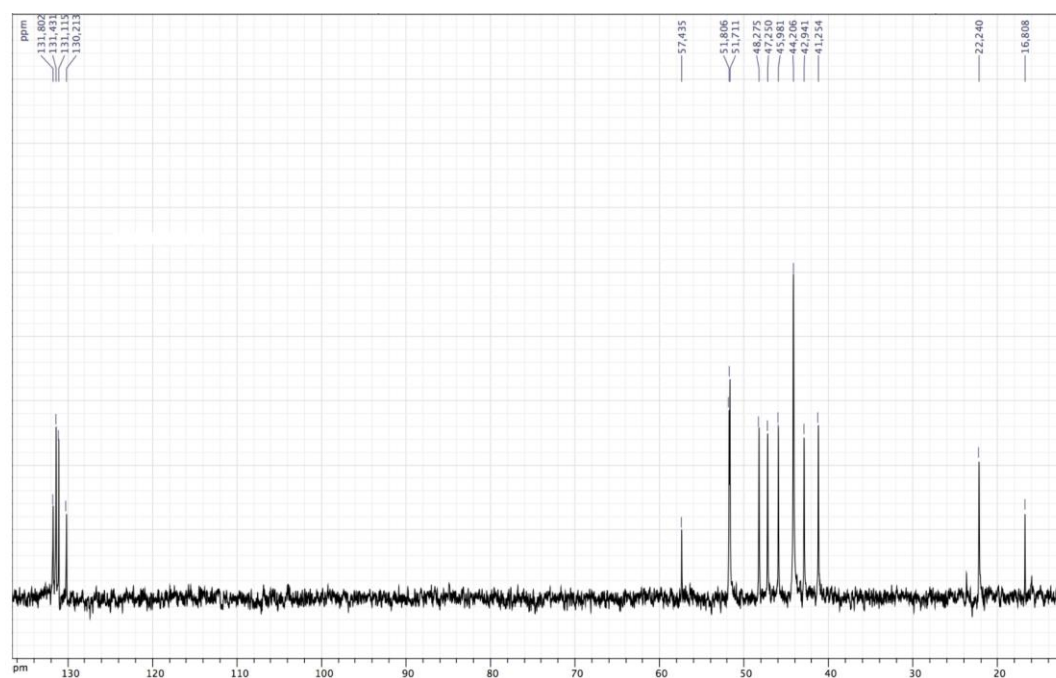


Figure 10: ^{13}C NMR of compound 5 (75 MHz, D_2O , 300 K)

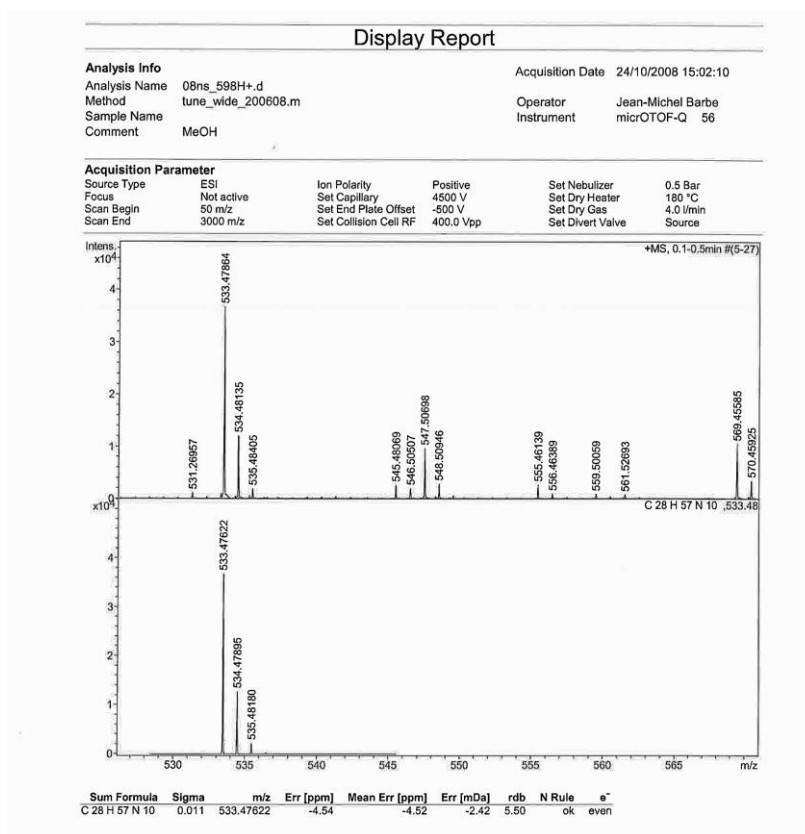


Figure 11: Mass spectrum of compound 5 (ESI-TOF)

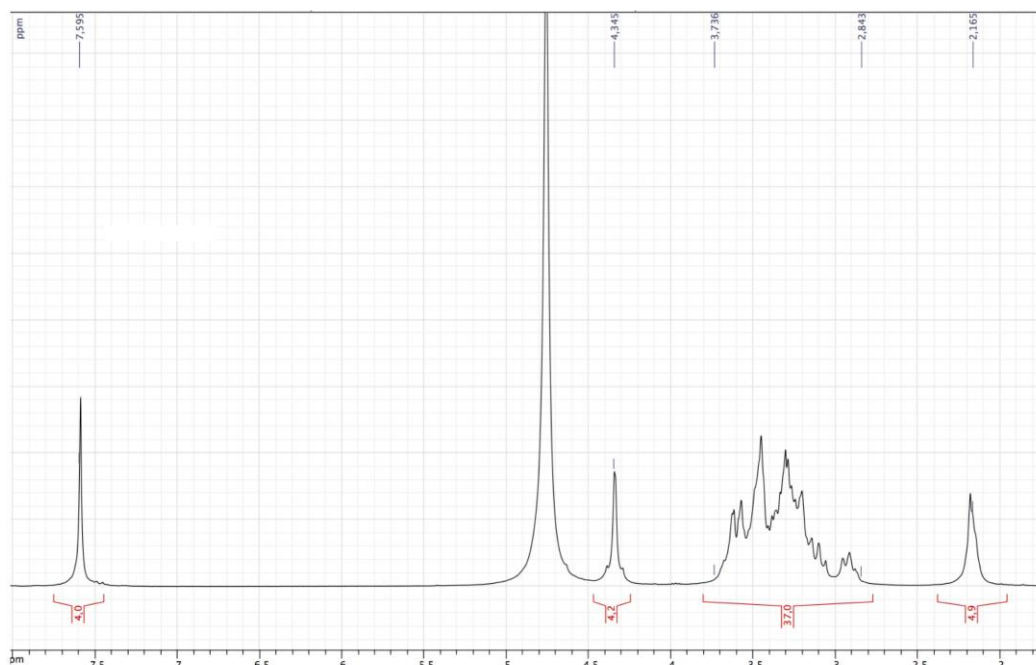


Figure 12: ¹H NMR of compound 6 (300 MHz, D₂O, 300 K)

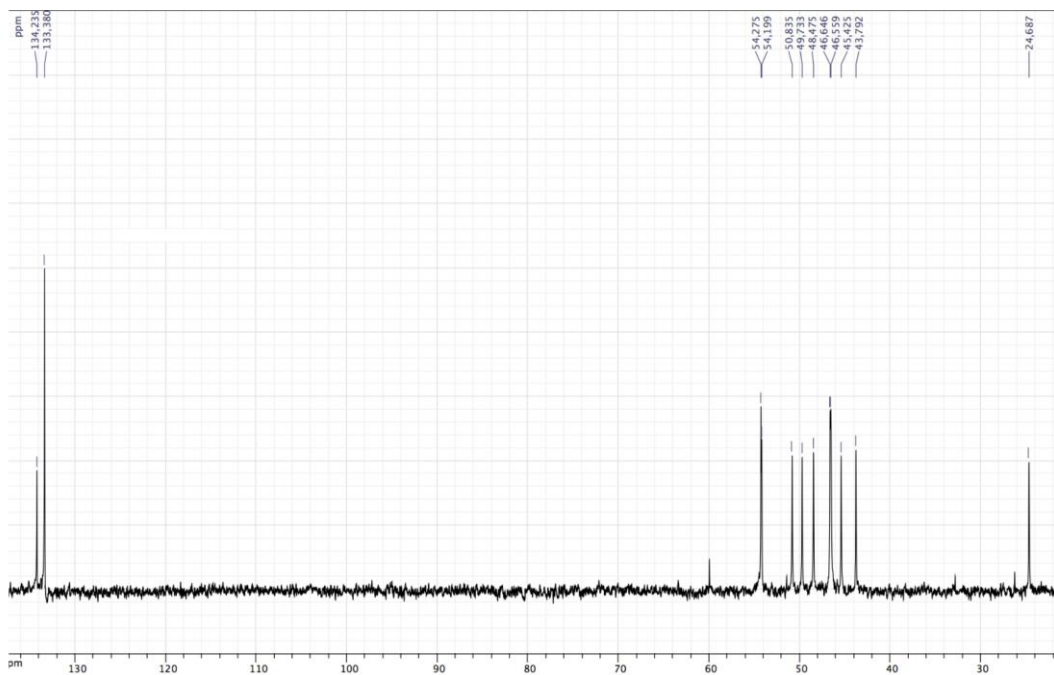


Figure 13: ^{13}C NMR of compound 6 (75 MHz, D_2O , 300 K)

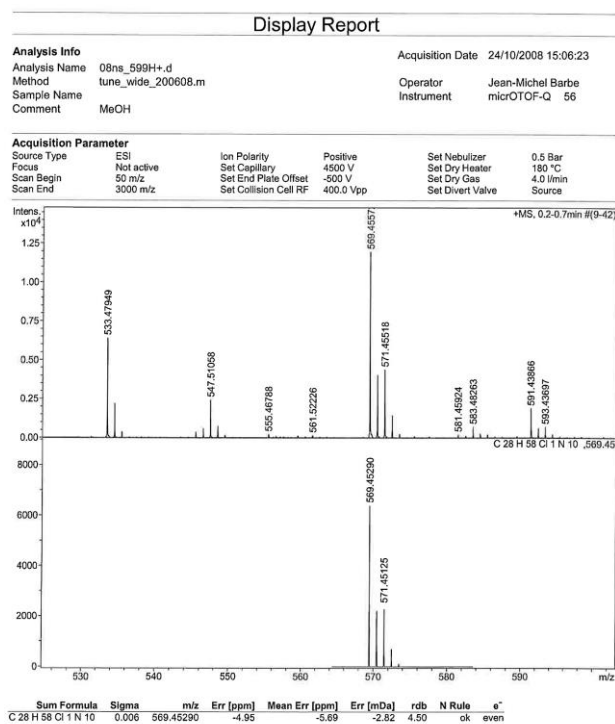


Figure 14: Mass spectrum of compound 6 (ESI-TOF)

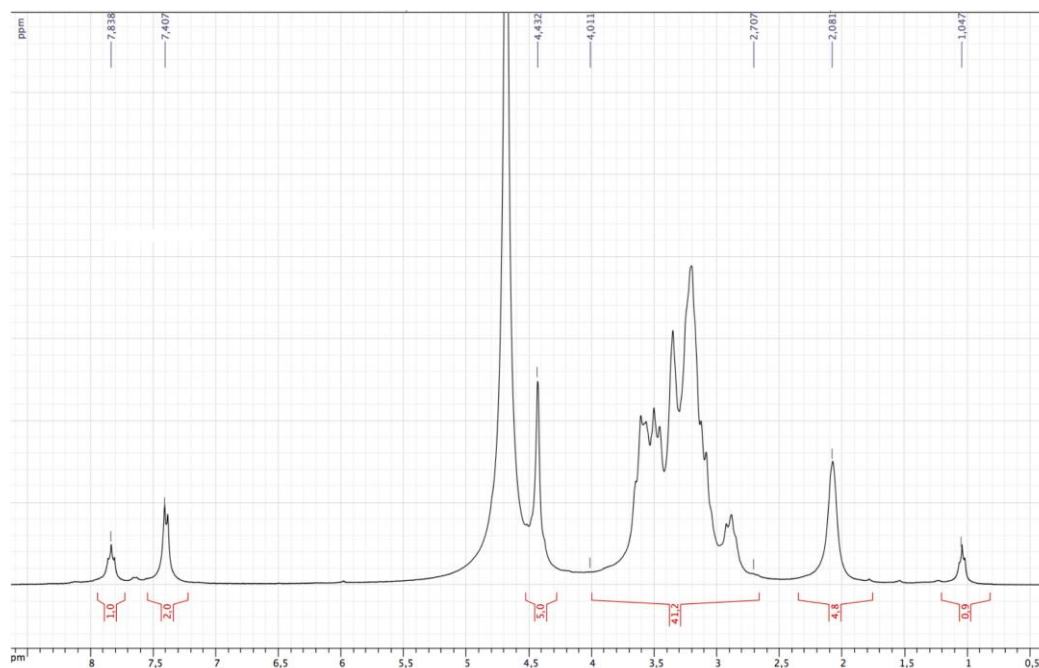


Figure 15: ^1H NMR of compound 7 (600 MHz, D_2O , 300 K)

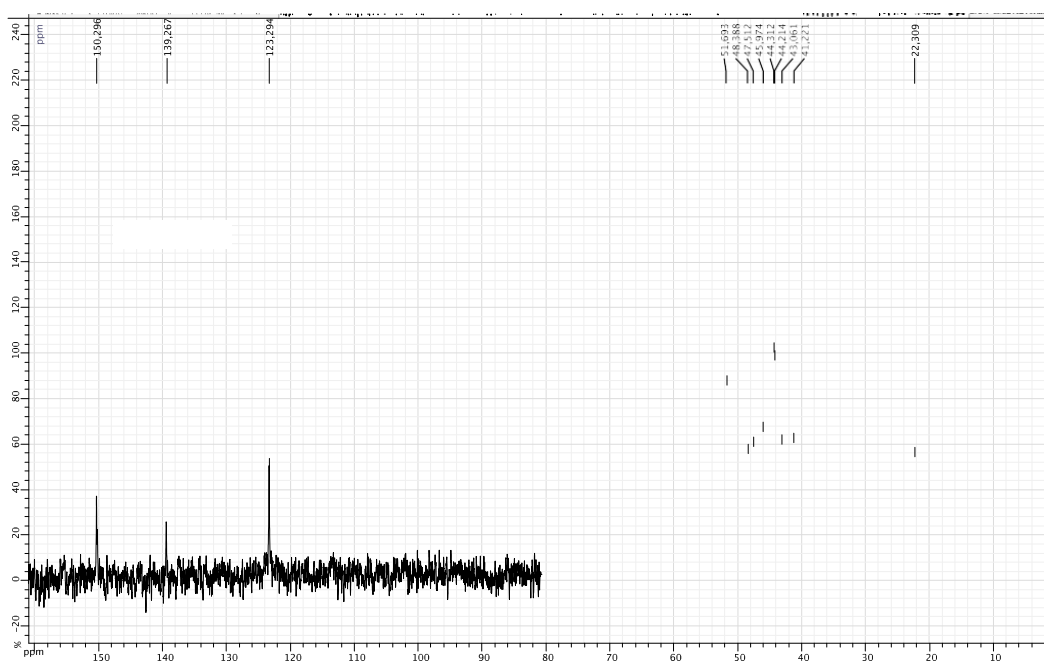


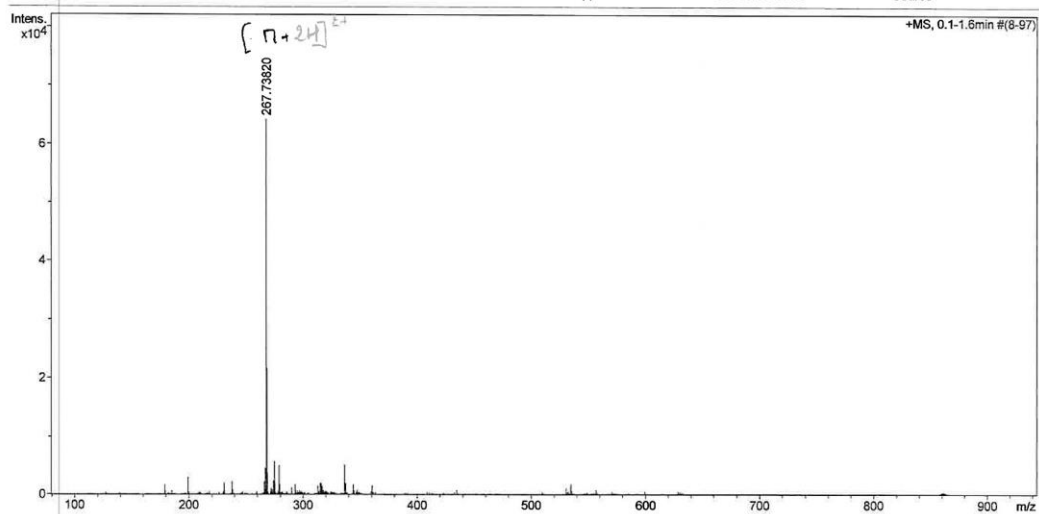
Figure 16: ^{13}C NMR of compound 7 (150 MHz, D_2O , 300 K)

Analysis Name 08ns_625H+.d
Method tune_wide.m
Sample Name
Comment MeOH

Operator Marie-José Penouilh
Instrument micrOTOF-Q 56

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



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Page 1 of 1

Figure 17: Mass spectrum of compound 7 (ESI-TOF)

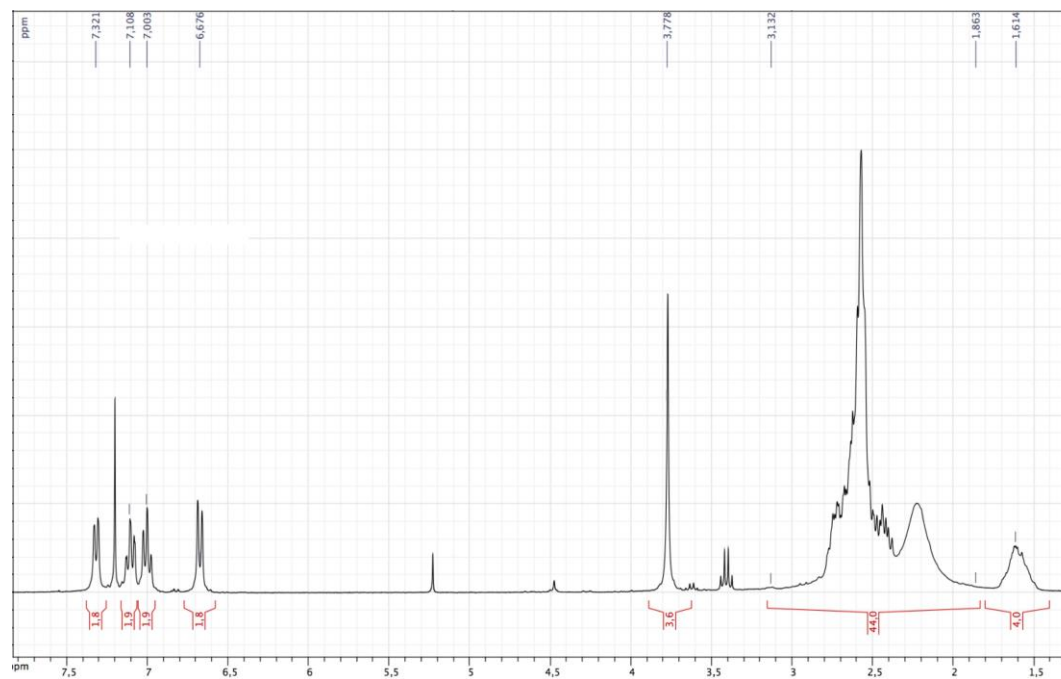


Figure 18: ^1H NMR of compound 8 (300 MHz, CDCl_3 , 300 K)

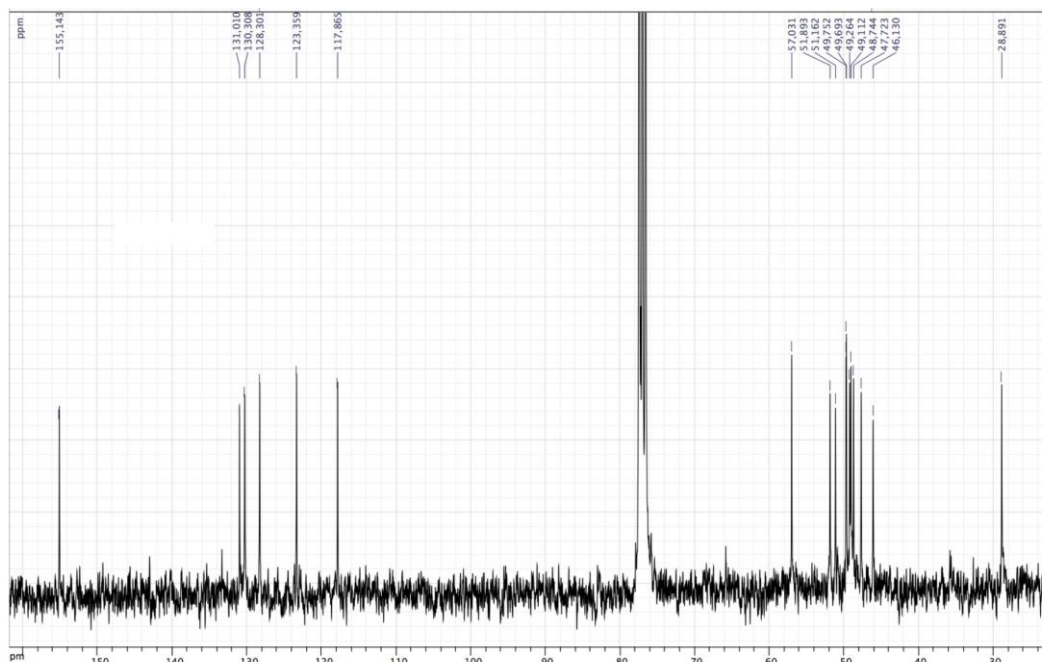


Figure 19: ^{13}C NMR of compound 8 (150 MHz, CDCl_3 , 300 K)

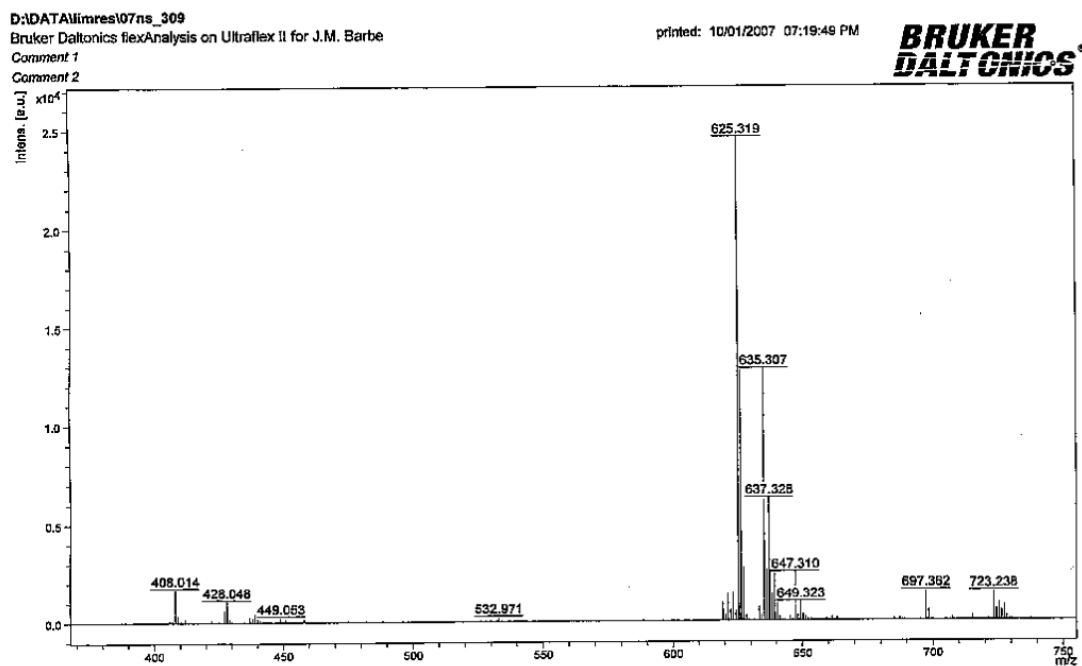


Figure 20: Mass spectrum of compound 8 (HRMS-MALDI-TOF)

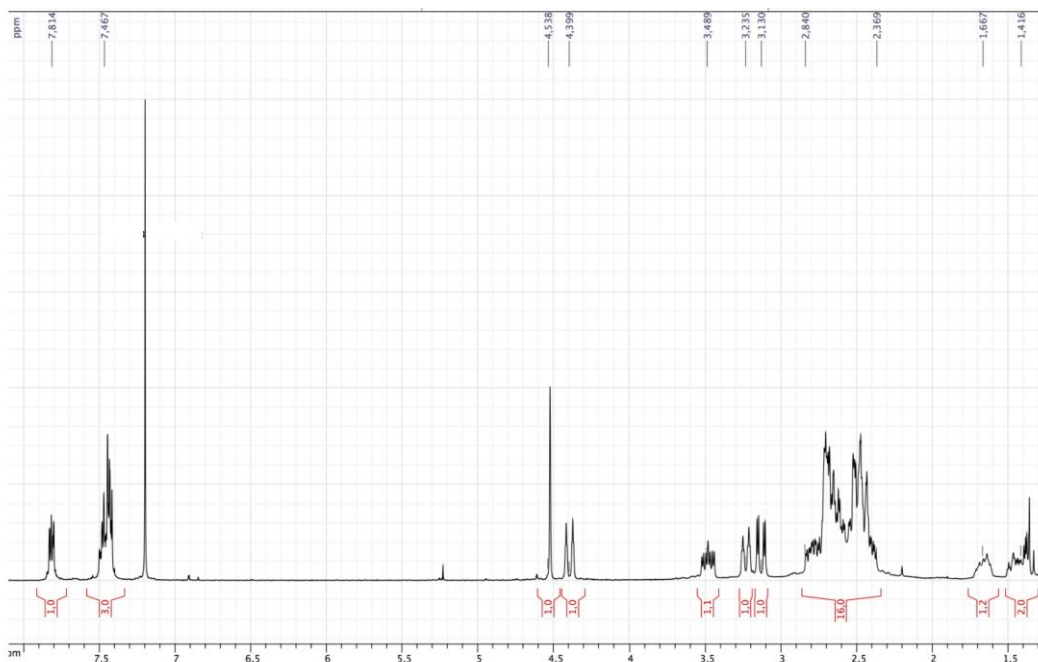


Figure 21: ^1H NMR of compound 9 (150 MHz, CDCl_3 , 300 K)

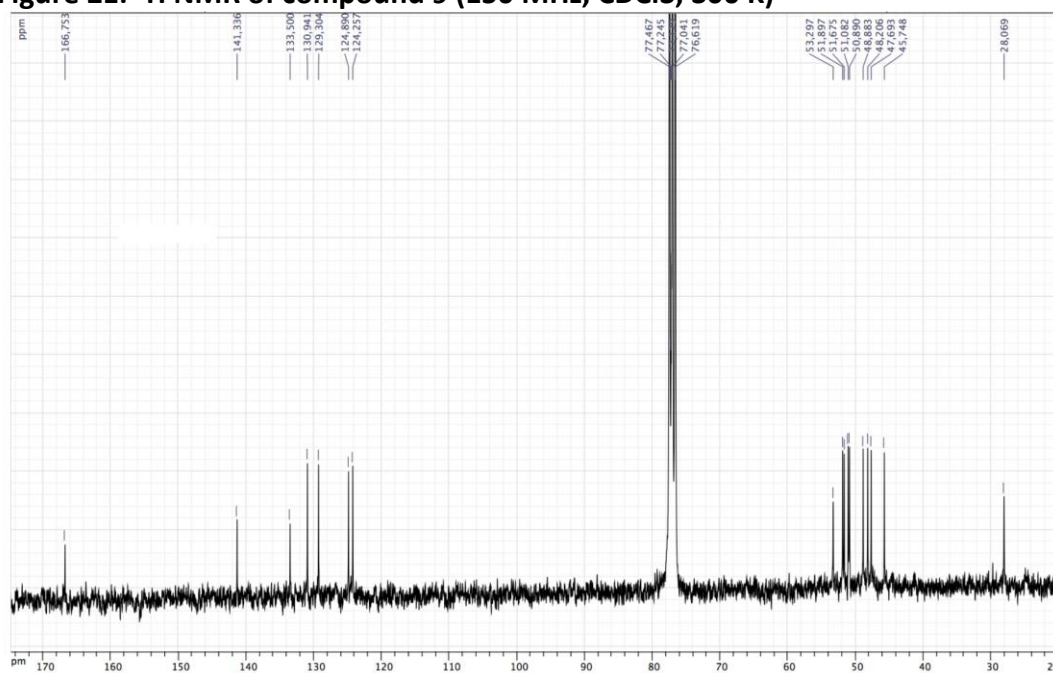


Figure 22: ^{13}C NMR of compound 9 (150 MHz, CDCl_3 , 300 K)

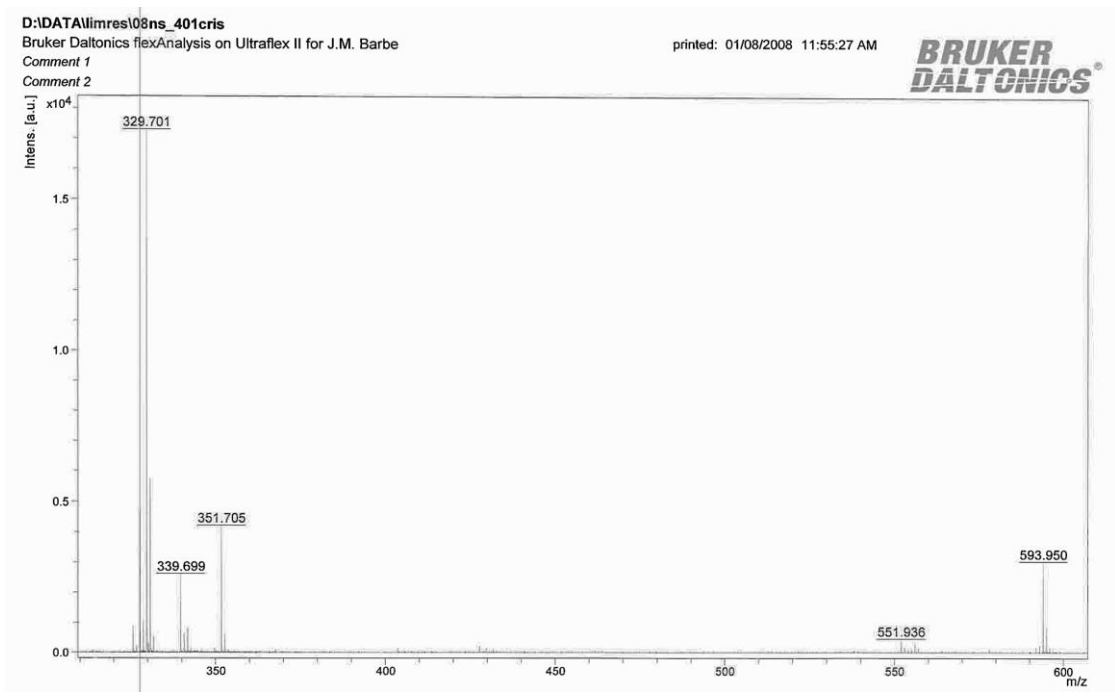


Figure 23: Mass spectrum of compound 9 (HRMS-MALDI-TOF)

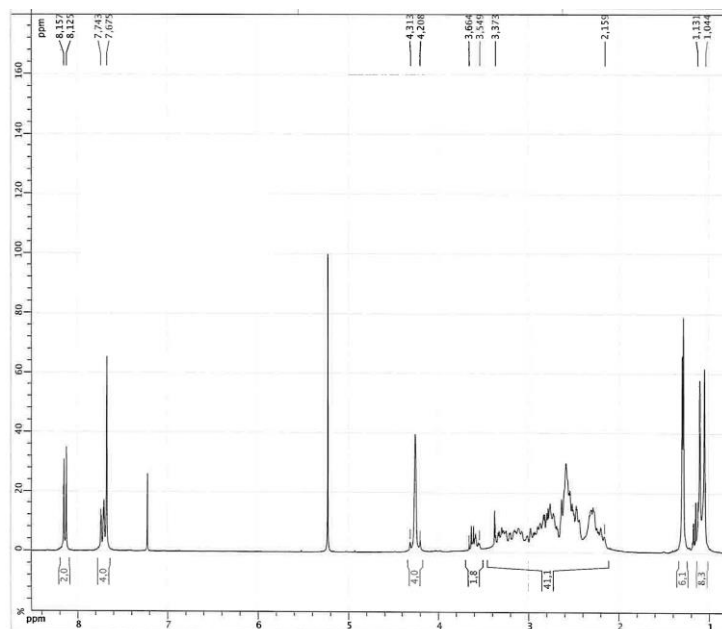


Figure 24: ¹H NMR of compound 11 (300 MHz, CDCl₃, 300 K)

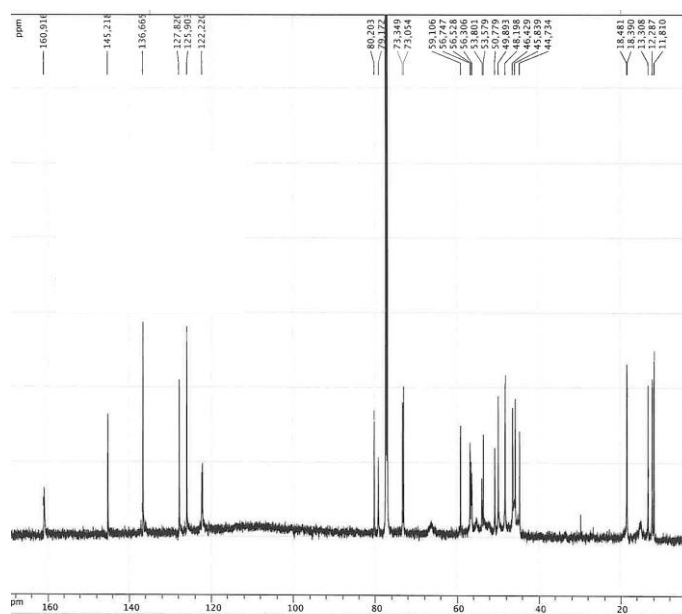


Figure 25: ^{13}C NMR of compound 11 (75 MHz, CDCl_3 , 300 K)

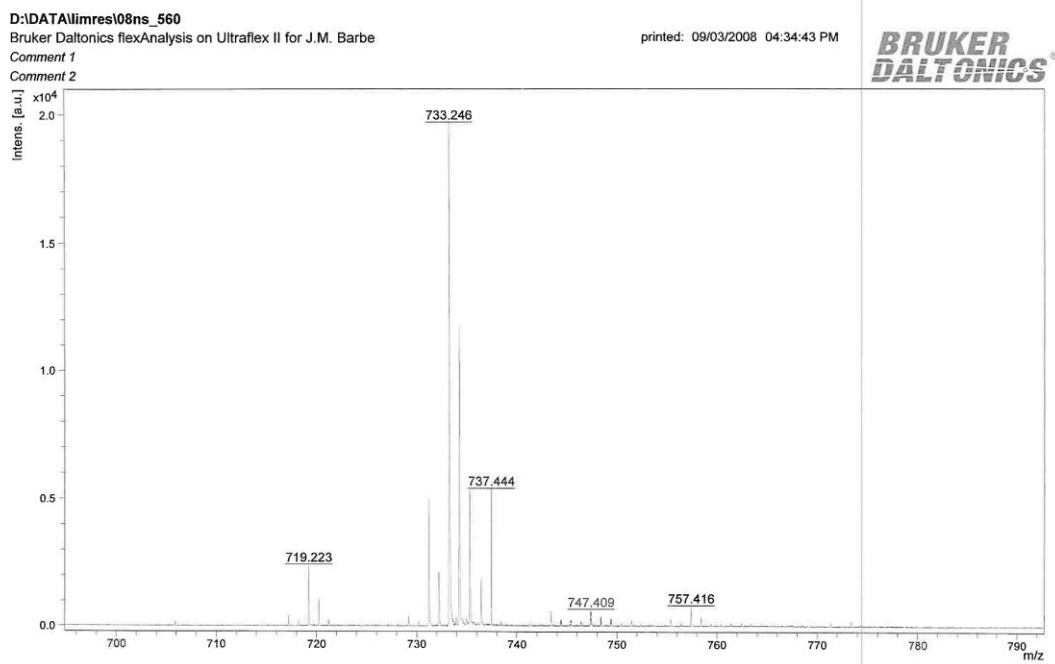


Figure 26: Mass spectrum of compound 11 (MALDI-TOF)

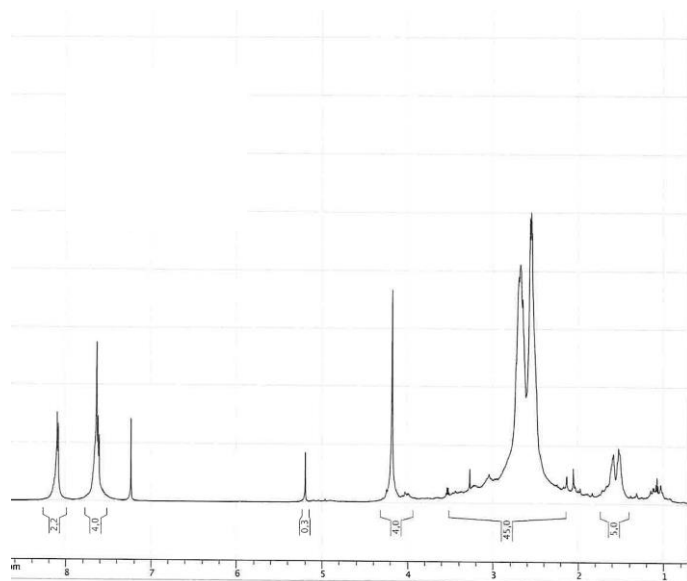


Figure 27: ^1H NMR of compound 12 (300 MHz, CDCl_3 , 300 K)

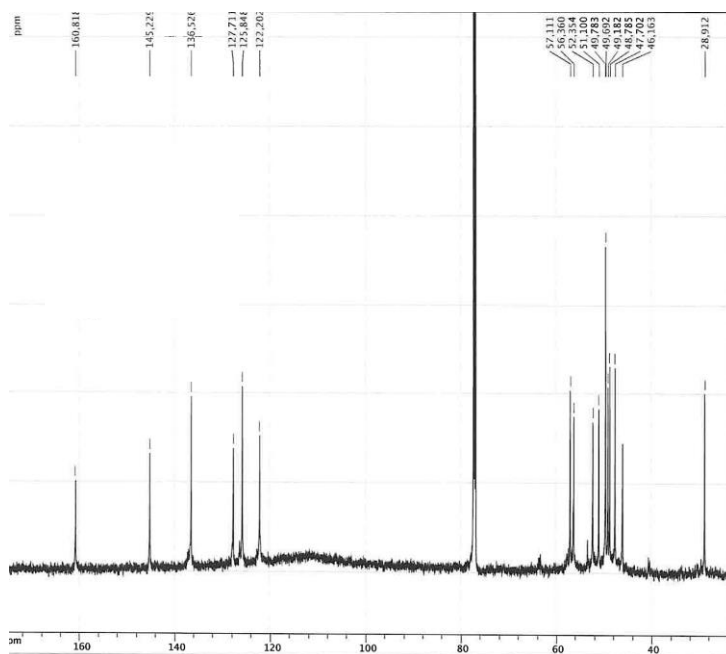


Figure 28: ^{13}C NMR of compound 12 (75 MHz, CDCl_3 , 300 K)

Analysis Info
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 Method tune_wide_200608.m Operator Jean-Michel Barbe
 Sample Name Instrument micrOTOF-Q 56
 Comment MeOH

Acquisition Parameter
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 Focus Not active Set Capillary 4500 V Set Dry Heater 180 °C
 Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 4.0 l/min
 Scan End 3000 m/z Set Collision Cell RF 400.0 Vpp Set Divert Valve Source

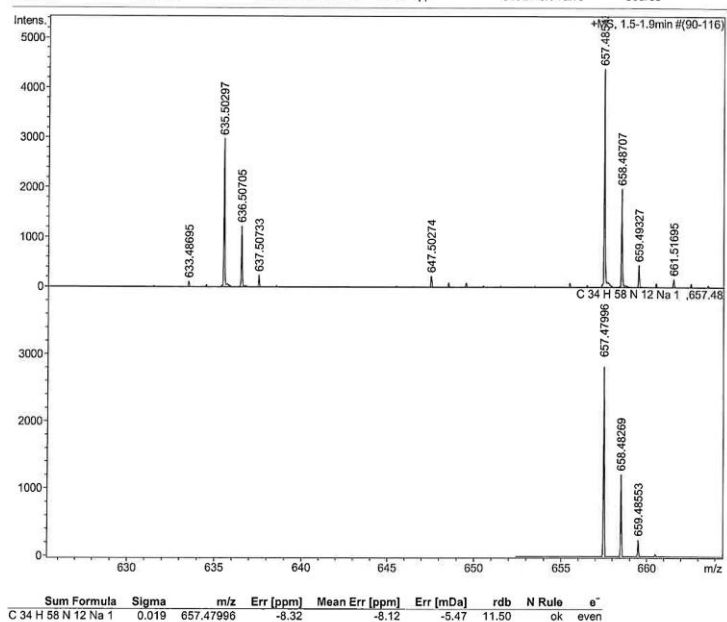


Figure 29: Mass spectrum of compound 12 (ESI-TOF)