

Supporting Information

Tetrahydropyran and Tetrahydrofuran Containing Diarylheptanoids from *Hedychium coronarium* Rhizomes

Yi-Shan Lin,[†] Jung-Hsin Lin,^{†,‡,§} Chia-Chuan Chang,[†] and Shoei-Sheng Lee^{*,†}

[†]School of Pharmacy, College of Medicine, National Taiwan University, 33 Linsen South Road, Taipei 100, Taiwan, Republic of China

[‡]Research Center for Applied Sciences, Academia Sinica, 128 Academia Rd., Sec. 2, Nankang, Taipei 115, Taiwan, Republic of China

[§]Institute of Biomedical Sciences, Academia Sinica, 128 Academia Rd., Sec. 2, Nankang, Taipei 115, Taiwan, Republic of China

Content

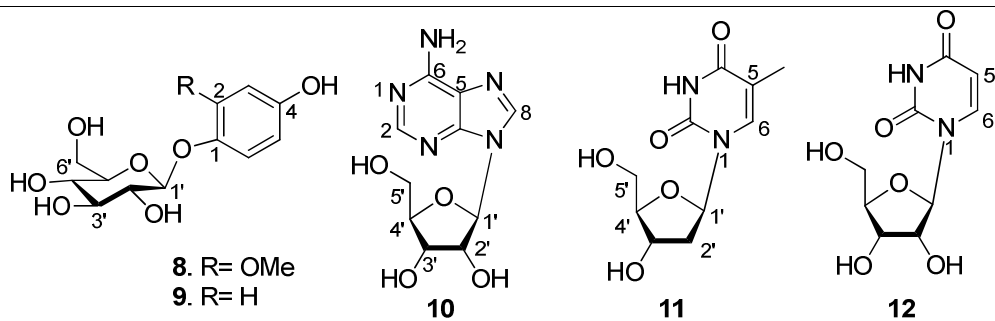
page

4. Table 1. ^1H and ^{13}C NMR spectroscopic data of compounds **8**–**12** (CD_3OD , AVIII-600)
5. S1. ^1H NMR spectrum of **1** (600MHz, CD_3OD)
6. S2. ^{13}C NMR spectrum of **1** (150MHz, CD_3OD)
7. S3. COSY spectrum of **1** (600MHz, CD_3OD)
8. S4. HSQC spectrum of **1** (600MHz, CD_3OD)
9. S5. HMBC spectrum of **1** (600MHz, CD_3OD)
10. S6. NOESY spectrum of **1** (600MHz, CD_3OD)
11. S7. Energy minimized conformation of **1** (6*R*) and **1a** (6*S*), obtained by MM2 calculation through molecular dynamic and energy minimization.
12. S8. ^1H NMR spectrum of **2** (600MHz, CD_3OD)
13. S9. ^{13}C NMR spectrum of **2** (150MHz, CD_3OD)
14. S10. COSY spectrum of **2** (600MHz, CD_3OD)
15. S11. HSQC spectrum of **2** (600MHz, CD_3OD)
16. S12. HMBC spectrum of **2** (600MHz, CD_3OD)
17. S13. NOESY spectrum of **2** (600MHz, CD_3OD)
18. S14. ^1H NMR spectrum of **3** (600MHz, CD_3OD)
19. S15. ^{13}C NMR spectrum of **3** (150MHz, CD_3OD)
20. S16. COSY spectrum of **3** (600MHz, CD_3OD)
21. S17. HSQC spectrum of **3** (600MHz, CD_3OD)
22. S18. HMBC spectrum of **3** (600MHz, CD_3OD)
23. S19. NOESY spectrum of **3** (600MHz, CD_3OD)
24. S20. Energy minimized conformation of **3** (6*R*) and **3a** (6*S*), obtained by MM2 calculation through molecular dynamic and energy minimization.
25. S21. ^1H NMR spectrum of **4** (600MHz, CD_3OD)
26. S22. ^{13}C NMR spectrum of **4** (150MHz, CD_3OD)
27. S23. COSY spectrum of **4** (600MHz, CD_3OD)
28. S24. HSQC spectrum of **4** (600MHz, CD_3OD)
29. S25. HMBC spectrum of **4** (600MHz, CD_3OD)
30. S26. NOESY spectrum of **4** (600MHz, CD_3OD)
31. S27. ^1H NMR spectrum of **5** (600MHz, CD_3OD)
32. S28. ^{13}C NMR spectrum of **5** (150MHz, CD_3OD)
33. S29. COSY spectrum of **5** (600MHz, CD_3OD)
34. S30. HSQC spectrum of **5** (600MHz, CD_3OD)
35. S31. HMBC spectrum of **5** (600MHz, CD_3OD)
36. S32. NOESY spectrum of **5** (600MHz, CD_3OD)
37. S33. ^1H NMR spectrum of **6** (600MHz, CD_3OD)
38. S34. ^{13}C NMR spectrum of **6** (150MHz, CD_3OD)
39. S35. COSY spectrum of **6** (600MHz, CD_3OD)
40. S36. HSQC spectrum of **6** (600MHz, CD_3OD)
41. S37. HMBC spectrum of **6** (600MHz, CD_3OD)
42. S38. NOESY spectrum of **6** (600MHz, CD_3OD)
43. S39. ^1H NMR spectrum of **7** (600MHz, CD_3OD)
44. S40. ^{13}C NMR spectrum of **7** (150MHz, CD_3OD)
45. S41. COSY spectrum of **7** (600MHz, CD_3OD)
46. S42. HSQC spectrum of **7** (600MHz, CD_3OD)
47. S43. HMBC spectrum of **7** (600MHz, CD_3OD)
48. S44. NOESY spectrum of **7** (600MHz, CD_3OD)

- 49. S45. ^1H NMR and 1D NOESY spectra of **4a** (600MHz, CD_3OD)
- 50. S46. ^1H NMR and 1D NOESY spectra of **7a** (600MHz, CD_3OD)
- 51. S47. HRESIMS⁻ of **1**
- 52. S48. HRESIMS⁻ of **2**
- 53. S49. HRESIMS⁻ of **3**
- 54. S50. HRESIMS⁻ of **4**
- 55. S51. HRESIMS⁻ of **5**
- 56. S52. HRESIMS⁻ of **6**
- 57. S53. HRESIMS⁻ of **7**
- 58. S54. HRESIMS⁻ of **4a**
- 59. S55. HRESIMS⁻ of **7a**
- 60. S56. ECD spectrum of **1**
- 61. S57. ECD spectrum of **2**
- 62. S58. ECD spectrum of **3**
- 63. S59. ECD spectrum of **4**
- 64. S60. ECD spectrum of **5**
- 65. S61. ECD spectrum of **6**
- 66. S62. ECD spectrum of **7**
- 67. S63. Calculated ECD spectra of Fragments **1**, **2**, and **4**.

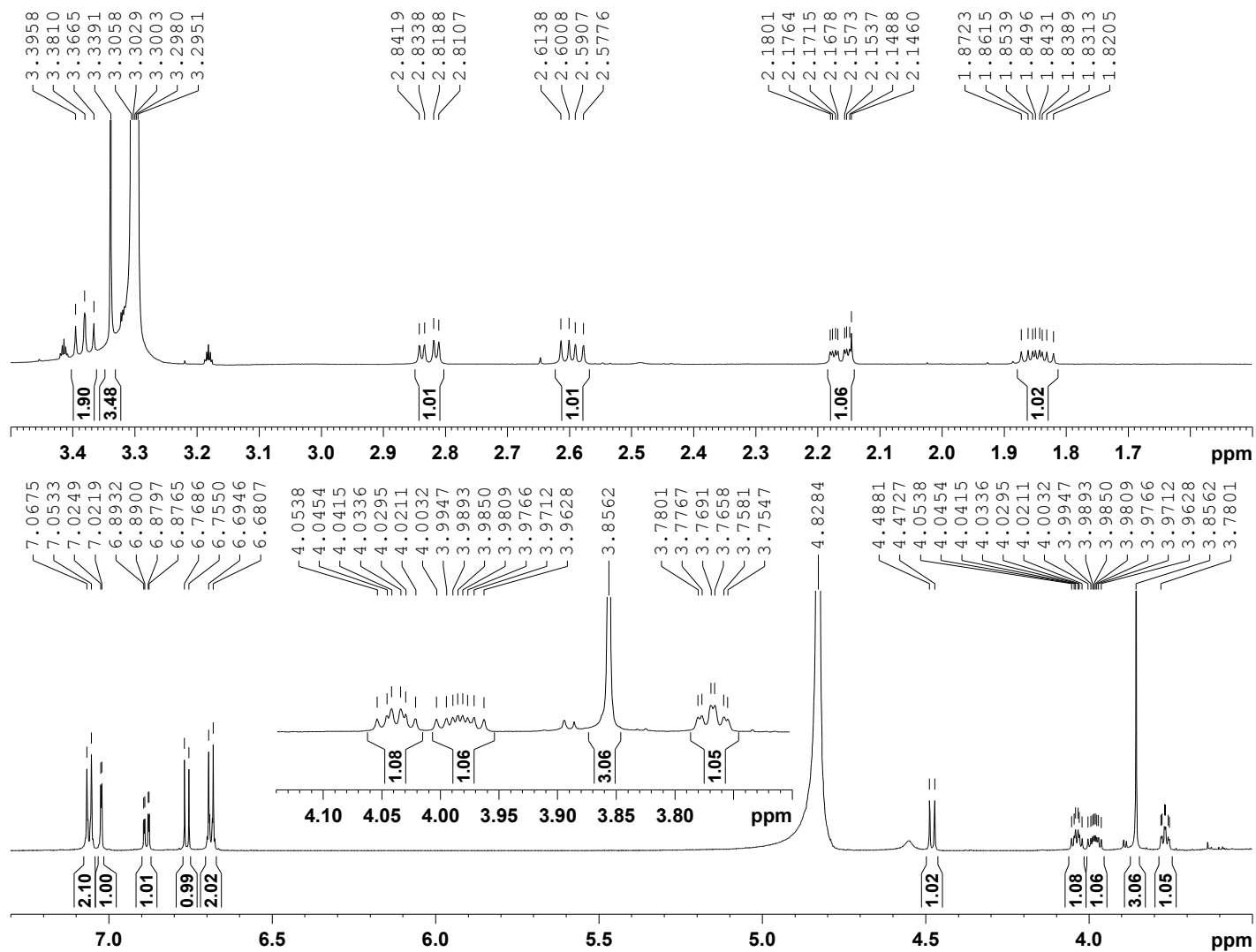
Table 2. ^1H and ^{13}C NMR spectroscopic data of compounds **8–12** (CD_3OD , AVIII-600)

No.	8		9		10		11		12	
	δ_{C} m	δ_{H} m (J/Hz)	δ_{C} m	δ_{H} m (J/Hz)	δ_{C} m	δ_{H} m (J/Hz)	δ_{C} m	δ_{H} m (J/Hz)	δ_{C} m	δ_{H} m (J/Hz)
1	141.1 C		153.8 C							
2	152.0 C		119.4 CH	6.95 d (9.1)	153.5 CH	8.17 s	152.4 C		152.4 C	
3	101.8 CH	6.46 d (2.6)	116.6 CH	6.68 d (8.9)						
4	154.9 C		152.5 C		150.0 C		166.4 C		166.2 C	
5	107.6 CH	6.29 dd (8.7, 2.5)	116.6 CH	6.68 d (8.9)	121.1 C		111.5 C		102.7 CH	5.70 d (8.1)
6	120.5 CH	7.01 d (8.8)	119.4 CH	6.95 d (9.1)	157.6 C		138.2 CH	7.80 s	142.7 CH	7.99 d (8.1)
8					142.0 CH	8.30 s				
2-OMe	56.5 CH ₃	3.80 s								
5-Me	56.5 CH ₃	3.80 s					12.4 CH ₃	1.87 s		
1'	104.3 CH	4.69 d (7.6)	103.7 CH	4.72 d (7.4)	91.3 CH	5.96 d (6.4)	86.3 CH	6.27 t (6.8)	90.7 CH	5.89 d (4.6)
2'	75.1 CH	3.39-3.45	75.0 CH	3.35-3.42	75.5 CH	4.73 br. t (5.9)	41.2 CH ₂	2.22 m/2H	75.7 CH	4.18 t (4.9)
3'	77.8 CH	3.39-3.45	78.0 CH	3.35-3.42	72.7 CH	4.31 dd (2.6, 5.0)	72.2 CH	4.39 dt (5.9, 3.4)	71.2 CH	4.14 t (4.9)
4'	71.4 CH	3.37 dd (9.5, 8.9)	71.5 CH	3.35-3.42	88.2 CH	4.16 dt (2.6, 2.5)	88.8 CH	3.89 q-like (3.4)	86.3 CH	4.00 dt (4.4, 2.9)
5'	78.1 CH	3.32 dd (5.6, 2.3)	78.1 CH	3.35-3.42	63.5 CH ₂	3.74 dd (12.5, 2.7) 3.88 dd (12.6, 2.5)	62.8 CH ₂	3.72 dd (12.1, 3.6) 3.79 dd (12.1, 3.2)	62.2 CH ₂	3.72 dd (12.3, 3.1) 3.83 dd (12.2, 2.7)
6'	62.6 CH ₂	3.68 dd (12.0, 5.4) 3.85 dd (11.9, 2.3)	62.6 CH ₂	3.68 dd (11.9, 5.0) 3.88 dd (11.8, 0.8)						



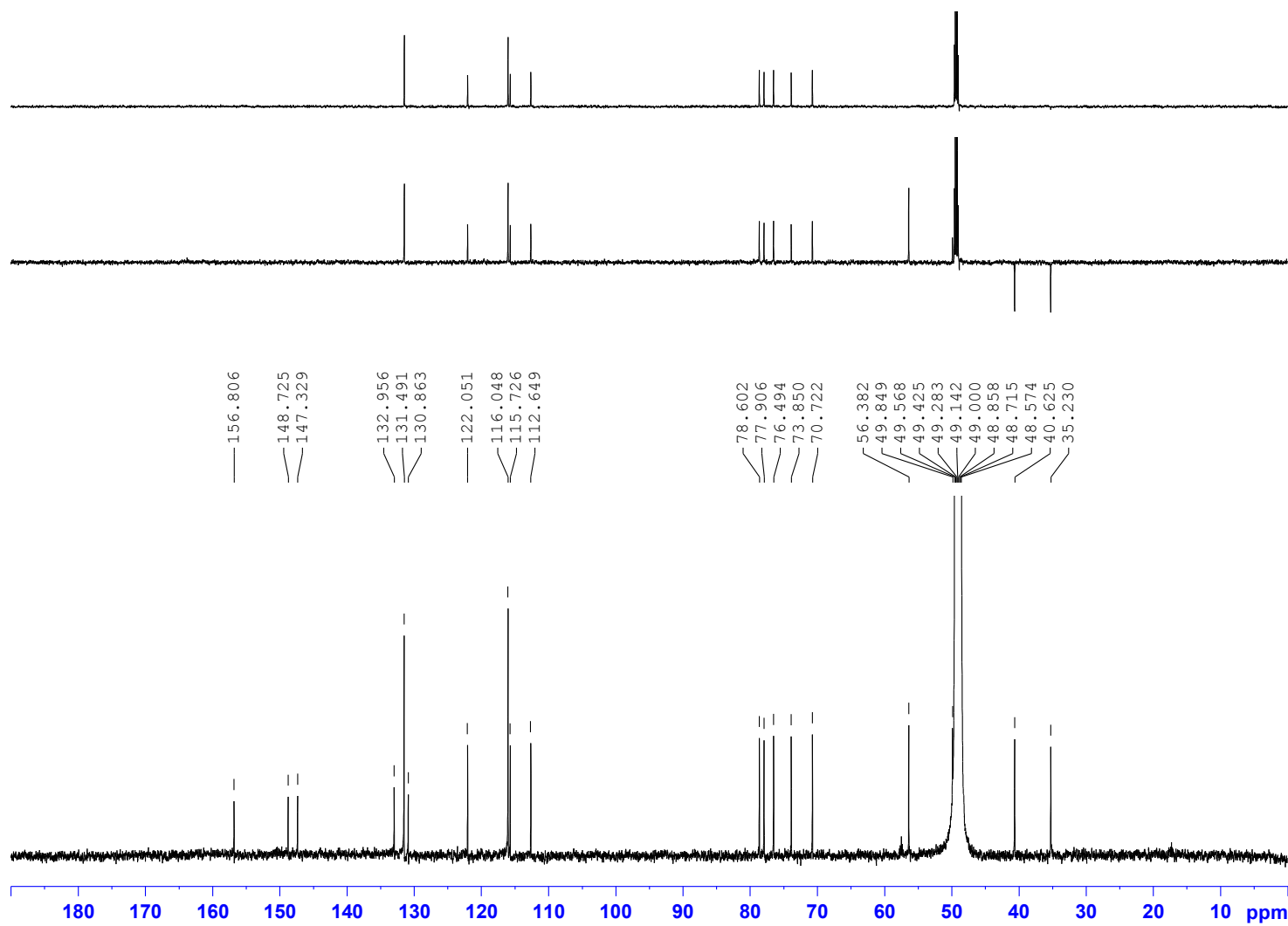
4-hydroxy-2-methoxyphenyl- β -glucopyranoside (**8**), 4-hydroxyphenyl- β -glucopyranoside (**9**), adenosine (**10**), thymidine (**11**), and uridine (**12**)

11006 ssl-ysl-3351883-fr.1-CD3OD-3.30 ppm-20120407, AV3-600, Cryo probe



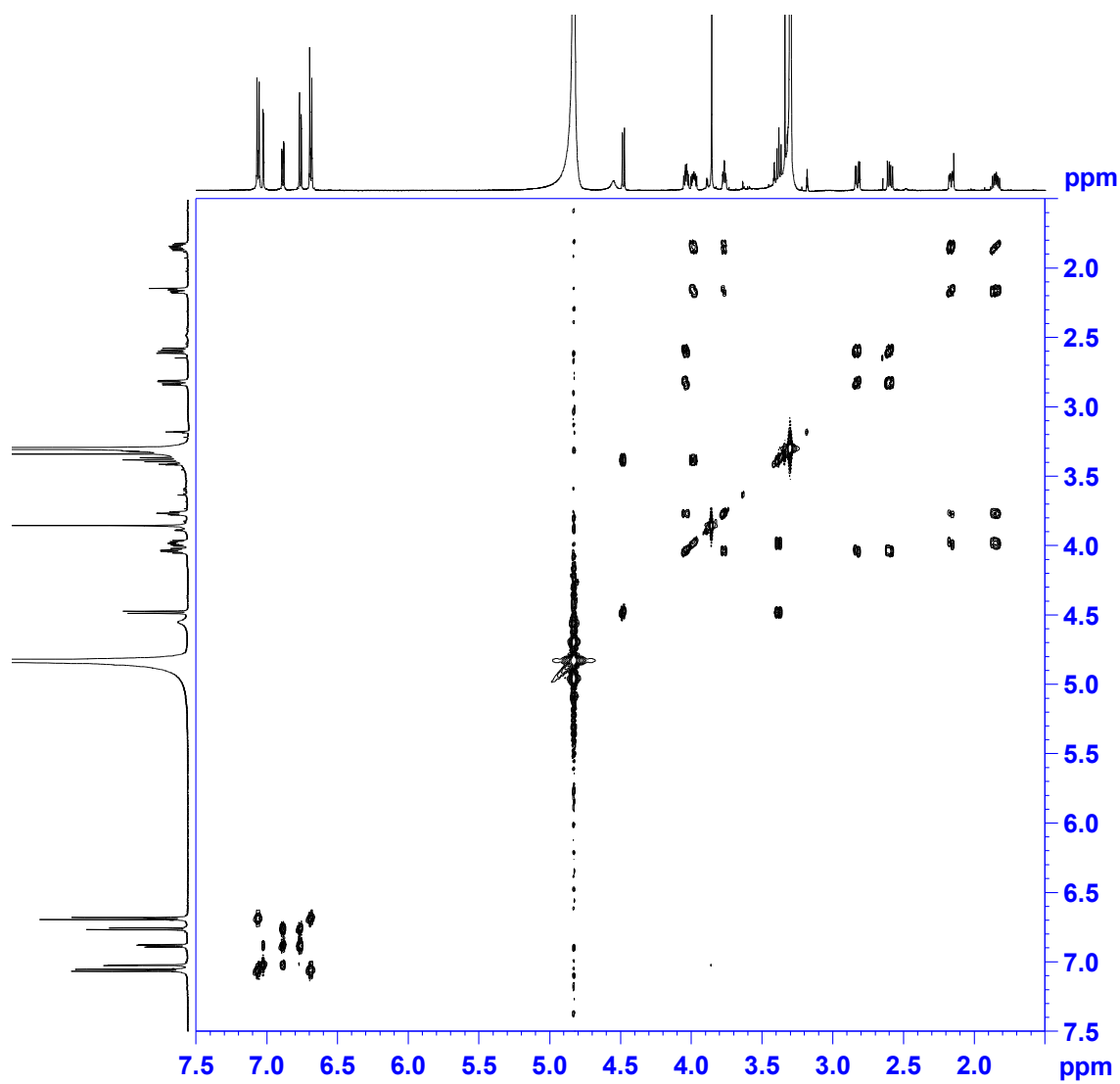
S1. ¹H NMR spectrum of **1** (600MHz, CD₃OD)

11006 ssl-ysl-3351883-fr.1-CD3OD-49.0 ppm-20120407, AV3-600, Cryo probe



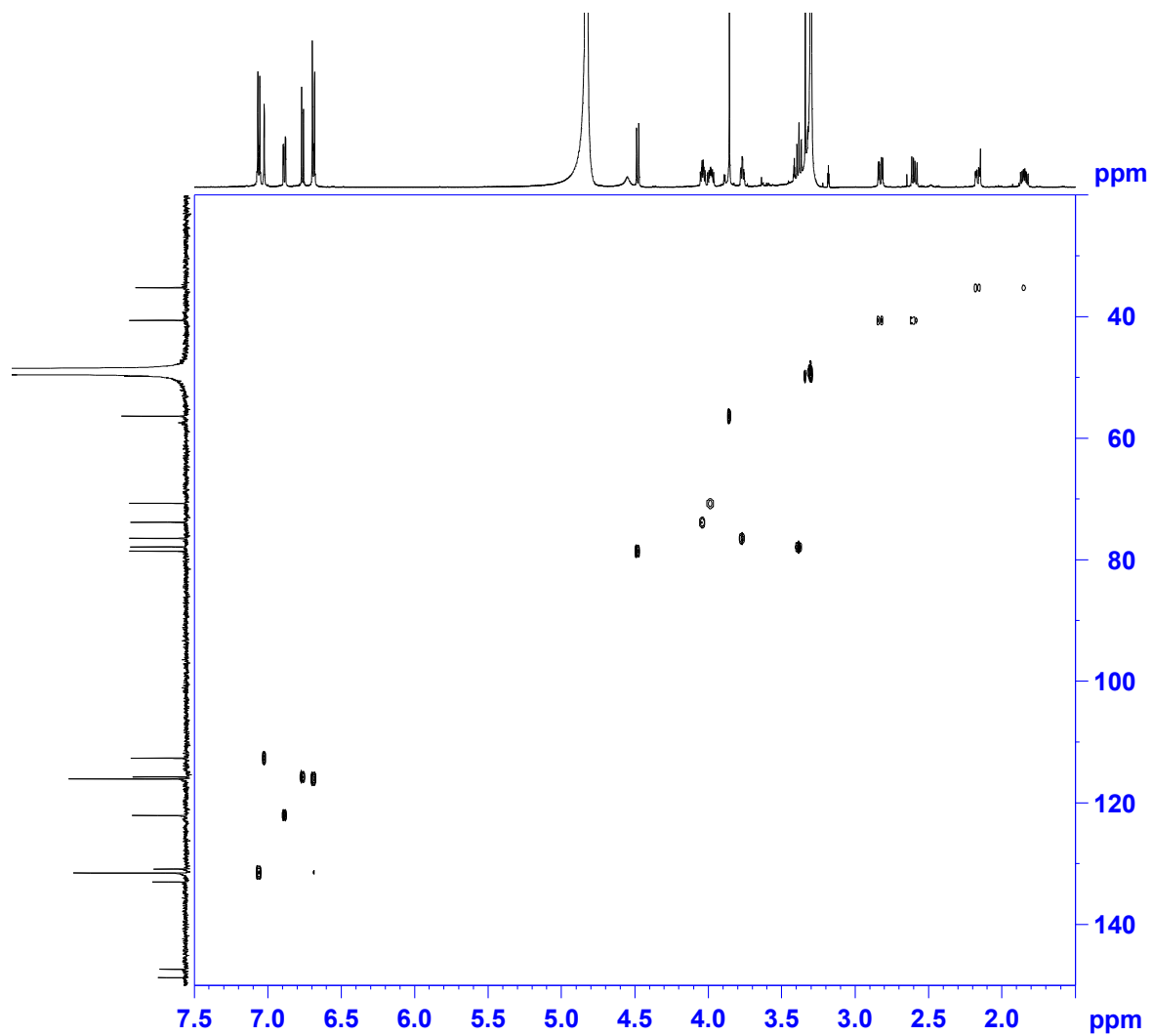
S2. ^{13}C NMR spectrum of **1** (150MHz, CD_3OD)

11006 ssl-ysl-3351883-fr.1-CD3OD-3.30 ppm-20120407, AV3-600, Cryo probe
COSY



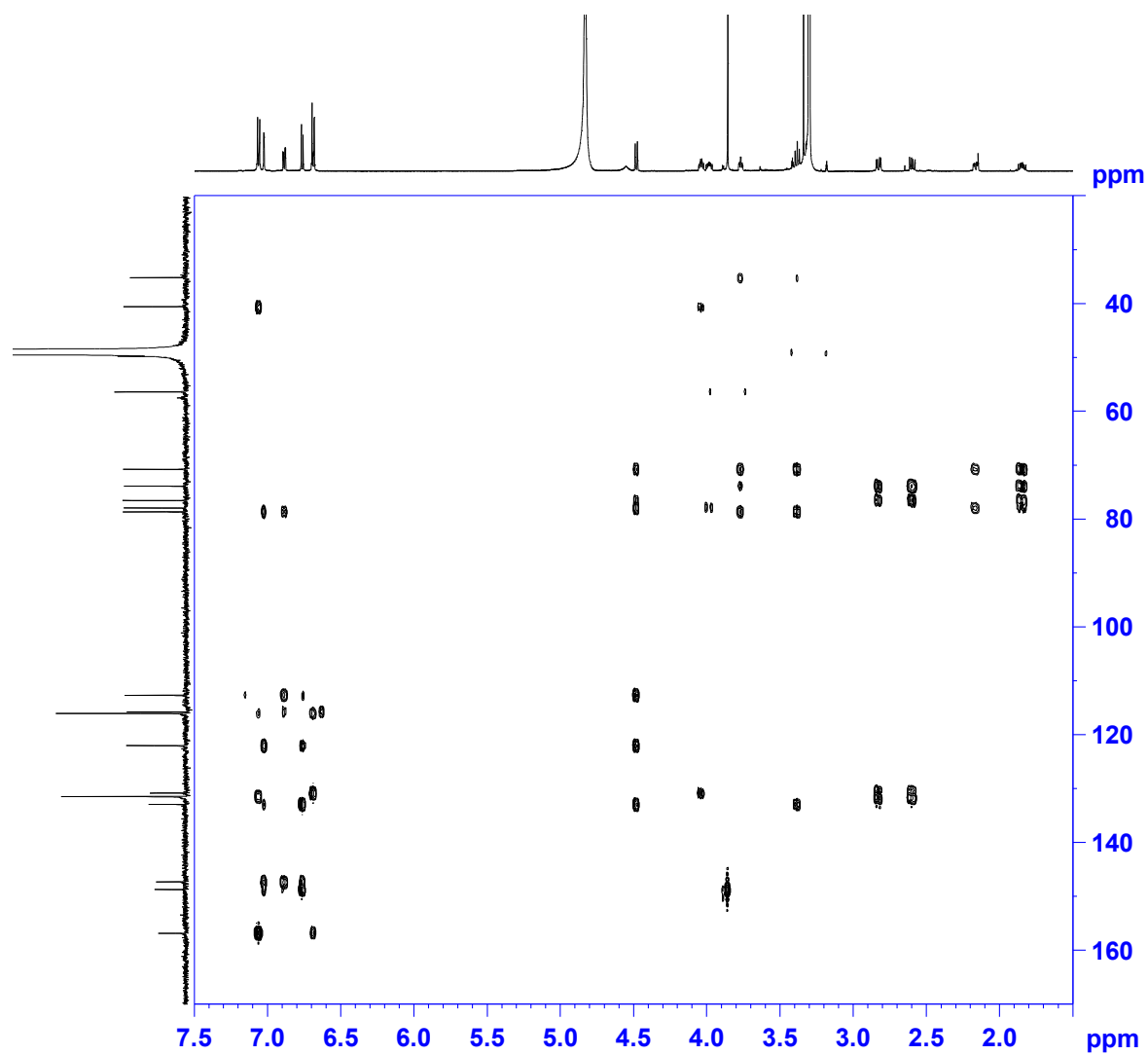
S3. COSY spectrum of **1** (600MHz, CD₃OD)

11006 ssl-ysl-3351883-fr.1-CD3OD-3.30 ppm-20120407, AV3-600, Cryo probe
HSQC



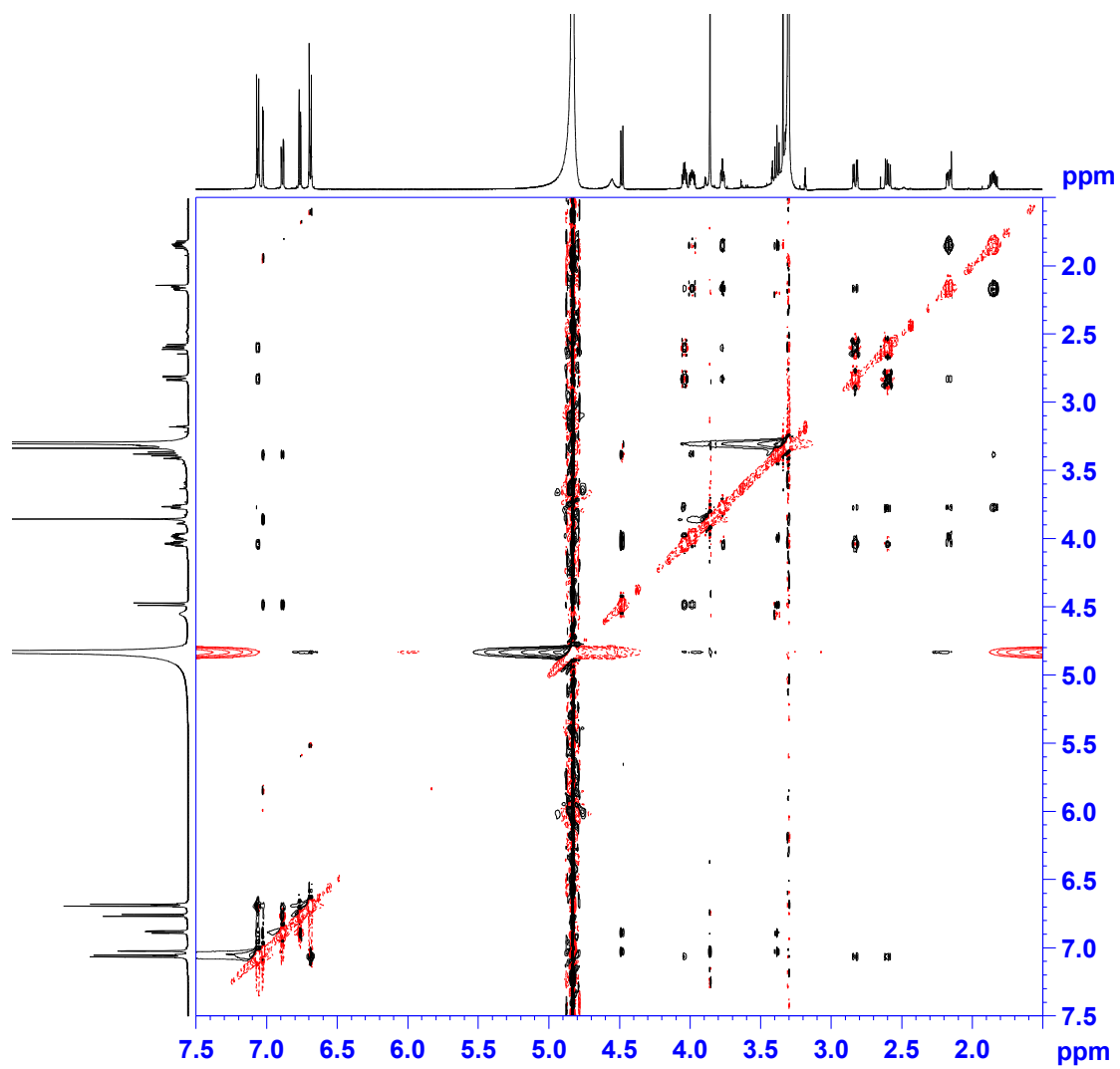
S4. HSQC spectrum of **1** (600MHz, CD_3OD)

11006 ssl-ysl-3351883-fr.1-CD3OD-3.30 ppm-20120407, AV3-600, Cryo probe
HMBC

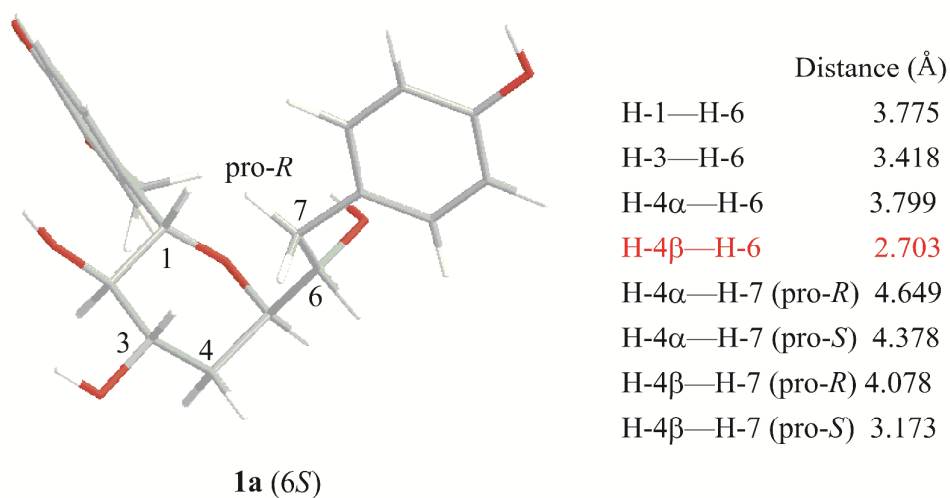
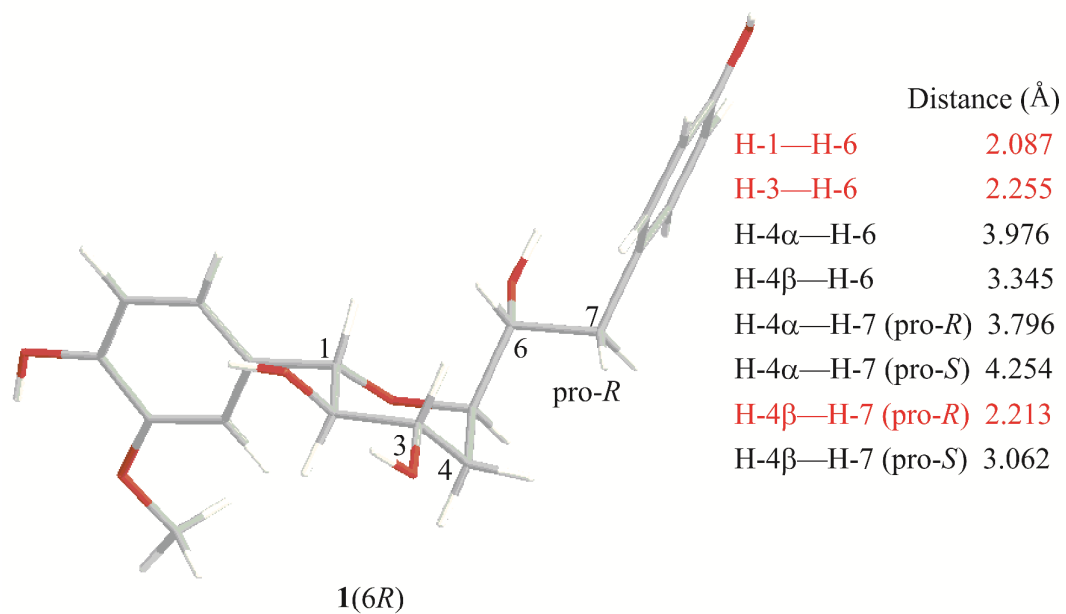


S5. HMBC spectrum of **1** (600MHz, CD_3OD)

11006 ssl-ysl-3351883-fr.1-CD3OD-3.30 ppm-20120407, AV3-600, Cryo probe
NOESY

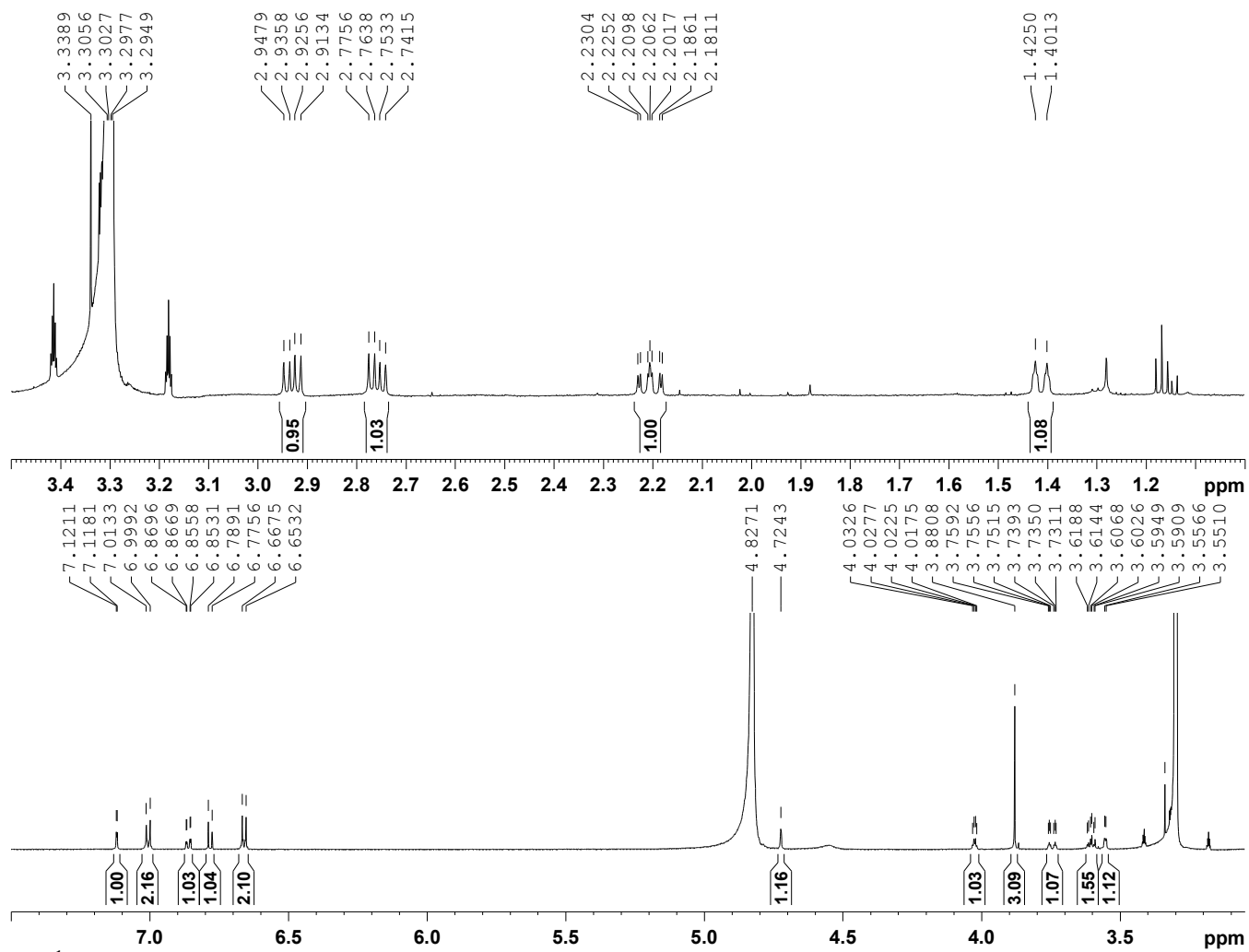


S6. NOESY spectrum of **1** (600MHz, CD₃OD)



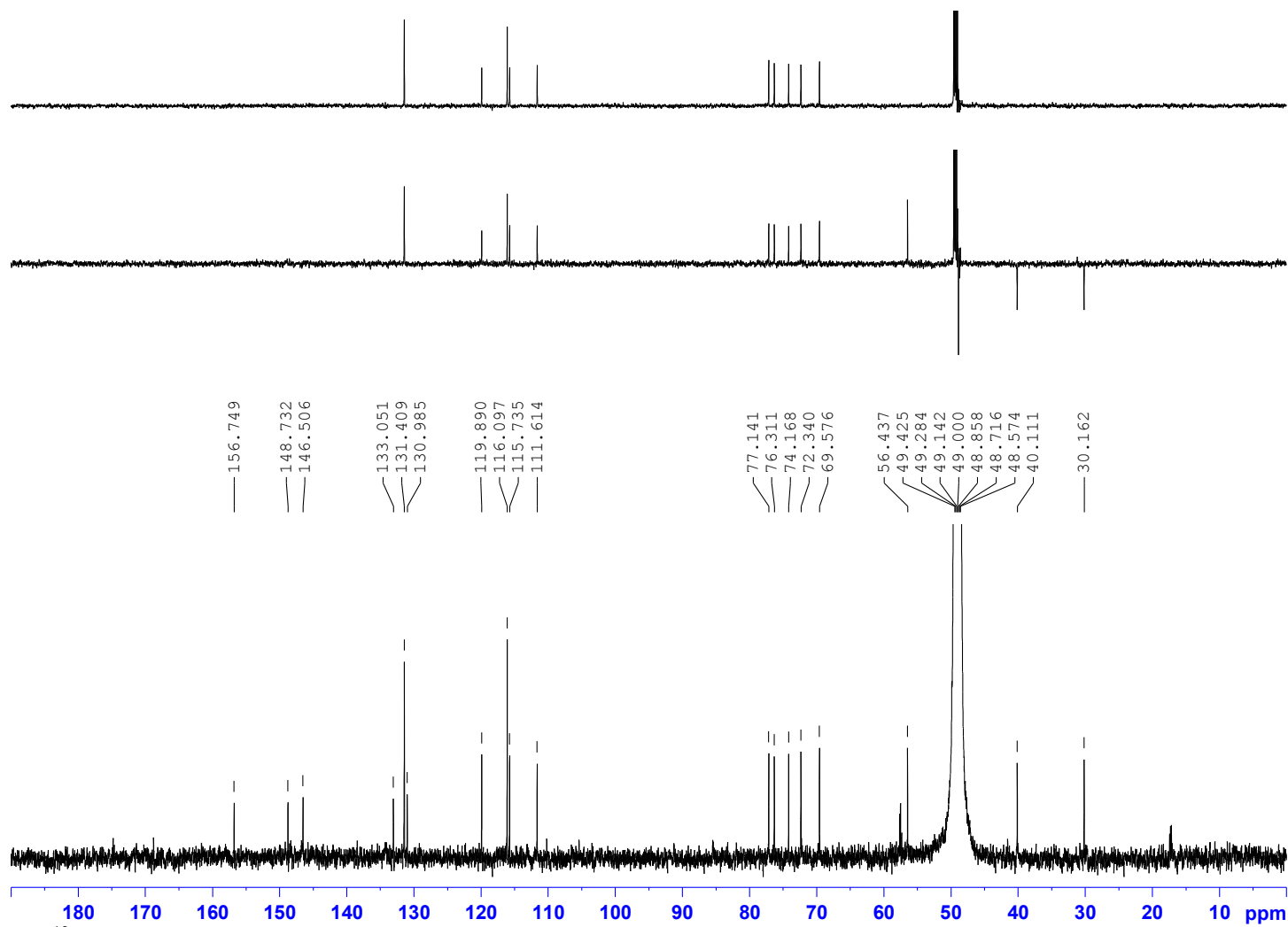
S7. Energy minimized conformation of **1** (6R) and **1a** (6S), obtained by MM2 calculation through molecular dynamic and energy minimization.

11006 ssl-ysl-3351886-fr.3-CD3OD-3.30 ppm-20120427, AV3-600, Cryo probe



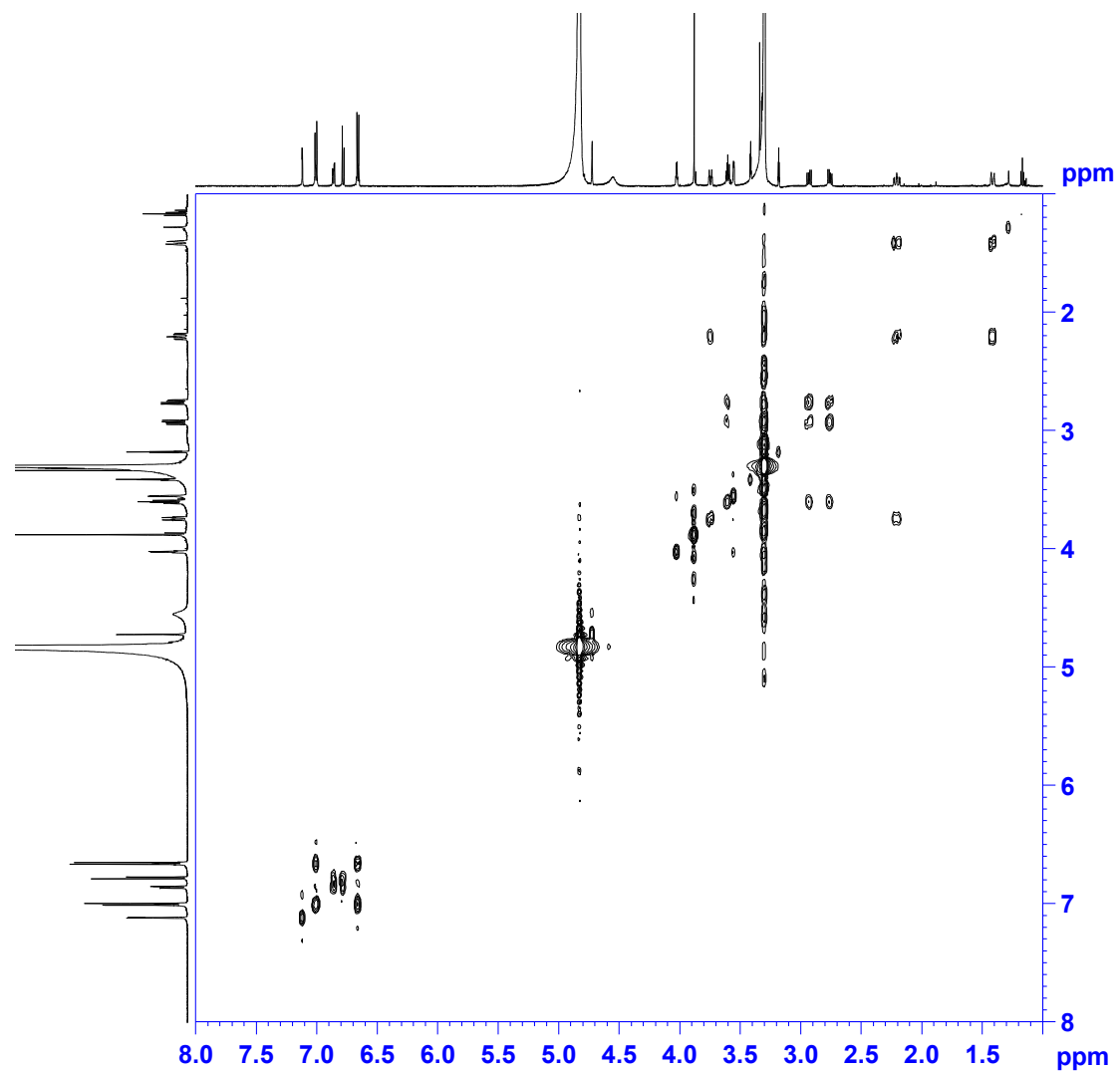
S8. ^1H NMR spectrum of **2** (600MHz, CD_3OD)

11006 ssl-ysl-3351886-fr.3-CD3OD-49.0 ppm-20120427, AV3-600, Cryo probe



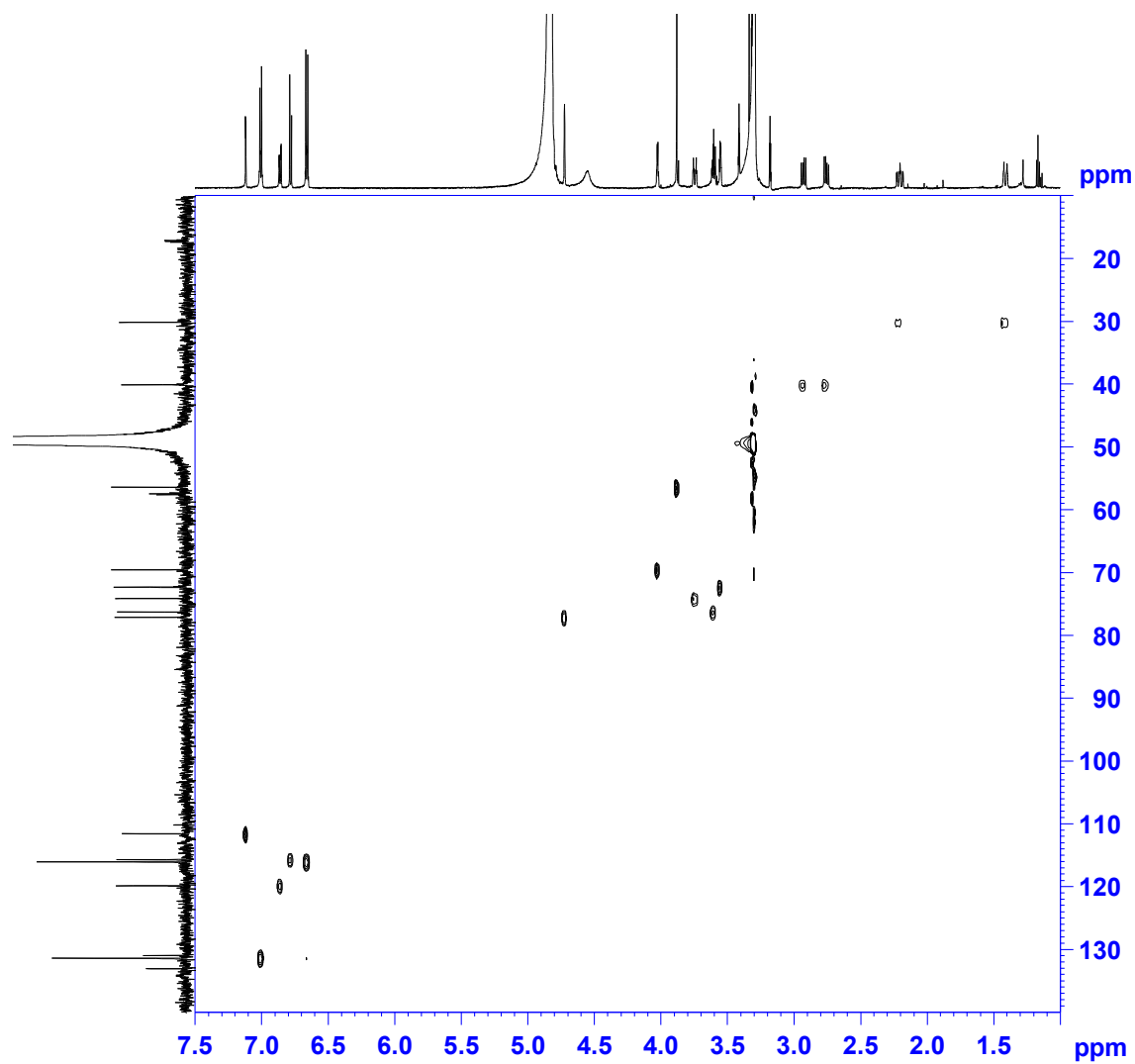
S9. ^{13}C NMR spectrum of **2** (150MHz, CD_3OD)

11006 ssl-ysl-3351886-fr.3-CD3OD-3.30 ppm-20120427, AV3-600, Cryo probe
COSY



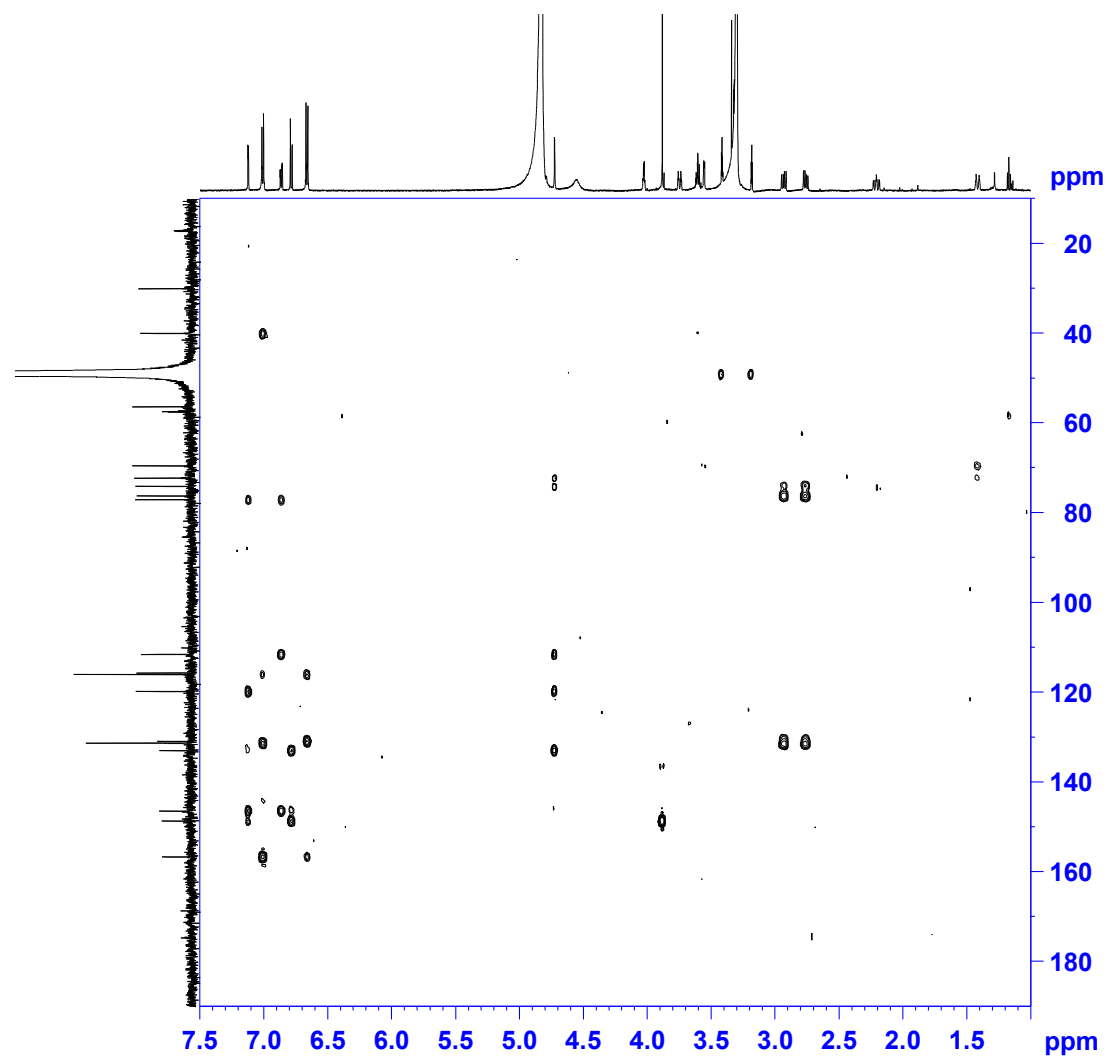
S10. COSY spectrum of **2** (600MHz, CD₃OD)

11006 ssl-ysl-3351886-fr.3-CD3OD-3.30, 49.0 ppm-20120427, AV3-600, Cryo probe
HSQC



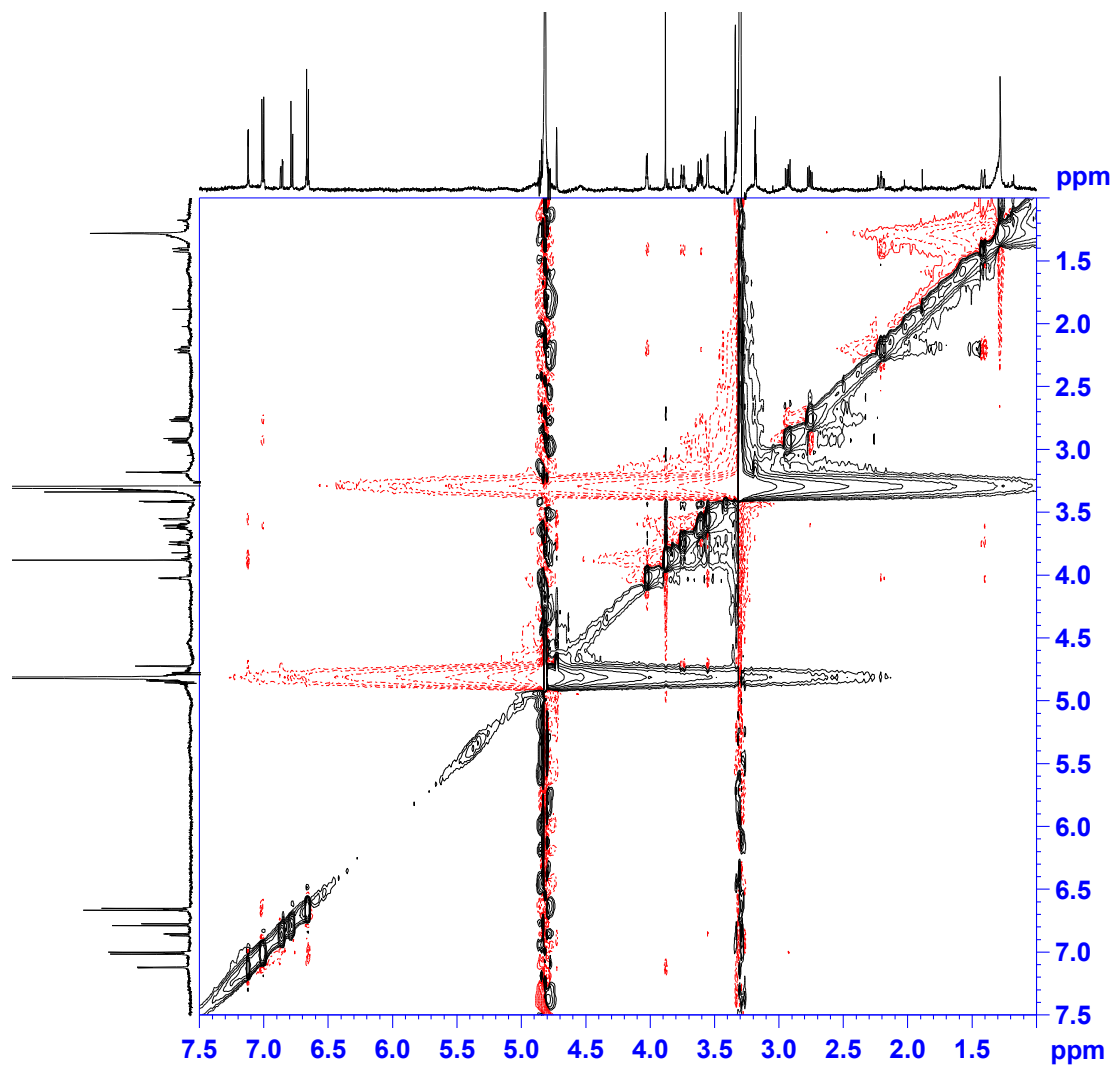
S11. HSQC spectrum of **2** (600MHz, CD_3OD)

11006 ssl-ysl-3351886-fr.3-CD3OD-3.30, 49.0 ppm-20120427, AV3-600, Cryo probe
HMBC

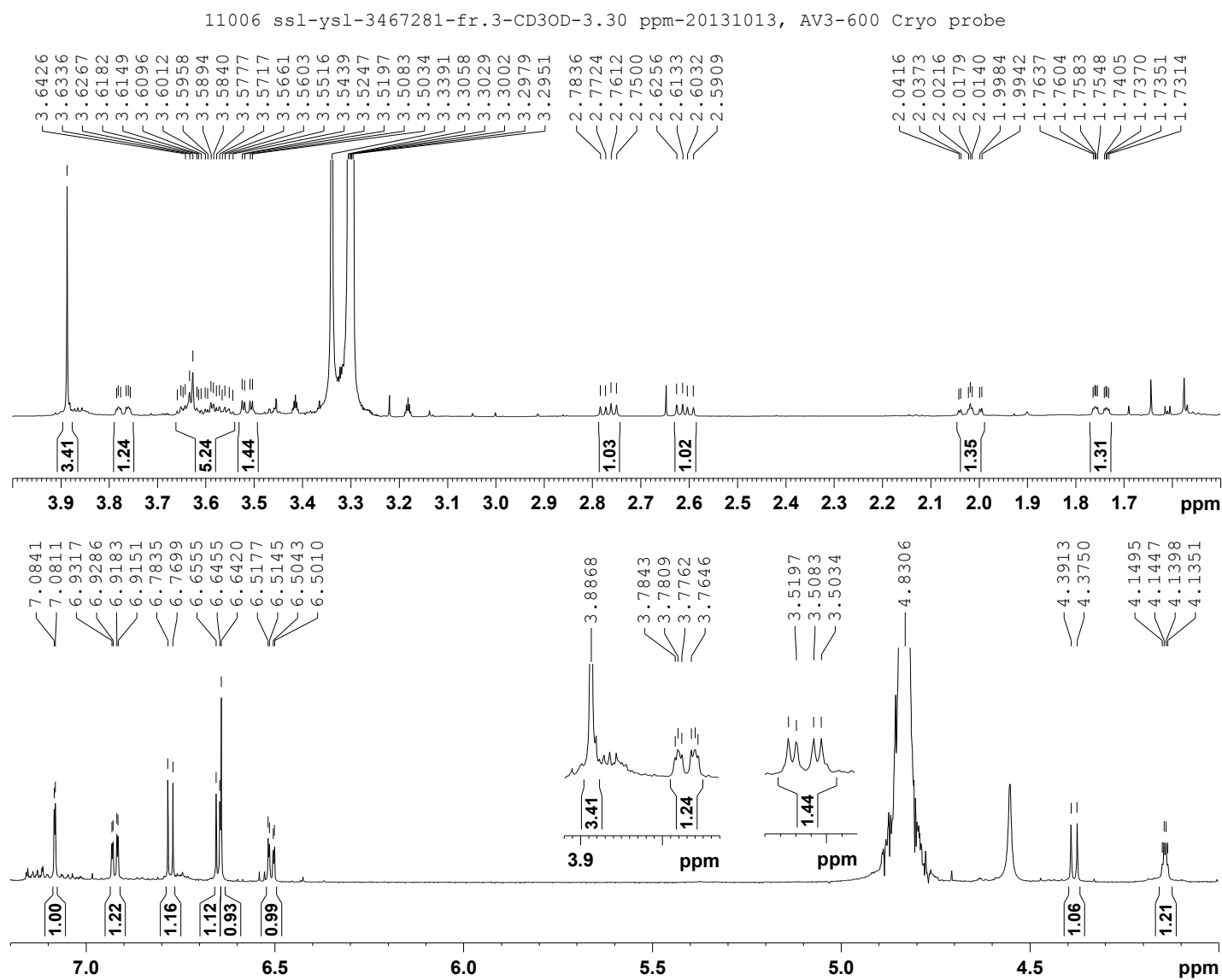


S12. HMBC spectrum of **2** (600MHz, CD_3OD)

11006 ssl-ysl-3351886-fr.3 (cpd12)-CD3OD-3.30 ppm-20140316, AV3-600
NOESY

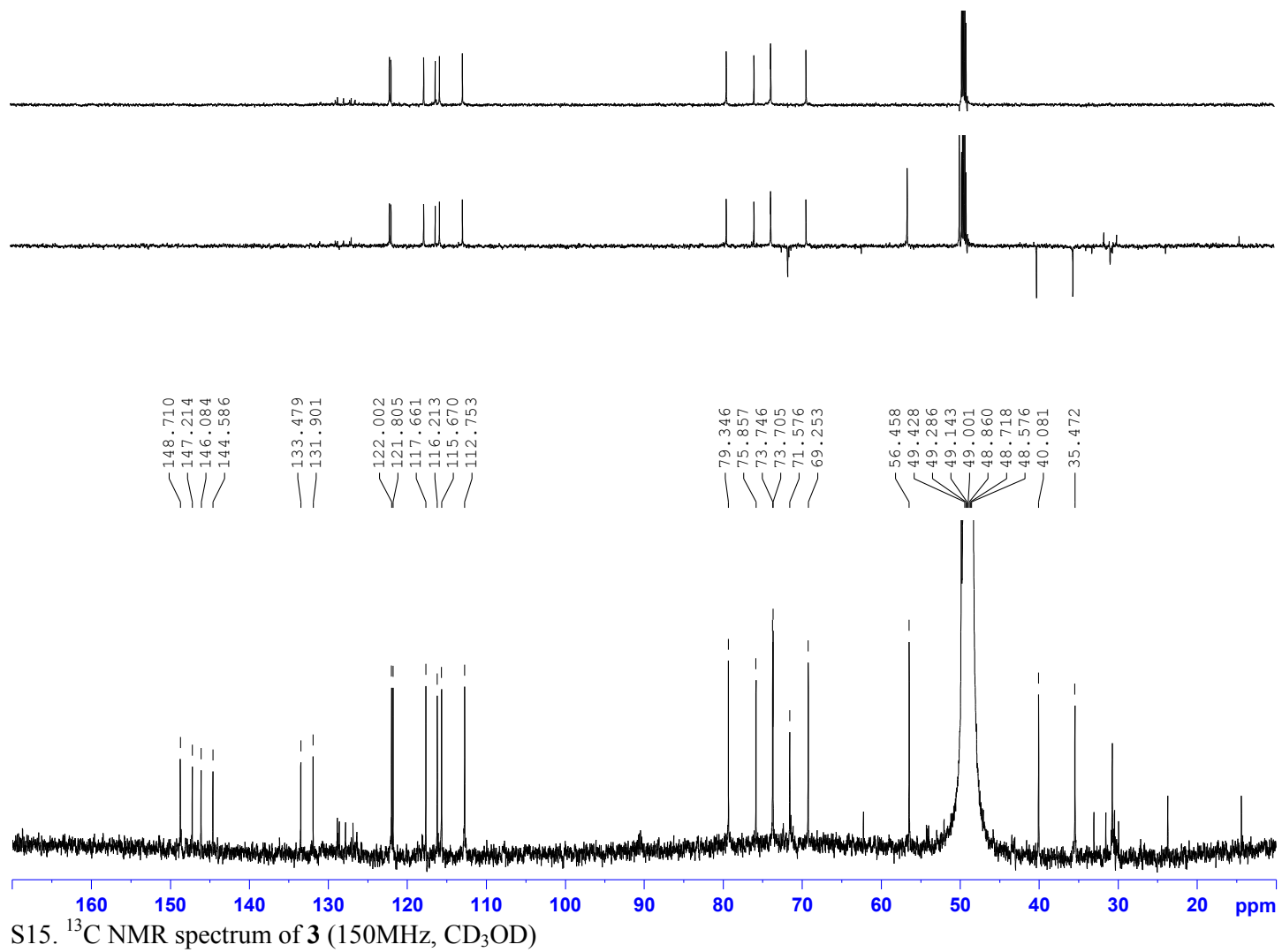


S13. NOESY spectrum of **2** (600MHz, CD₃OD)

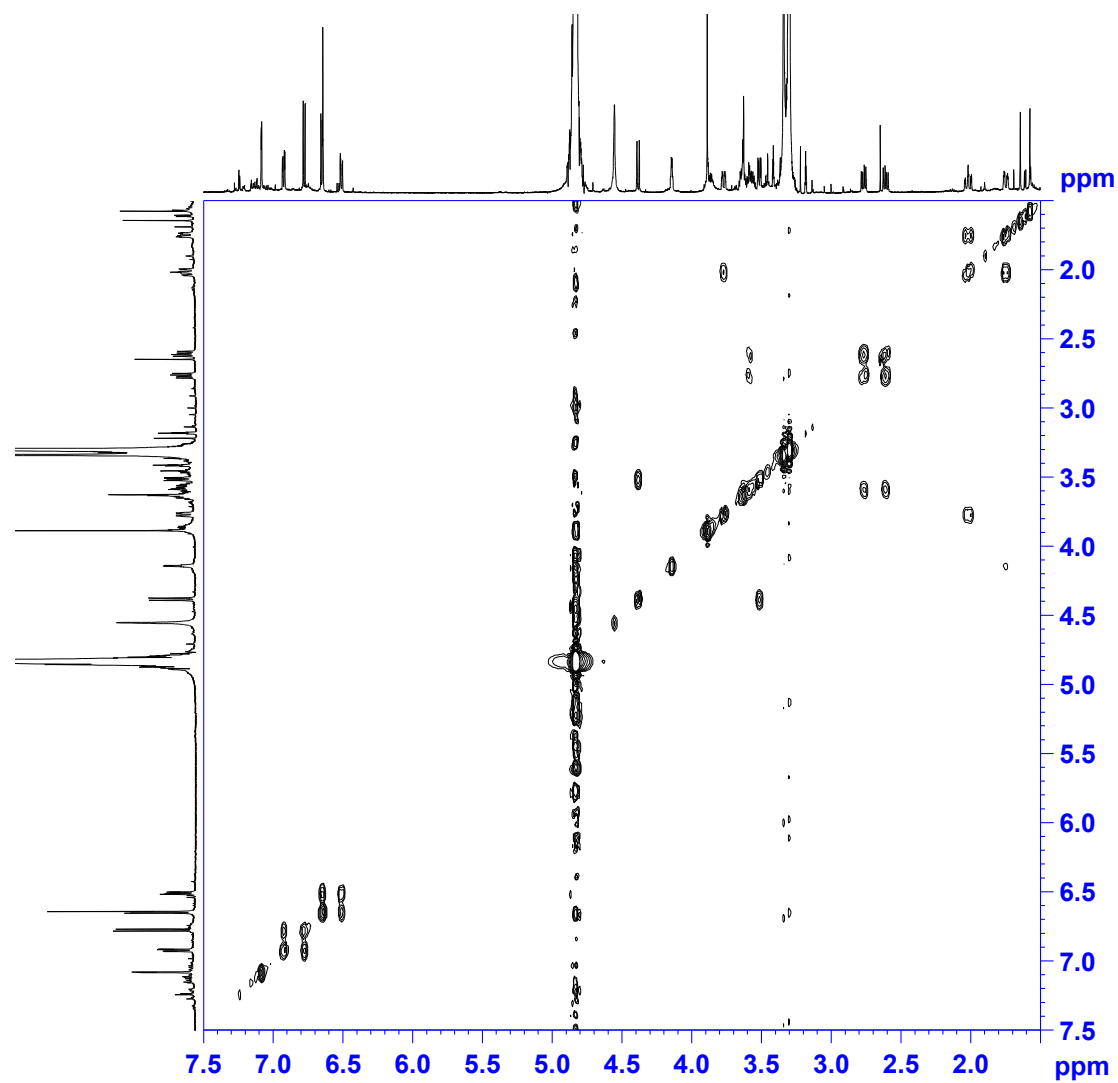


S14. ^1H NMR spectrum of **3** (600MHz, CD_3OD)

11006 ssl-ysl-3467281-fr.3-CD3OD-49.0 ppm-20131013, AV3-600 Cryo probe

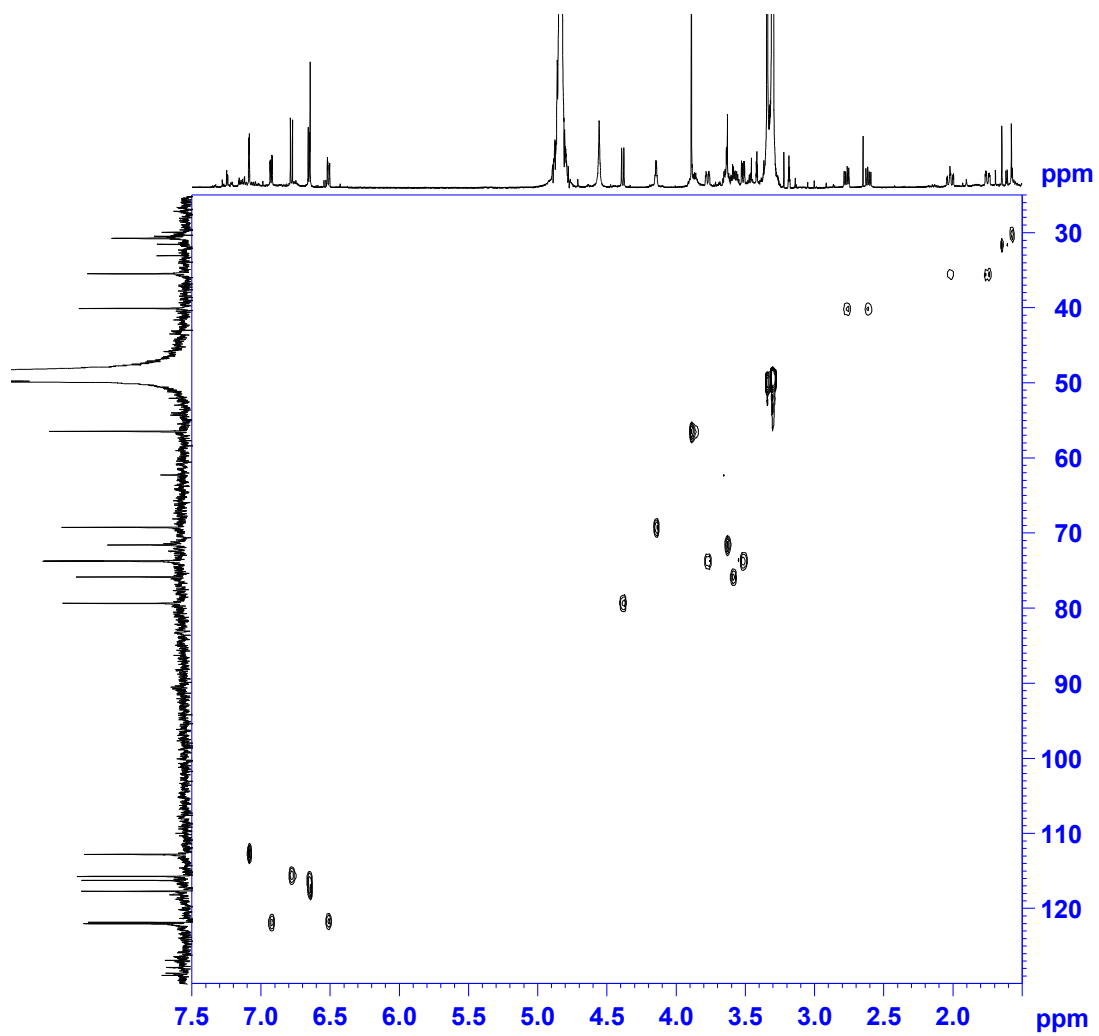


COSY 1006 ssl-ysl-3467281-fr.3-CD3OD-3.30 ppm-20131013, AV3-600 Cryo probe



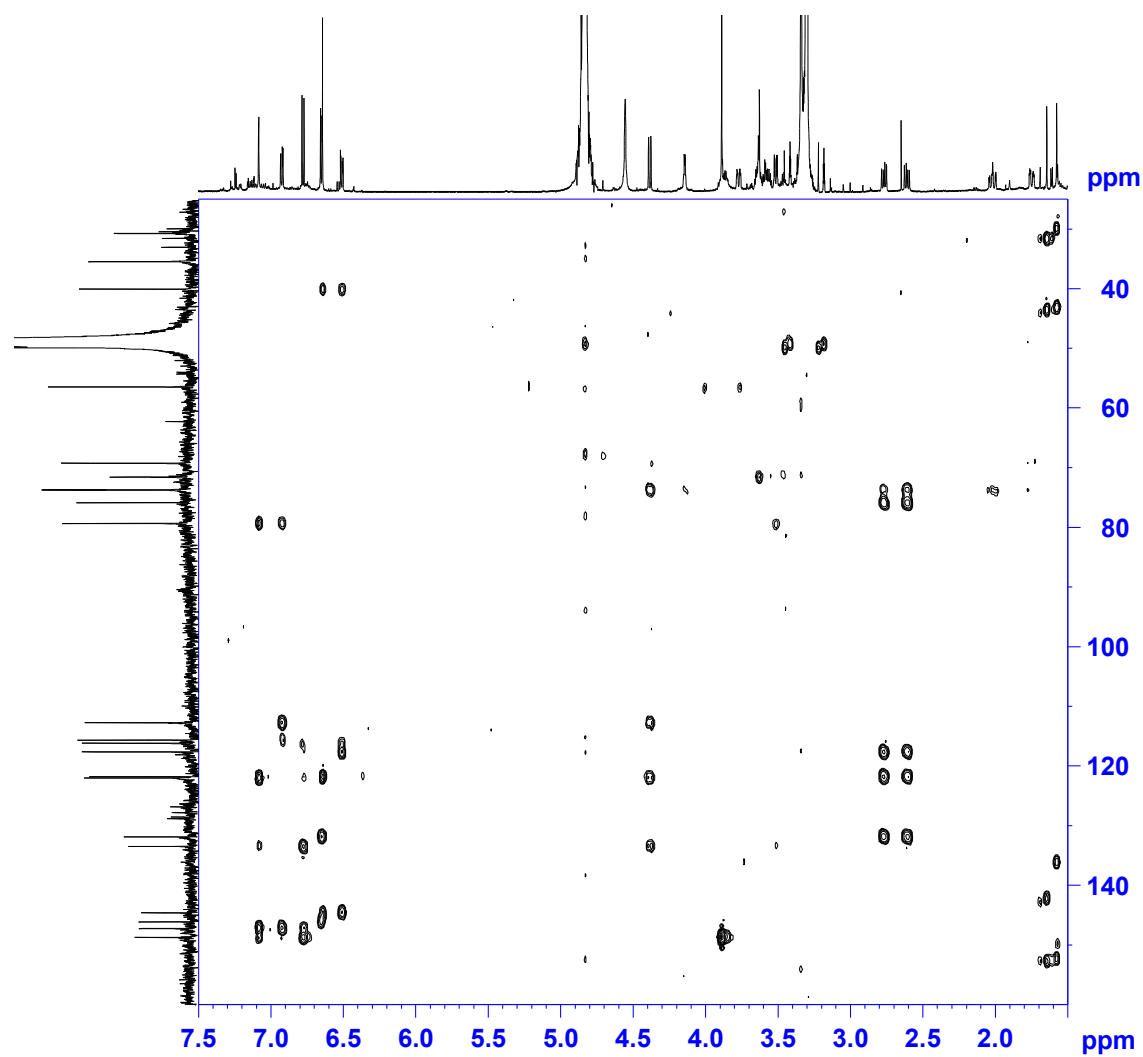
S16. COSY spectrum of **3** (600MHz, CD₃OD)

HSQC 11006 ssl-ysl-3467281-fr.3-CD3OD-3.30, 49.0 ppm-20131013, AV3-600 Cryo probe



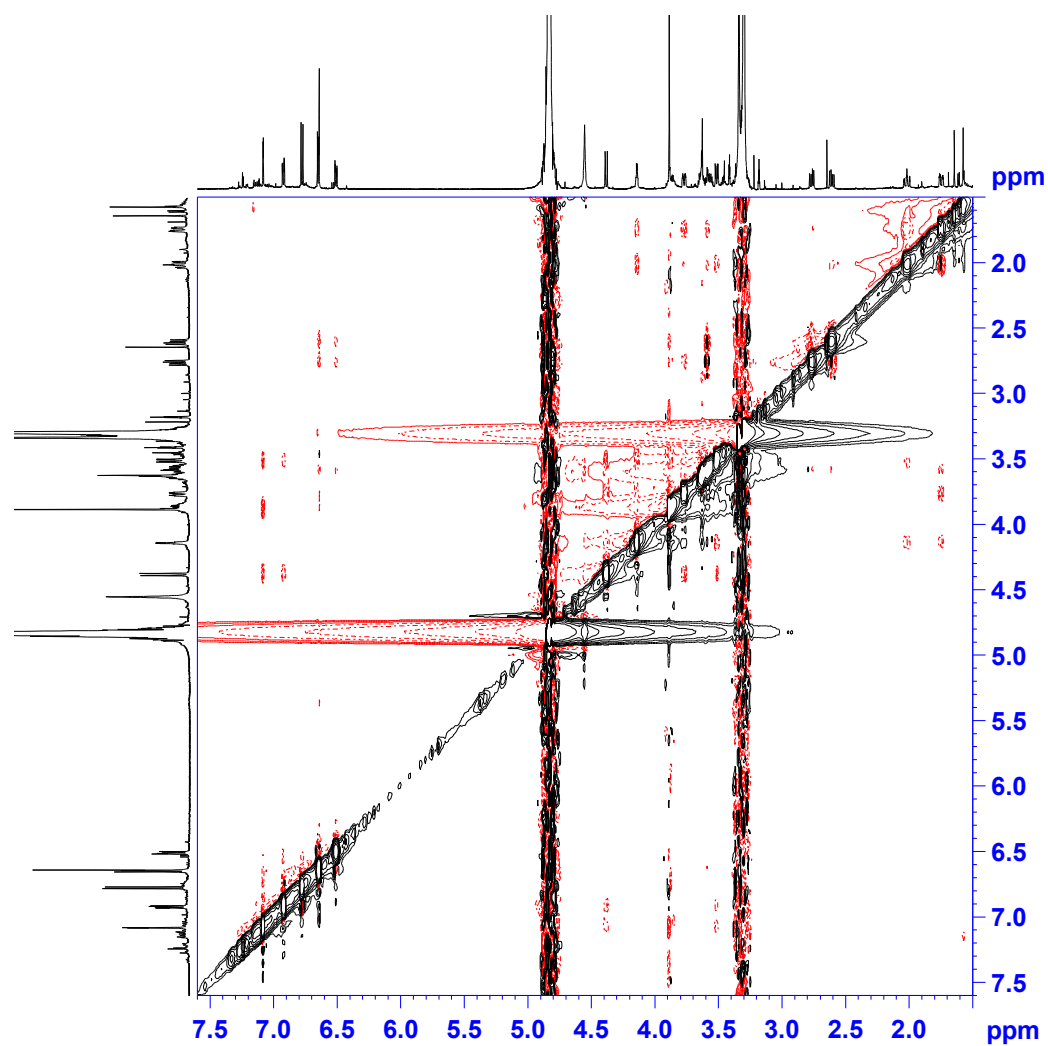
S17. HSQC spectrum of **3** (600MHz, CD_3OD)

HMBC 11006 ssl-ysl-3467281-fr.3-CD3OD-3.30, 49.0 ppm-20131013, AV3-600 Cryo probe

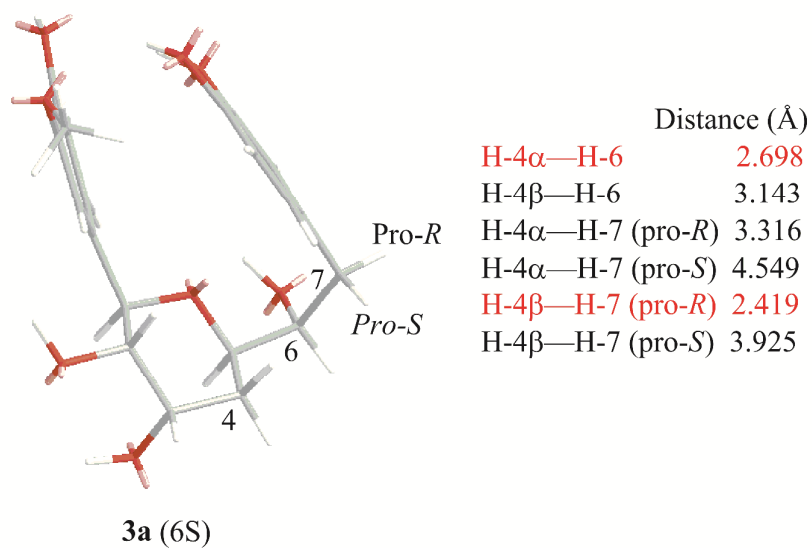
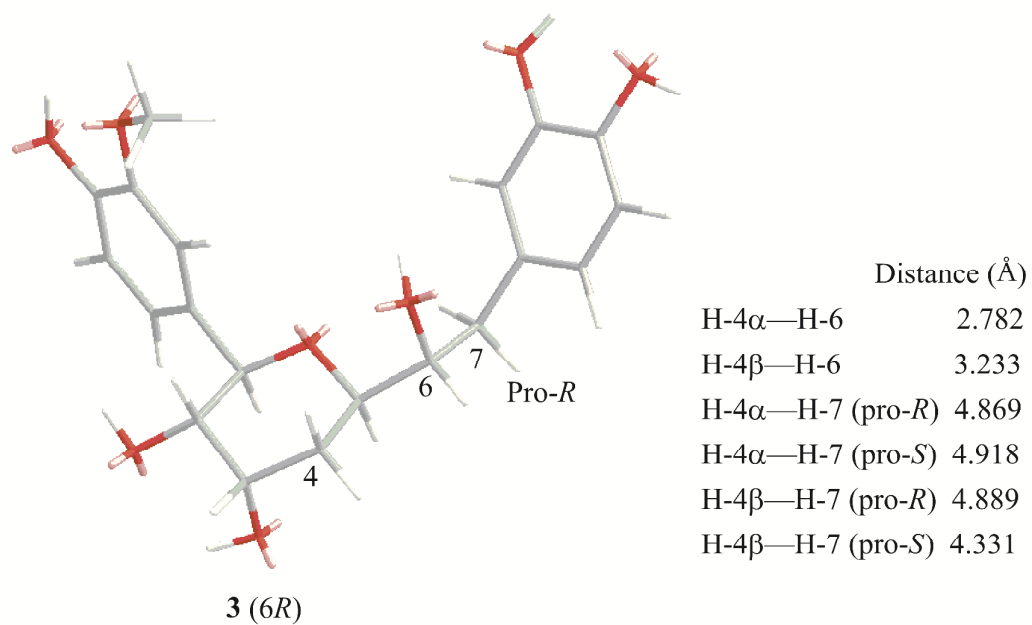


S18. HMBC spectrum of **3** (600MHz, CD₃OD)

NOESY 11006 ssl-ysl-3467281-fr.3-CD3OD-3.30 ppm-20131013, AV3-600 Cryo probe

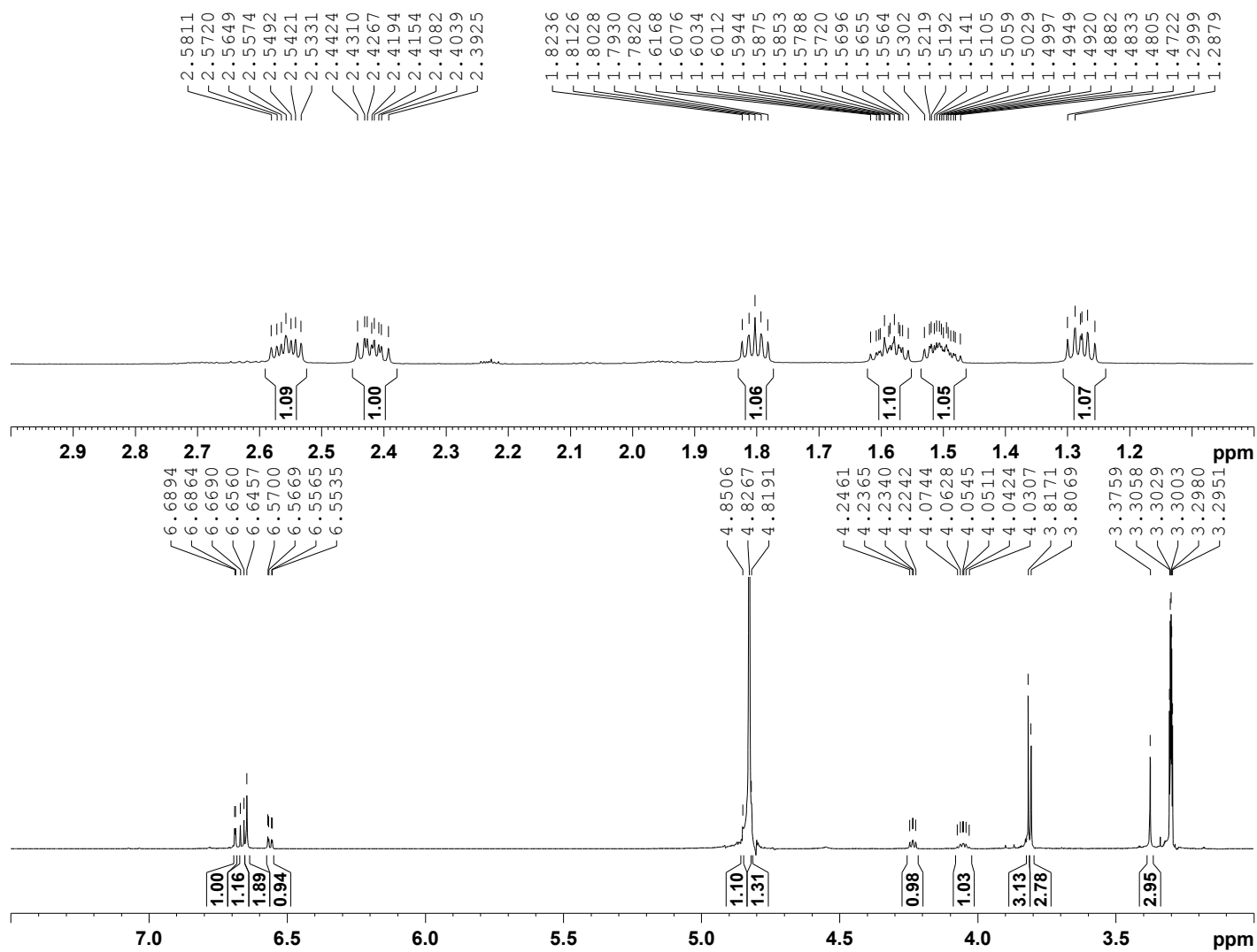


S19. NOESY spectrum of **3** (600MHz, CD₃OD)



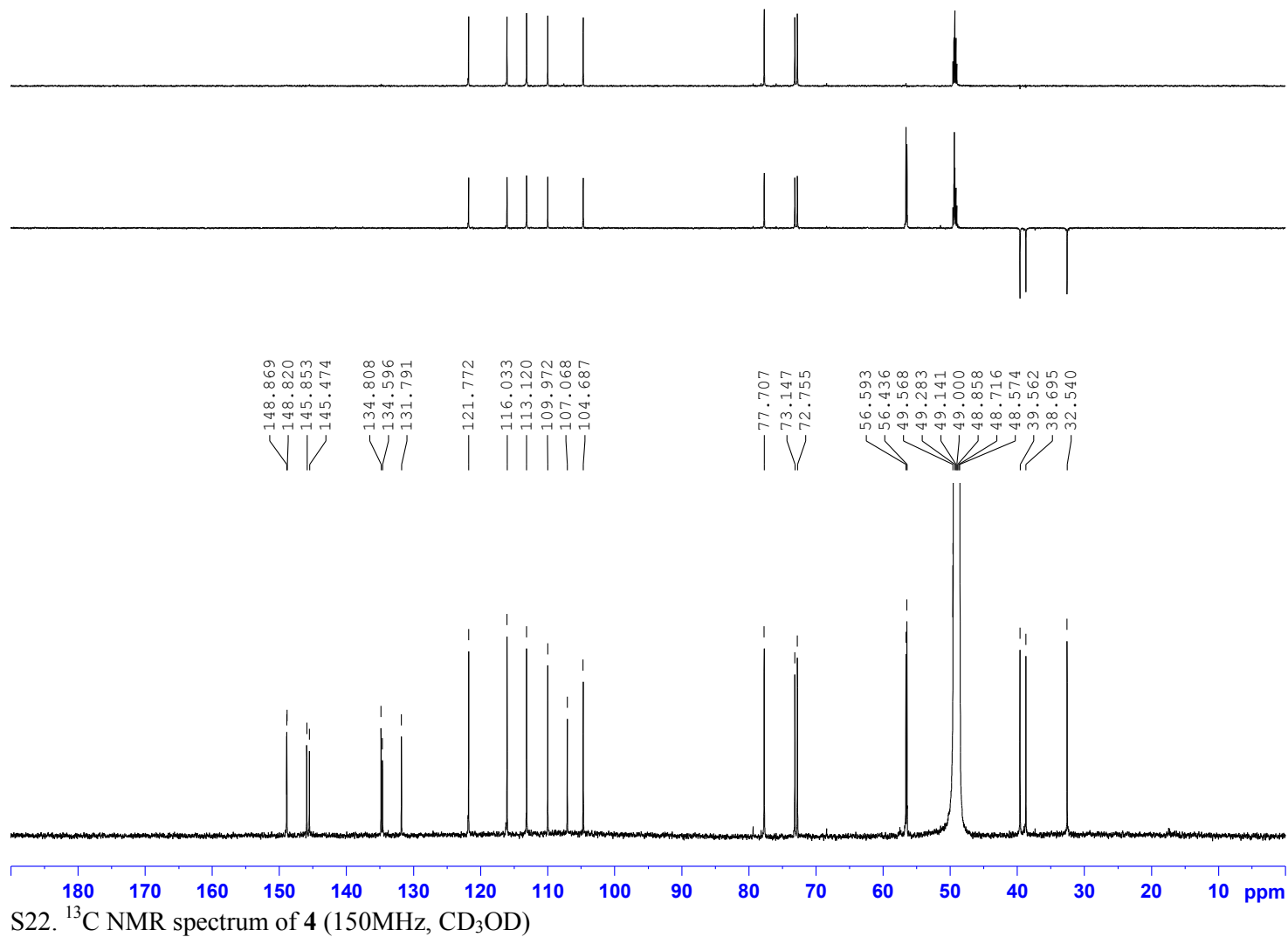
S20. Energy minimized conformation of **3** (6R) and **3a** (6S), obtained by MM2 calculation through molecular dynamic and energy minimization.

11006 ssl-ysl-3351873-fr.4 (30min, cpd5)-CD3OD-3.30 ppm-20120302, Bruker AV-III 600 MHz, Cryo probe

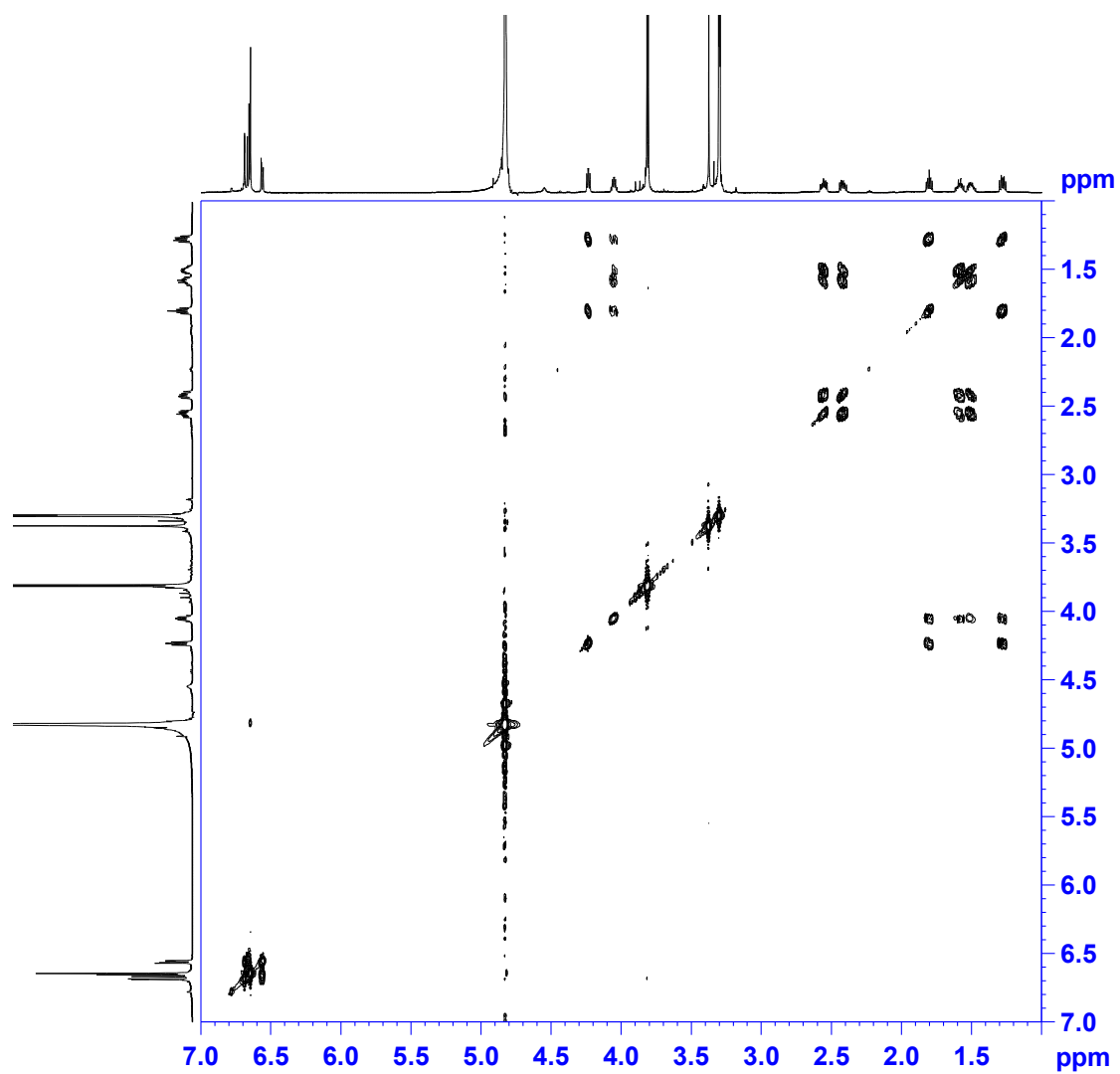


S21. ¹H NMR spectrum of **4** (600MHz, CD₃OD)

11006 ssl-ysl-3351873-fr.4 (cpd5)-CD3OD-49.0 ppm-20120302, AV3-600, Cryo probe

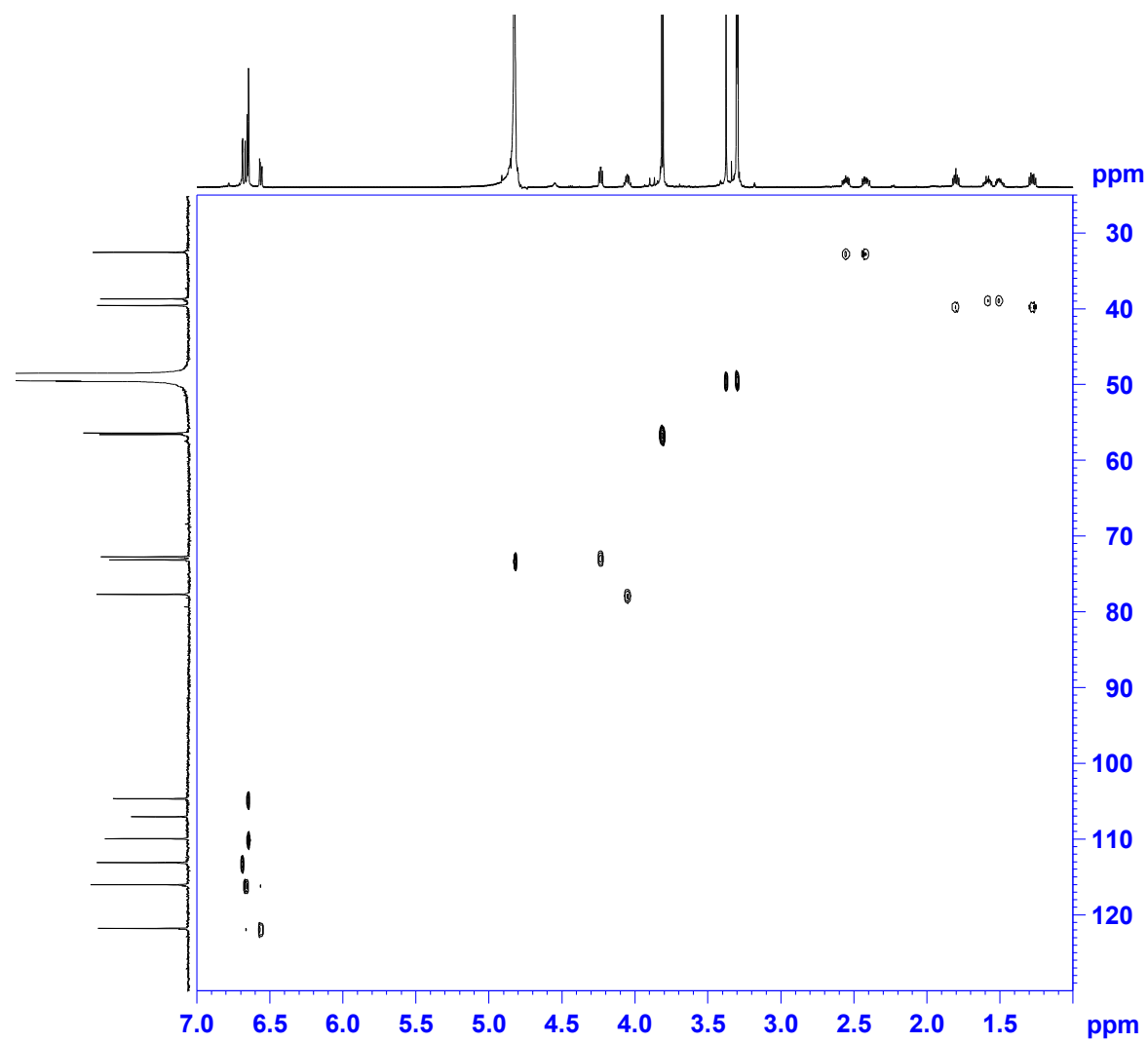


COSY 11006 ssl-ysl-3351873-fr.4(cpd5)-CD3OD-3.30 ppm-20120302, AV3-600, Cryo pr



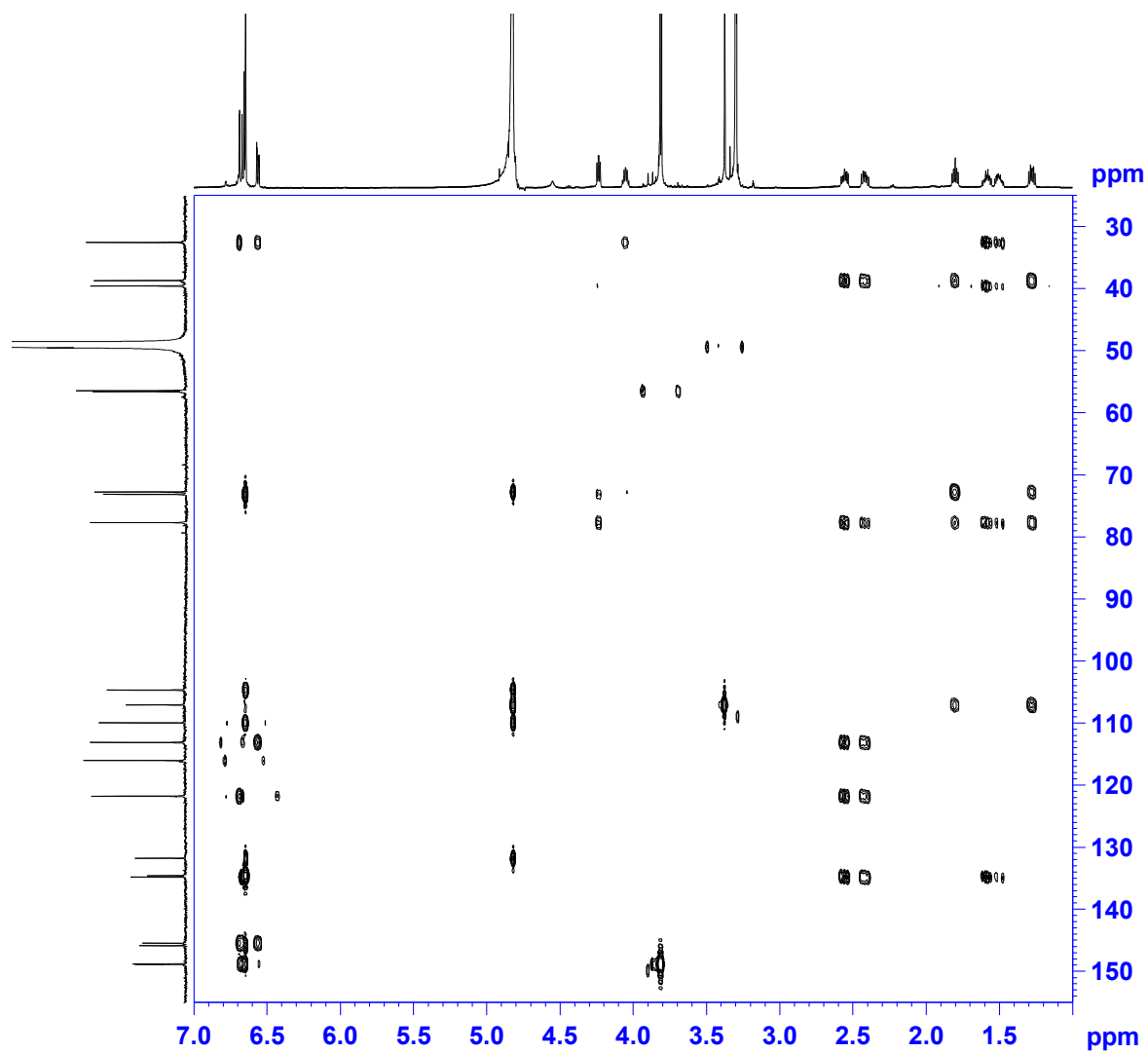
S23. COSY spectrum of **4** (600MHz, CD₃OD)

HSQC 11006 ssl-ysl-3351873-fr.4(cpd5)-CD3OD-3.30 ppm-20120302, AV3-600, Cryo pr



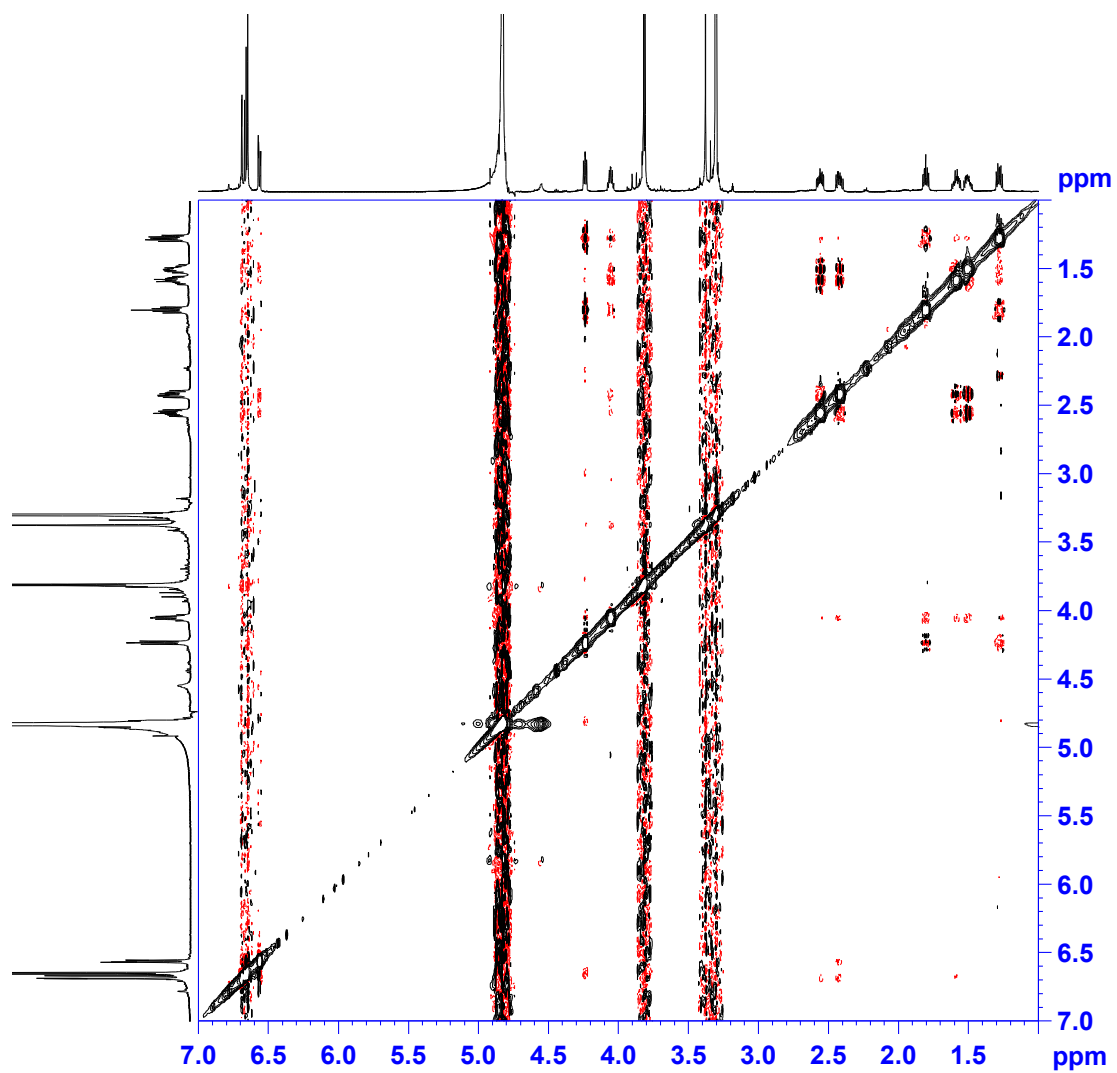
S24. HSQC spectrum of **4** (600MHz, CD_3OD)

HMBC 11006 ssl-ysl-3351873-fr.4(cpd5)-CD3OD-3.30, 49.0 ppm-20120302, AV3-600, C

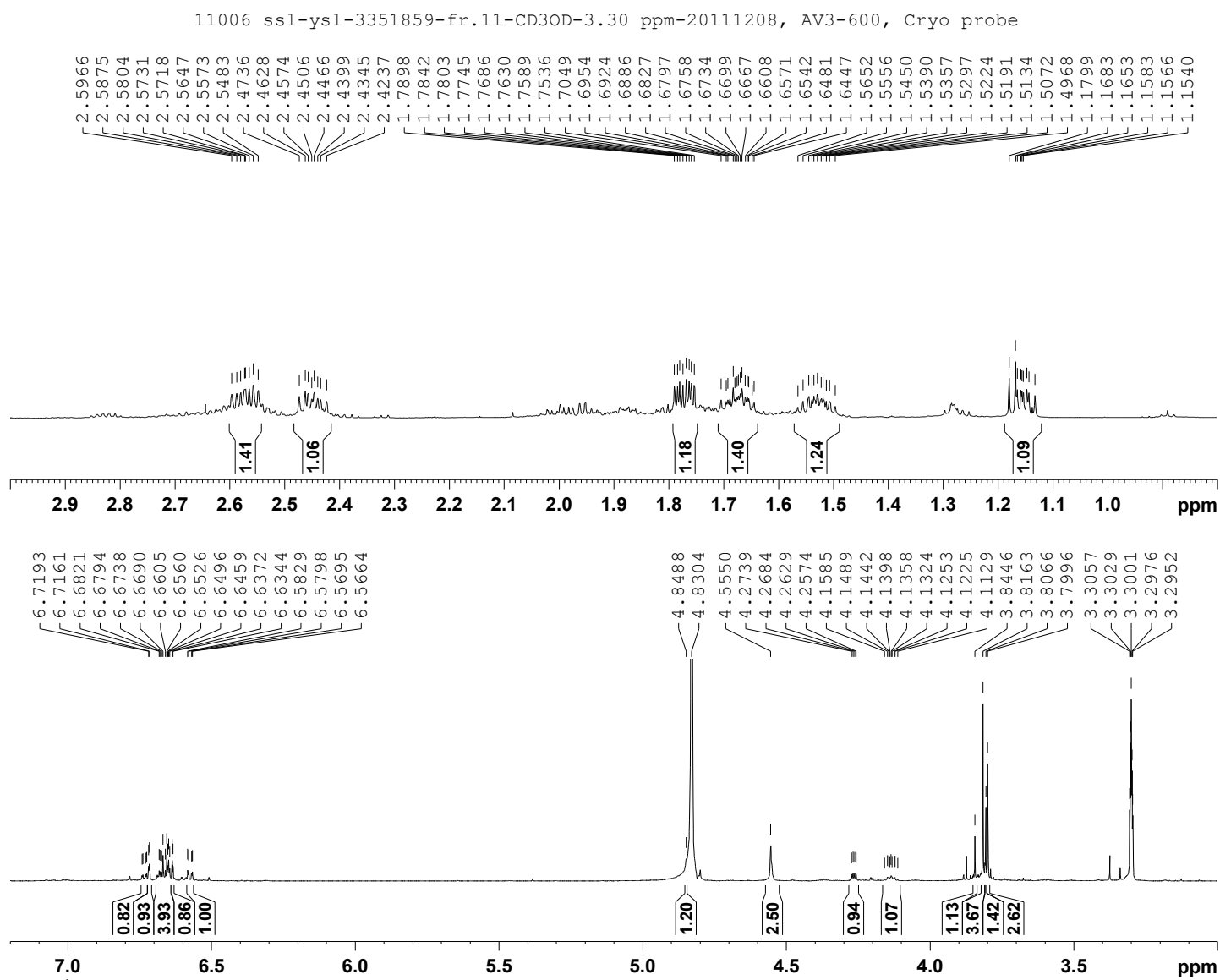


S25. HMBC spectrum of **4** (600MHz, CD₃OD)

11006 ssl-ysl-3351873-fr.4 (cpd5)-CD3OD-3.30 ppm-20120302, AV3-600, Cryo probe

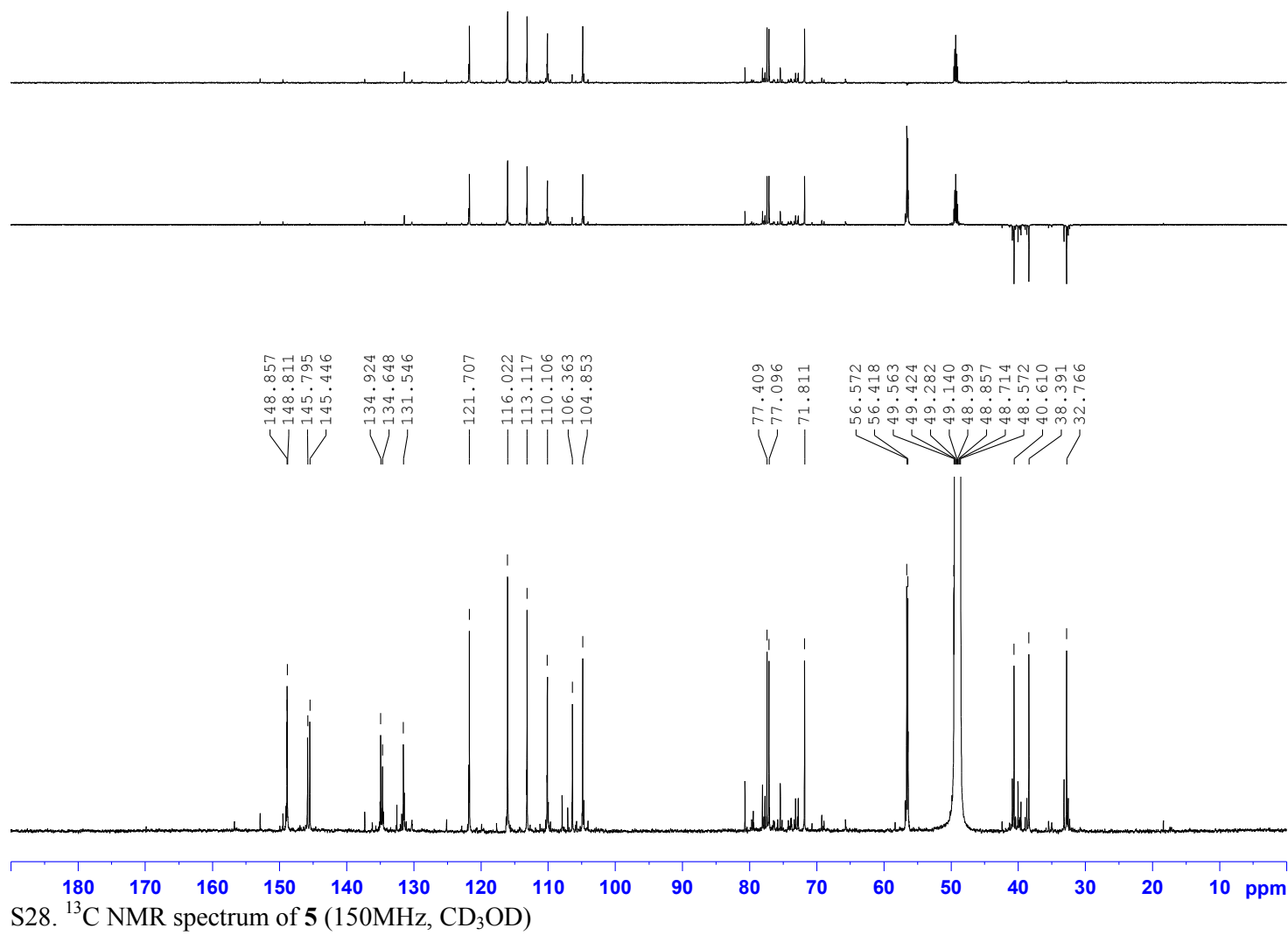


S26. NOESY spectrum of **4** (600MHz, CD₃OD)

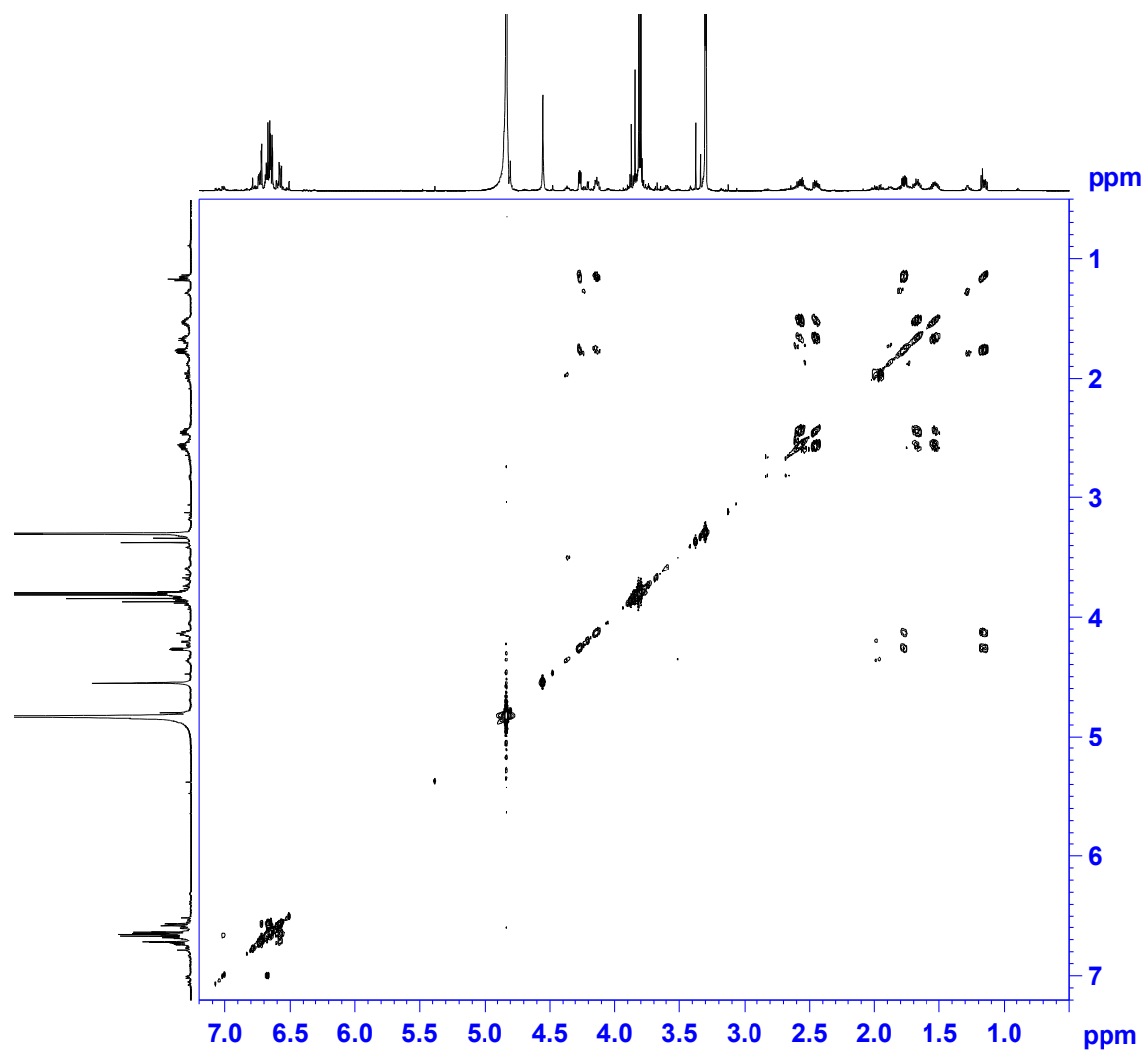


S27. ^1H NMR spectrum of **5** (600MHz, CD_3OD)

11006 ssl-ysl-3351859-fr.11-CD3OD-49.0 ppm-20111208, AV3-600, Cryo probe

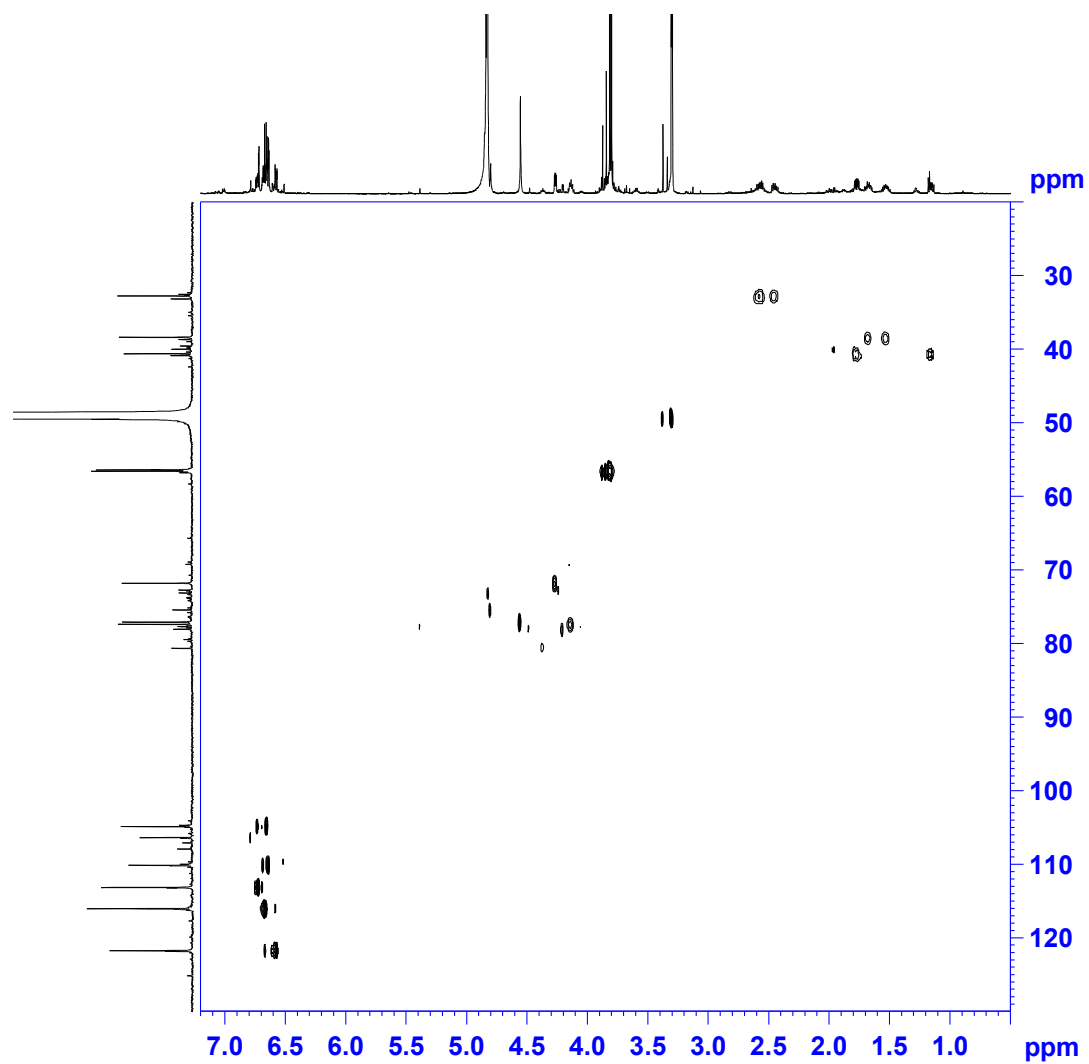


COSY 11006 ssl-ysl-3351859-fr.11-CD3OD-3.30 ppm-20111208, AV3-600, Cryo probe



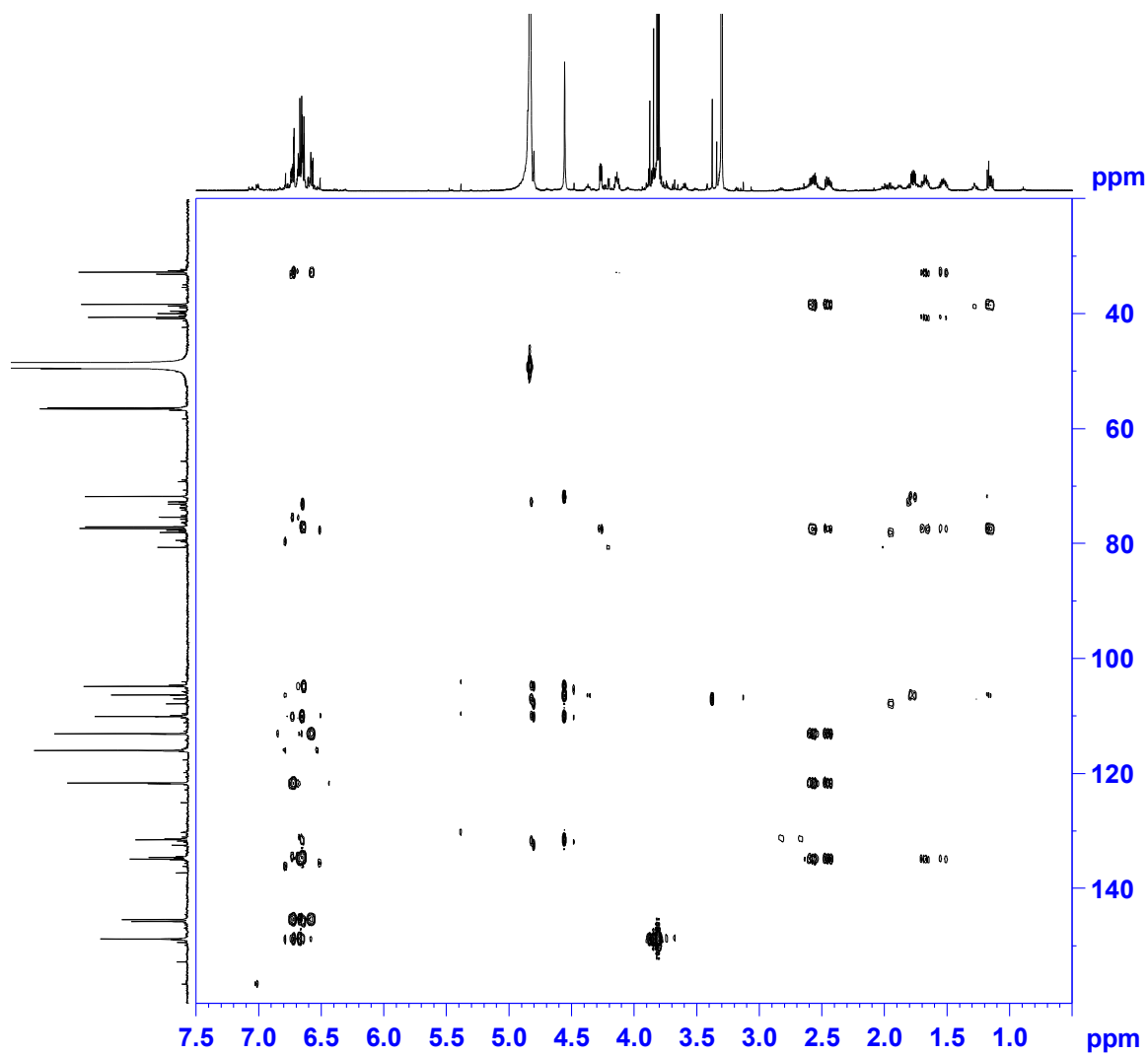
S29. COSY spectrum of **5** (600MHz, CD₃OD)

HSQC 11006 ssl-ysl-3351859-fr.11-CD3OD-3.30, 49.0 ppm-20111208, AV3-600, Cryo p



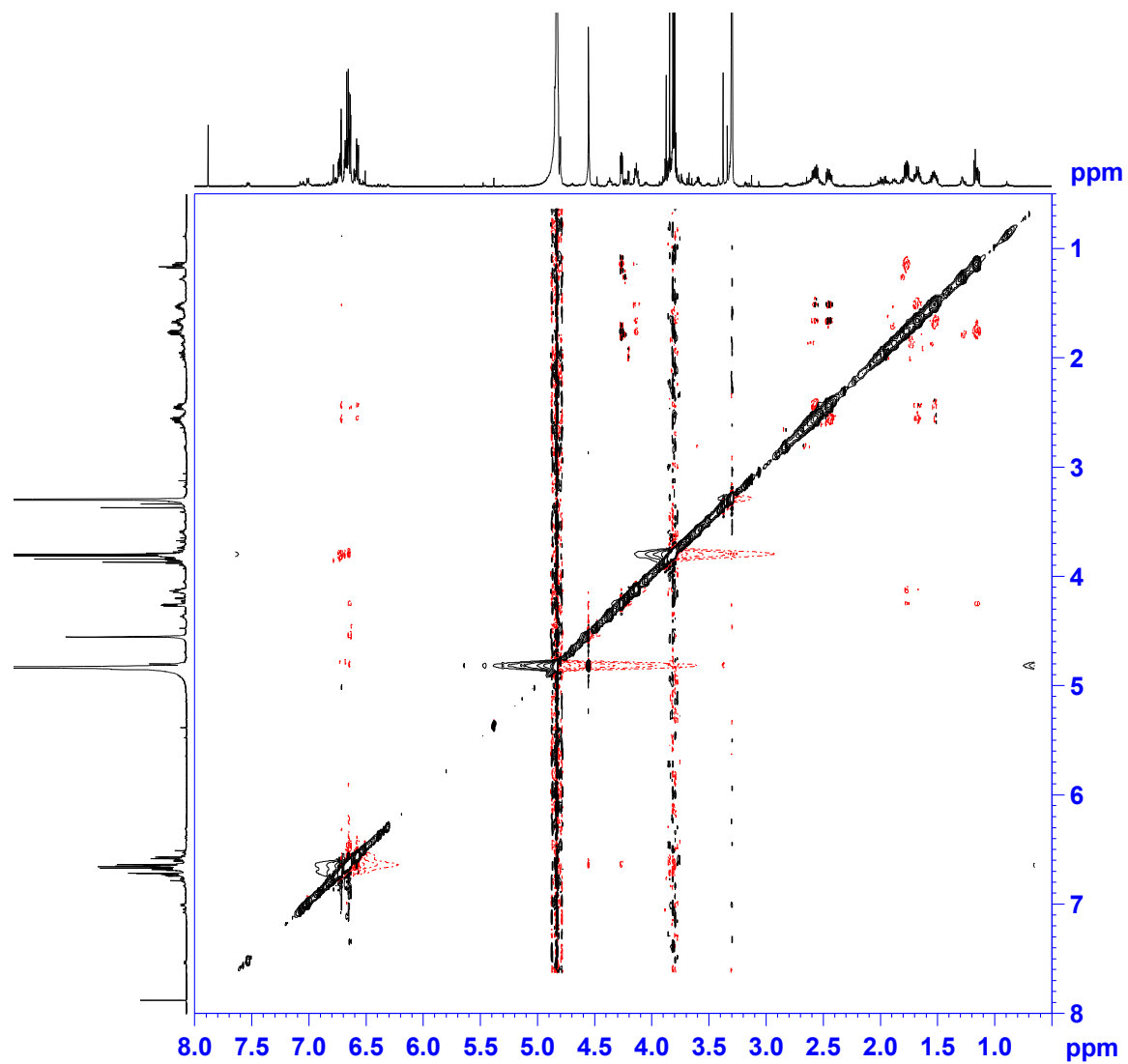
S30. HSQC spectrum of **5** (600MHz, CD_3OD)

HMBC 11006 ssl-y51-3351859-fr.11-CD3OD-3.30, 49.0 ppm-20111208, AV3-600, Cryo p



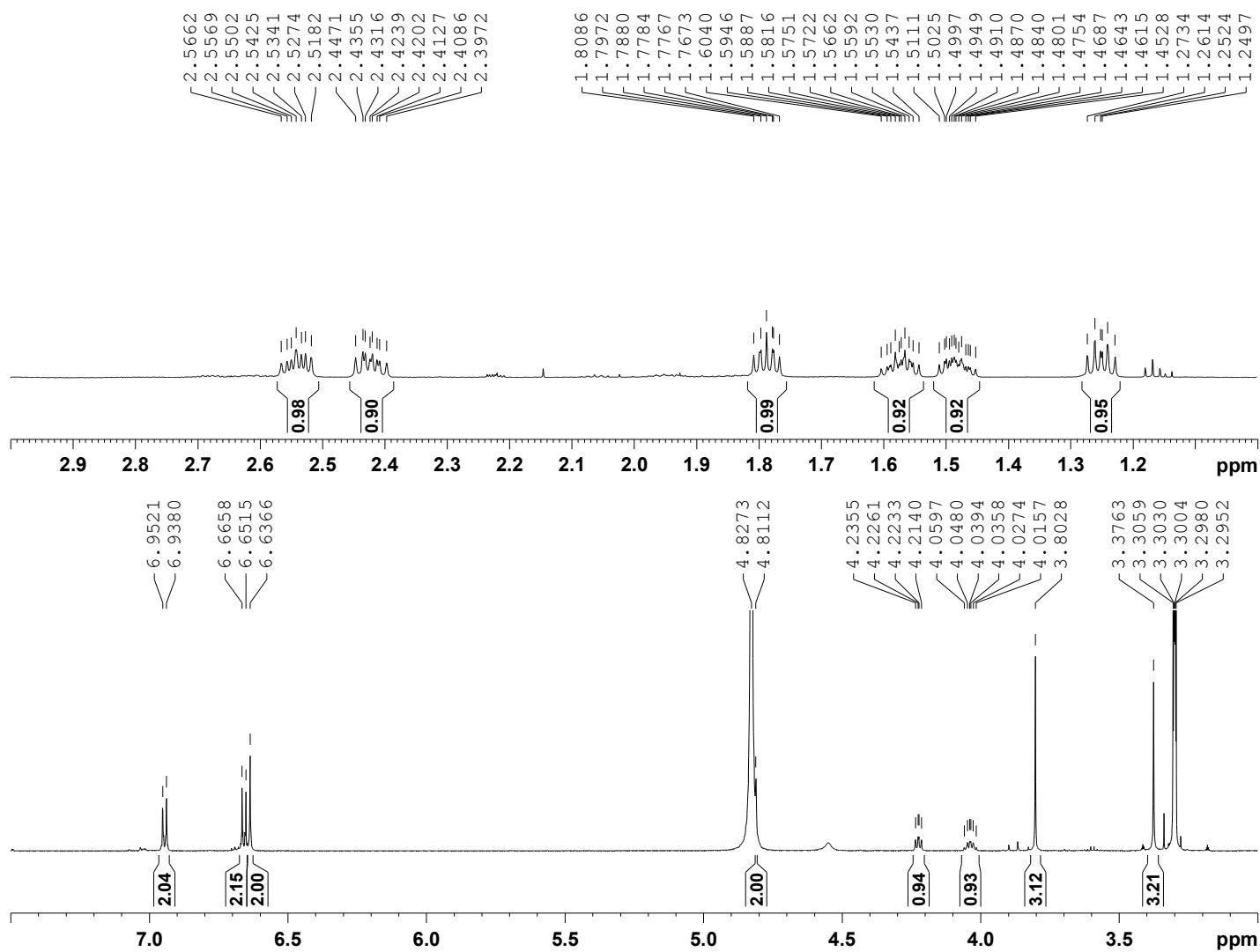
S31. HMBC spectrum of **5** (600MHz, CD₃OD)

NOESY 11006 ssl-ysl-3351859-fr.11-CD3OD-3.30 ppm-20111208, AV3-600, Cryo probe



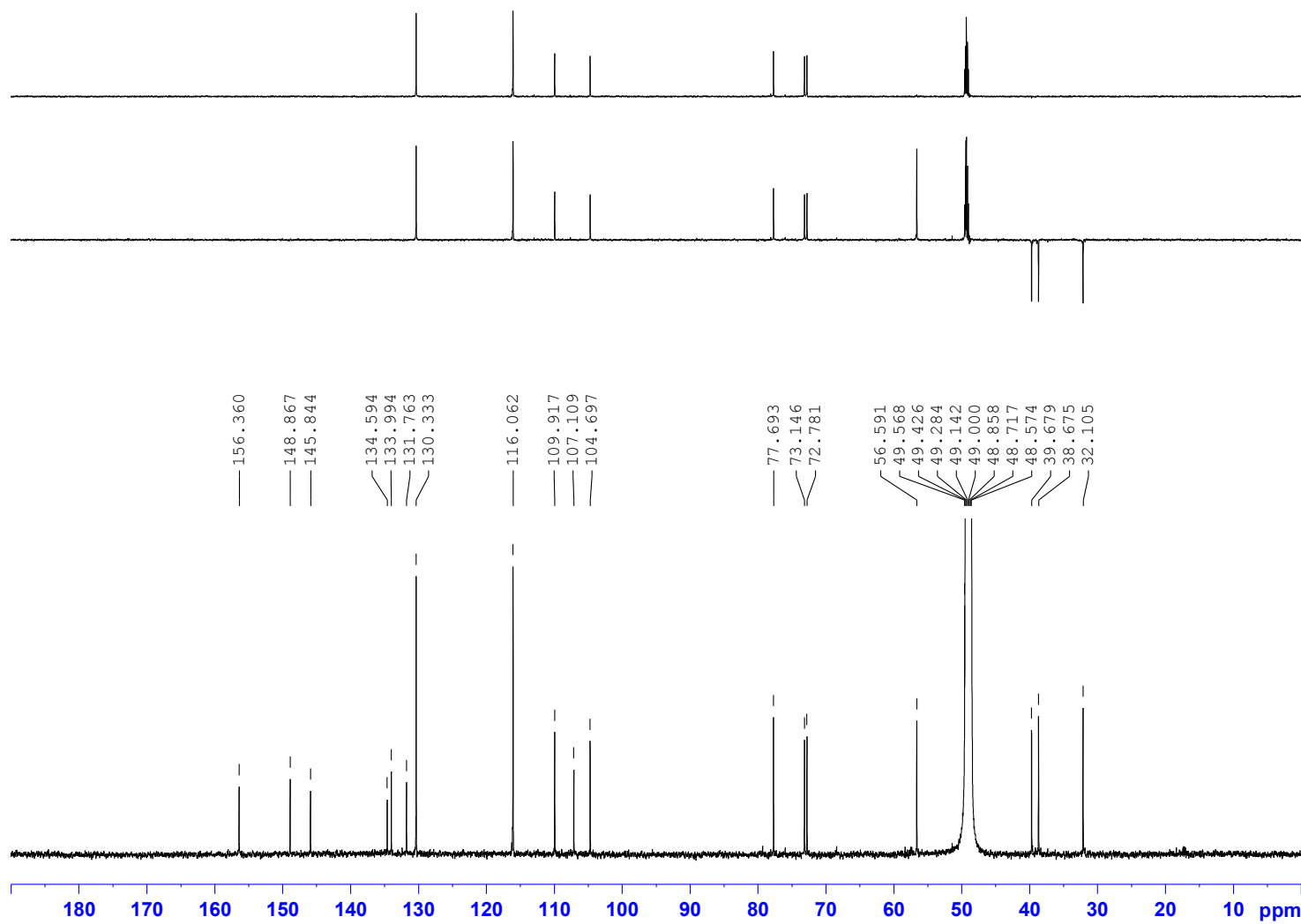
S32. NOESY spectrum of **5** (600MHz, CD₃OD)

11006 ssl-ysl-3351884-fr.3-CD3OD-3.30 ppm-20120420, Bruker AV-III 600 MHz, Cryo probe



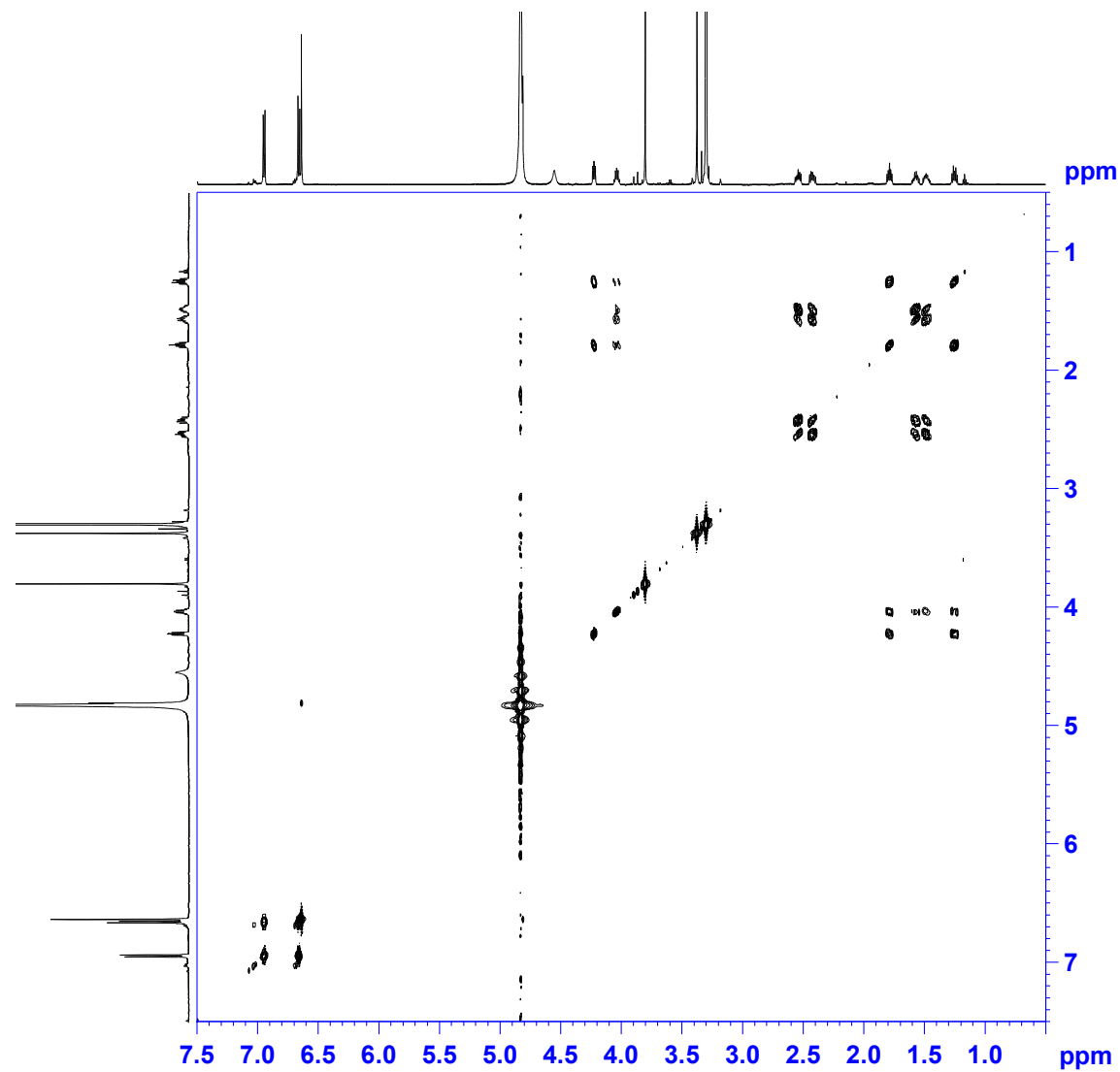
S33. ^1H NMR spectrum of **6** (600MHz, CD_3OD)

11006 ssl-ysl-3351884-fr.3(cpd 9)-CD3OD-49.0 ppm-20120420, AV3-600, Cryo probe



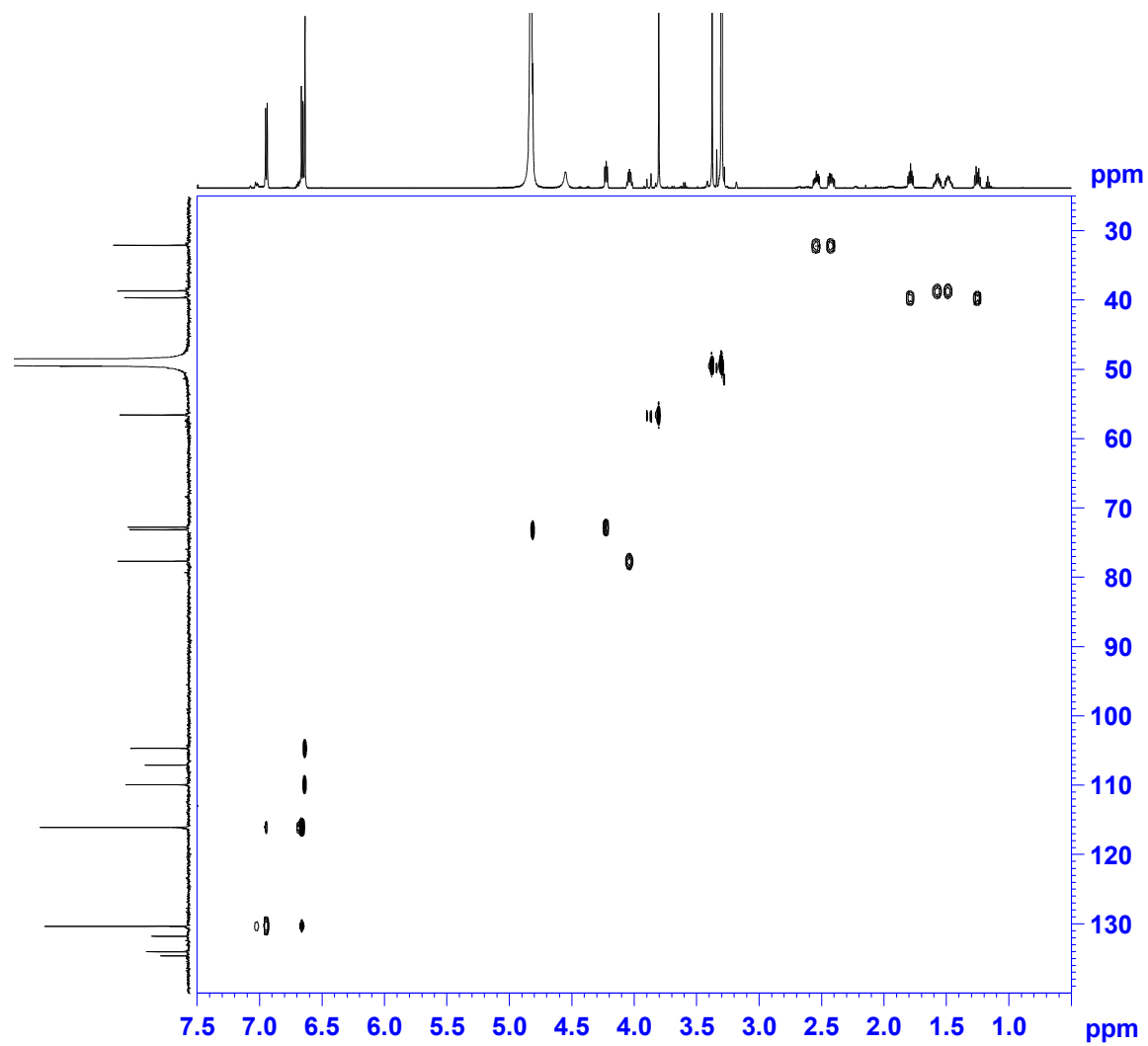
S34. ^{13}C NMR spectrum of **6** (150MHz, CD_3OD)

11006 ssl-ysl-3351884-fr.3(cpd 8)-CD3OD-3.30 ppm-20120420, AV3-600, Cryo probe
COSY



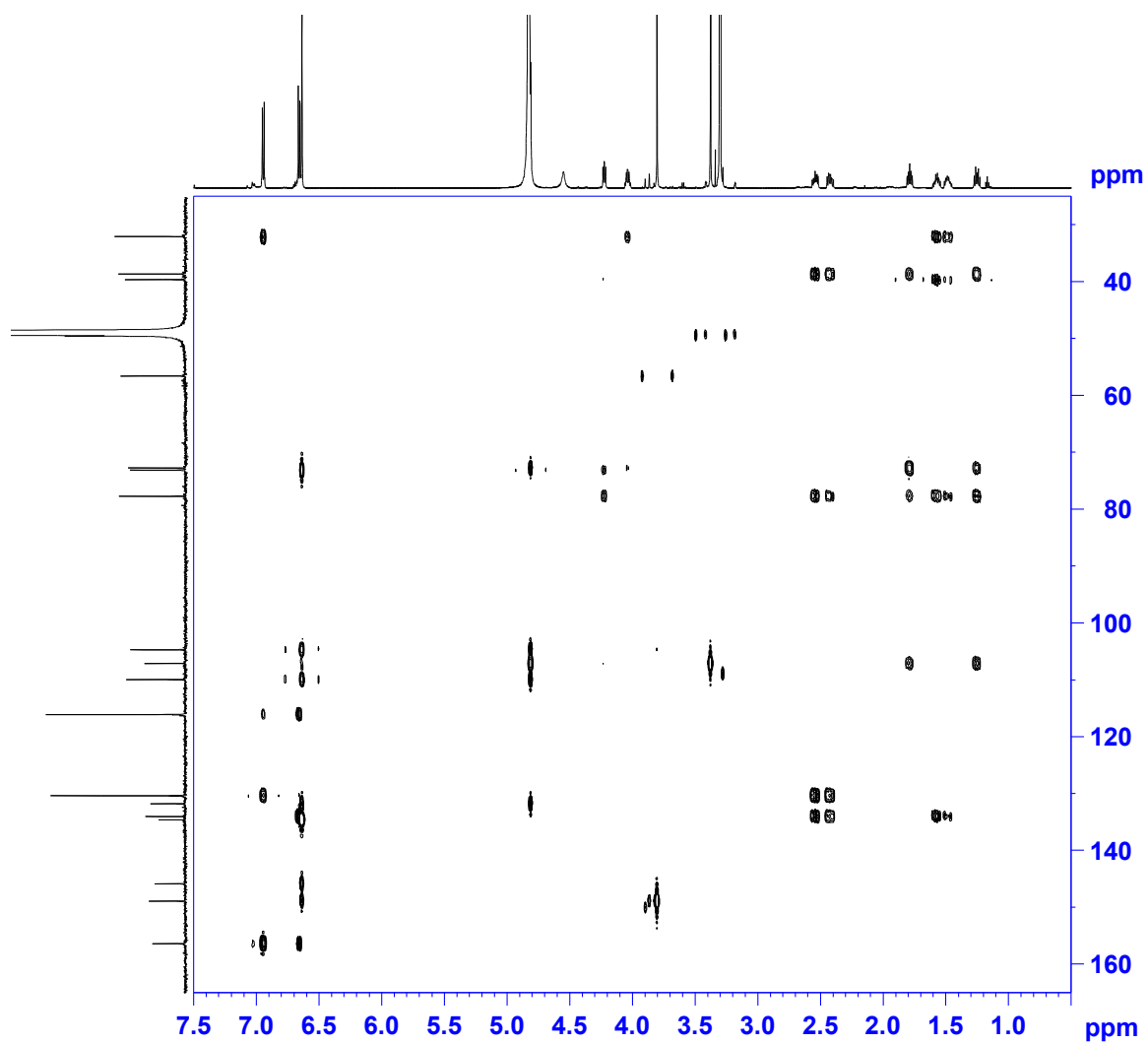
S35. COSY spectrum of **6** (600MHz, CD₃OD)

11006 ssl-ysl-3351884-fr.3(cpd 8)-CD3OD-3.30, 49.0 ppm-20120420, AV3-600, Cryo probe
HSQC



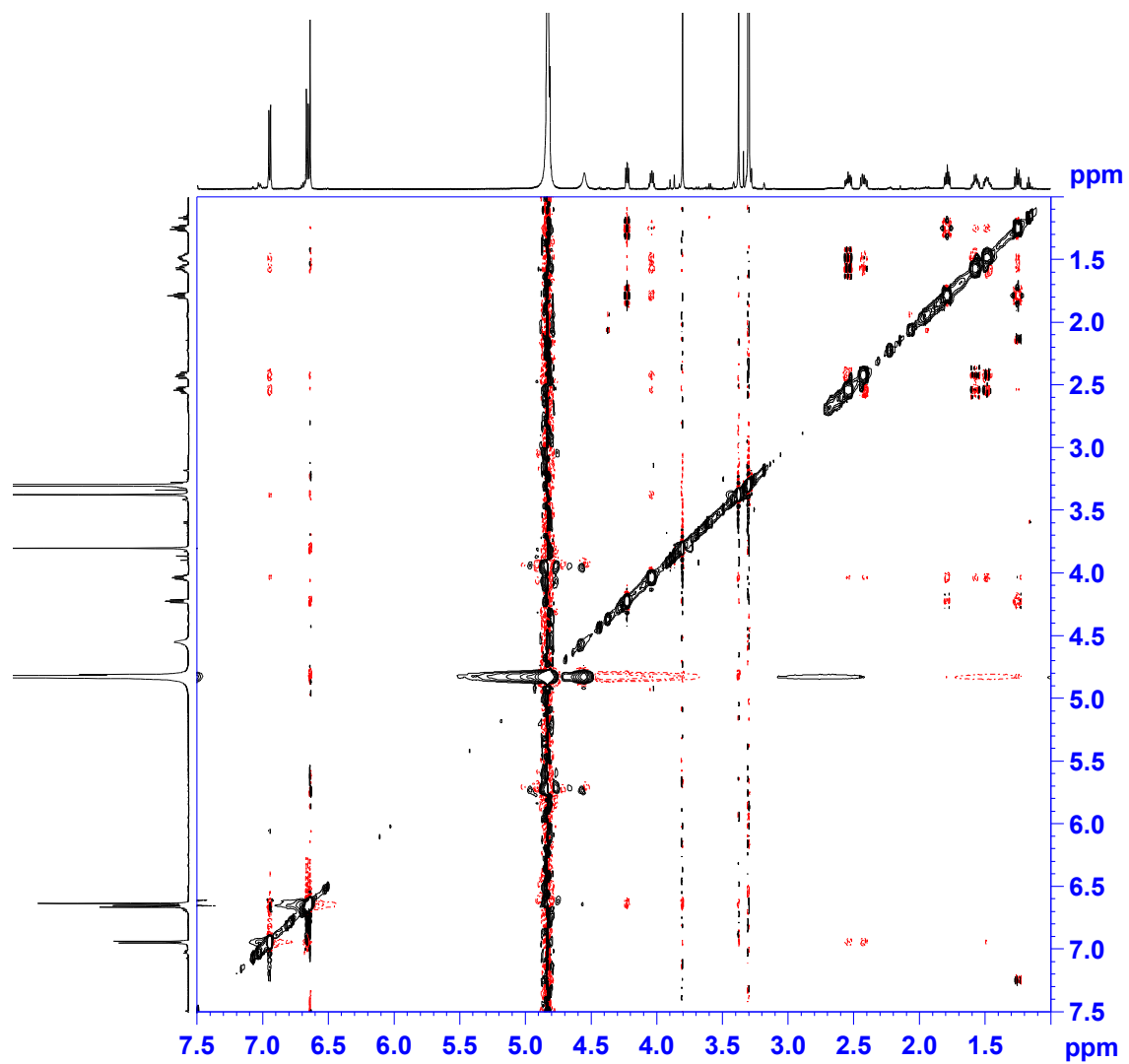
S36. HSQC spectrum of **6** (600MHz, CD₃OD)

11006 ssl-ysl-3351884-fr.3(cpd 8)-CD3OD-3.30, 49.0 ppm-20120420, AV3-600, Cryo probe
HMBC

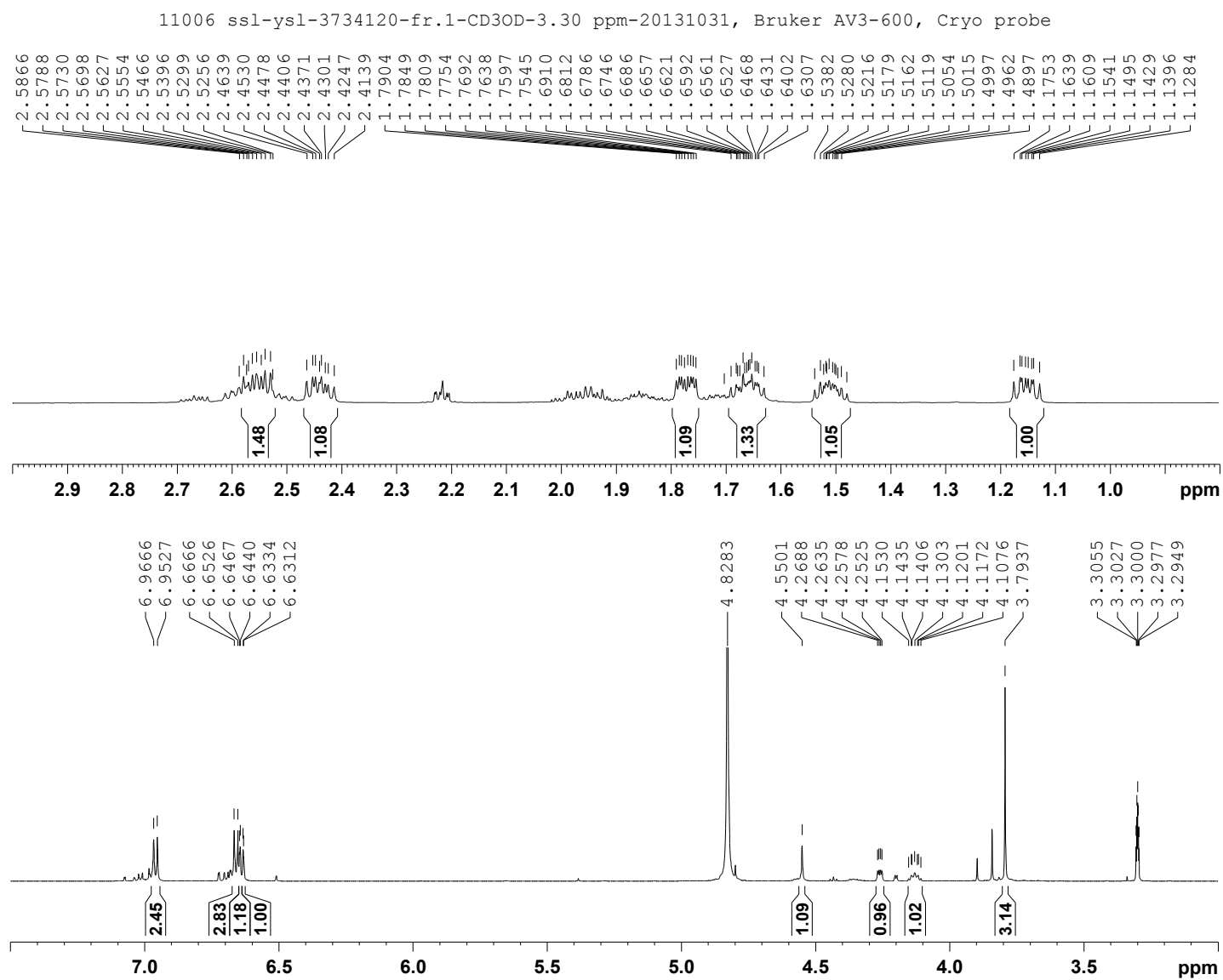


S37. HMBC spectrum of **6** (600MHz, CD₃OD)

11006 ssl-ysl-3351884-fr.3(cpd 9)-CD3OD-3.30 ppm-20120420, AV3-600, Cryo probe
NOESY

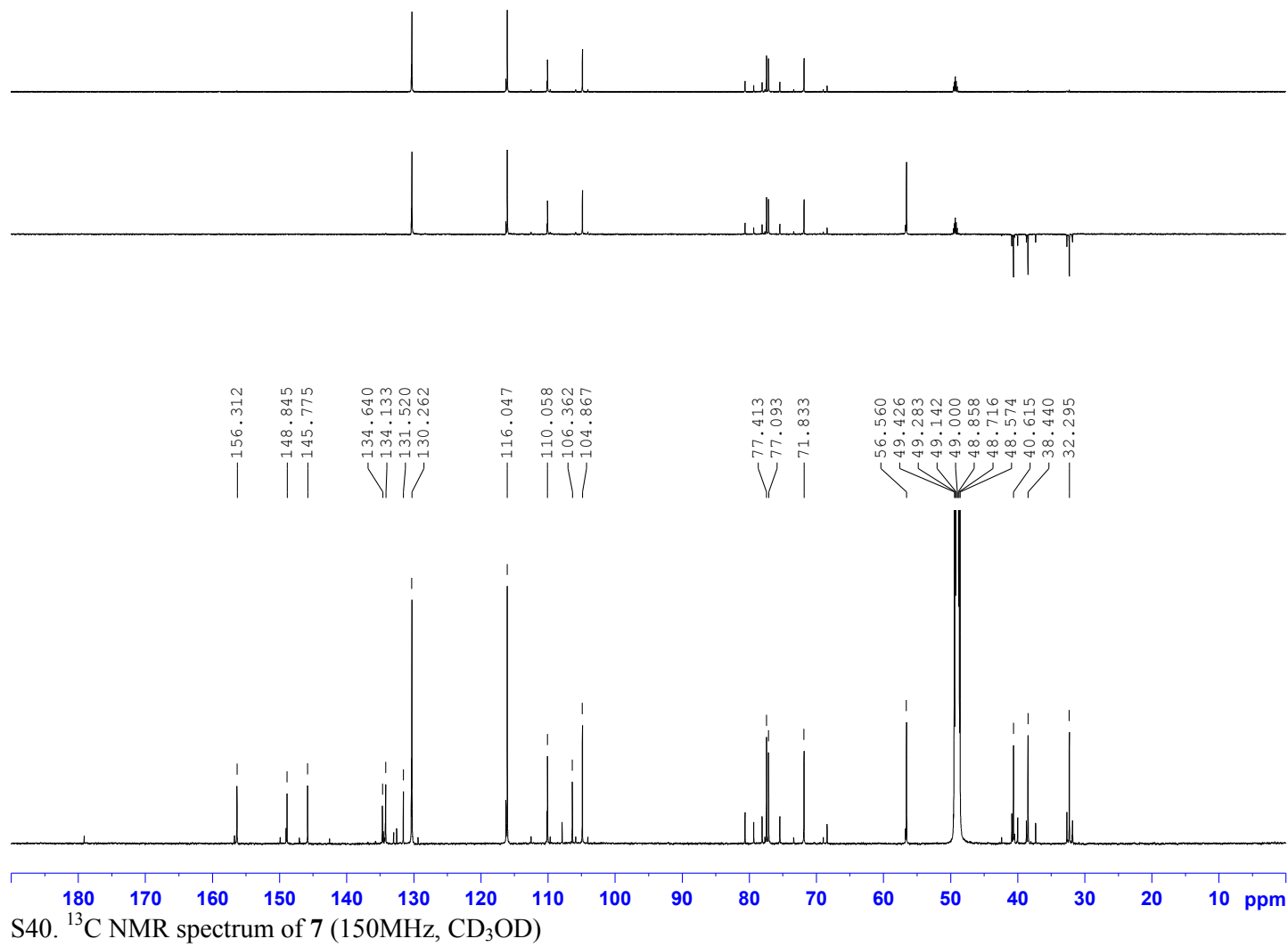


S38. NOESY spectrum of **6** (600MHz, CD₃OD)

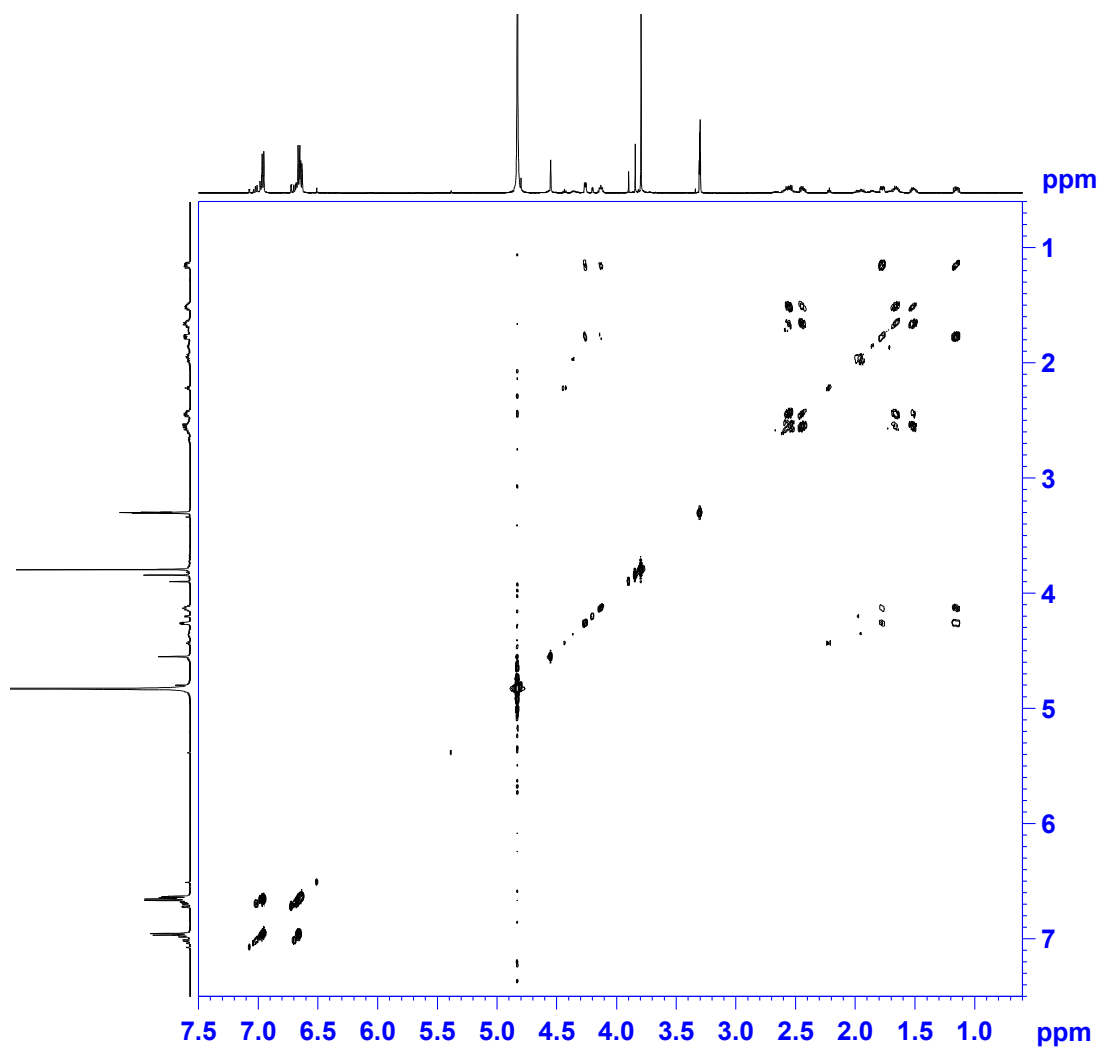


S39. ^1H NMR spectrum of **7** (600MHz, CD_3OD)

11006 ssl-ysl-3734120-fr.1-CD3OD-49.0 ppm-20131031, Bruker AV3-600, Cryo probe

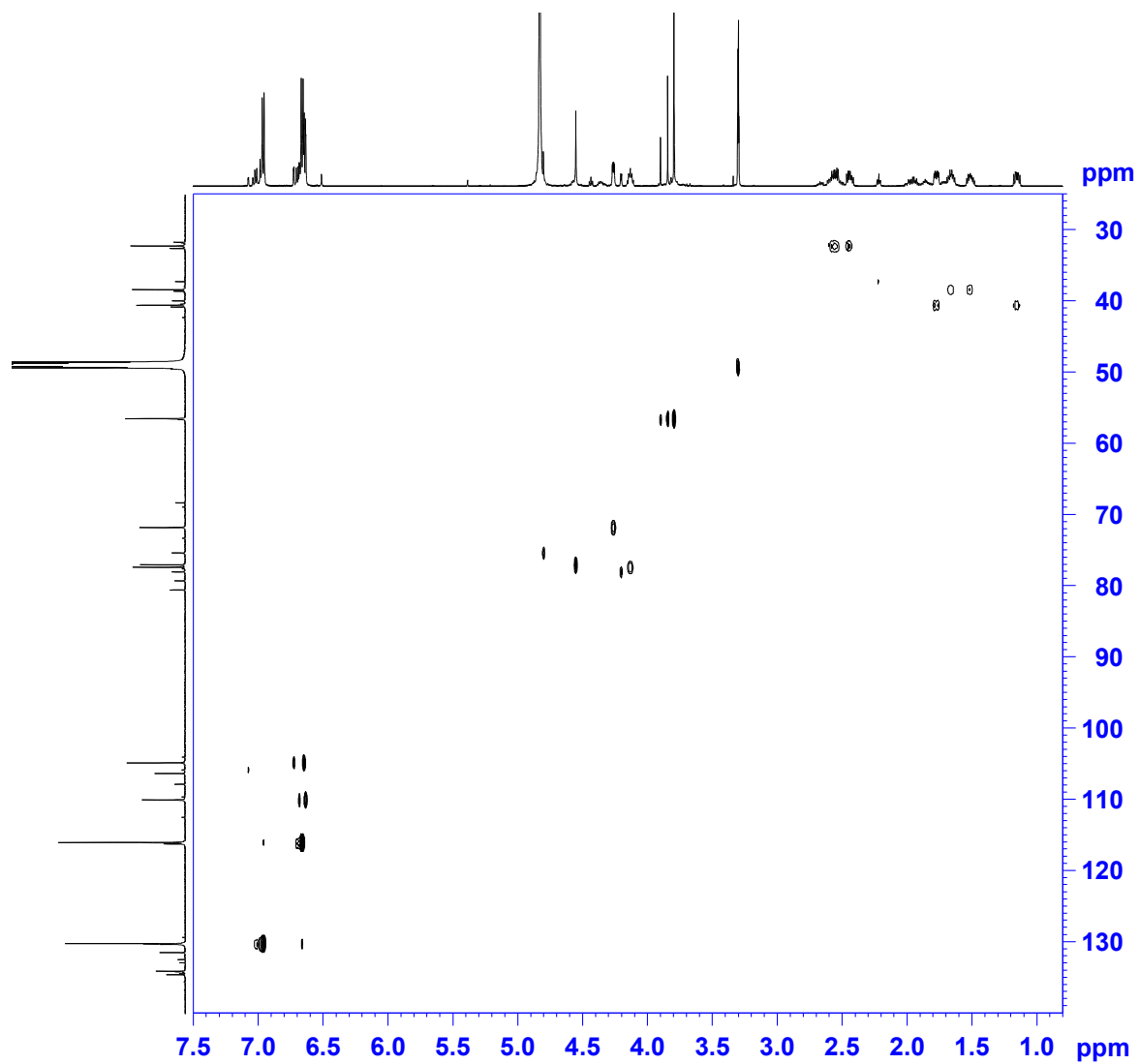


COSY 11006 ssl-ysl-3734120-fr.1-CD3OD-3.30 ppm-20131031, Bruker AV3-600, Cryo p



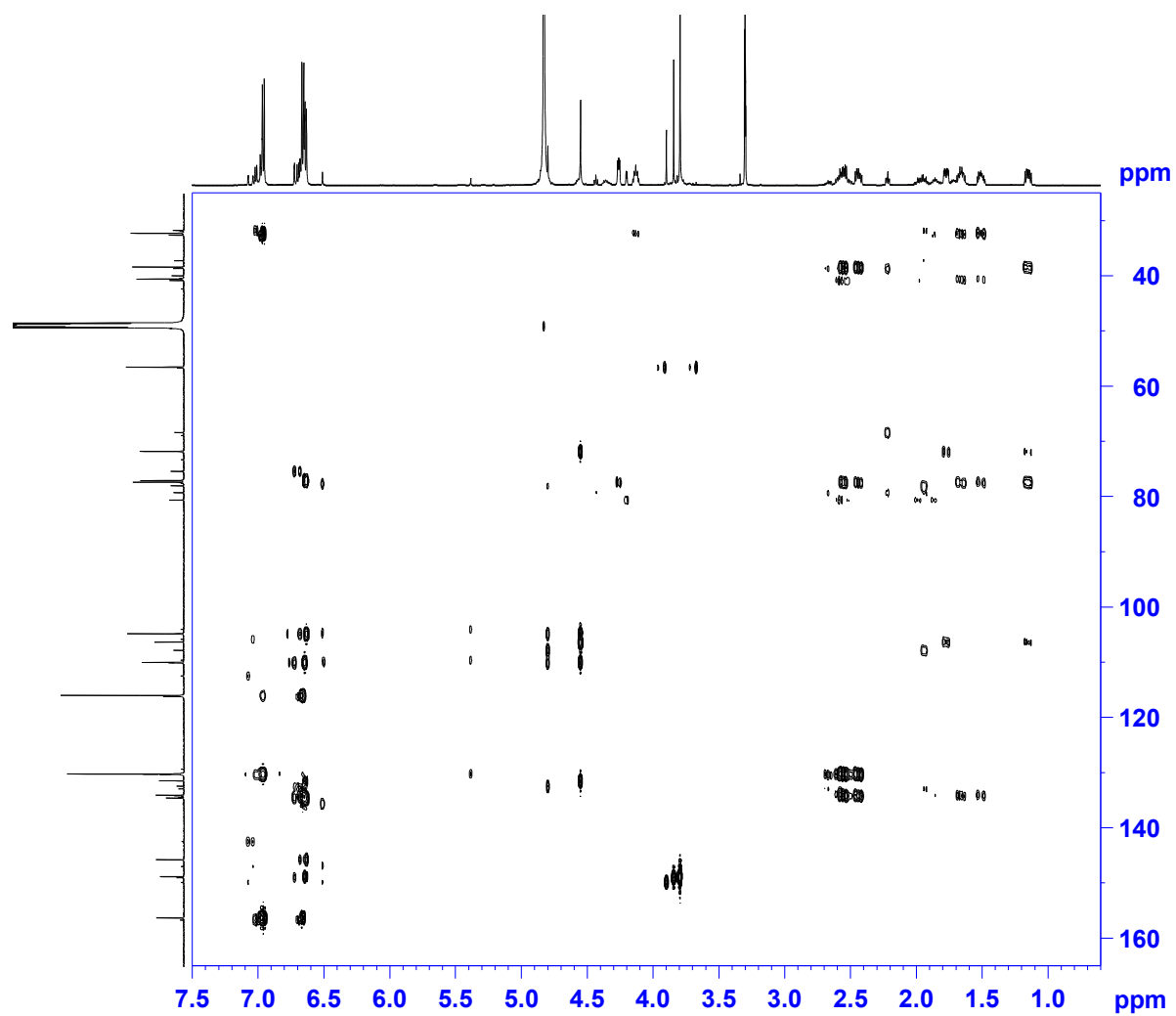
S41. COSY spectrum of **7** (600MHz, CD₃OD)

HSQC 11006 ssl-y5l-3734120-fr.1-CD3OD-3.30/49.0 ppm-20131031, Bruker AV3-600, C



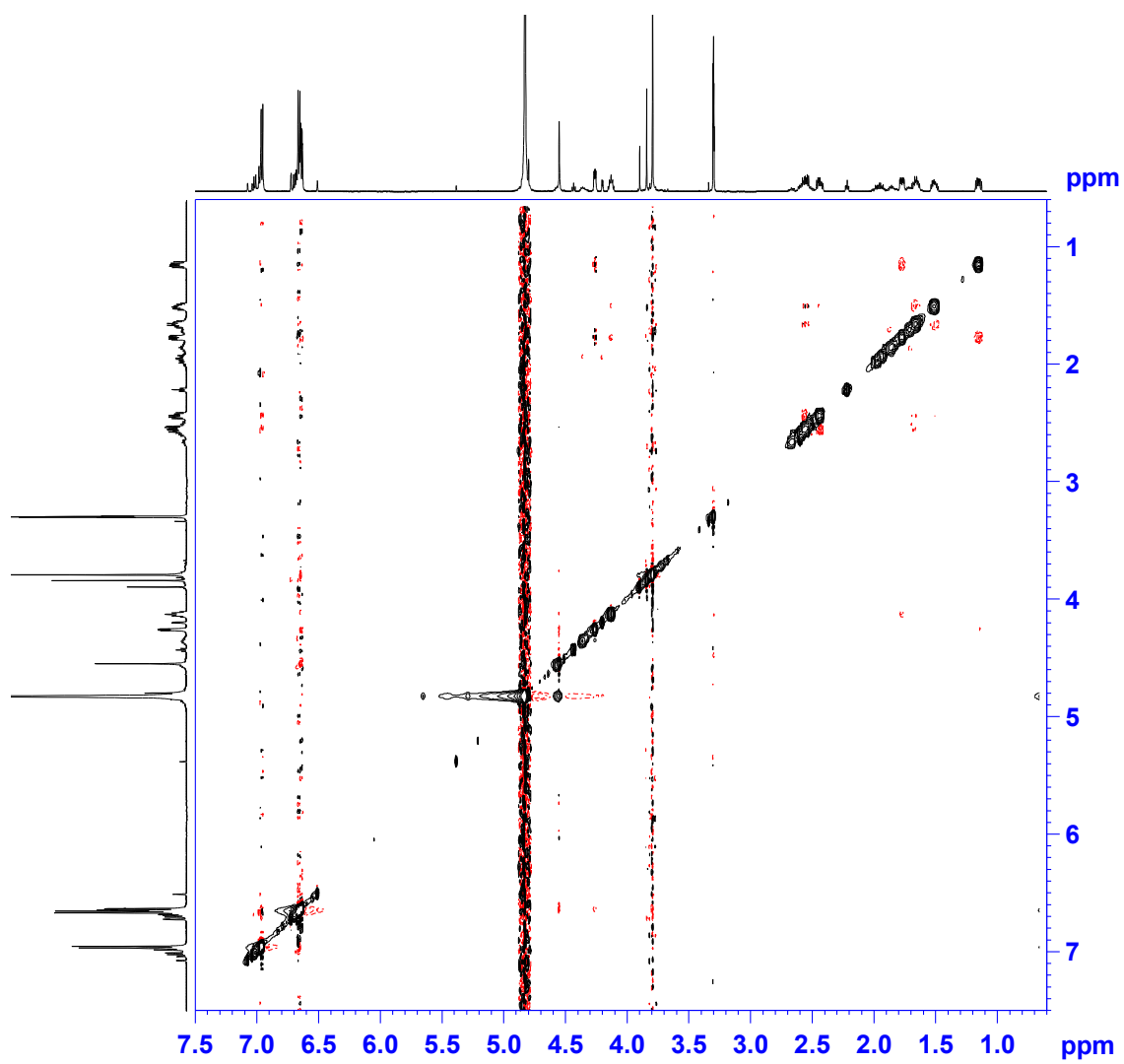
S42. HSQC spectrum of **7** (600MHz, CD_3OD)

HMBC 11006 ssl-ysl-3734120-fr.1-CD3OD-3.30/49.0 ppm-20131031, Bruker AV3-600, C:



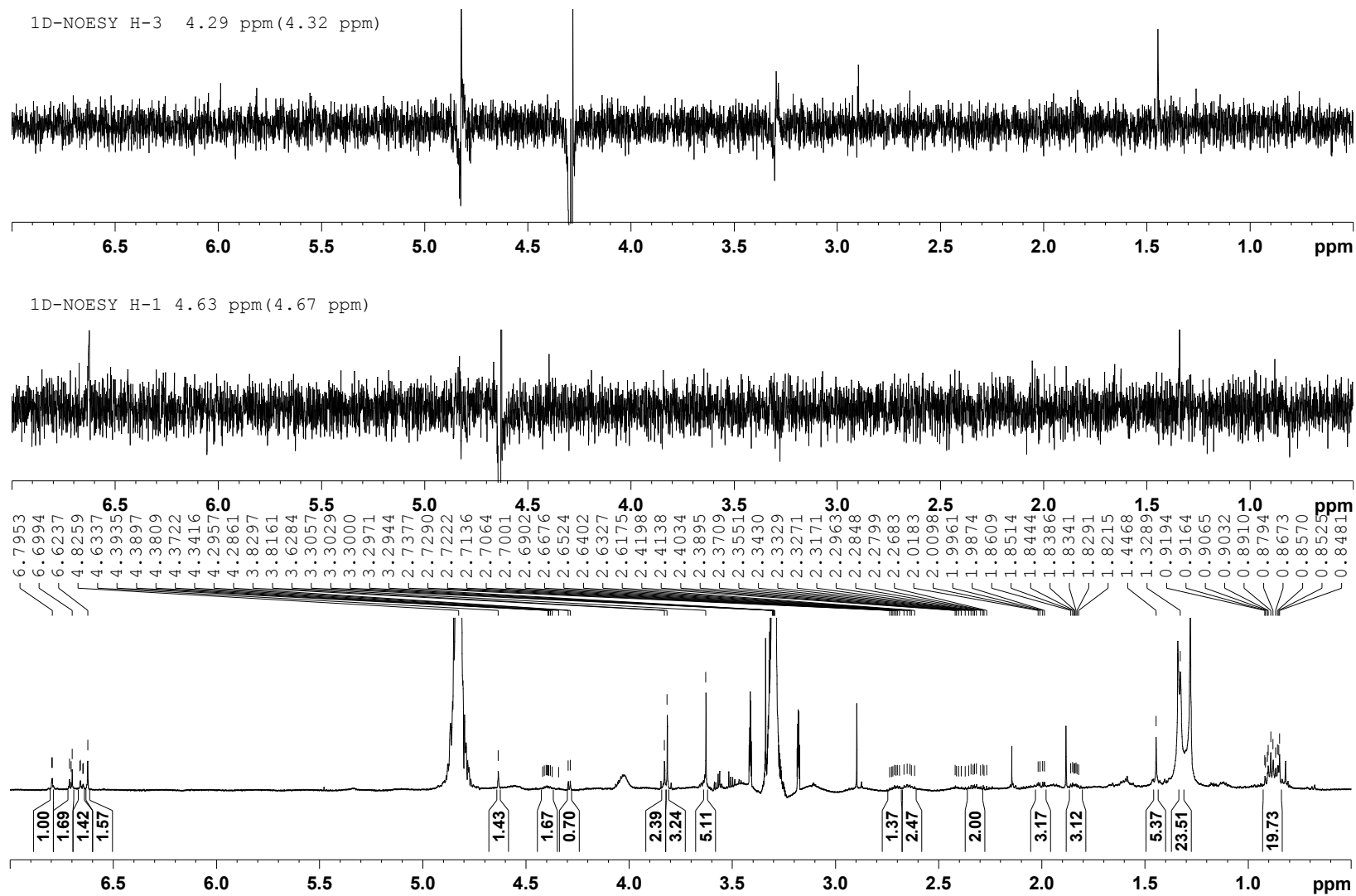
S43. HMBC spectrum of **7** (600MHz, CD₃OD)

NOESY 11006 ssl-ysl-3734120-fr.1-CD3OD-3.30 ppm-20131031, Bruker AV3-600, Cryo



S44. NOESY spectrum of **7** (600MHz, CD₃OD)

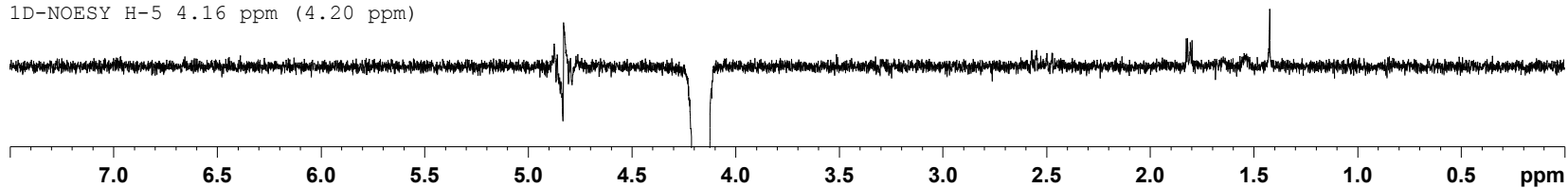
11006 ssl-ysl-3734129-fr.2-CD3OD-3.30 ppm-20131125, Bruker AV3-600, Cryo probe



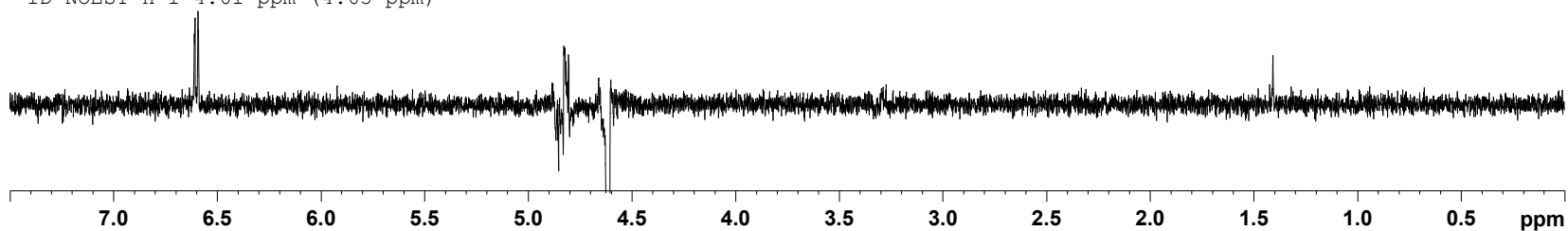
S45. ¹H NMR and 1D NOESY spectrum of **4a** (600MHz, CD₃OD)

11006 ssl-y5l-3734125-fr.2-CD3OD-3.30 ppm-20131031, Bruker AV-III 600 MHz, Cryo probe

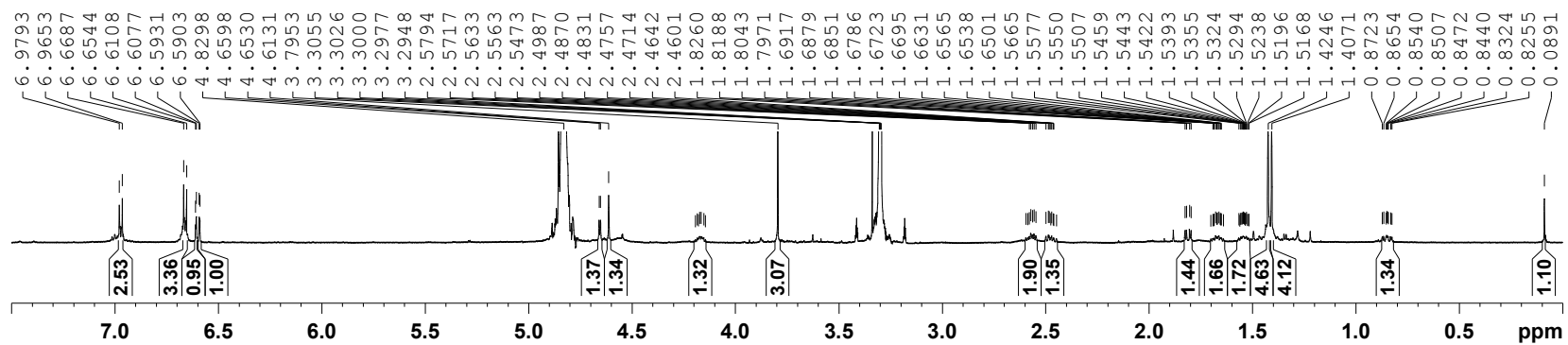
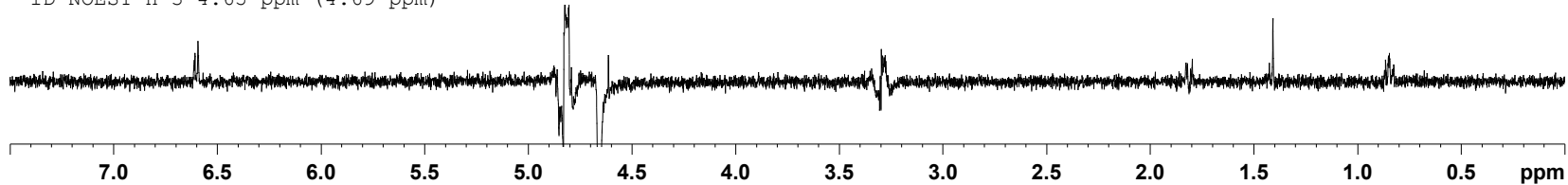
1D-NOESY H-5 4.16 ppm (4.20 ppm)



1D-NOESY H-1 4.61 ppm (4.65 ppm)



1D-NOESY H-3 4.65 ppm (4.69 ppm)



S46. ^1H NMR and 1D NOESY spectrum of **7a** (600MHz, CD_3OD)

Mass Spectrum SmartFormula Report

Analysis Info

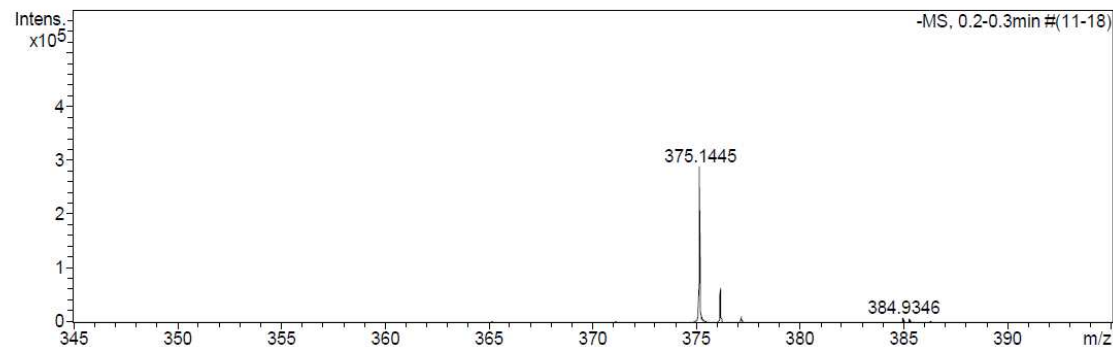
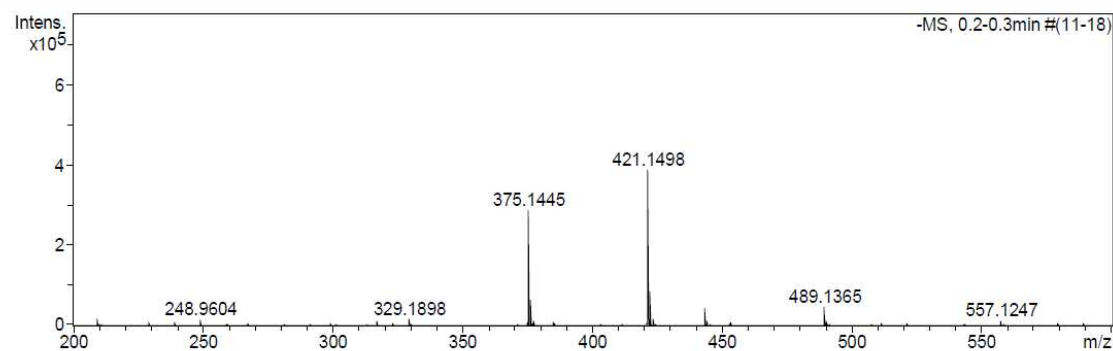
Analysis Name D:\Data\HRMS-YSL\11006\11006-cpd8.d
Method tune_low.m
Sample Name p.3351883-fr.1
Comment

Acquisition Date 2012/8/24 下午 06:17:48

Operator default
Instrument / Ser# micrOTOF 10247

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	200 度
Scan Begin	50 m/z	Set Capillary	4100 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [mDa]	err [ppm]	Mean err [ppm]	mSigma	Std Mean m/z	Std m/z Diff
375.1445	1	C ₂₀ H ₂₃ O ₇	375.1449	0.4	1.0	1.4	1.59	0.0006	0.0006
	2	C ₁₅ H ₂₃ N ₂ O ₉	375.1409	-3.6	-9.7	-9.5	28.57	0.0036	0.0006

S47. HRESIMS⁻ of 1

Mass Spectrum SmartFormula Report

Analysis Info

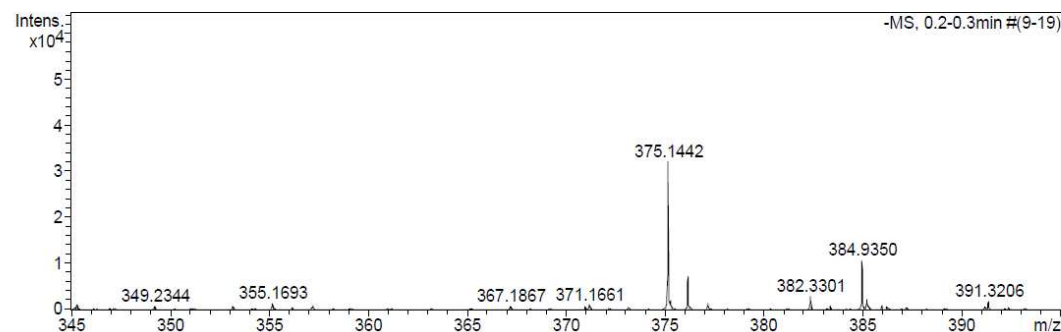
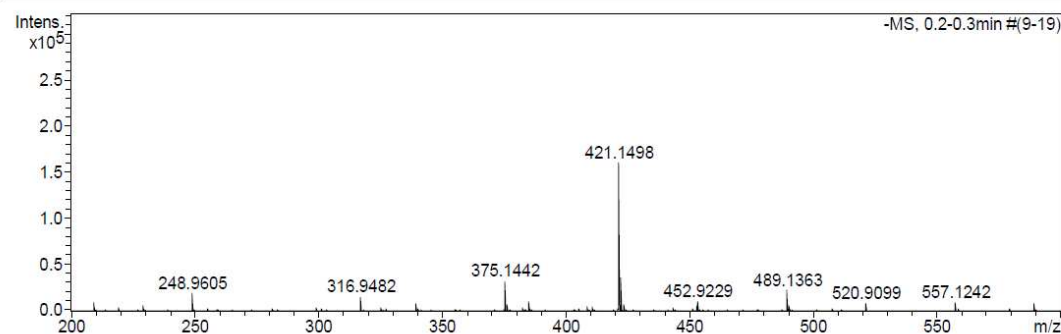
Analysis Name D:\Data\HRMS-YSL\11006\11006-cpd12.d
 Method tune_low.m
 Sample Name p.3351886-fr.3
 Comment

Acquisition Date 2012/8/24 下午 06:31:33

Operator default
 Instrument / Ser# microTOF 10247

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	200 度
Scan Begin	50 m/z	Set Capillary	4100 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [mDa]	err [ppm]	Mean err [ppm]	mSigma	Std Mean m/z	Std m/z Diff
375.1442									
	1	C 20 H 23 O 7	375.1449	0.7	2.0	2.6	7.56	0.0011	0.0014
	2	C 15 H 23 N 2 O 9	375.1409	-3.3	-8.8	-8.4	33.94	0.0032	0.0014

S48. HRESIMS⁻ of 2

Mass Spectrum SmartFormula Report

Analysis Info

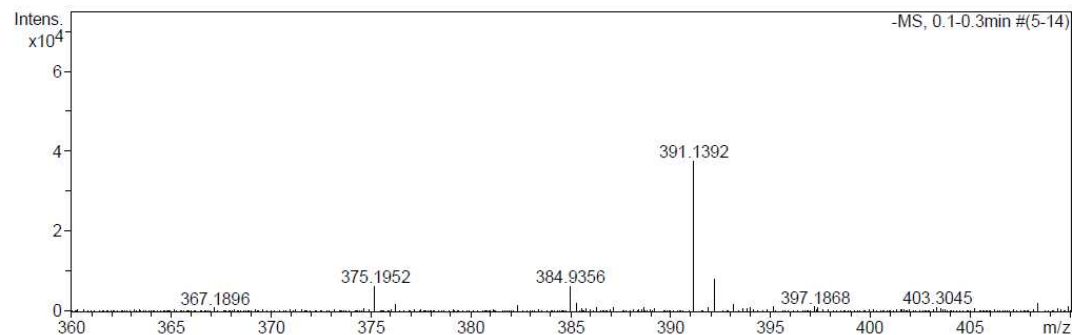
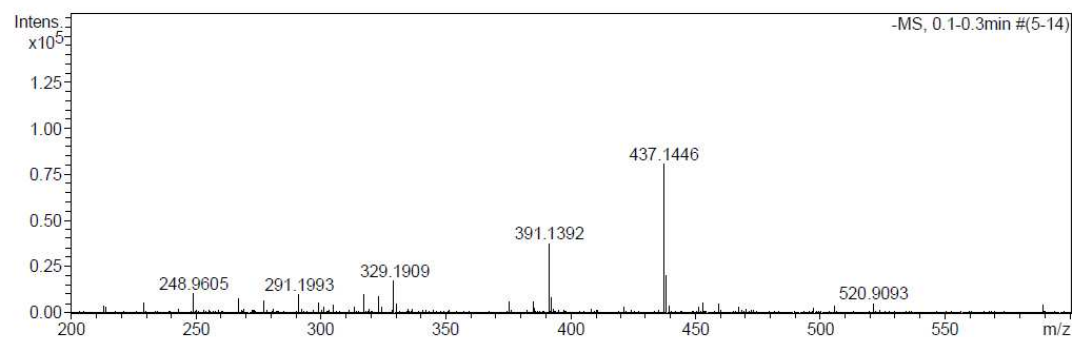
Analysis Name F:\YSL\TOF\11006\p.3467281-fr.3 (-).d
 Method tune_low.m
 Sample Name p.3467281-fr.3
 Comment

Acquisition Date 2013/12/22 下午 06:40:43

Operator default
 Instrument / Ser# microTOF 10247

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	250 度
Scan Begin	50 m/z	Set Capillary	4100 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [mDa]	err [ppm]	Mean err [ppm]	mSigma	Std Mean m/z	Std m/z Diff
391.1392									
	1	C 15 H 23 N 2 O 10	391.1358	-3.4	-8.7	-8.5	24.10	0.0033	0.0005
	2	C 13 H 27 O 13	391.1457	6.5	16.6	17.3	34.51	0.0071	0.0005

S49. HRESIMS⁻ of 3

Mass Spectrum SmartFormula Report

Analysis Info

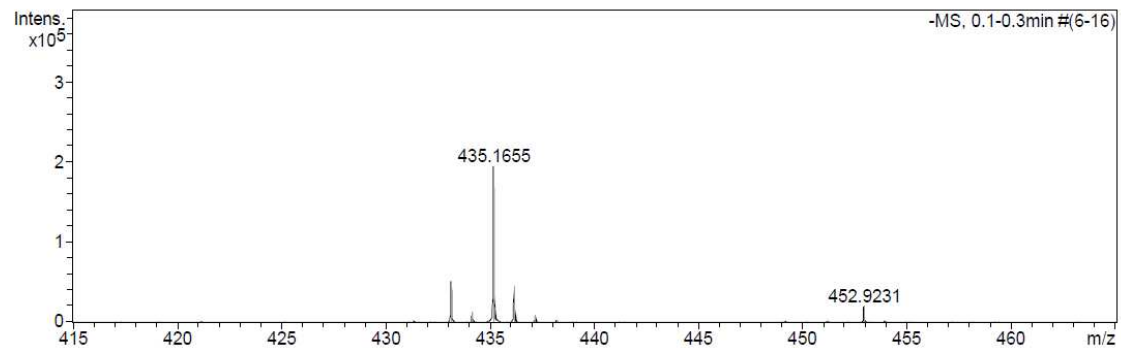
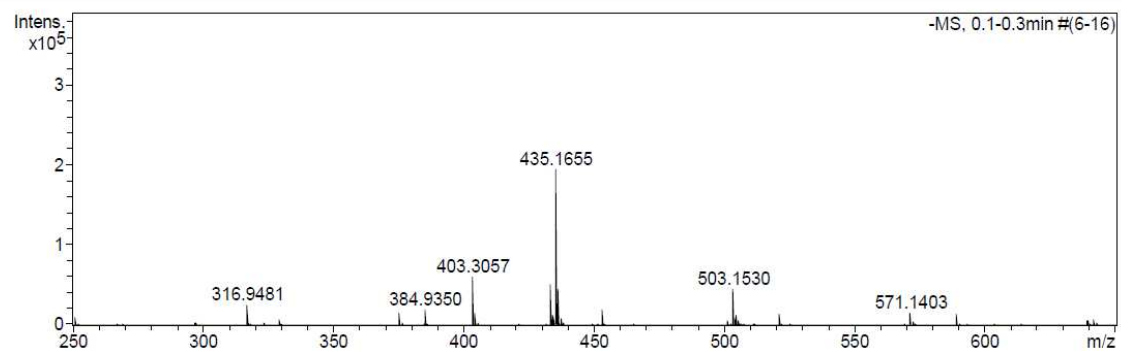
Analysis Name D:\Data\HRMS-YSL\11006\11006-cpd5(-).d
 Method tune_low.m
 Sample Name p.3351873-fr.4
 Comment

Acquisition Date 2012/8/24 下午 06:02:15

Operator default
 Instrument / Ser# micrOTOF 10247

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	200 度
Scan Begin	50 m/z	Set Capillary	4100 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [mDa]	err [ppm]	Mean err [ppm]	mSigma	Std Mean m/z	Std m/z Diff
435.1655	1	C 22 H 27 O 9	435.1661	0.5	1.2	1.7	4.64	0.0010	0.0011
	2	C 17 H 27 N 2 O 11	435.1620	-3.5	-8.0	-7.8	19.75	0.0035	0.0011

S50. HRESIMS⁻ of 4

Mass Spectrum SmartFormula Report

Analysis Info

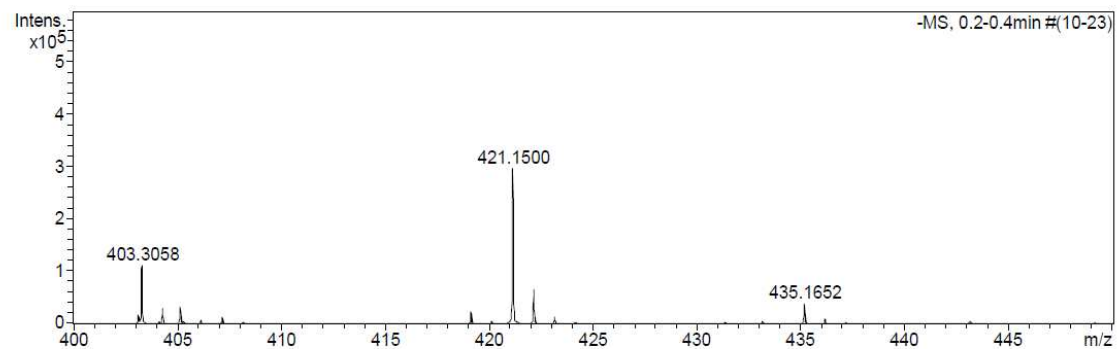
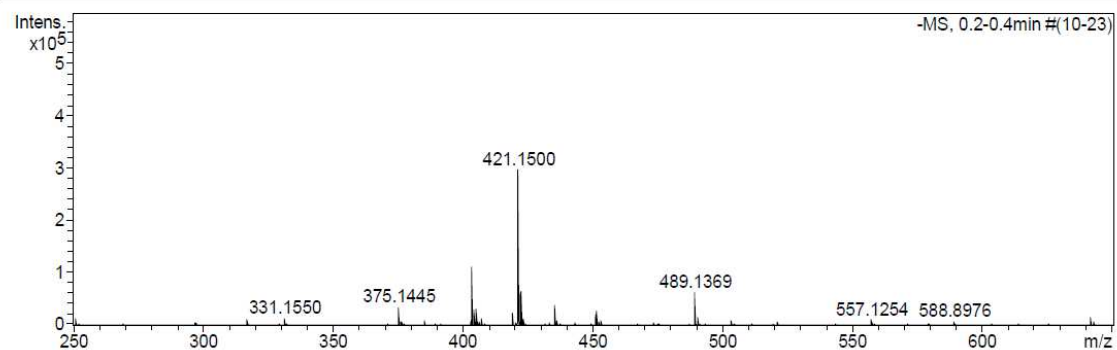
Analysis Name D:\Data\HRMS-YSL\11006\11006-cpd6.d
 Method tune_low.m
 Sample Name p.3351859-fr.11
 Comment

Acquisition Date 2012/8/24 下午 06:09:04

Operator default
 Instrument / Ser# micrOTOF 10247

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	200 度
Scan Begin	50 m/z	Set Capillary	4100 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [mDa]	err [ppm]	Mean err [ppm]	mSigma	Std Mean m/z	Std m/z Diff
421.1500	1	C 21 H 25 O 9	421.1504	0.4	1.0	1.2	2.47	0.0006	0.0008
	2	C 16 H 25 N 2 O 11	421.1464	-3.6	-8.6	-8.5	19.34	0.0036	0.0009

S51. HRESIMS⁻ of **5**

Mass Spectrum SmartFormula Report

Analysis Info

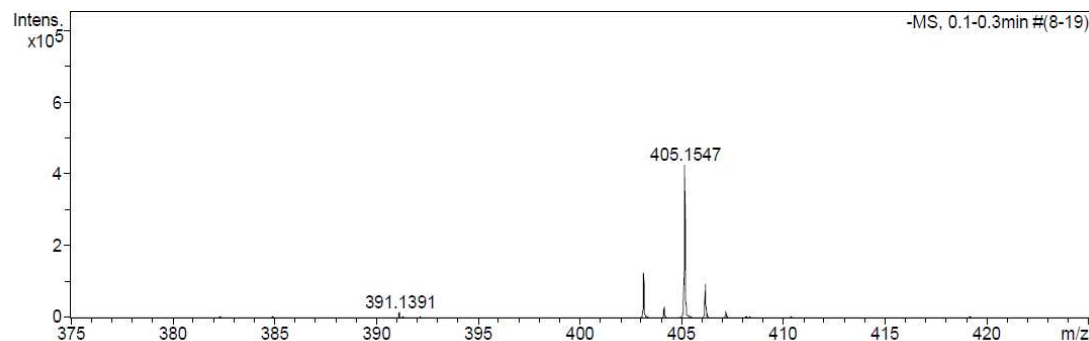
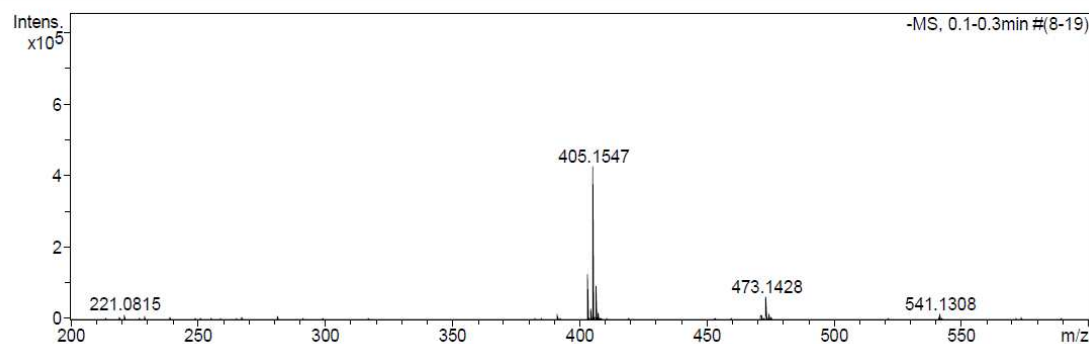
Analysis Name D:\Data\HRMS-YSL\11006\11006-cpd9.d
 Method tune_low.m
 Sample Name p.3351884-fr.3
 Comment

Acquisition Date 2012/8/24 下午 06:23:36

Operator default
 Instrument / Ser# microTOF 10247

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	200 秒
Scan Begin	50 m/z	Set Capillary	4100 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [mDa]	err [ppm]	Mean err [ppm]	mSigma	Std Mean m/z	Std m/z Diff
405.1547									
	1	C 21 H 25 O 8	405.1555	0.8	2.0	2.1	3.86	0.0009	0.0006
	2	C 16 H 25 N 2 O 10	405.1515	-3.2	-7.9	-8.1	18.41	0.0033	0.0009

S52. HRESIMS⁻ of 6

Mass Spectrum SmartFormula Report

Analysis Info

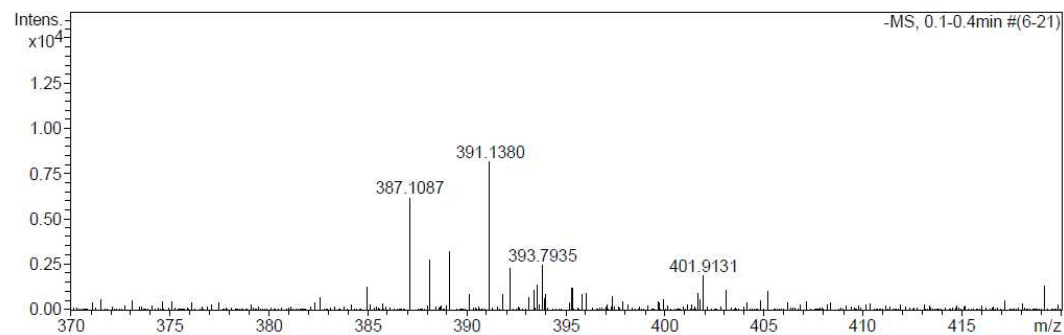
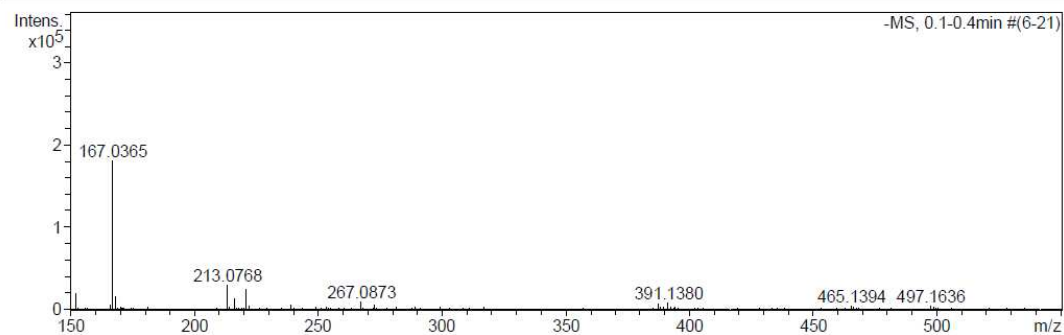
Analysis Name F:\YSL\TOF\11006\p.3734121 (-).d
 Method tune_low.m
 Sample Name p.3734121
 Comment

Acquisition Date 2013/12/22 下午 04:36:09

Operator default
 Instrument / Ser# microTOF 10247

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	250 度
Scan Begin	50 m/z	Set Capillary	4100 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [mDa]	err [ppm]	Mean err [ppm]	mSigma	Std Mean m/z	Std m/z Diff
391.1380	1	C ₂₀ H ₂₃ O ₈	391.1398	1.8	4.6	4.3	39.34	0.0017	0.0006

S53. HRESIMS⁻ of 7

Mass Spectrum SmartFormula Report

Analysis Info

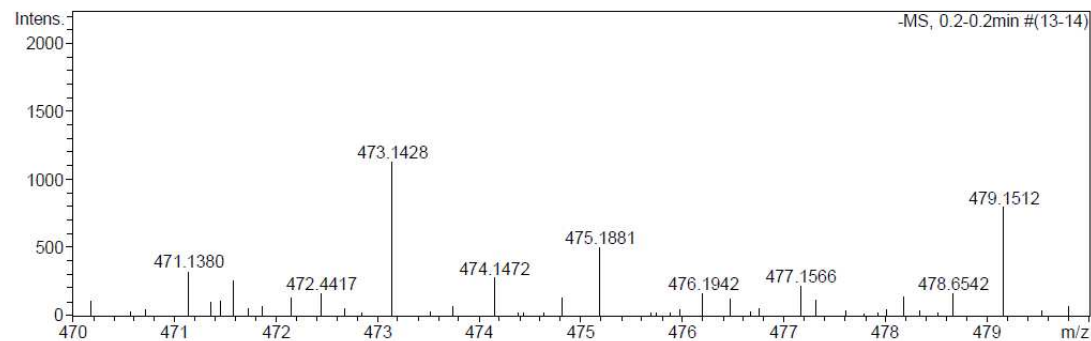
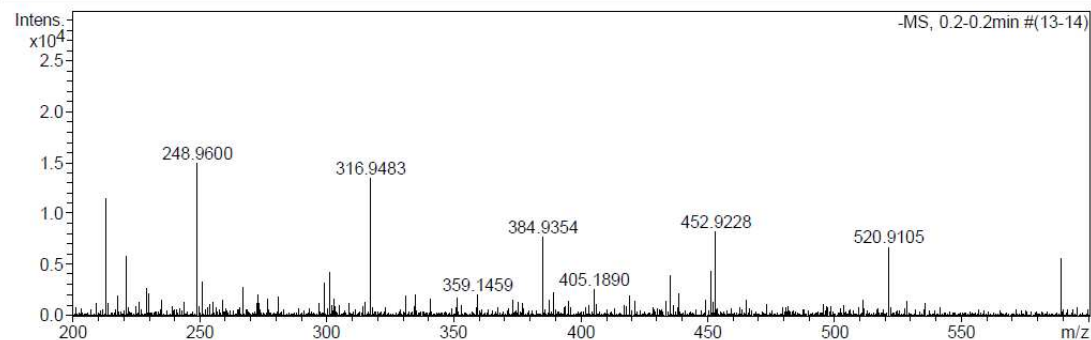
Analysis Name F:\YSL\TOF\11006\p.3734129-fr.2 (-)-4.d
 Method tune_low.m
 Sample Name p.3734129-fr.2
 Comment

Acquisition Date 2013/12/22 下午 05:18:52

Operator default
 Instrument / Ser# microTOF 10247

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	250 度
Scan Begin	50 m/z	Set Capillary	4100 V	Set Dry Gas	4.0 l/min
Scan End	700 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [mDa]	err [ppm]	Mean err [ppm]	mSigma	Std Mean m/z	Std m/z Diff
475.1881	1	C 25 H 31 O 9	475.1974	9.2	19.4	43.5	231.99	0.0267	0.0316

S54. HRESIMS⁻ of **4a**

Mass Spectrum SmartFormula Report

Analysis Info

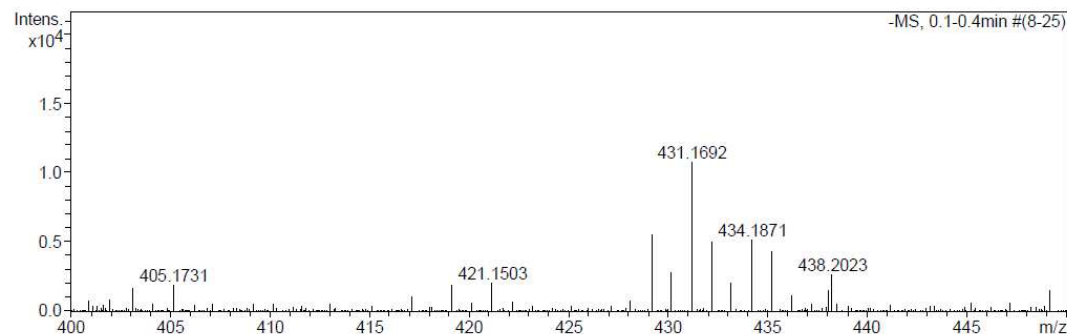
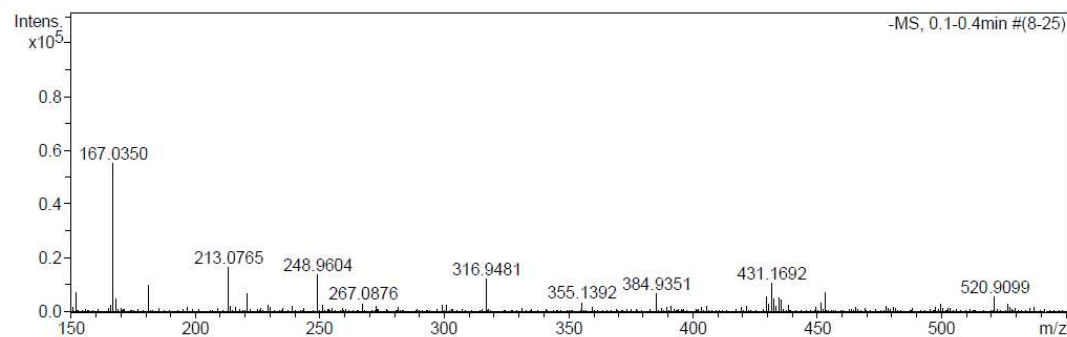
Analysis Name F:\YSL\TOF\11006\p.3734125 (-).d
 Method tune_low.m
 Sample Name p.3734125
 Comment

Acquisition Date 2013/12/22 下午 04:46:13

Operator default
 Instrument / Ser# micrOTOF 10247

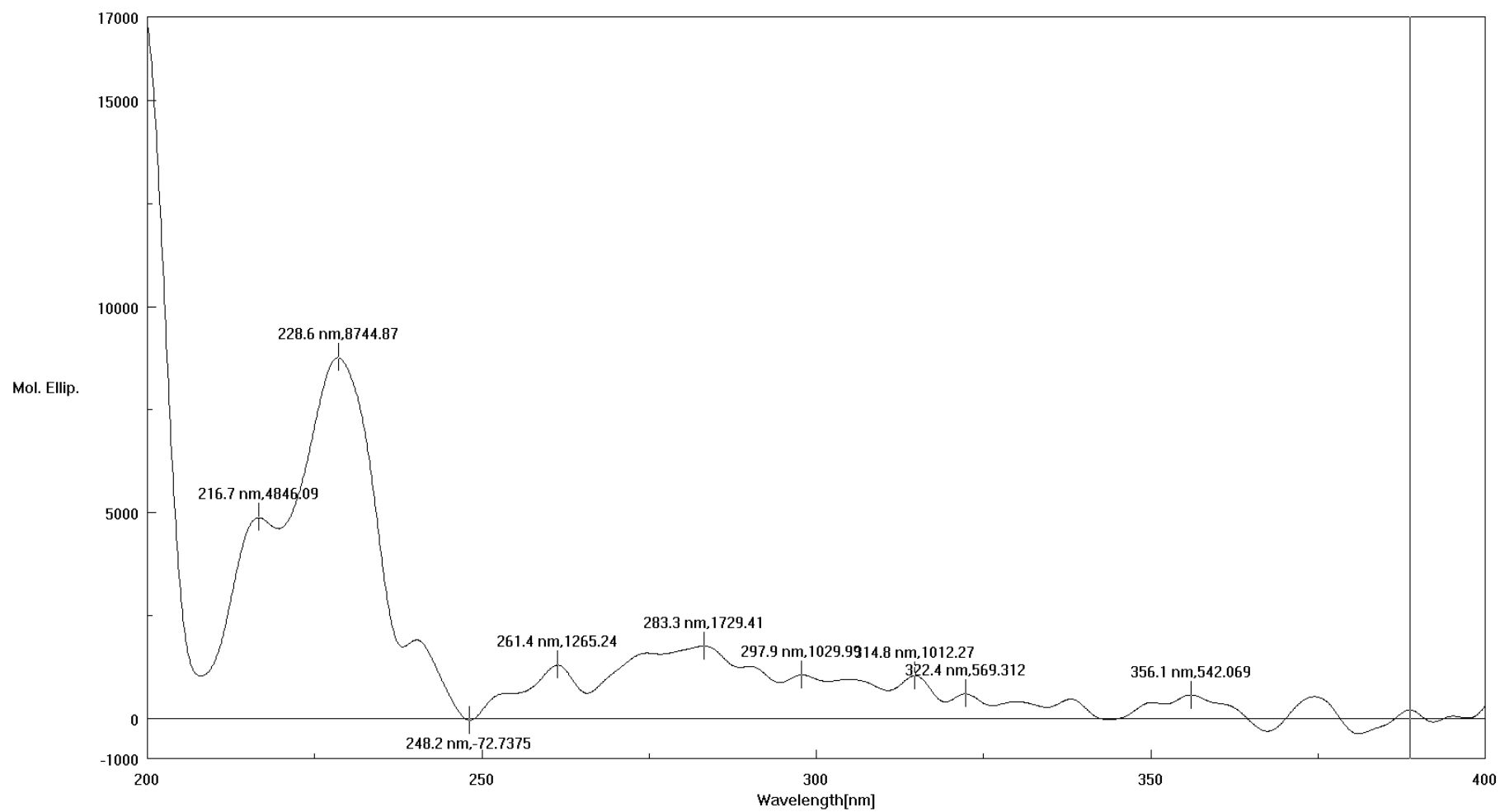
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	250 度
Scan Begin	50 m/z	Set Capillary	4100 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

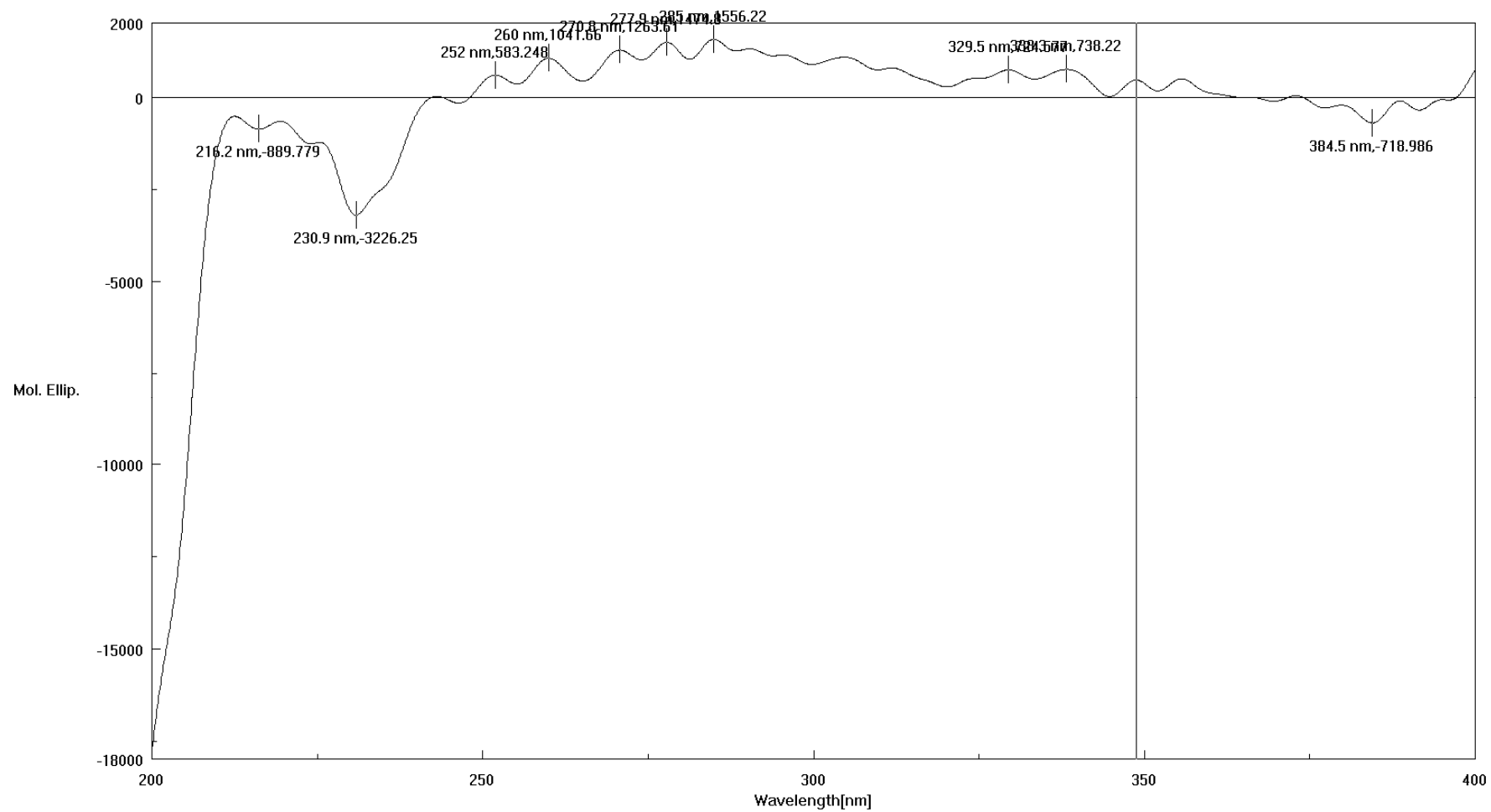


Meas. m/z	#	Formula	m/z	err [mDa]	err [ppm]	Mean err [ppm]	mSigma	Std	Mean m/z	Std m/z	Diff
431.1692	1	C ₂₃ H ₂₇ O ₈	431.1711	1.9	4.4	0.2	268.40	0.0058	0.0095		

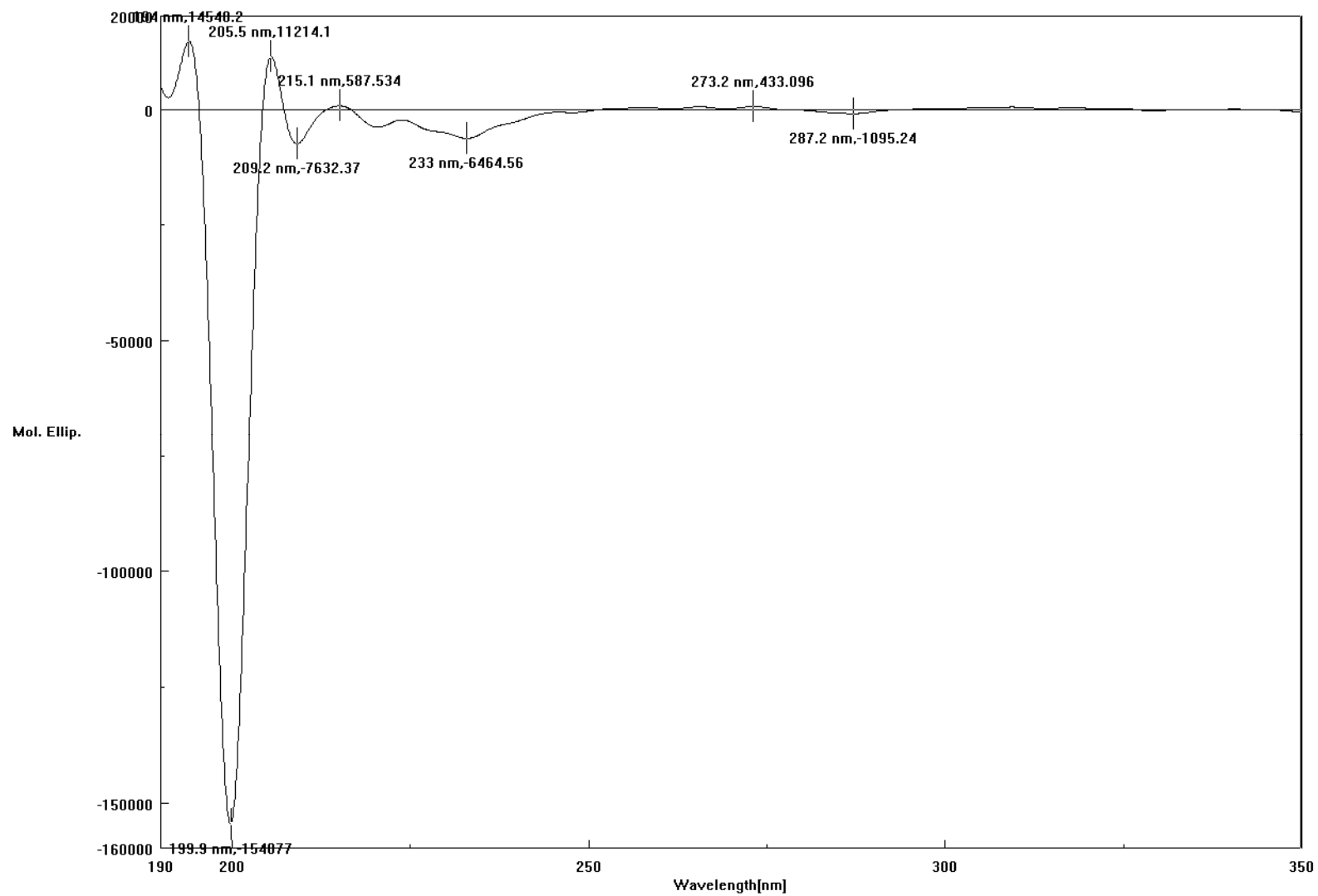
S55. HRESIMS⁻ of **7a**



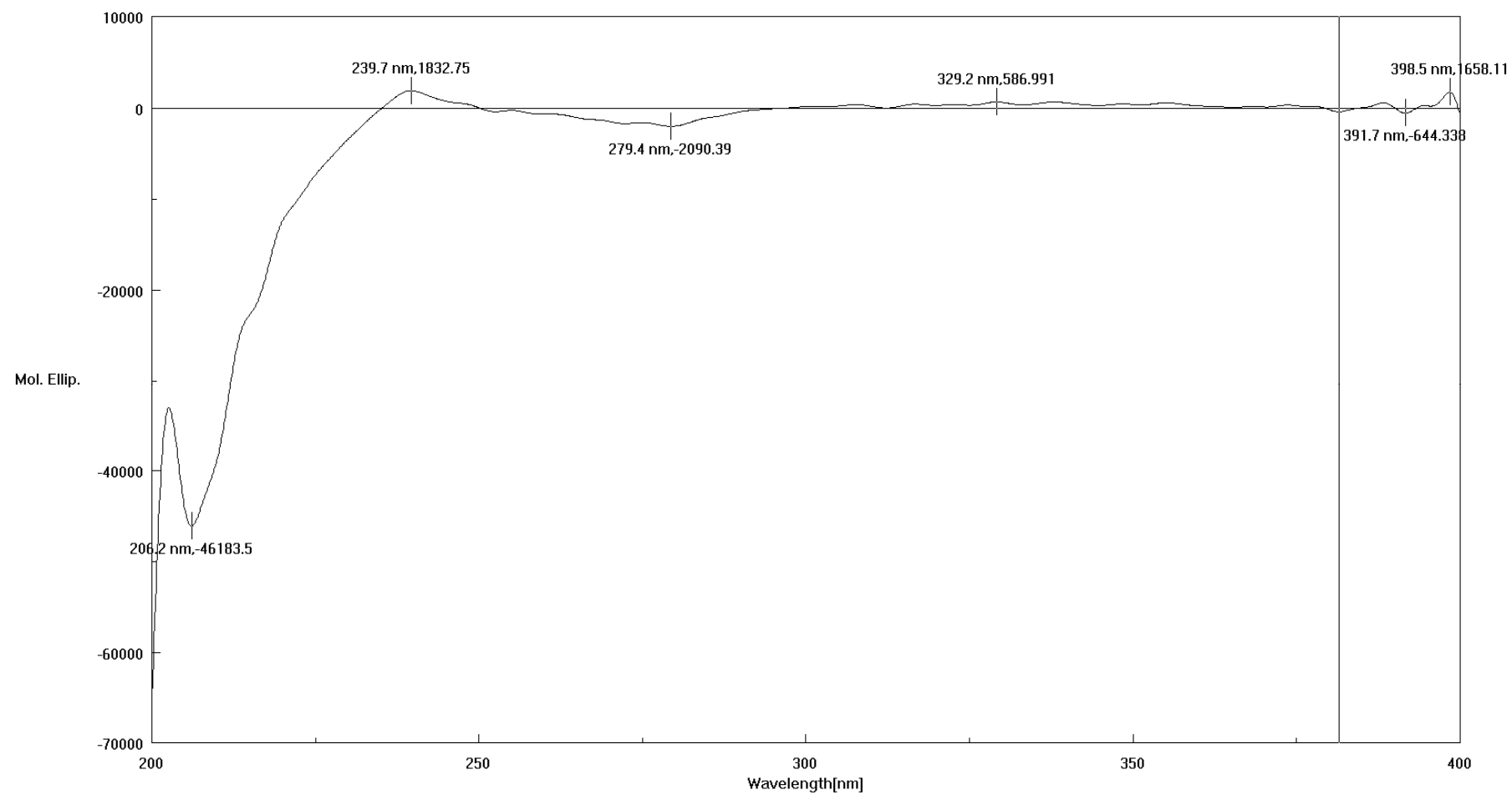
S56. ECD spectrum of **1** (MeCN)



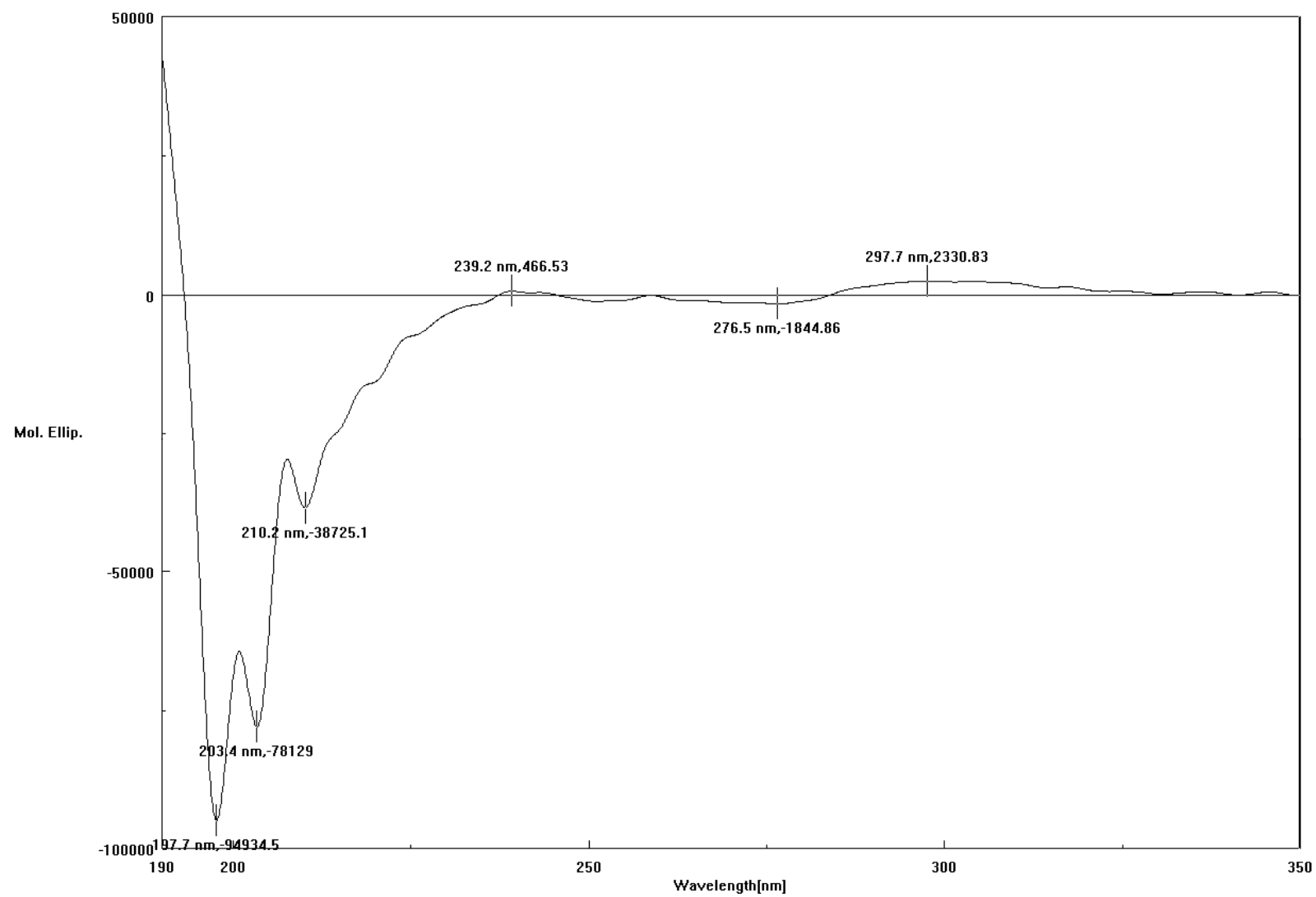
S57. ECD spectrum of **2** (MeCN)



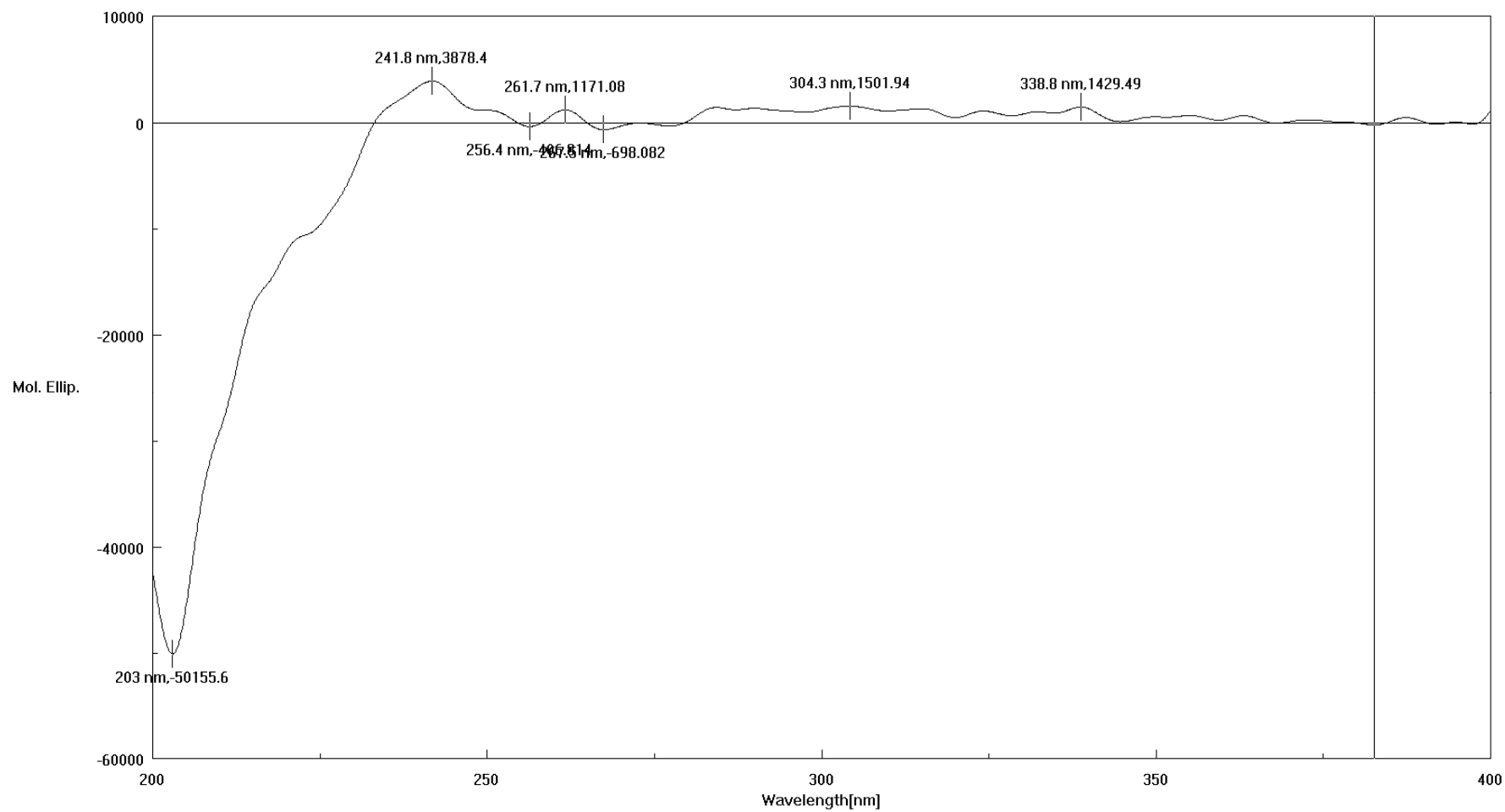
S58. ECD spectrum of **3** (MeCN)



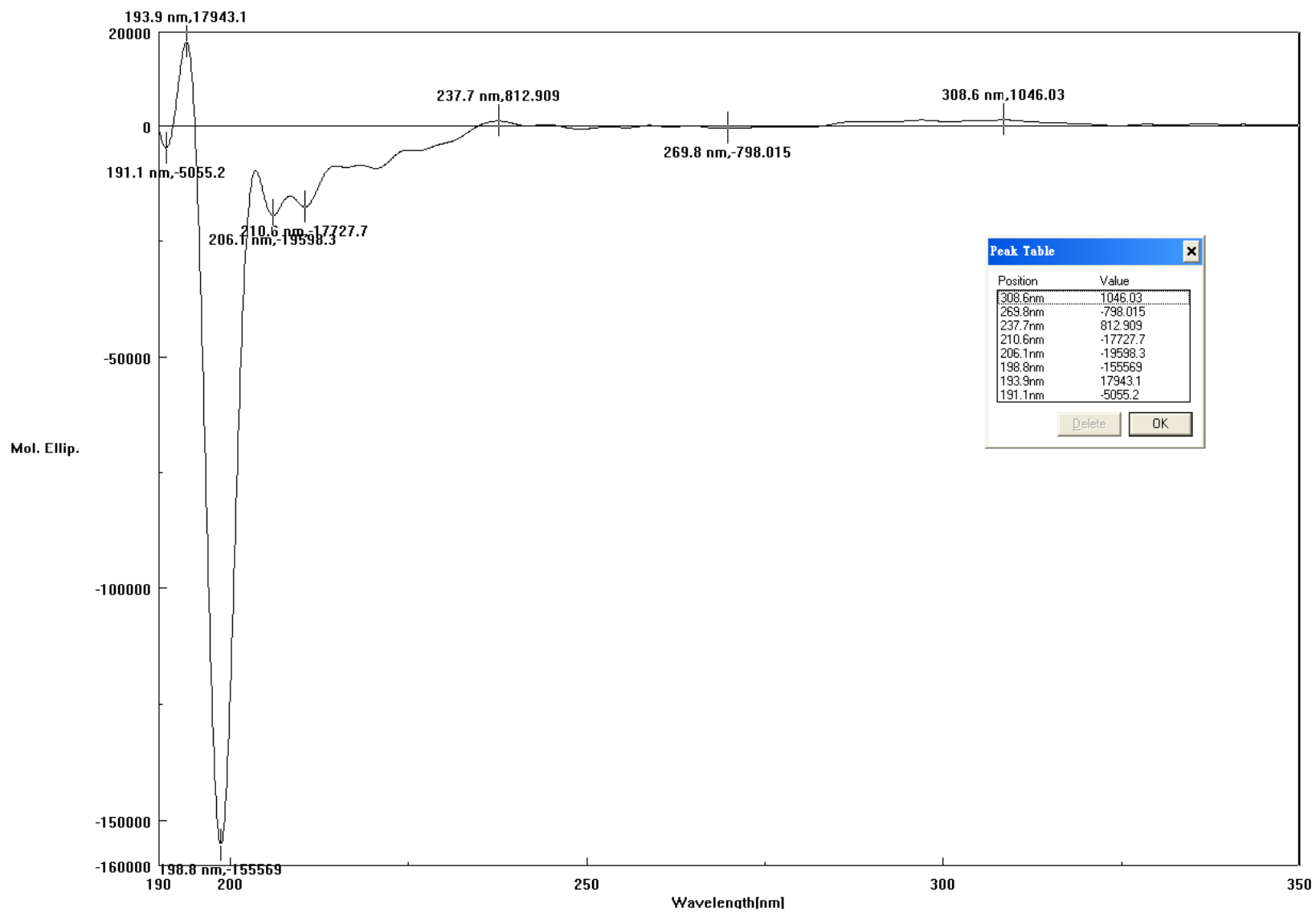
S59. ECD spectrum of **4** (MeCN)



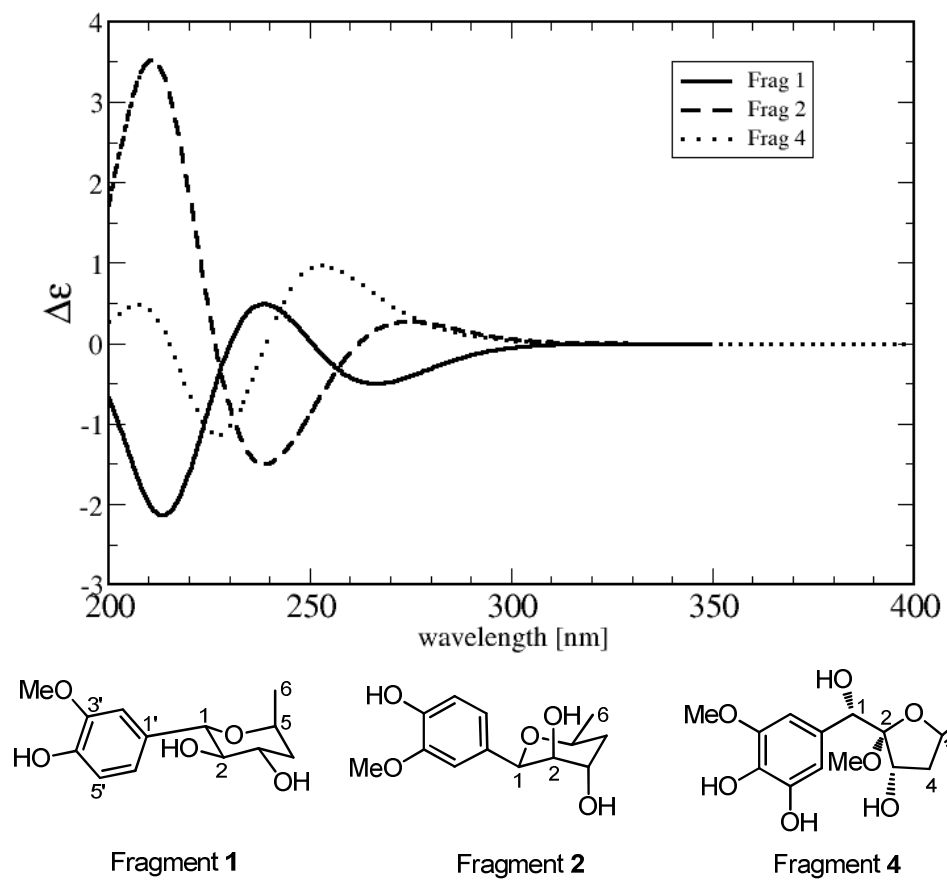
S60. ECD spectrum of **5** (MeOH)



S61. ECD spectrum of **6** (MeCN)



S62. ECD spectrum of **7** (MeOH)



S63. Calculated ECD spectra of Fragments **1**, **2**, and **4**