Bioactive Iridoid Glycosides from the Whole Plants of *Rehmannia chingii*

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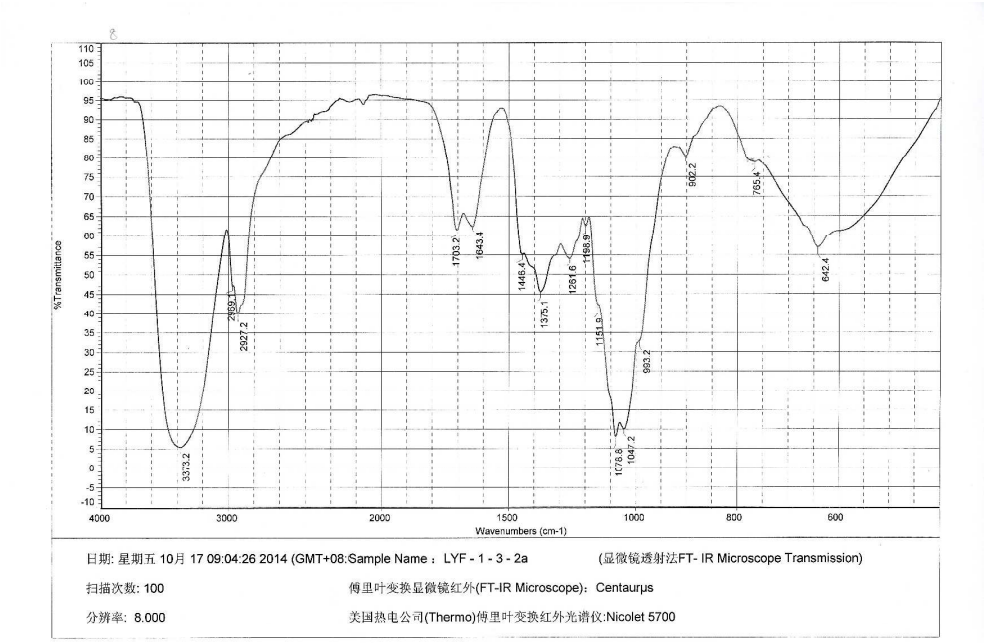
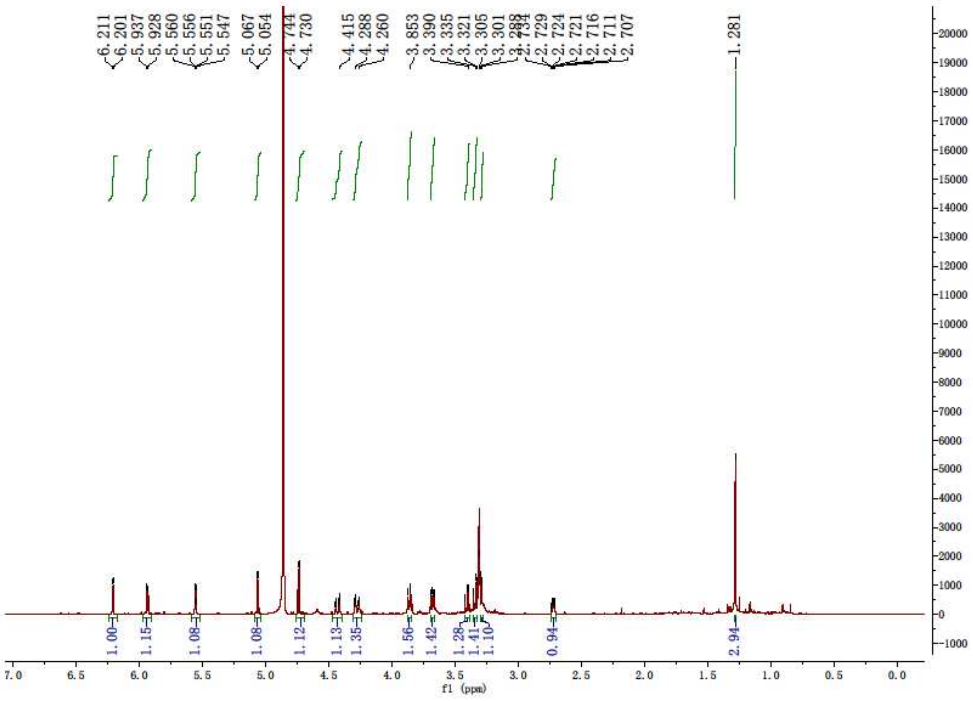
Supporting Information

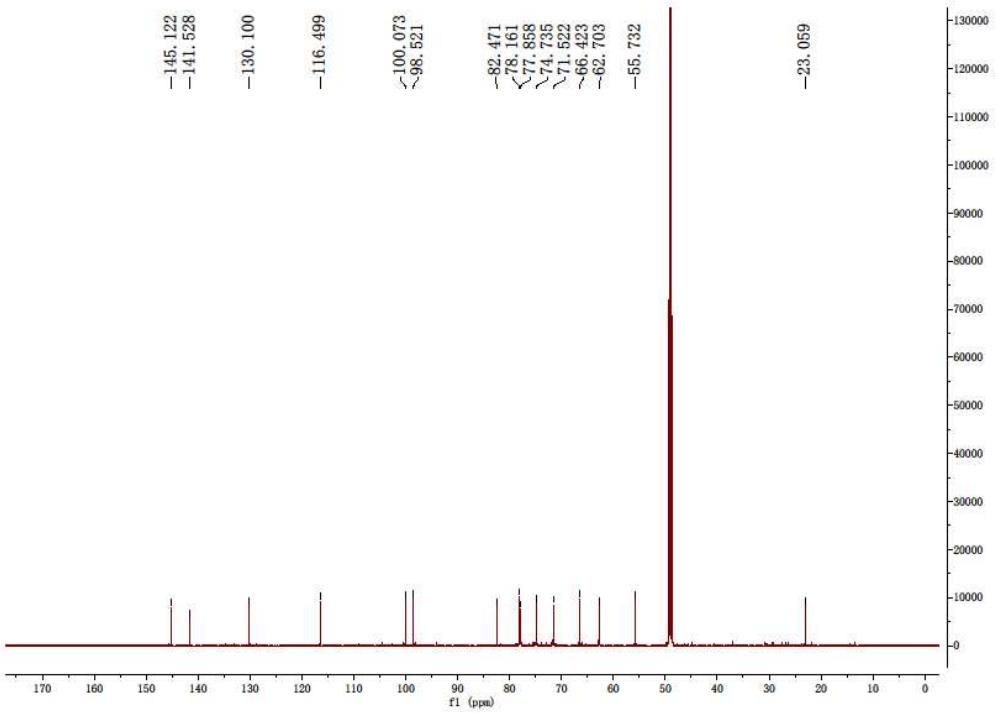
List of Supporting Information



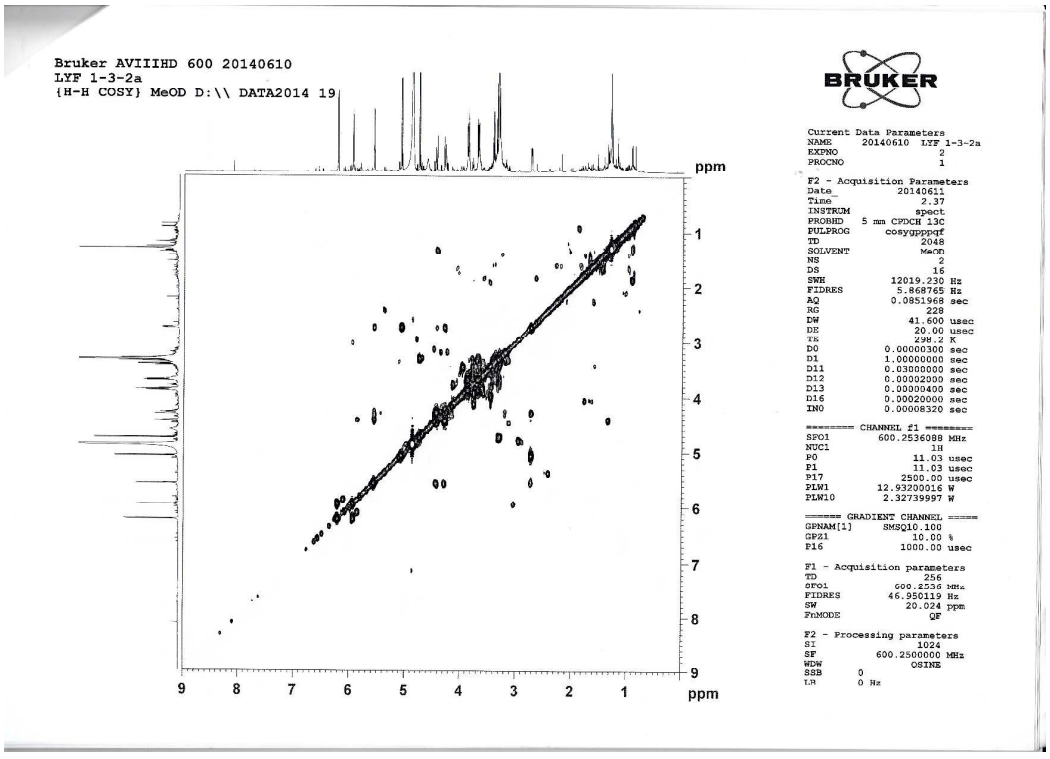
S1. IR Spectrum of compound **1**



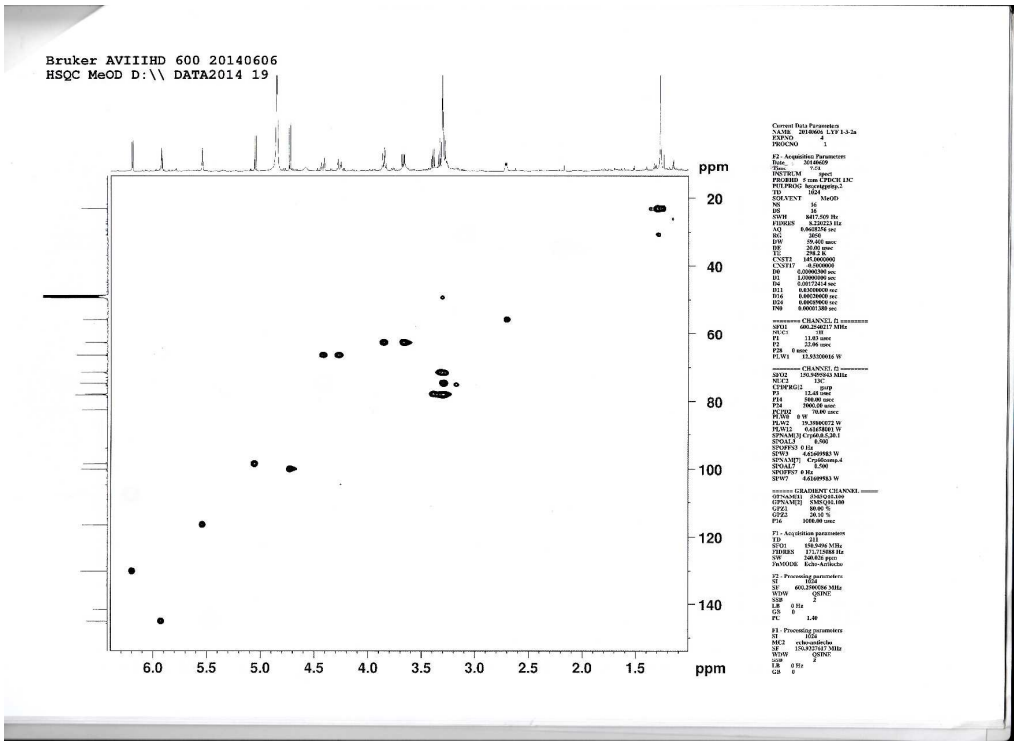
S2. ^{1}H NMR Spectrum of compound **1** (600MHz, Methanol-d_4)



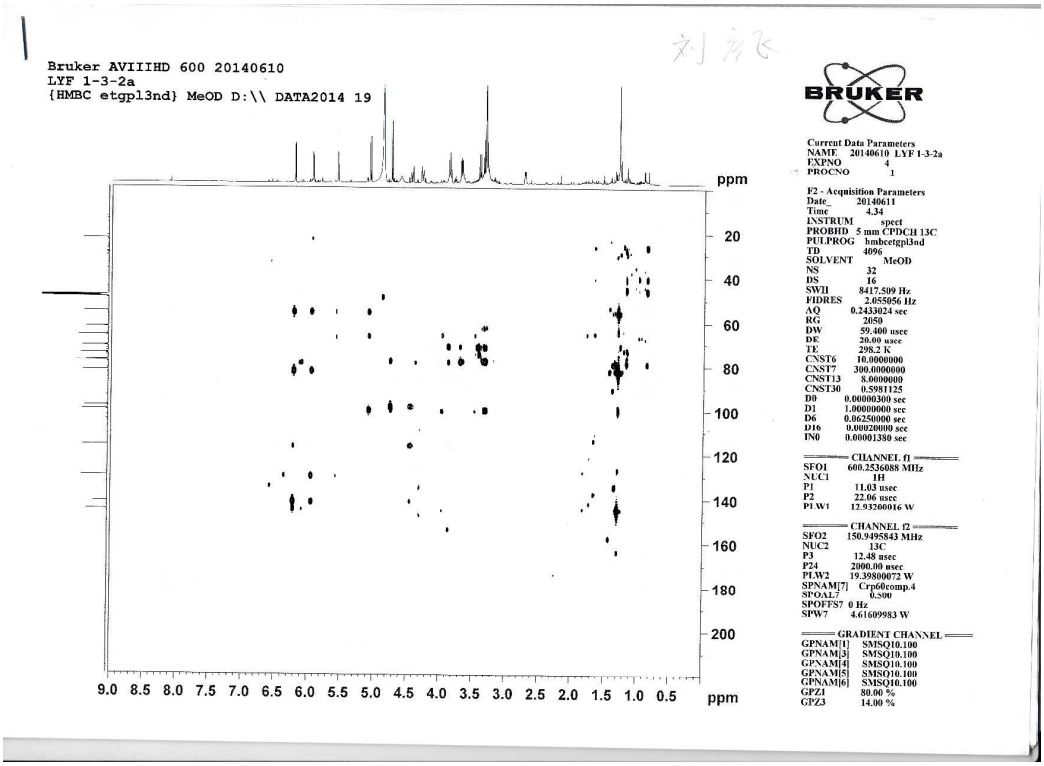
S3. ^{13}C NMR Spectrum of compound **1** (150 MHz, Methanol-d_4)



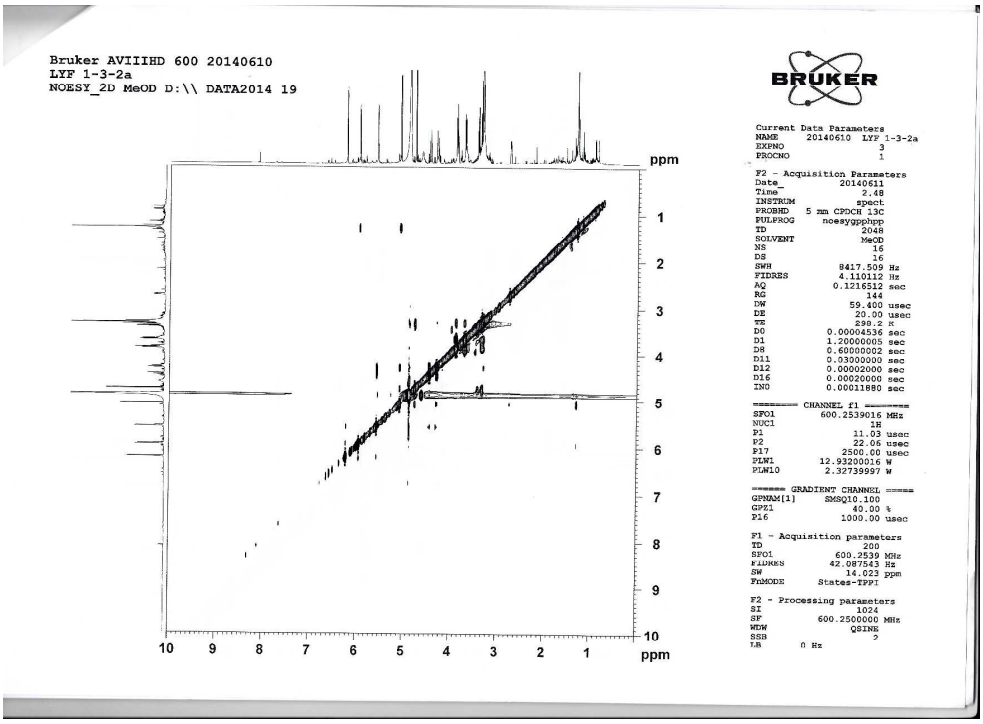
S4. ^{1}H–^{1}H COSY Spectrum of compound **1**



S5. HSQC Spectrum of compound **1**



S6. HMBC Spectrum of compound **1**



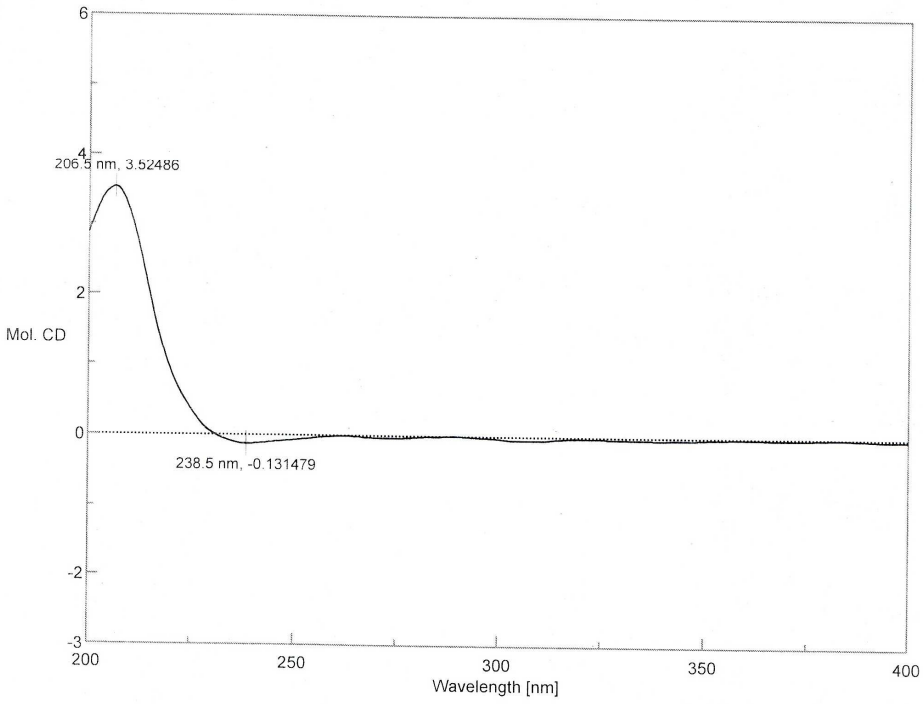
S7. NOESY Spectrum of compound **1**

MS Formula Results: + Scan (4.170 min) Sub (2014090903.d)

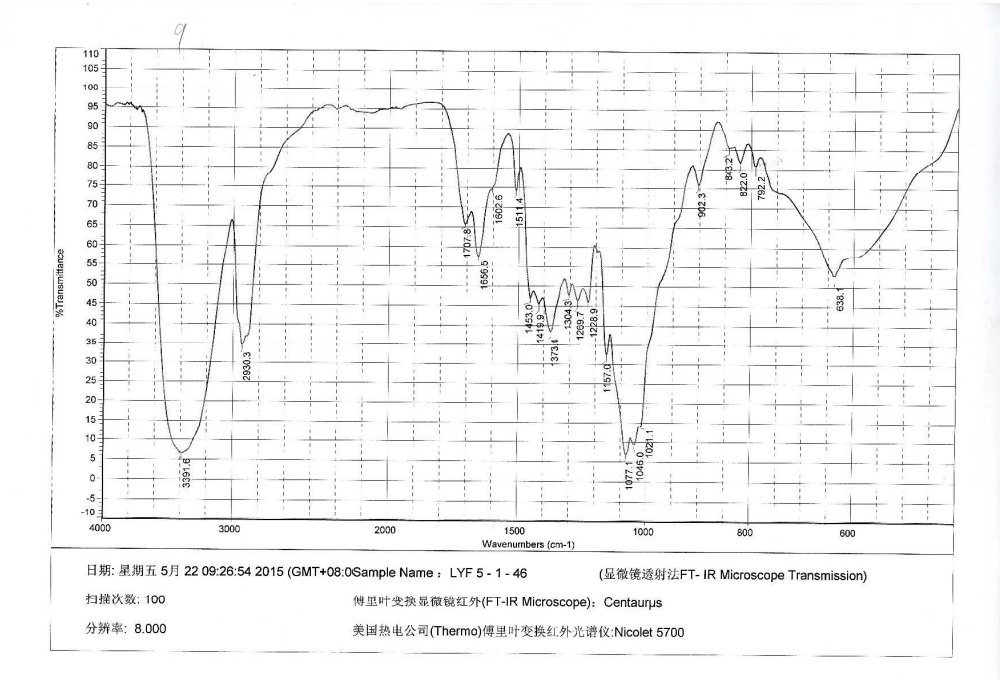
	m/z	Ion	Formula	Abundance
	353.1211	(M+Na)+	C15 H22 Na O8	481958.8

	Best	Formula (M)	Ion Formula	Score	Cross Score	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
1	✔	C15 H22 O8	C15 H22 Na O8	99.93		330.1319	330.1315	353.1207	-1.34	1.34	99.95	99.88	99.94	5

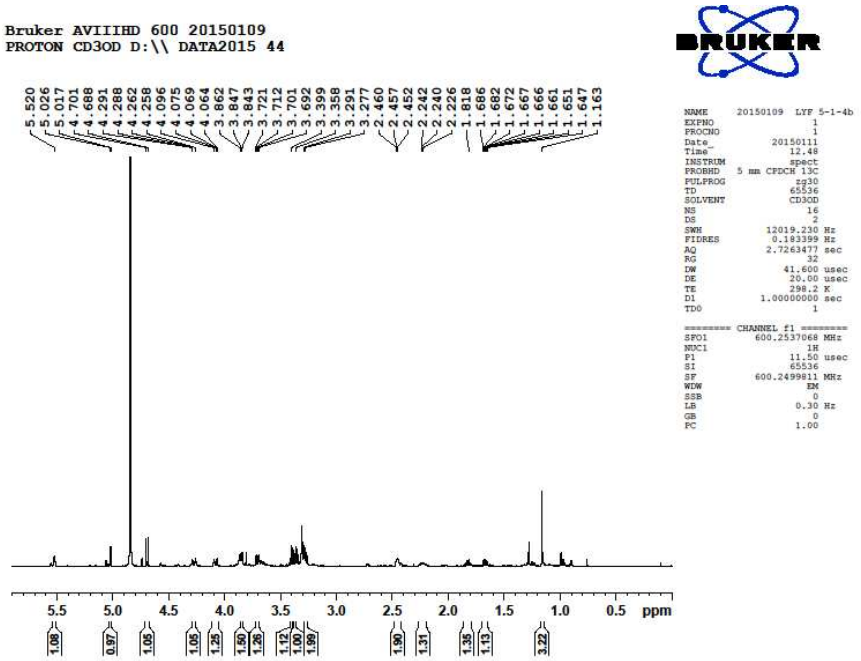
S8. HRESIMS Spectrum of compound **1**



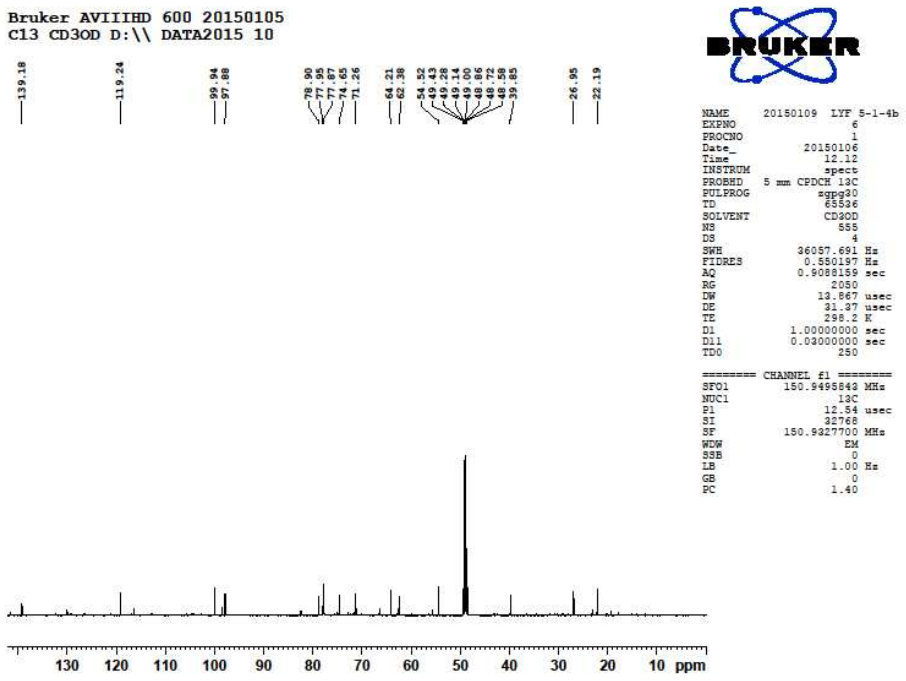
S9. CD Spectrum of compound **1** (CH_3OH)



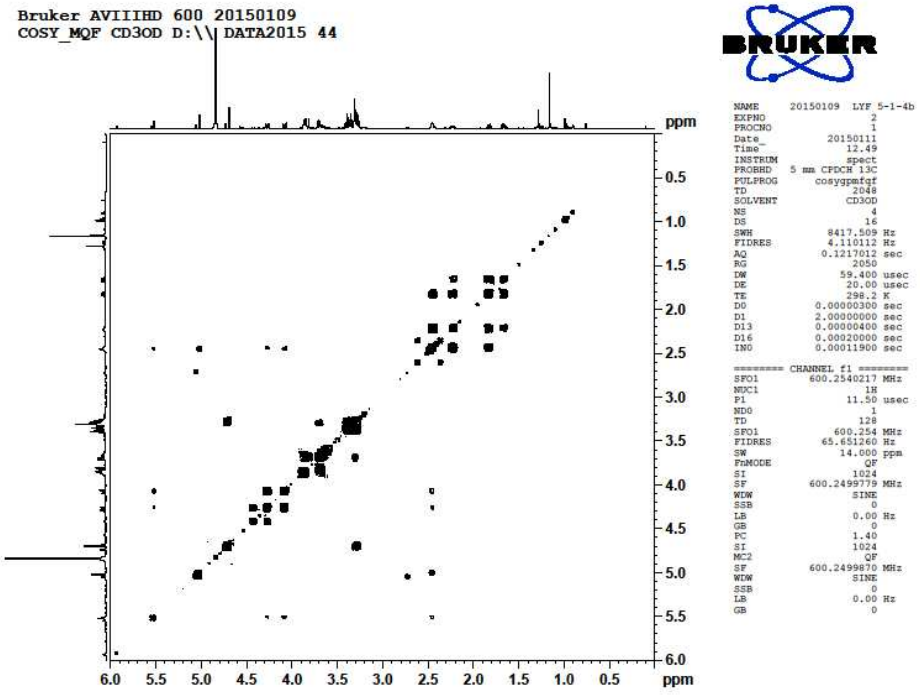
S10. IR Spectrum of compound **2**



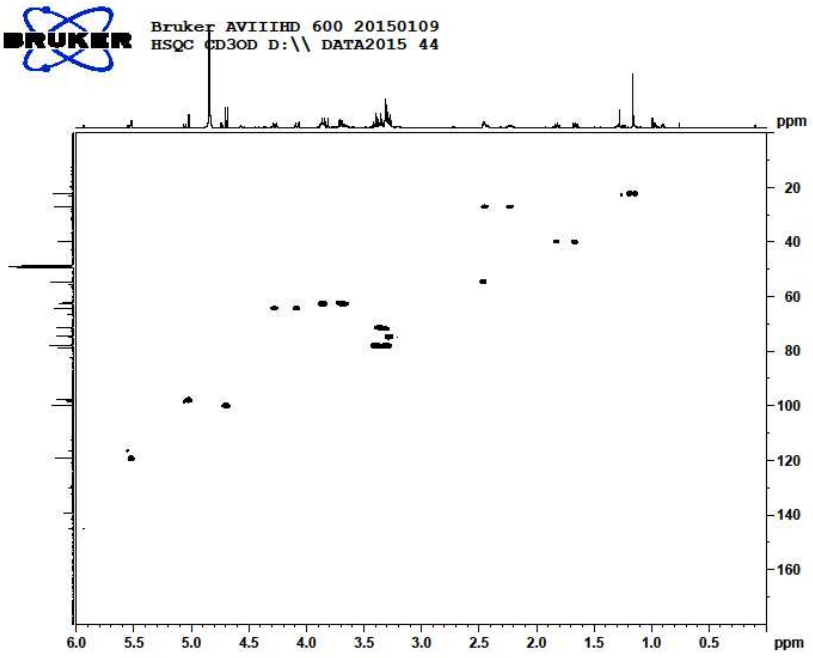
S11. ^{1}H NMR Spectrum of compound **2** (600 MHz, Methanol-d_4)



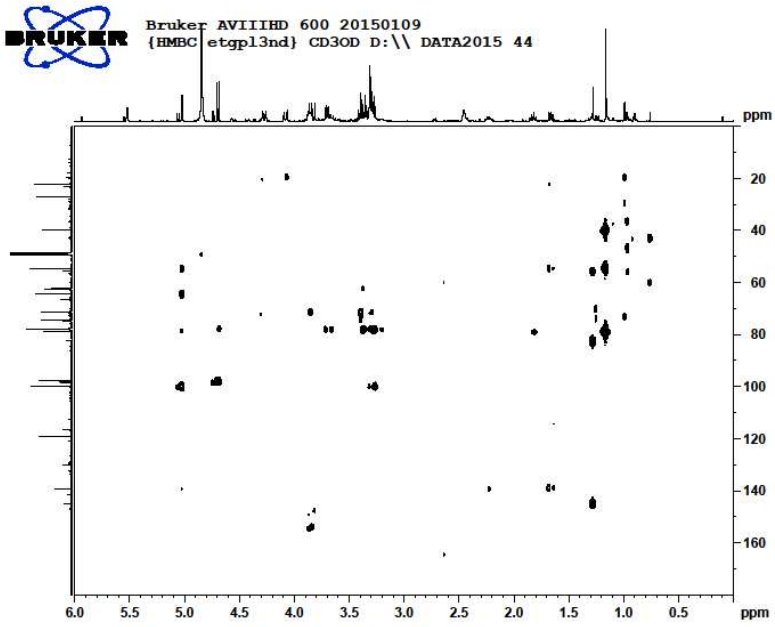
S12. ^{13}C NMR Spectrum of compound **2** (150 MHz, Methanol-d_4)



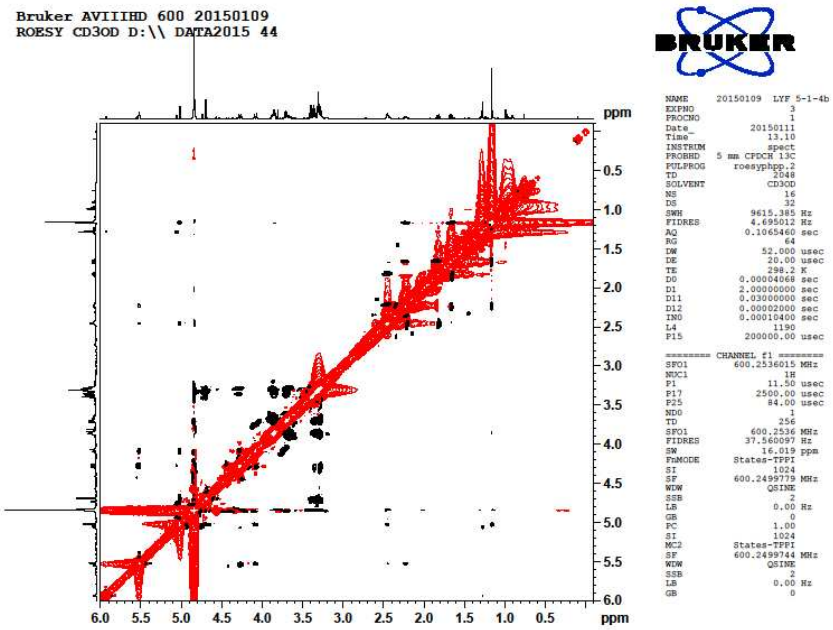
S13. ^{1}H–^{1}H COSY Spectrum of compound **2**



S14. HSQC Spectrum of compound **2**



S15. HMBC Spectrum of compound **2**



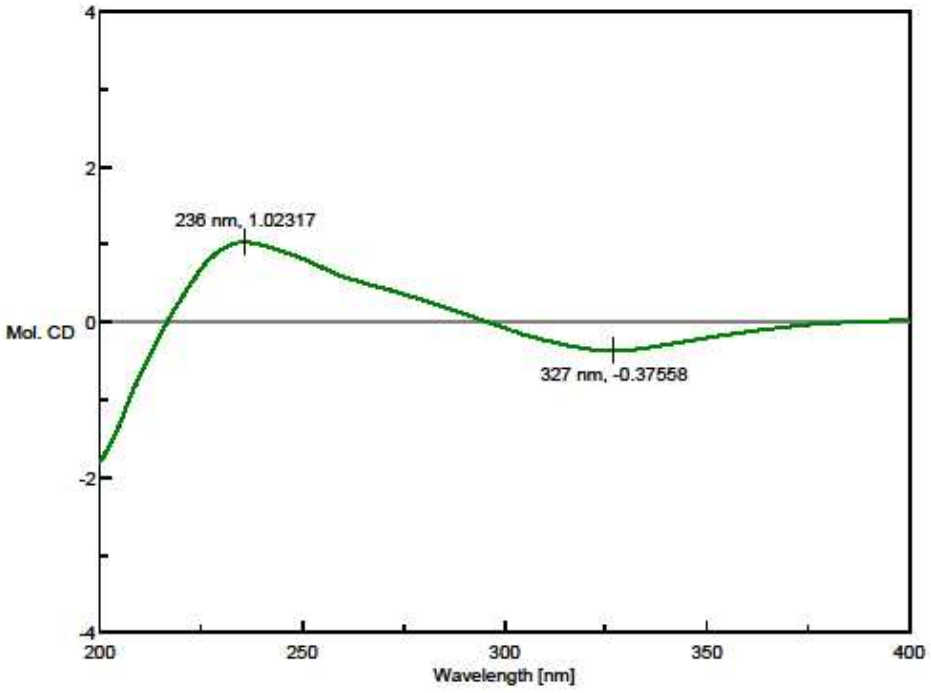
S16. ROESY Spectrum of compound **2**

MS Formula Results: + Scan (4.457 min) Sub (2015012103.d)

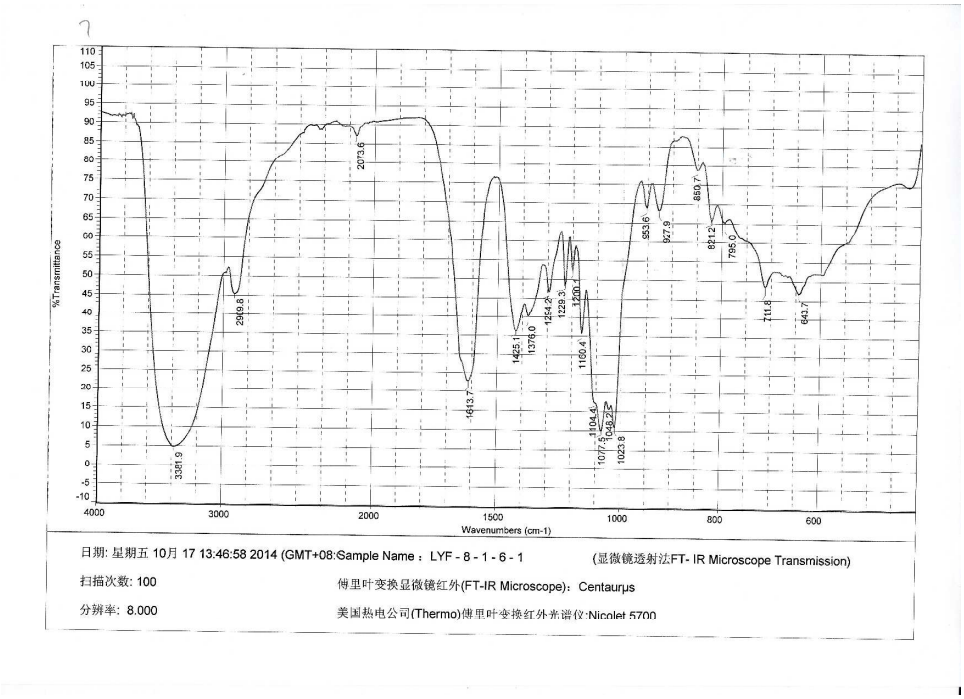
m/z	Ion	Formula	Abundance
355.136	(M+Na)+	C15 H24 Na O8	2087070

Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
✓	C15 H24 O8	C15 H24 Na O8	99.94		332.1467	332.1471	355.1363	1.12	1.12	99.96	99.89	99.93	4
	C16 H28 O3 S2	C16 H28 Na O3 S2	97.24		332.1467	332.148	355.1372	3.73	3.73	99.61	91.61	99.27	3

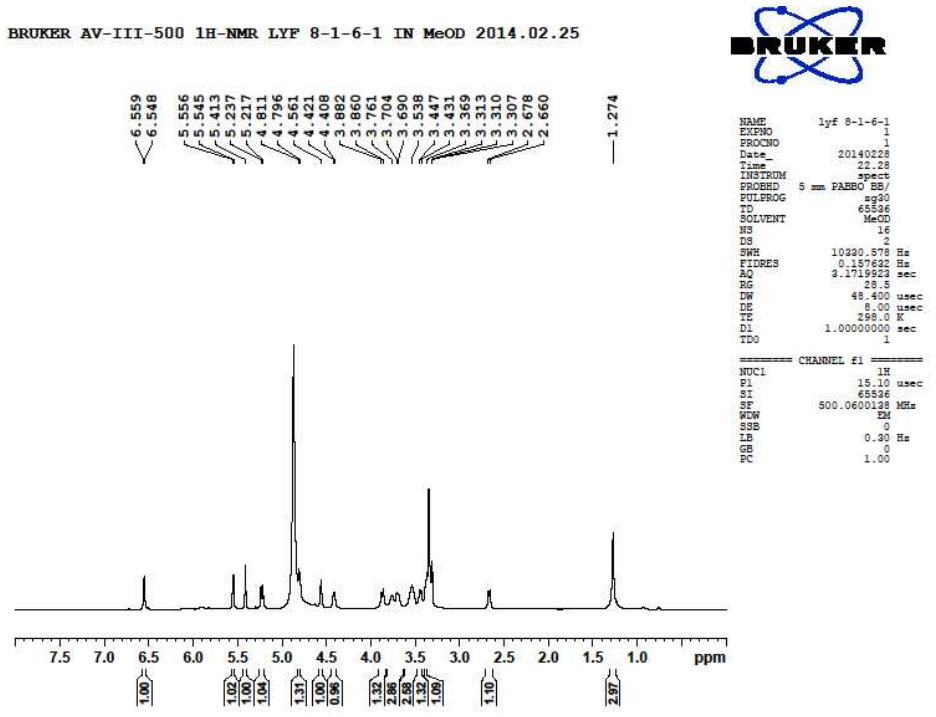
S17. HRESIMS Spectrum of compound **2**



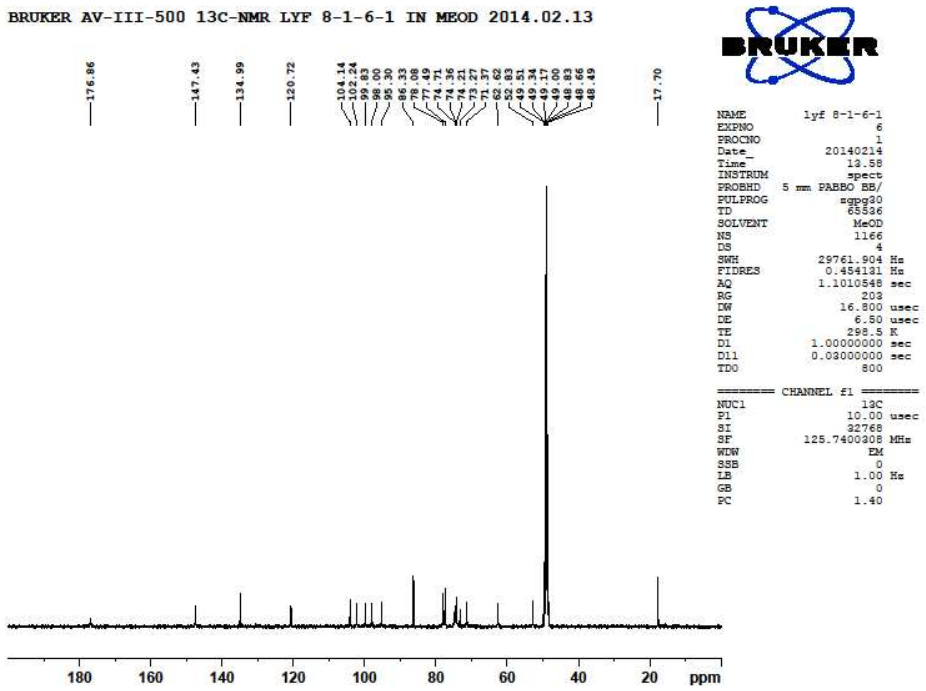
S18. CD Spectrum of compound **2** (CH_3OH)



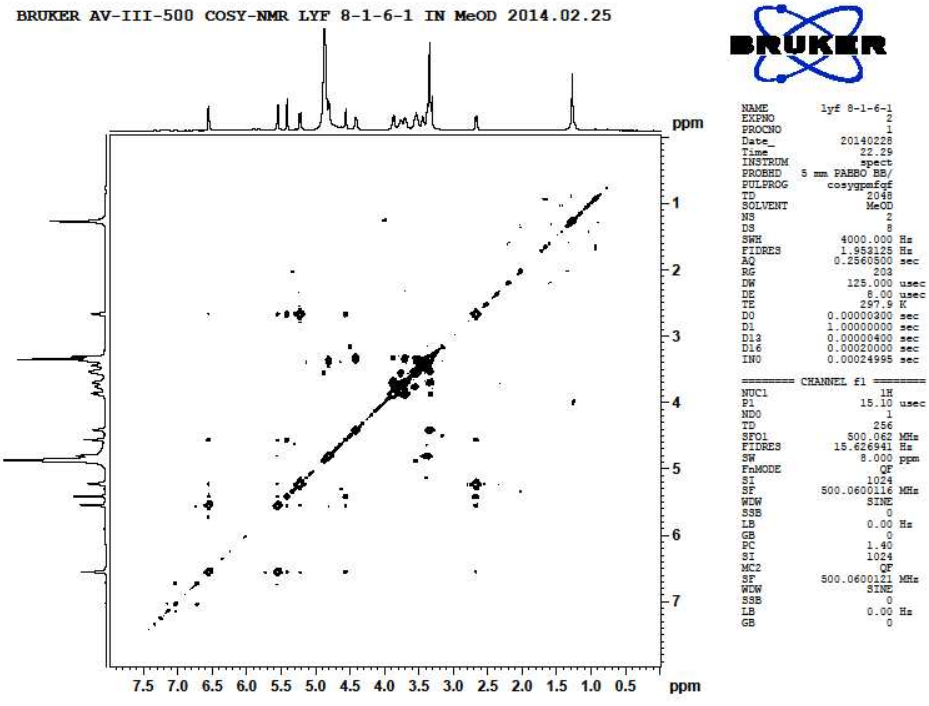
S19. IR Spectrum of compound **3**



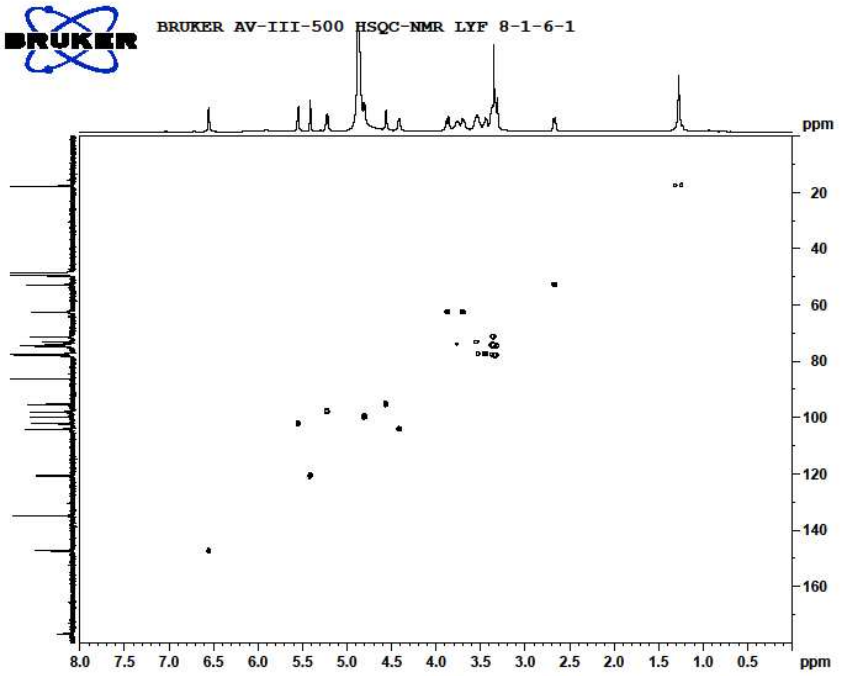
S20. ^{1}H NMR Spectrum of compound **3** (500MHz, Methanol-d_4)



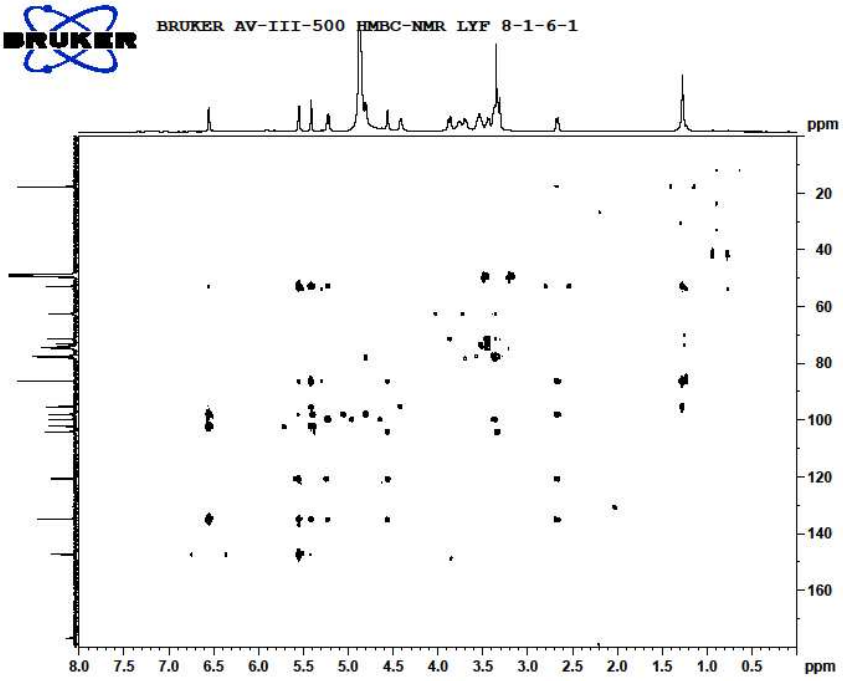
S21. ^{13}C NMR Spectrum of compound **3** (125 MHz, Methanol-d_4)



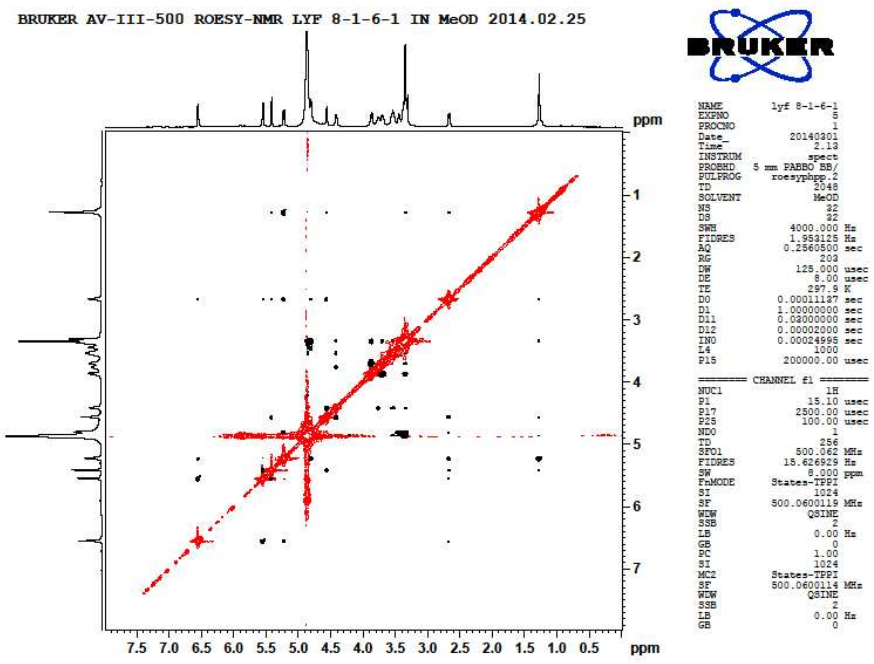
S22. ^{1}H–^{1}H COSY Spectrum of compound **3**



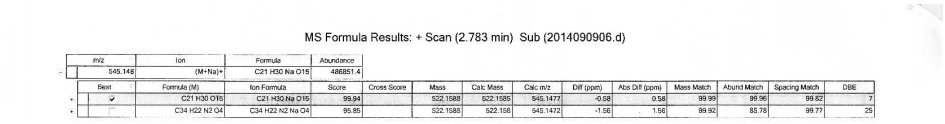
S23. HSQC Spectrum of compound **3**



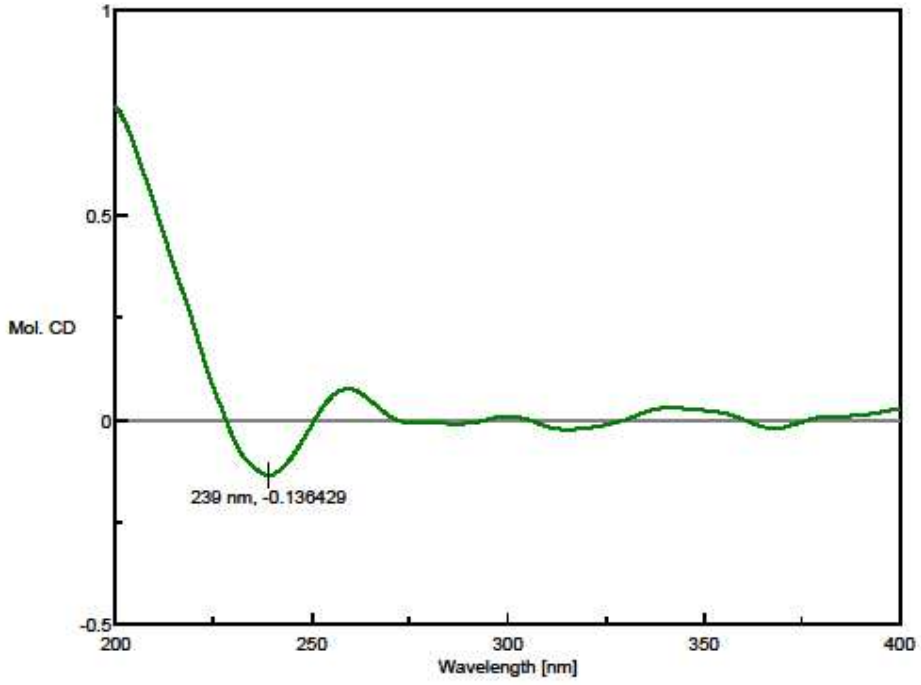
S24. HMBC Spectrum of compound **3**



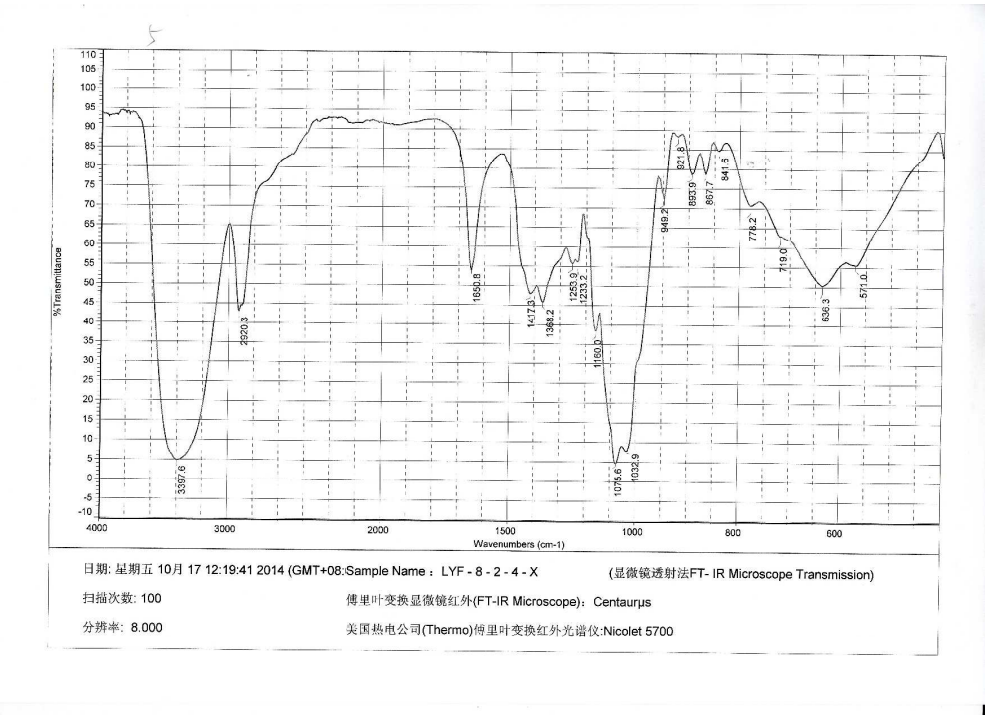
S25. ROESY Spectrum of compound **3**



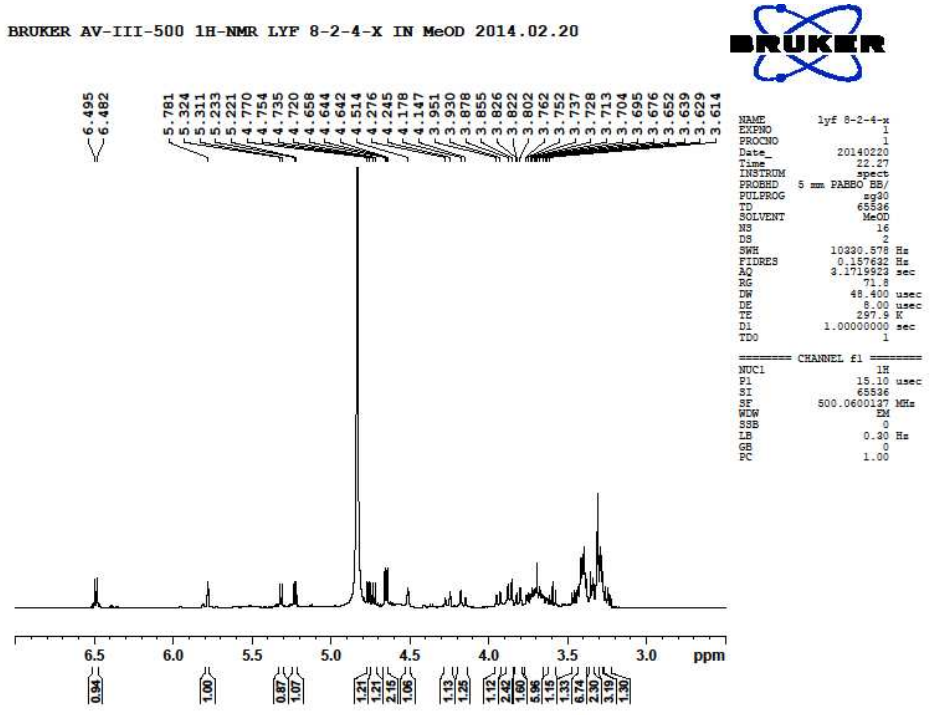
S26. HRESIMS Spectrum of compound **3**



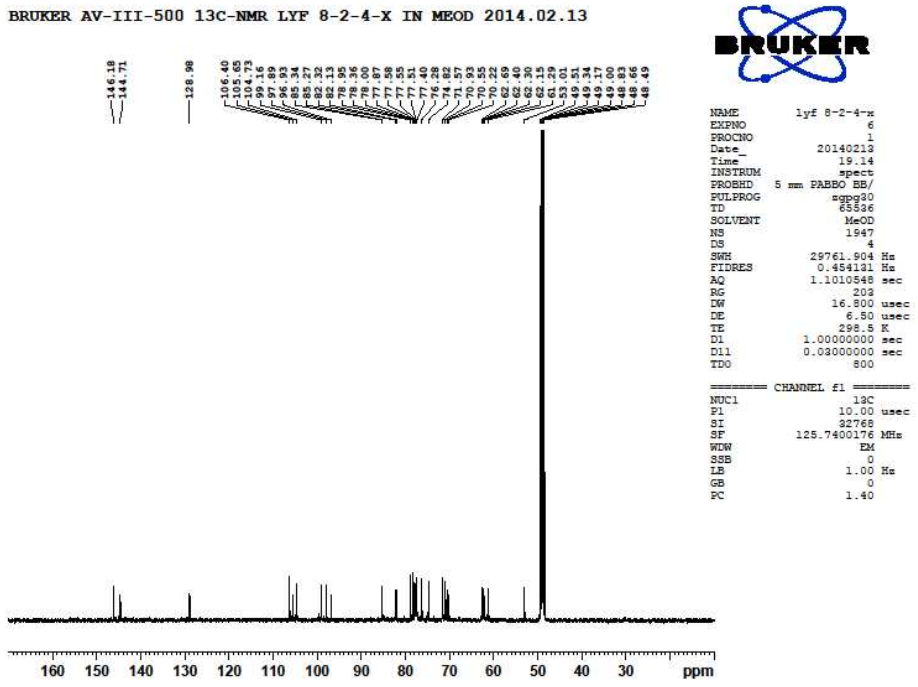
S27. CD Spectrum of compound **3** (CH_3OH)



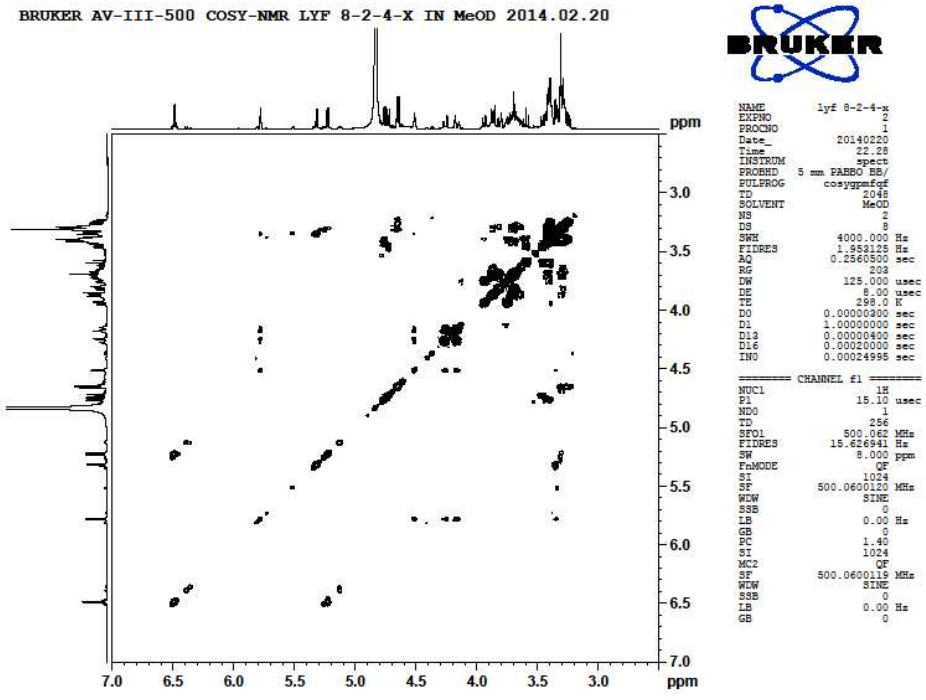
S28. IR Spectrum of compound **4**



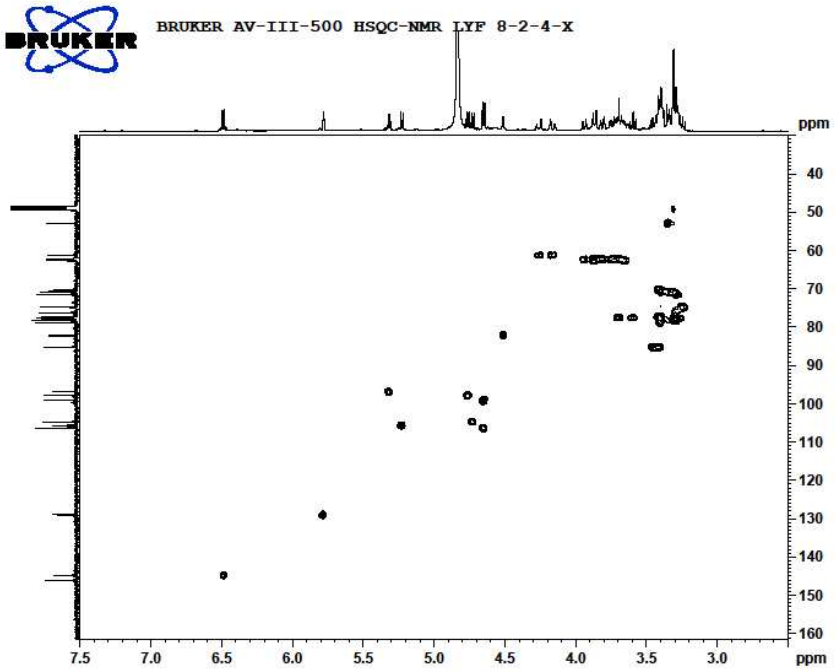
S29. ^{1}H NMR Spectrum of compound **4** (500MHz, Methanol-d_4)



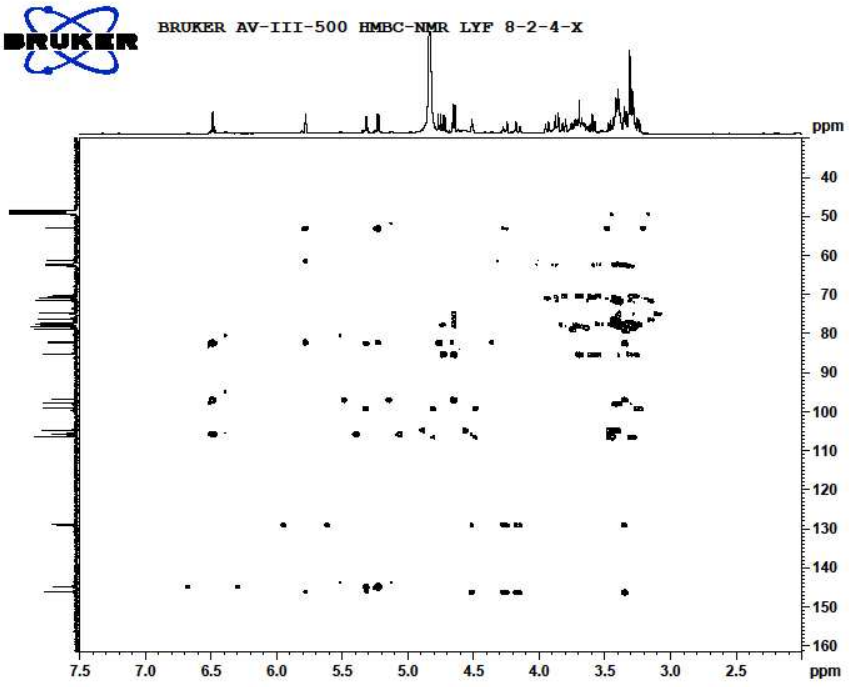
S30. ^{13}C NMR Spectrum of compound **4** (125 MHz, Methanol-d_4)



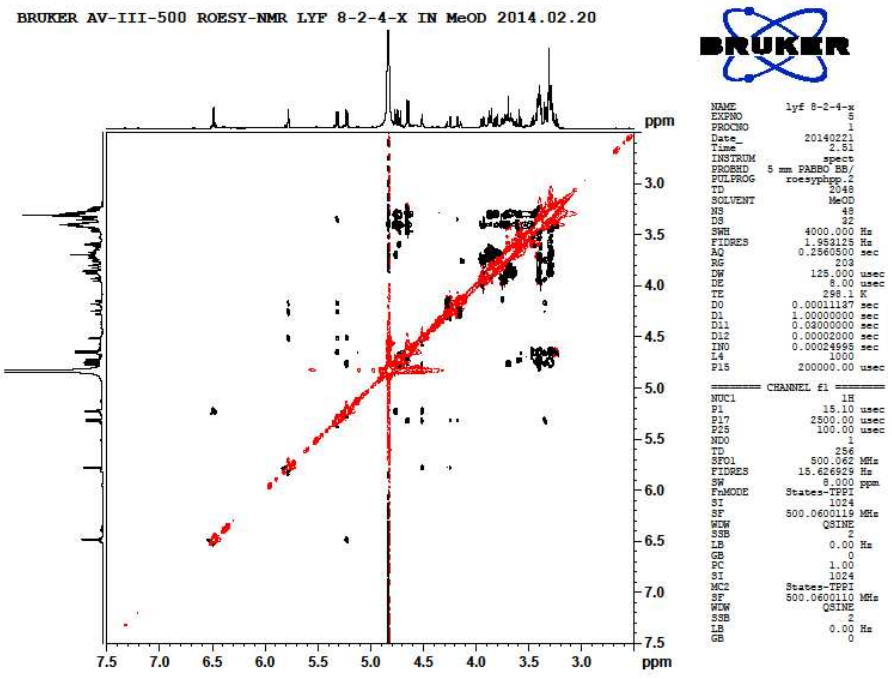
S31. ^{1}H–^{1}H COSY Spectrum of compound **4**



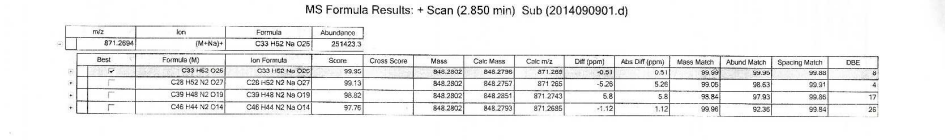
S32. HSQC Spectrum of compound **4**



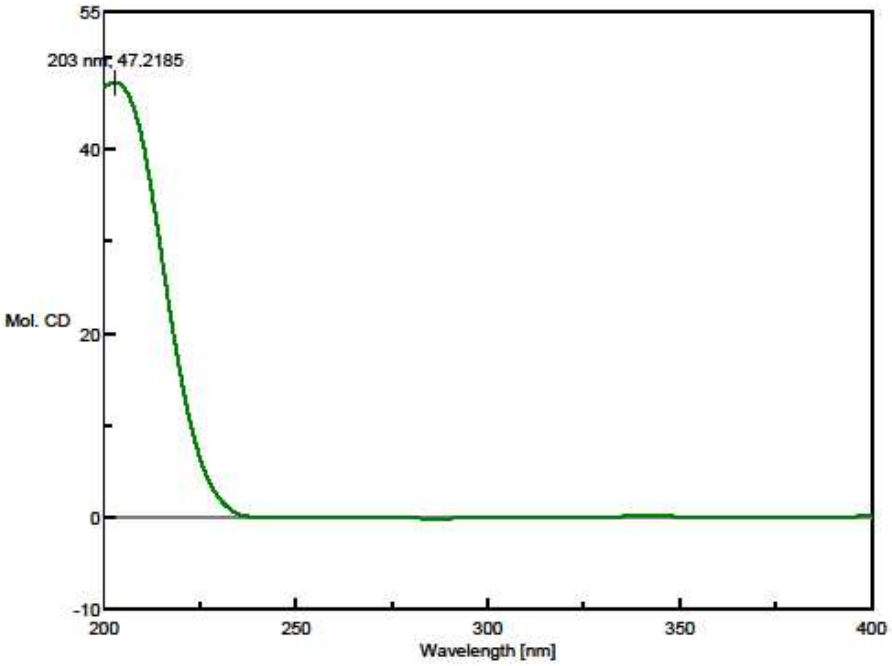
S33. HMBC Spectrum of compound **4**



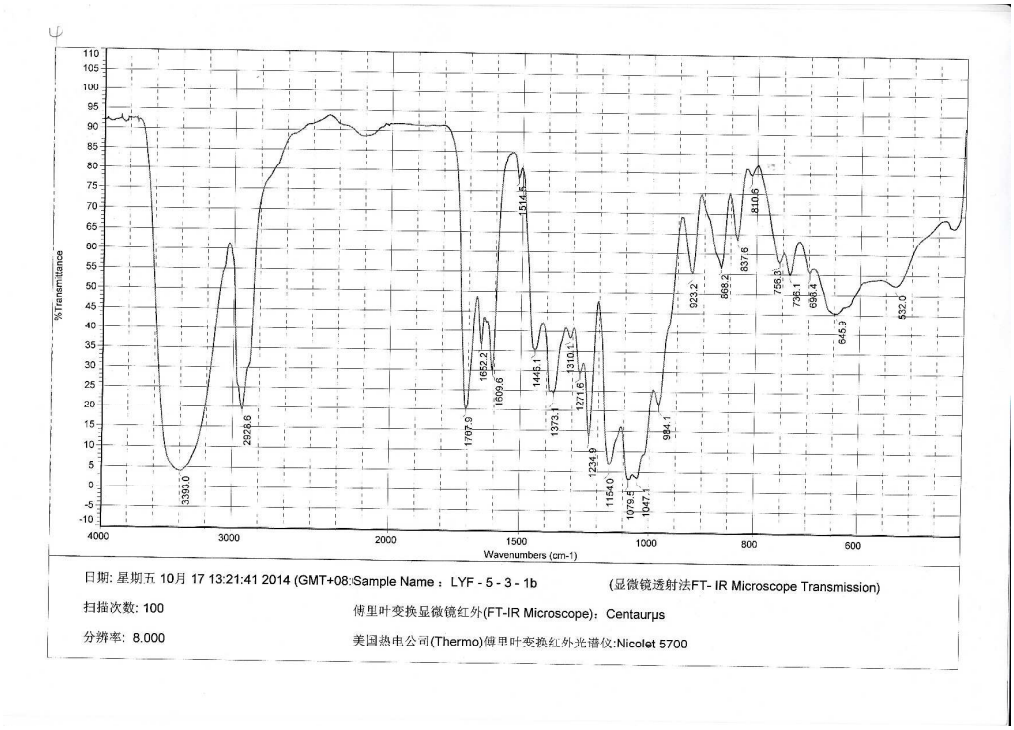
S34. ROESY Spectrum of compound **4**



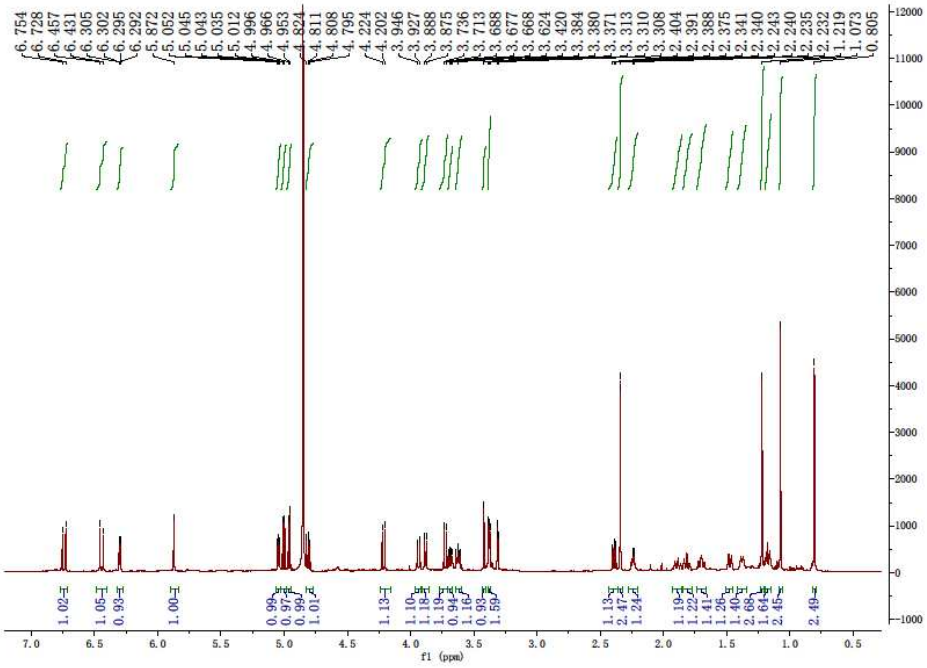
S35. HRESIMS Spectrum of compound **4**



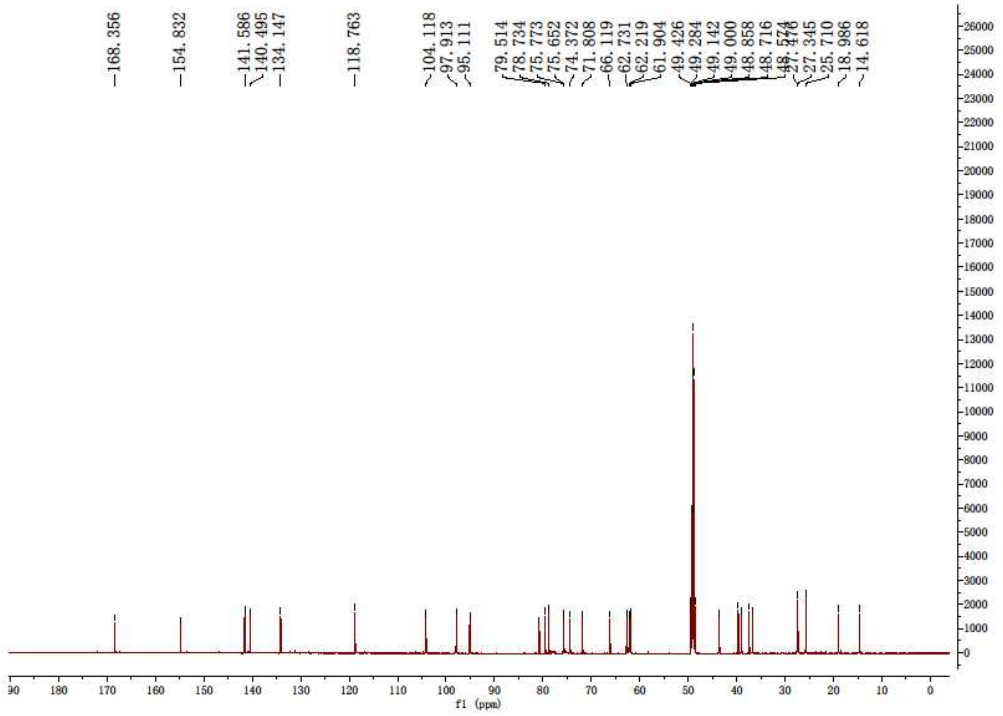
S36. CD Spectrum of compound **4** (CH_3OH)



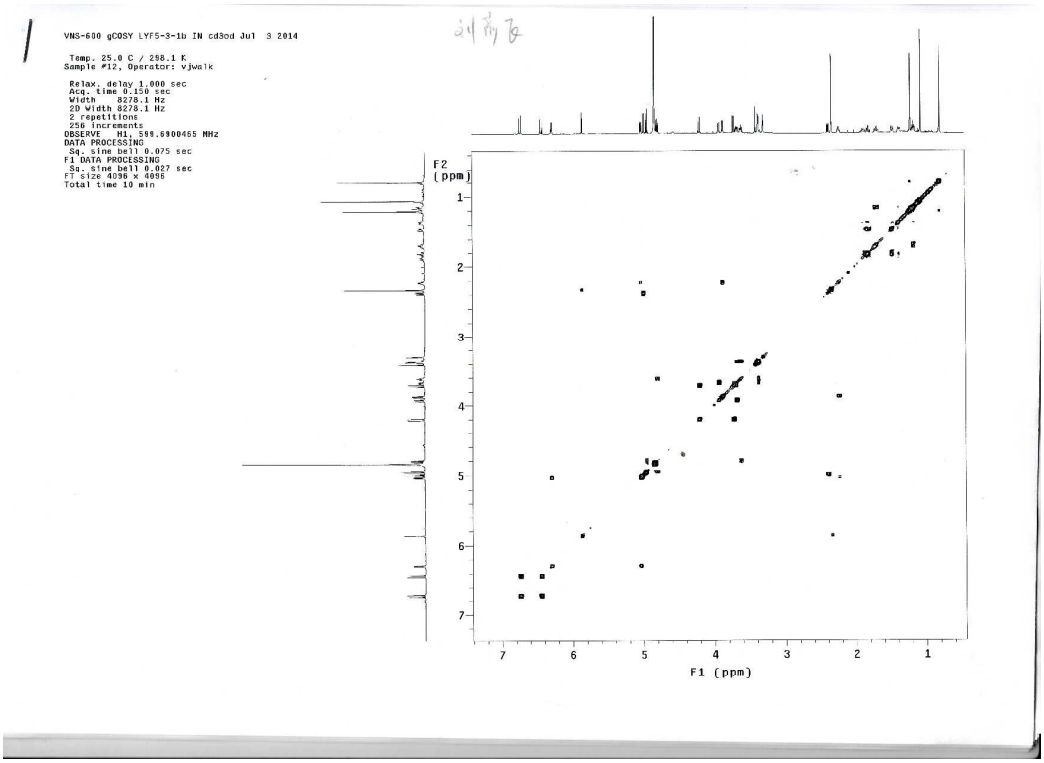
S37. IR Spectrum of compound **5**



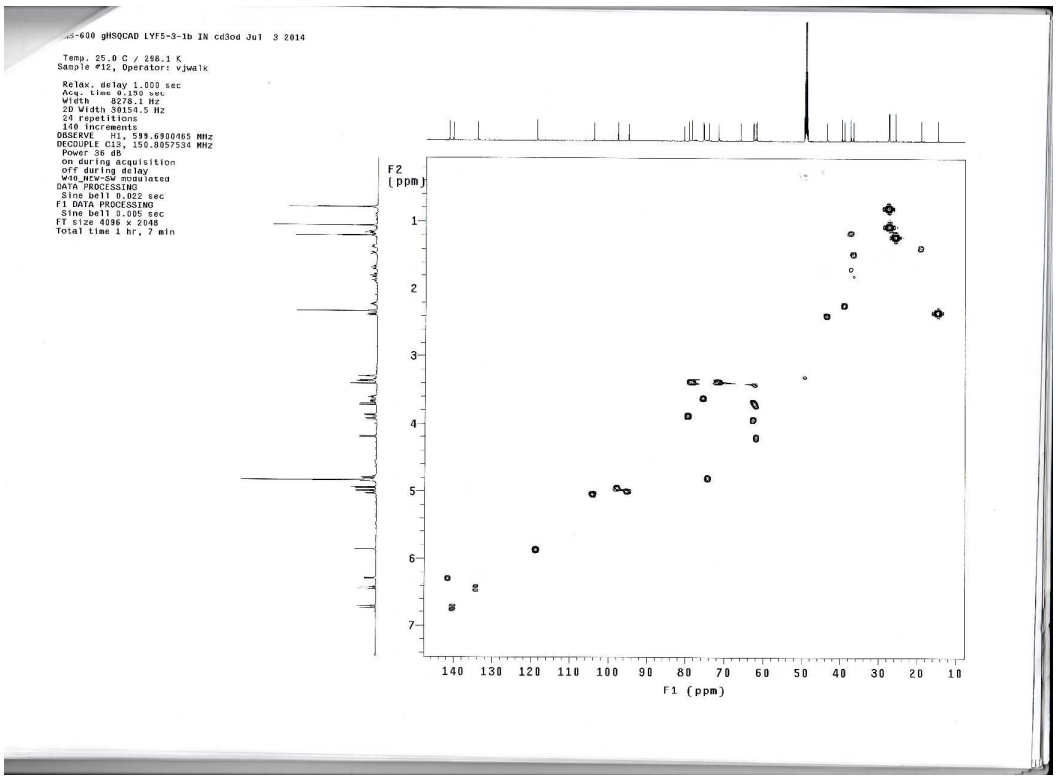
S38. ^{1}H NMR Spectrum of compound **5** (600 MHz, Methanol-d_4)



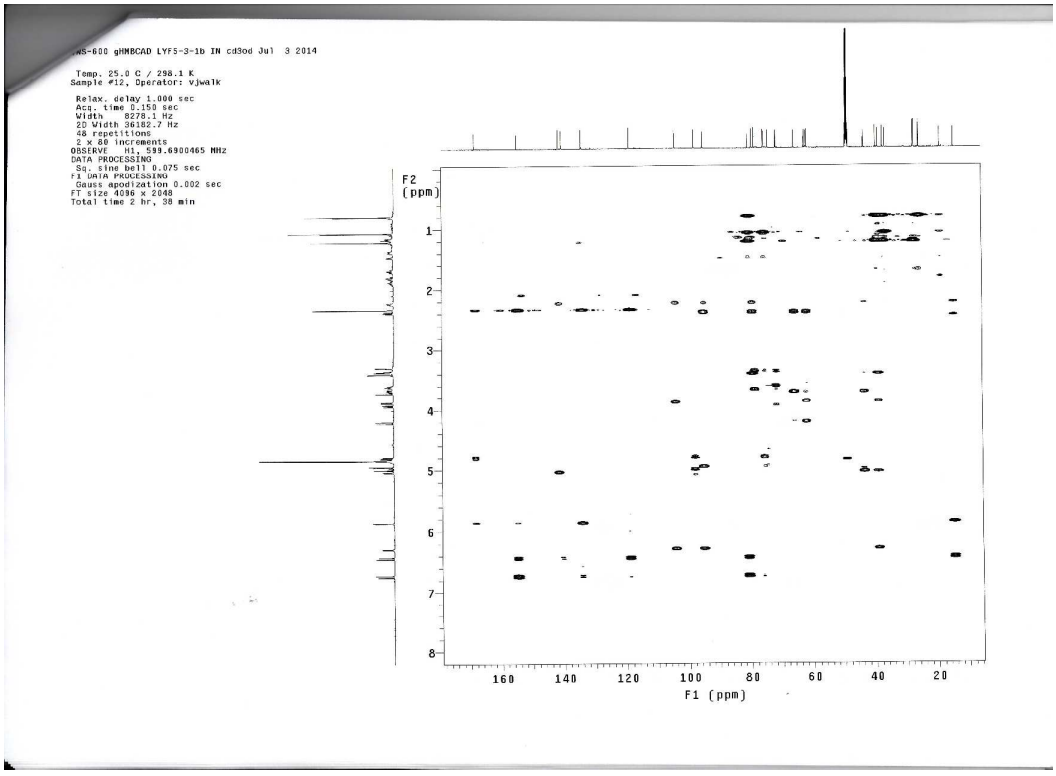
S39. ^{13}C NMR Spectrum of compound **5** (150 MHz, Methanol-d_4)



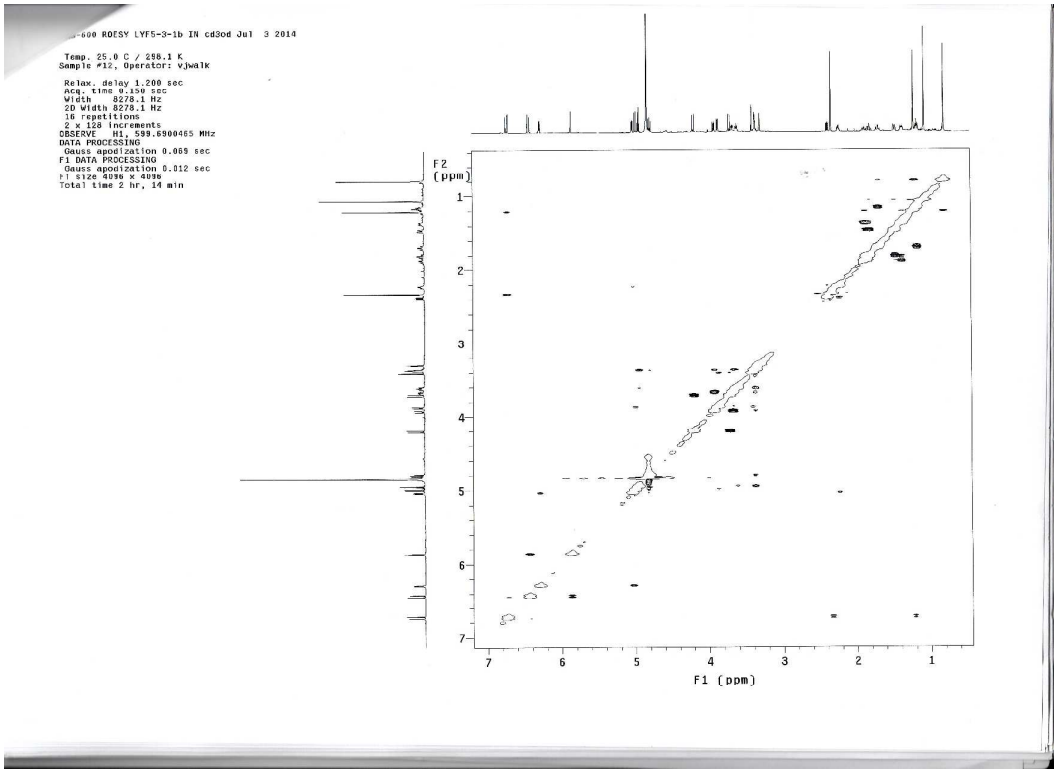
S40. ^{1}H–^{1}H COSY Spectrum of compound **5**



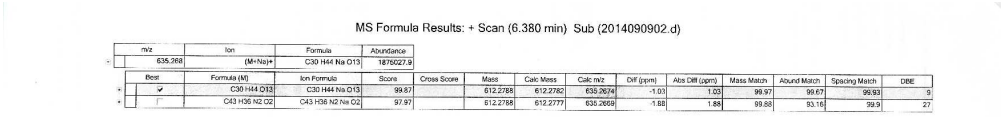
S41. HSQC Spectrum of compound **5**



S42. HMBC Spectrum of compound **5**



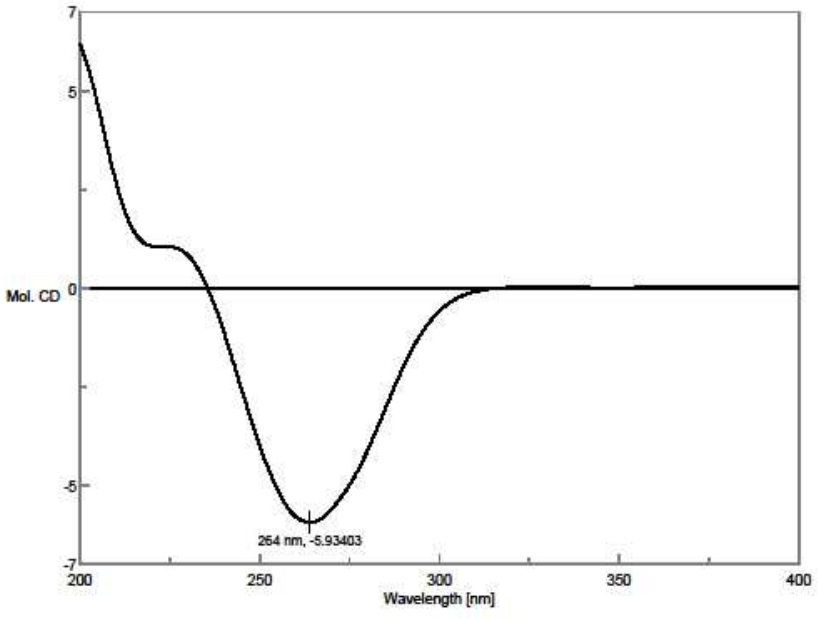
S43. ROESY Spectrum of compound **5**



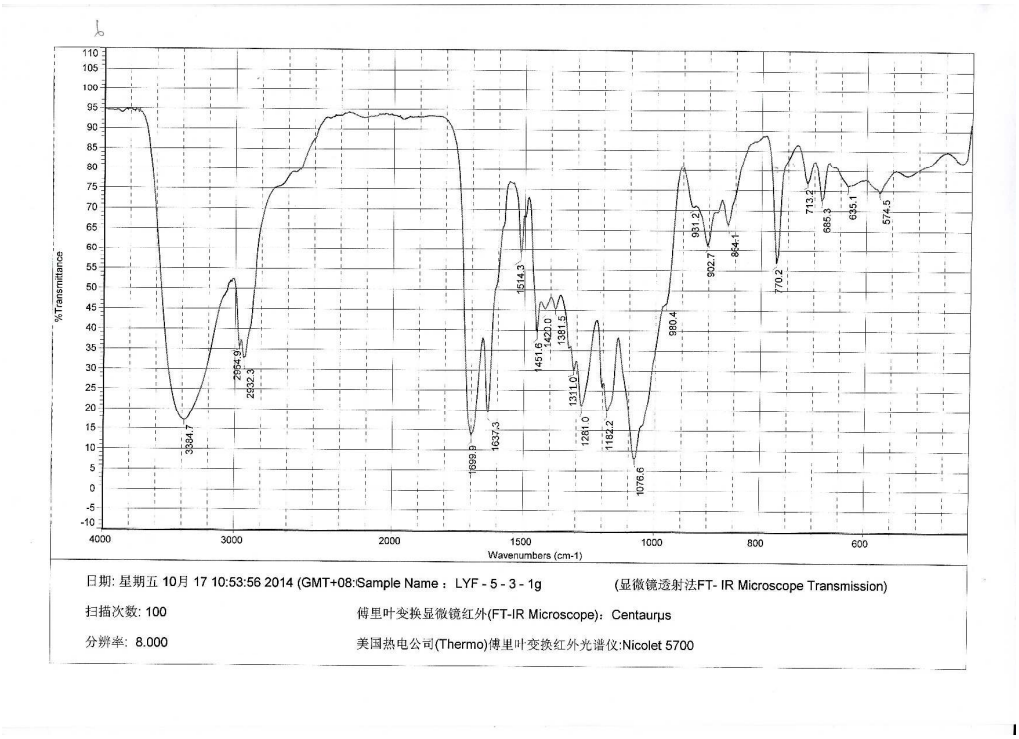
m/z	Ion	Formula	Abundance
635.268	(M+Na)+	C30 H44 Na O13	1876027.9

Best	Formula (M)	Ion Formula	Score	Cross Score	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
✔	C30 H44 O13	C30 H44 Na O13	99.87		612.2788	612.2782	635.2674	-1.03	1.03	99.97	99.67	99.93	9
	C43 H36 N2 O2	C43 H36 N2 Na O2	97.97		612.2788	612.2777	635.2669	-1.88	1.88	99.88	93.16	99.9	27

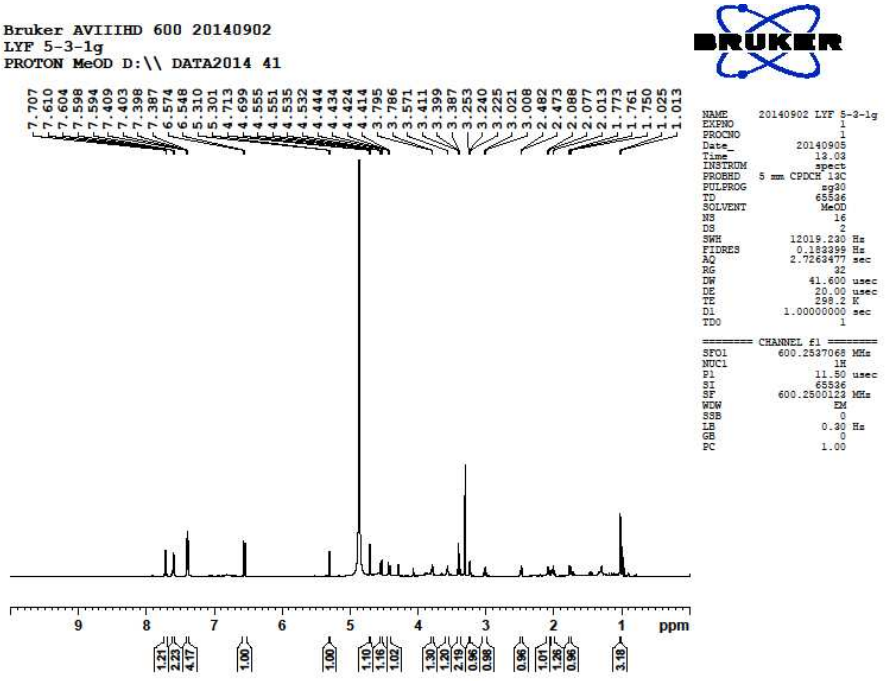
S44. HRESIMS Spectrum of compound **5**



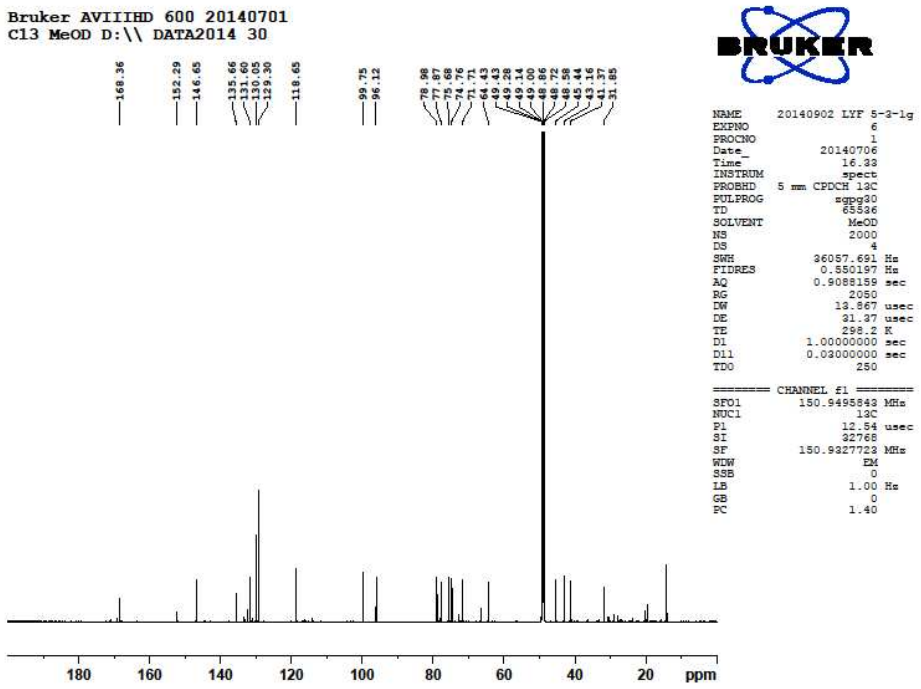
S45. CD Spectrum of compound **5** (CH_3OH)



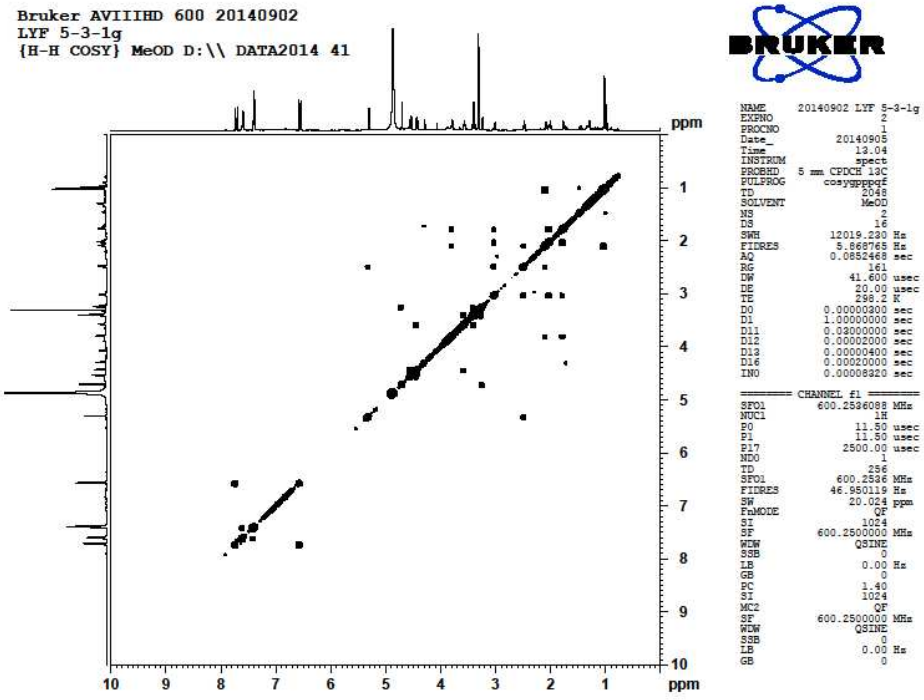
S46. IR Spectrum of compound **6**



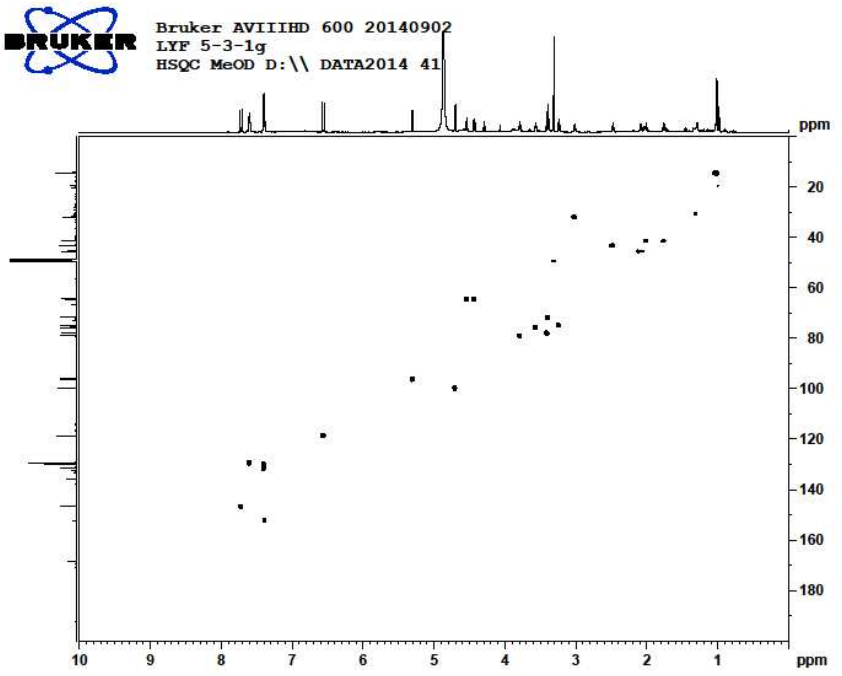
S47. ^{1}H NMR Spectrum of compound **6** (600MHz, Methanol-d_4)



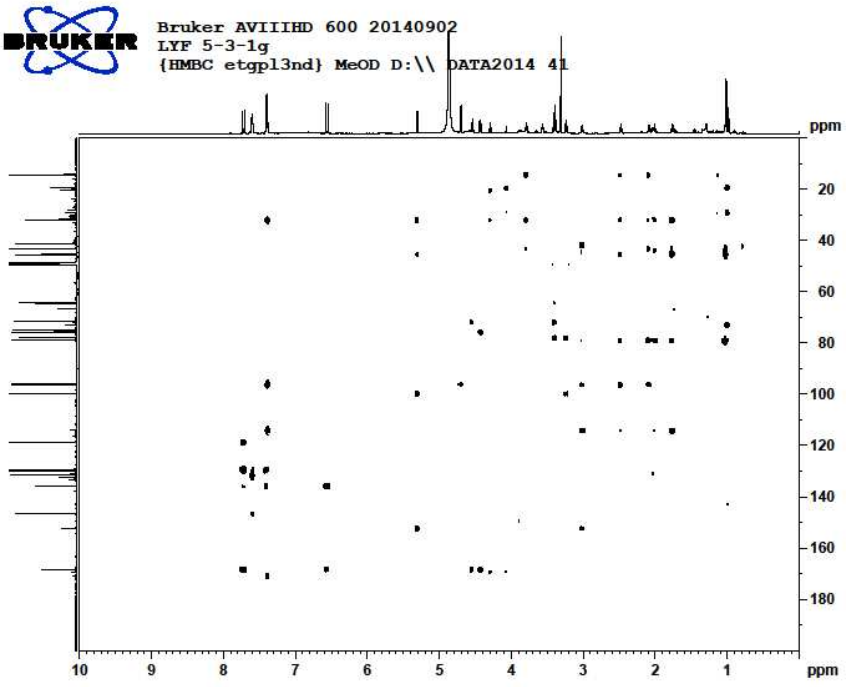
S48. ^{13}C NMR Spectrum of compound **6** (150 MHz, Methanol-d_4)



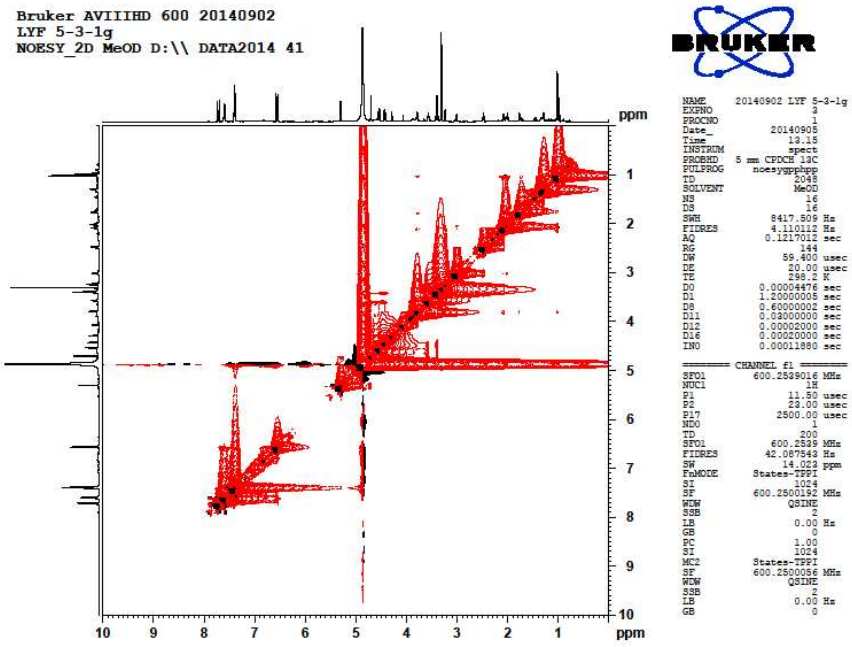
S49. ^{1}H–^{1}H COSY Spectrum of compound **6**



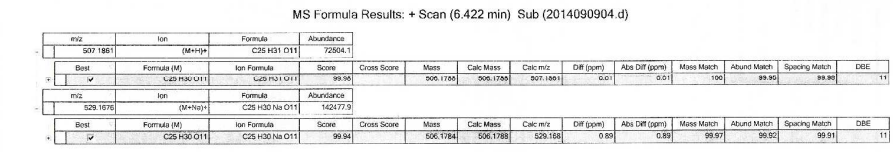
S450. HSQC Spectrum of compound **6**



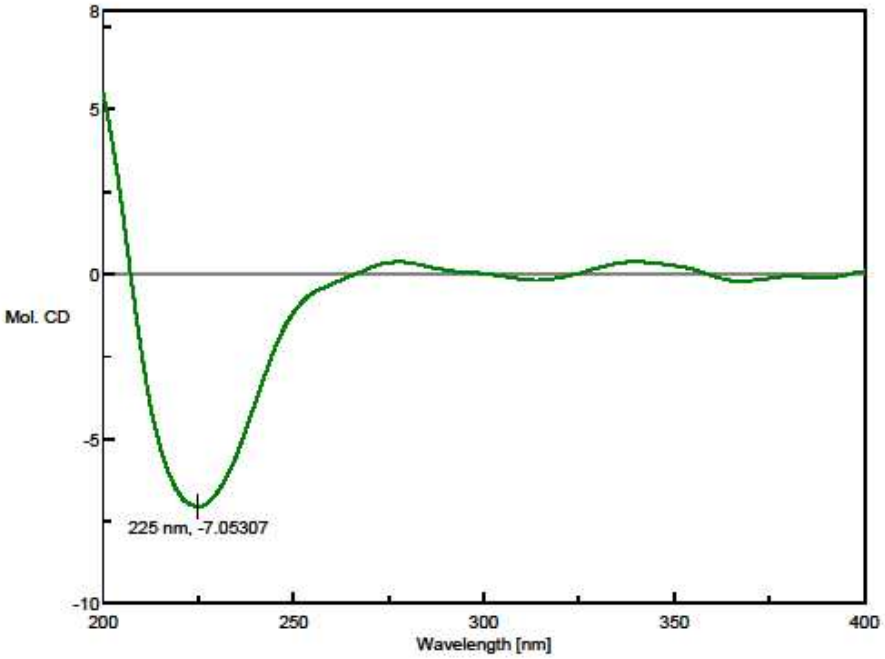
S51. HMBC Spectrum of compound **6**



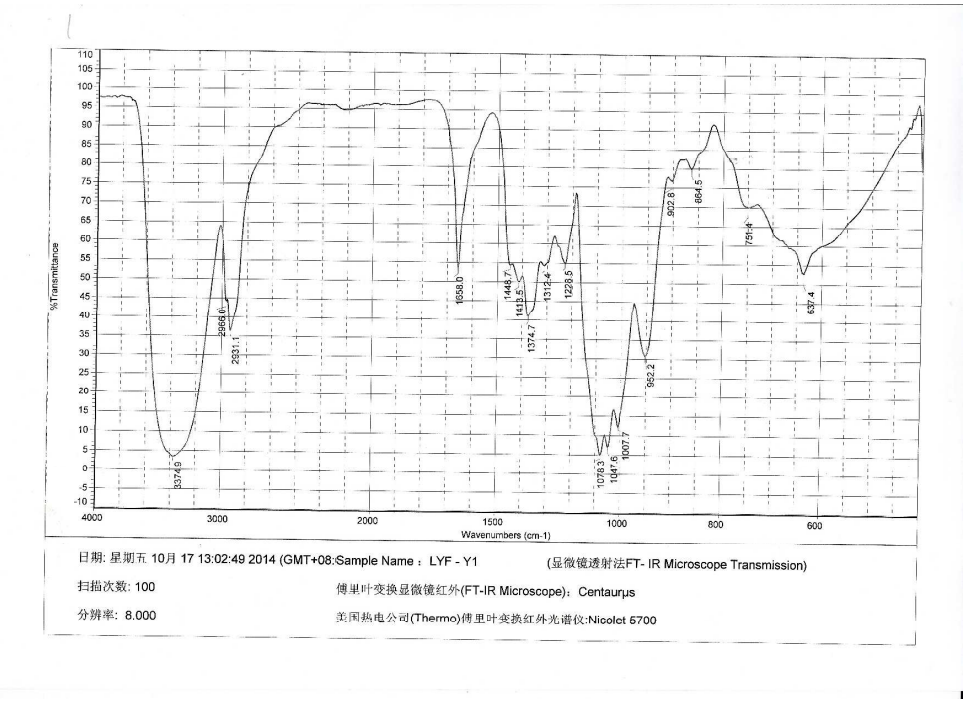
S52. NOESY Spectrum of compound **6**



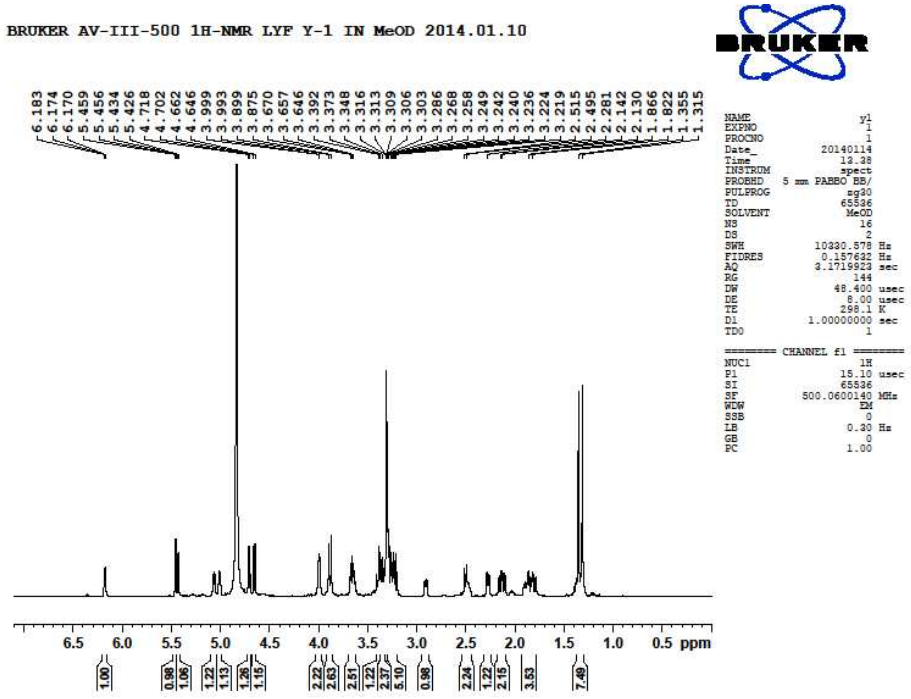
S53. HRESIMS Spectrum of compound **6**



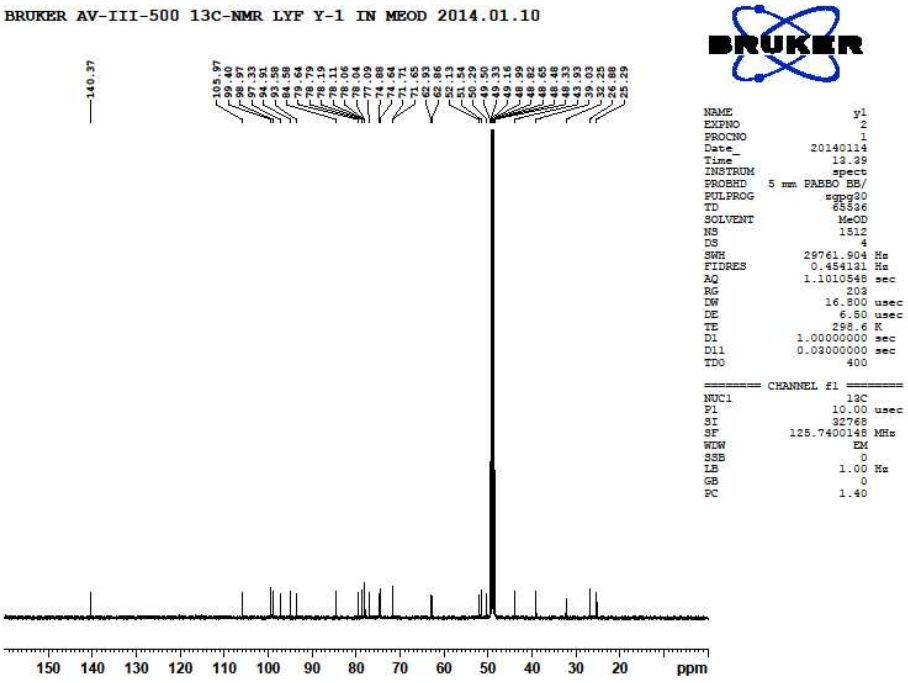
S54. CD Spectrum of compound **6** (CH_3OH)



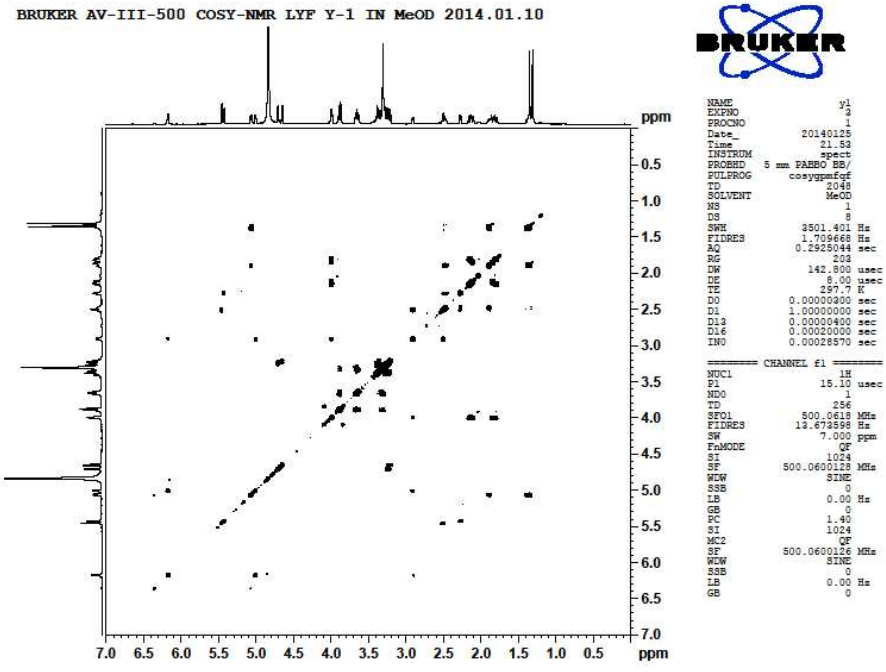
S55. IR Spectrum of compound **7**



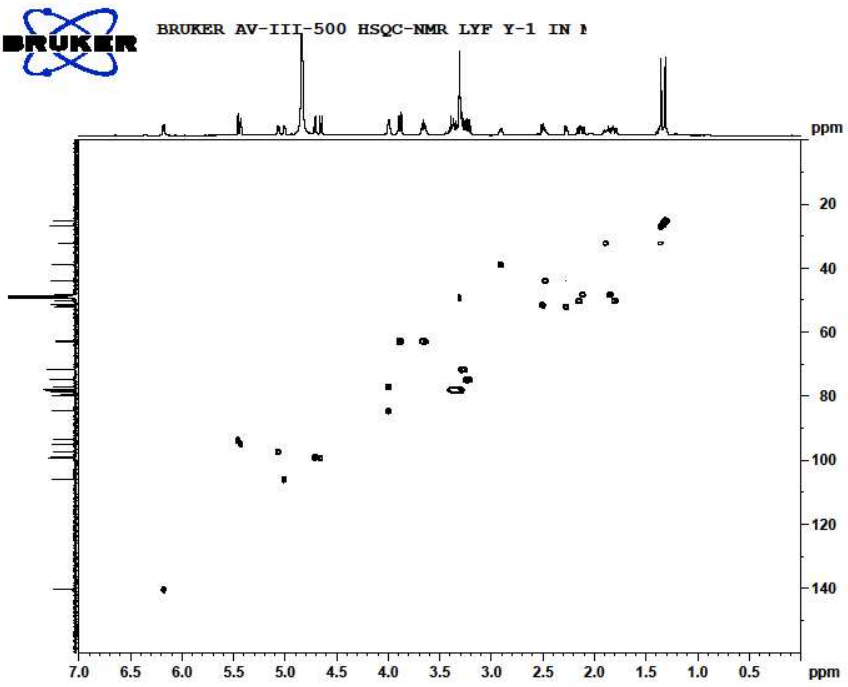
S56. ^{1}H NMR Spectrum of compound **7** (500MHz, Methanol-d_4)



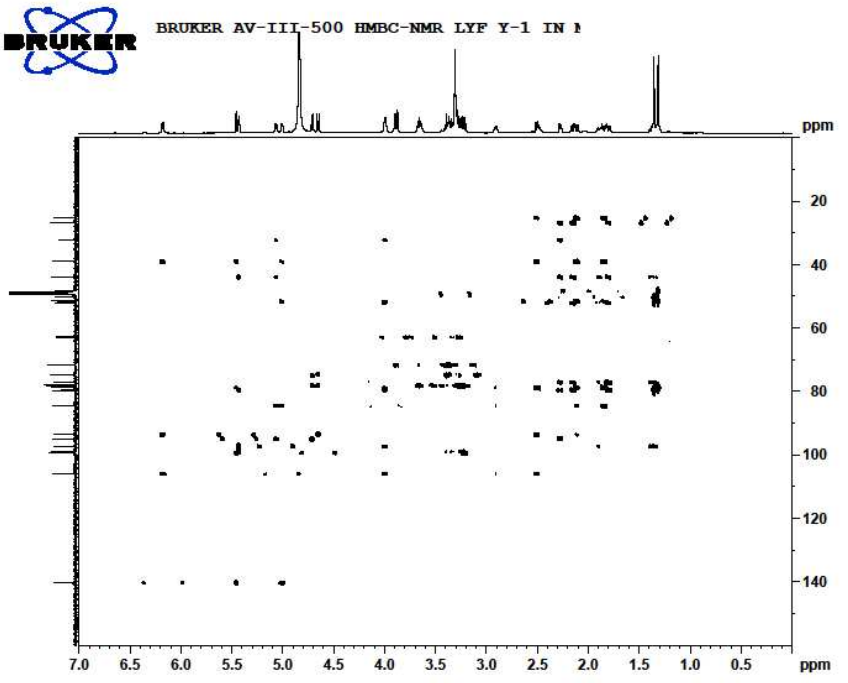
S57. ^{13}C NMR Spectrum of compound **7** (125 MHz, Methanol-d_4)



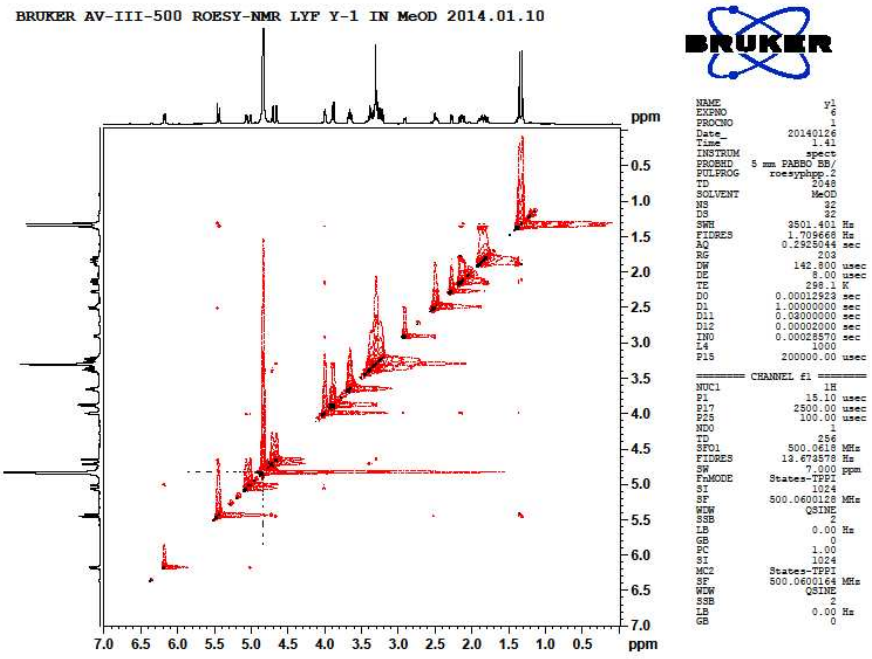
S58. ^{1}H–^{1}H COSY Spectrum of compound **7**



S59. HSQC Spectrum of compound **7**



S60. HMBC Spectrum of compound **7**



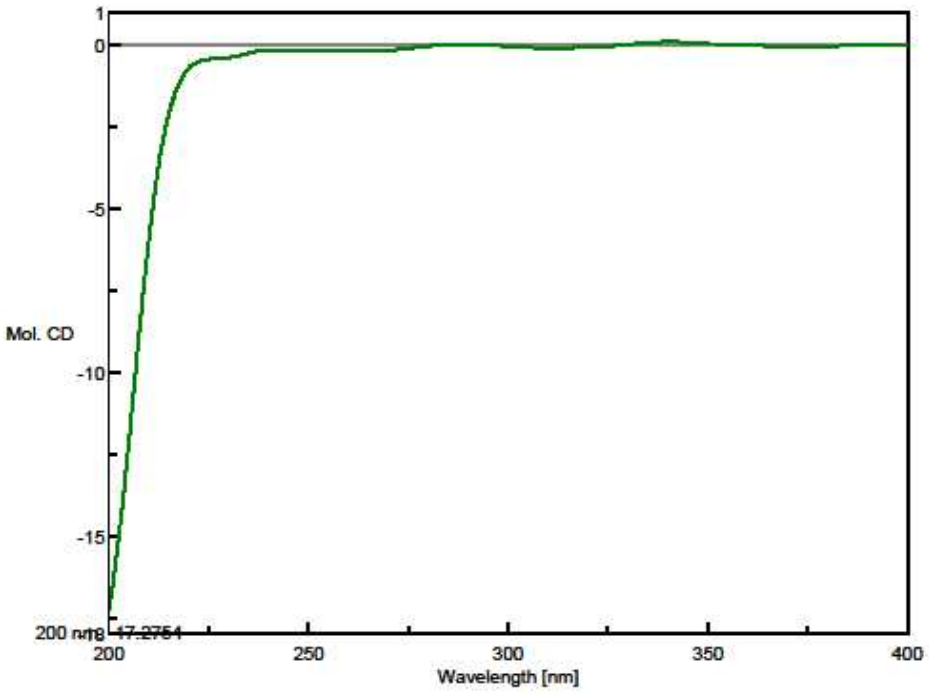
S61. ROESY Spectrum of compound **7**

MS Formula Results: + Scan (3.520 min) Sub (2014090501.d)

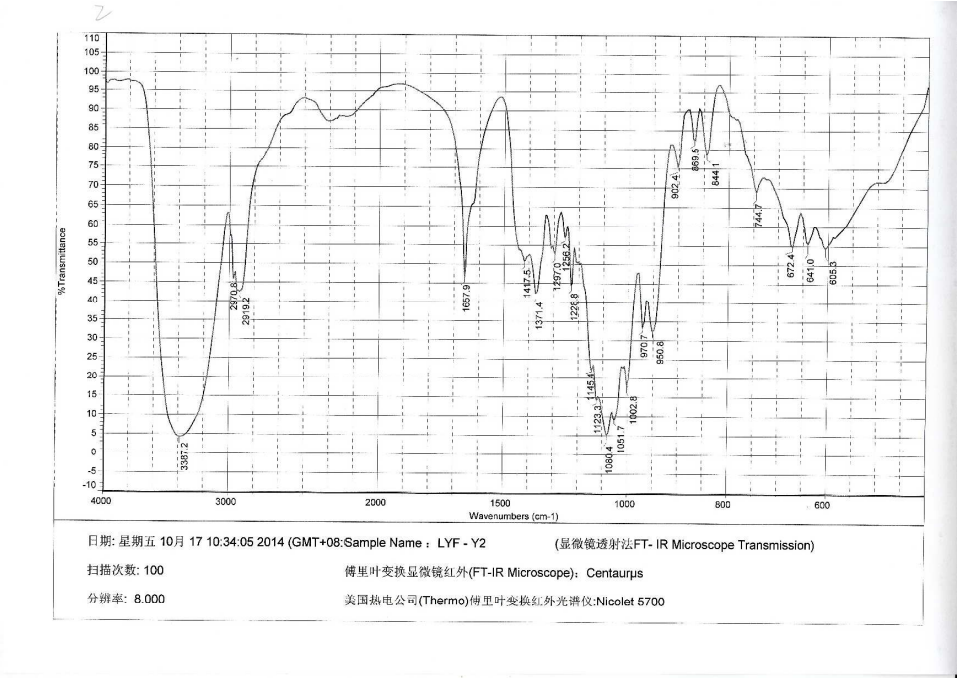
m/z	Ion	Formula	Abundance
719.2746	(M+Na)+	C30 H48 Na O18	411252.3

Best	Formula (M)	Ion Formula	Score	Cross Score	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
✓	C30 H48 O18	C30 H48 Na O18	99.89		696.2854	696.2841	719.2733	-1.85	1.85	99.89	99.92	99.88	7
	C36 H44 N2 O12	C36 H44 N2 Na O12	98.8		696.2854	696.2894	719.2786	5.84	5.84	98.88	97.82	99.87	16
	C43 H40 N2 O7	C43 H40 N2 Na O7	97.42		696.2854	696.2836	719.2728	-2.59	2.59	99.77	91.48	99.84	25

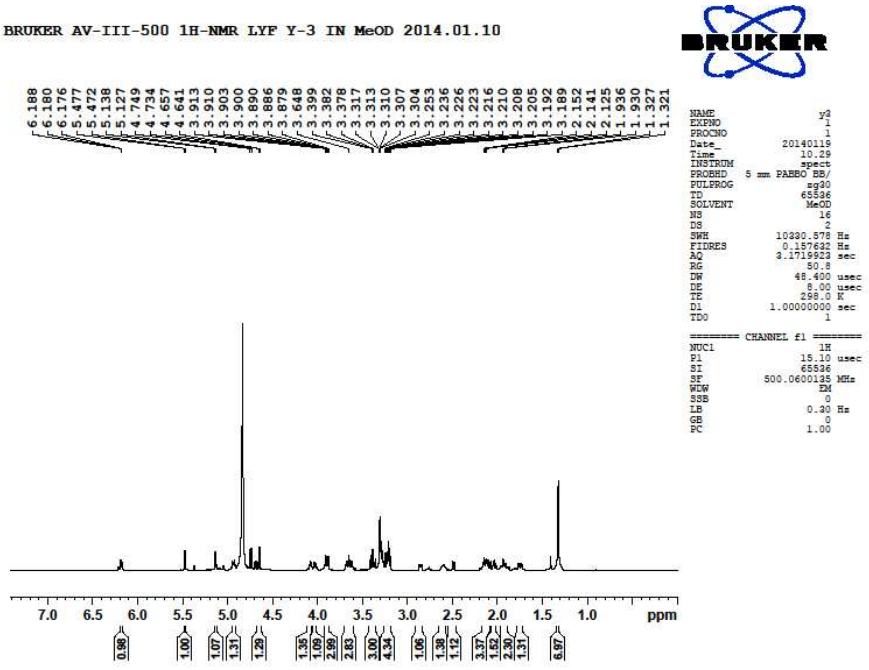
S62. HRESIMS Spectrum of compound **7**



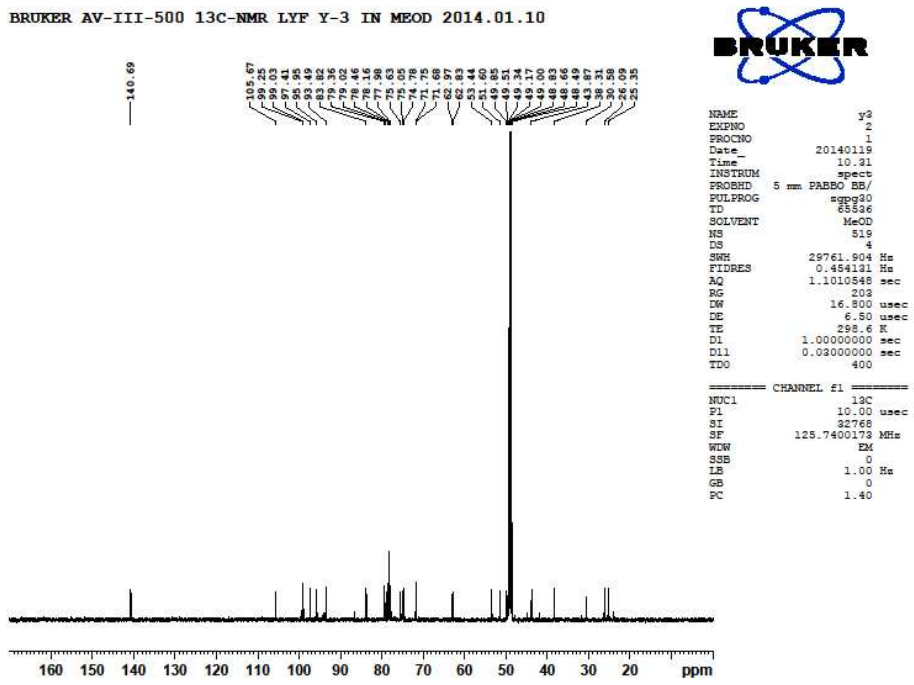
S63. CD Spectrum of compound **7** (CH_3OH)



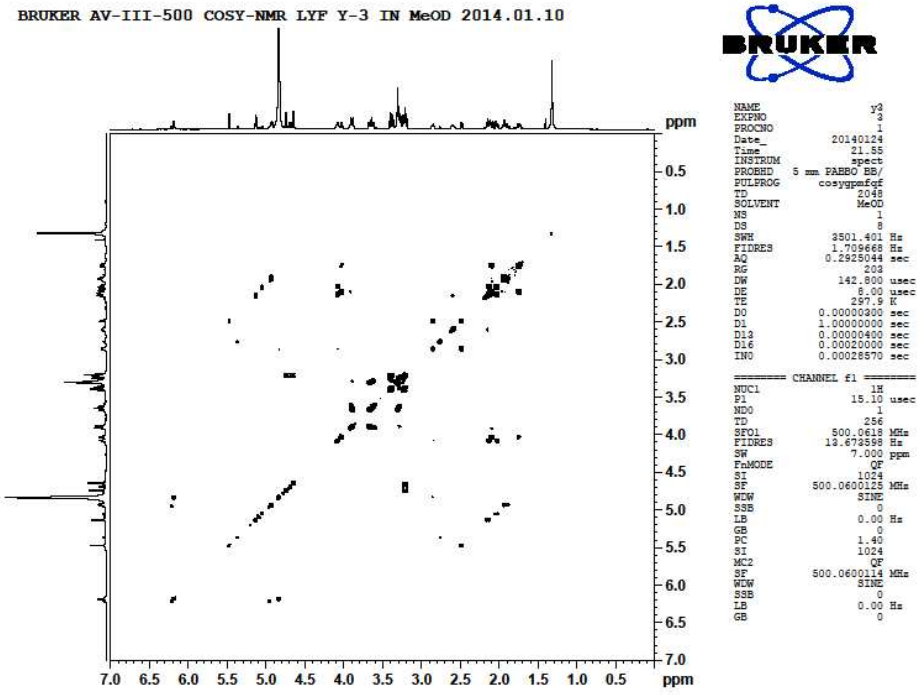
S64. IR Spectrum of compound **8**



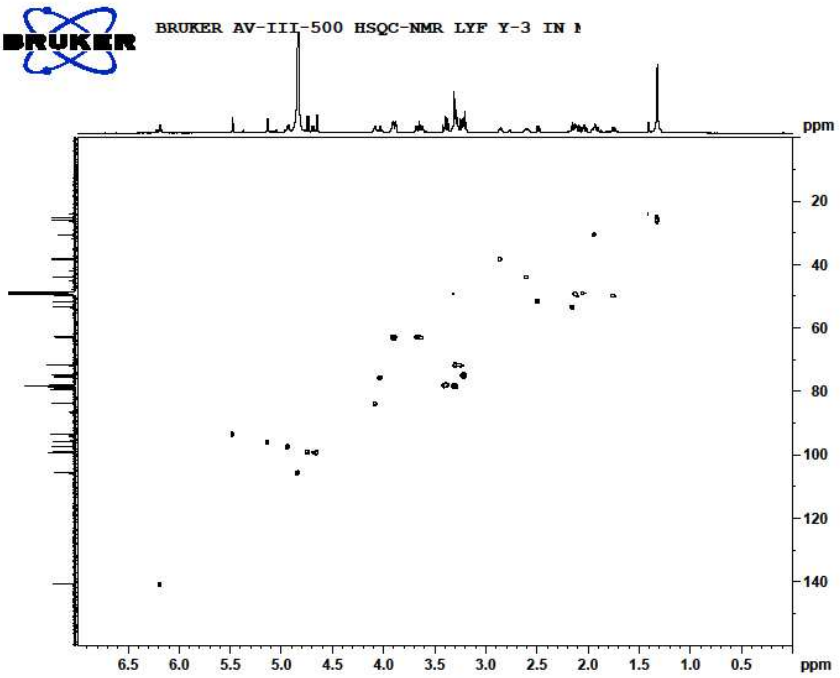
S65. ^{1}H NMR Spectrum of compound **8** (500MHz, Methanol-d_4)



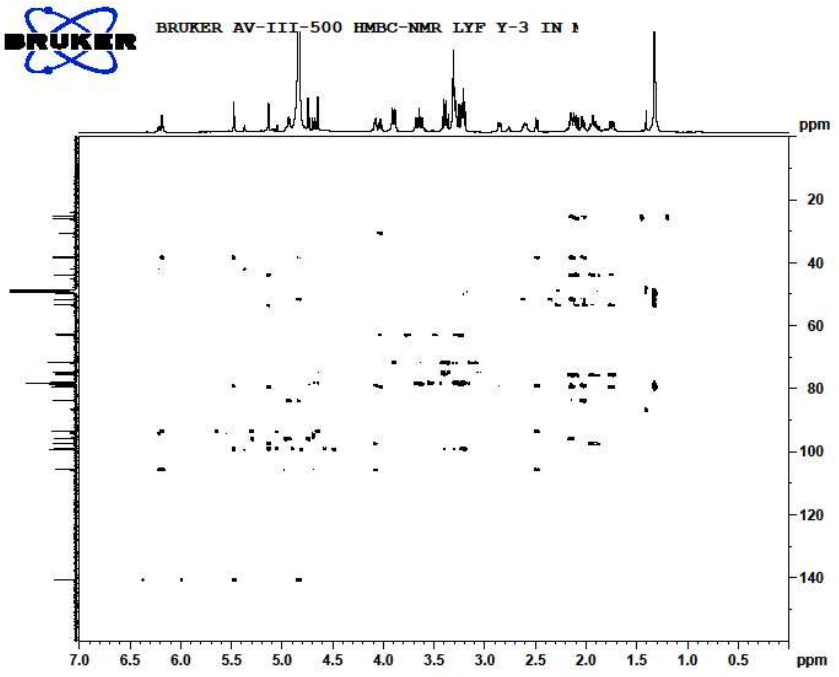
S66. ^{13}C NMR spectrum of compound **8** (125 MHz, Methanol-d_4)



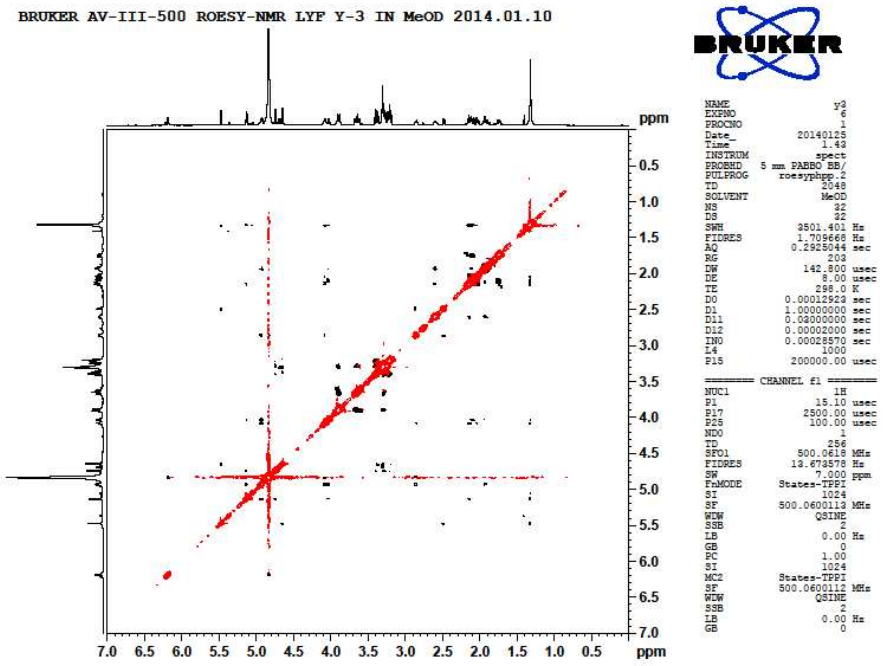
S67. ^{1}H–^{1}H COSY Spectrum of compound **8**



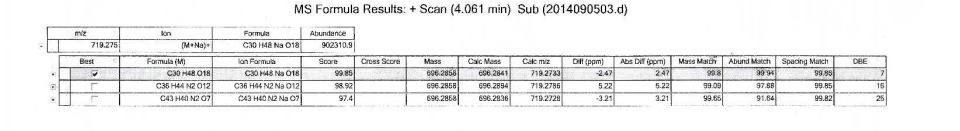
S68. HSQC Spectrum of compound **8**



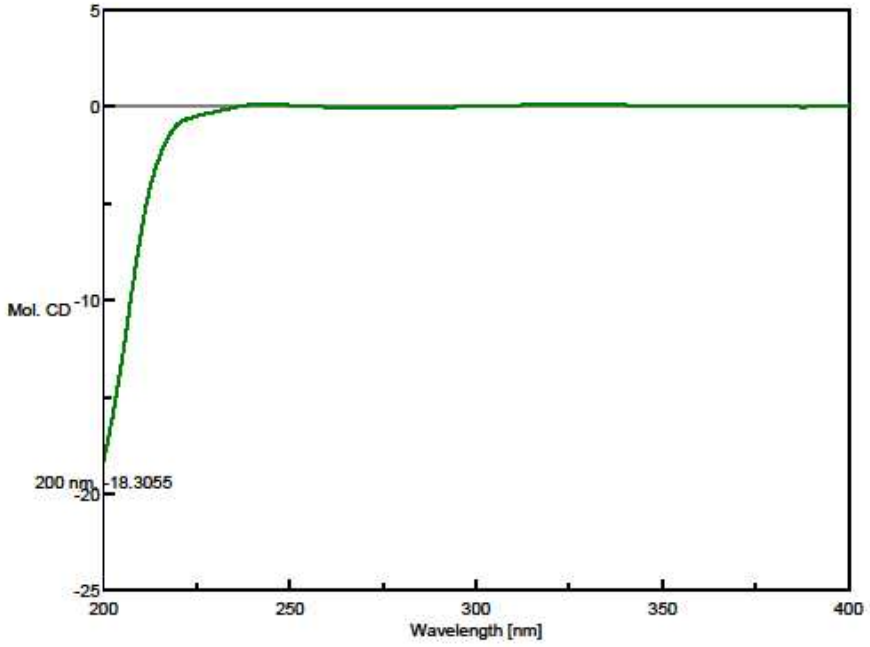
S69. HMBC Spectrum of compound **8**



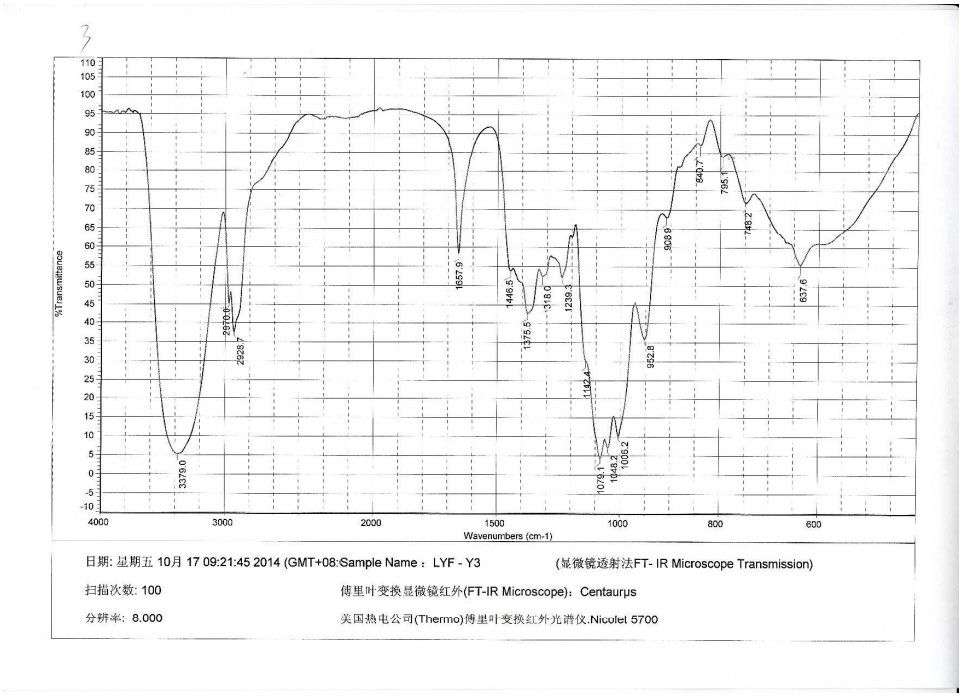
70. ROESY Spectrum of compound **8**



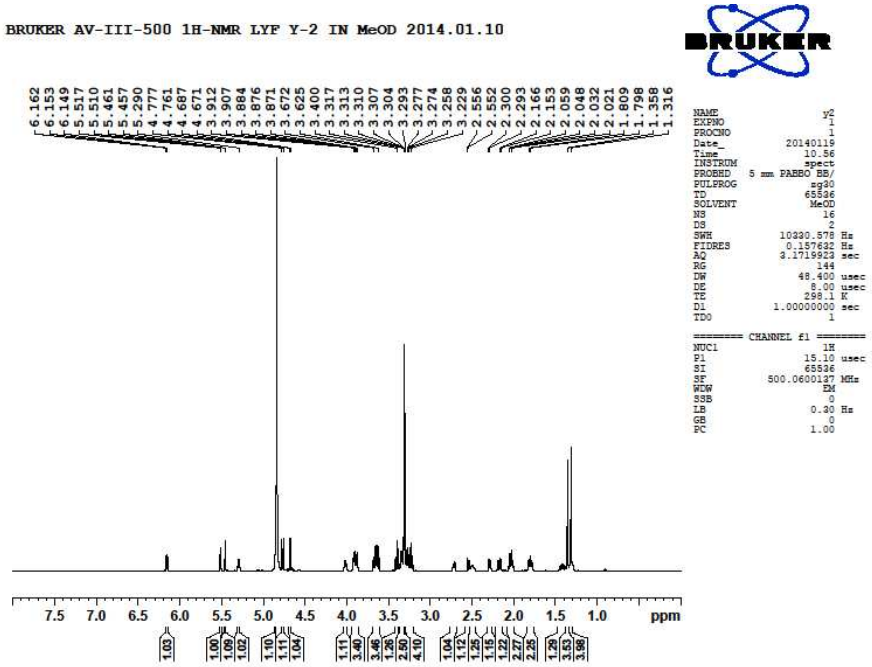
S71. HRESIMS Spectrum of compound **8**



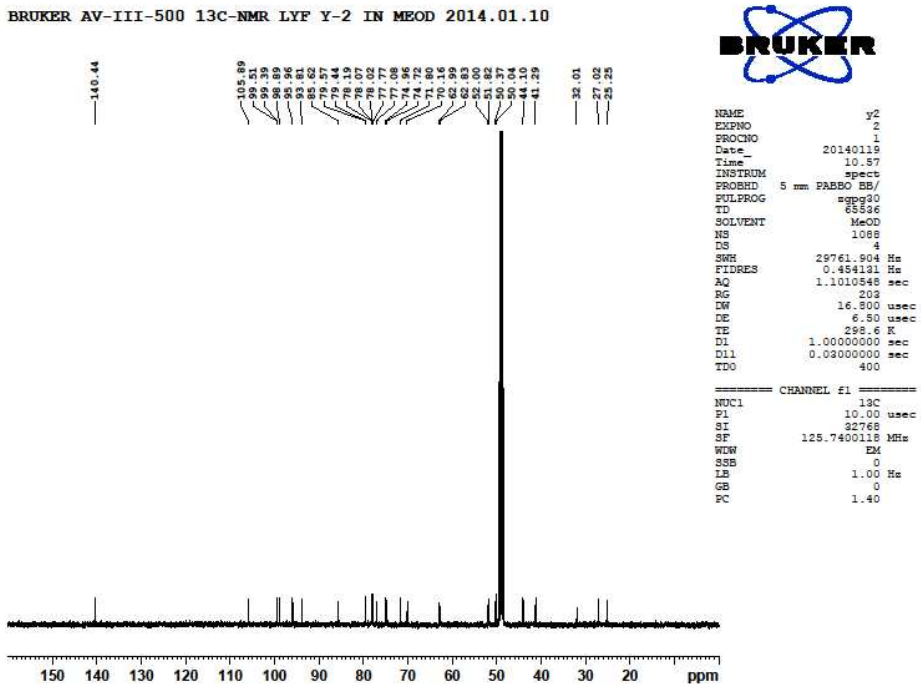
S72. CD Spectrum of compound **8** (CH_3OH)



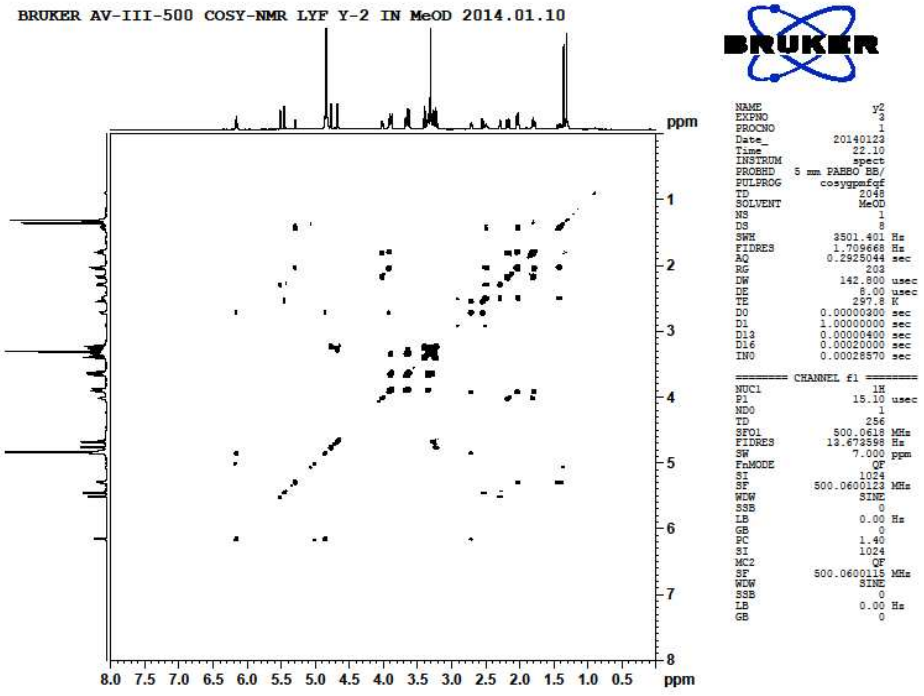
S73. IR Spectrum of compound **9**



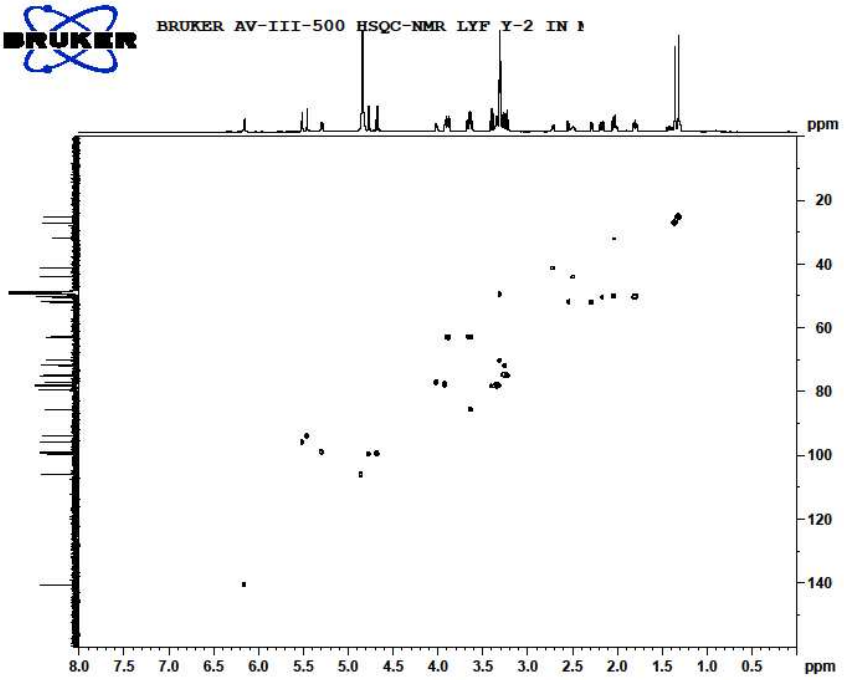
S74. ^{1}H NMR Spectrum of compound **9** (500MHz, Methanol-d_4)



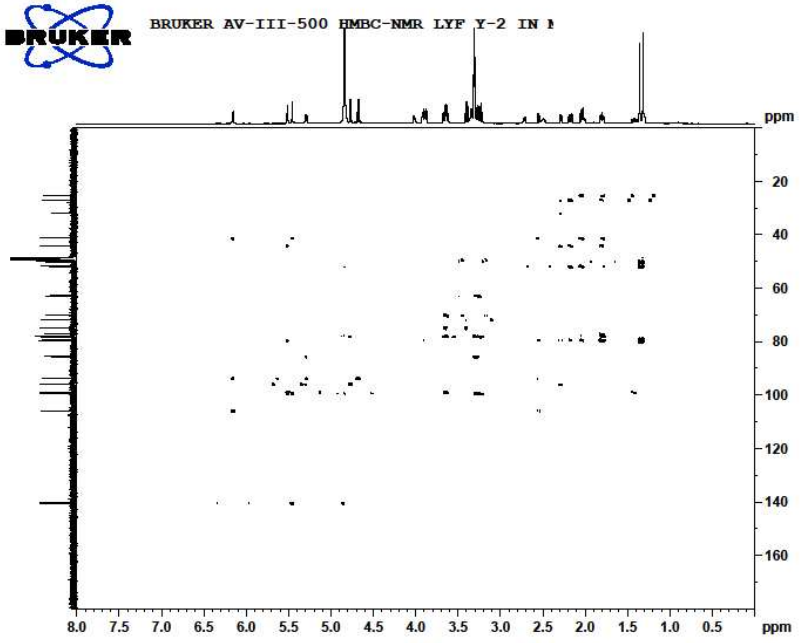
S75. ^{13}C NMR Spectrum of compound **9** (125 MHz, Methanol-d_4)



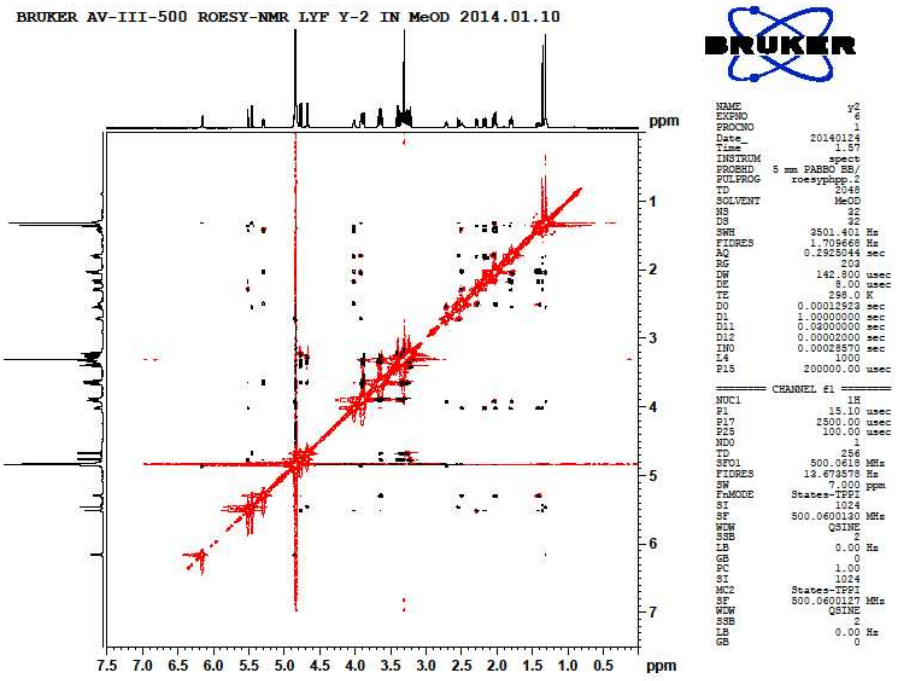
S76. ^{1}H–^{1}H COSY Spectrum of compound **9**



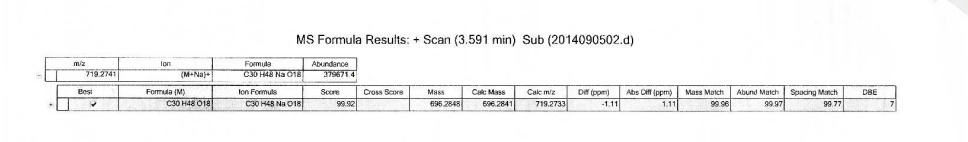
S77. HSQC Spectrum of compound **9**



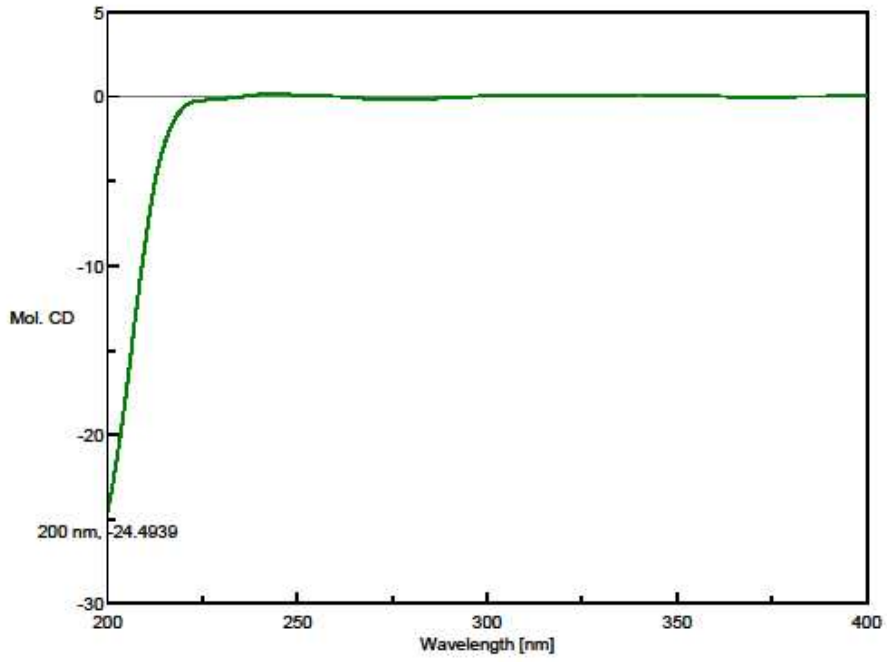
S78. HMBC Spectrum of compound **9**



S79. ROESY Spectrum of compound **9**



S80. HRESIMS Spectrum of compound **9**



S81. CD Spectrum of compound **9** (CH_3OH)