

**Spiromastixones A-O, Antibacterial Chlorodepsidones from a
Deep-Sea Derived *Spiromastix* sp. Fungus**

Supporting Information

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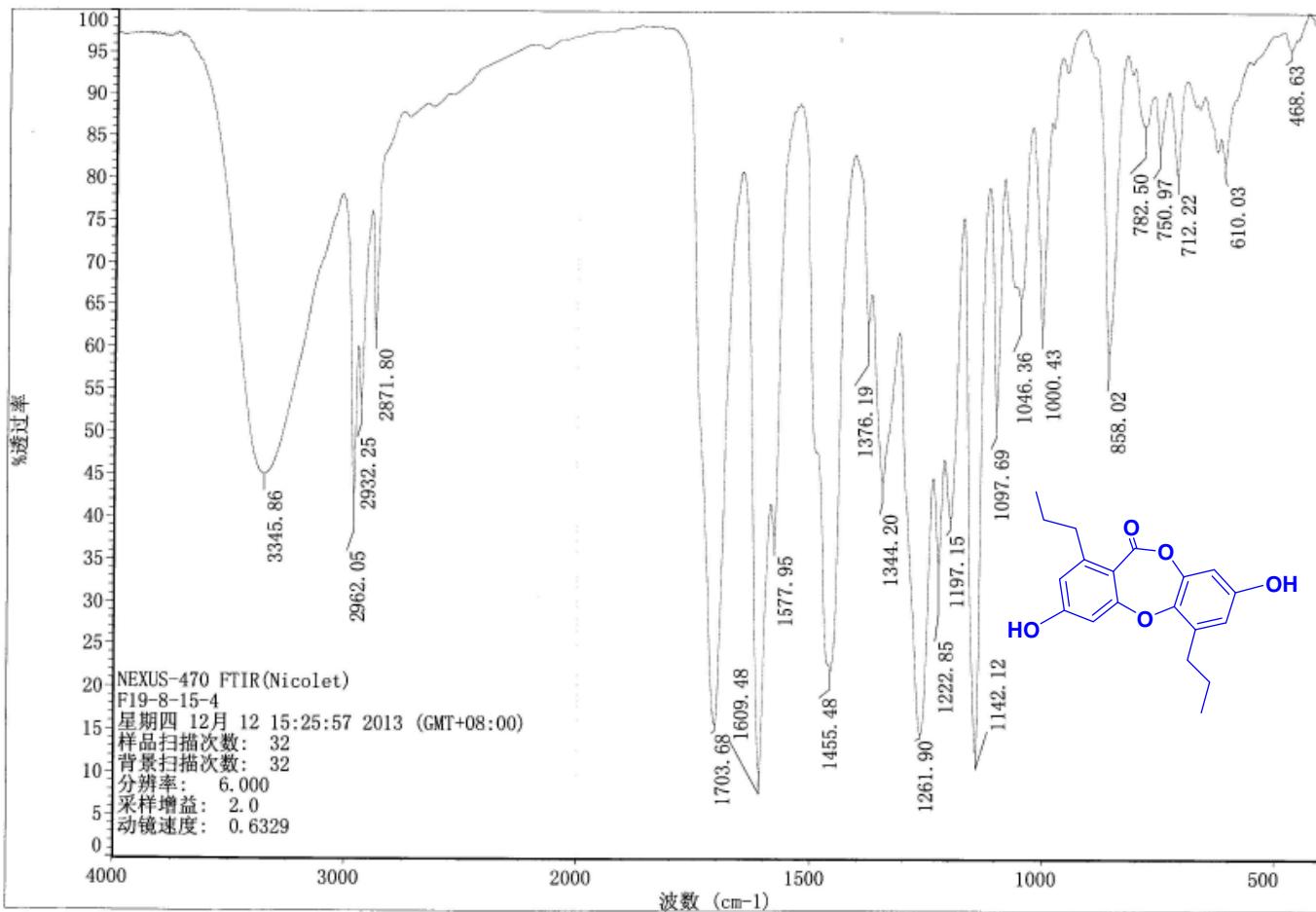


Figure S1. IR spectrum of **1**

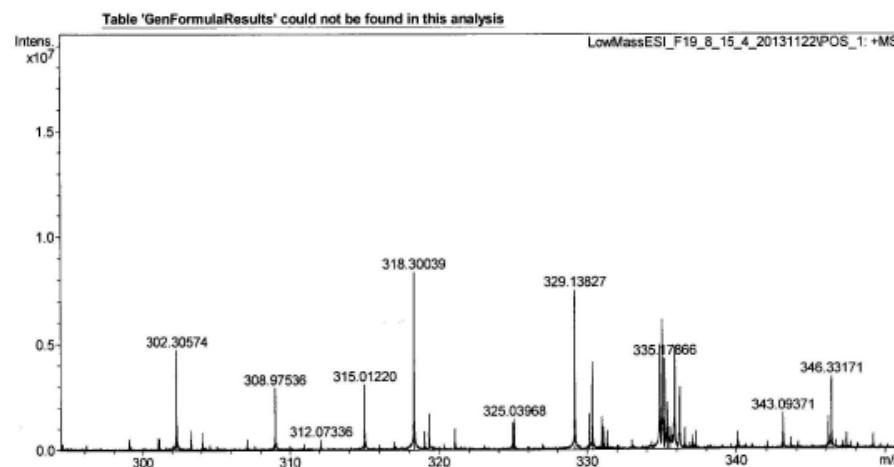
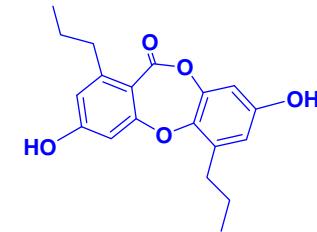


Figure S2. HRESIMS spectrum of **1**

F19-8-15-4 400 MHz DMSO

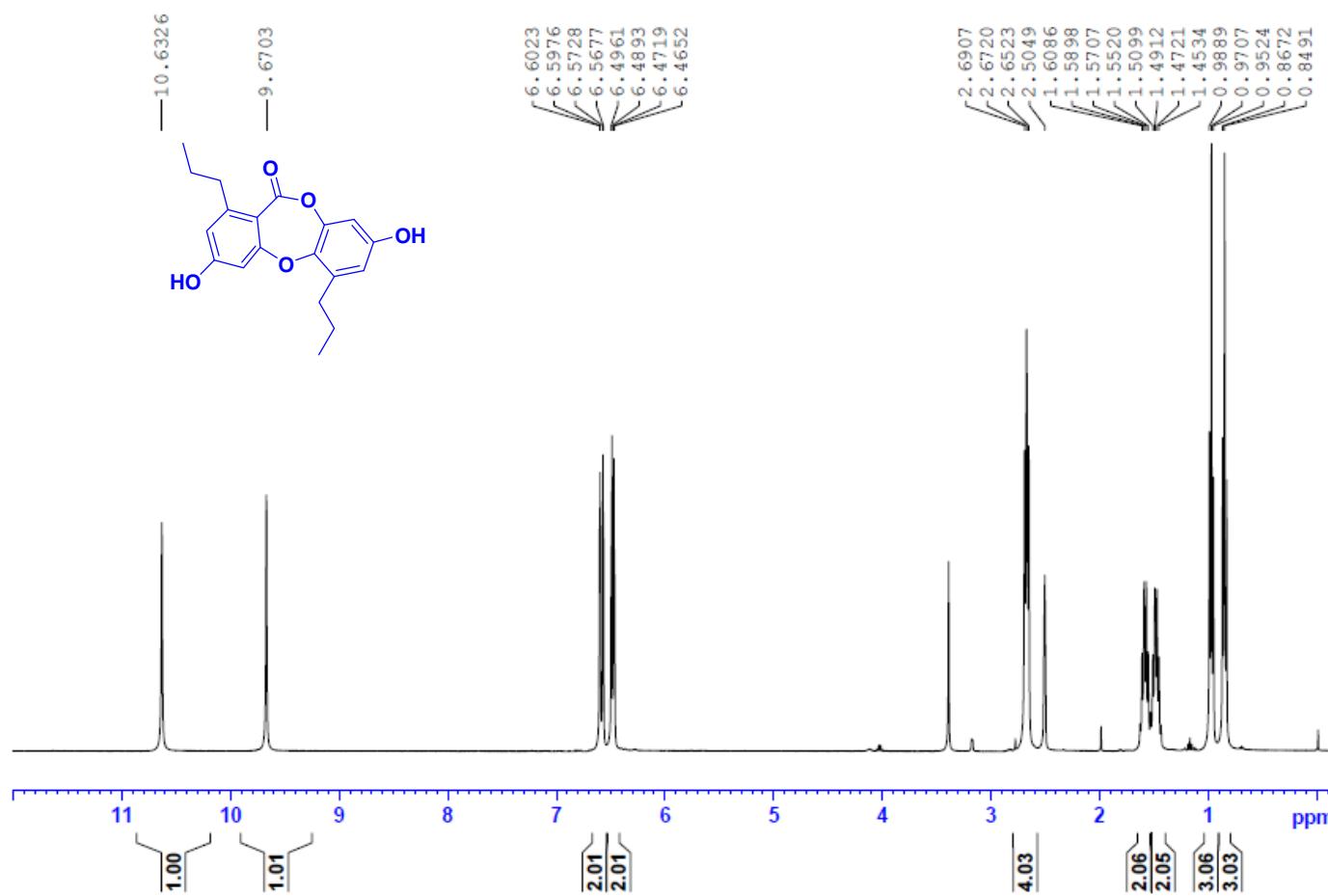


Figure S3. ^1H NMR spectrum of **1** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-15-4 APT

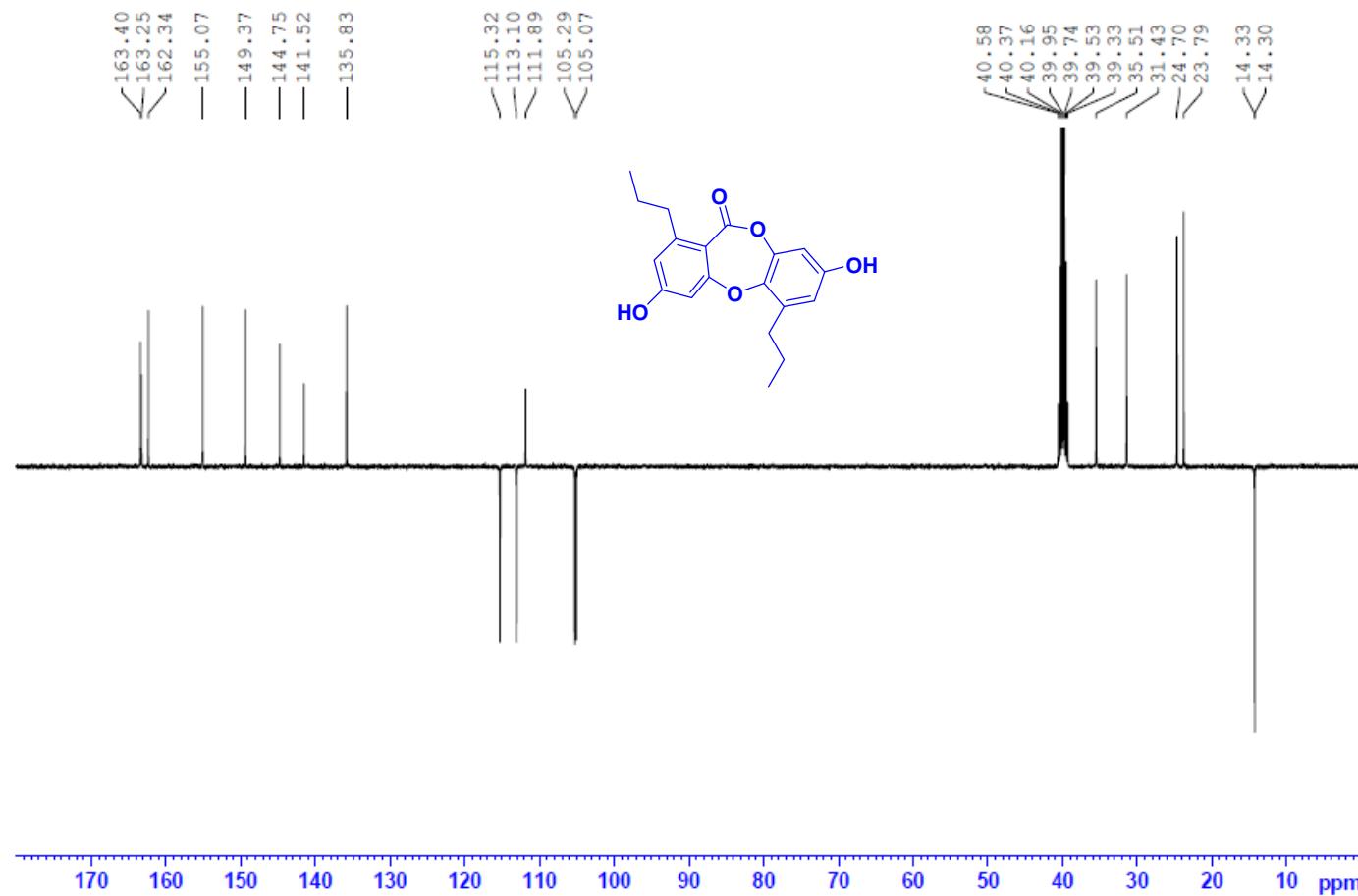


Figure S4. APT spectrum of **1** in $\text{DMSO}-d_6$ (100 MHz)

F19-8-15-4 HSQC

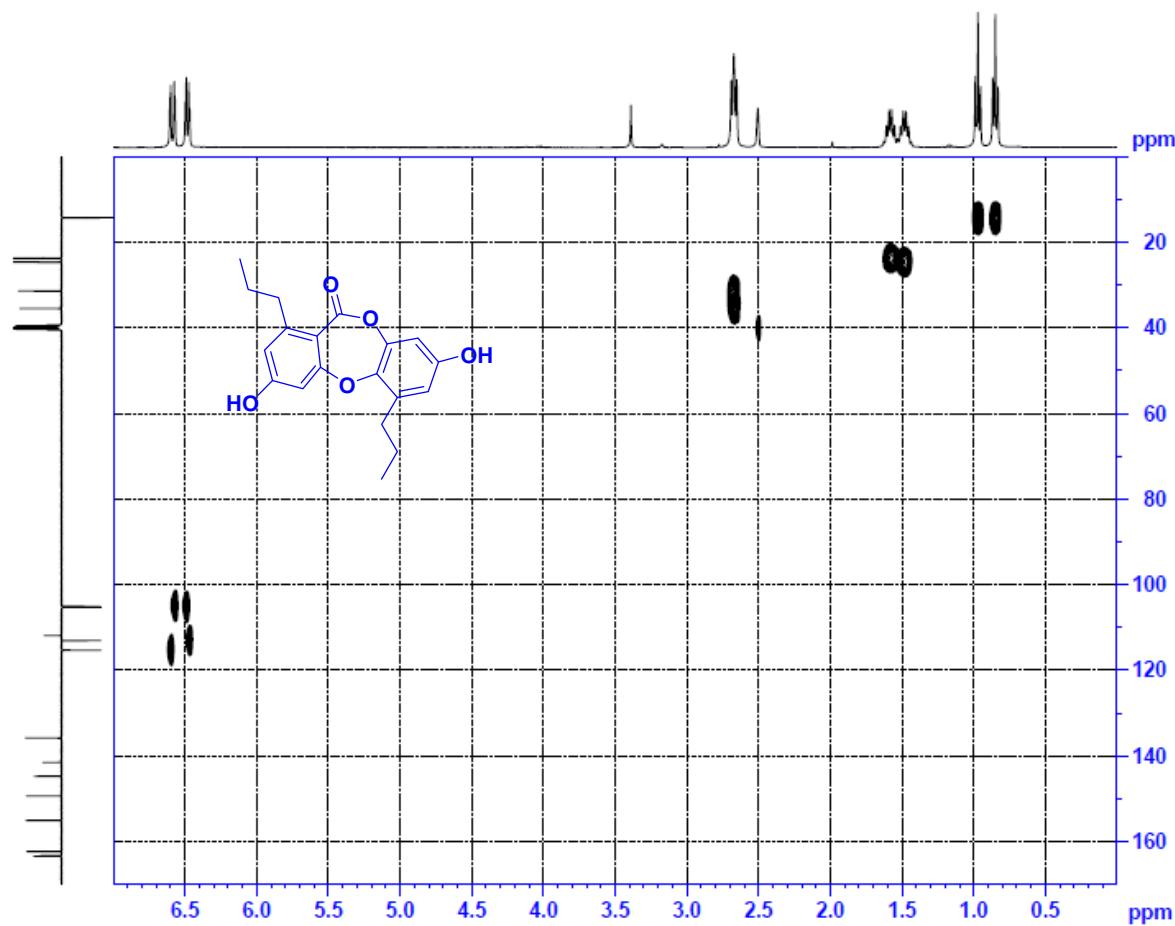


Figure S5. HSQC spectrum of **1** in DMSO-*d*₆ (400 MHz)

F19-8-15-4 COSY

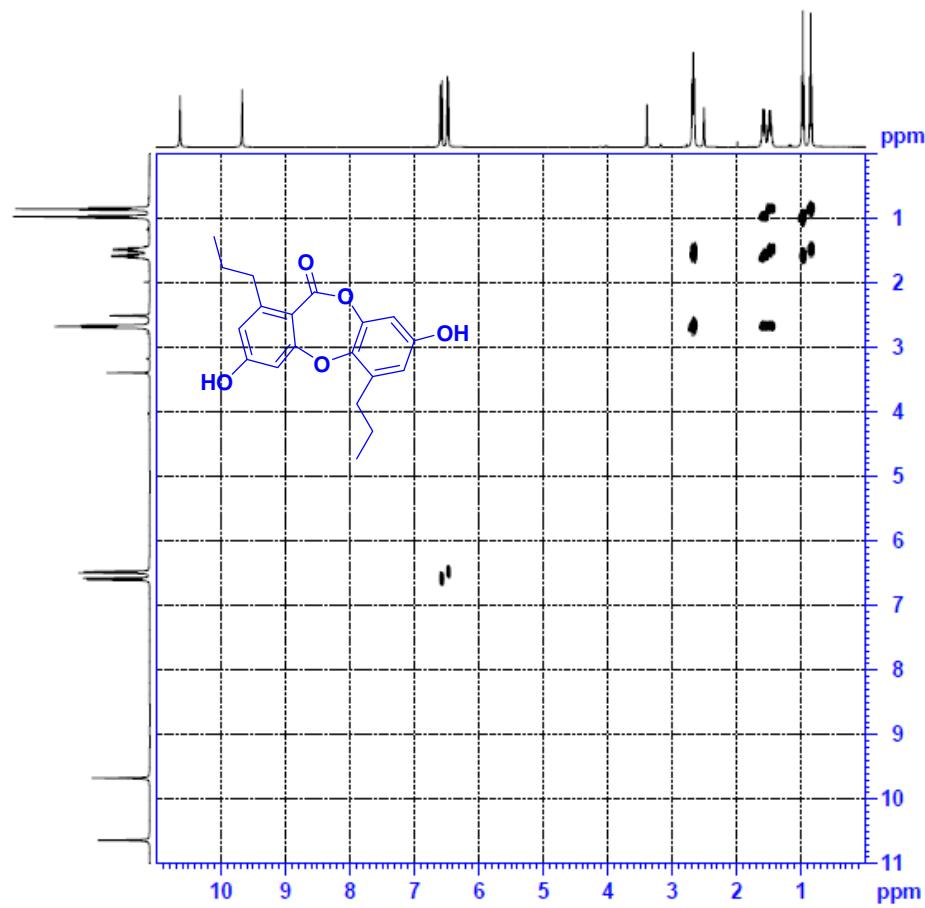


Figure S6. ^1H - ^1H COSY spectrum of **1** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-15-4 HMBC

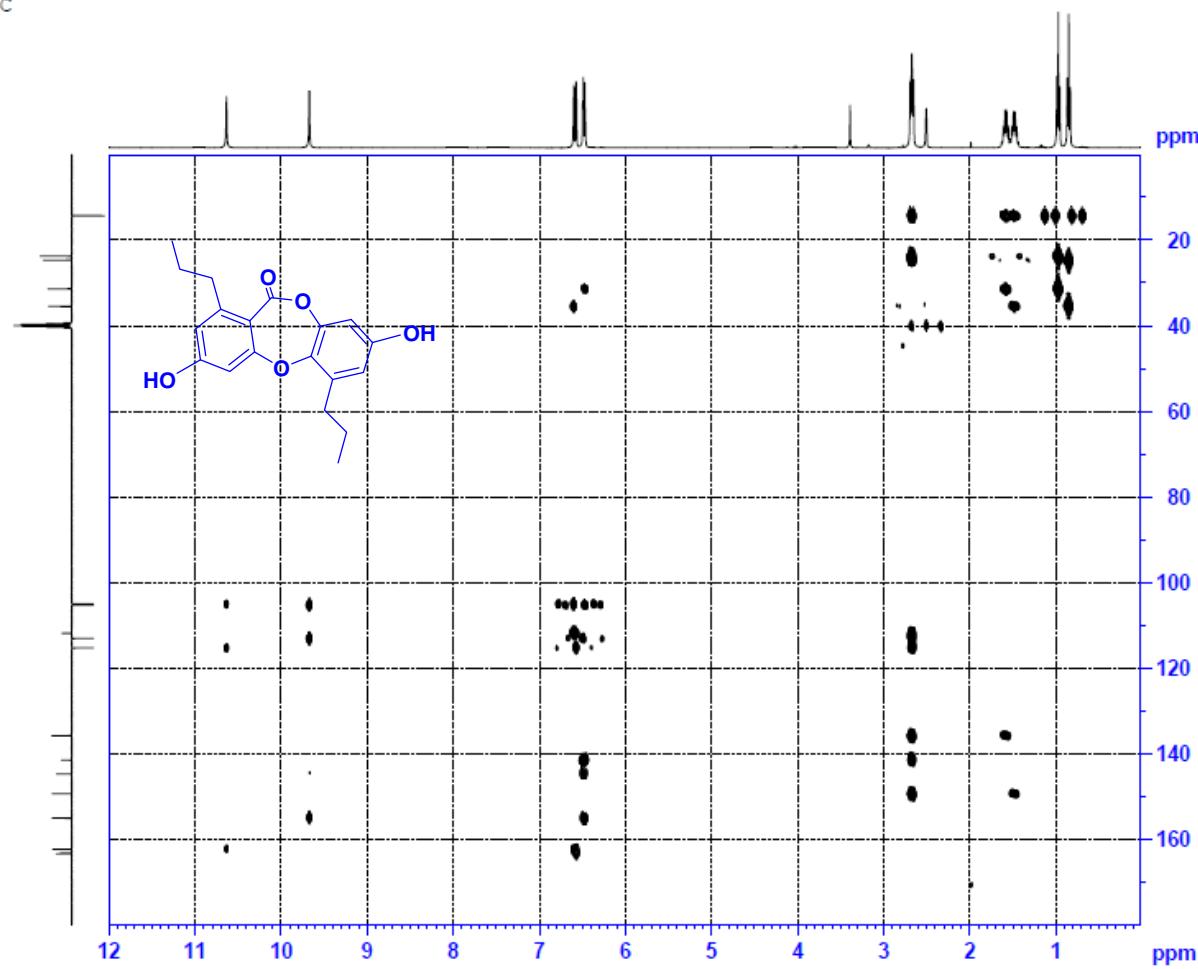


Figure S7. HMBC spectrum of **1** in $\text{DMSO}-d_6$ (400 MHz)

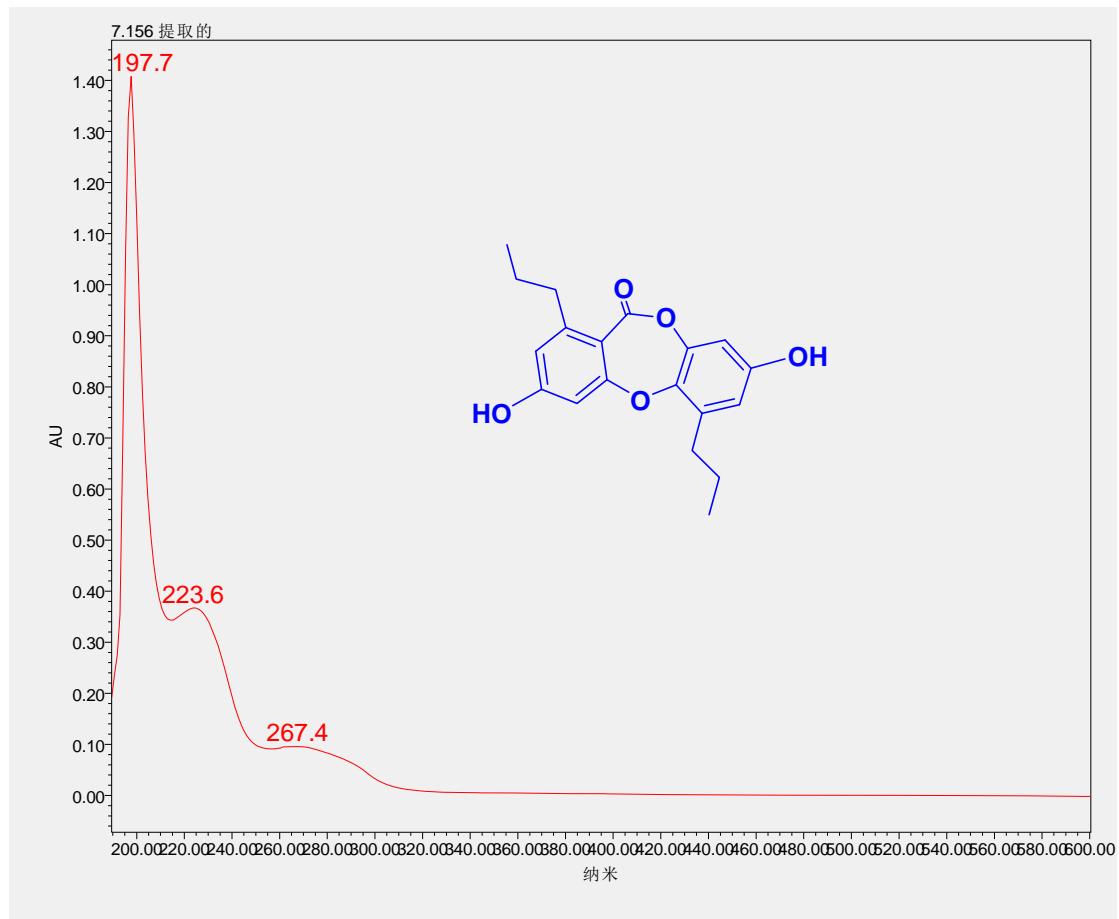


Figure S8. UV spectrum of **1** in MeOH

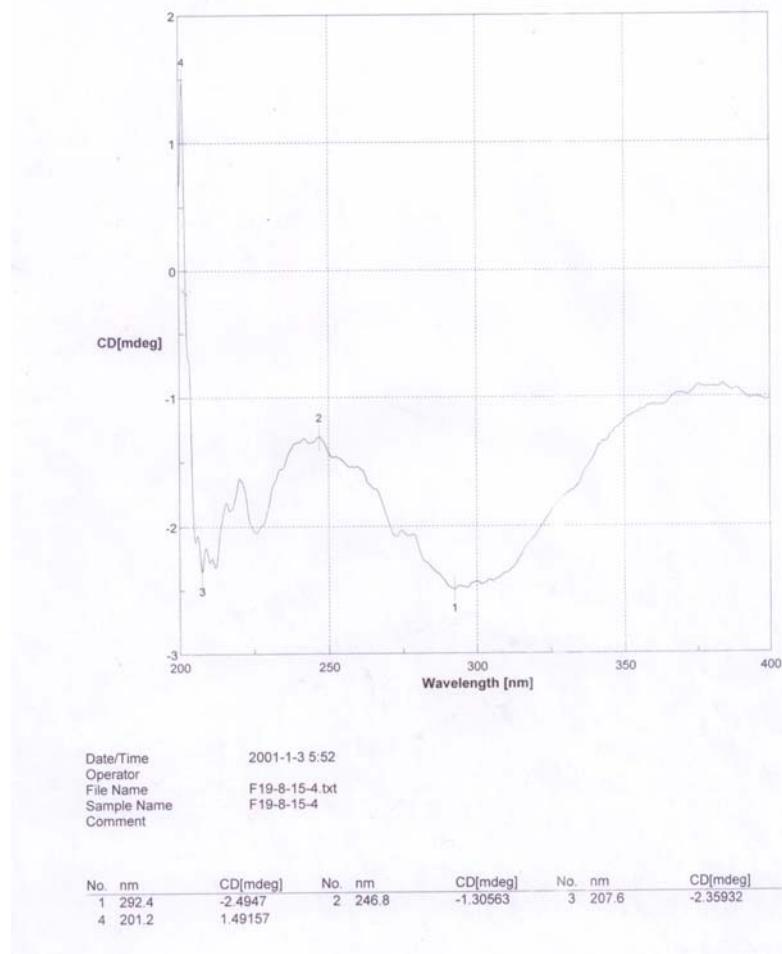


Figure S9. CD spectrum of **1** in MeOH

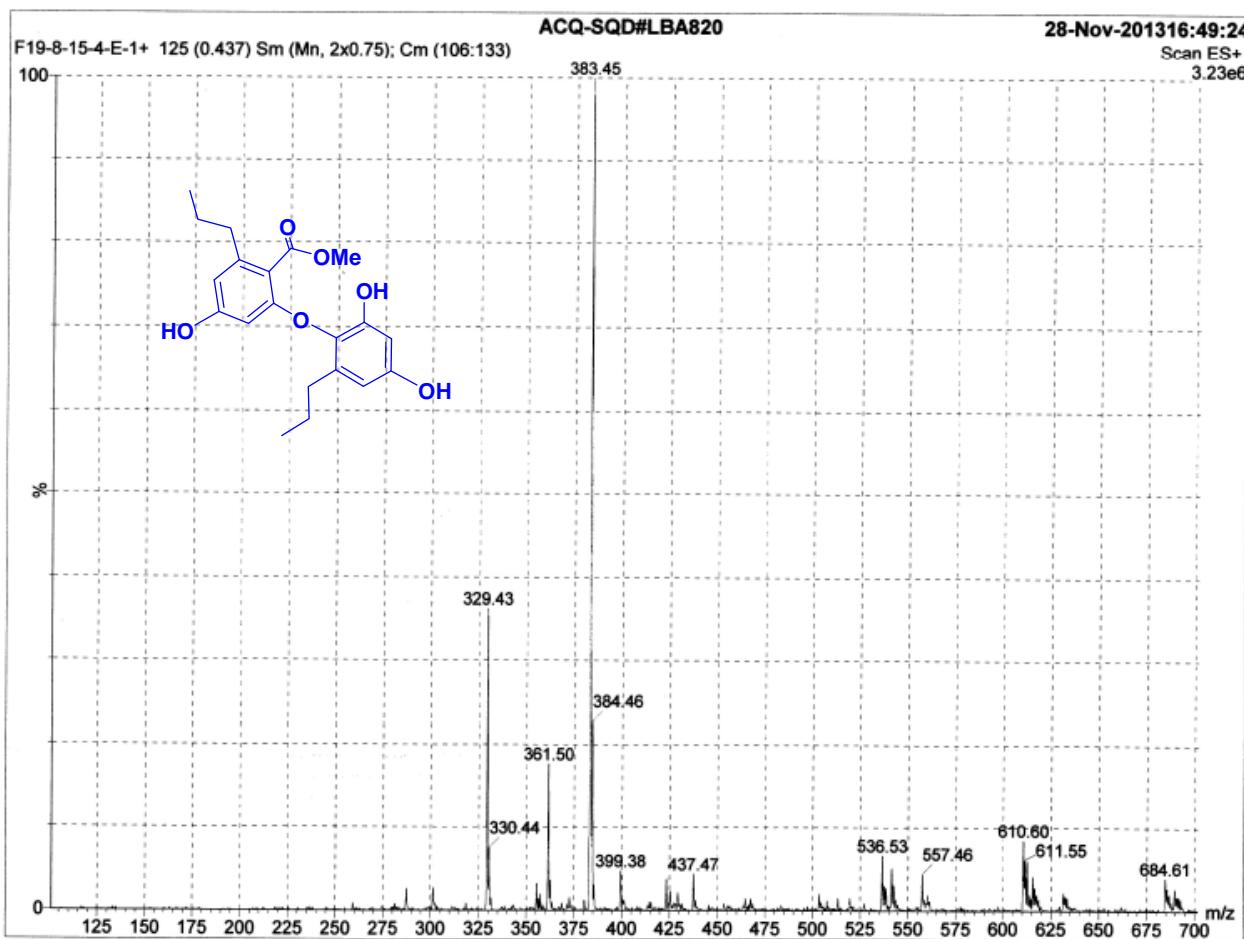


Figure S10. ESIMS spectrum of **1a**

F19-8-15-4-e 400 MHz DMSO

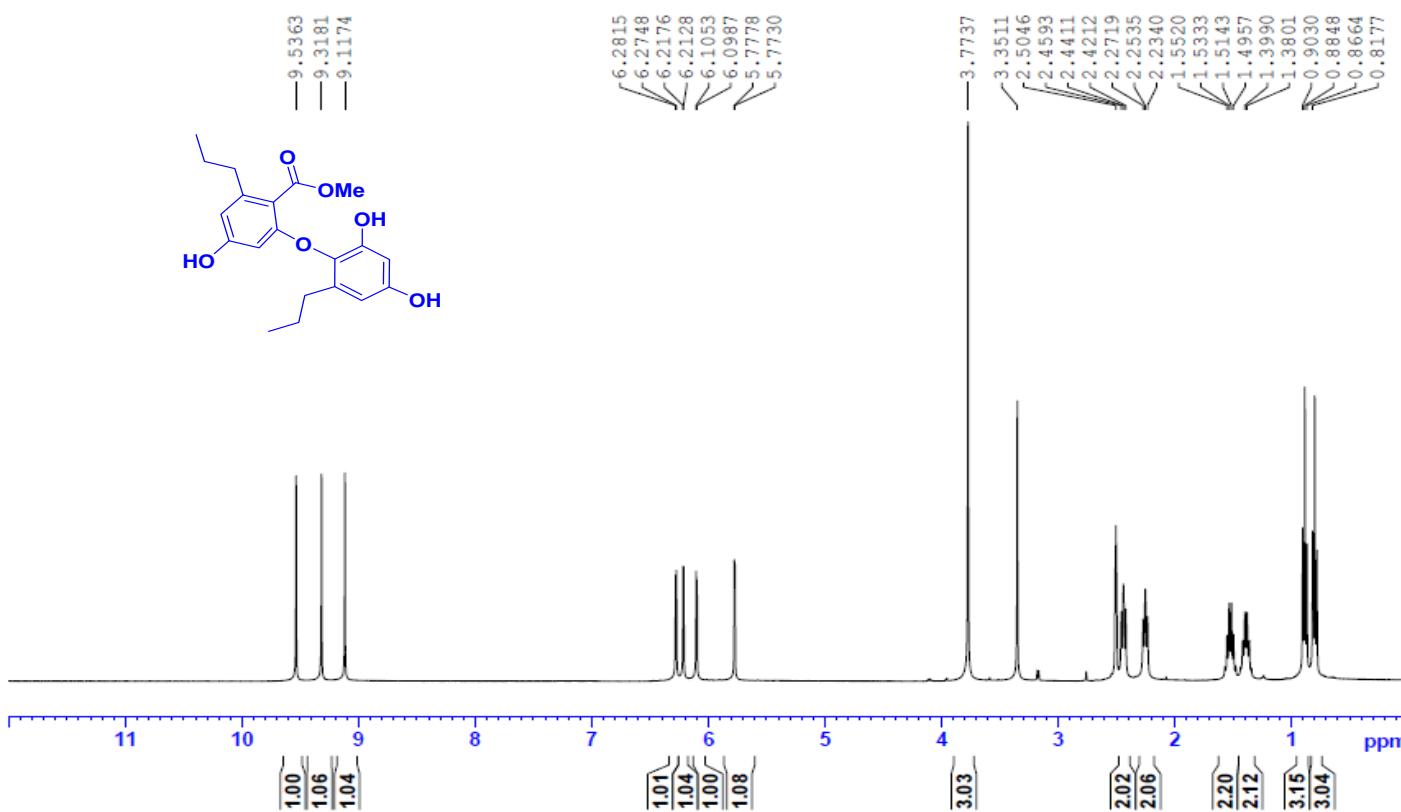


Figure S11. ^1H NMR spectrum of **1a** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-5-4-e APT

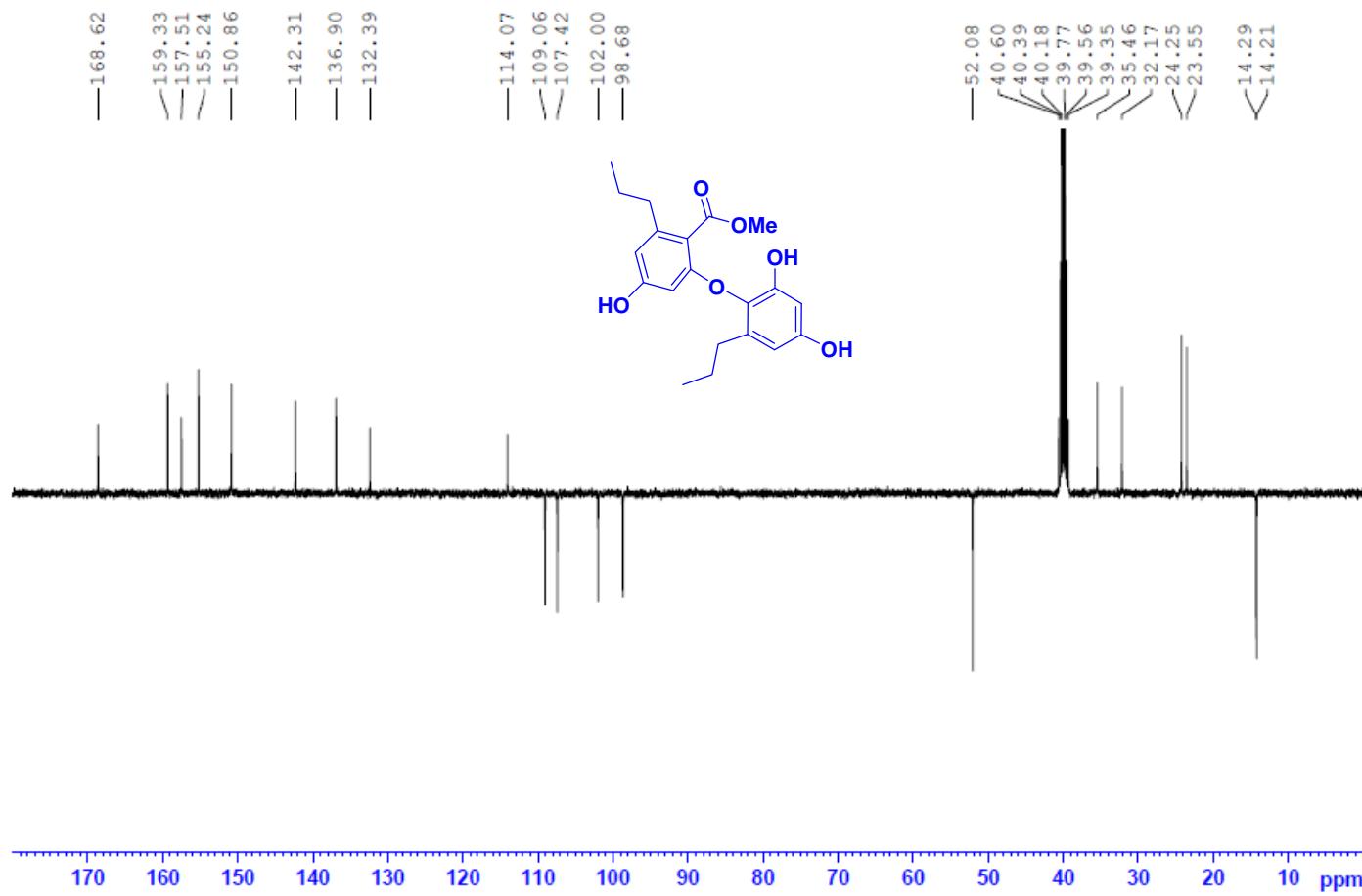


Figure S12. APT spectrum of **1a** in DMSO-*d*₆(100 MHz)

F19-8-15-4-e HSQC

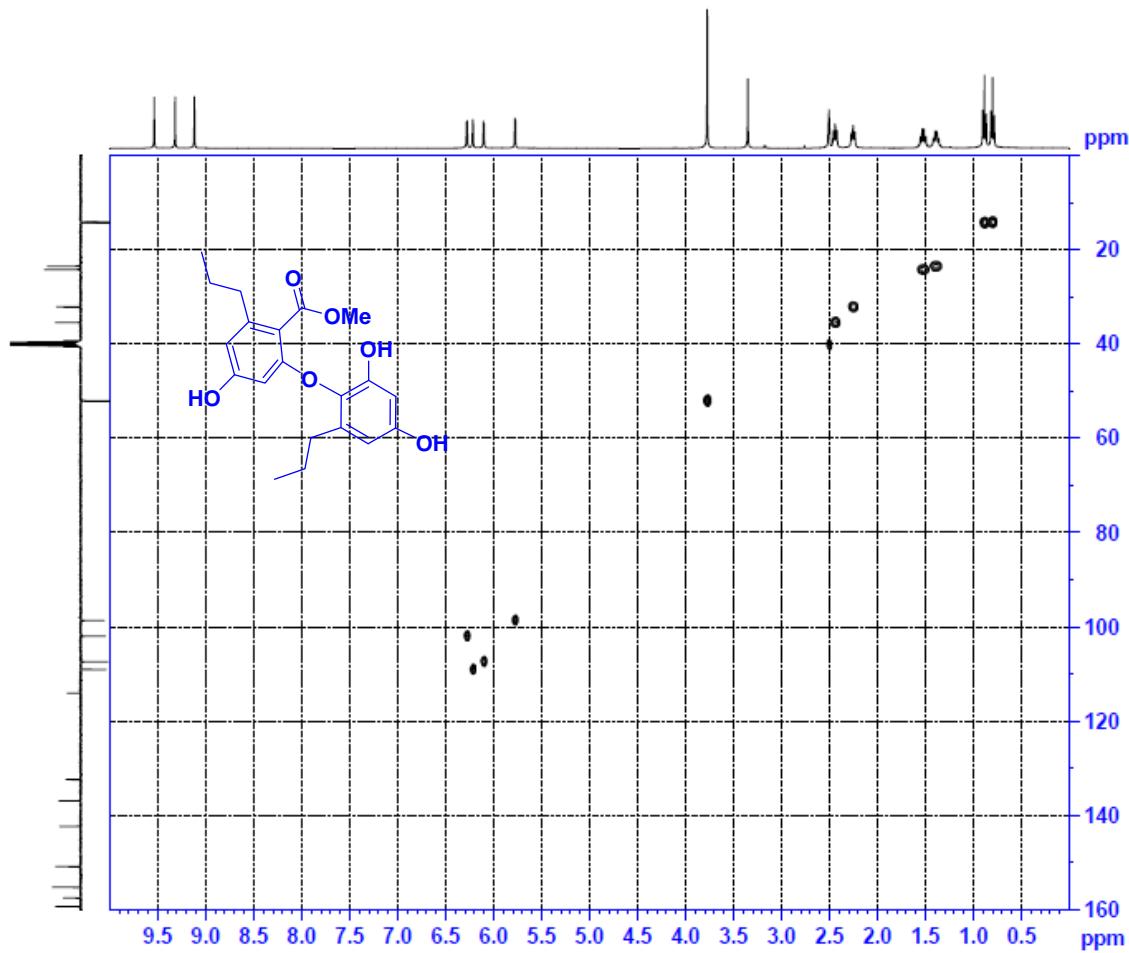


Figure S13. HSQC spectrum of **1a** in $\text{DMSO}-d_6$ (400 MHz for ^1H)

F19-8-15-4-e COSY

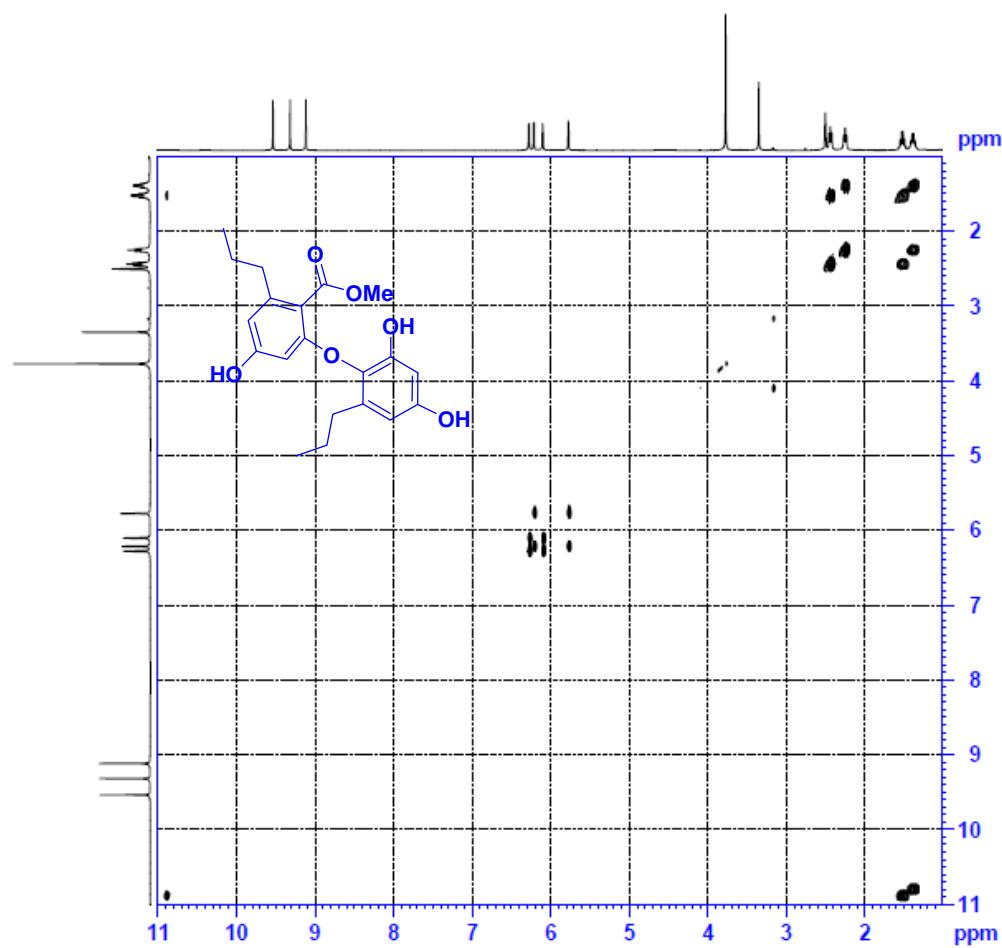


Figure S14. ^1H - ^1H COSY spectrum of **1a** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-15-4-e HMBC

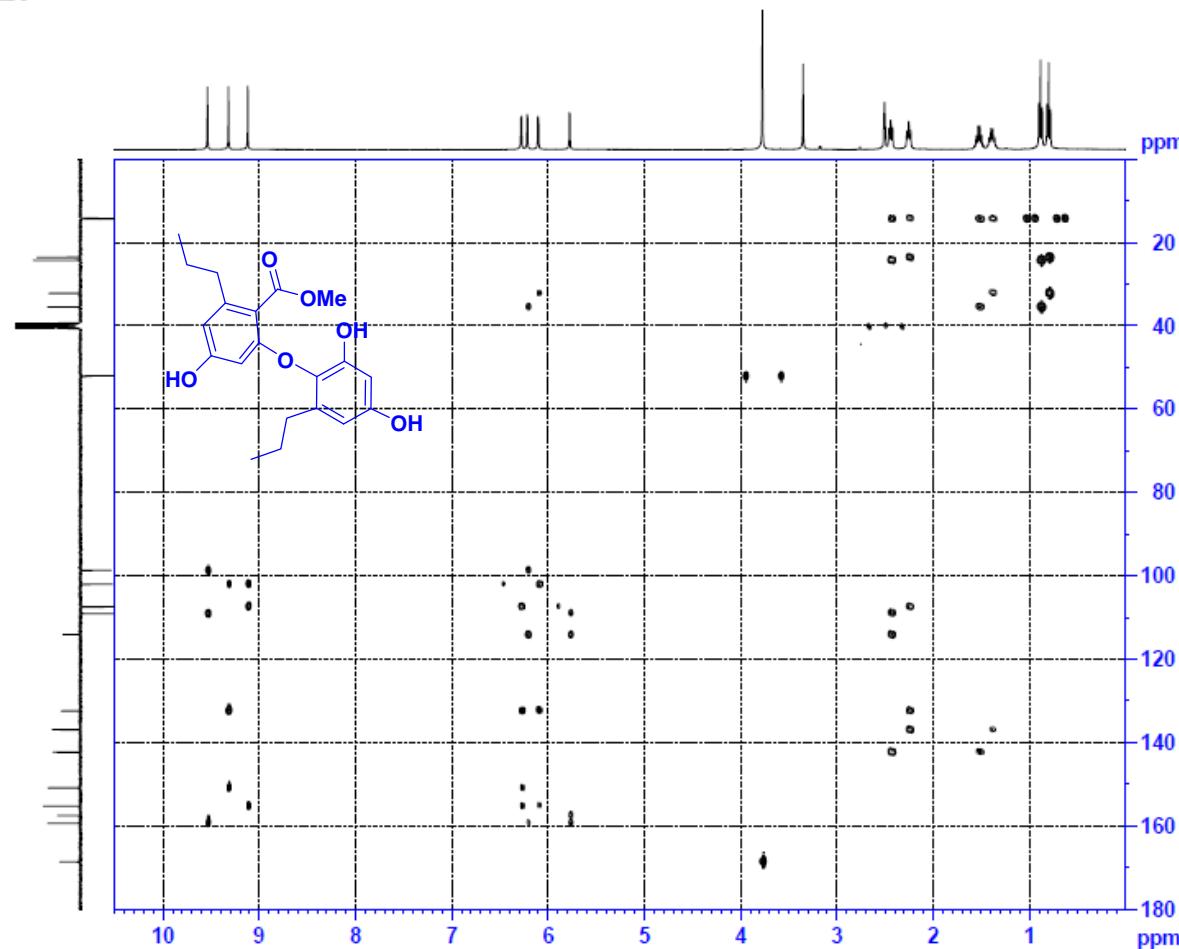


Figure S15. HMBC spectrum of **1a** in DMSO-*d*₆ (400 MHz for ¹H)

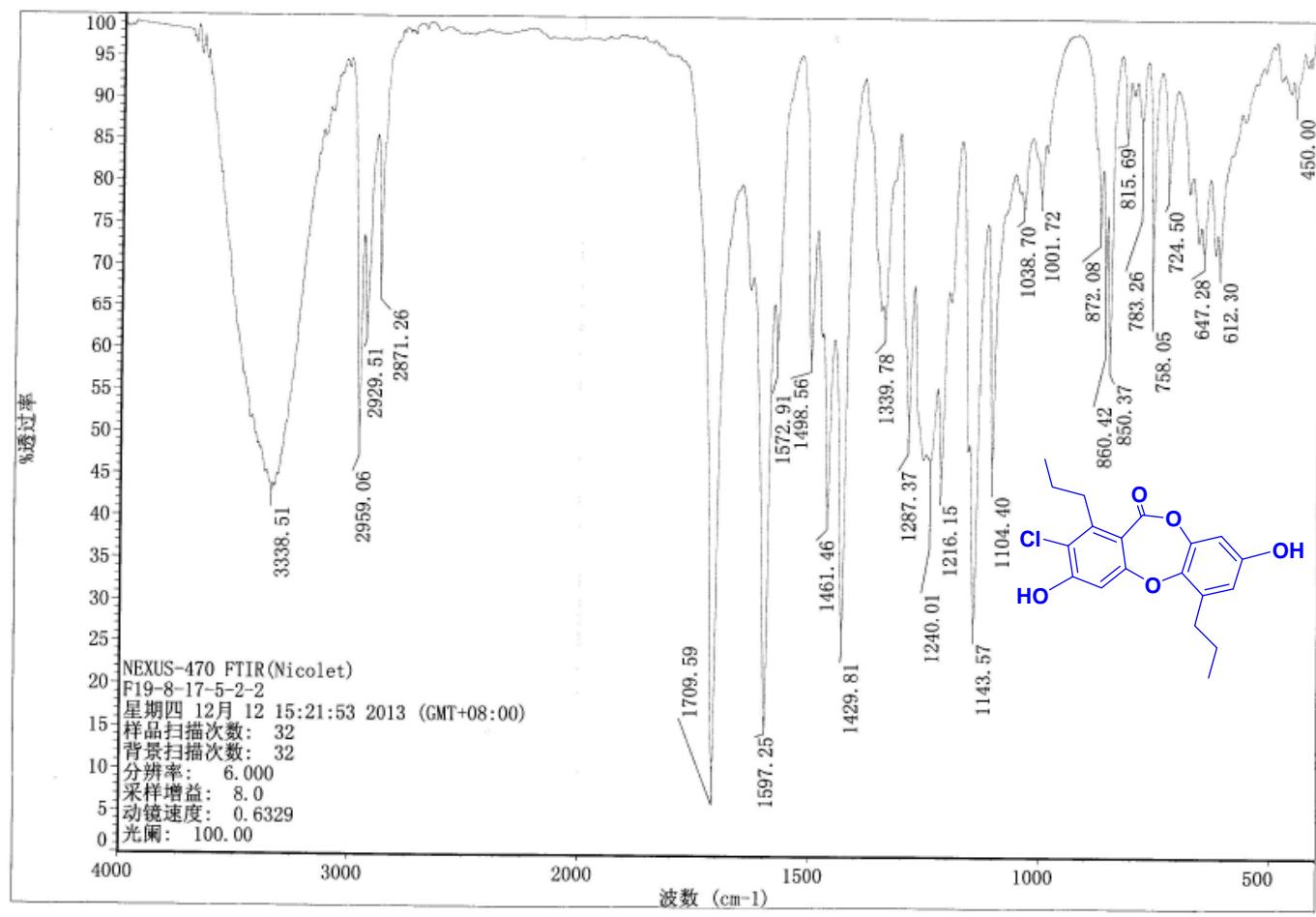


Figure S16. IR spectrum of 2



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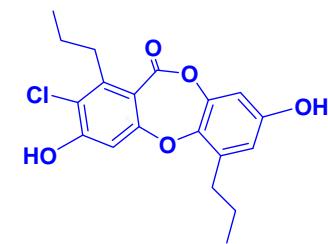
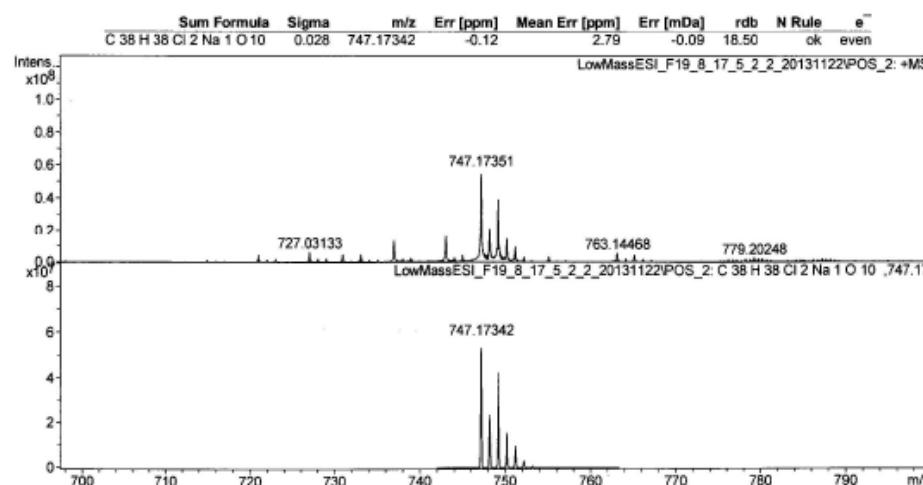
Analysis Name C:\data_sample\ESI_12131120_30\LowMassESI_F19_8_17_5_2_2_20131122\POS_2 Acquisition Date 11/22/2013 9:36:44 AM

Operator bpxsh@bjmu.edu.cn; Tel:010-82801

Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI □ C19H19O5Cl1 MW 362.09
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;826.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result Exact Mass Measured Mass Error (mDa) Error (ppm) Description





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Analysis Name C:\data_sample\ESI_12131120_30\LowMassESI_F19_8_17_5_2_2_20131122\POS_2 Acquisition Date 11/22/2013 9:36:44 AM
Operator bpxsh@bjmu.edu.cn; Tel:010-82801
Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI □ C19H19O5CL1 MW 362.09
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;8.26.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result	Exact Mass	Measured Mass	Error (mDa)	Error (ppm)	Description
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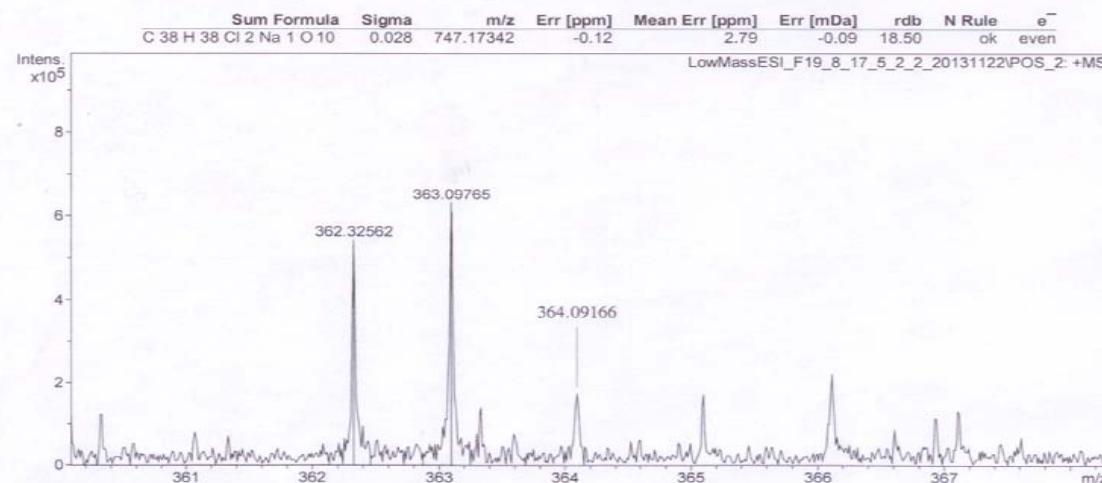


Figure S17. HRESIMS spectrum of 2

F19-8-17-5-2-2 400 MHz DMSO

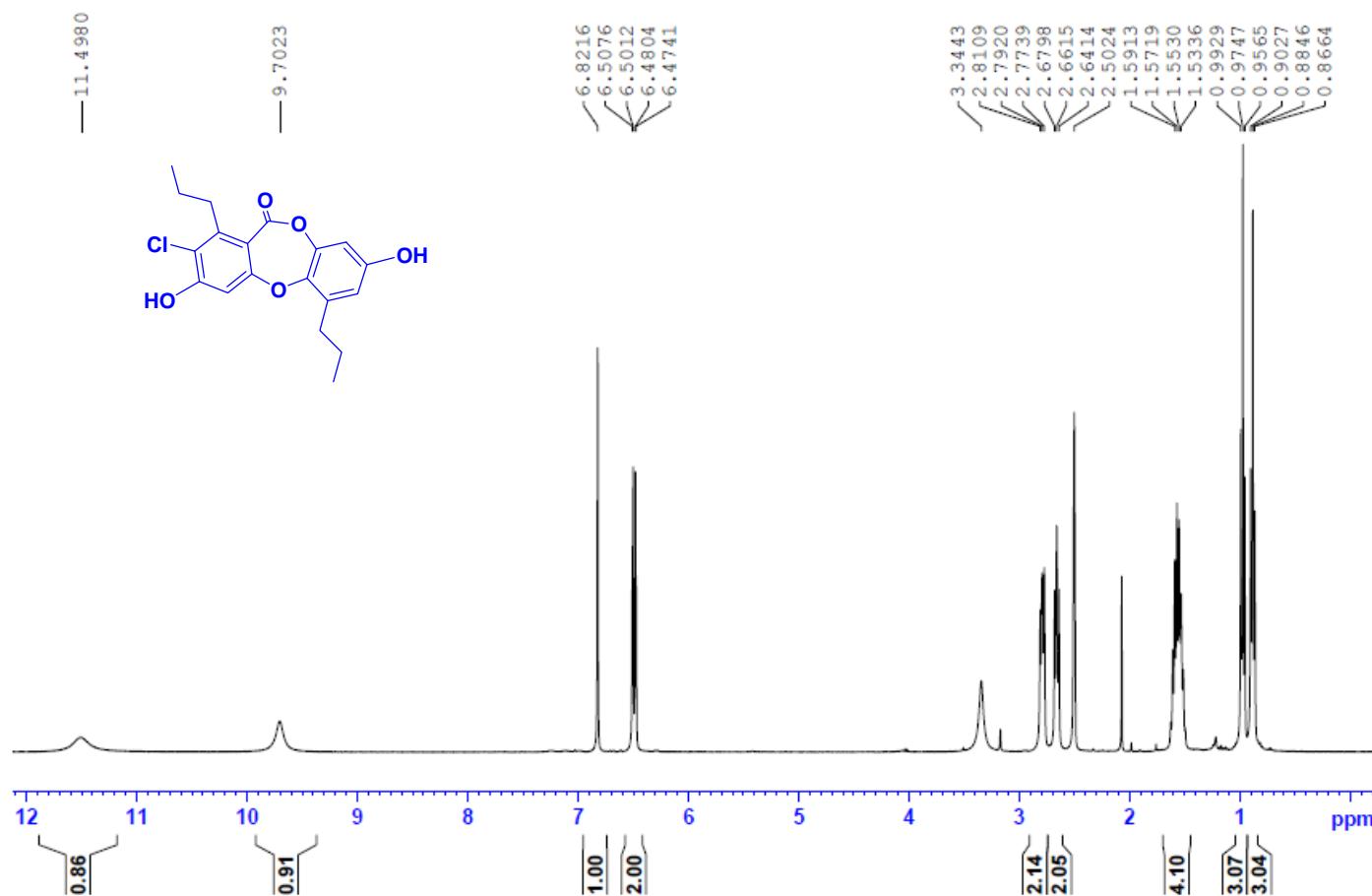


Figure S18. ^1H NMR spectrum of **2** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-17-5-2-2 APT

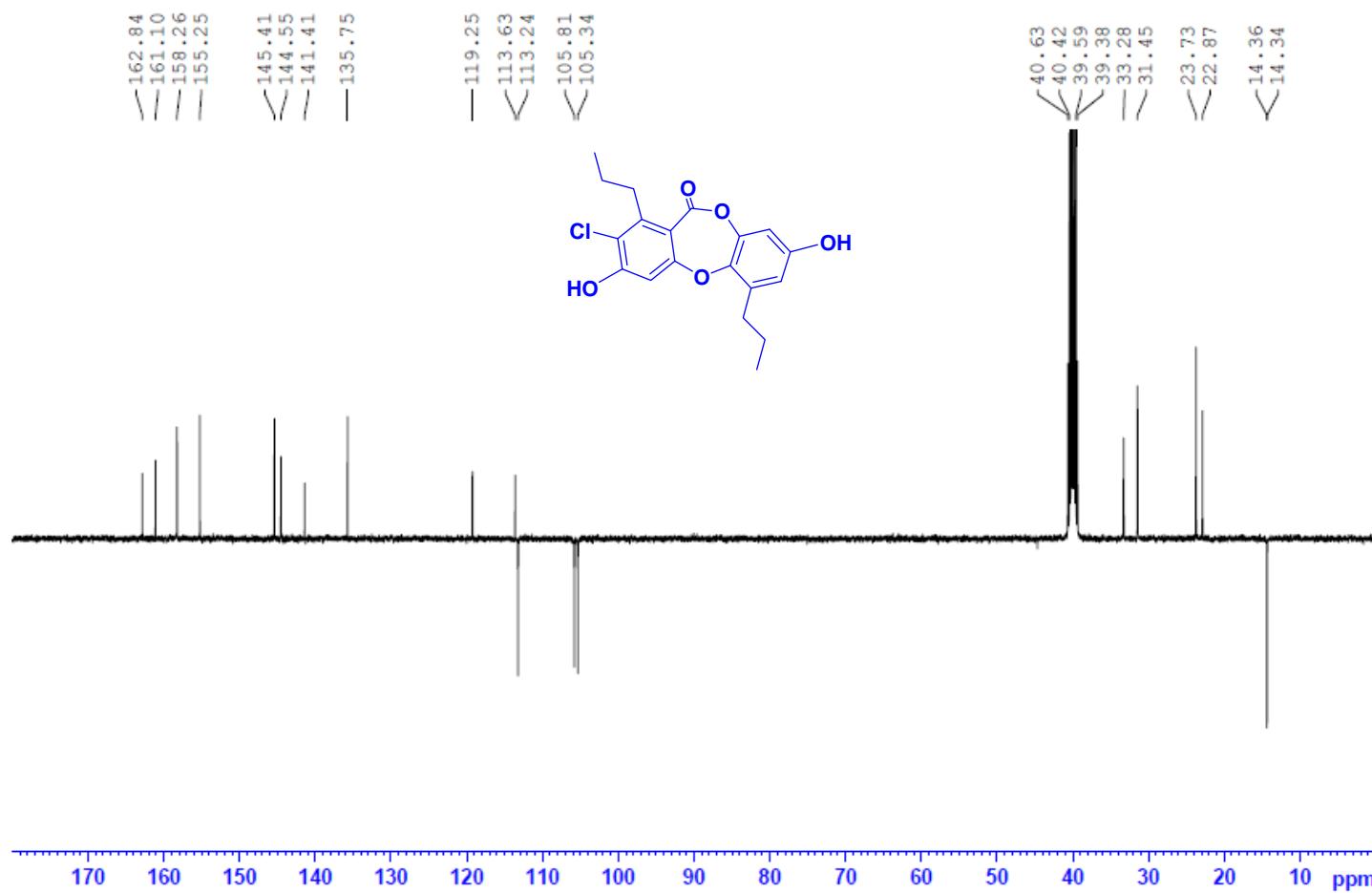


Figure S19. APT spectrum of **2** in DMSO-*d*₆ (100 MHz)

F19-8-17-5-2-2 HSQC

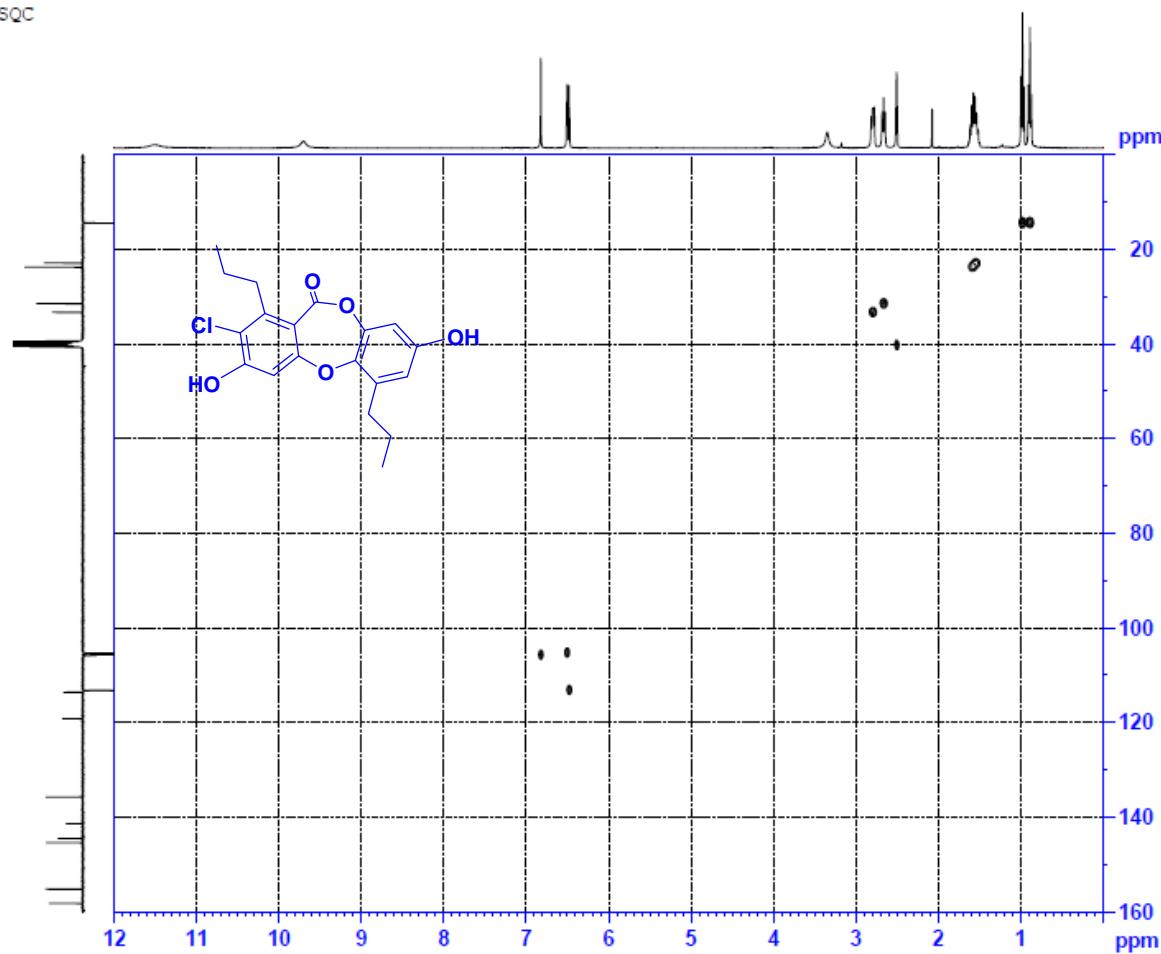


Figure S20. HSQC spectrum of **2** in $\text{DMSO}-d_6$ (400 MHz for ^1H)

F19-8-17-5-2-2 COSY

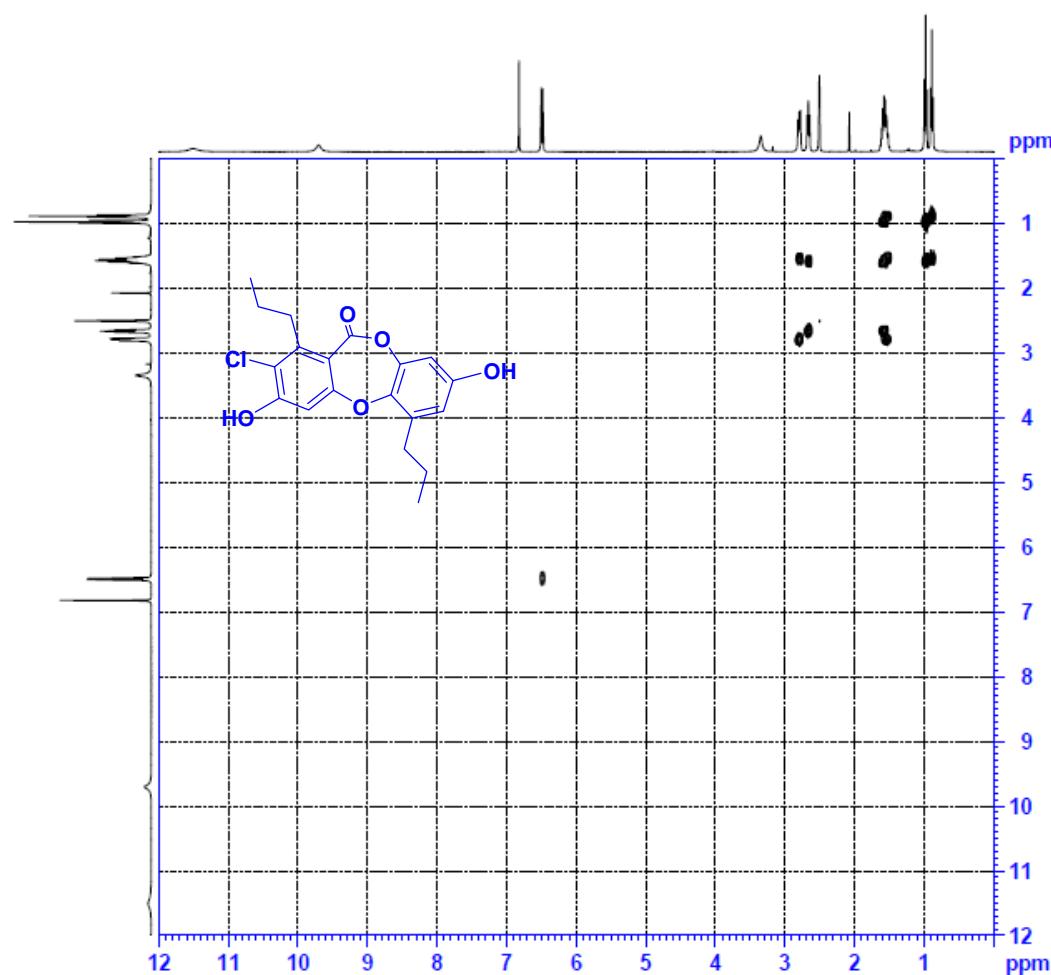


Figure S21. ^1H - ^1H COSY spectrum of **2** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-17-5-2-2 HMBC

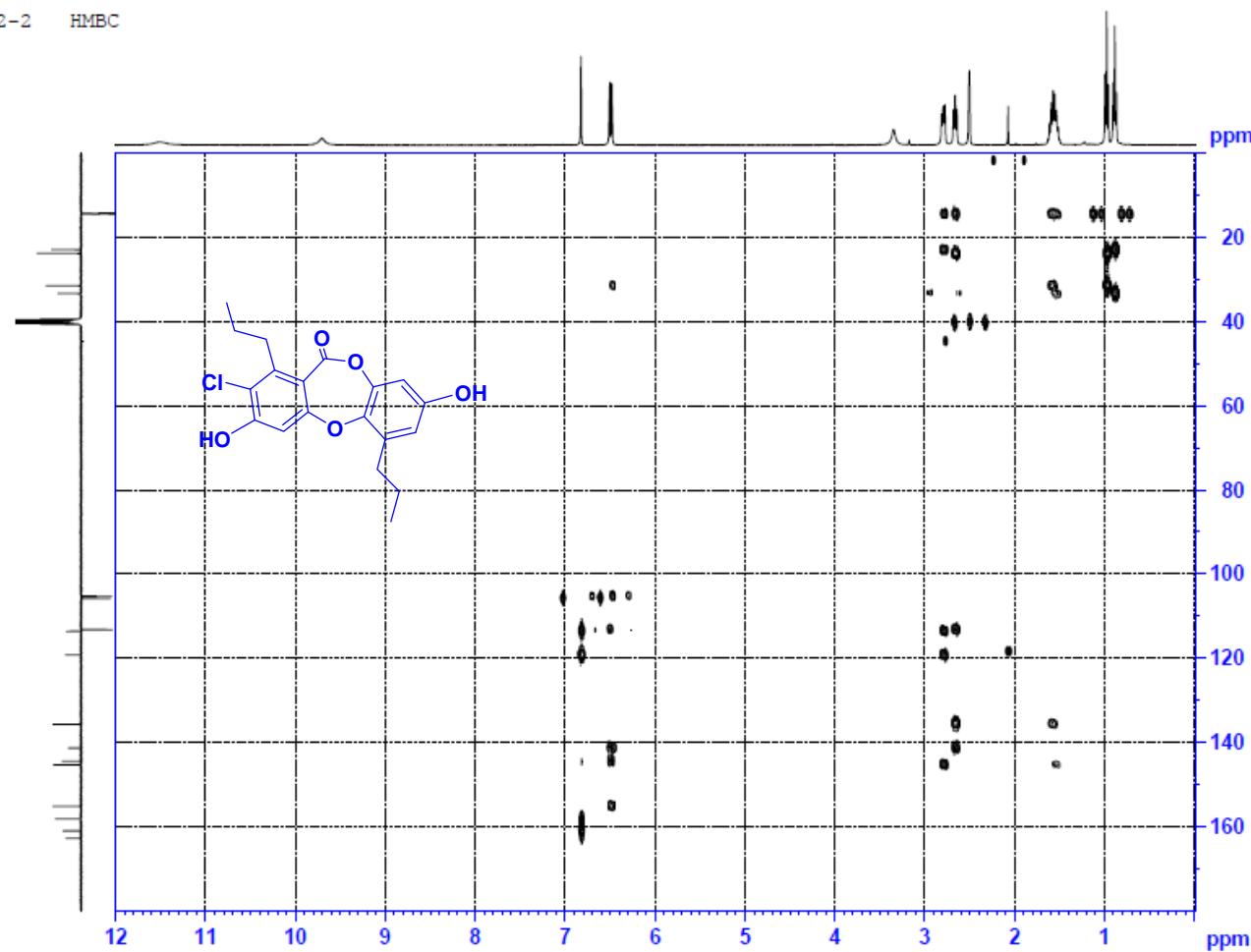
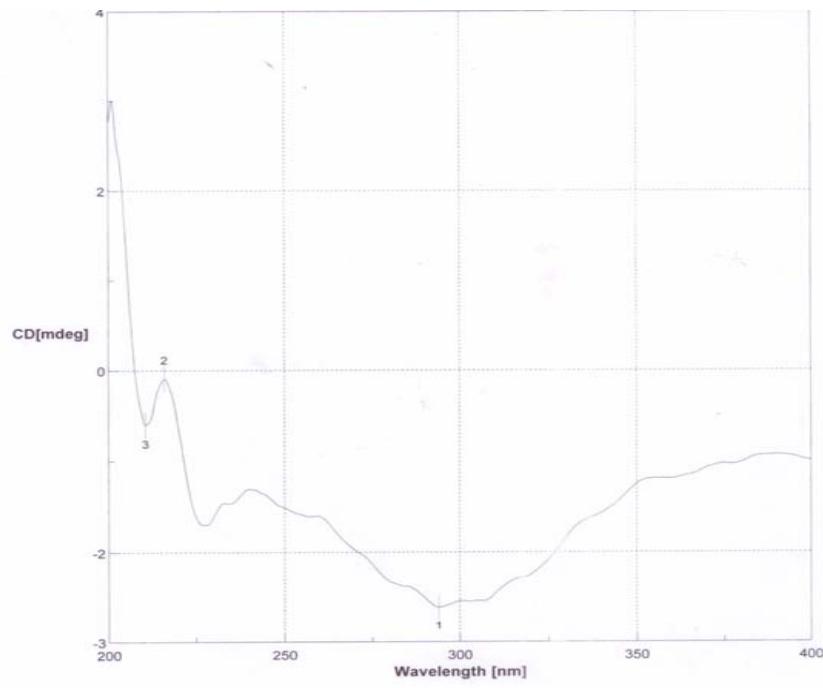


Figure S22. HMBC spectrum of **2** in $\text{DMSO}-d_6$ (400 MHz for ^1H)



Date/Time 2001-1-3 5:39
Operator
File Name F19-8-17-5-2-2.txt
Sample Name F19-8-17-5-2-2
Comment

No.	nm	CD[mdeg]	No.	nm	CD[mdeg]	No.	nm	CD[mdeg]
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Figure S23. CD spectrum of 2

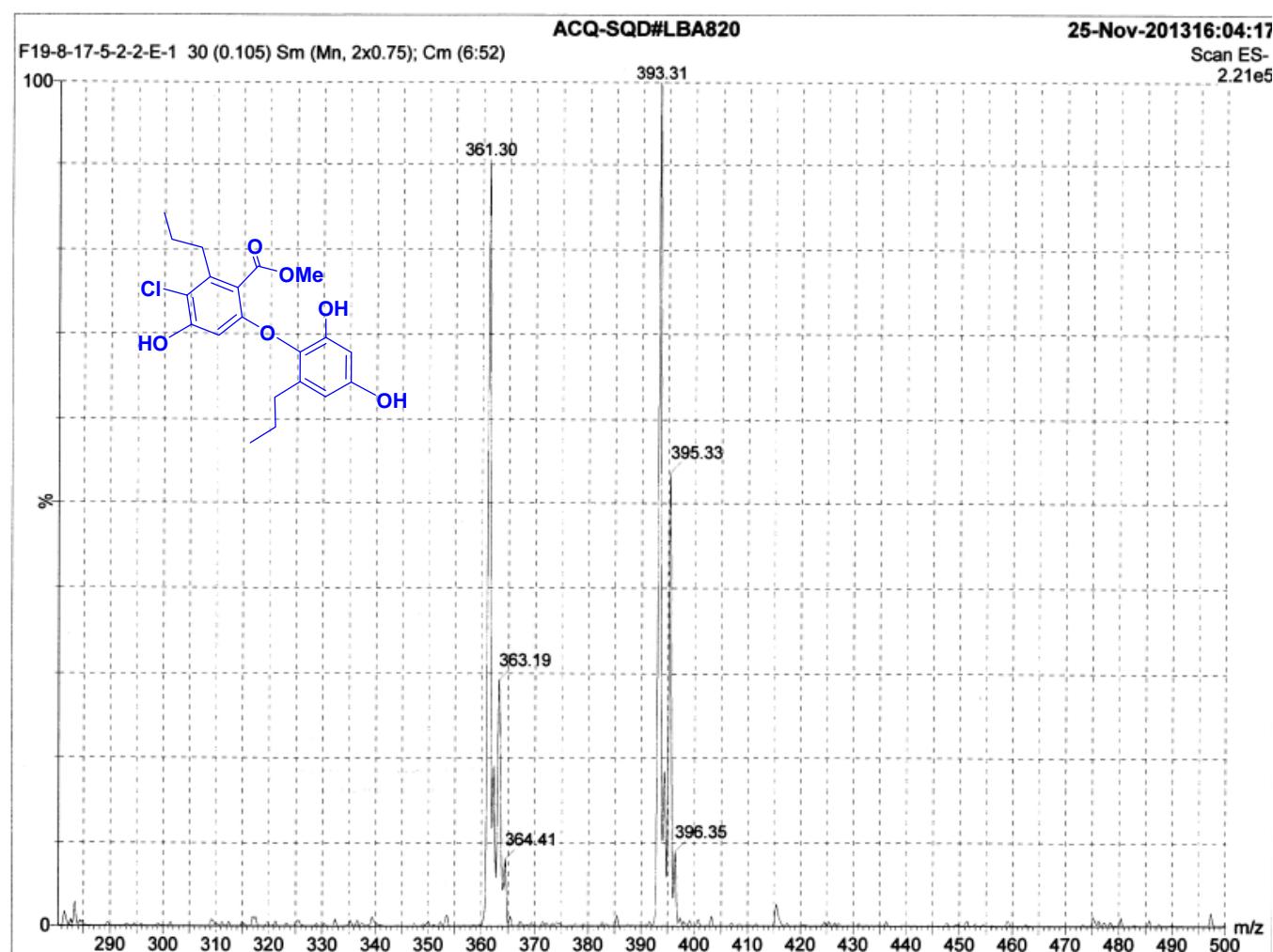


Figure S24. ESIMS spectrum of 2a

F19-8-17-5-2-2-e 400MHz DMSO

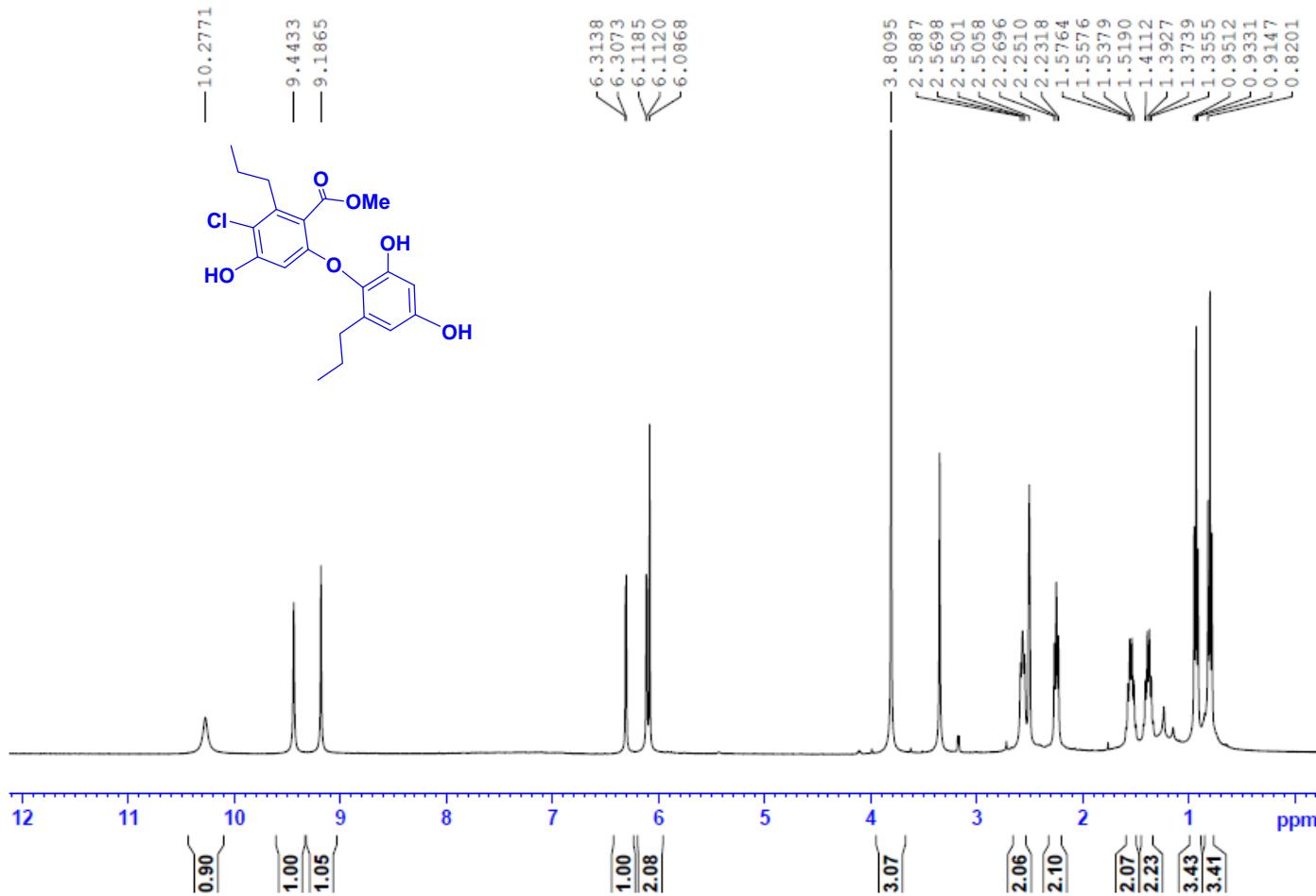


Figure S25. ^1H NMR spectrum of **2a** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-17-5-2-2-e APT

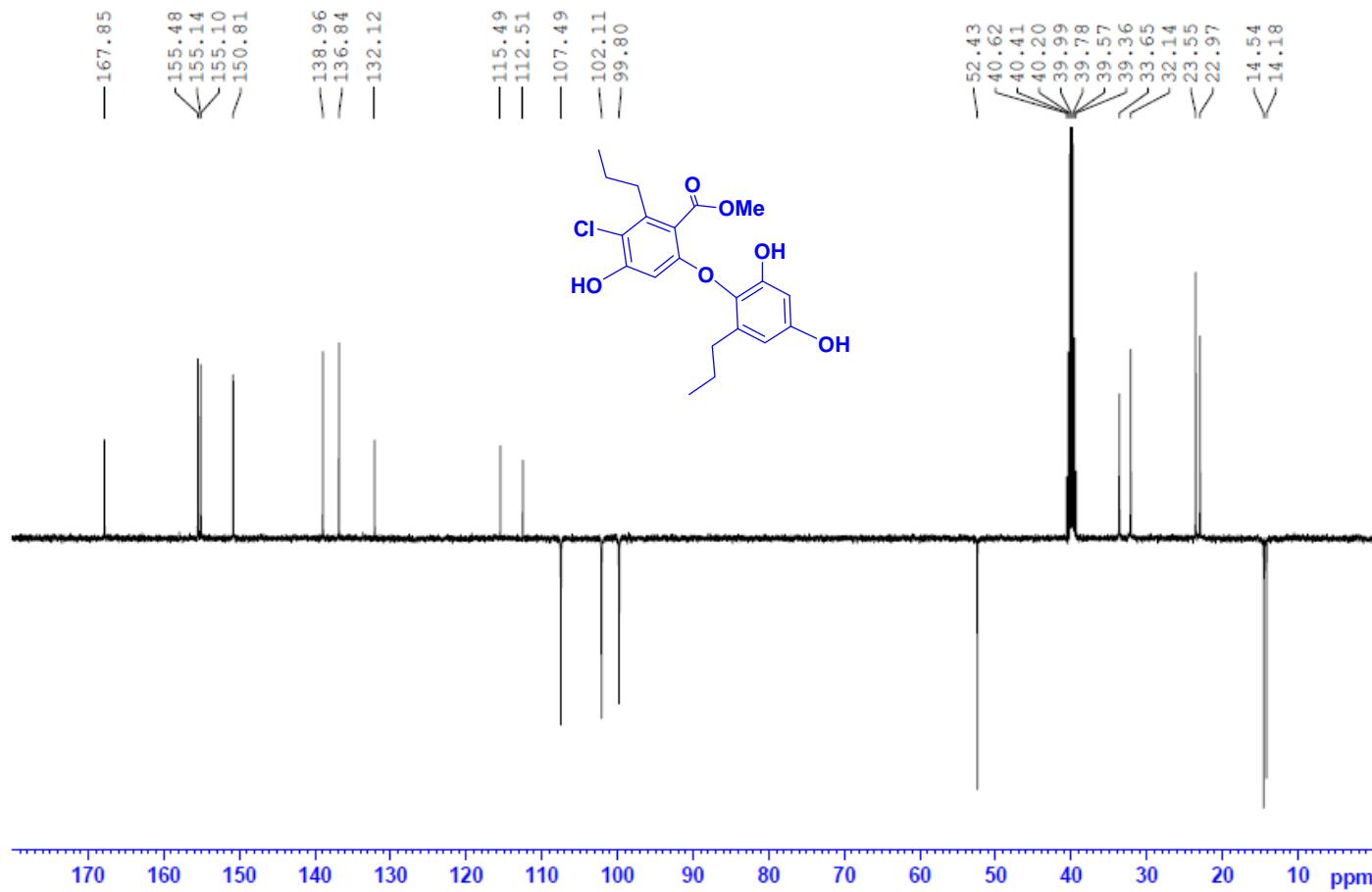


Figure S26. APT spectrum of **2a** in $\text{DMSO}-d_6$ (100 MHz)

F19-8-17-5-2-2-e HSQC

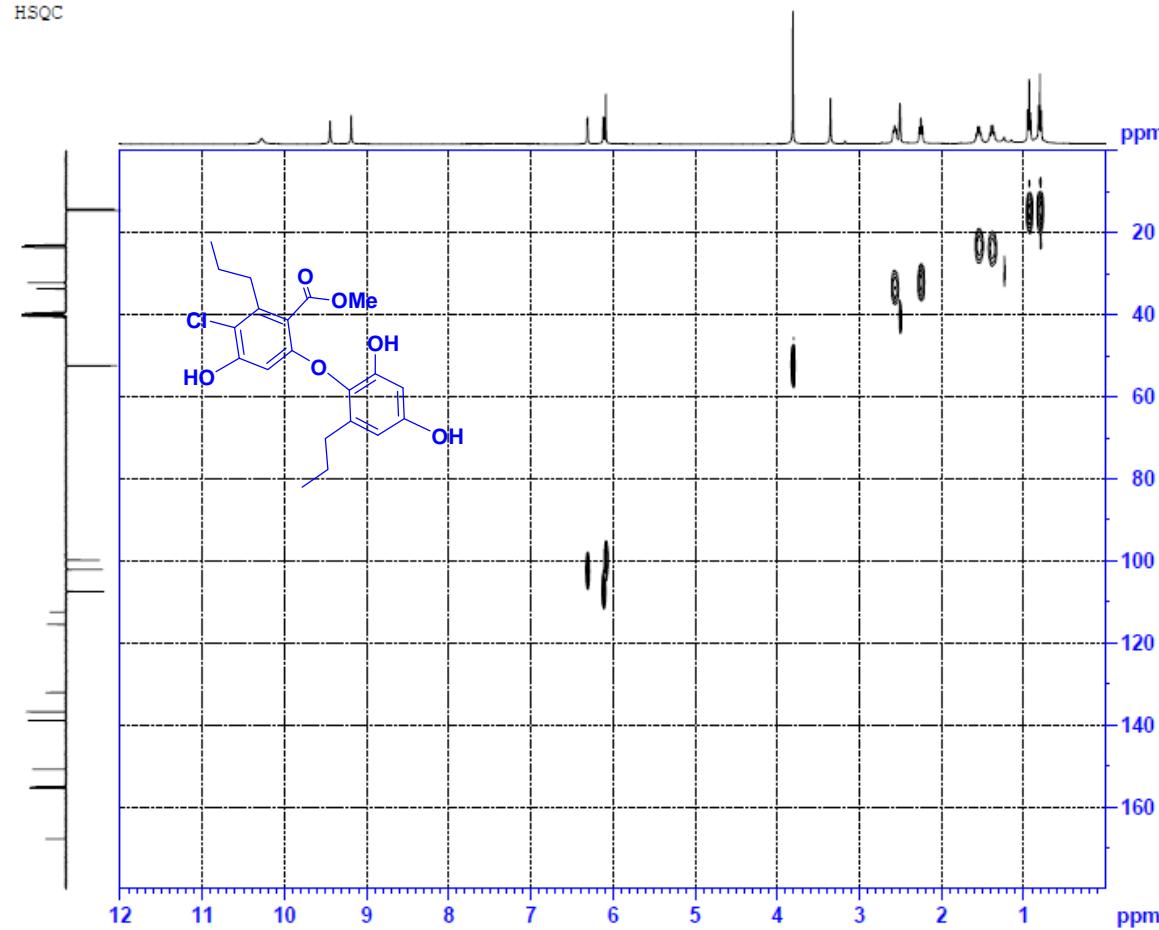


Figure S27. HSQC spectrum of **2a** in DMSO-*d*₆ (400 MHz for ¹H)

F19-8-17-5-2-2-e COSY

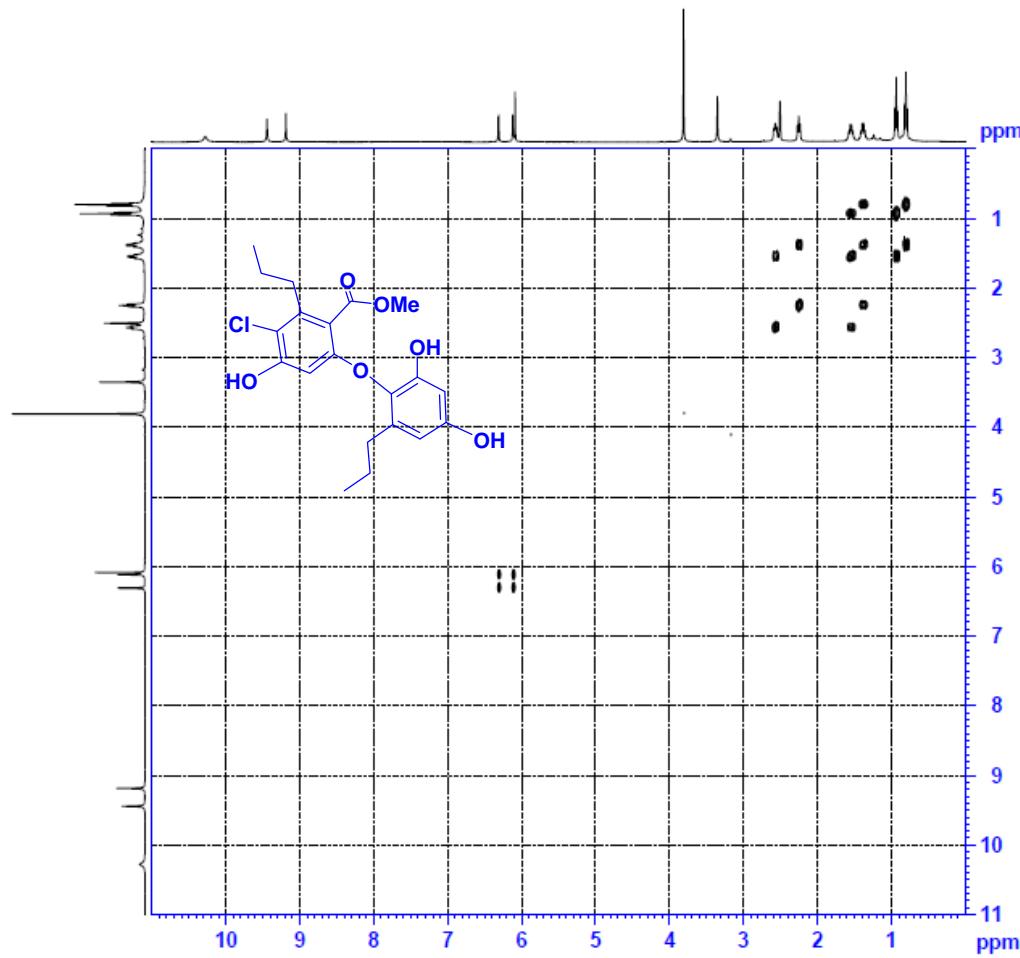


Figure S28. ^1H - ^1H COSY spectrum of **2a** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-17-5-2-2-e HMBC

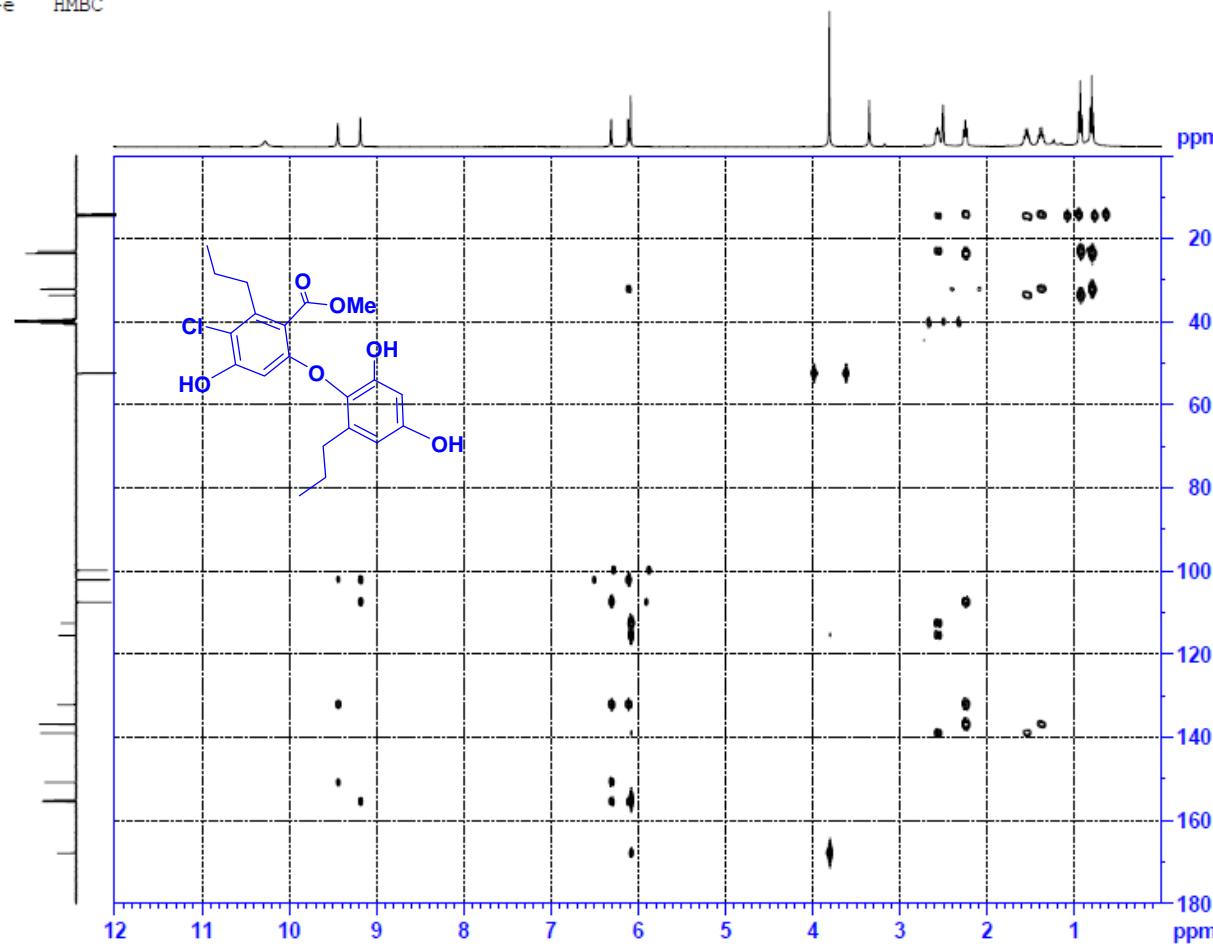


Figure S29. HMBC spectrum of **2a** in DMSO-*d*₆ (400 MHz for ¹H)

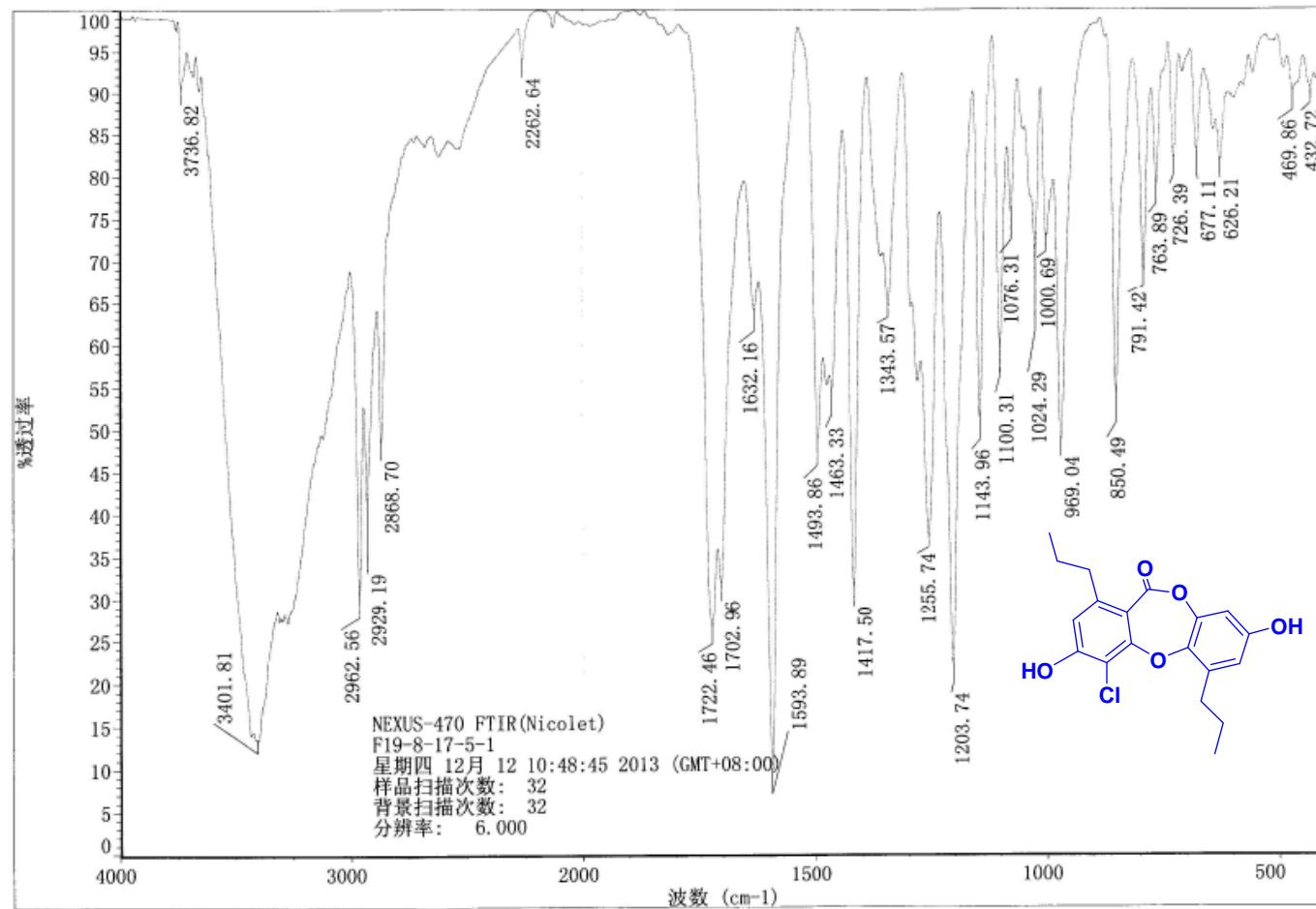


Figure S30. IR spectrum of 3



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Analysis Name C:\data\sample\ESI_12131120_30\LowMassESI_F19_8_17_5_1_20131122\POS_2

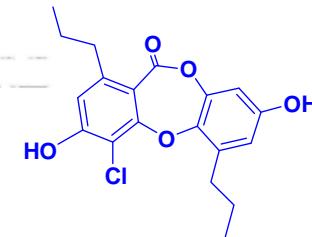
Acquisition Date 11/22/2013 9:54:29 AM

Operator bpxsh@bjmu.edu.cn; Tel:010-82801

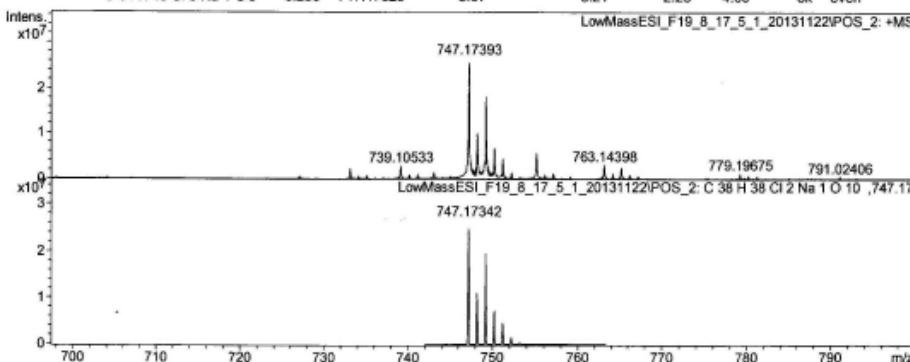
Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI □ C19H19O5Cl1 MW 362.09
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;8.26.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result Exact Mass Measured Mass Error (mDa) Error (ppm) Description



Sum Formula	Exact Mass	Measured Mass	Error (mDa)	Error (ppm)	Description
C 30 H 165 Cl 2 Na 1 O 8	747.17737	747.17737	4.60	7.21	3.44 -53.00 ok odd
C 36 H 39 Cl 2 Na 2 O 10	747.17102	747.17102	-3.90	-1.10	-2.92 15.50 ok even
C 38 H 38 Cl 2 Na 1 O 10	747.17342	747.17342	-0.68	2.21	-0.51 18.50 ok even
C 32 H 43 Cl 3 Na 1 O 12	747.17123	747.17123	-3.62	-0.92	-2.70 9.50 ok even
C 31 H 49 Cl 5 Na 1 O 8	747.17623	747.17623	3.07	5.21	2.29 4.50 ok even



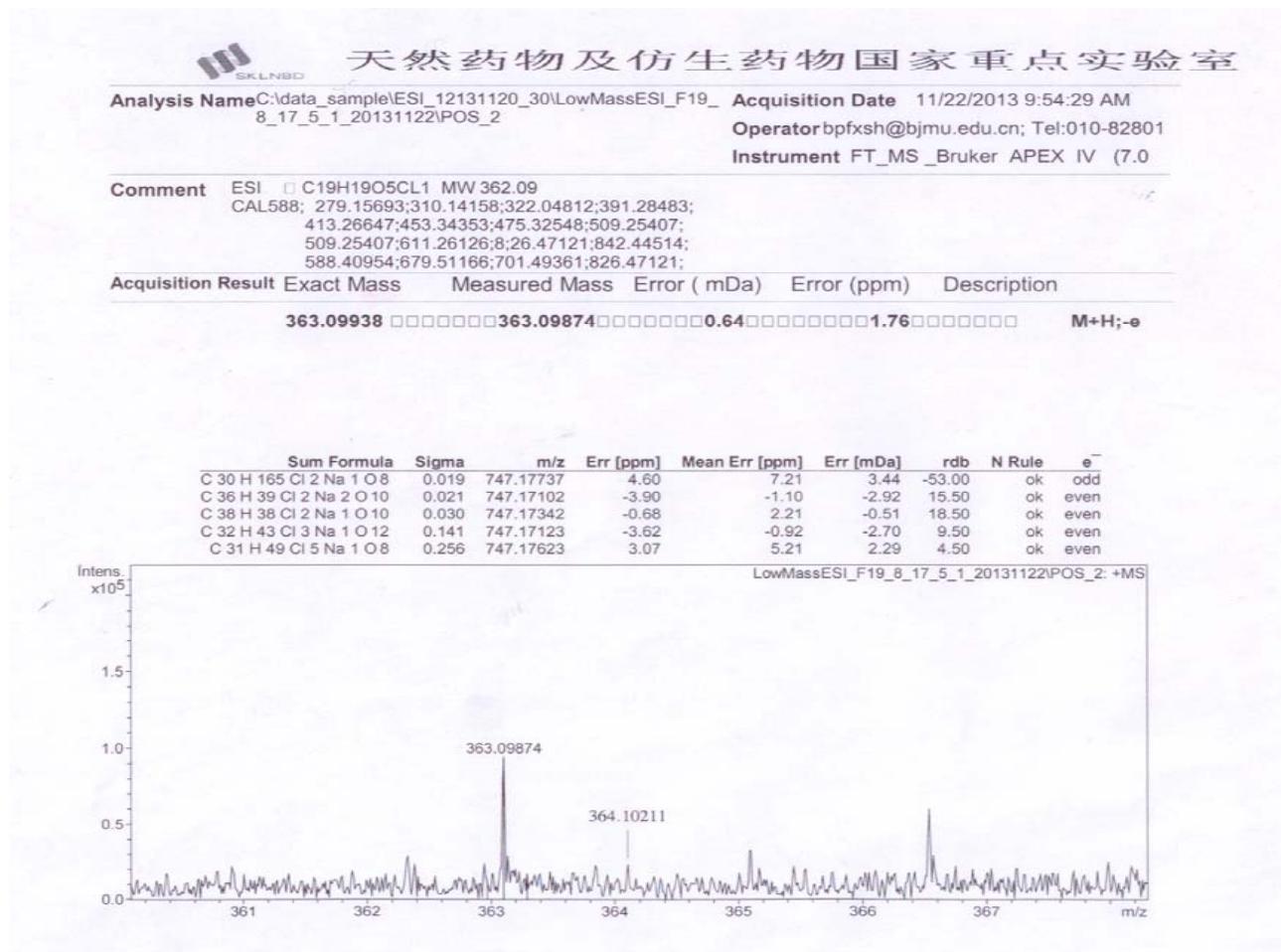


Figure S31. HRESIMS spectrum of **3**

F19-8-17-5-1 400 MHz DMSO

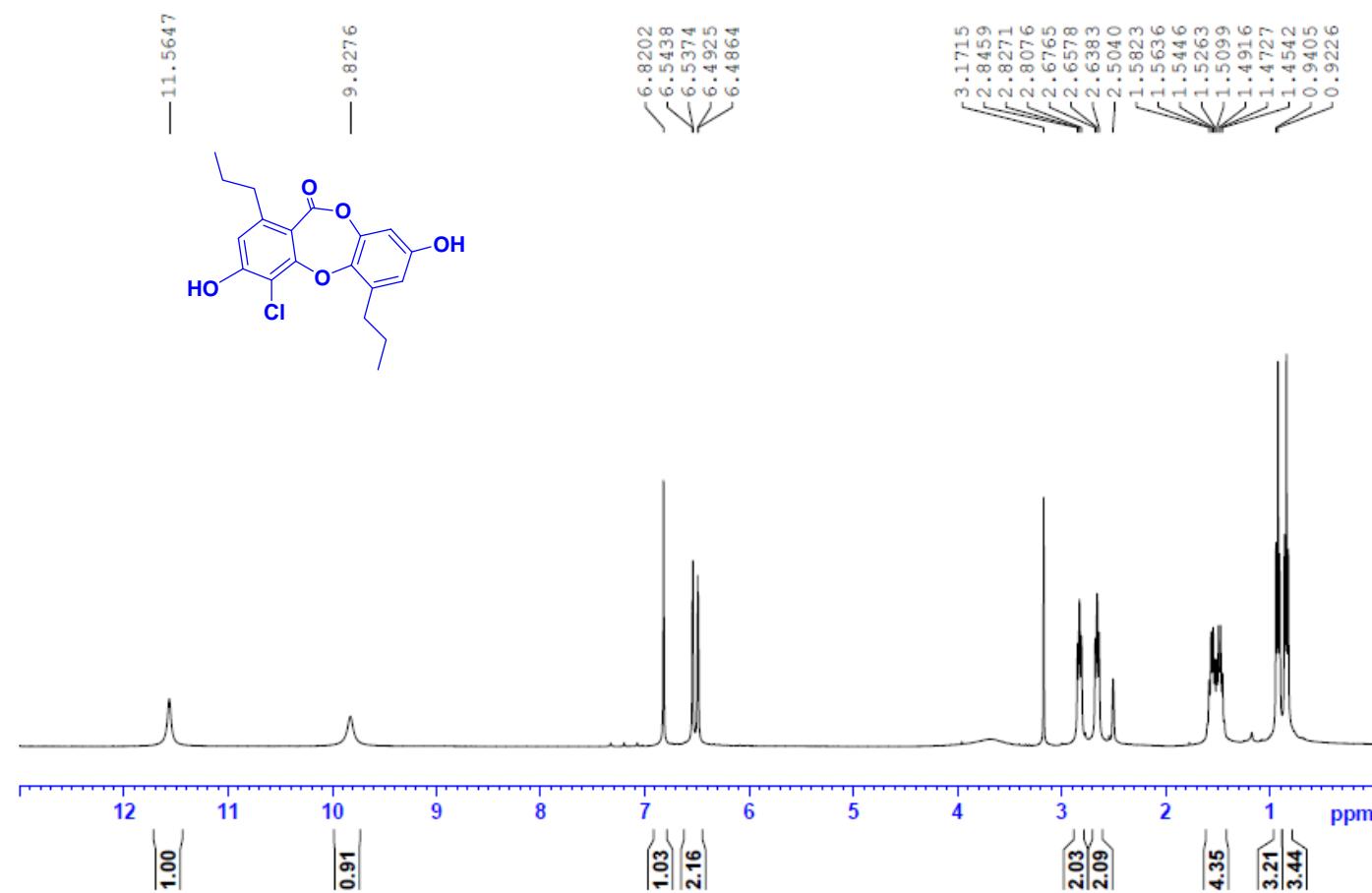


Figure S32. ^1H NMR spectrum of **3** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-17-5-1 APT

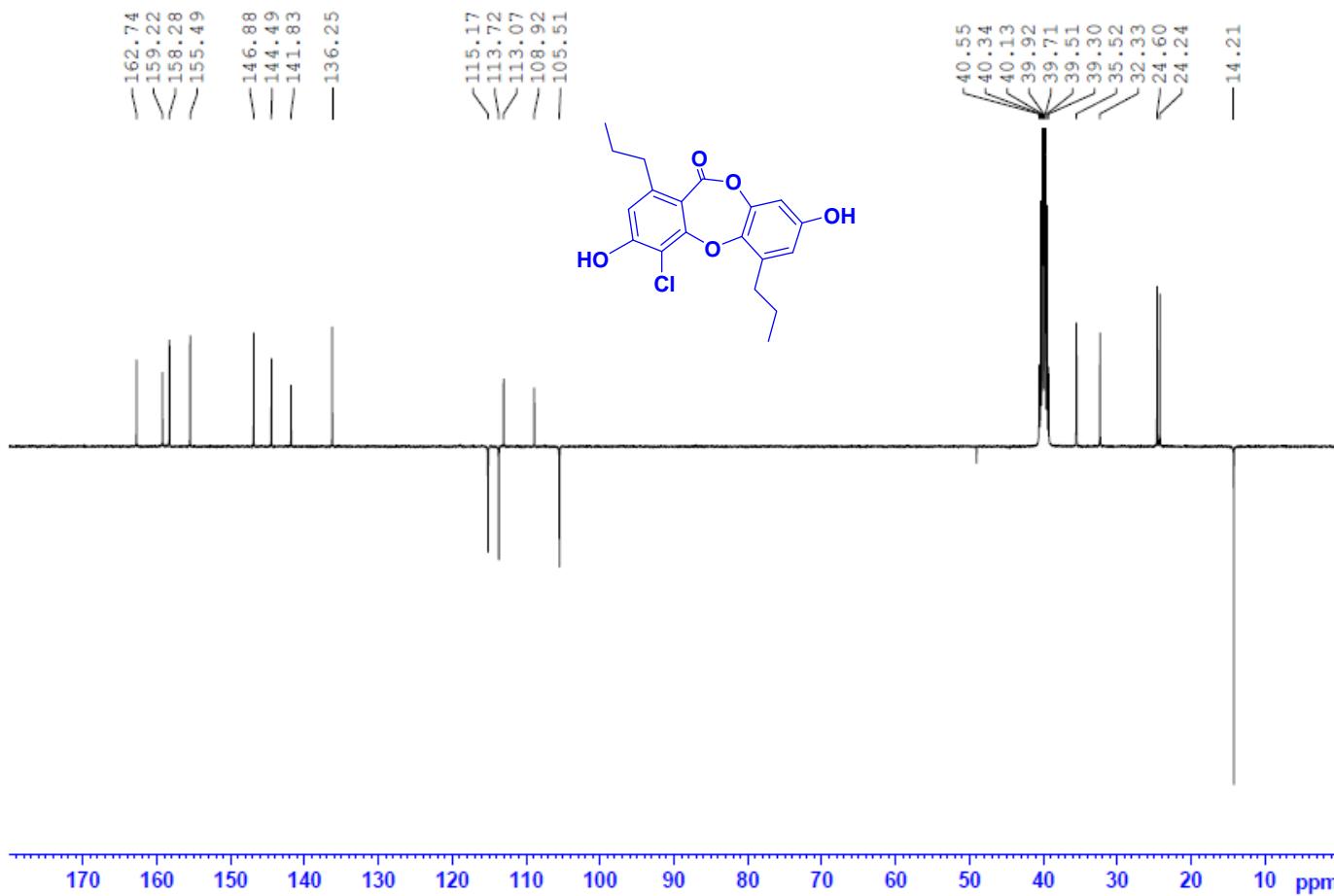


Figure S33. APT spectrum of **3** in ⁶DMSO (100 MHz)

F19-8-17-5-1 HSQC

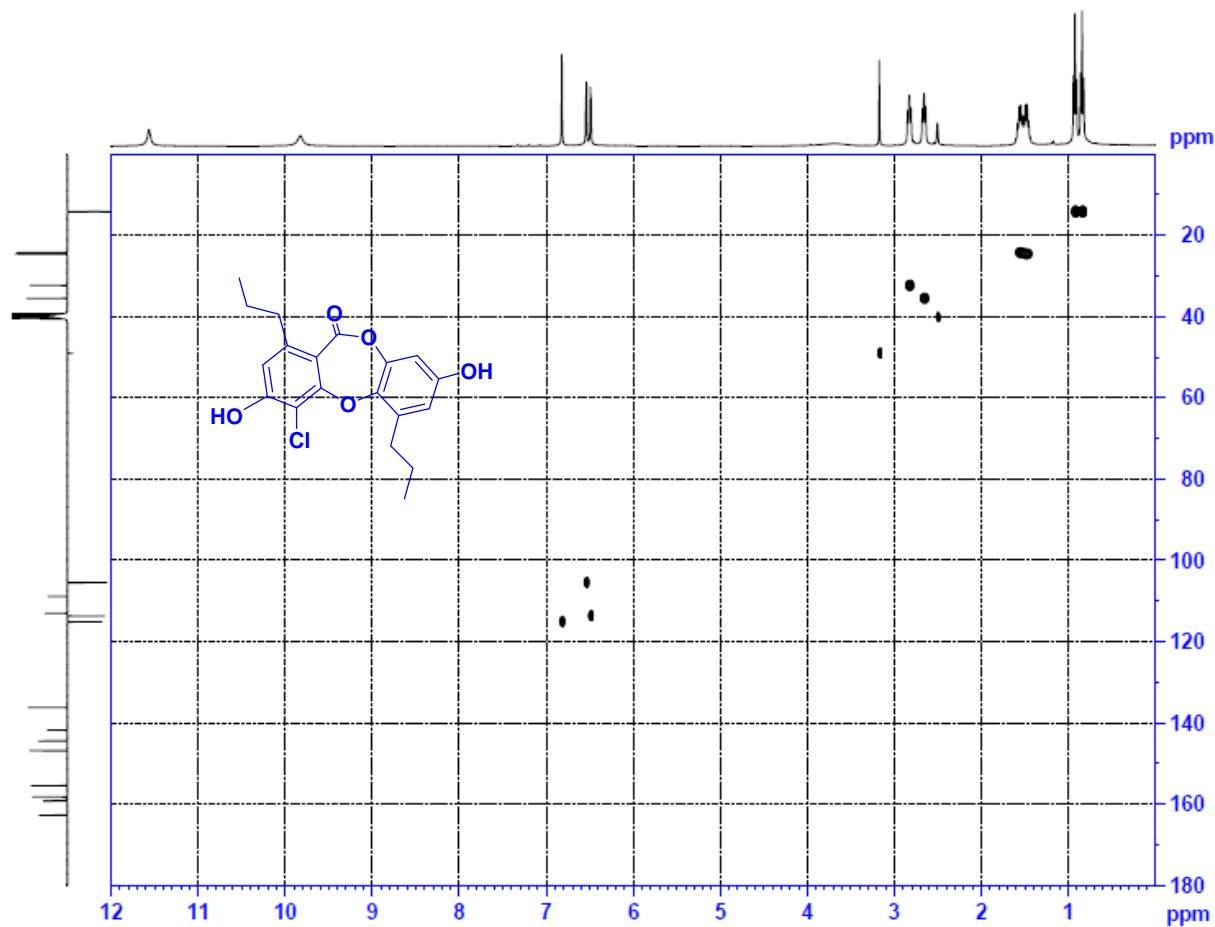


Figure S34. HSQC spectrum of **3** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-17-5-1 COSY

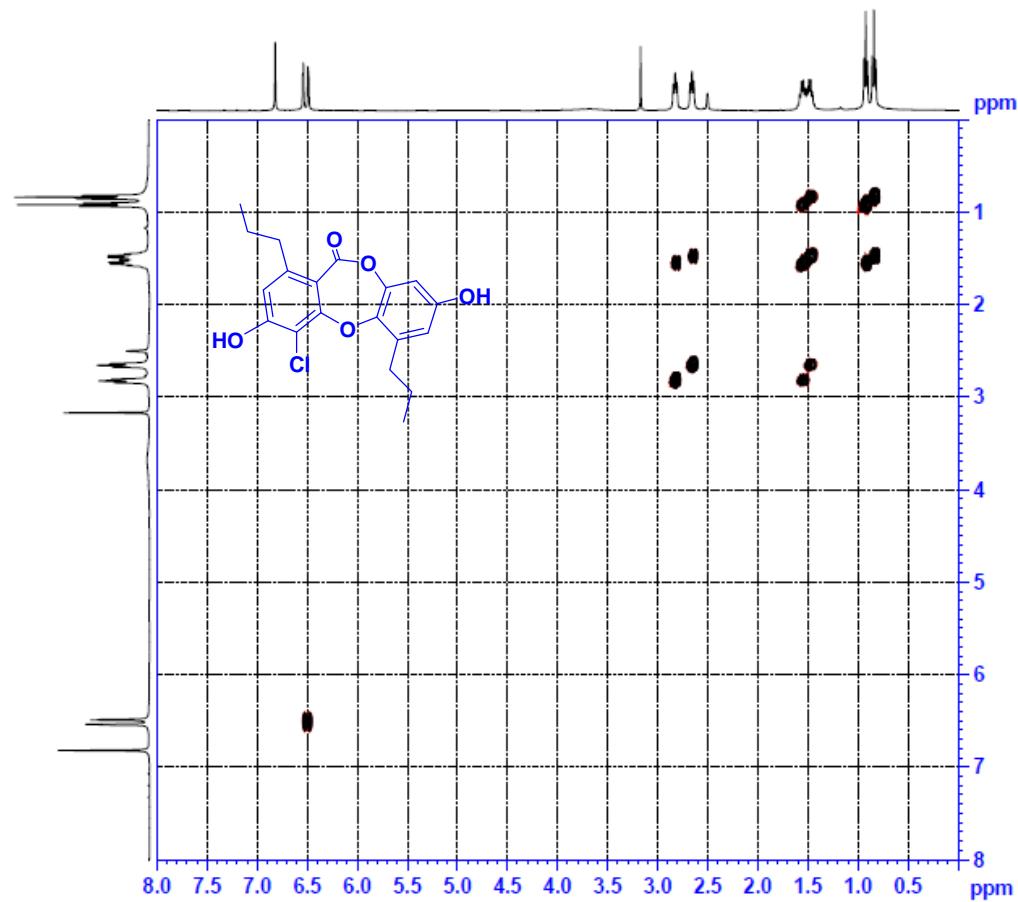


Figure S35. ^1H - ^1H COSY spectrum of 3 in $\text{DMSO}-d_6$ (400 MHz)

F19-8-17-5-1 HMBC

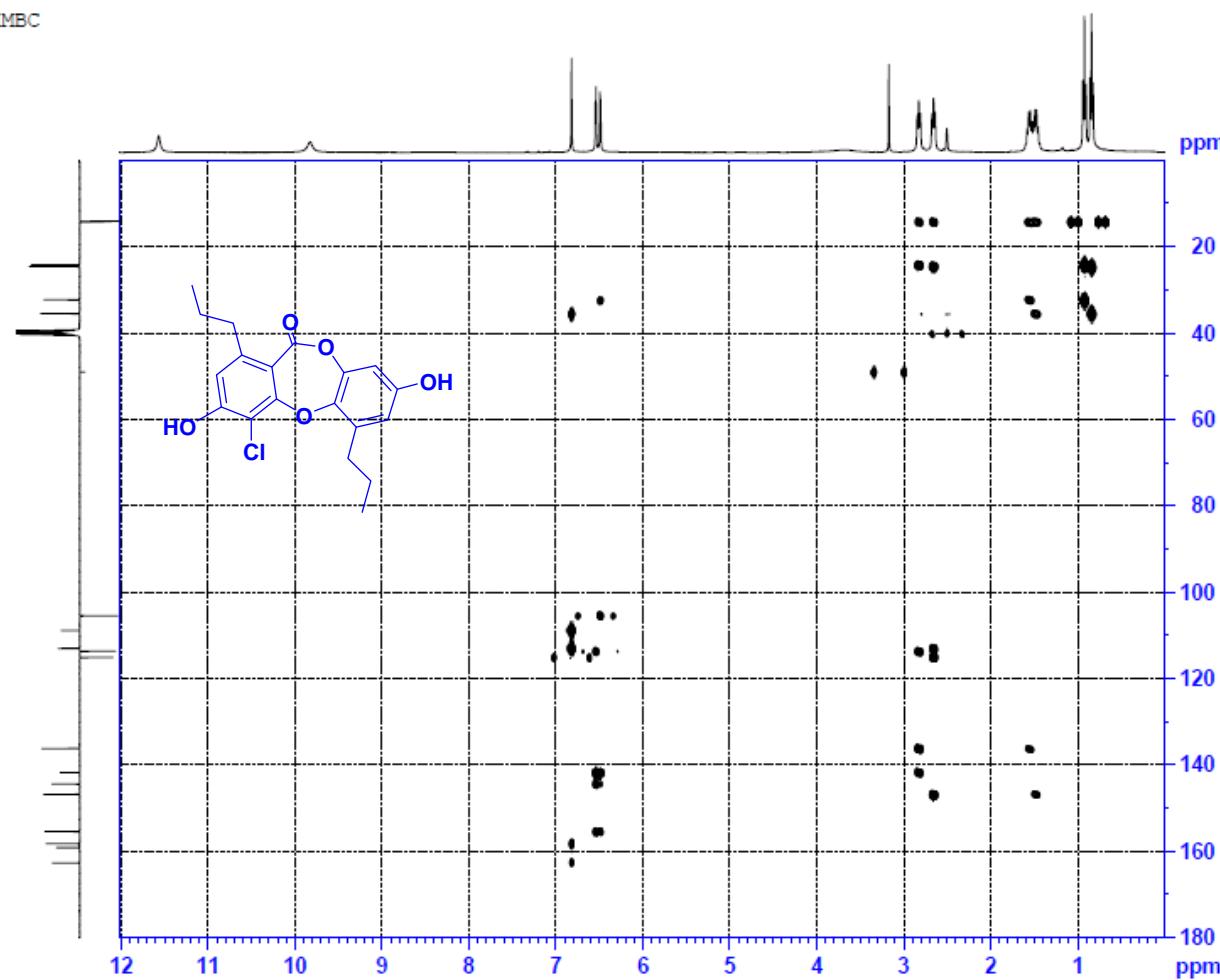
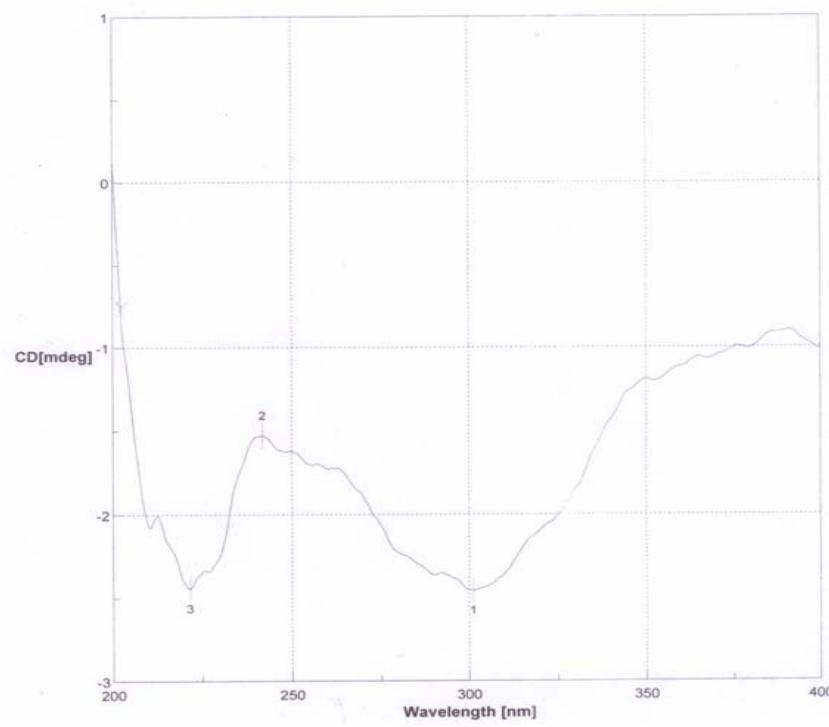


Figure S36. HMBC spectrum of **3** in $\text{DMSO}-d_6$ (400 MHz)



Date/Time 2001-1-3 5:26
Operator
File Name F19-8-17-5-1.txt
Sample Name F19-8-17-5-1
Comment

No.	nm	CD[mdeg]	No.	nm	CD[mdeg]	No.	nm	CD[mdeg]
1	301.2	-2.45526	2	241.8	-1.52621	3	221.6	-2.44318

Figure S37. CD spectrum of 3

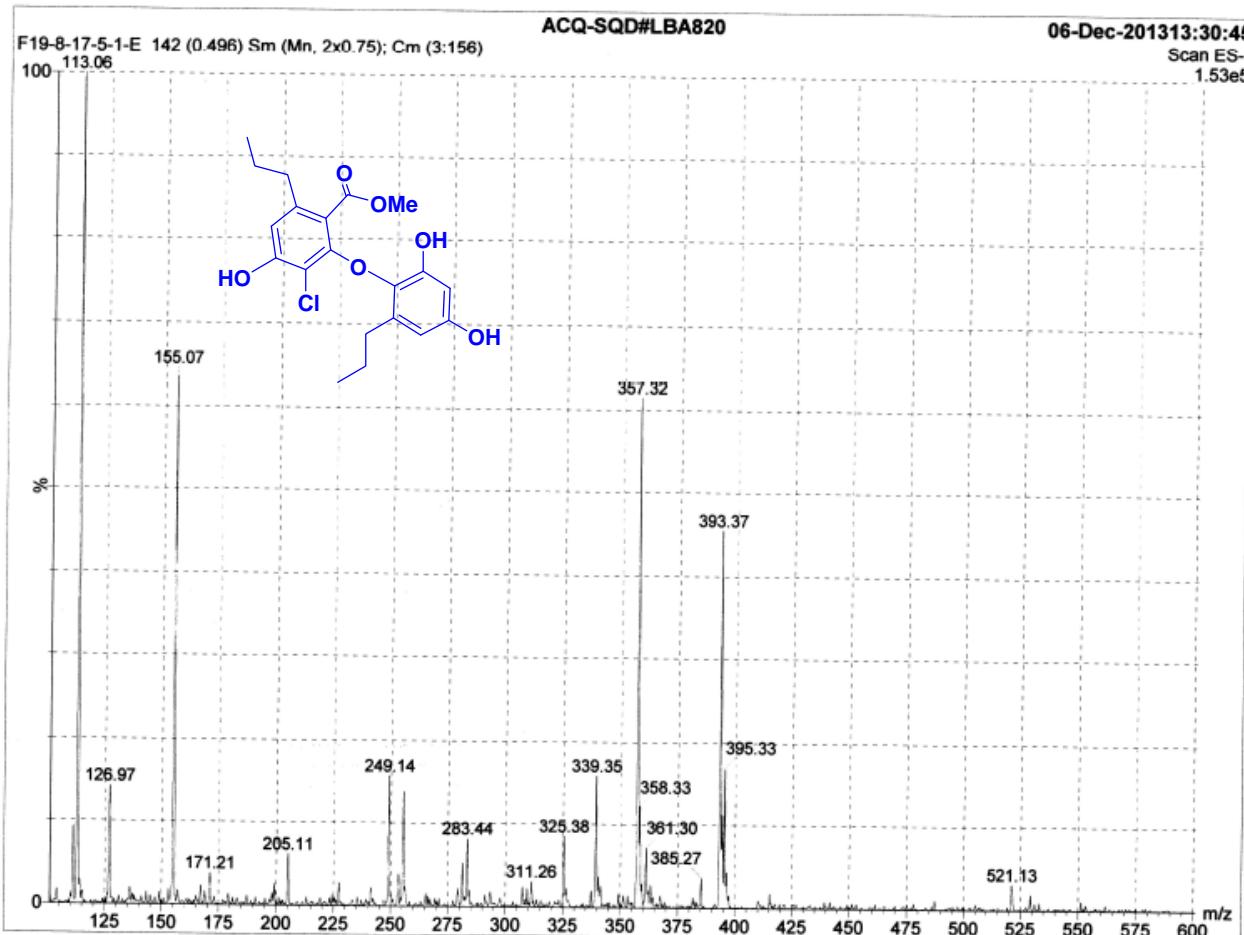


Figure S38. ESIMS spectrum of 3a

F19-8-17-5-1-e 400 MHz DMSO

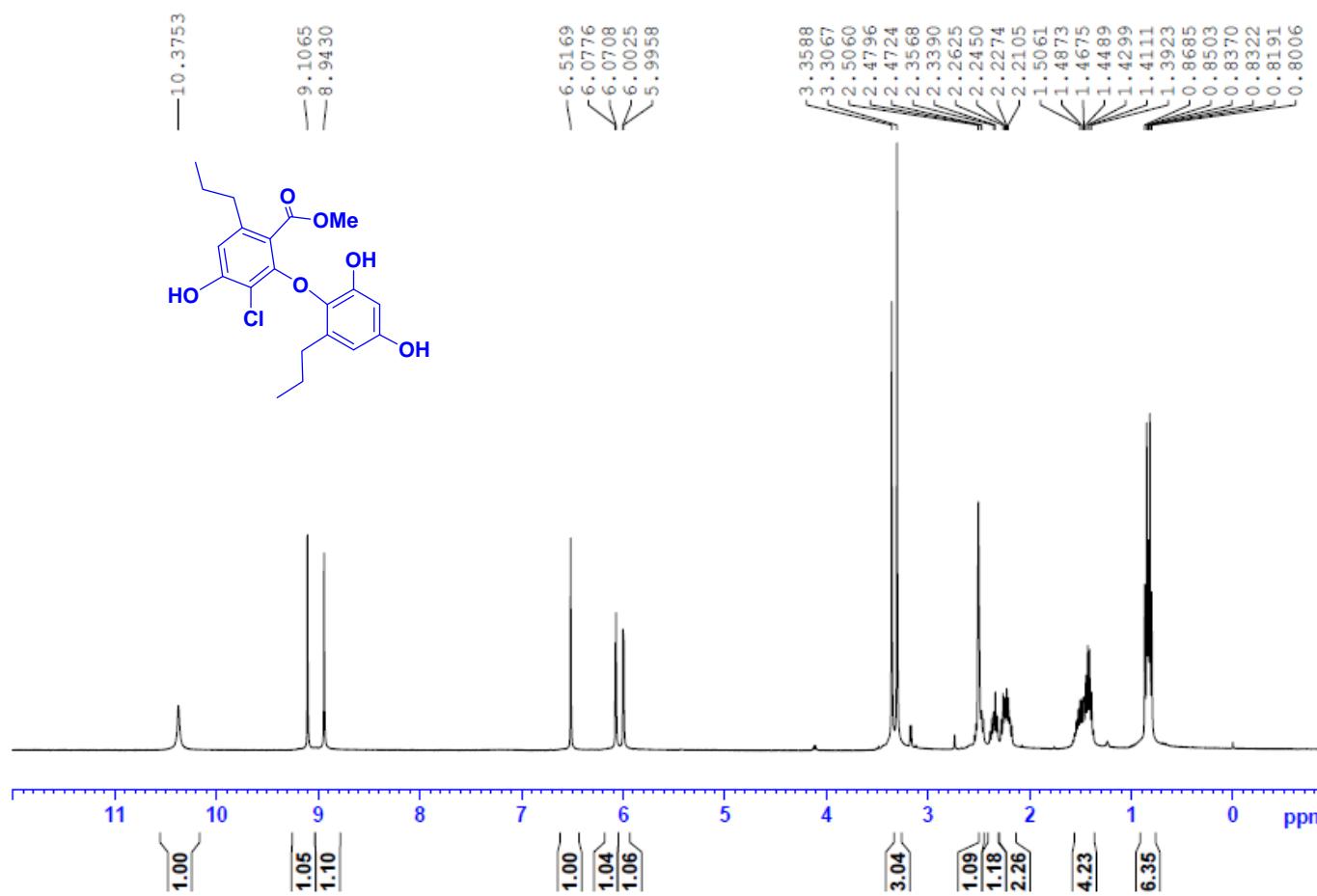


Figure S39. ^1H NMR spectrum of **3a** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-17-5-1-e APT

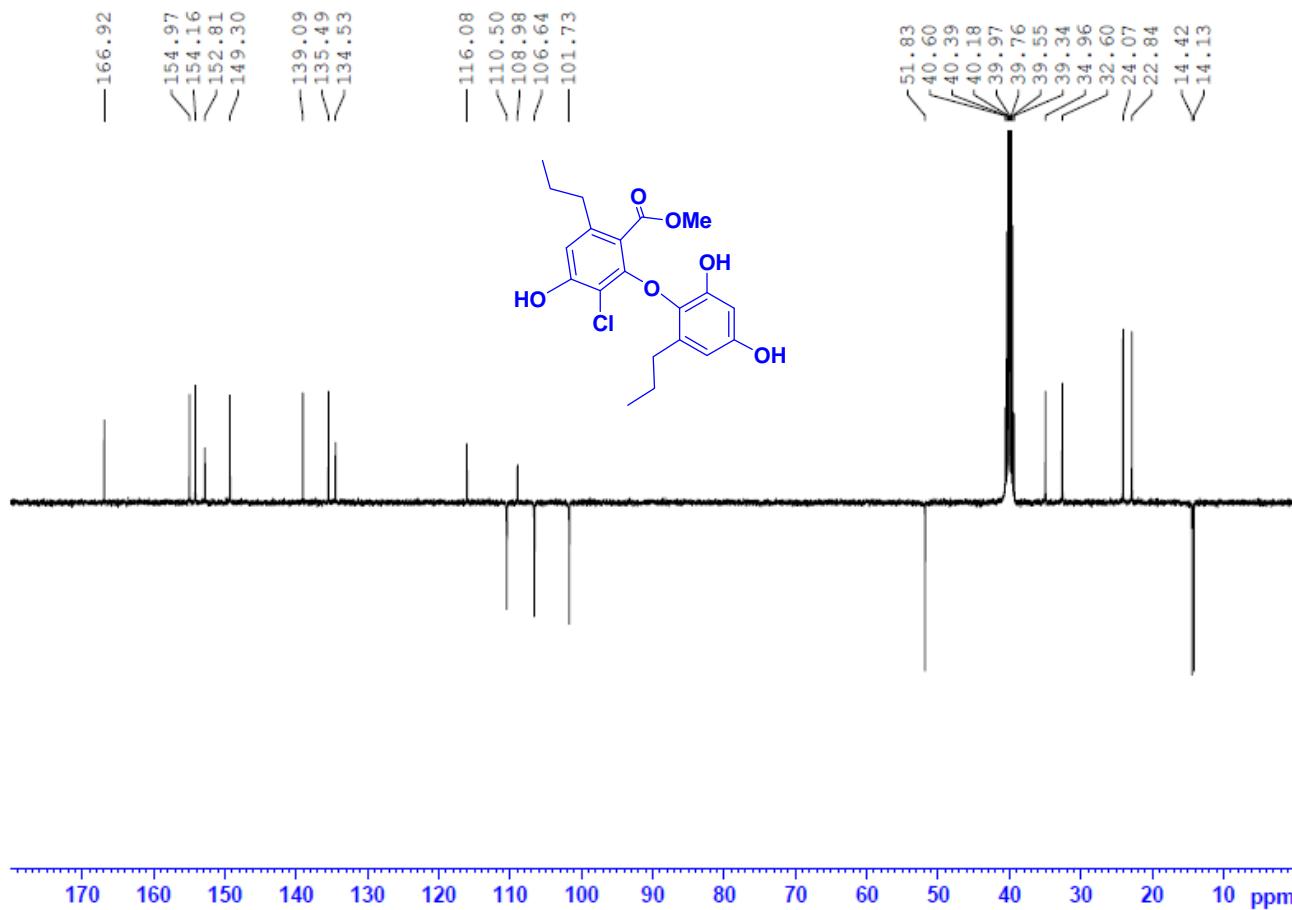


Figure S40. APT spectrum of 3a in DMSO-*d*₆ (100 MHz)

F19-8-17-5-1-e HSQC

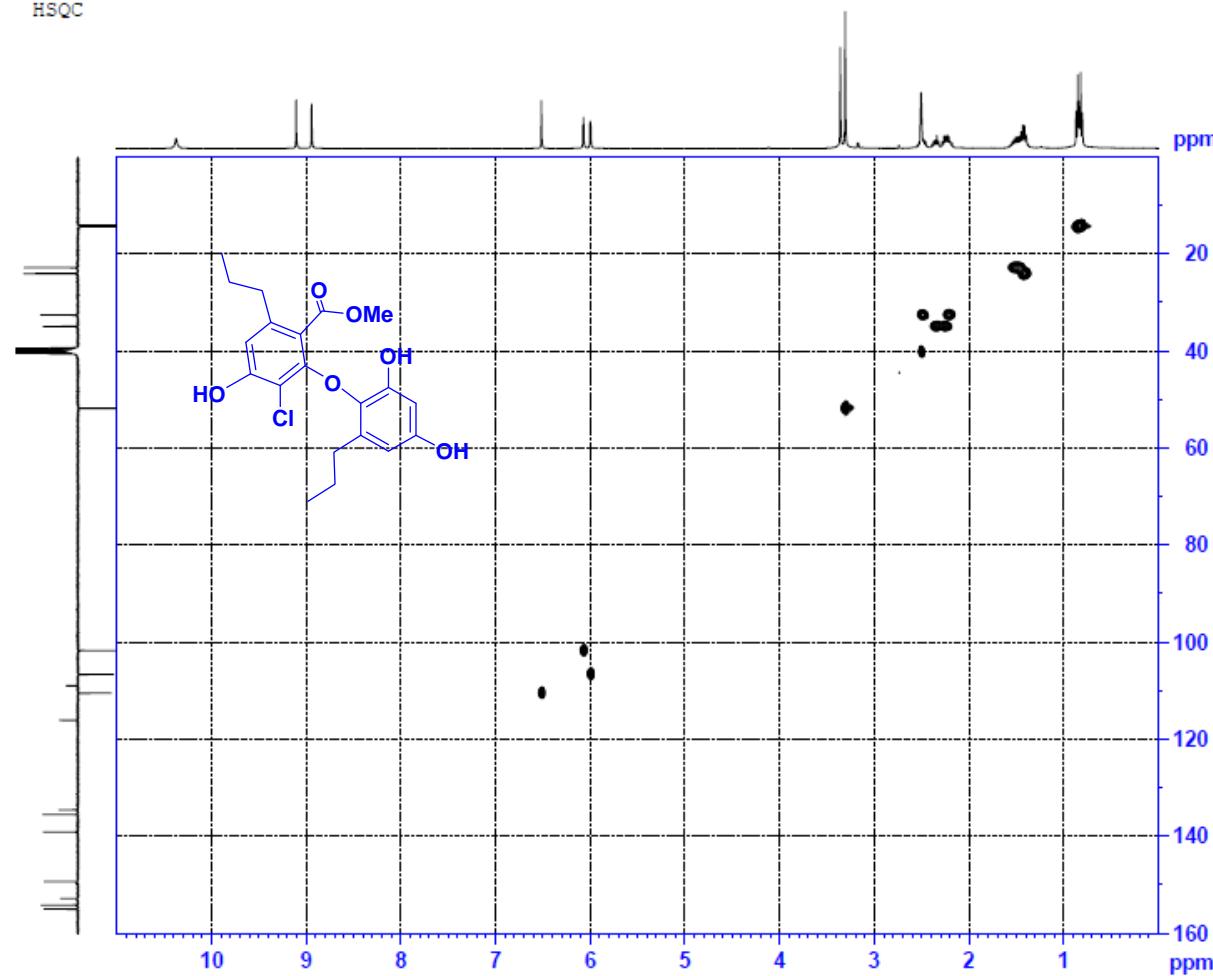


Figure S41. HSQC spectrum of **3a** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-17-5-1-e COSY

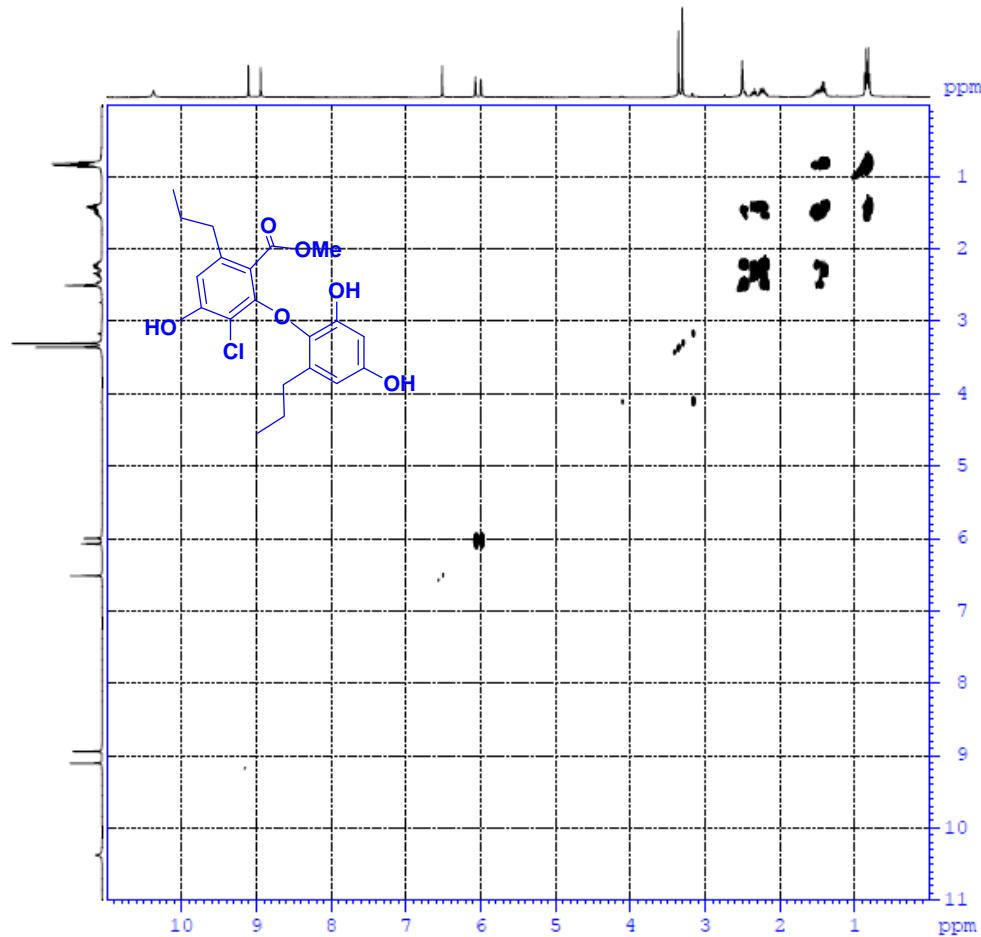


Figure S42. ^1H - ^1H COSY spectrum of **3a** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-17-5-1-e HMBC

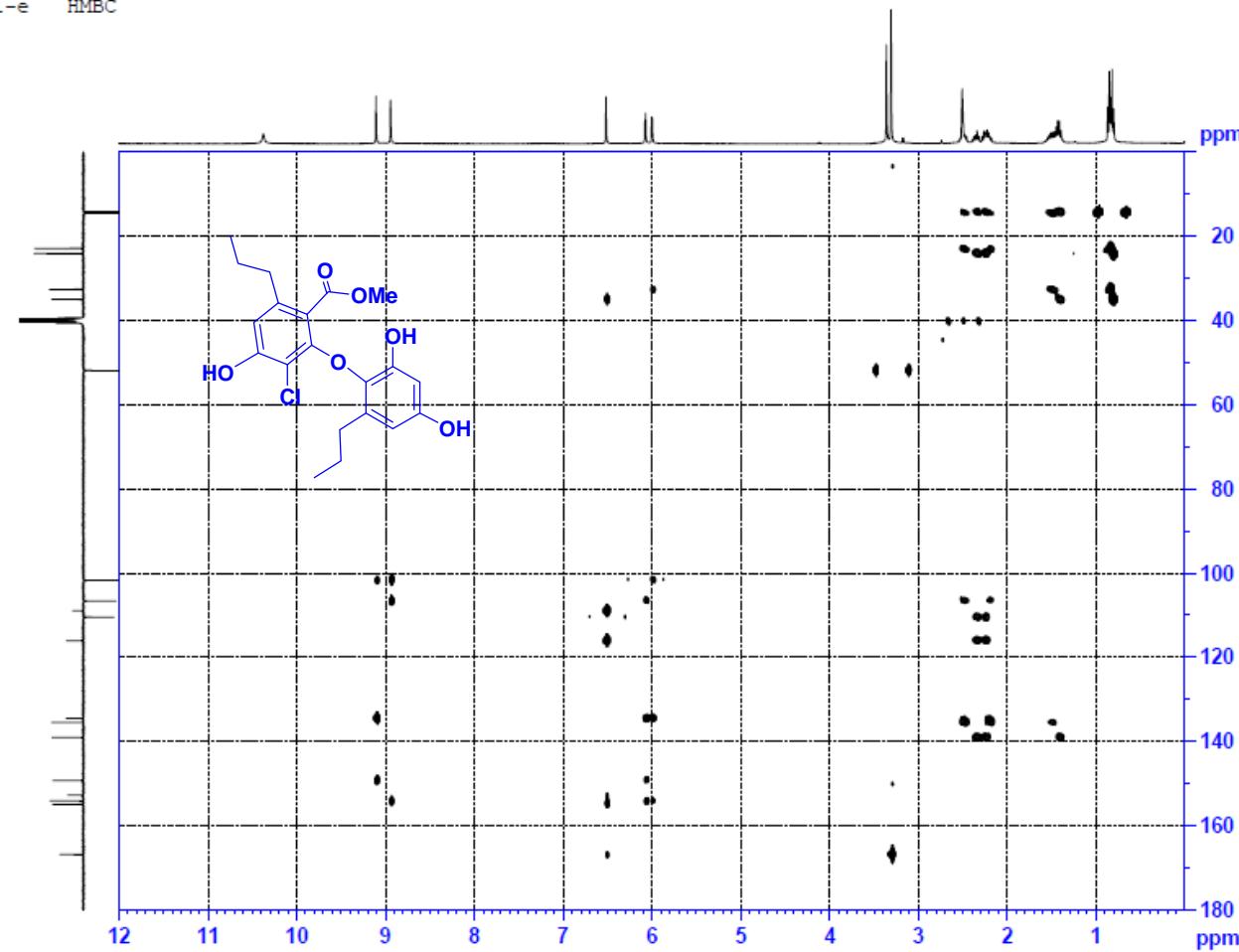


Figure S43. HMBC spectrum of **3a** in $\text{DMSO}-d_6$ (400 MHz)

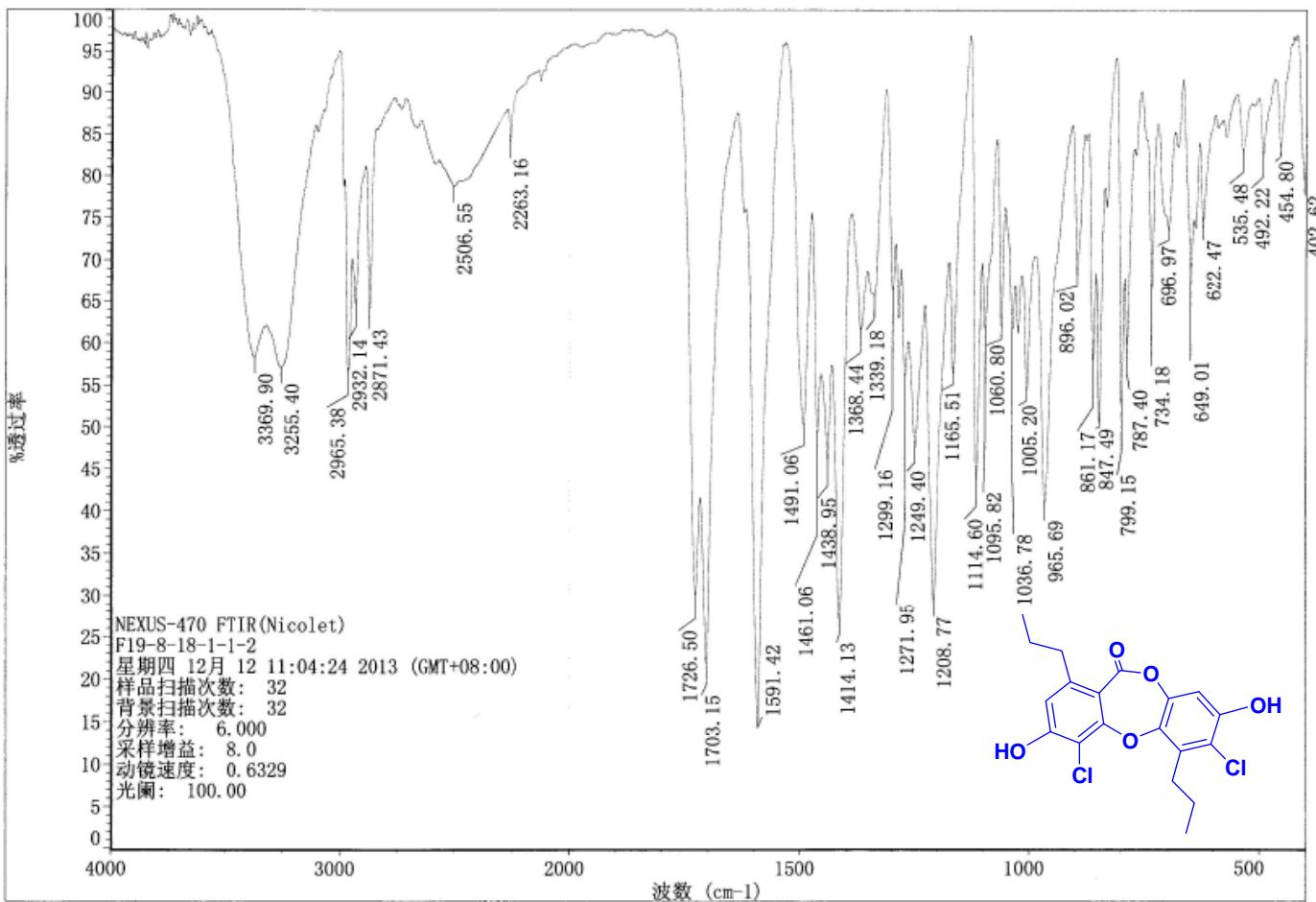


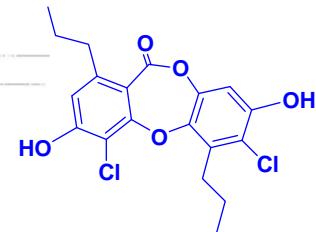
Figure S44. IR spectrum of 4

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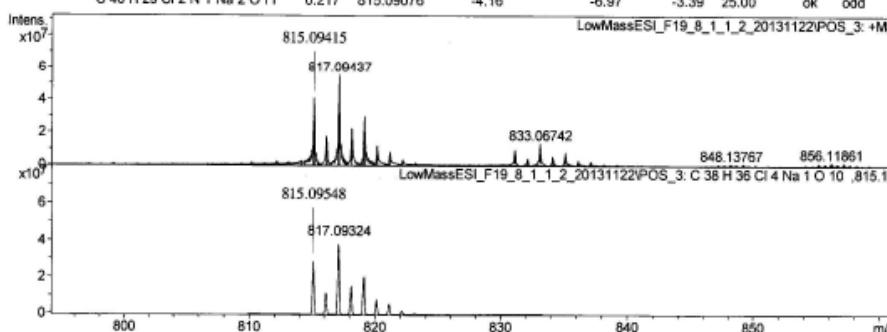
Analysis Name C:\data\sample\ESI_12131120_30\LowMassESI_F19_B Acquisition Date 11/22/2013 9:59:04 AM
 18_1_1_2_20131122\POS_3
 Operator bpxsh@bjmu.edu.cn; Tel:010-82801
 Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI □ C19H18O5Cl2 MW 396.05
 CAL588: 279.15693;310.14158;322.04812;391.28483;
 413.26647;453.34353;475.32548;509.25407;
 508.25407;611.26126;8.26.47121;842.44514;
 588.40954;679.51166;701.49361;826.47121;

Acquisition Result Exact Mass Measured Mass Error (mDa) Error (ppm) Description



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 40 H 35 Cl 4 O 10	0.012	815.09768	4.58	-0.17	3.73	21.50	ok	even
C 38 H 36 Cl 4 Na 1 O 10	0.014	815.09548	1.63	-3.08	1.33	18.50	ok	even
C 38 H 32 Cl 3 N 1 O 13	0.101	815.09337	-0.95	-4.70	-0.78	22.00	ok	odd
C 40 H 33 Cl 3 Na 3 O 8	0.104	815.09286	-1.58	-5.37	-1.29	21.50	ok	even
C 38 H 34 Cl 3 Na 4 O 8	0.106	815.09046	-4.53	-8.30	-3.70	18.50	ok	even
C 39 H 30 Cl 2 Na 1 O 14	0.216	815.09048	-4.50	-7.25	-3.67	23.50	ok	even
C 40 H 29 Cl 2 N 1 Na 2 O 11	0.217	815.09076	-4.16	-6.97	-3.39	25.00	ok	odd



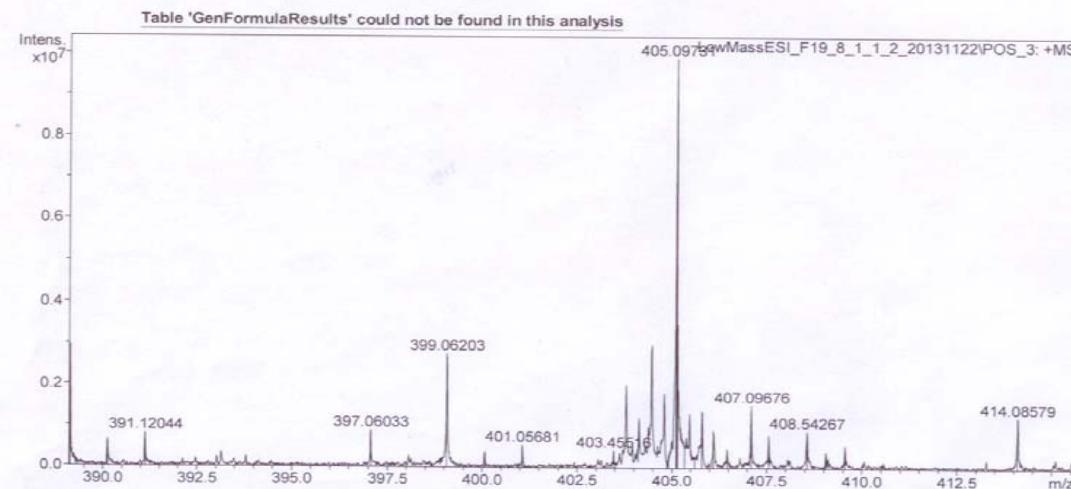


Figure S45. HRESIMS spectrum of **4**

F19-8-18-1-1-2 400 MHz DMSO

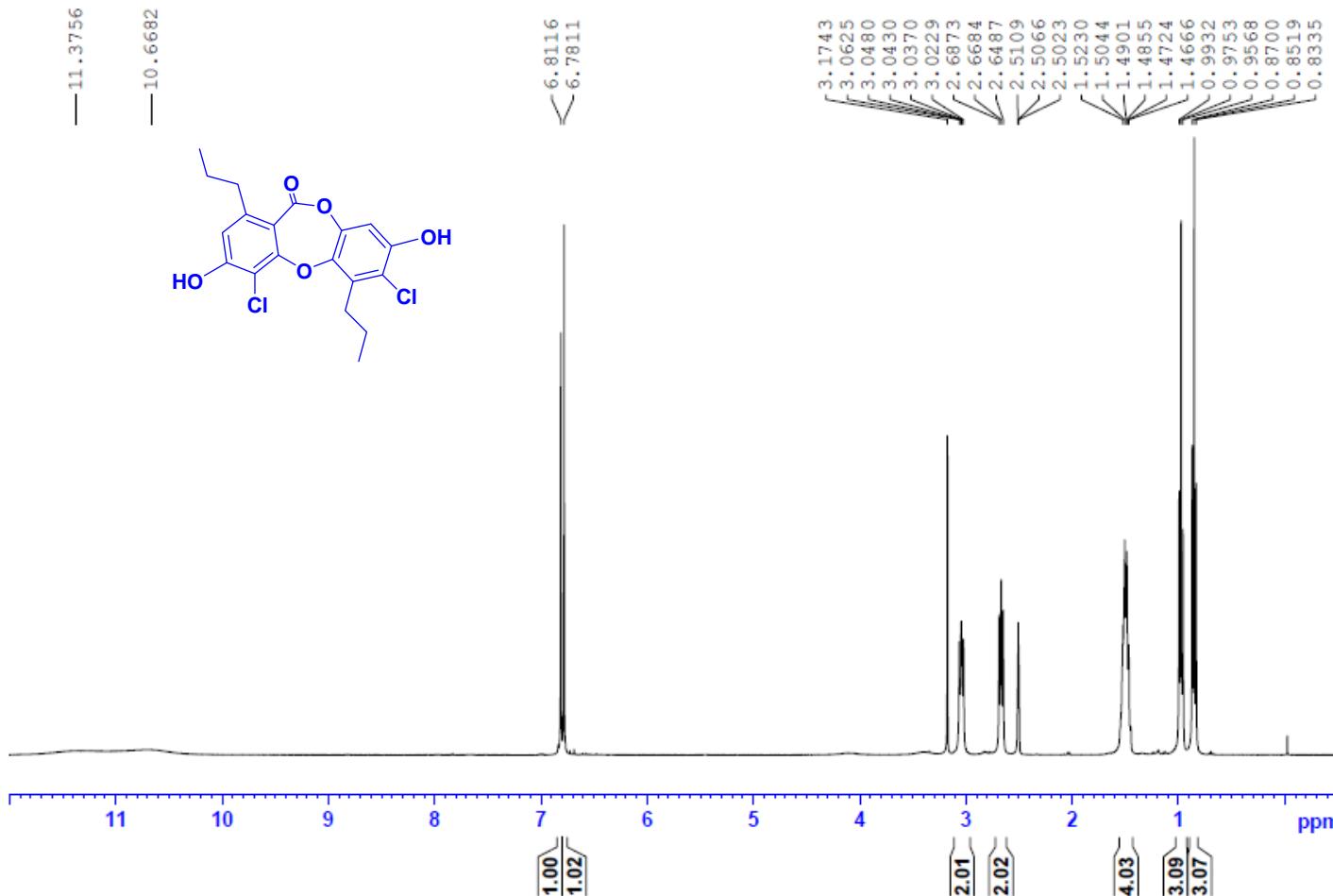


Figure S46. ¹H NMR spectrum of 4 in DMSO-*d*₆ (400 MHz)

F19-8-18-1-1-2 APT

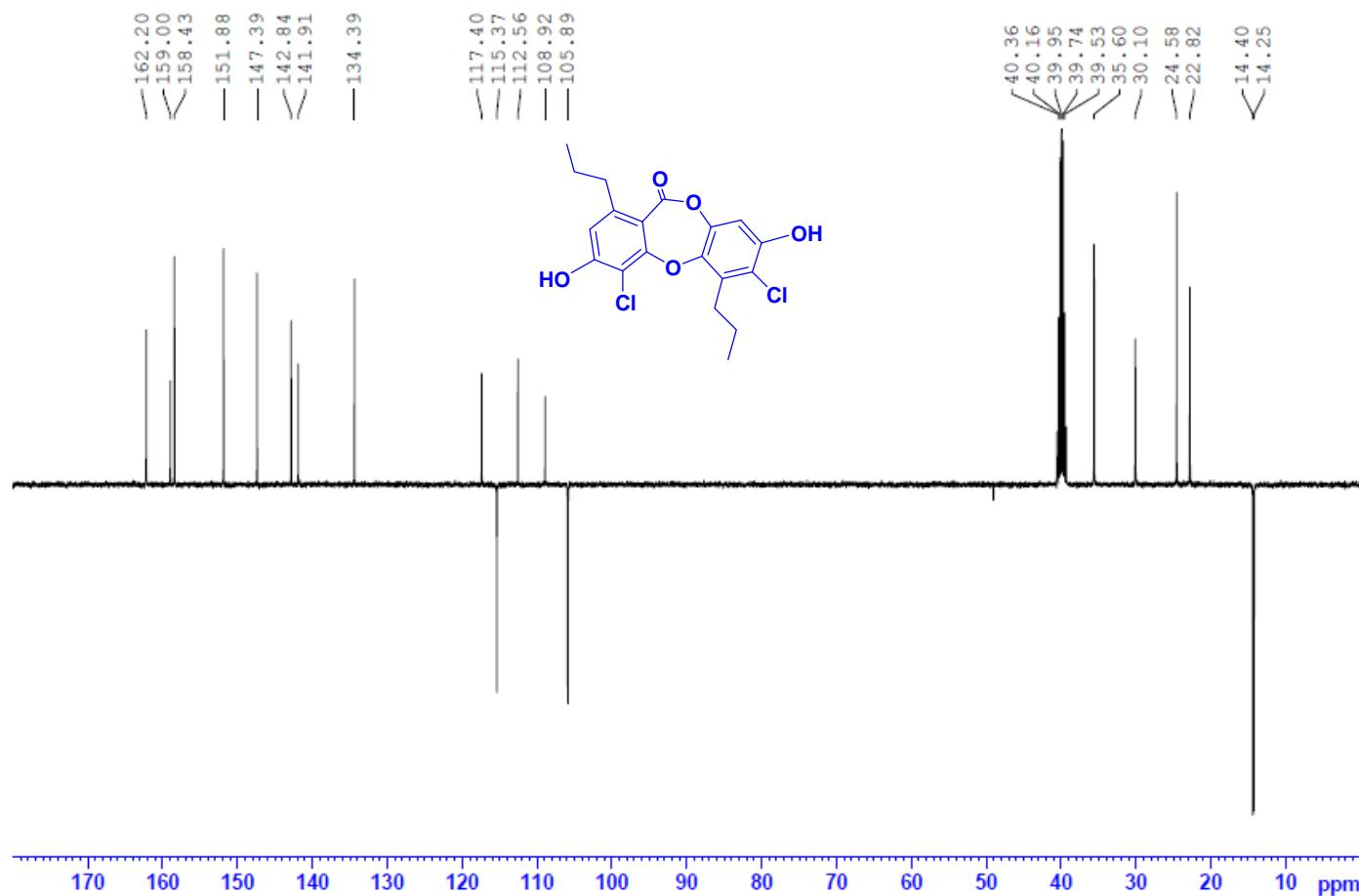


Figure S47. APT spectrum of **4** in $\text{DMSO}-d_6$ (100 MHz)

F19-8-18-1-1-2 HSQC

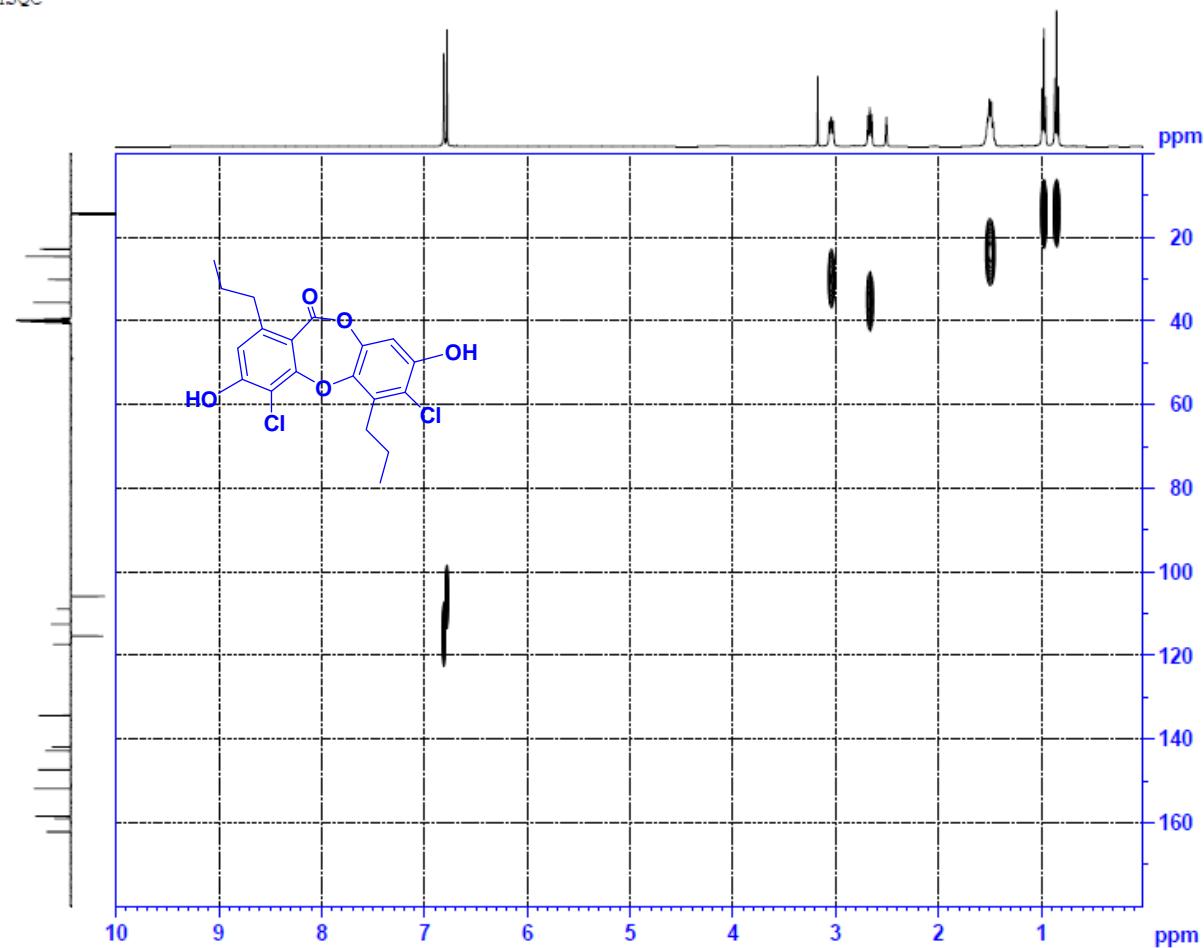


Figure S48. HSQC spectrum of **4** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-1-1-2 COSY

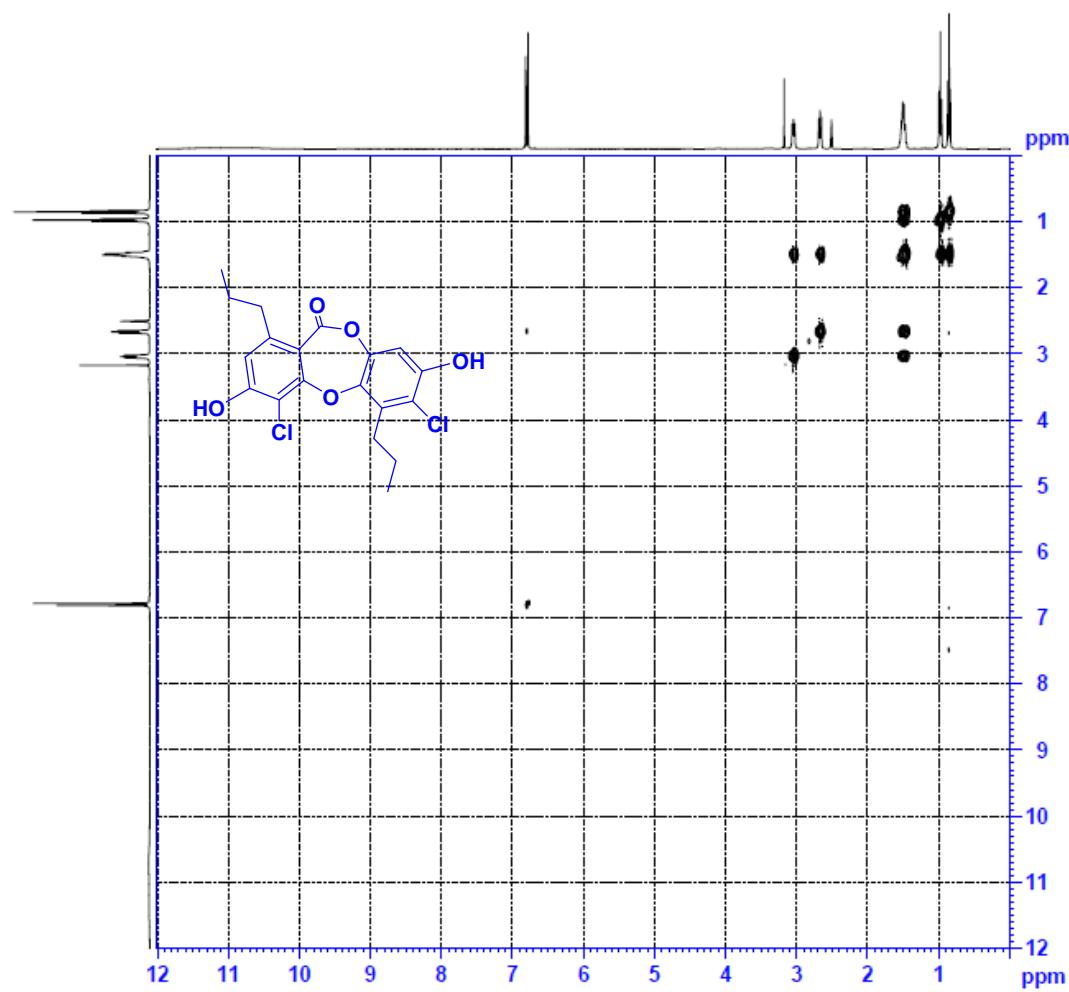


Figure S49. ^1H - ^1H COSY spectrum of **4** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-1-1-2 HMBC

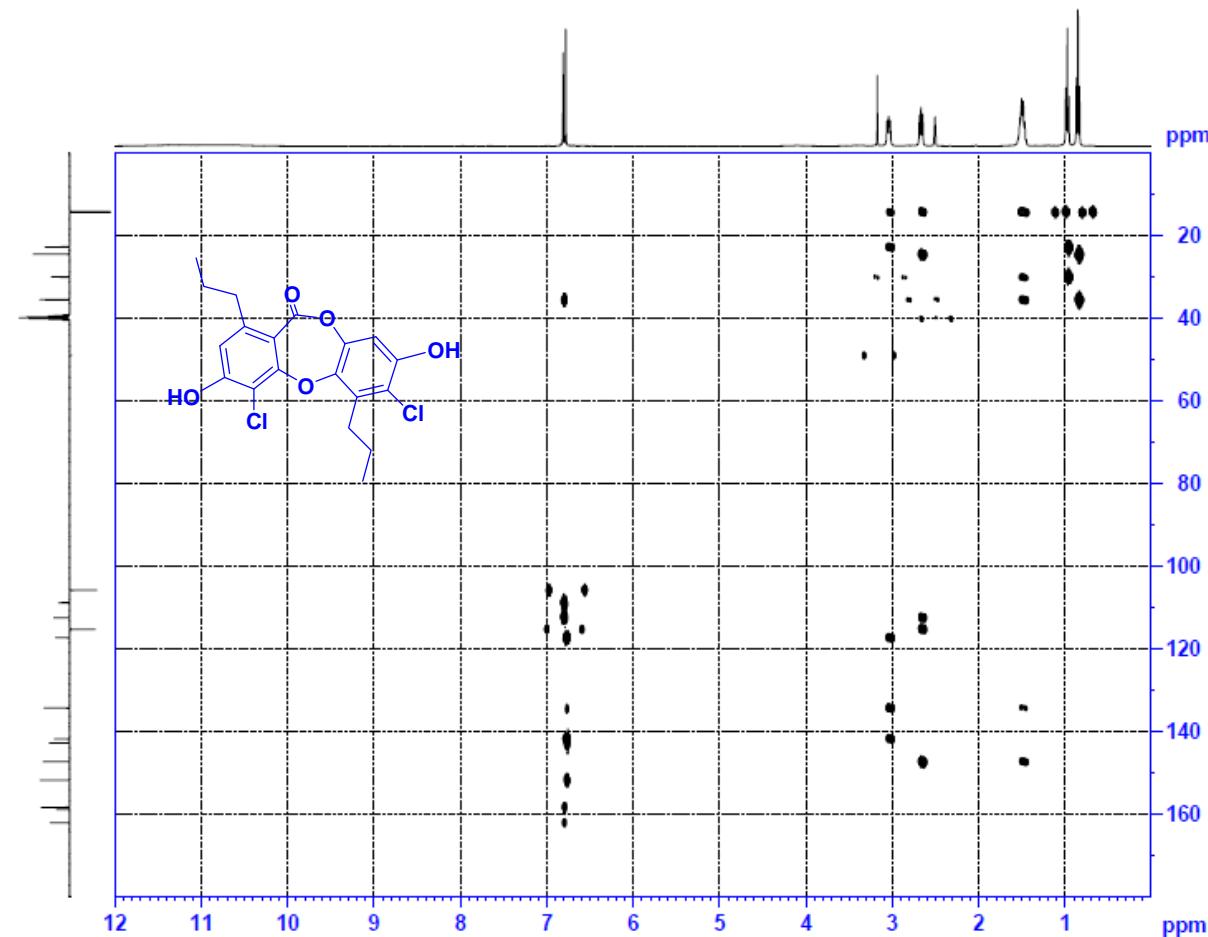
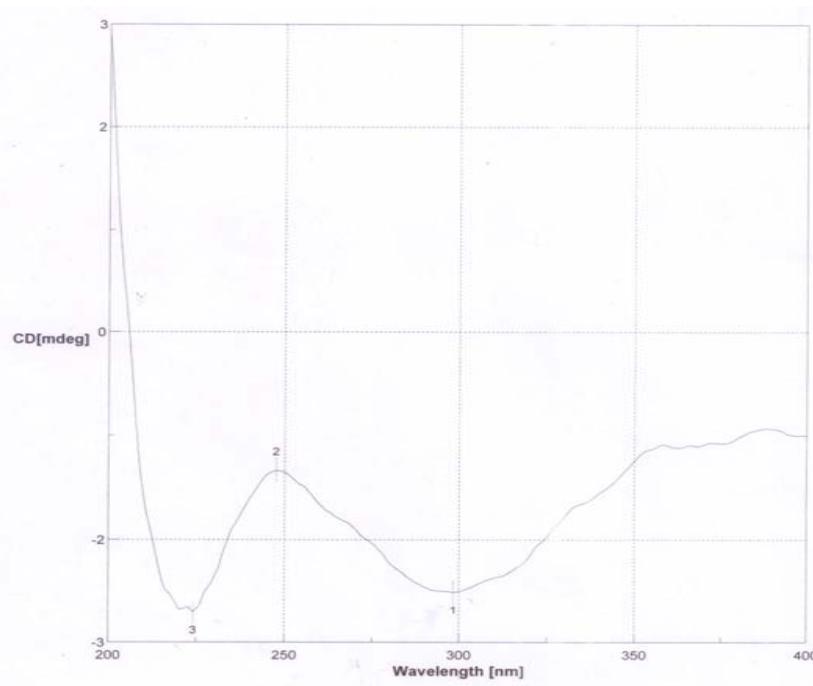


Figure S50. HMBC spectrum of **4** in $\text{DMSO}-d_6$ (400 MHz)



Date/Time 2001-1-3 5:48
Operator
File Name F19-8-18-1-1-2.txt
Sample Name F19-8-18-1-1-2
Comment

No.	nm	CD[mdeg]	No.	nm	CD[mdeg]	No.	nm	CD[mdeg]
1	298.4	-2.5073	2	247.6	-1.33419	3	224.2	-2.70522

Figure S51. CD spectrum of 4

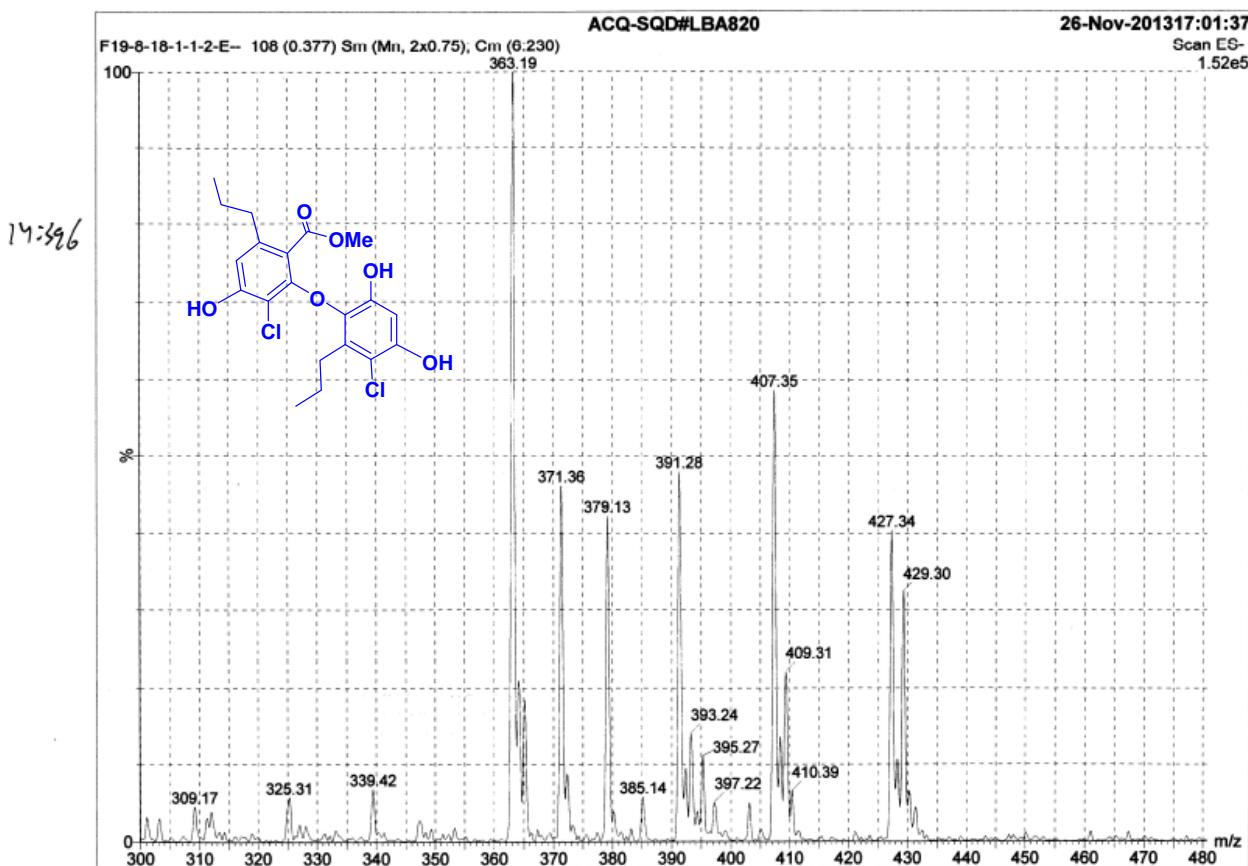


Figure S52. ESIMS spectrum of 4a

F19-8-18-1-1-2-e 400 MHz DMSO

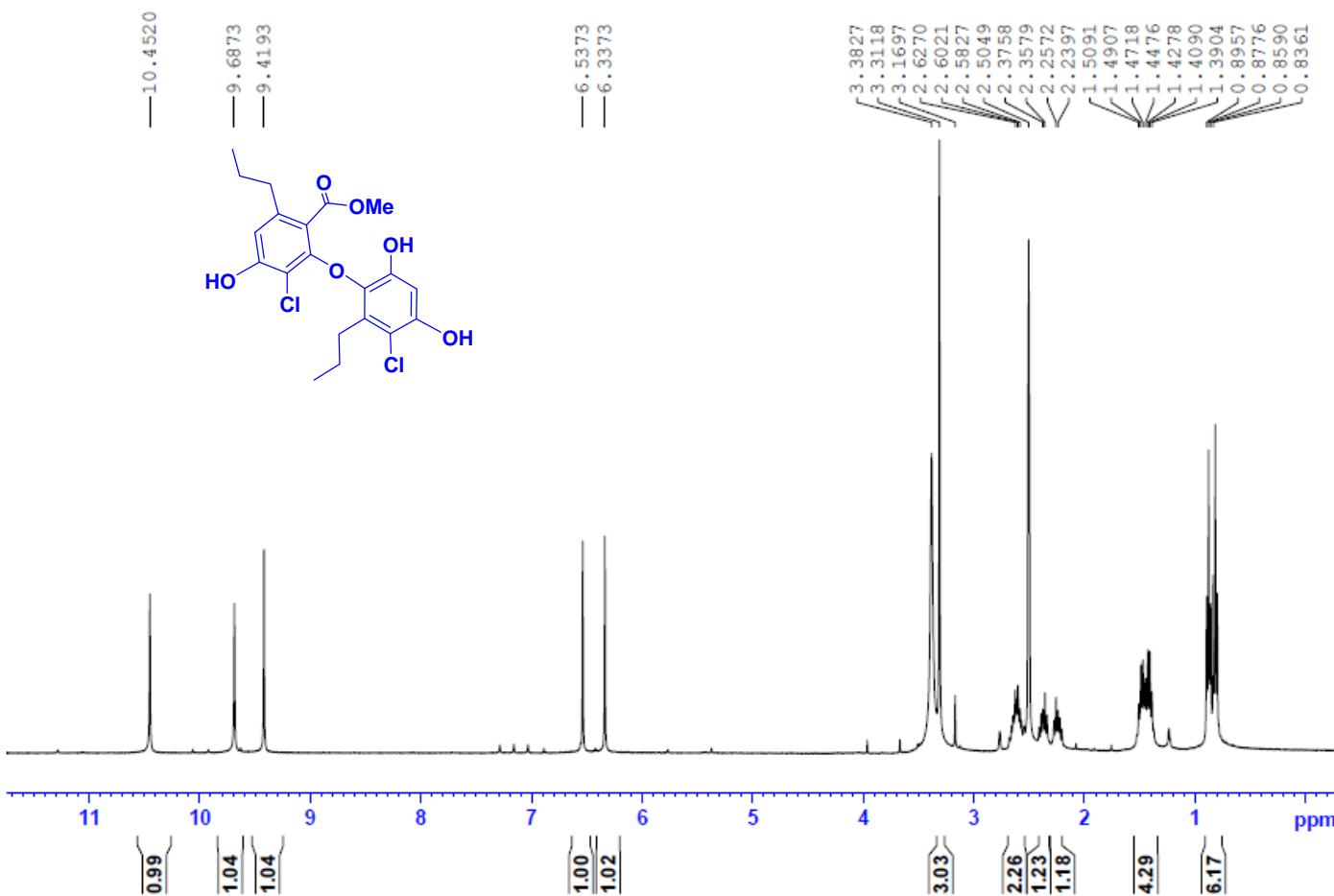


Figure S53. ^1H NMR spectrum of **4a** in $\text{DMSO}-d_6$ (400 MHz)

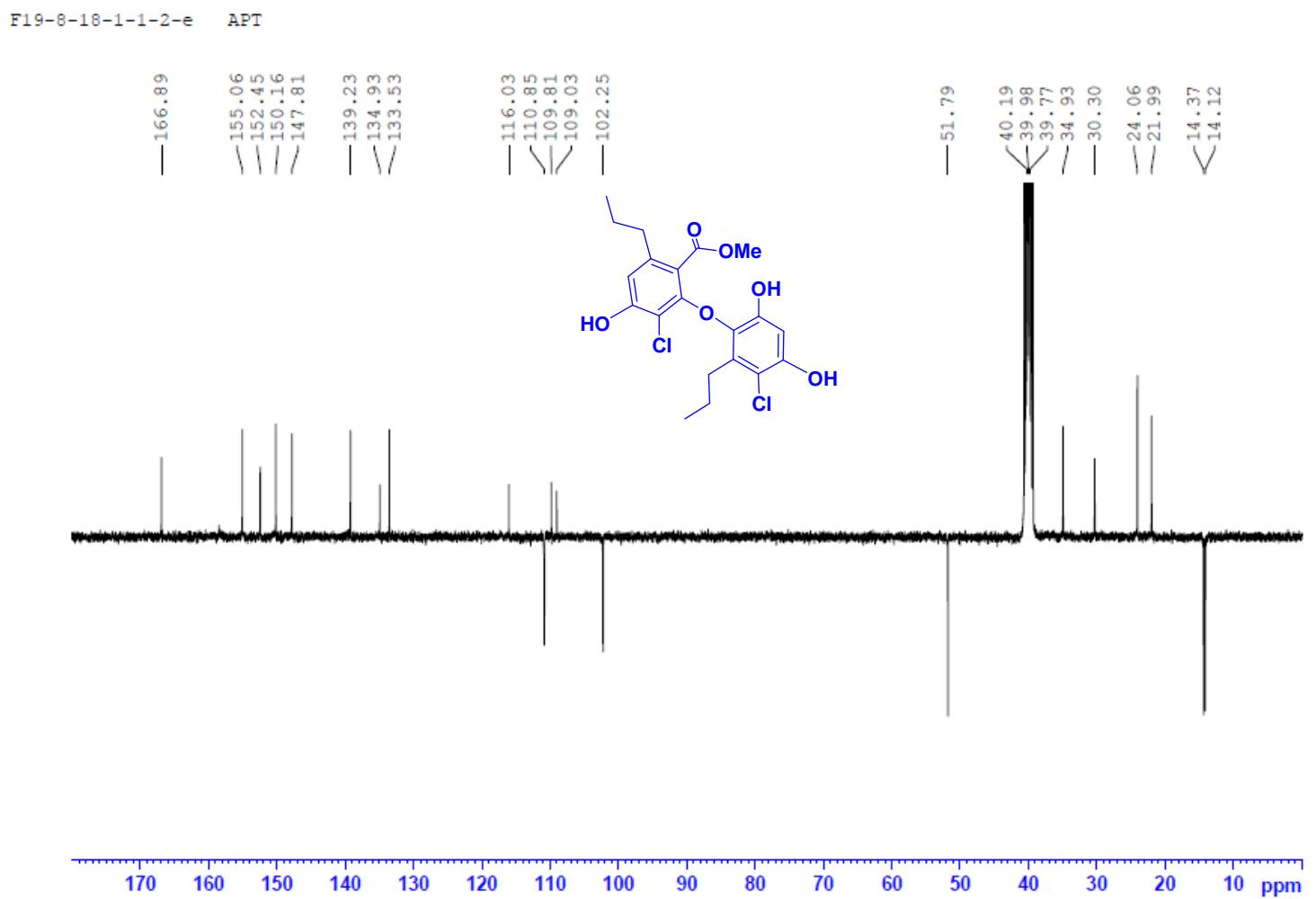


Figure S54. APT spectrum of **4a** in DMSO-*d*₆(100 MHz)

F19-8-18-1-1-2-e HSQC

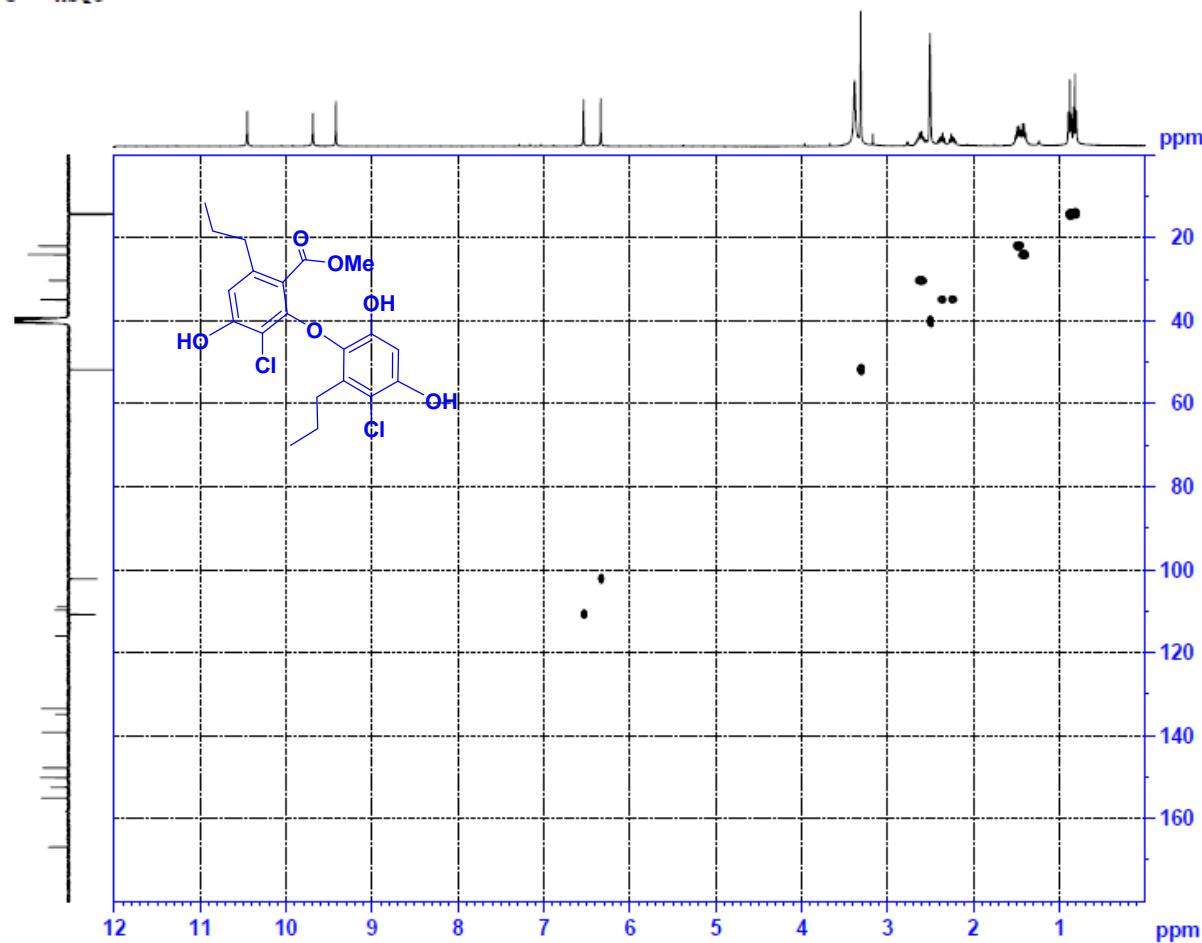


Figure S55. HSQC spectrum of **4a** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-1-1-2-e COSY

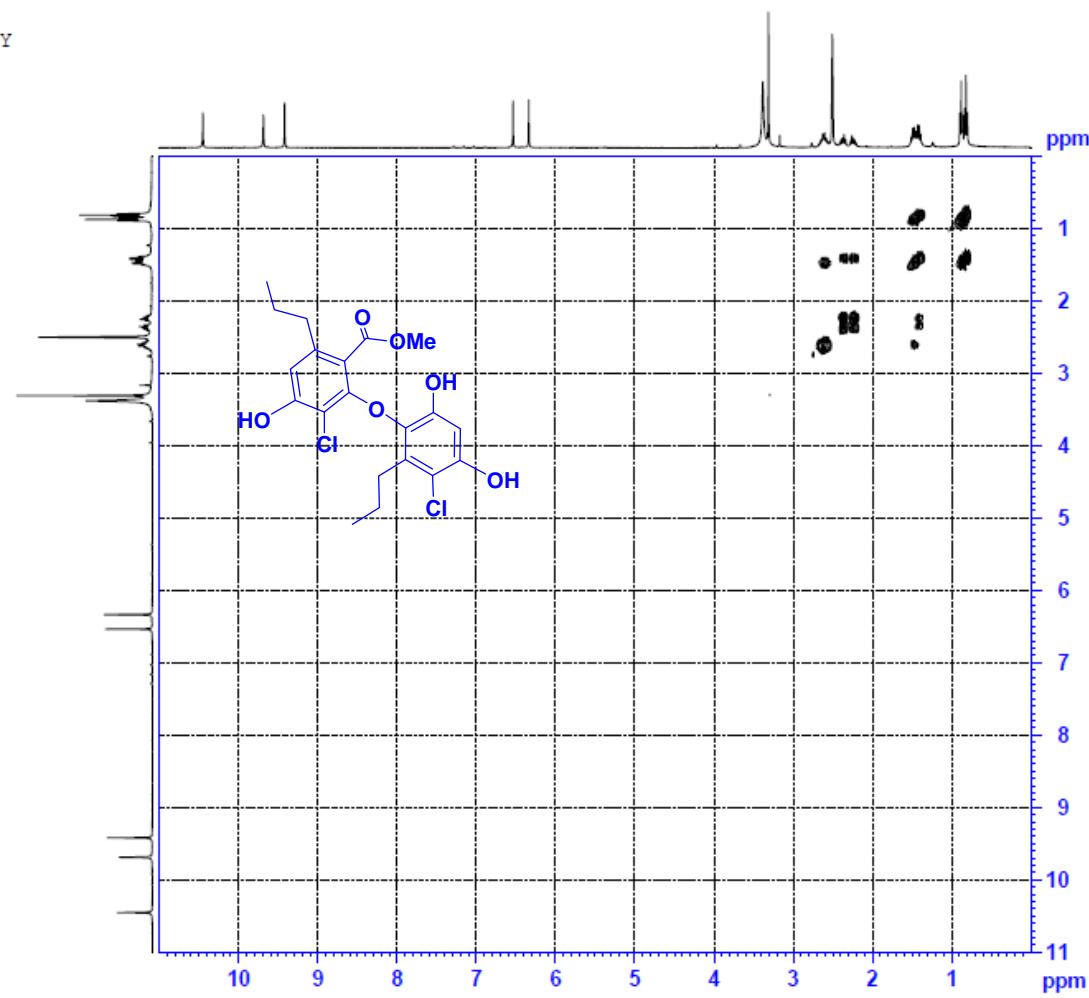


Figure S56. ^1H - ^1H COSY spectrum of **4a** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-1-1-2-e HMBC

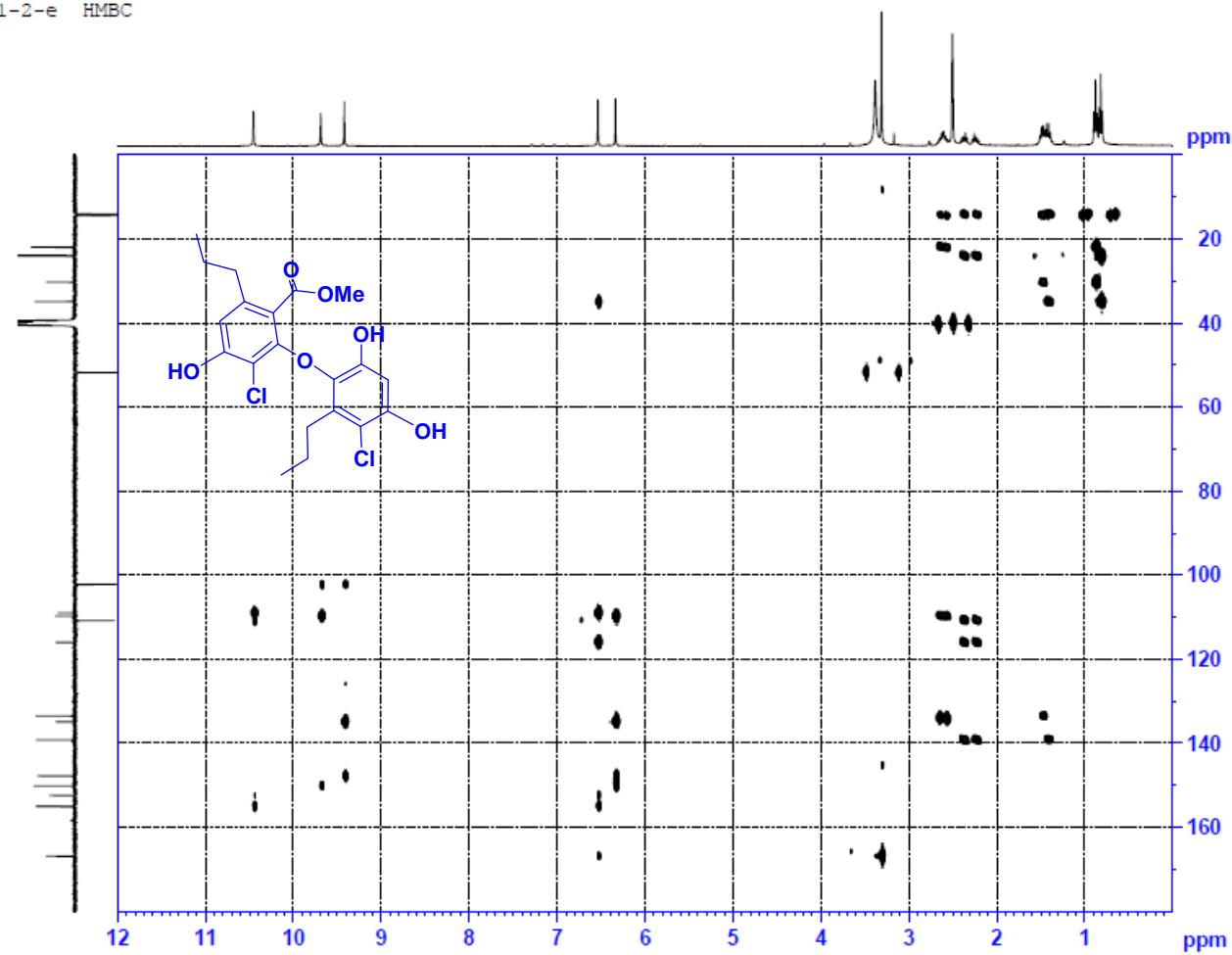


Figure S57. HMBC spectrum of **4a** in $\text{DMSO}-d_6$ (400 MHz)

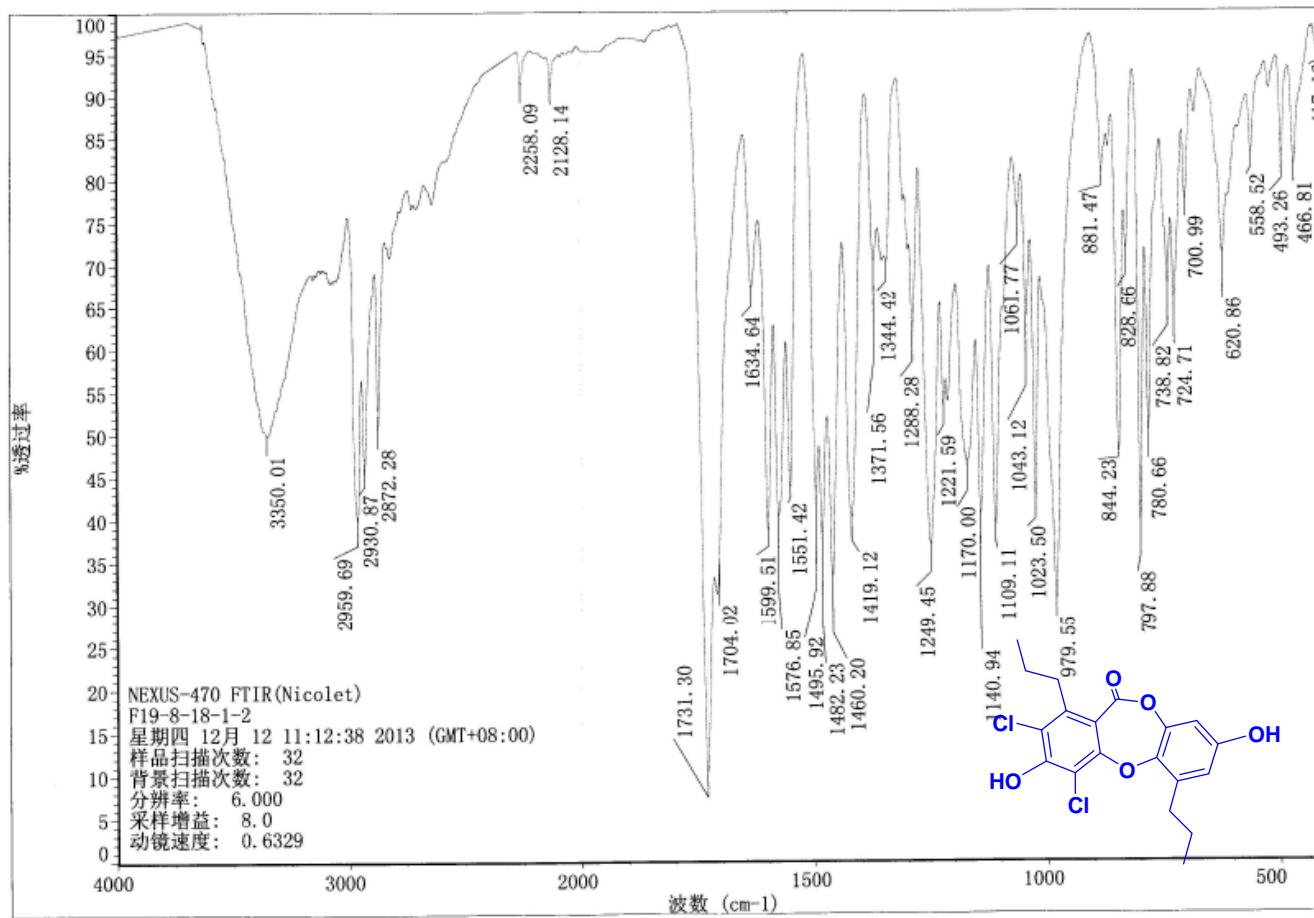


Figure S58. IR spectrum of 5



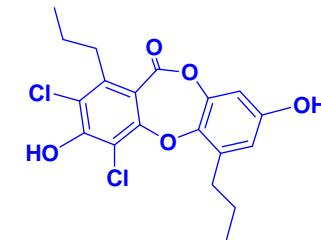
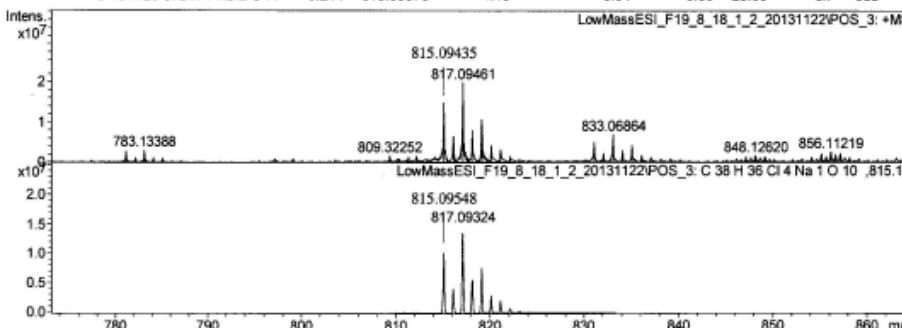
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Analysis Name C:\data_sample\ESI_12131120_30\LowMassESI_F19_8_18_1_2_20131122\POS_3
Acquisition Date 11/22/2013 10:12:26 AM
Operator bpxsh@bjmu.edu.cn; Tel:010-82801
Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI □ C19H18O5Cl2 MW 396.05
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;8.26.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result Exact Mass Measured Mass Error (mDa) Error (ppm) Description

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 40 H 35 Cl 4 O 10	0.017	815.09788	4.34	0.15	3.54	21.50	ok	even
C 38 H 36 Cl 4 Na 1 O 10	0.019	815.09548	1.39	-2.83	1.13	18.50	ok	even
C 38 H 32 Cl 3 N 1 O 13	0.100	815.09337	-1.19	-4.63	-0.97	22.00	ok	odd
C 40 H 33 Cl 3 Na 3 O 8	0.103	815.09286	-1.82	-5.29	-1.48	21.50	ok	even
C 38 H 34 Cl 3 Na 4 O 8	0.105	815.09046	-4.77	-8.25	-3.89	18.50	ok	even
C 39 H 30 Cl 2 Na 1 O 14	0.214	815.09048	-4.74	-7.23	-3.86	23.50	ok	even
C 40 H 29 Cl 2 N 1 Na 2 O 11	0.214	815.09076	-4.40	-6.94	-3.59	25.00	ok	odd





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Analysis Name C:\data_sample\ESI_12131120_30\LowMassESI_F19_8_18_1_2_20131122\POS_3 Acquisition Date 11/22/2013 10:12:26 AM
Operator bpxsh@bjmu.edu.cn; Tel:010-82801
Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI □ C19H18O5CL2 MW 396.05
CAL588: 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;8;26.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result	Exact Mass	Measured Mass	Error (mDa)	Error (ppm)	Description
	397.06041	397.06091	-0.50	-1.27	M+H;e

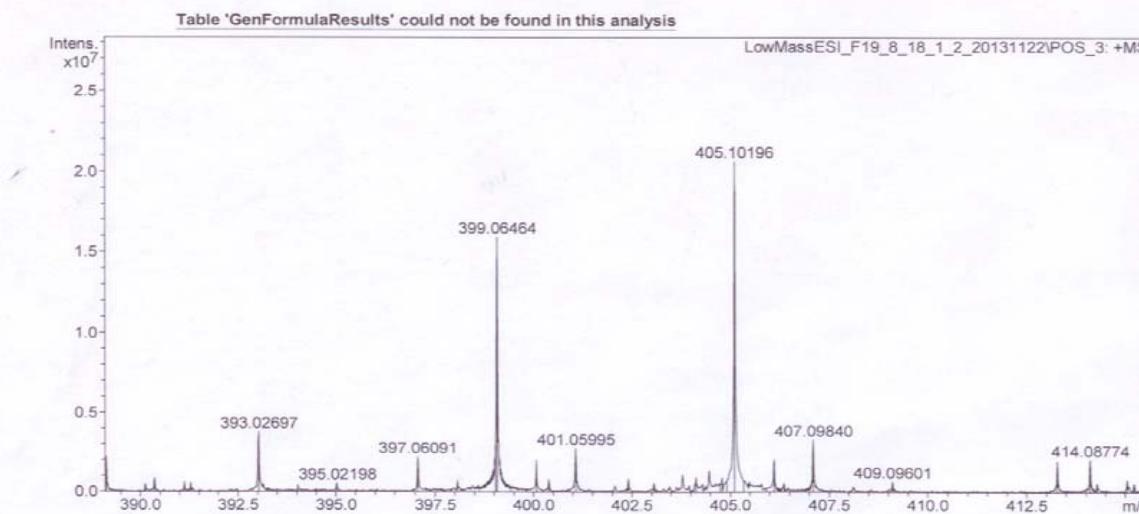


Figure S59. HRESIMS spectrum of 5

F19-8-18-1-2 400 MHz DMSO

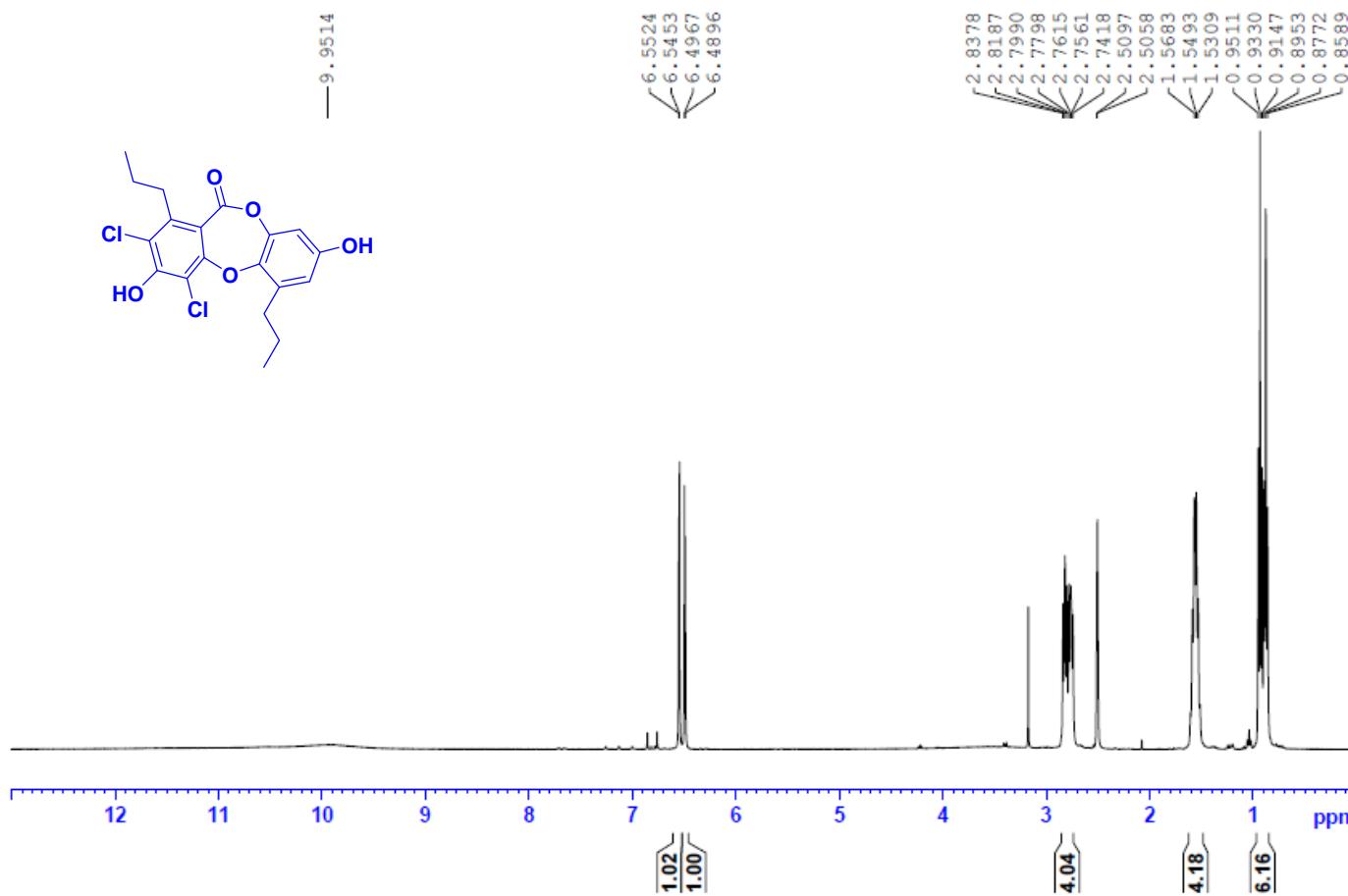


Figure S60. ^1H NMR spectrum of **5** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-1-2 APT

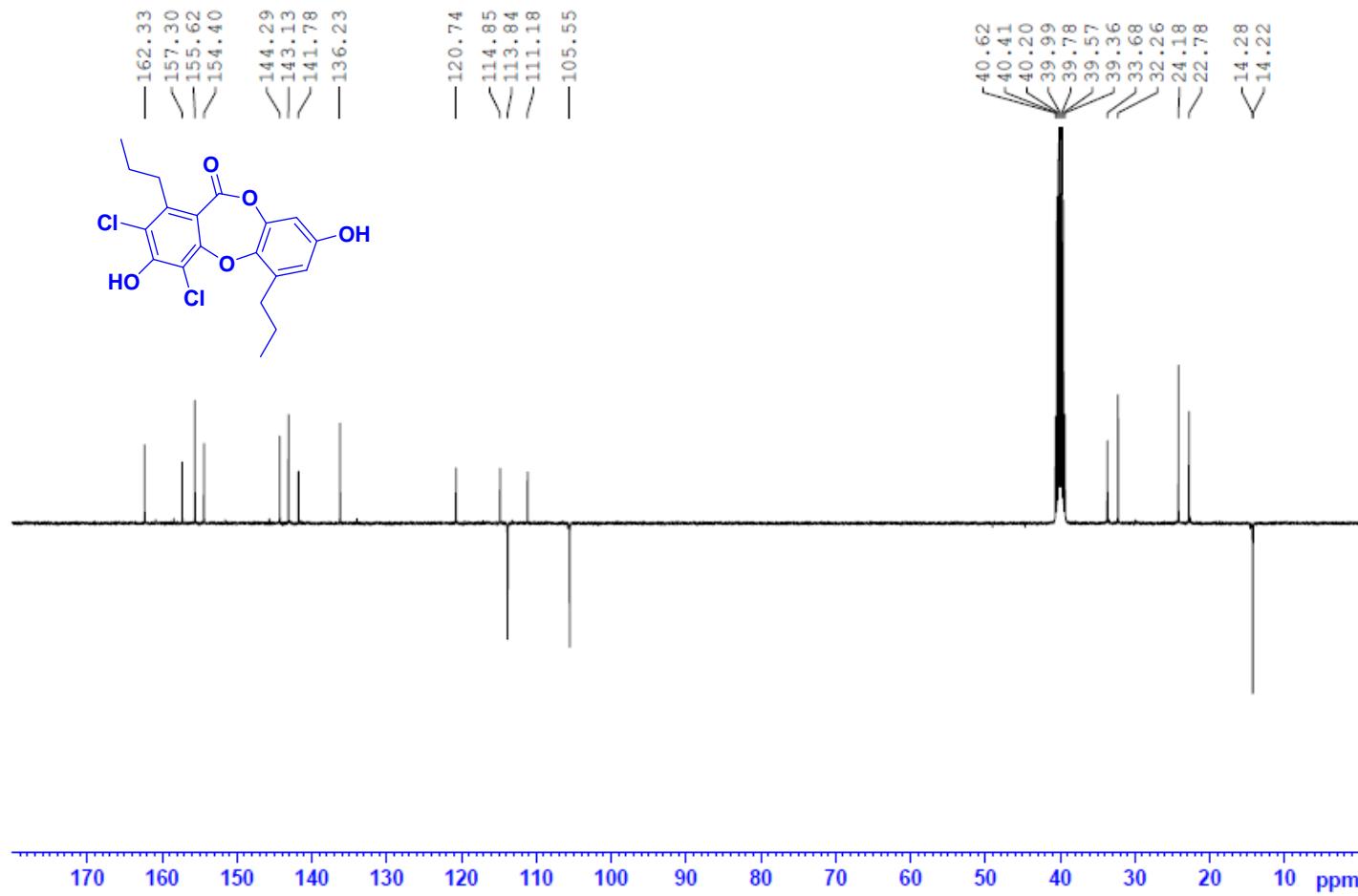


Figure S61. APT spectrum of **5** in $\text{DMSO}-d_6$ (100 MHz)

F19-8-18-1-2 HSQC

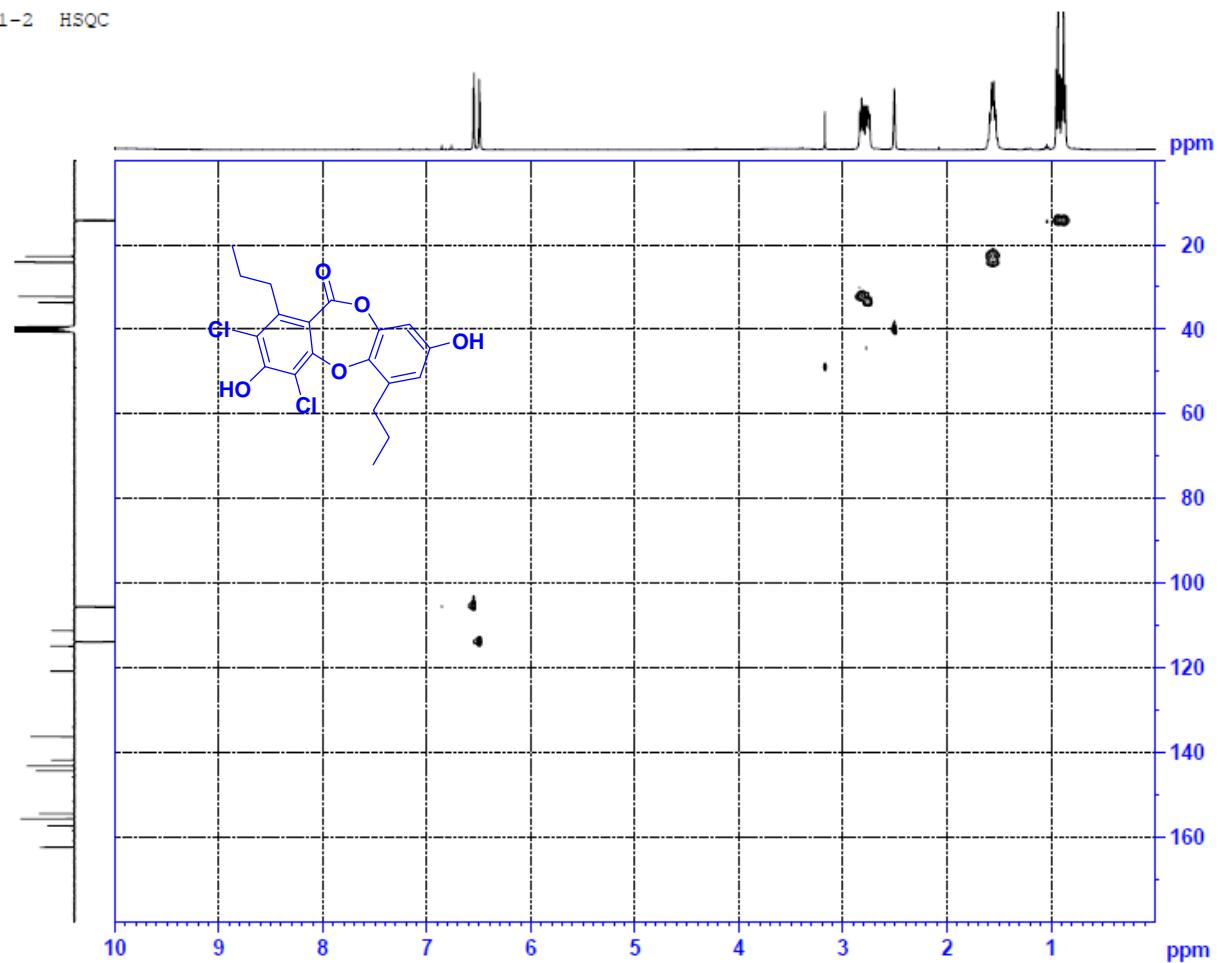


Figure S62. HSQC spectrum of **5** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-1-2 COSY

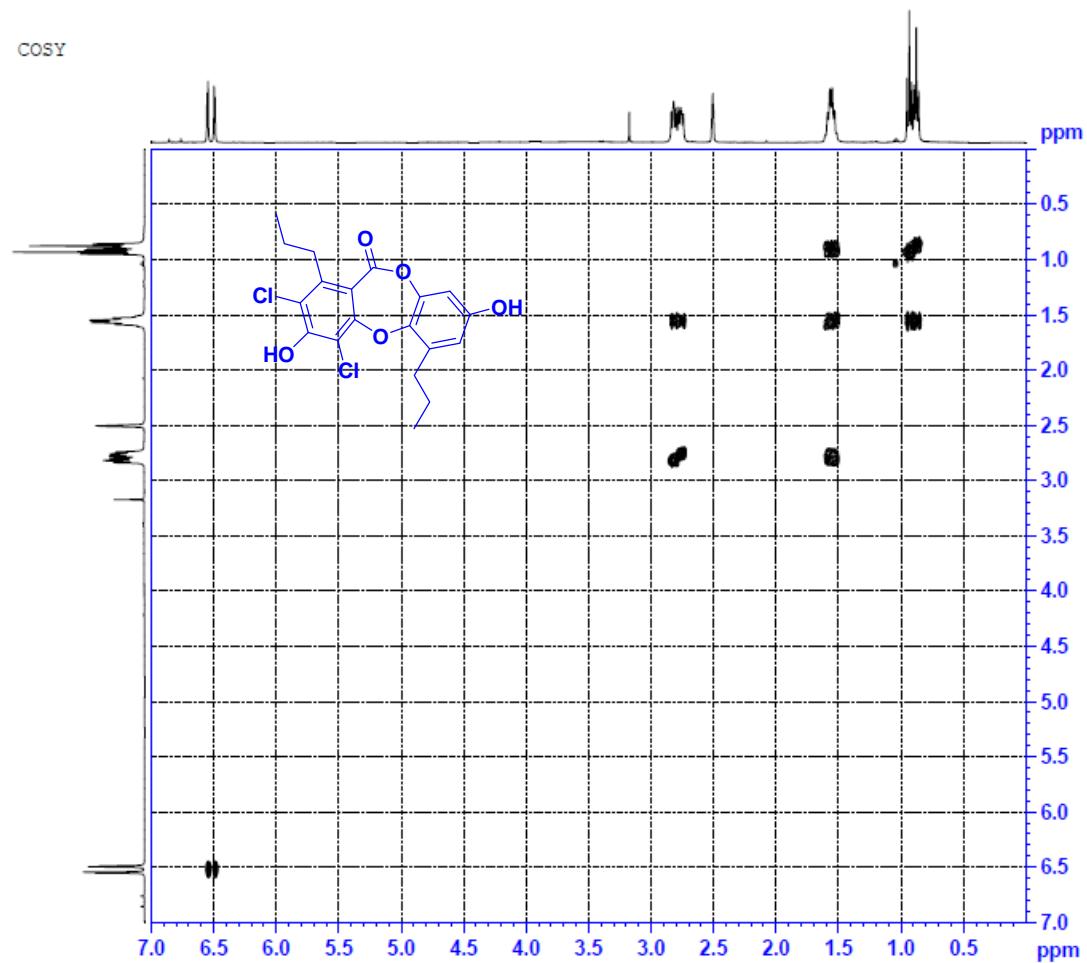


Figure S63. ^1H - ^1H COSY spectrum of **5** in $\text{DMSO}-d_6$ (400 MHz)

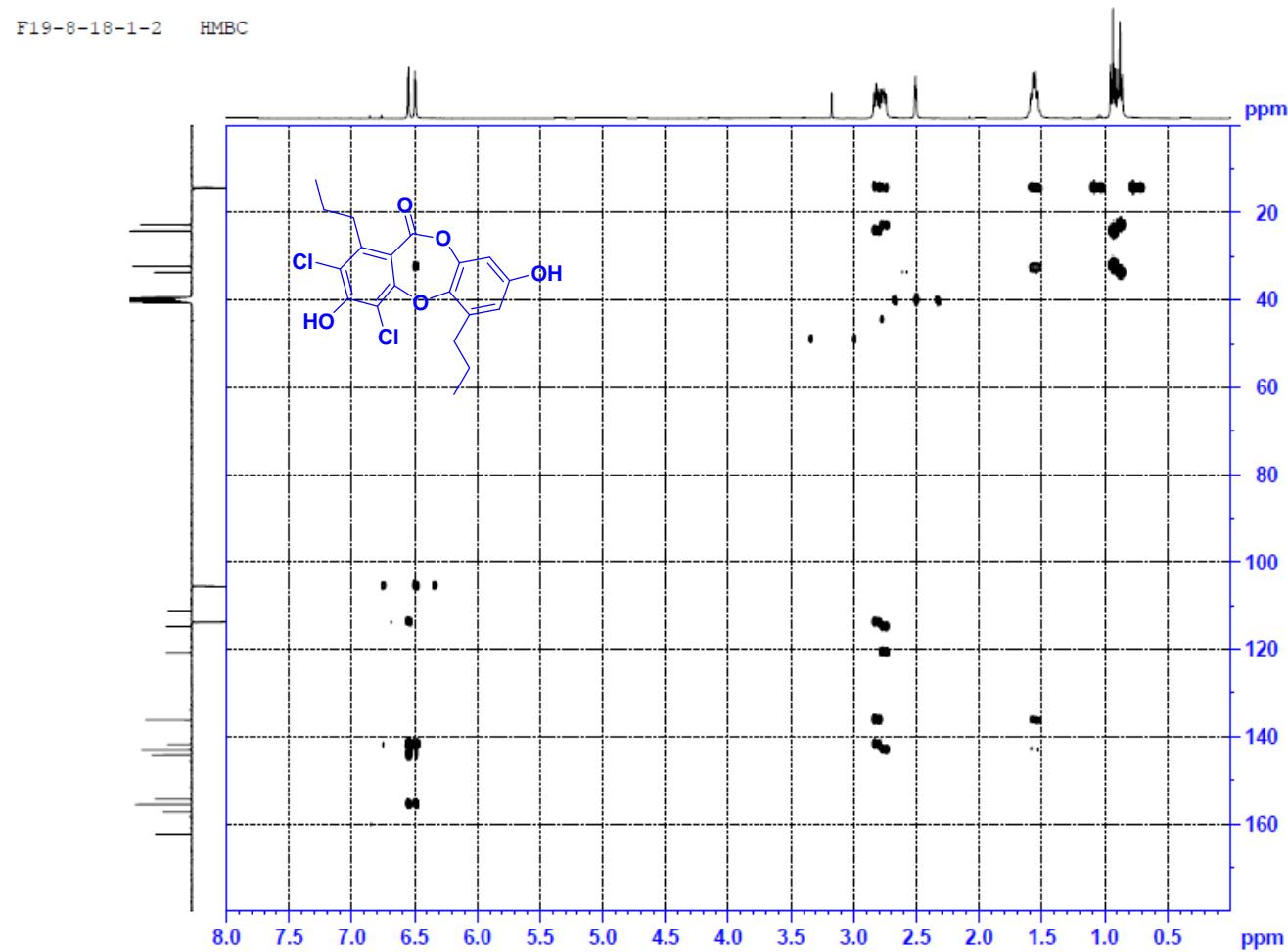
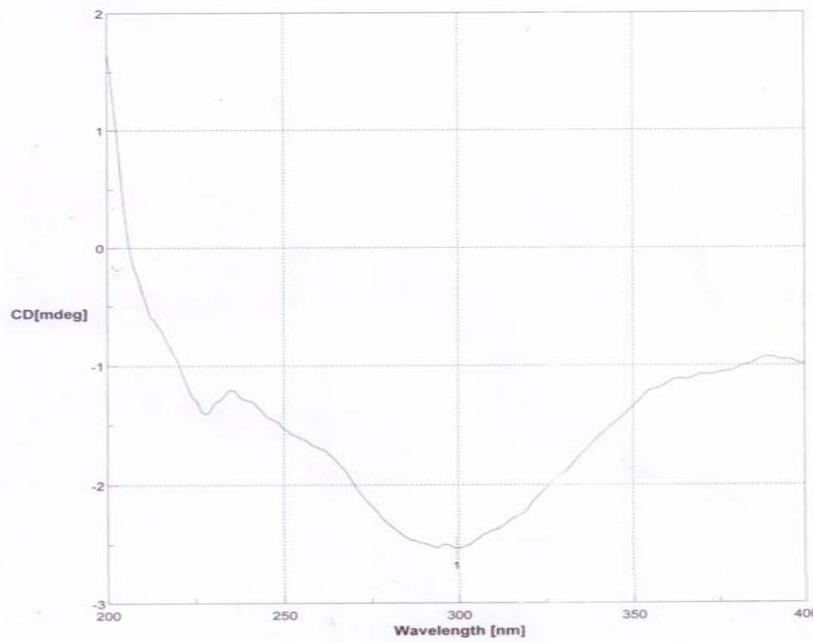


Figure S64. HMBC spectrum of **5** in $\text{DMSO}-d_6$ (400 MHz)



Date/Time 2001-1-3 5:15
Operator
File Name F19-8-18-1-2.txt
Sample Name F19-8-18-1-2
Comment

No. nm CD[mdeg]
1 299.4 -2.53153

Figure S65. CD spectrum of **5**

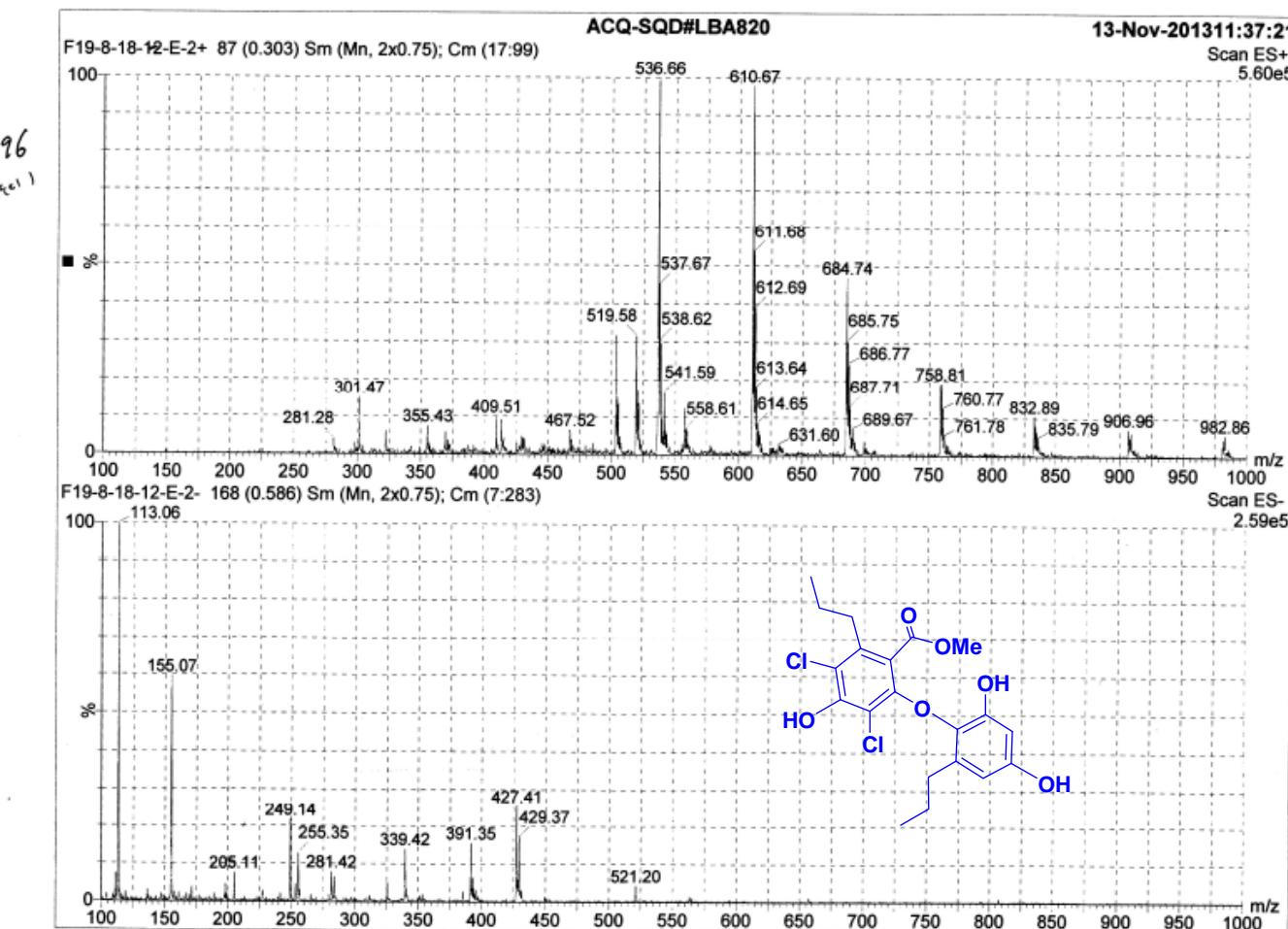


Figure S66. ESIMS spectrum of **5a**

F19-8-18-1-2-e-1 400 MHz DMSO

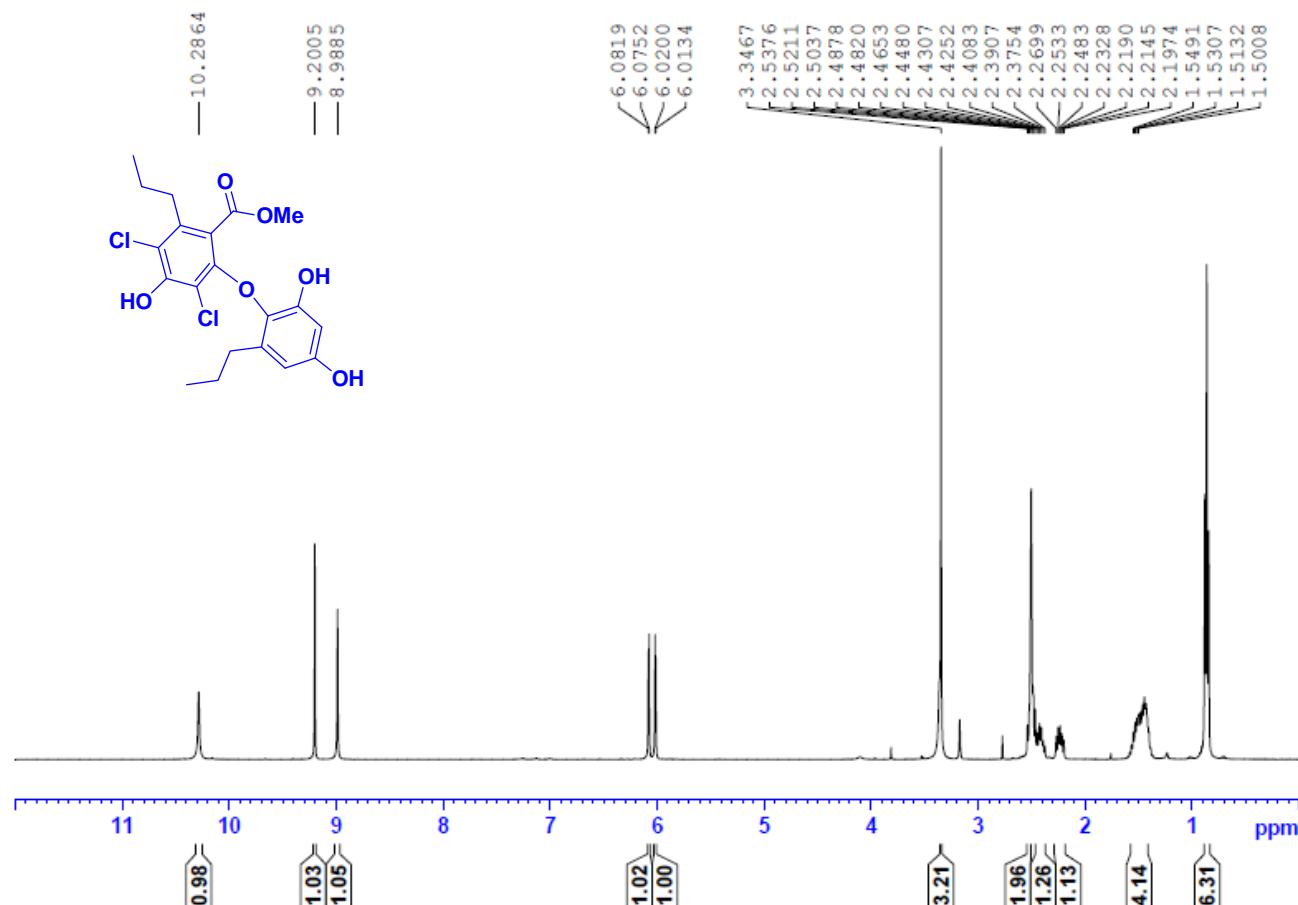


Figure S67. ^1H NMR spectrum of **5a** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-1-2-e-1 APT

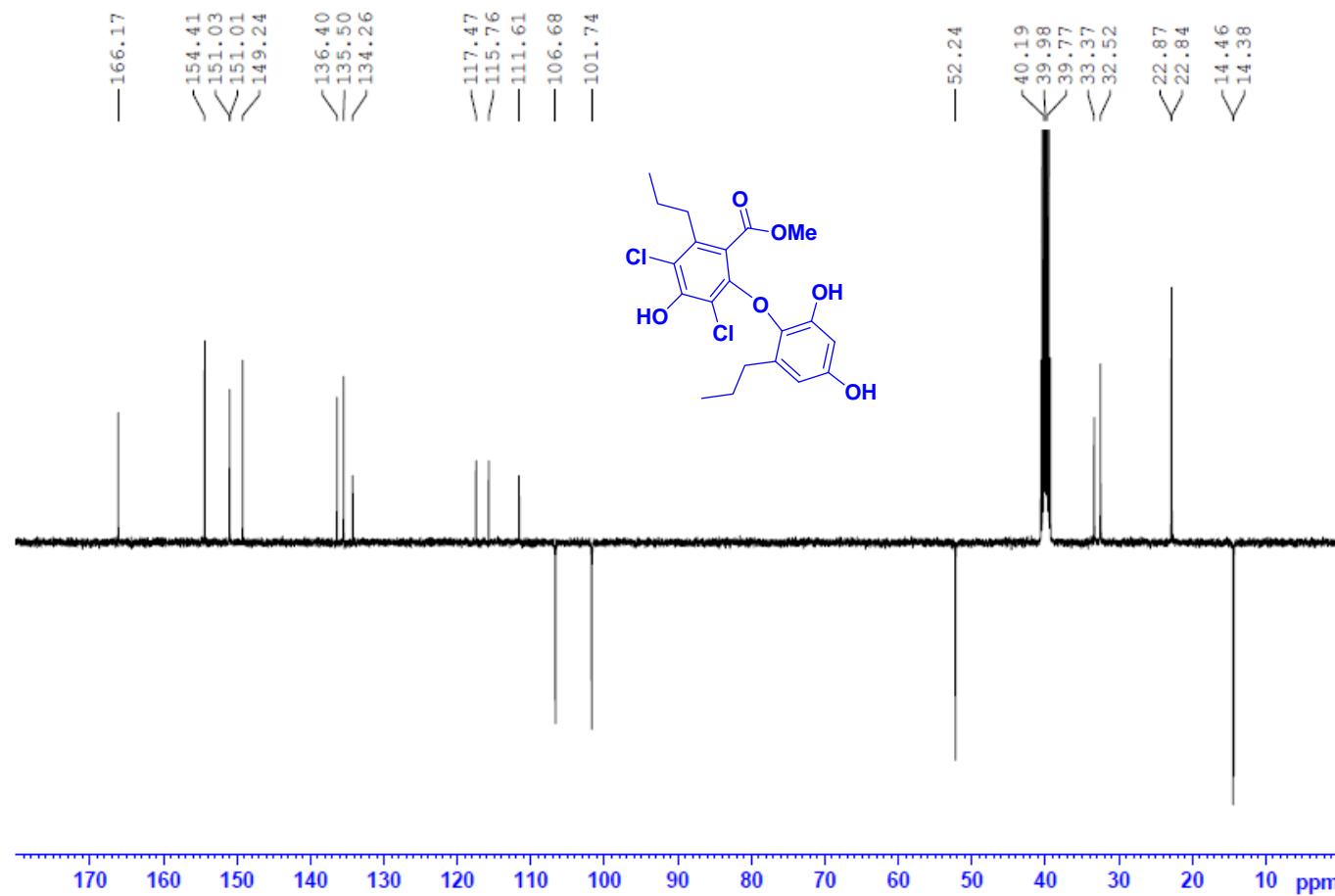


Figure S68. APT spectrum of **5a** in DMSO-*d*₆ (100 MHz)

F19-8-18-1-2-e-1 HSQC

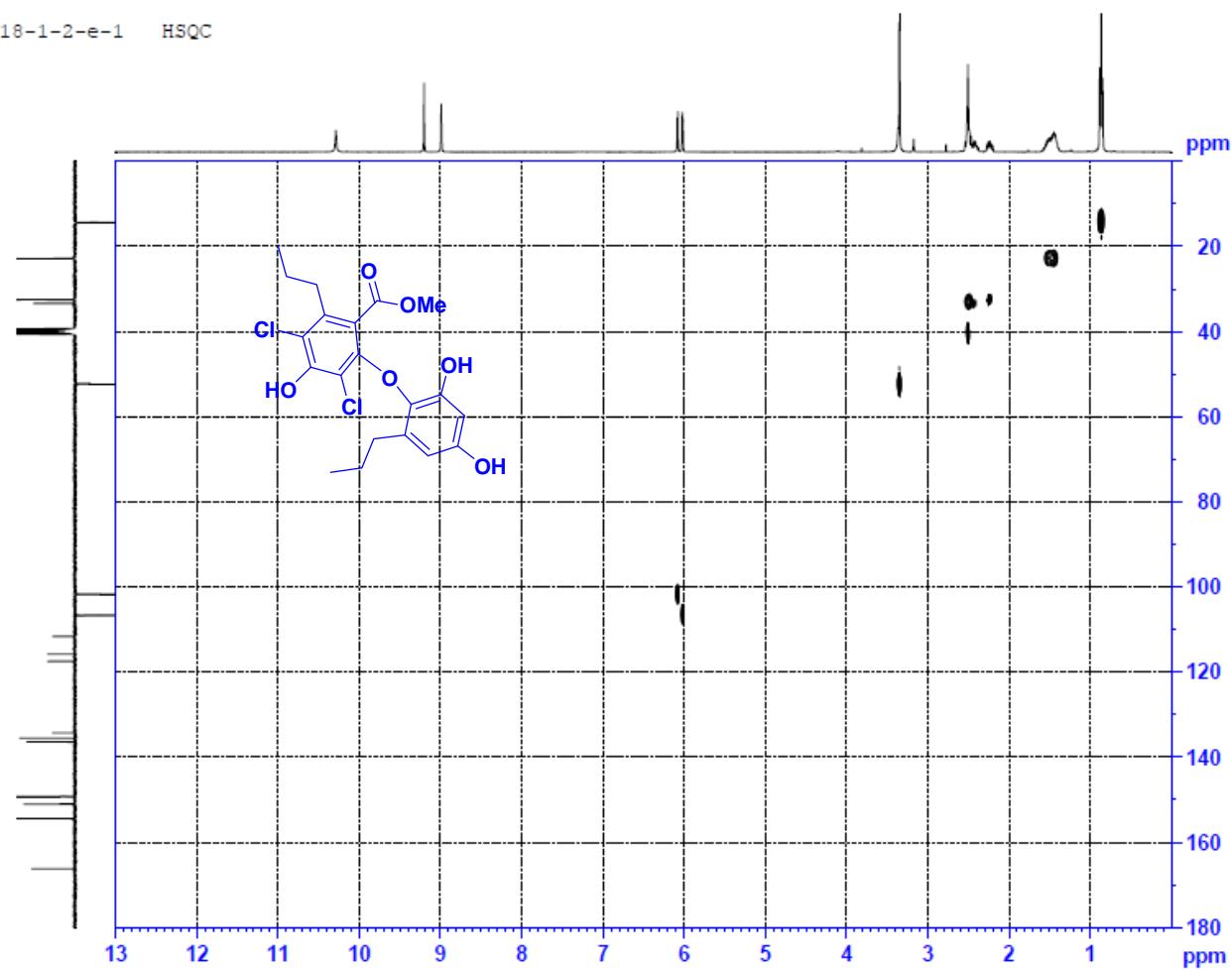


Figure S69. HSQC spectrum of **5a** in DMSO-*d*₆ (400 MHz)

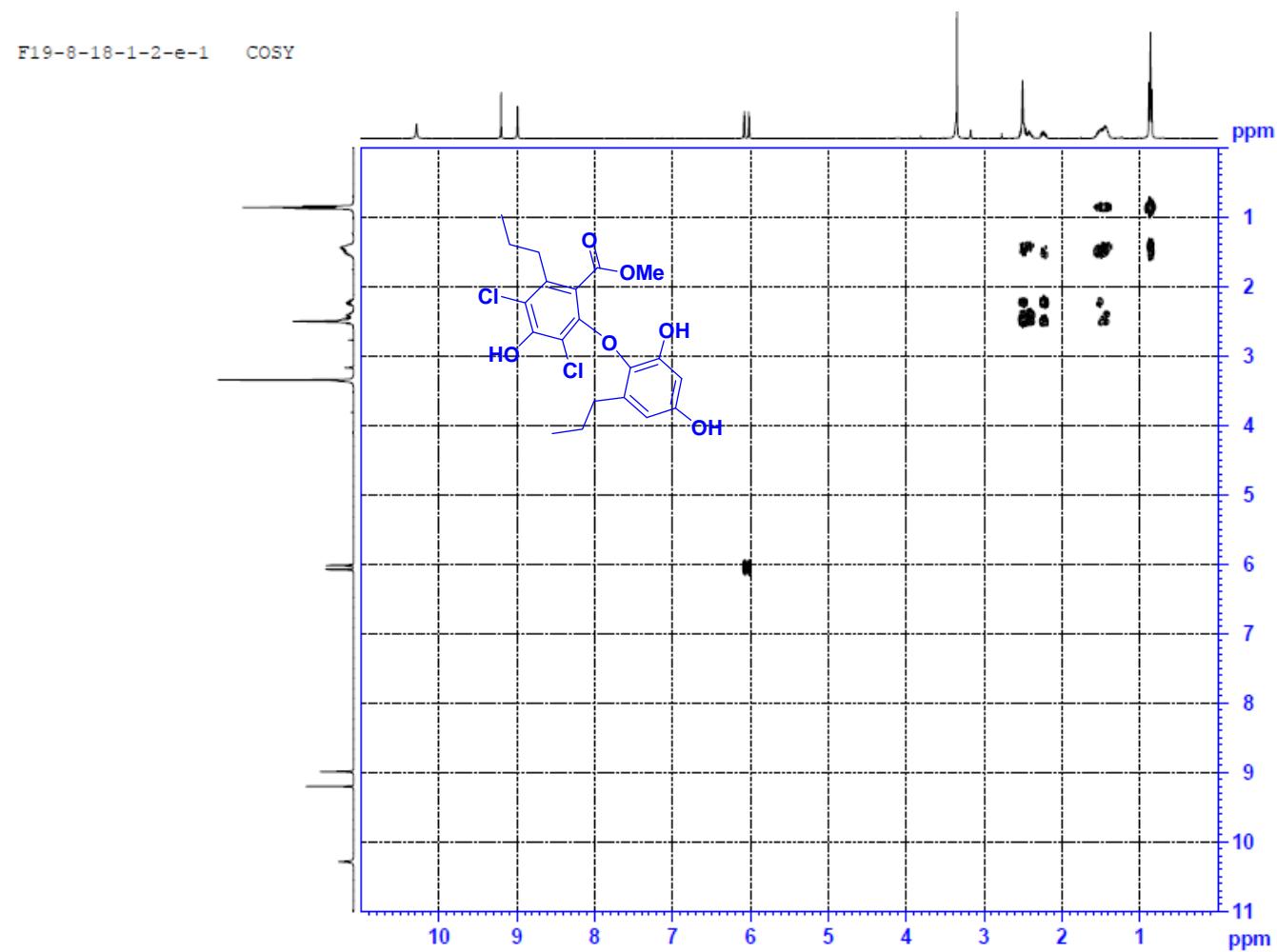


Figure S70. ^1H - ^1H COSY spectrum of **5a** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-1-2-e-1 HMBC

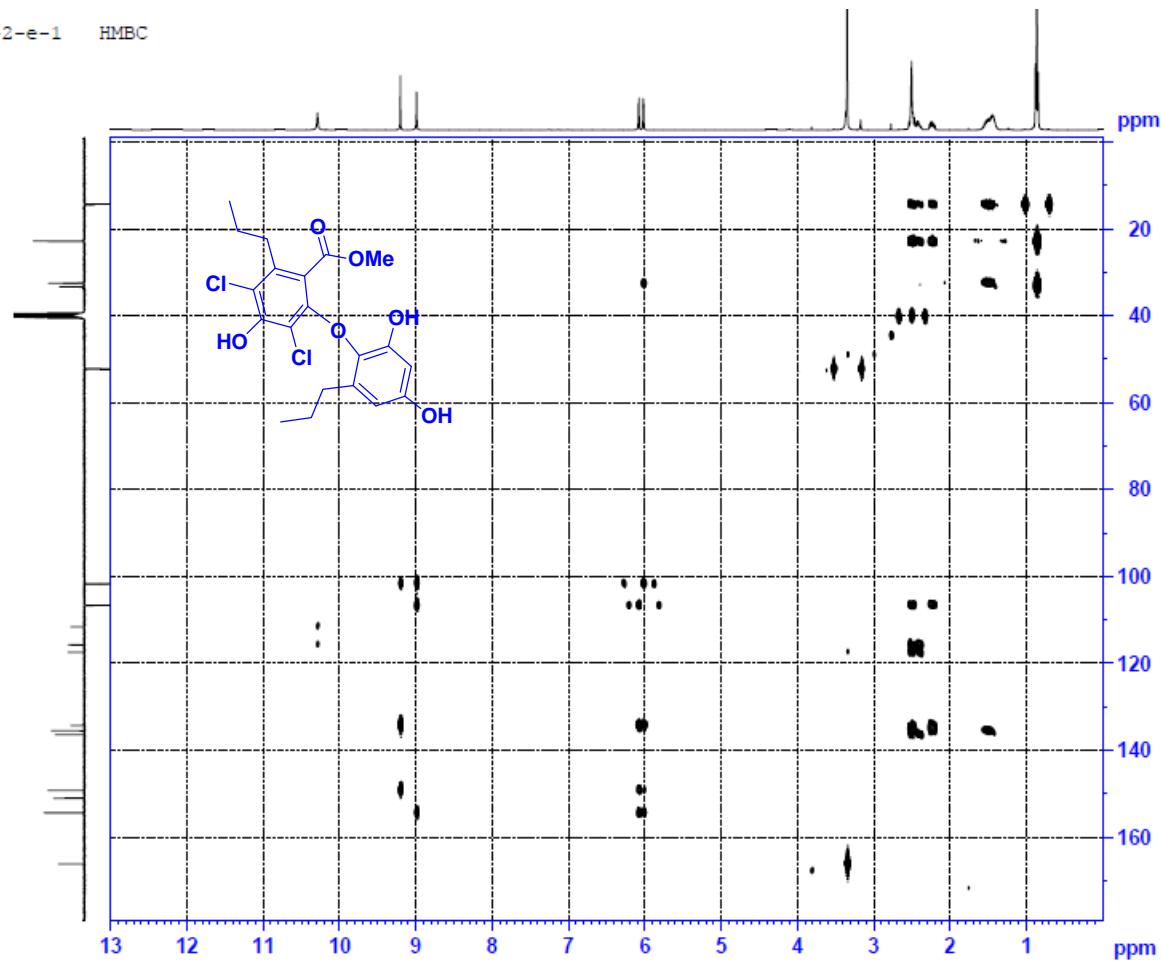


Figure S71. HMBC spectrum of **5a** in $\text{DMSO}-d_6$ (400 MHz)

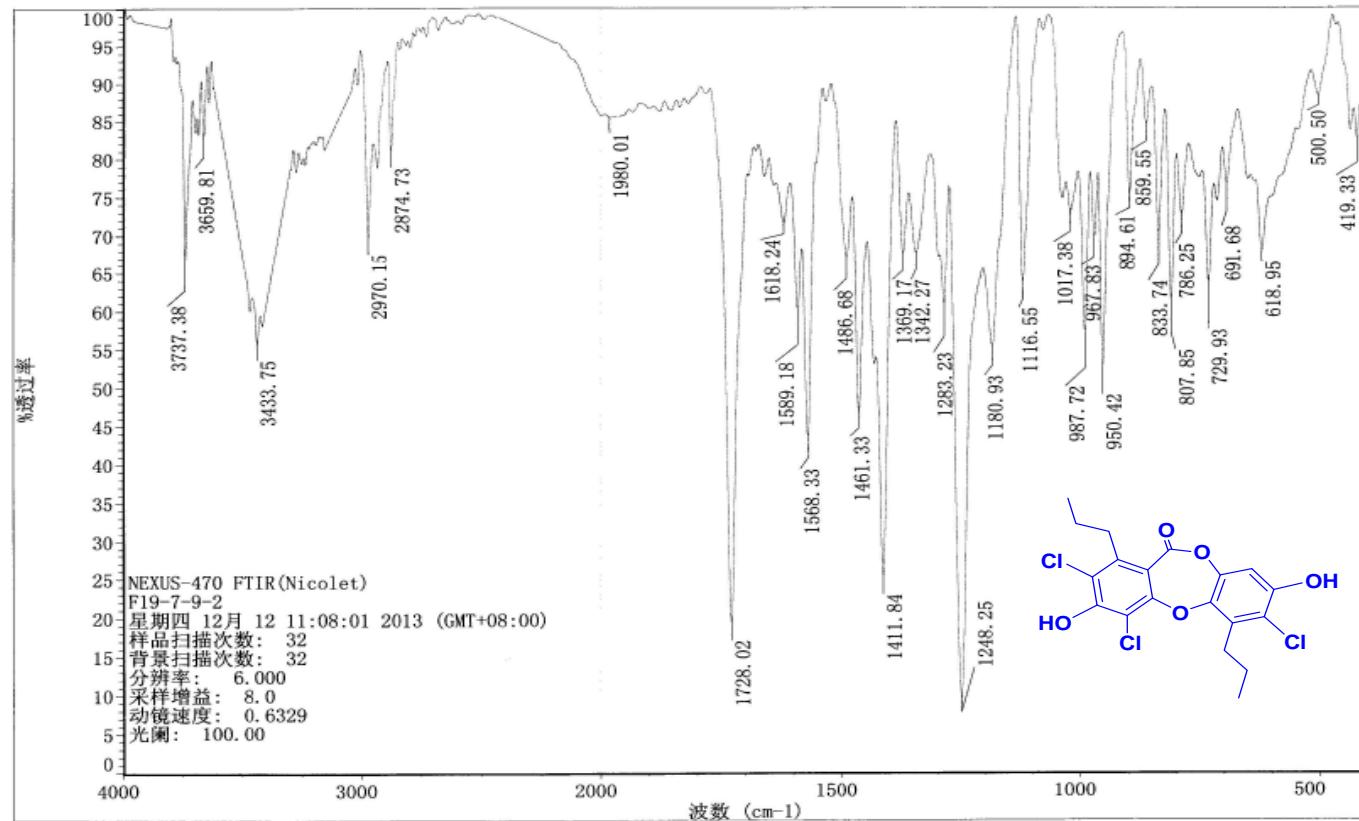


Figure S72. IR spectrum of **6**



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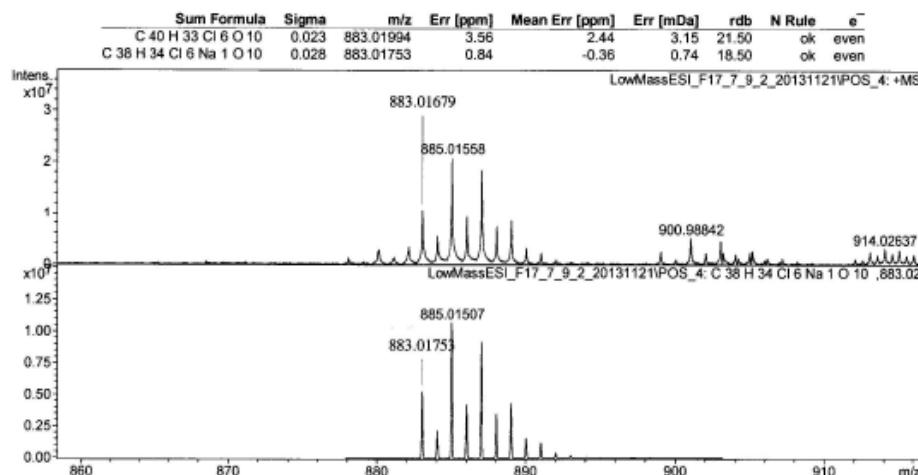
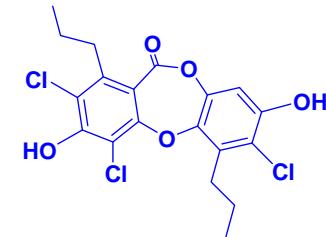
Analysis Name C:\data\sample\ESI_12131120_30\LowMassESI_F17_7_9_2_20131121\POS_4 Acquisition Date 11/20/2013 2:31:22 PM

Operator bpxsh@bjmu.edu.cn; Tel:010-82801

Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI pos □ C19H17CL3O5 MW 430
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;826.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result Exact Mass Measured Mass Error (mDa) Error (ppm) Description





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Analysis Name C:\data_sample\ESI_12131120_30\LowMassESI_F17_7_9_2_20131121\POS_4 Acquisition Date 11/20/2013 2:31:22 PM
Operator bpxsh@bjmu.edu.cn; Tel:010-82801
Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI pos □ C19H17CL3O5 MW 430
CAL588: 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;826.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result Exact Mass Measured Mass Error (mDa) Error (ppm) Description

431.02143 □□□□□□ 431.02178 □□□□□□ -0.35 □□□□□□□□ -0.80 □□□□□□□□ M+H;-e

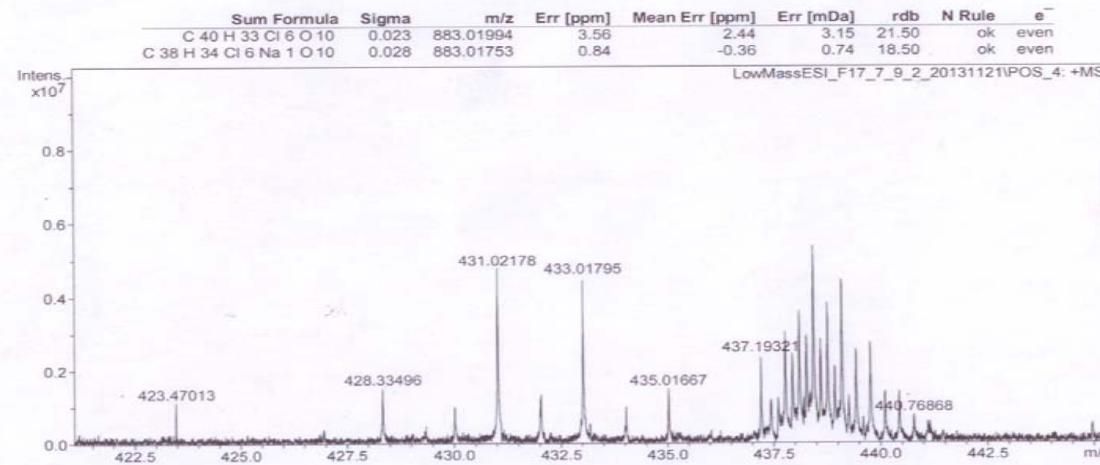


Figure S73. HRESIMS spectrum of 6

F19-7-9-2 400 MHz DMSO

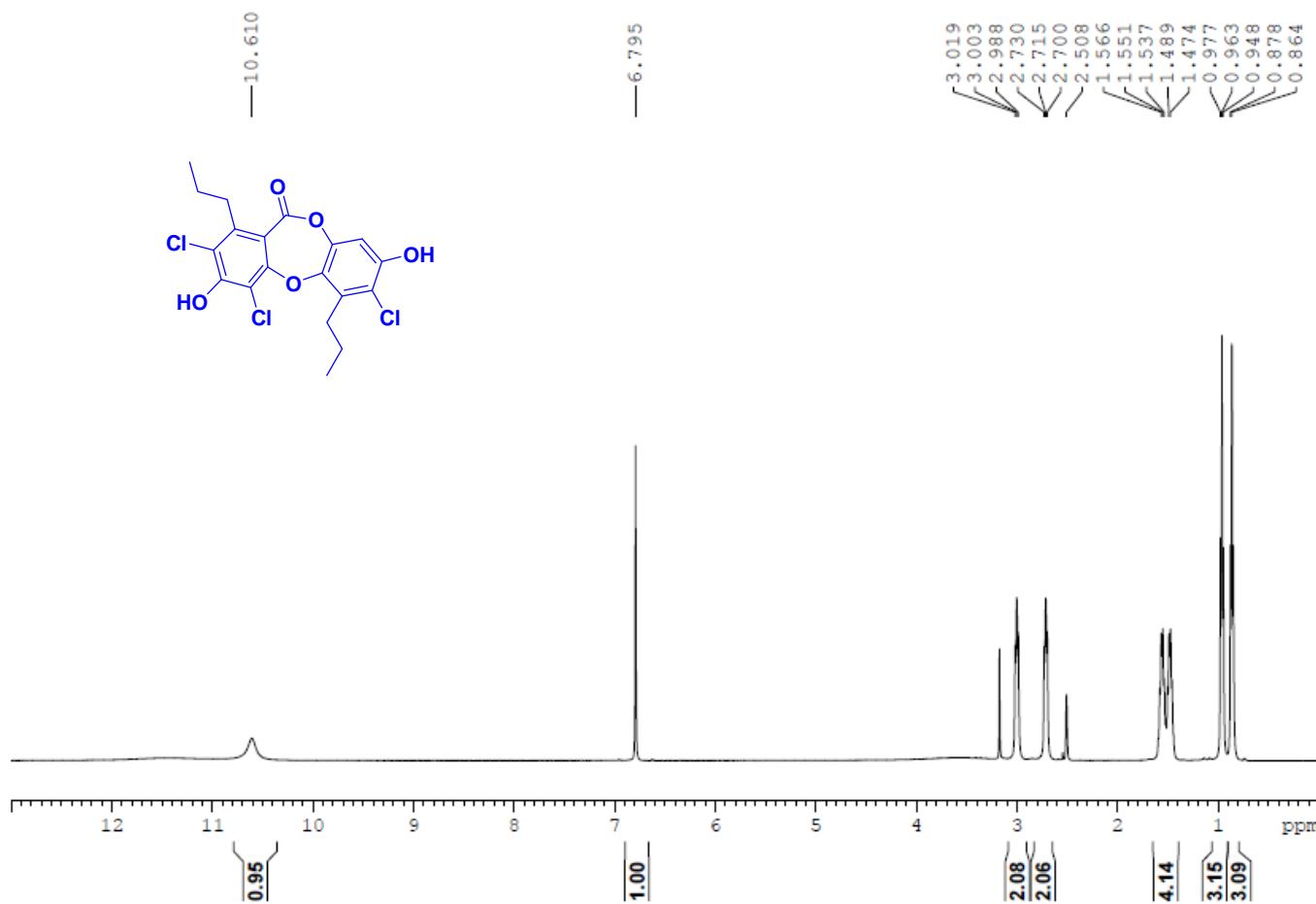


Figure S74. ^1H NMR spectrum of **6** in $\text{DMSO}-d_6$ (400 MHz)

F19-7-9-2 APT

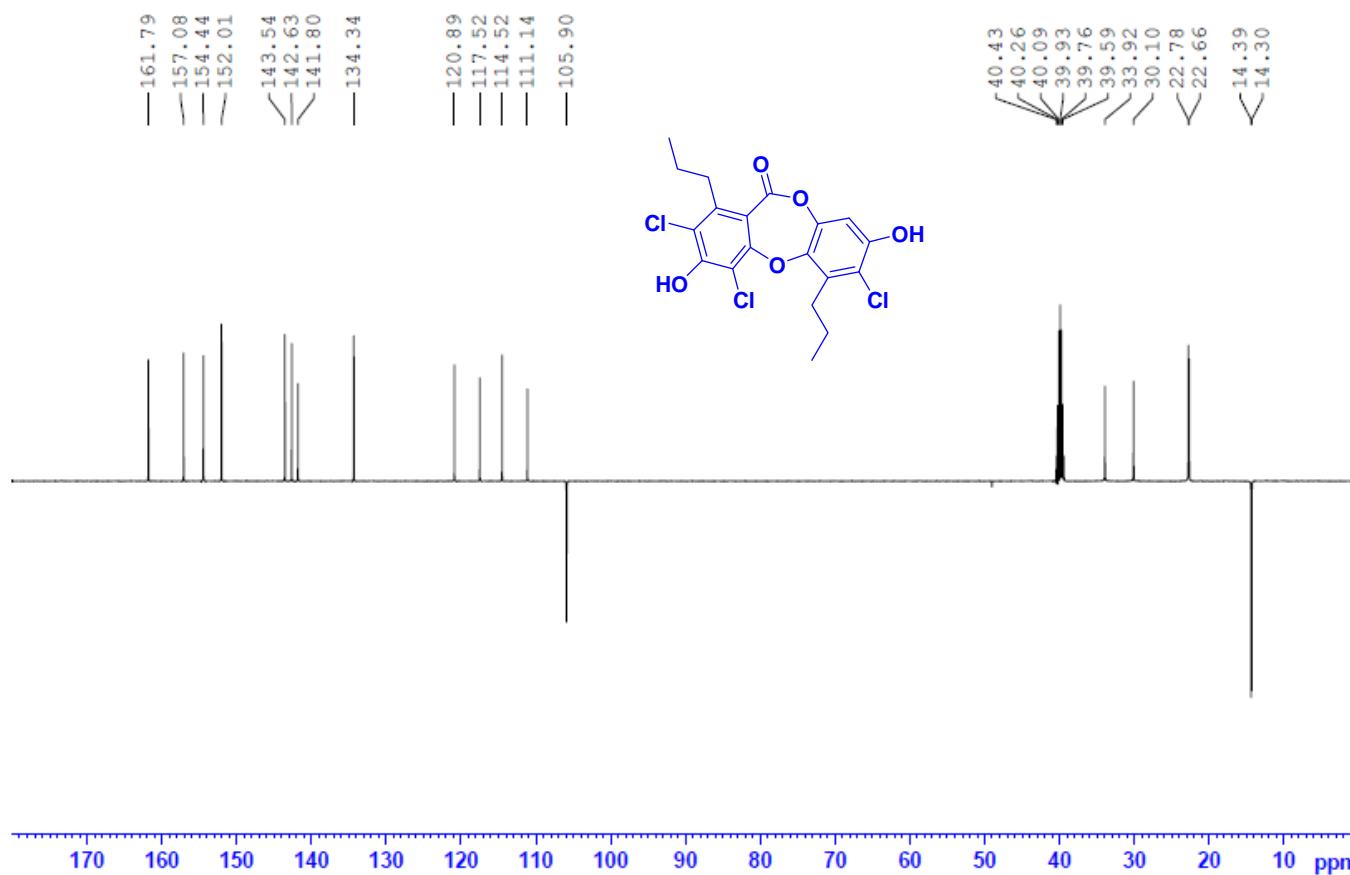


Figure S75. APT spectrum of **6** in $\text{DMSO}-d_6$ (100 MHz)

F19-7-9-2 HSQC

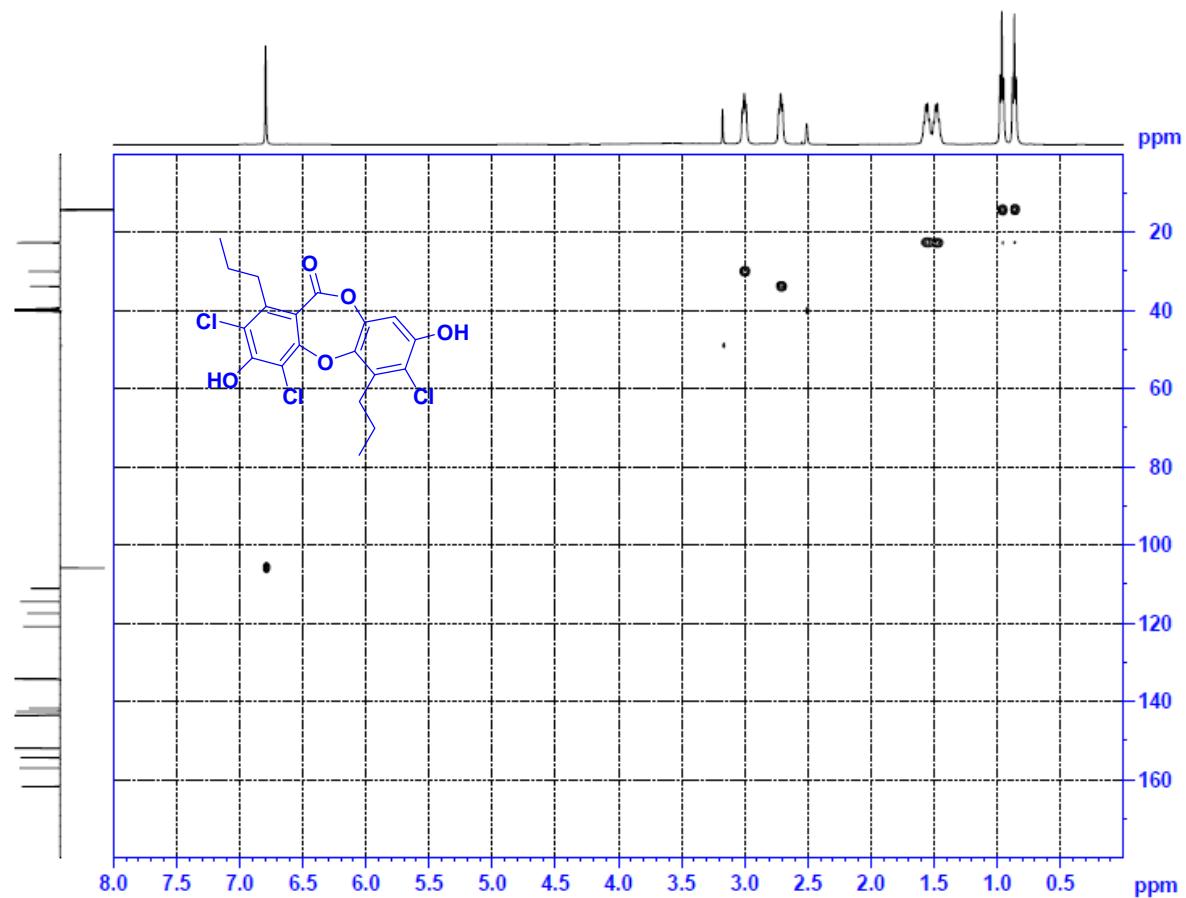


Figure S76. HSQC spectrum of **6** in $\text{DMSO}-d_6$ (400 MHz)

F19-7-9-2 COSY

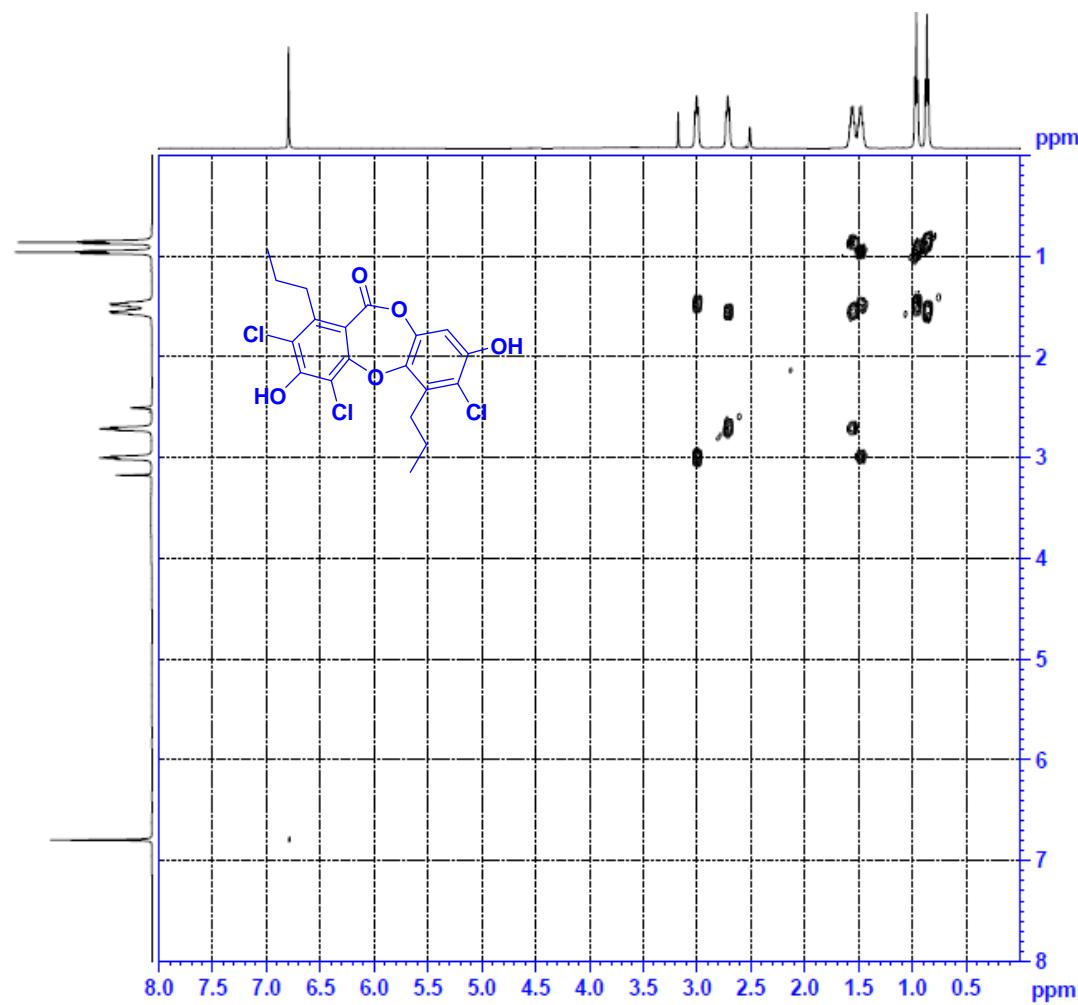


Figure S77. ^1H - ^1H COSY spectrum of **6** in $\text{DMSO}-d_6$ (400 MHz)

F19-7-9-2 HMBC

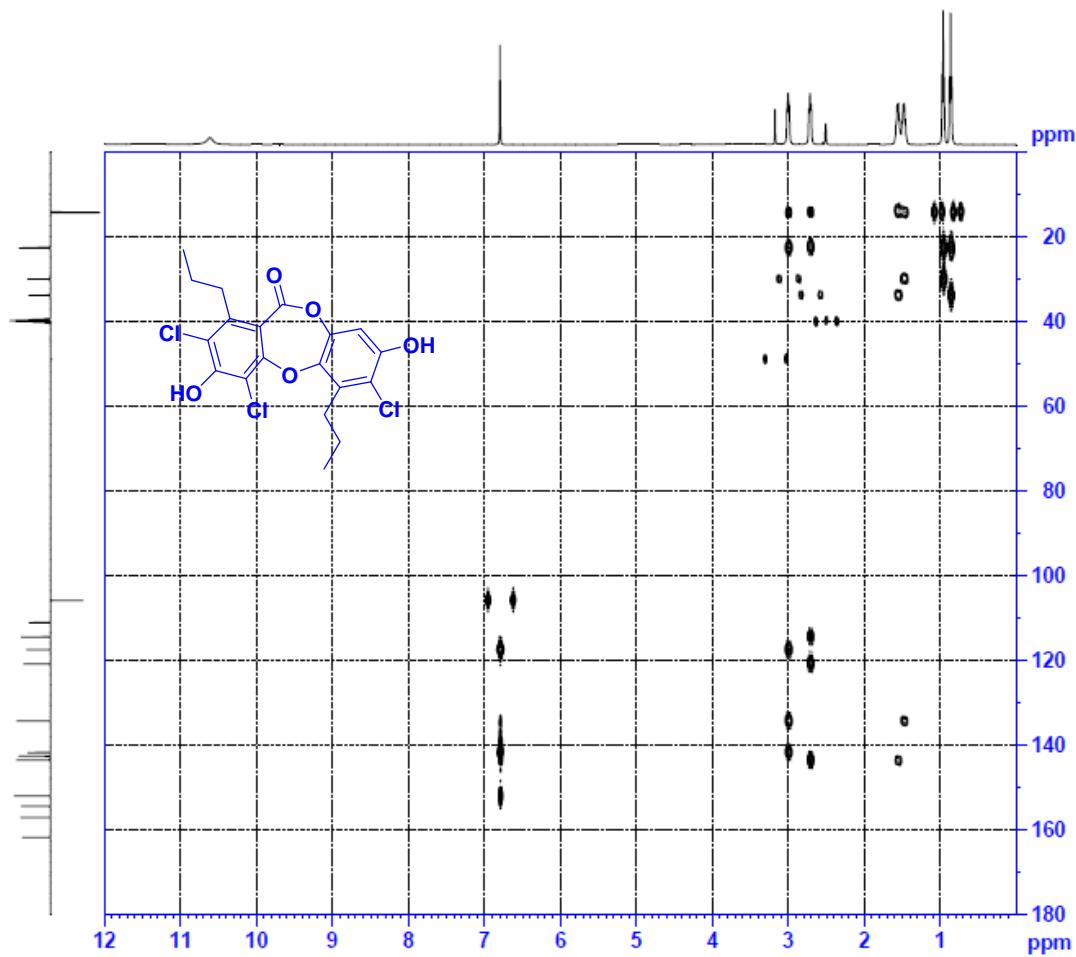
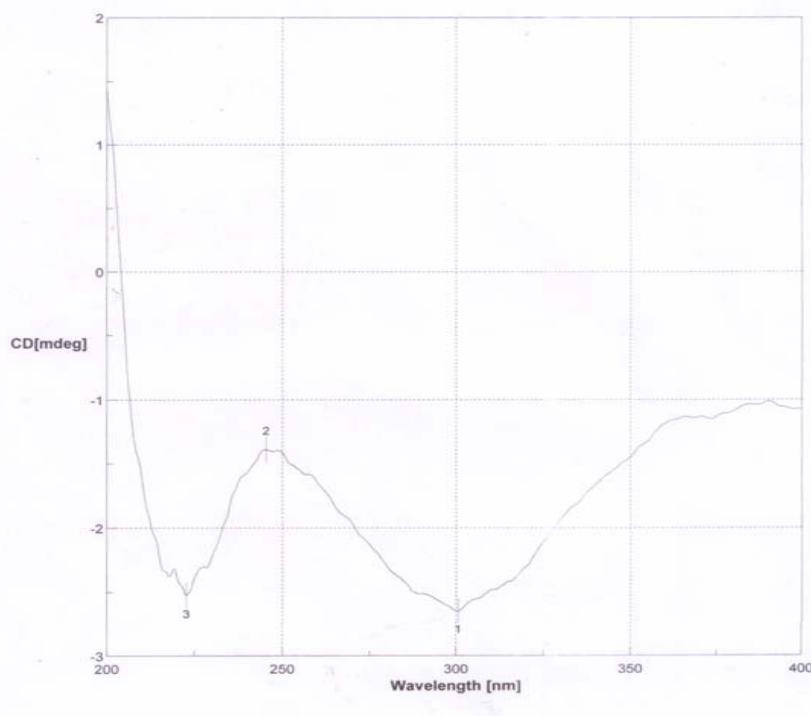


Figure S78. HMBC spectrum of **6** in $\text{DMSO}-d_6$ (400 MHz)



Date/Time 2001-1-3 4:21
Operator F19-7-9-2.txt
File Name F19-7-9-2
Sample Name
Comment

No.	nm	CD[mdeg]	No.	nm	CD[mdeg]	No.	nm	CD[mdeg]
1	300.6	-2.64777	2	245.4	-1.38954	3	222.8	-2.5228

Figure S79. CD spectrum of **6**

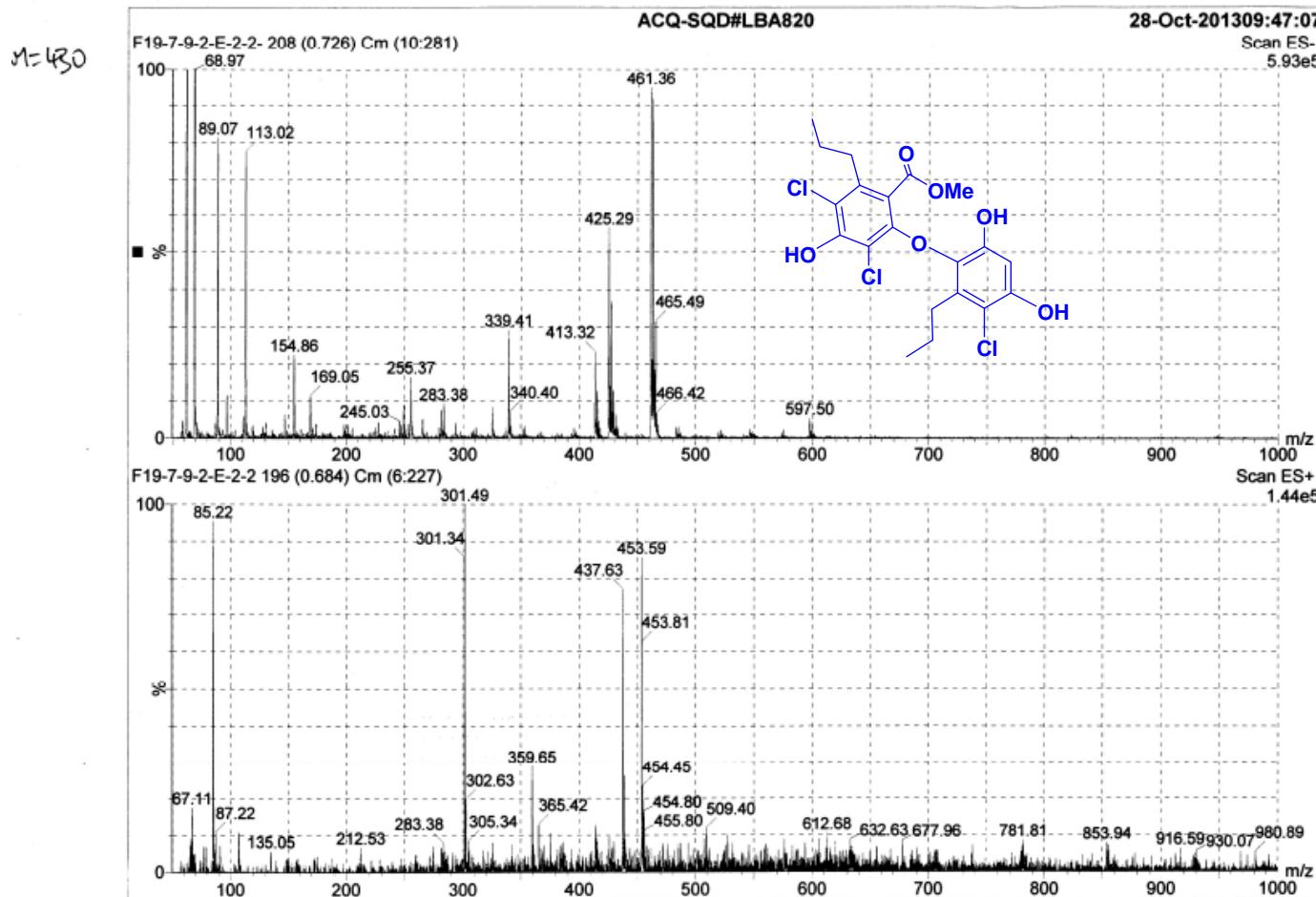


Figure S80. ESIMS spectrum of **6a**

F19-7-9-2-e-2 400 MHz DMSO

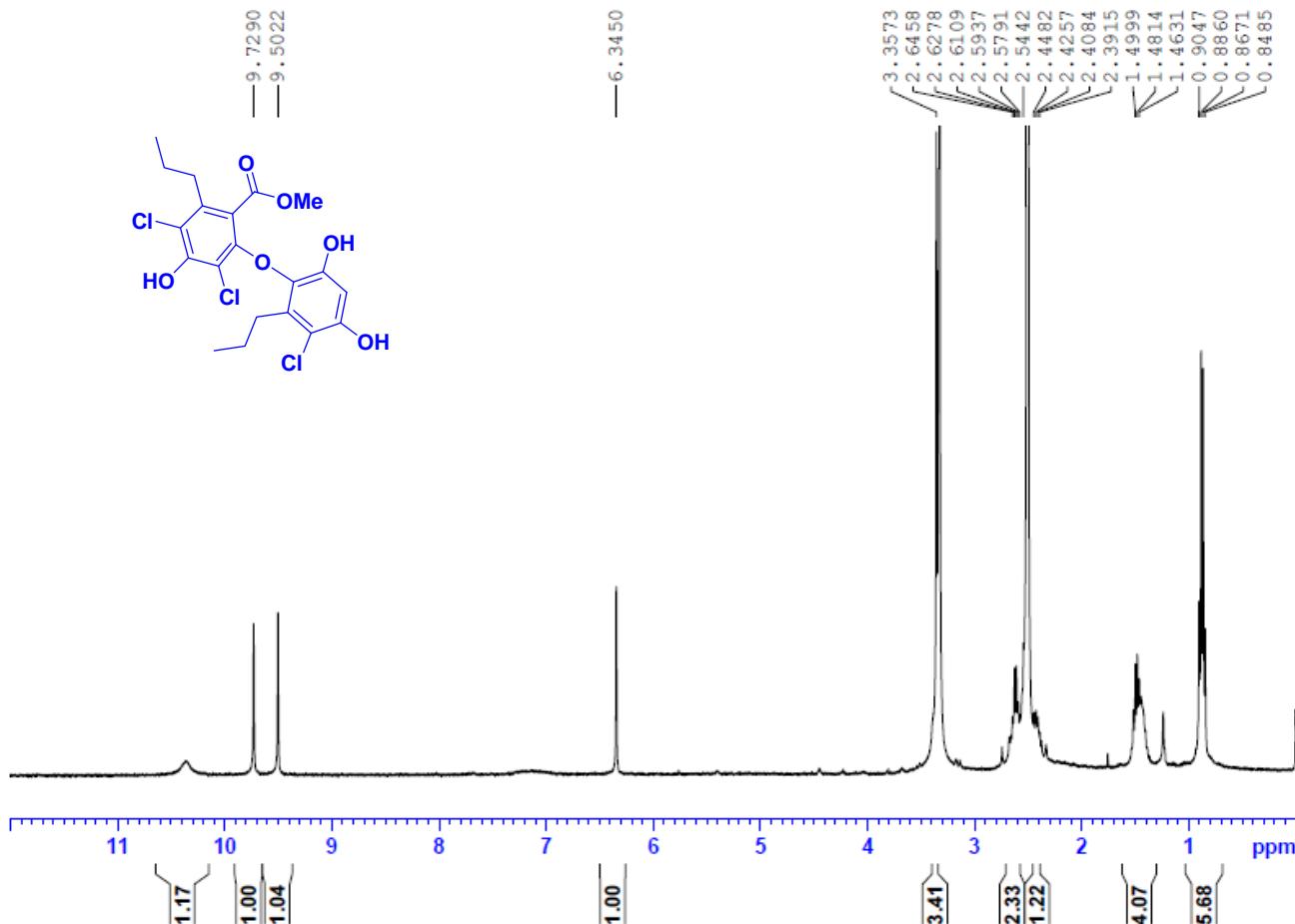


Figure S81. ^1H NMR spectrum of **6a** in $\text{DMSO}-d_6$ (400 MHz)

F19-7-9-2-e-2 APT

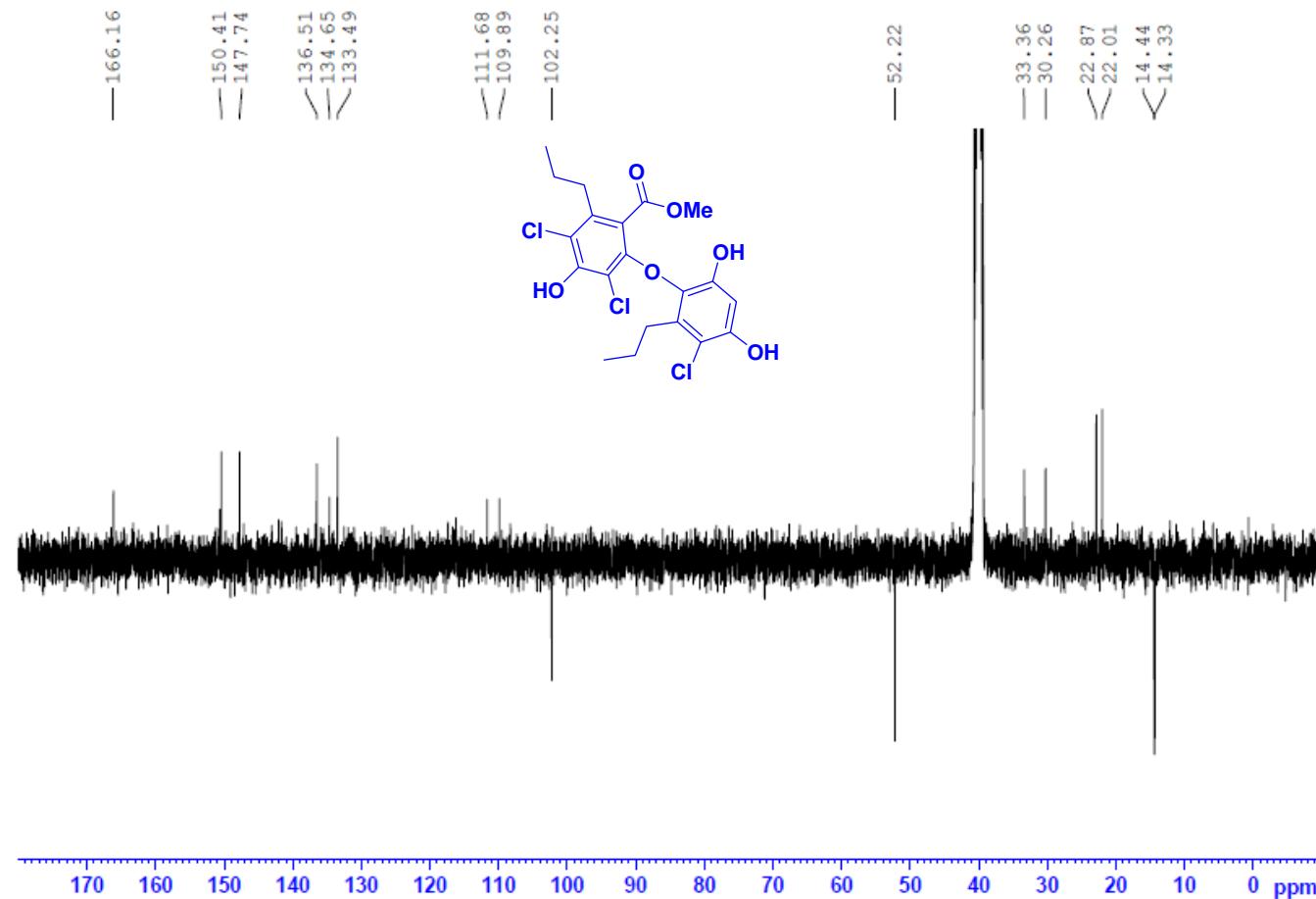


Figure S82. APT spectrum of **6a** in $\text{DMSO}-d_6$ (100 MHz)

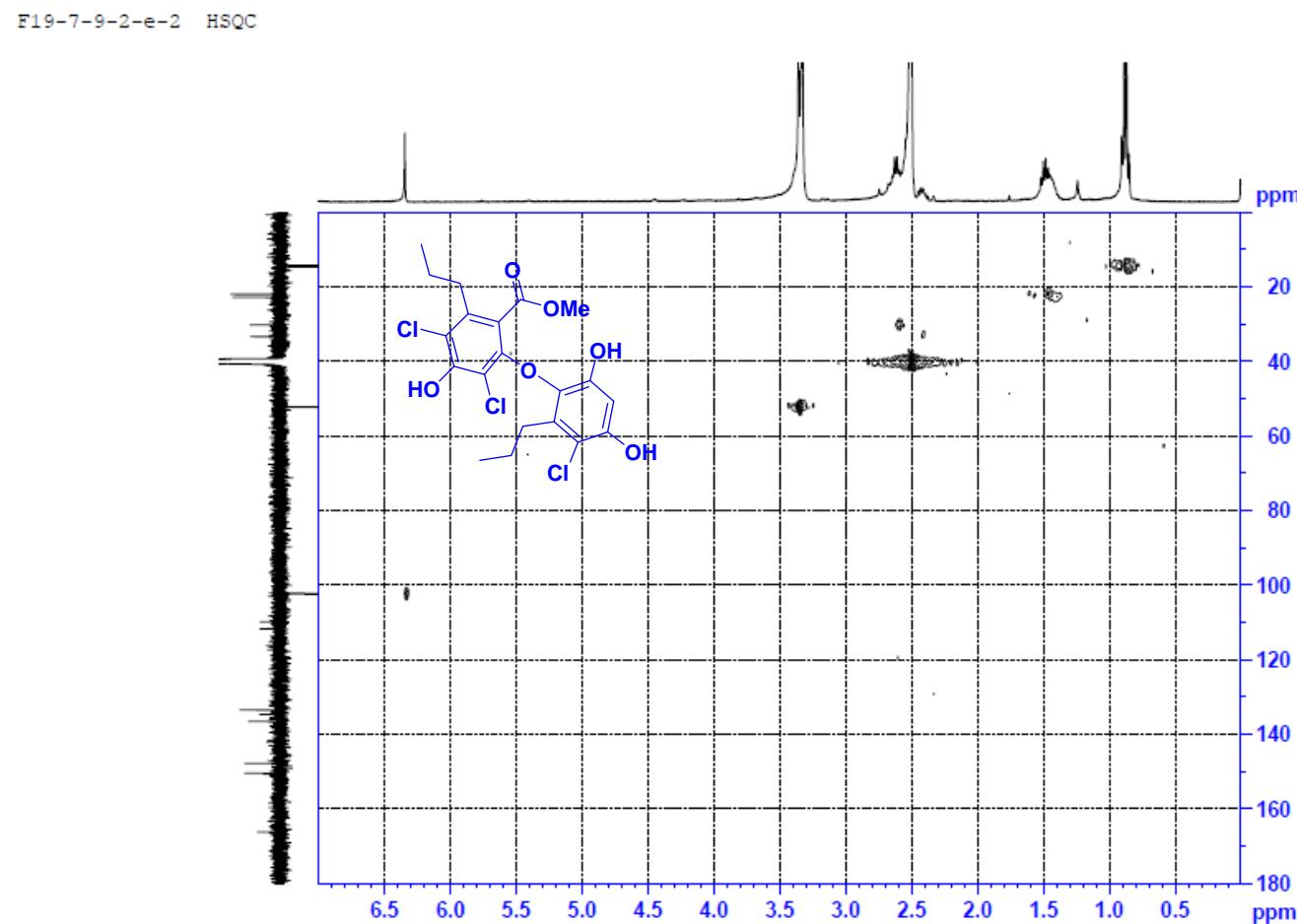


Figure S83. HSQC spectrum of **6a** in DMSO-*d*₆ (400 MHz)

F19-7-9-2-e-2 COSY

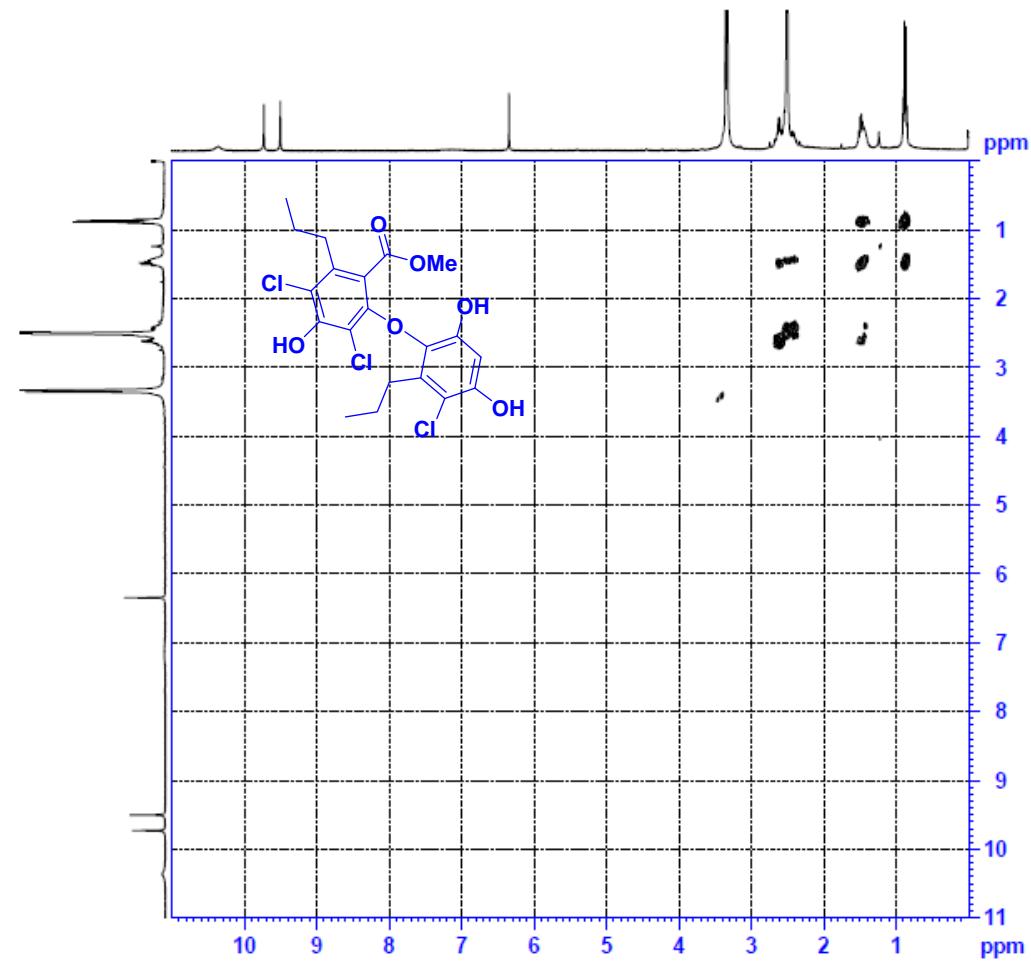


Figure S84. ^1H - ^1H COSY spectrum of **6a** in $\text{DMSO}-d_6$ (400 MHz)

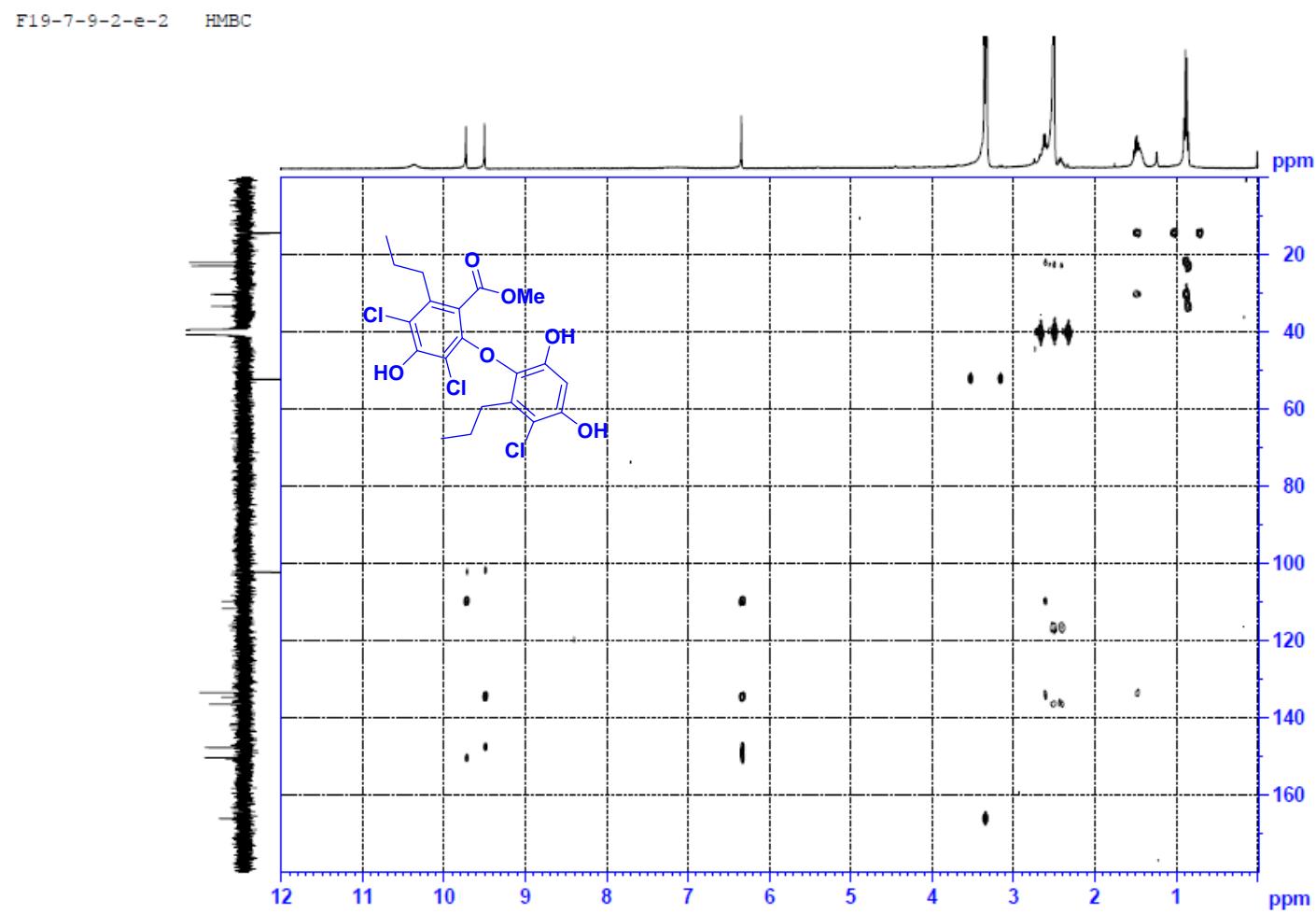


Figure S85. HMBC spectrum of **6a** in DMSO-*d*₆ (400 MHz)

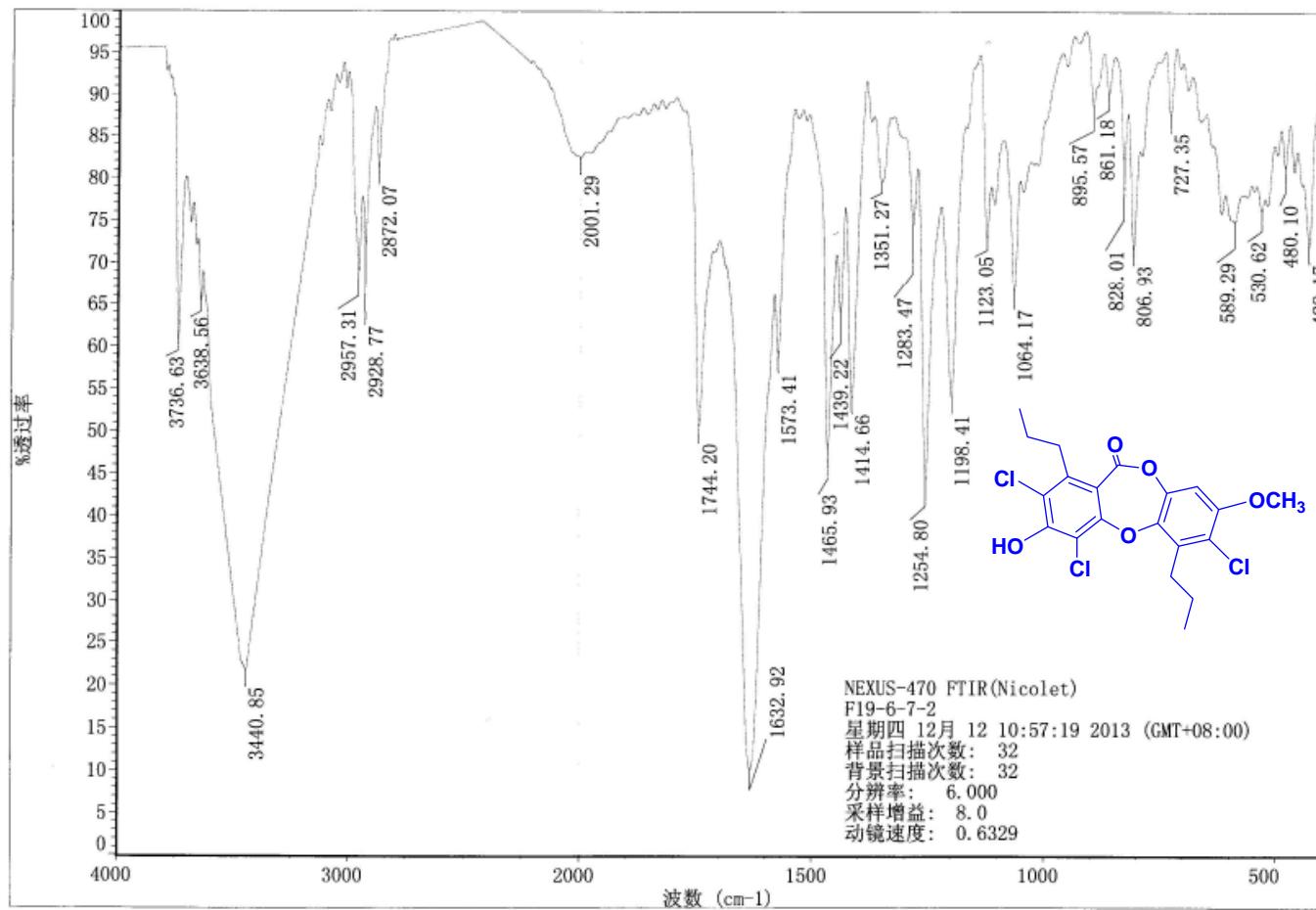


Figure 86. IR spectrum of 7



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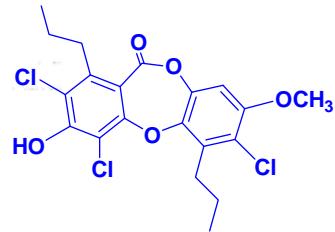
Analysis Name C:\data\sample\ESI_12131120_30\LowMass\ESI_F19_6_7_2_20131121\POS_2 Acquisition Date 11/20/2013 10:34:43 AM

Operator bpxsh@bjmu.edu.cn; Tel:010-82801

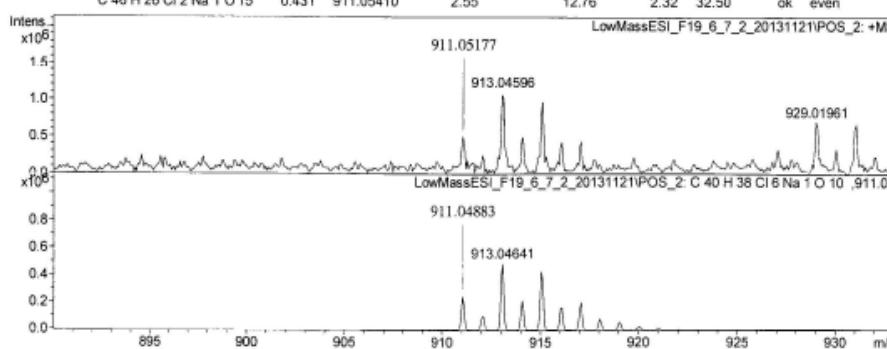
Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI pos C20H19Cl3O5 MW 444
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;826.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result Exact Mass Measured Mass Error (mDa) Error (ppm) Description



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 40 H 38 Cl 6 Na 1 O 10	0.092	911.04883	-3.23	4.14	-2.94	18.50	ok	even
C 46 H 33 Cl 5 Na 1 O 8	0.127	911.05103	-0.82	6.91	-0.75	27.50	ok	even
C 45 H 39 Cl 7 Na 1 O 4	0.134	911.05602	4.67	11.77	4.25	22.50	ok	even
C 46 H 40 Cl 8 Na 1 O 1	0.173	911.04796	-4.19	2.97	-3.81	22.50	ok	even
C 40 H 31 Cl 3 Na 1 O 17	0.312	911.05190	0.14	8.69	0.13	23.50	ok	even
C 46 H 26 Cl 2 Na 1 O 15	0.431	911.05410	2.55	12.76	2.32	32.50	ok	even





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Analysis Name C:\data_sample\ESI_12131120_30\LowMassESI_F19_6_7_2_20131121\POS_2
Acquisition Date 11/20/2013 10:34:43 AM
Operator bpxsh@bjmu.edu.cn; Tel:010-82801
Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI pos □ C₂₀H₁₉Cl₃O₅ MW 444
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;826.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result	Exact Mass	Measured Mass	Error (mDa)	Error (ppm)	Description
	445.03708	445.03675	0.33	0.75	M+H ⁺ ;e ⁻

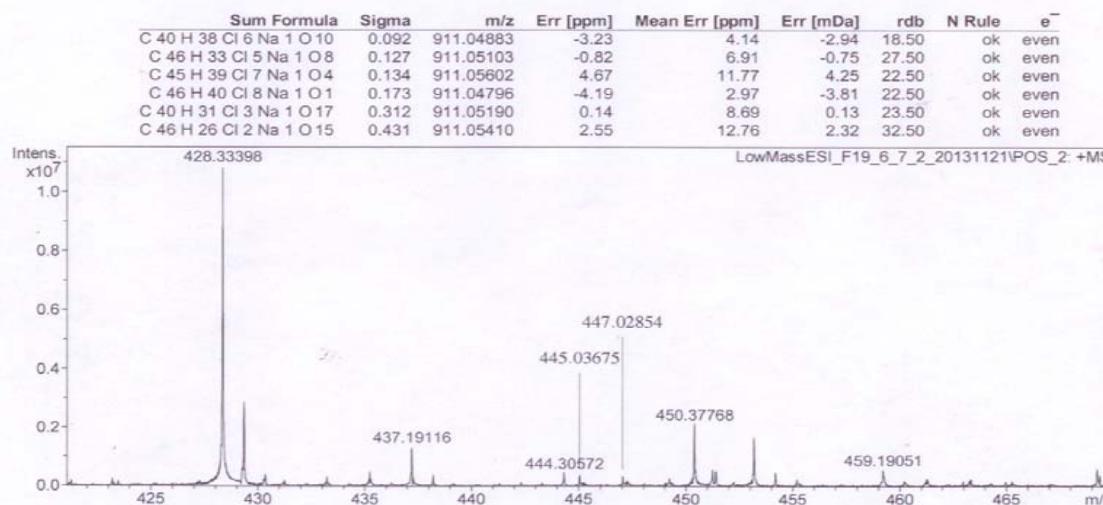


Figure S87. HRESIMS spectrum of 7

F19-6-7-2 400 MHz DMSO

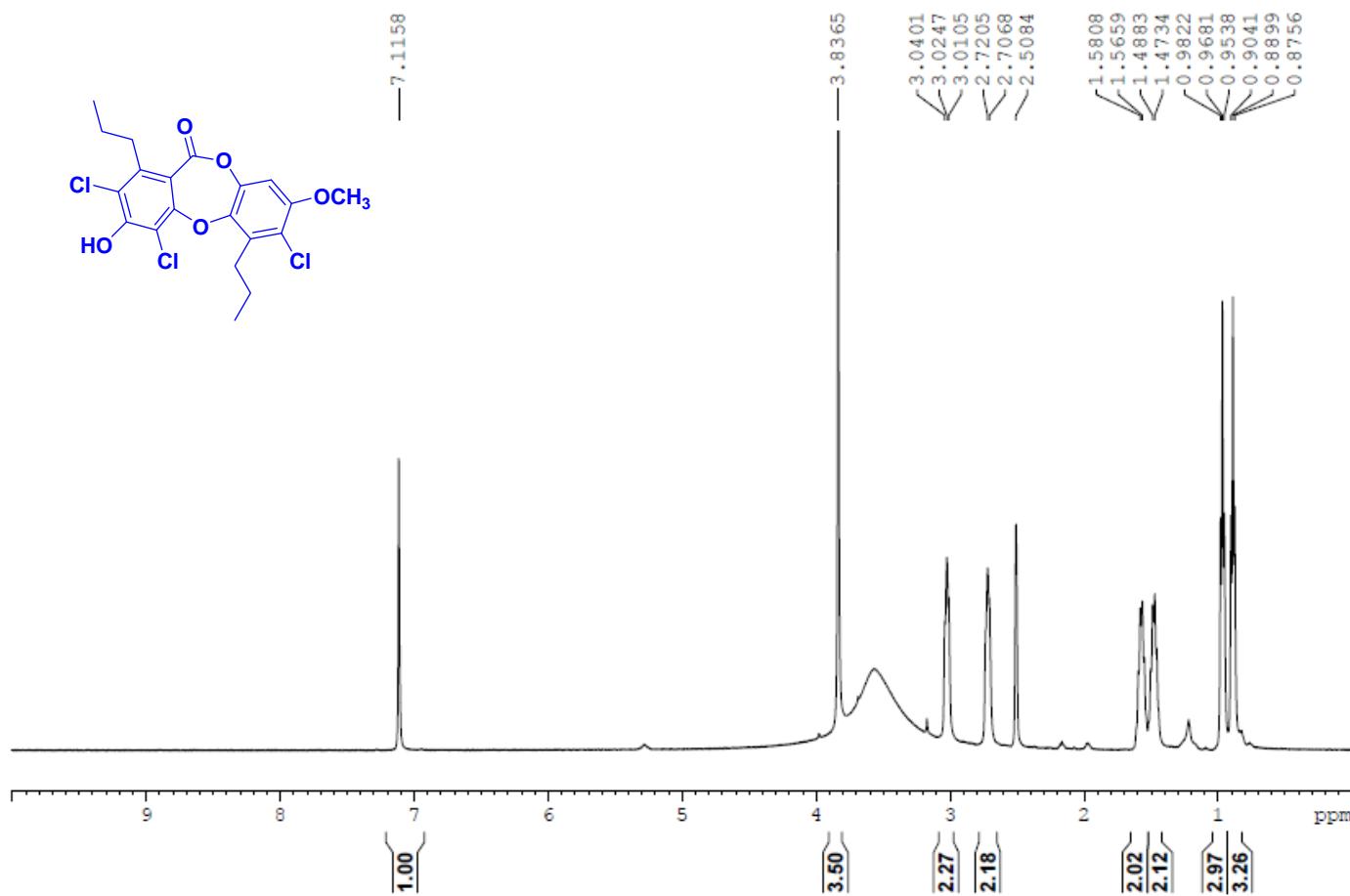


Figure S88. ^1H NMR spectrum of **7** in $\text{DMSO}-d_6$ (400 MHz)

F19-6-7-2 APT

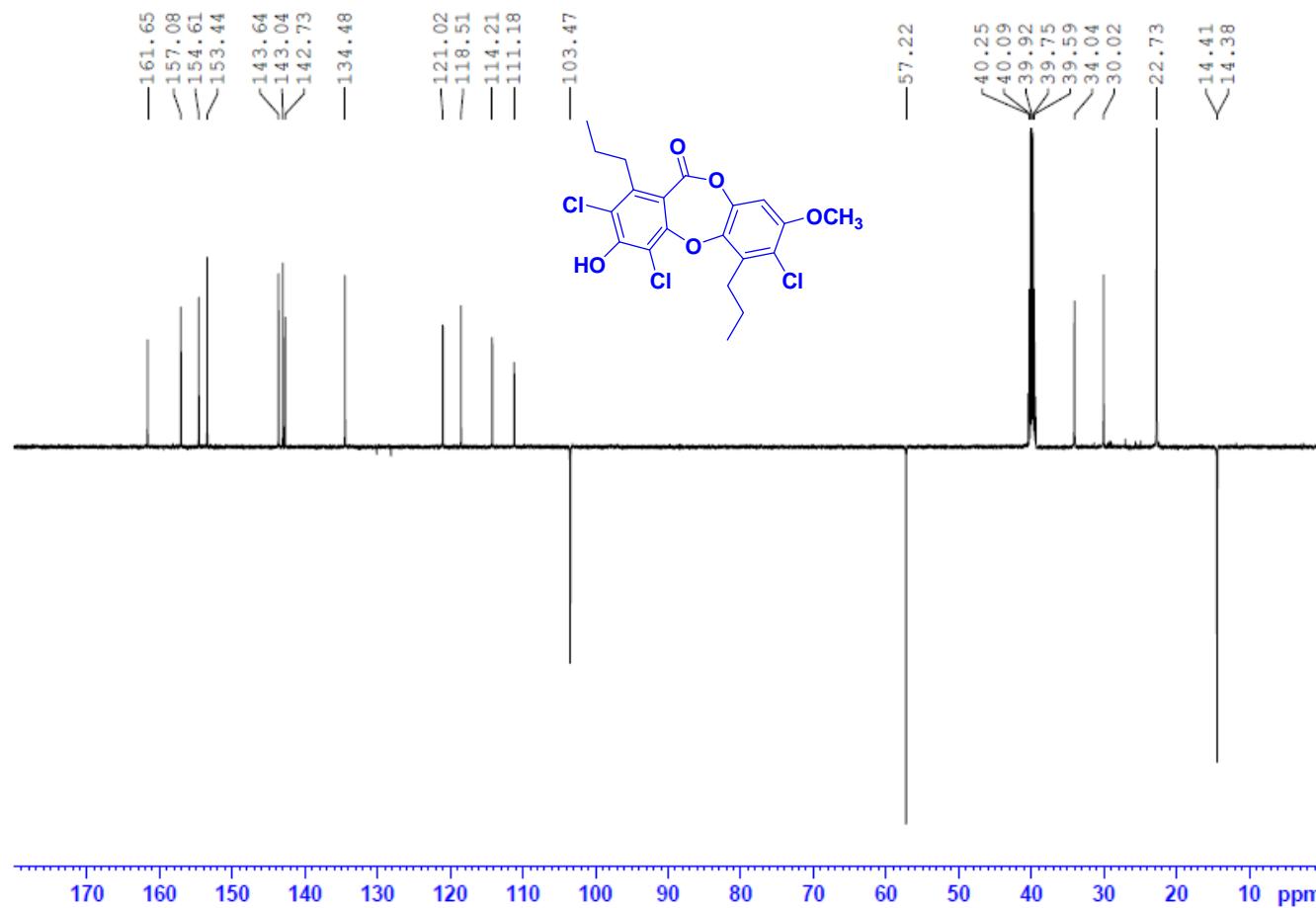


Figure S89. APT spectrum of **7** in $\text{DMSO}-d_6$ (100 MHz)

F19-6-7-2 HSQC

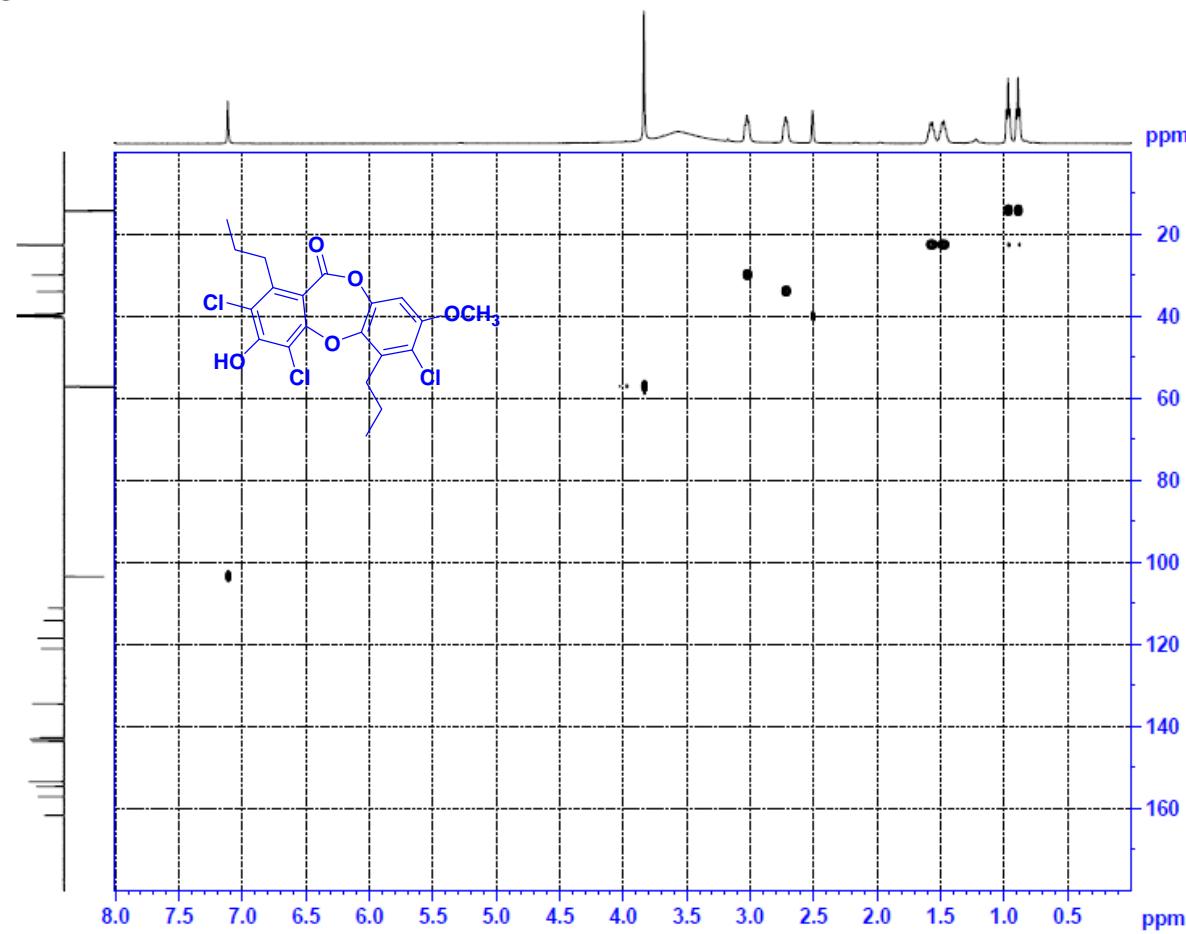


Figure S90. HSQC spectrum of **7** in $\text{DMSO}-d_6$ (400 MHz)

F19-6-7-2 COSY

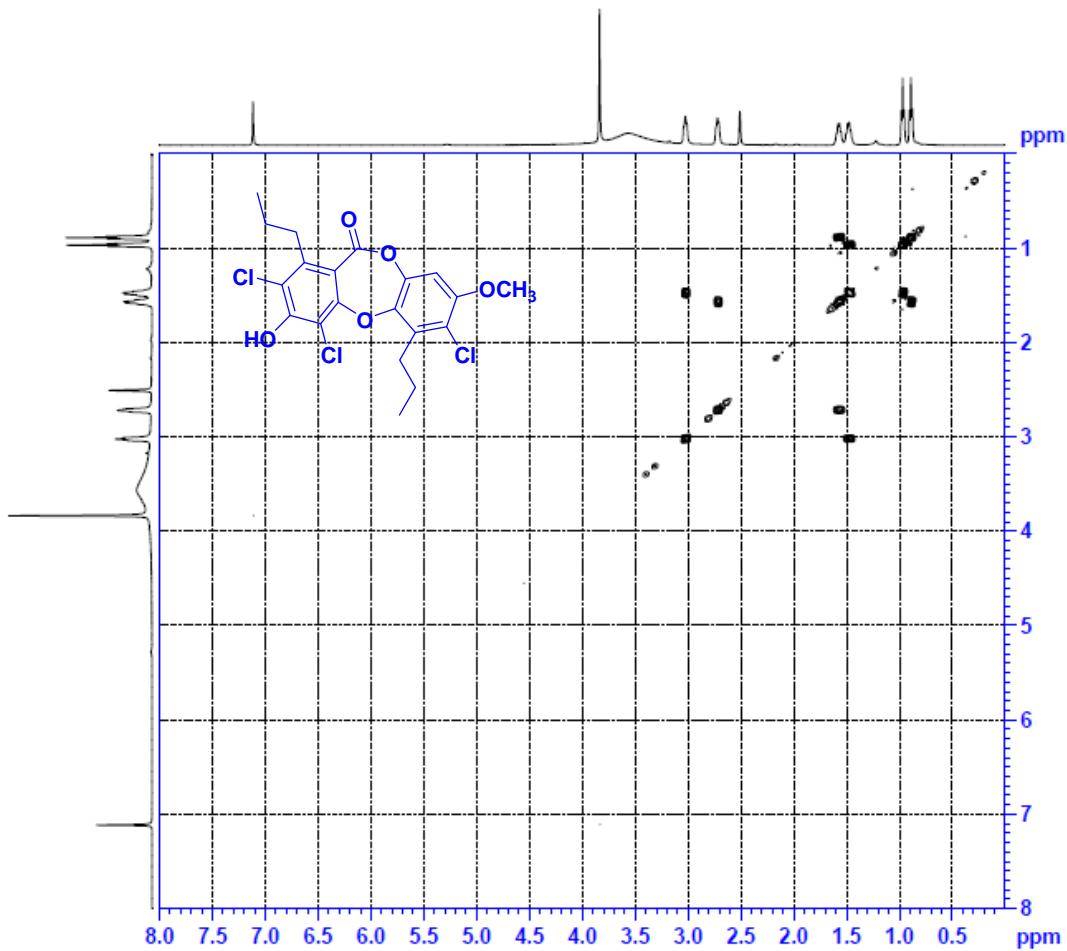


Figure S91. ^1H - ^1H COSY spectrum of **7** in $\text{DMSO}-d_6$ (400 MHz)

F19-6-7-2 HMBC

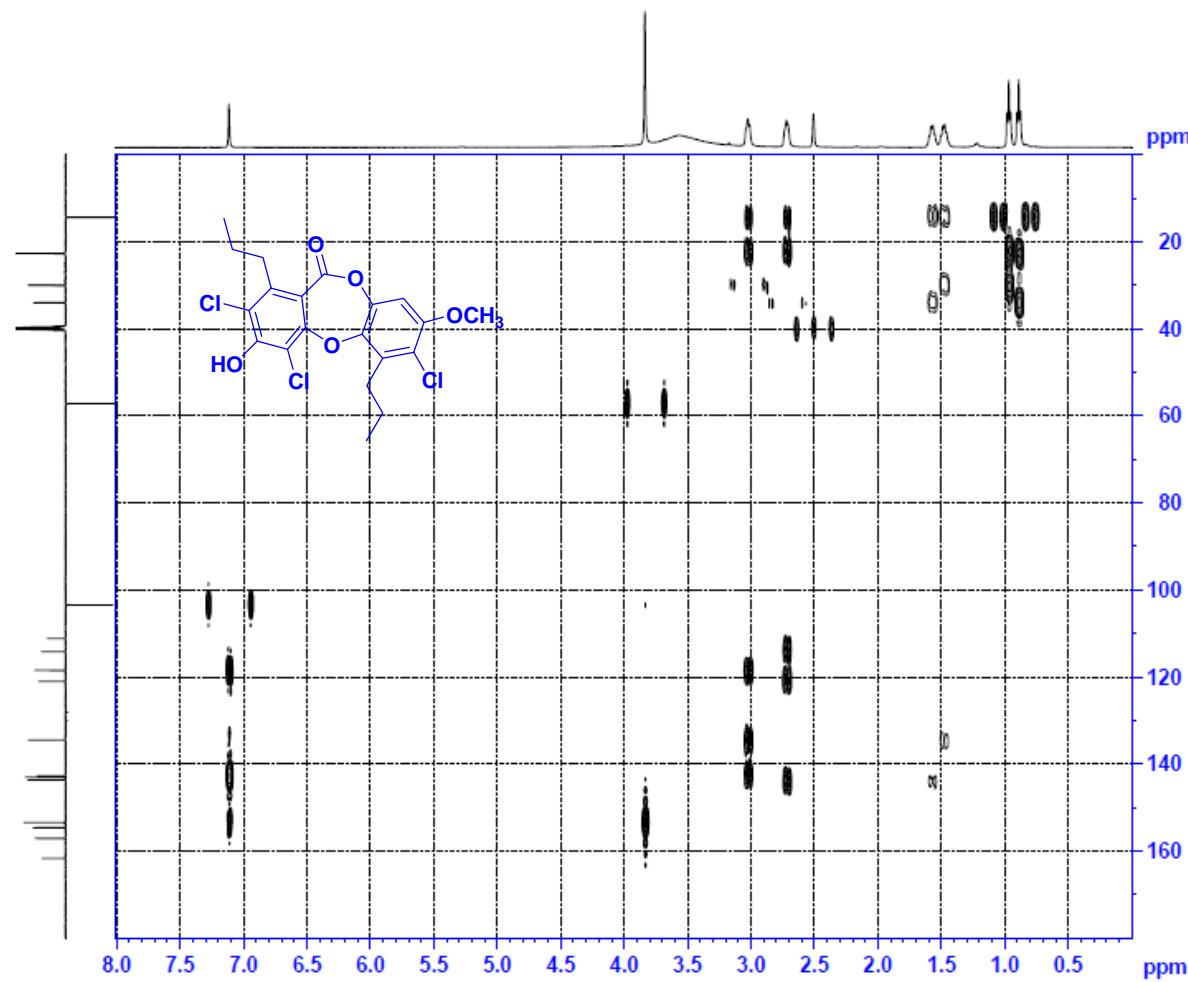
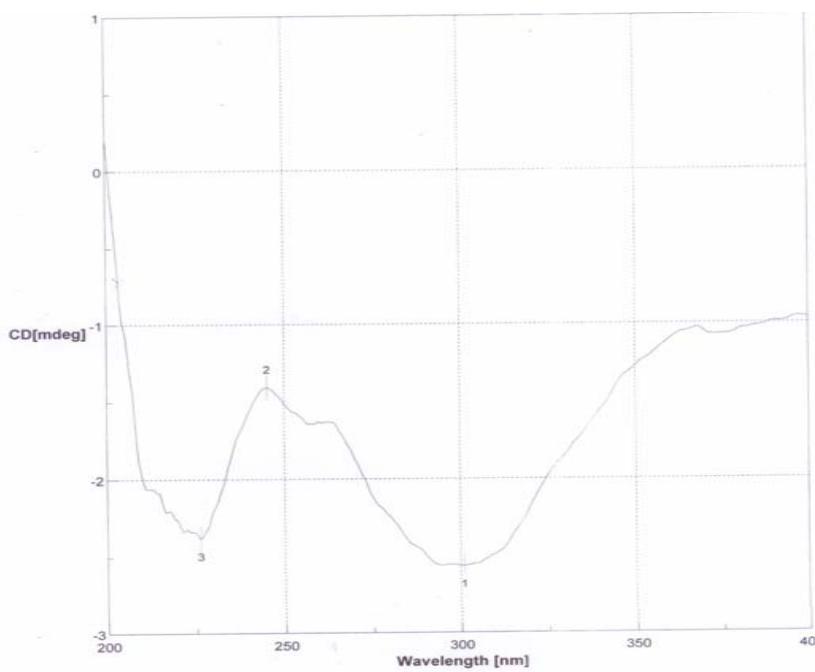


Figure S92. HMBC spectrum of **7** in $\text{DMSO}-d_6$ (400 MHz)



Date/Time 2001-1-3 5:30
Operator
File Name F19-6-7-2.txt
Sample Name F19-6-7-2
Comment

No.	nm	CD[mdeg]	No.	nm	CD[mdeg]	No.	nm	CD[mdeg]
1	301	-2.56119	2	245.2	-1.40787	3	226.4	-2.3779

Figure S93. CD spectrum of 7

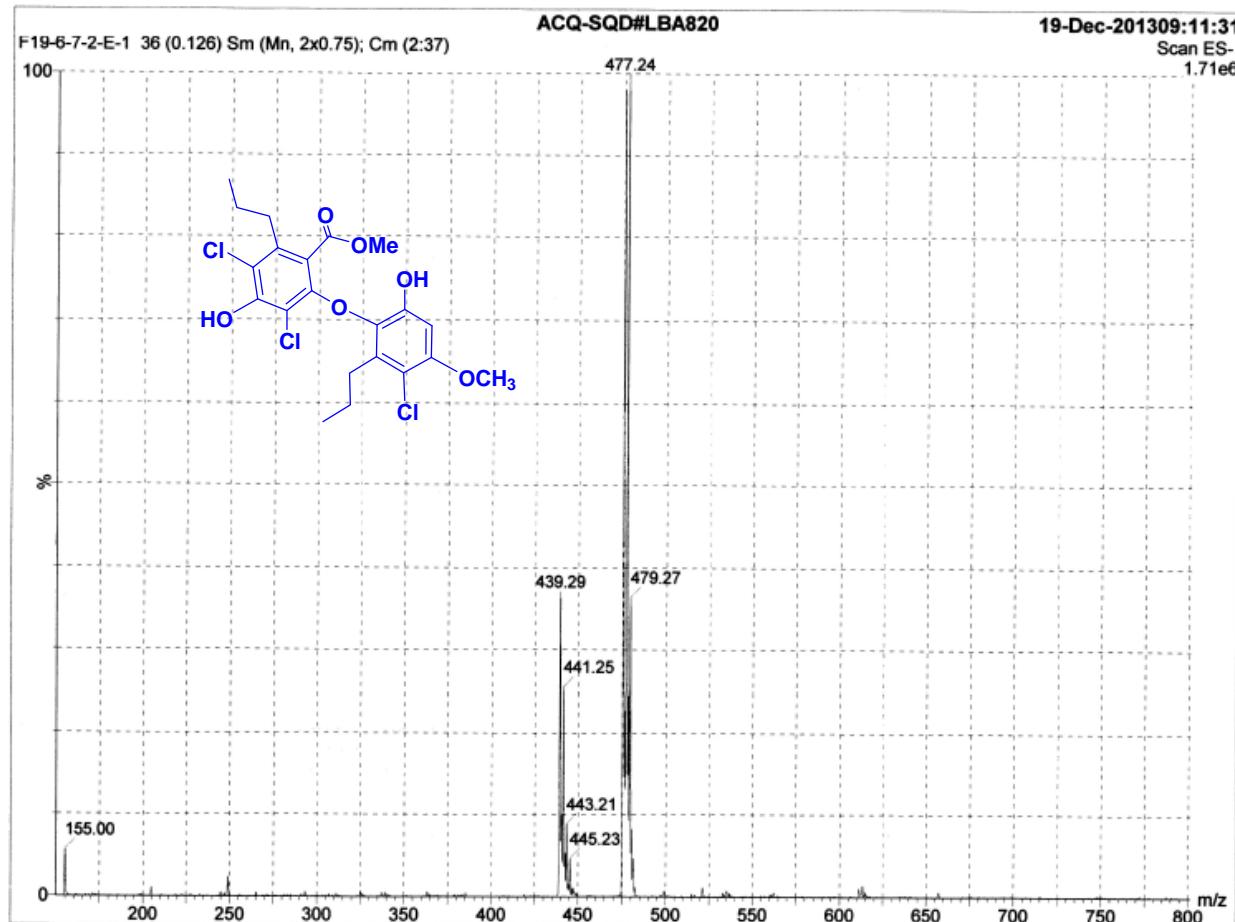


Figure S94. ESIMS spectrum of 7a

F19-6-7-2-e-1 400 MHz DMSO

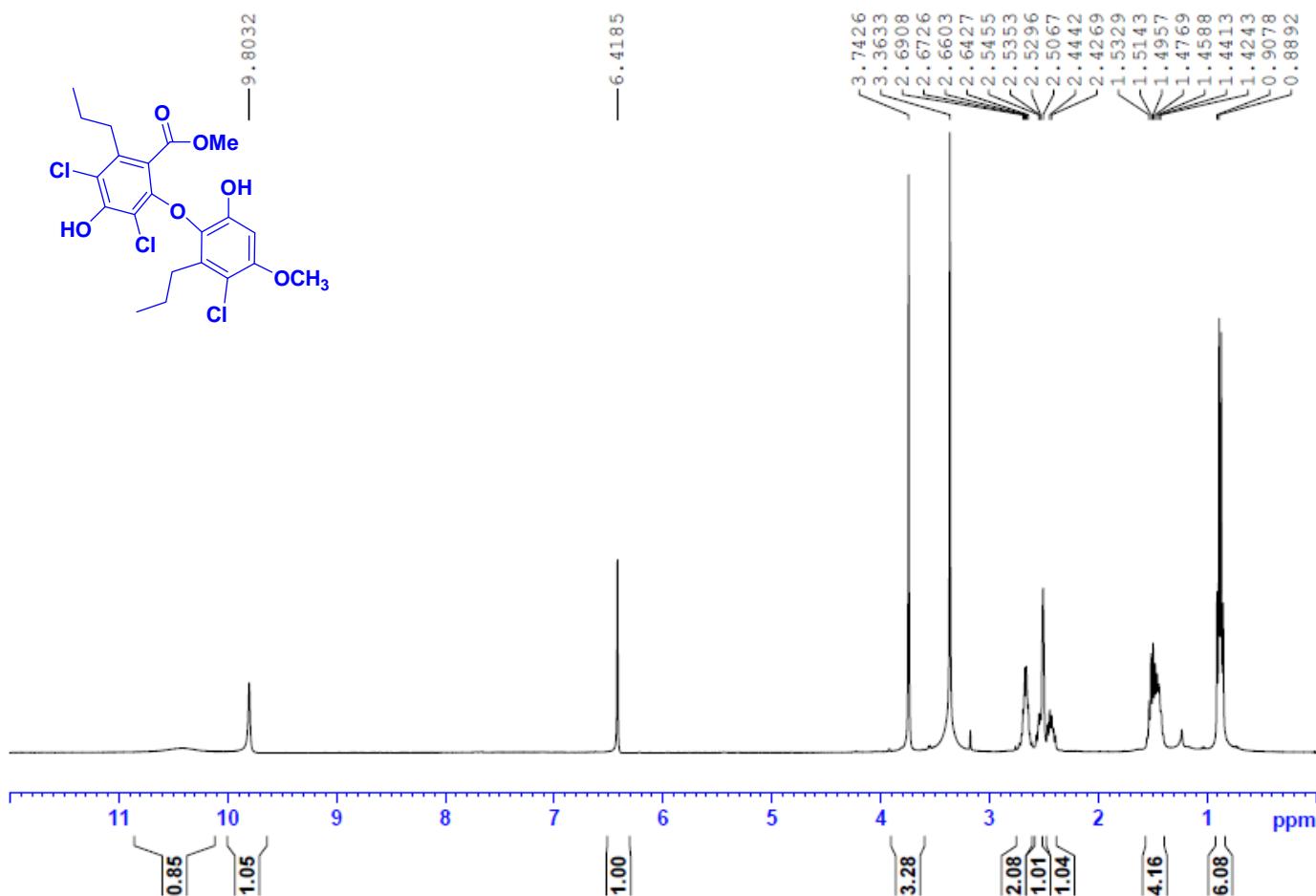


Figure S95. ^1H NMR spectrum of **7a** in $\text{DMSO}-d_6$ (400 MHz)

F19-6-7-2-e-1 APT

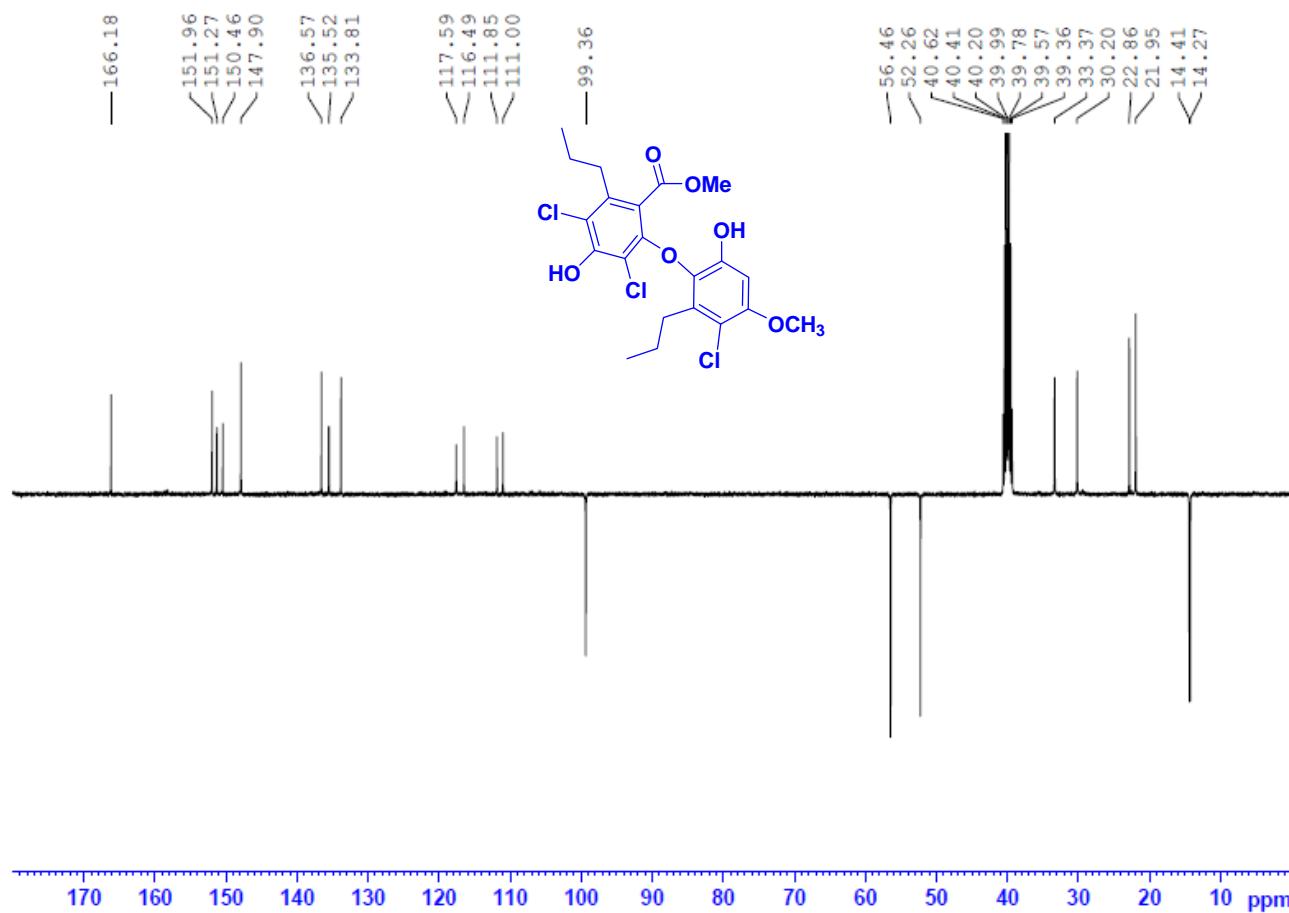


Figure S96. APT spectrum of **7a** in DMSO-*d*₆ (100 MHz)

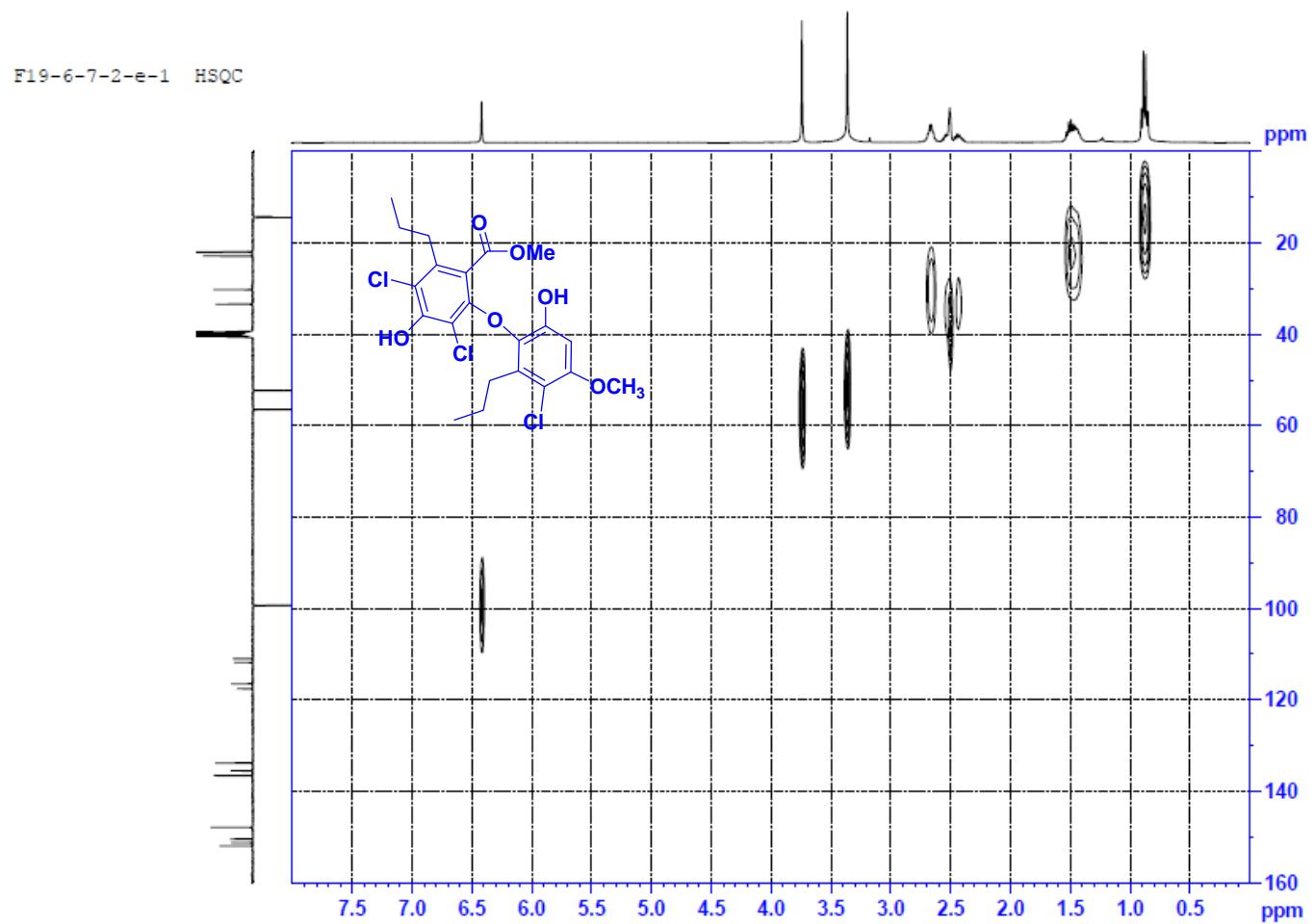


Figure S97. HSQC spectrum of **7a** in DMSO-*d*₆ (400 MHz)

F19-6-7-2-e-1 COSY

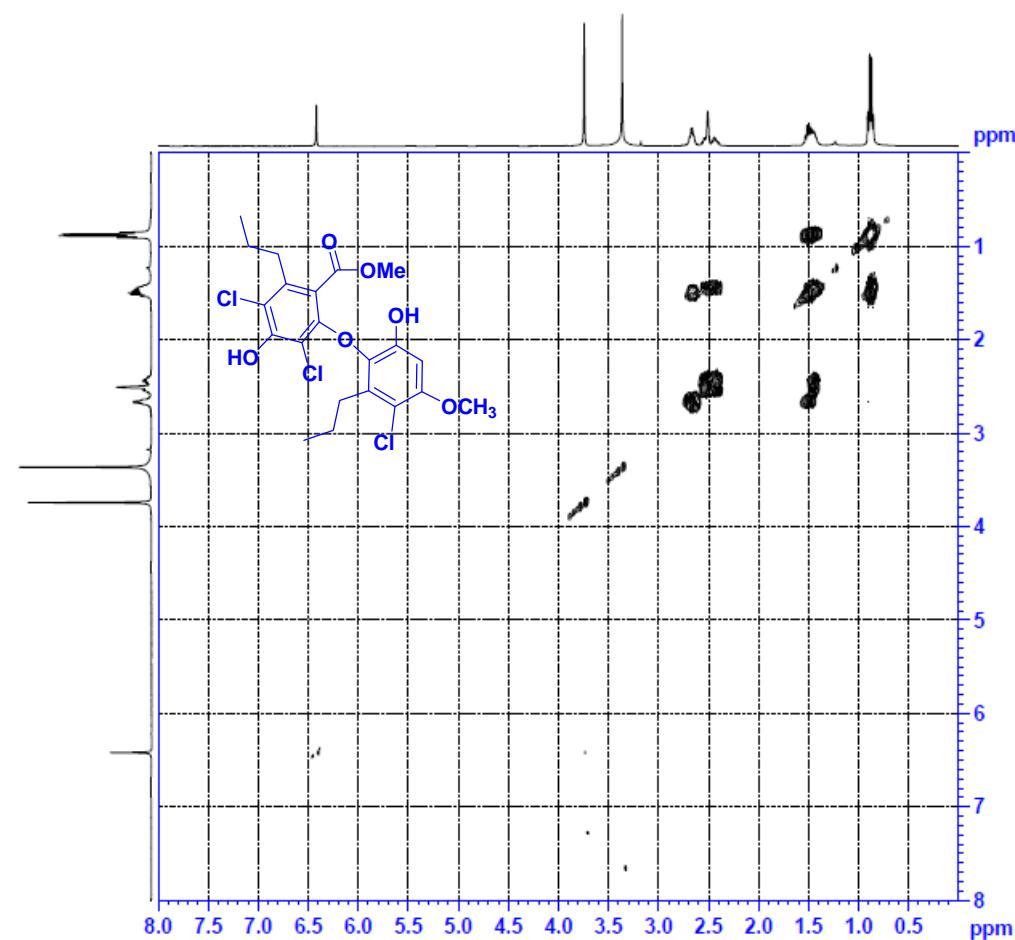


Figure S98. ^1H - ^1H COSY spectrum of **7a** in DMSO- d_6 (400 MHz)

F19-6-7-2-e-1 HMBC

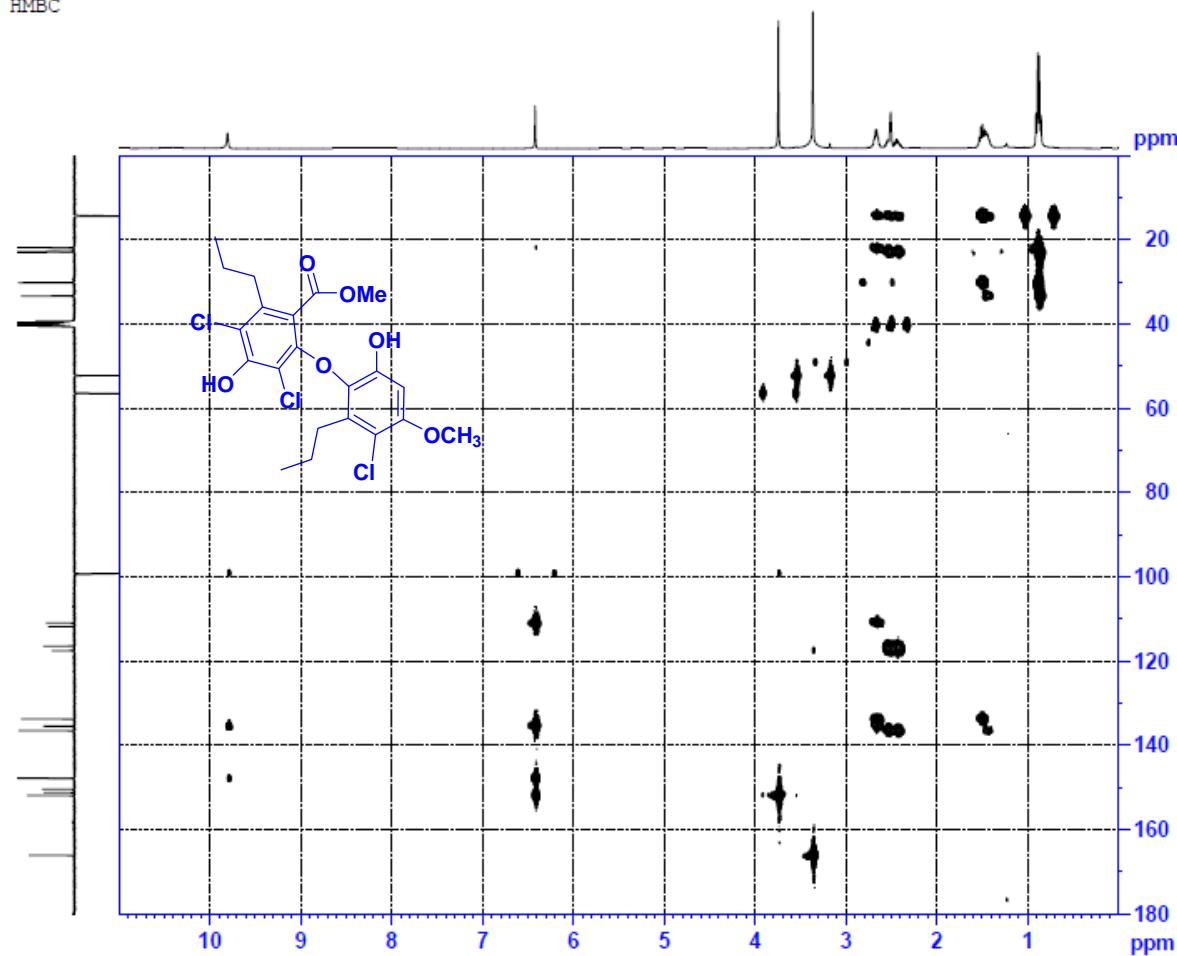


Figure S99. HMBC spectrum of **7a** in DMSO-*d*₆ (400 MHz)

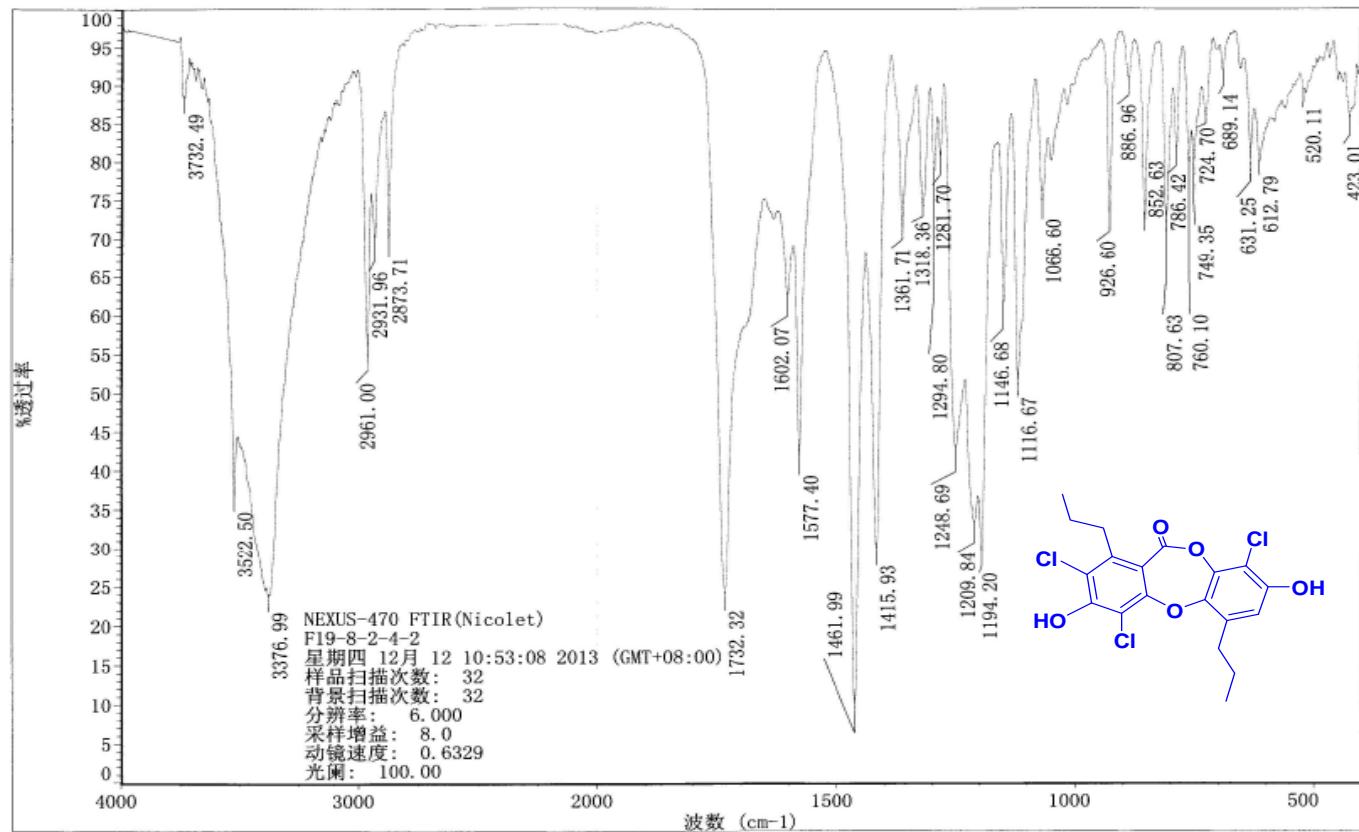


Figure S100. IR spectrum of 8

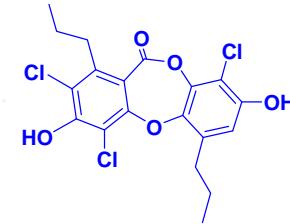


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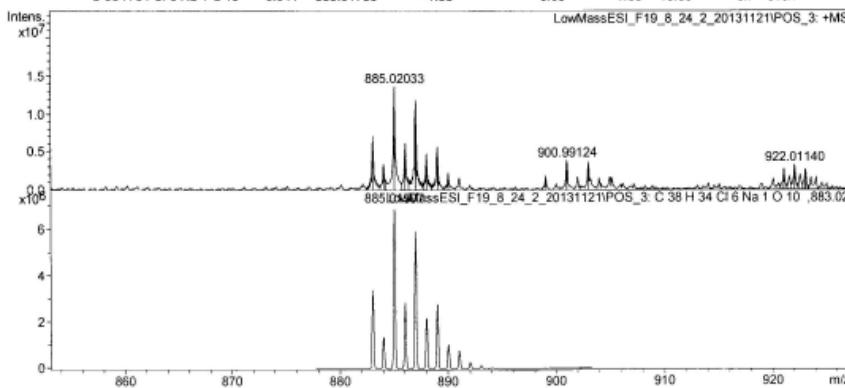
Analysis Name C:\data_sample\ESI_12131120_30\LowMassESI_F19_8_24_2_20131121\POS_3 Acquisition Date 11/20/2013 2:41:51 PM
Operator bpxsh@bjmu.edu.cn; Tel:010-82801
Instrument FT_MS_Bruker APEX IV_7.0

Comment ESI pos | C19H17Cl3O5 MW 430
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;8,26.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result Exact Mass Measured Mass Error (mDa) Error (ppm) Description



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 40 H 33 Cl 6 O 10	0.040	883.01994	0.88	-0.87	0.77	21.50	ok	even
C 38 H 34 Cl 6 Na 1 O 10	0.041	883.01753	-1.85	-3.68	-1.63	18.50	ok	even



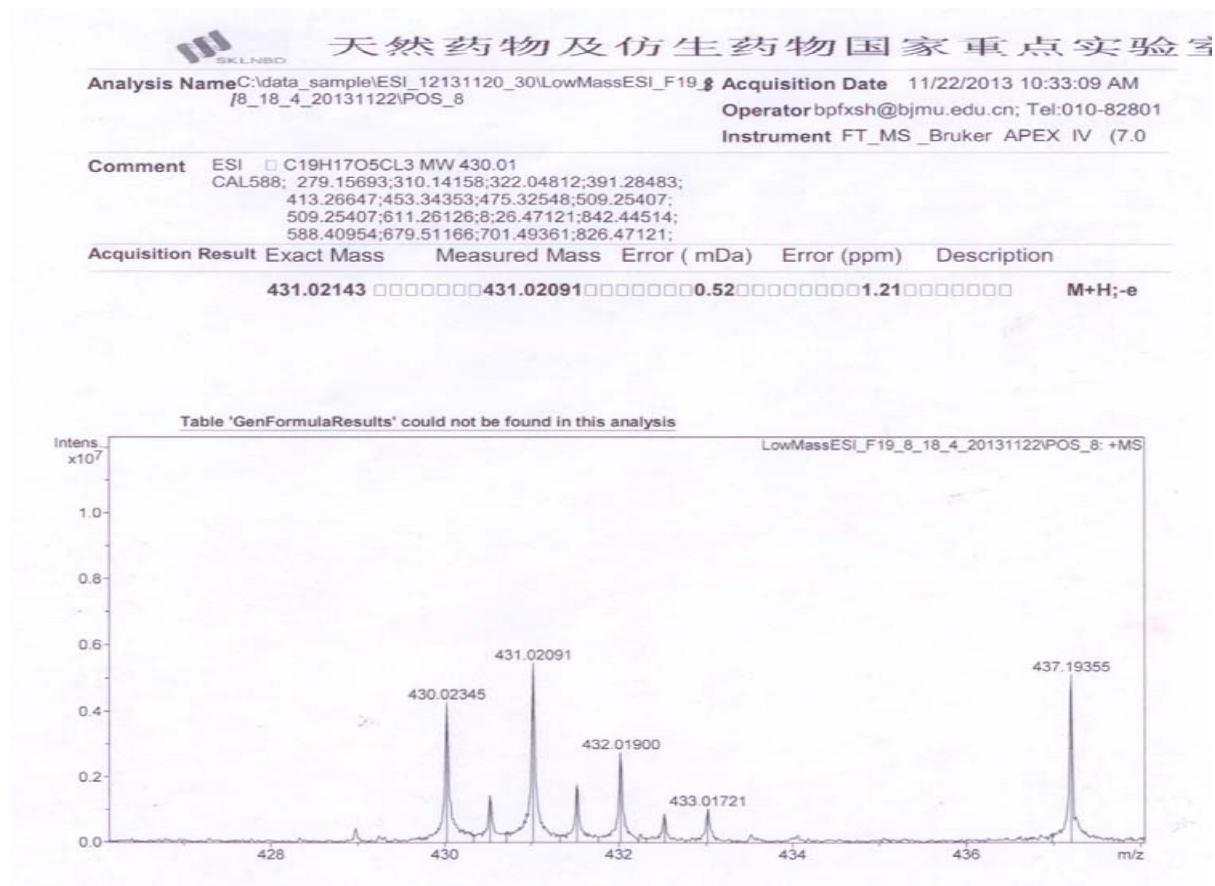


Figure S101. HRESIMS spectrum of **8**

F19-8-18-4 400 MHz DMSO

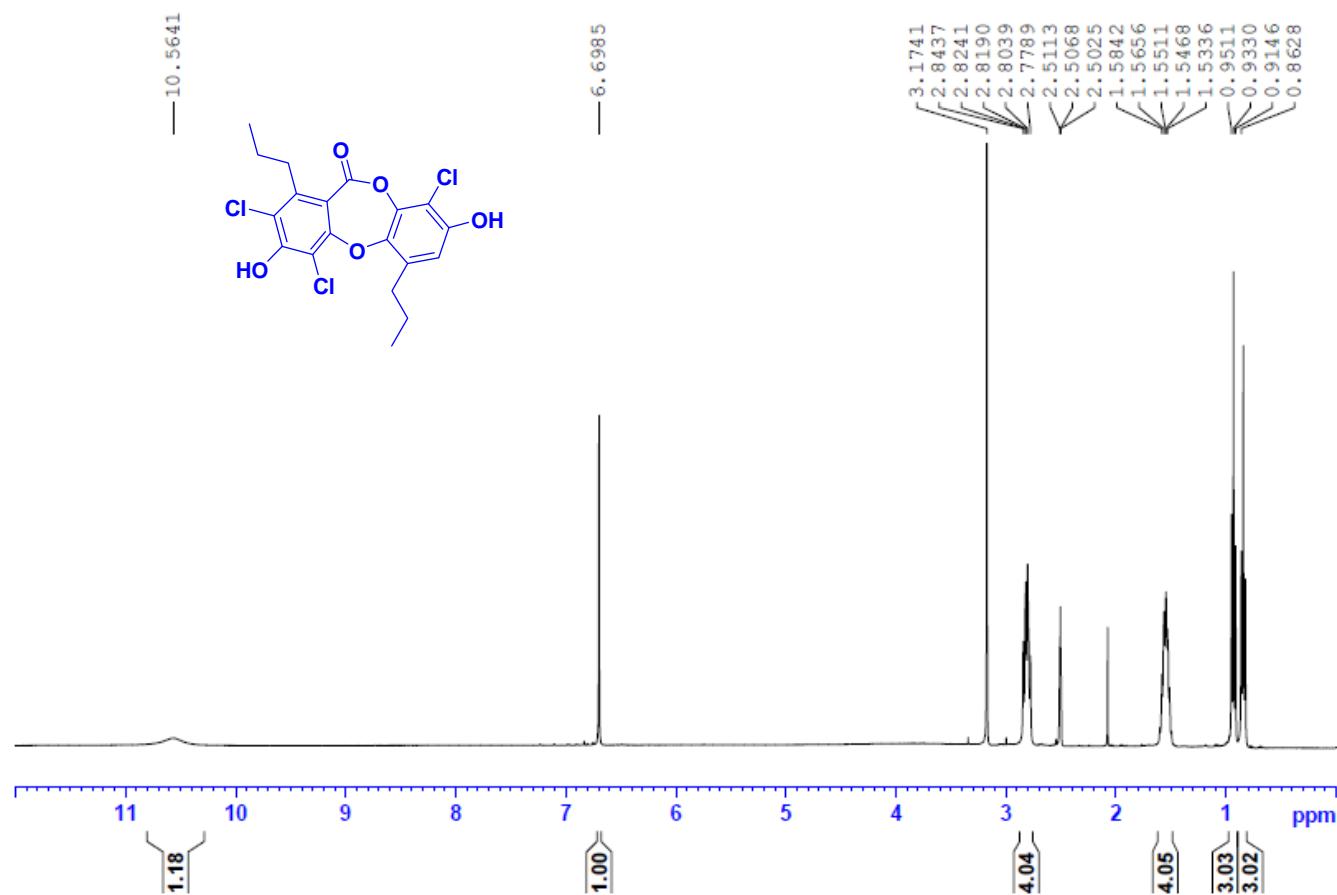


Figure S102. ^1H NMR spectrum of **8** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-4 APT

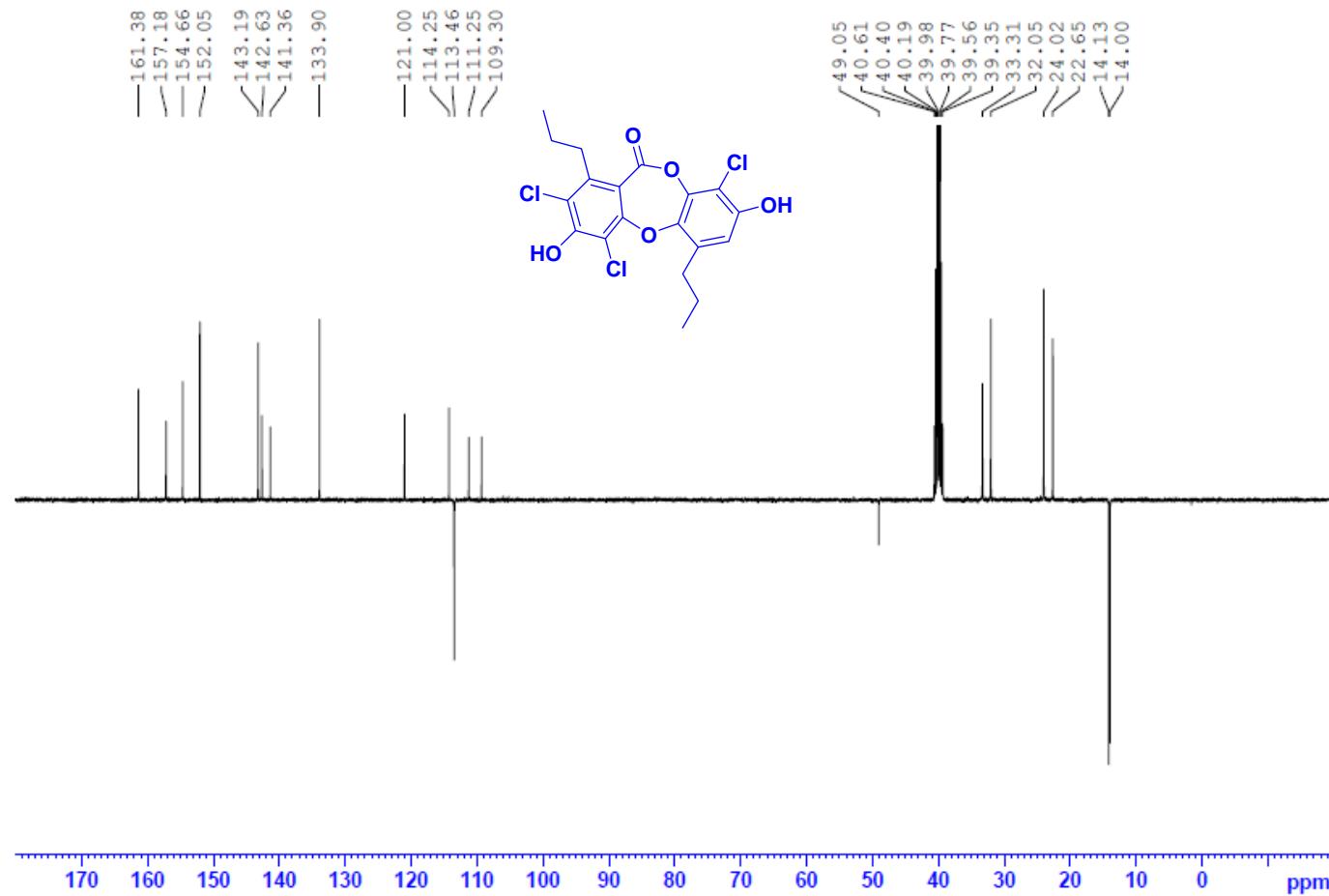


Figure S103. APT spectrum of **8** in $\text{DMSO}-d_6$ (100 MHz)

F19-8-18-4 HSQC

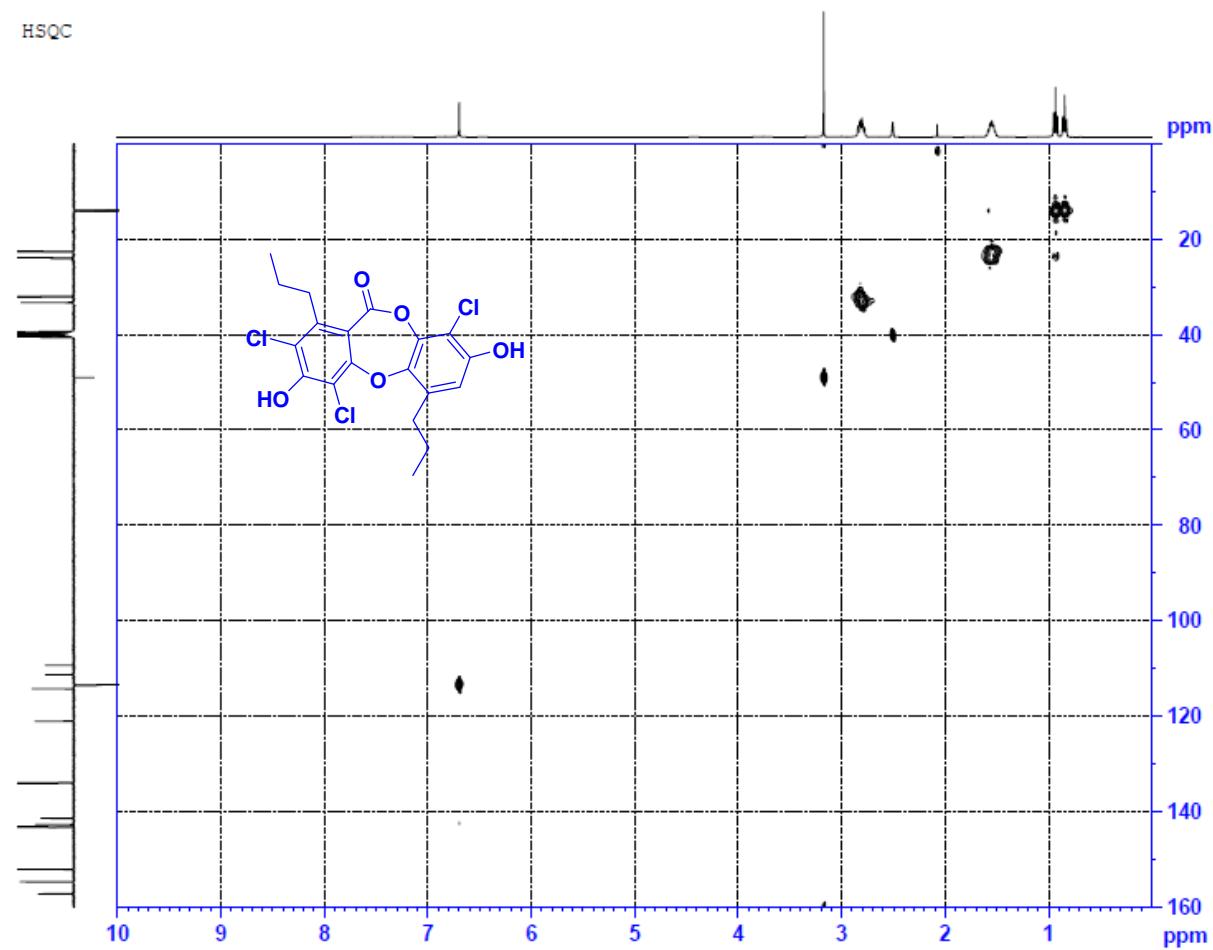


Figure S104. HSQC spectrum of **8** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-4 COSY

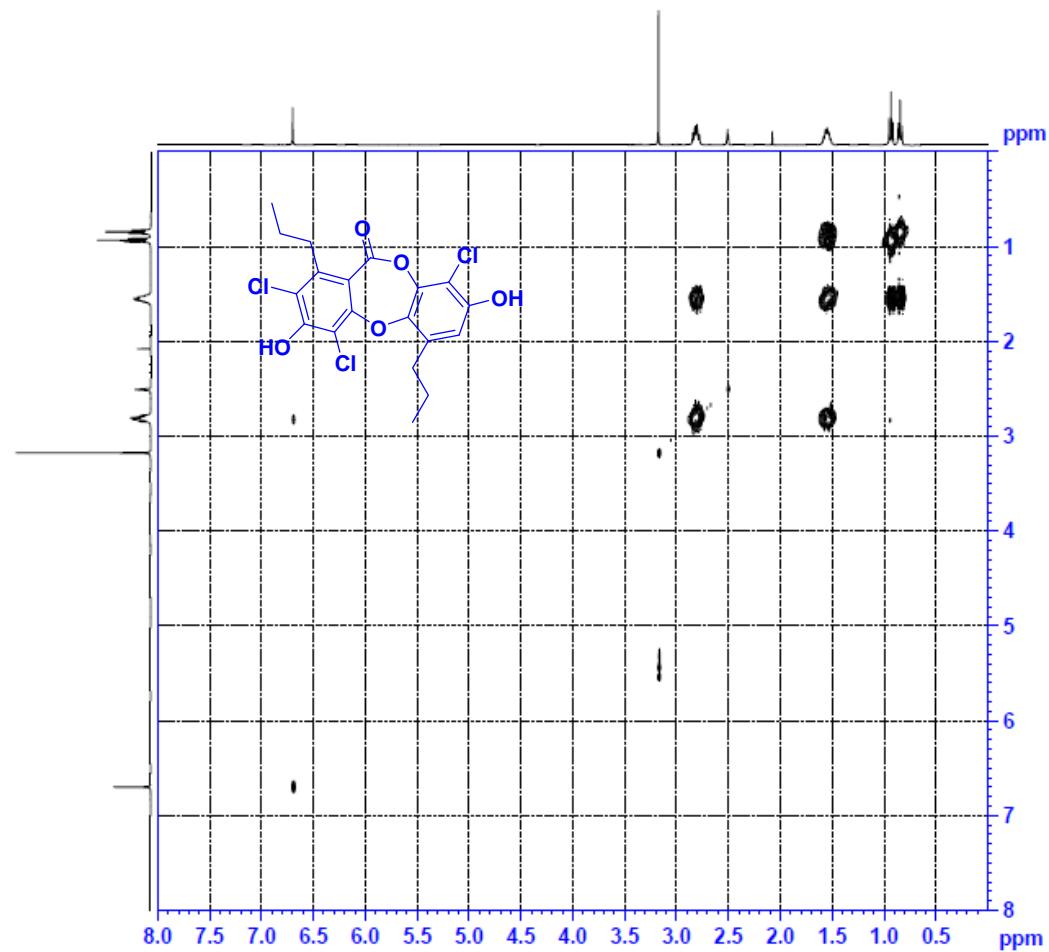


Figure S105. ^1H - ^1H COSY spectrum of **8** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-4 HMBC

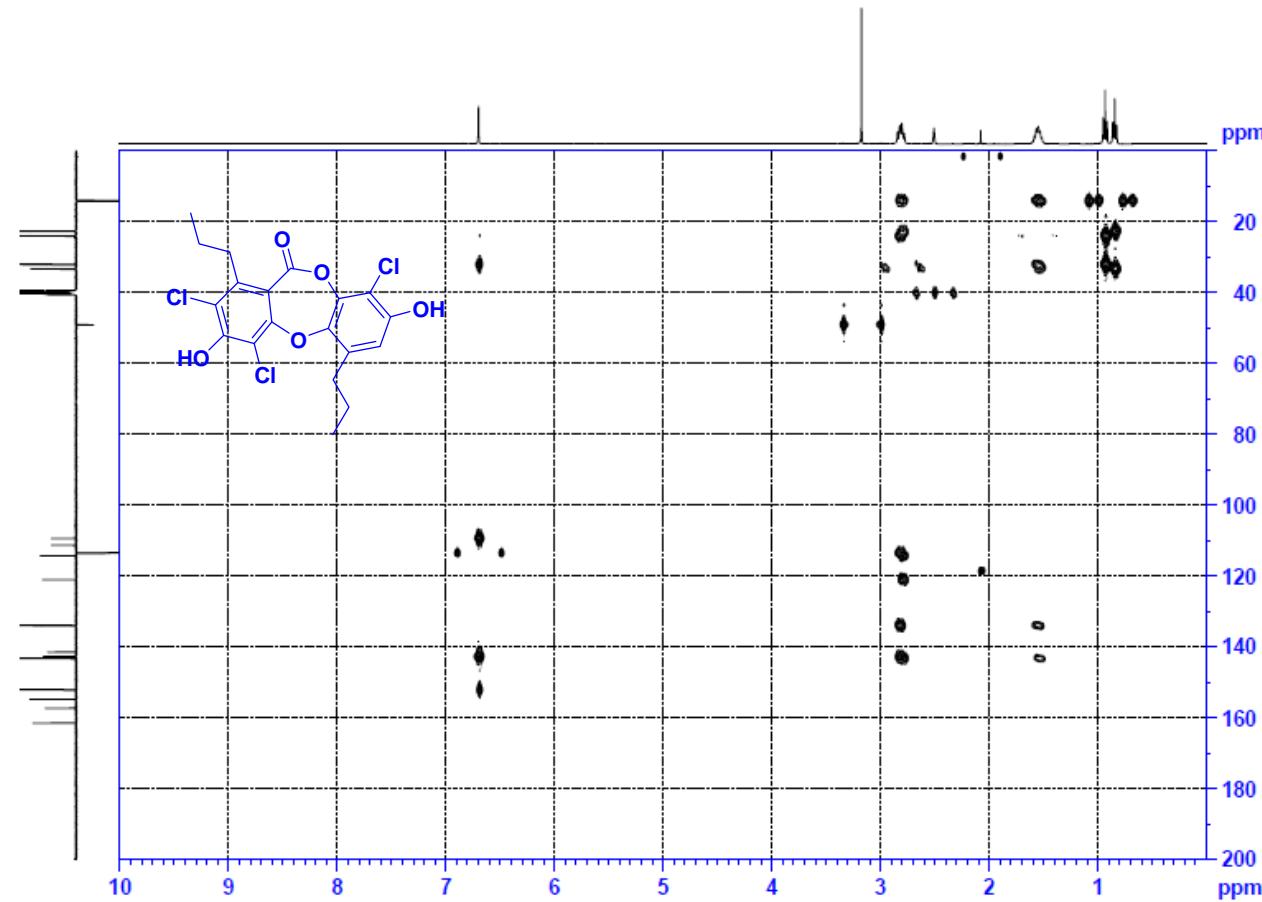
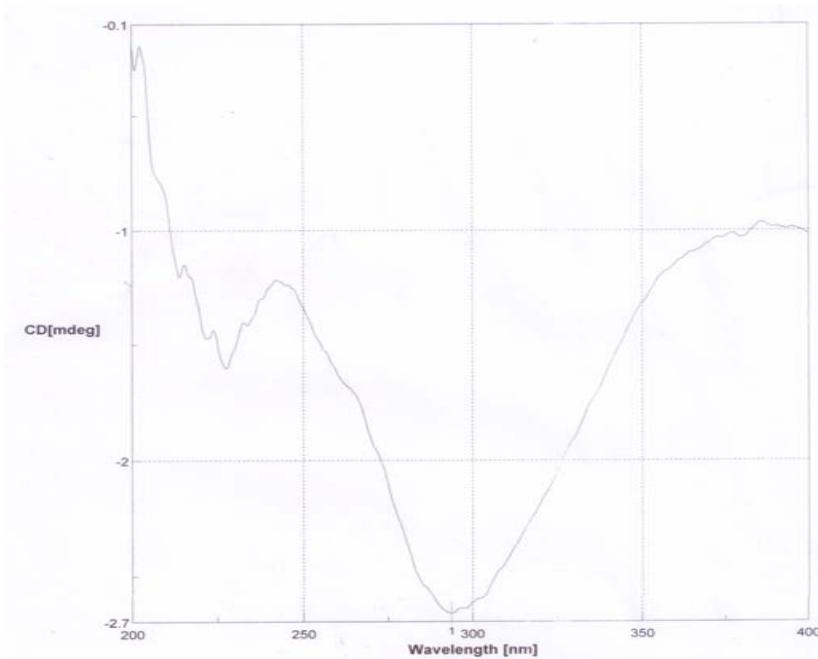


Figure S106. HMBC spectrum of **8** in $\text{DMSO}-d_6$ (400 MHz)



Date/Time 2001-1-3 6:01
Operator
File Name F19-8-18-4.txt
Sample Name F19-8-18-4
Comment

No.	nm	CD[mdeg]
1	293.8	-2.66392

Figure S107. CD spectrum of **8**

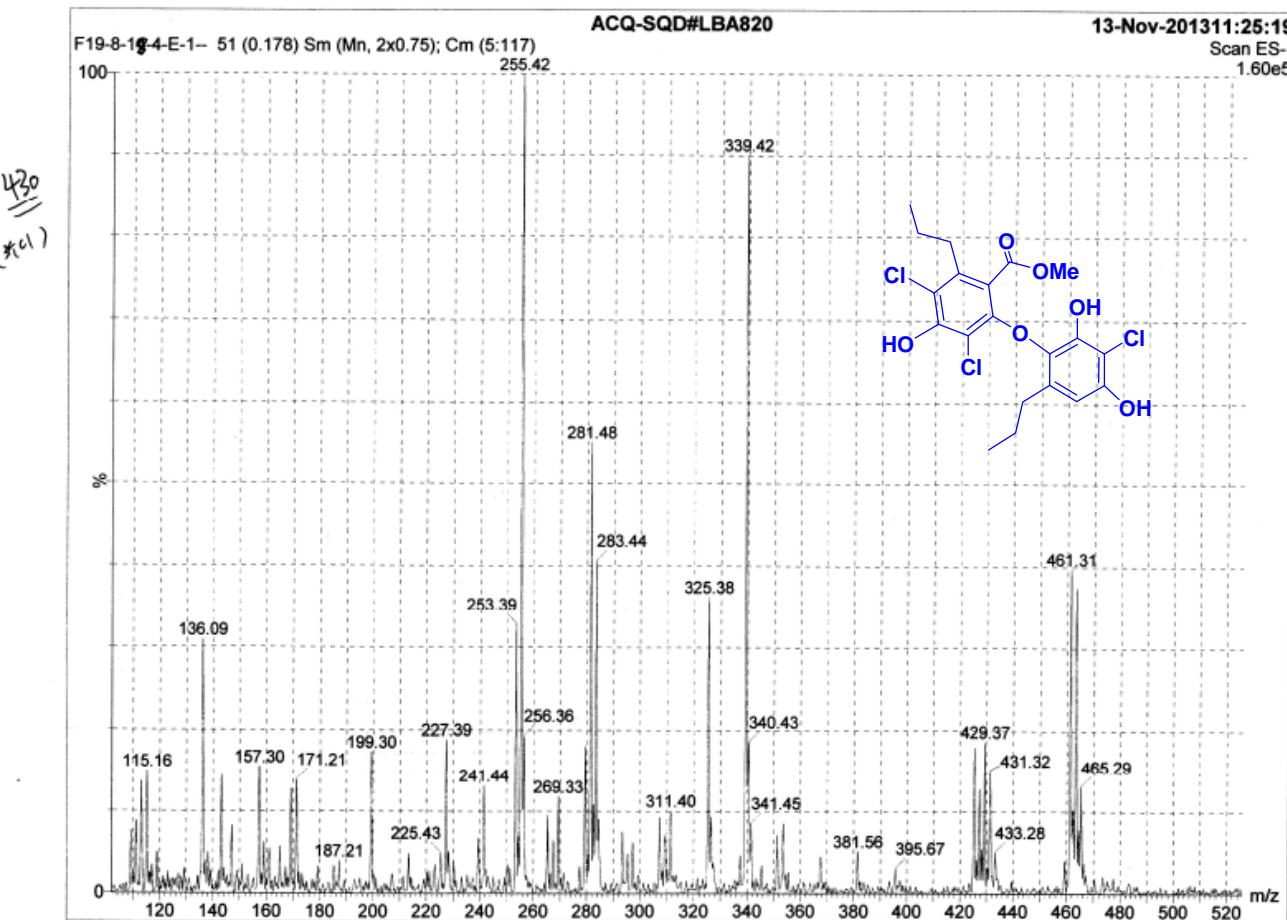


Figure S108. ESIMS spectrum of **8a**

F19-8-18-4-e-1 400 MHz DMSO

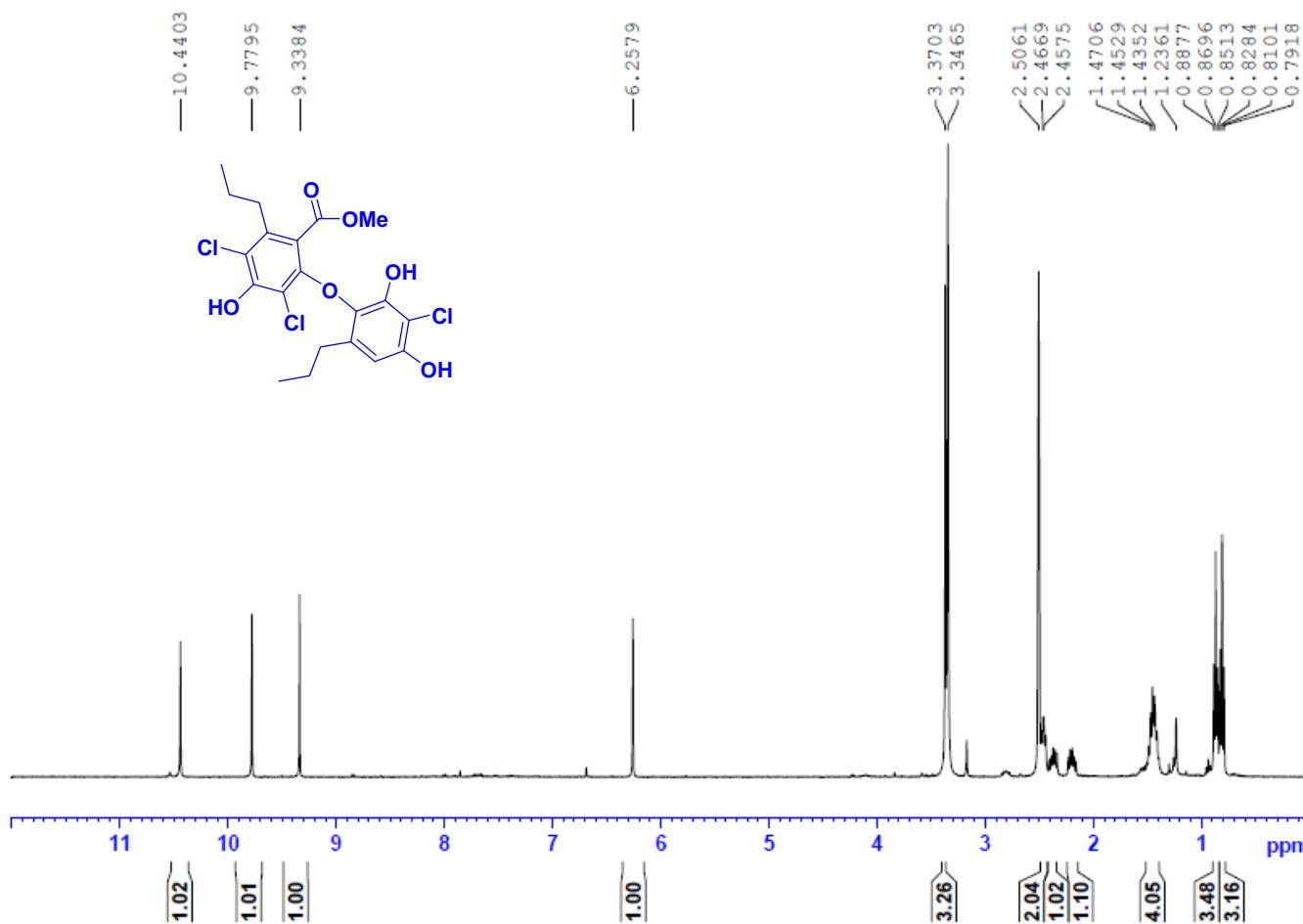


Figure S109. ^1H NMR spectrum of **8a** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-4-e-1 APT

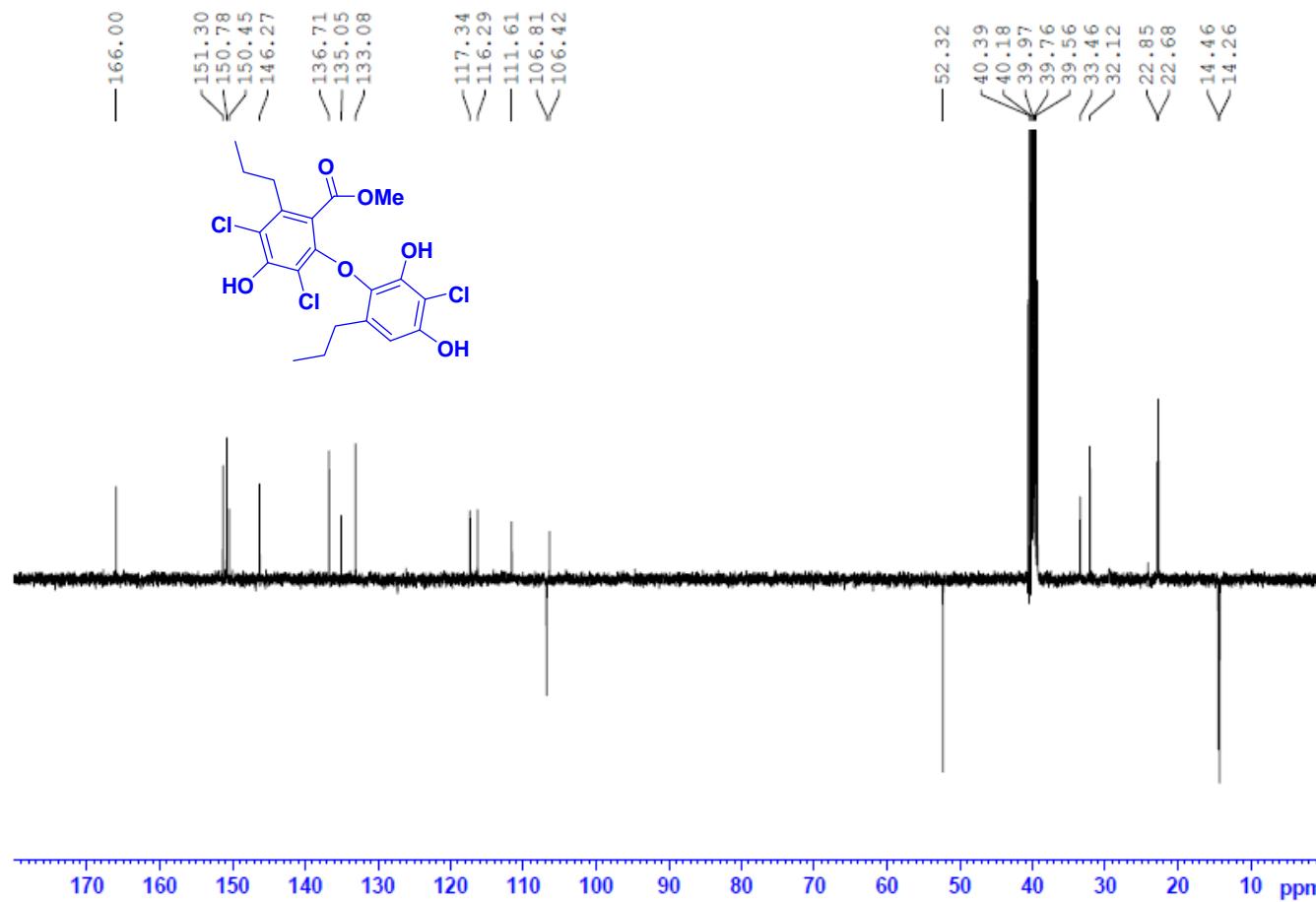


Figure S110. APT spectrum of **8a** in DMSO-*d*₆ (100 MHz)

F19-8-18-4-e-1 HSQC

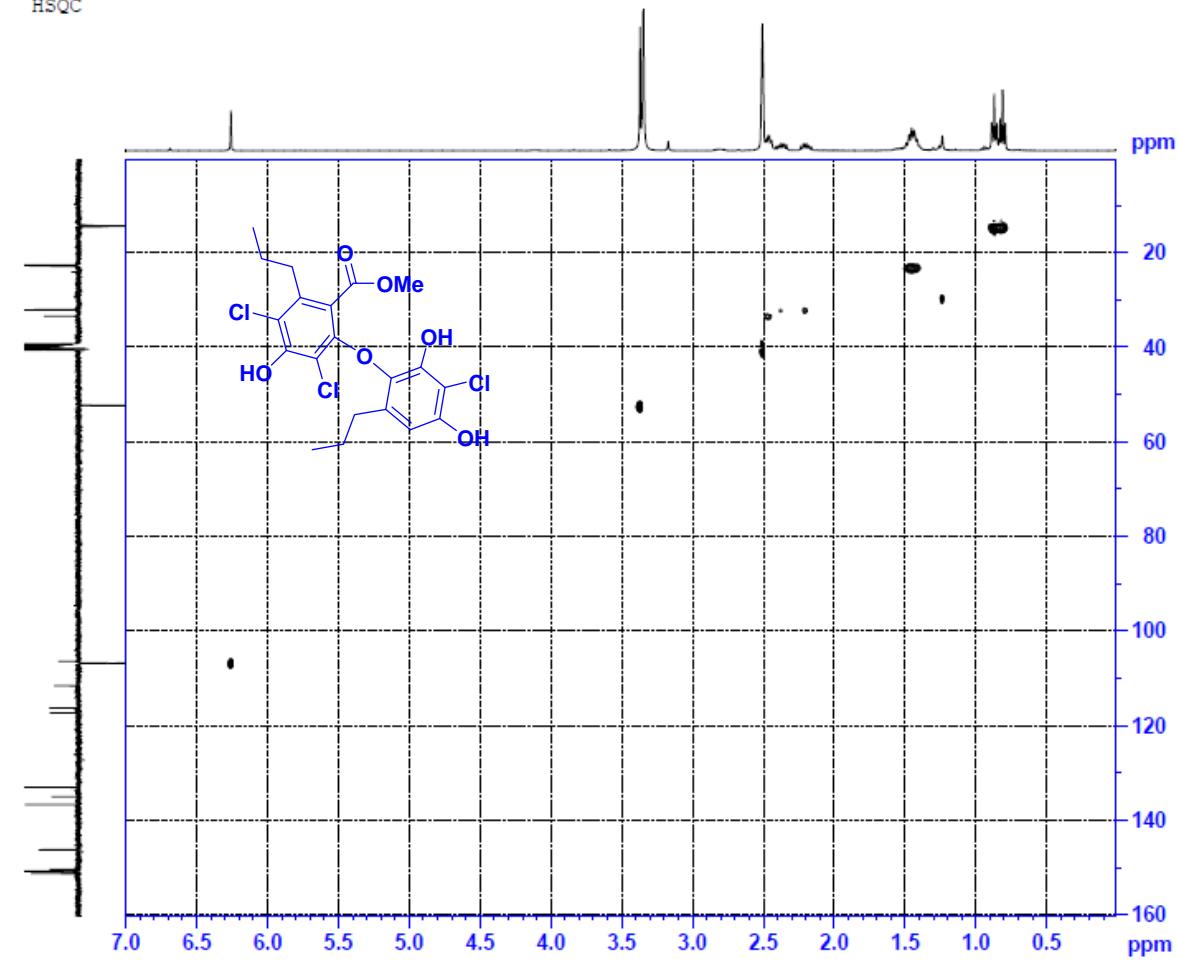


Figure S111. HSQC spectrum of **8a** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-4-e-1

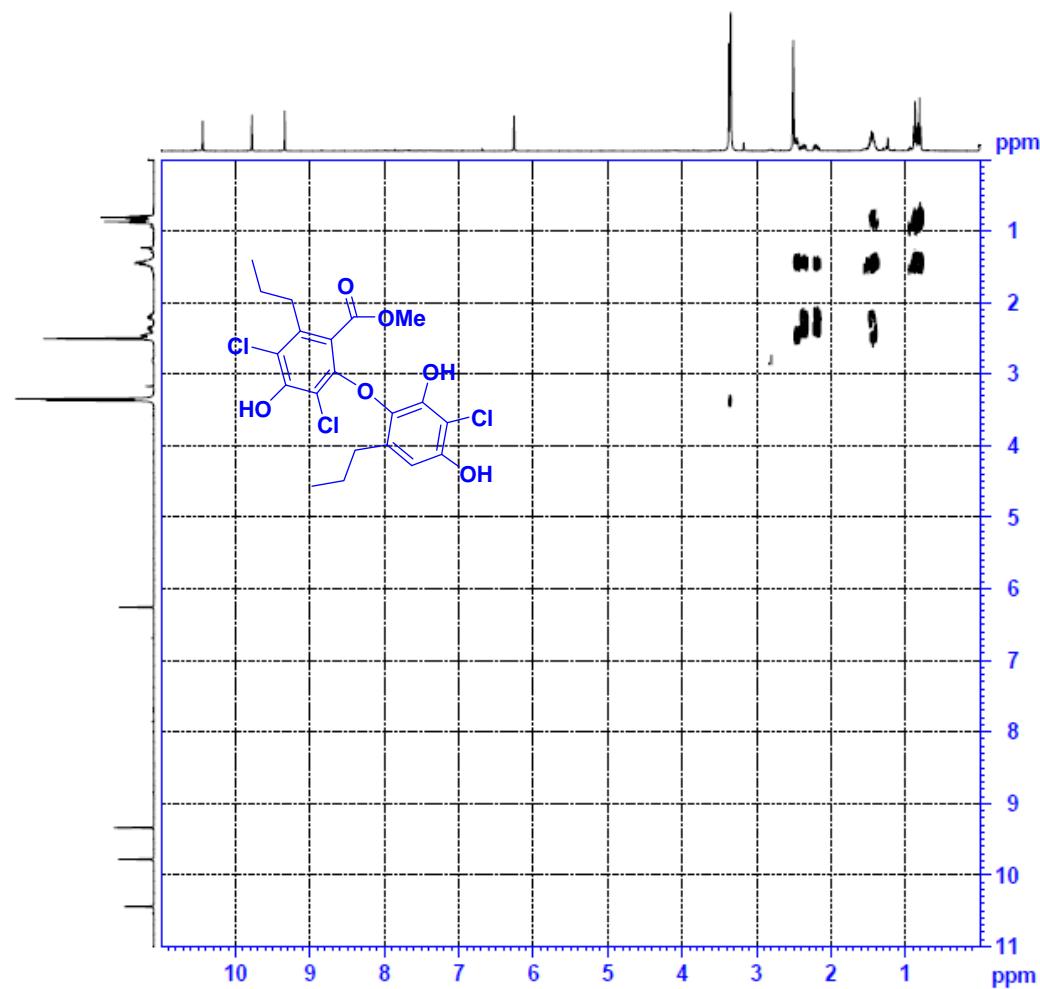


Figure S112. ^1H - ^1H COSY spectrum of **8a** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-4-e-1 HMBC

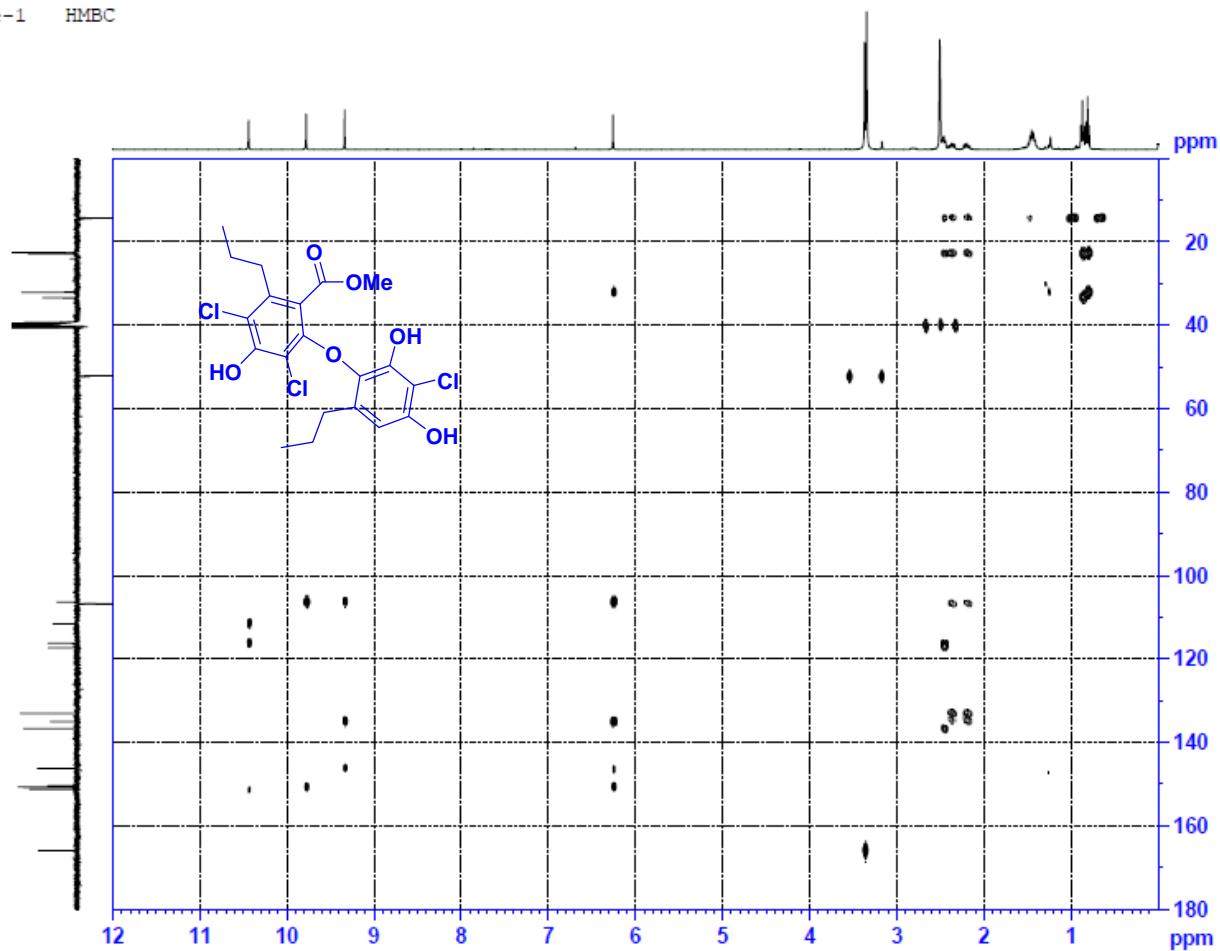


Figure S113. HMBC spectrum of **8a** in DMSO-*d*₆ (400 MHz)

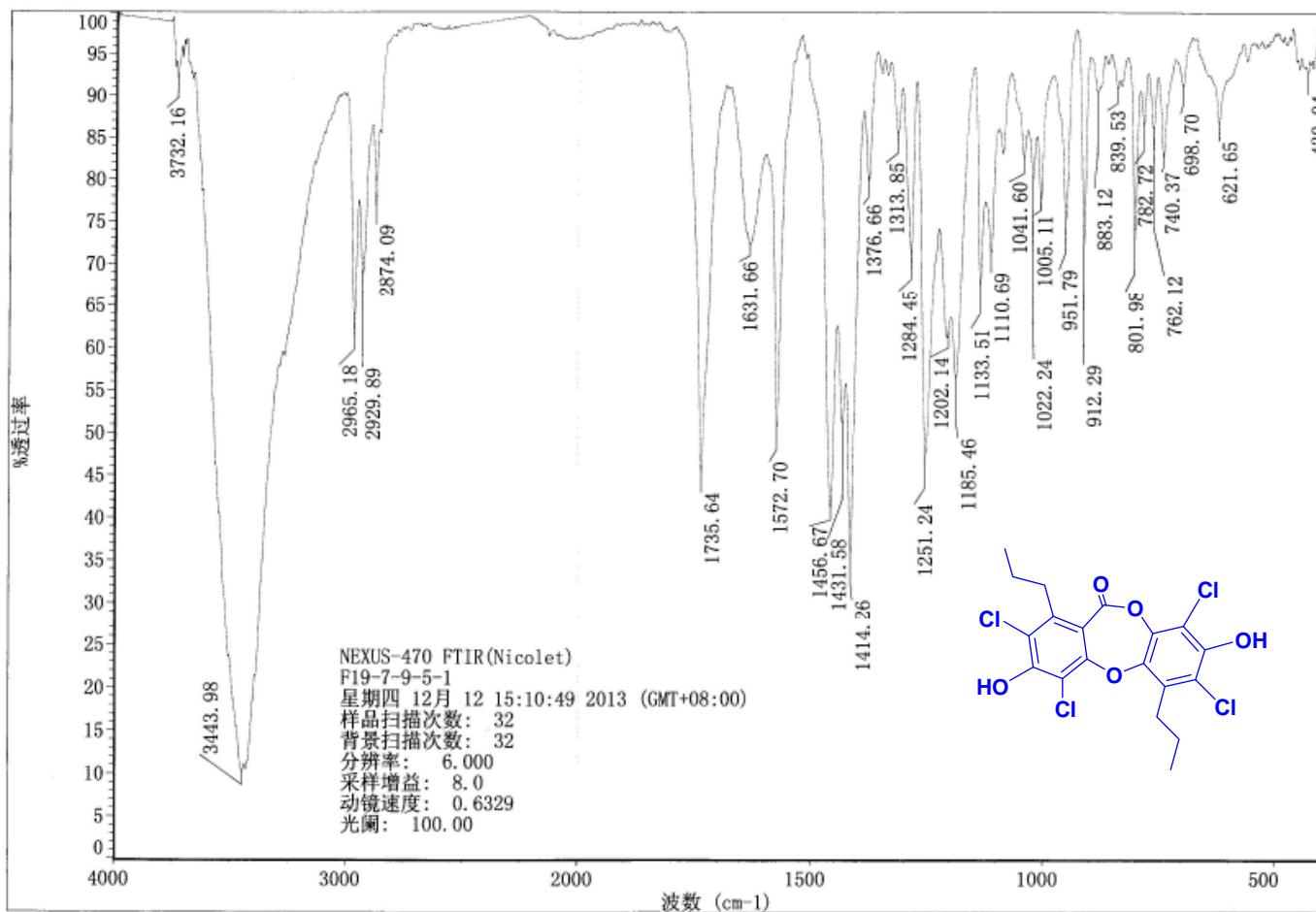


Figure S114. IR spectrum of 9



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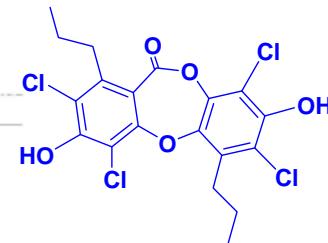
Analysis Name C:\data\sample\ESI_12131120_30\LowMassESI_F17_7_9_5_1_20131121\POS_2 Acquisition Date 11/20/2013 2:04:08 PM

Operator bpxsh@bjmu.edu.cn; Tel:010-82801

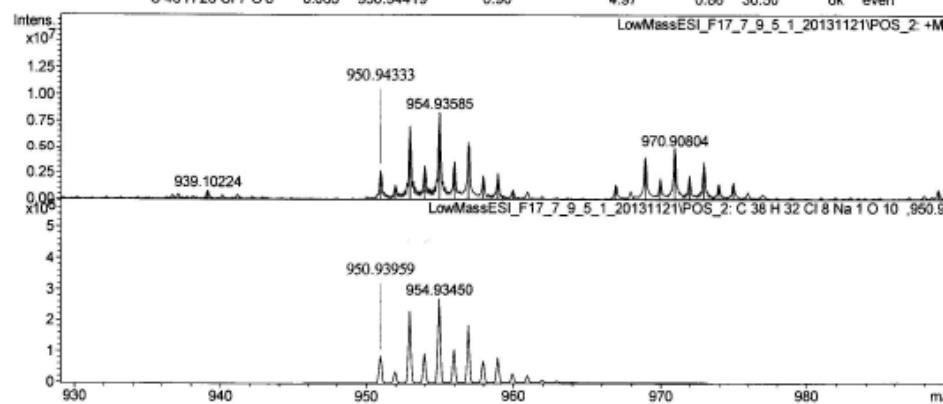
Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI pos □ C19H16Cl4O5 MW 464
CAL588: 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;8.26.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result Exact Mass Measured Mass Error (mDa) Error (ppm) Description



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 40 H 31 Cl 8 O 10	0.028	950.94200	-1.41	2.37	-1.34	21.50	ok	even
C 38 H 32 Cl 8 Na 1 O 10	0.029	950.93959	-3.94	-0.22	-3.74	18.50	ok	even
C 44 H 27 Cl 7 Na 1 O 8	0.062	950.94178	-1.63	2.38	-1.55	27.50	ok	even
C 46 H 26 Cl 7 O 8	0.063	950.94419	0.90	4.97	0.86	30.50	ok	even





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Analysis Name C:\data_sample\ESI_12131120_30\LowMassESI_F17_7_9_5_1_20131121\POS_2 Acquisition Date 11/20/2013 2:04:08 PM
Operator bpxsh@bjmu.edu.cn; Tel:010-82801
Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI pos □ C19H16Cl4O5 MW 464
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;8;26.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result	Exact Mass	Measured Mass	Error (mDa)	Error (ppm)	Description
	464.98246	464.98089	1.57	3.38	M+H ⁺ ;e ⁻

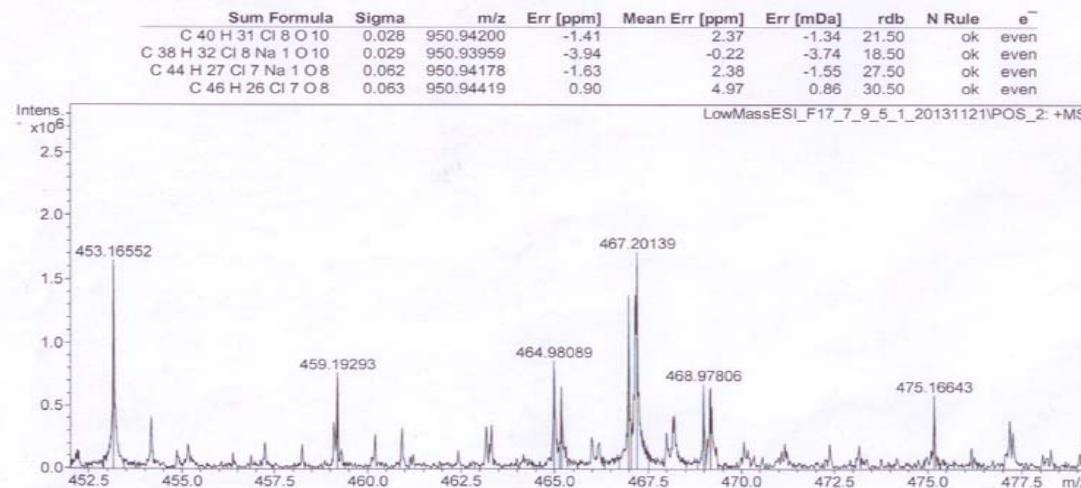


Figure S115. HRESIMS spectrum of 9

F19-7-9-5-1 400 MHz DMSO

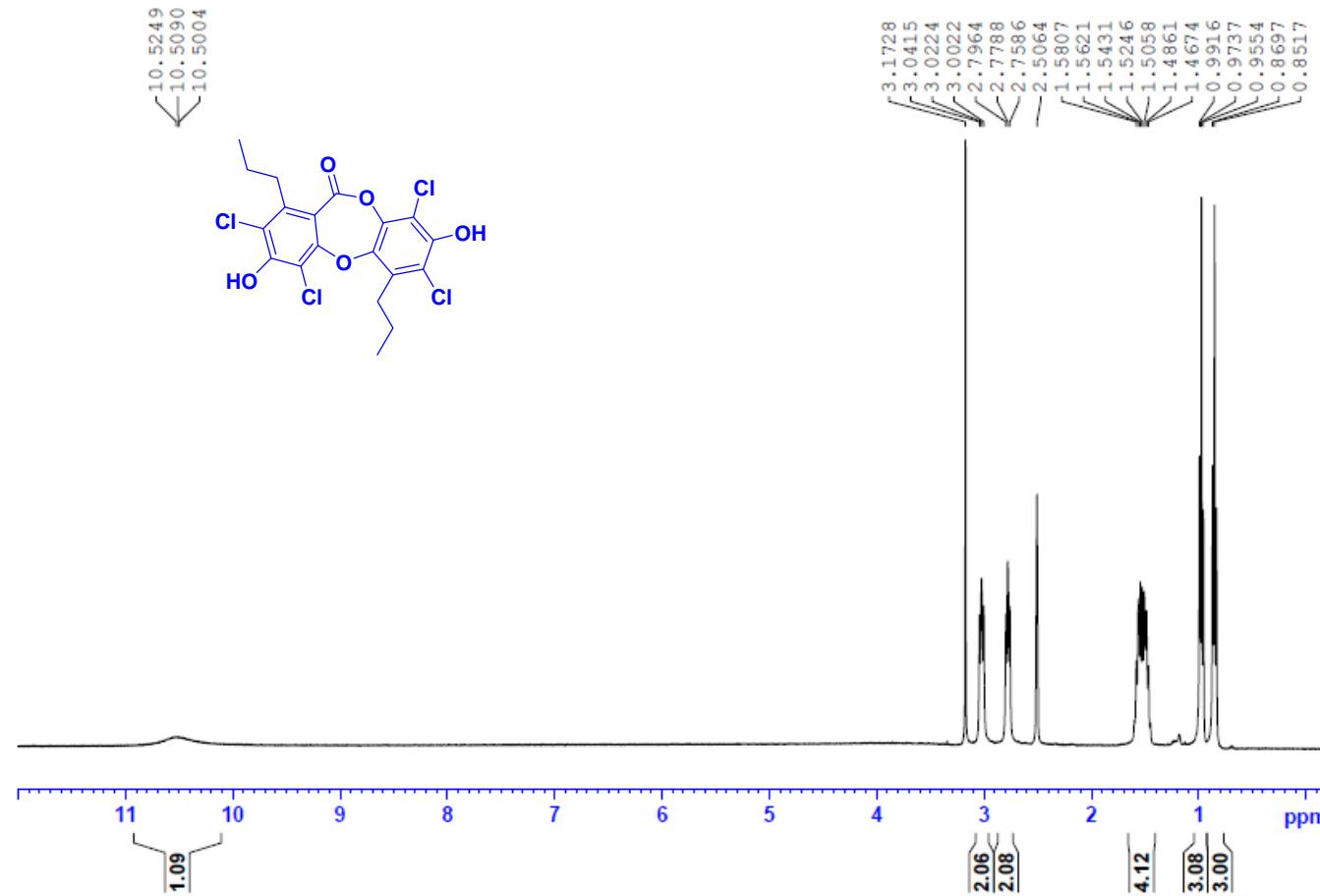
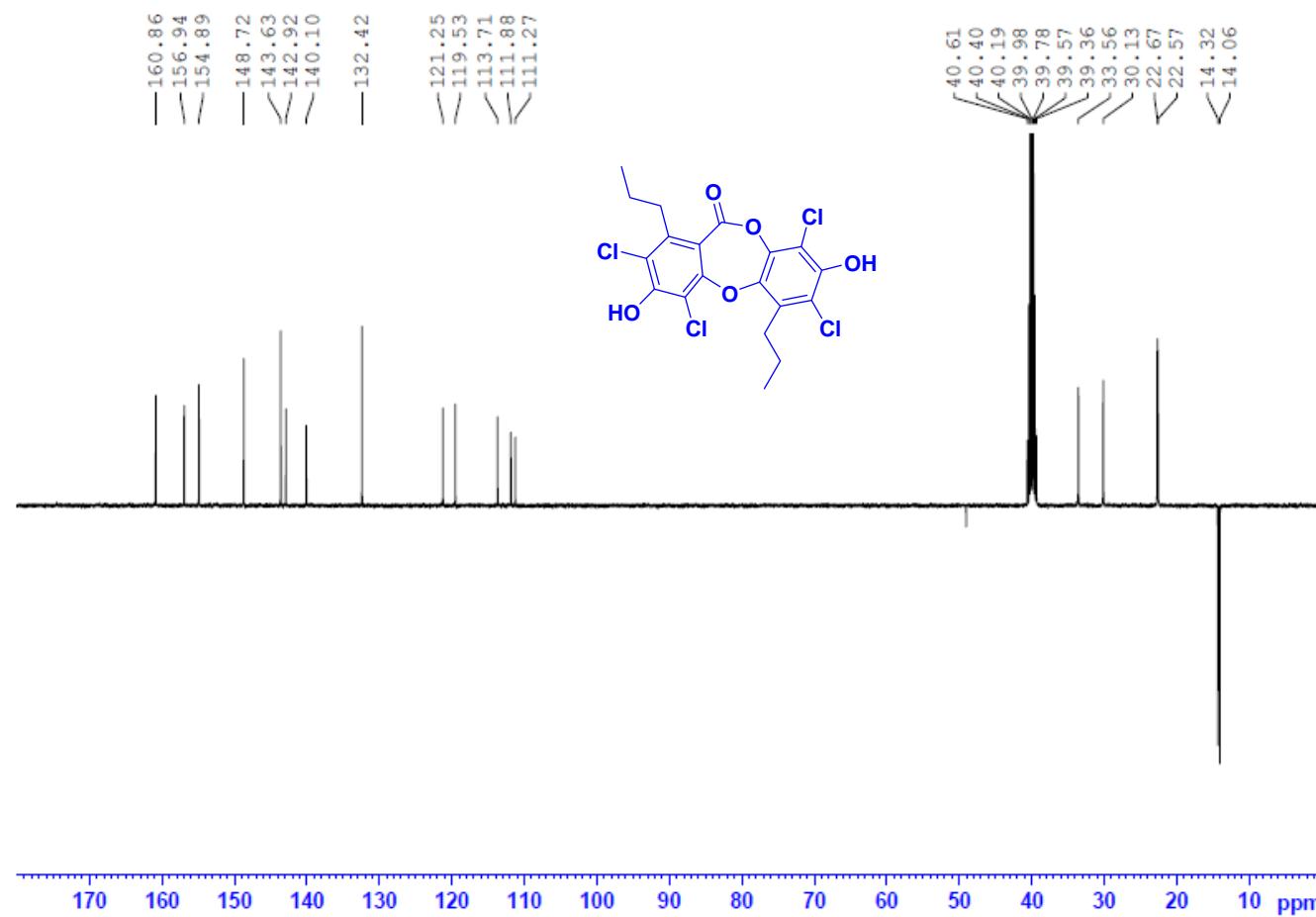


Figure S116. ^1H NMR spectrum of **9** in $\text{DMSO}-d_6$ (400 MHz)

F19-7-9-5-1 APT



F19-7-9-5-1 HSQC

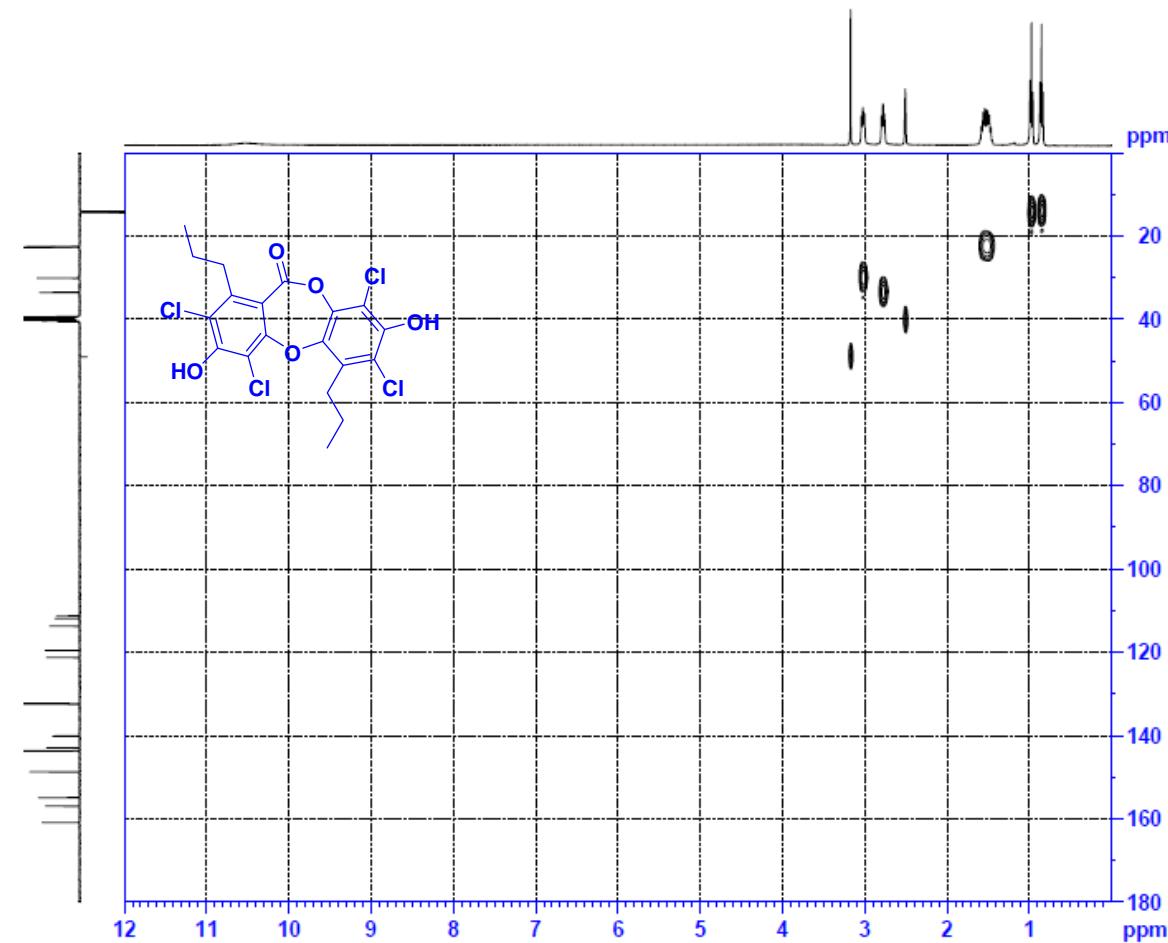


Figure S118. HSQC spectrum of **9** in $\text{DMSO}-d_6$ (400 MHz)

F19-7-9-5-1 COSY

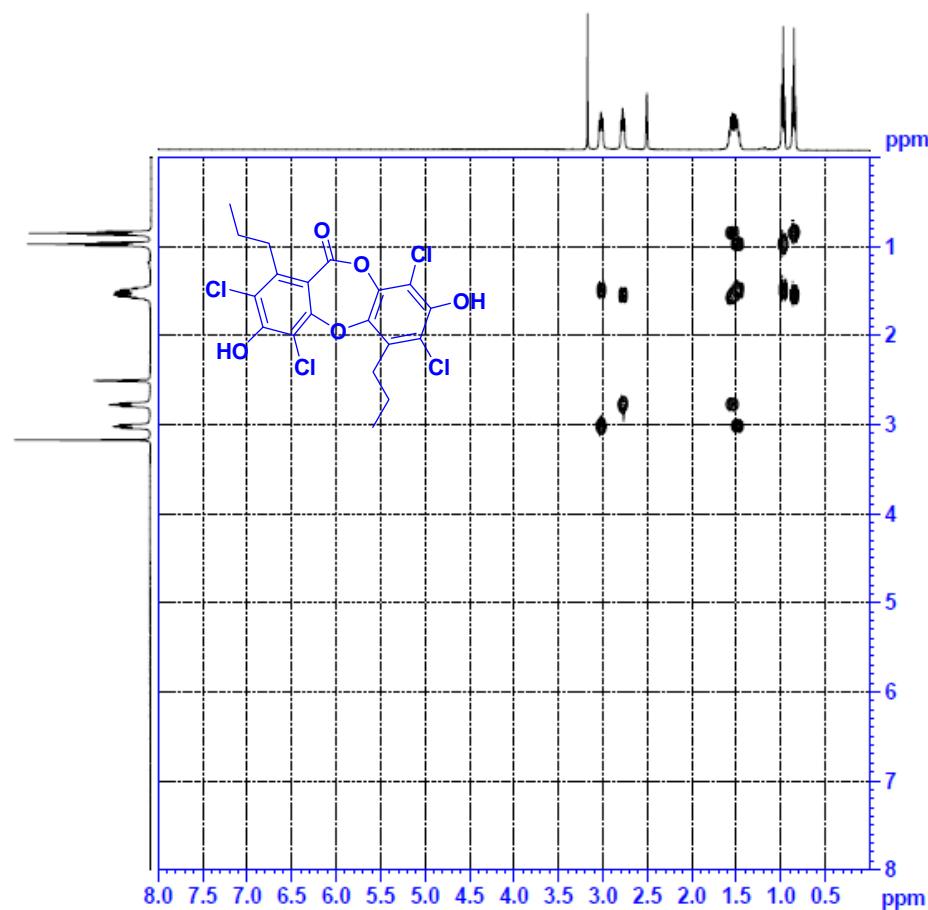


Figure S119. ^1H - ^1H COSY spectrum of **9** in $\text{DMSO}-d_6$ (400 MHz)

F19-7-9-5-1 HMBC

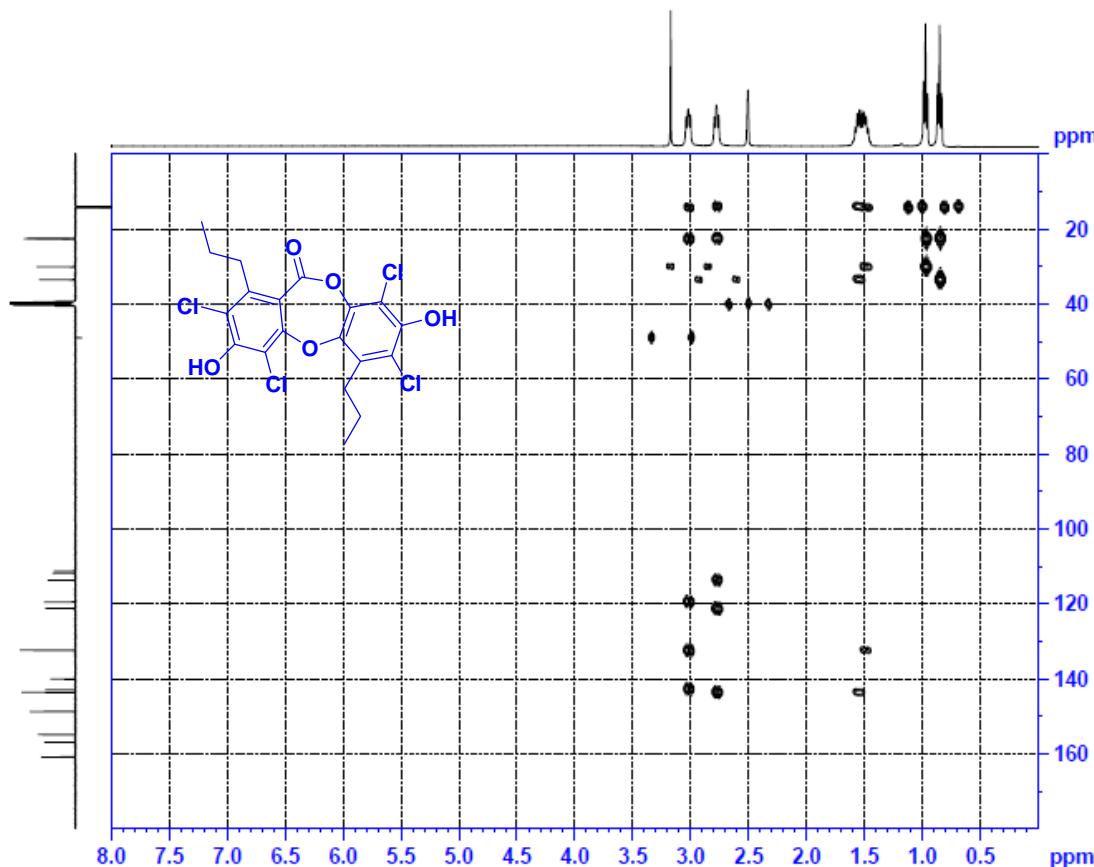
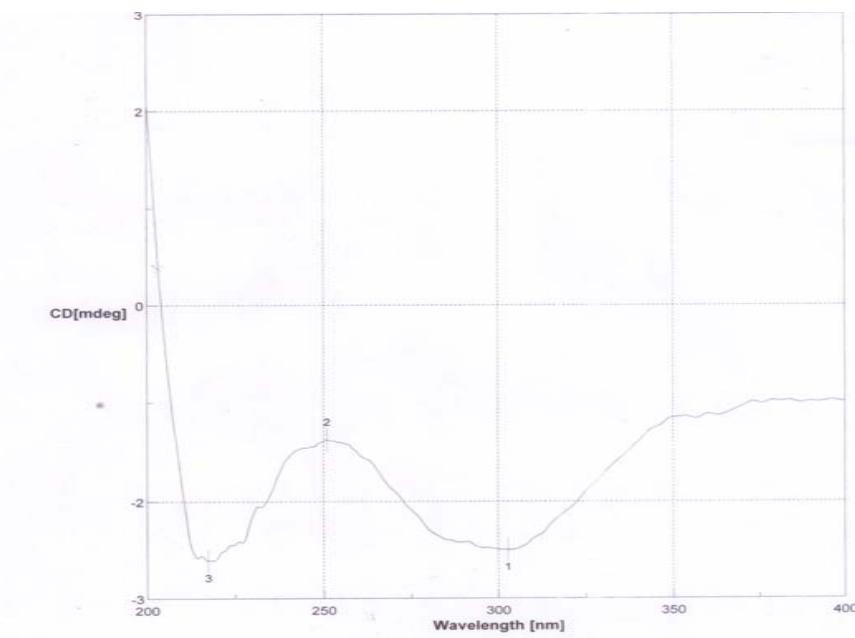


Figure S120. HMBC spectrum of **9** in DMSO-*d*₆ (400 MHz)



Date/Time 2001-1-3 6:11
Operator
File Name F19-7-9-5-1.txt
Sample Name F19-7-9-5-1
Comment

No.	nm	CD[mdeg]	No.	nm	CD[mdeg]	No.	nm	CD[mdeg]
1	302.8	-2.49479	2	251	-1.37738	3	217.4	-2.60624

Figure S121. CD spectrum of **9**

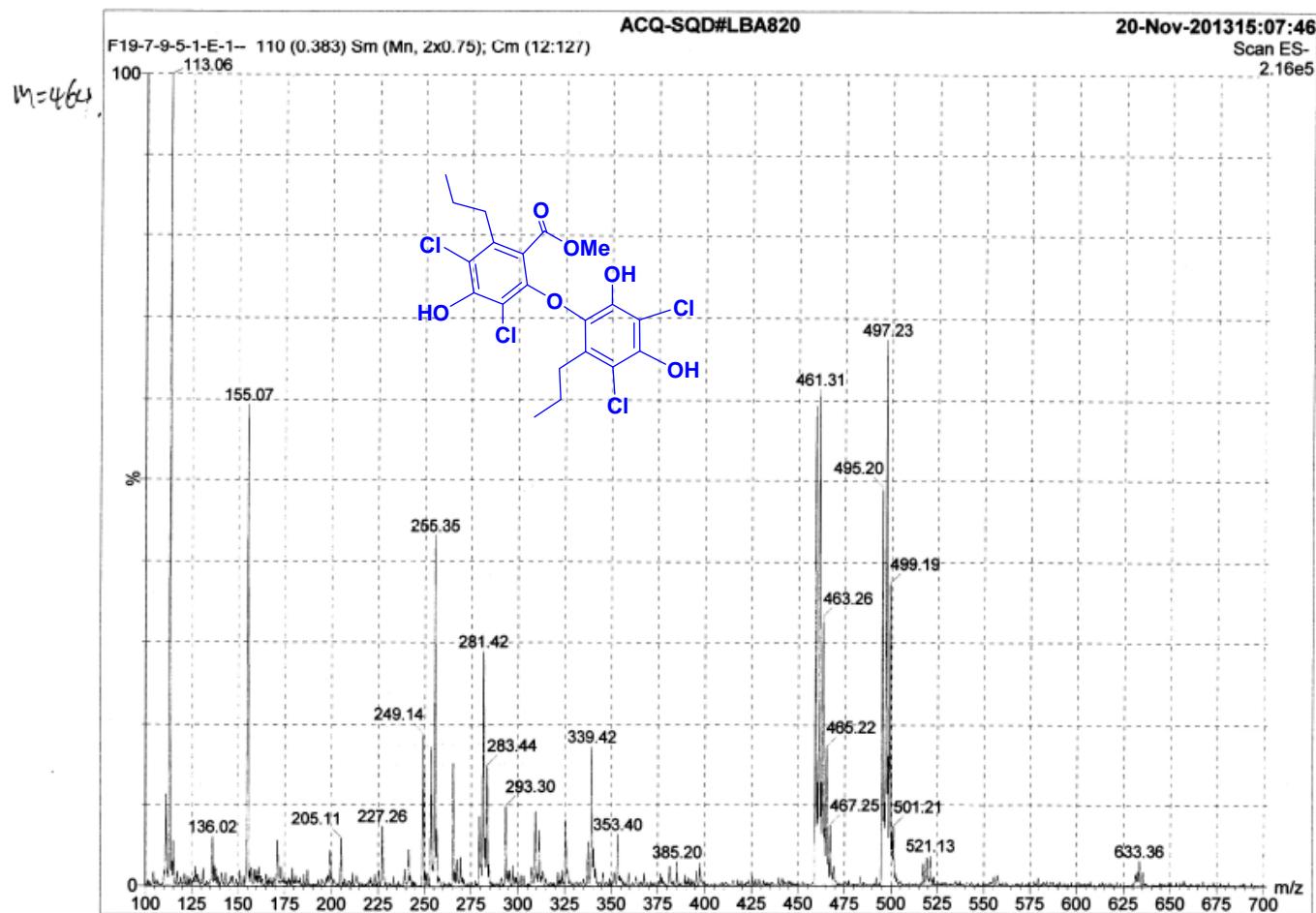


Figure S122. ESIMS spectrum of **9a**

F19-7-9-5-1-e-1 400 MHz DMSO

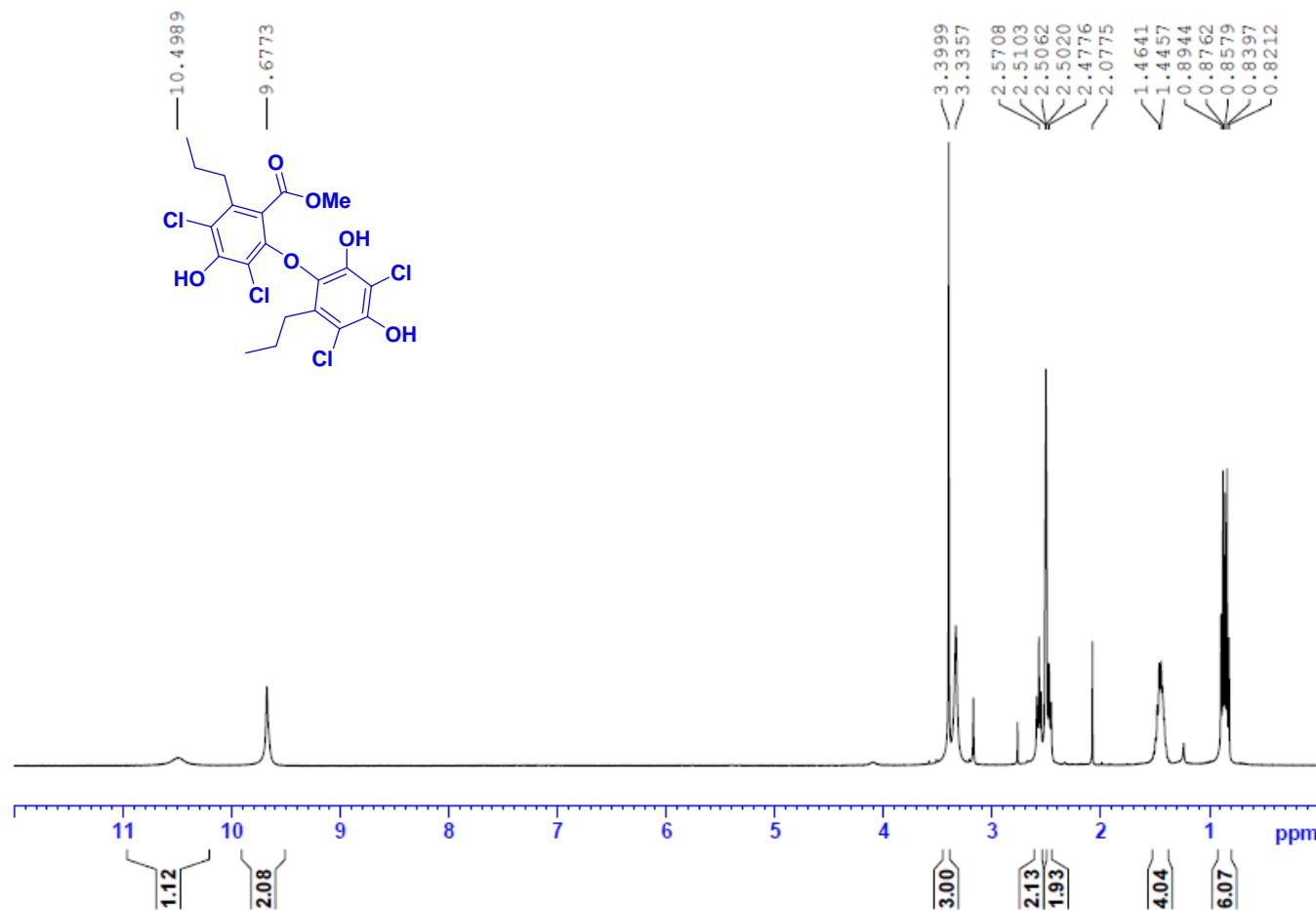


Figure S123. ^1H NMR spectrum of **9a** in $\text{DMSO}-d_6$ (400 MHz)

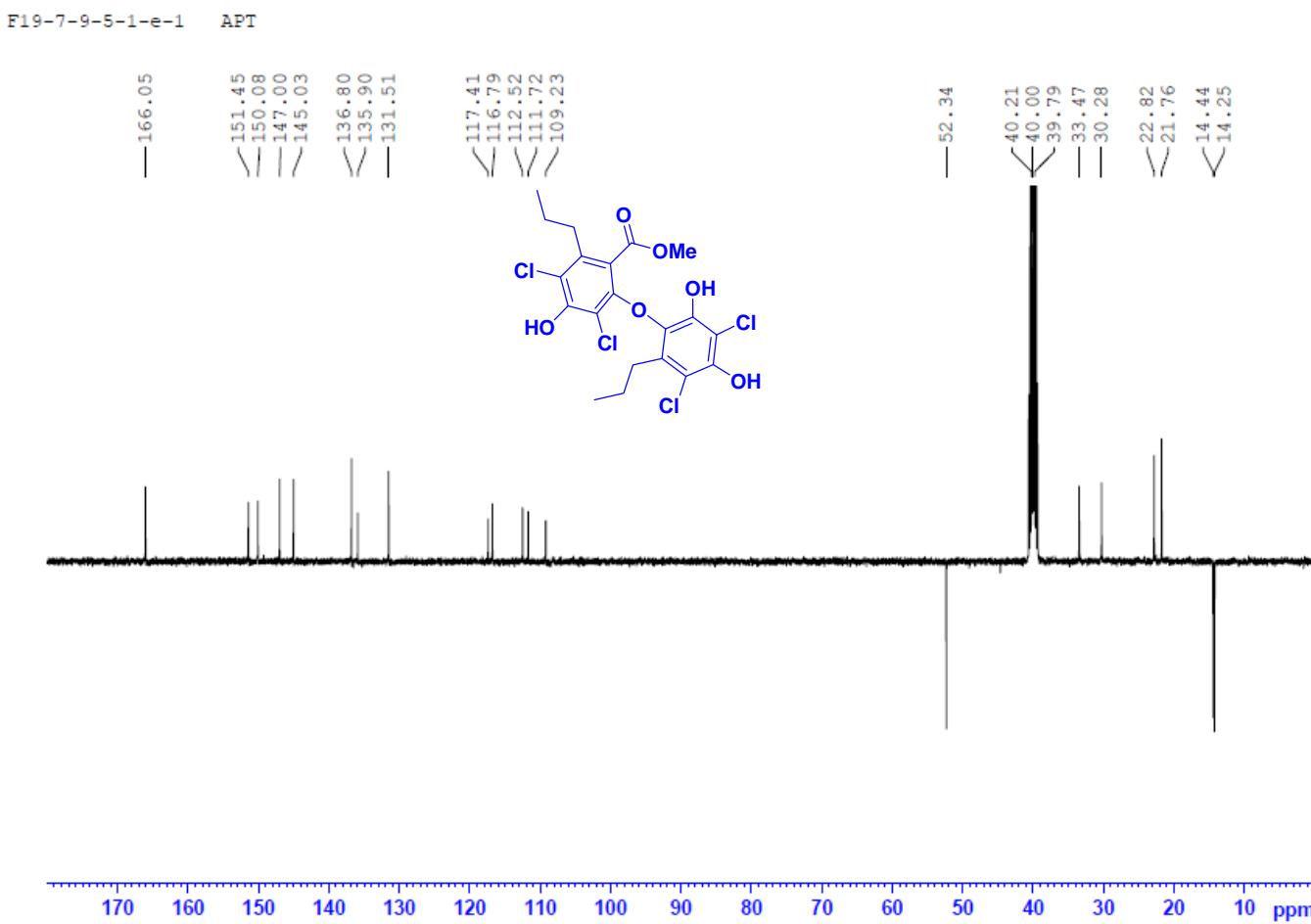


Figure S124. APT spectrum of **9a** in DMSO-*d*₆ (100 MHz)

F19-7-9-5-1-e-1 HSQC

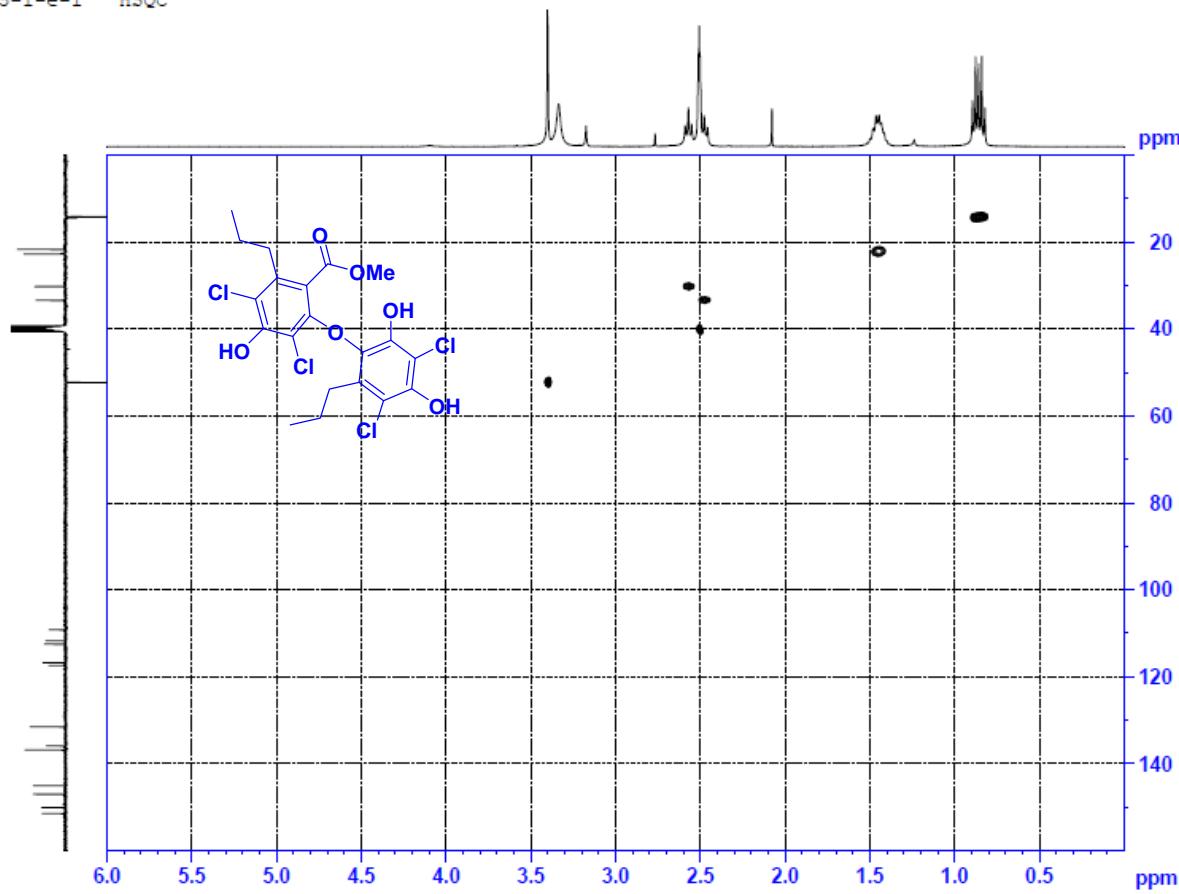


Figure S125. HSQC spectrum of **9a** in DMSO-*d*₆ (400 MHz)

F19-7-9-5-1-e-1 COSY

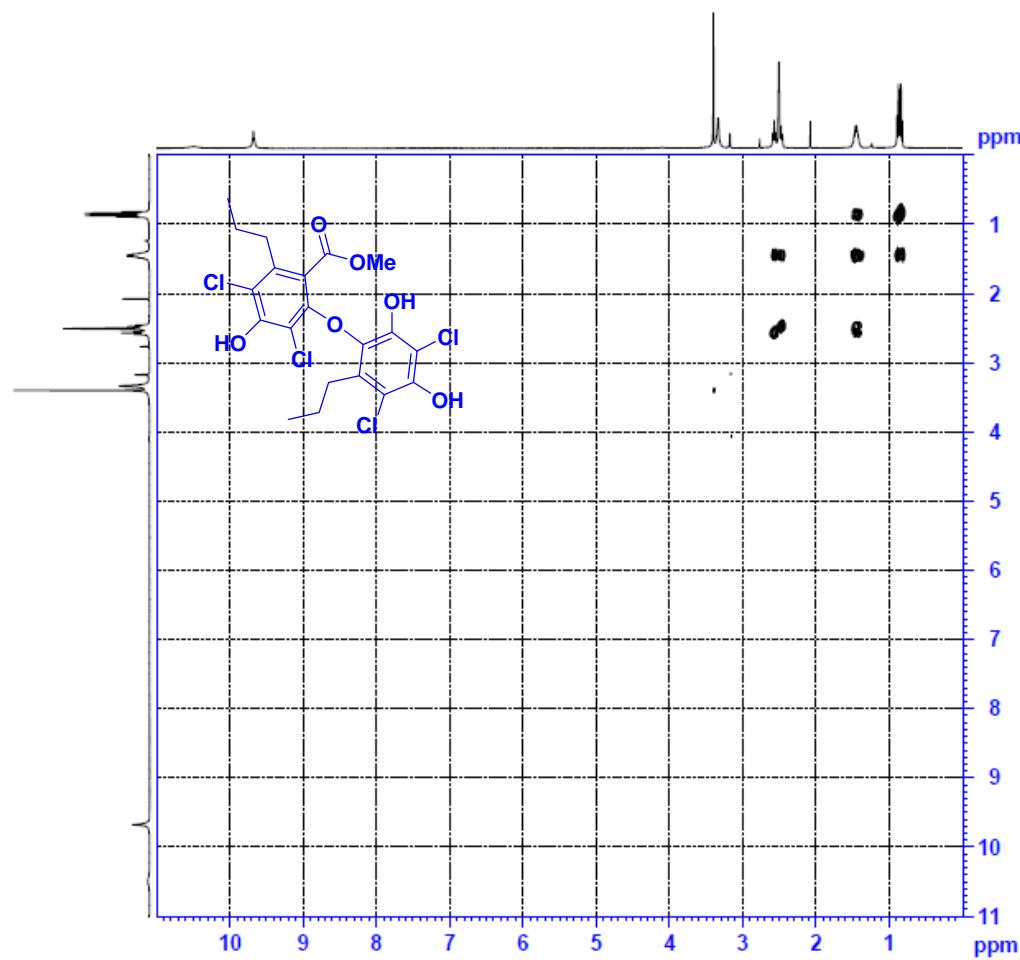


Figure S126. ^1H - ^1H COSY spectrum of **9a** in $\text{DMSO}-d_6$ (400 MHz)

F19-7-9-5-1-e-1 HMBC

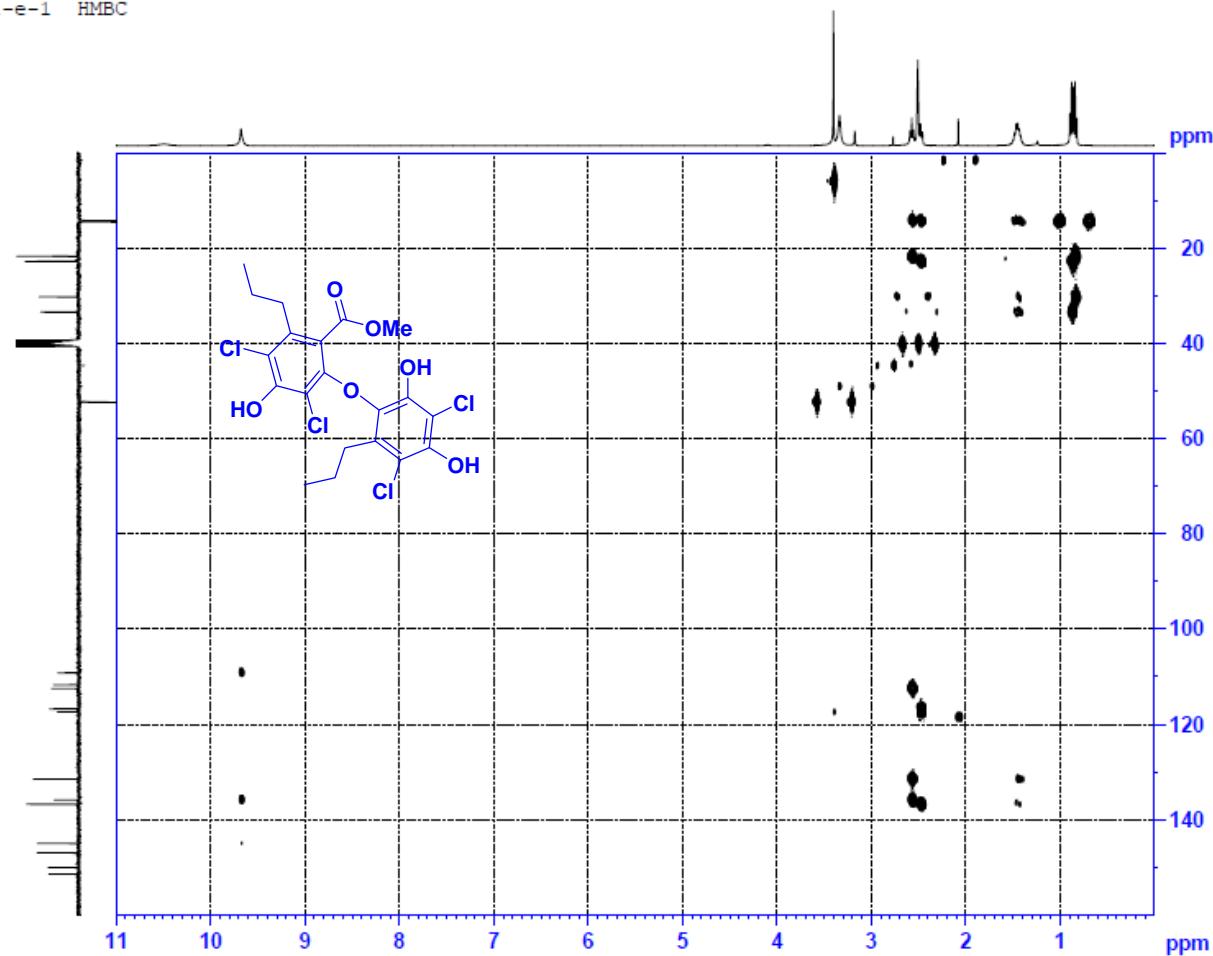


Figure S127. HMBC spectrum of **9a** in $\text{DMSO}-d_6$ (400 MHz)

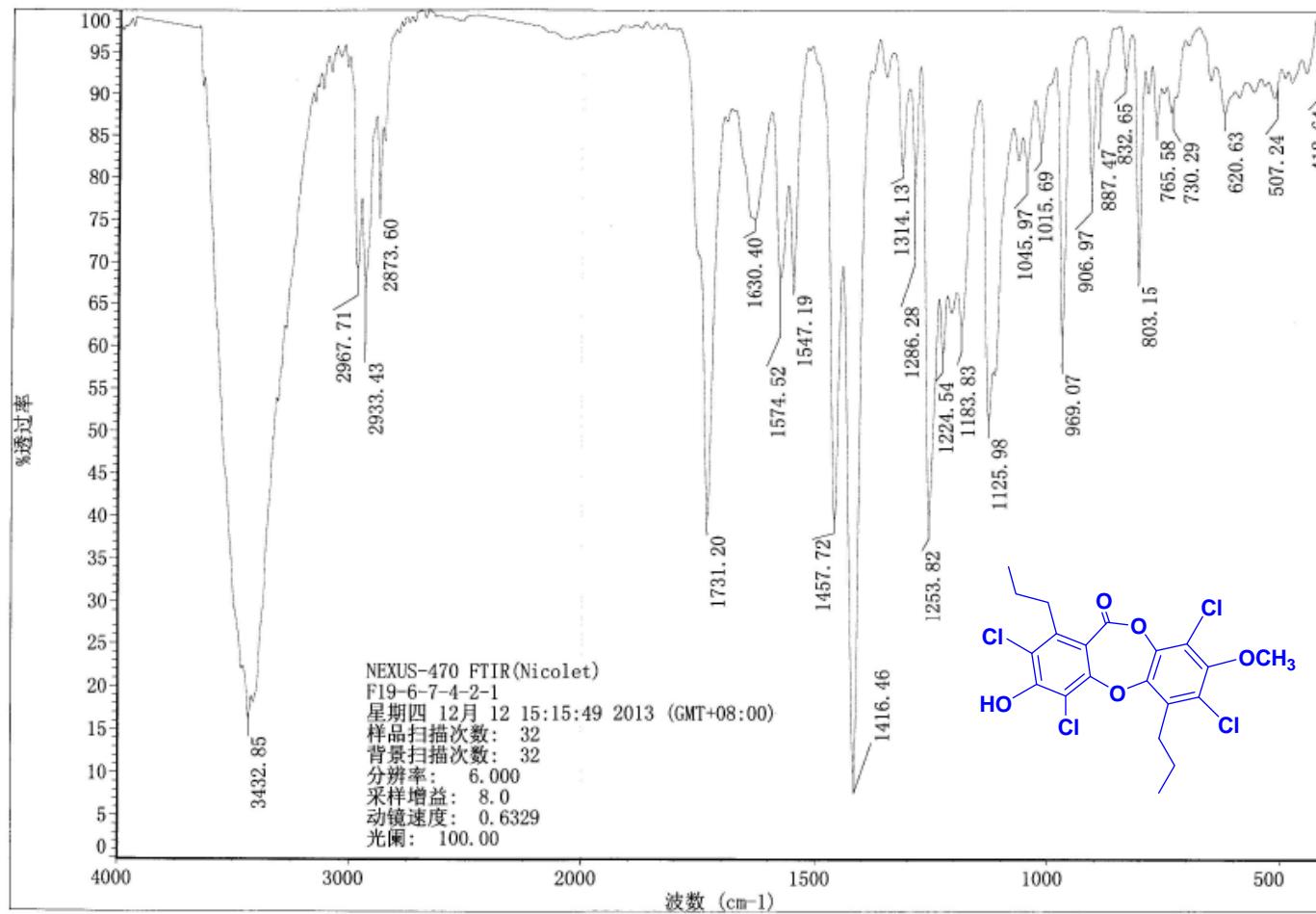


Figure S128. IR spectrum of **10**

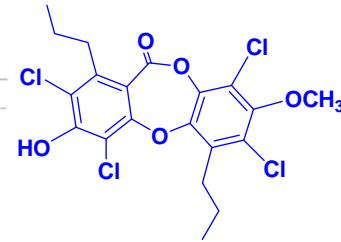


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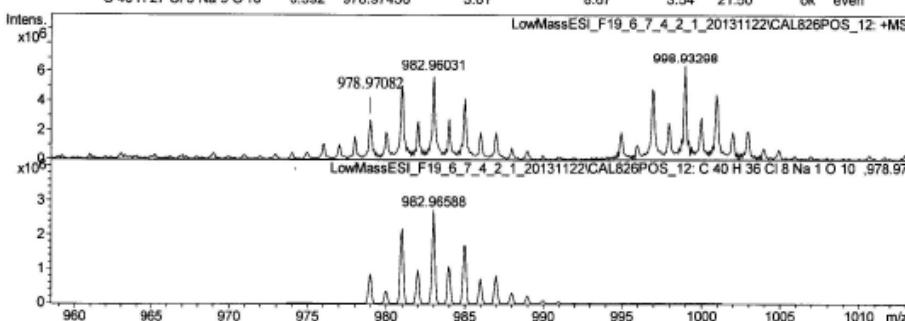
Analysis Name: C:\data\sample\ESI_12131120_30\LowMassESI_F19_6_7_4_2_1_20131122\CAL826POS_12
Acquisition Date: 11/22/2013 9:15:42 AM
Operator: bpxsh@bjmu.edu.cn; Tel: 010-82801
Instrument: FT_MS_Bruker APEX IV (7.0)

Comment: ESI □ C20H18O5Cl4 MW 477.99
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;826.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result Exact Mass Measured Mass Error (mDa) Error (ppm) Description



Sum Formula	Sigma	m/z	Err (ppm)	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 40 H 36 Cl 8 Na 1 O 10	0.080	978.97089	0.07	4.43	0.07	18.50	ok	even
C 40 H 29 Cl 5 Na 1 O 17	0.220	978.97396	3.20	7.82	3.14	23.50	ok	even
C 40 H 27 Cl 4 Na 4 O 15	0.302	978.96894	-1.93	3.15	-1.89	23.50	ok	even
C 40 H 29 Cl 4 Na 6 O 12	0.304	978.97938	8.74	13.70	8.56	21.50	ok	even
C 40 H 146 Cl 3 Na 1 O 14	0.387	978.96704	-3.87	1.47	-3.78	-34.00	ok	odd
C 40 H 148 Cl 3 Na 3 O 11	0.389	978.97748	6.80	12.02	6.66	-36.00	ok	odd
C 40 H 25 Cl 3 Na 7 O 13	0.390	978.96391	-7.06	-1.87	-6.91	23.50	ok	even
C 40 H 27 Cl 3 Na 9 O 10	0.392	978.97436	3.61	8.67	3.54	21.50	ok	even





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Analysis Name C:\data_sample\ESI_12131120_30\LowMassESI_F19_6_7_4_2_1_20131122\CAL826POS_10
Acquisition Date 11/22/2013 9:15:42 AM
Operator bpxsh@bjmu.edu.cn; Tel:010-82801
Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI □ C20H18O5CL4 MW 477.99
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;826.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result	Exact Mass	Measured Mass	Error (mDa)	Error (ppm)	Description
	478.99811	478.9962	1.91	3.99	M+H ⁺ ;e

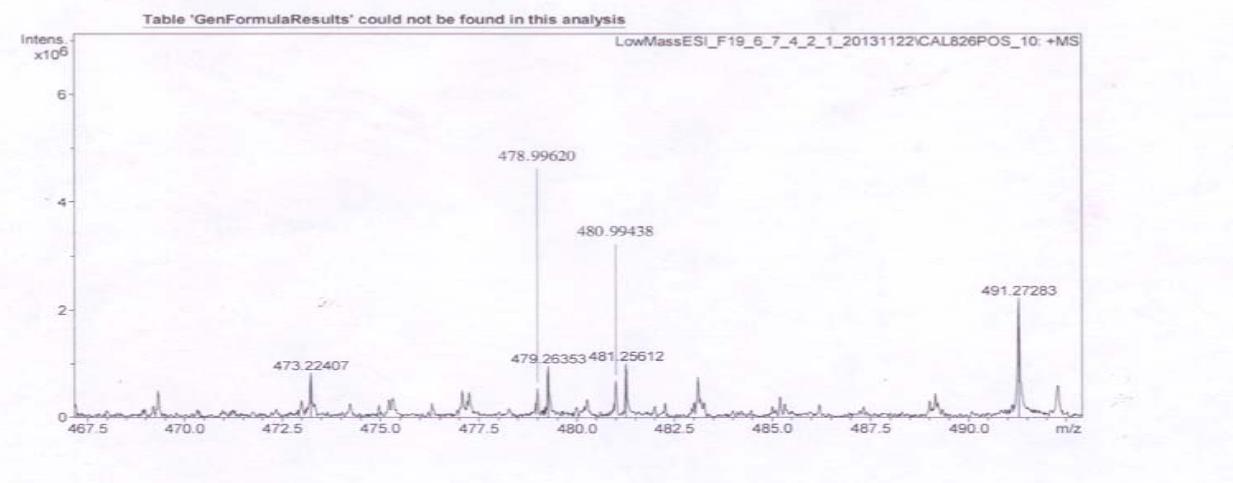


Figure S129. HRESIMS spectrum of **10**

F19-6-7-4-2-1 DMSO 400MHz

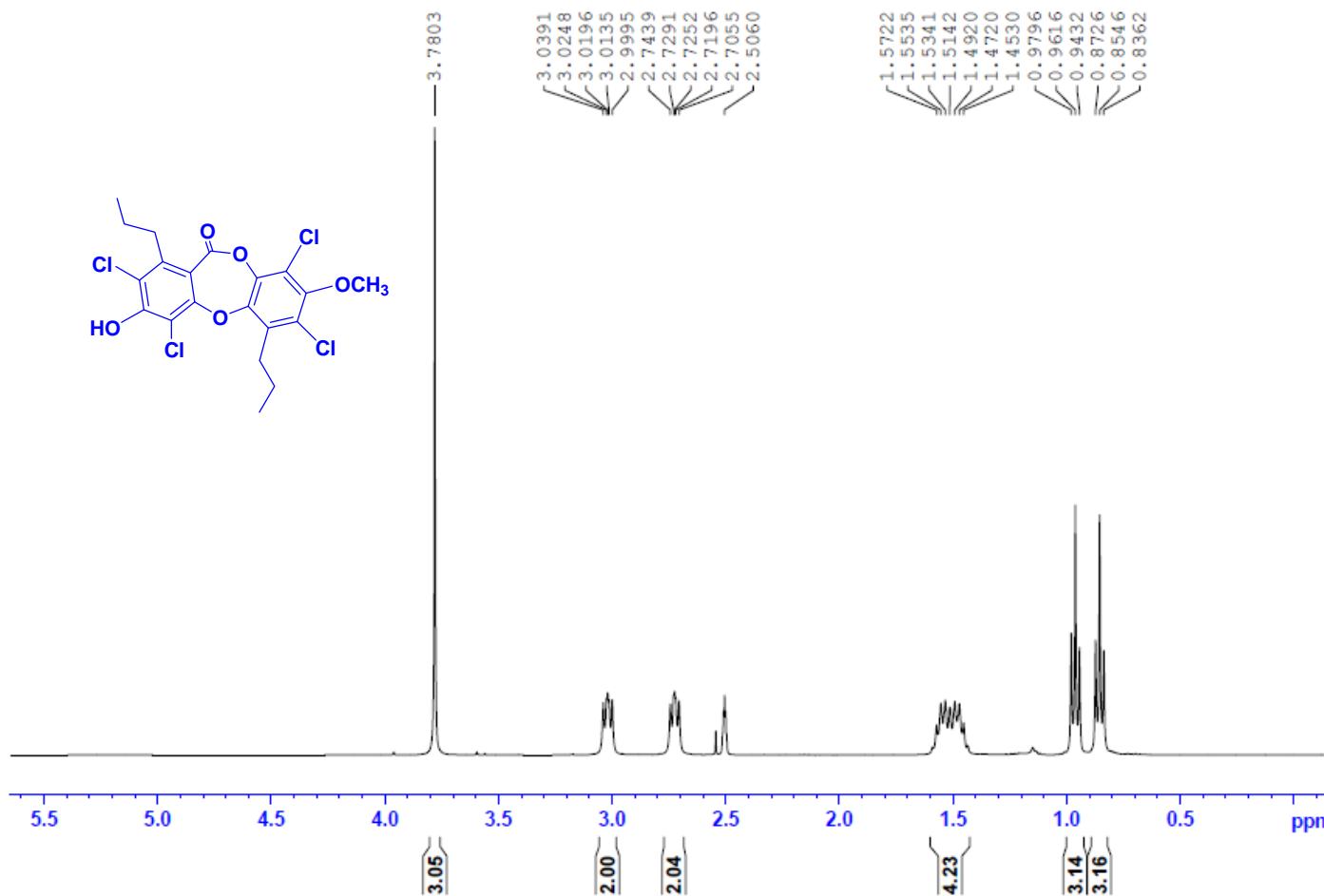
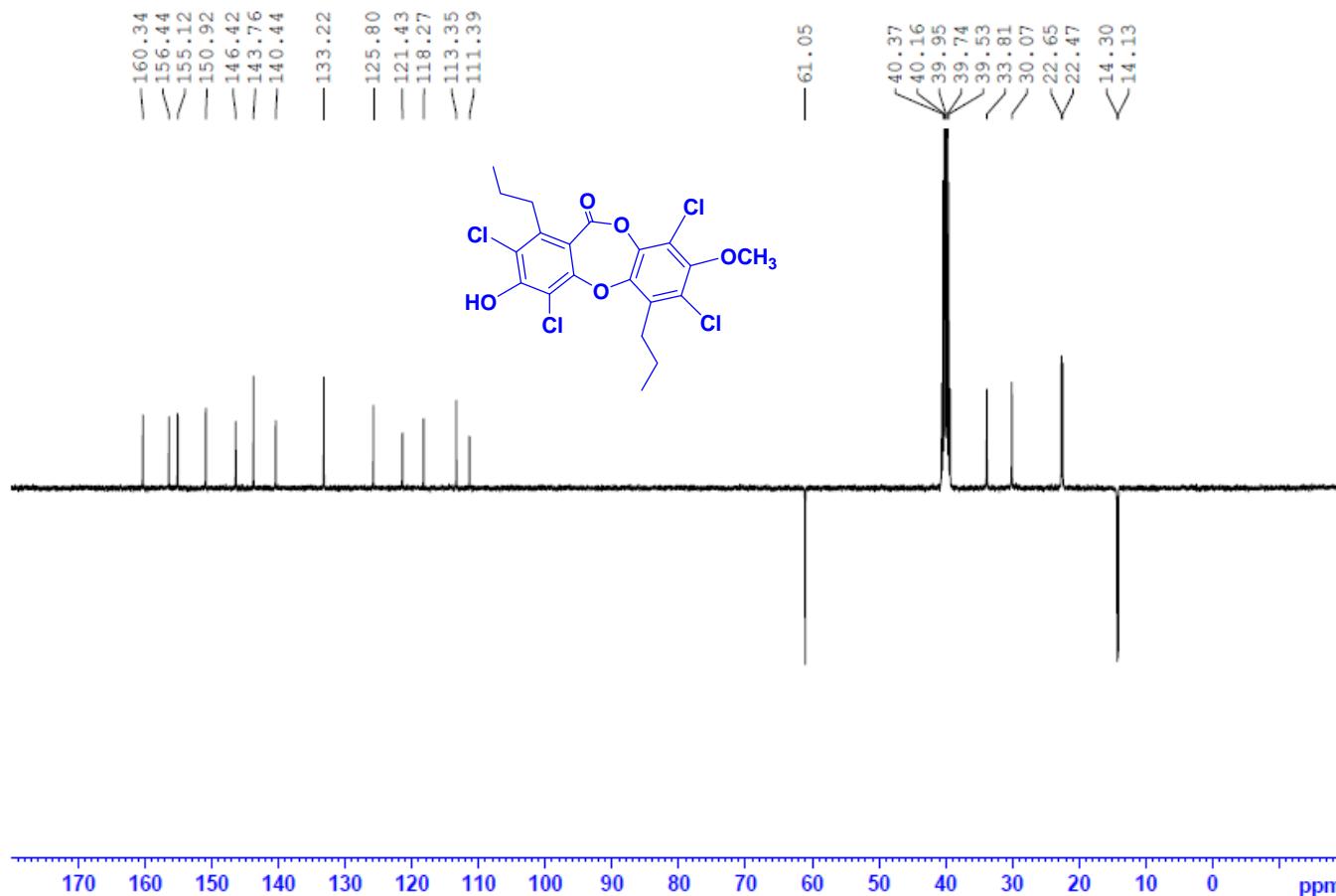


Figure S130. ^1H NMR spectrum of **10** in $\text{DMSO}-d_6$ (400 MHz)

F19-6-7-4-2-1 APT



F19-6-7-4-2-1 HSQC

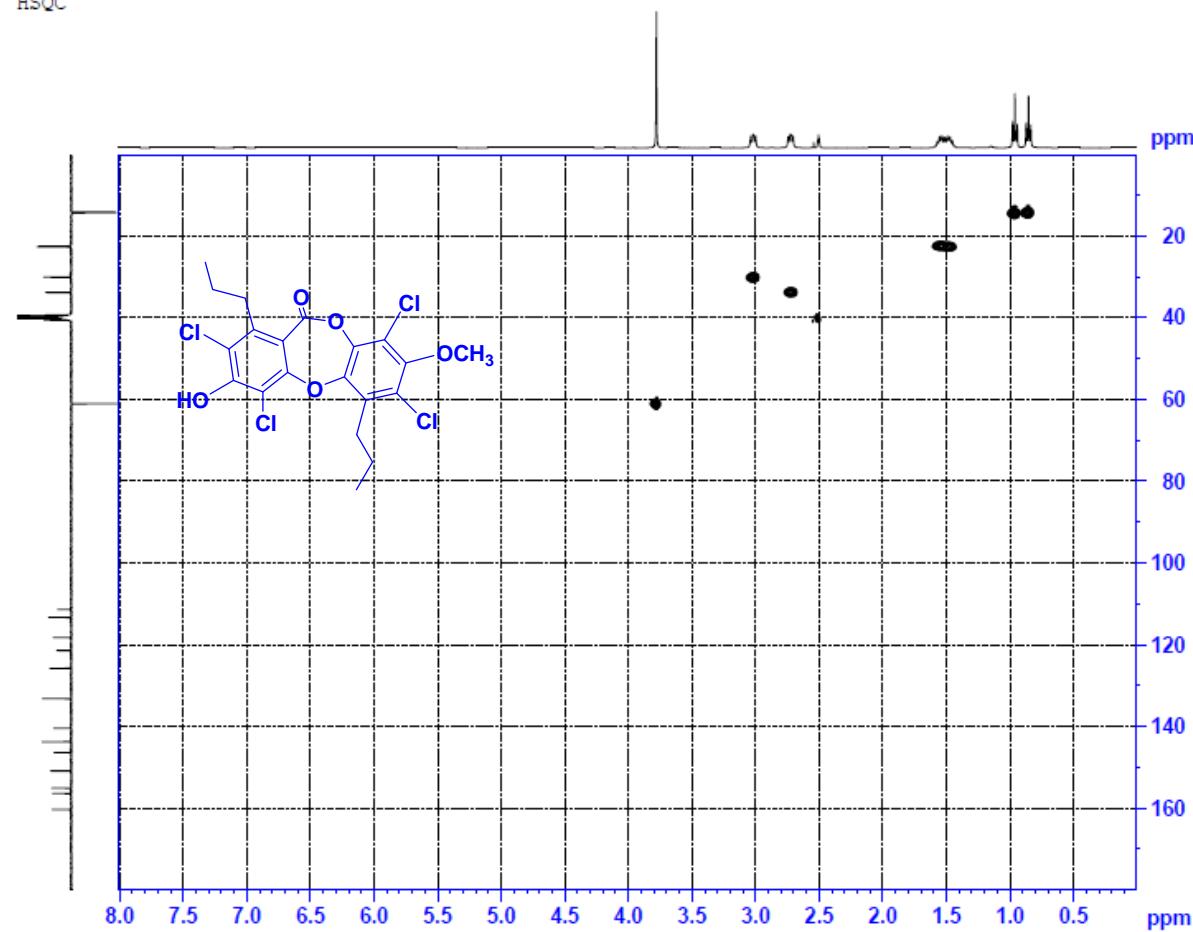


Figure S132. HSQC spectrum of **10** in $\text{DMSO}-d_6$ (400 MHz)

F19-6-7-4-2-1 COSY

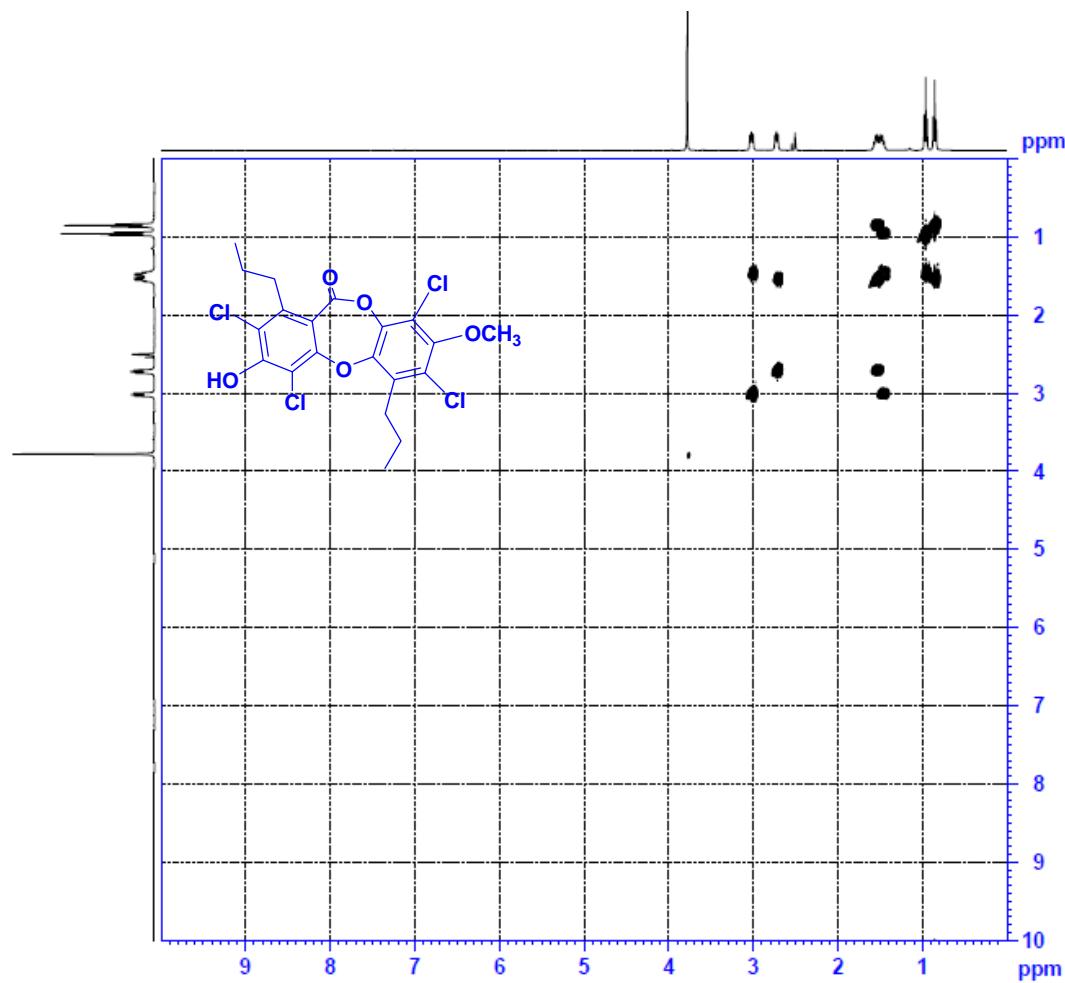


Figure S133. ^1H - ^1H COSY spectrum of **10** in $\text{DMSO}-d_6$ (400 MHz)

F19-6-7-4-2-1 HMBC

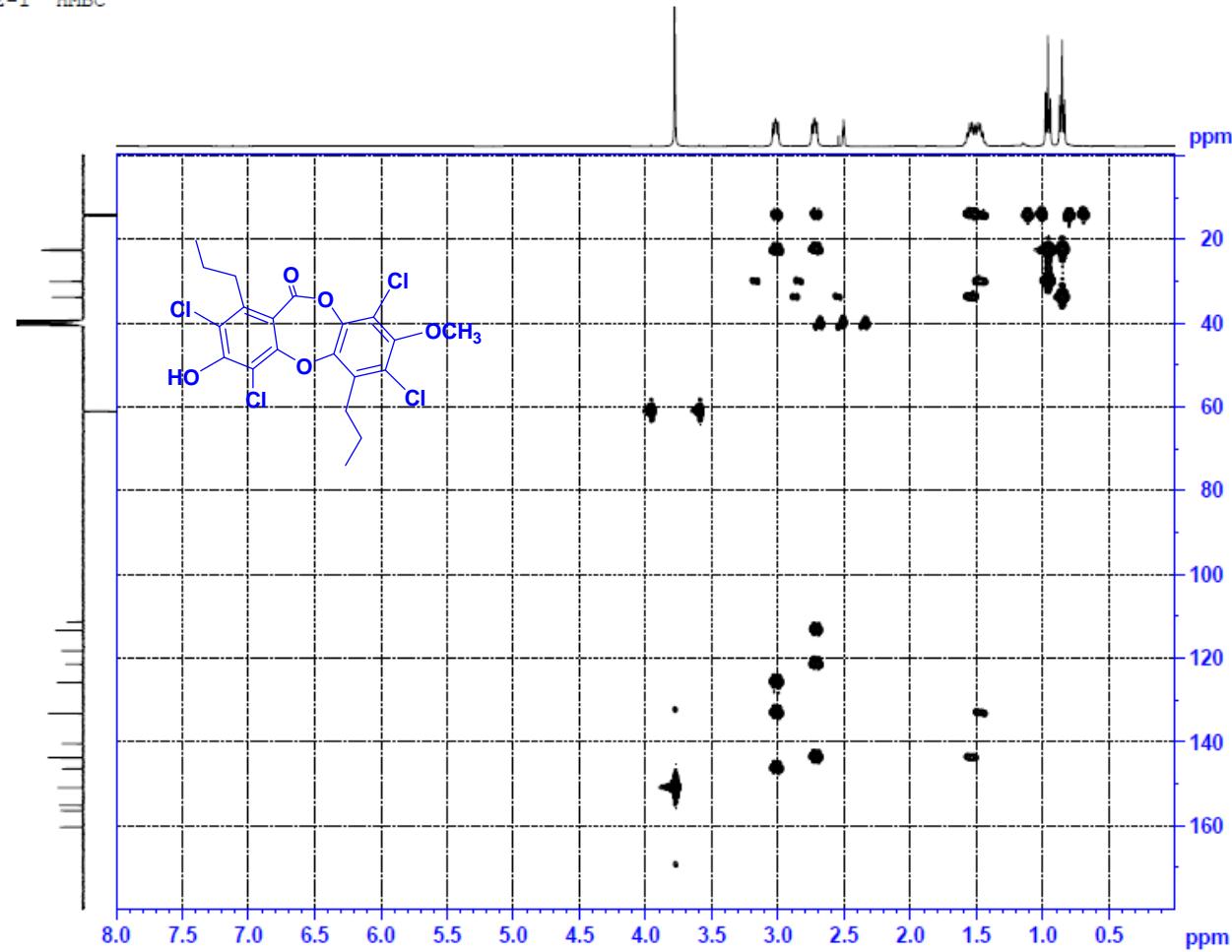
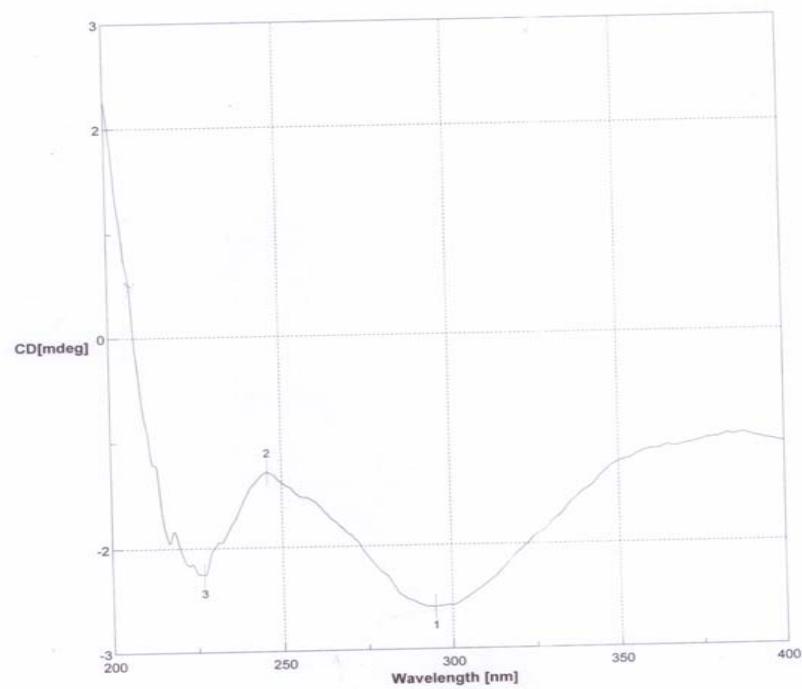


Figure S134. HMBC spectrum of **10** in $\text{DMSO}-d_6$ (400 MHz)

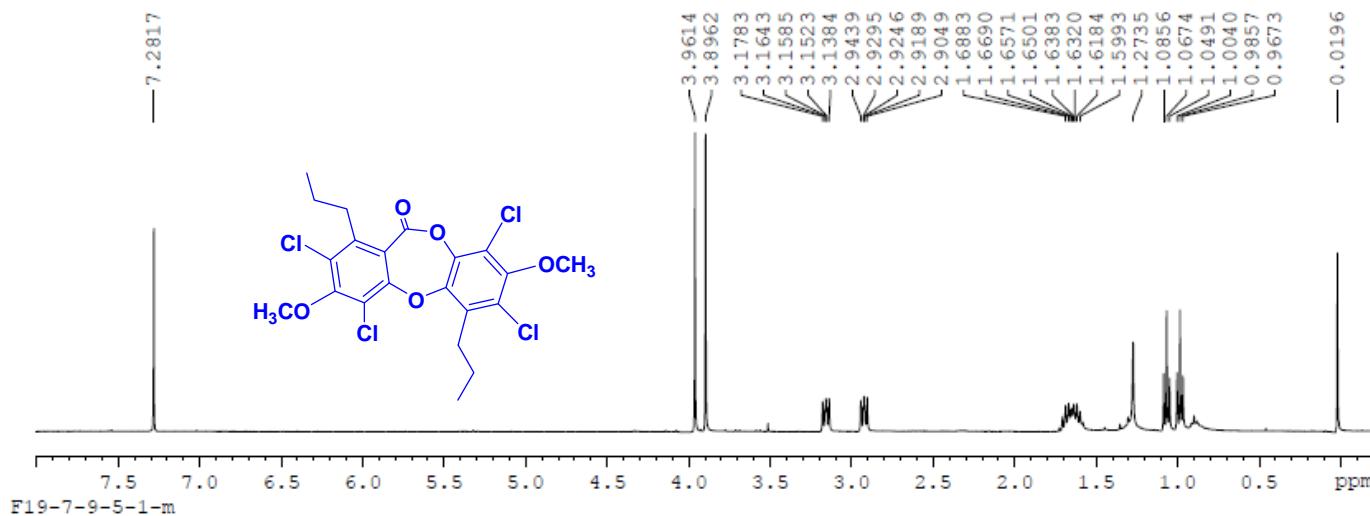


Date/Time	2001-1-3 5:57
Operator	F19-6-7-4-2-1.txt
File Name	F19-6-7-4-2-1
Sample Name	
Comment	

No.	nm	CD[mdeg]	No.	nm	CD[mdeg]	No.	nm	CD[mdeg]
1	295	-2.59481	2	245.8	-1.28982	3	227	-2.25719

Figure S135. CD spectrum of **10**

F19-6-7-4-2-1-m 400 MHz CDCl₃



F19-7-9-5-1-m

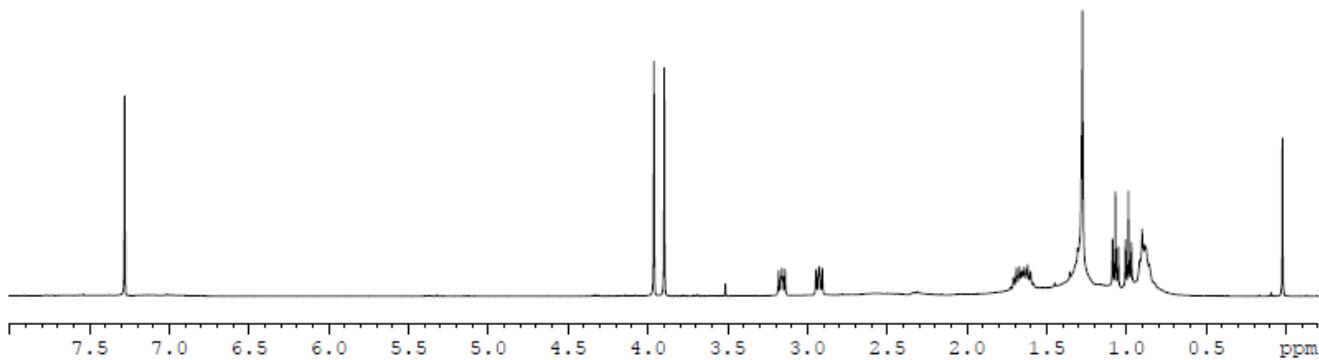


Figure S136. ¹H NMR Spectra of **9b** in CDCl₃ (400 MHz) derived from **9** and **10**

F19-6-7-4-2-1-m 100 MHz CDCl₃

— 160.41
< 156.51
< 156.47
— 151.10
— 146.60
— 144.22
— 140.13
— 133.49
— 128.16
— 126.32
— 119.75
— 118.52

F19-7-9-5-1-m

— 160.41
— 156.52
— 151.11
— 146.60
— 144.22
— 140.13
— 133.49
— 128.16
— 126.32
— 119.75
— 118.52

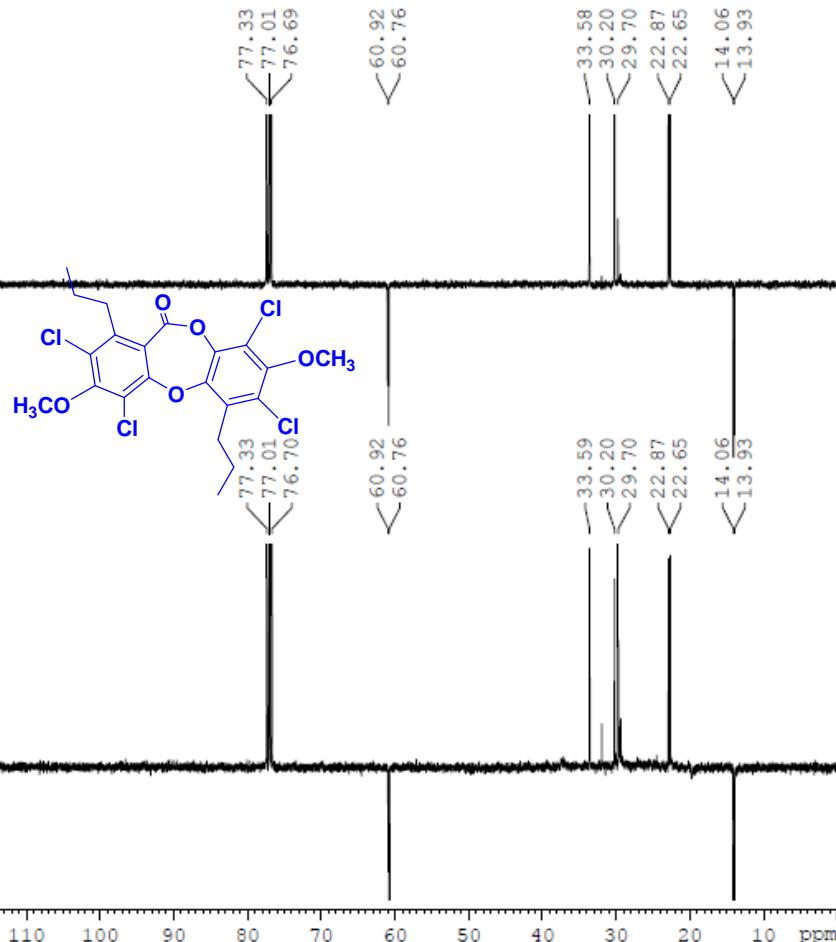


Figure S137. APT Spectra of **9b** in CDCl₃ (400 MHz) derived from **9** and **10**

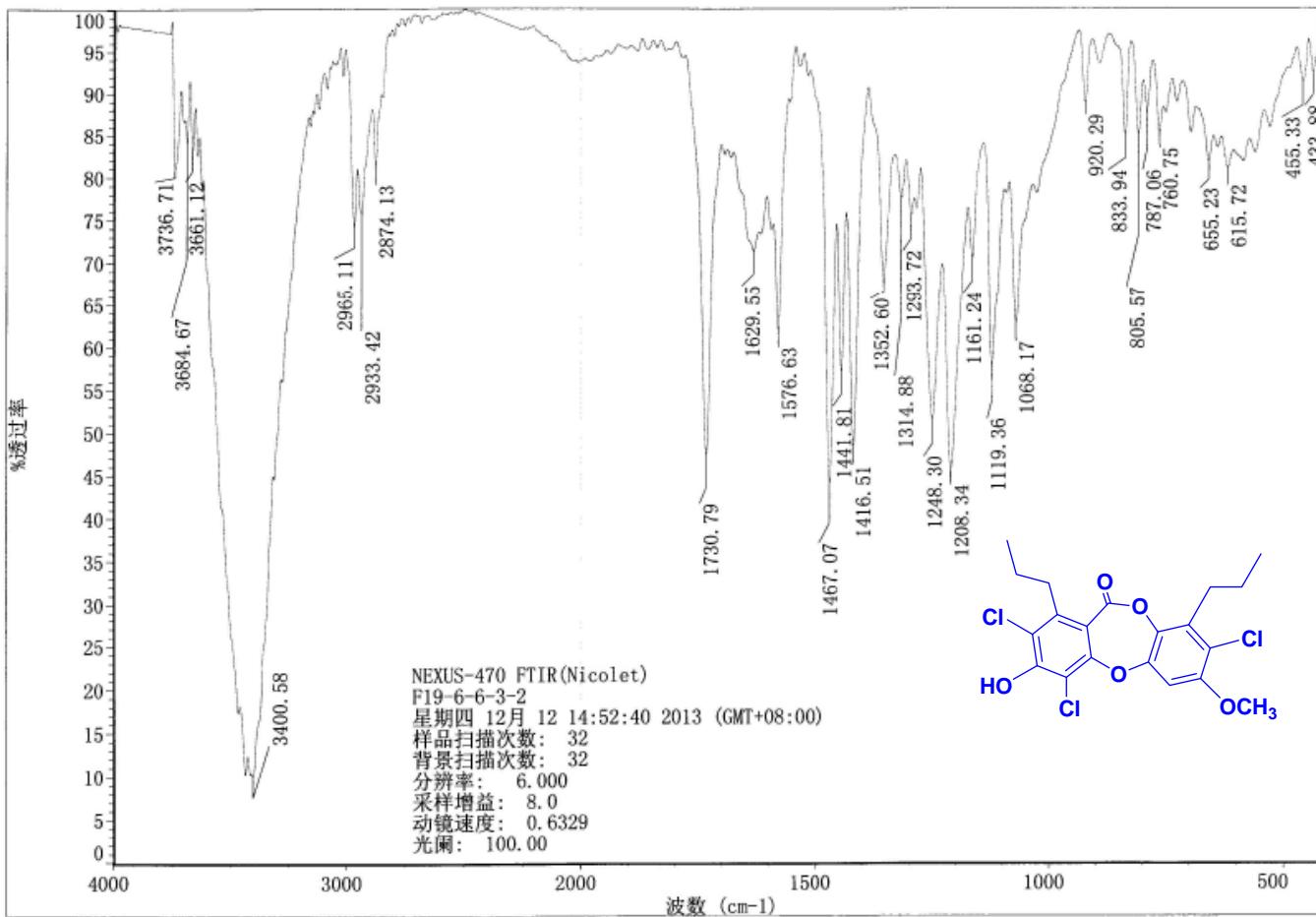


Figure S138. IR spectrum of **11**



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Analysis Name C:\data_sample\ESI_12131120_30\LowMassESI_F19_6_6_3_2_20131121\POS_6 Acquisition Date 11/20/2013 10:24:34 AM

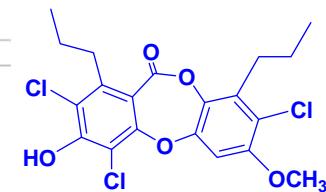
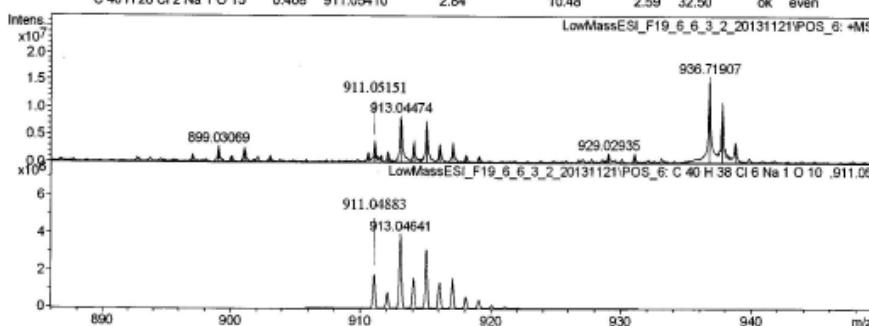
Operator bpxsh@bjmu.edu.cn; Tel:010-82801

Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI pos C20H19CL3O5 MW 444
CAL588; 279.15693,310.14158,322.04812391,28483;
413.26647,453.34353,47532548,509.25407;
509.25407,611.26126,8.26 47121,842.44514;
588.40954,679.51166,70149361,826.47121;

Acquisition Result Exact Mass Measured Mass Error (mDa) Error (ppm) Description

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 40 H 38 Cl 6 Na 1 O 10	0.029	911.04883	-2.93	2.36	-2.67	18.50	ok	even
C 45 H 39 Cl 7 Na 1 O 4	0.072	911.05602	4.96	10.03	4.52	22.50	ok	even
C 46 H 33 Cl 5 Na 1 O 8	0.095	911.05103	-0.53	5.17	-0.48	27.50	ok	even
C 39 H 44 Cl 8 Na 1 O 6	0.121	911.05383	2.55	7.35	2.32	13.50	ok	even
C 46 H 40 Cl 8 Na 1 O 1	0.127	911.04796	-3.90	1.22	-3.55	22.50	ok	even
C 40 H 31 Cl 3 Na 1 O 17	0.295	911.05190	0.43	6.80	0.40	23.50	ok	even
C 46 H 26 Cl 2 Na 1 O 15	0.408	911.05410	2.84	10.48	2.59	32.50	ok	even



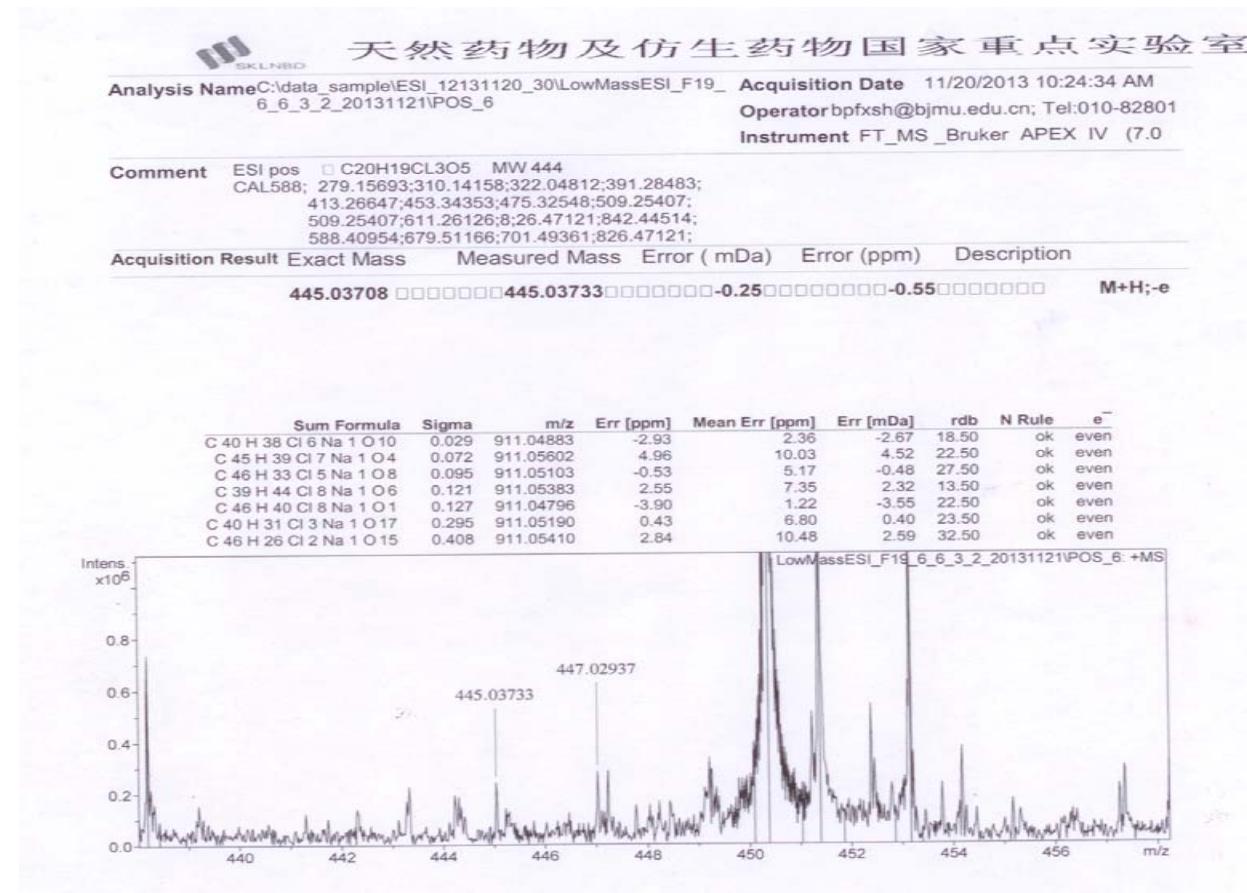


Figure S139. HRESIMS spectrum of **11**

F19-6-6-3-2 400 MHz DMSO

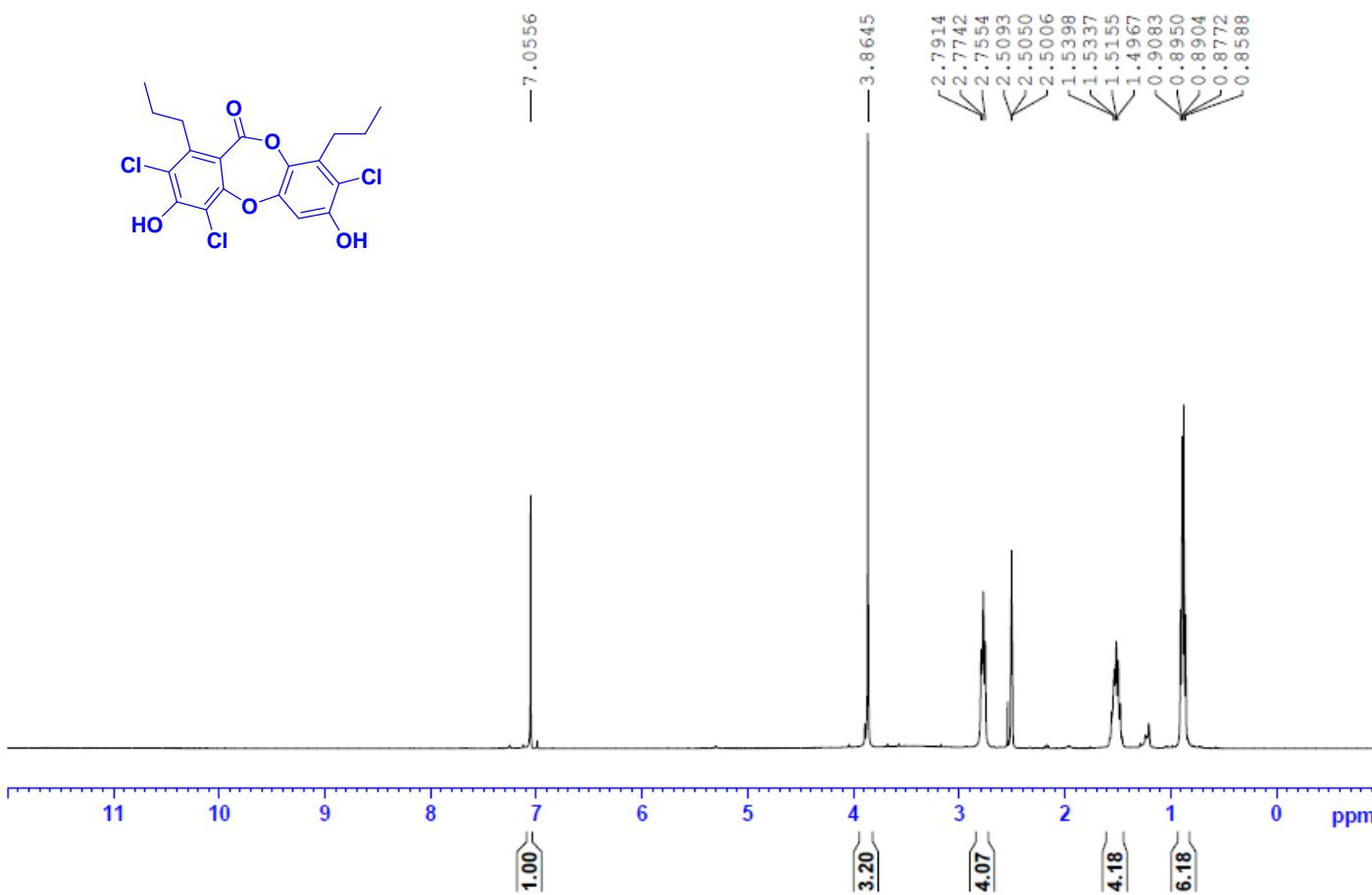


Figure S140. ^1H NMR spectrum of **11** in $\text{DMSO}-d_6$ (400 MHz)

F19-6-6-3-2 APT

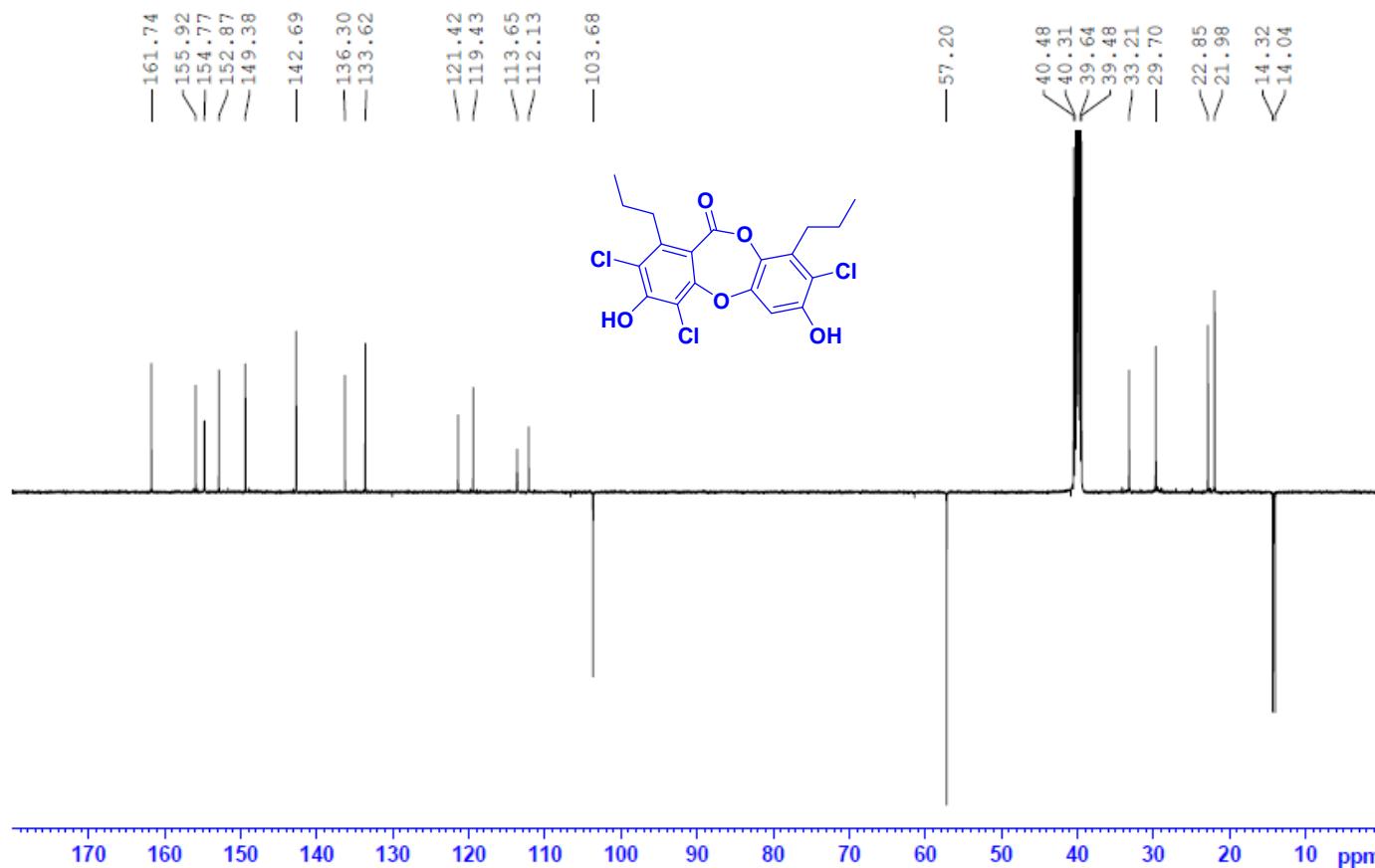


Figure S141. APT spectrum of **11** in DMSO-*d*₆ (100 MHz)

F19-6-6-3-2 HSQC

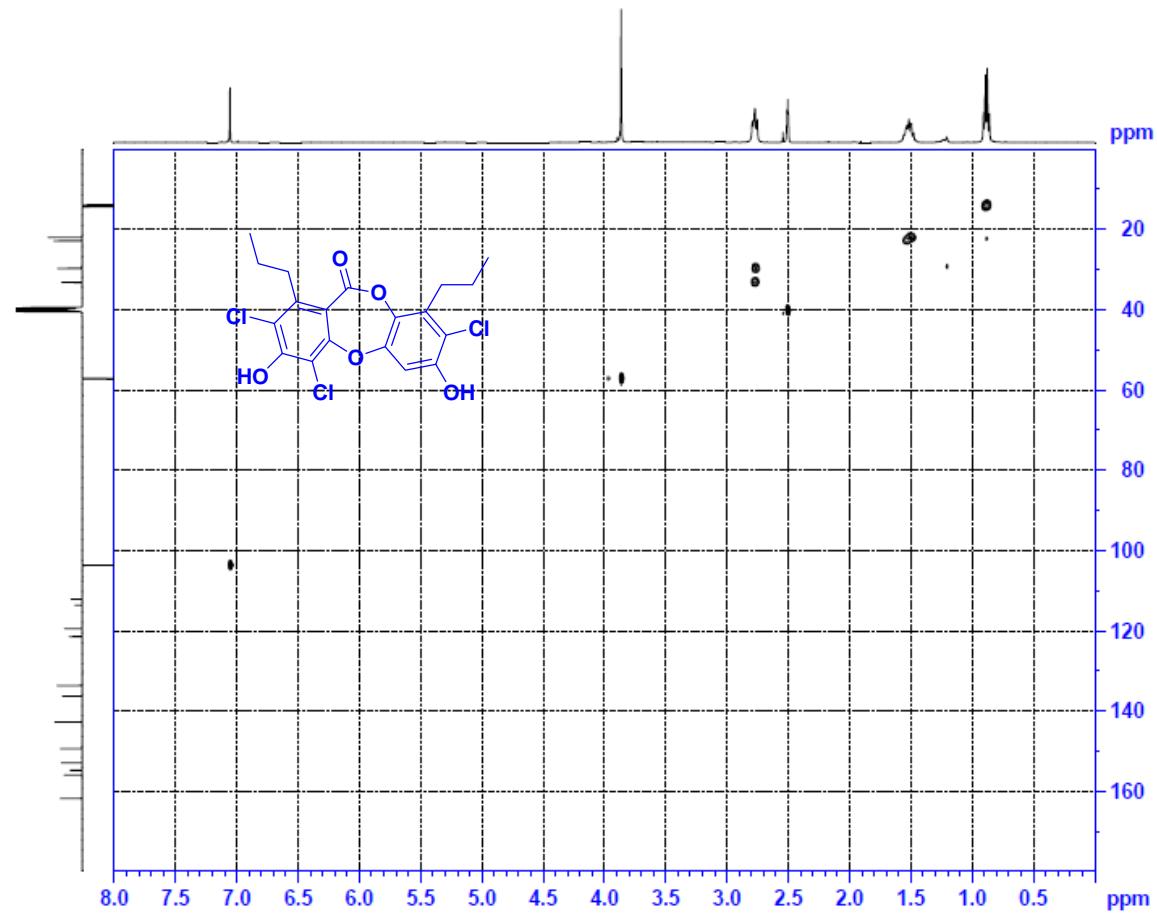


Figure S142. HSQC spectrum of **11** in $\text{DMSO}-d_6$ (400 MHz)

F19-6-6-3-2 COSY

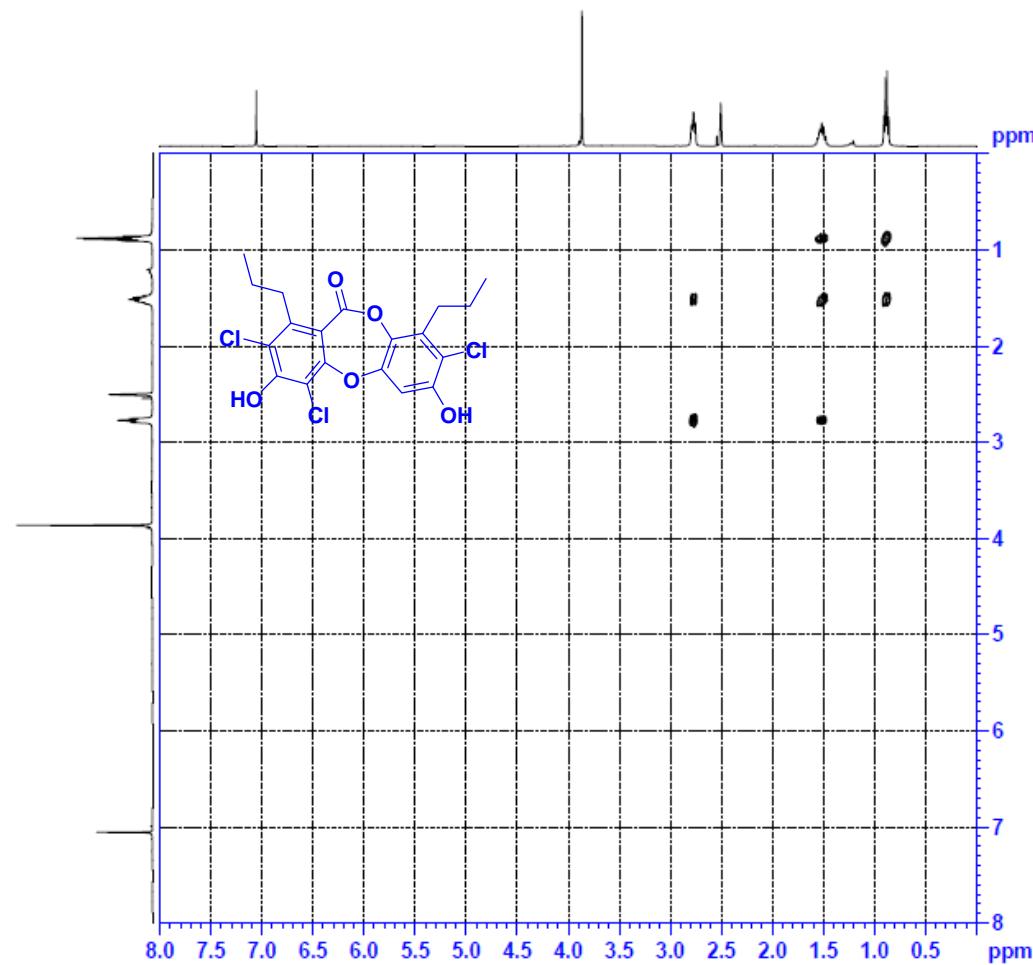


Figure S143. ^1H - ^1H COSY spectrum of **11** in $\text{DMSO}-d_6$ (400 MHz)

F19-6-6-3-2 HMBC

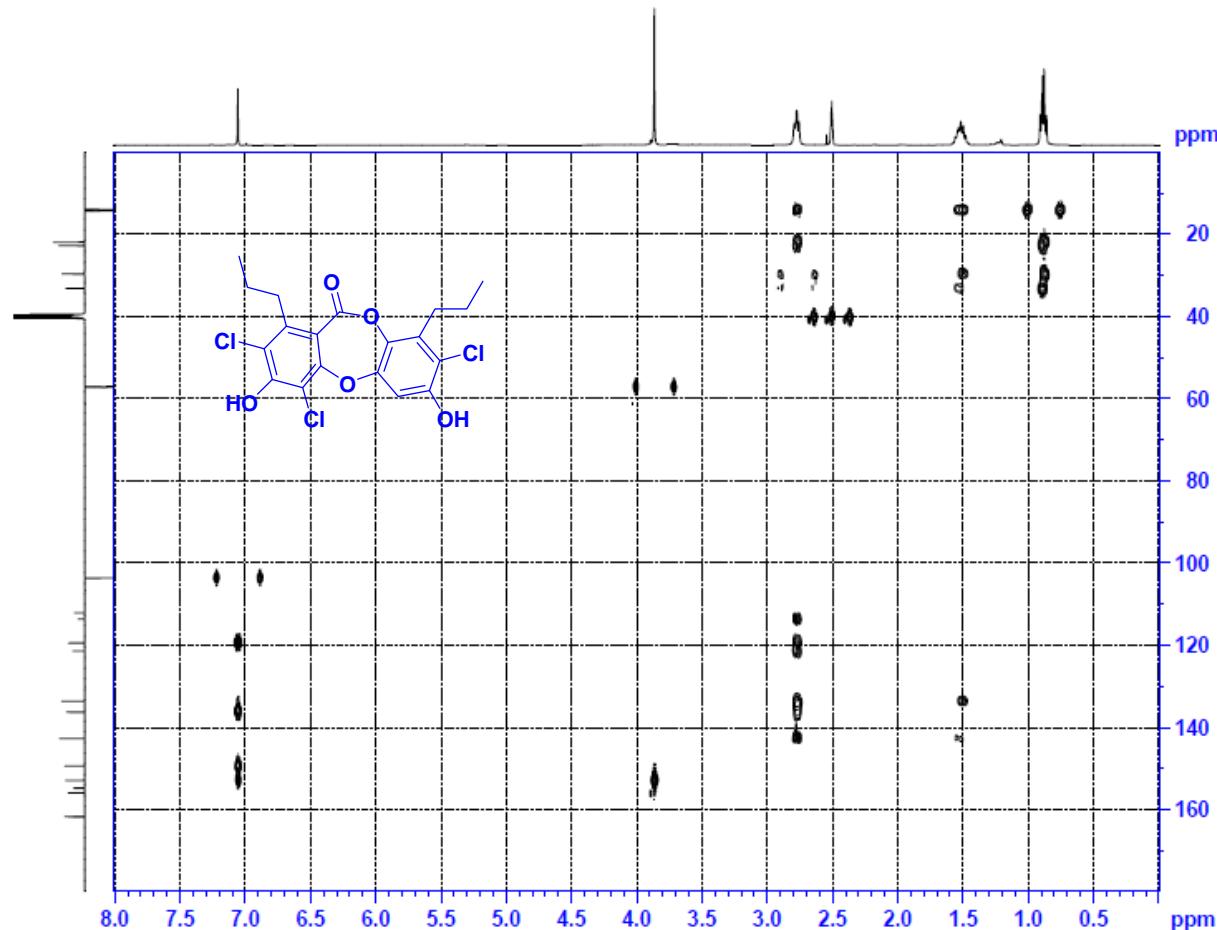
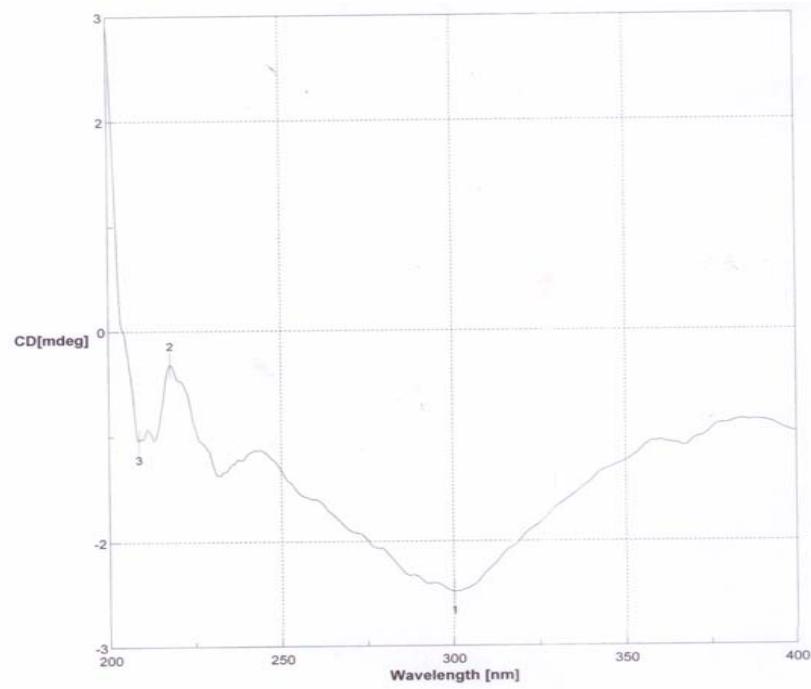


Figure S144. HMBC spectrum of **11** in $\text{DMSO}-d_6$ (400 MHz)



Date/Time 2001-1-3 5:44
Operator
File Name F19-6-3-2.txt
Sample Name F19-6-3-2
Comment

No.	nm	CD[mdeg]	No.	nm	CD[mdeg]	No.	nm	CD[mdeg]
1	300.2	-2.47715	2	218	-0.319702	3	208.8	-1.04183

Figure S145. CD spectrum of **11**

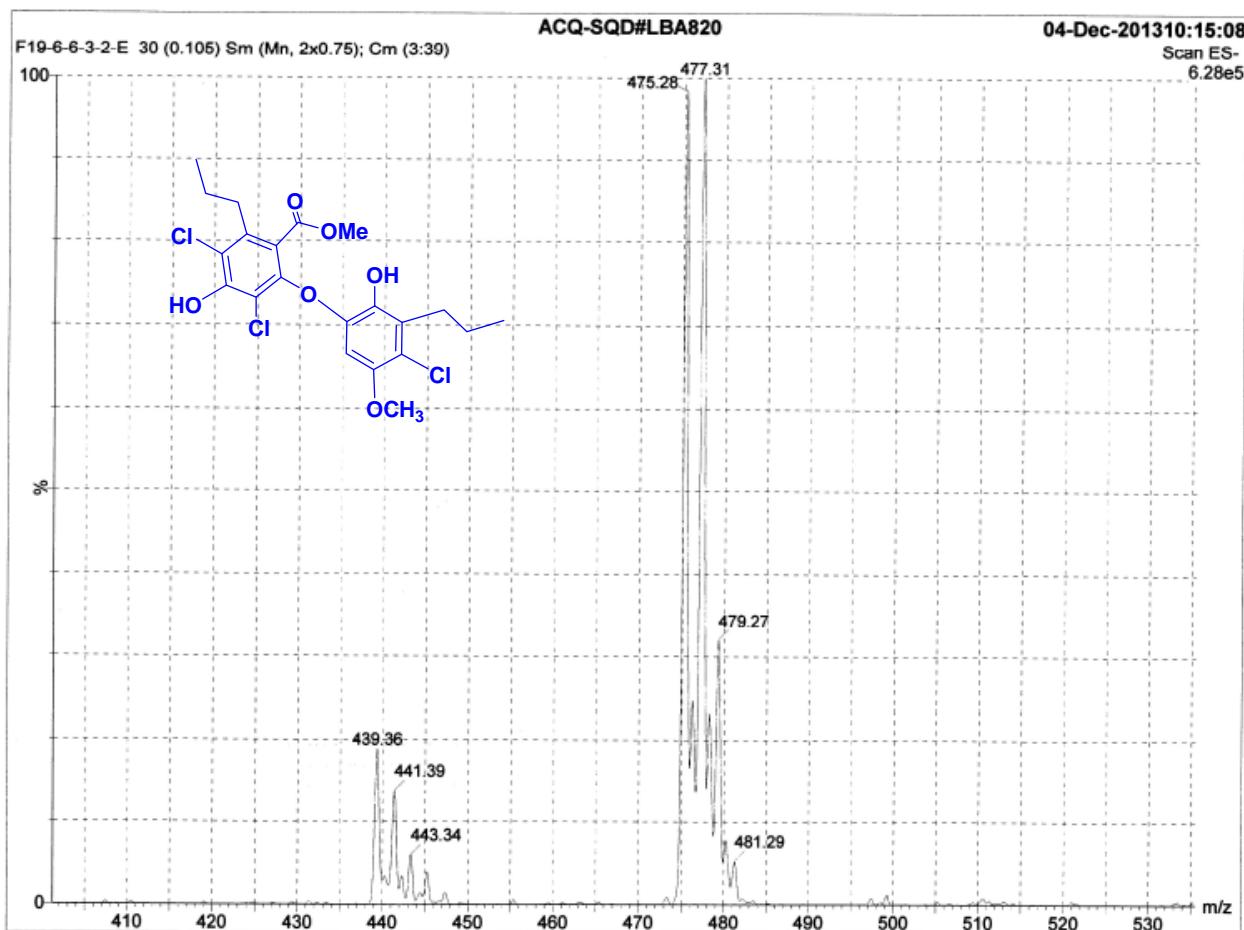


Figure S146. ESIMS spectrum of **11a**

F19-6-6-3-2-e

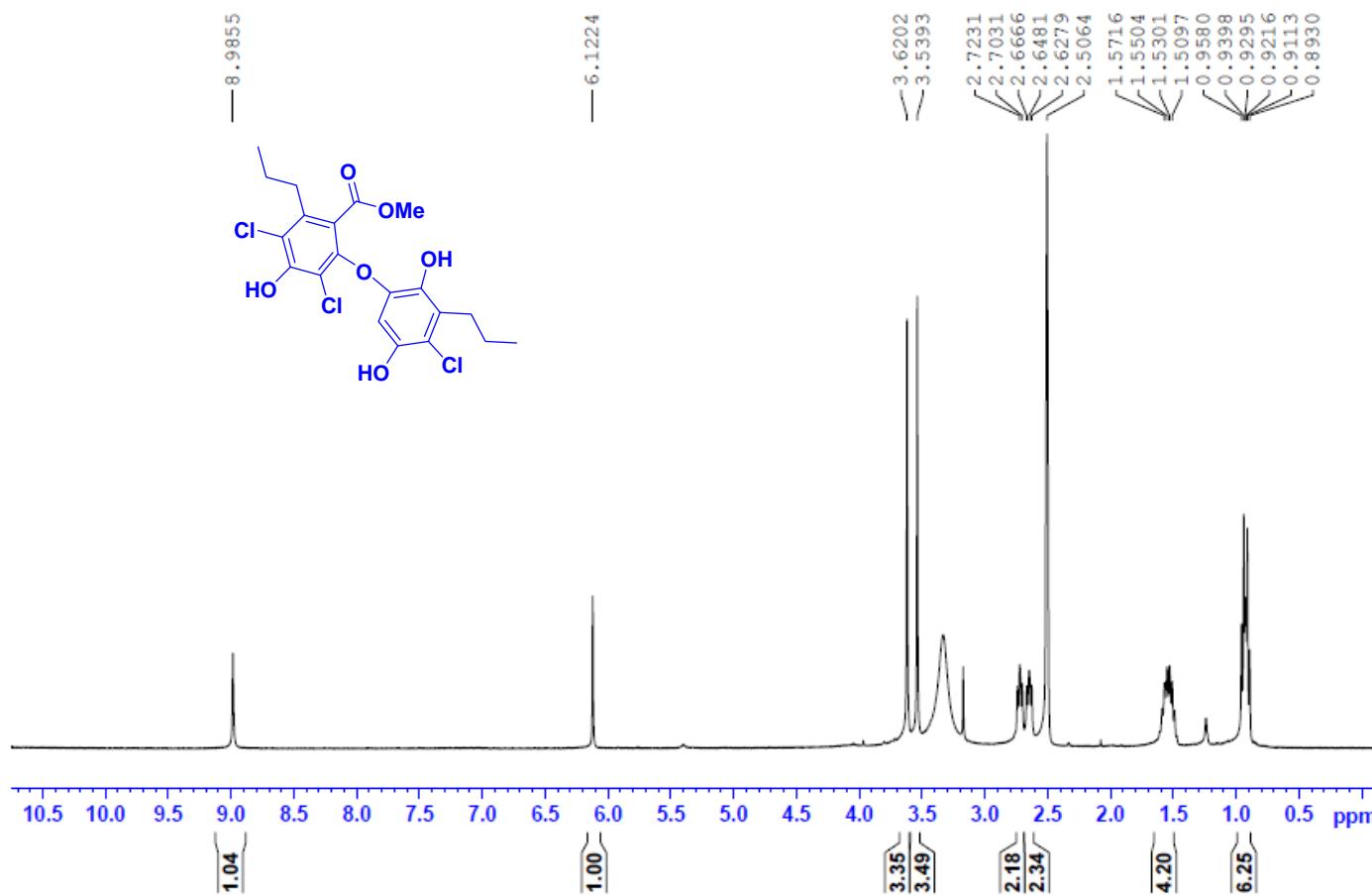


Figure S147. ^1H NMR spectrum of **11a** in $\text{DMSO}-d_6$ (400 MHz)

F19-6-6-3-2-e APT

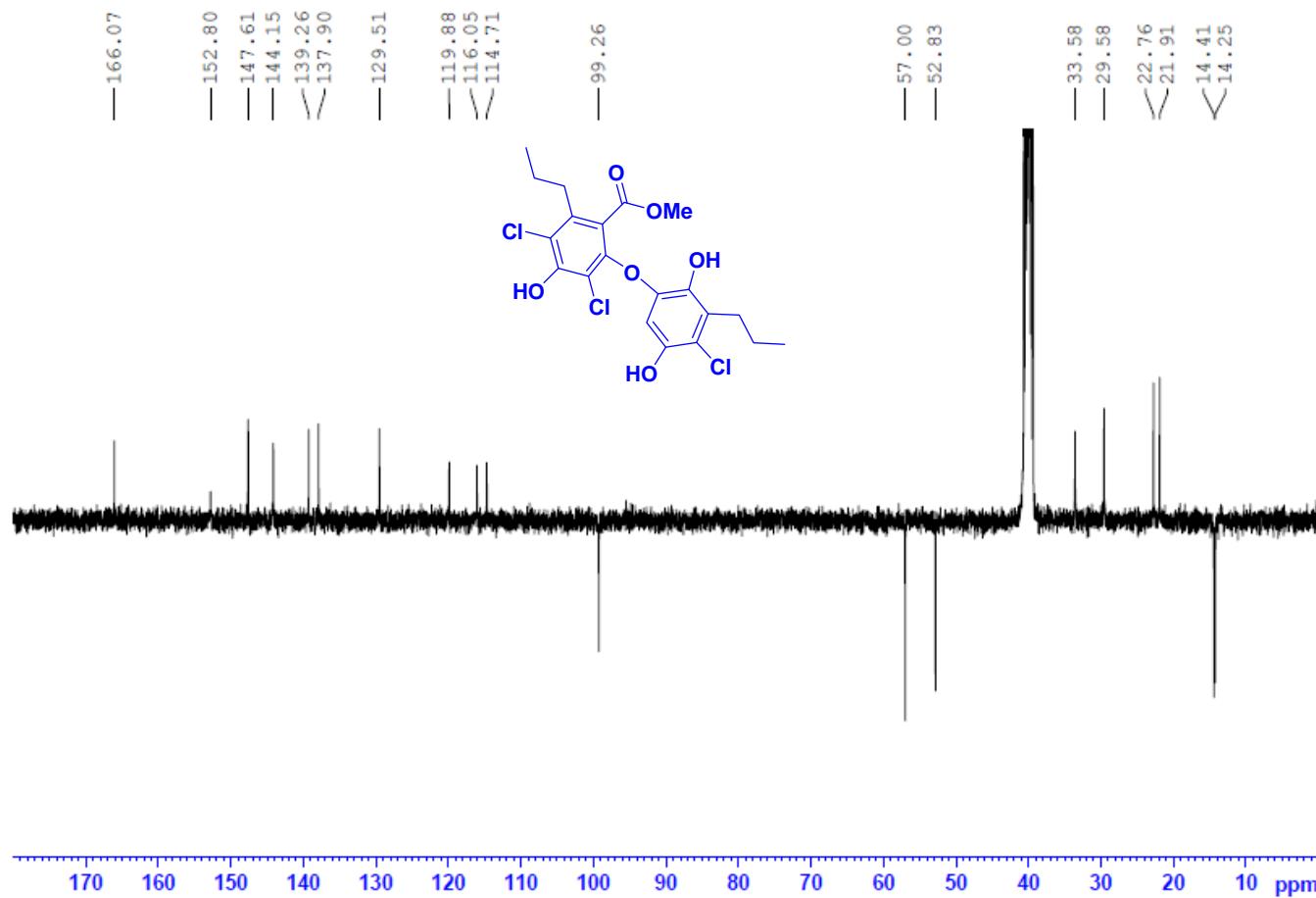


Figure S148. APT spectrum of **11a** in $\text{DMSO}-d_6$ (100 MHz)

F19-6-6-3-2-e HSQC

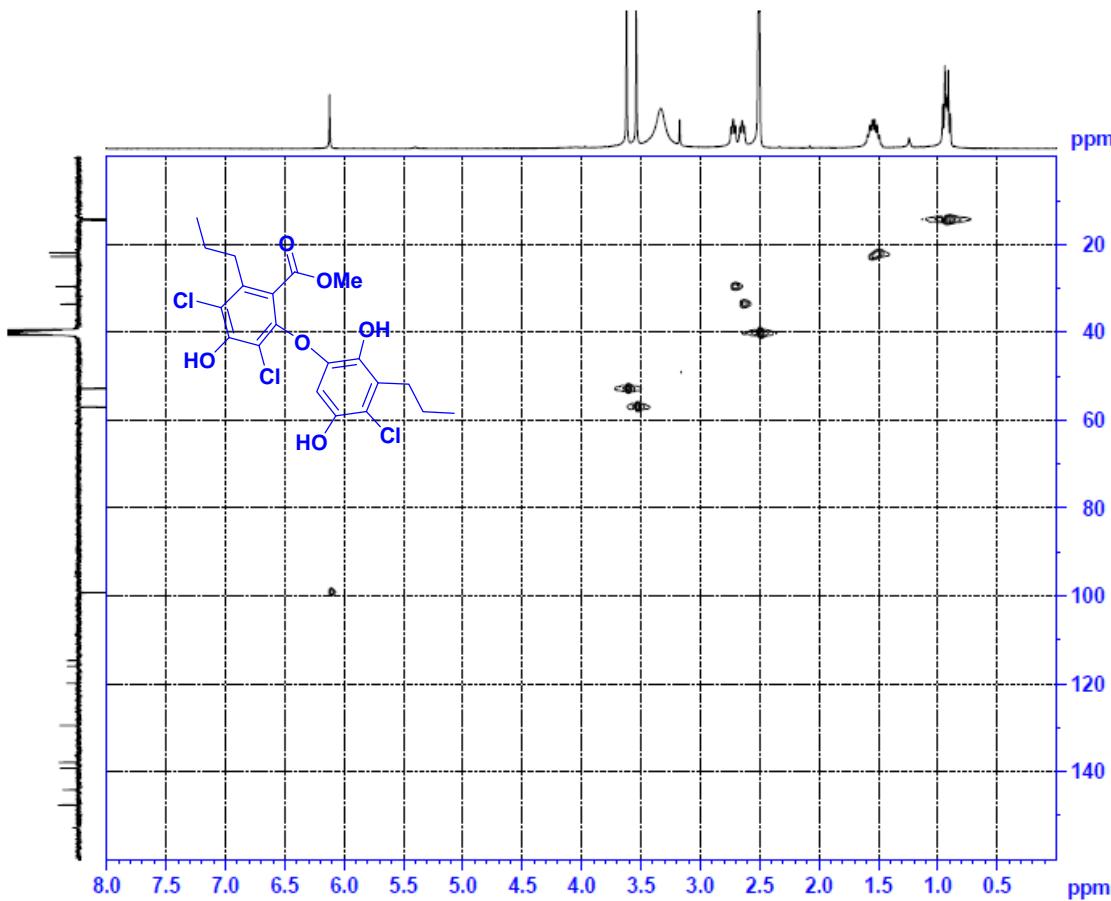


Figure S149. HSQC spectrum of **11a** in $\text{DMSO}-d_6$ (400 MHz)

F19-6-6-3-2-e COSY

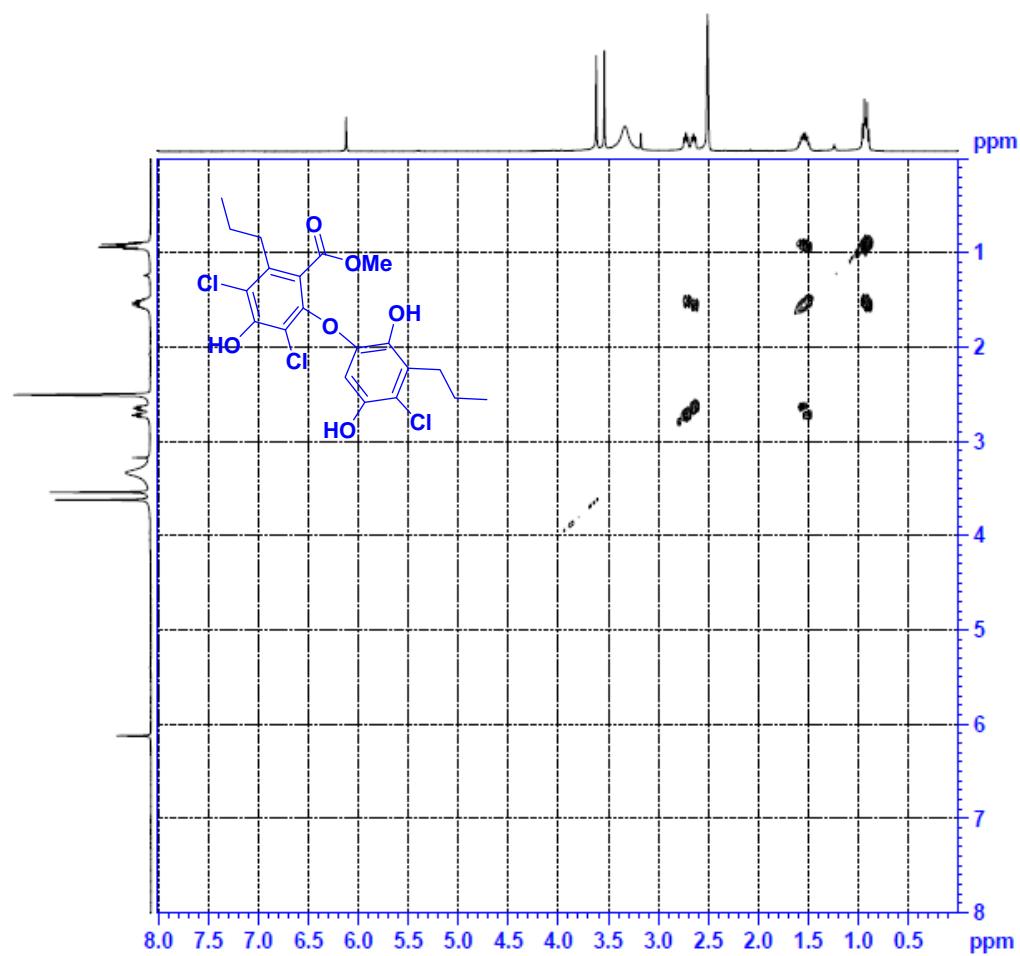


Figure S150. ^1H - ^1H COSY spectrum of **11a** in $\text{DMSO}-d_6$ (400 MHz)

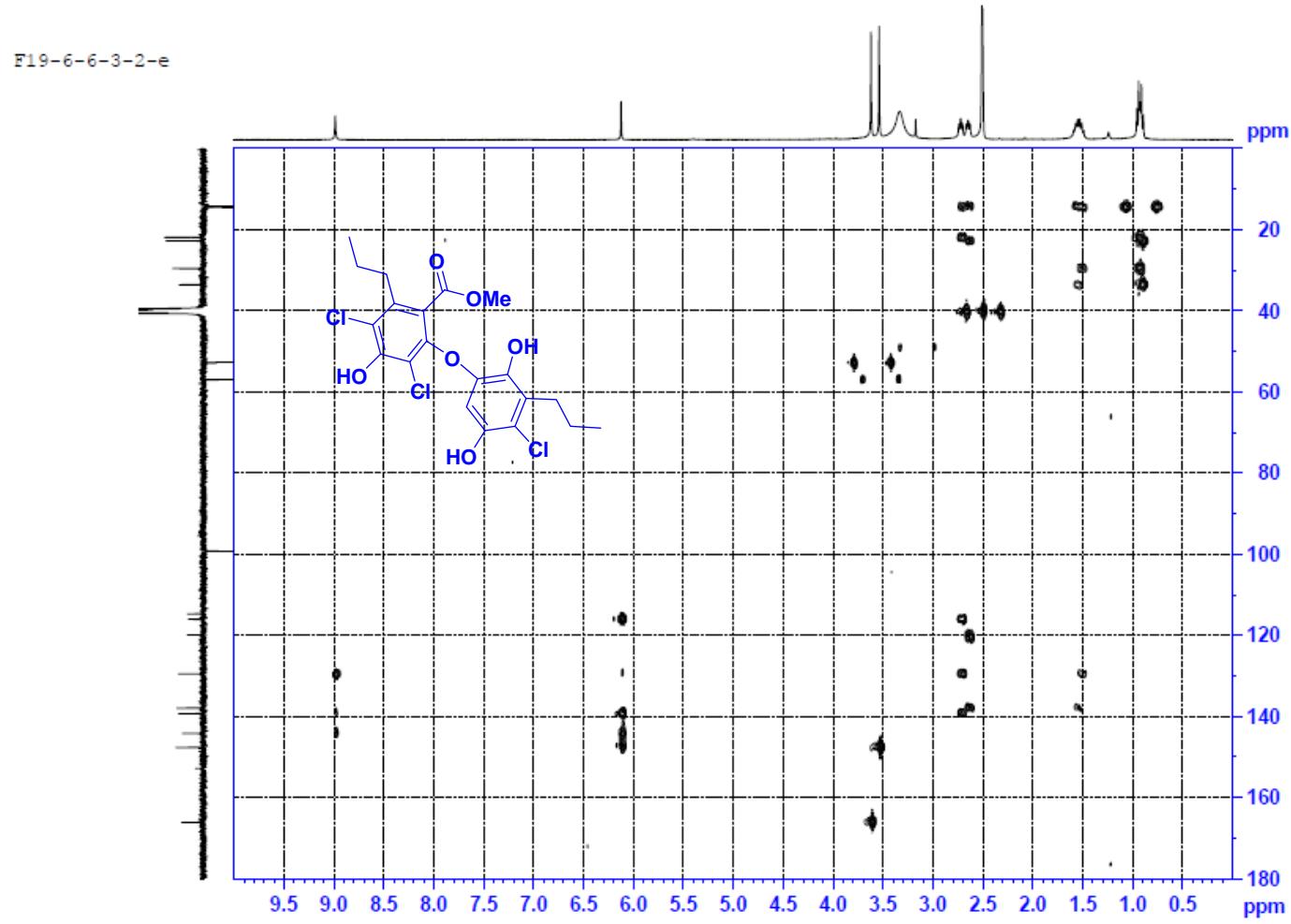


Figure S151. HMBC spectrum of **11a** in $\text{DMSO}-d_6$ (400 MHz)

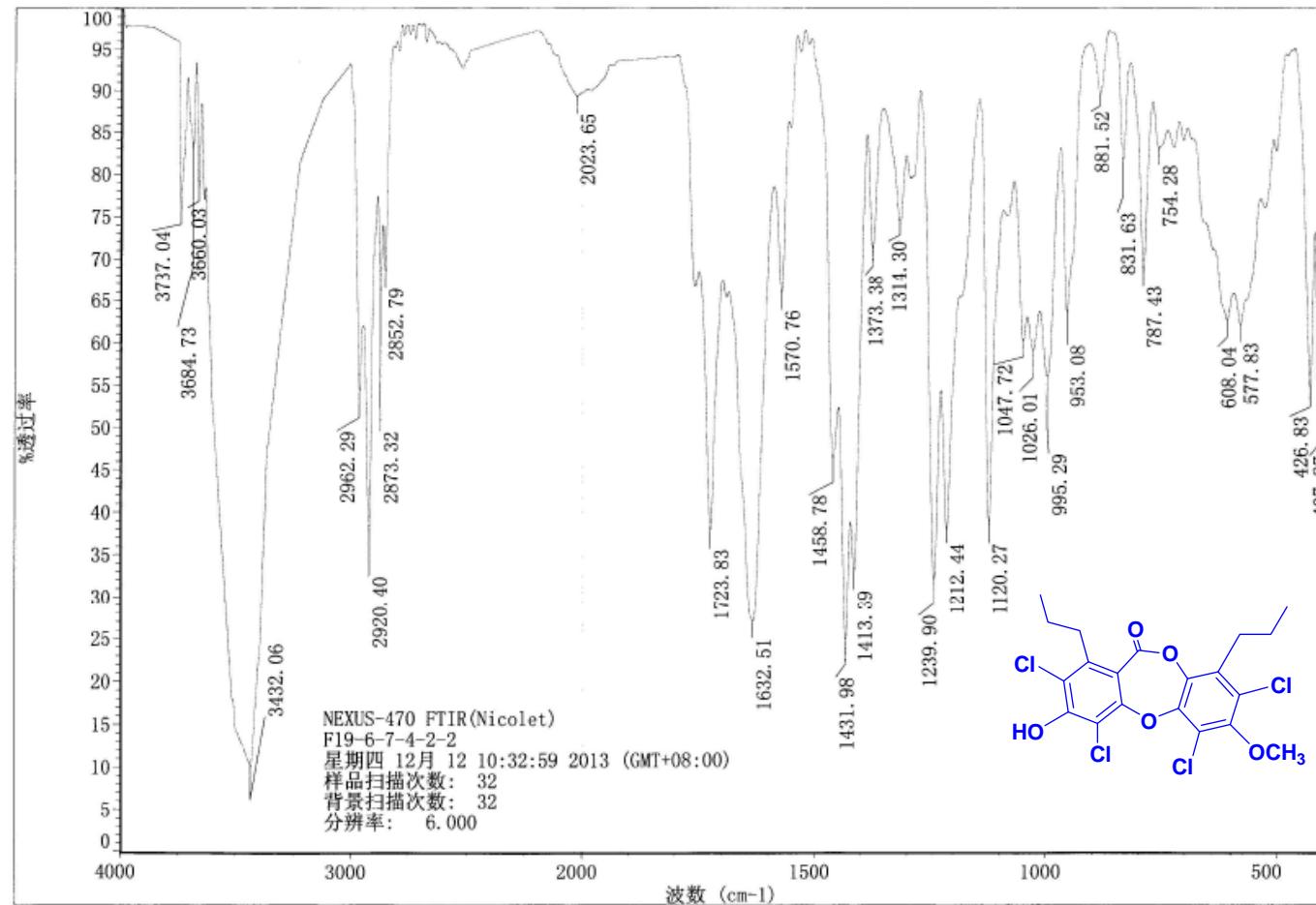


Figure S152. IR spectrum of **12**

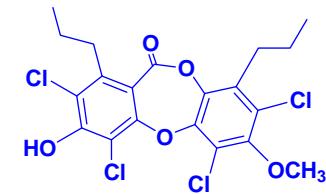


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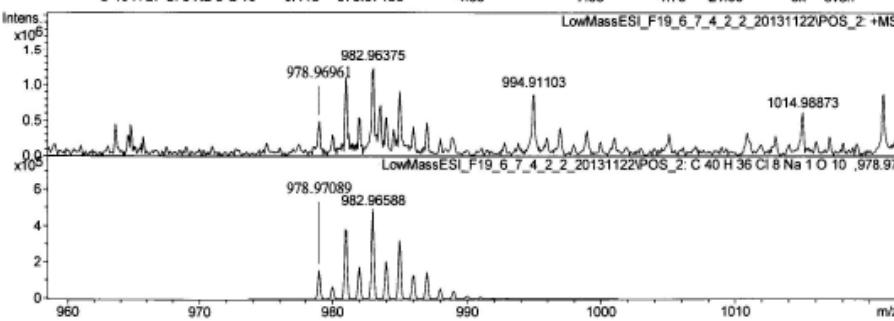
Analysis Name C:\data_sample\ESI_12131120_30\LowMassESI_F19_6_7_4_2_2_20131122\POS_2 Acquisition Date 11/22/2013 9:29:36 AM
Operator bpxsh@bjmu.edu.cn; Tel:010-82801
Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI □ C₂₀H₁₈O₅Cl₄ MW 477.99
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;8.26.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result Exact Mass Measured Mass Error (mDa) Error (ppm) Description



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 40 H 36 Cl 8 Na 1 O 10	0.135	978.97089	1.31	2.94	1.28	18.50	ok	even
C 40 H 29 Cl 5 Na 1 O 17	0.252	978.97395	4.44	6.92	4.35	23.50	ok	even
C 40 H 27 Cl 4 Na 4 O 15	0.331	978.98894	-0.69	2.21	-0.68	23.50	ok	even
C 40 H 29 Cl 4 Na 6 O 12	0.333	978.97938	9.98	12.73	9.77	21.50	ok	even
C 40 H 146 Cl 3 Na 1 O 14	0.414	978.96704	-2.63	0.77	-2.57	-34.00	ok	odd
C 40 H 25 Cl 3 Na 7 O 13	0.416	978.96391	-5.82	-2.59	-5.70	23.50	ok	even
C 40 H 148 Cl 3 Na 3 O 11	0.417	978.97748	8.04	11.31	7.87	-36.00	ok	odd
C 40 H 27 Cl 3 Na 9 O 10	0.418	978.97436	4.85	7.95	4.75	21.50	ok	even





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Analysis Name C:\data_sample\ESI_12140210_20\MassESI_f19_6_7_4_2_2_20140214\NEG_8 Acquisition Date 2/14/2014 9:10:46 AM
Operator bpxsh@bjmu.edu.cn; Tel:010-82801
Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI C20H18O5CL4 MW 477.9
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;8.26.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result	Exact Mass	Measured Mass	Error (mDa)	Error (ppm)	Description
	476.98356	476.98441	-0.85	-1.79	M-H ⁺ e

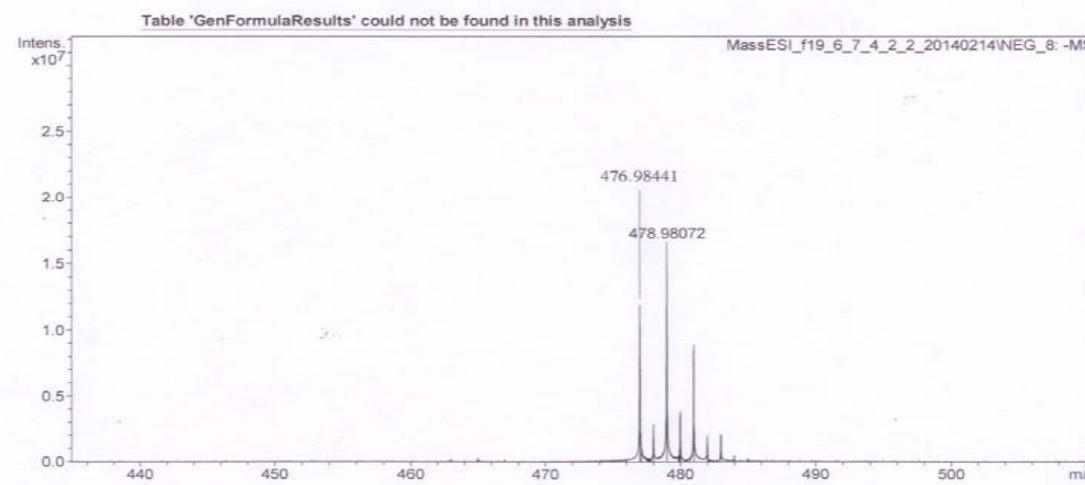


Figure S153. HRESIMS spectrum of **12**

F19-6-7-4-2-2 400 MHz DMSO

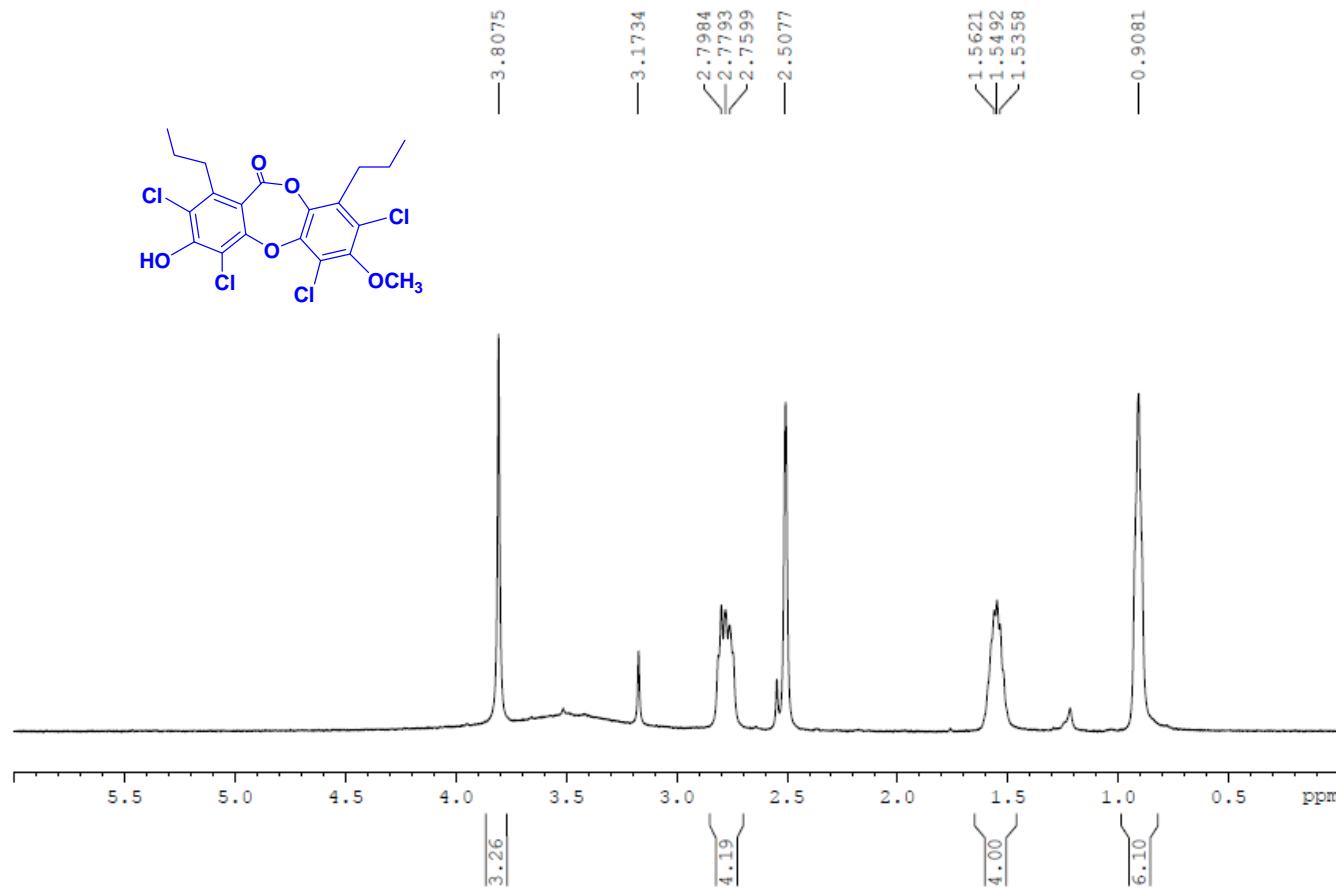


Figure S154. ^1H NMR spectrum of **12** in $\text{DMSO}-d_6$ (400 MHz)

F19-6-7-4-2-2 APT

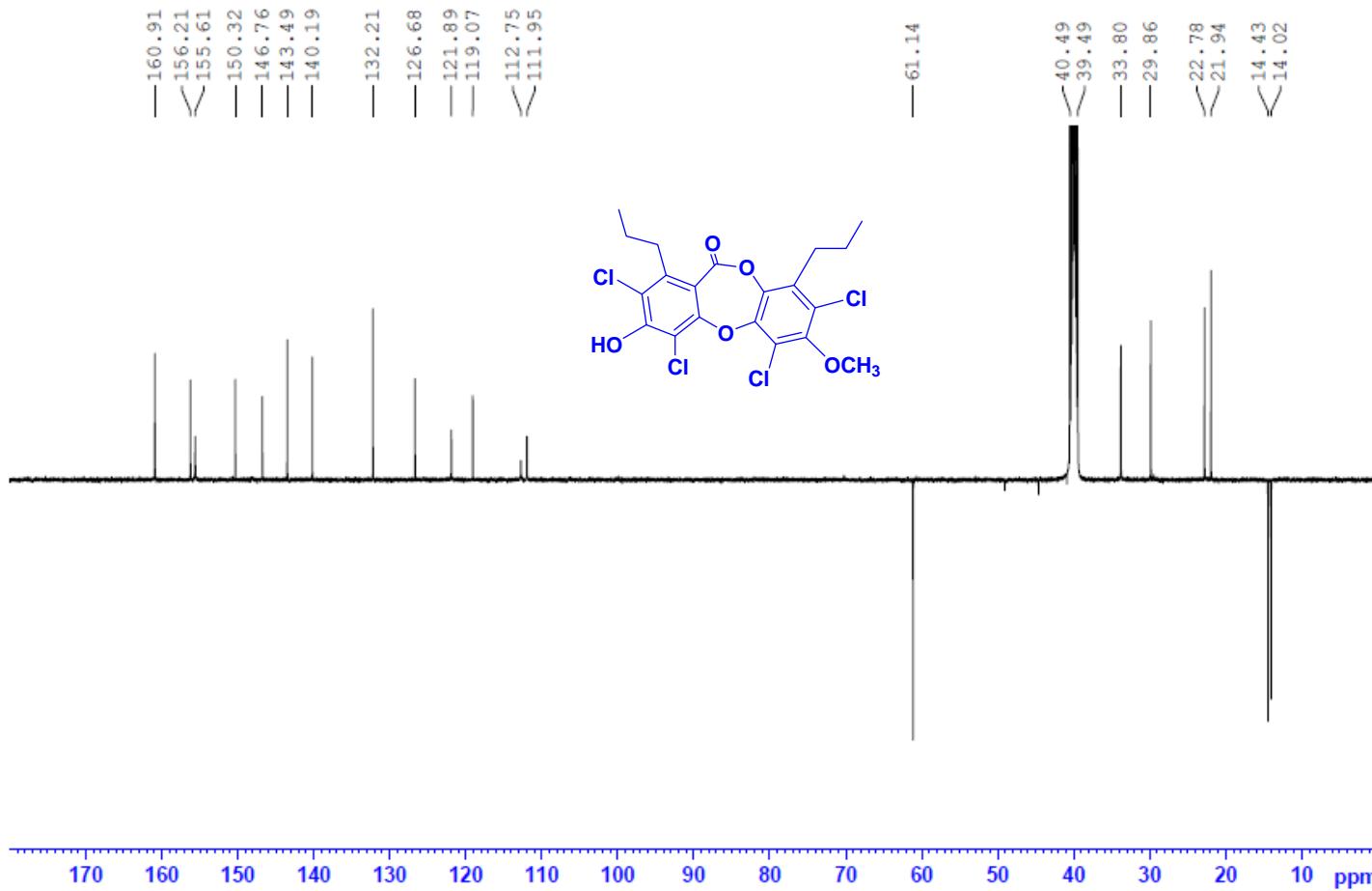


Figure S155. APT spectrum of **12** in *DMSO-d*₆ (100 MHz)

F19-6-7-4-2-2 HSQC

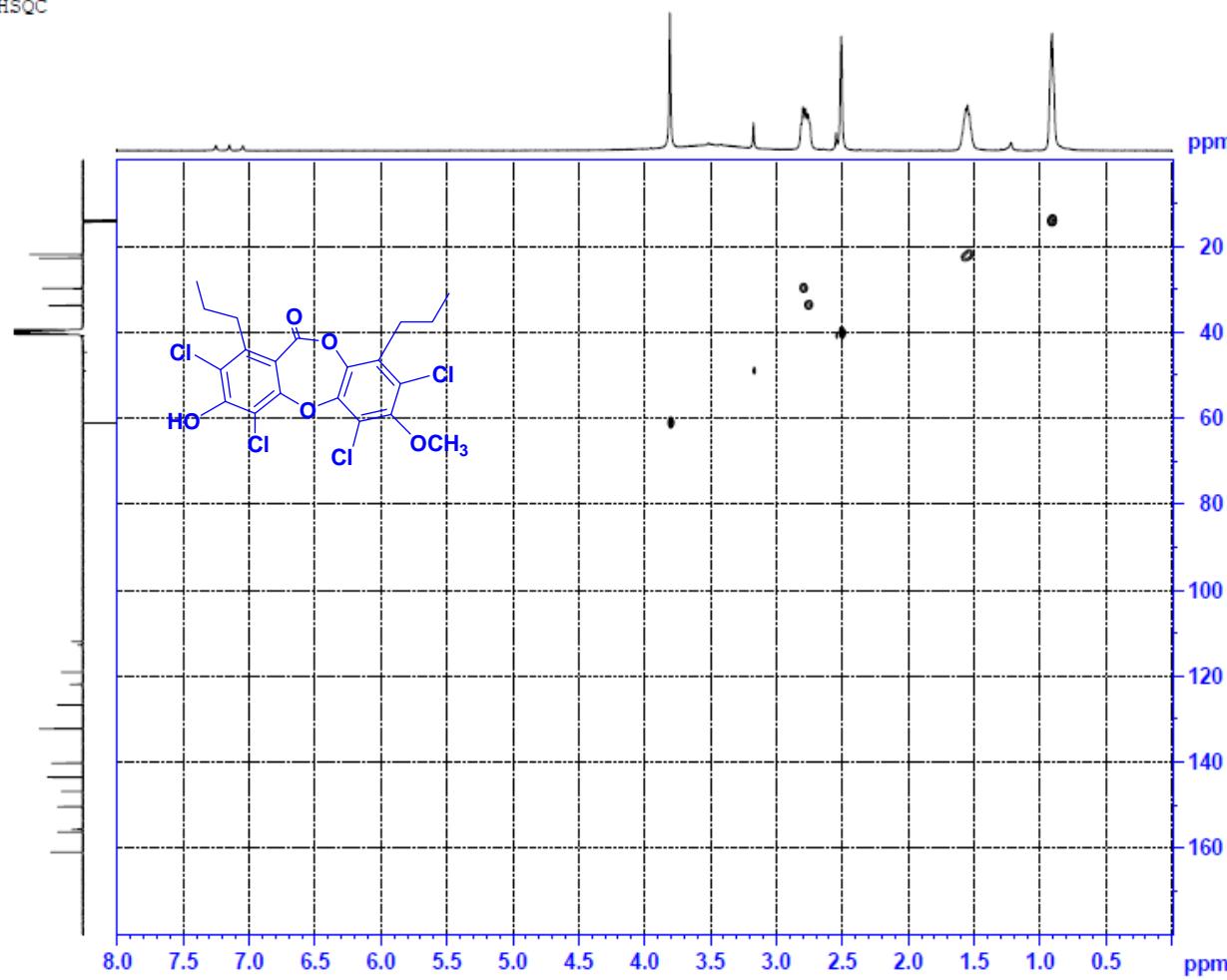


Figure S156. HSQC spectrum of **12** in $\text{DMSO}-d_6$ (400 MHz)

F19-6-7-4-2-2 COSY

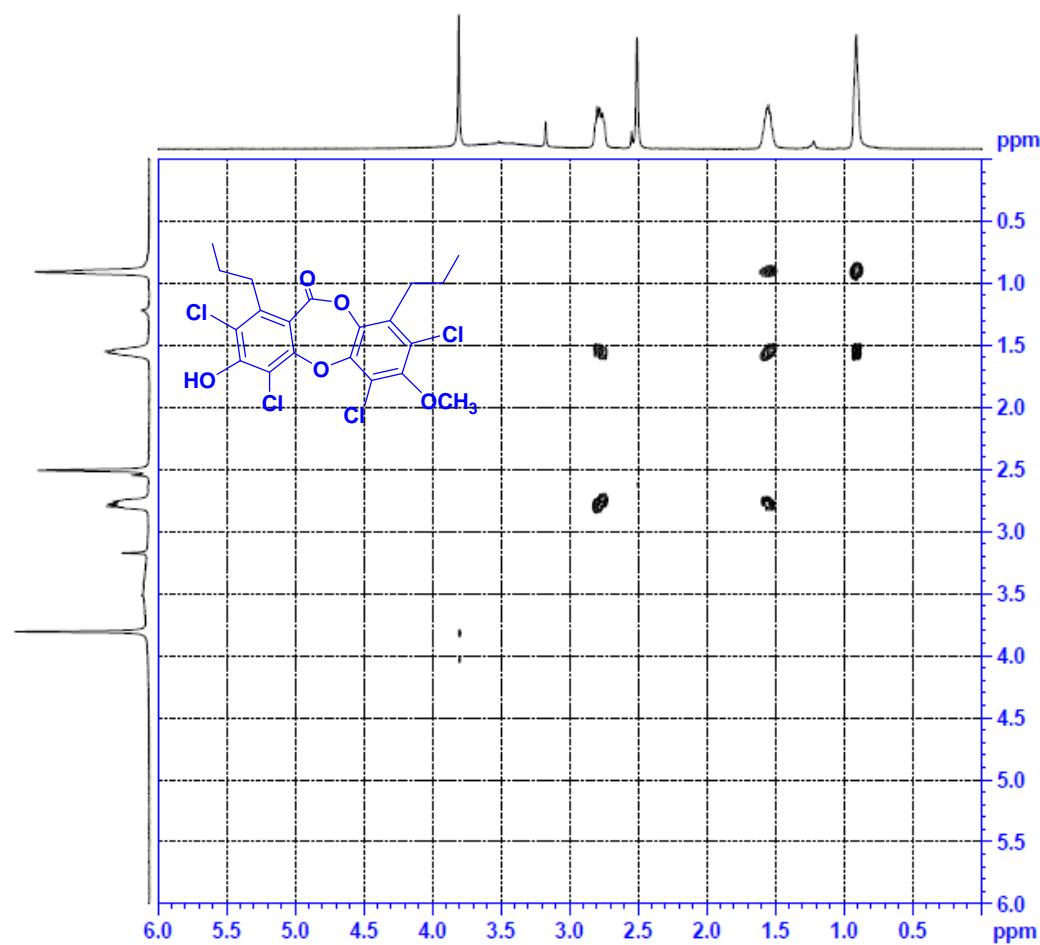


Figure S157. ^1H - ^1H COSY spectrum of **12** in DMSO-*d*₆ (400 MHz)

F19-6-7-4-2-2 HMBC

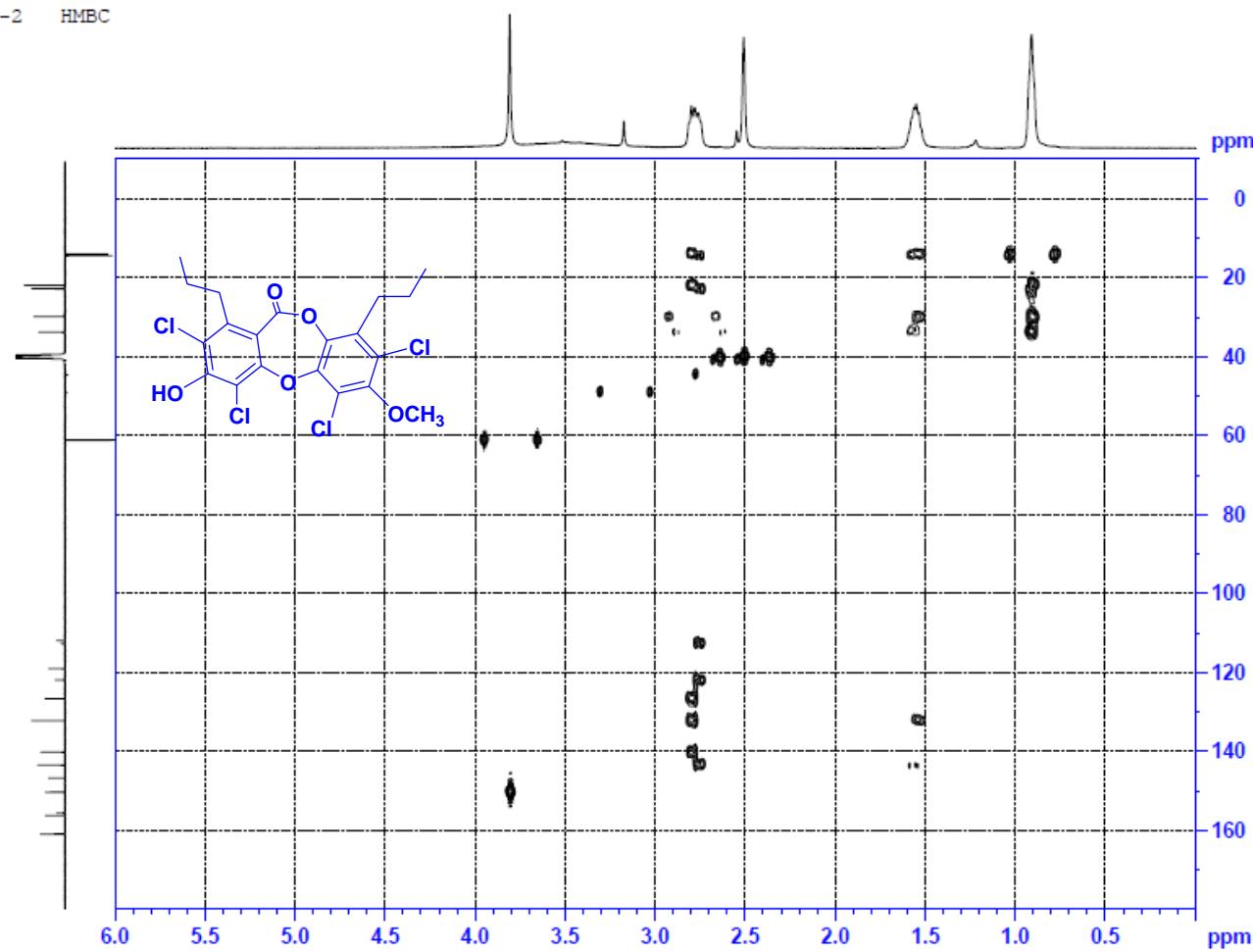
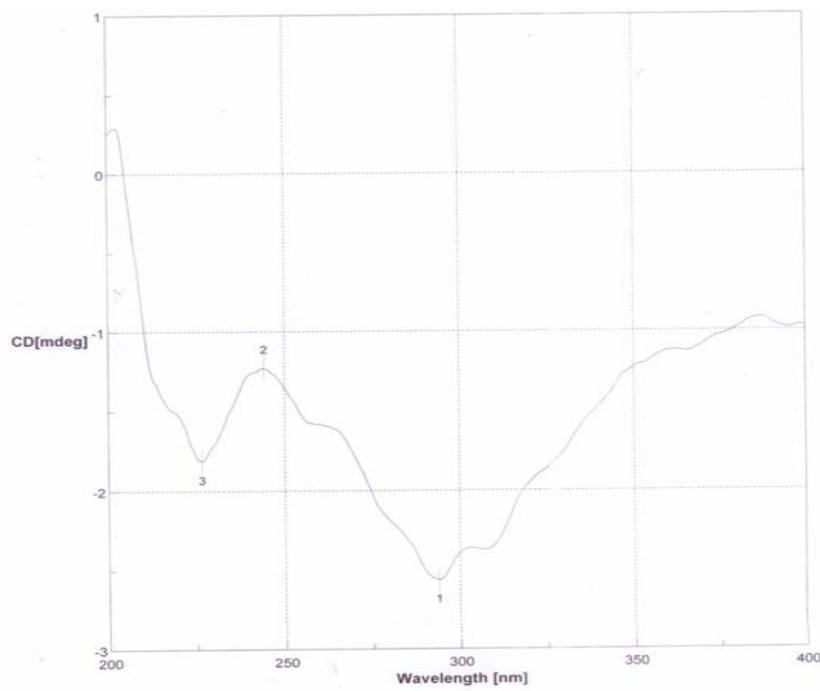


Figure S158. HMBC spectrum of **12** in $\text{DMSO}-d_6$ (400 MHz)



Date/Time
2001-1-3 6:23
Operator
F19-6-7-4-2-2.txt
File Name
F19-6-7-4-2-2 L
Sample Name
Comment

No.	nm	CD[mdeg]	No.	nm	CD[mdeg]	No.	nm	CD[mdeg]
1	294	-2.56362	2	244.2	-1.23014	3	226.6	-1.81393

Figure S159. CD spectrum of **12**

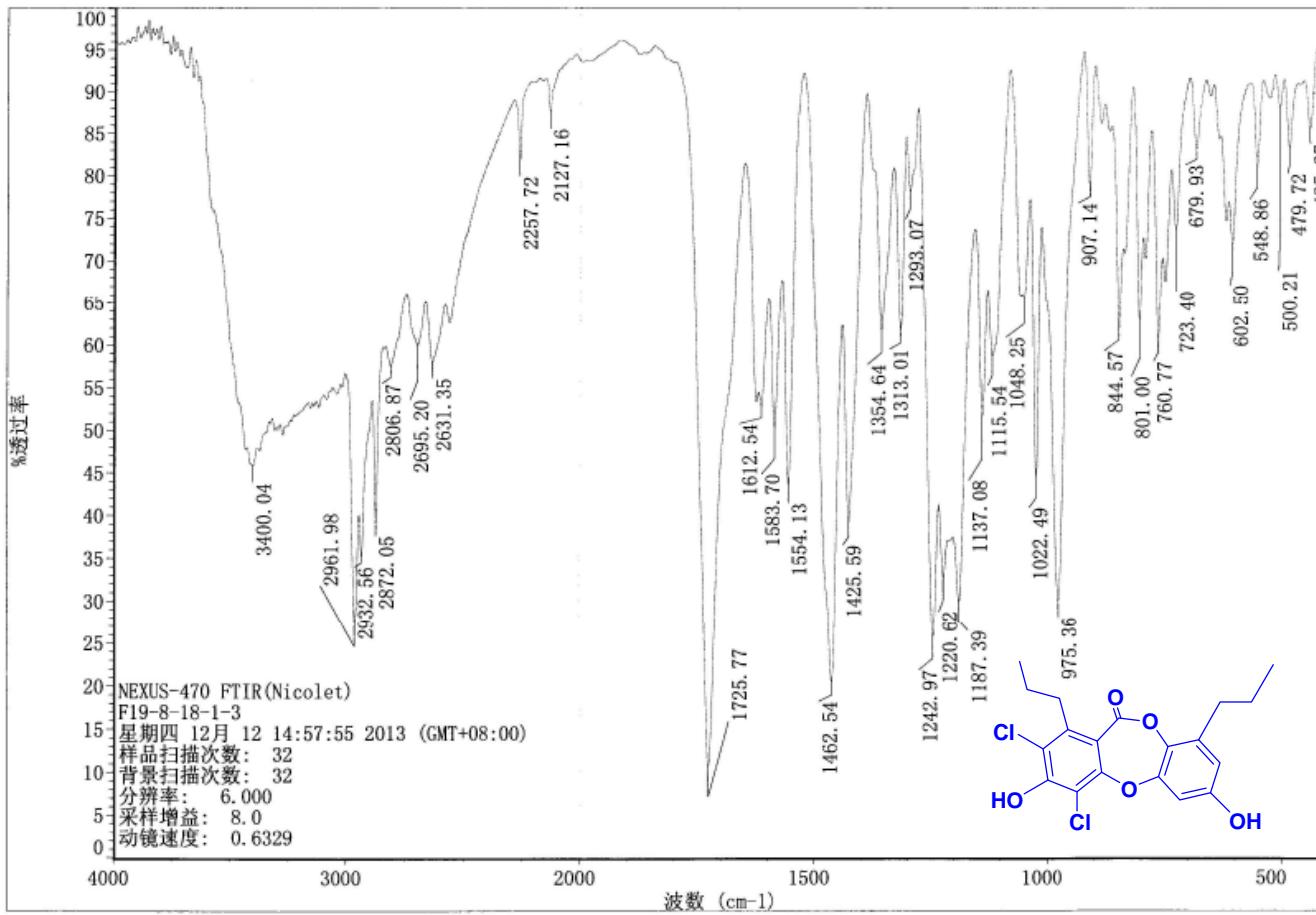


Figure S160. IR spectrum of **13**

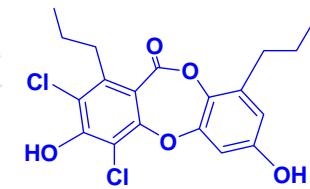


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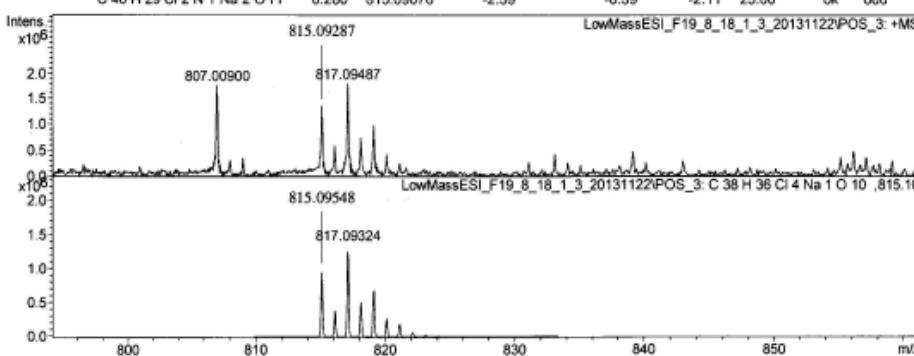
Analysis Name C:\data_sample\ESI_12131120_30\LowMassESI_F19_8_18_1_3_20131122\POS_3 Acquisition Date 11/22/2013 10:07:16 AM
Operator bpxsh@bjmu.edu.cn; Tel:010-82801
Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI □ C19H18O5Cl2 MW 396.05
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;826.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result Exact Mass Measured Mass Error (mDa) Error (ppm) Description



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 38 H 36 Cl 4 Na 1 O 10	0.188	815.09548	3.21	-1.59	2.61	18.50	ok	even
C 38 H 32 Cl 3 N 1 O 13	0.223	815.09337	0.62	-3.86	0.51	22.00	ok	odd
C 38 H 34 Cl 3 Na 4 O 8	0.223	815.09046	-2.96	-7.57	-2.41	18.50	ok	even
C 40 H 33 Cl 3 Na 3 O 8	0.230	815.09286	-0.01	-4.49	-0.01	21.50	ok	even
C 39 H 30 Cl 2 Na 1 O 14	0.276	815.09048	-2.93	-6.73	-2.38	23.50	ok	even
C 40 H 29 Cl 2 N 1 Na 2 O 11	0.280	815.09076	-2.59	-6.39	-2.11	25.00	ok	odd





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Analysis Name C:\data_sample\ESI_12140210_20\MassESI_f19_8_18
_1_3_20140214\NEG_6 Acquisition Date 2/14/2014 8:51:20 AM
Operator bpxsh@bjmu.edu.cn; Tel:010-82801
Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI C19H18O5CL2 MW 396.05
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;8;26.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result	Exact Mass	Measured Mass	Error (mDa)	Error (ppm)	Description
	395.04585	395.04622	-0.37	-0.93	M-H ⁺ e

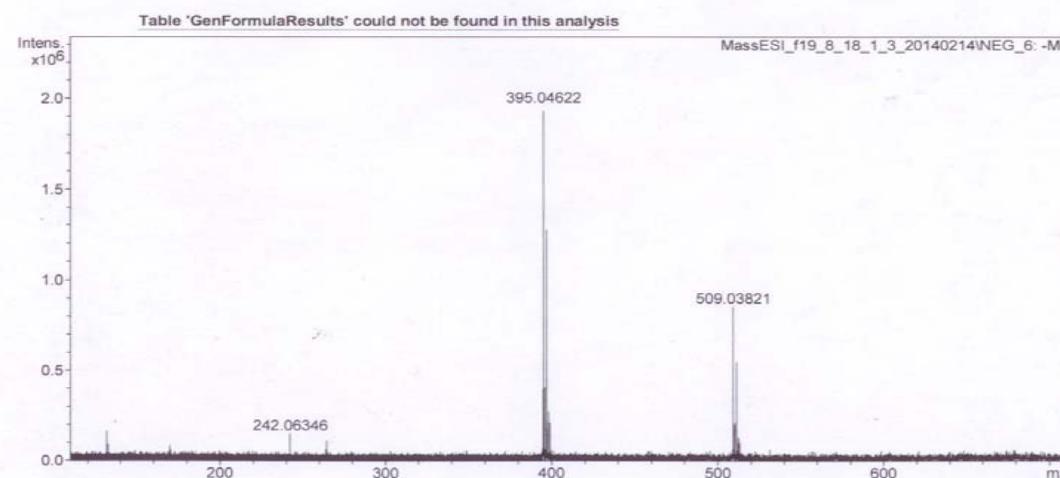


Figure S161. HRESIMS spectrum of **13**

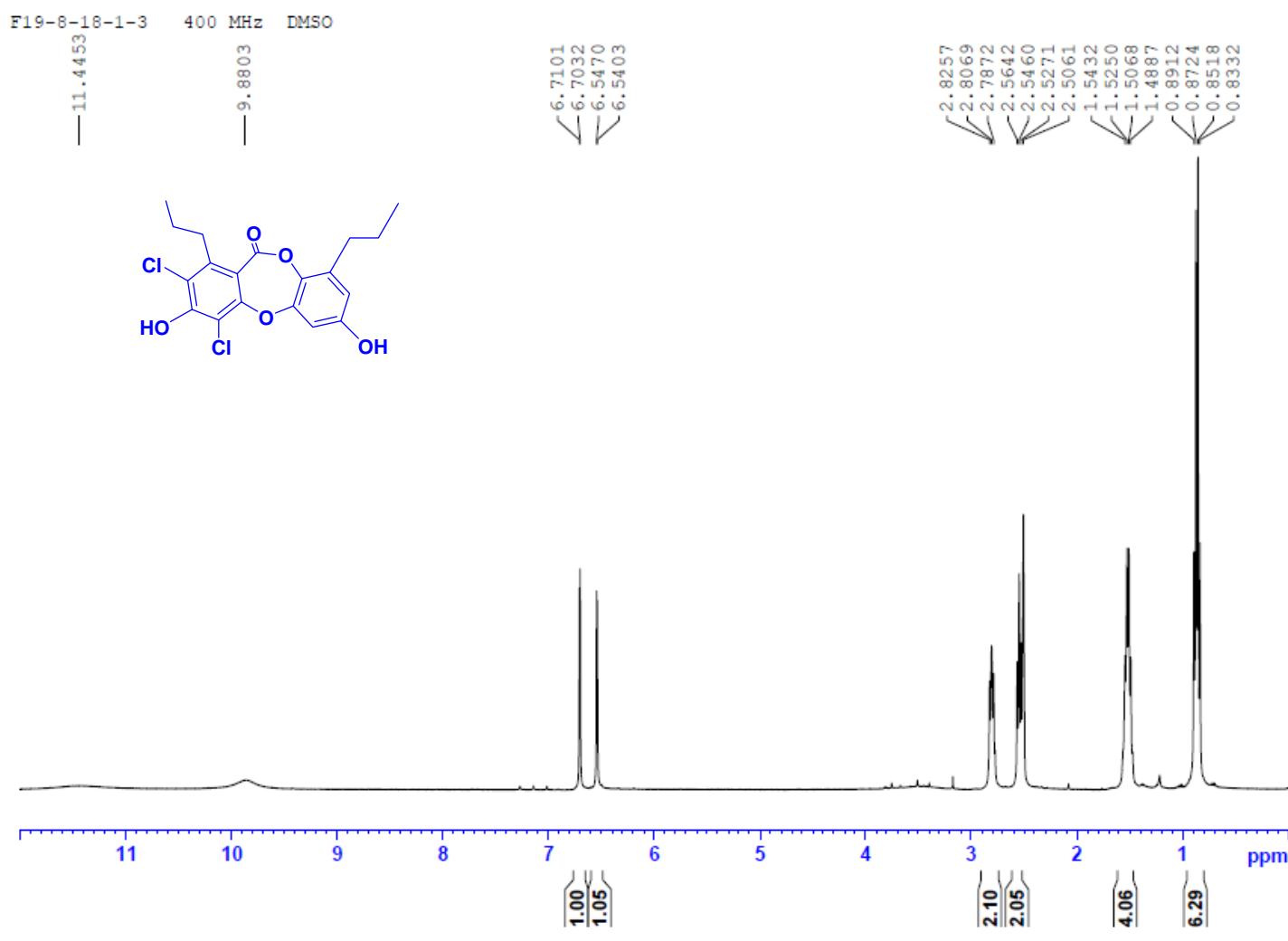


Figure S162. ^1H NMR spectrum of **13** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-1-3 APT

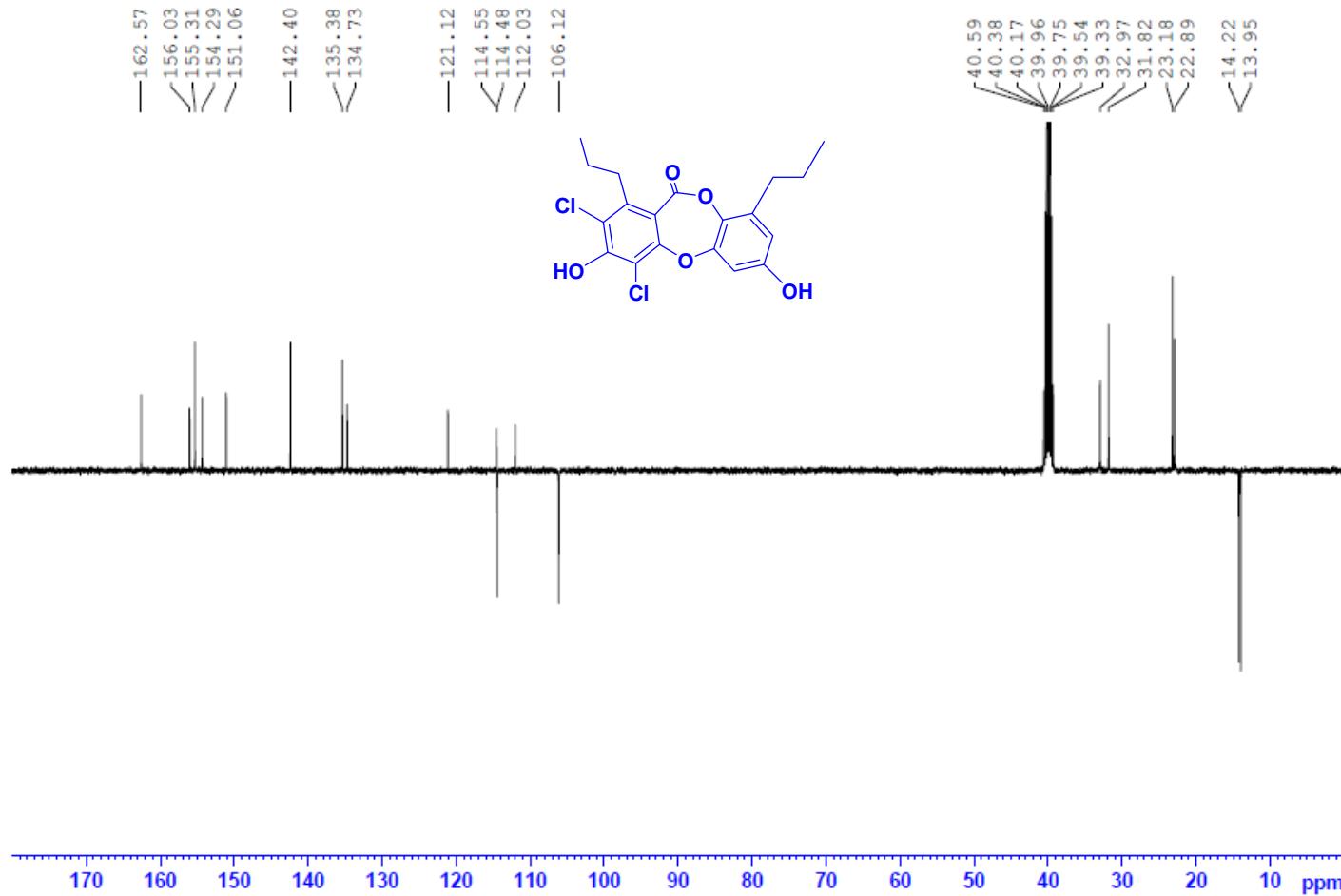


Figure S163. APT spectrum of **13** in $\text{DMSO}-d_6$ (100 MHz)

F19-8-18-1-3 HSQC

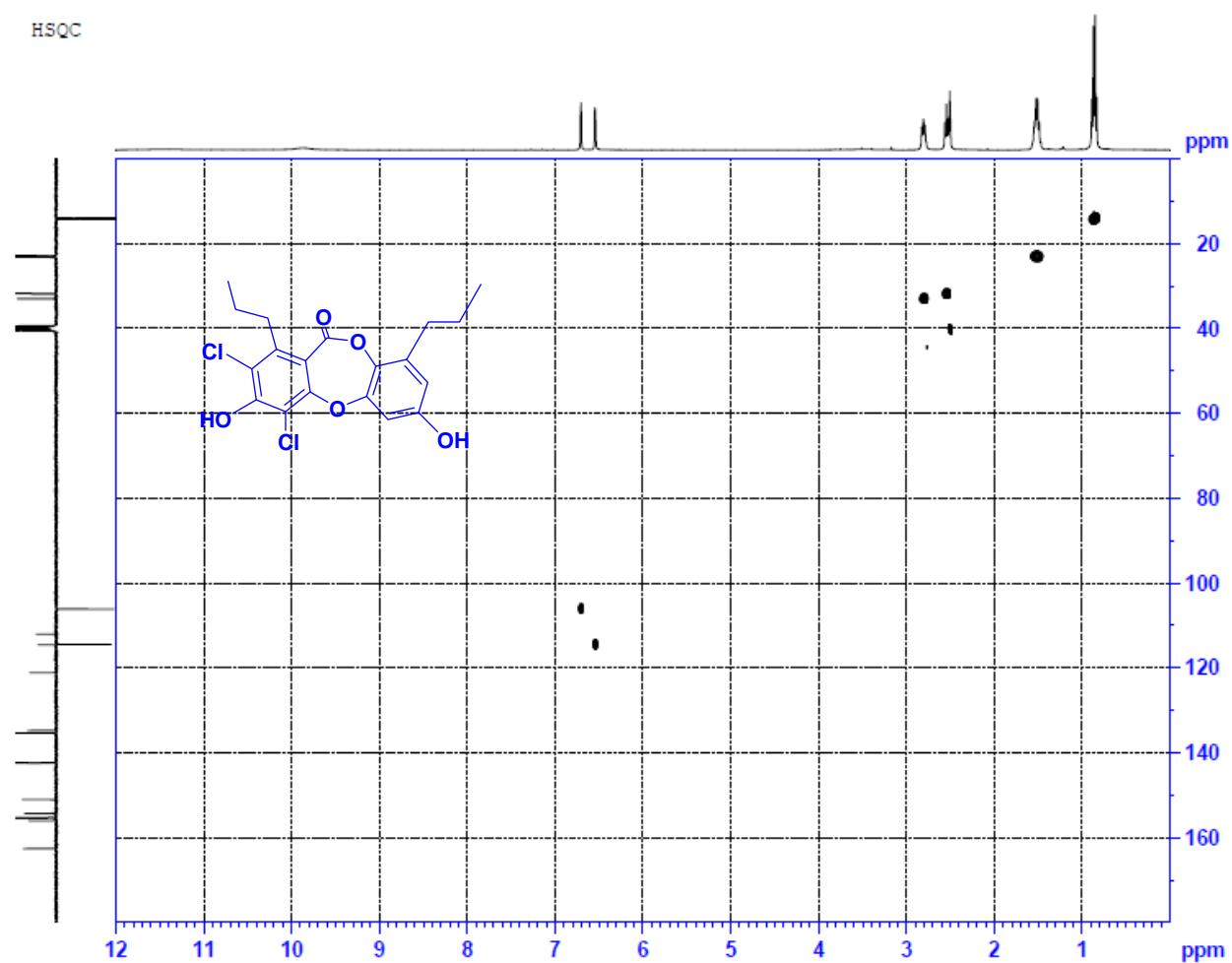


Figure S164. HSQC spectrum of **13** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-1-3 COSY

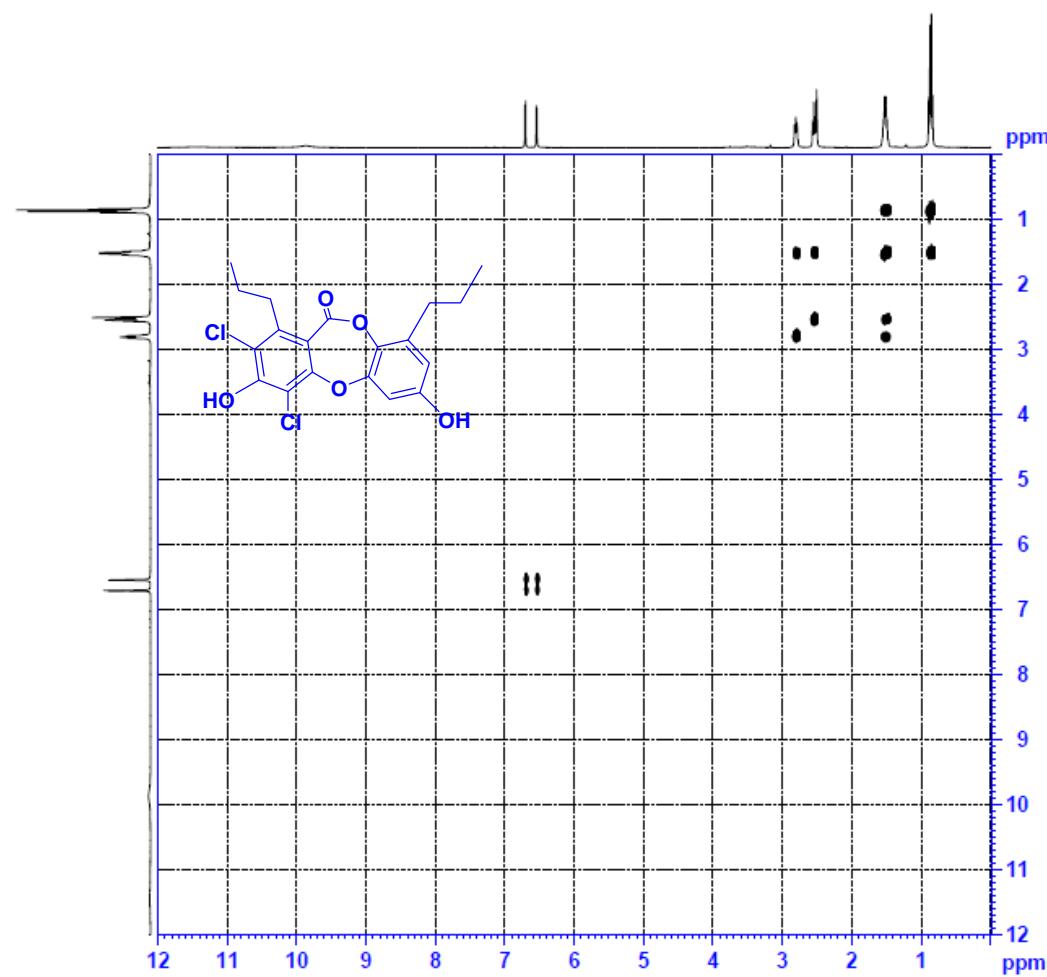


Figure 165. ^1H - ^1H COSY spectrum of **13** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-18-1-3 HMBC

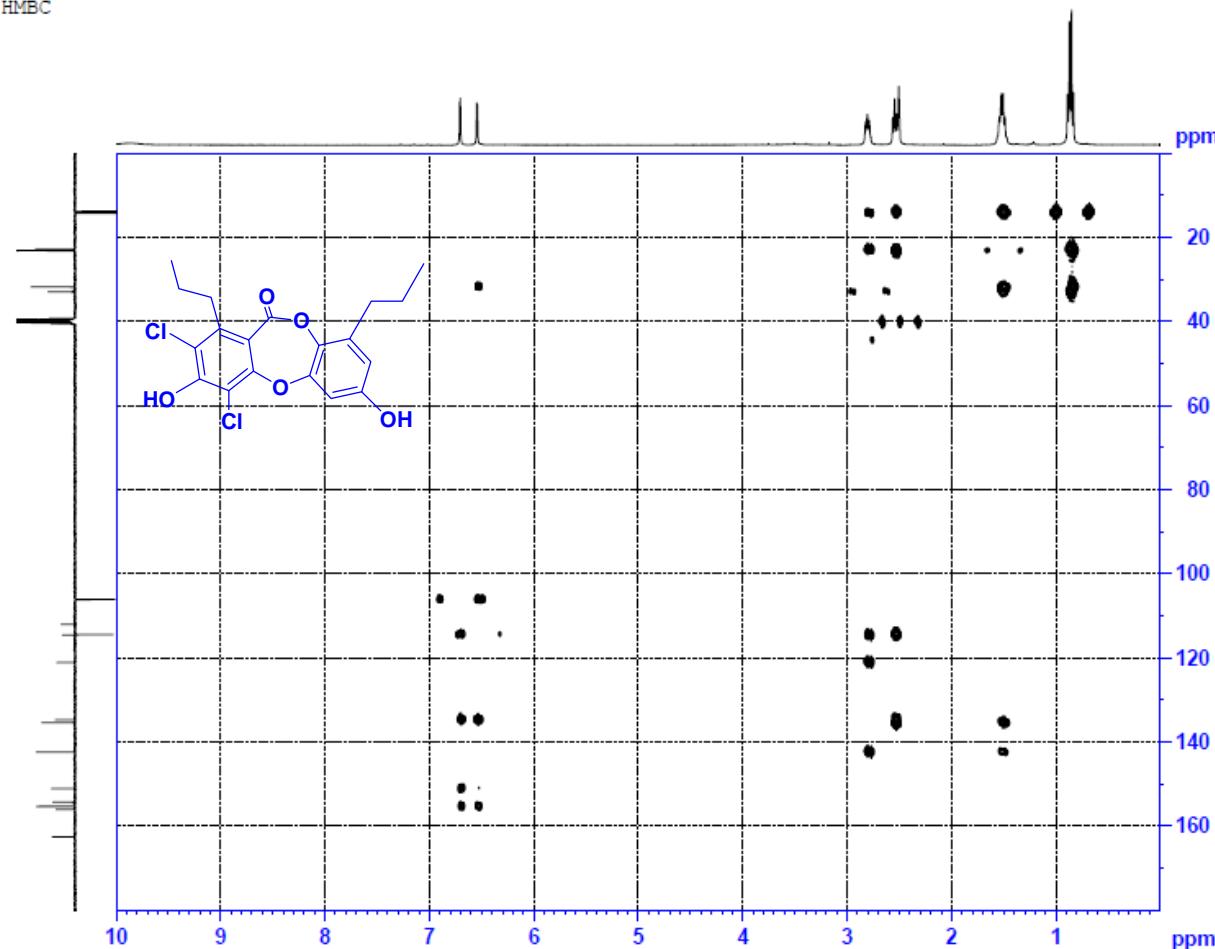
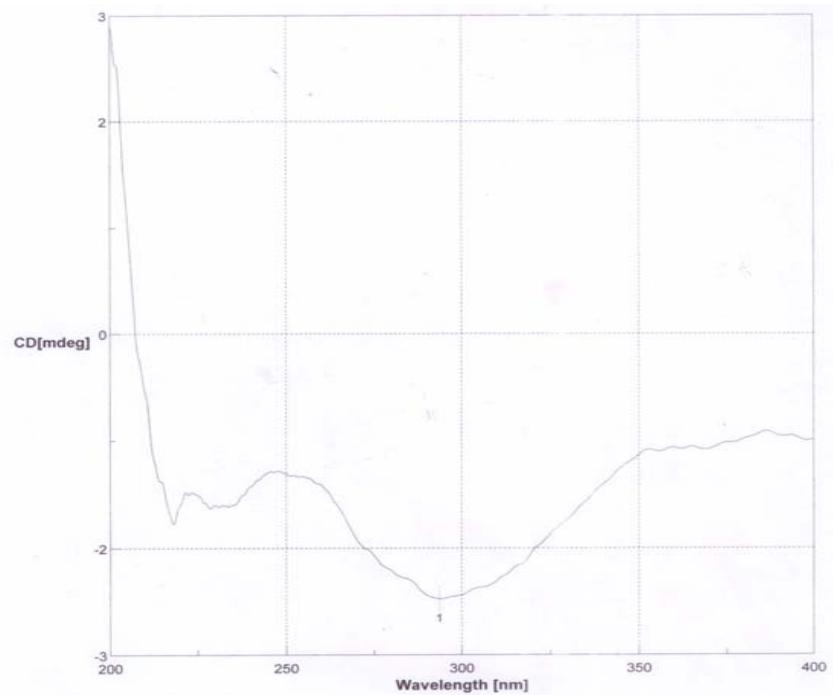


Figure S166. HMBC spectrum of **13** in $\text{DMSO}-d_6$ (400 MHz)



Date/Time 2001-1-3 5:35
Operator
File Name F19-8-18-1-3.txt
Sample Name F19-8-18-1-3
Comment

No. nm CD[mdeg]
1 293.6 -2.47295

Figure S167. CD spectrum of **13**

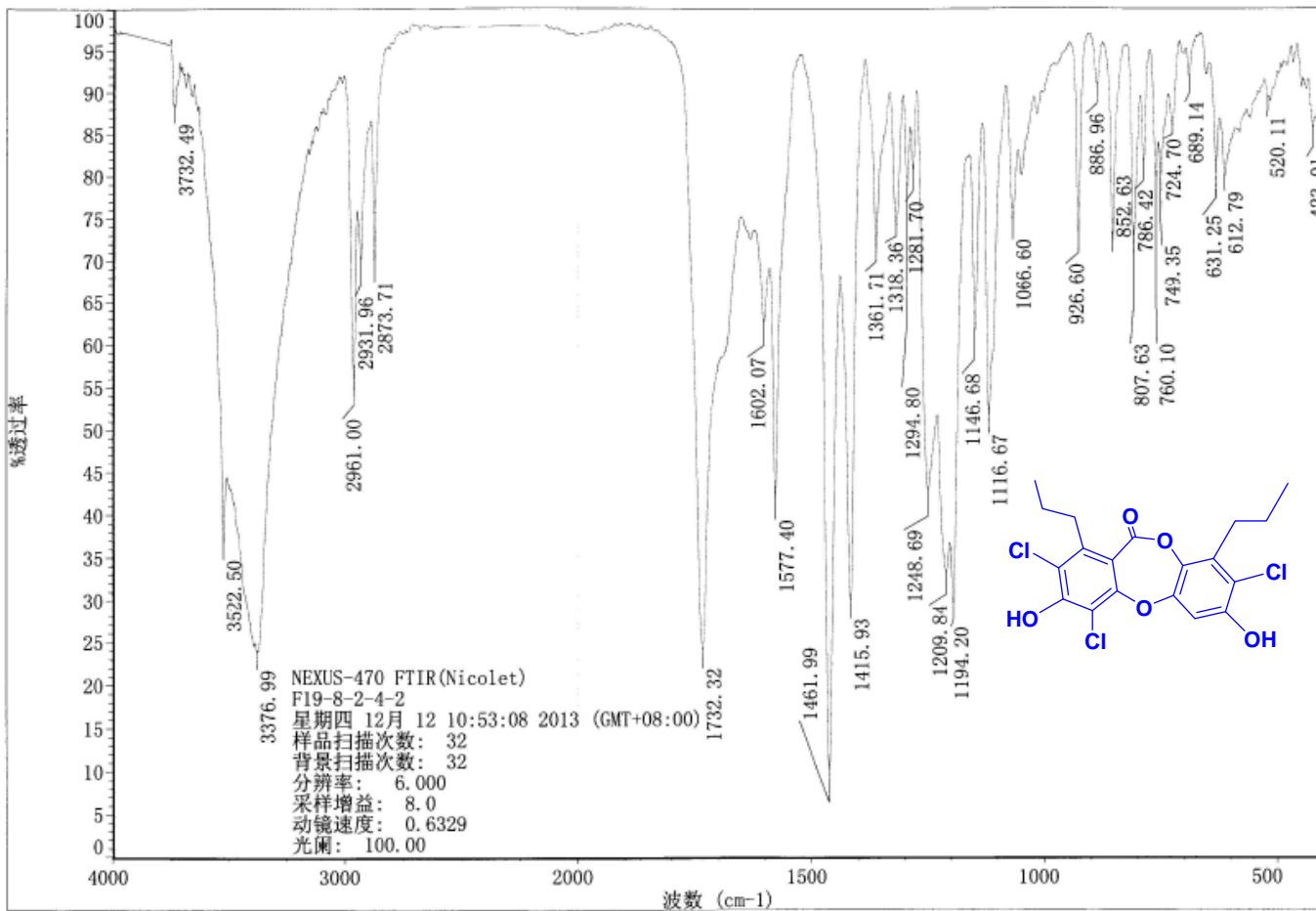


Figure S168. IR spectrum of **14**



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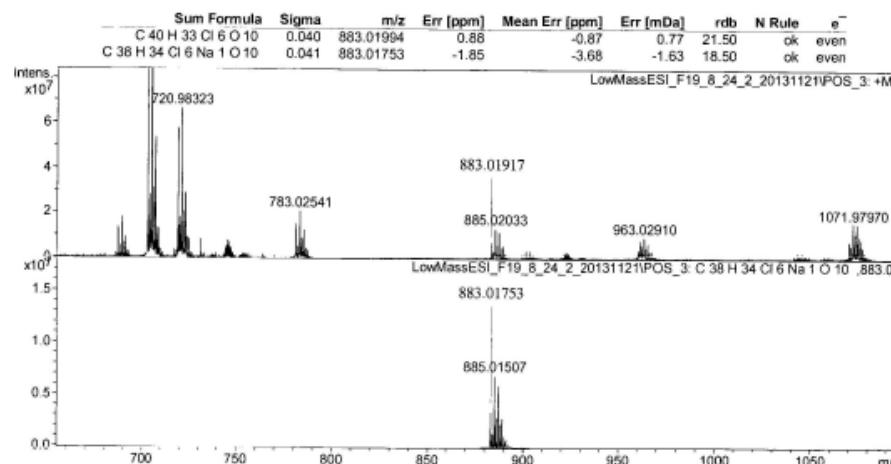
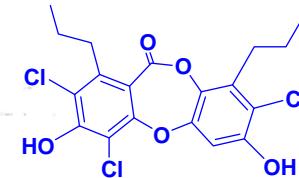
Analysis Name C:\data\sample\ESI_12131120_30\LowMassESI_F19_8_24_2_20131121\POS_3 Acquisition Date 11/20/2013 2:41:51 PM

Operator bpxsh@bjmu.edu.cn; Tel:010-82801

Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI pos C19H17CL3O5 MW 430
CAL588: 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;826.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result Exact Mass Measured Mass Error (mDa) Error (ppm) Description





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Analysis Name C:\data_sample\ESI_12131120_30\LowMassESI_F19_8_24_2_20131121\POS_3 Acquisition Date 11/20/2013 2:41:51 PM

Operator bpxsh@bjmu.edu.cn; Tel:010-82801

Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI pos □ C19H17Cl3O5 MW 430
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;826.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result Exact Mass Measured Mass Error (mDa) Error (ppm) Description

431.02143 □□□□□□□ 431.02199 □□□□□□□ -0.56 □□□□□□□ -1.29 □□□□□□□ M+H;-e

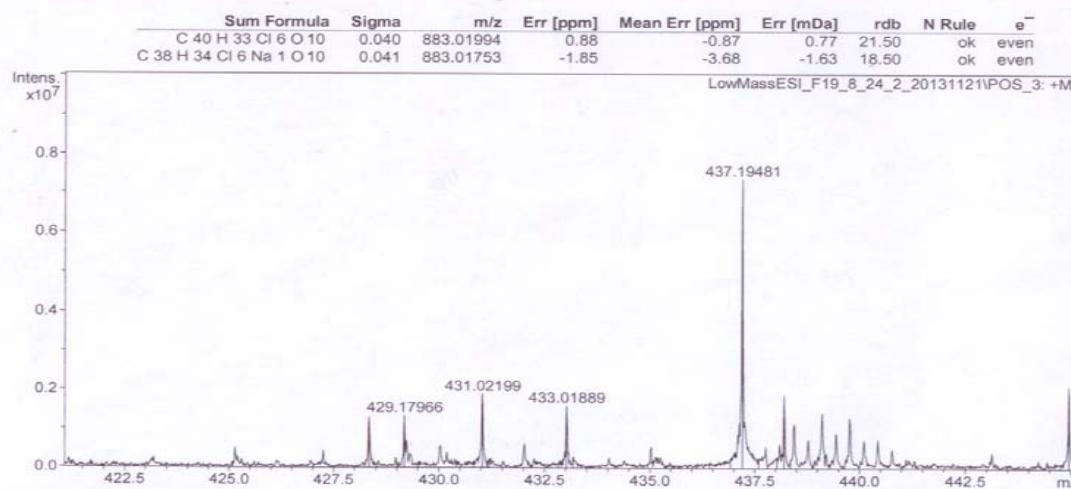


Figure S169. HRESIMS spectrum of 14

F19-8-24-2 400 MHz DMSO

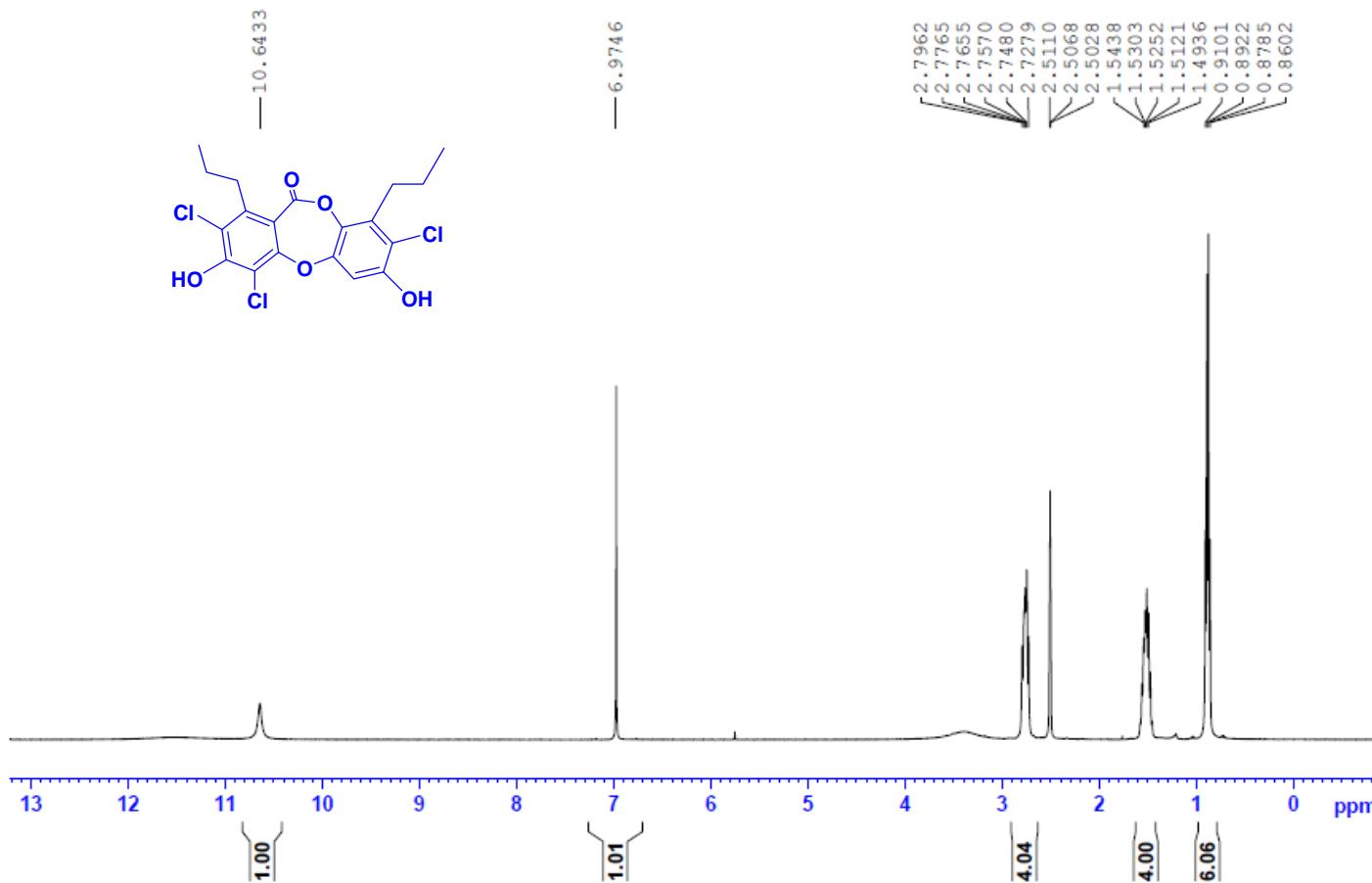


Figure S170. ^1H NMR spectrum of **14** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-24-2 APT

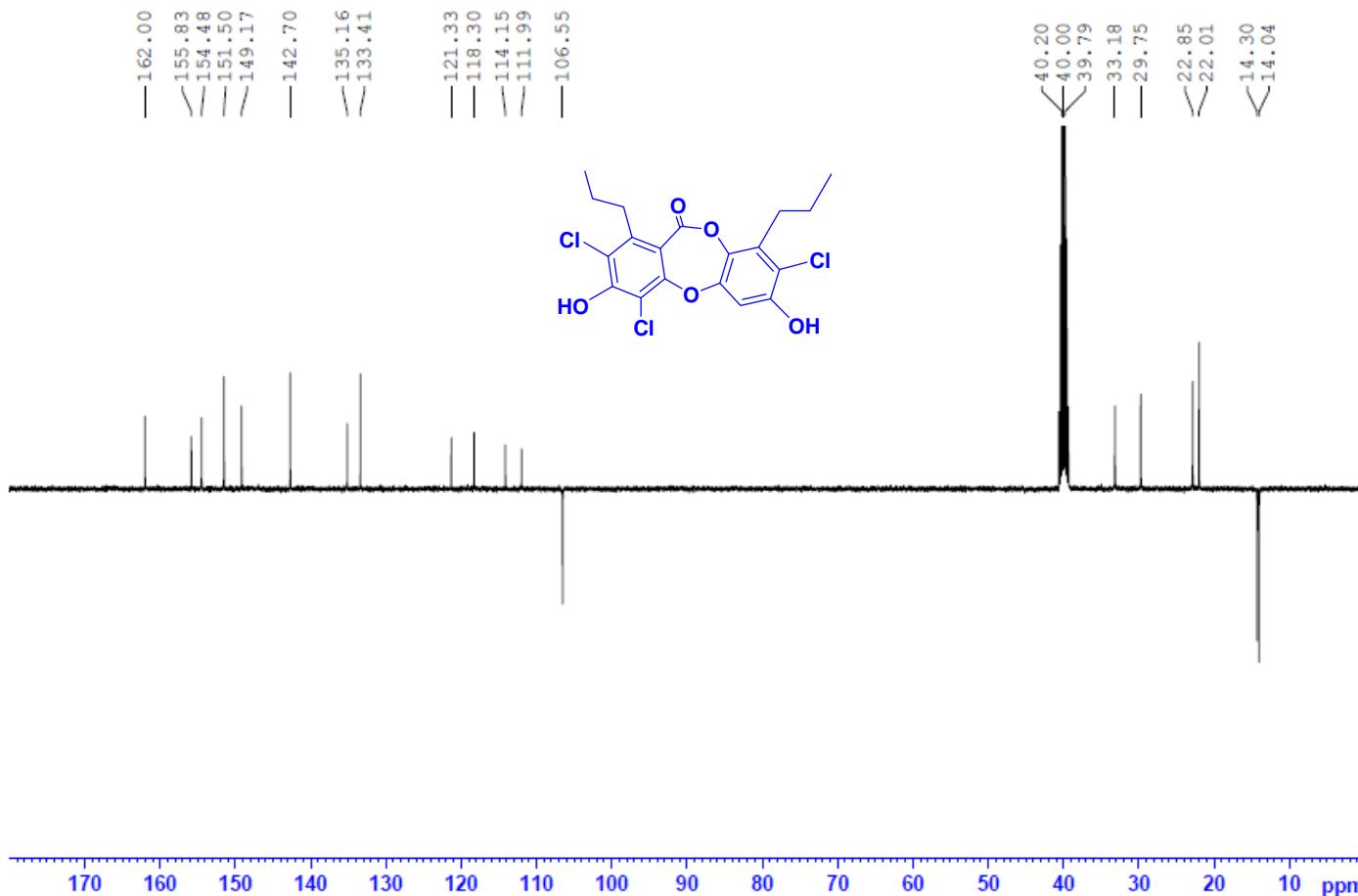


Figure S171. APT spectrum of **14** in $\text{DMSO}-d_6$ (100 MHz)

F19-8-24-2 HSQC

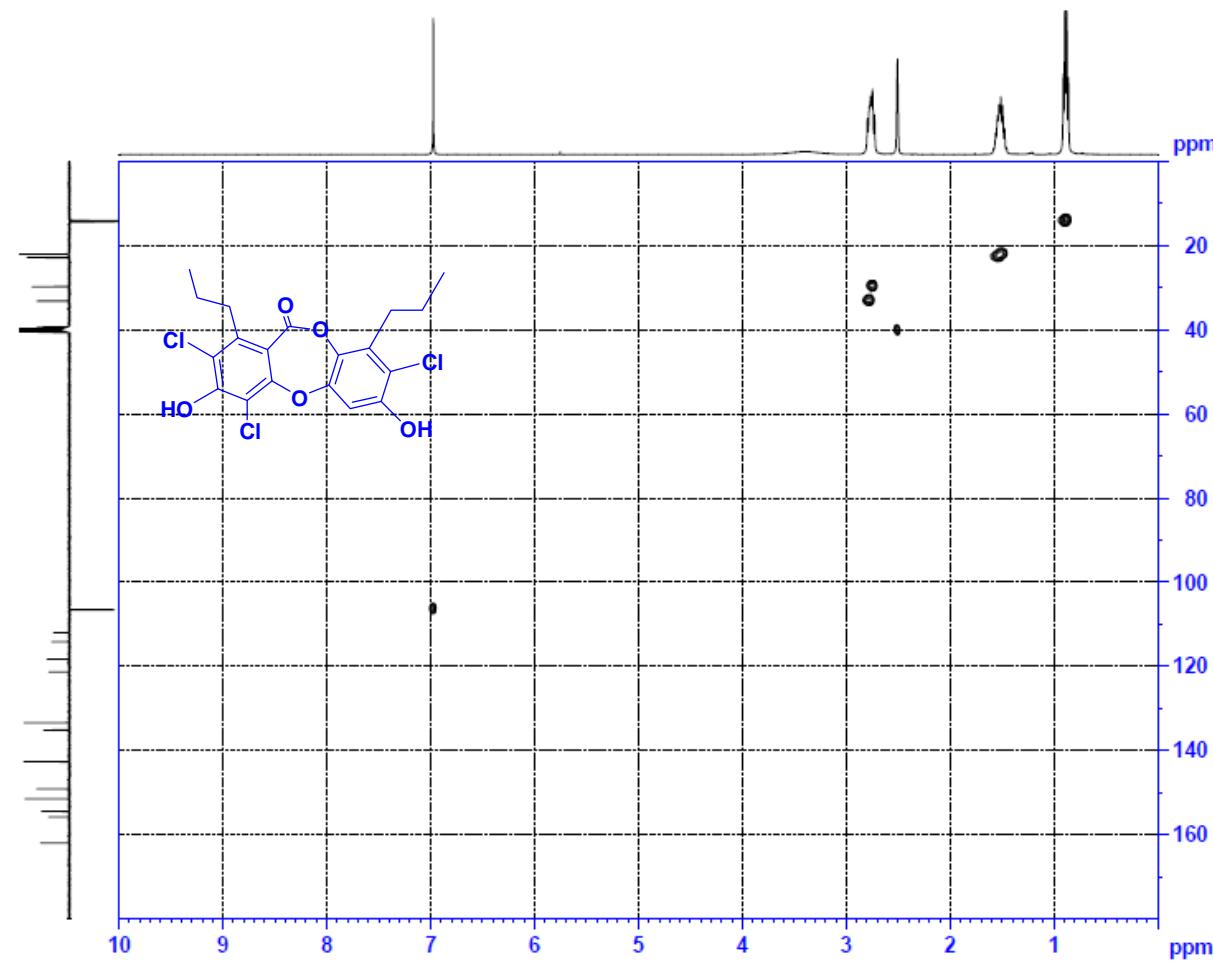


Figure S172. HSQC spectrum of **14** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-24-2 COSY

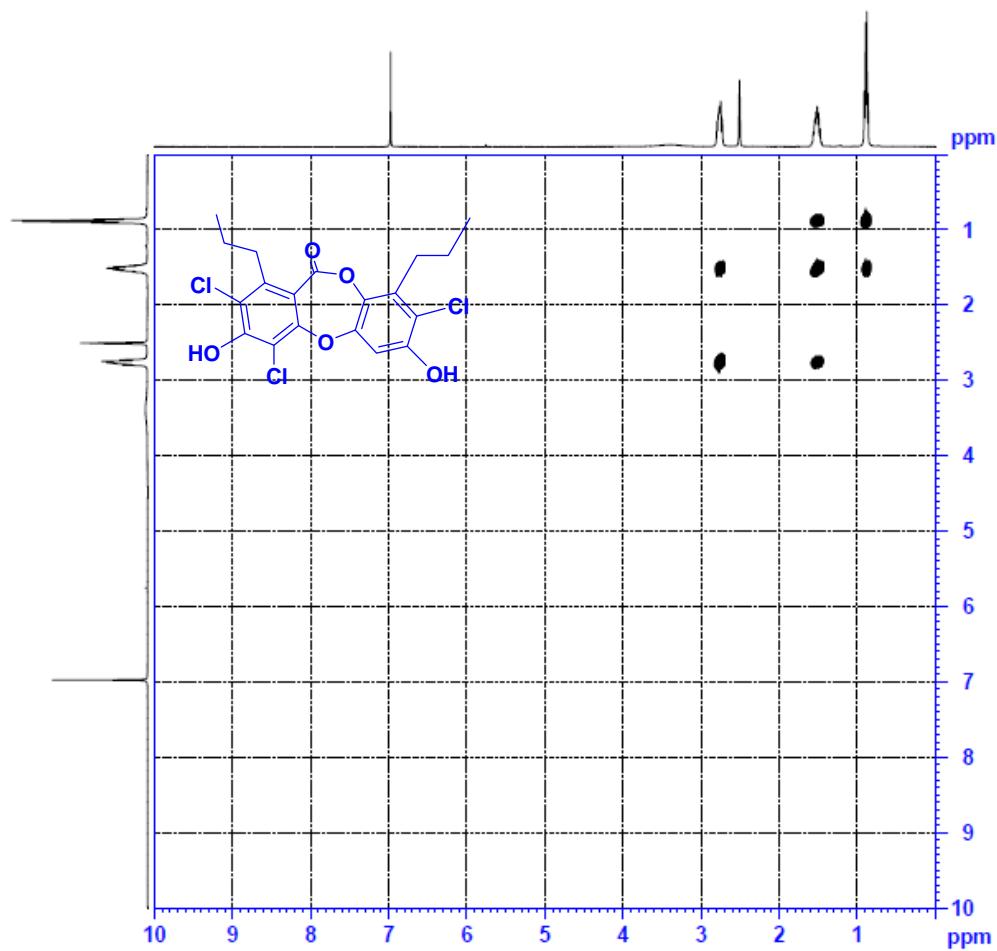


Figure S173. ^1H - ^1H COSY spectrum of **14** in $\text{DMSO}-d_6$ (400 MHz)

F19-8-24-2 HMBC

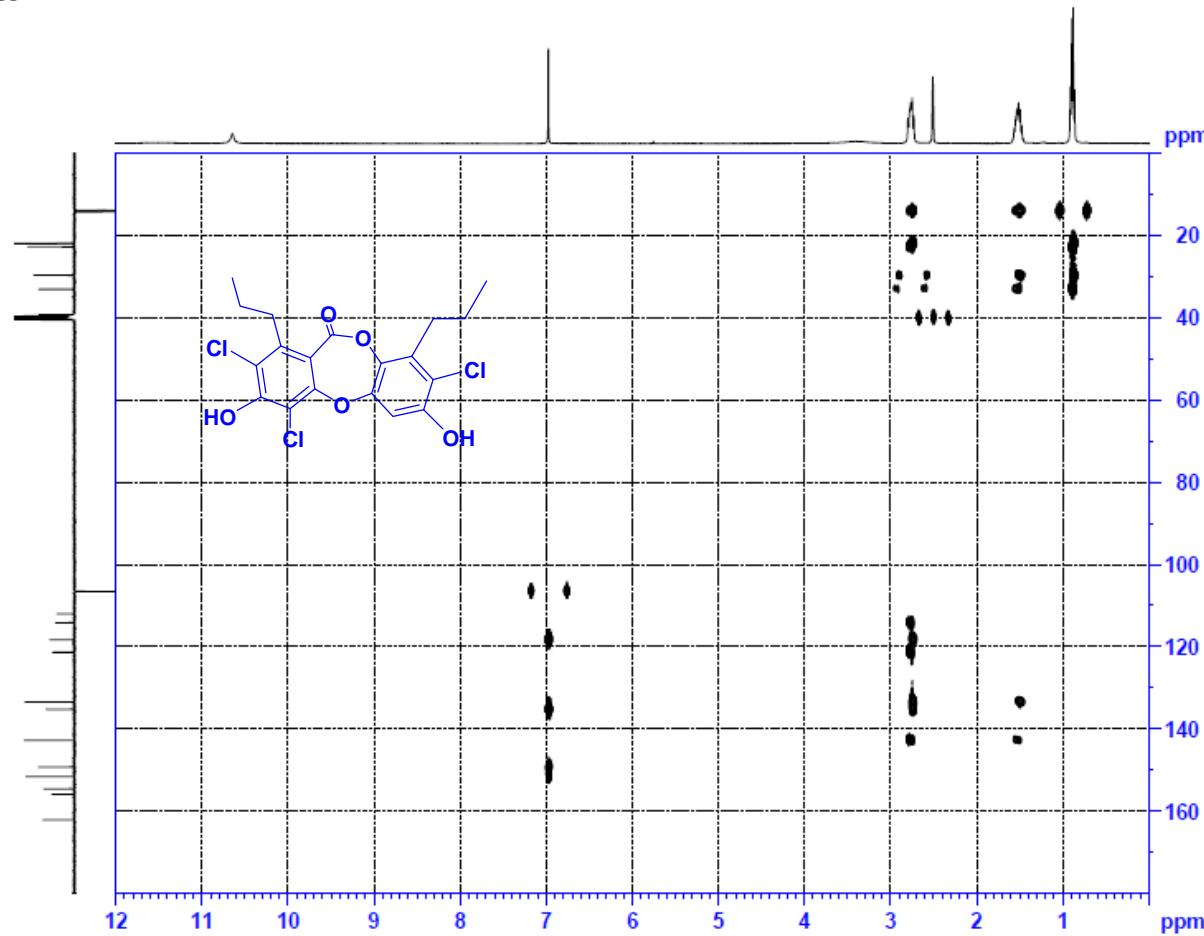
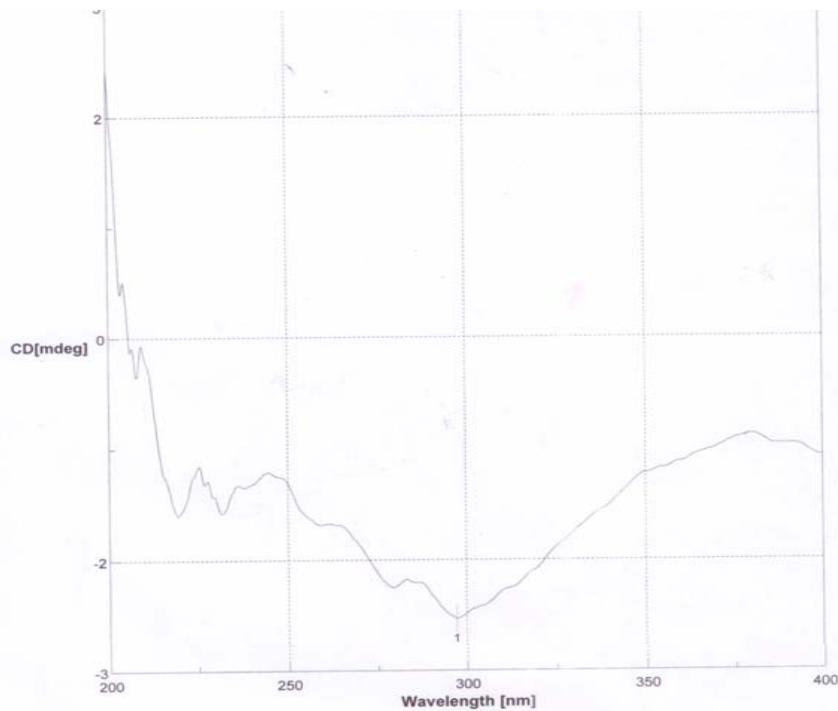


Figure S174. HMBC spectrum of **14** in DMSO-*d*₆ (400 MHz)



Date/Time 2001-1-3 5:04
Operator
File Name Memory#3
Sample Name F19-8-24-2
Comment

No. nm CD[mdeg]
1 297.2 -2.5273

Figure S175. CD spectrum of **14**

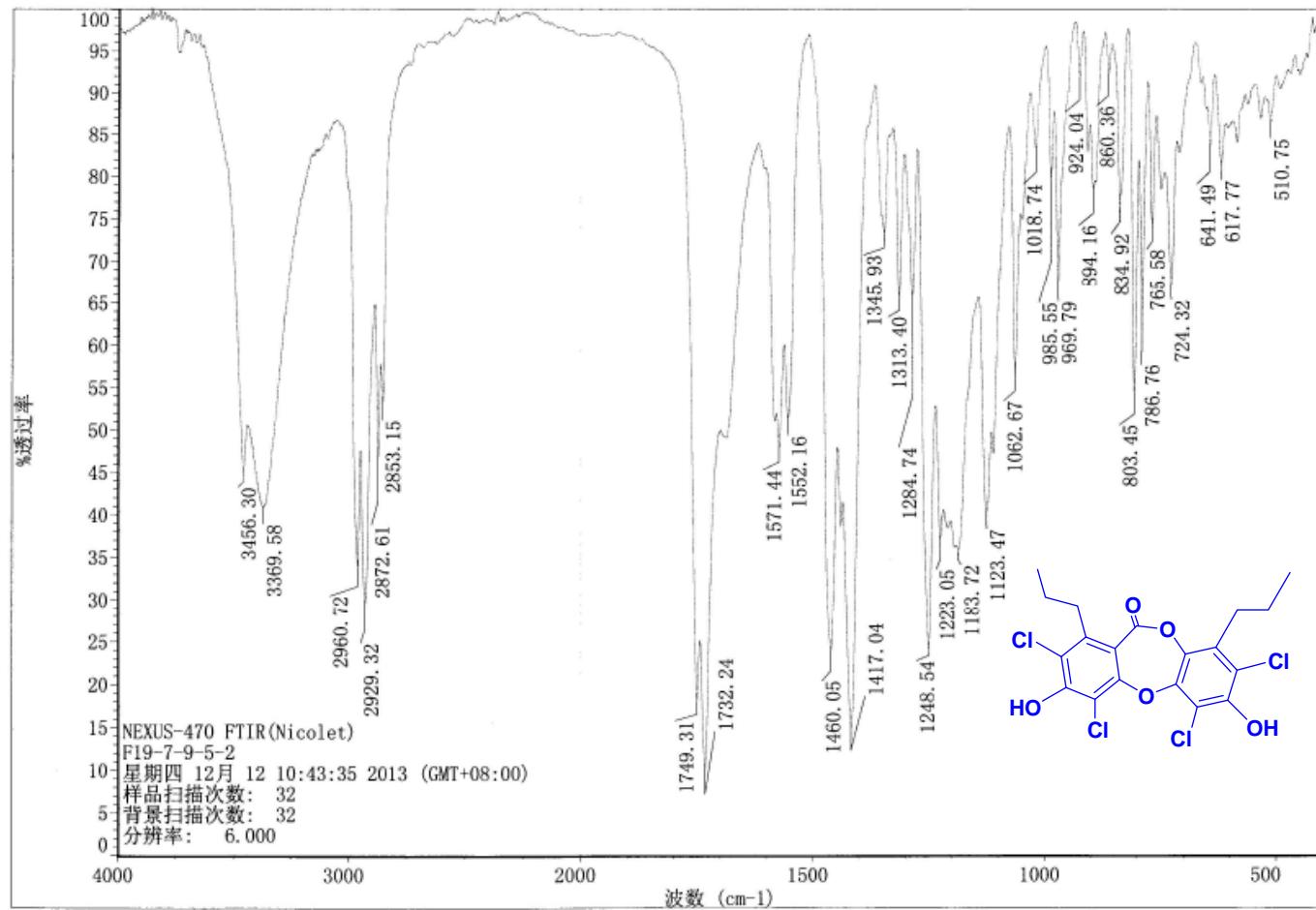


Figure S176. IR spectrum of **15**



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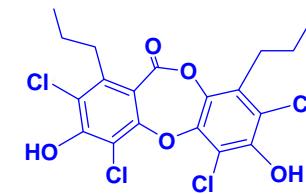
Analysis Name C:\data_sample\ESI_12131120_30\LowMassESI_F17_7_9_5_2_20131121\POS_3 Acquisition Date 11/20/2013 2:13:27 PM

Operator bpxsh@bjmu.edu.cn; Tel:010-82801

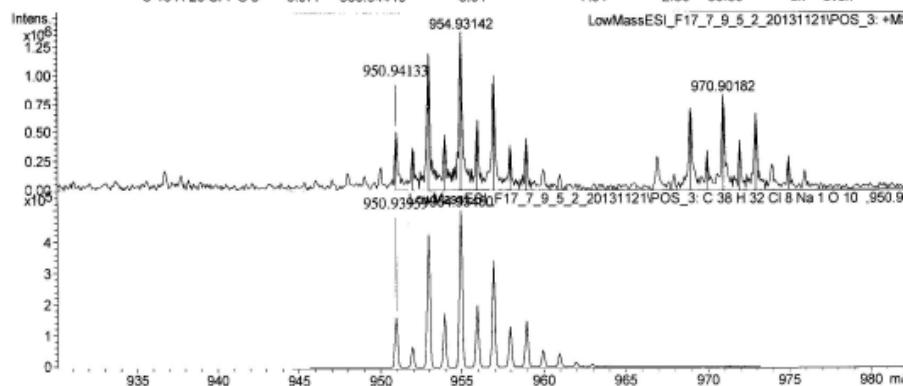
Instrument FT_MS_Bruker APEX IV (7.0)

Comment ESI pos C19H16Cl4O5 MW 464
CAL588; 279.15693;310.14158;322.04812;391.28483;
413.26647;453.34353;475.32548;509.25407;
509.25407;611.26126;8;26.47121;842.44514;
588.40954;679.51166;701.49361;826.47121;

Acquisition Result Exact Mass Measured Mass Error (mDa) Error (ppm) Description



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 40 H 31 Cl 8 O 10	0.058	950.94200	0.70	5.01	0.67	21.50	ok	even
C 38 H 32 Cl 8 Na 1 O 10	0.058	950.93959	-1.83	2.42	-1.74	18.50	ok	even
C 44 H 27 Cl 7 Na 1 O 8	0.076	950.94178	0.48	4.97	0.46	27.50	ok	even
C 46 H 26 Cl 7 O 8	0.077	950.94419	3.01	7.54	2.86	30.50	ok	even





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Analysis Name C:\data_sample\ESI_12140210_20\MassESI_f19_7_9_5_2_20140214\NEG_8 Acquisition Date 2/14/2014 9:04:11 AM
Operator bpxsh@bjmu.edu.cn; Tel:010-82801
Instrument FT_MS_Bruker APEX IV (7.0)

Comment	ESI	C19H16O5CL4	MW	464	CAL588; 279.15693;310.14158;322.04812;391.28483; 413.26647;453.34353;475.32548;509.25407; 509.25407;611.26126;826.47121;842.44514; 588.40954;679.51166;701.49361;826.47121;
Acquisition Result	Exact Mass	Measured Mass	Error (mDa)	Error (ppm)	Description
	462.96791	462.96842	-0.51	-1.11	M-H ;+e

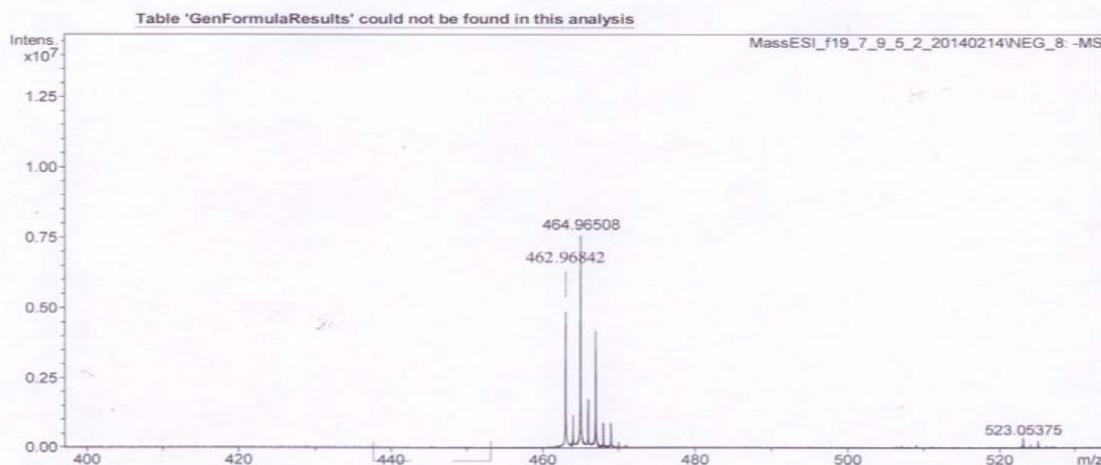


Figure S177. HRESIMS spectrum of **15**

F19-7-9-5-2 400 MHz DMSO

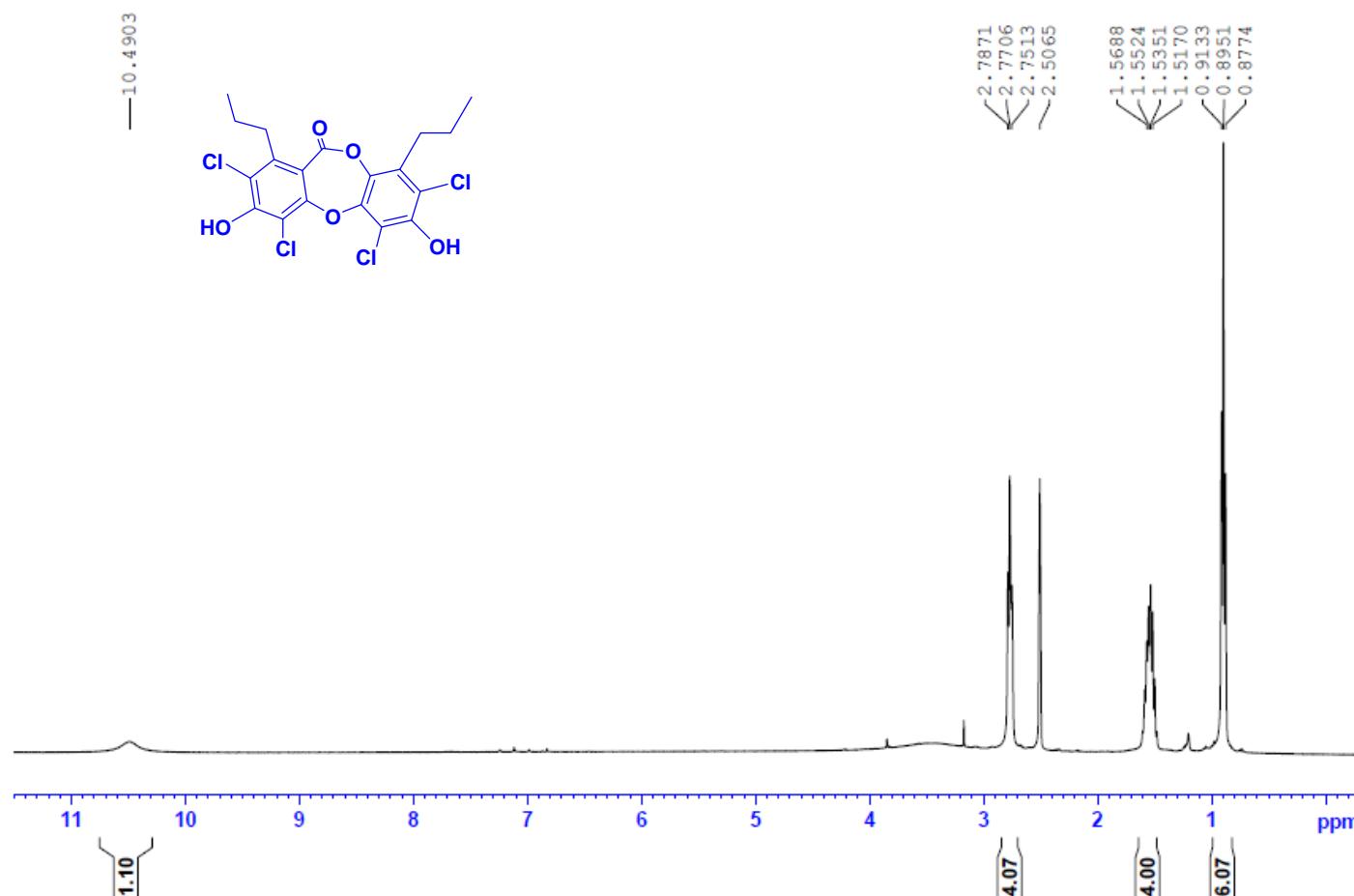


Figure S178. ^1H NMR spectrum of **15** in $\text{DMSO}-d_6$ (400 MHz)

F19-7-9-5-2 APT

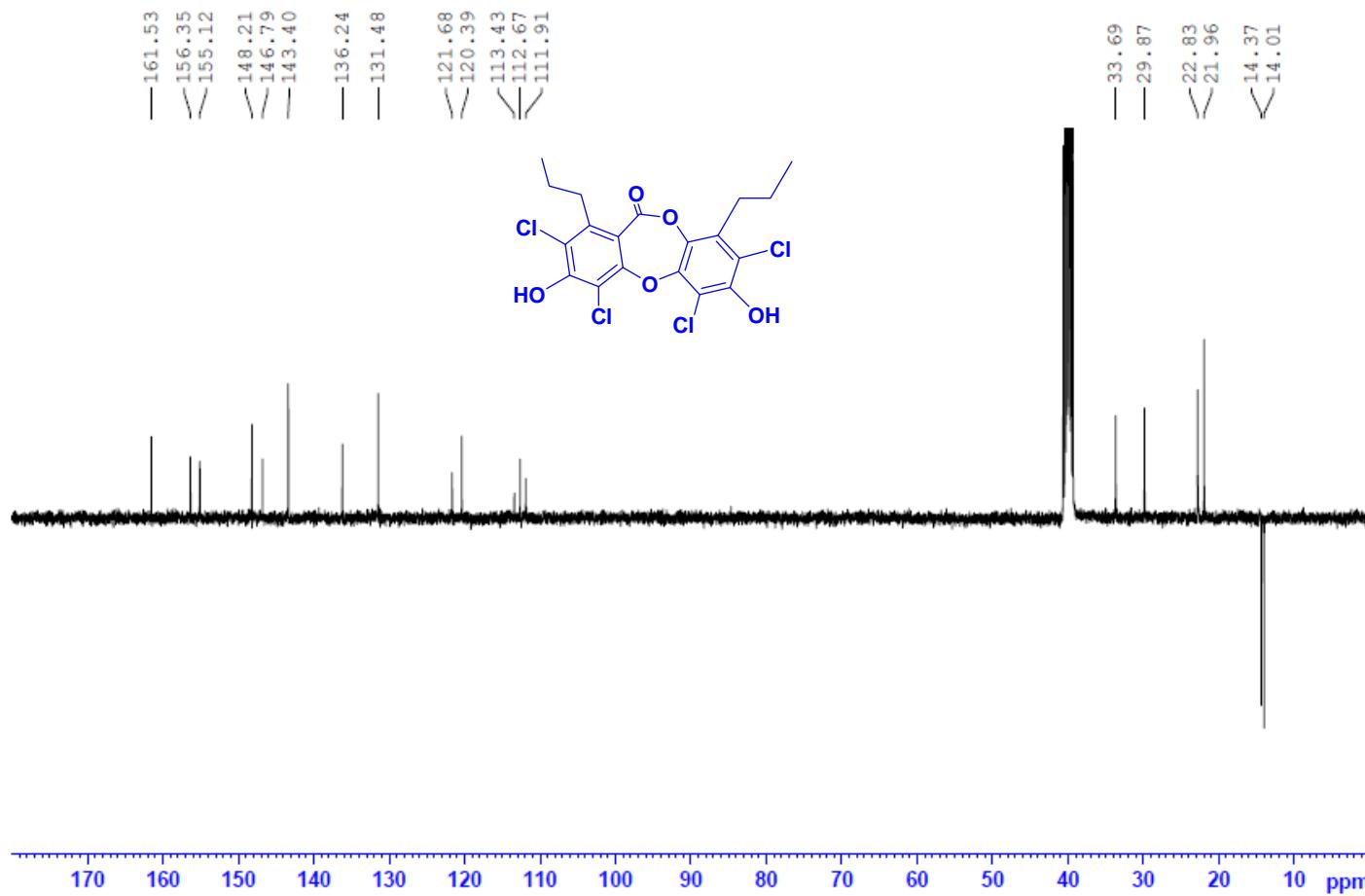


Figure S179. APT spectrum of **15** in $\text{DMSO}-d_6$ (100 MHz)

F19-7-9-5-2 HSQC

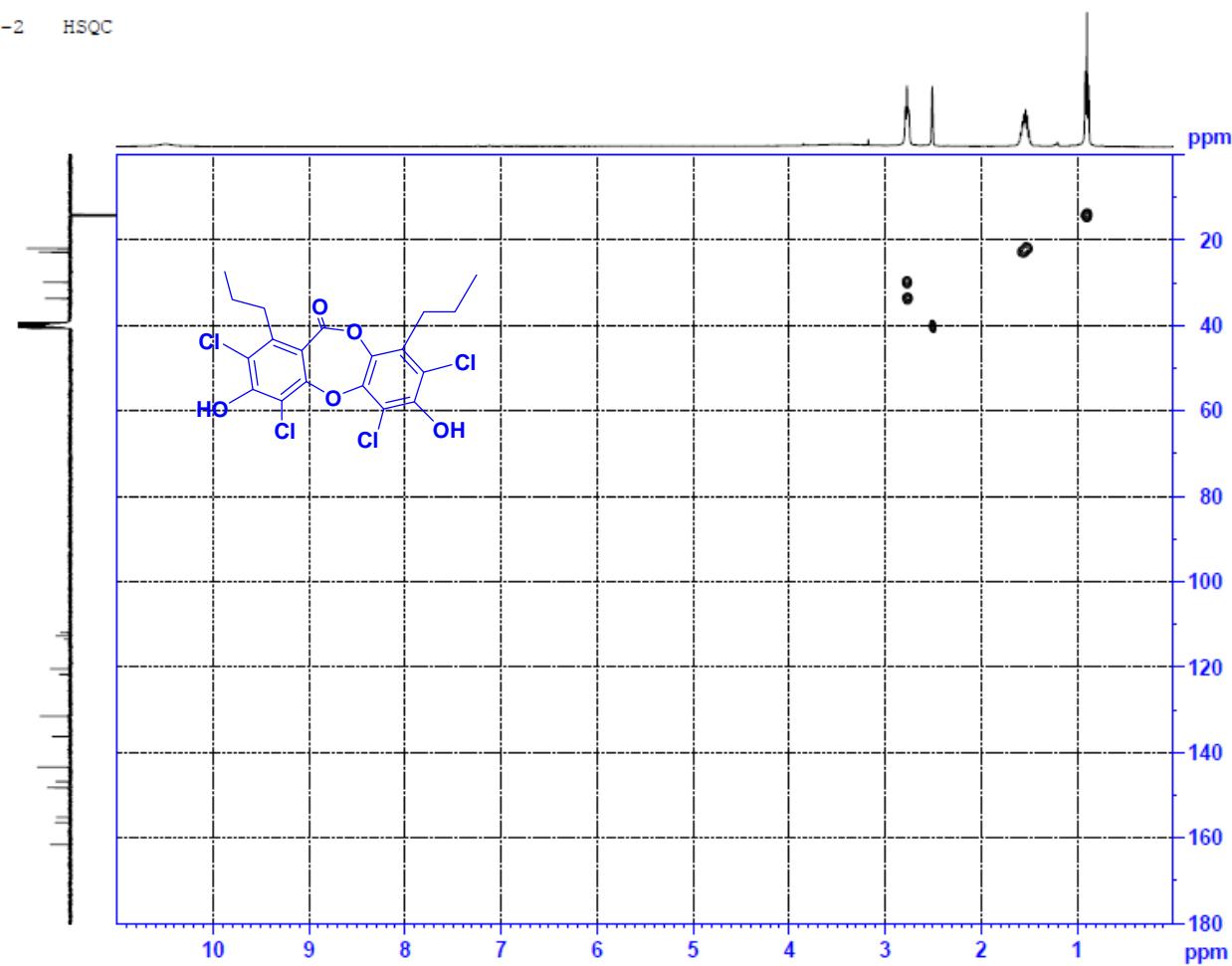


Figure S180. HSQC spectrum of **15** in $\text{DMSO}-d_6$ (400 MHz)

F19-7-9-5-2 COSY

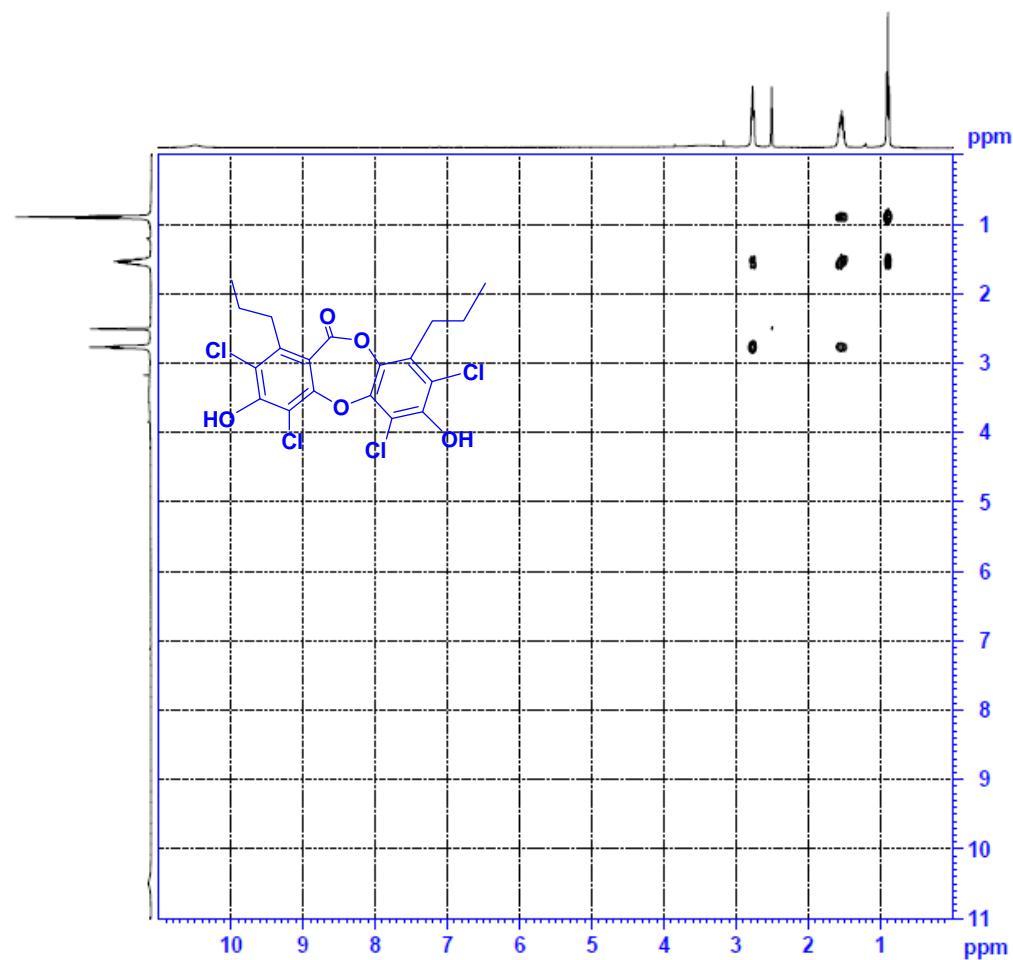


Figure S181. ^1H - ^1H COSY spectrum of **15** in $\text{DMSO}-d_6$ (400 MHz)

F19-7-9-5-2 HMBC

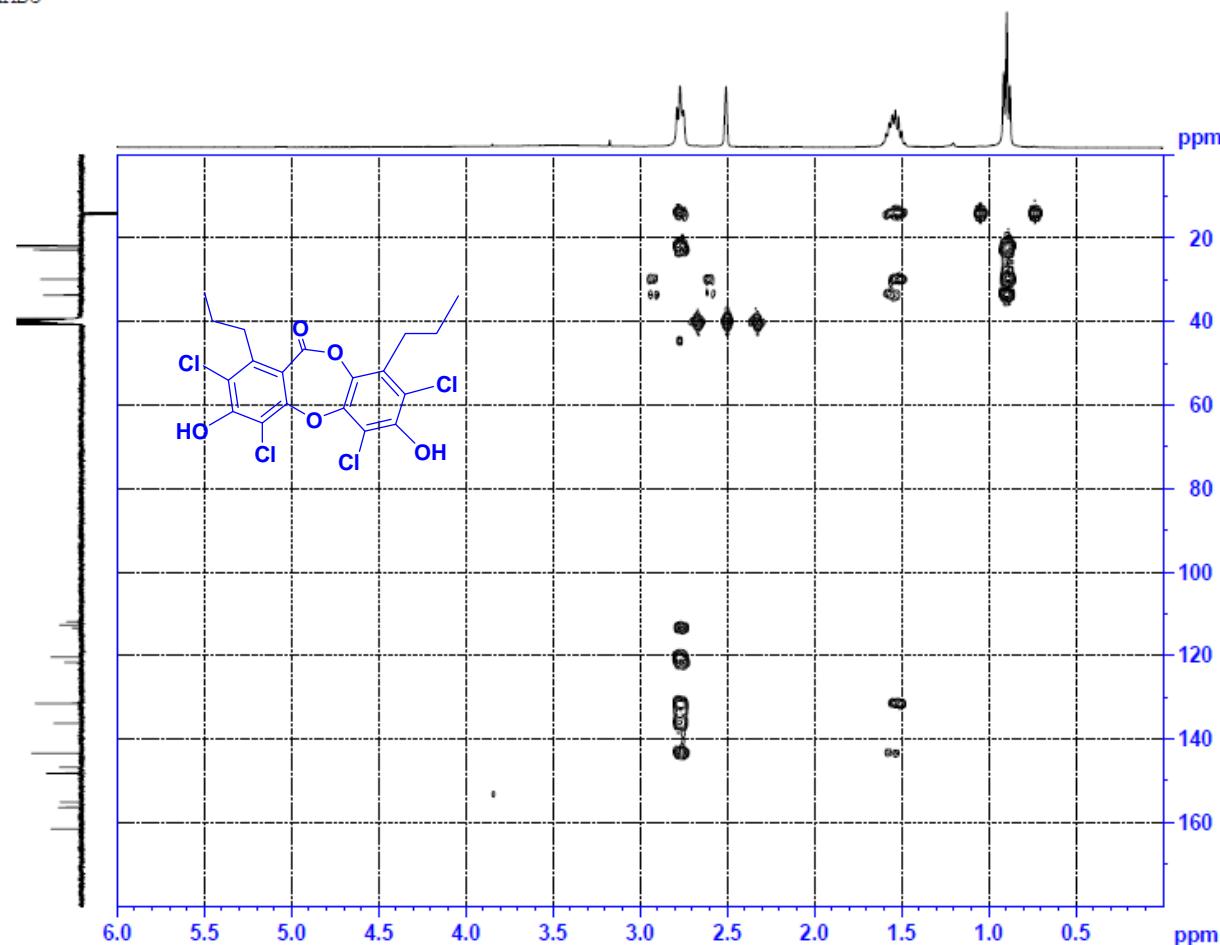
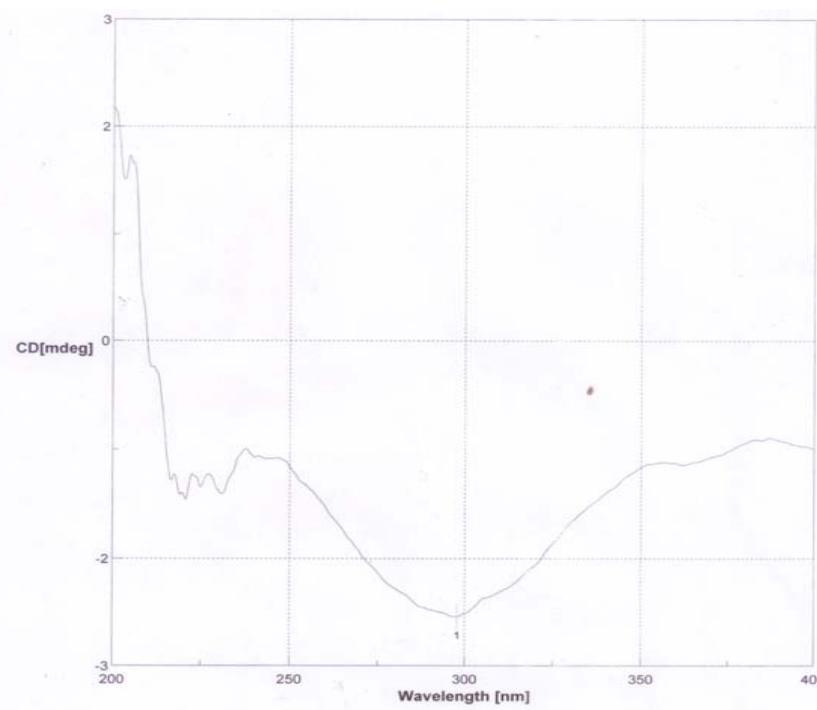


Figure S182. HMBC spectrum of **15** in DMSO-*d*₆ (400 MHz)



Date/Time 2001-1-3 5:20
Operator
File Name F19-7-9-5-2.txt
Sample Name F19-7-9-5-2
Comment

No. nm CD[mdeg]
1 297.8 -2.5388

Figure S183. CD spectrum of **15**