**SUPPLEMENTARY MATERIAL**

**Cytotoxicity and molecular docking analysis of new** **sesquiterpenoids from the leaves of** ***Datura stramonium* L.**

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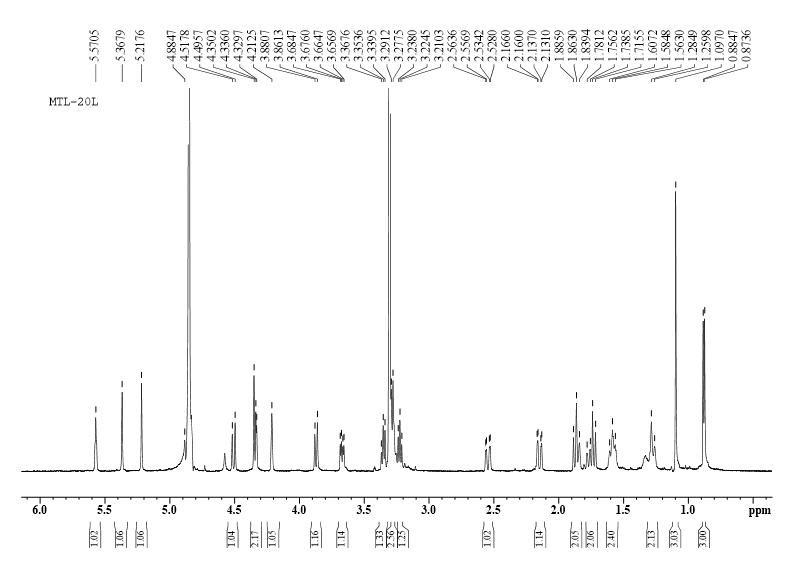
Bing-you Yang, Email: ybywater@163.com, Tel.: +86-451-82193007.

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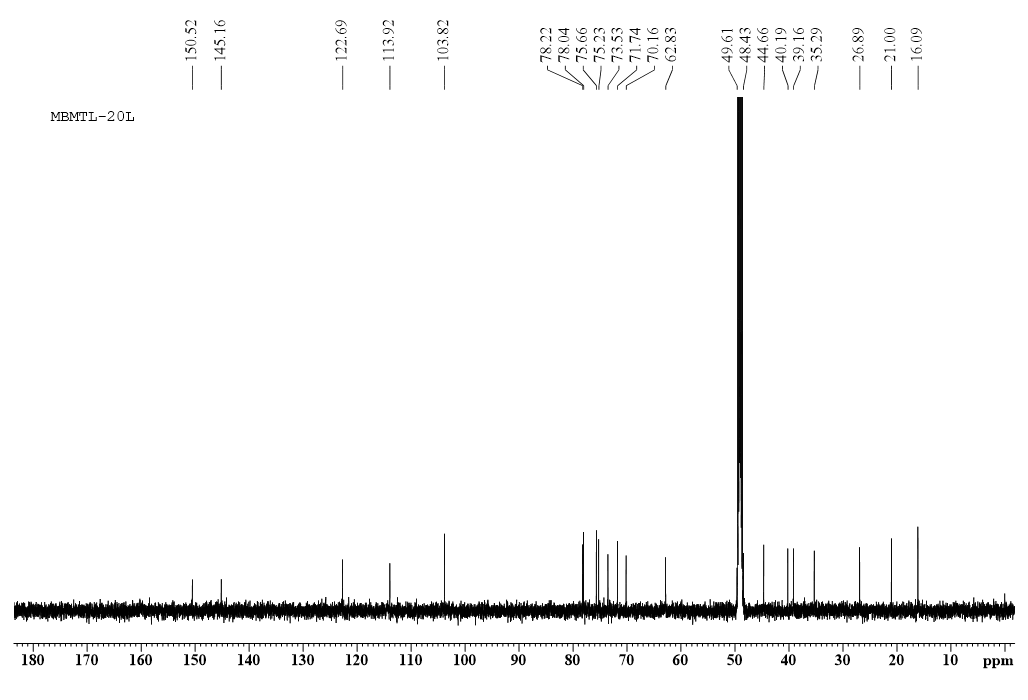
**Figure S1**. HR-ESI-MS spectrum of **1**.



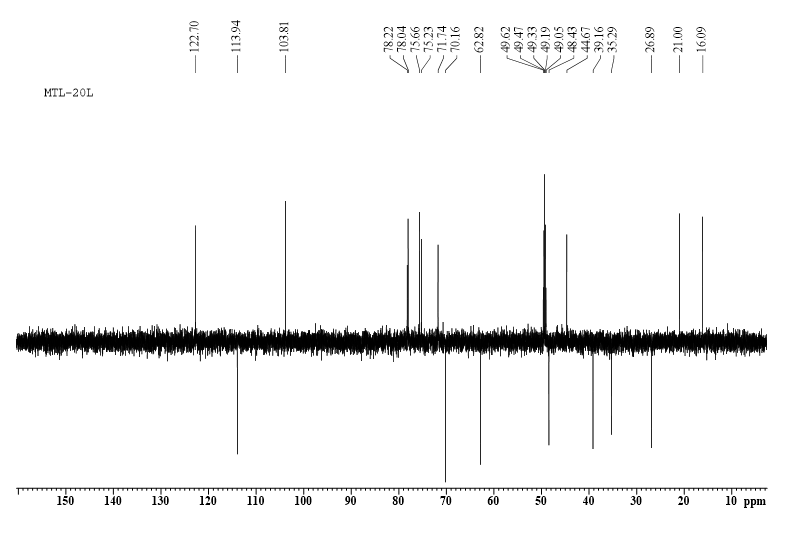
**Figure S2**. 1H NMR spectrum of **1**.



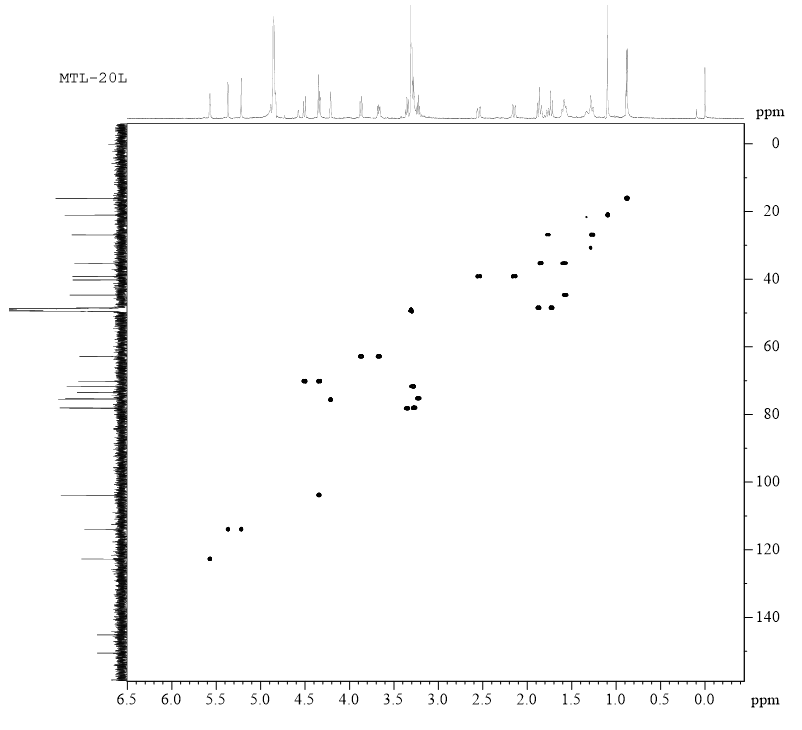
**Figure S3**. 13C NMR spectrum of **1**.



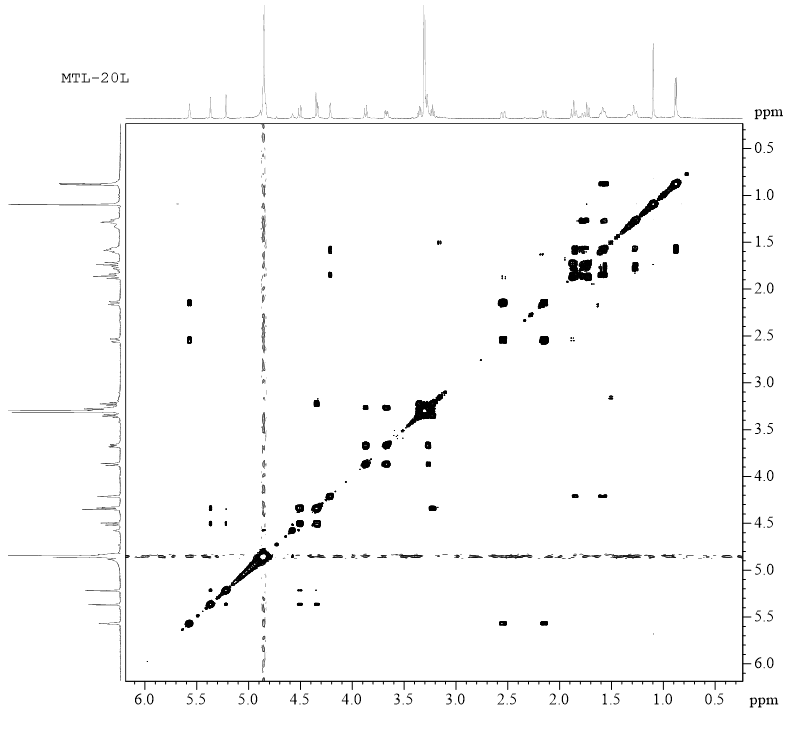
**Figure S4**. DEPT 135 spectrum of **1**.



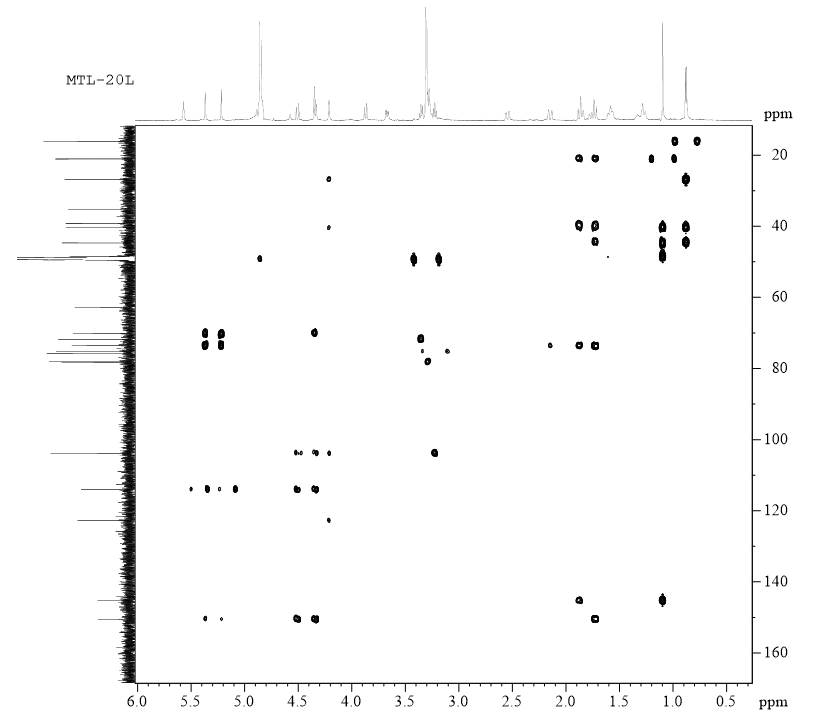
**Figure S5**. HSQC spectrum of **1**.



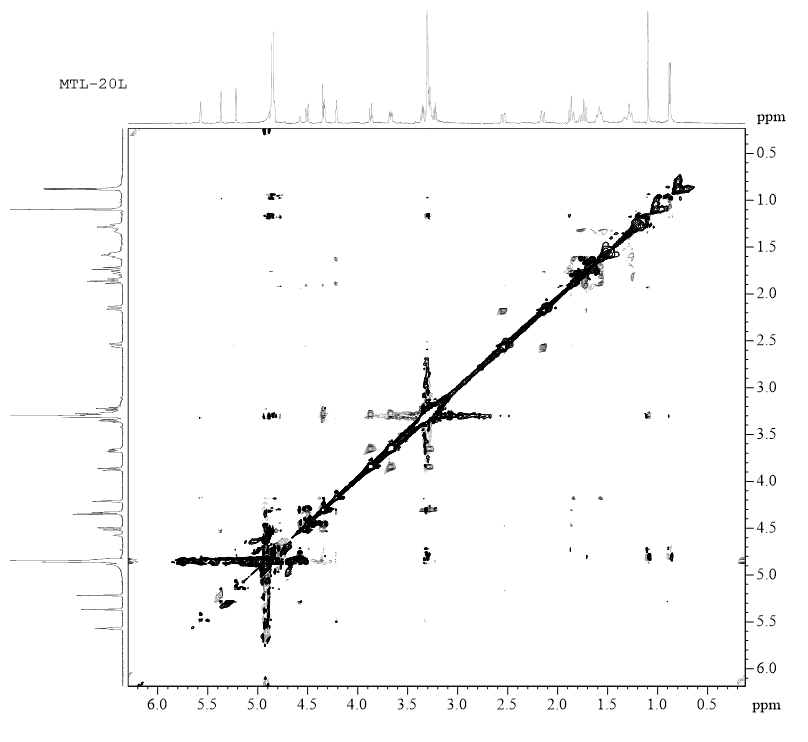
**Figure S6.** 1H-1H COSY spectrum of **1.**



**Figure S7.** HMBC spectrum of **1.**



**Figure S8**. NOESY spectrum of **1**.



**Figure S9**. UV spectrum of **1**.



**Figure S10**.CD spectrum of **1**.



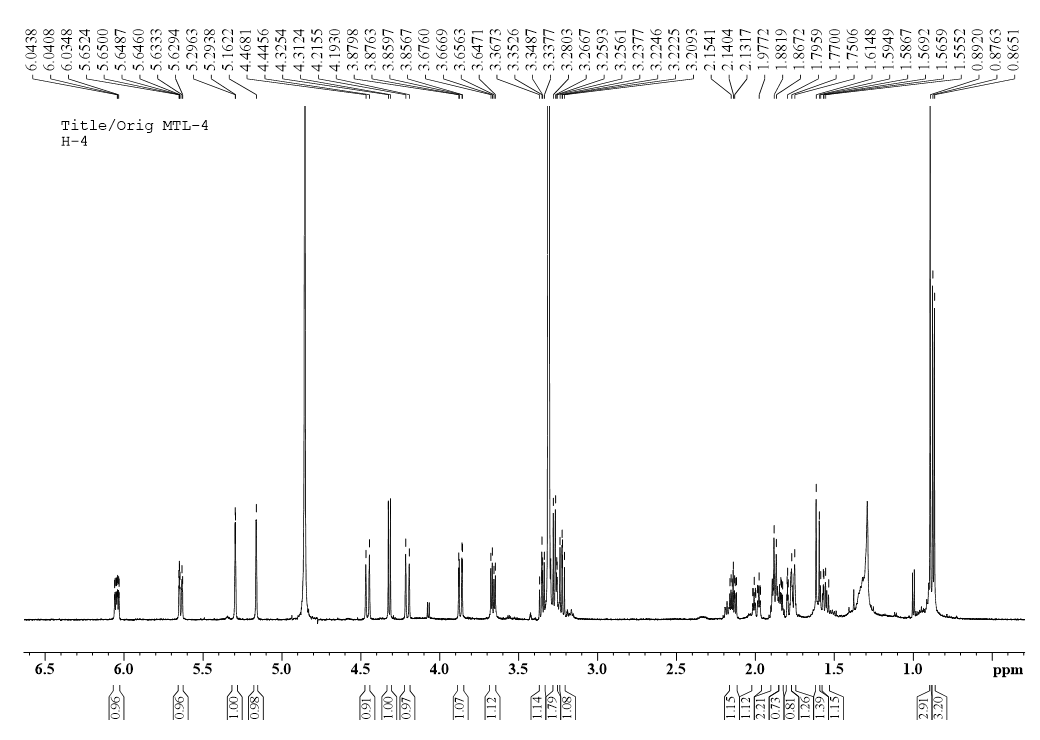
**Figure S11**. IR spectrum of **1**.



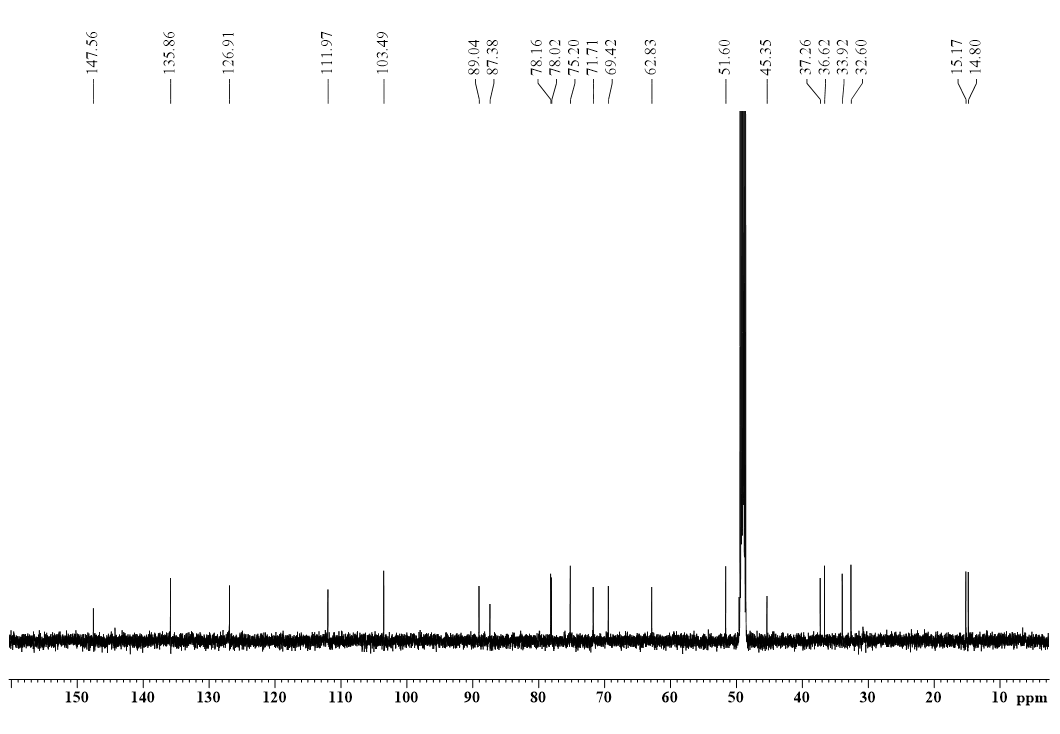
**Figure S12.** HR-ESI-MS spectrum of **2.**

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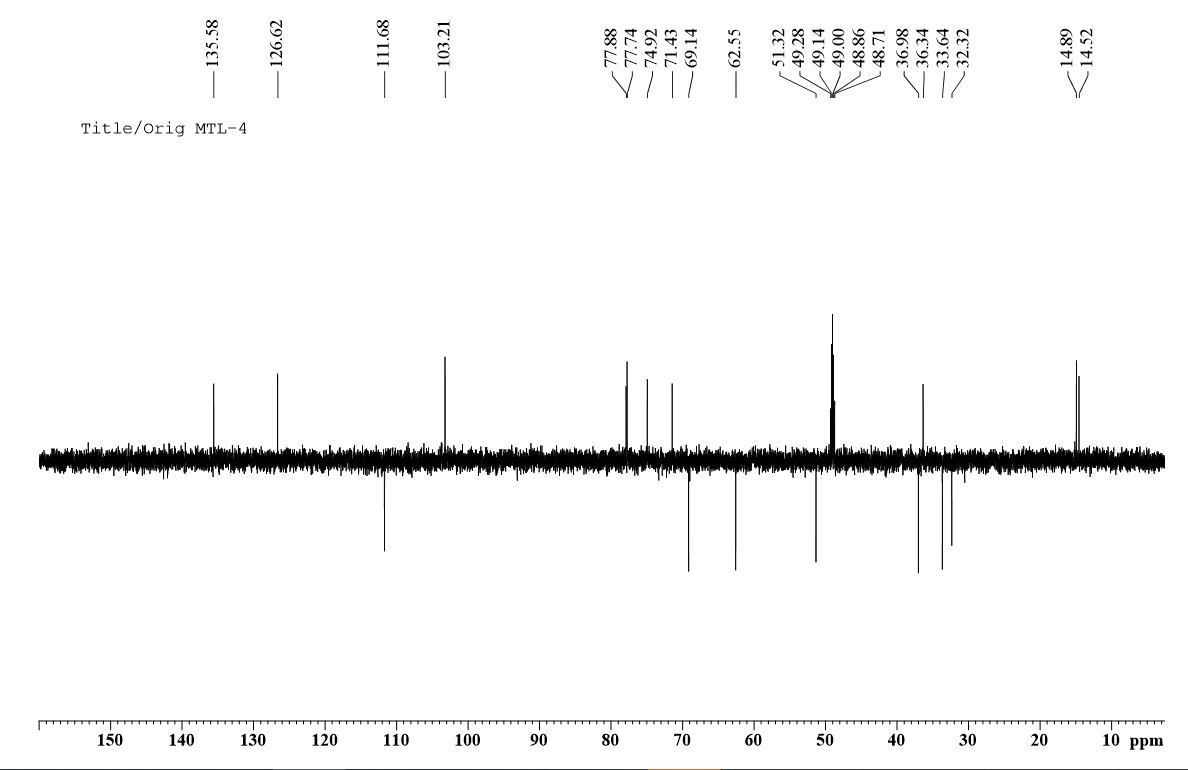
**Figure S13.** 1H NMR spectrum of **2**.



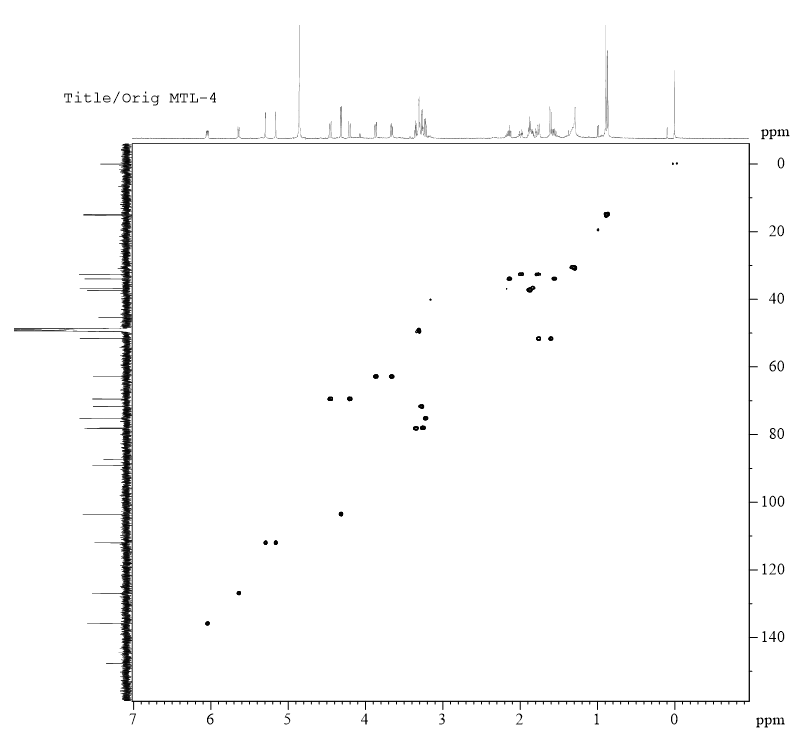
**Figure S14.** 13C NMR spectrum of **2**.



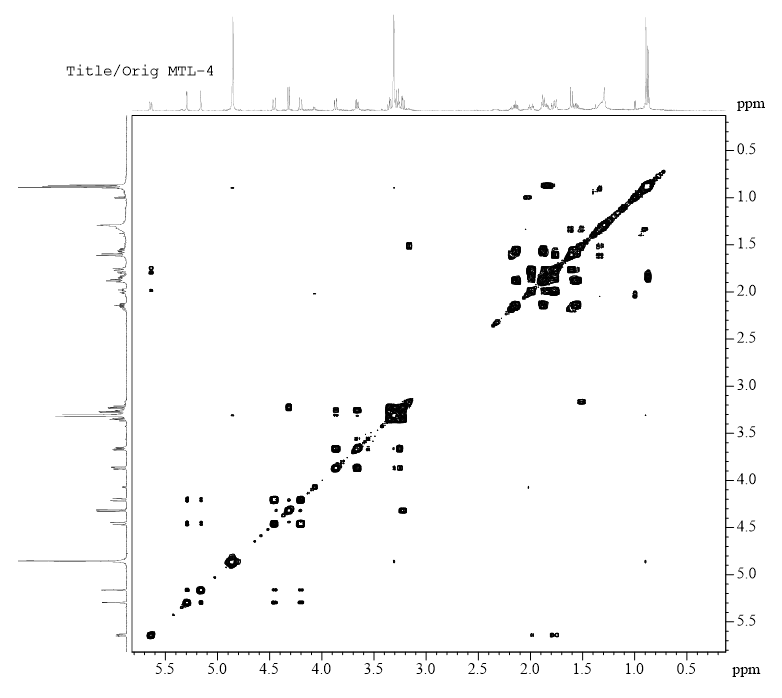
**Figure S15.** DEPT 135 spectrum of **2**.



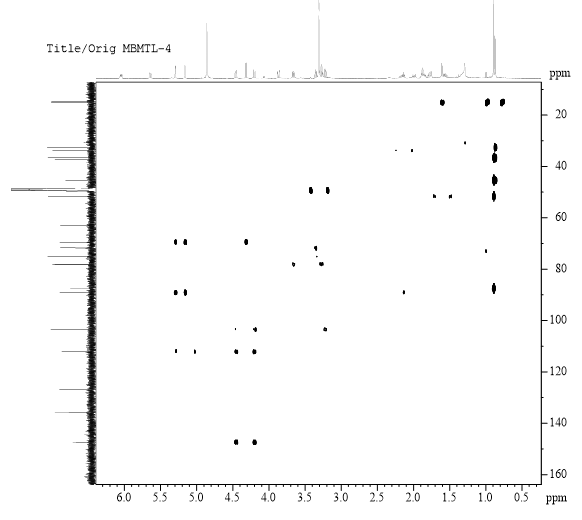
**Figure S16.** HSQC spectrum of **2**.



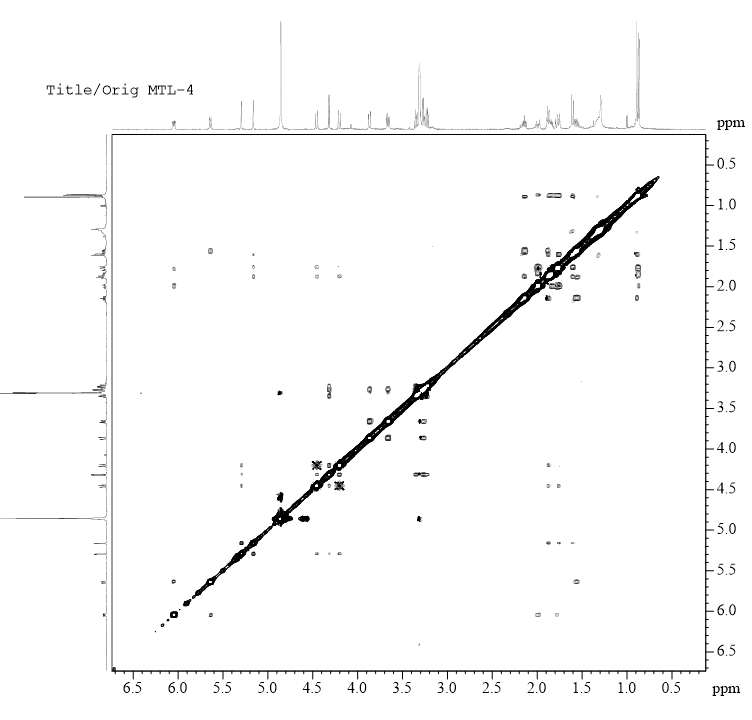
**Figure S17.** 1H-1H COSY spectrum of **2**.



**Figure S18.** HMBC spectrum of **2**.



**Figure S19.** NOESY spectrum of **2**.



**Figure S20**. UV spectrum of **2**.



**Figure S21**. CD spectrum of **2**.



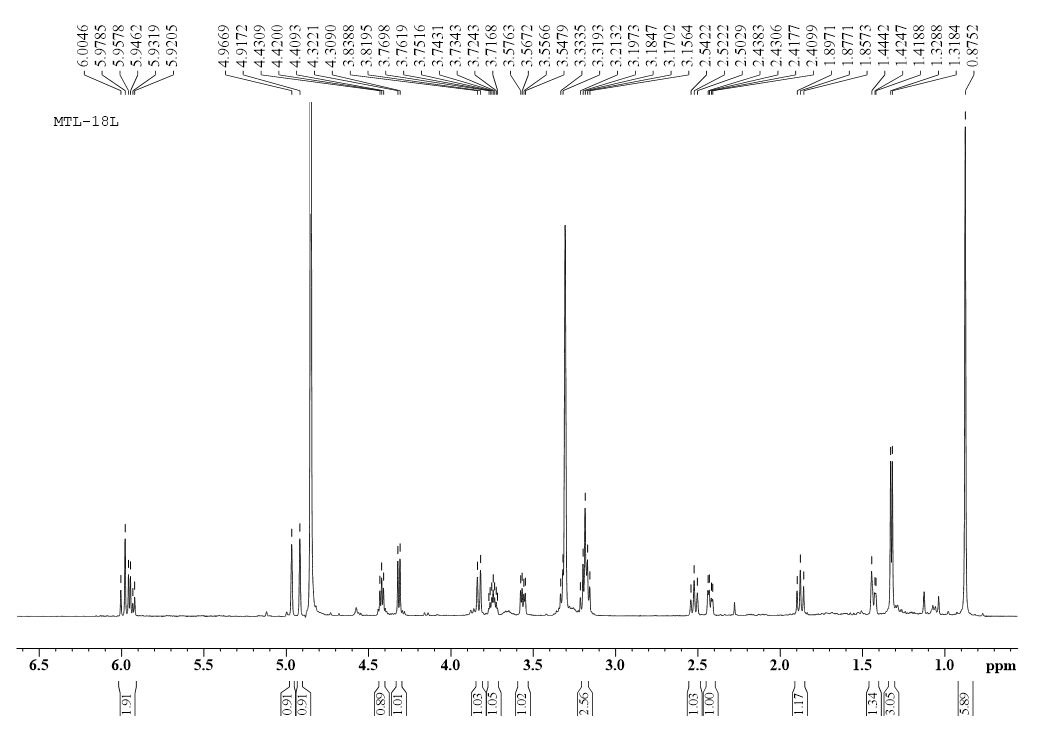
**Figure S22.** IR spectrum of **2**



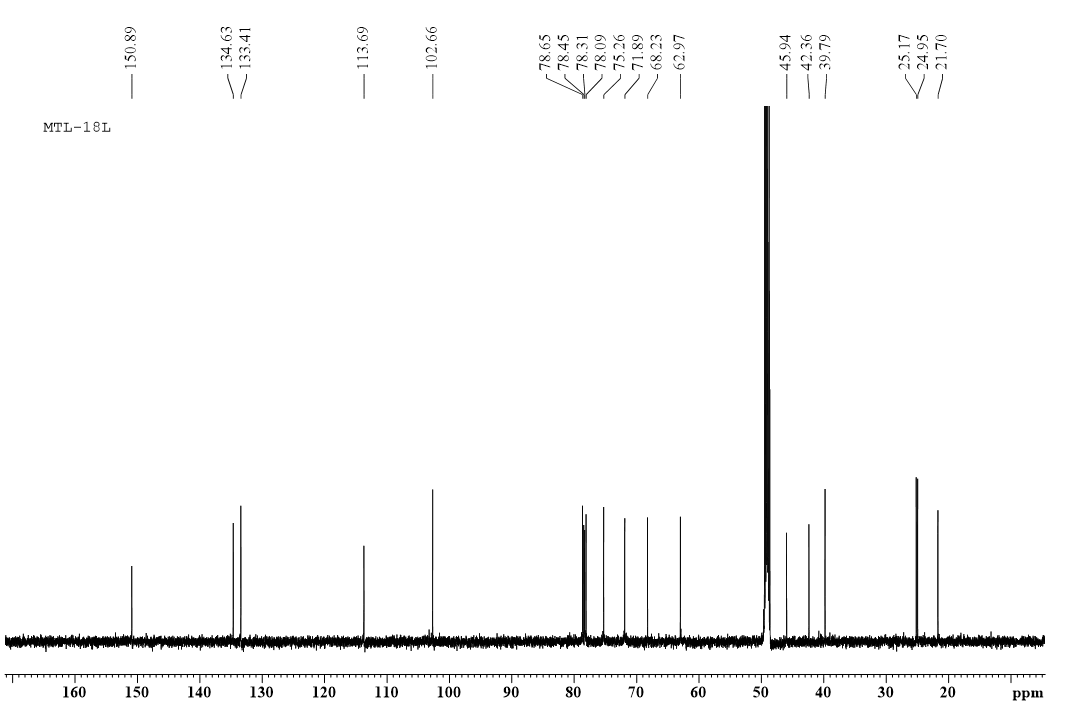
**Figure S23**. HR-ESI-MS spectrum of **3**.

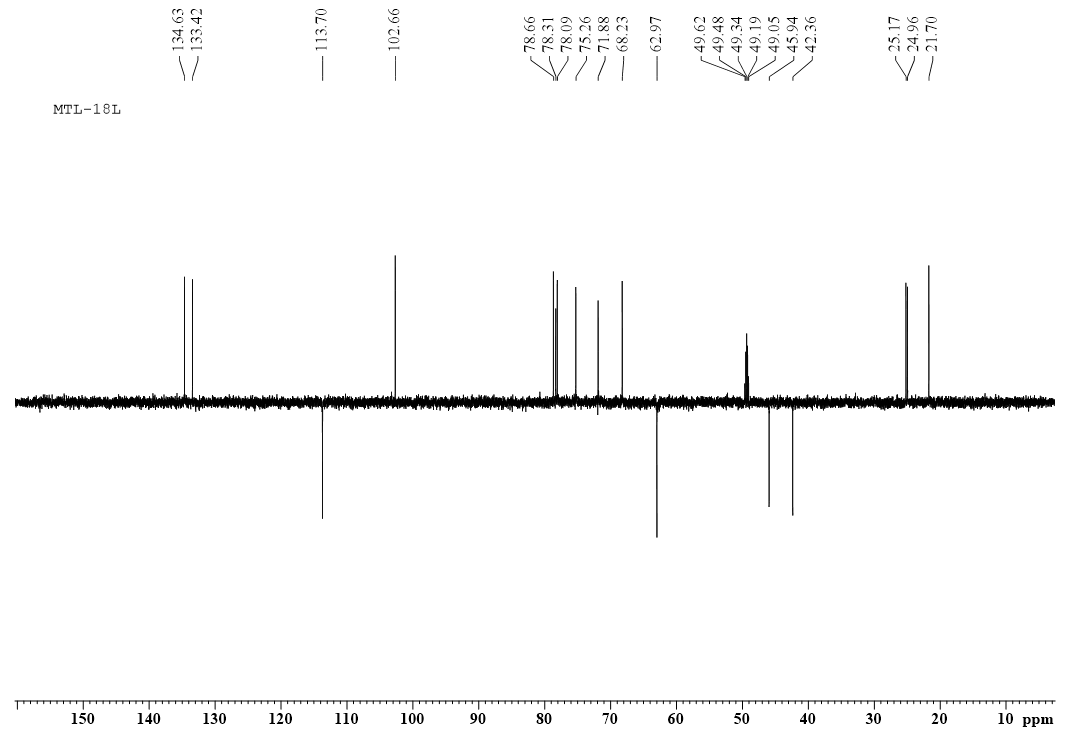


**Figure S24**. 1H NMR spectrum of **3**.

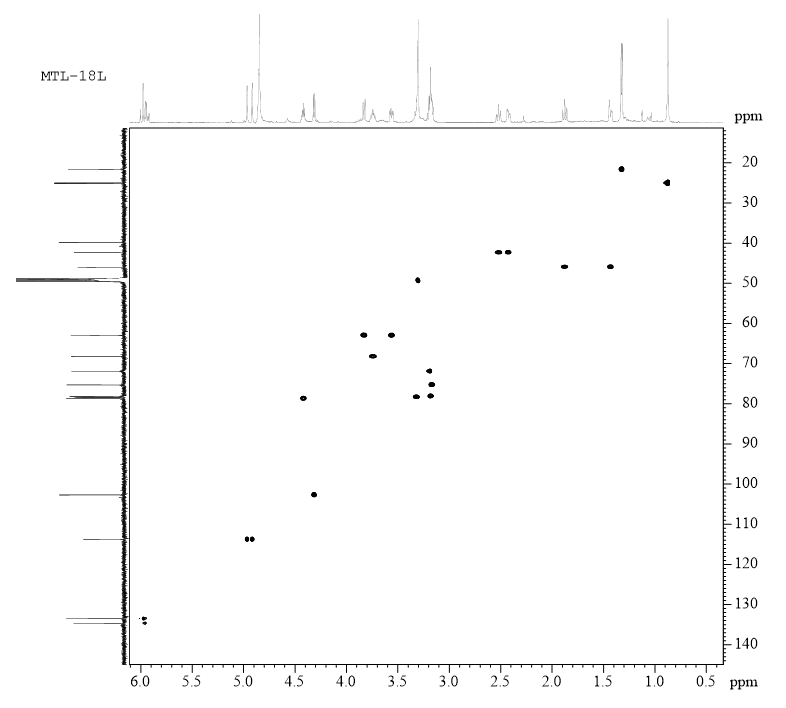


**Figure S25**. 13C NMR spectrum of **3**

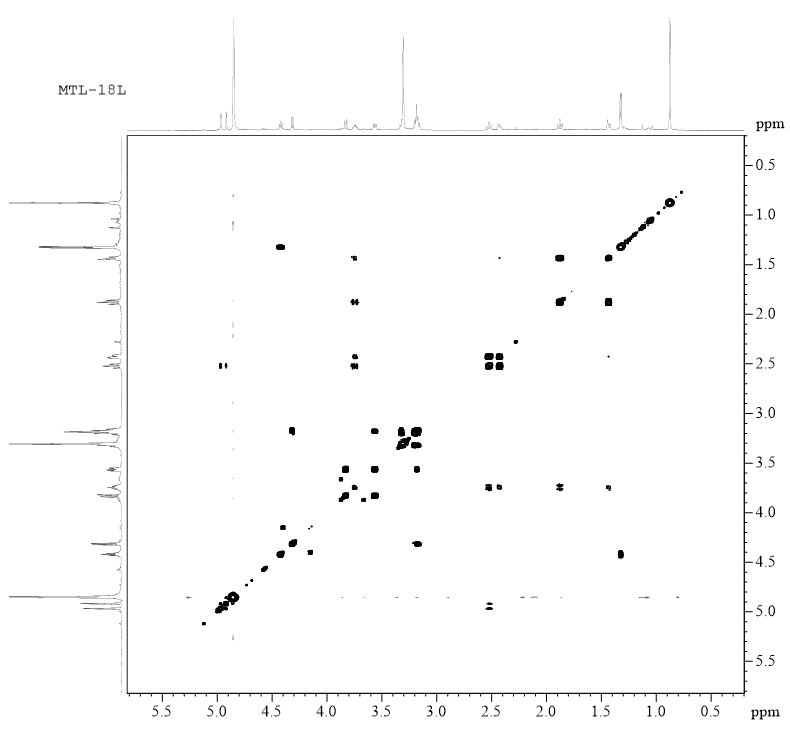
 **Figure S26**. DEPT 135 spectrum of **3**.



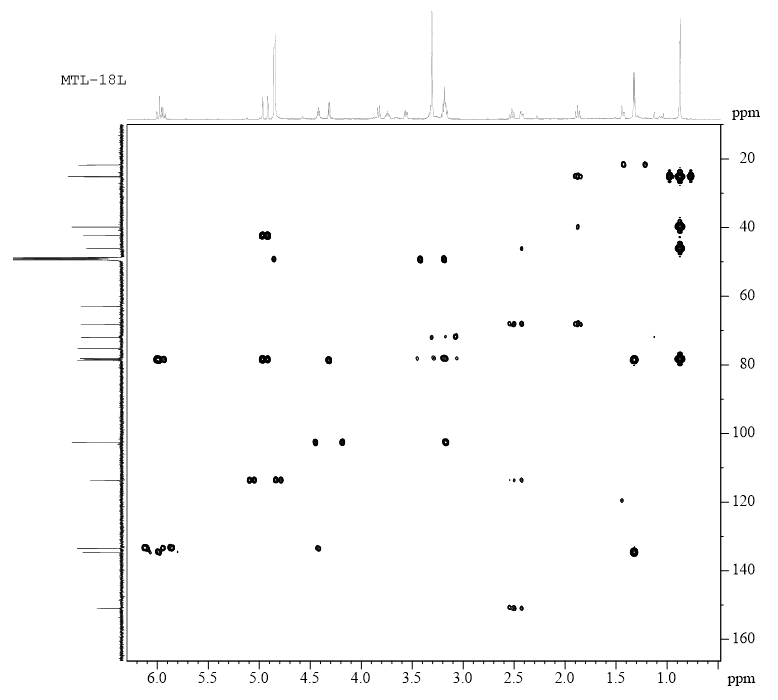
**Figure S27**. HSQC spectrum of **3**.



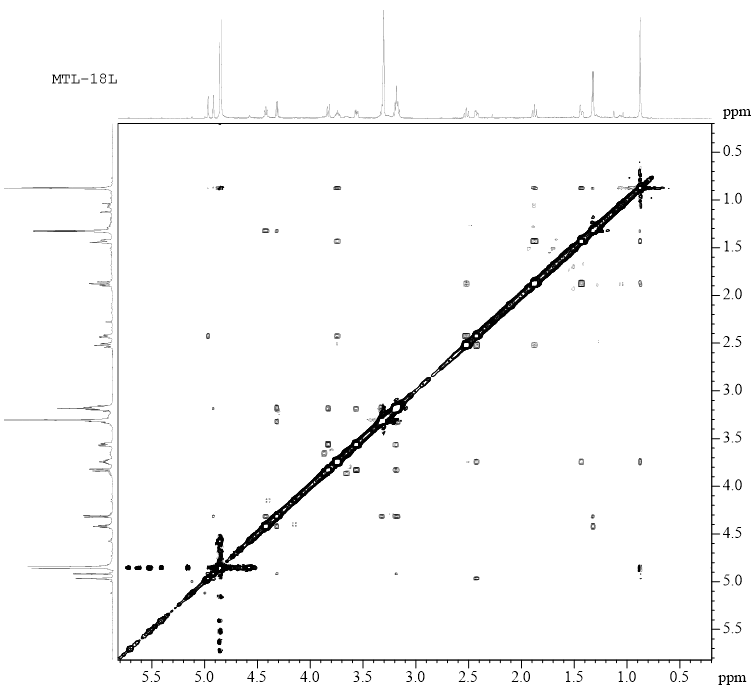
**Figure S28**. 1H-1H COSY spectrum of **3**.



**Figure S29**. HMBC spectrum of **3**.



**Figure S30**. NOESY spectrum of **3**.



**Figure S31**. UV spectrum of **3**.



**Figure S32**. CD spectrum of **3**.



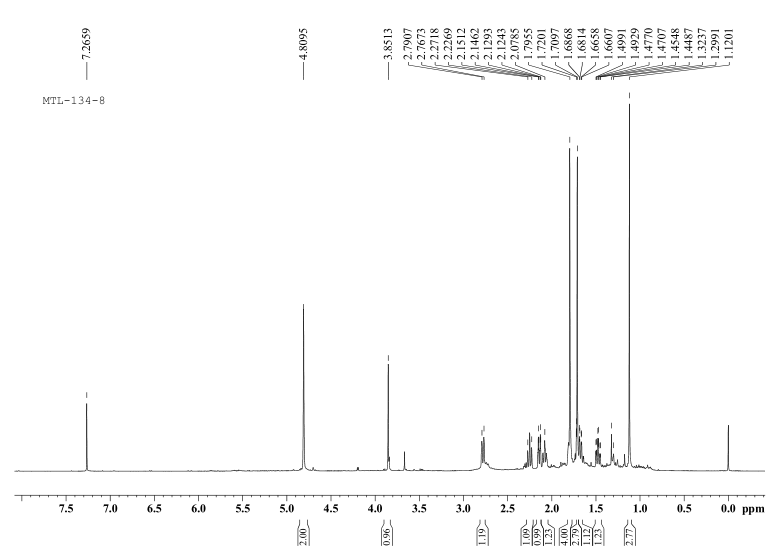
**Figure S33**. IR spectrum of **3**.



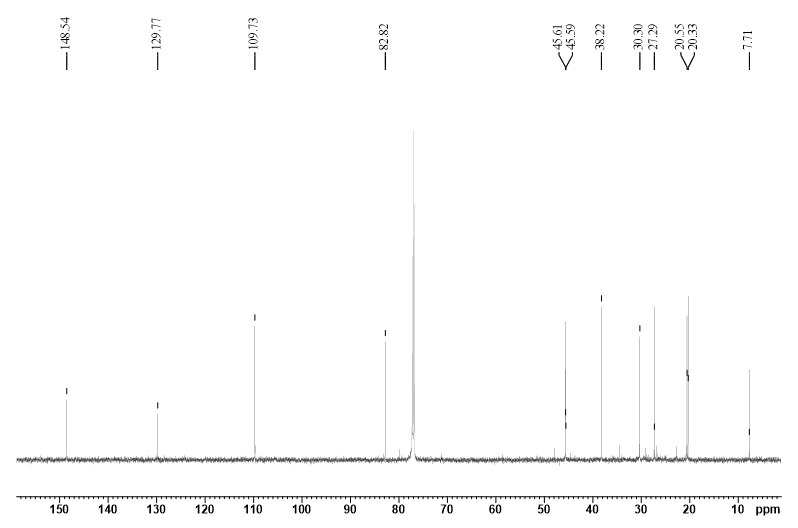
**Figure S34**. HR-ESI-MS spectrum of **4**.

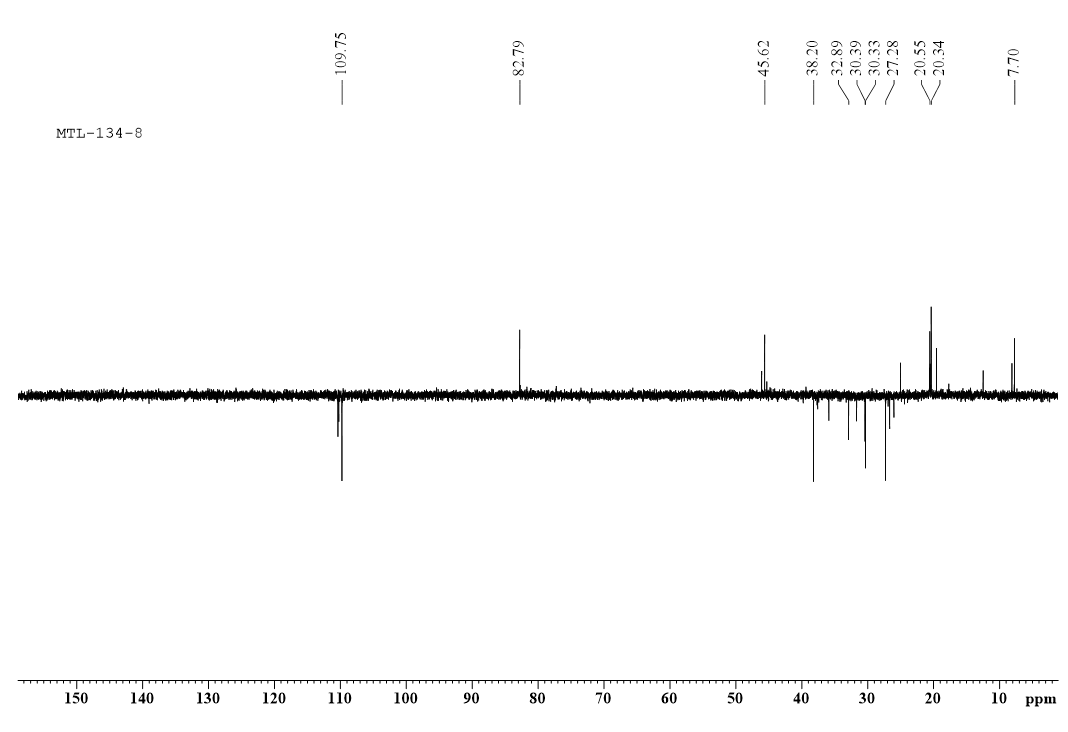


**Figure S35**. 1H NMR spectrum of **4**.

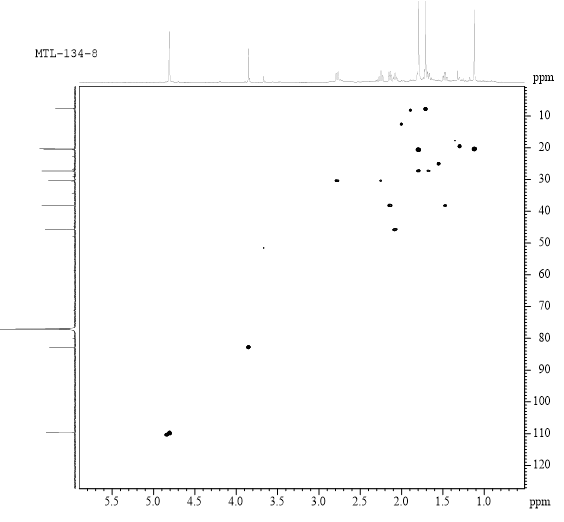


**Figure S36**. 13C NMR spectrum of **4**.

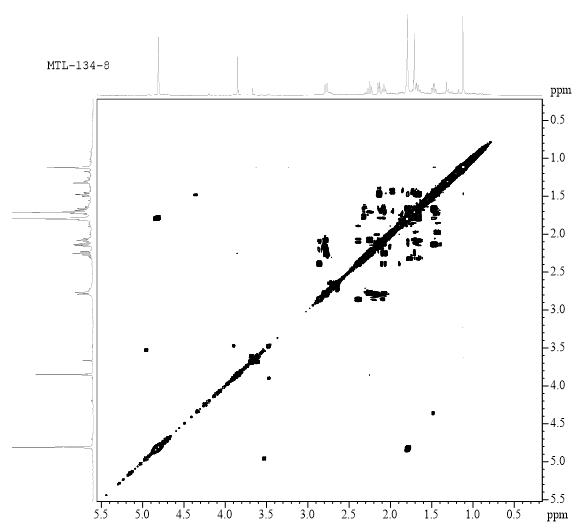
 **Figure S37**. DEPT 135 spectrum of **4**.



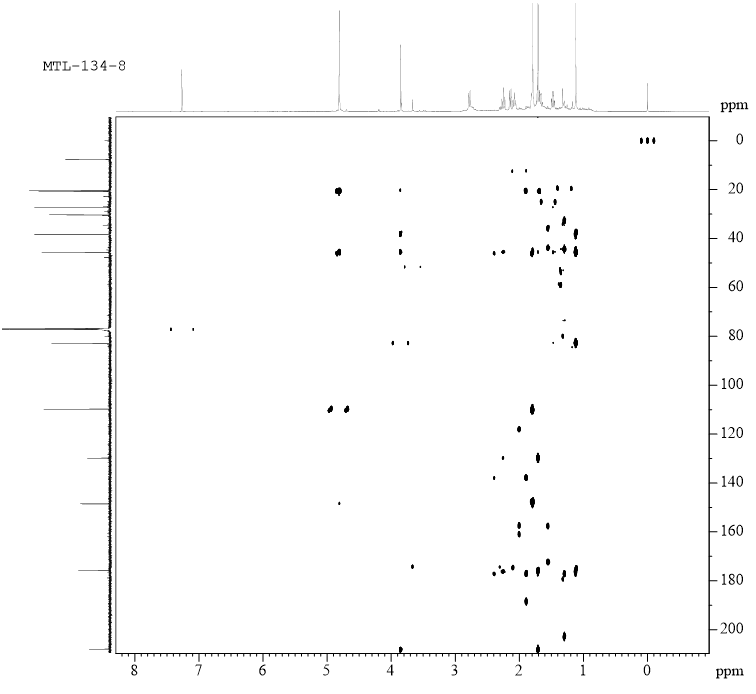
**Figure S38**. HSQC spectrum of **4**.



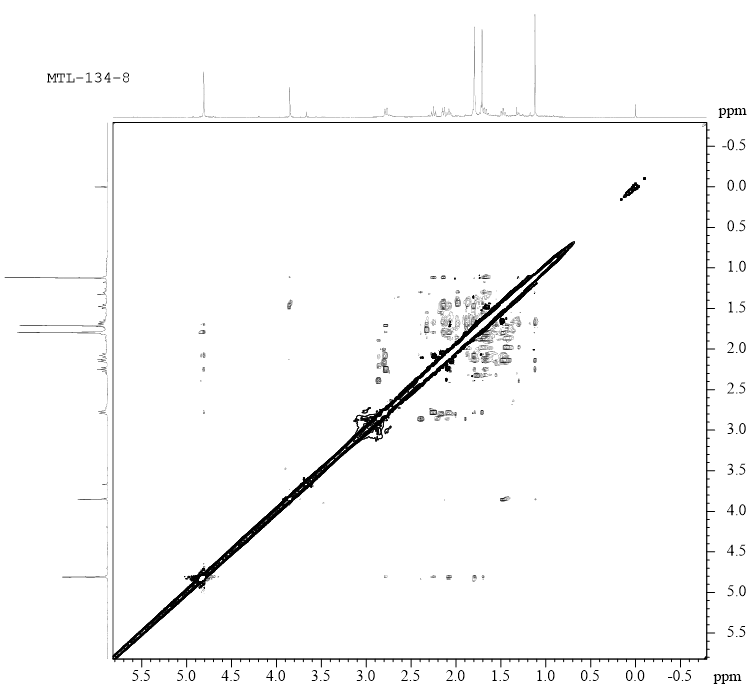
**Figure S39**. 1H-1H COSY spectrum of **4**.



**Figure S40**. HMBC spectrum of **4**.



**Figure S41**. NOESY spectrum of **4**.



**Figure S42**. UV spectrum of **4**.



**Figure S43**. CD spectrum of **4**.

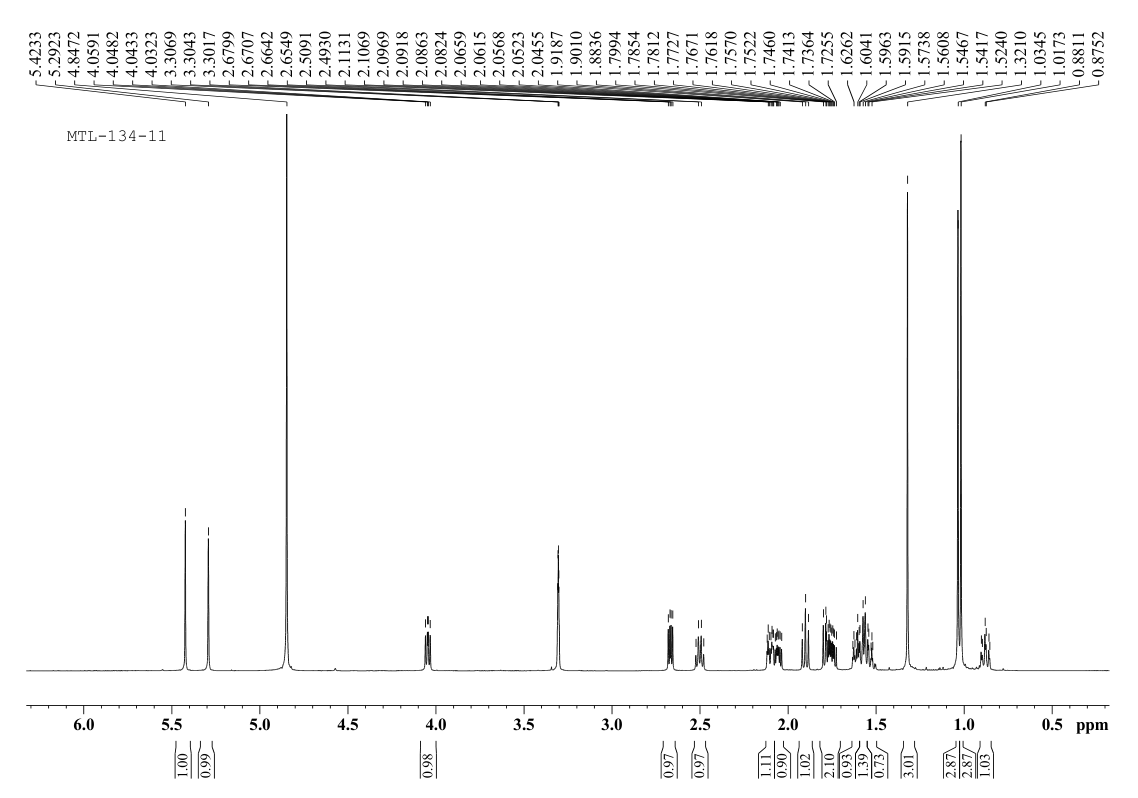


**Figure S44**. IR spectrum of **4**.

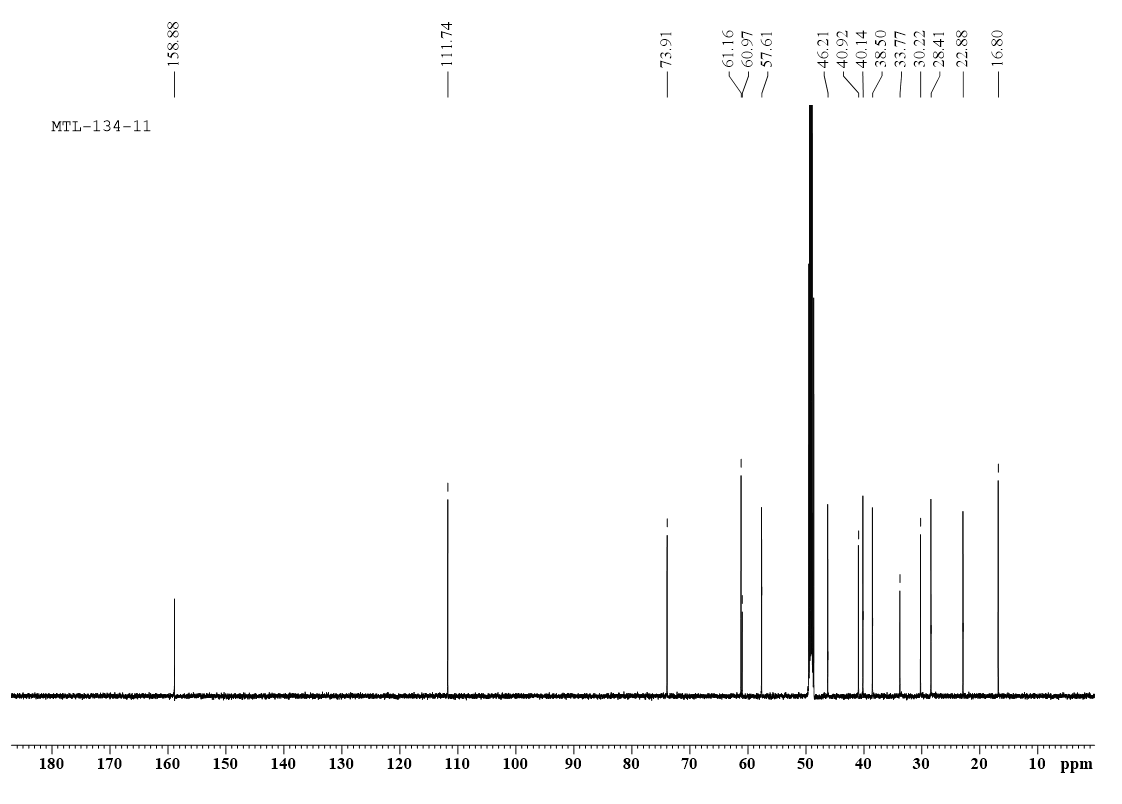


**Figure S45**. HR-ESI-MS spectrum of **5**.

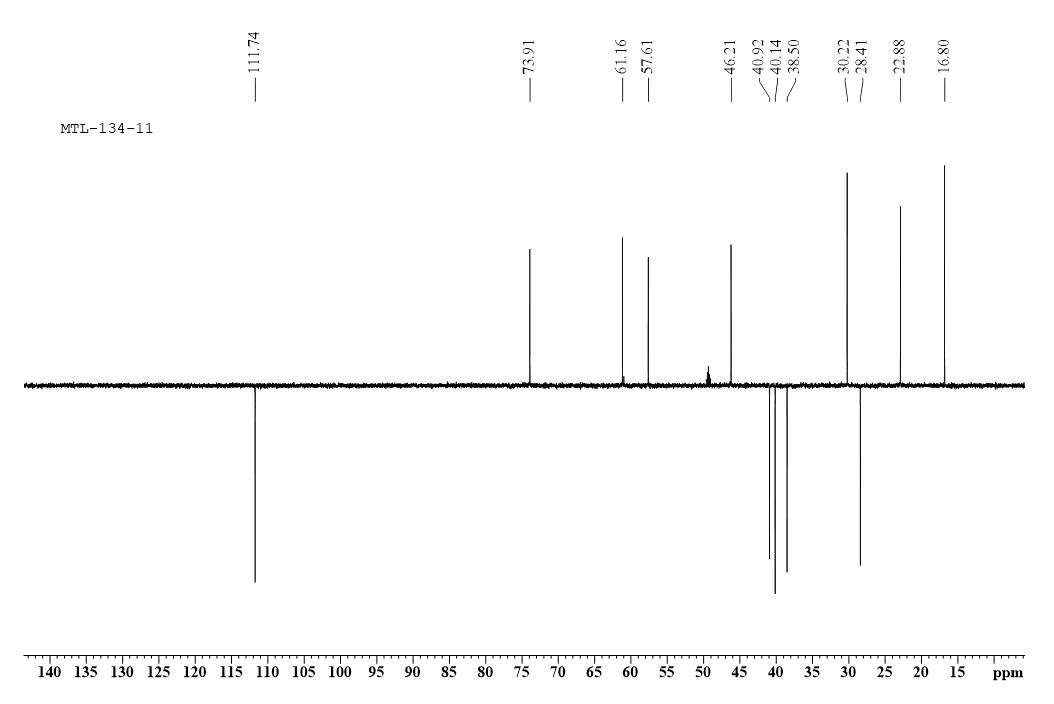
**Figure S46**. 1H NMR spectrum of **5**.



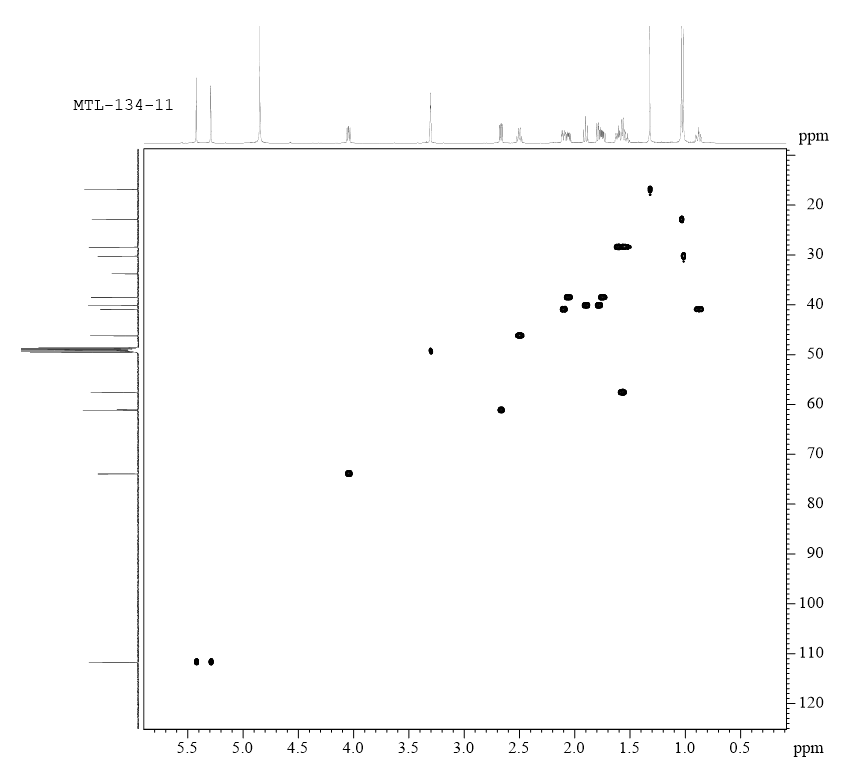
**Figure S47**. 13C NMR spectrum of **5.**



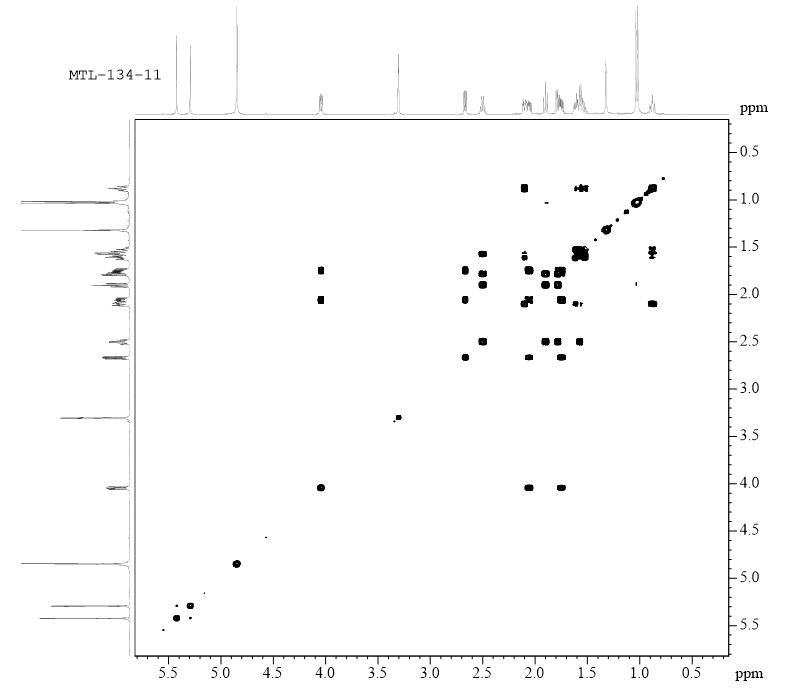
**Figure S48**. DEPT 135 spectrum of **5**.



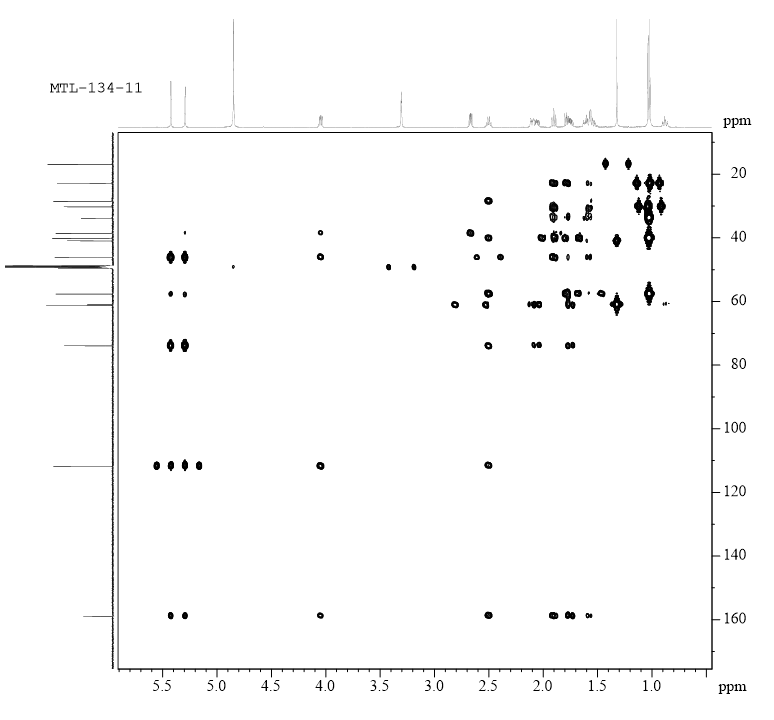
**Figure S49**. HSQC spectrum of **5**.



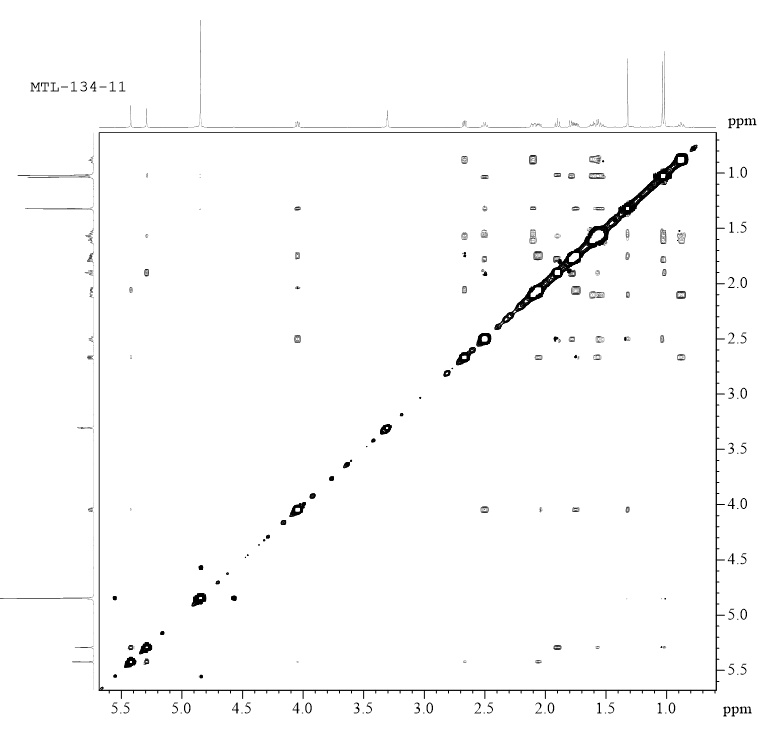
**Figure S50**. 1H-1H COSY spectrum of **5**.



**Figure S51**. HMBC spectrum of **5**.



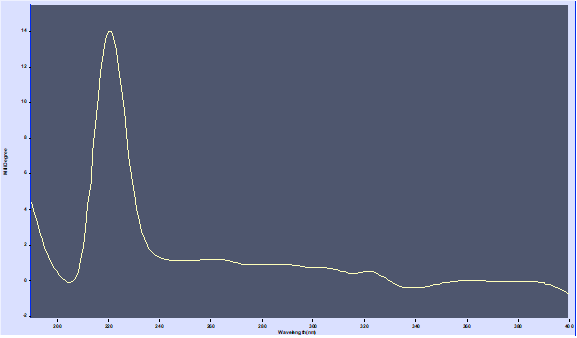
**Figure S52**. NOESY spectrum of **5**.



**Figure S53**. UV spectrum of **5**.



**Figure S54**. CD spectrum of **5**.



**Figure S55**. IR spectrum of **5**.



**Figure S56.** GC-MS chromatogram of the sugars of compounds **1-3.**

**Fig.S56-1** the GC chromatogram of hydrolyzed *D*-glucose



**Fig.S56-2** the GC chromatogram of compound **1** after hydrolysis



**Fig.S56-3** the GC chromatogram of compound **2** after hydrolysis



**Fig.S56-4** the GC chromatogram of compound **3** after hydrolysis



**Table S57** 13C-NMR data of compounds **6-8** (MeOD, *δ* in ppm)

|  |  |  |  |
| --- | --- | --- | --- |
| **NO.** | **6** | **7** | **8** |
| **1** | 49.0 | 204.6 | 50.7 |
| **2** | 26.5 | 125.6 | 27.5 |
| **3** | 28.7 | 153.5 | 39.8 |
| **4** | 62.8 | 70.7 | 59.1 |
| **5** | 65.0 | 52.2 | 57.5 |
| **6** | 30.2 | 26.4 | 34.6 |
| **7** | 33.5 | 45.0 | 69.3 |
| **8** | 151.4 | 26.3 | 61.1 |
| **9** | 49.9 | 34.8 | 42.9 |
| **10** | 39.9 | 44.7 | 33.8 |
| **11** | 34.5 | 149.7 | 32.9 |
| **12** | 21.4 | 108.8 | 16.3 |
| **13** | 29.9 | 21.1 | 45.0 |
| **14** | 62.1 | 22.3 | 30.0 |
| **15** | 113.3 | 18.1 | 22.8 |