



## Supporting Information

for

### **Sesquiterpenes from the soil-derived fungus *Trichoderma citrinoviride* PSU-SPSF346**

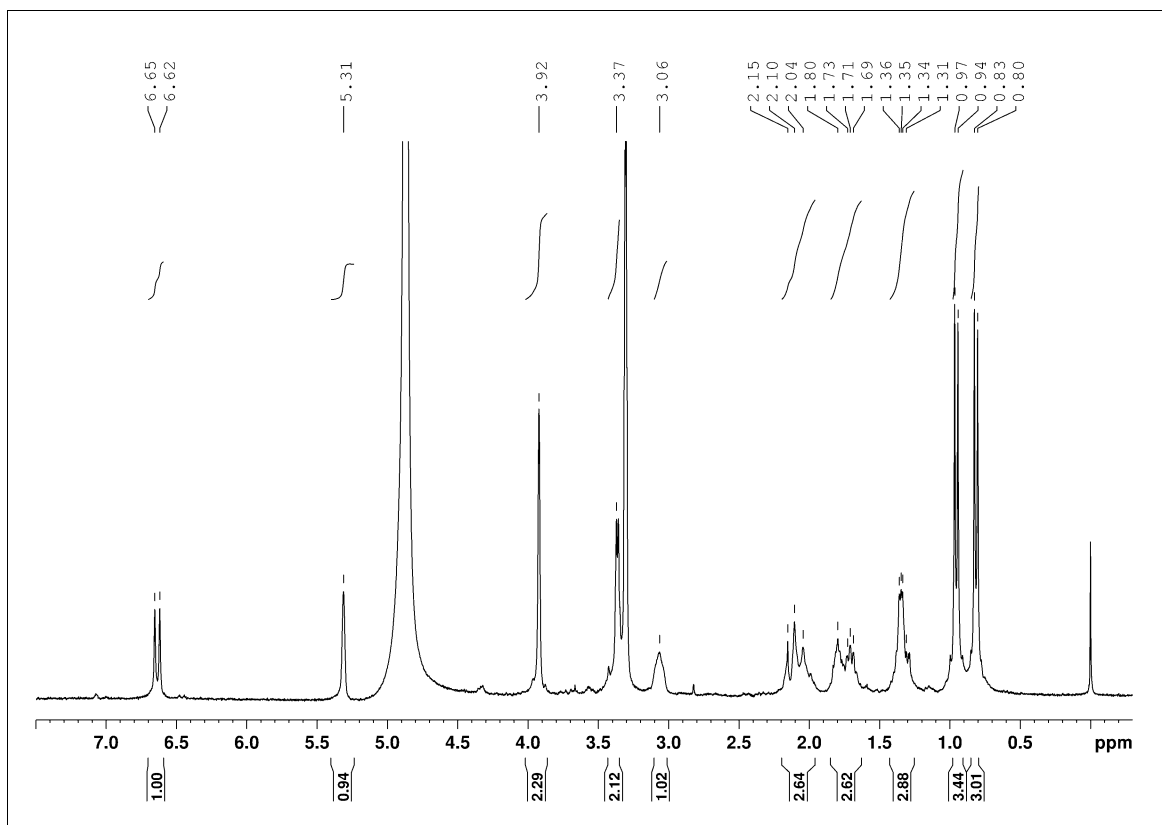
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*Beilstein J. Org. Chem.* **2022**, *18*, 479–485. [doi:10.3762/bjoc.18.50](https://doi.org/10.3762/bjoc.18.50)

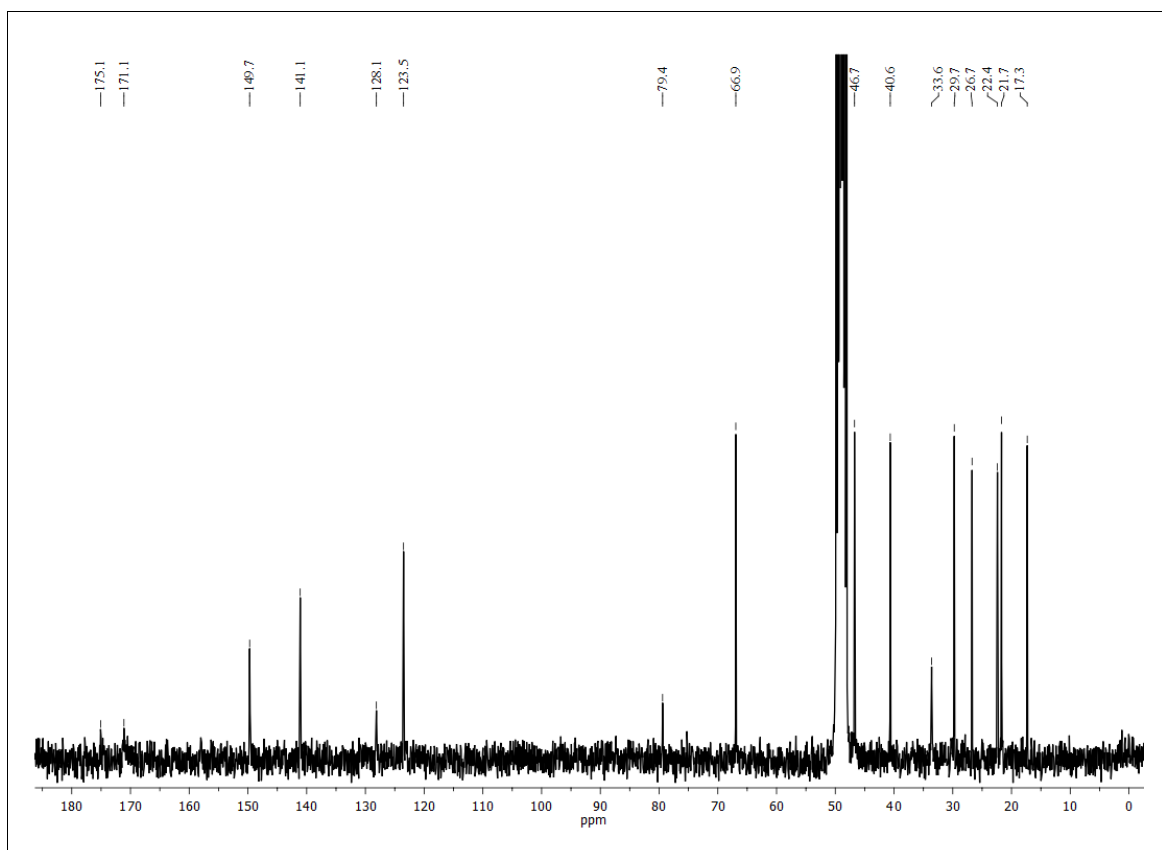
### **HRESIMS profiles for compounds 1 and 2 and copies of NMR spectra for compounds 1–7**

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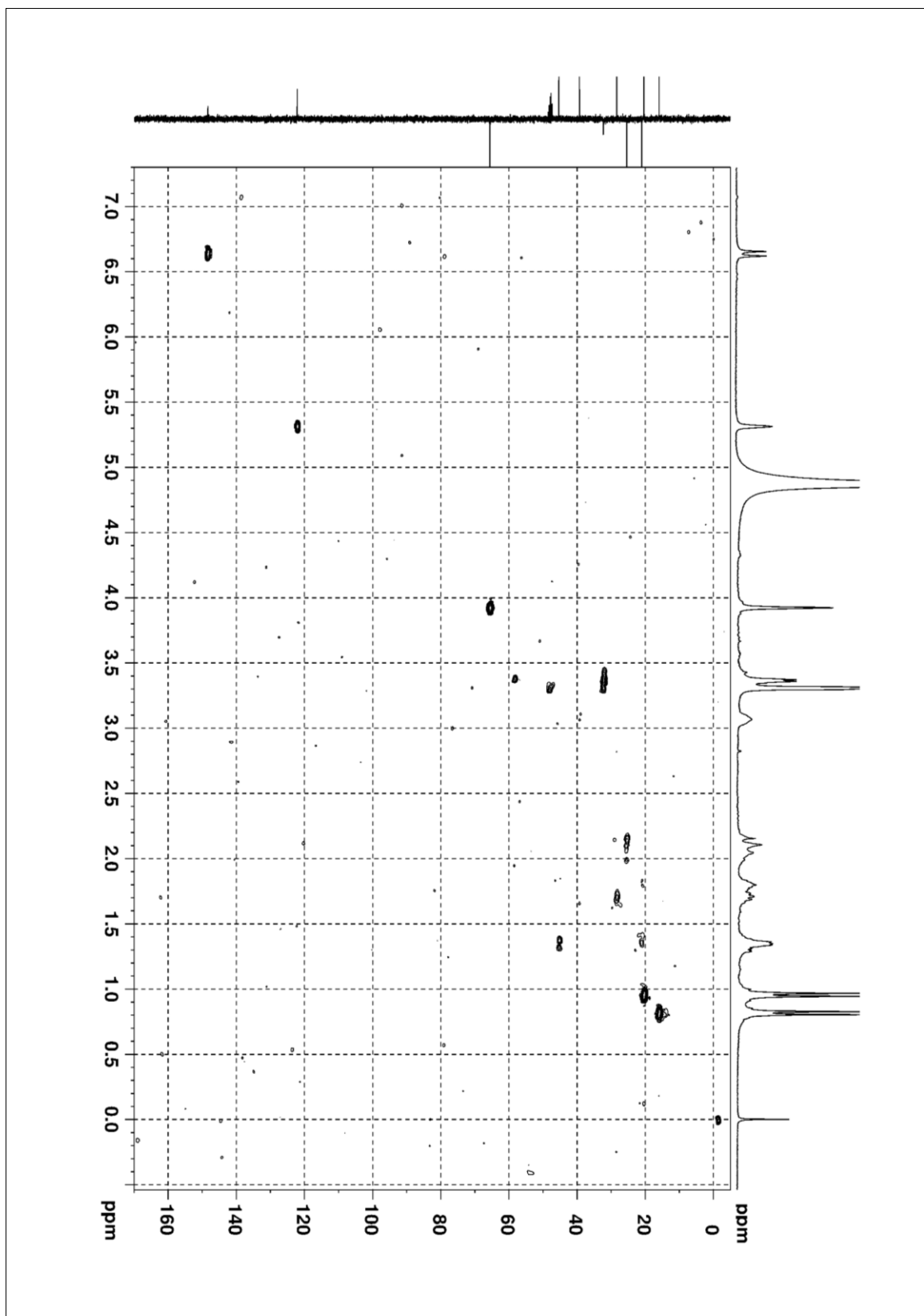
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**Figure S1.**  $^1\text{H}$  NMR spectrum (300 MHz,  $\text{CD}_3\text{OD}$ ) of compound **1**



**Figure S2.**  $^{13}\text{C}$  NMR spectrum (75 MHz,  $\text{CD}_3\text{OD}$ ) of compound **1**



**Figure S3.** HMQC spectrum (CD<sub>3</sub>OD) of compound 1

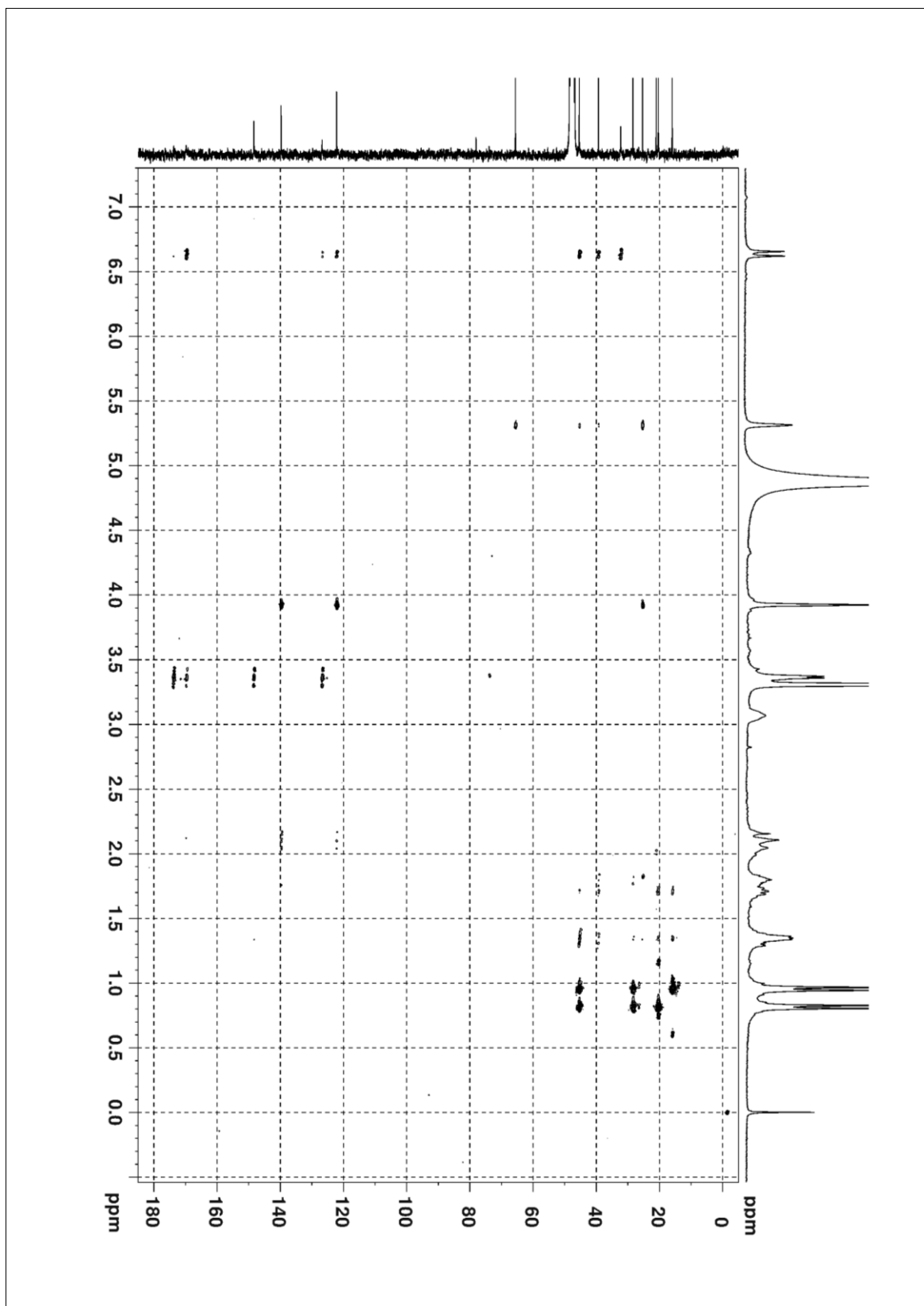


Figure S4. HMBC spectrum (CD<sub>3</sub>OD) of compound 1

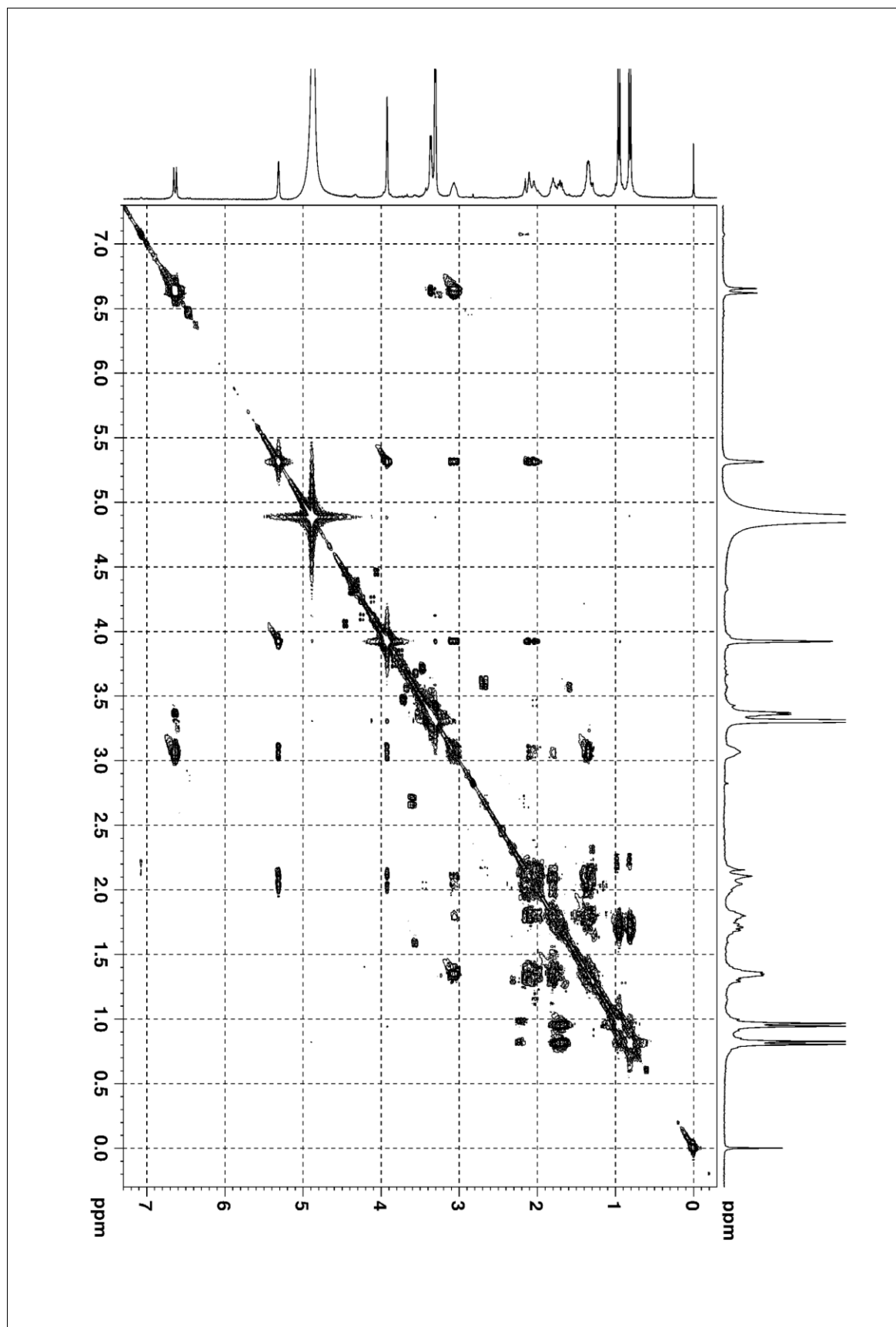
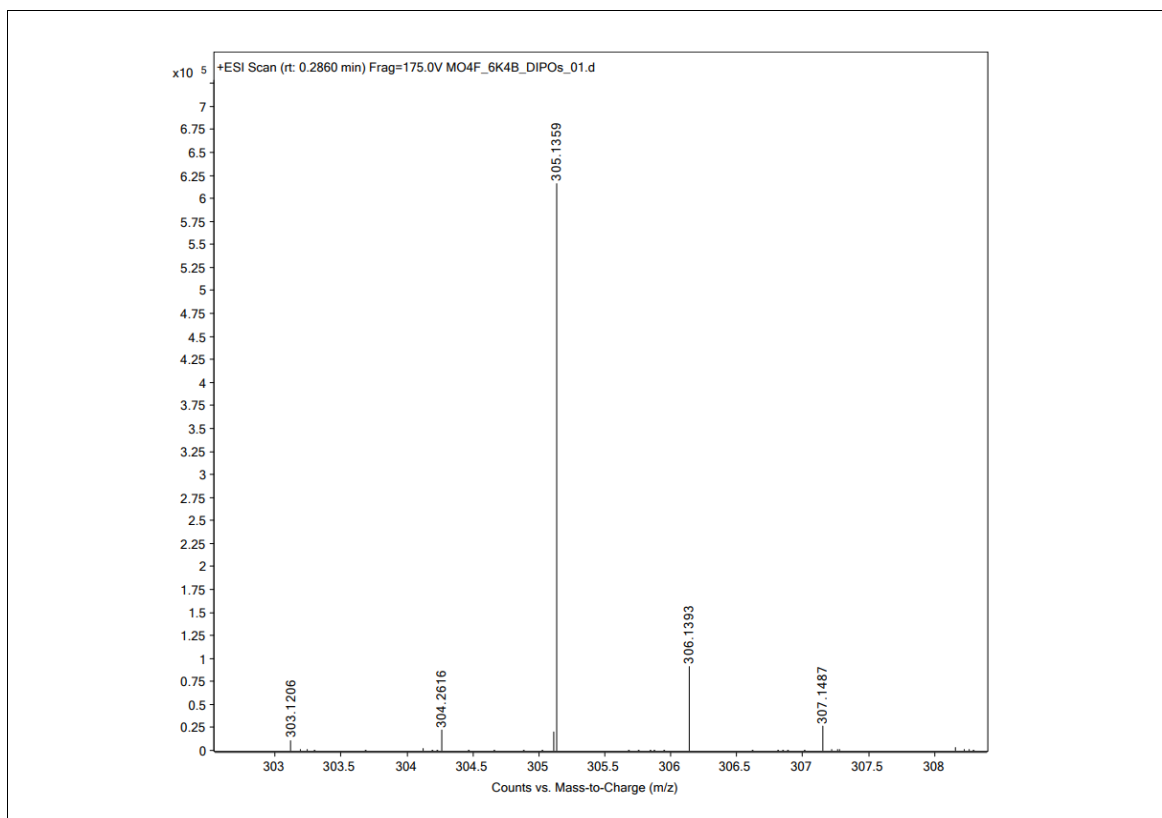
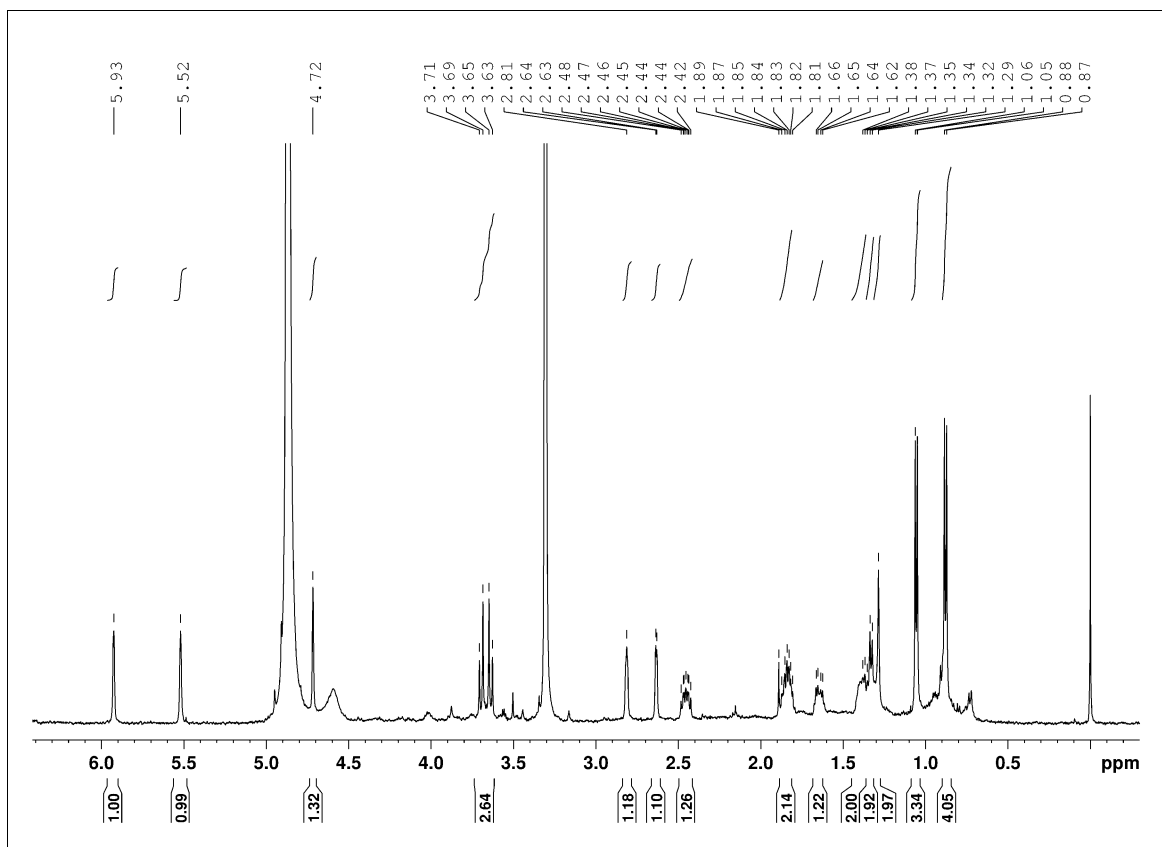


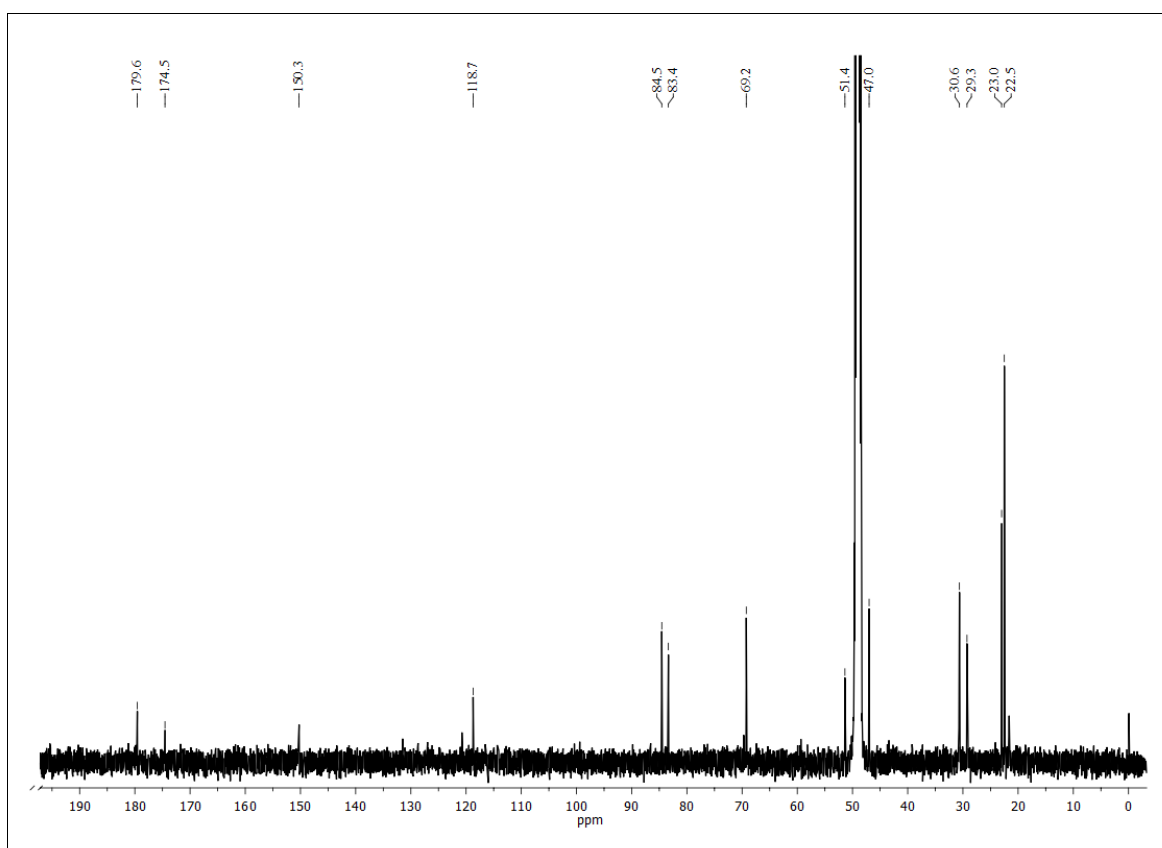
Figure S5.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum ( $\text{CD}_3\text{OD}$ ) of compound 1



**Figure S6.** HRESI mass spectrum of compound **1**



**Figure S7.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CD}_3\text{OD}$ ) of compound **2**



**Figure S8.**  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CD}_3\text{OD}$ ) of compound **2**



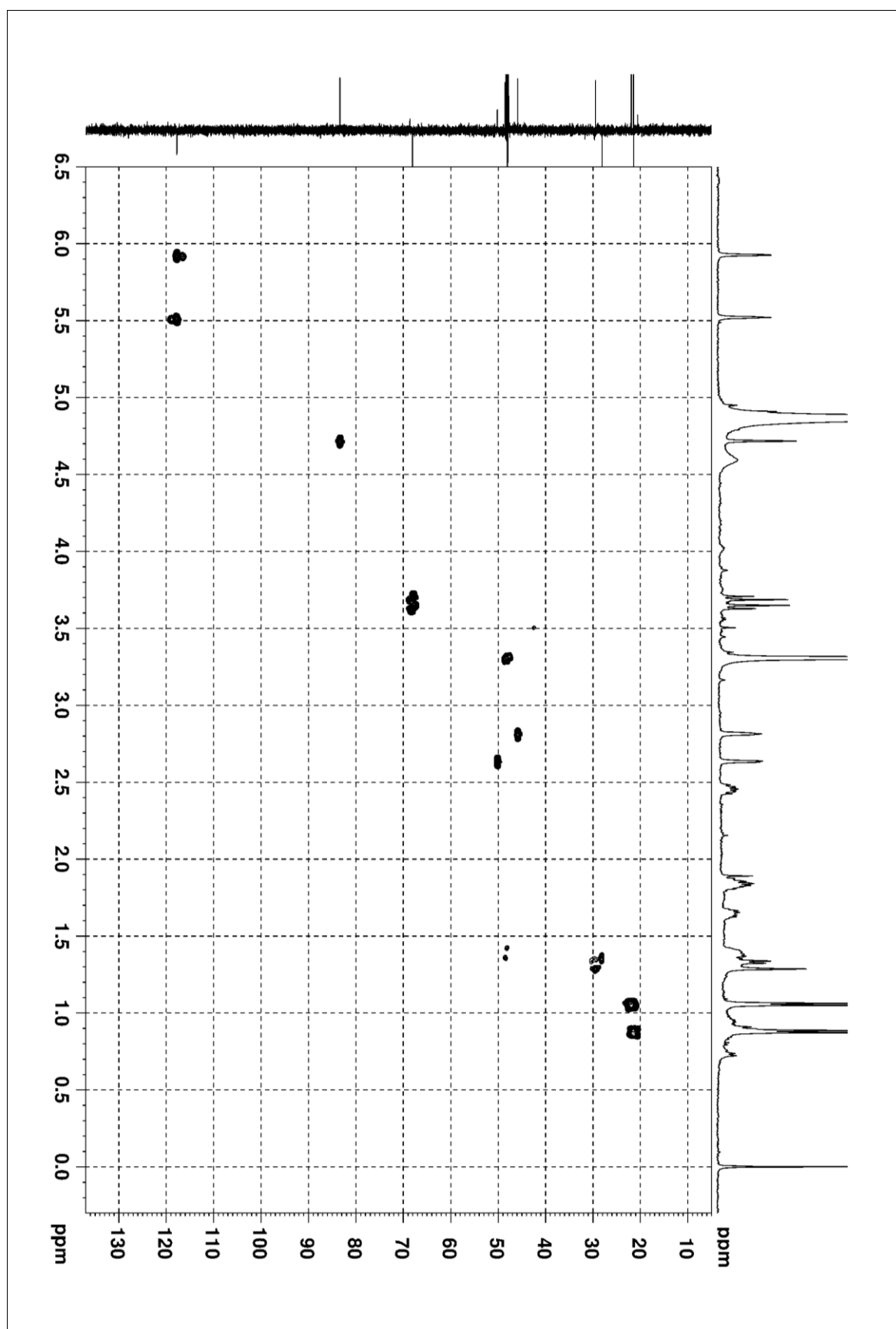
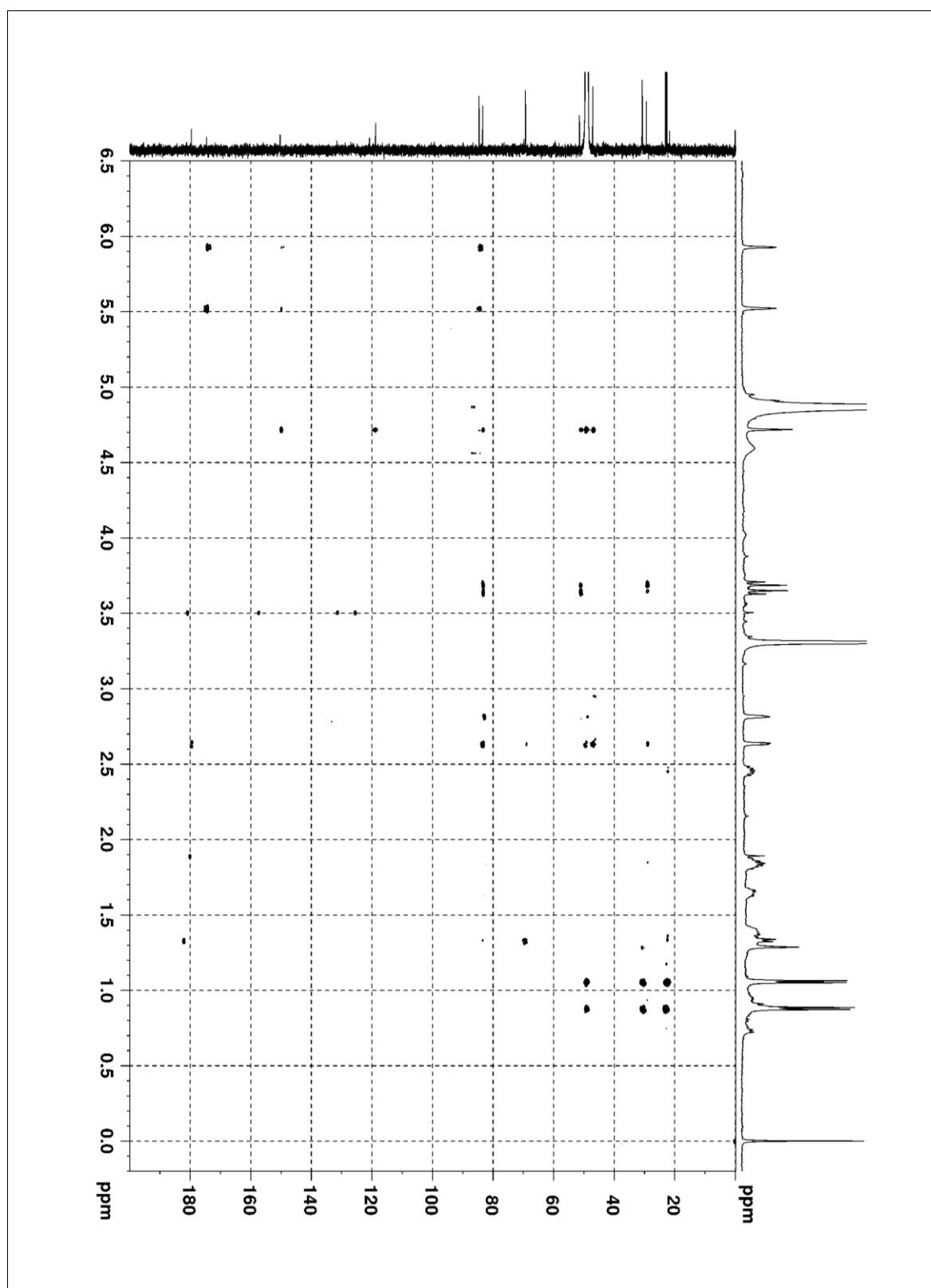


Figure S9. HMQC spectrum ( $\text{CD}_3\text{OD}$ ) of compound 2



**Figure S10.** HMBC spectrum (CD<sub>3</sub>OD) of compound 2

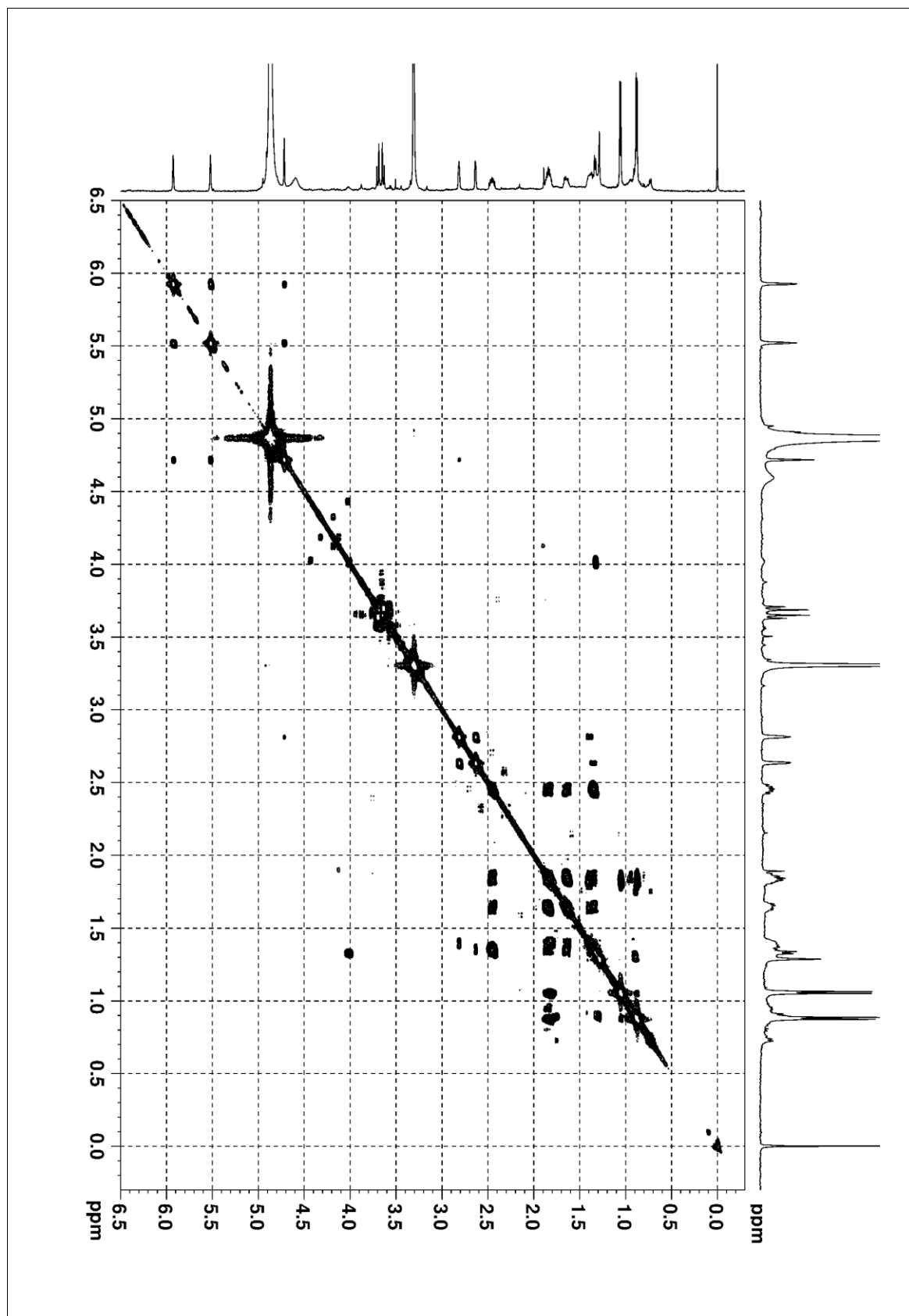
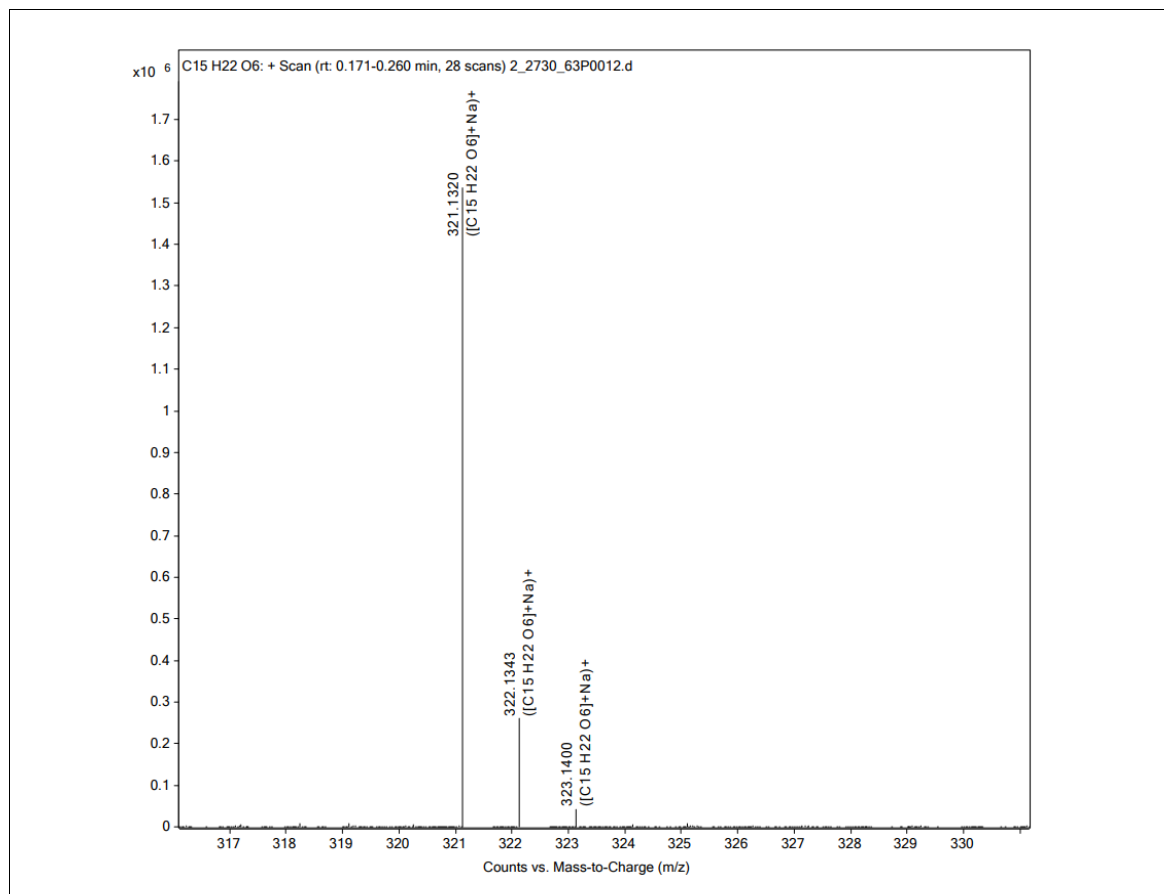
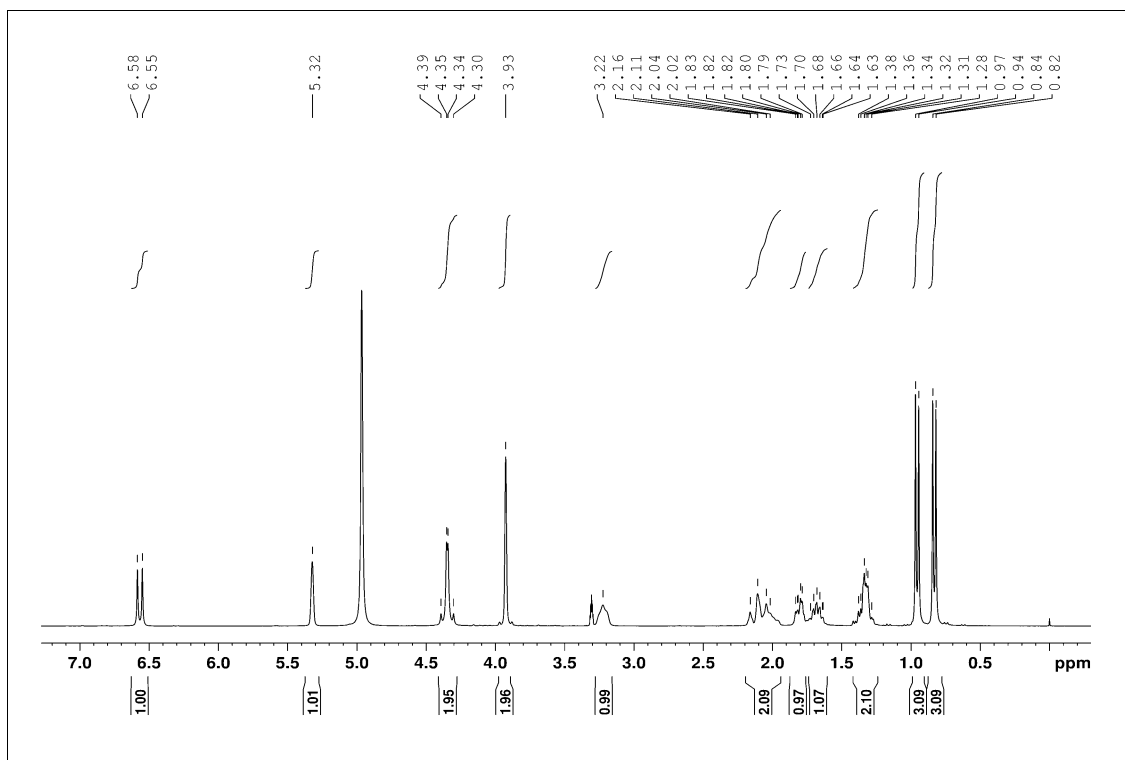


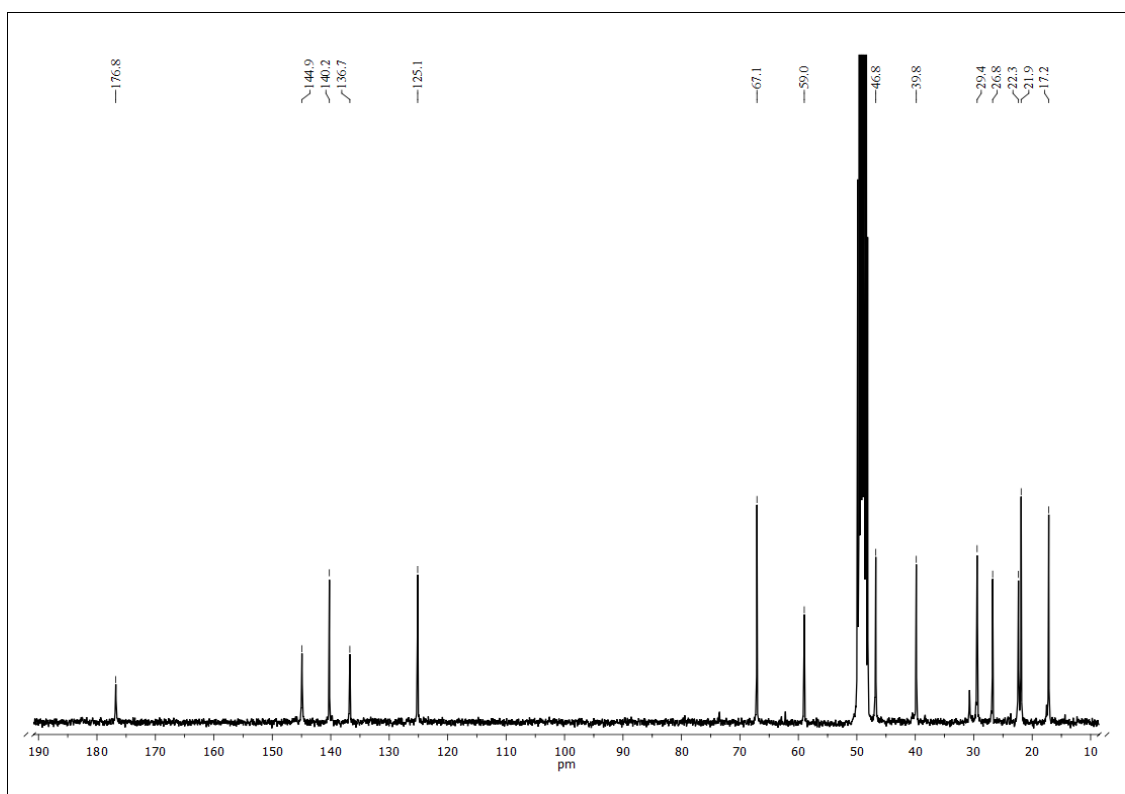
Figure S11.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum ( $\text{CD}_3\text{OD}$ ) of compound 2



**Figure S12.** HRESI mass spectrum of compound **2**

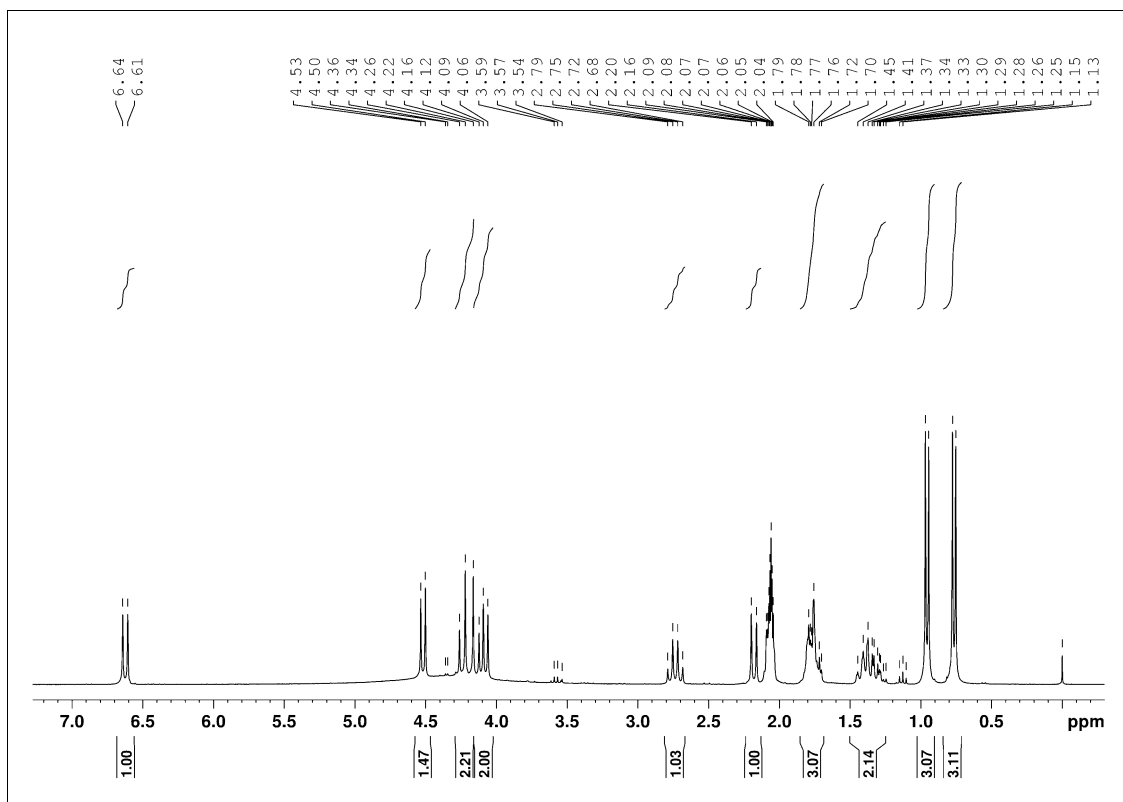


**Figure S13.**  $^1\text{H}$  NMR spectrum (300 MHz,  $\text{CD}_3\text{OD}$ ) of compound **3**

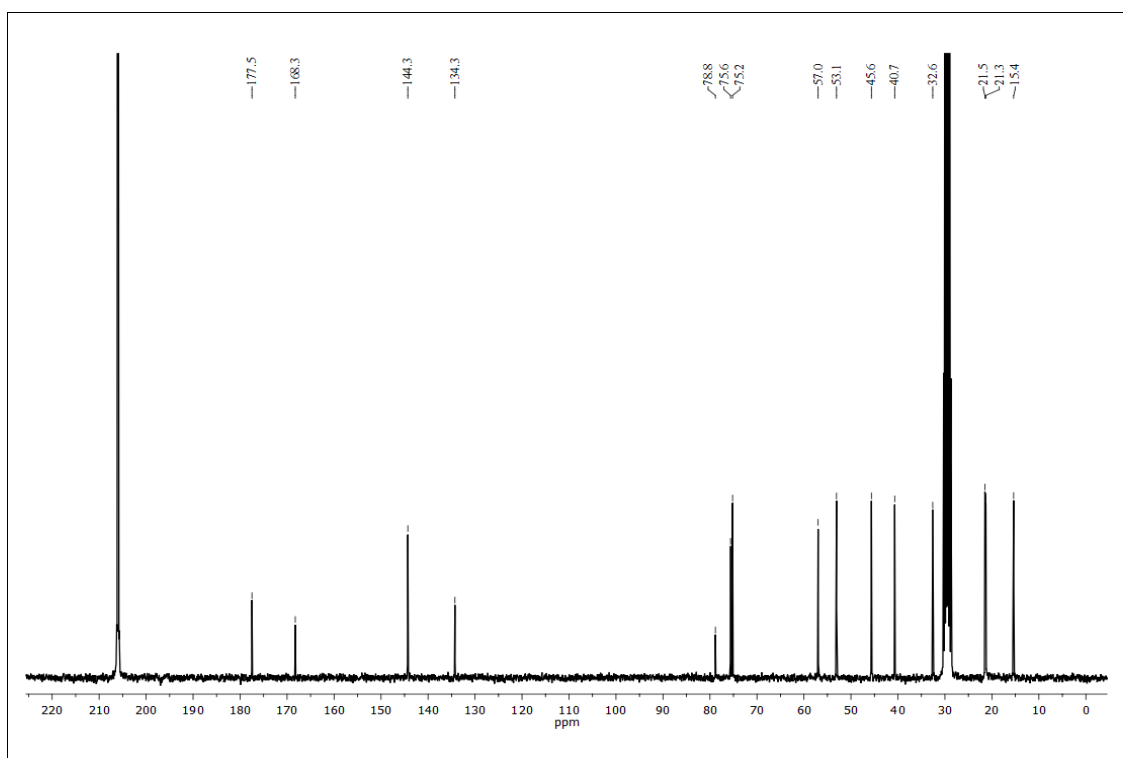


**Figure S14.**  $^{13}\text{C}$  NMR spectrum (75 MHz,  $\text{CD}_3\text{OD}$ ) of compound **3**

Colorless gum;  $[\alpha]_D^{25} +44.3$  ( $c$  0.67, MeOH), Ref.  $[\alpha]_D^{25} +41.4$  ( $c$  0.67, MeOH) [1]; UV (MeOH)  $\lambda_{\text{max}}$  ( $\log \epsilon$ ) 210 (3.72); ECD ( $c$  0.0008 M, MeOH)  $\lambda_{\text{max}}$  ( $\Delta\epsilon$ ): 227 (+4.6) nm, Ref. ECD ( $c$  0.0008 M, MeOH)  $\lambda_{\text{max}}$  ( $\Delta\epsilon$ ): 227 (+4.8) nm [1]; IR (neat)  $\nu_{\text{max}}$  3429, 1656, 1640  $\text{cm}^{-1}$ .

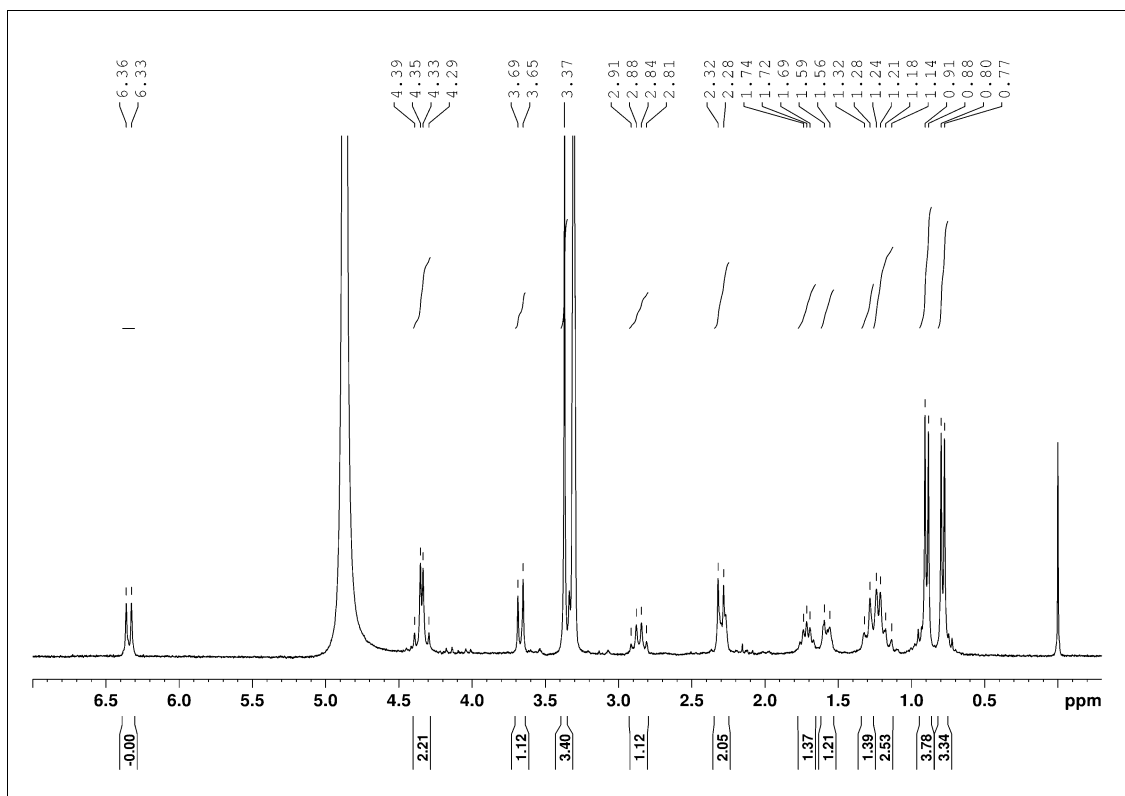


**Figure S15.**  $^1\text{H}$  NMR spectrum (300 MHz, acetone- $d_6$ ) of compound **4**

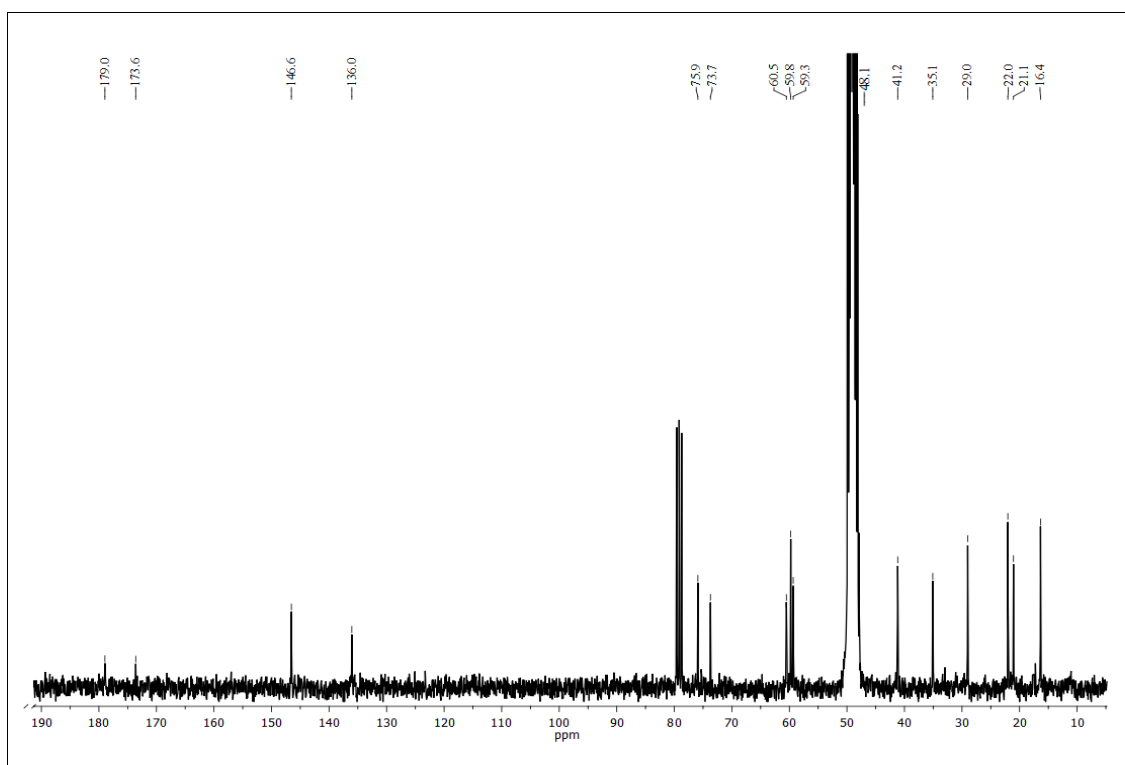


**Figure S16.**  $^{13}\text{C}$  NMR spectrum (75 MHz, acetone- $d_6$ ) of compound **4**

Colorless gum;  $[\alpha]_D^{25} +39.8$  (c 0.83, MeOH), Ref.  $[\alpha]_D^{25} +37.0$  (c 0.83, MeOH) [1]; UV (MeOH)  $\lambda_{\text{max}}$  (log  $\epsilon$ ) 210 (4.14); ECD (c 0.0007 M, MeOH)  $\lambda_{\text{max}}$  ( $\Delta\epsilon$ ): 209 (+11.7), 230 (-5.0) nm, Ref. ECD (c 0.0007 M, MeOH)  $\lambda_{\text{max}}$  ( $\Delta\epsilon$ ): 208 (+9.1), 230 (-4.8) nm [1]; IR (neat)  $\nu_{\text{max}}$  3407, 1761, 1684, 1654  $\text{cm}^{-1}$ .

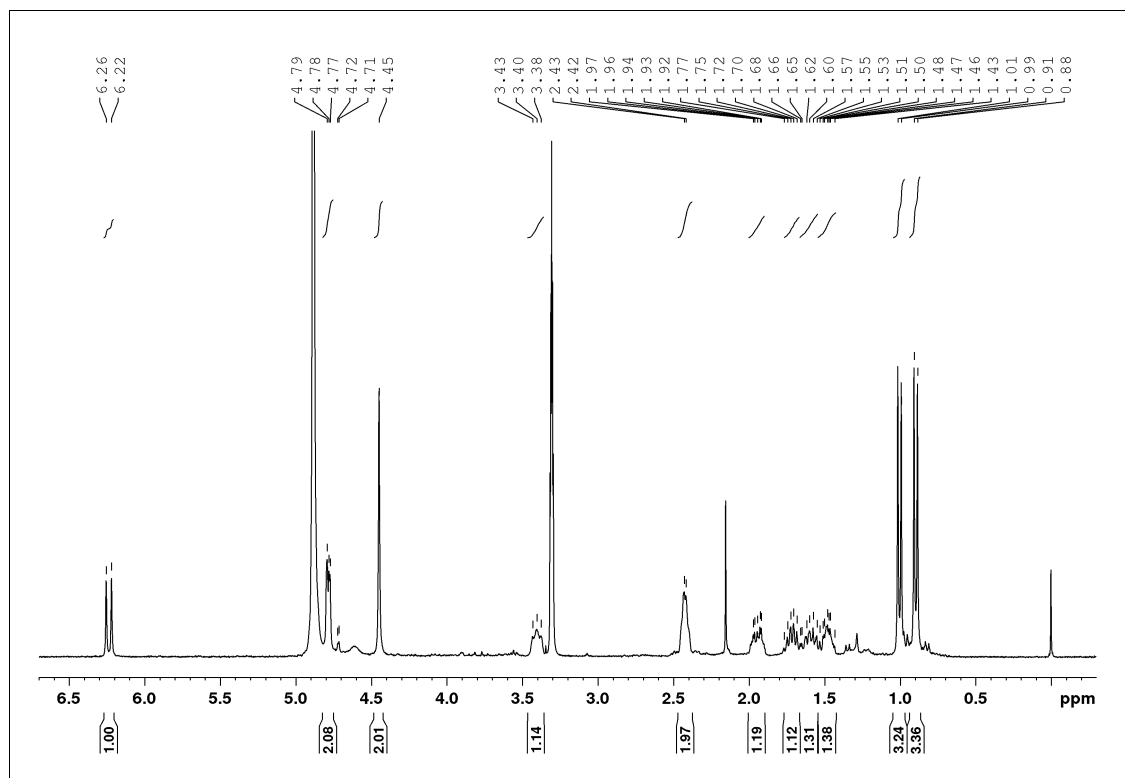


**Figure S17.**  $^1\text{H}$  NMR spectrum (300 MHz,  $\text{CD}_3\text{OD}$ ) of compound **5**

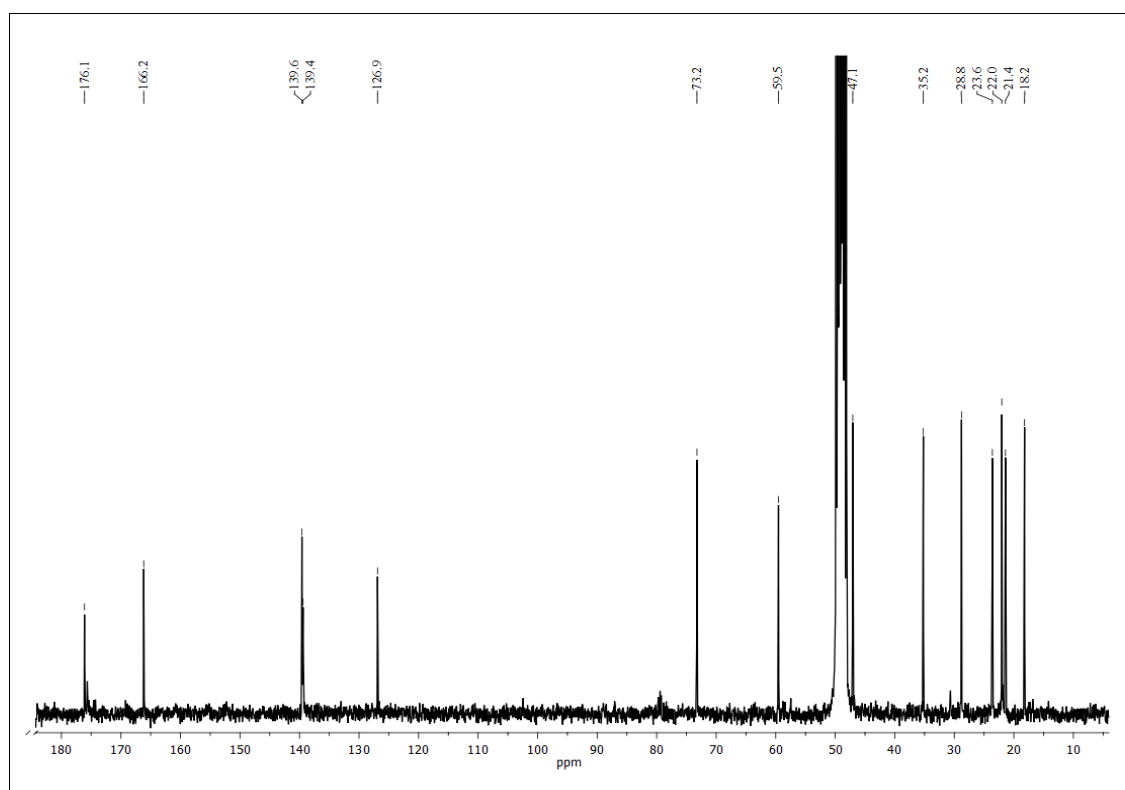


**Figure S18.**  $^{13}\text{C}$  NMR spectrum (75 MHz,  $\text{CD}_3\text{OD}$ ) of compound **5**

Colorless gum;  $[\alpha]_D^{25} +30.2$  (*c* 0.79, MeOH), Ref.  $[\alpha]_D^{25} +28.0$  (*c* 0.79, MeOH) [1]; UV (MeOH)  $\lambda_{\text{max}}$  ( $\log \epsilon$ ) 210 (4.14); ECD (*c* 0.0006 M, MeOH)  $\lambda_{\text{max}}$  ( $\Delta\epsilon$ ): 214 (+7.3), 235 (−5.5) nm, Ref. ECD (*c* 0.0006 M, MeOH)  $\lambda_{\text{max}}$  ( $\Delta\epsilon$ ): 209 (+1.8), 244 (−1.2), 270 (1.0), 289 (−1.1) nm [1]; IR (neat)  $\nu_{\text{max}}$  3422, 1686, 1639  $\text{cm}^{-1}$ .



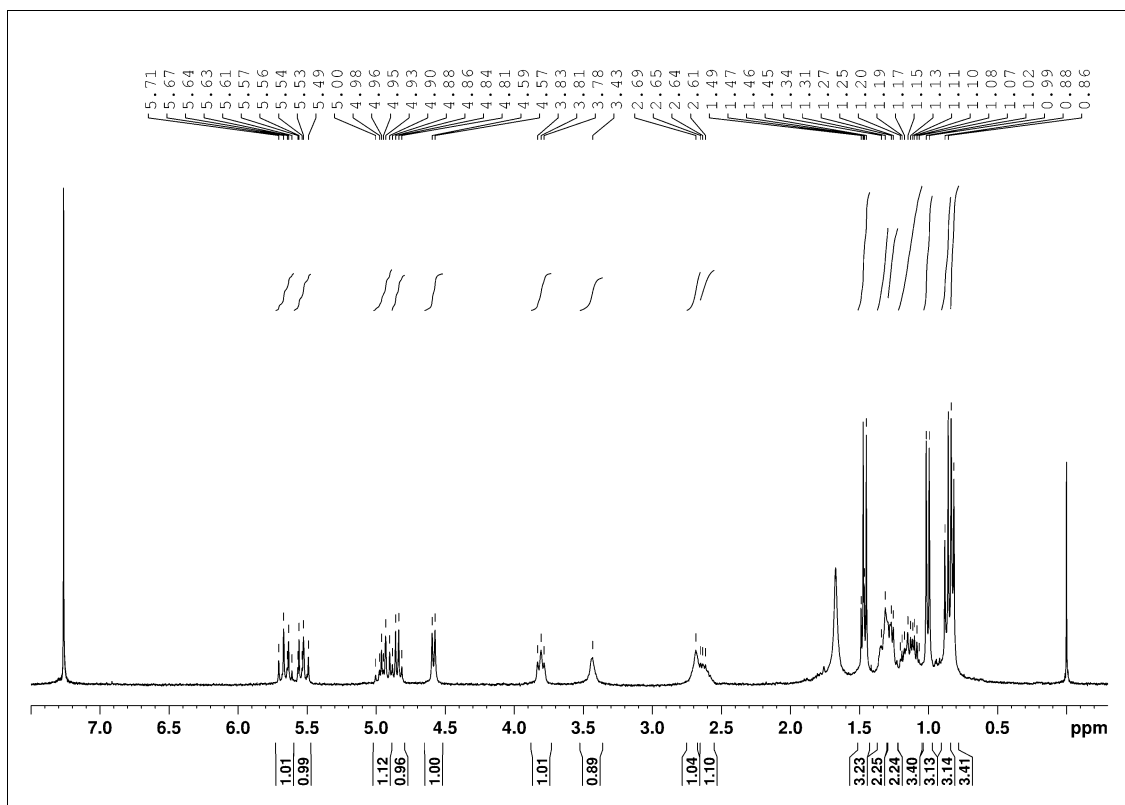
**Figure S19.**  $^1\text{H}$  NMR spectrum (300 MHz,  $\text{CD}_3\text{OD}$ ) of compound **6**



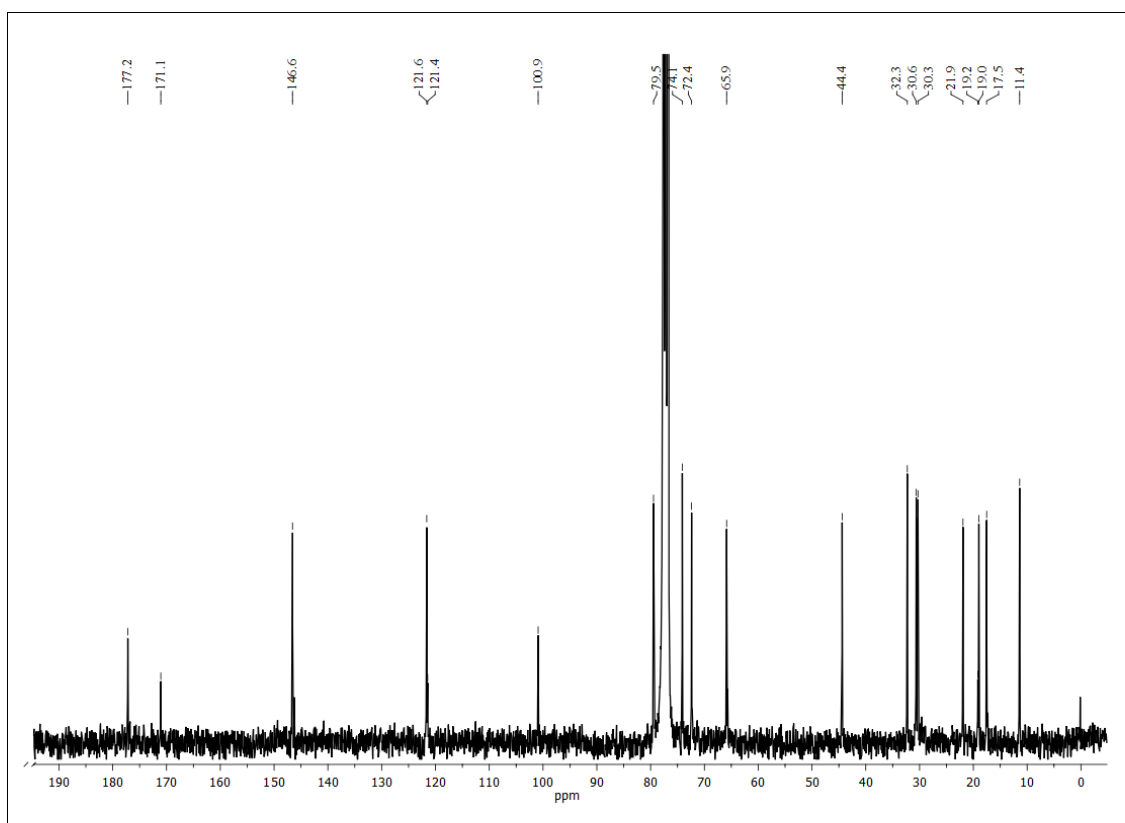
**Figure S20.**  $^{13}\text{C}$  NMR spectrum (75 MHz,  $\text{CD}_3\text{OD}$ ) of compound **6**

Colorless gum;  $[\alpha]_D^{25} +75.6$  (*c* 0.70, MeOH), Ref.  $[\alpha]_D^{25} +74.4$  (*c* 0.70, MeOH) [1]; UV (MeOH)  $\lambda_{\text{max}}$  ( $\log \epsilon$ ) 219 (4.26); ECD (*c* 0.0007 M, MeOH)  $\lambda_{\text{max}}$  ( $\Delta\epsilon$ ): 225 (+11.6), 248 (-1.4) nm, Ref. ECD (*c* 0.0007 M, MeOH)  $\lambda_{\text{max}}$  ( $\Delta\epsilon$ ): 225 (+22.9), 248 (-3.4) nm [1]; IR (neat)  $\nu_{\text{max}}$  3423, 1684, 1638  $\text{cm}^{-1}$ .





**Figure S21.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of compound **7**



**Figure S22.**  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ ) of compound **7**

Colorless gum;  $[\alpha]_D^{25} +9.5$  ( $c$  1.2,  $\text{CH}_2\text{Cl}_2$ ), Ref.  $[\alpha]_D^{25} +8.2$  ( $c$  1.2,  $\text{CH}_2\text{Cl}_2$ ) [2]; UV (MeOH)  $\lambda_{\text{max}}$  (log  $\epsilon$ ) 228 (4.15); IR (neat)  $\nu_{\text{max}}$  3423, 1684, 1638  $\text{cm}^{-1}$ .

## References

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doi:10.1002/cbdv.201100026
2. Krohn, K.; Biele, C.; Drogies, K.-H.; Steingröver, K.; Aust, H.-J.; Draeger, S.; Schulz, B. *J. Org. Chem.* **2002**, *14*, 2331–2336. doi:10.1002/1099-0690(200207)2002:14<2331::AID-EJOC2331>3.0.CO;2-P