Supporting Information

for

New furoisocoumarins and isocoumarins from the mangrove endophytic fungus *Aspergillus* sp. 085242

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1D and 2D NMR, HREIMS, and HRESIMS spectra of the new compounds

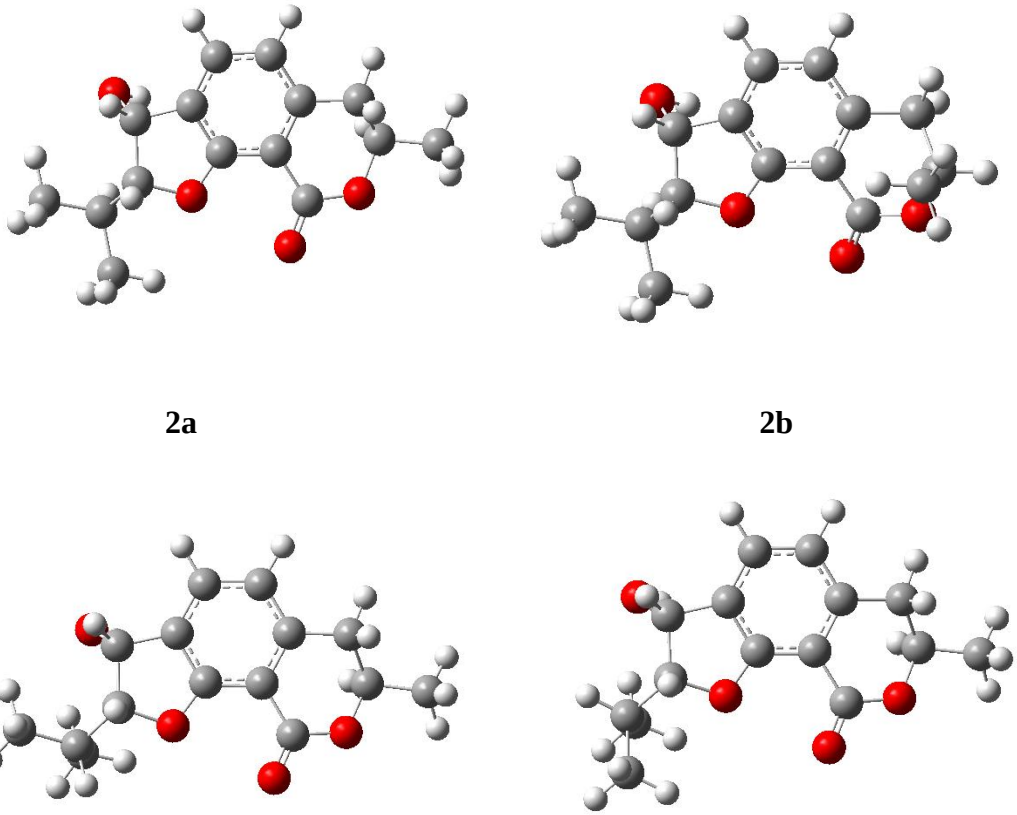
Computational details

Molecular Merck force field (MMFF) and DFT/TD-DFT calculations were carried out with Spartan' 14 software (Wavefunction Inc., Irvine, CA, USA) and Gaussian 09 program, respectively. Conformers within 10 kcal/mol energy window were generated and optimized using DFT calculations at B3LYP/6-31G(d) level. Conformers with Boltzmann distribution over 1% were chosen for ECD calculations in methanol at B3lYP/6-311+g(2d,p) level. The IEF-PCM solvent model for MeOH was used. ECD spectra were generated using the program SpecDis 3.0 (University of Würzburg, Würzburg, Germany) and OriginPro 8.5 (OriginLab, Ltd., Northampton, MA, USA) from dipole-length rotational strengths by applying Gaussian band shapes with sigma = 0.30 eV and UV shift = +21 nm. All calculations were performed with High-Performance Grid Computing Platform of Sun Yat-Sen University.

Result

Table S1: Energy Analysis for the Conformers of (2*R*,3*R*,7*R*)-**2**.

compound	Conformation	G (Hartree)	G (Kcal/mol)	ΔG (Kcal/mol)	Boltzmann Dist (%)
(2*R*,3*R*,7*R*)-**2**	**2a**	−883.632283748	−554481.8206	0.0000	87.18
	2b	−883.629991994	−554480.3825	1.4380	7.68
	2c	−883.628769196	−554479.6152	2.2053	2.10
	2d	−883.629048220	−554479.7903	2.0303	2.83



2a **2b**

2c **2d**

Figure S1: B3LYP/6-31G(d) optimized low-energy conformers of **2**

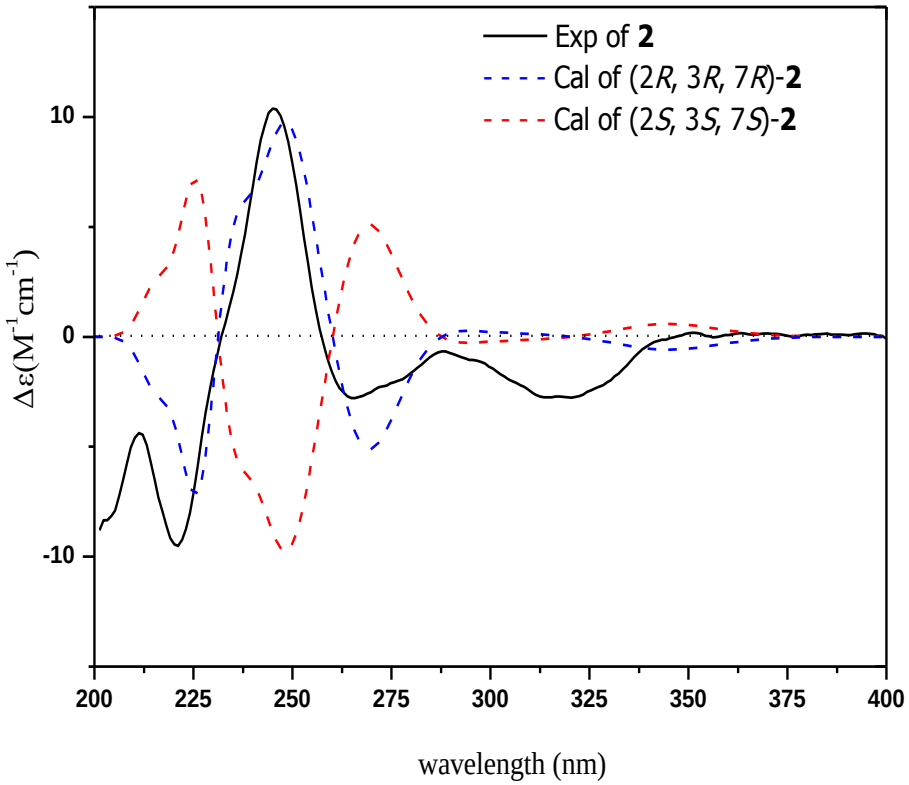


Figure S2: Comparison of the experimental ECD spectra of **2** with the B3lYP/6-311+g(2d,p) calculated spectrum of (2*R*,3*R*,7*R*)-**2** and (2*S*,3*S*,7*S*)-**2** in MeOH. σ = 0.30 eV.

References

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, revision C.01. Gaussian, Inc.: Wallingford CT, 2010.Bruhn, T.; Schaumlöffel, A.; Hemberger, Y.; Bringmann, G. SpecDis: Quantifying the comparison of calculated and experimental electronic circular dichroism spectra. Chirality 2013, 25, 243–249.

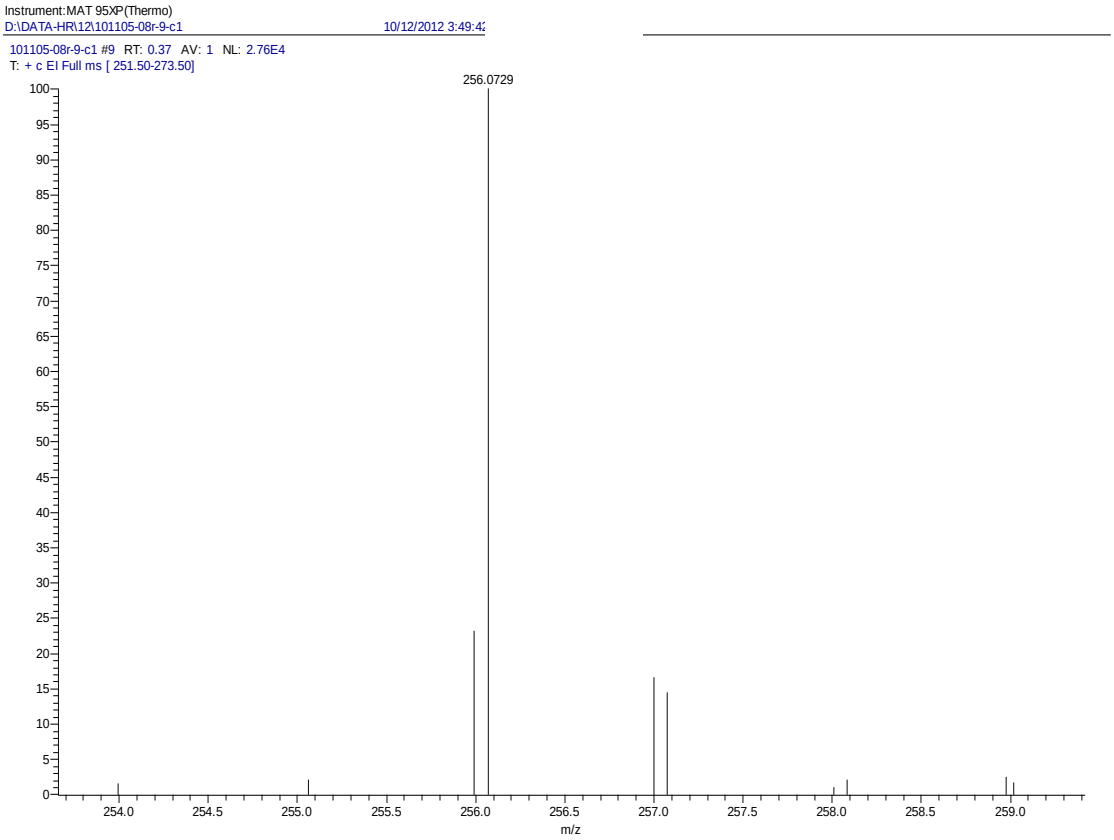


Figure S3 HREIMS spectrum of **1**

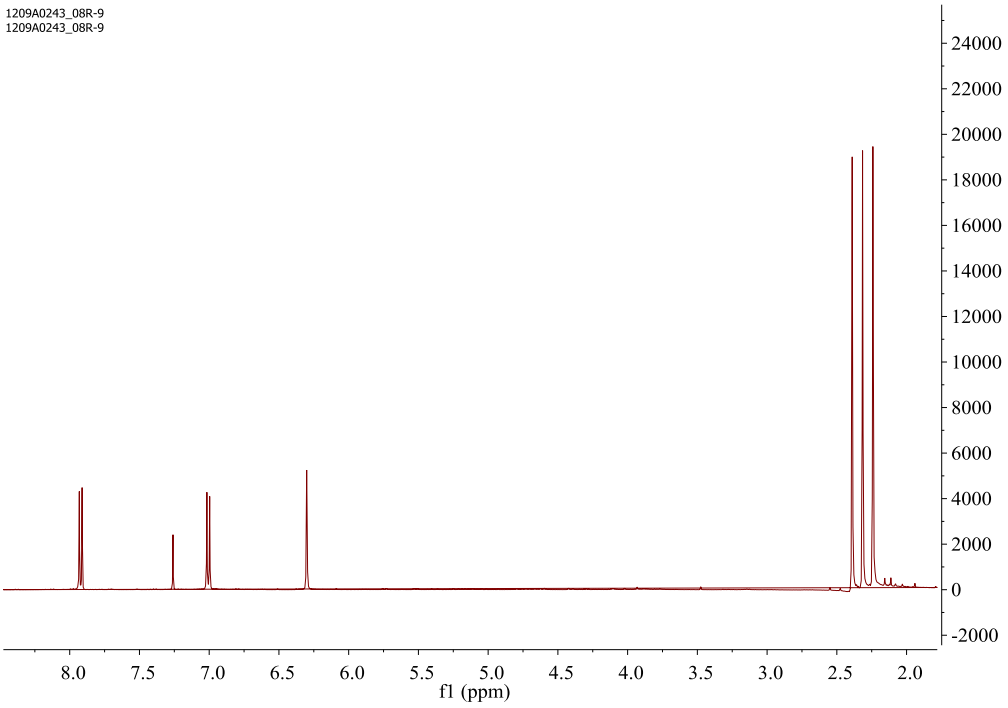


Figure S4 ^{1}H NMR spectrum of **1** in $CDCl_3$

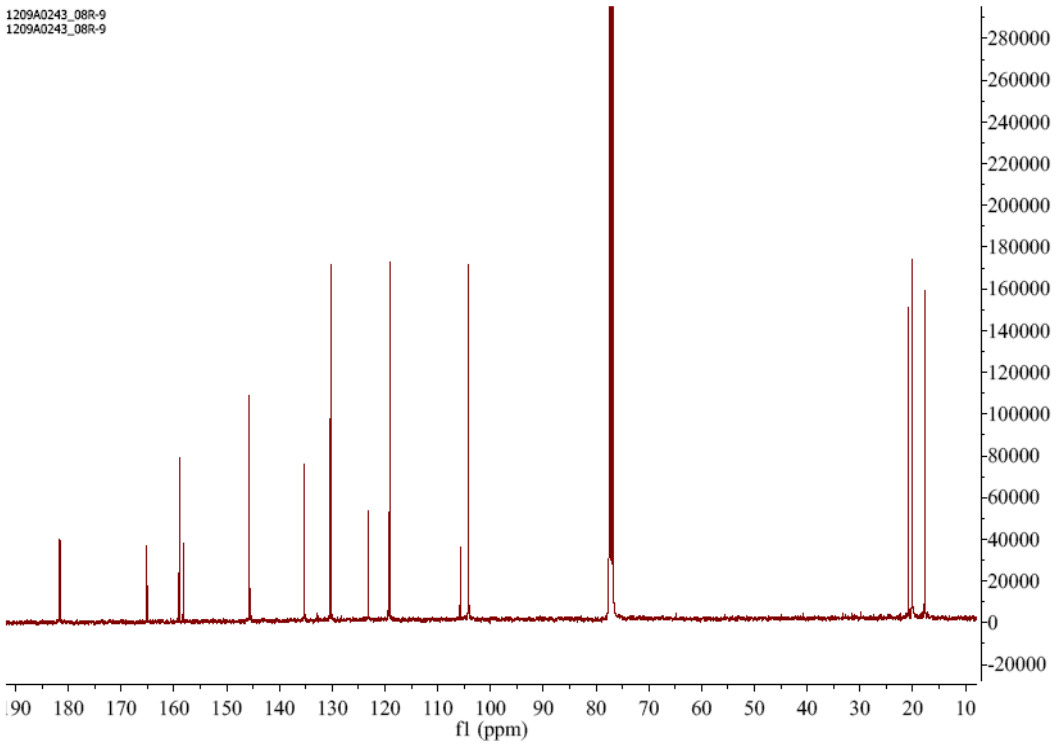


Figure S5 ^{13}C NMR spectrum of **1** in $CDCl_3$

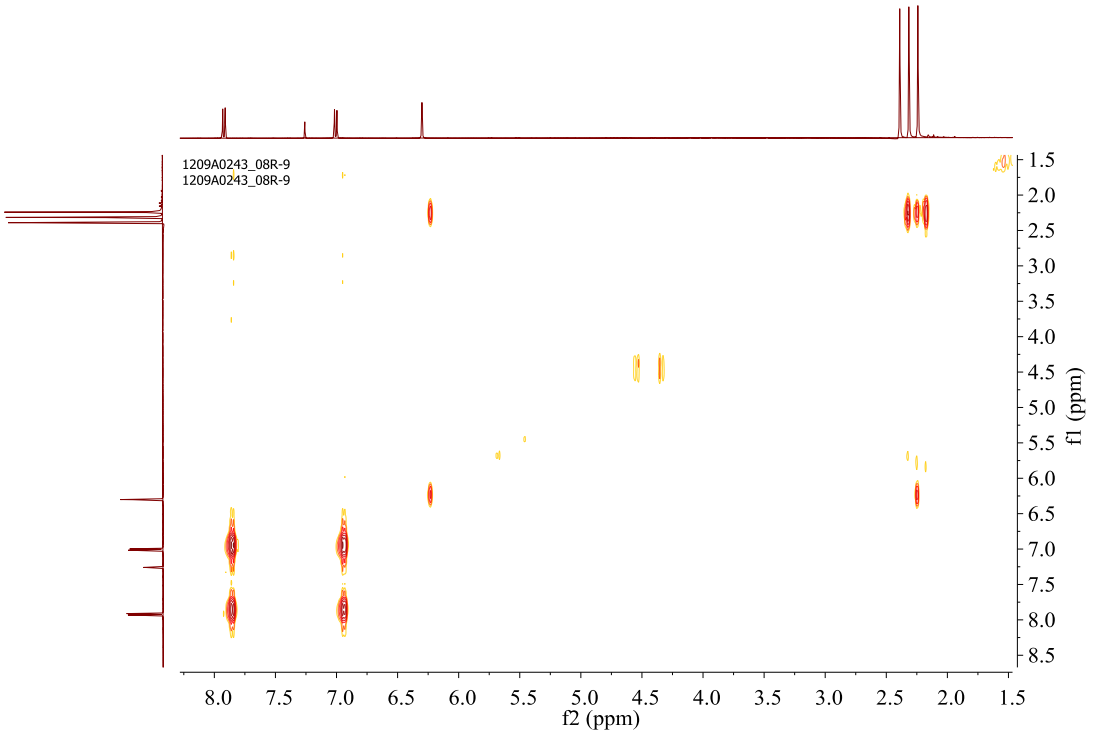


Figure S6 ^{1}H–^{1}H COSY spectrum of **1** in $CDCl_3$

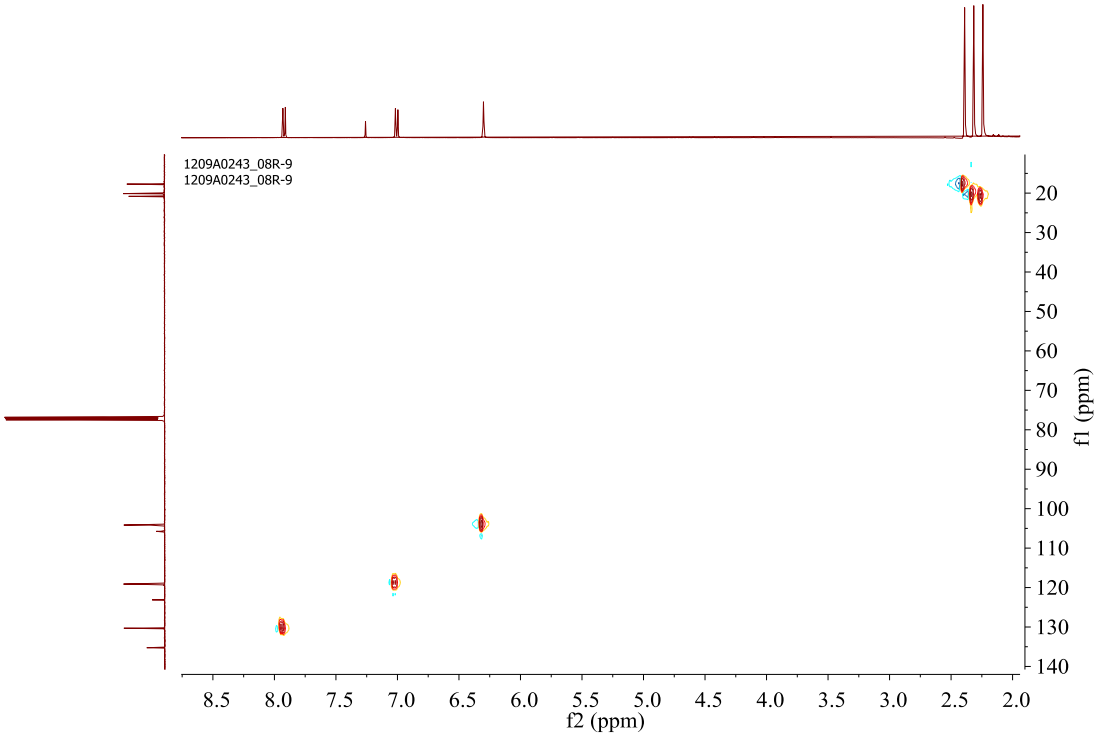


Figure S7 HSQC spectrum of **1** in $CDCl_3$

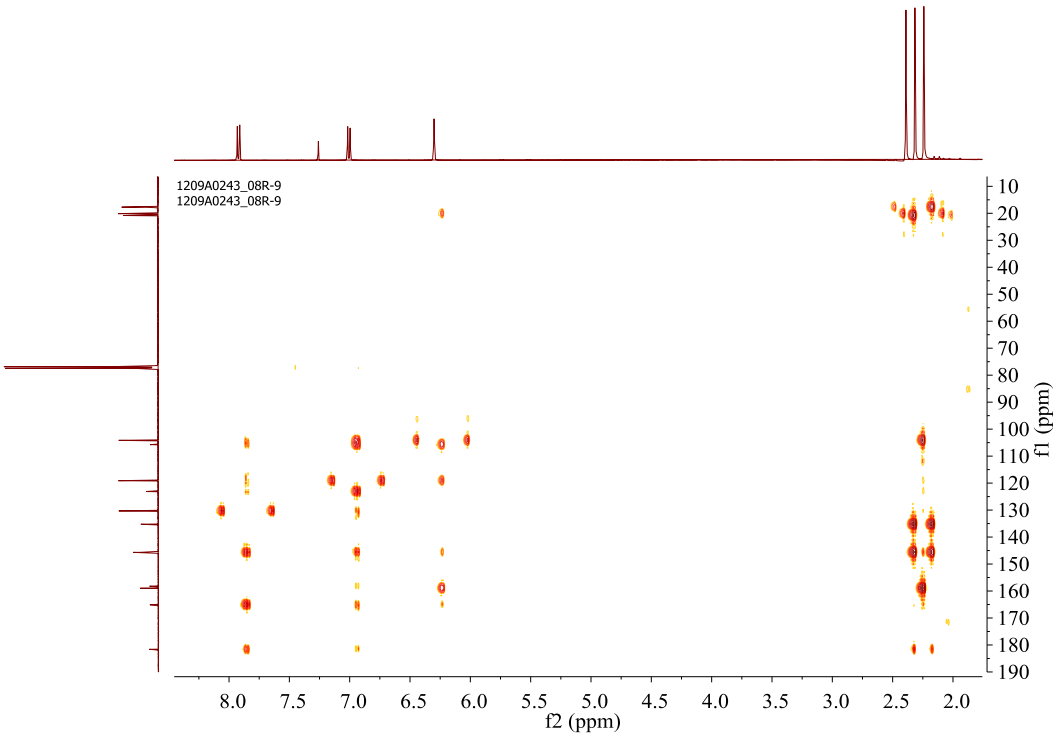


Figure S8 HMBC spectrum of **1** in $CDCl_3$

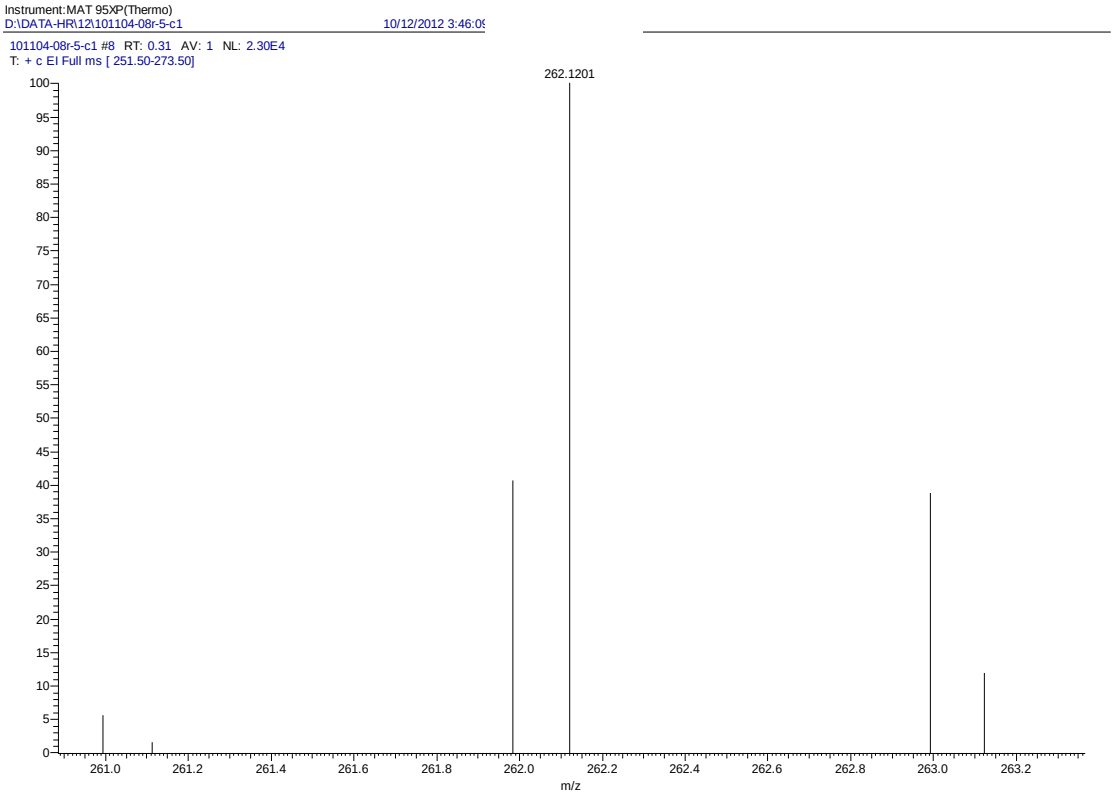


Figure S9 HREIMS spectrum of **2**

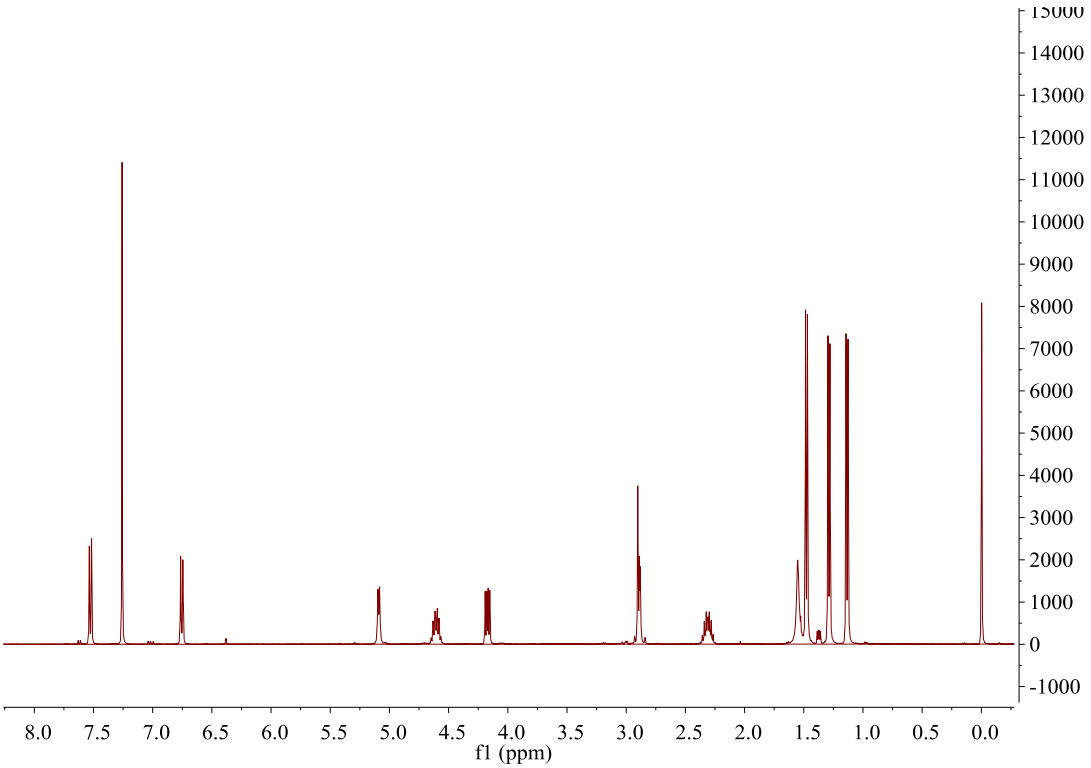


Figure S10 ^{1}H NMR spectrum of **2** in $CDCl_3$

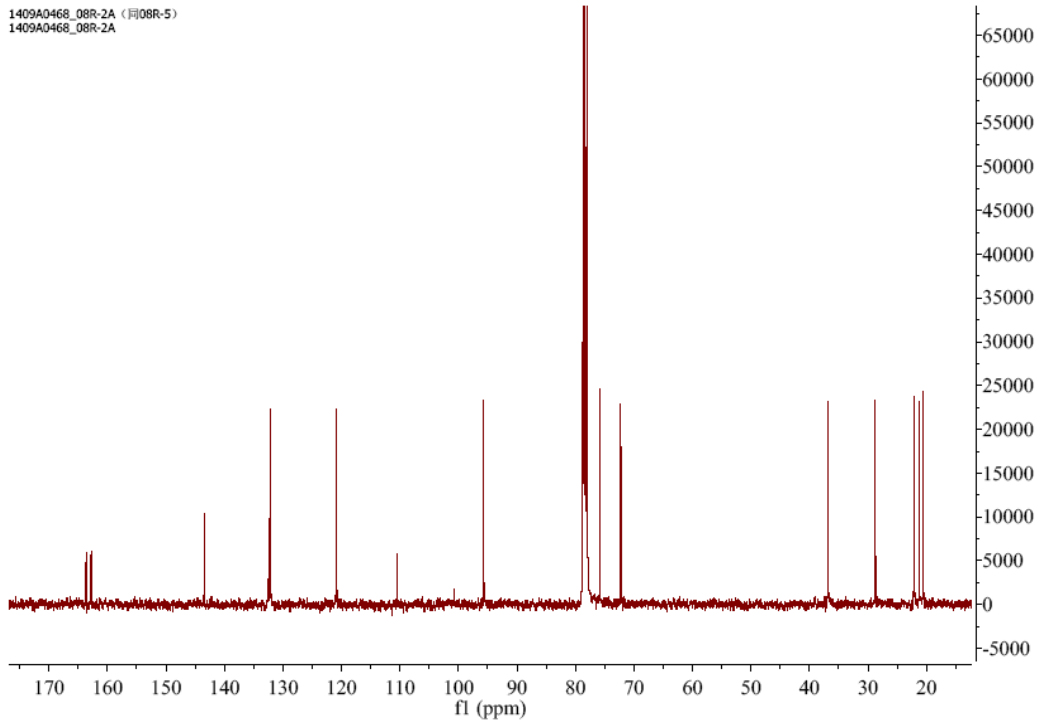


Figure S11 ^{13}C NMR spectrum of **2** in $CDCl_3$

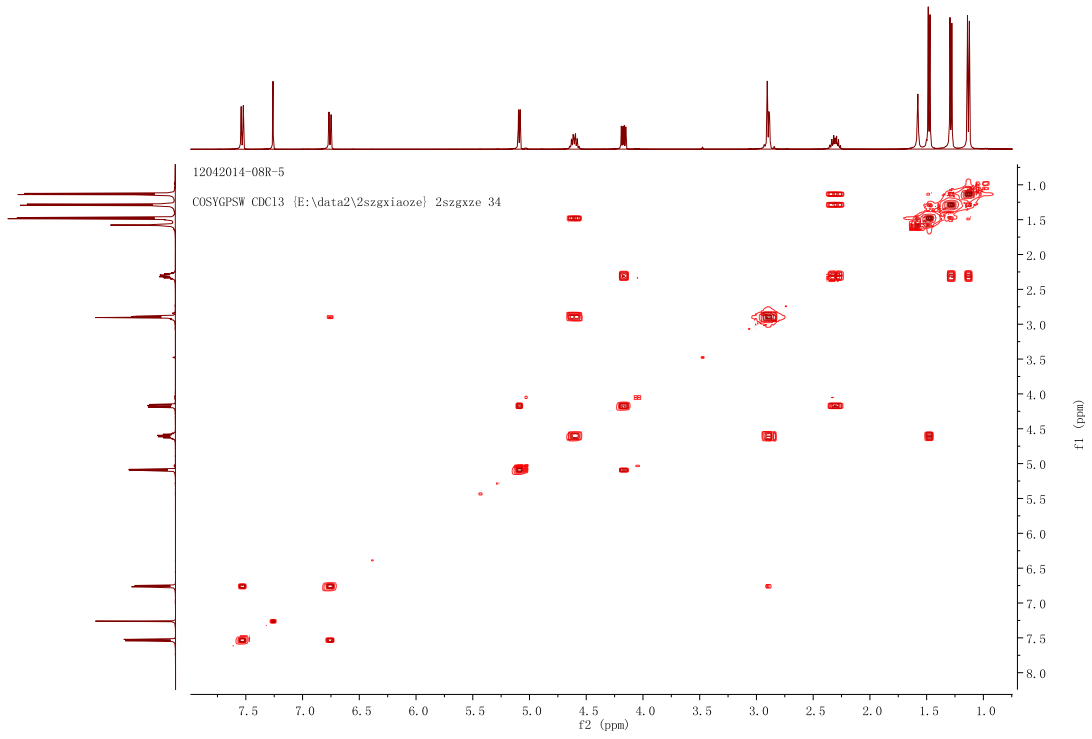


Figure S12 ^{1}H–^{1}H COSY spectrum of **2** in $CDCl_3$

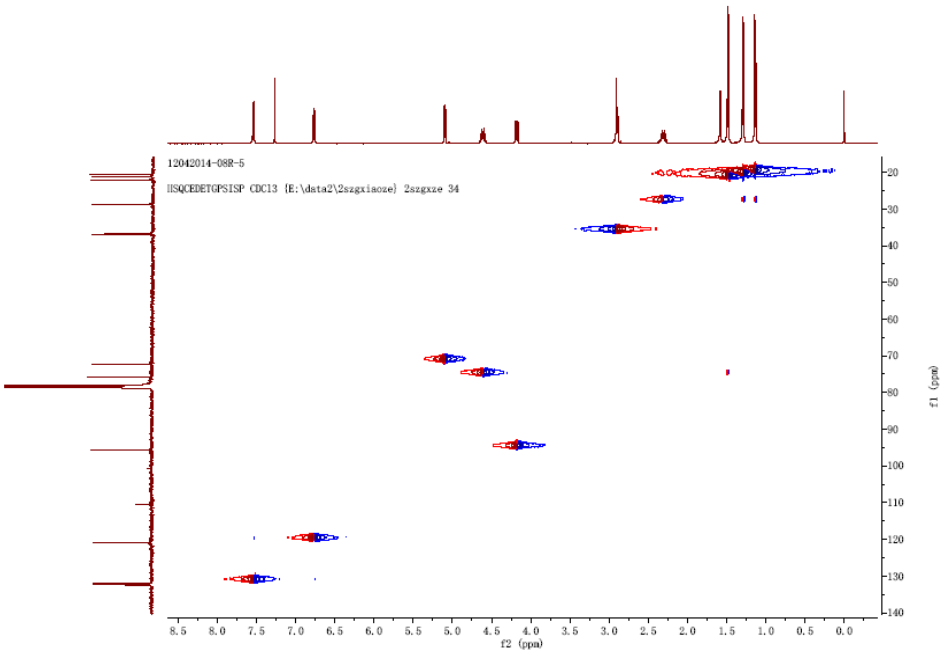


Figure S13 HSQC spectrum of **2** in $CDCl_3$

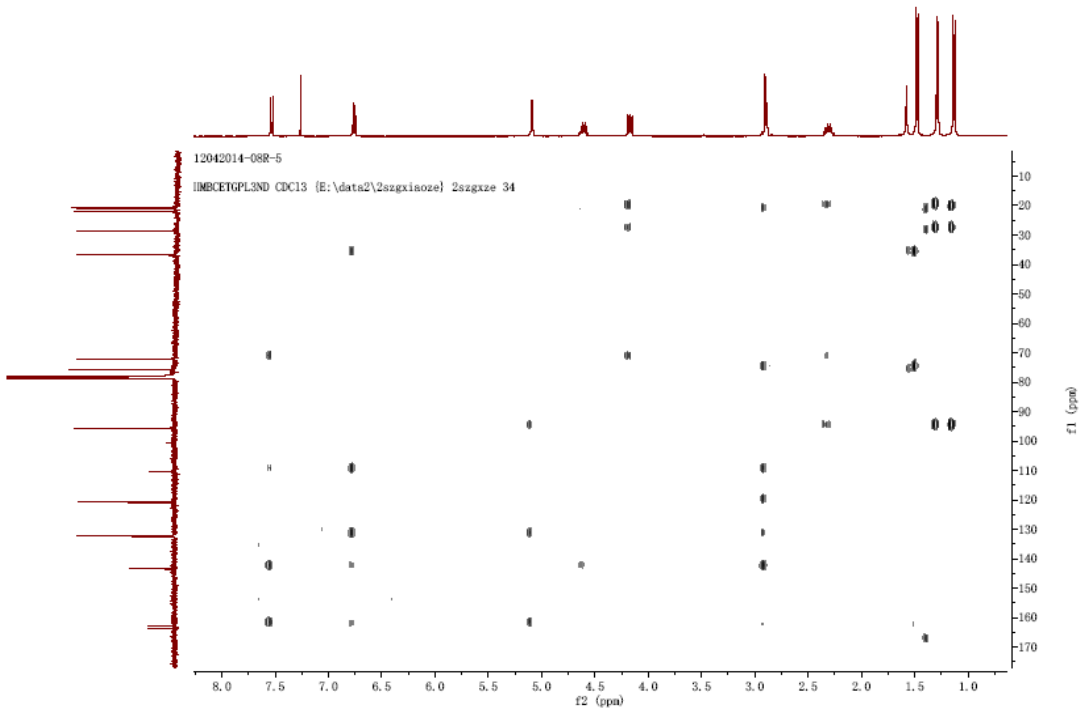


Figure S14 HMBC spectrum of **2** in $CDCl_3$

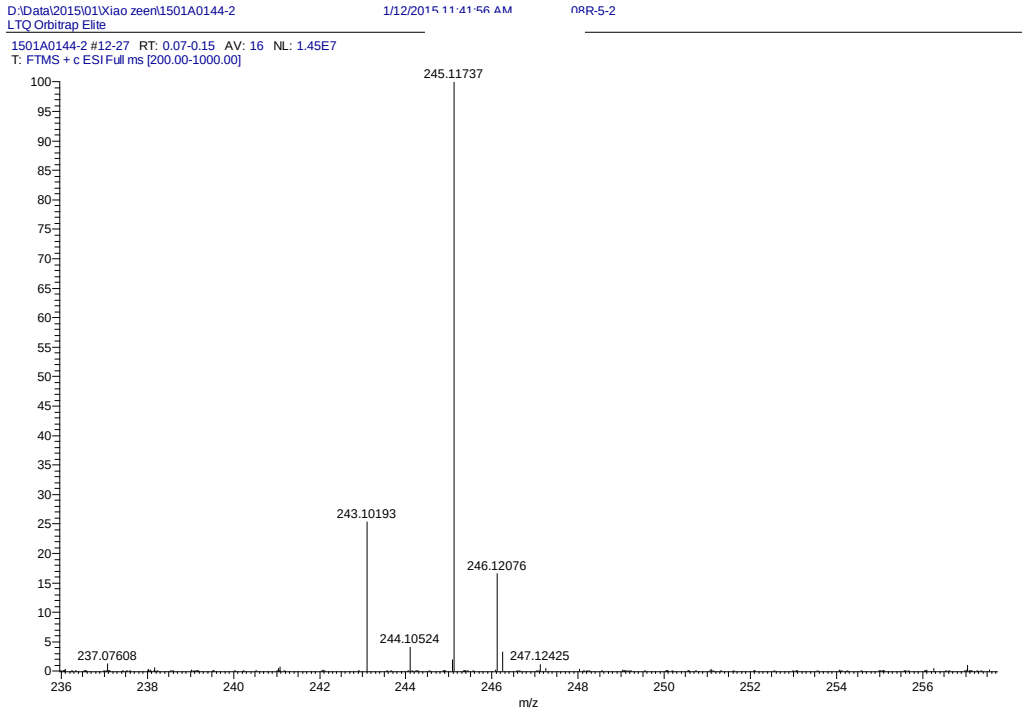


Figure S15 HRESIMS spectrum of **3**

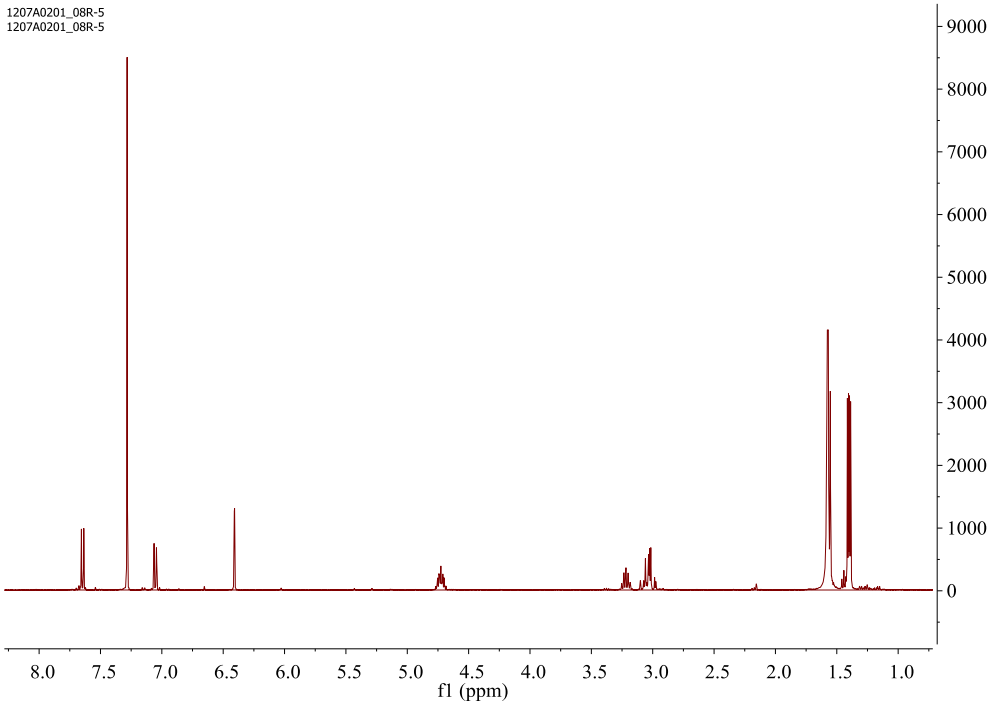


Figure S16 ^{1}H NMR spectrum of **3** in $CDCl_3$

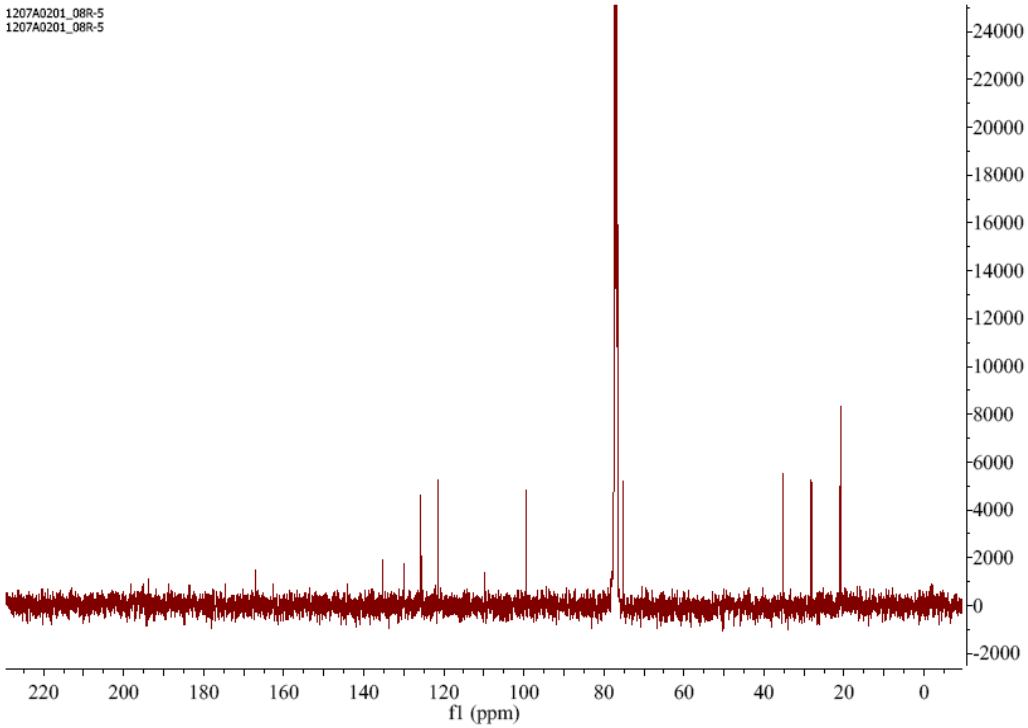


Figure S17 ^{13}C NMR spectrum of **3** in $CDCl_3$

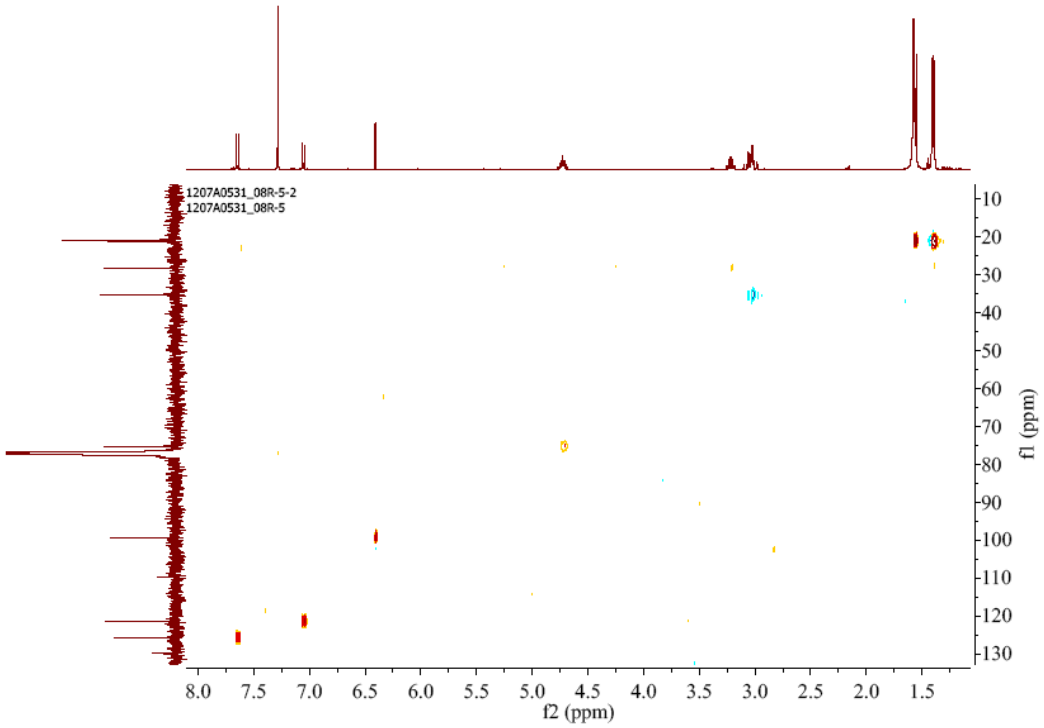


Figure S18 HSQC spectrum of **3** in $CDCl_3$

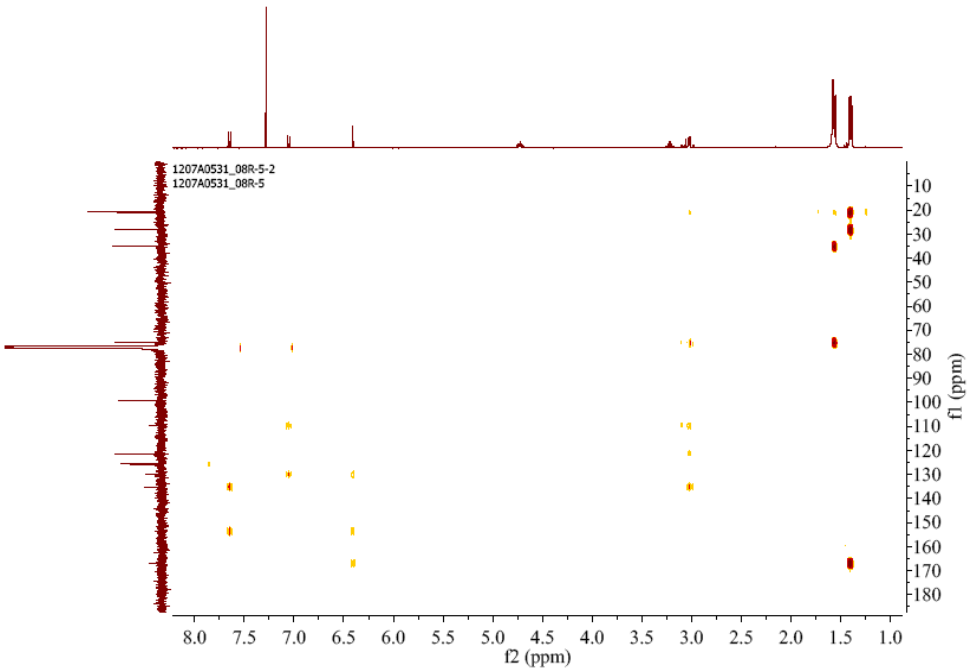


Figure S19 HMBC spectrum of **3** in $CDCl_3$

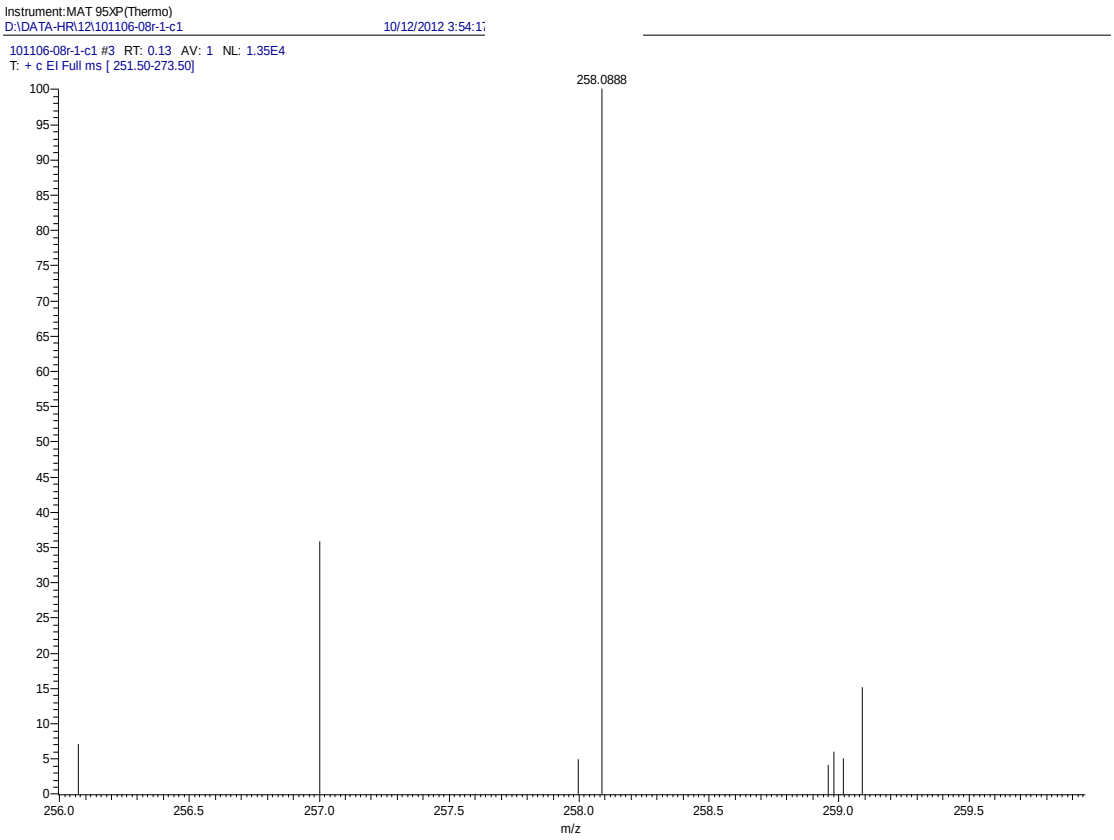


Figure S20 HRESIMS spectrum of **4**

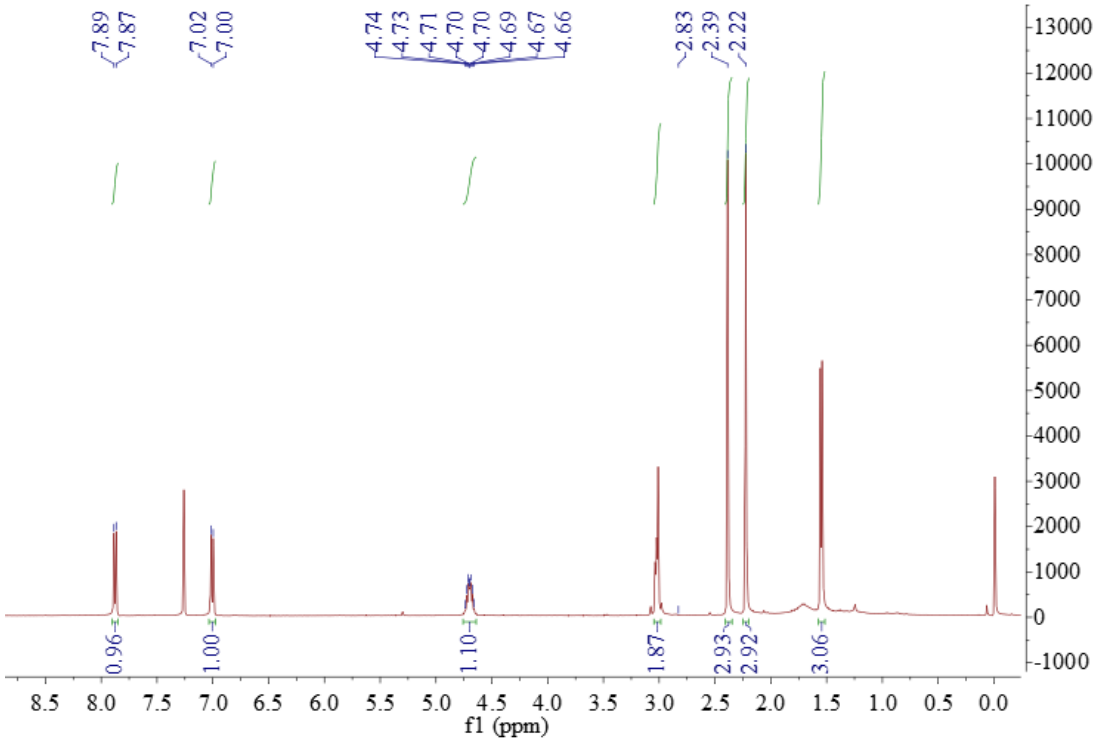


Figure S21 ^{1}H NMR spectrum of **4** in $CDCl_3$

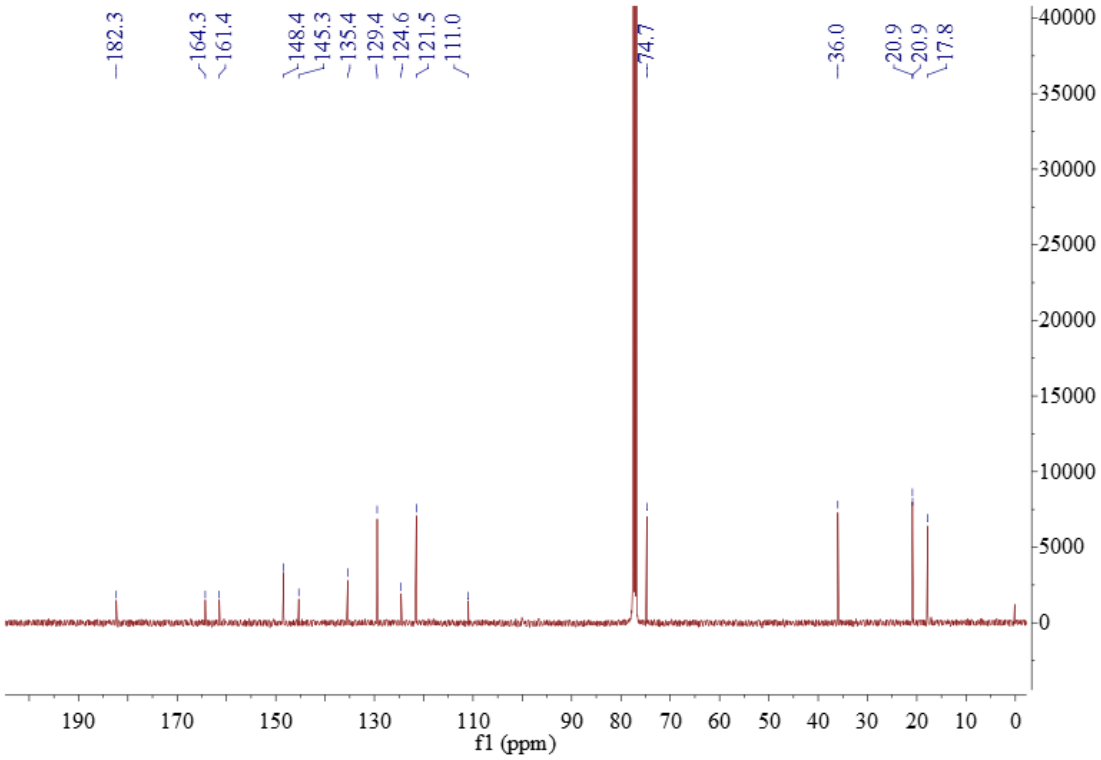


Figure S22 ^{13}C NMR spectrum of **4** in $CDCl_3$

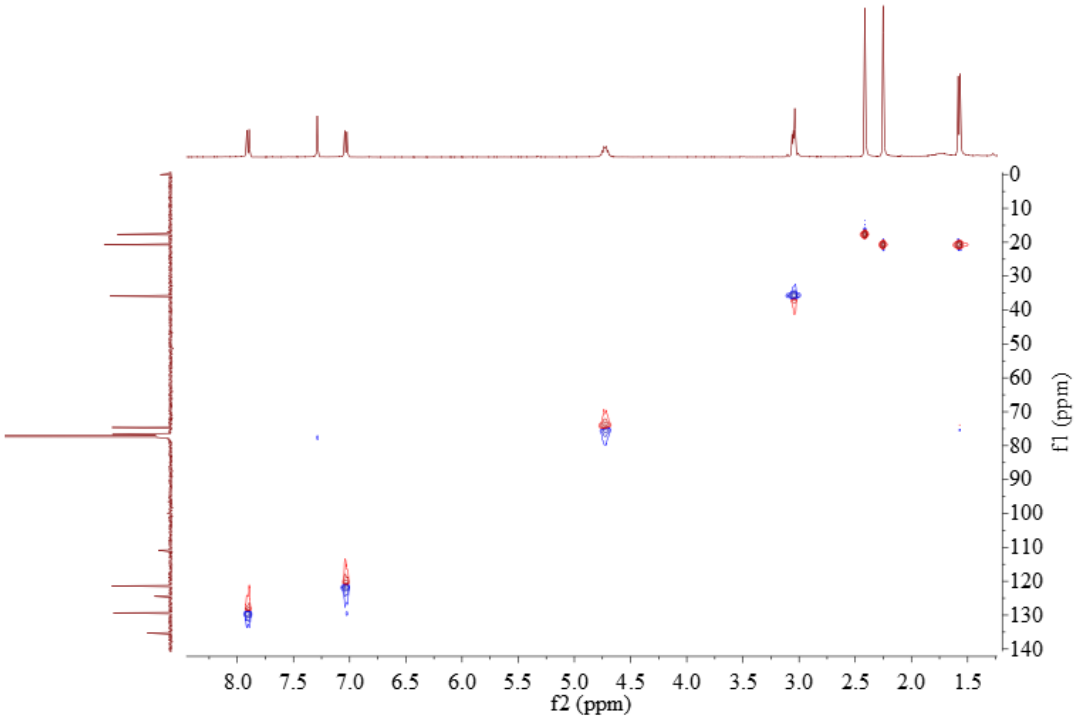


Figure S23 HSQC spectrum of **4** in $CDCl_3$

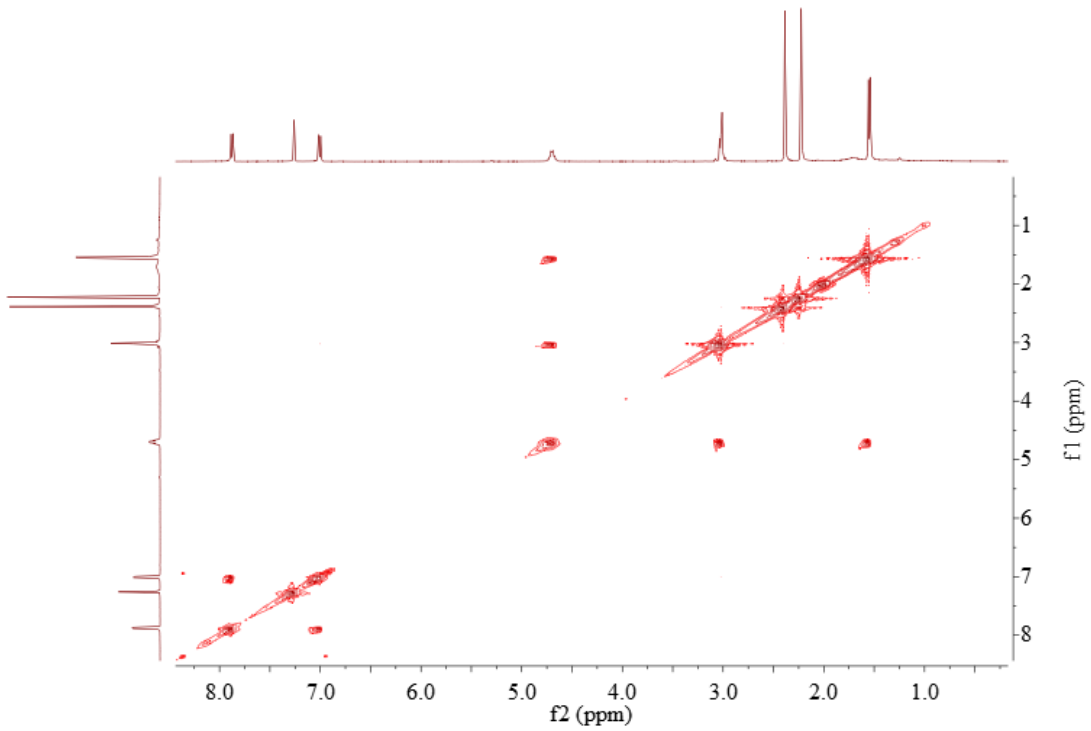


Figure S24 ^{1}H–^{1}H spectrum of **4** in $CDCl_3$

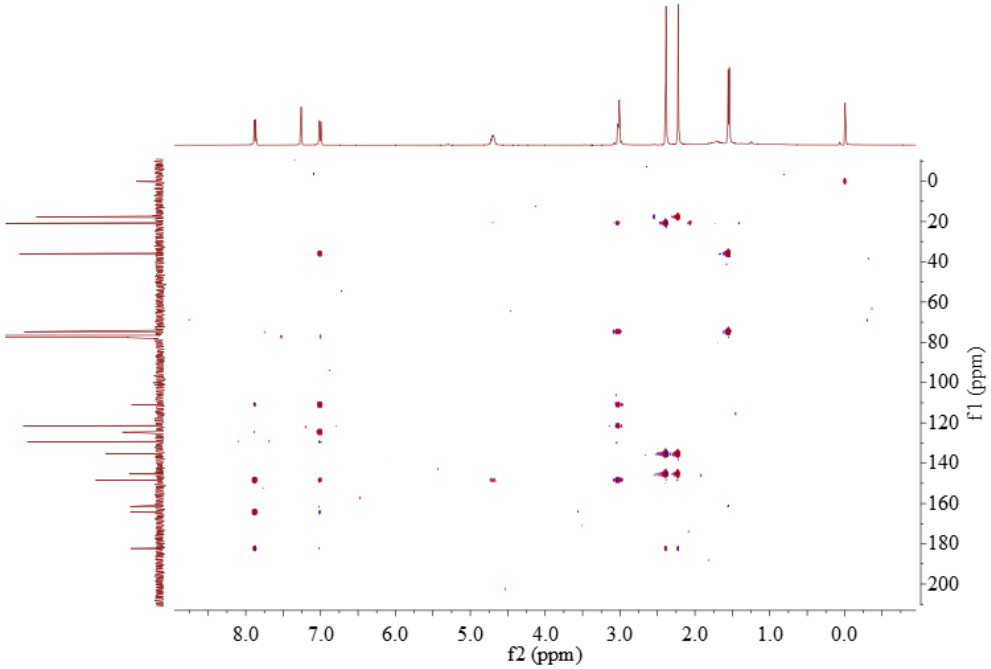


Figure S25 HMBC spectrum of **4** in $CDCl_3$

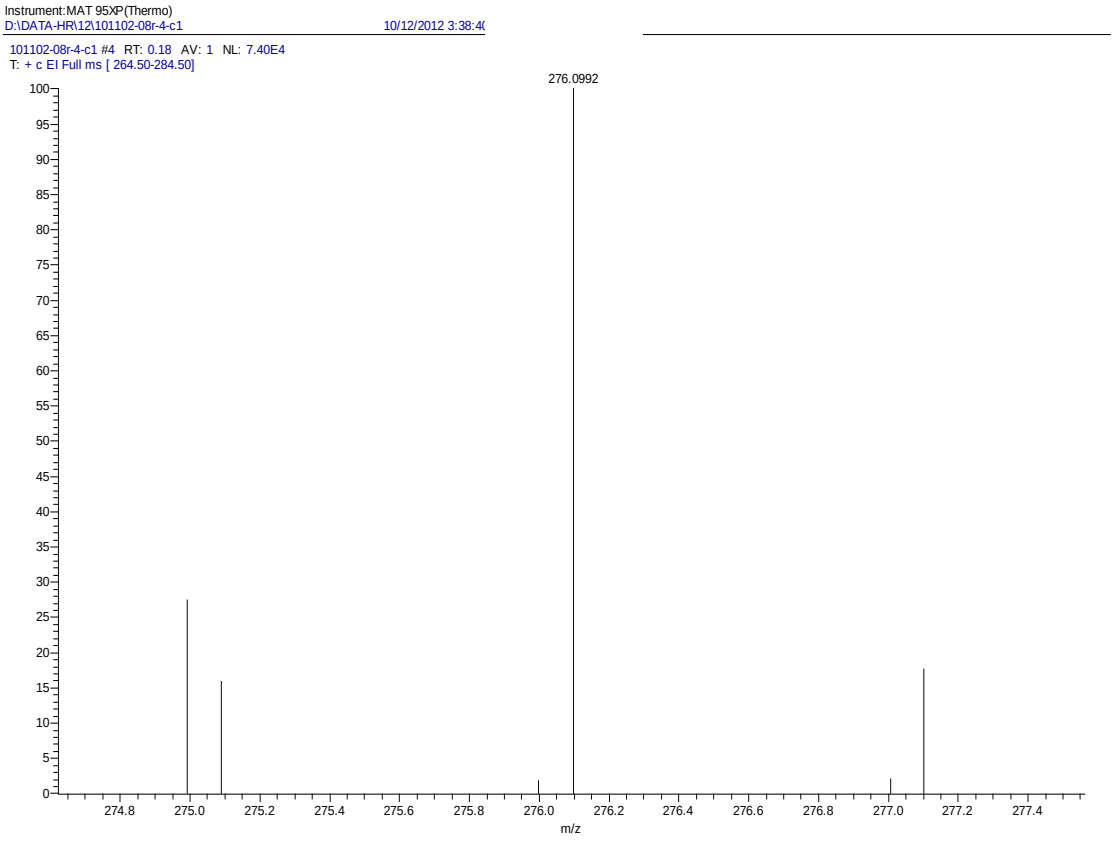


Figure S26 HREIMS spectrum of **5**

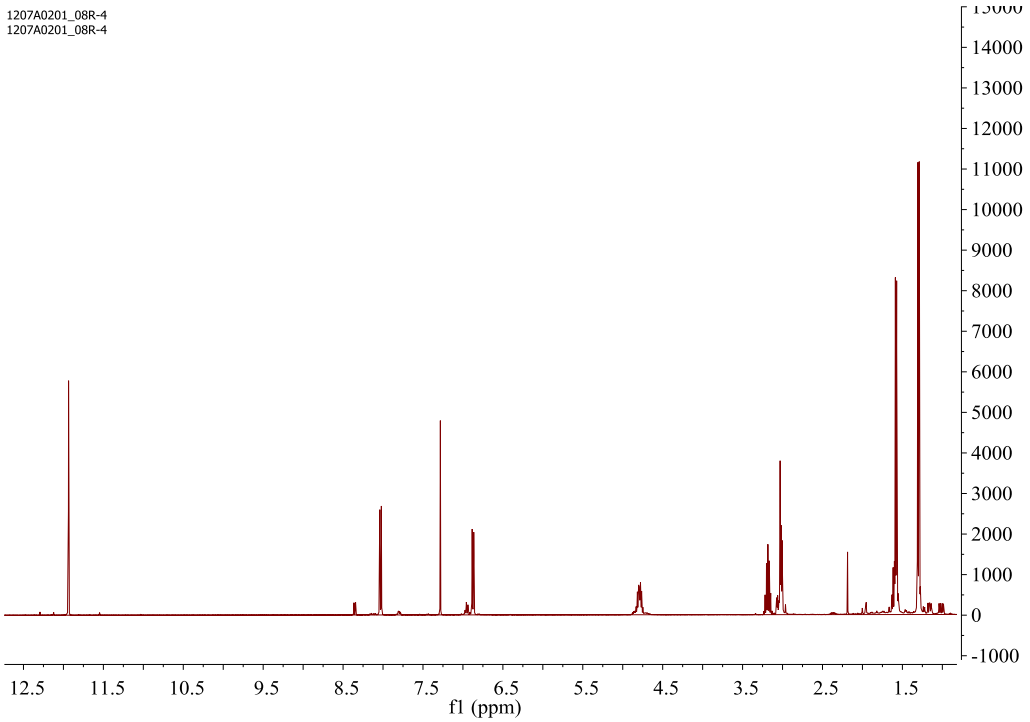


Figure S27 ^{1}H NMR spectrum of **5** in $CDCl_3$

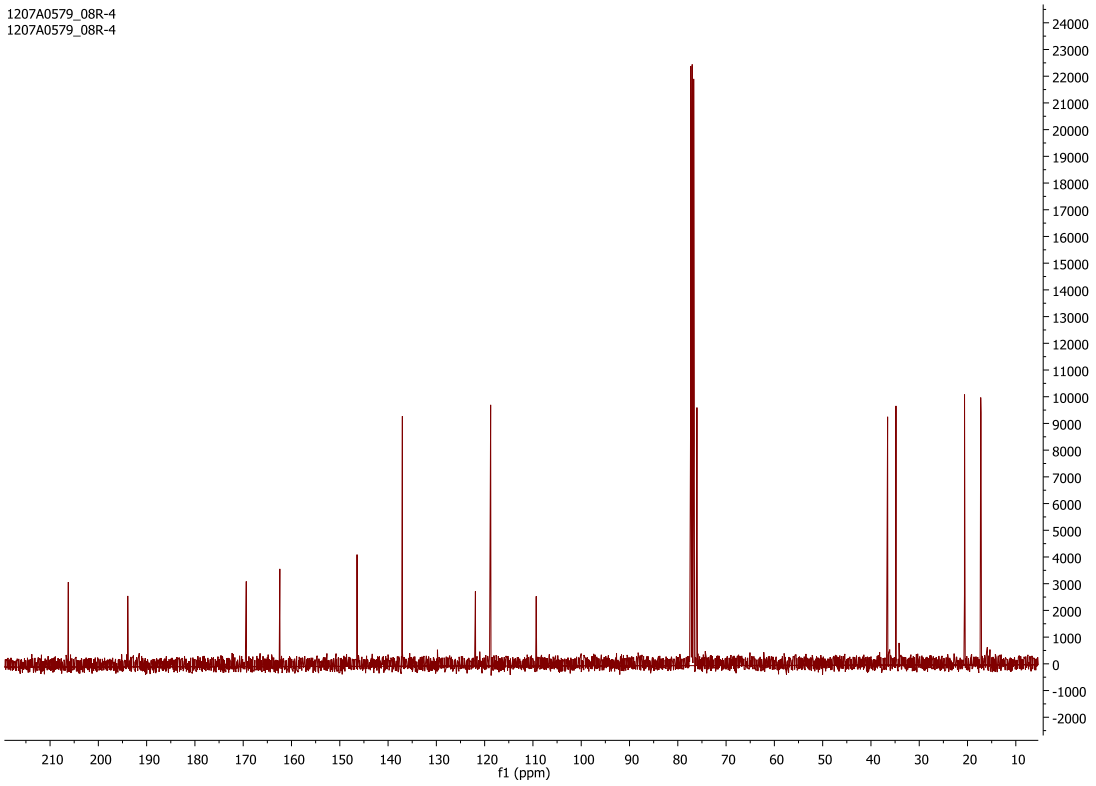


Figure S28 ^{13}C NMR spectrum of **5** in $CDCl_3$

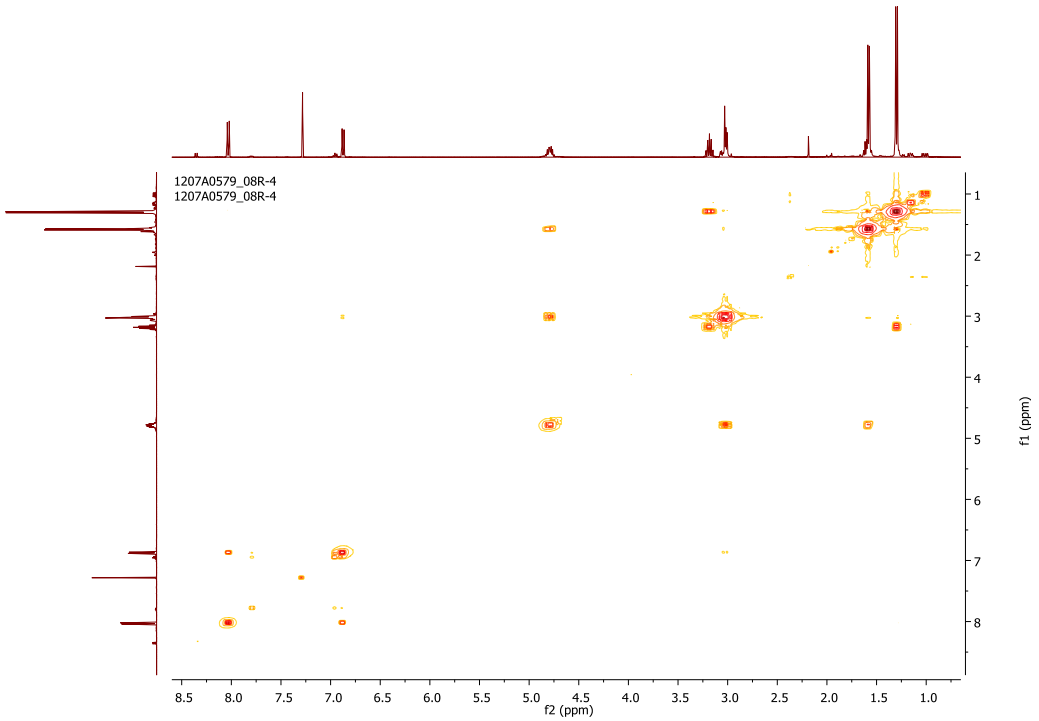


Figure S29 ^{1}H–^{1}H COSY spectrum of **5** in $CDCl_3$

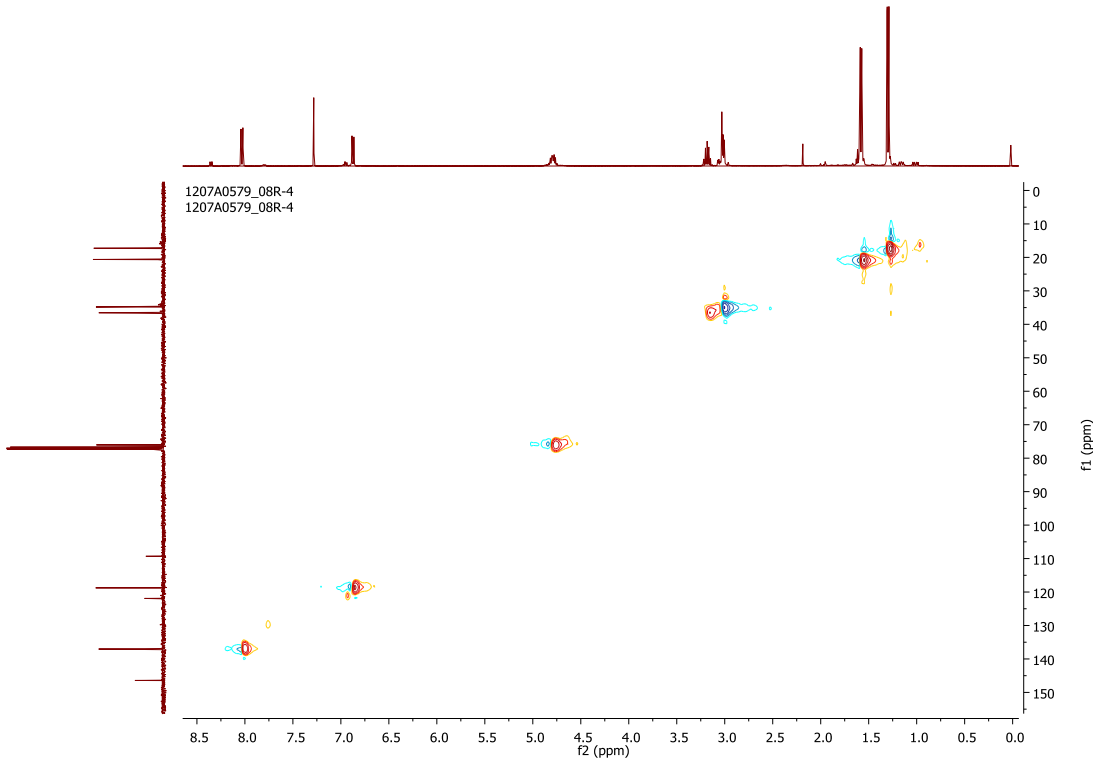


Figure S30 HSQC spectrum of **5** in $CDCl_3$

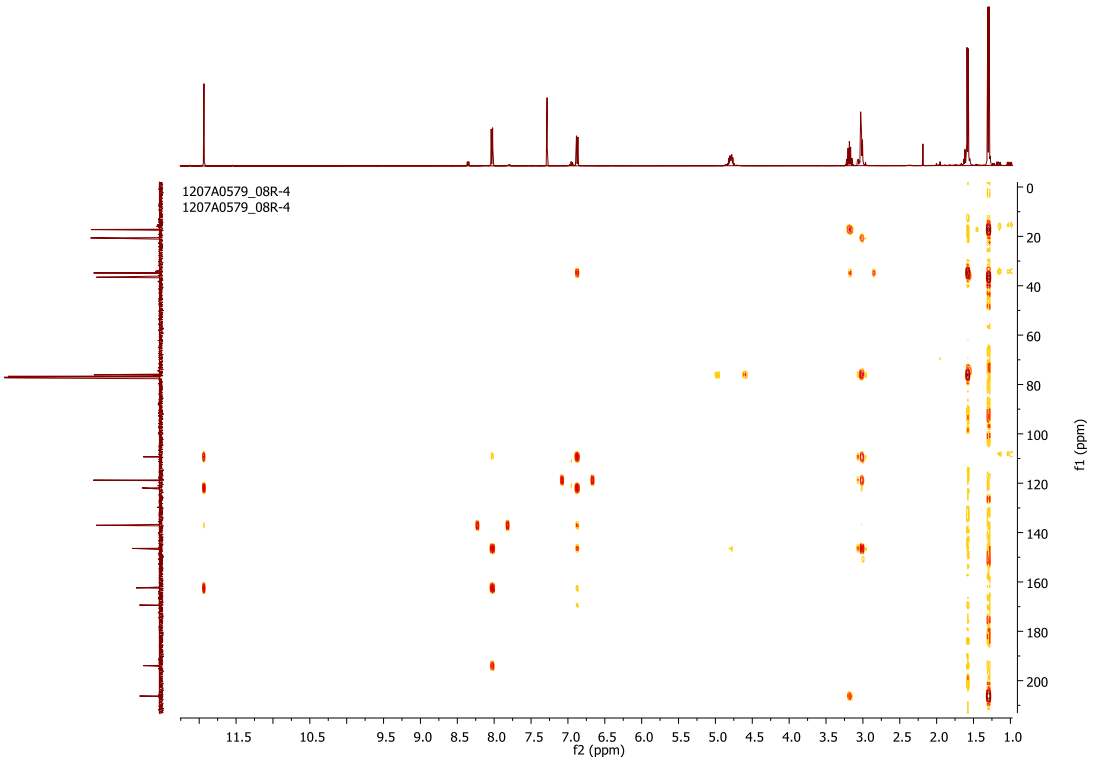


Figure S31 HMBC spectrum of **5** in $CDCl_3$

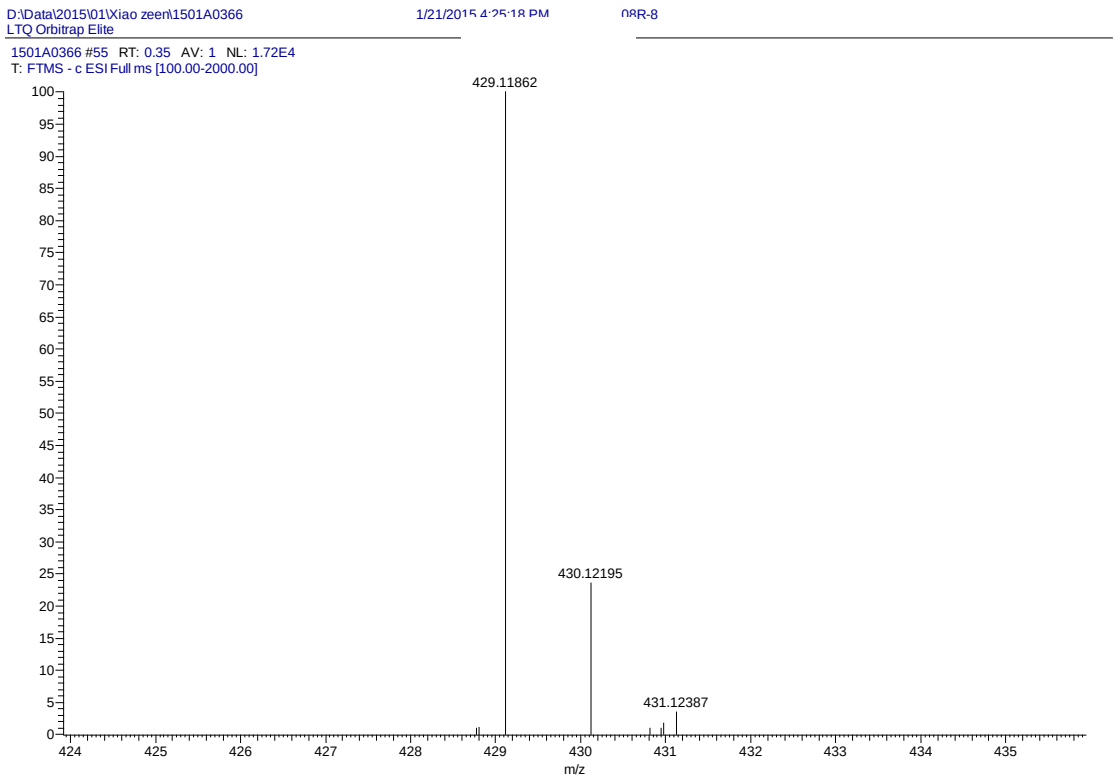


Figure S32 HRESIMS spectrum of **6**

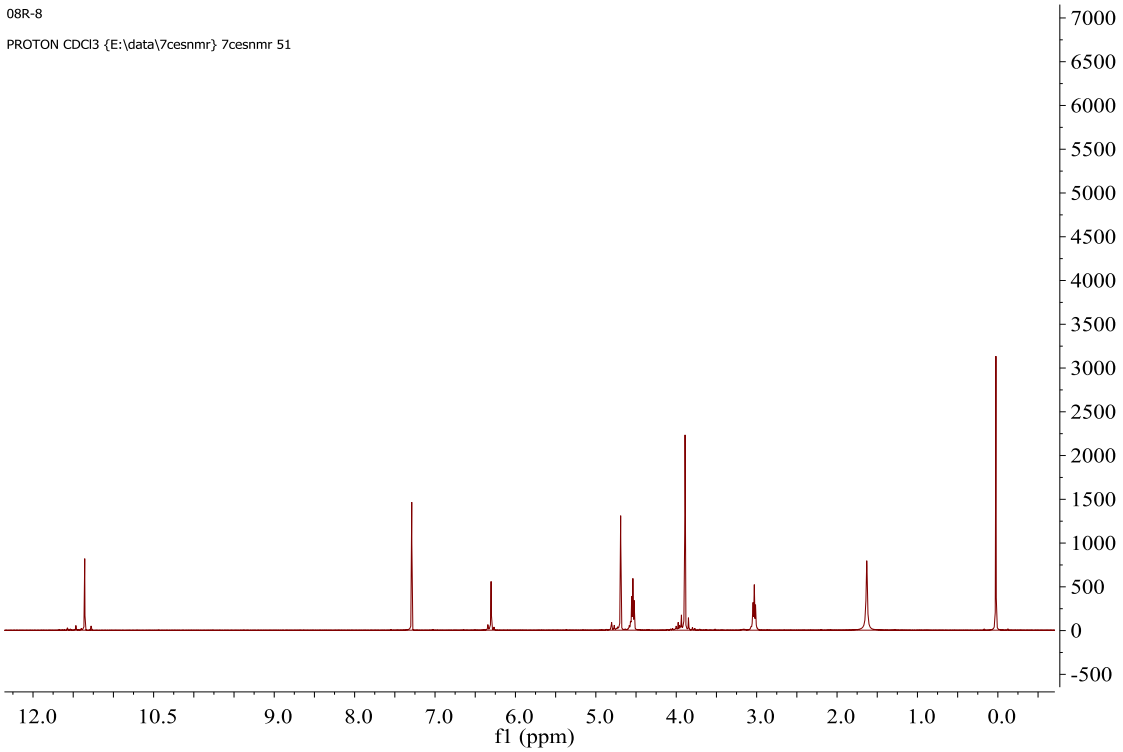


Figure S33 ^{1}H NMR spectrum of **6** in $CDCl_3$

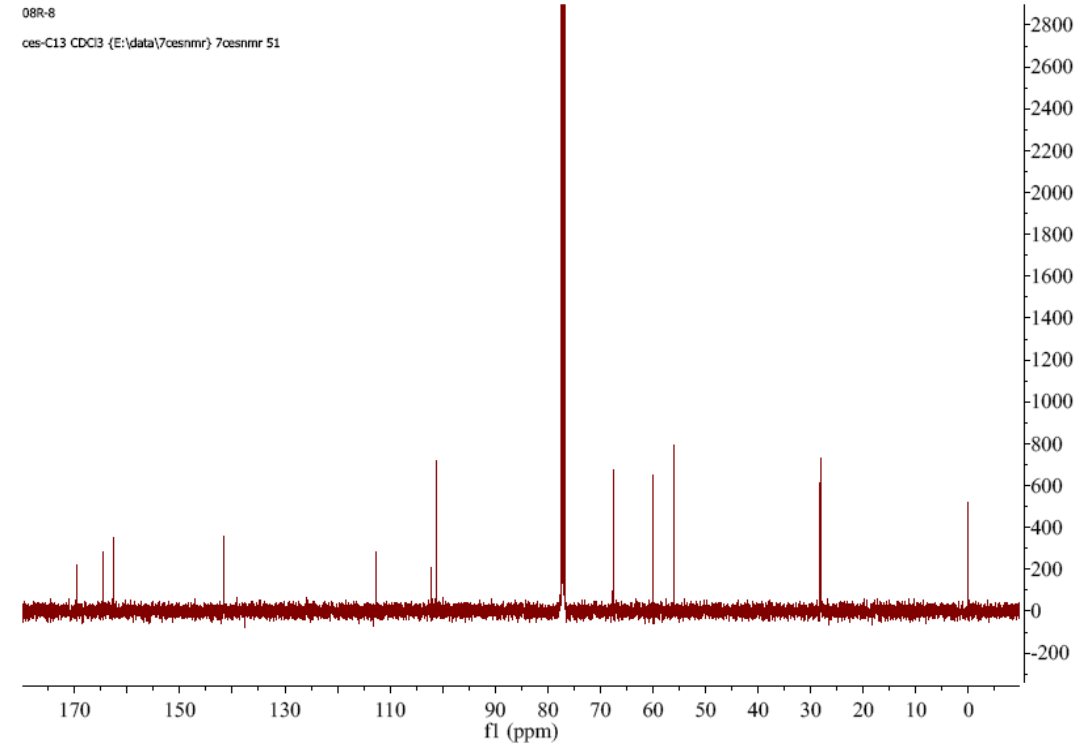


Figure S34 ^{13}C NMR spectrum of **6** in $CDCl_3$

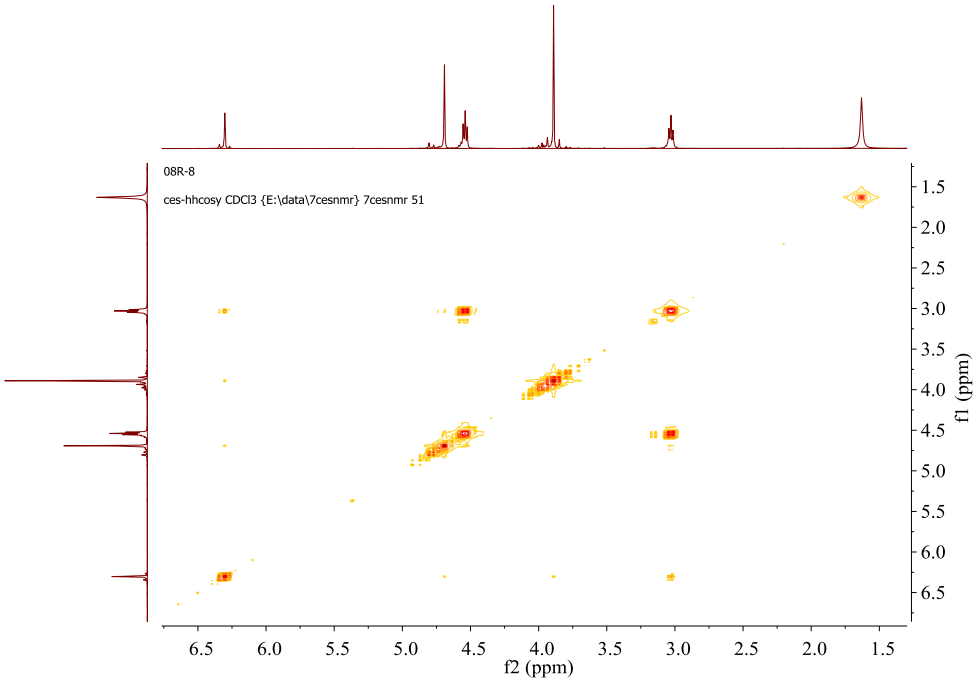


Figure S35 ^{1}H–^{1}H COSY spectrum of **6** in $CDCl_3$

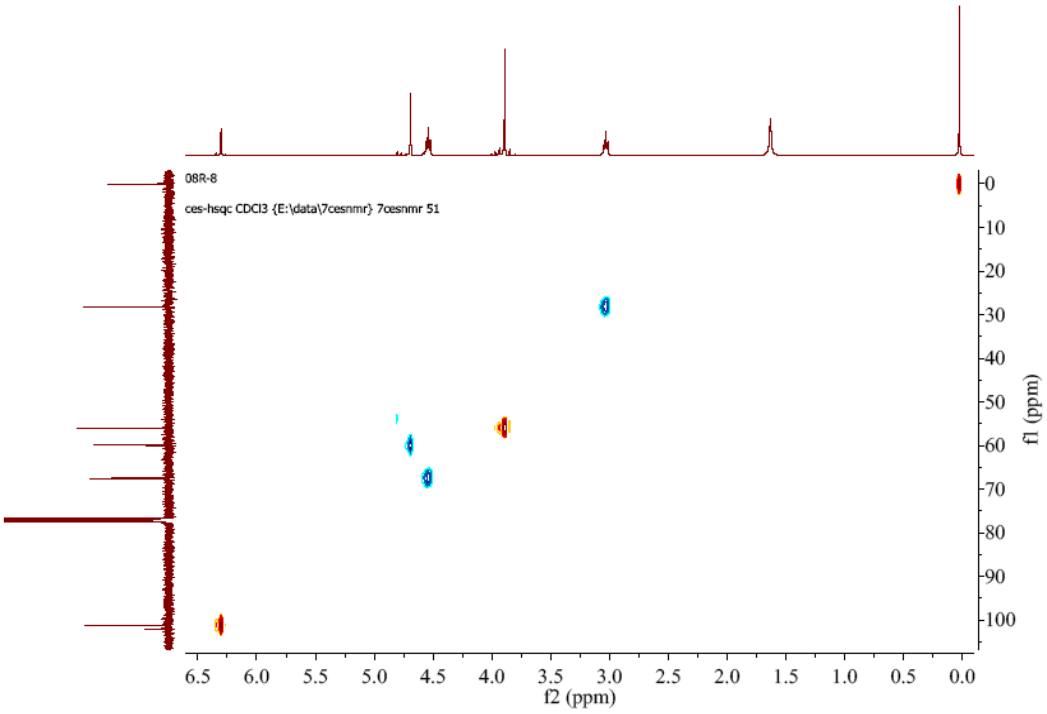


Figure S36 HSQC spectrum of **6** in $CDCl_3$

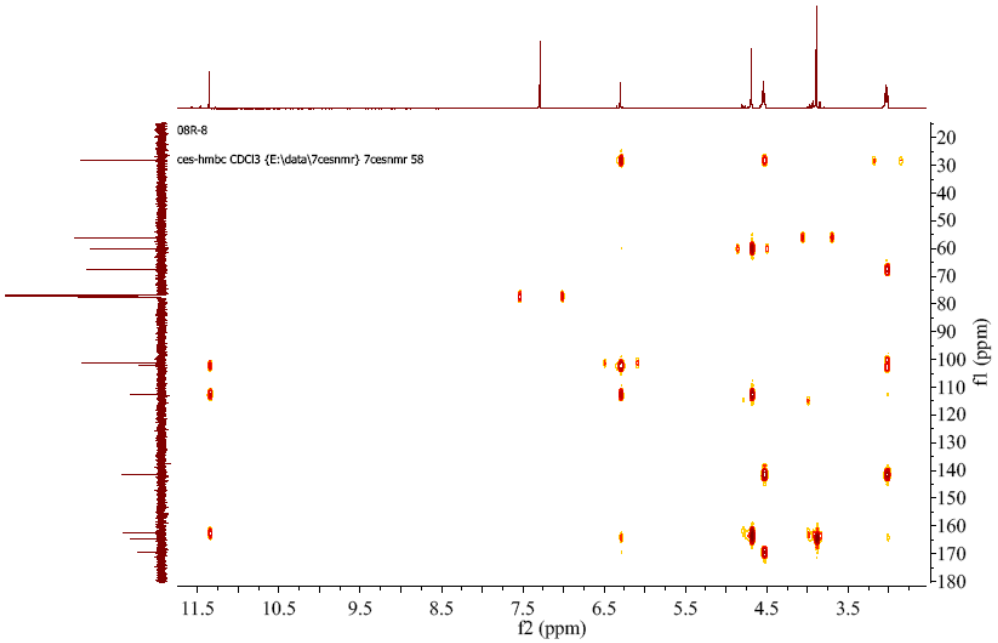


Figure S37 HMBC spectrum of **6** in $CDCl_3$