Supporting Information

Neobraclactones A–C, three unprecedented chaise longue-shaped xanthones from *Garcinia bracteata*

Sheng-Li Niu,[a,b†] Da-Hong Li,[a†] Yue-Tong Wang,[c] Kai-Bo Wang,[a] Bin Lin,[d] Yong-Kui Jing,[c] Hui-Ming Hua,[a] Jiao Bai[*a] and Zhan-Lin Li[*a]

[a] *Key Laboratory of Structure-Based Drug Design & Discovery, Ministry of Education; School of Traditional Chinese Materia Medica, Shenyang Pharmaceutical University, Shenyang 110016, P. R. China.*
[b] *Key laboratory of Zoonosis, Shengyang Agricultural University, Shenyang 110866, P. R. China*
[c] *School of Life Science and Biopharmaceutics, Shenyang Pharmaceutical University, Shenyang 110016, P. R. China*
[d] *School of Pharmaceutical Engineering, Shenyang Pharmaceutical University, Shenyang 110016, P. R. China*

Corresponding Author

* E-mail: lzl1030@hotmail.com
* E-mail: baijiao@hotmail.com
⊥ These authors contributed equally to this work.

Contents

Computational methods of ECD of compound 1

The CONFLEX[1, 2] searches based on molecular mechanics with MMFF94S force fields were performed for (6*R*, 7*R*, 8*R*, 17*R*, 22*S*)-**1** and its enantiomer (6*S*, 7*S*, 8*S*, 17*S*, 22*R*)-**1**, which gave 8 stable conformers. Selected conformers of (6*R*, 7*R*, 8*R*, 17*R*, 22*S*)-**1** and (6*S*, 7*S*, 8*S*, 17*S*, 22*R*)-**1** with the lowest energy were further optimized by the density functional theory method at the B3LYP/6-31+G** level in Gaussian 03 program package,[3] which was further checked by frequency calculation and resulted in no imaginary frequencies. The ECD of the conformer of **1** was then calculated by the TDDFT method at the B3LYP/6-31+G** level, and at the B3LYP/6-311++G**//B3LYP/6-31+G** levels with the PCM model in methanol solution. The calculated ECD curve was generated using SpecDis 1.51[4] with σ = 0.16 ev, and UV shift -5 nm.

References

[1] Goto, H.; Osawa, E.; *J. Am. Chem. Soc.*1989, ***111***, 8950–8951.

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[3]. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb,M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.;Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.;Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.;Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.;Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li,X.; Knox, J. E.; Hratchian, H. P.; 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.; Ayala, P. Y.; Morokuma, K.;Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich,S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.;Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.;Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz,P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.;Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson,B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, revision D.01; Gaussian, Inc.: Wallingford, CT, 2005.

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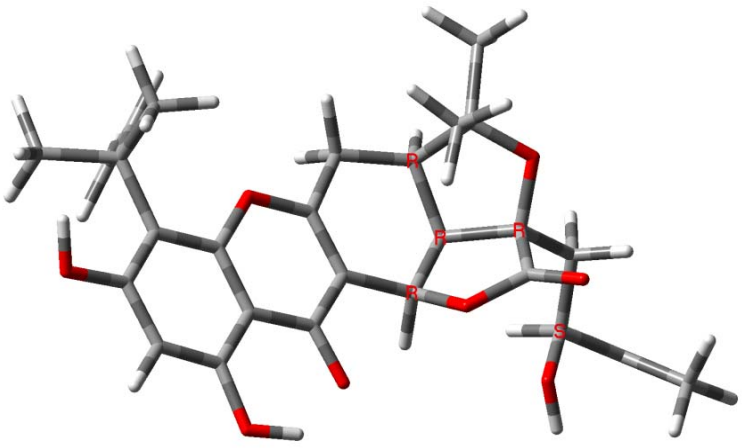


Figure S1. B3LYP/6-31+G** optimized lowest energy 3D conformer of **1**

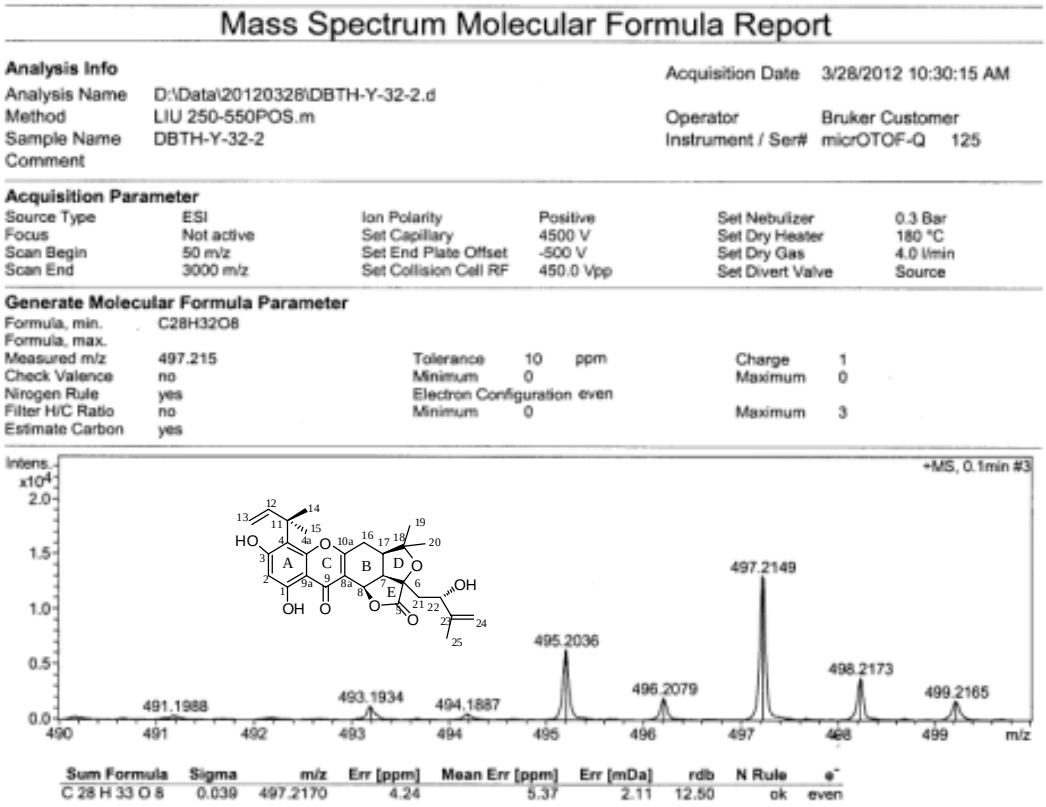


Figure S2. The HR-ESIMS spectrum of neobraclactone A (**1**)

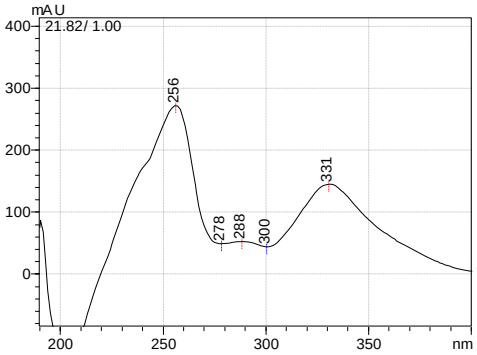


Figure S3. The UV spectrum of neobraclactone A (**1**) in CH_3OH

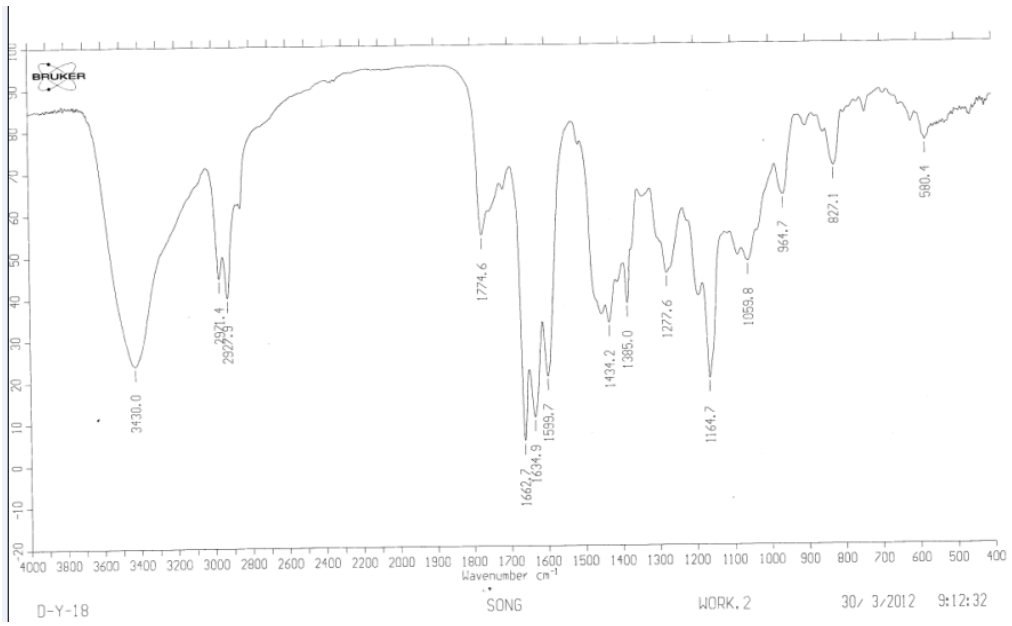


Figure S4. The IR spectrum of neobraclactone A (**1**)

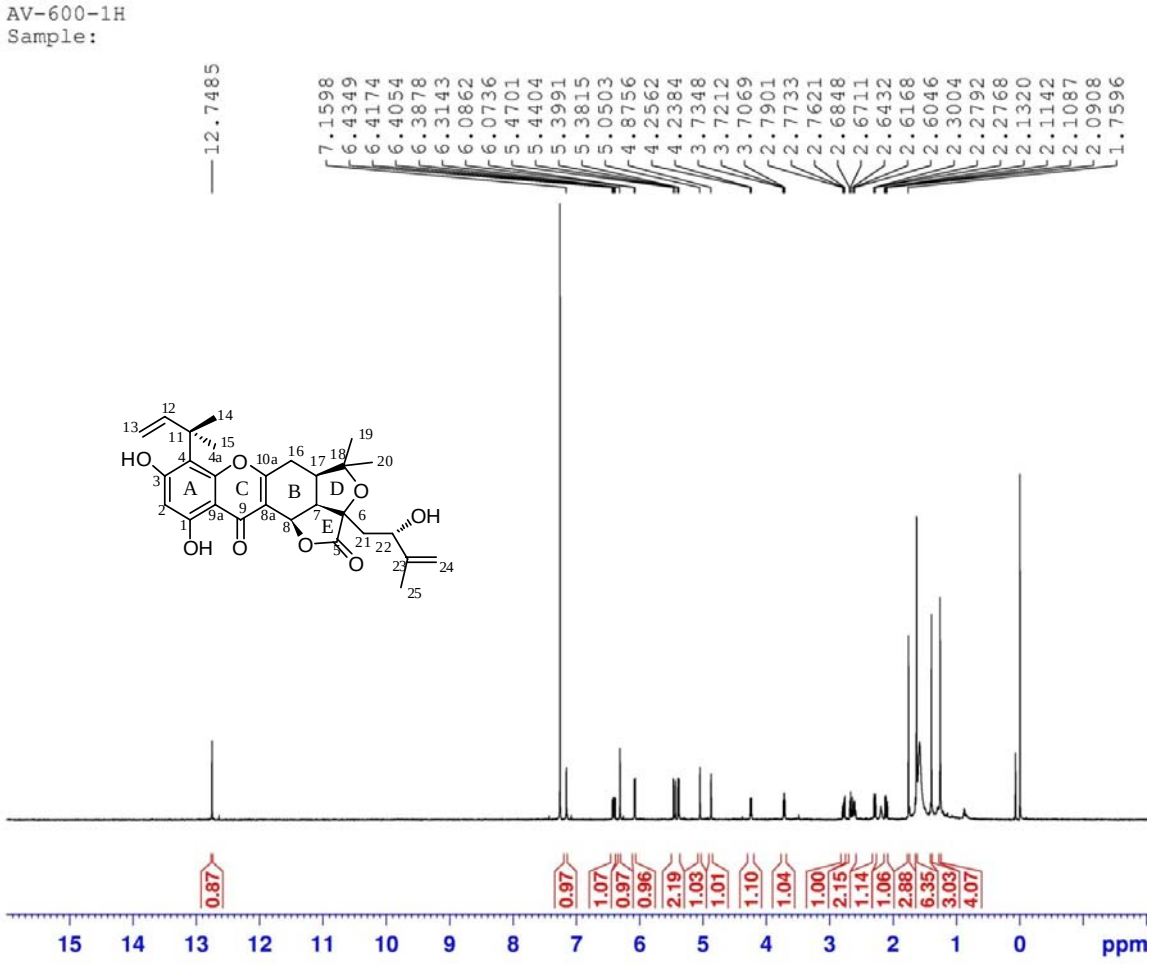


Figure S5. The ^{1}H NMR spectrum of neobraclactone A (**1**) in $CDCl_3$

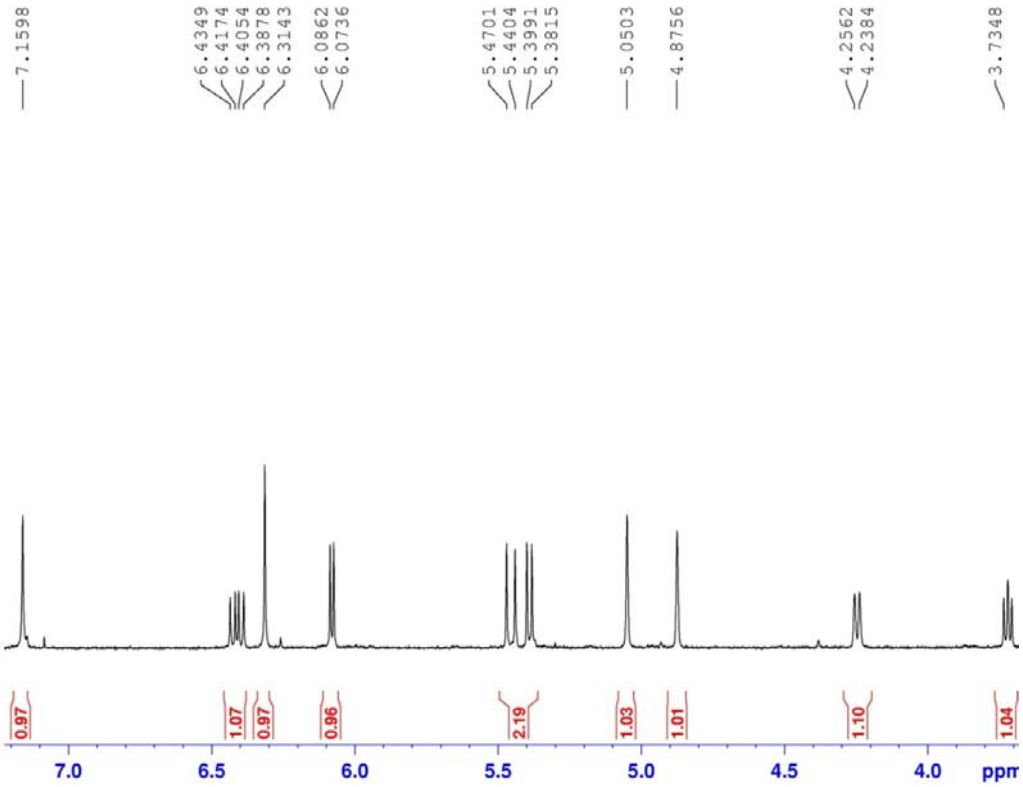


Figure S6. The expanded ^{1}H NMR spectrum of neobraclactone A (**1**) in $CDCl_3$

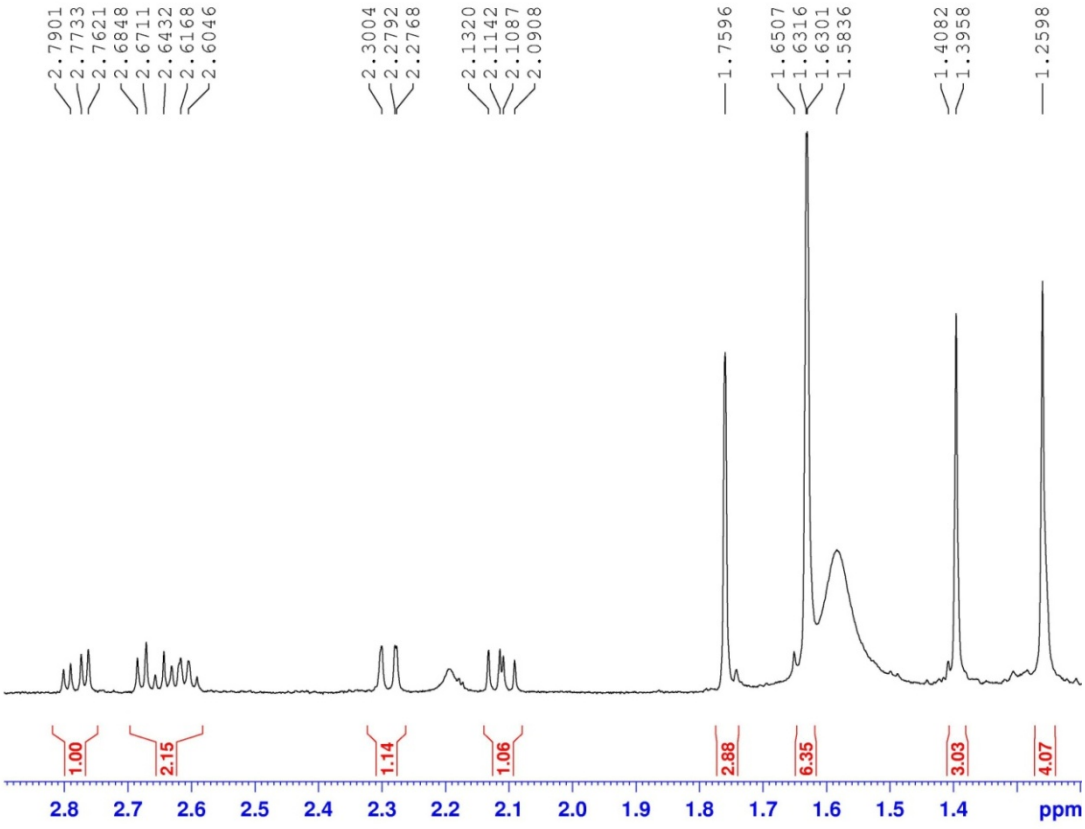


Figure S7. The expanded ^{1}H NMR spectrum of neobraclactone A (**1**) in $CDCl_3$

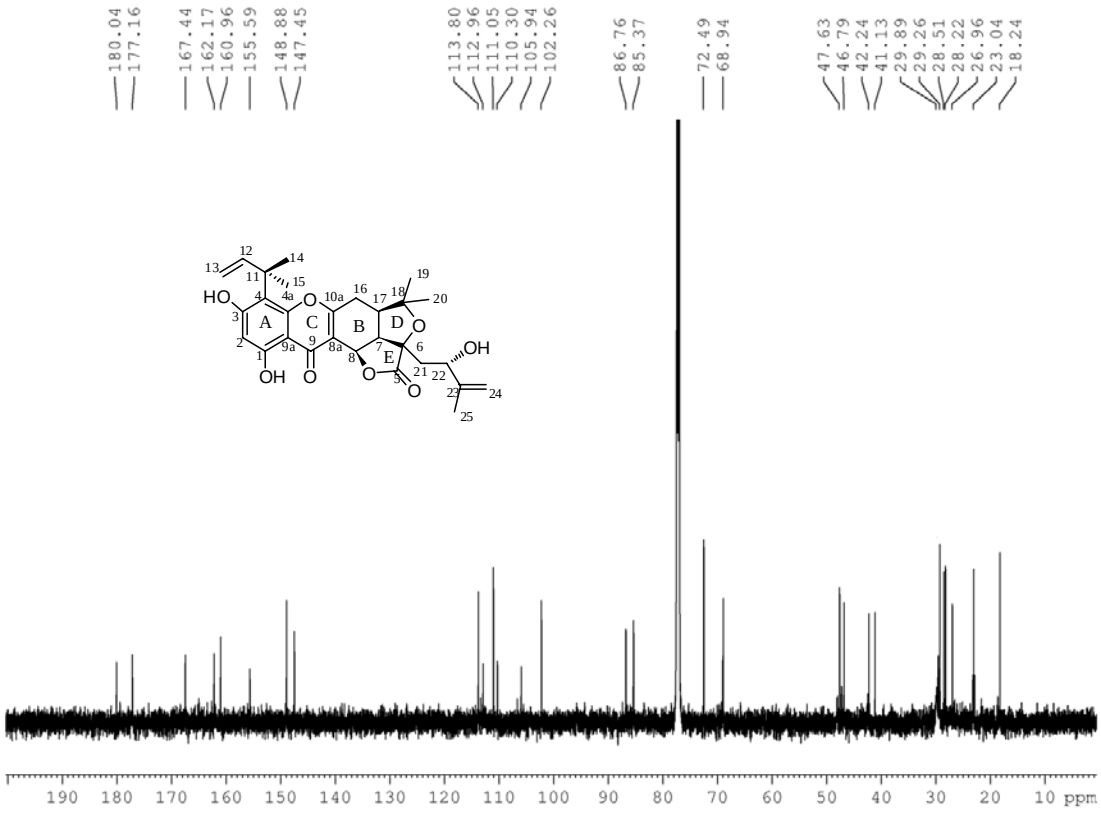


Figure S8. The ^{13}C NMR spectrum of neobraclactone A (**1**) in $CDCl_3$

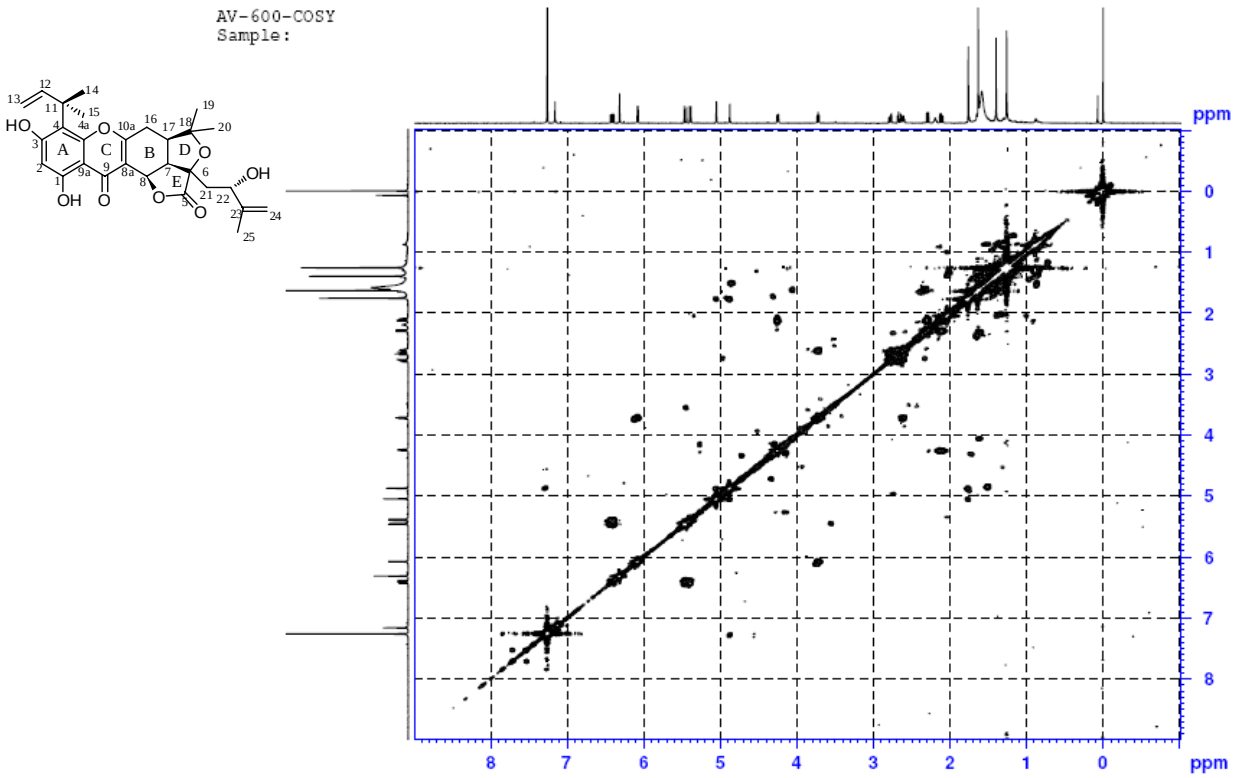


Figure S9. The ^{1}H-^{1}H COSY spectrum of neobraclactone A (**1**) in $CDCl_3$

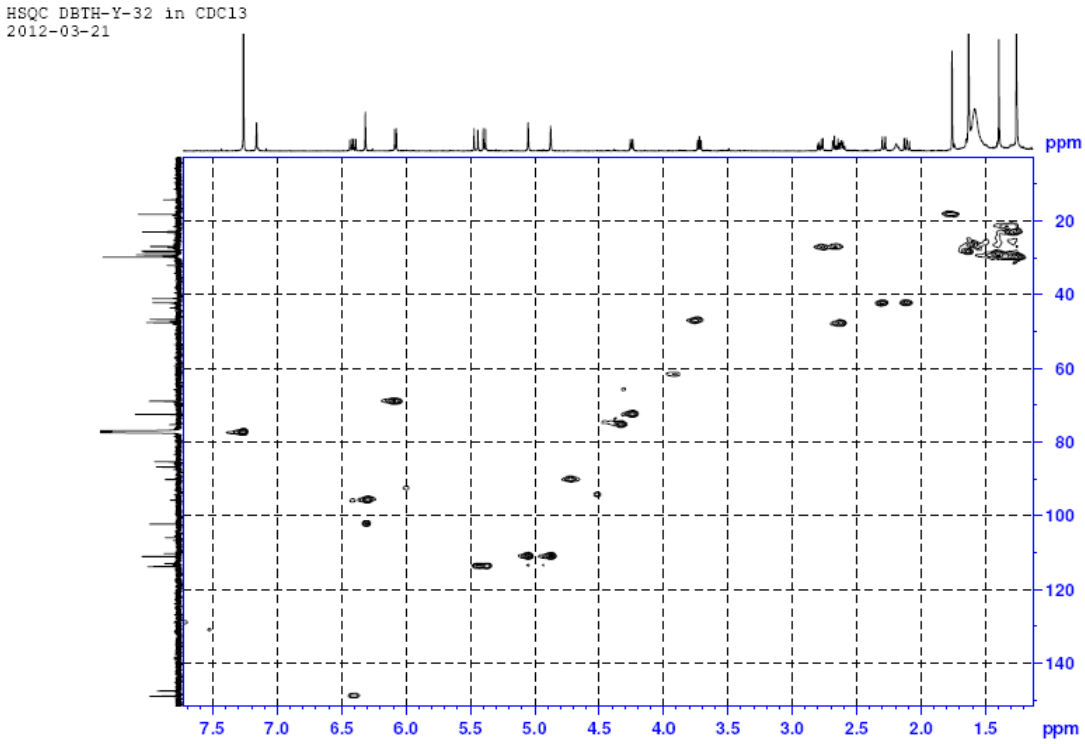
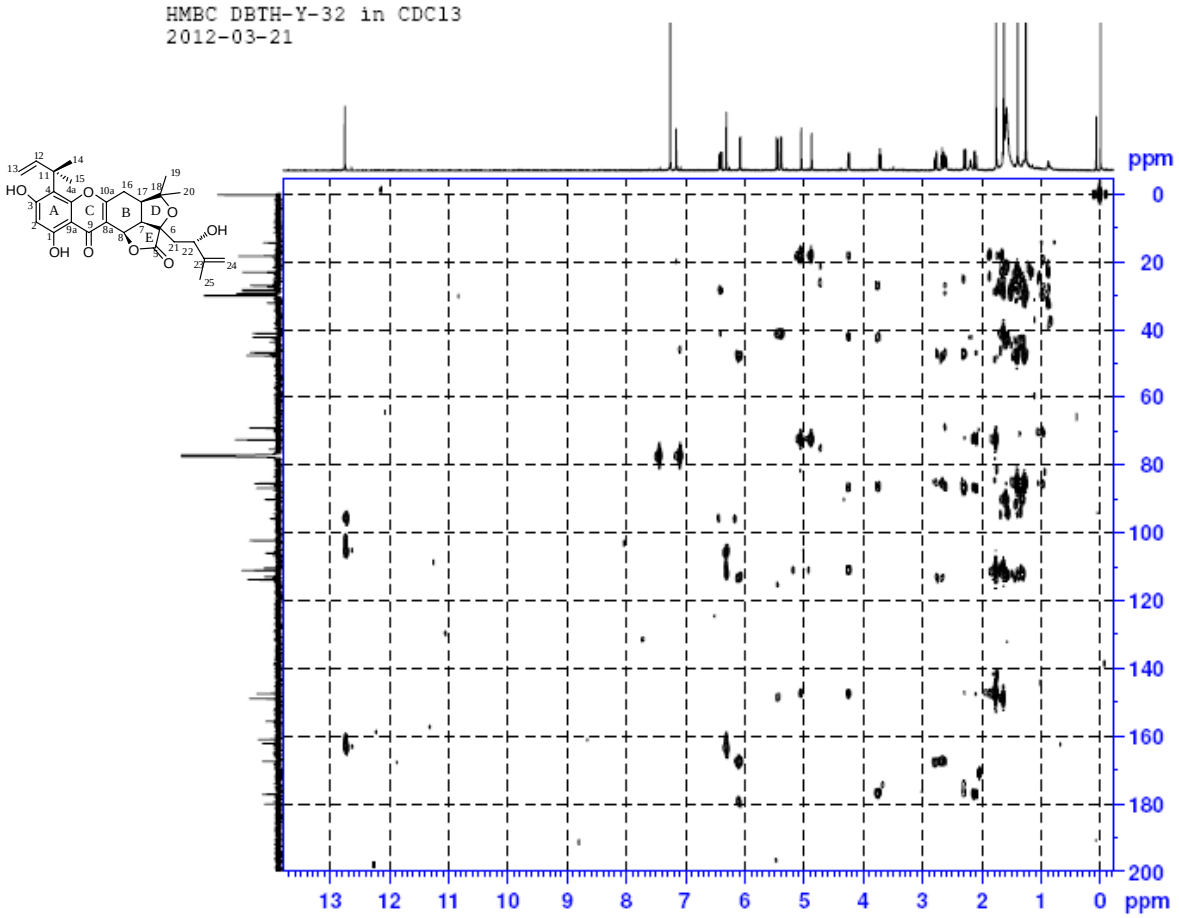


Figure S10. The HSQC spectrum of neobraclactone A (**1**) in $CDCl_3$



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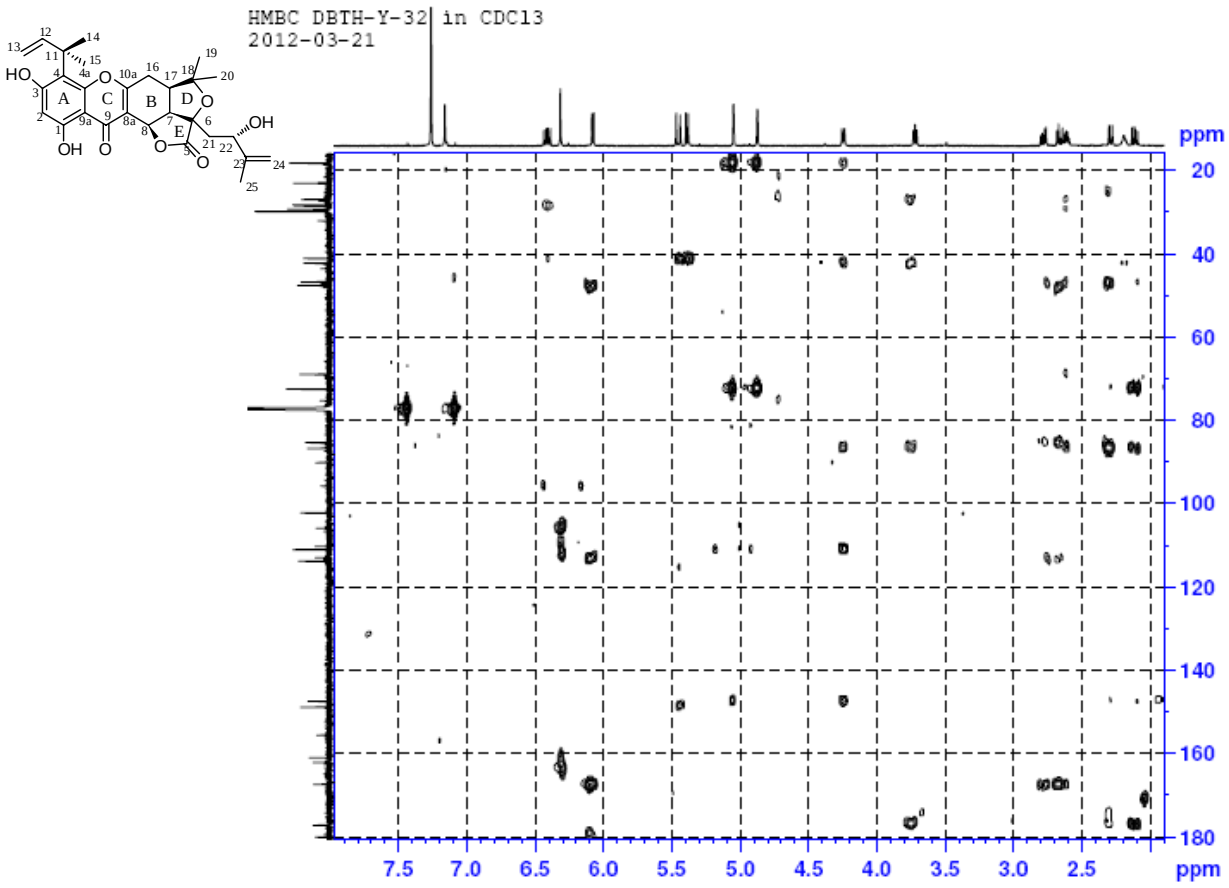


Figure S12. The expanded HMBC spectrum of neobraclactone A (**1**) in $CDCl_3$

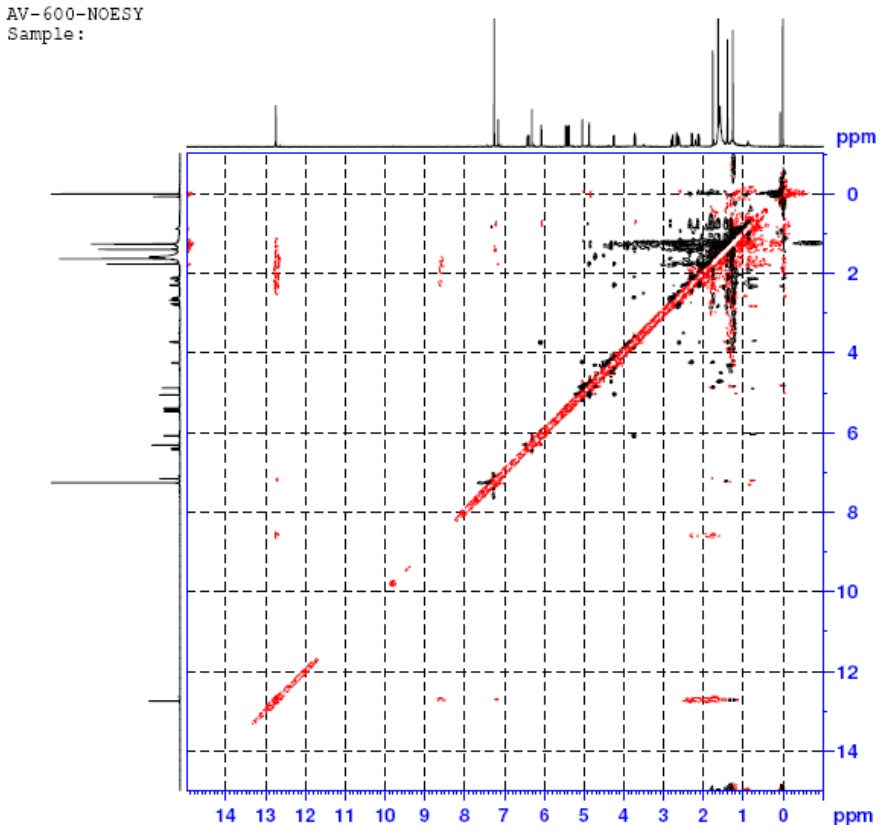


Figure S13. The NOESY spectrum of neobraclactone A (**1**) in $CDCl_3$

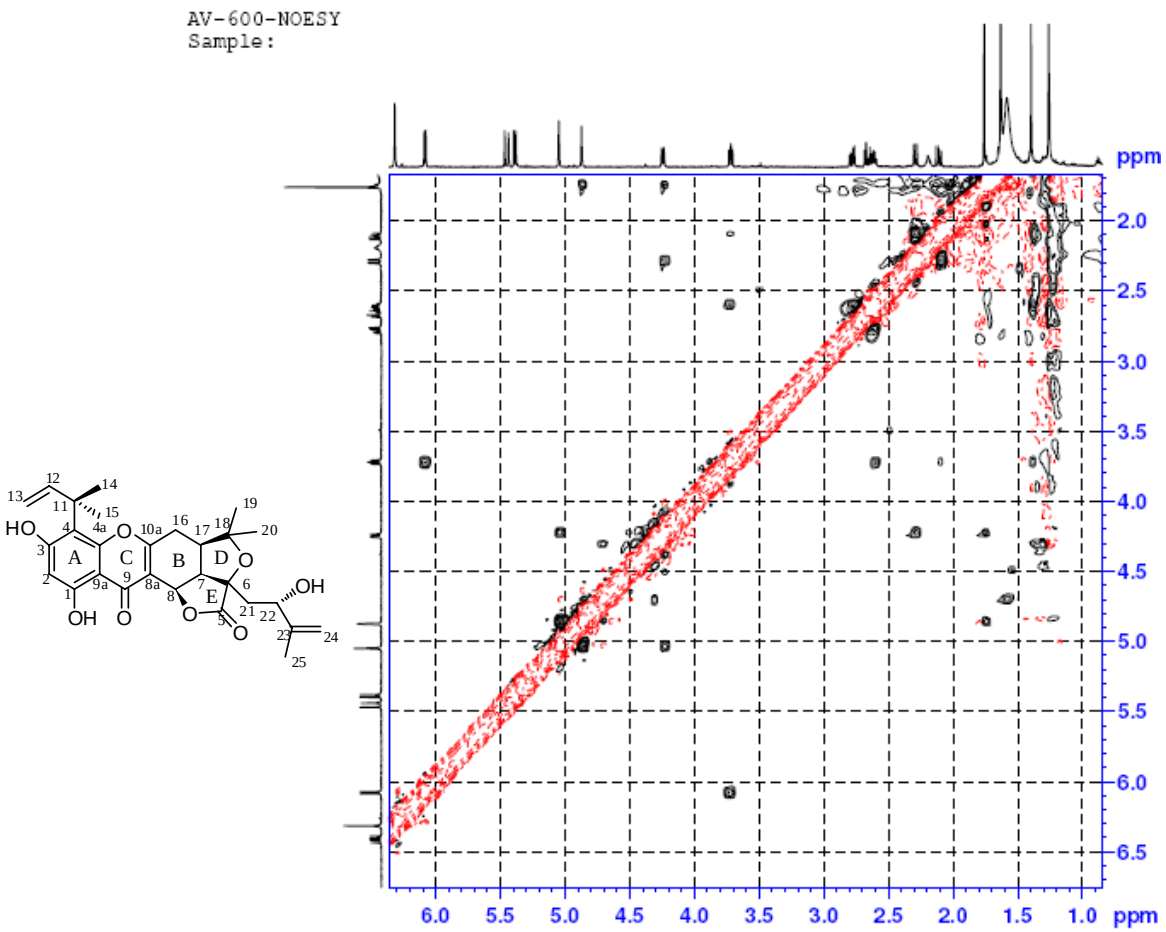


Figure S14. The expanded NOESY spectrum of neobraclactone A (**1**) in $CDCl_3$

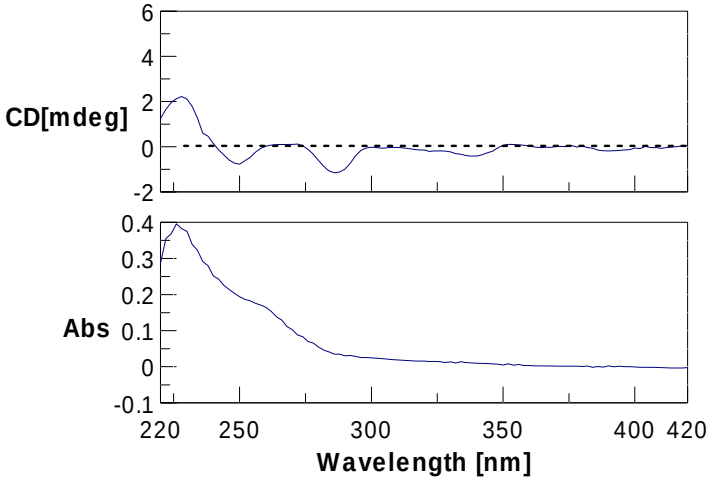


Figure S15. ECD spectrum of neobraclactone A (**1**)

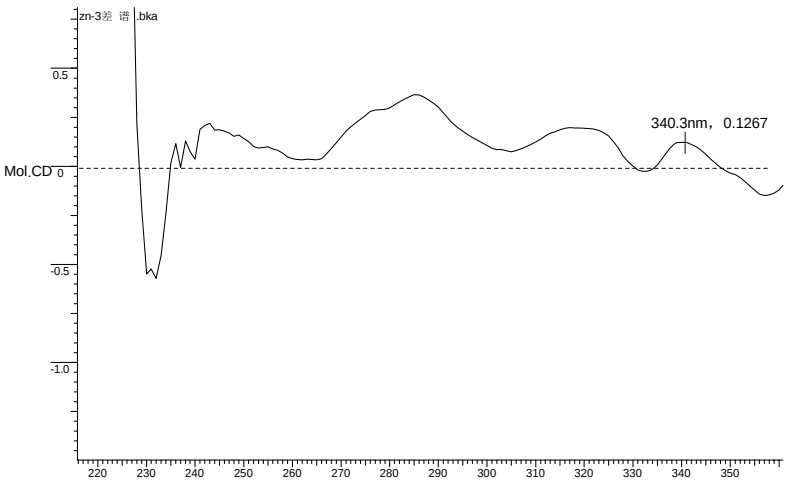


Figure S16. The $Rh_2(OCOCF_3)_4$ induced ECD spectrum of neobraclactone A (**1**)

Figure S17. The bulkiness rule for secondary alcohols applied

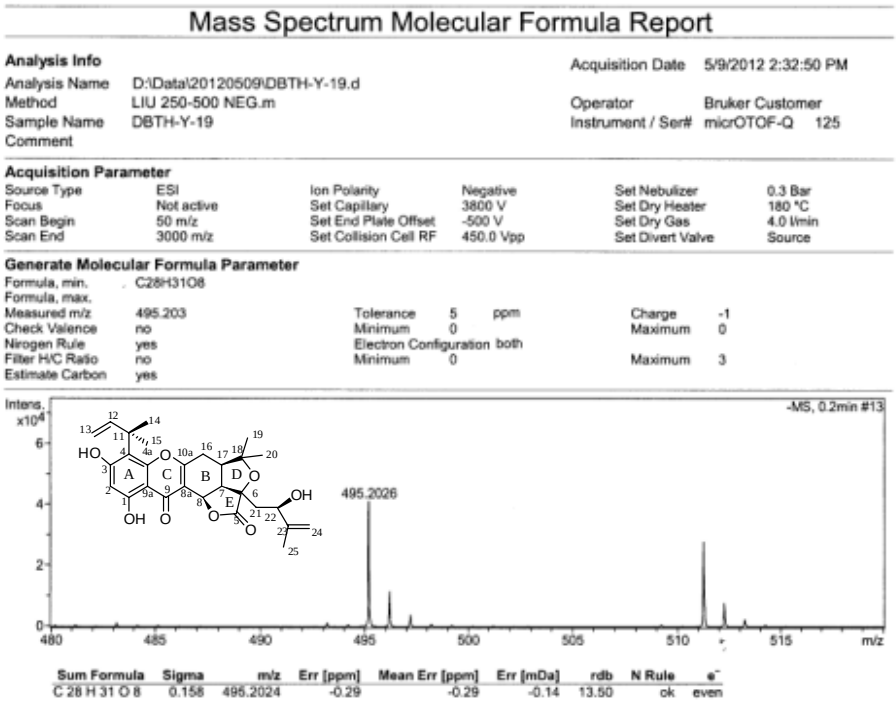


Figure S18. The HR-ESIMS spectrum of neobraclactone B (**2**)

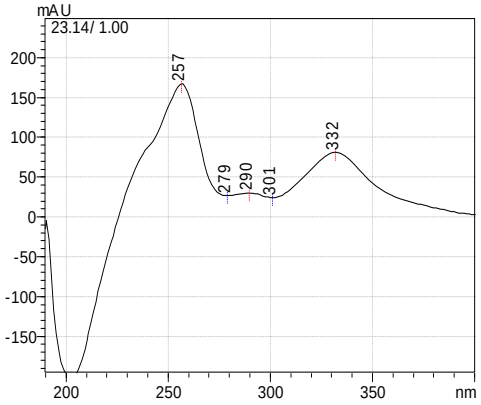
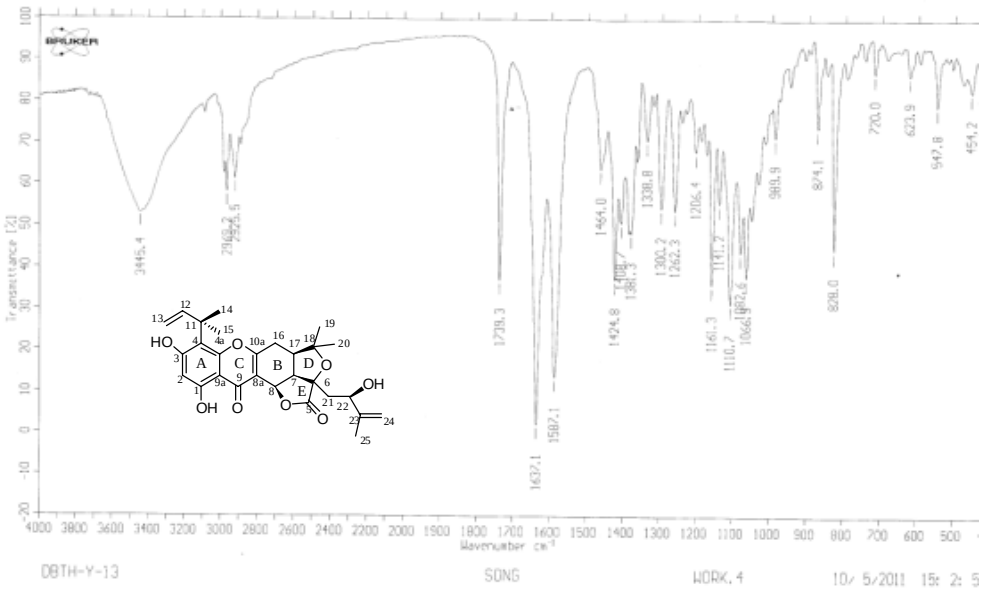


Figure S19. The UV spectrum of neobraclactone B (**2**)



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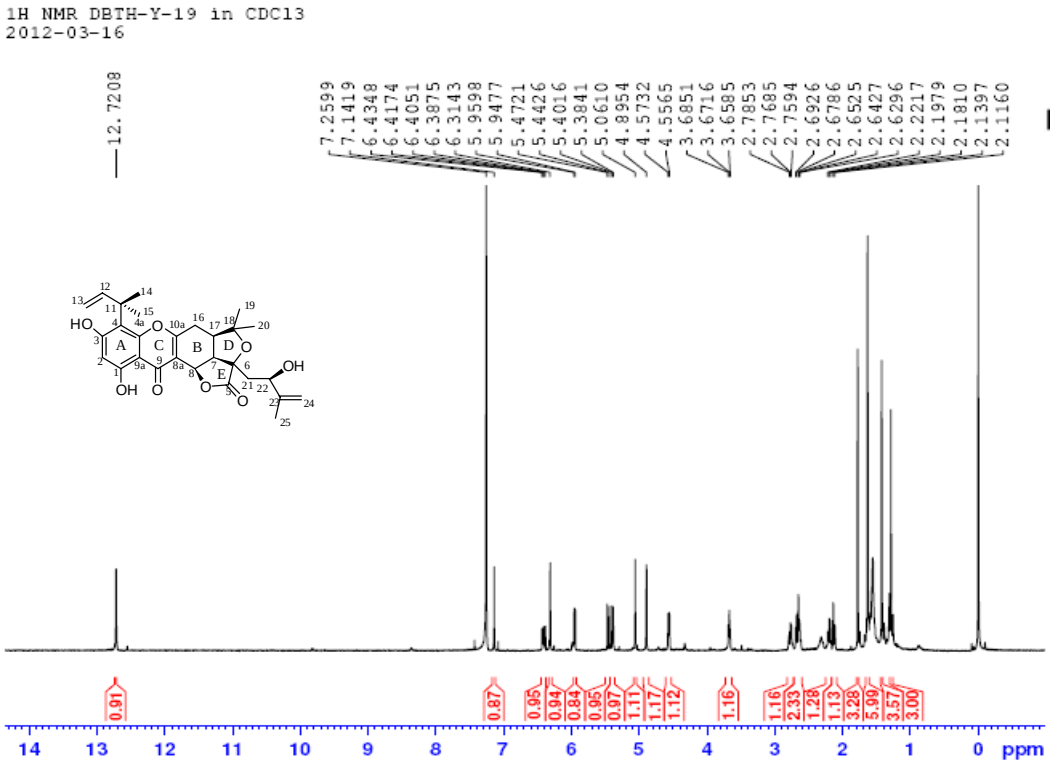

Figure S21. The ^{1}H NMR spectrum of neobraclactone B (**2**) in $CDCl_3$

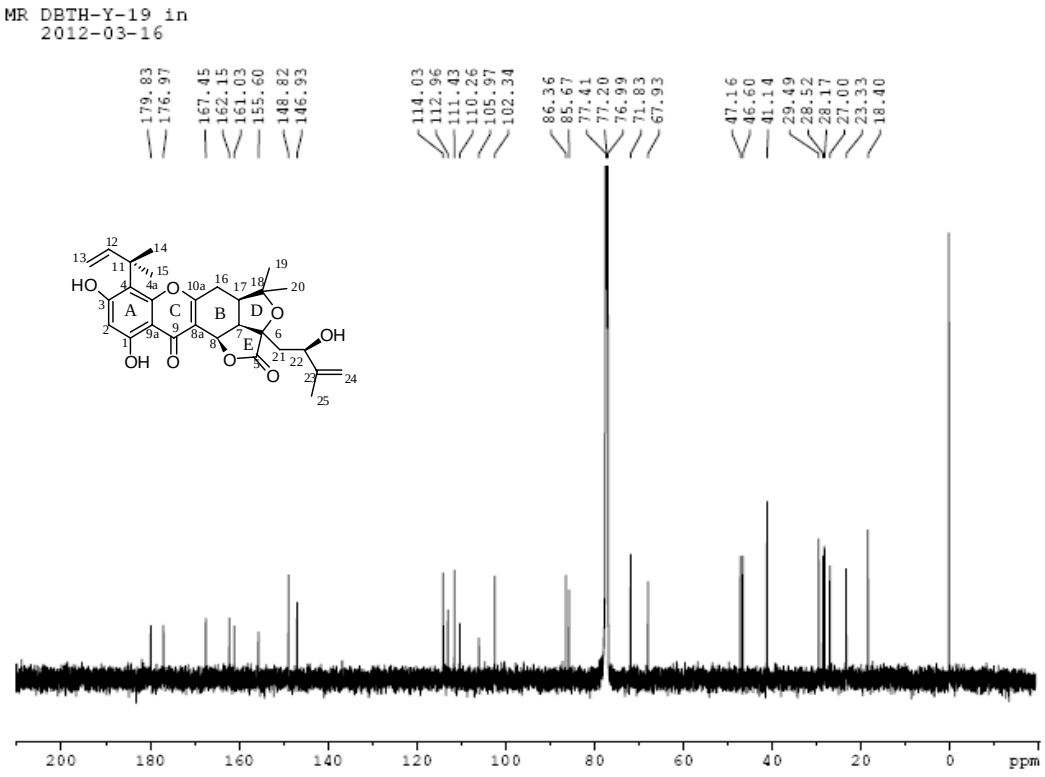

Figure S22. The ^{13}C NMR spectrum of neobraclactone B (**2**) in $CDCl_3$

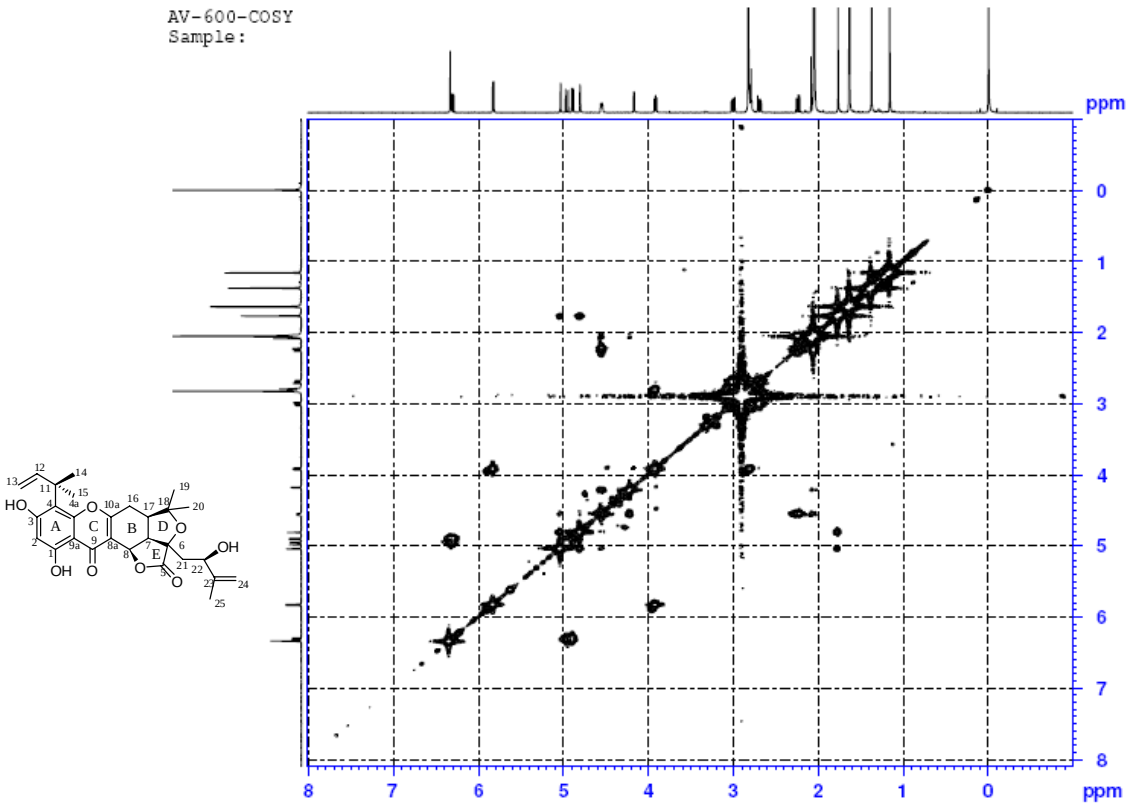

Figure S23. The ^{1}H-^{1}H COSY spectrum of neobraclactone B (**2**) in $CDCl_3$

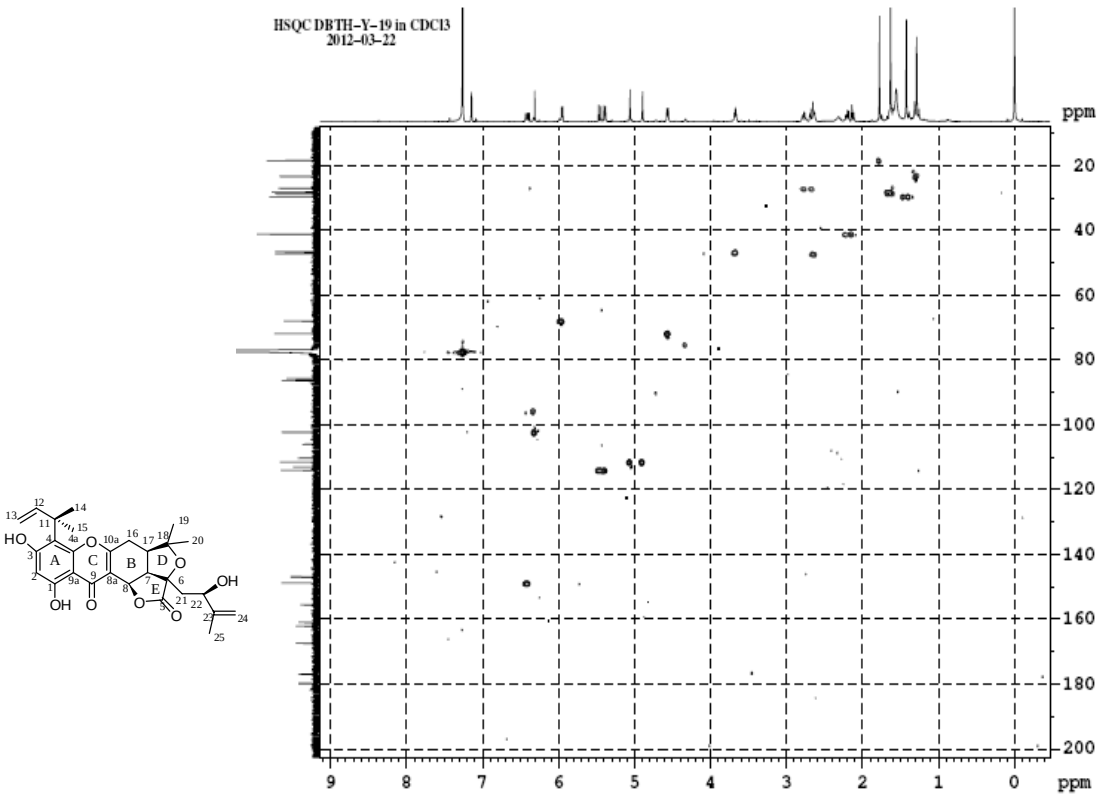

Figure S24. The HSQC spectrum of neobraclactone B (**2**) in $CDCl_3$

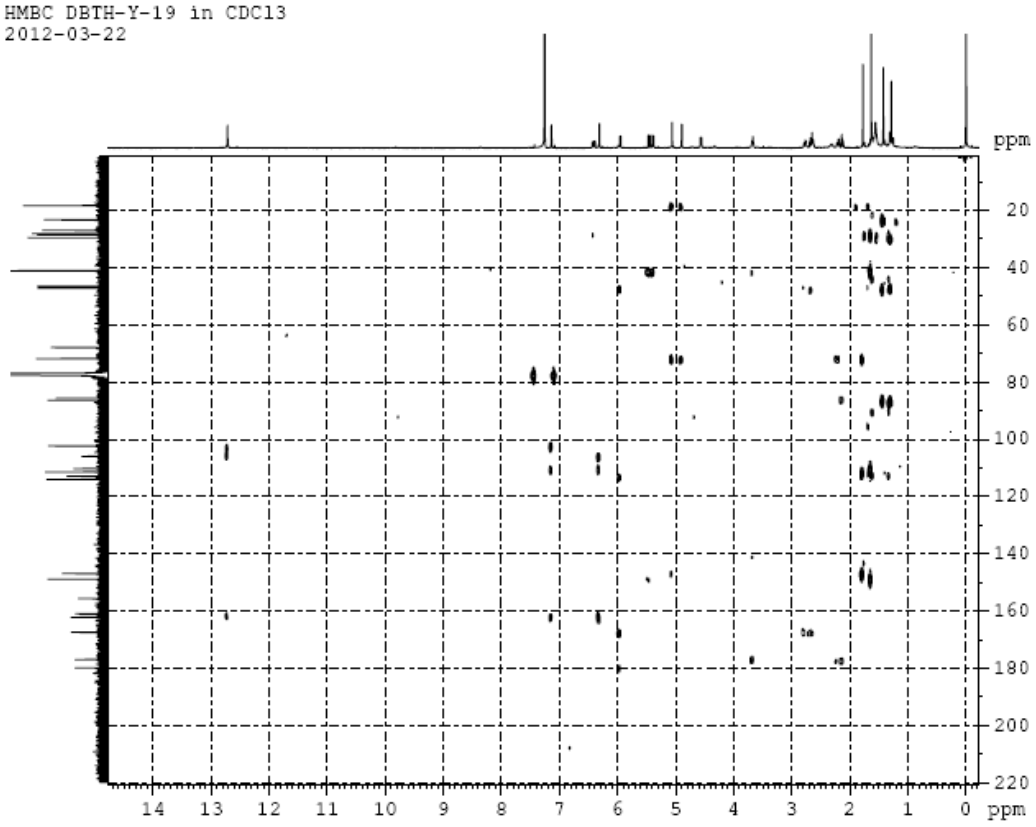

Figure S25. The HMBC spectrum of neobraclactone B (**2**) in $CDCl_3$

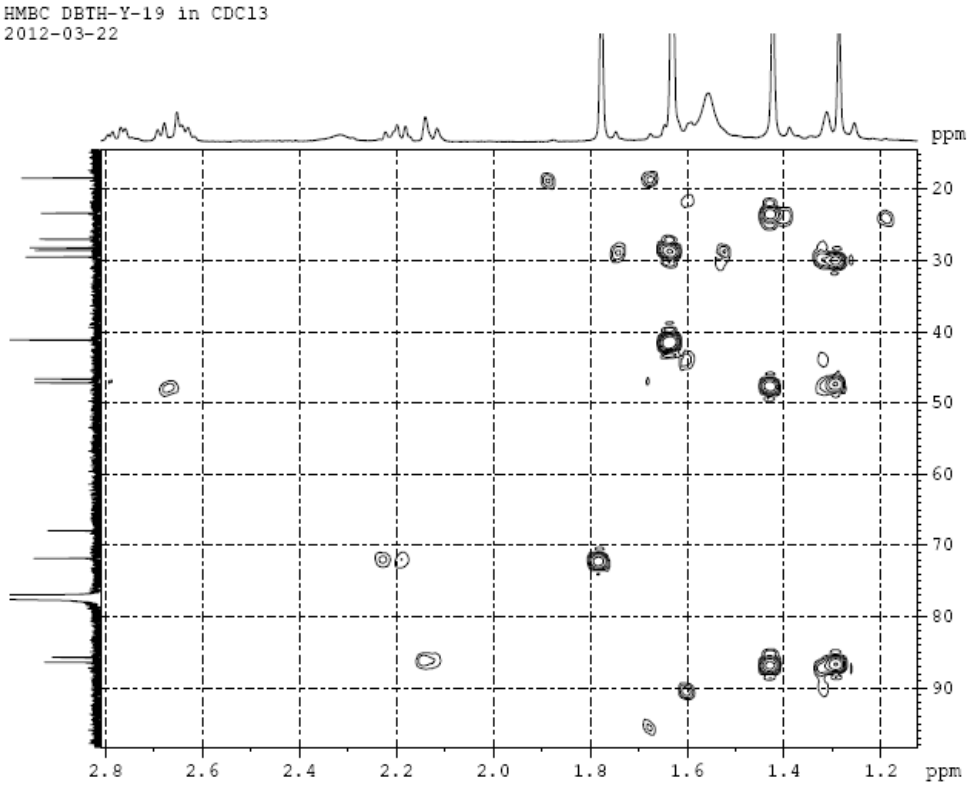

Figure S26. The expanded HMBC spectrum of neobraclactone B (**2**) in $CDCl_3$

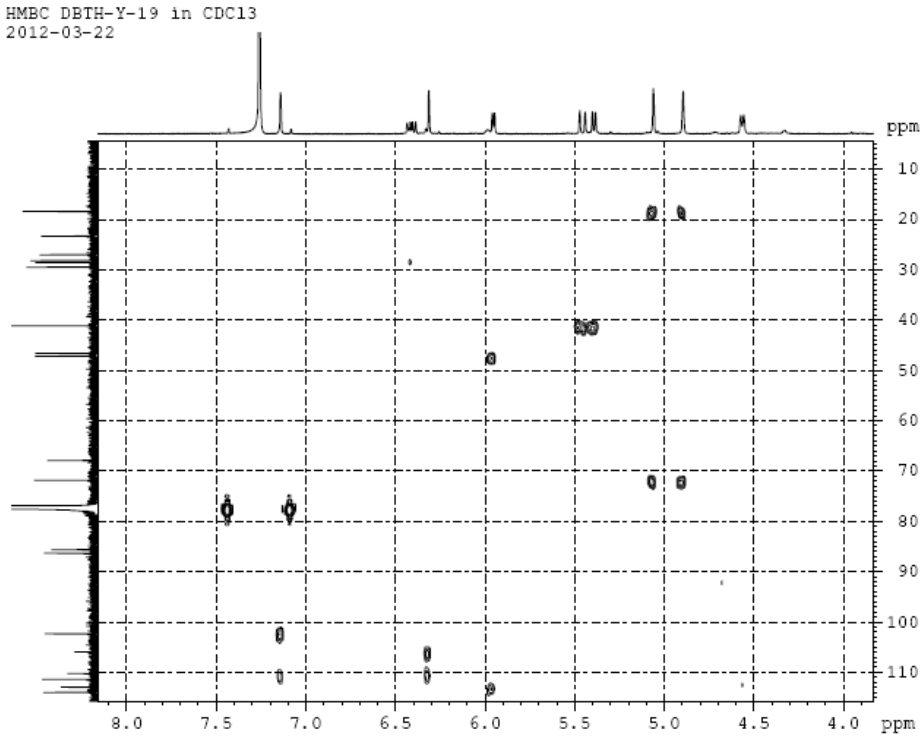

Figure S27. The expanded HMBC spectrum of neobraclactone B (**2**) in $CDCl_3$

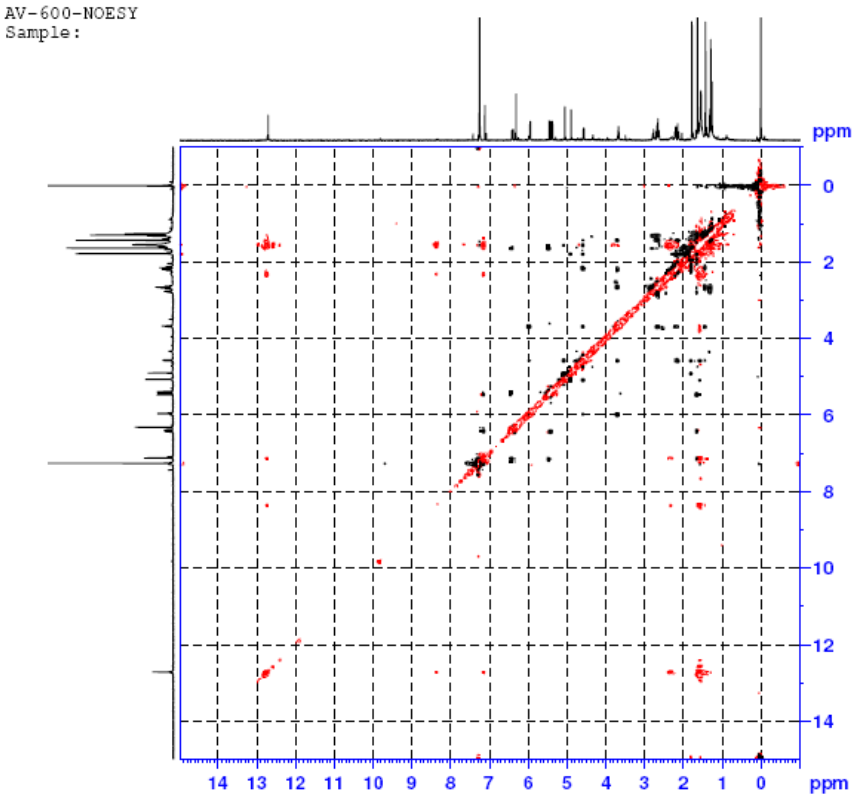

Figure S28. The NOESY spectrum of neobraclactone B (**2**) in $CDCl_3$

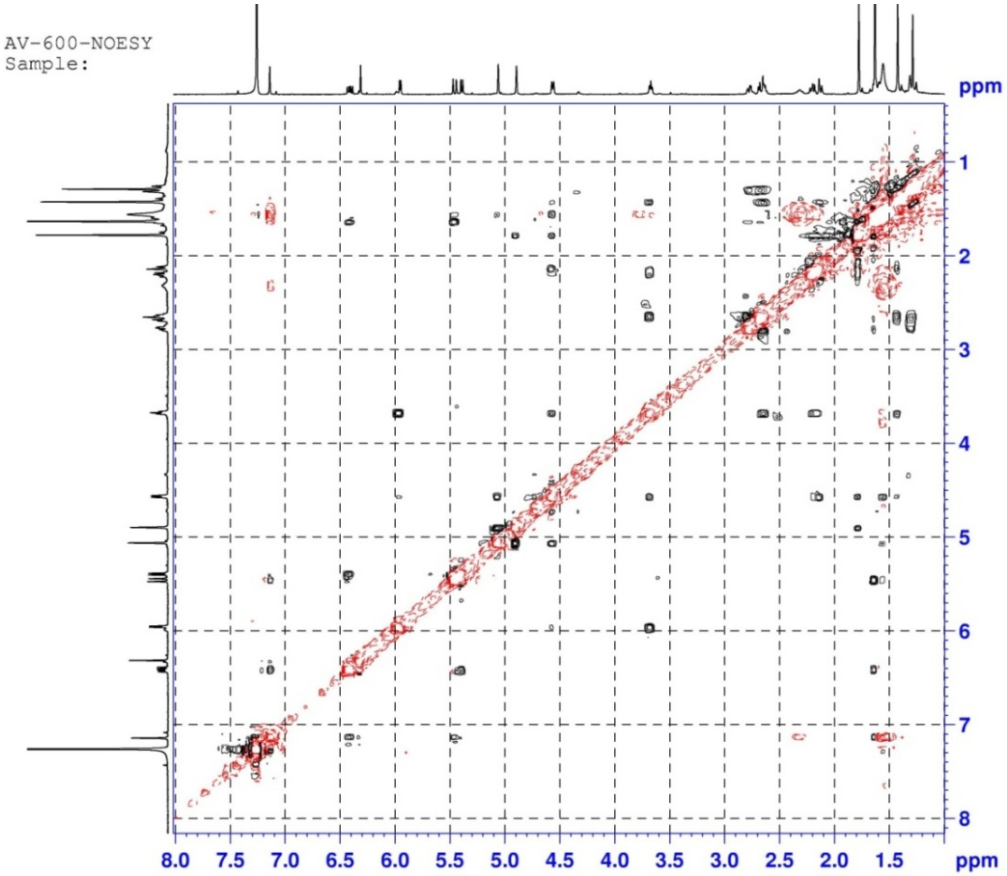

Figure S29. The expanded NOESY spectrum of neobraclactone B (**2**) in $CDCl_3$

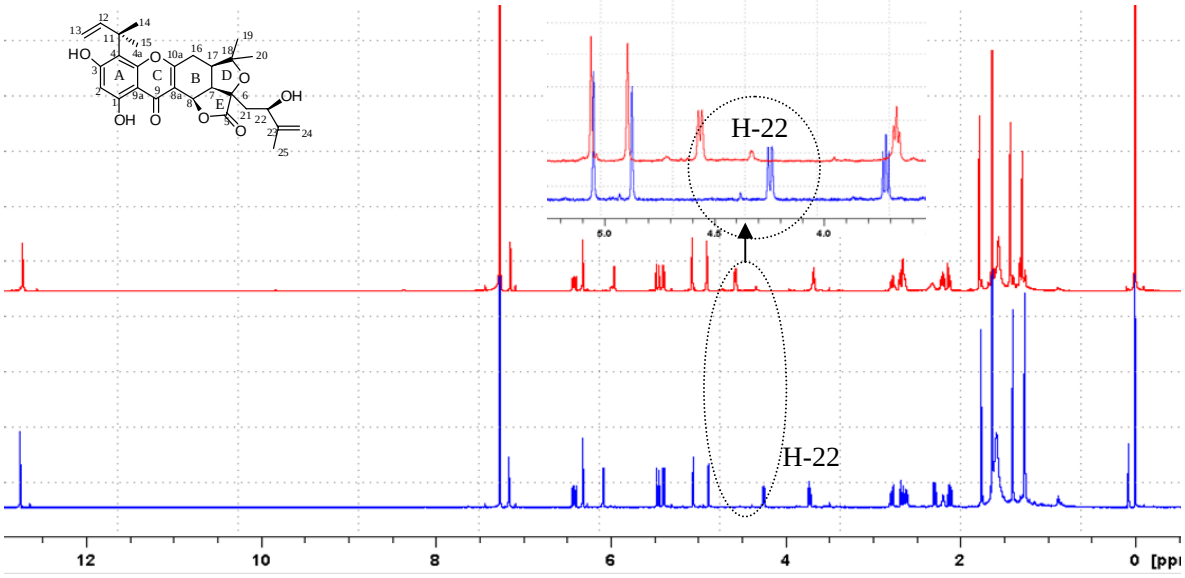

Figure S30. The comparison of the ^{1}H NMR spectra of compounds **1** (blue) and **2** (red) in $CDCl_3$

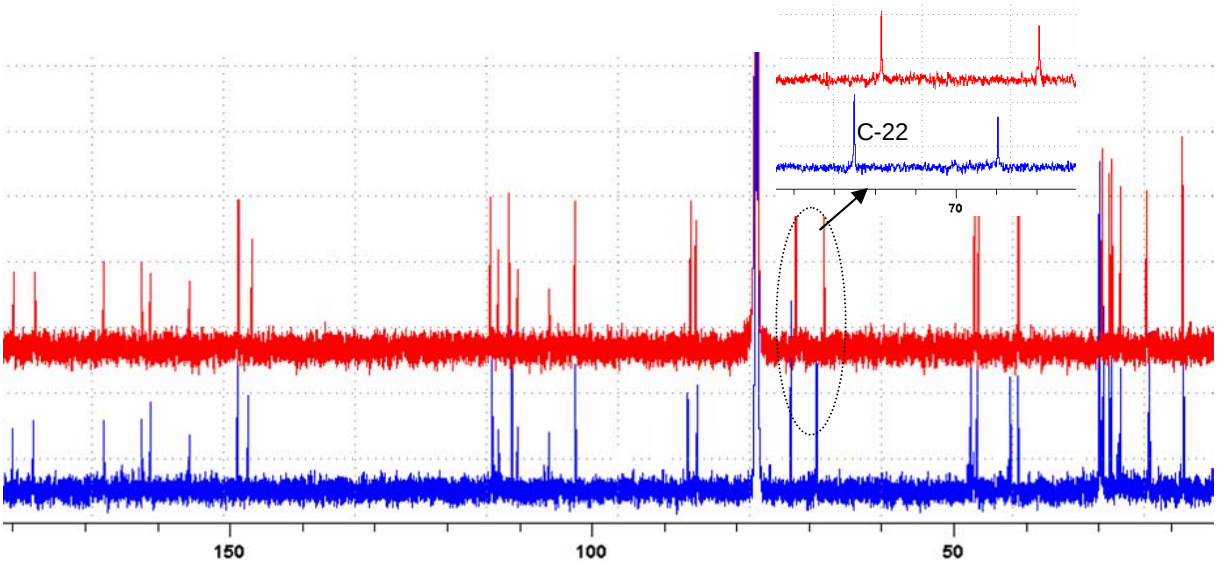

Figure S31. The comparison of the ^{13}C NMR spectra of compounds **1** (blue) and **2** (red) in $CDCl_3$

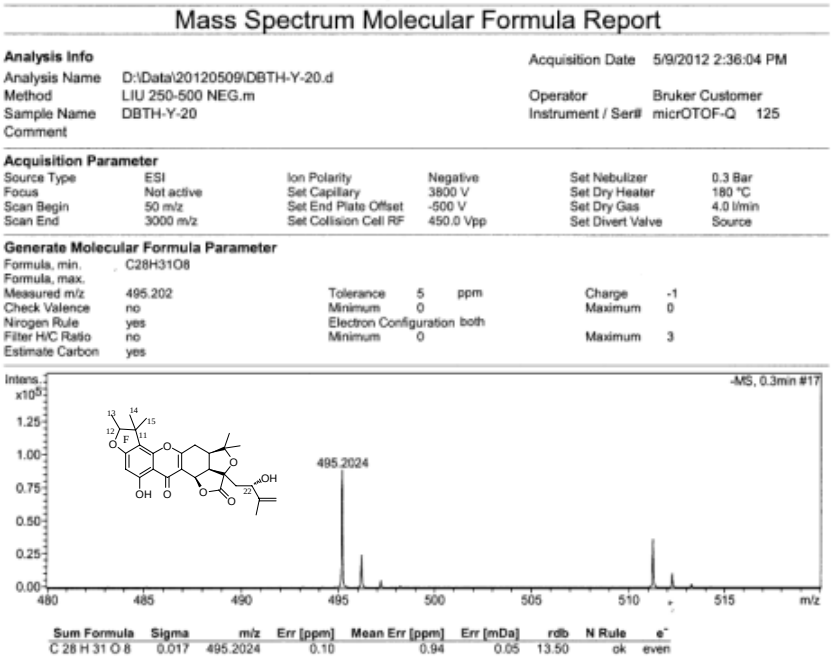

Figure S32. The HR-ESIMS spectrum of neobraclactone C (**3**) in $CDCl_3$

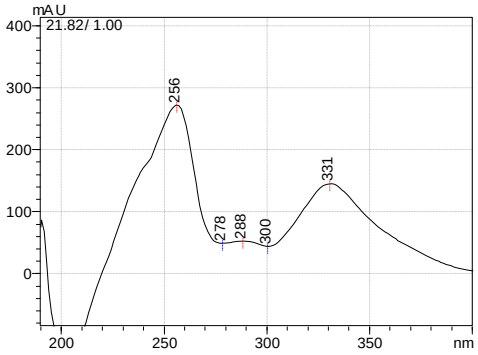

Figure S33. The UV spectrum of neobraclactone C (**3**) in $CDCl_3$

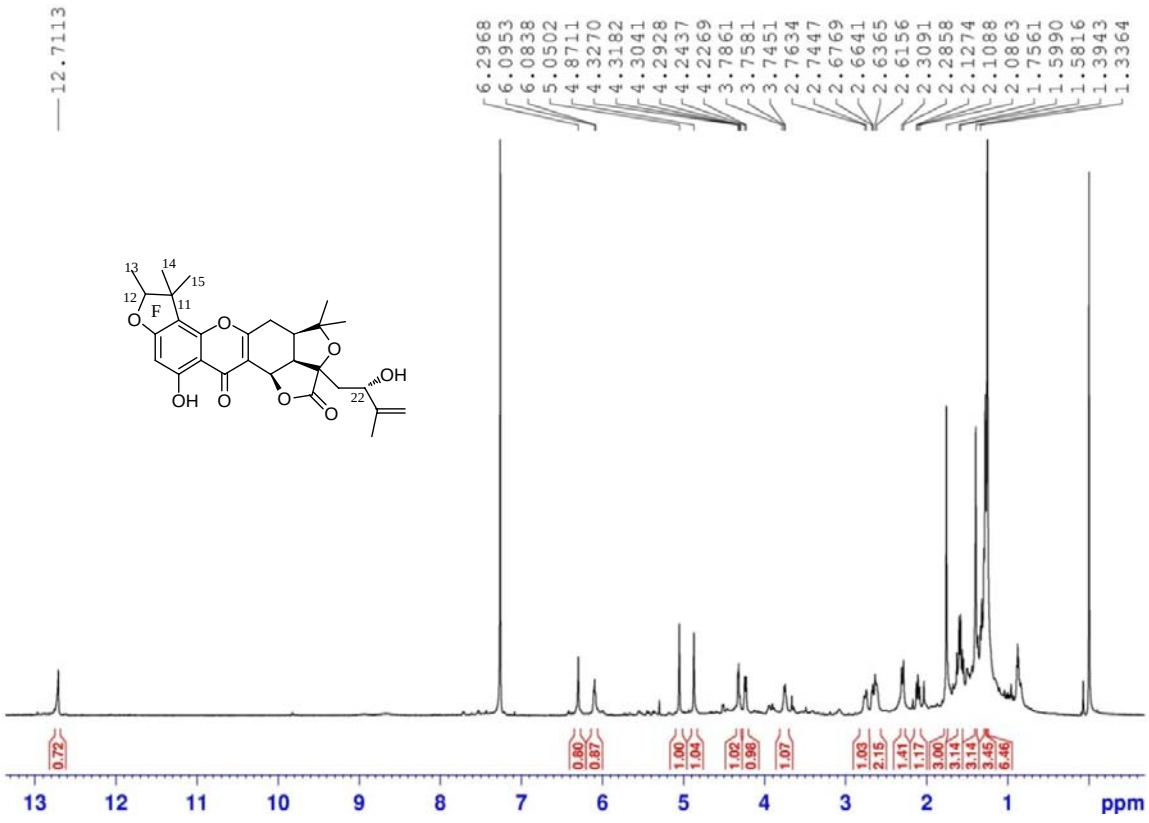

Figure S34. The ^{1}H NMR spectrum of neobraclactone C (**3**) in $CDCl_3$

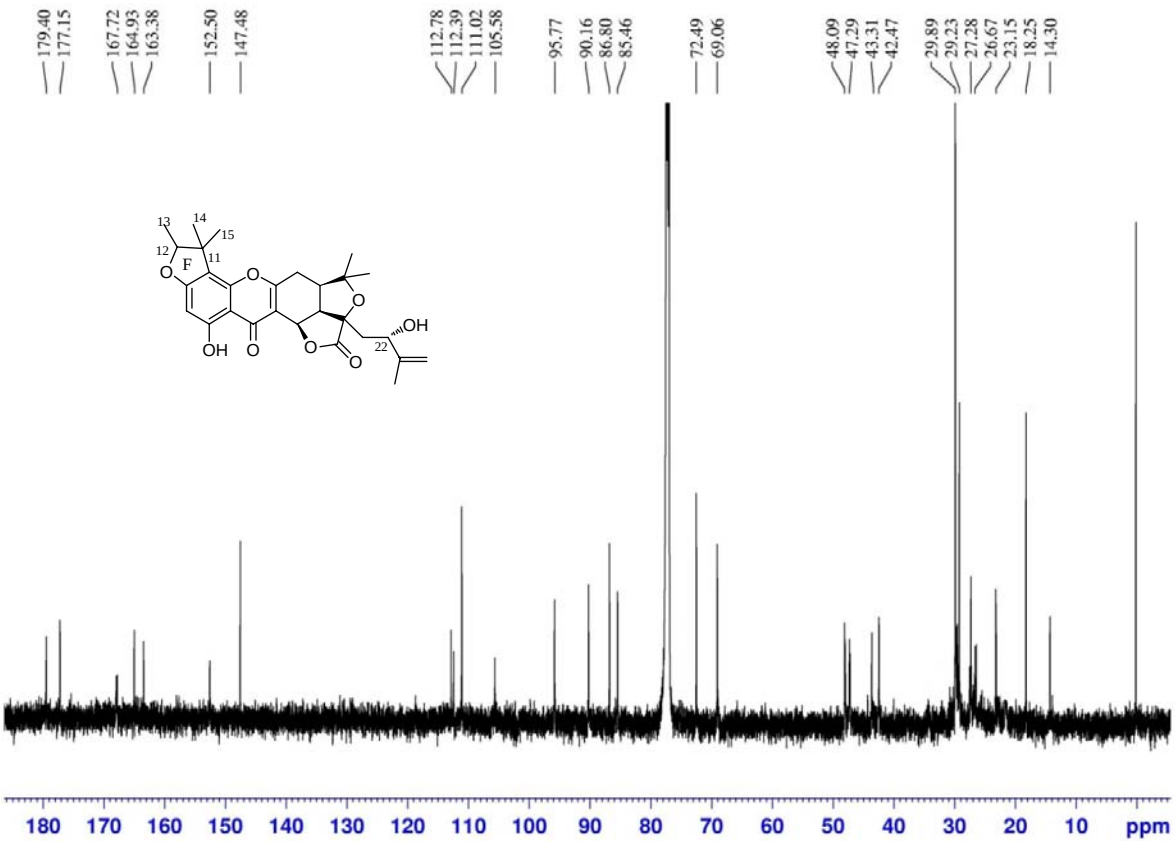

Figure S35. The ^{13}C NMR spectrum of neobraclactone C (**3**) in $CDCl_3$

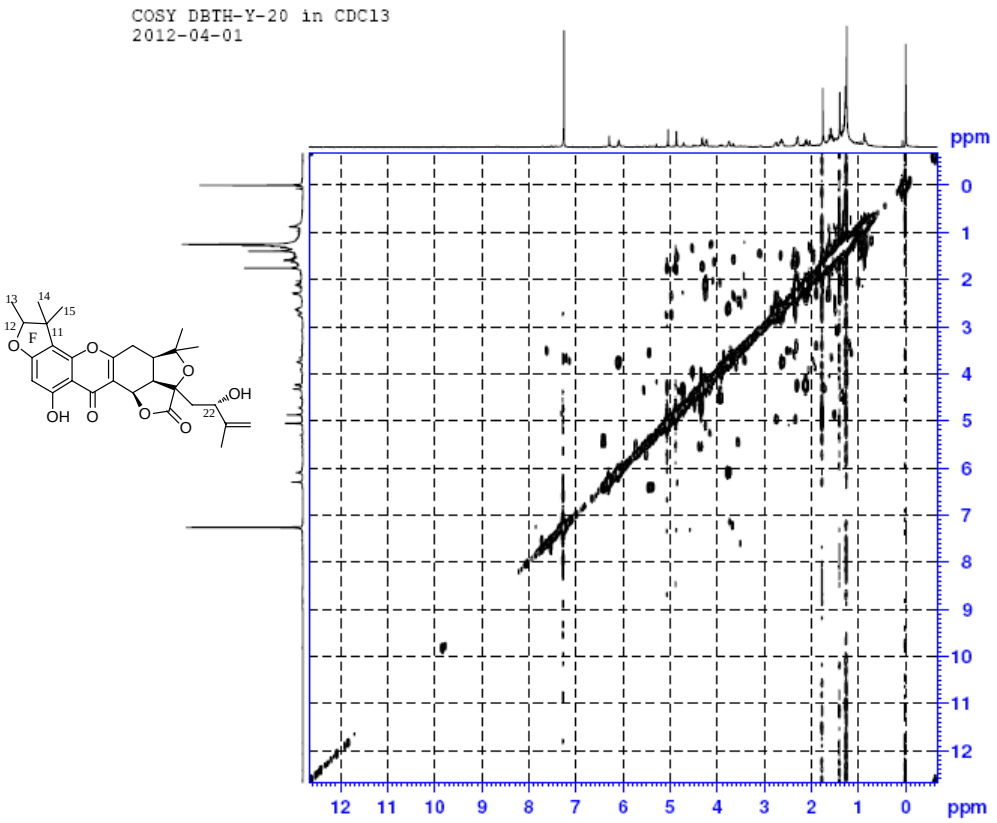

Figure S36. The ^{1}H-^{1}H COSY spectrum of neobraclactone C (**3**) in $CDCl_3$

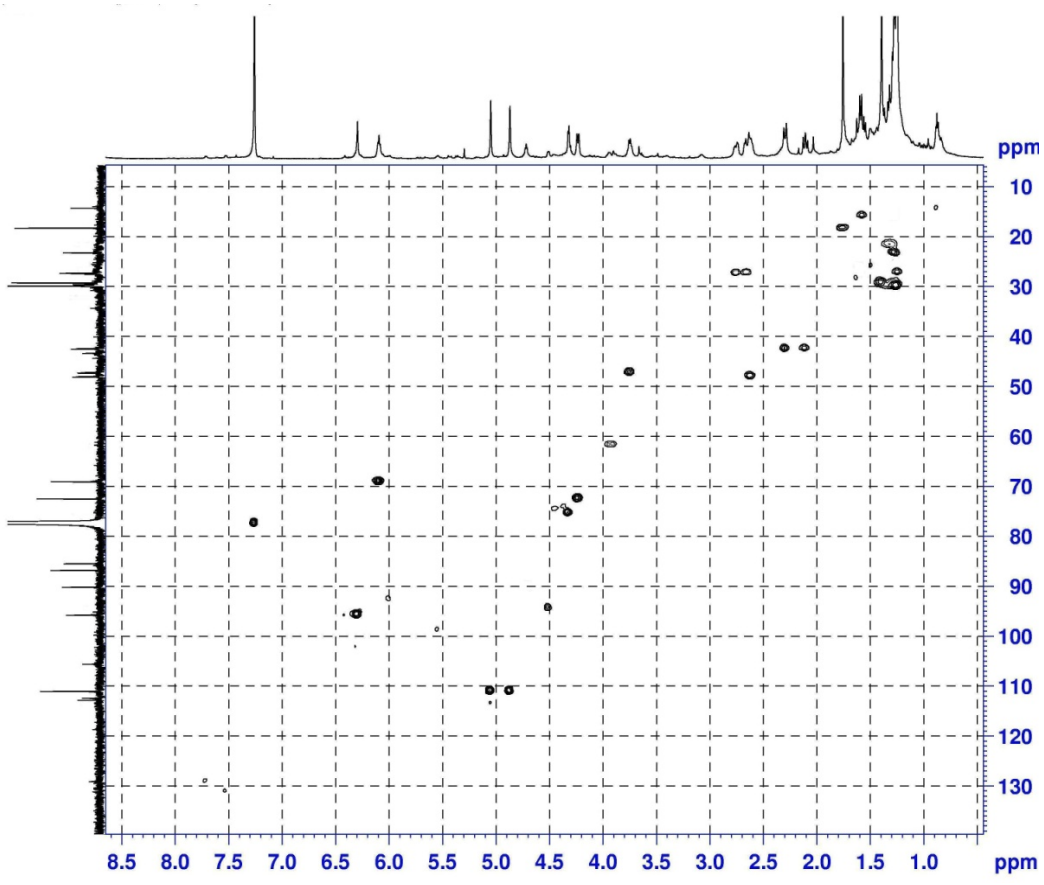

Figure S37. The HSQC spectrum of neobraclactone C (**3**) in $CDCl_3$

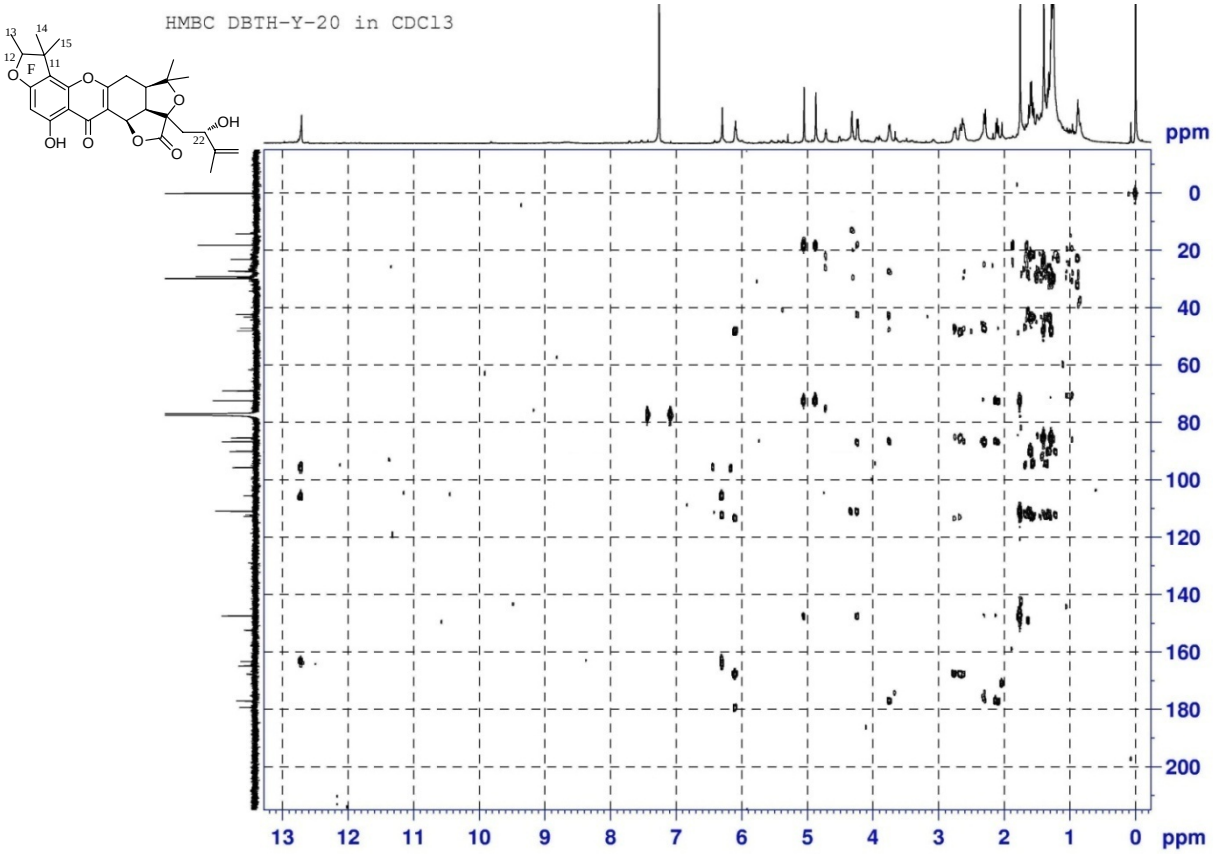

Figure S38. The HMBC spectrum of neobraclactone C (**3**) in $CDCl_3$

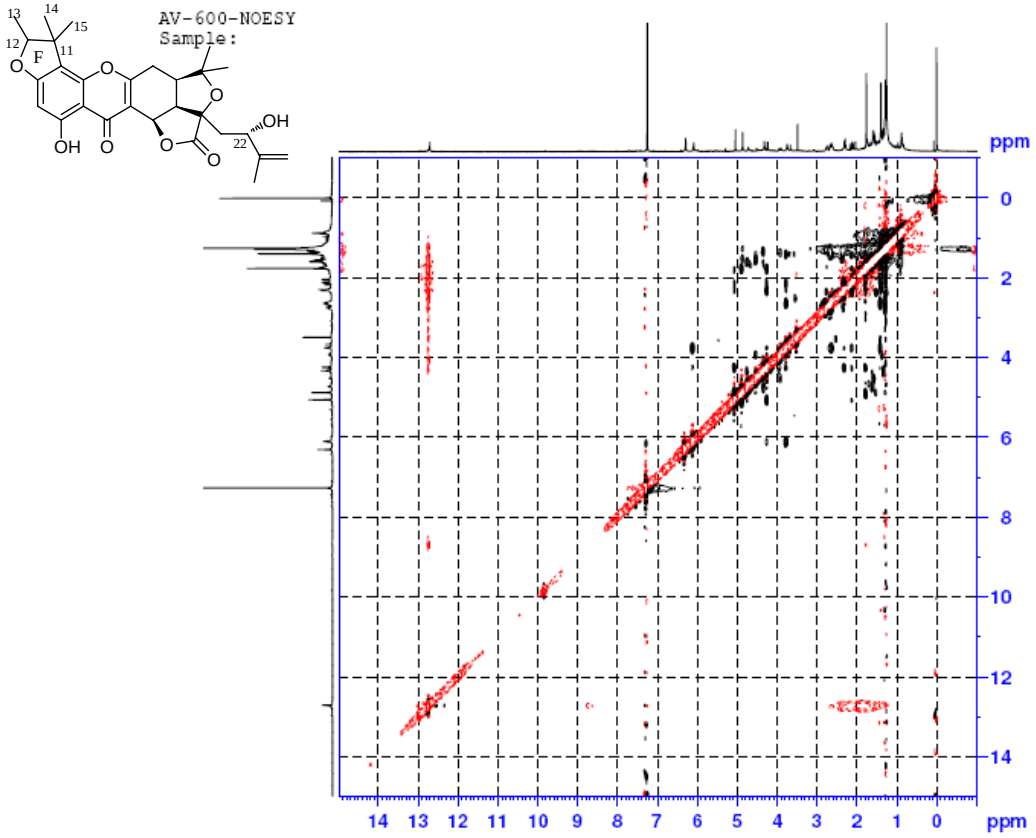

Figure S39. The NOESY spectrum of neobraclactone C (**3**) in $CDCl_3$

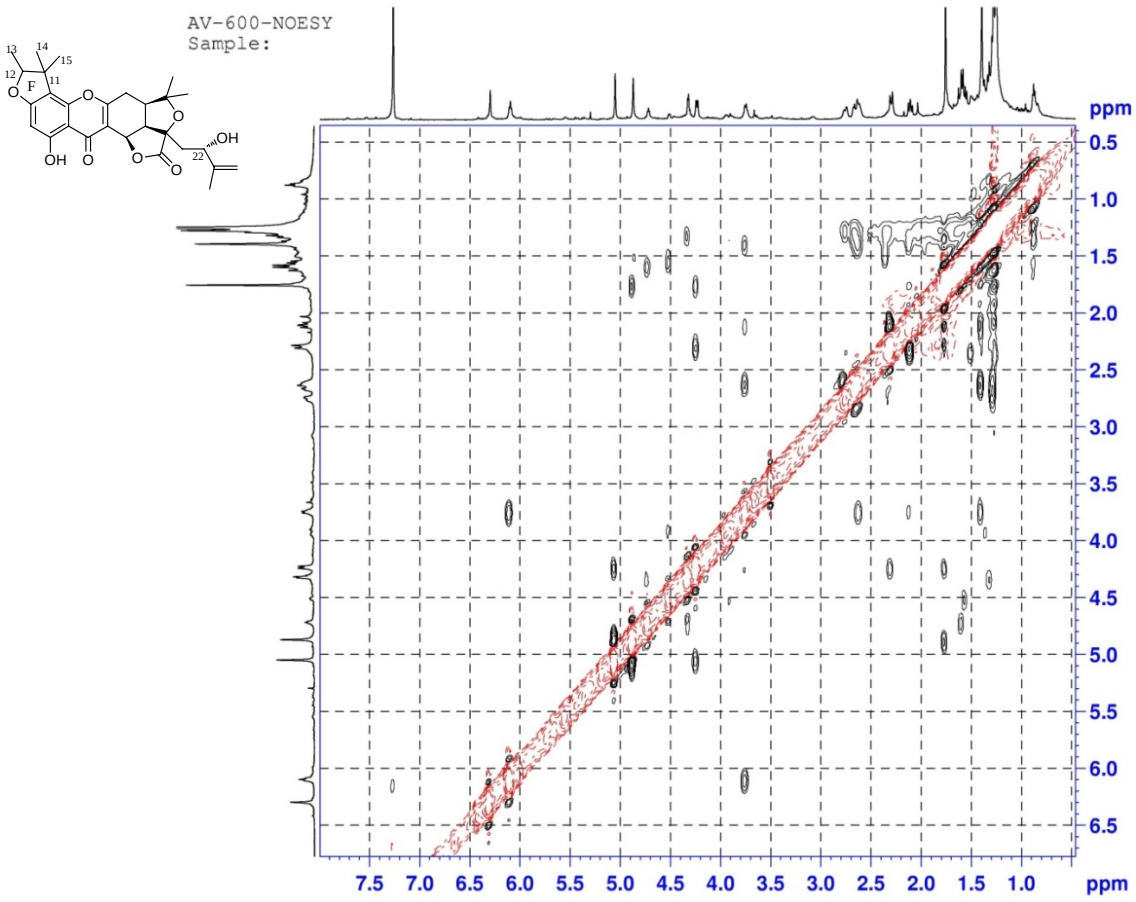

Figure S40. The expanded NOESY spectrum of neobraclactone C (**3**) in $CDCl_3$