

Supporting Information

Anti-influenza Virus Polyketides from the Acid-tolerant Fungus *Penicillium purpurogenum* JS03-21

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List of Supporting Information

Anti-influenza A Virus (H1N1) Bioassay	S3
The 18S rRNA sequences data of <i>Penicillium purpurogenum</i> JS03-21	S4
Figure S1. CD curves of compounds 1–3	S4
Figure S2. The ¹ H-NMR spectrum of purpurquinone A (1) in DMSO.....	S5
Figure S3. The ¹³ C-NMR spectrum of purpurquinone A (1) in DMSO.....	S6
Figure S4. The DEPT spectrum of purpurquinone A (1) in DMSO.....	S7
Figure S5. The HMQC spectrum of purpurquinone A (1) in DMSO.....	S8
Figure S6. The ¹ H- ¹ H COSY spectrum of purpurquinone A (1) in DMSO	S9
Figure S7. The HMBC spectrum of purpurquinone A (1) in DMSO.....	S10
Figure S8. The NOESY spectrum of purpurquinone A (1) in DMSO.....	S11
Figure S9. The ¹ H-NMR spectrum of purpurquinone B (2) in DMSO.....	S12
Figure S10. The ¹³ C-NMR spectrum of purpurquinone B (2) in DMSO.....	S13
Figure S11. The DEPT spectrum of purpurquinone B (2) in DMSO.....	S14
Figure S12. The HMQC spectrum of purpurquinone B (2) in DMSO.....	S15
Figure S13. The ¹ H- ¹ H COSY spectrum of purpurquinone B (2) in DMSO.....	S16
Figure S14. The HMBC spectrum of purpurquinone B (2) in DMSO	S17
Figure S15. The NOESY spectrum of purpurquinone B (2) in DMSO.....	S18

Figure S16. The ¹ H-NMR spectrum of purpurquinone C (3) in DMSO.....	S19
Figure S17. The ¹³ C-NMR spectrum of purpurquinone C (3) in DMSO.....	S20
Figure S18. The DEPT spectrum of purpurquinone C (3) in DMSO.....	S21
Figure S19. The NOESY spectrum of purpurquinone C (3) in DMSO.....	S22
Figure S20. The ¹ H-NMR spectrum of purpurester A (4) in DMSO.....	S23
Figure S21. The ¹³ C-NMR spectrum of purpurester A (4) in DMSO.....	S24
Figure S22. The DEPT spectrum of purpurester A (4) in DMSO.....	S25
Figure S23. The HMQC spectrum of purpurester A (4) in DMSO.....	S26
Figure S24. The ¹ H- ¹ H COSY spectrum of purpurester A (4) in DMSO.....	S27
Figure S25. The HMBC spectrum of purpurester A (4) in DMSO	S28
Figure S26. The ¹ H-NMR spectrum of purpurester B (5) in DMSO.....	S29
Figure S27. The ¹³ C-NMR spectrum of purpurester B (5) in DMSO.....	S30
Figure S28. The DEPT spectrum of purpurester B (5) in DMSO.....	S31
Figure S29. The ¹ H-NMR spectrum of compound 6 in DMSO.....	S32
Figure S30. The ¹³ C-NMR spectrum of compound 6 in DMSO.....	S33
Figure S31. The DEPT spectrum of compound 6 in DMSO.....	S34
Figure S32. HPLC profiles (360 nm) of secondary metabolites from <i>P. purpurogenum</i> JS03-21 cultivated at pH 2 and pH 7	S35
Figure S33. Key NOESY correlations of compounds 1–3	S35

Anti-influenza A Virus (H1N1) Bioassay

The antiviral activity against H1N1 was evaluated by the CPE inhibition assay. Confluent MDCK cell monolayers were firstly incubated with influenza virus (A/Puerto Rico/8/34 (H1N1), PR/8) at 37 °C for 1 h. After removing the virus dilution, cells were maintained in infecting media (RPMI 1640, 4 µg/mL of trypsin) containing different concentrations of test compounds at 37 °C. After 48 h incubation at 37 °C, the Cells were fixed with 100 µL of 4% formaldehyde for 20 min at room temperature. After removal of the formaldehyde, the cells were stained with 0.1% crystal violet for 30 min. The plates were washed and dried, and the intensity of crystal violet staining for each well was measured in a microplate reader (Bio-Rad, USA) at 570 nm. The IC₅₀ was calculated as the compound concentration required inhibiting influenza virus yield at 48 h post-infection by 50%. Ribavirin was used as the positive control with the IC₅₀ values of 100.8 µM.

The 18S rRNA sequence data of *Penicillium purpurogenum* JS03-21

ACTTTCCTCTAATGACCAAGTTTGACCAACTTTCGGGCTCTGGGCGGTCGTTGCCAACCCCCCTGAGCC
AGTCCGAAGGCCTCACTGAGCCATTCAATCGGTAGTAGCGACGGGCGGTGTGTACAAAGGGCAGGGA
CGTAATCGGCACGAGCTGATGACTCGTGCCTACTAGGCATTCTCGTTGAAGAGCAATAATTGCAATGC
TCTATCCCCAGCACGACAGGGTTTAAACAAGATTACCCAGGCCTCTCGGCCAAGGTGATGTAAGTCTG
GCCCTGTCAGTGTAGCGCGCGTGC GGCCAGAACATCTAAGGGCATCACAGACCTGTTATTGCCACGT
ACTTCCATCGGCTTGAGCCGATAGTCCCCCTAAGAAGCCAGCGGCCCGCAAACGCGGACCGGGCTATT
TAAGGGCCGAGGTCTCGTTCGTTATCGCAATTAAGCAGACAAATCACTCCACCAACTAAGAACGGCCA
TGCACCACCATCCAAAAGATCAAGAAAGAGCTCTCAATCTGTCAATCCTTATTTTGTCTGGACCTGGTG
AGTTTCCCCGTGTTGAGTCAAATTAAGCCGAGGCTCCACGCCTTGTGGTGCCCTTCCGTCAATTTCTT
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CGGCAGGACGGGCCCCAAGTTCAACTACGAGCTTTTAACTGCAACAACCTTAAATATACGCTATTGGAG
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TCTCATTCCAATTACAAGACCCAAAAGAGCCCTGTATCAGTATTTATTGTCACTACCTCCCCGTATCGGG
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TCGAACCCTAATTCCTCGTTACCCGTTGCCACCATGGTAGGCCACTATCCTACCATCGAAAGTTGATAG
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AGGAGCCCCGAGGGGCATTGGTTTTTTATCTAATAAATACACCCCTTCCGAAGTCGGGGTTTTGCGCAT
GTATTAGCTCTAGAATTACCACAGGTATCCATGTAGTAGGGTACTATCAAATAAACGATAACTGATTTAAT
GAGCCATTCGCAGTTTCACGGTACAAGAGTGCTTATAACCTA

Figure S1. CD curves of compounds 1–3

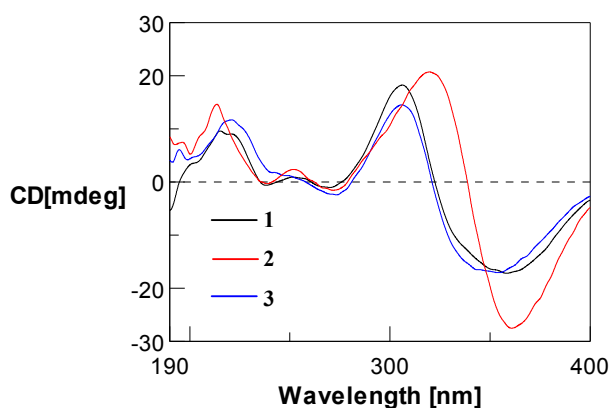


Figure S2. The ^1H NMR spectrum of purpurquinone A (**1**) in DMSO

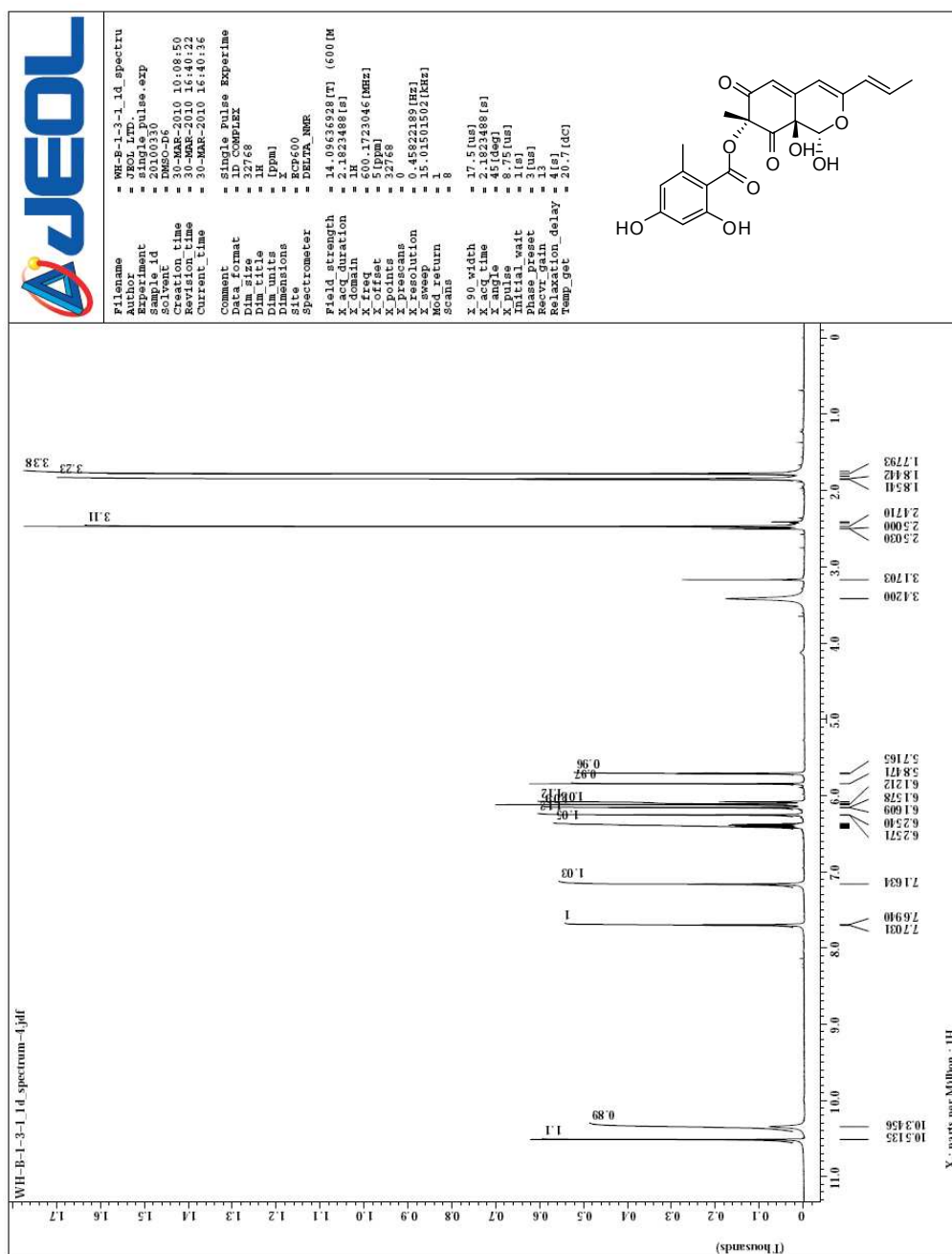


Figure S3. The ^{13}C NMR spectrum of purpurquinone A (**1**) in DMSO

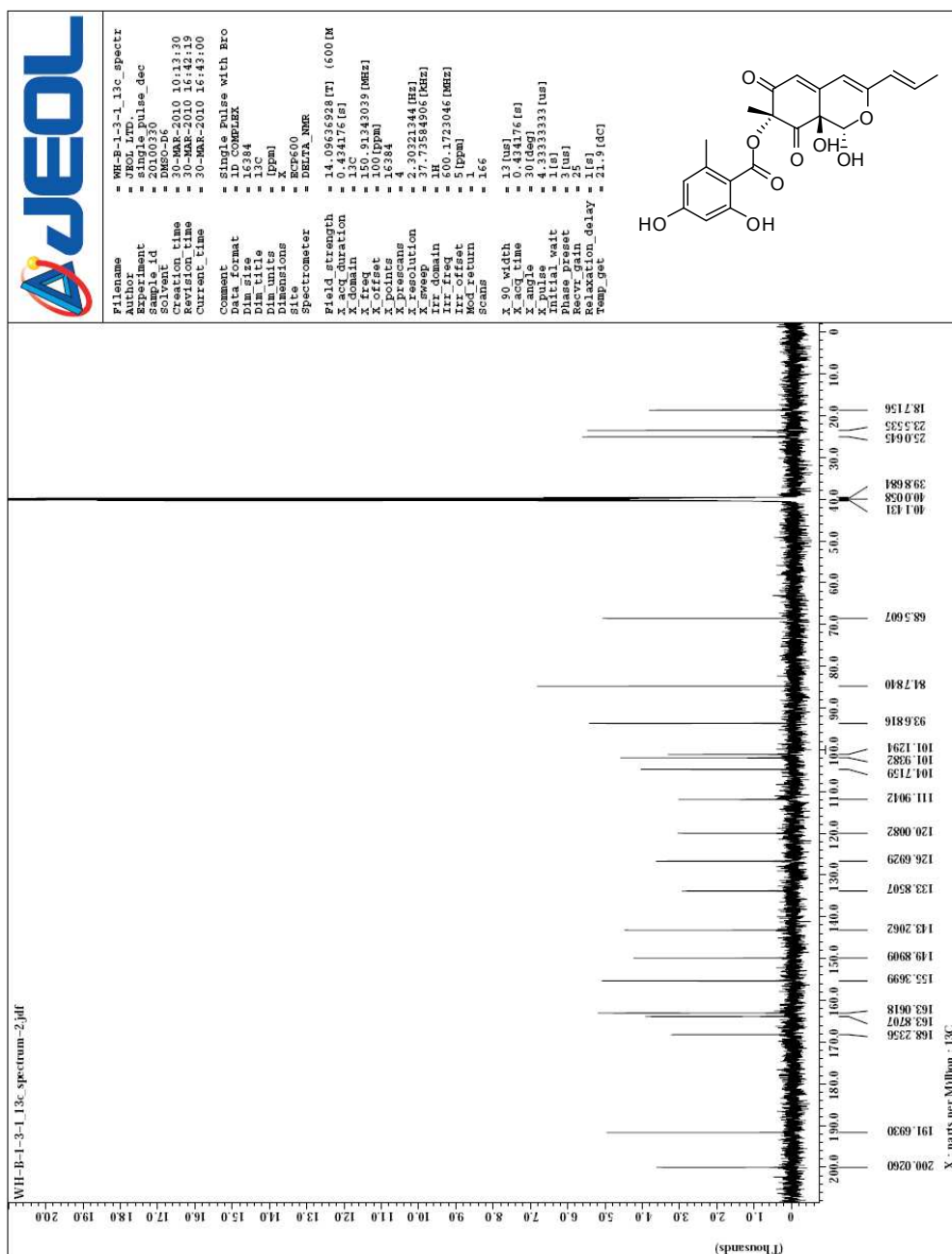


Figure S4. The DEPT spectrum of purpurquinone A (**1**) in DMSO

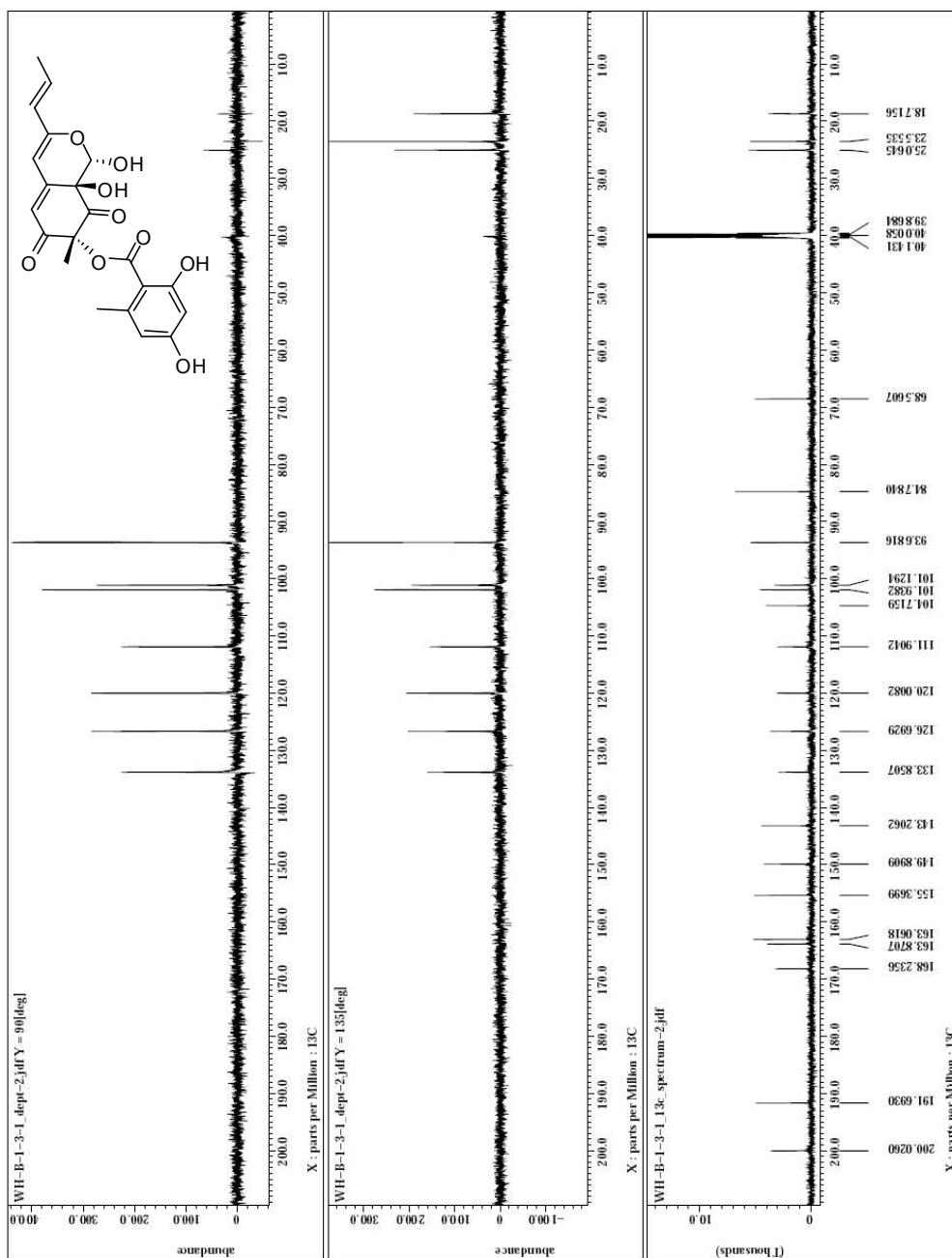


Figure S5. The HMQC spectrum of purpurquinone A (**1**) in DMSO

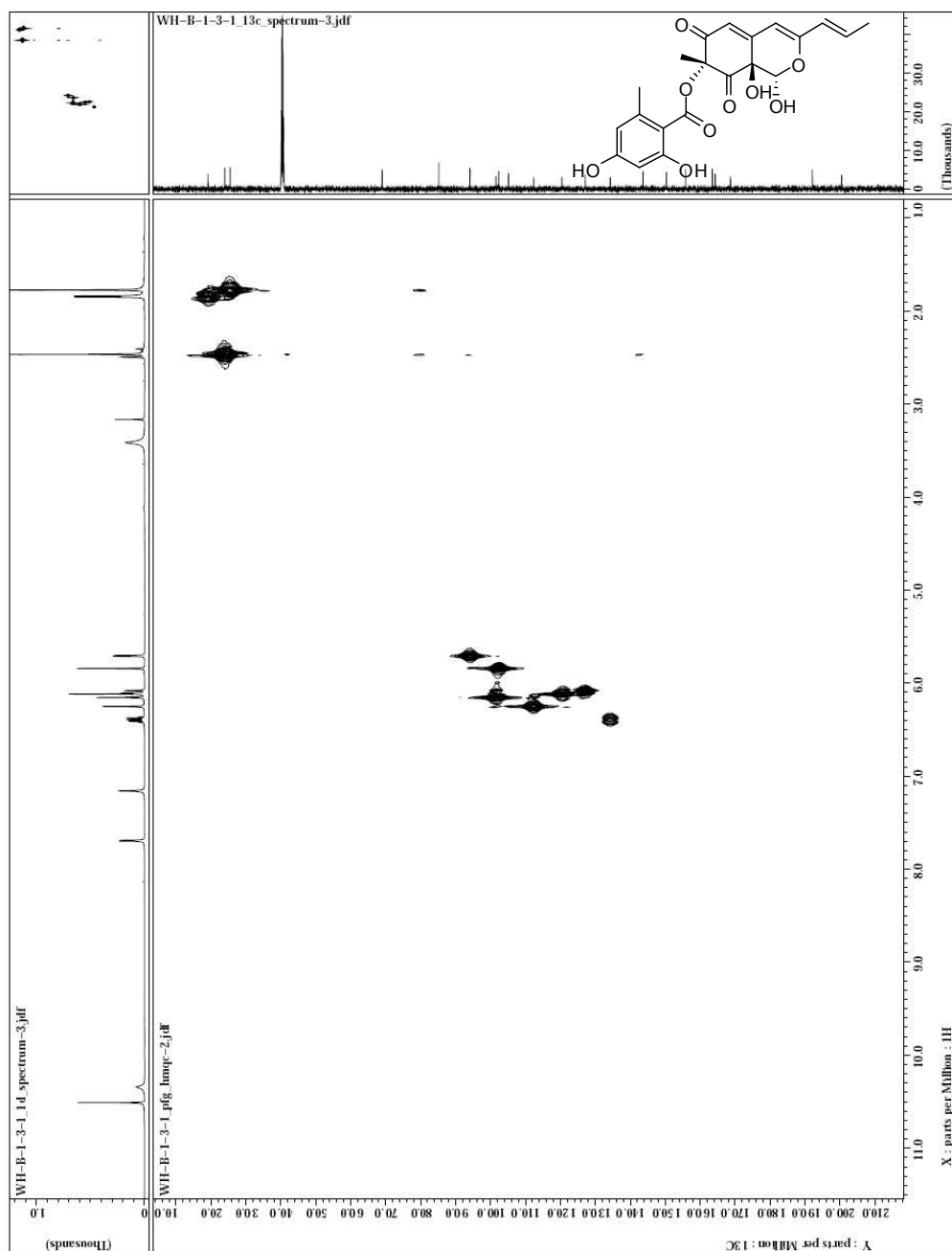


Figure S6. The ^1H - ^1H COSY spectrum of purpurquinone A (**1**) in DMSO

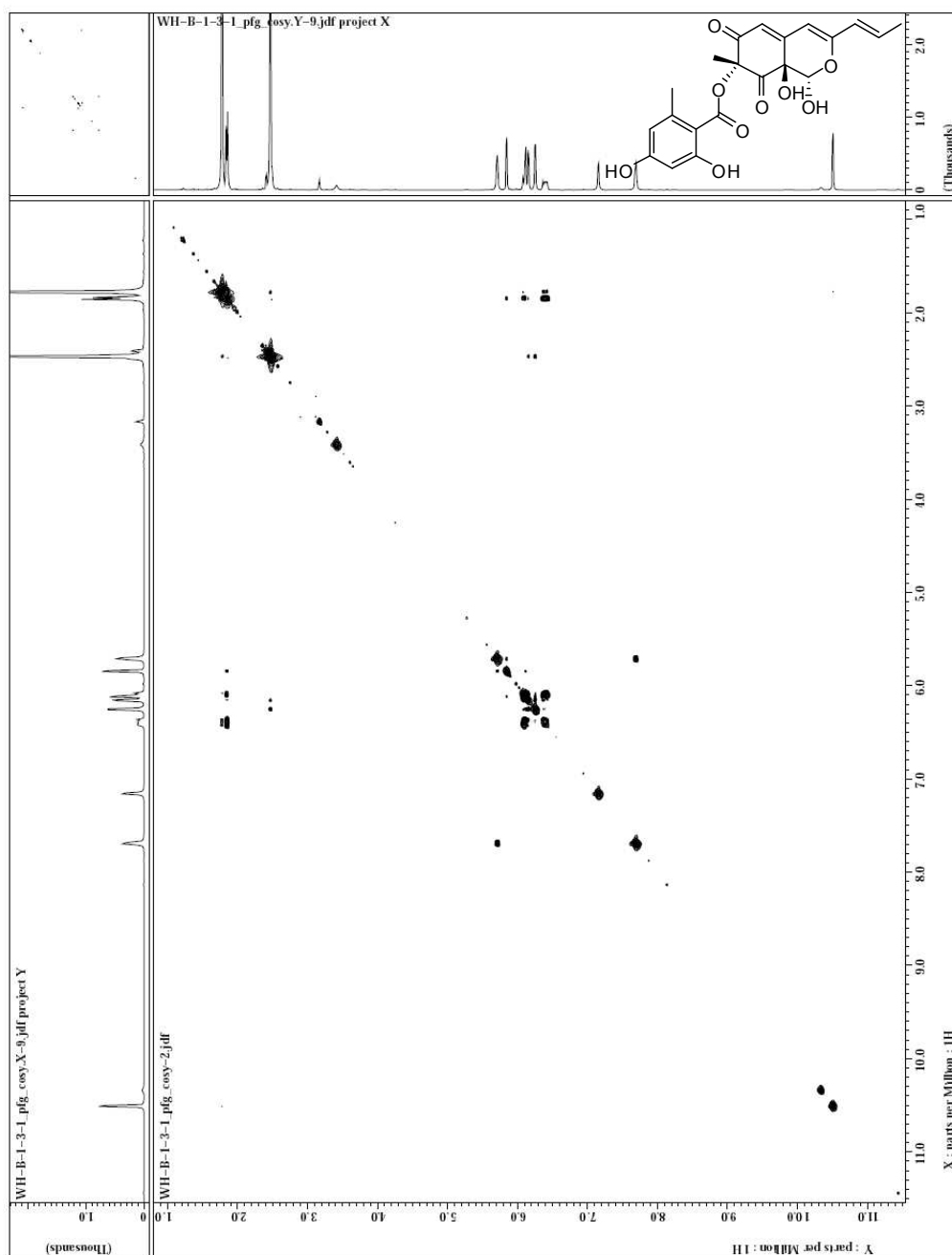


Figure S7. The HMBC spectrum of purpurquinone A (**1**) in DMSO

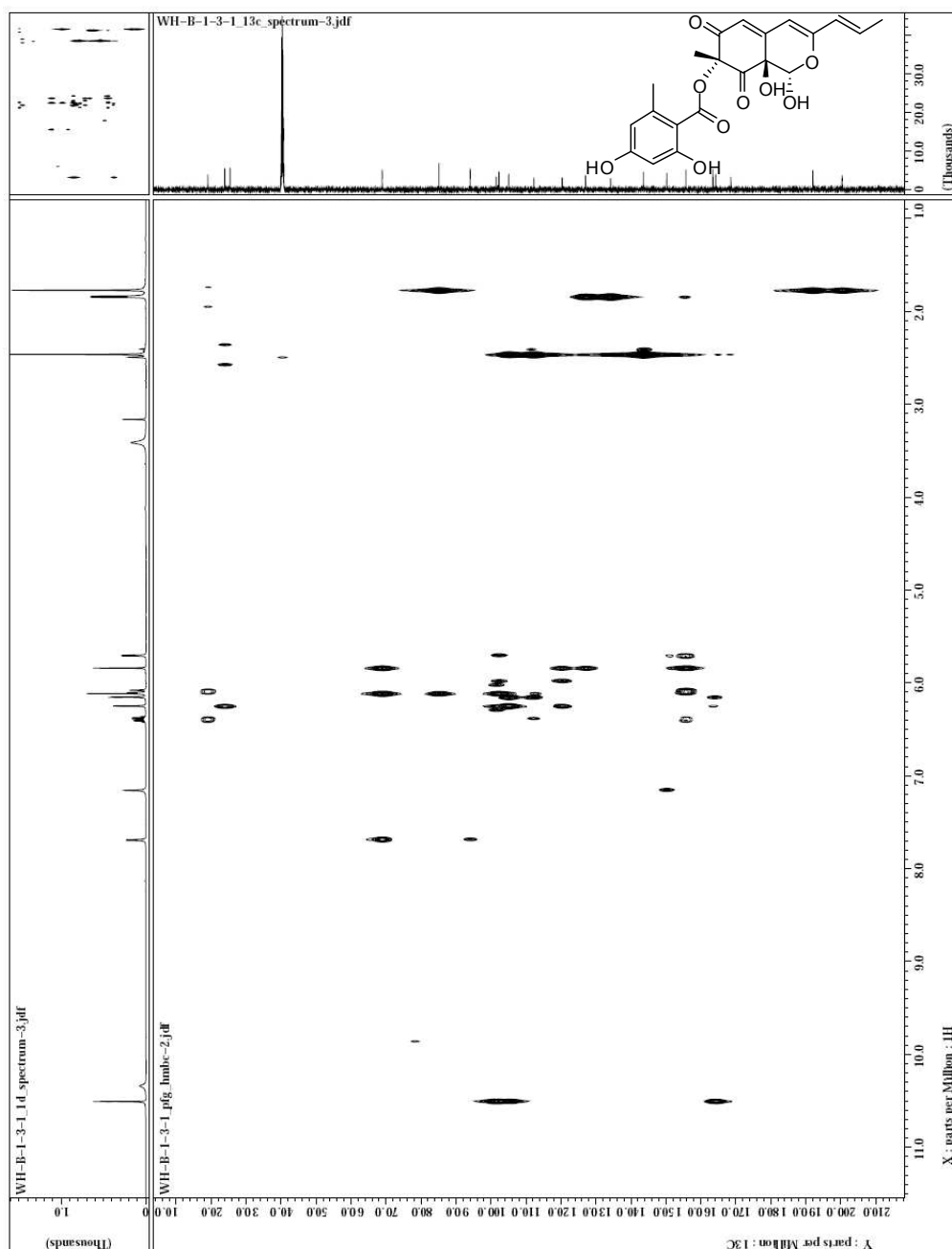


Figure S8. The NOESY spectrum of purpurquinone A (**1**) in DMSO

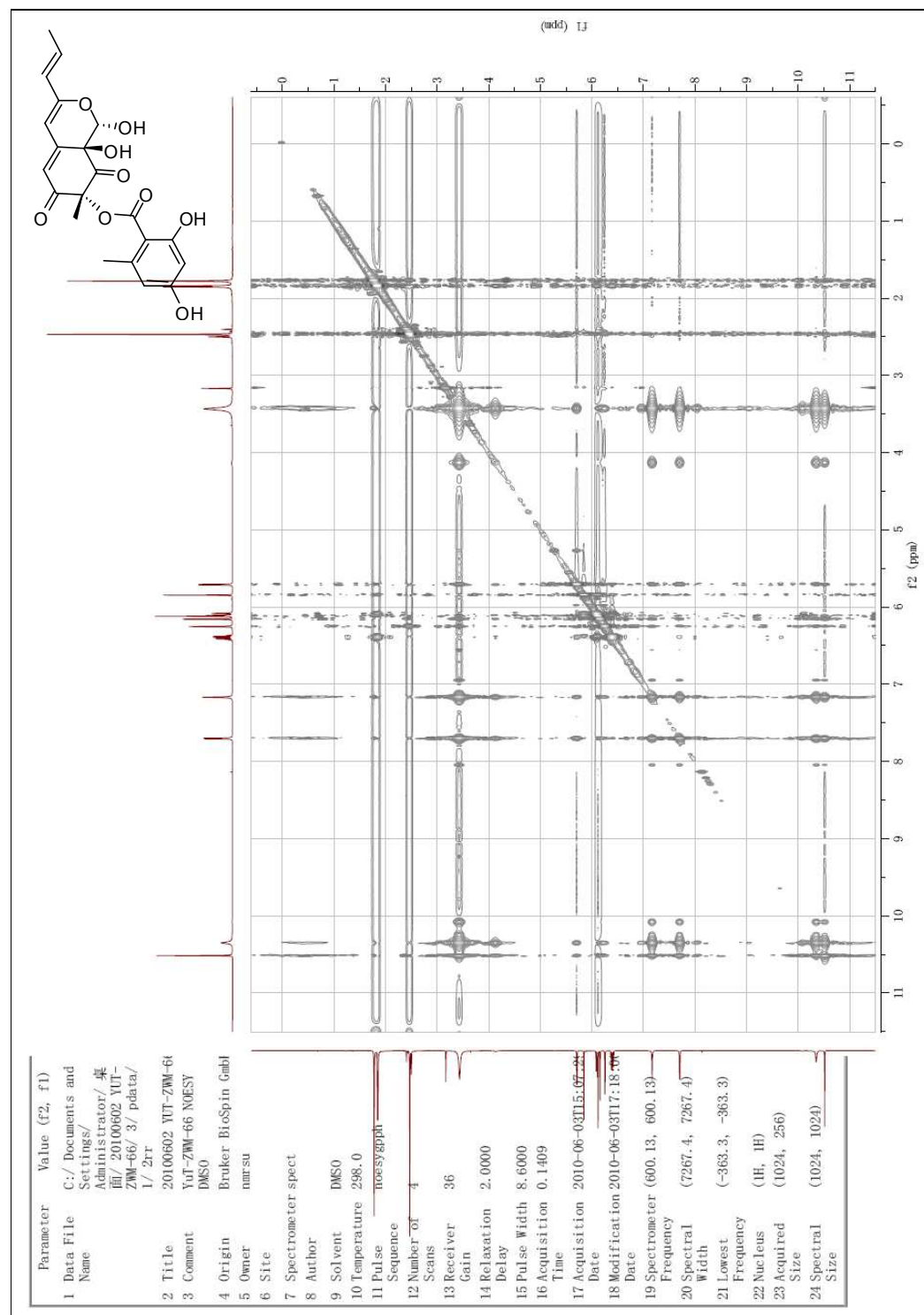


Figure S9. The ^1H NMR spectrum of purpurquinone B (**2**) in DMSO

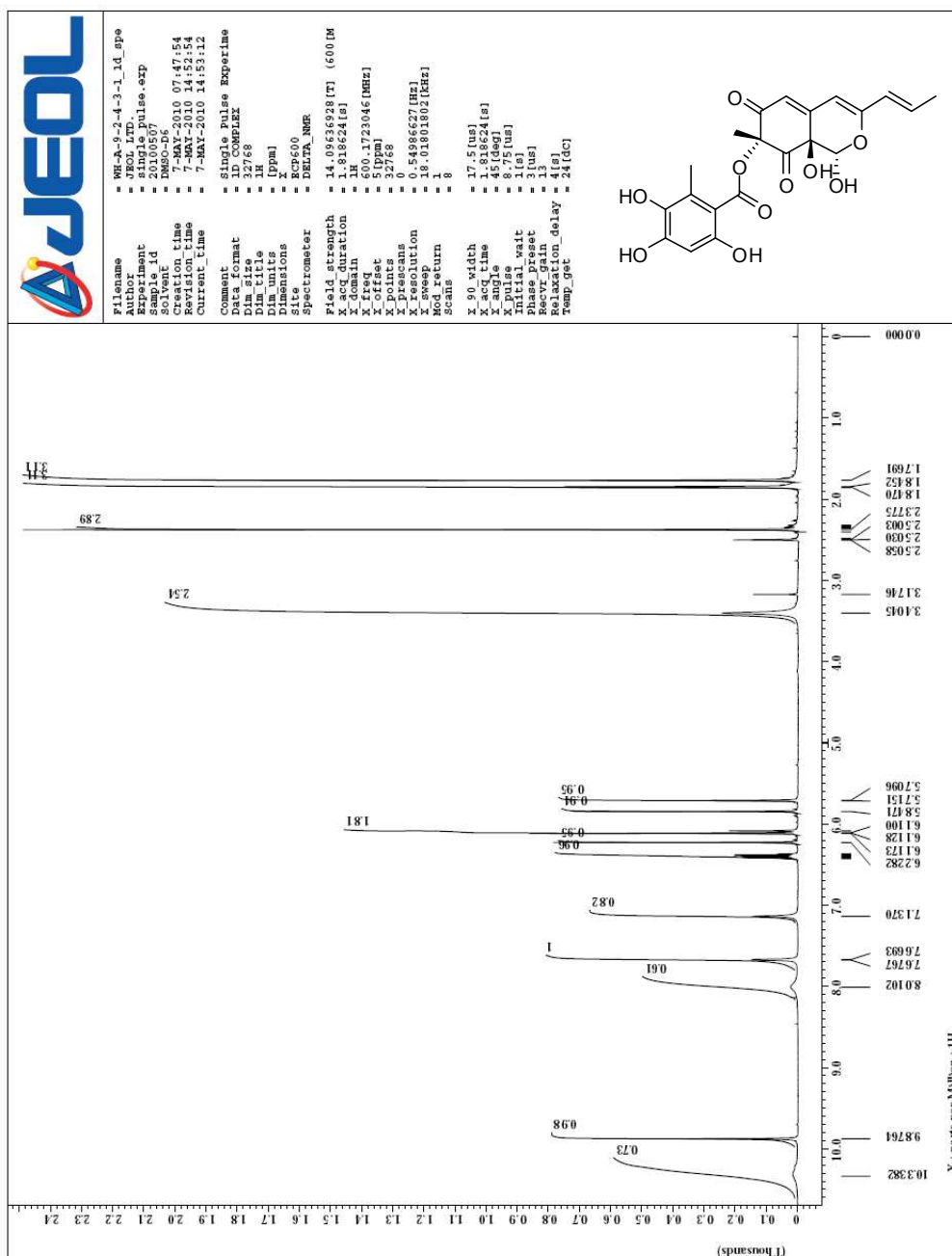


Figure S10. The ^{13}C NMR spectrum of purpurquinone B (**2**) in DMSO

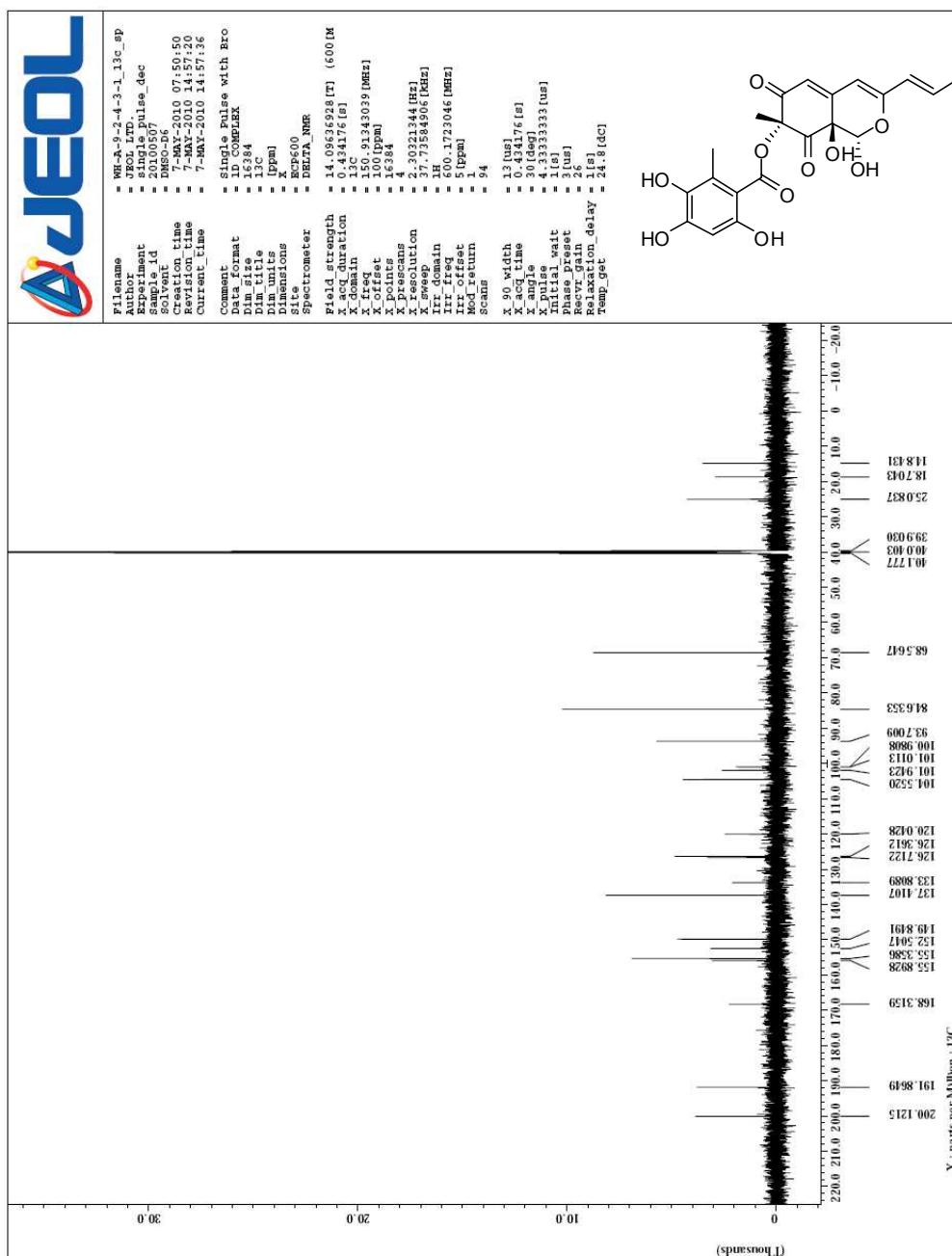


Figure S11. The DEPT spectrum of purpurquinone B (**2**) in DMSO

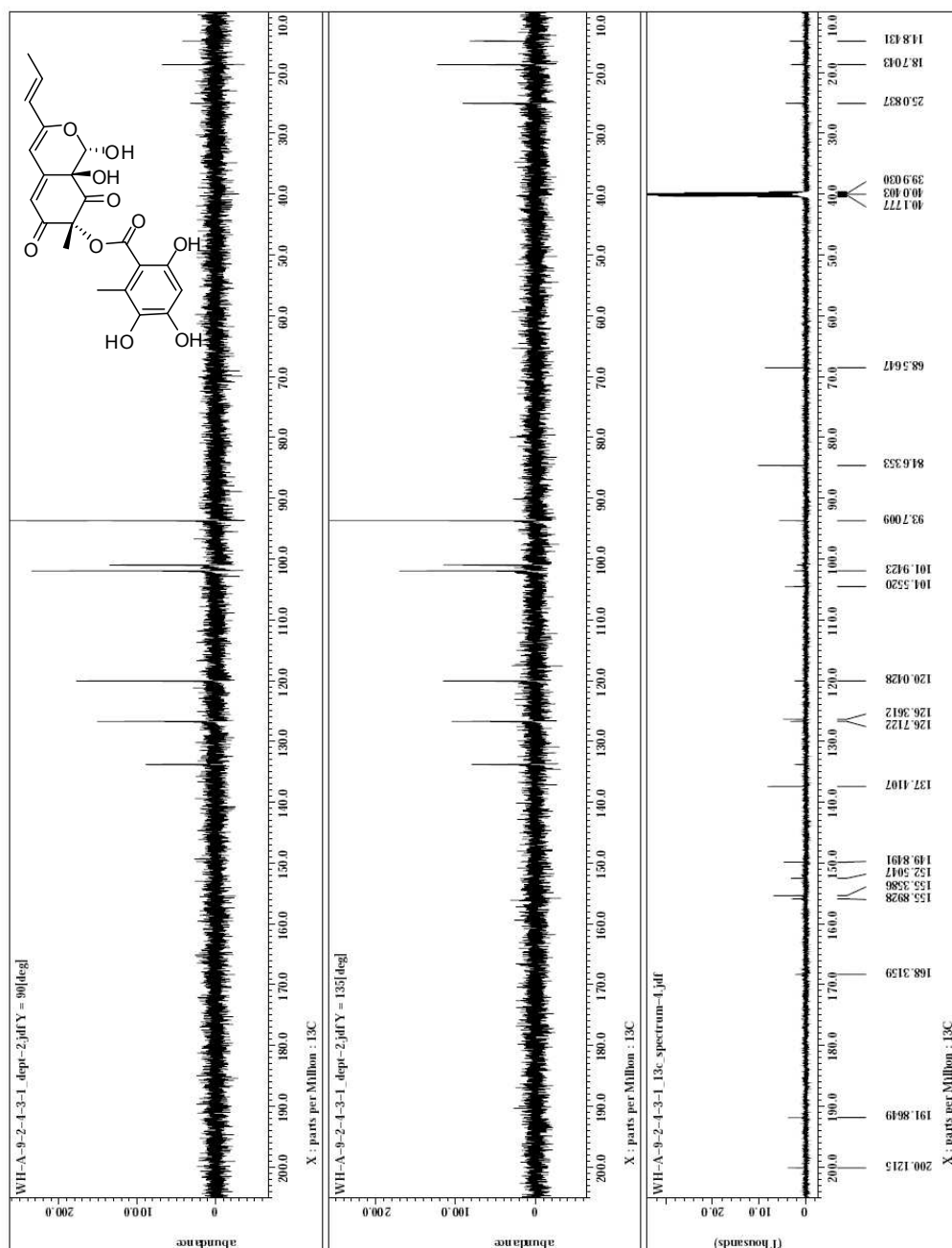


Figure S12. The HMQC spectrum of purpurquinone B (**2**) in DMSO

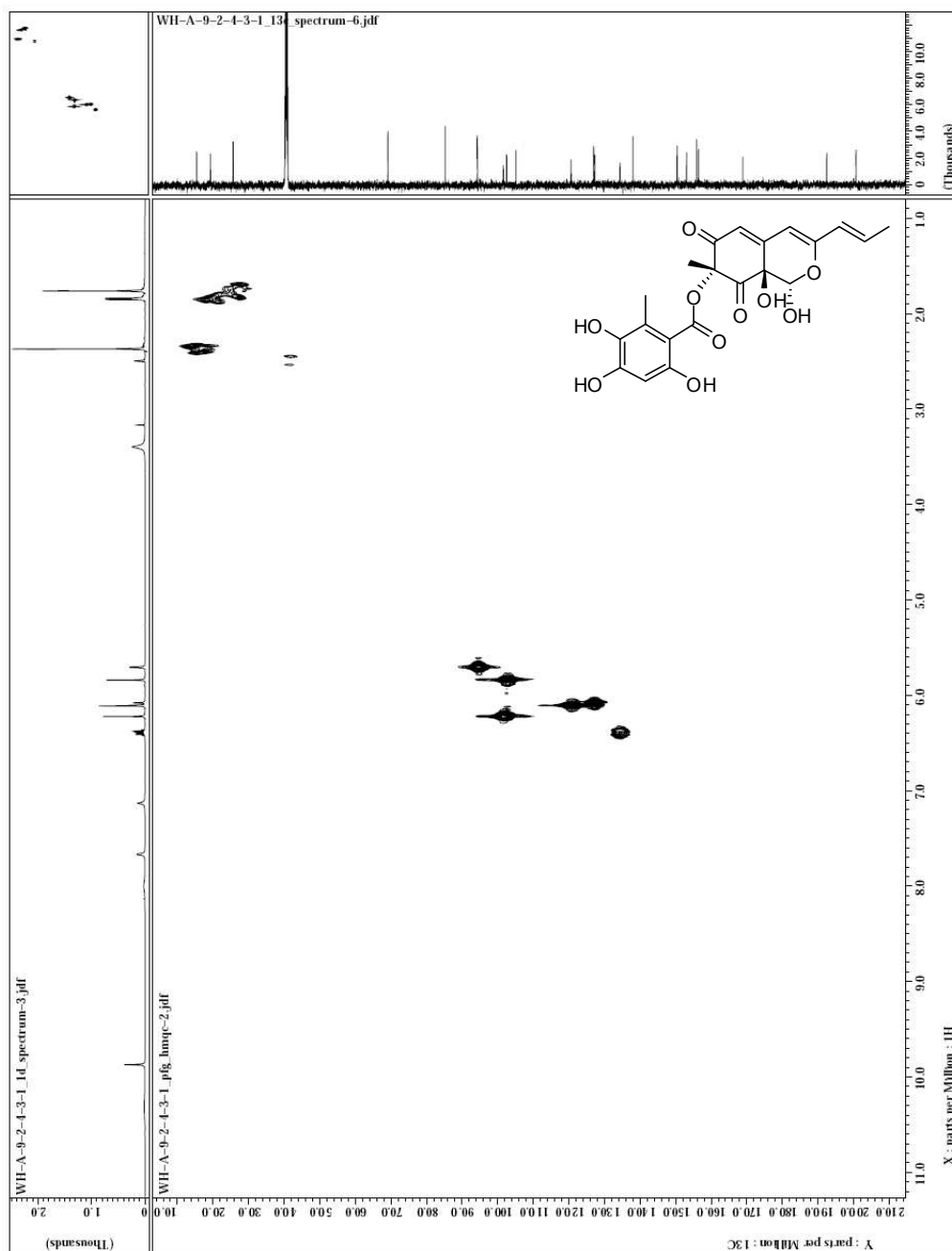


Figure S13. The ^1H - ^1H COSY spectrum of purpurquinone B (**2**) in DMSO

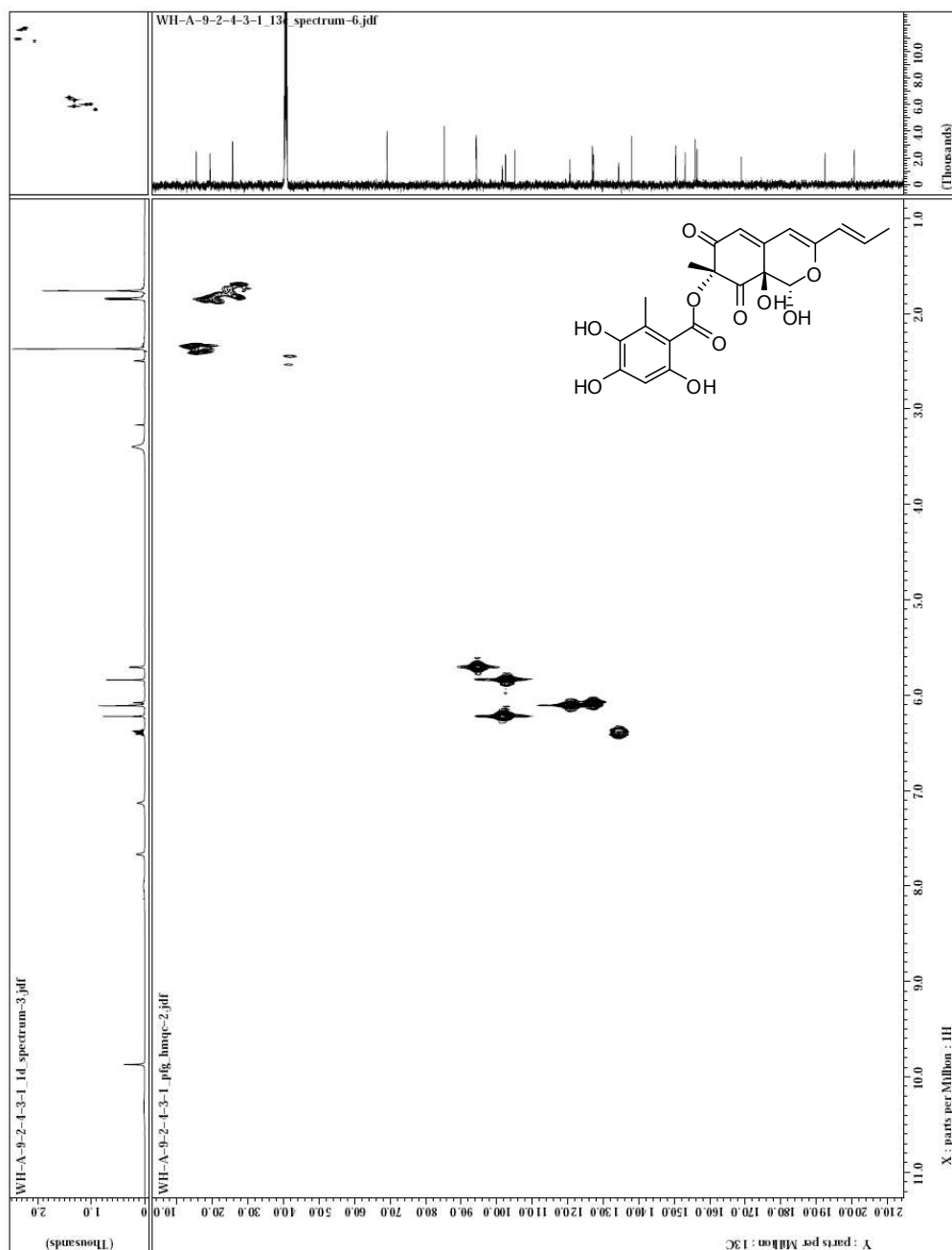


Figure S14. The HMBC spectrum of purpurquinone B (**2**) in DMSO

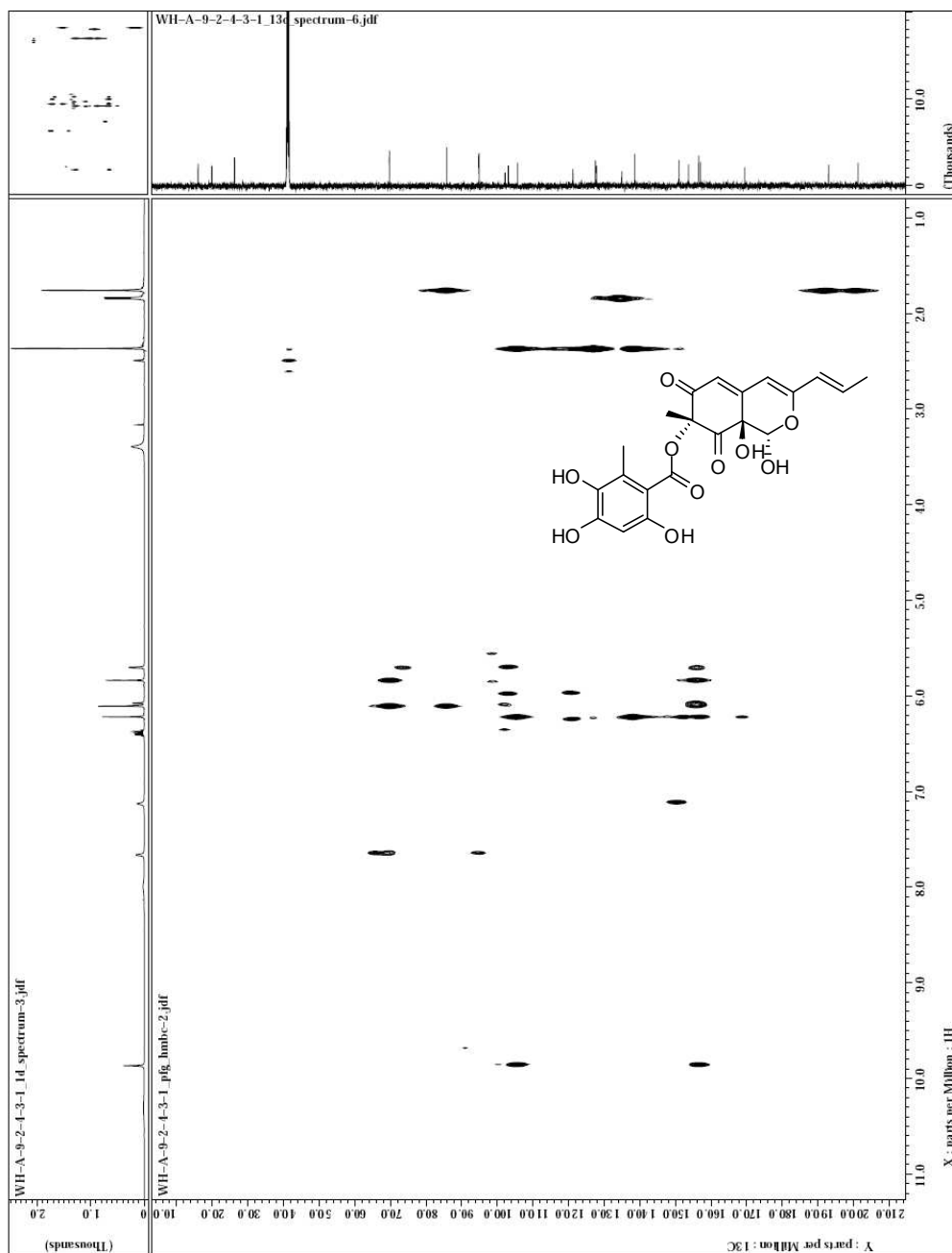


Figure S15. The NOESY spectrum of purpurquinone B (**2**) in DMSO

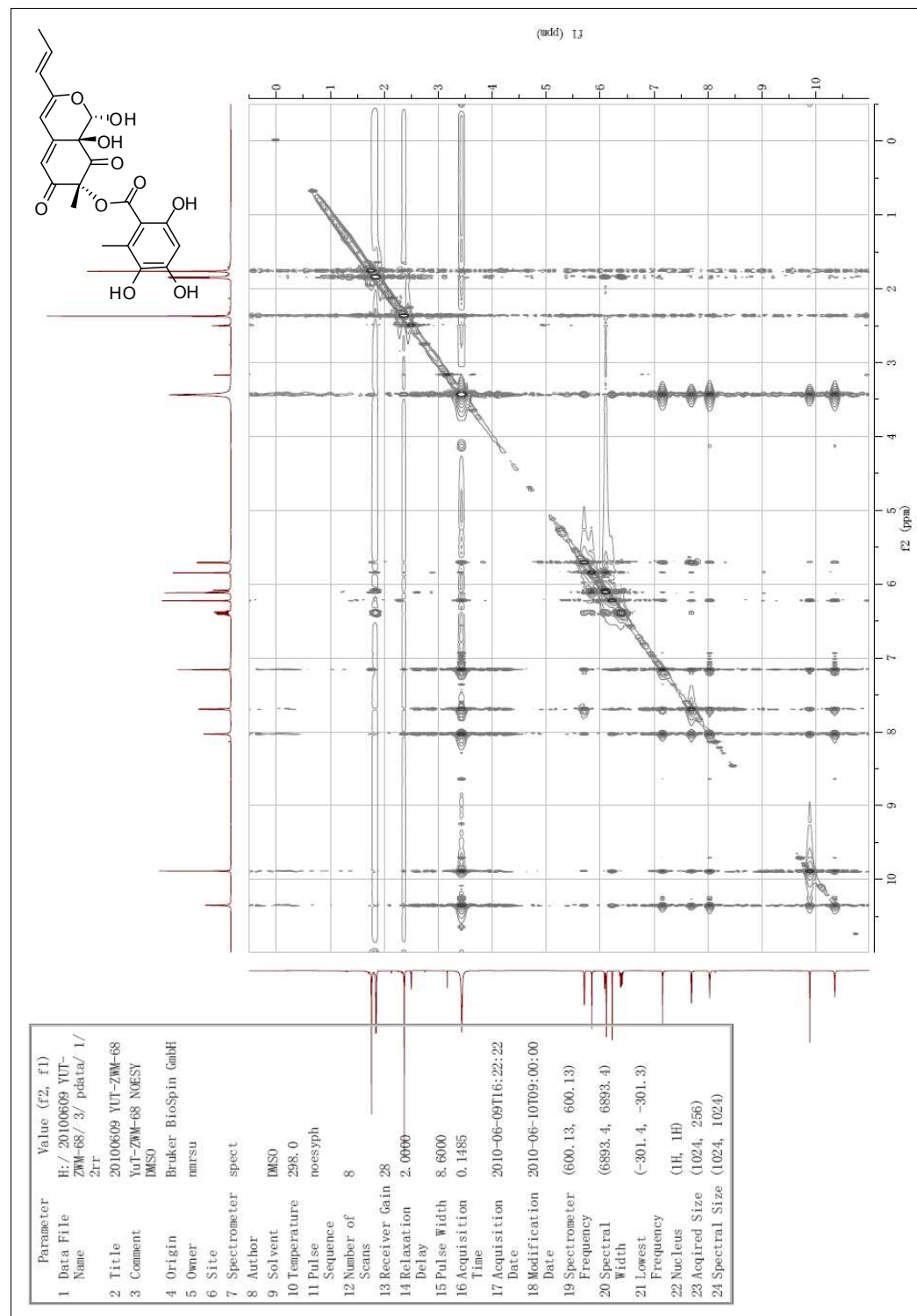


Figure S16. The ^1H NMR spectrum of purpurquinone C (**3**) in DMSO

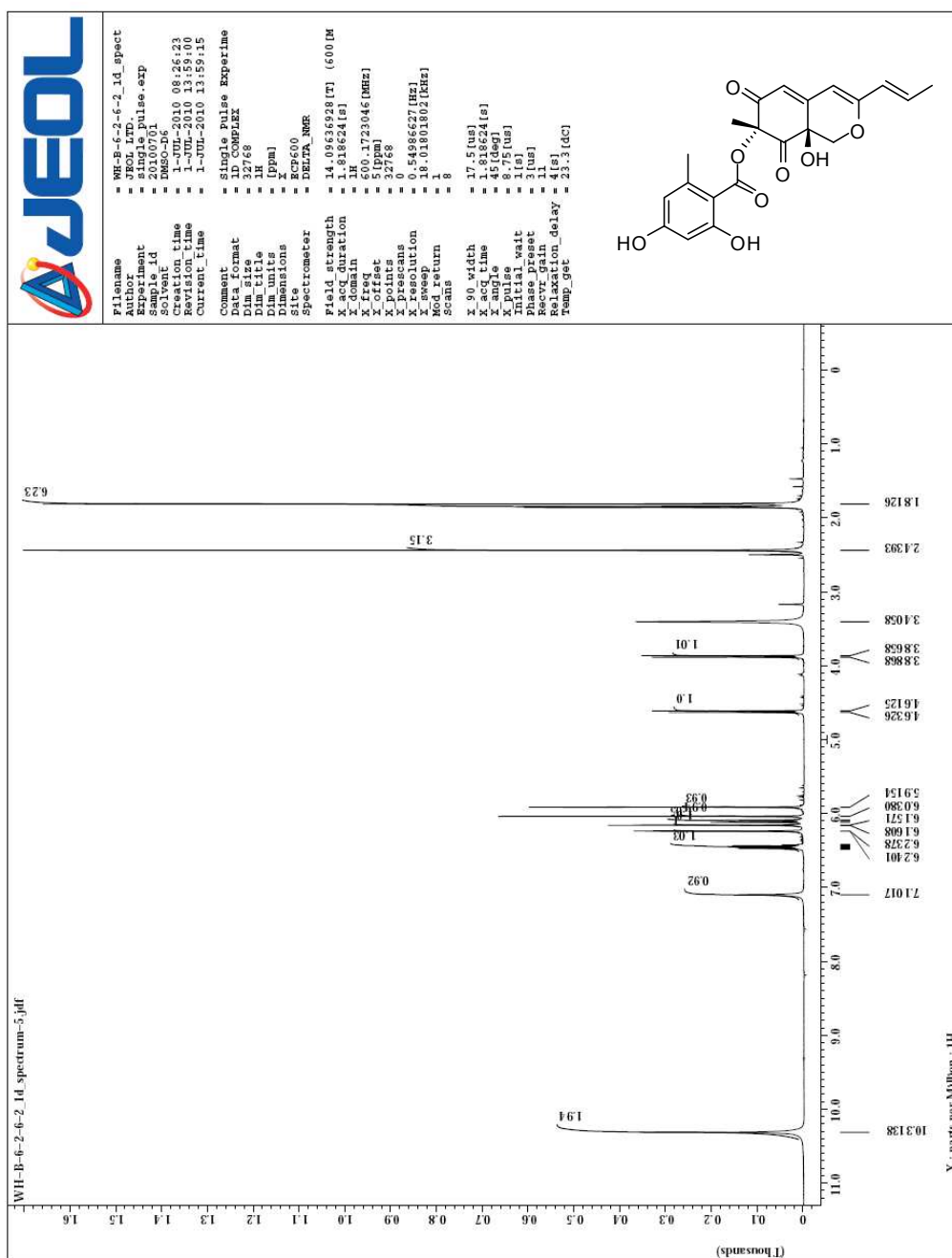


Figure S17. The ^{13}C NMR spectrum of purpurquinone C (**3**) in DMSO

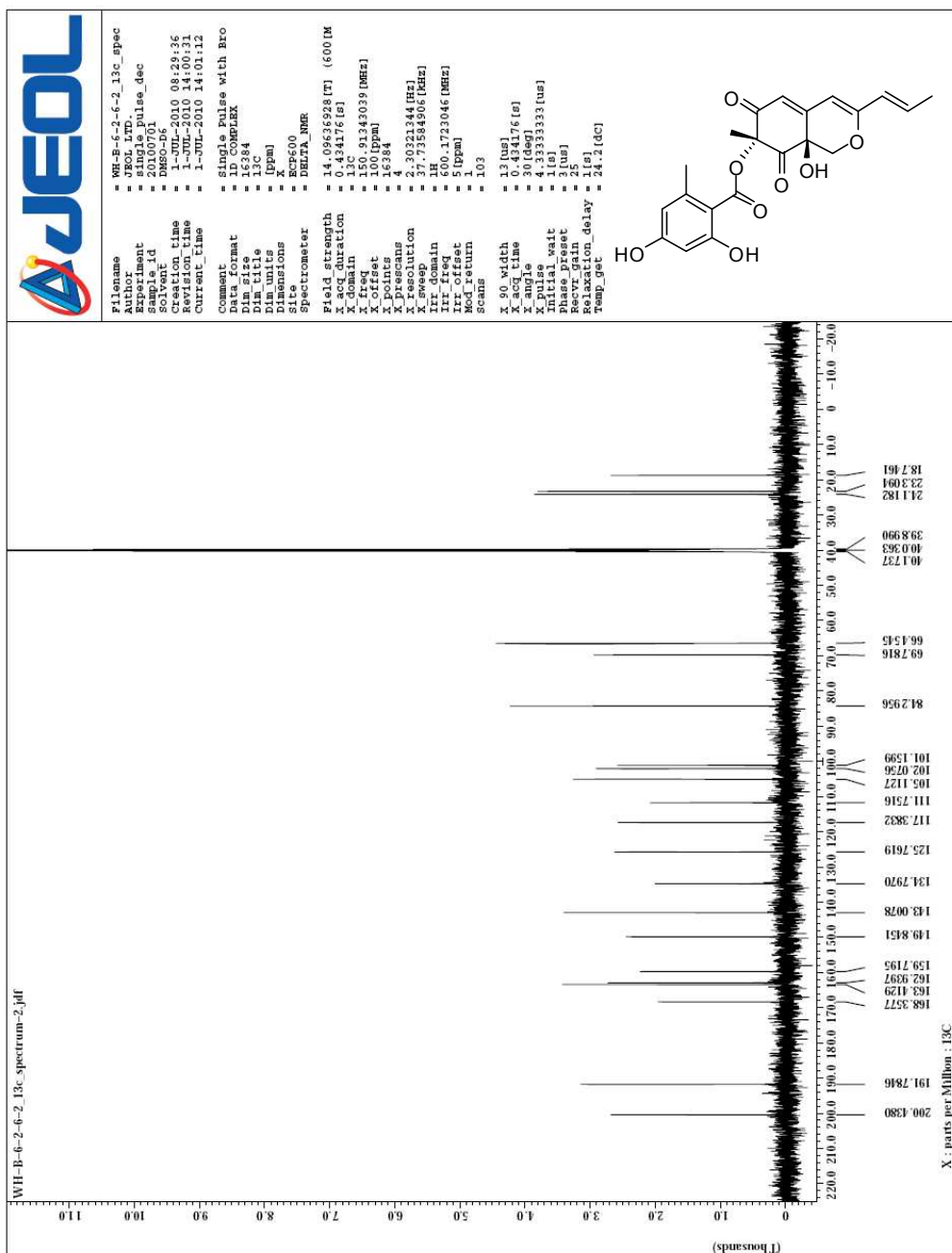


Figure S18. The DEPT spectrum of purpurquinone C (**3**) in DMSO

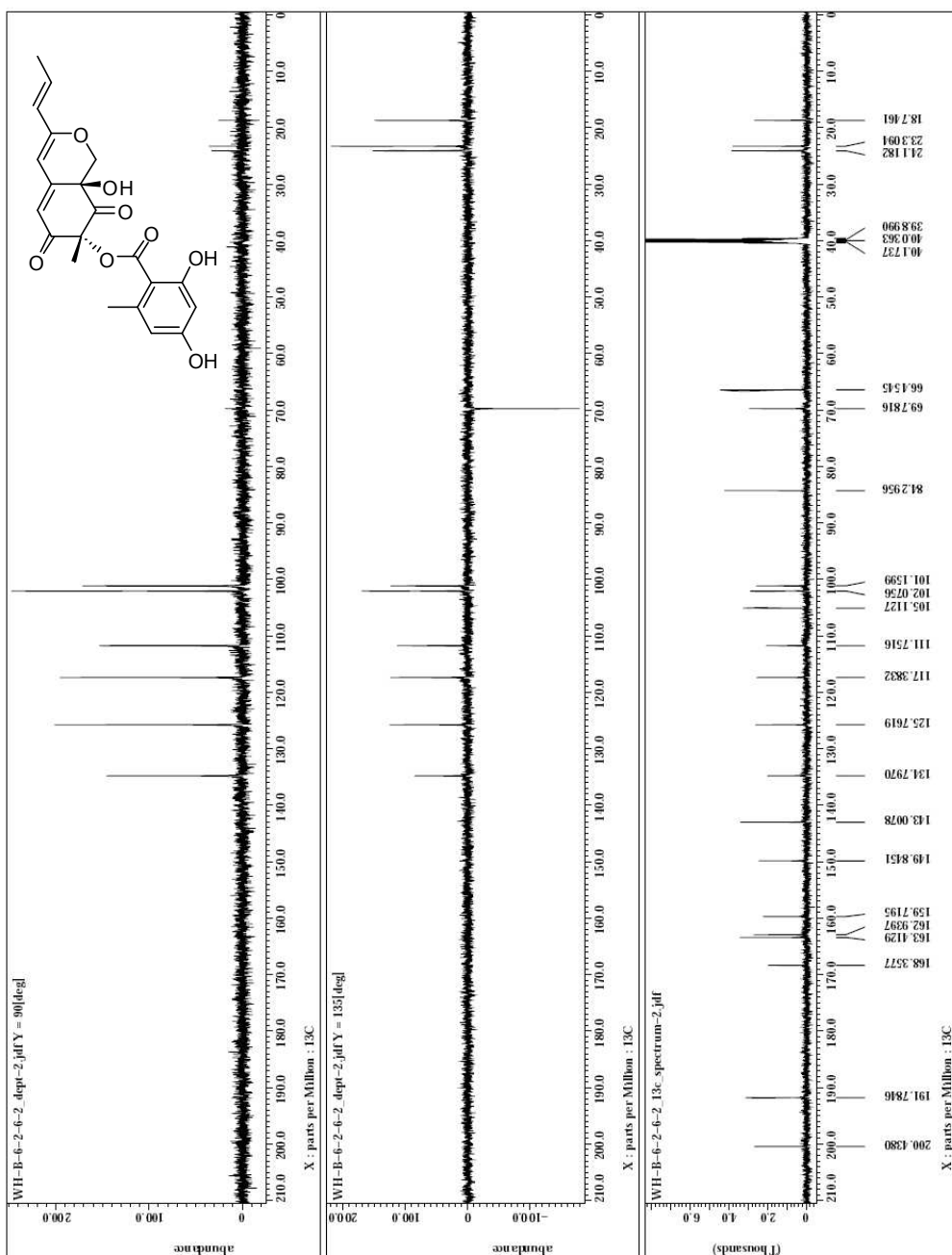


Figure S19. The NOESY spectrum of purpurquinone C (**3**) in DMSO

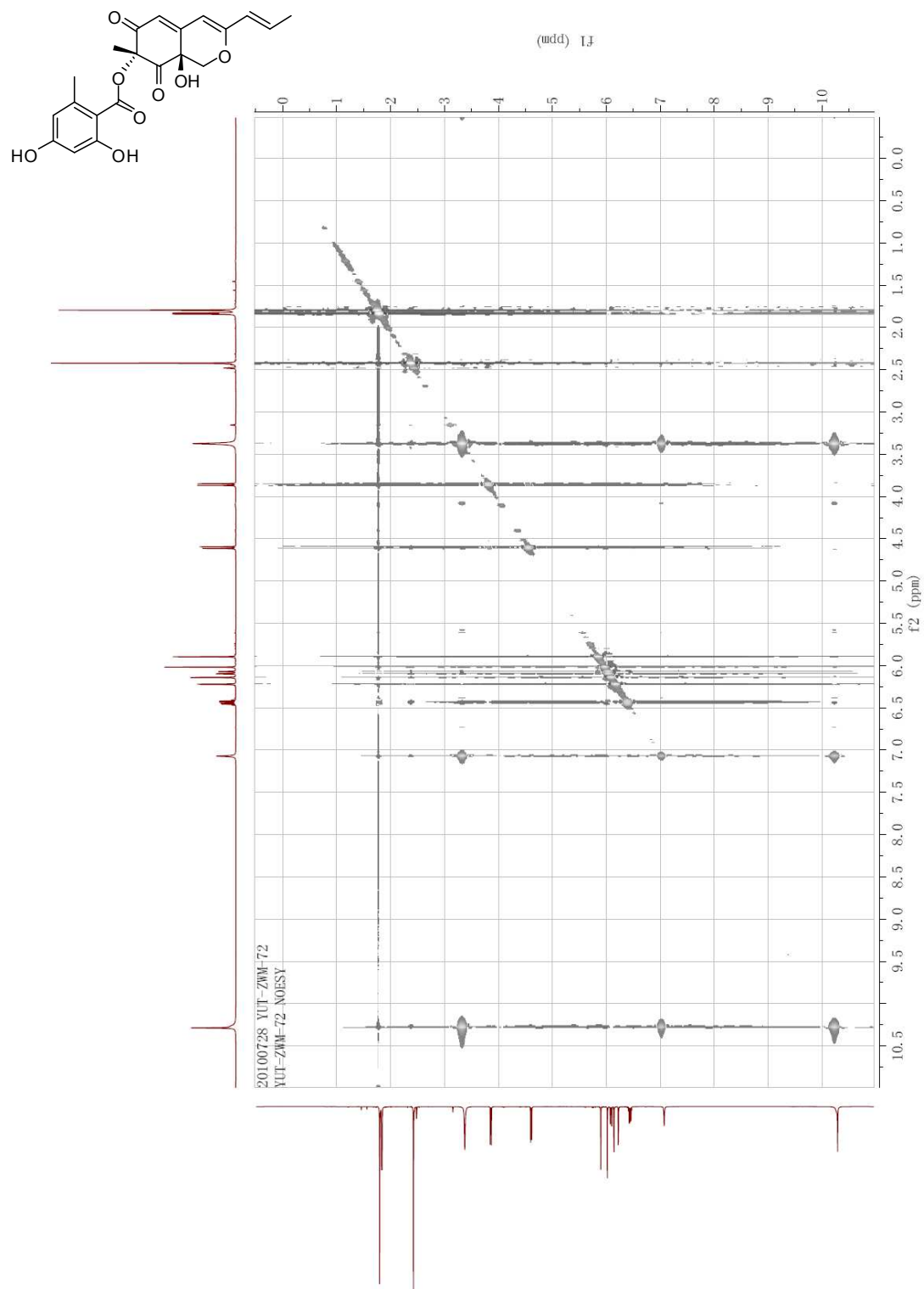


Figure S20. The ^1H NMR spectrum of purpurester A (4) in DMSO

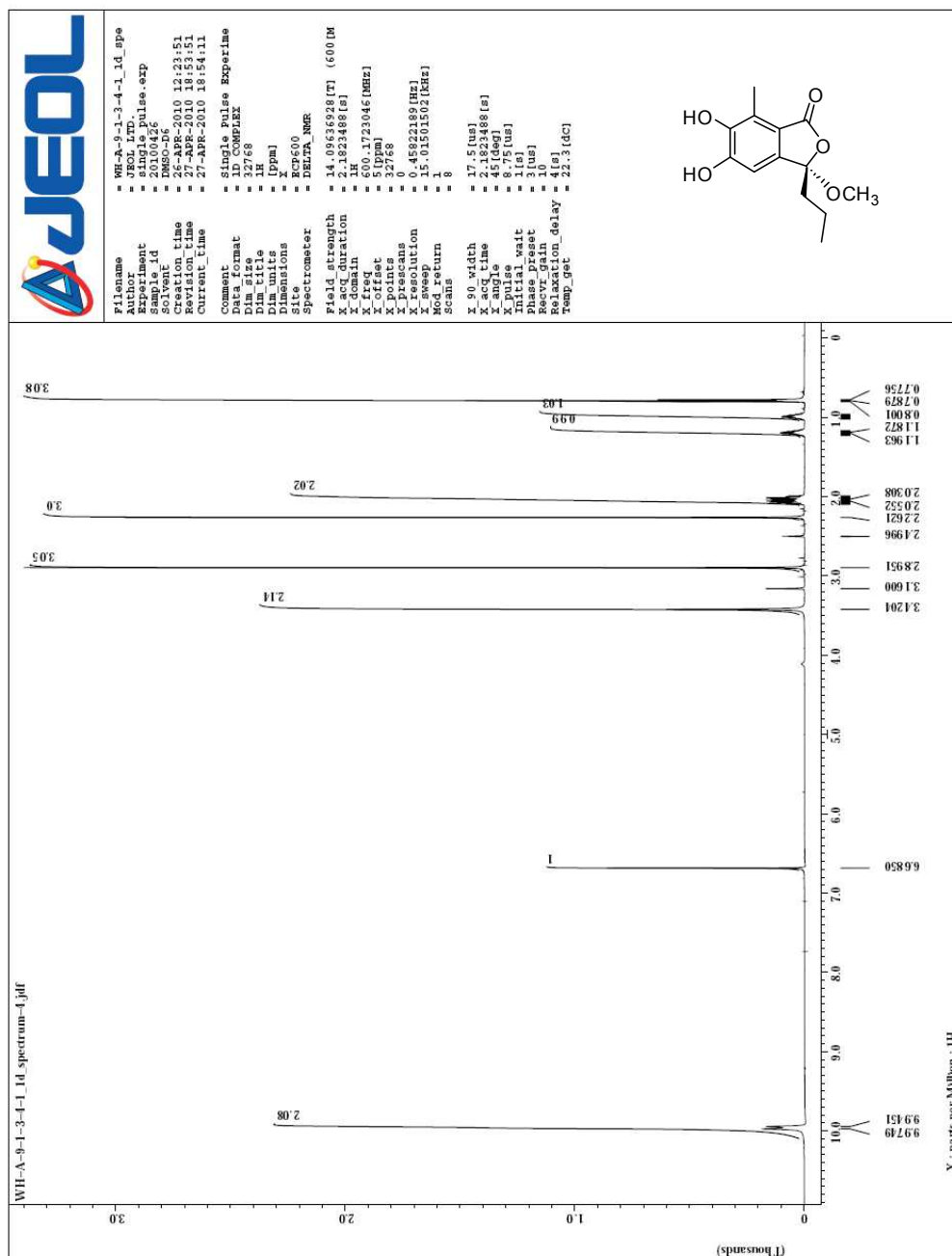


Figure S21. The ^{13}C NMR spectrum of purpurester A (4) in DMSO

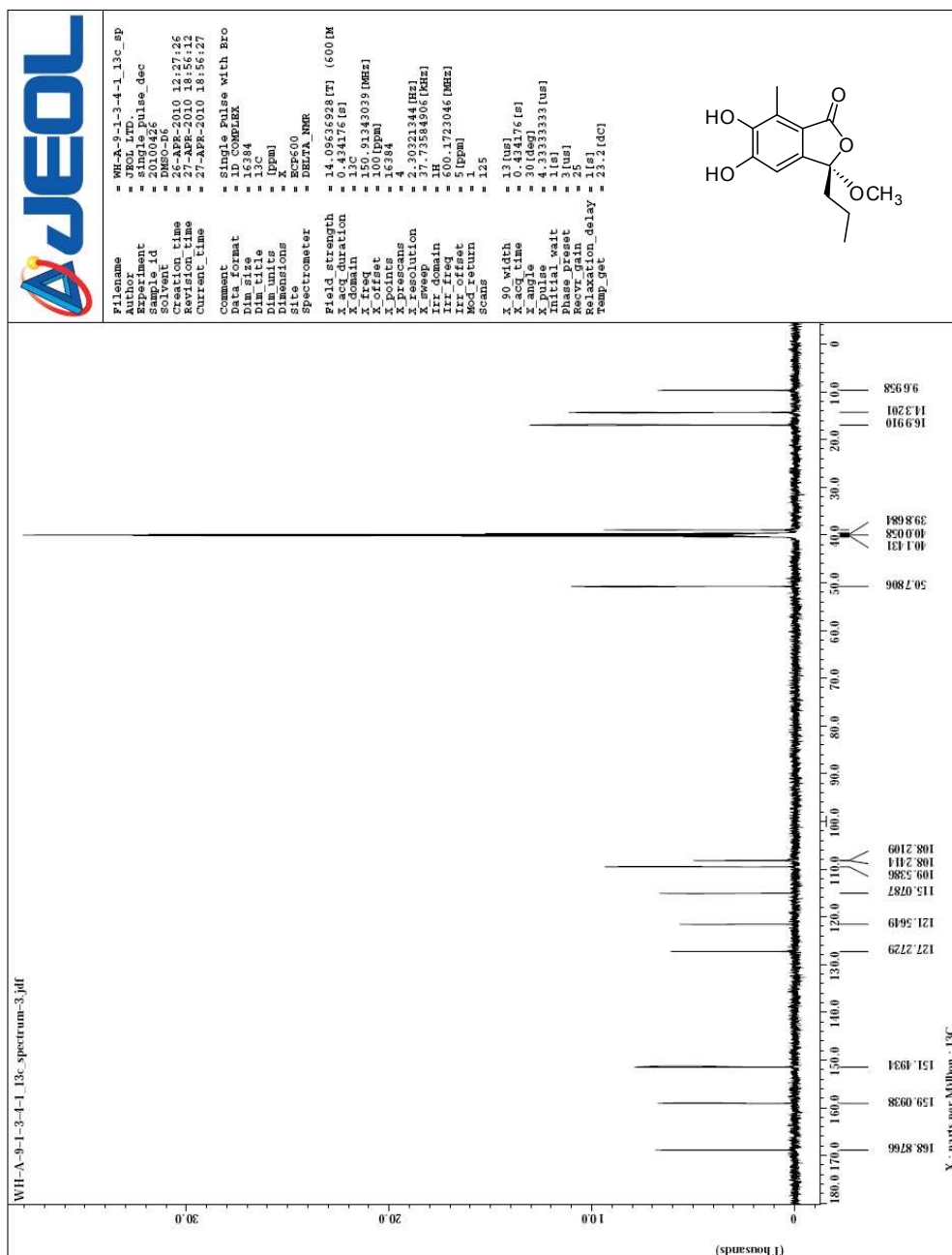


Figure S22. The DEPT spectrum of purpurester A (4) in DMSO

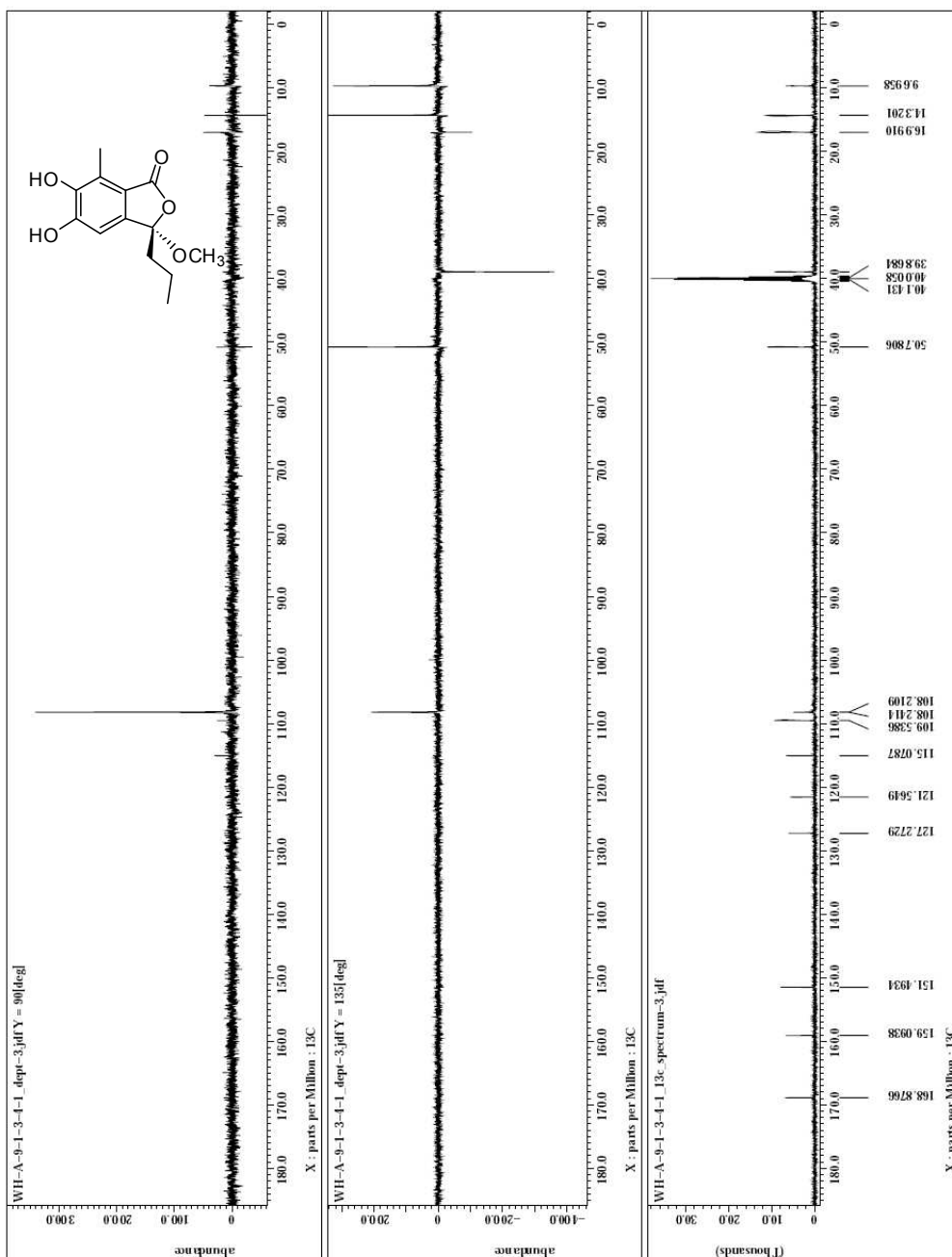


Figure S23. The HMQC spectrum of purpurester A (4) in DMSO

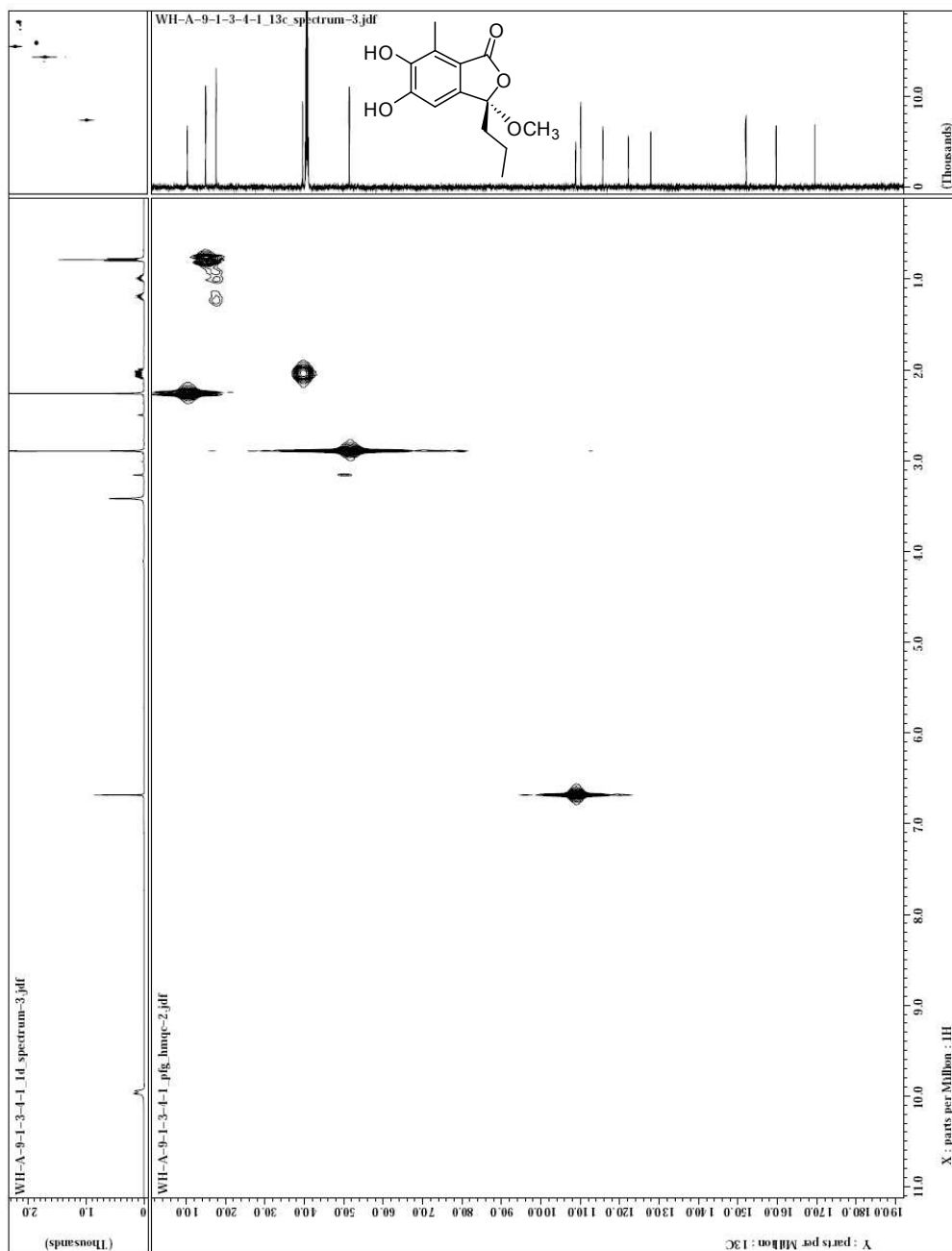


Figure S24. The ^1H - ^1H COSY spectrum of purpurester A (**4**) in DMSO

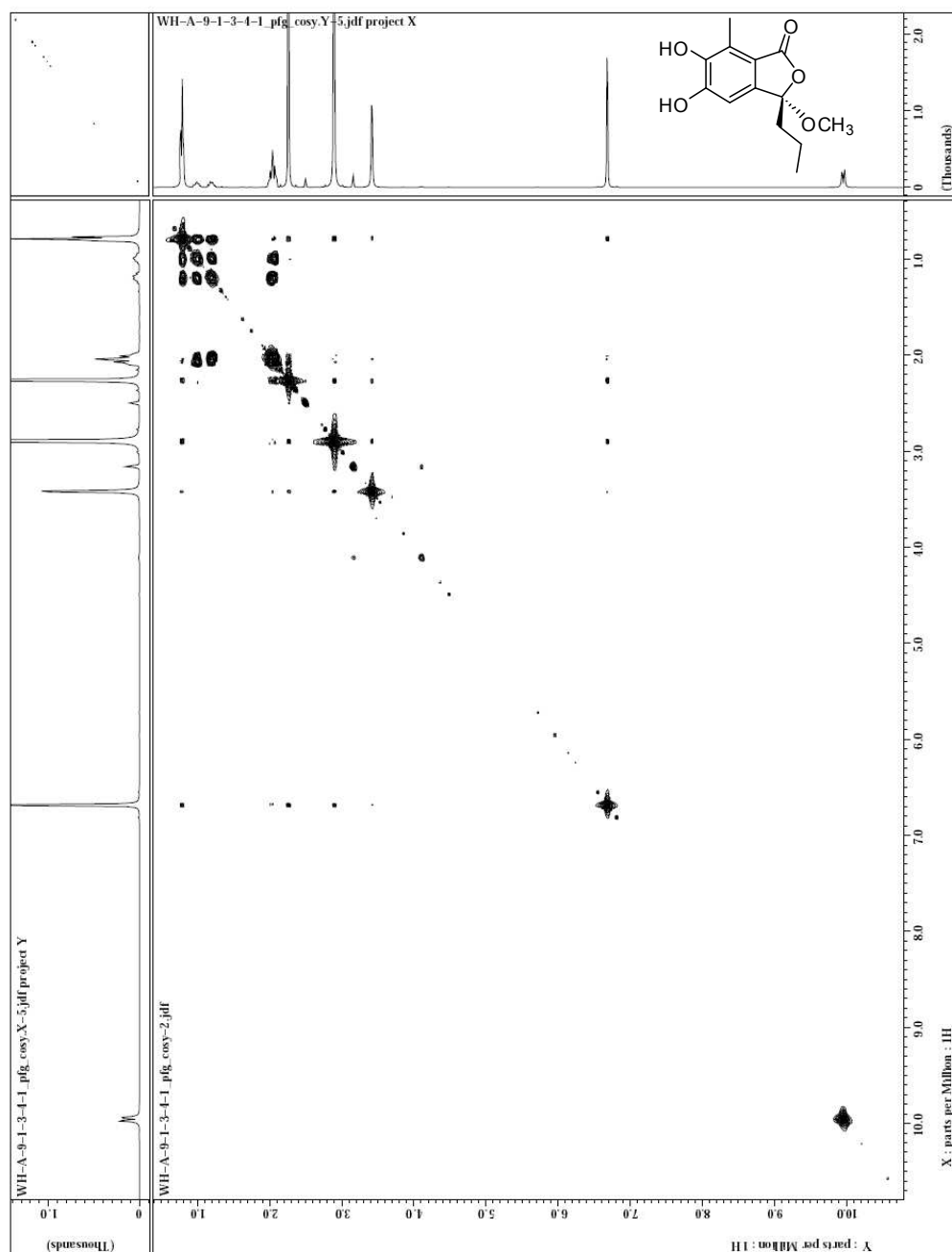


Figure S25. The HMBC spectrum of purpurester A (4) in DMSO

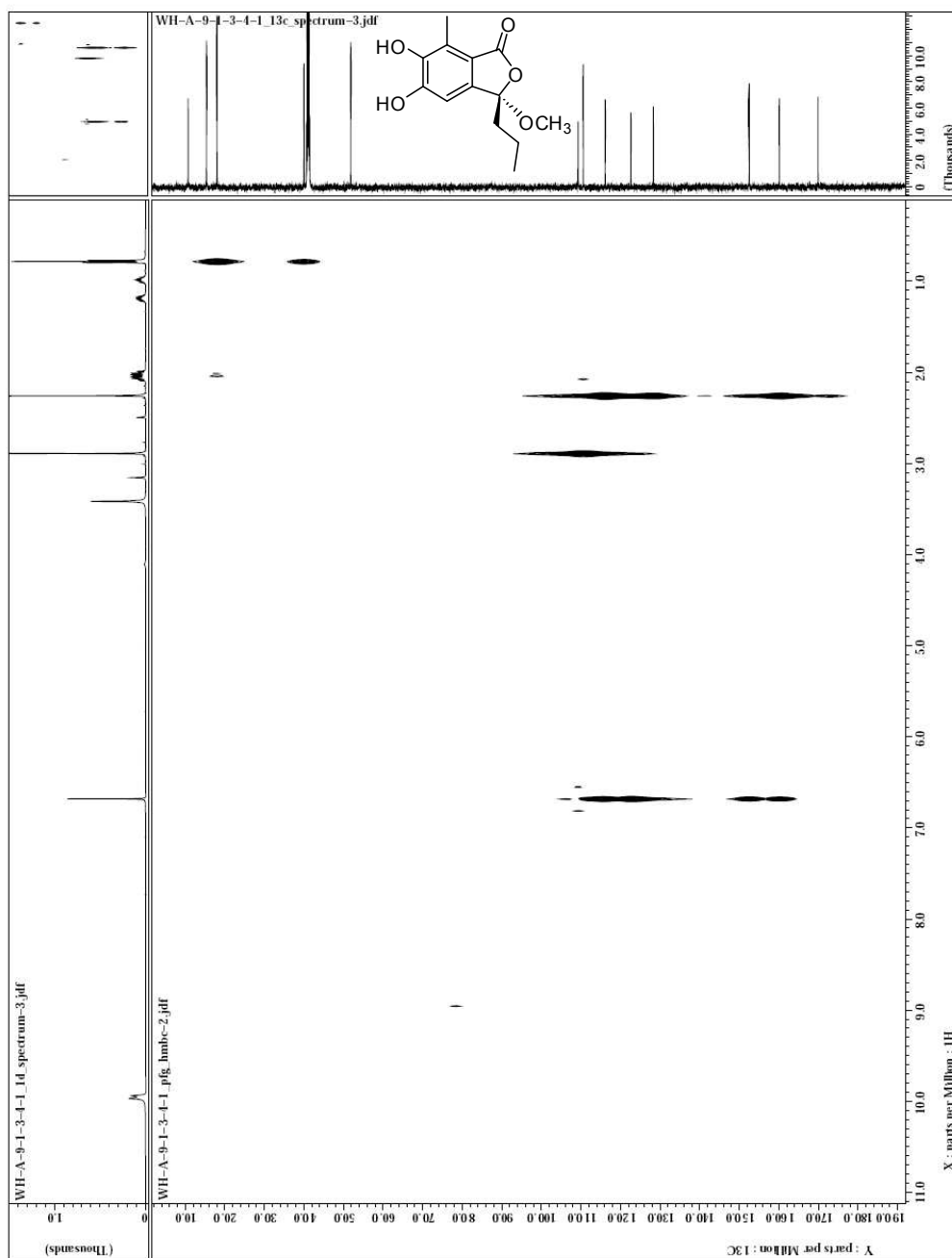


Figure S26. The ^1H NMR spectrum of purplester B (**5**) in DMSO

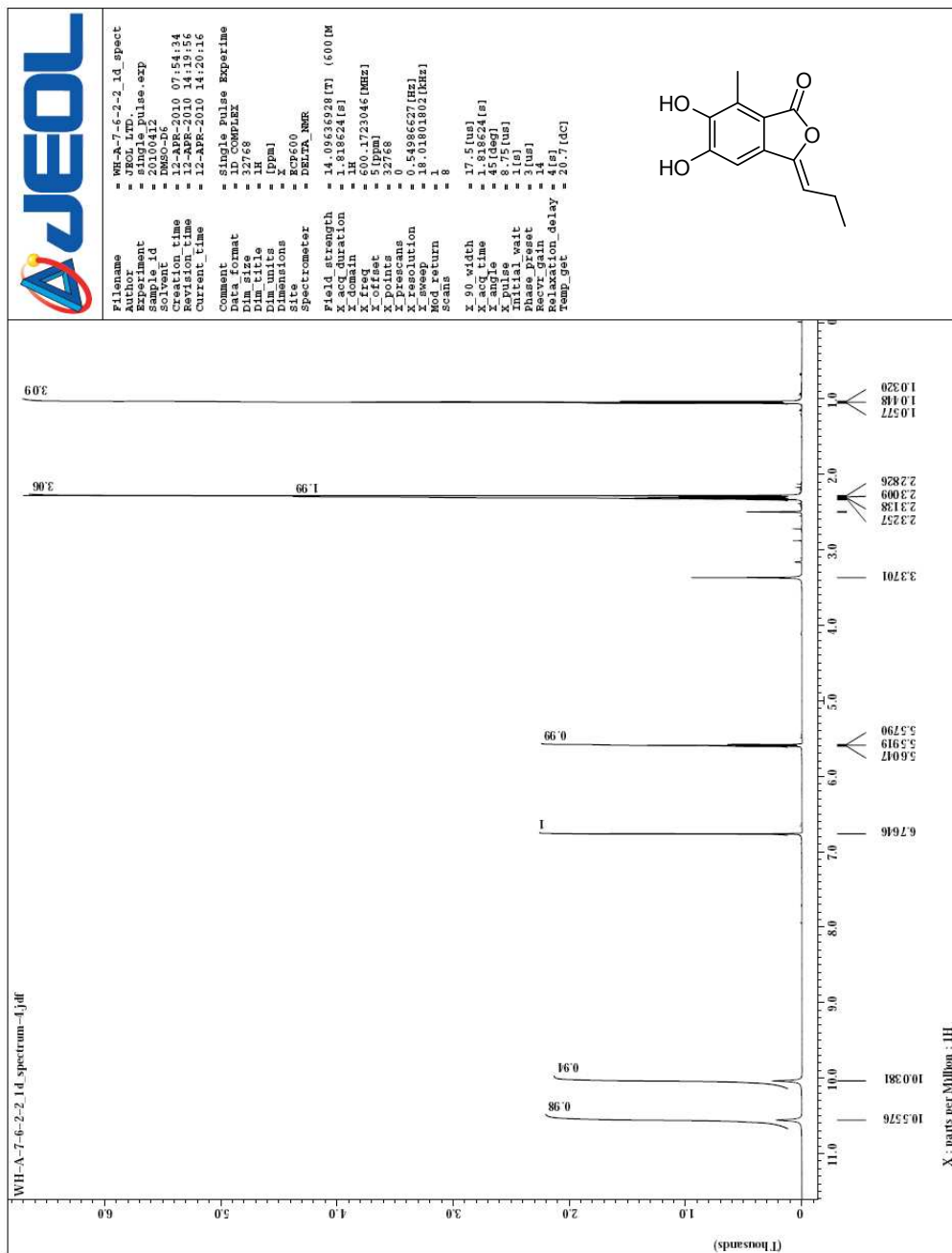


Figure S27. The ^{13}C NMR spectrum of purplester B (**5**) in DMSO

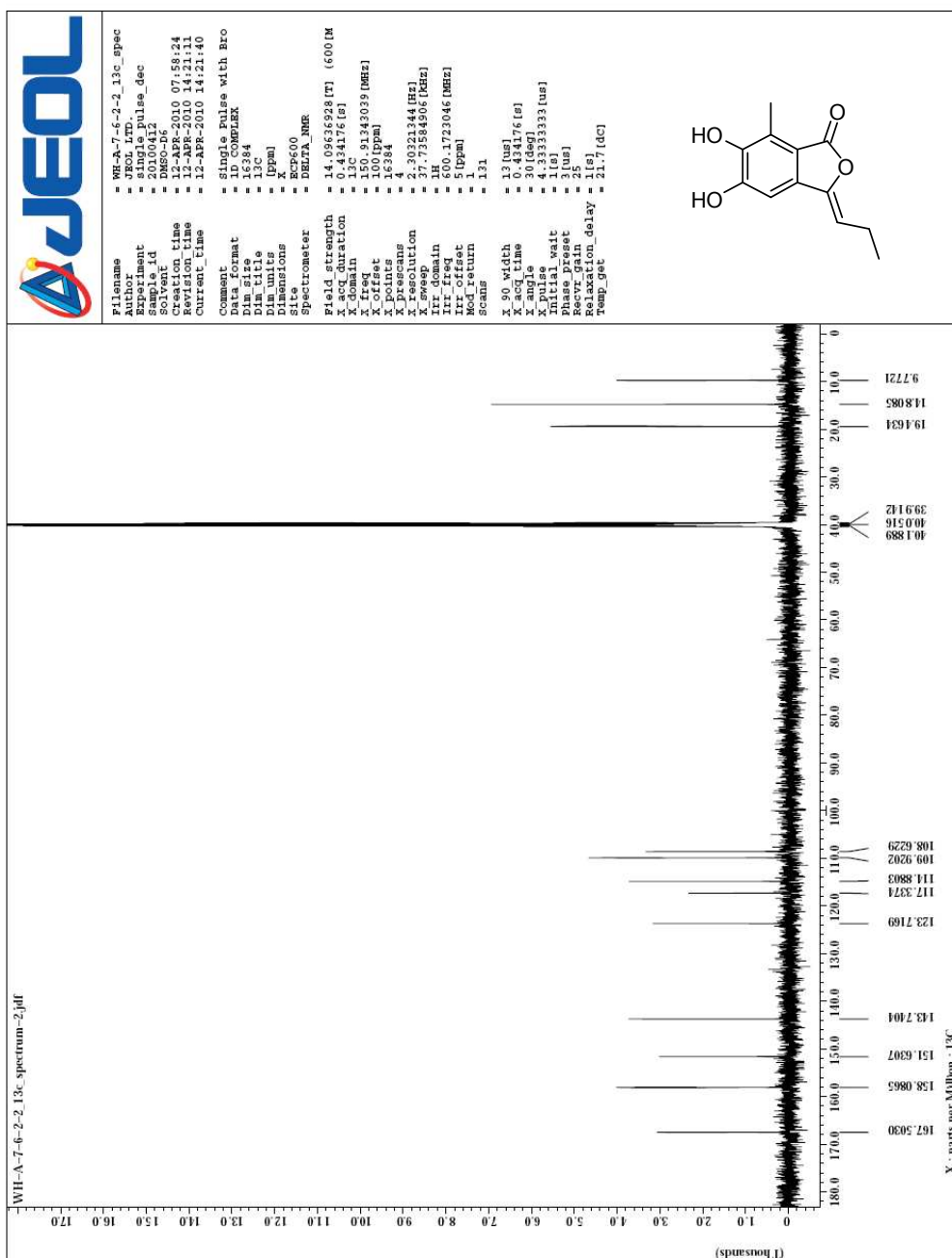


Figure S28. The DEPT spectrum of purplester B (**5**) in DMSO

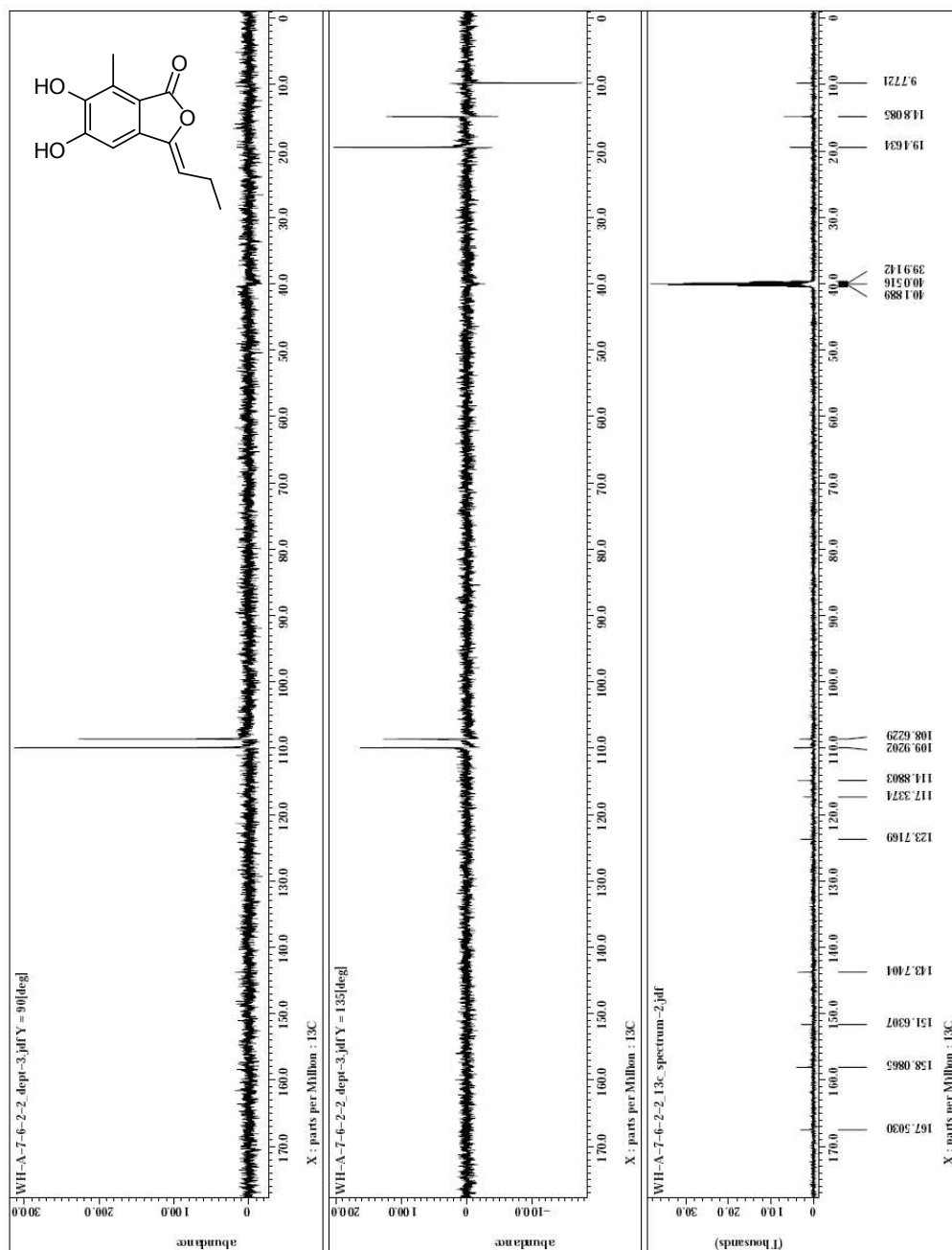


Figure S29. The ^1H NMR spectrum of compound **6** in DMSO

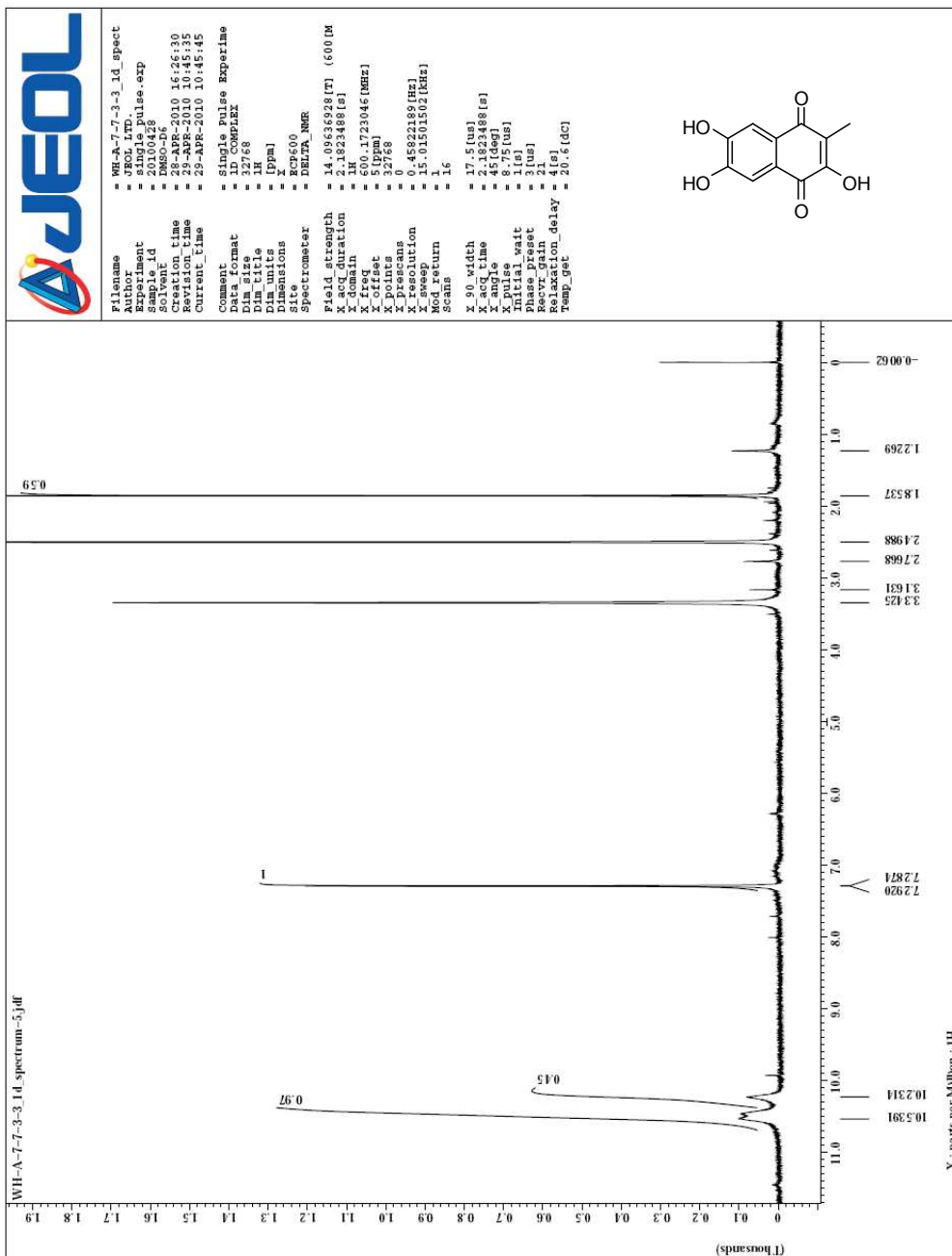


Figure S30. The ^{13}C NMR spectrum of compound **6** in DMSO

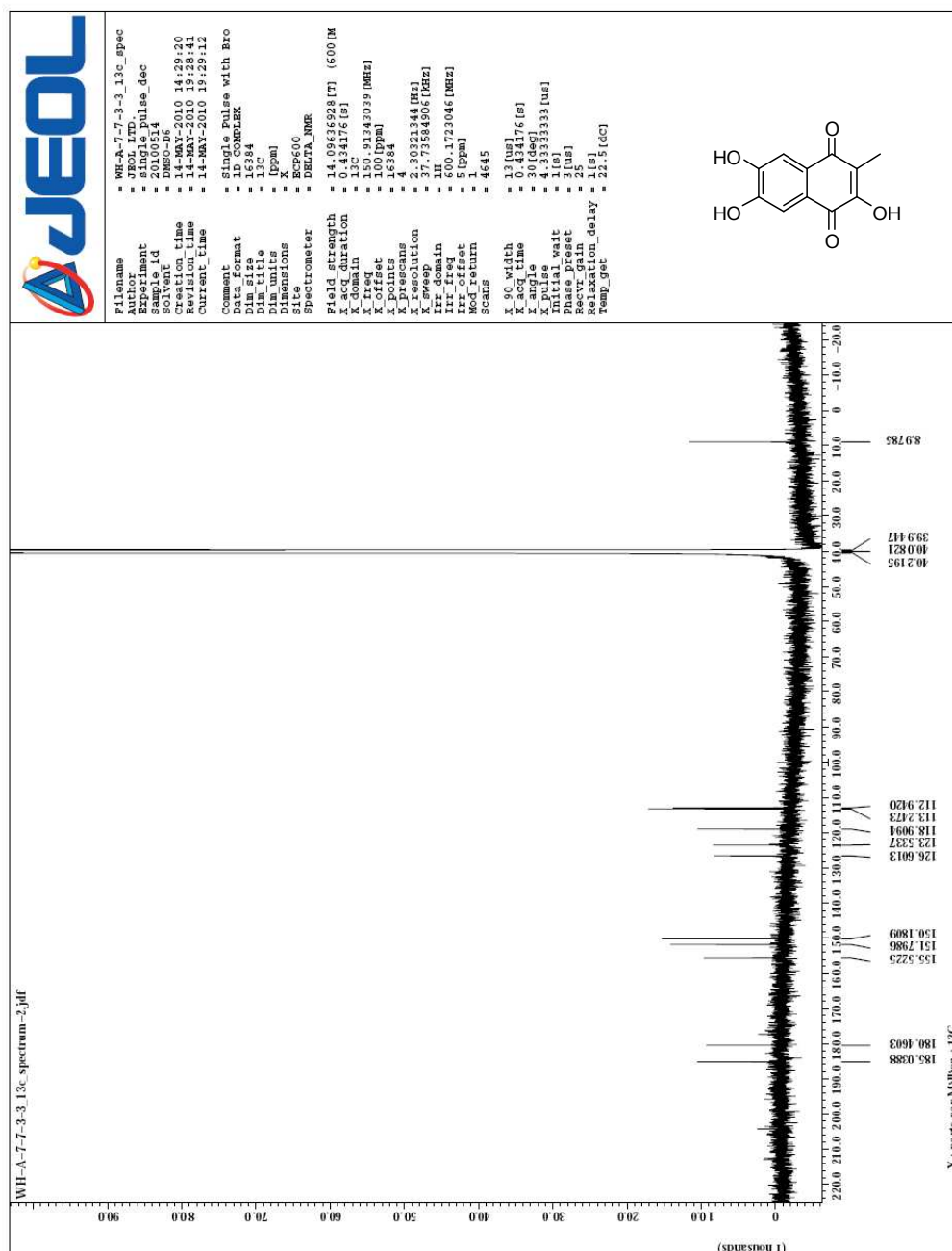


Figure S31. The DEPT spectrum of compound **6** in DMSO

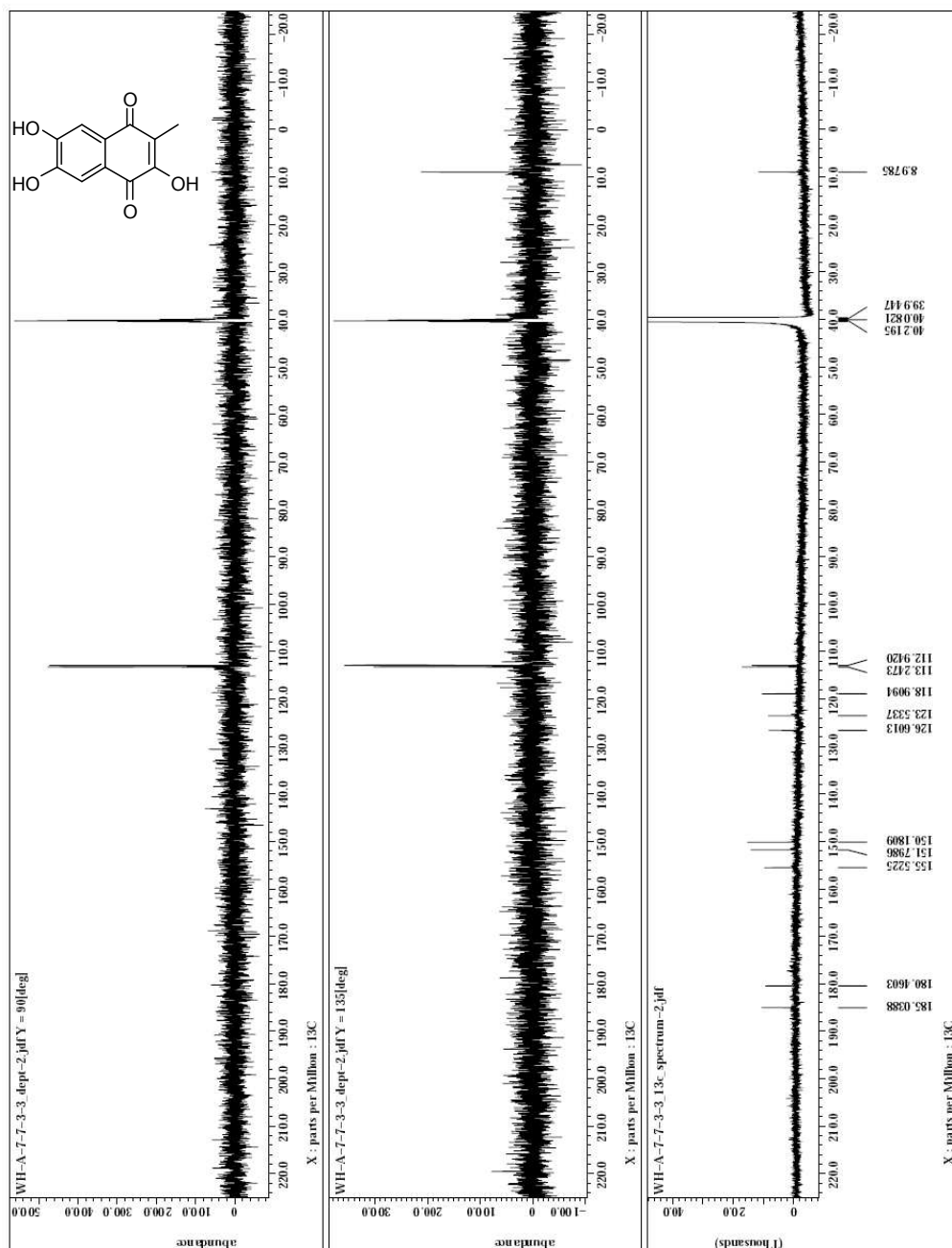


Figure S32. HPLC profiles (360 nm) of secondary metabolites from *P. purpurogenum* JS03-21 cultivated at pH 2 and pH 7.

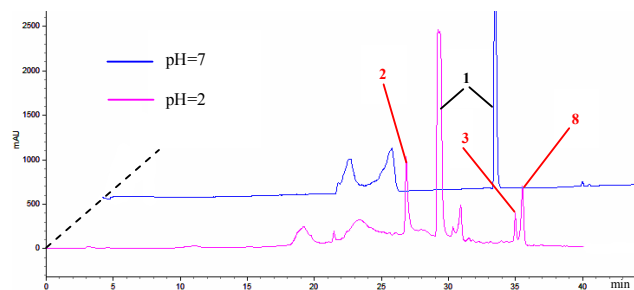


Figure S33. Key NOESY correlations of compounds 1–3.

