### **Supporting Information**

Rec. Nat. Prod. 17:3 (2023) 555-560

# An Undescribed Triterpenoid Saponin Isolated from

## Zornia diphylla

# Jiahui Li<sup>1</sup>, Mengfei Xue<sup>1</sup>, Meng Wang<sup>1</sup>, Peng Li<sup>3</sup> and Zhenliang Sun<sup>2</sup>

<sup>1</sup> Anhui University of Science and Technology School of Medicine, Huainan, China

<sup>&</sup>lt;sup>3</sup> State Key Laboratory of Quality Research in Chinese Medicine, Institute of Chinese Medical Sciences, University of Macau, Macau 999078, China

Table of contents	Page
Figure S1: HRESIMS data of zordiphylloside I	3
Figure S2: <sup>1</sup> H-NMR spectrum of zordiphylloside I	3
Figure S3: DEPT and <sup>13</sup> C-NMR spectra of zordiphylloside I	4
Figure S4: <sup>1</sup> H- <sup>1</sup> H COSY spectrum of zordiphylloside I	4
Figure S5: HSQC spectrum of zordiphylloside I	5
Figure S6: HMBC spectrum of zordiphylloside I	5
Figure S7: ROESY spectrum of zordiphylloside I	6
Figure S8: UV spectrum of zordiphylloside I	6
Figure S9: IR spectrum of zordiphylloside I	7
Figure S10. <sup>1</sup> H-NMR spectrum of compound 2	7
Figure S11. <sup>13</sup> C-NMR spectrum of compound 2	7
Figure S12. <sup>1</sup> H-NMR spectrum of compound 3	8
Figure S13. <sup>13</sup> C-NMR spectrum of compound 3	8
Figure S14. <sup>1</sup> H-NMR spectrum of compound 4	9
Figure S15. <sup>13</sup> C-NMR spectrum of compound 4	9
Figure S16. <sup>1</sup> H-NMR spectrum of compound 5	10
Figure S17. <sup>13</sup> C-NMR spectrum of compound 5	10
Figure S18. <sup>1</sup> H-NMR spectrum of compound 6	11
Figure S19. <sup>13</sup> C-NMR spectrum of compound 6	11
Figure S20. <sup>1</sup> H-NMR spectrum of compound 7	12
Figure S21. <sup>1</sup> H-NMR spectrum of compound 8	13

<sup>&</sup>lt;sup>2</sup> Fengxian Hospital affiliated to Anhui University of Science and Technology, Shanghai, China

Figure S22. <sup>13</sup> C-NMR spectrum of compound 8	13
Figure S23. <sup>1</sup> H-NMR spectrum of compound 9	14
Figure S24. <sup>13</sup> C-NMR and DEPT spectra of compound 9	14
Figure S25. <sup>1</sup> H-NMR spectrum of compound 10	15
Figure S26. <sup>13</sup> C-NMR spectrum of compound 10	15
Figure S27. <sup>1</sup> H-NMR spectrum of compound 11	16
Figure S28. <sup>13</sup> C-NMR and DEPT spectra of compound 11	16
Figure S29. <sup>1</sup> H-NMR spectrum of compound 12	17
Figure S30. DEPT and <sup>13</sup> C-NMR spectra of compound 12	17
Figure S31. <sup>1</sup> H-NMR spectrum of compound 13	18
Figure S32. <sup>13</sup> C-NMR spectrum of compound 13	18
Figure S33. <sup>1</sup> H-NMR spectrum of compound 14	19
Figure S34. DEPT and <sup>13</sup> C-NMR spectra of compound 14	19
Figure S35. <sup>1</sup> H-NMR spectrum of compound 15	20
Figure S36. <sup>1</sup> H-NMR spectrum of compound 16	21
Figure S37. <sup>13</sup> C-NMR spectrum of compound 16	21
Figure S38. <sup>1</sup> H-NMR spectrum of compound 17	22
Figure S39. DEPT and <sup>13</sup> C-NMR spectra of compound 17	22
Figure S40. <sup>13</sup> C-NMR spectrum of compound 18	23
Figure S41. <sup>1</sup> H-NMR spectrum of compound 19	23
Figure S42. <sup>13</sup> C-NMR spectrum of compound 19	24
Figure S43. <sup>1</sup> H-NMR spectrum of compound 20	25
Figure S44. <sup>13</sup> C-NMR spectrum of compound 20	25
Figure S45. <sup>1</sup> H-NMR spectrum of compound 21	26
Figure S46. <sup>13</sup> C-NMR spectrum of compound 21	26
Figure S47. <sup>1</sup> H-NMR spectrum of compound 22	27
Figure S48. <sup>13</sup> C-NMR spectrum of compound 22	27
Figure S49. <sup>1</sup> H-NMR spectrum of compound 23	28
Figure S50. <sup>13</sup> C-NMR spectrum of compound 23	28
Figure S51. <sup>1</sup> H-NMR spectrum of compound 24	29
Figure S52. <sup>13</sup> C-NMR and DEPT spectra of compound 24	29
Figure S53. <sup>1</sup> H-NMR spectrum of compound 25	30
Figure S54. <sup>13</sup> C-NMR and DEPT spectra of compound 25	30
Figure S55. <sup>1</sup> H-NMR spectrum of compound 26	31
Figure S56. <sup>13</sup> C-NMR and DEPT spectra of compound 26	31
Scifinder search report	32

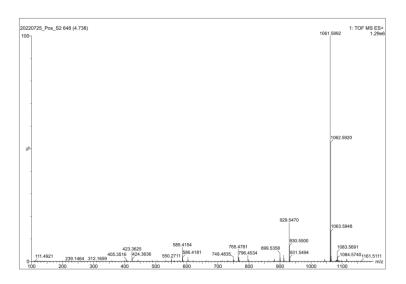


Figure S1: HRESIMS spectrum of zordiphylloside I

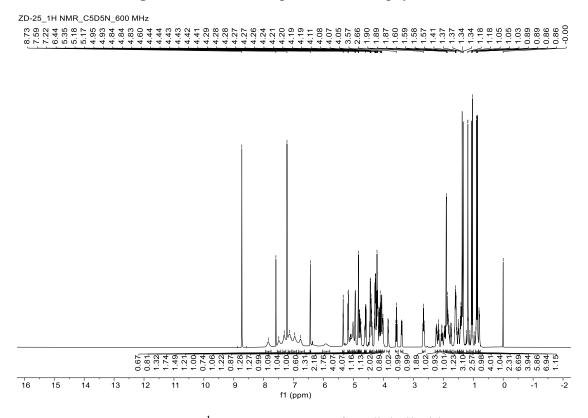


Figure S2: <sup>1</sup>H-NMR spectrum of zordiphylloside I

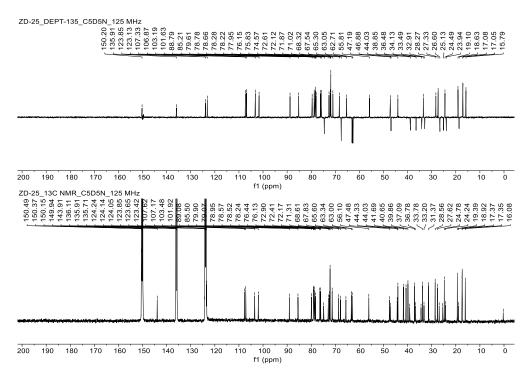


Figure S3: DEPT and <sup>13</sup>C NMR spectra of zordiphylloside I

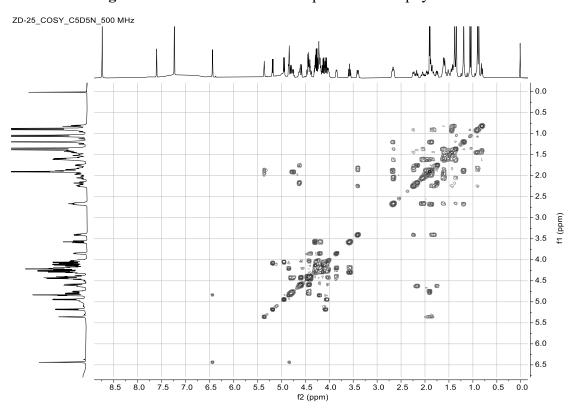


Figure S4: <sup>1</sup>H-<sup>1</sup>H COSY spectrum of zordiphylloside I

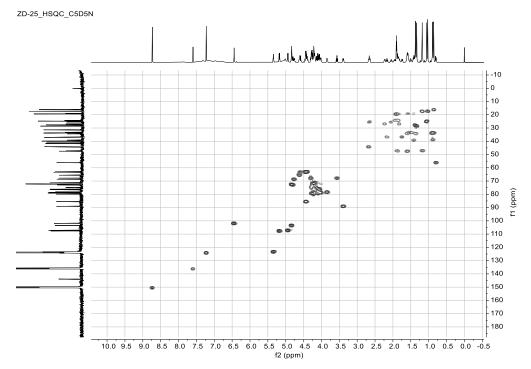


Figure S5: HSQC spectrum of zordiphylloside I

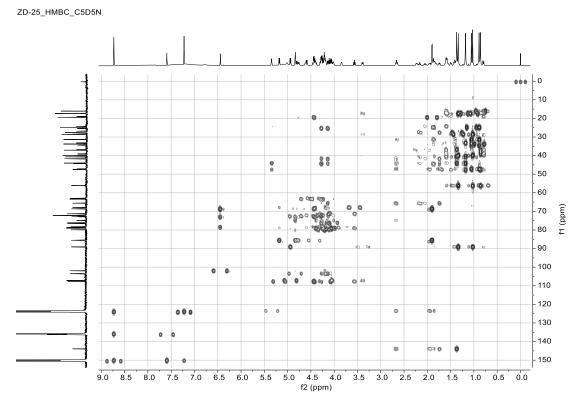


Figure S6: HMBC spectrum of zordiphylloside I

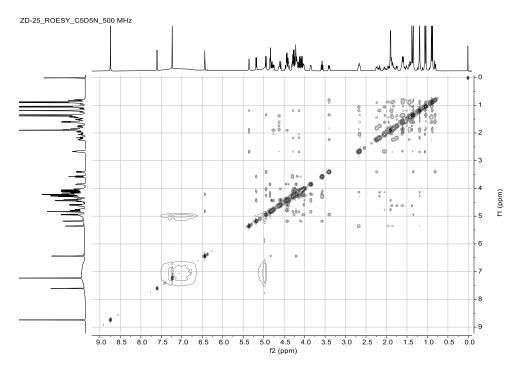


Figure S7: ROESY spectrum of zordiphylloside I

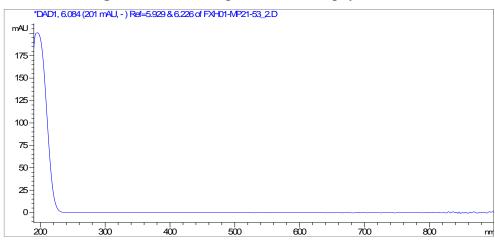
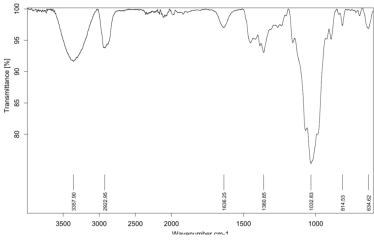


Figure S8: UV spectrum of zordiphylloside I



**Figure S9:** IR spectrum of zordiphylloside I © 2023 ACG Publications. All rights reserved.



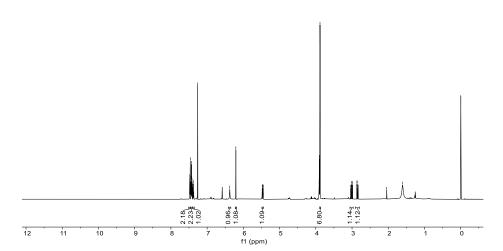


Figure S10: <sup>1</sup>H-NMR spectrum of compound 2

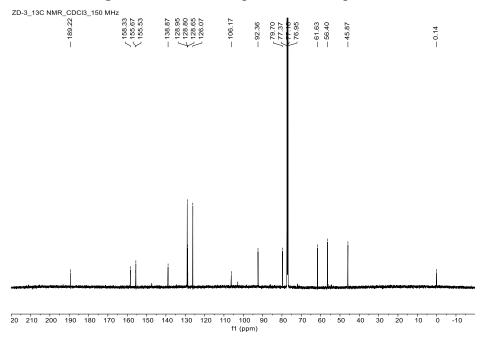


Figure S11: <sup>13</sup>C-NMR spectrum of compound 2

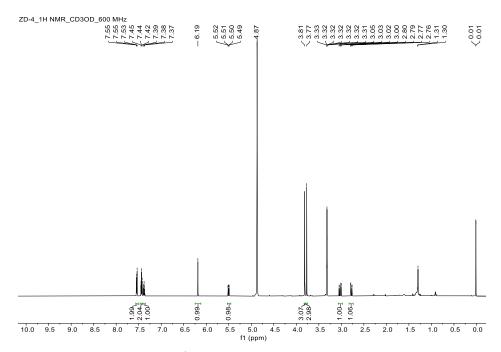


Figure S12: <sup>1</sup>H-NMR spectrum of compound 3

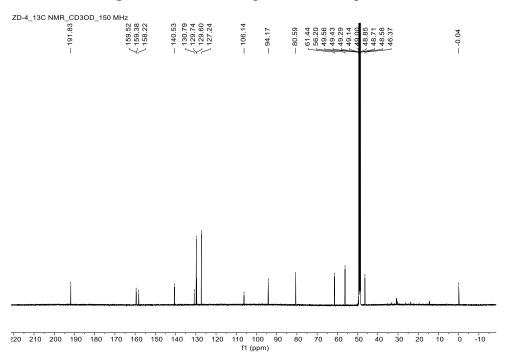


Figure S13: <sup>13</sup>C-NMR spectrum of compound 3

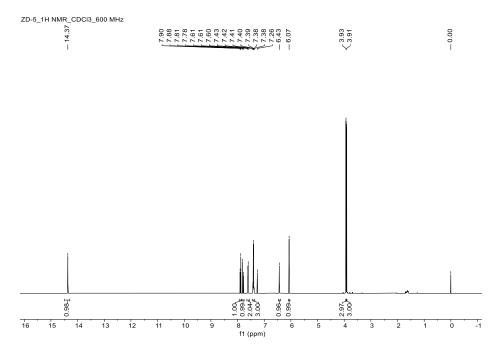


Figure S14: <sup>1</sup>H-NMR spectrum of compound 4



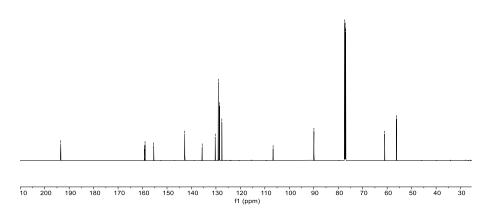


Figure S15: <sup>13</sup>C-NMR spectrum of compound 4



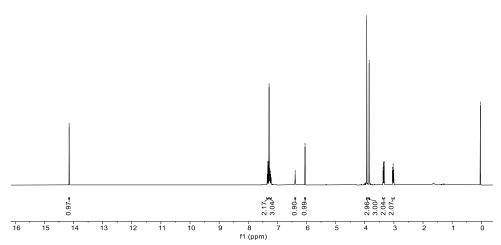


Figure S16: <sup>1</sup>H-NMR spectrum of compound 5

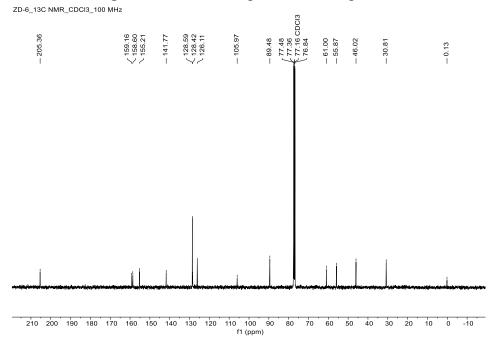


Figure S17: <sup>13</sup>C-NMR spectrum of compound 5



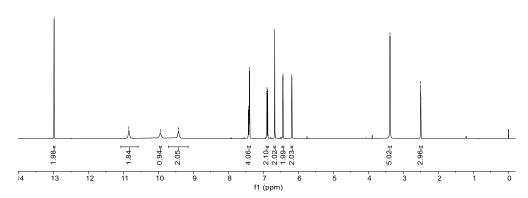


Figure S18: <sup>1</sup>H-NMR spectrum of compound 6

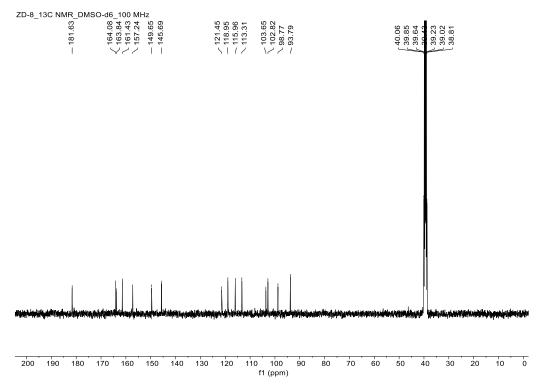


Figure S19: <sup>13</sup>C-NMR spectrum of compound 6

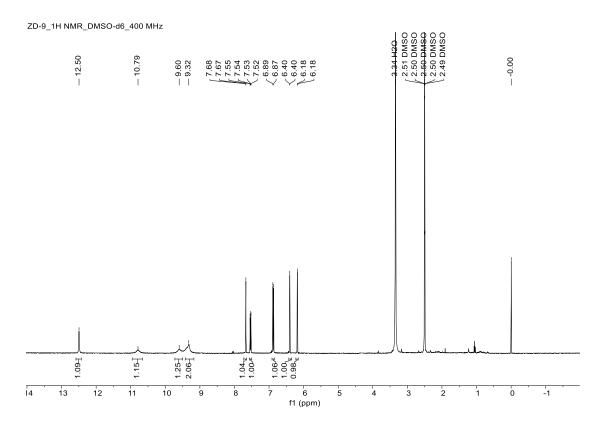


Figure S20: <sup>1</sup>H-NMR spectrum of compound 7

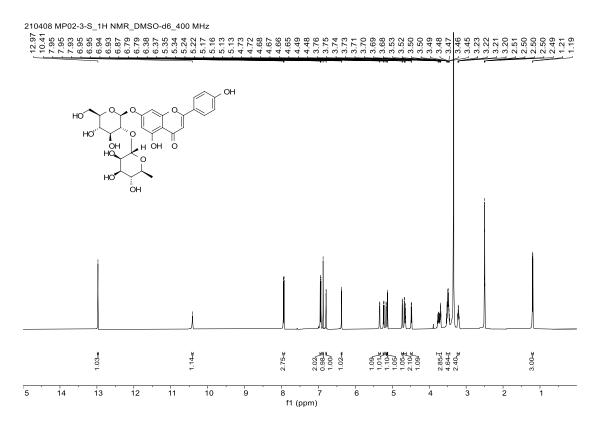


Figure S21: <sup>1</sup>H-NMR spectrum of compound 8

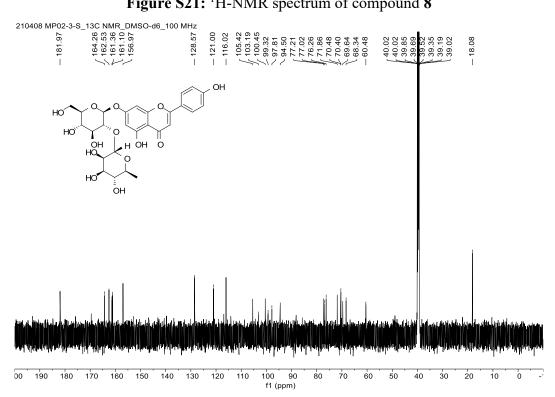
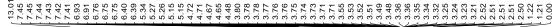


Figure S22: <sup>13</sup>C-NMR spectrum of compound 8



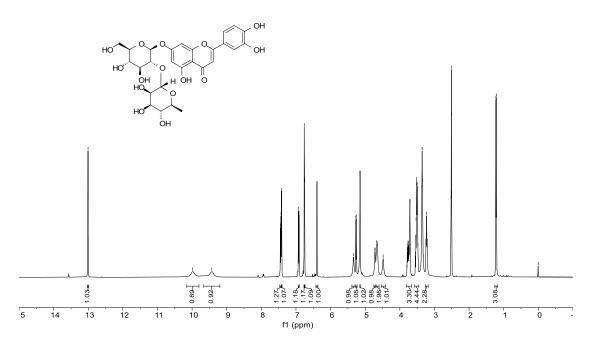


Figure S23: <sup>1</sup>H-NMR spectrum of compound 9

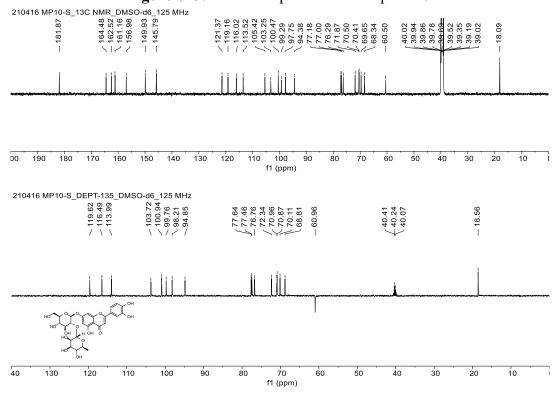


Figure S24: <sup>13</sup>C-NMR and DEPT135 spectra of compound 9

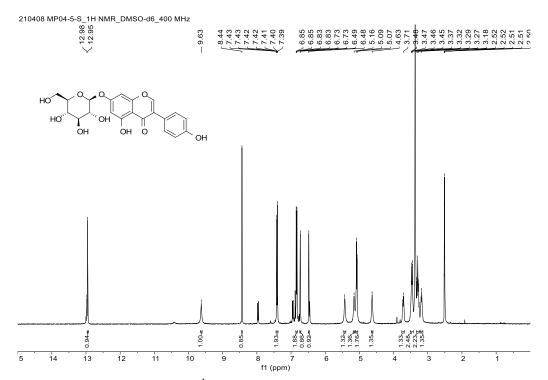


Figure S25: <sup>1</sup>H-NMR spectrum of compound 10

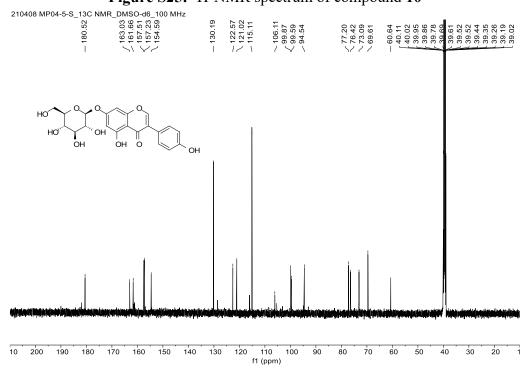


Figure S26: <sup>13</sup>C-NMR spectrum of compound 10

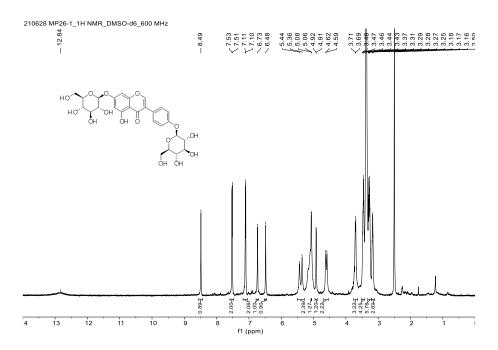


Figure S27: <sup>1</sup>H-NMR spectrum of compound 11

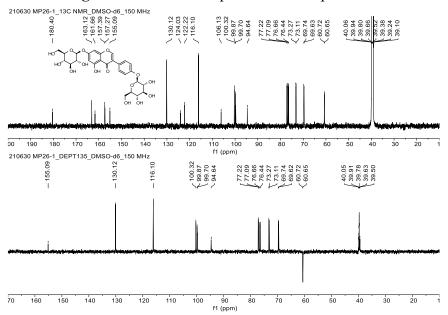


Figure S28: <sup>13</sup>C-NMR and DEPT135 spectra of compound 11

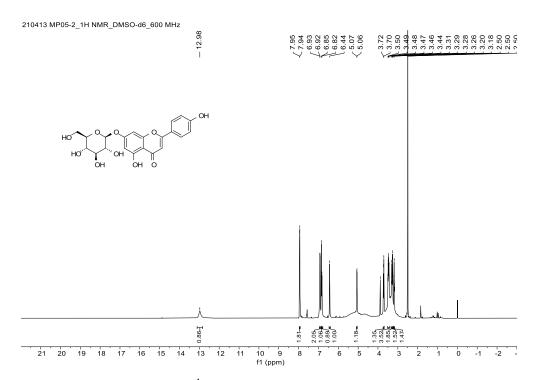


Figure S29: <sup>1</sup>H-NMR spectrum of compound 12

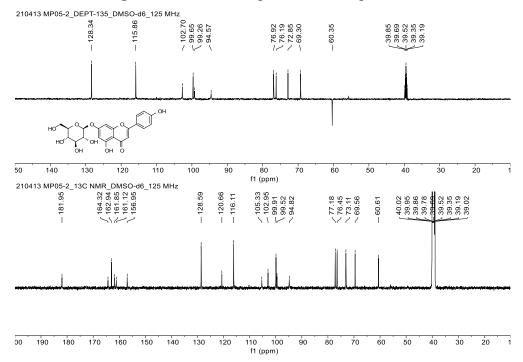


Figure S30: DEPT and <sup>13</sup>C-NMR spectra of compound 12

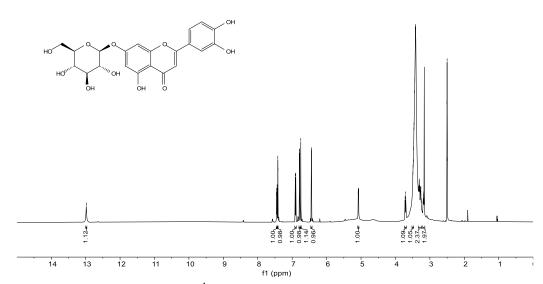


Figure S31: <sup>1</sup>H-NMR spectrum of compound 13

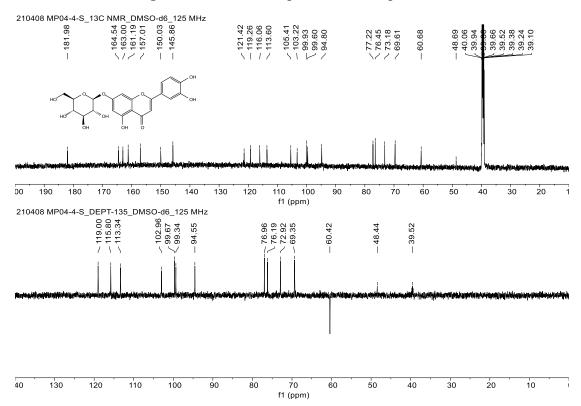


Figure S32: <sup>13</sup>C-NMR and DEPT135 spectra of compound 13

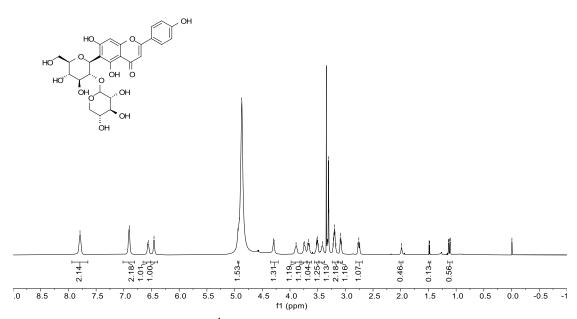


Figure S33: <sup>1</sup>H-NMR spectrum of compound 14

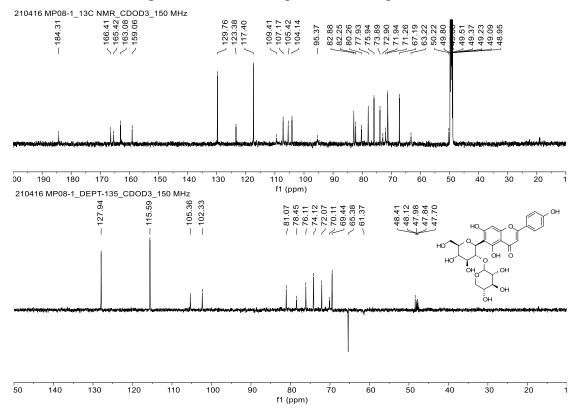


Figure S34: <sup>13</sup>C-NMR and DEPT135 spectra of compound 14

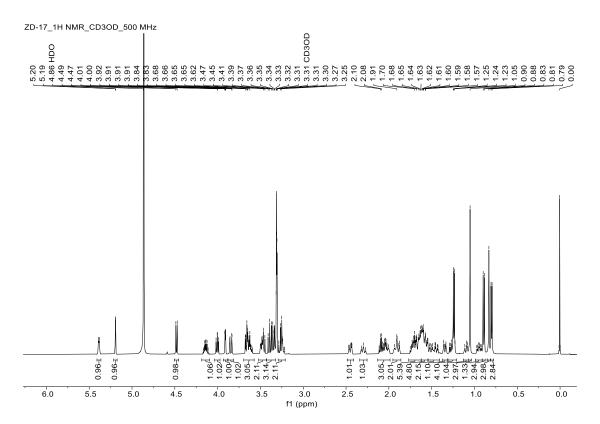


Figure S35: <sup>1</sup>H-NMR spectrum of compound 15

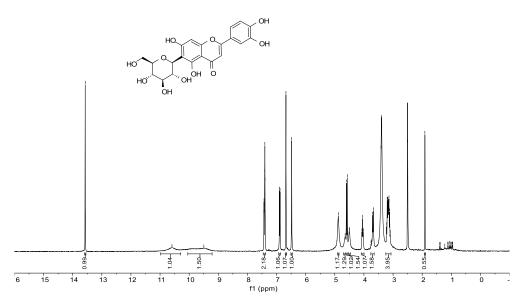


Figure S36: <sup>1</sup>H-NMR spectrum of compound 16

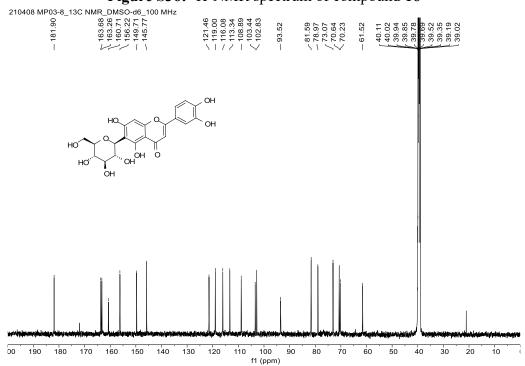


Figure S37: <sup>13</sup>C-NMR spectrum of compound 16



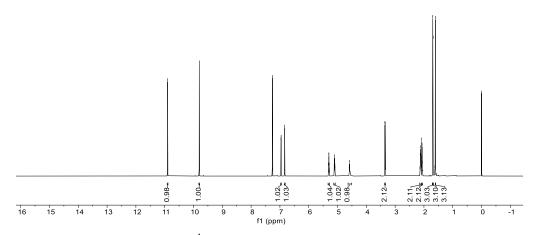


Figure S38: <sup>1</sup>H-NMR spectrum of compound 17

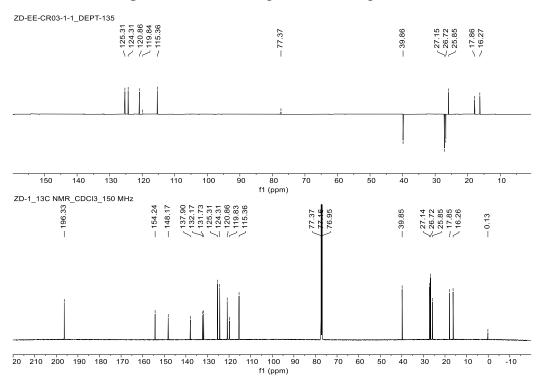


Figure S39: DEPT and <sup>13</sup>C-NMR spectra of compound 17

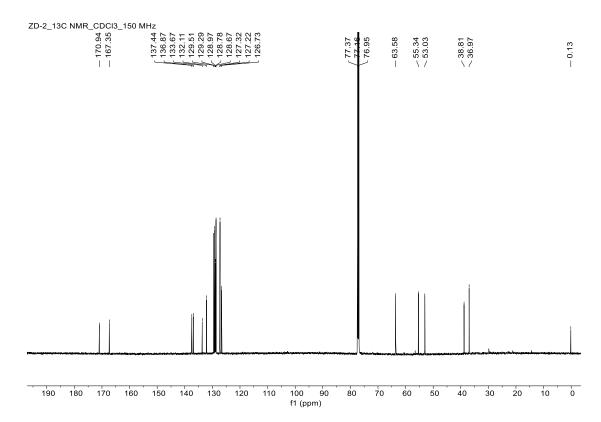


Figure \$40: <sup>13</sup>C-NMR spectrum of compound 18

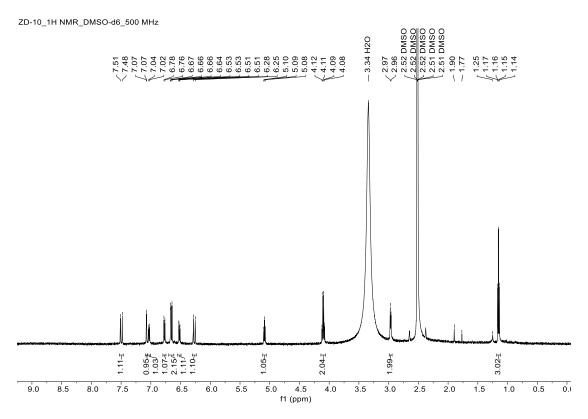


Figure S41: <sup>1</sup>H NMR spectrum of compound 19

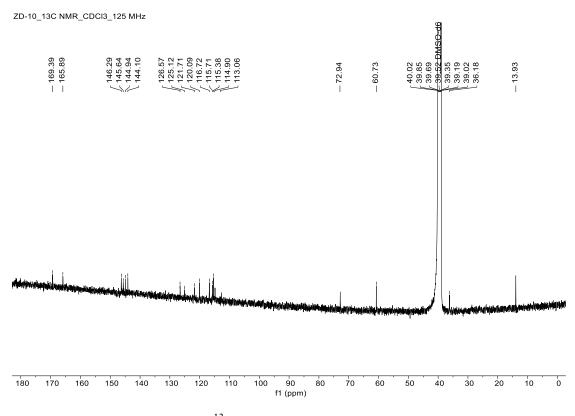


Figure S42: <sup>13</sup>C-NMR spectrum of compound 19

© 2023 ACG Publications. All rights reserved.



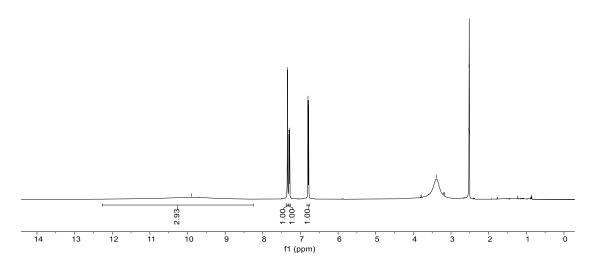


Figure S43: <sup>1</sup>H NMR spectrum of compound 20

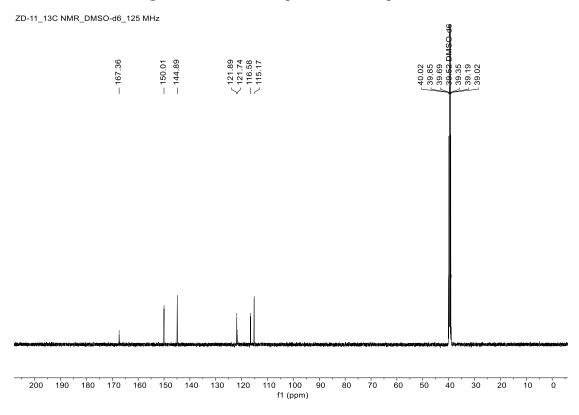


Figure S44: <sup>13</sup>C-NMR spectrum of compound 20

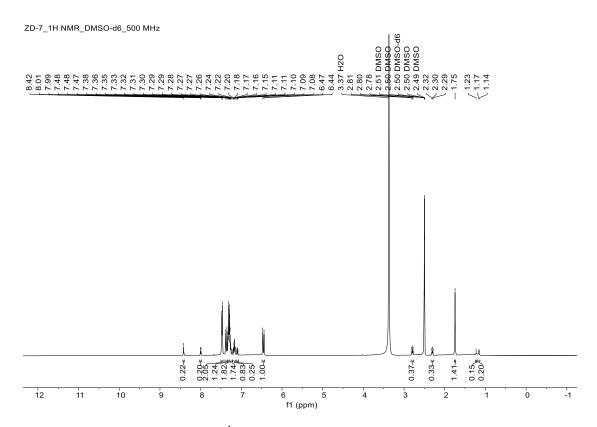


Figure S45: <sup>1</sup>H-NMR spectrum of compound 21

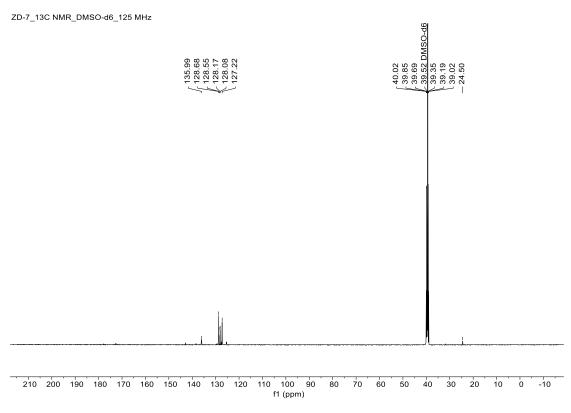


Figure S46: <sup>13</sup>C-NMR spectrum of compound 21

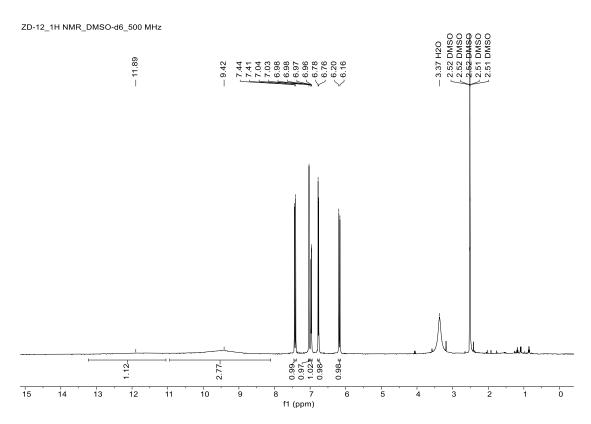


Figure S47: <sup>1</sup>H-NMR spectrum of compound 22

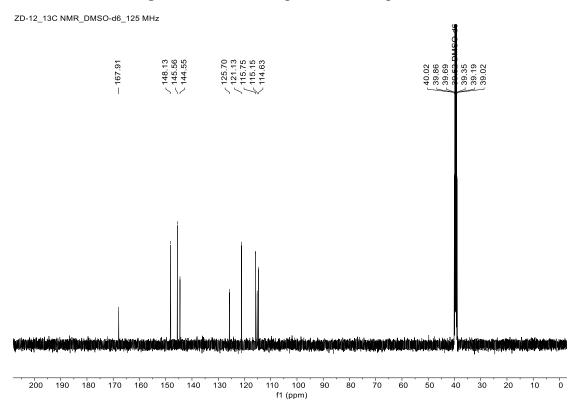
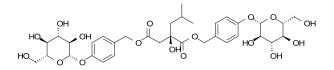


Figure S48: <sup>13</sup>C-NMR spectrum of compound 22



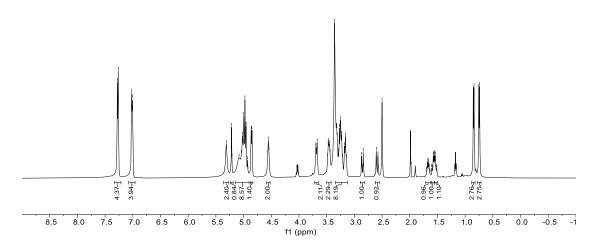


Figure S49: <sup>1</sup>H-NMR spectrum of compound 23

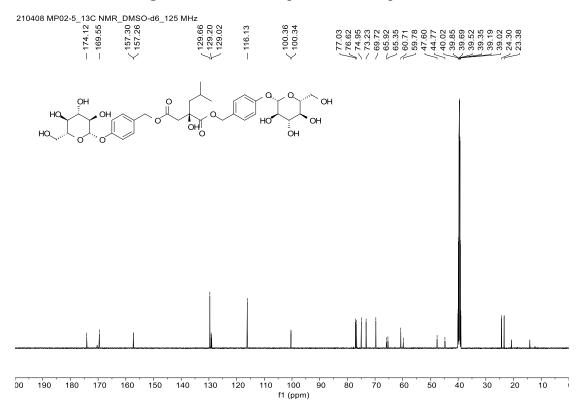


Figure S50: <sup>13</sup>C-NMR spectrum of compound 23

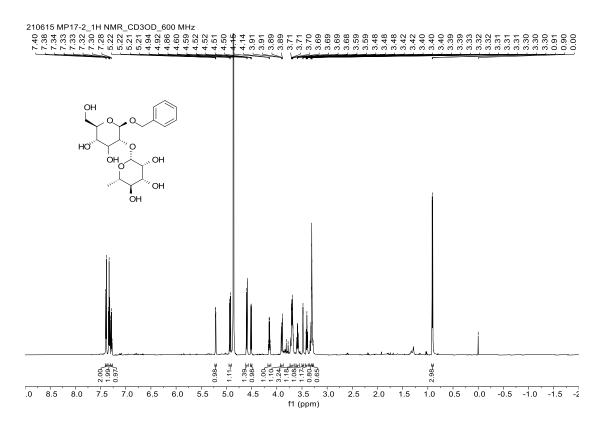


Figure S51: <sup>1</sup>H NMR spectrum of compound 24

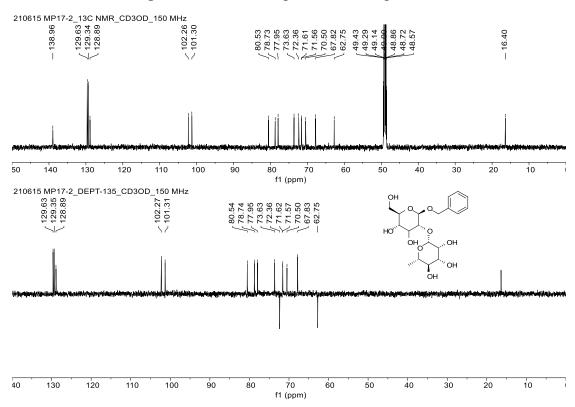


Figure S52: <sup>13</sup>C-NMR and DEPT spectra of compound 24

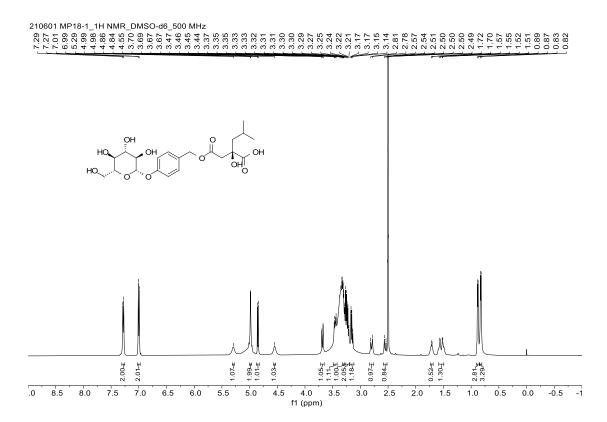


Figure S53: <sup>1</sup>H NMR spectrum of compound 25

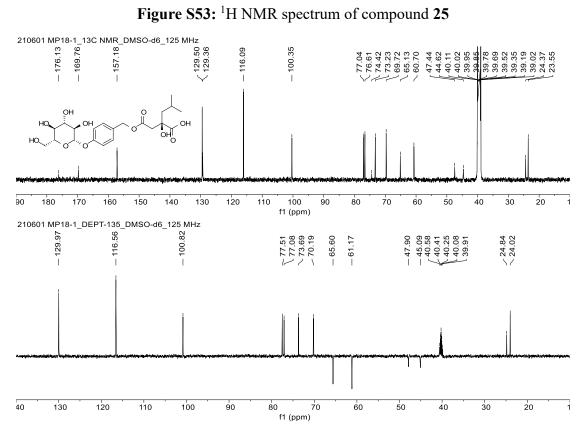


Figure S54: <sup>13</sup>C-NMR and DEPT spectra of compound 25

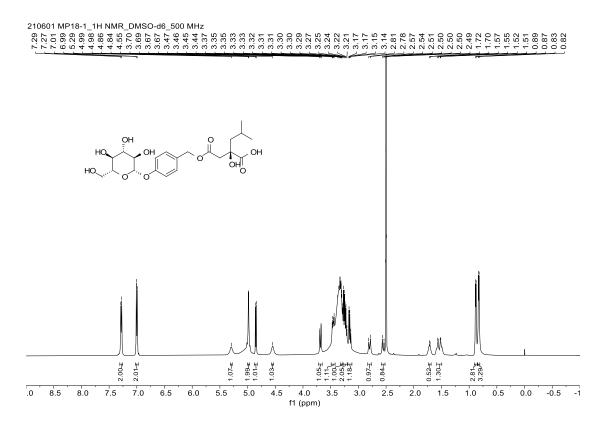


Figure S55: <sup>1</sup>H-NMR spectrum of compound 26

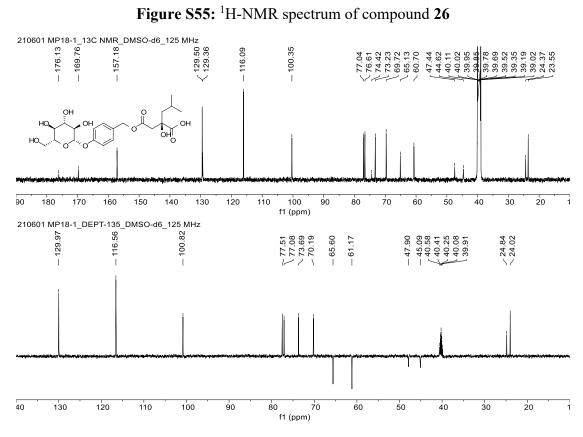
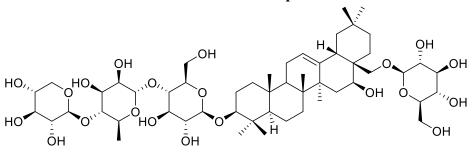
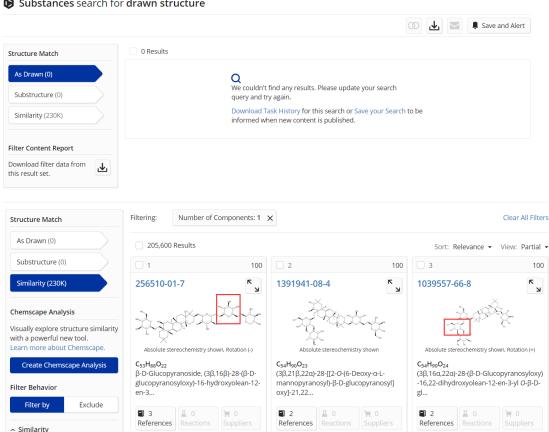


Figure S56: <sup>13</sup>C-NMR and DEPT spectra of compound 26

#### Scifinder search report



Substances search for drawn structure



The most similar three compounds to compound 1. The sugar unit and sugar chain are different from compound 1.