Synthesis, characterization and cytotoxic activity evaluation of ginsengdiol oxidation and nitrogen hybrid derivatives

Yumeng Zhang a, Weihui Yuan a, Xude Wang a, Hongyu Zhang a, Yuanyuan Sun a, Xiaoshu Zhang a,b*, Yuqing Zhao a,b*

a Department of Traditional Chinese Medicine Chemical, Shenyang Pharmaceutical University, Shenyang 110016, China

b Key Laboratory of Structure-based Drug Design and Discovery, Ministry of Education, Shenyang Pharmaceutical University, Shenyang 110016, China

*Corresponding author: Tel: +86 24 43520309. Fax: +86 24 43520300; E-mail address: zyq4885@126.com (Y. Zhao) or Tel: +86 24 43520309. Fax: +86 24 43520300; E-mail address: xiaoshu2397@163.com (X. Zhang)

1H NMR and 13NMR Spectrum of Compounds
Figure S1. $^1$H-NMR of Compound PD

Figure S2. $^{13}$C-NMR of Compound PD
Figure S3. $^1$H-NMR of Compound 1

Figure S4. $^{13}$C-NMR of Compound 1
Figure S5. ESI-MS of Compound 1

Figure S6. $^1$H-NMR of Compound 1a
Figure S7. $^{13}$C-NMR of Compound 1a

Analysis Name: 17051210.d
Sample Name: PD-3
Instrument: LC-MSD-Trap-SL
Operator: Administrator
Print Date: 5/12/2017 3:15:39 PM
Acq. Date: 5/12/2017 3:14:34 PM

Figure S8. ESI-MS of Compound 1a
Figure S9. $^1$H-NMR of Compound 1b

Figure S10. $^{13}$C-NMR of Compound 1b
Figure S11. ESI-MS of Compound 1b

Figure S12. $^1$H-NMR of Compound 1c
Figure S13. $^{13}$C-NMR of Compound 1c

Figure S14. HSQC of Compound 1c
Figure S15. HMBC of Compound 1c
**Figure S16. HR-ESI-TOF-MS of Compound 1c**
Figure S17. $^1$H-NMR of Compound 1d

Figure S18. $^{13}$C-NMR of Compound 1d
Figure S19. HR-ESI-TOF-MS of Compound 1d
Figure S20. $^1$H-NMR of Compound 1e

Figure S21. $^{13}$C-NMR of Compound 1e
Figure S22. $^1$H-NMR of Compound 1f

Figure S23. $^{13}$C-NMR of Compound 1f
Figure S24. HSQC of Compound 1f

Figure S25. HMBC of Compound 1f
Figure S26. HR-ESI-TOF-MS of Compound 1f
Figure S27. $^1$H-NMR of Compound 1g

Figure S28. $^{13}$C-NMR of Compound 1g
Figure S29. HR-ESI-TOF-MS of Compound 1g
Figure S30. $^1$H-NMR of Compound 1h

Figure S31. $^{13}$C-NMR of Compound 1h
Figure S32. ESI-MS of Compound 1h

Figure S33. 1H-NMR of Compound 1i
Figure S34. $^{13}$C-NMR of Compound 1i

Figure S35. HSQC of Compound 1i
Figure S36. HMBC of Compound 1i
Figure S37. HR-ESI-TOF-MS of Compound 1i
Figure S38. $^1$H-NMR of Compound 1j

Figure S39. $^{13}$C-NMR of Compound 1j
Figure S40. HR-ESI-TOF-MS of Compound 1j
Figure S41. $^1$H-NMR of Compound 1k

Figure S42. $^{13}$C-NMR of Compound 1k
Figure S43. HSQC of Compound 1k

Figure S44. HMBC of Compound 1k
Figure S45. HR-ESI-TOF-MS of Compound 1k
Figure S46. $^1$H-NMR of Compound 1m

Figure S47. $^{13}$C-NMR of Compound 1m
Figure S48. HR-ESI-TOF-MS of Compound 1m
Figure S49. $^1$H-NMR of Compound 1n

Figure S50. $^{13}$C-NMR of Compound 1n
Figure S51. HSQC of Compound 1n

Figure S52. HMBC of Compound 1n
Figure S53. HR-ESI-TOF-MS of Compound 1n
Figure S54. $^1$H-NMR of Compound 2a

Figure S55. $^{13}$C-NMR of Compound 2a
Figure S56. HR-ESI-TOF-MS of Compound 2a
Figure S57. $^1$H-NMR of Compound 2b

Figure S58. $^{13}$C-NMR of Compound 2b
Figure S59. HR-ESI-TOF-MS of Compound 2b
Figure S60. $^1$H-NMR of Compound 2c

Figure S61. $^{13}$C-NMR of Compound 2c
Figure S62. HR-ESI-TOF-MS of Compound 2c
Figure S63. $^1$H-NMR of Compound 2d

Figure S64. $^{13}$C-NMR of Compound 2d
Figure S65. HR-ESI-TOF -MS of Compound 2d
Figure S66. ¹H-NMR of Compound 2e

Figure S67. ¹³C-NMR of Compound 2e

Figure S68. HSQC of Compound 2e
Figure S69. HMBC of Compound 2e
Figure S70. HR-ESI-TOF-MS of Compound 2e
Figure S71. $^1$H-NMR of Compound 2f

Figure S72. $^{13}$C-NMR of Compound 2f
Figure S73. HSQC of Compound 2f

Figure S74. HMBC of Compound 2f
Figure S75. HR-ESI-TOF-MS of Compound 2f
Figure S76. $^1$H-NMR of Compound 2g

Figure S77. $^{13}$C-NMR of Compound 2g
Figure S78. HR-ESI-TOF-MS of Compound 2g
Figure S79. $^1$H-NMR of Compound 3a

Figure S80. $^{13}$C-NMR of Compound 3a
Figure S81. HR-ESI-TOF-MS of Compound 3a
Figure S82. $^1$H-NMR of Compound 3b

Figure S83. $^{13}$C-NMR of Compound 3b
Figure S84. HR-ESI-TOF-MS of Compound 3b
Figure S85. $^1$H-NMR of Compound 3c

Figure S86. $^{13}$C-NMR of Compound 3c
Figure S87. HR-ESI-TOF-MS of Compound 3c
Figure S88. $^1$H-NMR of Compound 3d

Figure S89. $^{13}$C-NMR of Compound 3d
Figure S90. HR-ESI-TOF-MS of Compound 3d
Figure S91. $^1$H-NMR of Compound 3e

Figure S92. $^{13}$C-NMR of Compound 3e
Figure S93. HR-ESI-TOF-MS of Compound 3e