#### Supplementary information

# Bicyclic basic merbarone analogues as antiproliferative agents

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Figure 579. H-NMR (200 MHz,  $CDCI_3$ ) spectrum of compound oc

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Figure S81. IR (KBr) spectrum of compound 6c

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Figure S84. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 6d

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Figure S86. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 6e

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### Figure S1. <sup>1</sup>H-NMR (200 MHz, d<sub>6</sub>-DMSO) spectrum of compound 7



Figure S2. <sup>13</sup>C-NMR (101 MHz, d<sub>6</sub>-DMSO) spectrum of compound 7





Figure S3. IR (KBr) spectrum of compound 7





# Figure S5. <sup>1</sup>H-NMR (200 MHz, d<sub>6</sub>-DMSO) spectrum of compound 8



Figure S6. <sup>13</sup>C-NMR (101 MHz, d<sub>6</sub>-DMSO) spectrum of compound 8





Figure S7. IR (KBr) spectrum of compound 8

Figure S8. Mass spectrum of compound 8



### Figure S9. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 9



Figure S10. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 9





Figure S11. IR (KBr) spectrum of compound 9

Figure S12. Mass spectrum of compound 9



Figure S13. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 10



Figure S14. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 10





Figure S15. IR (KBr) spectrum of compound 10

Figure S16. Mass spectrum of compound 10







Figure S18. <sup>13</sup>C-NMR (75 MHz, d<sub>6</sub>-DMSO) spectrum of compound 11





Figure S19. IR (KBr) spectrum of compound 11

Figure S20. Mass spectrum of compound 11



### Figure S21. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 12



Figure S22. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 12





Figure S23. IR (KBr) spectrum of compound 12

Figure S24. Mass spectrum of compound 12



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# Figure S25. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 3a



Figure S26. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 3a





Figure S27. IR (KBr) spectrum of compound 3a

Figure S28. Mass spectrum of compound 3a



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### Figure S29. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 3b



Figure S30. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 3b





Figure S31. IR (KBr) spectrum of compound 3b



Figure S32. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 3c

Figure S33. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 3c





Figure S34. IR (KBr) spectrum of compound 3c

# Figure S35. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 3d



Figure S36. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 3d





Figure S37. IR (KBr) spectrum of compound 3d

### Figure S38. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 3e



Figure S39. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 3e





Figure S40. IR (KBr) spectrum of compound 3e

#### Figure S41. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 4a



Figure S42. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 4a





Figure S43. IR (KBr) spectrum of compound 4a

### Figure S44. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 4b









Figure S46. IR (KBr) spectrum of compound 4b



Figure S47. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 4c

Figure S48. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 4c





Figure S49. IR (KBr) spectrum of compound 4c



Figure S50. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 4d

Figure S51. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 4d





Figure S52. IR (KBr) spectrum of compound 4d

### Figure S53. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 4e



Figure S54. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 4e





Figure S55. IR (KBr) spectrum of compound 4e

Figure S56. Mass spectrum of compound 4e







Figure S58. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 5a





# Figure S59. IR (KBr) spectrum of compound 5a

### Figure S60. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 5b



Figure S61. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 5b





Figure S62. IR (KBr) spectrum of compound 5b

### Figure S63. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 5c



Figure S64. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 5c





Figure S65. IR (KBr) spectrum of compound 5c

### Figure S66. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 5d



Figure S67. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 5d





Figure S68. IR (KBr) spectrum of compound 5d





#### 0.043 0.043 0.041 0.036 0.033 0.020 Pulse Sequence: s2pul Solvent: CDC13 Ambient temperature SEMINI-200 "gem2000 -2.332 -2.325 -1.741 -1.466 -1.431 Pulse 28.8 degrees Acq. time 2.000 sec Width 4000.0 Hz 144 repetitions OSSERVE H1, 199.9417676 DATA PROCESSING FT size 65536 Total time 17 min, 58 sec -2.376 7.633 -7.620 -7.634 -7.558 -7.558 -7.328 -7.283 -4.935 .530 12 11 10 9 8 7 6 5 4 3 2 1 ppm لېا لېا 6.65 8.86 لب لب 18.18 5.51 8.85 4.65 2.42 39.19 5.70

Figure S70. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 5e

Figure S71. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 5e





Figure S72. IR (KBr) spectrum of compound 5e



Figure S73. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 6a

Figure S74. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 6a





Figure S75. IR (KBr) spectrum of compound 6a

# Figure S76. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 6b



Figure S77. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 6b





Figure S78. IR (KBr) spectrum of compound 6b



### Figure S79. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 6c

Figure S80. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 6c





Figure S81. IR (KBr) spectrum of compound 6c





#### Figure S83. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 6d



Figure S84. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 6d





Figure S85. IR (KBr) spectrum of compound 6d

#### Figure S86. <sup>1</sup>H-NMR (200 MHz, CDCl<sub>3</sub>) spectrum of compound 6e



Figure S87. <sup>13</sup>C-NMR (101 MHz, CDCl<sub>3</sub>) spectrum of compound 6e





Figure S88. IR (KBr) spectrum of compound 6e