## **Supporting Information**

## Pregnenolone derivatives for the treatment of Alzheimer's disease: Synthesis, in-vitro inhibition of amyloid $\beta_{1-42}$ peptide aggregation, acetylcholinesterase and carbonic anhydrase-II

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**Figure S-1.** 2-D interaction plot of inhibitor **15** with Aβ protofibrils (PDB ID: 2BEG)



Figure S-2. 2-D interaction plot of inhibitor 23 with Aβ protofibrils (PDB ID: 2BEG)



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Figure S-3: <sup>1</sup>H-NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound **12** 



Figure S-4. <sup>1</sup>H-NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound



Figure S-5. <sup>1</sup>H-NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 15



Figure S-6. <sup>1</sup>H-NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 16



Figure S-7. <sup>1</sup>H-NMR spectrum (400 MHz, CDCl<sub>3</sub>) expansion of compound 16



Figure S-8. <sup>1</sup>H-NMR spectrum (400 MHz, CDCl<sub>3</sub>) expansion of compound 16



Figure S-9. <sup>1</sup>H-NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 23



Figure S-10. <sup>13</sup>C-NMR spectrum (100 MHz, CDCl<sub>3</sub>) of compound 23



Figure S-11. <sup>1</sup>H-NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 24



Figure S-12. <sup>1</sup>H-NMR spectrum (400 MHz, CDCl<sub>3</sub>) expansion of compound 24



Figure S-13. <sup>1</sup>H-NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 25



Figure S-14. <sup>1</sup>H-NMR spectrum (400 MHz, CDCl<sub>3</sub>) expansions of compound 25



Figure S-15. <sup>1</sup>H-NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 26



Figure S-16. <sup>13</sup>C-NMR spectrum (100 MHz, CDCl<sub>3</sub>) of compound 26



Figure S-17. <sup>1</sup>H-NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 27



Figure S-18. <sup>13</sup>C-NMR spectrum (100 MHz, CDCl<sub>3</sub>) of compound 26



Figure S-19. <sup>1</sup>H-NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 28



Figure S-20. <sup>13</sup>C-NMR spectrum (100 MHz, CDCl<sub>3</sub>) of compound 28



Figure S-21. HPLC chromatogram of compound 23



Figure S-22. HPLC chromatogram of compound 25



Figure S-23. HPLC chromatogram of compound 26



Figure S-24. HPLC chromatogram of compound 27



Figure S-25. HPLC chromatogram of compound 28