Supplementary Material

Secoyanhusamine A, an oxidatively ring opened isoquinoline inner salt from Corydalis yanhusuo

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Supplementary Material

Contents

Supplementary Figure 1. The $^1$H NMR spectrum of compound 1 in MeOH-$d_4$ (600 MHz) .................3

Supplementary Figure 2. The $^{13}$C NMR spectrum of compound 1 in MeOH-$d_4$ (150 MHz) ............4

Supplementary Figure 3. The $^{19}$F NMR spectrum of compound 1 in MeOH-$d_4$ (400 MHz) ............5

Supplementary Figure 4. The $^1$H-$^1$H COSY spectrum of compound 1 in MeOH-$d_4$ (600 MHz) .......6

Supplementary Figure 5. The HSQC spectrum of compound 1 in MeOH-$d_4$ (600 MHz) .................7

Supplementary Figure 6. The HMBC spectrum of compound 1 in MeOH-$d_4$ (600 MHz) ...............8

Supplementary Figure 7. The NOESY spectrum of compound 1 in MeOH-$d_4$ (600 MHz) ............9

Supplementary Figure 8. The IR spectrum of compound 1 ..............................................................10

Supplementary Figure 9. The HRMS spectrum of compound 1 in MeOH .................................11

Supplementary Figure 10. The UV spectrum of compound 1 in MeOH .................................11

Supplementary Figure 11. Bioassay for anti-cholinesterase activity ...........................................12

Molecular docking studies ...............................................................12
Supplementary Figure 1. The $^1$H NMR spectrum of compound 1 in MeOH-$d_4$ (600 MHz)
Supplementary Figure 2. The $^{13}$C NMR spectrum of compound 1 in MeOH-$_d_4$ (150 MHz)
Supplementary Figure 3. The $^{19}$F NMR spectrum of compound 1 in MeOH-$d_4$ (400 MHz)
Supplementary Figure 4. The $^1$H-$^1$H COSY spectrum of compound 1 in MeOH-$d_4$ (600 MHz)
Supplementary Figure 5. The HSQC spectrum of compound 1 in MeOH-\textit{d}_4 (600 MHz)
Supplementary Figure 6. The HMBC spectrum of compound 1 in MeOH-$d_4$ (600 MHz)
Supplementary Figure 7. The NOESY spectrum of compound 1 in MeOH-$d_4$ (600 MHz)
Supplementary Figure 8. The IR spectrum of compound 1
**Supplementary Figure 9.** The HRMS spectrum of compound 1 in MeOH

| m/z<sup>1</sup> | Theo. Mass<sup>1</sup> | Delta (ppm)<sup>1</sup> | RDB equiv.<sup>1</sup> | Composition<sup>1</sup> |      |
|-----------------|------------------------|-------------------------|------------------------|------------------------|------|
| 370.1299<sup>-</sup> | 370.1285<sup>-</sup> | 3.69<sup>-</sup>       | 11.5<sup>-</sup>    | C20 H20 O6 N<sup>-</sup> | M+H<sup>-</sup> |
| 739.2518<sup>-</sup> | 739.2498<sup>-</sup> | 2.81<sup>-</sup>       | 22.5<sup>-</sup>    | C40 H39 O12 N2<sup>-</sup> | 2M+H<sup>-</sup> |

**Supplementary Figure 10.** The UV spectrum of compound 1 in MeOH
Molecular docking studies

Molecular docking analyses in this study were performed using the software Discovery Studio 2016. The structural coordinates of AChE was based on the crystal structure of AChE, which was acquired from the PDB database (PDB: 4EY7). The protein and ligands were prepared by a standard procedure using Discovery Studio 2016. The location and the size of the active pocket was confined by the native ligand of AChE. The docking was performed using the "CDOCKER" procedure of Discovery Studio 2016.