Supplementary Data

Development of Novel N-(6-Methanesulfonyl-benzothiazol-2-yl)-3-(4-substituted-piperazin-1-yl)-propionamidewithcholinesterase inhibition, anti-β-amyloid aggregation, neuroprotection and cognition enhancing properties for the therapy of Alzheimer’s disease

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Supplementary Data

**Supplementary Figure S1:** Time evolution plot of secondary structures, AChE (A) and AChE-12complex (B), during the simulation in water at 300 K.

**Supplementary Figure S2:** Structural contents of AChE (A) and AChE-12complex (B), during the simulation in water at 300 K.
Supplementary Figure S3: Time evolution plot of secondary structures, Aβ_{1-42} (A) and Aβ_{1-42-12}complex (B), during the simulation in water at 300 K.

Supplementary Figure S4: Structural contents of Aβ_{1-42} (A) and Aβ_{1-42-12}complex (B), during the simulation in water at 300 K.
$^1$HNMR of Compound 4

![HNMR Spectrum of Compound 4](image-url)
Supplementary Data

$^{13}$C NMR of Compound 4

X : parts per Million  | Carbon13
Supplementary Data

Mass spectra of compound 4

| Compound Label | m/z  | RT  | Algorithm                  | Mass   |
|----------------|------|-----|----------------------------|--------|
| Cpd 19: C21 H24 N4 O3 S2 | 445.1393 | 0.096 | Find by Molecular Feature | 444.1321 |

MFE MS Spectrum:

- Cpd 19: C21 H24 N4 O3 S2: +ESI MFE Spectrum (0.034-0.551 min) Frag=175.0V C8-21.d
- Mass = 889.2686 (2M+H)+

MFE MS Zoomed Spectrum:

- Cpd 19: C21 H24 N4 O3 S2: +ESI MFE Spectrum (0.034-0.551 min) Frag=175.0V C8-21.d
- Mass = 889.2686 (2M+H)+
Supplementary Data

$^1$HNMR of compound 5
$^{13}$C NMR of compound 5
Supplementary Data

Mass spectra of Compound 5

Qualitative Compound Report

| Compound Label | RT   | Mass | Formula     | MFG Formula | MFG Diff (ppm) | DB Formula |
|---------------|------|------|-------------|-------------|----------------|------------|
| Cpd 5: C21 H23 F N4 O3 S2 | 0.096 | 462.1194 | C21 H23 F N4 O3 S2 | C21 H23 F N4 O3 S2 | 0.44 | C21 H23 F N4 O3 S2 |

| Compound Label | m/z  | RT   | Algorithm                  | Mass     |
|---------------|------|------|----------------------------|----------|
| Cpd 5: C21 H23 F N4 O3 S2 | 463.1266 | 0.096 | Find by Molecular Feature  | 462.1194 |

MFE MS Spectrum

MFE MS Zoomed Spectrum
Supplementary Data

$^1$H NMR of compound 6

![NMR Spectrum Image]
Supplementary Data

$^{13}$C NMR of compound 6
Mass spectra of Compound 6
$^1$H NMR of Compound 7
C NMR of compound 7
Supplementary Data

Mass spectra of 7
$^1$H NMR of Compound 8
Supplementary Data

$^{13}$C NMR of Compound 8

![NMR Spectrum](Image)

X : parts per Million / Carbon13
Mass spectra of Compound 8
Supplementary Data

$^1$H NMR of Compound 9
$^{13}$C NMR of Compound 9
Supplementary Data

Mass spectra of compound 9

| Compound Label | RT | Mass   | MFG Formula | MFG TDP (ppm) | DB Formula |
|----------------|----|--------|-------------|---------------|------------|
| Cpd 3: C22 H26 N4 O4 S2 | 0.095 | 474.1429 | C22 H26 N4 O4 S2 | -7.03 | C22 H26 N4 O4 S2 |

| Compound Label | m/z | RT | Algorithm      | Mass   |
|----------------|-----|----|----------------|--------|
| Cpd 3: C22 H26 N4 O4 S2 | 475.1501 | 0.095 | Find by Molecular Feature | 474.1429 |

**MFE MS Spectrum**

Cpd 3: C22 H26 N4 O4 S2: ESI MFE Spectrum (0.043-0.710 min) Frag=175.0V CB-22.d

**MFE MS Zoomed Spectrum**

Cpd 3: C22 H26 N4 O4 S2: ESI MFE Spectrum (0.043-0.710 min) Frag=175.0V CB-22.d
Supplementary Data

$^1$H NMR of Compound 10
$^{13}$C NMR of Compound 10
Mass spectra of compound 10
Supplementary Data

$^1$H NMR of Compound 11
Supplementary Data

$^{13}$C NMR of Compound 11
Supplementary Data

Mass spectra of compound 11
Supplementary Data

$^1$HNMR spectra of Compound 12
$^{13}$CNMR of Compound 12
Supplementary Data

Mass spectra of Compound 12
Supplementary Data

$^1$H NMR of Compound 13
Supplementary Data

$^{13}$C NMR of Compound 13
Supplementary Data

Mass spectra of Compound 13
Supplementary Data

$^1$H NMR of Compound 14
Supplementary Data

$^{13}$C NMR of Compound 14

![NMR Spectrum](image-url)
Supplementary Data

Mass spectra of Compound 14

| Compound Table |
|----------------|
| Compound Label | RT    | Mass | Formula | MFE Formula | DB Formula |
| Cpd 3: 0.121   | 0.121 | 462.1021 | C24 H14 N8 O5 | C24 H14 N8 O5 | C24 H14 N8 O5 |

| Compound Label | m/z  | RT    | Algorithm             | Mass     |
|----------------|------|-------|-----------------------|----------|
| Cpd 3: 0.121   | 463.1095 | 0.121 | Find by Molecular Feature | 462.1021 |

MFE MS Spectrum

Cpd 3: 0.121: +ESI MFE Spectrum (0.050-0.600 min) Frag=175.0V CB-20.d
* 463.1095
(M+H)+

MFE MS Zoomed Spectrum

Cpd 3: 0.121: +ESI MFE Spectrum (0.050-0.600 min) Frag=175.0V CB-20.d
* 463.1095
(M+H)+
Supplementary Data

$^1$H NMR of Compound 15
13C spectra of Compound 15
Supplementary Data

Mass spectra of Compound 15
Supplementary Data

$^1$H NMR of Compound 16
$^{13}$C NMR of Compound 16
Supplementary Data

Mass spectra of Compound 16
Supplementary Data

$^1$H NMR of Compound 17

![NMR Spectrogram](image)
Supplementary Data

$^{13}$C NMR of Compound 17
Supplementary Data

Mass spectra of Compound 17

| Compound Label | RT  | Mass   | Formula        | MFG Formula | MFG Diff (ppm) | DB Formula   |
|----------------|-----|--------|----------------|-------------|----------------|--------------|
| Cpd 4: C22 H23 F3 N4 O3 S2 | 0.089 | 512.1182 | C22 H23 F3 N4 O3 S2 | C22 H23 F3 N4 O3 S2 | -3.66 | C22 H23 F3 N4 O3 S2 |

| Compound Label | m/z  | RT   | Algorithm        | Mass  |
|----------------|------|------|------------------|-------|
| Cpd 4: C22 H23 F3 N4 O3 S2 | 513.1257 | 0.089 | Find by Molecular Feature | 512.1182 |

**MFE MS Spectrum**

**MFE MS Zoomed Spectrum**
Supplementary Data