



Supplementary Materials: Click-Free Synthesis of a Multivalent Tricyclic Peptide as a Molecular Transporter

Sumit Kumar, Dindyal Mandal, Shaima Ahmed El-Mowafi, Saghar Mozaffari, Rakesh Kumar Tiwari and Keykavous Parang

Content

Representative MALDI Spectra and HPLC of Intermediate and Synthesized Compounds (Page 3-15).







Exact Mass: 1815.9586





Exact Mass: 1775.9273





Exact Mass: 1611.8436





Peptide #8 after Dde deprotection.



Exact Mass: 1642.9222



Peptide # 9/10 with Dde



Exact Mass: 1624.9116

Peptide #12

Exact Mass: 1596.8327

HPLC of compound 20

Tricyclic peptide **20** was purified using reverse phase-high performance liquid chromatography (RP-HPLC) using Hitachi L-2455 system (Canby, OR, USA) with a C18 Phenomenex column (Prodigy, 10 μ m, 2.1 cm × 25 cm), at a flow rate of 10 mL/min with the detection at 214 nm using a gradient of 0-100% acetonitrile (0.1% trifluoracetic acid (TFA)) and water (0.1% TFA) over 60 min.

Figure S1. Preparatory RP-HPLC profile of tricyclic peptide 20.

The analytical HPLC (HITACHI LaChrom ULTRA) was run with a gradient system of acetonitrile and water with 0.1% TFA (v/v) using a reversed-phase VyDAC column (218TP54, 5 μ m, 4.60 mm x 150 mm) and flow rate of 1 mL/min with the detection at 214 nm.

Figure S2. Analytical RP-HPLC profile of tricyclic peptide 20.

| UV-VIS | | | | | | | 0 | |
|------------------|--|--|--|--|--|---|----------------|--------|
| 3000 | Time: 3 02117 Minutes - Amplitude: 53 9025 mAU UV V13 | | | | | | | 3000 |
| 2500- | | | | | | | | -2500 |
| 2000- | | | | | | | | -2000 |
| 1500- | | | | | | | | - 1500 |
| 1000- | | | | | | | | 1000 |
| 600- | | | | | | | | 500 |
| | | ~~ | | | | ~ | | 0 |
| 10 | 1 2 | 5 4 6 | 7 8 9 | 12 11 12 Minutes | 13 14 15 | 16 17 1 <u>5</u> | 9 | 122 |
| Result | Sequence | | | | | | -0- | |
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Figure S3. Analytical RP-HPLC profile of peptide 7.

Figure S4. Analytical RP-HPLC profile of peptide 10.

Figure S5. Analytical RP-HPLC profile of peptide 16.

Figure S6. Analytical RP-HPLC profile of peptide 18.

Figure S7. Analytical RP-HPLC profile of crude peptide 12.