Ligations of O-acyl threonine units to give native peptides via 5-, 8-, 9- and 10-membered cyclic transition states

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SUPPORTING INFORMATION

1. Copy of 1H, 13C NMR and CHN/HRMS spectra for compounds 3, 4, 8a-c, and 9a-c

2. HPLC-MS spectra for compounds 4-6, 9b, 10b and 11b
HPLC chromatograms and ESI-MS for chemical ligation of 4 in buffer

Summary Chromatogram: HPLC/(+)ESI-MS integrated ion-peaks for the 4 (top, rt 34.61), 5 (middle, rt 38.08), and 6 (bottom, rt 60.58).
MW 324-LP 5 (top) and MW 324-SM 4 (bottom): (+)ESI-MS.
MW 324-LP 5 (top) and MW 324-SM 4 (bottom): (±)ESI-MS/MS of the m/z 347 [M+Na]+ ions.
MW 324-LP 5 (top two) and MW 324-SM 4 (bottom two): (+)ESI-MS/MS (top and 3rd) and –MS/MS/MS (2nd and bottom) of the m/z 325 [M+H]+ ions.
Summary Chromatogram: HPLC/(+)-ESI-MS integrated ion-peaks for the 4 (top, rt 34.61), 5 (middle, rt 38.08), and 6 (bottom, rt 60.58).
MW 395 isomers: (+)ESI-MS for RT 59.5 min LP 10b (top) and SM 9b (bottom).

MW 395, RT 59.5 min: (+)ESI-MS/MS of m/z 396 [M+H]+ ions for LP (top) and SM (bottom).