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Short synthesis of polyfunctional sp³-rich threonine-derived morpholine scaffolds

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ELECTRONIC SUPPLEMENTARY INFORMATION

¹ H and ¹³ C NMR spectra for compounds 8–11, 13, 16, 18-22	S2-S15
Energy minimization of compound 19 conformers	S16
NOESY-1D spectra for compound 19	S17

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Figure S2. ¹³C NMR spectrum of compound **8a** (100 MHz, CDCl₃).



Figure S4. ¹³C NMR spectrum of compound **8b** (100 MHz, CDCl₃).



Figure S6. ¹H NMR spectrum of compound 9 (50 MHz, CDCl₃).

6.13 6.13 6.13 6.13 6.13 6.13 6.13


¹¹⁵⁵ ¹⁵⁰ ¹⁴⁵ ¹⁴⁰ ¹³⁵ ¹³⁰ ¹²⁵ ¹²⁰ ¹¹⁵ ¹¹⁰ ¹⁰⁵ ¹⁰⁰ ⁹⁵ ⁹⁰ ⁸⁵ ⁸⁰ ⁷⁵ ⁷⁰ ⁶⁵ ⁶⁰ ⁵⁵ ⁵⁰ ⁴⁵ ⁴⁰ ³⁵ ³⁰ ²⁵ ²⁰ ¹⁵ ¹⁰ ⁵ ⁵ ⁵⁰ ¹⁴⁵ ¹³C NMR spectrum of compound **10** (100 MHz, CDCl₃).

 $<_{1.46}^{1.48}$ -6.31 -6.21 slir ss s Ph 11a 1.00 J 212 120 4 ٣ -10.70-1.04 -1.05 0.97 2.96 6.5 2.5 8.0 7.5 6.0 5.5 5.0 4.5 4.0 f1 (ppm) 3.0 1.5 7.0 3.5 2.0 1.0 0.5 Figure S9. ¹H NMR spectrum of compound **11a** (400 MHz, CDCl₃). 139.50 136.63 134.33 134.33 134.33 124.35 128.67 128.66 127.29 126.42

 $_{55}$ $_{150}$ $_{145}$ $_{140}$ $_{135}$ $_{130}$ $_{125}$ $_{120}$ $_{115}$ $_{110}$ $_{105}$ $_{100}$ $_{95}$ $_{90}$ $_{85}$ $_{80}$ $_{75}$ $_{70}$ $_{65}$ $_{60}$ $_{55}$ $_{50}$ $_{45}$ $_{40}$ $_{35}$ $_{30}$ $_{25}$ $_{20}$ $_{15}$ $_{10}$ Figure S10. 13 C NMR spectrum of compound **11a** (100 MHz, CDCl₃).



Figure S12. ¹³C NMR spectrum of compound **11b** (100 MHz, CDCl₃).

L136

<7.33 <7.31



Figure S14. ¹³C NMR spectrum of compound **13** (100 MHz, CDCl₃).



Figure S16. ¹³C NMR spectrum of compound **16** (100 MHz, CDCl₃).



Figure S18. ¹³C NMR spectrum of compound **18a** (100 MHz, CDCl₃).



Figure S20. ¹³C NMR spectrum of compound **18b** (100 MHz, CDCl₃).



Figure S22. ¹³C NMR spectrum of compound **19** (100 MHz, CDCl₃).



Figure S26. ¹³C NMR spectrum of compound **20** (100 MHz, CDCl₃).



Figure S28. ¹³C NMR spectrum of compound **21** (100 MHz, CDCl₃).



Figure S30. ¹³C NMR spectrum of compound **22** (100 MHz, CDCl₃).



Figure S31. Minimum energy conformations of **19** resulting from geometry optimization using the AM1 semiempirical method and ab initio single point calculation of the electronic properties at the 3-21G*/HF level of quantum chemical theory (SPARTAN software, v. 5.147).





Figure S32. 1D-NOESY spectrum of compound **19** (400 MHz, CDCl₃), using 500 ms as mixing time.