

Description of Additional Supplementary items

File name: Supplementary file 1

Description: Contains ^1H , ^{13}C , and ^{19}F NMR chemical shift assignments for synthesized compounds

File name: Supplementary file 2

Description: Contains ^1H , ^{13}C , and ^{19}F NMR spectra for synthesized compounds

File name: Supplementary file 3

Description: HPLC traces for synthesized compounds

File name: Supplementary file 4

Description: Initial coordinate and simulation input file for 25CN-NBOH MD simulation

File name: Supplementary file 5

Description: Final coordinate and simulation output file for 25CN-NBOH MD simulation

File name: Supplementary file 6

Description: Initial coordinate and simulation input file for 25N-N1-Nap (16) MD simulation

File name: Supplementary file 7

Description: Final coordinate and simulation output file for 25N-N1-Nap (16) MD simulation