

Supplementary Materials

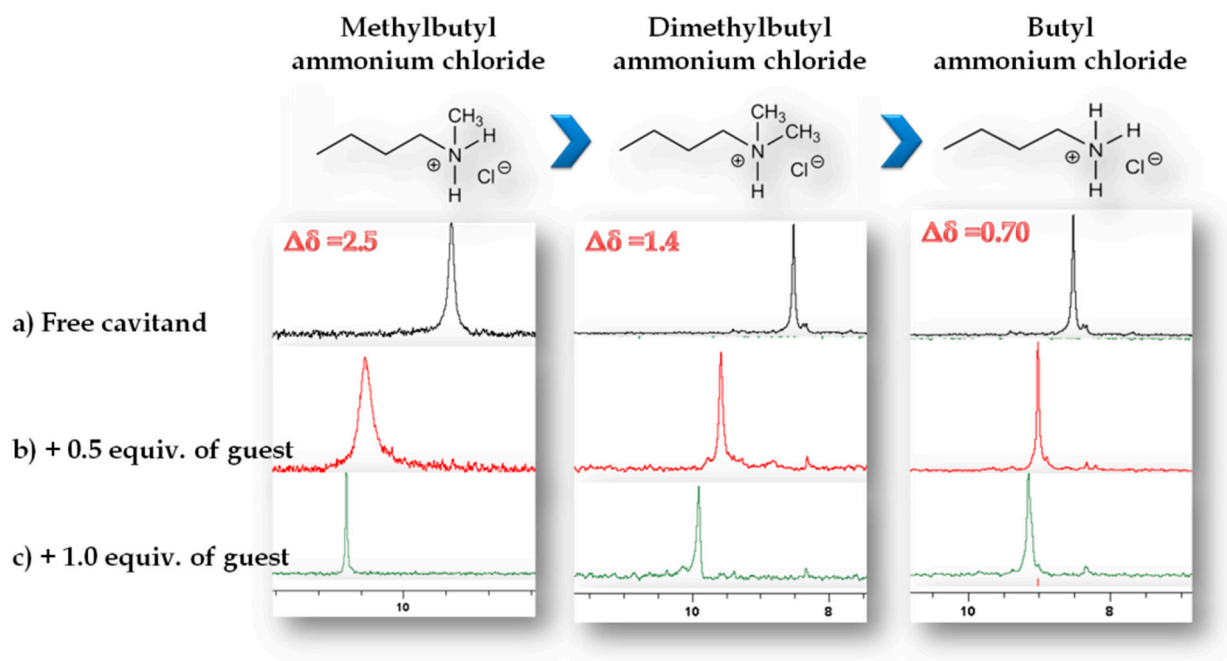
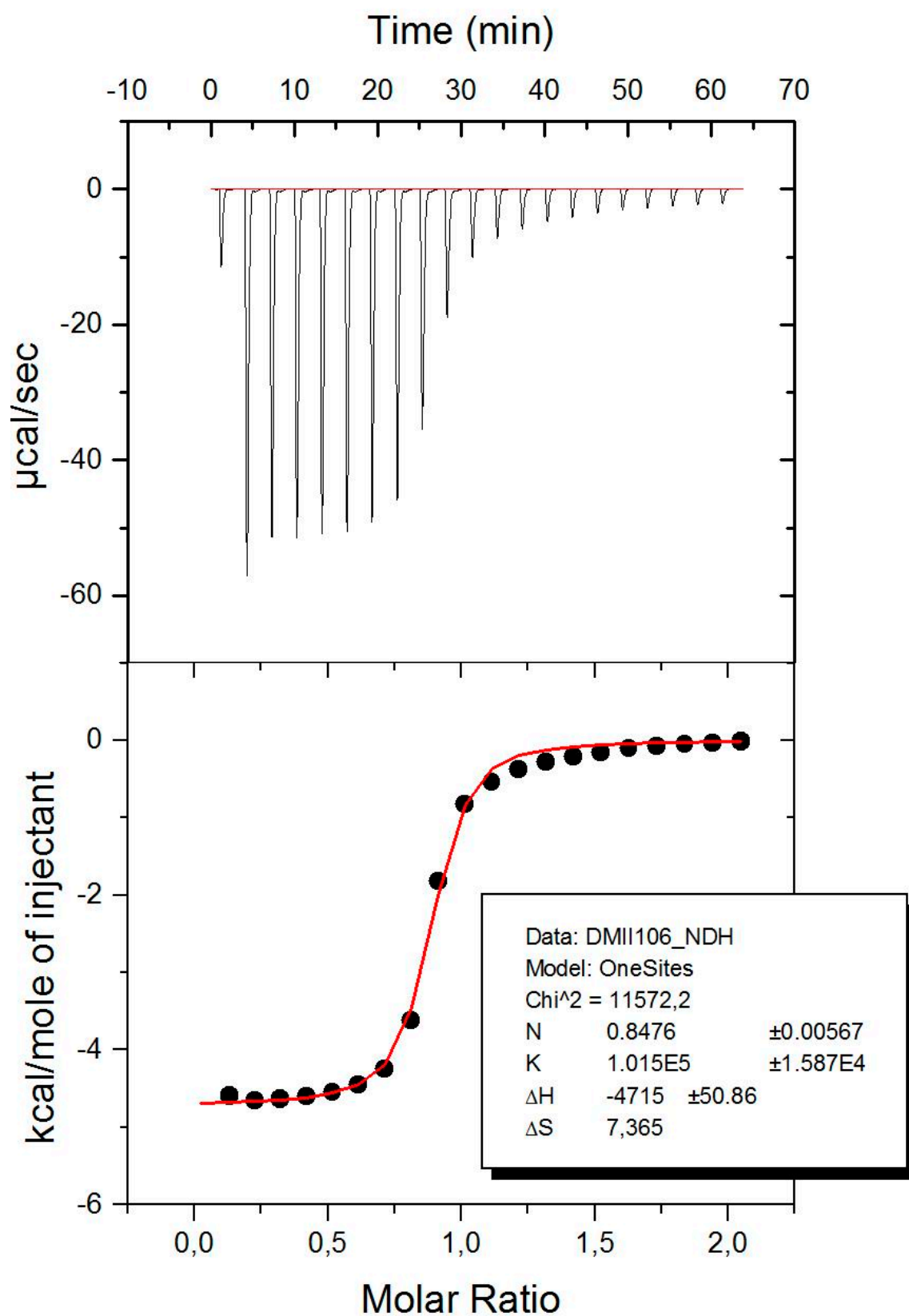


Figure S1. ^{31}P NMR of $\text{Ti}^{4+}[\text{C}_3\text{H}_7, \text{CH}_3, \text{Ph}]$ ·methylbutyl/dimethylbutyl/butyl ammonium chloride qualitative complexation test: (a) spectra of the free cavitand; (b) spectra recorded after the addition of 0.5 equivalents of the guest; (c) spectra recorded after the addition of 1.0 equivalent of the guest. All spectra were recorded in MeOD.

ITC curves and fittings

**Figure S2.** ITC trace and fitting of 1@Tiini.

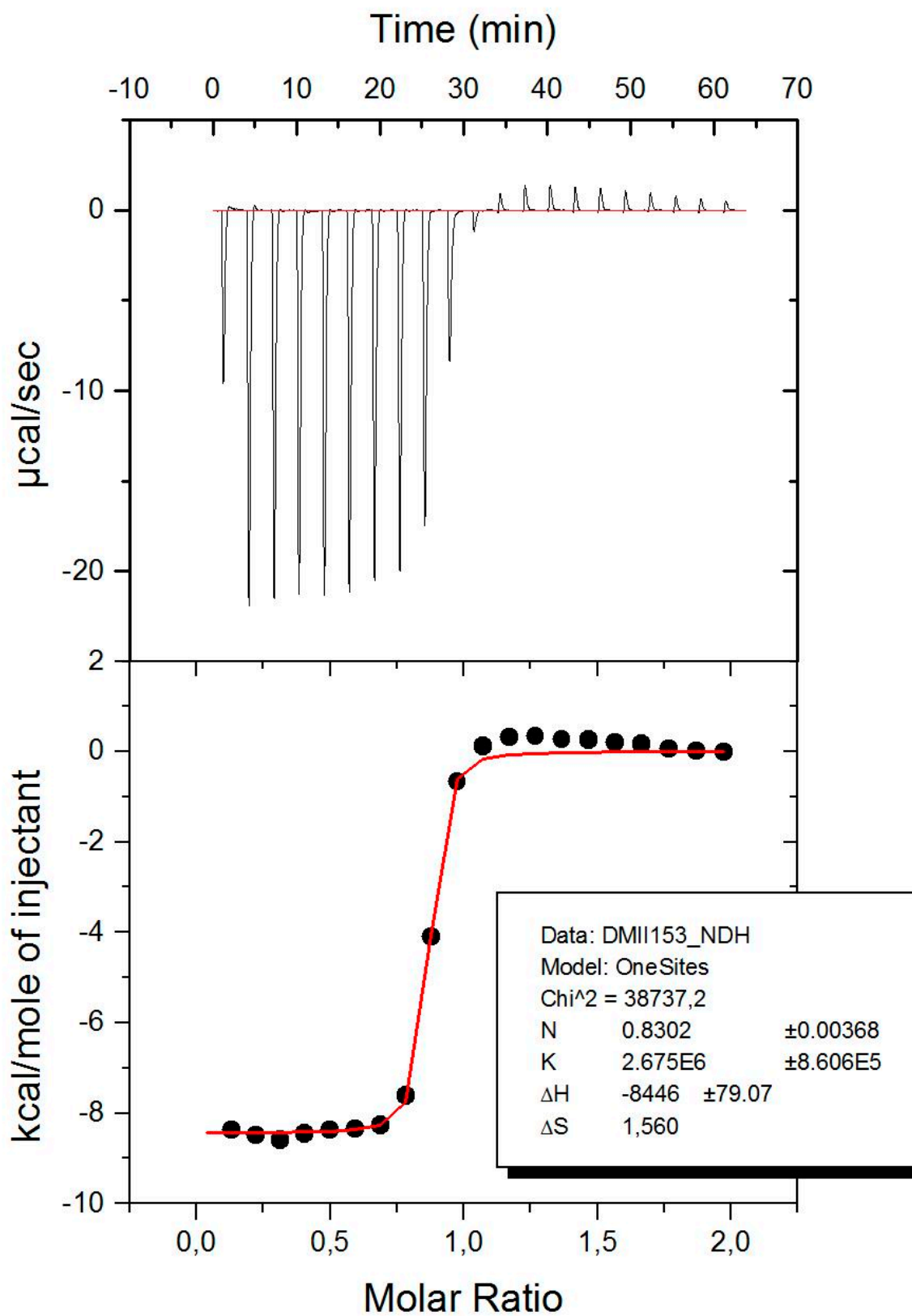


Figure S3. ITC trace and fitting of 1@3POiii1PSi.

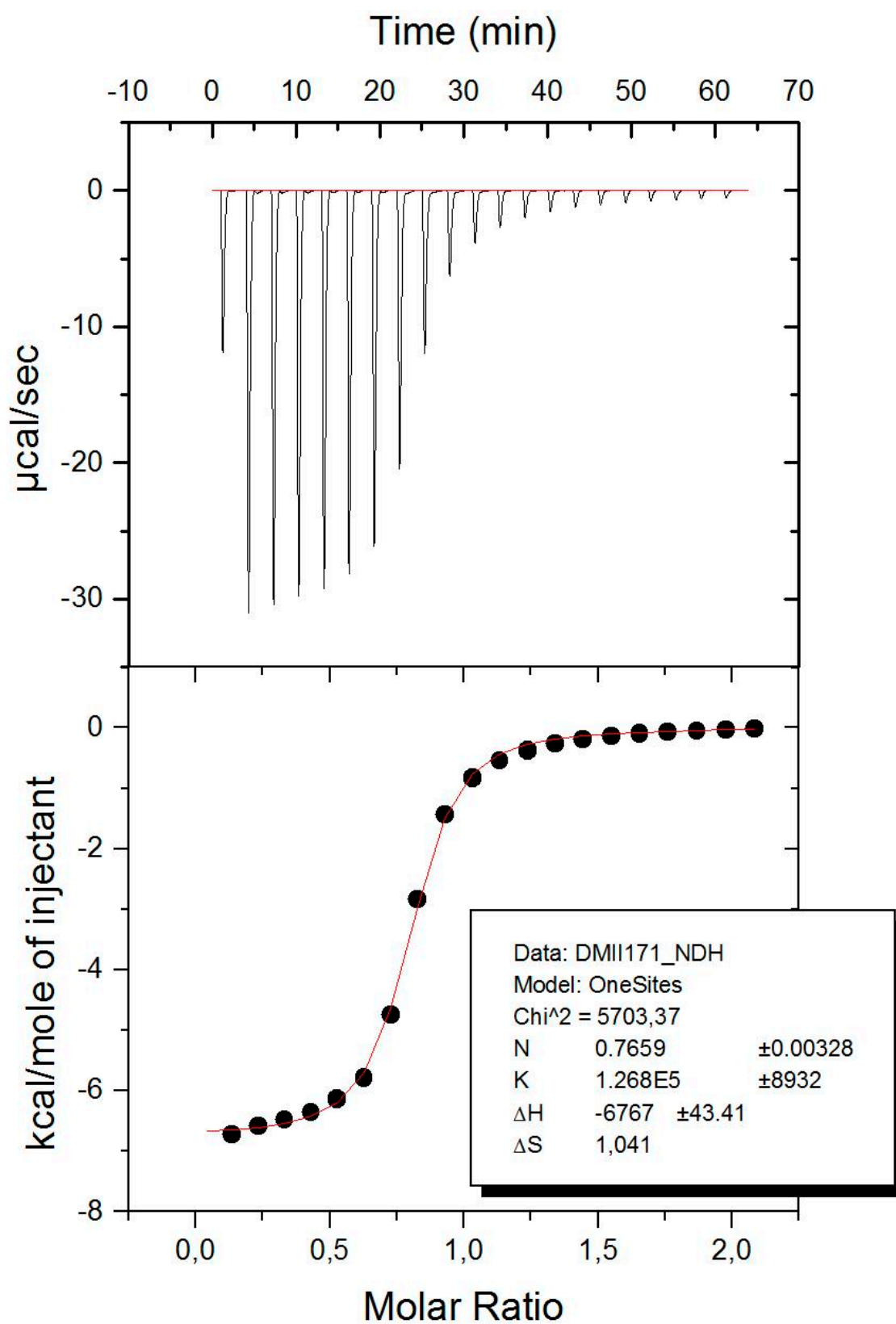


Figure S4. ITC trace and fitting of 1@AB2POii2PSii first run.

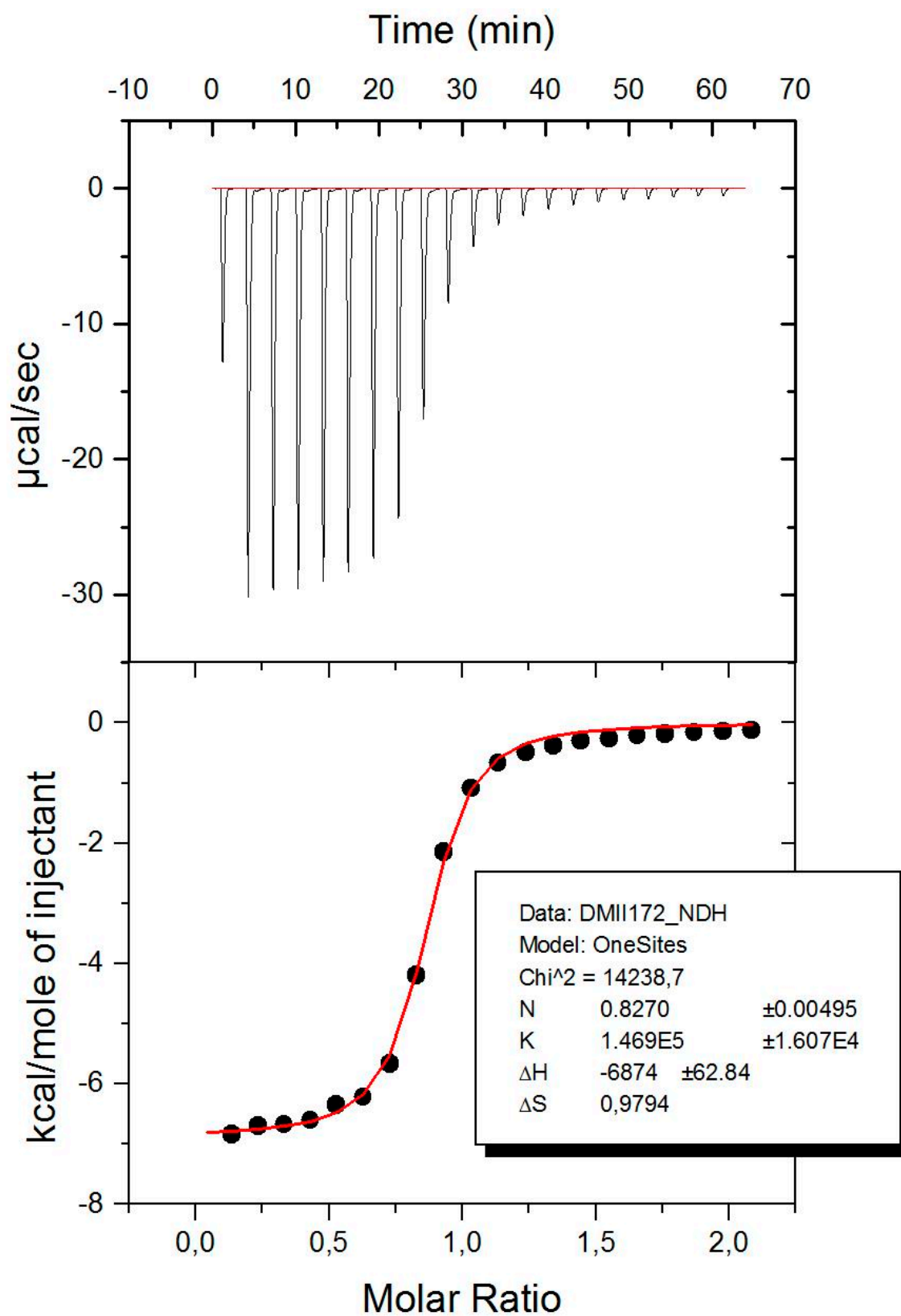


Figure S5. ITC trace and fitting of 1@AB2POii2PSii second run.

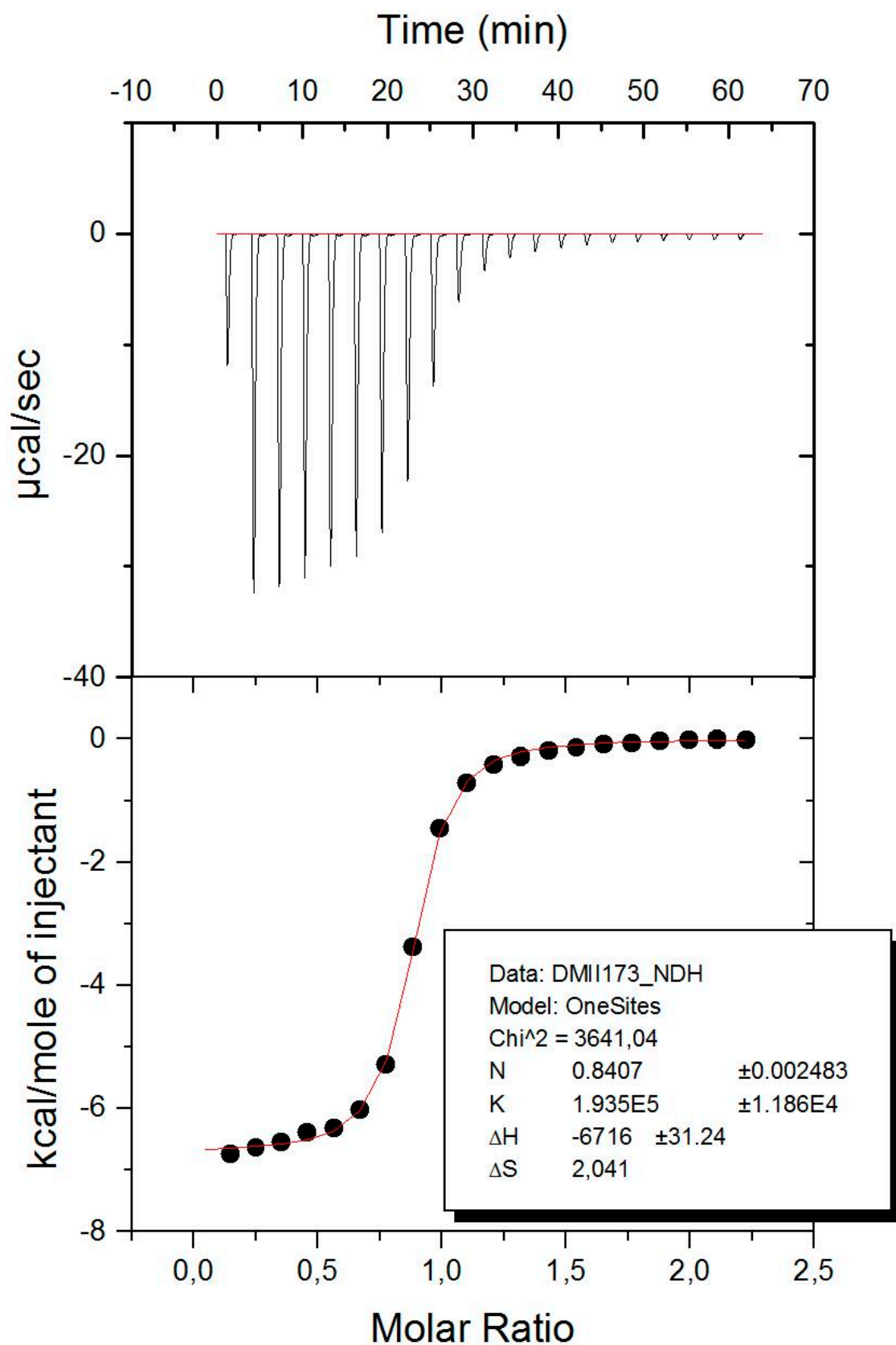


Figure S6. ITC trace and fitting of 1@AB2POii2PSii third run.

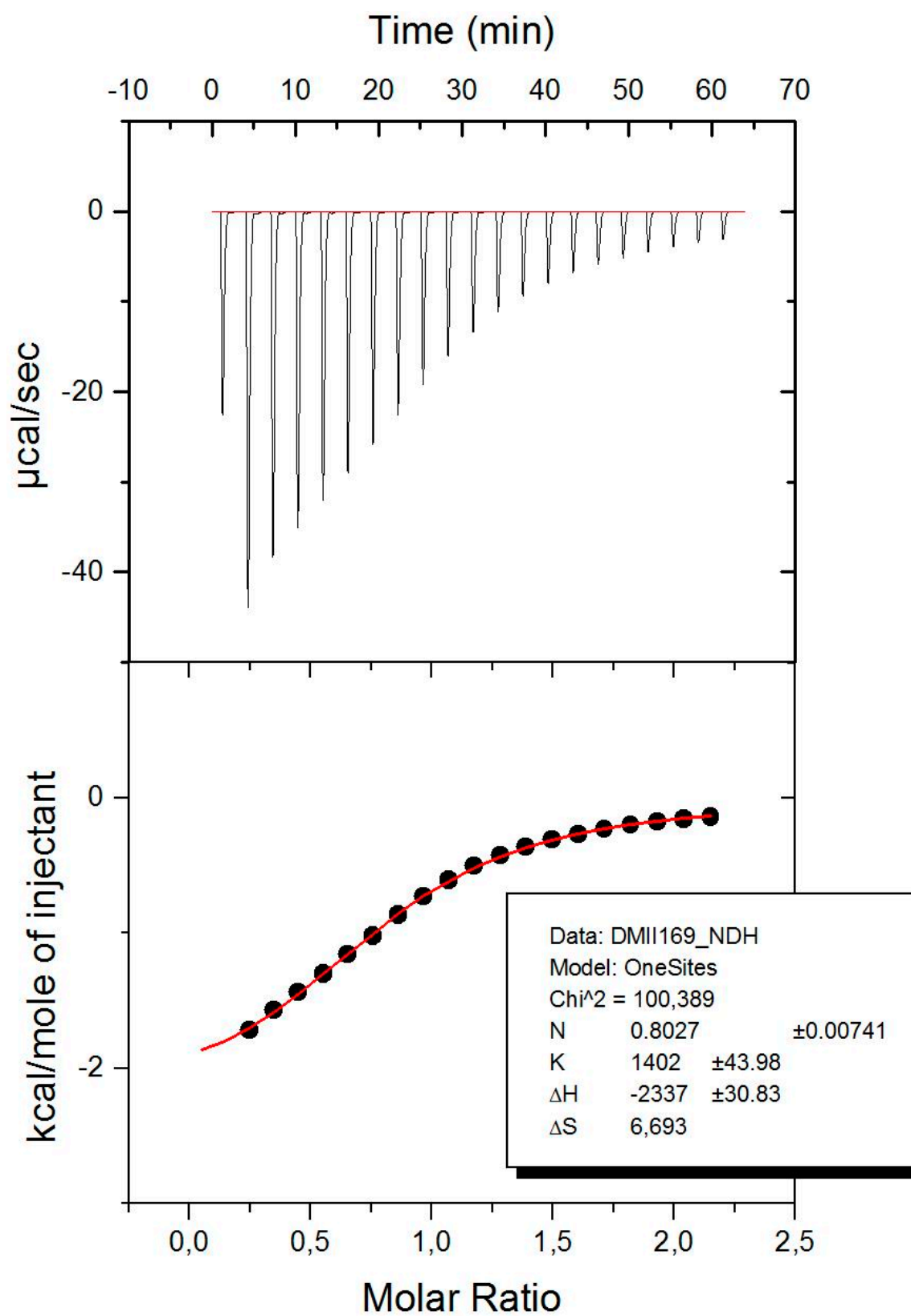


Figure S7. ITC trace and fitting of 1@AC2POii2PSii.

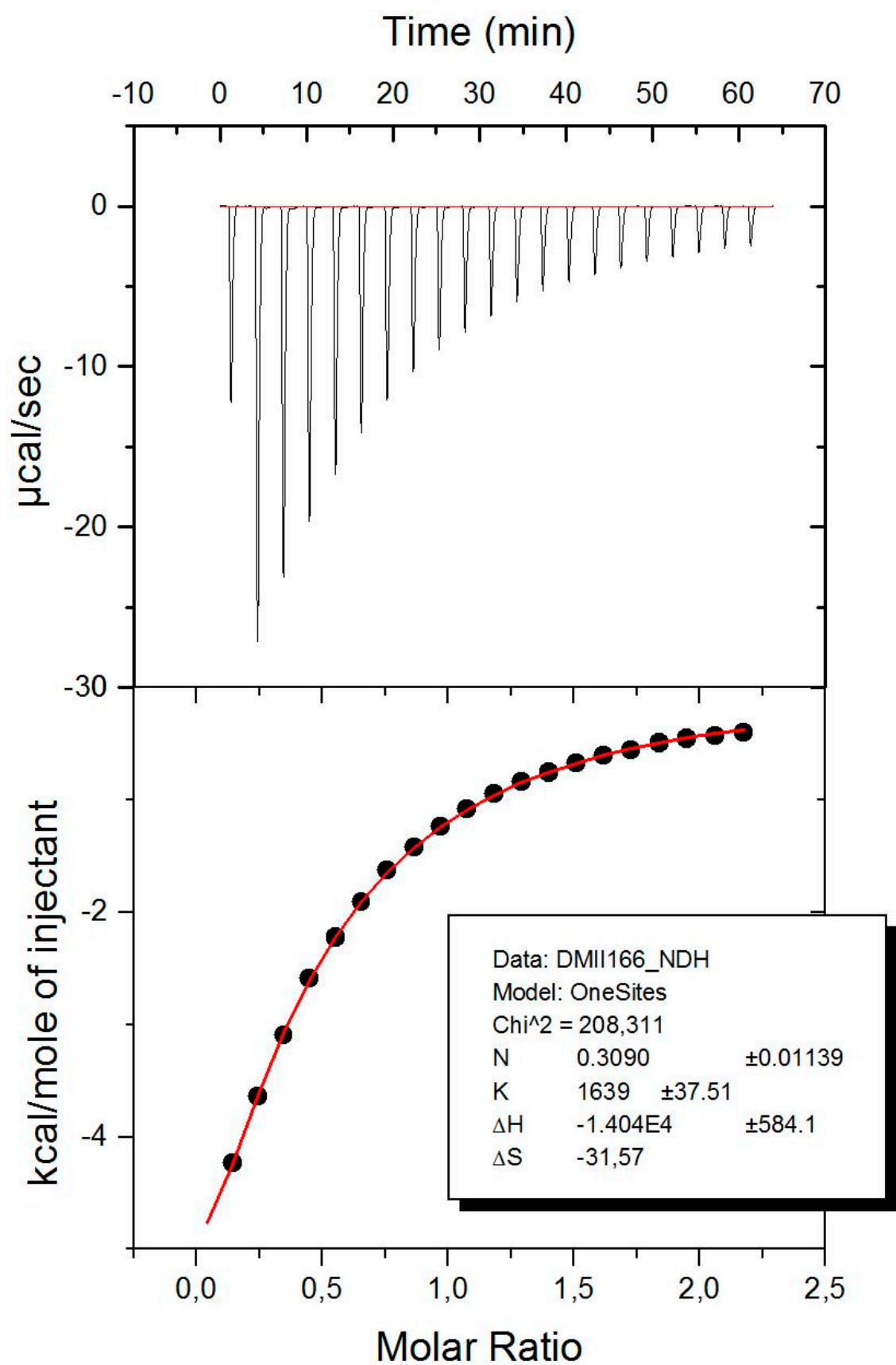


Figure S8. ITC trace and fitting of 1@1POi3PSiii.

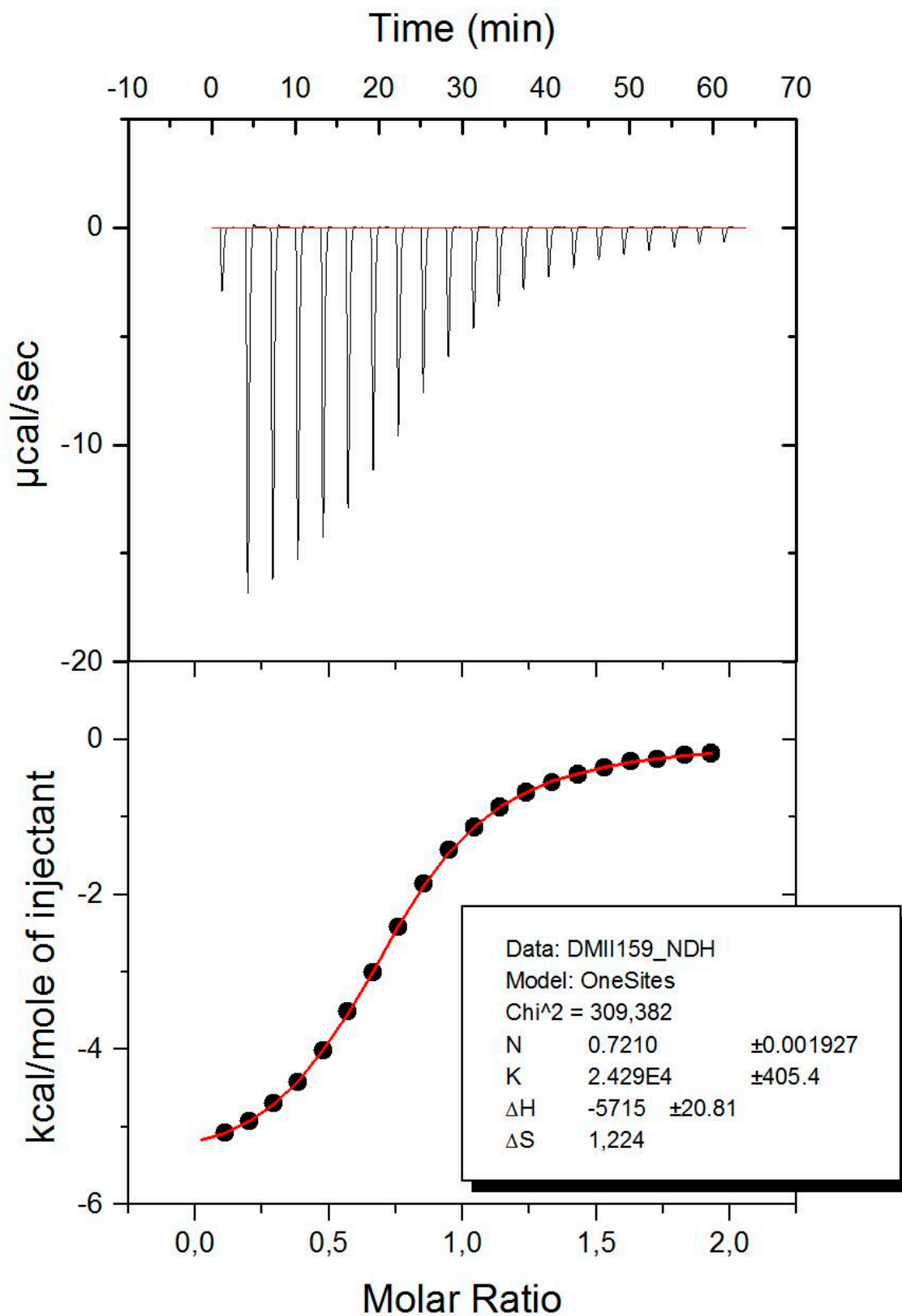
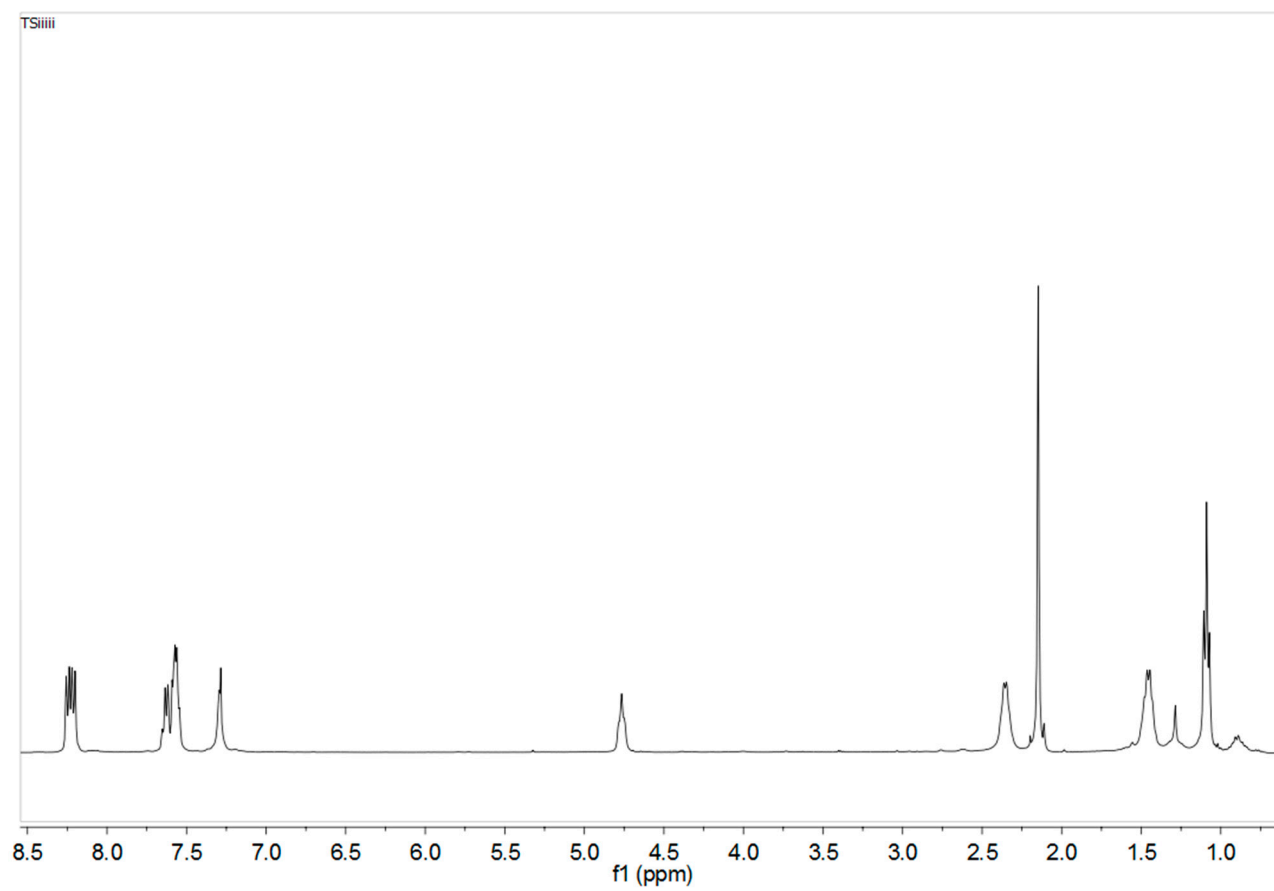


Figure S9. ITC trace and fitting of 1@3POiii1CH₂.

^1H and ^{31}P -NMR of the new cavitands**Figure S10.** ^1H -NMR of TSiiii.

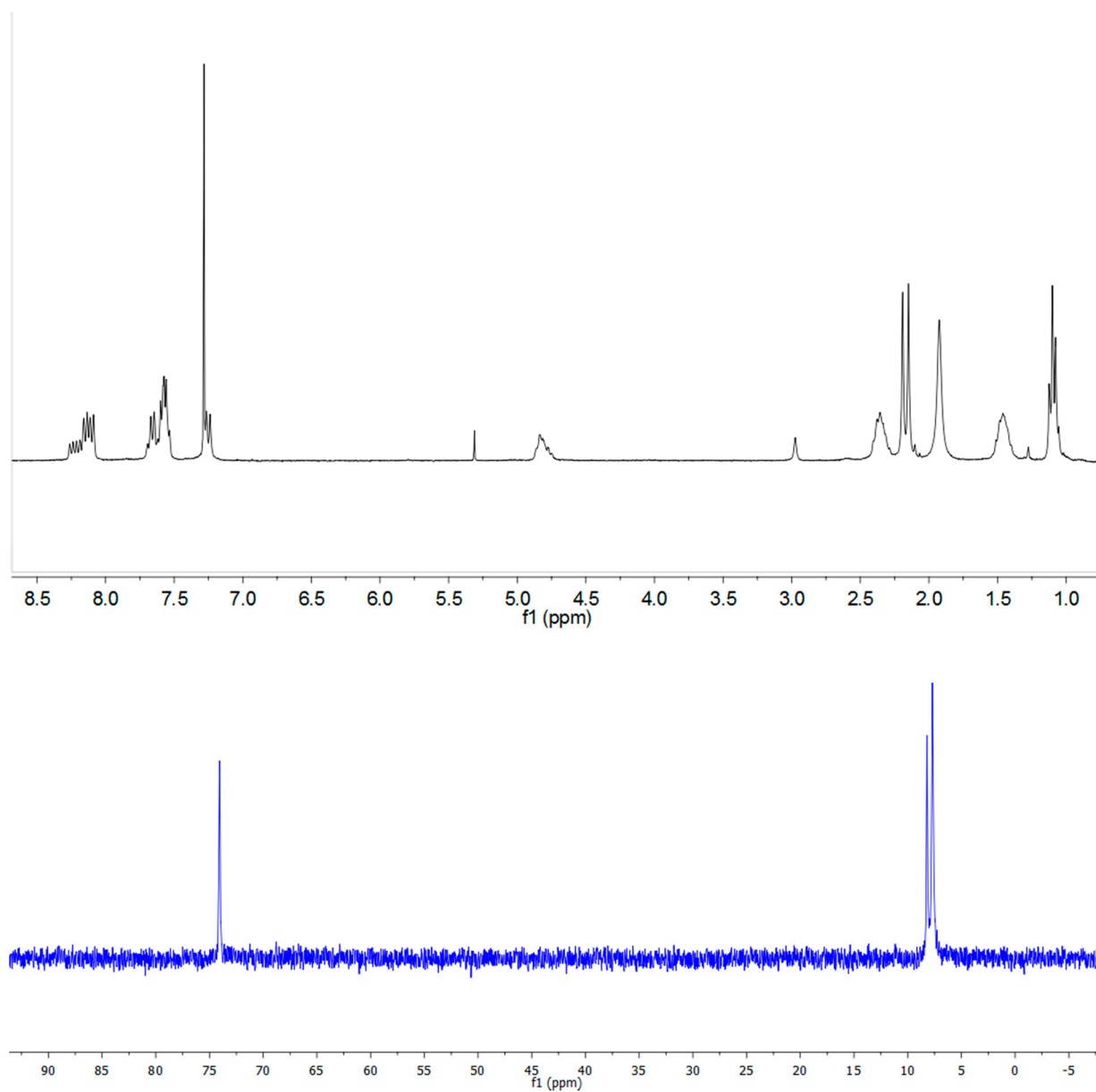


Figure S11. ^1H and ^{31}P -NMR of 3POiii1Psi.

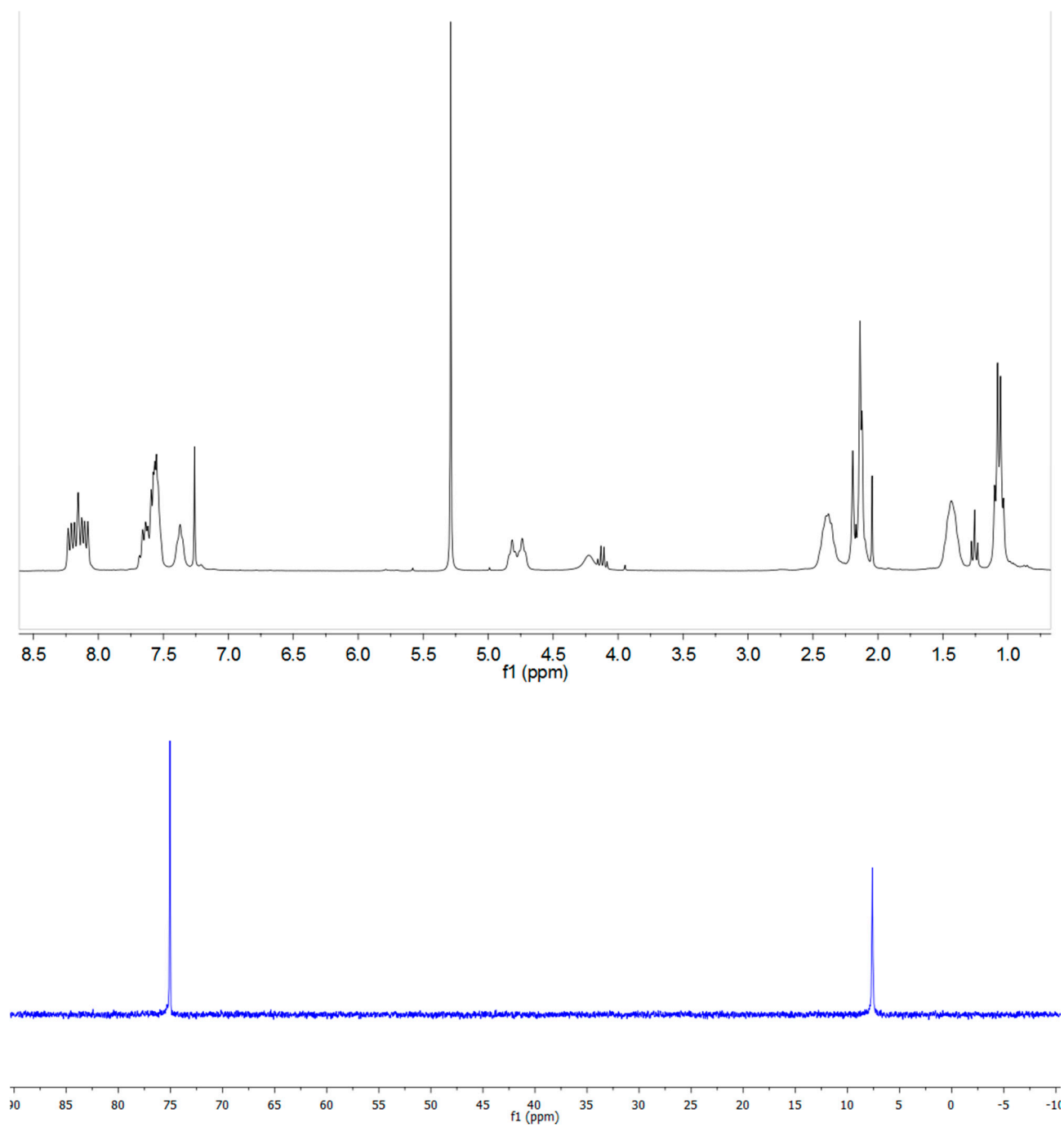


Figure S12. ¹H and ³¹P-NMR of AB₂POii₂PSii.

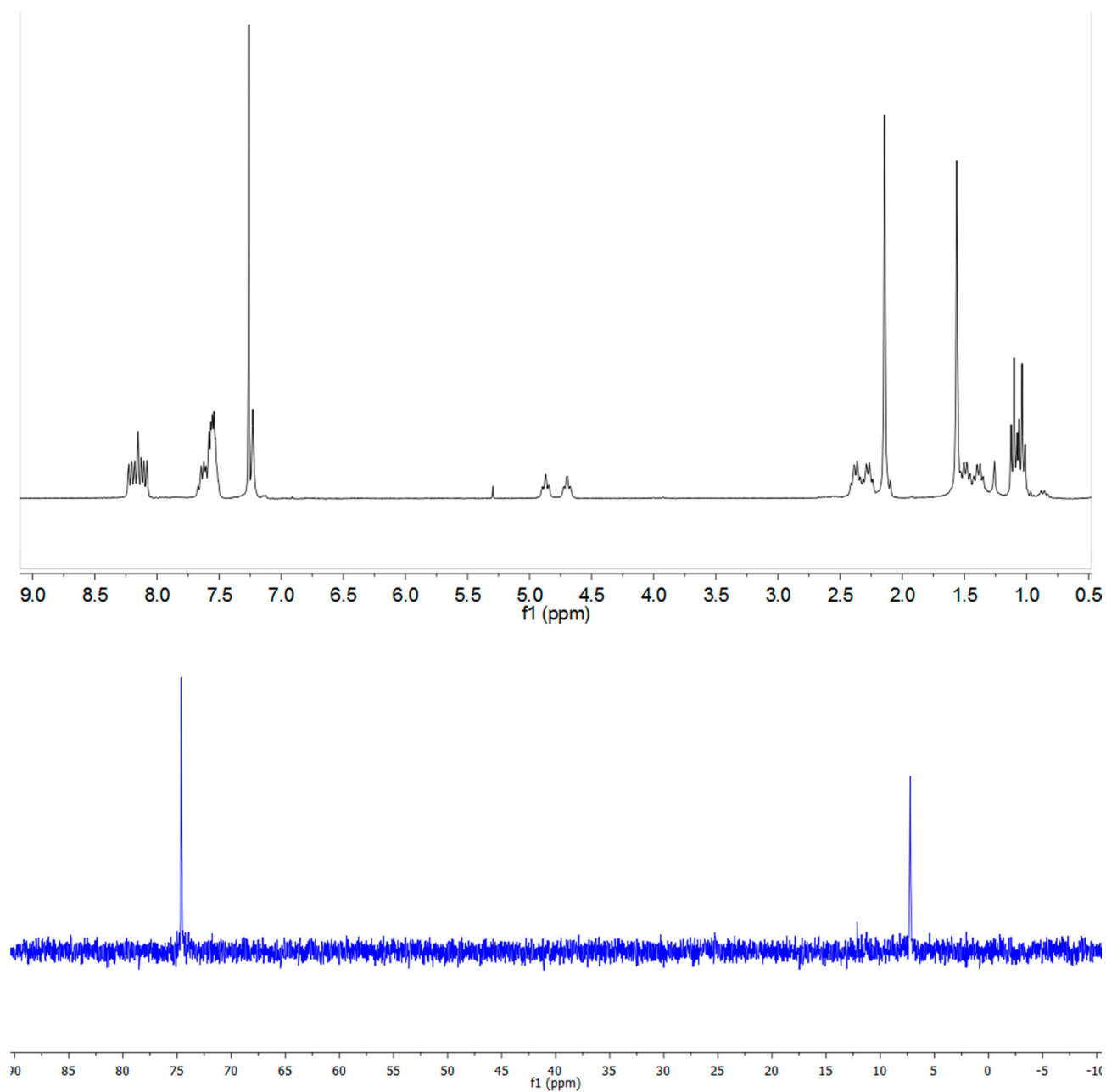


Figure S13. ^1H and ^{31}P -NMR of AC2POii2PSii.

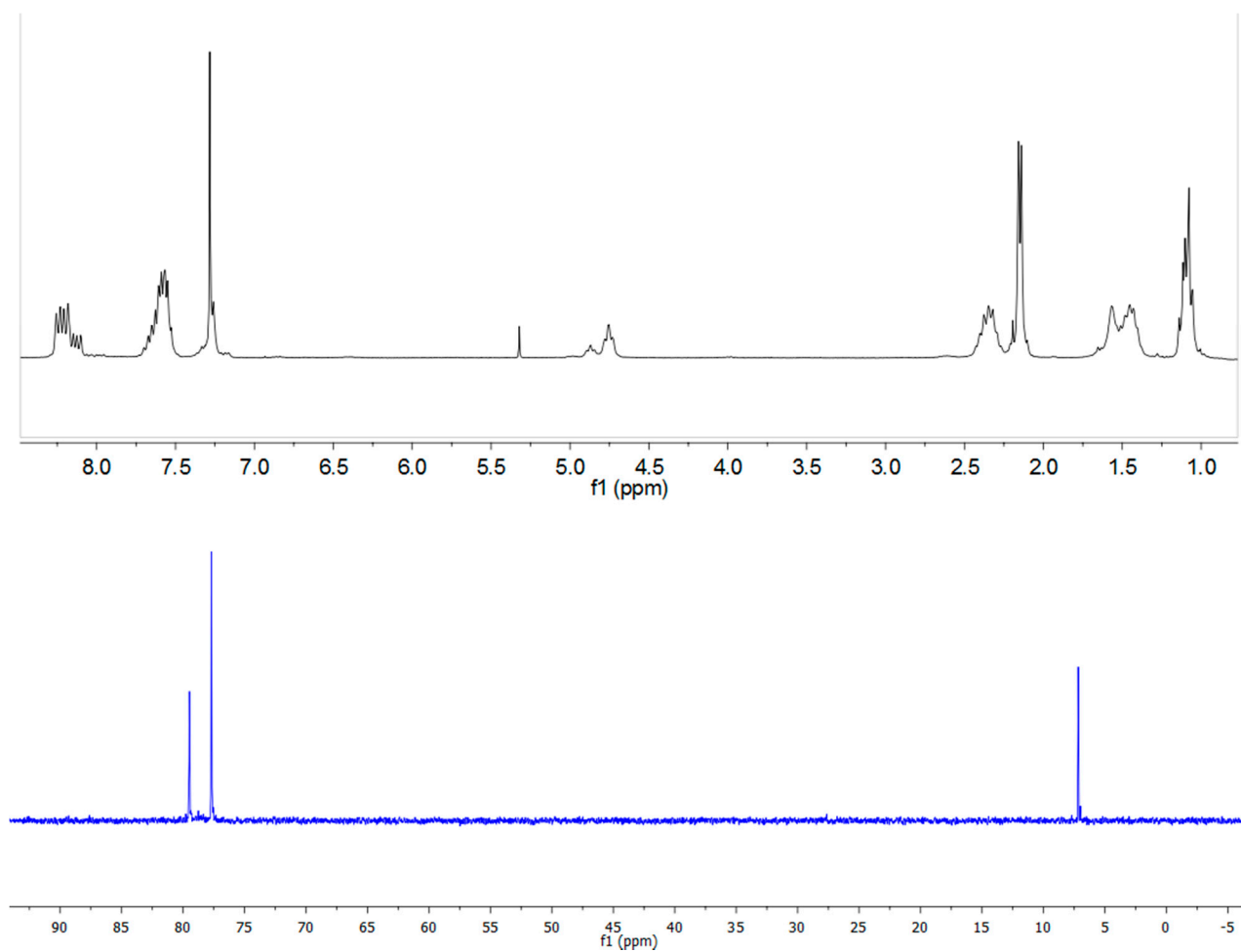


Figure S14. ^1H and ^{31}P -NMR of 1POi3PSiii.

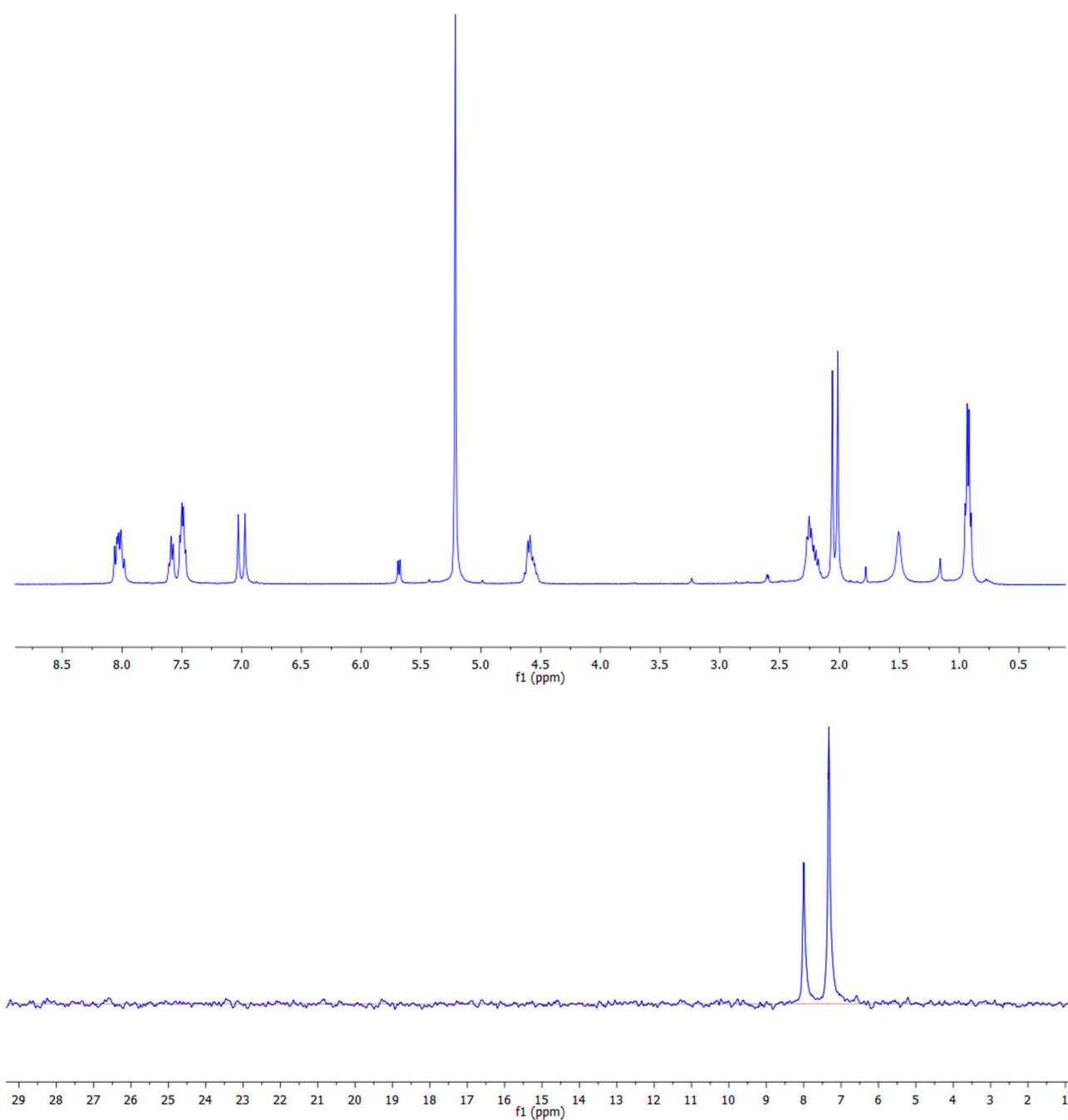


Figure S15. ¹H and ³¹P-NMR of 3POiii1CH₂.