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Supporting Information

for

Stereodiscrimination of guests in chiral organosilica aerogels studied by ESR spectroscopy

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Materials characterization and ESR spectra

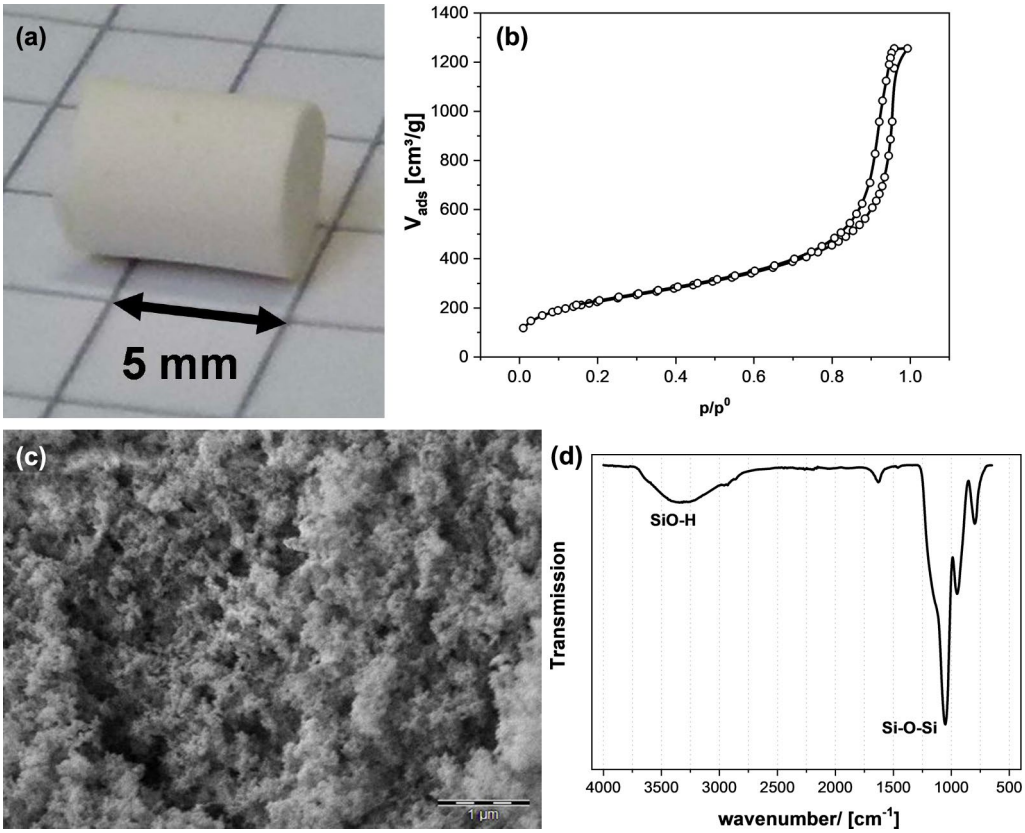

Figure S1: SIL-AG as achiral reference material. (a) Photographic image of silica monolith after supercritical drying. (b) Porosity analysis using N_2 physisorption measurements (A_{BET} = 946 $m^2 \cdot g^{-1}$). (c) SEM micrograph. (d) FTIR spectrum.

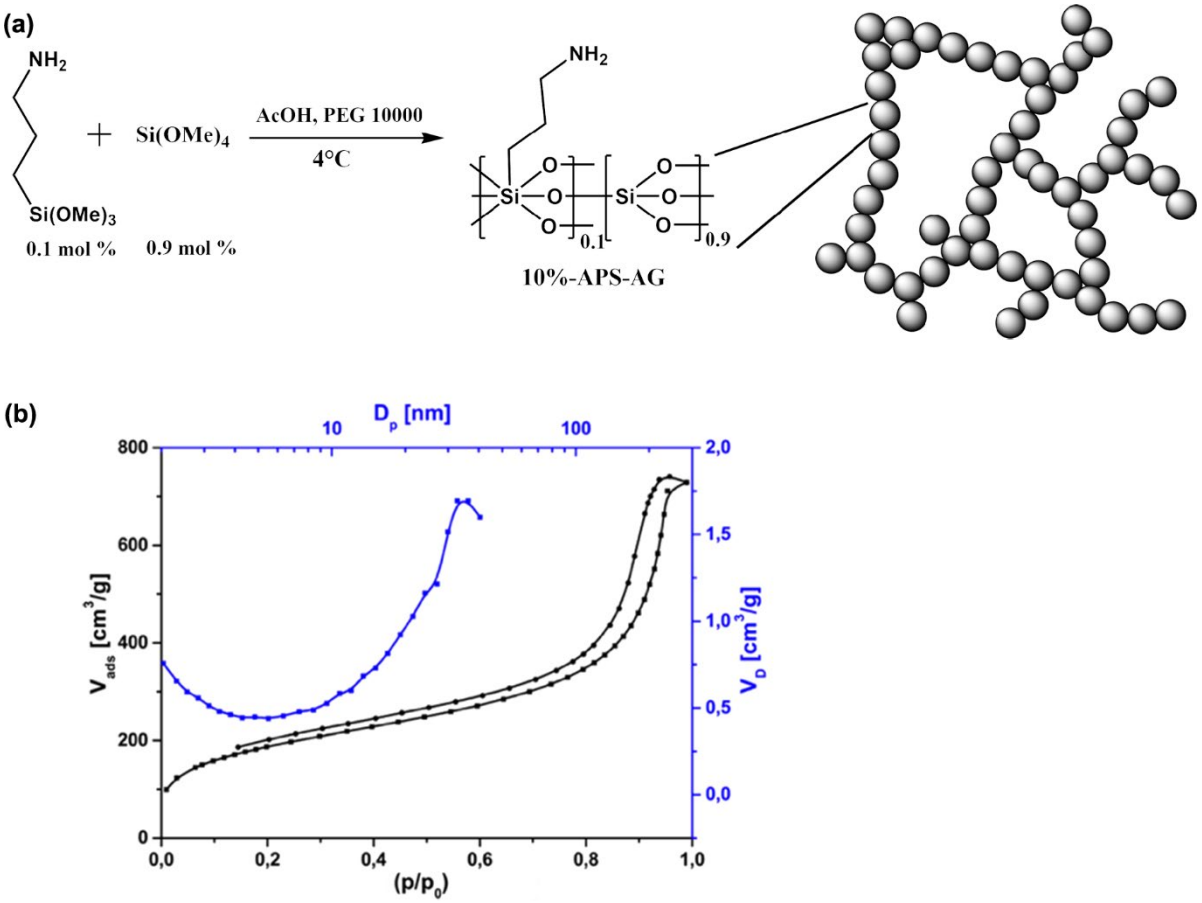

Figure S2: NH_xSIL. (a) Synthesis scheme. (b) Nitrogen physisorption analysis (black, A_{BET} = 681 $m^2 \cdot g^{-1}$) and pore-size distribution (blue).

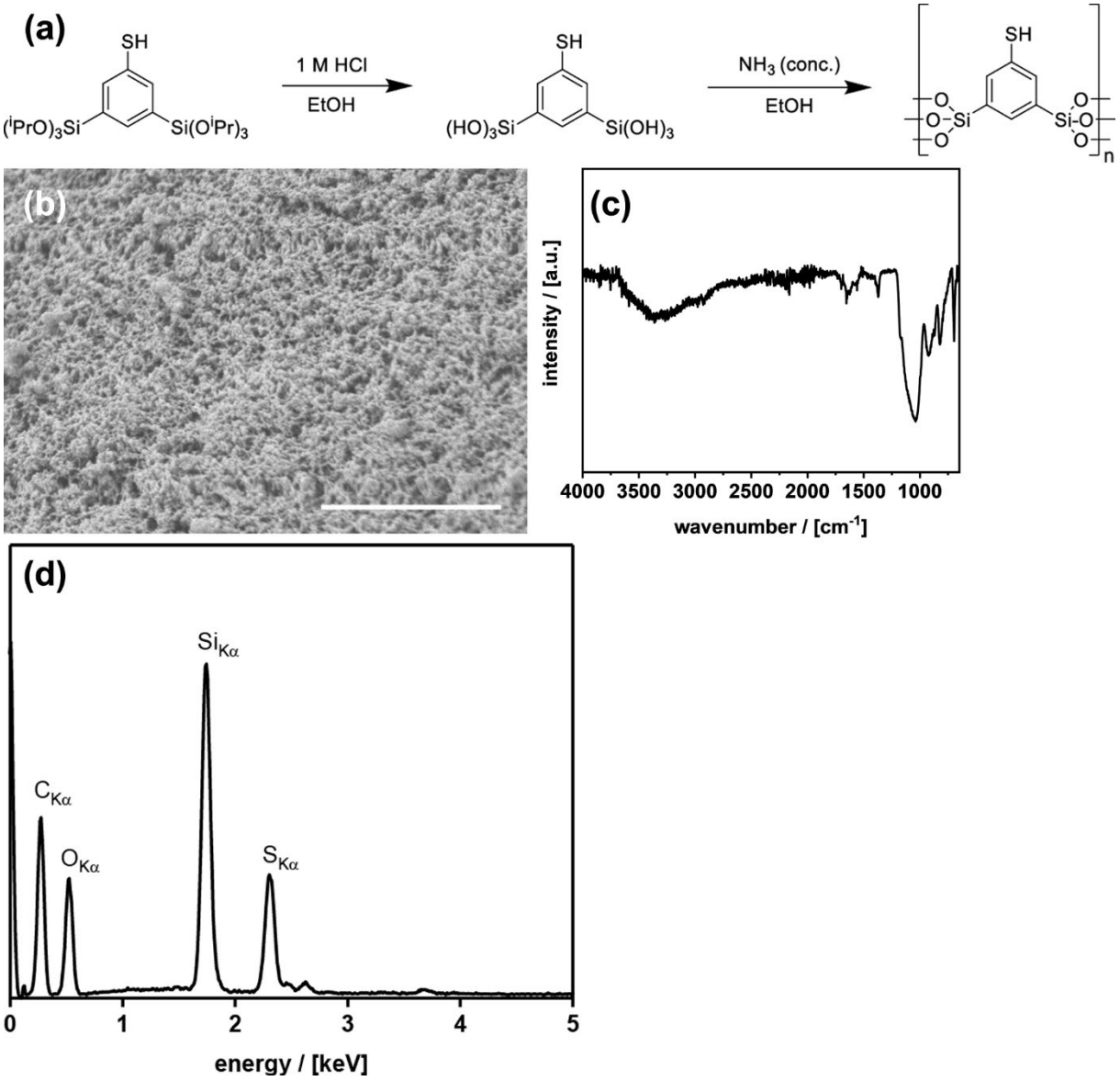

Figure S3: SH-AG as achiral reference material. (a) Sol–gel preparation. (b) SEM micrograph (scale bar = 2 µm). (c) FTIR spectrum (v [cm^{-1}] = 3000–3200 (CH-arom), 1100 (Si–O–Si), 600–700 (CS deformation). (d) EDX spectrum.

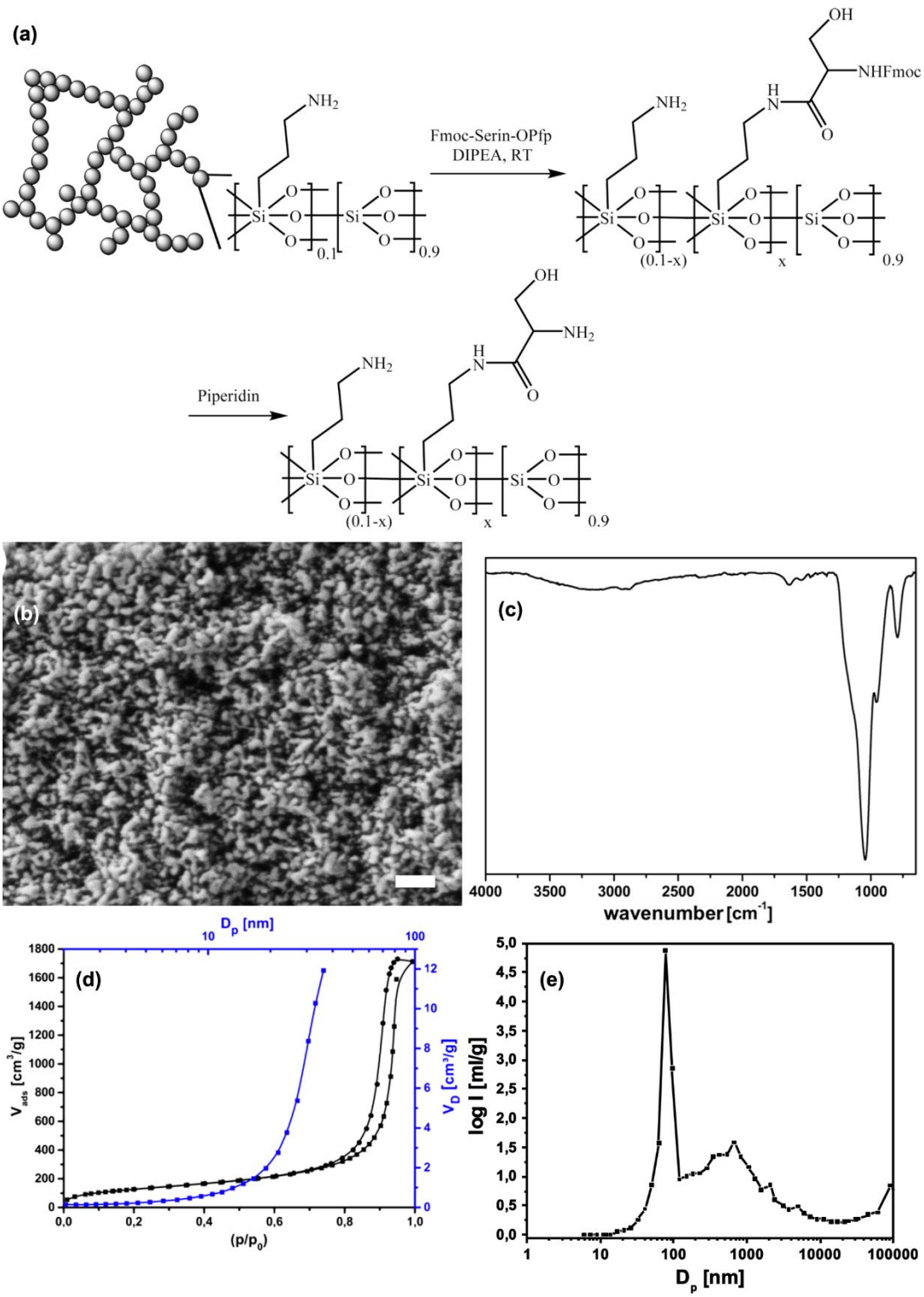

Figure S4: SerNH$_{10}$SIL. (a) Synthesis scheme. (b) SEM micrograph; scale bar = 200 nm. (c) Nitrogen physisorption analysis (black) (A_{BET} = 472 m^2·g^{-1}) and pore-size distribution (blue). (d) FTIR (ATR, v = 3200 cm^{-1} (OH), 2860–2970 cm^{-1} (CH), 1637 and 1541 cm^{-1} (amid I & II), 1049 cm^{-1} (SiO)). (e) Mercury intrusion porosimetry.

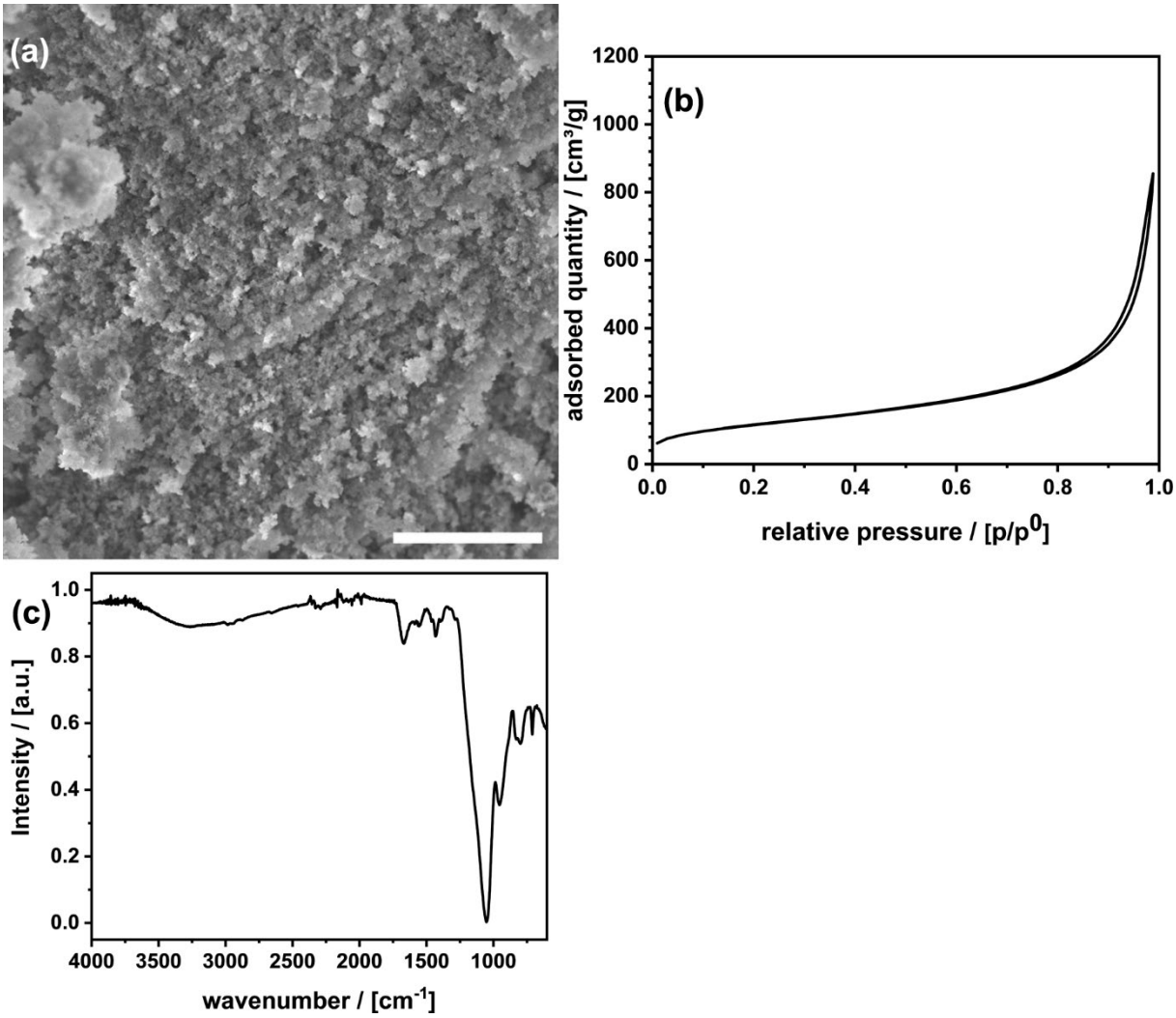

Figure S5: AlaNH15oSIL. (a) SEM micrograph; scale bar = 2 µm. (b) Nitrogen physisorption isotherm (A_{BET} = 404 $m^2 \cdot g^{-1}$). (c) FTIR (ATR, v = 3400 cm^{-1} (NH), 3200 cm^{-1} (OH), 2978 & 2858 cm^{-1} (CH), 1668 cm^{-1} (amid I), 1548 cm^{-1} (amid II), 1368–1577 cm^{-1} (aliph. + arom. C–C); 1044 cm^{-1} (SiO).

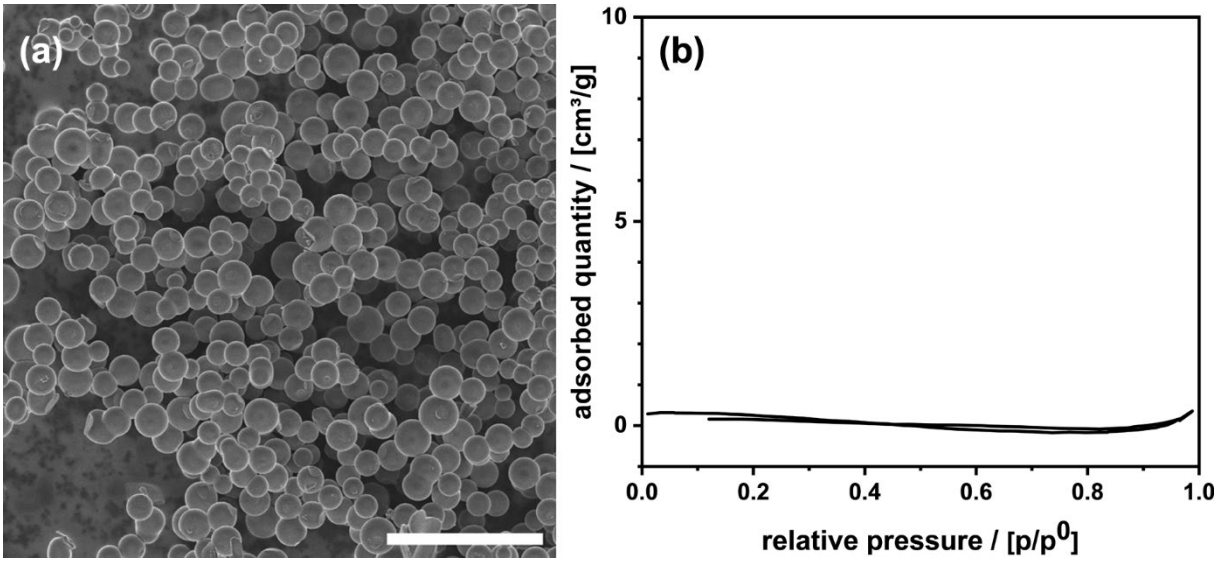

Figure S6: AlaNH15oSIL. (a) SEM micrograph; scale bar = 20 µm. (b) Nitrogen physisorption isotherm.

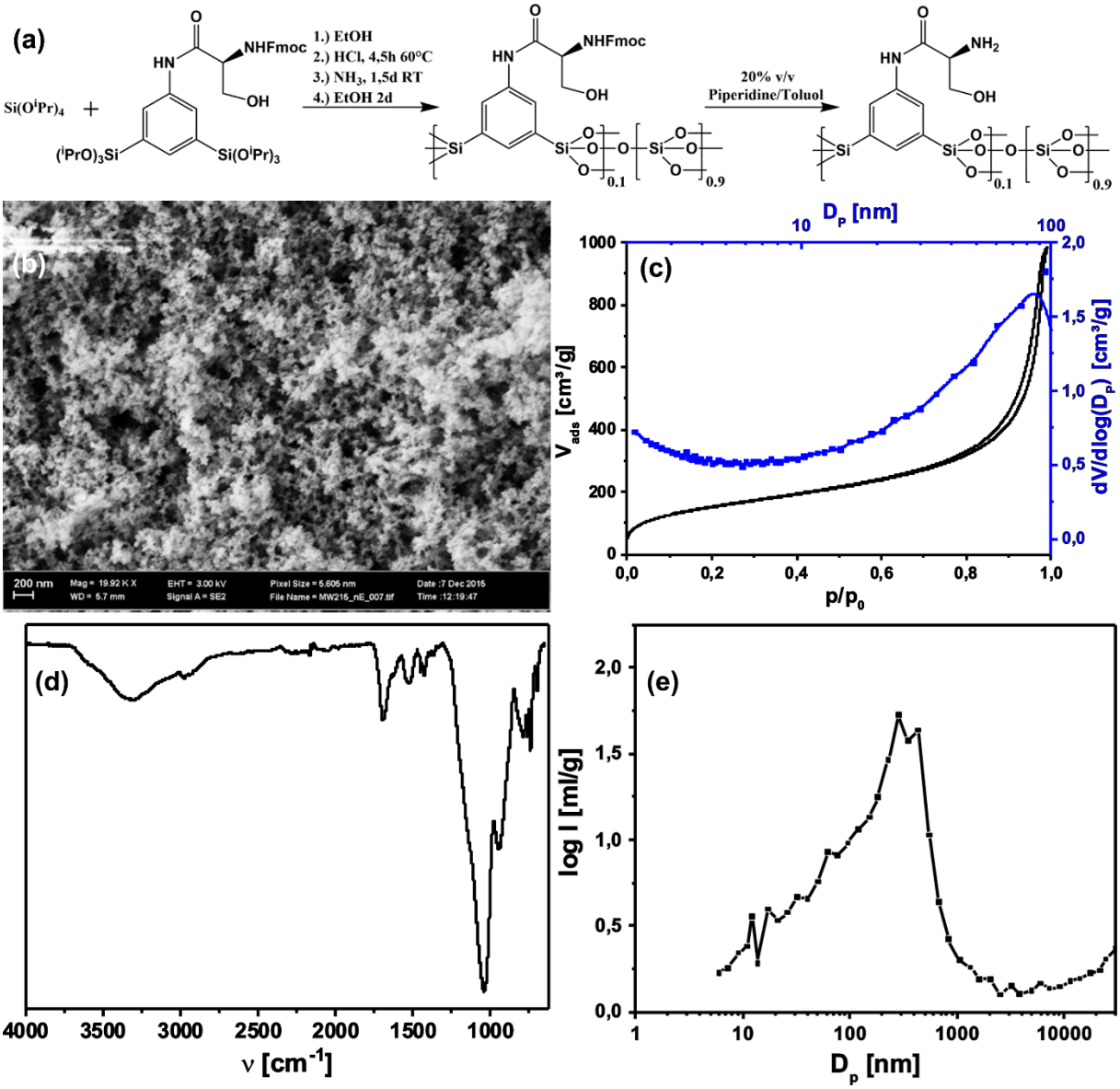

Figure S7: SerNH10oSIL. (a) Synthesis scheme. (b) SEM micrograph; scale bar = 200 nm. (c) Nitrogen physisorption analysis (black, A_{BET} = 552 $m^2 \cdot g^{-1}$) and pore-size distribution (blue). (d) FTIR spectroscopy (ATR, ν = 3000–3500 cm^{-1} (NH & OH), 2985 & 2945 & 2874 cm^{-1} (CH), 1673 cm^{-1} (arom. amid I), 1582 cm^{-1} (arom. amid II), 1423 cm^{-1} (amine), 1047 & 950 cm^{-1} (SiO)). (e) Mercury intrusion porosimetry.

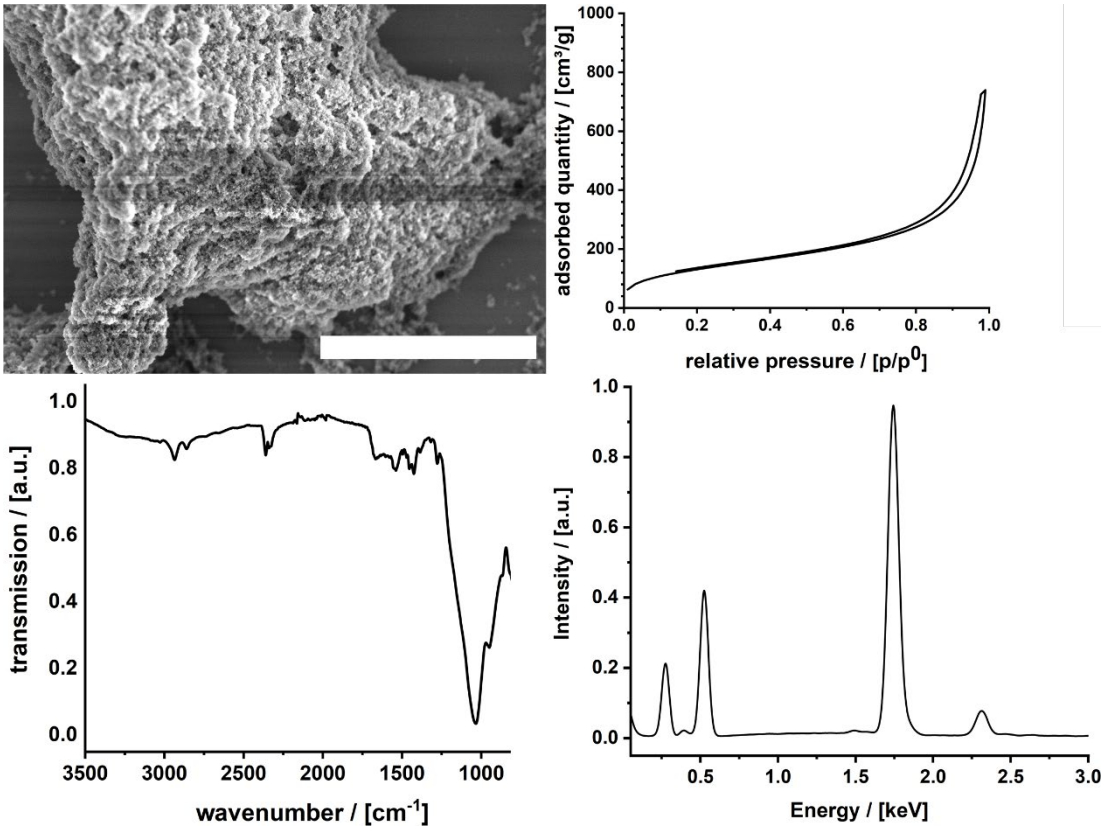

Figure S8: SH-AlaNH10oSIL. (a) SEM micrograph; scale bar = 5 µm. (b) Nitrogen physisorption analysis (black, A_{BET} = 478 $m^2 \cdot g^{-1}$). (c) FTIR spectroscopy (ATR, v = 2937 & 2858 cm^{-1} (CH), 1666 cm^{-1} (amid I), 1548 cm^{-1} (amid II), 1368–1466 (aliph. + arom. C–C); 1033 cm^{-1} (SiO)). (d) EDX analysis (0.28 eV (C), 0.4 eV (N), 0.52 eV (O), 1.43 eV (Al), 1.74 eV (Si), 2.32 eV (S)).

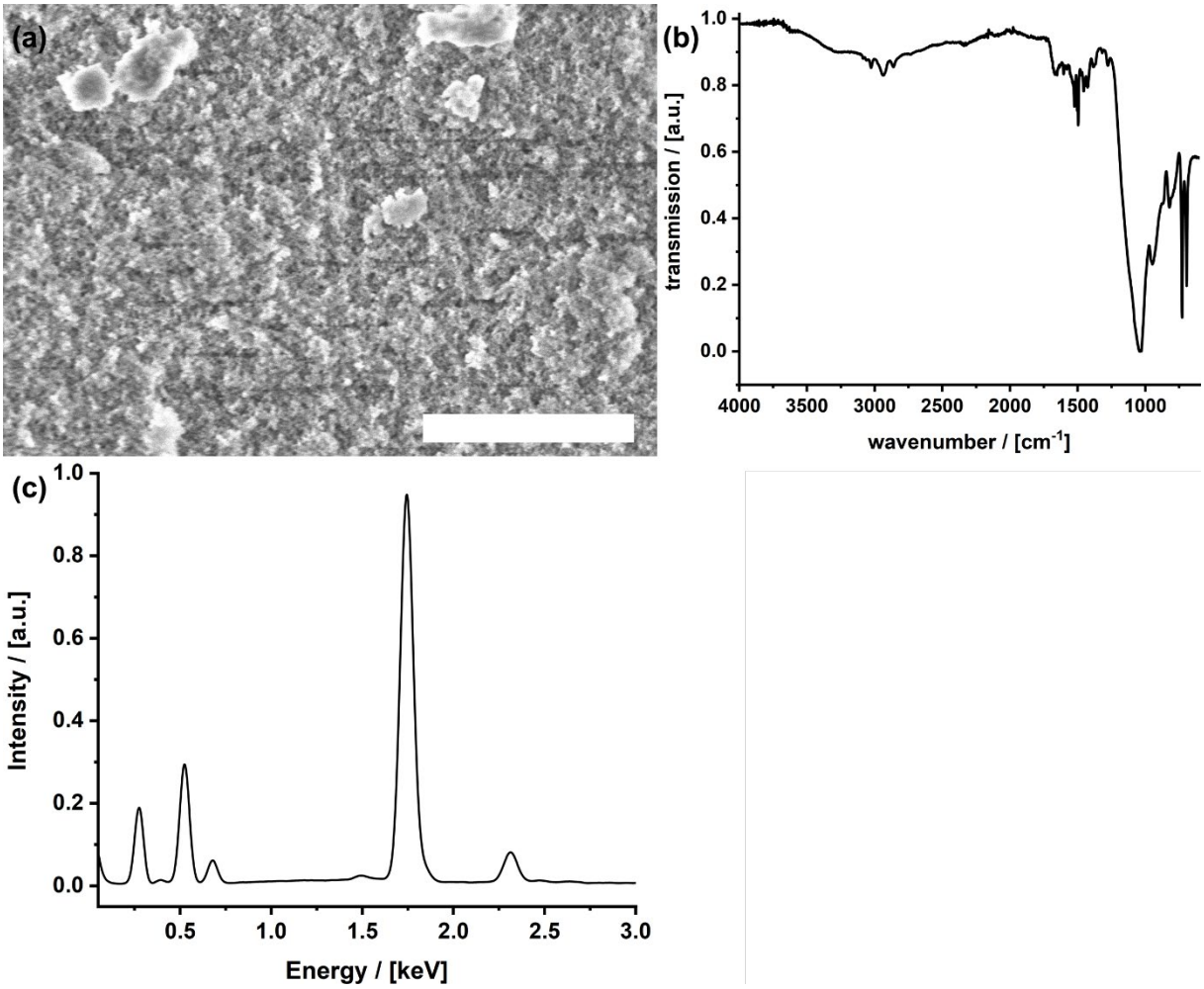

Figure S9: ArFSH-AlaNH10oSIL. (a) SEM micrograph; scale bar = 5 µm. (b) FTIR spectroscopy (ATR, v = 3296 cm^{-1} (O–H), 2935 & 2860 cm^{-1} (CH), 1669 cm^{-1} (amid I), 1544 cm^{-1} (amid II), 1522 cm^{-1} (C–F), 1368–1449 (aliph. + arom. C–C); 1029 cm^{-1} (Si–O)). (c) EDX analysis.

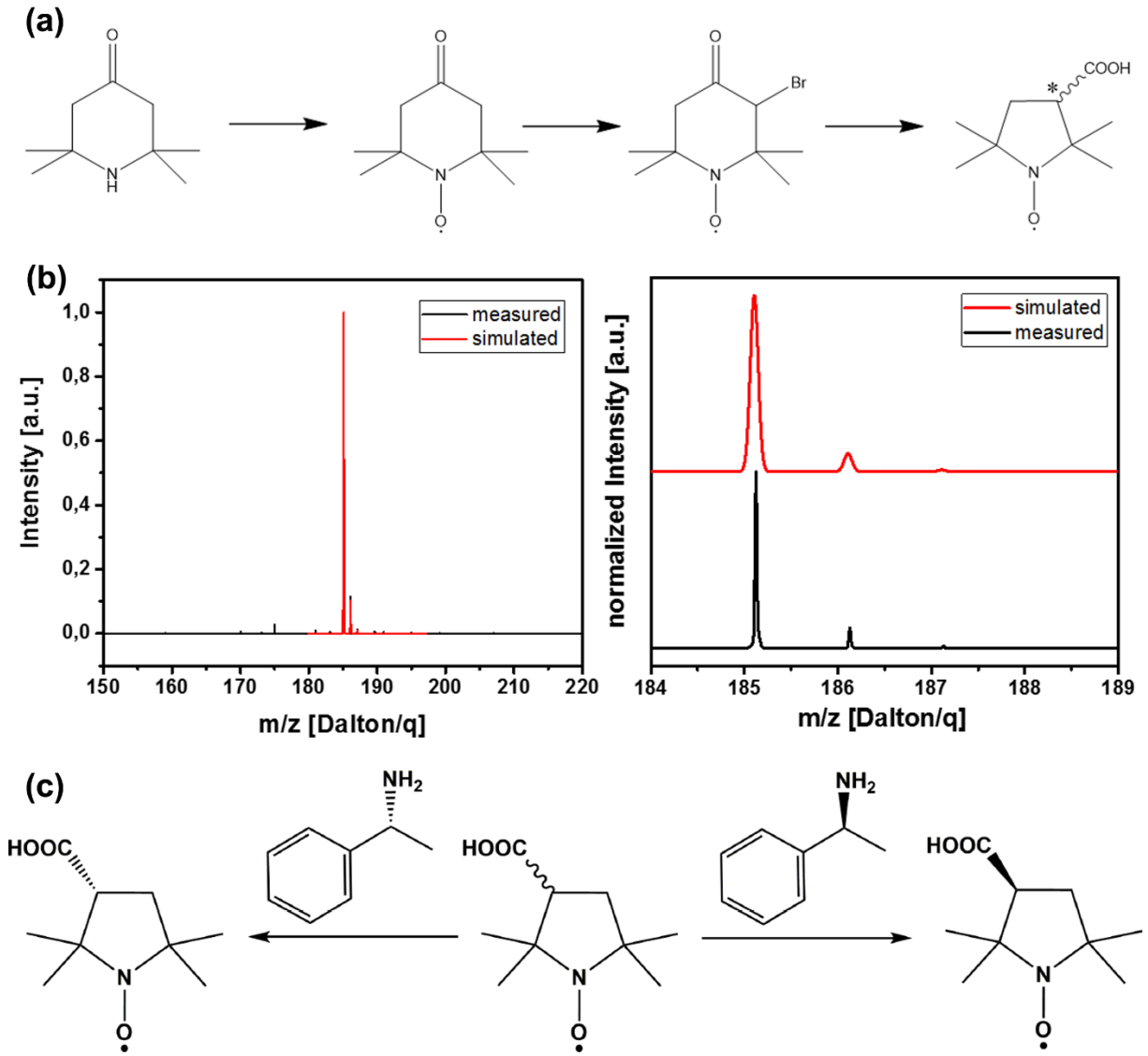

Figure S10: The 3CP spin probe. (a) Synthesis scheme. (b) Selected data for molecular characterization: ESI-MS. (c) Racemate separation of (+)-3CP.

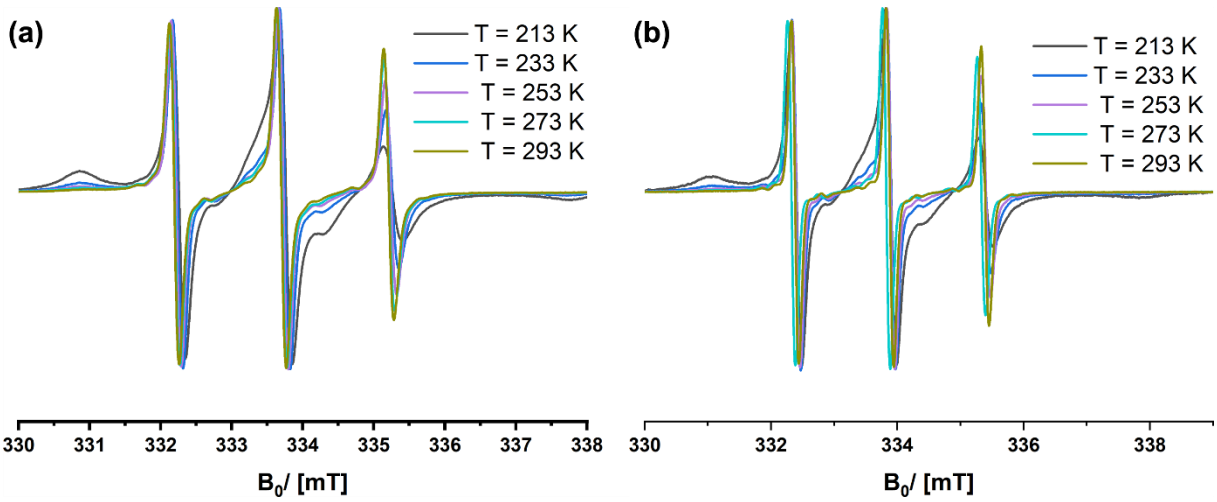

Figure 11: cw-ESR; SerNH10oSil; EtOH; temperature series. (a) (+)-3CP. (b) (−)-3CP.

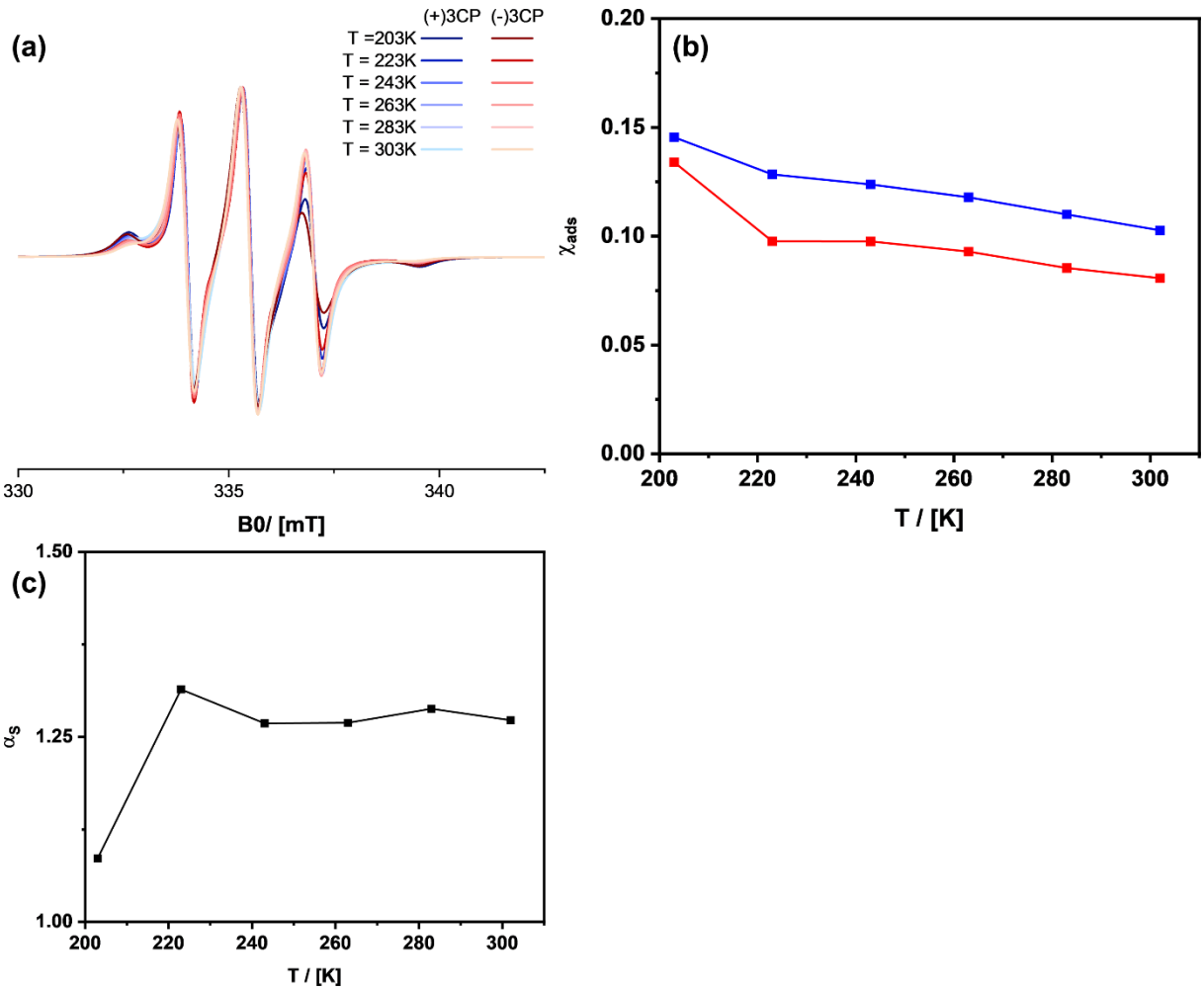

Figure 12: (a) cw-ESR; host material: AlaNH15oSIL; solvent ethanol/pentane 20:80. (b) Quantification of immobile species; (+)-3CP (blue), (−)-3CP (red). (c) Quantification of selectivity factor.

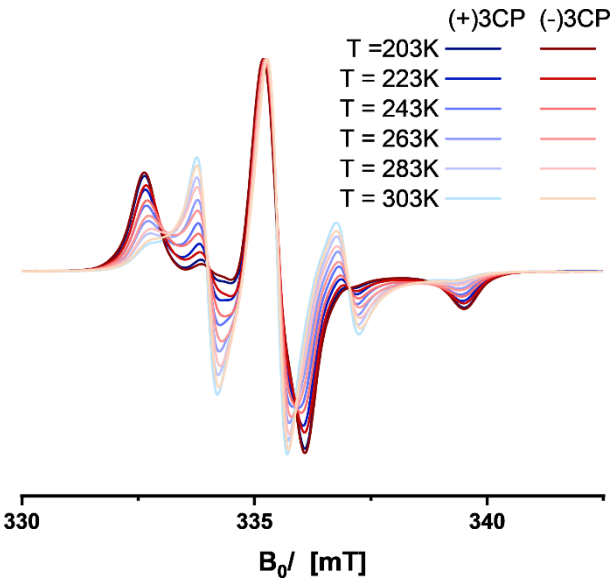

Figure S13: cw-ESR; host material: ArFSHAlaNH10oSIL; solvent: ethanol/pentane.