

Supporting Information

Superfluorinated, Highly Water Soluble Polyphosphazenes as potential ^{19}F Magnetic Resonance Imaging (MRI) Contrast Agents

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Polymer Characterization:

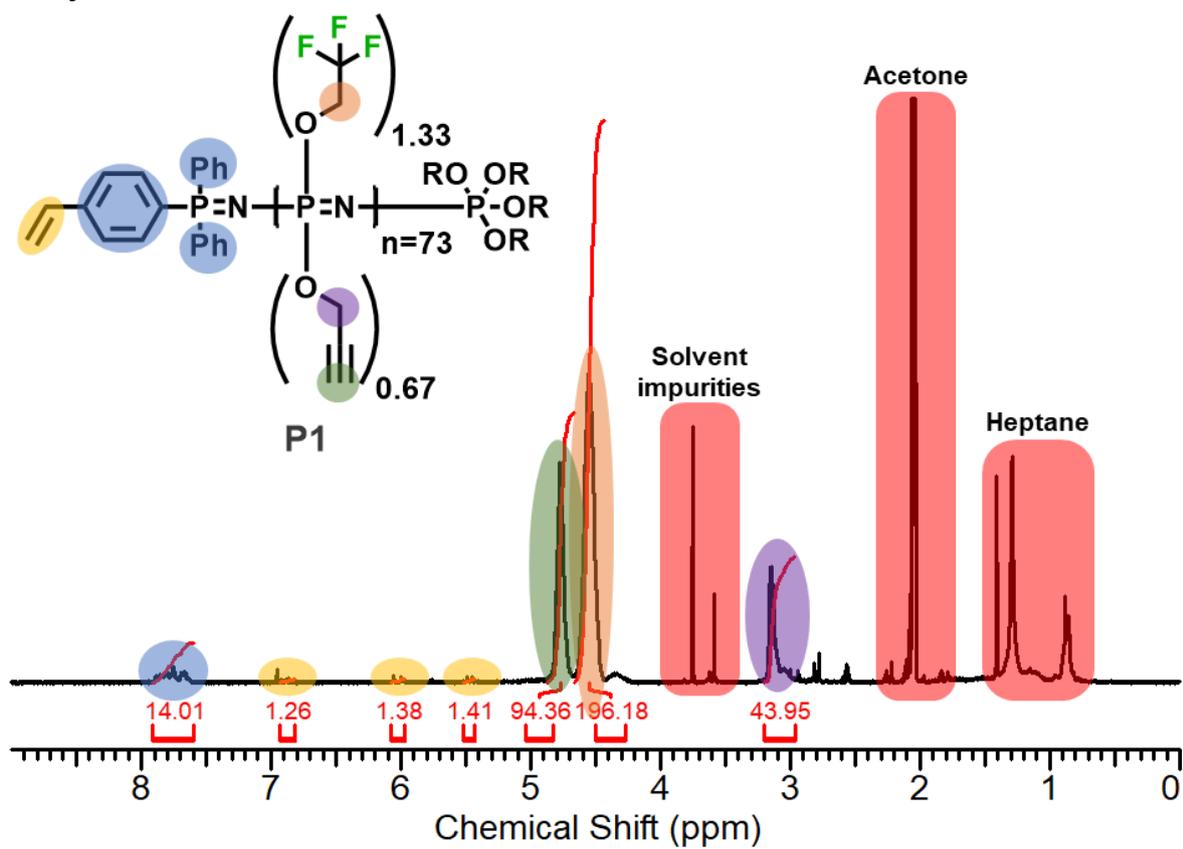


Figure S1: ¹H-NMR spectrum of TFE-Propargyl-PPz P1 in (CD₃)₂CO, including peak assignment.

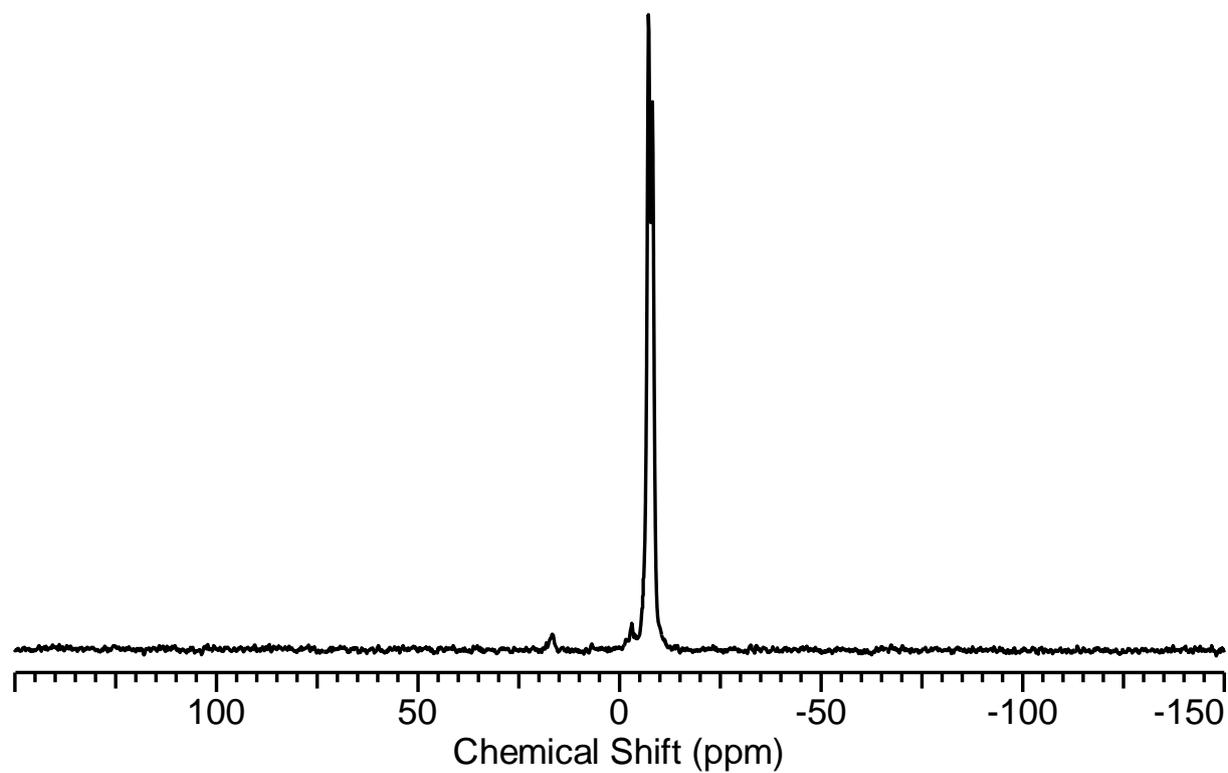


Figure S2: ³¹P-NMR spectrum of TFE-Propargyl-PPz P1 in (CD₃)₂CO.

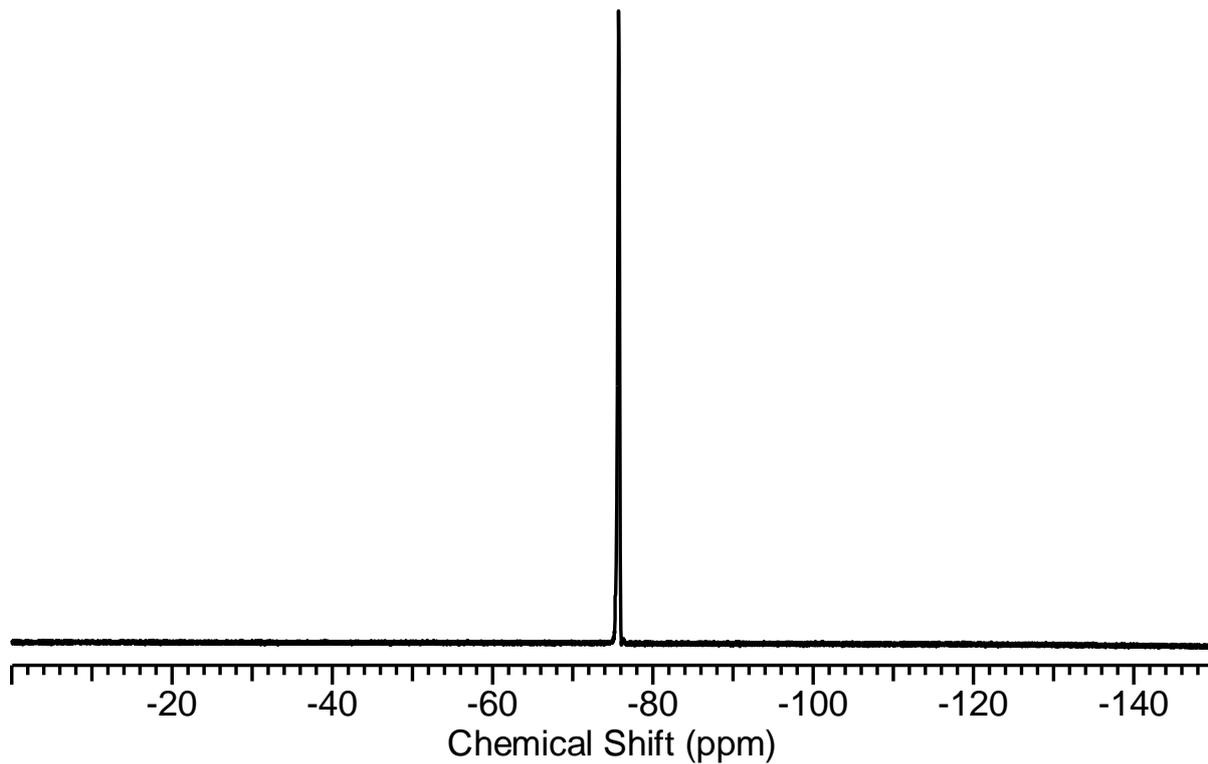


Figure S3: ^{19}F -NMR spectrum of TFE-Propargyl-PPz P1 in $(\text{CD}_3)_2\text{CO}$.

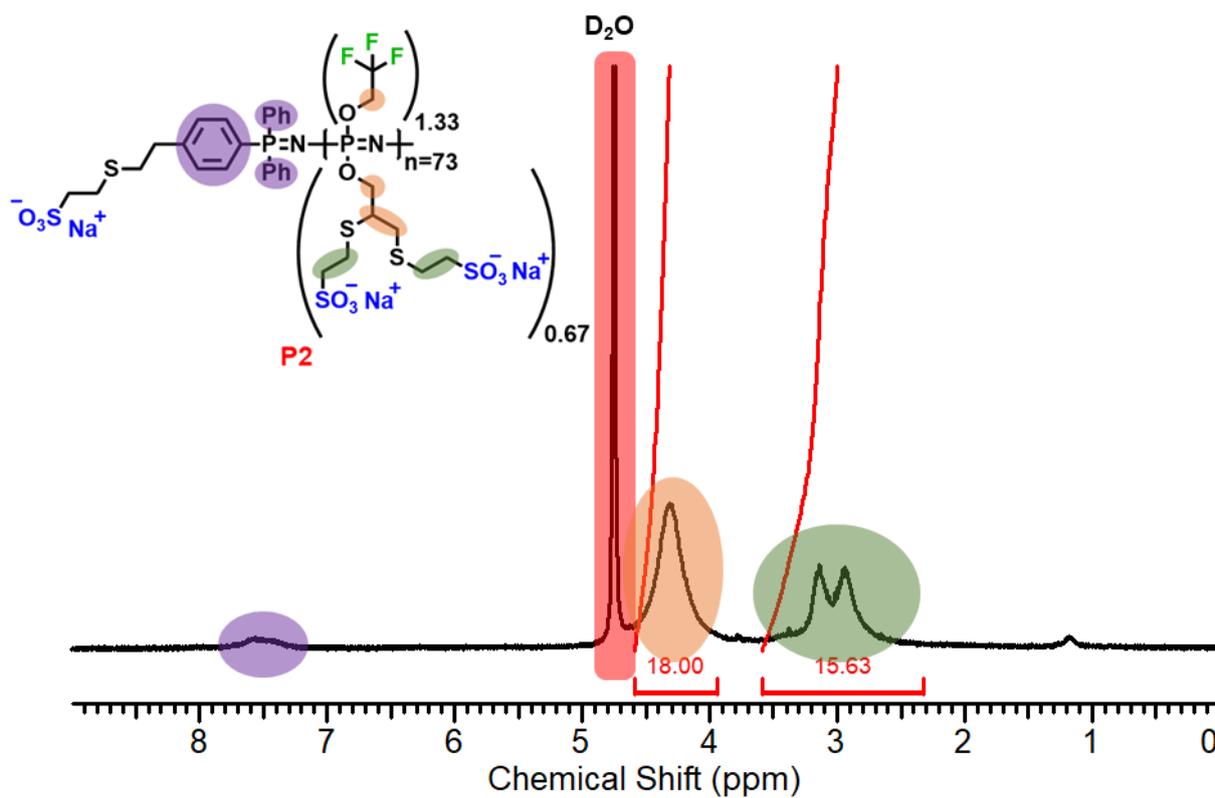


Figure S4: ^1H -NMR spectrum of TFE-MESNa-PPz P2 in D_2O .

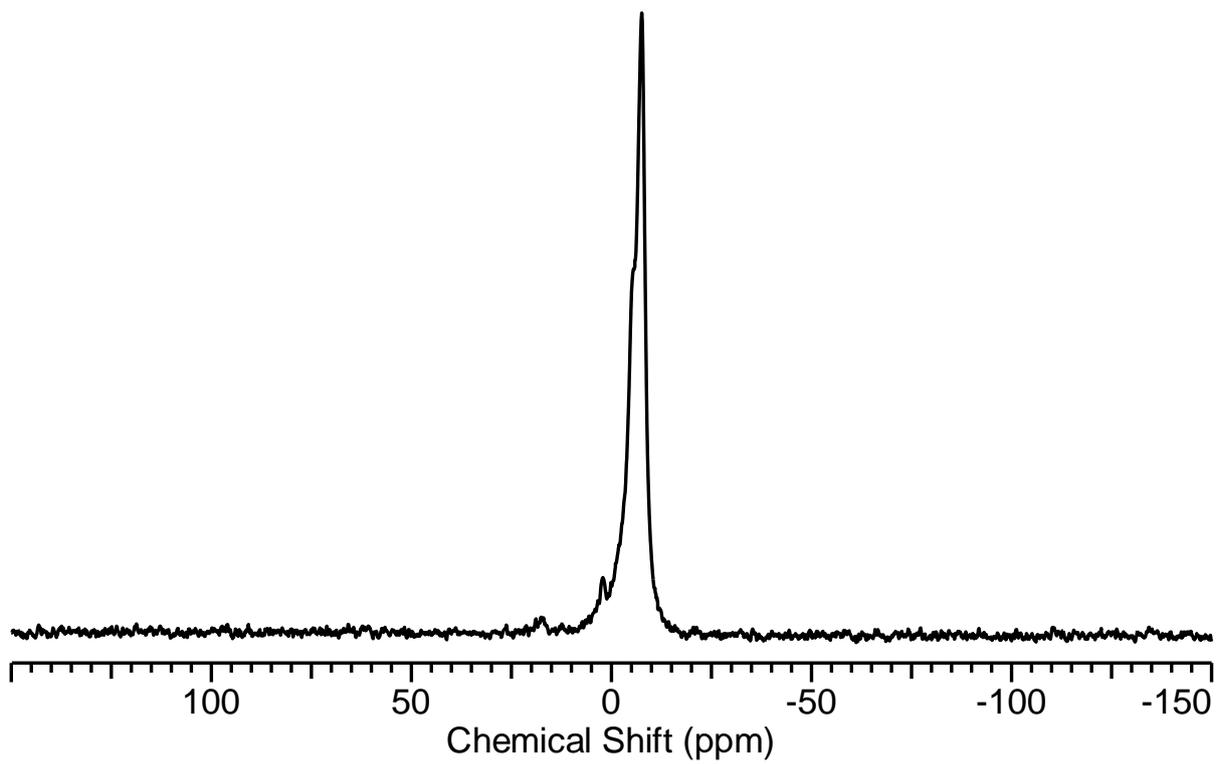


Figure S5: ^{31}P -NMR spectrum of TFE-MESNa-PPz P2 in D_2O .

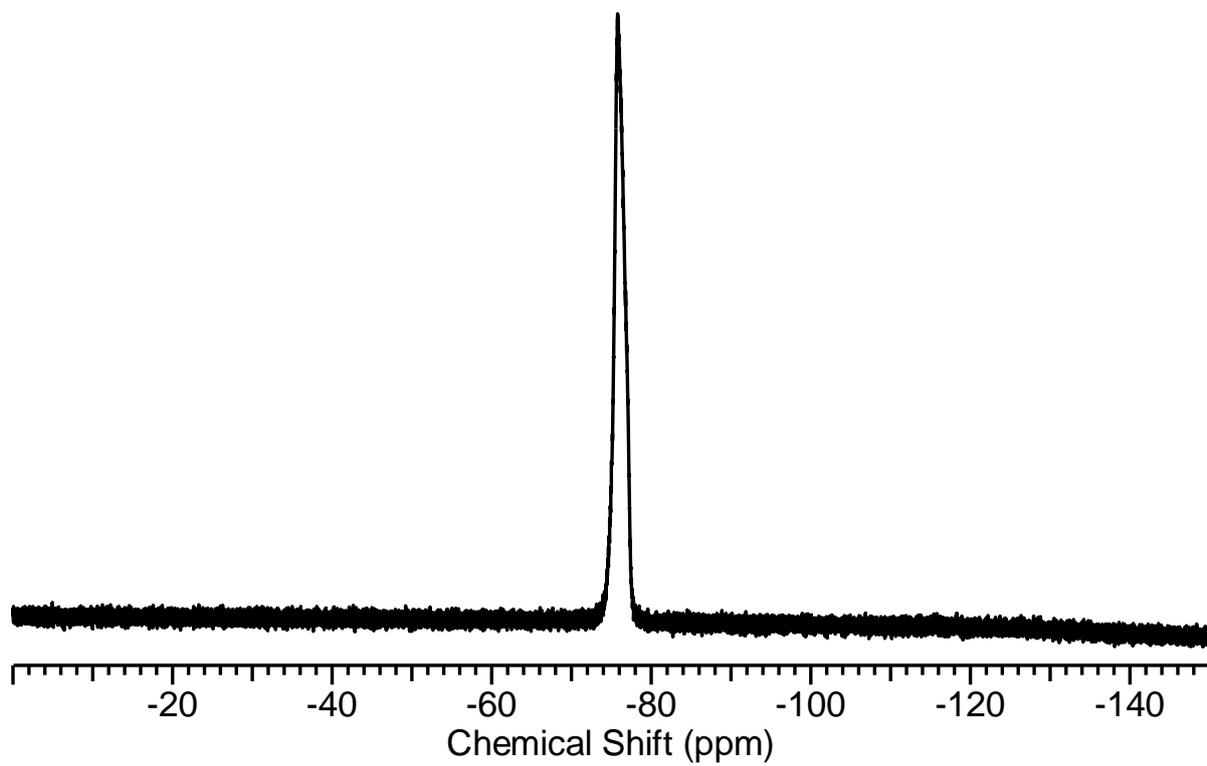


Figure S6: ^{19}F -NMR spectrum of TFE-MESNa-PPz P2 in D_2O .

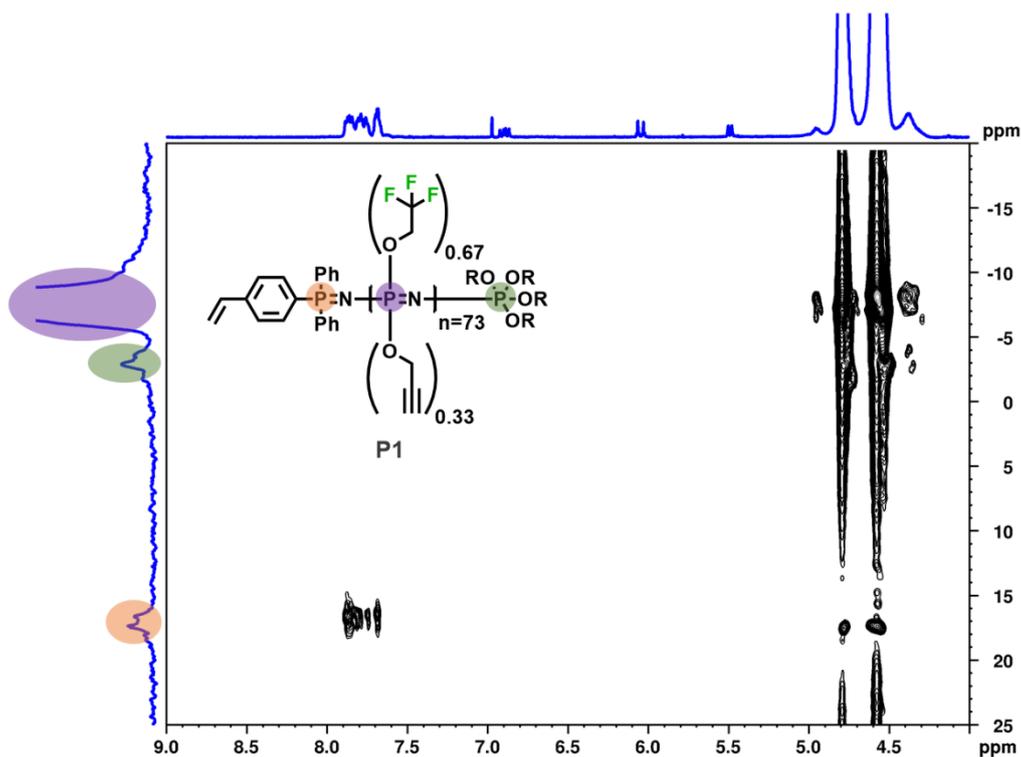


Figure S7. ^1H - ^{31}P – heteronuclear multiple bond correlation (HMBC) spectrum of TFE-Propargyl-PPz **P1** in $(\text{CD}_3)_2\text{CO}$. The spectrum confirms a correlation between the aromatic protons and the phosphorus atom of the phosphine end-group at around 17 ppm (orange). Additionally, the phosphorus signal at around -7.5 ppm can be assigned to the repeating units of the polymer (violet) and the signal at around -2.8 ppm to the opposite chain end (green).

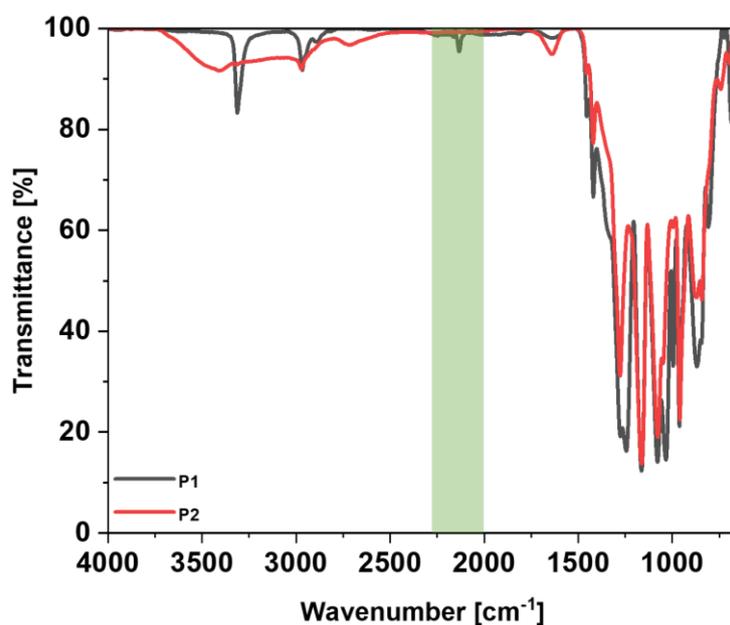


Figure S8: FT-IR spectra of TFE-Propargyl-PPz **P1** and TFE-MESNa-PPz **P2** showing complete disappearance of the signal corresponding to the triple bond at around 2130 cm^{-1} , highlighted in green.

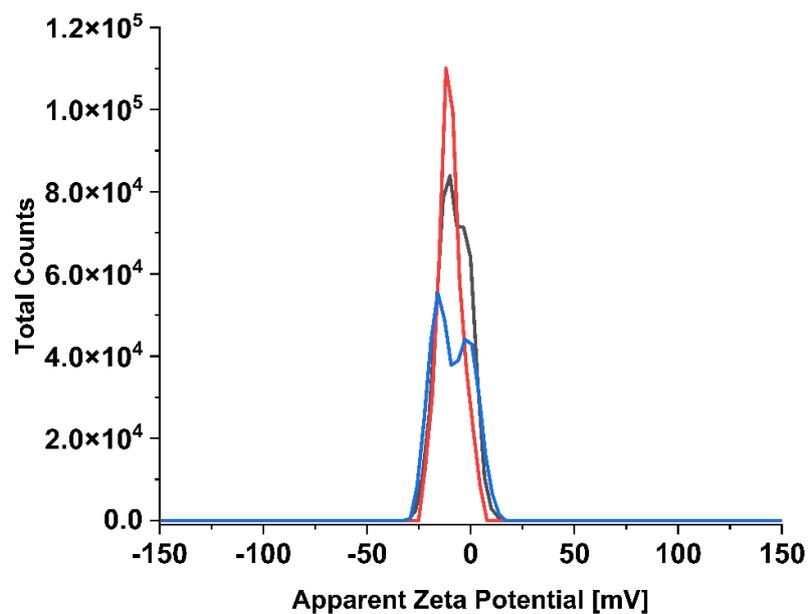


Figure S9: Evaluation of zeta-potential of TFE-MESNa-PPz. Measurement was carried out in triplicates (blue, black and red) and in nanopure water as a dispersant (viscosity = 0.8872 cP and refractive index, RI = 1.330) after calibration with Zeta Potential Transfer Standard ($-40 \text{ mV} \pm 5.8 \text{ mV}$) showing an average ζ -potential of $-12.5 \text{ mV} \pm 0.8 \text{ mV}$.

MRI evaluation:

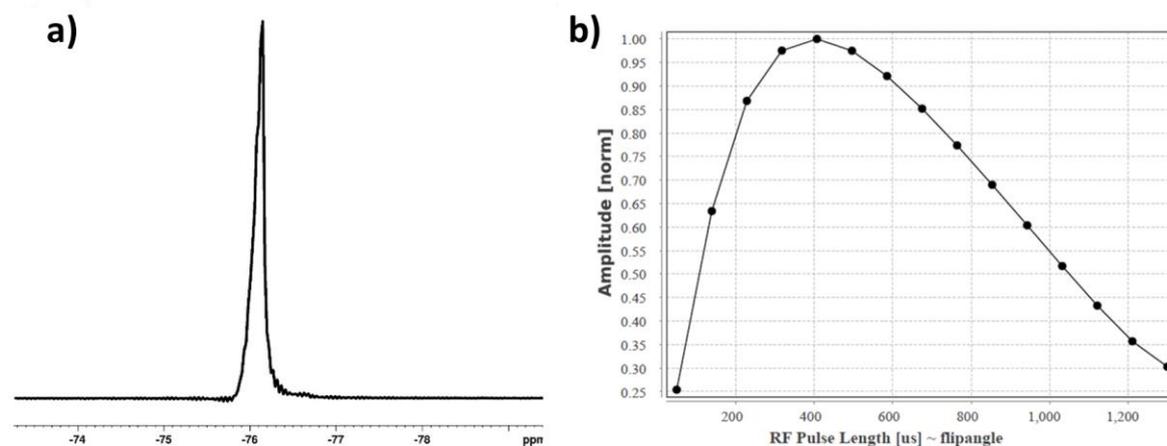


Figure S10: Flip angle graph for TFA as a positive control: a) Isolated peak of TFA in a ^{19}F -spectrum recorded via an ISIS spectroscopy sequence. b) Dependence of the signal amplitude of TFA at -76.1 ppm on radio frequency pulse length, as determined by the AdjRefPowX procedure, showing the maximum at a pulse length of 407.243 μs .

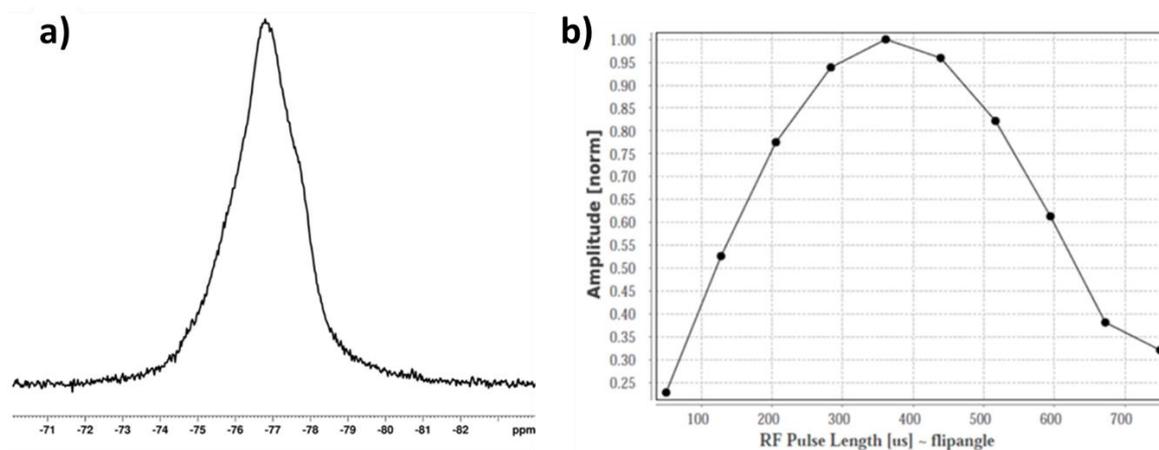


Figure S11: Evaluation of the 90-degree flip angle of P2. a) Isolated peak of P2 in a ^{19}F -spectrum recorded via an ISIS spectroscopy sequence. b) Dependence of the signal amplitude of P2 at -76.7 ppm on radio frequency pulse length, as determined by the AdjRefPowX procedure, showing the maximum at a pulse length of 361.111 μs .

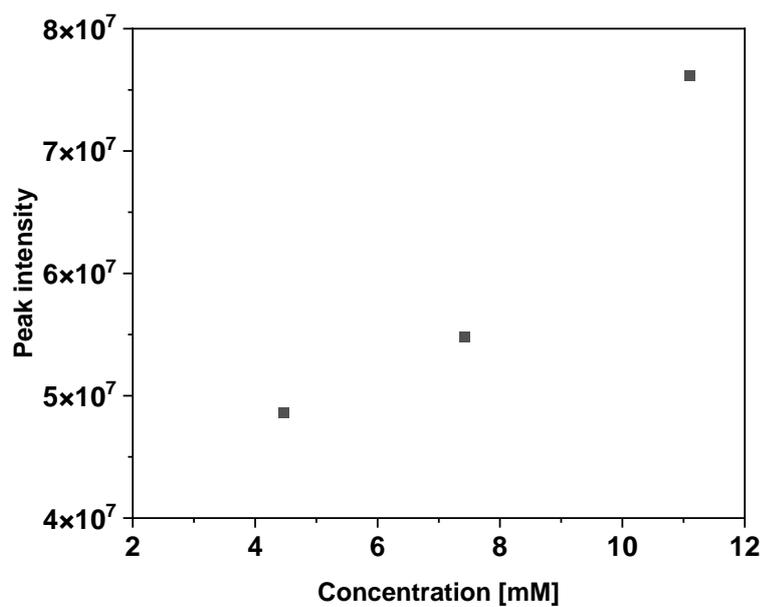


Figure S12: Quantitative evaluation of TFE-MESNa-PPz by MRS, based on the arbitrary peak intensity at -76.6 ppm in the respective ^{19}F -spectra using an ISIS spectroscopic sequence.