

# Supporting Information

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

**Paul Strasser <sup>1</sup>, Verena Schinegger <sup>1</sup>, Joachim Friske <sup>2</sup>, Oliver Brüggemann <sup>1</sup>, Thomas H. Helbich <sup>2</sup>,  
Ian Teasdale <sup>1,\*</sup> and Irena Pashkunova-Martic <sup>2,\*</sup>**

<sup>1</sup> Institute of Polymer Chemistry, Johannes Kepler University Linz, Altenberger Straße 69,  
A-4040 Linz, Austria

<sup>2</sup> Department of Biomedical Imaging and Image-Guided Therapy, Division of Structural and Molecular  
Preclinical Imaging, Medical University of Vienna and General Hospital of Vienna, 18–20 Währinger  
Gürtel, 1090 Vienna, Austria

\* Correspondence: [ian.teasdale@jku.at](mailto:ian.teasdale@jku.at) (I.T.); [irena.pashkunova-martic@meduniwien.ac.at](mailto:irena.pashkunova-martic@meduniwien.ac.at) (I.P.-M.)

## Polymer Characterization:

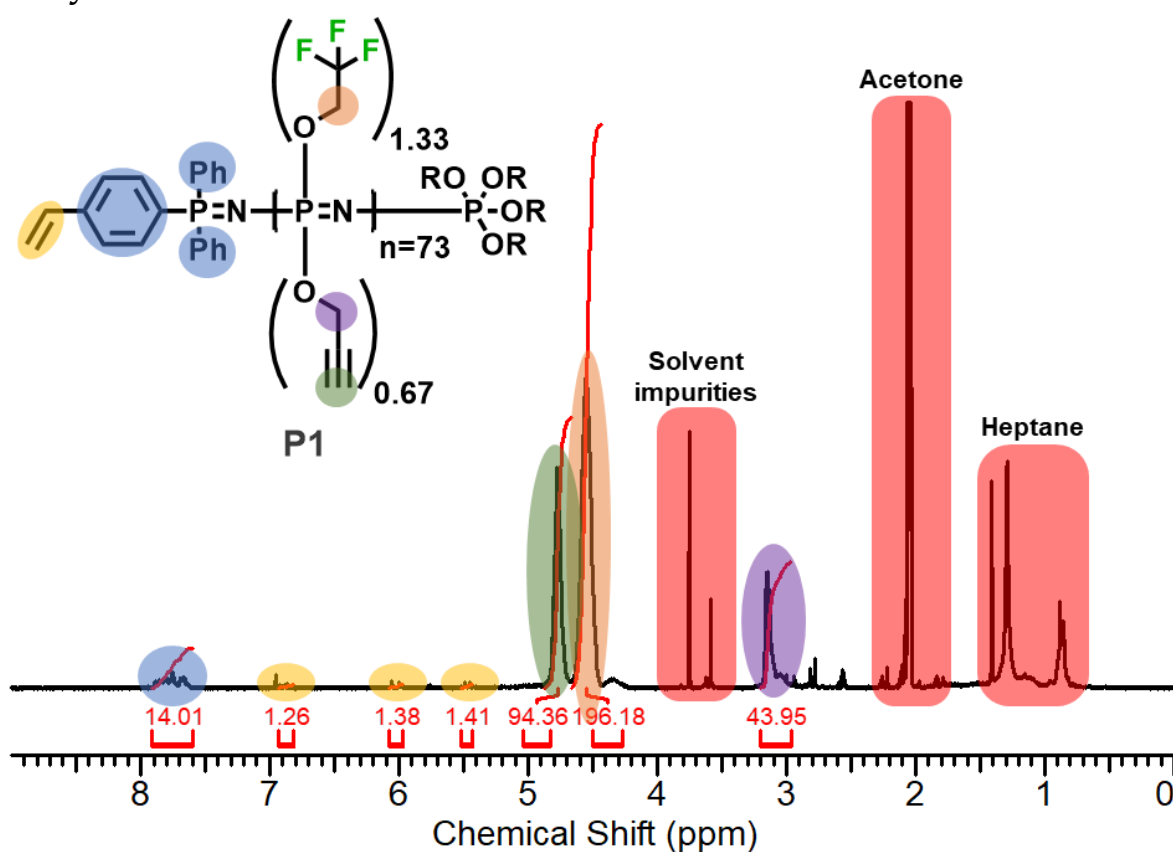


Figure S1:  $^1\text{H}$ -NMR spectrum of TFE-Propargyl-PPz **P1** in  $(\text{CD}_3)_2\text{CO}$ , including peak assignment.

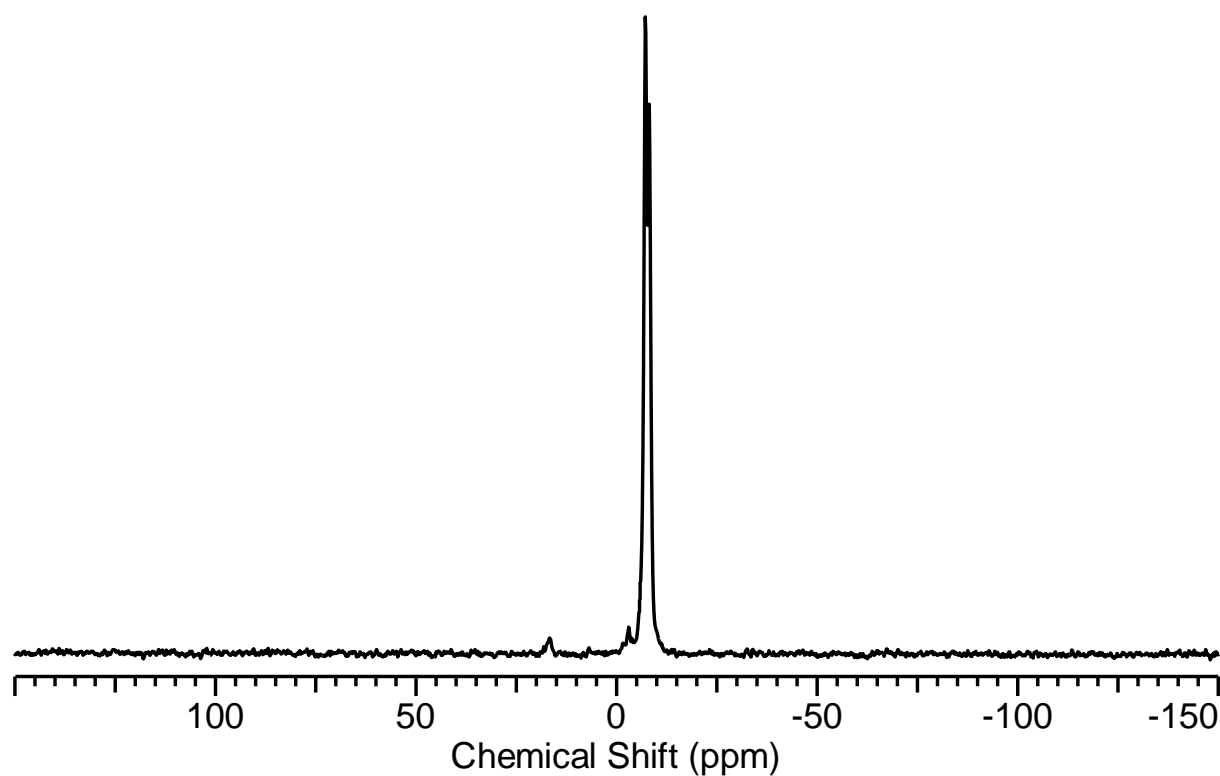


Figure S2:  $^{31}\text{P}$ -NMR spectrum of TFE-Propargyl-PPz **P1** in  $(\text{CD}_3)_2\text{CO}$ .

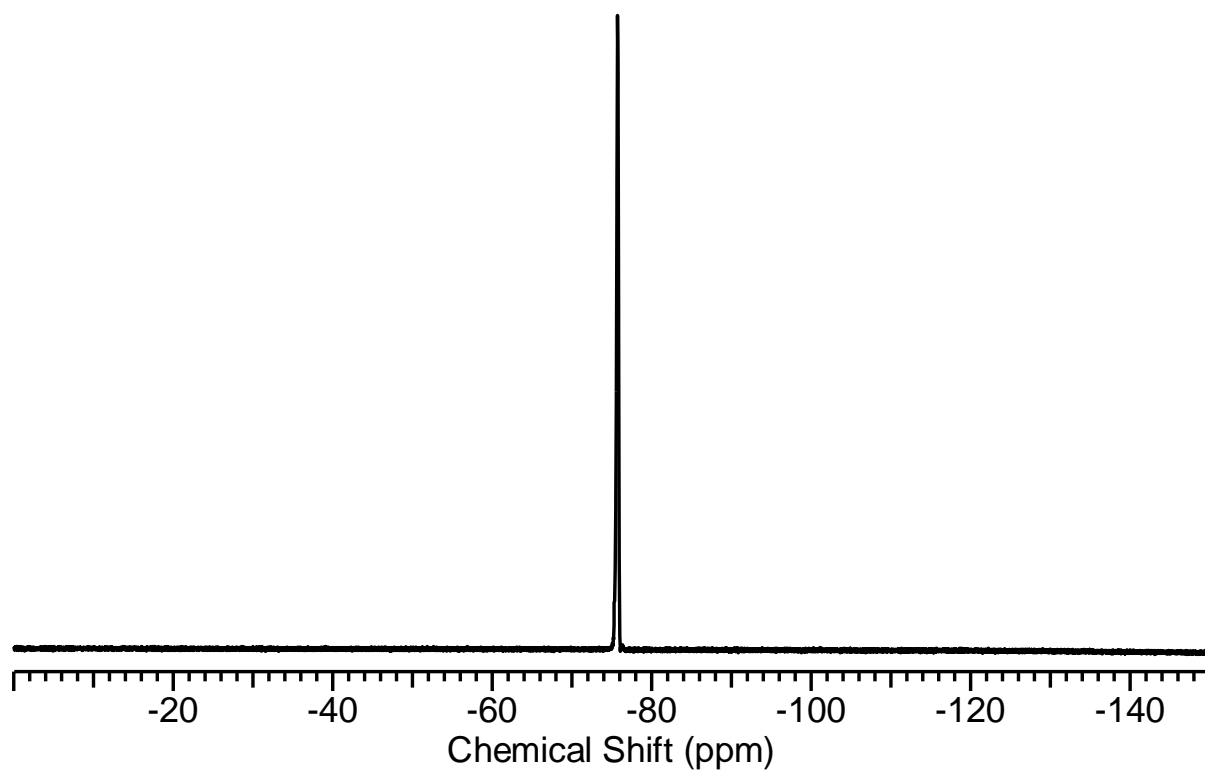


Figure S3:  $^{19}\text{F}$ -NMR spectrum of TFE-Propargyl-PPz **P1** in  $(\text{CD}_3)_2\text{CO}$ .

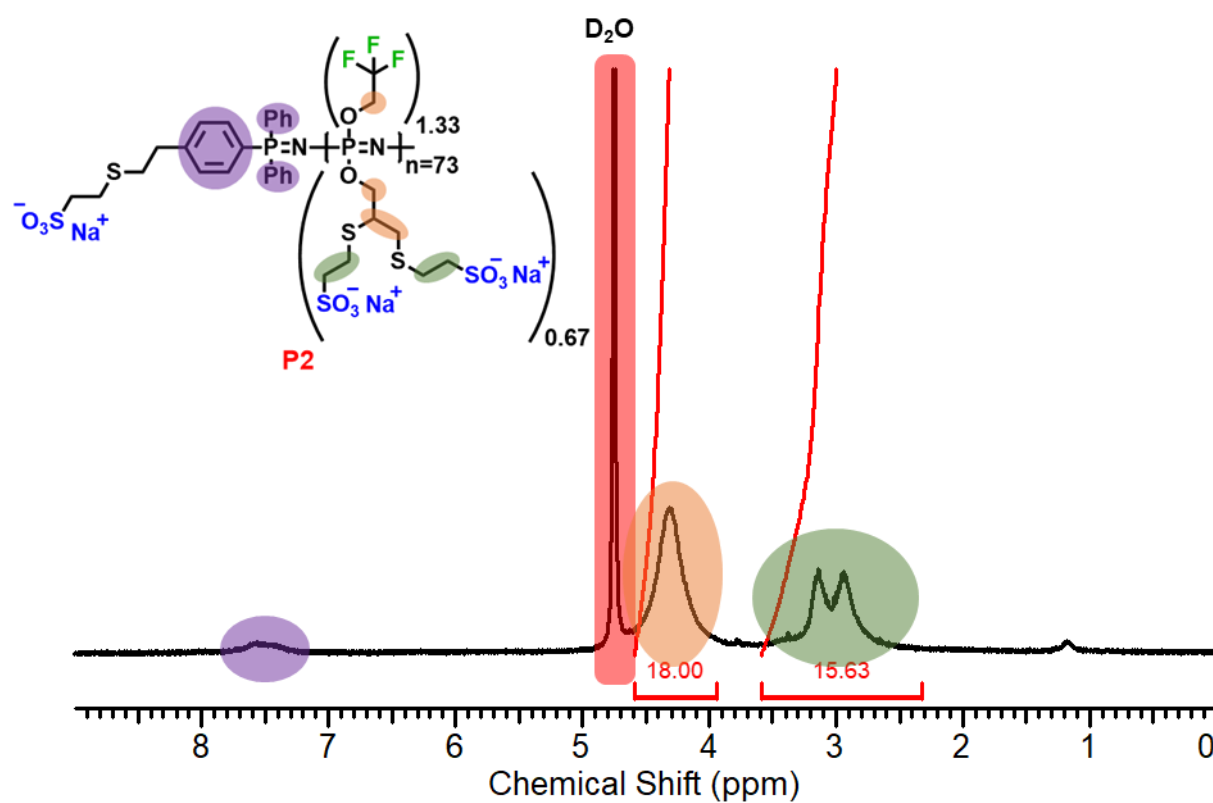


Figure S4:  $^1\text{H}$ -NMR spectrum of TFE-MESNa-PPz **P2** in  $\text{D}_2\text{O}$ .

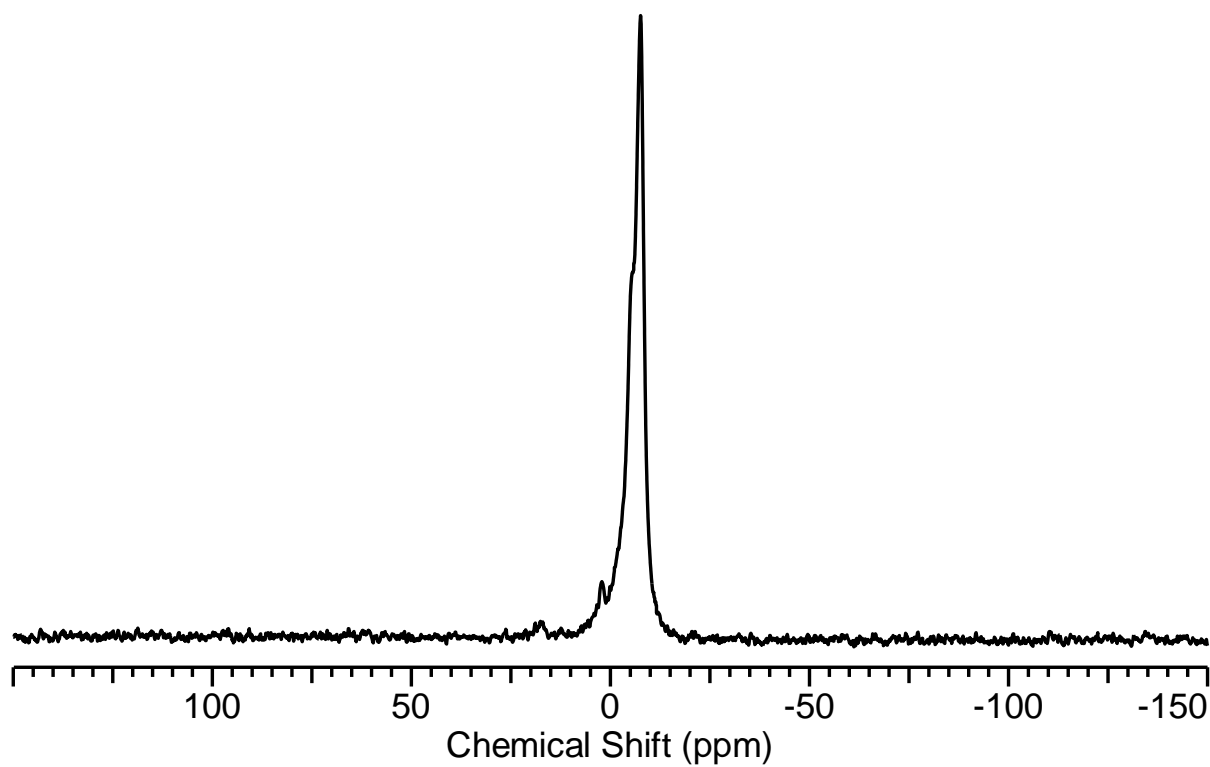


Figure S5:  $^{31}\text{P}$ -NMR spectrum of TFE-MESNa-PPz **P2** in  $\text{D}_2\text{O}$ .

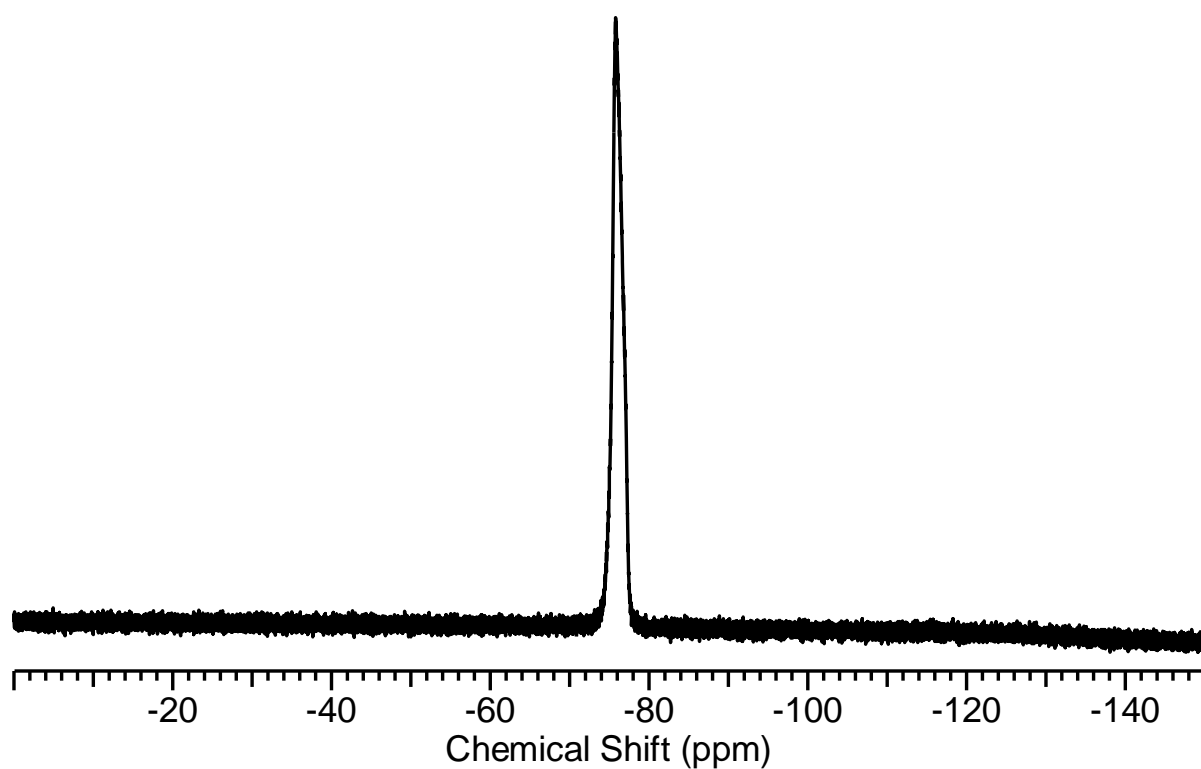


Figure S6:  $^{19}\text{F}$ -NMR spectrum of TFE-MESNa-PPz **P2** in  $\text{D}_2\text{O}$ .

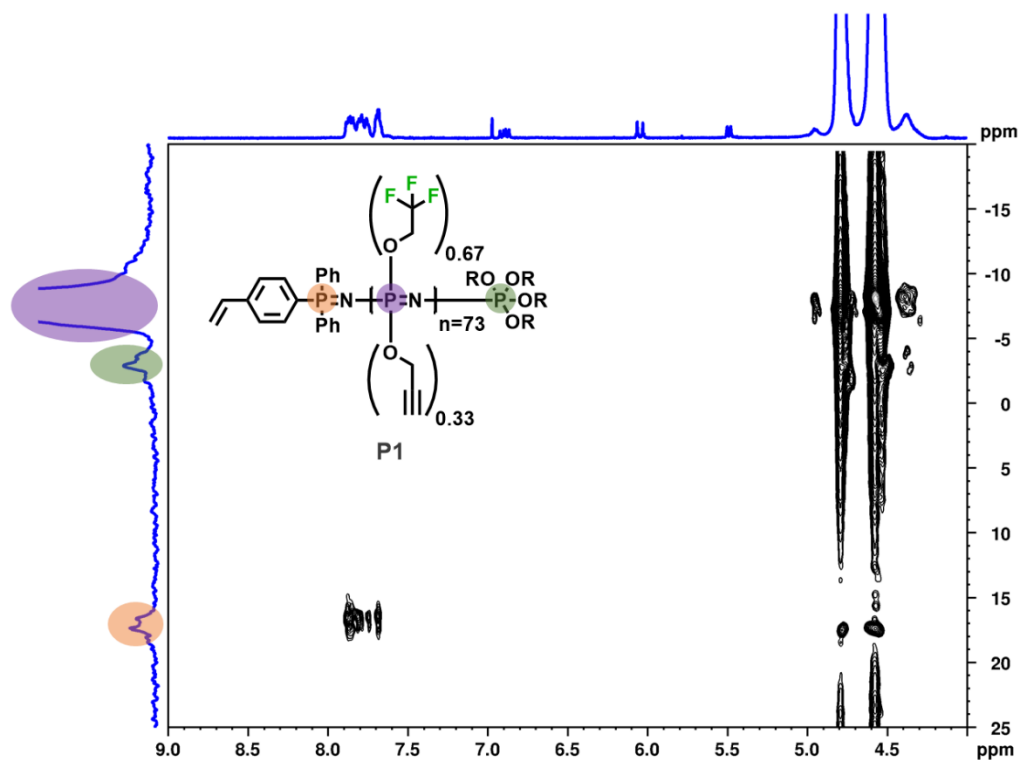


Figure S7.  $^1\text{H}$ - $^{31}\text{P}$  – heteronuclear multiple bond correlation (HMBC) spectrum of TFE-Propargyl-PPz **P1** in  $(\text{CD}_3)_2\text{CO}$ . The spectrum confirms a correlation between the aromatic protons and the phosphorus atom of the phosphine end-group at around 17 ppm (orange). 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).

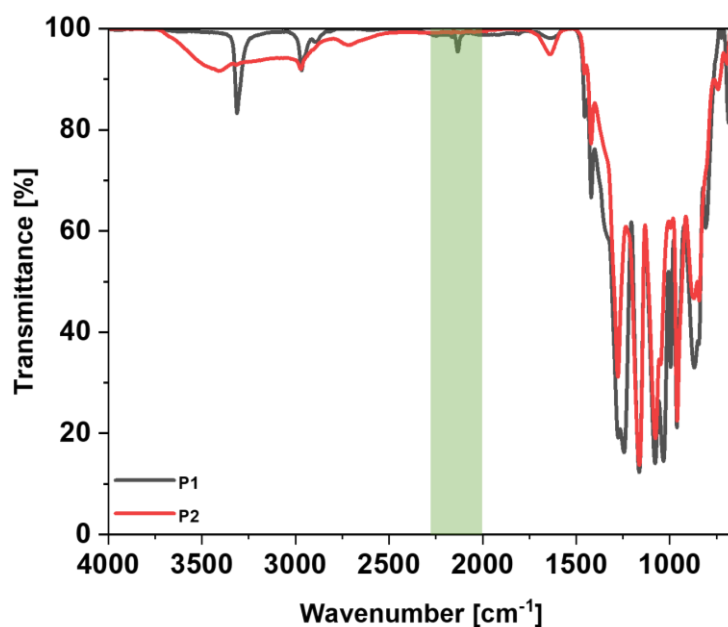


Figure S8: FT-IR spectra of TFE-Propargyl-PPz **P1** and TFE-MESNa-PPz **P2** showing complete disappearance of the signal corresponding to the triple bond at around  $2130\text{ cm}^{-1}$ , highlighted in green.

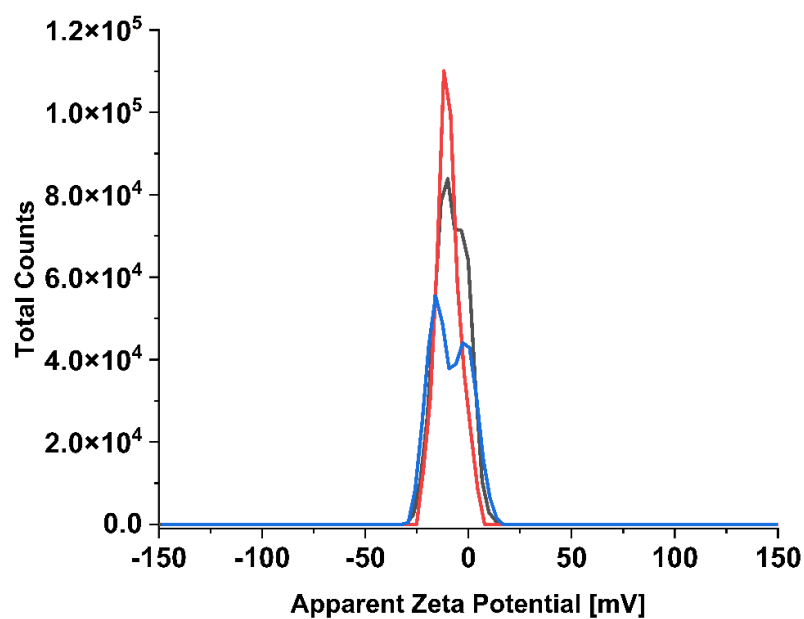


Figure S9: Evaluation of zeta-potential of TFE-MESNa-PPz. Measurement was carried out in triplicates (blue, black and red) and in nanopure water as a dispersant (viscosity = 0.8872 cP and refractive index, RI = 1.330) after calibration with Zeta Potential Transfer Standard ( $-40 \text{ mV} \pm 5.8 \text{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

## MRI evaluation:

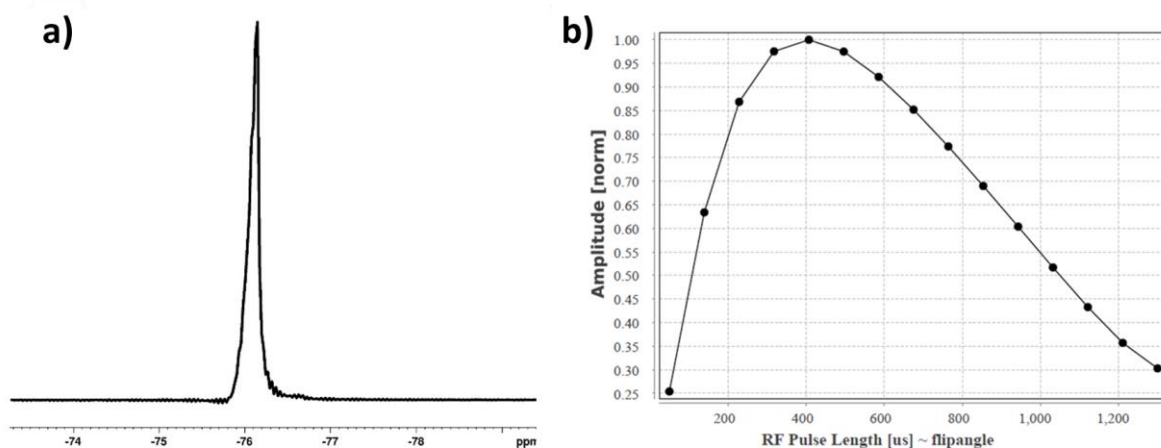


Figure S10: Flip angle graph for TFA as a positive control: a) Isolated peak of **TFA** in a  $^{19}\text{F}$ -spectrum recorded via an ISIS spectroscopy sequence. b) Dependence of the signal amplitude of **TFA** at -76.1 ppm on radio frequency pulse length, as determined by the AdjRefPowX procedure,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

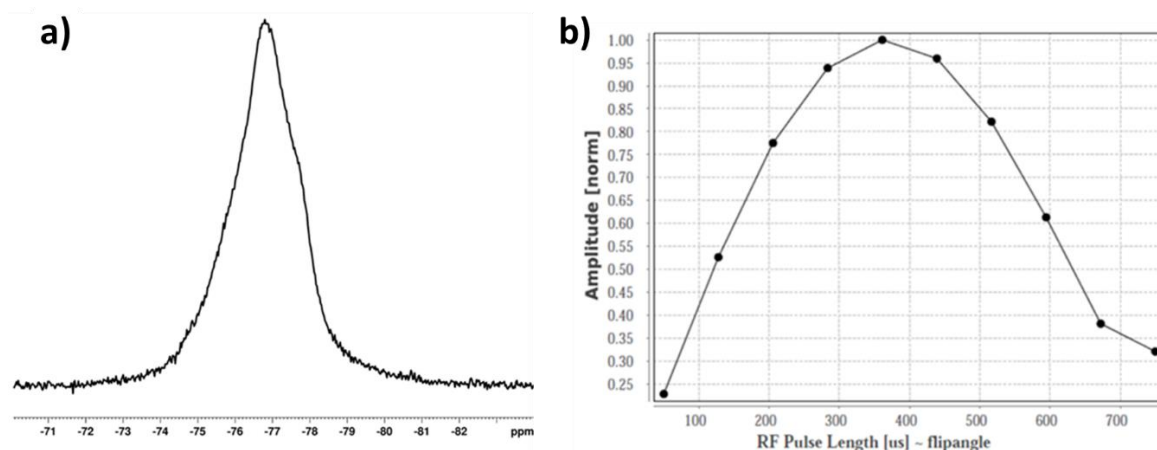


Figure S11: Evaluation of the 90-degree flip angle of **P2**. a) Isolated peak of **P2** in a  $^{19}\text{F}$ -spectrum recorded via an ISIS spectroscopy sequence. b) Dependence of the signal amplitude of **P2** at -76.7 ppm on radio frequency pulse length, as determined by the AdjRefPowX procedure,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

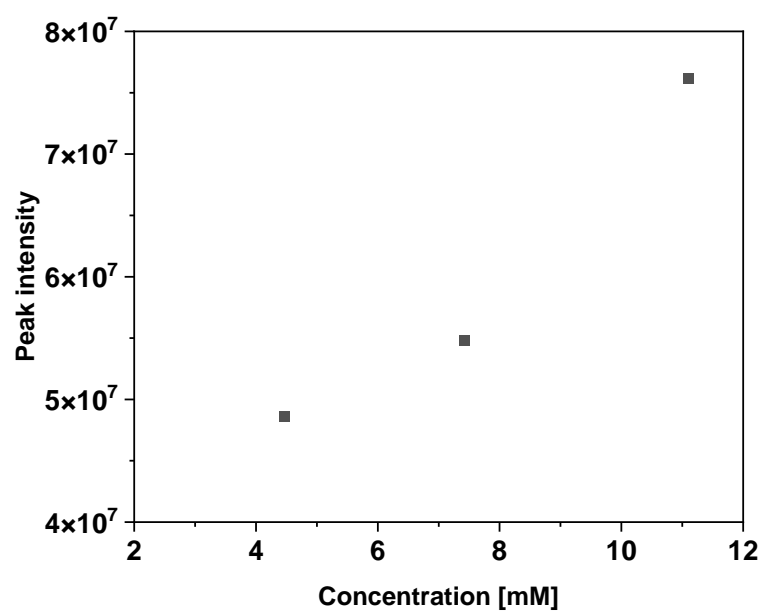


Figure S12: Quantitative evaluation of TFE-MESNa-PPz by MRS, based on the arbitrary peak intensity at  $-76.6$  ppm in the respective  $^{19}\text{F}$ -spectra using an ISIS spectroscopic sequence.