Supplementary Information

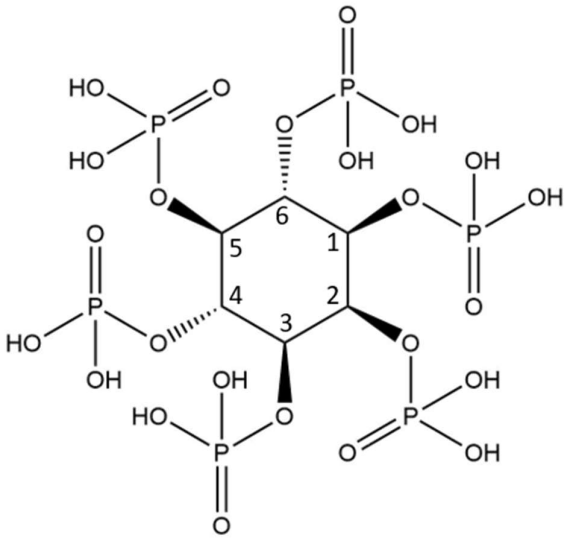

Figure SI-1. Structural formula of *myo*-inositol hexakisphosphate (*myo*-IP_6). The carbon positions of the inositol ring have been identifed (1-6). ChemDraw Professional 17.0, ©PerkinElmer Informatics Inc.

Analysis of *myo*-IP_6 standard

Doolette and Smernik (2018) reported the P impurities of commercially available 'phytate' standards. The authors reported that concentrations of *myo*-IP_6 in the standards ranged from 8 % to 93 % of the P_{tot}. Consequently, the phytate standard (Sigma-Aldrich, product no. P5681) used in this study was analyzed using solution ^{31}P NMR spectroscopy prior to the spiking experiments. The spectrum (Figure SI-2) revealed P impurities similar to that reported by Doolette and Smernik (2018), which comprised 28.97 % of P_{tot} in the purchased standard.

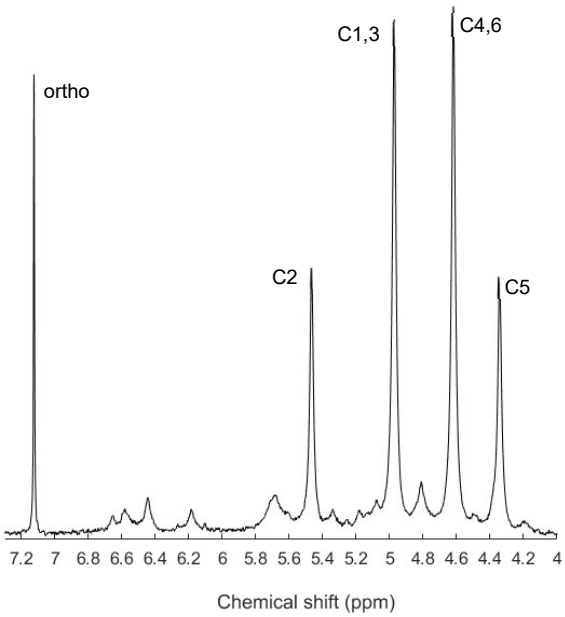

Figure SI-2. Solution ^{31}P NMR spectrum (500 MHz) of *myo*-IP_6 standard (Sigma Aldrich, product no. P5681), 0.2 mg P in 150 µL D2O and 400 µL NaOD. Identified are P peaks of *myo*-IP_6 labeled with corresponding carbons C1-6 and orthophosphate (ortho).

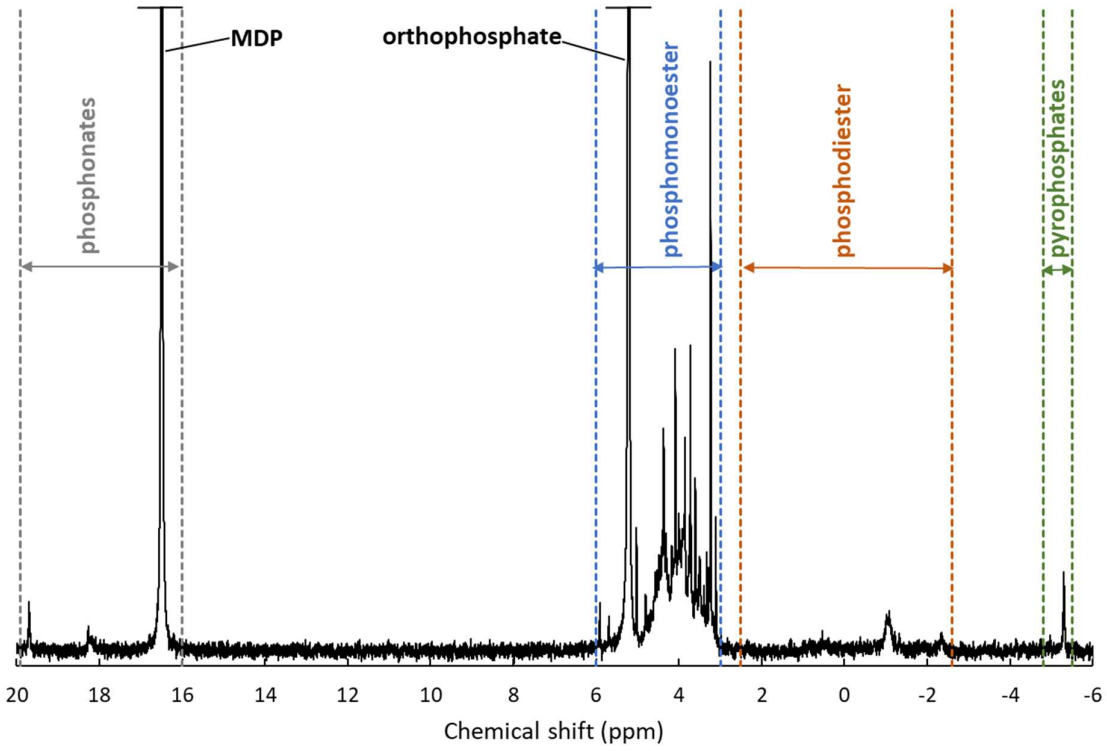

Figure SI-3. Solution ^{31}P NMR spectrum (500 MHz) of 0.25 M NaOH + 0.05 M EDTA soil extract S4 (black) with marked integral regions of phosphonates, phosphomonoester, phosphodiester and pyrophosphates. Signal intensities were normalized to the MDP peak intensity and the vertical axis has been increased by factor 2.

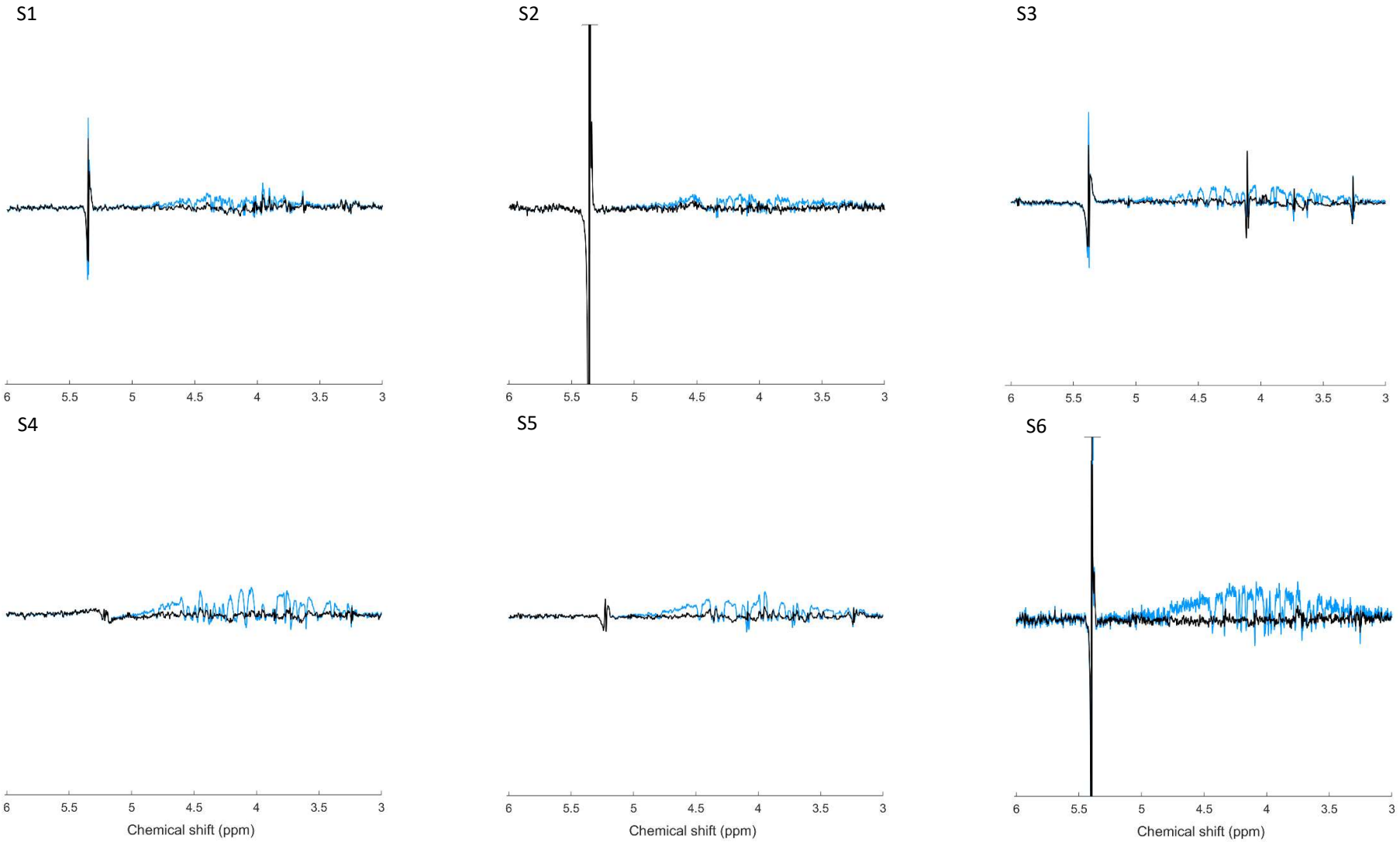

Figure SI-4. Residues of the spectral deconvolution fitting (SDF) procedure of solution ^{31}P NMR spectra of unspiked 0.25 M NaOH + 0.05 M EDTA soil extracts. The residues of the SDF approach including an underlying broad signal are shown in black and the approach without an underlying broad signal in blue. Residue intensities were normalized to the MDP peak intensity and the vertical axes of the spectra have been increased by a factor of 1.7 for soils S3, S4 and S5, and by a factor of 10 for soils S1, S2 and S6 for direct comparison with the initial soil spectra before SDF (Figure 2).

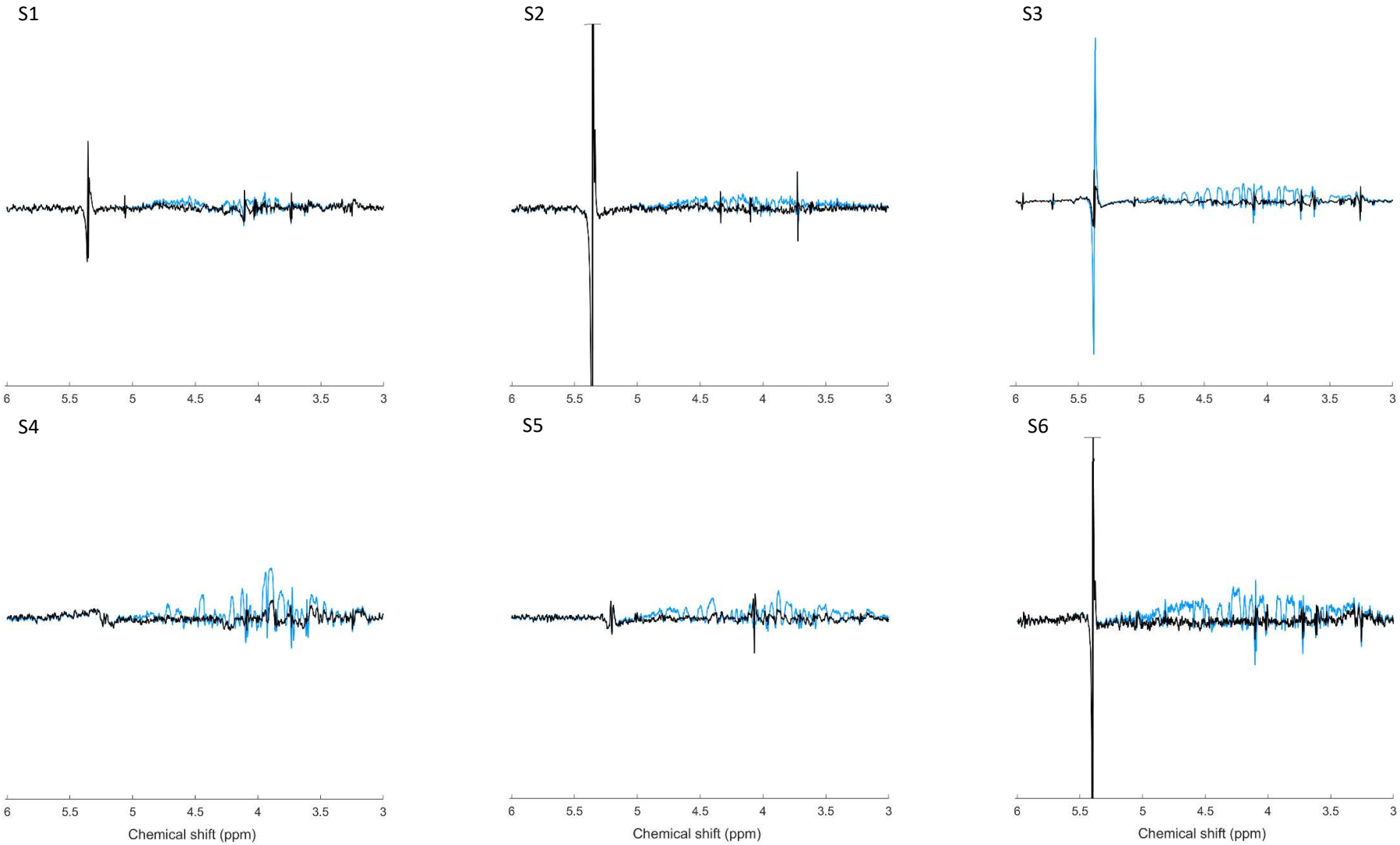

Figure SI-5. Residues of the spectral deconvolution fitting (SDF) procedure of solution ^{31}P NMR spectra of spiked 0.25 M NaOH + 0.05 M EDTA soil extracts. The residues of the SDF approach including an underlying broad signal are shown in black and the approach without an underlying broad signal in blue. Residue intensities were normalized to the MDP peak intensity and the vertical axes of the spectra have been increased by a factor of 1.7 for soils S3, S4 and S5, and by a factor of 10 for soils S1, S2 and S6 for direct comparison with the initial soil spectra before SDF (Figure 2).

Table SI-1. Goodness of fit parameters of the spectral deconvolution fitting carried out with the non-linear optimization algorithm in MATLAB®. The Root-mean-square fitting error, R^2 and Chi^2 for the fitted spectra with and without an underlying broad signal are listed. Chi^2 was calculated using the chemical shift range from δ 5.2 to 3.0 ppm in order to avoid the domination of the orthophosphate peak and its residuals in the calculations. The variances of the 'noise' of the spectra were calculated over the chemical shift range δ 14.1 to 8.1 ppm.

	With underlying broad signal			Without underlying broad signal		
Soil	**Root-mean-square fitting error**	**R^2**	**Chi^2**	**Root-mean-square fitting error**	**R^2**	**Chi^2**
S1	0.33	0.997	4.6	0.40	0.995	19.2
S1 spiked	0.17	0.999	4.4	0.70	0.987	9.0
S2	0.29	0.997	1.7	0.39	0.993	10.5
S2 spiked	0.30	0.997	2.7	0.35	0.996	9.5
S3	0.43	0.988	27.5	0.44	0.988	62.9
S3 spiked	0.43	0.988	16.1	0.44	0.988	151.1
S4	0.23	0.999	4.3	0.56	0.994	52.2
S4 spiked	0.25	0.999	7.5	0.44	0.997	53.1
S5	0.21	0.999	5.5	0.62	0.993	48.5
S5 spiked	0.28	0.999	6.7	0.67	0.993	23.0
S6	0.33	0.994	1.6	0.46	0.985	34.2
S6 spiked	0.34	0.994	2.6	0.40	0.992	21.2

Table SI-2. Chemical shift, linewidth at half height and area of the underlying broad signal as determined by the MATLAB® bootstrap function of the spectral deconvolution fitting procedure. Mean values with standard deviation in parentheses (100 trials).

Soil	**Chemical shift (ppm)**	**Linewidth (Hz)**	**Area (-)**
S1	4.20 (1.1E-06)	162 (3.1E-04)	1130800 (839)
S1 spiked	4.22 (2.5E-03)	162 (8.4E-03)	1144189 (2754)
S2	4.06 (1.2E-03)	212 (8.4E-01)	621167 (1450)
S2 spiked	4.04 (1.1E-03)	219 (7.2E-01)	661114 (1422)
S3	4.10 (2.2E-04)	229 (1.7E-01)	4370326 (2026)
S3 spiked	4.11 (9.9E-04)	202 (1.6E-03)	3644372 (3649)
S4	4.05 (2.0E-04)	217 (5.8E-02)	8564373 (3212)
S4 spiked	4.10 (9.4E-08)	202 (3.7E-05)	9035211 (2375)
S5	4.03 (4.5E-04)	221 (2.3E-01)	7383970 (5627)
S5 spiked	4.04 (1.2E-04)	243 (5.7E-05)	6842632 (3397)
S6	4.10 (2.3E-06)	223 (5.5E-03)	2535481 (846)
S6 spiked	4.15 (4.7E-06)	233 (2.4E-03)	2414768 (1338)