Electronic Supplementary Material (ESI) for MedChemComm.

Supporting Information

Mechanism of thienopyridone and iminothienopyridinedione inhibition of protein phosphatases

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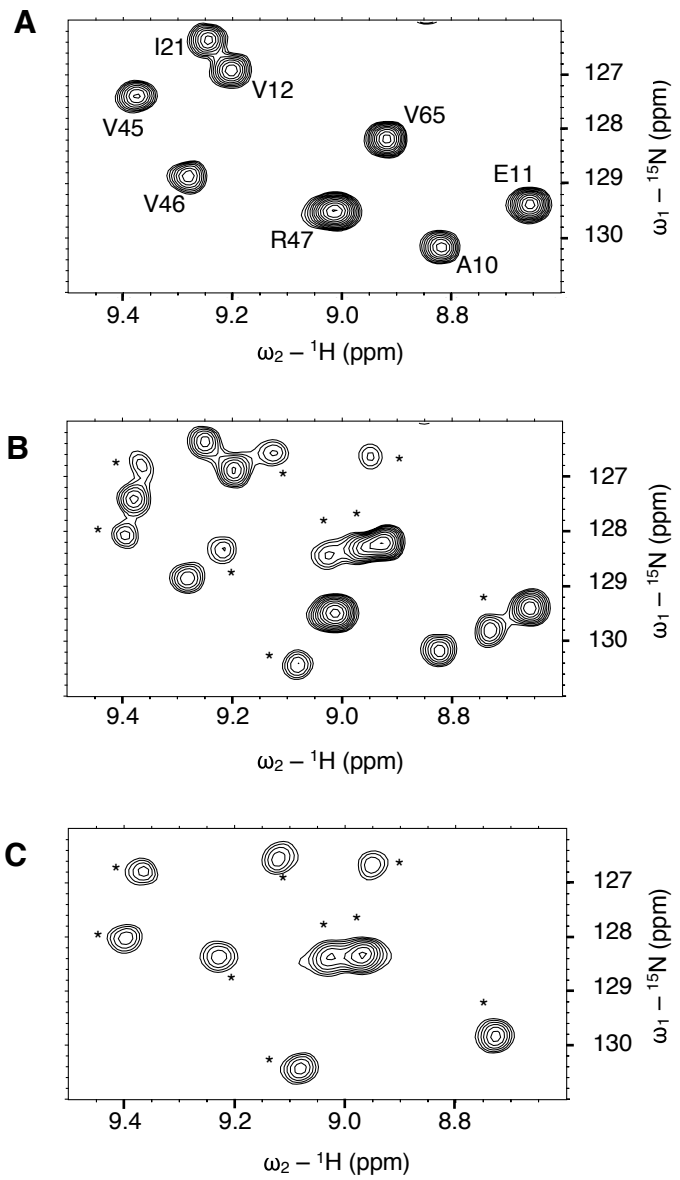

Figure S1. Titration of PRL-3 with TP. ^{15}N-^{1}H correlation spectra of reduced human PRL-3 (0.2 mM) in the absence of TP (A), in the presence of 1:2 (B) and 1:5 (C) ratios of PRL-3 to TP showed no binding. Upon addition of TP, PRL-3 was converted to the oxidized form but no other changes indicative of an interaction were observed. Peaks corresponding to oxidized PRL-3 are marked with asterisks.

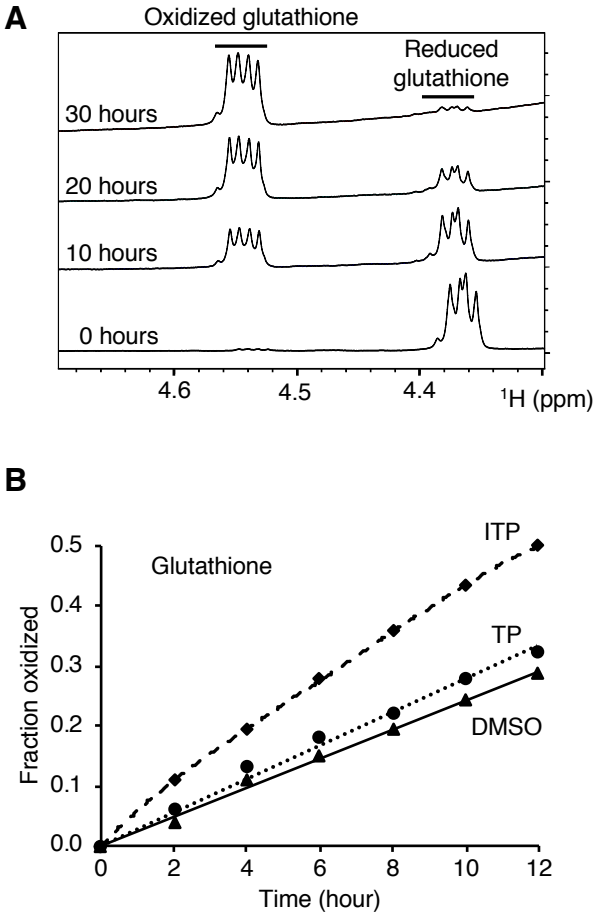

Figure S2. Oxidation of glutathione by TP and ITP. (A) ^{1}H NMR of reduced glutathione (10 mM) incubated with ITP (1 mM) in 80% d6-DMSO and 20% D_2O. (B) Fraction of oxidized glutathione obtained from NMR peak integration showing the increase in oxidation of glutathione.

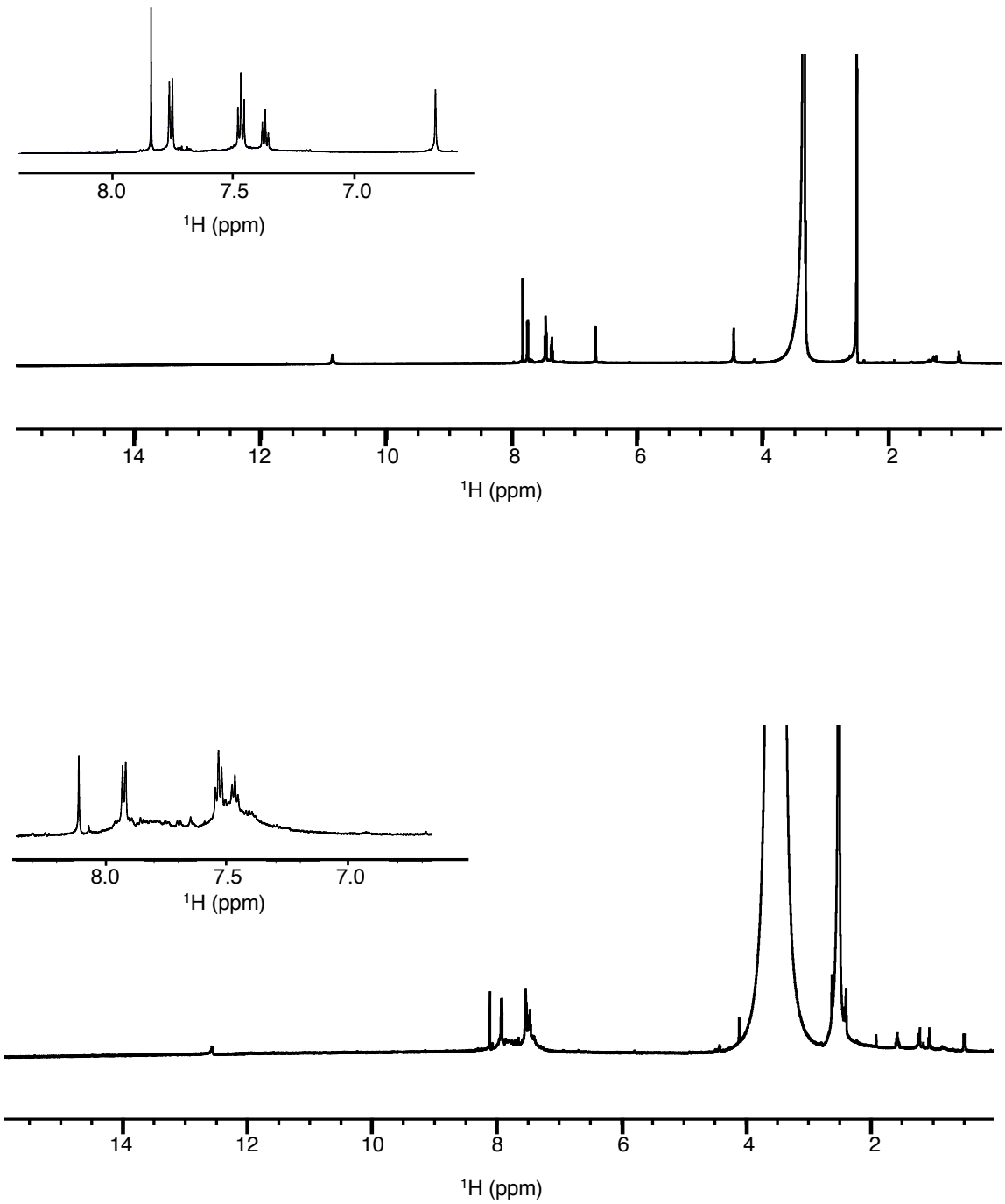

Figure S3. ^{1}H NMR of TP and ITP to confirm identity and purity of the reagents. The 1D NMR spectra were obtained for TP (*upper panel*) and ITP (*lower panel*) in 100% d6-DMSO at 30 ℃.