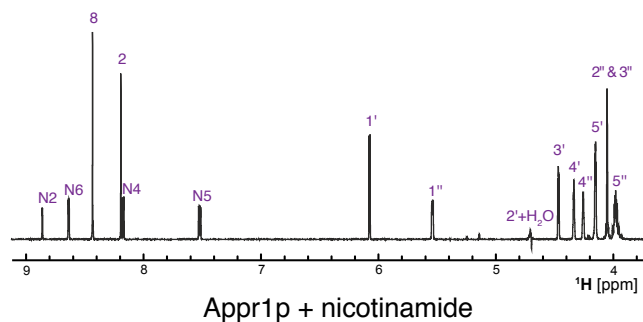
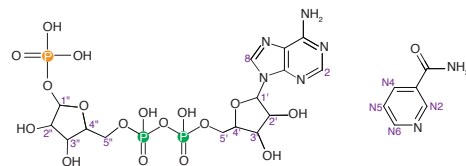
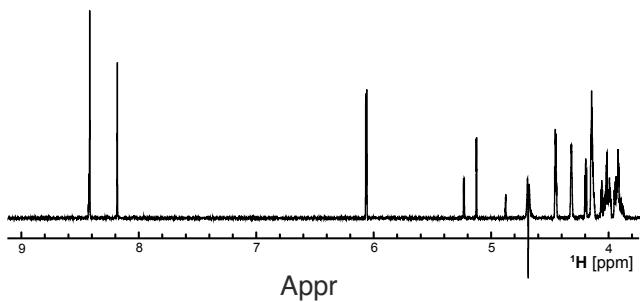
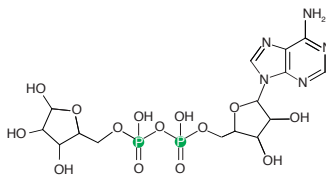
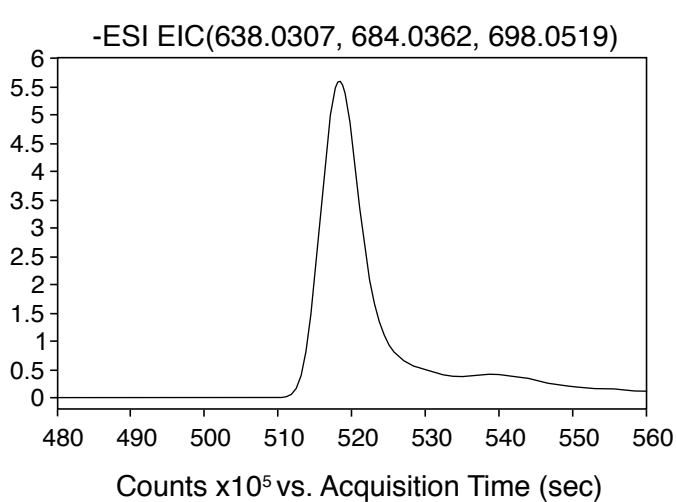
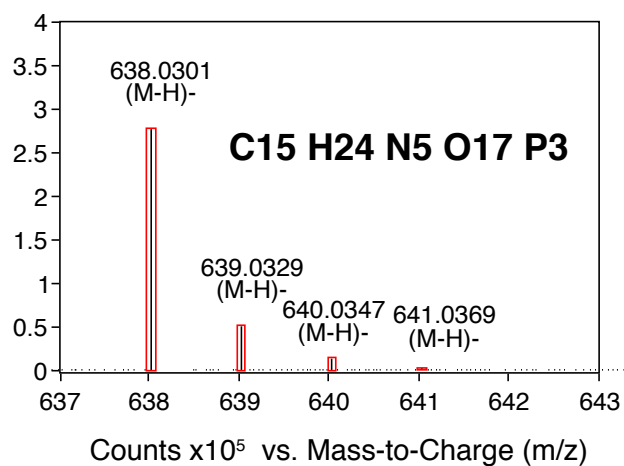
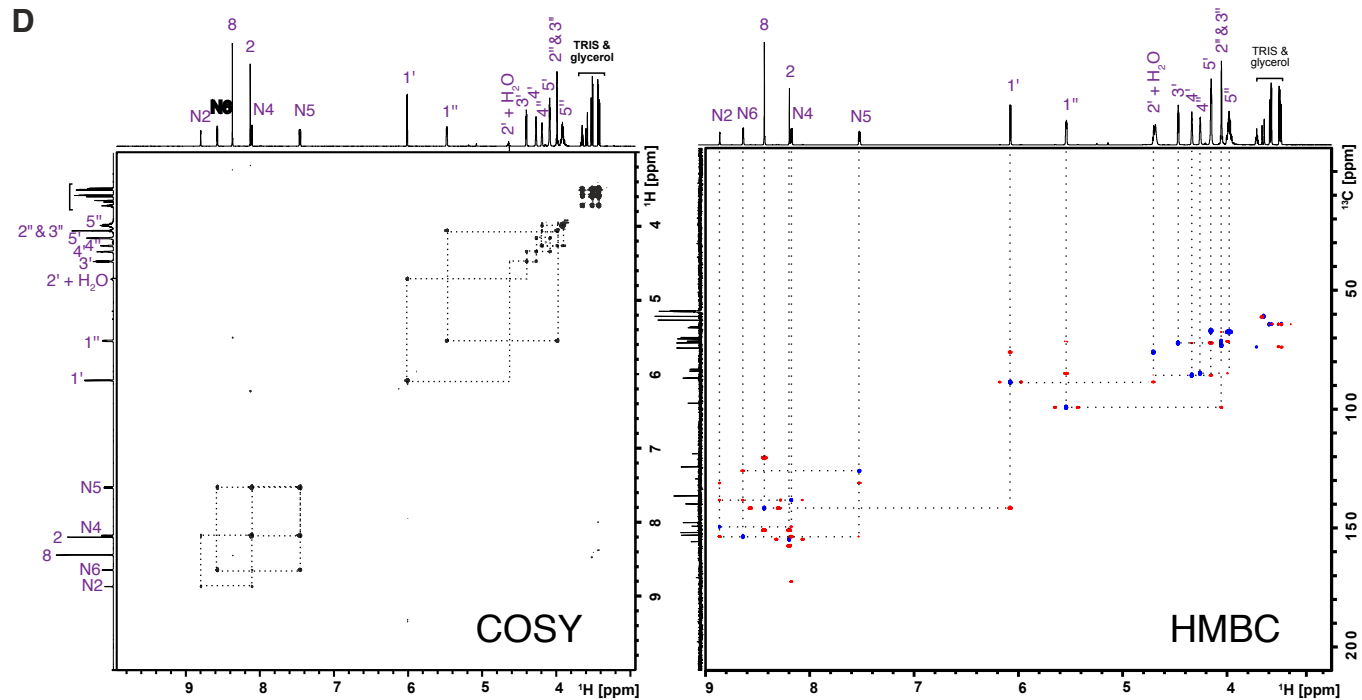


A**B****C****D**

1D and COSY HMBC NMR spectrum. Related to Figure 3.

(A) ^1H NMR spectra of the reaction products of NAD^+ (5 mM) after incubation with MbcT (10 mM) and, for reference, of pure ADP-ribose (5 mM). Reaction conditions were Tris (30 mM), NaCl (200 mM), sodium phosphate (30 mM) in D_2O (pD 7.4). Signals were assigned via the ^1H - ^1H COSY and ^1H - ^{13}C HMBC experiments. Phosphate atoms from the ADP-ribose moiety are coloured green, while the phosphate atom derived from orthophosphate is highlighted in orange.

(B) Extracted ion chromatogram (left) and mass spectrum (right) of the ions with m/z 638.0307, 684.0362 and 698.0519 ascribed to Appr1p (C15 H24 N5 O17 P3).

(C) ^1H - ^1H Correlation spectroscopy (DQF-COSY) and ^1H - ^{13}C Heteronuclear Multiple Bond Correlation (HMBC) experiments of the reaction products of NAD^+ (5 mM) after incubation with MbcT (10 mM) in Tris (30 mM), NaCl (200 mM), sodium phosphate (30 mM) in D_2O (pD 7.4). The HMBC data were acquired with (blue) and without (red) decoupling, the latter optimized for long-range couplings with suppression of one-bond correlations. Phosphate atoms from the ADP-ribose moiety are coloured green, while the phosphate atom derived from orthophosphate is highlighted in orange.