

Fig. S1 Zoomed mass spectra of doubly charged ions, showing their isotopic behaviour.

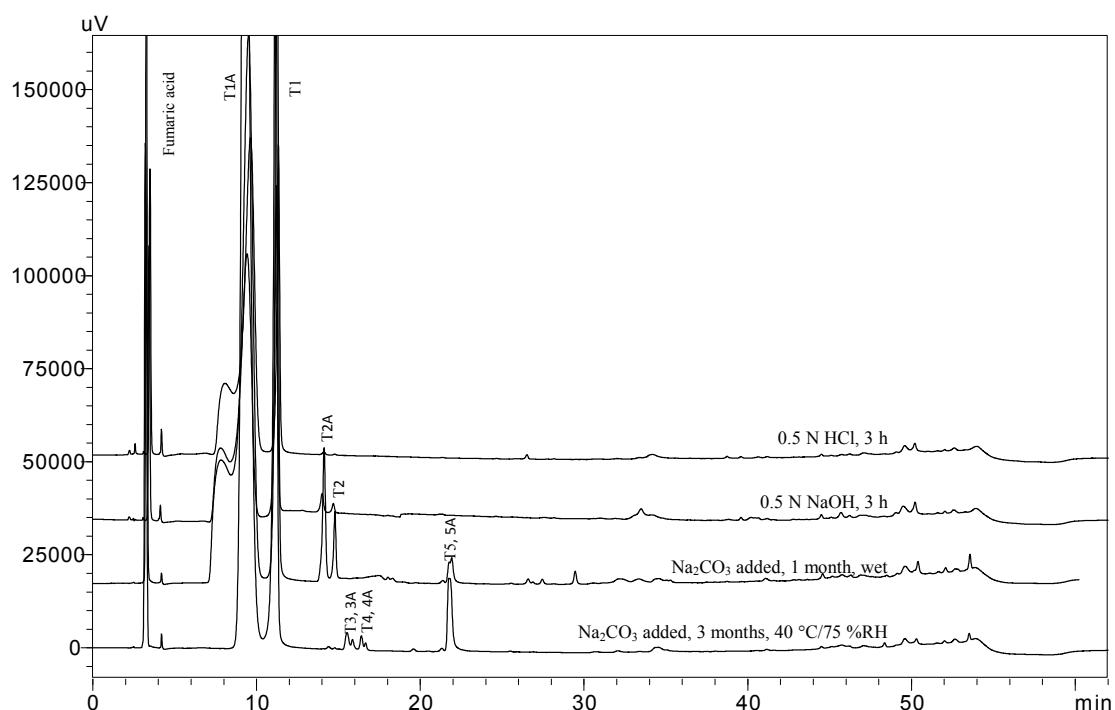
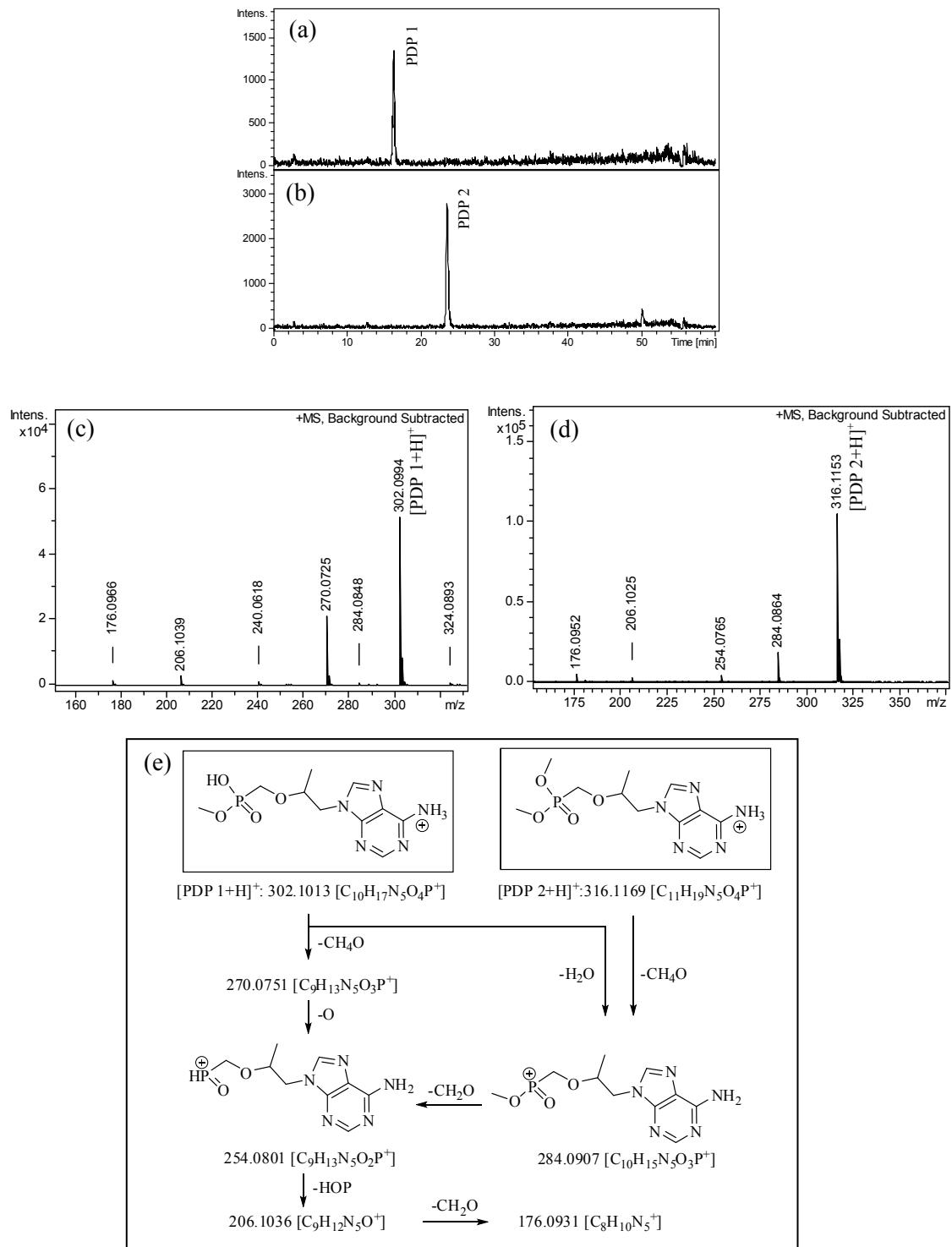


Fig. S2 HPLC chromatograms showing effect of CH<sub>3</sub>CN used as a diluent during sample preparation. Here the products T1, T2, T3, and T4 were seen as pairs with peaks labelled as T1A, T2A, T3A, and T4A, respectively. There is near overlapping of T5 and T5A in this figure, but they were seen as separated peaks when LC-HRMS studies were carried out to determine their mass.



**Fig. S3** Extracted ion chromatograms of pseudo degradation products PDP 1 (a) and PDP 2 (b), LC-HRMS spectra of PDP 1 (c) and PDP 2 (d), structures and fragmentation behaviour of the same (e). See Fig. 2 for the structures of fragments not shown in this figure. The structures of pseudo degradation products are shown in solid boxes.