Supporting Information:

Analysis and Identification of 2'-Deoxyadenosine-derived Adducts in Lung and Liver DNA of F-344 Rats Treated with the Tobacco-Specific Carcinogen 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanone and Enantiomers of its Metabolite 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanol

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Figure S1: Representative chromatograms obtained from the LC-NSI-HRMS/MS analyses of POB- and PHB-DNA adducts in the lungs of rats chronically treated with 5 ppm NNK for 50 weeks. Each channel is monitoring the two most abundant product ions from MS^2-fragmentation of a particular DNA adduct. Adduct identity and product ions are the following: A) N^1-POB-dIno (400 → 283.1300, 265.1194), (B) N^1-PHB-dIno (402 → 286.1296, 268.1191), (C) N^6-POB-dAdo (399 → 283.1300, 265.1194), (D) [D_4]N^6-POB-dAdo (403 → 285.1456, 267.1350), (E) N^6-PHB-dAdo (401 → 287.1550, 269.1445), (F) [$^{15}N_5$]N^6-PHB-dAdo (406 → 290.1307, 272.1202) .

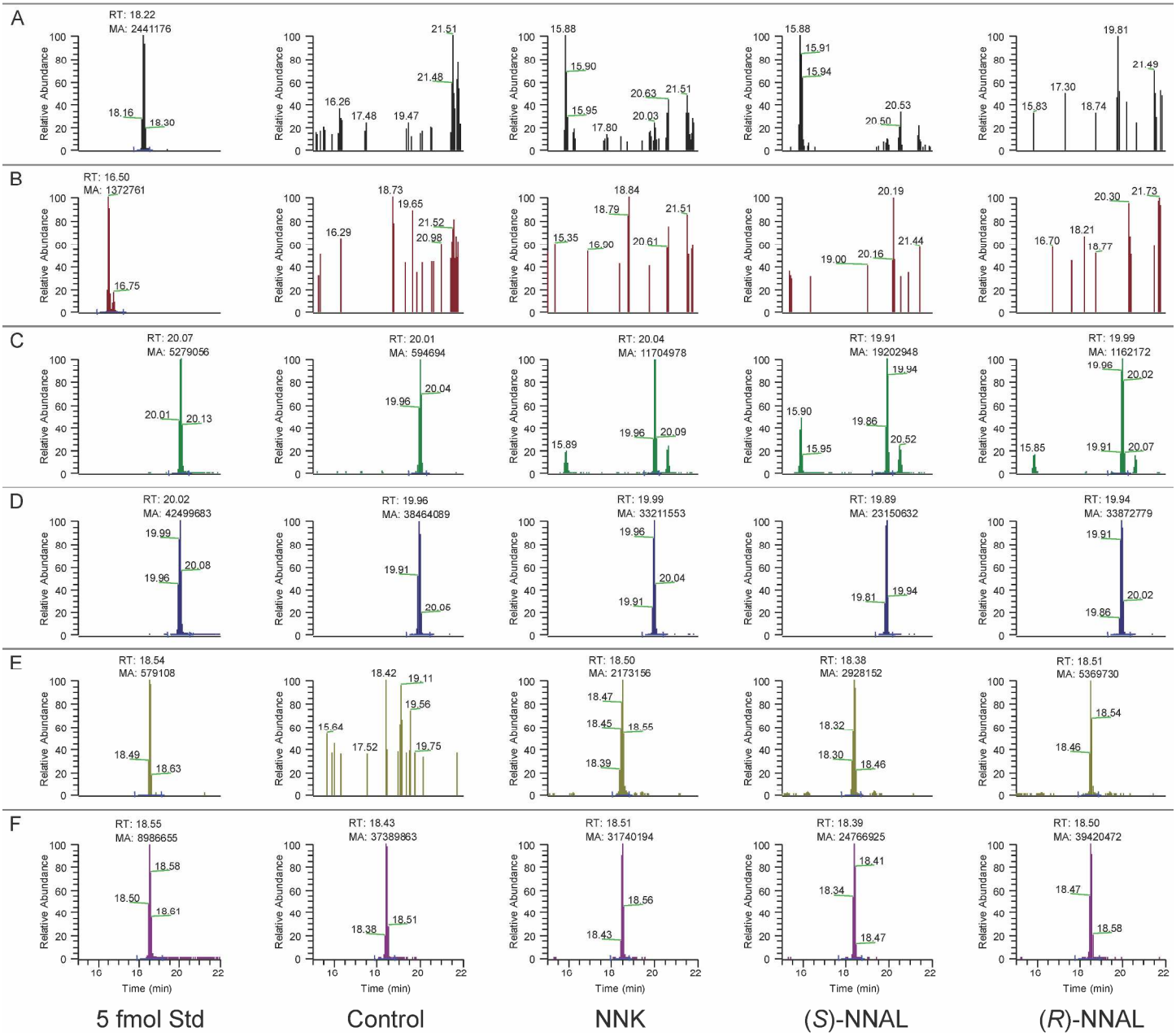
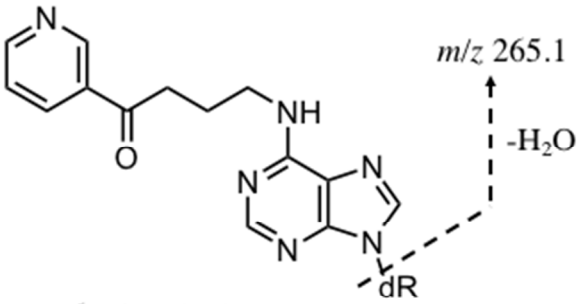
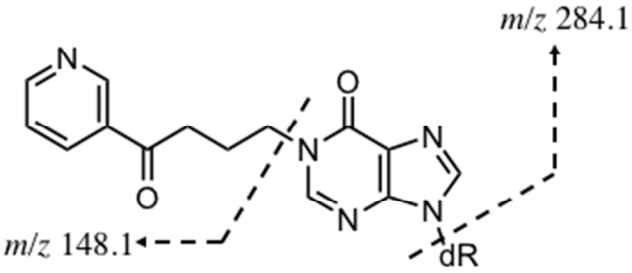


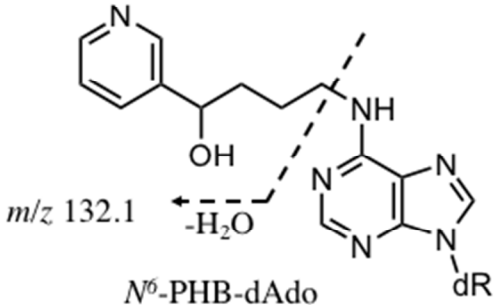
Figure S2: Structures and fragmentation patterns for the monitored N^6-dAdo and N^1-dIno adducts. dR: 2'-deoxyribose.



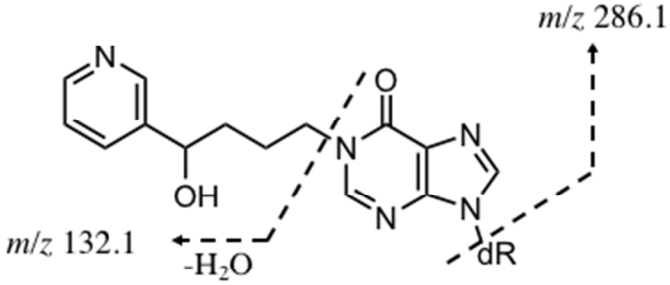
N^6-POB-dAdo
[M+H] = *m/z* 399.1



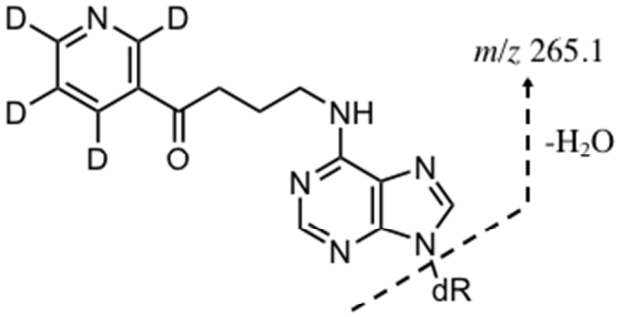
N^1-POB-dIno
[M+H] = *m/z* 400.1



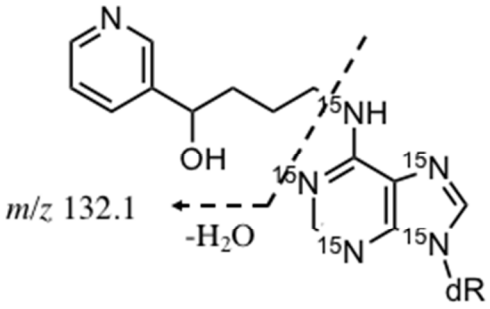
N^6-PHB-dAdo
[M+H] = *m/z* 401.1



N^1-PHB-dIno
[M+H] = *m/z* 402.1



[Pyridine-D_4]*N6*-POB-dAdo
[M+H] = *m/z* 403.1



[$^{15}N_5$]N^6-PHB-dAdo
[M+H] = *m/z* 406.1