

Supporting Information

Biocatalytic Separation of N-7/N-9 Guanine Nucleosides

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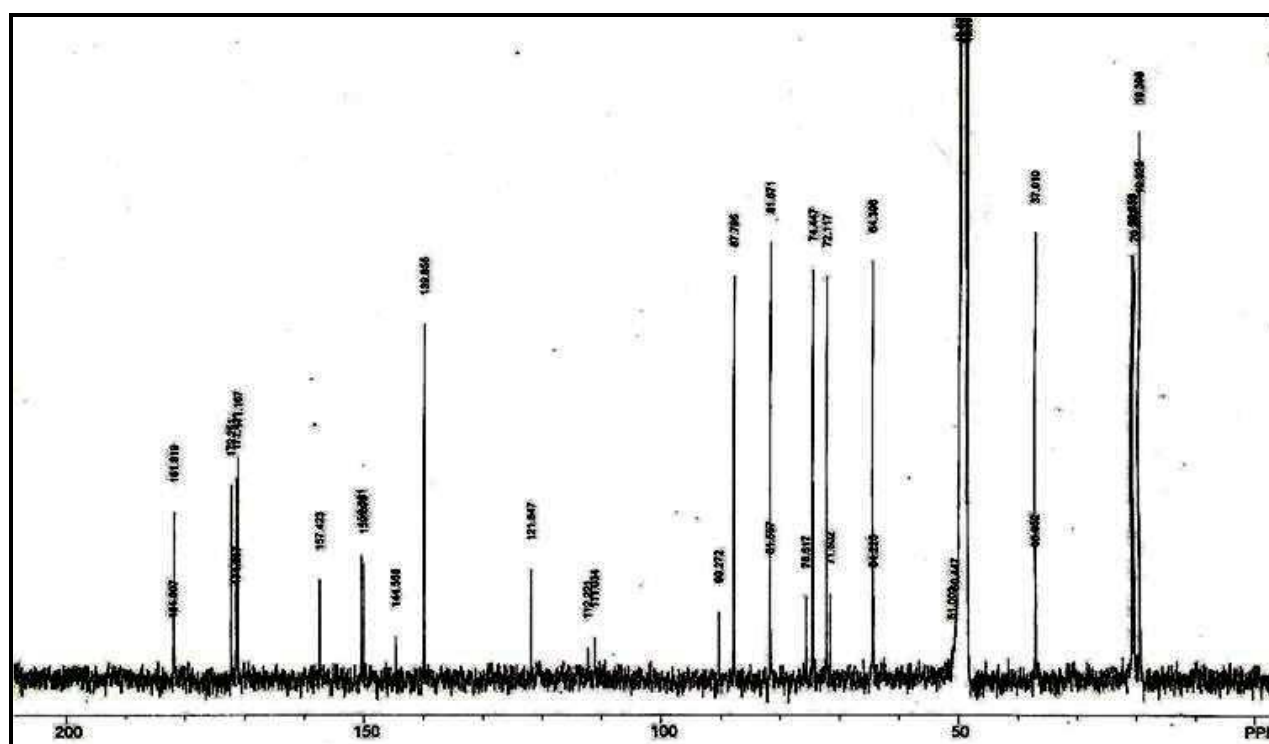
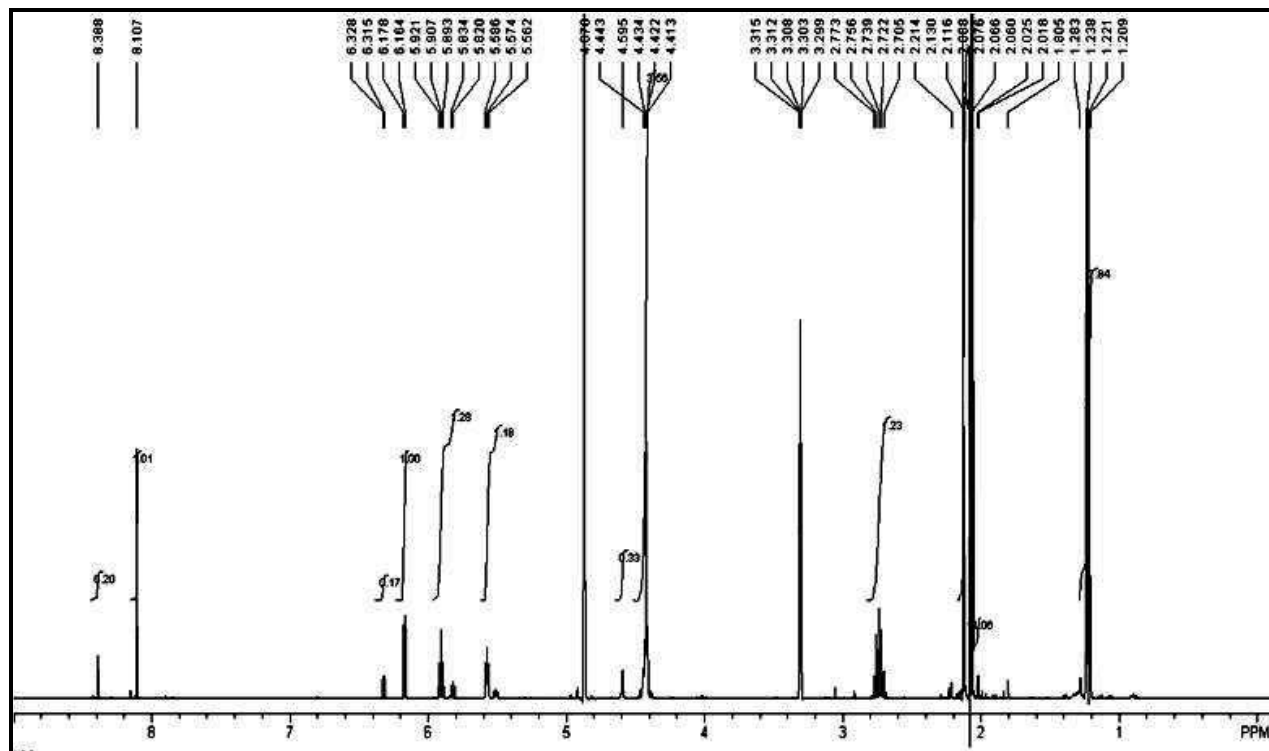
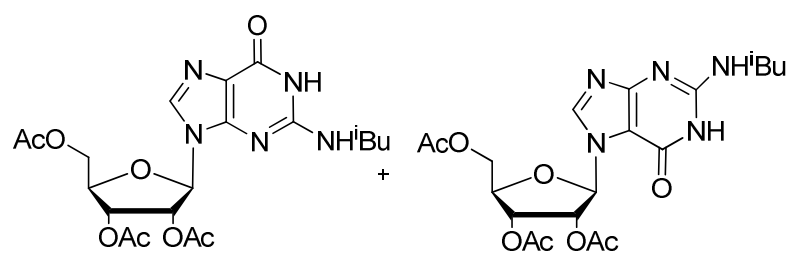
General experimental note

Melting points were determined on a Mettler FP 62 instrument or in a sulfuric acid bath and were uncorrected. The IR spectra were recorded on a FT-IR spectrometer by making KBr disc for solid samples and thin film for oils. The specific rotations were measured with Rudolph autopol II automatic polarimeter using light of 546 nm wavelength. The ^1H NMR spectra were recorded on 400/300 MHz spectrometer and ^{13}C NMR spectra were recorded on 100.6/75.5 MHz, respectively, using TMS as internal standard. The chemical shift values are on δ scale and the coupling constants (J) are in Hz. HRMS analysis was carried out on a microTOF-Q instrument from Bruker Daltonics, Bremen. They were run in ESI positive mode. The *Candida antarctica* lipase B immobilized on lewattite was used after storing *in vacuo* over P_2O_5 for more than 24 hours. THF was dried over Na wire distilled and kept over Na wire prior to use. The spots on analytical TLCs were detected either under UV light or by charring with 4% alcoholic H_2SO_4 . Silica gel (100-200 mesh) was used for column chromatography.

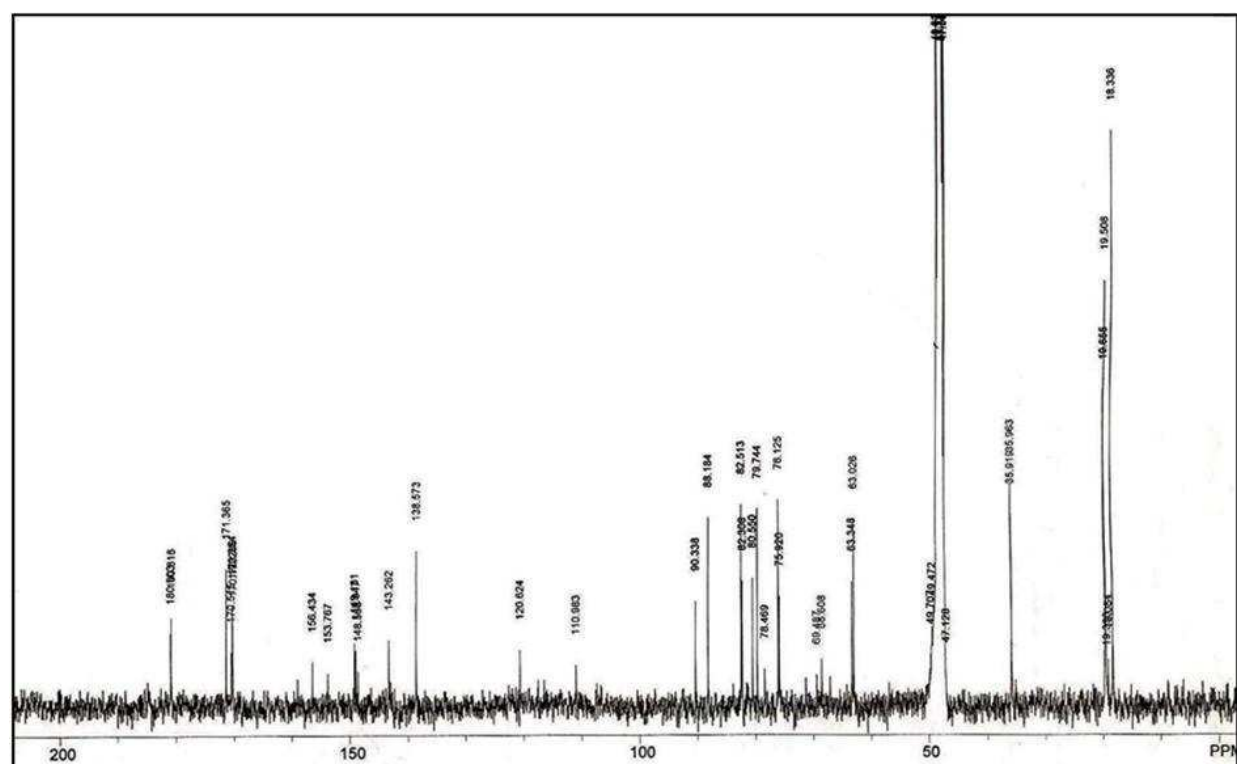
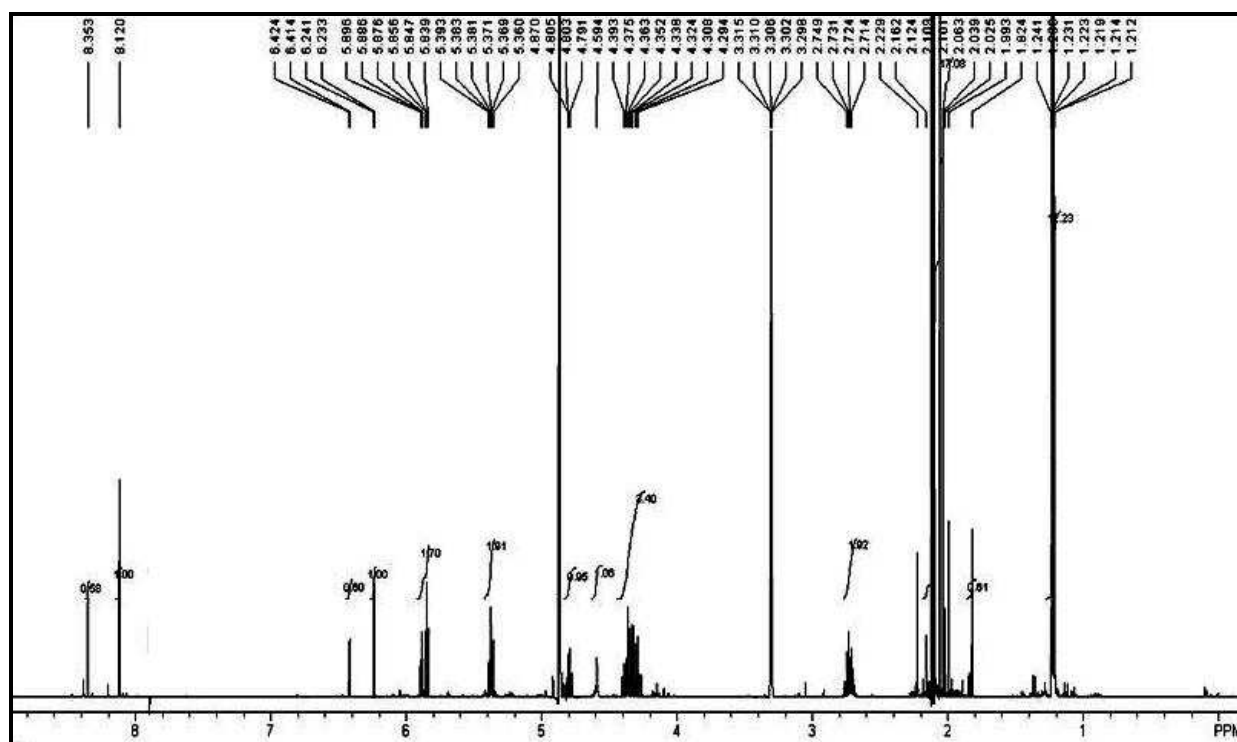
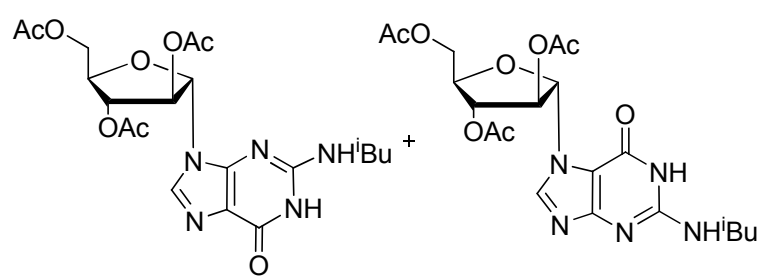
General procedure for the preparation of guanine nucleosides **6** & **7**, **8** & **9** and **10** & **11**

2-*N*-isobutanoylguanine **2** (3.12 g, 14.15 mmol) was coupled with 1,2,3,5-tetra-*O*-acetyl- β -D-ribofuranose (**3**), 1,2,3,5-tetra-*O*-acetyl- α,β -D-arabinofuranose (**4**) and 1,2,3,5-tetra-*O*-acetyl- α,β -L-arabinofuranose (**5**) (3.0 g, 9.4 mmol) in the presence of BSA (10.3 mL, 41.32 mmol) as silylating agent and TMSOTf (3.8 mL, 21.03 mmol) as Lewis acid catalyst following the method of Vorbrüggen, *et al.*¹¹ After completion of reaction on analytical TLC, reaction mixture was poured on ice-cold water and was extracted with chloroform (3 x 100 mL). The combined organic layer was washed with sodium hydrogen carbonate (2 x 50 mL) and brine (2 x 50 mL). Excess of solvent was evaporated under reduced pressure and the crude product thus obtained was purified by silica gel column chromatography to afford mixtures of 9-(2',3',5'-tri-*O*-acetyl- β -D-ribofuranosyl)-*N*²-isobutanoylguanine (**6**) & 7-(2',3',5'-tri-*O*-acetyl- β -D-ribofuranosyl)-*N*²-isobutanoylguanine (**7**) (87:13), 9-(2',3',5'-tri-*O*-acetyl- α -D-arabinofuranosyl)-*N*²-isobutanoylguanine (**8**) & 7-(2',3',5'-tri-*O*-acetyl- α -D-arabinofuranosyl)-*N*²-isobutanoylguanine (**9**) (63:37) and 9-(2',3',5'-tri-*O*-acetyl- α -L-arabinofuranosyl)-*N*²-isobutanoylguanine (**10**) & 7-(2',3',5'-tri-*O*-acetyl- α -L-arabinofuranosyl)-*N*²-isobutanoylguanine (**11**) (76:24) in 60, 62 and 65% yields, respectively.

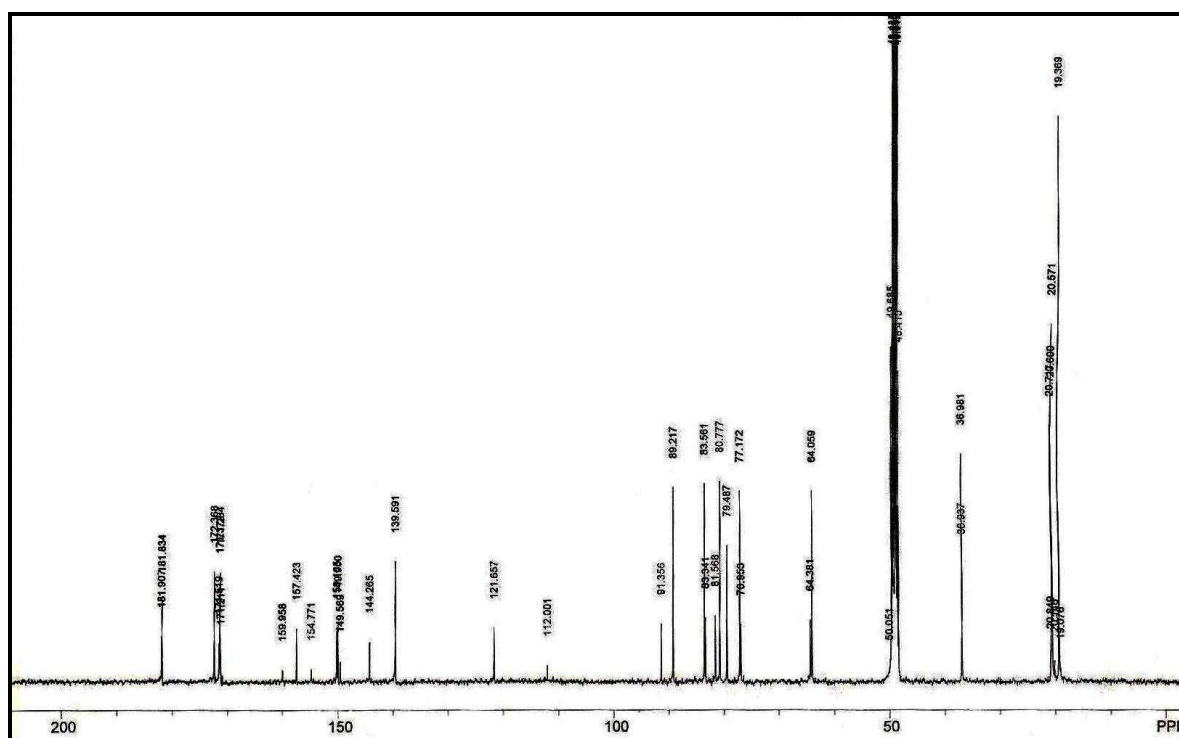
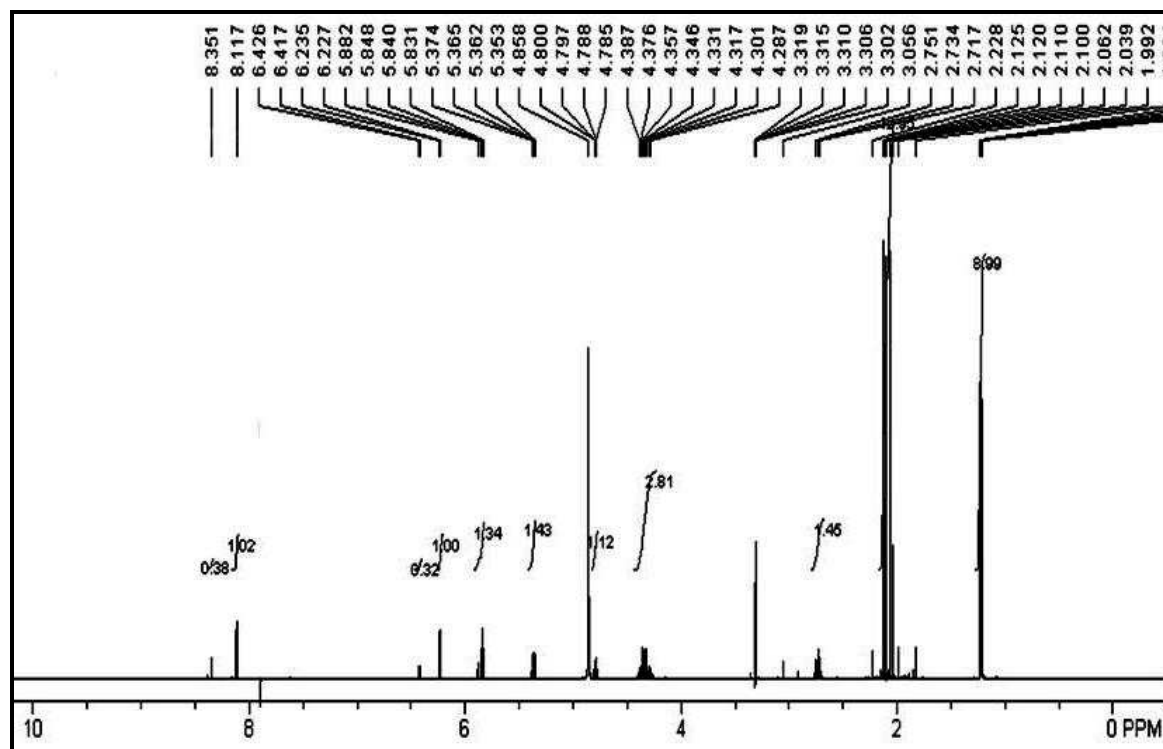
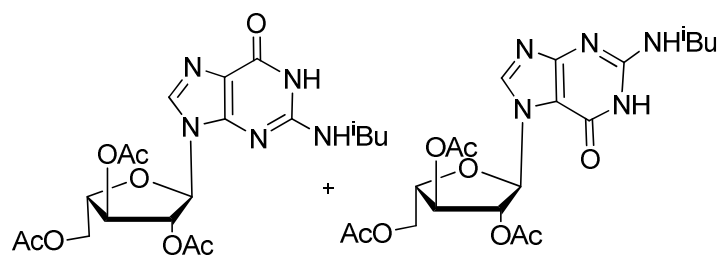
Mixture of Compounds 6 & 7



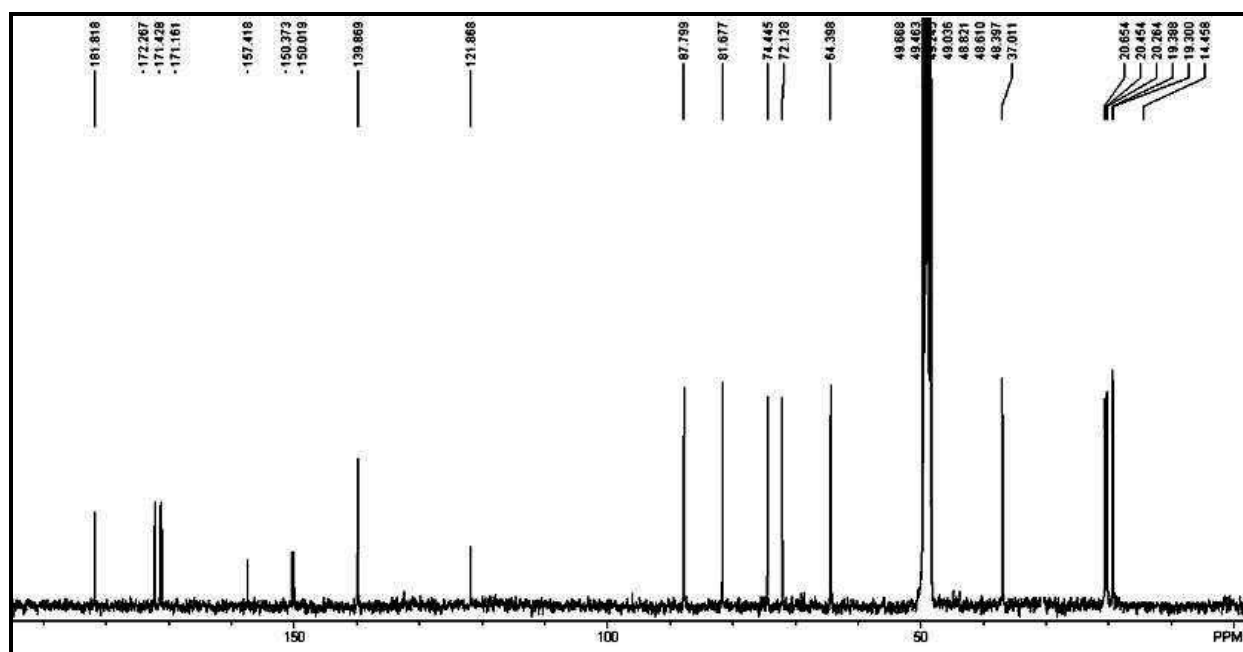
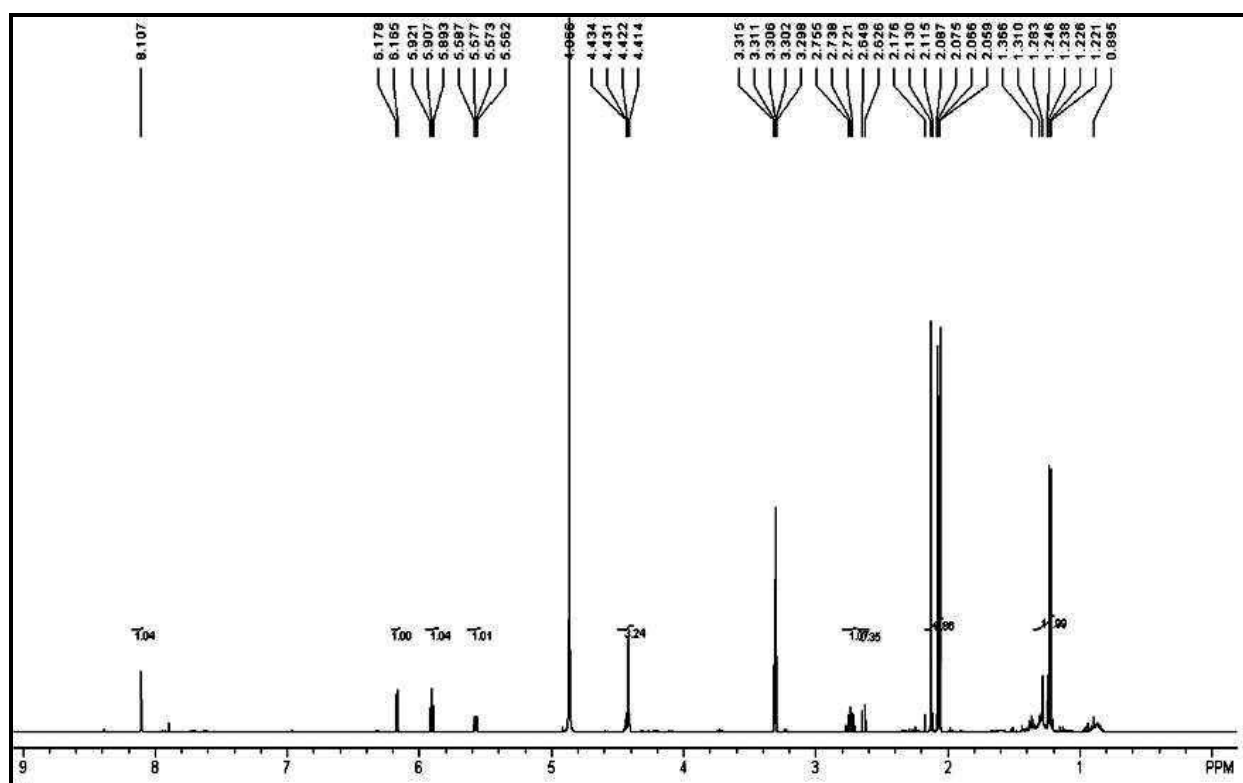
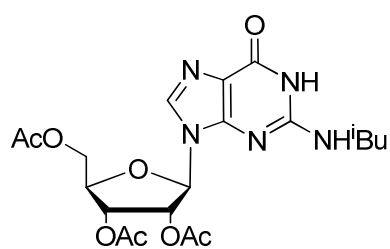
Mixture of Compounds 8 & 9



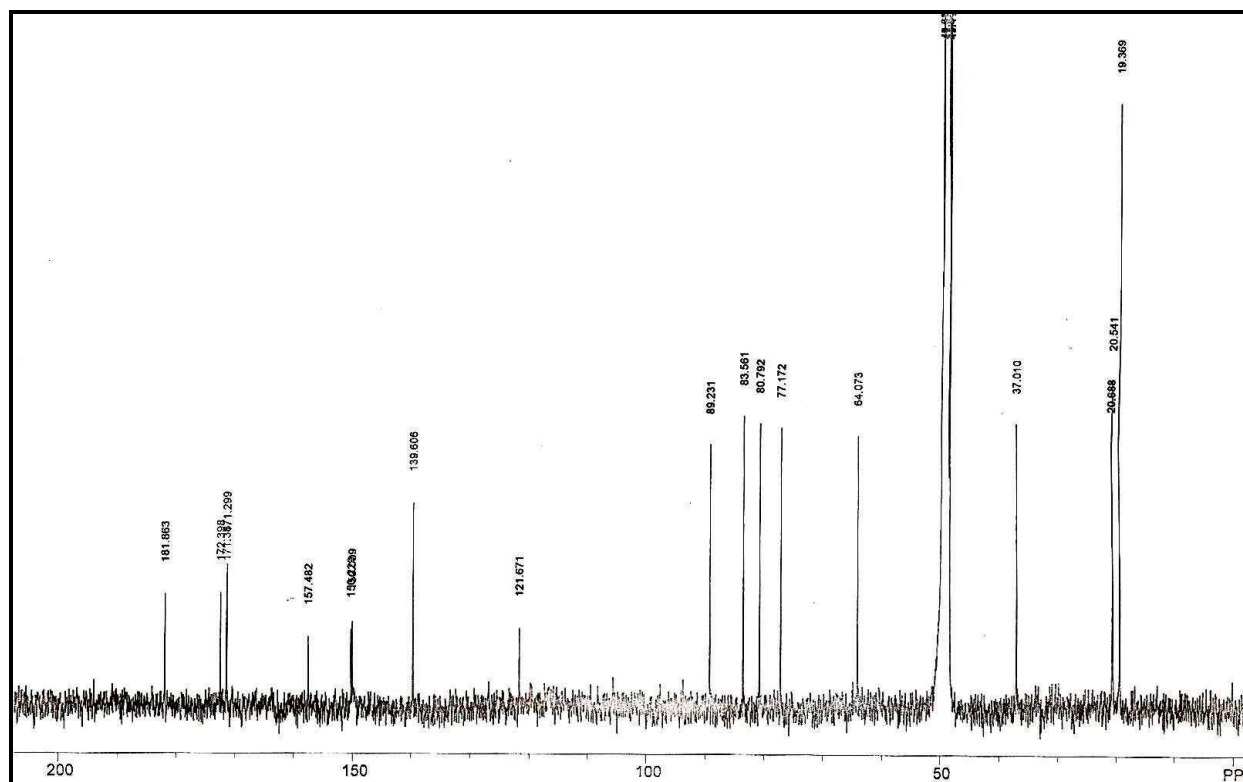
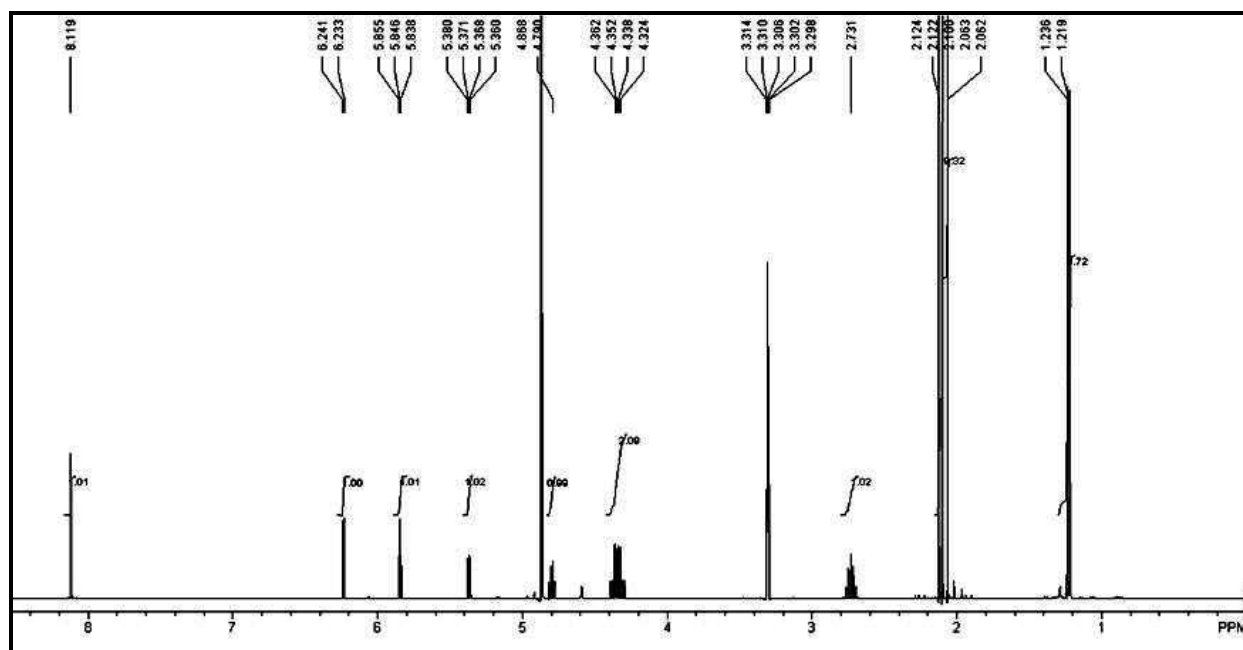
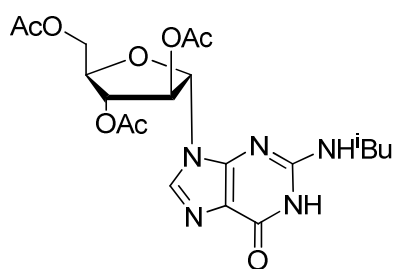
Mixture of Compounds 10 & 11



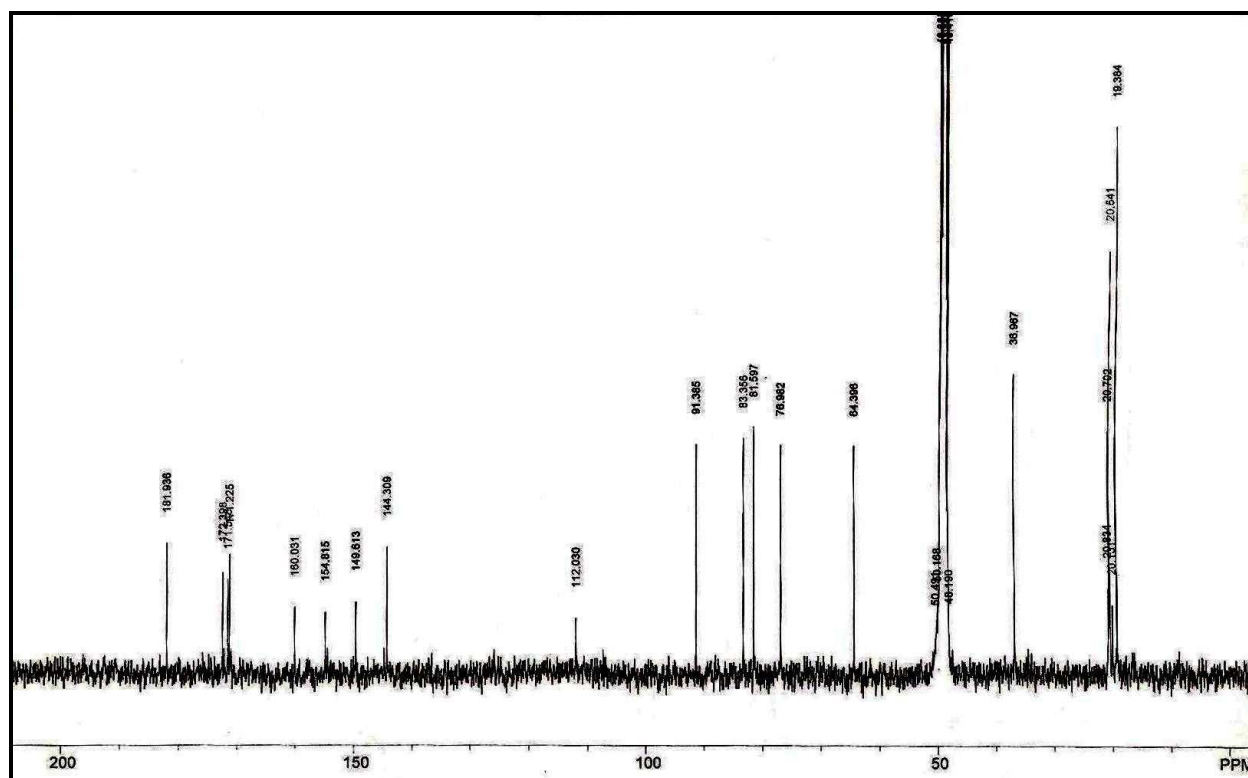
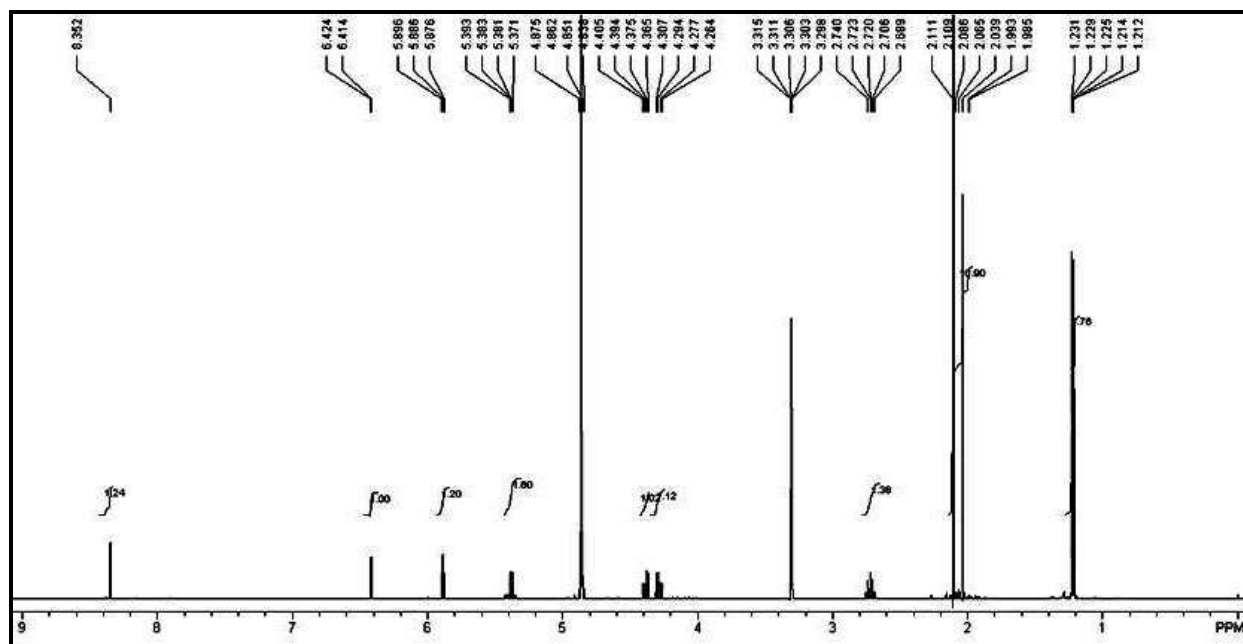
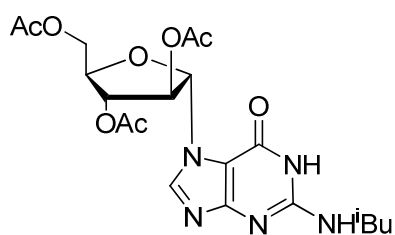
Compound 6



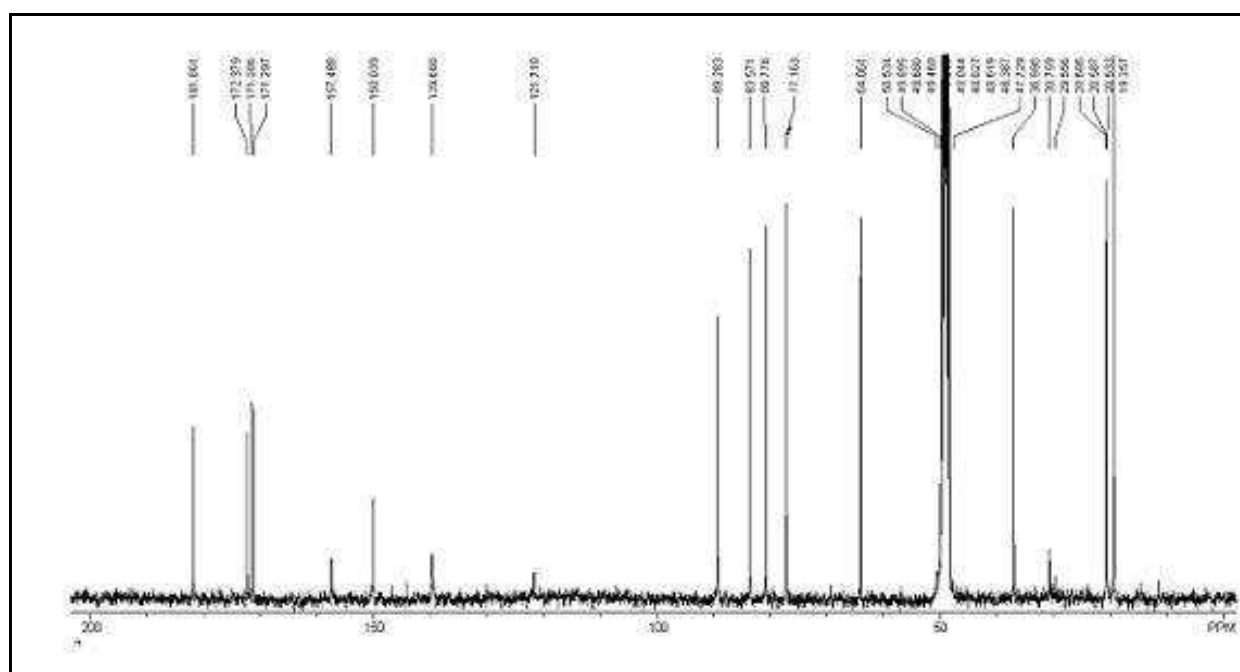
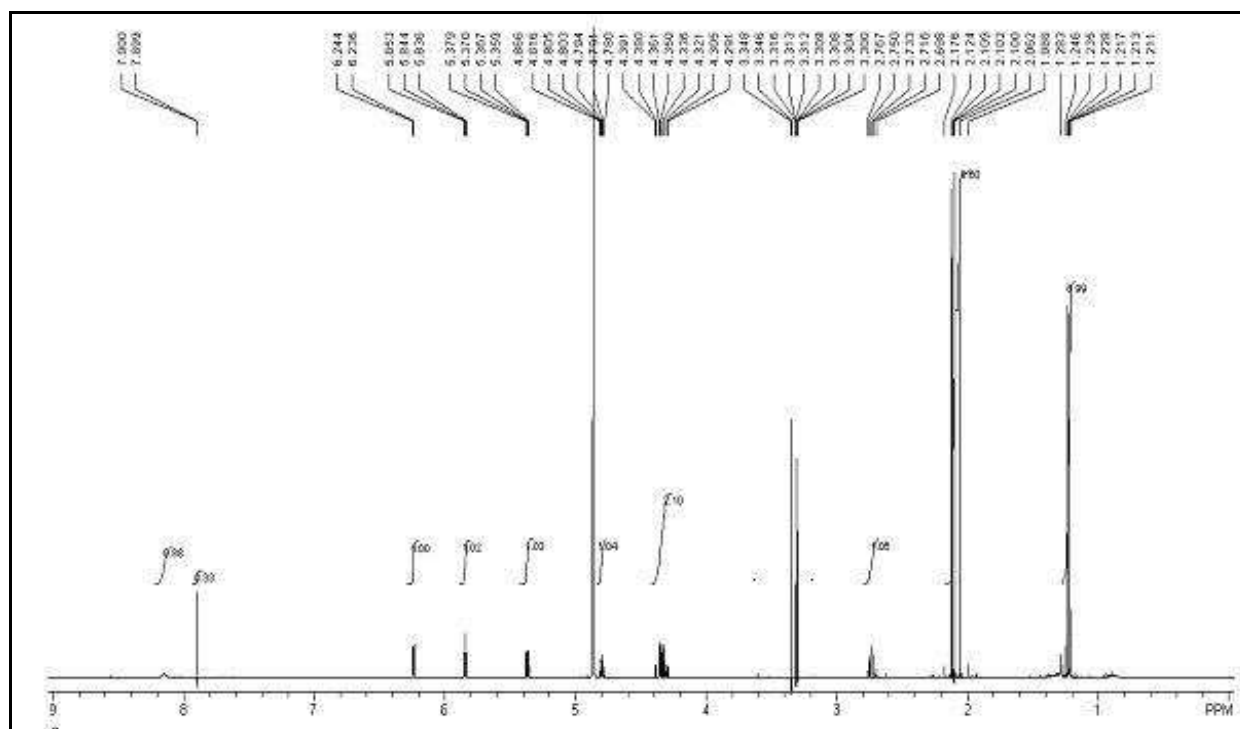
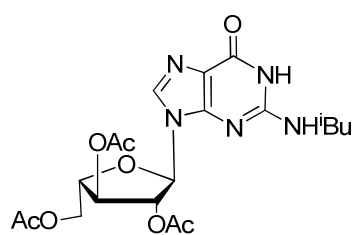
Compound 8



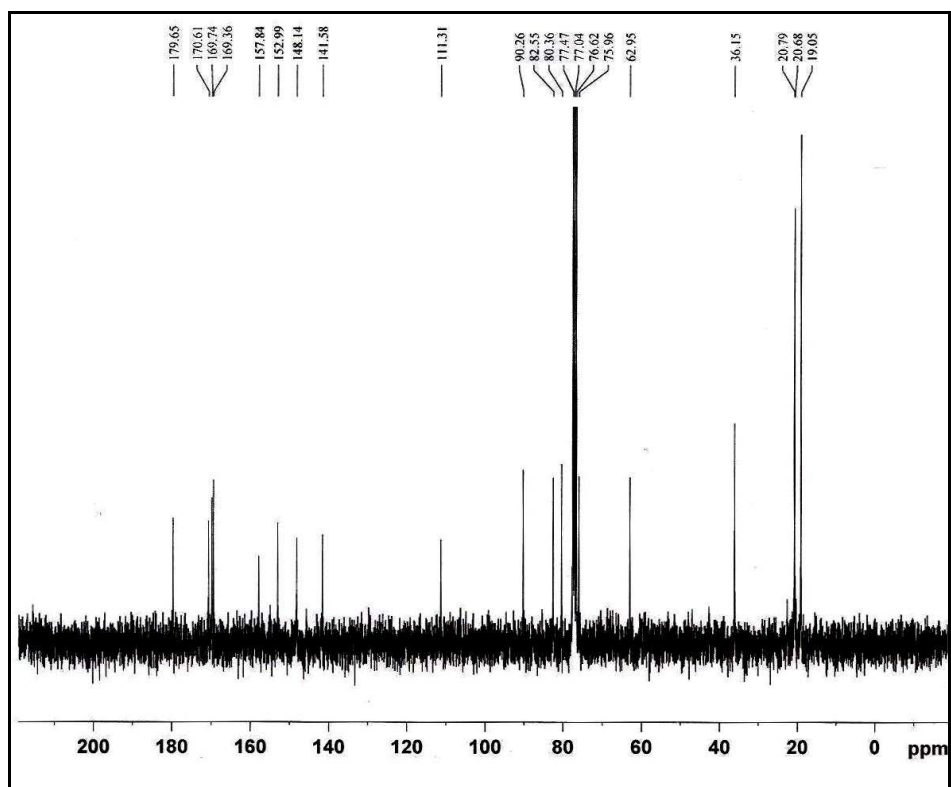
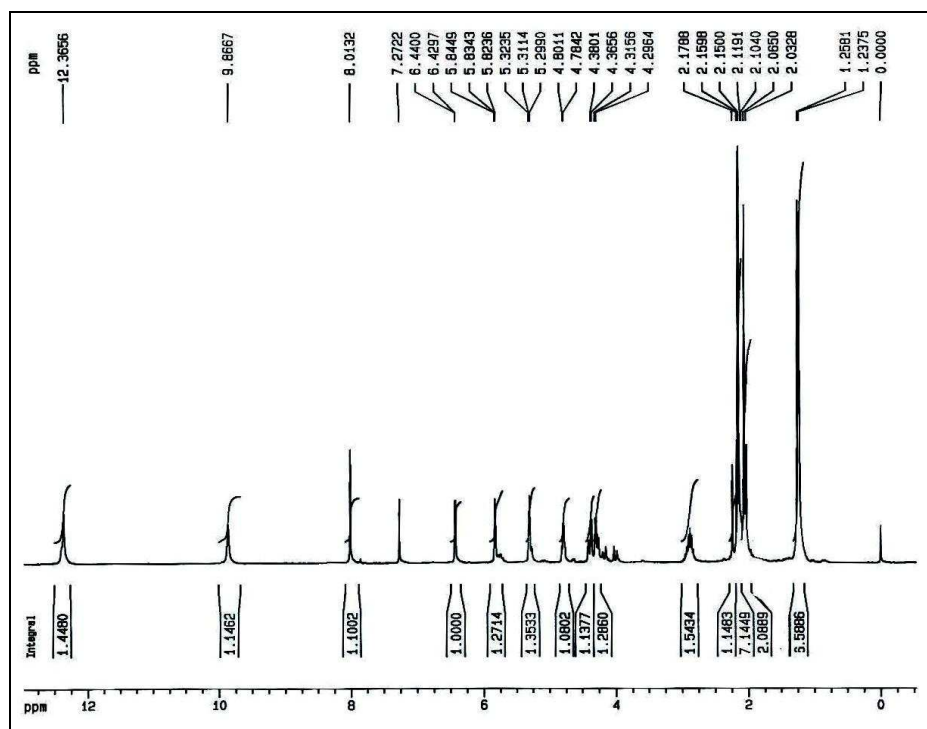
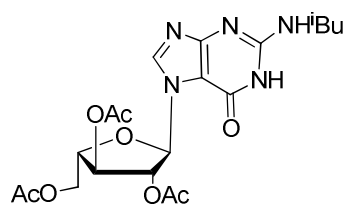
Compound 9



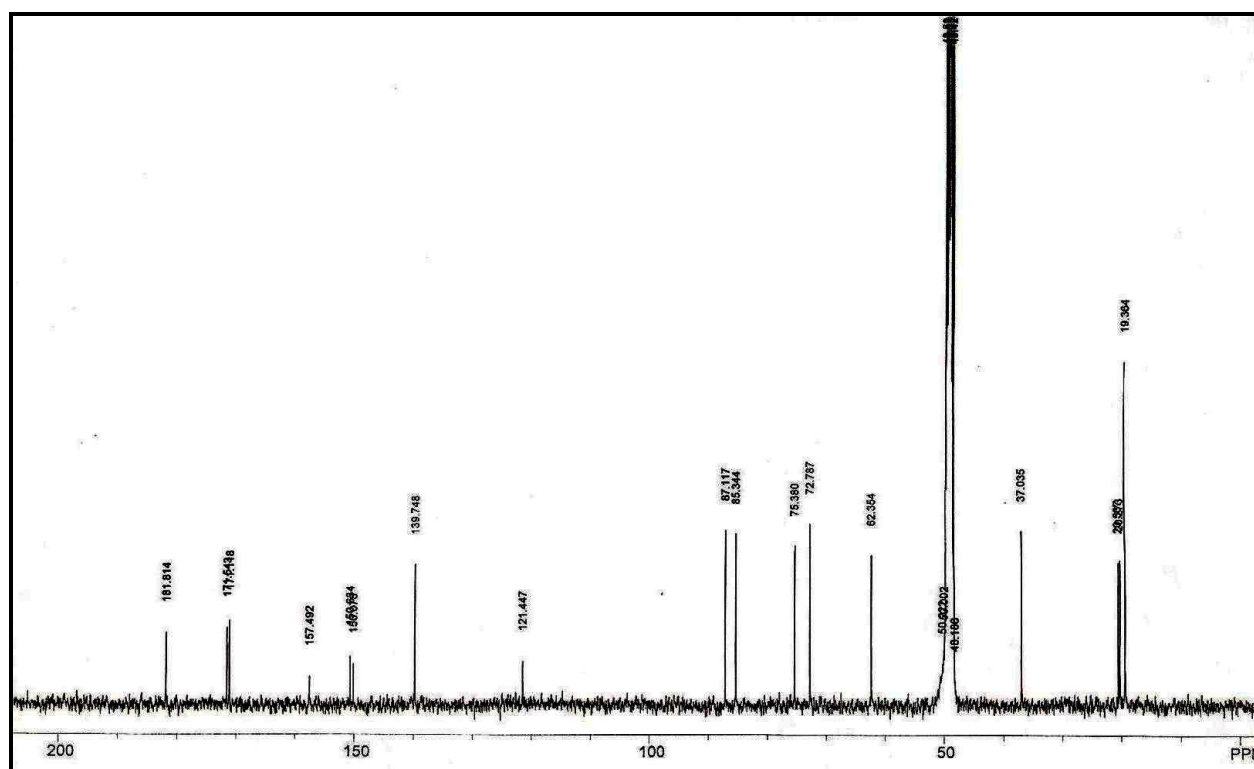
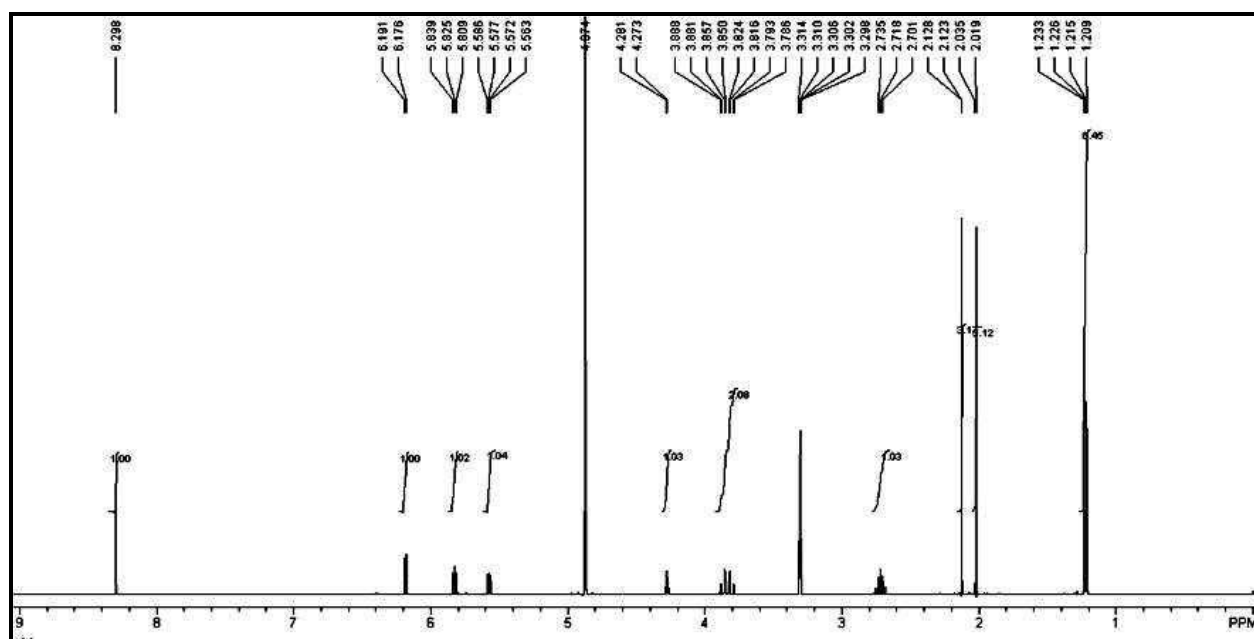
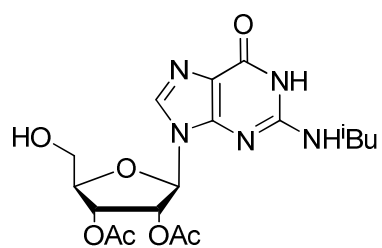
Compound 10



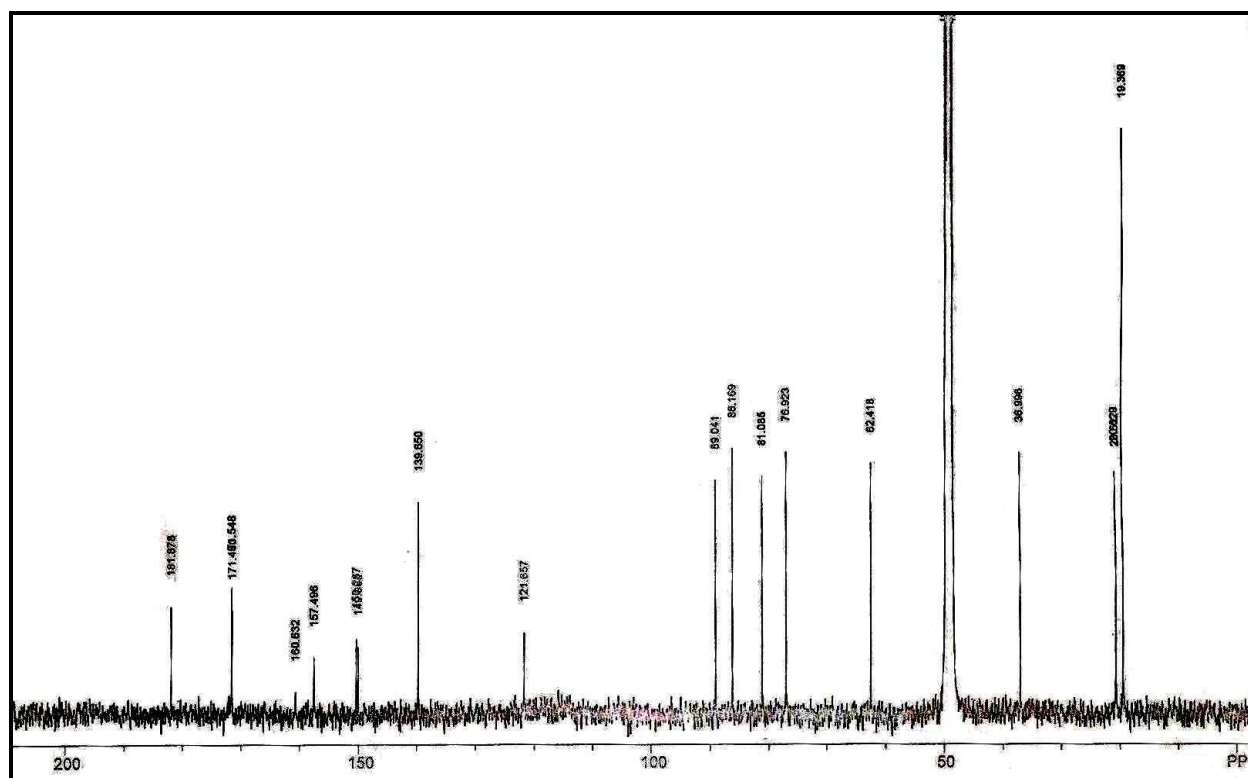
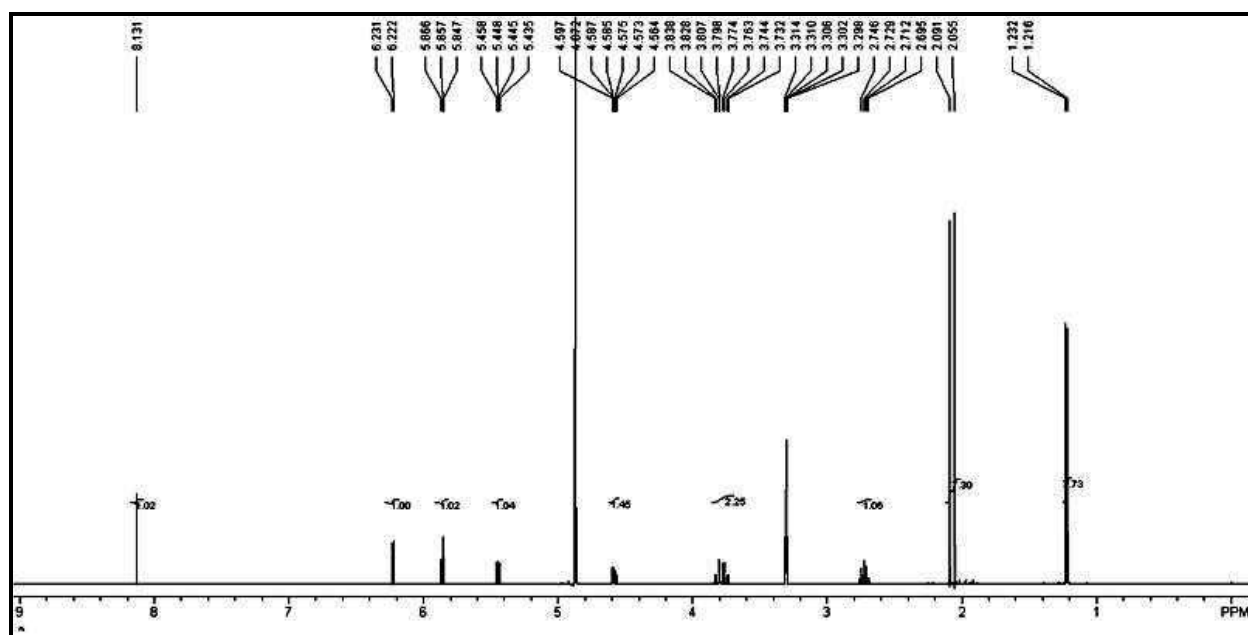
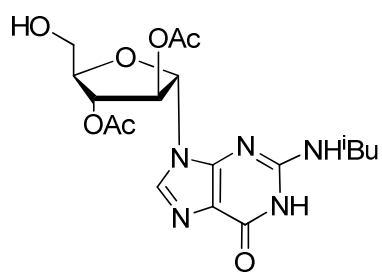
Compound 11



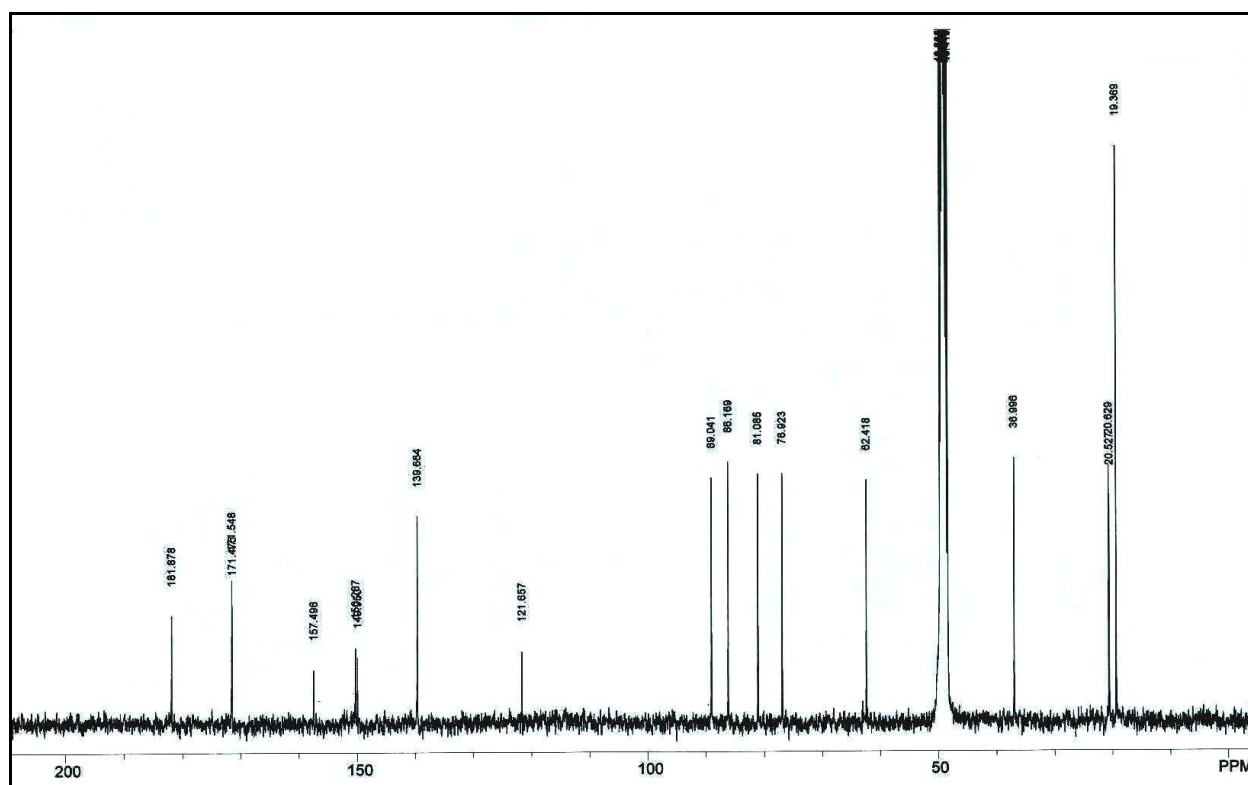
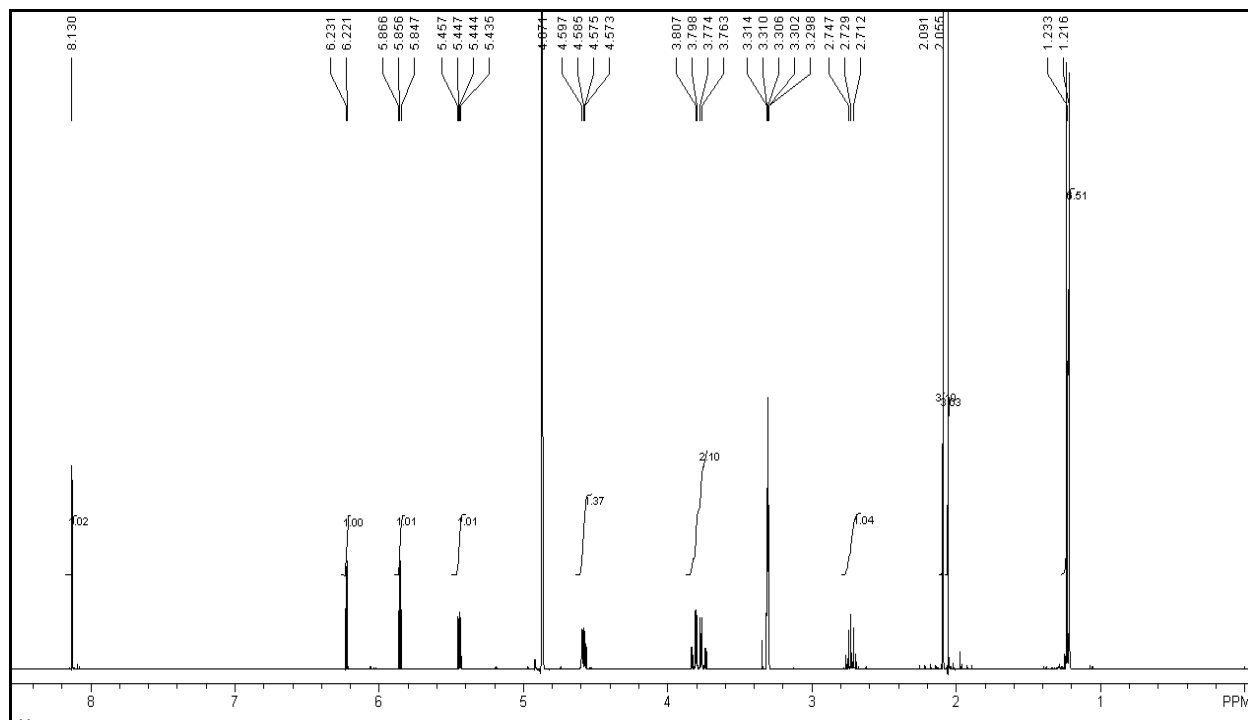
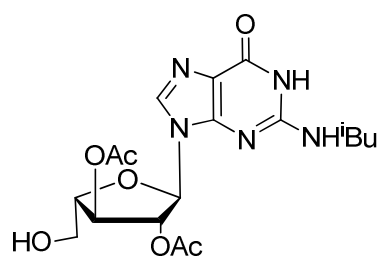
Compound 12



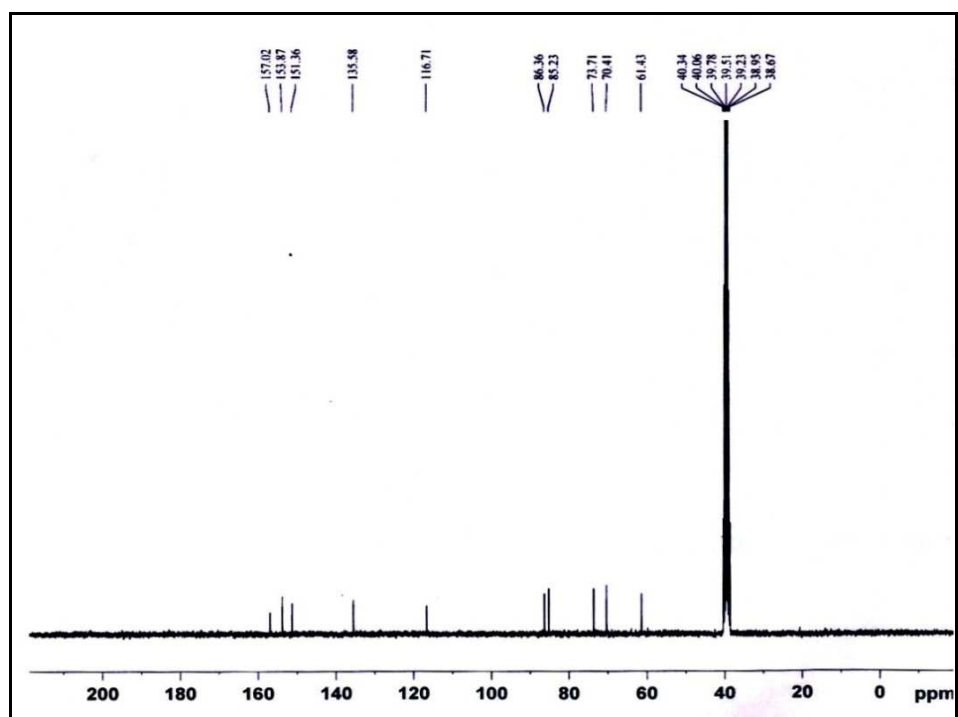
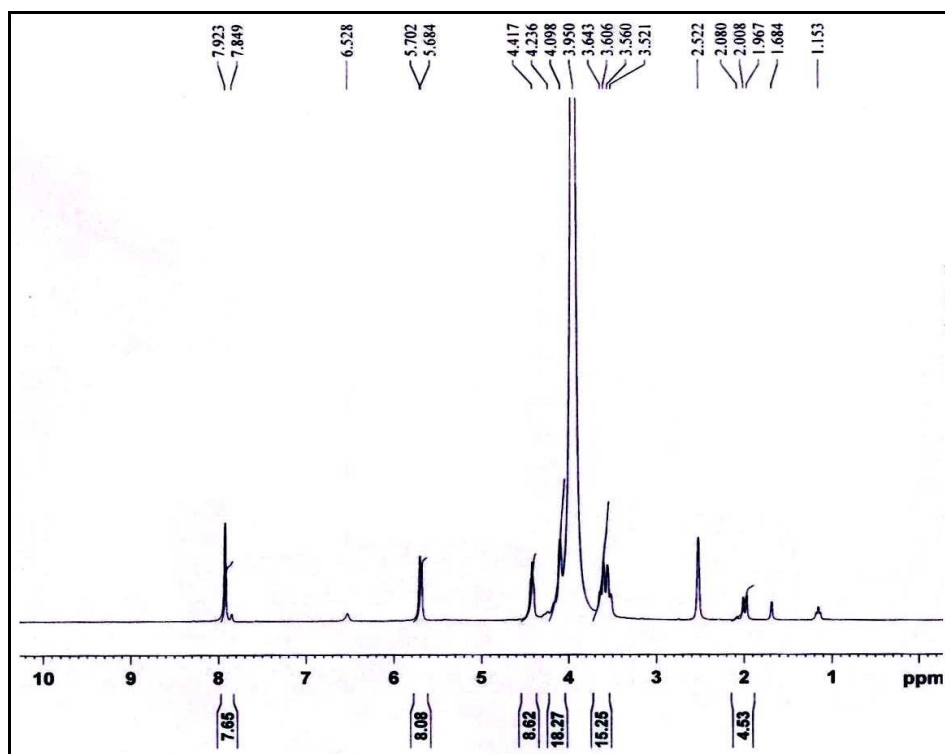
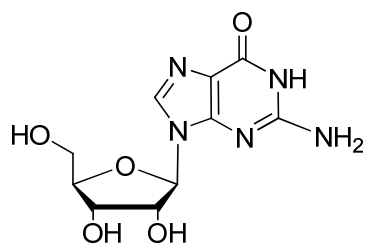
Compound 13



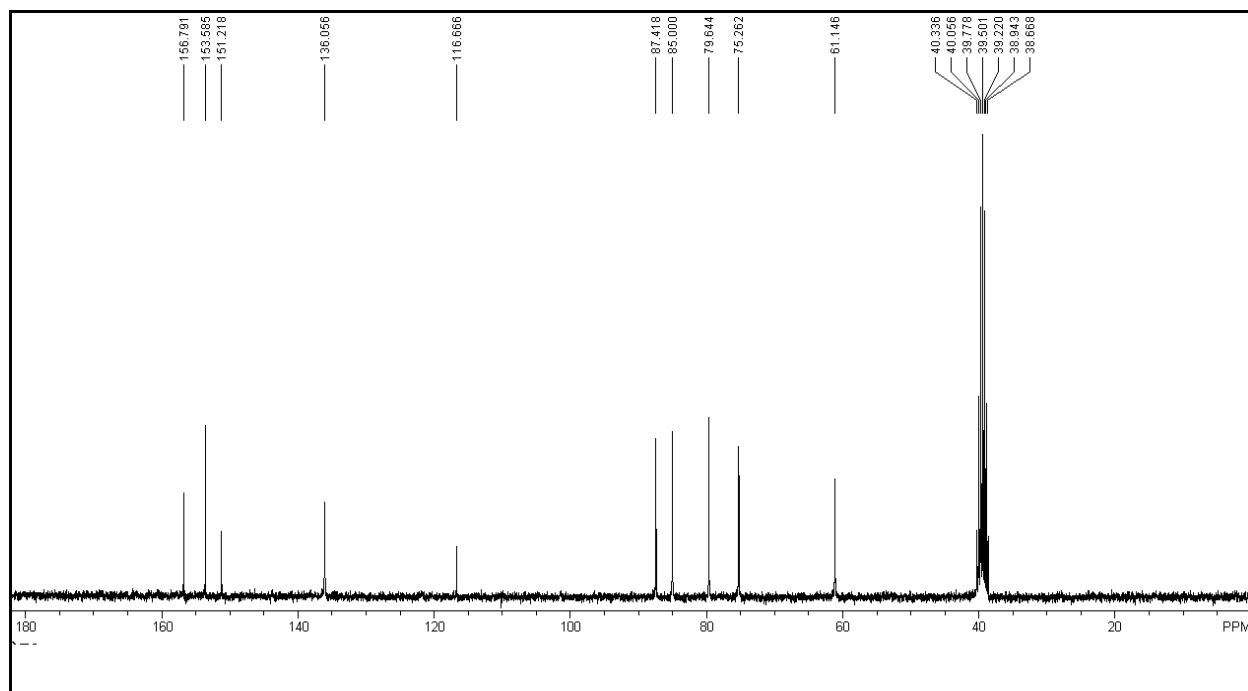
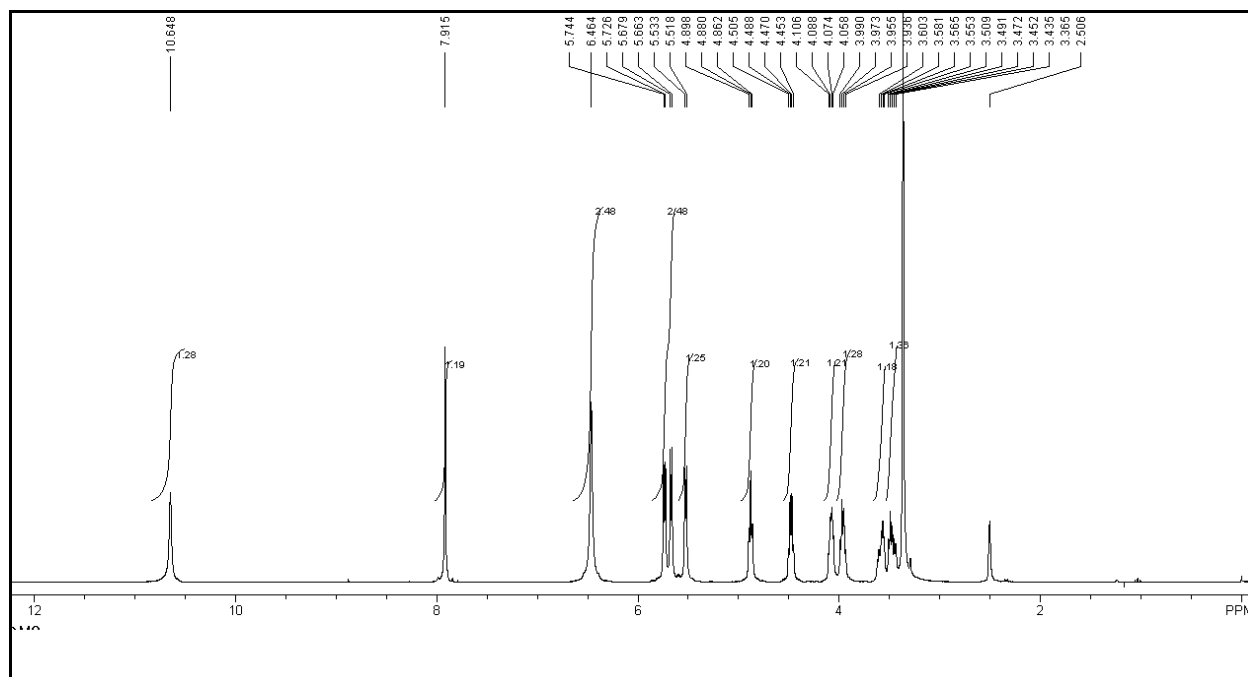
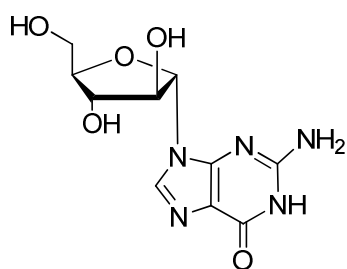
Compound 14



Compound 15



Compound 16



Compound 17

