Supporting Information

Water-Soluble Pd-Imidate Complexes: Broadly Applicable Catalysts for the Synthesis of Chemically Modified Nucleosides via Pd-Catalysed Cross-Coupling

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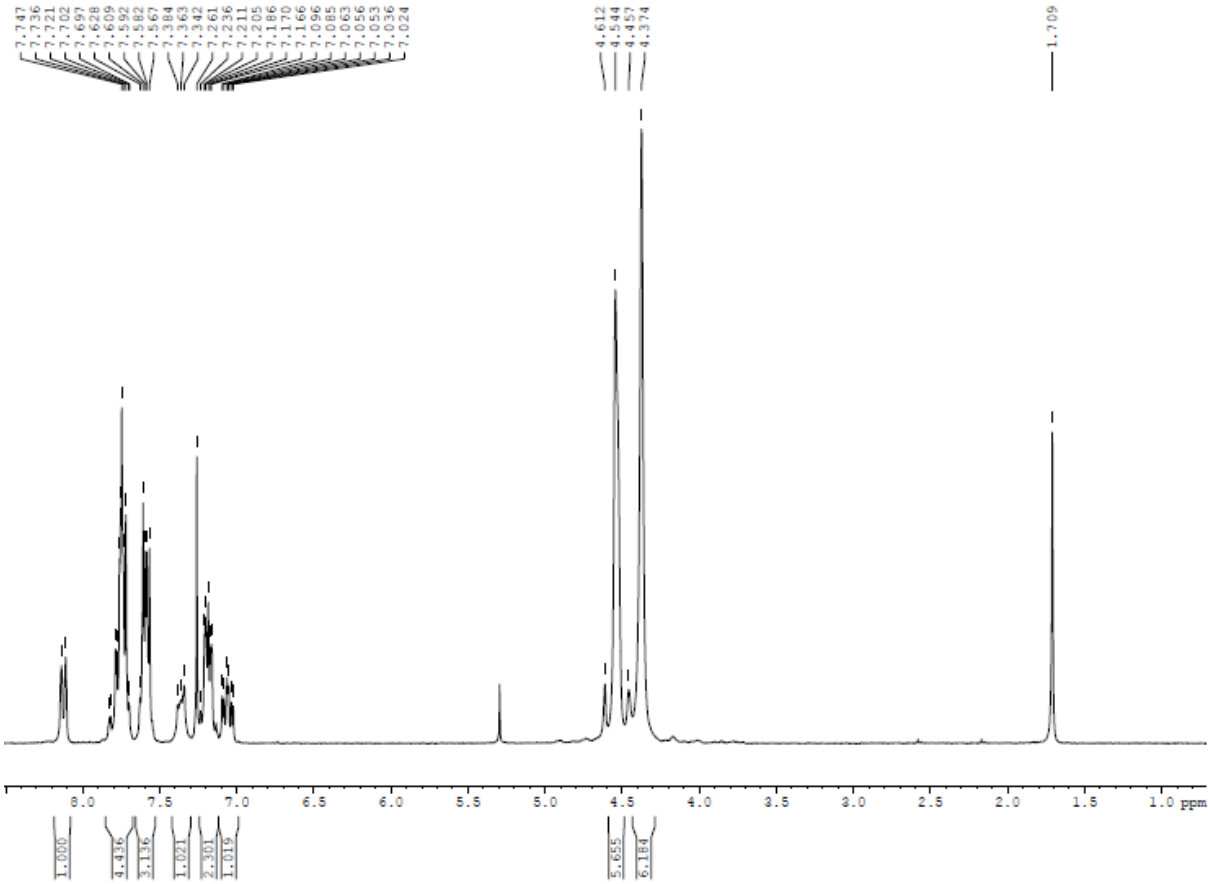
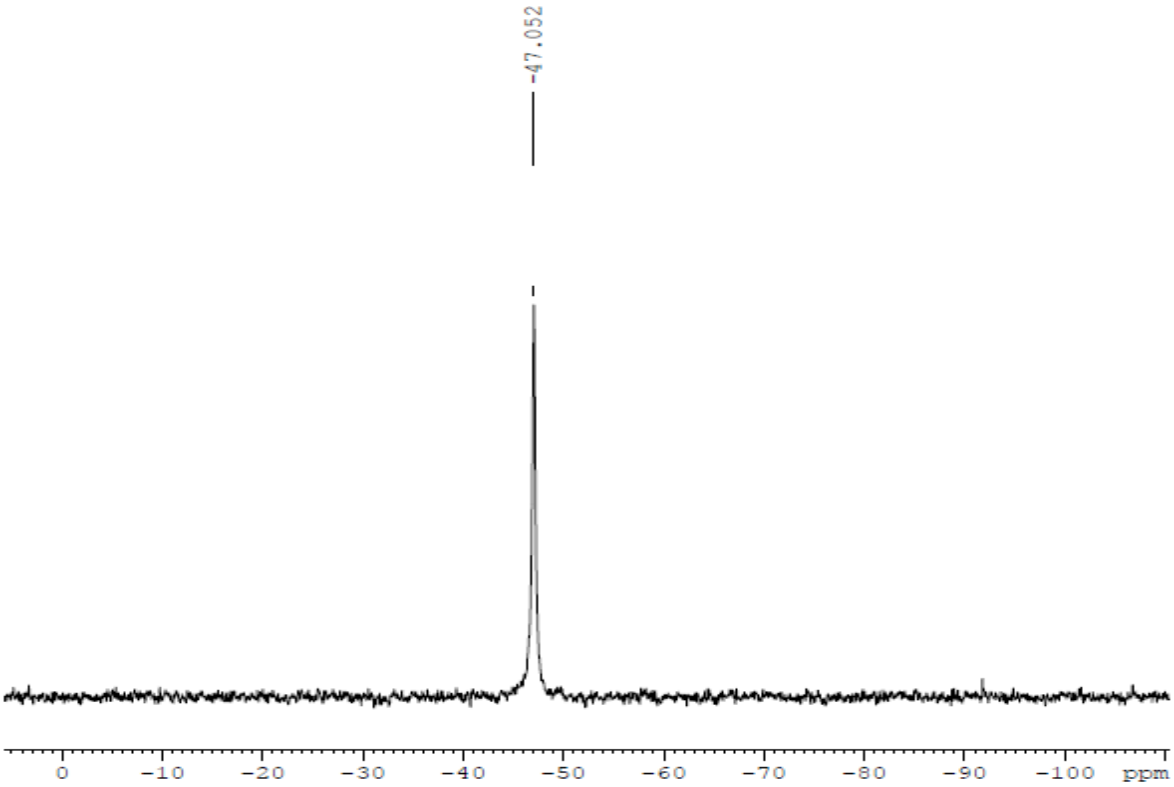
[Pd(Phpy)(Phthalimidate)(PTA)] IIa





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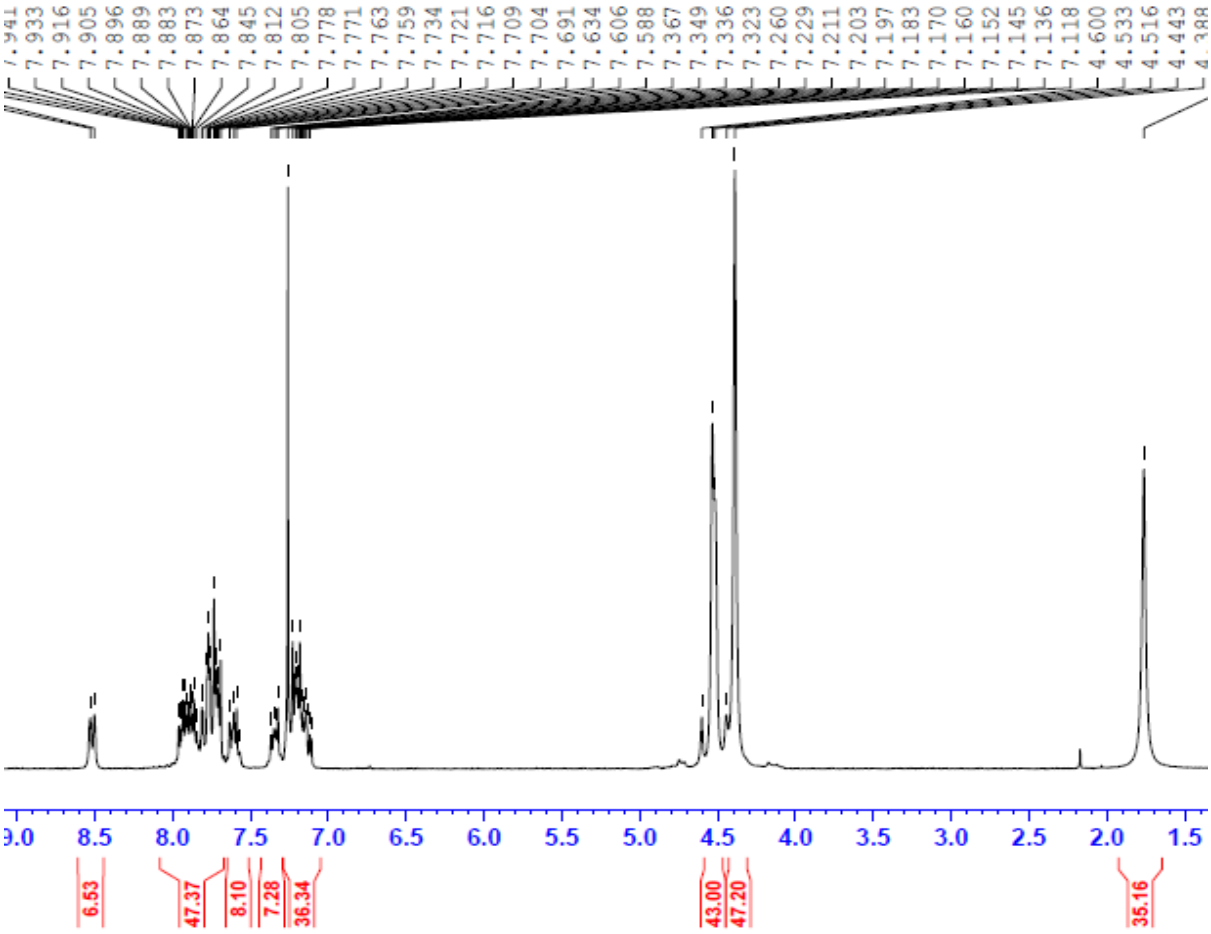
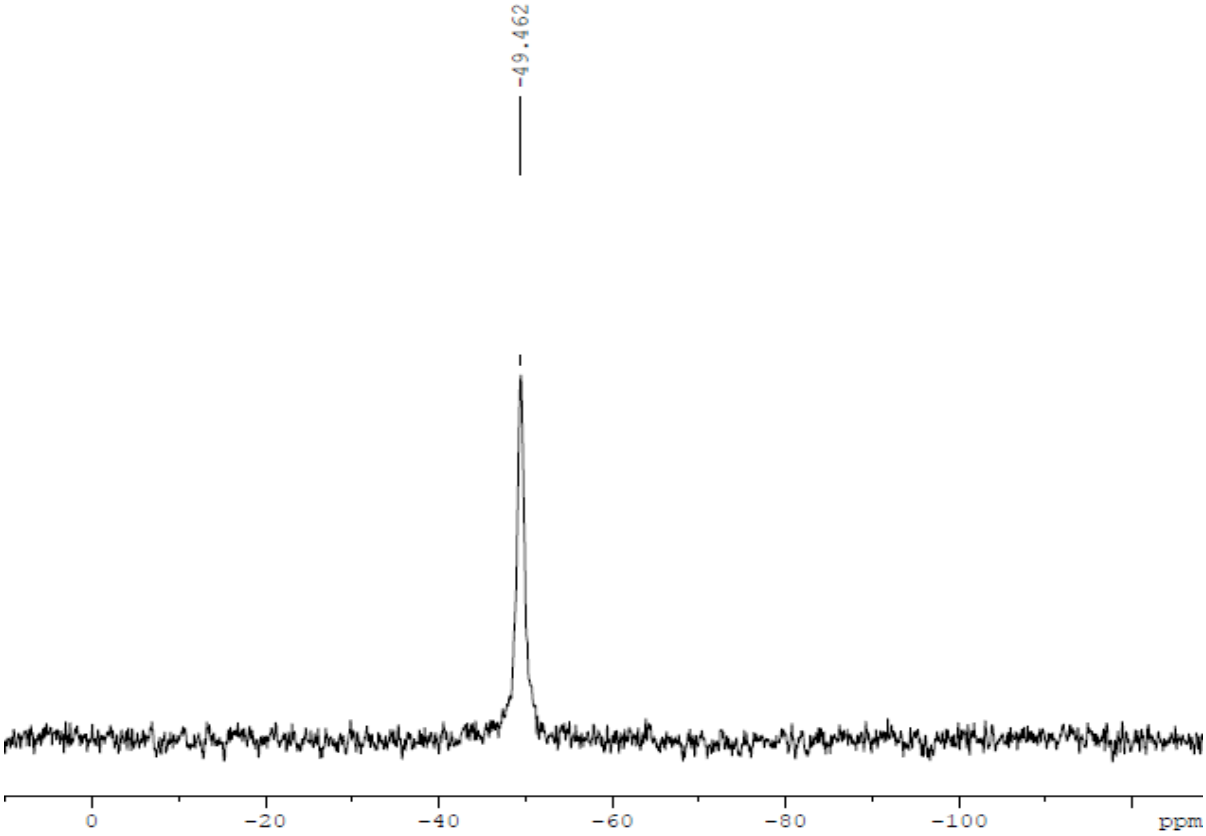
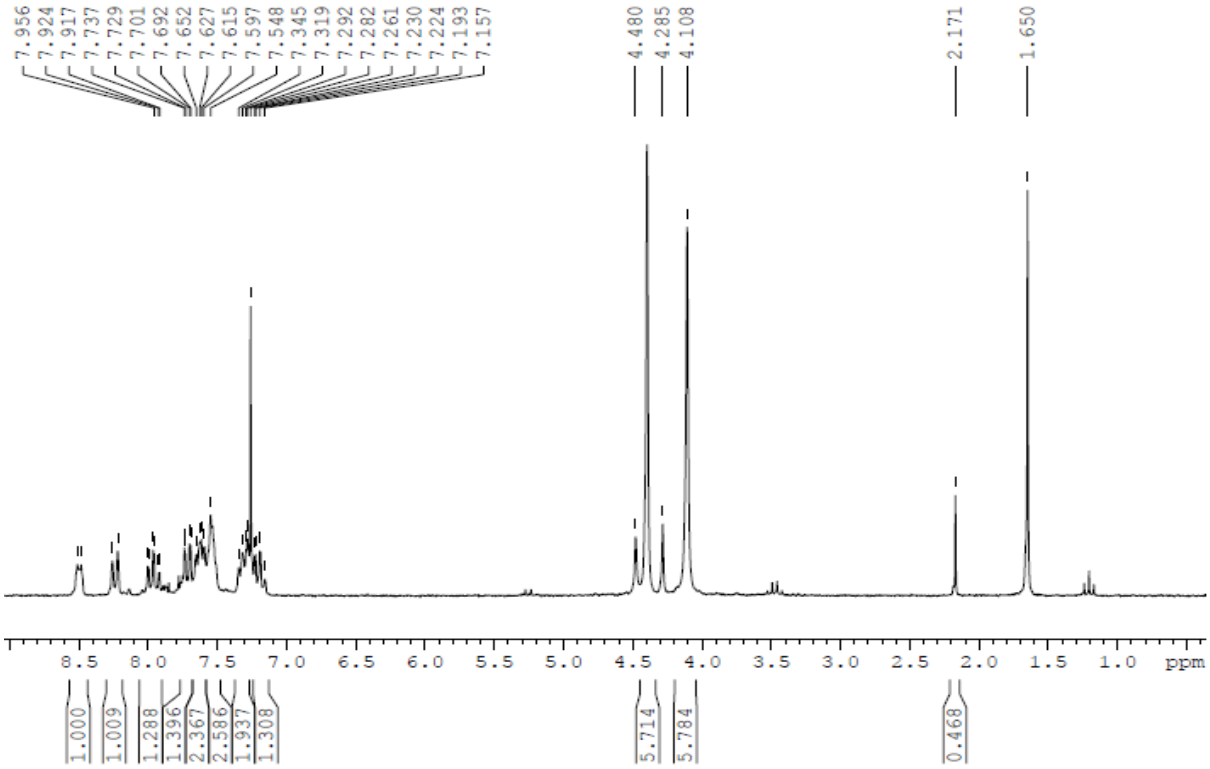
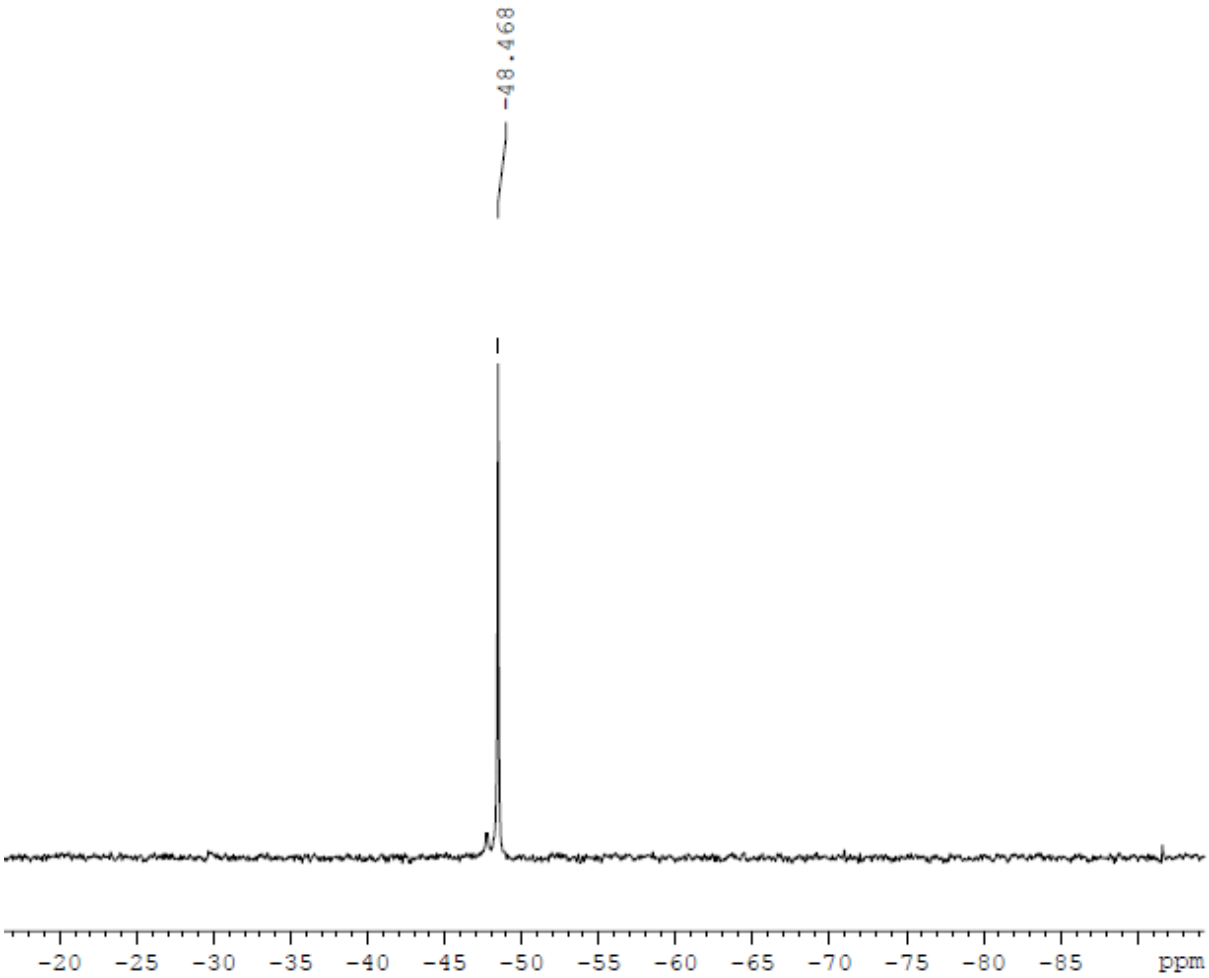


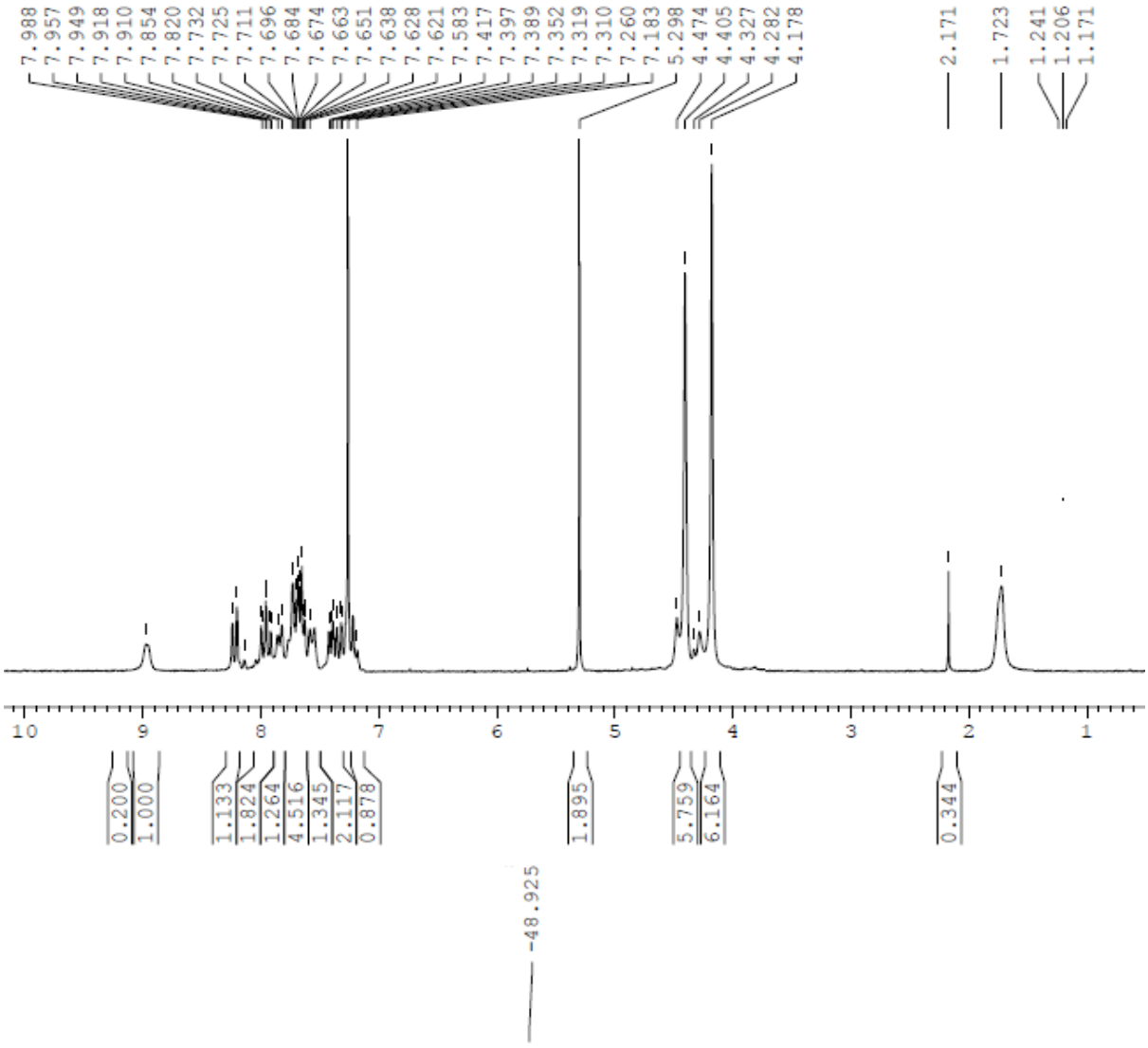


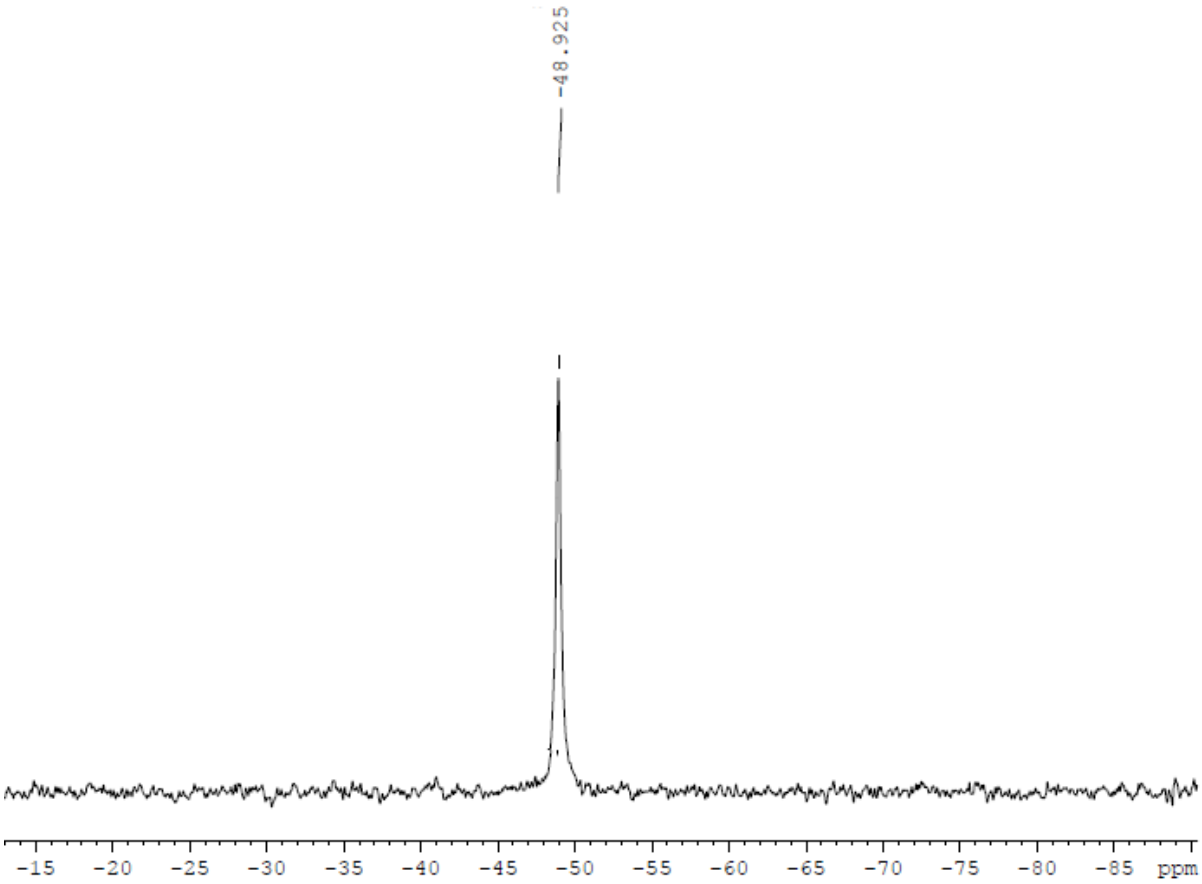
[Pd(Bzpy)(Phthalimidate)(PTA)] IIIa



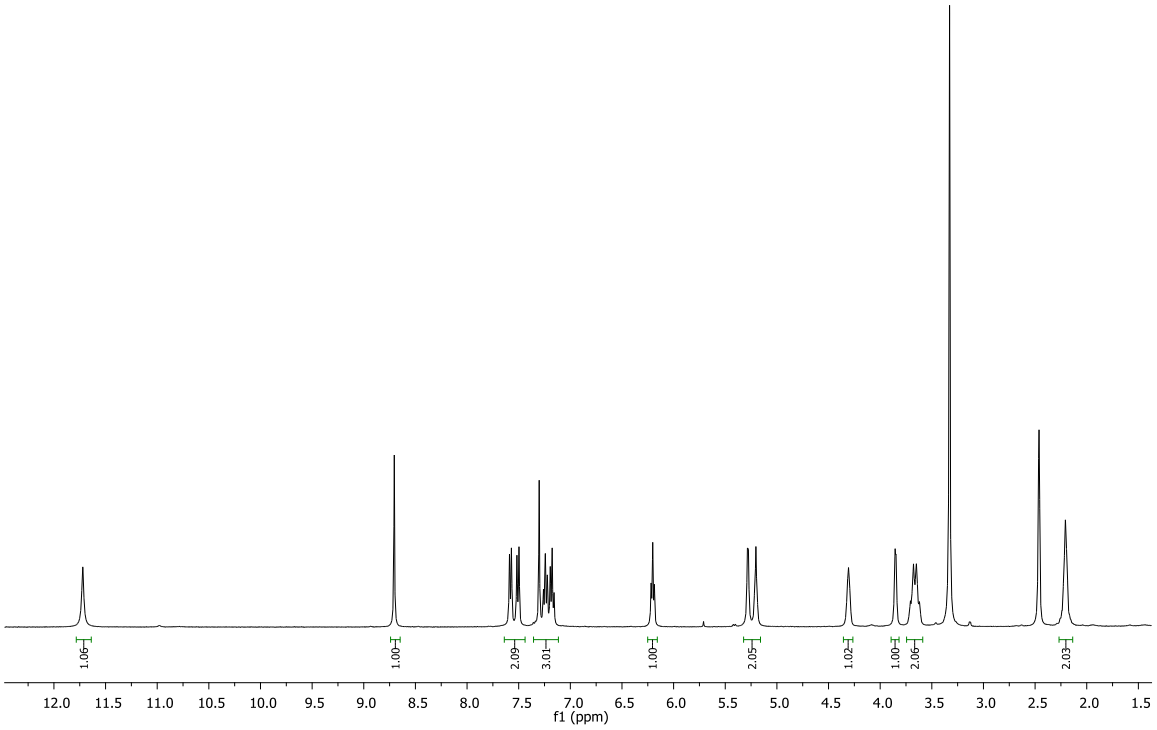


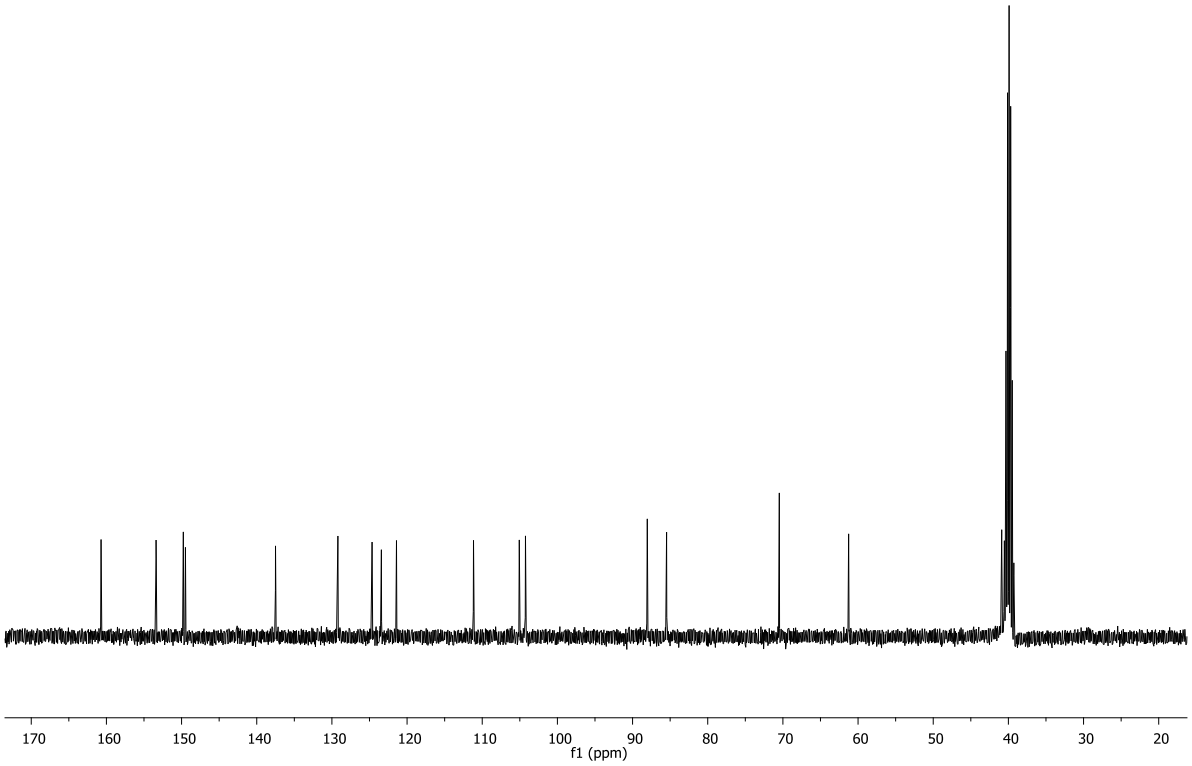
[Pd(Bzpy)(Saccharinate)(PTA)] IIIb





5-(2-Benzofuranyl)-2'-deoxyuridine (3a):-





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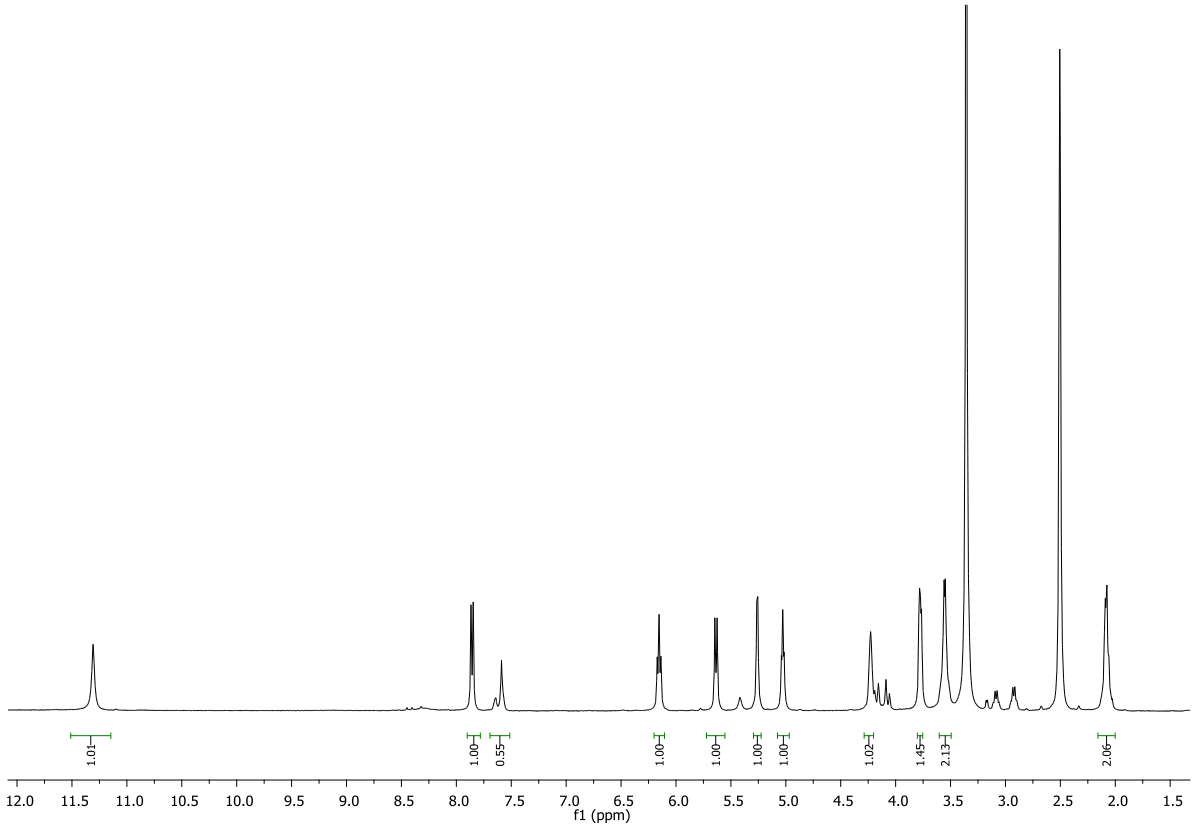

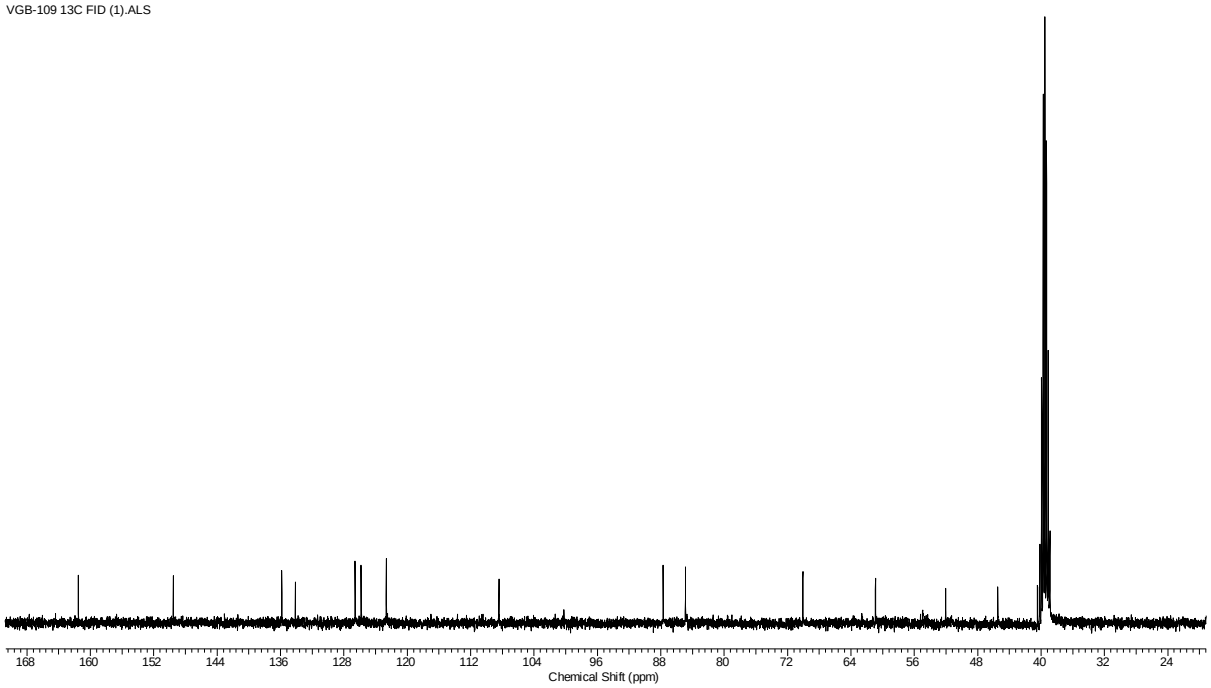

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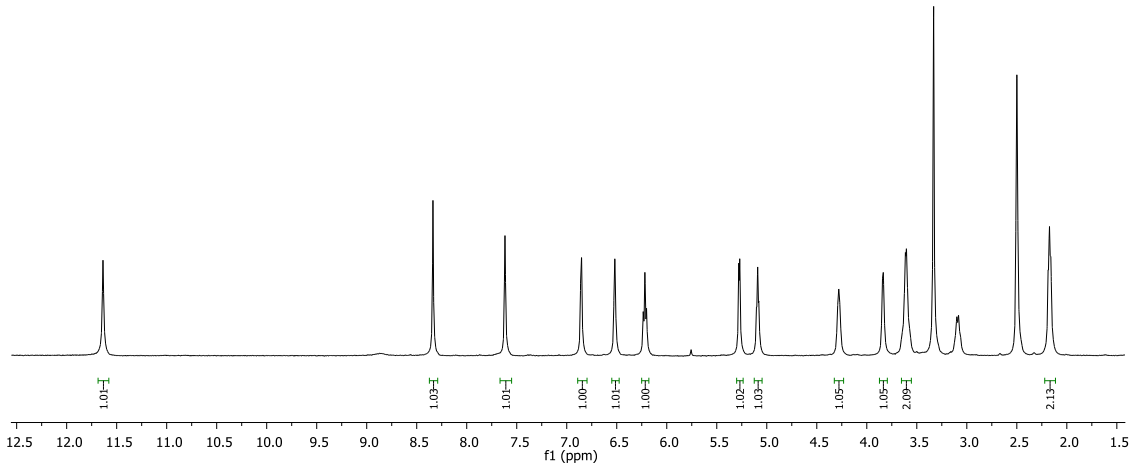
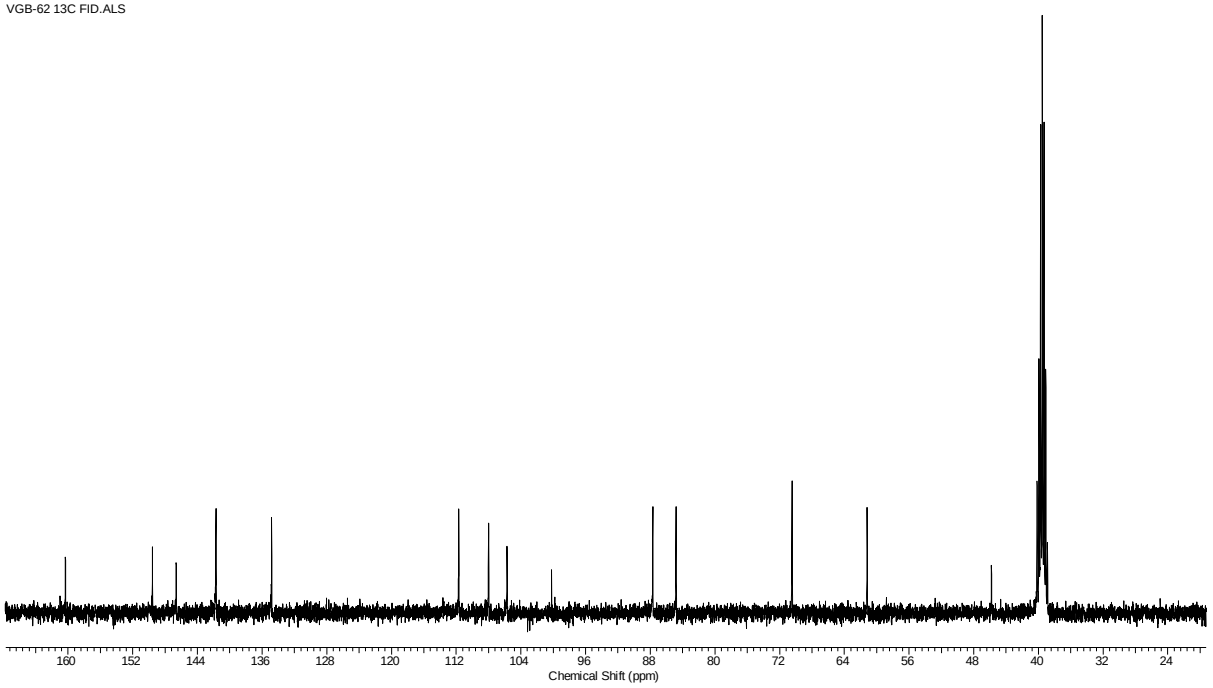
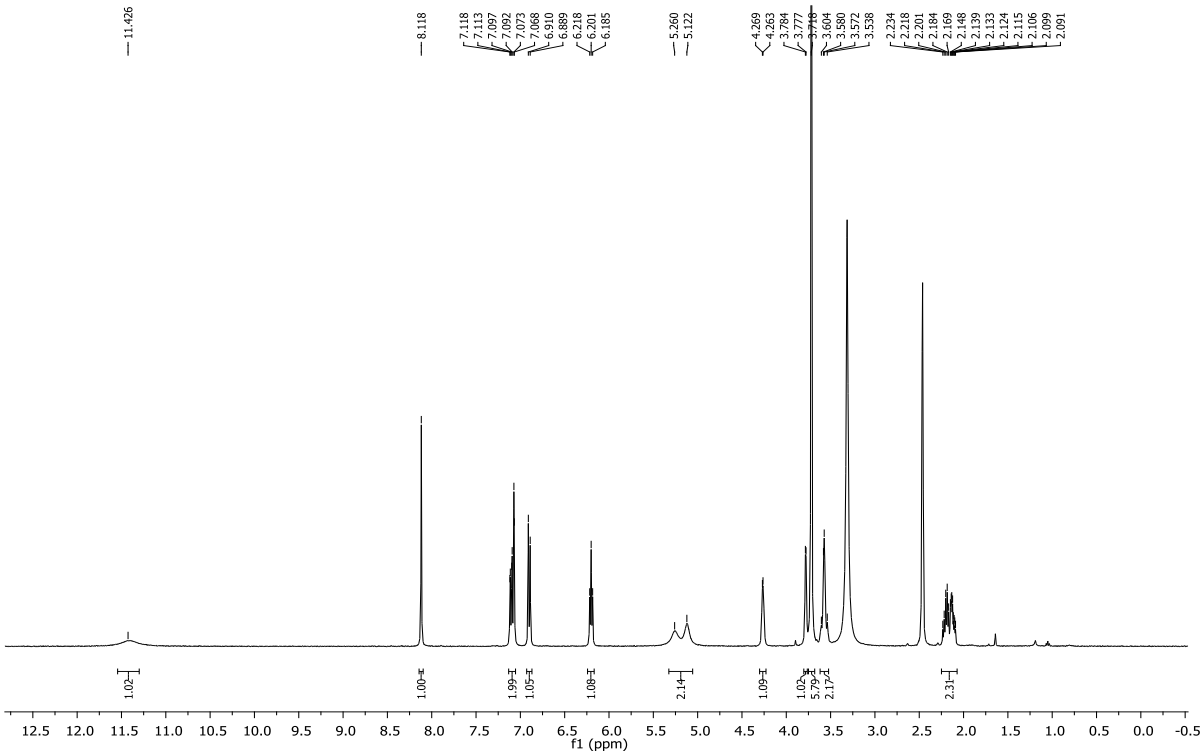
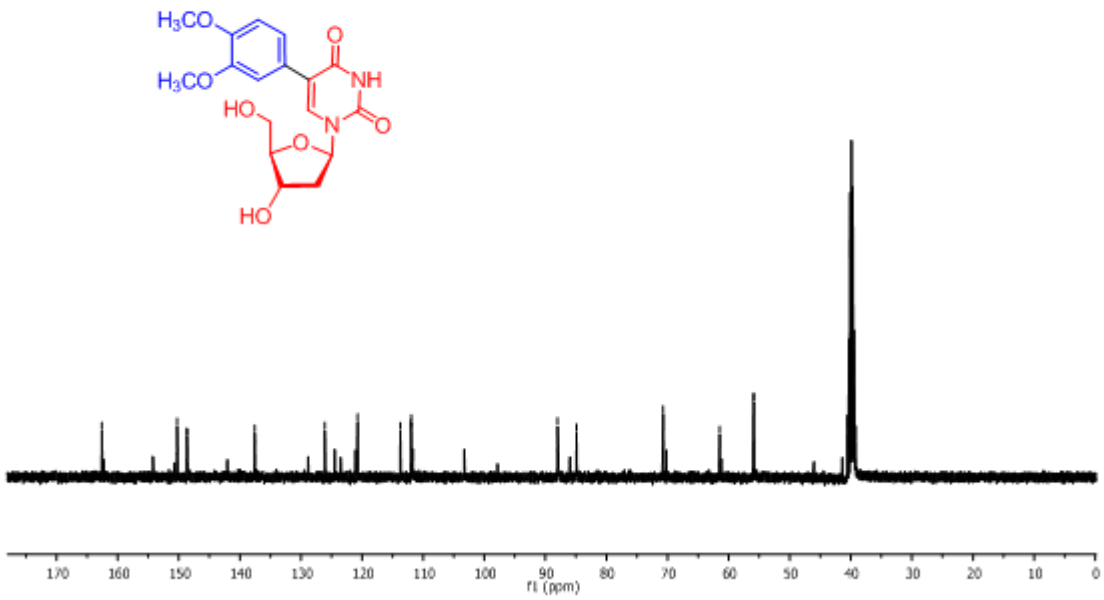




5-(3,4-Dimethoxy phenyl)-2'-deoxyuridine (3d):-





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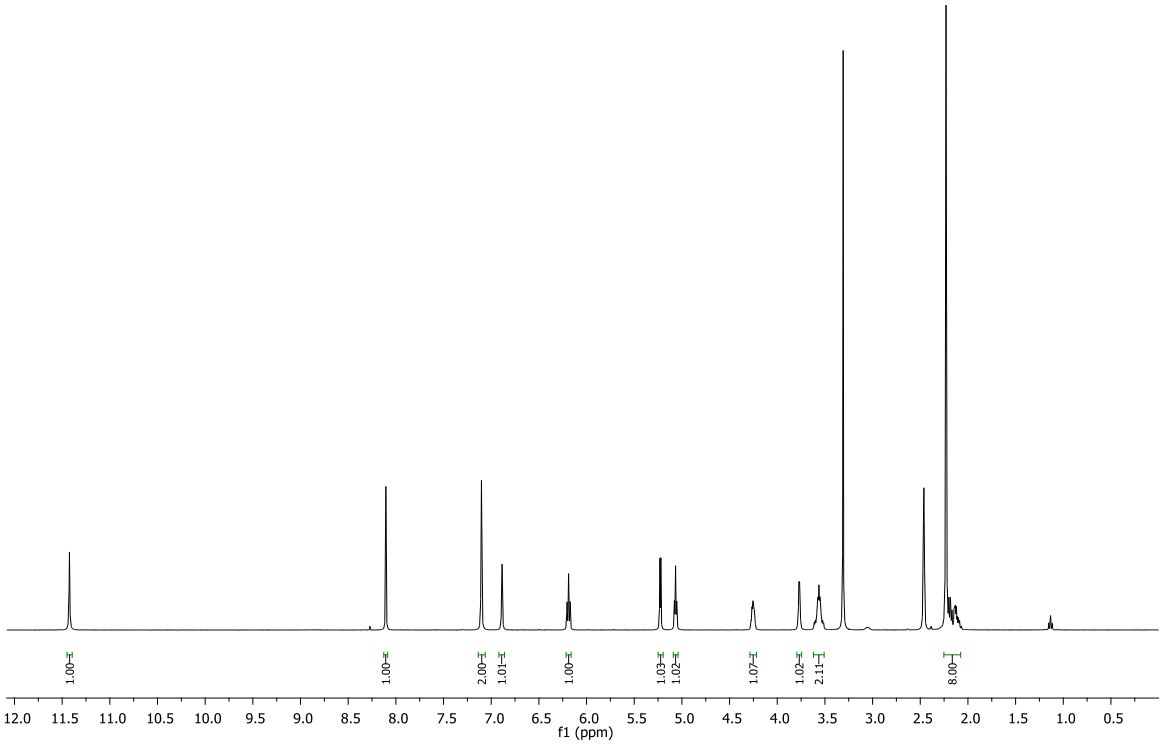

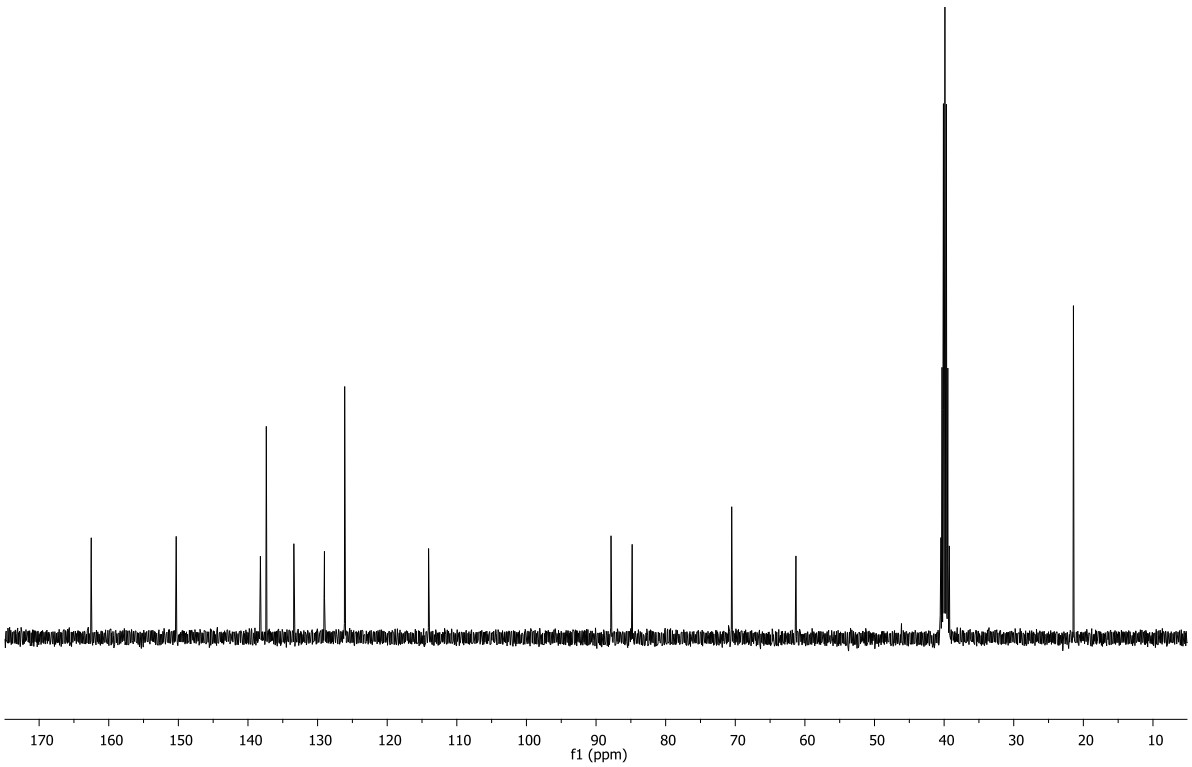

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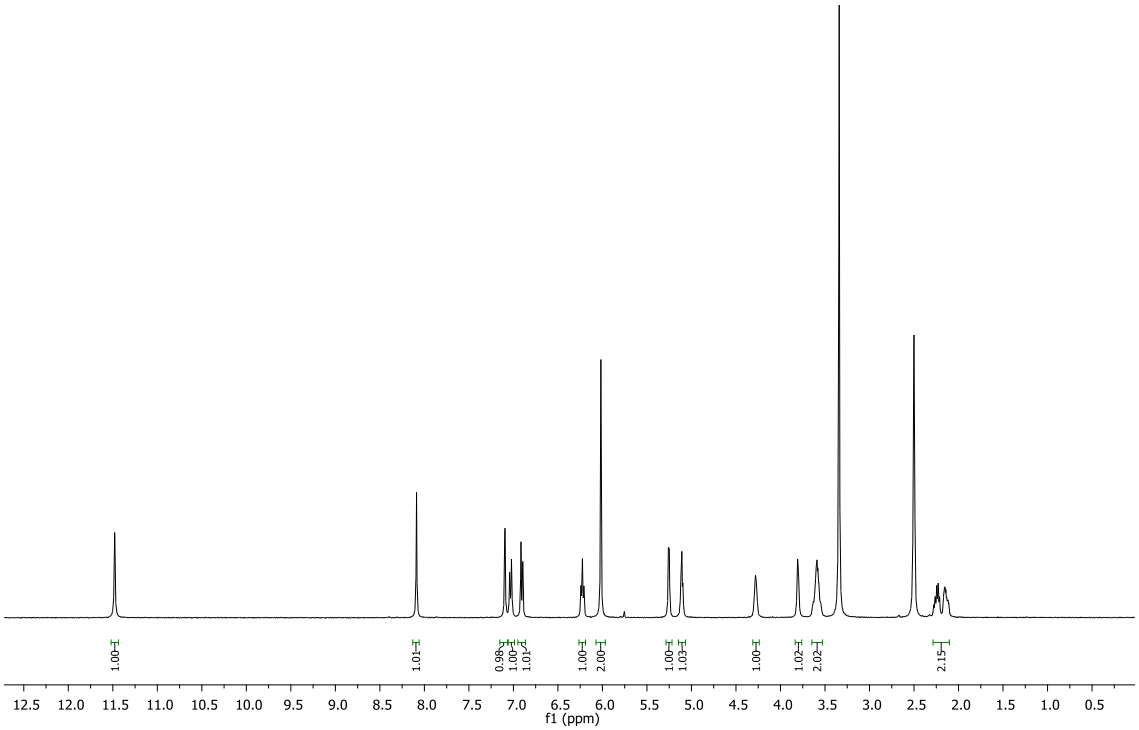
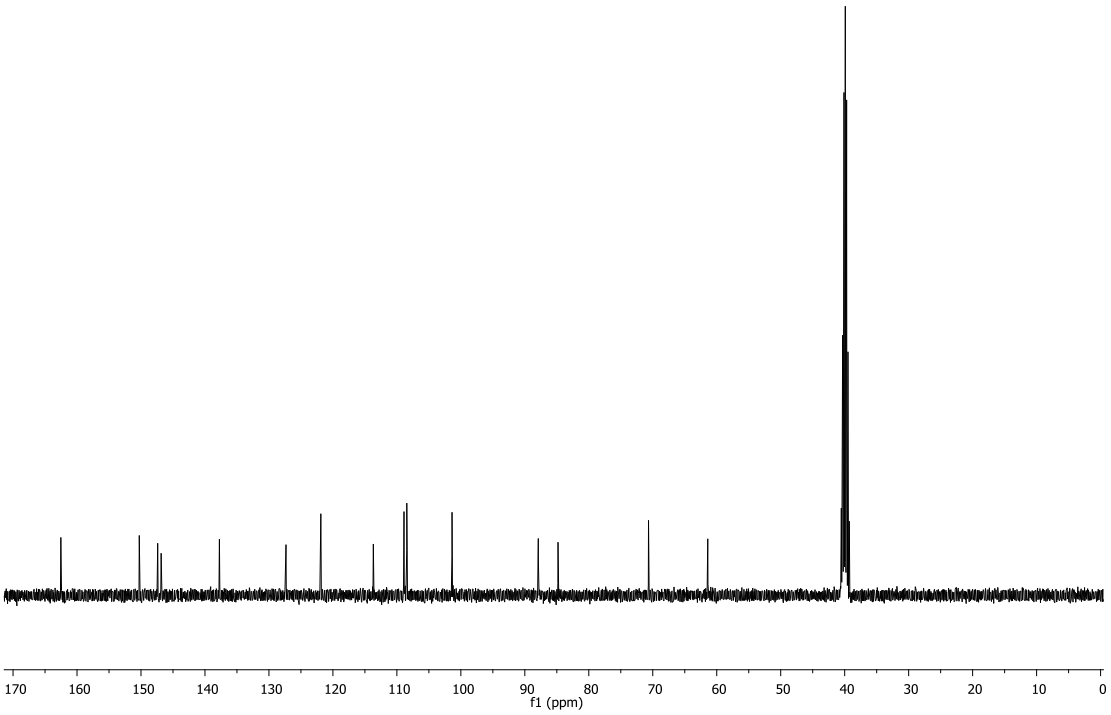
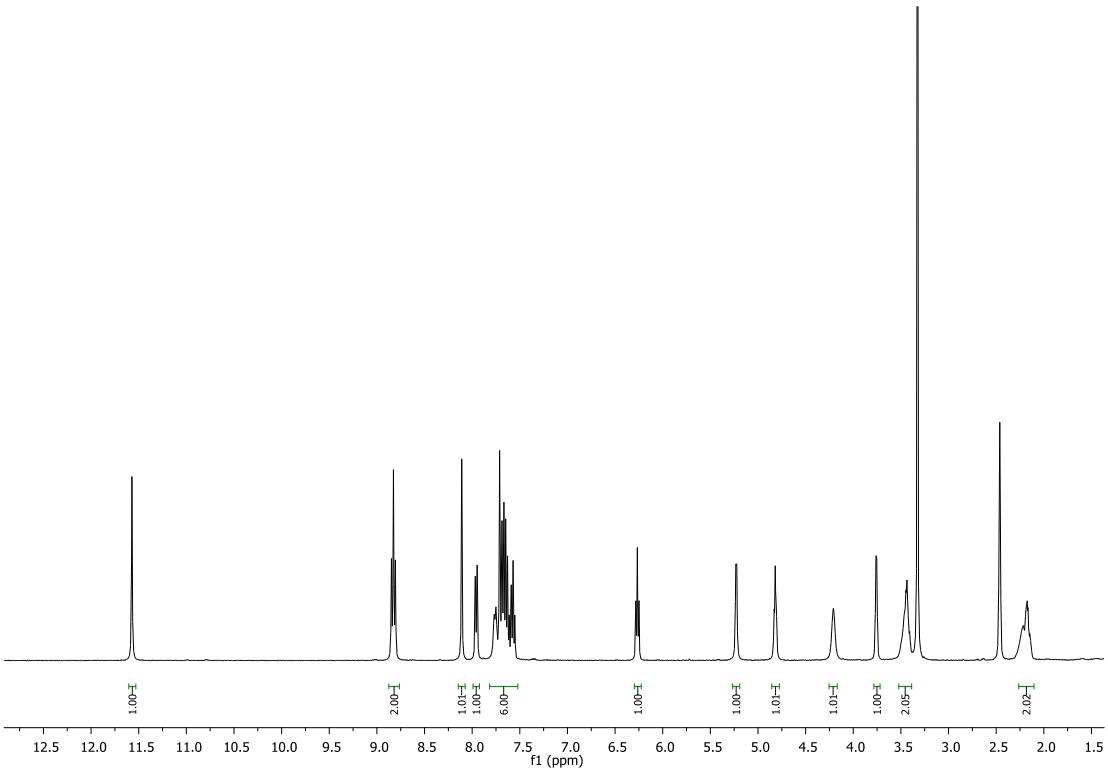
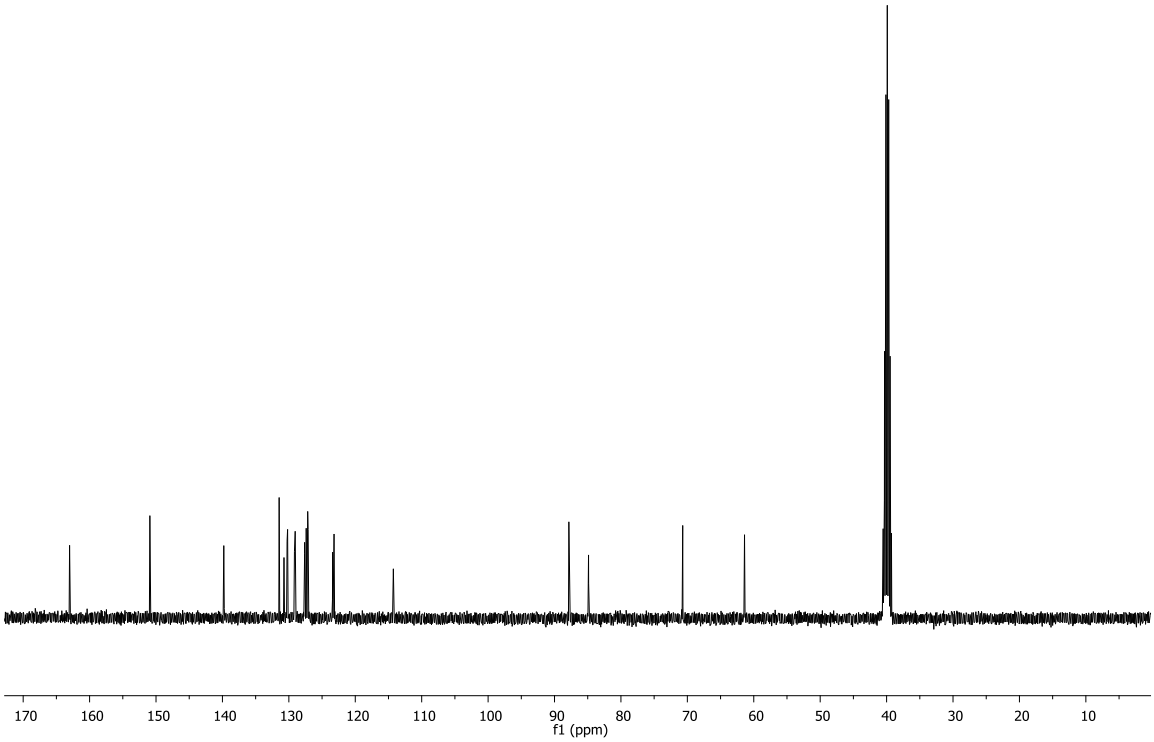




5-(Phenanthren-9-yl)-2'-deoxyuridine (3g)





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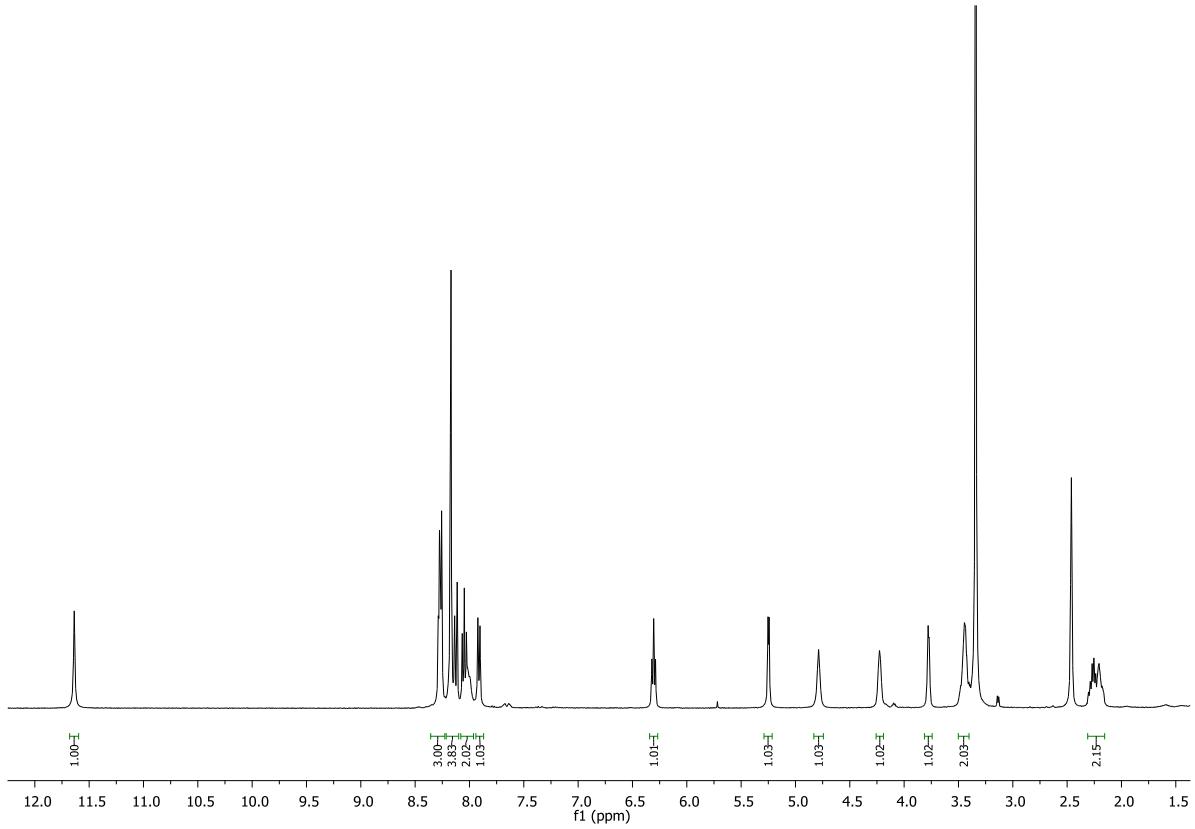

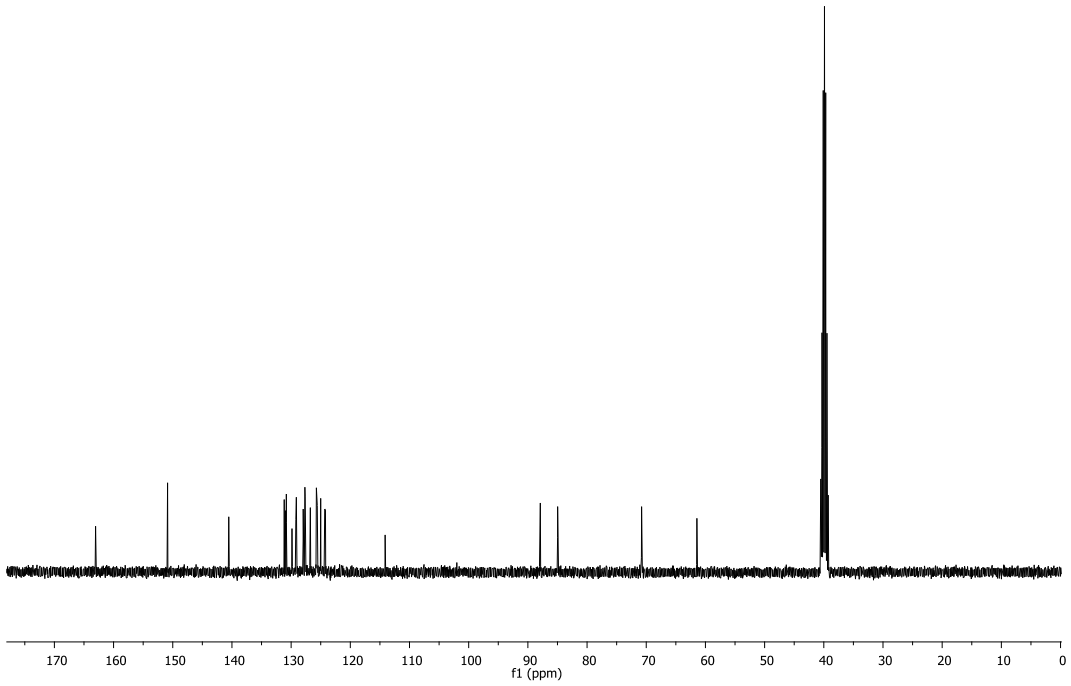

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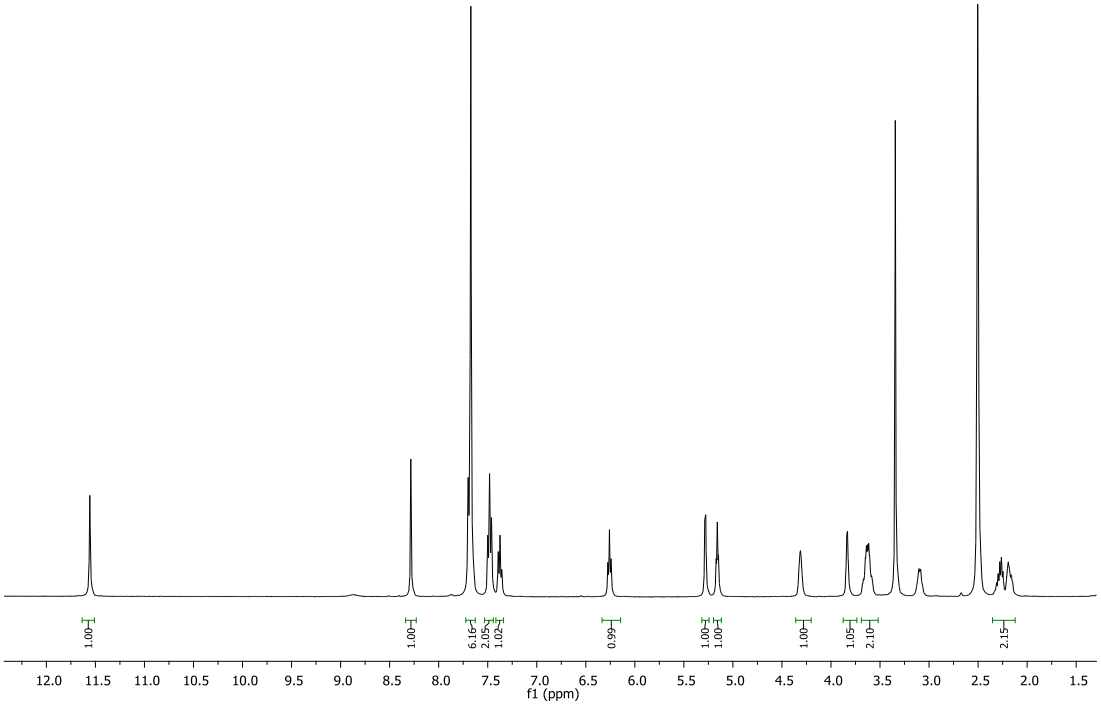
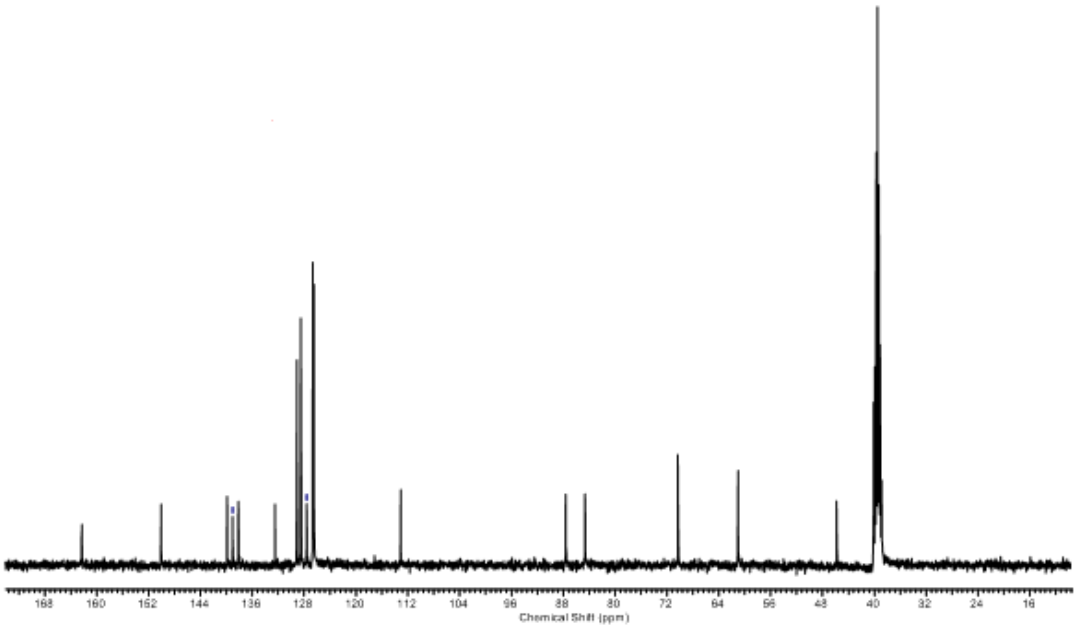
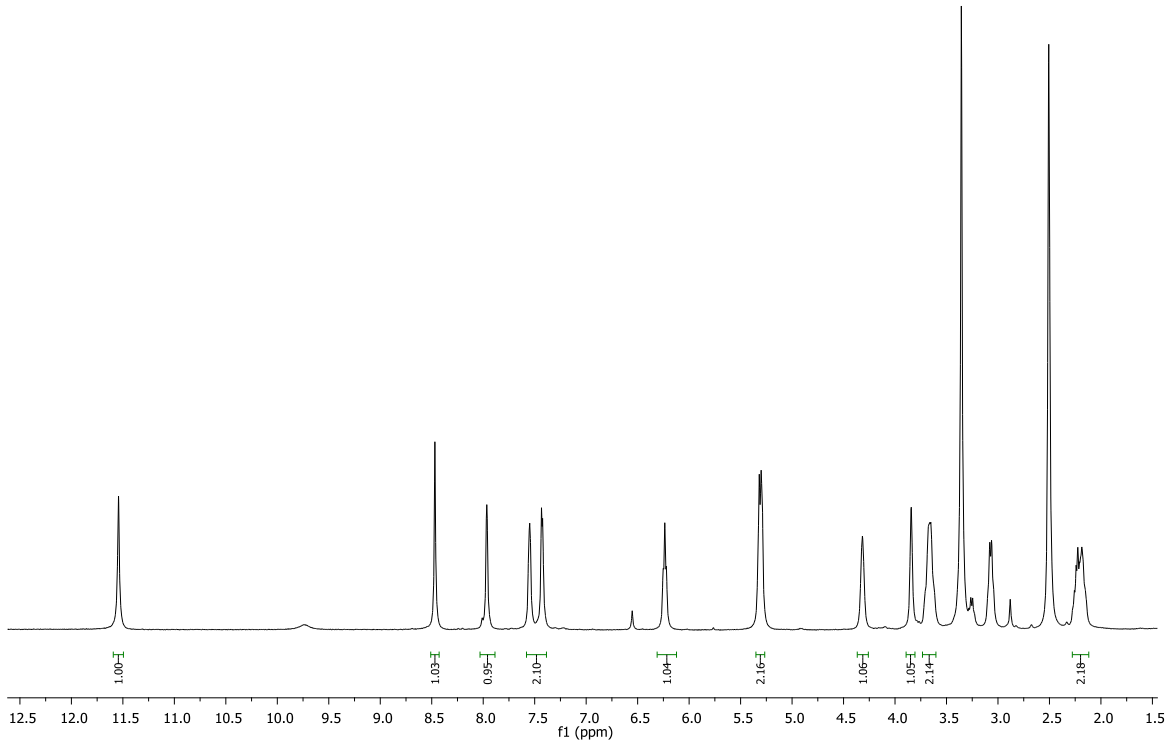
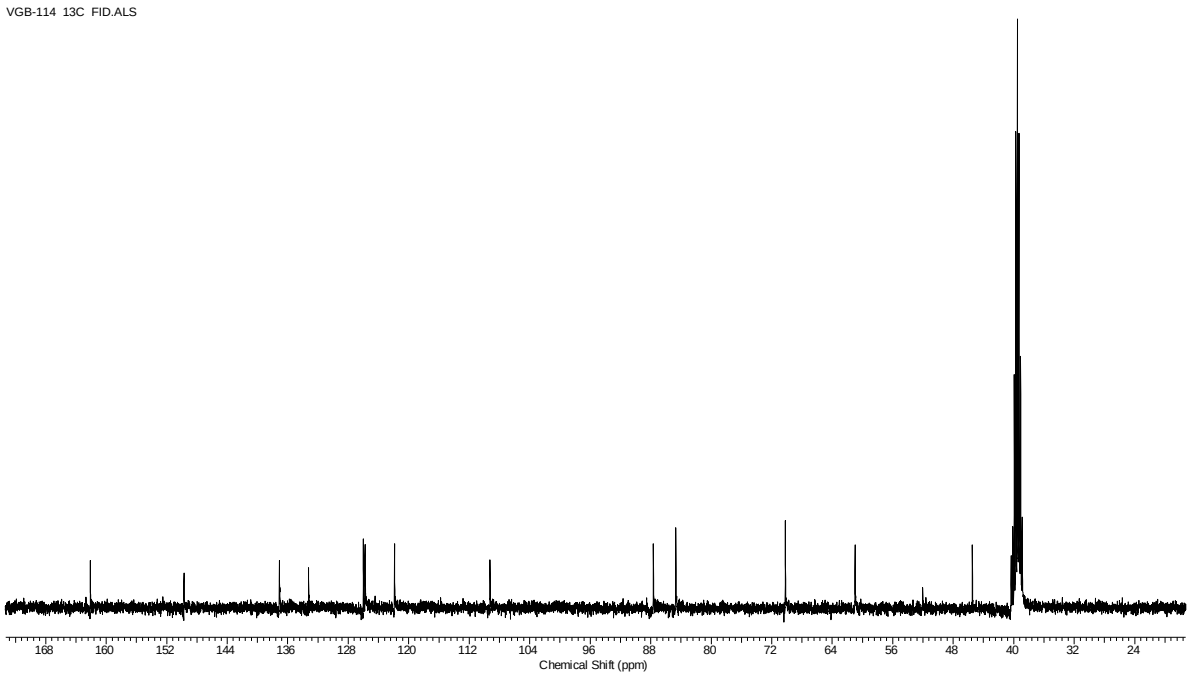


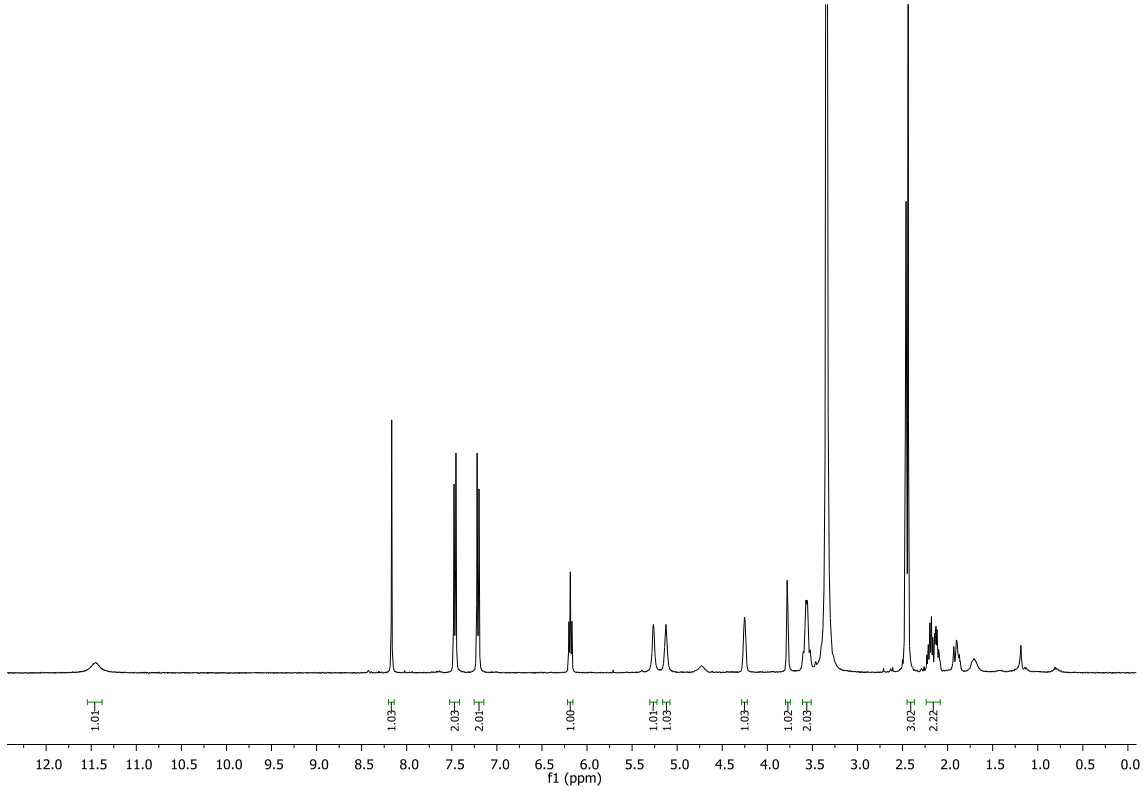


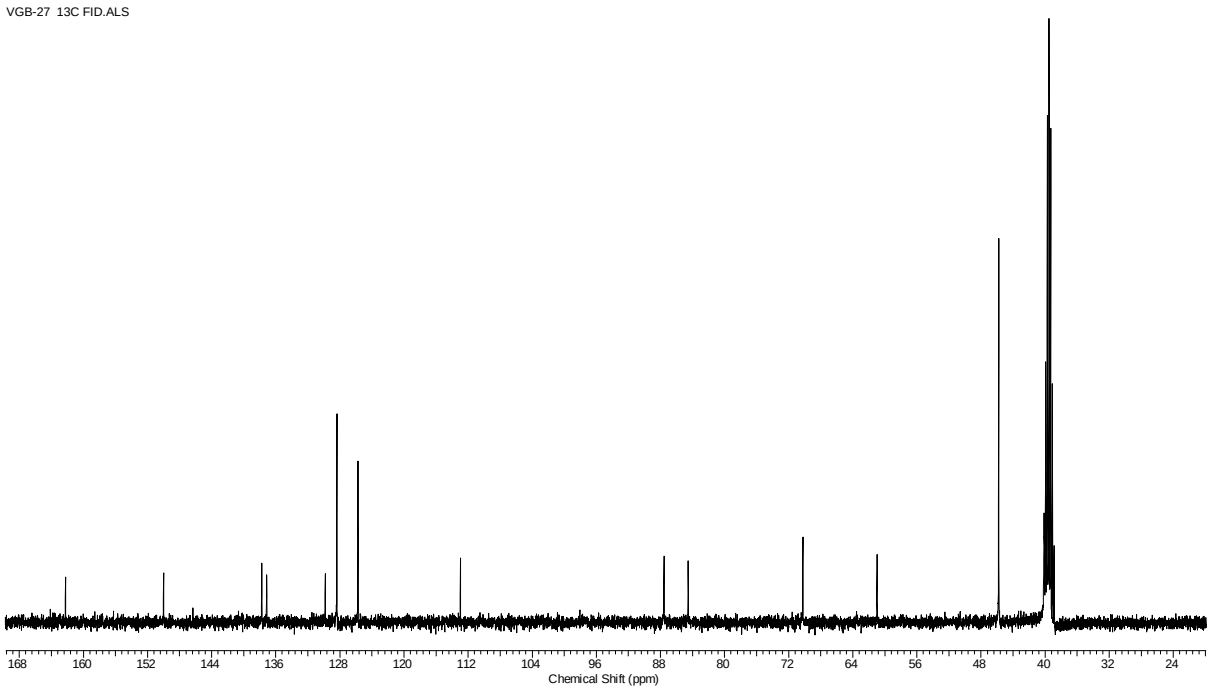
5-(Thiophen-3-yl)- 2'-deoxyuridine (3j)





5-(4-(Methylthio)phenyl)-2'-deoxyuridine (3k):-





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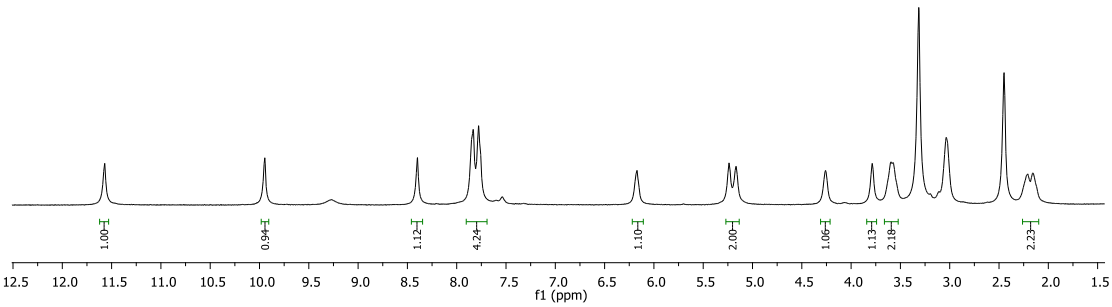
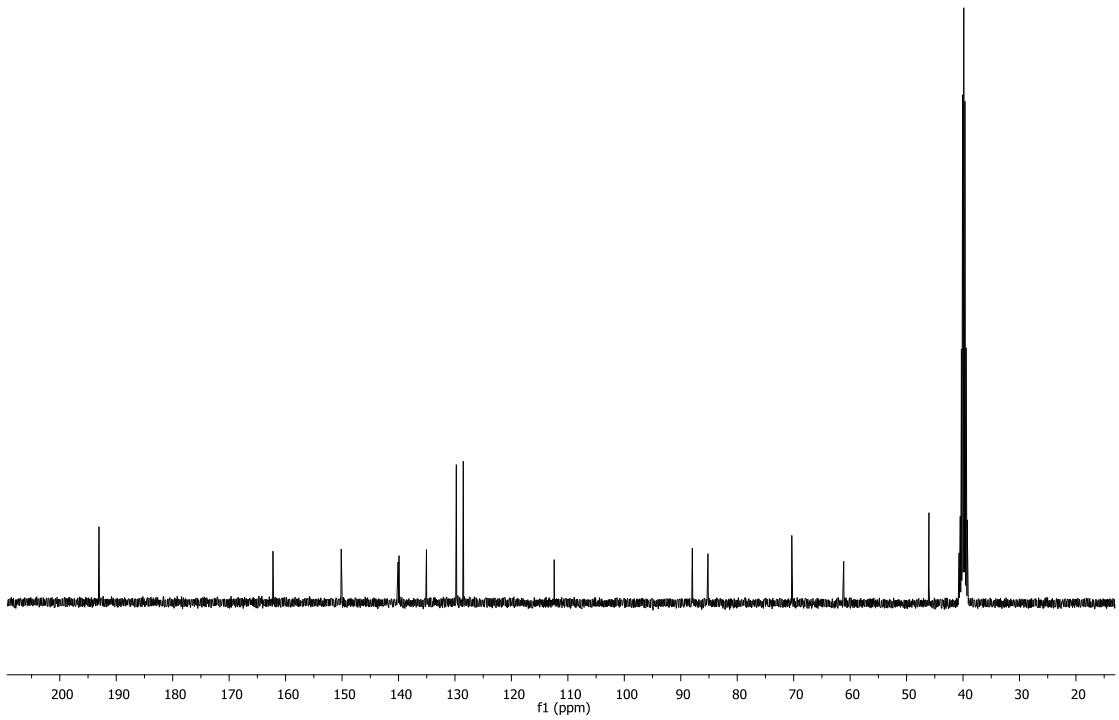
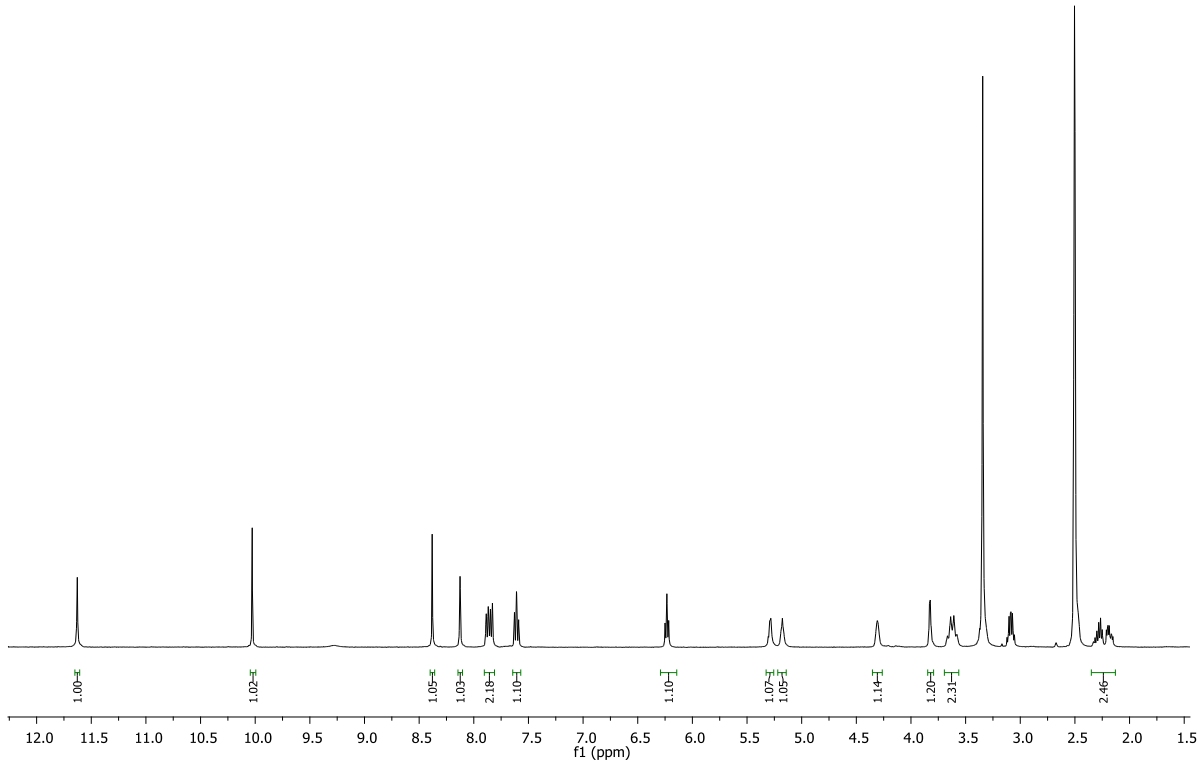
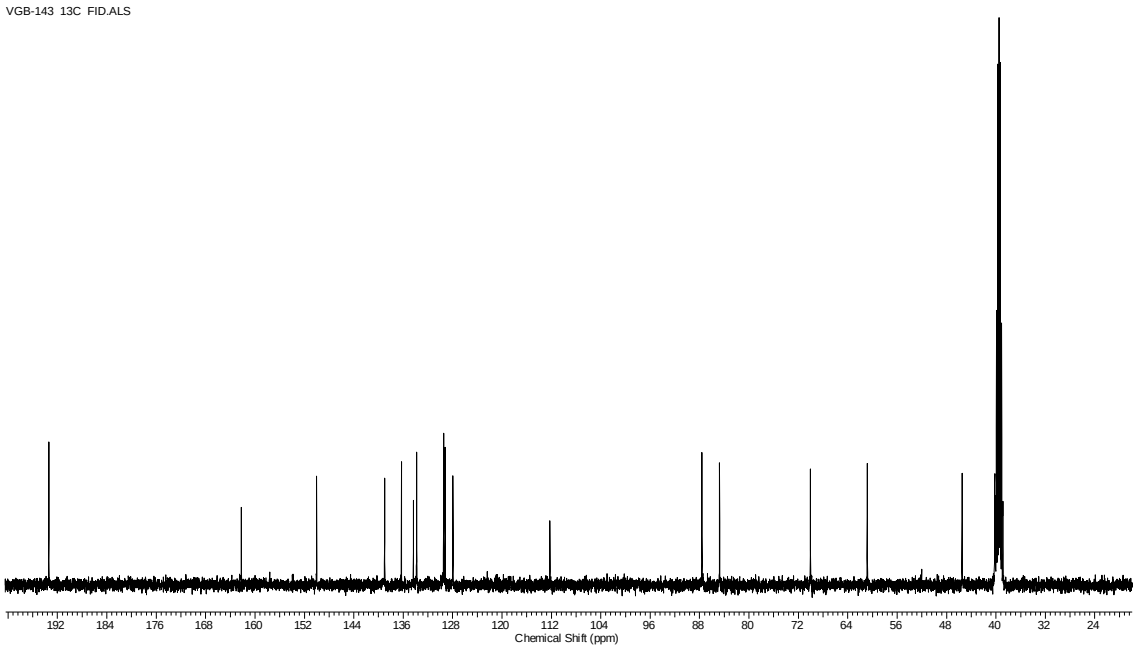


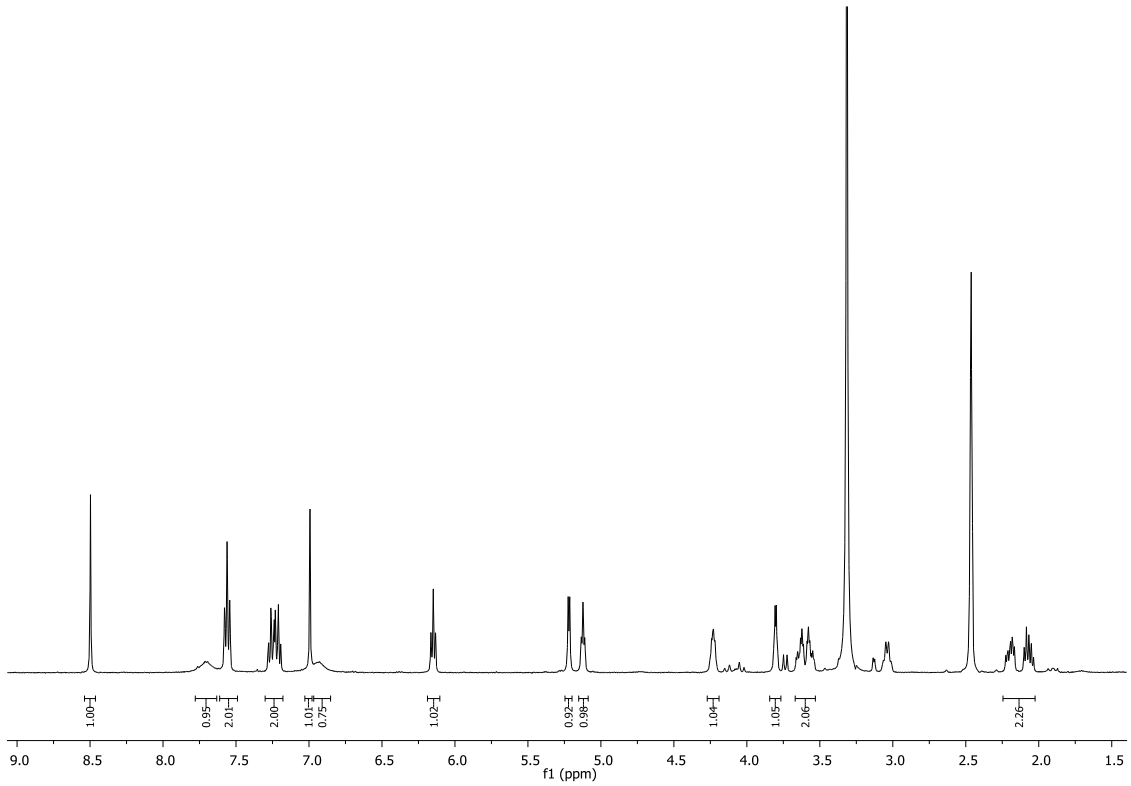


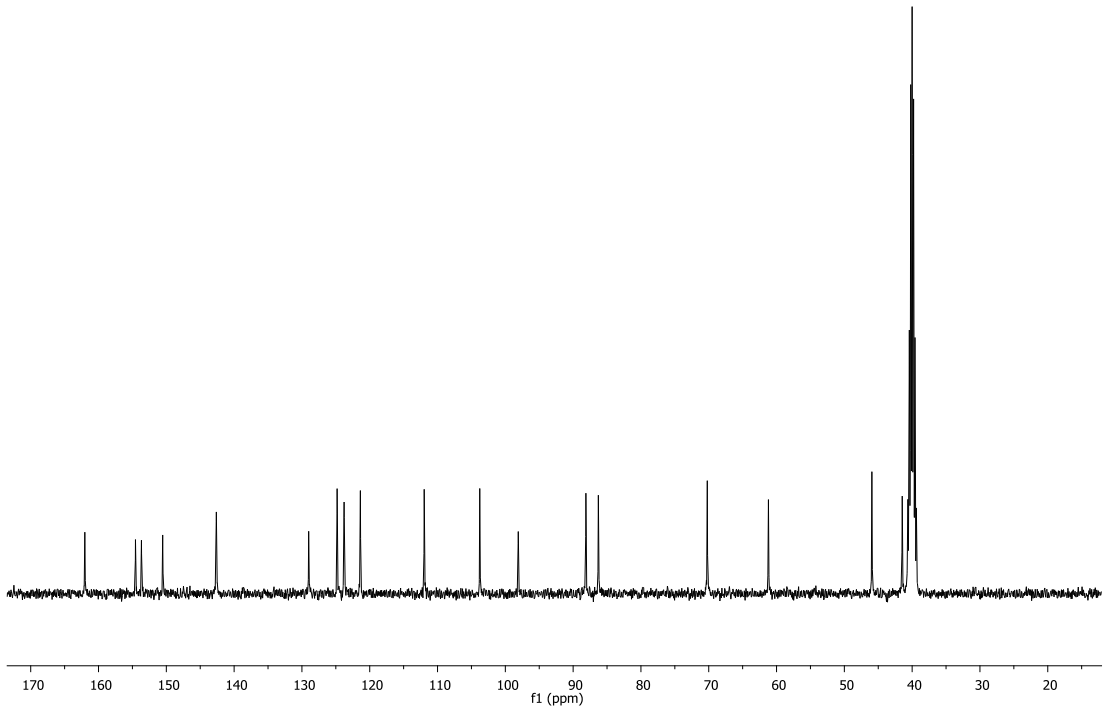
5-(3-Formyl phenyl)-2'-deoxyuridine (3m)



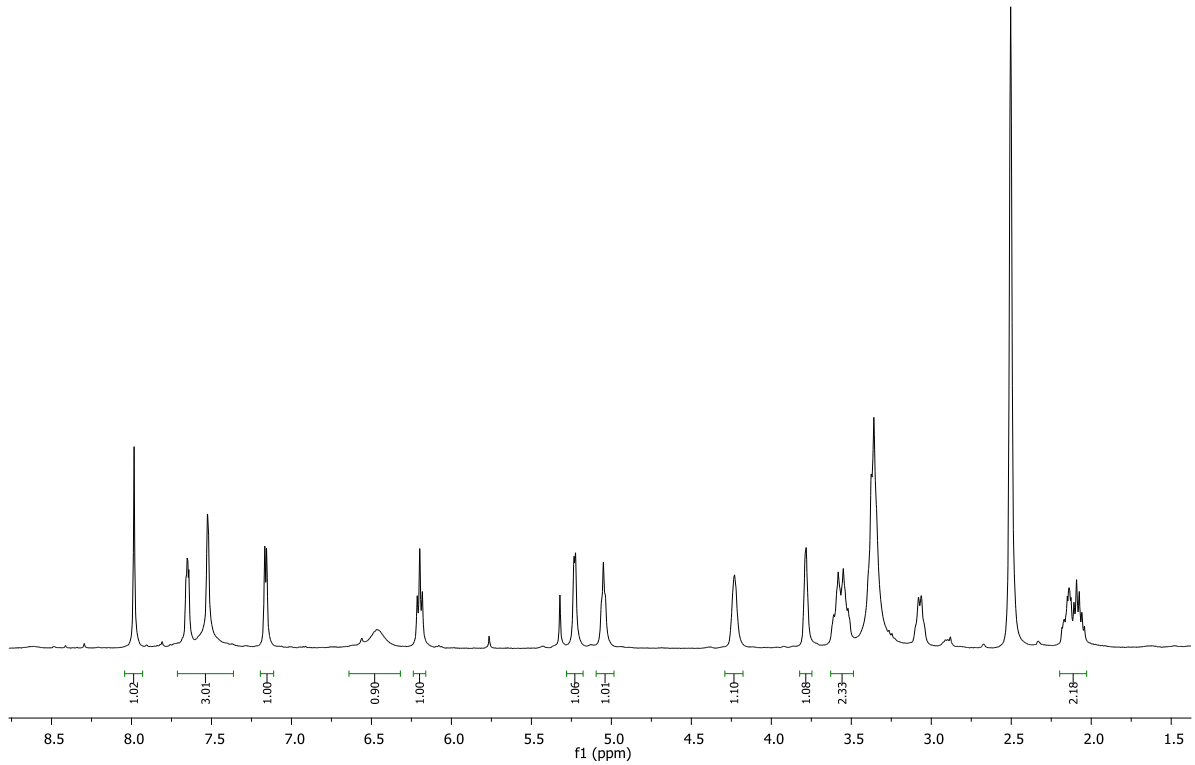


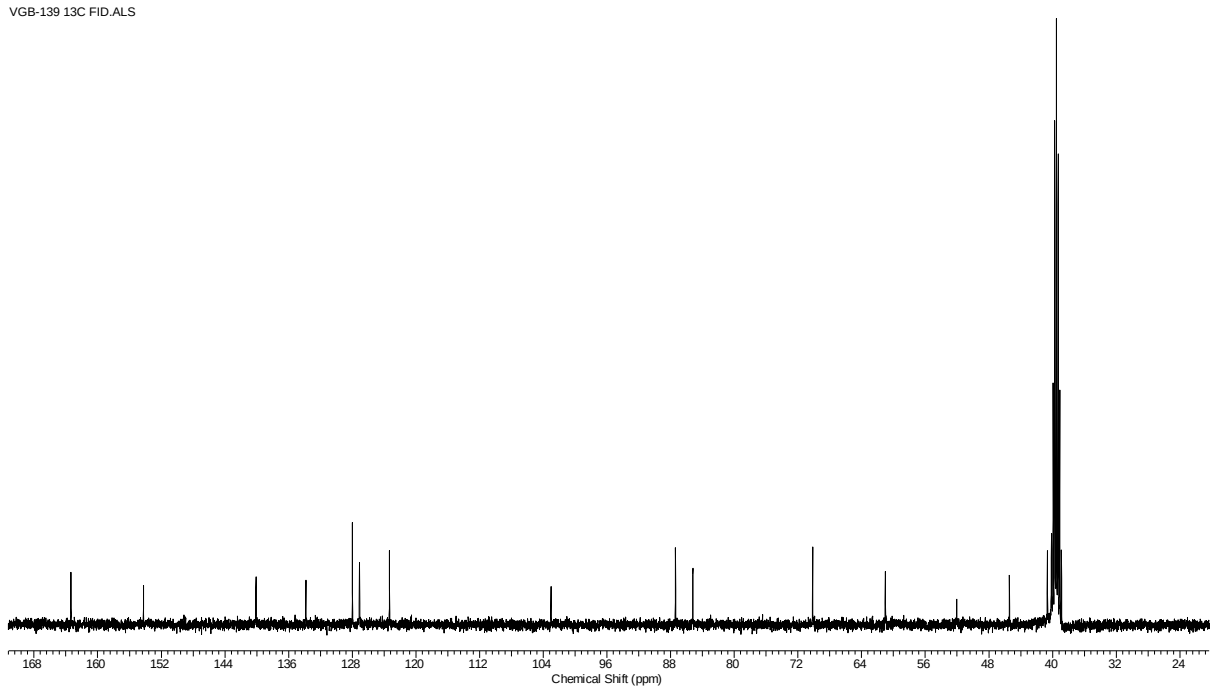
5-(2-Benzofuranyl)-2'-deoxycytidine (5a)



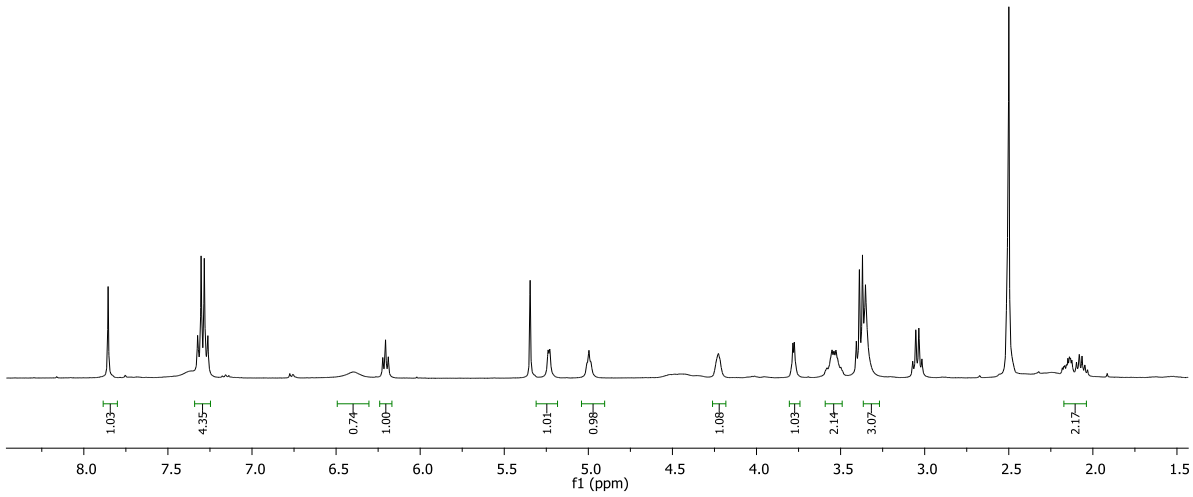


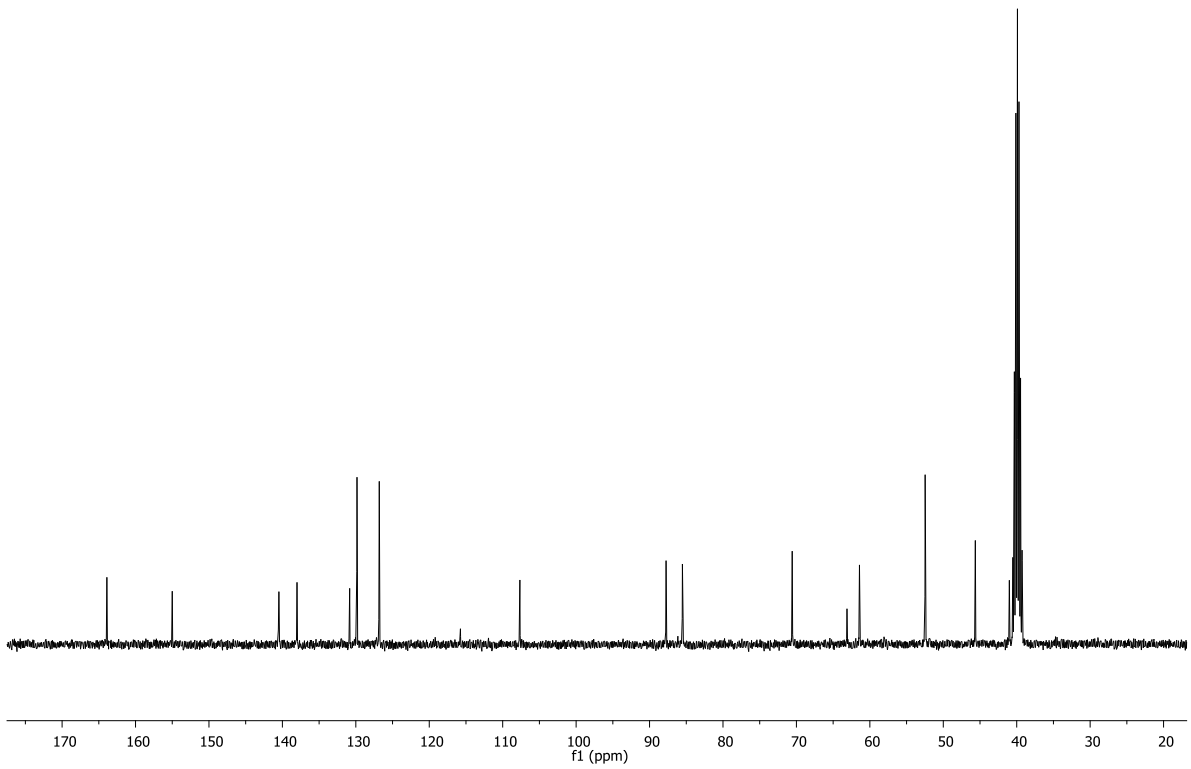
5-(Thiophen-3-yl)-2'-deoxycytidine (5b):-



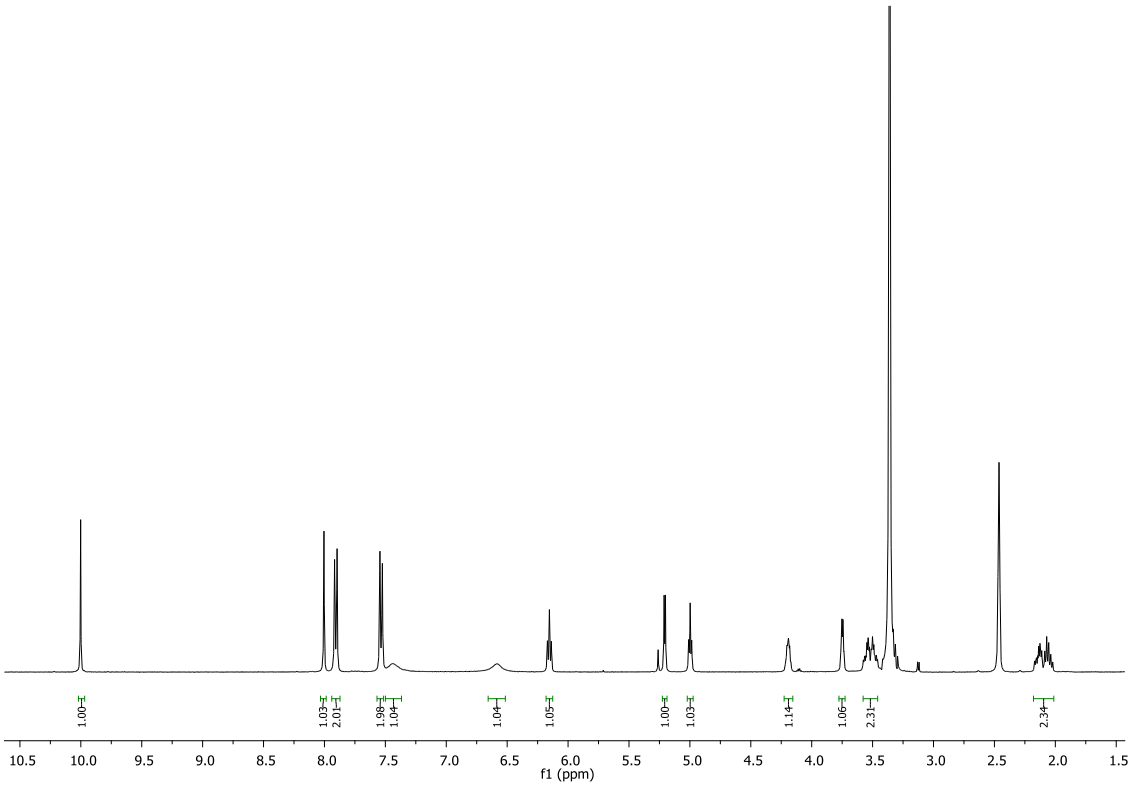


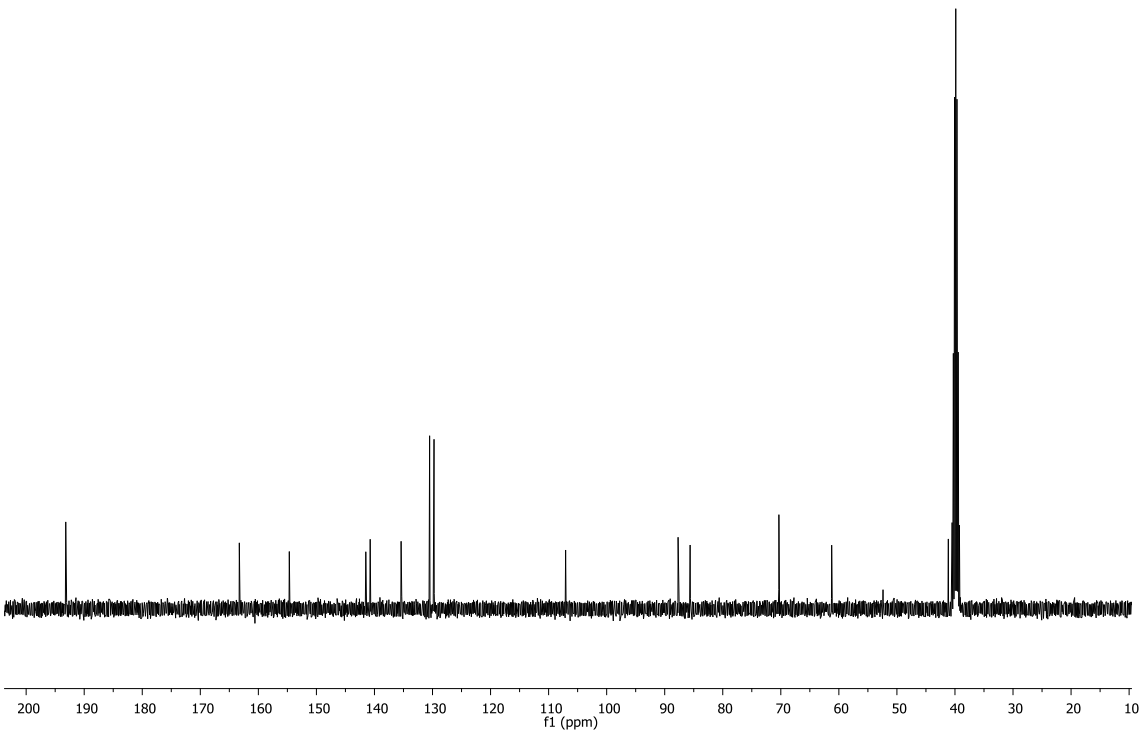
5-(4-(Methylthio)phenyl)-2'-deoxycytidine (5c)



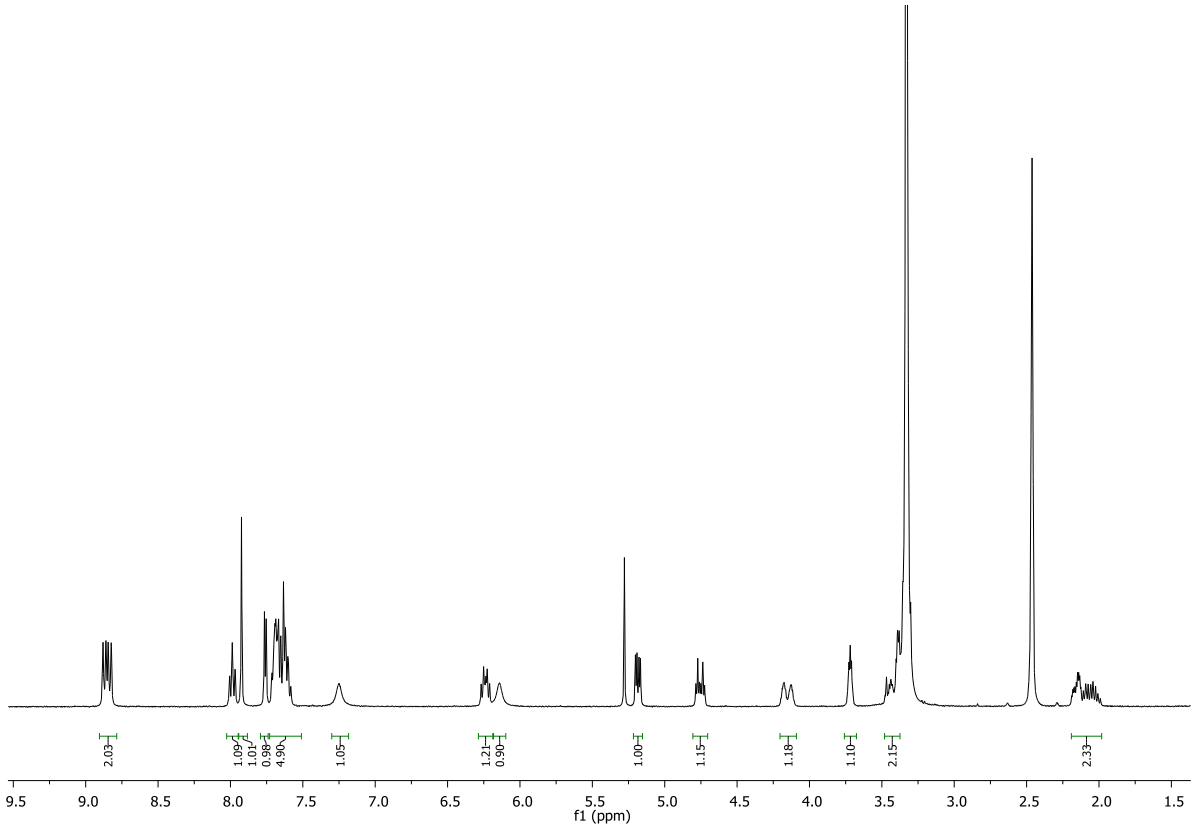


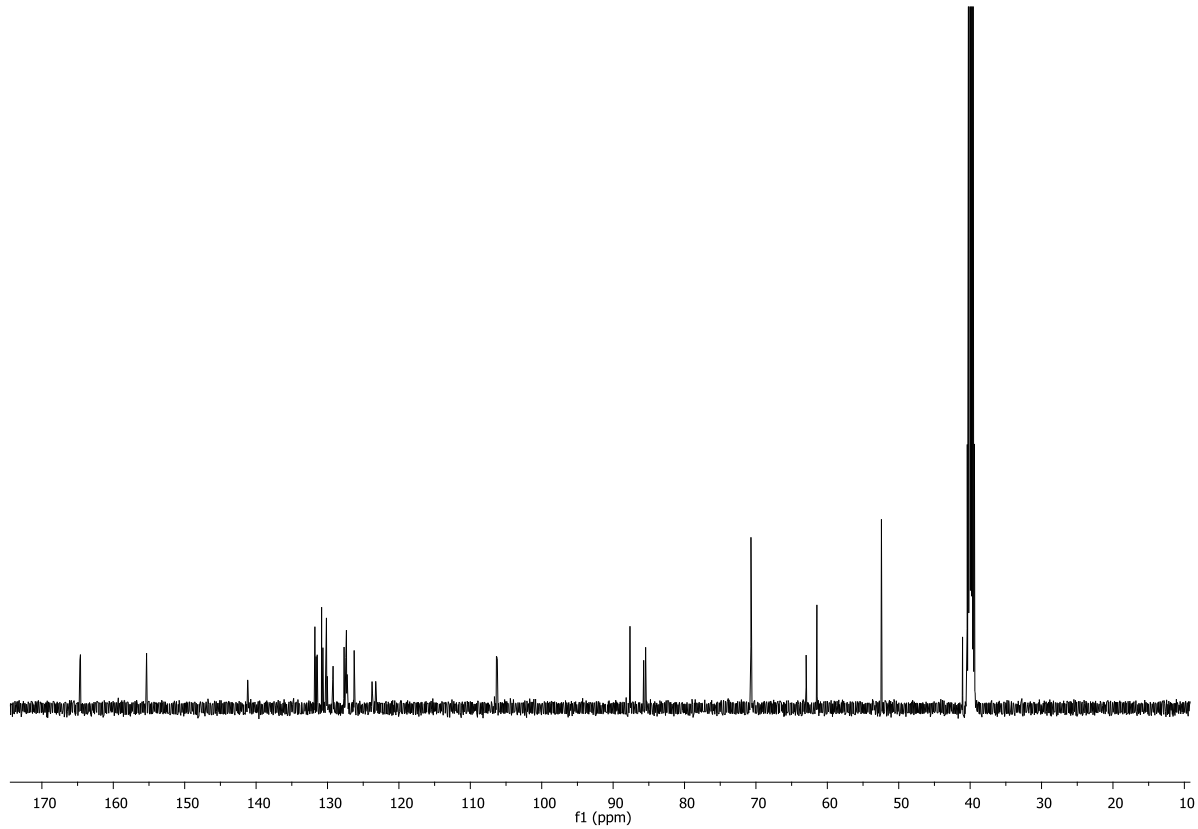
5-(4-Formyl phenyl)-2'-deoxycytidine (5d)



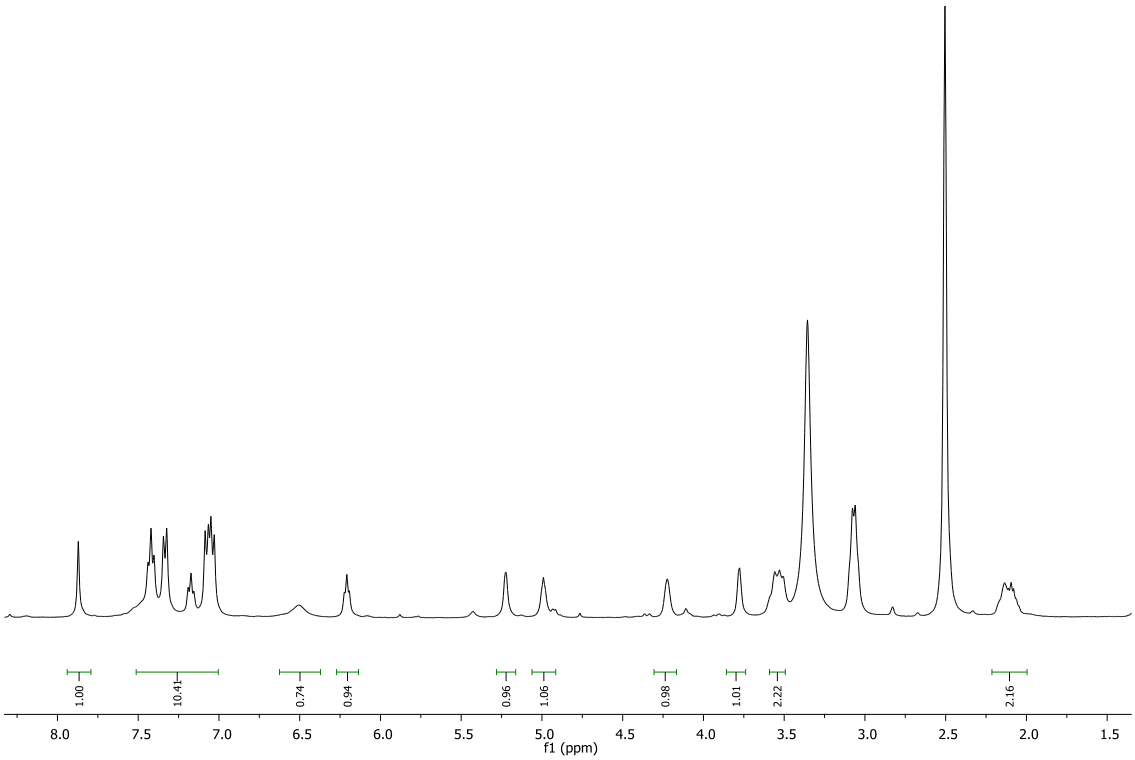


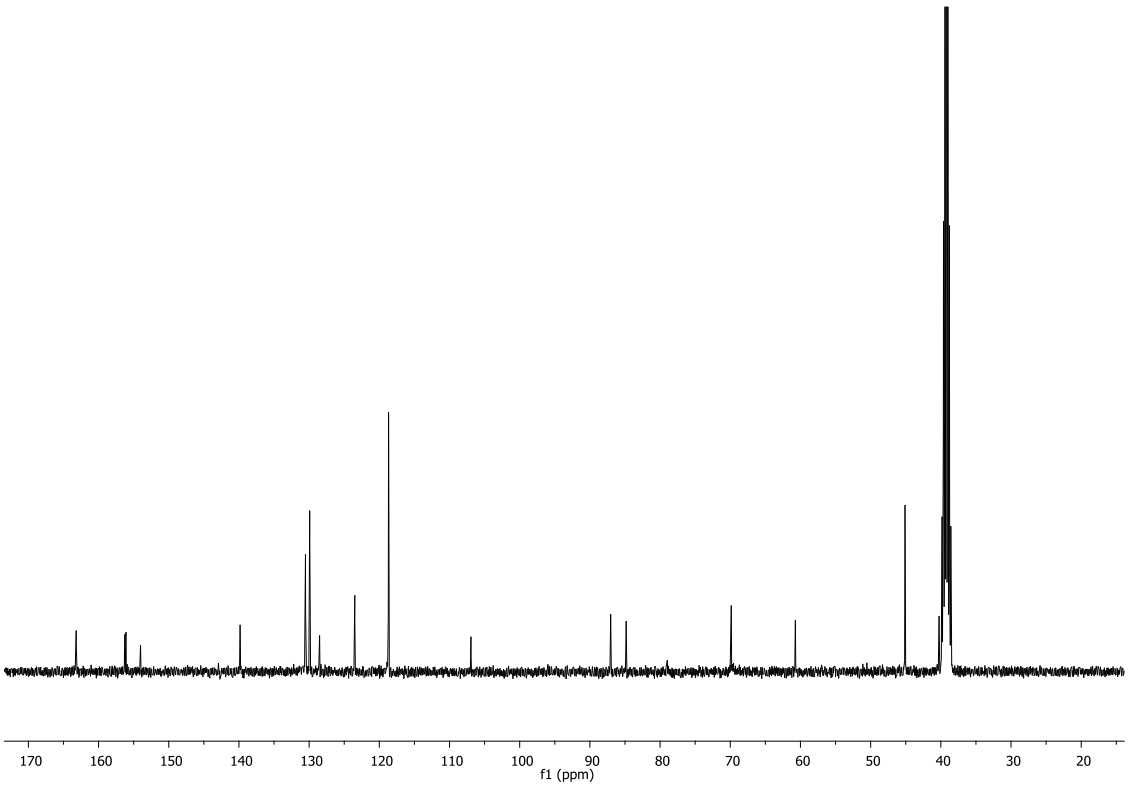
5-(Phenanthren-9-yl)-2'-deoxycytidine (5e)



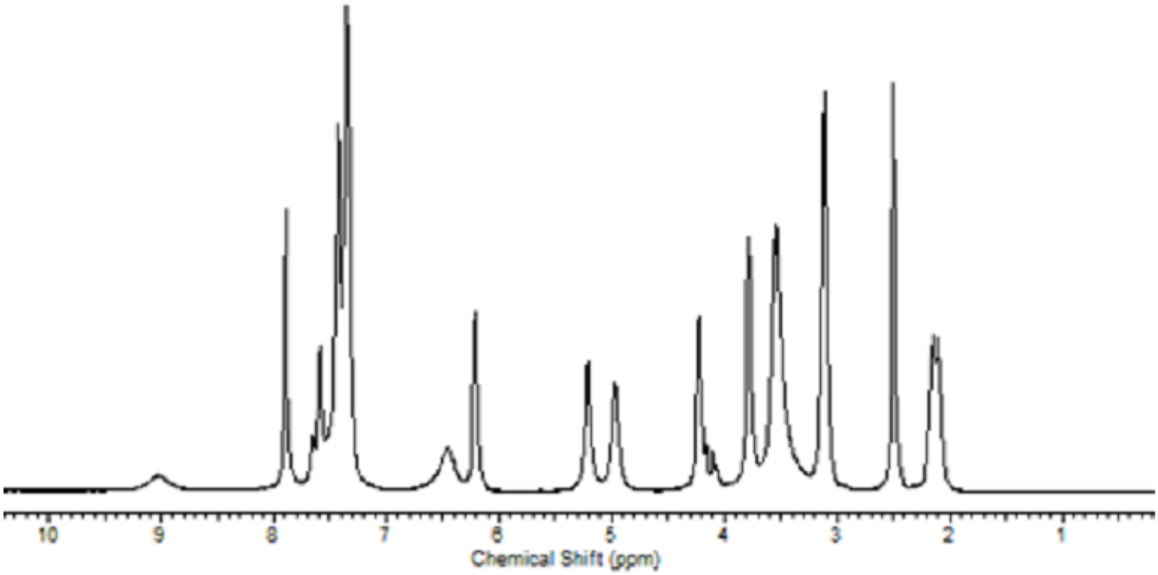


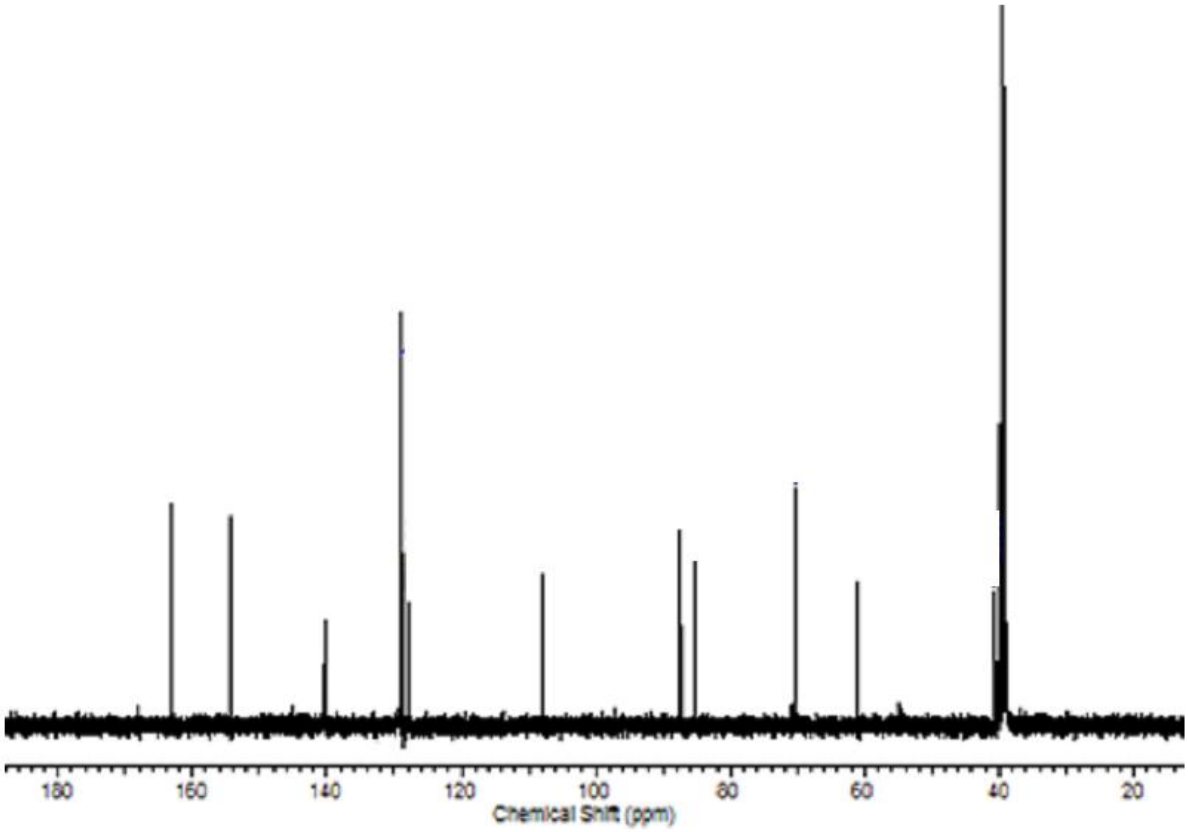
5-(4-Phenoxyphenyl)-2'-deoxycytidine (5f)



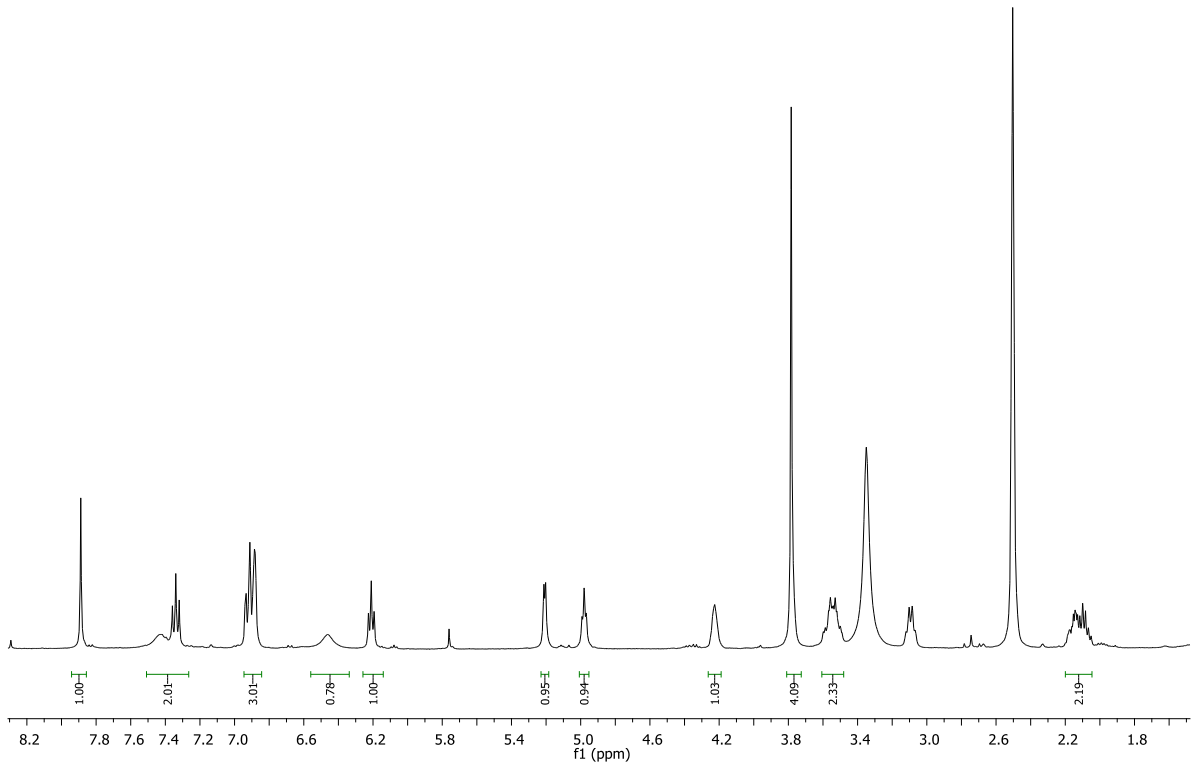


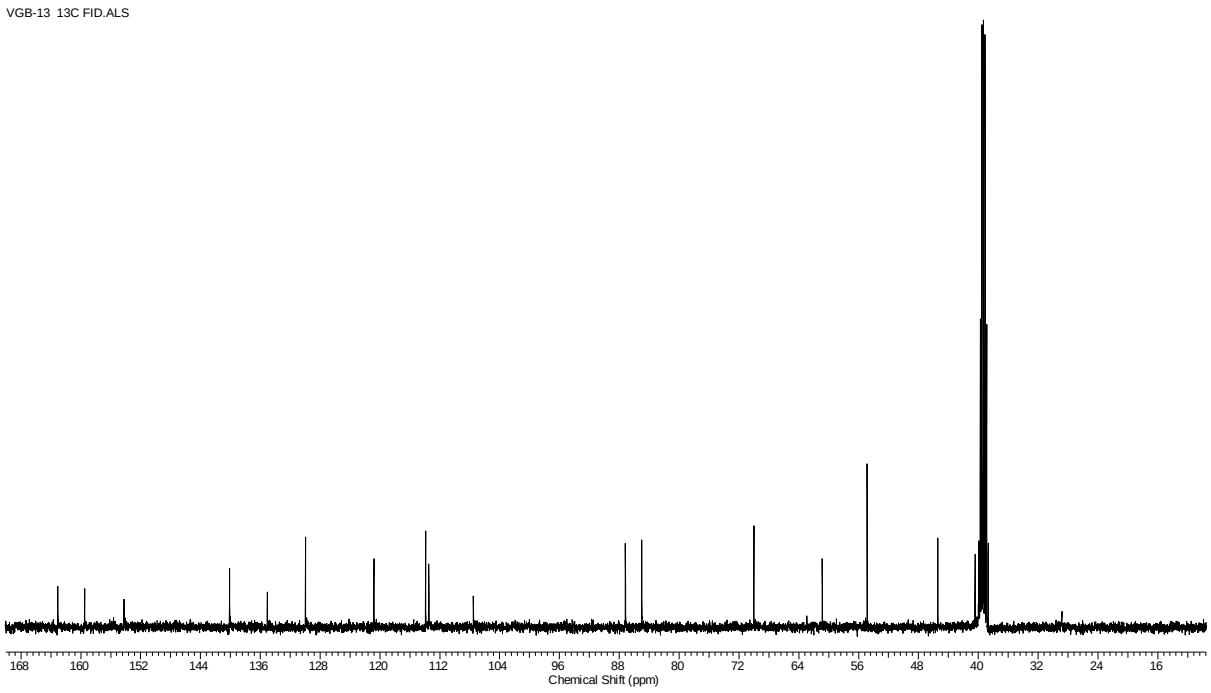
5-Phenyl-2´-deoxycytidine (5g)



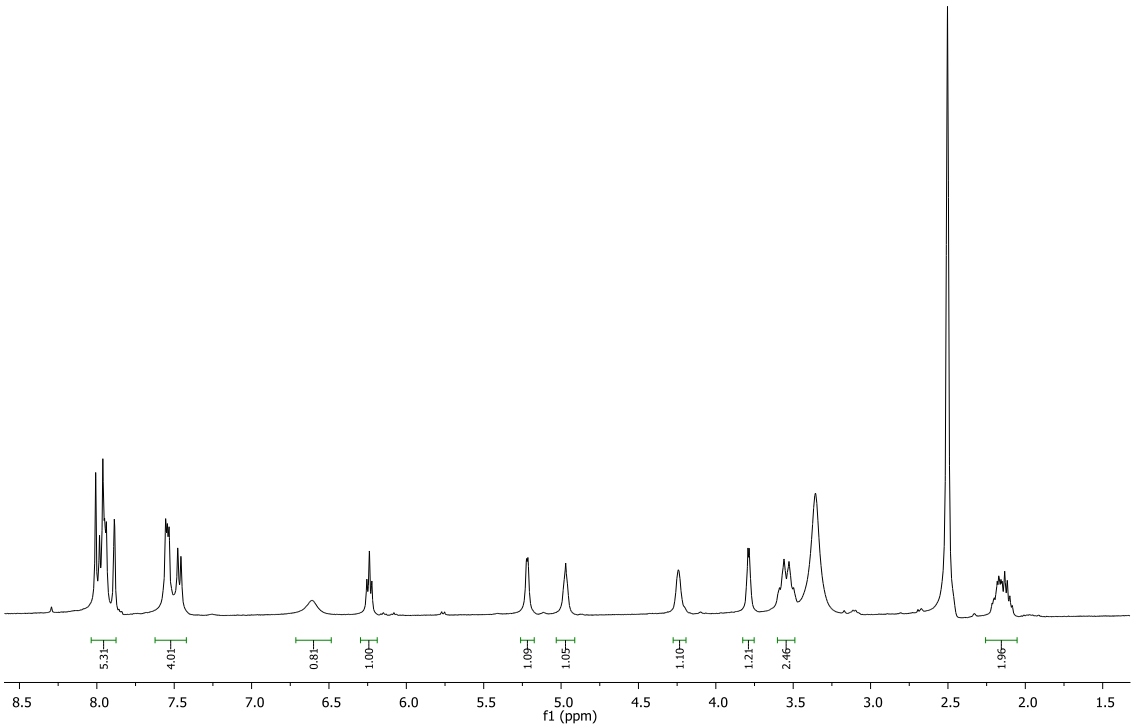


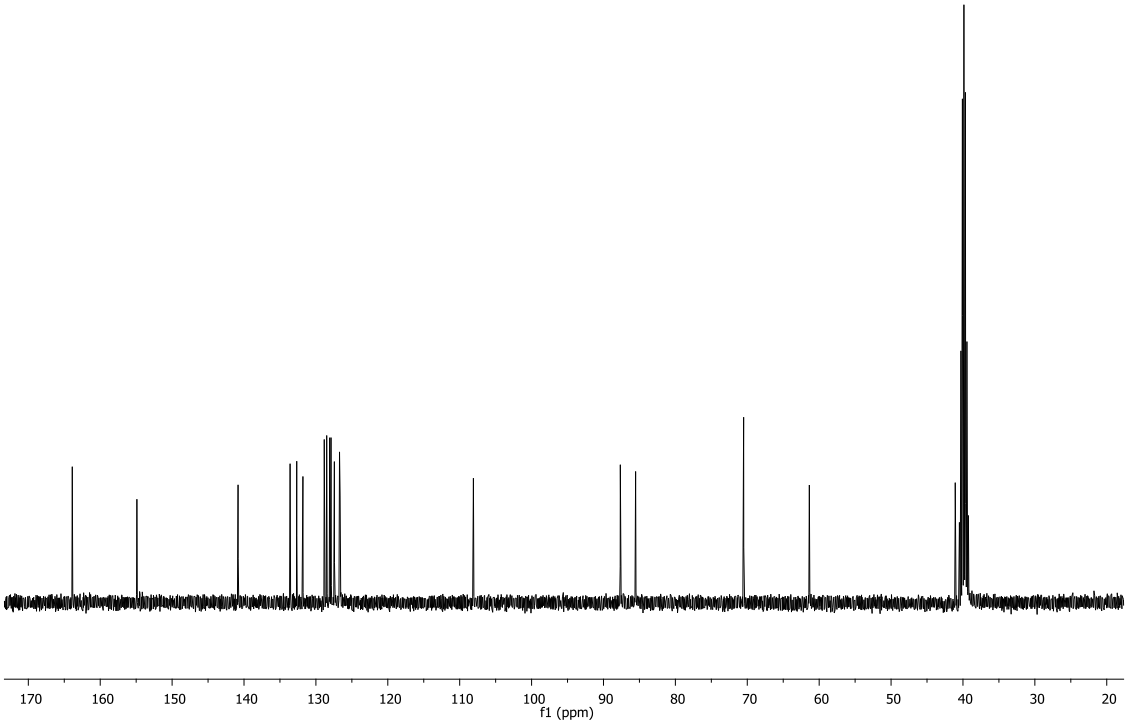
5-(3-Methoxy phenyl)-2'-deoxycytidine (5h)



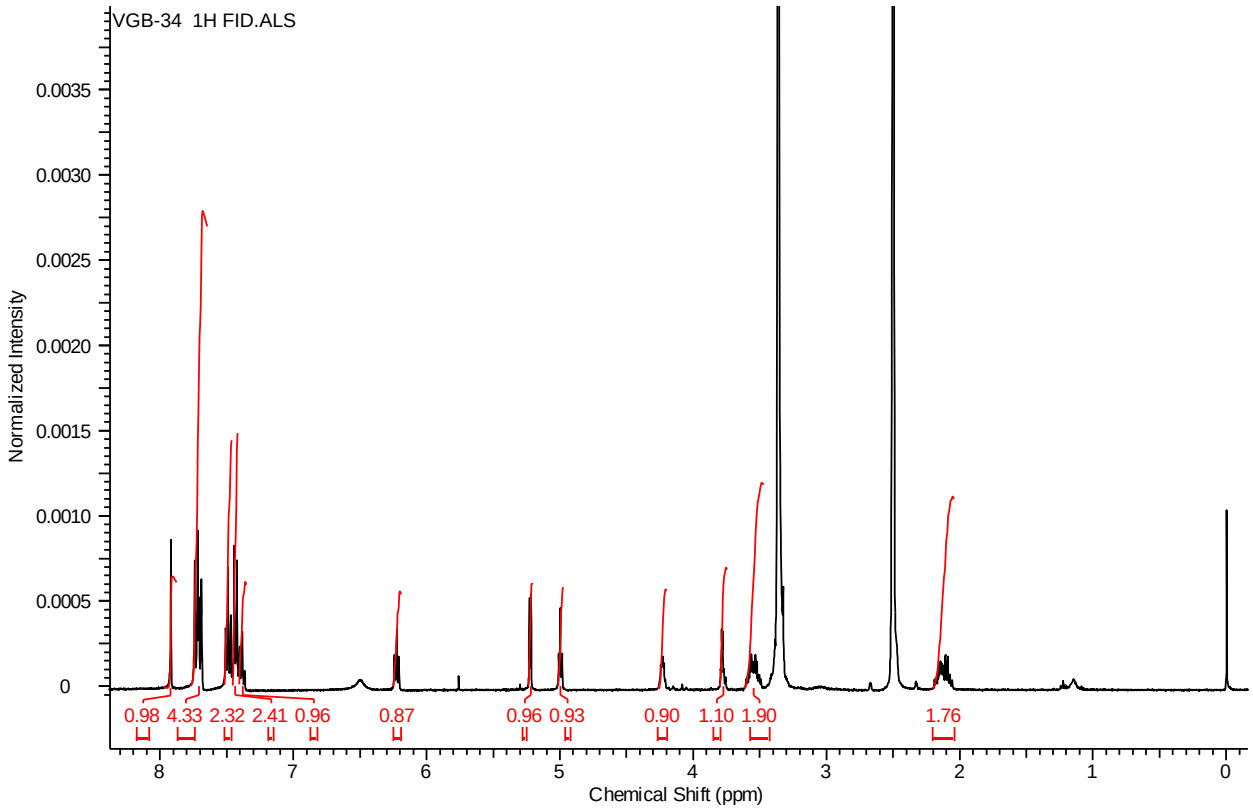


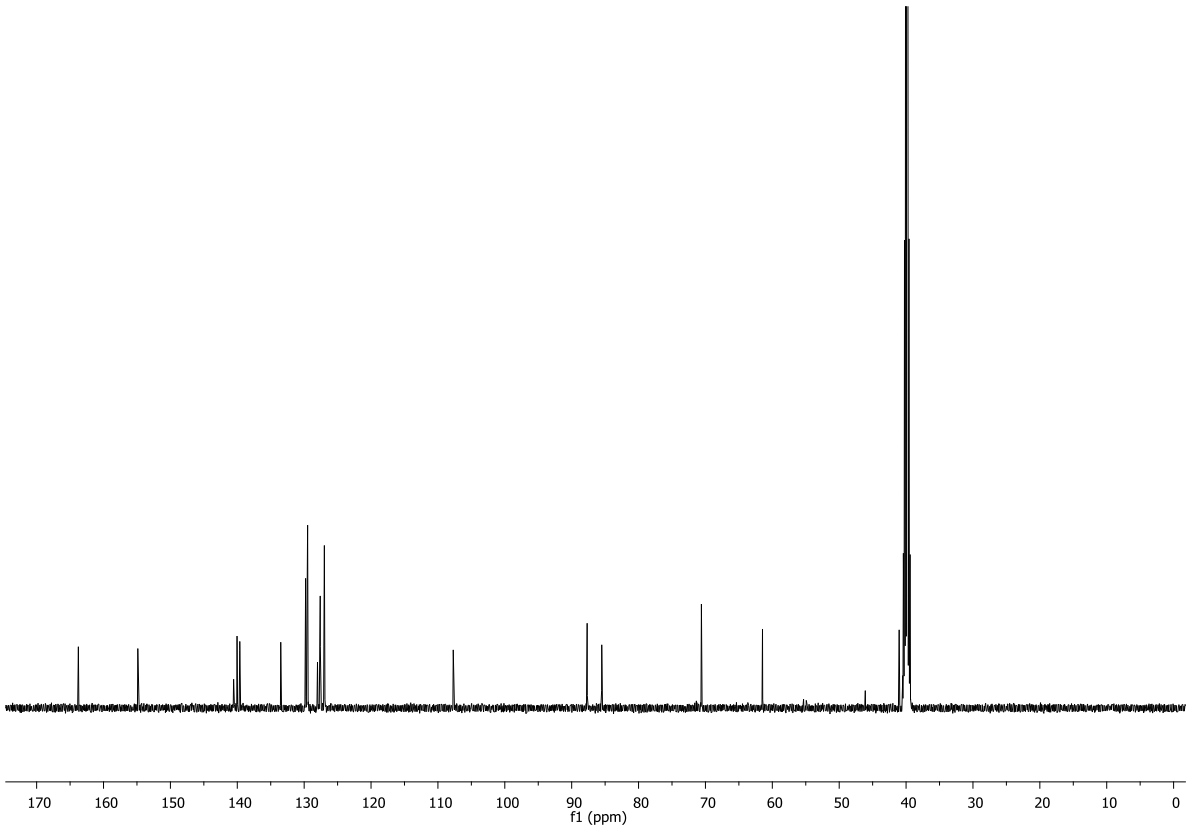
5-(2-Naphthyl)-2'-deoxycytidine (5i)



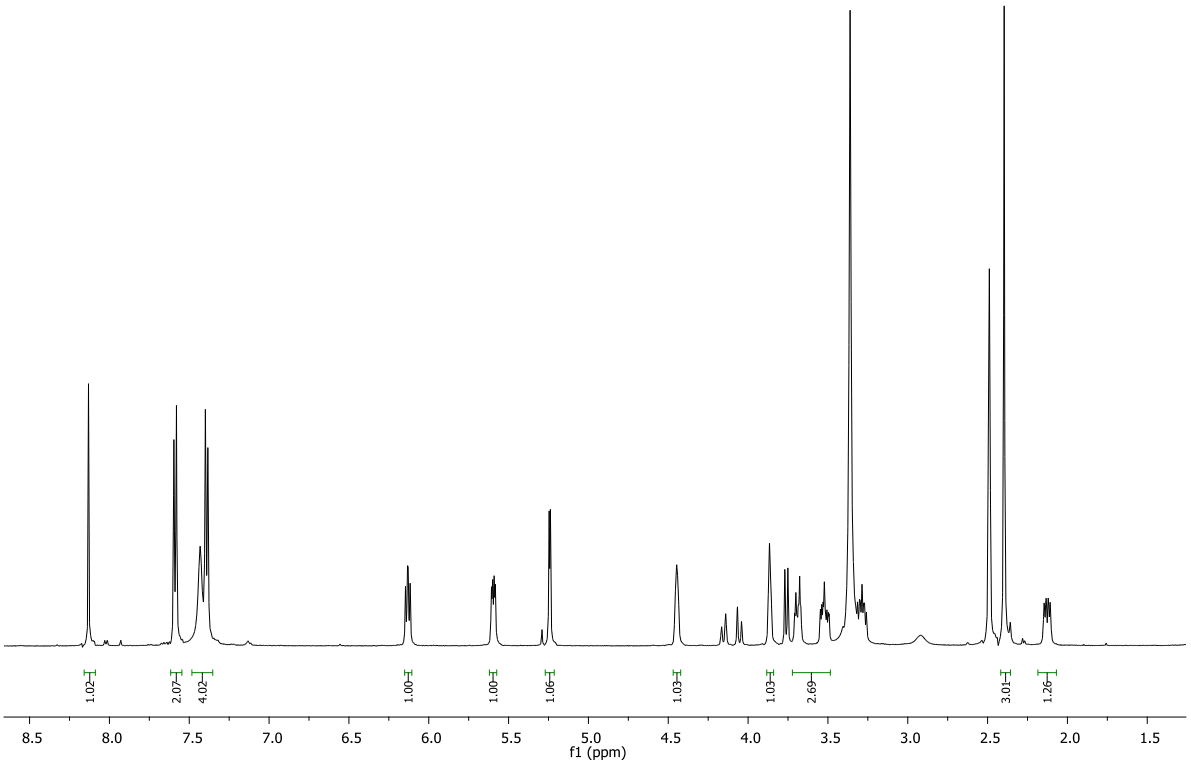


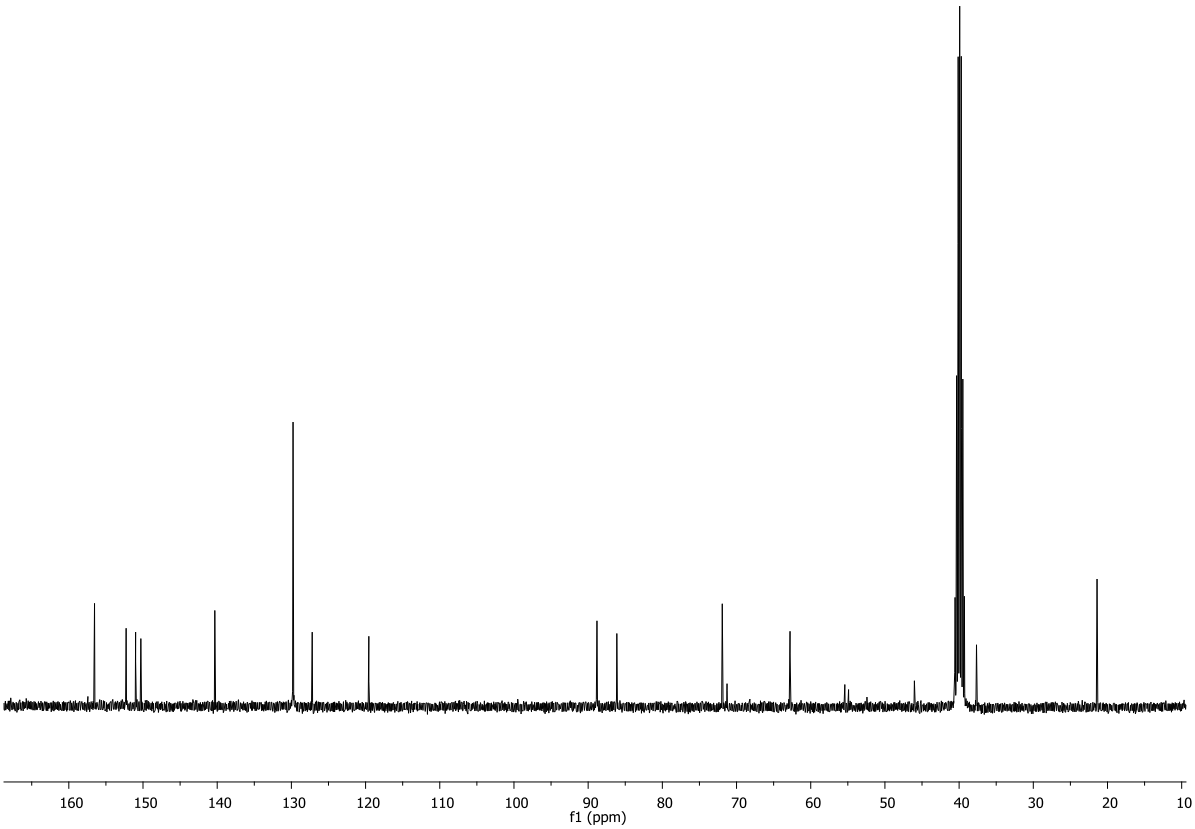
5-(4-Biphenyl)-2'-deoxycytidine (5j):-



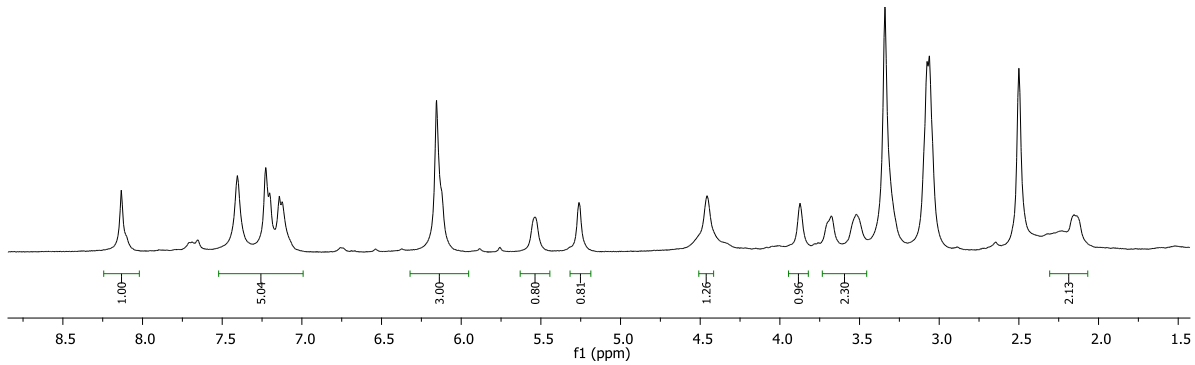


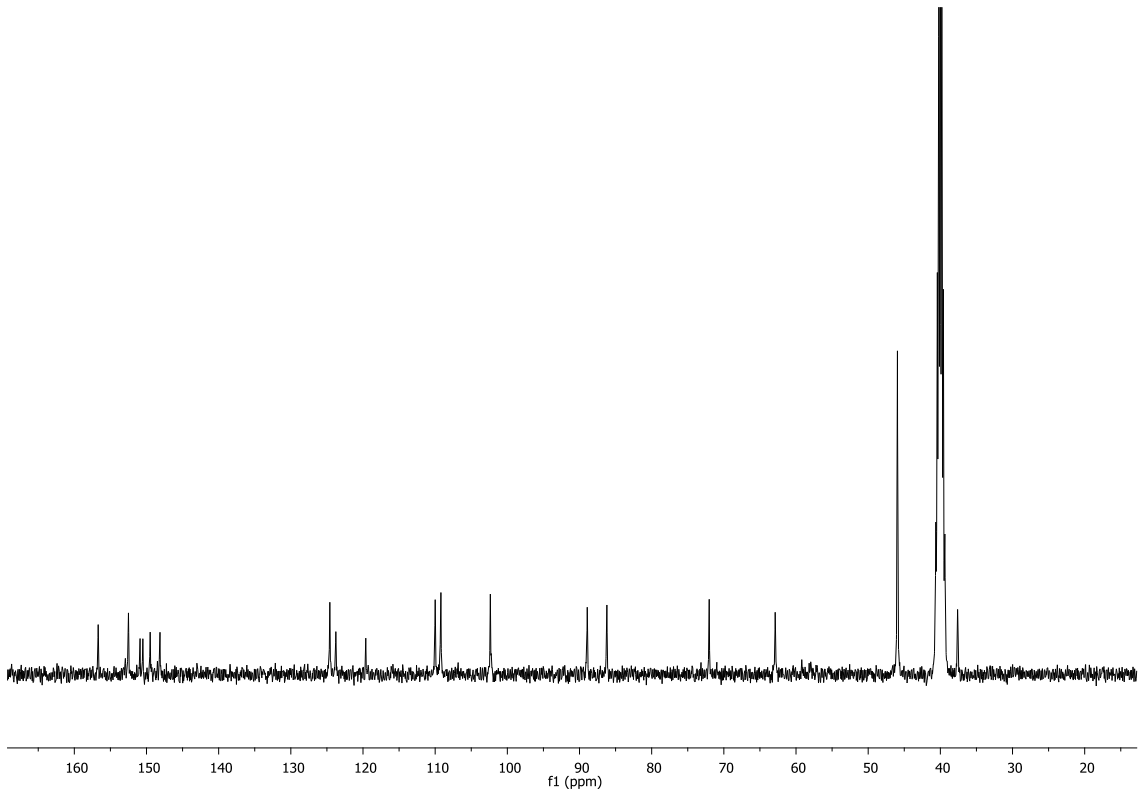
8-(4-(Thiomethyl)phenyl)-2'-deoxyadenosine (7a)



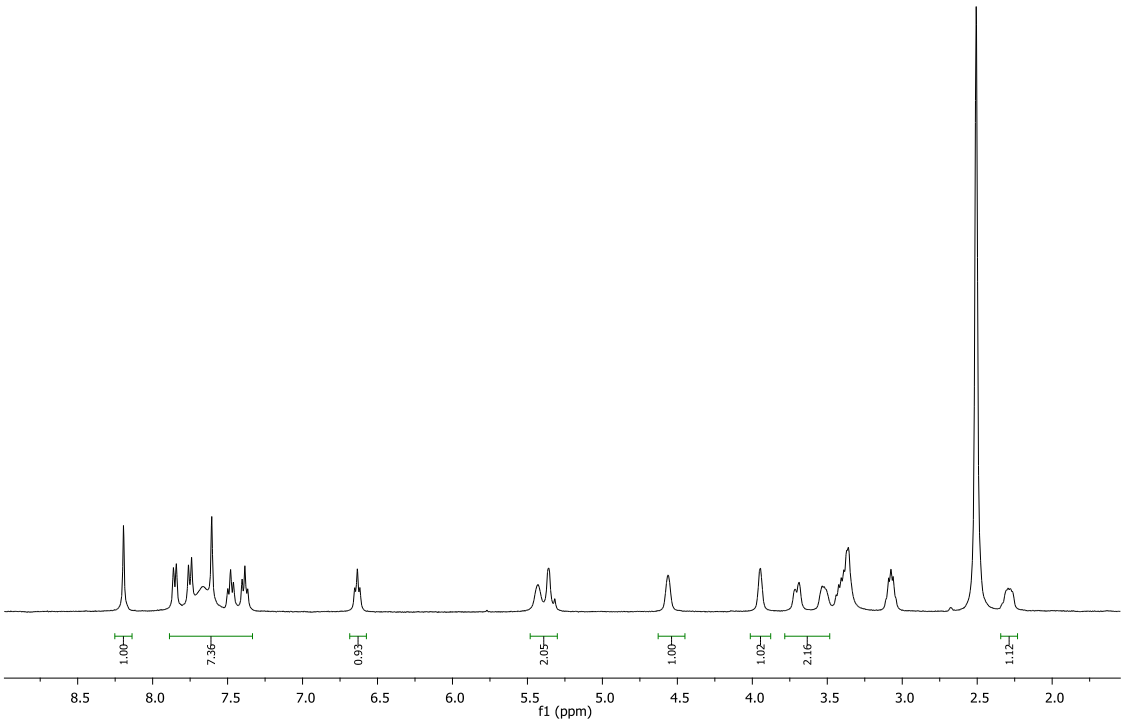


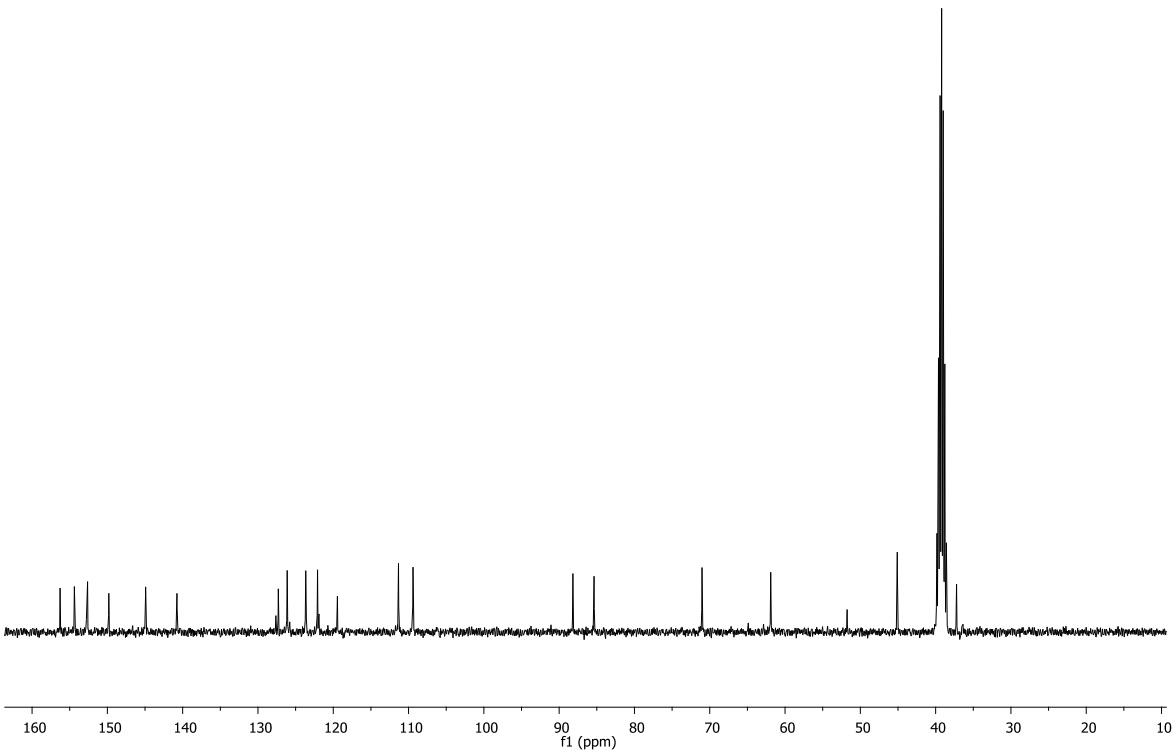
8-(3,4-(Methylenedioxy)phenyl)-2'-deoxyadenosine (7b)



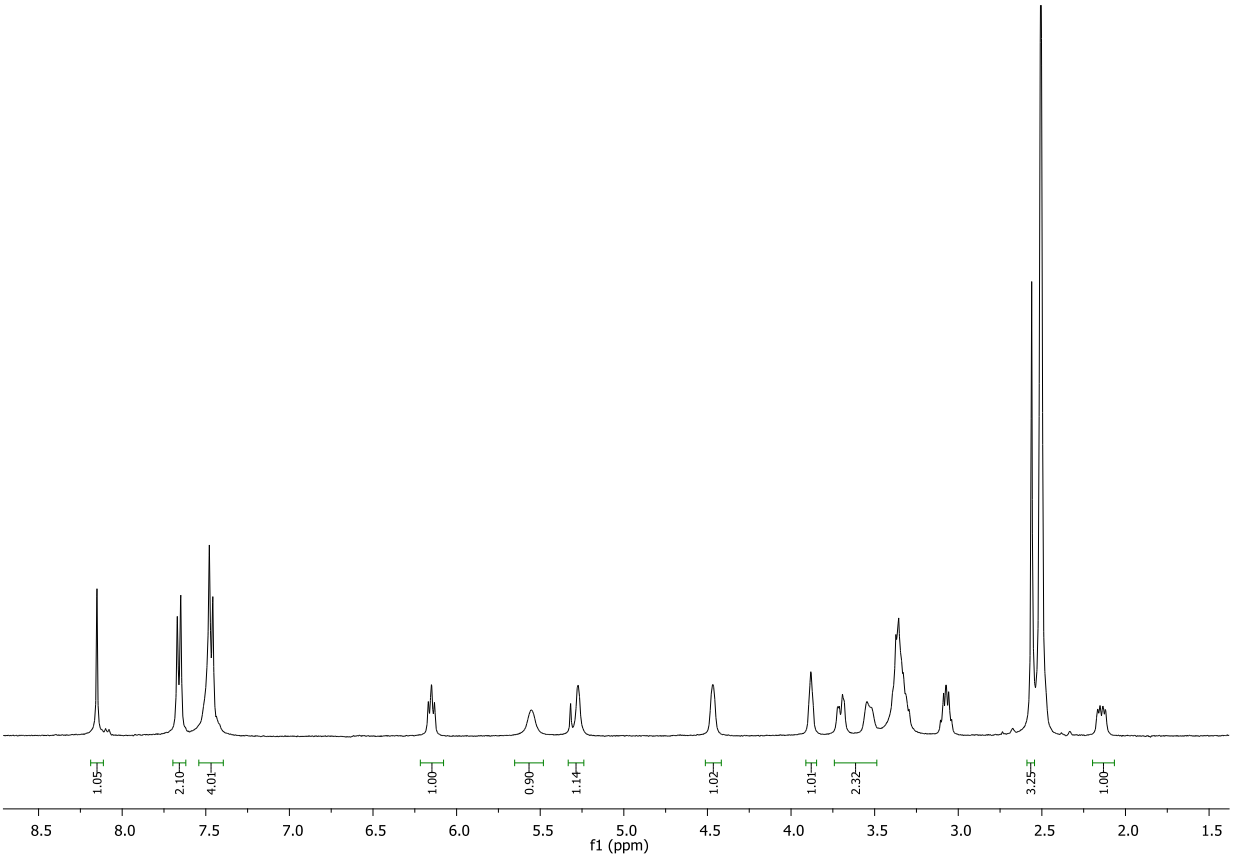


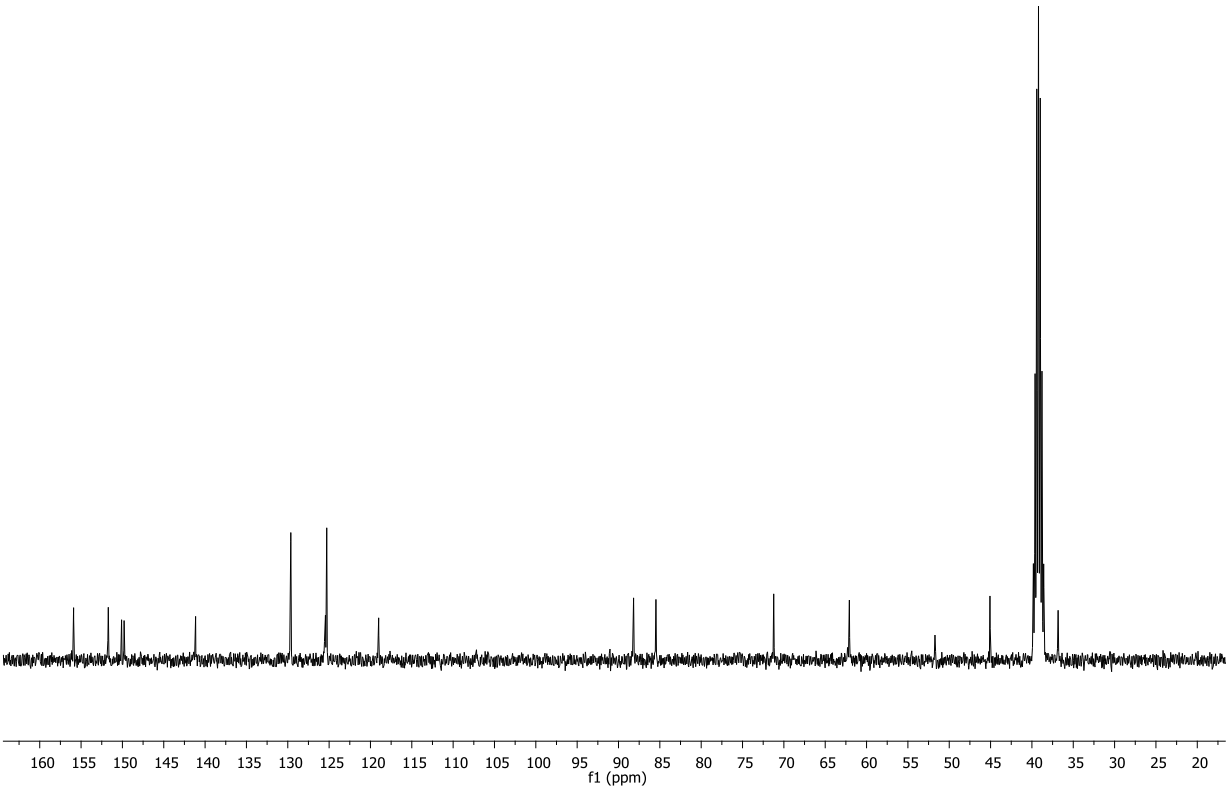
8-(2-Benzofuranyl)-2'-deoxyadenosine (7c)



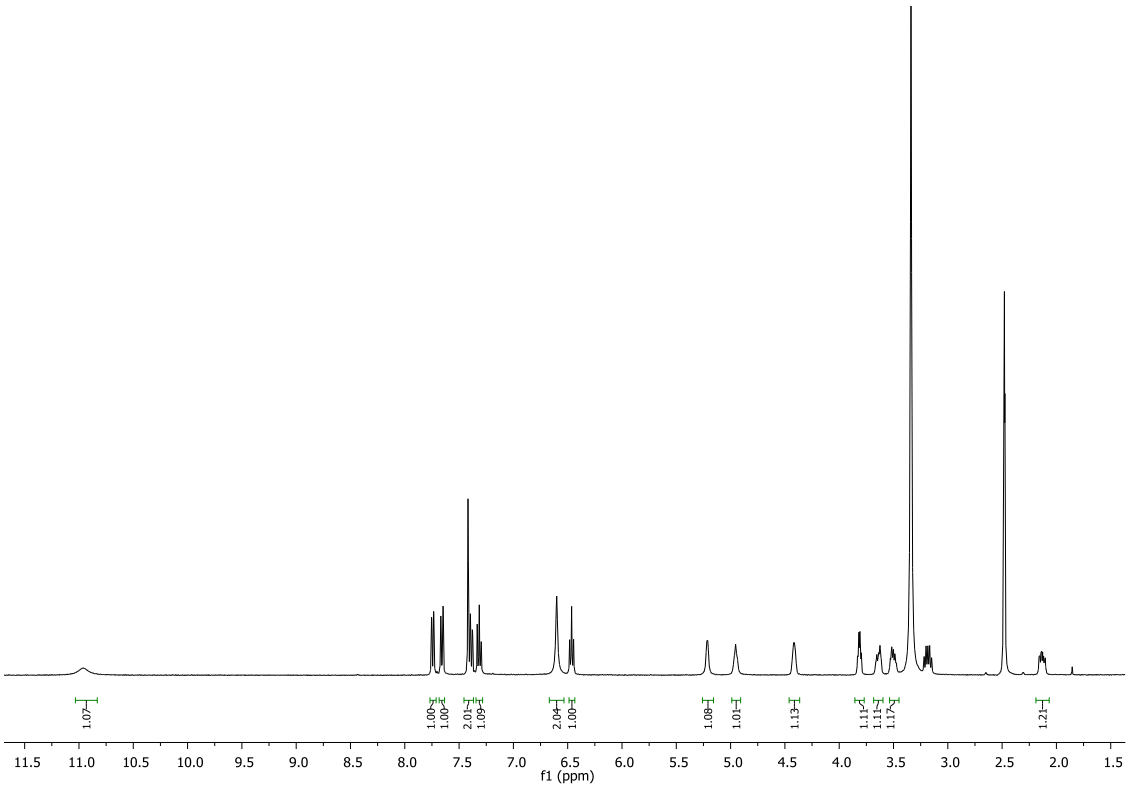


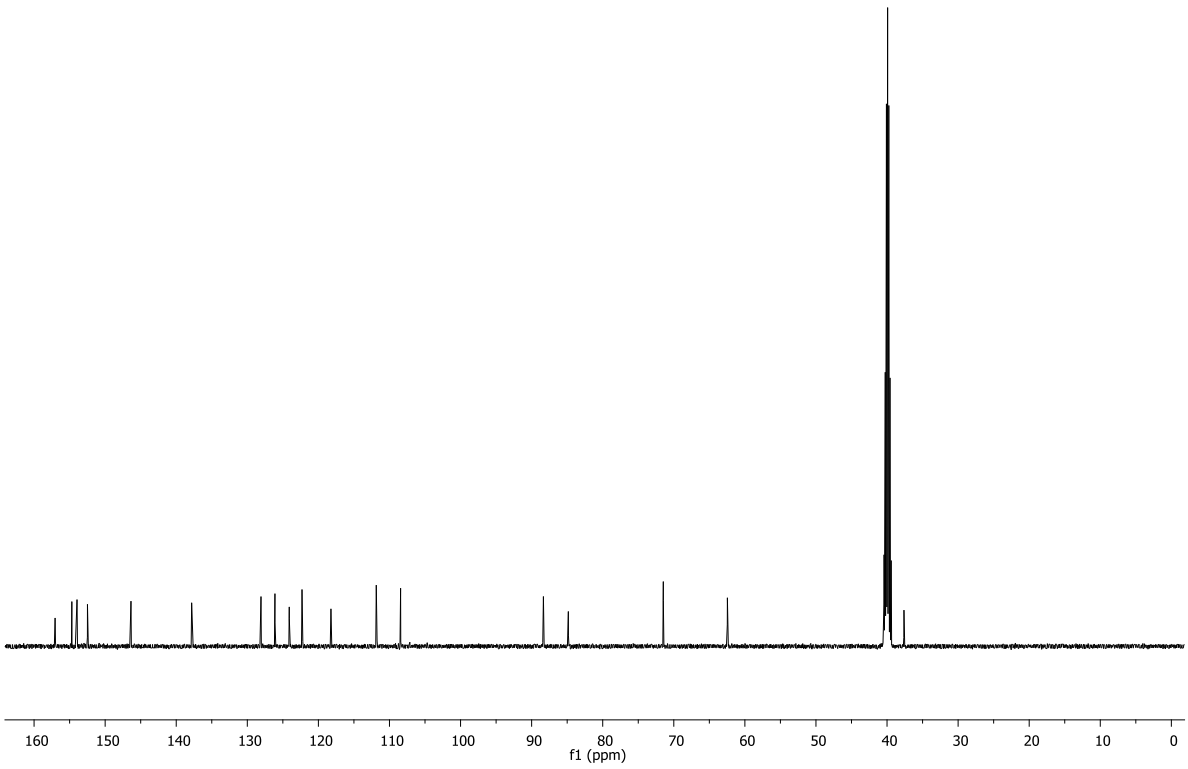
8-(4-(Methyl)phenyl)-2'-deoxyadenosine (7d)



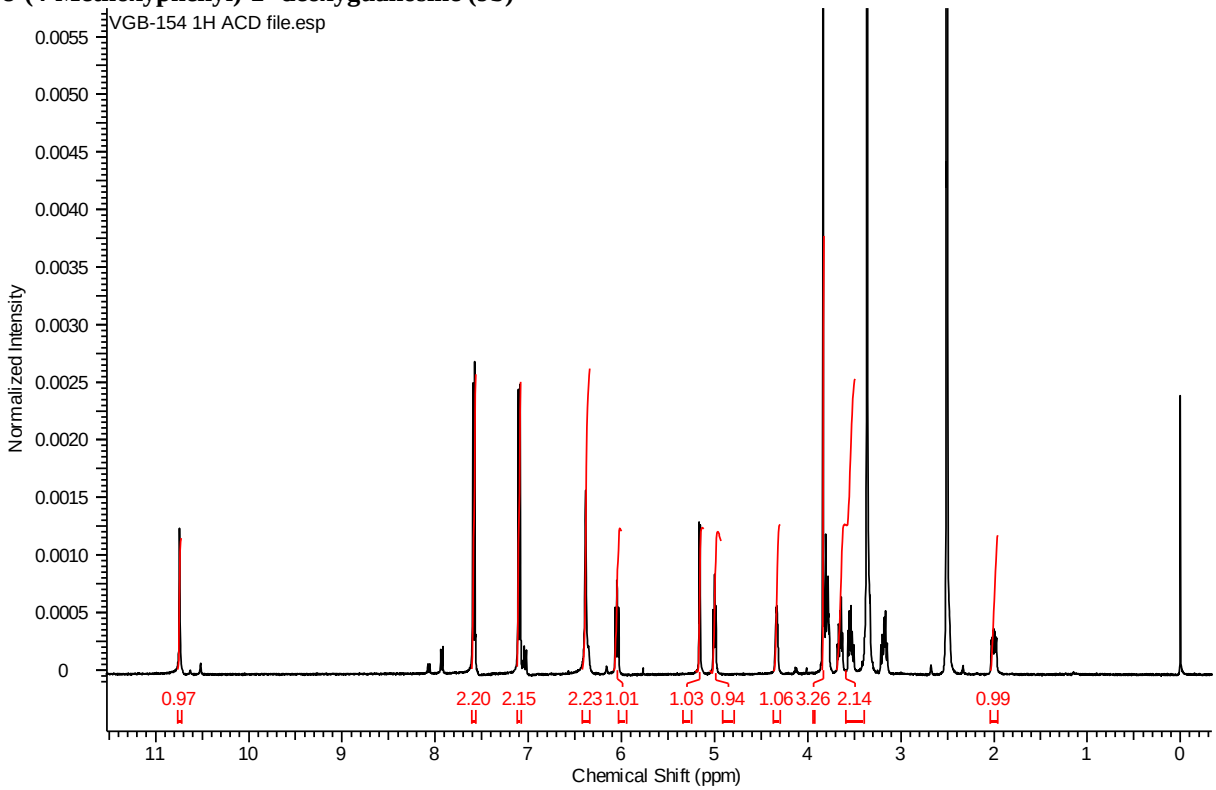


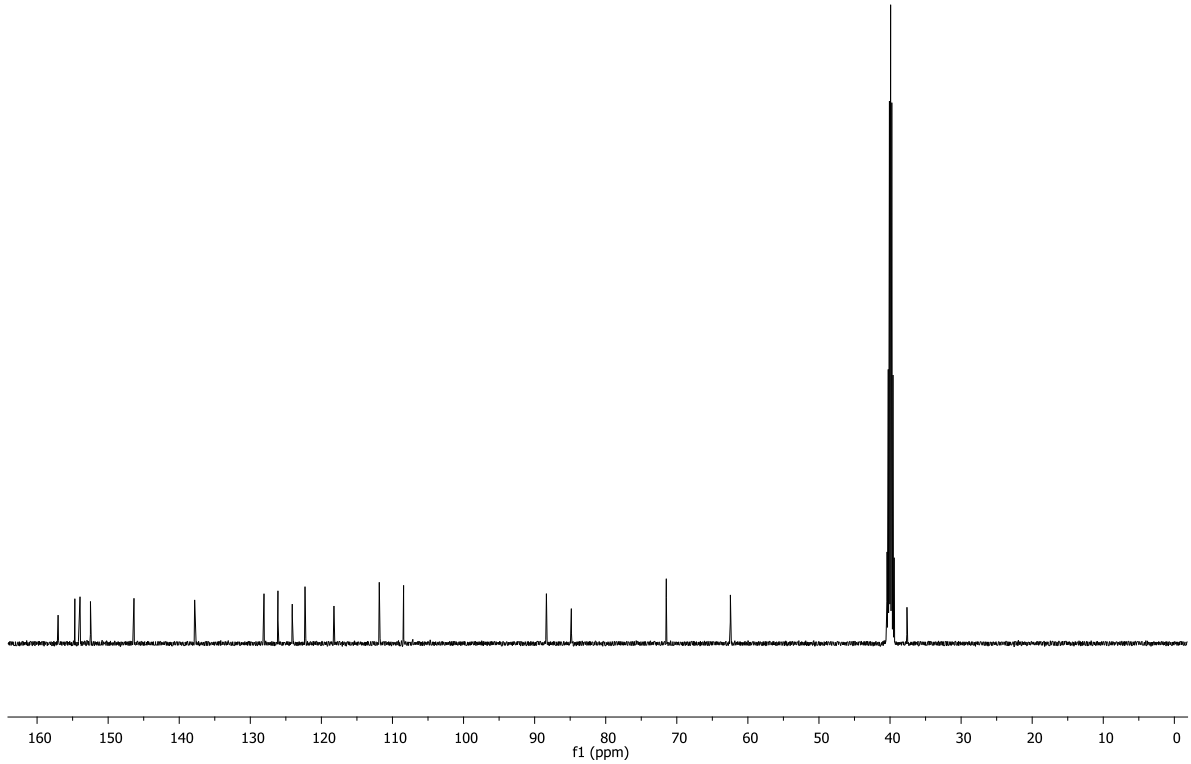
8-(2-Benzofuranyl)-2'-deoxyguanosine (9a)



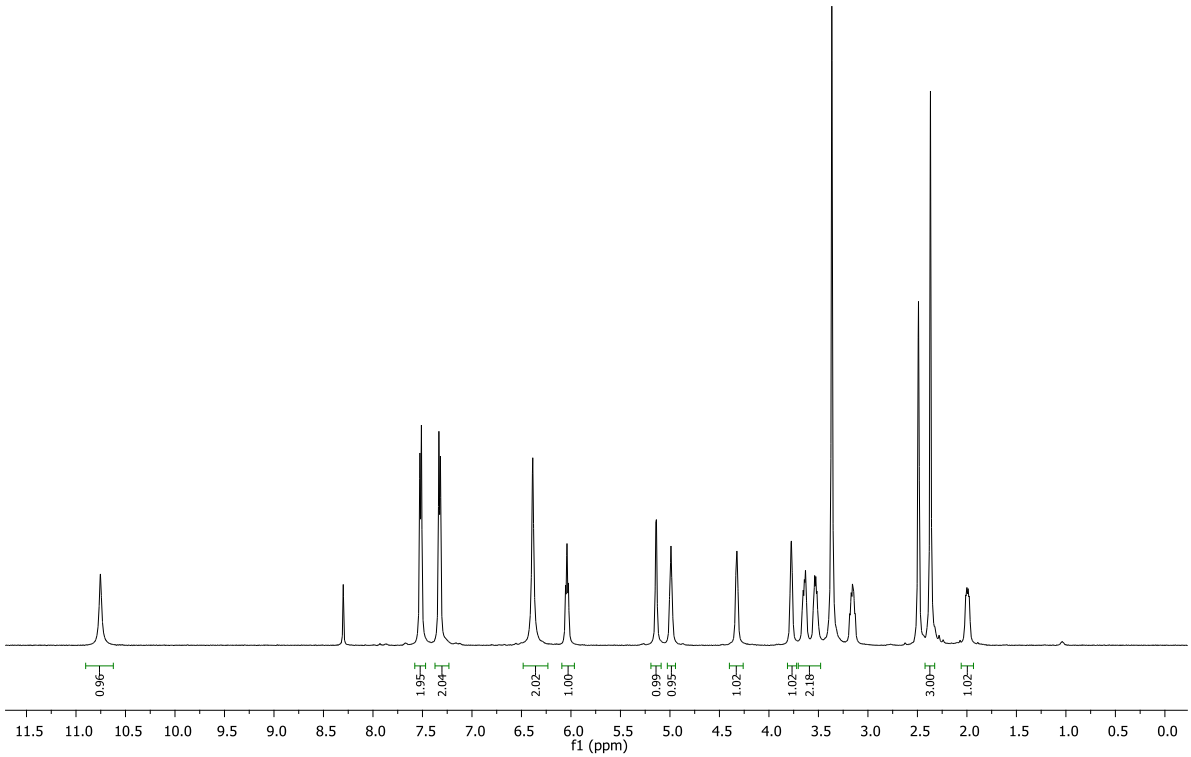


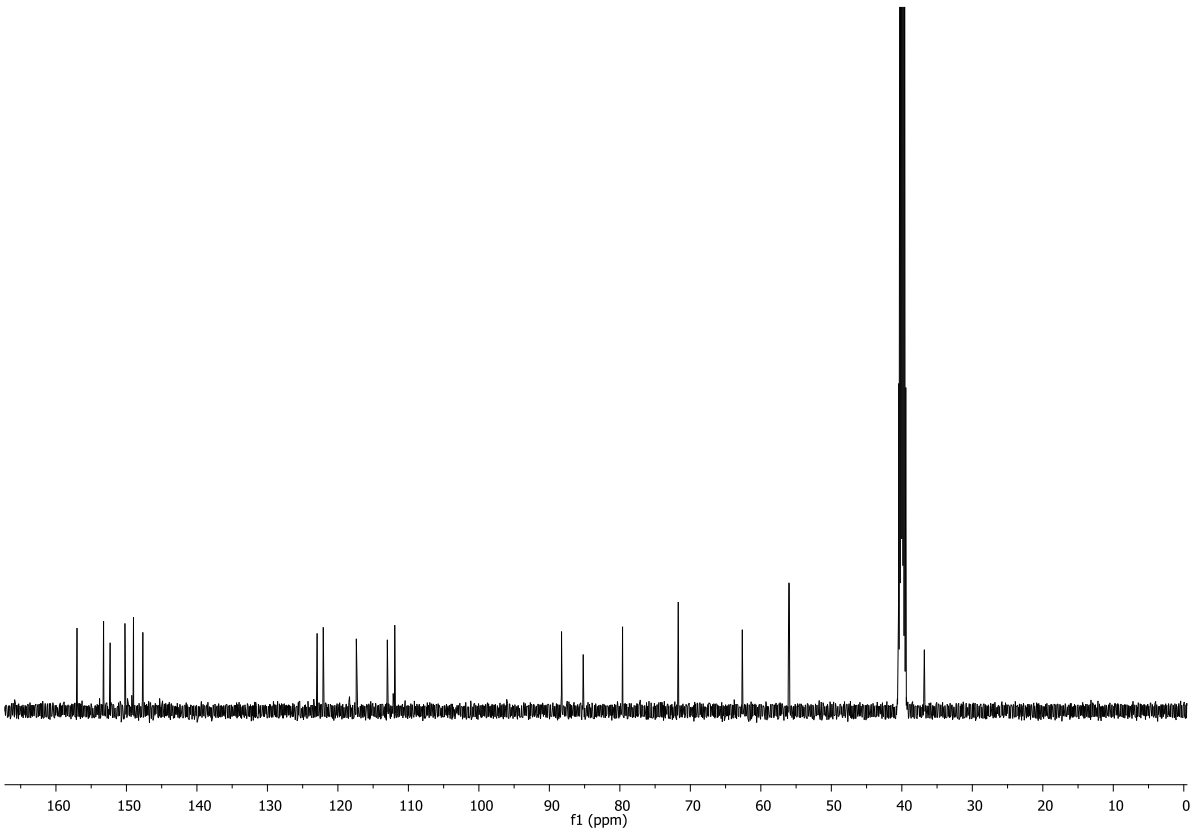
8-(4-Methoxyphenyl)-2'-deoxyguanosine (9b)



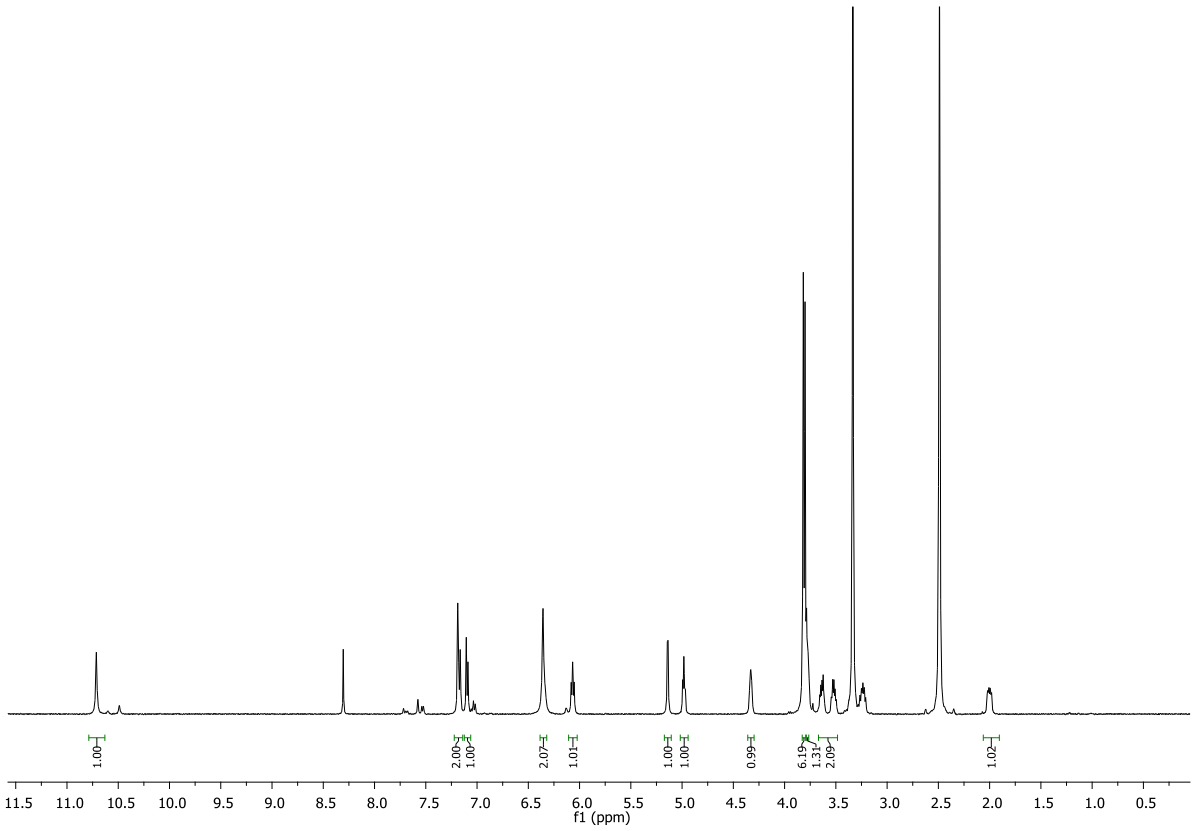


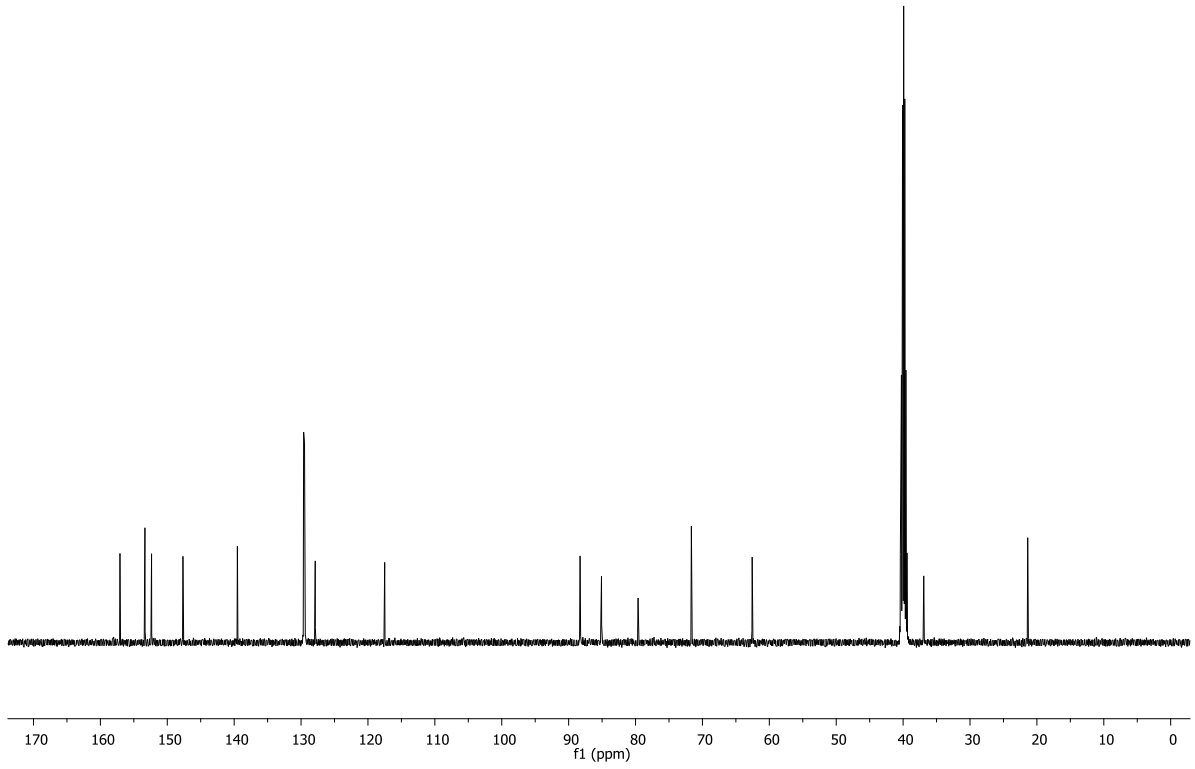
8-(4-Methylphenyl) 2'-deoxyguanosine (9c)



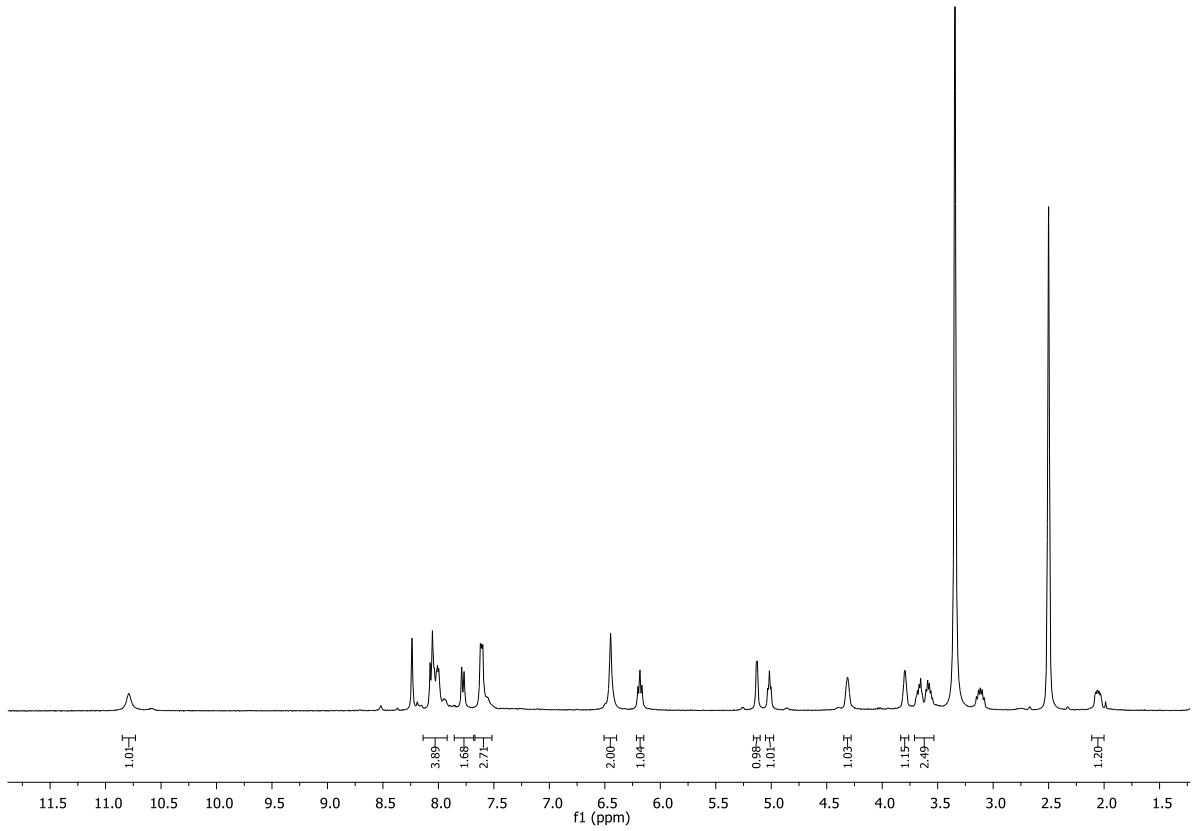


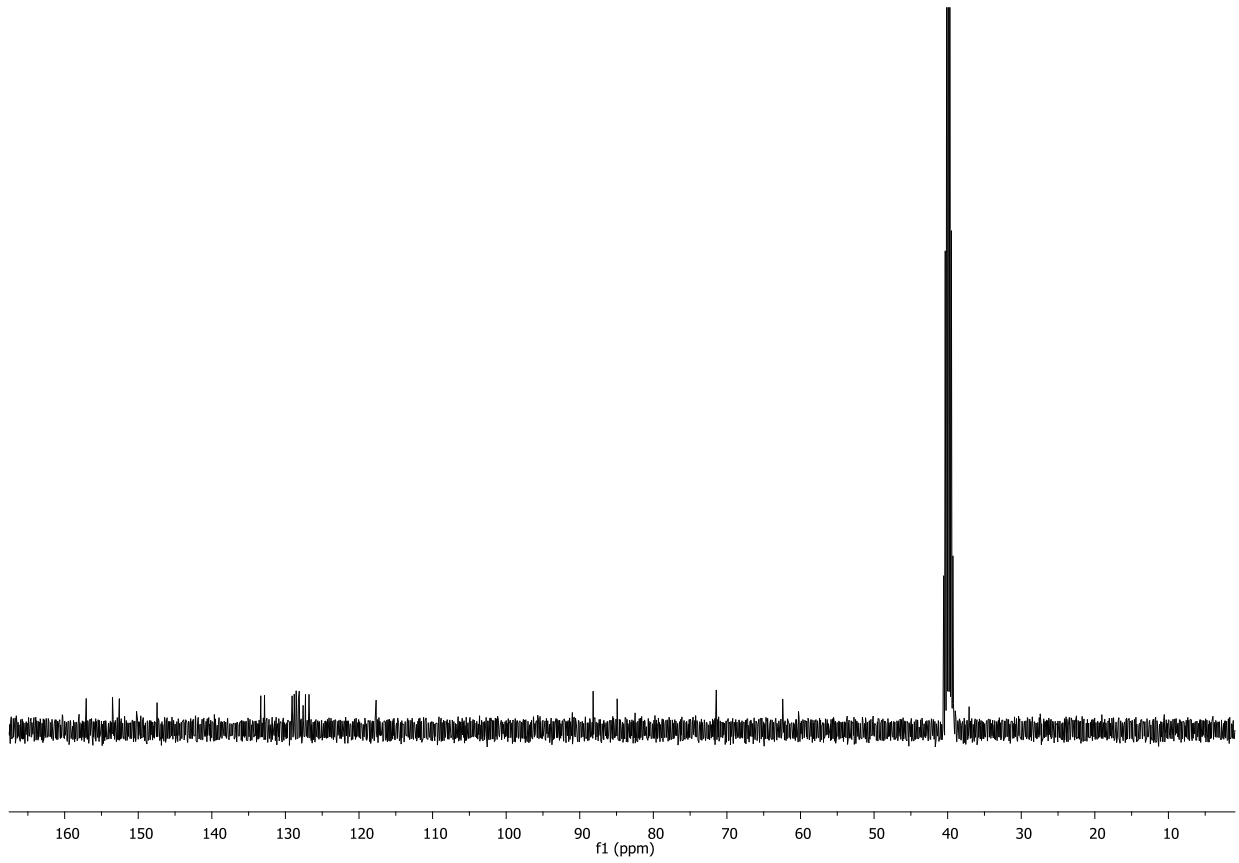
8-(3,4-Dimethoxylphenyl) 2'-deoxyguanosine (9d)



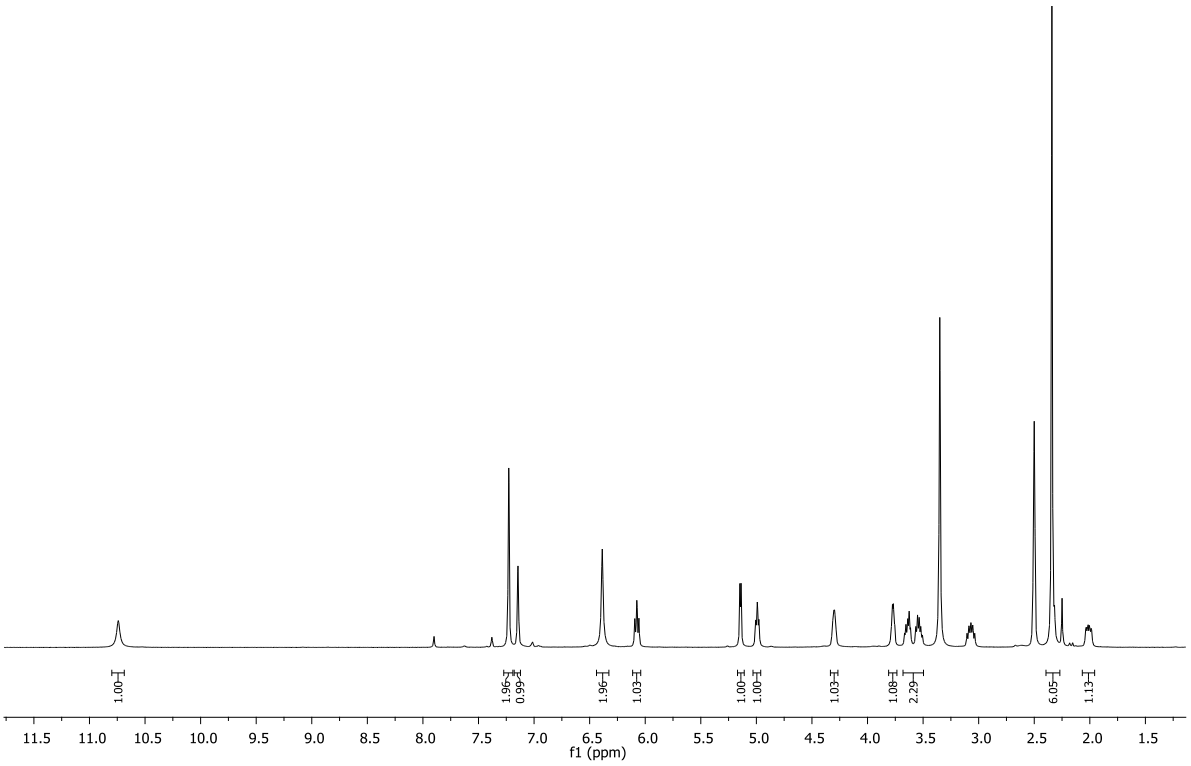


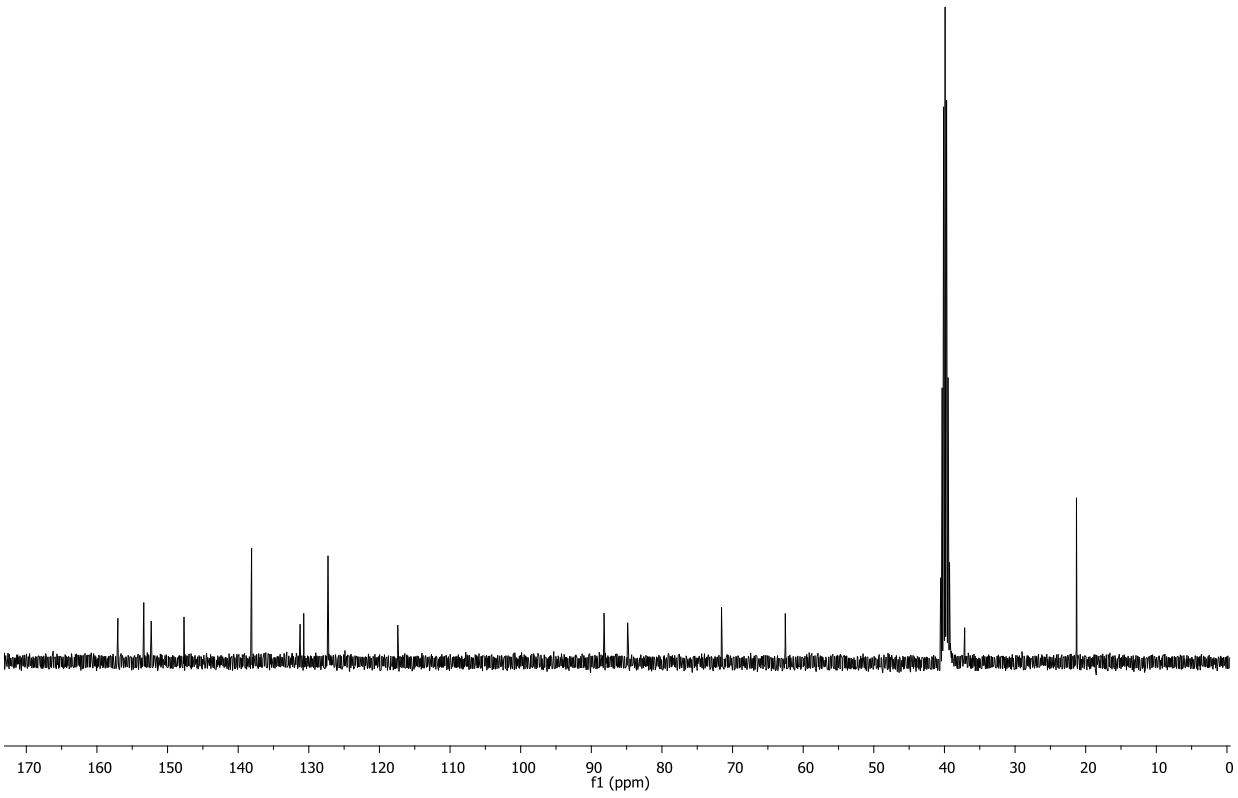
8-(4-Biphenyl) 2'-deoxyguanosine (9e)



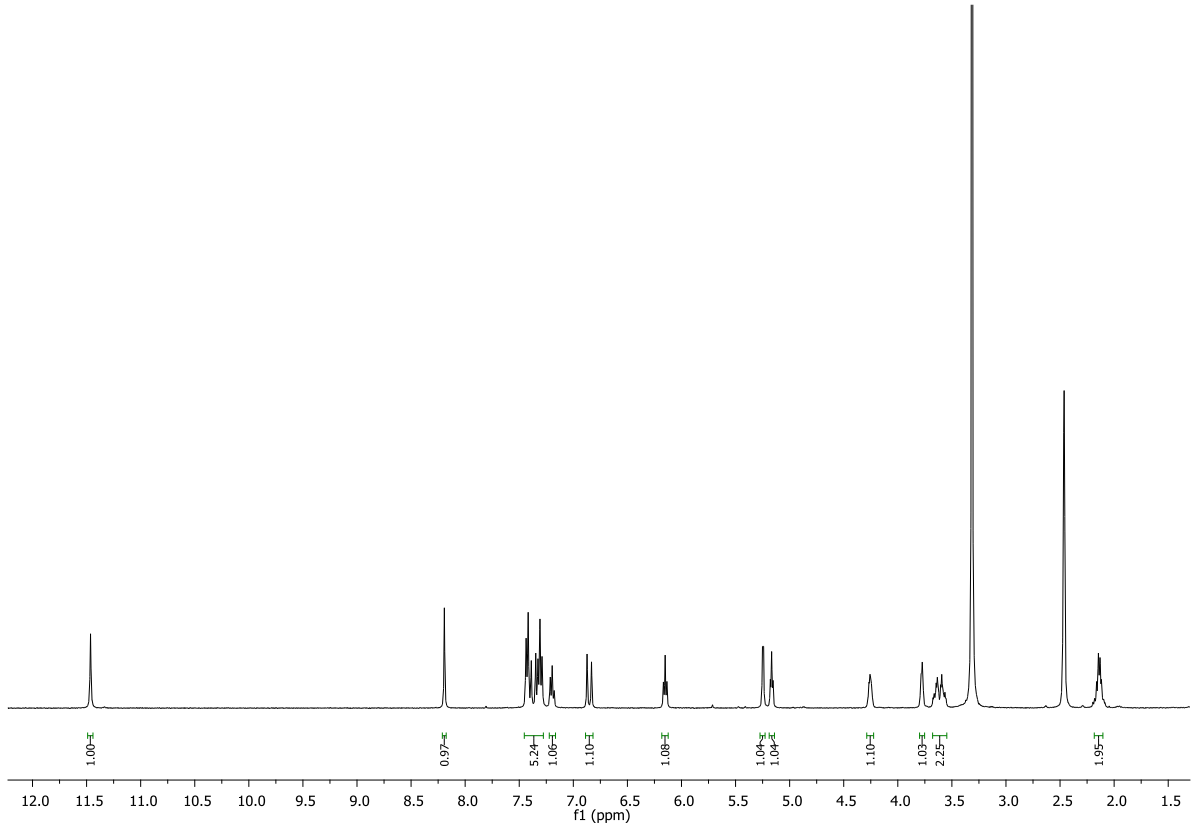


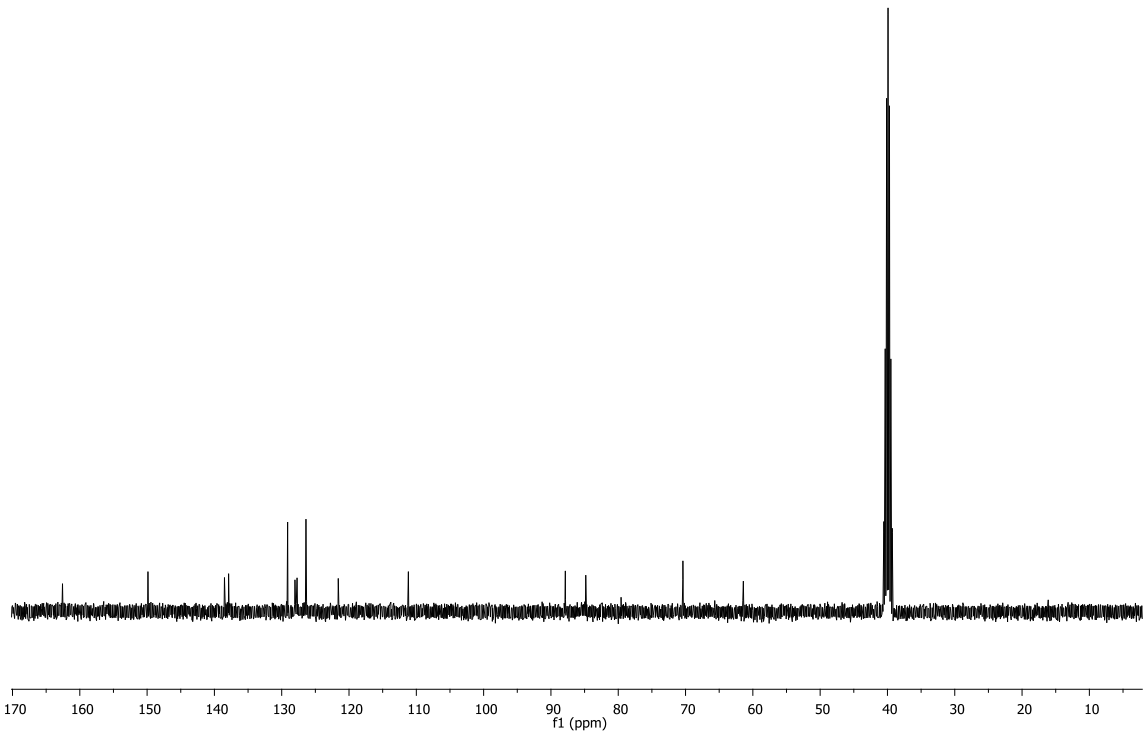
8-(3,5-Dimethylphenyl) 2'-deoxyguanosine (9f)



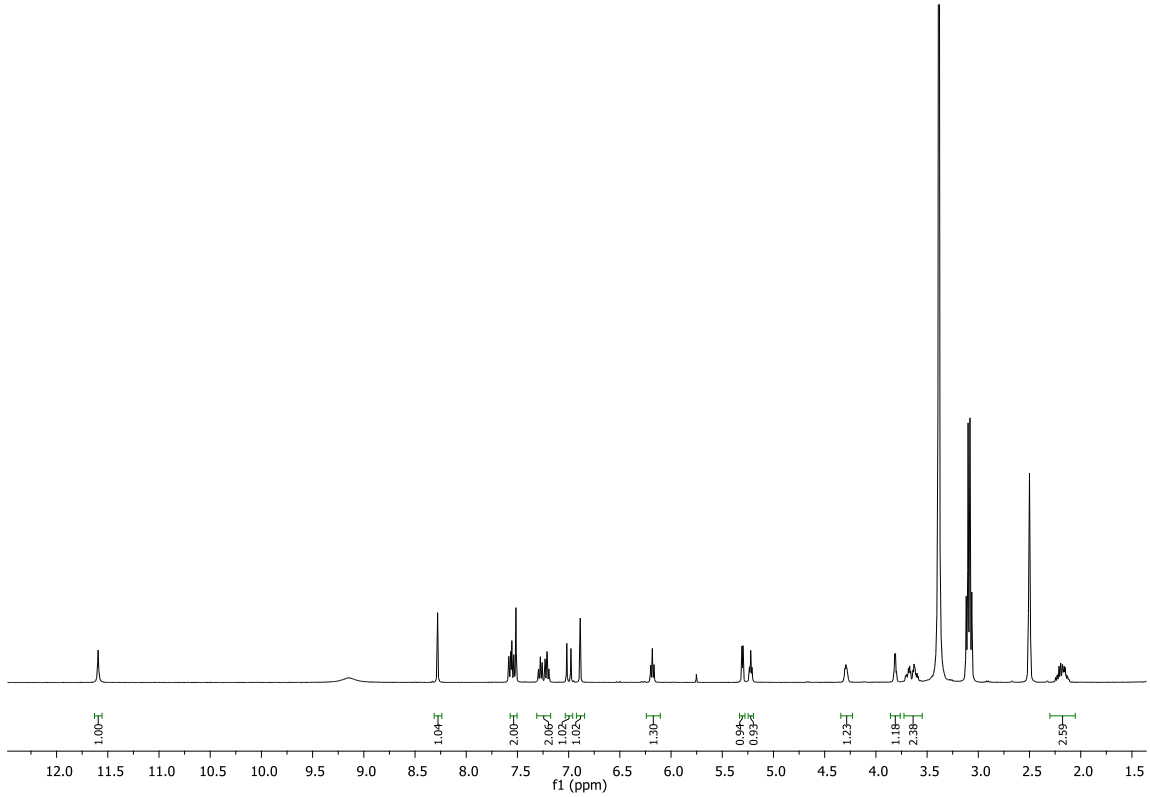


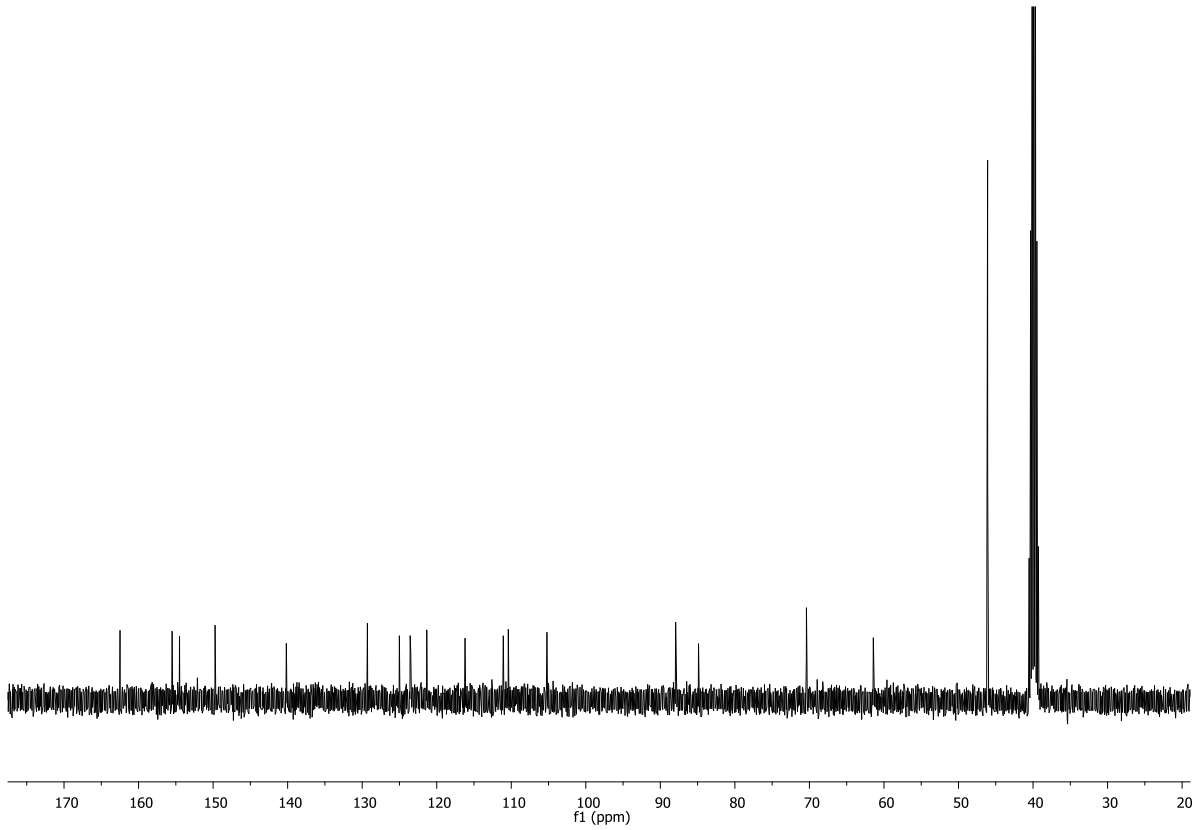
5-((E)-2-Phenylethenyl)-2′-deoxyuridine (11a)

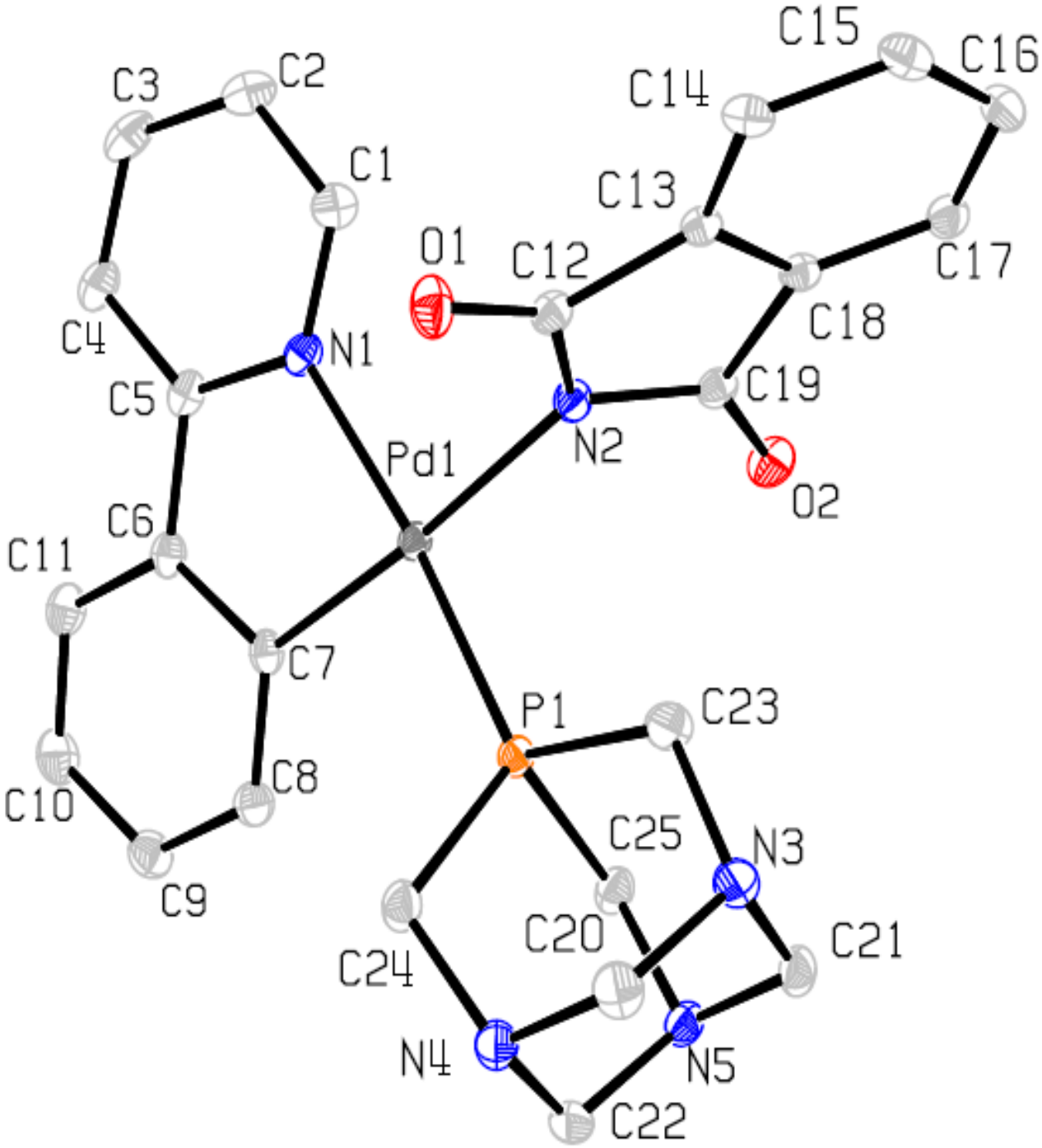




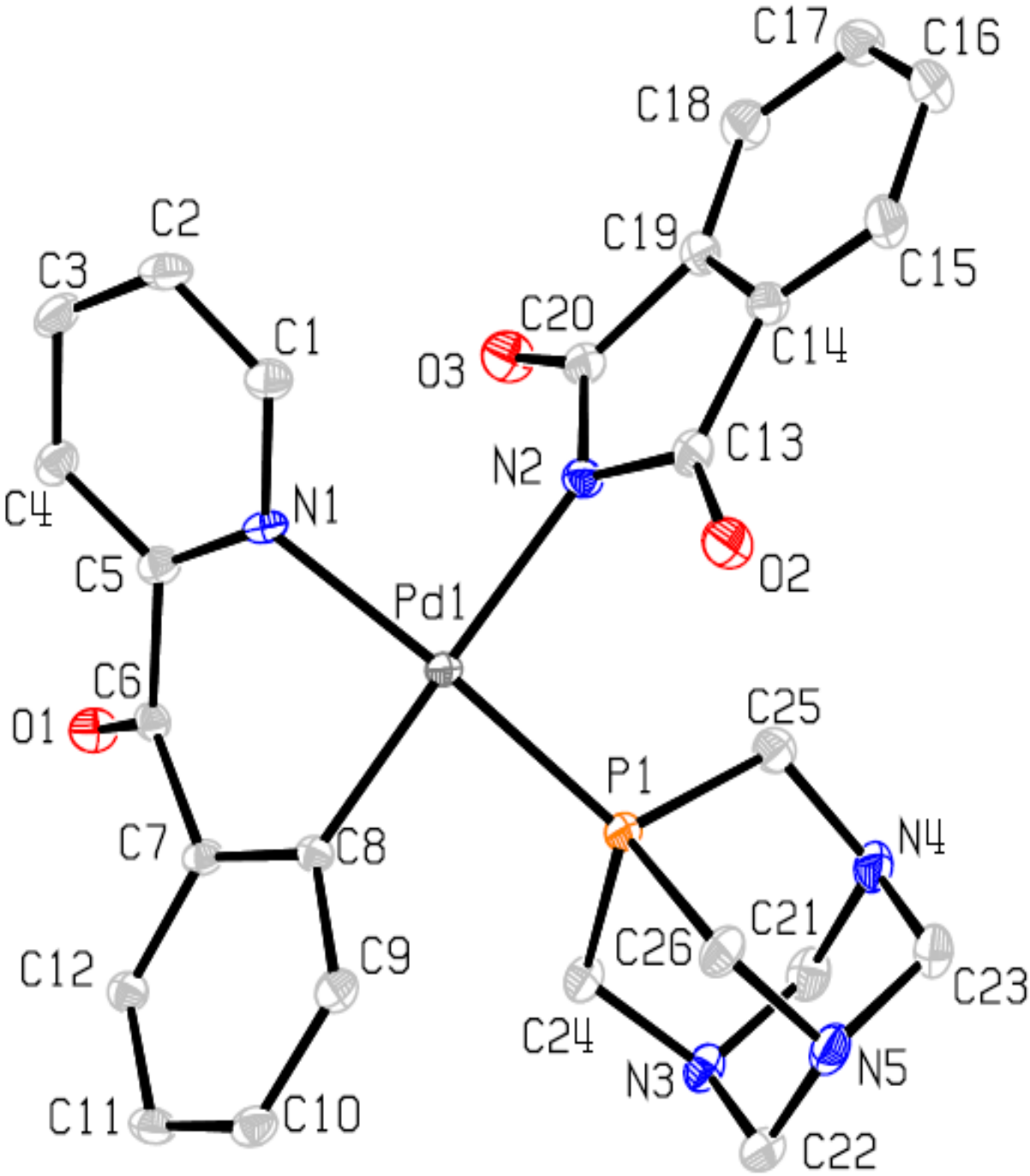
5-((E)-2-Benzofuranylethenyl)-2′-deoxyuridine (11b)



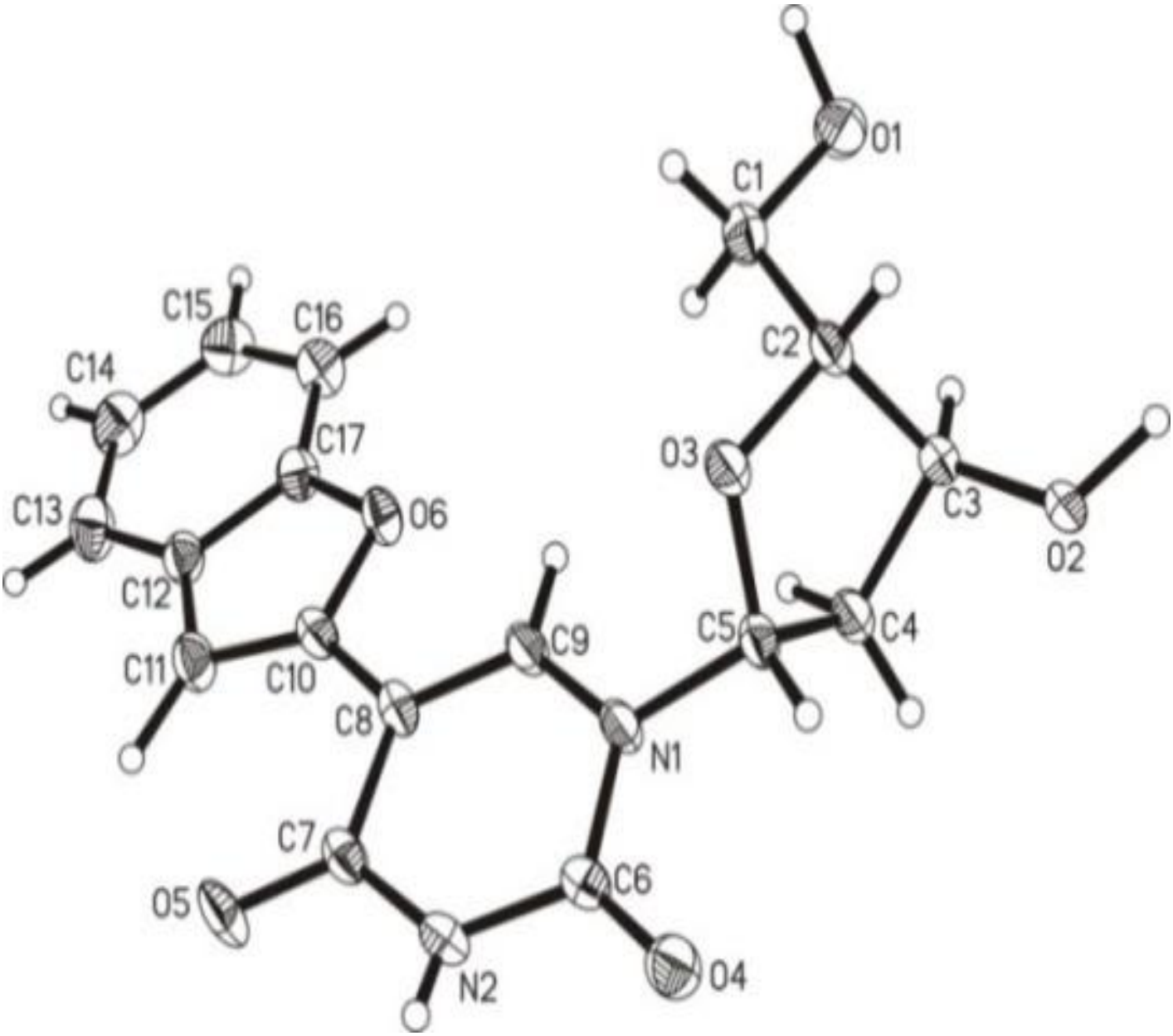




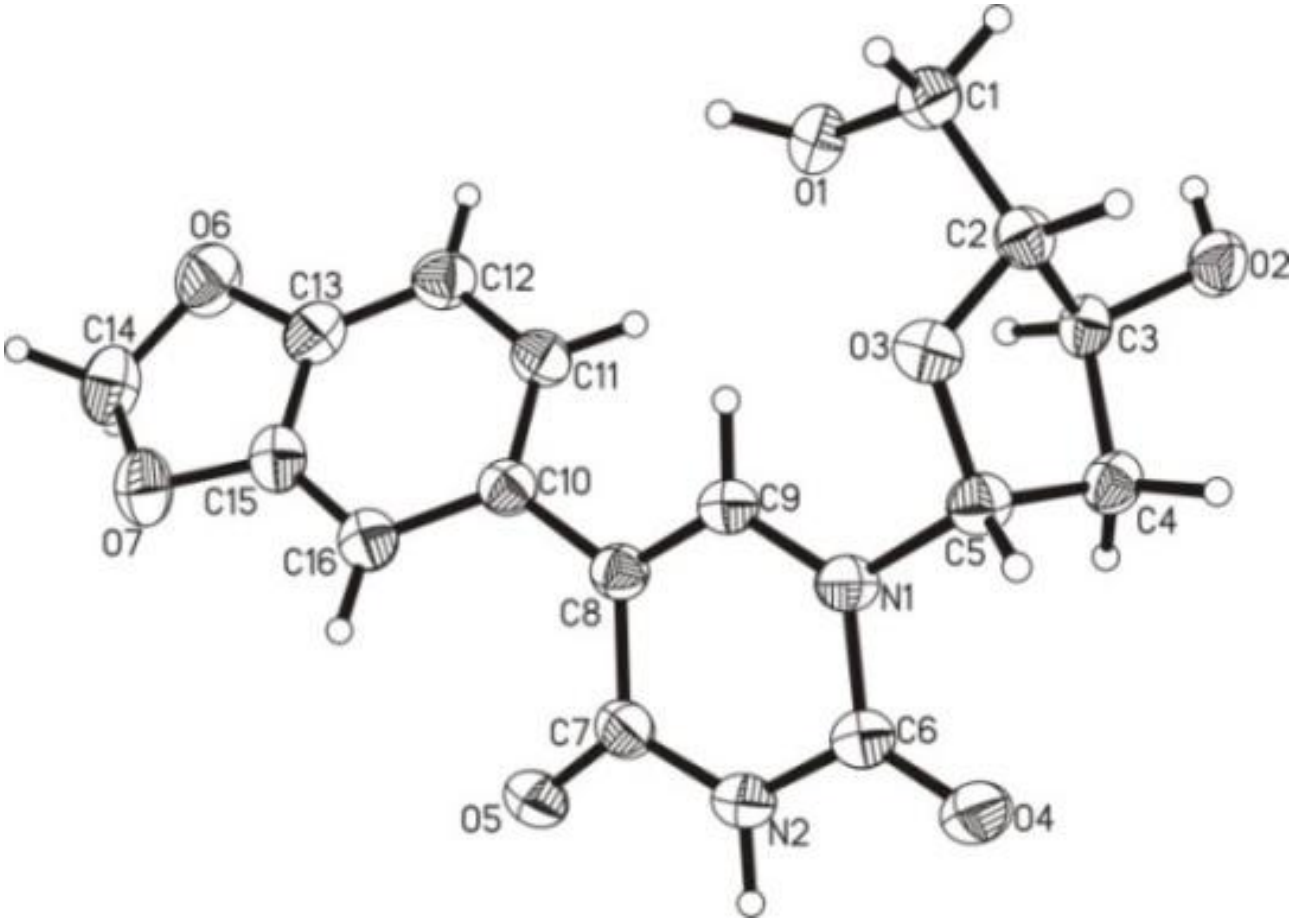
Single crystal X-ray structure for **IIa**. Ellipsoids are shown with 50% probability.



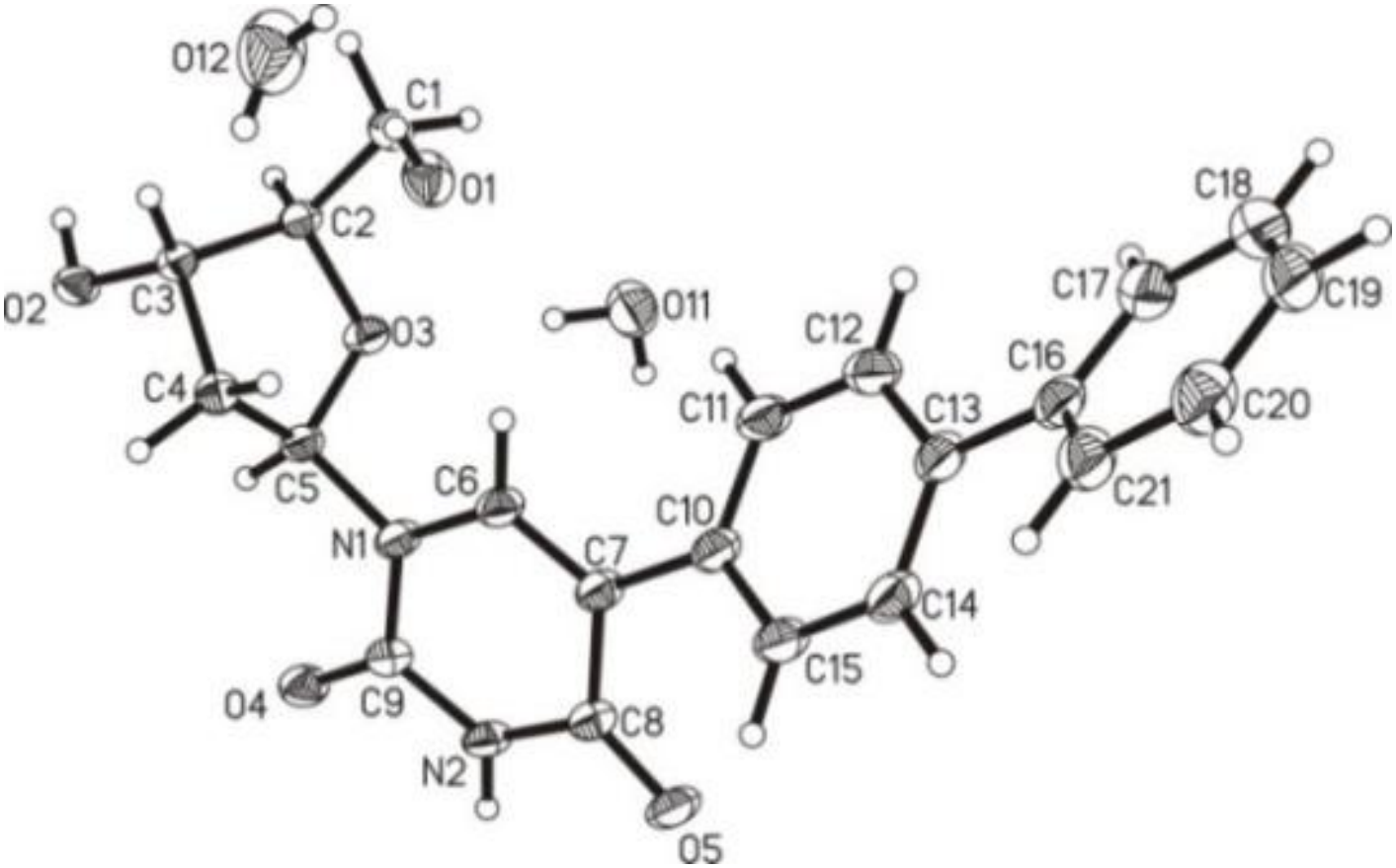
Single crystal X-ray structure for **IIIa**. Ellipsoids are shown with 50% probability.



Single crystal X-ray structure for **3a**. Ellipsoids are shown with 50% probability.



Single crystal X-ray structure for **3f**. Ellipsoids are shown with 50% probability.



Single crystal X-ray structure for **3i**. Ellipsoids are shown with 50% probability.