

Carbohydrates as reagent in a multicomponent reaction: One-pot access to a new library of hydrophilic substituted pyrimidine-fused heterocycles

Maryam Nourisefat, Farhad Panahi* and Ali Khalafi-Nezhad*

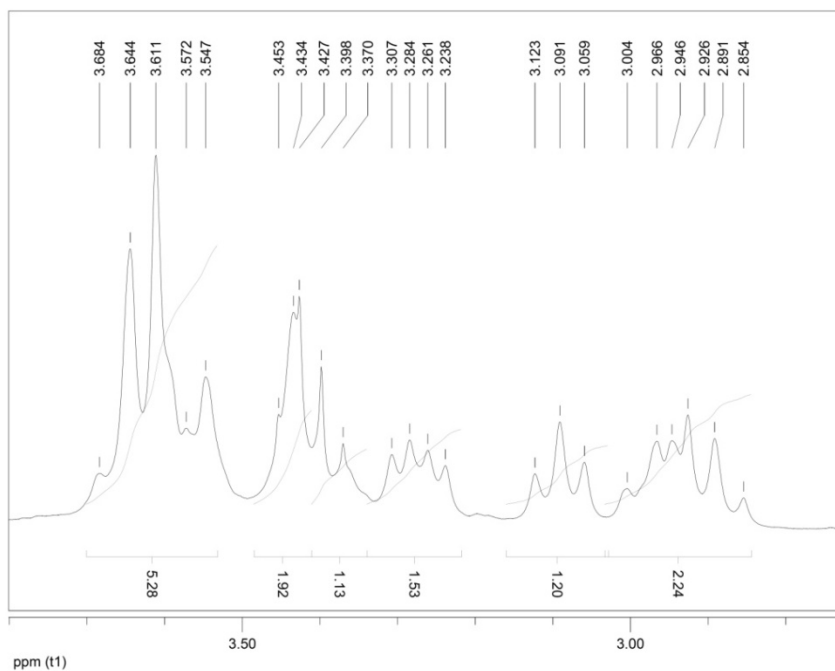
Department of Chemistry, College of Sciences, Shiraz University, Shiraz, 71454, Iran

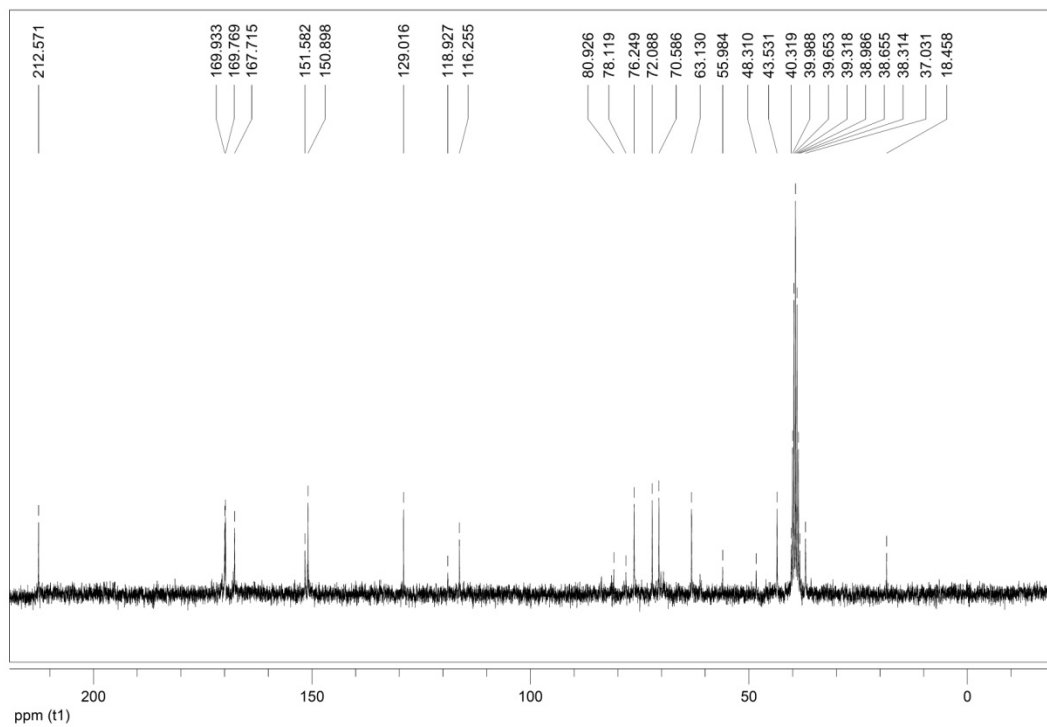
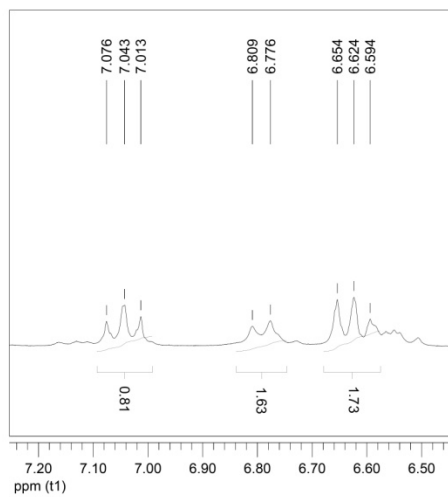
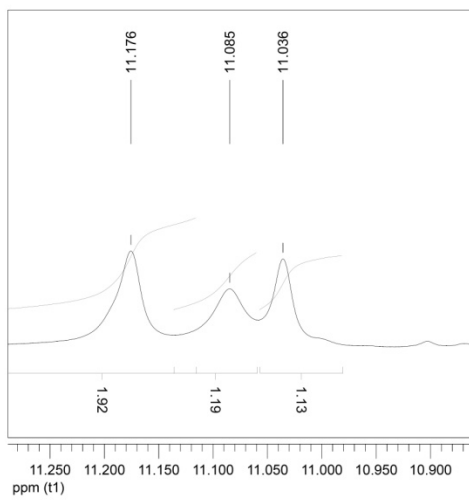
khalafi@chem.susc.ac.ir; panahi@shirazu.ac.ir

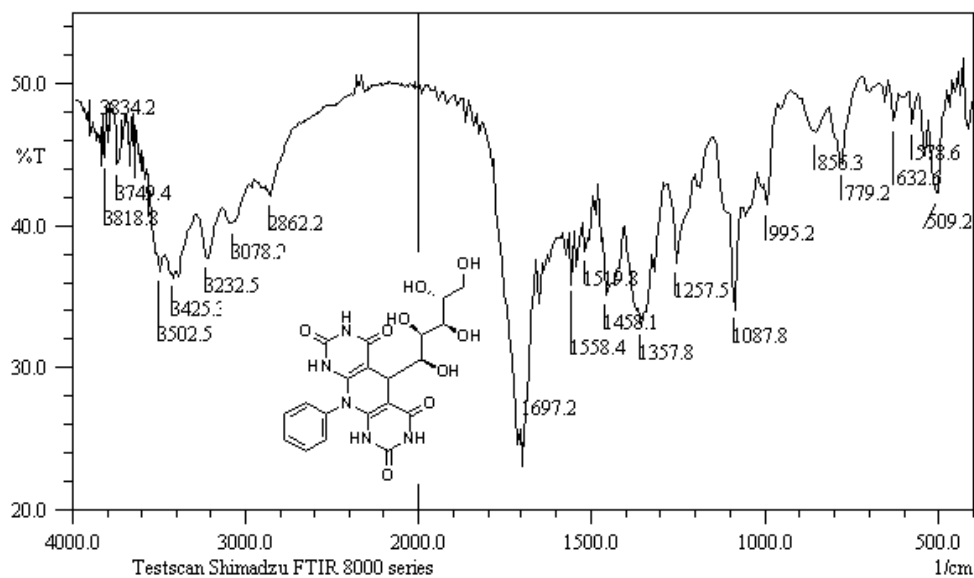
Outline

Copy of ^1H NMR, ^{13}C NMR and IR of synthesized compounds

1. 5-((1S,2R,3R,4R)-1,2,3,4,5-pentahydroxypentyl)-10-phenyl-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (4a)

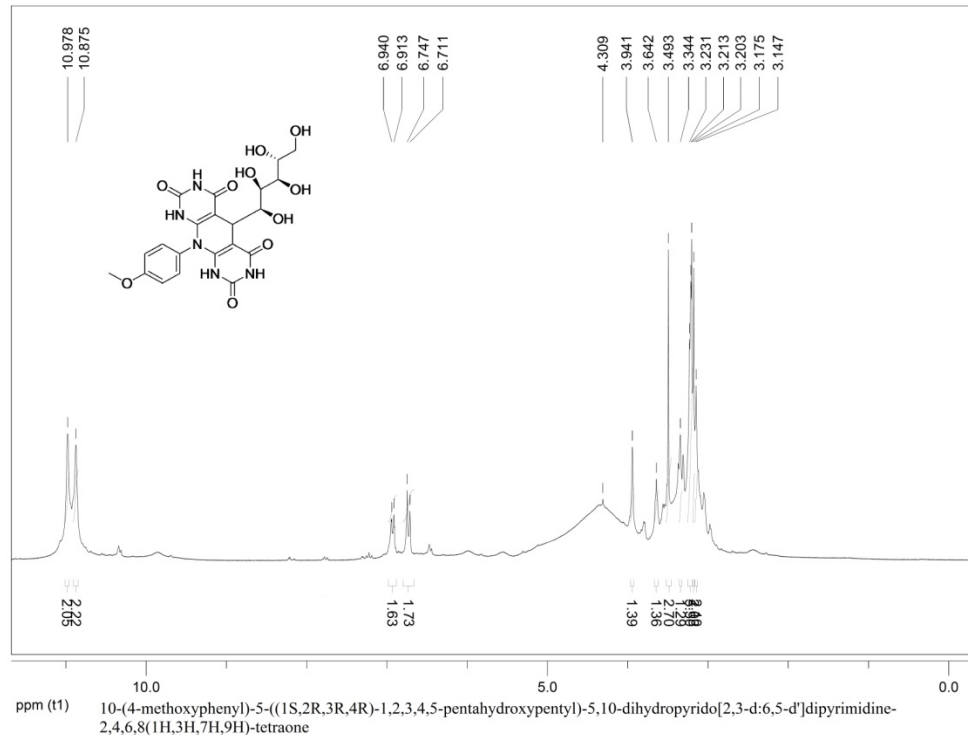


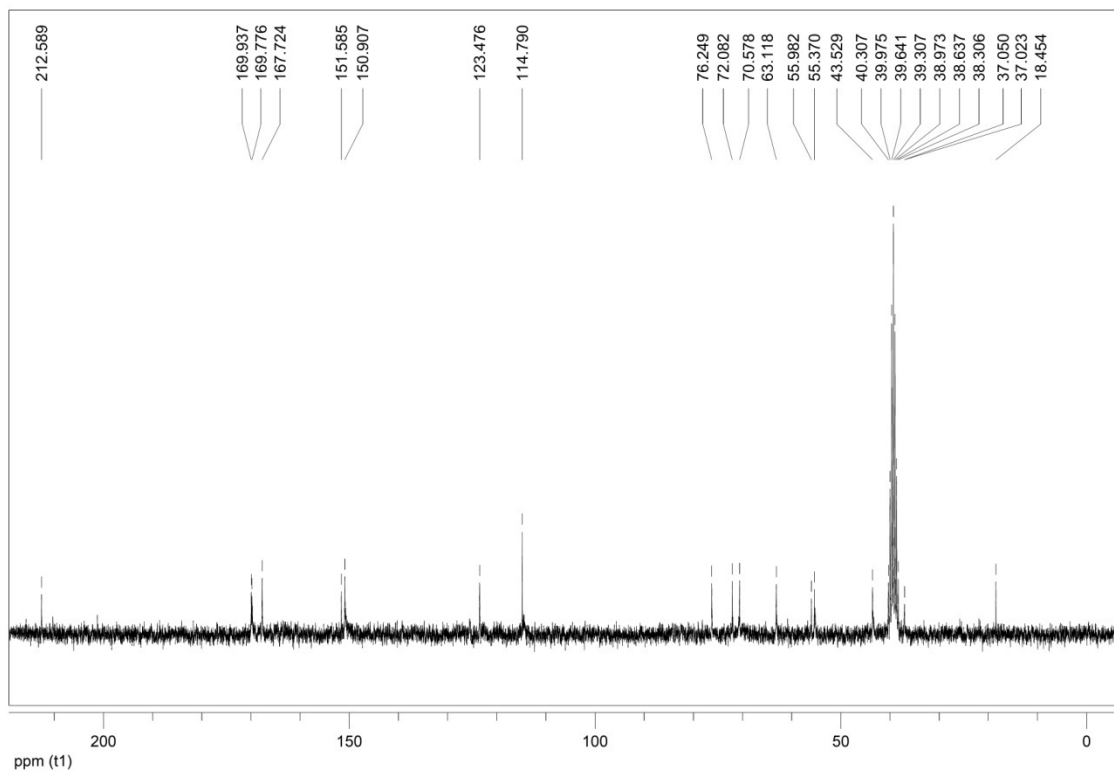
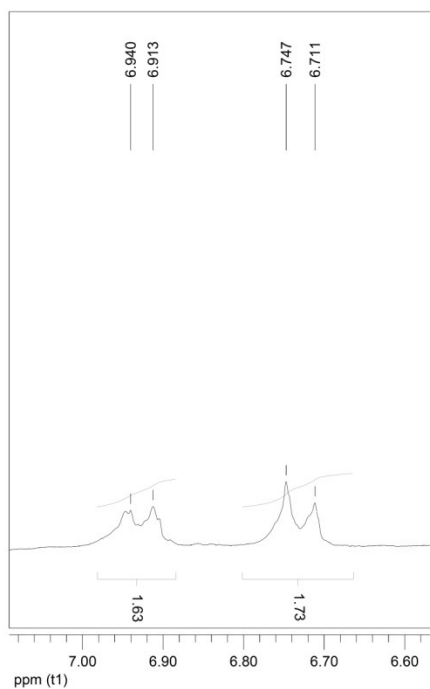
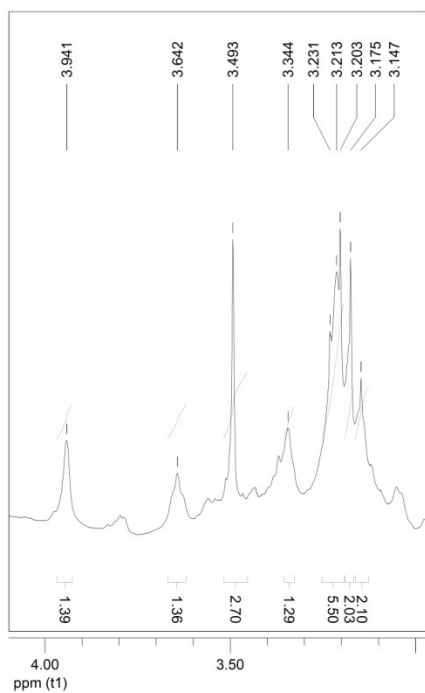


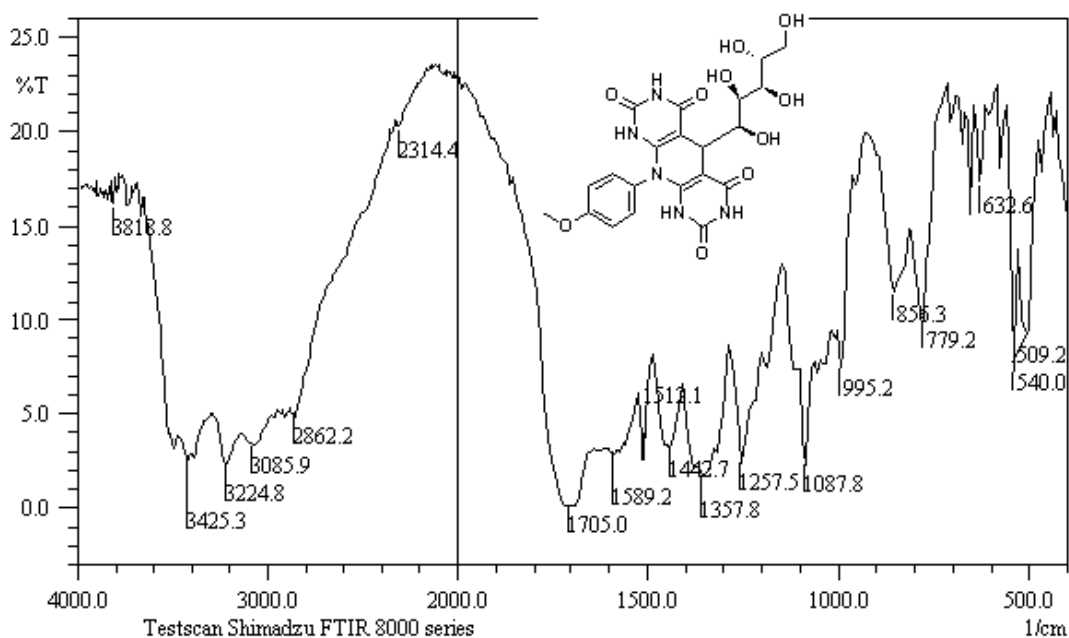


5-((1S,2R,3R,4R)-1,2,3,4,5-pentahydroxypentyl)-10-phenyl-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone

2. 10-(4-methoxyphenyl)-5-((1S,2R,3R,4R)-1,2,3,4,5-pentahydroxypentyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (4b)

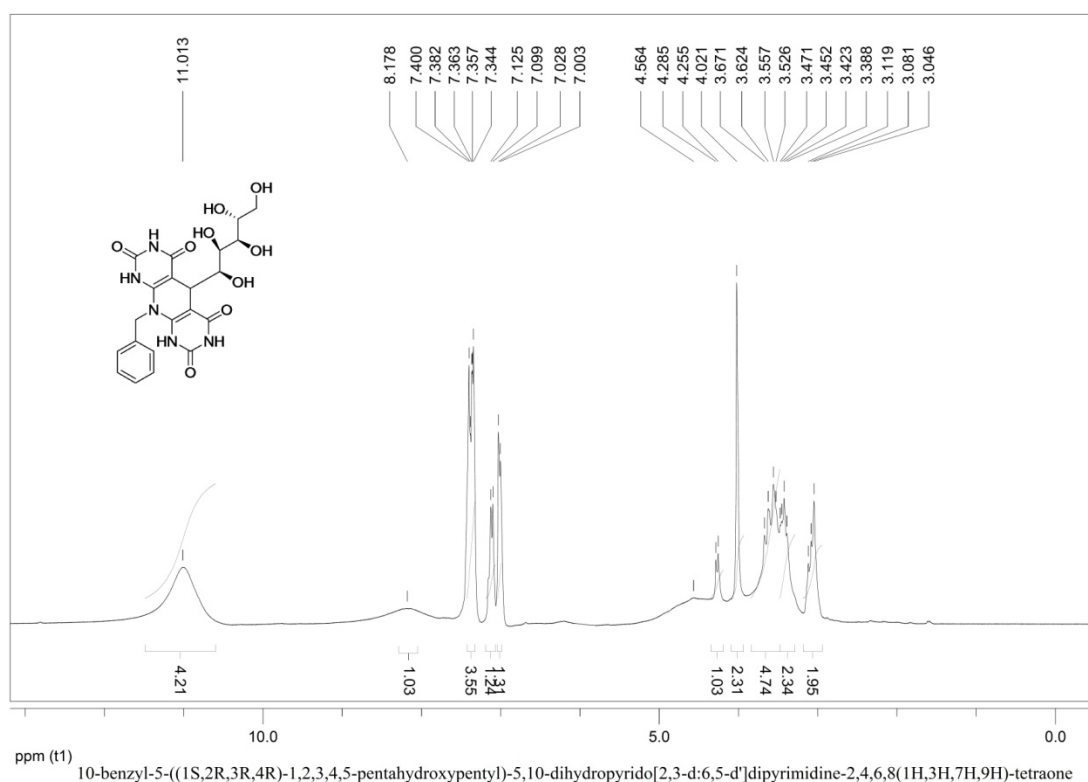


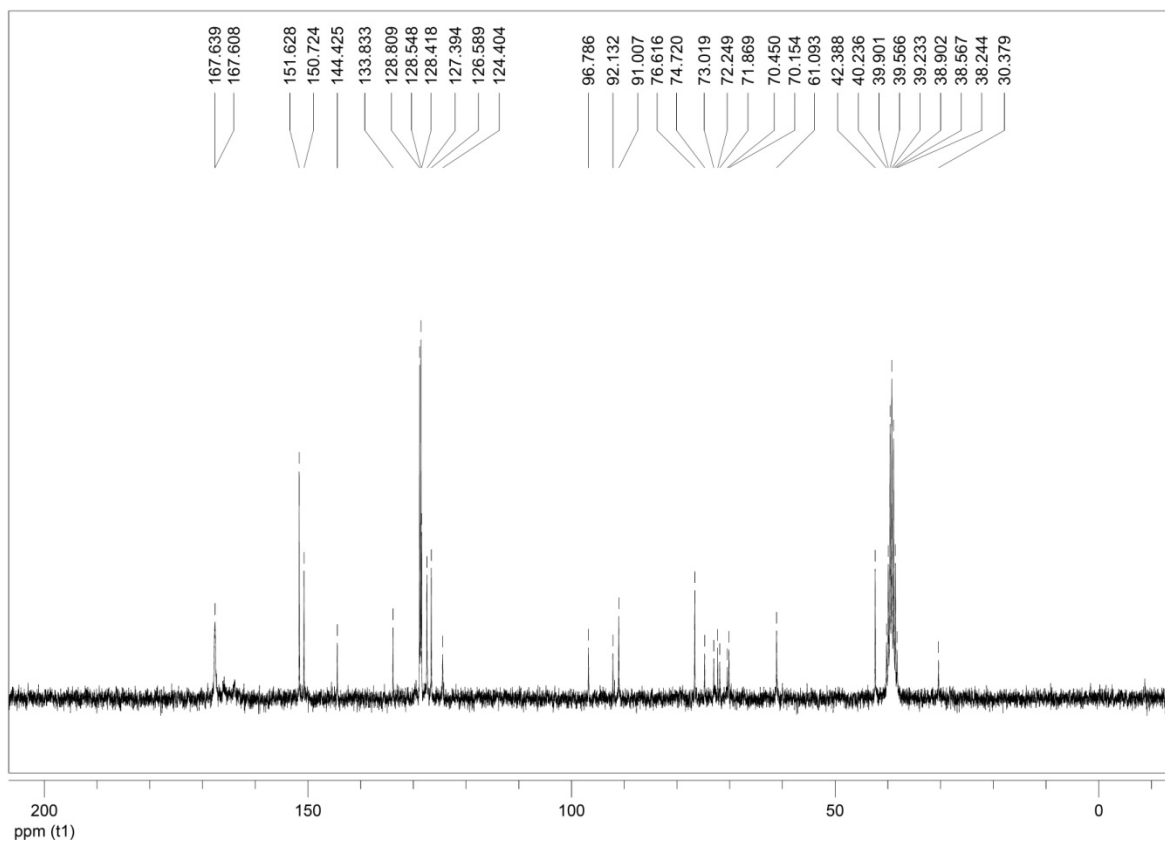
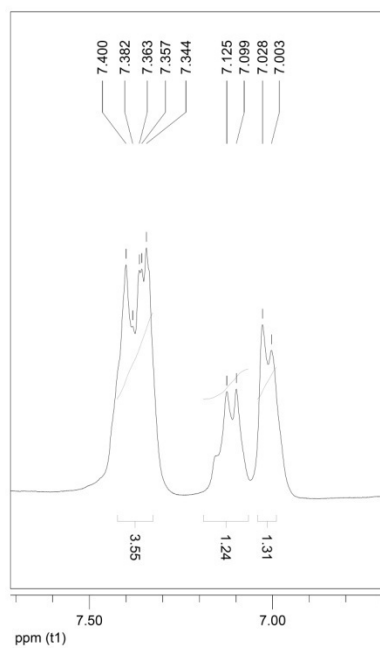
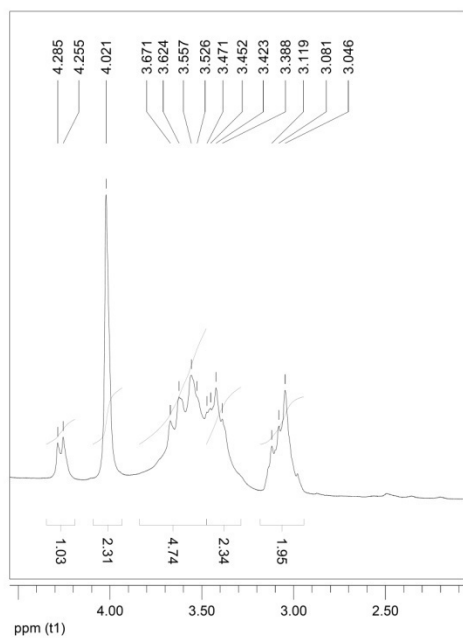


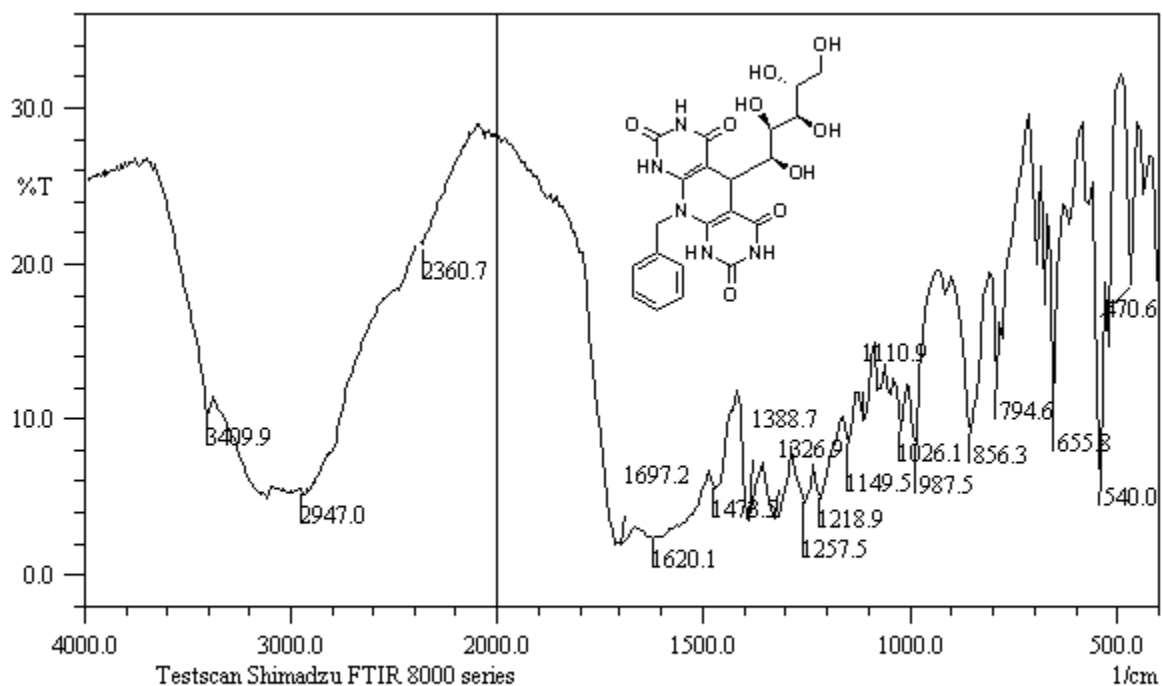


10-(4-methoxyphenyl)-5-((1S,2R,3R,4R)-1,2,3,4,5-pentahydroxypentyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone

3. 10-benzyl-5-((1S,2R,3R,4R)-1,2,3,4,5-pentahydroxypentyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (4c)

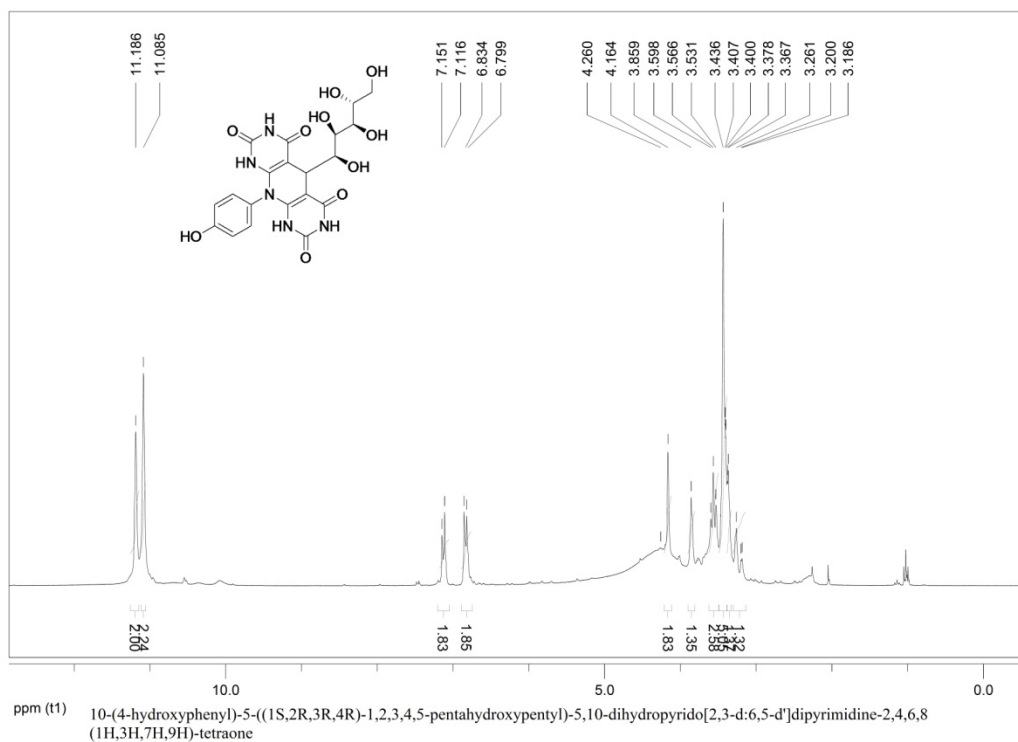


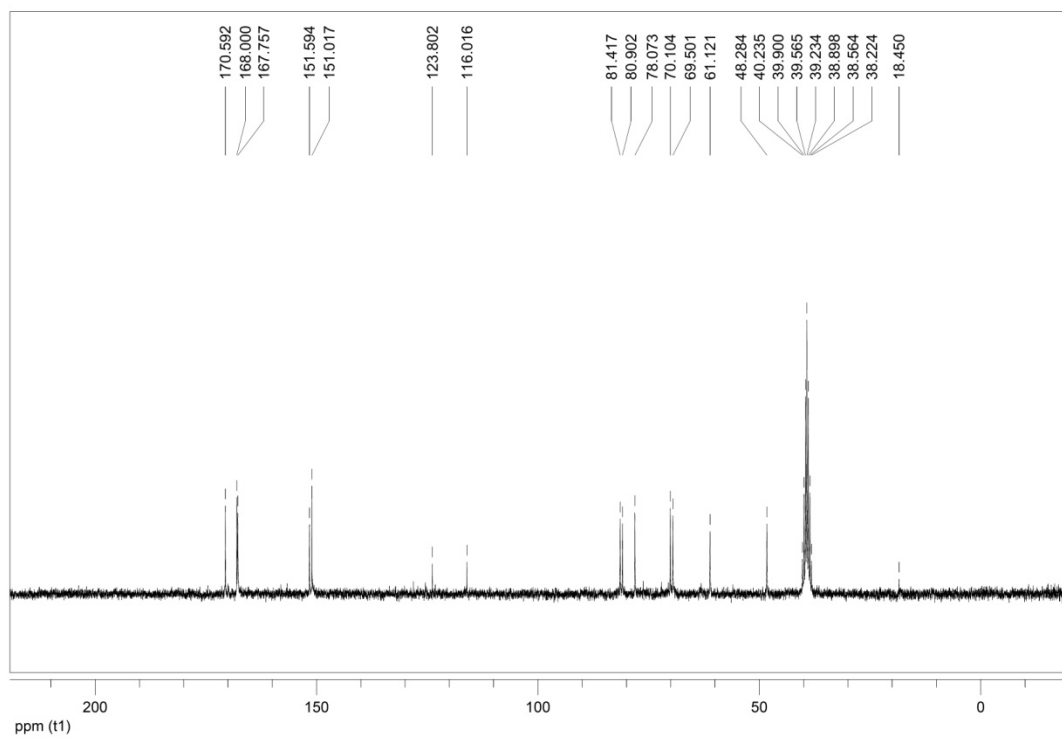
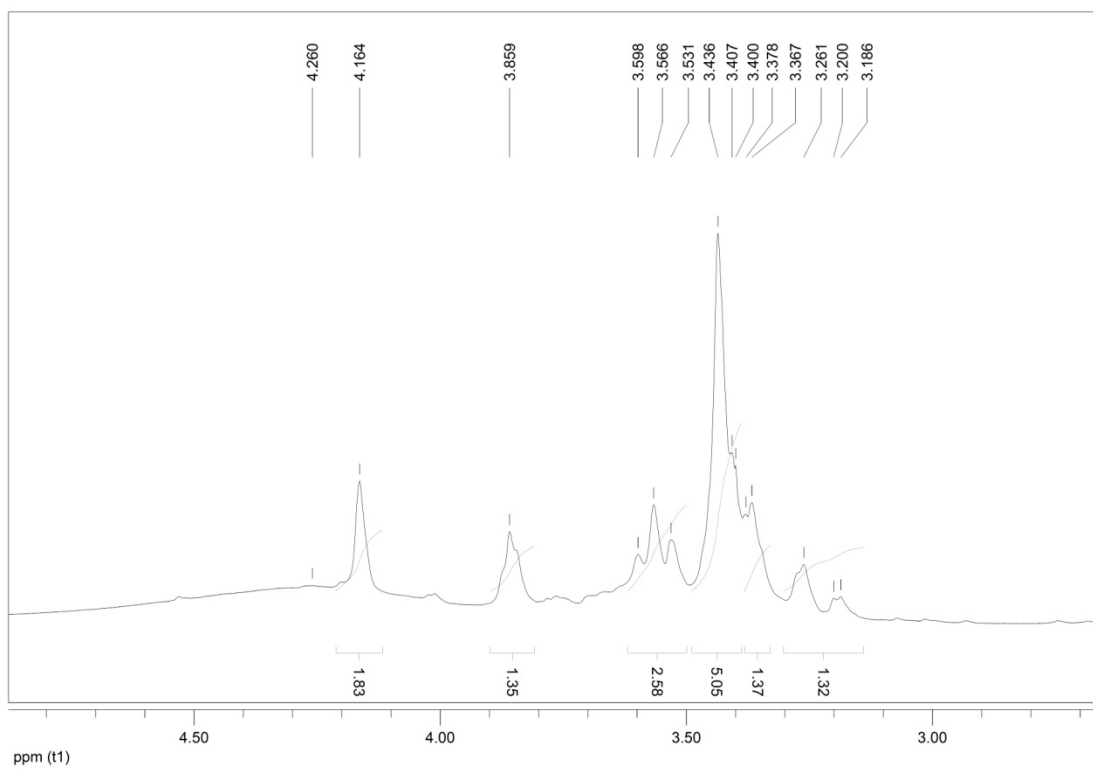


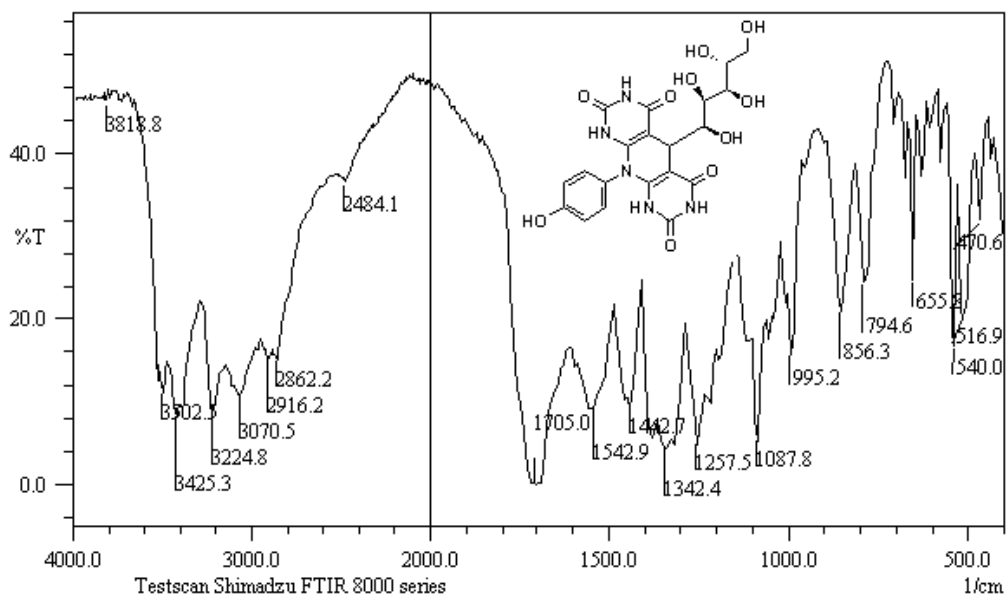


10-benzyl-5-((1S,2R,3R,4R)-1,2,3,4,5-pentahydroxypentyl)-5,10-dihydropyrido[2,3-d,6,5-d']
dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone

4. 10-(4-hydroxyphenyl)-5-((1S,2R,3R,4R)-1,2,3,4,5-pentahydroxypentyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (4d)

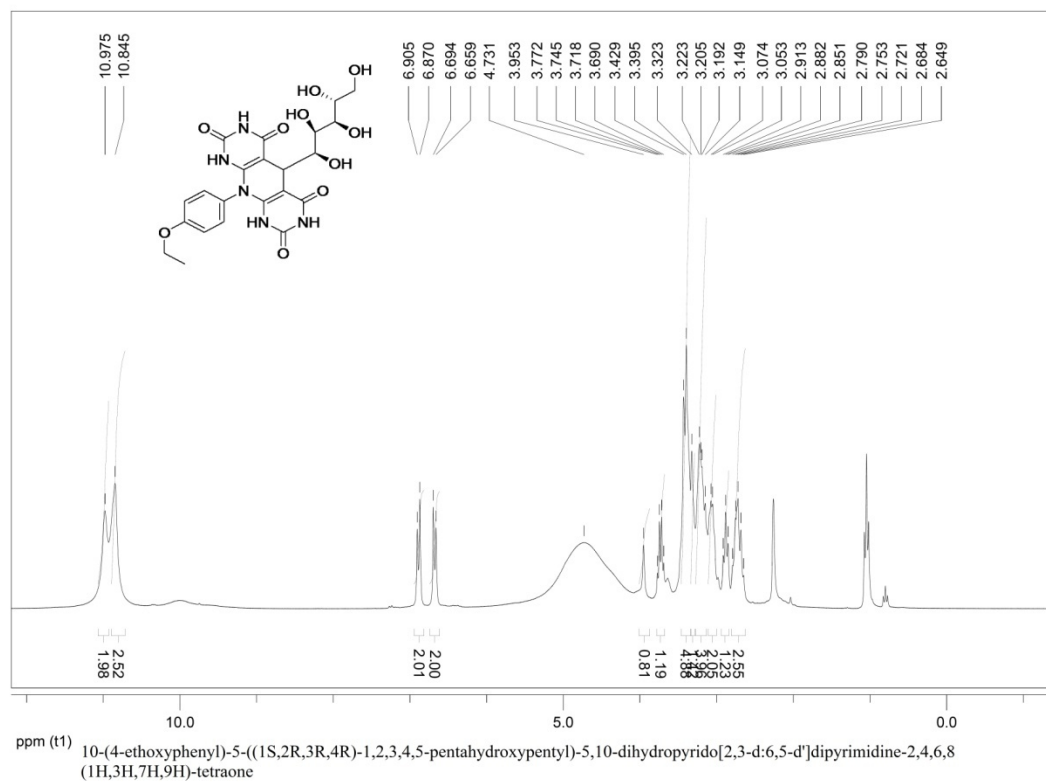


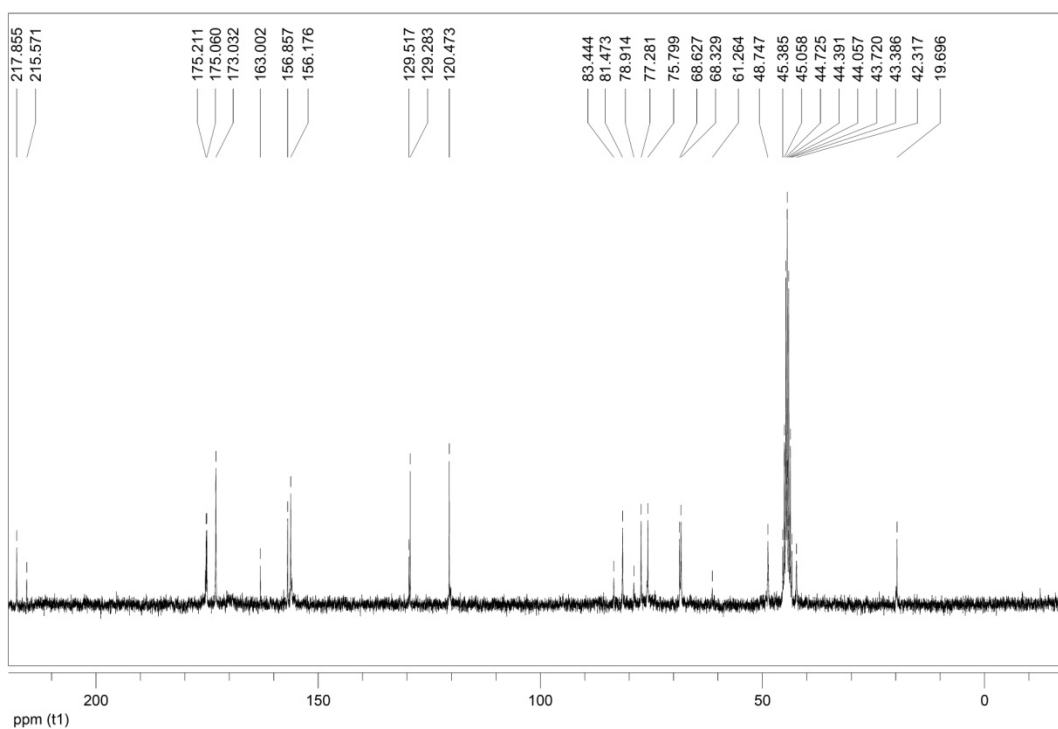
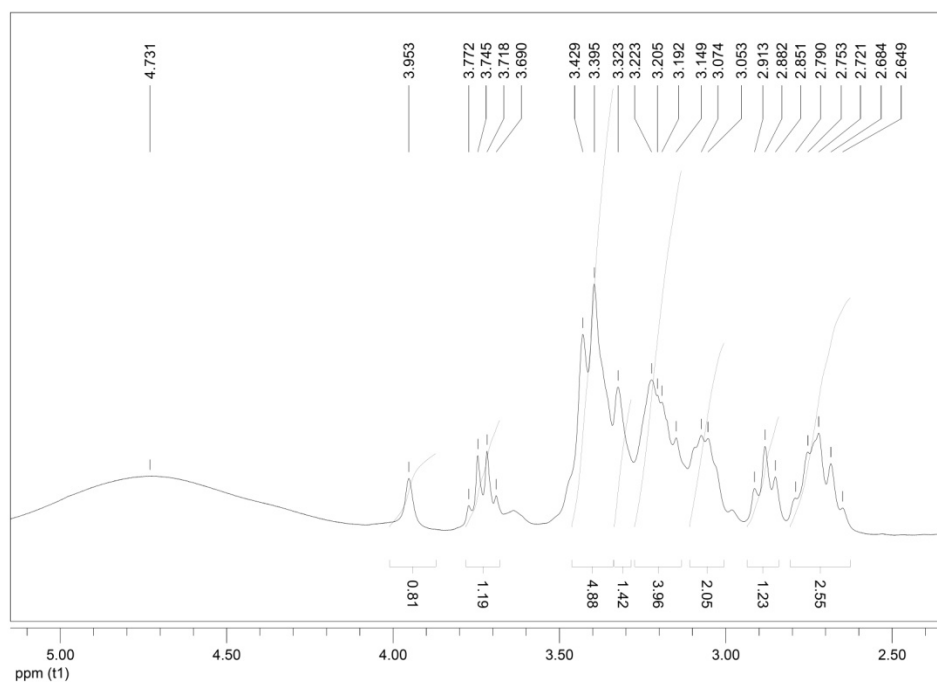


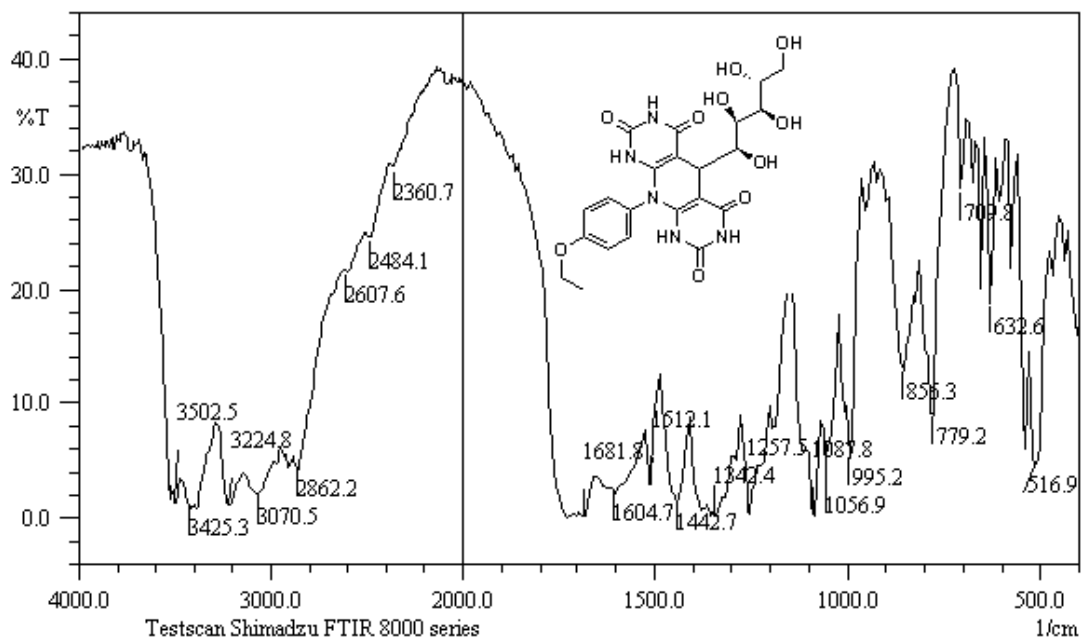


10-(4-hydroxyphenyl)-5-((1S,2R,3R,4R)-1,2,3,4,5-pentahydroxypentyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone

5. 10-(4-ethoxyphenyl)-5-((1S,2R,3R,4R)-1,2,3,4,5-pentahydroxypentyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (4e)

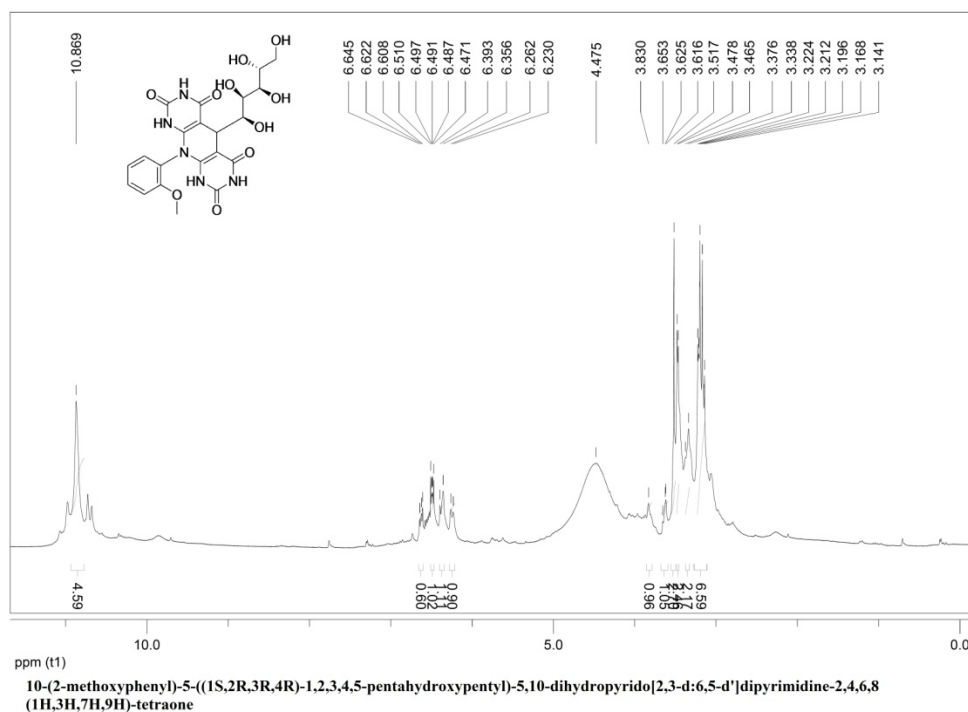


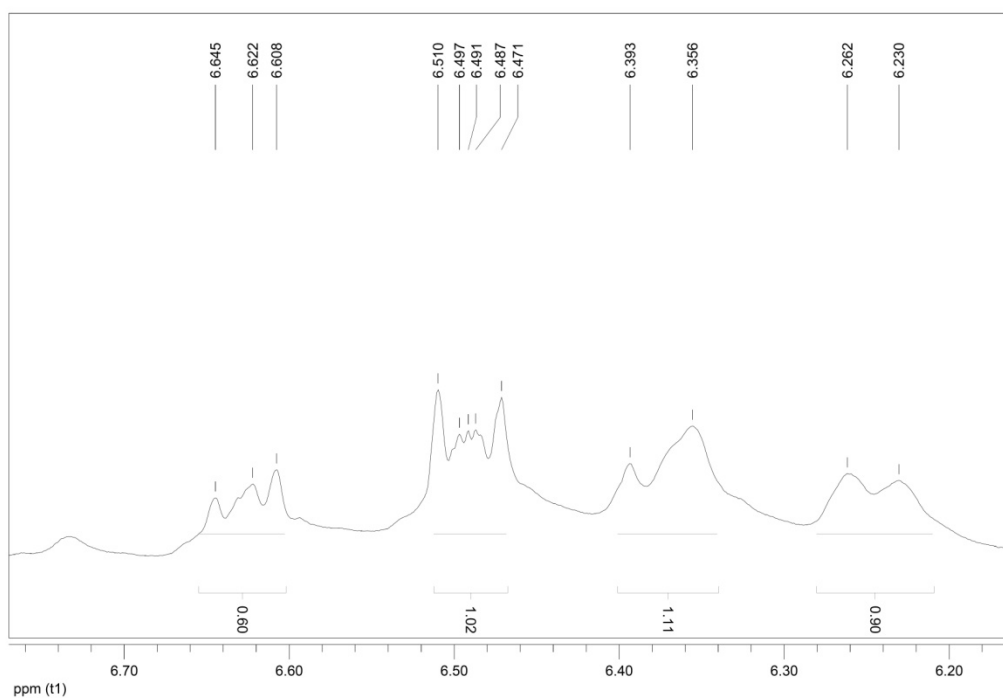
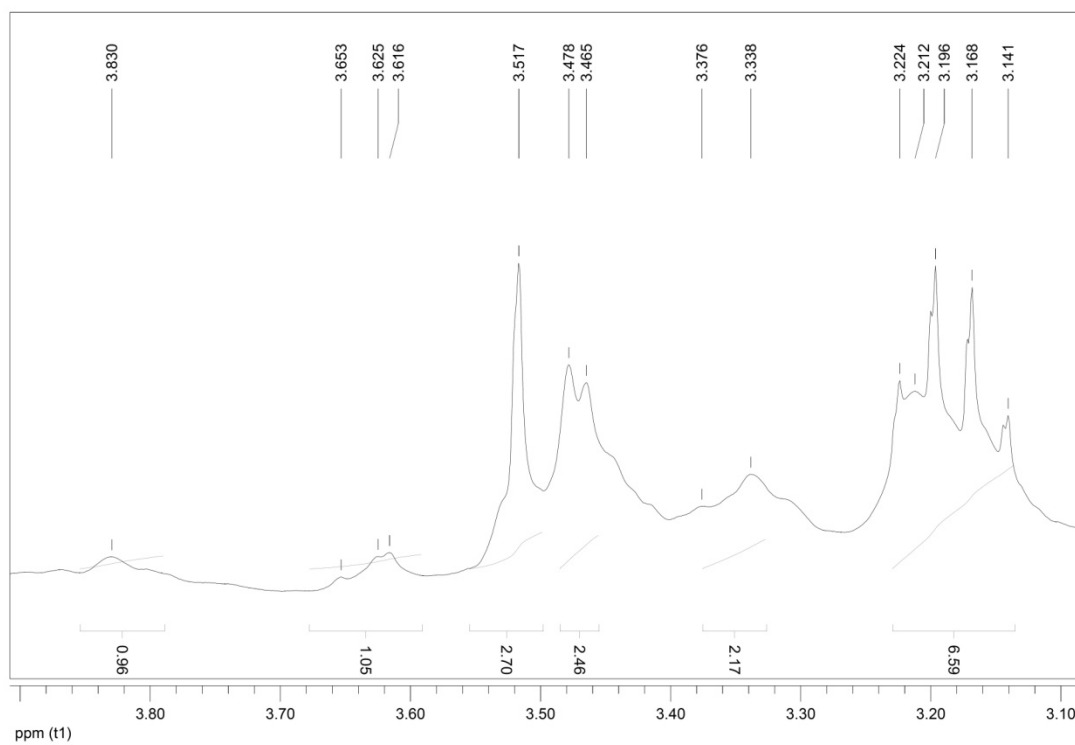


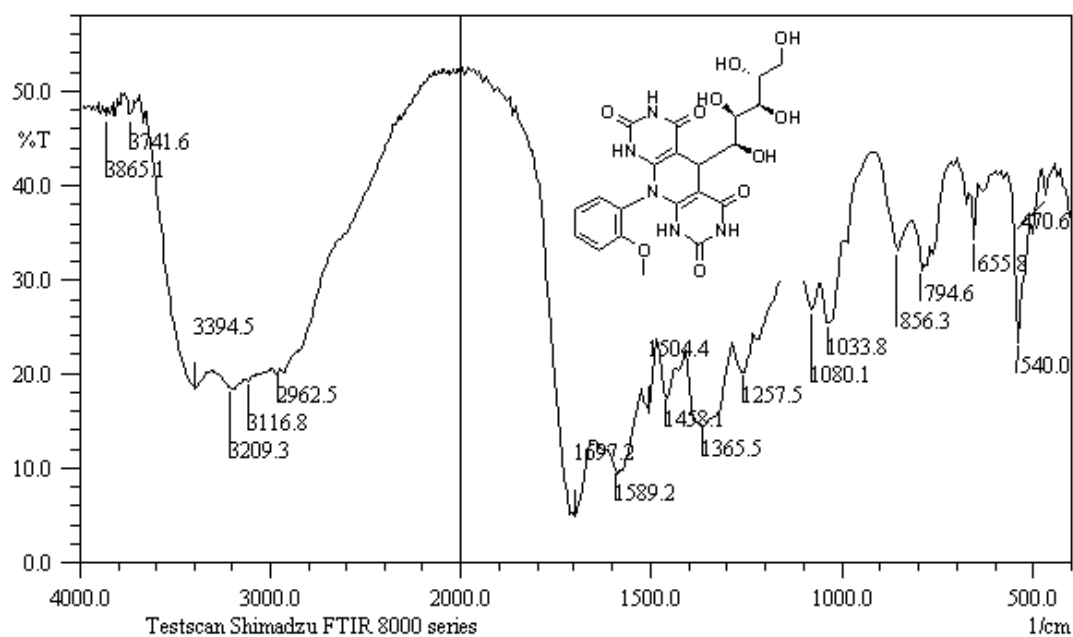
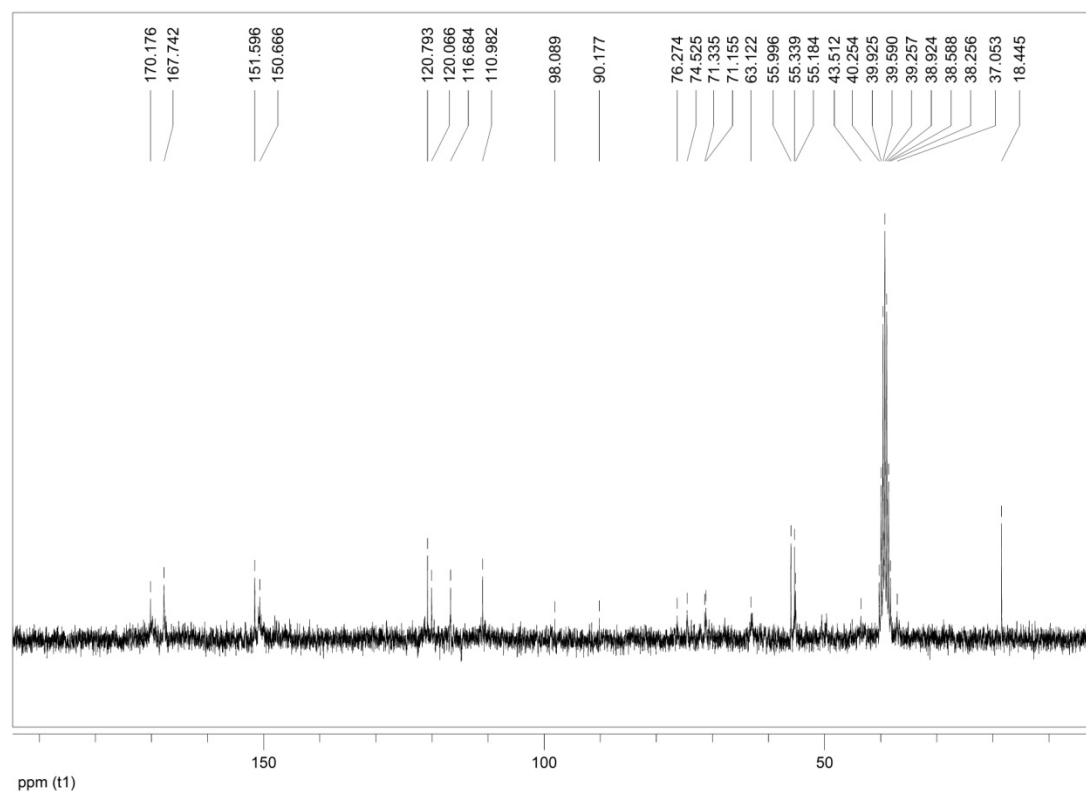


10-(4-ethoxyphenyl)-5-((1S,2R,3R,4R)-1,2,3,4,5-pentahydroxypentyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone

6. 10-(2-methoxyphenyl)-5-((1S,2R,3R,4R)-1,2,3,4,5-pentahydroxypentyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (4f)

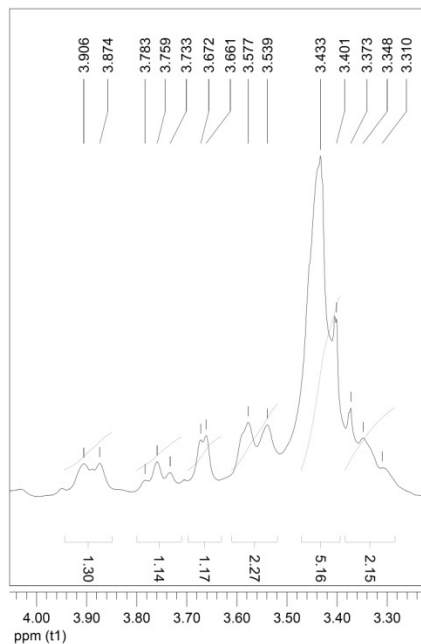
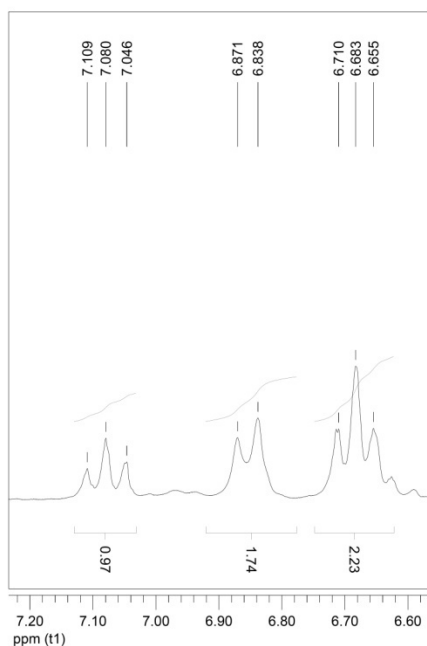
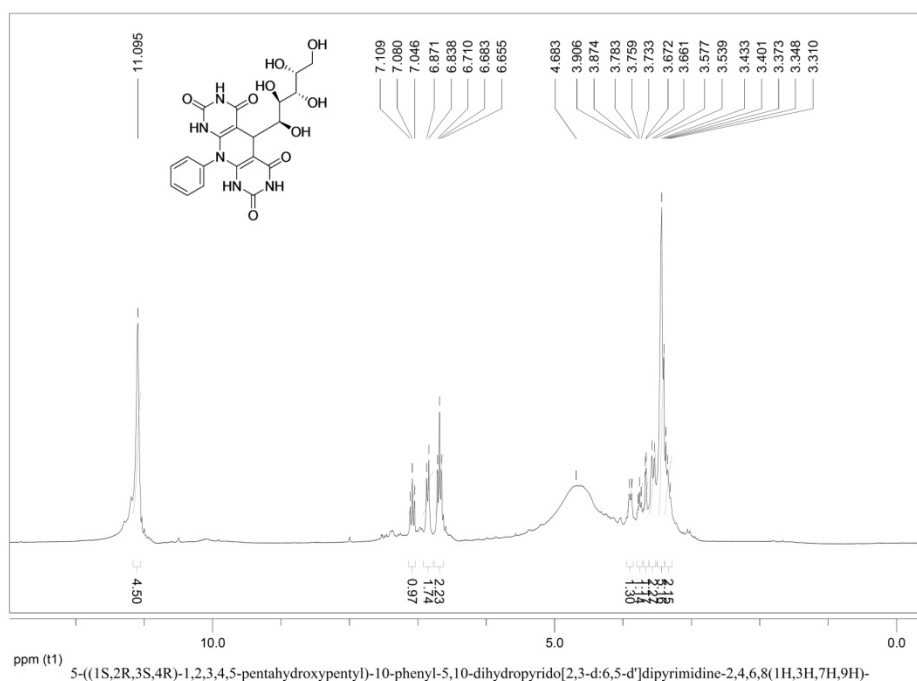


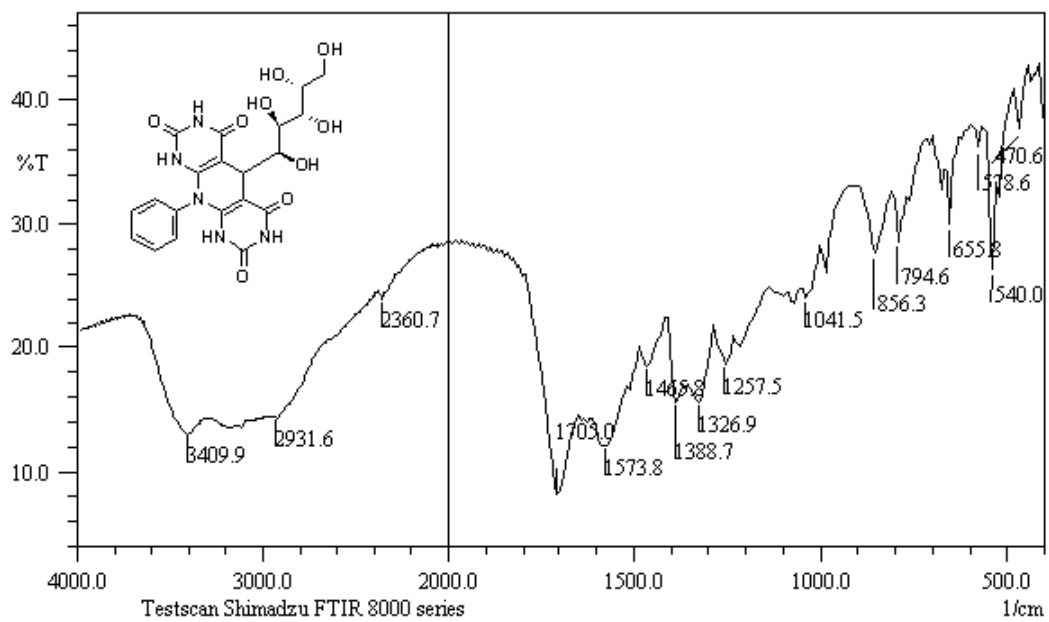
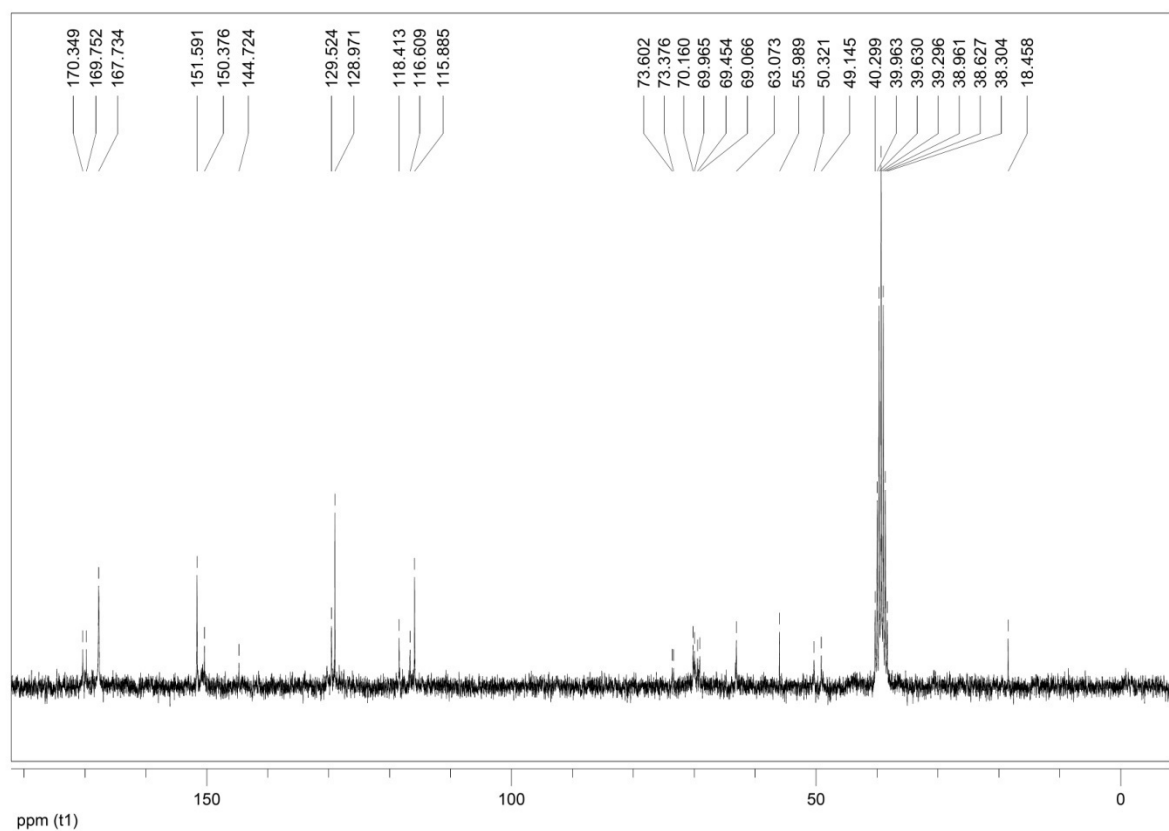




10-(2-methoxyphenyl)-5-((1S,2R,3R,4R)-1,2,3,4,5-pentahydroxypentyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone

7. 5-((1S,2R,3S,4R)-1,2,3,4,5-pentahydroxypentyl)-10-phenyl-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (4g)



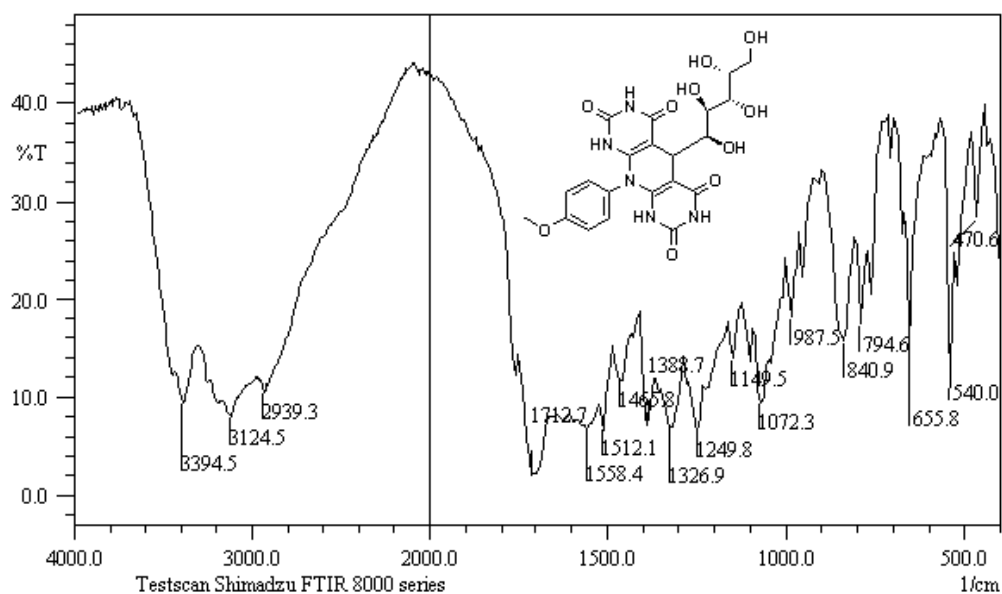
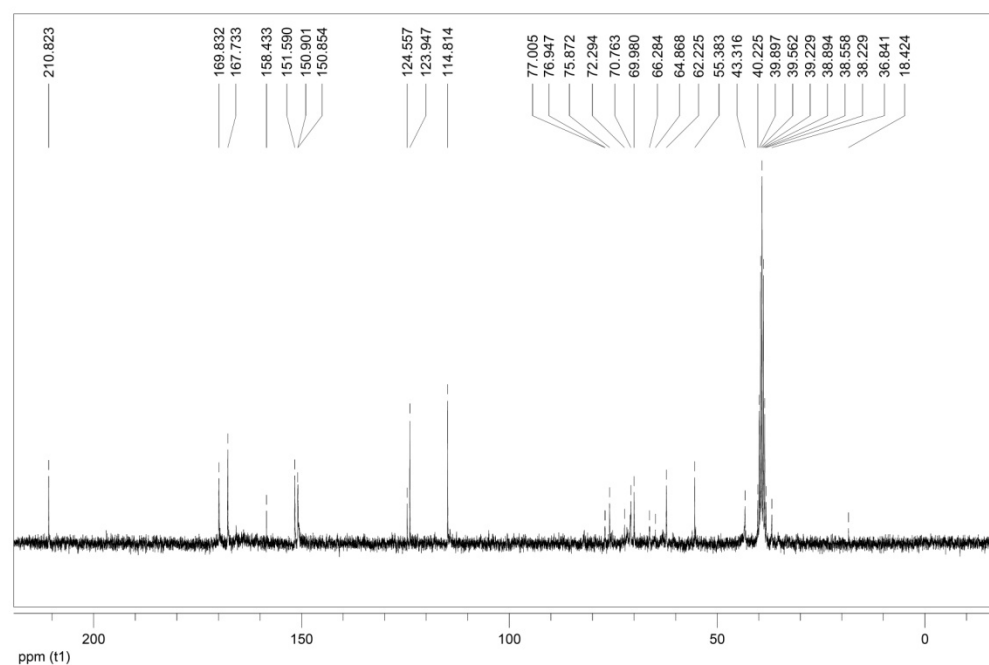


10-(4-methoxyphenyl)-5-((1S,2R,3R,4R)-1,2,3,4,5-pentahydroxypentyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone

Chemical structure of 10: 10-(4-methoxyphenyl)-5-((1S,2R,3S,4R)-1,2,3,4,5-pentahydroxypentyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8-tetraone.

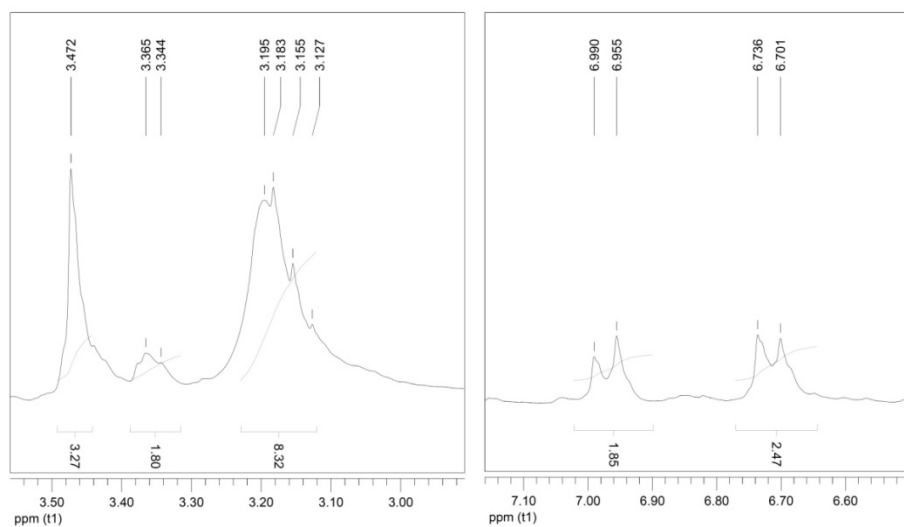
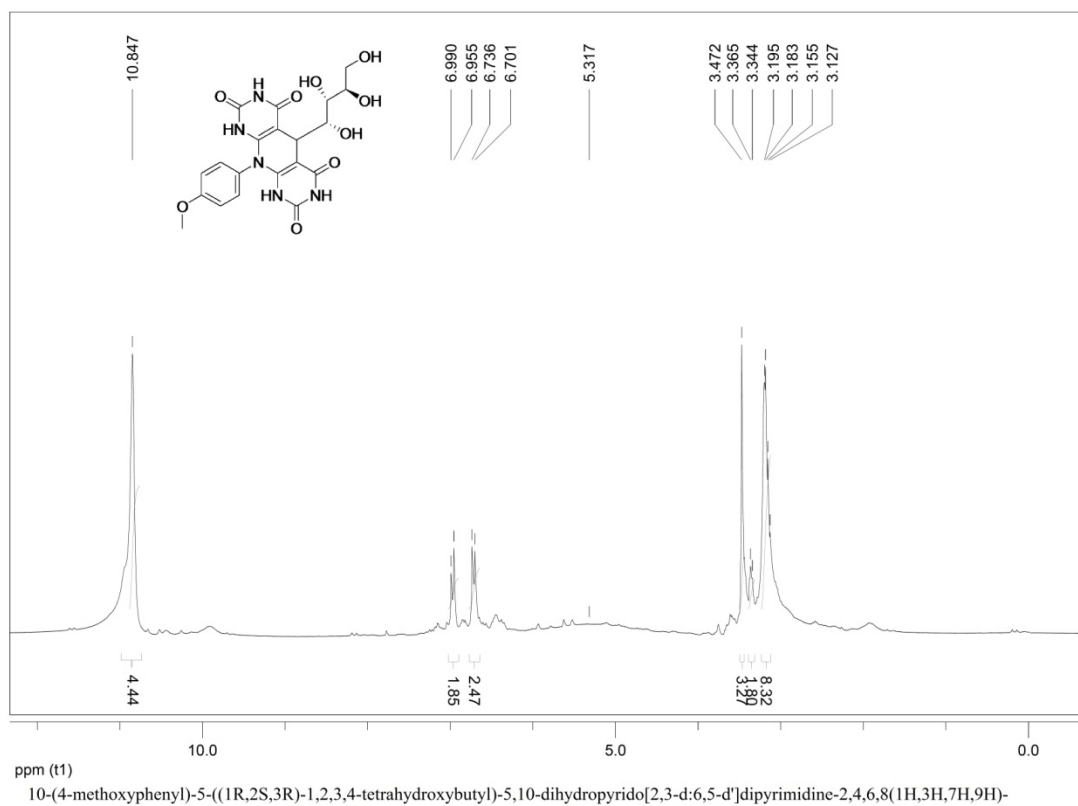
¹H NMR spectrum (DMSO-d₆) of compound 10. The spectrum shows peaks at 10.963 ppm (s, 1H), 7.10-7.14 ppm (m, 3H), 4.47-4.74 ppm (m, 5H), and 3.62-3.96 ppm (m, 9H).

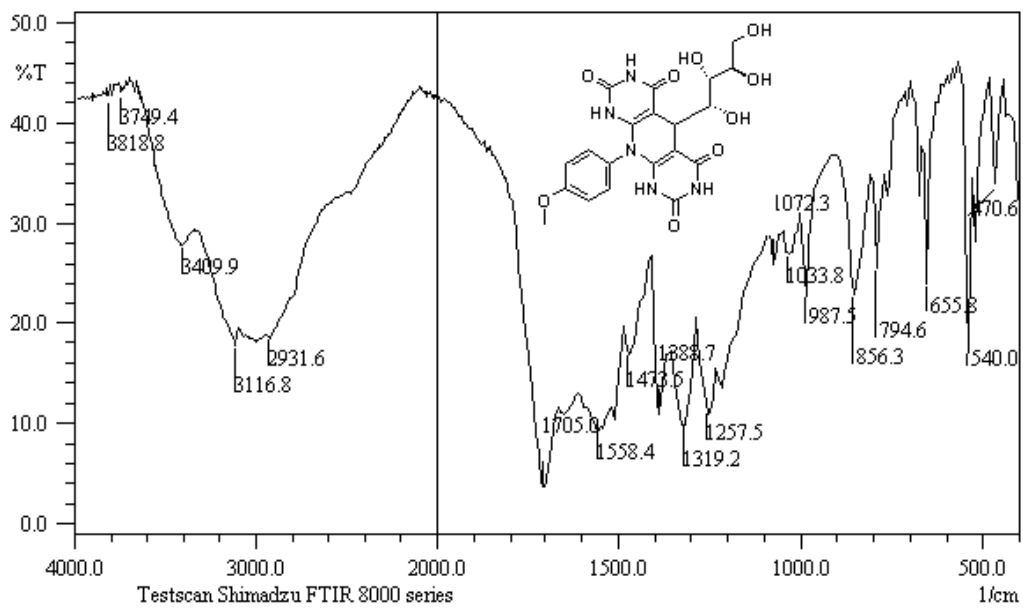
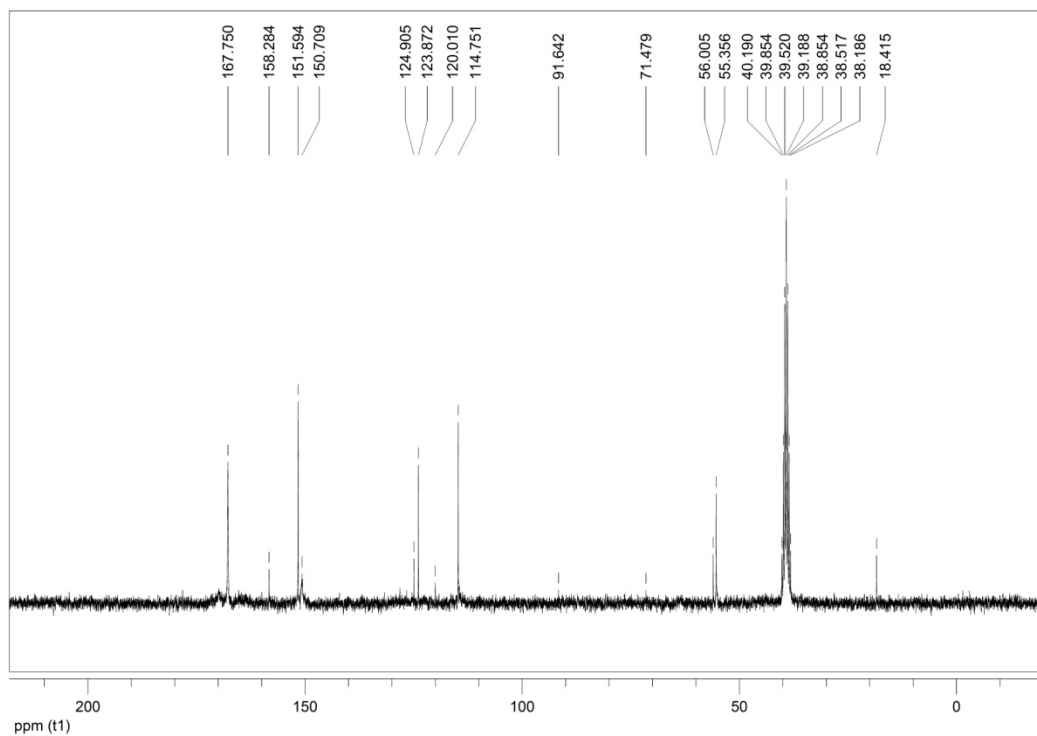




10-(4-methoxyphenyl)-5-((1S,2R,3S,4R)-1,2,3,4,5-pentahydroxypentyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone

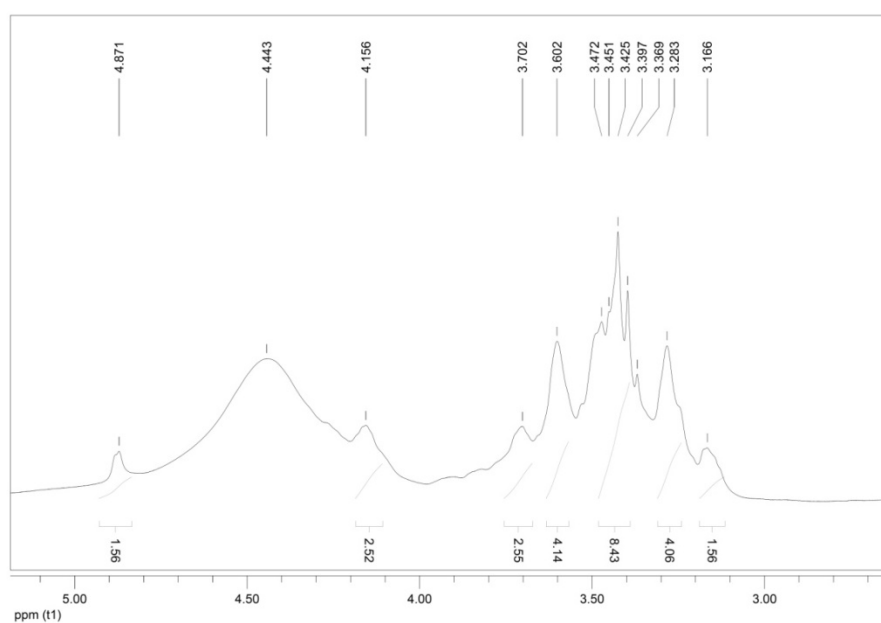
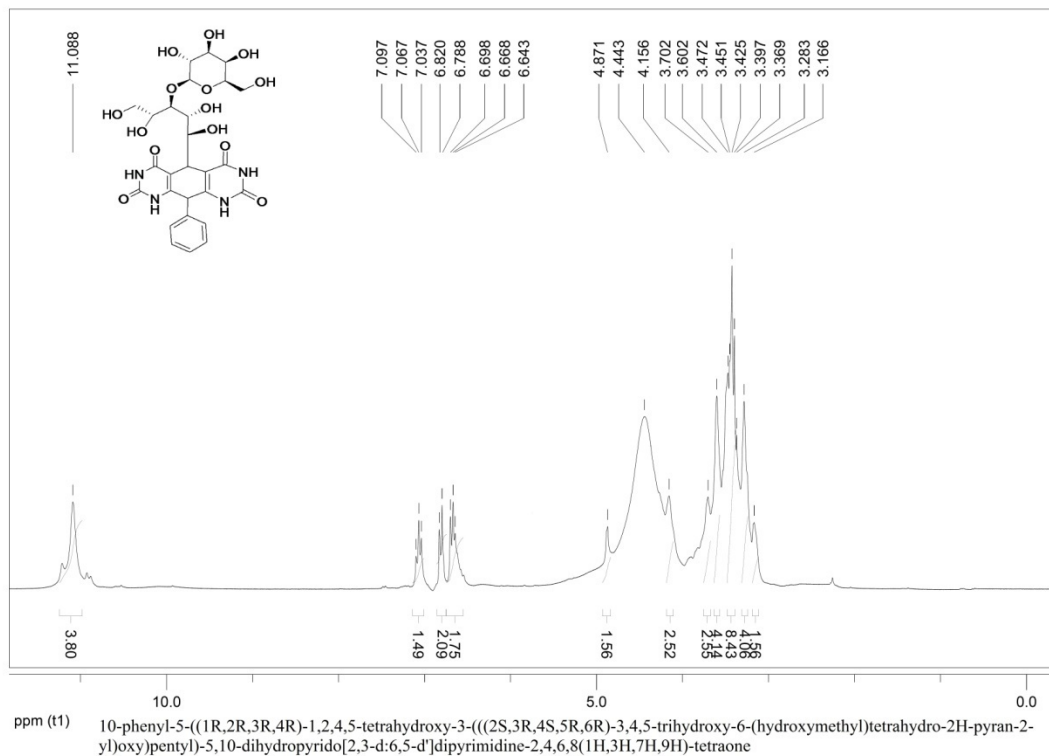
9. 10-(4-methoxyphenyl)-5-((1R,2S,3R)-1,2,3,4-tetrahydroxybutyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (4i)

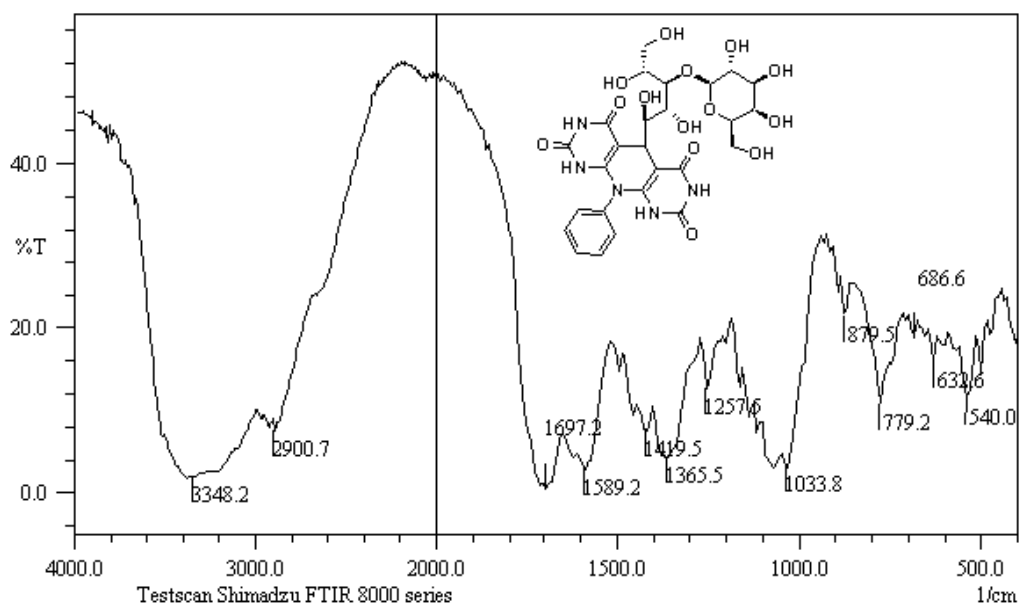
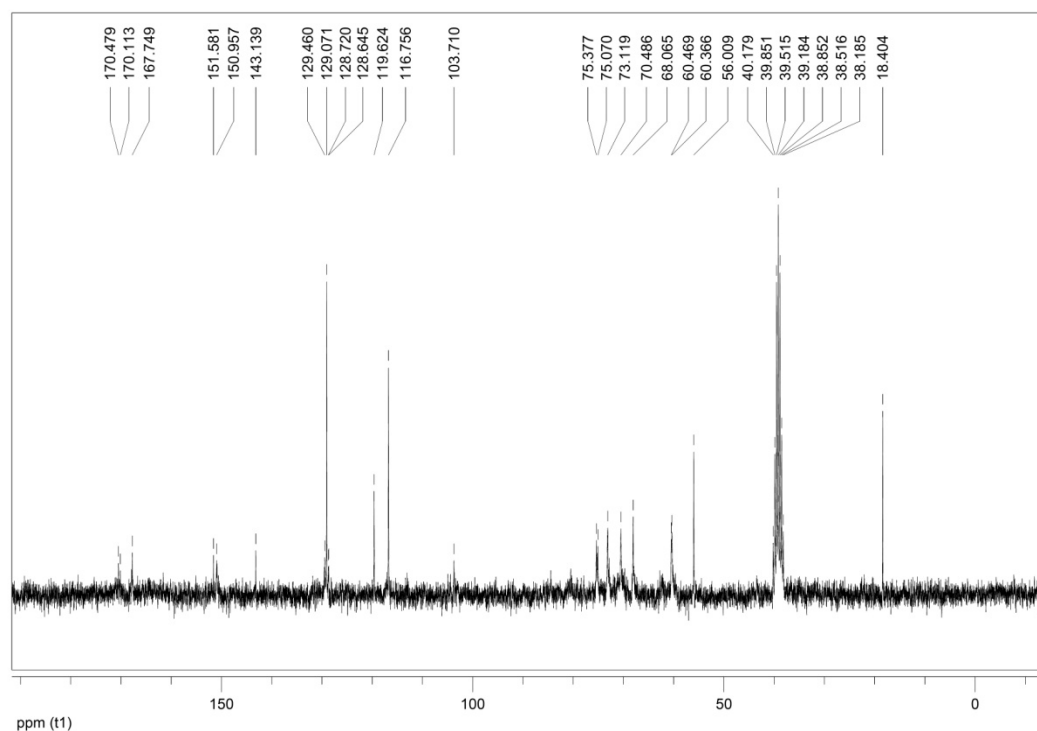




10-(4-methoxyphenyl)-5-((1R,2S,3R)-1,2,3,4-tetrahydroxybutyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone

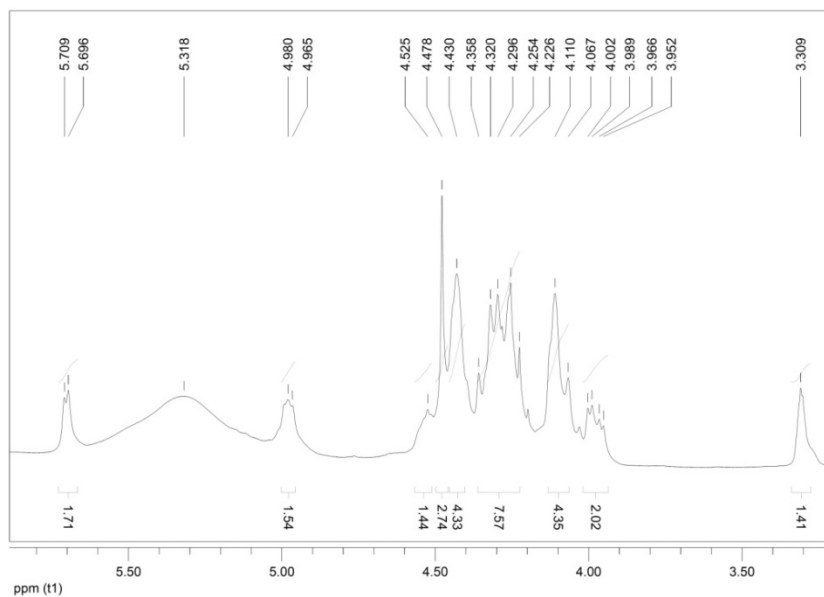
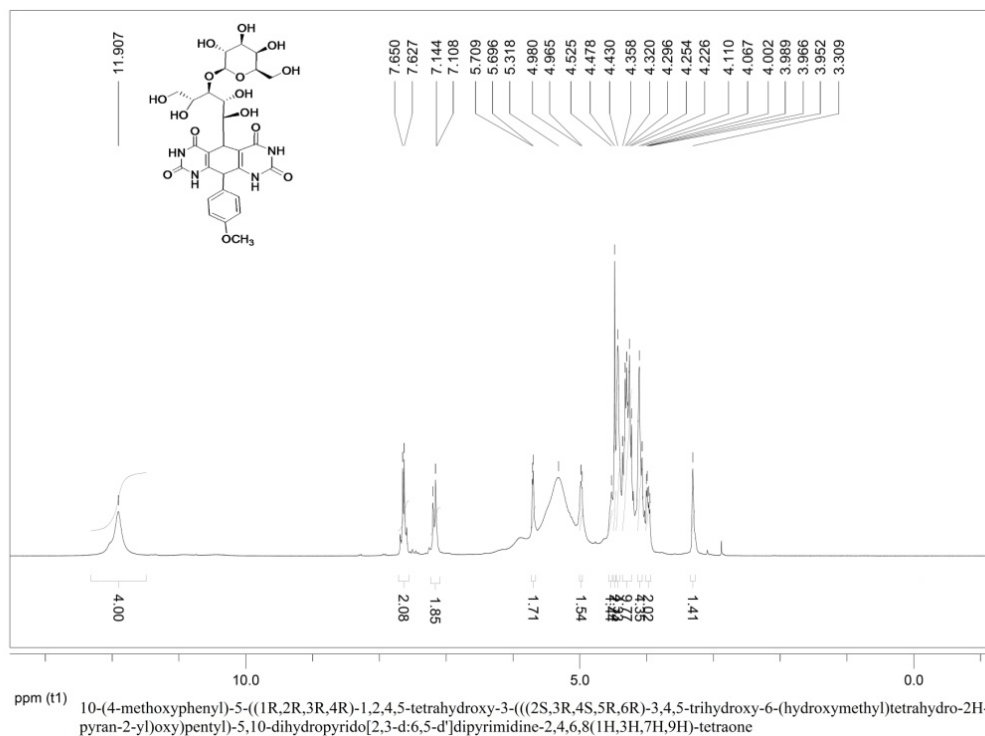
10. 10-phenyl-5-((1R,2R,3R,4R)-1,2,4,5-tetrahydroxy-3-(((2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)pentyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (4j)

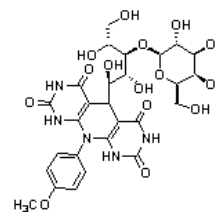
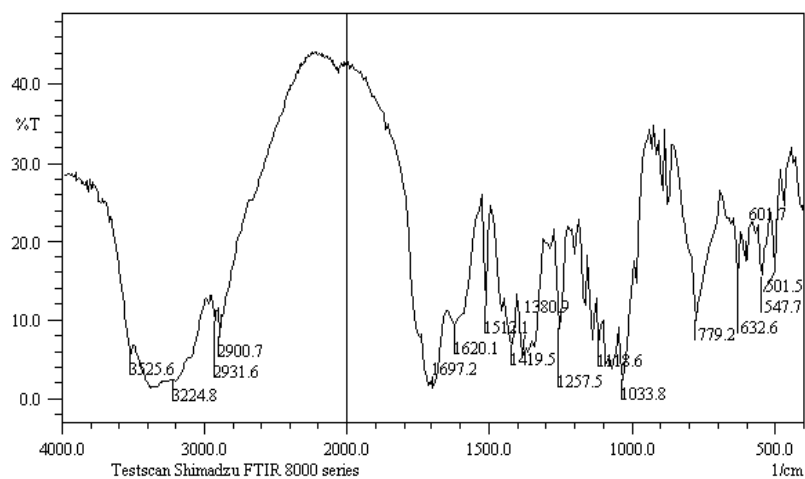
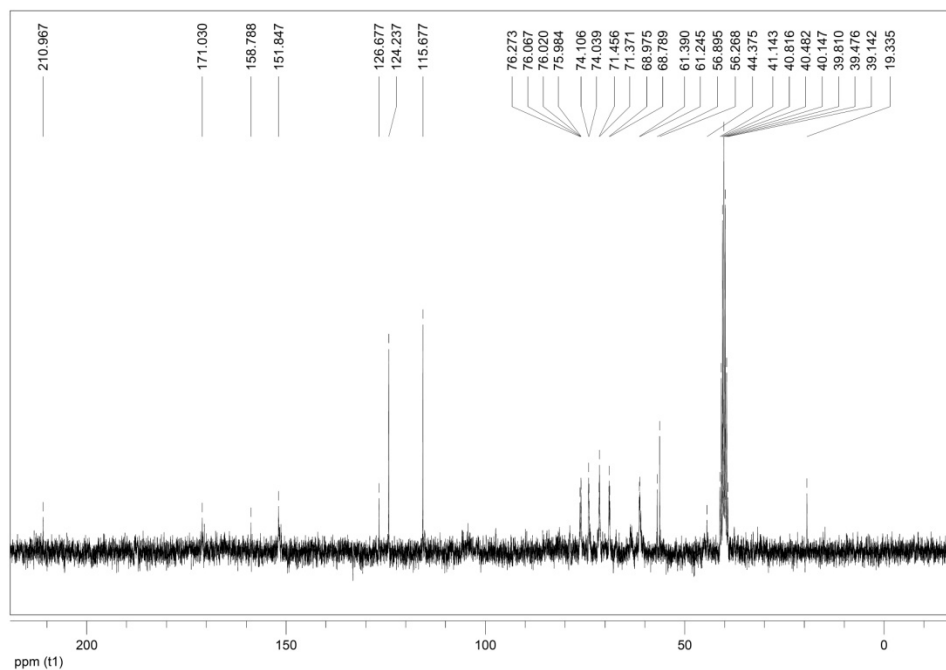




10-phenyl-5-((1R,2R,3R,4R)-1,2,4,5-tetrahydroxy-3-(((2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)pentyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone

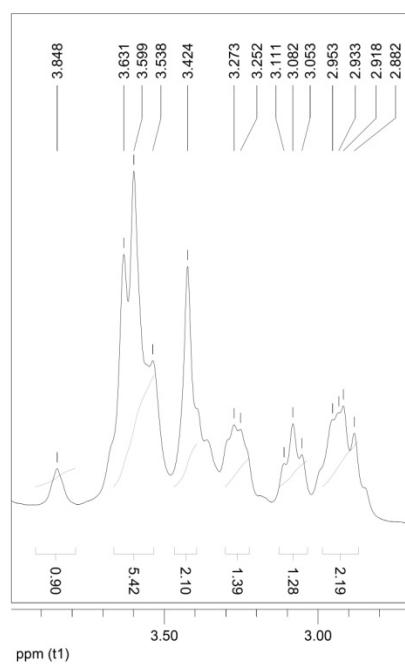
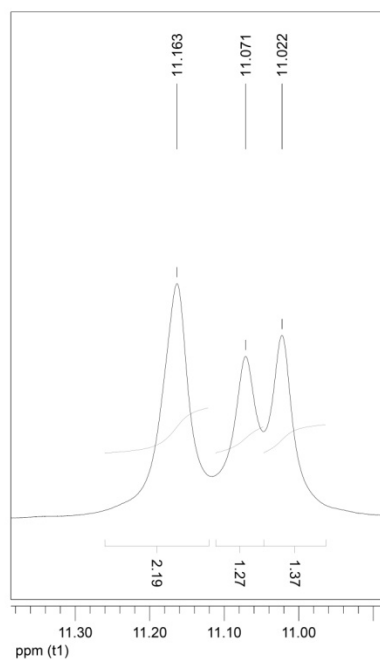
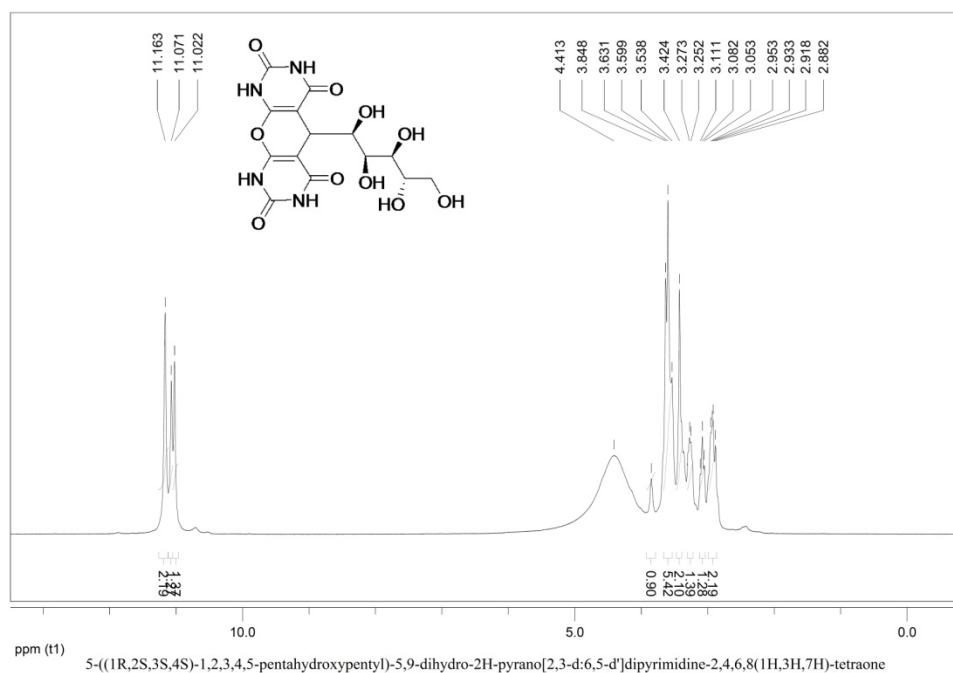
11. 10-(4-methoxyphenyl)-5-((1R,2R,3R,4R)-1,2,4,5-tetrahydroxy-3-(((2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)pentyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (4k)

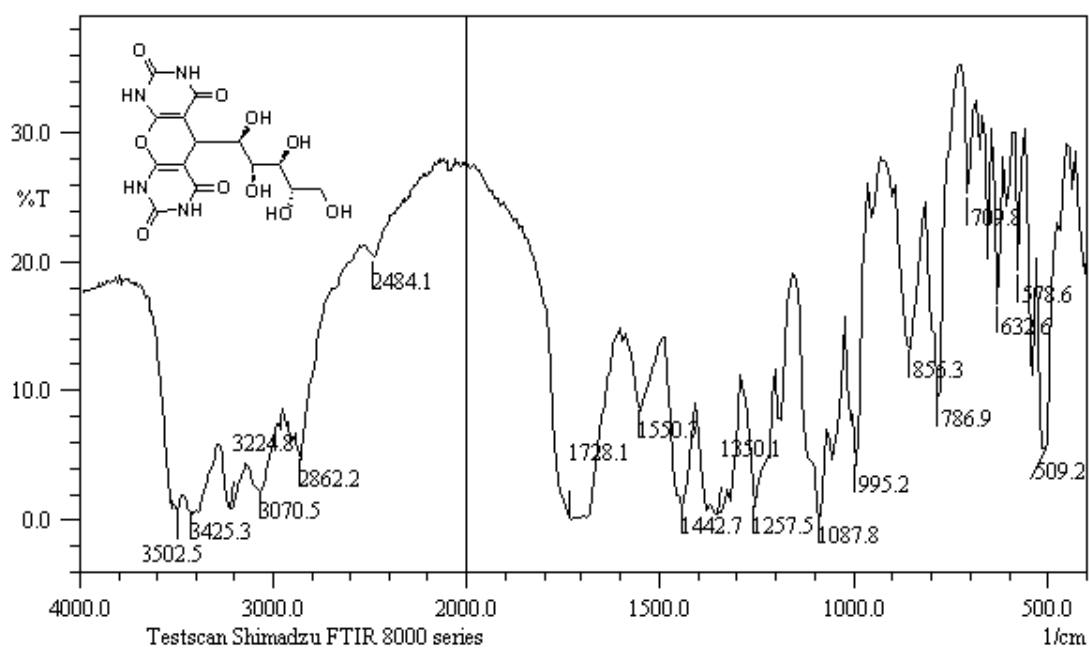
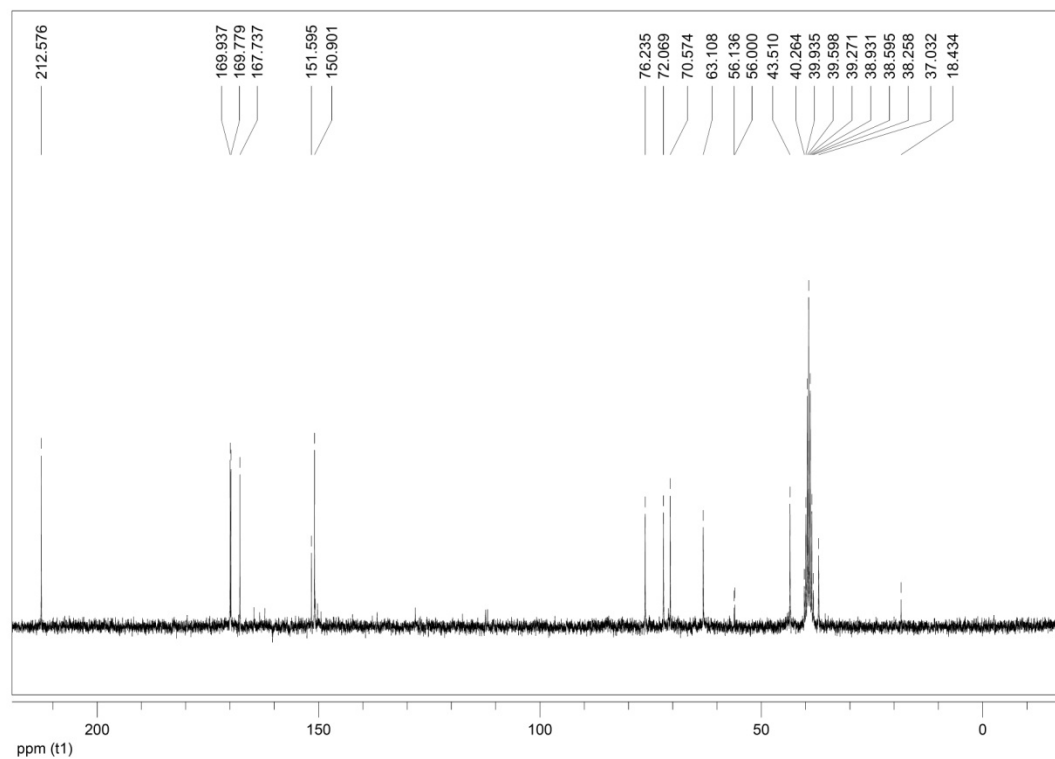




10-(4-methoxyphenyl)-5-(((1R,2R,3R,4R)-1,2,4,5-tetrahydroxy-3-(((2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)pentyl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone

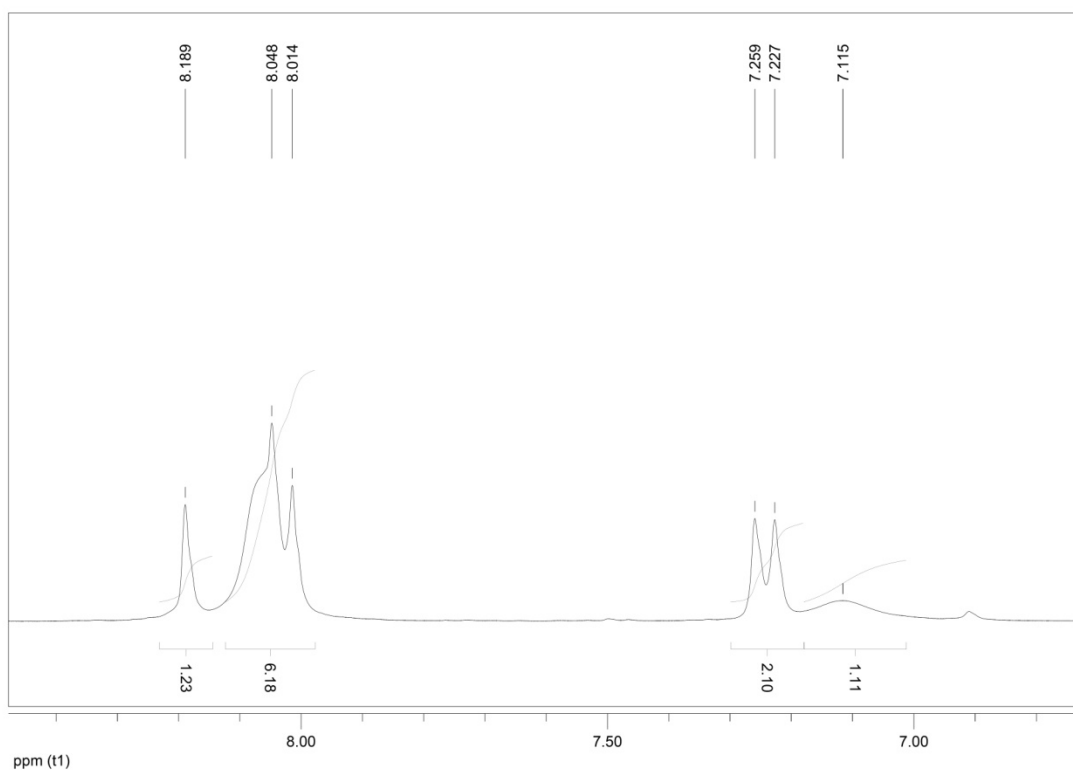
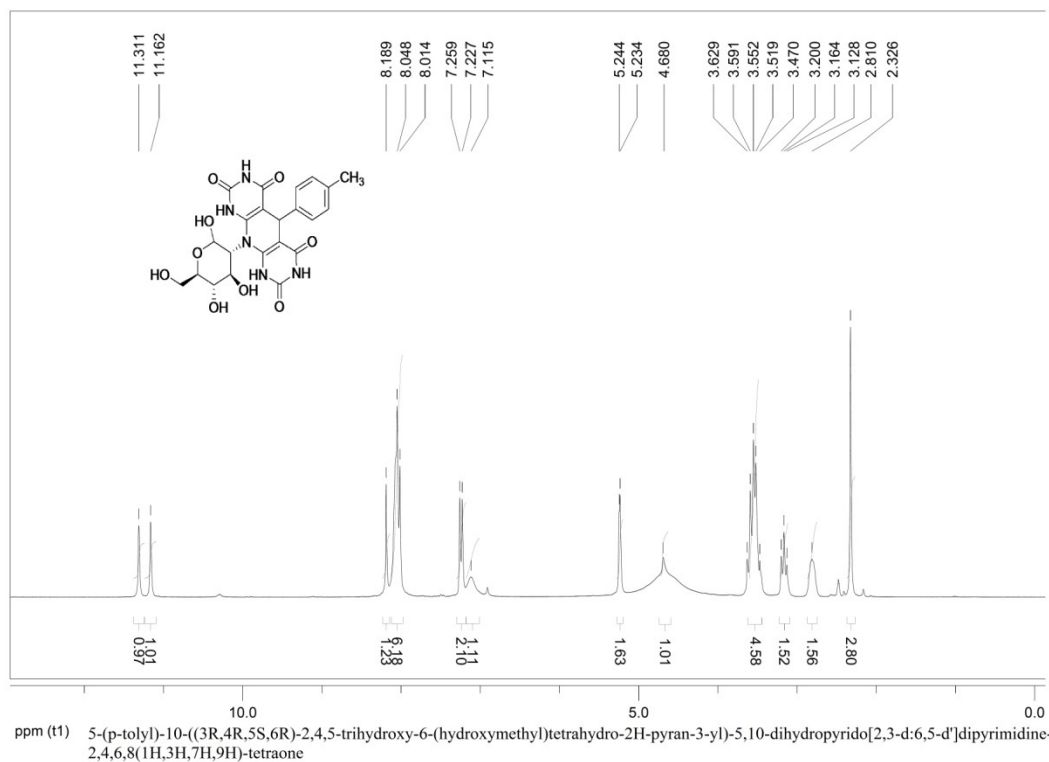
12. 5-((1R,2S,3S,4S)-1,2,3,4,5-pentahydroxypentyl)-5,9-dihydro-2H-pyrano[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H)-tetraone (4l)

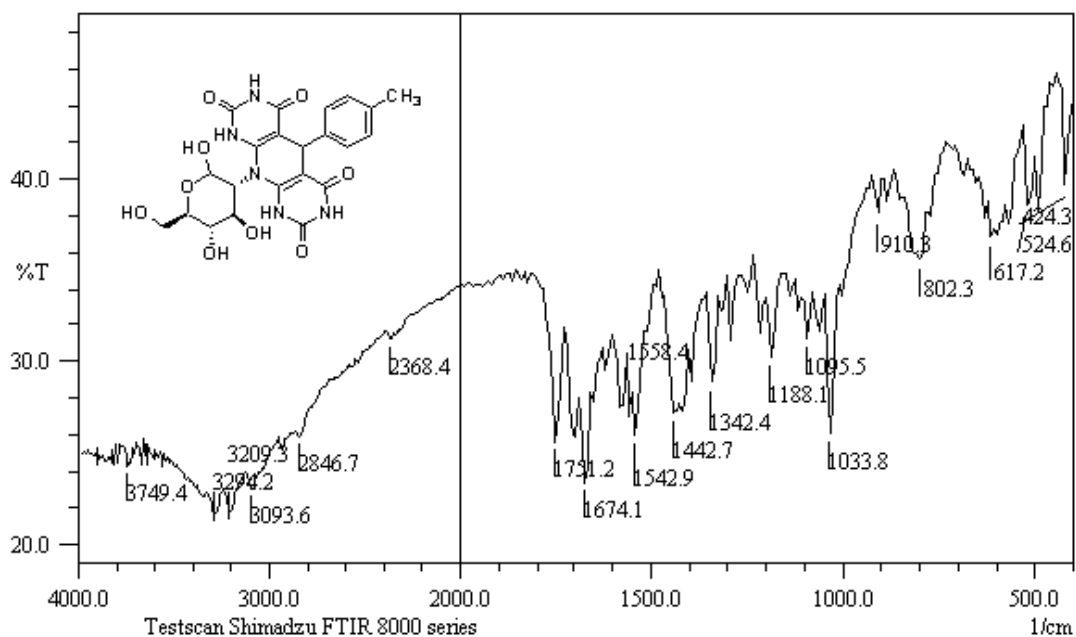
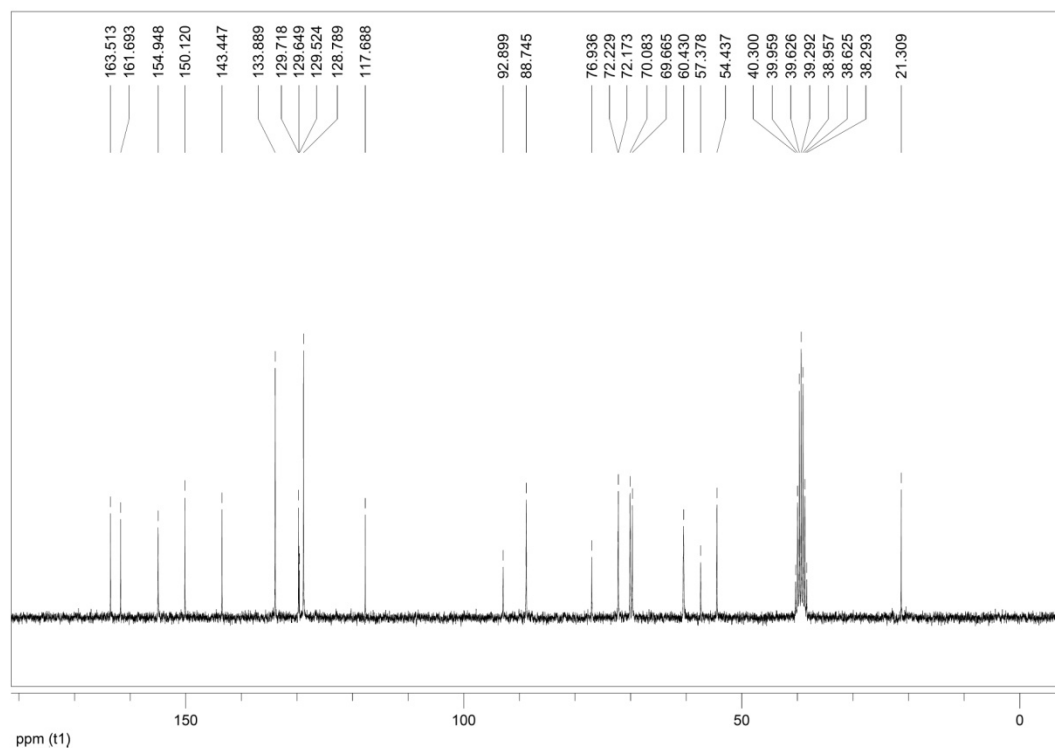




5-((1R,2S,3S,4S)-1,2,3,4,5-pentahydroxypentyl)-5,9-dihydro-2H-pyrano[2,3-d:6,5-d']dipyrimidine-2,4,6,8-(1H,3H,7H)-tetraone

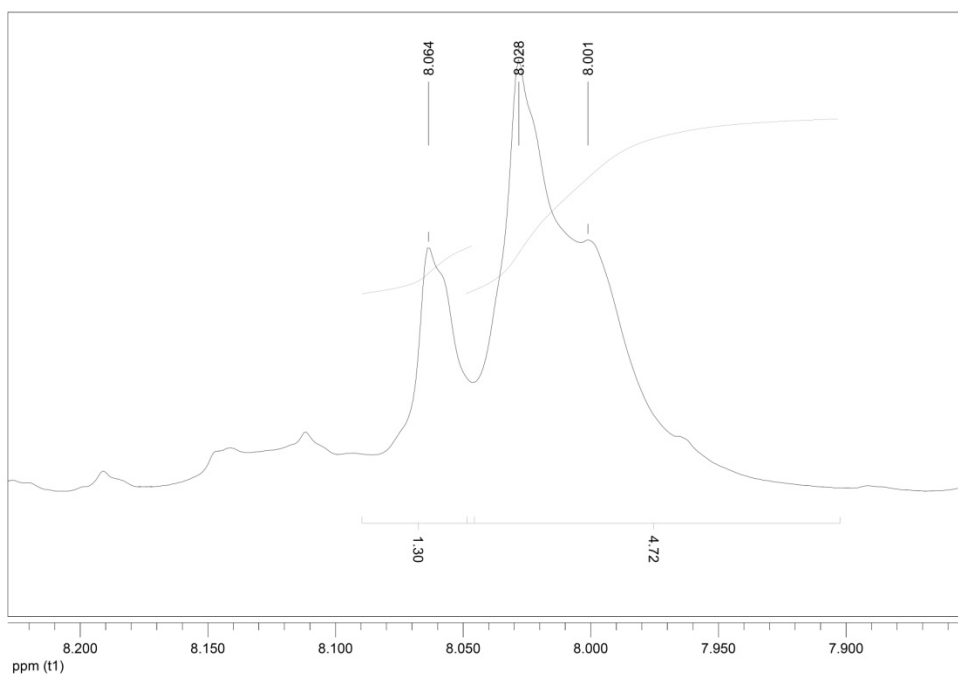
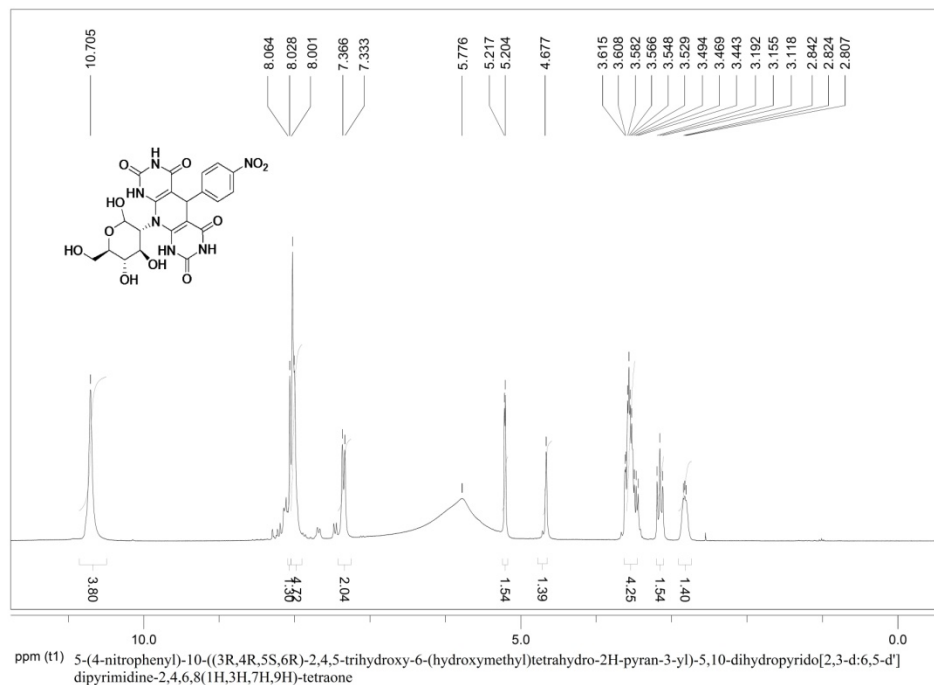
13. 5-(p-tolyl)-10-((3R,4R,5S,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-3-yl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (6a)

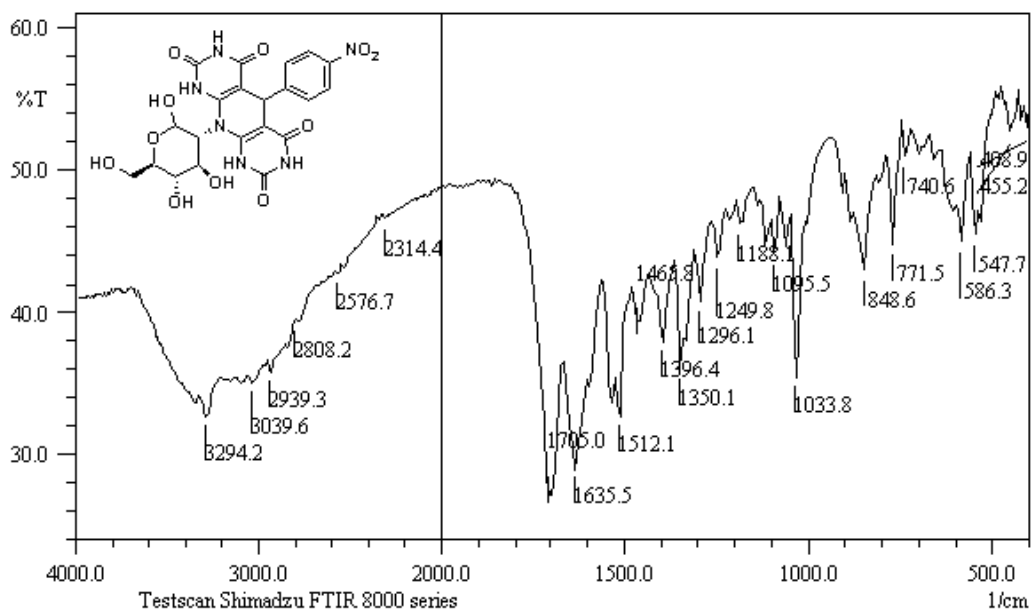
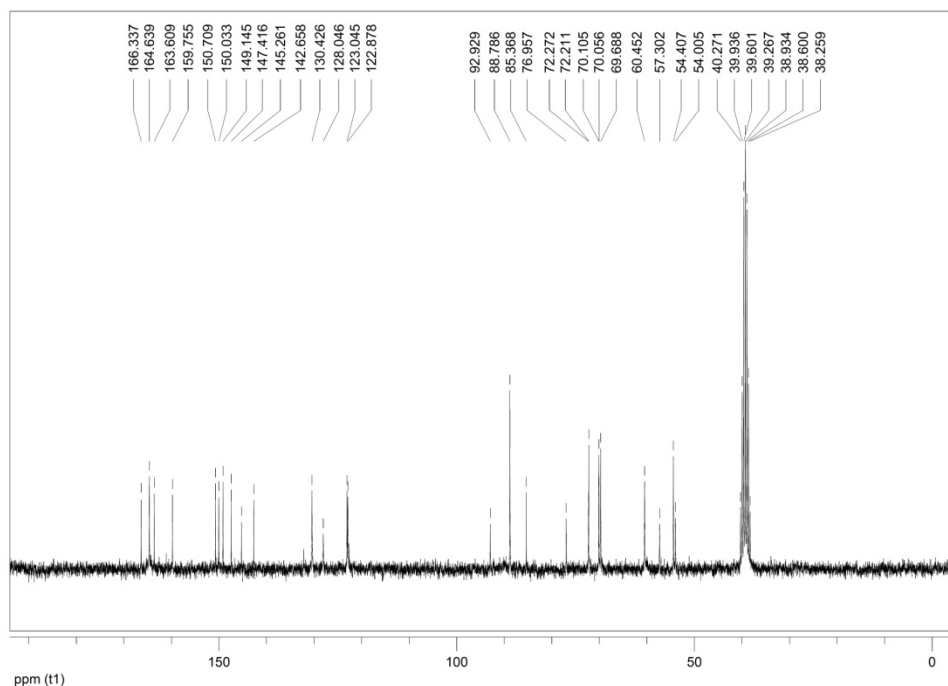




5-(p-tolyl)-10-((3R,4R,5S,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-3-yl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone

14. 5-(4-nitrophenyl)-10-((3R,4R,5S,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-3-yl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (6b)





5-(4-nitrophenyl)-10-((3R,4R,5S,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-3-yl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone

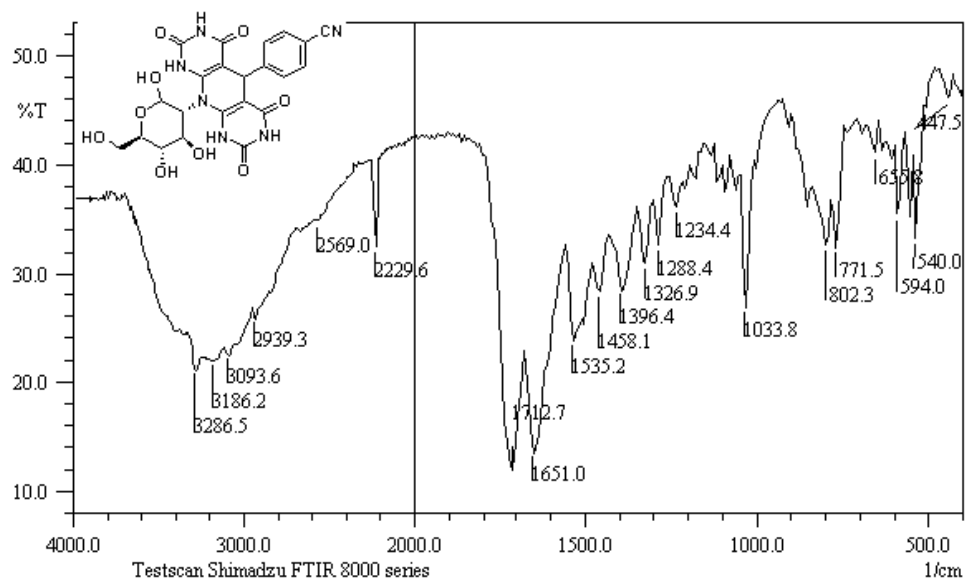
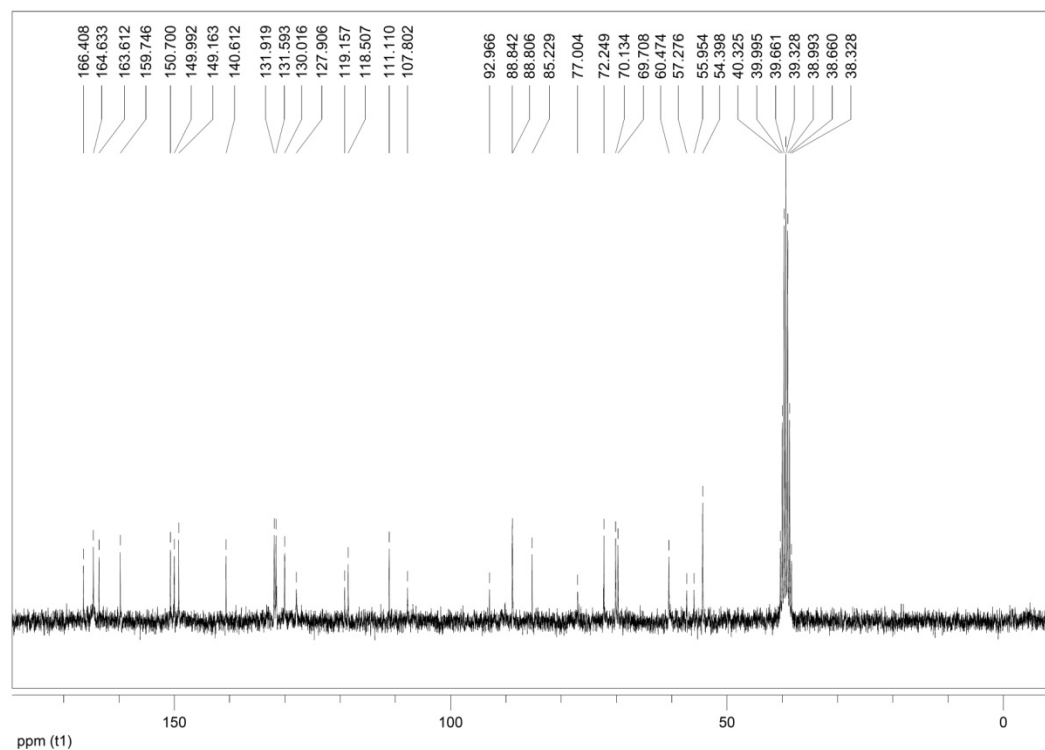
Chemical structure of 4-(2,4,6,8-tetraoxo-10-((3R,4R,5S,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-3-yl)-1,2,3,4,5,6,7,8,9,10-decahydropyrido[2,3-d:6',5'-d']dipyrimidin-5-yl)benzonitrile:

N#Cc1ccc(cc1)c2nc3c(nc(=O)[nH]3)c4c(nc(=O)[nH]4)[C@H]5O[C@H](CO)[C@@H](O)[C@H]5O

¹H NMR spectrum (DMSO-d₆) showing chemical shifts (ppm) and integration values:

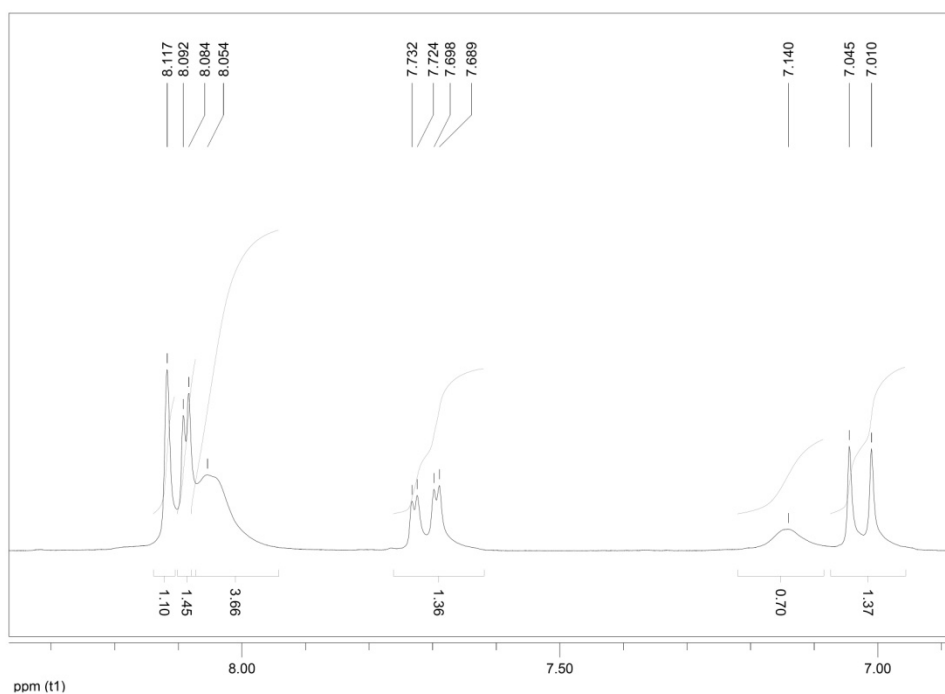
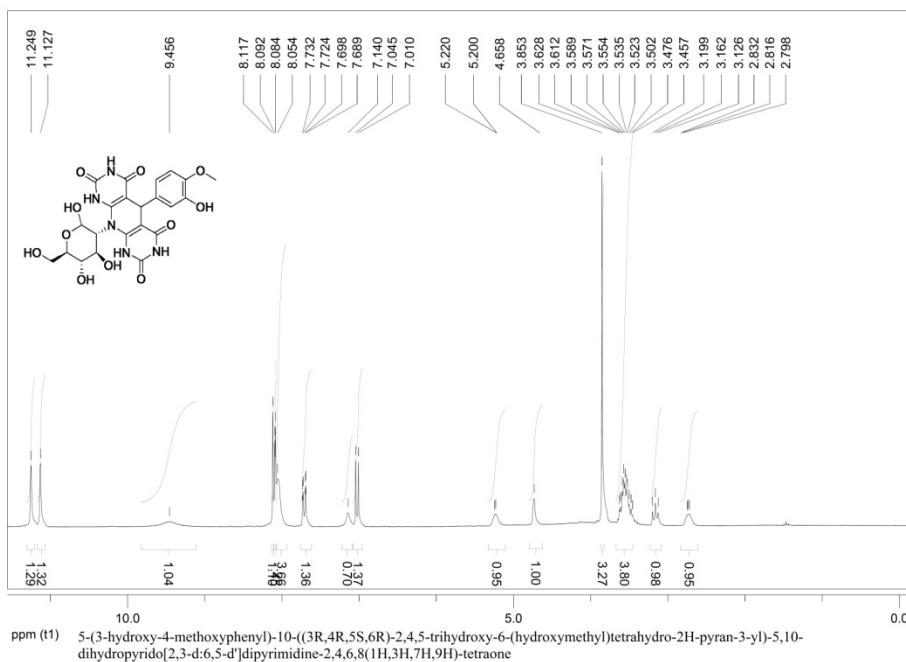
Chemical Shift (ppm)	Integration
10.651	4.05
7.982, 7.947, 7.643, 7.643, 7.197, 7.101, 7.269, 6.160	3.81
5.216, 5.203	2.22
5.640	2.17
5.132	1.32
4.084	0.84
3.630, 3.582, 3.556, 3.547, 3.525, 3.505, 3.479, 3.457, 3.447, 3.430, 3.402, 3.374, 3.200, 3.163, 3.126, 2.847, 2.829, 2.812	4.58
1.24	1.24

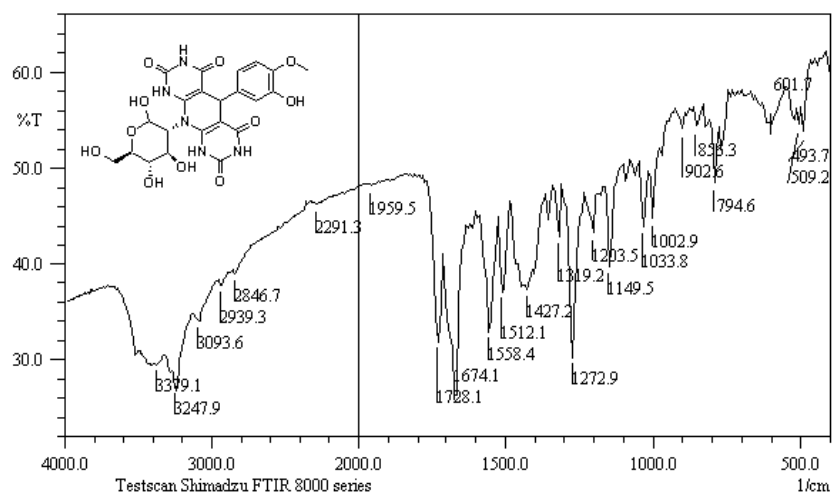
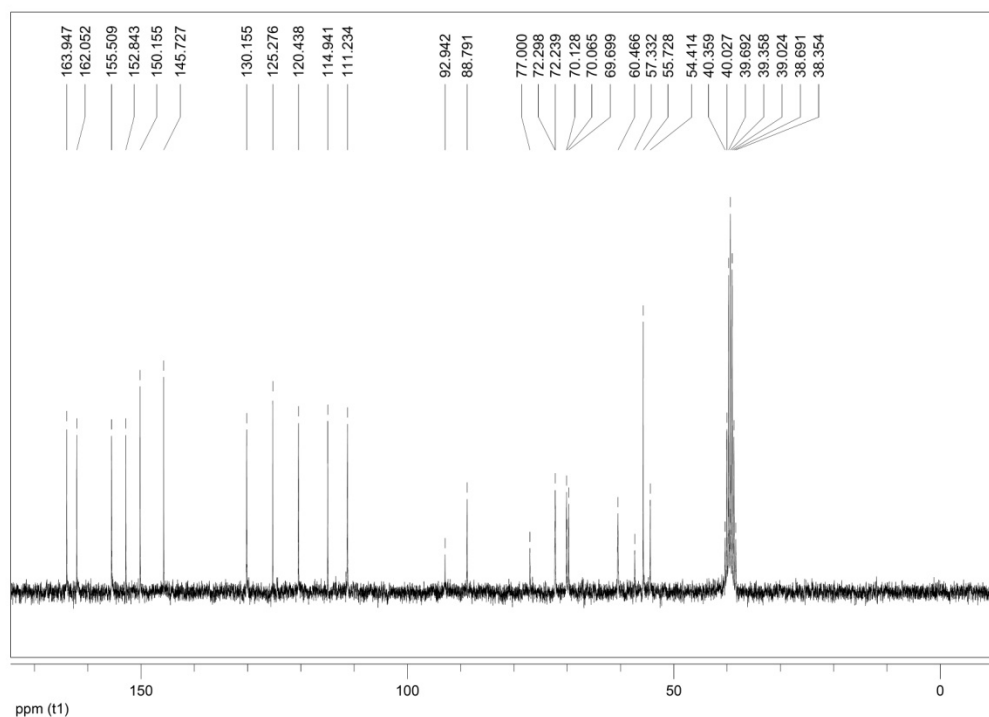




4-(2,4,6,8-tetraoxo-10-((3R,4R,5S,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-3-yl)-1,2,3,4,5,6,7,8,9,10-decahydropyrido[2,3-d:6,5-d']dipyrimidin-5-yl)benzonitrile

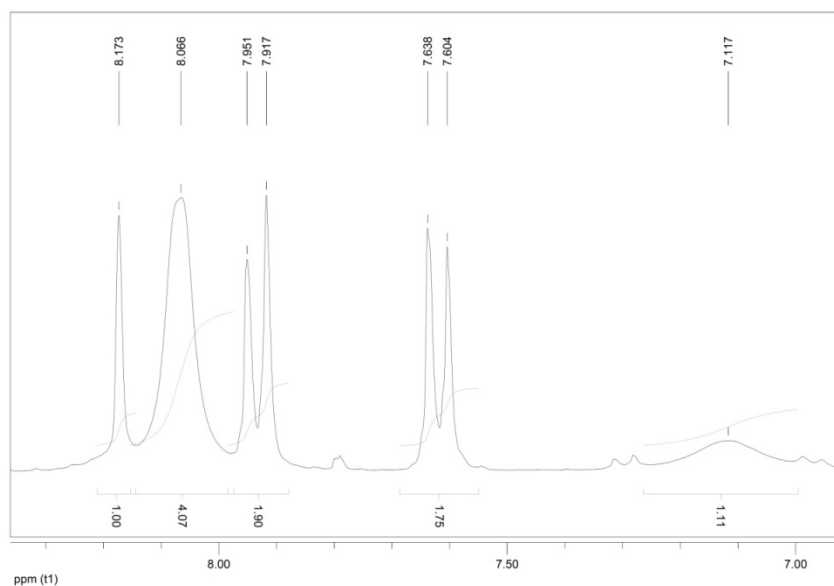
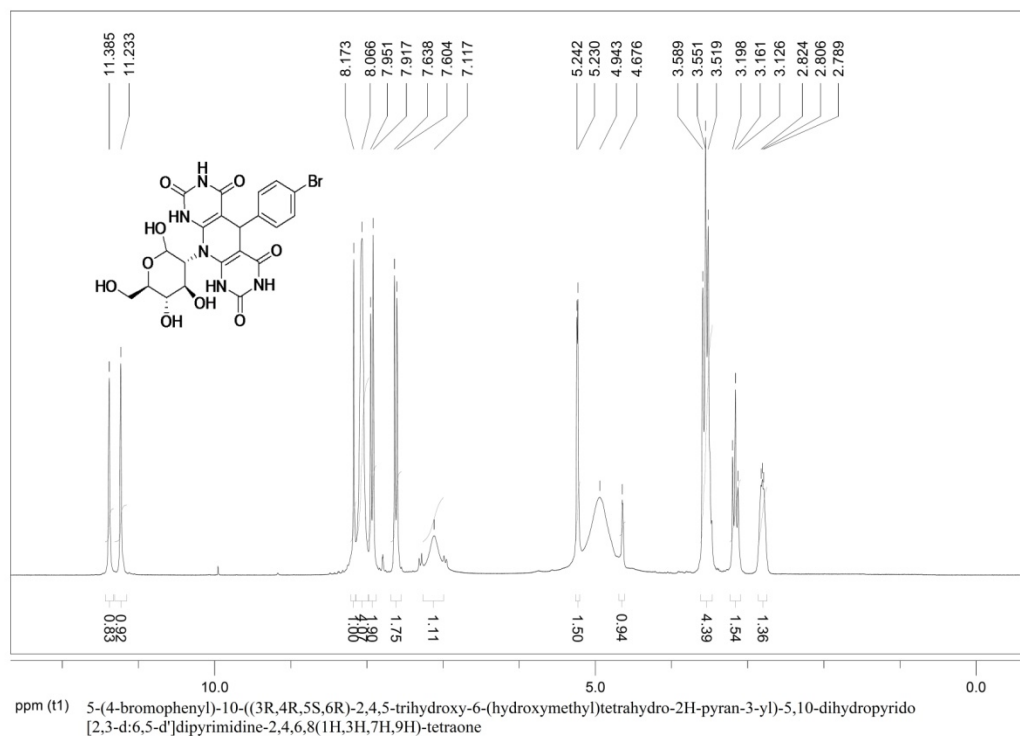
16. 5-(3-hydroxy-4-methoxyphenyl)-10-((3R,4R,5S,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-3-yl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (6d)

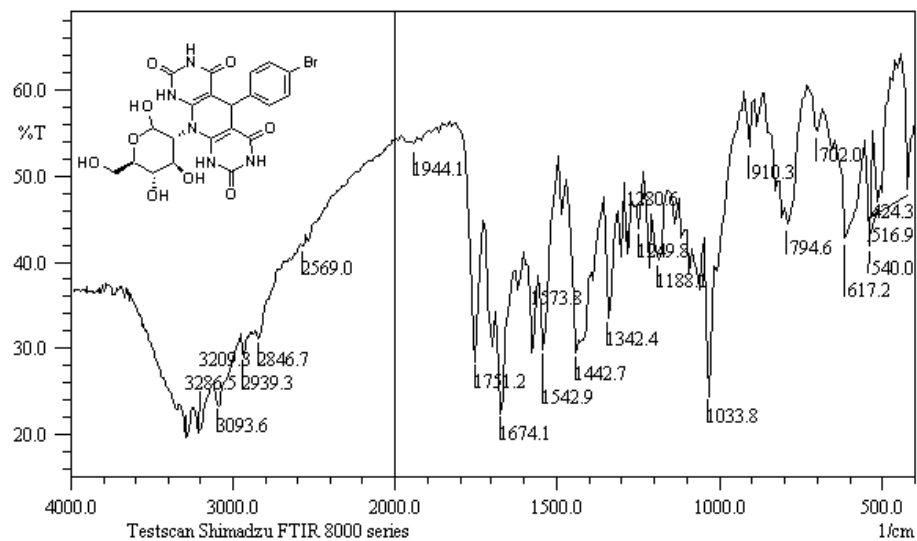
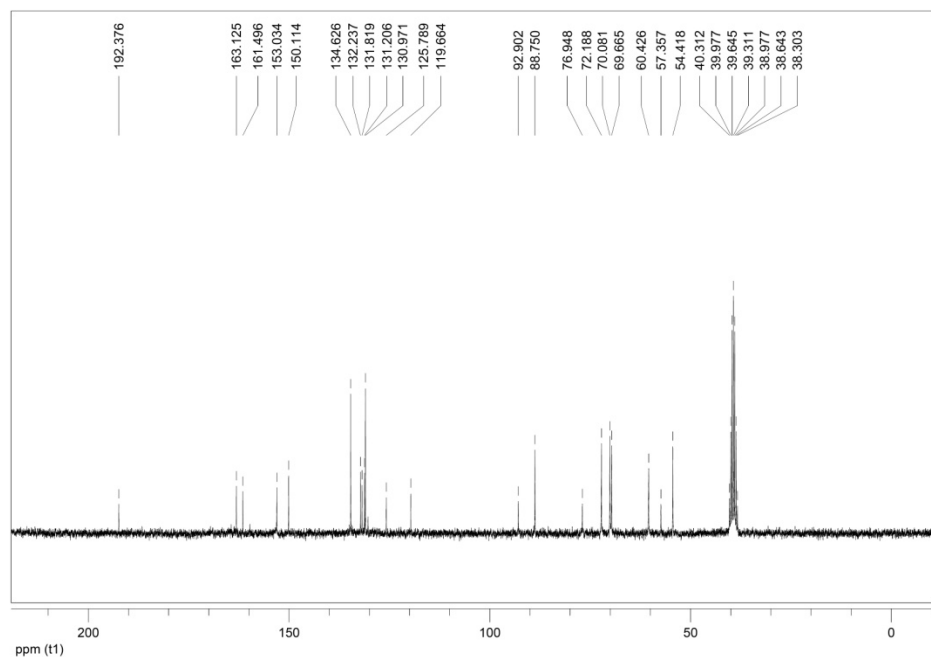




5-(3-hydroxy-4-methoxyphenyl)-10-((3R,4R,5S,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-3-yl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone

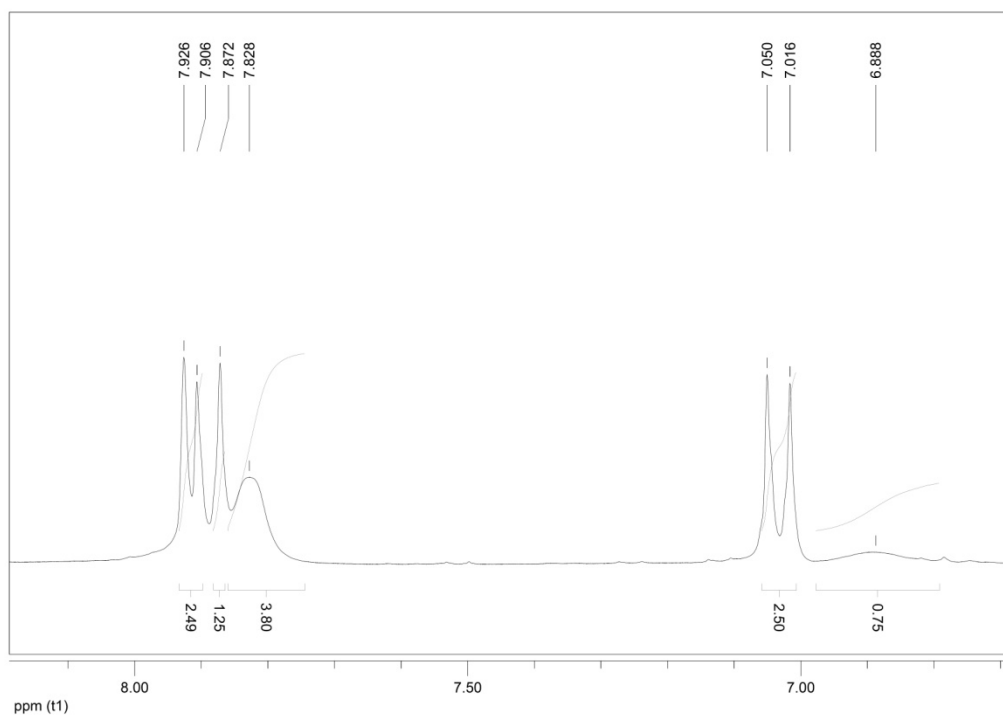
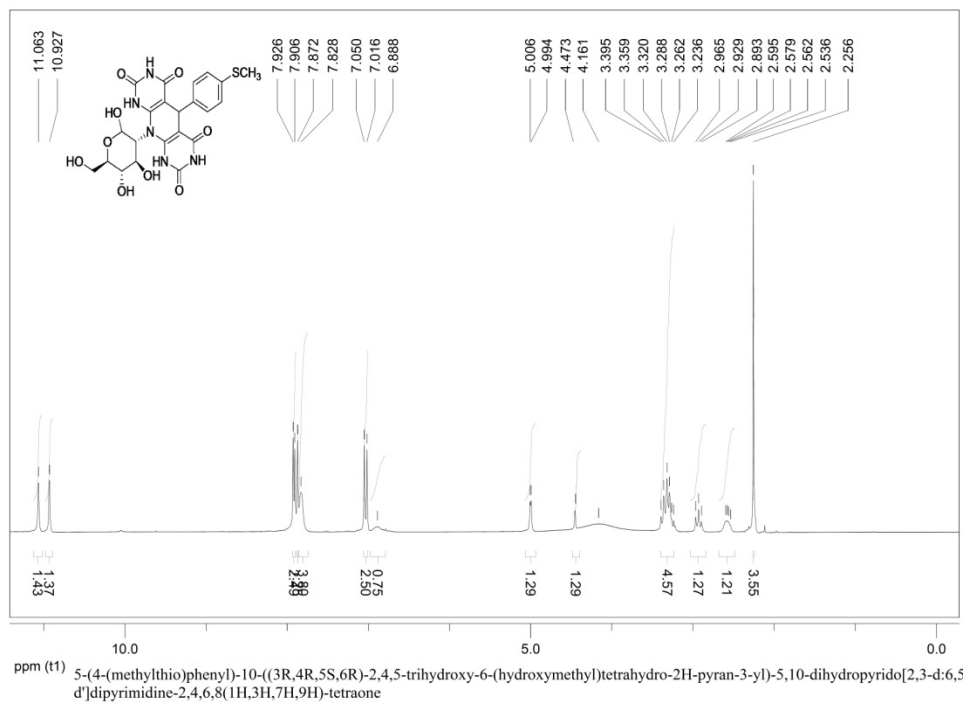
17. 5-(4-bromophenyl)-10-((3R,4R,5S,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-3-yl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (6e)

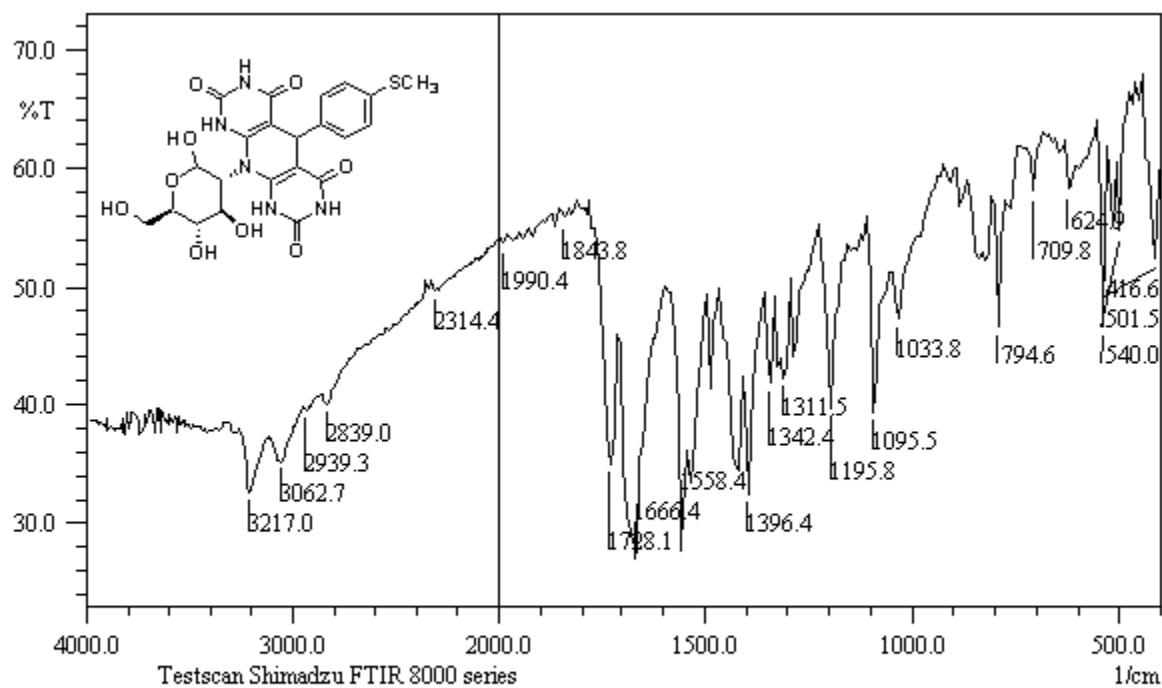
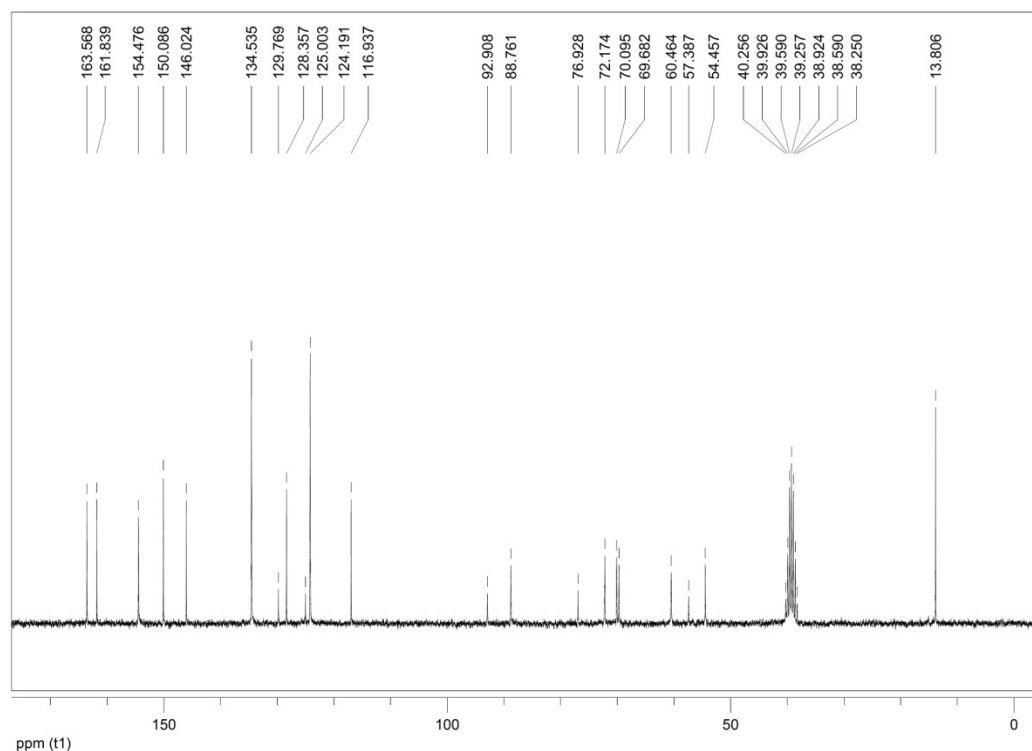




5-(4-bromophenyl)-10-((3R,4R,5S,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-3-yl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone

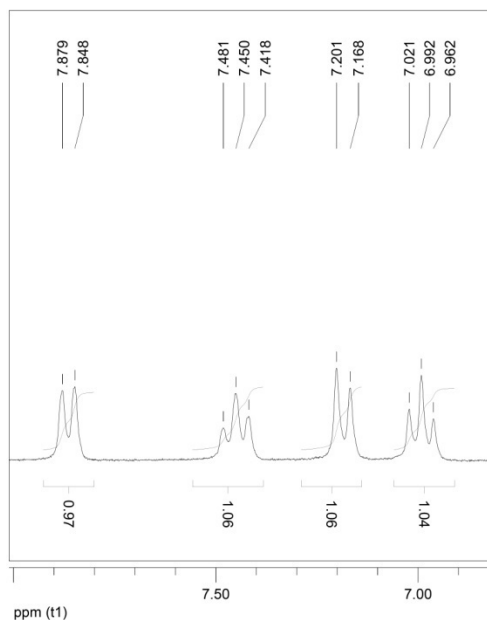
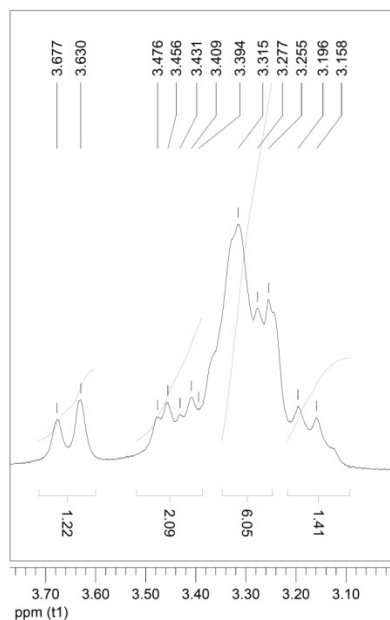
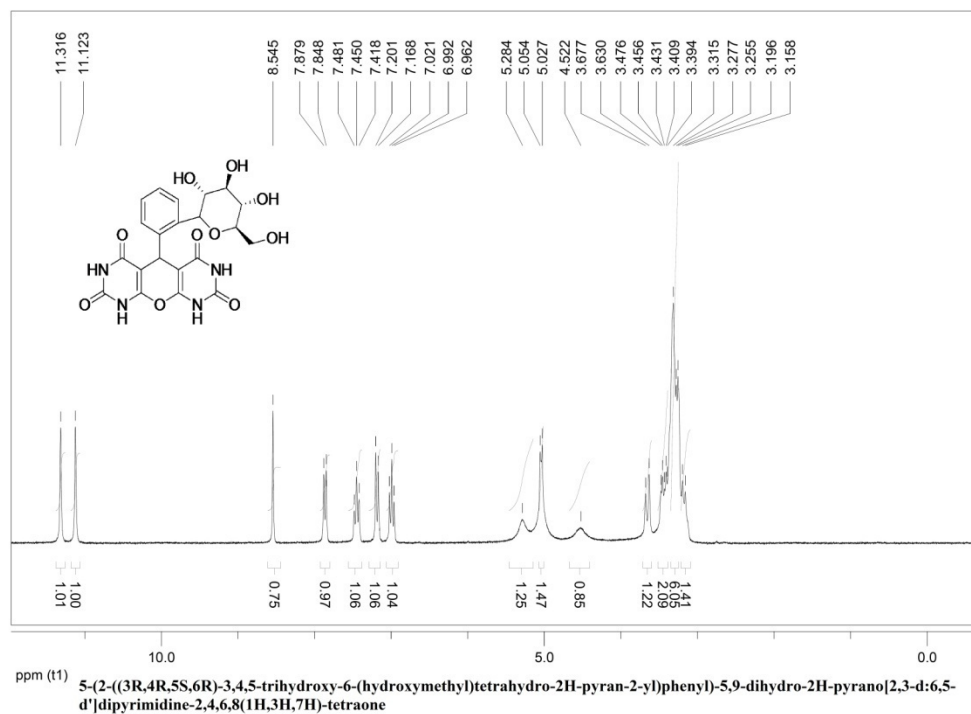
18. 5-(4-(methylthio)phenyl)-10-((3R,4R,5S,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-3-yl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone (6f)

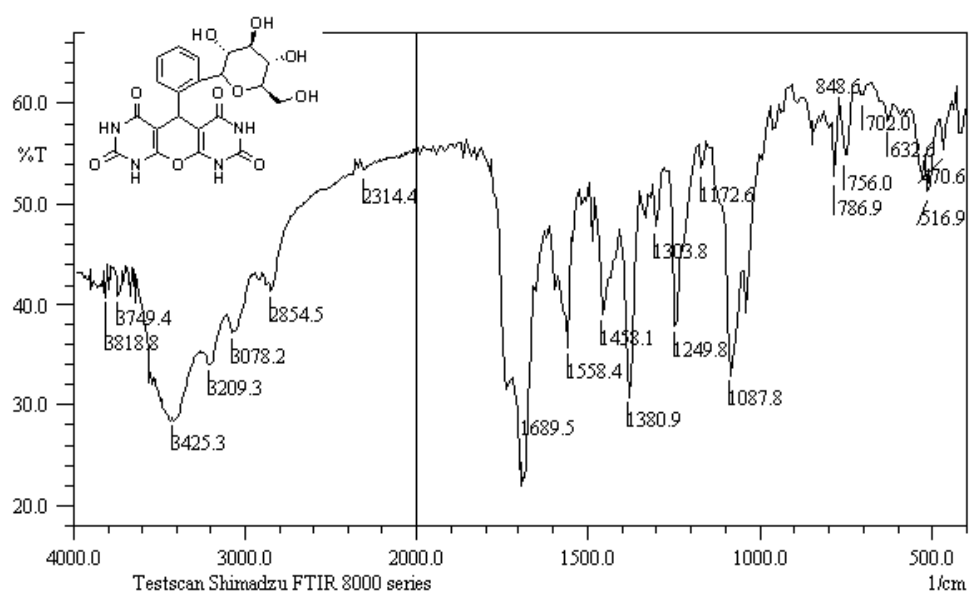
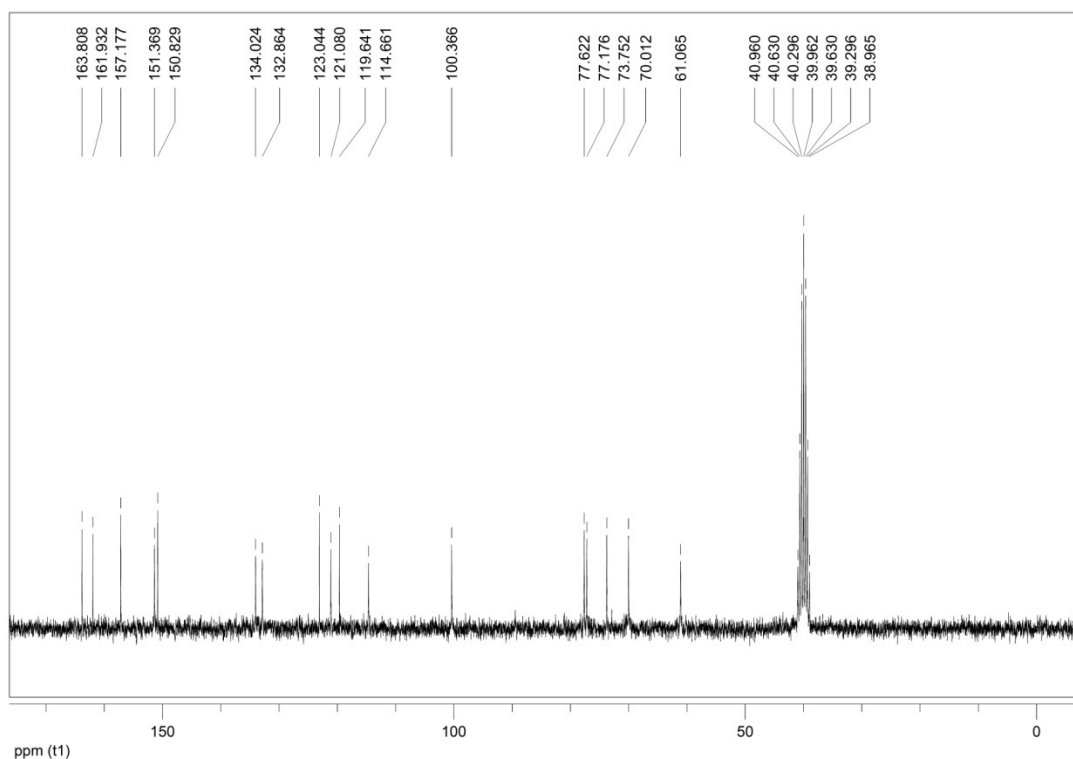




5-(4-(methylthio)phenyl)-10-((3R,4R,5S,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-3-yl)-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H,9H)-tetraone

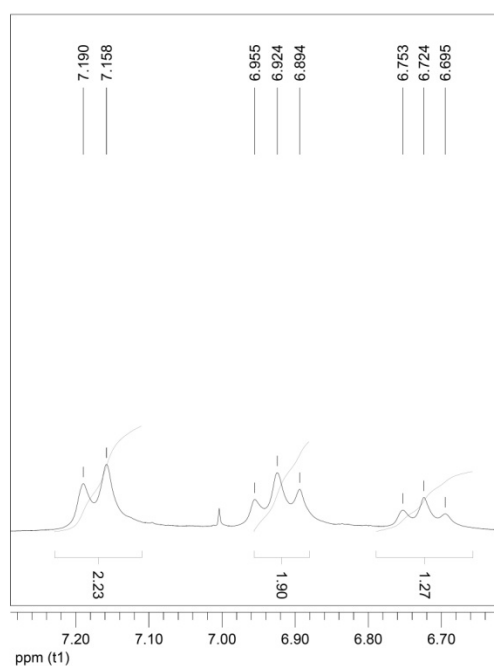
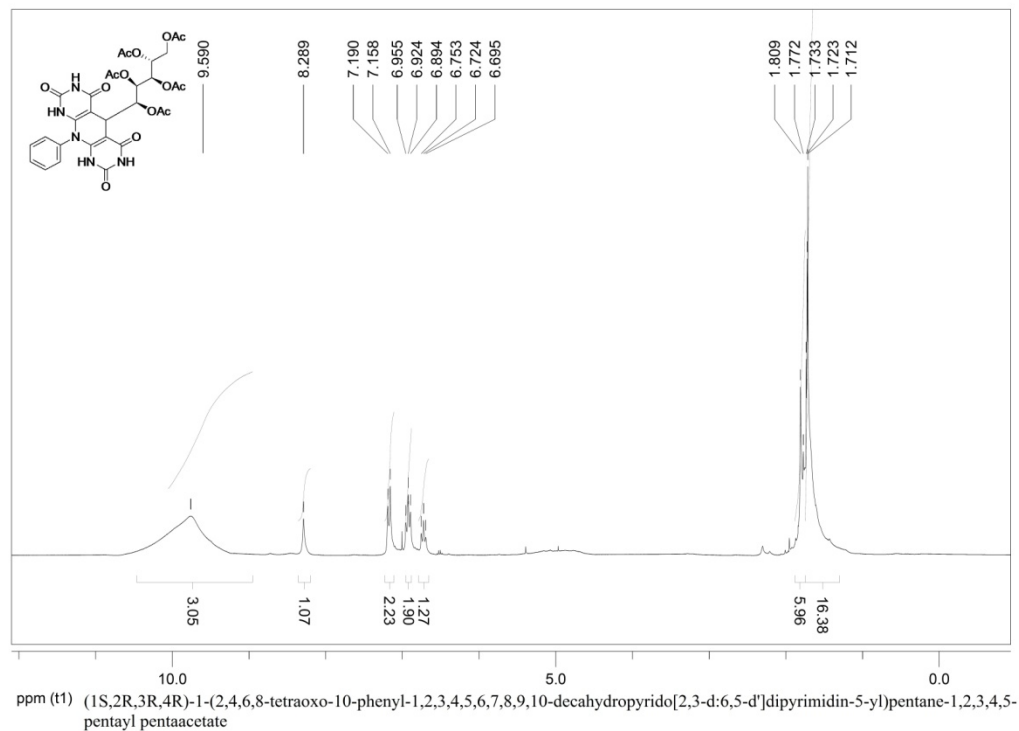
19. 5-(2-((3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)phenyl)-5,9-dihydro-2H-pyrano[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H)-tetraone (7)

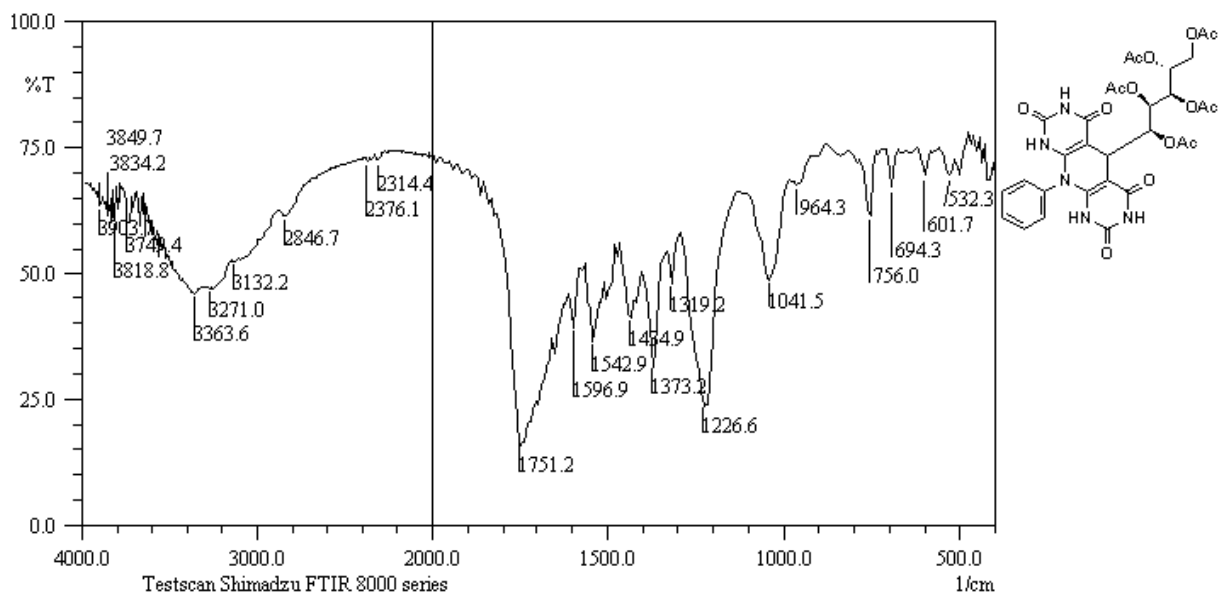
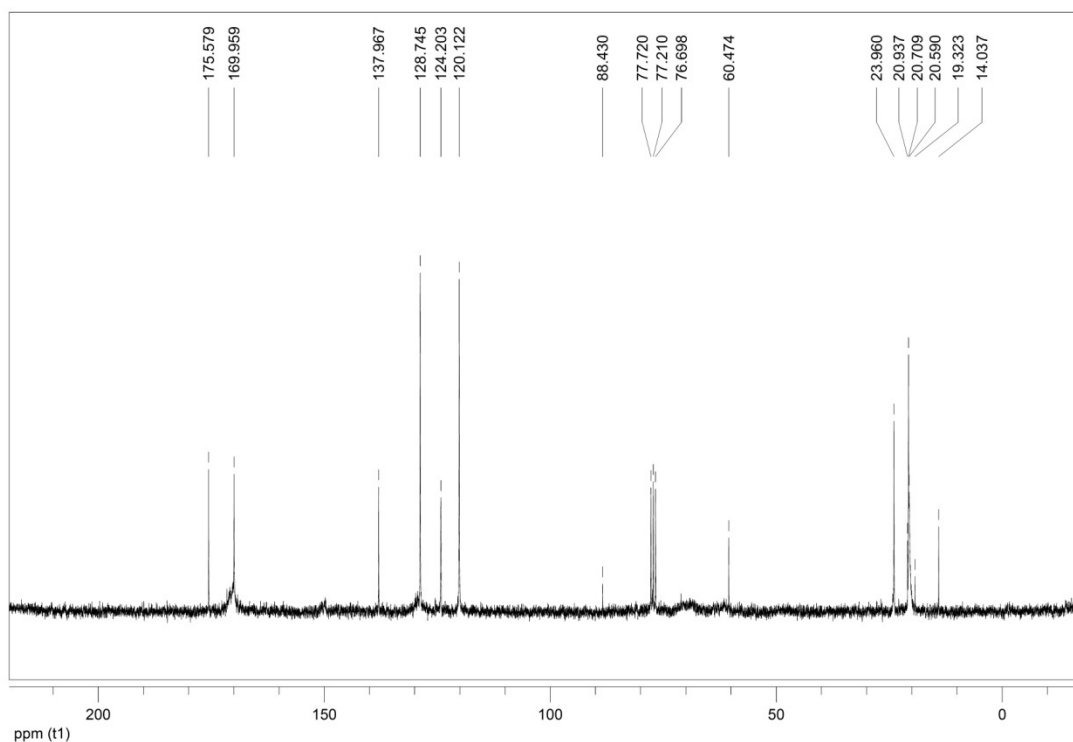




5-(2-((3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)phenyl)-5,9-dihydro-2H-pyrano[2,3-d:6,5-d']dipyrimidine-2,4,6,8(1H,3H,7H)-tetraone

20. (1S,2R,3R,4R)-1-(2,4,6,8-tetraoxo-10-phenyl-1,2,3,4,5,6,7,8,9,10-decahydropyrido[2,3-d:6,5-d']dipyrimidin-5-yl)pentane-1,2,3,4,5-pentayl pentaacetate (8a)





(1S,2R,3R,4R)-1-(2,4,6,8-tetraoxo-10-phenyl-1,2,3,4,5,6,7,8,9,10-decahydropyrido[2,3-d:6,5-d']dipyrimidin-5-yl)pentane-1,2,3,4,5-pentayl pentaacetate

21. (1S,2R,3R,4R)-1-(10-(4-methoxyphenyl)-2,4,6,8-tetraoxo-1,2,3,4,5,6,7,8,9,10-decahydropyrido[2,3-d:6,5-d']dipyrimidin-5-yl)pentane-1,2,3,4,5-pentayl pentaacetate (8b)

