

Electronic Supplementary Information

Diazepinium perchlorate: A neutral catalyst for mild, solvent-free acyl transfer reactions of carbohydrates and other substances

Santosh Kumar Giri, Rajesh Gour and K. P. Ravindranathan Kartha*

Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research, S.A.S Nagar, Punjab-160062, India.

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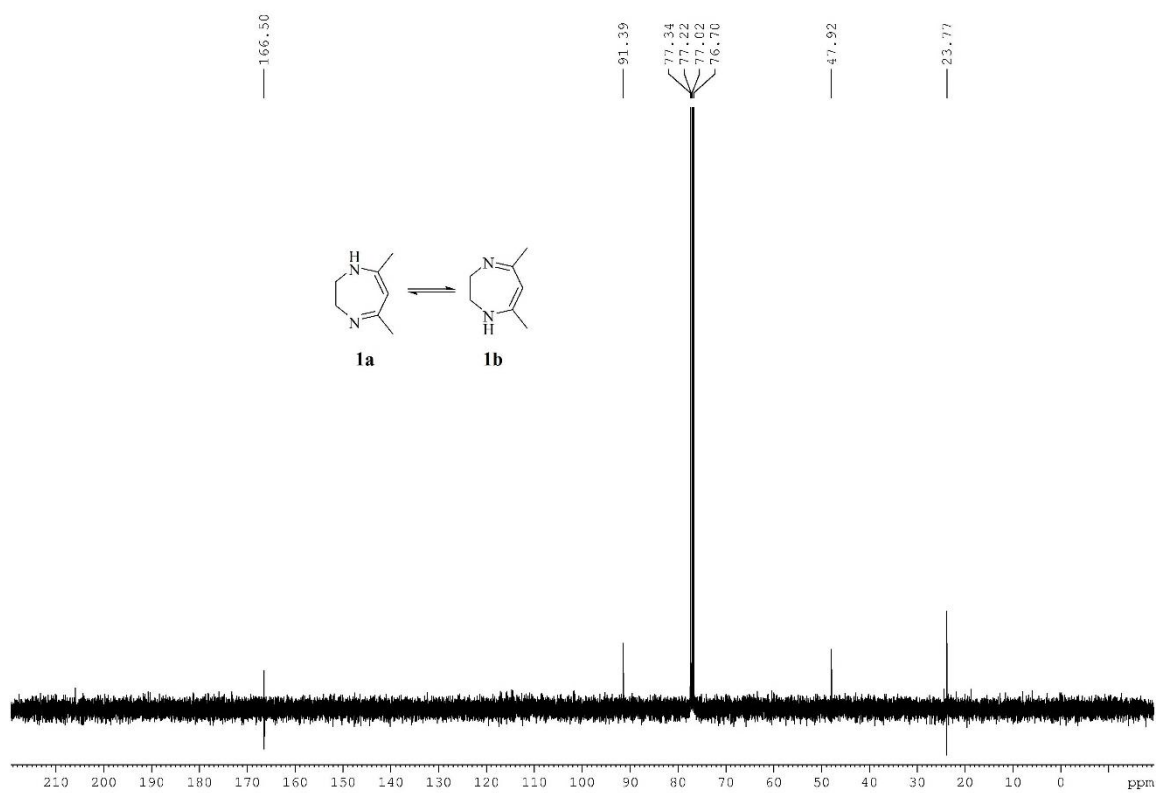
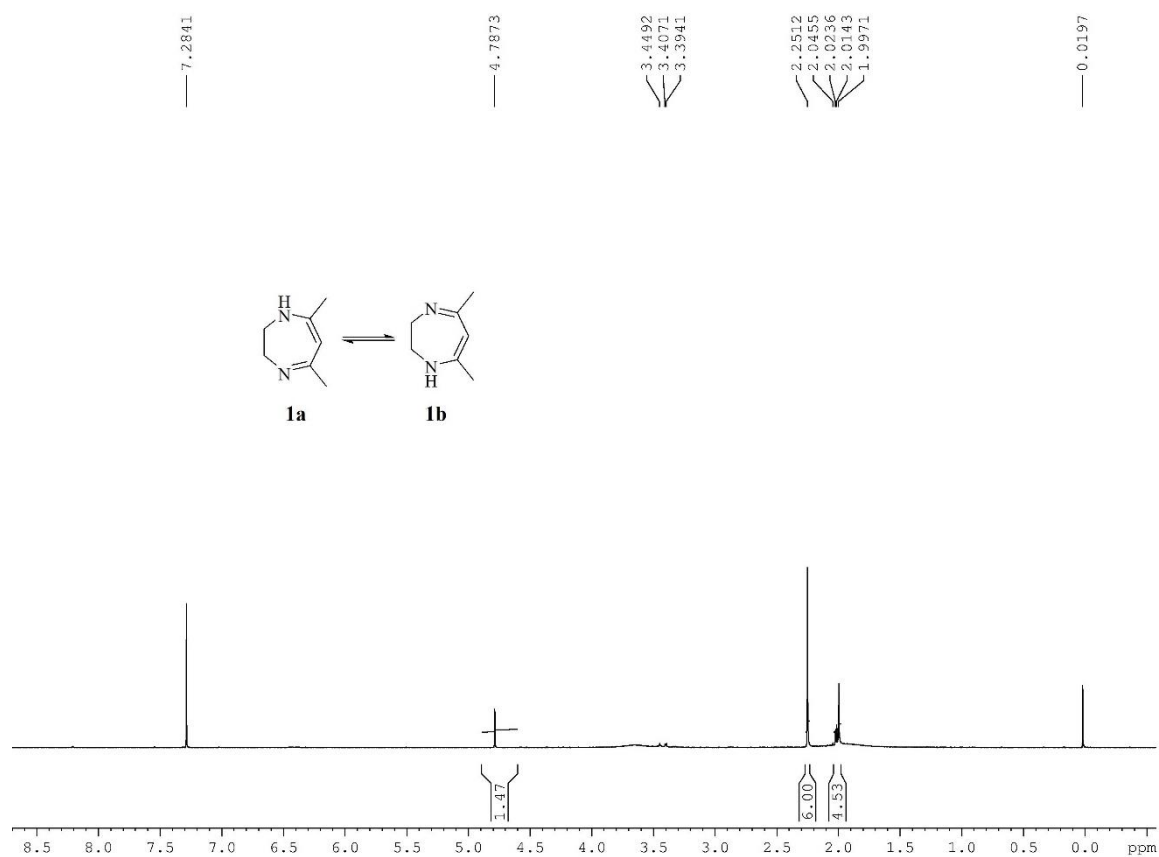
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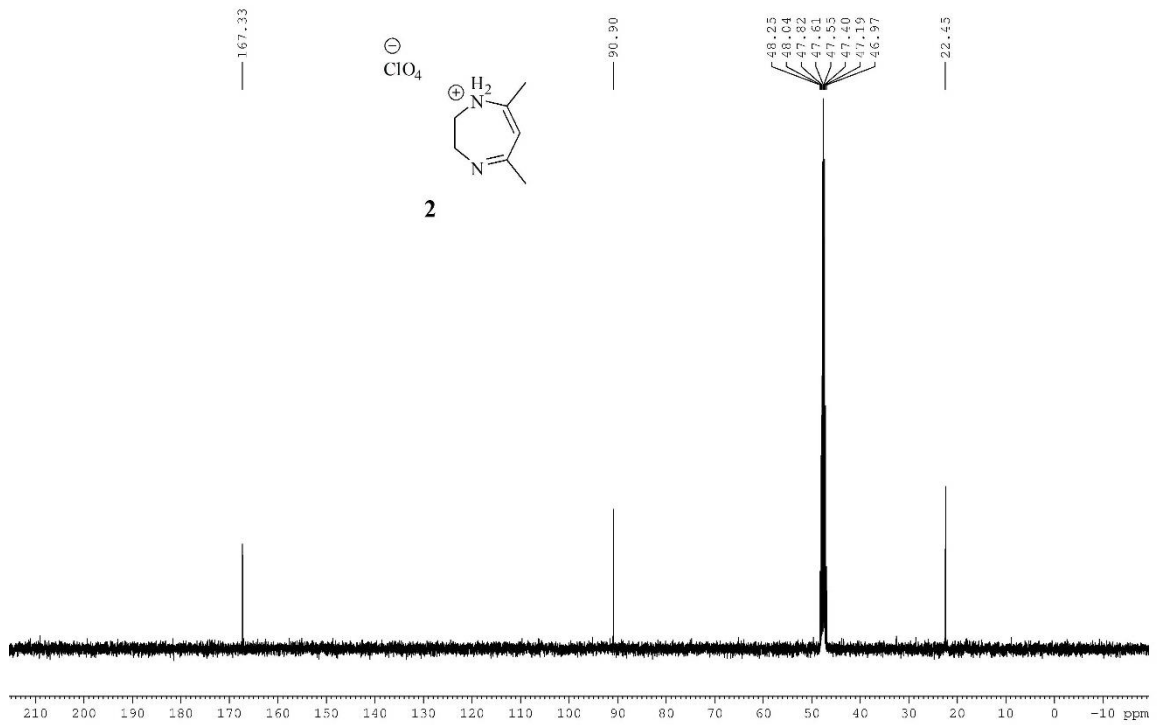
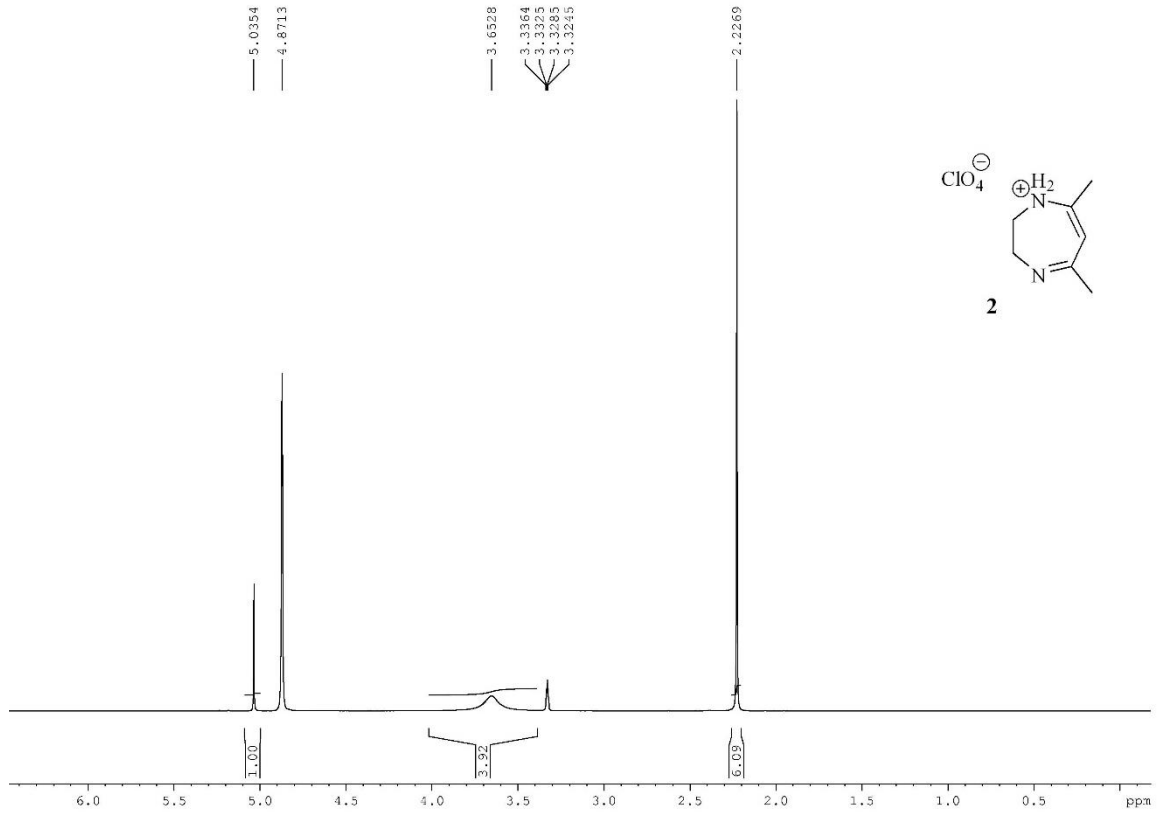
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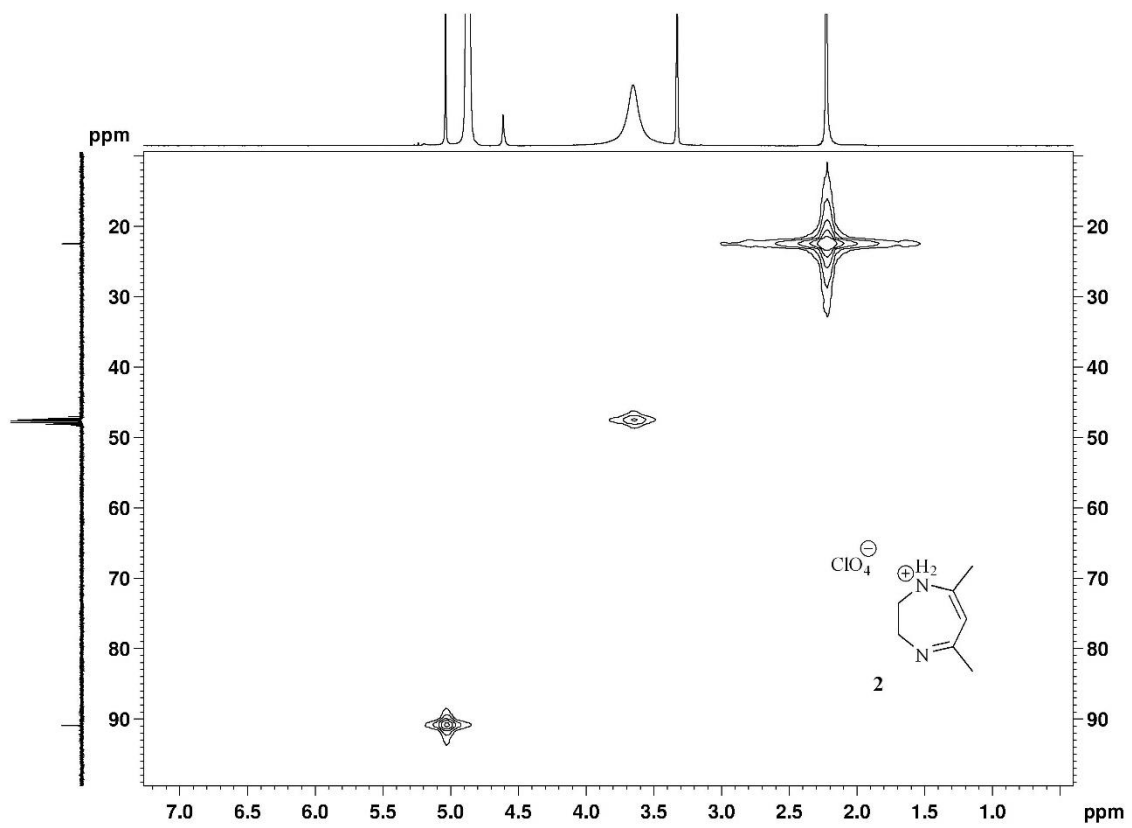
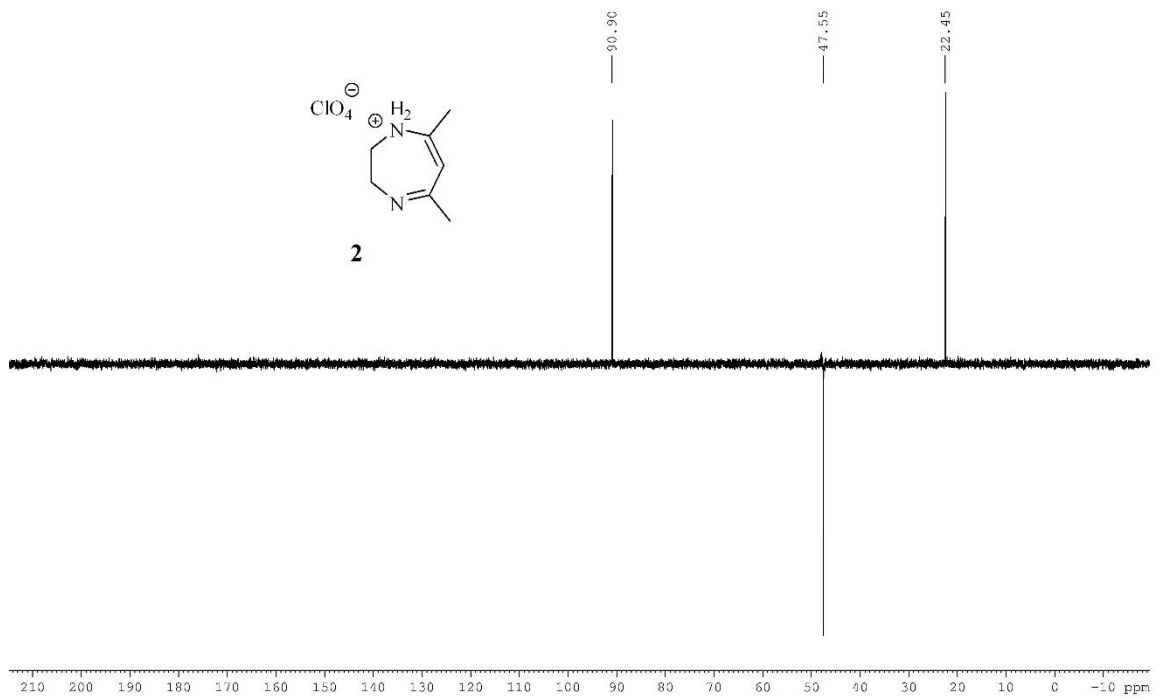
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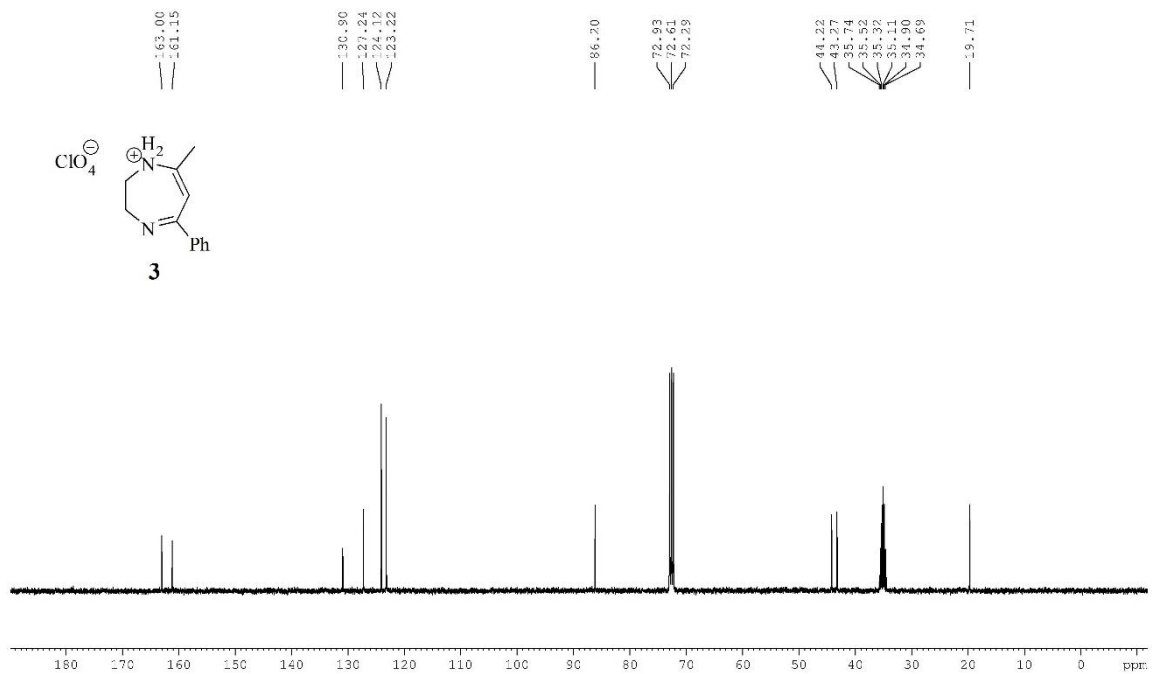
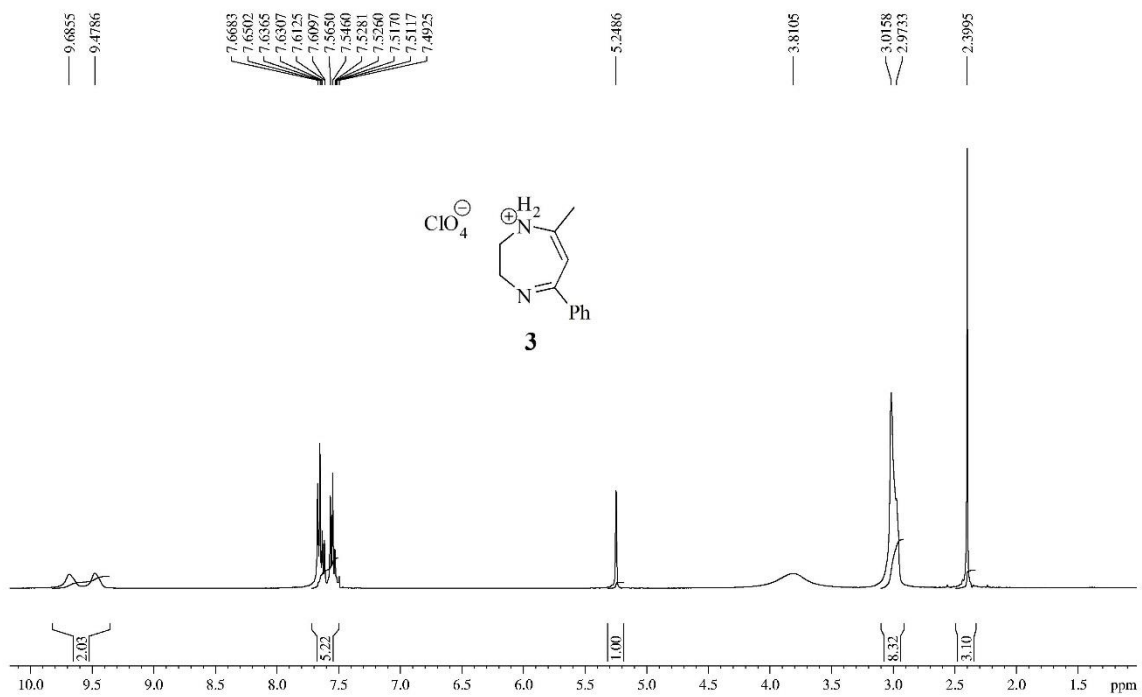
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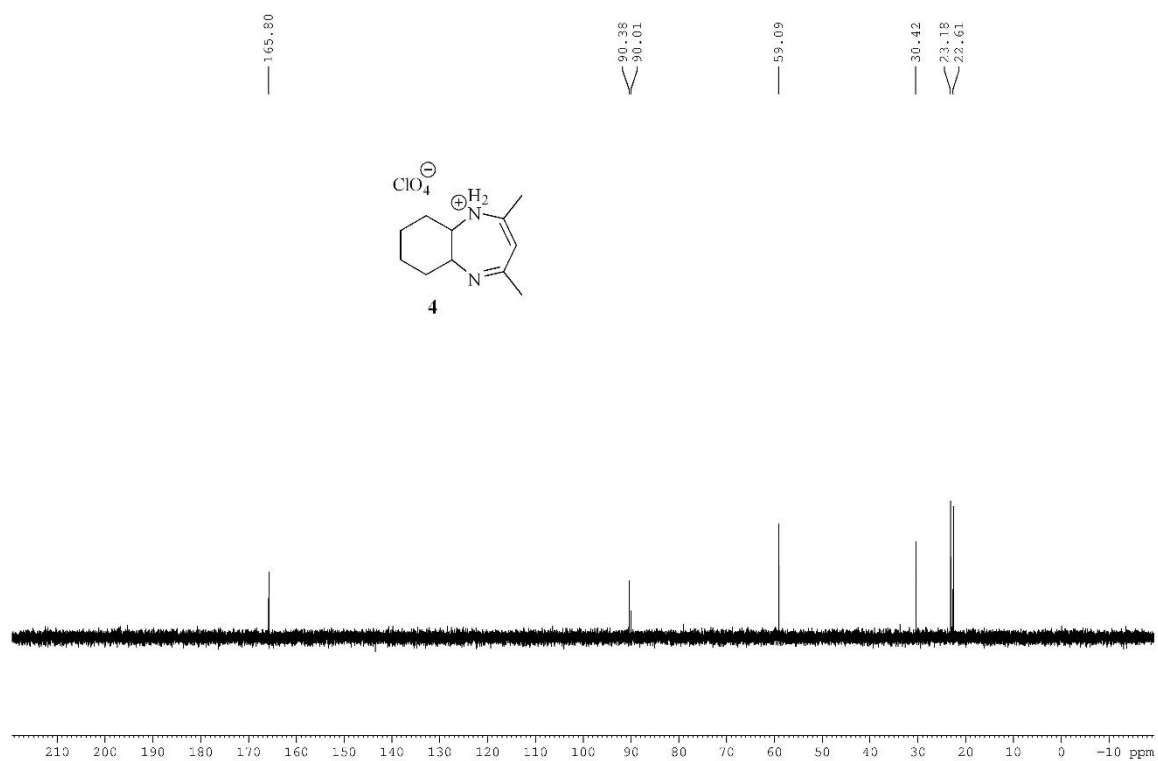
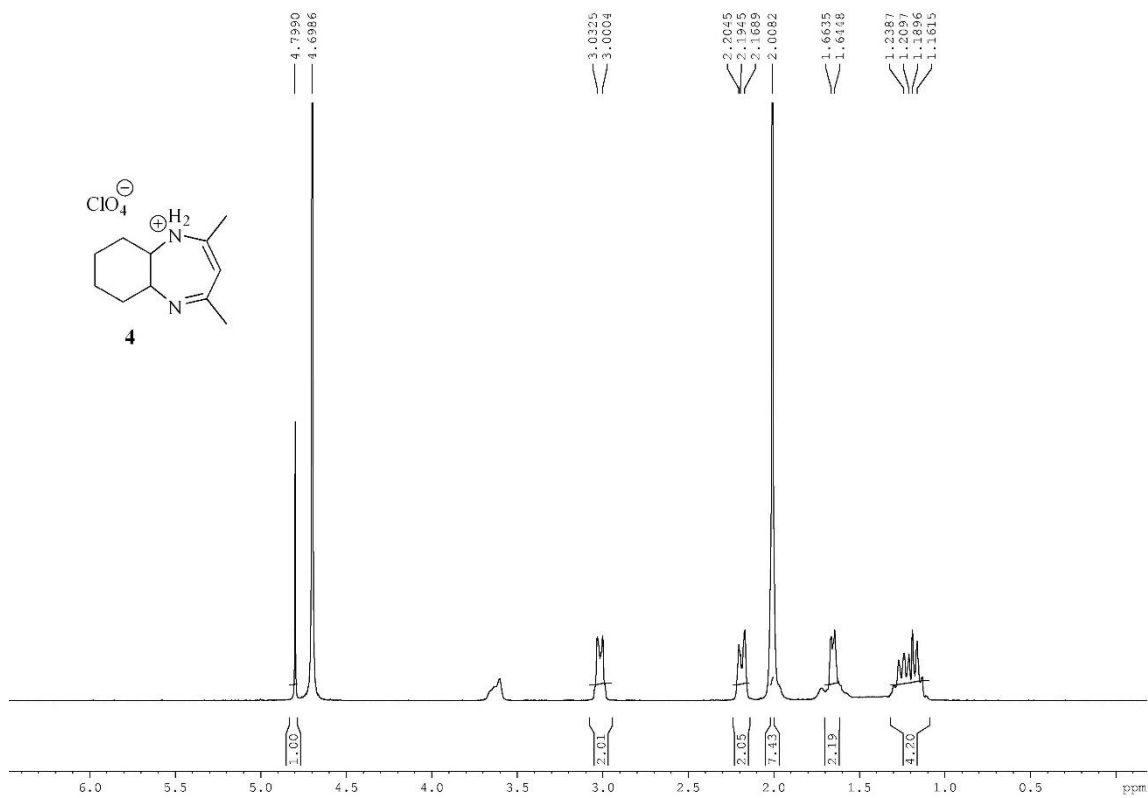
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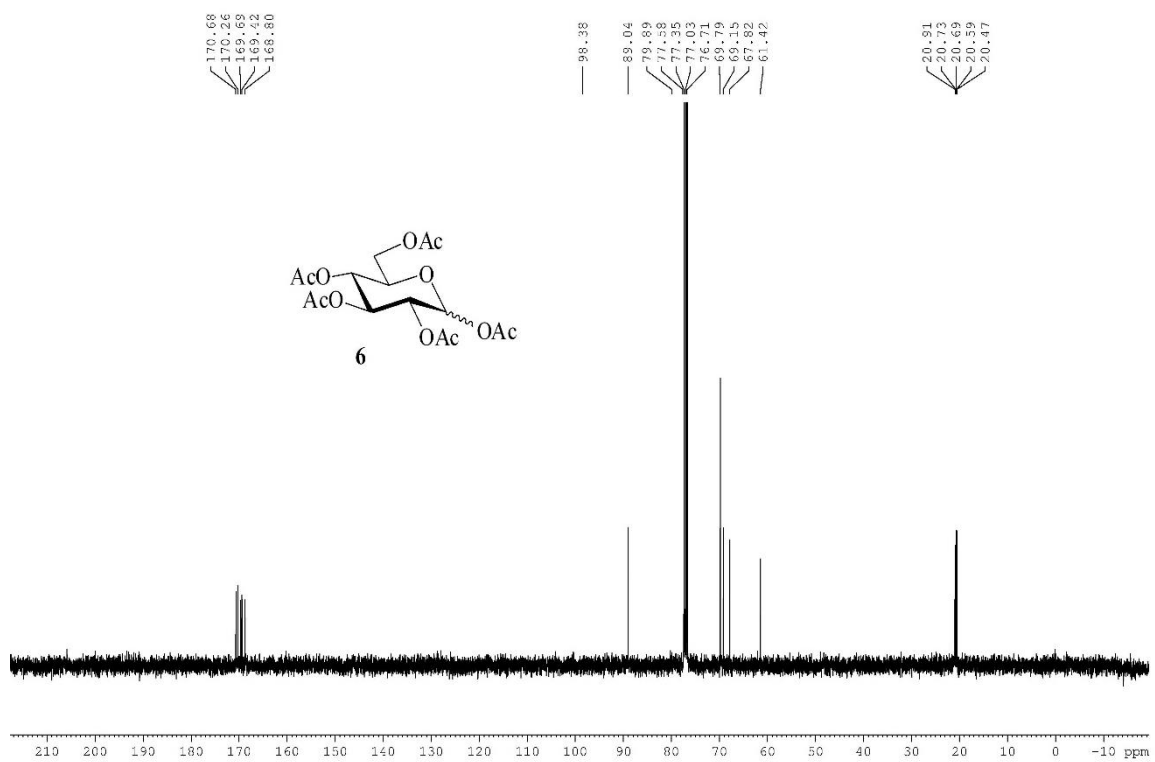
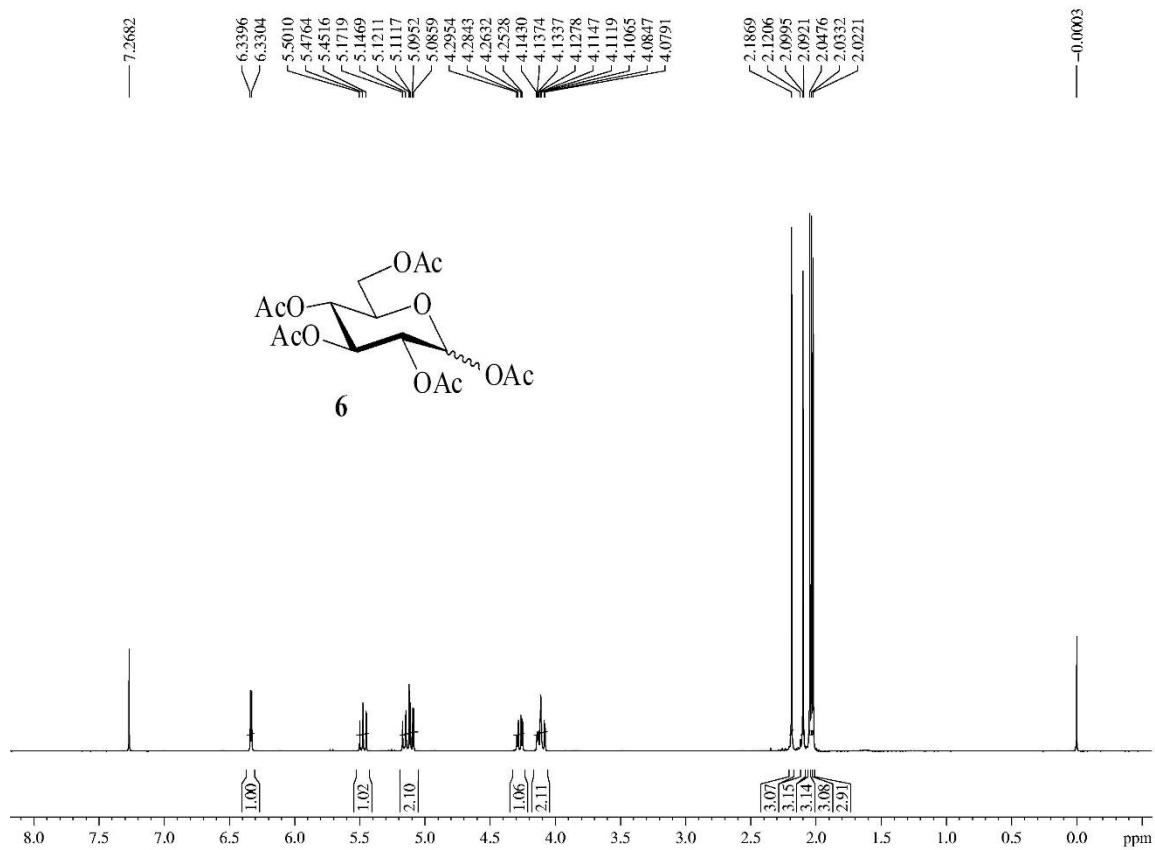


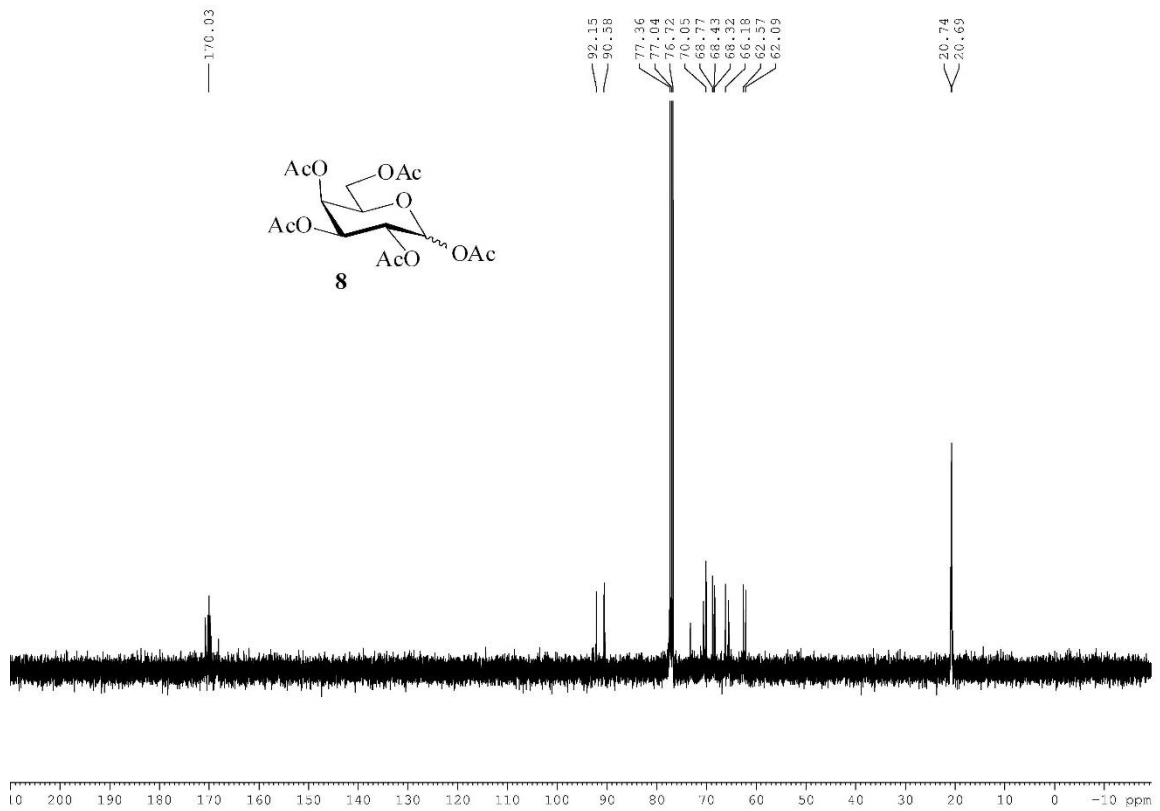
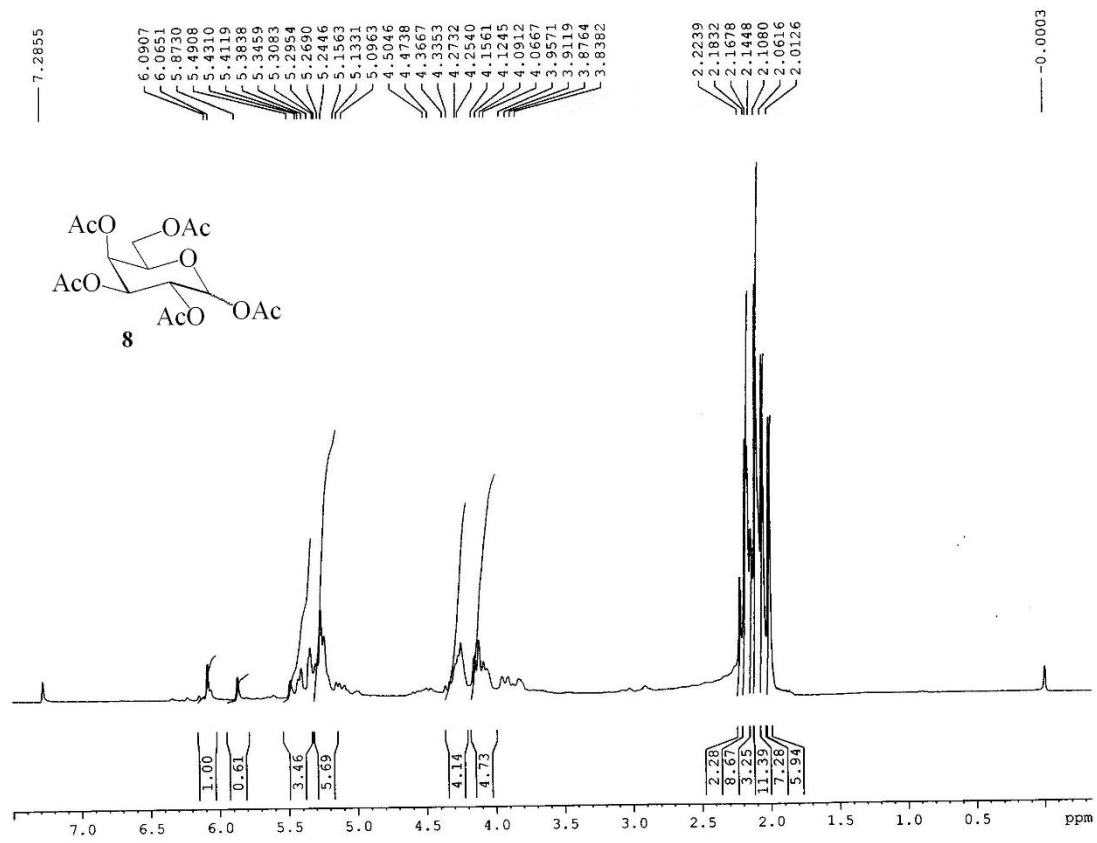


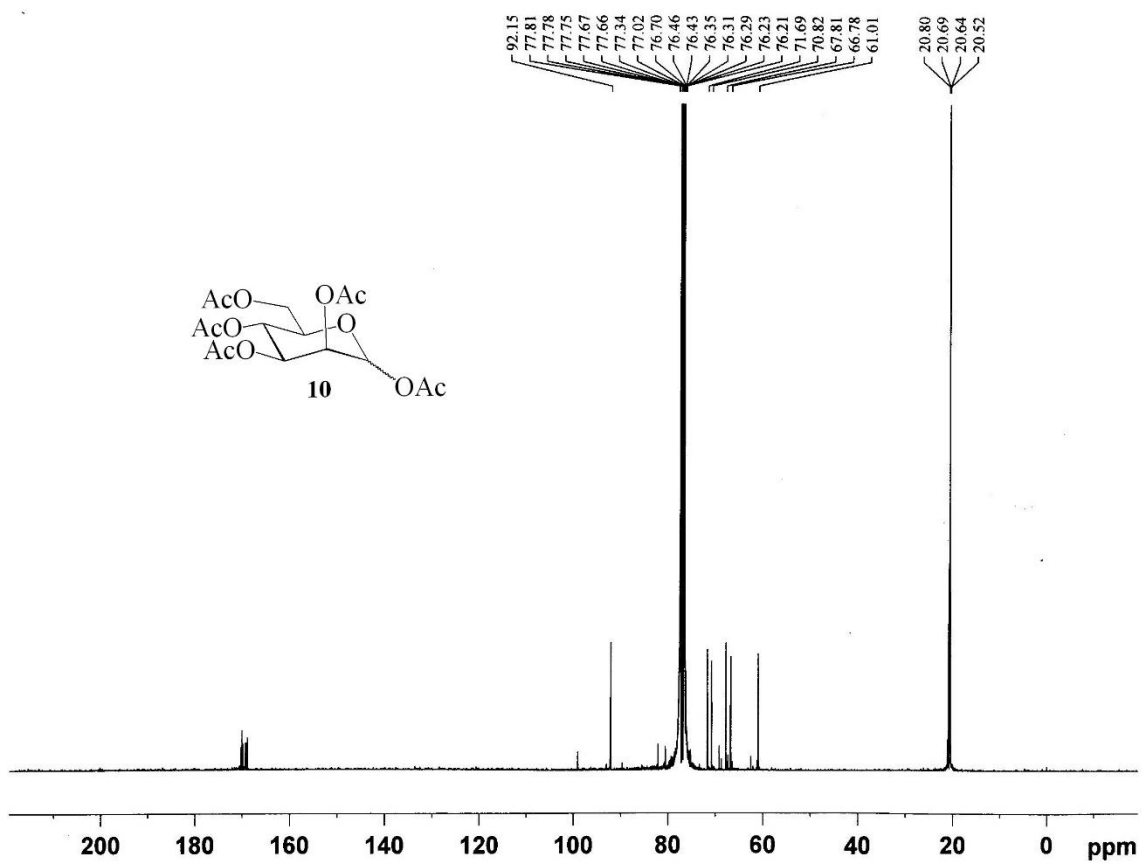
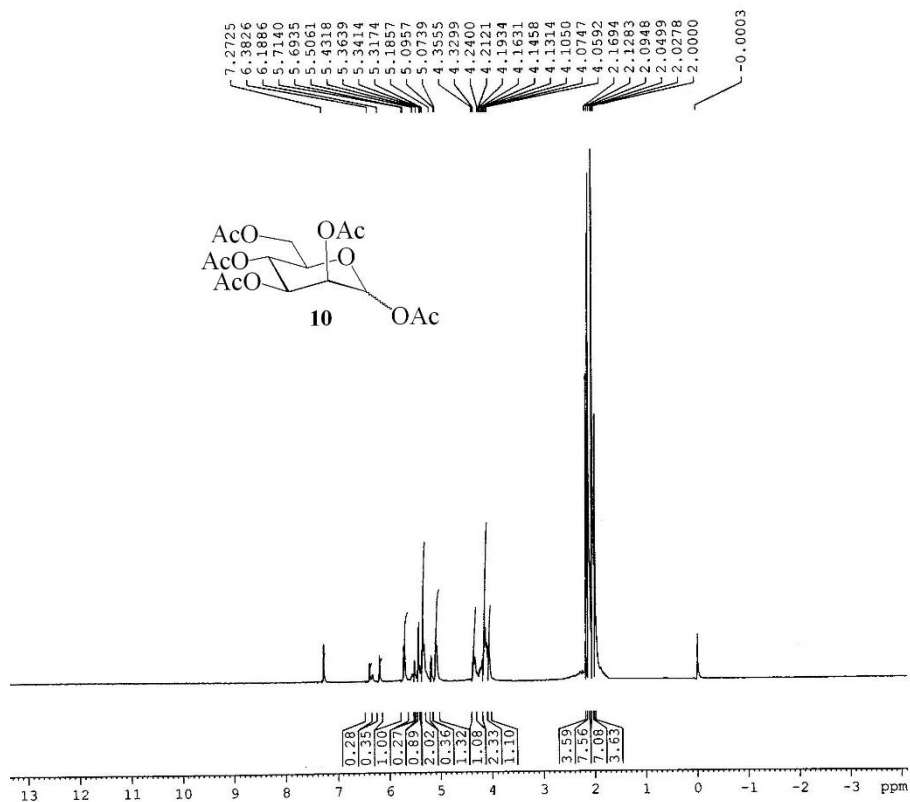


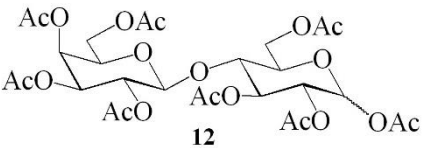
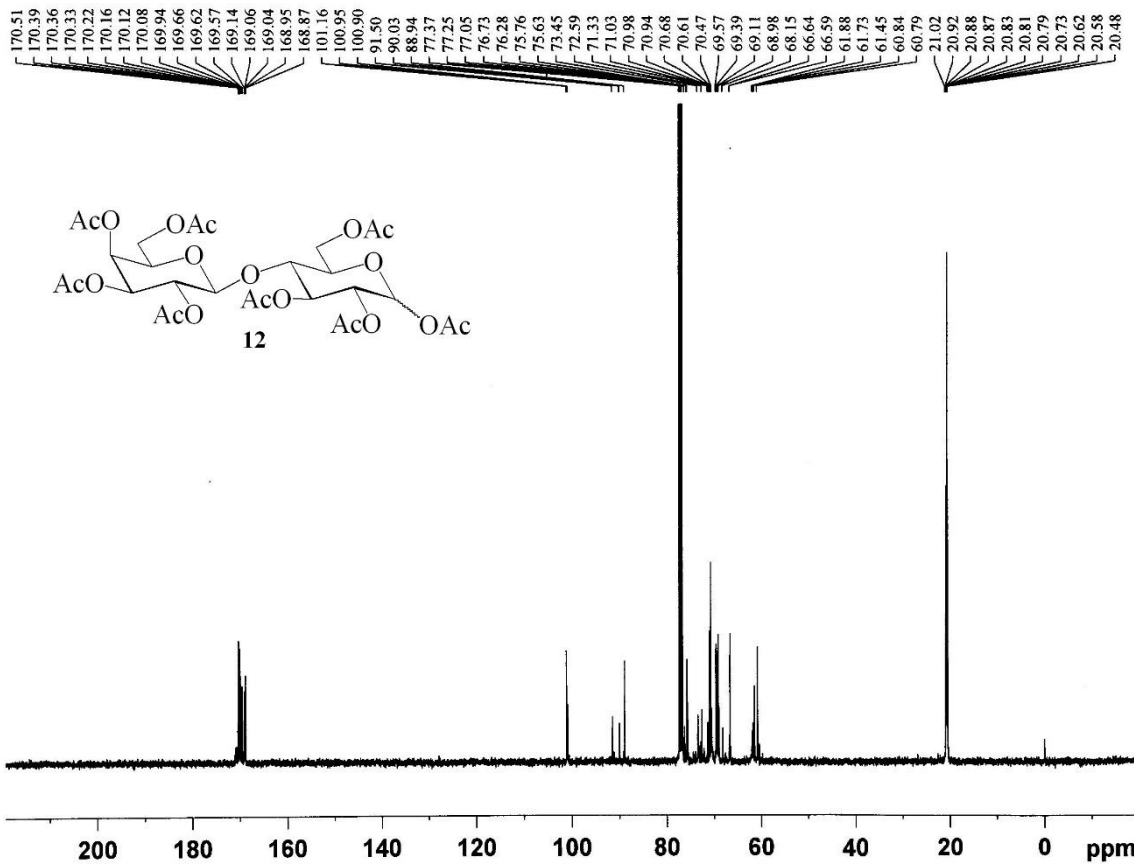
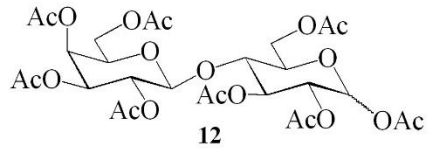
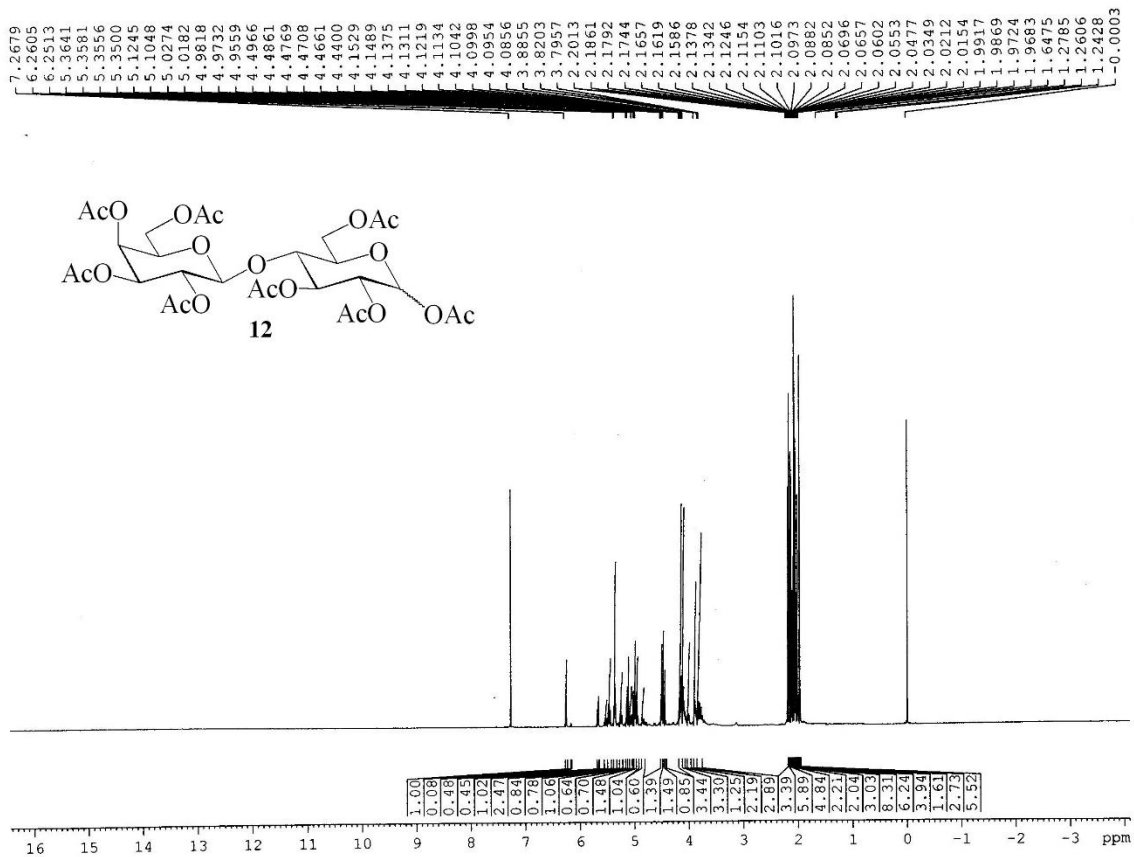


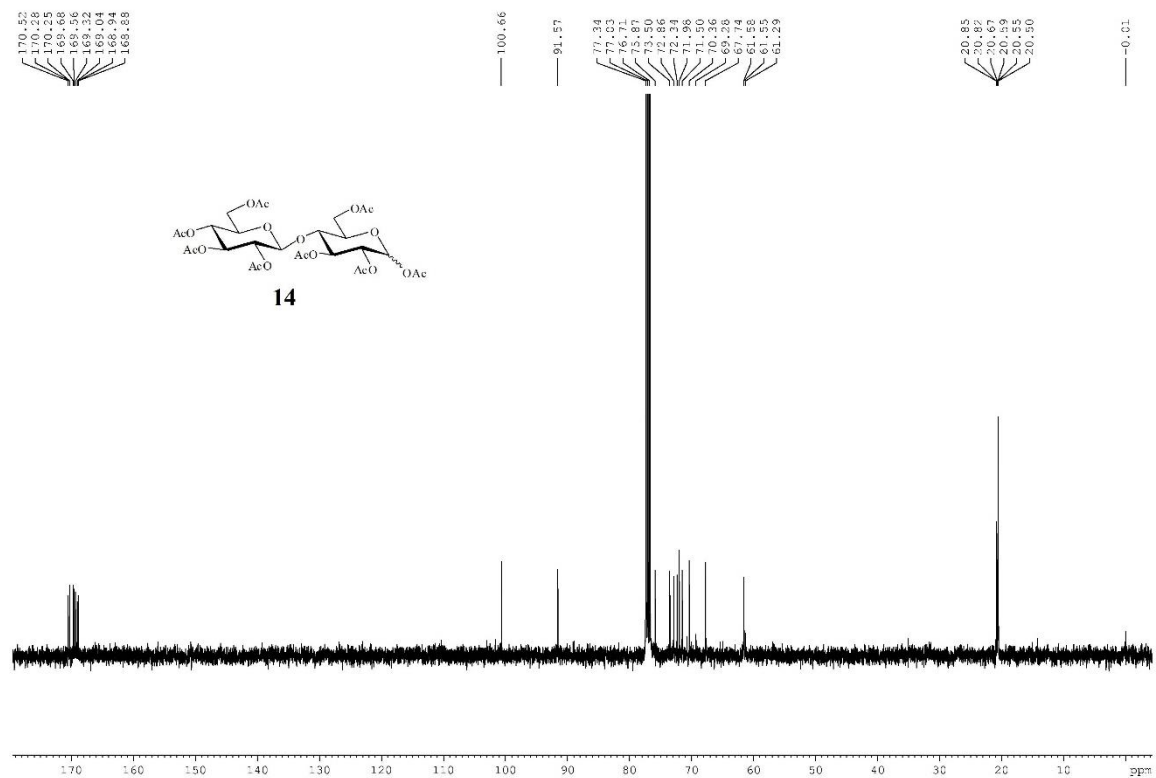
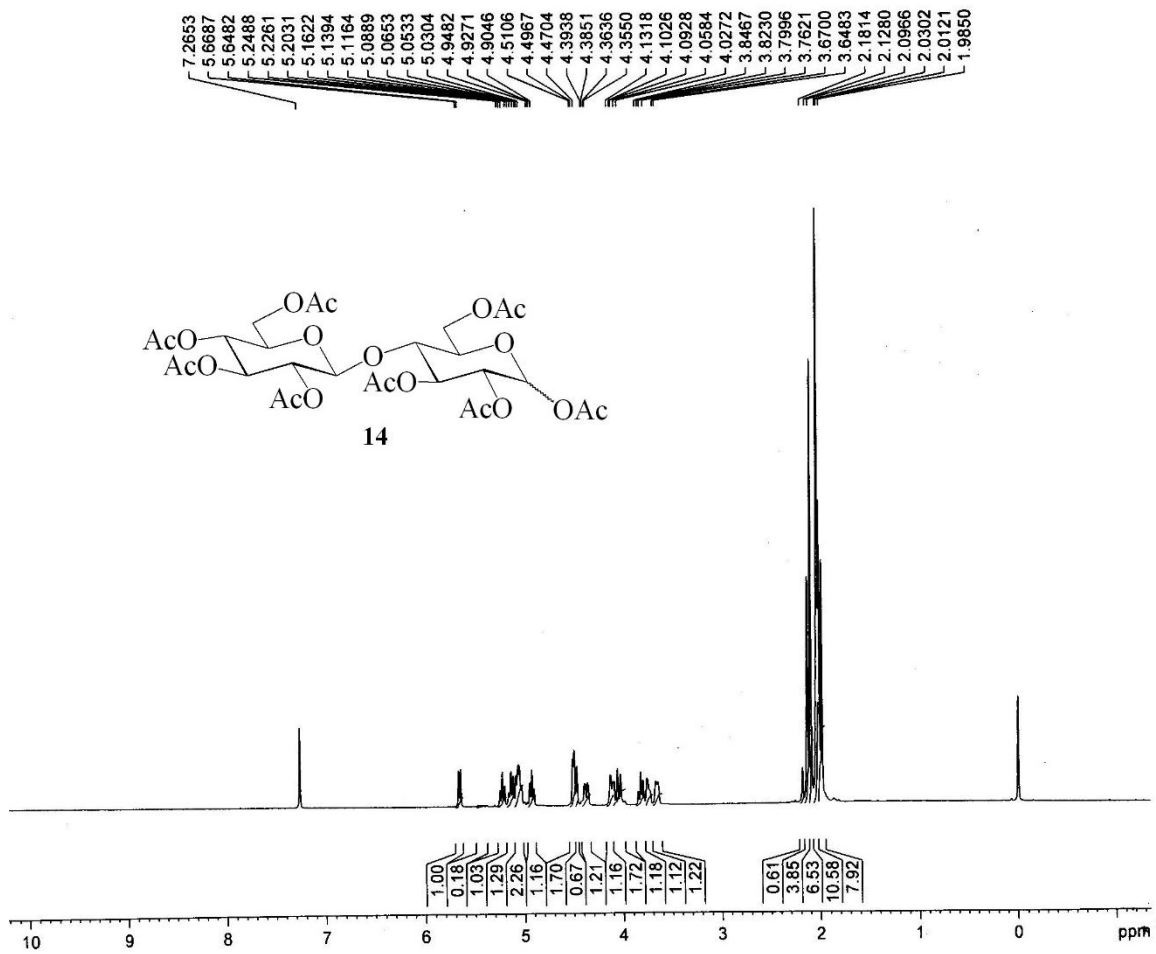


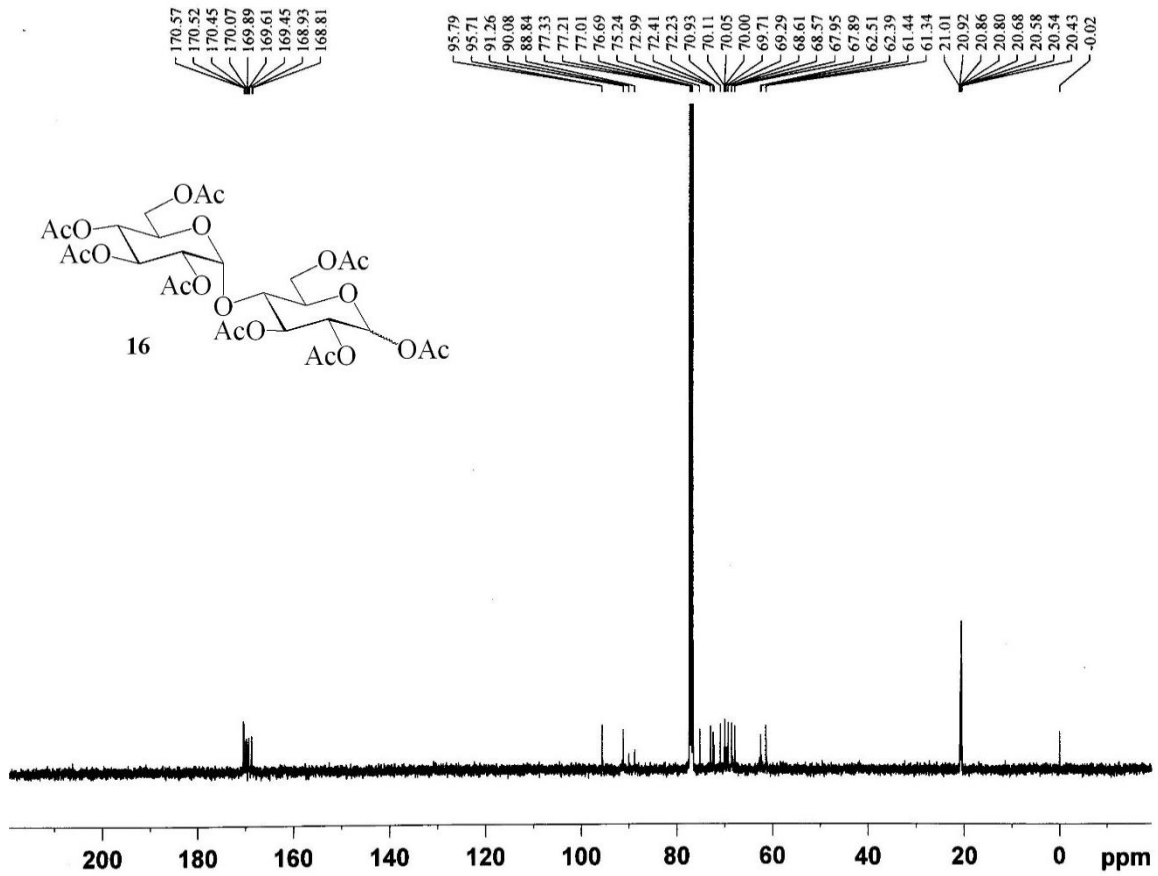
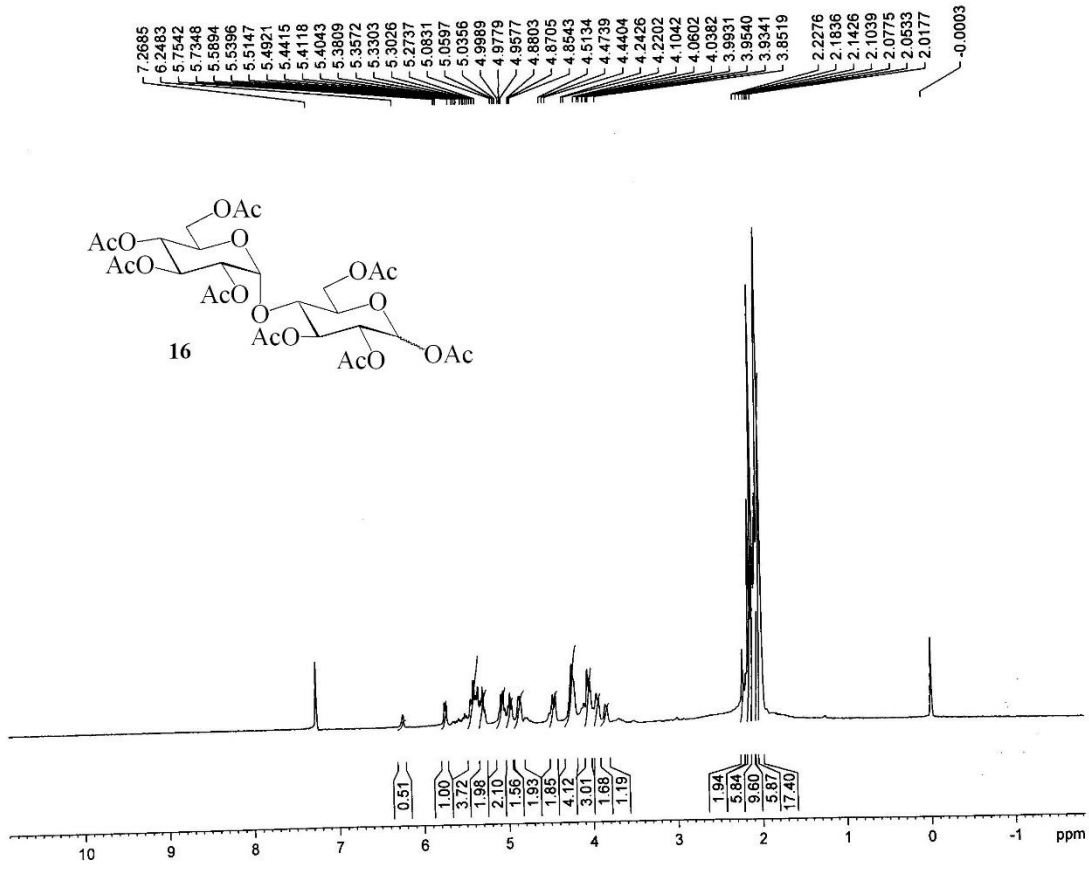


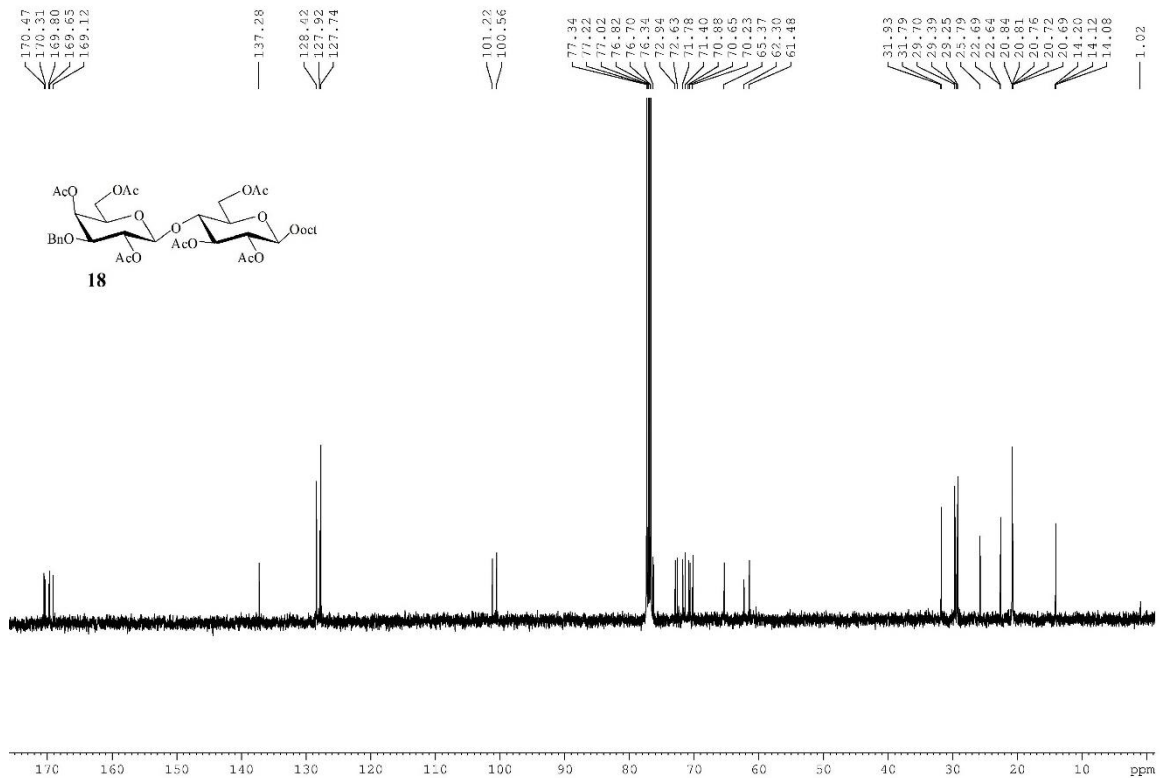
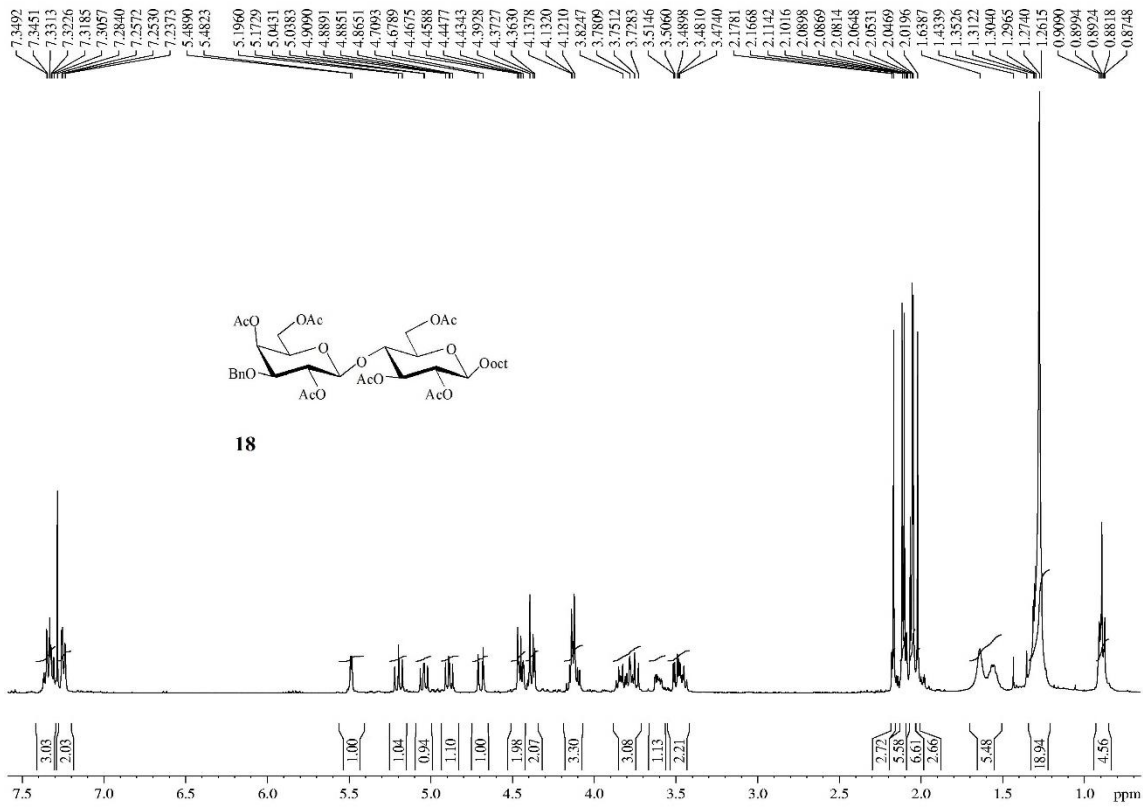


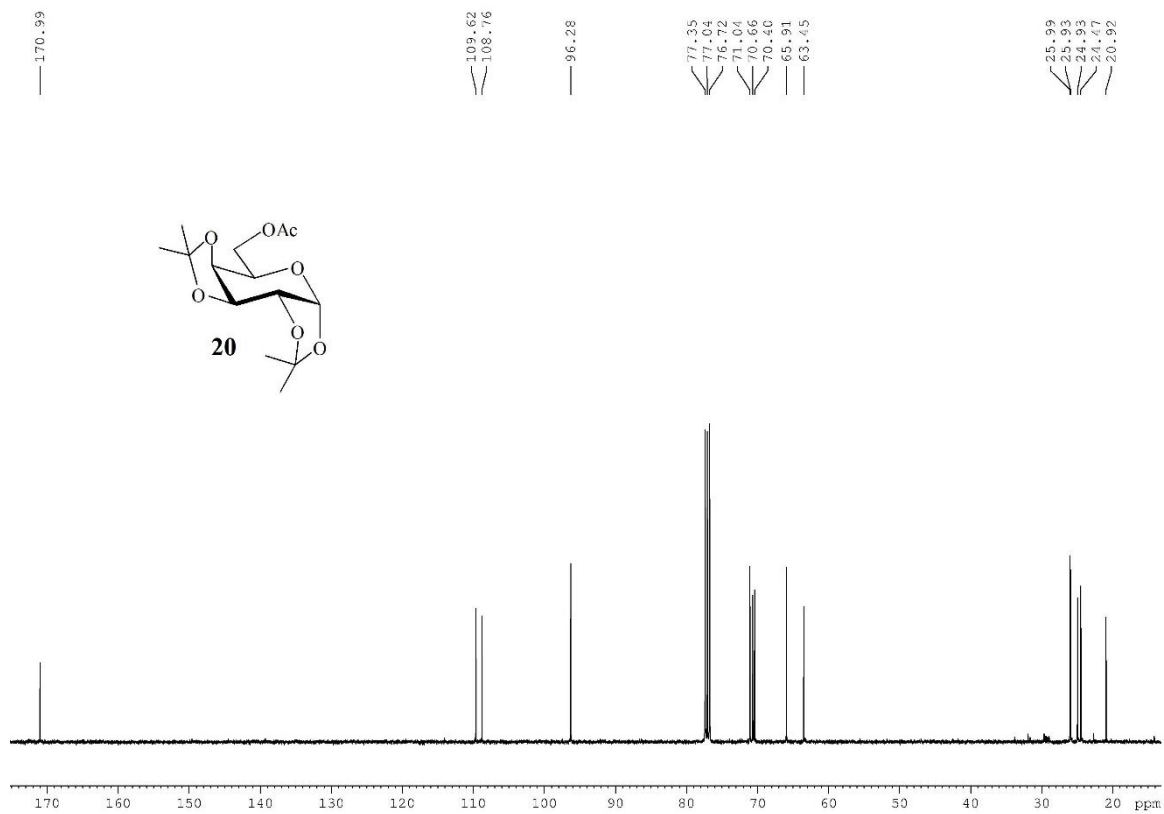
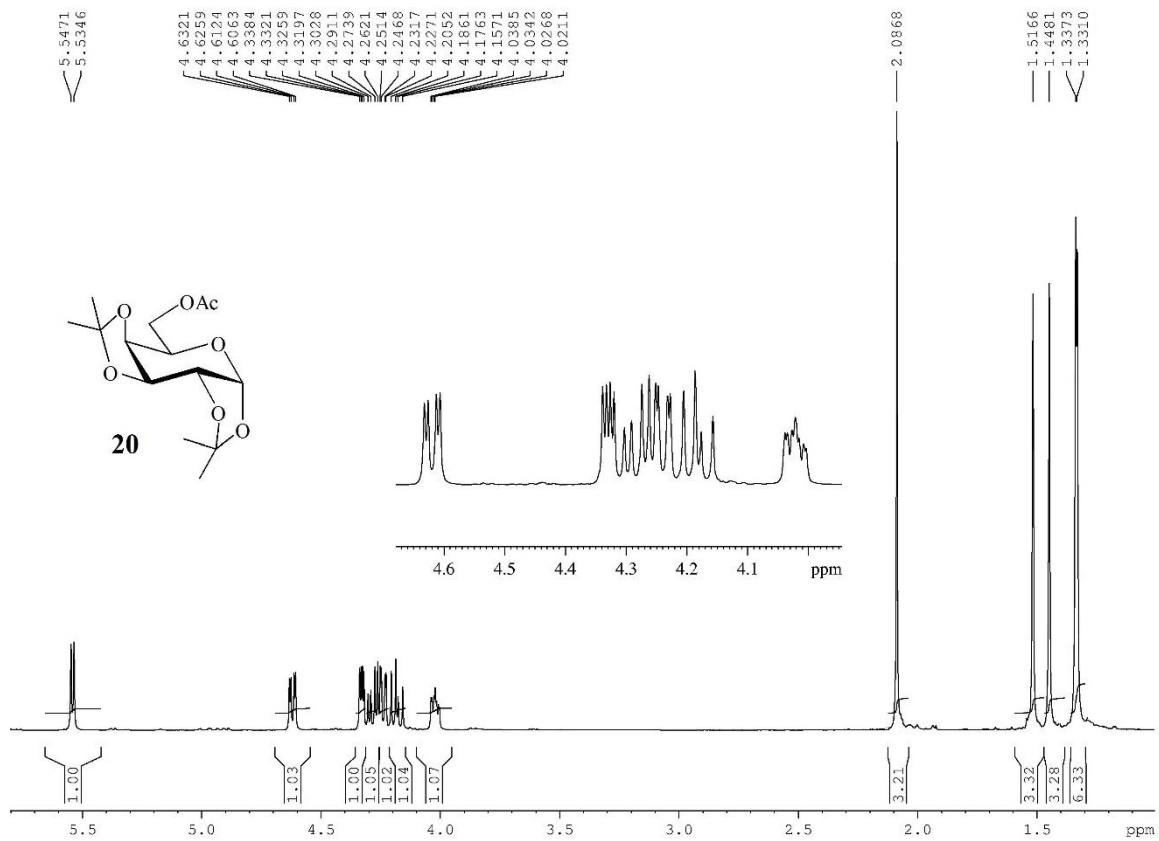


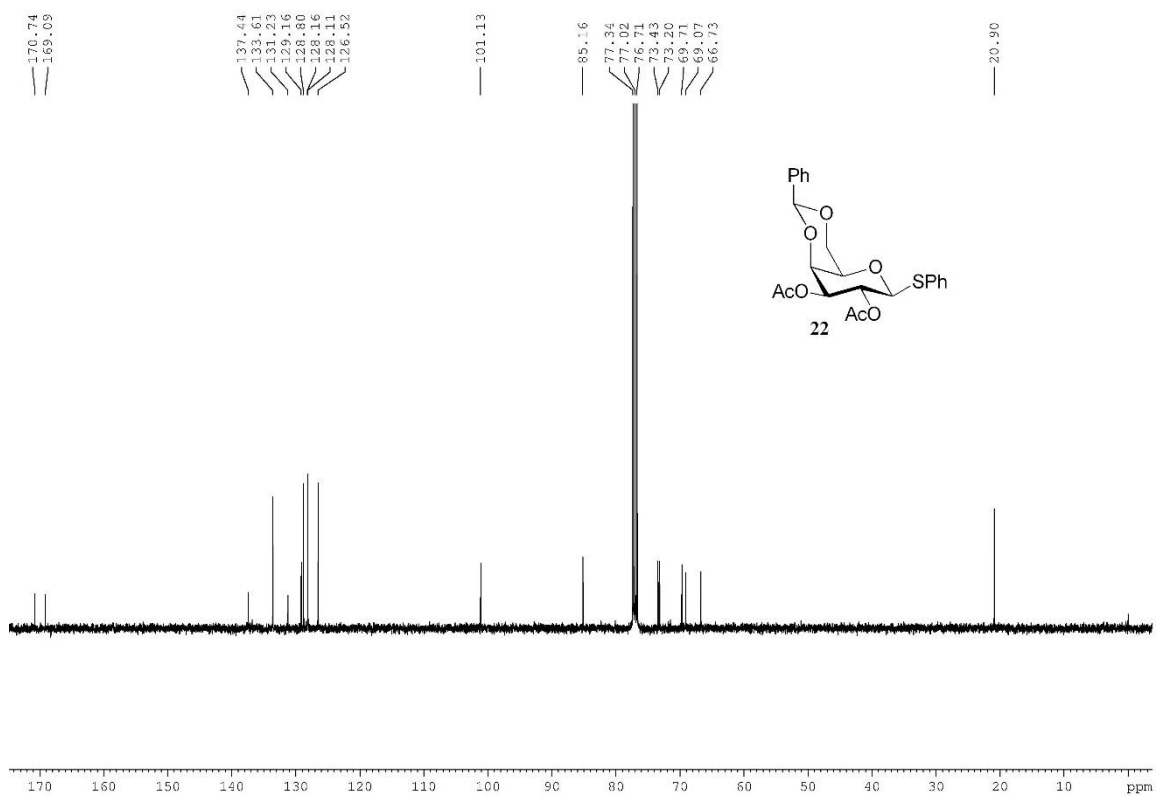
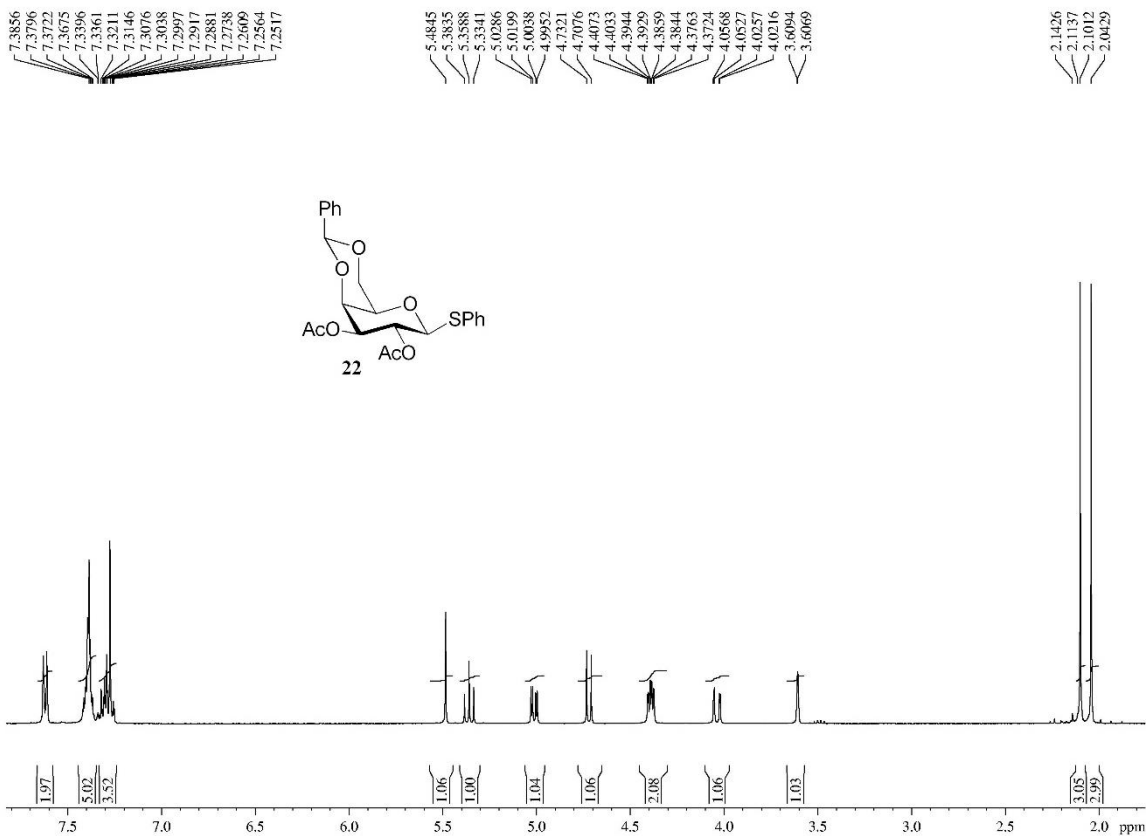


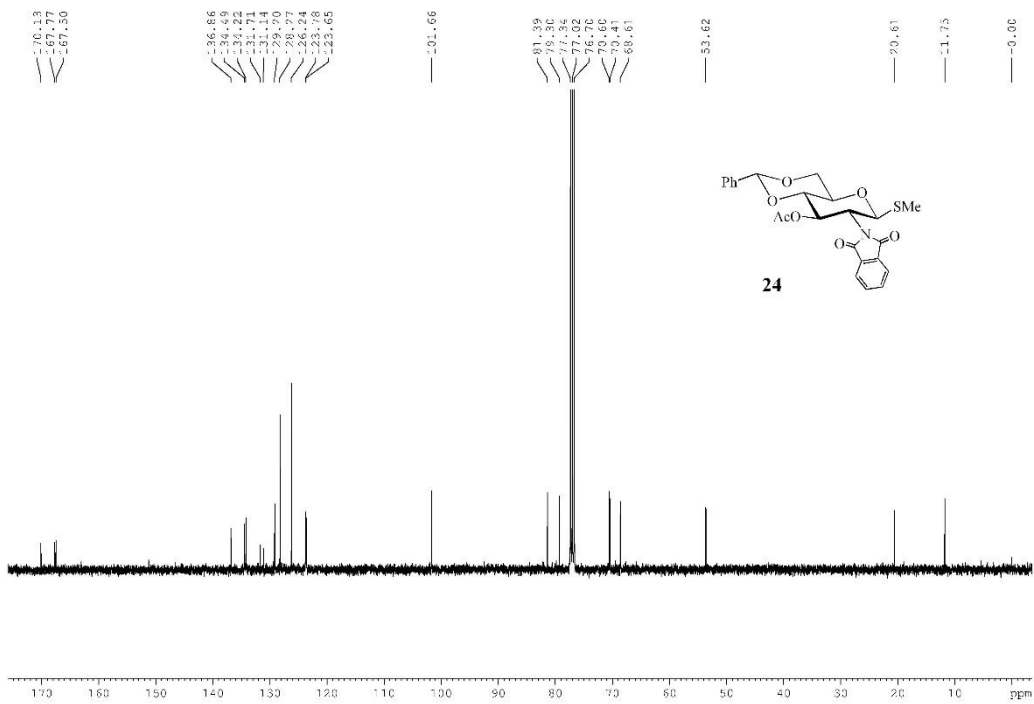
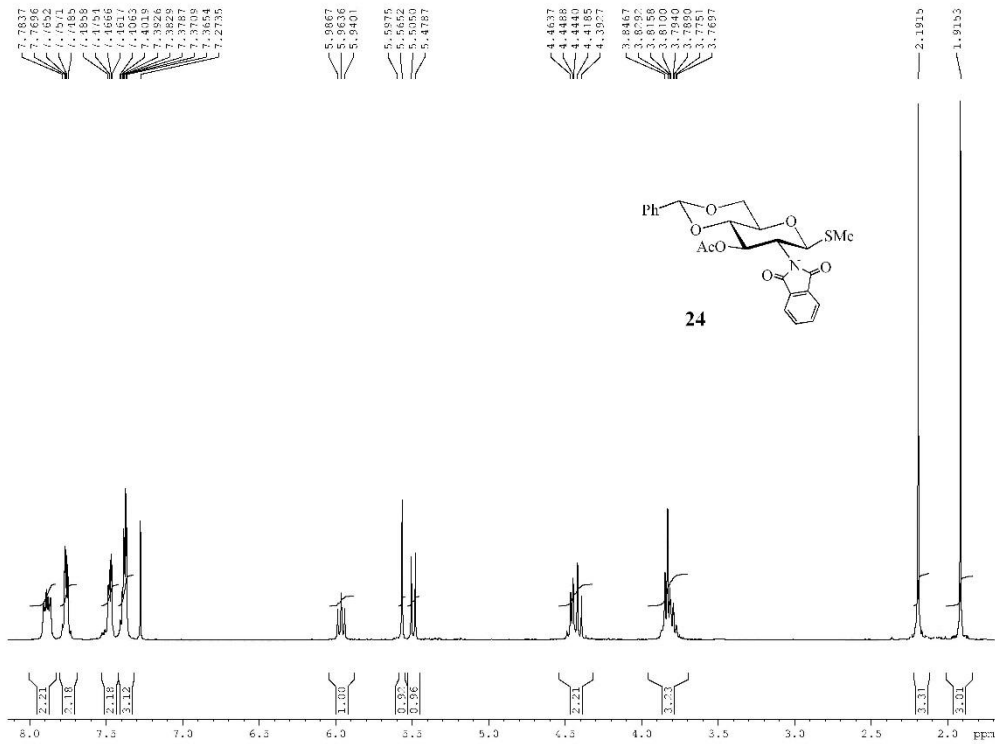




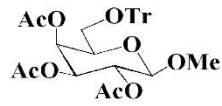




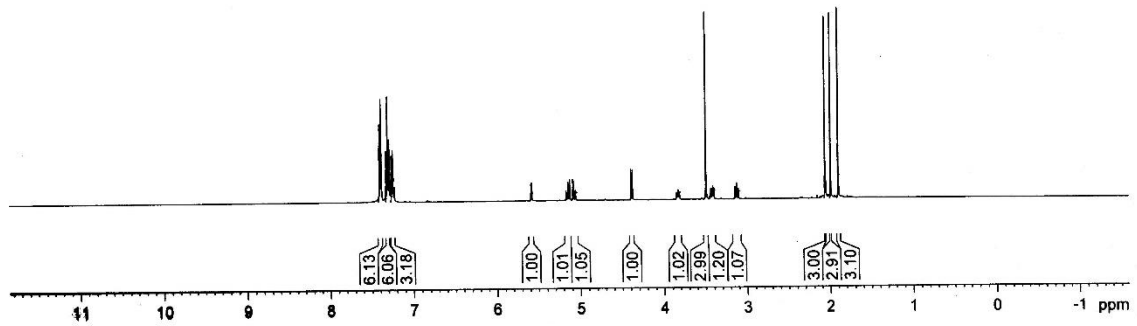




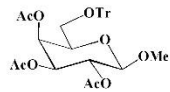
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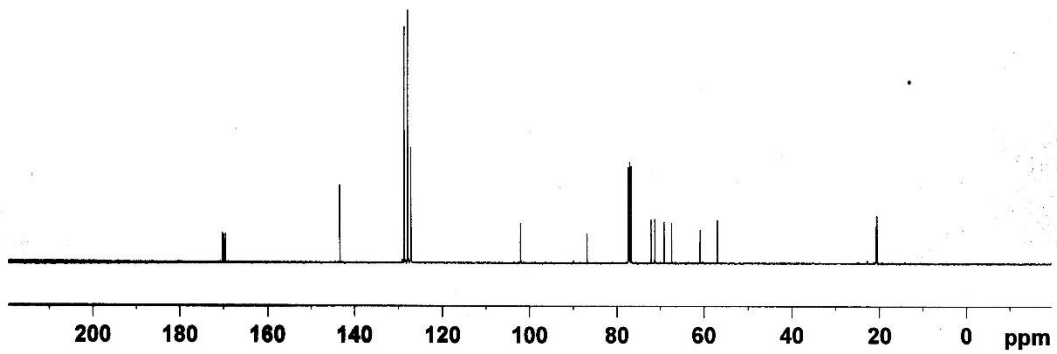
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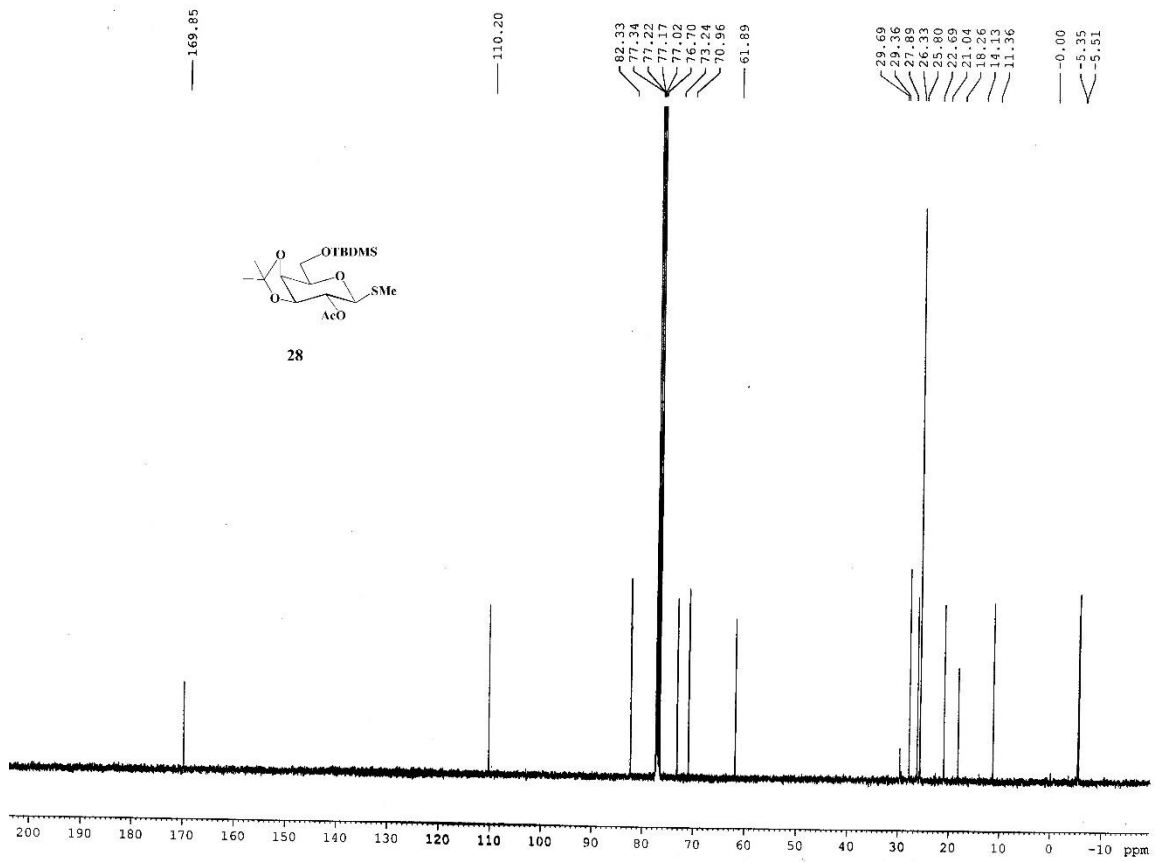
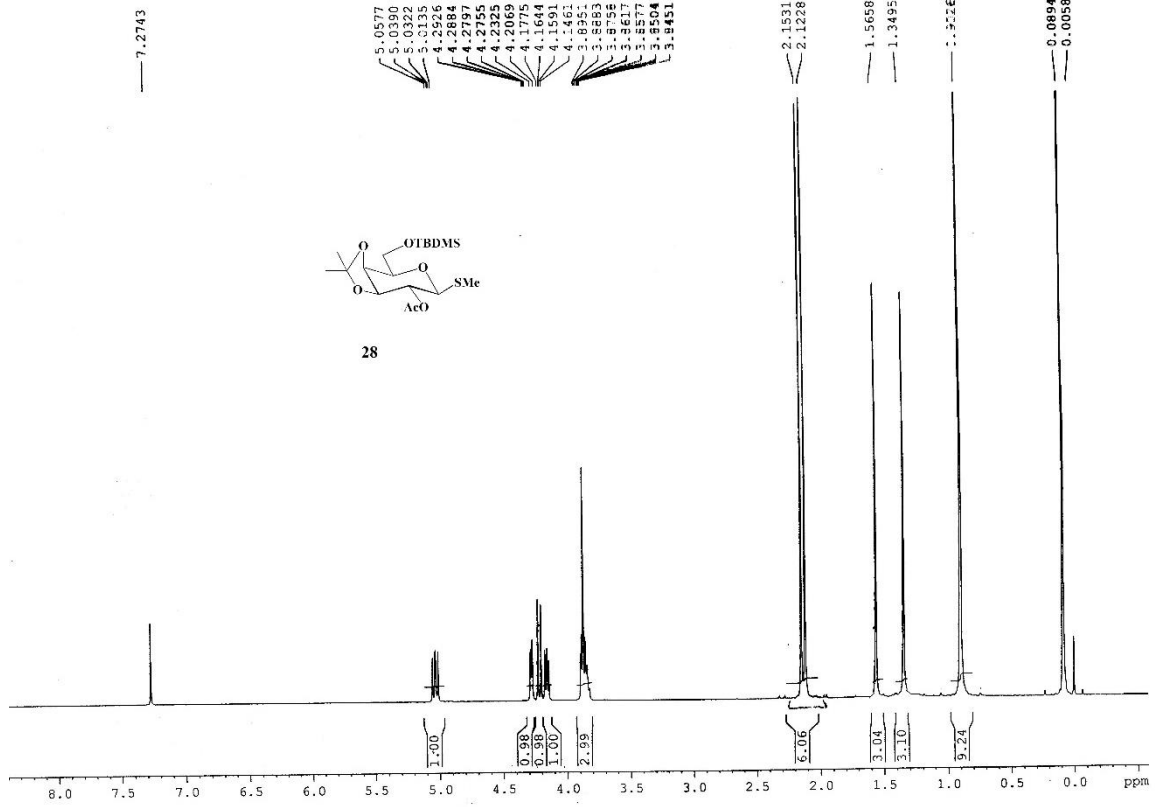


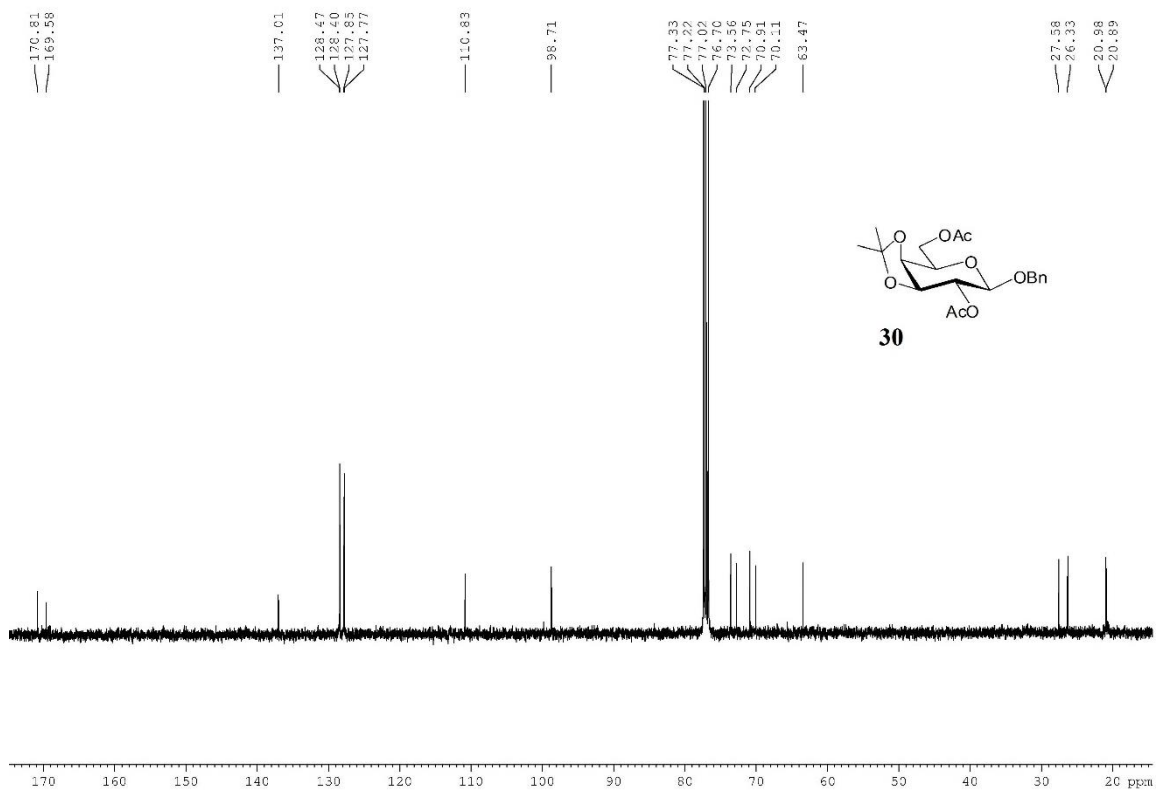
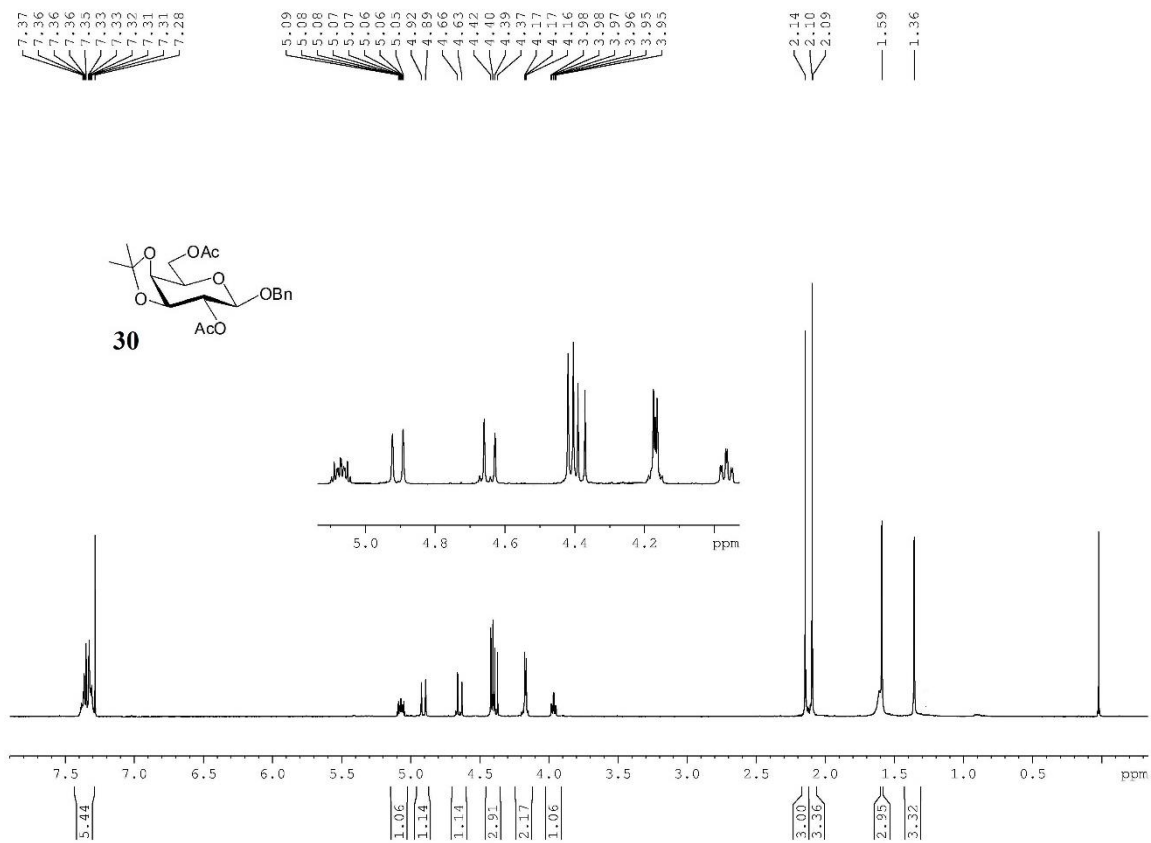
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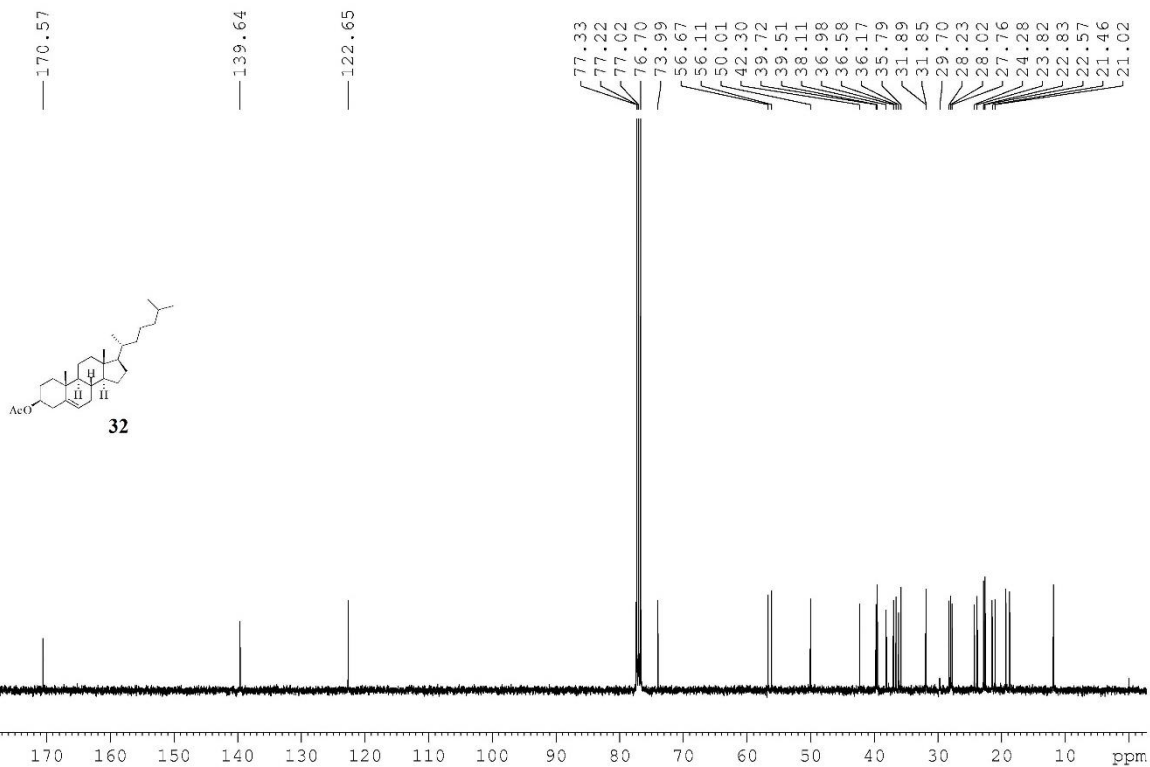
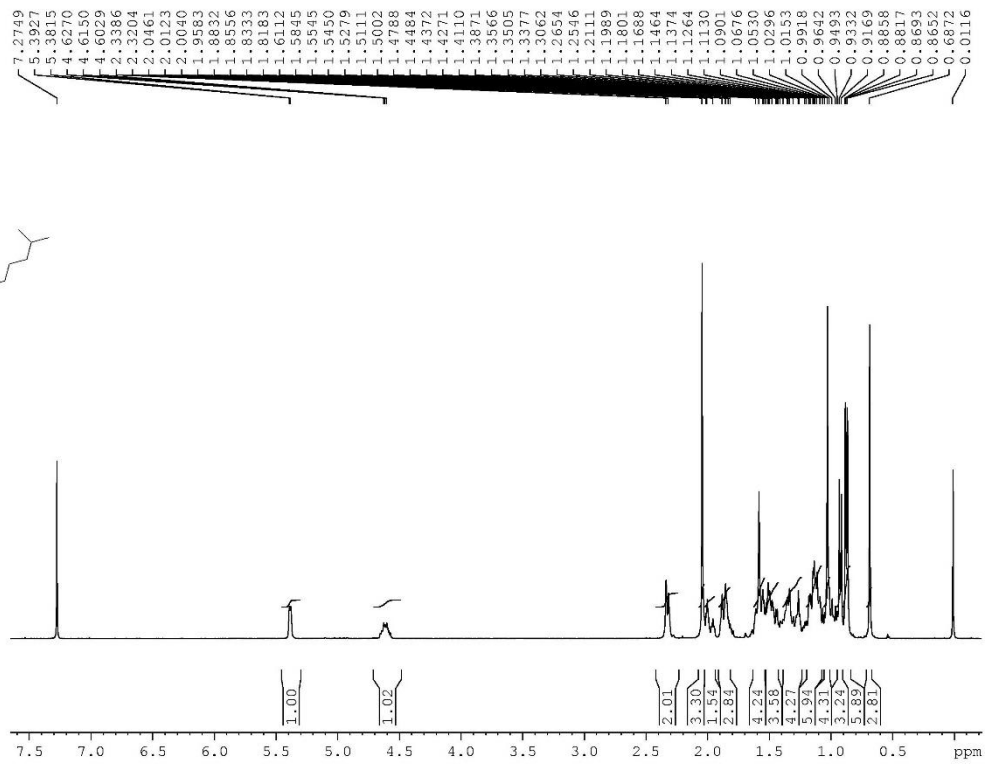
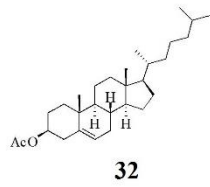


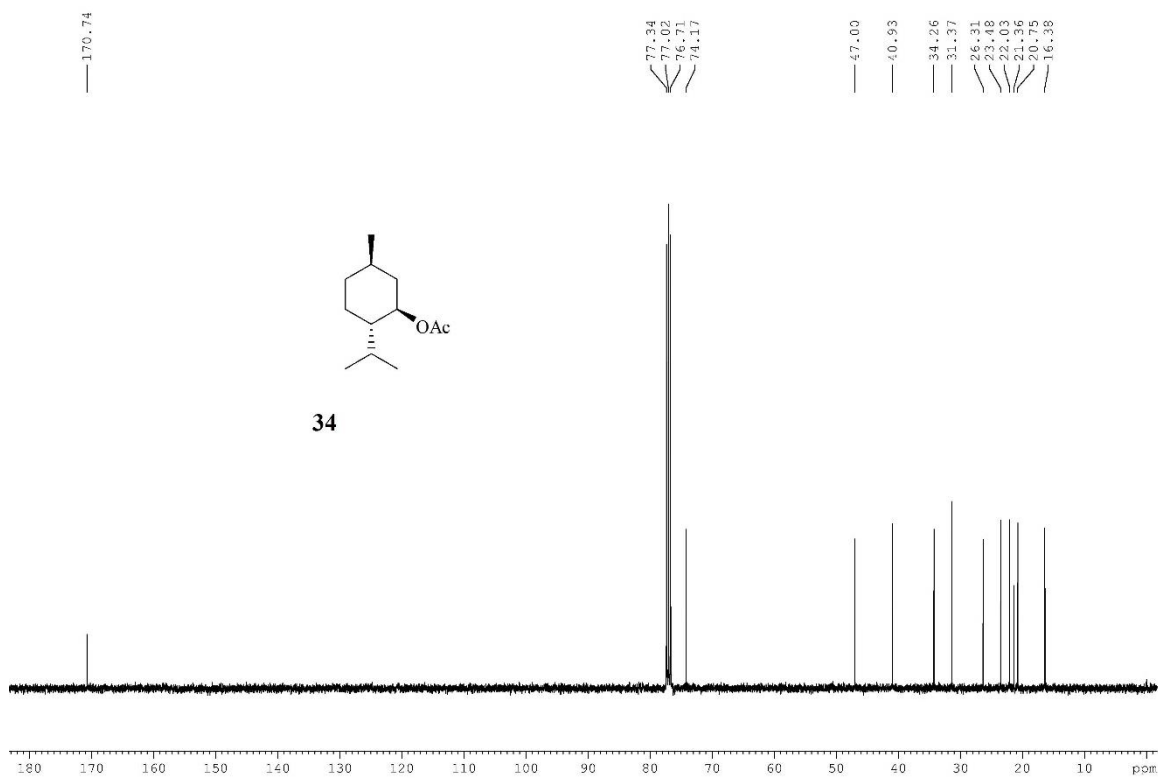
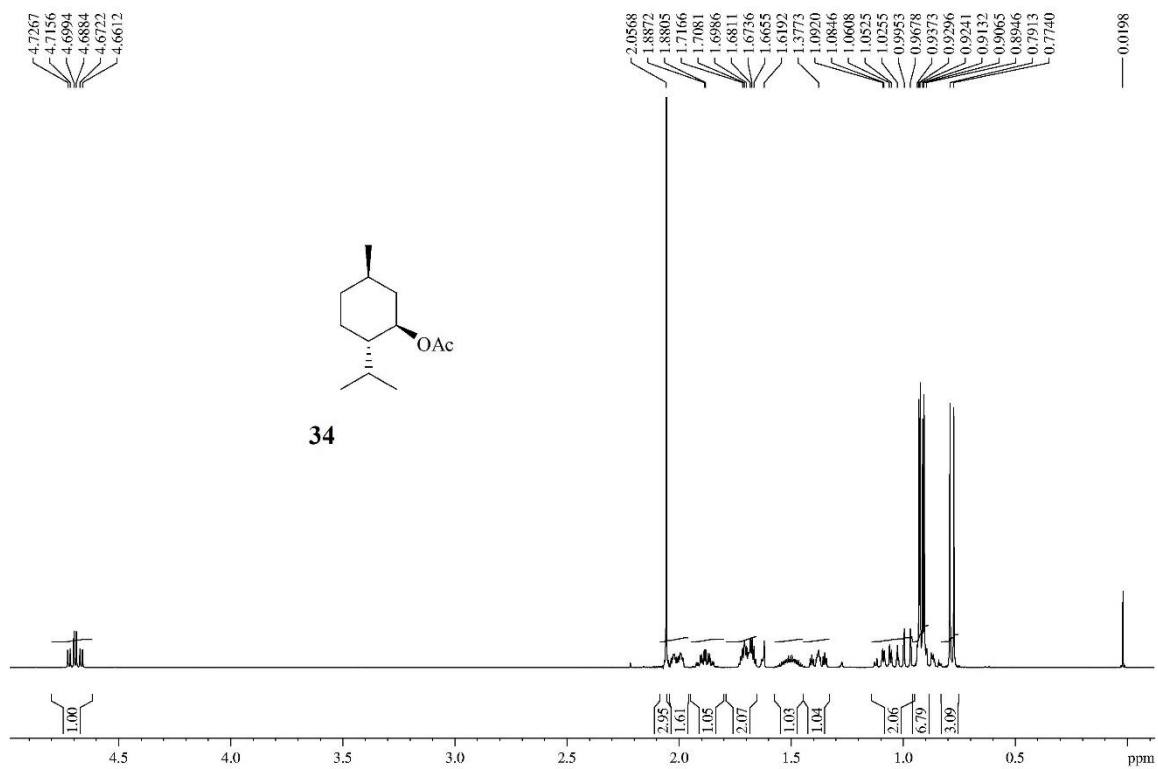
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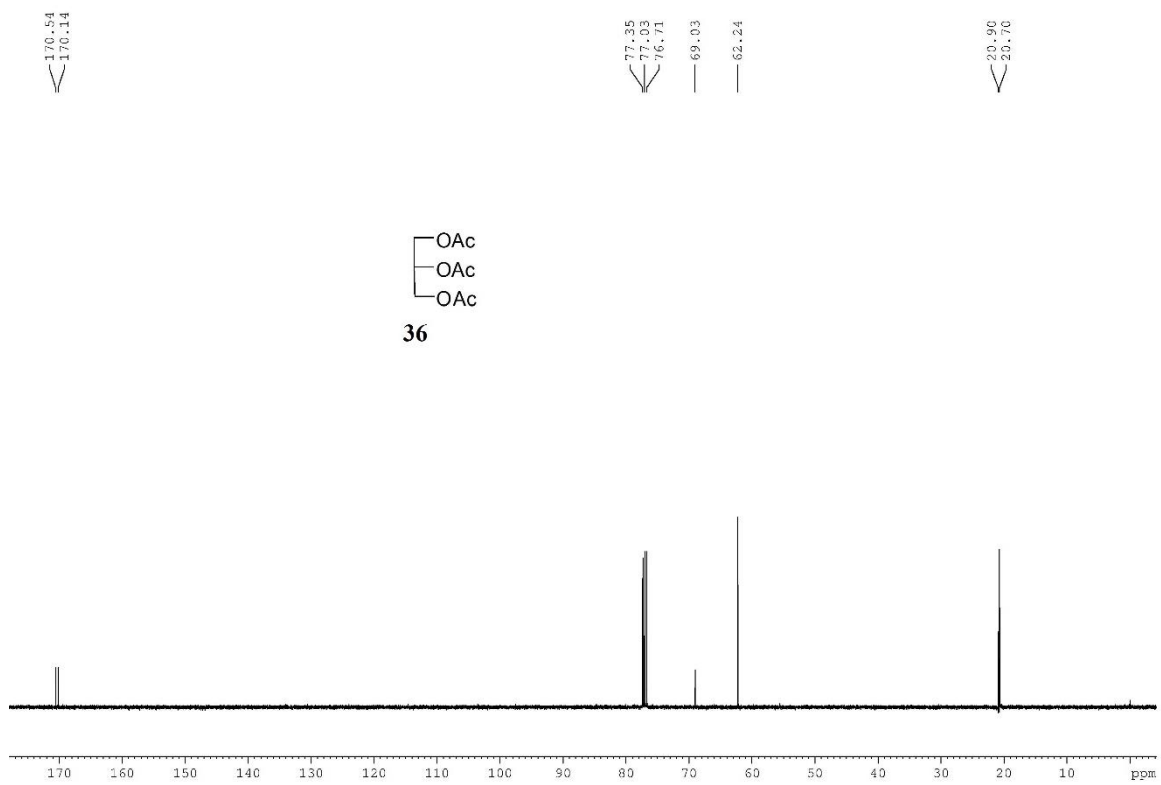
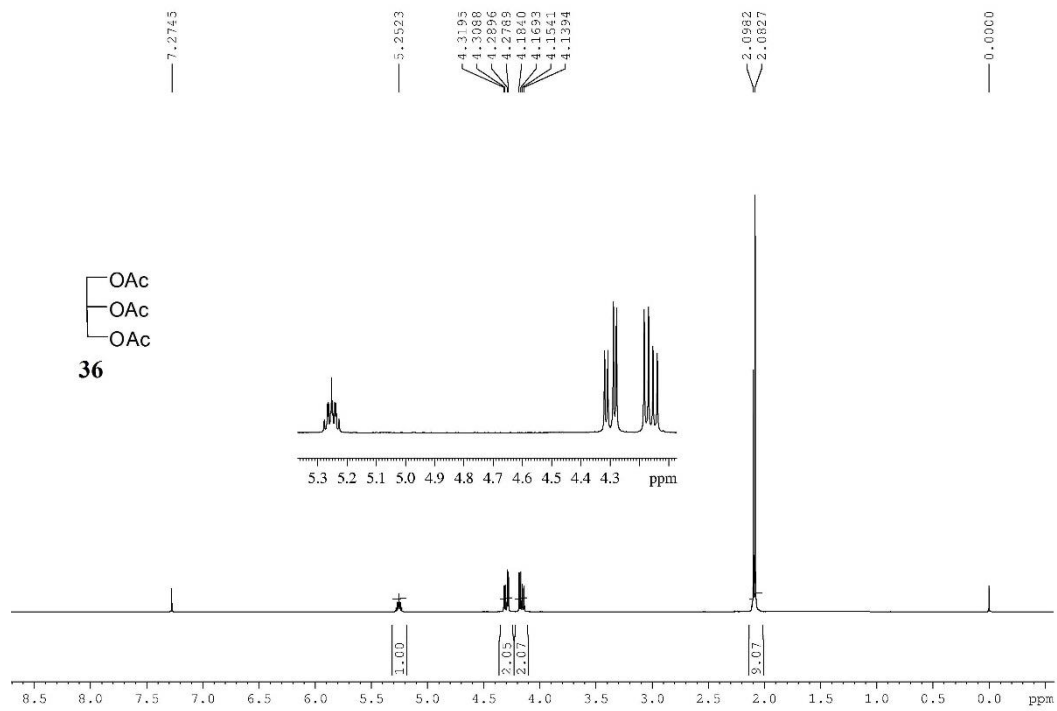


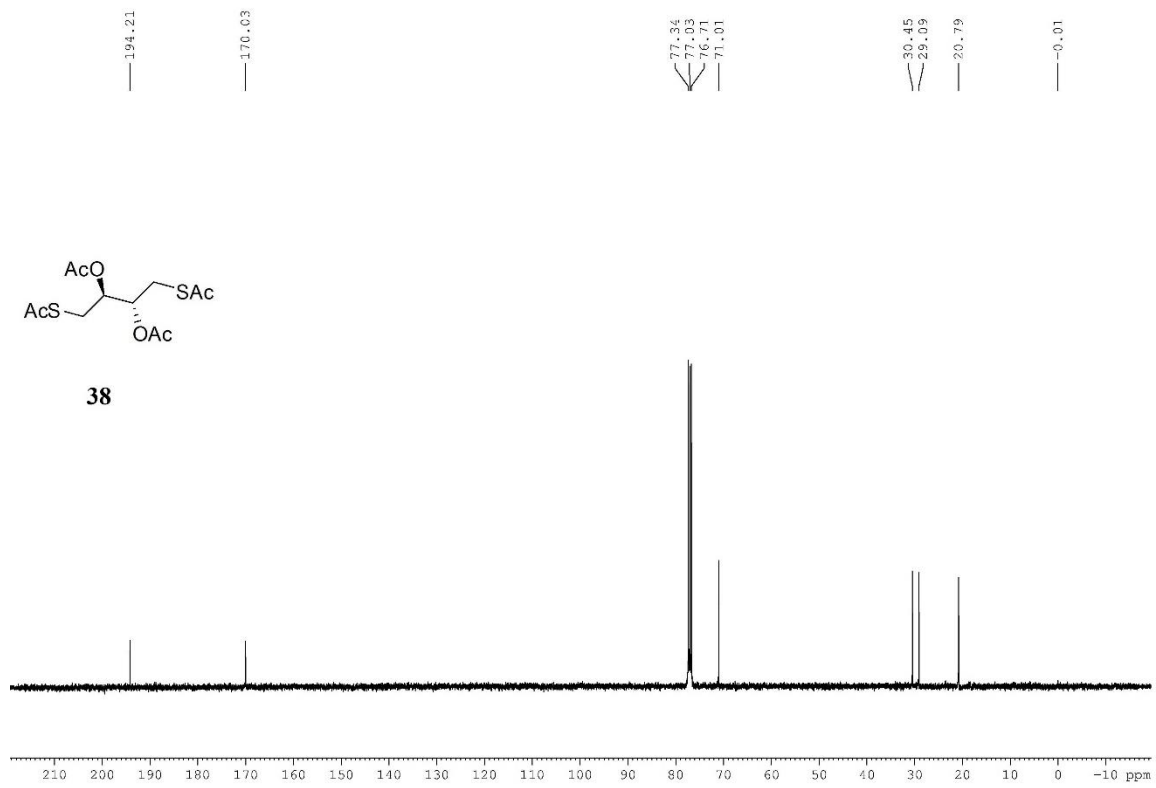
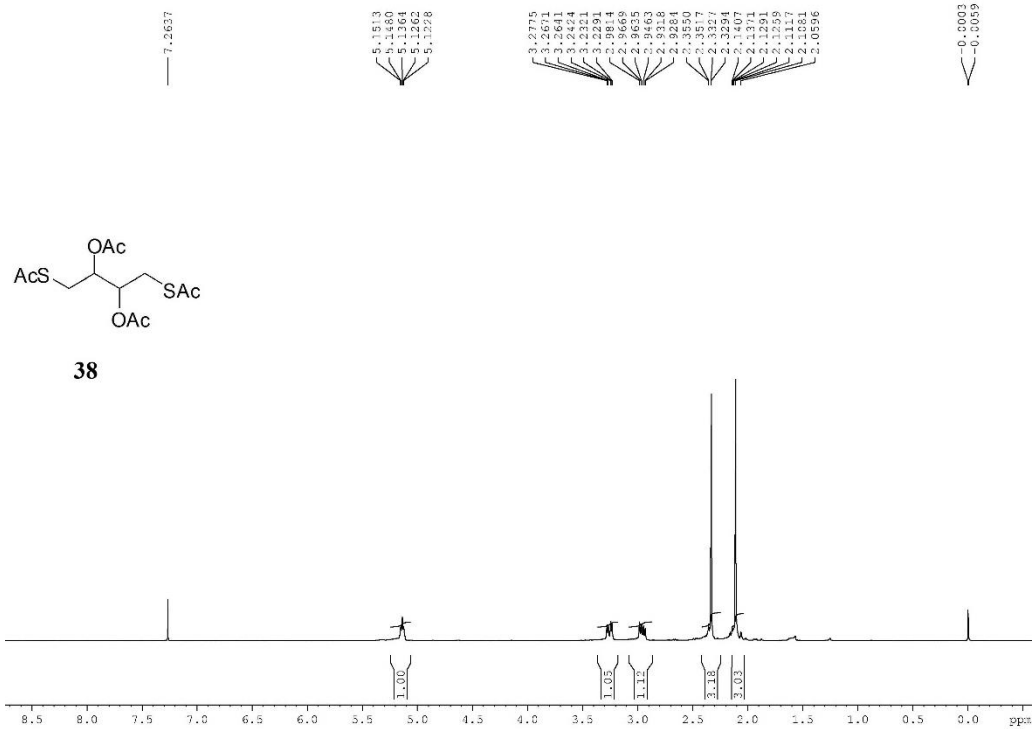


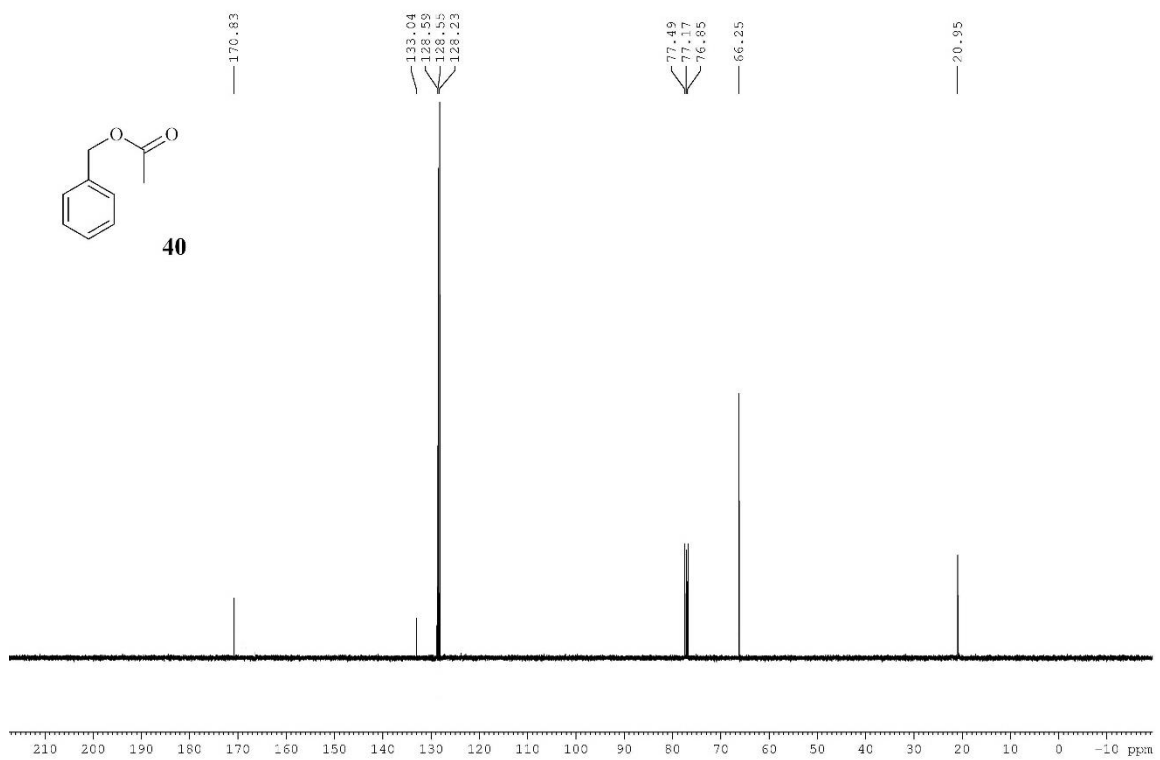
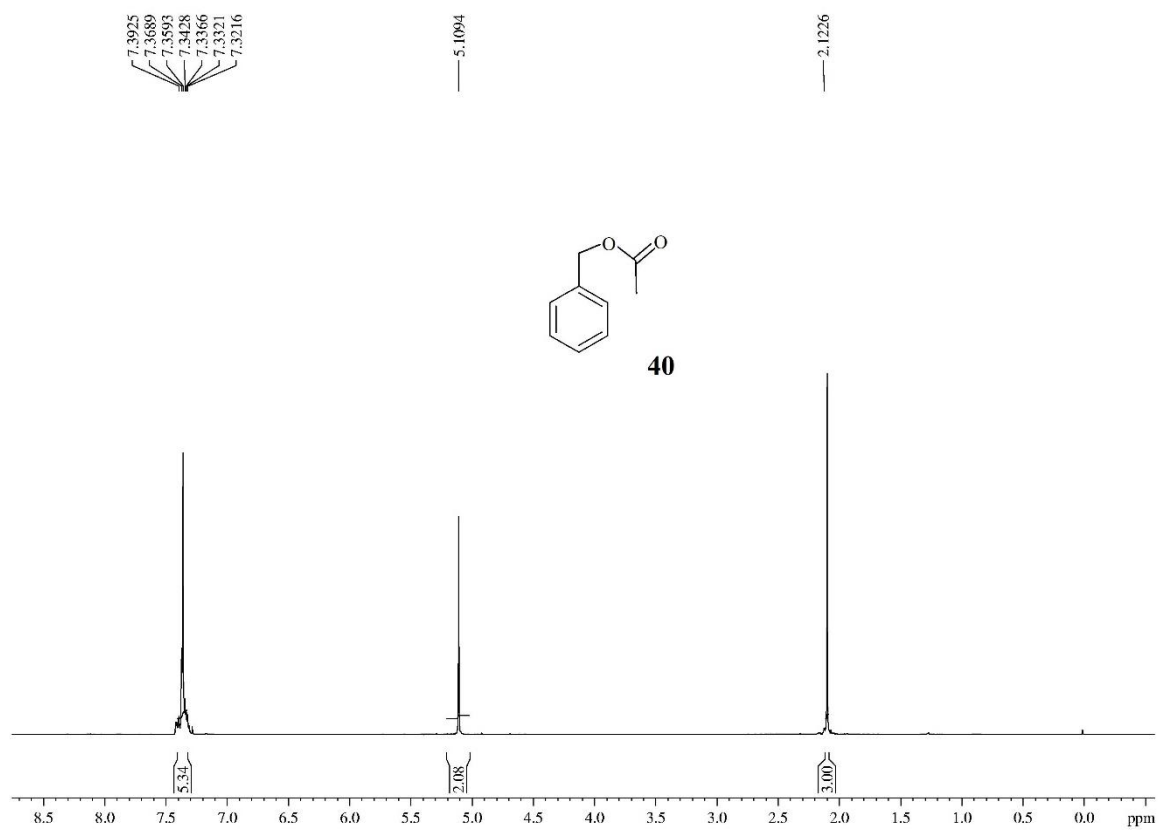


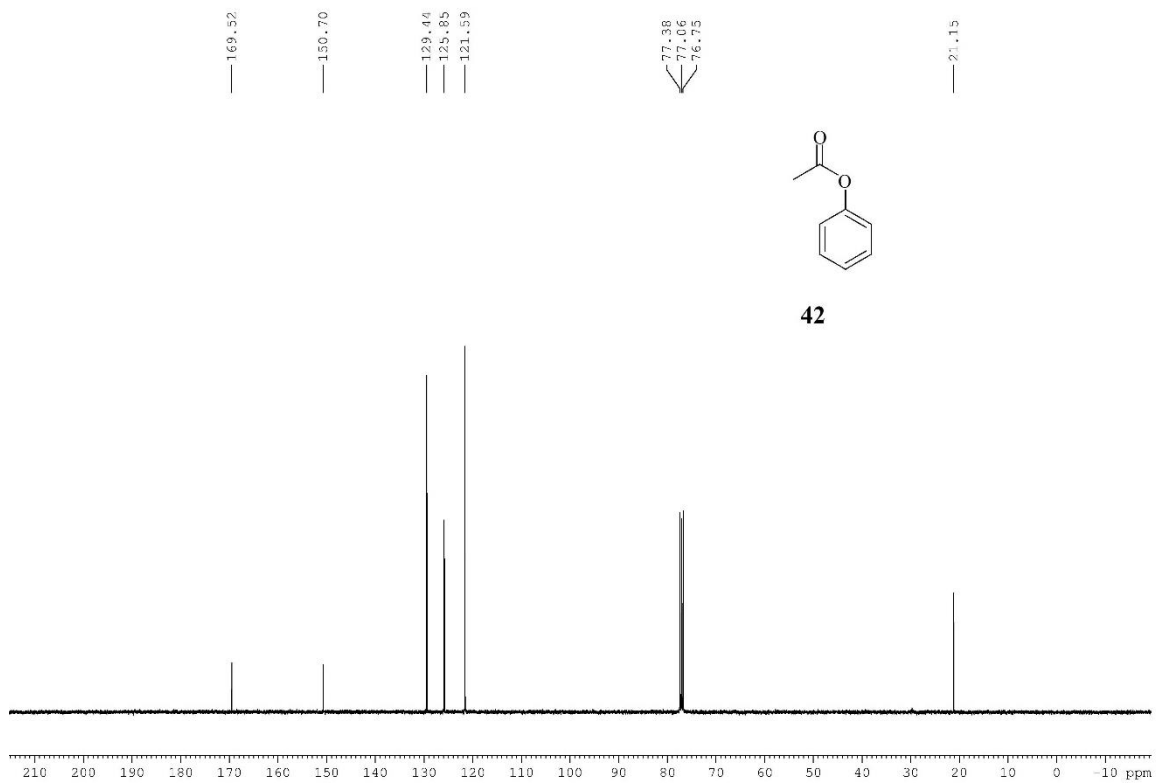
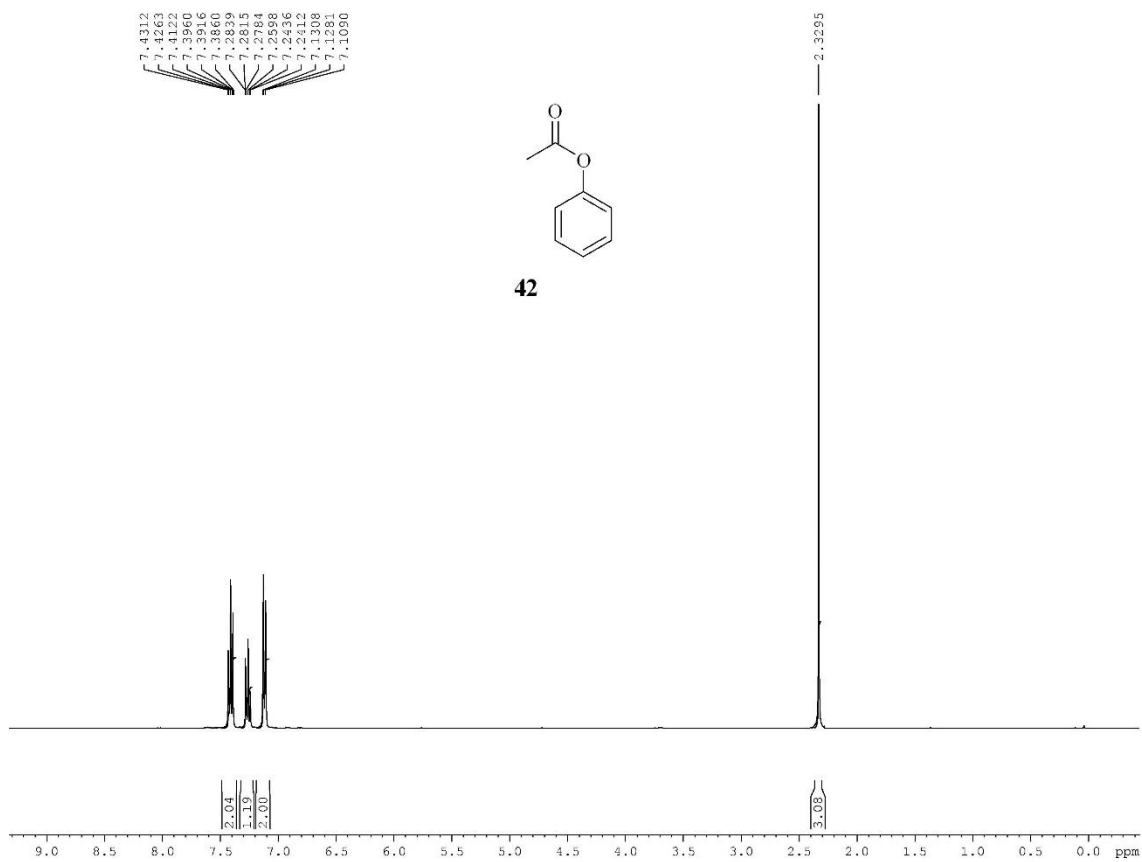


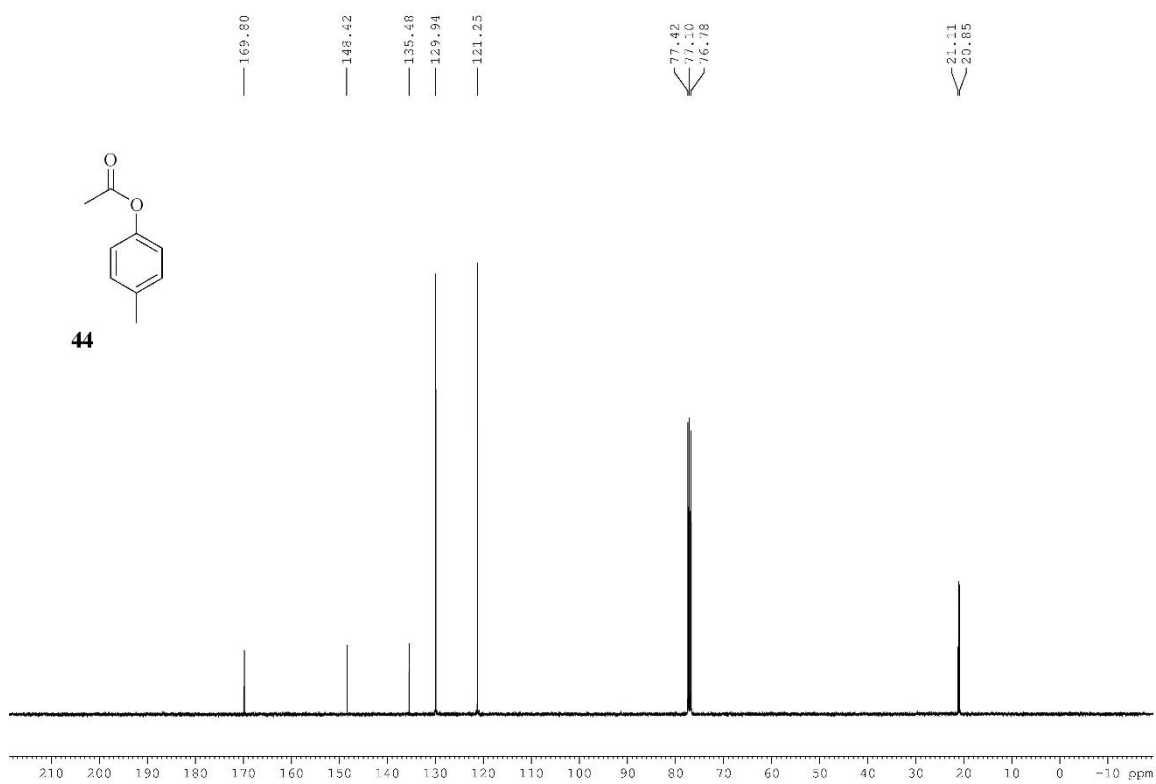
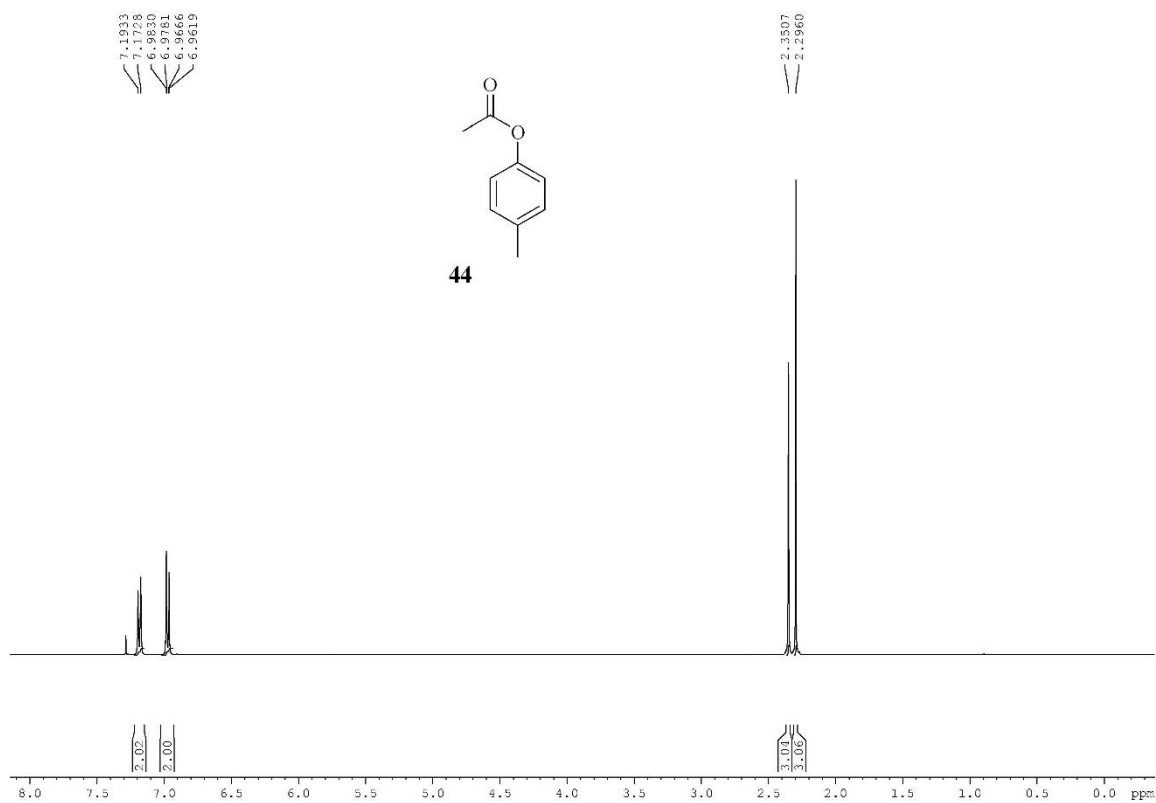


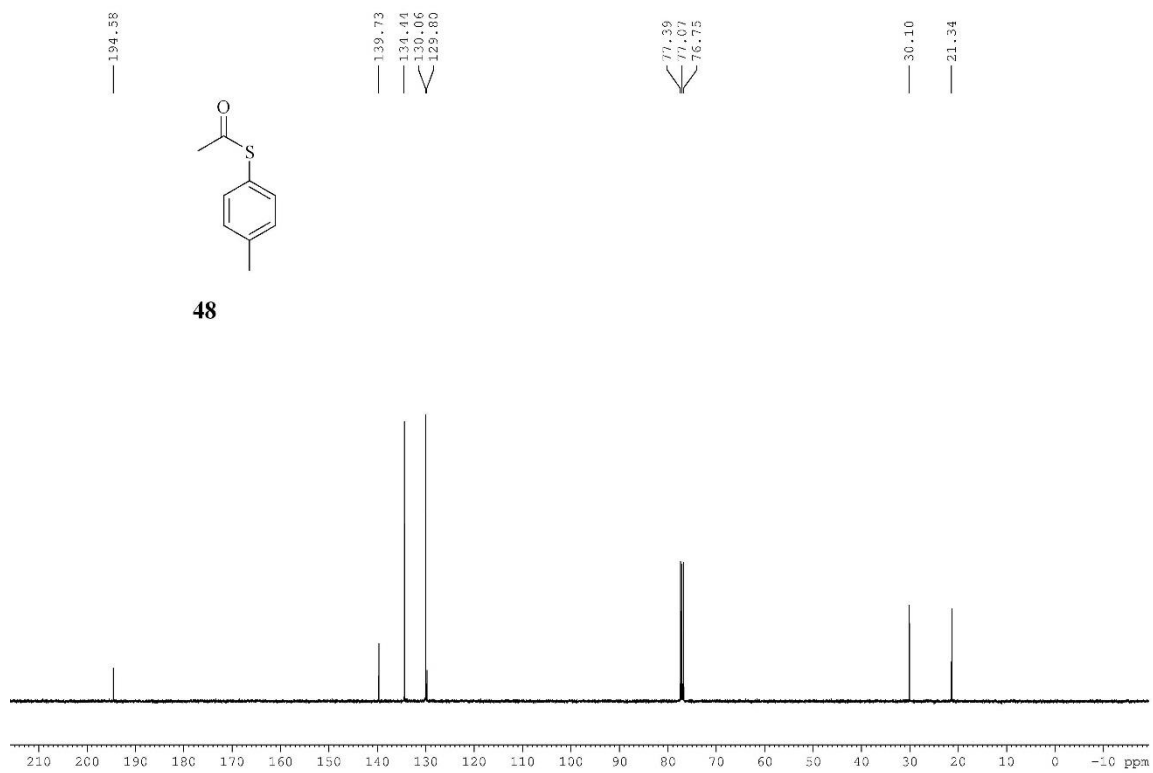
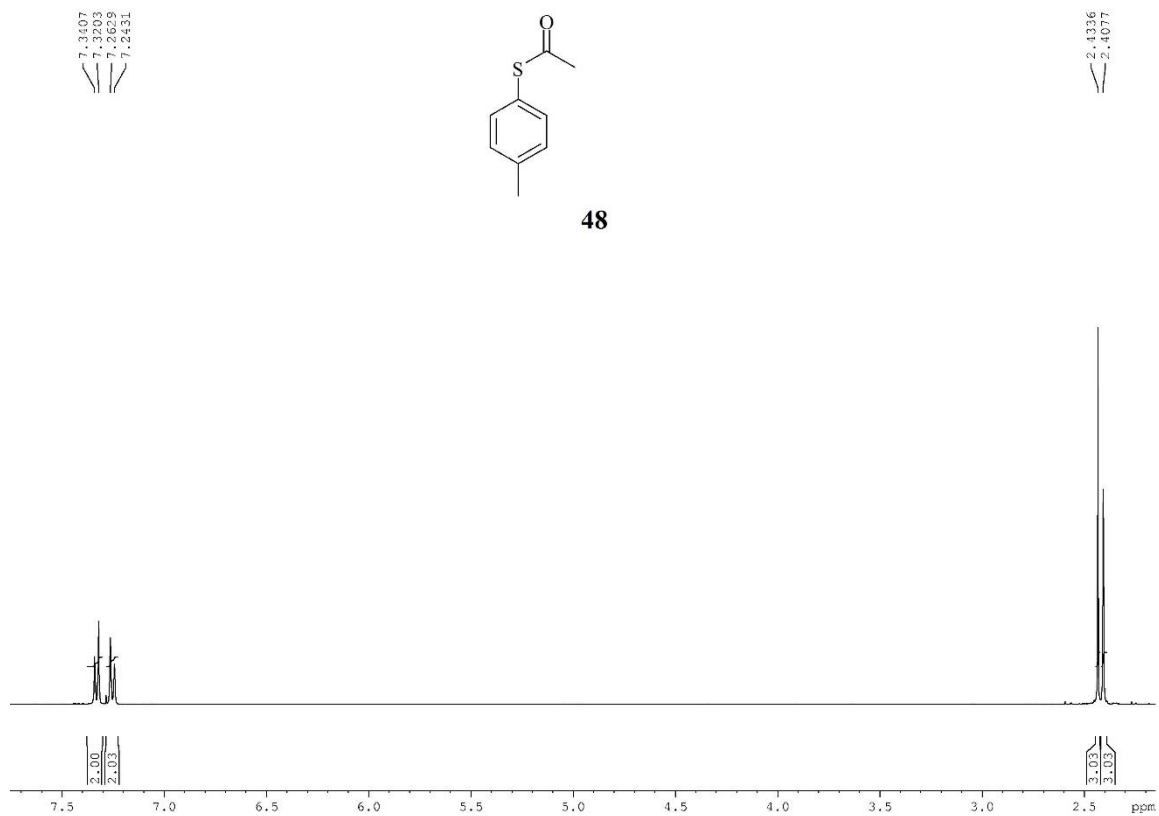


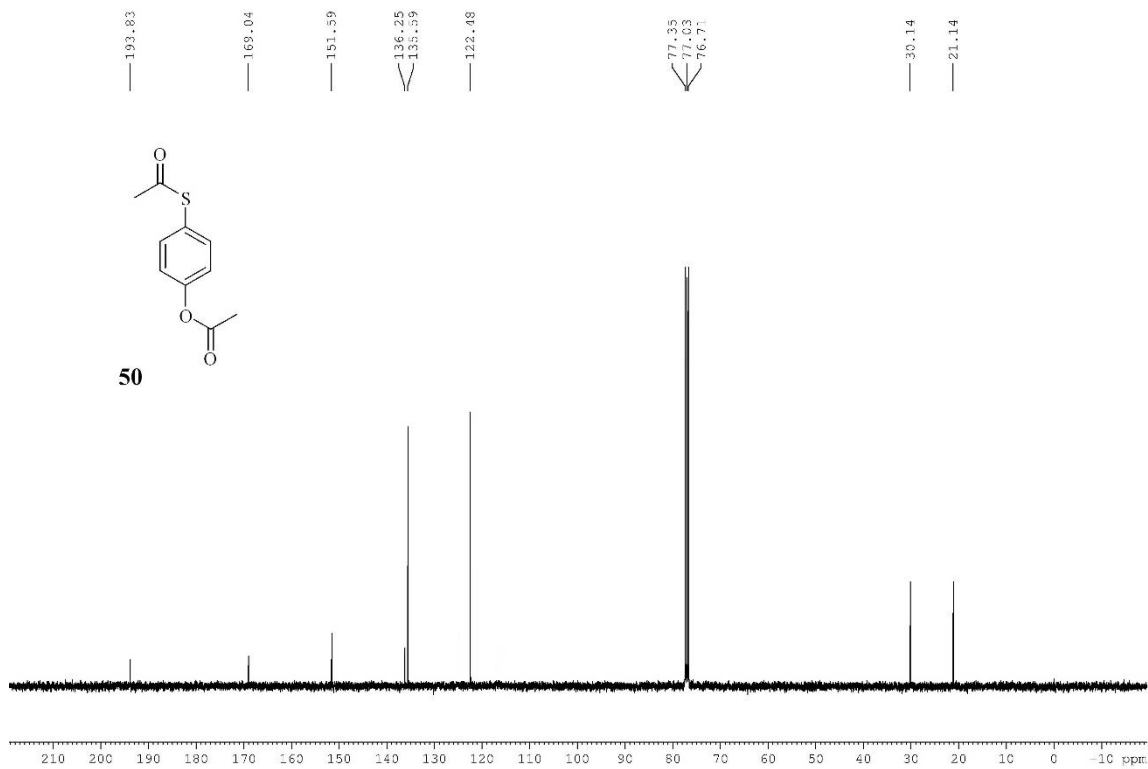
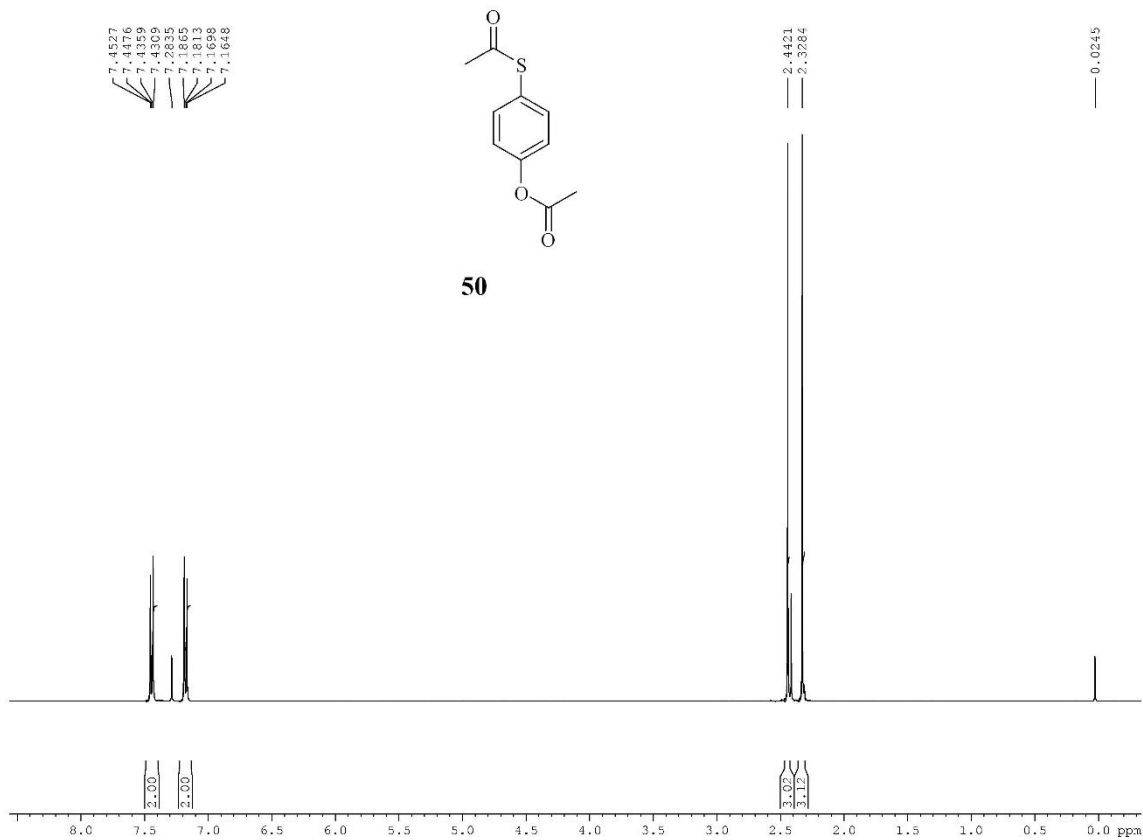


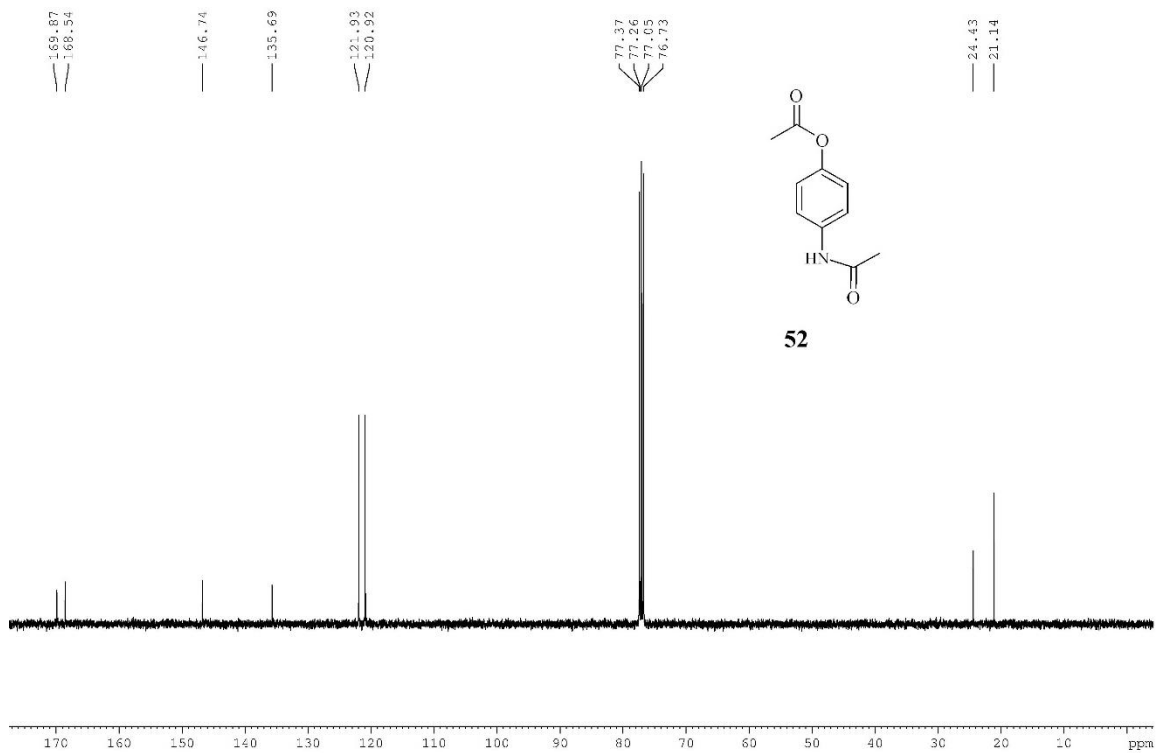
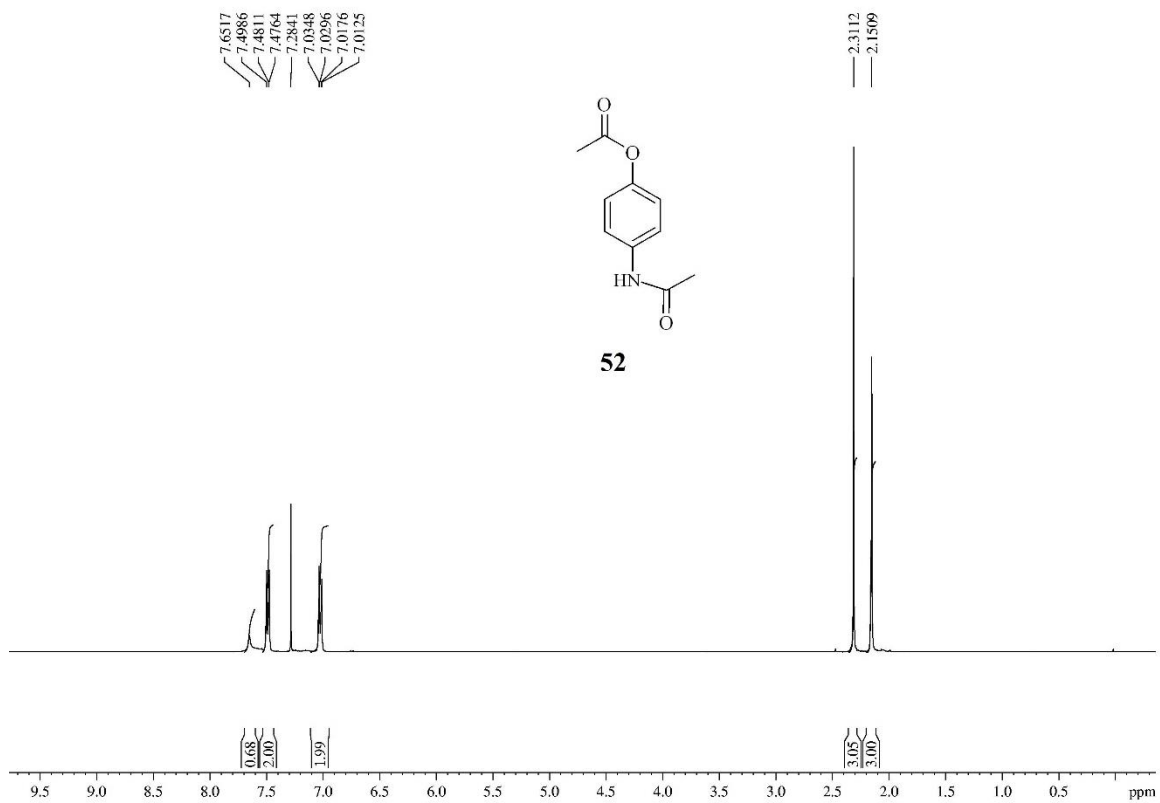


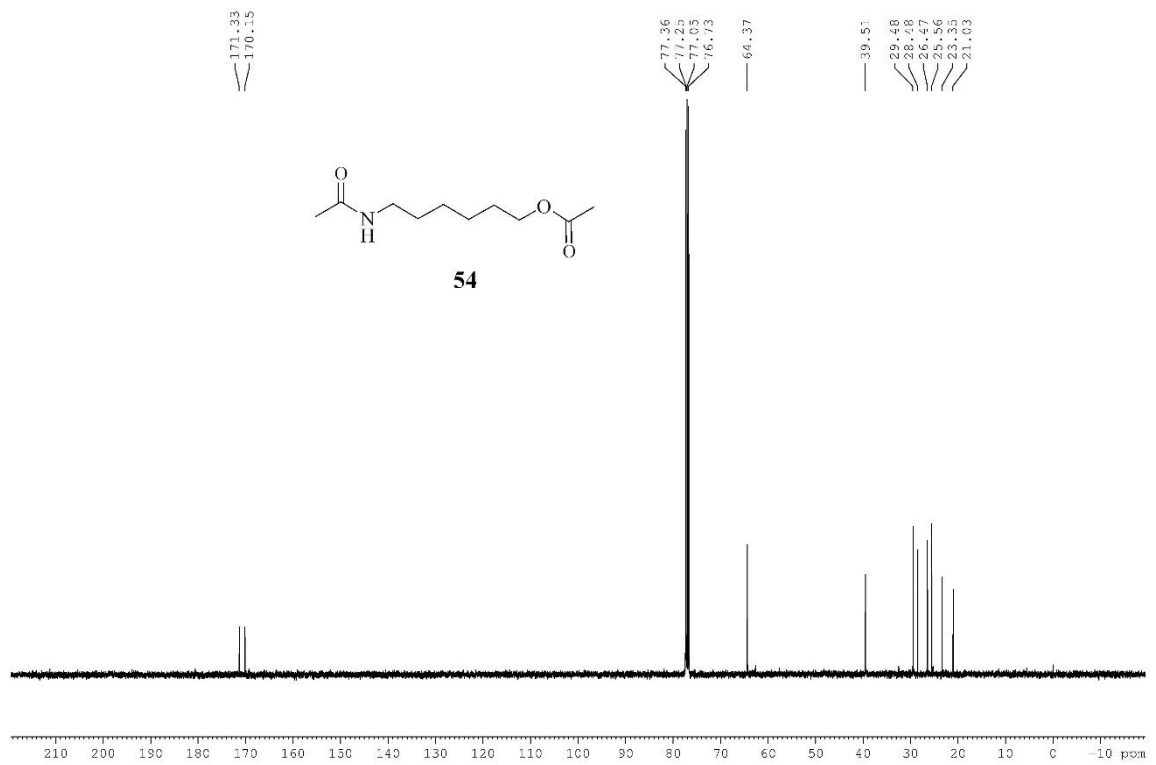
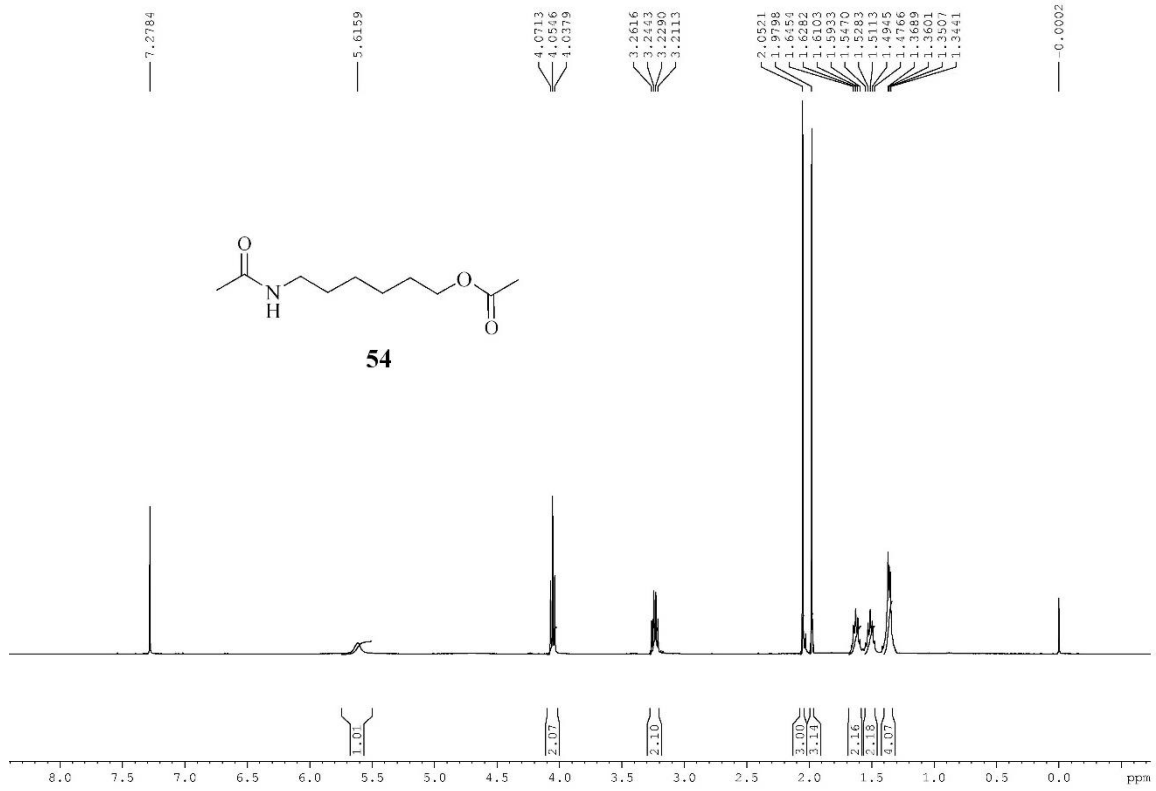


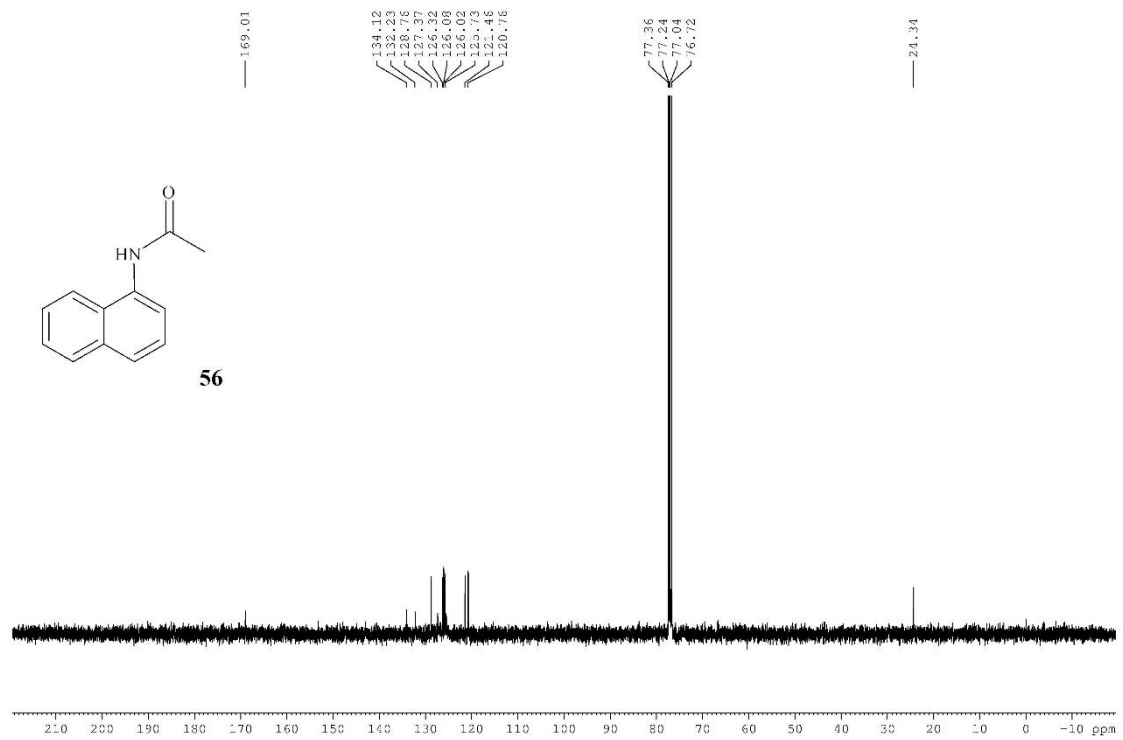
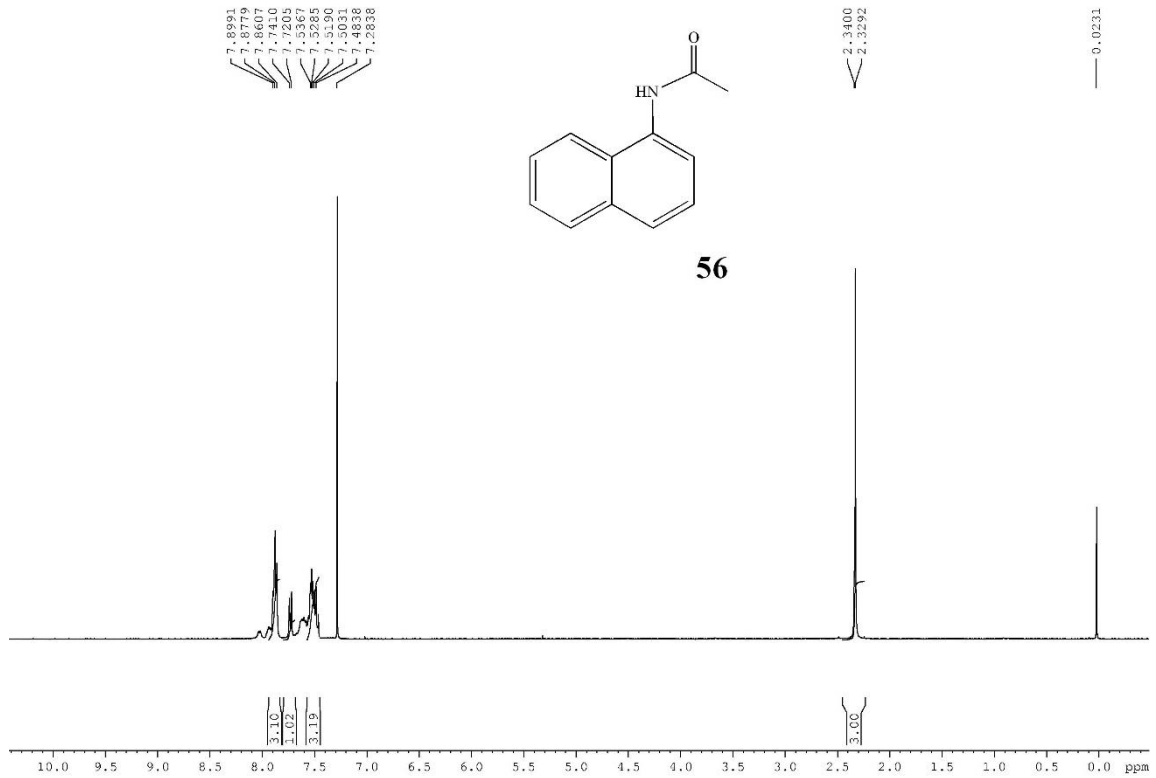


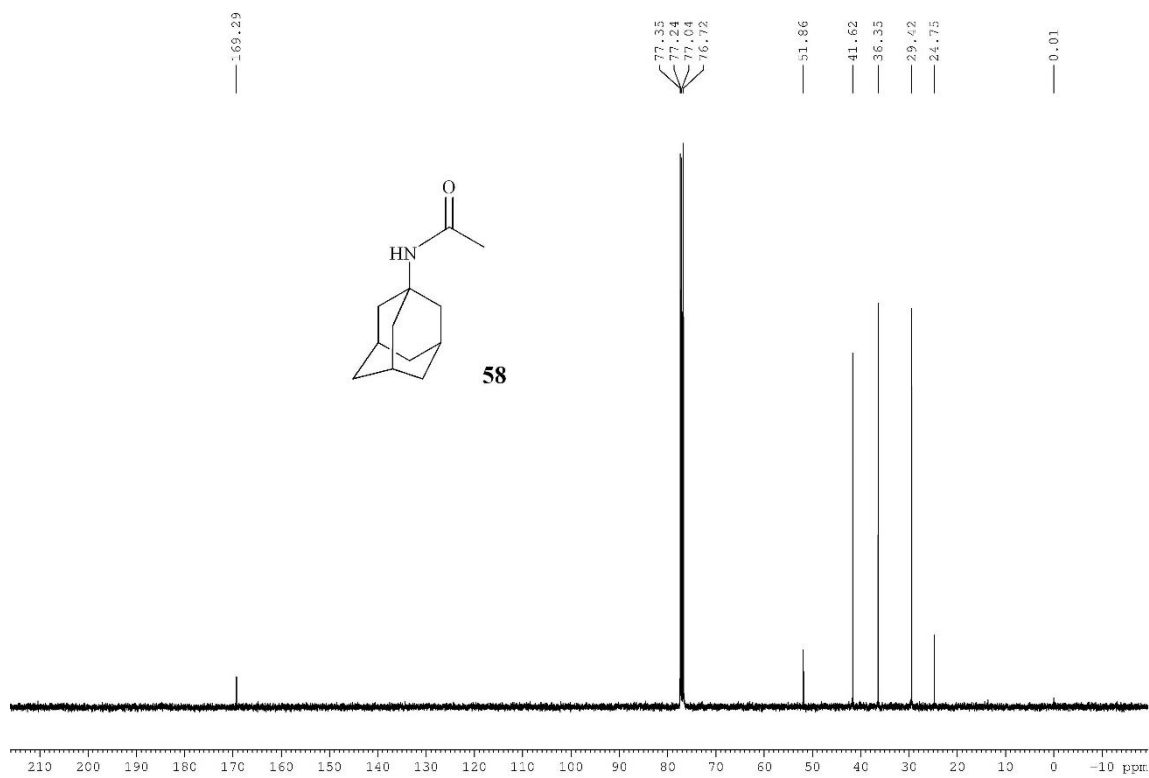
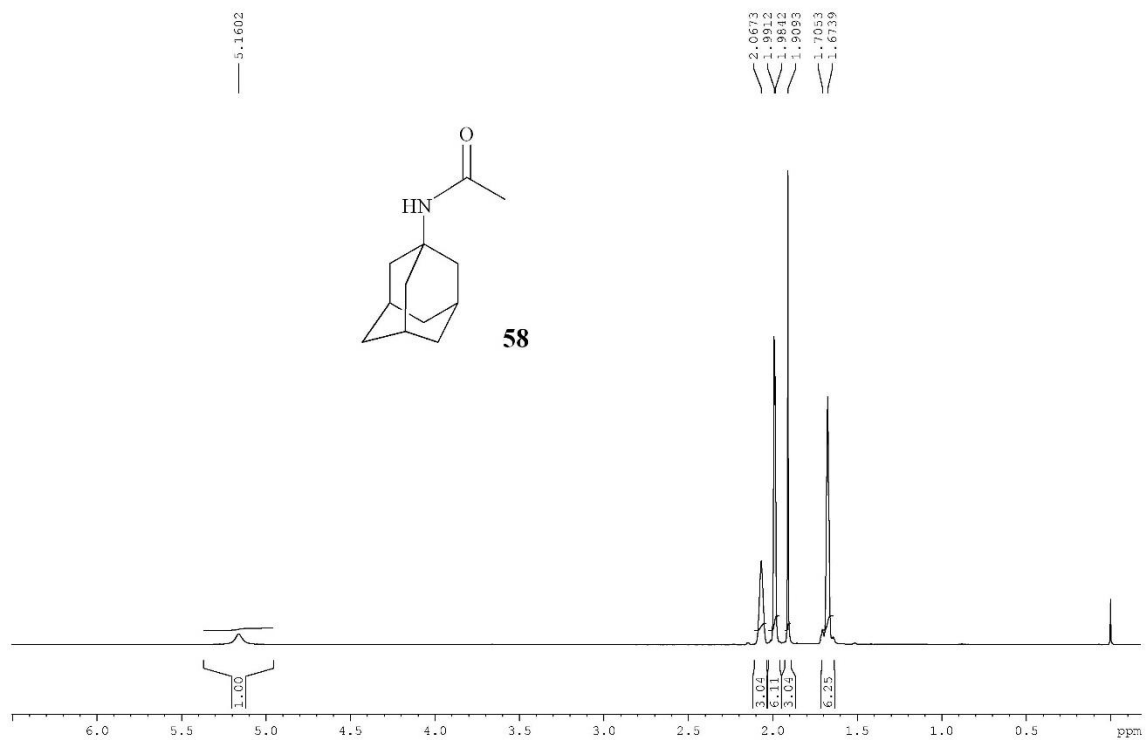


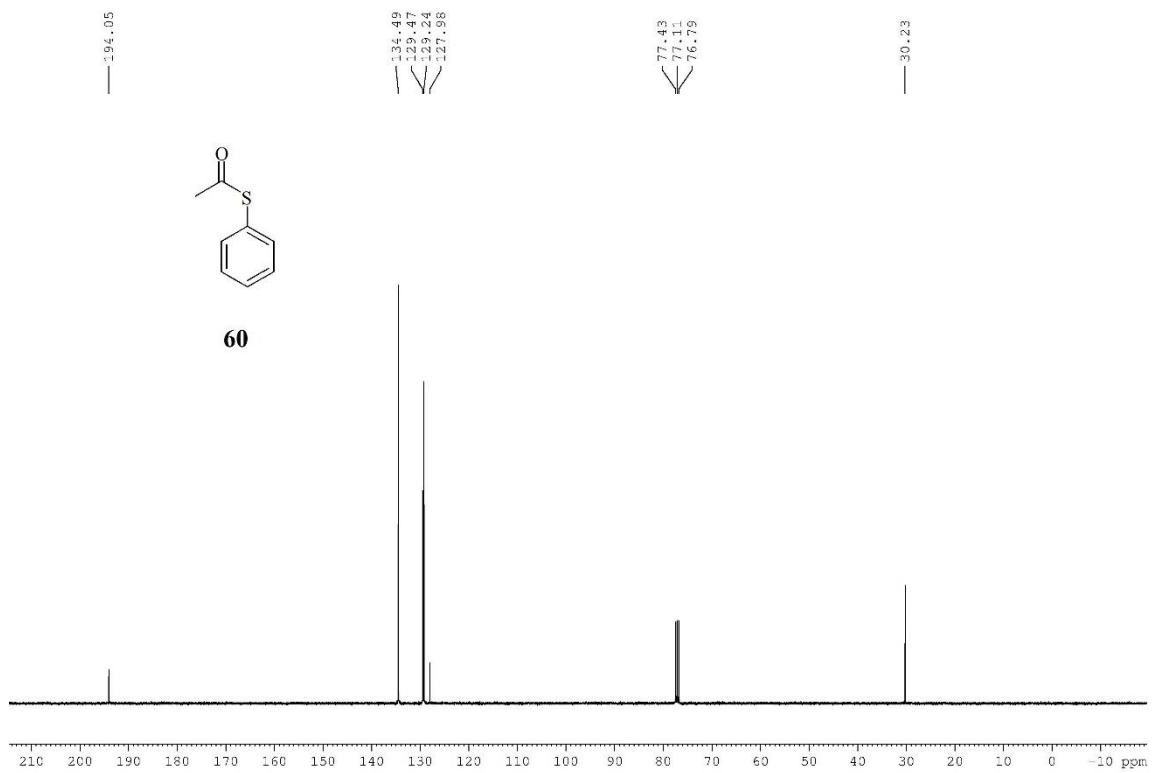
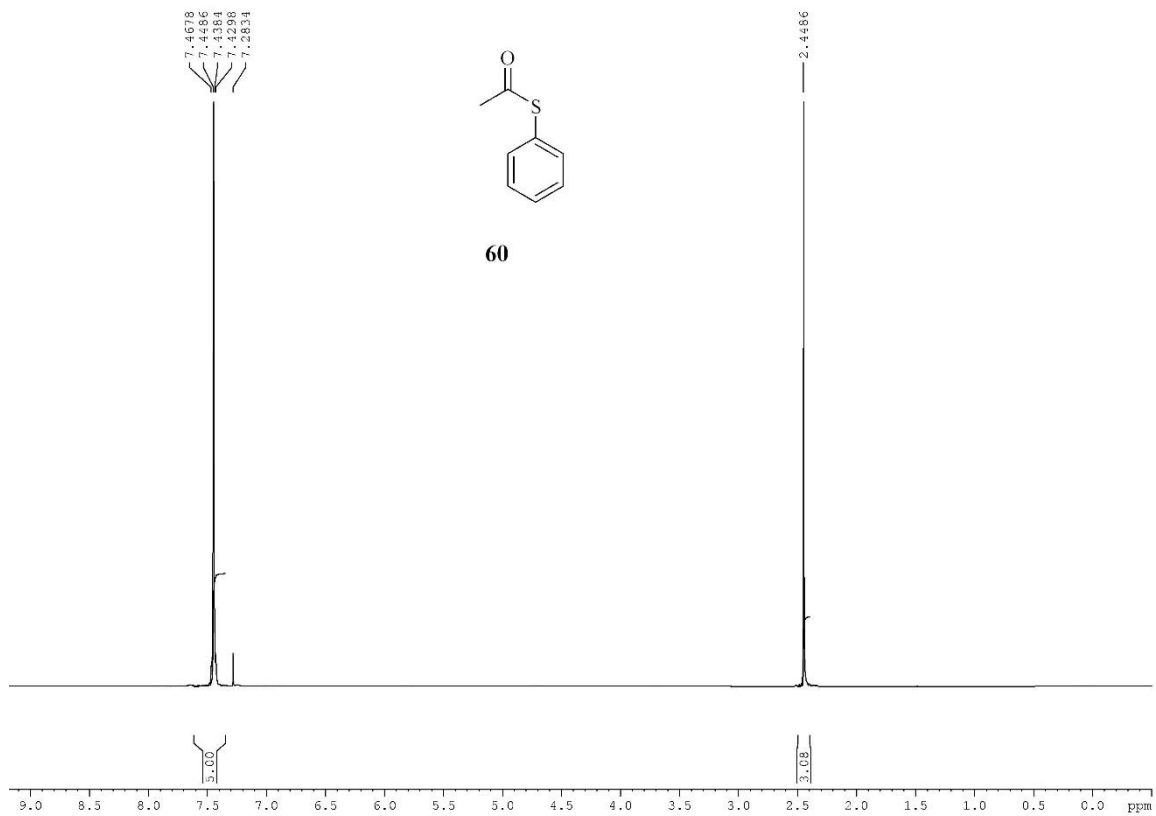


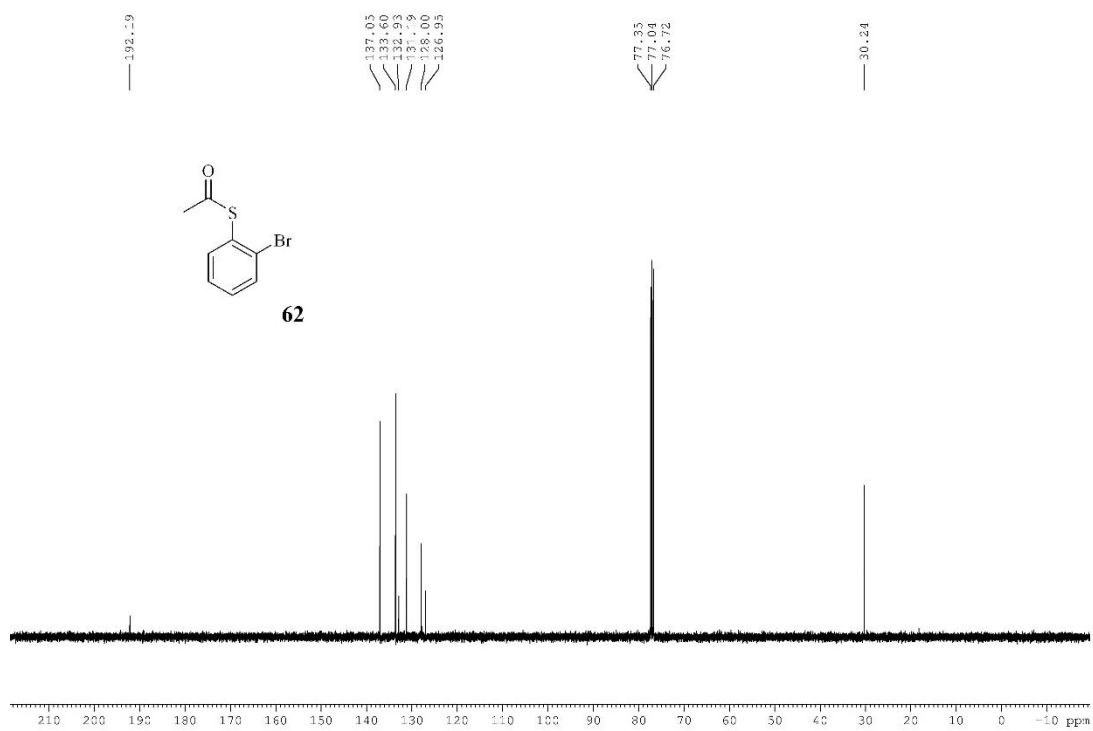
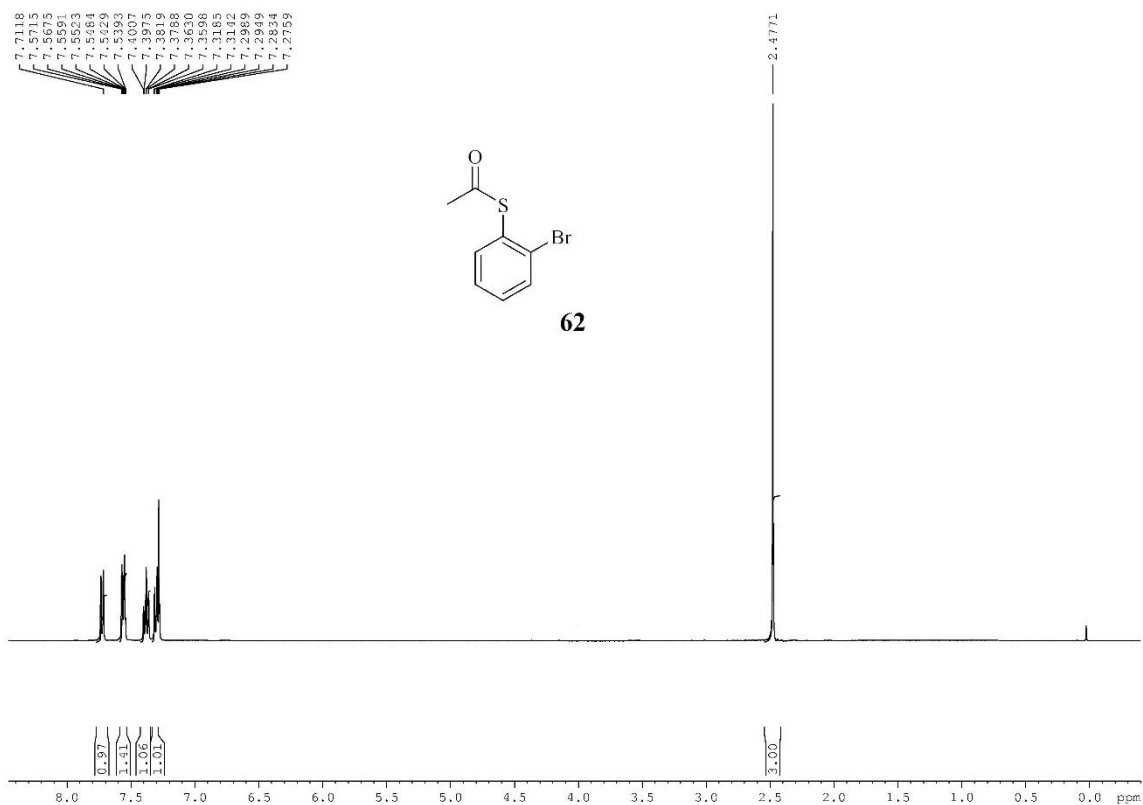


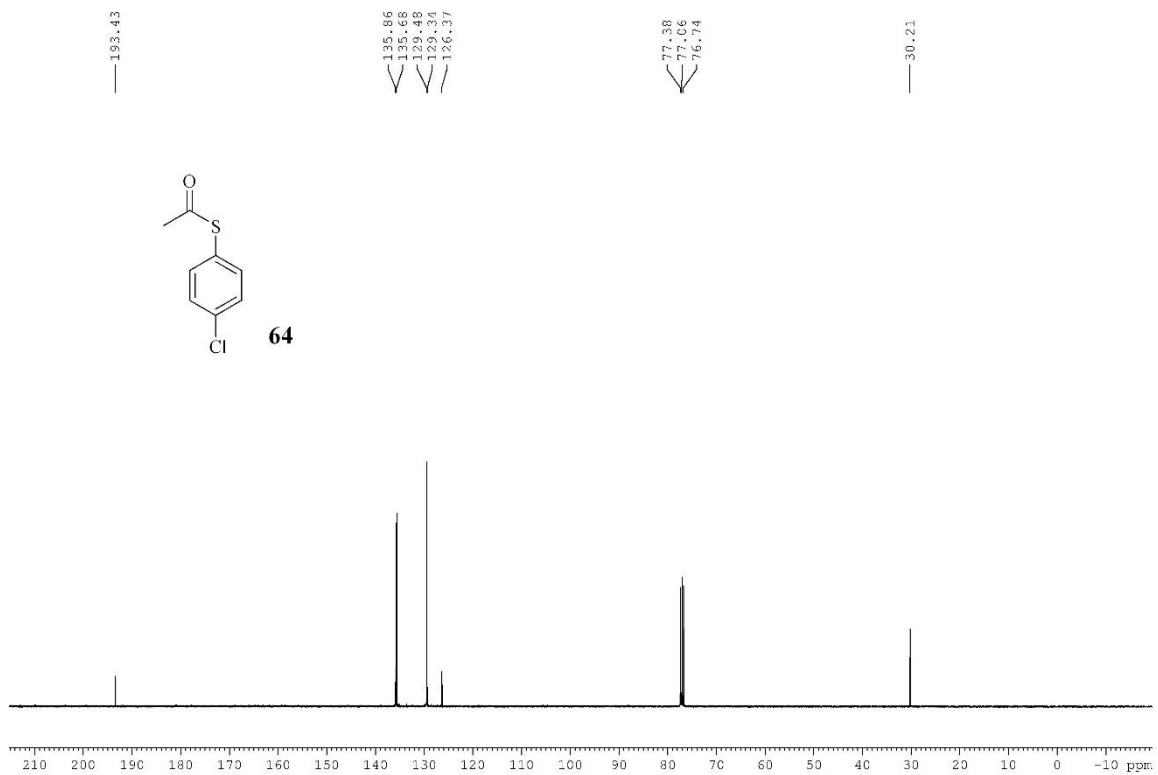
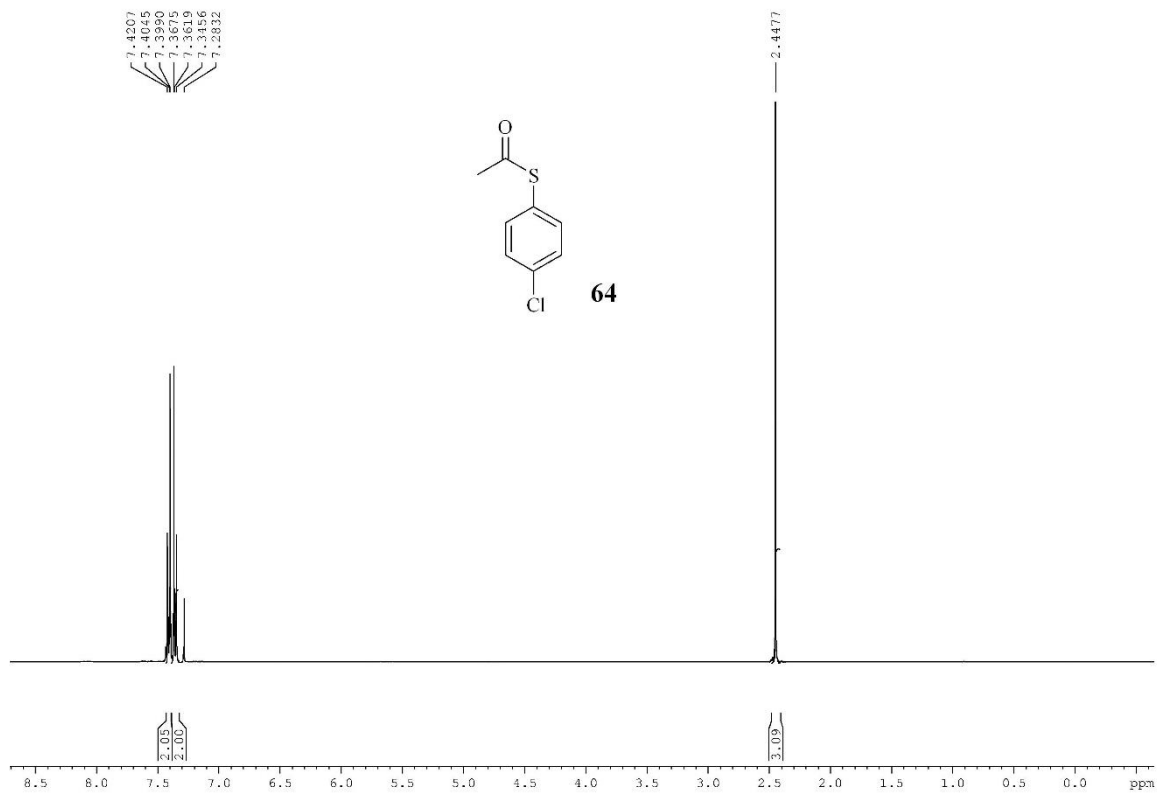


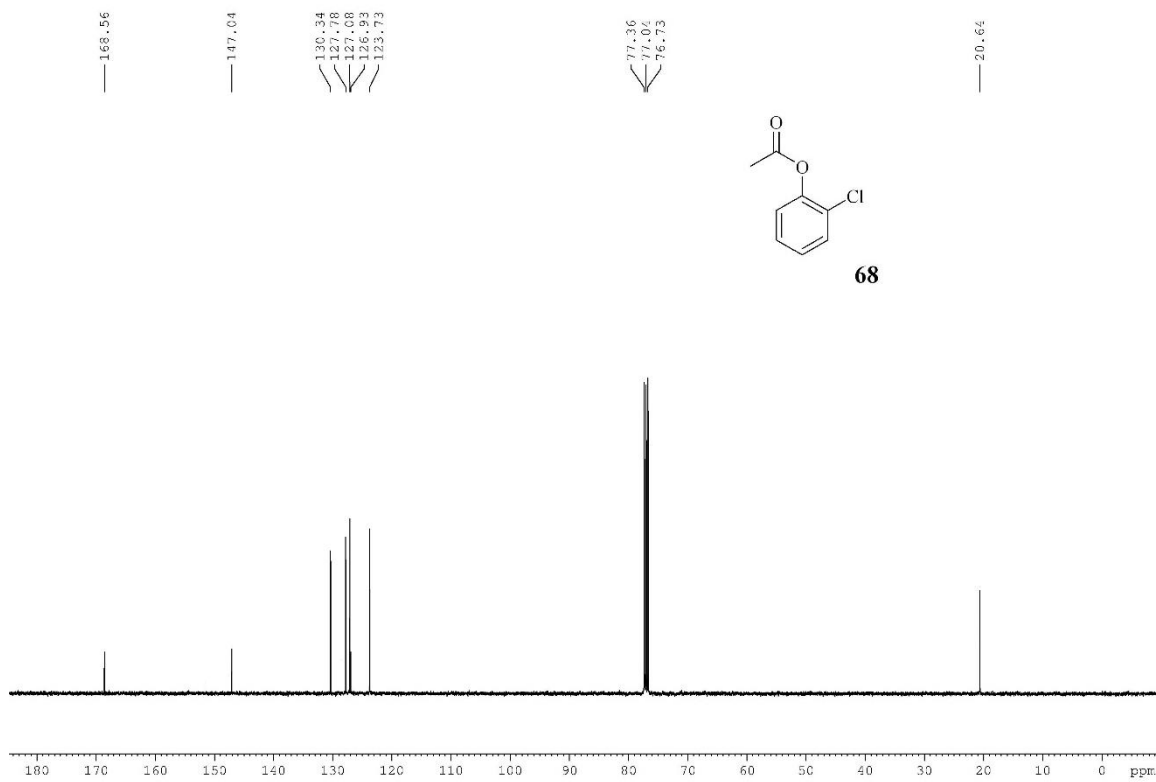
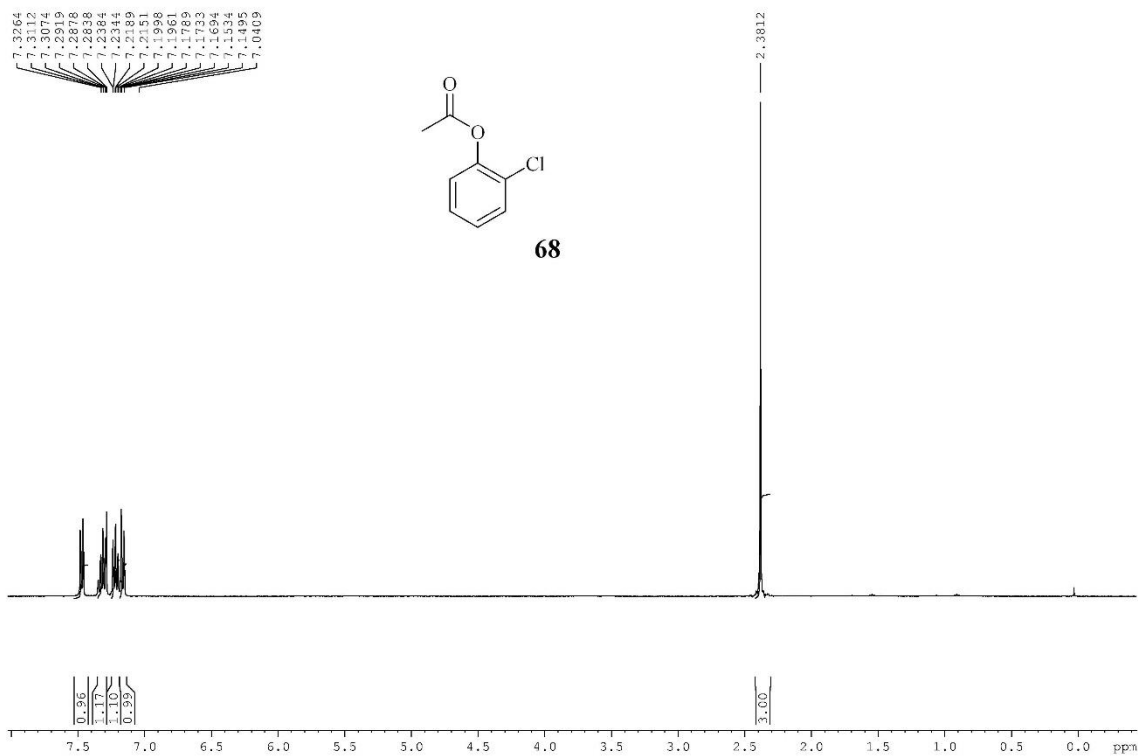


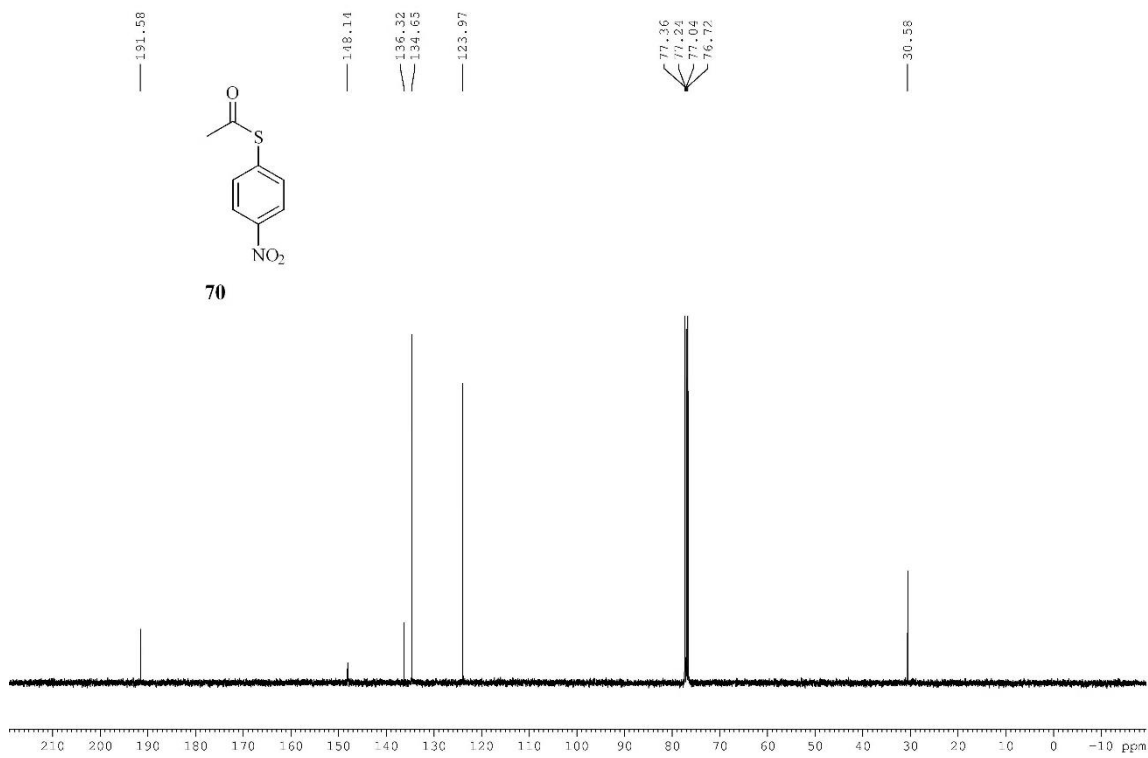
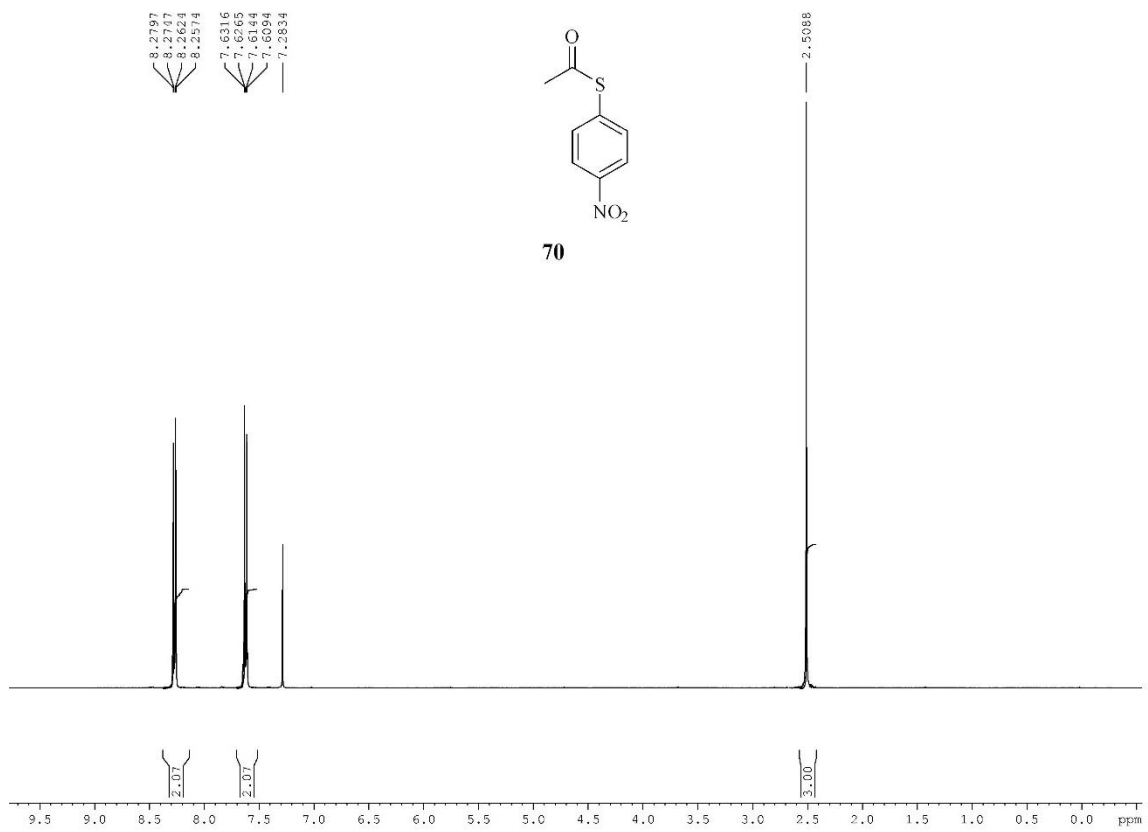


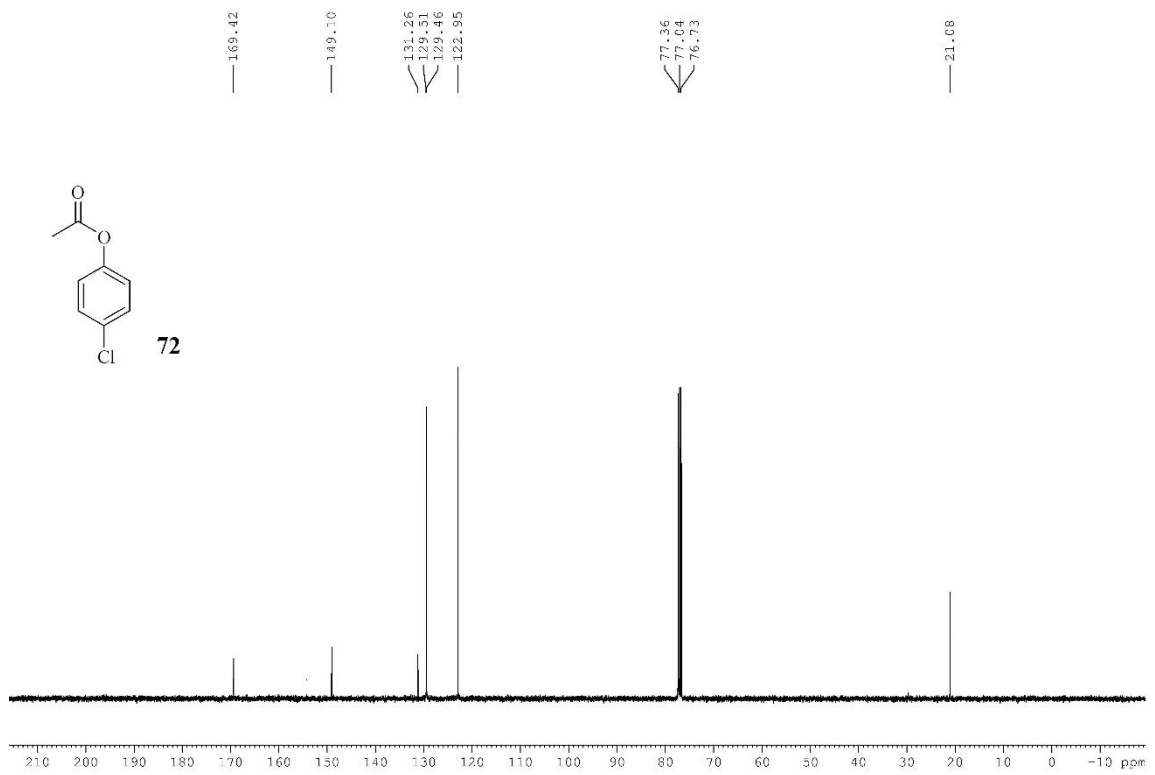
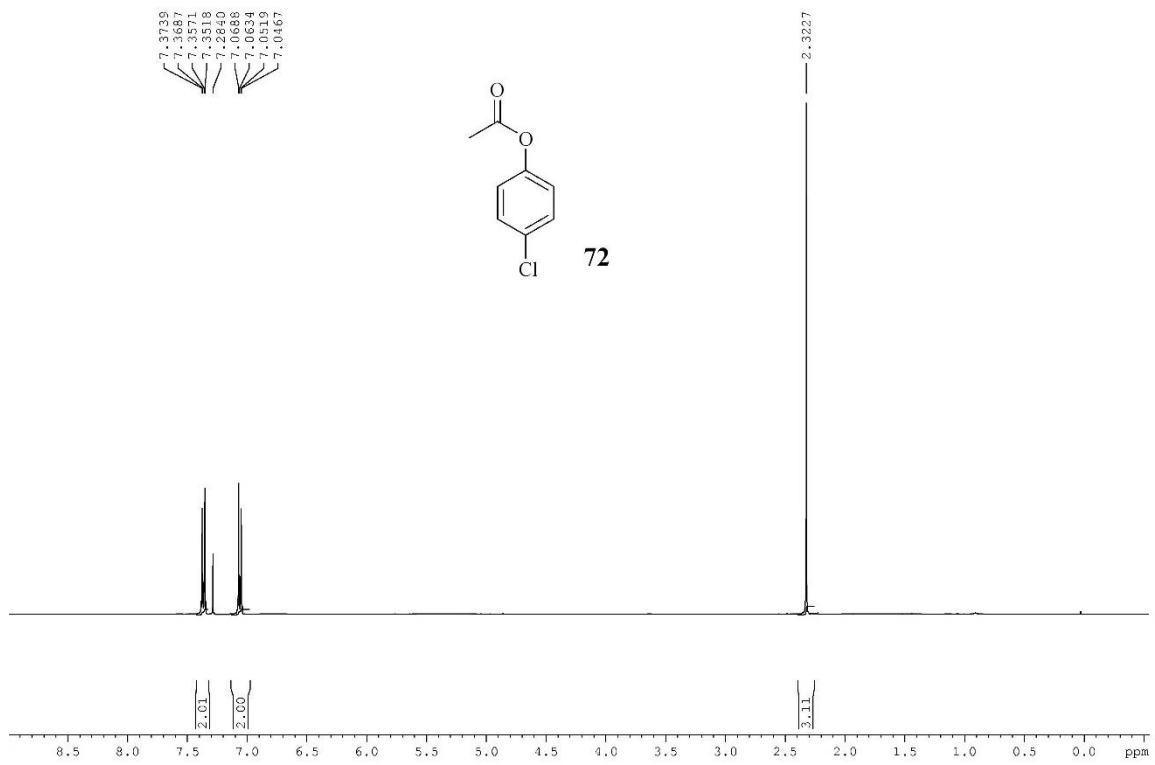


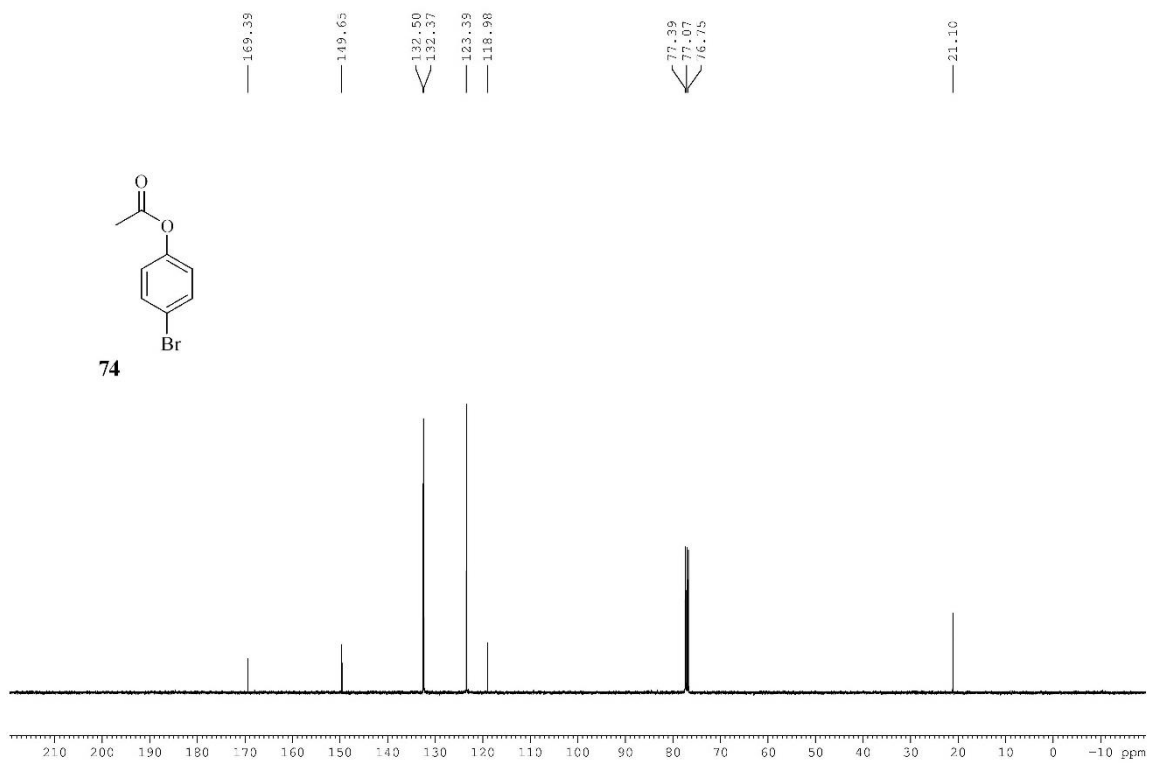
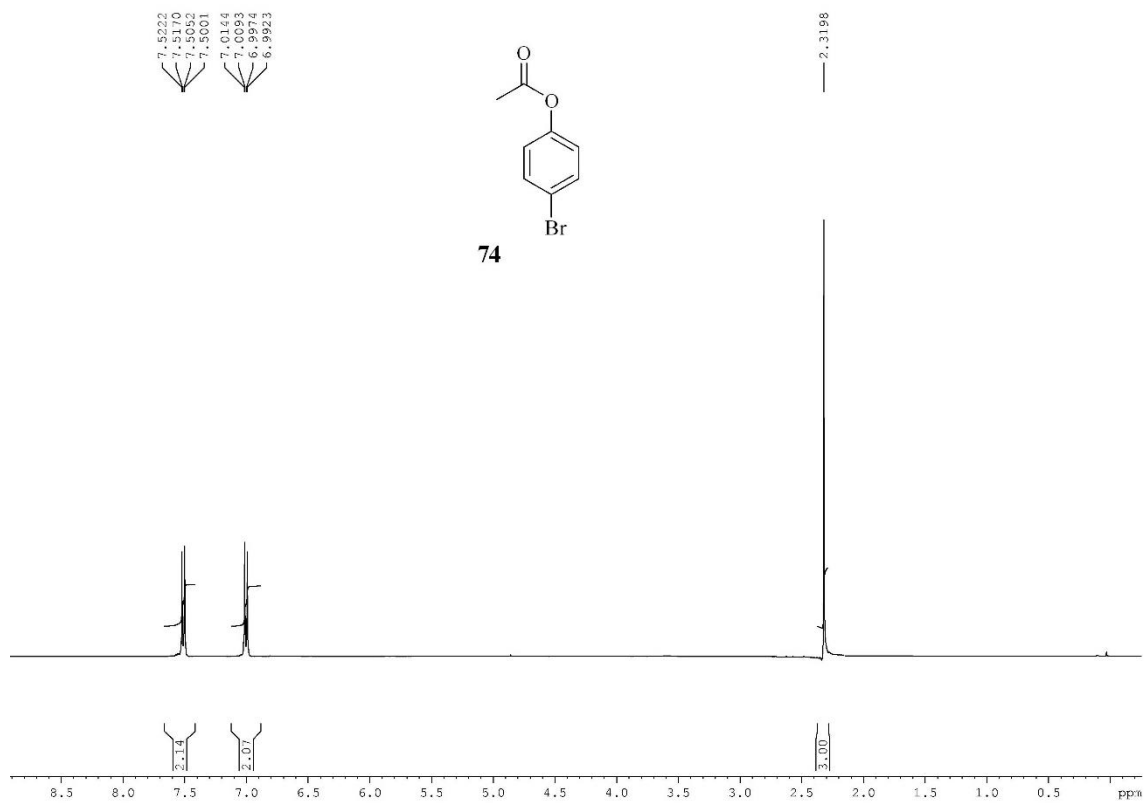


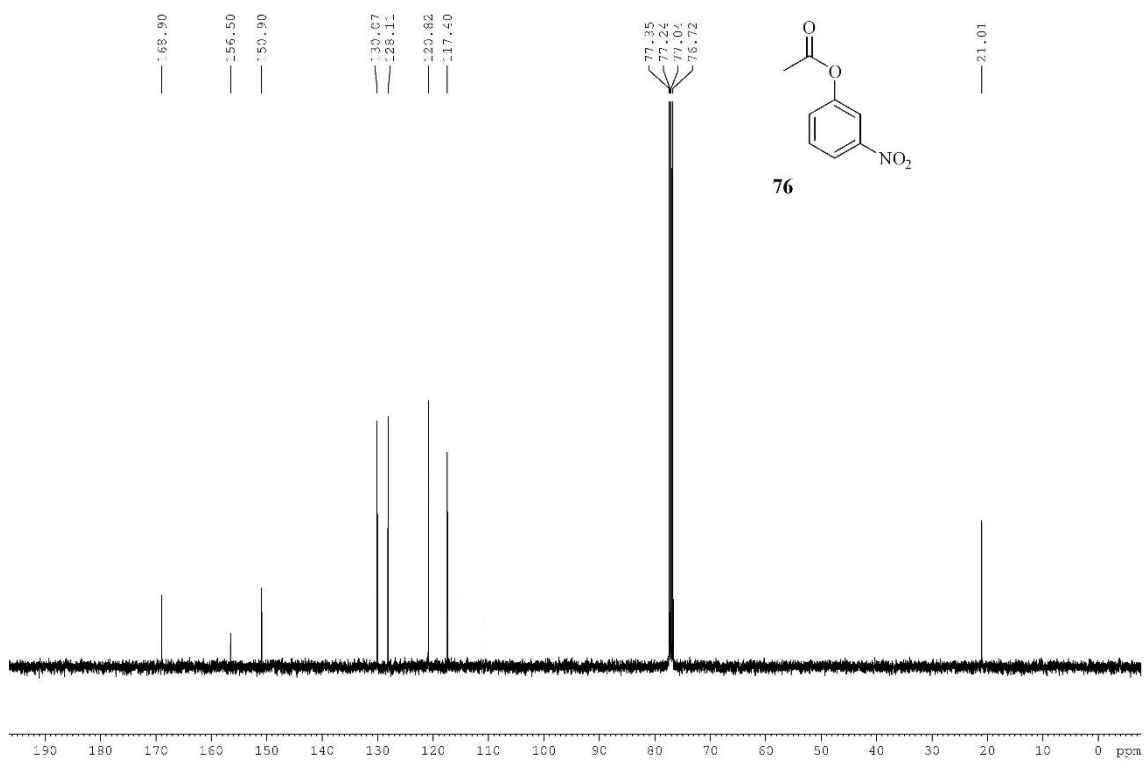
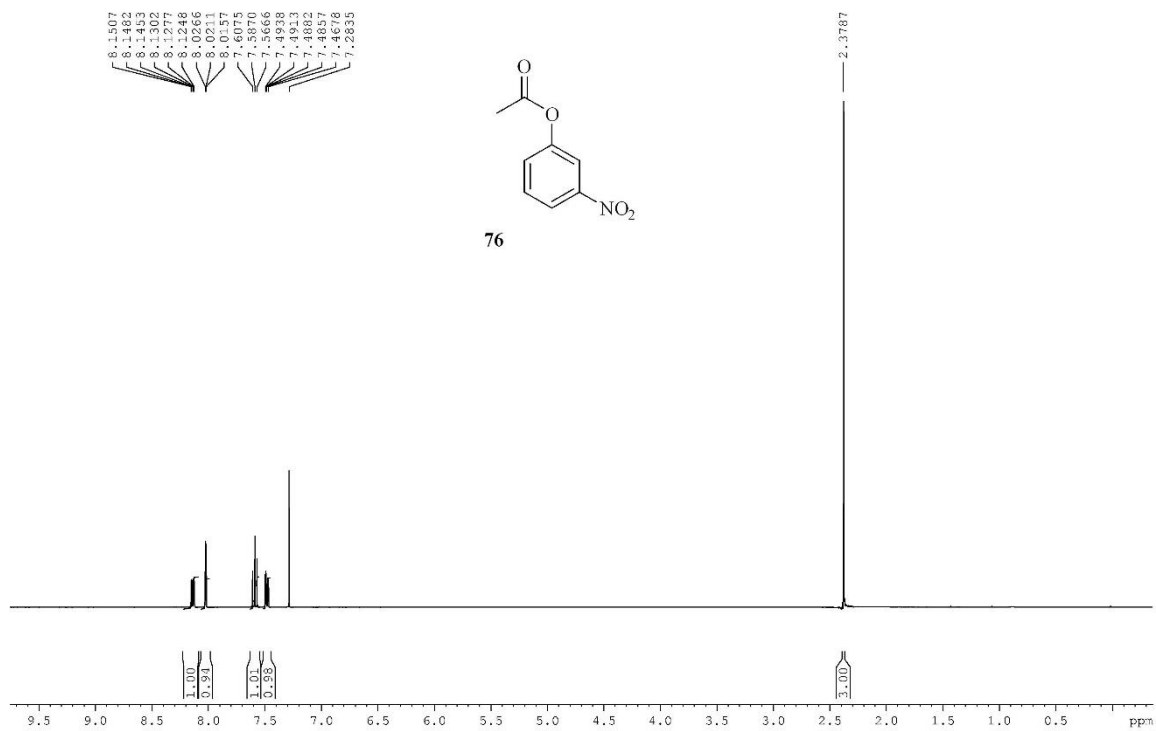


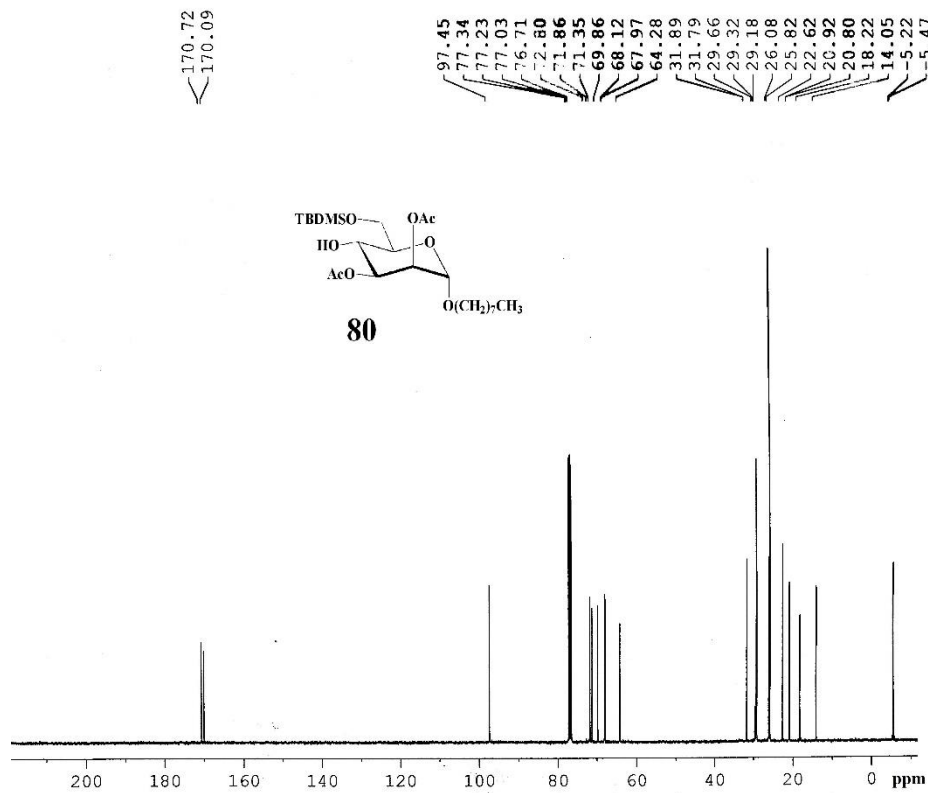
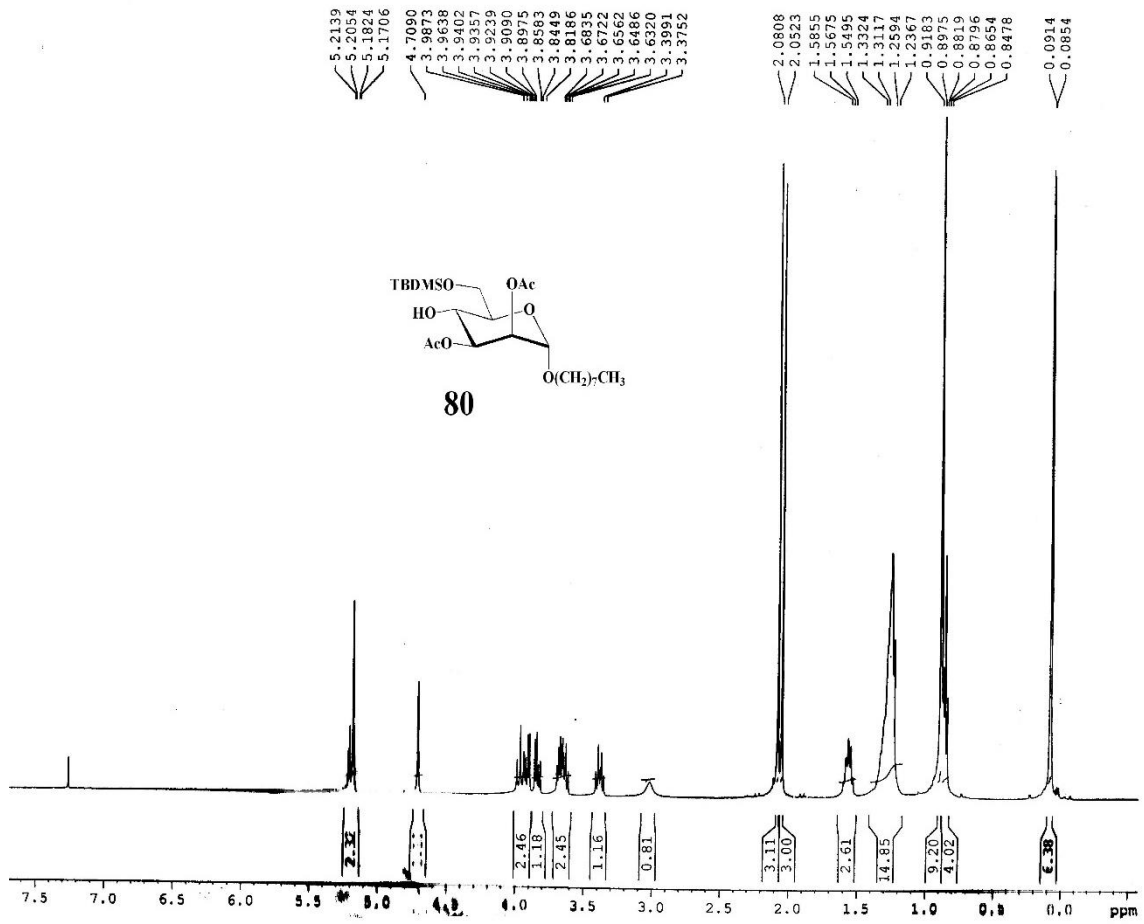


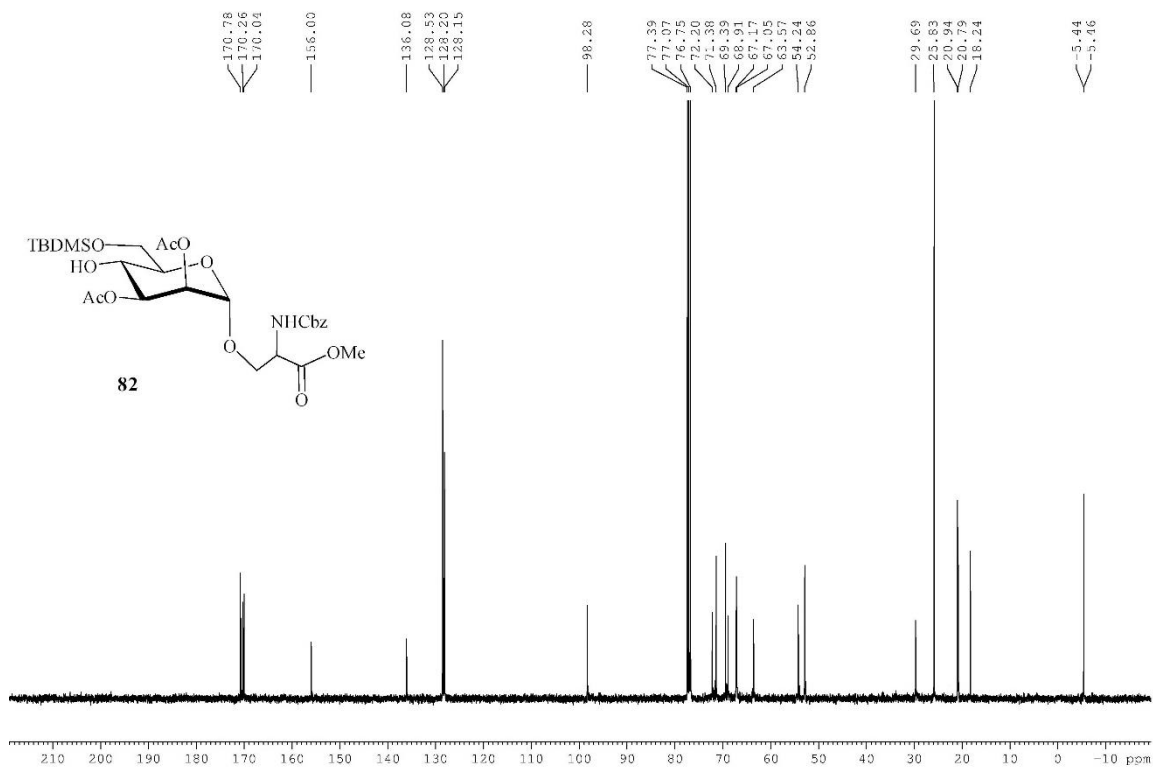
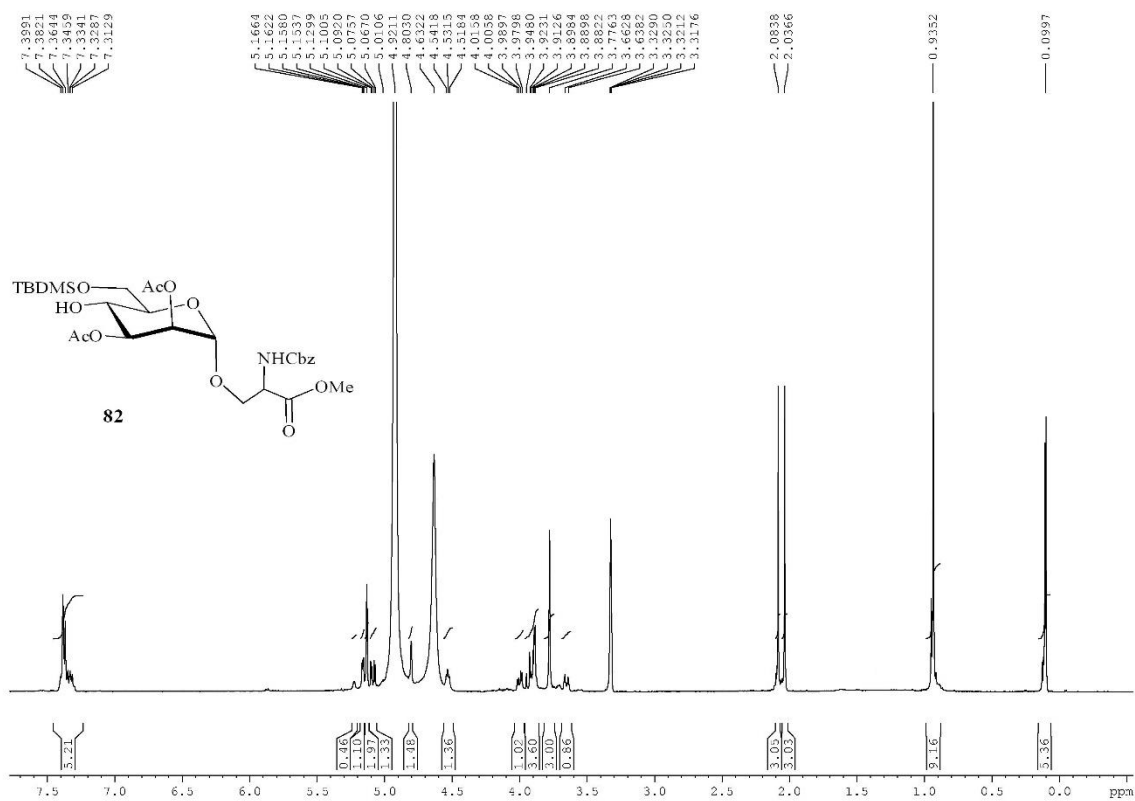


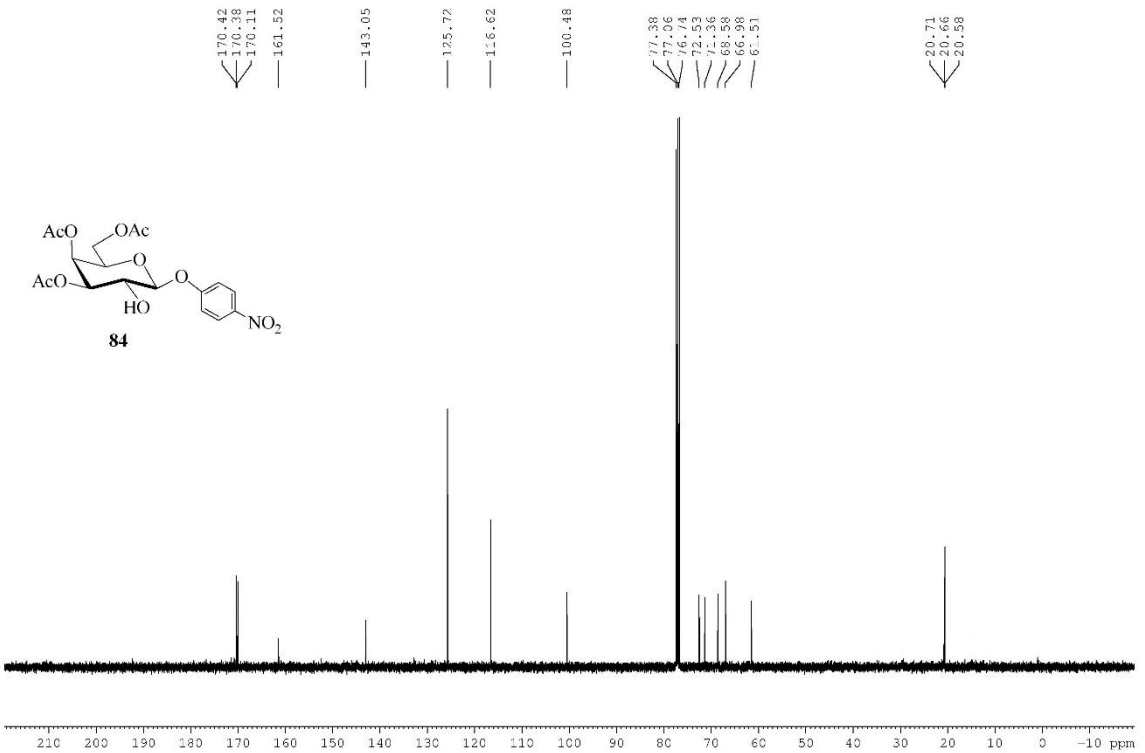
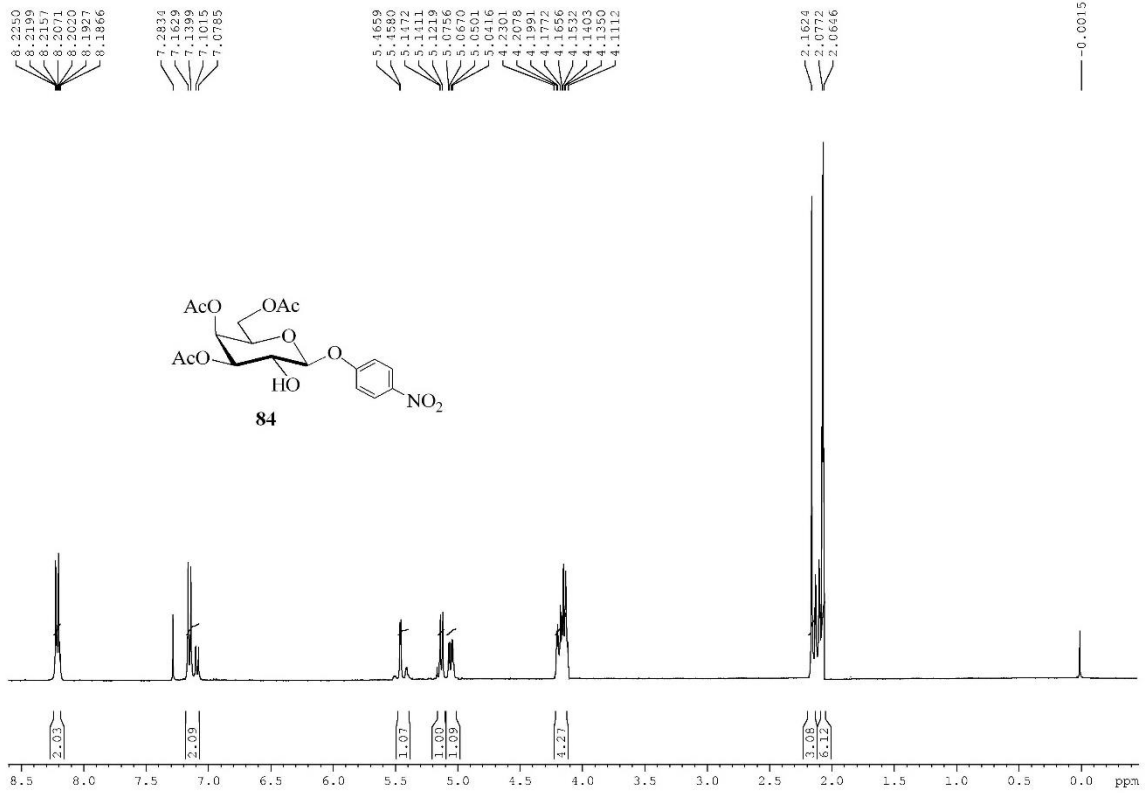


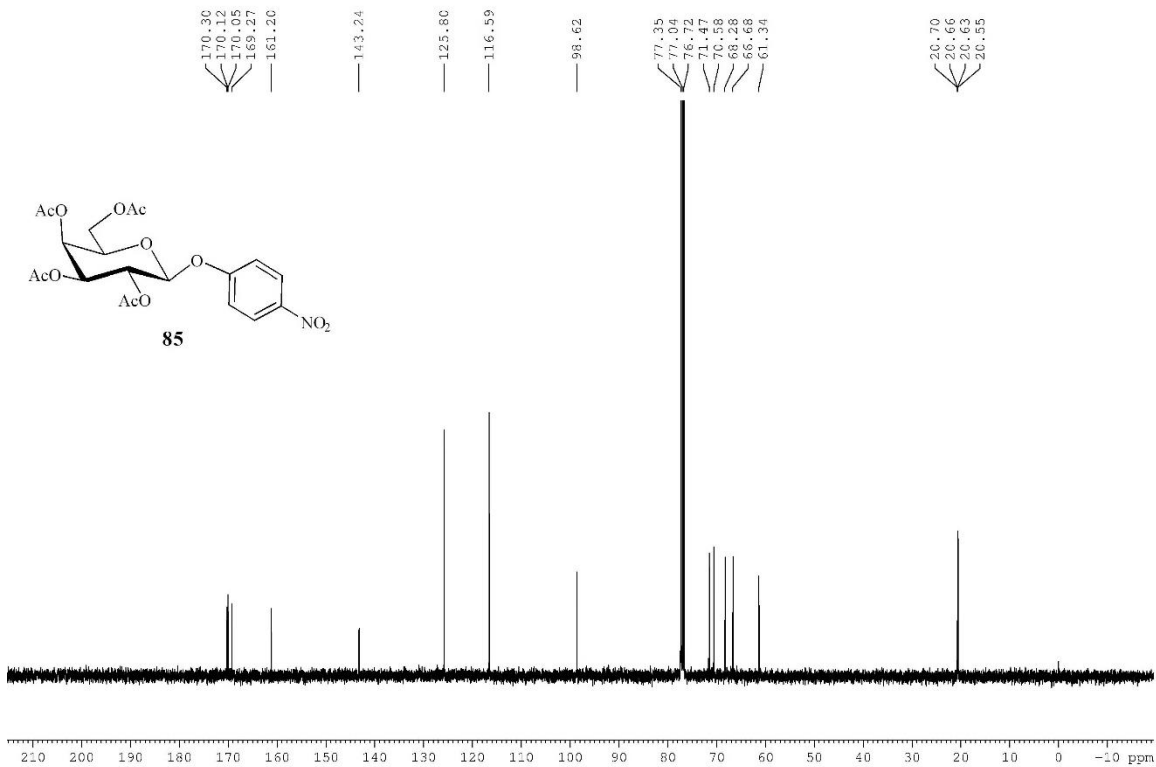
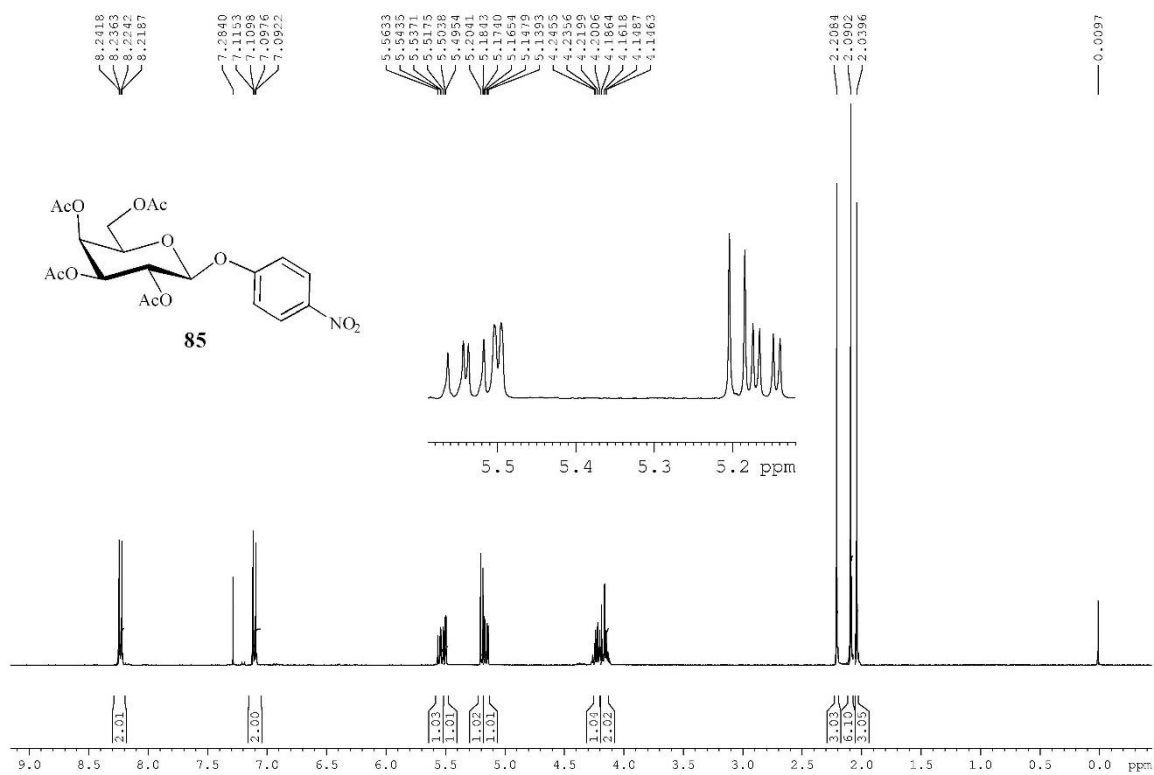


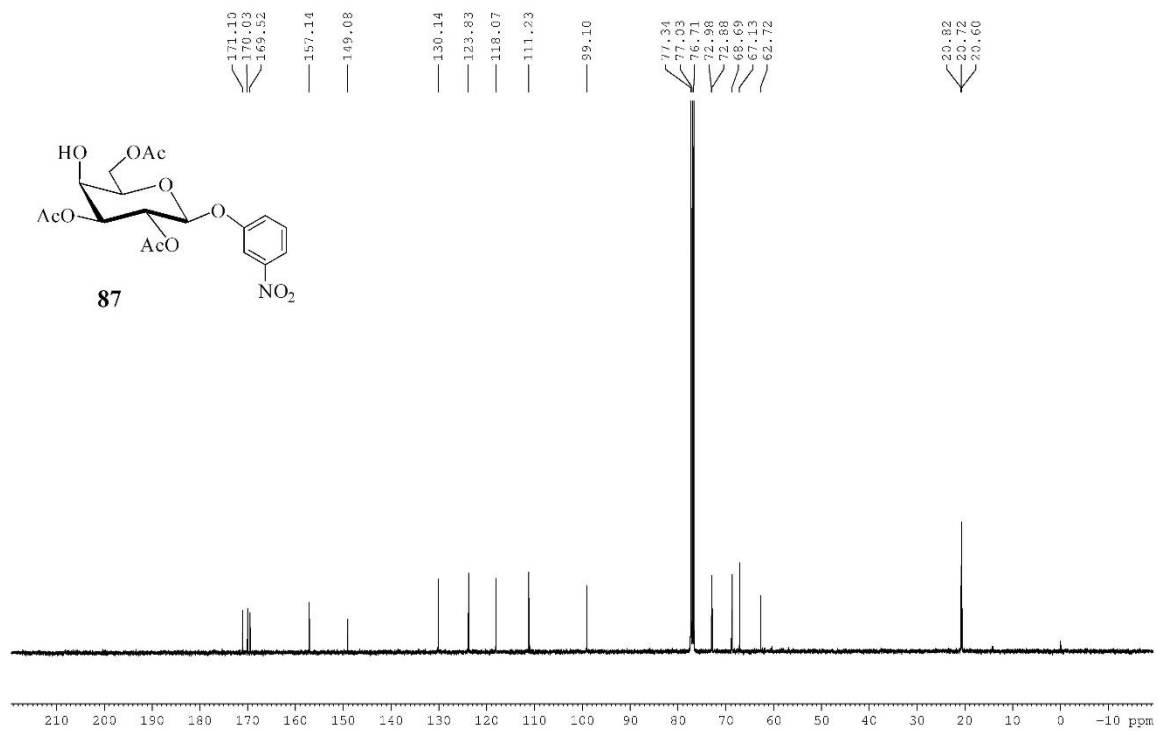
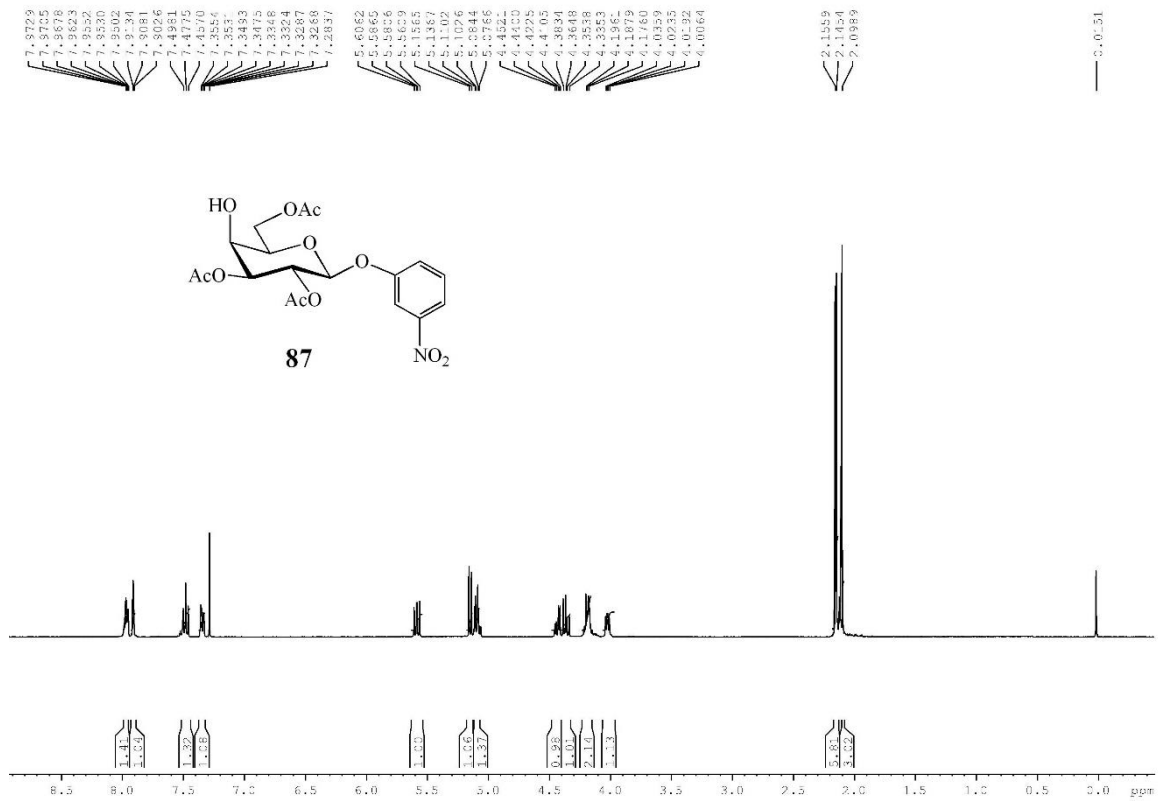


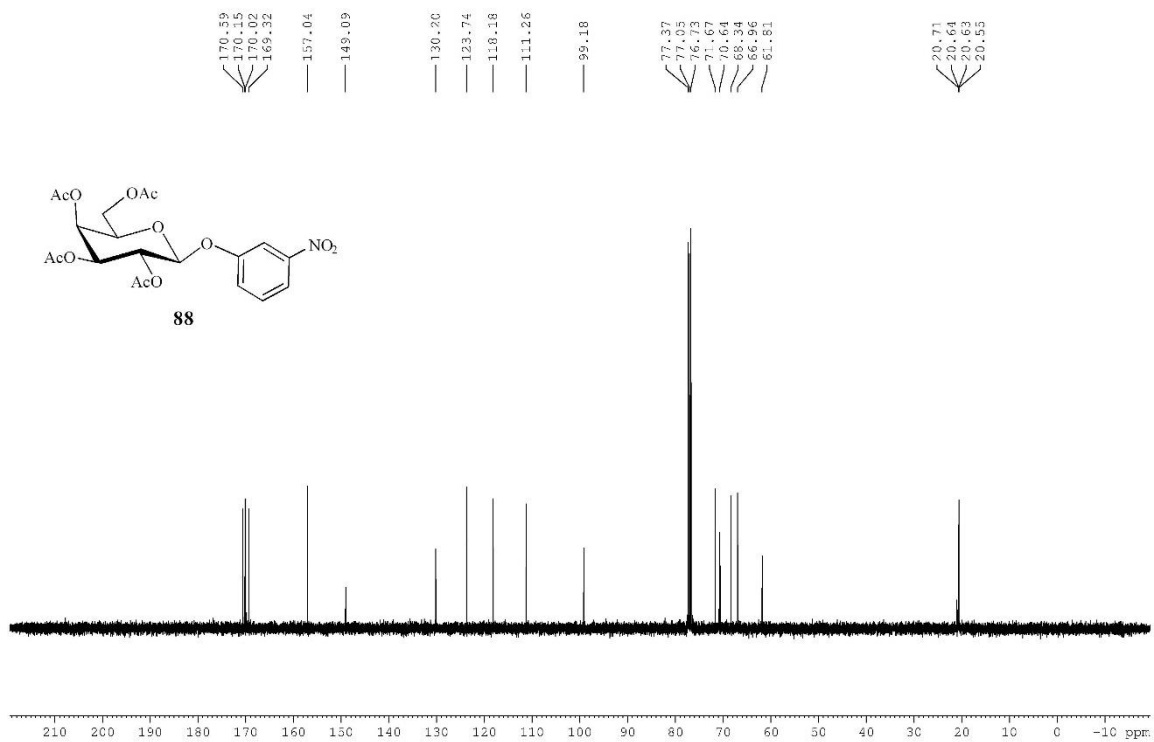
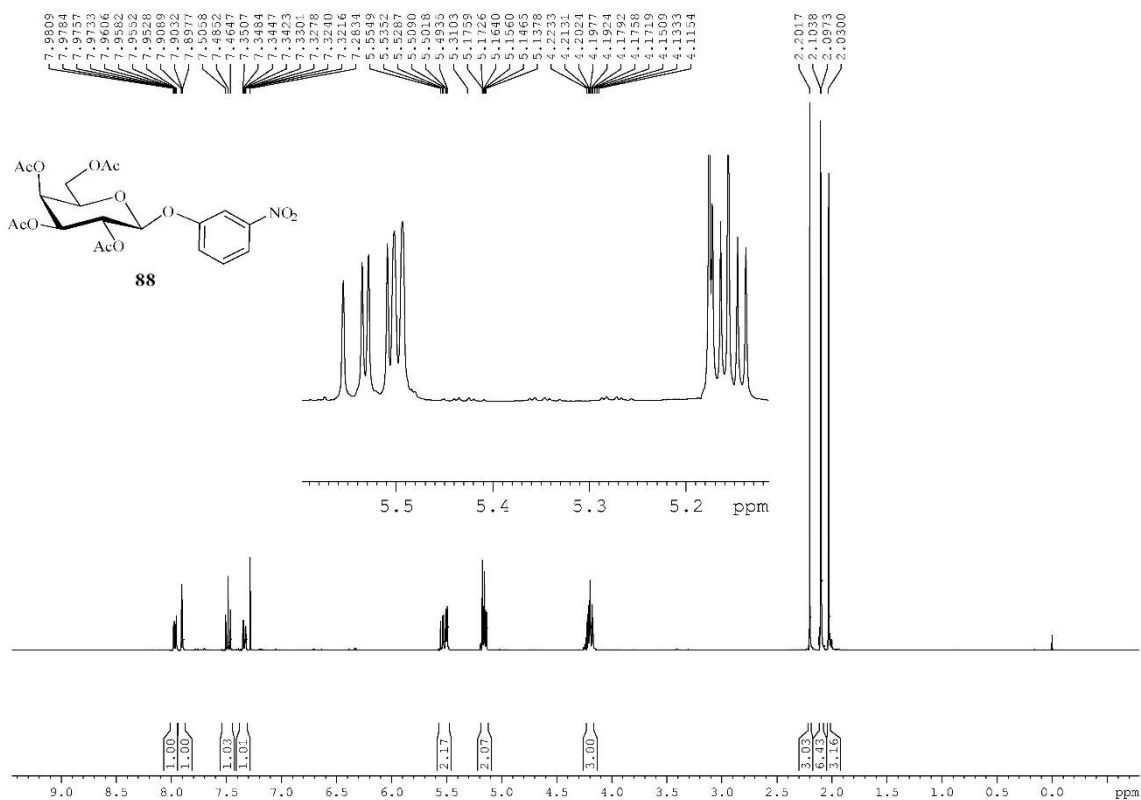


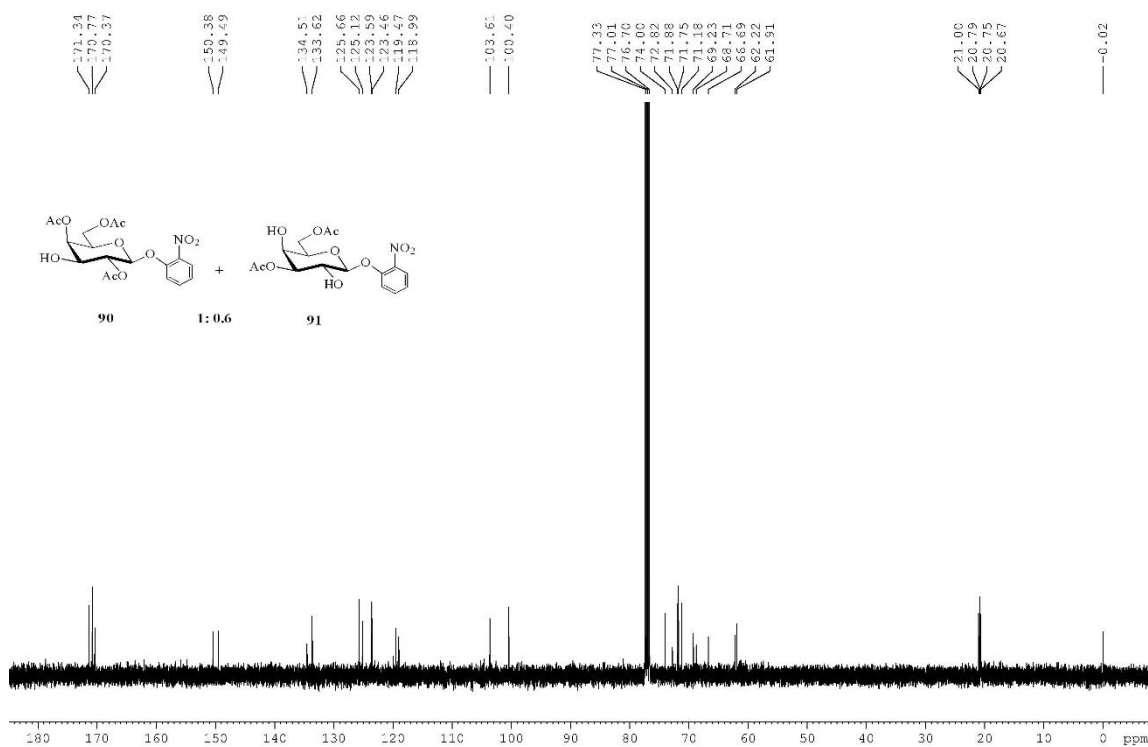
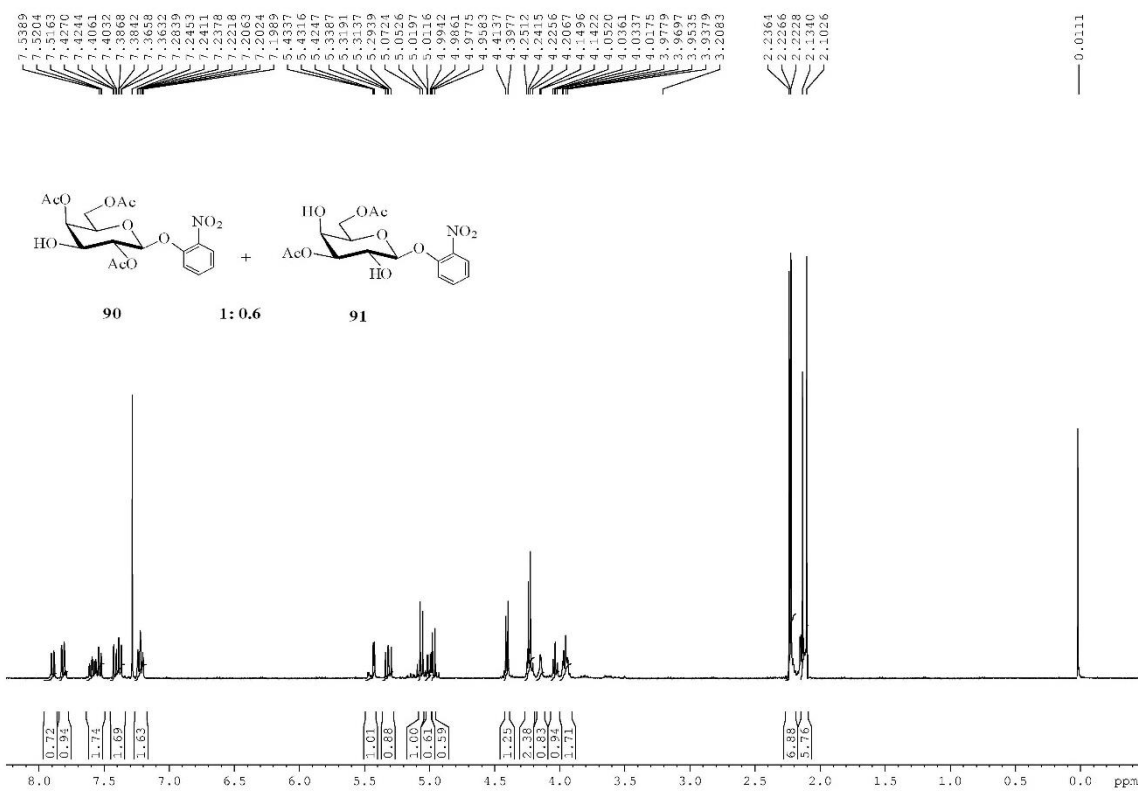


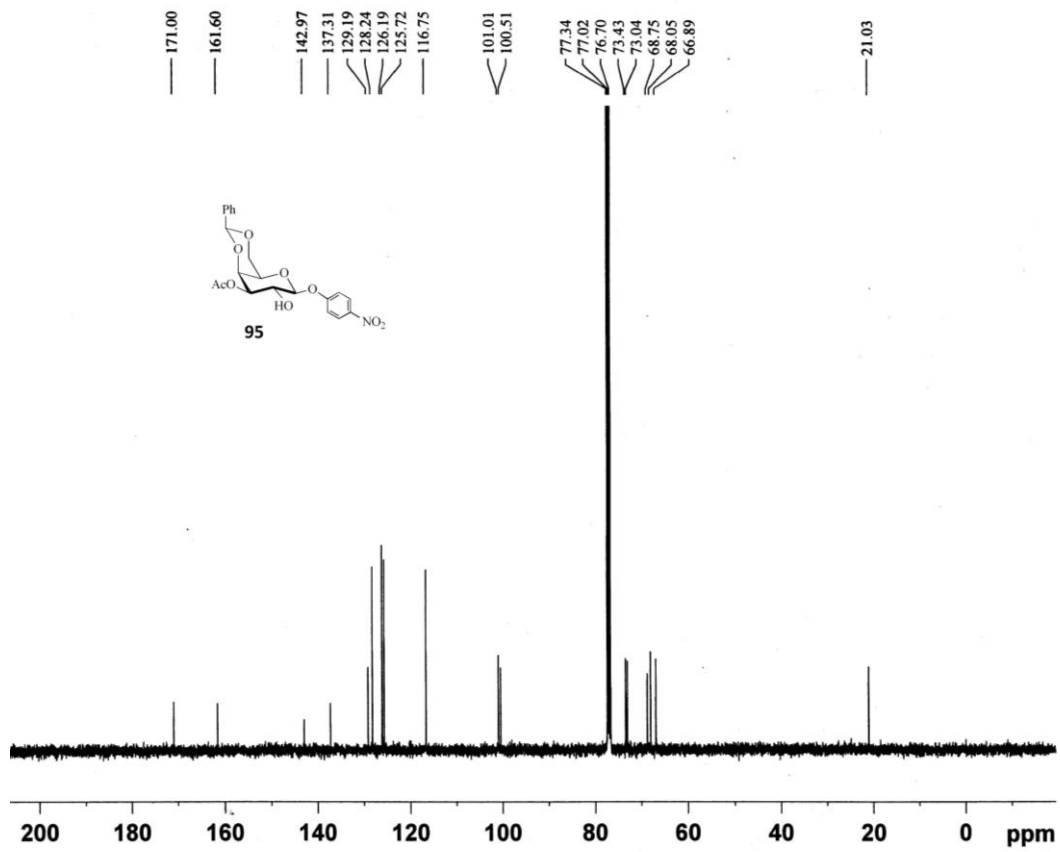
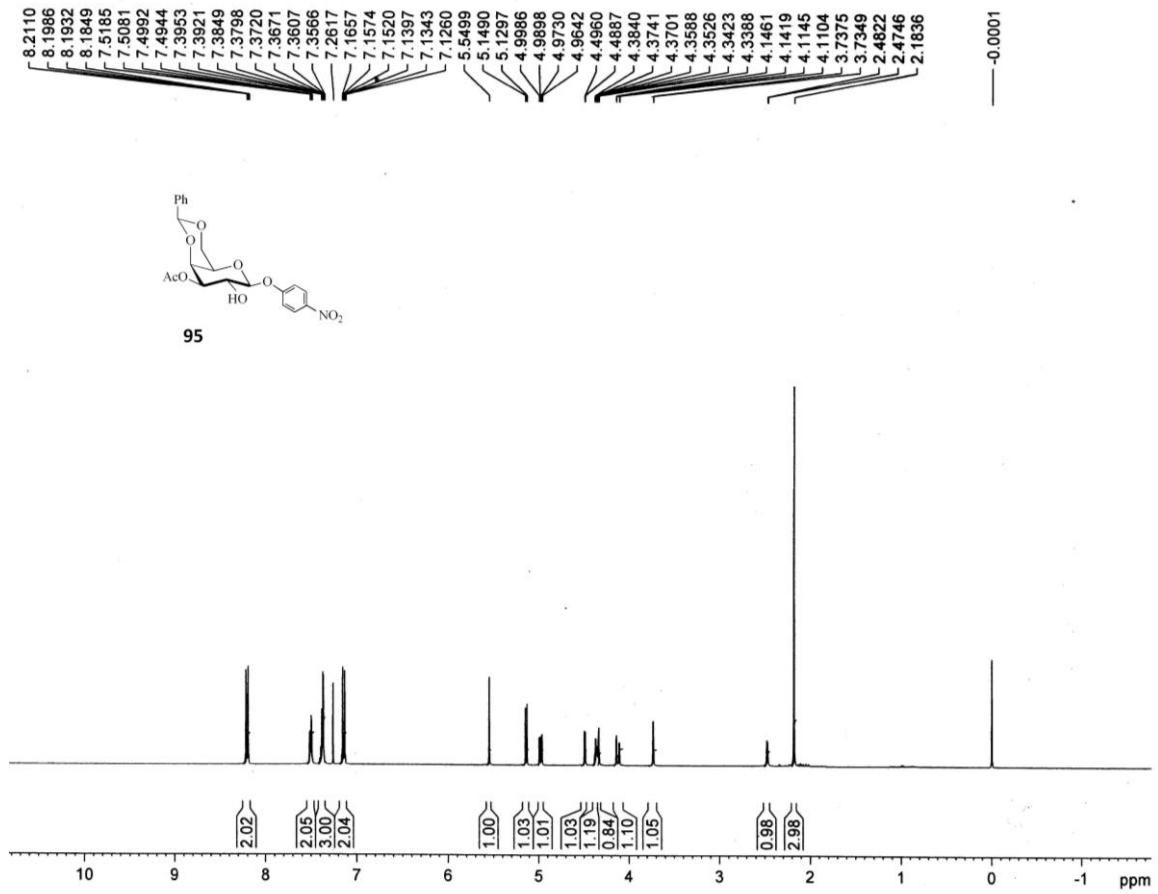




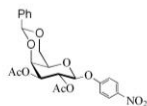




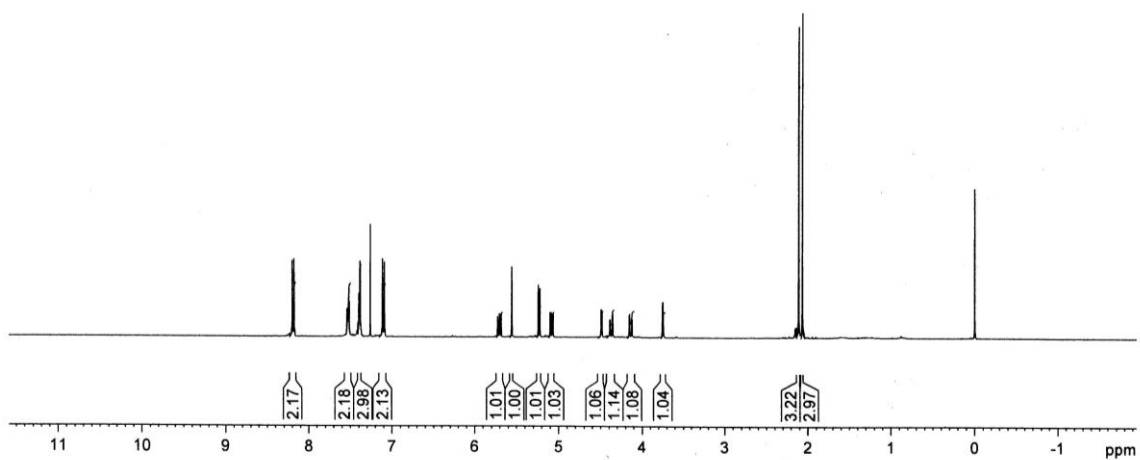




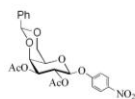
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8.1813
8.1730
7.5400
7.5332
7.5292
7.5207
7.5160
7.4119
7.4093
7.4005
7.3945
7.3871
7.3826
7.3772
7.3752
7.3713
7.2622
7.1251
7.1168
7.1115
7.0991
7.0937
7.0854
5.7309
5.7112
5.7048
5.6851
5.5597
5.2442
5.2244
5.1030
5.0941
5.0789
5.0681
4.4978
4.4891
4.3936
4.3897
4.3621
4.3583
4.1586
4.1544
4.1270
4.1229
3.7540
3.7515
2.1579
2.1414
2.1141
2.0700
2.0605
2.0559



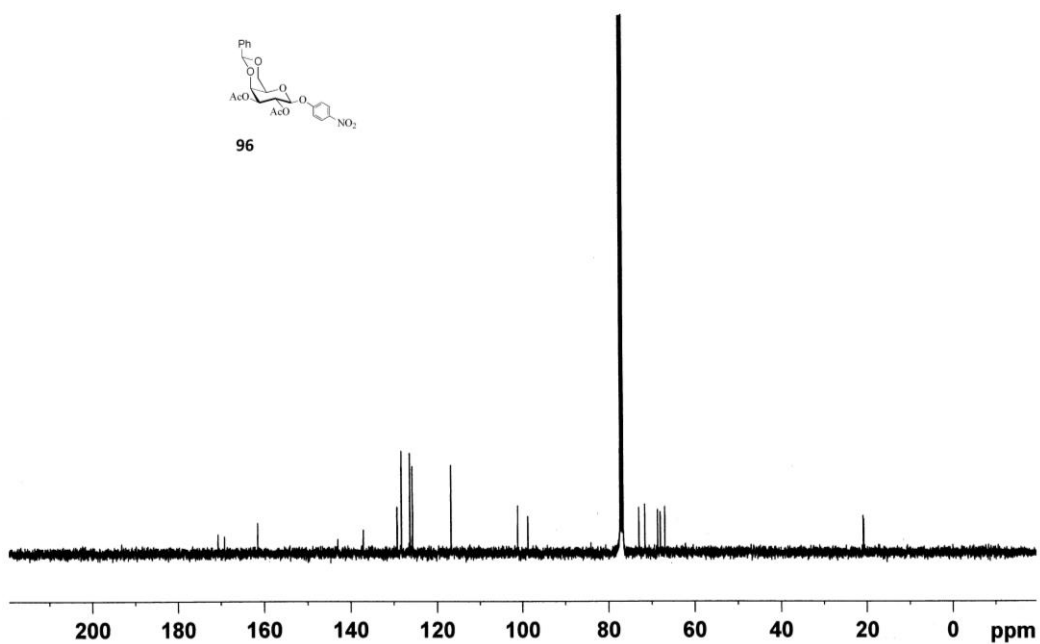
96

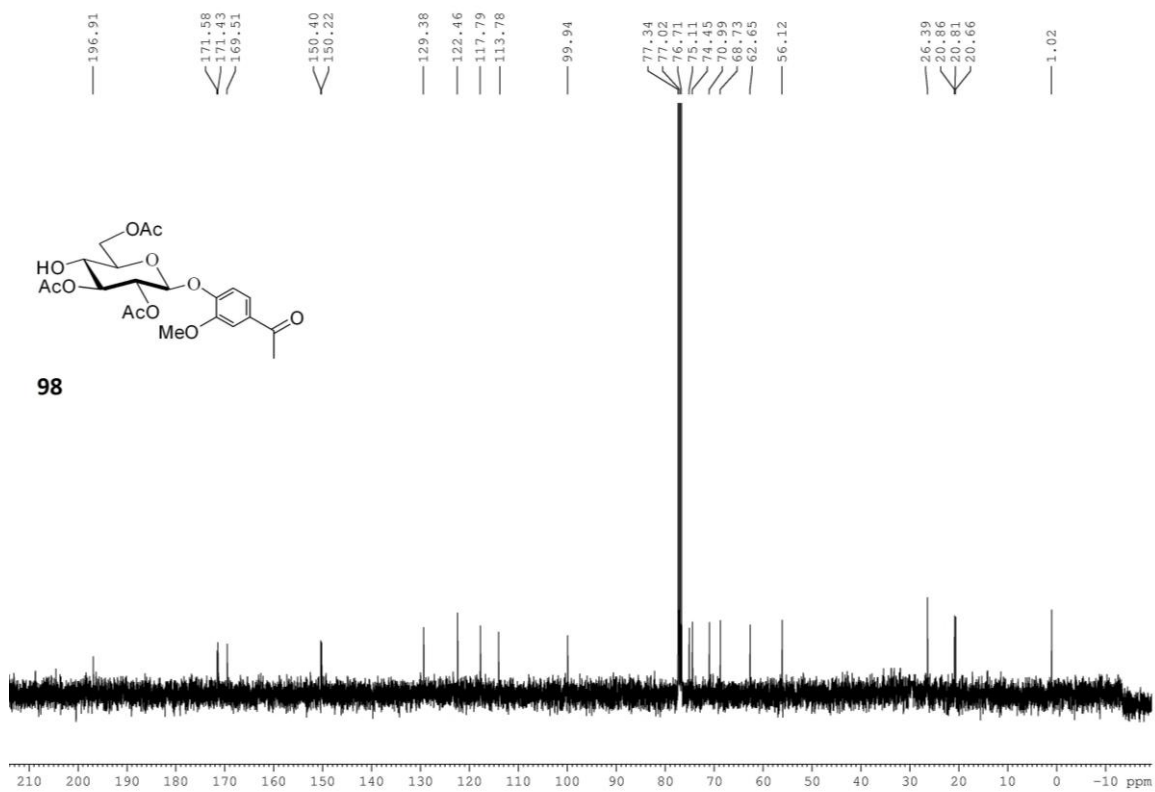
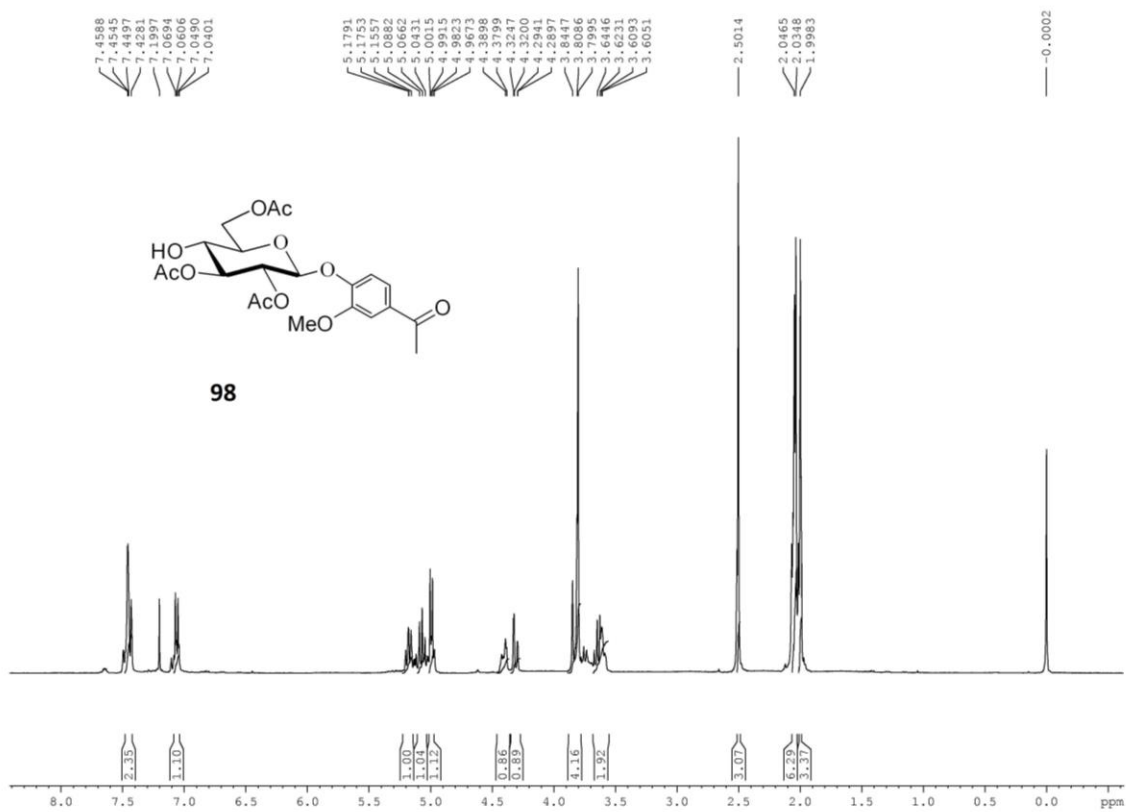


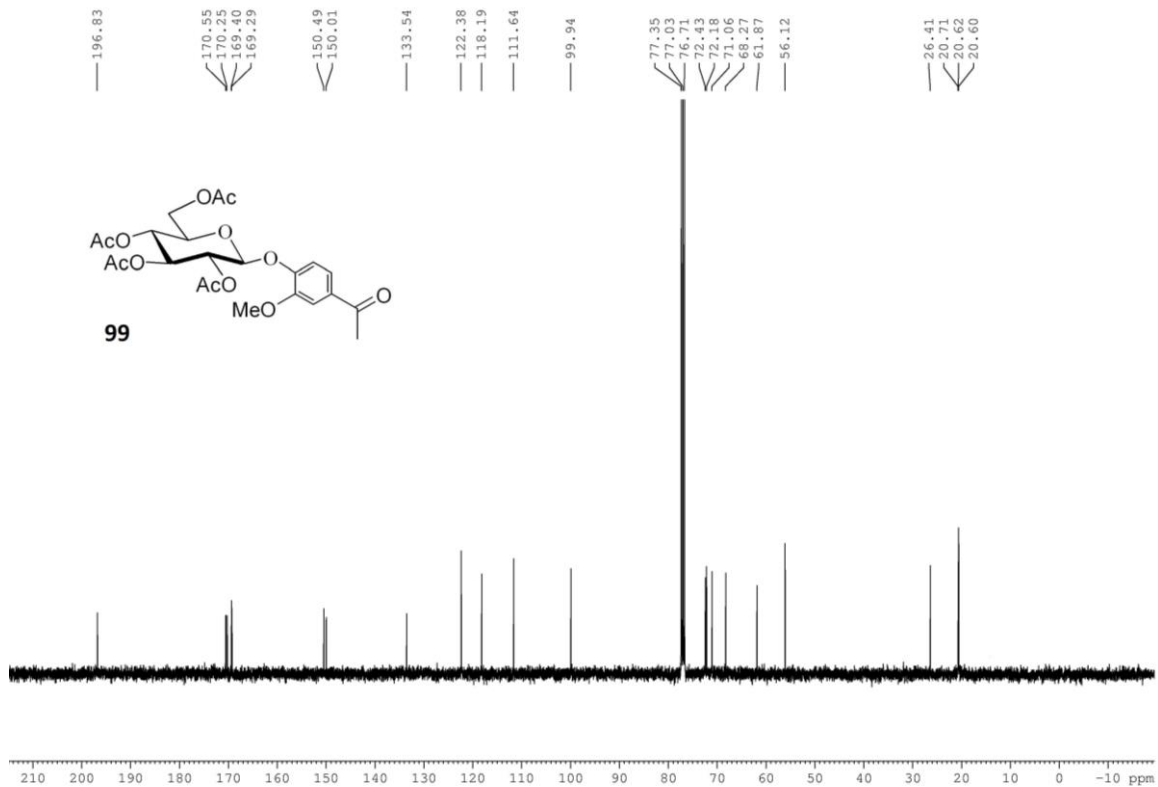
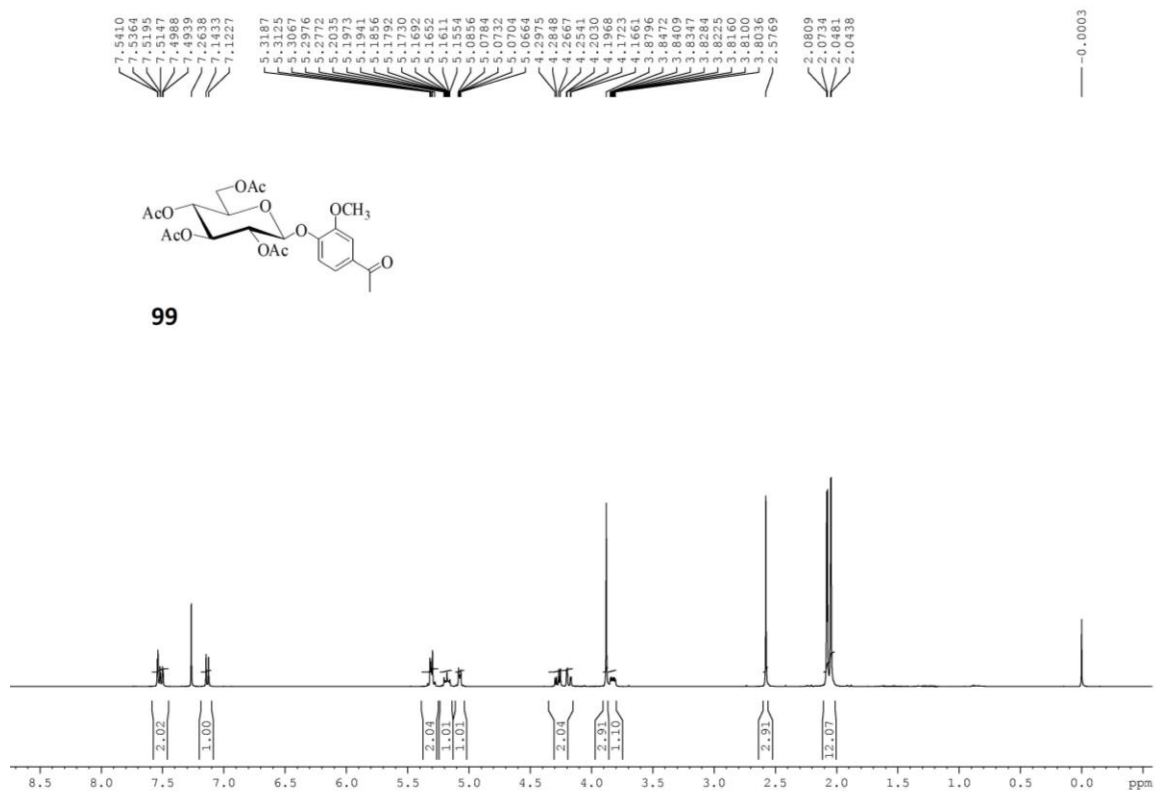
170.70
169.13
161.47
143.02
137.11
129.26
128.26
126.29
125.73
116.77
101.13
98.75
77.33
77.01
76.70
72.97
71.58
68.62
67.99
66.91
20.85
20.72

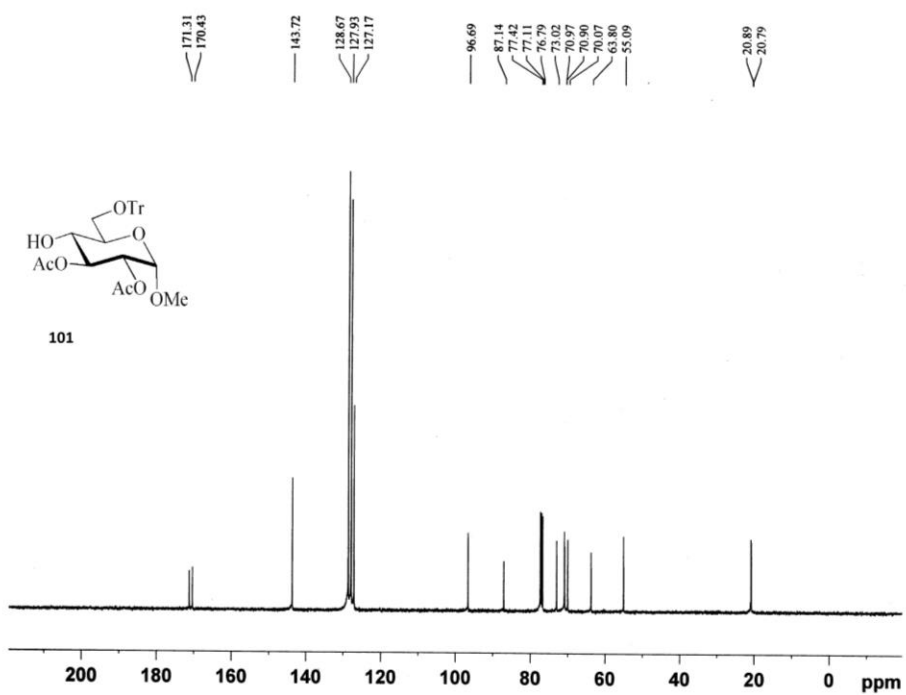
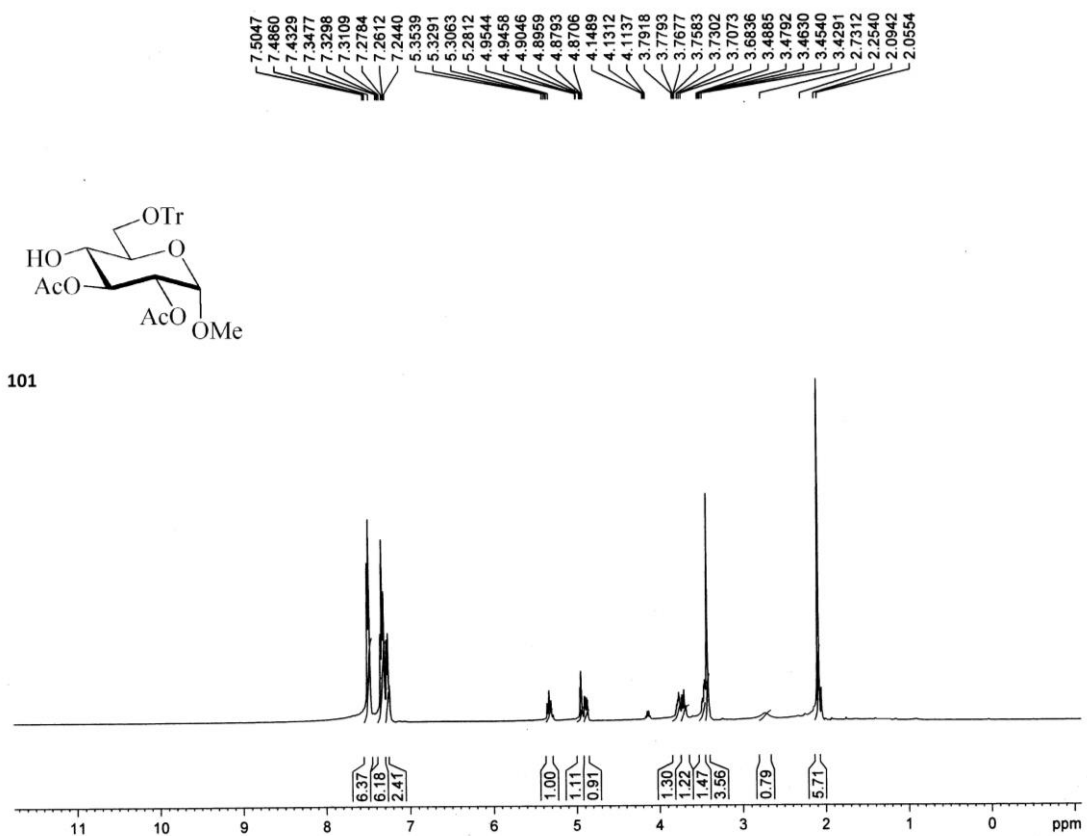


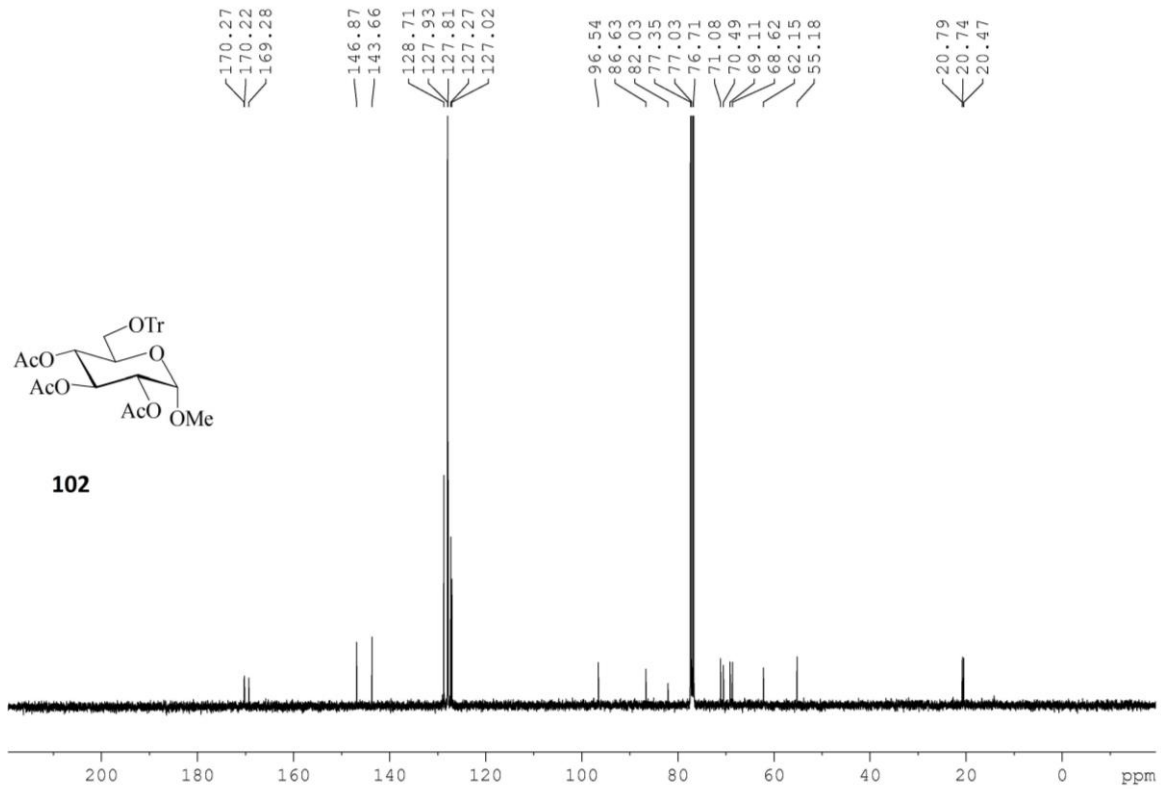
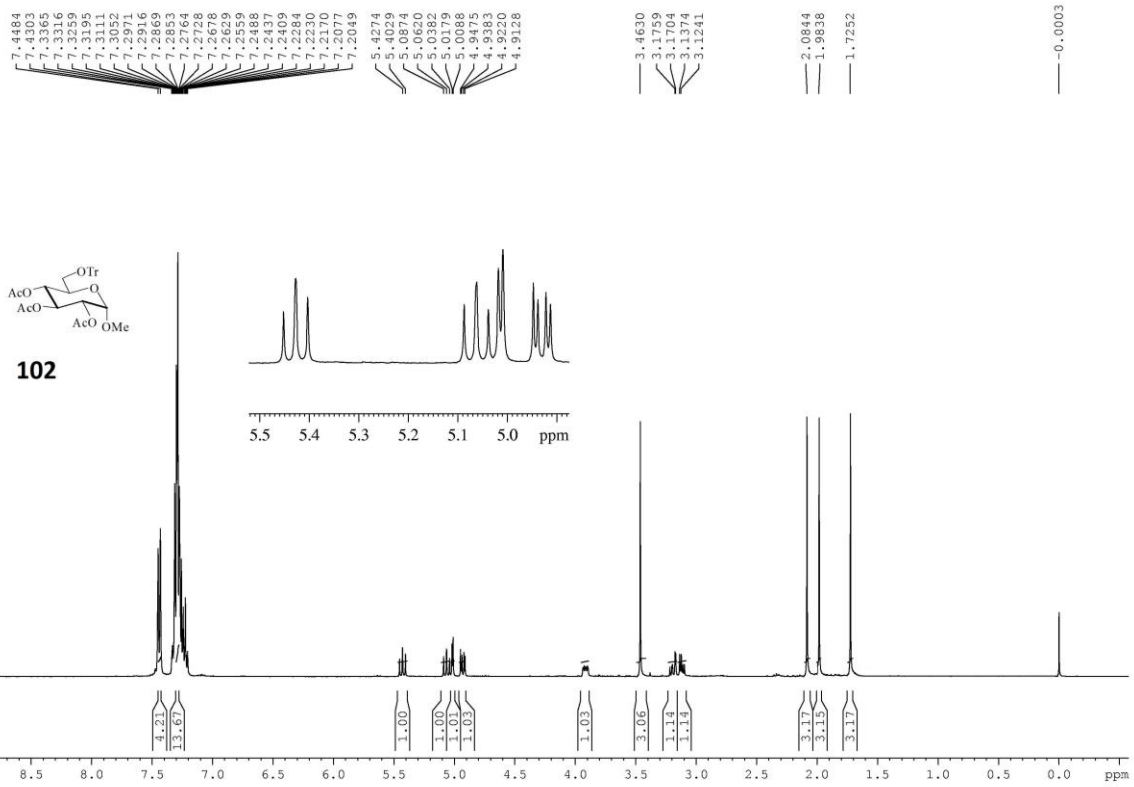
96

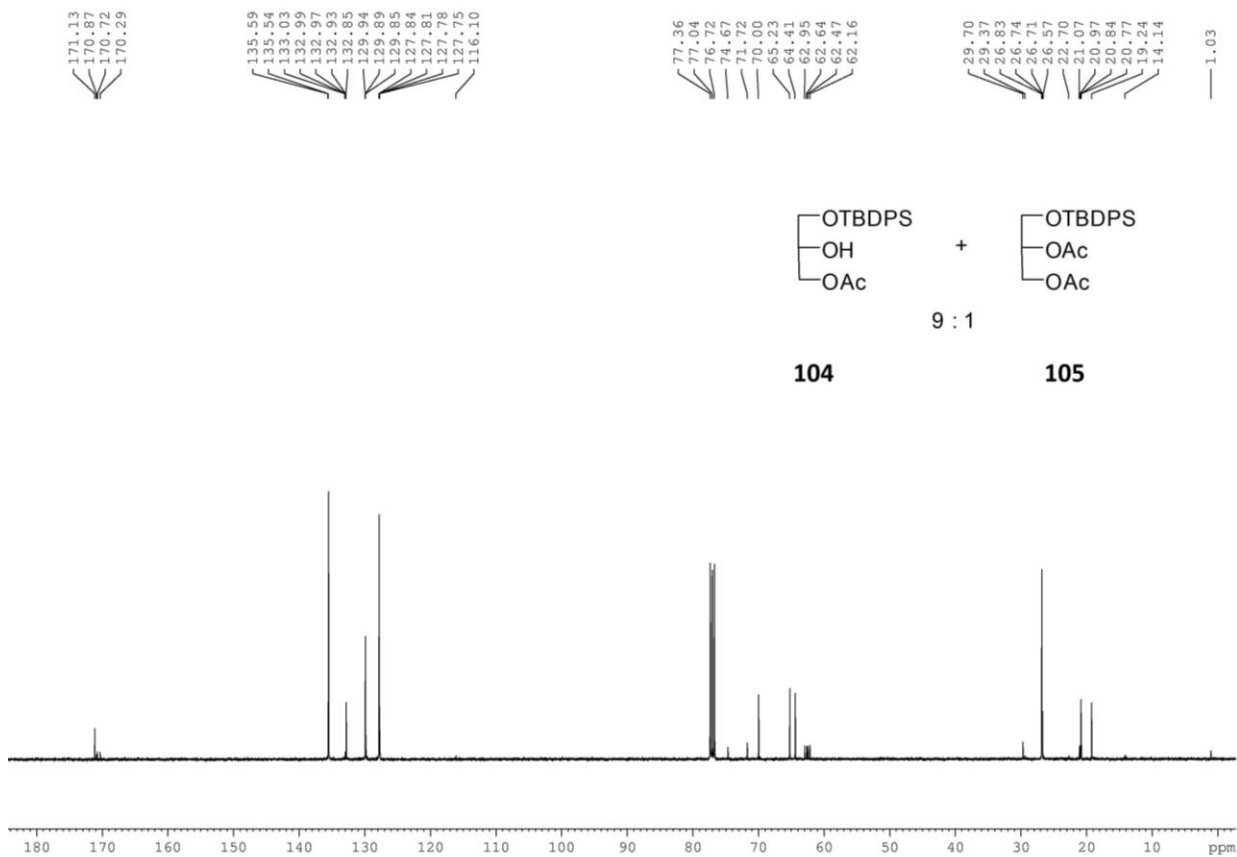
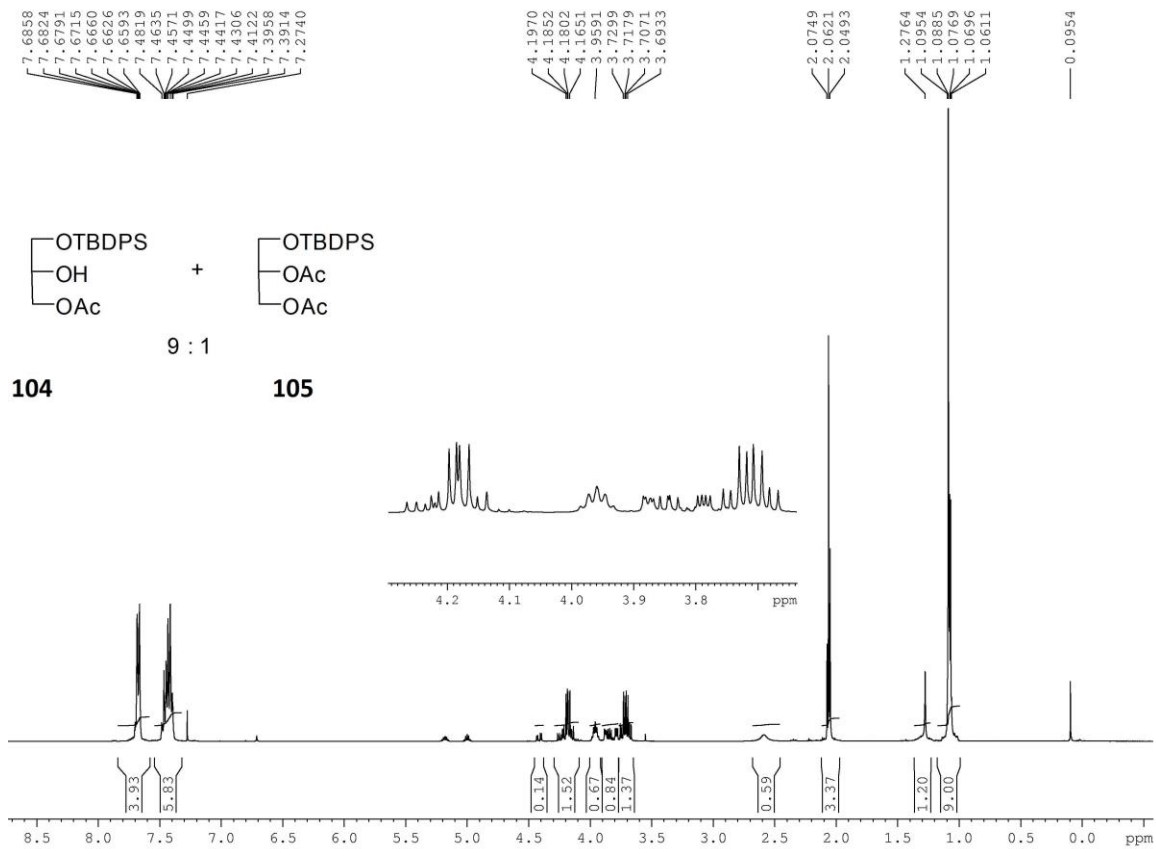










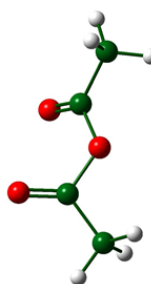


2. Computational Details

2.1. Cartesian coordinates of compounds Ac₂O, MeSO₃H, 2, 2b, 2d optimized at B3LYP/6-31+G(d) in gas phase

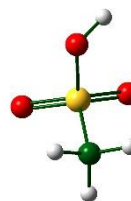
Ac₂O

0 1			
C	2.35011300	-0.74812100	0.34850900
H	2.27763400	-0.83023200	1.43942500
H	3.29620500	-0.27760900	0.07692100
H	2.29917200	-1.76258600	-0.06012300
C	1.20701200	0.08343800	-0.16611000
O	-0.00002200	-0.60228600	-0.00009000
C	-1.20699400	0.08344400	0.16609400
C	-2.35018500	-0.74801800	-0.34848100
H	-2.29927000	-1.76250600	0.06010200
H	-3.29623100	-0.27746900	-0.07679800
H	-2.27779000	-0.83008200	-1.43940500
O	1.27749500	1.15843500	-0.69519200
O	-1.27739800	1.15835300	0.69525700



MeSO₃H

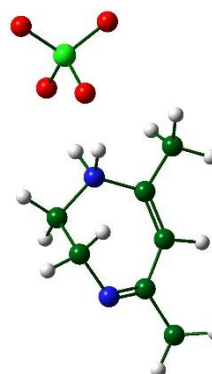
0 1			
S	-0.09003200	0.15220000	0.04696200
O	-0.72163300	-1.15390600	-0.74764000
O	-0.65045100	0.13562200	1.40065600
O	-0.22695900	1.32042700	-0.81213000
C	1.63611600	-0.34625200	0.07929700
H	2.19168600	0.47350500	0.54053100
H	1.72729500	-1.25972400	0.66855500
H	1.96573000	-0.50150900	-0.94953100
H	-1.46855300	-1.48710300	-0.21381400



2

0 1			
C	-1.13945500	1.06840400	0.05845100
C	-2.47455600	1.07356700	-0.09979600
C	-1.02305100	-1.42297800	0.65596100
C	-2.04106400	-1.83989700	-0.40473600
H	-1.50194500	-1.30908000	1.63229700
H	-2.15423000	-2.92719700	-0.35169600

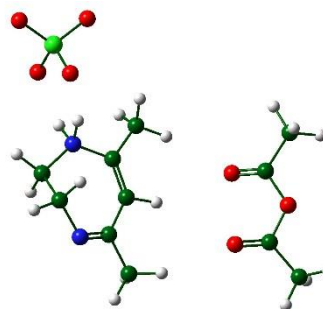
H	-2.88805000	2.06809700	-0.25501200
H	-0.21645600	-2.15557700	0.74360300
H	-1.64751900	-1.61825300	-1.40926200
N	-0.34461300	-0.13464700	0.31730500
H	0.38757000	0.06248900	1.03957200
C	-0.27781100	2.29838800	-0.00767800
H	-0.87938100	3.17471400	-0.25801000
H	0.22722600	2.48220700	0.94950400
H	0.51348600	2.18892800	-0.76007500
C	-4.92254500	0.53328300	0.05529700
H	-5.62864800	-0.29877200	0.04710400
H	-5.03379800	1.09339300	0.99305900
H	-5.17099400	1.22256100	-0.76287100
N	-3.36279500	-1.25763300	-0.24234000
C	-3.51150500	0.00760500	-0.09746300
Cl	2.93049000	-0.08197100	-0.05412000
O	4.03421700	-1.05484700	0.02290100
O	3.39064700	1.27663300	-0.42813600
O	1.89730800	-0.56112400	-1.09166400
O	2.19482100	-0.01724700	1.28576800
H	0.33024300	-0.30159500	-0.48410100



2b

0 1

C	-0.55122800	0.49793400	0.59918200
C	0.53742900	1.27919400	0.49391600
C	-2.22044600	2.40274200	0.15704200
C	-1.36192200	3.02222300	-0.94542600
H	-2.05656800	2.91322500	1.10996000
H	-1.90286400	3.88424000	-1.34836100
H	1.46719500	0.76516000	0.72915100
H	-3.28454000	2.44941300	-0.08928800
H	-1.25165800	2.30774400	-1.77673600
N	-1.92630000	0.94965200	0.34778300
H	-2.56955900	0.56708100	1.07381400
C	-0.51583900	-0.95313900	0.98829900
H	0.51495400	-1.29173300	1.10431500
H	-1.05194500	-1.12114200	1.93216400
H	-1.01406100	-1.57659100	0.23444400
C	2.07154900	3.26539400	0.56555300
H	2.14988000	4.31131900	0.26260700
H	2.18954500	3.19459800	1.65538300
H	2.88919900	2.68831600	0.11678600
N	-0.06099900	3.49280800	-0.49996400
C	0.73202500	2.71017200	0.13675800
Cl	-4.40025000	-1.20701100	-0.16559300
O	-5.81919800	-1.08365700	-0.55102200

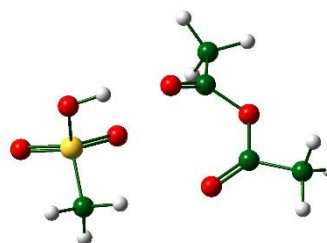


O	-3.97408800	-2.61966100	-0.01744800
O	-3.52227900	-0.53127500	-1.23564100
O	-4.14500200	-0.45705000	1.13897600
H	-2.33135100	0.41374000	-0.47162300
C	6.59559100	0.11750800	-0.24838700
H	6.96487300	-0.15614200	0.74686600
H	6.75342700	1.18284400	-0.42162900
H	7.15895000	-0.47215600	-0.97894300
C	5.12865000	-0.19671500	-0.34432100
O	4.93162600	-1.57825000	-0.28277100
C	3.71865300	-2.13406100	0.12189100
C	3.57501600	-3.52294200	-0.43421600
H	4.47215800	-4.11315400	-0.22130900
H	2.69573200	-4.00289600	-0.00255800
H	3.46983700	-3.47027100	-1.52428500
O	4.23079500	0.58665600	-0.49974100
O	2.94755800	-1.56445000	0.84862800

2d

0 1

S	-2.30863800	-0.16116200	-0.17150400
O	-1.96309400	0.36153100	1.33096700
O	-1.42068700	0.52797900	-1.11936900
O	-3.75635500	-0.07036000	-0.30775200
C	-1.82367000	-1.89151400	-0.09342100
H	-2.06993600	-2.33424000	-1.06164600
H	-0.74911400	-1.94479300	0.09310400
H	-2.39650300	-2.36828500	0.70390800
H	-1.00775000	0.61630600	1.38218100
C	4.08930400	-1.17762600	-0.17066500
H	4.51983000	-0.76305100	-1.08808200
H	4.20471600	-2.26216400	-0.15534600
H	4.62940100	-0.73393200	0.67386000
C	2.63222400	-0.82546000	-0.07473600
O	2.46336800	0.55577400	-0.25566900
C	1.37759700	1.23394500	0.26456000
C	1.09987400	2.49187900	-0.49932300
H	0.42724900	2.23291700	-1.32643400
H	0.58888100	3.20934200	0.14557600
H	2.01784600	2.91910600	-0.90974300
O	1.71282400	-1.58135200	0.07971700
O	0.77914600	0.83393300	1.23813000

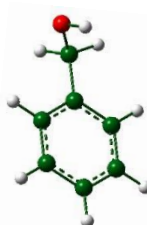


2.2. Cartesian coordinates of compounds 39-78 optimized at B3LYP/6-31+G(d) in gas phase

39

0 1

C	1.45929600	1.30348300	0.03311700
C	0.08976400	1.11054900	0.21783400
C	-0.45554600	-0.18353600	0.22070800
C	0.39995100	-1.27652800	0.03334800
C	1.77458900	-1.08714700	-0.14707300
C	2.30669100	0.20377800	-0.14821400
H	1.86852900	2.31080900	0.03424200
H	-0.56915800	1.96467700	0.35433000
H	-0.01040700	-2.28471500	0.02950900
H	2.42515700	-1.94633000	-0.29052900
H	3.37383800	0.35482200	-0.29022500
C	-1.94300900	-0.38590200	0.42273200
H	-2.18471700	-1.45803300	0.37403400
H	-2.25530100	-0.02192100	1.40735700
O	-2.74661200	0.35559600	-0.50140000
H	-2.46546600	0.12774100	-1.40222800



41

0 1

C	-1.17217600	-1.19242400	-0.00001100
C	0.22230400	-1.22457000	0.00001100
C	0.94012400	-0.02338700	0.00001400
C	0.26357400	1.20142500	-0.00000800
C	-1.13436900	1.22034600	-0.00001300
C	-1.86000600	0.02682400	-0.00001600
H	-1.72522400	-2.12838200	-0.00001300
H	0.76711400	-2.16401700	0.00002900
H	0.82425600	2.13506300	-0.00002800
H	-1.65305000	2.17576900	-0.00002100
H	-2.94616700	0.04486800	-0.00002500
O	2.30987500	-0.11129400	-0.00000500
H	2.69736400	0.77776600	0.00023900



43

0 1

C	-0.66436100	-1.19693800	-0.00002100
C	0.72847400	-1.22076800	0.00000700
C	1.44207400	-0.01699700	0.00001700



C	0.75177600	1.19679000	-0.00000600
C	-0.64752600	1.20076100	-0.00002600
C	-1.38323800	0.01068000	-0.00003100
H	-1.20605100	-2.14107200	-0.00003500
H	1.27550900	-2.15909500	0.00001500
H	1.29839000	2.13883300	-0.00002200
H	-1.16999000	2.15516400	-0.00004500
O	2.81394800	-0.09591700	0.00001800
H	3.19376000	0.79635600	0.00019600
C	-2.89582000	0.01518900	0.00000800
H	-3.29000600	1.03715600	-0.00059800
H	-3.30075900	-0.49669200	-0.88266200
H	-3.30070800	-0.49561500	0.88333000

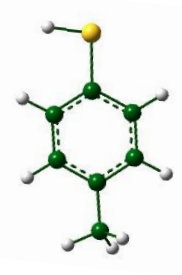
45

0 1			
C	-0.01272900	1.22319900	-0.00022300
C	1.37544000	1.22902500	-0.00023800
C	2.07781600	0.01455200	-0.00002200
C	1.38565800	-1.20577900	0.00022100
C	-0.00522200	-1.21417300	0.00019000
C	-0.69218000	0.00069800	-0.00003500
H	-0.57578900	2.14886400	-0.00039700
H	1.93215000	2.16044000	-0.00040900
H	1.93308200	-2.14588500	0.00041900
H	-0.55941100	-2.14518500	0.00034200
O	3.43698300	0.08749400	0.00007700
H	3.82542800	-0.80208800	0.00044300
N	-2.15574600	-0.00666700	-0.00005200
O	-2.72818200	-1.10033400	0.00013200
O	-2.73854300	1.08101400	-0.00013400



47

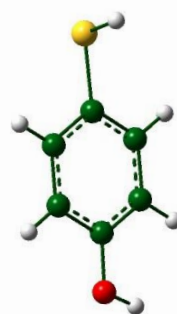
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C	-1.10593400	-1.19556400	0.00010700
C	0.28774100	-1.20568500	0.00020800
C	1.00355000	0.00128800	0.00012100
C	0.29456500	1.20775400	0.00007800
C	-1.10324700	1.20137600	0.00005300
C	-1.83171000	0.00598700	0.00004700
H	-1.63935100	-2.14437100	0.00014500
H	0.81922100	-2.15426400	0.00032600
H	0.82338200	2.15777800	0.00004000
H	-1.63265500	2.15205400	0.00003500
C	-3.34359400	0.00102300	-0.00018300
H	-3.74501900	1.01987700	0.00147100



H	-3.74302500	-0.51272200	-0.88406900
H	-3.74333100	-0.51575400	0.88178200
S	2.78992900	-0.08411500	-0.00023700
H	3.01368200	1.24617200	0.00148900

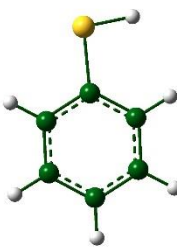
49

0 1			
C	1.13951000	-1.22390600	-0.00308300
C	-0.25364300	-1.21029900	-0.01422700
C	-0.96055100	0.00170400	-0.00246400
C	-0.24427700	1.20414700	-0.00632800
C	1.15247700	1.20007500	0.00035500
C	1.84518800	-0.01535600	0.00491800
H	1.69175000	-2.15882500	-0.00764200
H	-0.79995700	-2.14876700	-0.03320200
H	-0.77937400	2.14911900	-0.01273400
H	1.69811700	2.14227400	0.00004800
S	-2.76137700	0.01737400	-0.07431700
O	3.21288400	-0.08831800	0.01285300
H	3.59358900	0.80386900	0.01100500
H	-2.99738700	-0.09730100	1.25375600



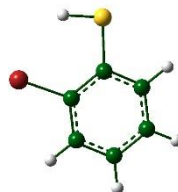
59

0 1			
C	1.59642700	-1.20322400	-0.00000900
C	0.20062800	-1.21017800	0.00001100
C	-0.50909000	0.00015400	0.00000900
C	0.19585600	1.21208400	-0.00000800
C	1.59285400	1.20891000	-0.00001400
C	2.30084100	0.00438000	-0.00001900
H	2.13352900	-2.14839000	-0.00001000
H	-0.33623600	-2.15557100	0.00003600
H	-0.33915600	2.15848600	-0.00001900
H	2.12644400	2.15619100	-0.00001900
H	3.38730800	0.00636800	-0.00002800
S	-2.29494400	-0.08353900	-0.00000400
H	-2.51787900	1.24678000	0.00028200



61

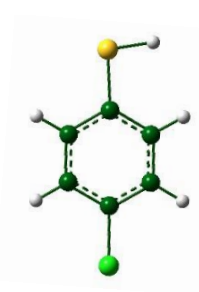
0 1			
C	2.87604600	-0.57257600	0.00005400
C	2.22152300	0.65509200	-0.00009800
C	0.81637700	0.73394300	-0.00005800
C	0.08745800	-0.46604400	-0.00002700



C	0.74492200	-1.69941600	0.00017700
C	2.13713300	-1.75930900	0.00022500
H	3.96220200	-0.60098700	0.00005500
H	2.79915800	1.57592500	-0.00022400
H	0.15898400	-2.61315500	0.00029600
H	2.63488700	-2.72466000	0.00036400
S	0.12808300	2.37650700	-0.00028000
H	-1.16848500	2.00889300	-0.00050700
Br	-1.82105200	-0.48629300	0.00008200

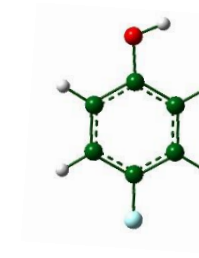
63

0 1			
C	-0.71275400	-1.21135900	-0.00000600
C	0.68198500	-1.20815700	0.00007100
C	1.39387600	0.00069300	0.00006900
C	0.68384700	1.20914600	0.00000000
C	-0.71232700	1.21237700	-0.00002600
C	-1.40324800	0.00124400	-0.00004500
H	-1.25777100	-2.14991400	-0.00000600
H	1.21453300	-2.15568700	0.00016400
H	1.21163300	2.15922200	-0.00004000
H	-1.25609600	2.15176000	-0.00005400
S	3.17761700	-0.08178100	0.00001600
H	3.39913000	1.24866000	0.00107300
Cl	-3.16127000	0.00181200	-0.00010400



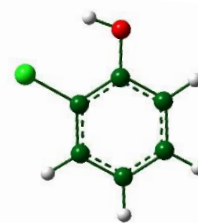
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0 1			
C	-0.72034900	1.21391100	-0.00001900
C	0.67442800	1.22366100	0.00001500
C	1.38313100	0.01658300	0.00003300
C	0.69414600	-1.20104900	0.00001600
C	-0.70435400	-1.21621400	-0.00001400
C	-1.38580300	-0.00737800	-0.00003300
H	-1.28874400	2.13867400	-0.00003300
H	1.22458300	2.15950000	0.00003000
H	1.24187000	-2.14155900	0.00002400
H	-1.25633300	-2.15079200	-0.00002600
O	2.75393100	0.09549900	0.00005400
H	3.13793800	-0.79488000	0.00015900
F	-2.74866100	-0.01689100	-0.00006400



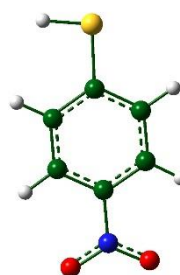
67

0 1			
C	-0.44893100	-1.47042900	0.00016700
C	0.39023700	-0.35726200	-0.00002200
C	-0.12748900	0.94679800	-0.00005600
C	-1.51763200	1.11570900	0.00010700
C	-2.36100100	0.00671200	0.00029700
C	-1.83272000	-1.28907500	0.00032700
H	-0.01464000	-2.46528200	0.00018800
H	-3.43730200	0.15571200	0.00042100
H	-2.48913500	-2.15419100	0.00047500
O	0.65206700	2.06222000	-0.00023600
H	1.59063100	1.80455700	-0.00034200
Cl	2.14293100	-0.56947600	-0.00022600
H	-1.91070200	2.12782600	0.00008000



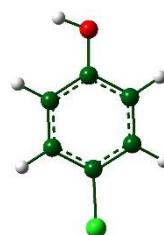
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0 1			
C	-0.44188600	-1.21772000	-0.00001100
C	0.94813500	-1.21384600	-0.00000500
C	1.65738900	0.00097500	0.00000600
C	0.94899600	1.21497100	0.00001000
C	-0.44214200	1.21750600	0.00000400
C	-1.12480400	0.00036500	-0.00000700
H	-0.99901100	-2.14710800	-0.00001900
H	1.48516400	-2.15818100	-0.00000800
H	1.48048500	2.16226800	0.00001800
H	-0.99941400	2.14693200	0.00000700
N	-2.59065300	0.00133900	-0.00001700
O	-3.16594100	1.09273600	0.00000000
O	-3.16721600	-1.08917700	-0.00001400
S	3.43146900	-0.08149500	0.00001400
H	3.65499300	1.24864600	0.00002100



71

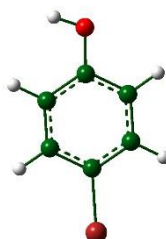
0 1			
C	-0.27533100	1.21480300	-0.00000600
C	1.11842700	1.22253700	0.00001300
C	1.82506600	0.01481400	0.00001900
C	1.13149800	-1.19990200	0.00000800
C	-0.26581500	-1.20974800	-0.00000200
C	-0.96113900	-0.00206700	-0.00001400
H	-0.82651400	2.14980800	-0.00001000
H	1.66922400	2.15814400	0.00002700
H	1.67523600	-2.14288500	0.00000500
H	-0.80517400	-2.15159300	-0.00000800
O	3.19351100	0.08938800	0.00002000



H	3.57602600	-0.80182700	0.00022300
Cl	-2.72194900	-0.00996300	-0.00003000

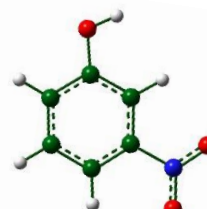
73

0 1			
C	0.37655400	-1.20577500	-0.00038100
C	1.77338900	-1.20002400	-0.00043600
C	2.46740600	0.01384800	-0.00043300
C	1.76383000	1.22275200	-0.00039500
C	0.37050800	1.21530300	-0.00037300
C	-0.31943600	0.00111800	-0.00054800
H	-0.16074100	-2.14868500	-0.00013800
H	2.31562100	-2.14381300	-0.00033800
H	2.31598600	2.15749700	-0.00027100
H	-0.17588100	2.15300200	-0.00012100
O	3.83605900	0.08603800	-0.00031200
Br	-2.22266800	-0.00524100	0.00054700
H	4.21639400	-0.80620100	-0.00039500



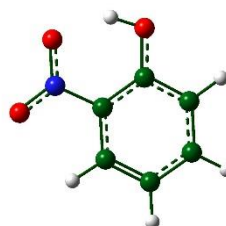
75

0 1			
C	1.06640700	1.85727400	0.00001800
C	2.07478200	0.89490300	0.00008000
C	1.74111400	-0.46702800	0.00007900
C	0.40266500	-0.86295800	0.00001500
C	-0.58048800	0.12745400	-0.00004500
C	-0.28147500	1.48743500	-0.00004500
H	1.33228200	2.91031400	0.00002000
H	3.12306300	1.17704100	0.00013100
H	-1.07799800	2.22069500	-0.00009200
O	2.77372500	-1.36161200	0.00013700
H	2.43372700	-2.27054500	0.00016200
H	0.11248100	-1.90820400	0.00001000
N	-1.99365300	-0.29593900	-0.00011100
O	-2.85649900	0.58234400	-0.00009900
O	-2.23047700	-1.50575700	-0.00004700



77

0 1			
C	-2.55784600	-0.17179600	0.00002200
C	-1.83583600	1.01179200	0.00004300
C	-0.42905900	0.99587300	0.00004200
C	0.21873800	-0.26611400	-0.00000700



C	-0.52162600	-1.46144400	-0.00001700
C	-1.90492600	-1.41873900	-0.00000300
H	-3.64382300	-0.13099600	0.00003400
H	-2.32779200	1.97930400	0.00008500
H	0.01755500	-2.40138400	-0.00005900
H	-2.47744700	-2.34071700	-0.00002300
O	0.20421900	2.17728400	0.00014800
H	1.17434200	1.99439000	0.00031400
N	1.66362800	-0.36131200	-0.00010400
O	2.19323600	-1.46862200	0.00007900
O	2.32693300	0.70273200	-0.00024100