Synthesis and stereochemical determination of batzelladine C methyl ester

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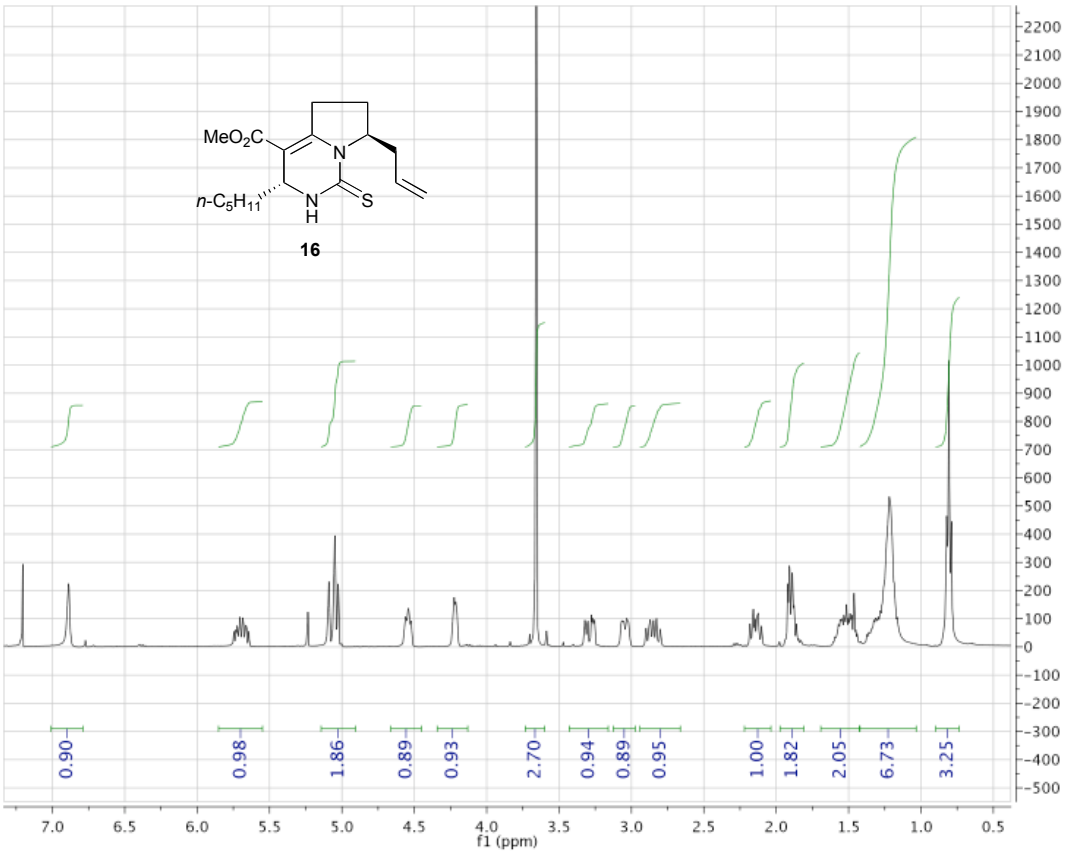
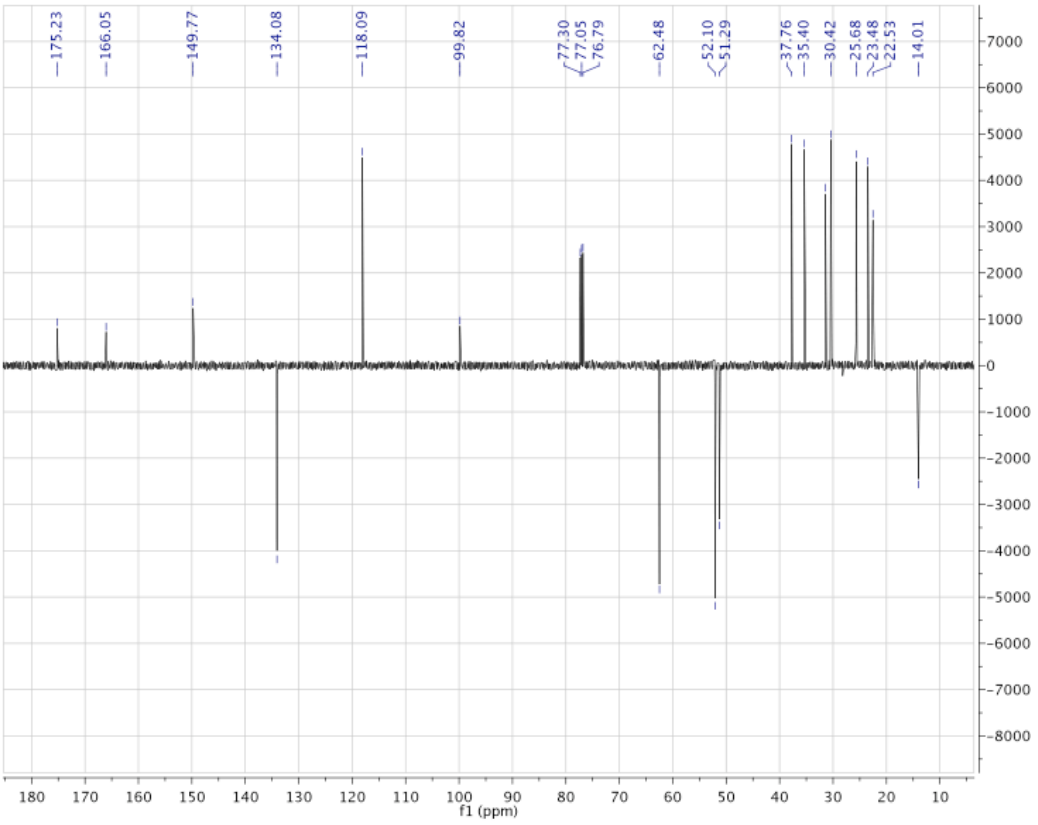
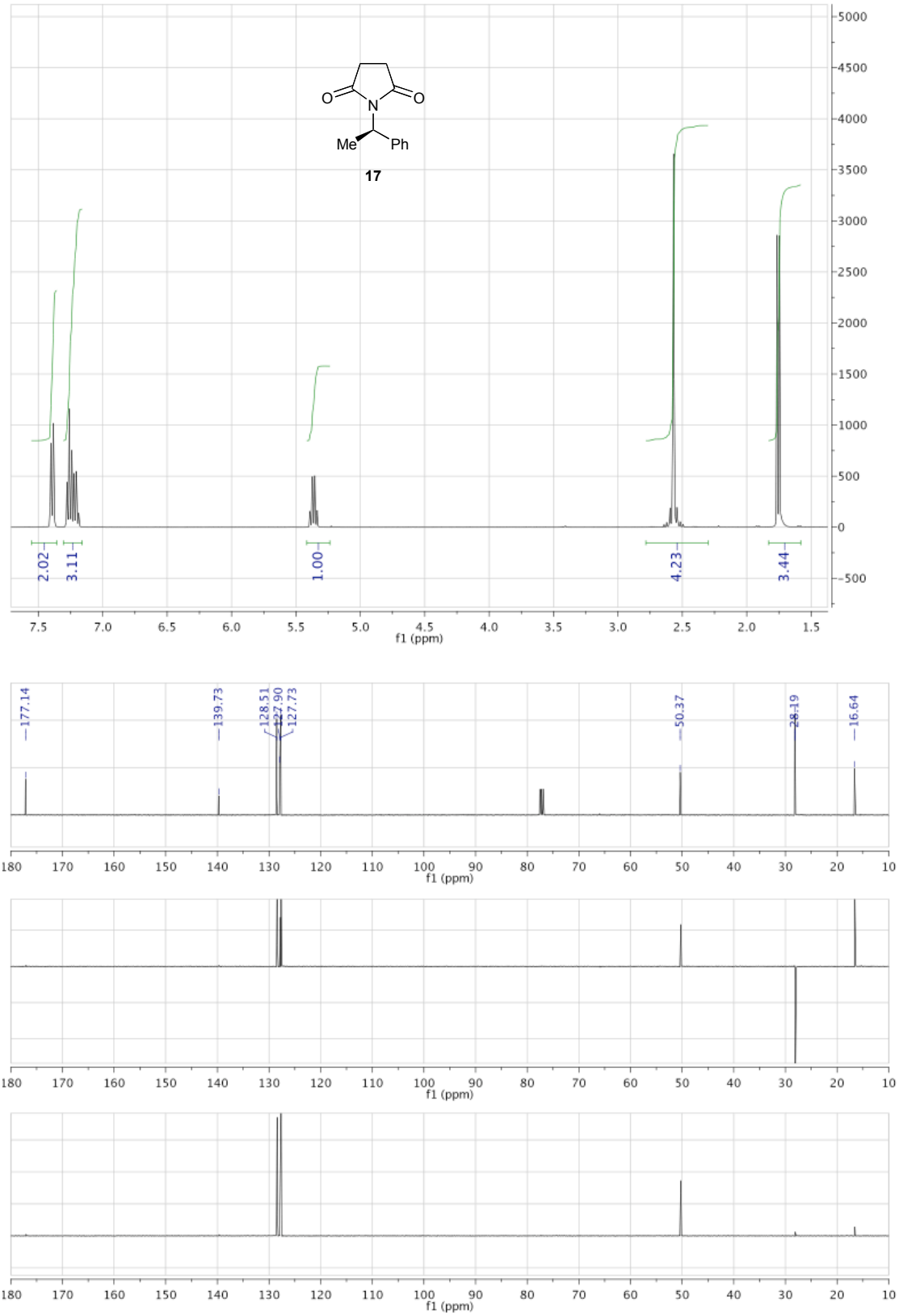
(3*R*,7*S*)-Methyl 7-allyl-1,2,3,5,6-hexahydro-3-pentyl-1-thioxopyrrolo[1,2-*c*]pyrimidine-4-carboxylate (16)

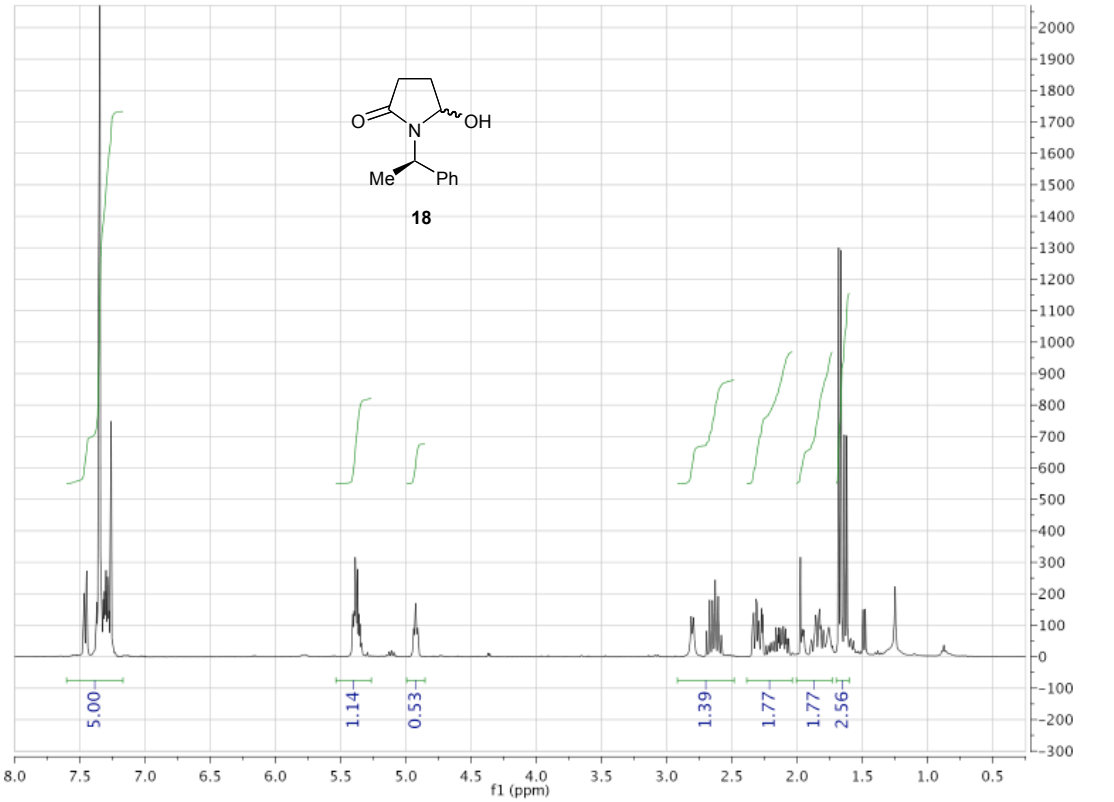


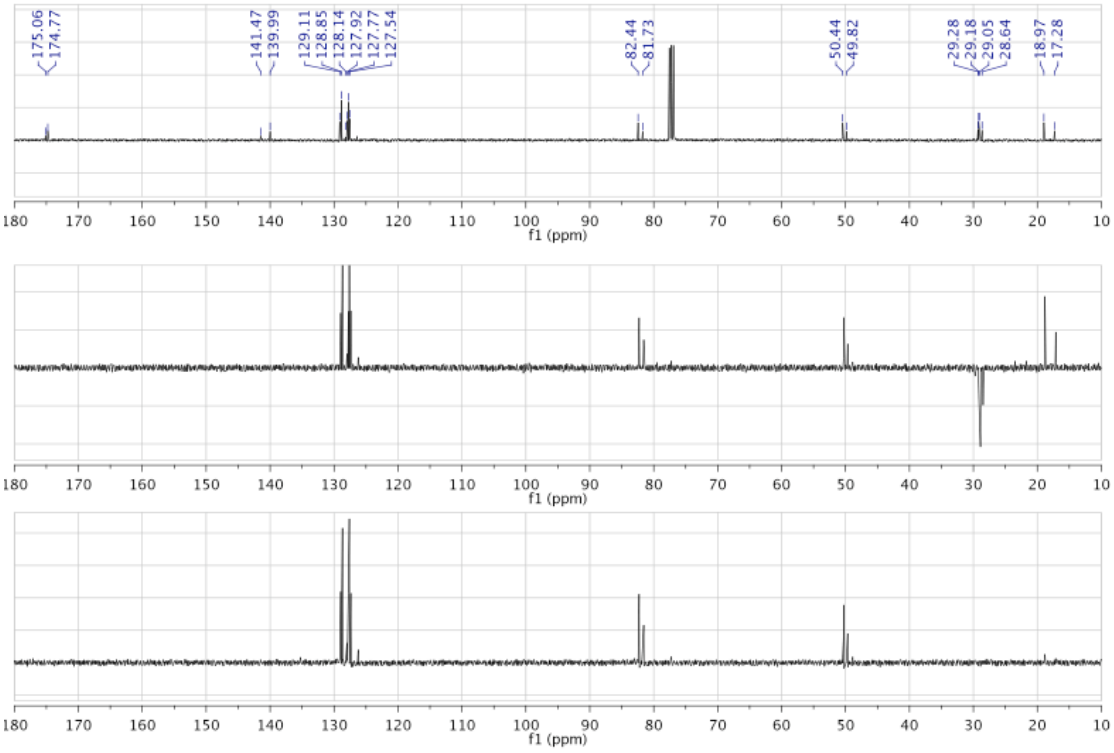


(*R*)-1-(1-Phenylethyl)pyrrolidin-2,5-dione (17)

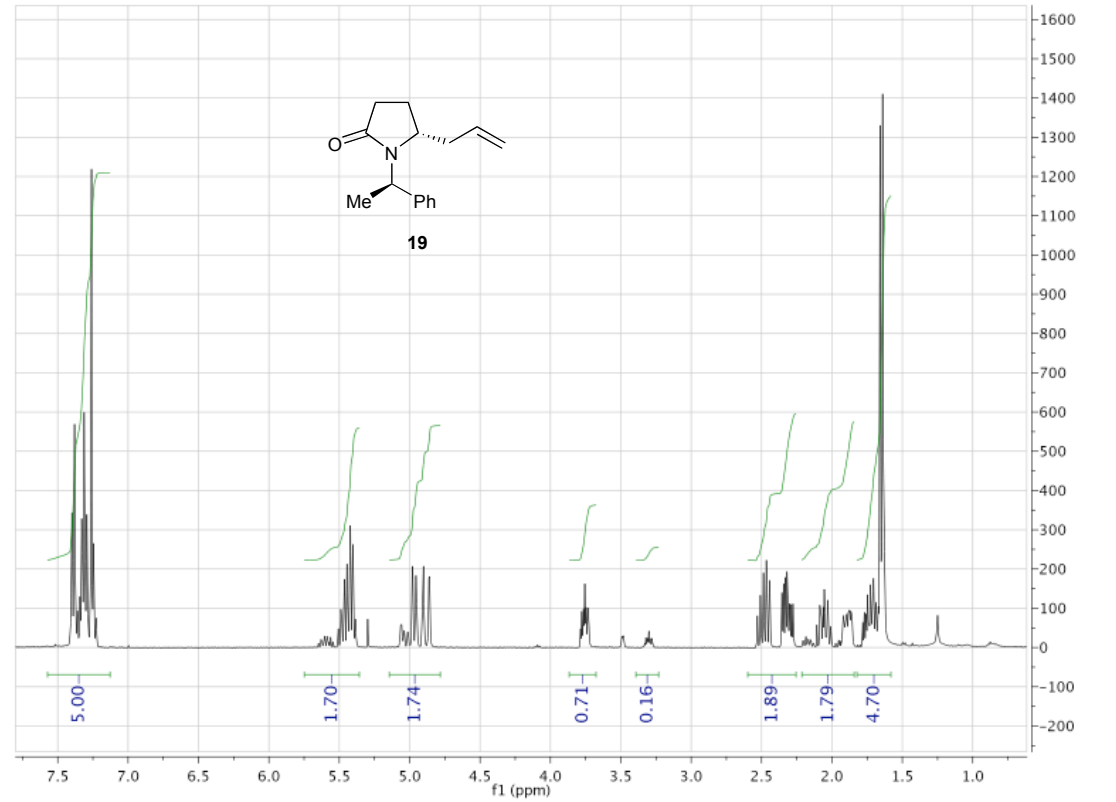


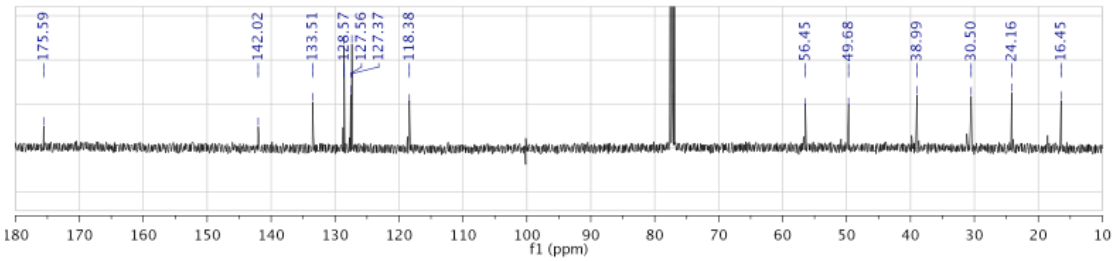
5-Hydroxy-1-((*R*)-1-phenylethyl)pyrrolidin-2-one (18)

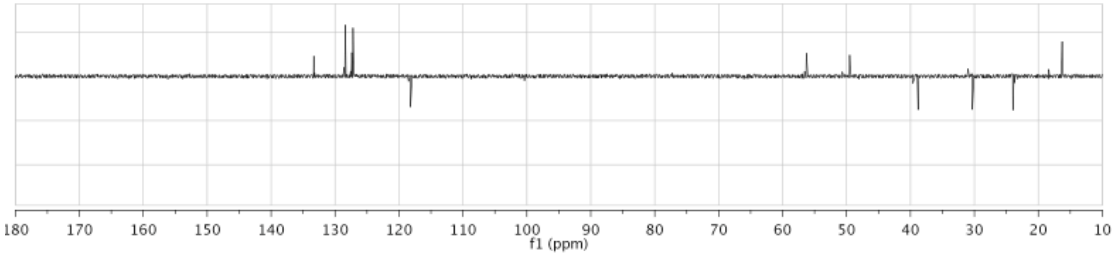


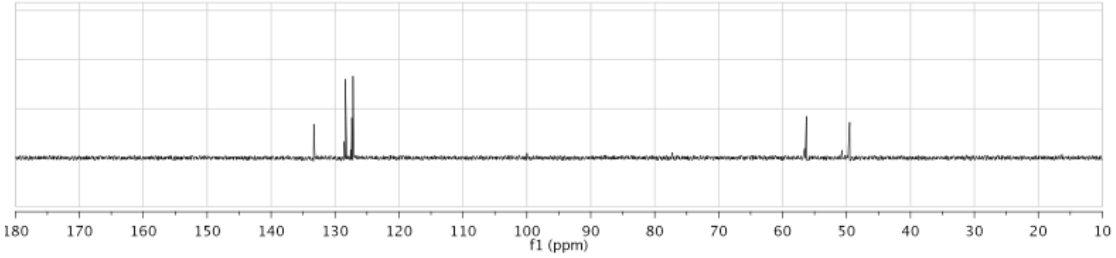


(*R*)-5-Allyl-1-((*R*)-1-phenylethyl)pyrrolidin2-one (19)

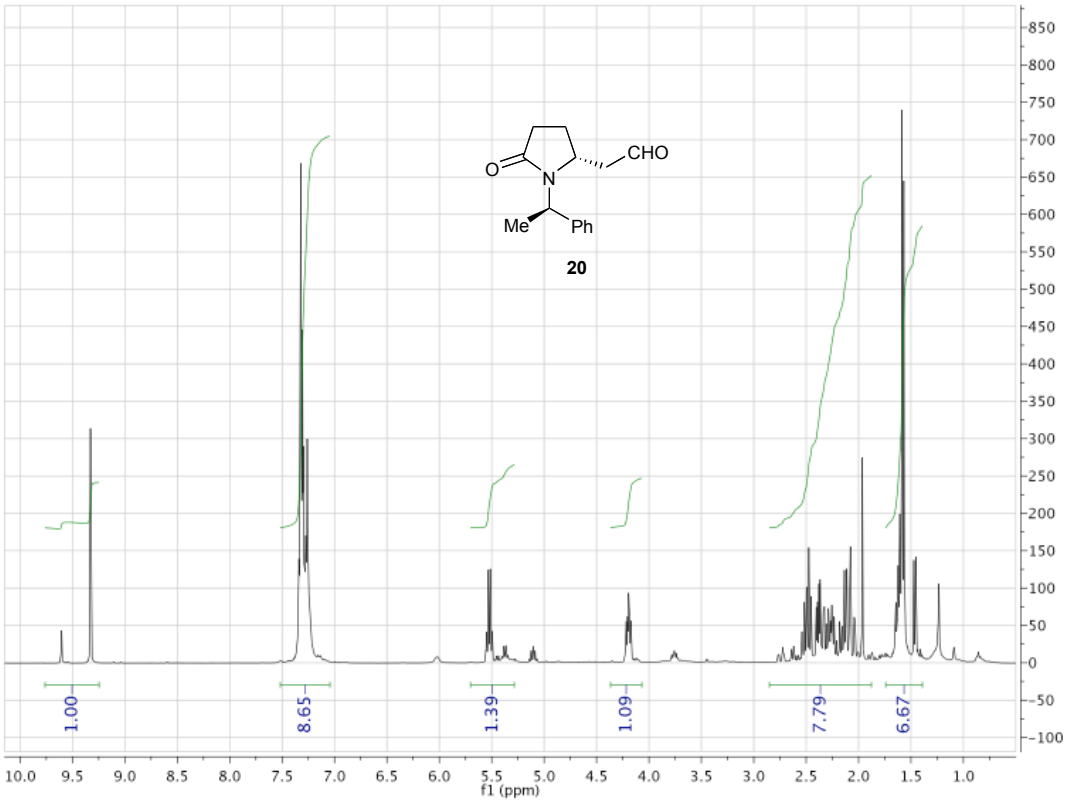


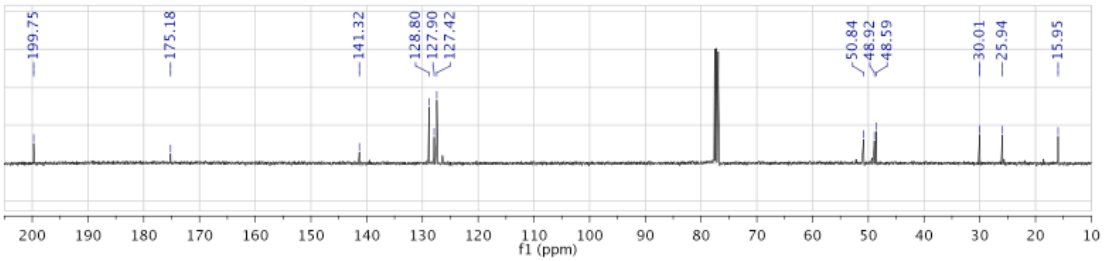


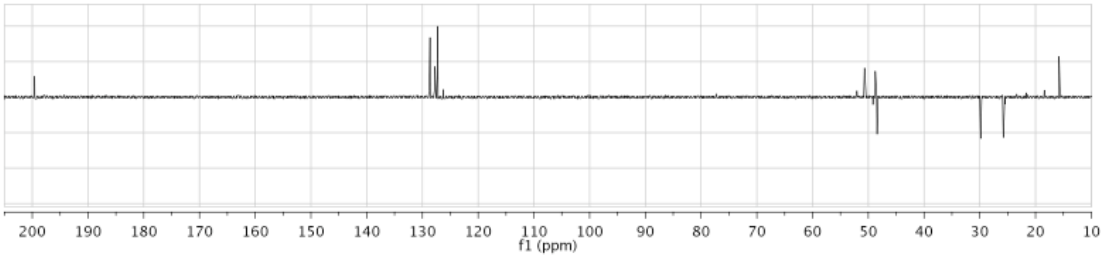


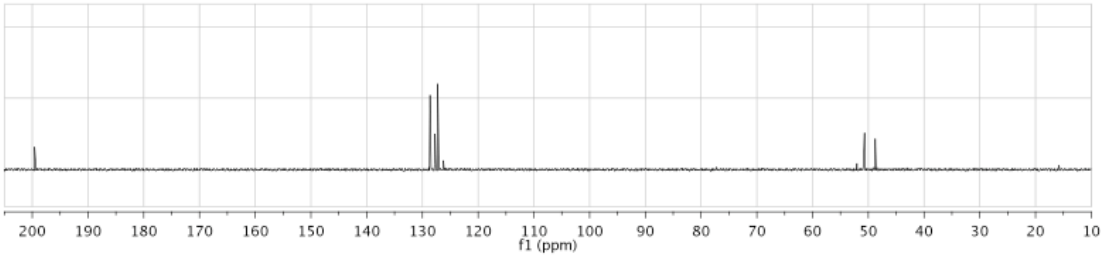


2-(*R*)-5-Oxo-1-((*R*)-1-phenylethyl)pyrrolidin-2-yl)acetaldehyde (20)

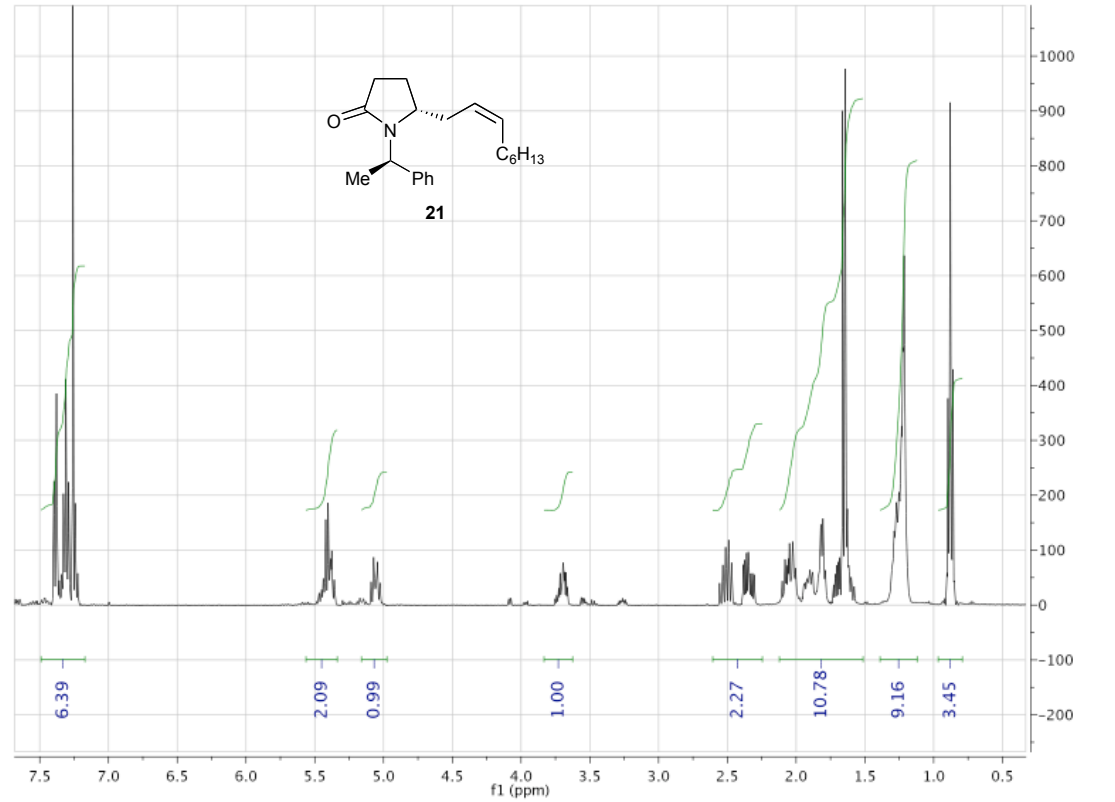


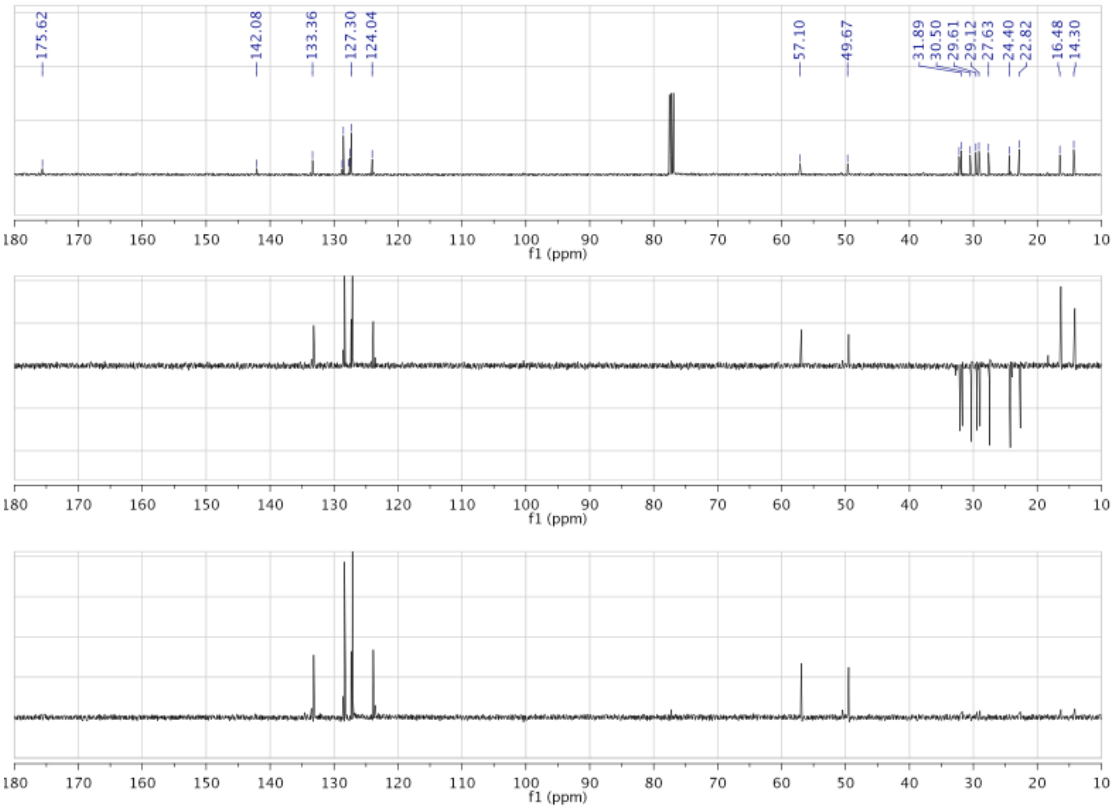




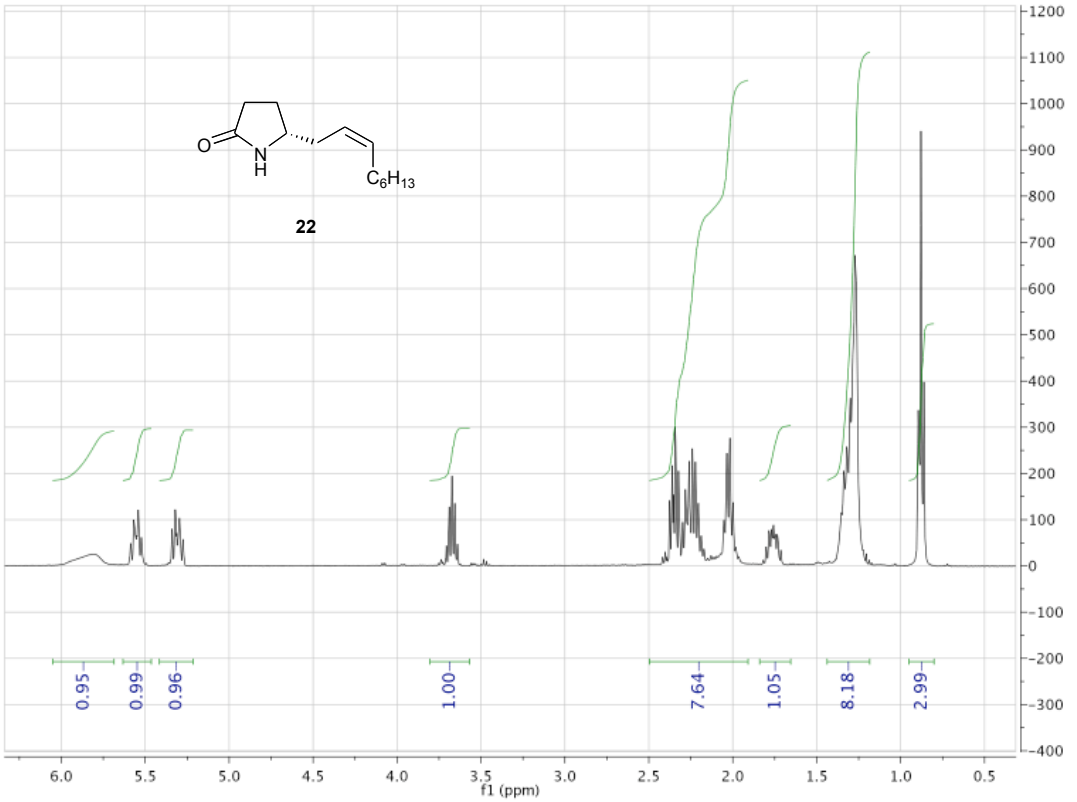


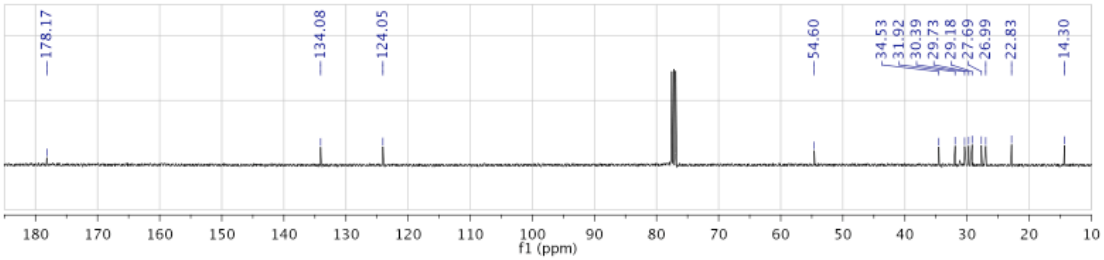
(*R*)-5-((*Z*)-Non-2-enyl)-1-((*R*)-1-phenylethyl)pyrrolidin-2-one (21)

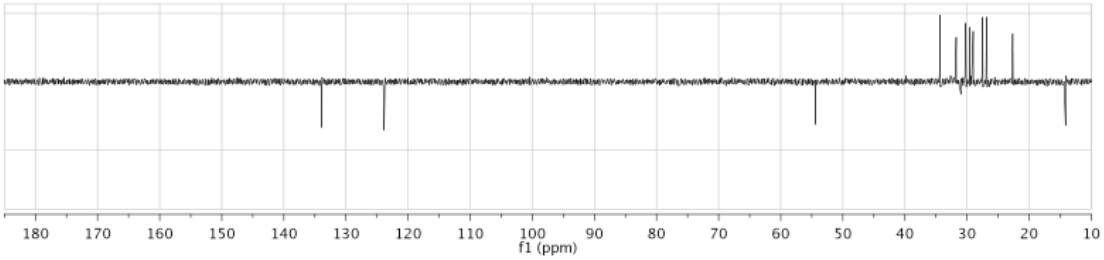


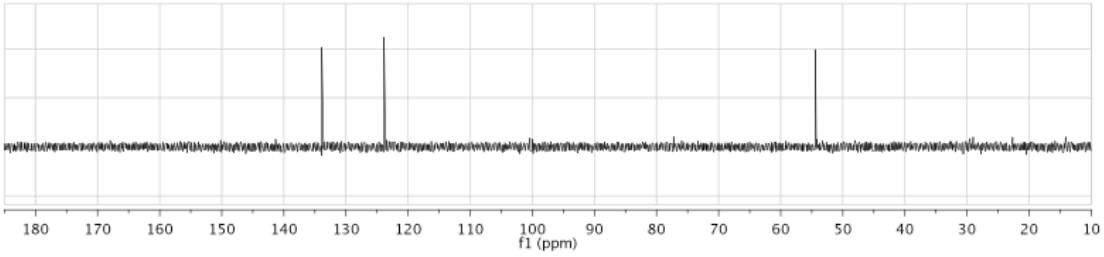


(*R*,*Z*)-5-Non-2-enyl)pyrrolidine-2-one (22)

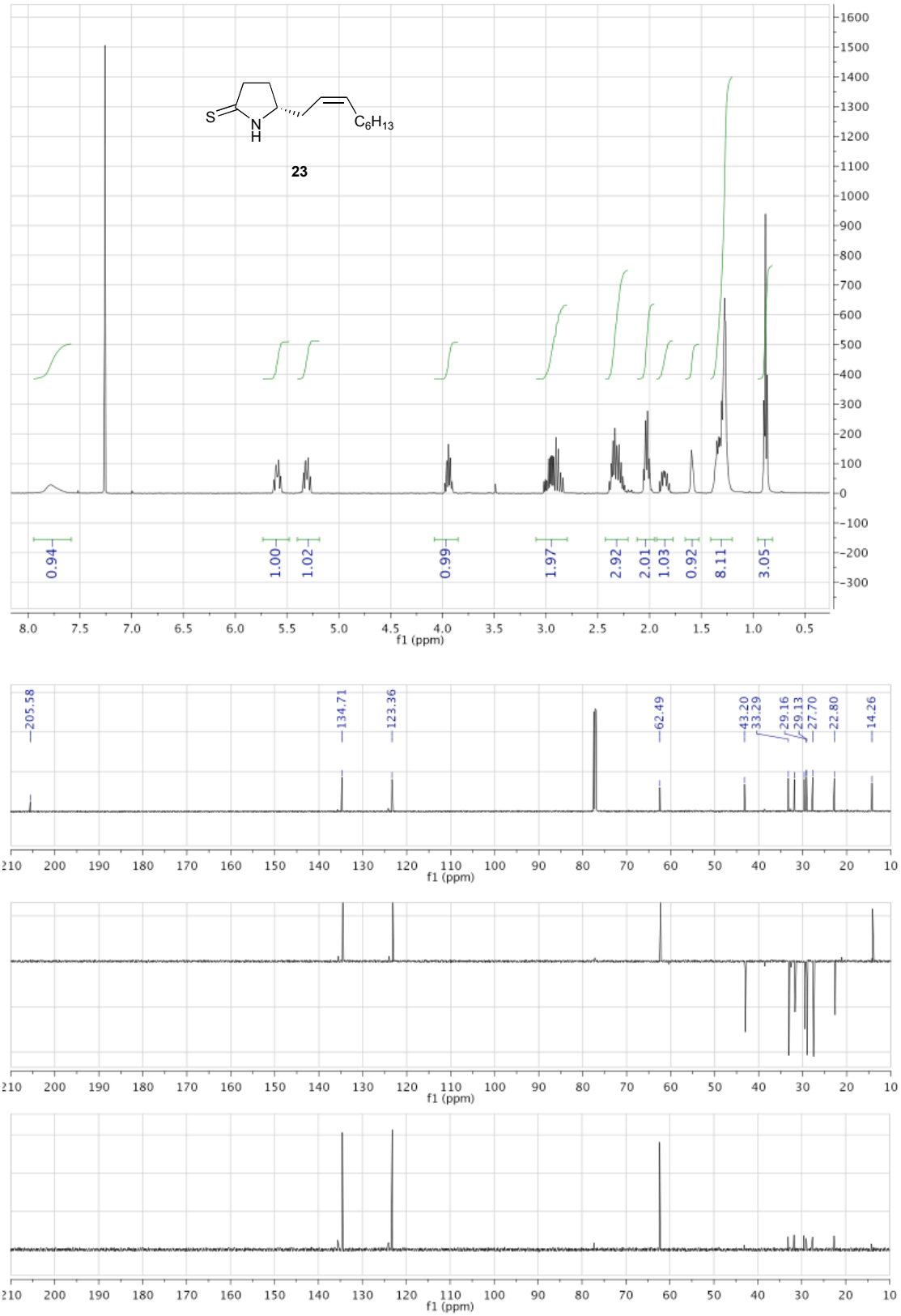




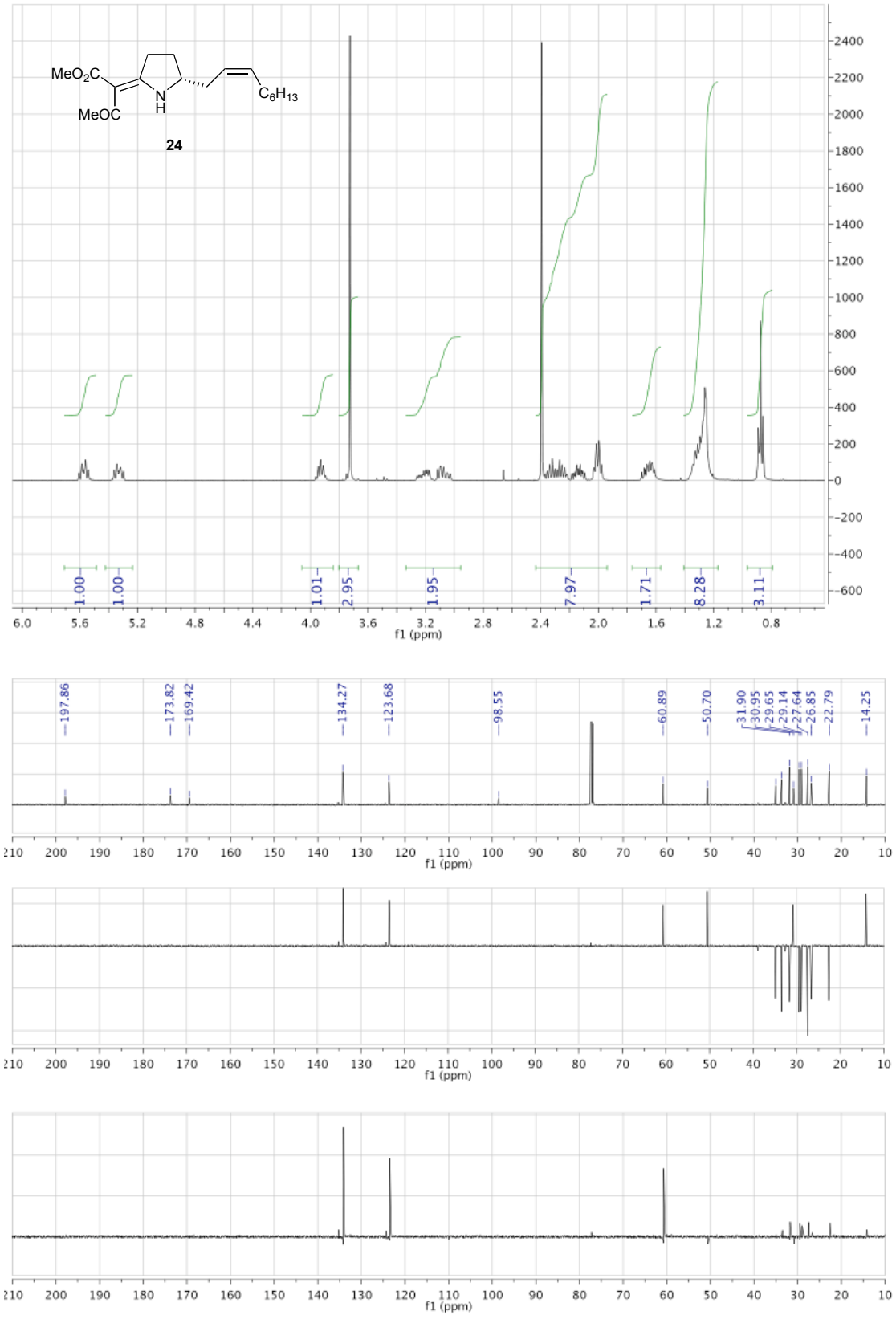




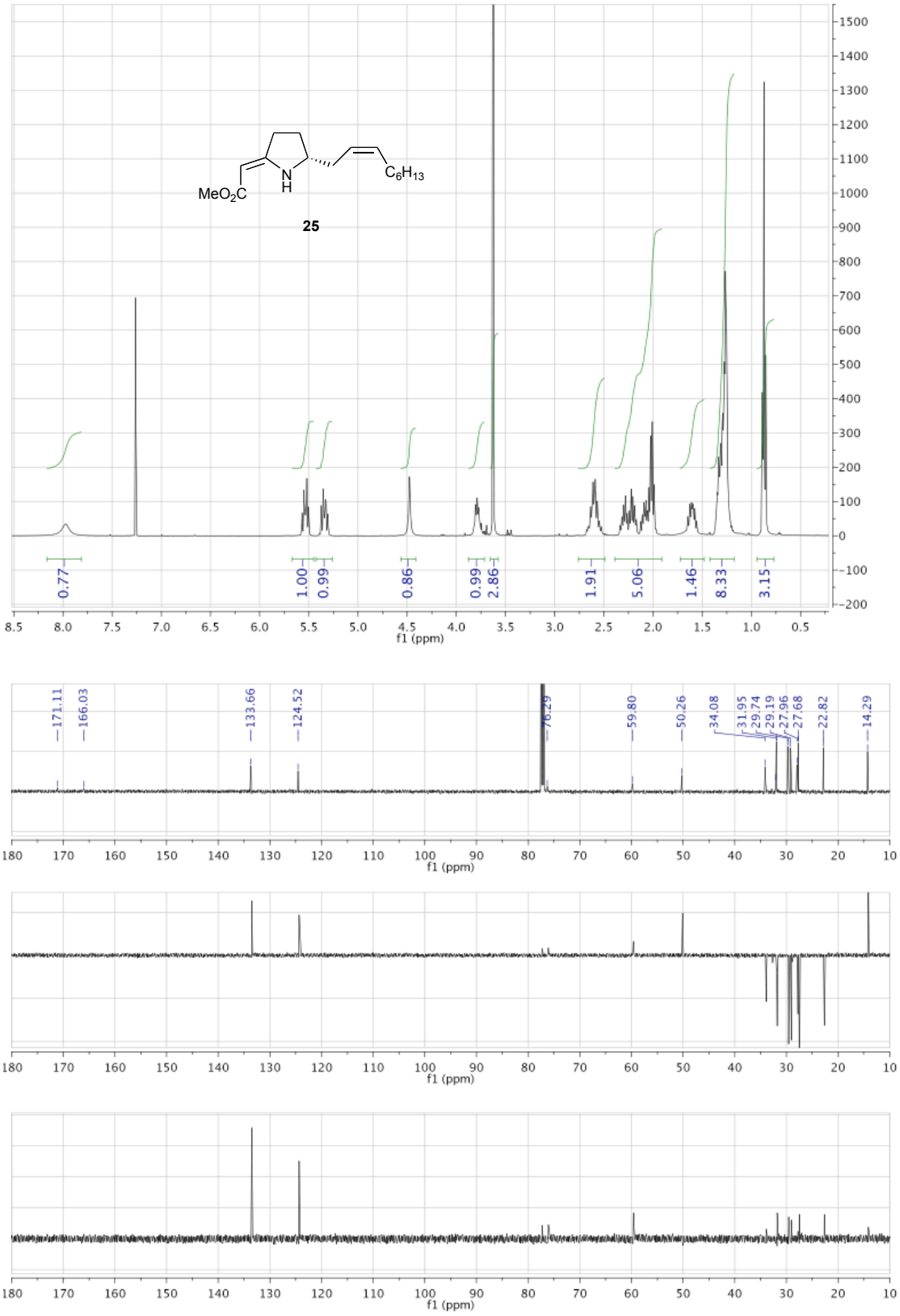
(*R*,*Z*)-5-Non-2-enyl)pyrrolidine-2-thione (23)



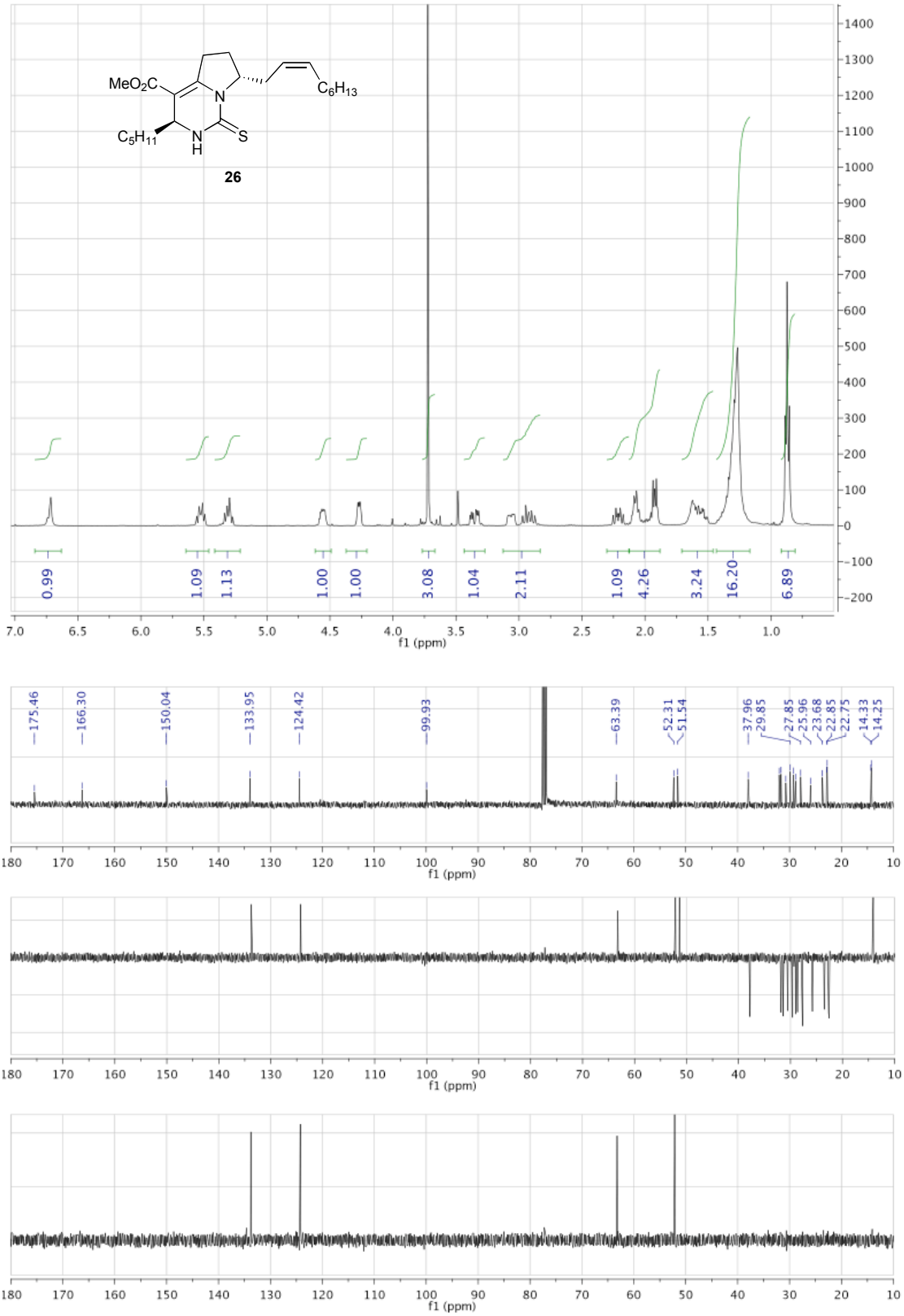
(*E*)-Methyl 2-((*R*)-5-((*Z*)-non-2-enyl)pyrrolidin-2-ylidene)-3-oxobutanoate (24)



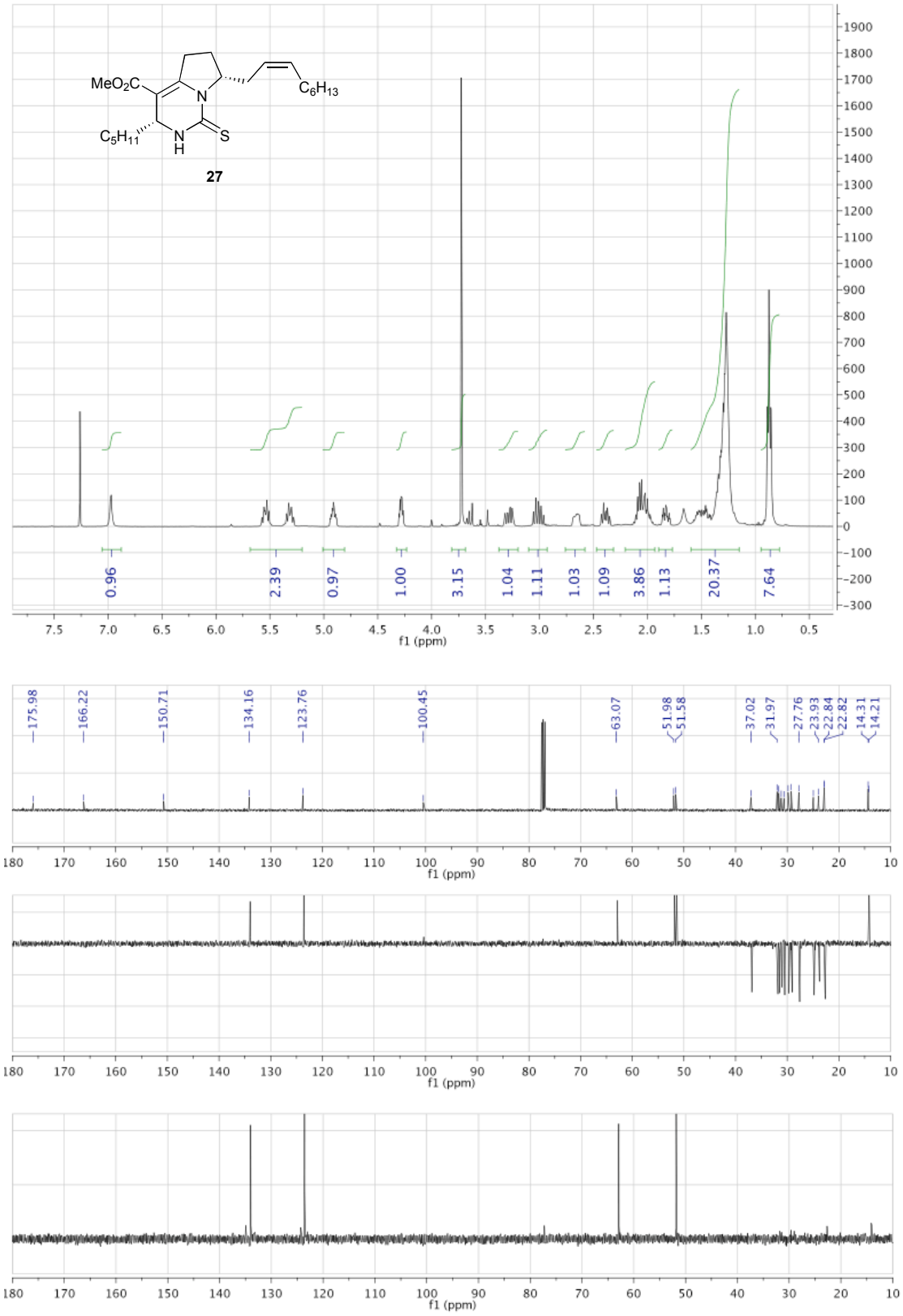
(*Z*)-Methyl 2-(*R*)-5-((*Z*)-non-2-enyl)pyrrolidin-2-ylidene)acetate (25)



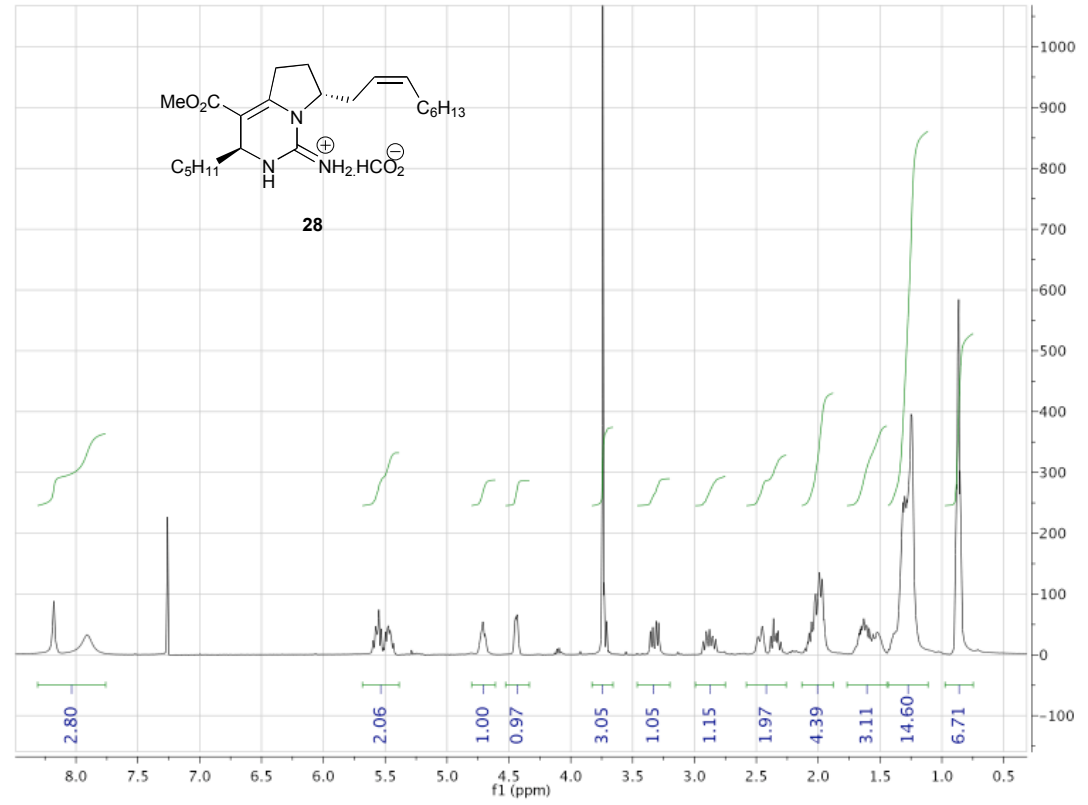
(3*S*,7*R*)-Methyl 1,2,3,5,6,7-hexahydro-7-((*E*)-non-2-enyl)-3-pentyl-1-thioxopyrrolo[1,2-*c*]pyrimidine-4-carboxylate (26)

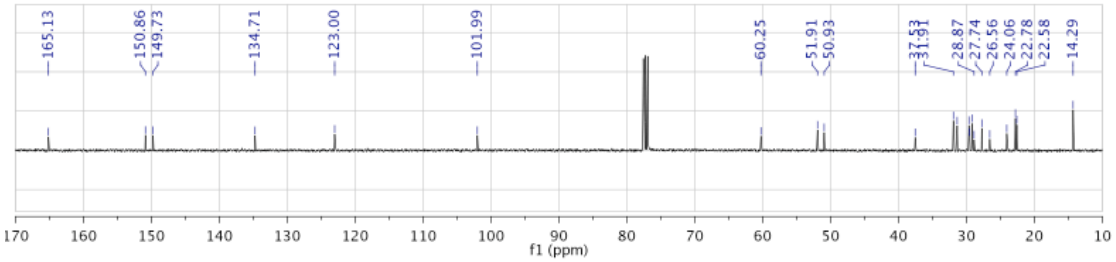


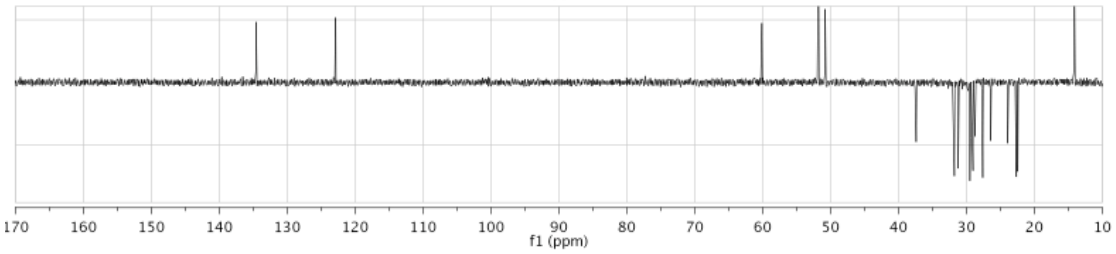
(3*R*,7*R*)-Methyl 1,2,3,5,6,7-hexahydro-7-((*E*)-non-2-enyl)-3-pentyl-1-thioxopyrrolo[1,2-*c*]pyrimidine-4-carboxylate (27)

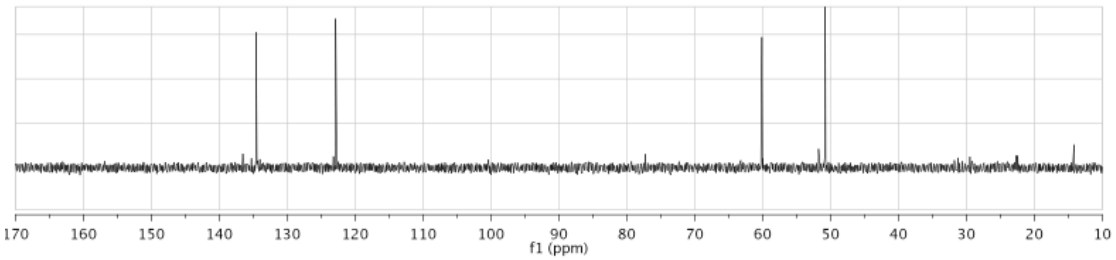


(3*S*,7*R*)-7-((*Z*)-Non-2-enyl)-4-(methoxycarbonyl)-3-pentyl-2,3,6,7-tetrahydropyrrolo[1,2-*c*]pyrimidine-1(5*H*)-iminium formate (28)

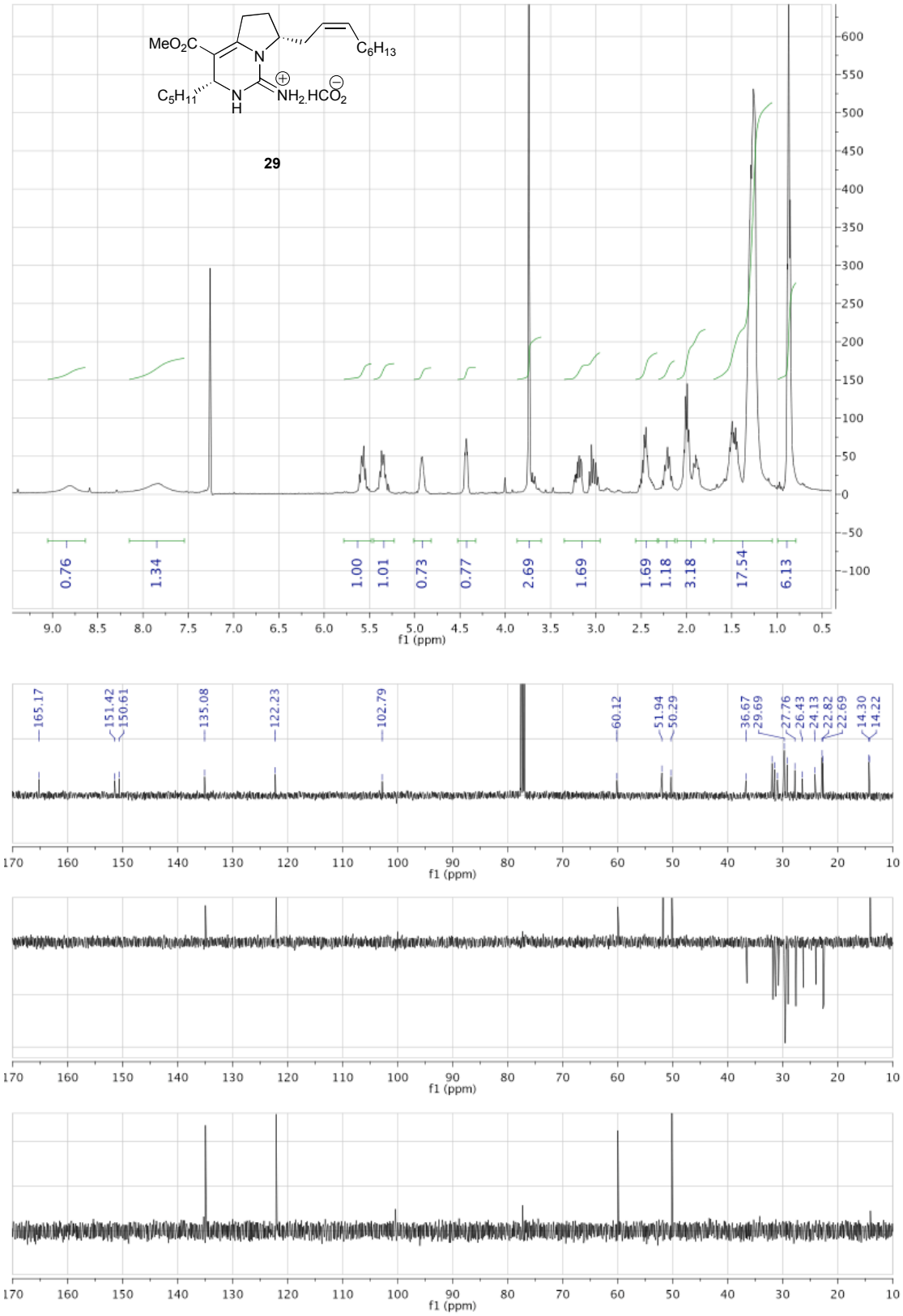






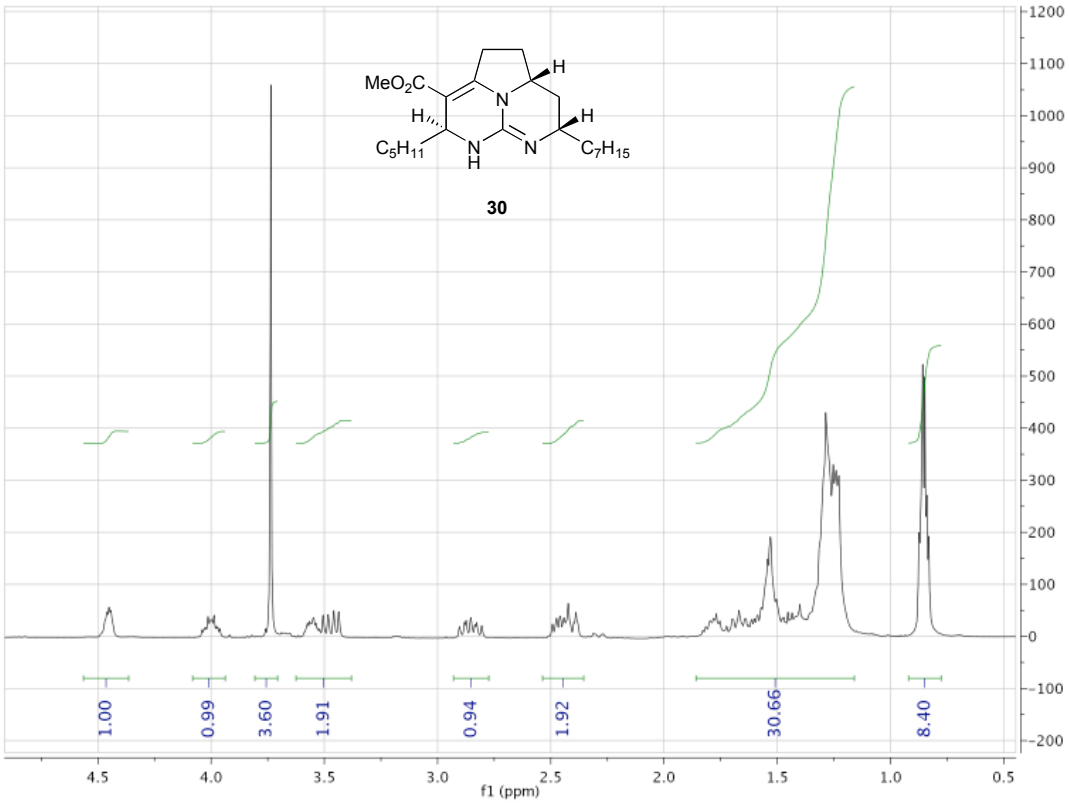


(3*R*,7*R*)-7-((*Z*)-Non-2-enyl)-4-(methoxycarbonyl)-3-pentyl-2,3,6,7-tetrahydropyrrolo[1,2-*c*]pyrimidine-1(5*H*)-iminium formate (29)

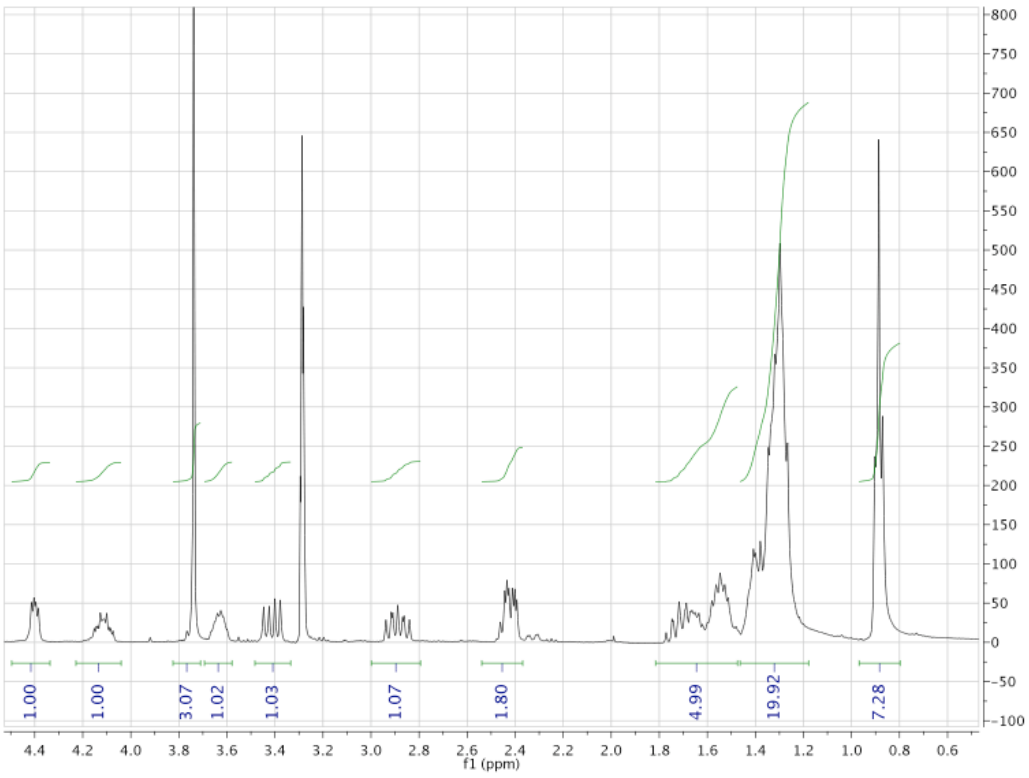


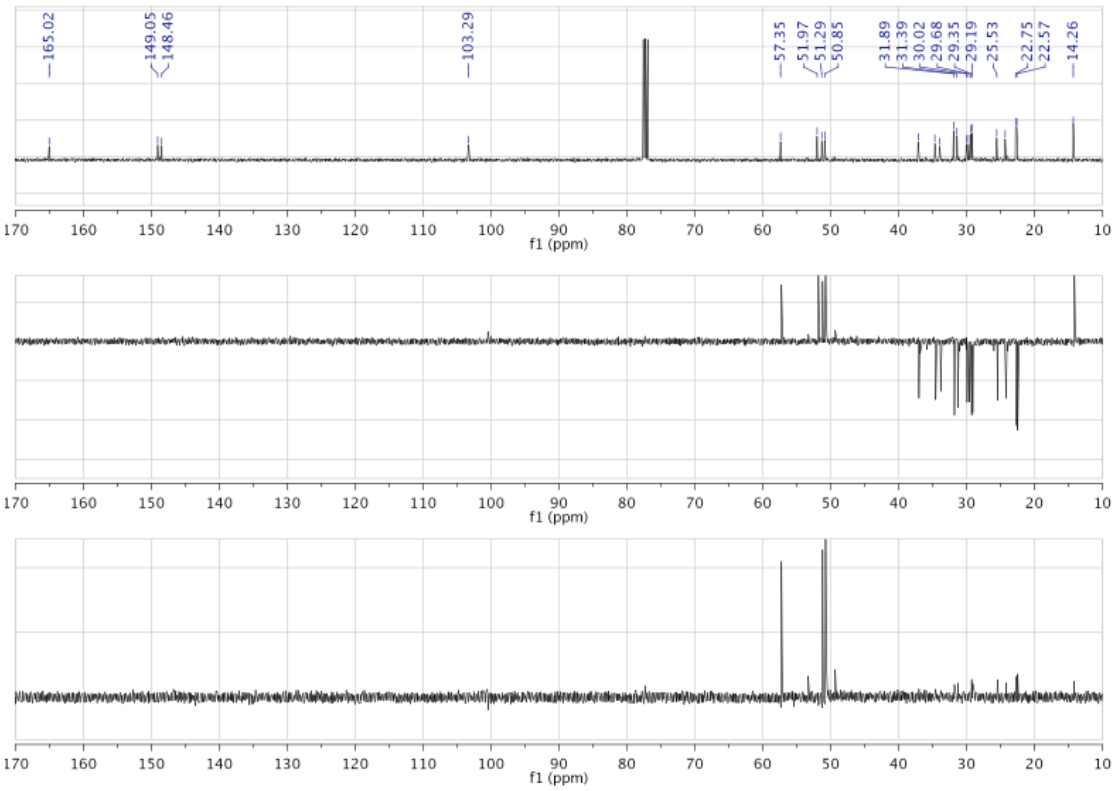
(4*S*,7*S*,8a*R*)-Methyl 7-heptyl-4-pentyl-1,2,4,5,7,8-hexahydro-11a*H*-2a^1,5,6-triaza-acenaphthylene-3-carboxylate (30)

In $CDCl_3$

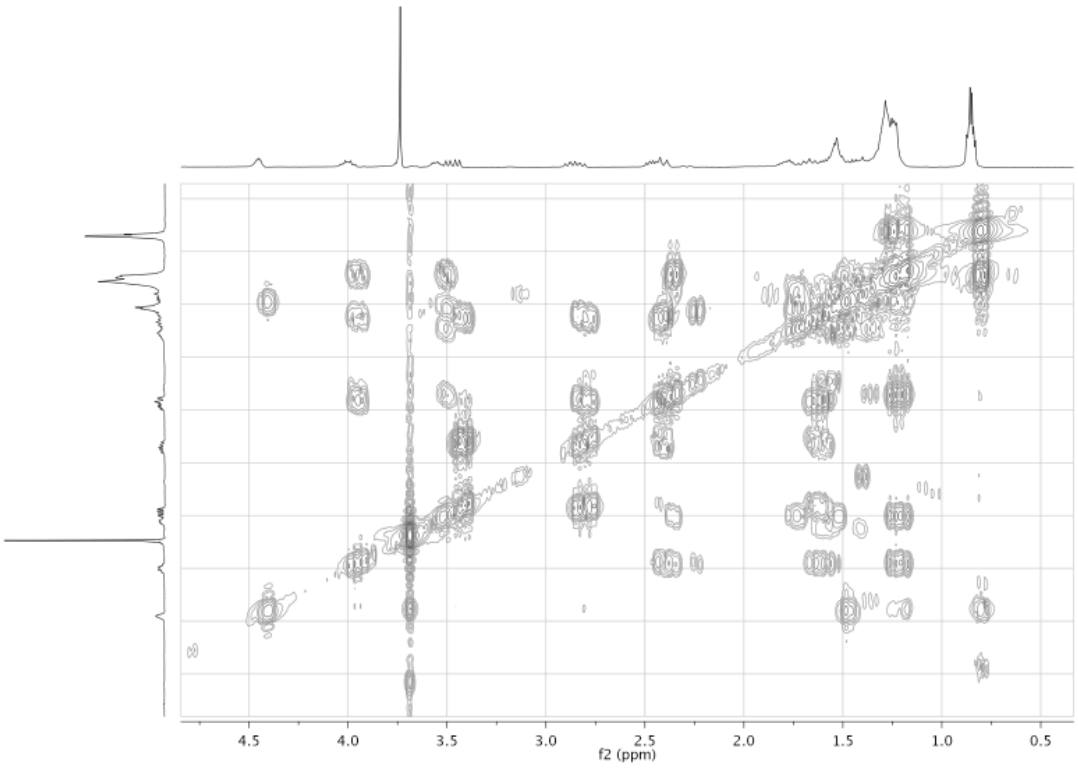


In CD_3OD

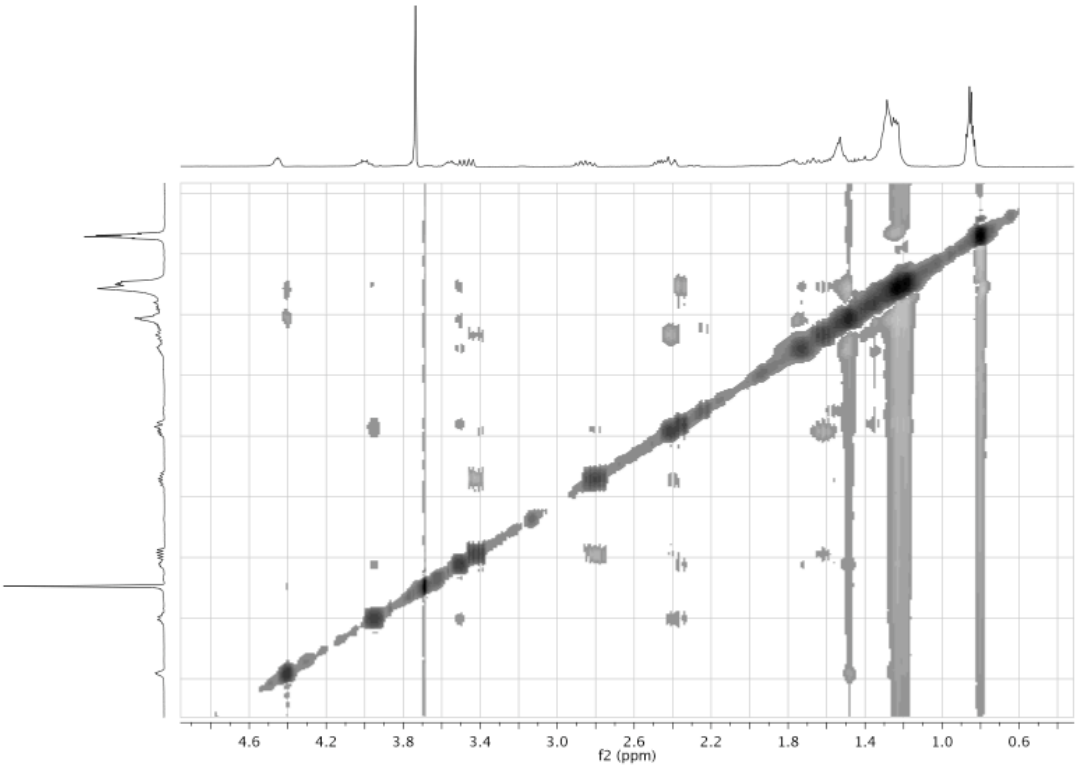



165.02
149.05
148.46
103.29
57.35
51.97
51.29
50.85
31.89
31.39
30.02
29.68
29.35
29.19
25.53
22.75
22.57
14.26
f1 (ppm)

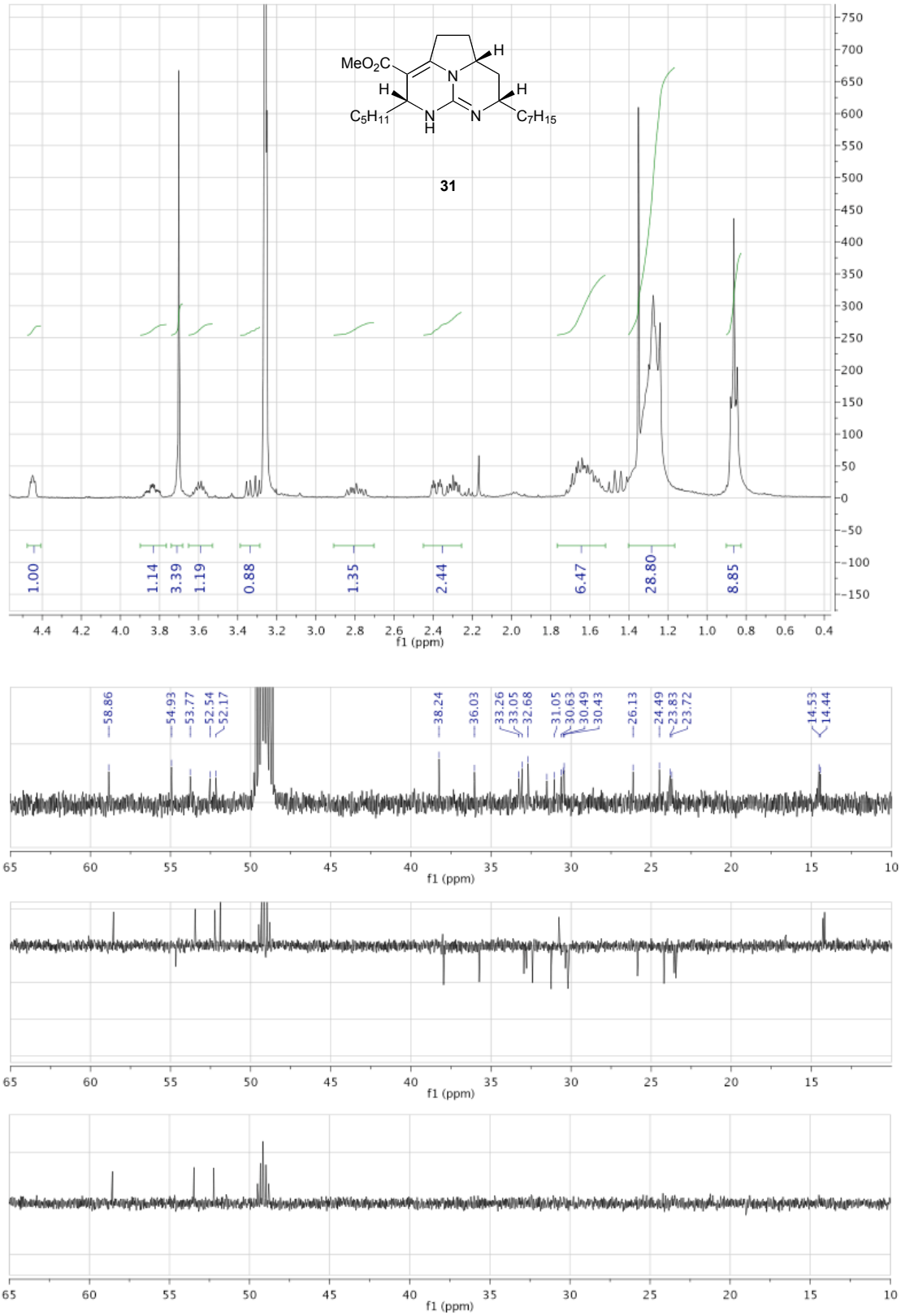
^{1}H-^{1}H COSY


f2 (ppm)

g-NOESY

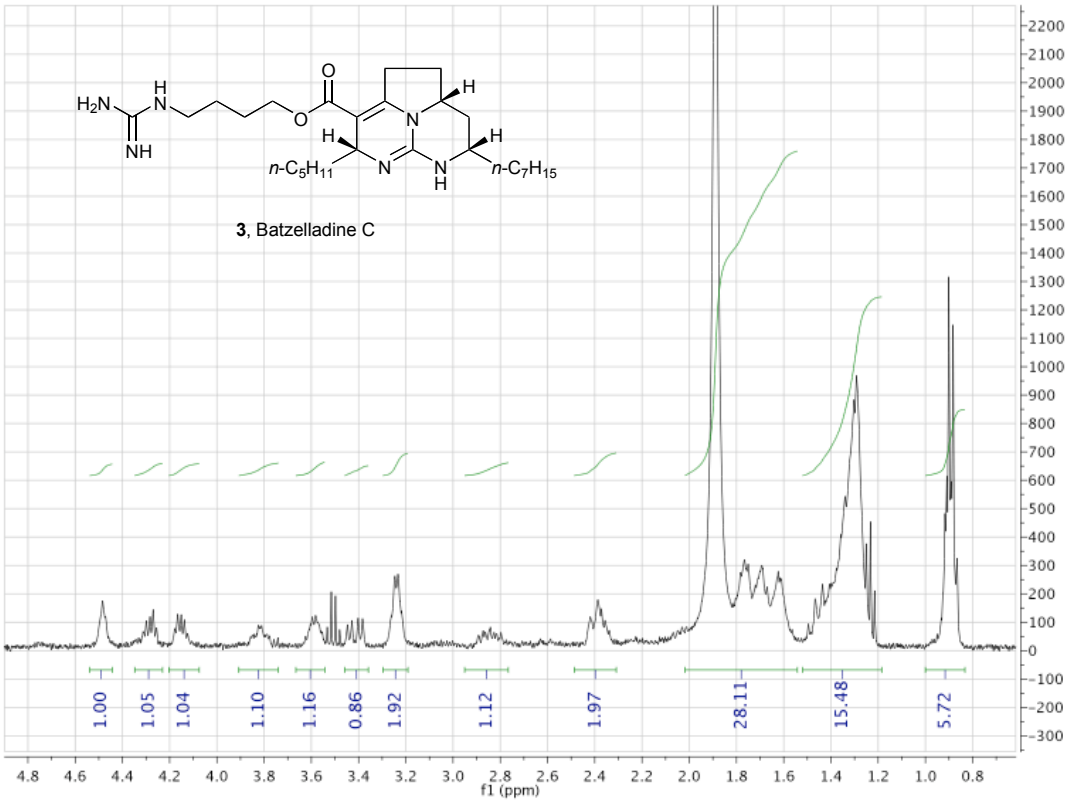


(4*R*,7*S*,8a*R*)-Methyl 7-heptyl-4-pentyl-1,2,4,5,7,8-hexahydro-11a*H*-2a^1,5,6-triaza-acenaphthylene-3-carboxylate (batzelladine C methyl ester) (31)



Batzelladine C (3)

In $CDCl_3$



In CD_3OD