

Supporting Information, Part D

Small-Molecule Inhibitors of Protein Geranylgeranyltransferase Type I

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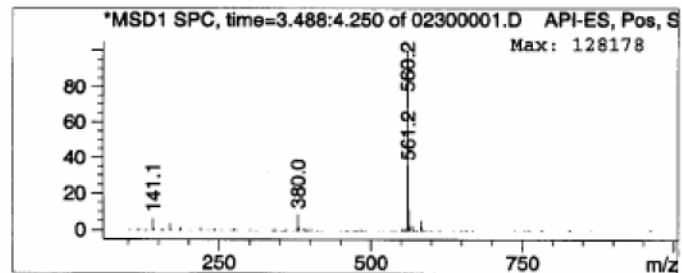
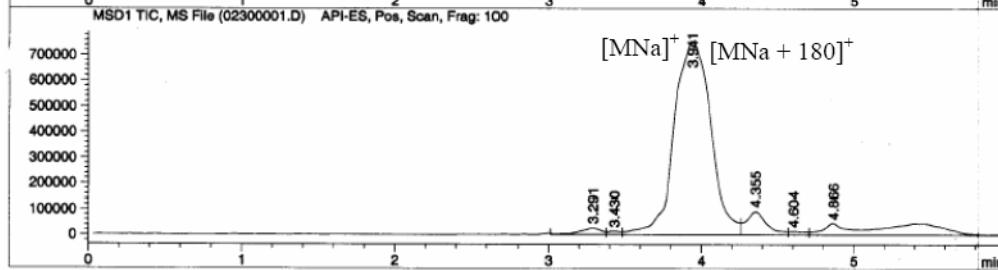
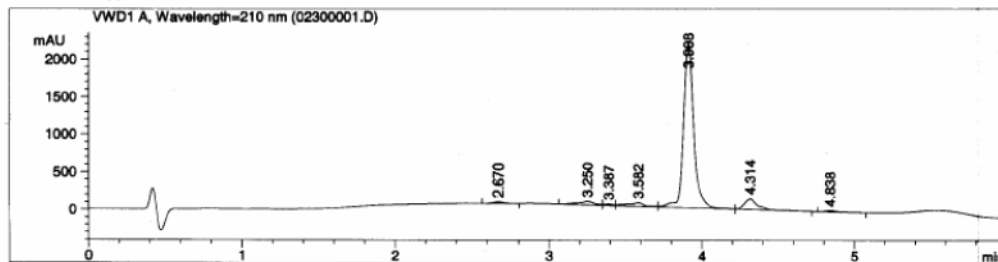
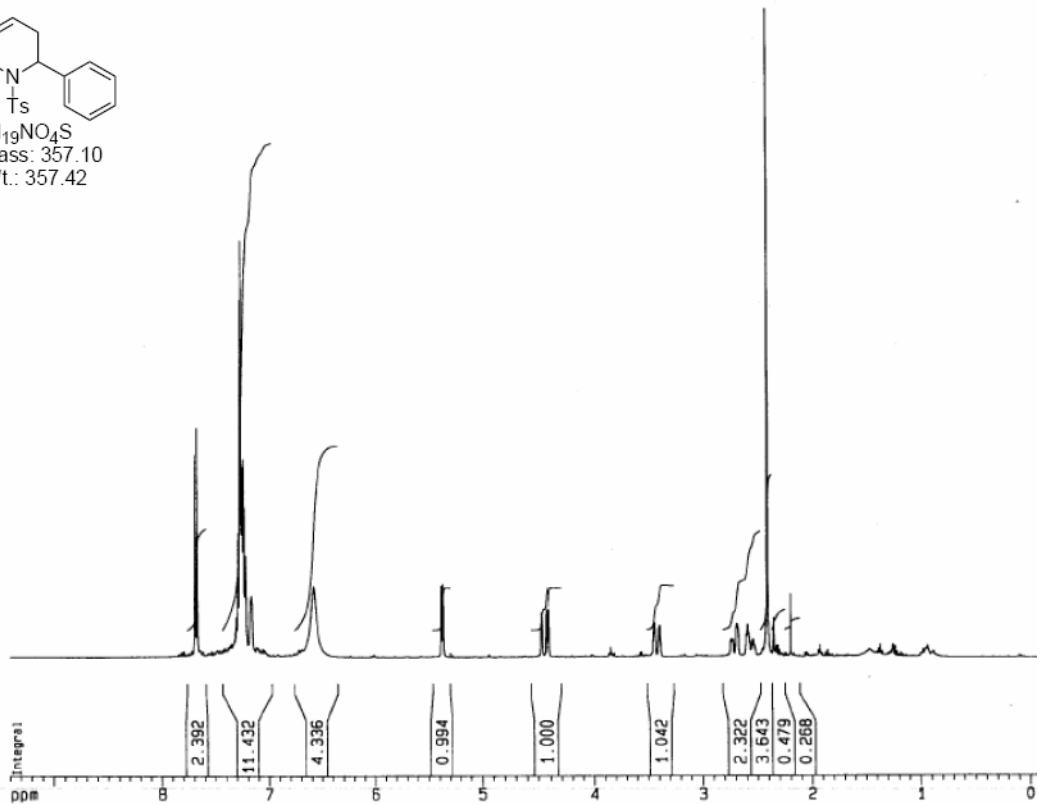
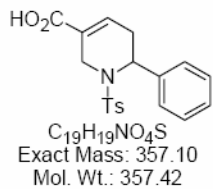
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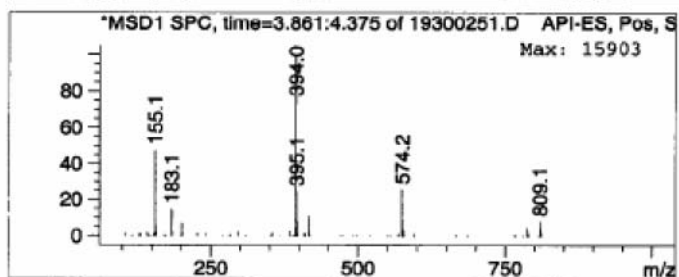
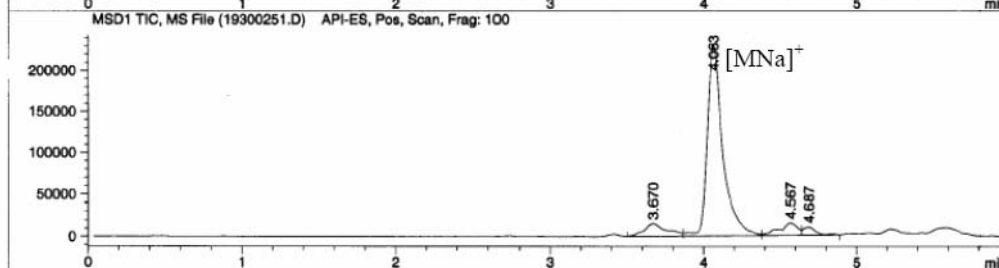
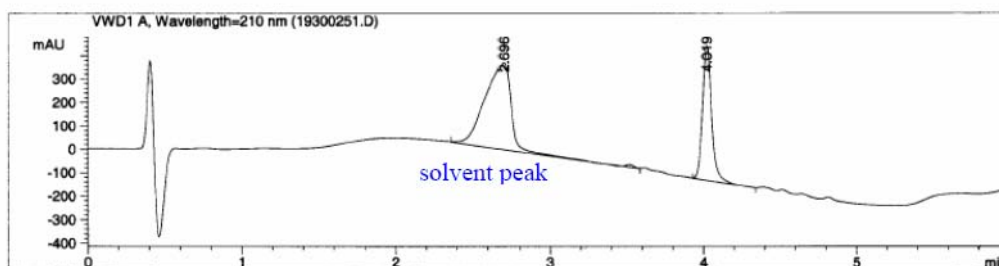
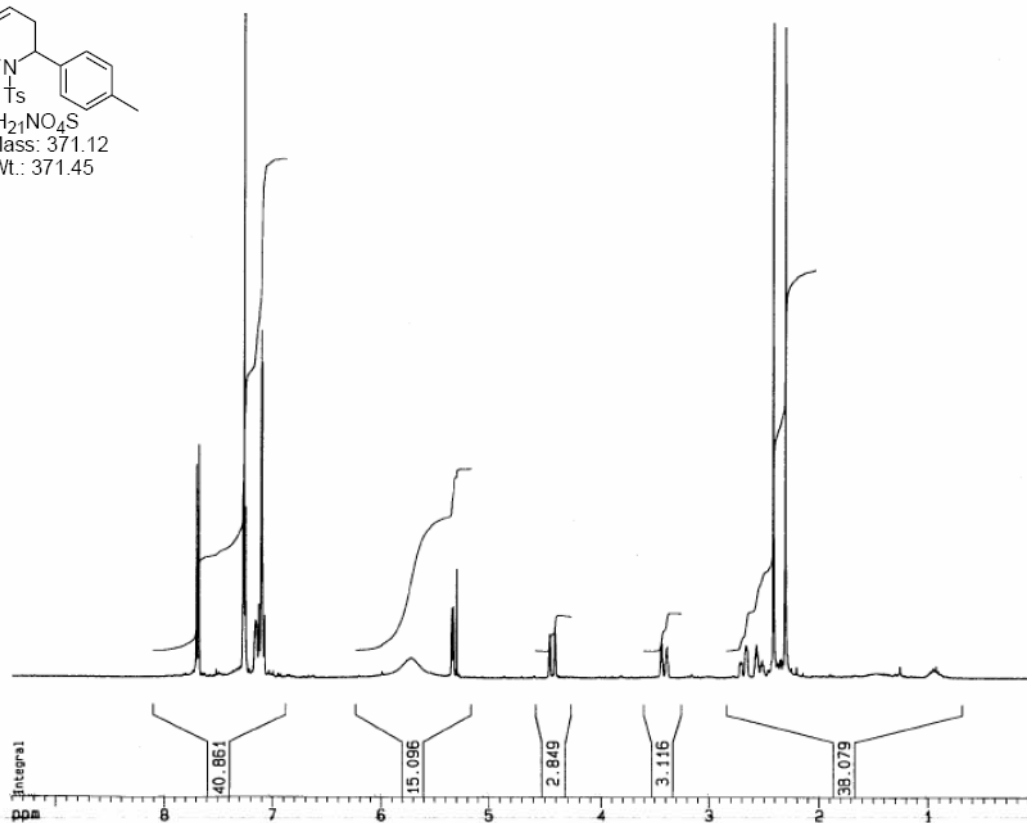
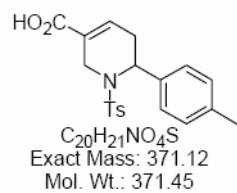
¹ Department of Microbiology, Immunology and Molecular Genetics

Spectral Data for Table 6

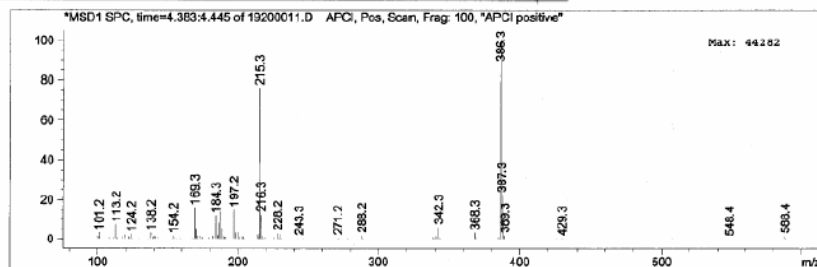
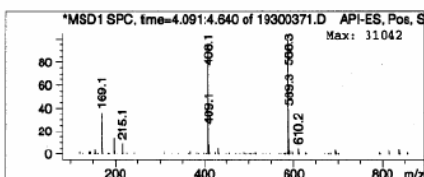
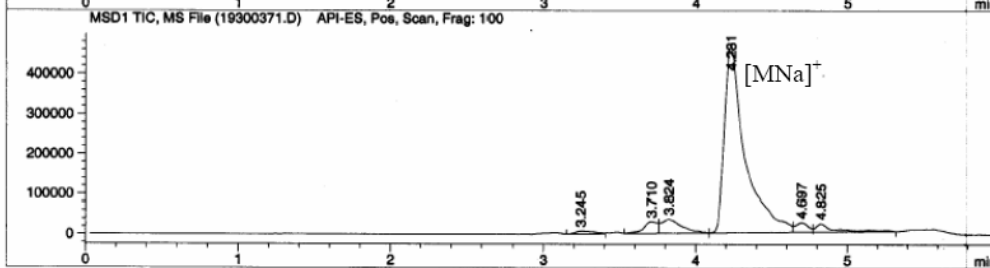
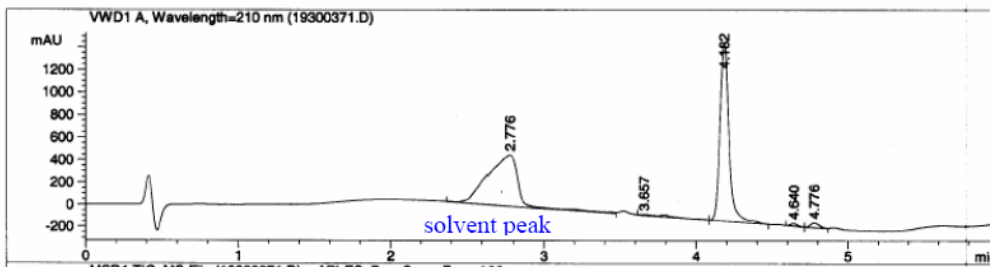
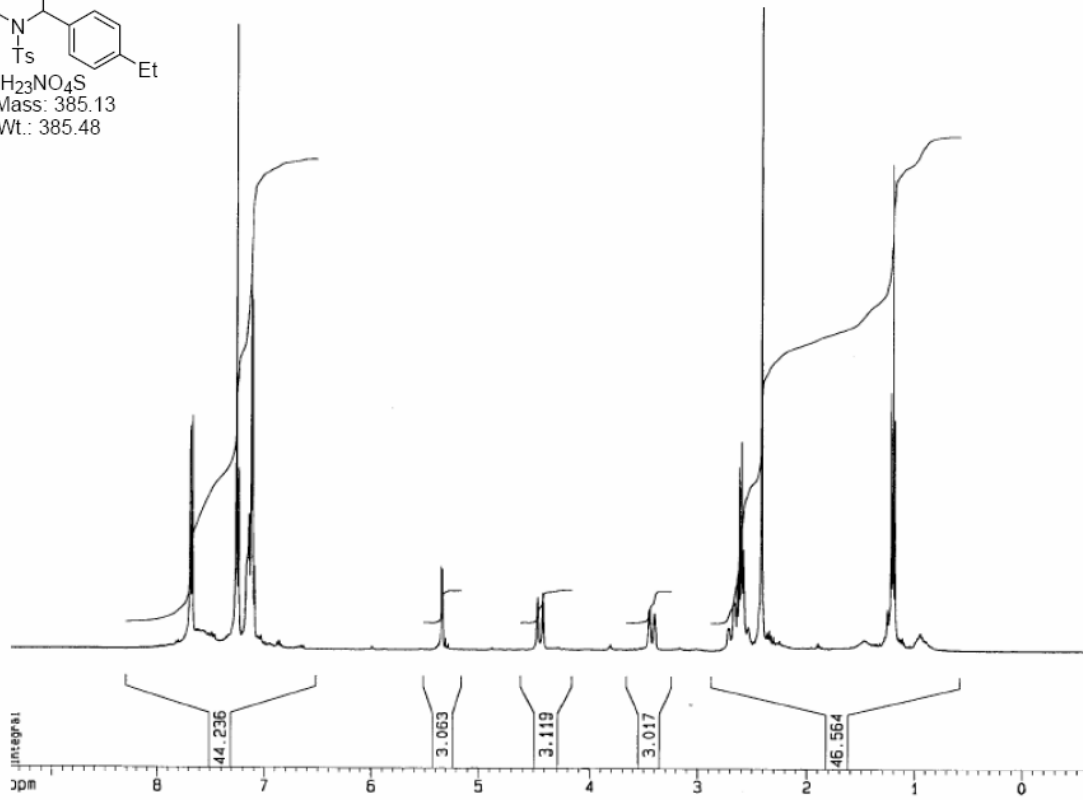
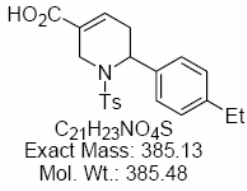
6-Phenyl-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C01)



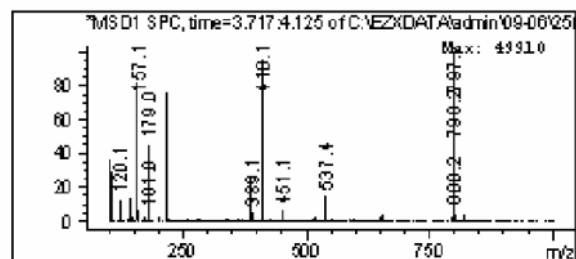
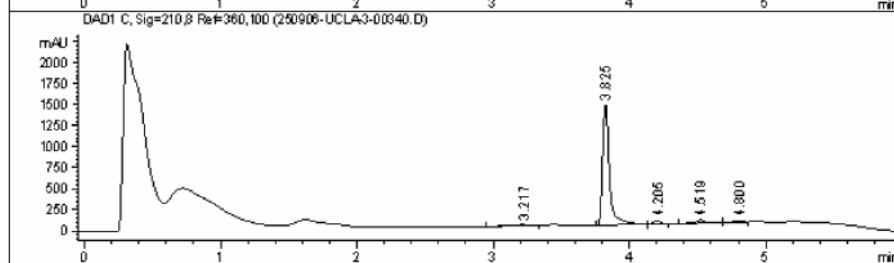
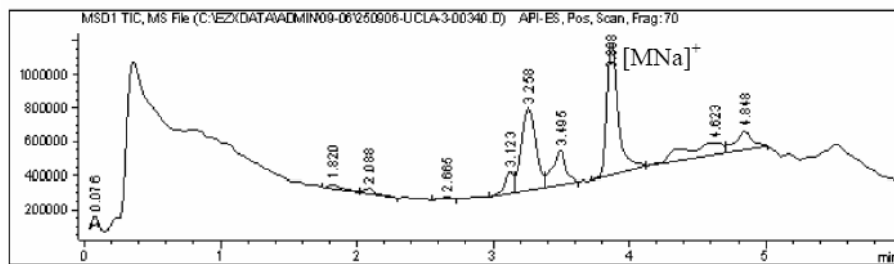
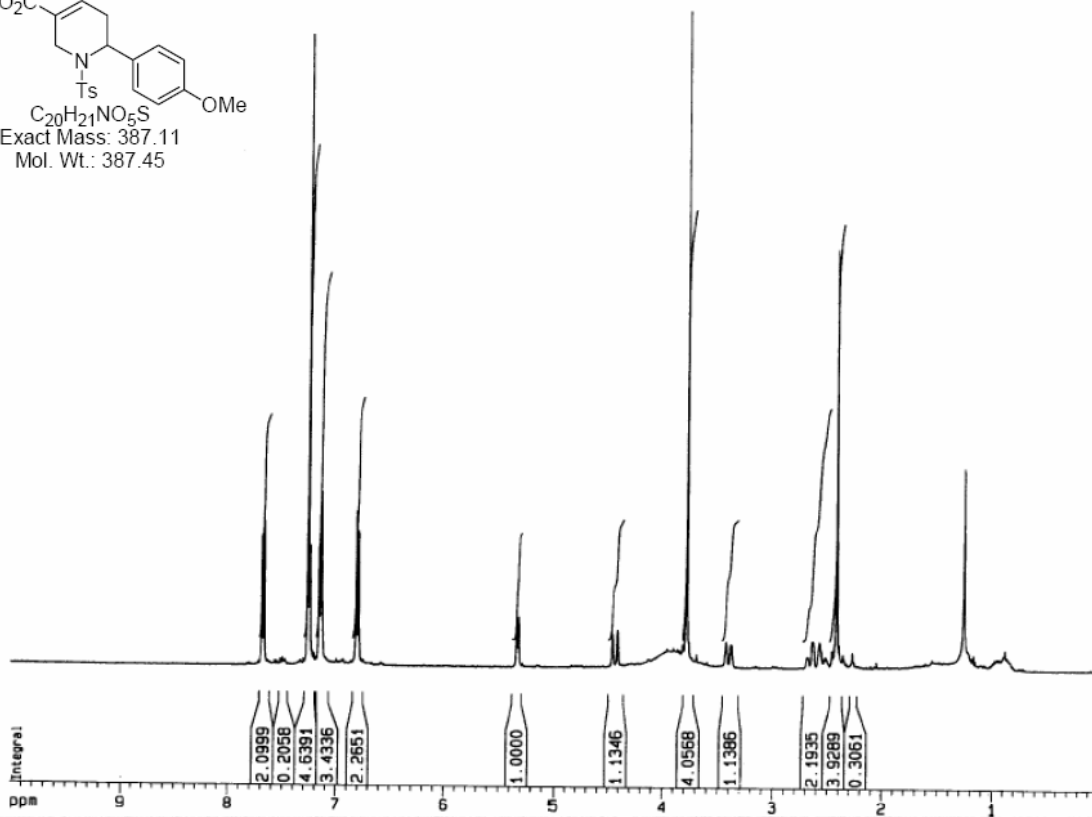
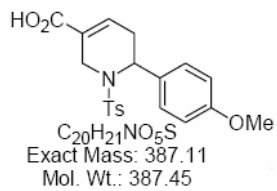
1-(4-Toluenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C02)



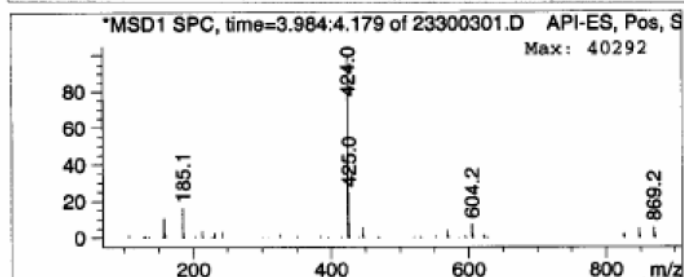
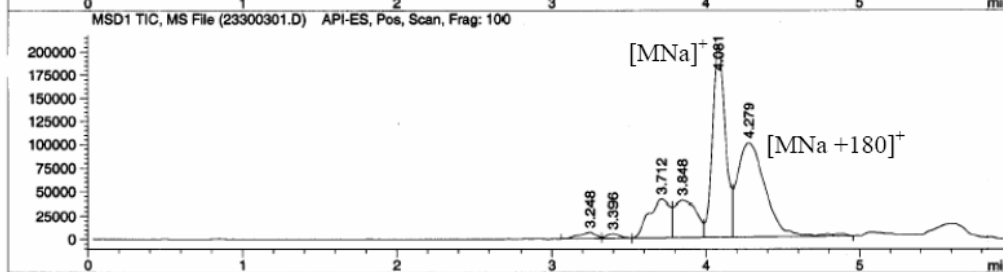
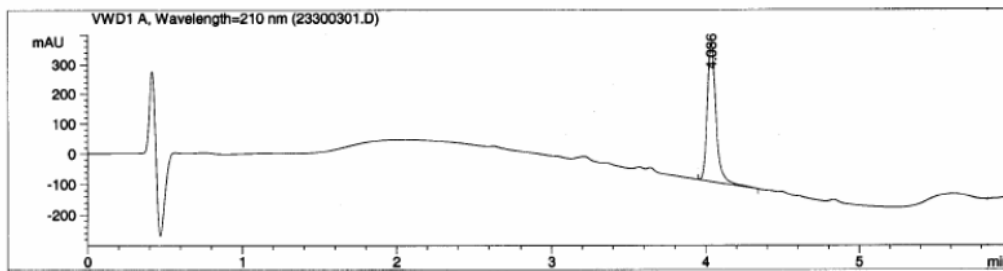
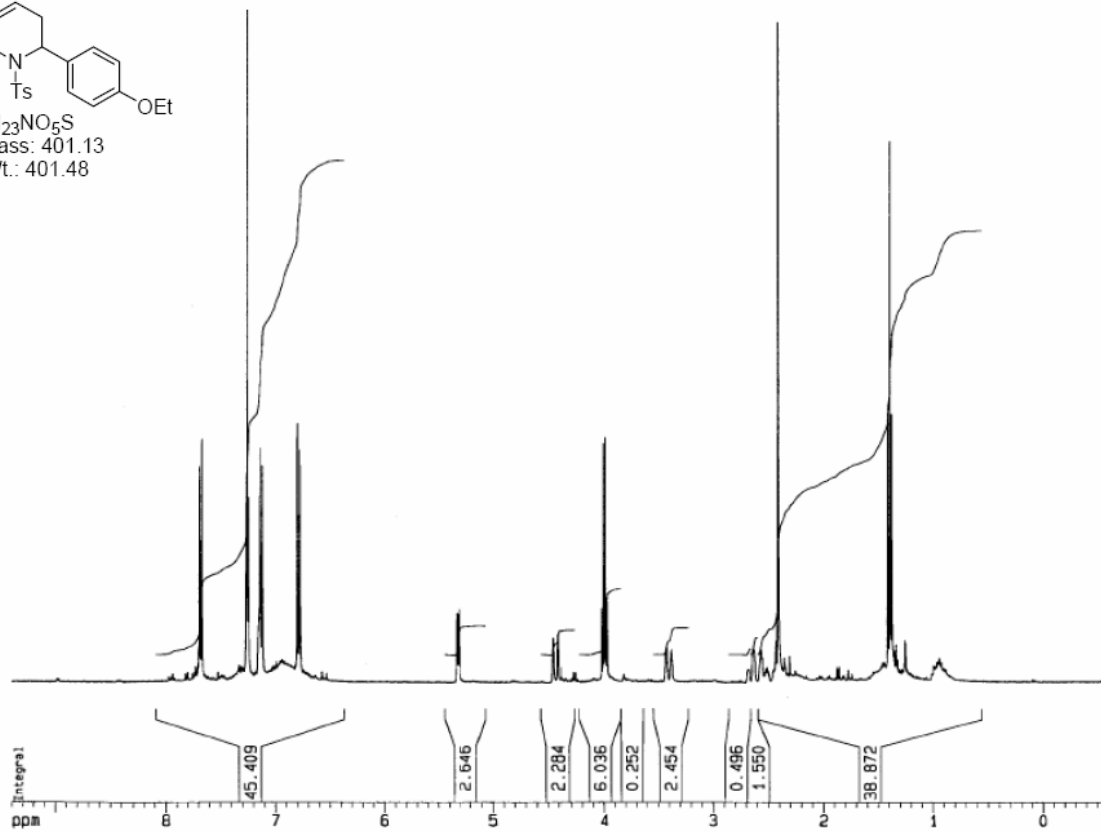
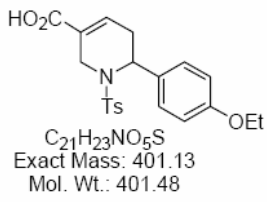
6-(4-Ethylphenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C03)



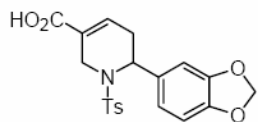
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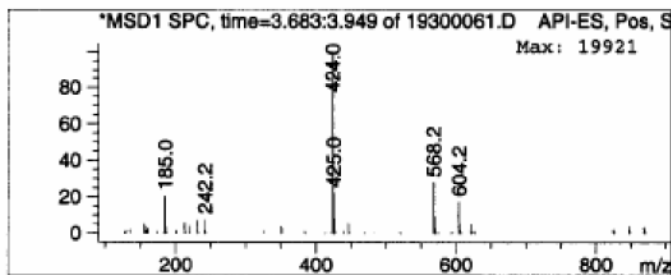
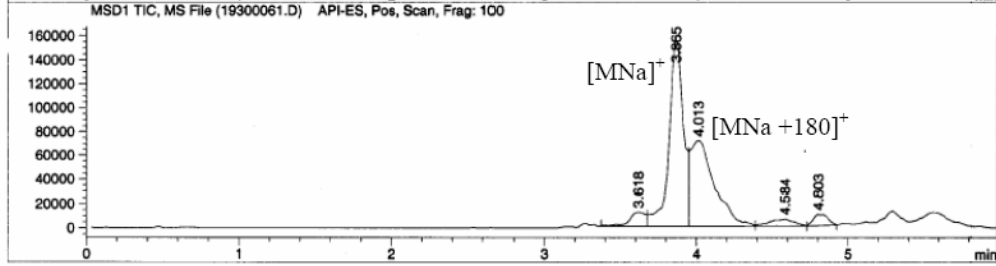
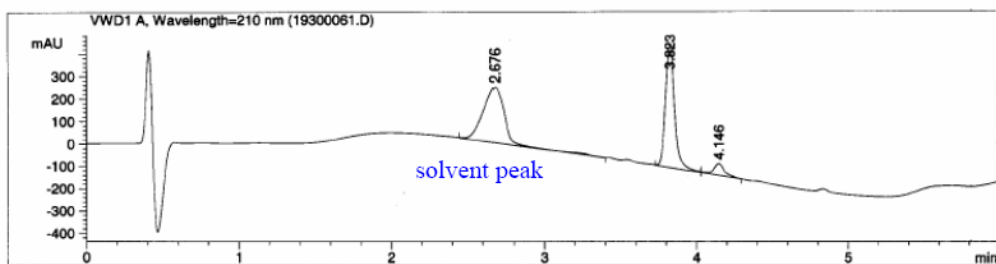
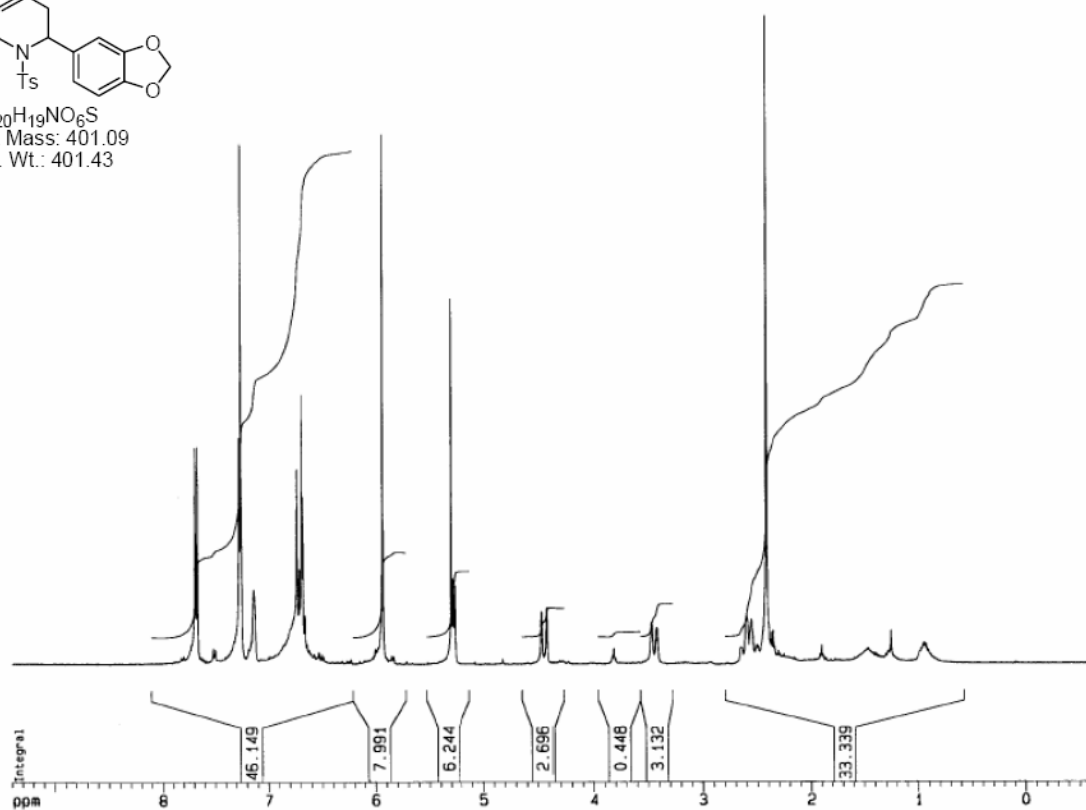
6-(4-Ethoxyphenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C05)



6-(Benzo[1,3]dioxol-5-yl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C06)

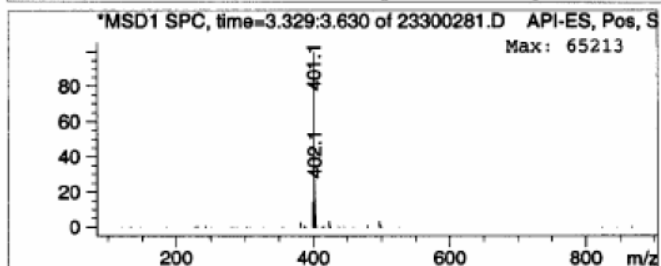
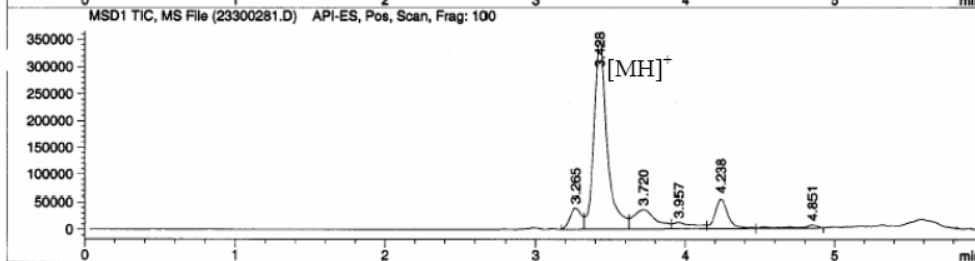
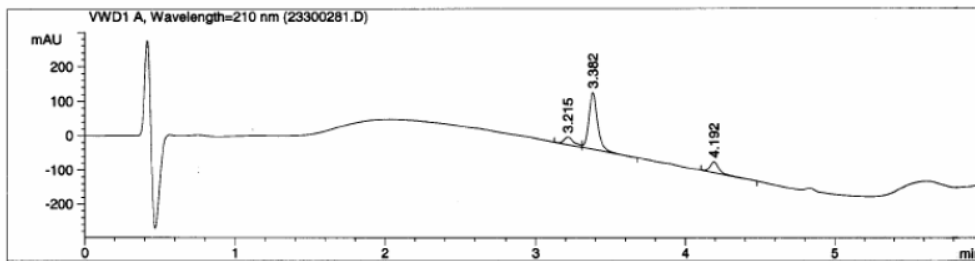
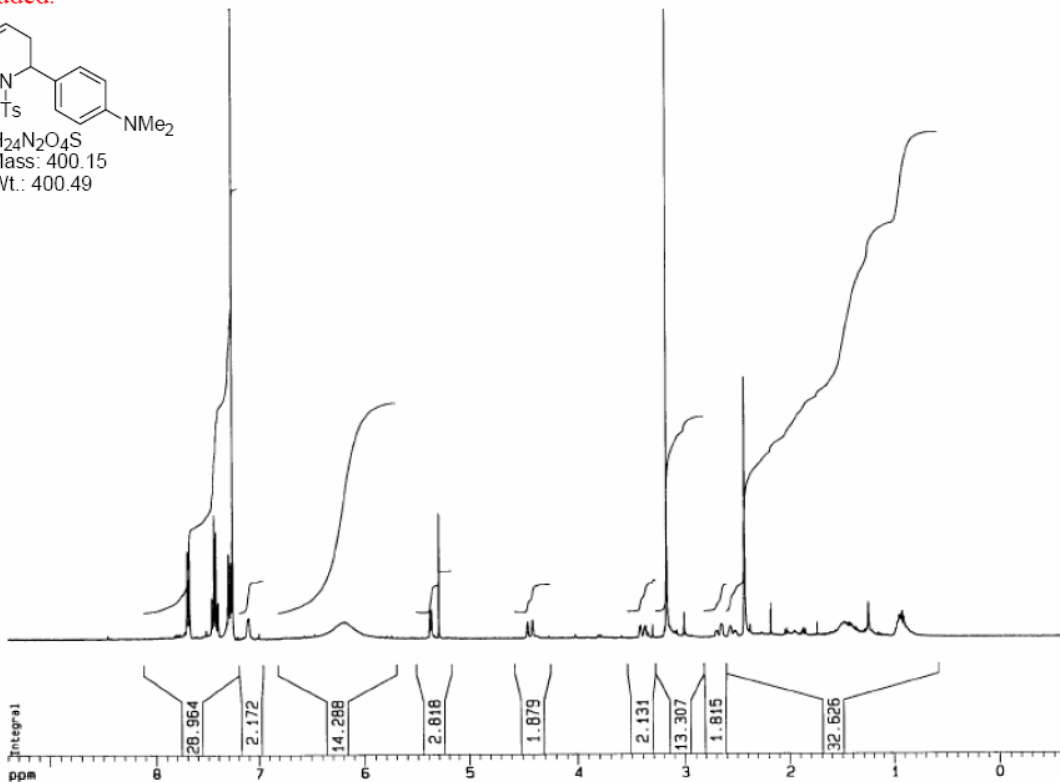
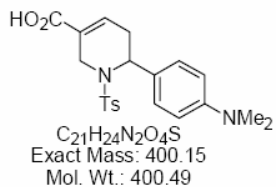


C₂₀H₁₉NO₆S
 Exact Mass: 401.09
 Mol. Wt.: 401.43



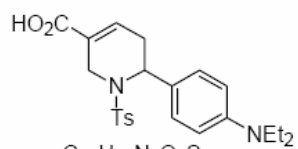
6-(4-Dimethylaminophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C07)

Not included.

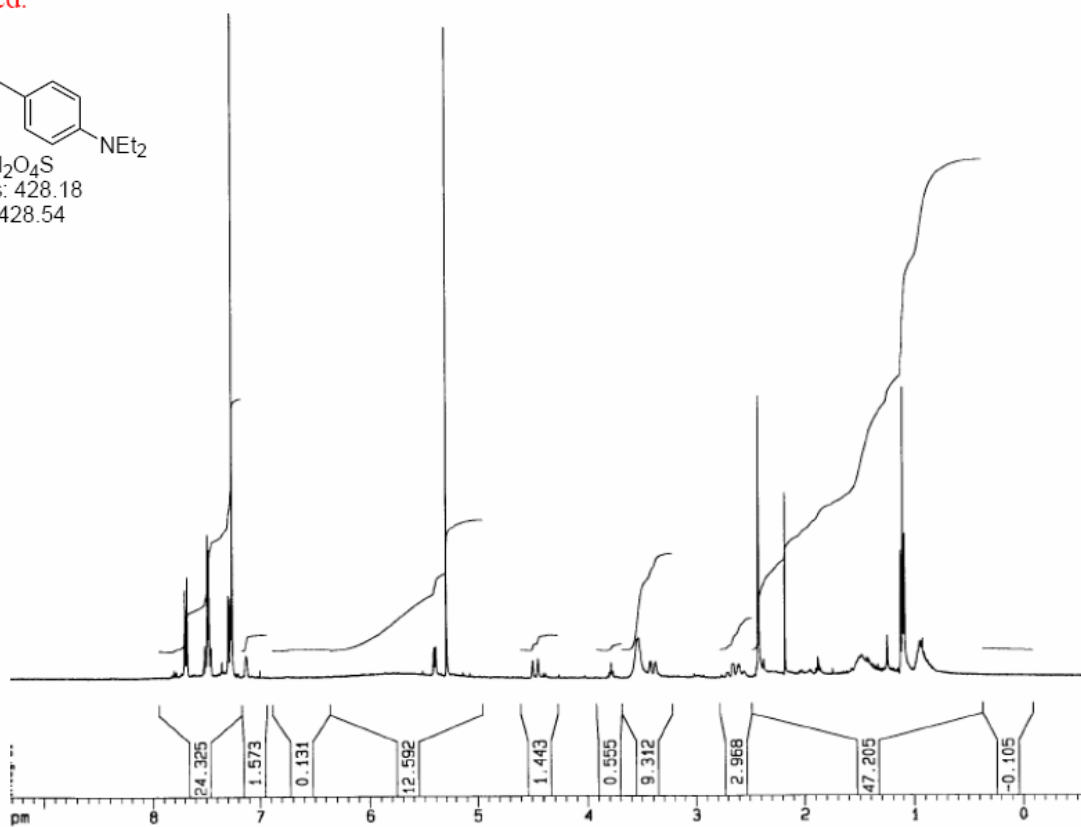


6-(4-Diethylaminophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C08)

Not included.

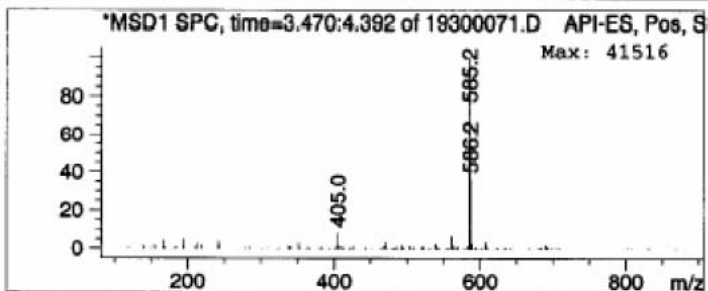
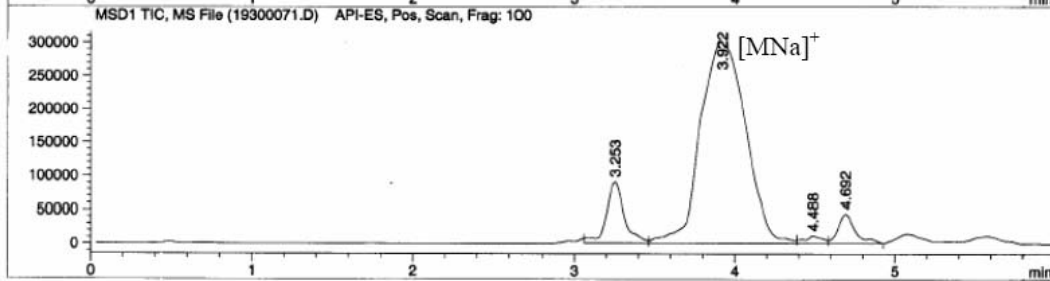
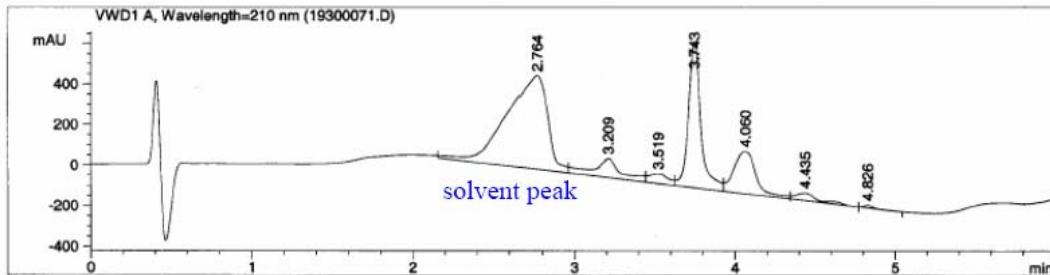
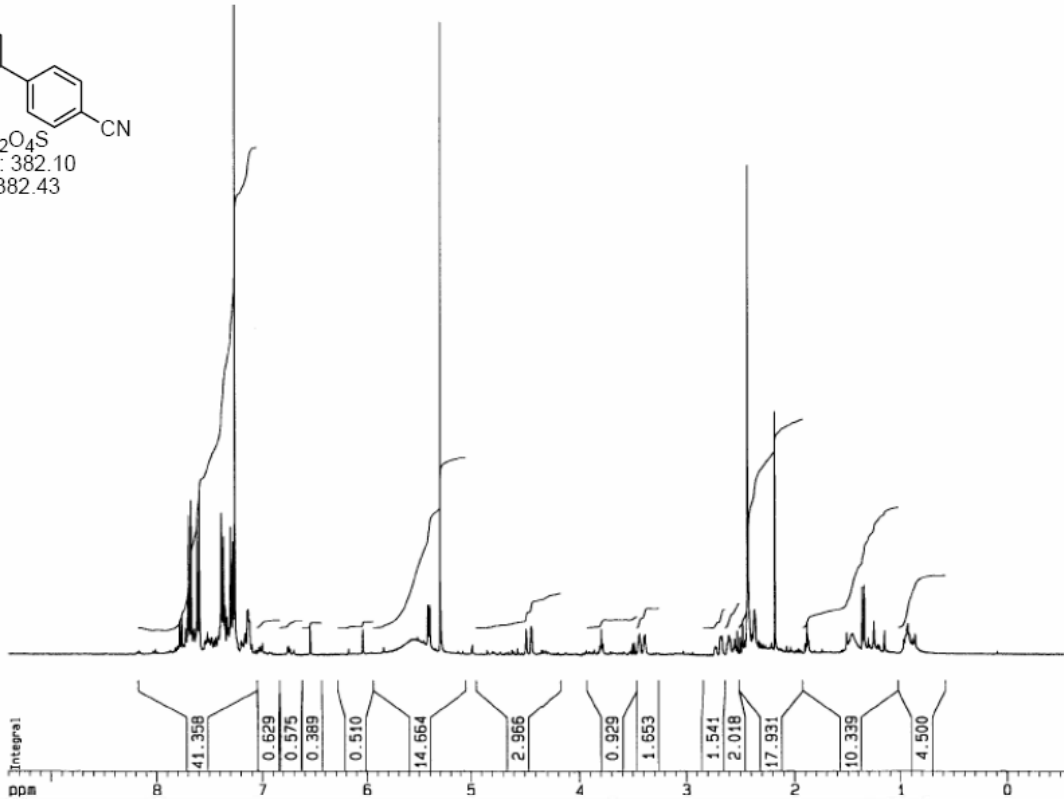
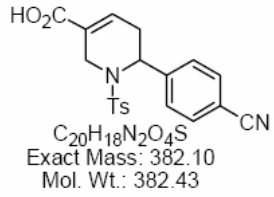


$C_{23}H_{28}N_2O_4S$
Exact Mass: 428.18
Mol. Wt.: 428.54

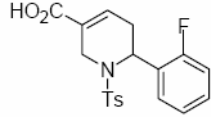


6-(4-Cyanophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C09)

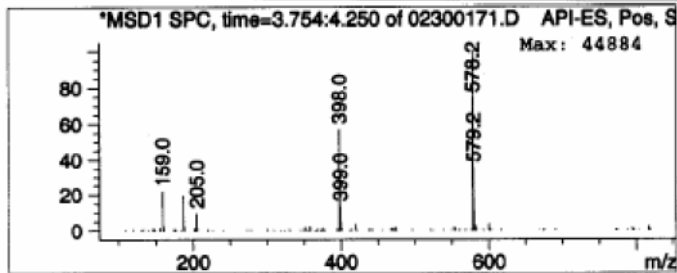
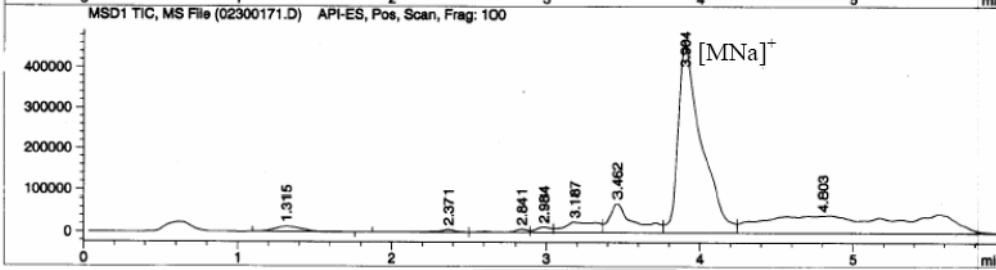
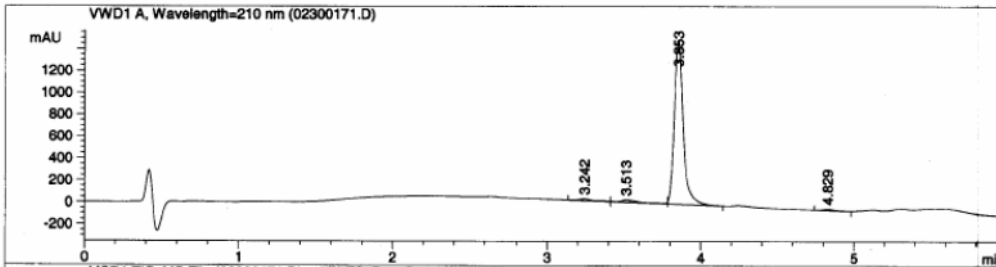
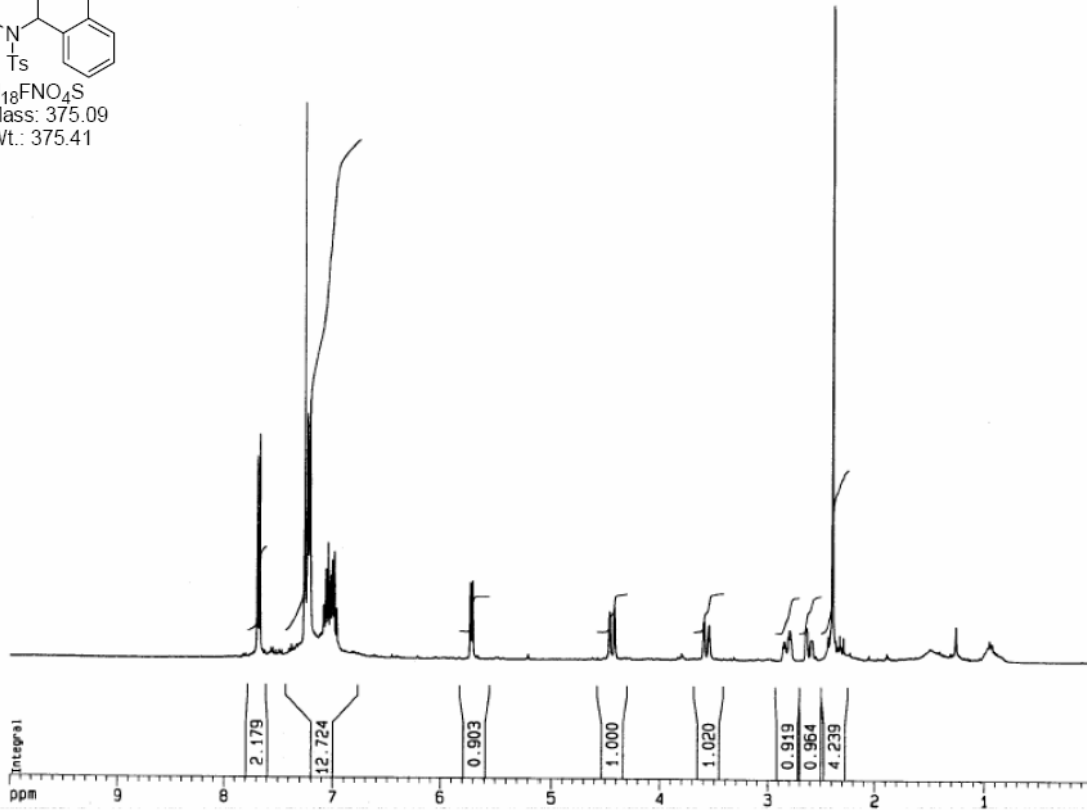
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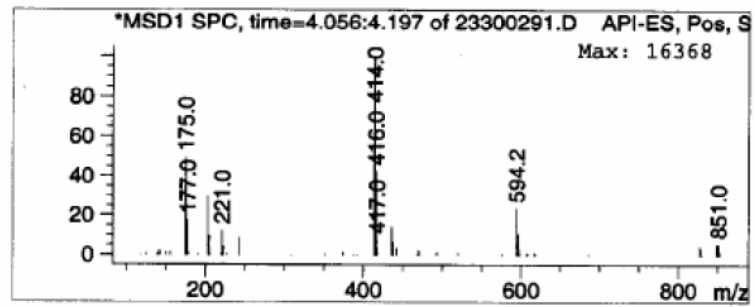
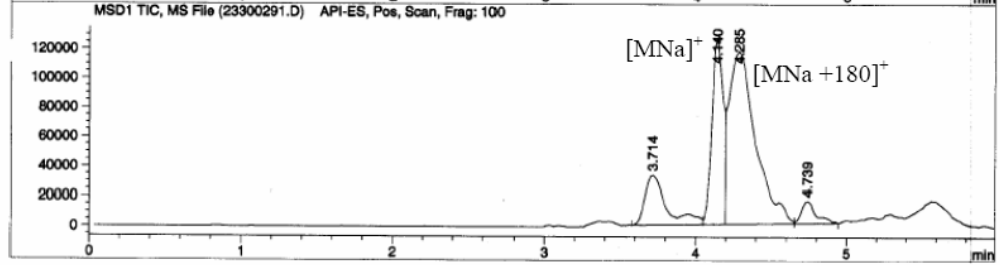
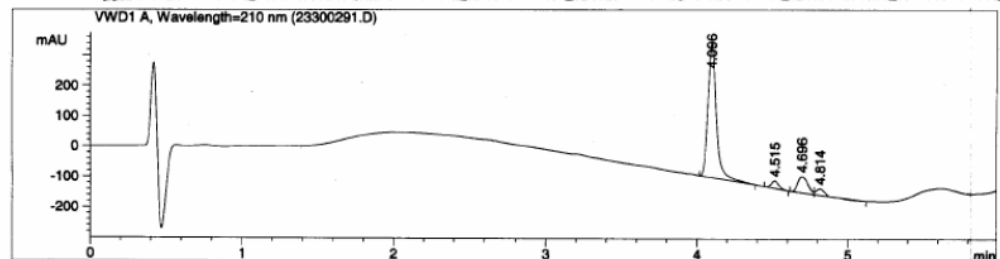
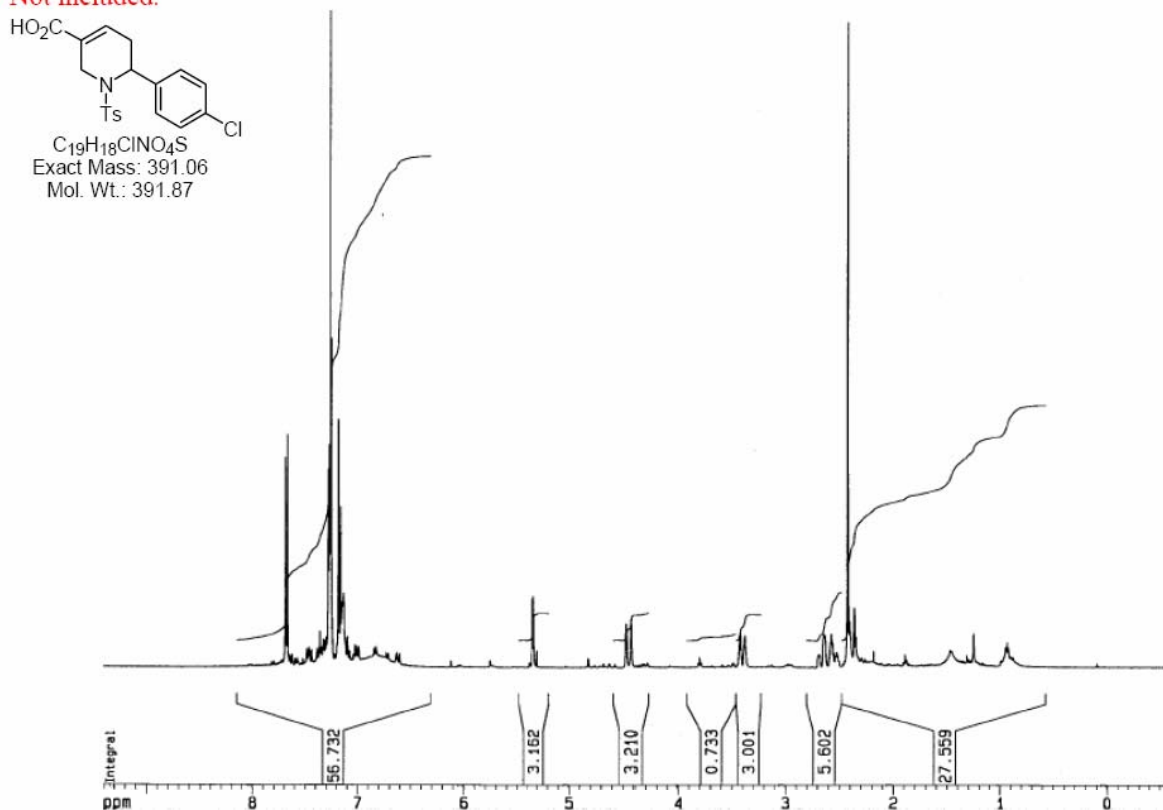
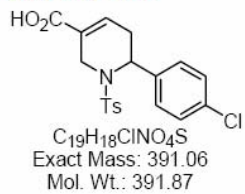


C₁₉H₁₈FNO₄S
 Exact Mass: 375.09
 Mol. Wt.: 375.41

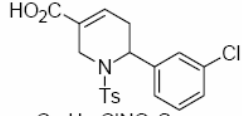


6-(4-Chlorophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C11)

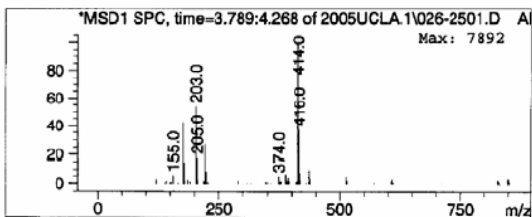
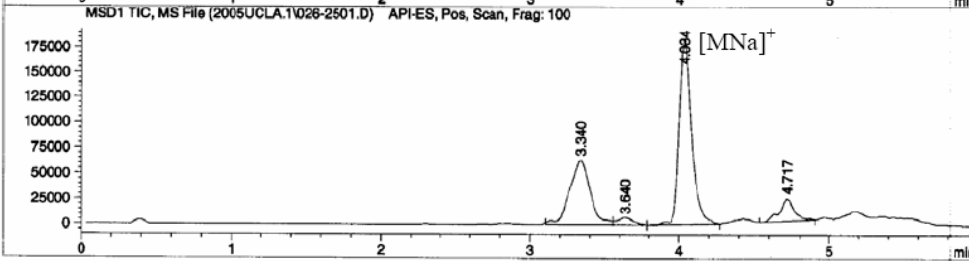
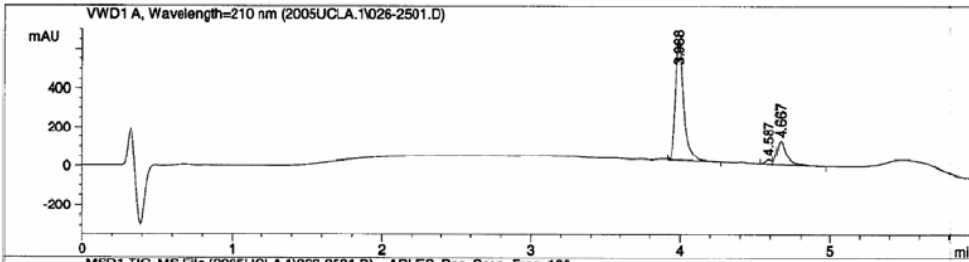
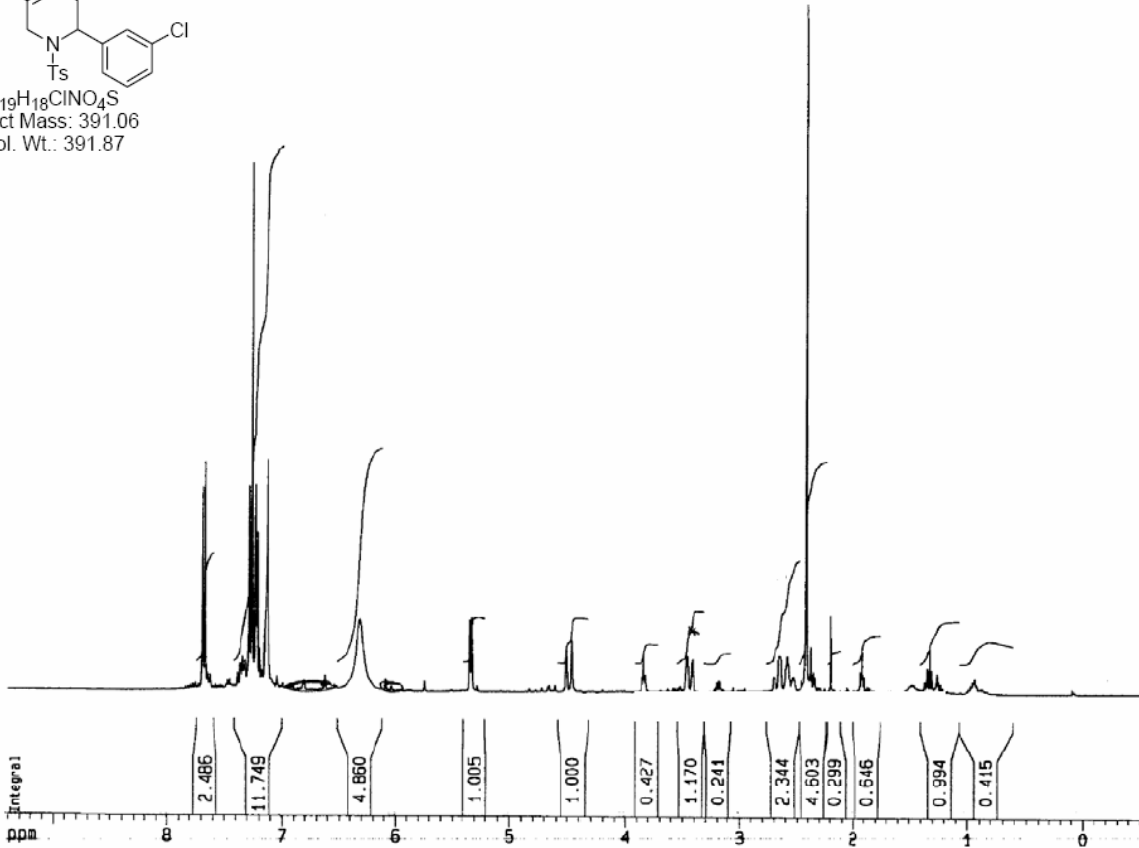
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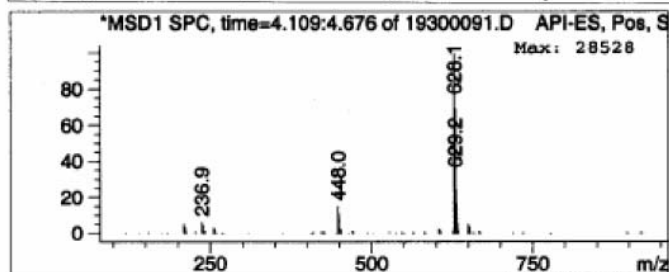
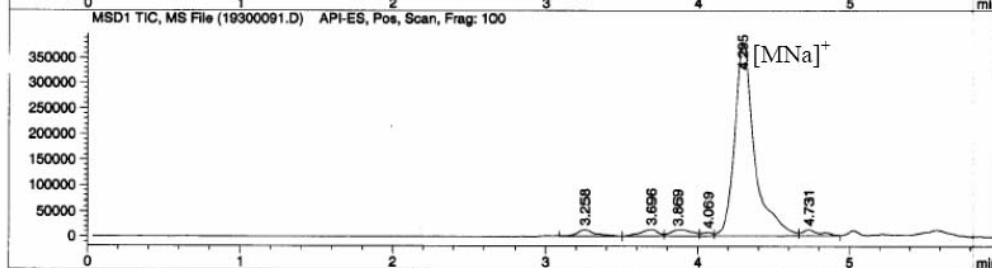
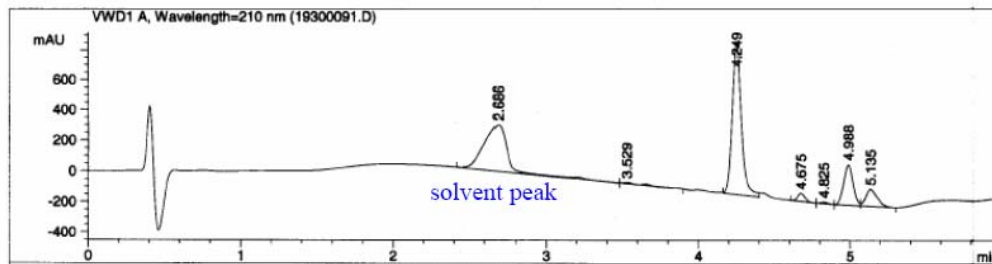
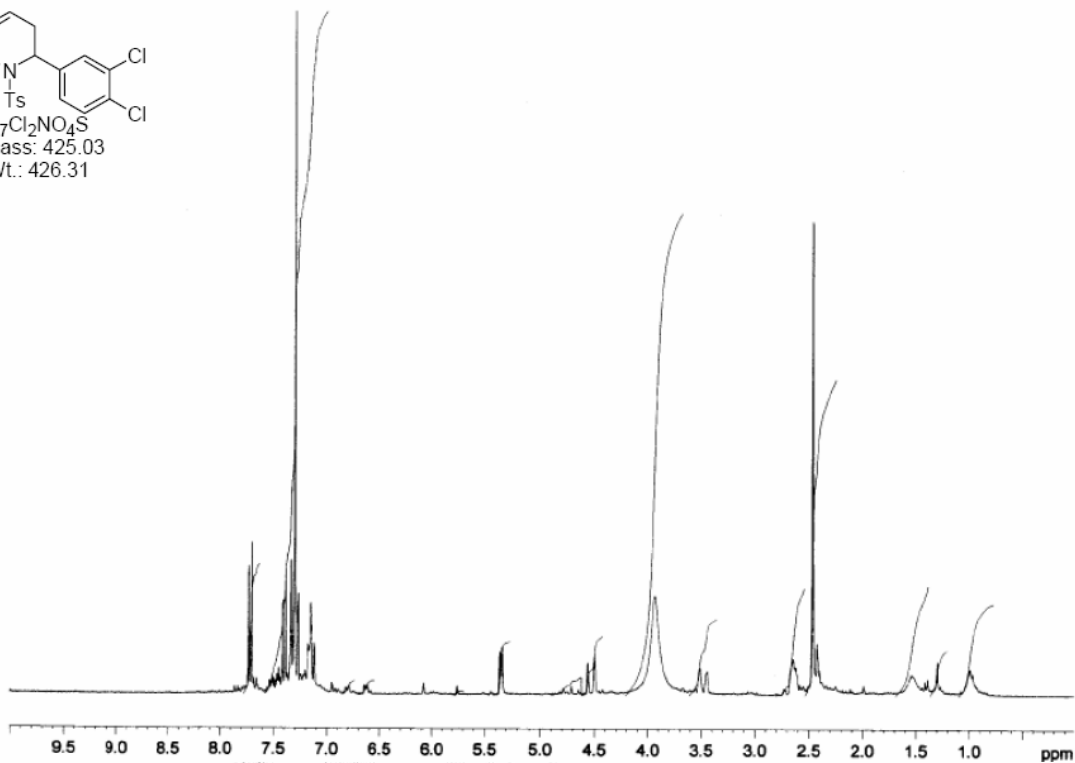
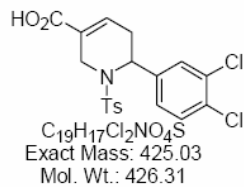
6-(3-Chlorophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C12)



C₁₉H₁₈ClNO₄S
 Exact Mass: 391.06
 Mol. Wt.: 391.87

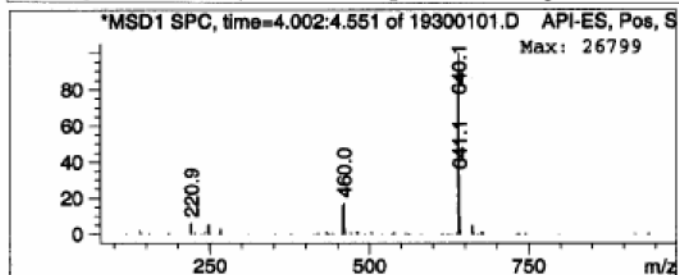
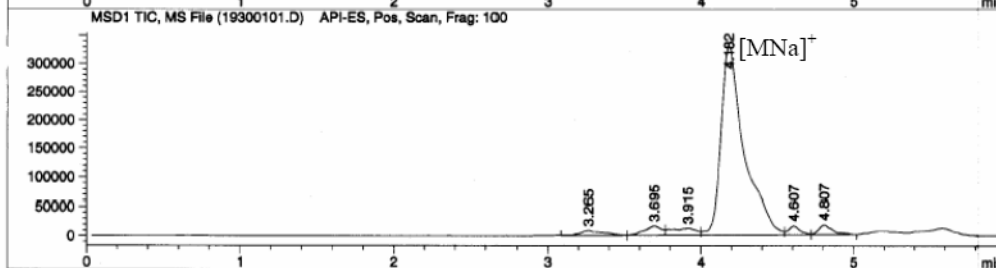
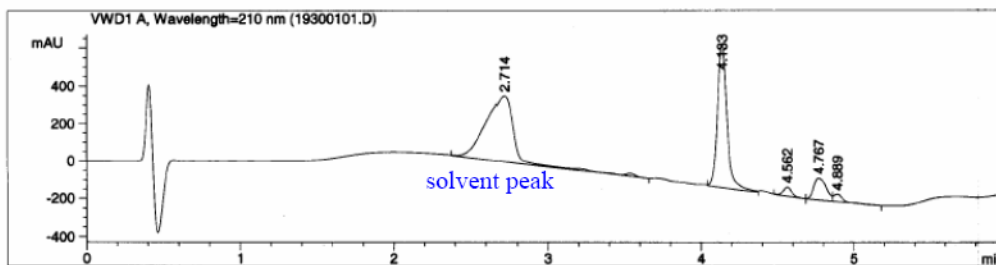
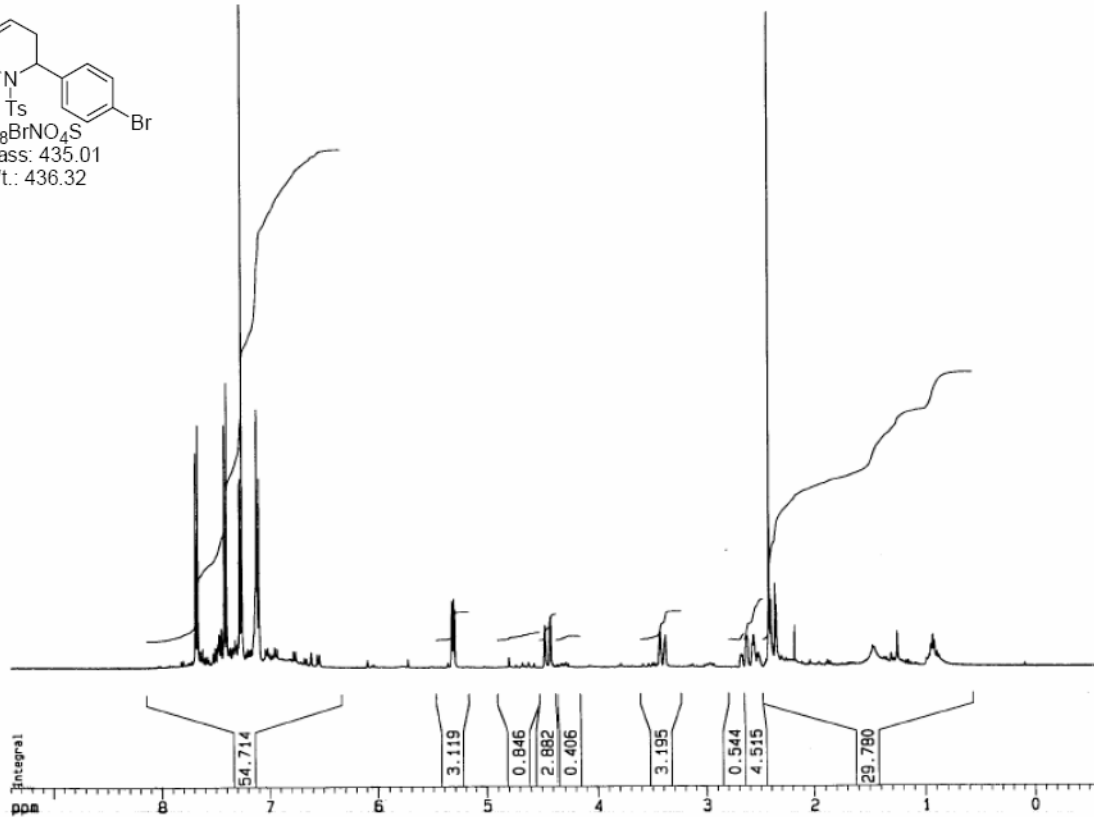
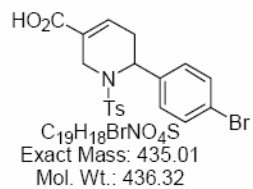


6-(3,4-Dichlorophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C13)
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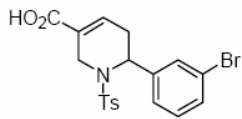


6-(4-Bromophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C14)

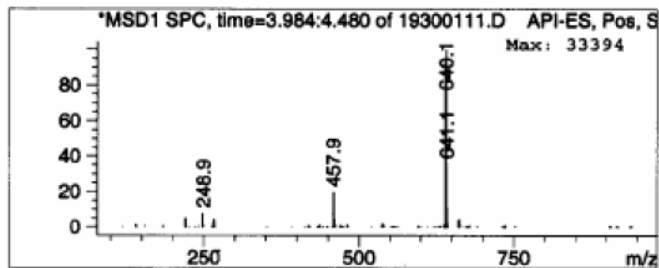
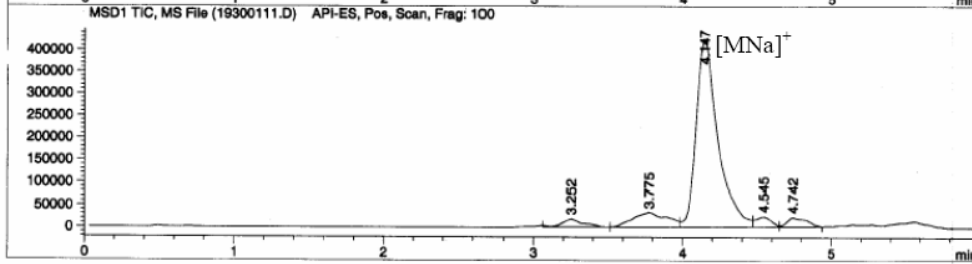
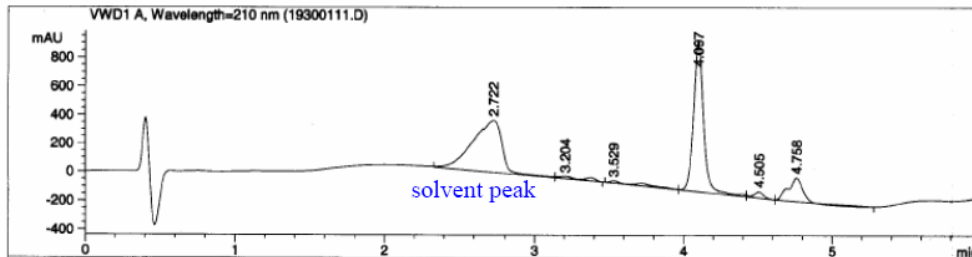
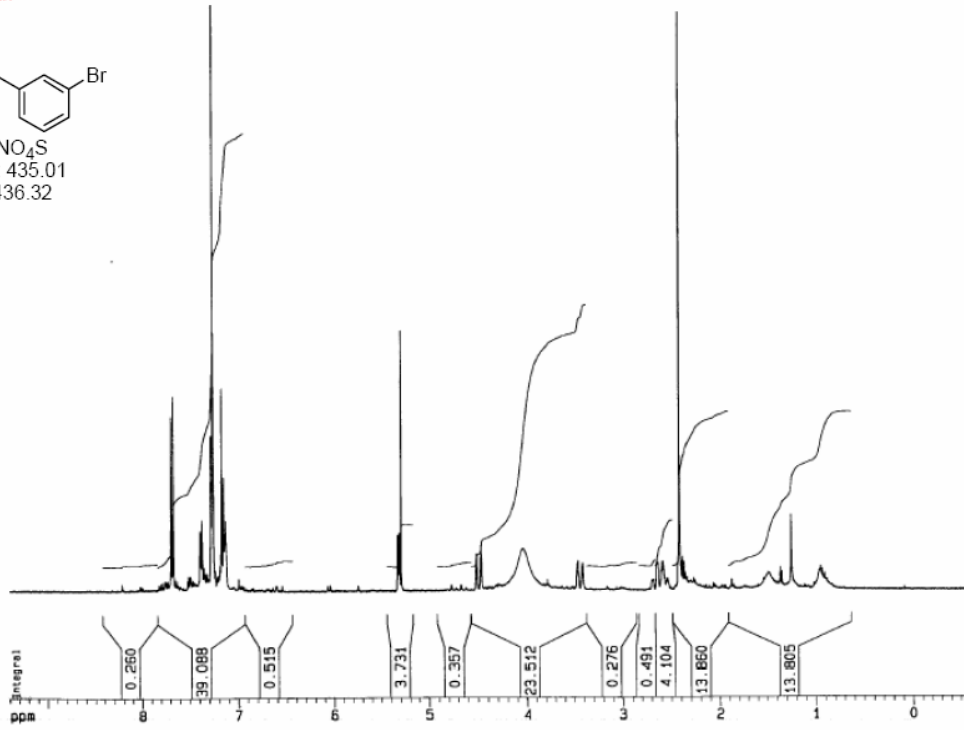
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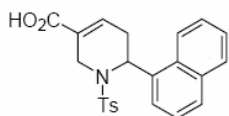
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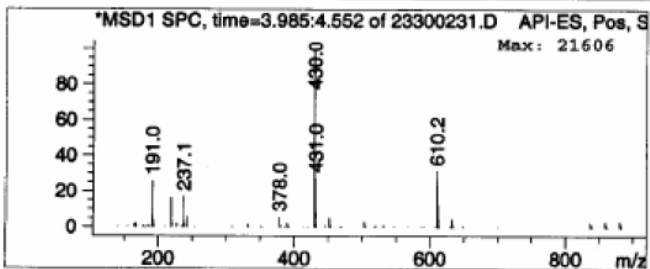
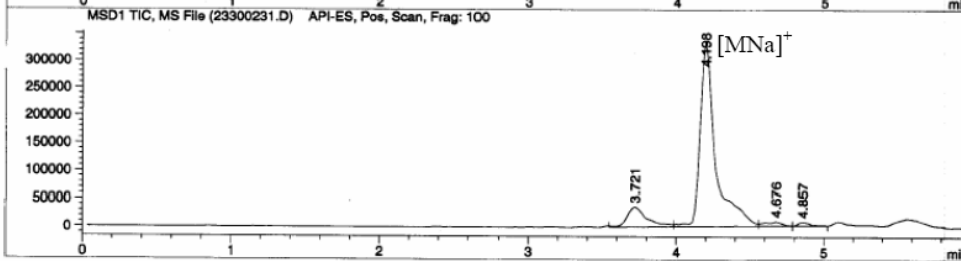
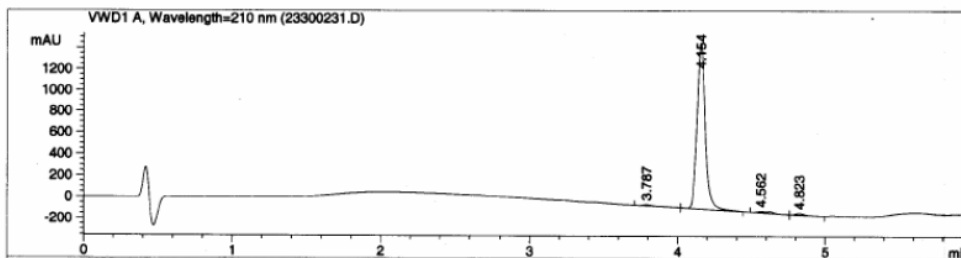
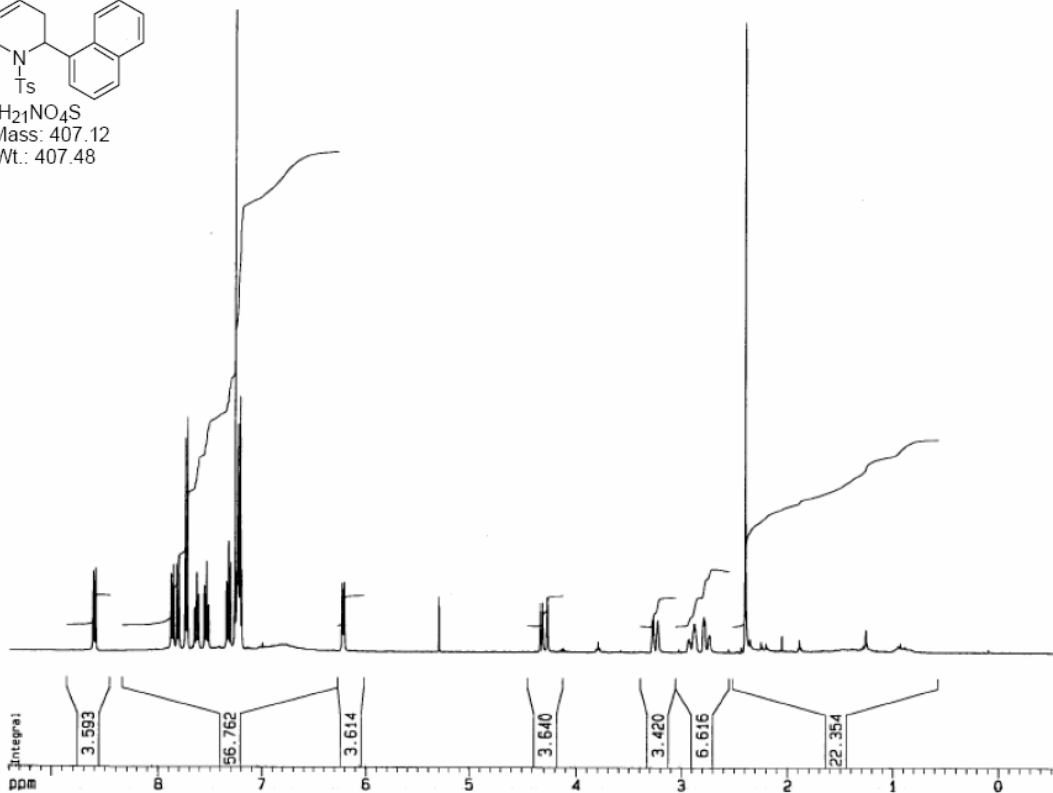
C₁₉H₁₈BrNO₄S
 Exact Mass: 435.01
 Mol. Wt.: 436.32



6-(Naphthalen-1-yl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C16)

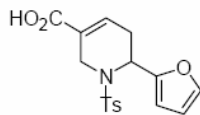


C₂₃H₂₁NO₄S
 Exact Mass: 407.12
 Mol. Wt.: 407.48



6-(Furan-2-yl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C17)

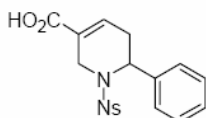
Not included.



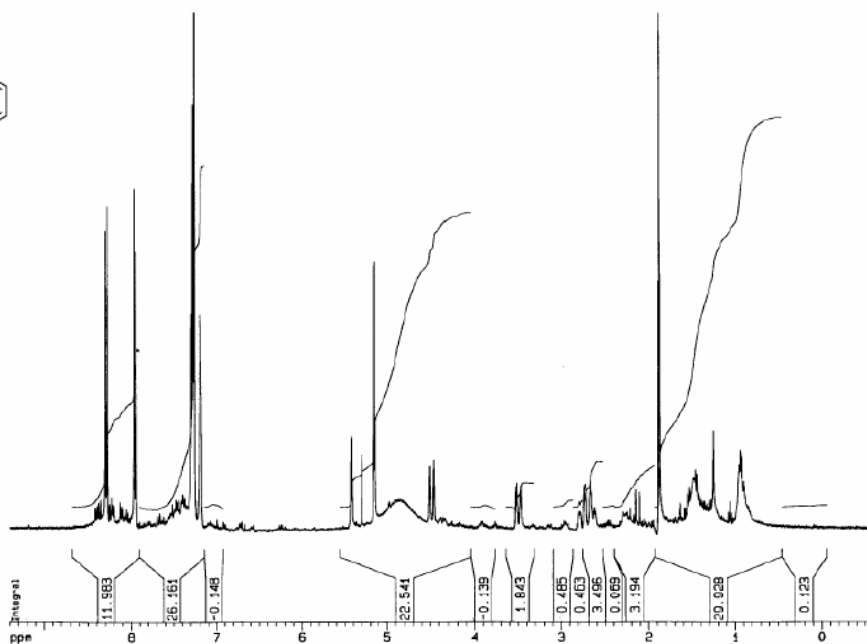
C₁₇H₁₇NO₅S
Exact Mass: 347.08
Mol. Wt.: 347.39

1-(4-Nitrobenzenesulfonyl)-6-phenyl-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C18)

Not included.

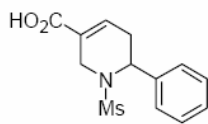


C₁₈H₁₆N₂O₆S
Exact Mass: 388.07
Mol. Wt.: 388.39

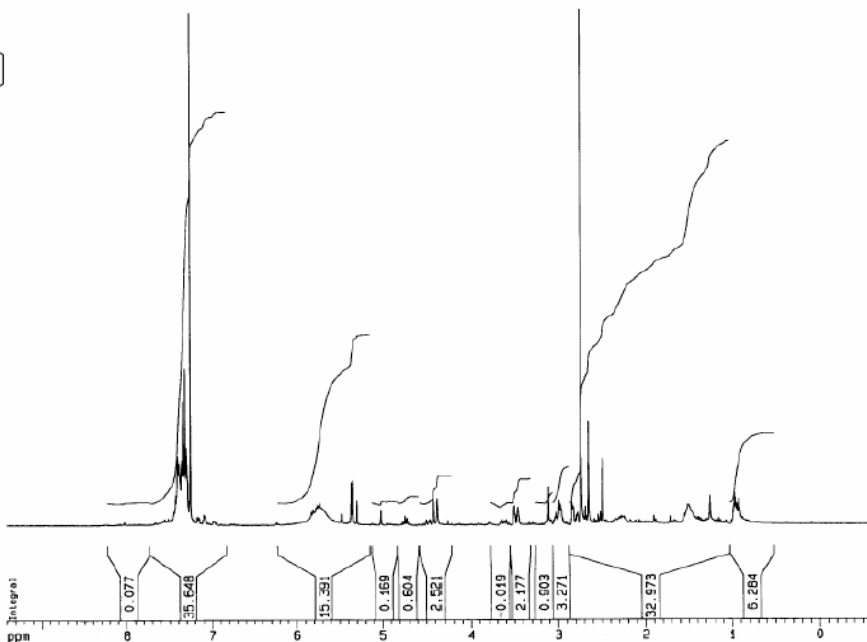


1-Methanesulfonyl-6-phenyl-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C19)

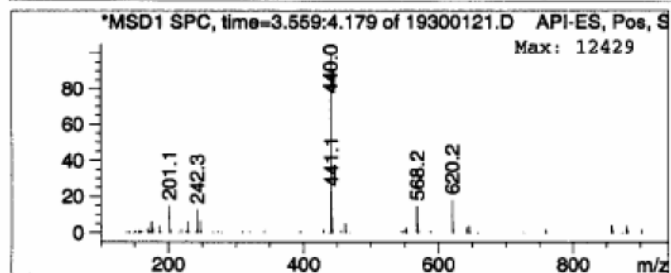
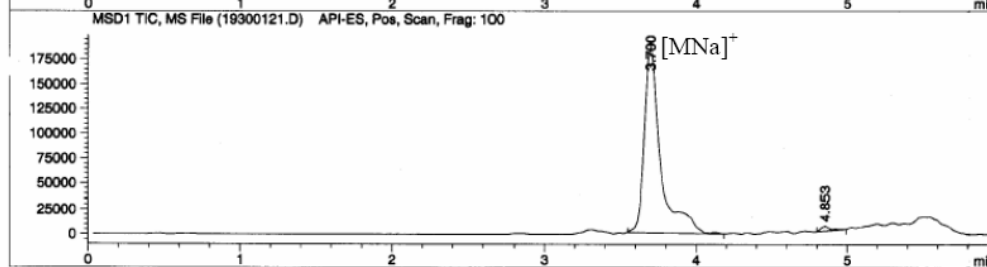
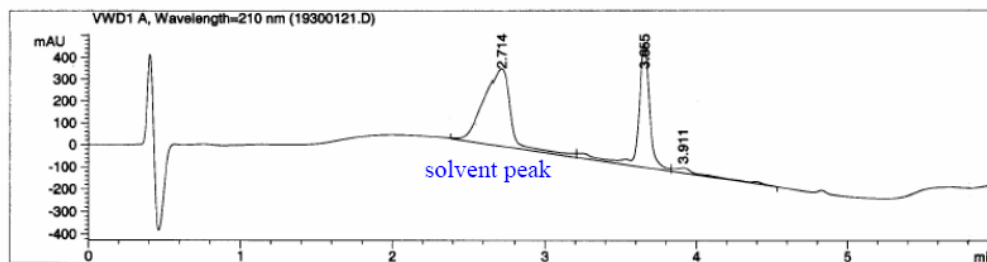
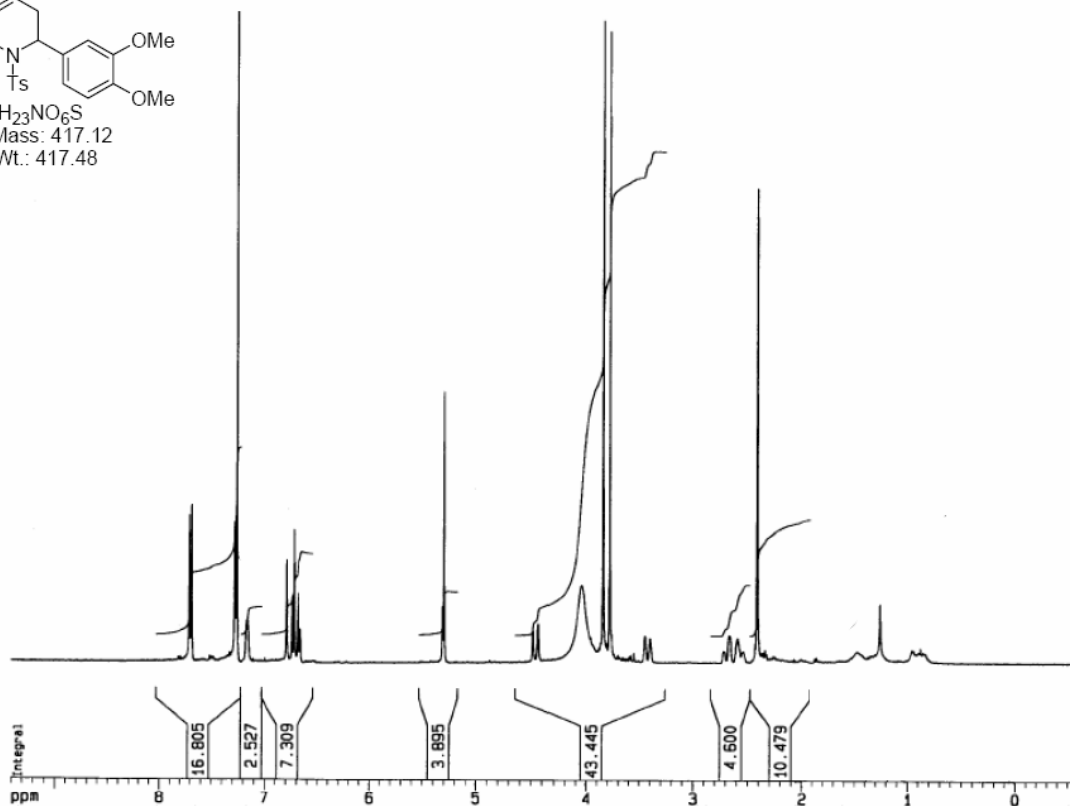
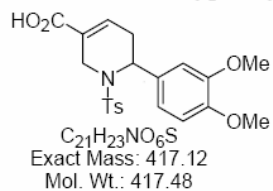
Not included.



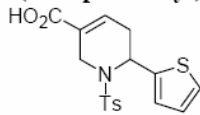
C₁₃H₁₅NO₄S
Exact Mass: 281.07
Mol. Wt.: 281.33



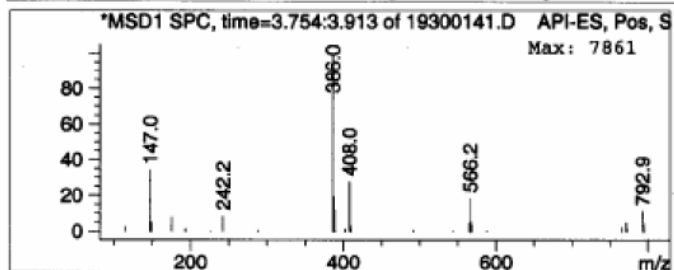
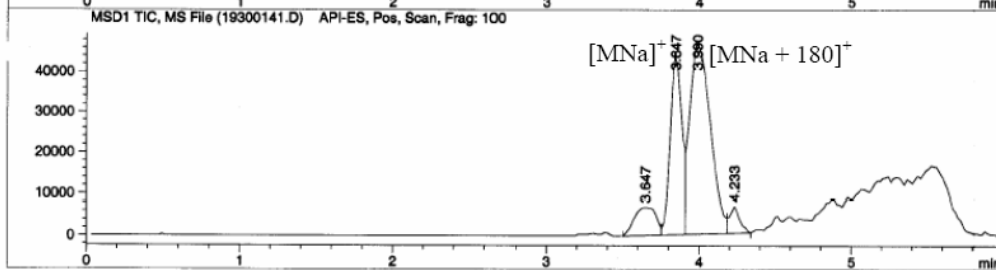
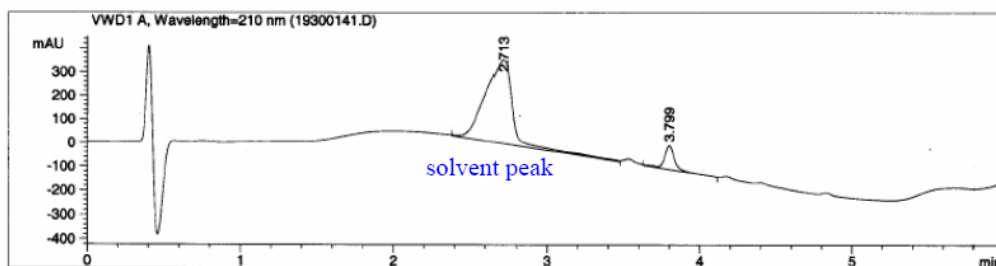
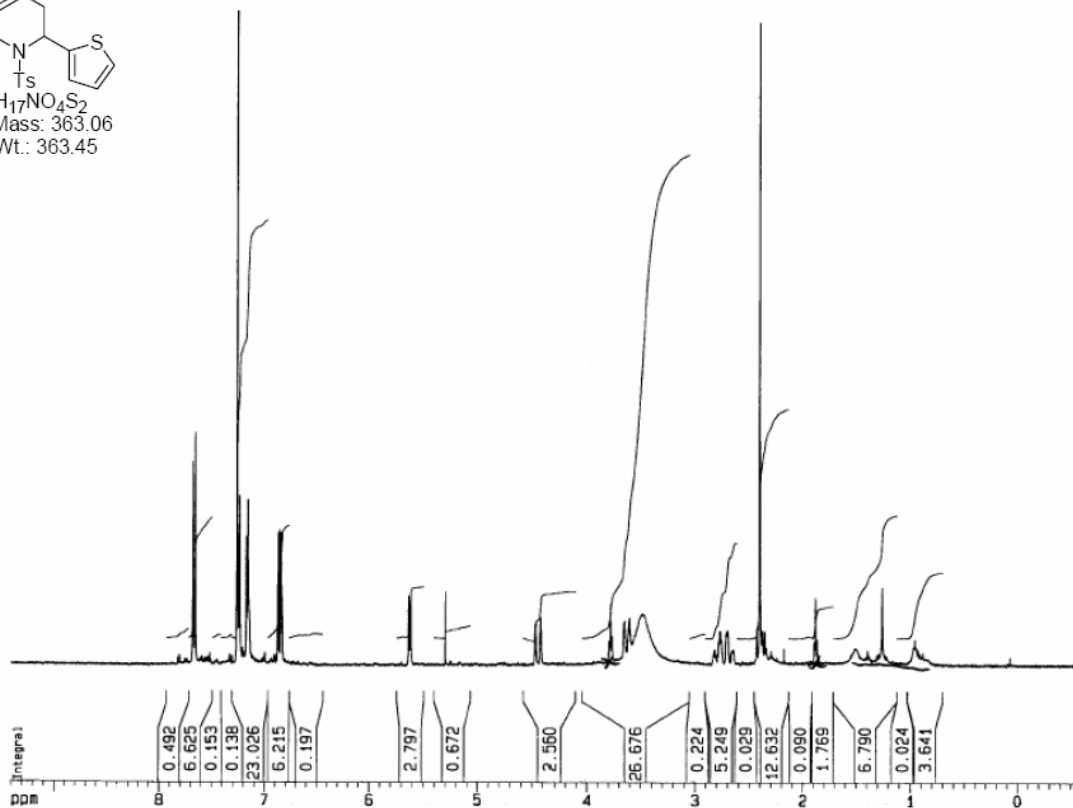
6-(3,4-Dimethoxyphenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C20)



6-(Thiophen-2-yl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C21)

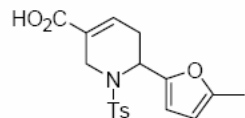


C₁₇H₁₇NO₄S₂
 Exact Mass: 363.06
 Mol. Wt.: 363.45

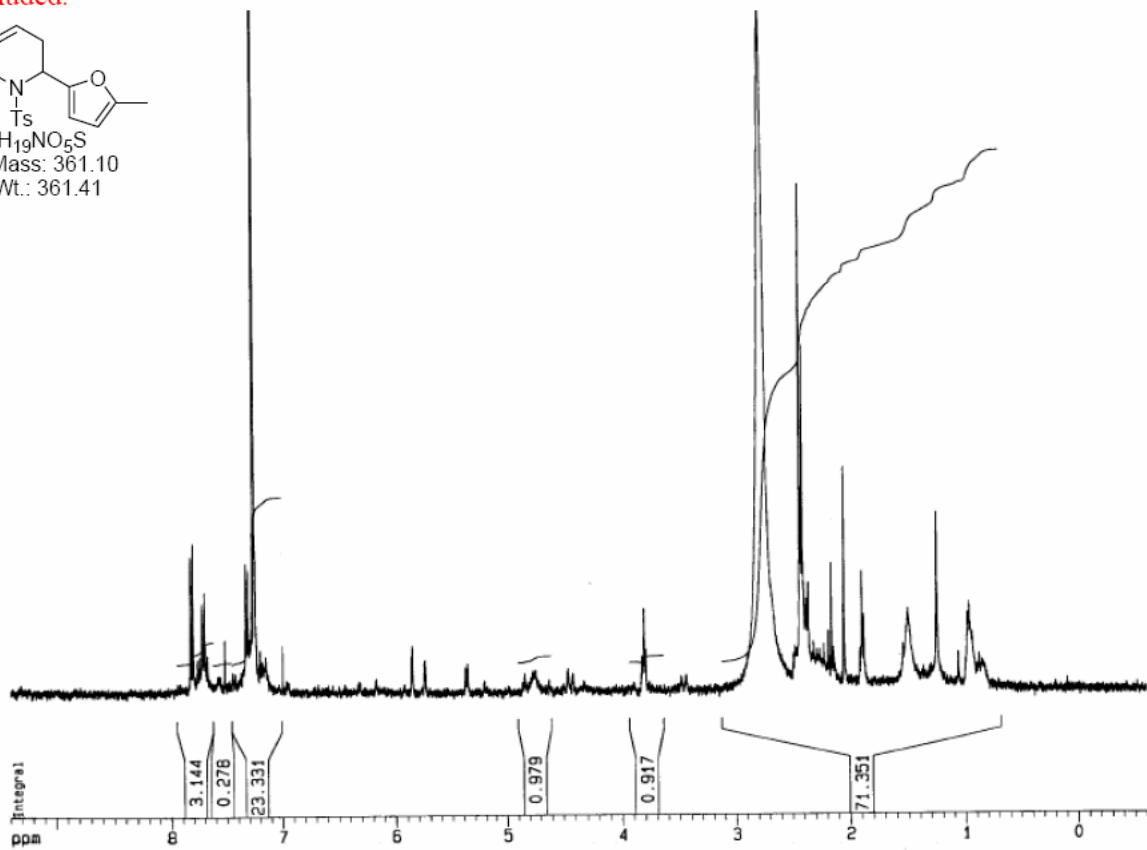


6-(5-Methylfuran-2-yl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C22)

Not included.

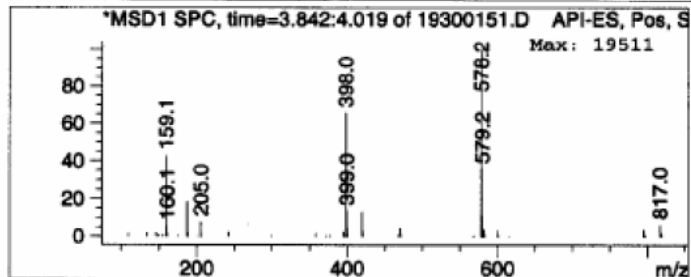
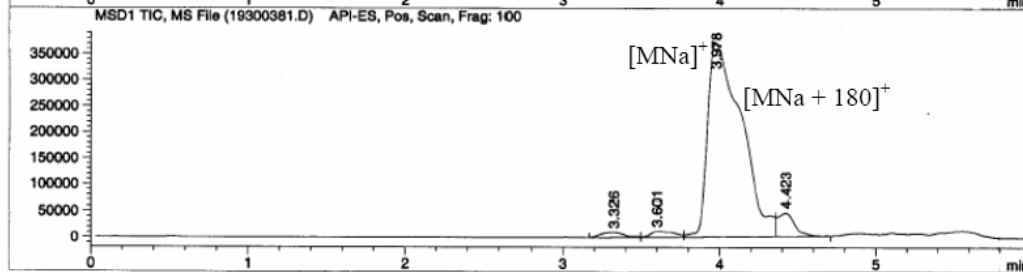
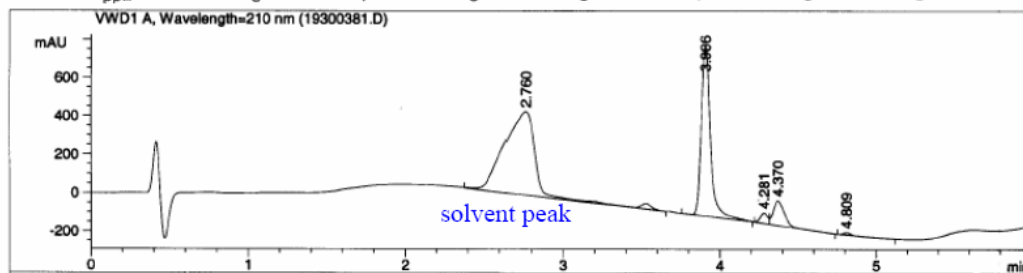
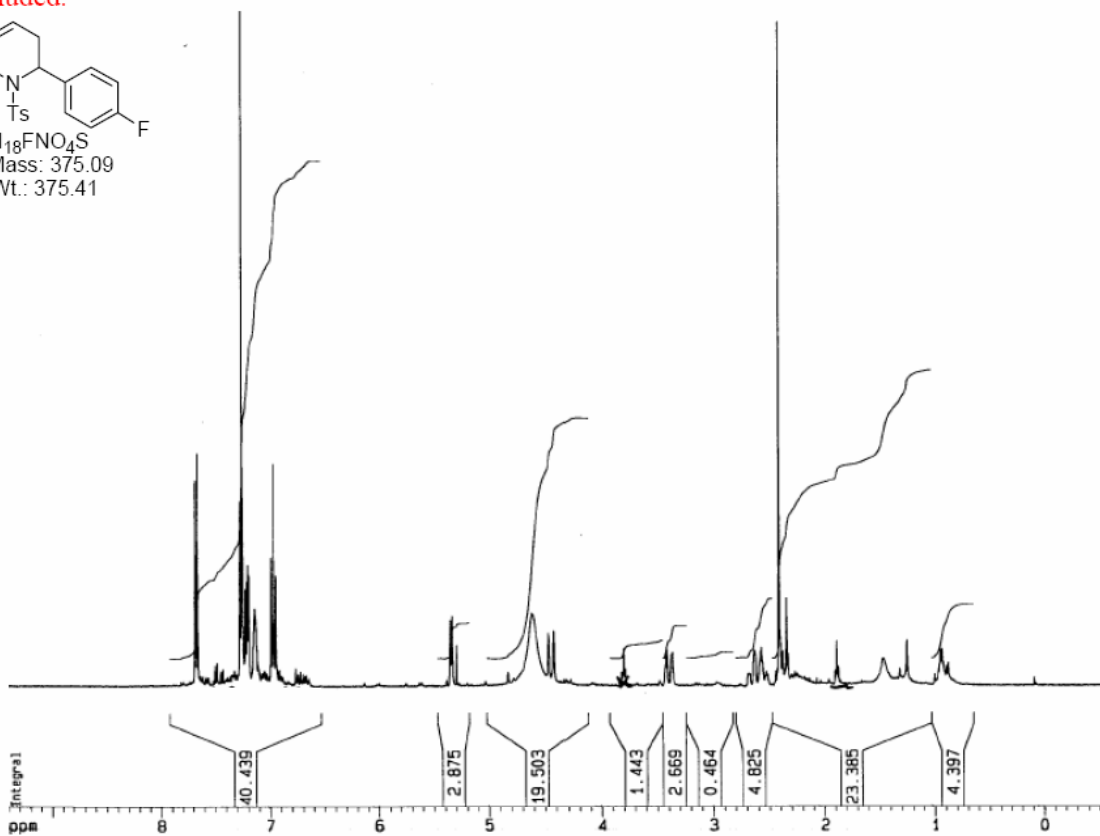
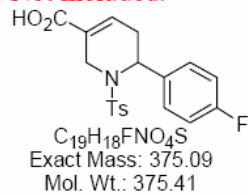


$C_{18}H_{19}NO_5S$
Exact Mass: 361.10
Mol. Wt.: 361.41

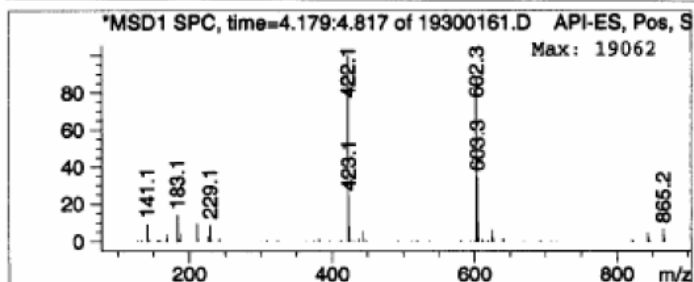
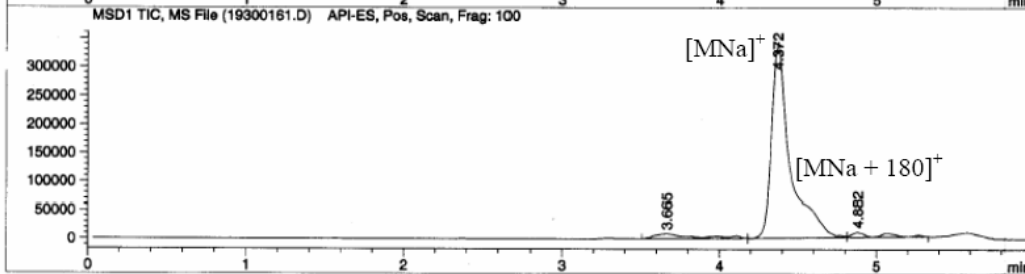
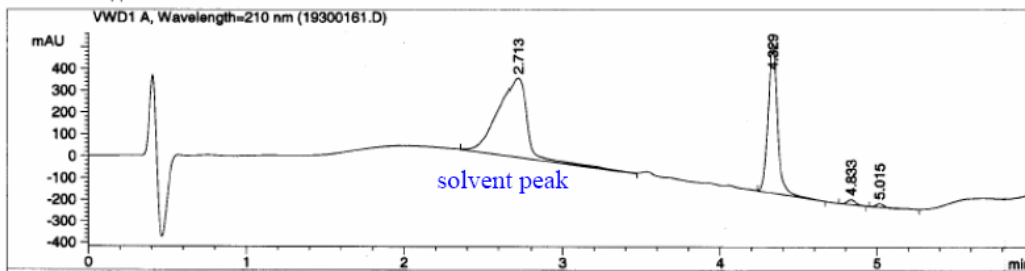
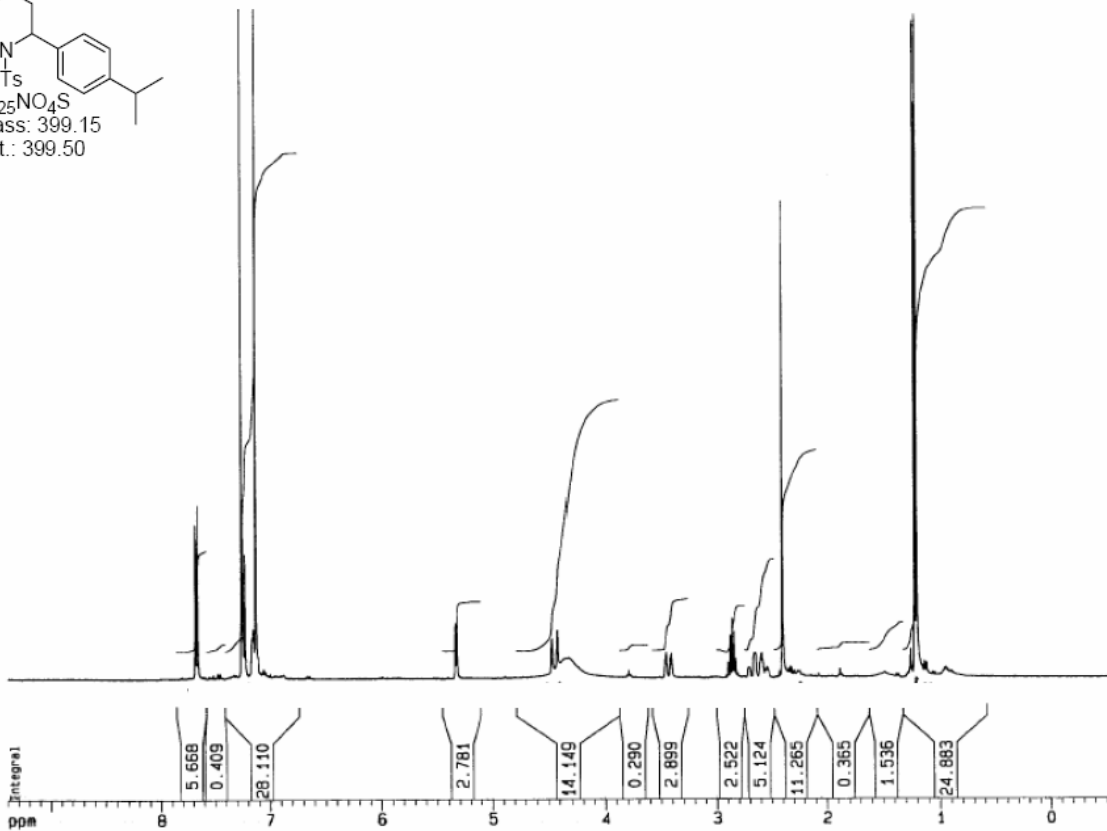
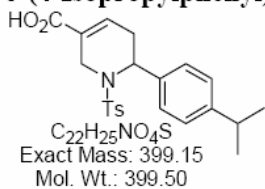


6-(4-Fluorophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C23)

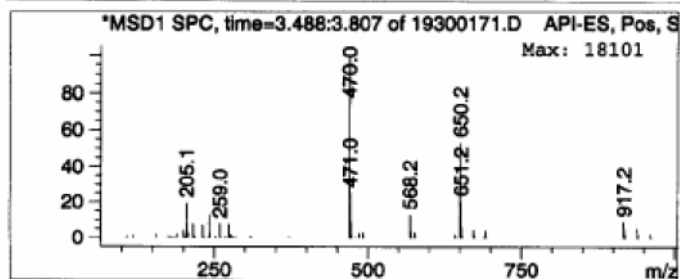
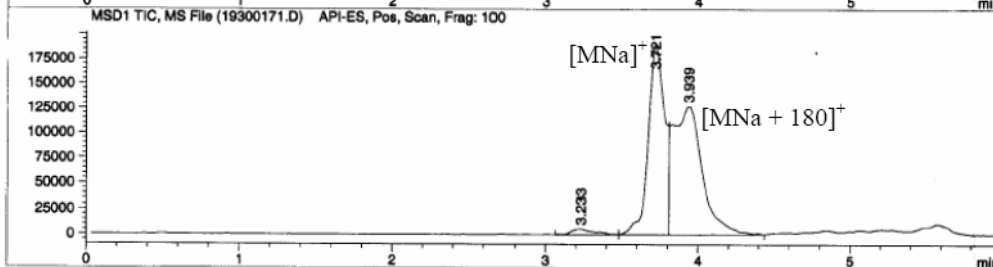
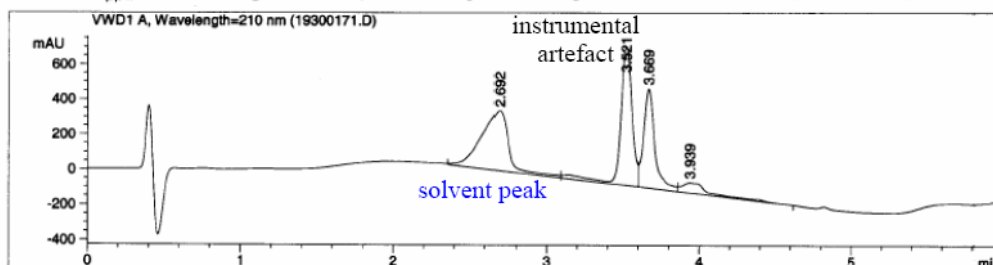
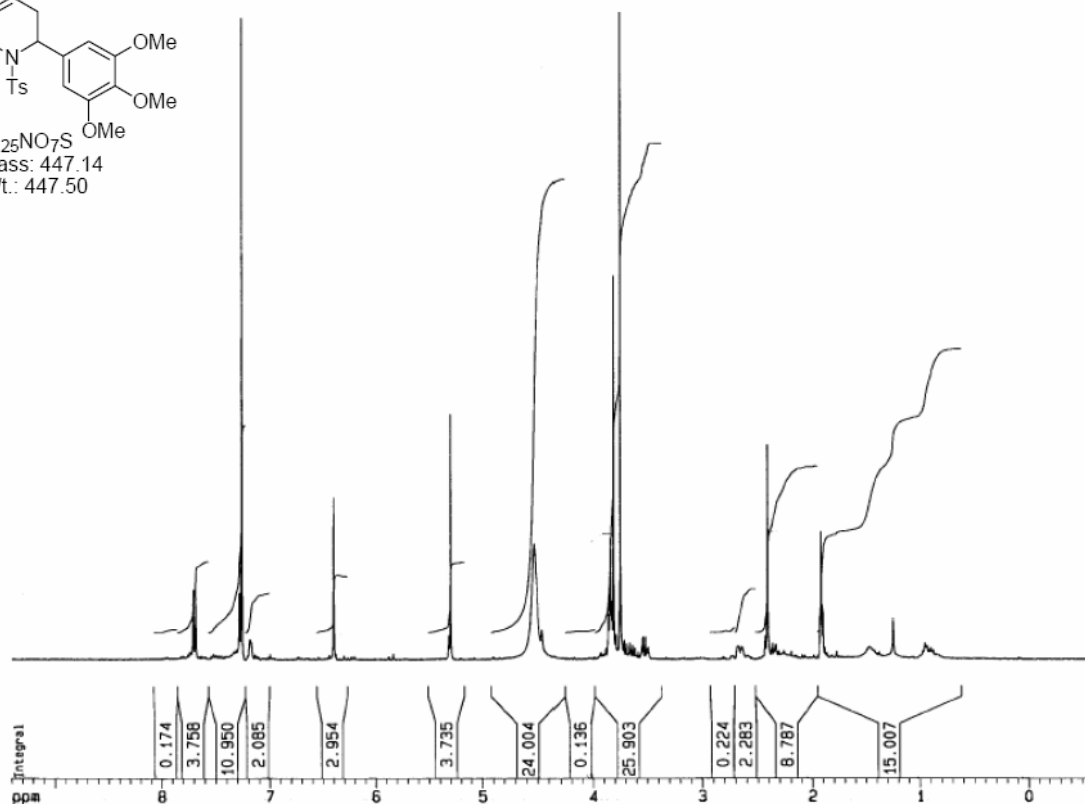
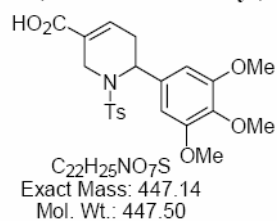
Not included.



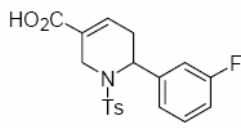
6-(4-Isopropylphenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C24)



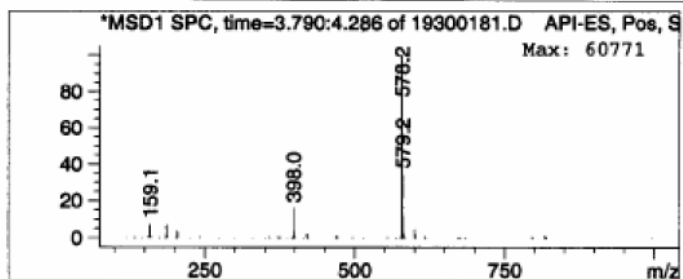
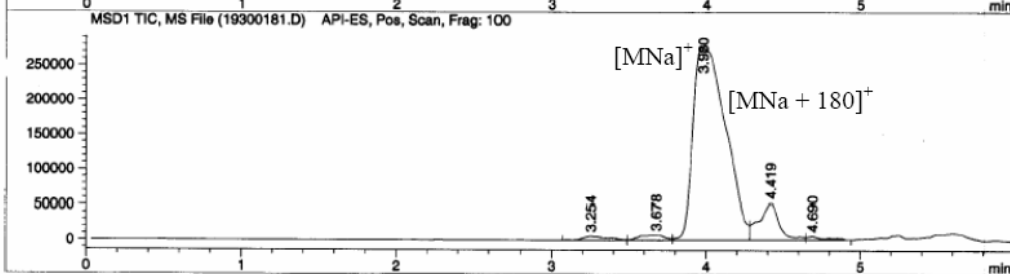
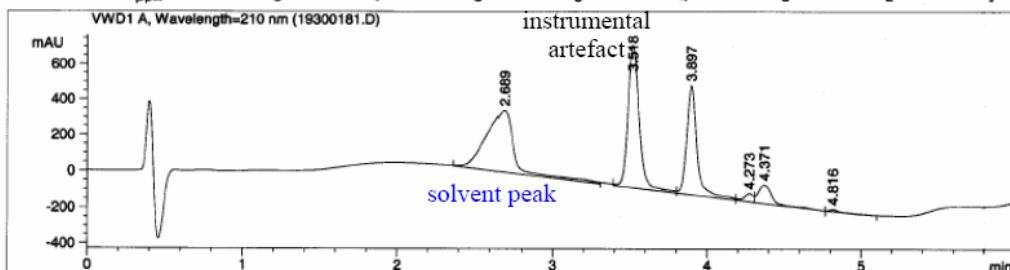
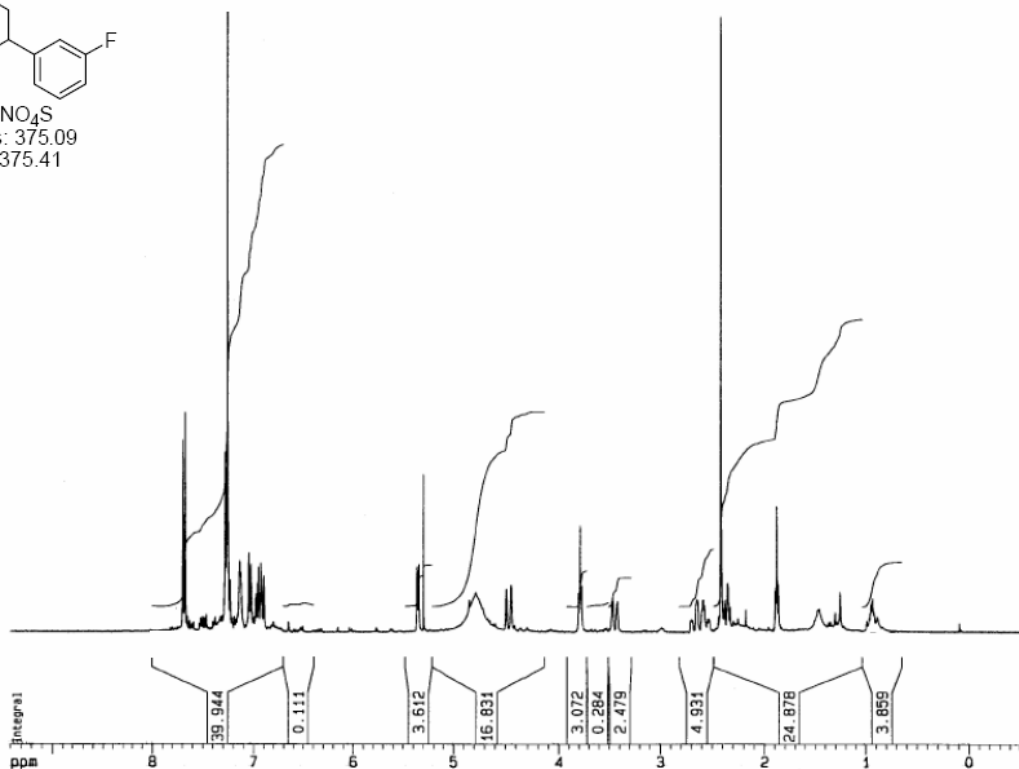
1-(4-Toluenesulfonyl)-6-(3,4,5-trimethoxyphenyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C25)



6-(3-Fluorophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C26)
Not included.

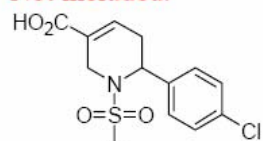


C₁₉H₁₈FNO₄S
Exact Mass: 375.09
Mol. Wt.: 375.41

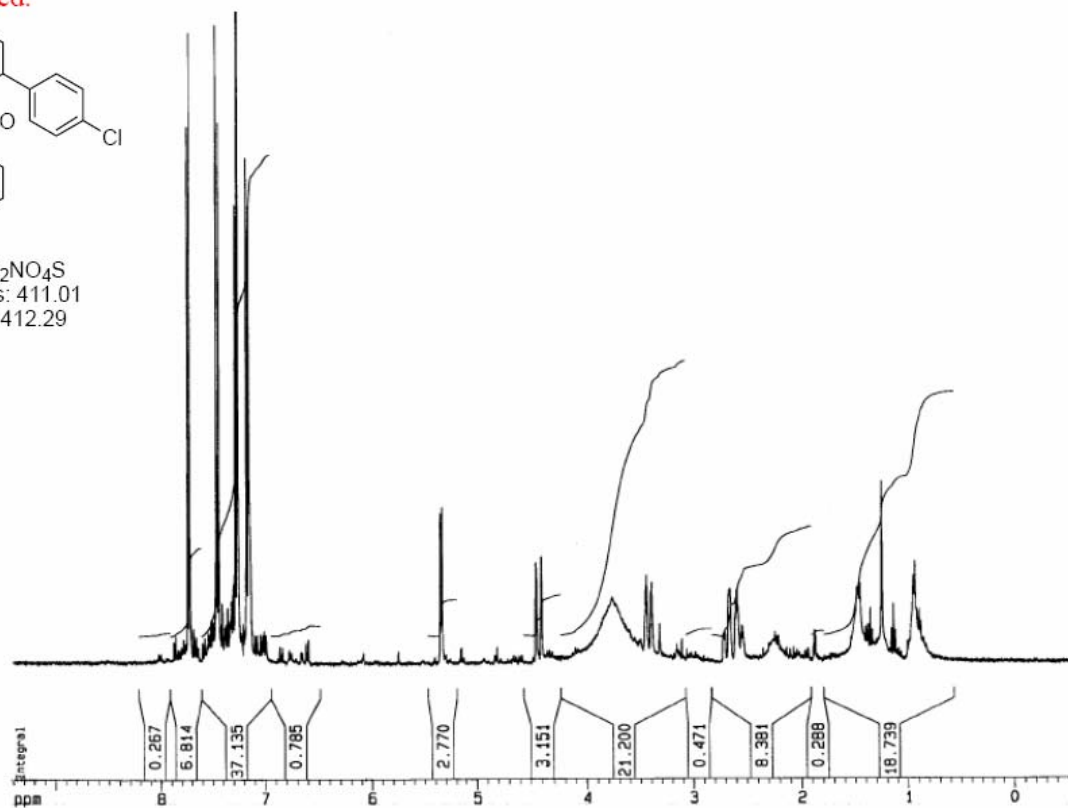


1-(4-Chlorobenzenesulfonyl)-6-(4-chlorophenyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C27)

Not included.

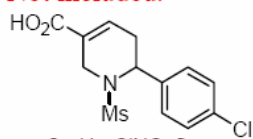


C₁₈H₁₅Cl₂NO₄S
Exact Mass: 411.01
Mol. Wt.: 412.29

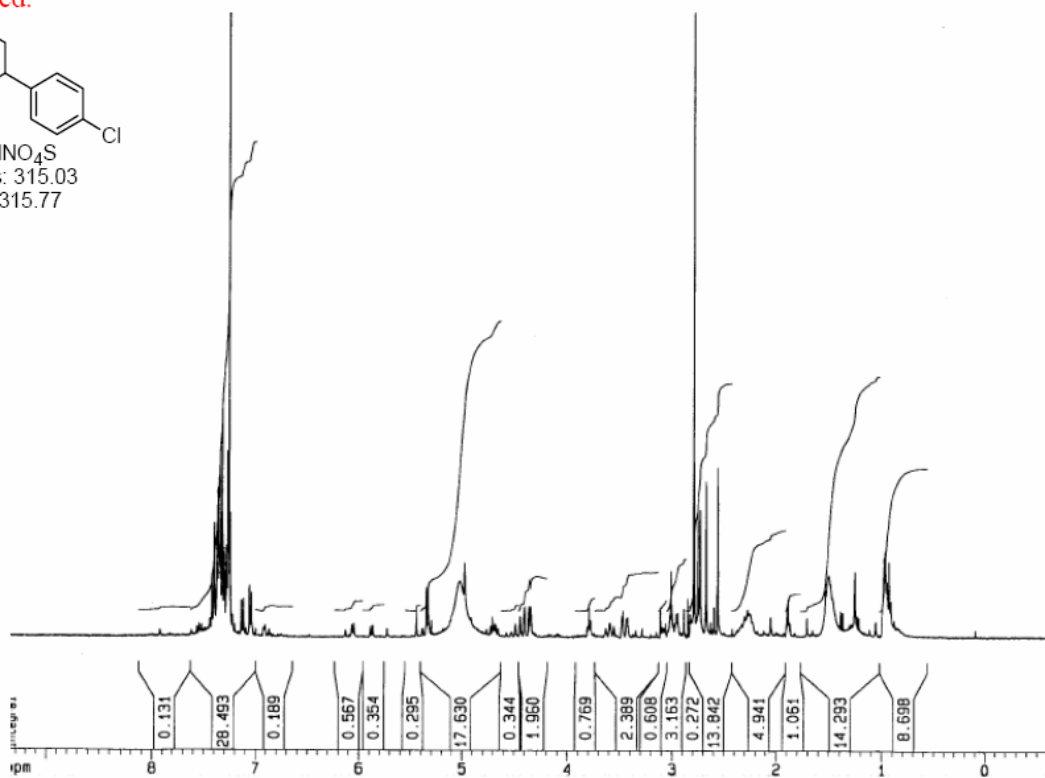


6-(4-Chlorophenyl)-1-methanesulfonyl-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C28)

Not included.

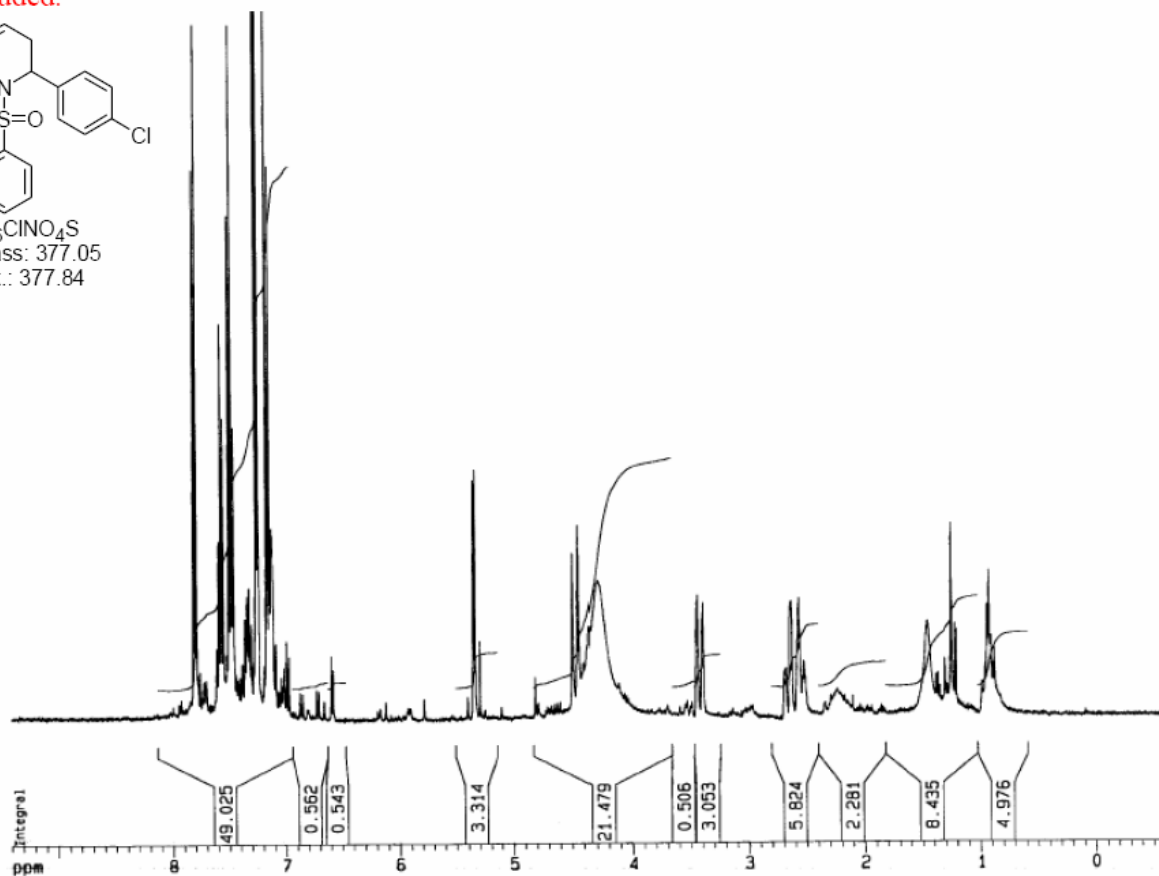
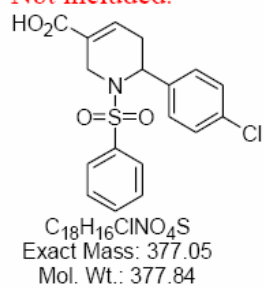


$C_{13}H_{14}ClNO_4S$
Exact Mass: 315.03
Mol. Wt.: 315.77

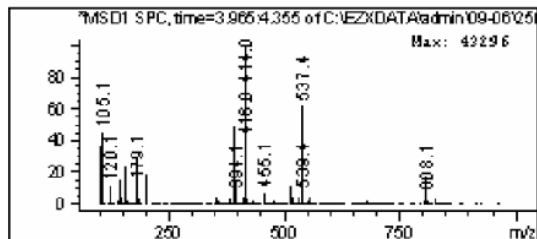
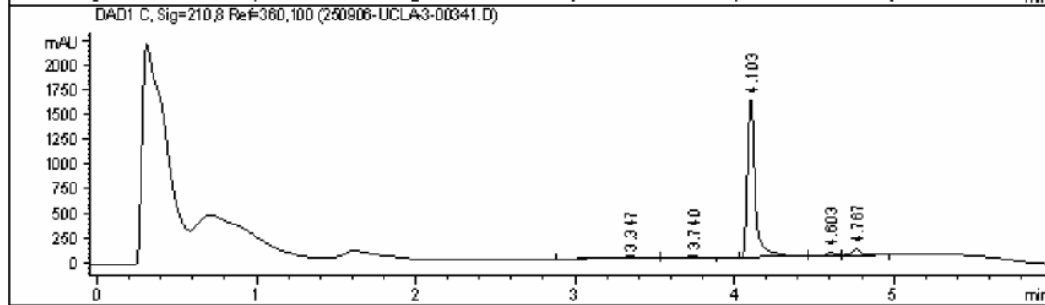
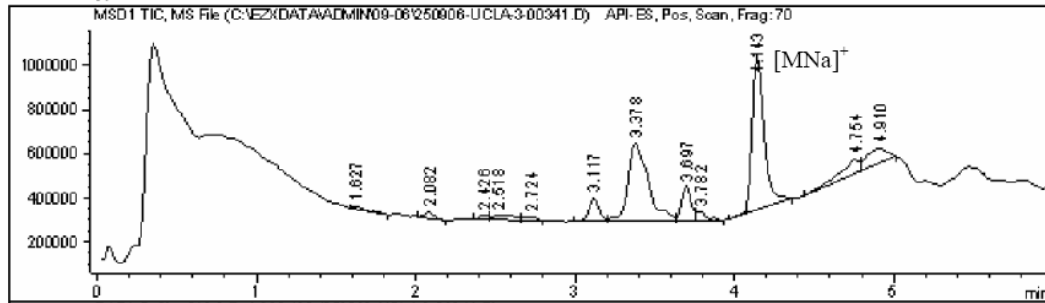
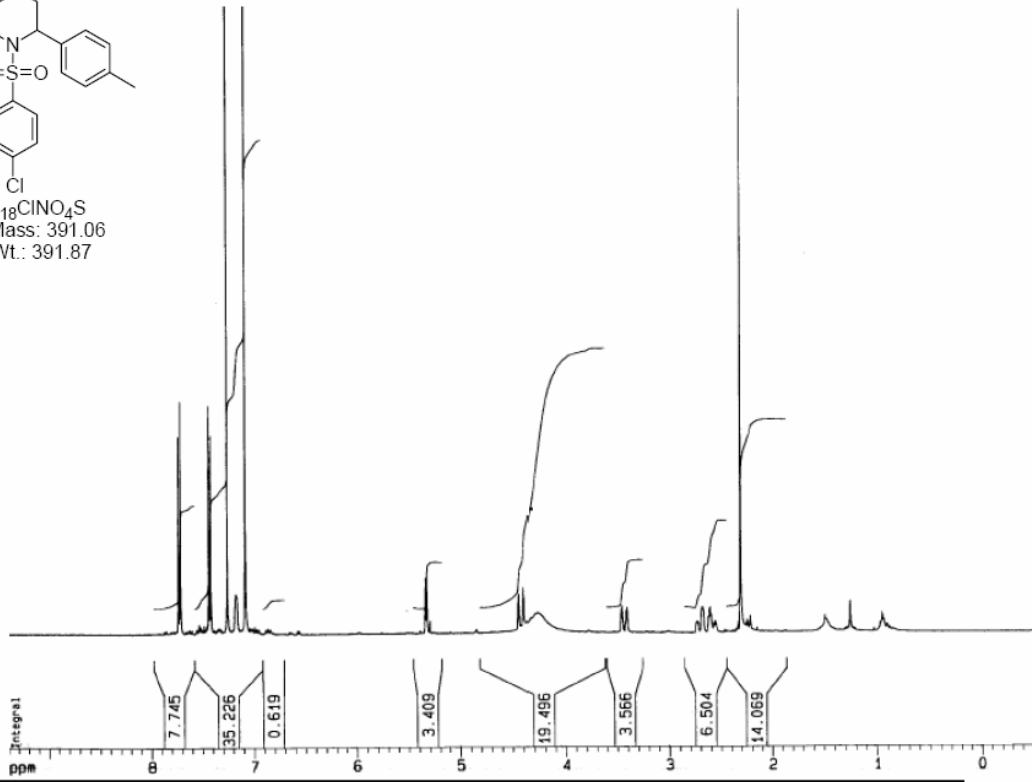
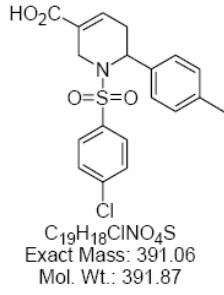


Benzenesulfonyl-6-(4-chlorophenyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C29)

Not included.

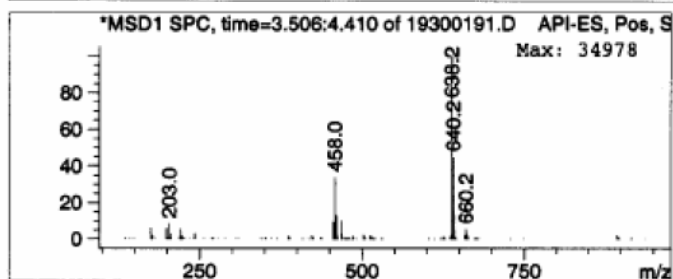
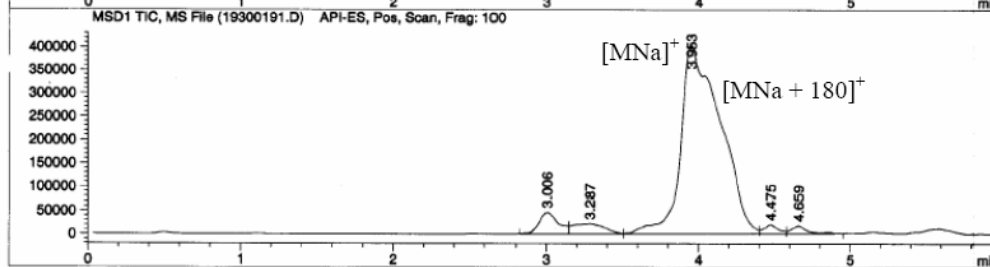
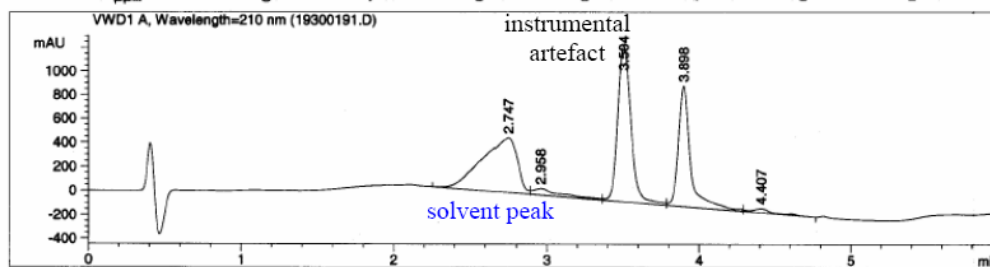
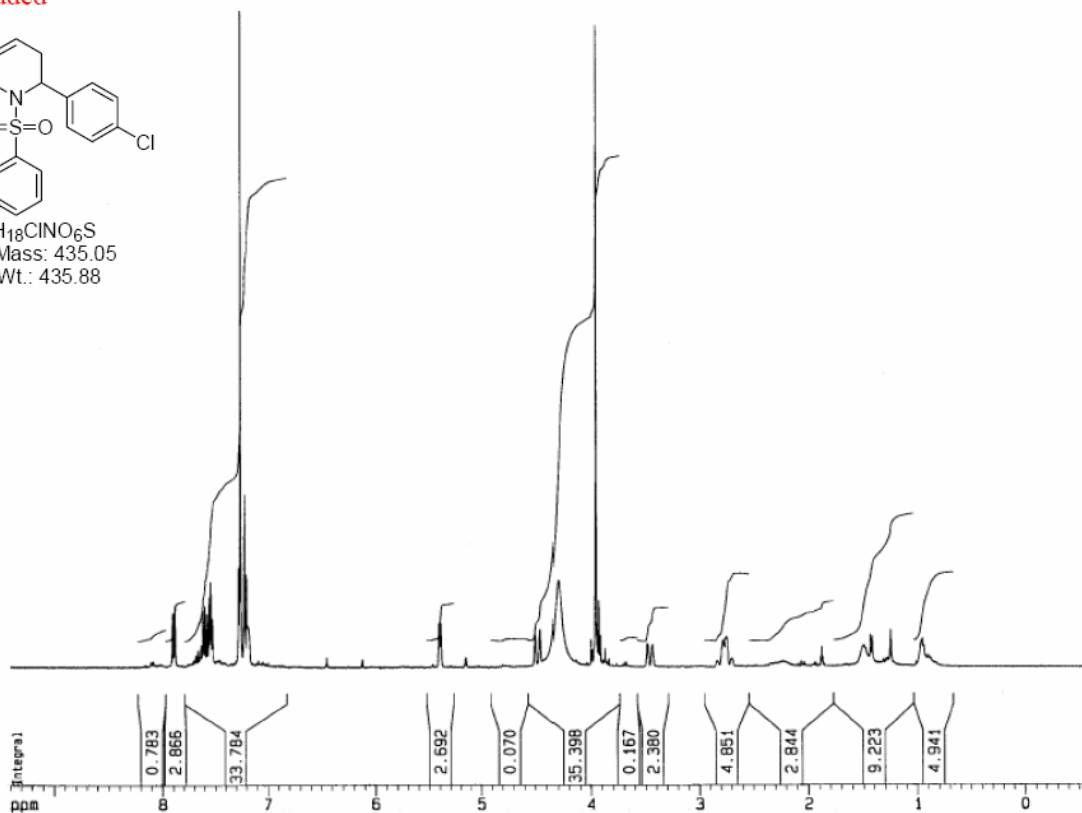
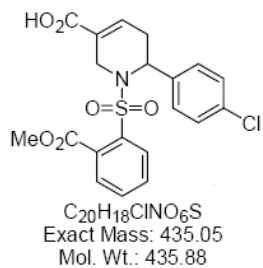


1-(4-Chlorobenzenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C30)

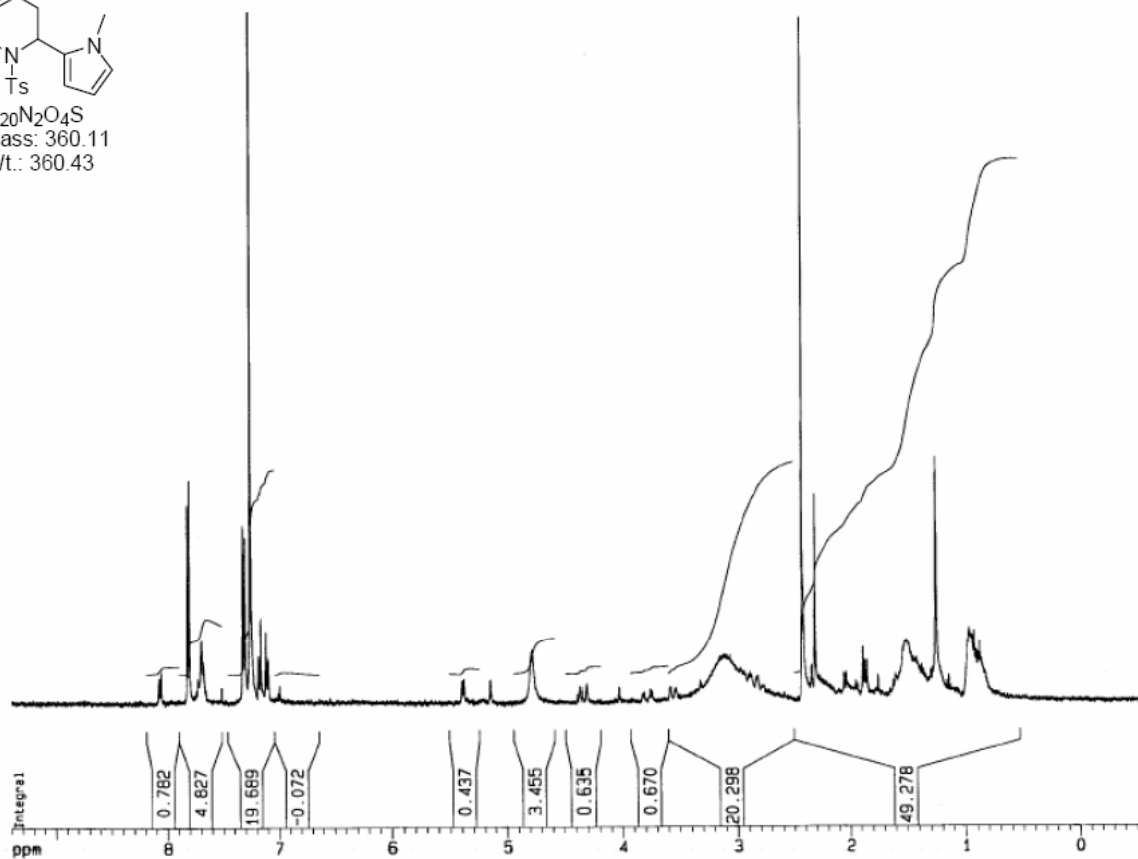
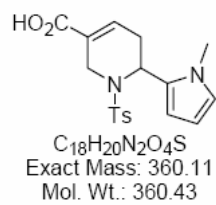


6-(4-Chlorophenyl)-1-(2-methoxycarbonylbenzenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C31)

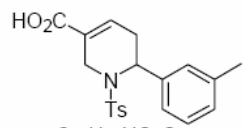
Not included



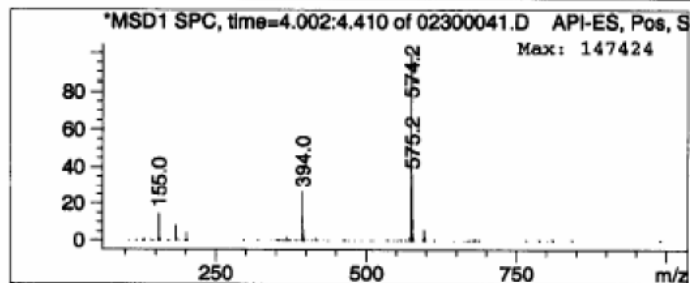
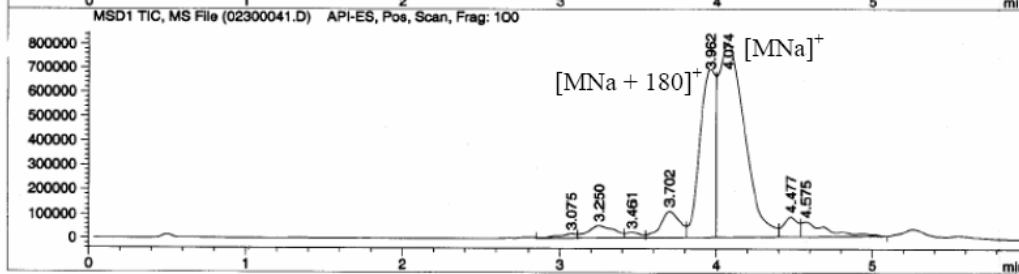
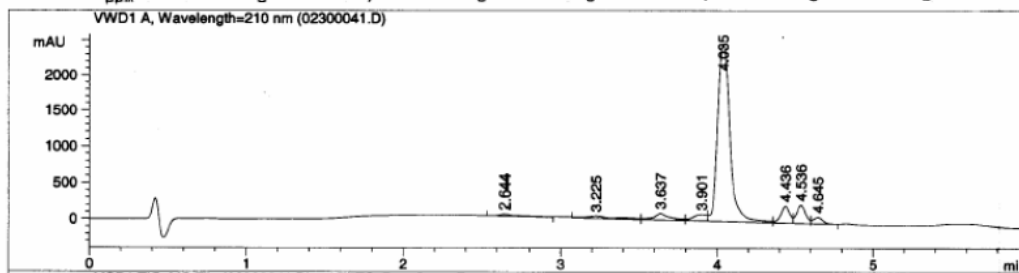
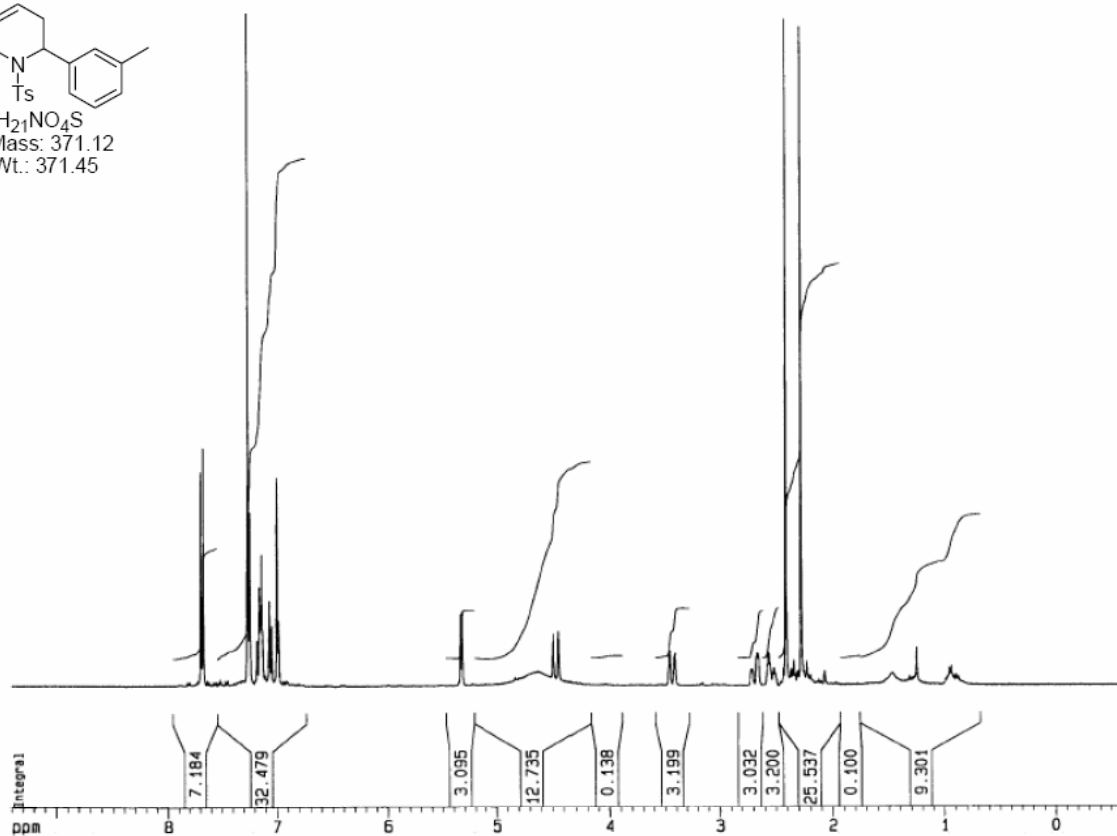
6-(1-Methyl-1H-pyrrol-2-yl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C32)
Not included.



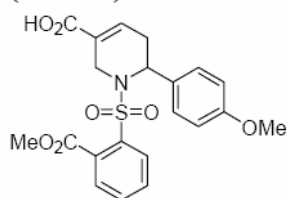
1-(4-Toluenesulfonyl)-6-(*m*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C33)



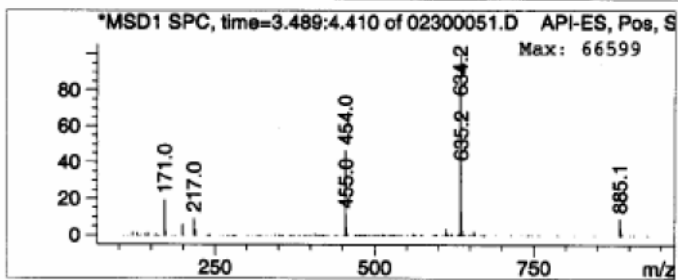
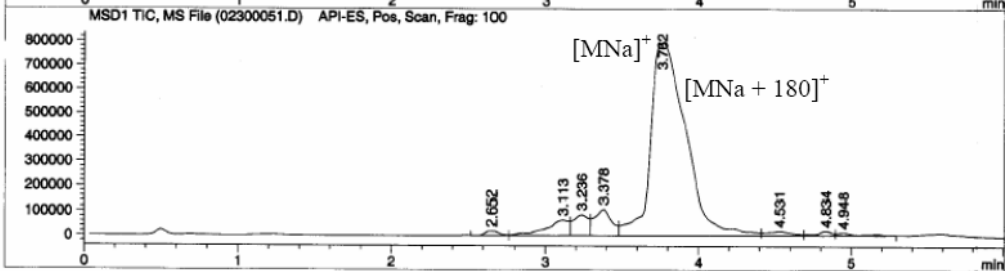
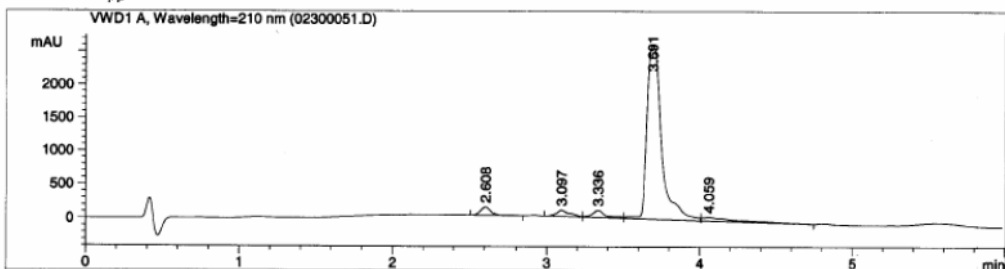
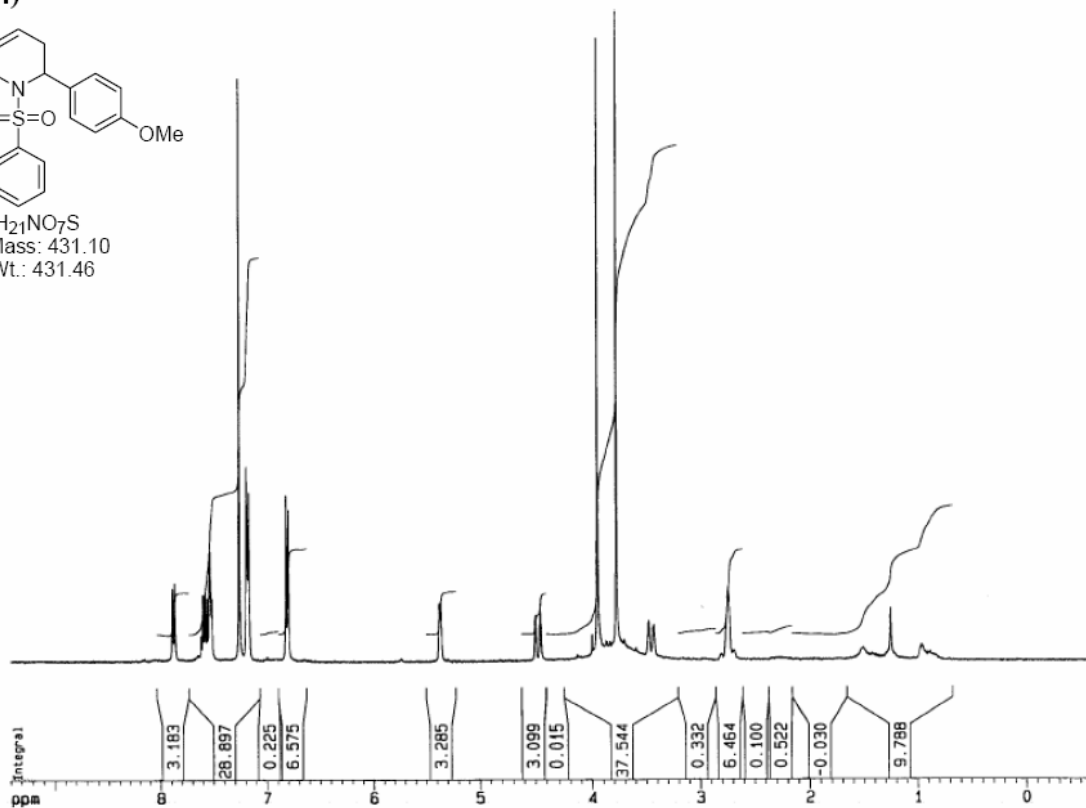
C₂₀H₂₁NO₄S
 Exact Mass: 371.12
 Mol. Wt.: 371.45



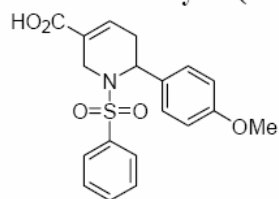
1-(2-Methoxycarbonylbenzenesulfonyl)-6-(4-methoxyphenyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C34)



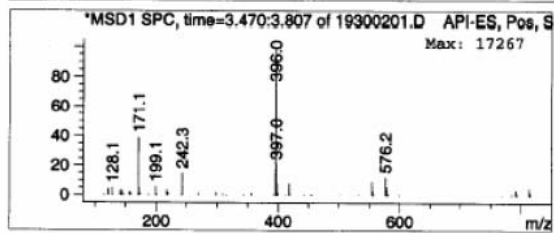
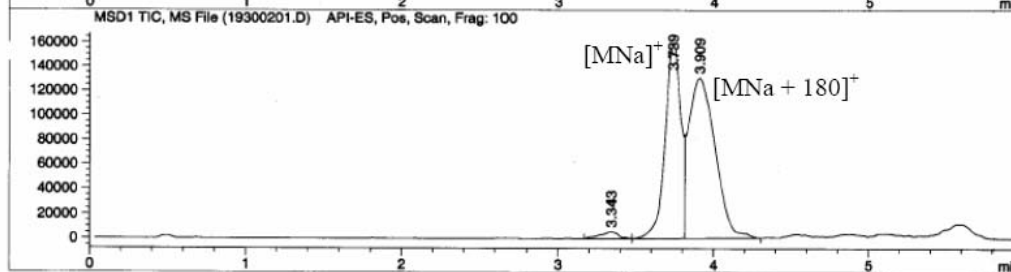
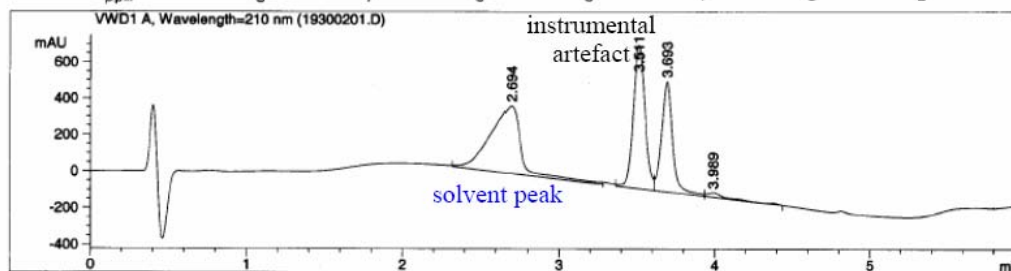
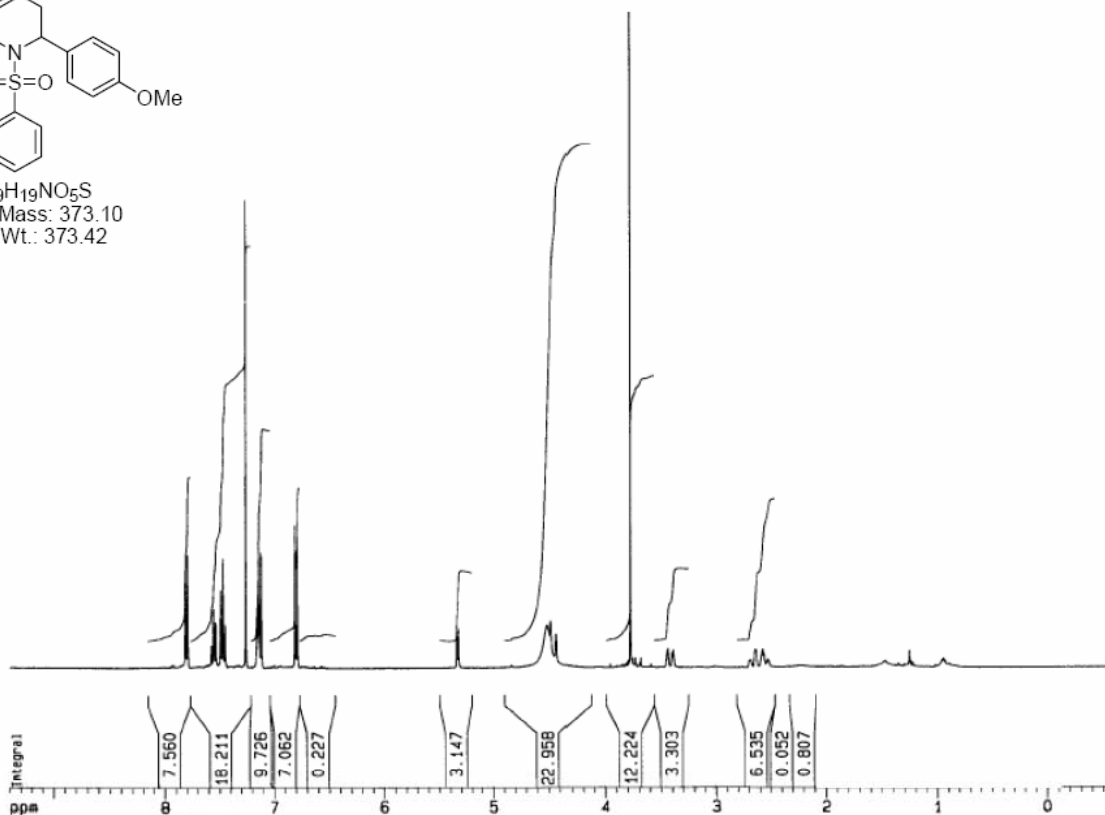
C₂₁H₂₁NO₇S
 Exact Mass: 431.10
 Mol. Wt.: 431.46



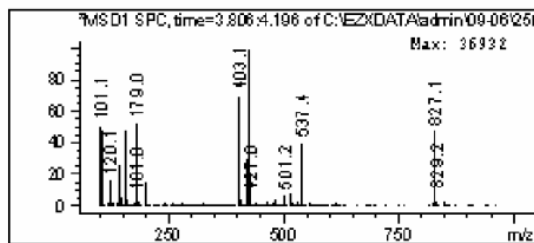
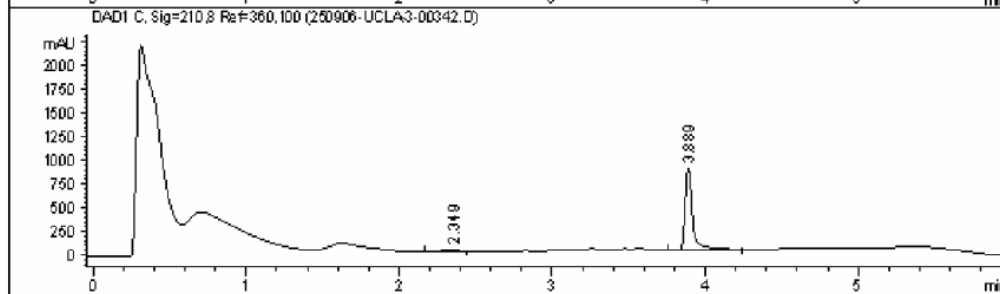
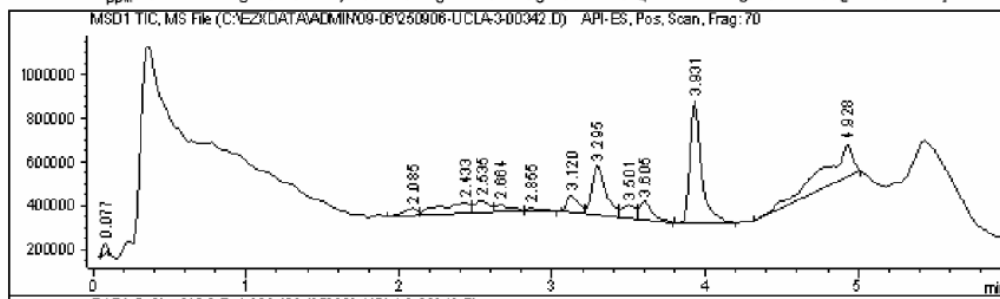
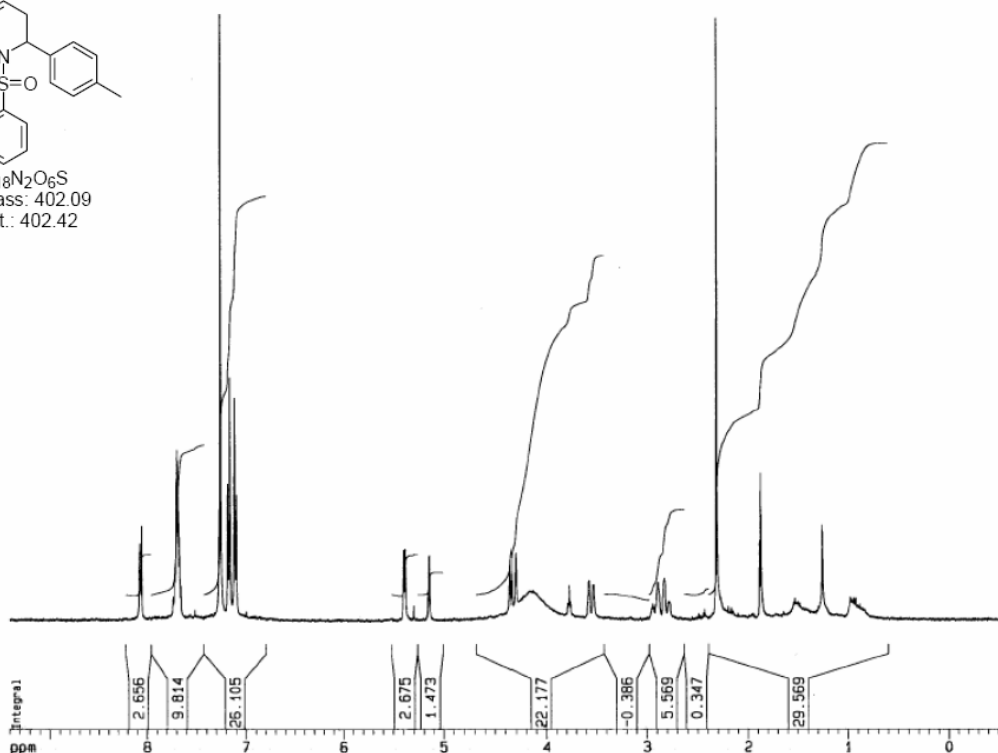
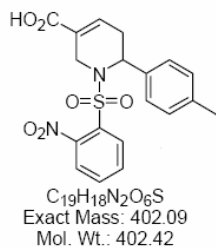
Benzenesulfonyl-6-(4-methoxyphenyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C35)



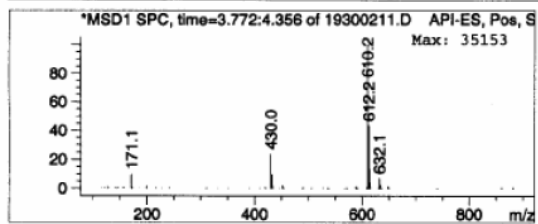
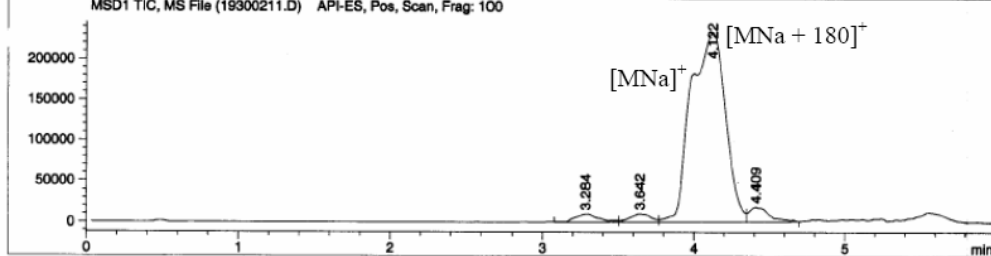
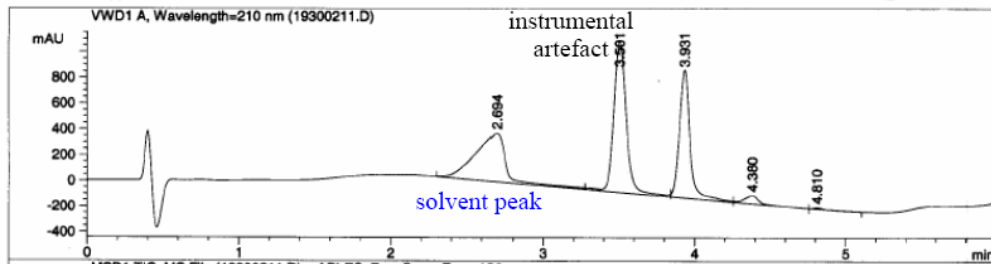
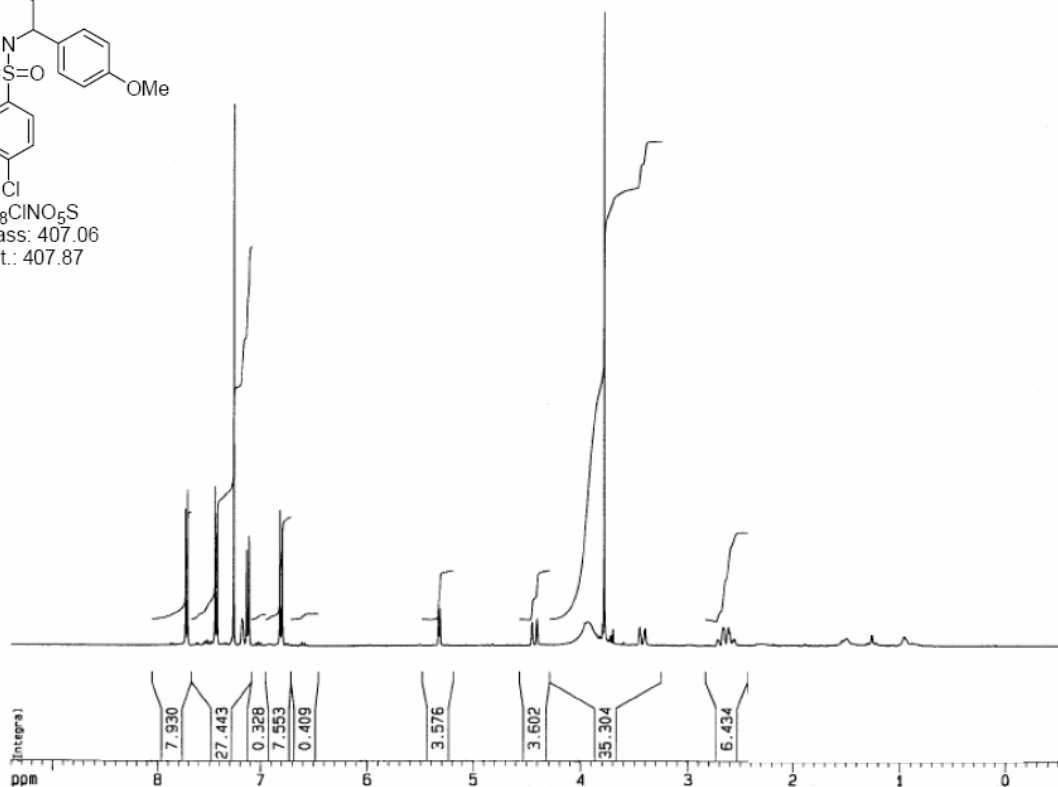
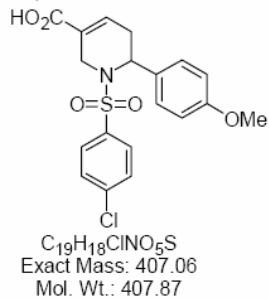
C₁₉H₁₉NO₅S
 Exact Mass: 373.10
 Mol. Wt.: 373.42



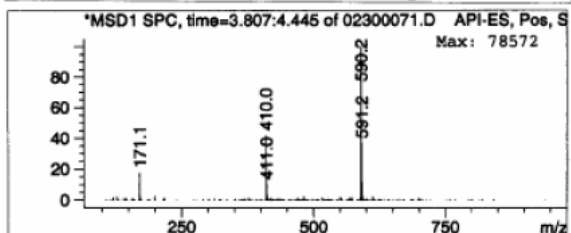
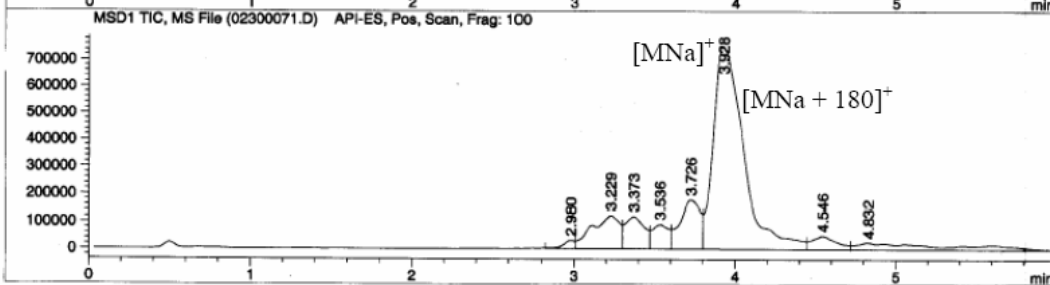
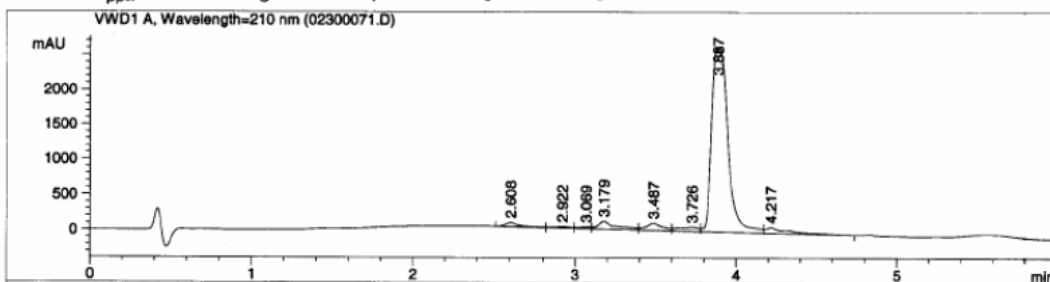
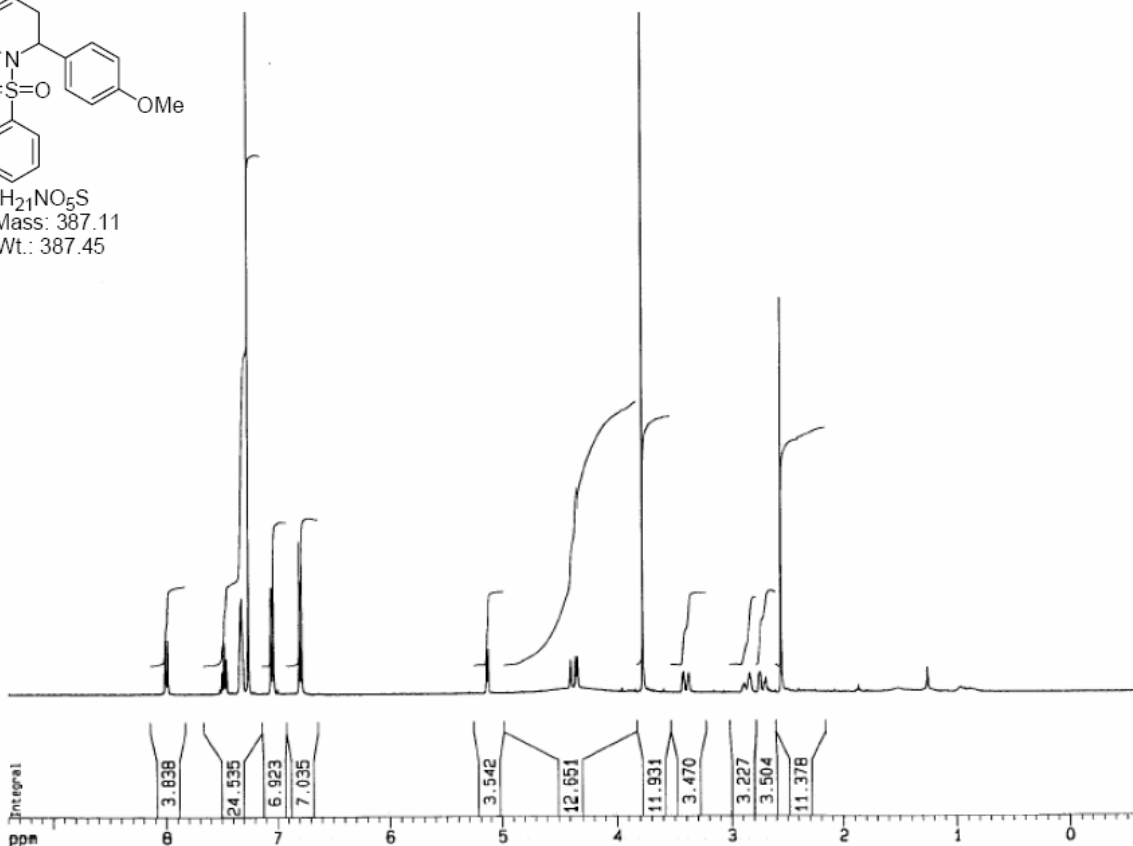
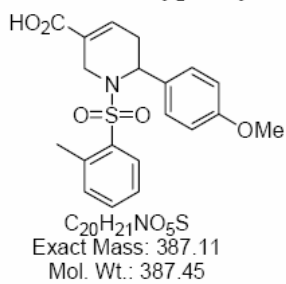
1-(2-Nitrobenzenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C36)



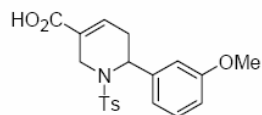
1-(4-Chlorobenzenesulfonyl)-6-(4-methoxyphenyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C37)



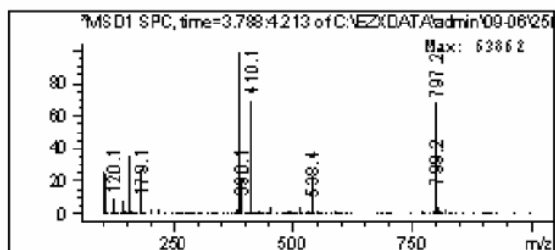
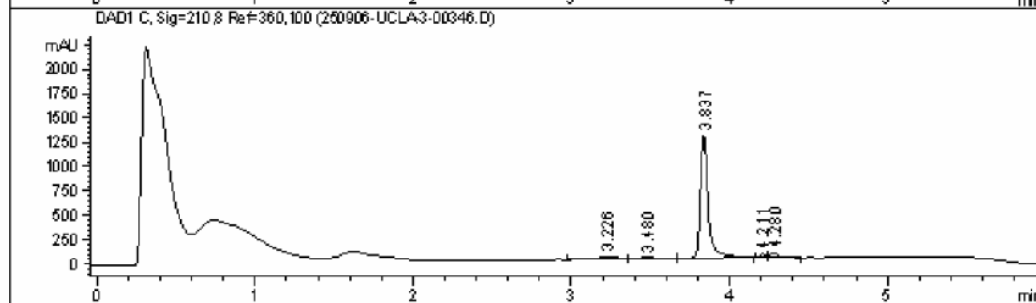
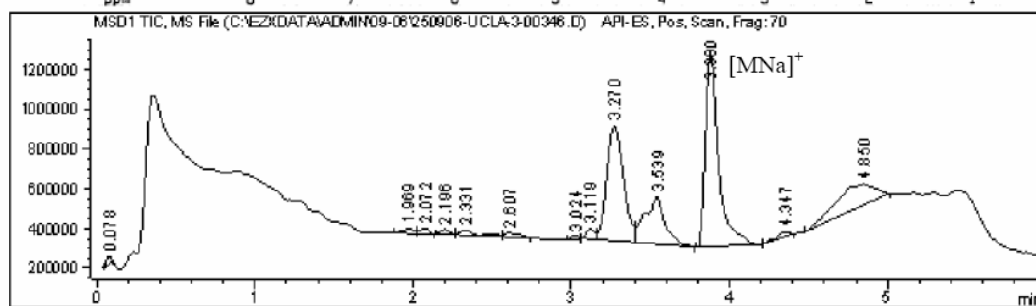
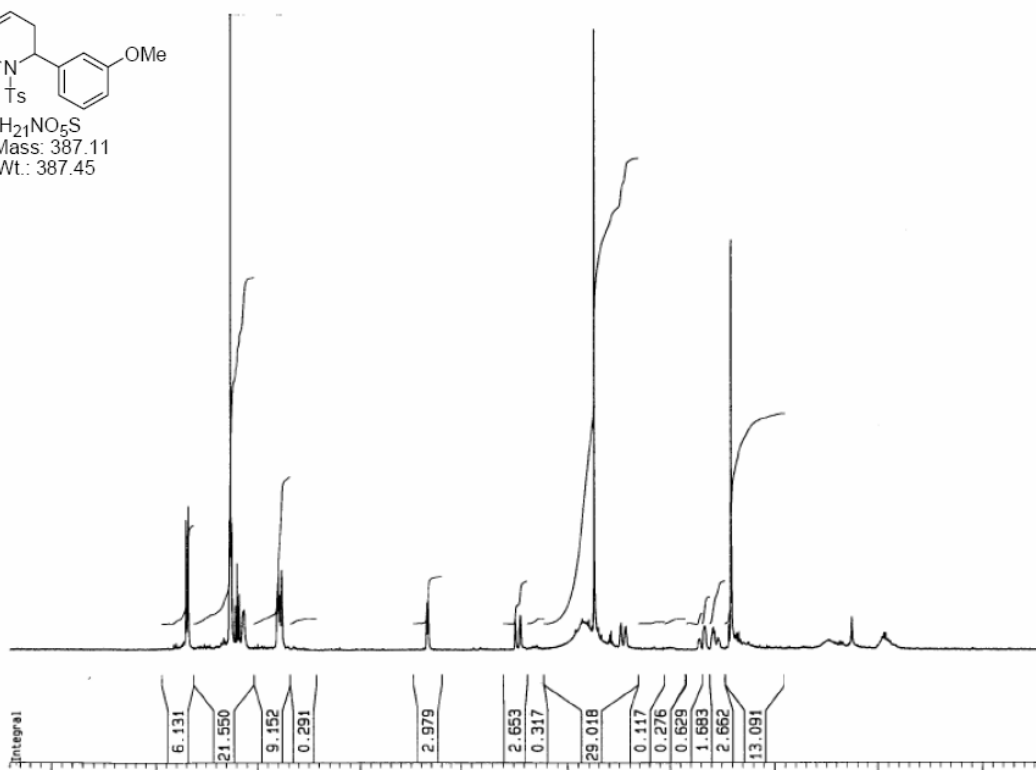
6-(4-Methoxyphenyl)-1-(2-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C38)



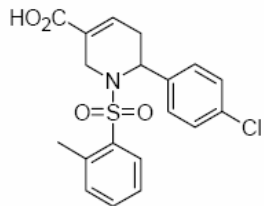
6-(3-Methoxyphenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C39)



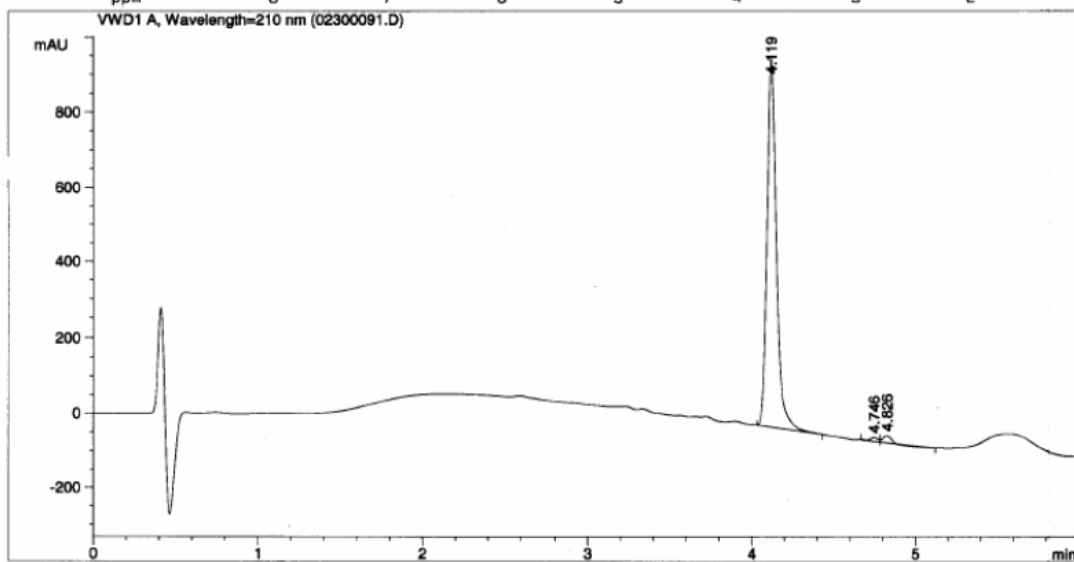
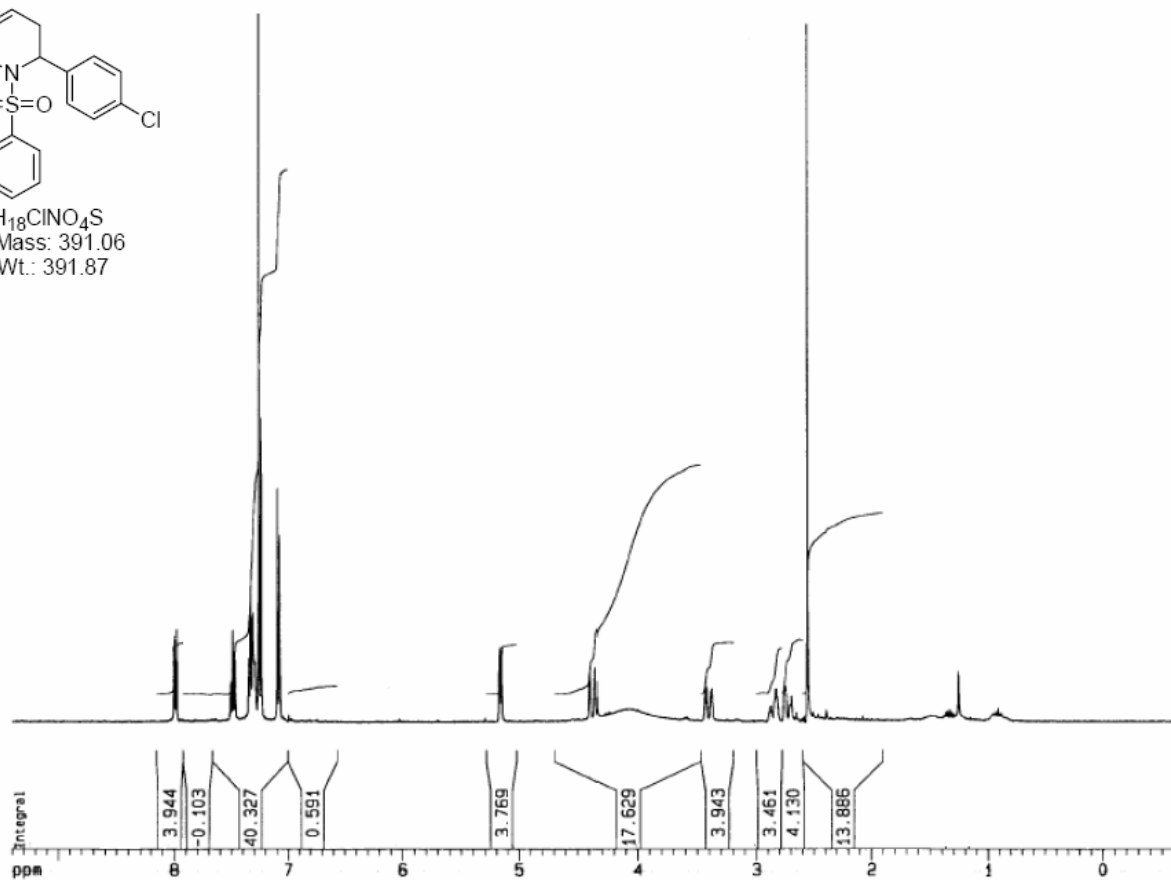
C₂₀H₂₁NO₅S
 Exact Mass: 387.11
 Mol. Wt.: 387.45



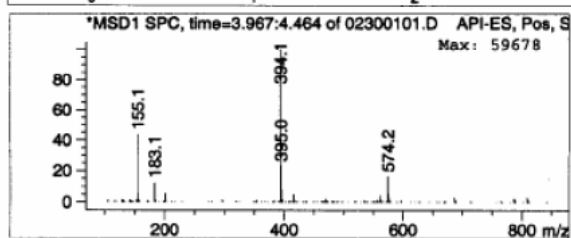
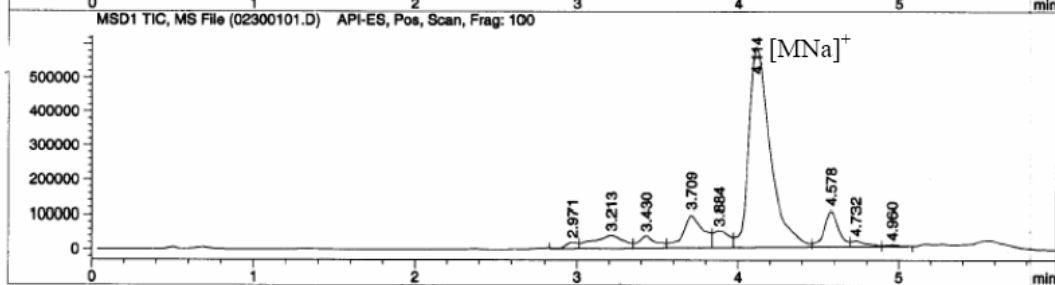
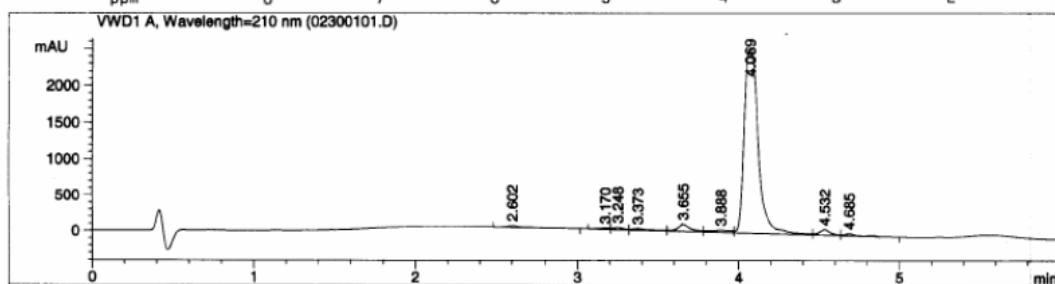
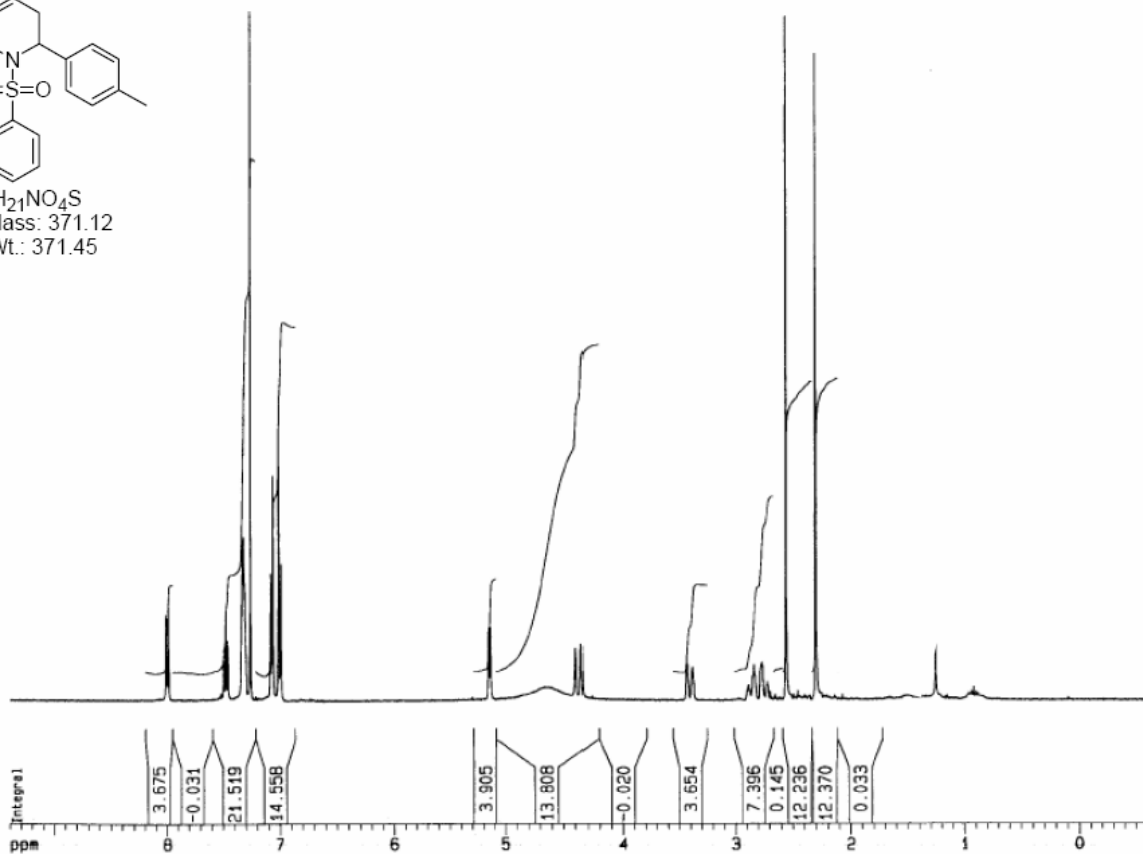
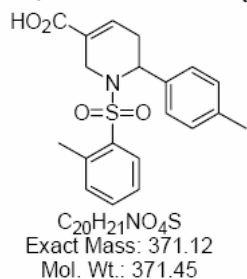
6-(4-Chlorophenyl)-1-(2-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C40)



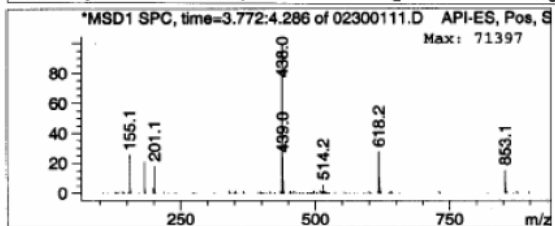
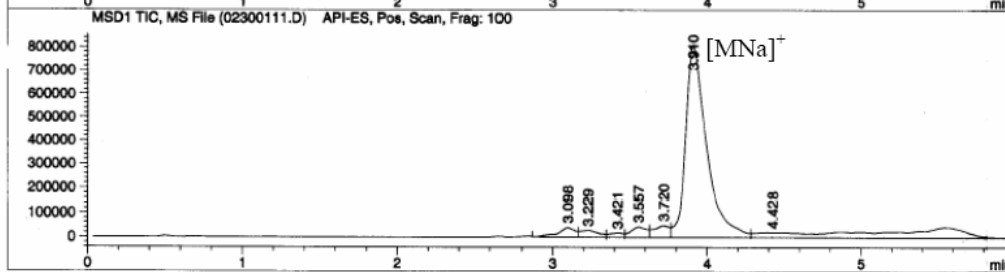
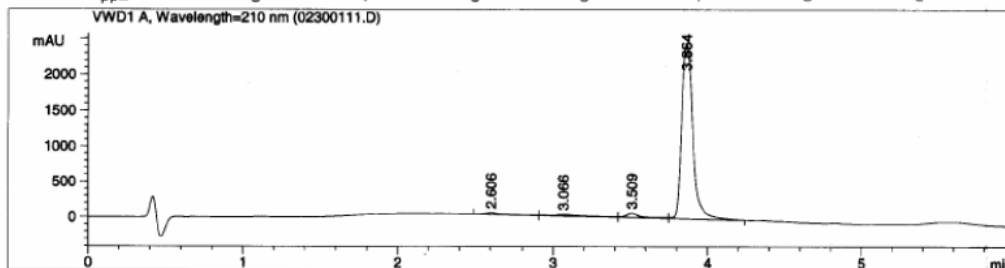
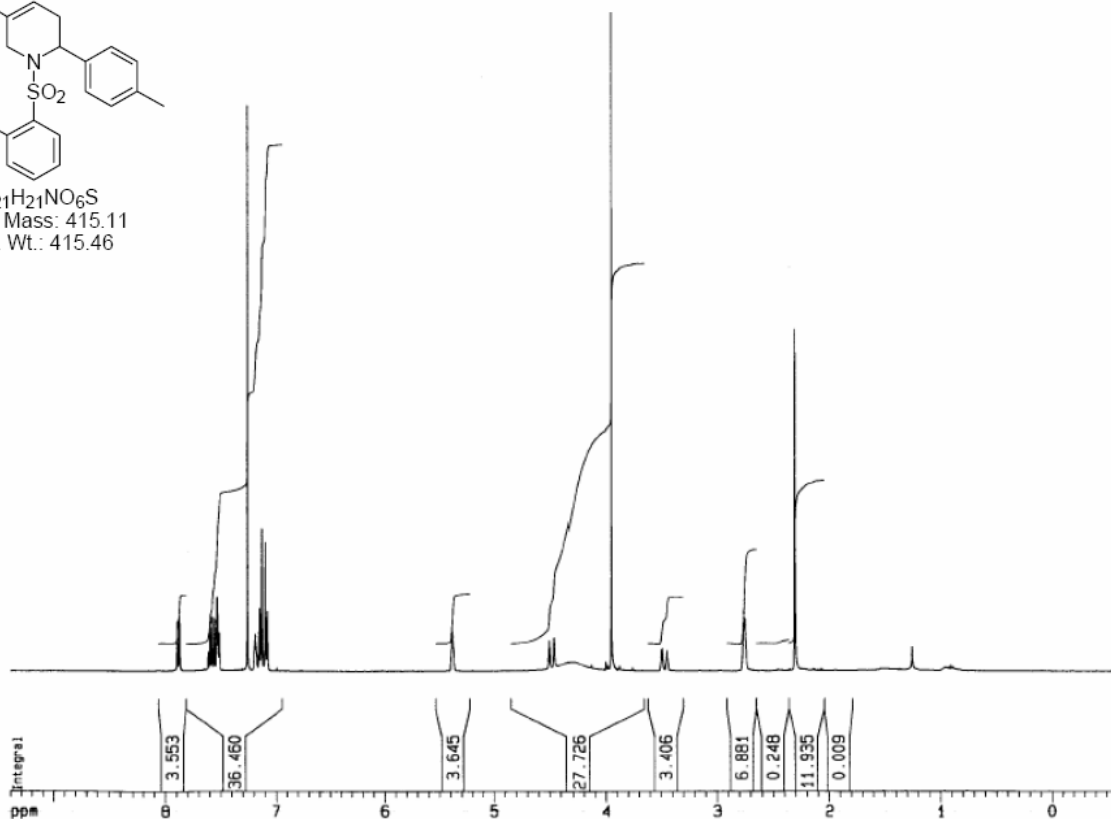
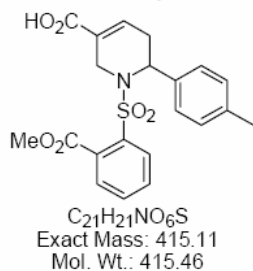
C₁₉H₁₈ClNO₄S
Exact Mass: 391.06
Mol. Wt.: 391.87



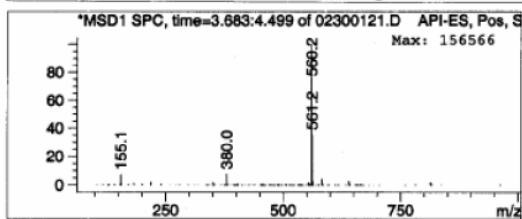
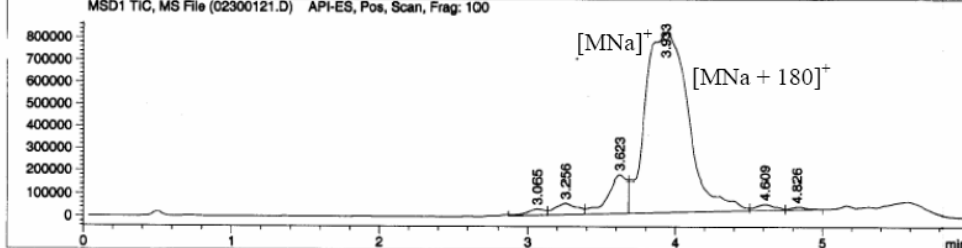
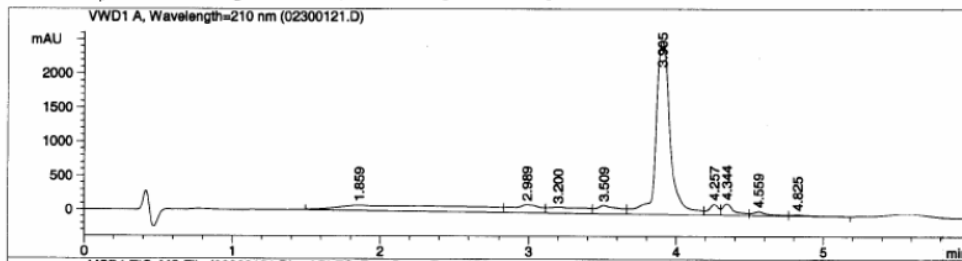
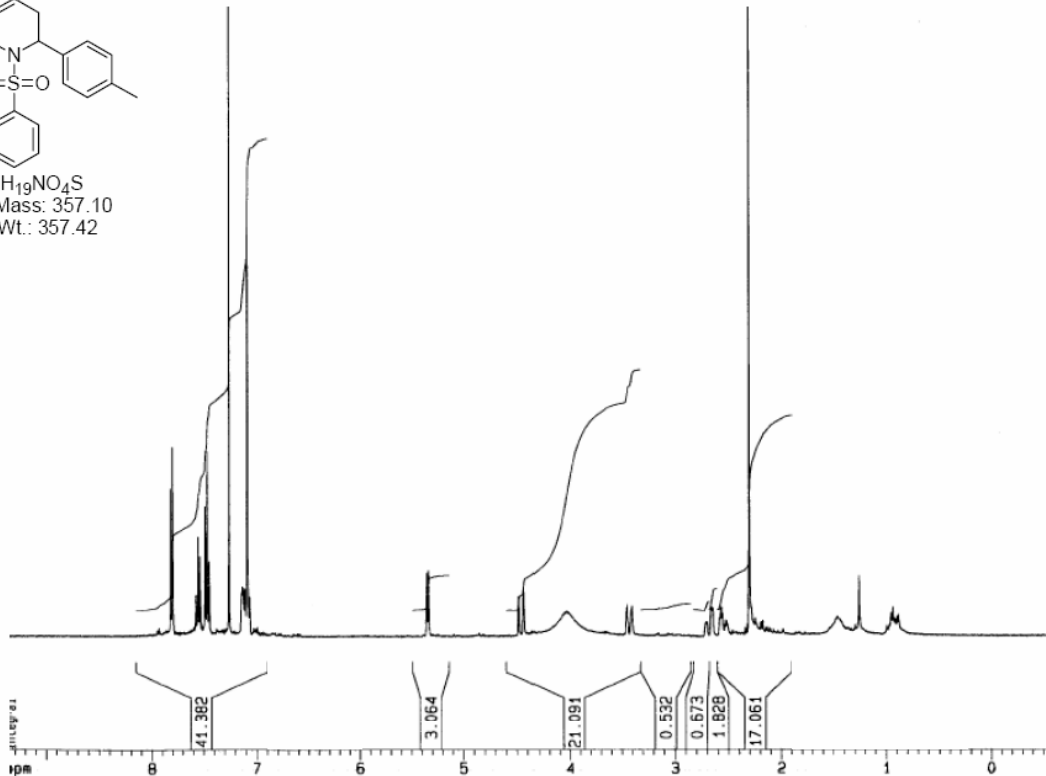
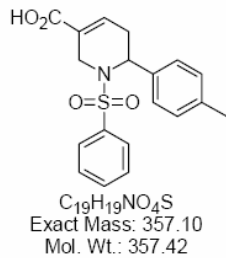
1-(2-Toluenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C41)



1-(2-Methoxycarbonylbenzenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C42)

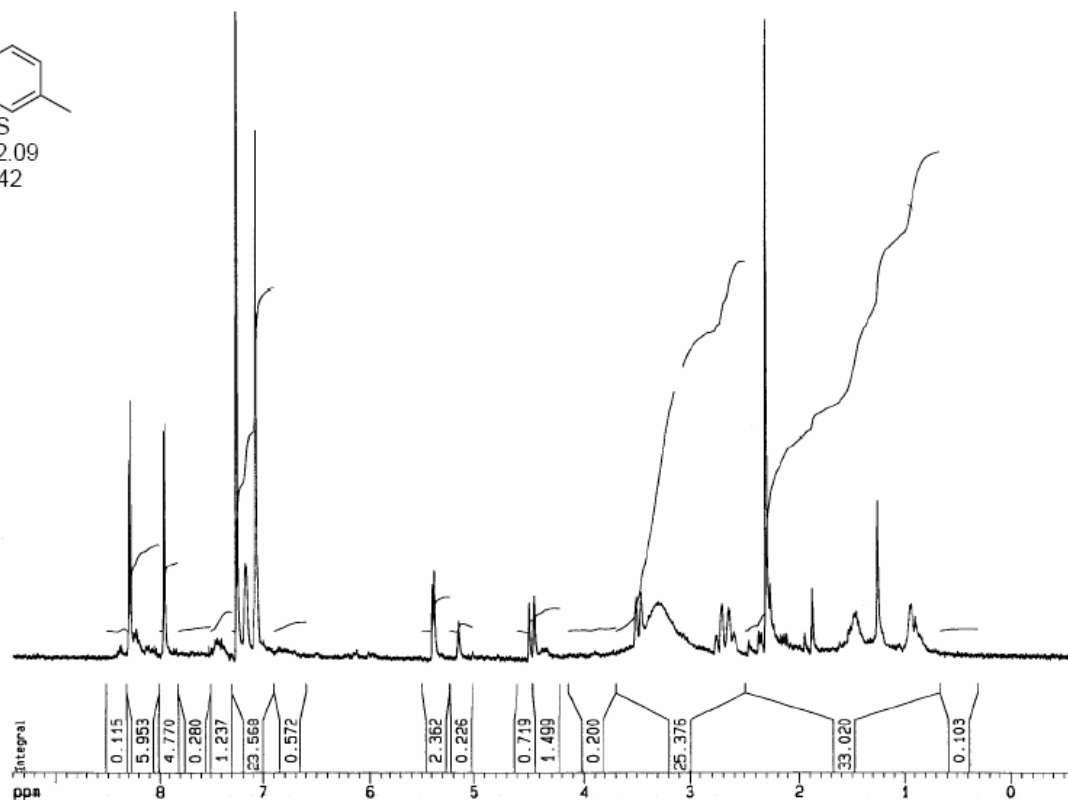
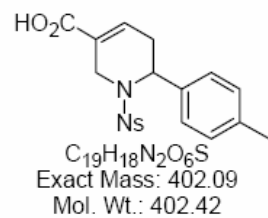


1-Benzenesulfonyl-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C43)



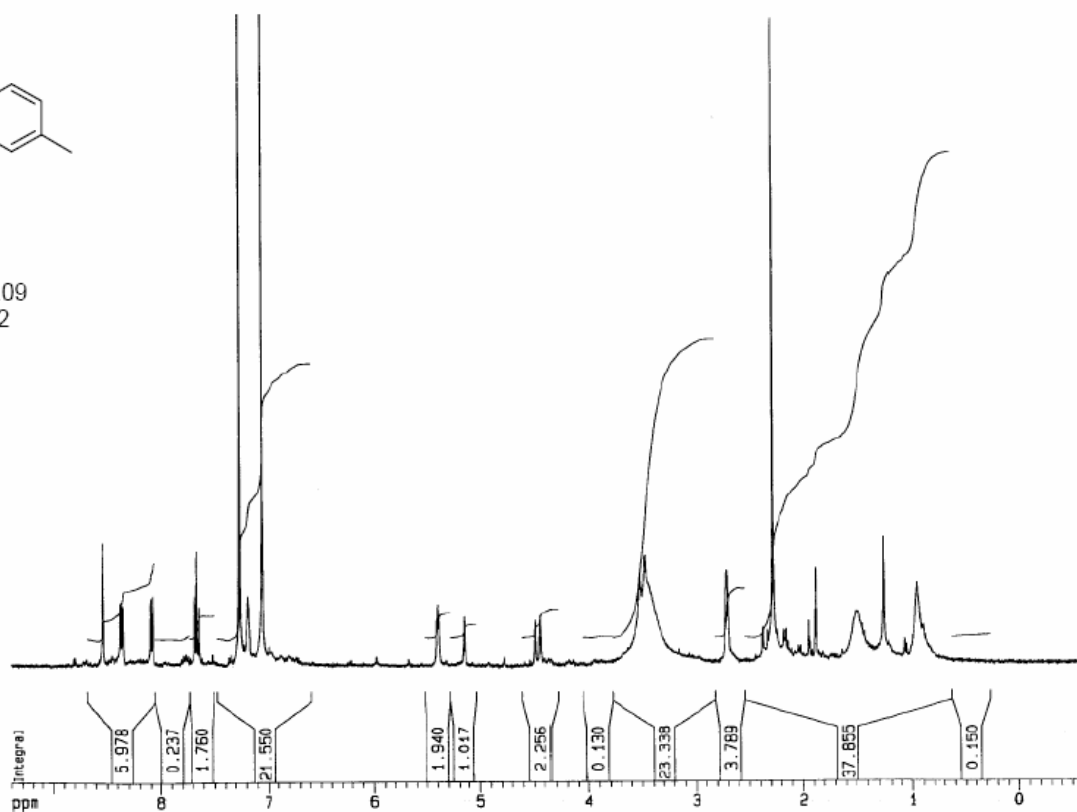
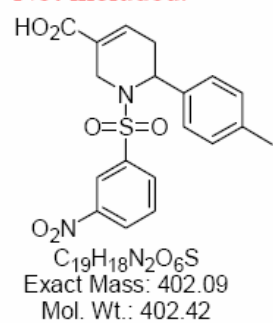
1-(4-Nitrobenzenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C44)

Not included.



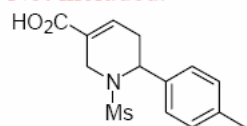
1-(3-Nitrobenzenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C45)

Not included.

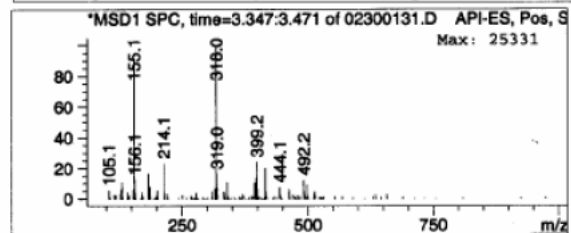
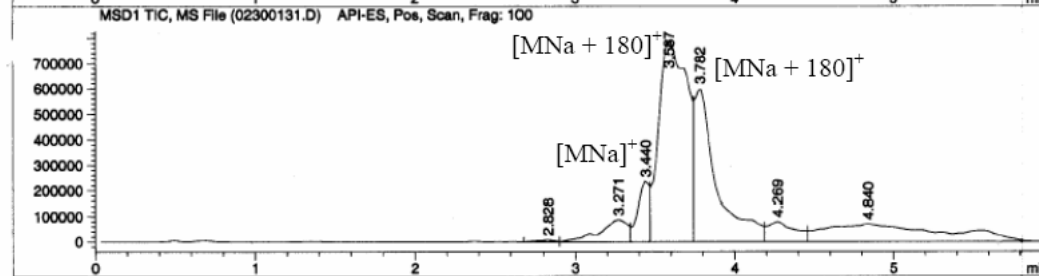
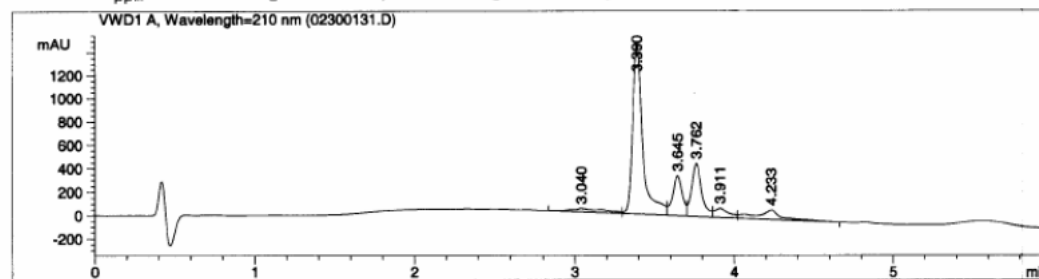
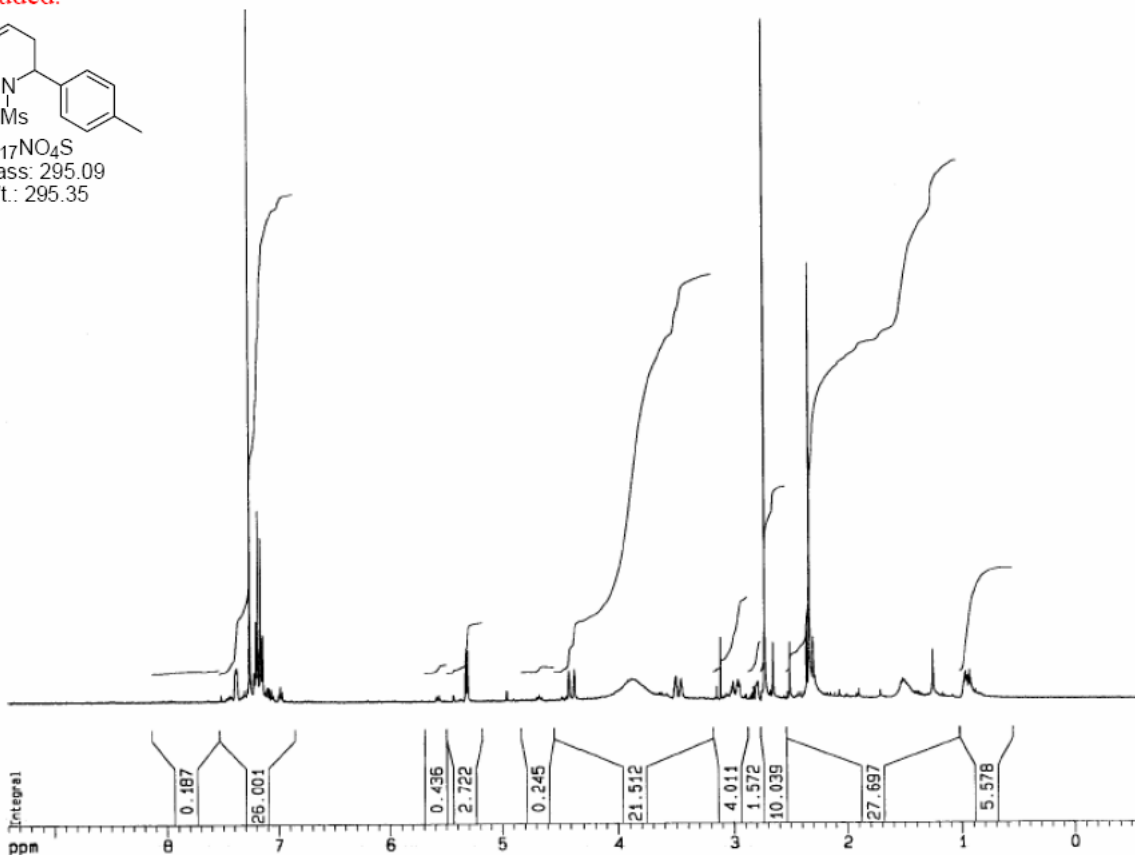


1-Methanesulfonyl-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B01C46)

Not included.

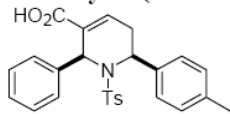


C₁₄H₁₇NO₄S
Exact Mass: 295.09
Mol. Wt.: 295.35

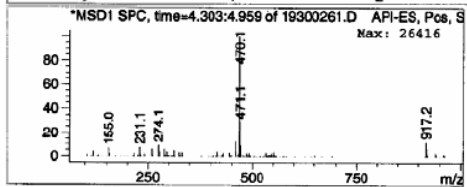
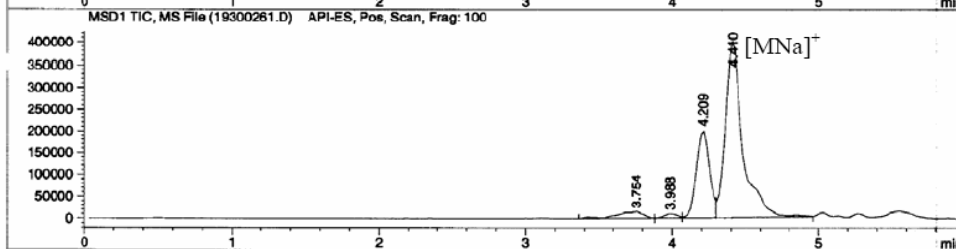
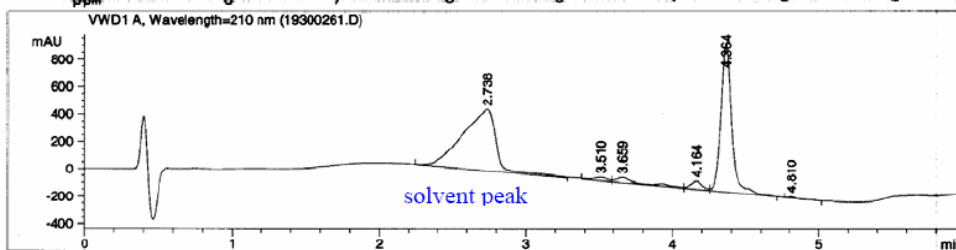
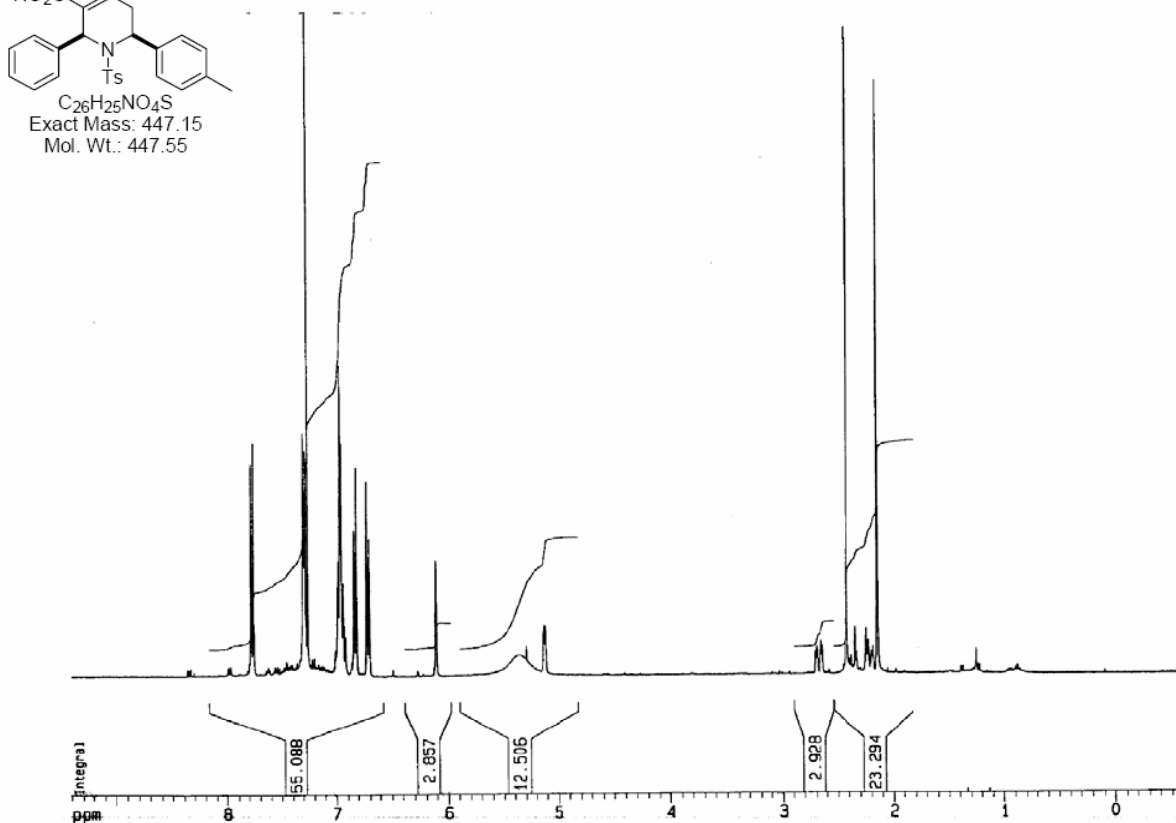


Spectral data for Table 7

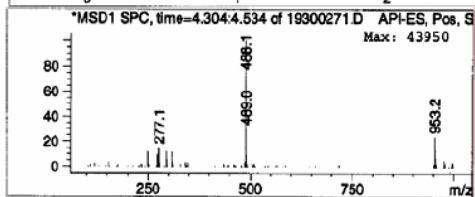
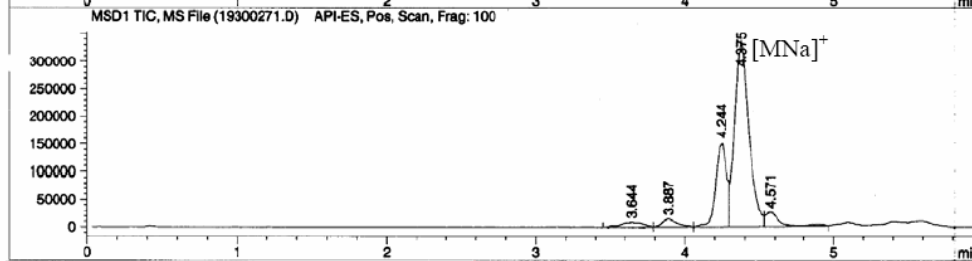
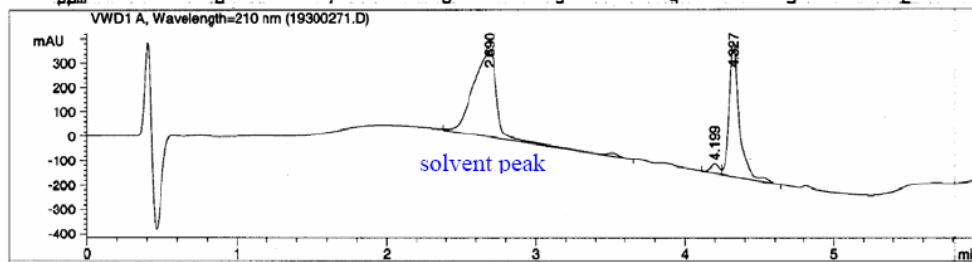
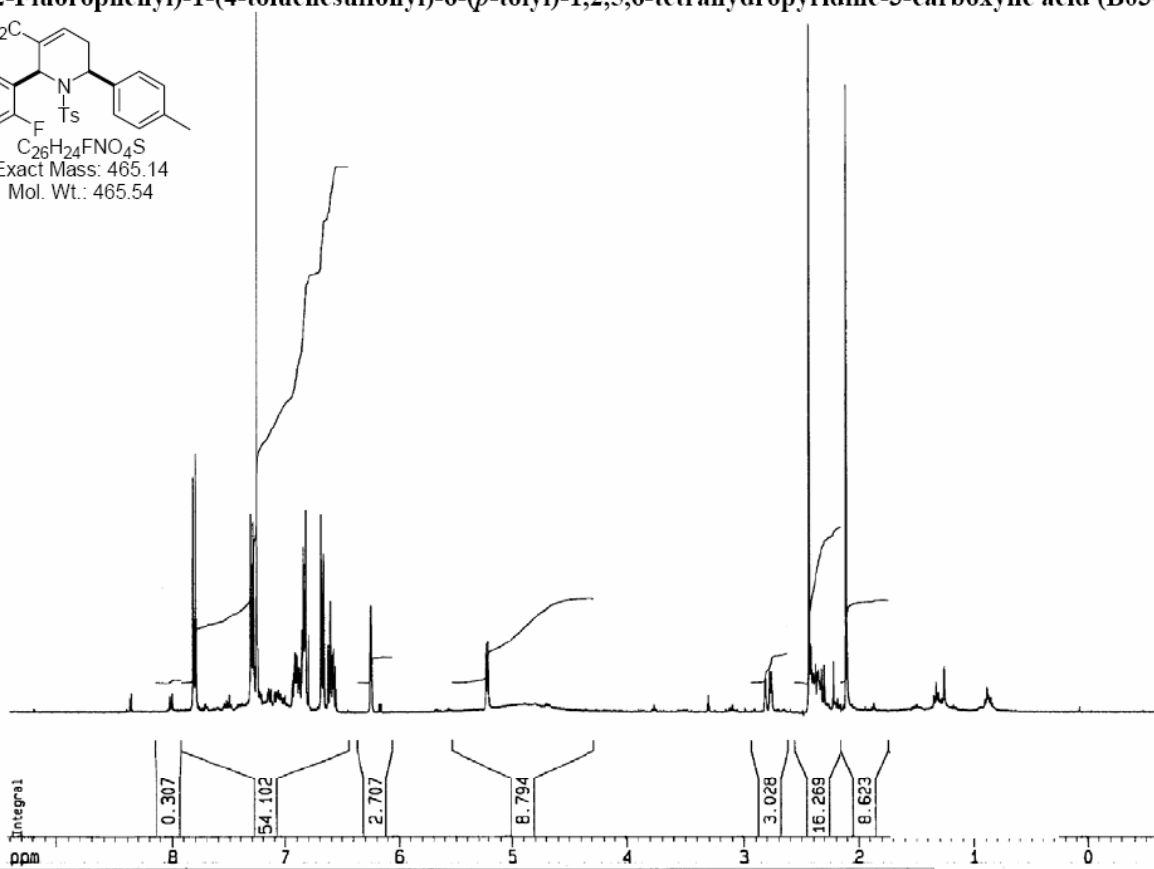
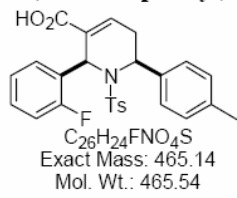
2-Phenyl-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B02C02)



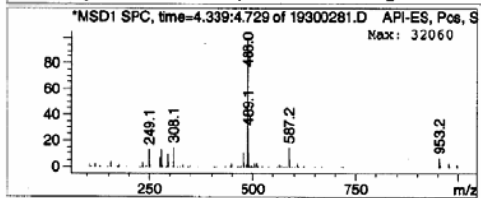
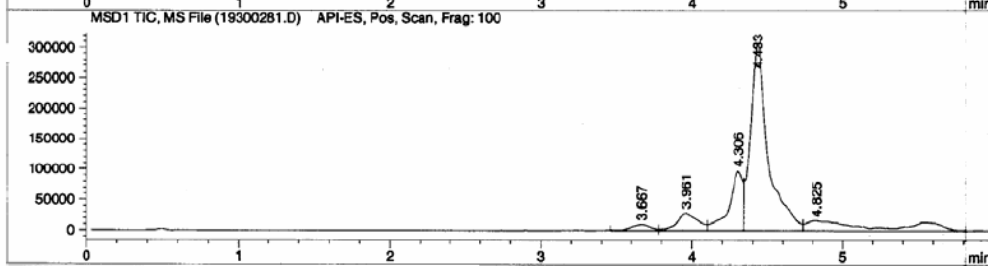
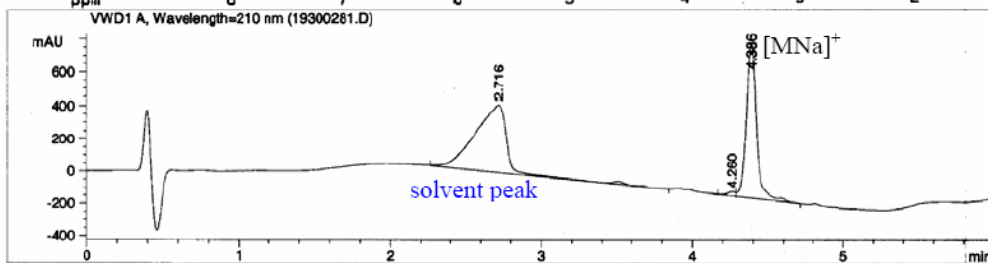
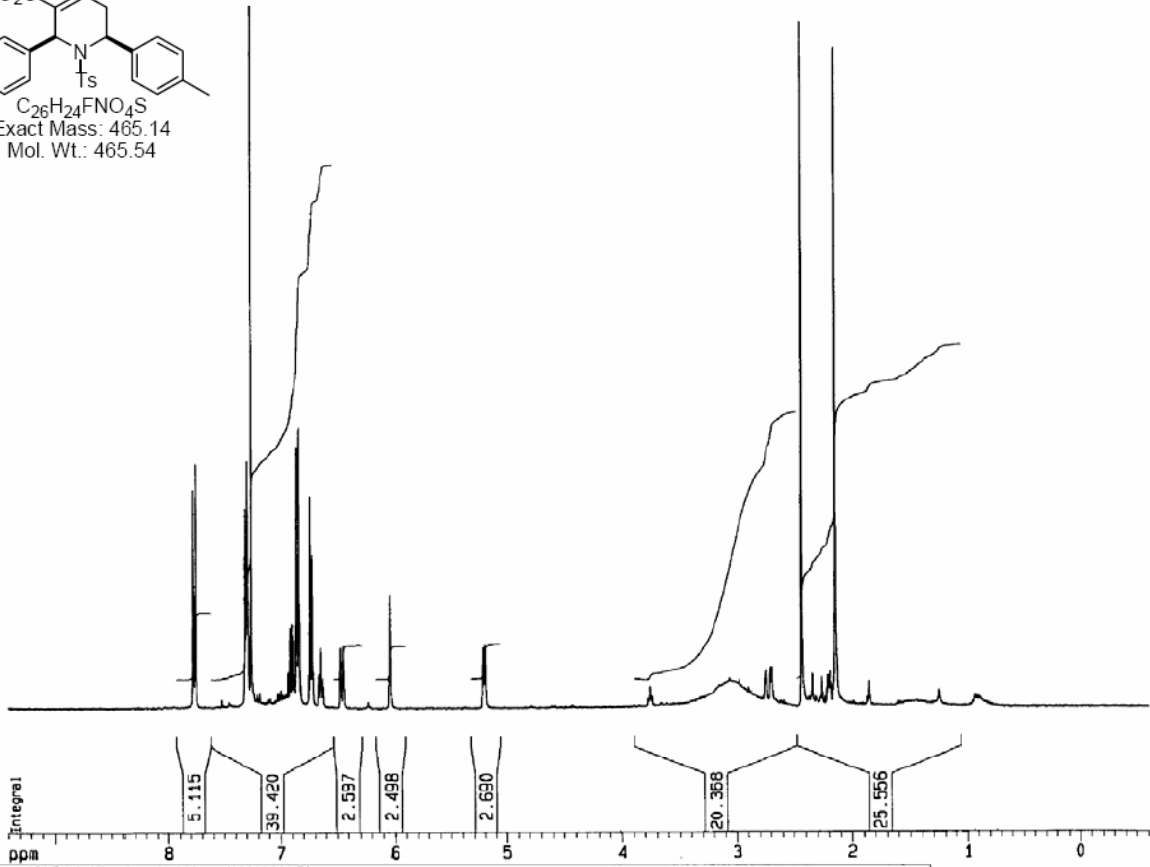
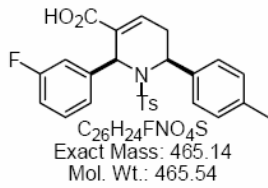
C₂₆H₂₅NO₄S
 Exact Mass: 447.15
 Mol. Wt.: 447.55



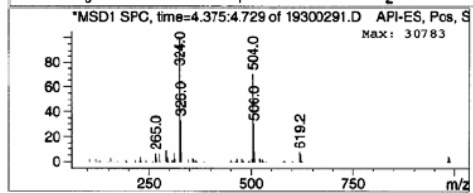
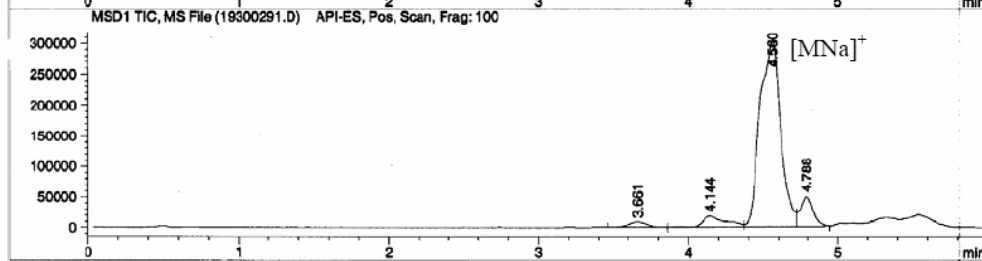
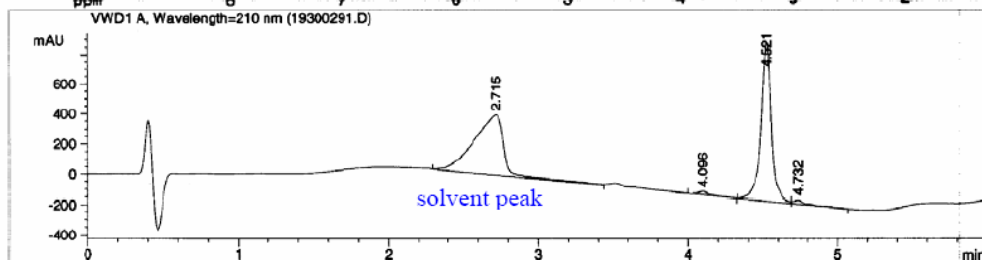
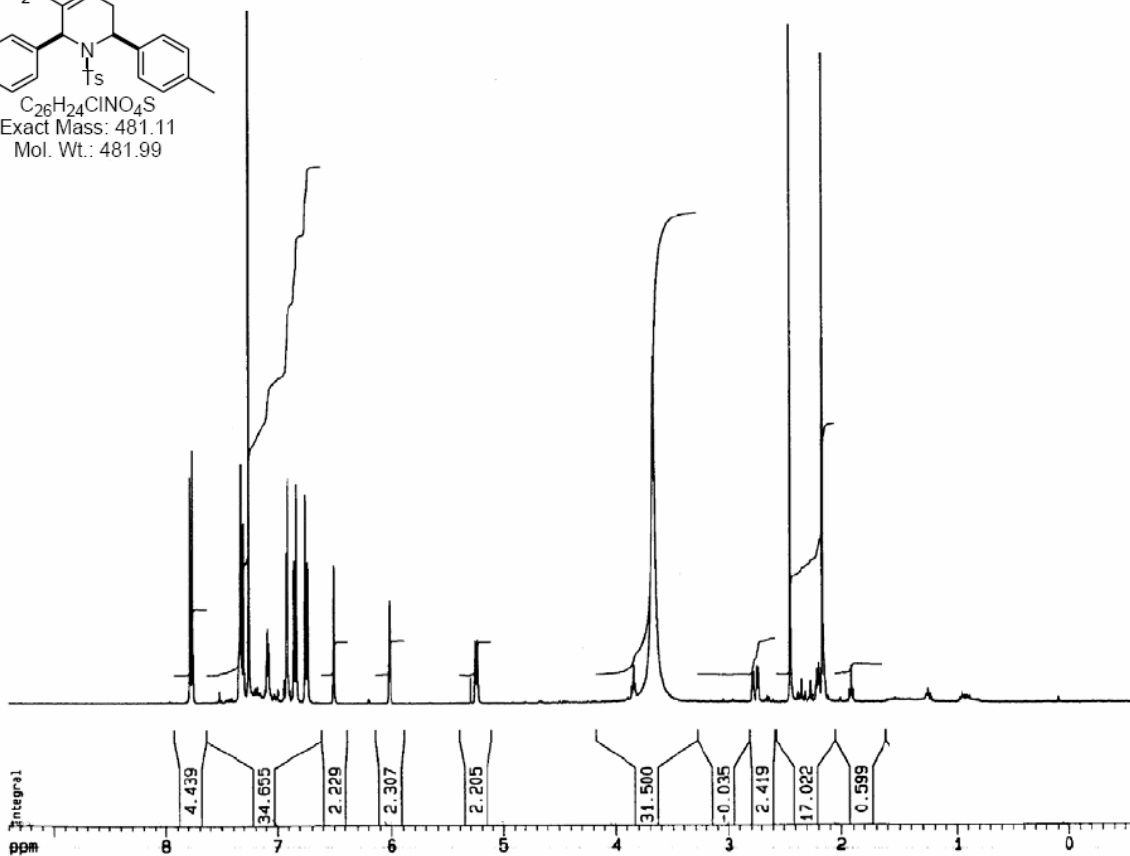
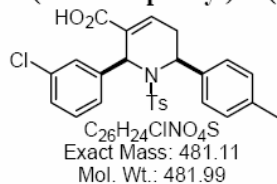
2-(2-Fluorophenyl)-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B03C02)



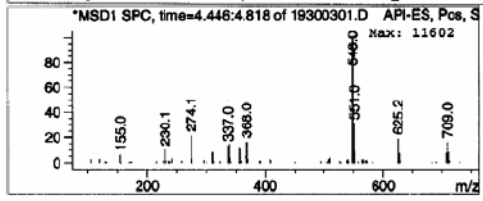
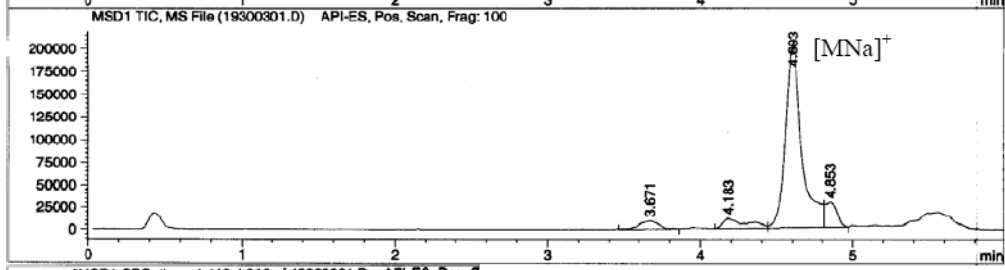
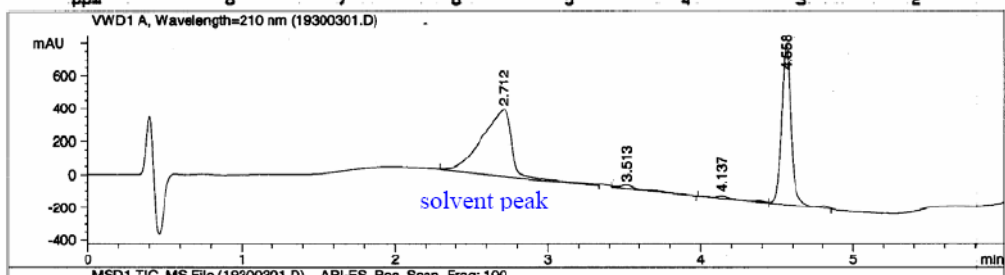
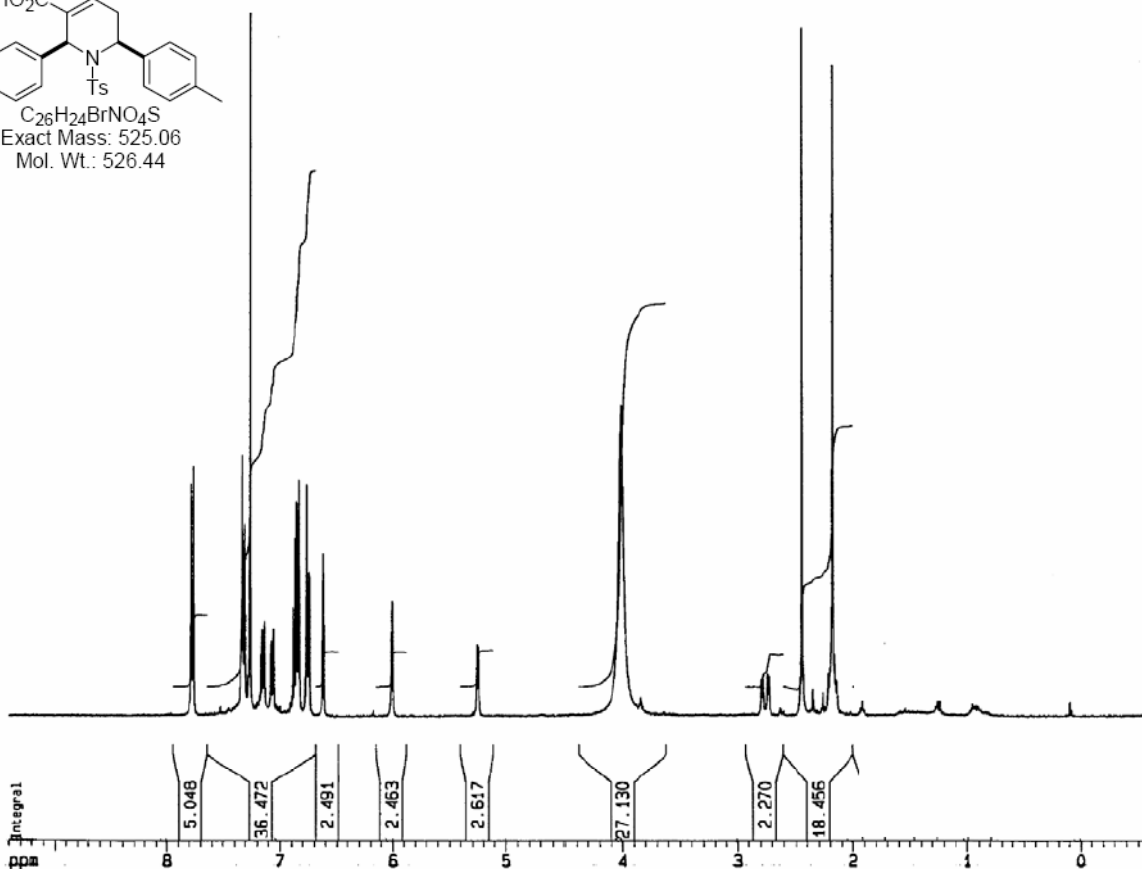
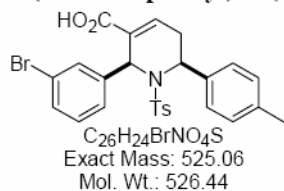
2-(3-Fluorophenyl)-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B04C02)



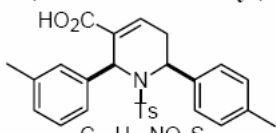
2-(3-Chlorophenyl)-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C02)



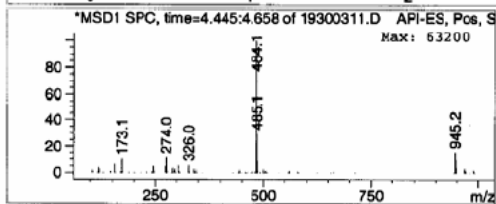
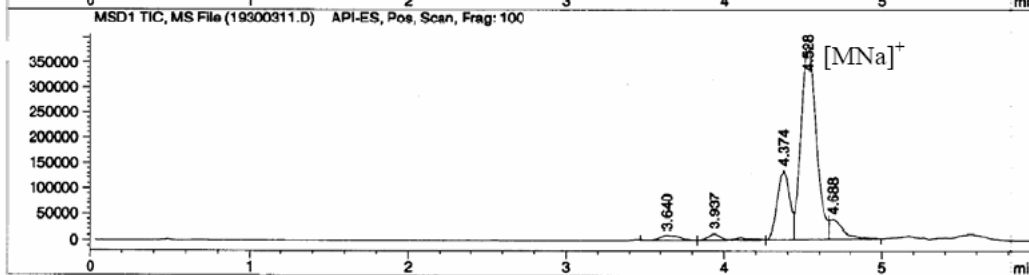
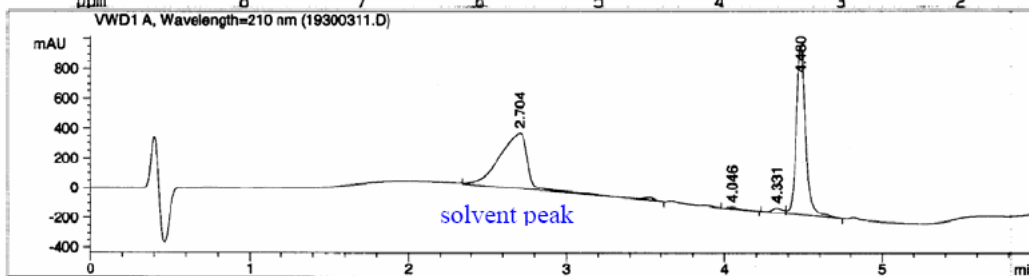
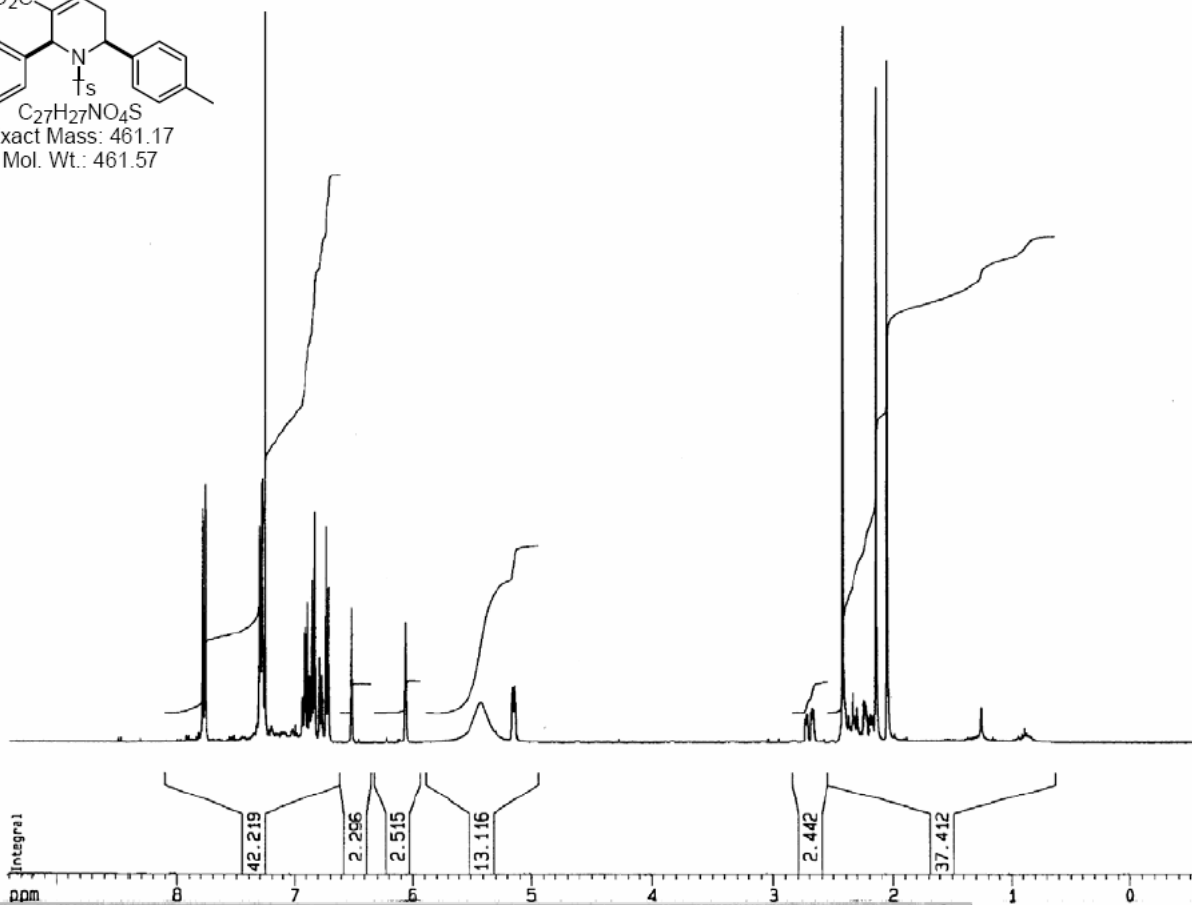
2-(3-Bromophenyl)-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B06C02)



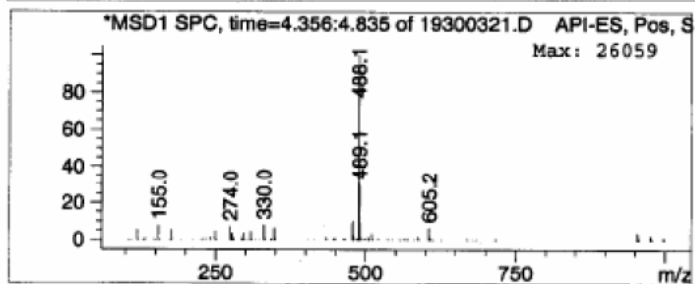
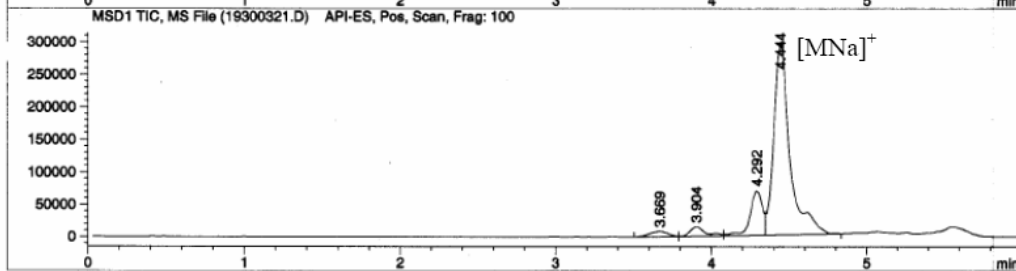
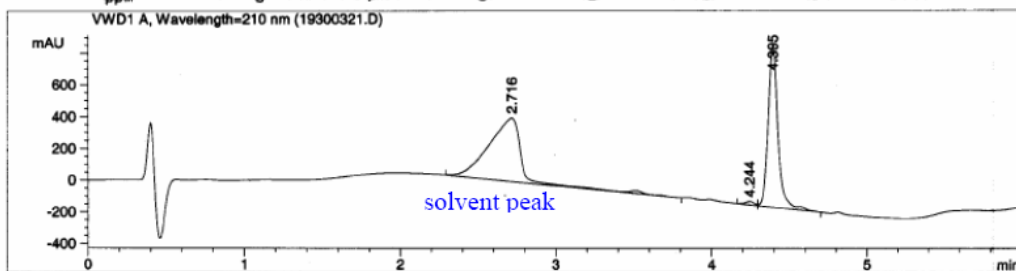
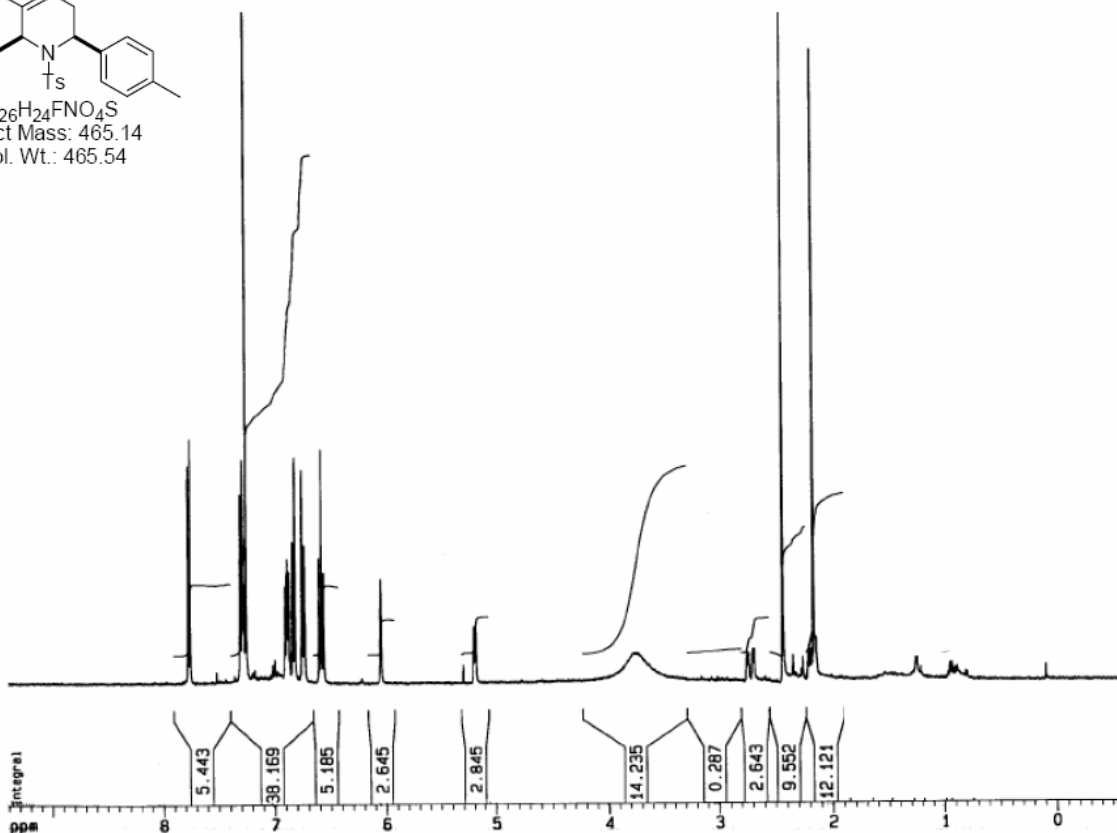
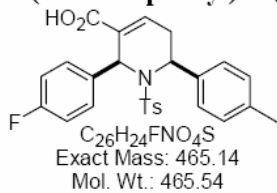
1-(4-Toluenesulfonyl)-2-(*m*-tolyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B07C02)



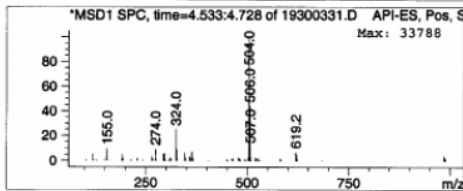
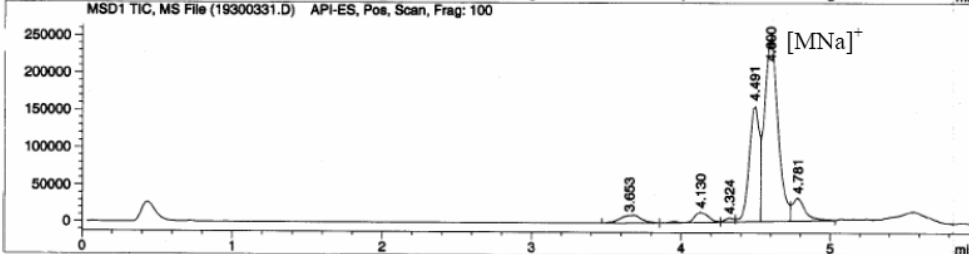
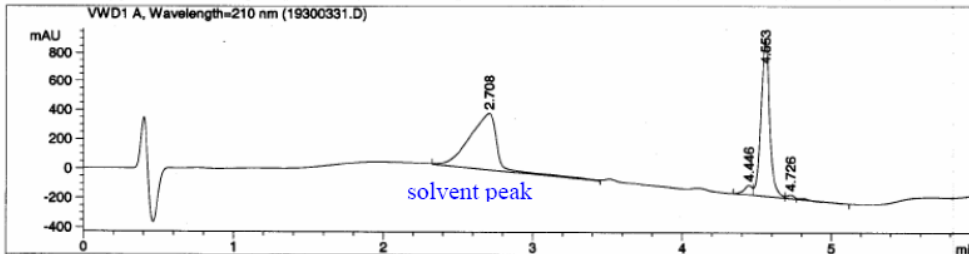
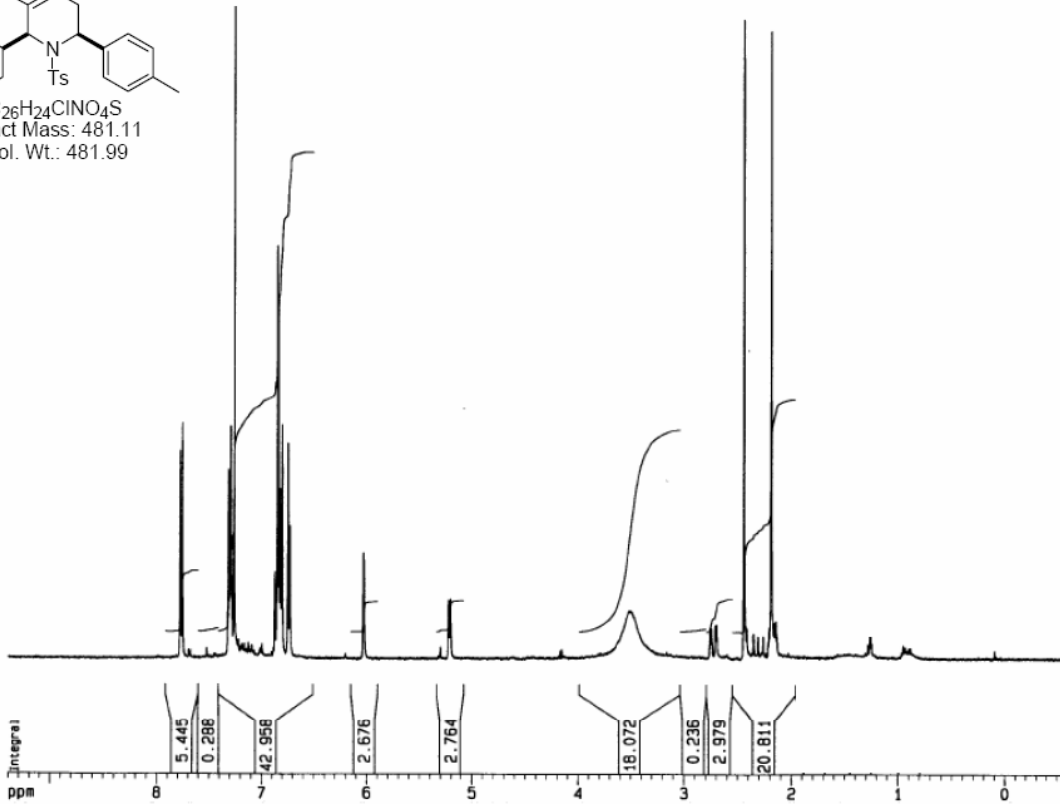
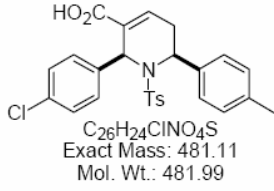
C₂₇H₂₇NO₄S
 Exact Mass: 461.17
 Mol. Wt.: 461.57



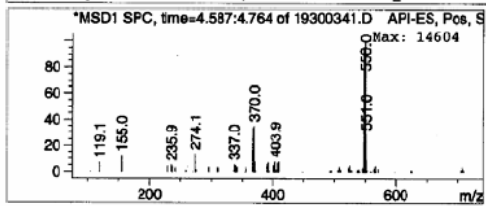
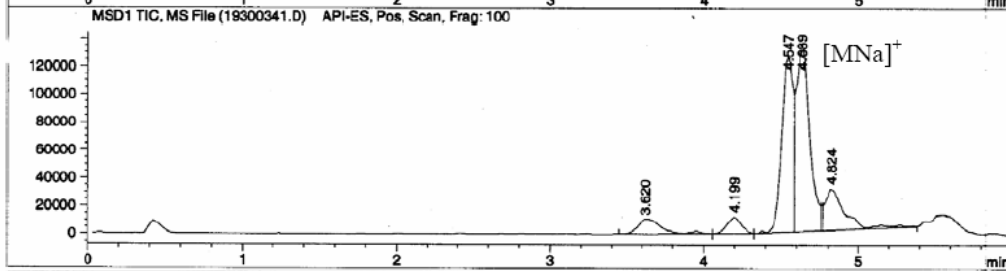
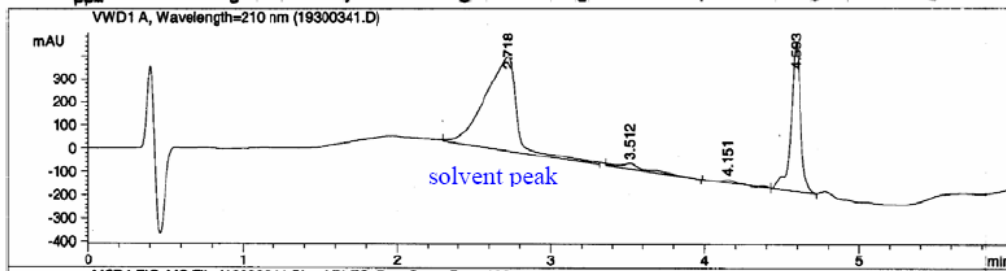
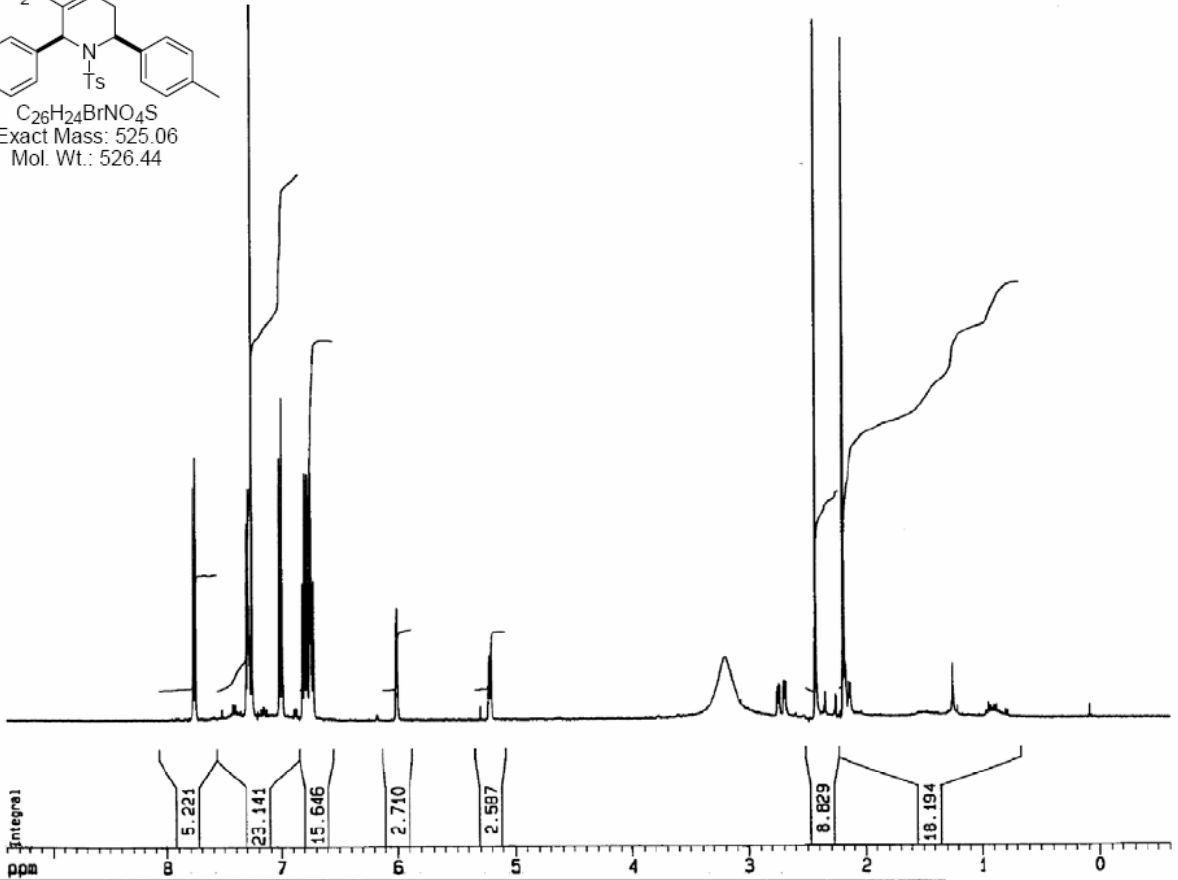
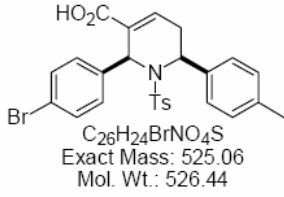
2-(4-Fluorophenyl)-1-(4-toluenesulfonyl)-6-(p-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B08C02)



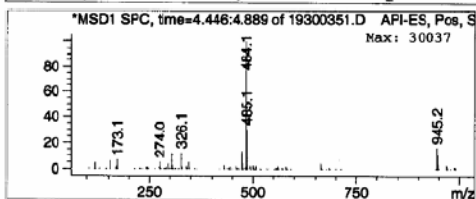
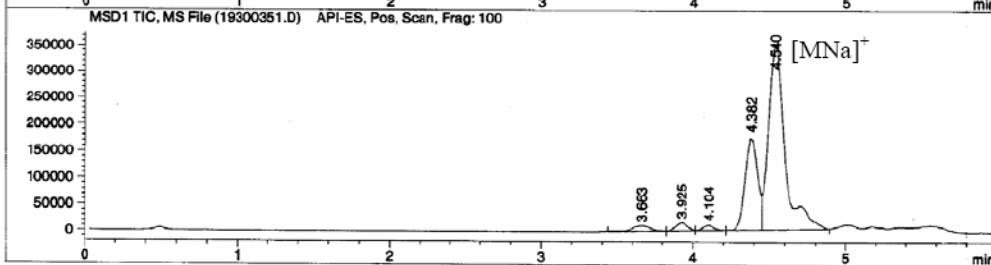
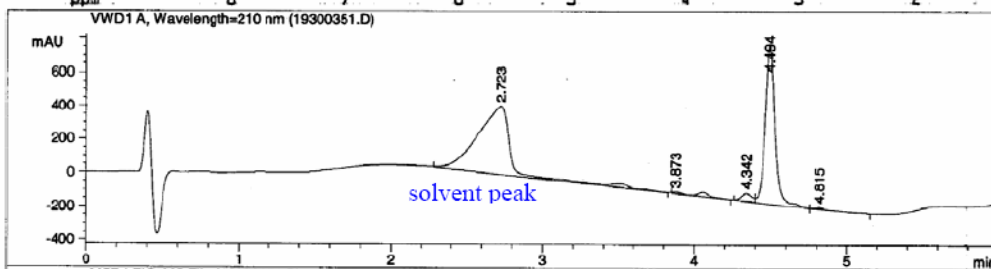
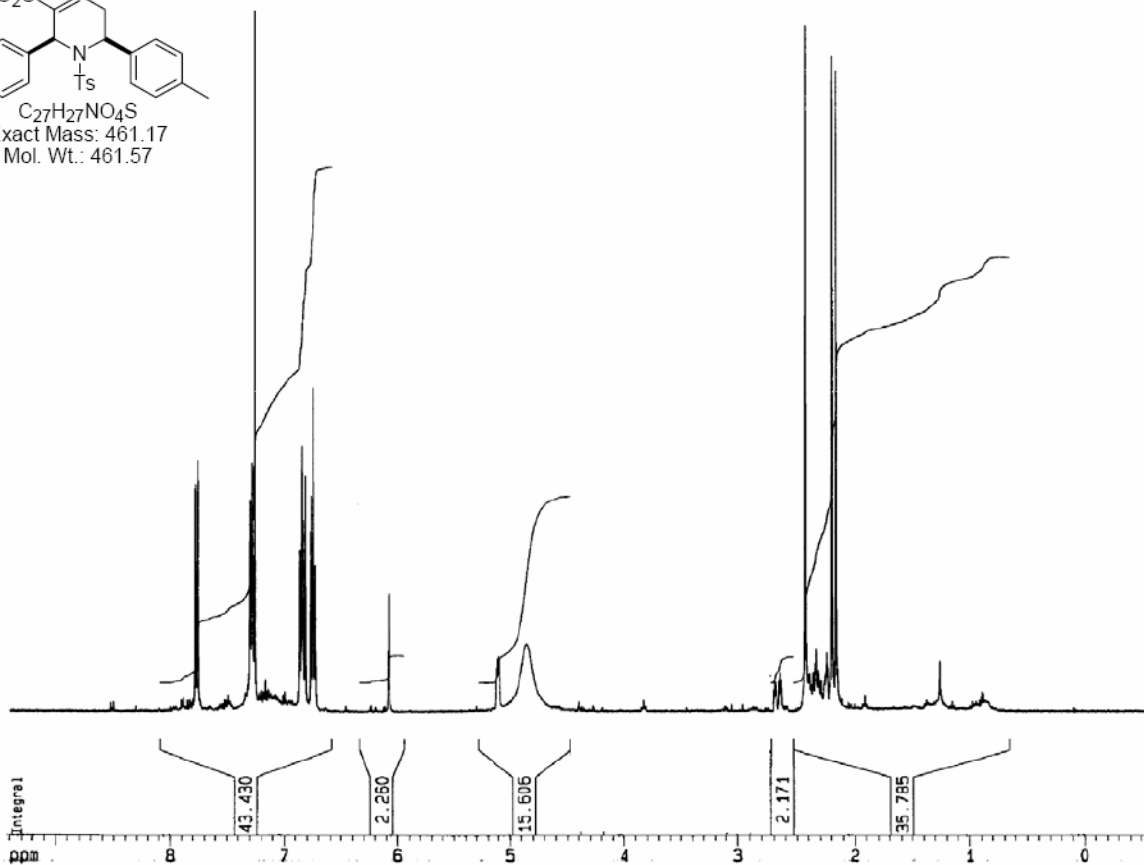
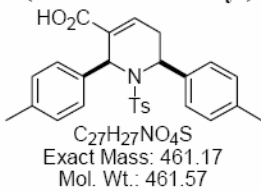
2-(4-Chlorophenyl)-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B09C02)



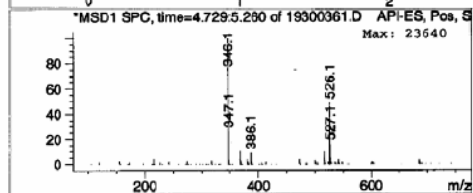
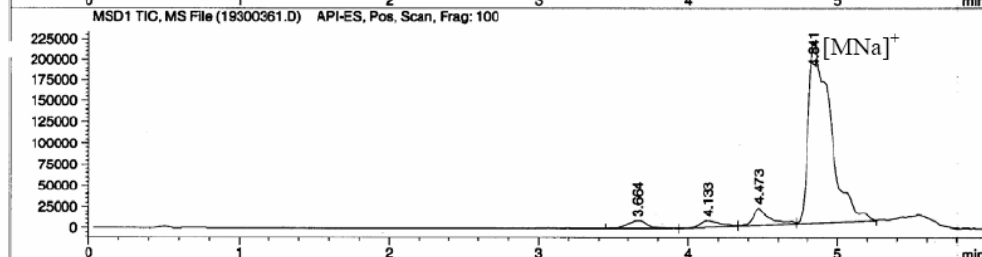
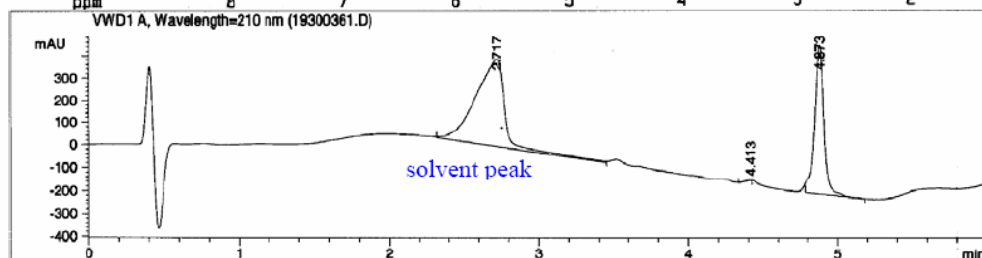
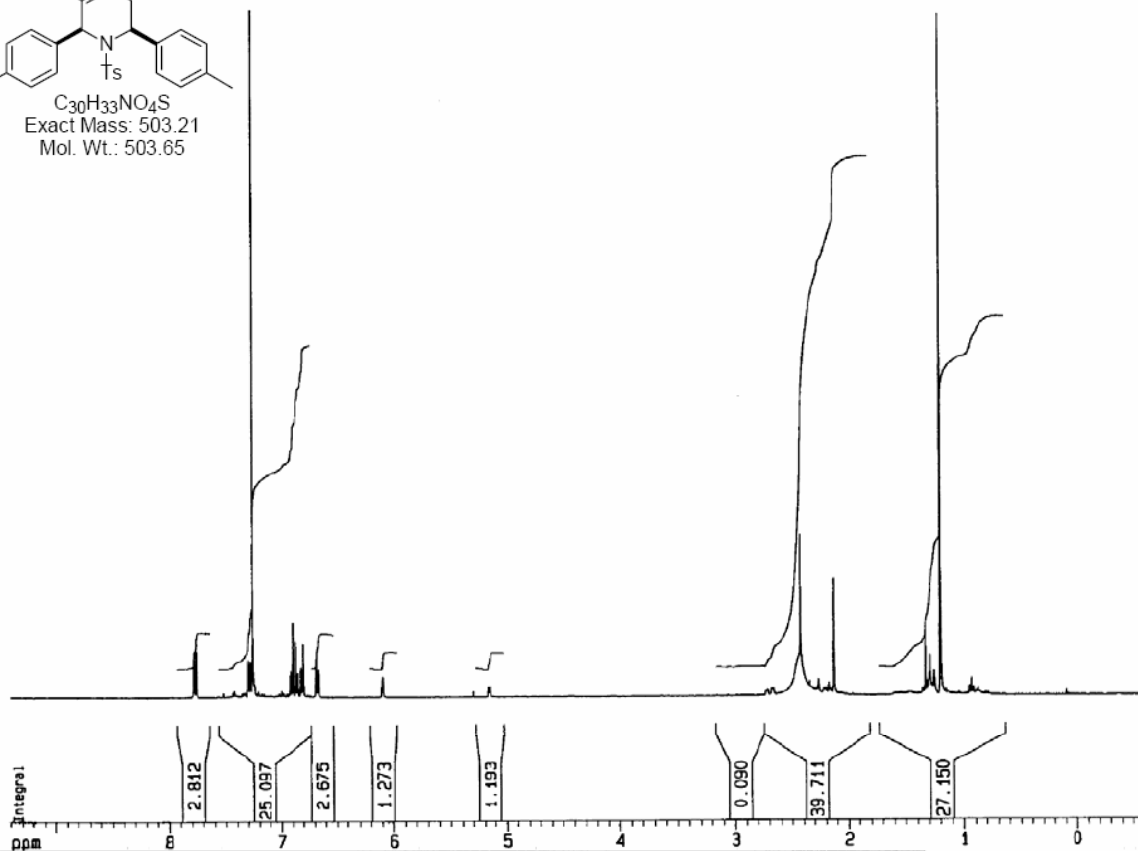
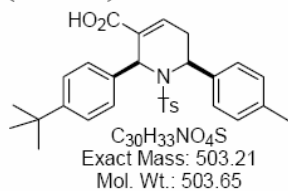
2-(4-Bromophenyl)-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B10C02)



1-(4-Toluenesulfonyl)-2,6-di-(p-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B11C02)

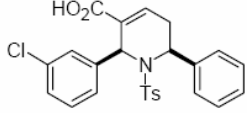


2-(4-*tert*-Butylphenyl)-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid acid

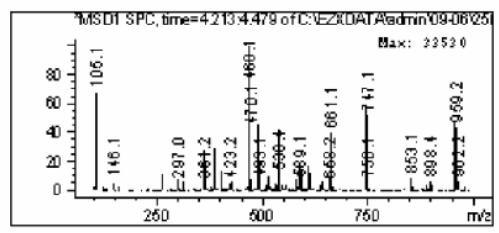
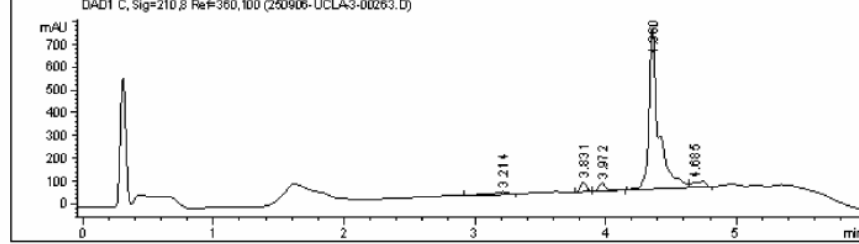
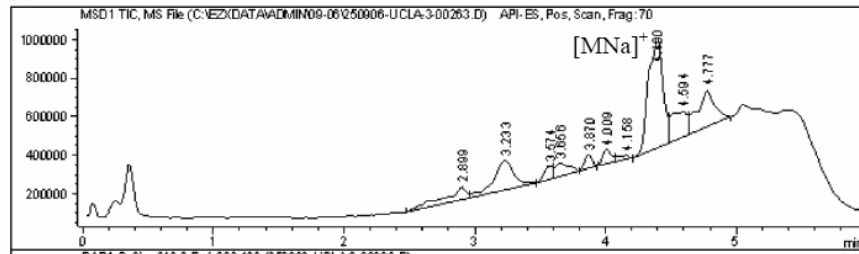
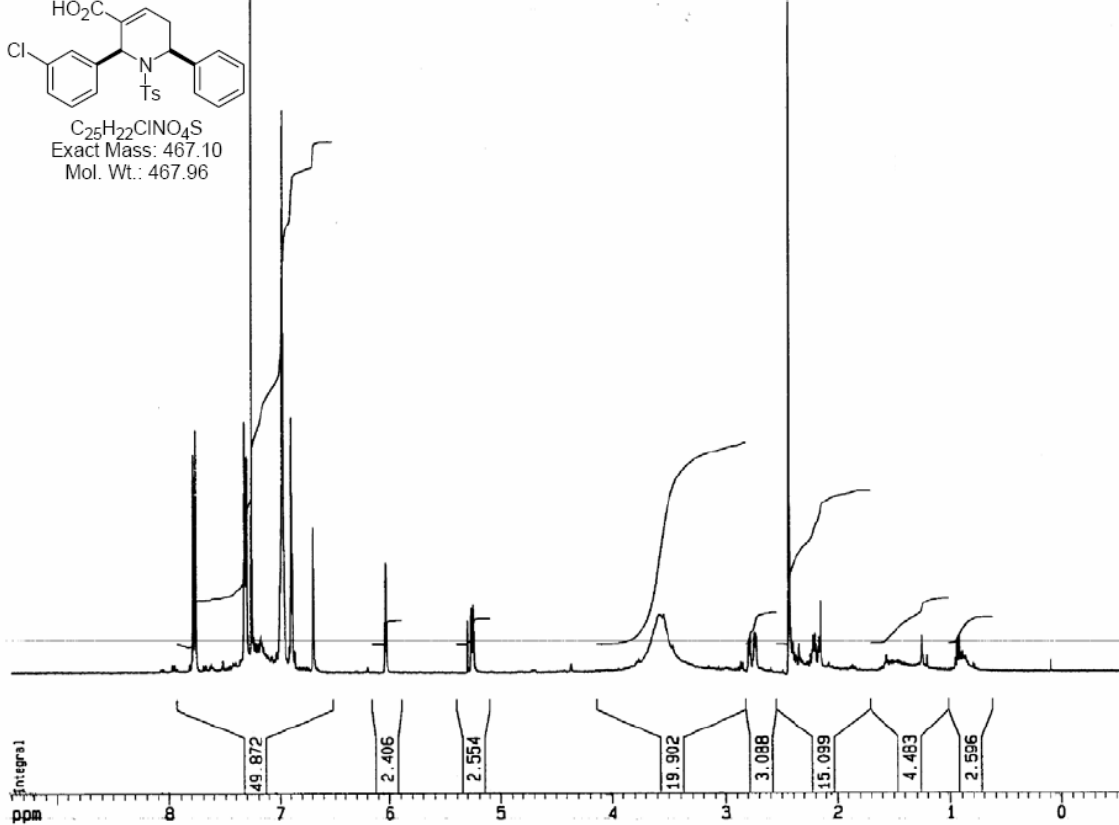


Spectral data for Table 8

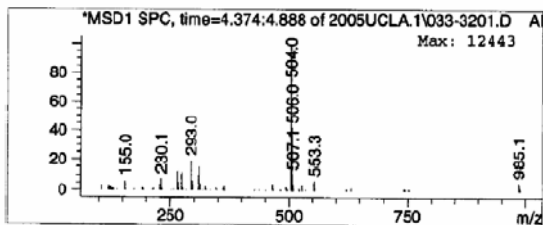
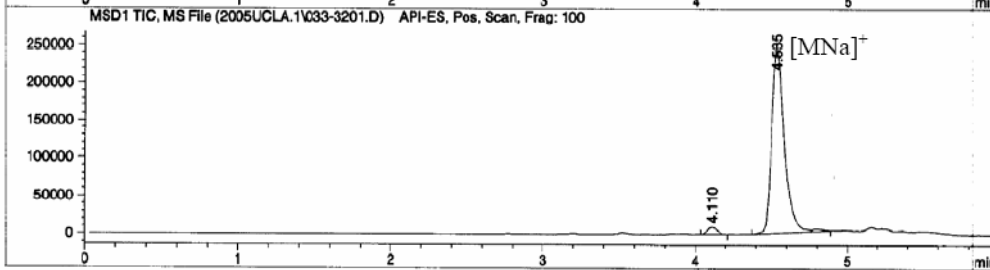
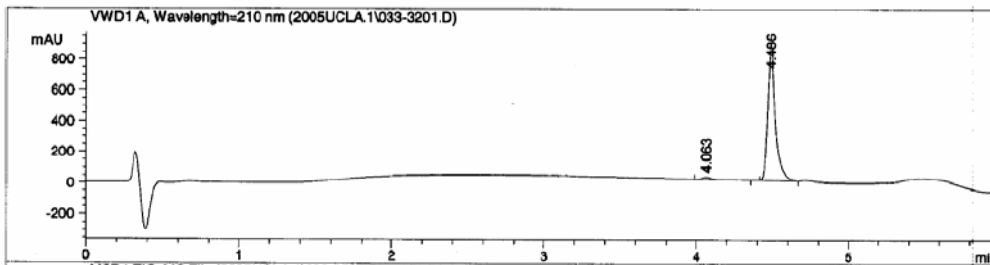
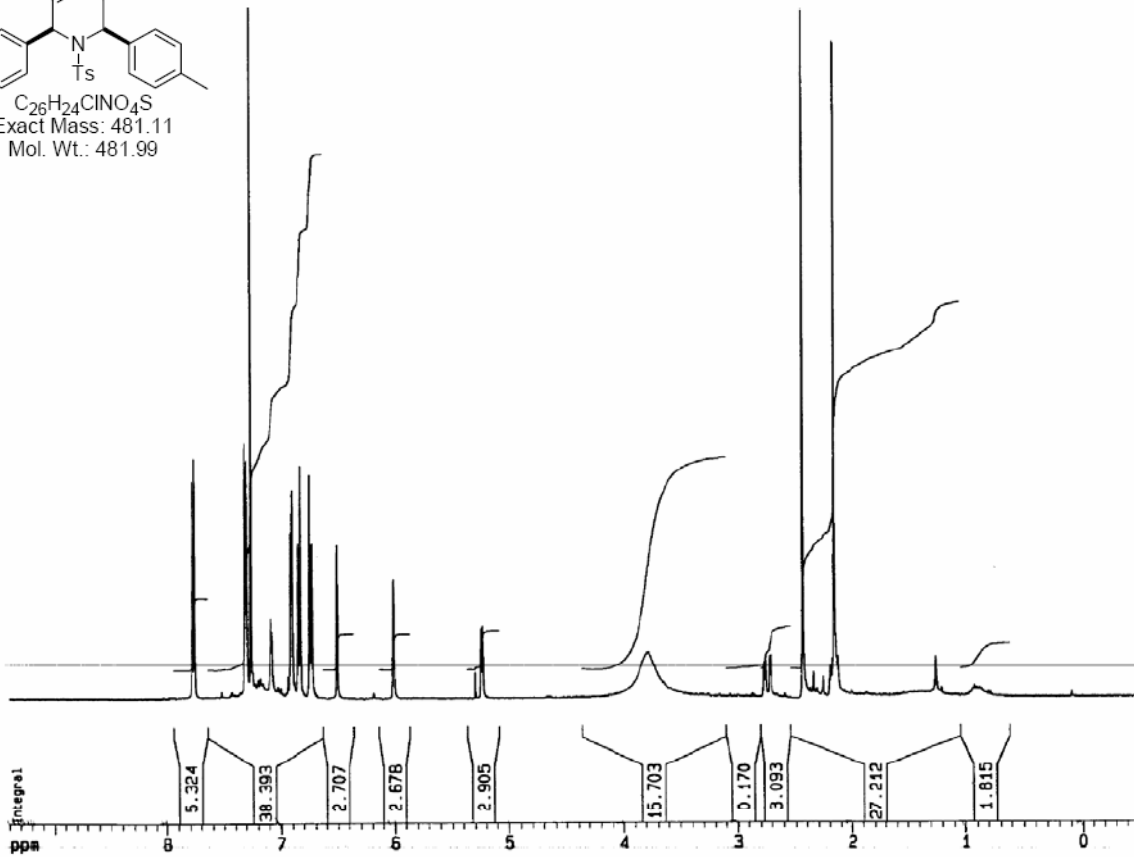
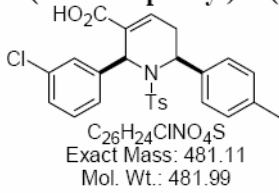
2-(3-Chlorophenyl)-6-phenyl-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C01)



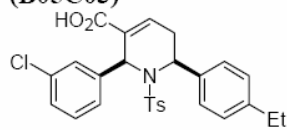
C₂₅H₂₂ClNO₄S
 Exact Mass: 467.10
 Mol. Wt.: 467.96



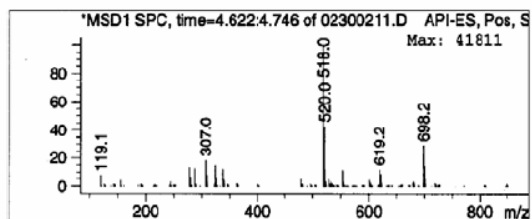
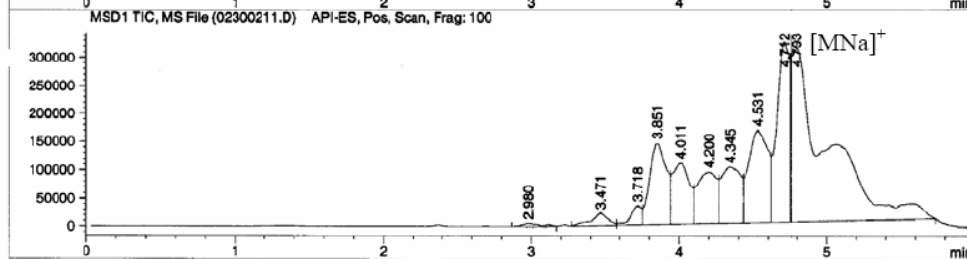
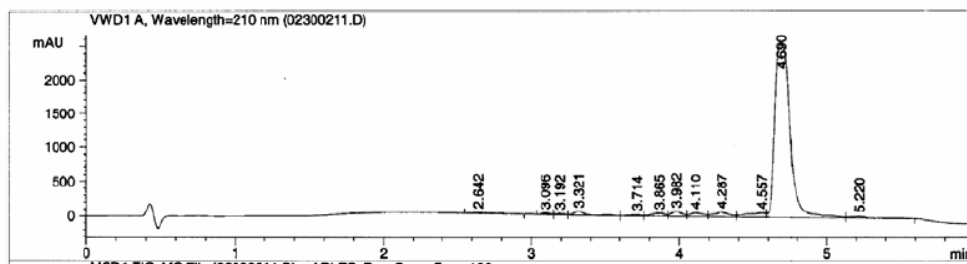
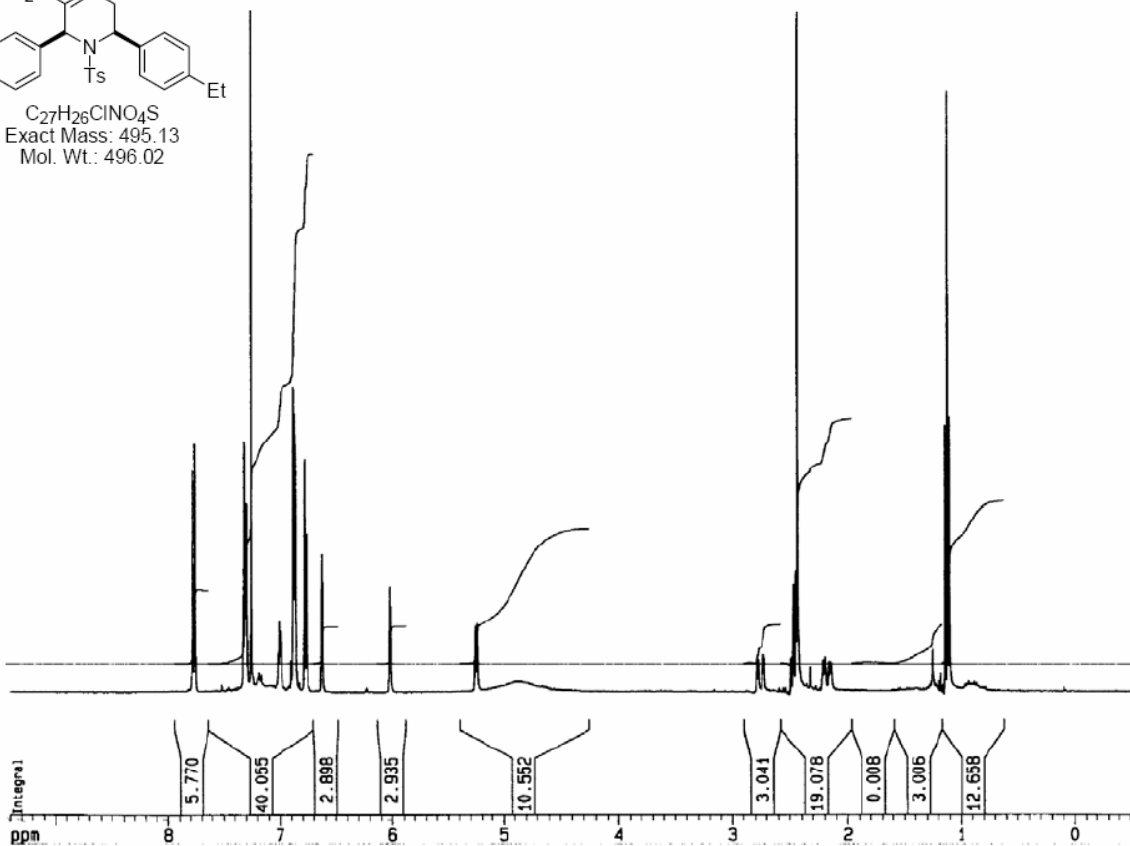
2-(3-Chlorophenyl)-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C02)



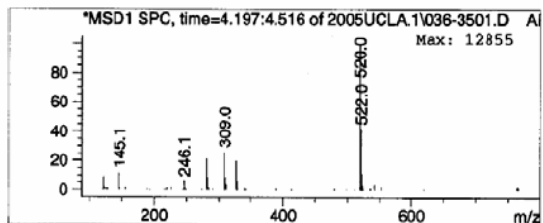
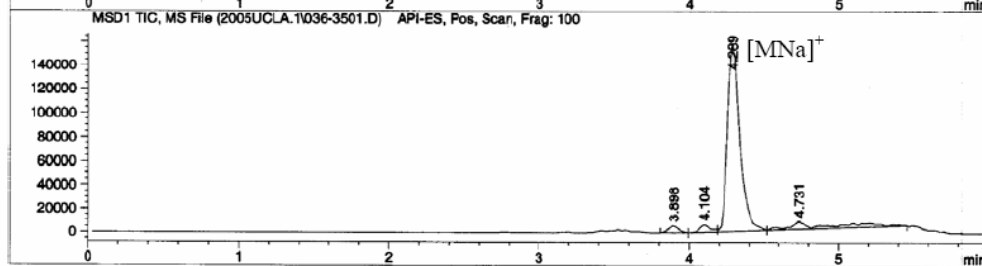
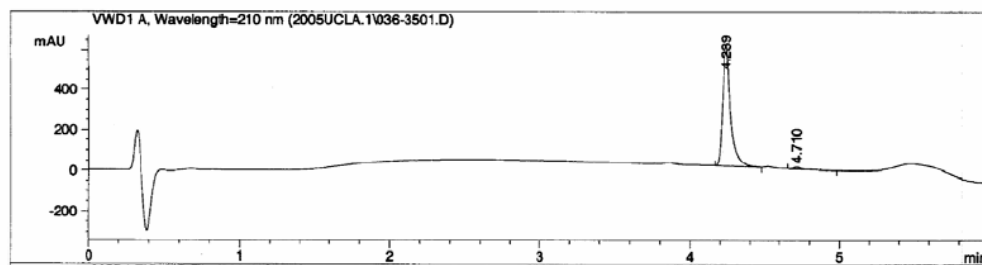
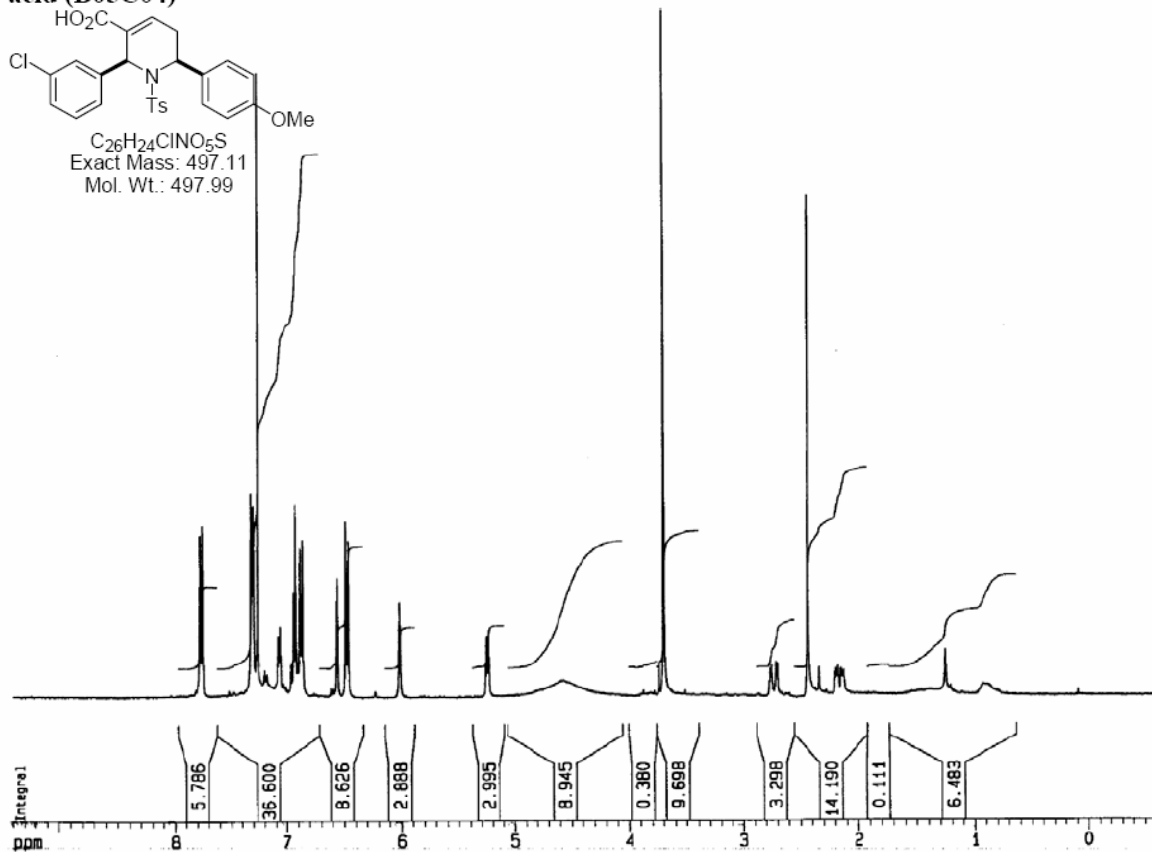
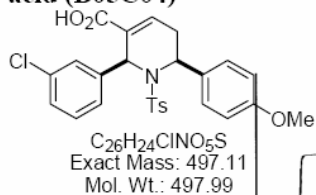
2-(3-Chlorophenyl)-6-(4-ethylphenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C03)



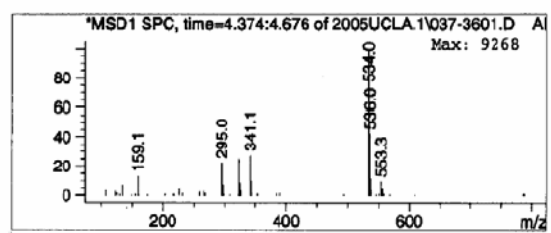
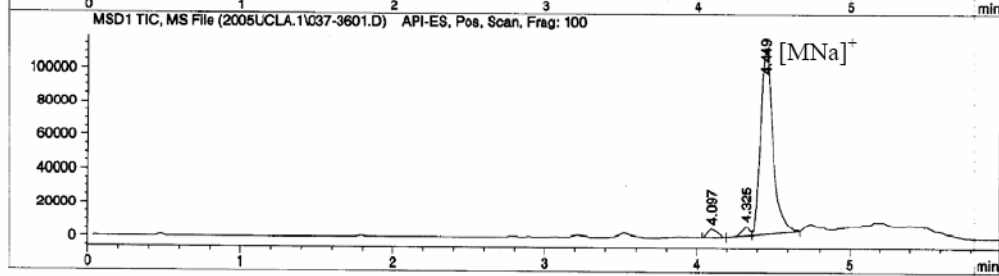
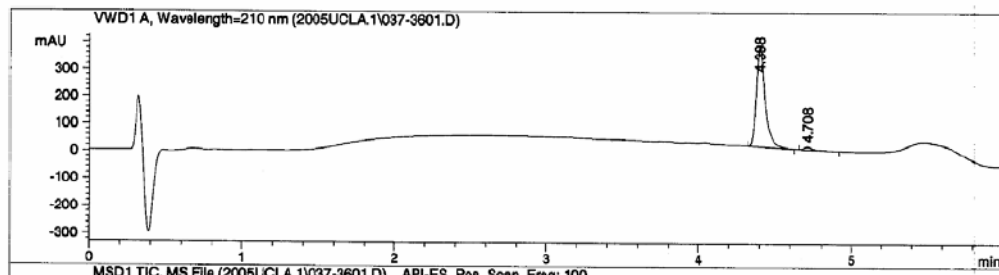
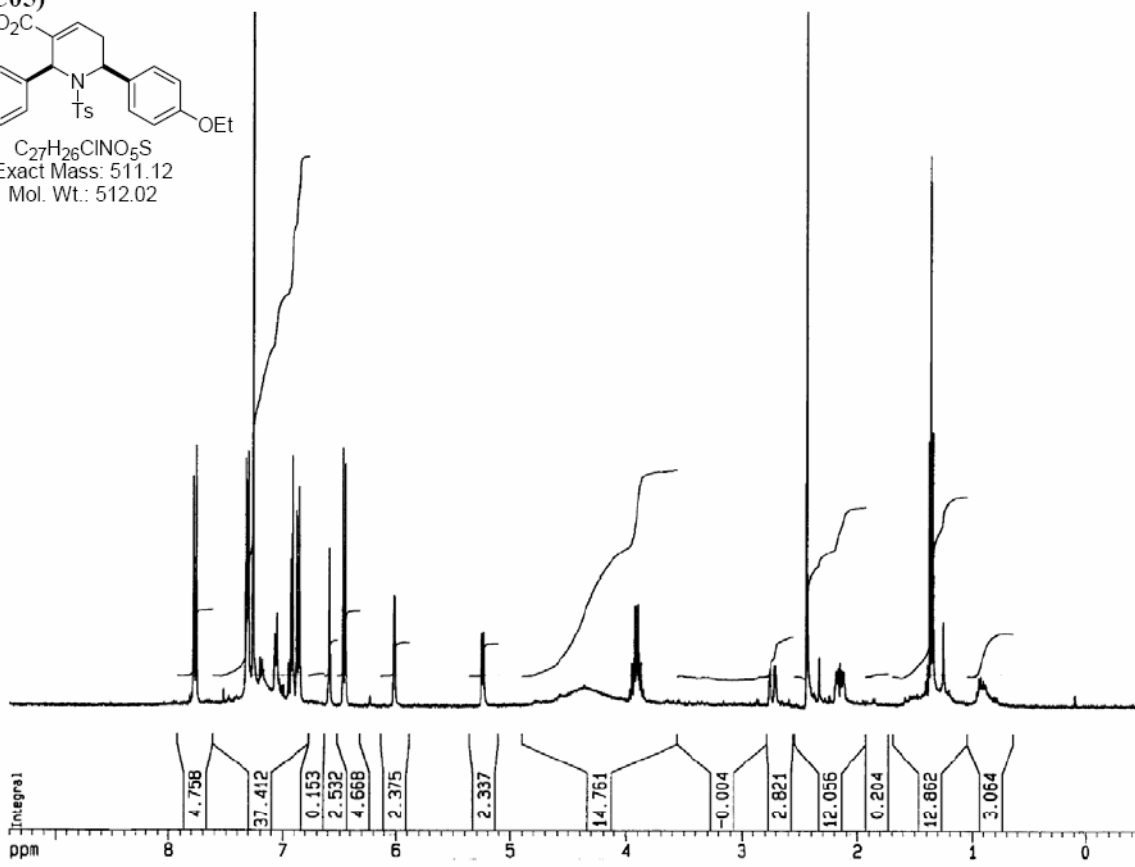
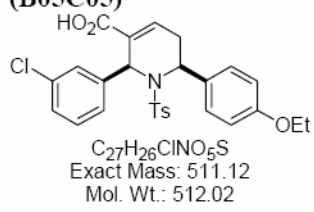
C₂₇H₂₆ClNO₄S
 Exact Mass: 495.13
 Mol. Wt.: 496.02



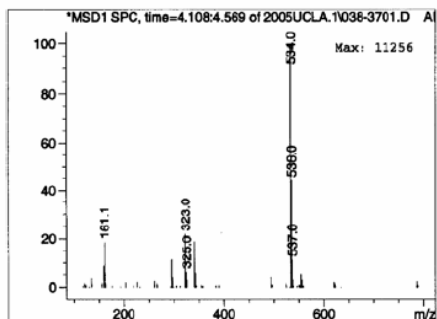
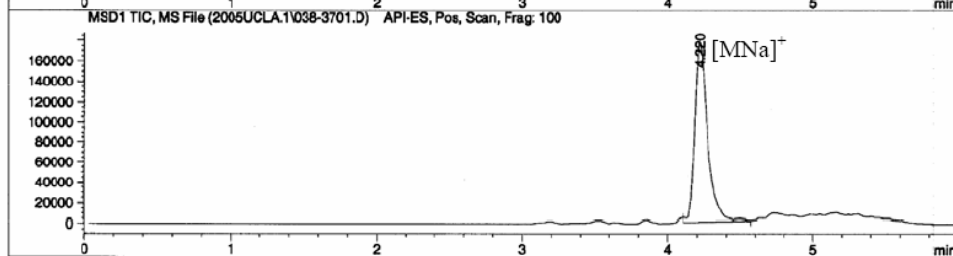
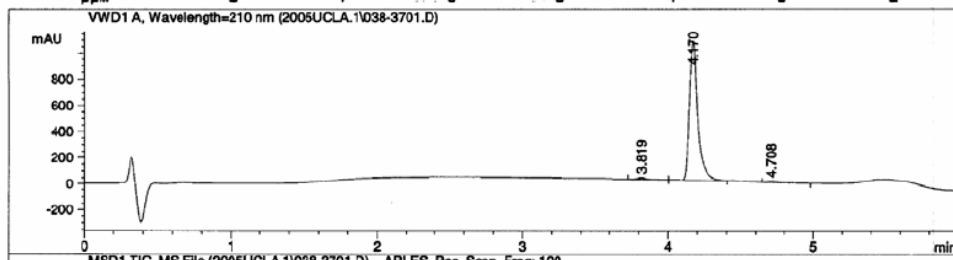
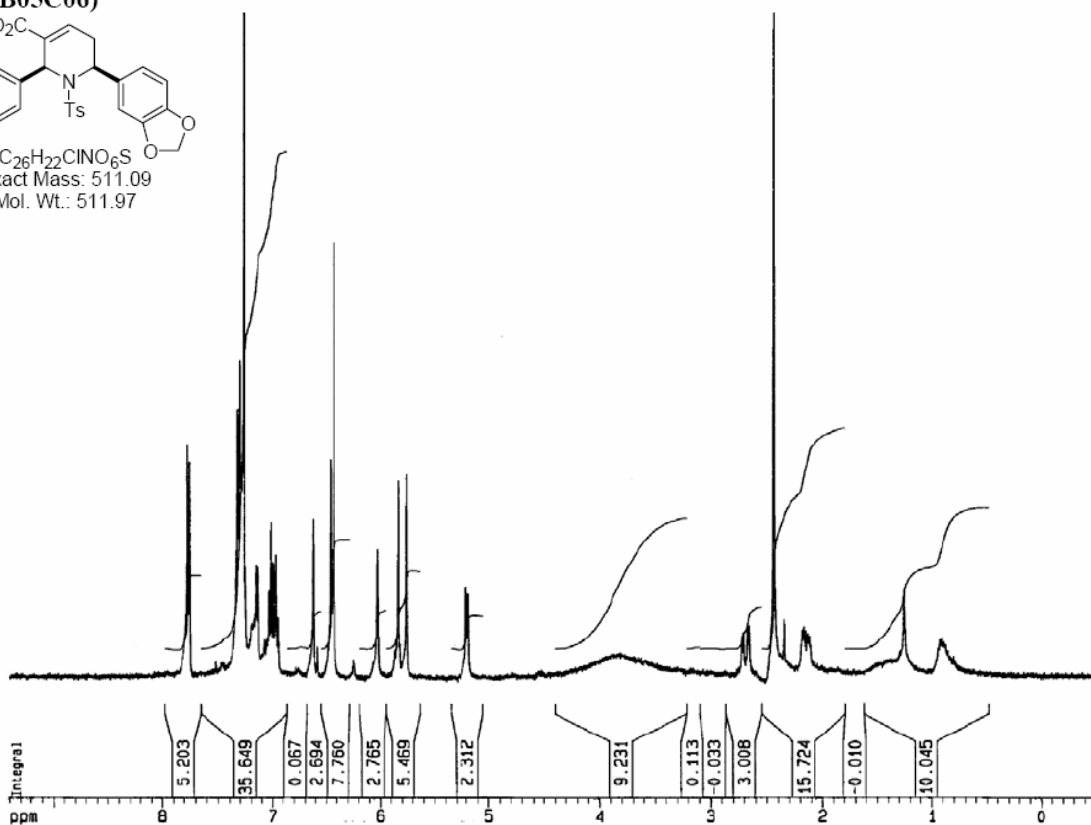
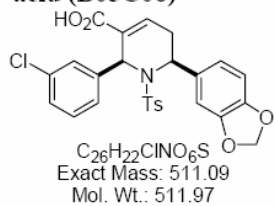
2-(3-Chlorophenyl)-6-(4-methoxyphenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C04)



2-(3-Chlorophenyl)-6-(4-ethoxyphenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C05)

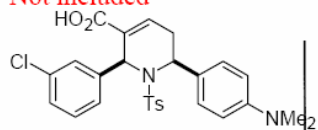


6-(Benzo[1,3]dioxol-5-yl)-2-(3-chlorophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C06)

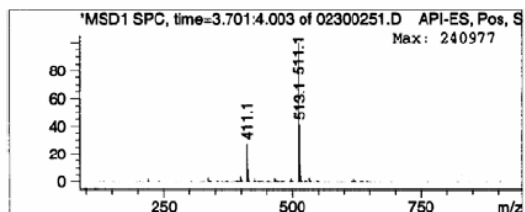
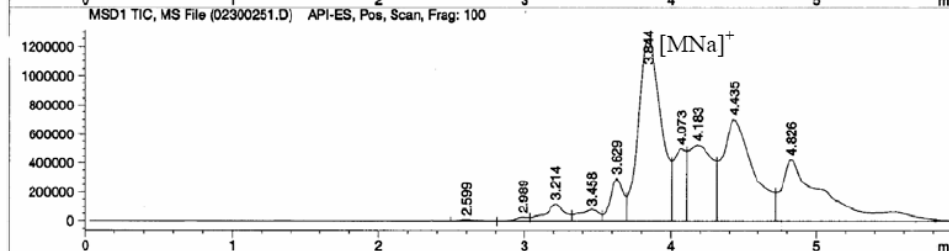
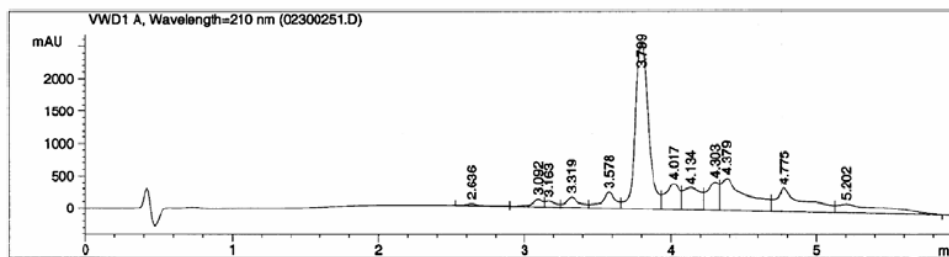
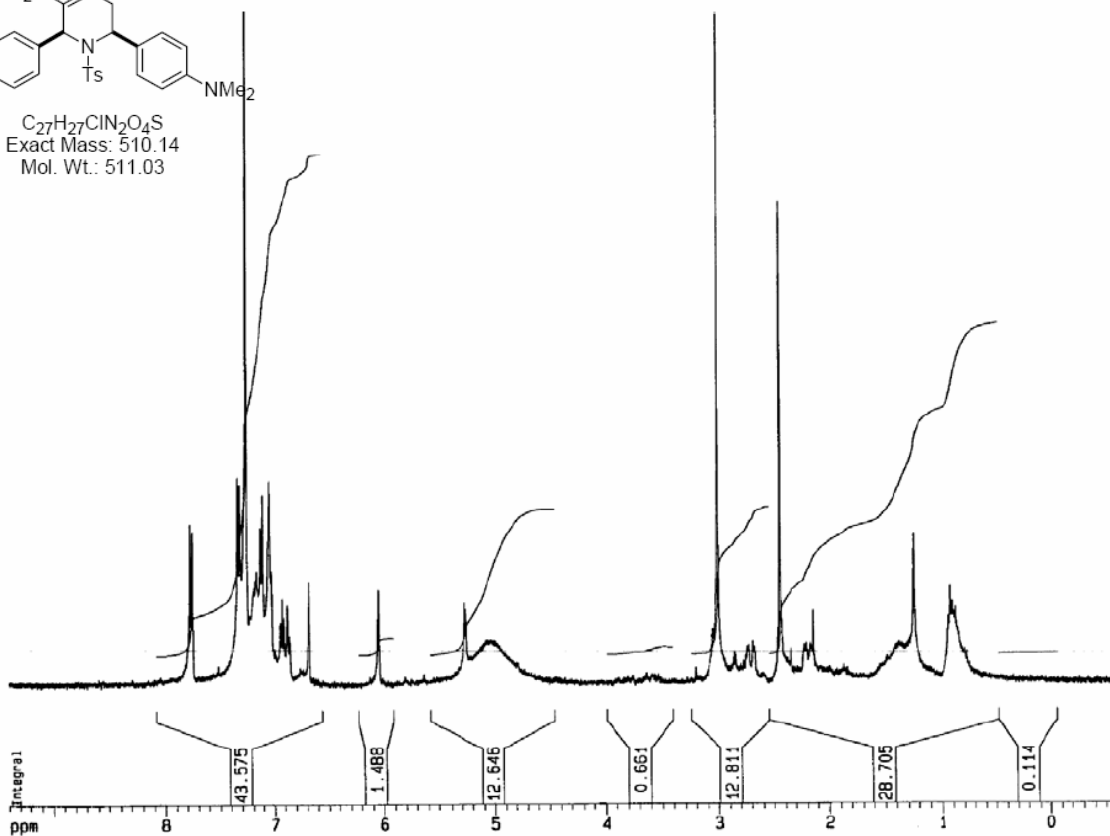


2-(3-Chlorophenyl)-6-(4-dimethylaminophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C07)

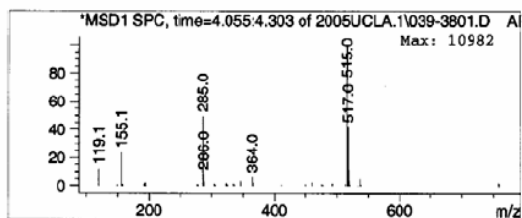
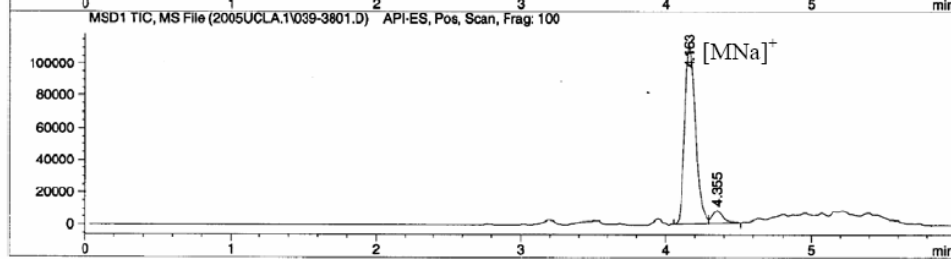
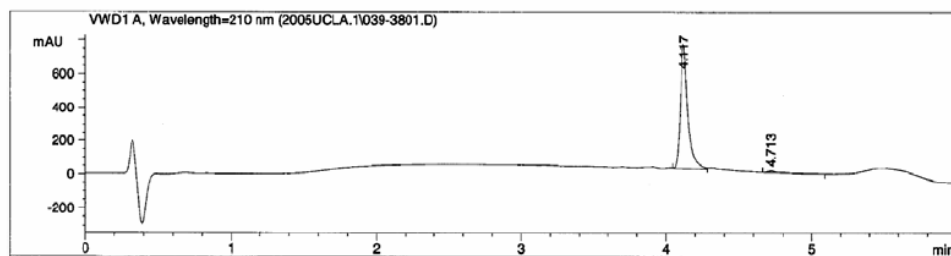
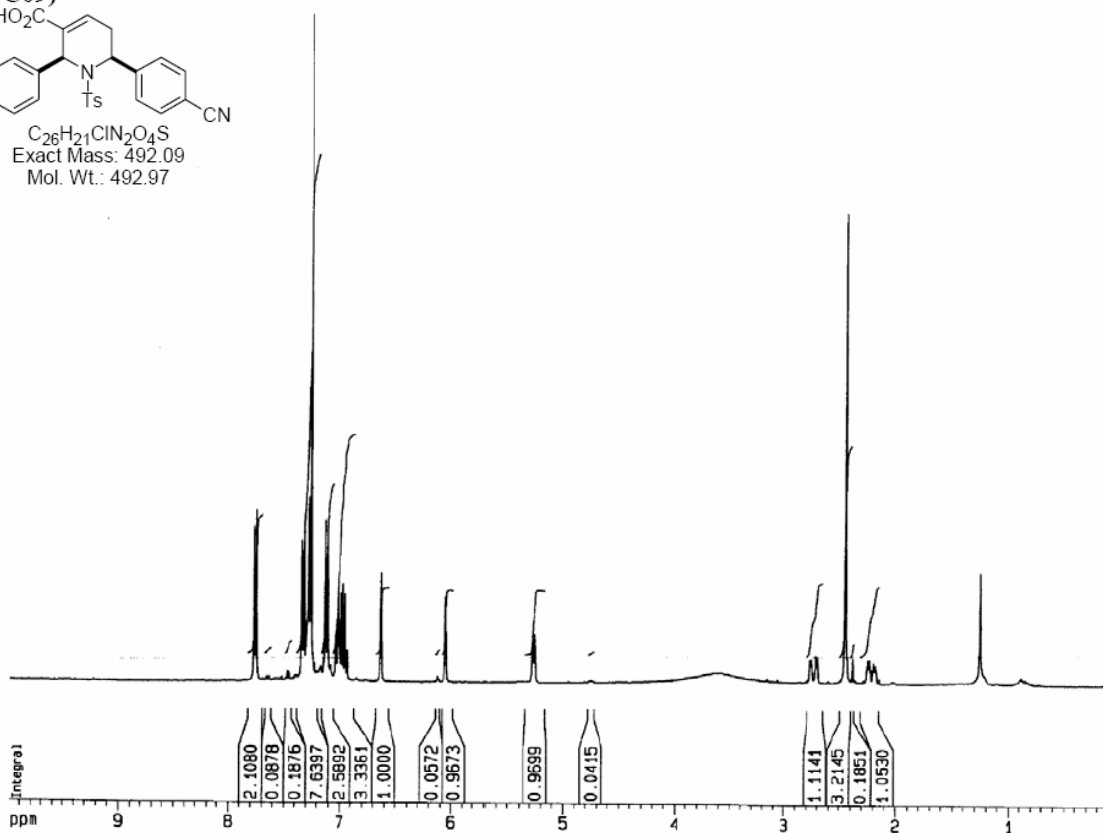
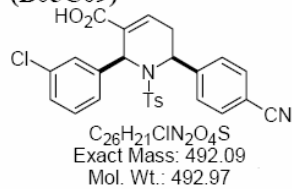
Not included



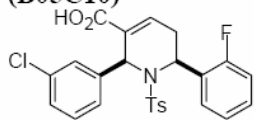
C₂₇H₂₇ClN₂O₄S
Exact Mass: 510.14
Mol. Wt.: 511.03



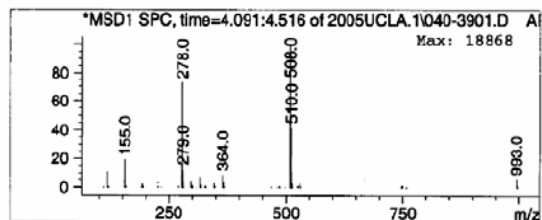
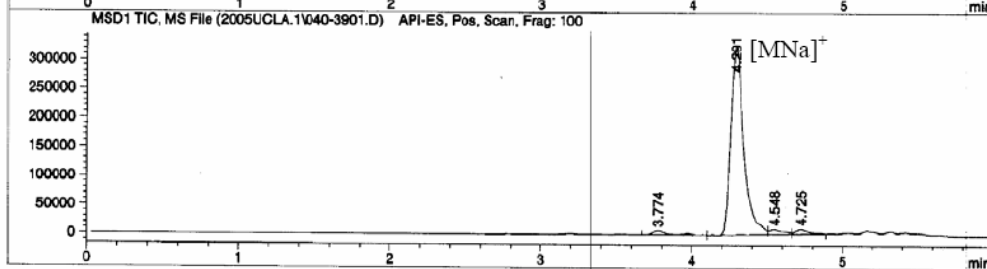
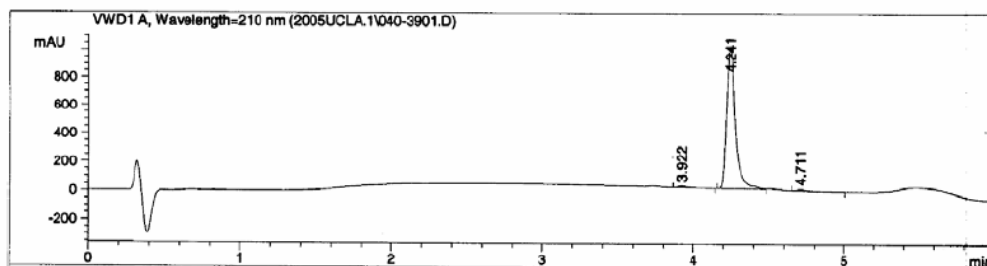
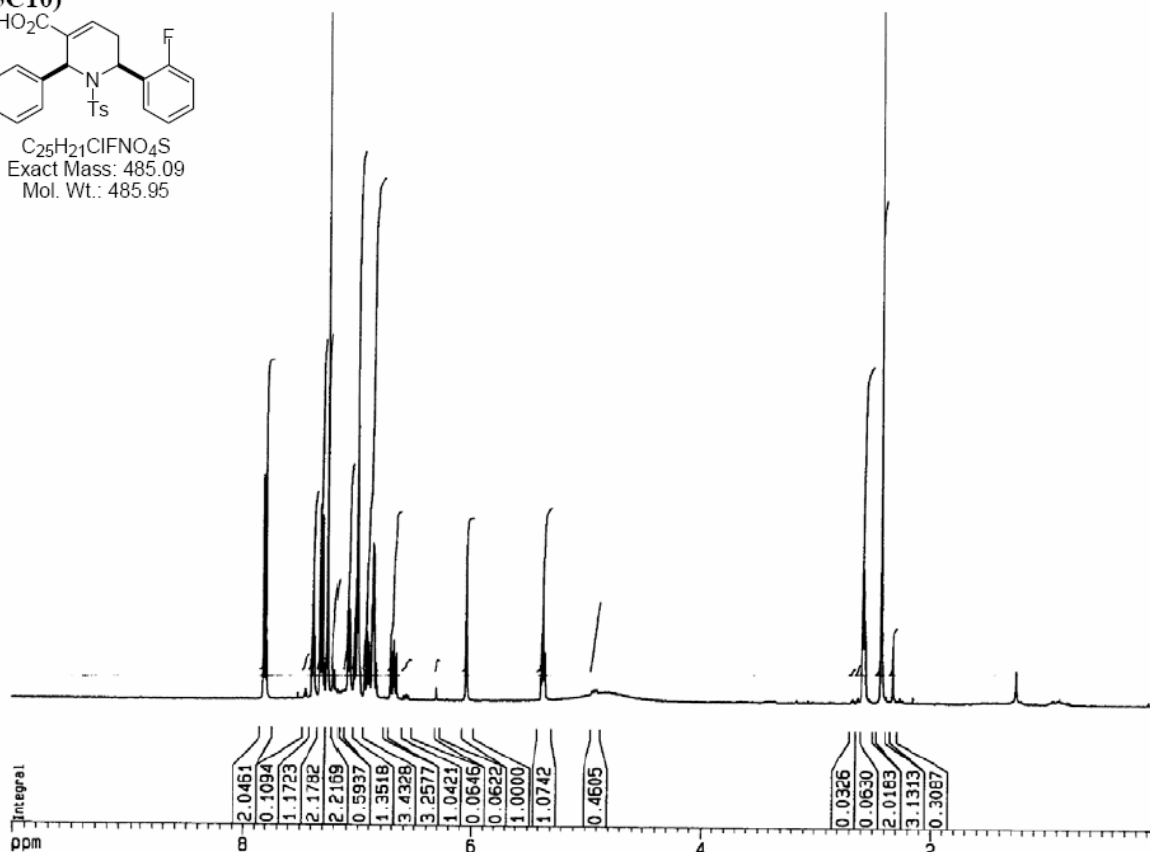
2-(3-Chlorophenyl)-6-(4-cyanophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C09)



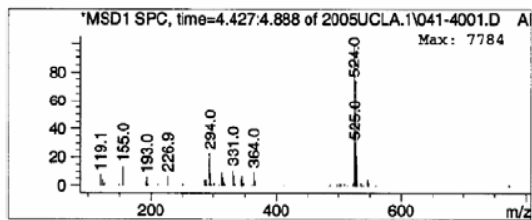
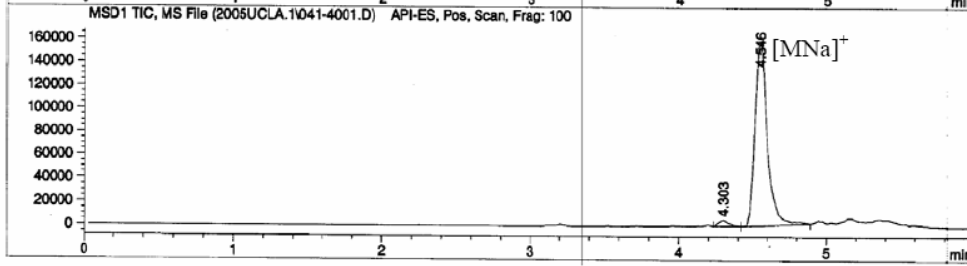
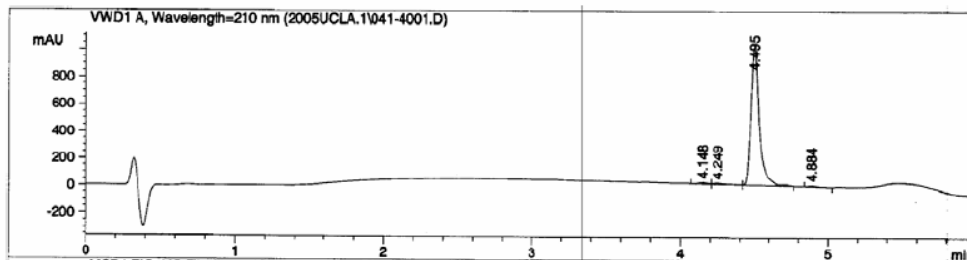
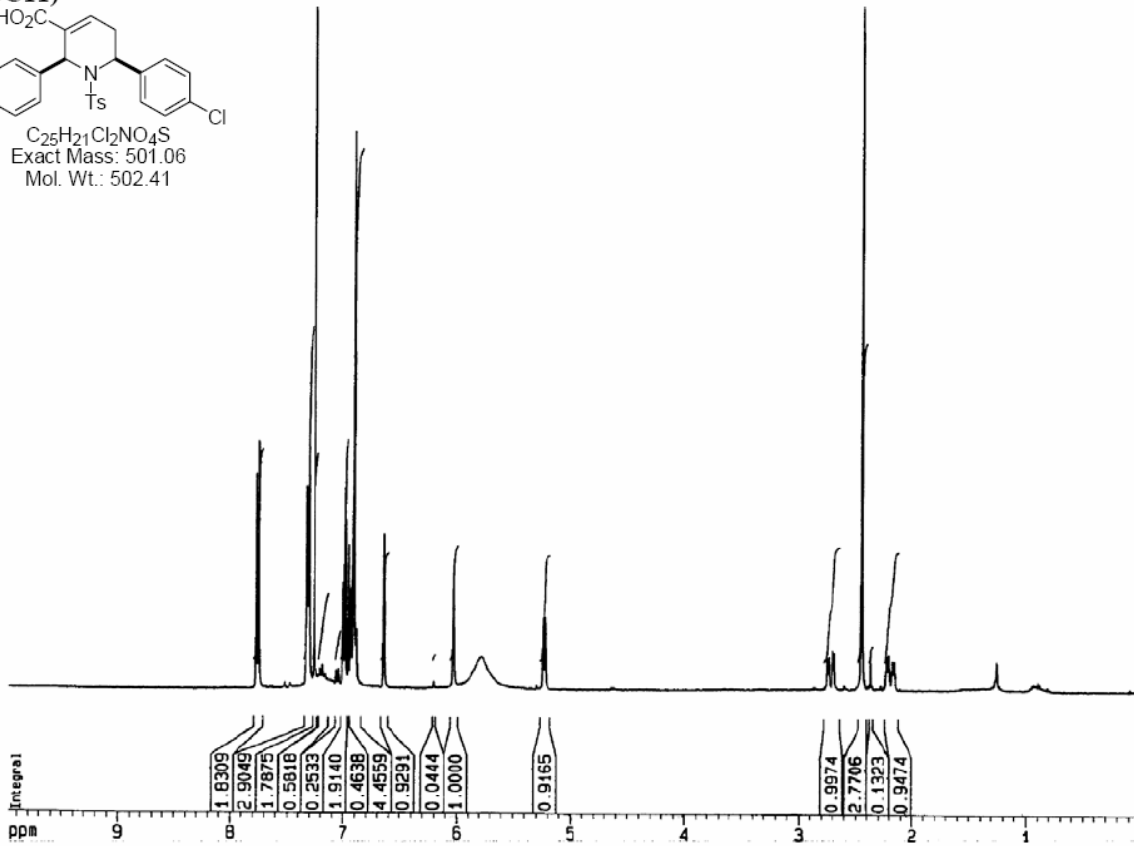
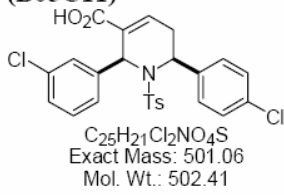
2-(3-Chlorophenyl)-6-(2-fluorophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C10)



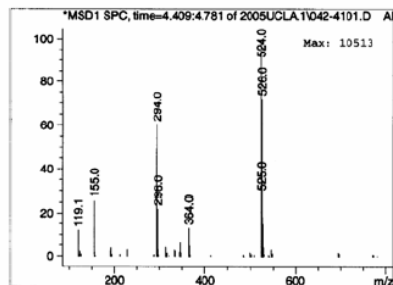
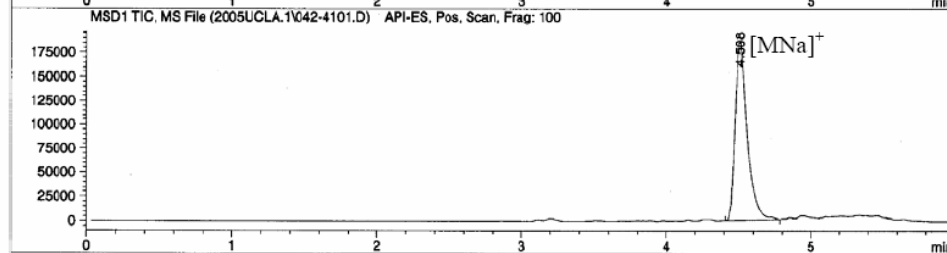
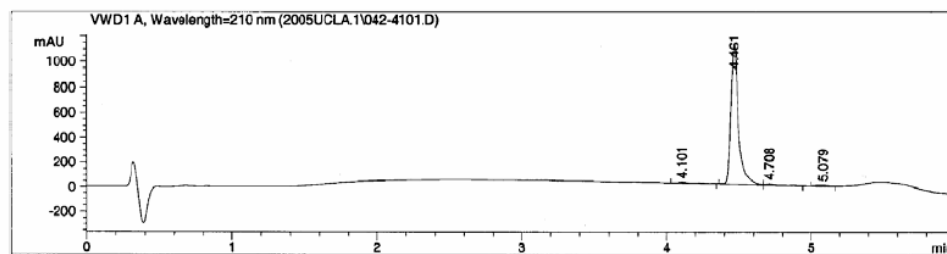
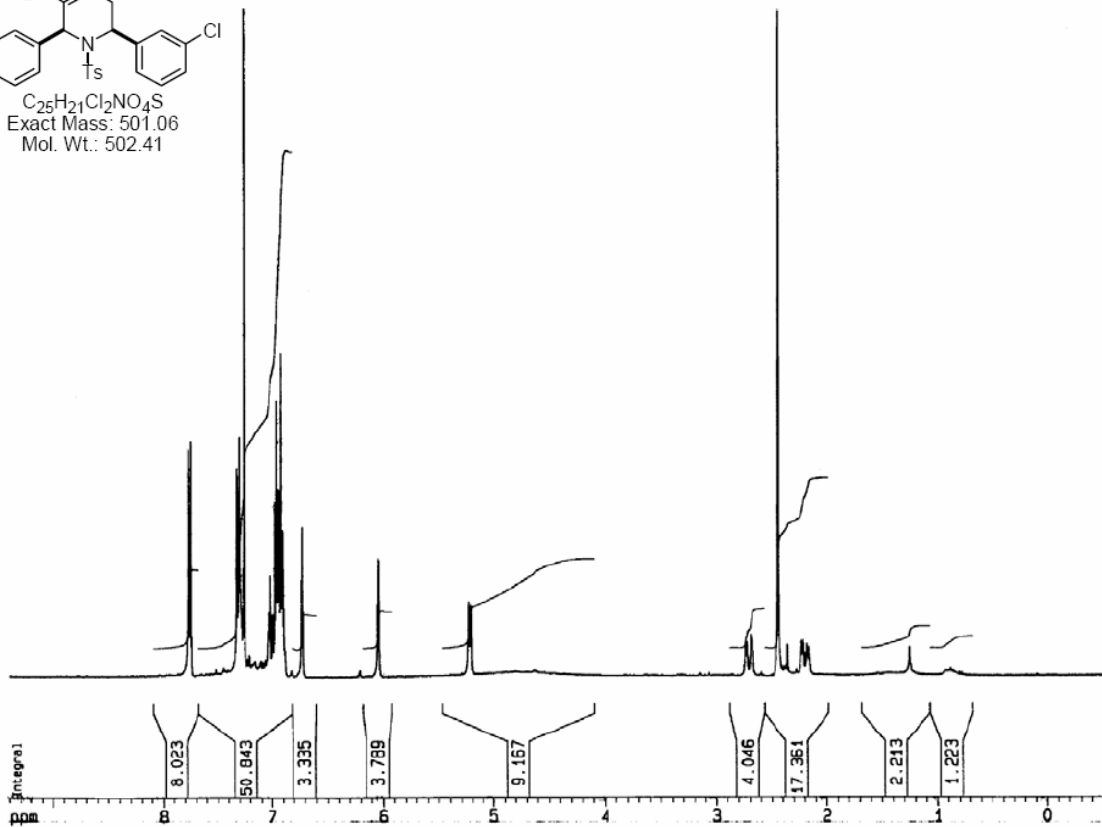
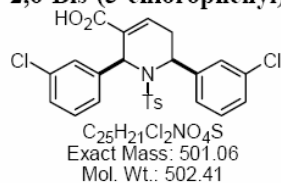
C₂₅H₂₁ClFNO₄S
 Exact Mass: 485.09
 Mol. Wt.: 485.95



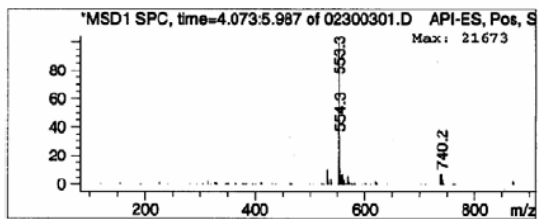
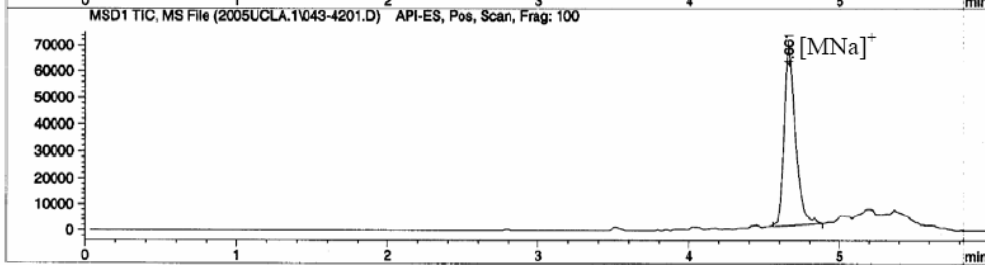
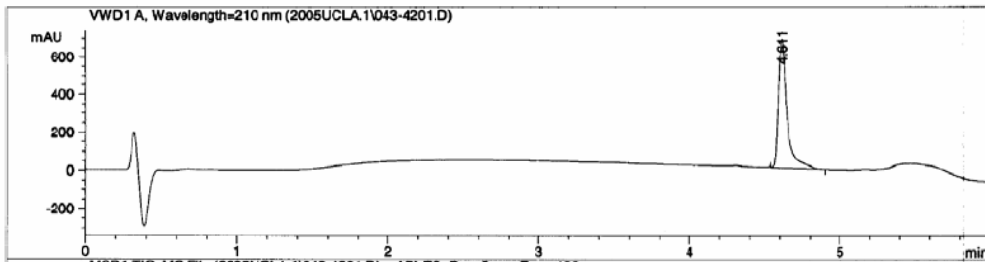
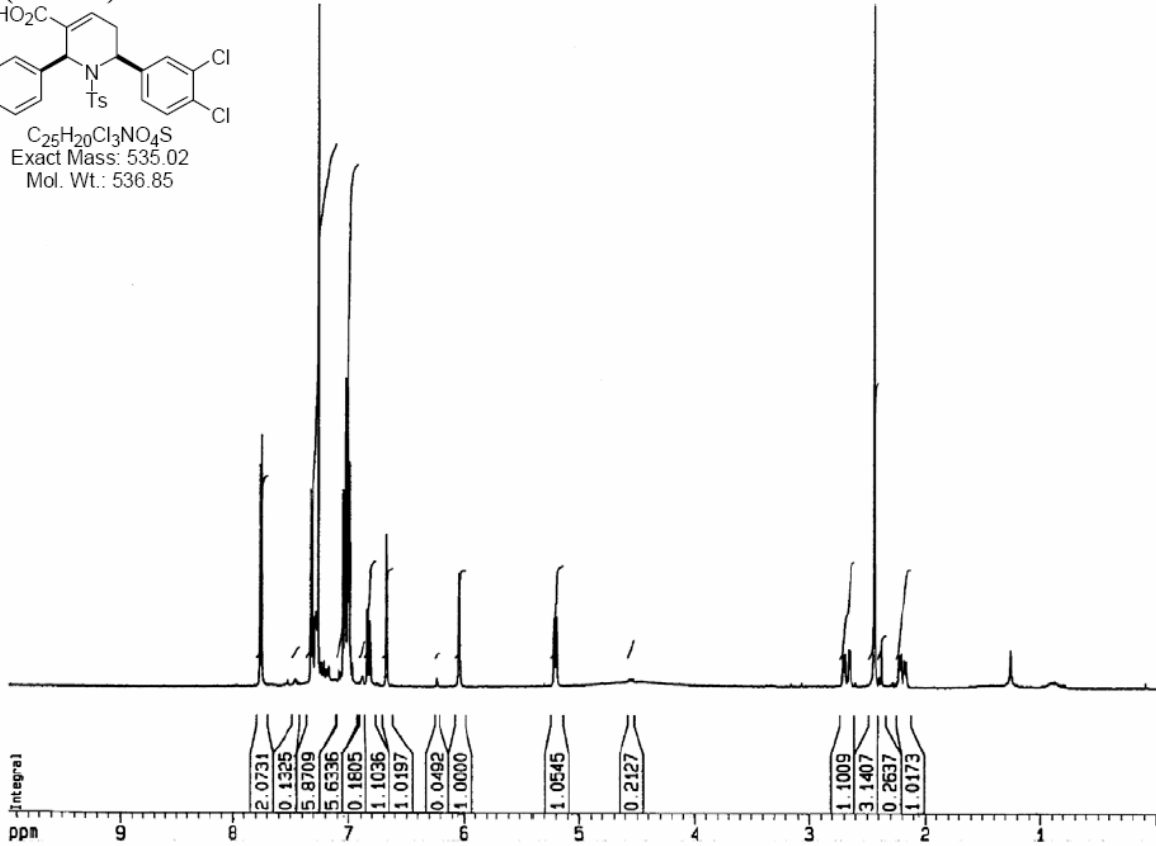
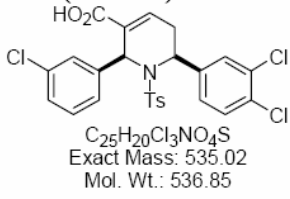
6-(4-Chlorophenyl)-2-(3-chlorophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C11)



2,6-Bis-(3-chlorophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C12)

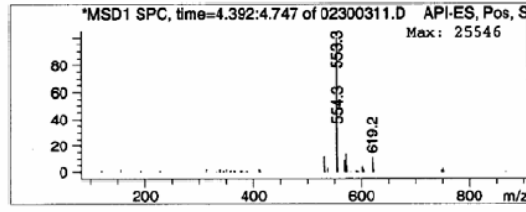
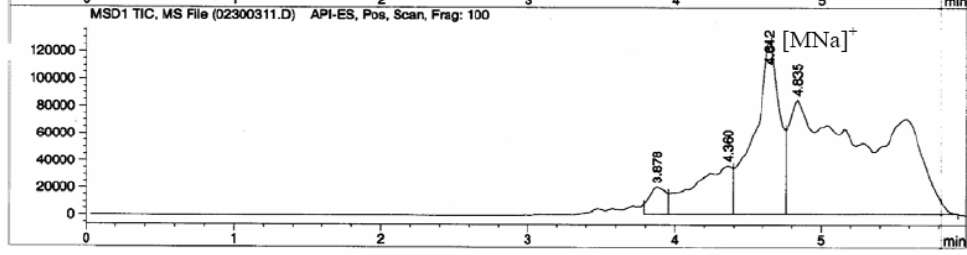
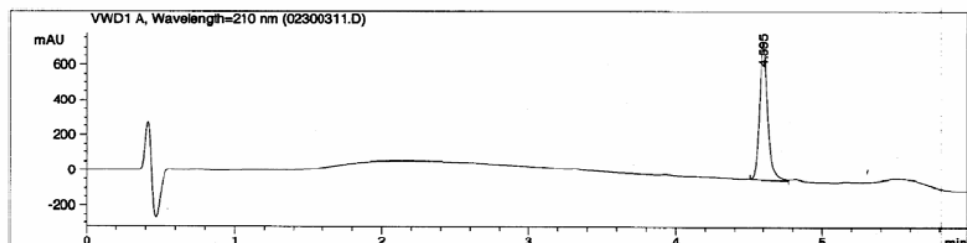
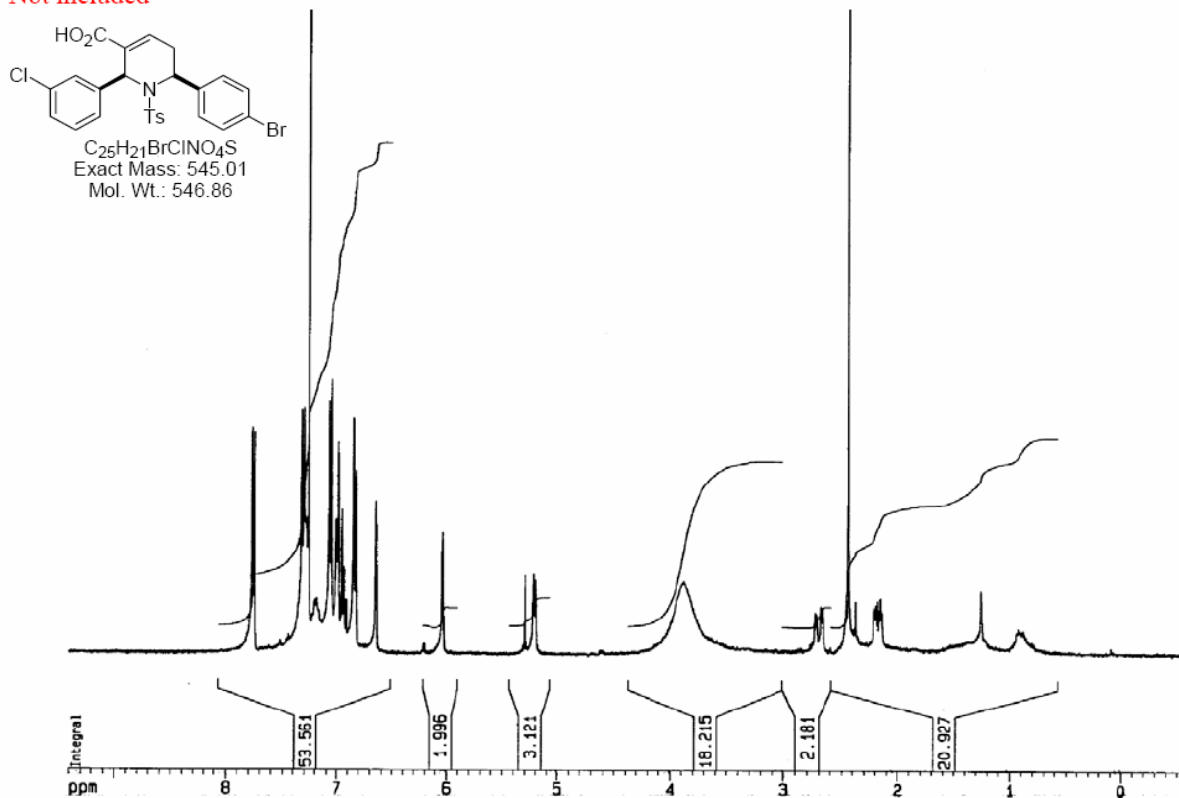


2-(3-Chlorophenyl)-6-(3,4-dichlorophenyl)-1-(toluene-4-sulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C13)



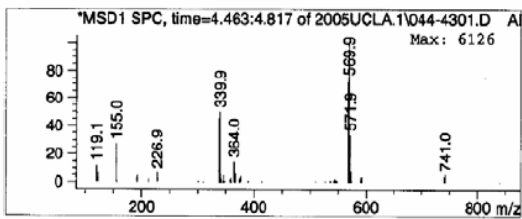
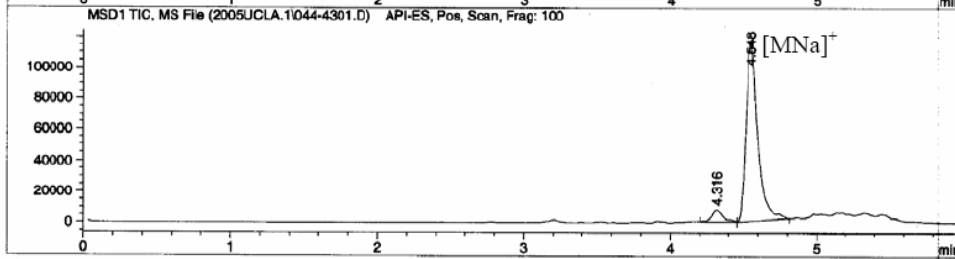
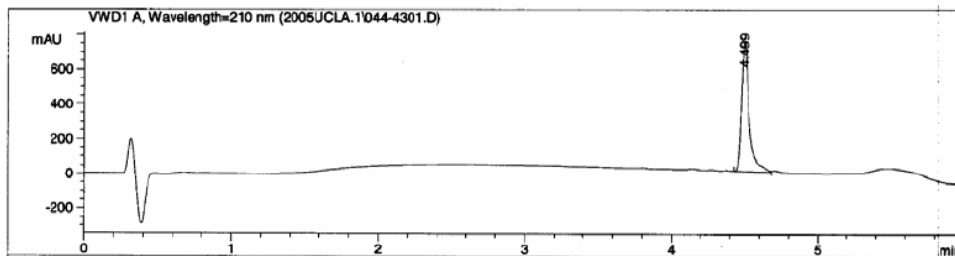
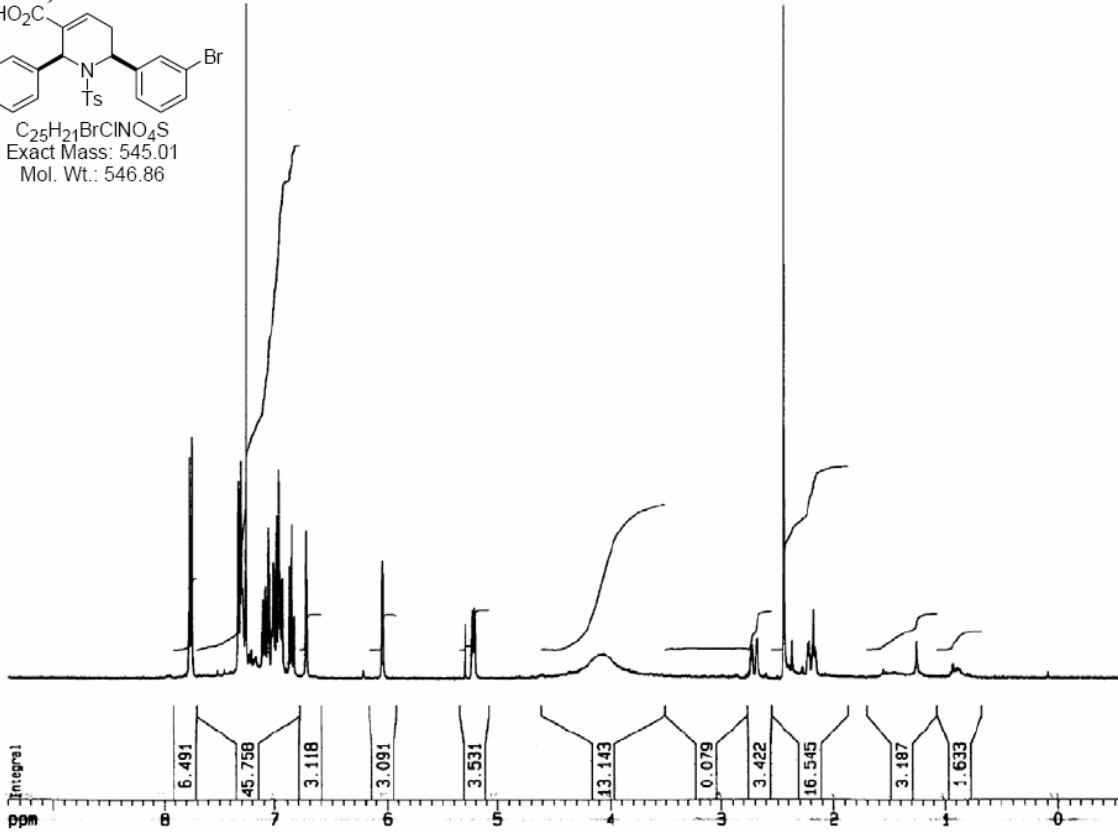
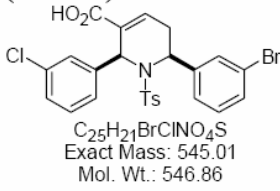
6-(4-Bromophenyl)-2-(3-chlorophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C14)

Not included



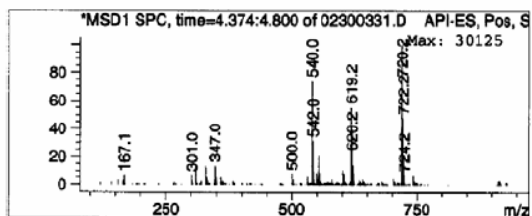
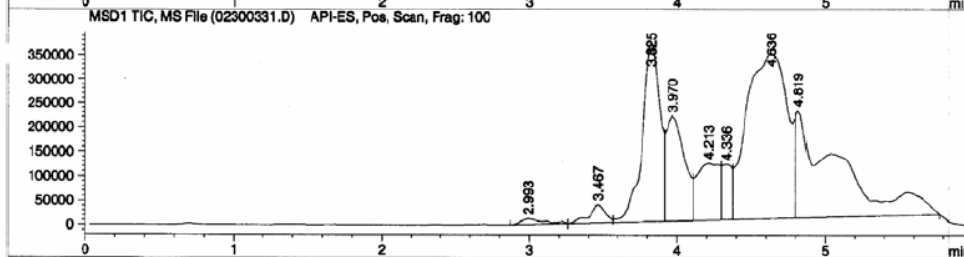
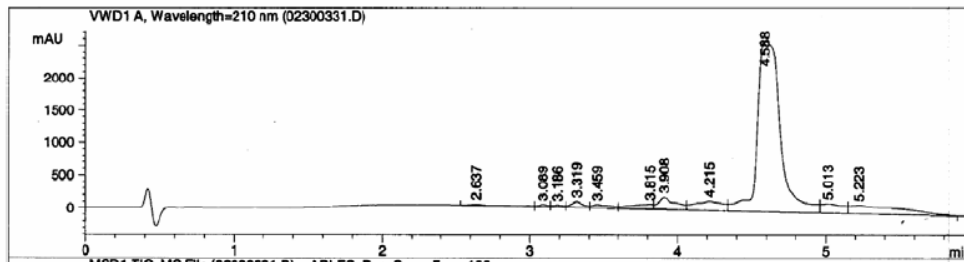
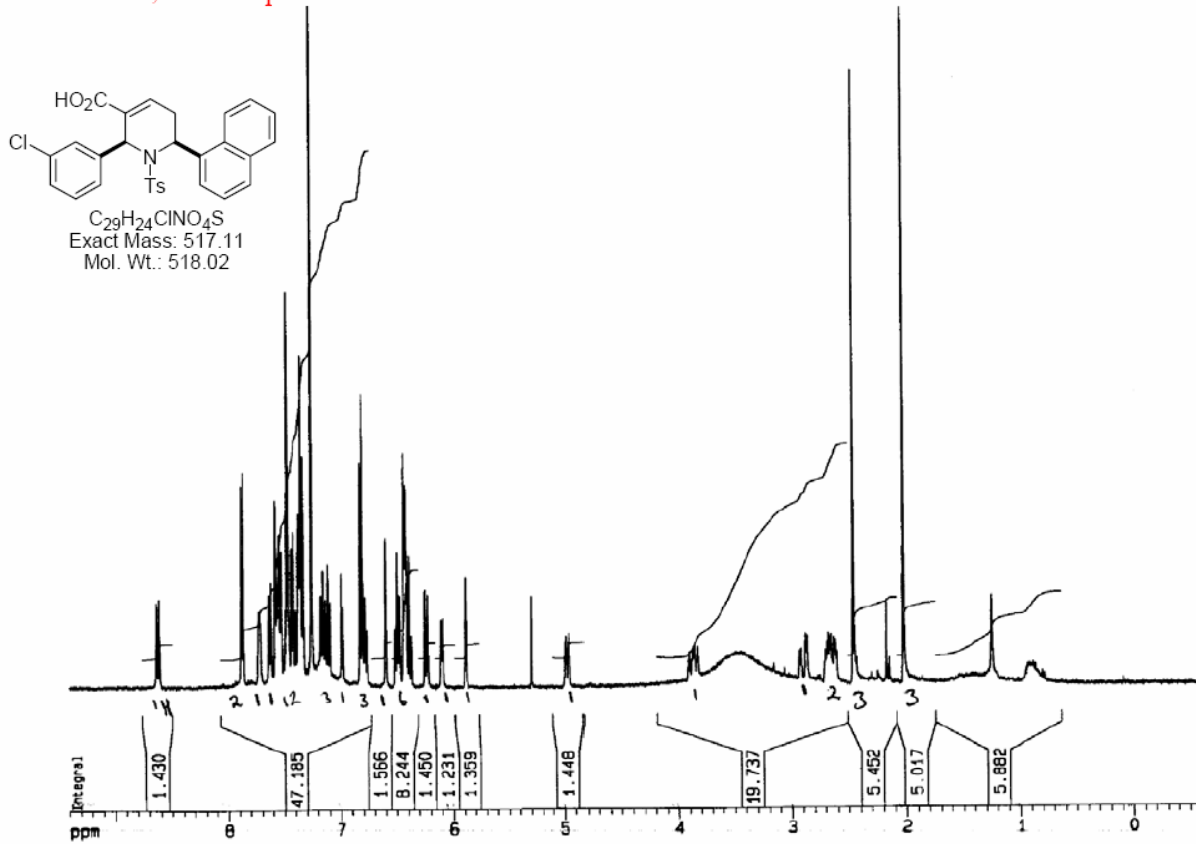
Component 3: Peak at Scan 261.3. Top ions are 553 570 568

6-(3-Bromophenyl)-2-(3-chlorophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C15)



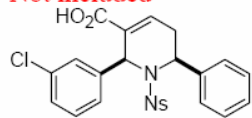
2-(3-Chlorophenyl)-6-(naphthalen-1-yl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C16)

Not included, different product formed

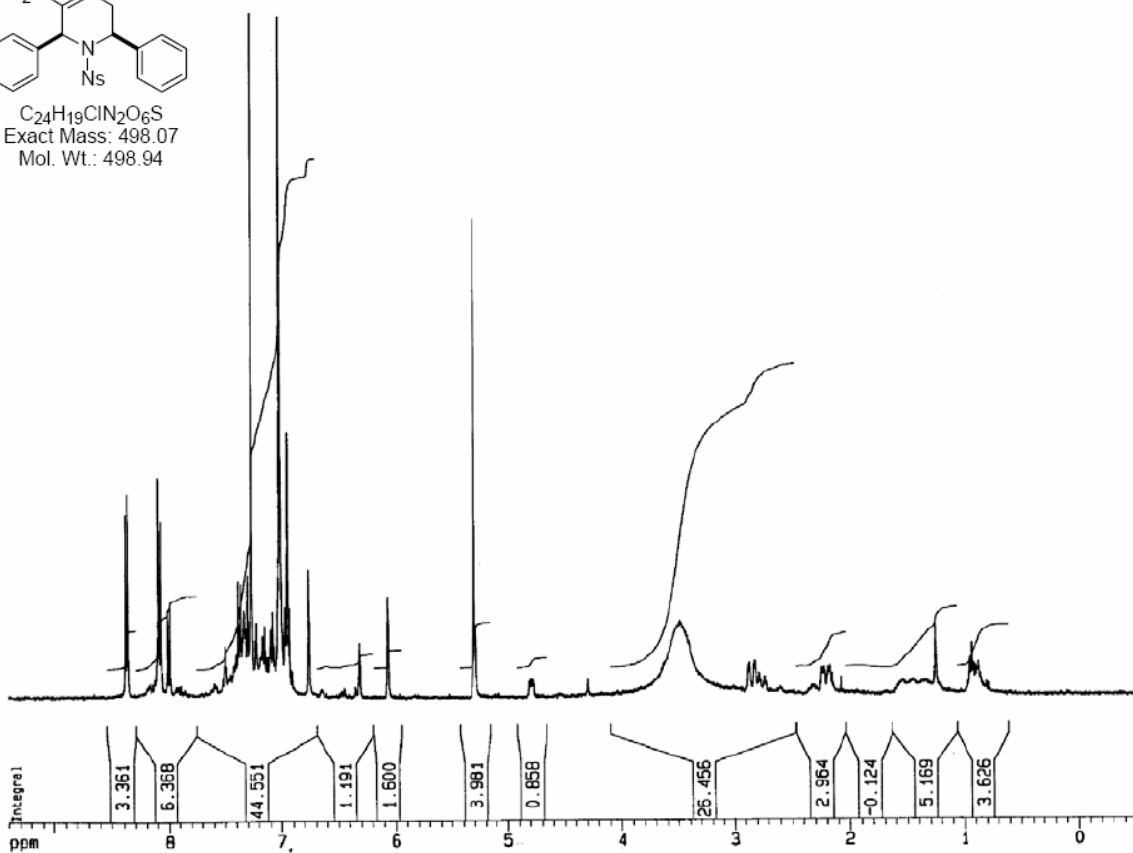


2-(3-Chlorophenyl)-1-(4-nitrobenzenesulfonyl)-6-phenyl-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C18)

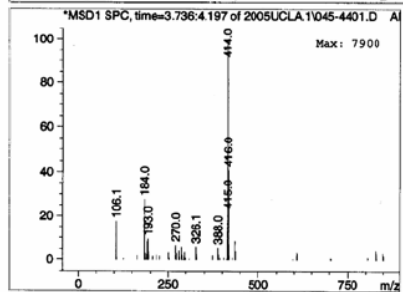
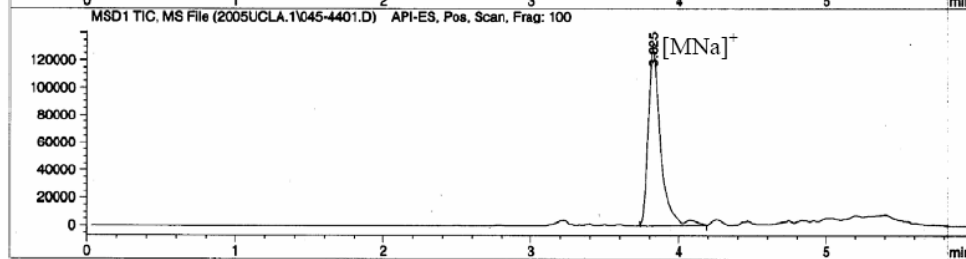
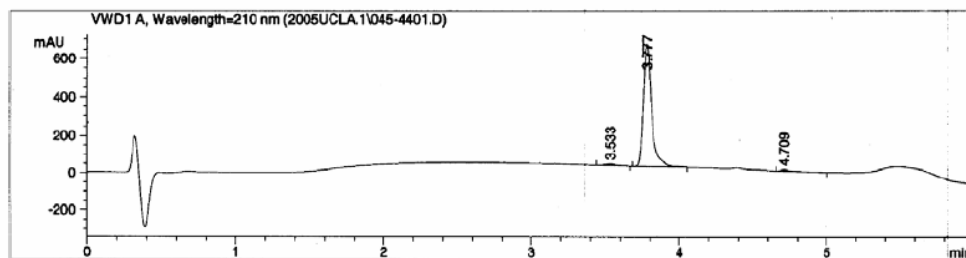
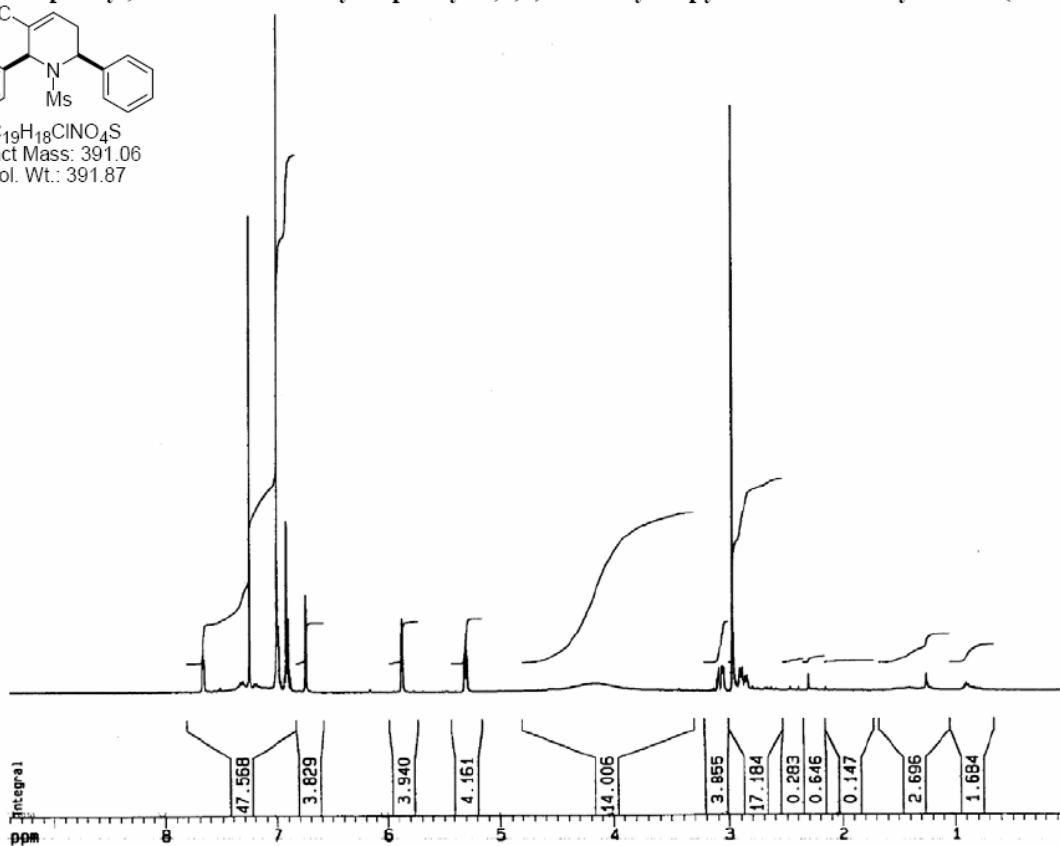
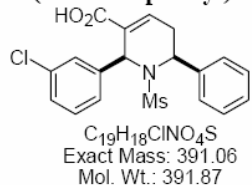
Not included



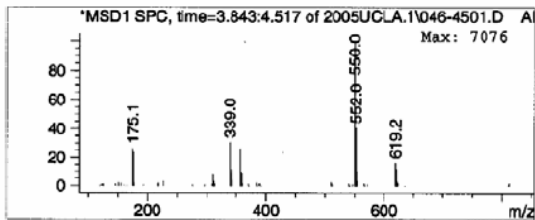
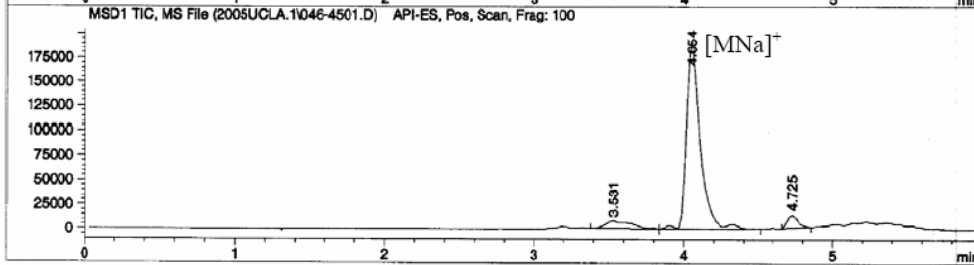
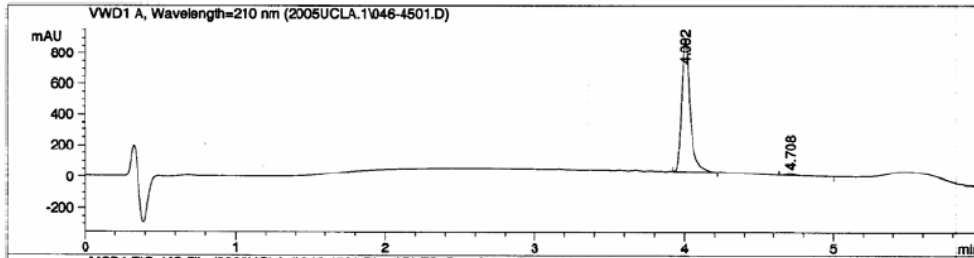
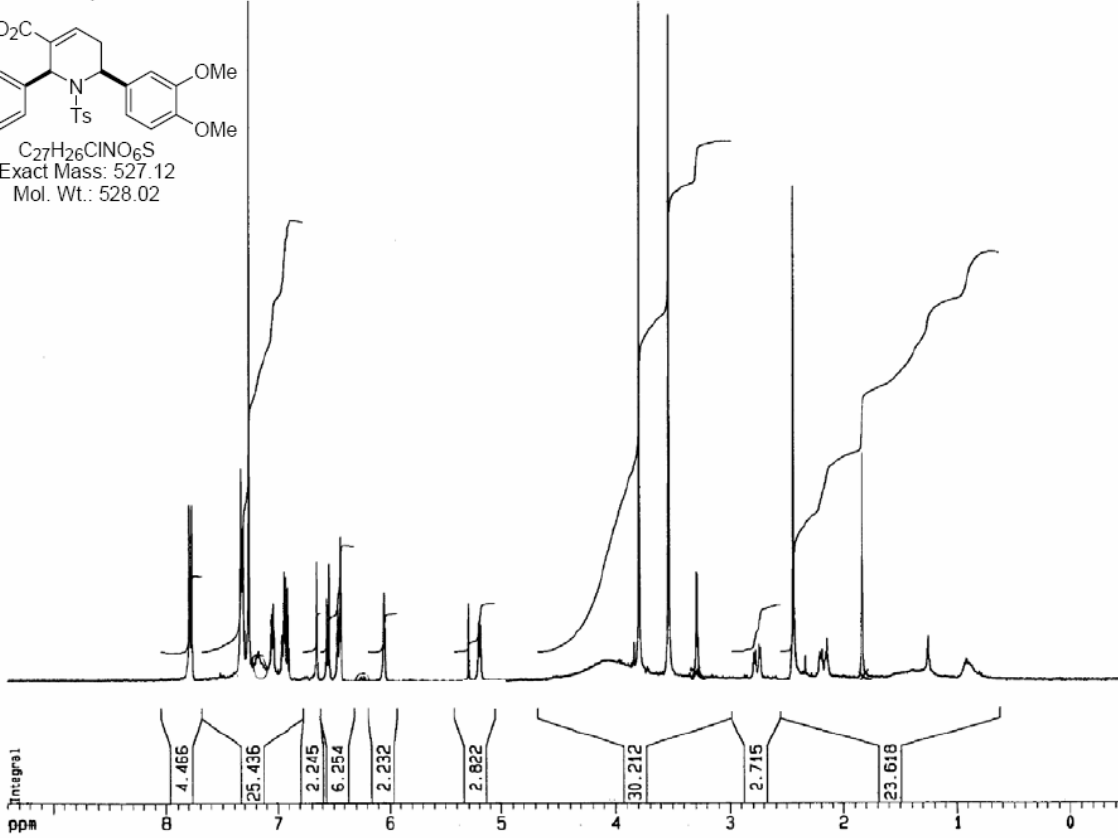
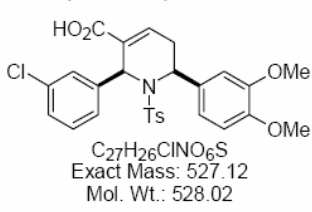
C₂₄H₁₉ClN₂O₆S
Exact Mass: 498.07
Mol. Wt.: 498.94



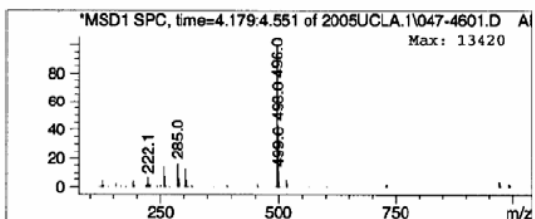
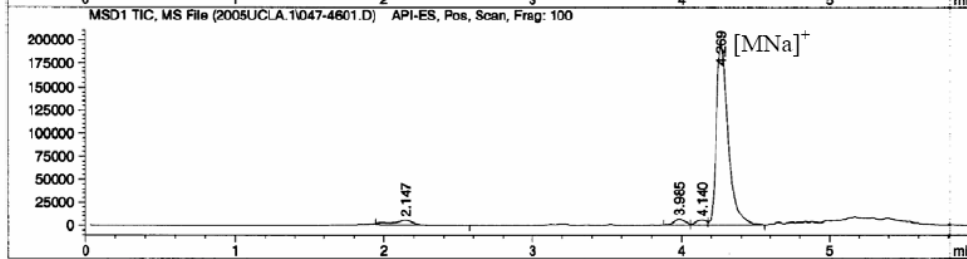
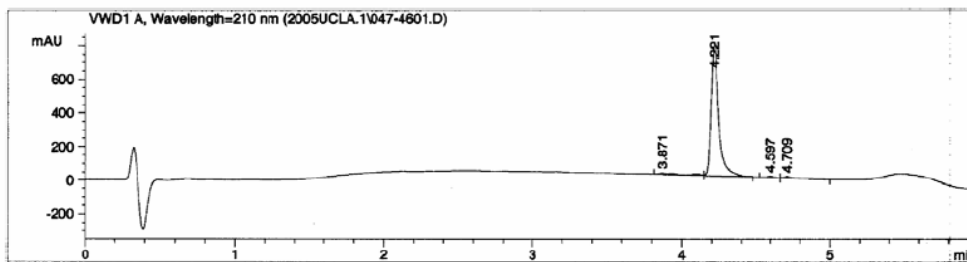
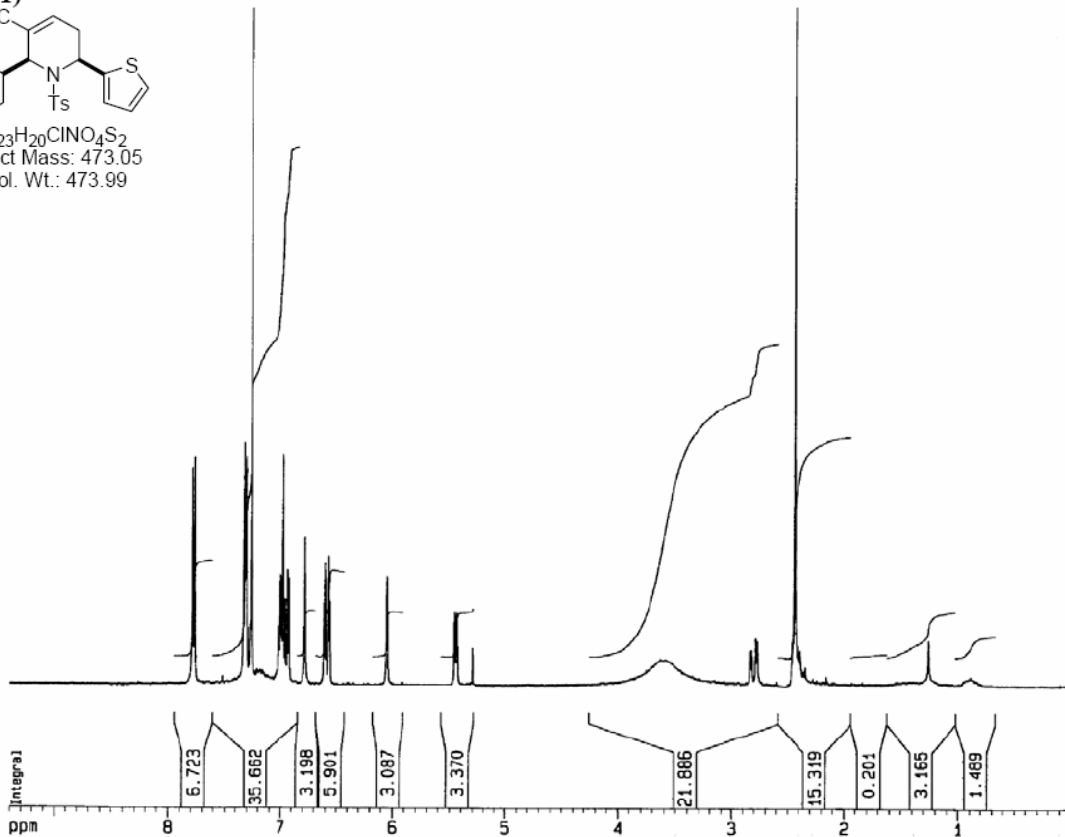
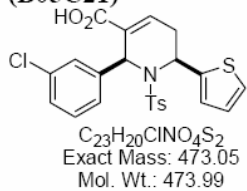
2-(3-Chlorophenyl)-1-methanesulfonyl-6-phenyl-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C19)



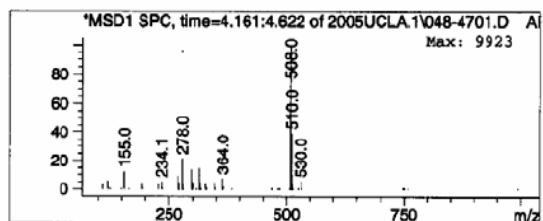
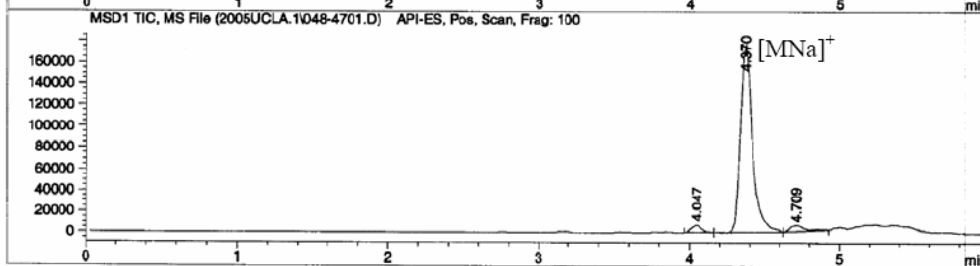
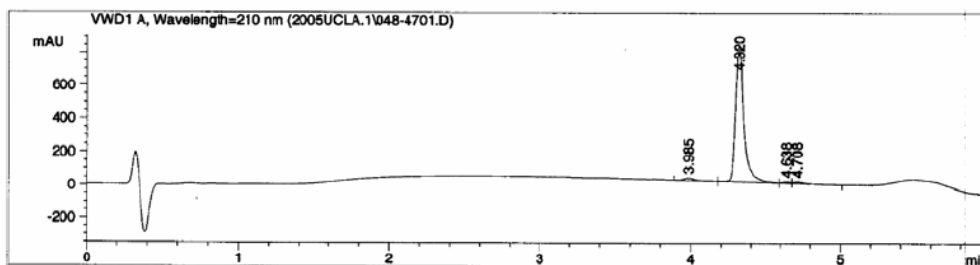
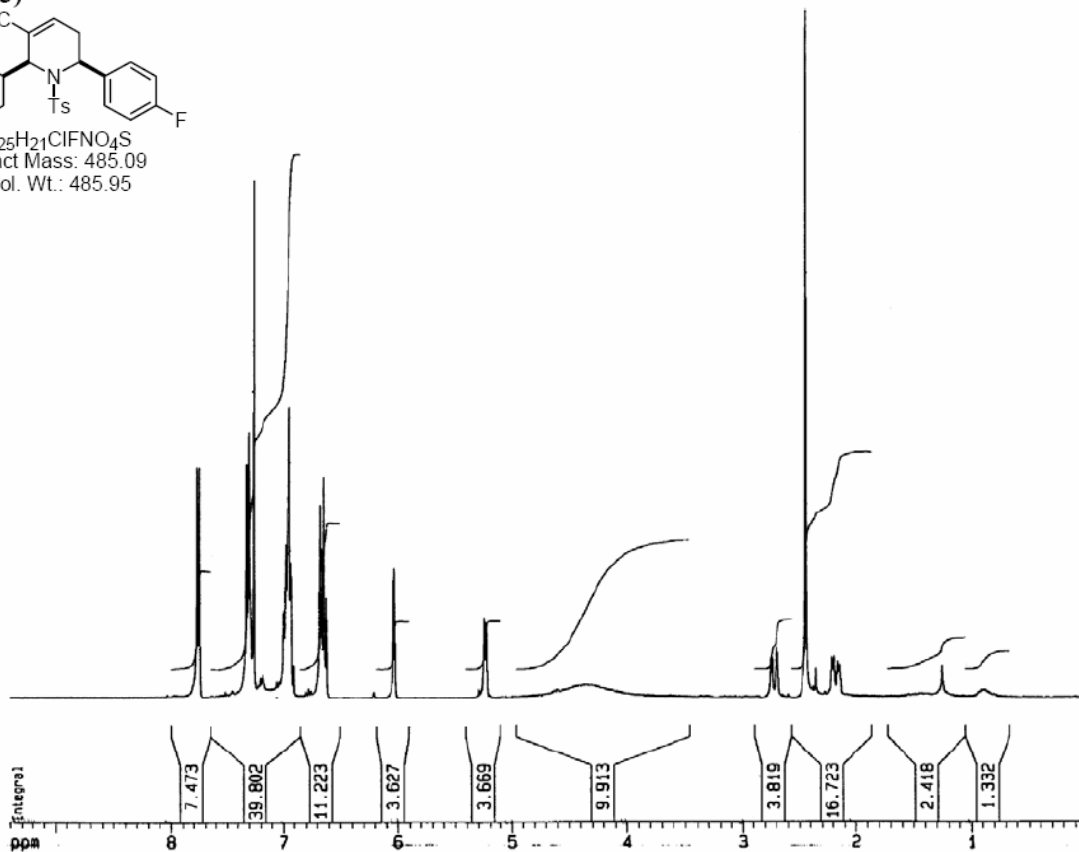
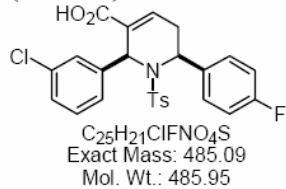
2-(3-Chlorophenyl)-6-(3,4-dimethoxyphenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C20)



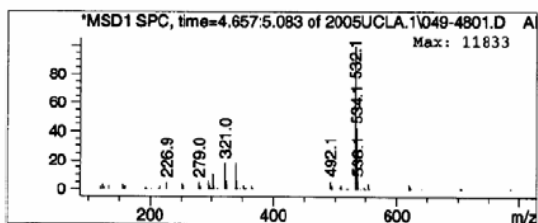
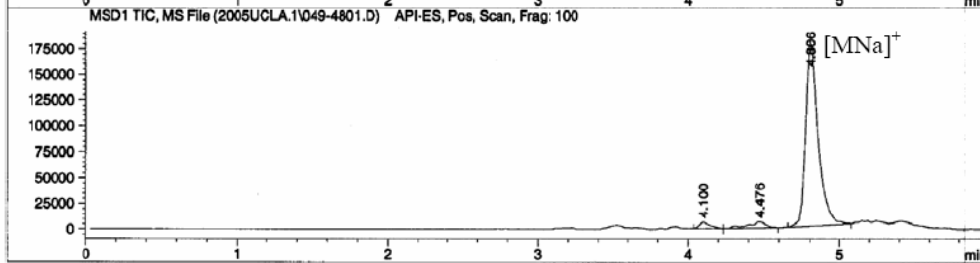
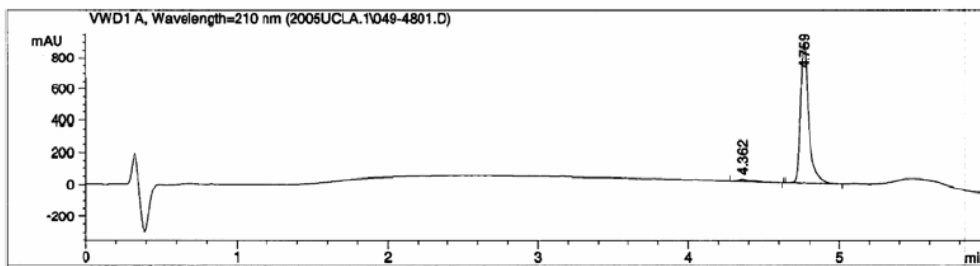
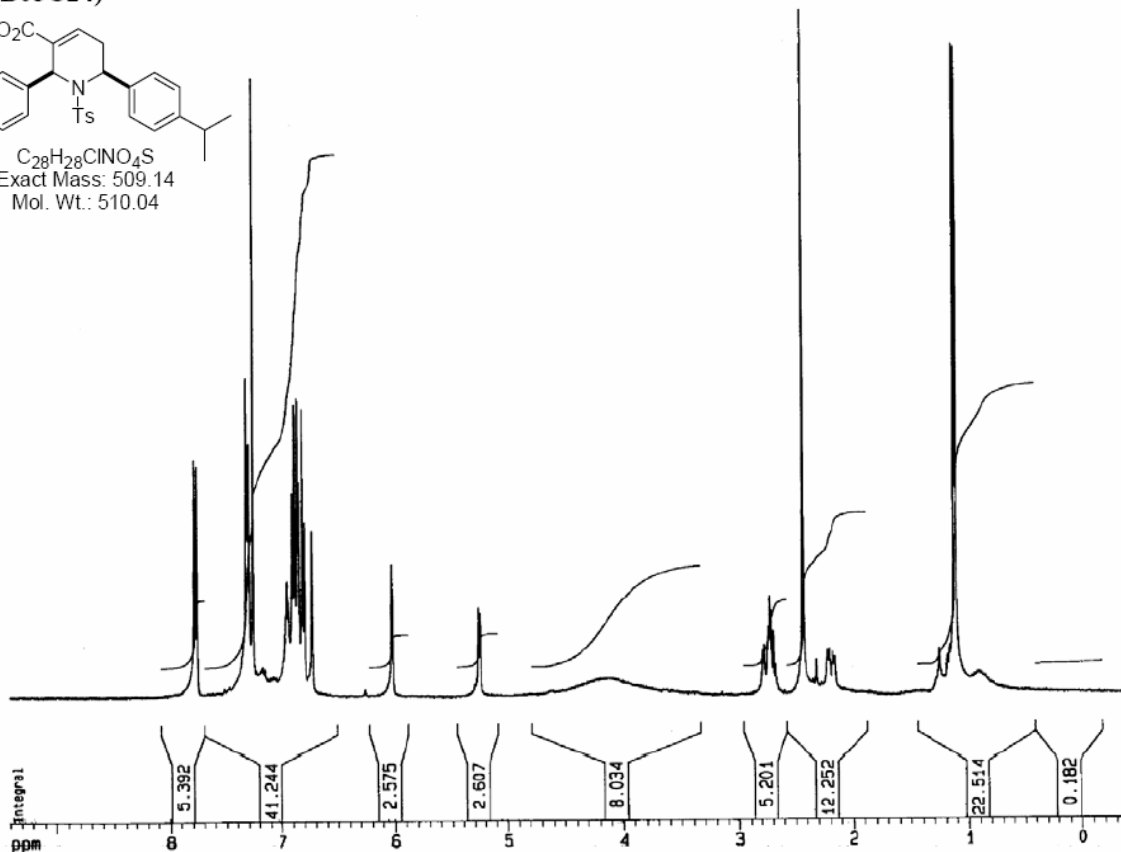
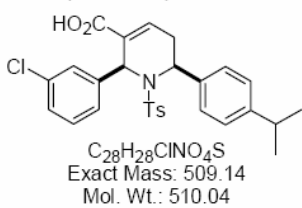
2-(3-Chlorophenyl)-6-(thiophen-2-yl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C21)



2-(3-Chlorophenyl)-6-(4-fluorophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C23)

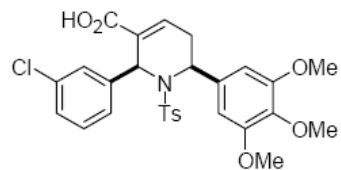


2-(3-Chlorophenyl)-6-(4-isopropylphenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C24)

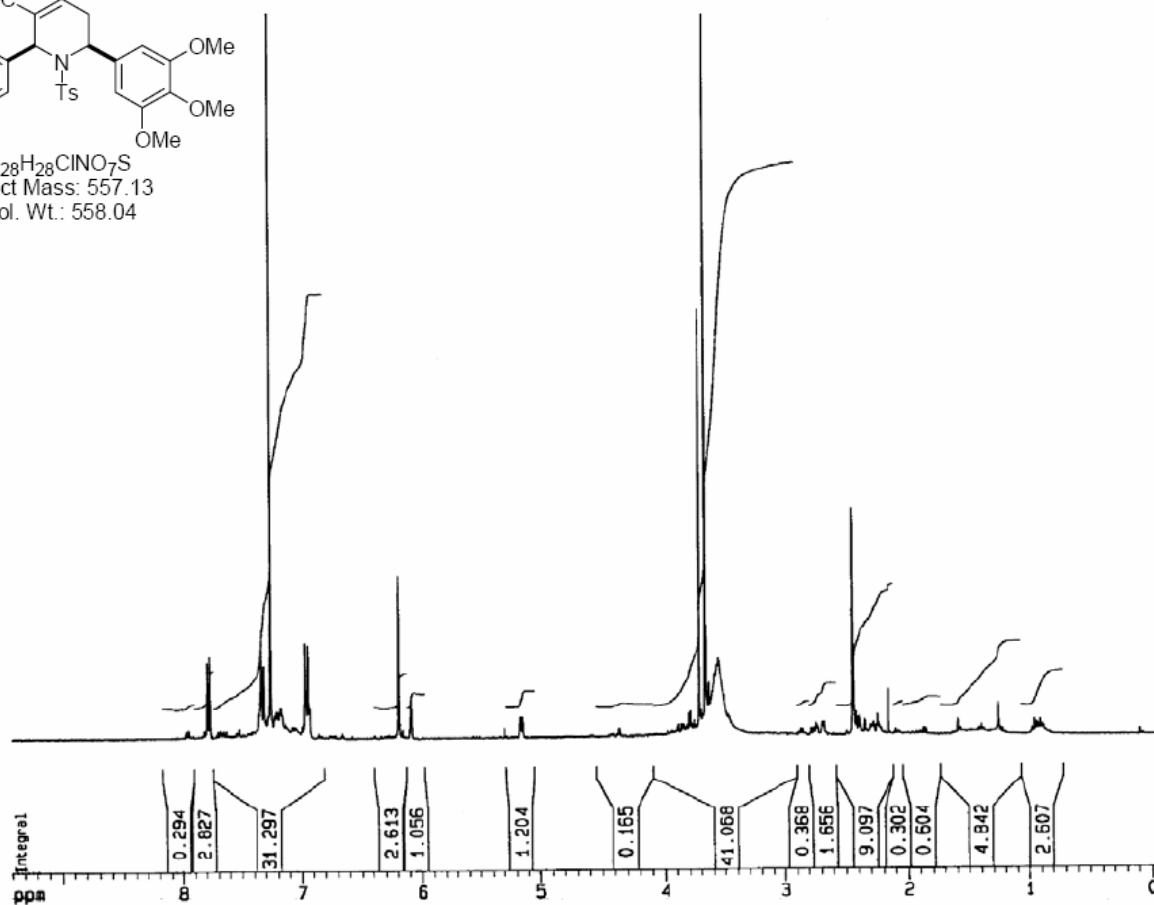


2-(3-Chlorophenyl)-1-(4-toluenesulfonyl)-6-(3,4,5-trimethoxyphenyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C25)

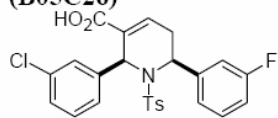
Not included



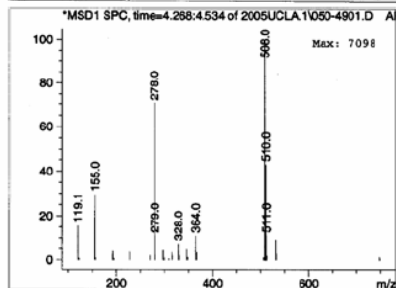
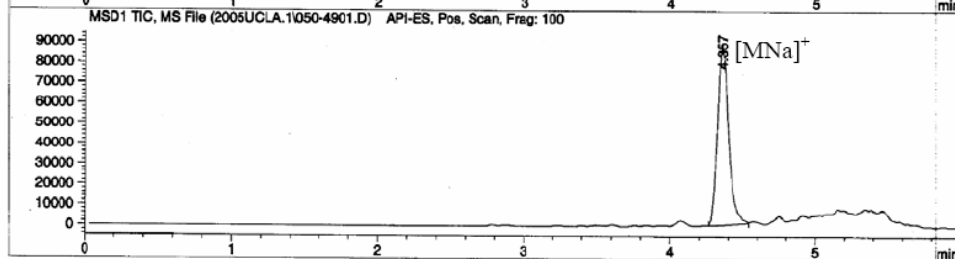
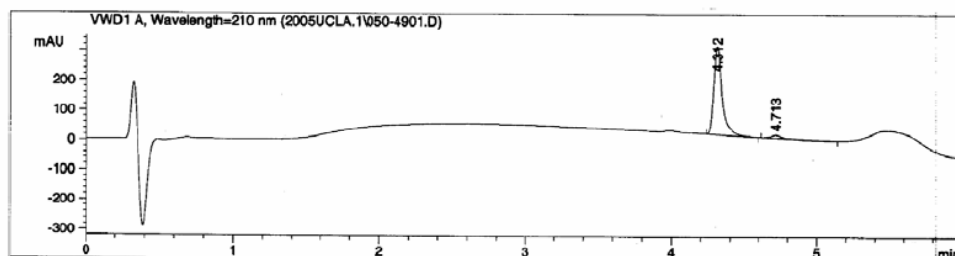
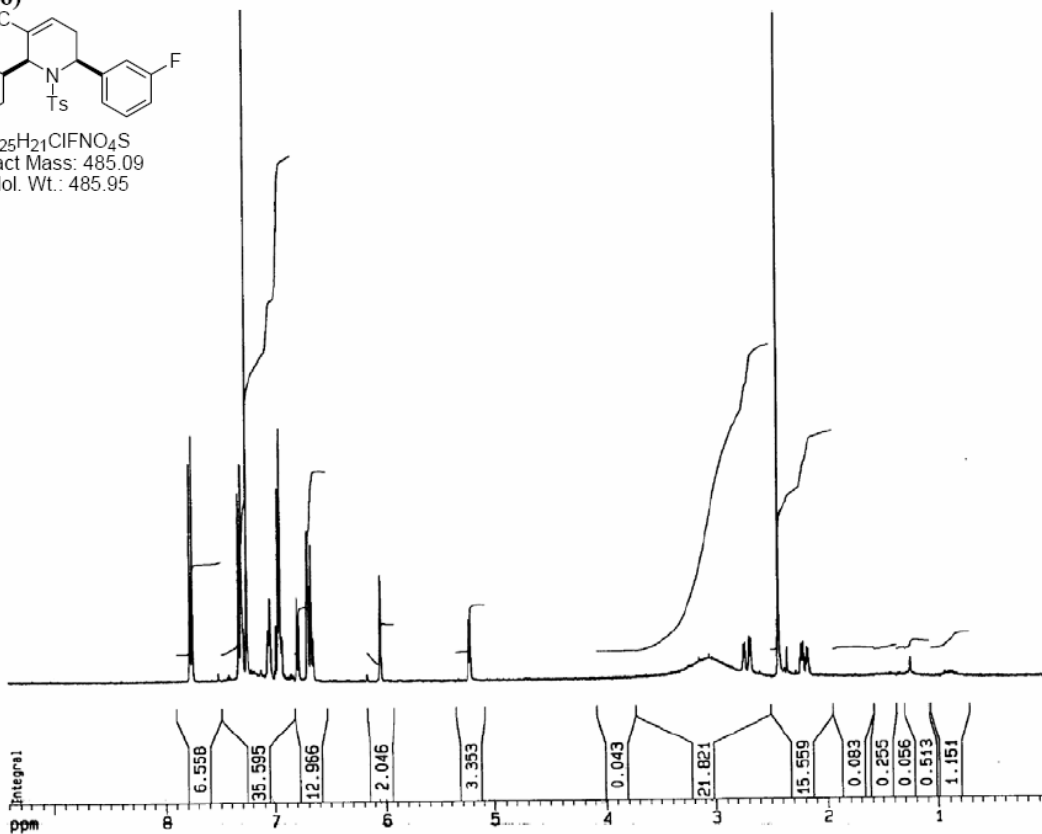
$C_{28}H_{28}ClNO_7S$
Exact Mass: 557.13
Mol. Wt.: 558.04



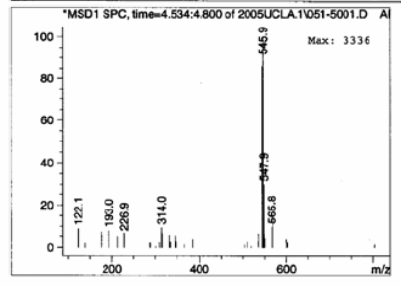
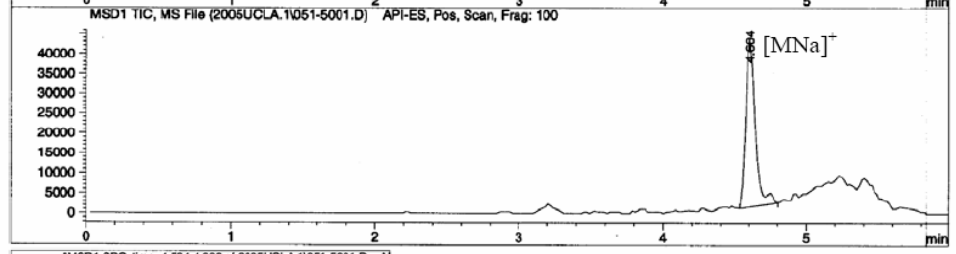
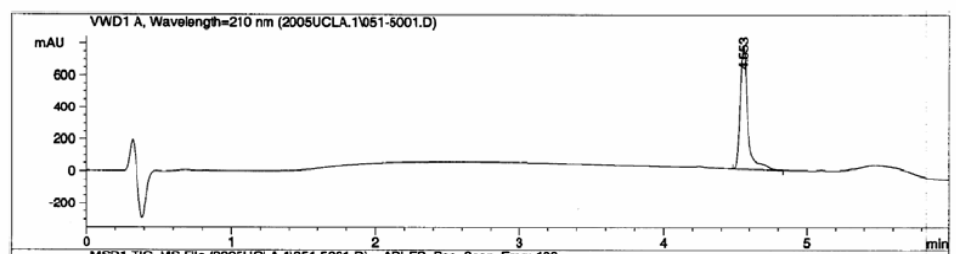
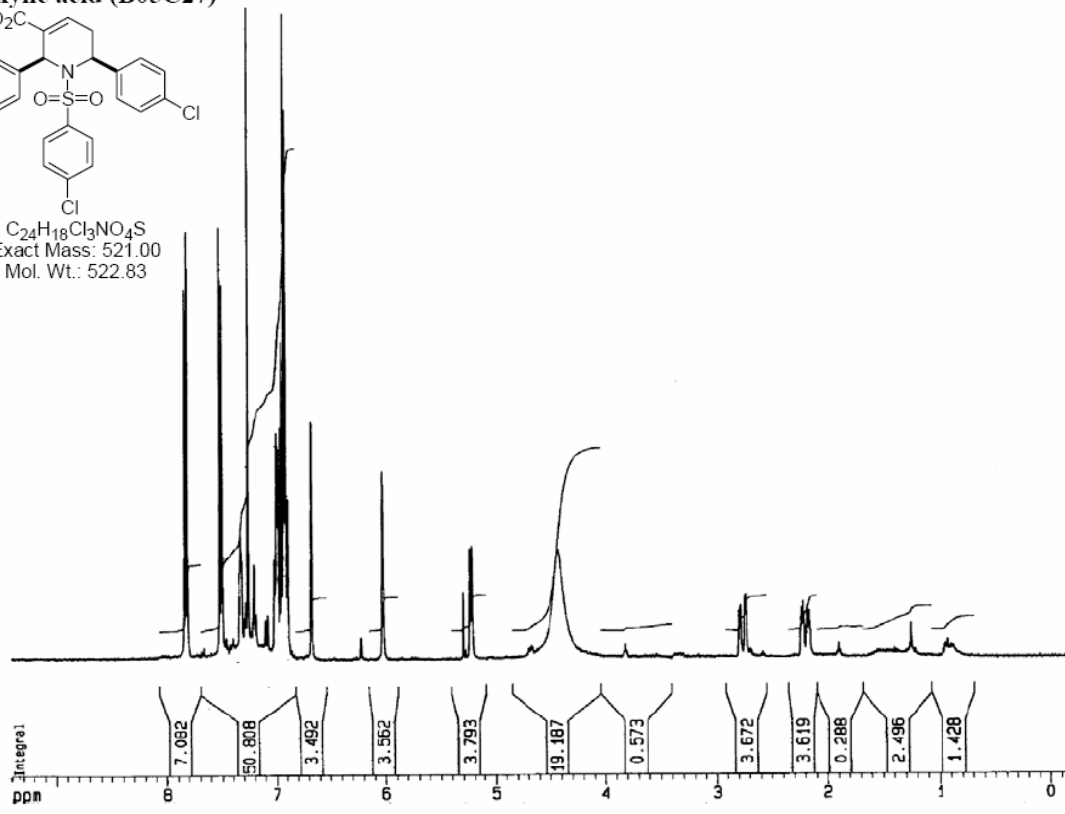
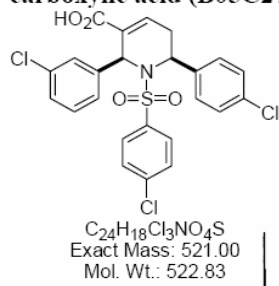
2-(3-Chlorophenyl)-6-(3-fluorophenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C26)



C₂₅H₂₁ClFNO₄S
 Exact Mass: 485.09
 Mol. Wt.: 485.95

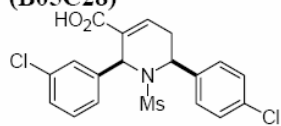


1-(4-Chlorobenzenesulfonyl)-6-(4-chlorophenyl)-2-(3-chlorophenyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C27)

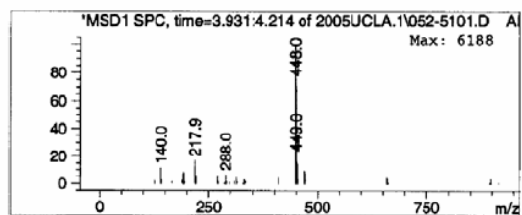
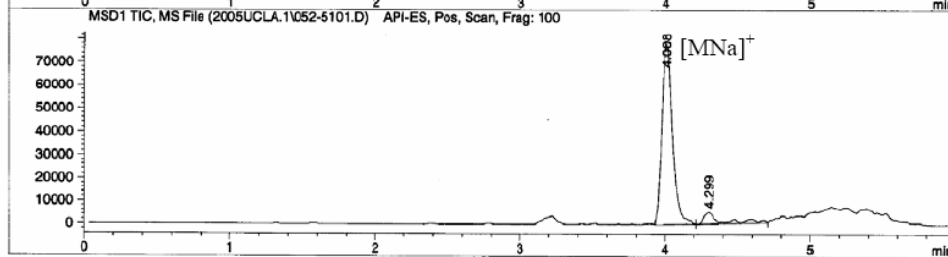
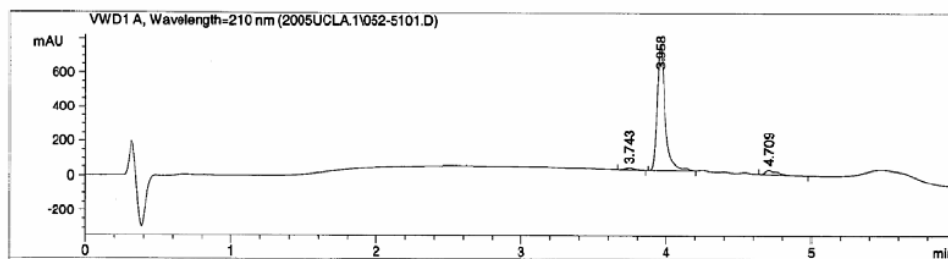
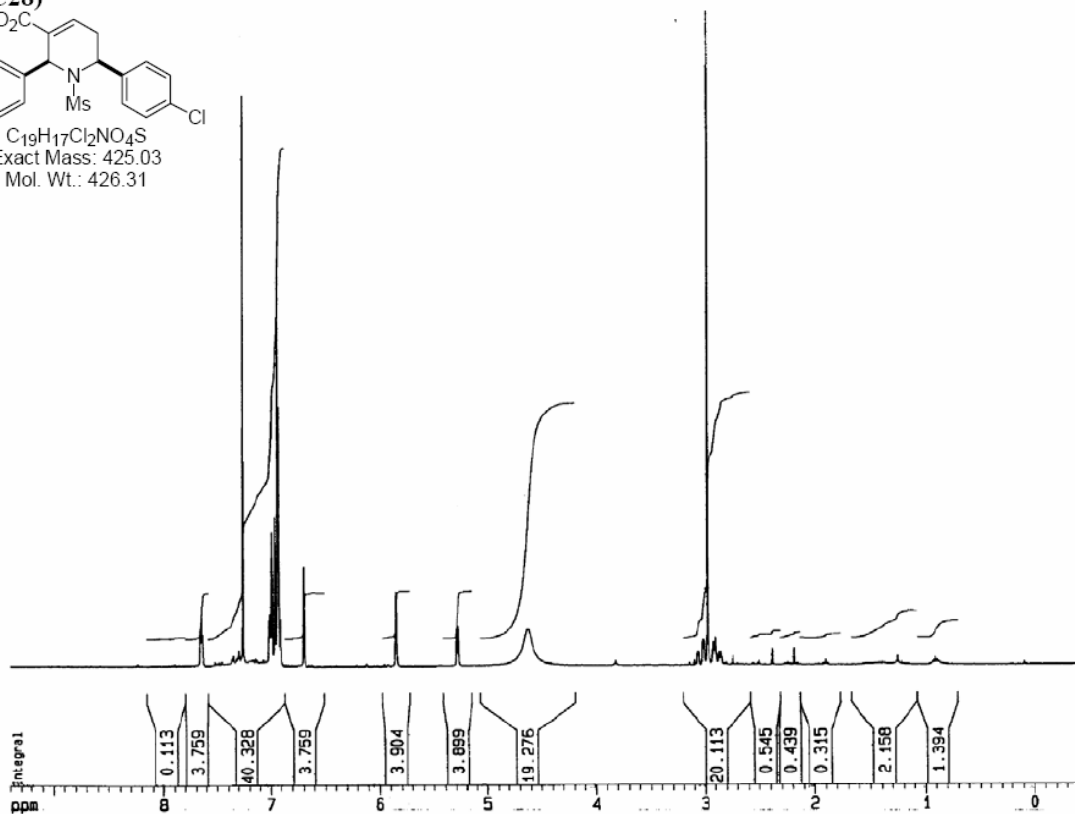


Component 2: Peak at Scan 258.9. Top ions are 546 544 548

6-(4-Chlorophenyl)-2-(3-chlorophenyl)-1-methanesulfonyl-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C28)

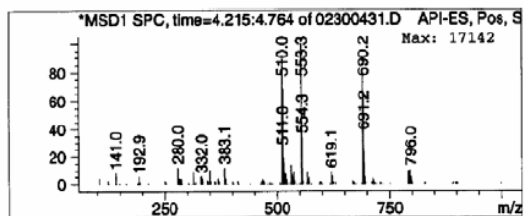
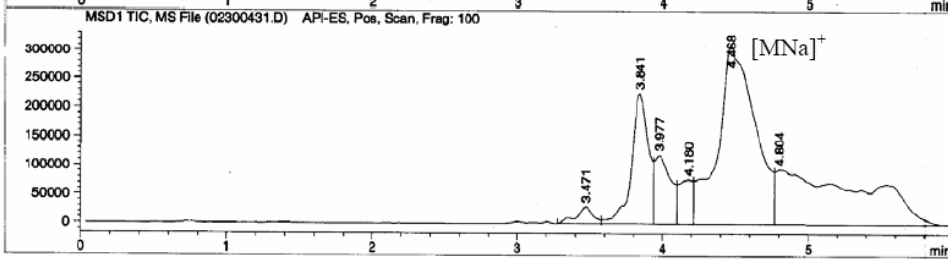
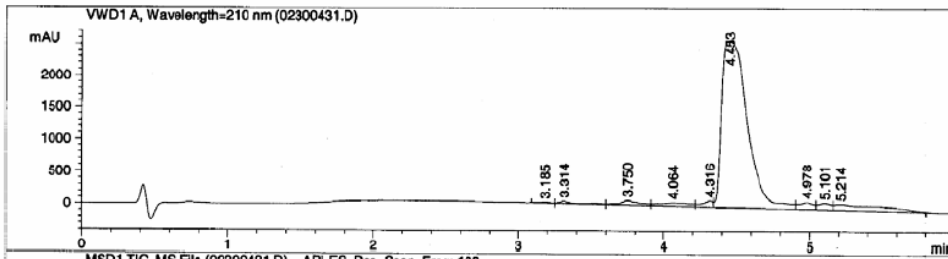
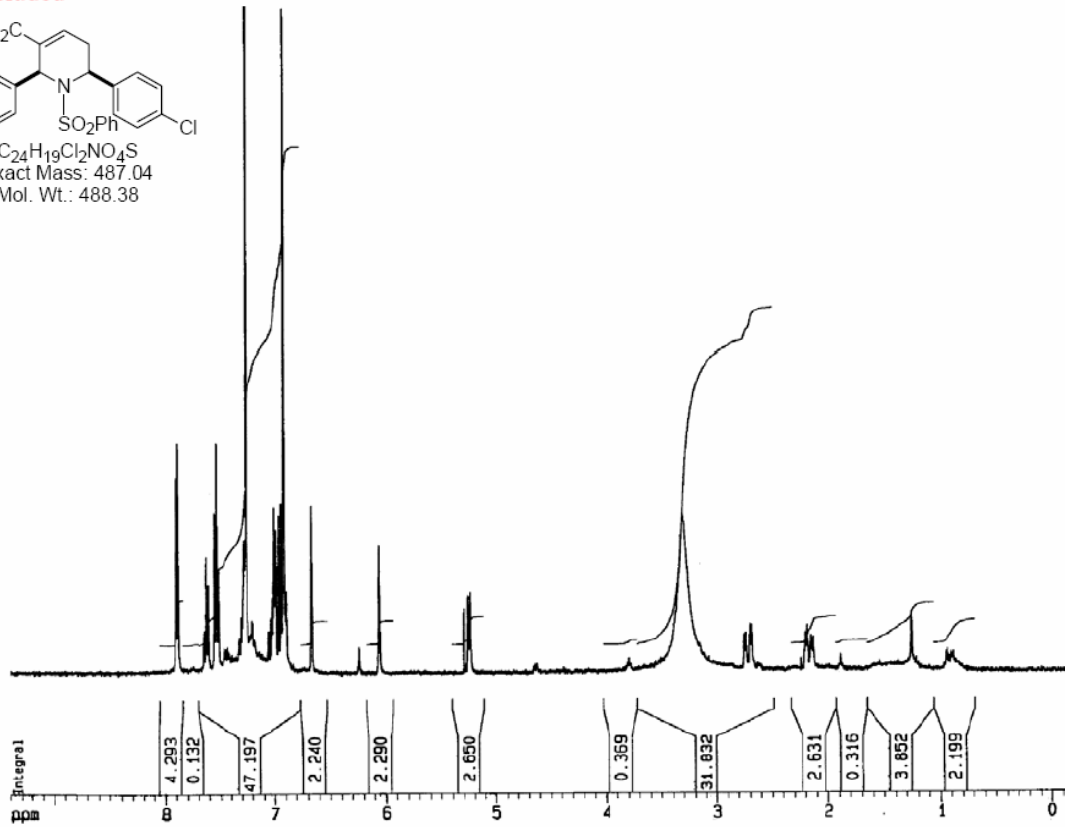
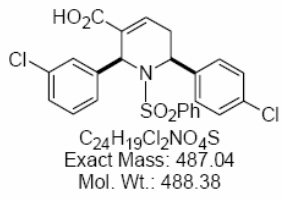


C₁₉H₁₇Cl₂NO₄S
 Exact Mass: 425.03
 Mol. Wt.: 426.31

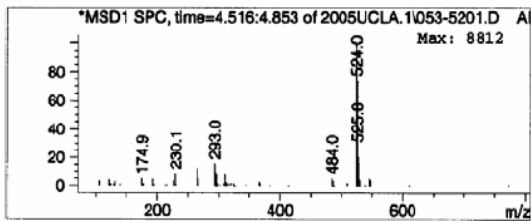
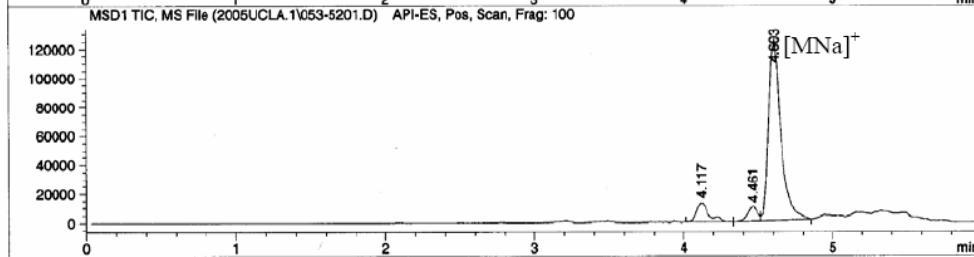
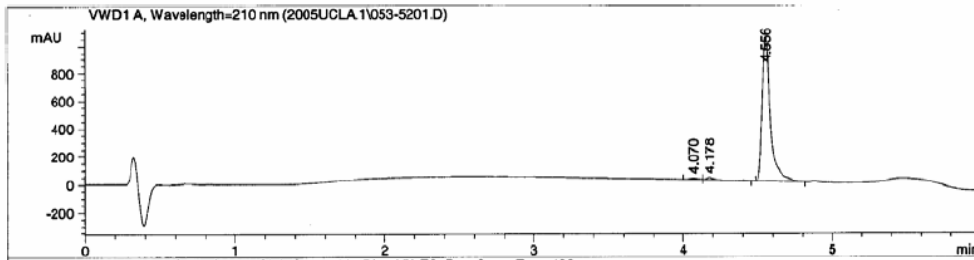
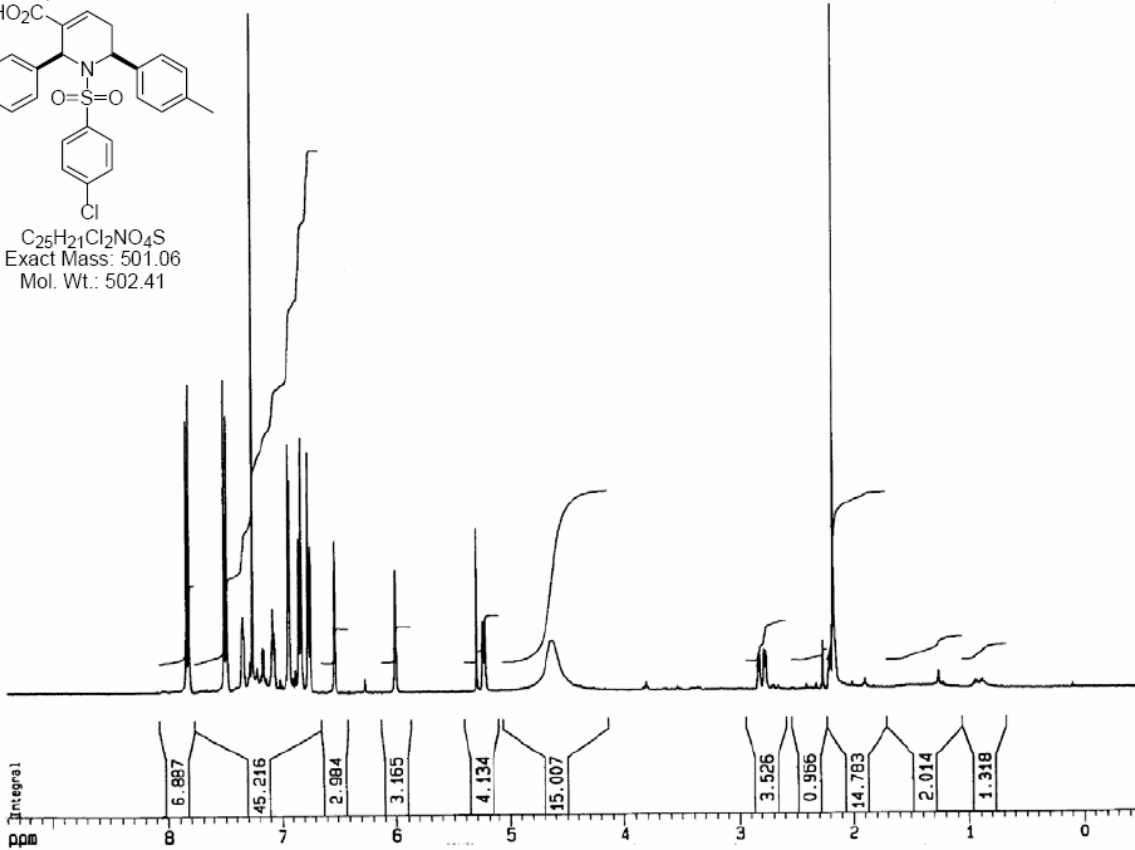
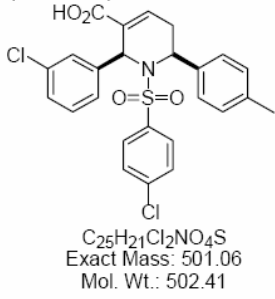


1-Benzenesulfonyl-6-(4-chlorophenyl)-2-(3-chlorophenyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C29)

Not included

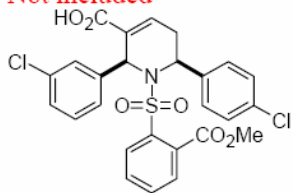


1-(4-Chlorobenzenesulfonyl)-2-(3-chlorophenyl)-6-(p-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C30)

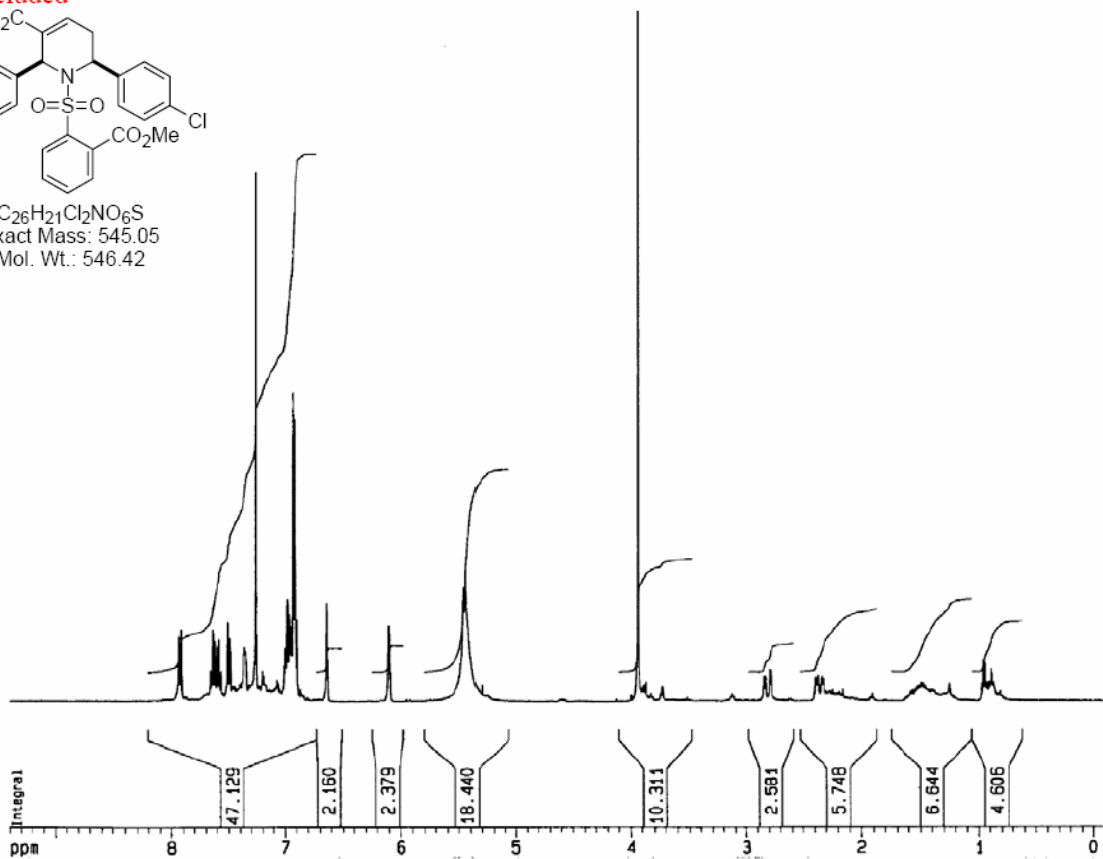


6-(4-Chlorophenyl)-2-(3-chlorophenyl)-1-(2-methoxycarbonylbenzenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C31)

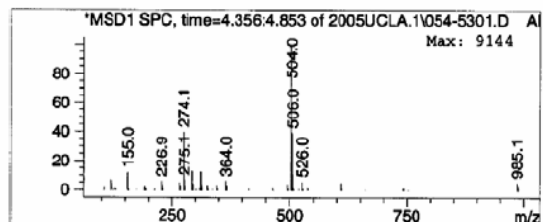
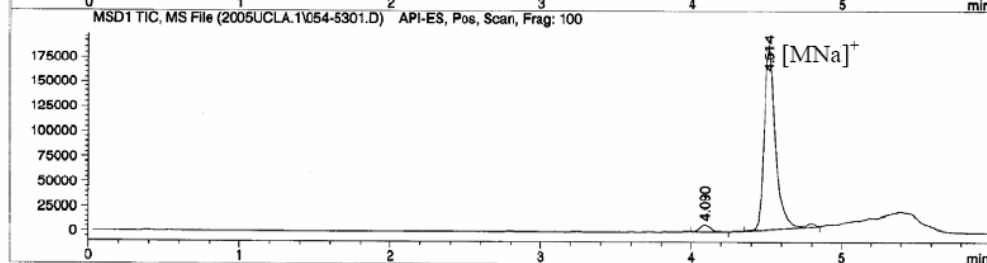
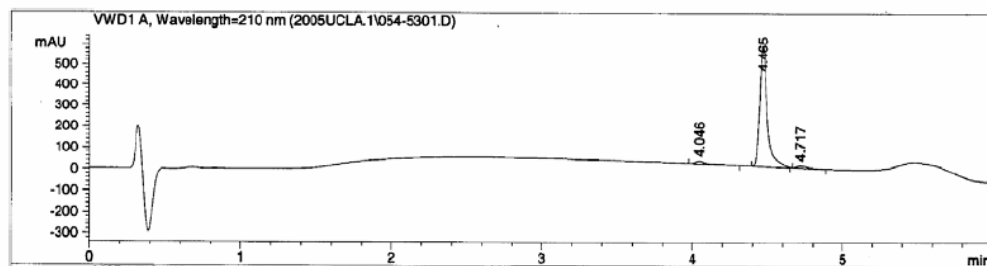
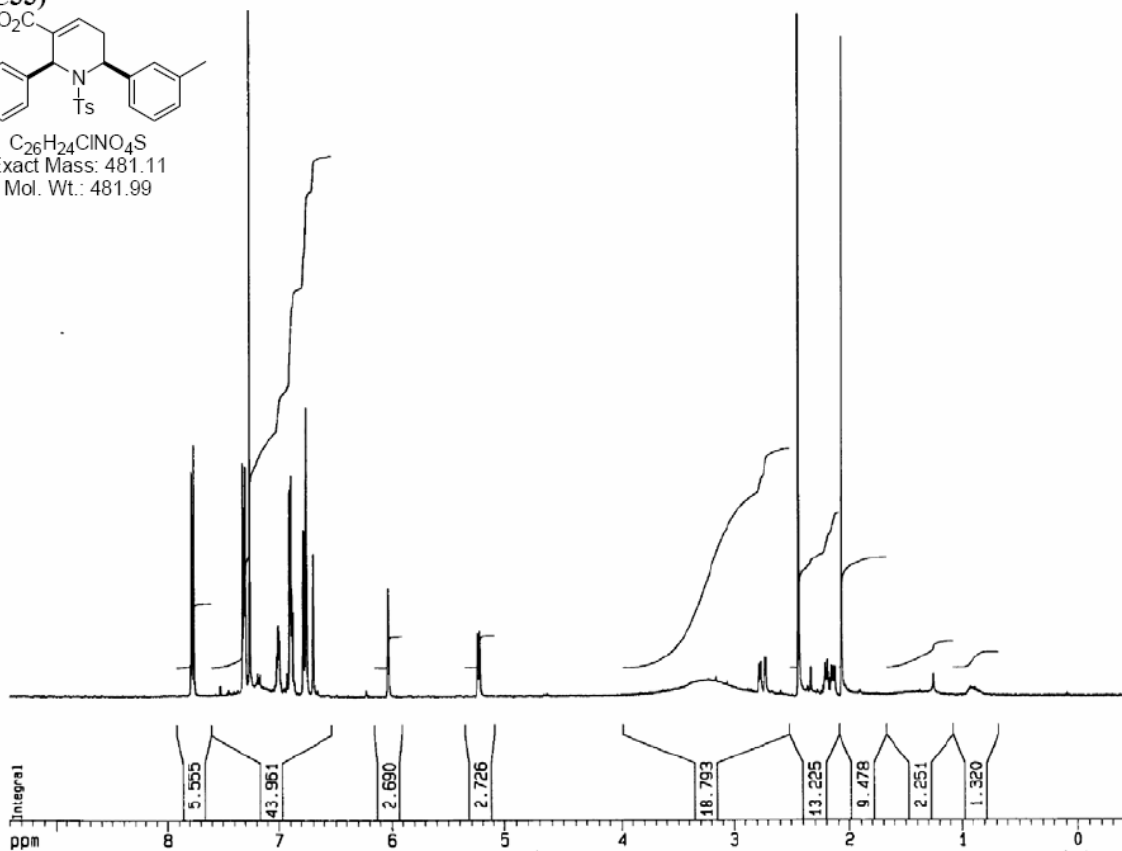
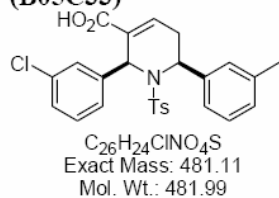
Not included



C₂₆H₂₁Cl₂NO₆S
Exact Mass: 545.05
Mol. Wt.: 546.42

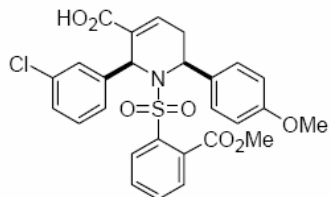


2-(3-Chlorophenyl)-1-(4-toluenesulfonyl)-6-(*m*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C33)

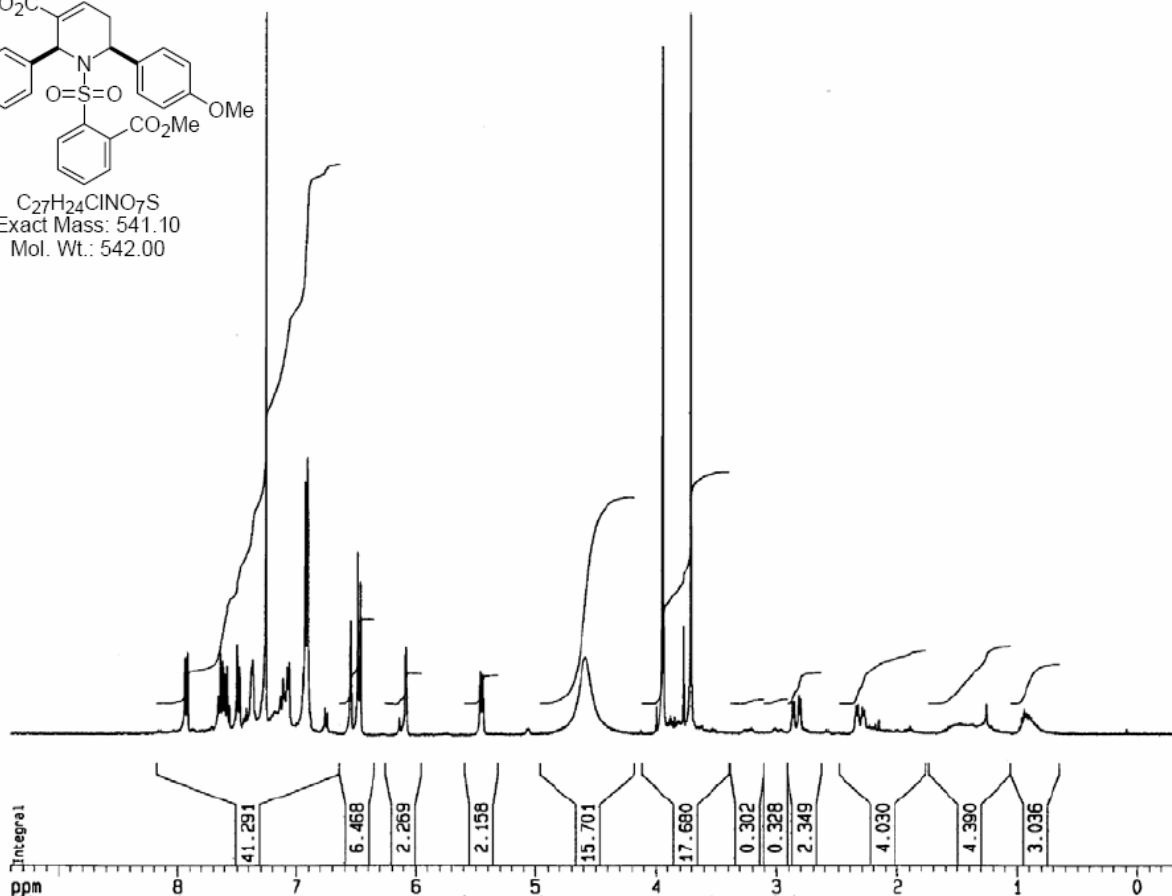


2-(3-Chlorophenyl)-1-(2-methoxycarbonylbenzenesulfonyl)-6-(4-methoxyphenyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C34)

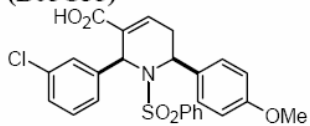
Not included



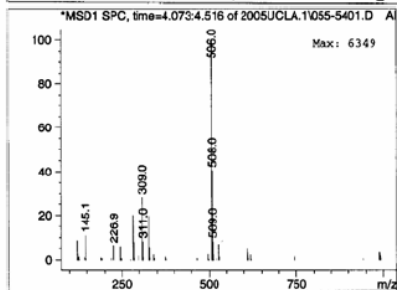
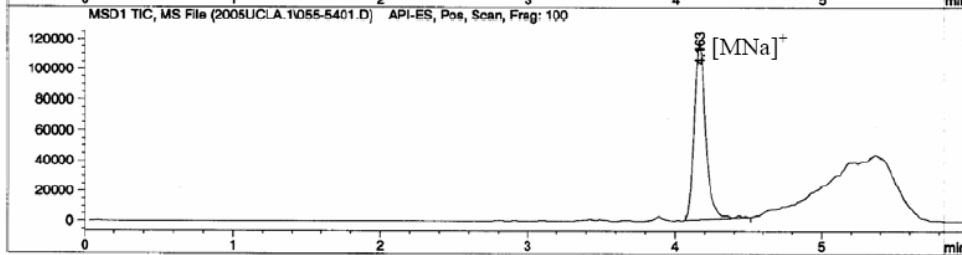
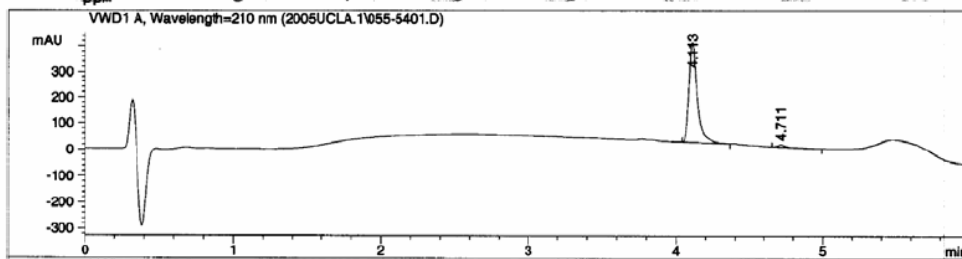
C₂₇H₂₄ClNO₇S
Exact Mass: 541.10
Mol. Wt.: 542.00



1-Benzenesulfonyl-2-(3-chlorophenyl)-6-(4-methoxyphenyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C35)

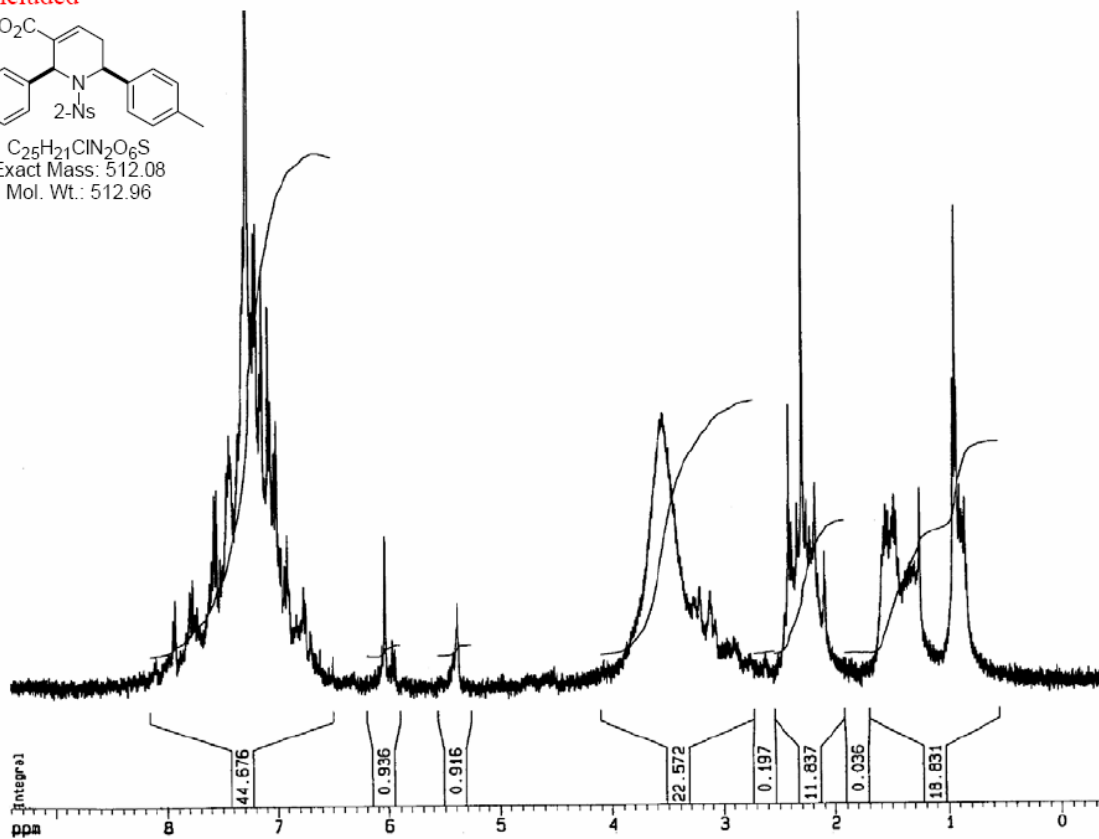
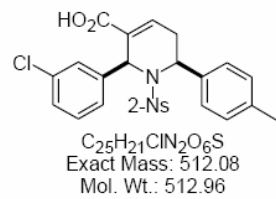


C₂₅H₂₂ClNO₆S
 Exact Mass: 483.09
 Mol. Wt.: 483.96

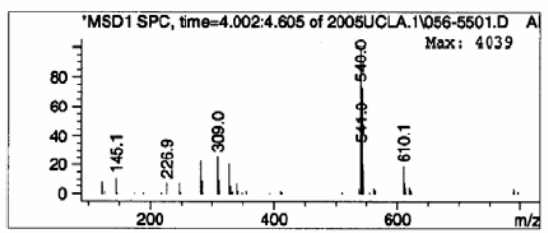
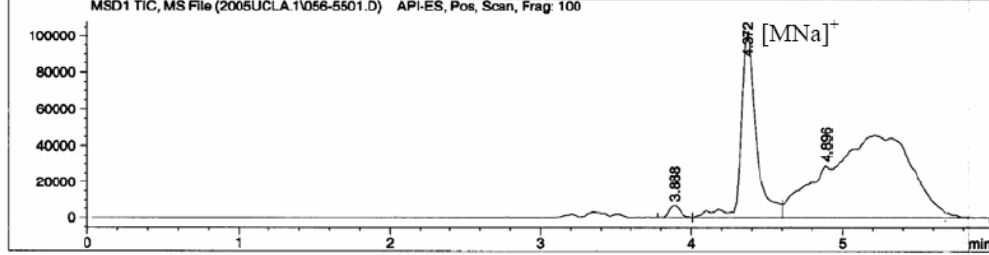
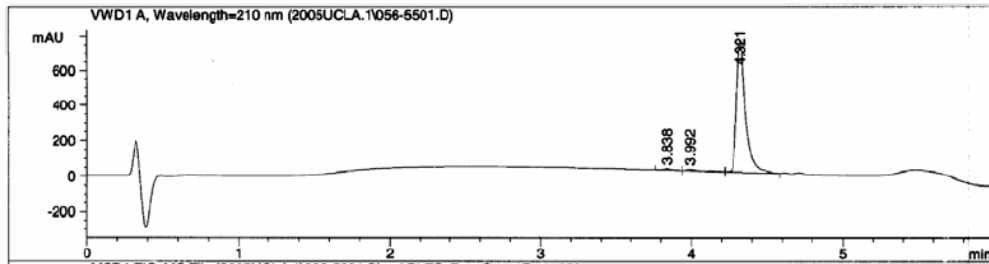
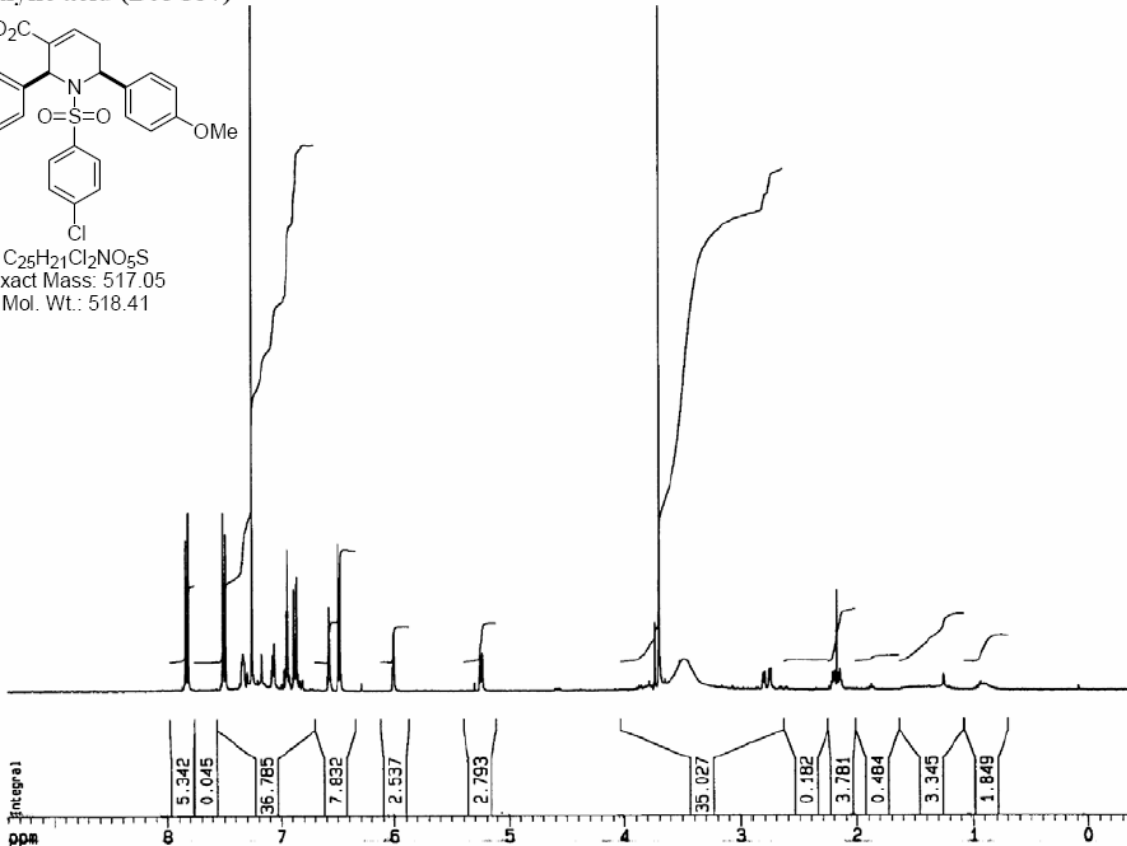
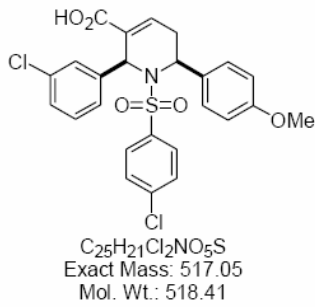


2-(3-Chlorophenyl)-1-(2-nitrobenzenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C36)

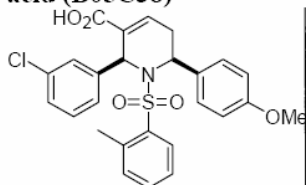
Not included



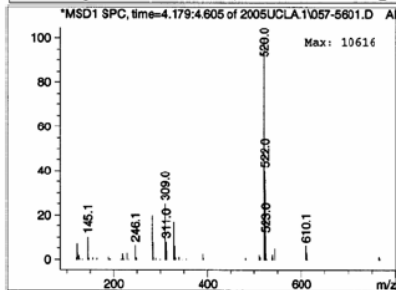
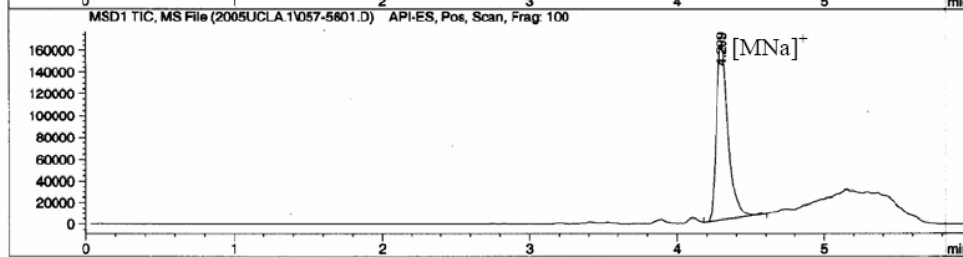
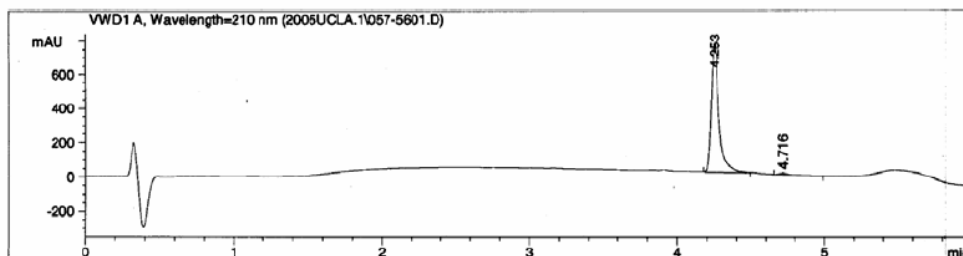
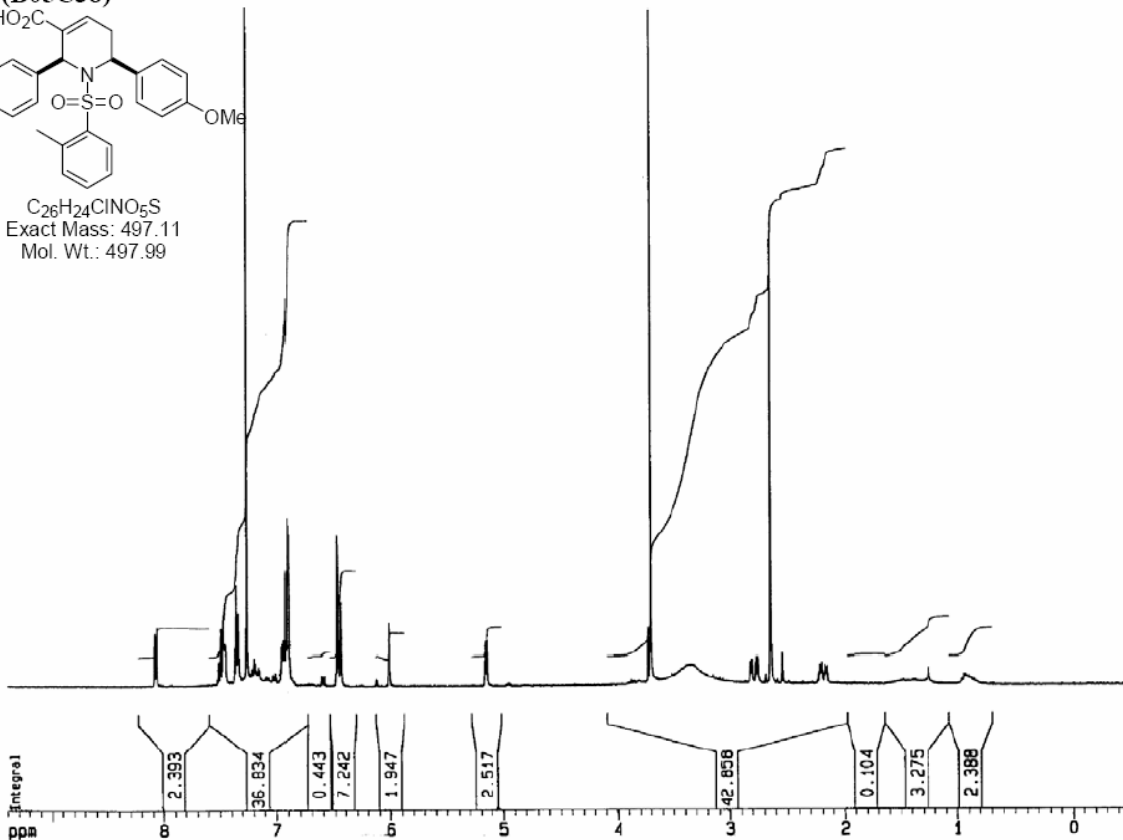
1-(4-Chlorobenzenesulfonyl)-2-(3-chlorophenyl)-6-(4-methoxyphenyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C37)



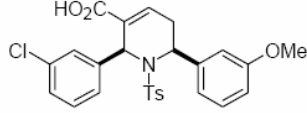
2-(3-Chlorophenyl)-6-(4-methoxyphenyl)-1-(2-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C38)



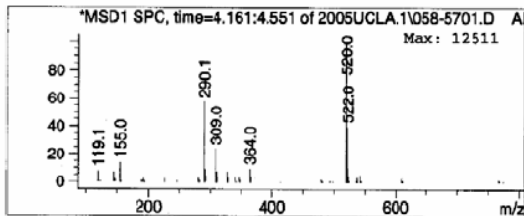
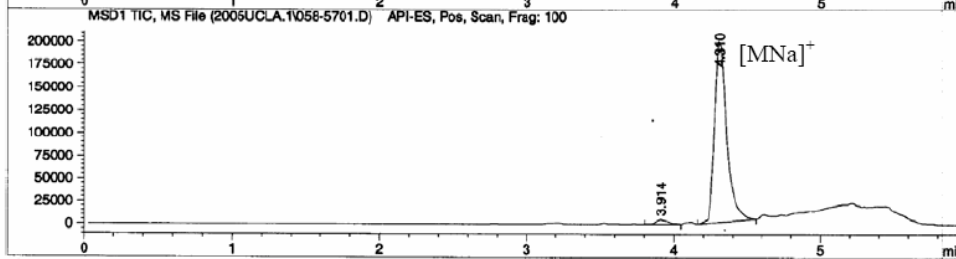
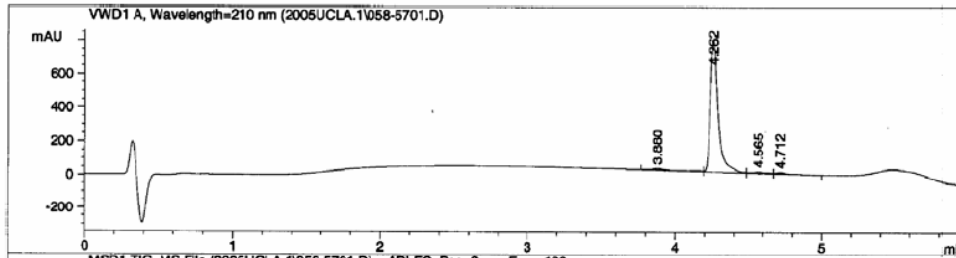
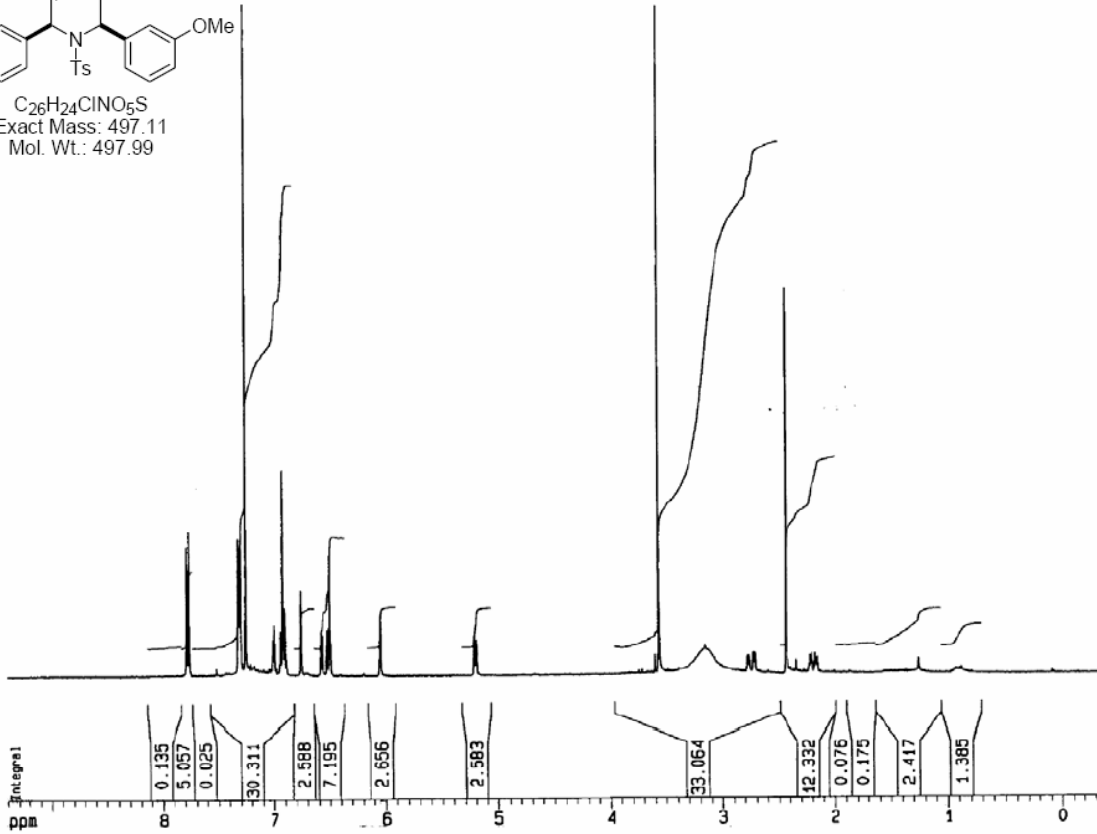
C₂₆H₂₄ClNO₅S
 Exact Mass: 497.11
 Mol. Wt.: 497.99



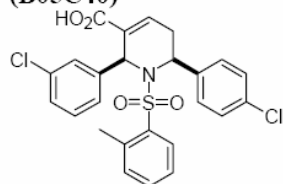
2-(3-Chlorophenyl)-6-(3-methoxyphenyl)-1-(4-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C39)



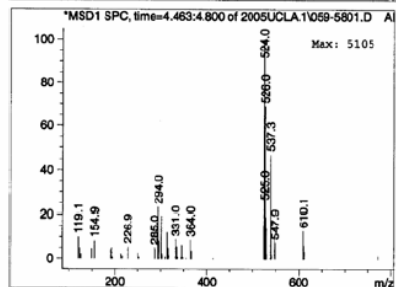
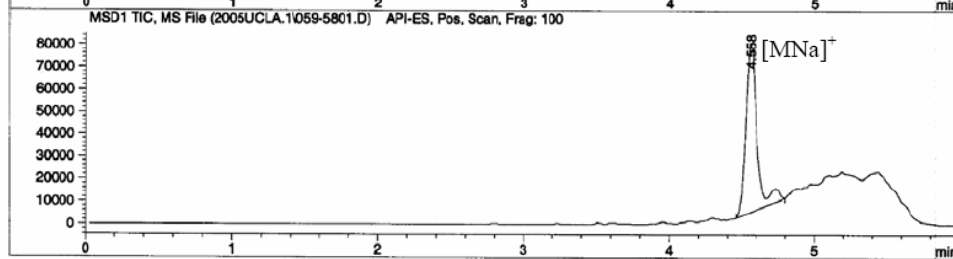
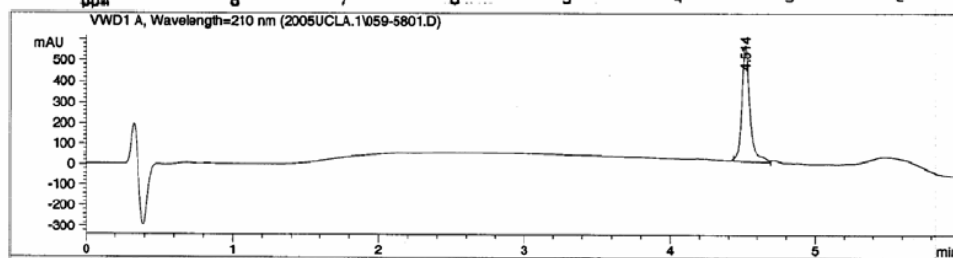
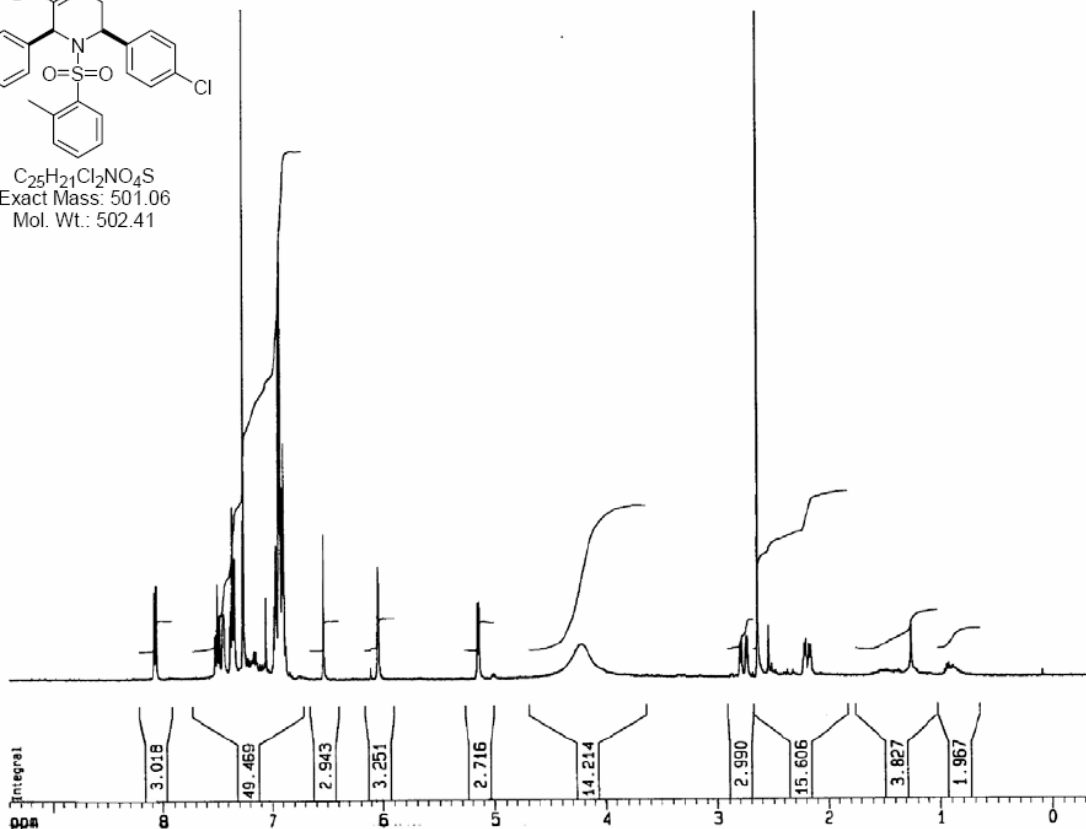
C₂₆H₂₄ClNO₅S
 Exact Mass: 497.11
 Mol. Wt.: 497.99



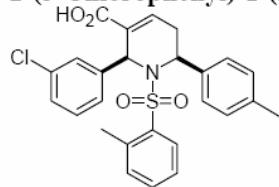
6-(4-Chlorophenyl)-2-(3-chlorophenyl)-1-(2-toluenesulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C40)



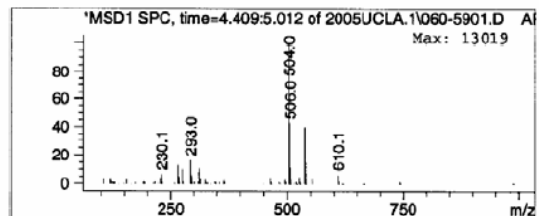
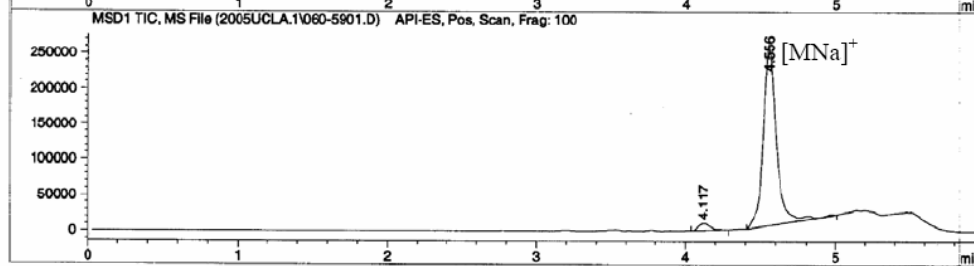
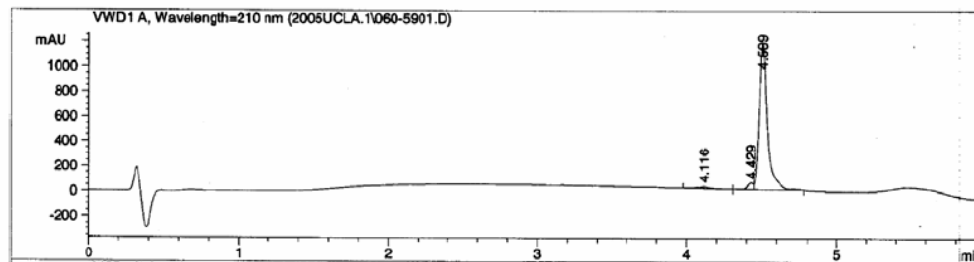
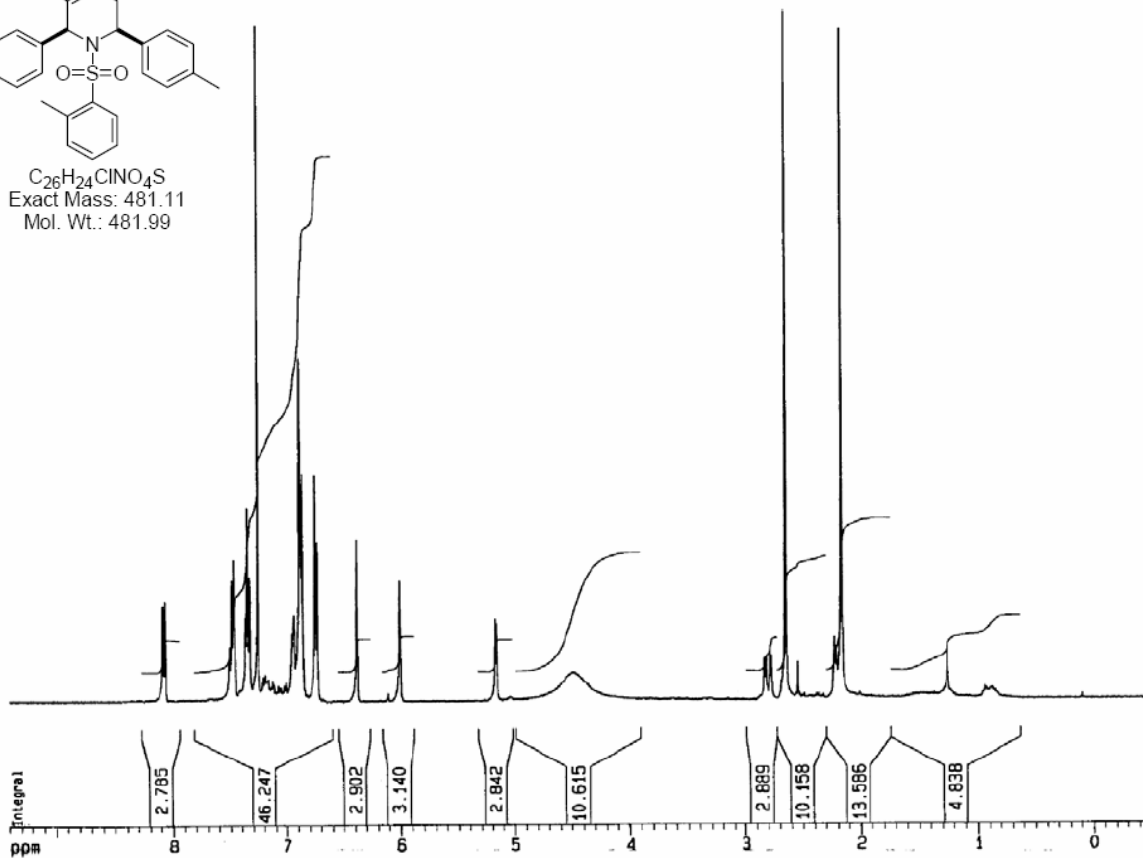
C₂₅H₂₁Cl₂NO₄S
 Exact Mass: 501.06
 Mol. Wt.: 502.41



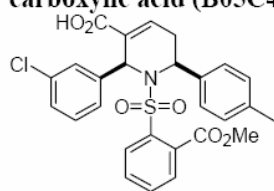
2-(3-Chlorophenyl)-1-(2-toluenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C41)



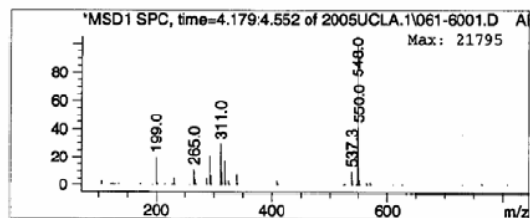
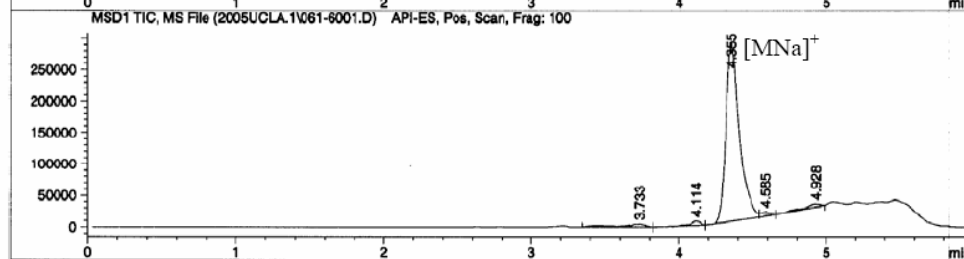
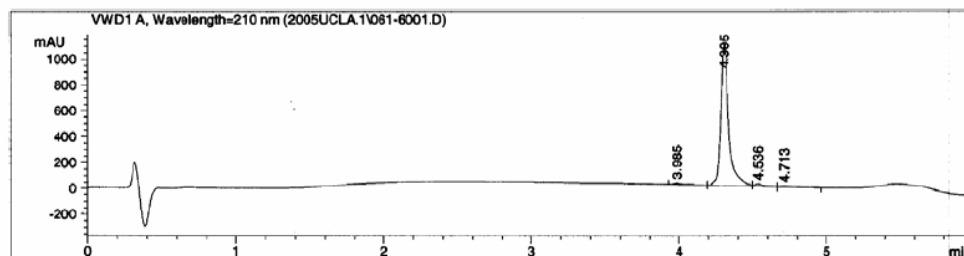
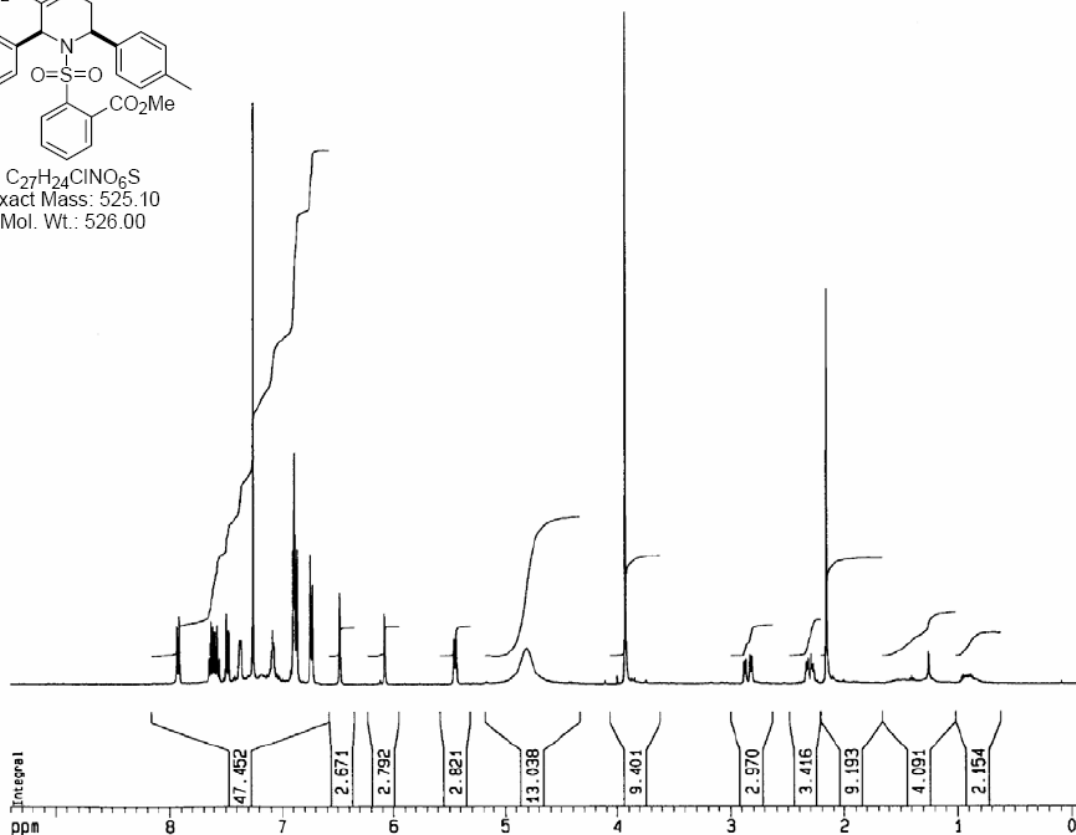
C₂₆H₂₄ClNO₄S
 Exact Mass: 481.11
 Mol. Wt.: 481.99



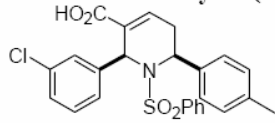
2-(3-Chlorophenyl)-1-(2-methoxycarbonylbenzenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C42)



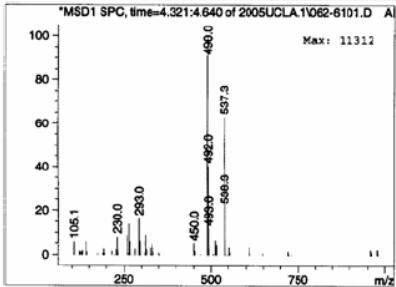
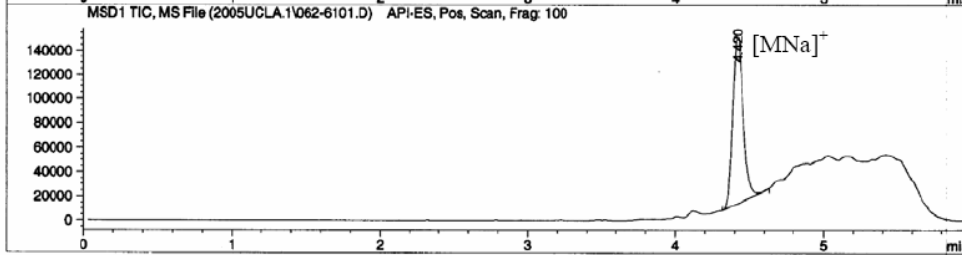
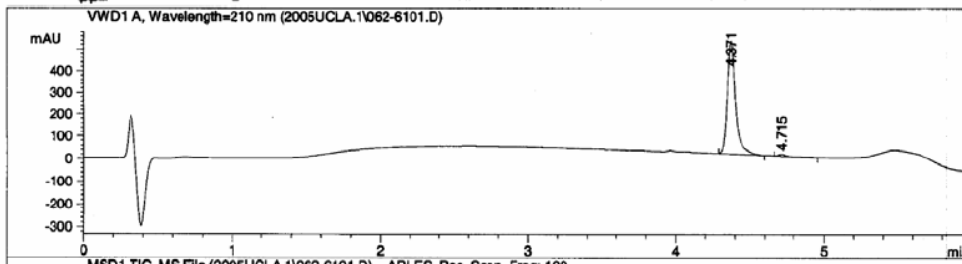
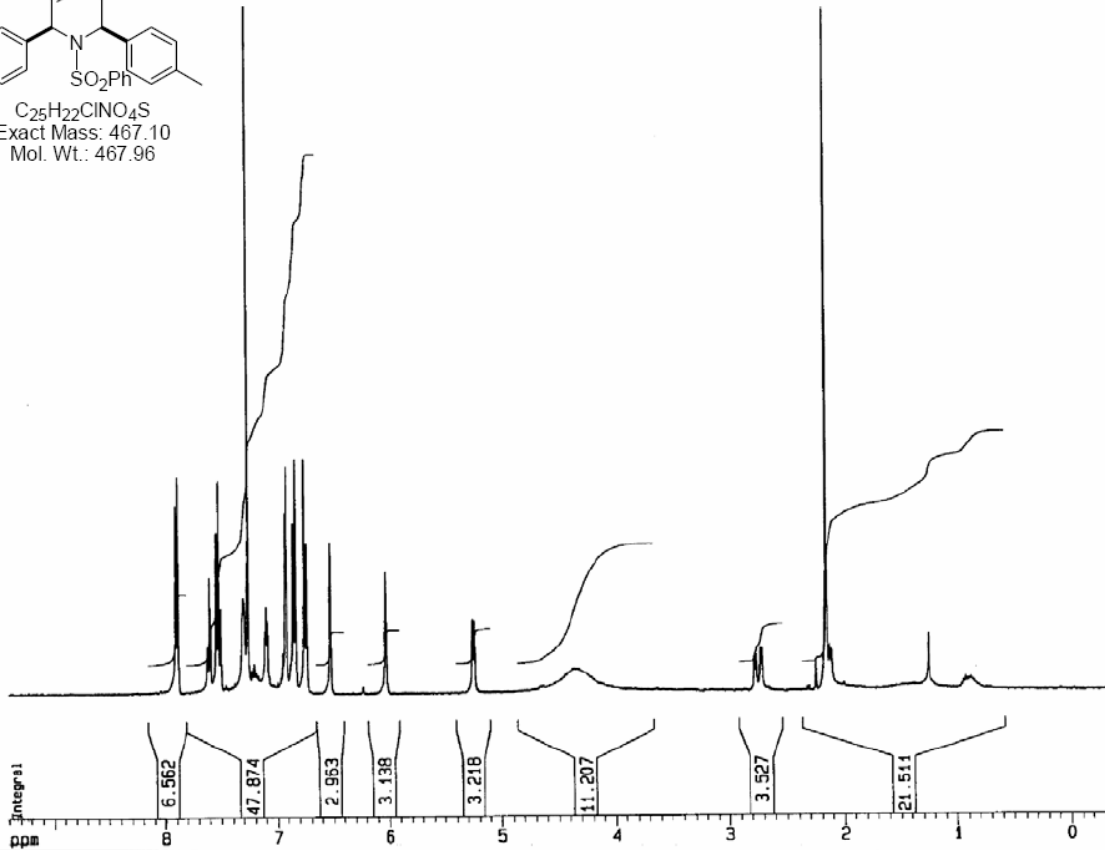
C₂₇H₂₄ClNO₆S
 Exact Mass: 525.10
 Mol. Wt.: 526.00



1-Benzenesulfonyl-2-(3-chlorophenyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C43)

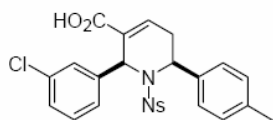


C₂₅H₂₂ClNO₄S
 Exact Mass: 467.10
 Mol. Wt.: 467.96

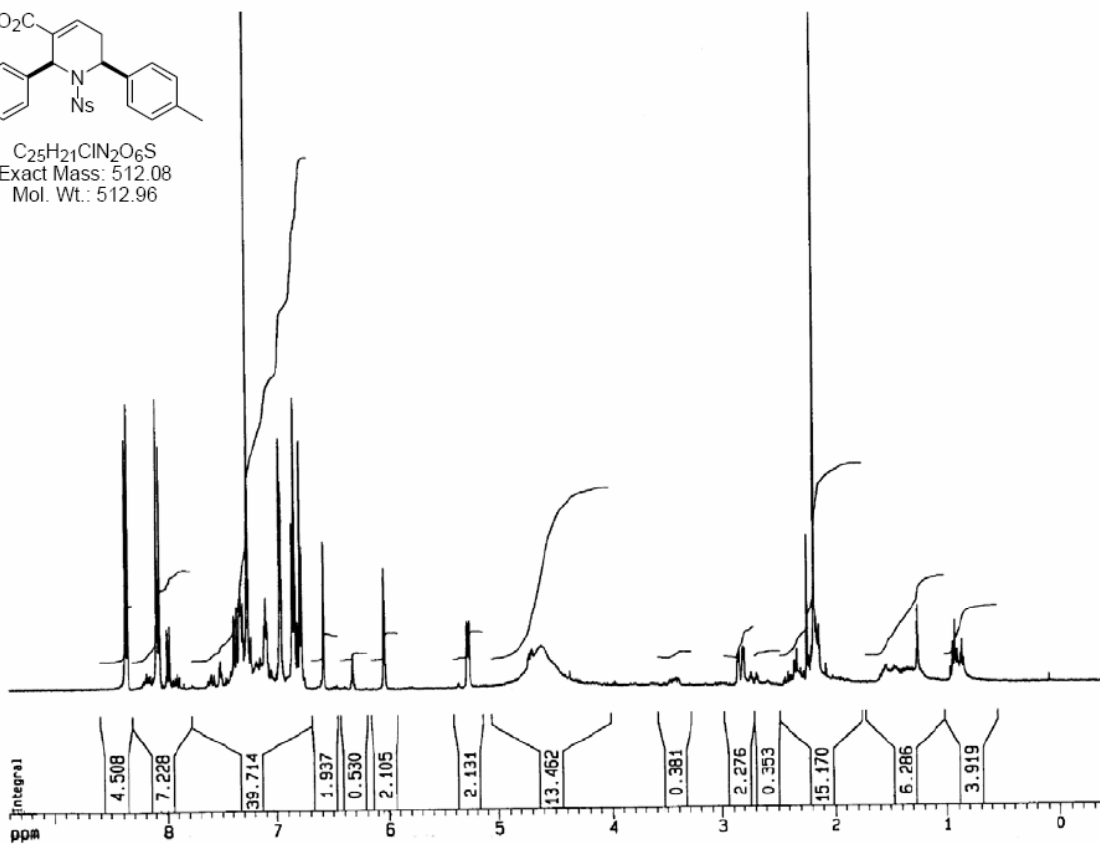


2-(3-Chlorophenyl)-1-(4-nitrobenzenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C44)

Not included

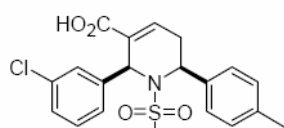


C₂₅H₂₁ClN₂O₆S
Exact Mass: 512.08
Mol. Wt.: 512.96

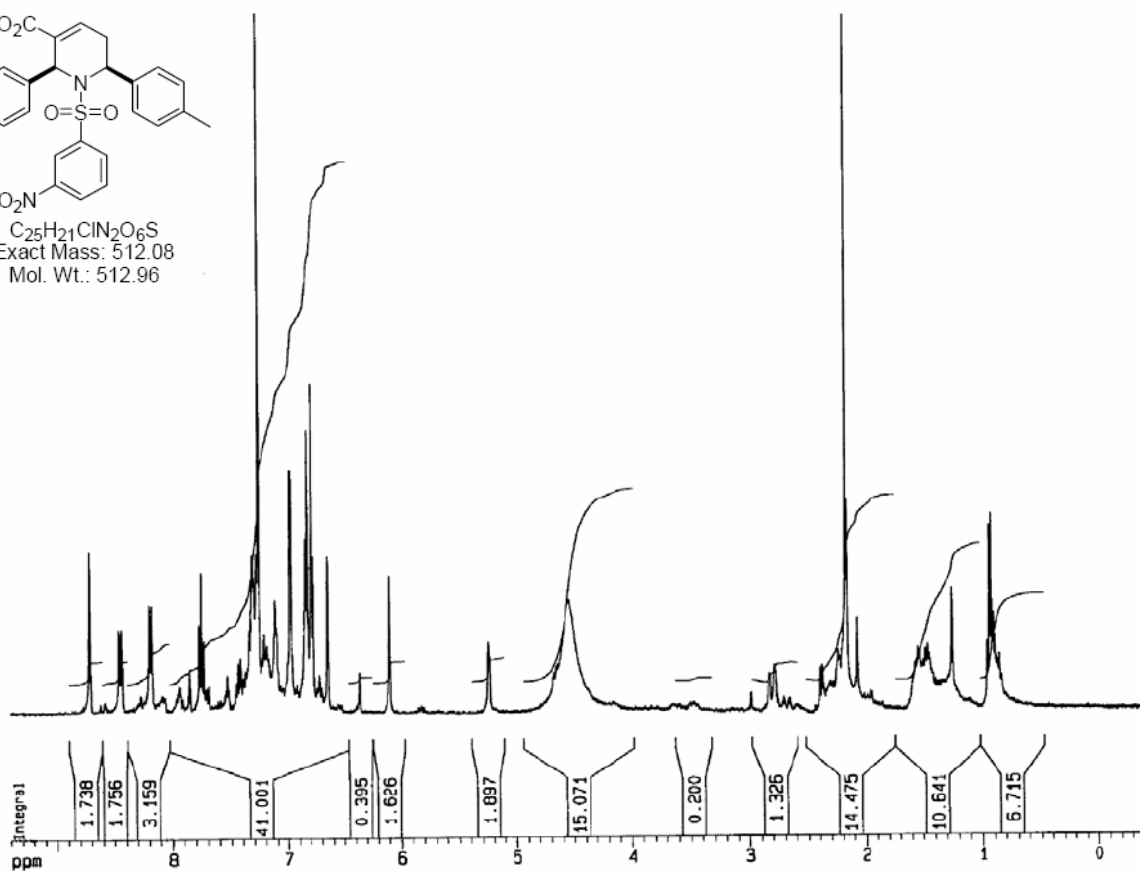


2-(3-Chlorophenyl)-1-(3-nitrobenzenesulfonyl)-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C45)

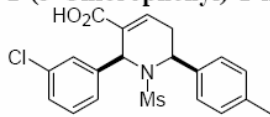
Not included



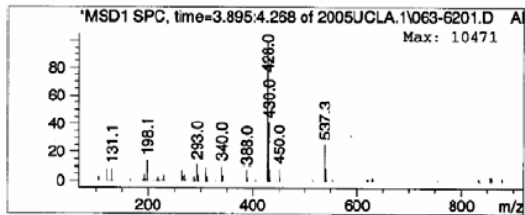
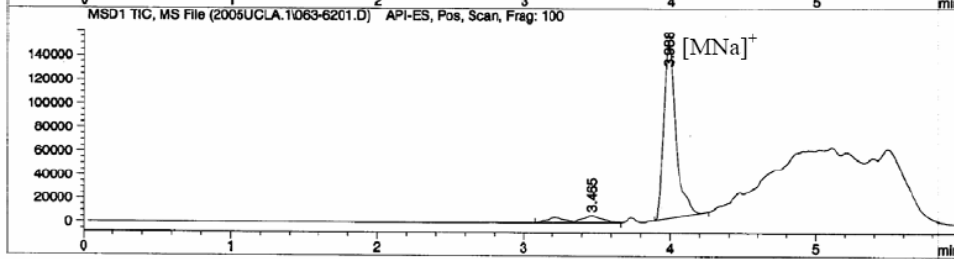
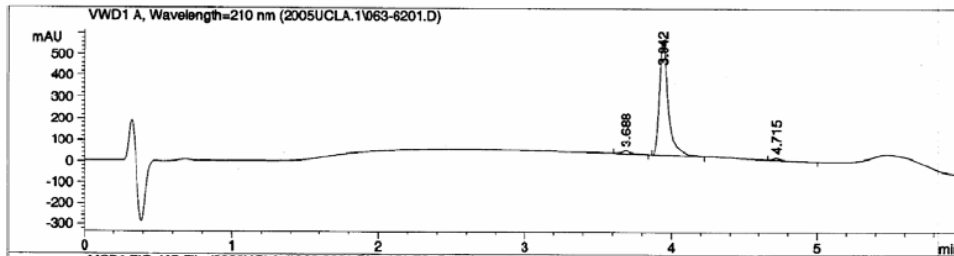
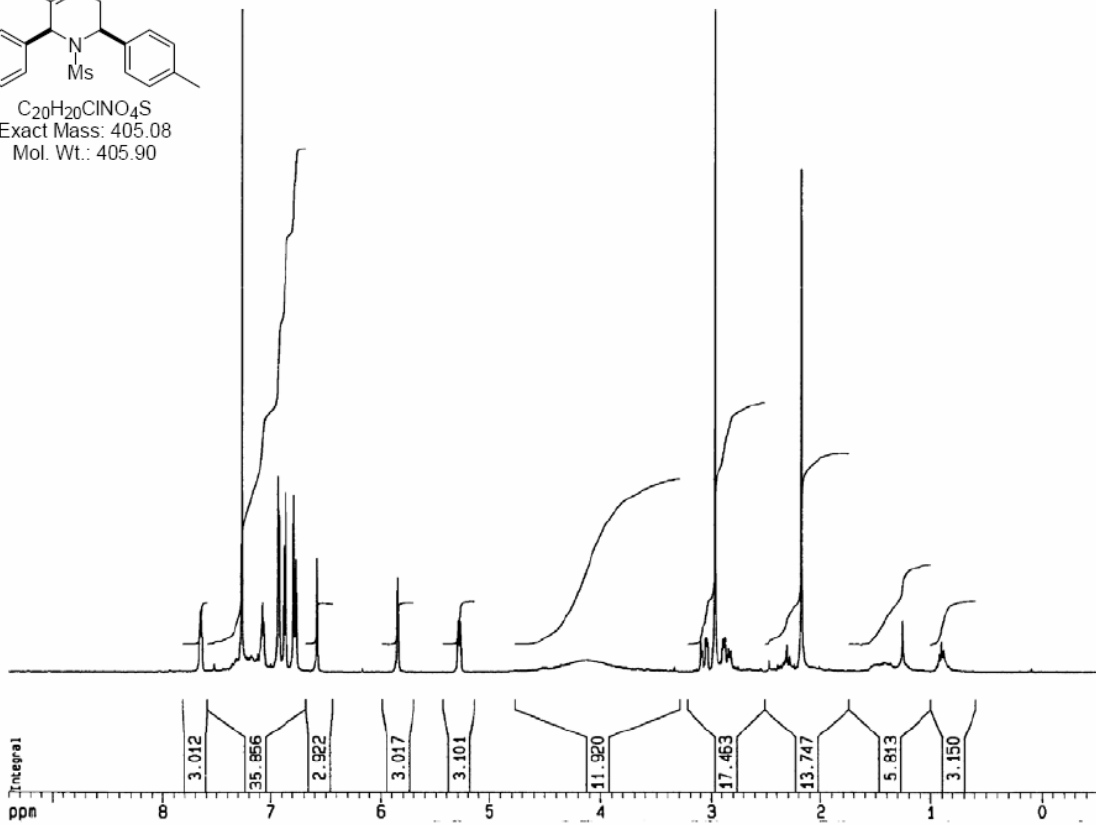
C₂₅H₂₁ClN₂O₆S
Exact Mass: 512.08
Mol. Wt.: 512.96



2-(3-Chlorophenyl)-1-methanesulfonyl-6-(*p*-tolyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B05C46)

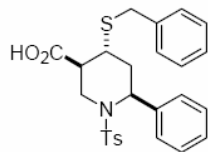


C₂₀H₂₀ClNO₄S
 Exact Mass: 405.08
 Mol. Wt.: 405.90

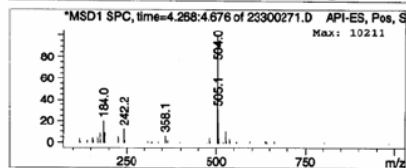
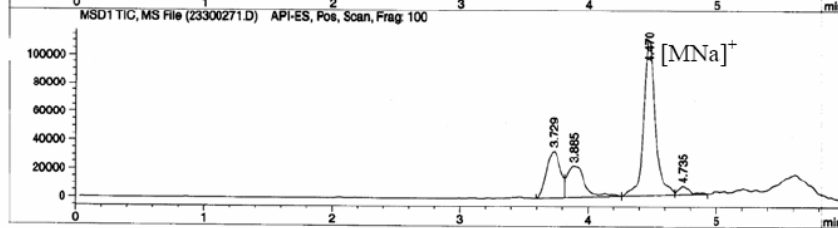
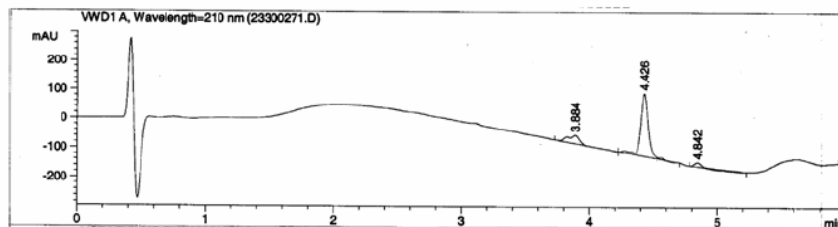
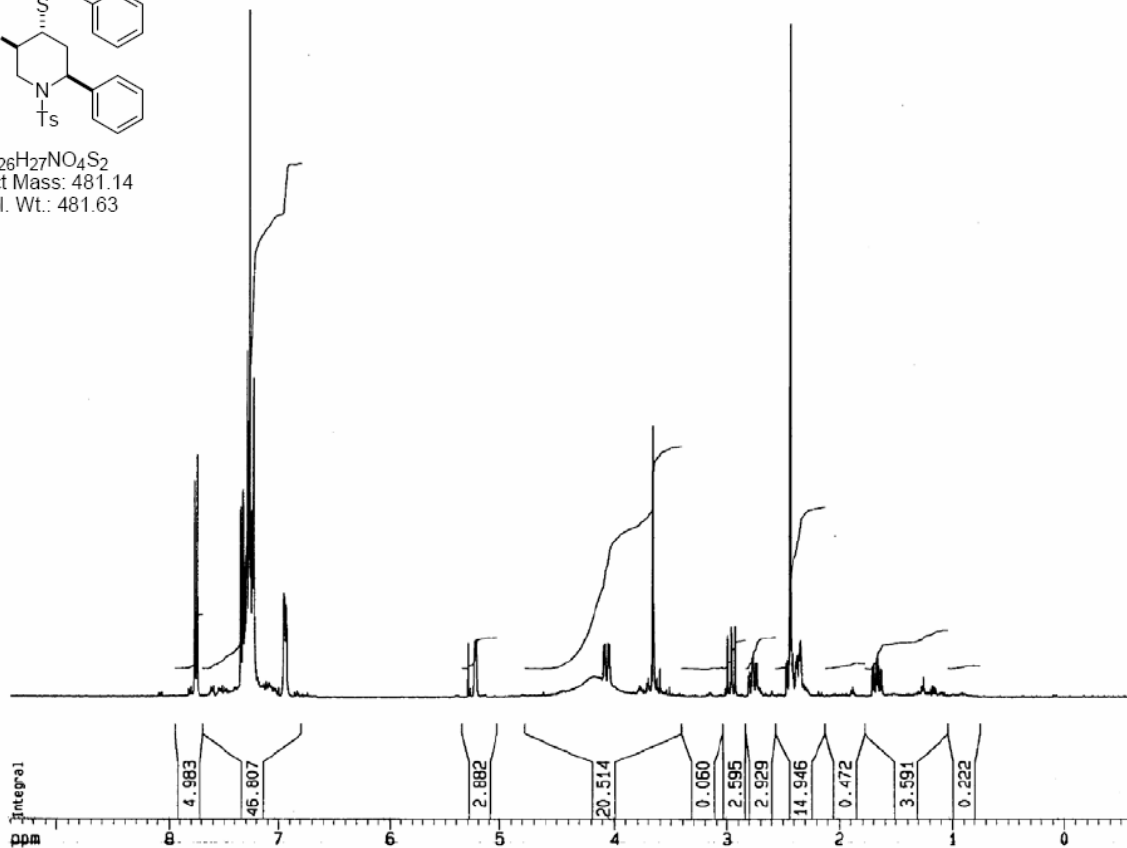


Spectral data for Table 12

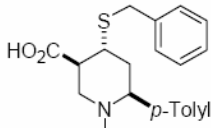
4-Benzylsulfanyl-6-phenyl-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C01E06)



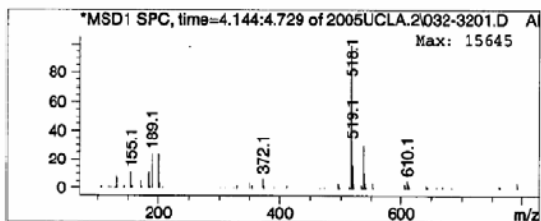
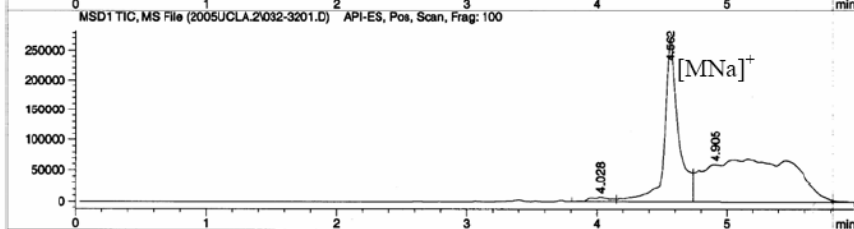
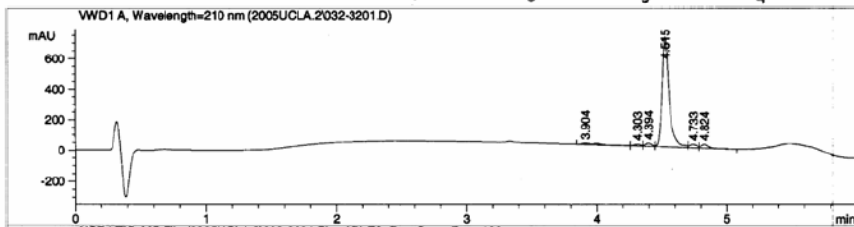
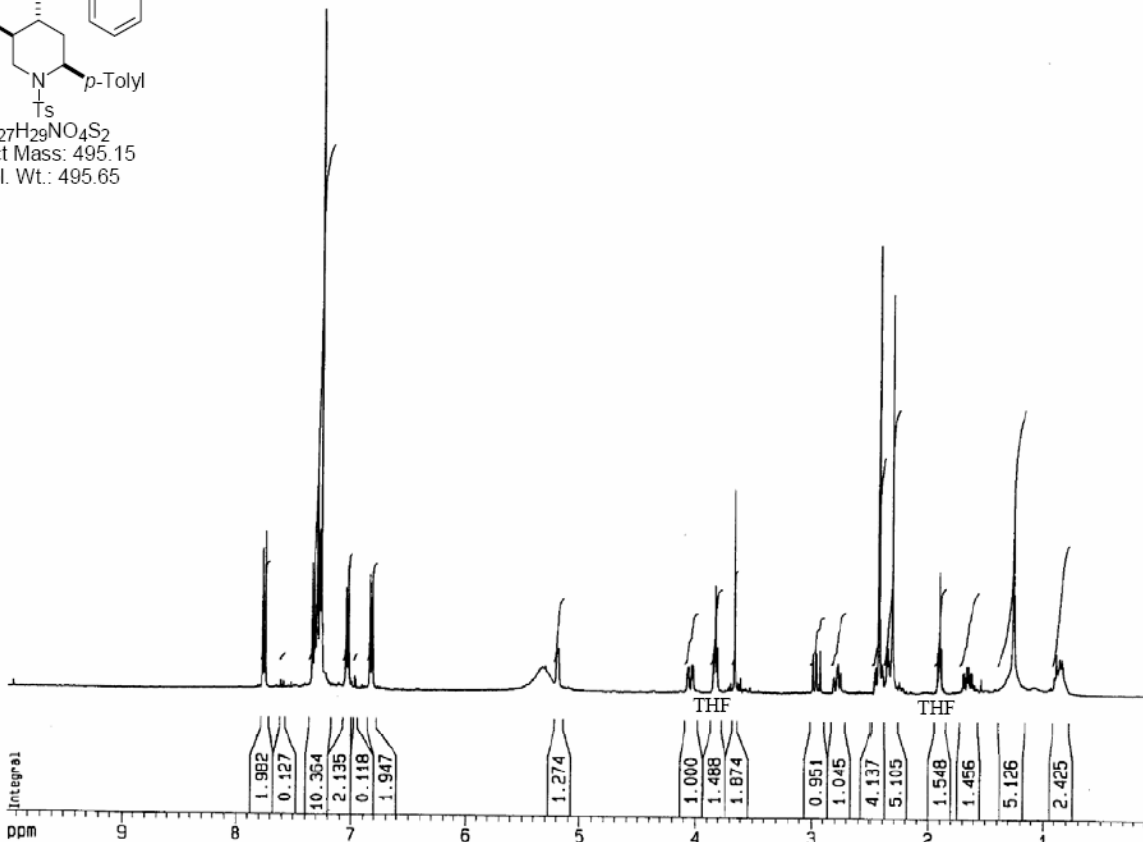
C₂₆H₂₇NO₄S₂
 Exact Mass: 481.14
 Mol. Wt.: 481.63



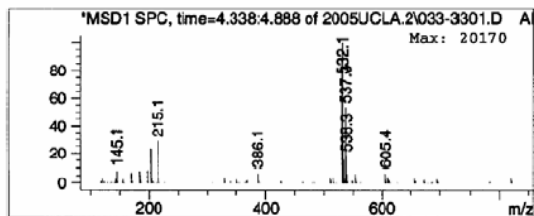
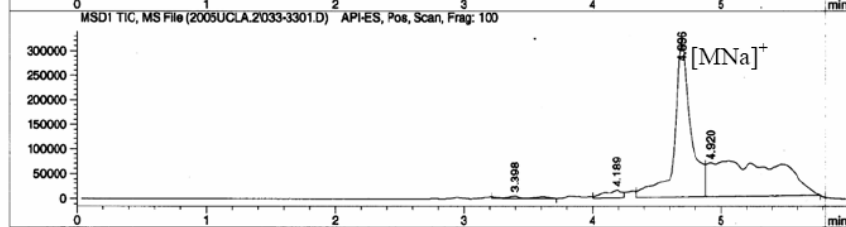
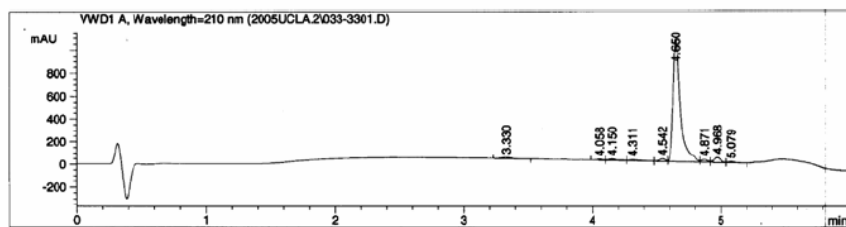
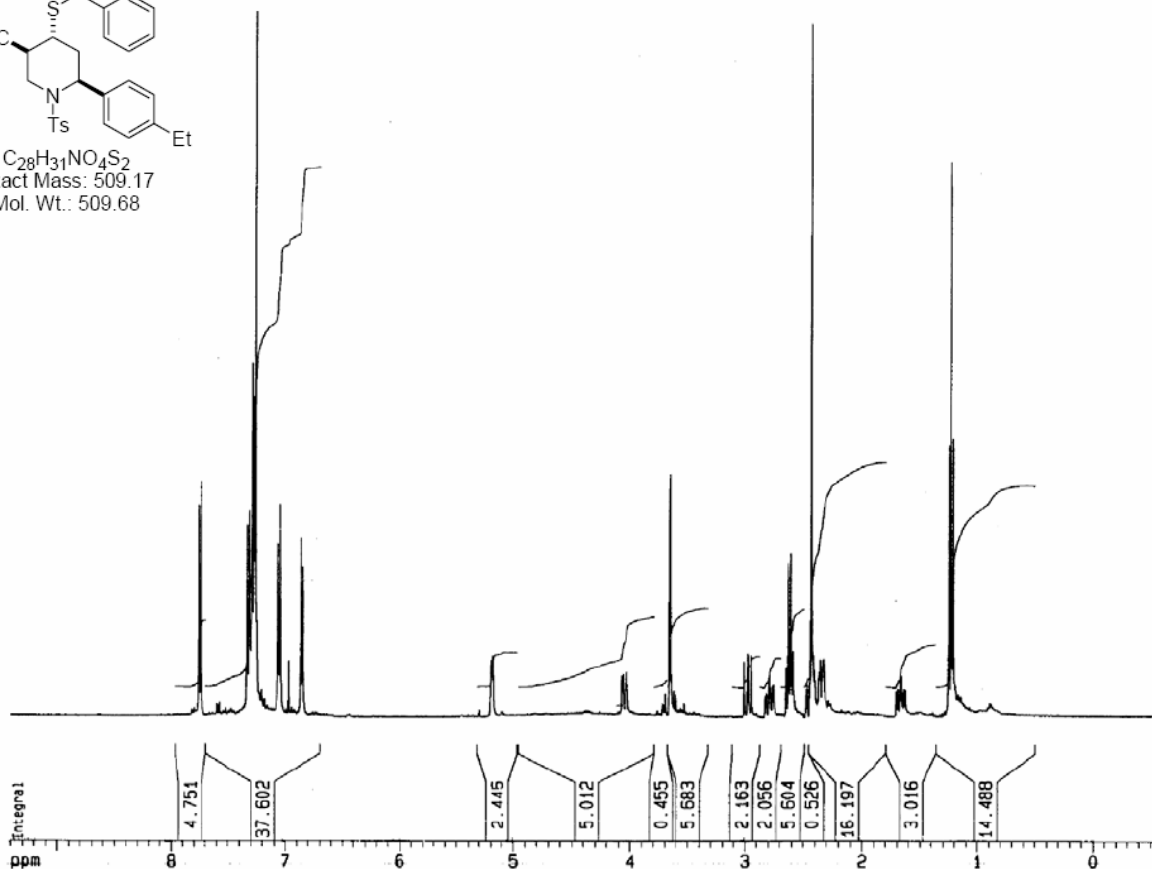
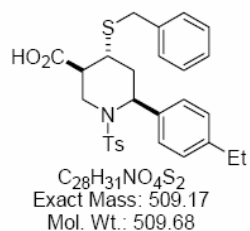
4-Benzylsulfanyl-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C02E06)



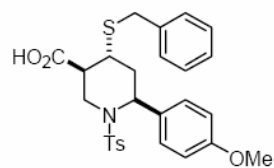
C₂₇H₂₉NO₄S₂
 Exact Mass: 495.15
 Mol. Wt.: 495.65



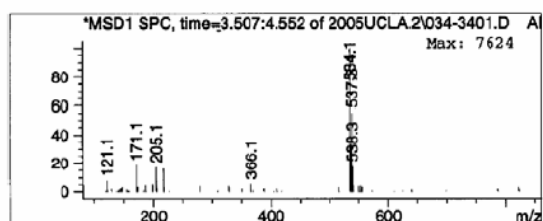
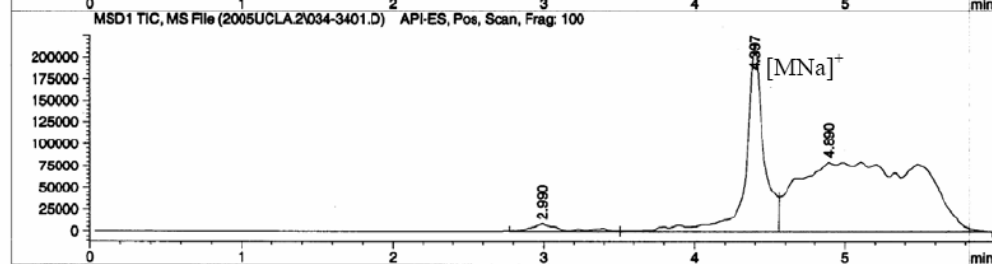
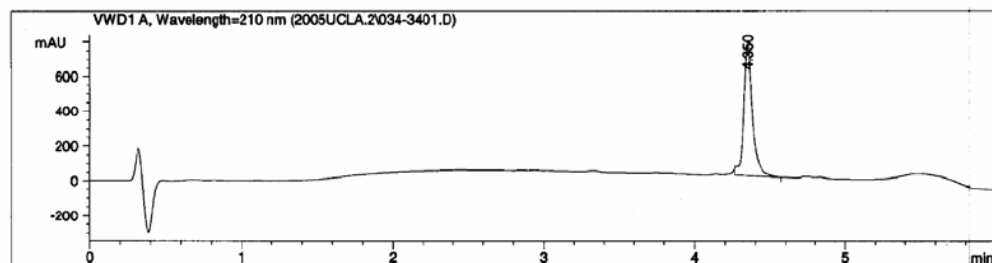
4-Benzylsulfanyl-6-(4-ethylphenyl)-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C03E06)



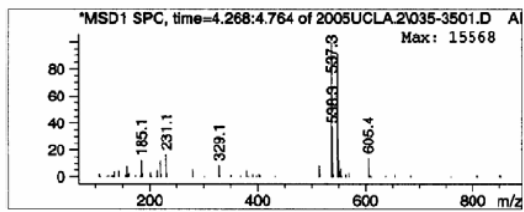
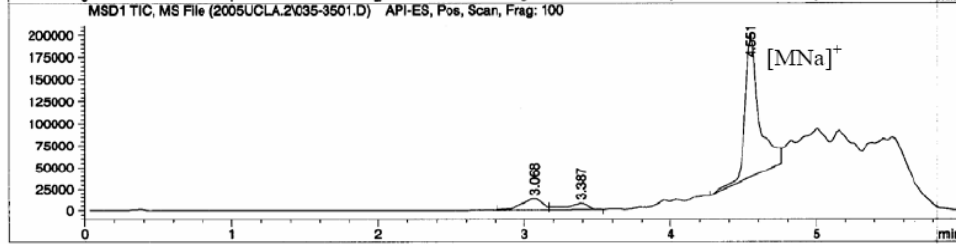
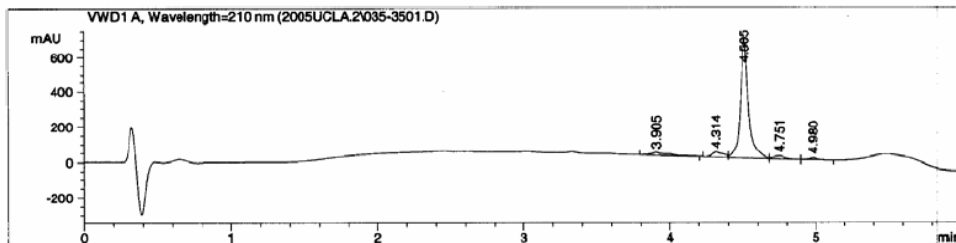
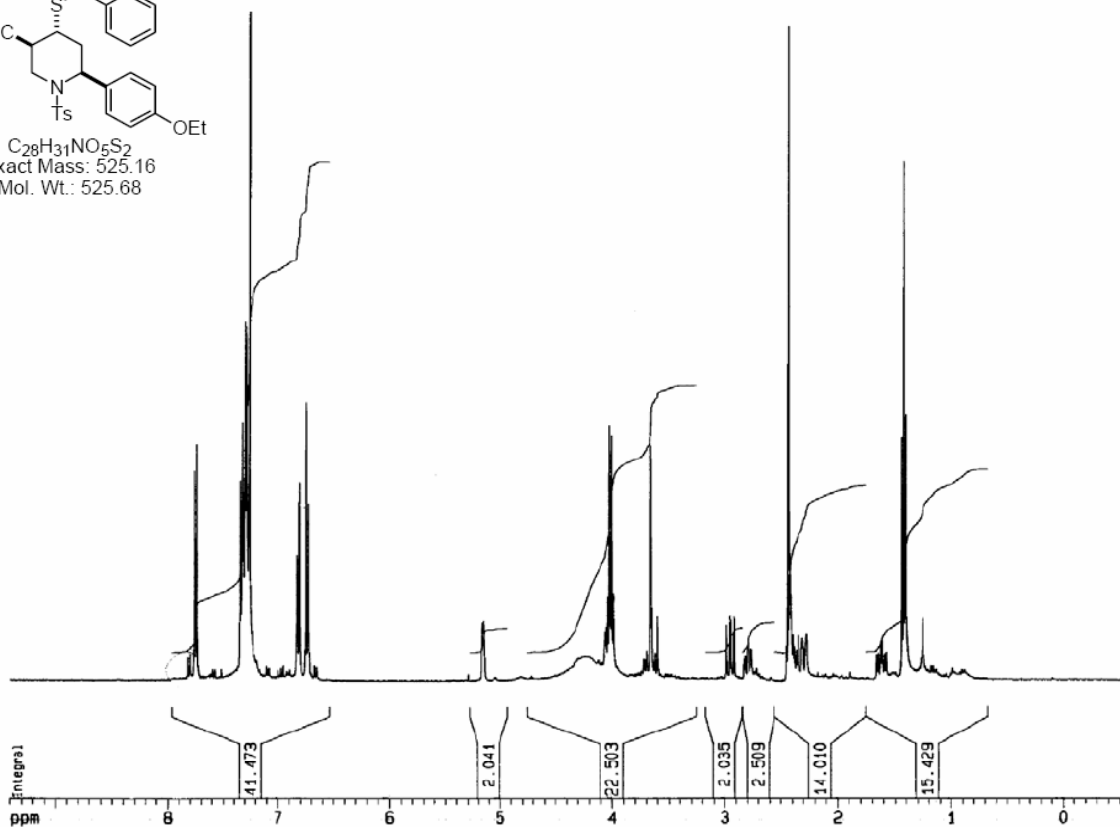
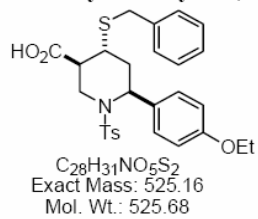
4-Benzylsulfanyl-6-(4-methoxyphenyl)-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C04E06)



C₂₇H₂₉NO₅S₂
Exact Mass: 511.15
Mol. Wt.: 511.65

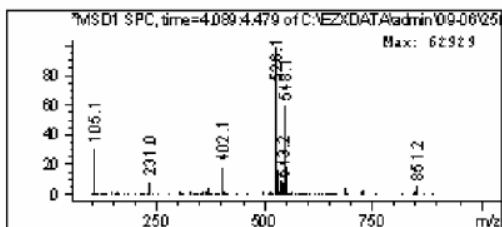
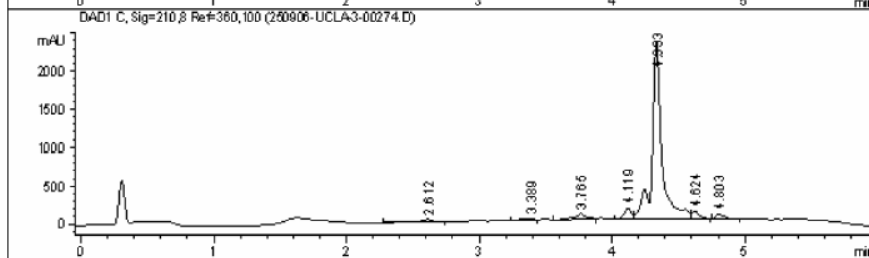
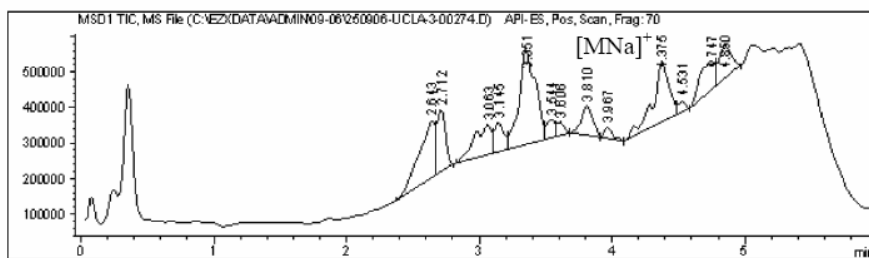
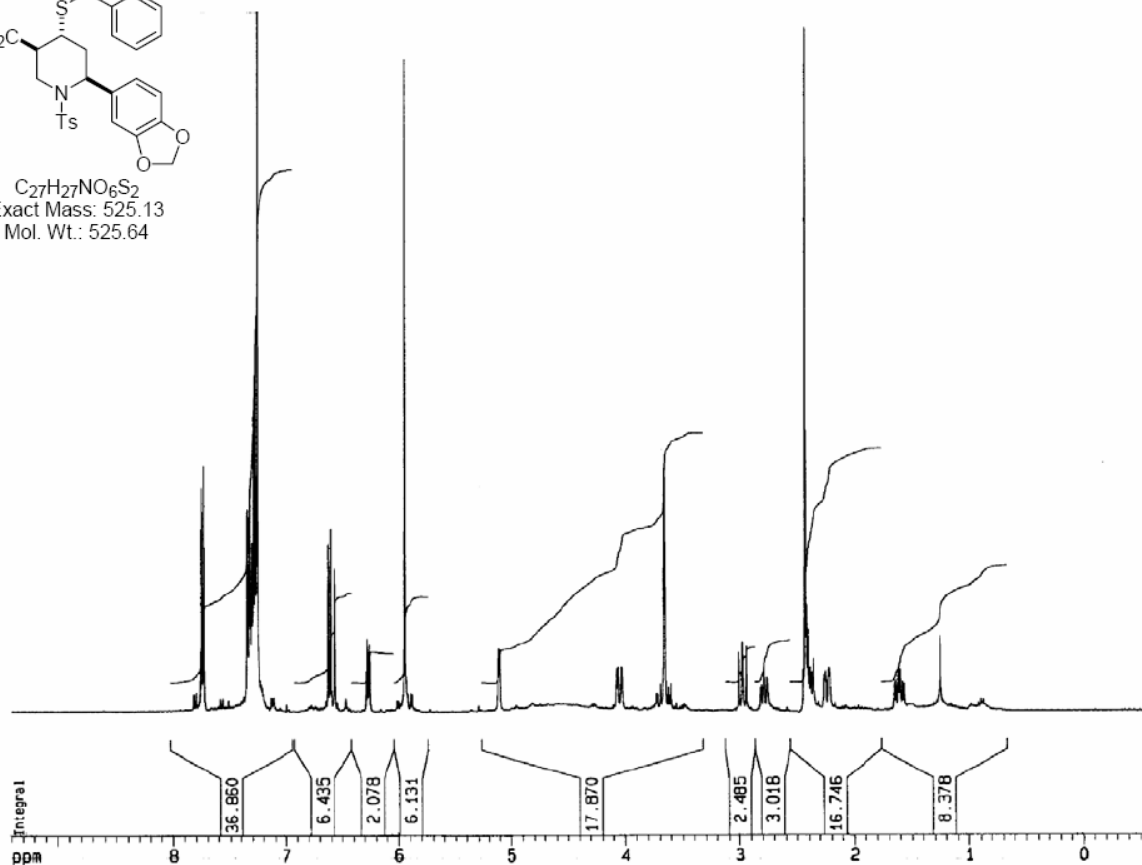
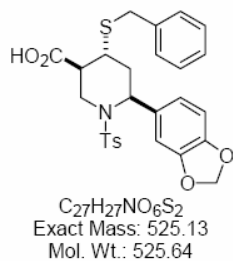


4-Benzylsulfanyl-6-(4-ethoxyphenyl)-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C05E06)



Component 1: Peak at Scan 255.9. Top ions are 548 549 231

6-(Benzo[1,3]dioxol-5-yl)-4-benzylsulfanyl-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C06E06)

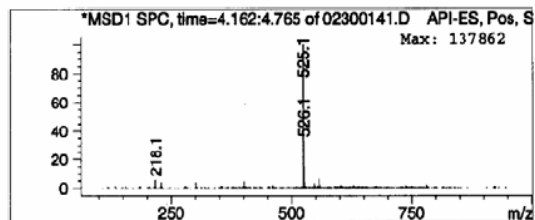
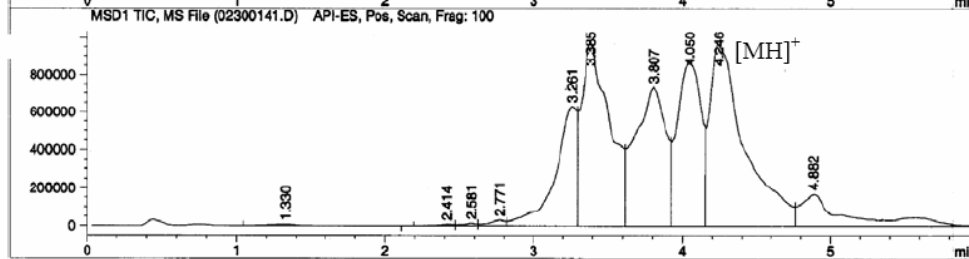
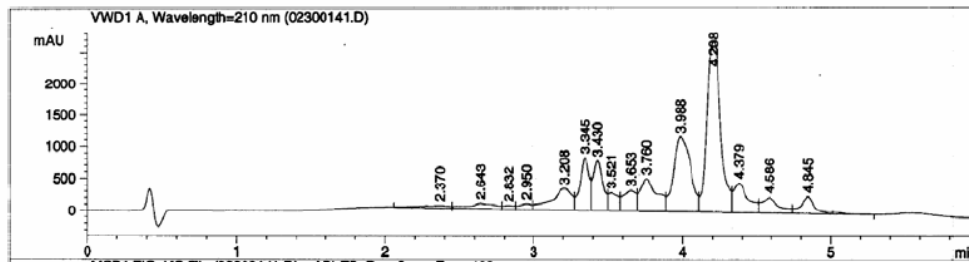
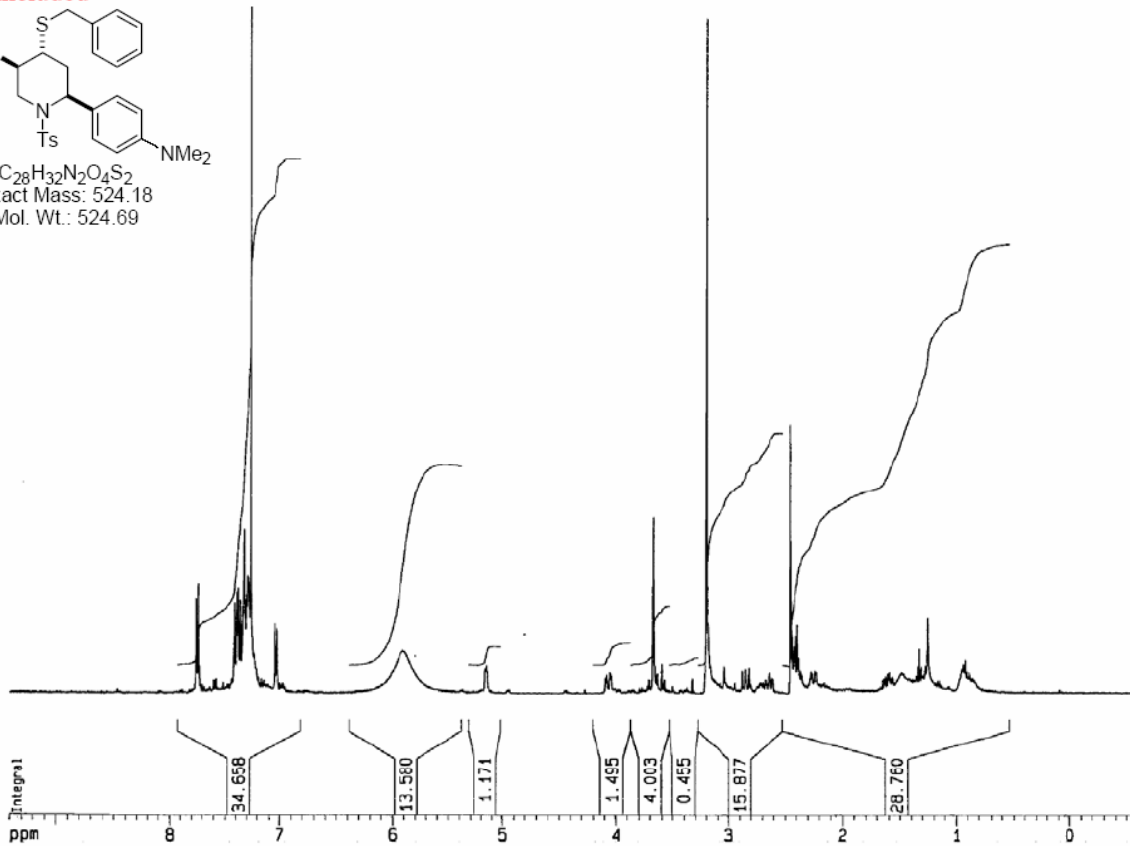
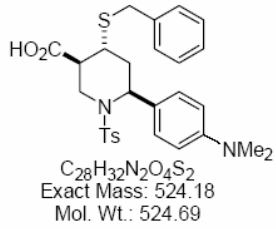


4-Benzylsulfanyl-6-(4-dimethylaminophenyl)-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid

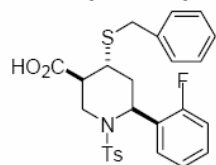
acid

(B01C07E06)

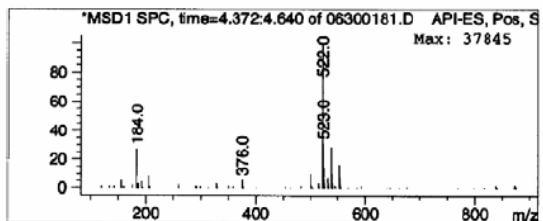
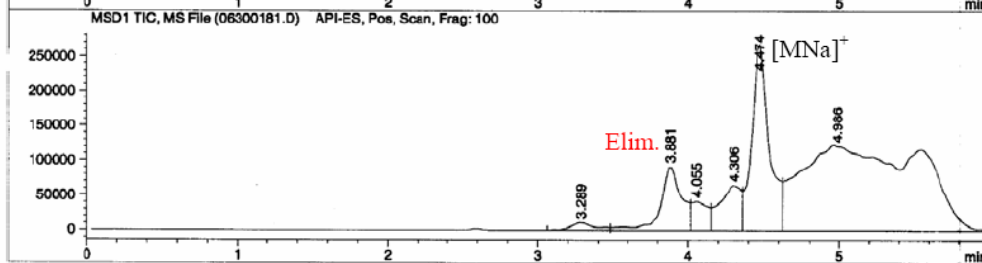
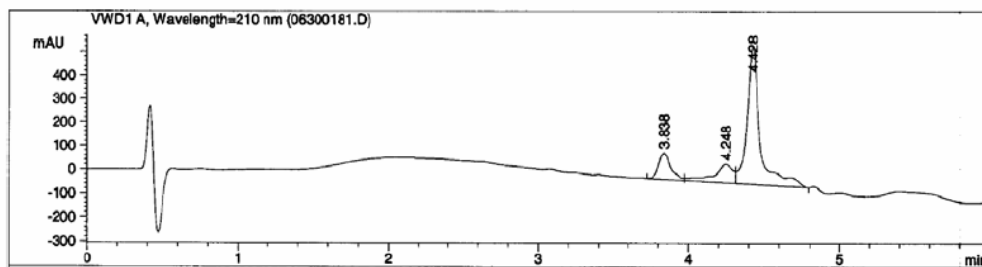
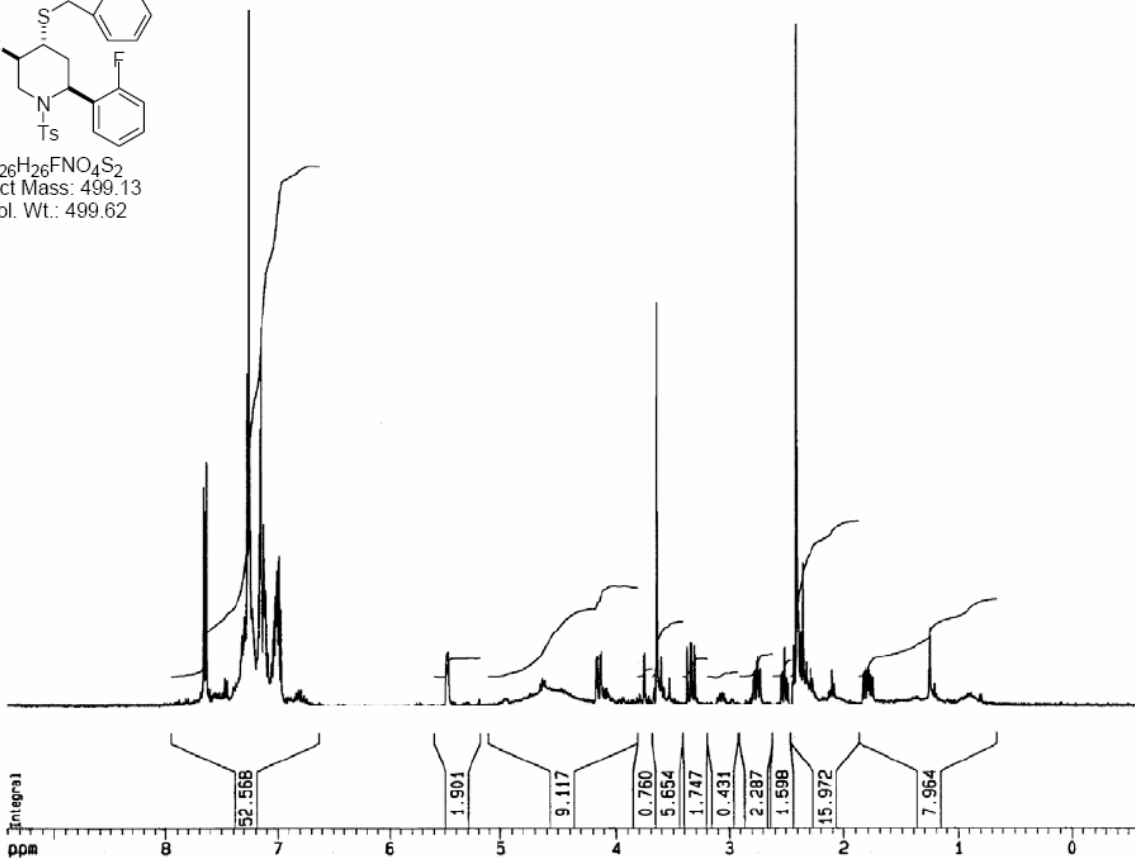
Not included



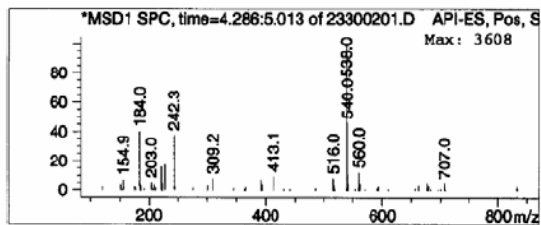
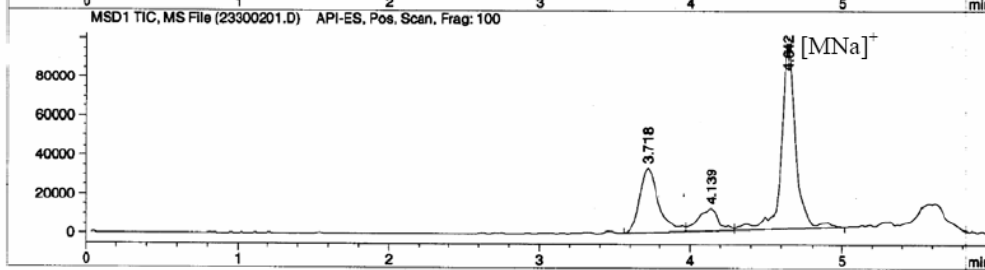
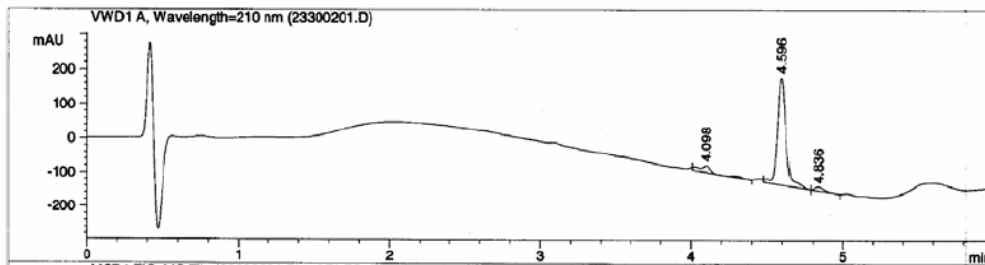
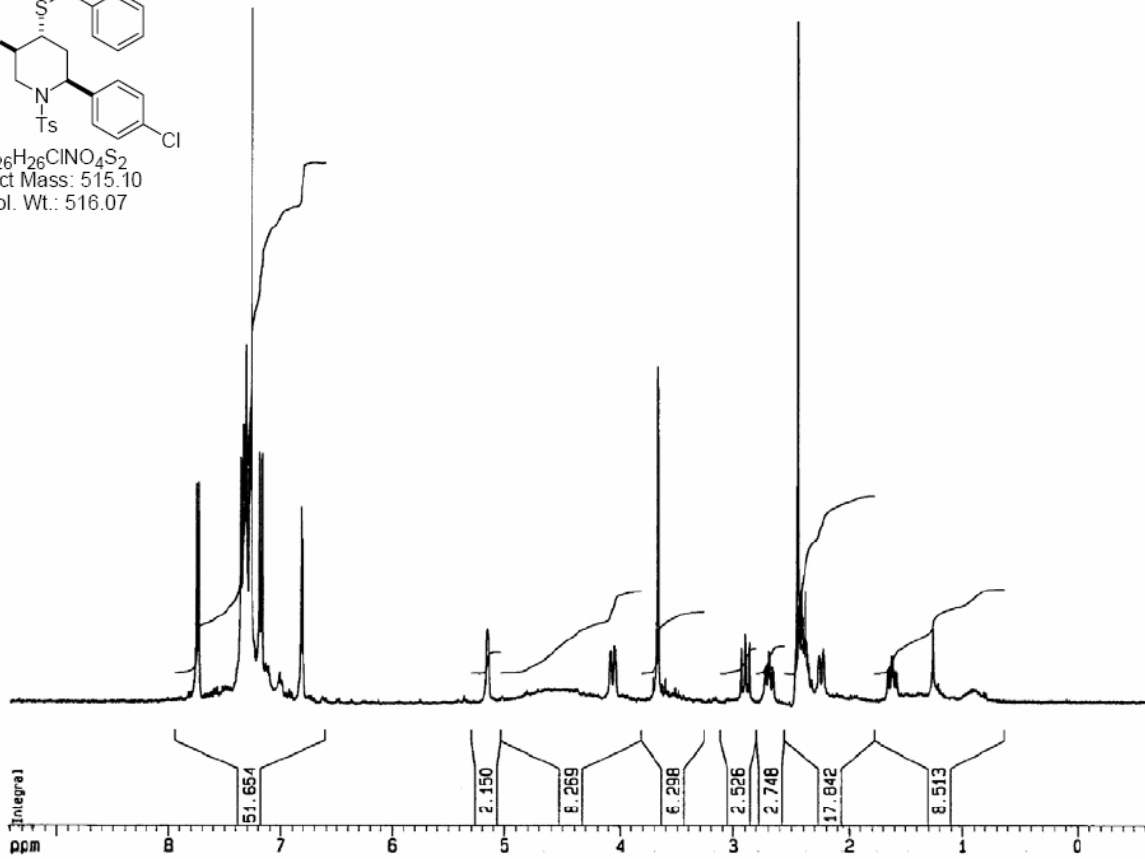
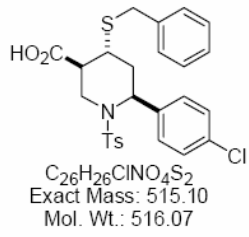
4-Benzylsulfanyl-6-(2-fluorophenyl)-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C10E06)



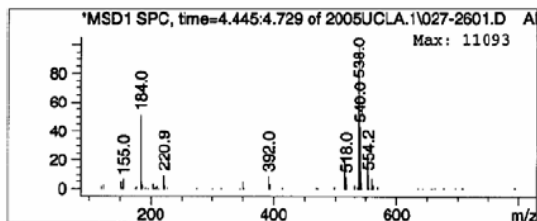
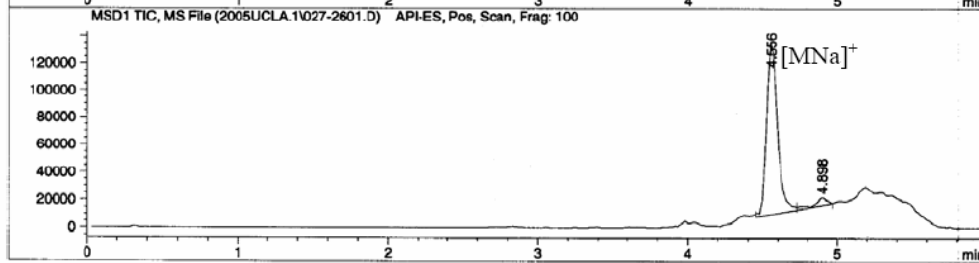
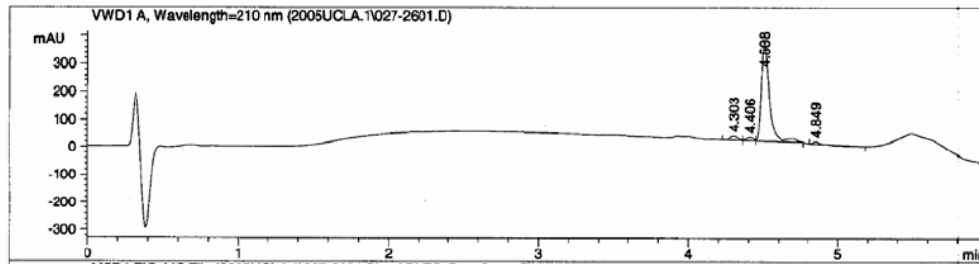
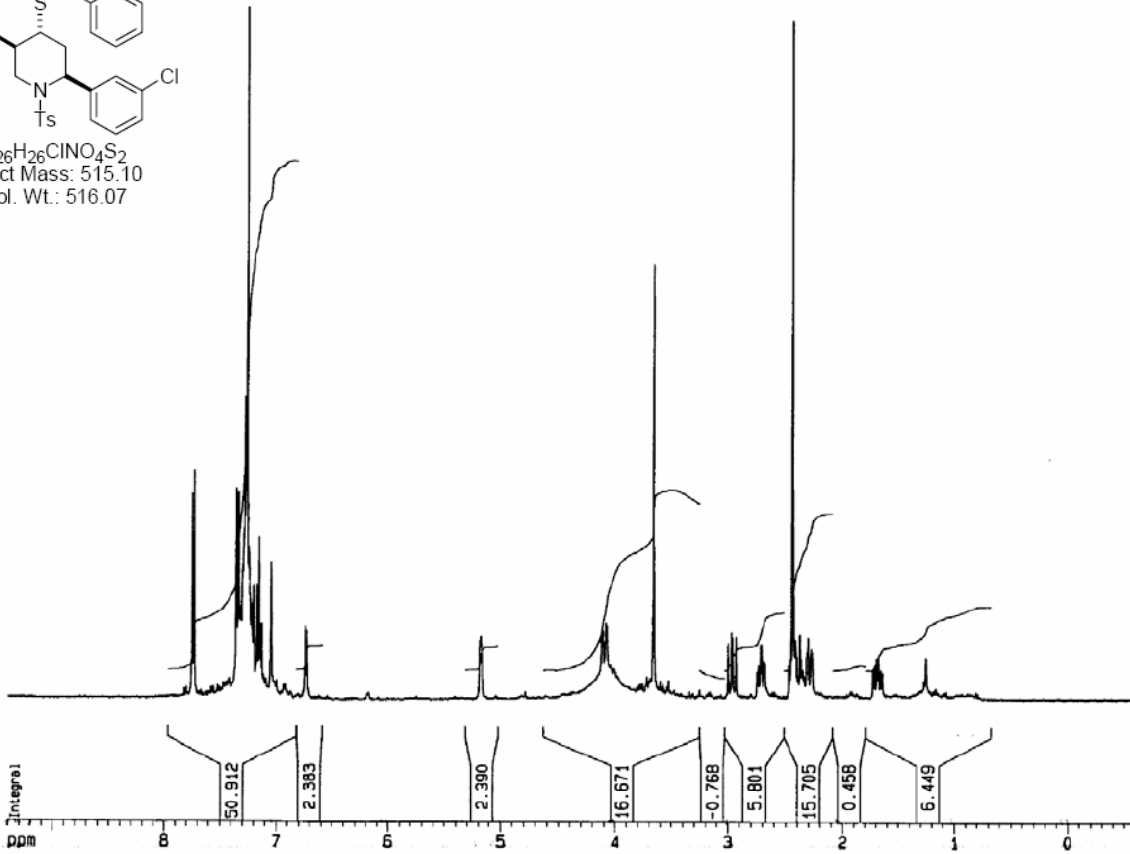
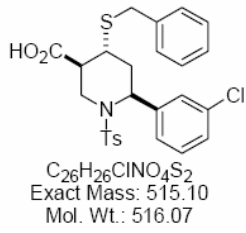
C₂₆H₂₆FNO₄S₂
 Exact Mass: 499.13
 Mol. Wt.: 499.62



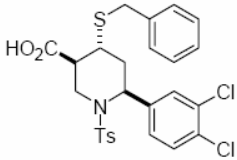
4-Benzylsulfanyl-6-(4-chlorophenyl)-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C11E06)



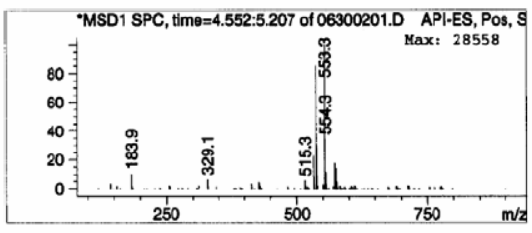
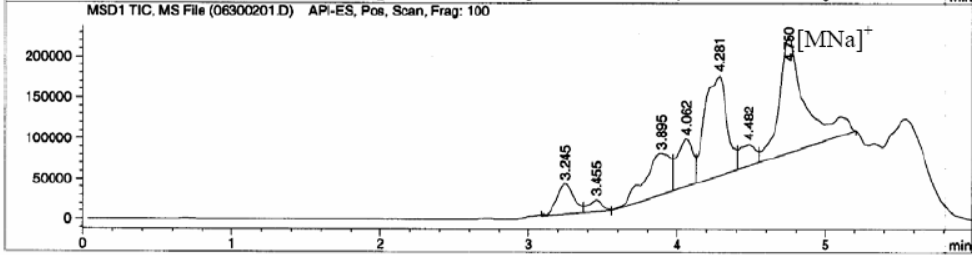
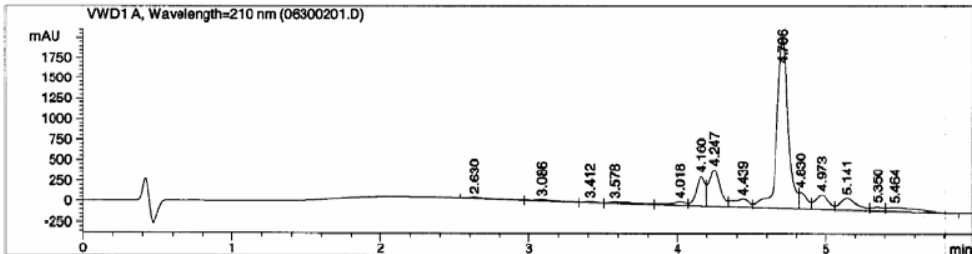
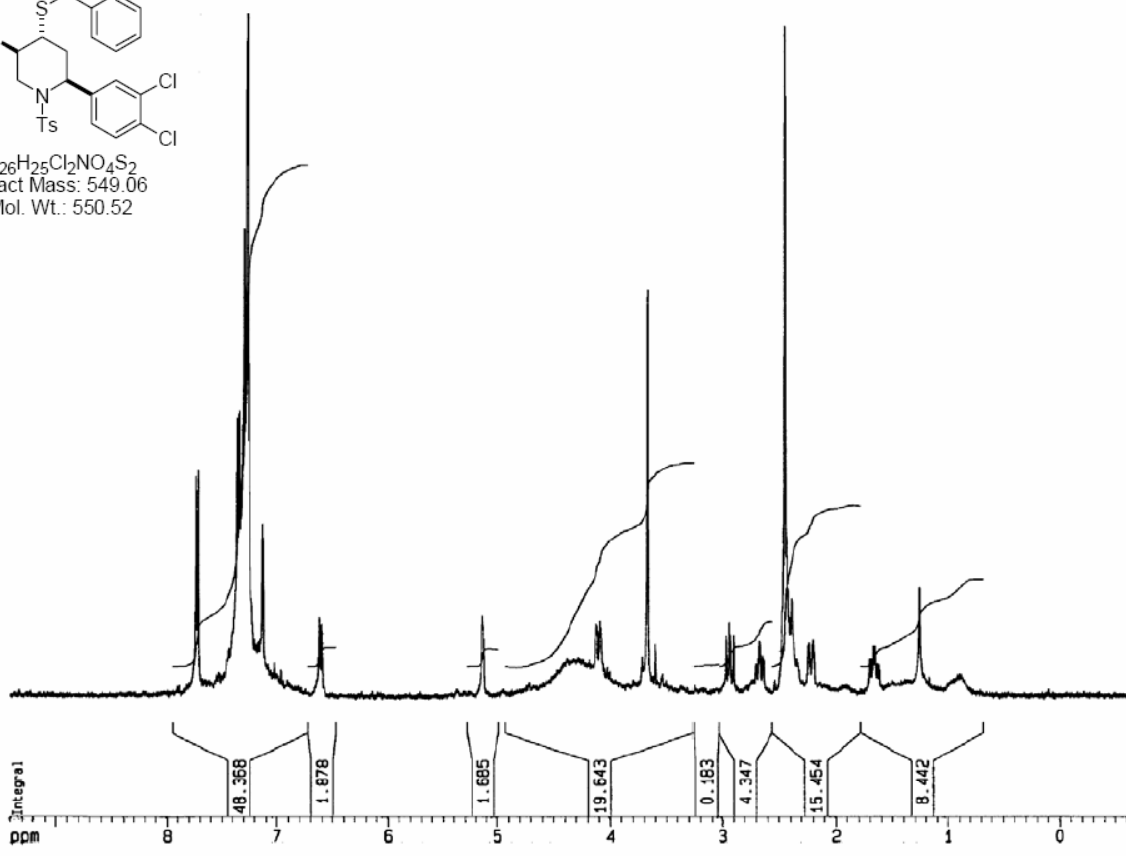
4-Benzylsulfanyl-6-(3-chlorophenyl)-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C12E06)



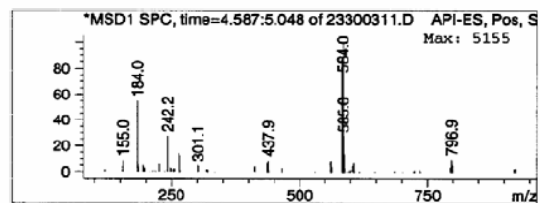
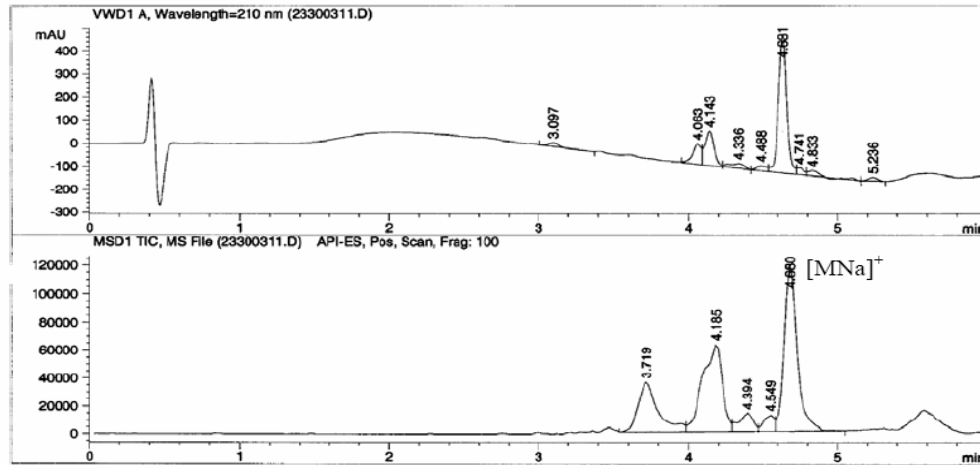
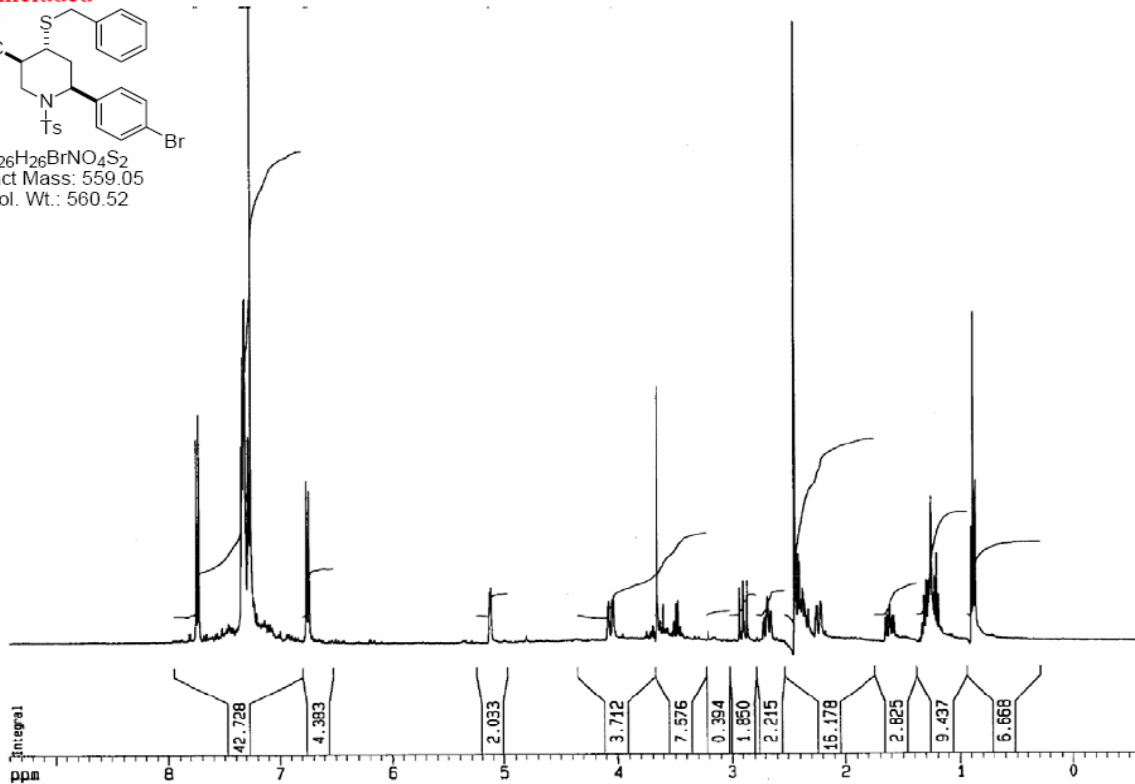
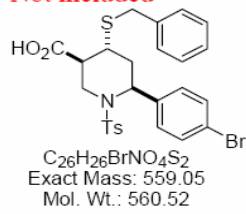
4-Benzylsulfanyl-6-(3,4-dichlorophenyl)-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C13E06)
Not included



C₂₆H₂₅Cl₂NO₄S₂
 Exact Mass: 549.06
 Mol. Wt.: 550.52

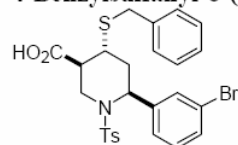


4-Benzylsulfanyl-6-(4-bromophenyl)-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C14E06)
Not included

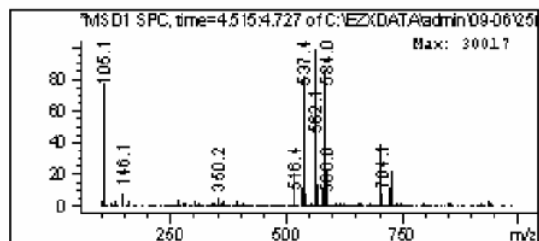
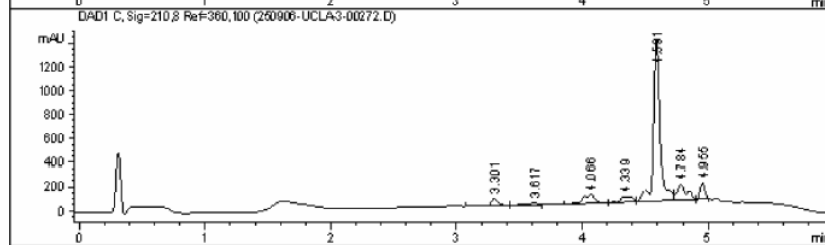
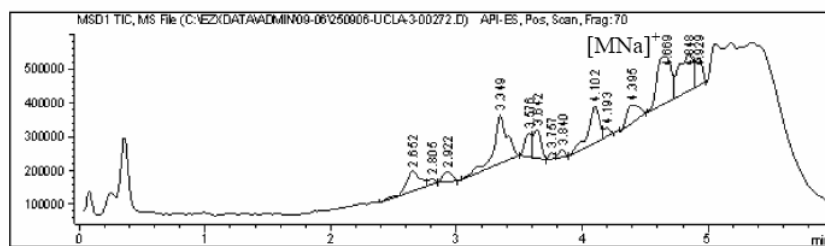
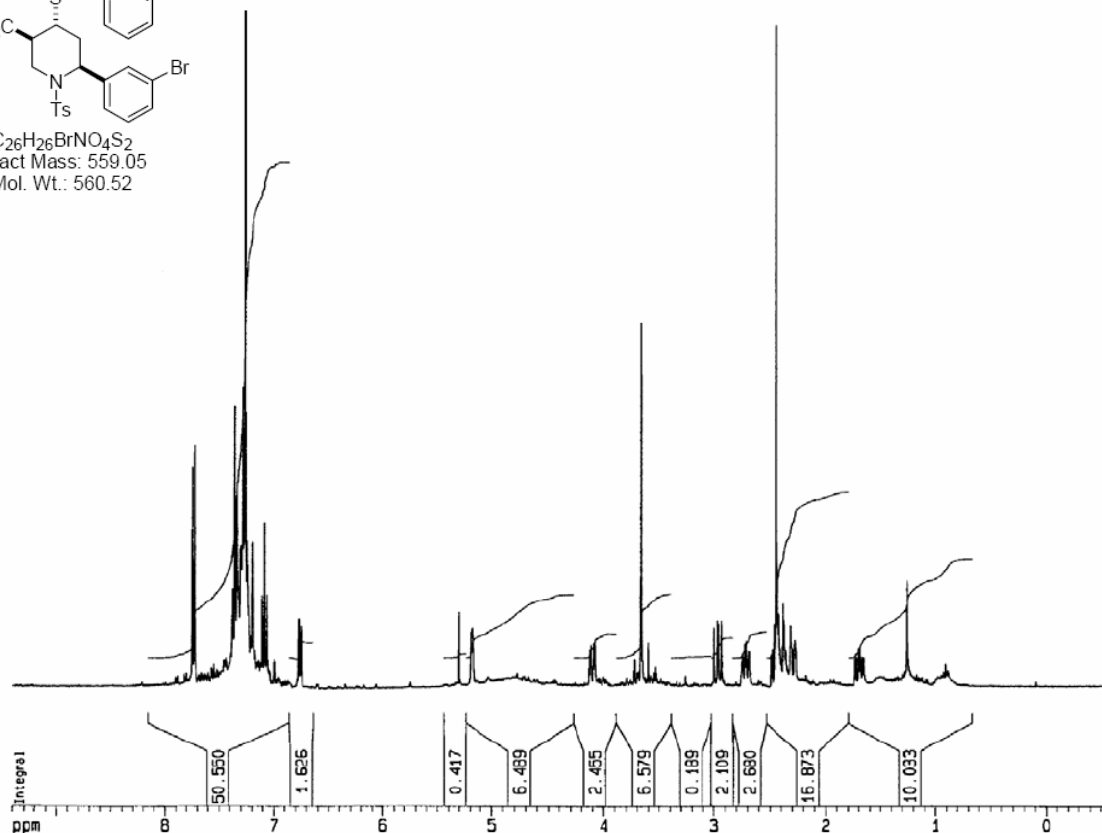


Component 3: Peak at Scan 261.6. Top ions are 584 582 583

4-Benzylsulfanyl-6-(3-bromophenyl)-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C15E06)



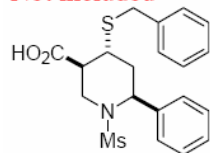
C₂₆H₂₆BrNO₄S₂
 Exact Mass: 559.05
 Mol. Wt.: 560.52



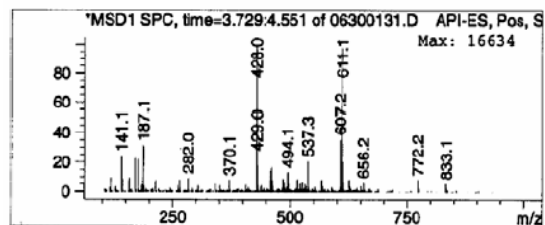
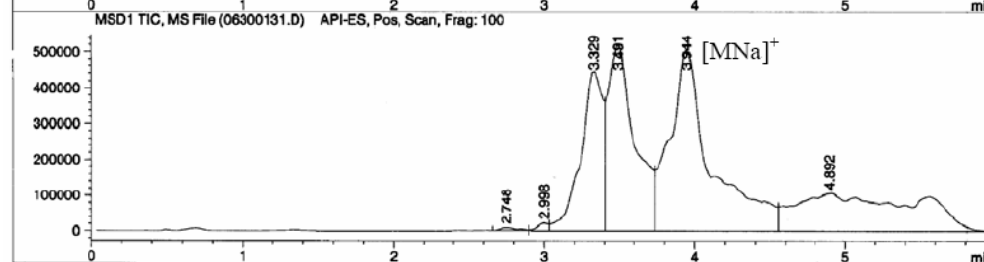
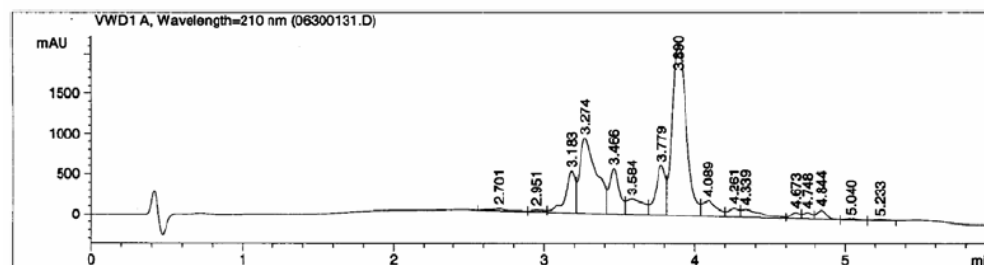
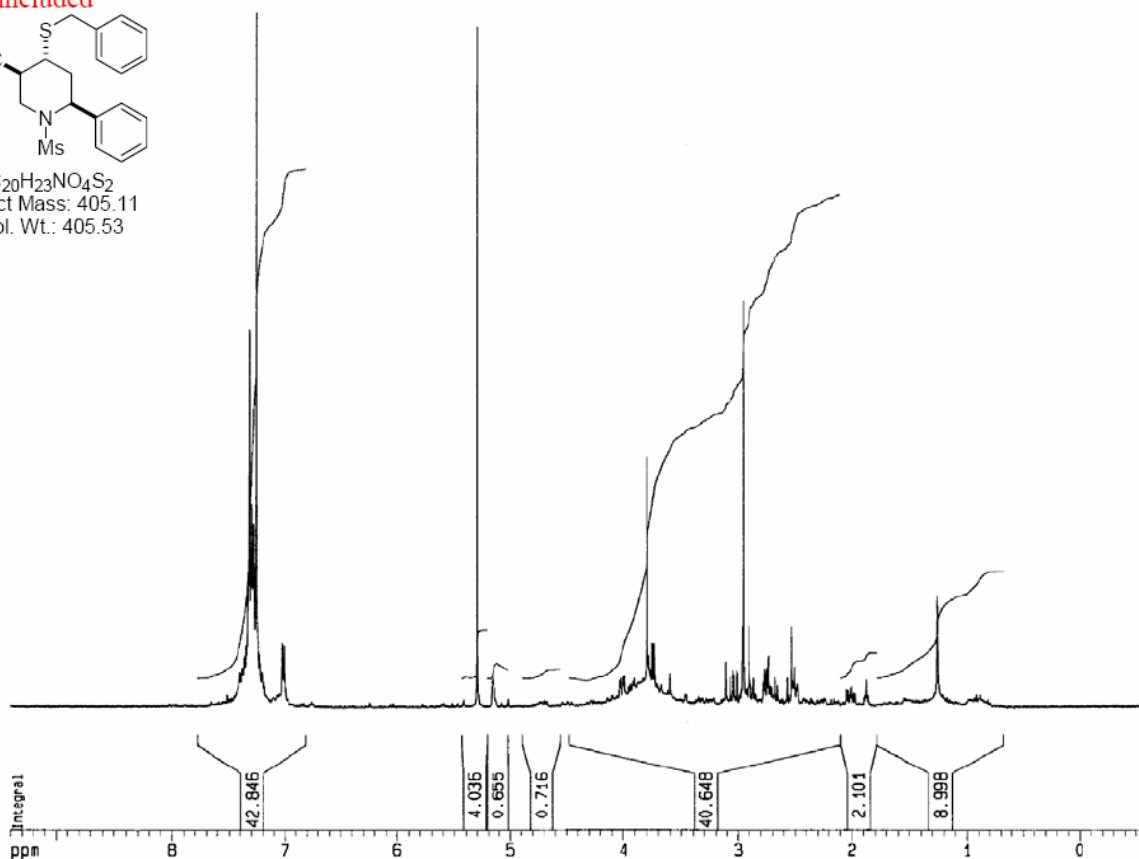
Component 2: Peak at Scan 260.8. Top ions are 562 560 584

4-Benzylsulfanyl-1-methanesulfonyl-6-phenylpiperidine-3-carboxylic acid (B01C19E06)

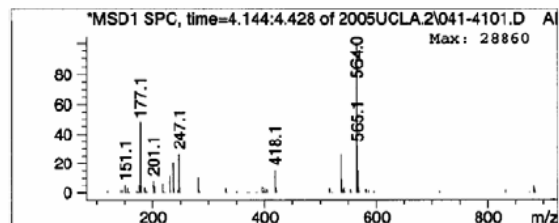
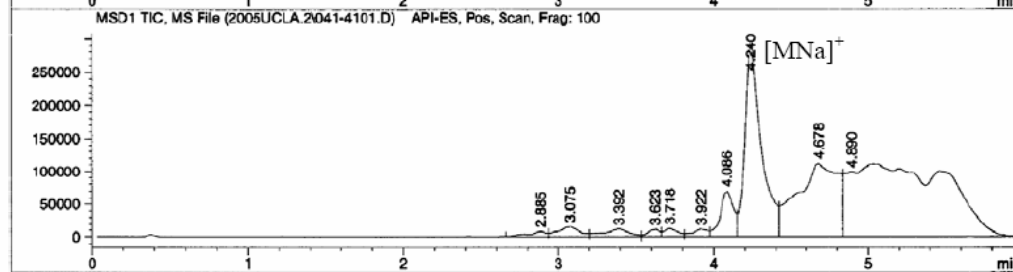
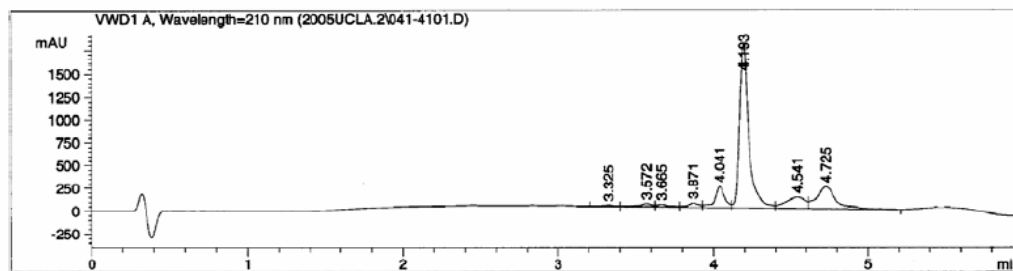
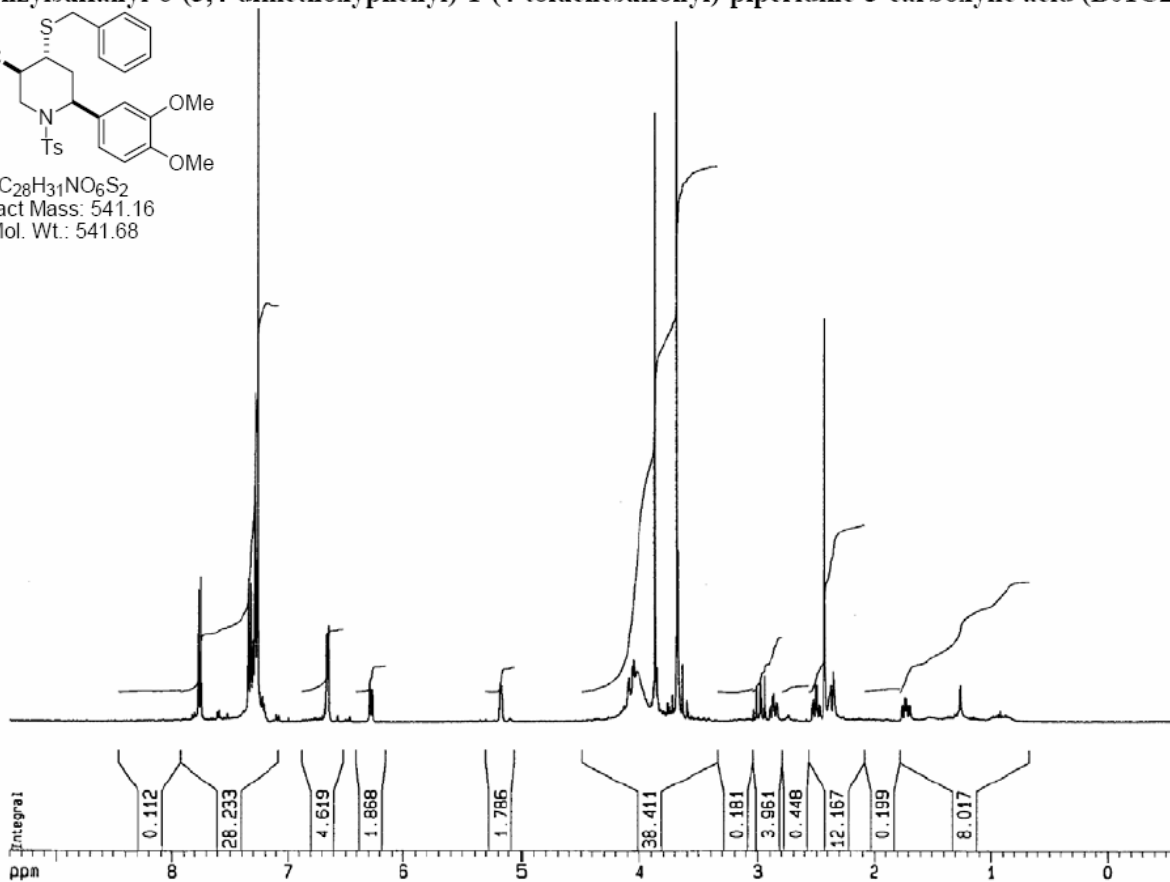
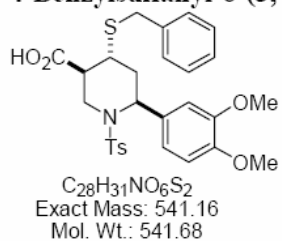
Not included



C₂₀H₂₃NO₄S₂
Exact Mass: 405.11
Mol. Wt.: 405.53

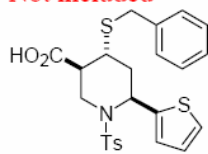


4-Benzylsulfanyl-6-(3,4-dimethoxyphenyl)-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C20E06)

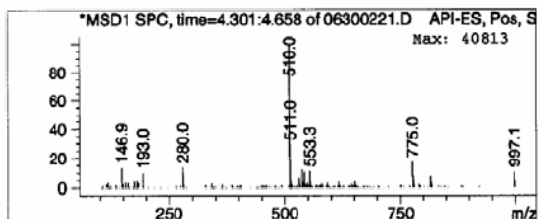
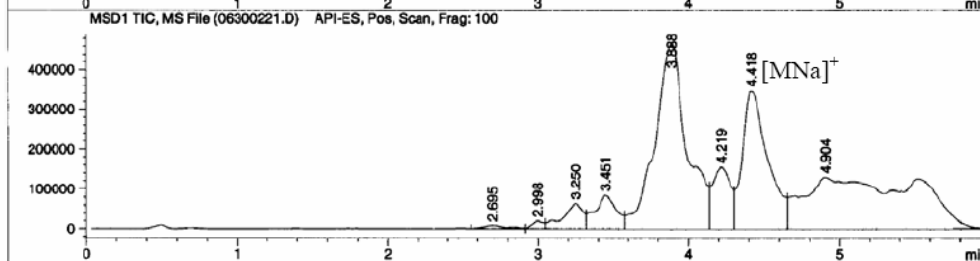
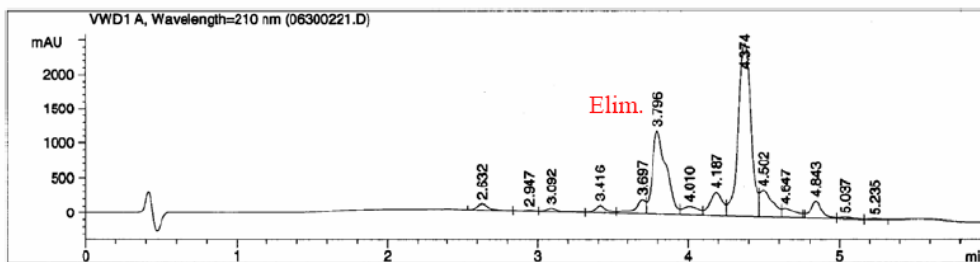
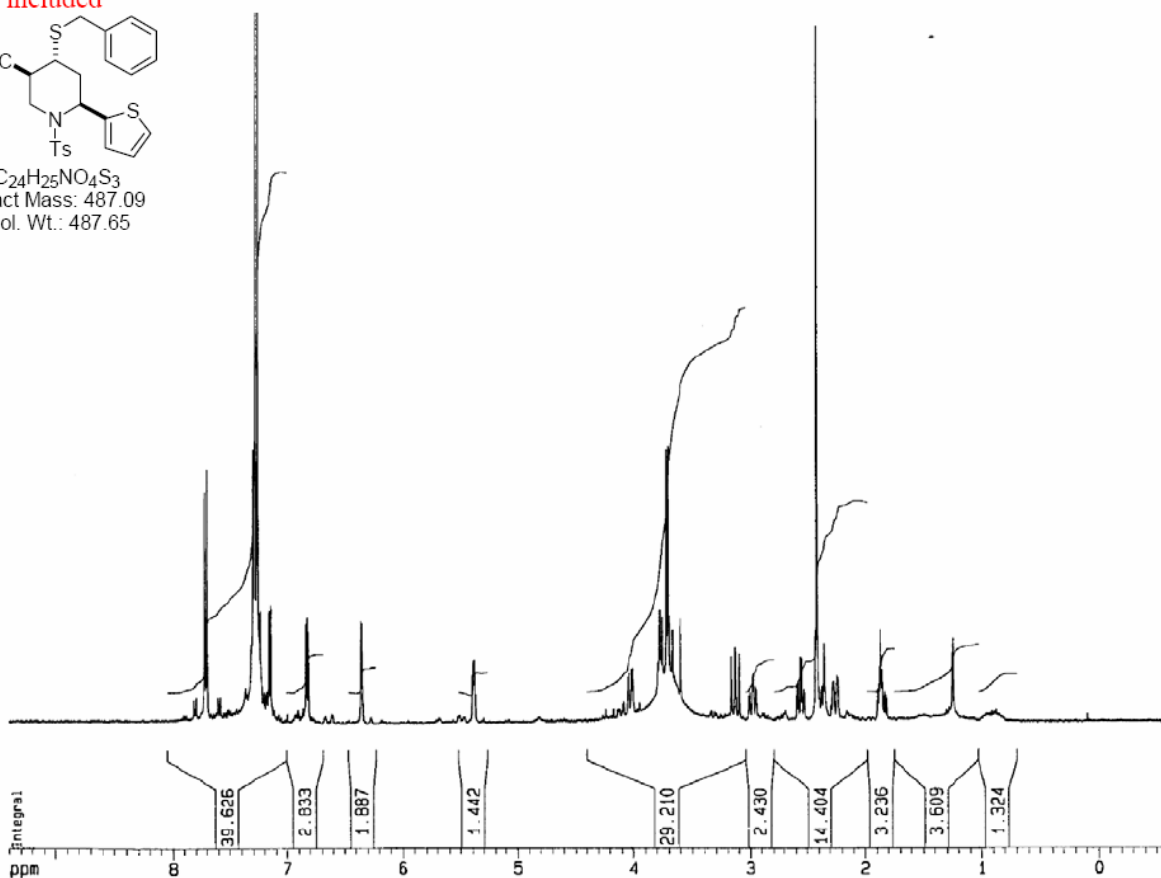


4-Benzylsulfanyl-6-(thiophen-2-yl)-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C21E06)

Not included

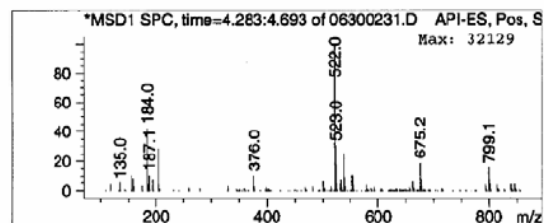
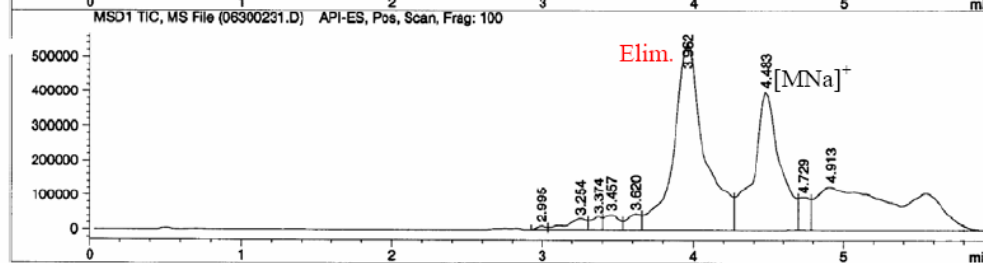
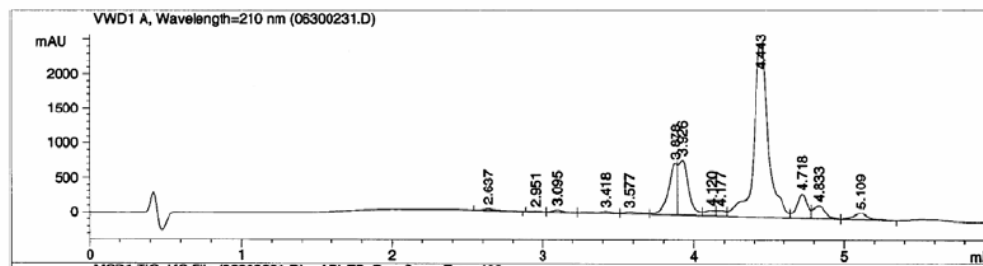
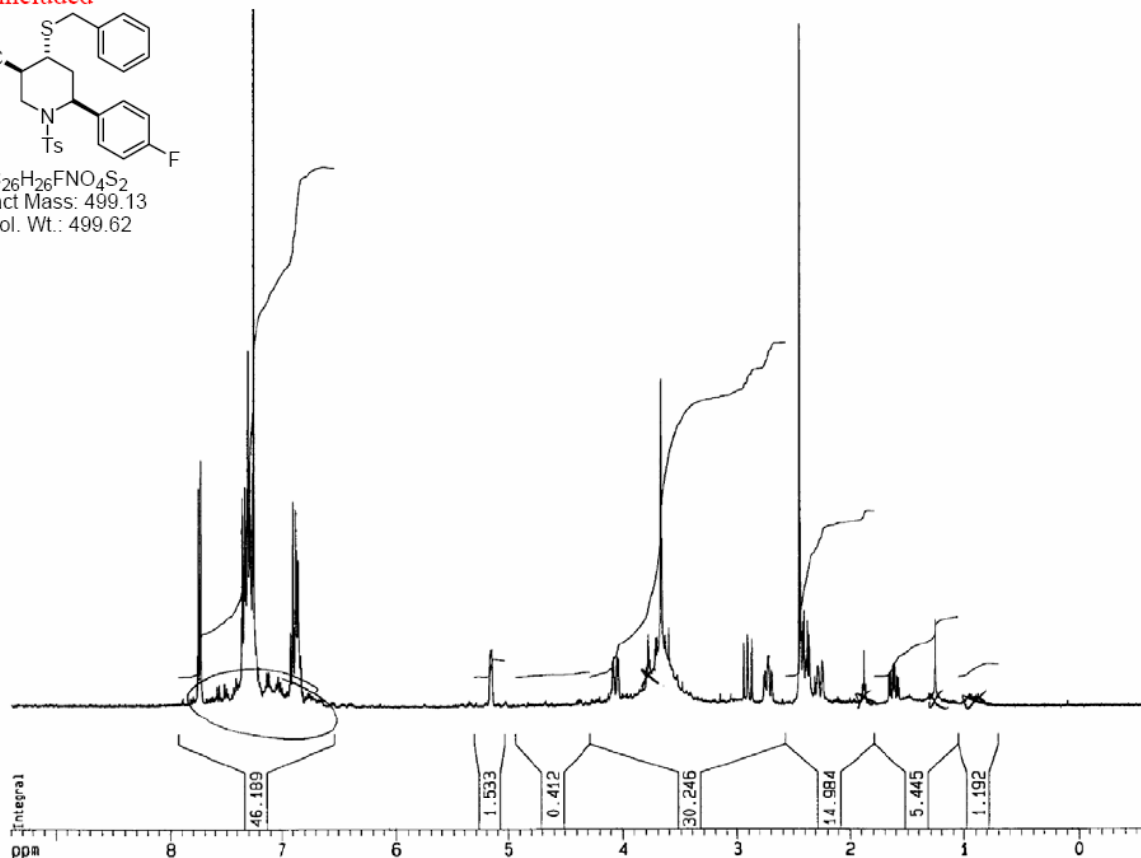
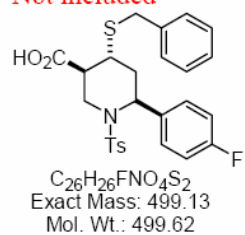


C₂₄H₂₅NO₄S₃
Exact Mass: 487.09
Mol. Wt.: 487.65

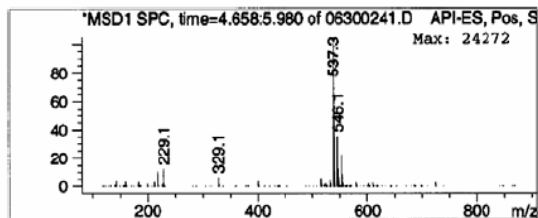
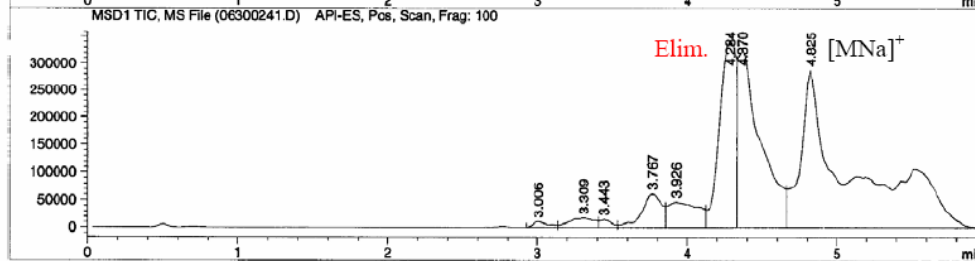
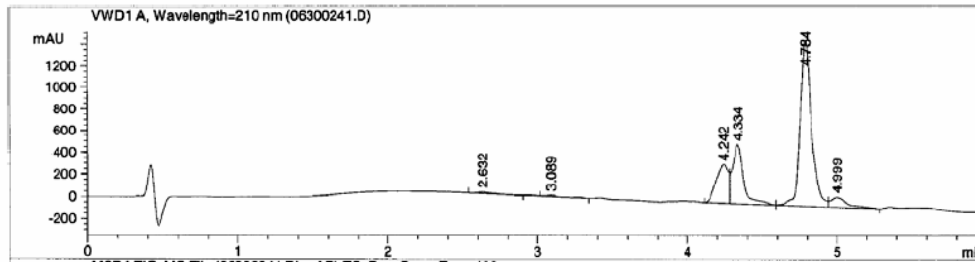
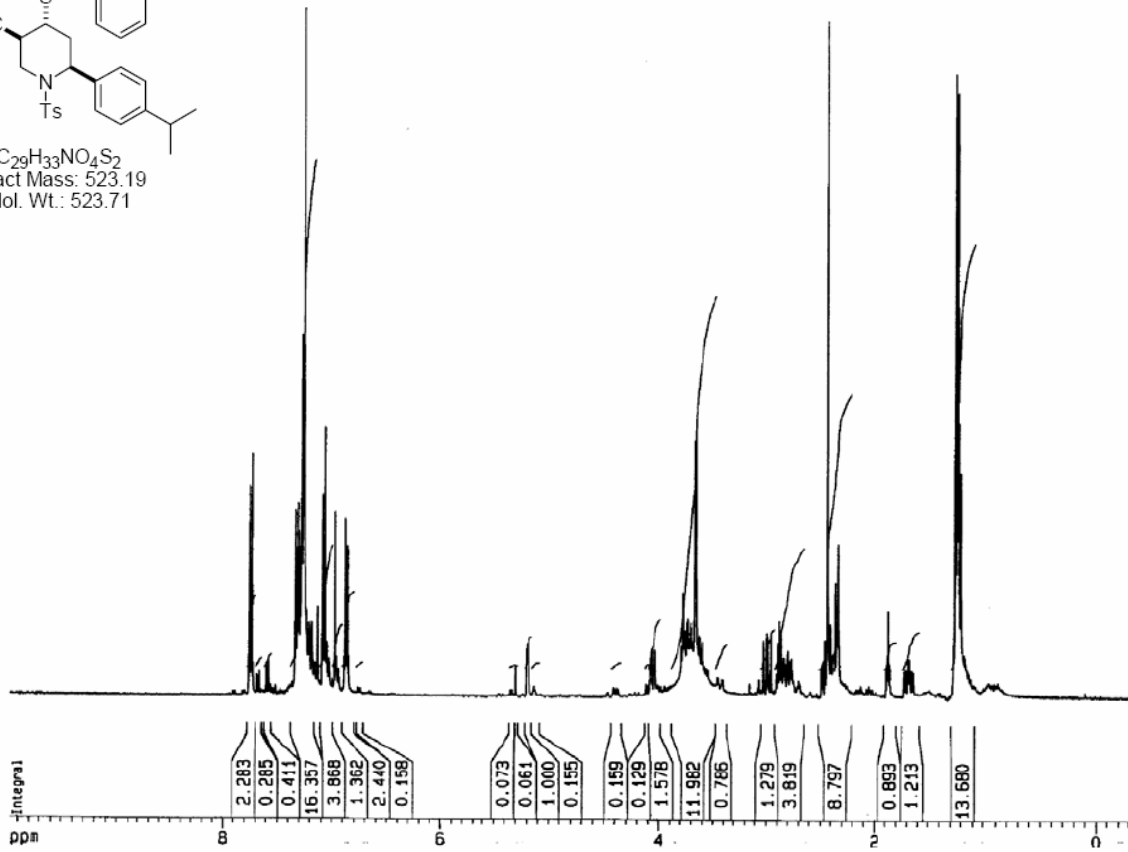
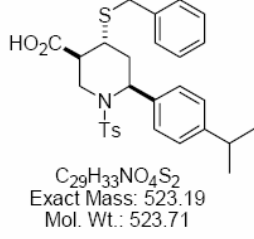


4-Benzylsulfanyl-6-(4-fluorophenyl)-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C23E06)

Not included

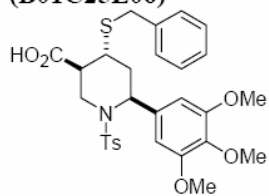


4-Benzylsulfanyl-6-(4-isopropylphenyl)-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C24E06)
 Not included

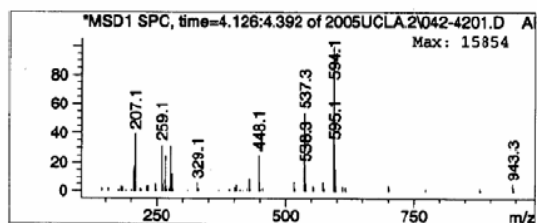
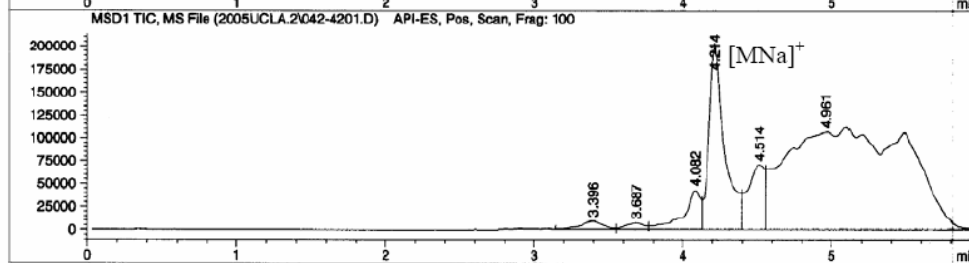
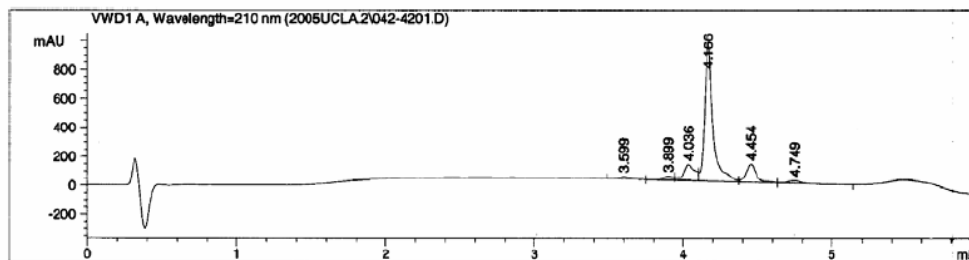
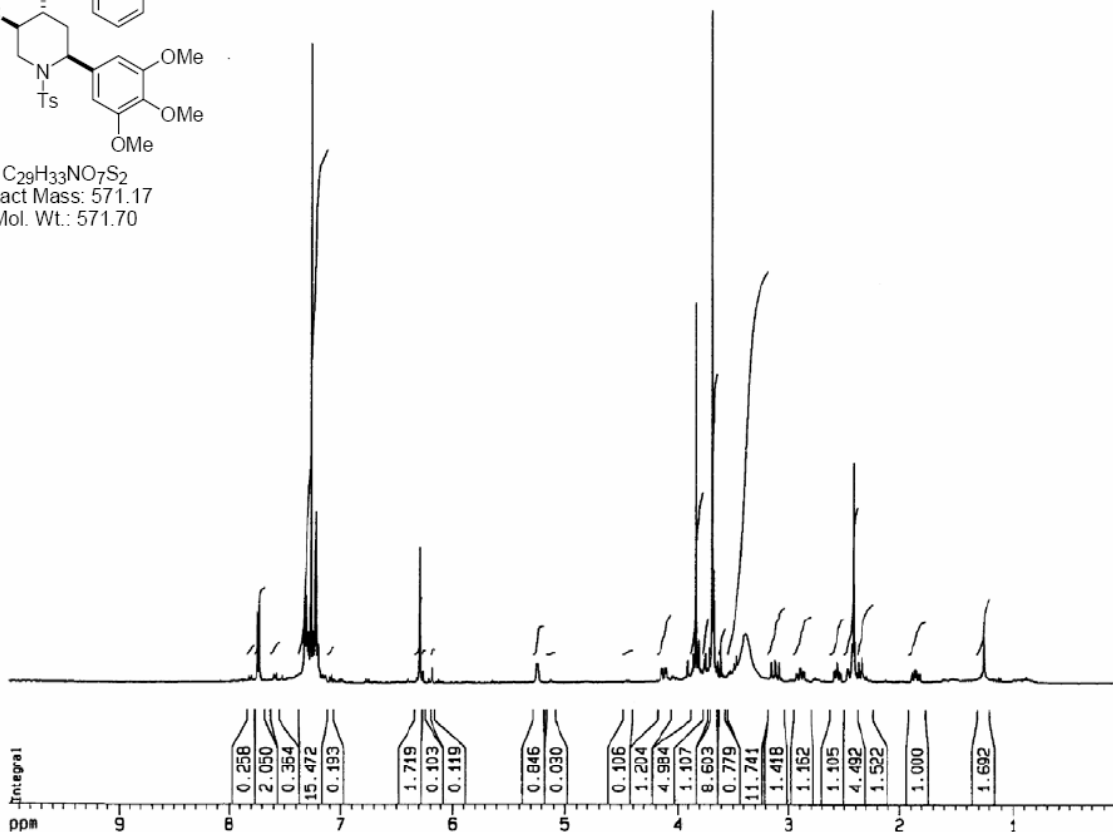


4-Benzylsulfanyl-1-(4-toluenesulfonyl)-6-(3,4,5-trimethoxyphenyl)-piperidine-3-carboxylic acid (B01C25E06)

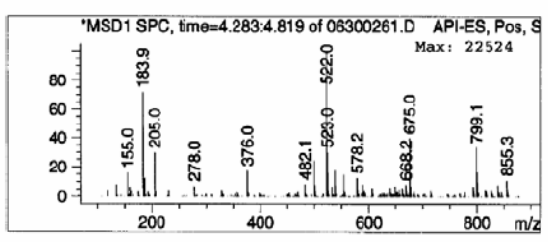
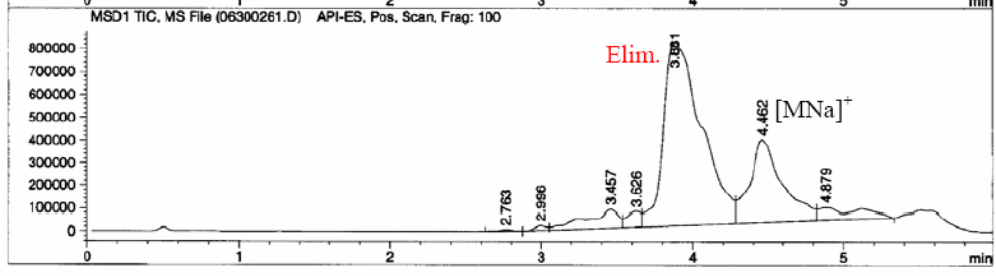
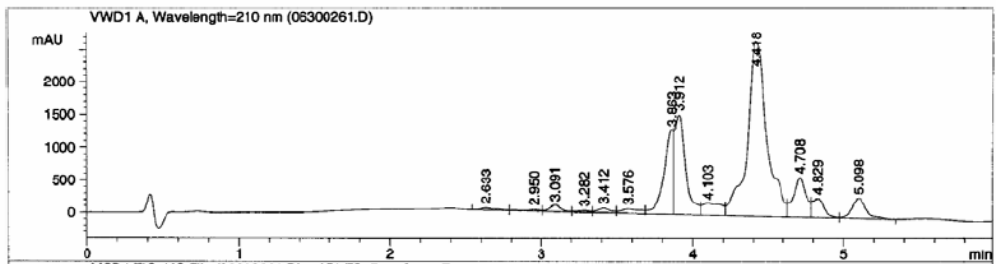
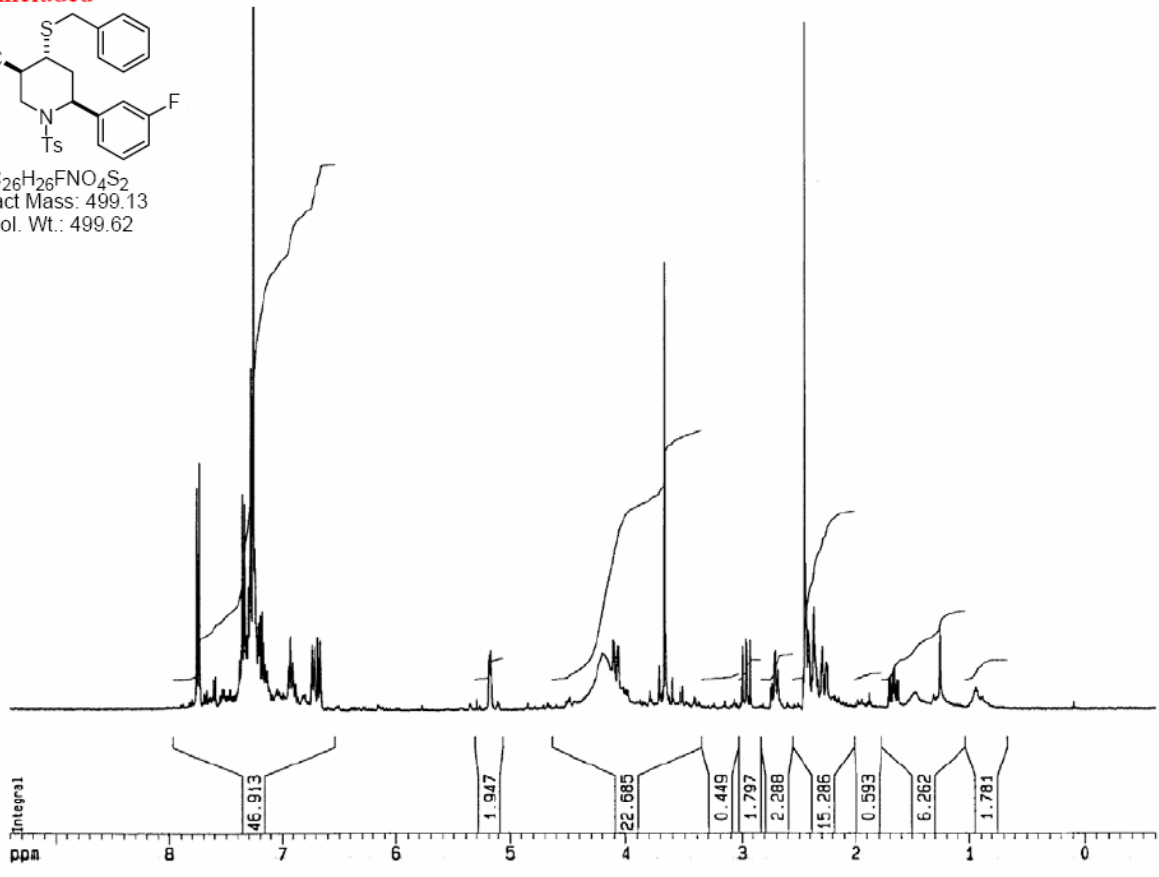
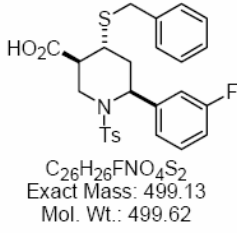
acid



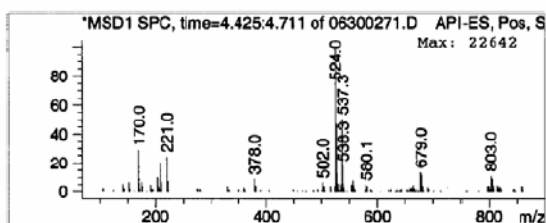
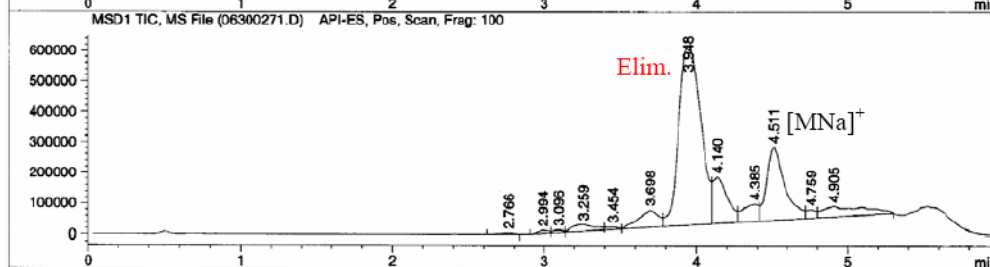
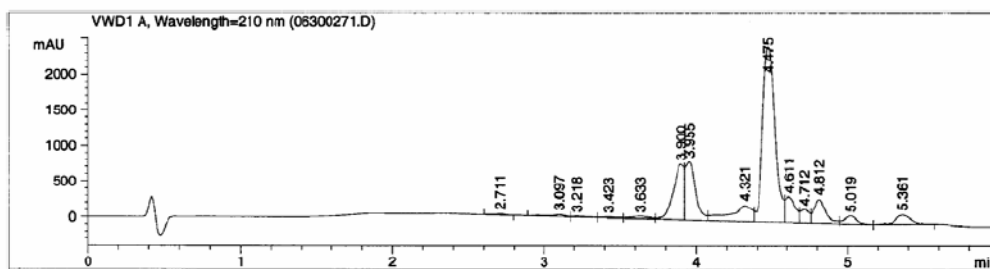
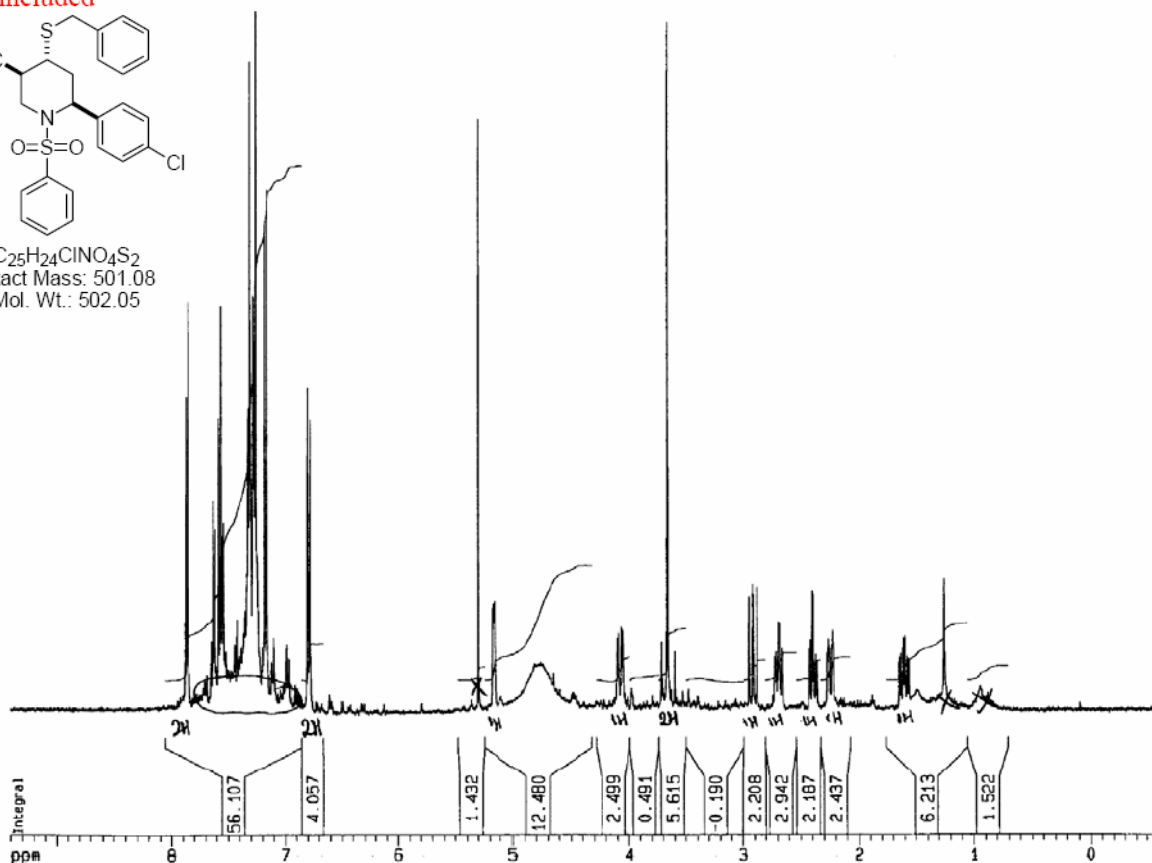
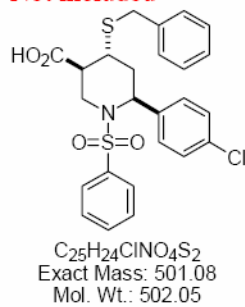
C₂₉H₃₃NO₇S₂
 Exact Mass: 571.17
 Mol. Wt.: 571.70



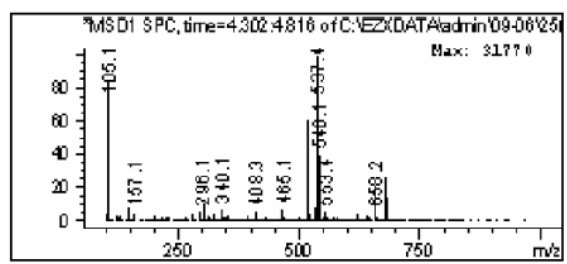
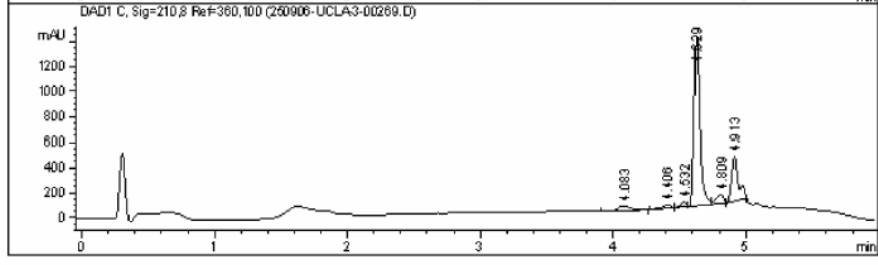
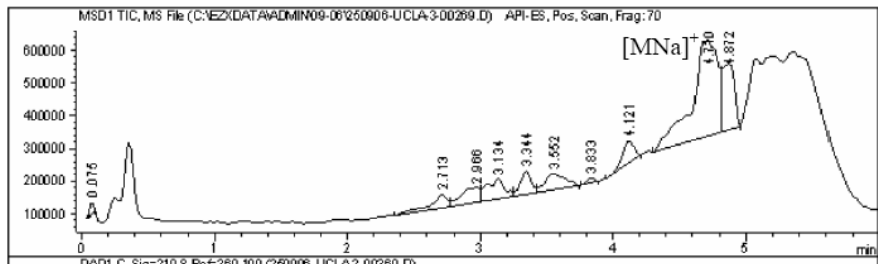
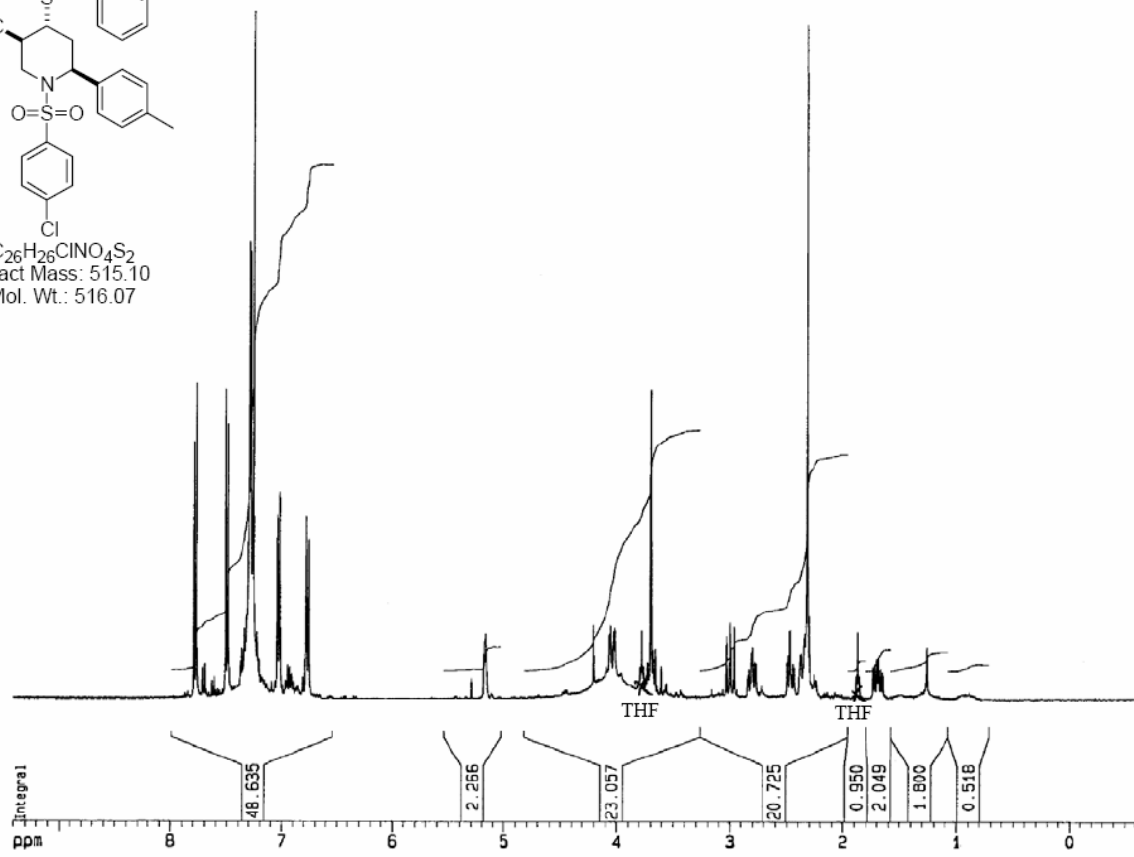
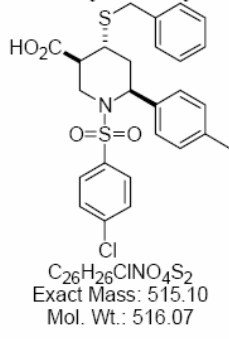
4-Benzylsulfanyl-6-(3-fluorophenyl)-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C26E06)
Not included



1-Benzenesulfonyl-4-benzylsulfanyl-6-(4-chlorophenyl)-piperidine-3-carboxylic acid (B01C29E06)
 Not included



4-Benzylsulfanyl-1-(4-chlorobenzenesulfonyl)-6-(p-tolyl)-piperidine-3-carboxylic acid (B01C30E06)

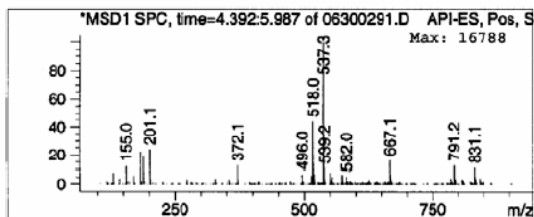
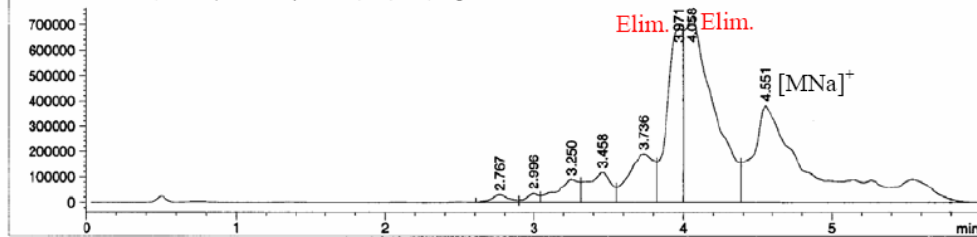
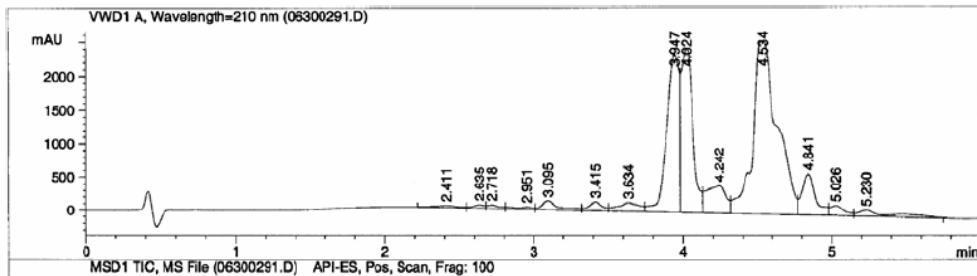
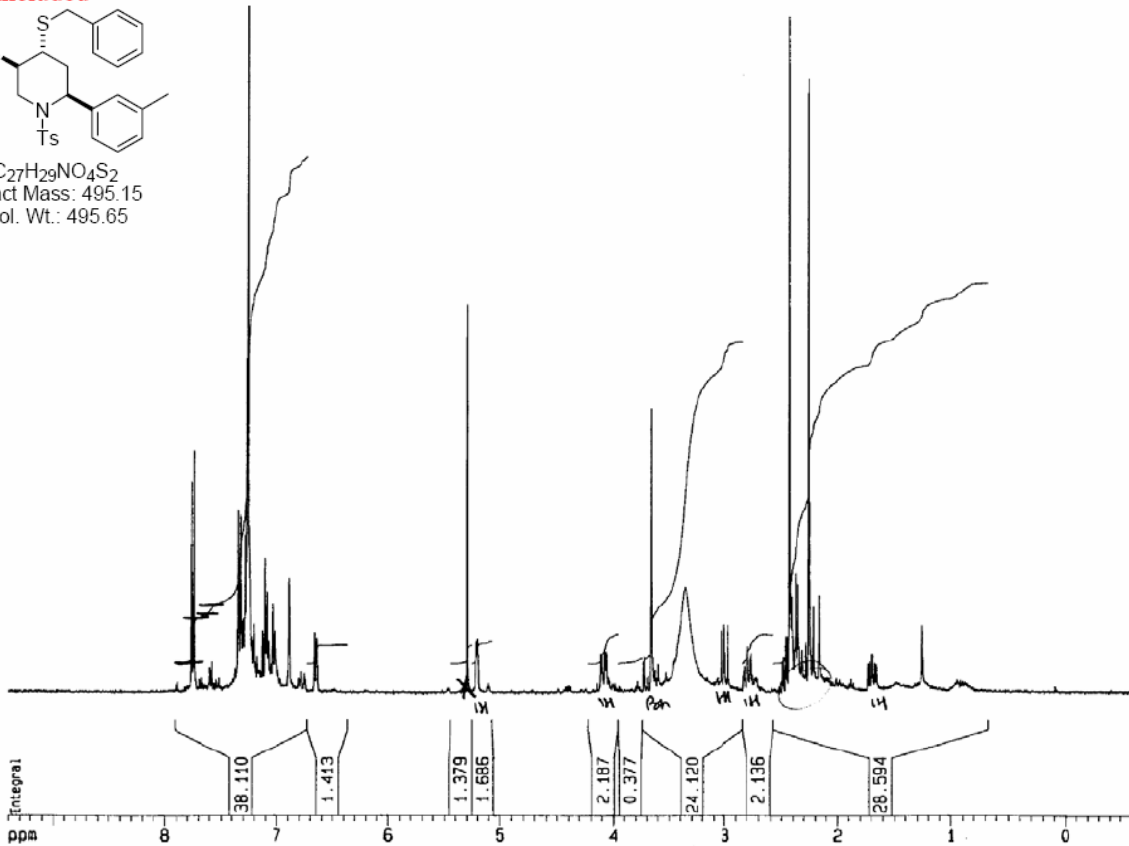
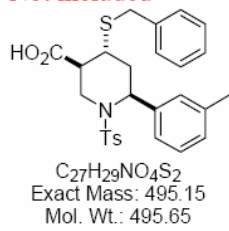


Peak #9 at 4.710 min (4.302 to 4.816 min)
 -> The analysis found 3 components, indicating an impure peak. <-

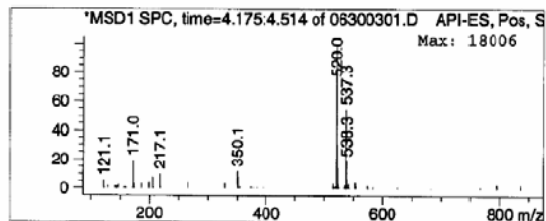
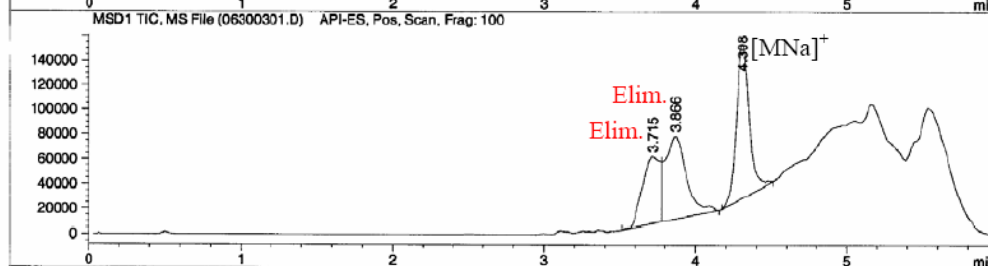
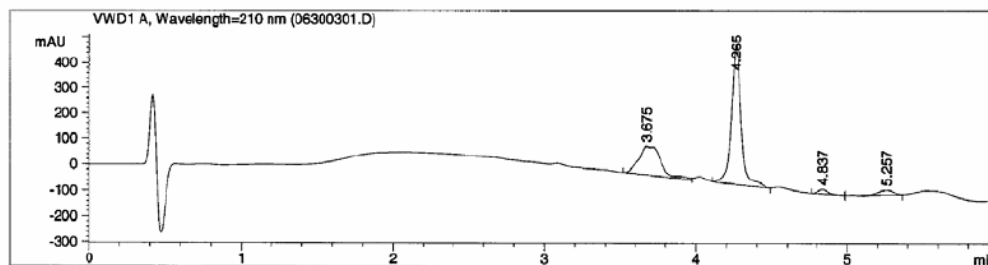
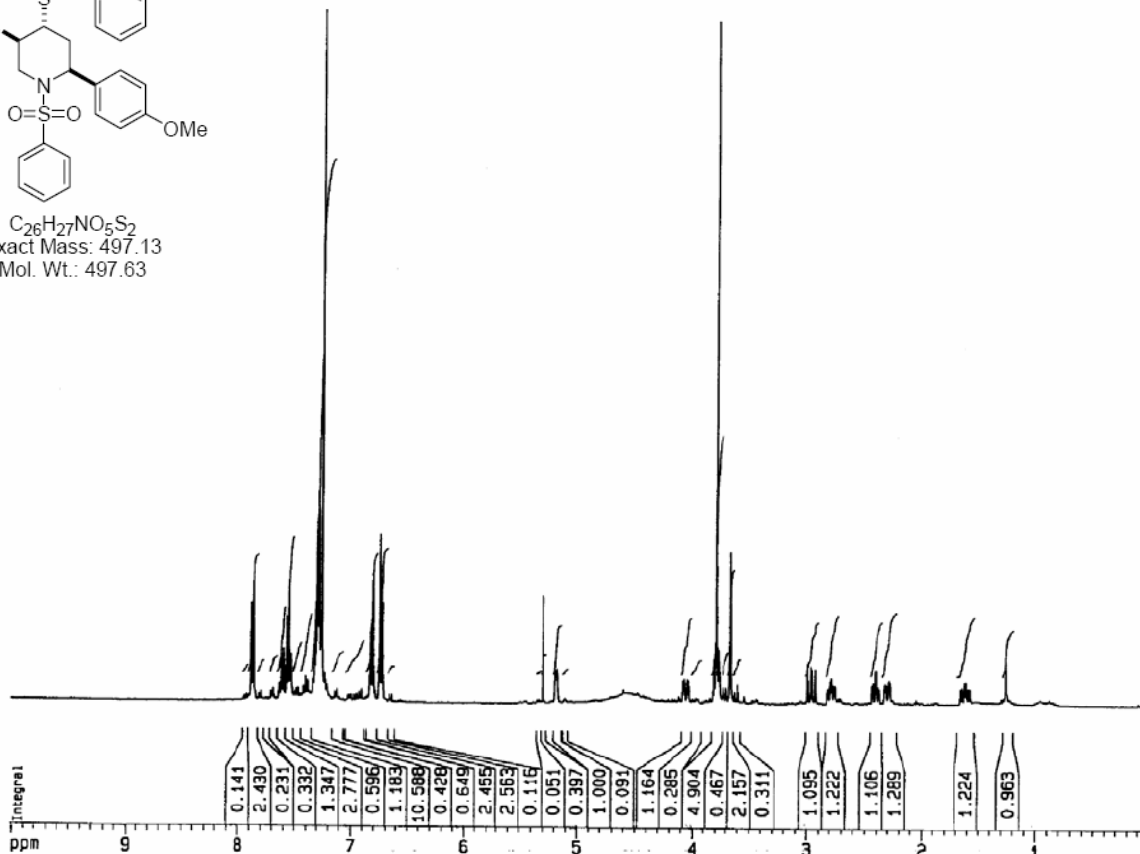
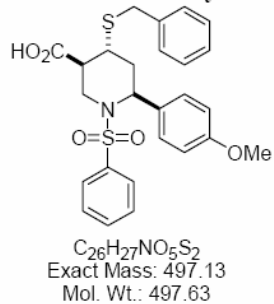
Component 1: Peak at Scan 248.8, Top ions are 678 656
 Component 2: Peak at Scan 262.9, Top ions are 538 516 540
 Component 3: Peak at Scan 268.1, Top ions are 537 301

4-Benzylsulfanyl-1-(4-toluenesulfonyl)-6-(*m*-tolyl)-piperidine-3-carboxylic acid (B01C33E06)

Not included

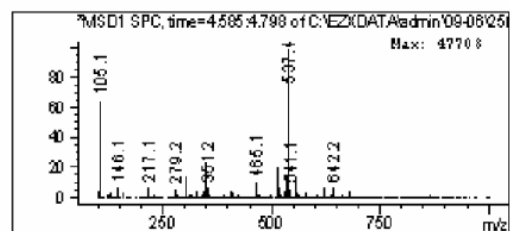
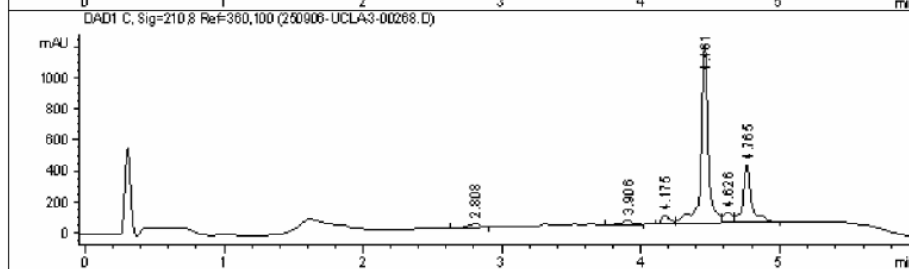
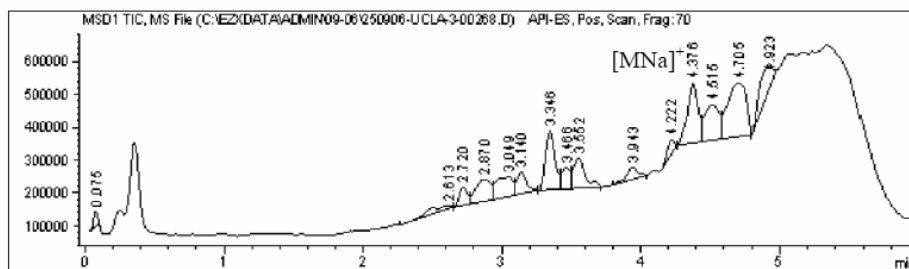
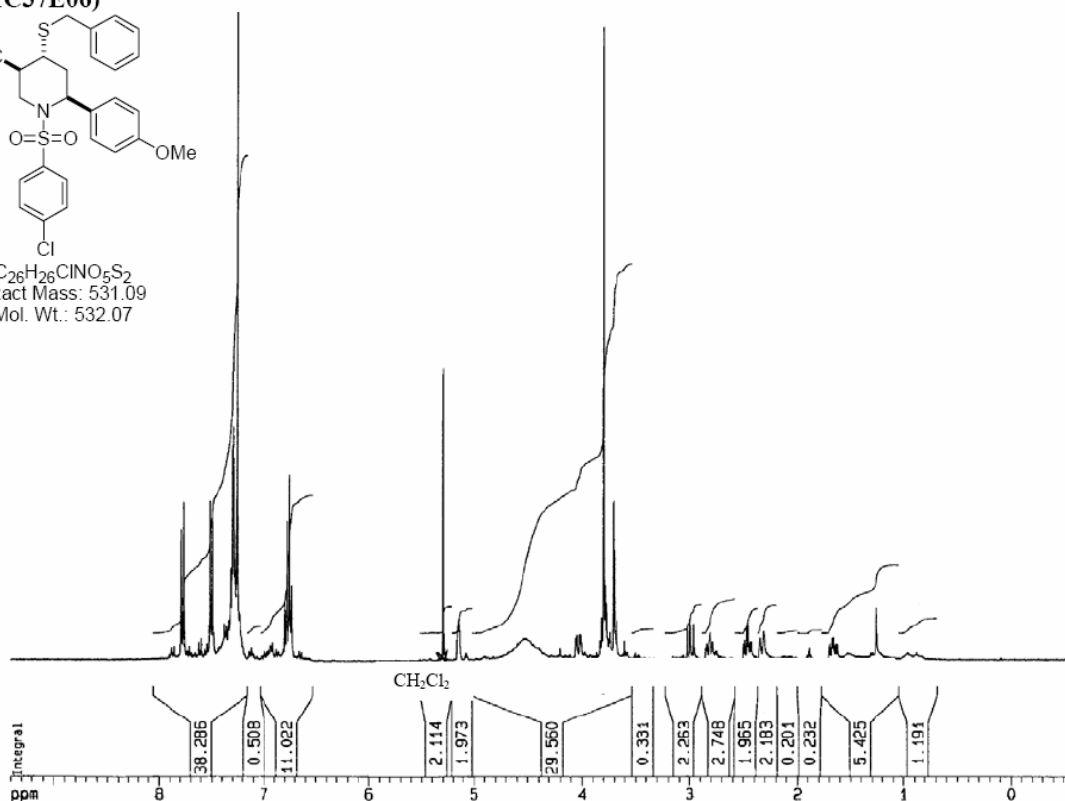
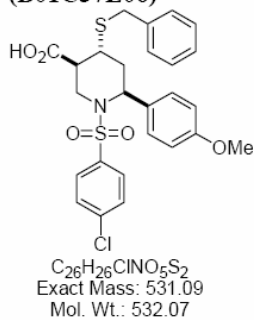


1-Benzenesulfonyl-4-benzylsulfanyl-6-(4-methoxyphenyl)-piperidine-3-carboxylic acid (B01C35E06)



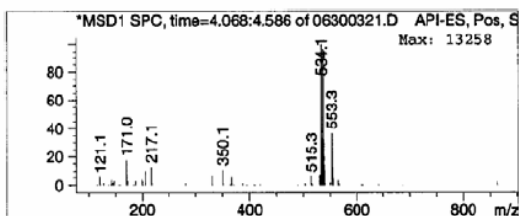
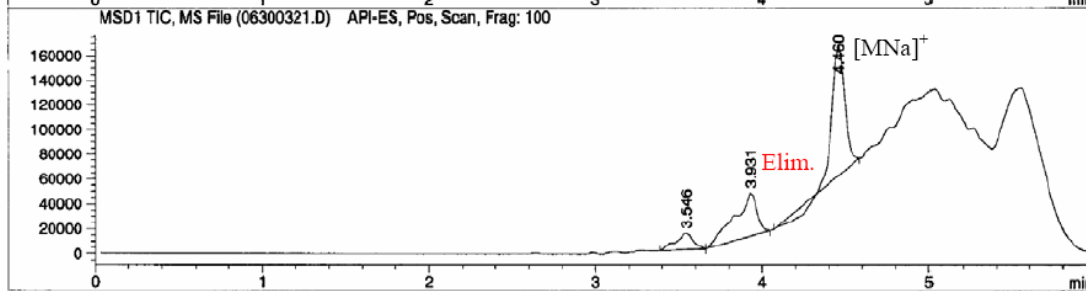
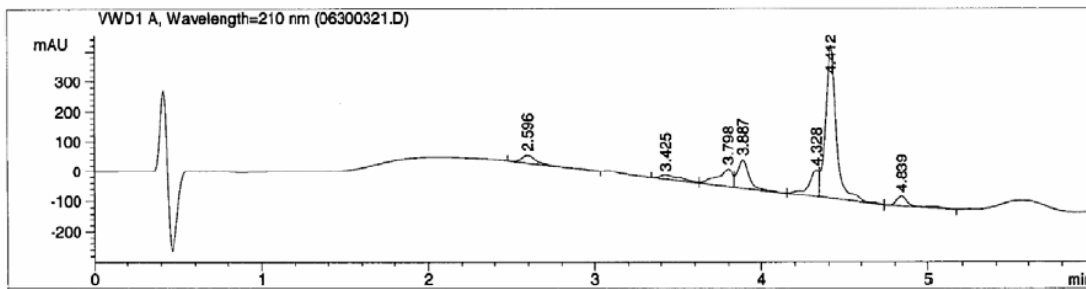
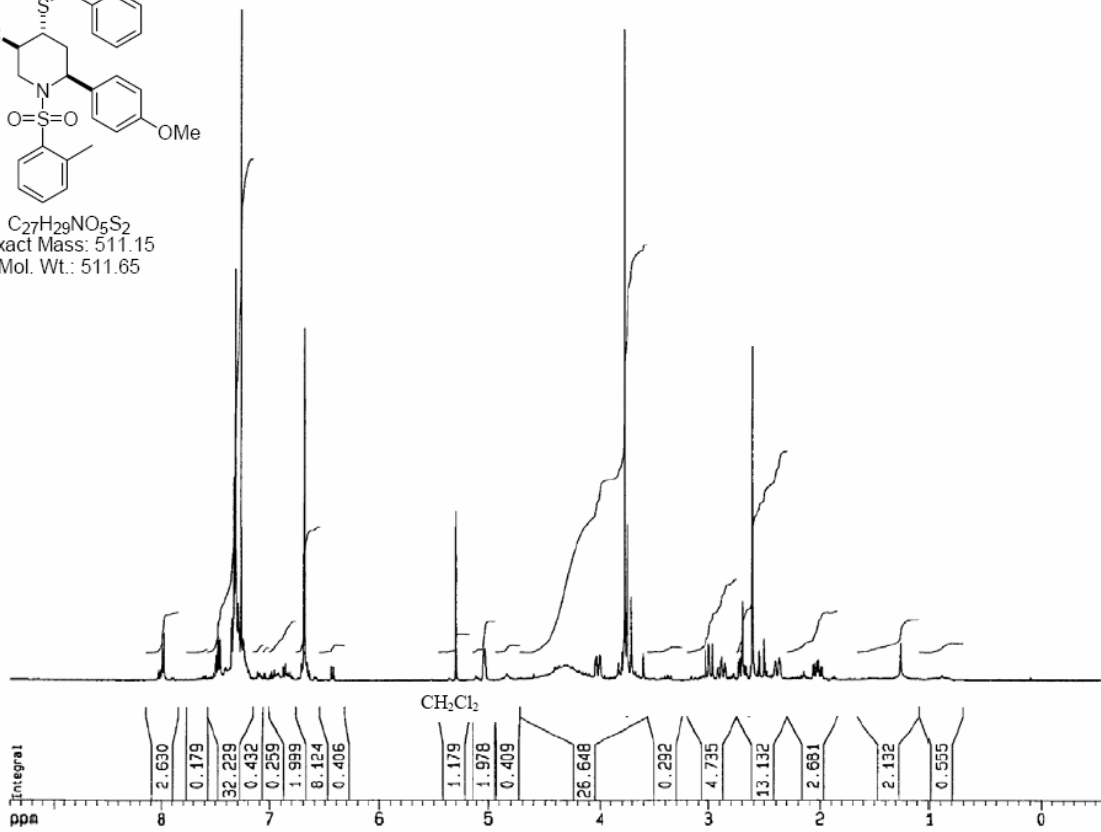
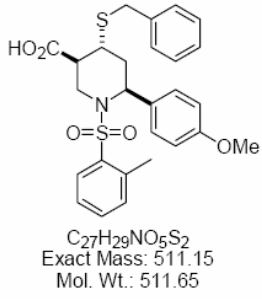
4-Benzylsulfanyl-1-(4-chlorobenzenesulfonyl)-6-(4-methoxyphenyl)-piperidine-3-carboxylic acid (B01C37E06)

acid

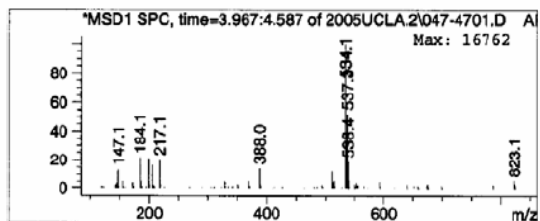
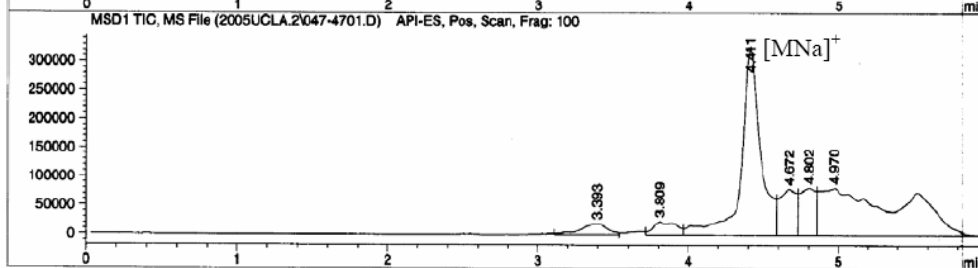
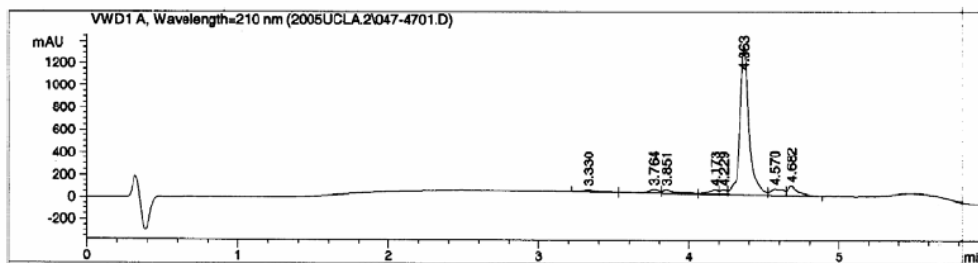
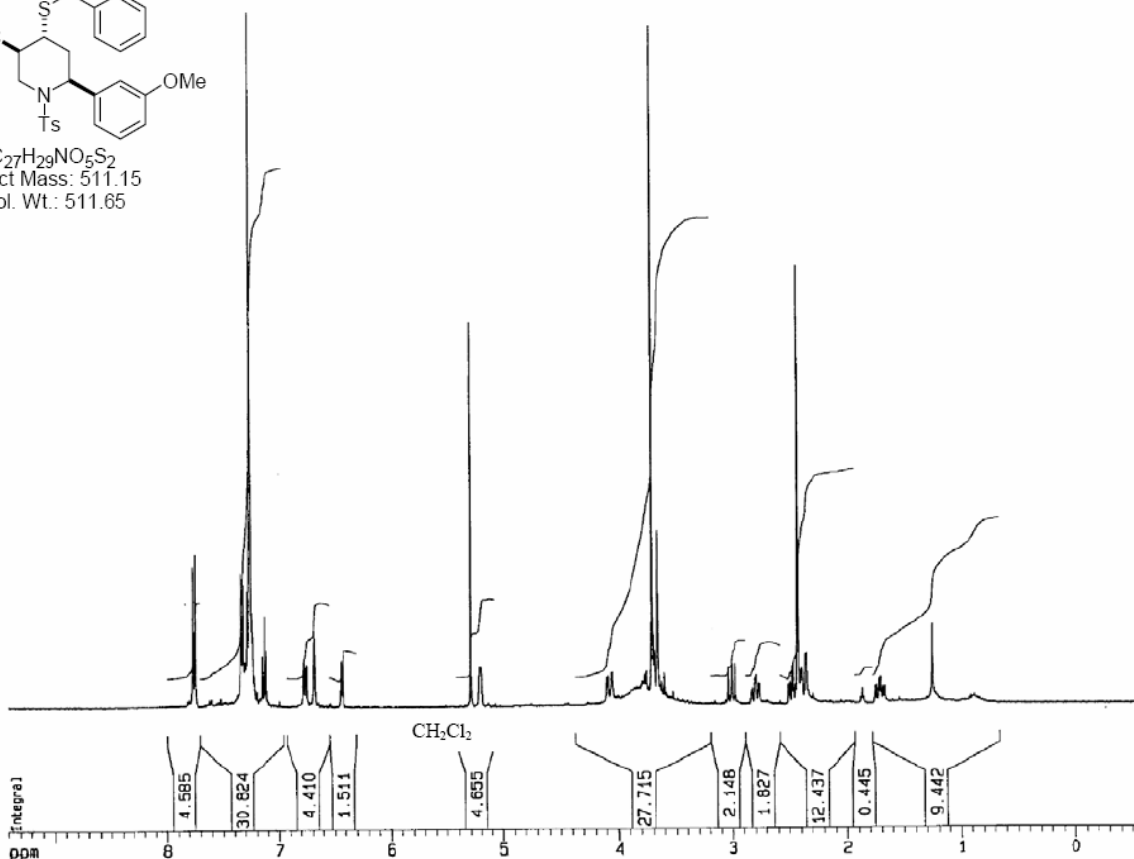
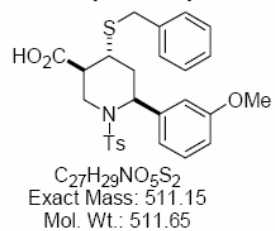


Component 1: Peak at Scan 253.2. Top ions are 554 532 534

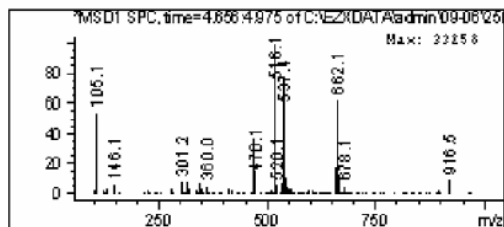
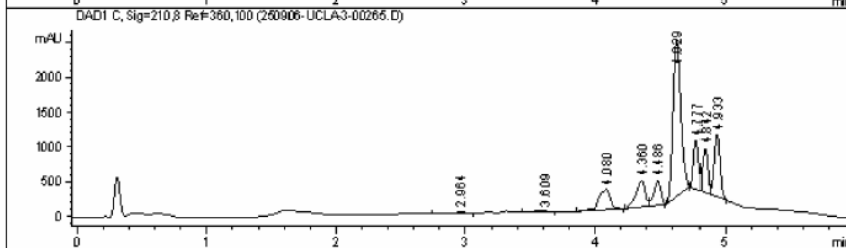
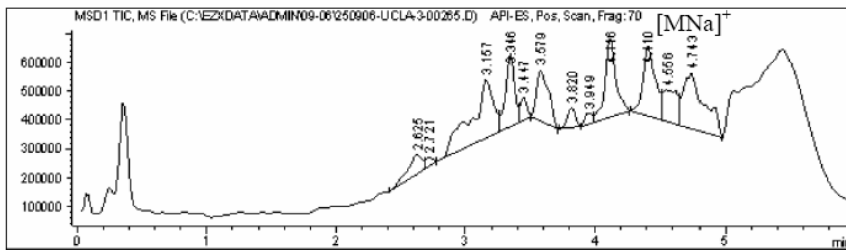
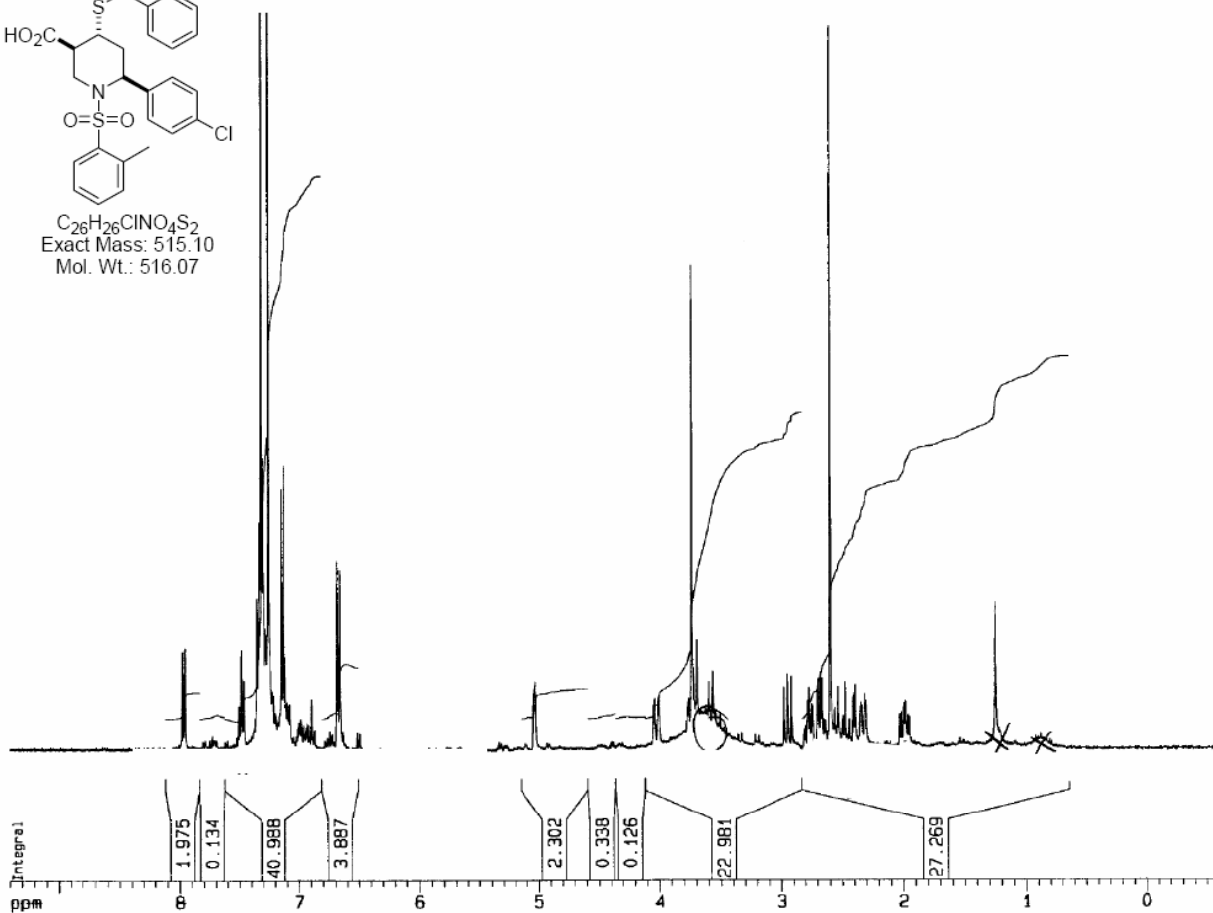
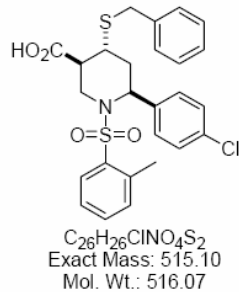
4-Benzylsulfanyl-6-(4-methoxyphenyl)-1-(2-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C38E06)



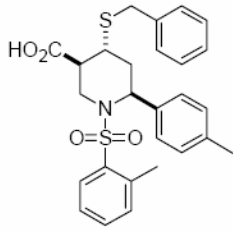
4-Benzylsulfaul-6-(3-methoxyphenyl)-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C39E06)



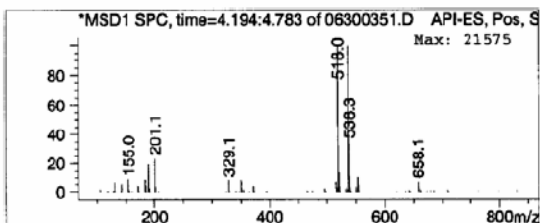
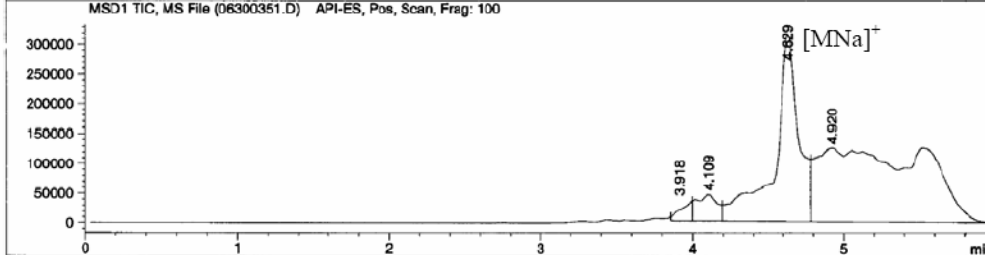
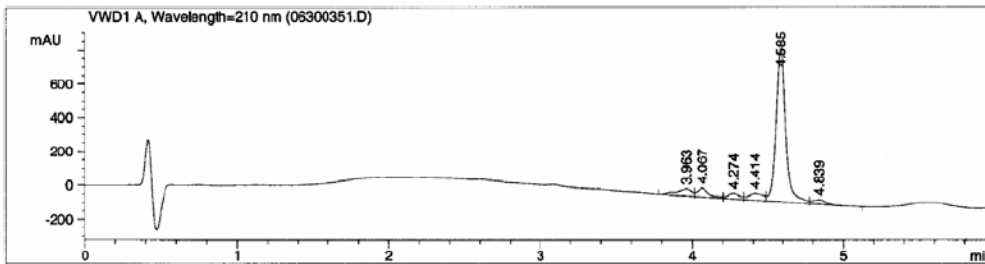
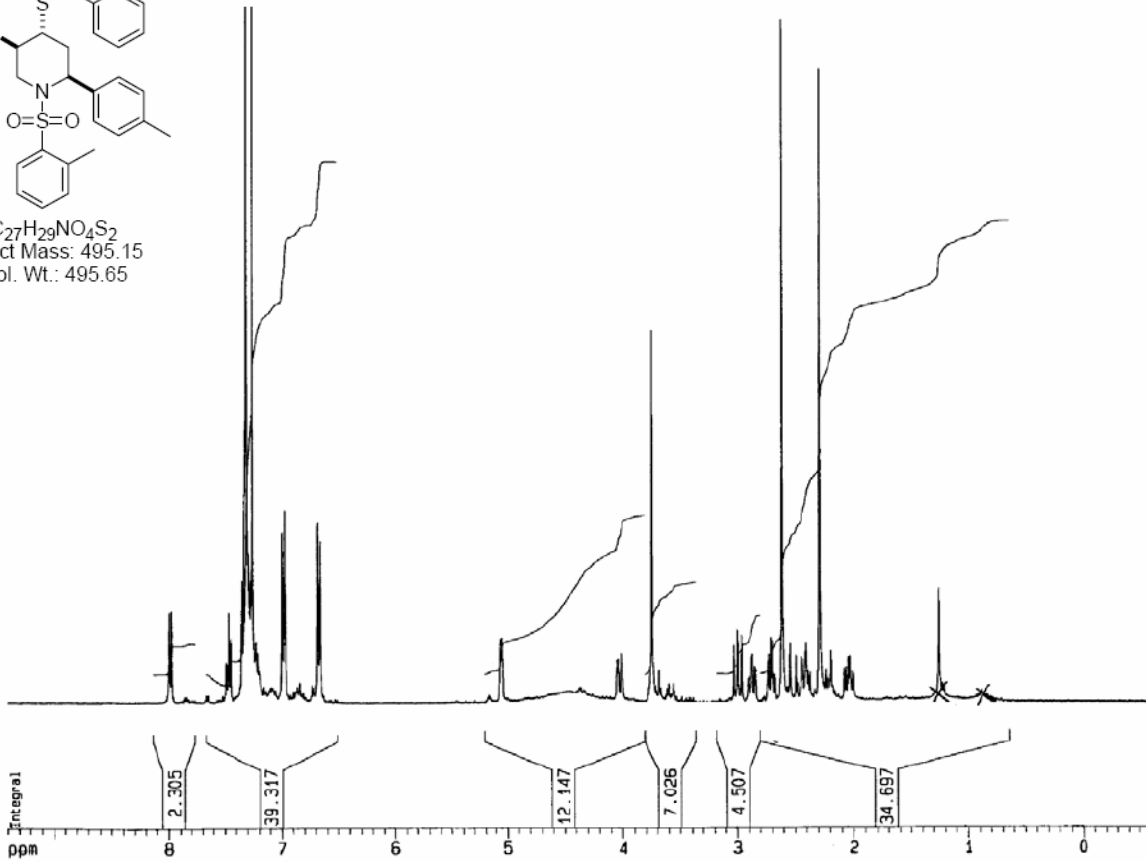
4-Benzylsulfanyl-6-(4-chlorophenyl)-1-(2-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C40E06)



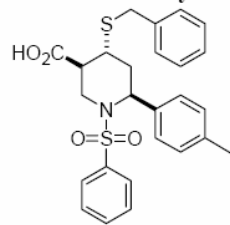
4-Benzylsulfanyl-1-(2-toluenesulfonyl)-6-(*p*-tolyl)piperidine-3-carboxylic acid (B01C41E06)



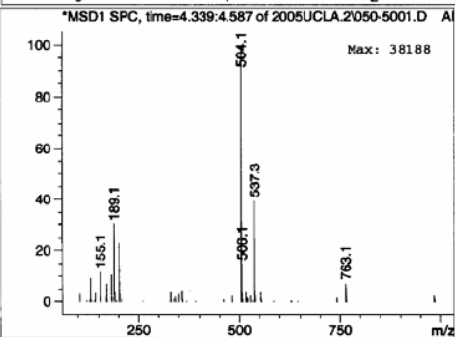
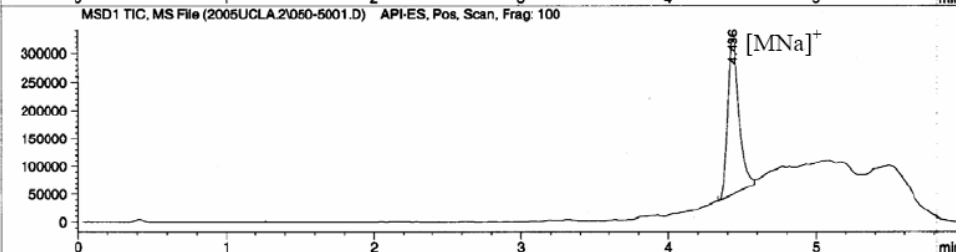
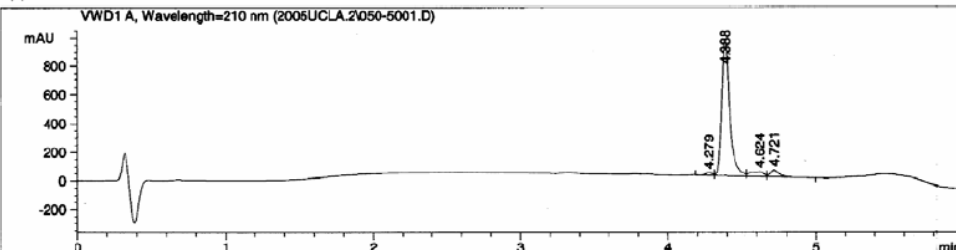
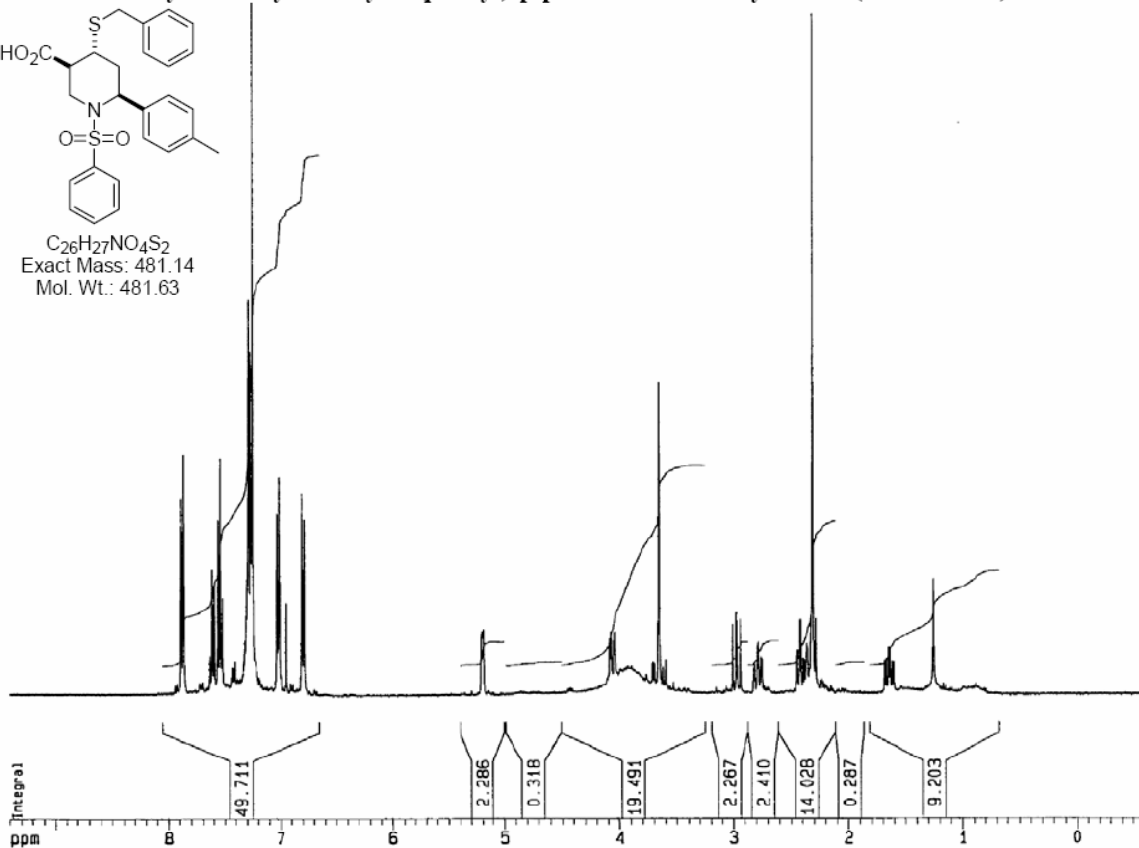
C₂₇H₂₉NO₄S₂
 Exact Mass: 495.15
 Mol. Wt.: 495.65



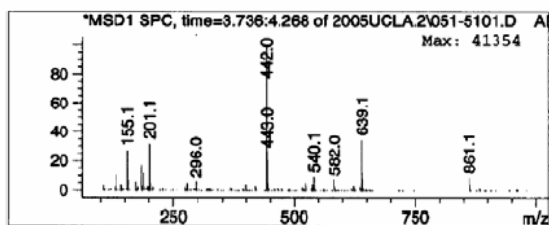
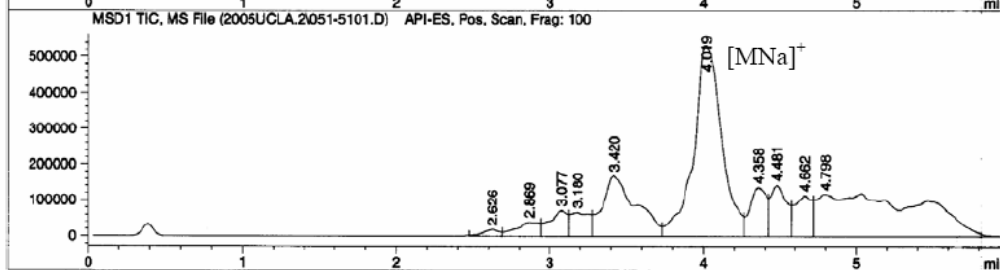
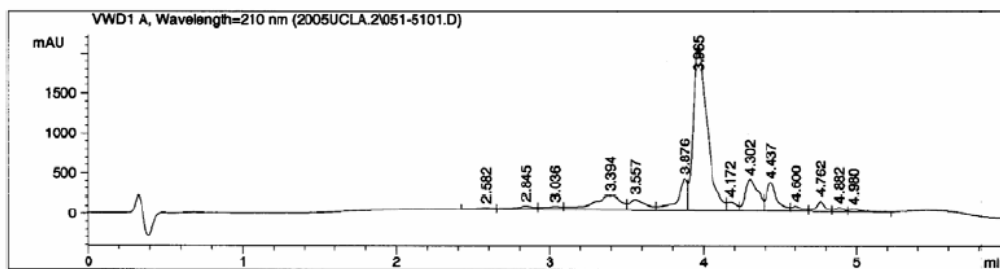
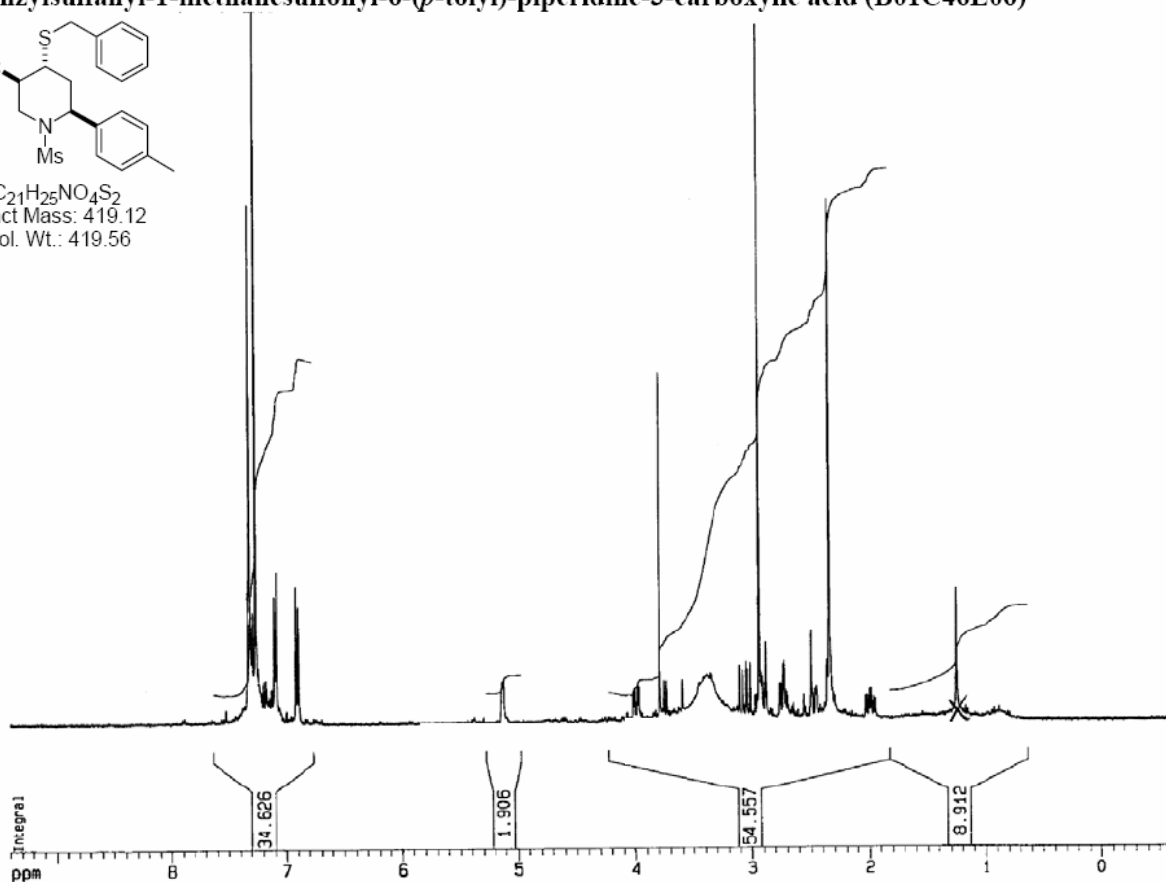
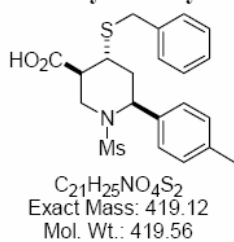
Benzenesulfonyl-4-benzylsulfanyl-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C43E06)



C₂₆H₂₇NO₄S₂
 Exact Mass: 481.14
 Mol. Wt.: 481.63

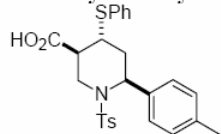


4-Benzylsulfanyl-1-methanesulfonyl-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C46E06)

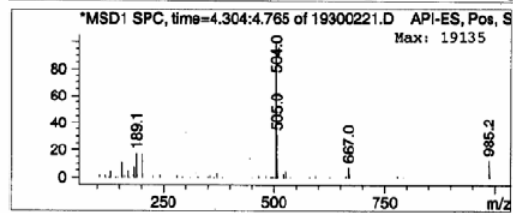
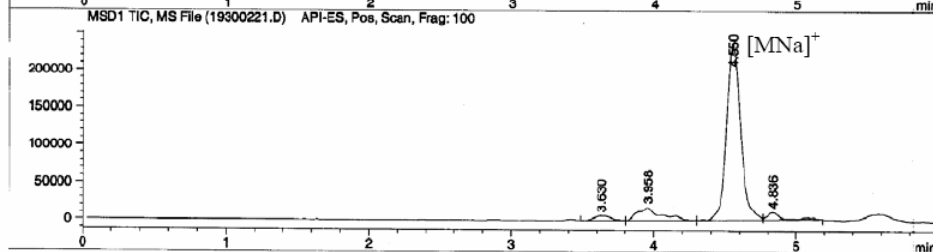
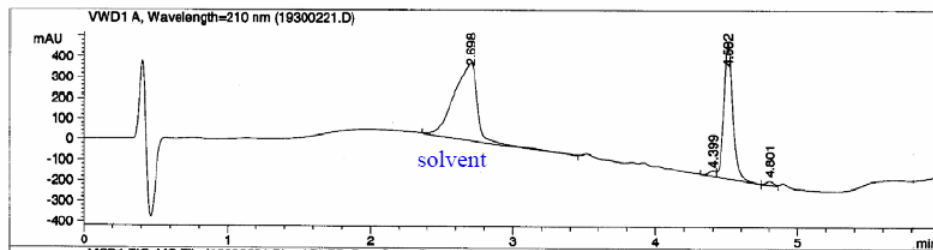
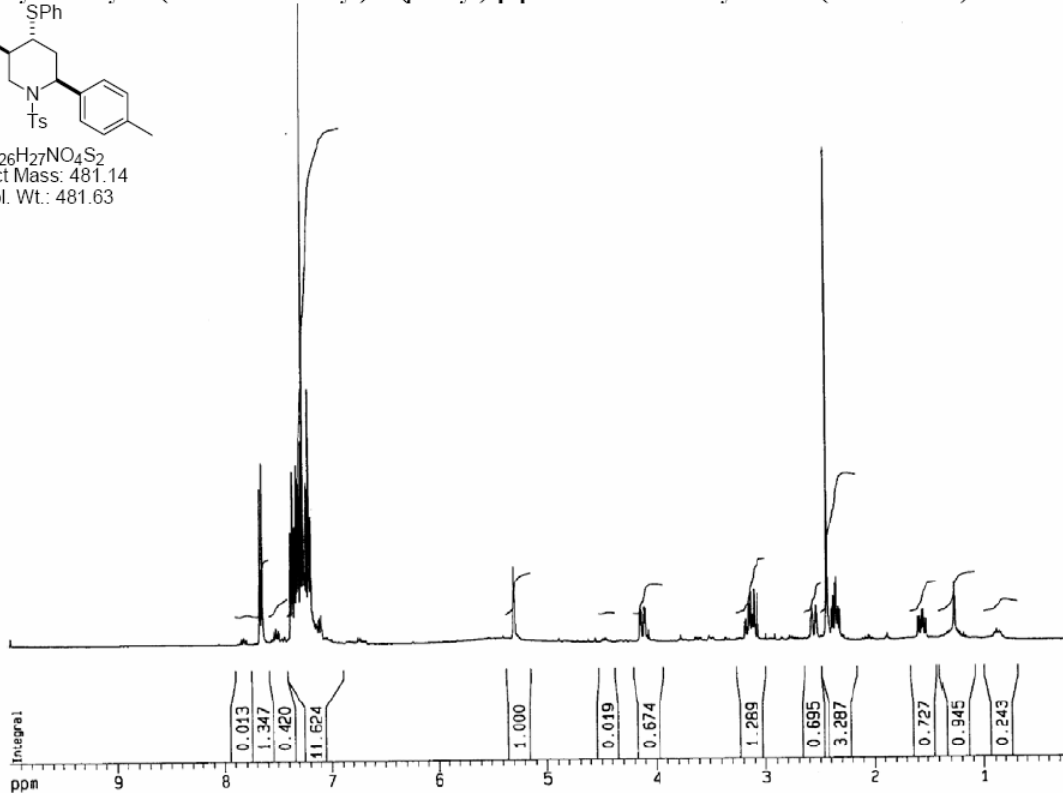


Spectral data for Table 13

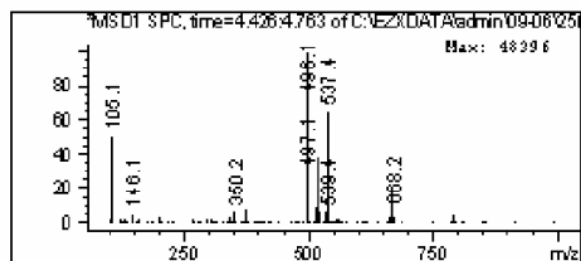
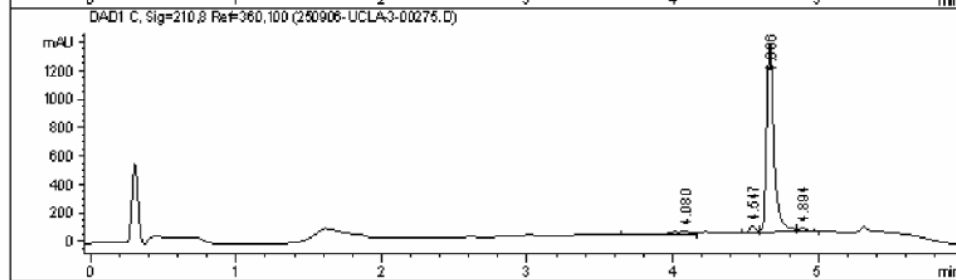
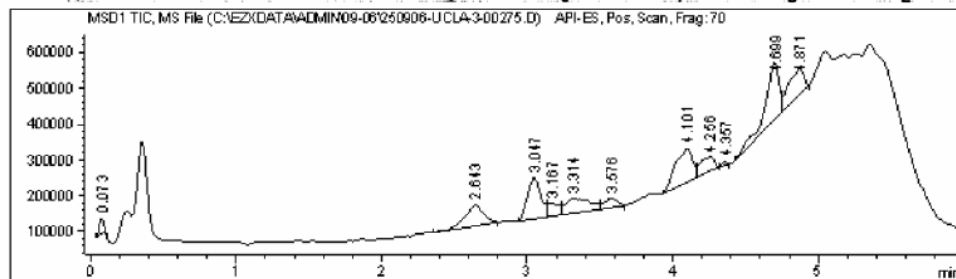
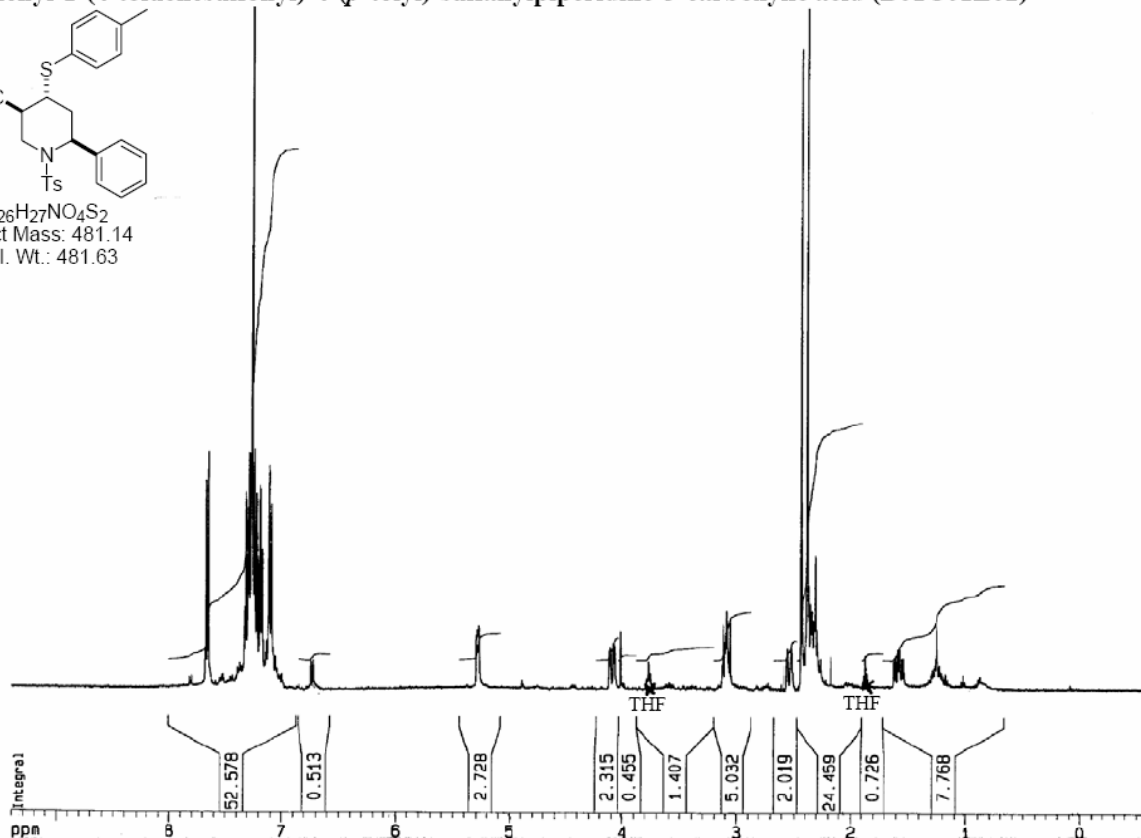
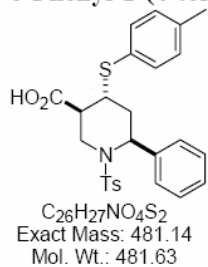
4-Phenylsulfanyl-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C02E01)



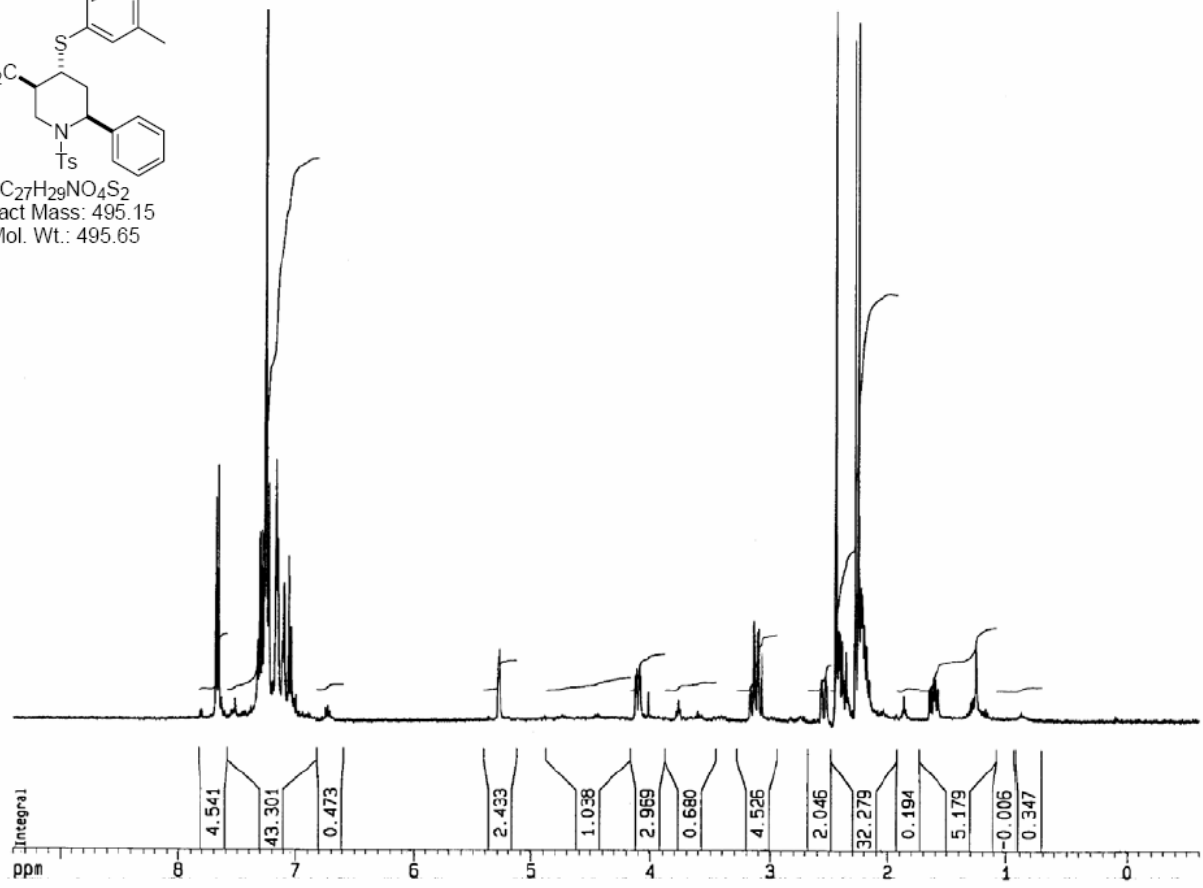
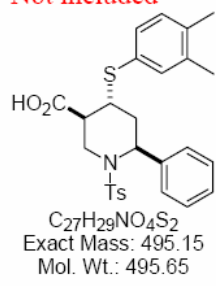
C₂₆H₂₇NO₄S₂
 Exact Mass: 481.14
 Mol. Wt.: 481.63



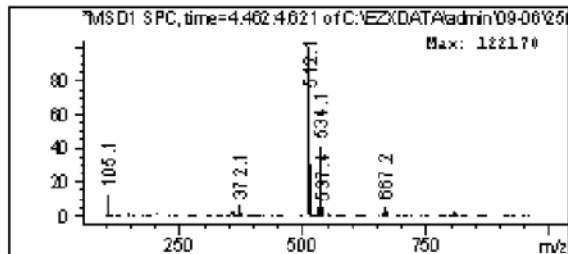
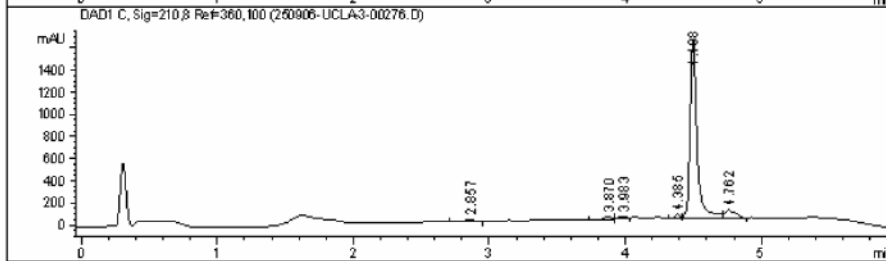
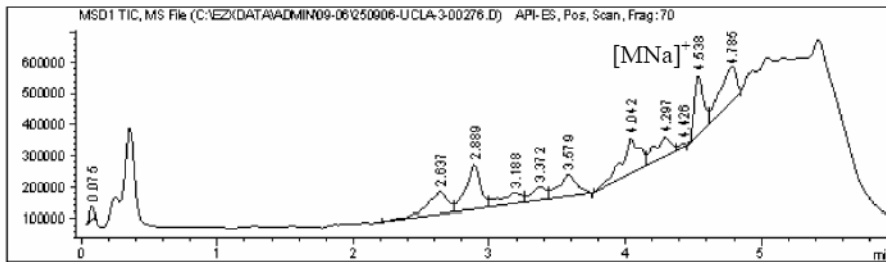
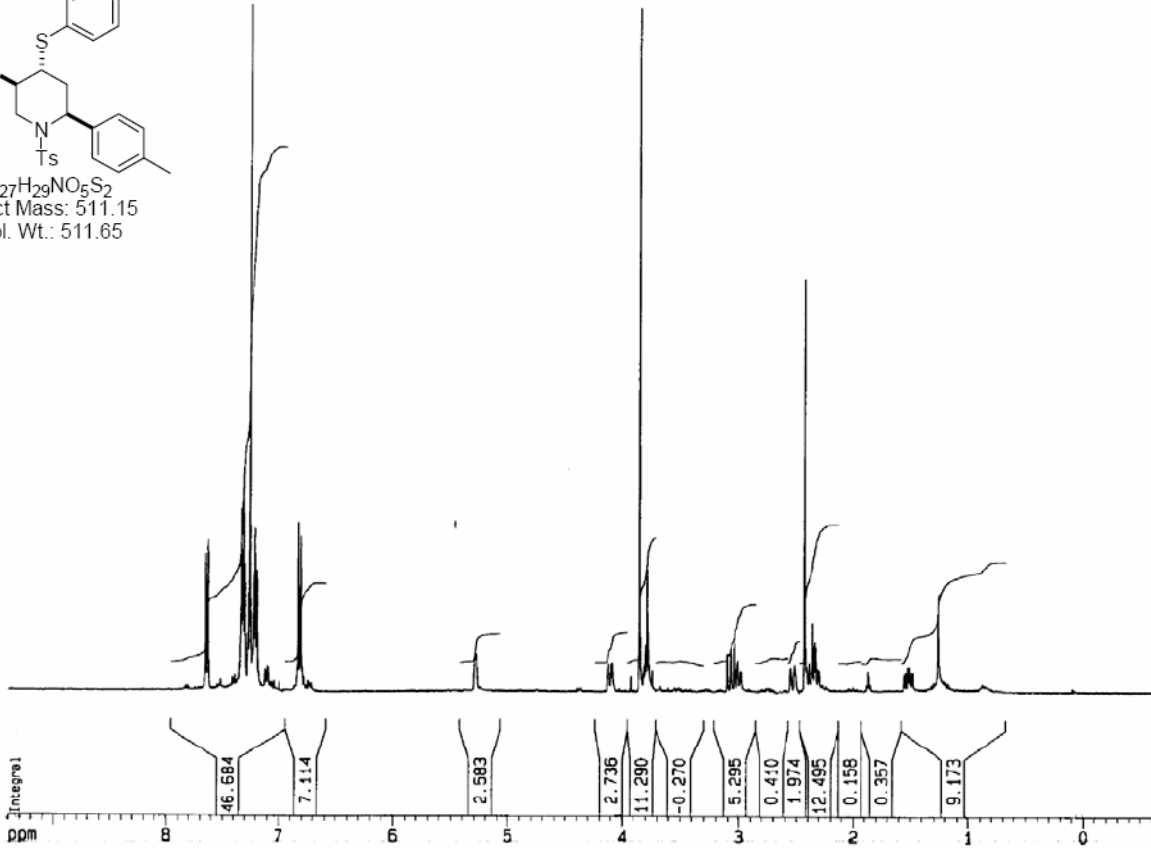
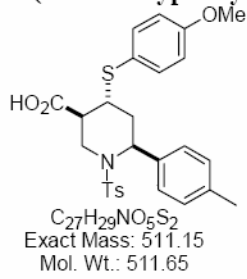
6-Phenyl-1-(4-toluenesulfonyl)-4-(p-tolyl)-sulfanyl piperidine-3-carboxylic acid (B01C01E02)



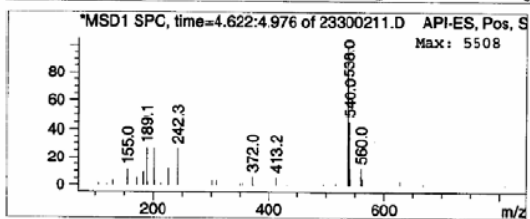
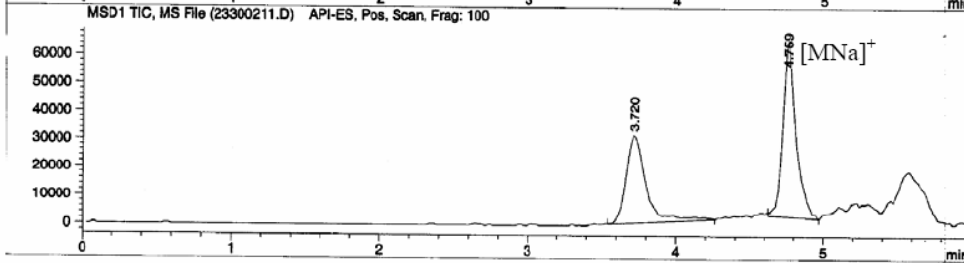
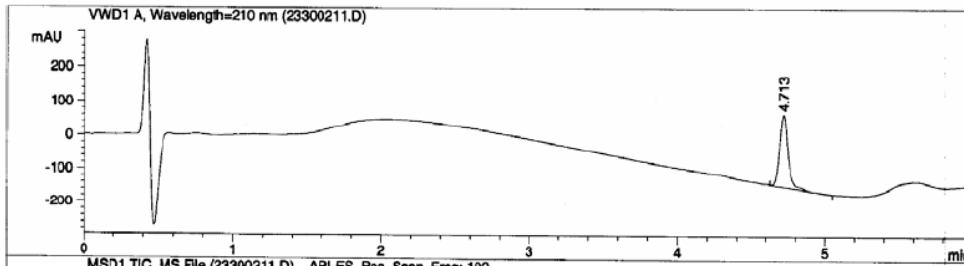
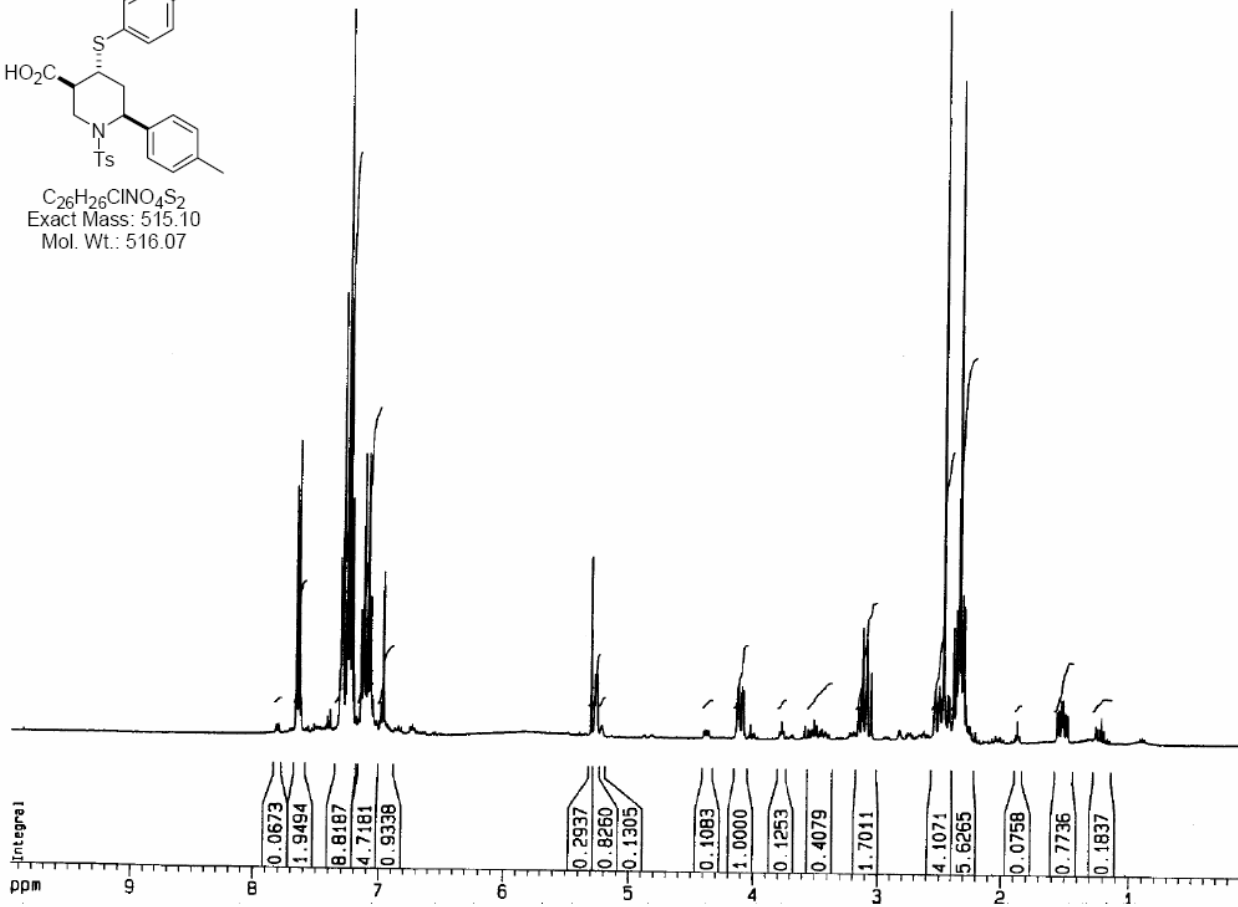
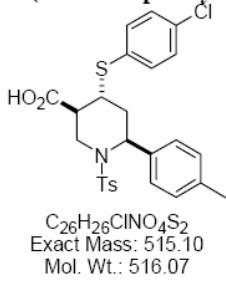
4-(3,4-Dimethylphenylsulfanyl)-6-phenyl-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C01E03)
Not included



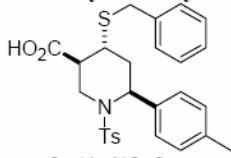
4-(4-Methoxyphenylsulfanyl)-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C02E04)



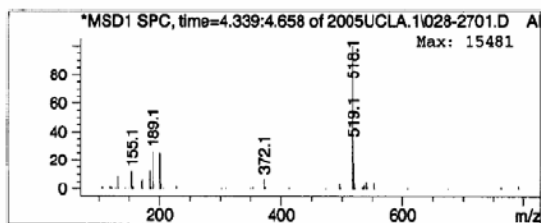
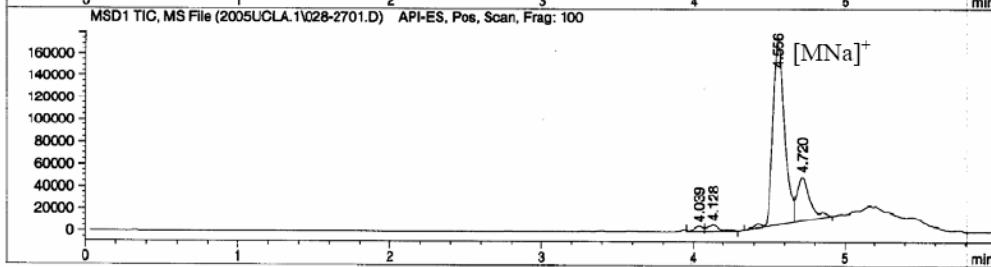
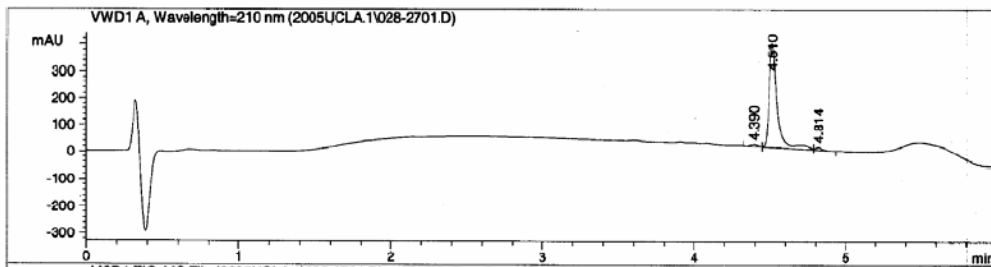
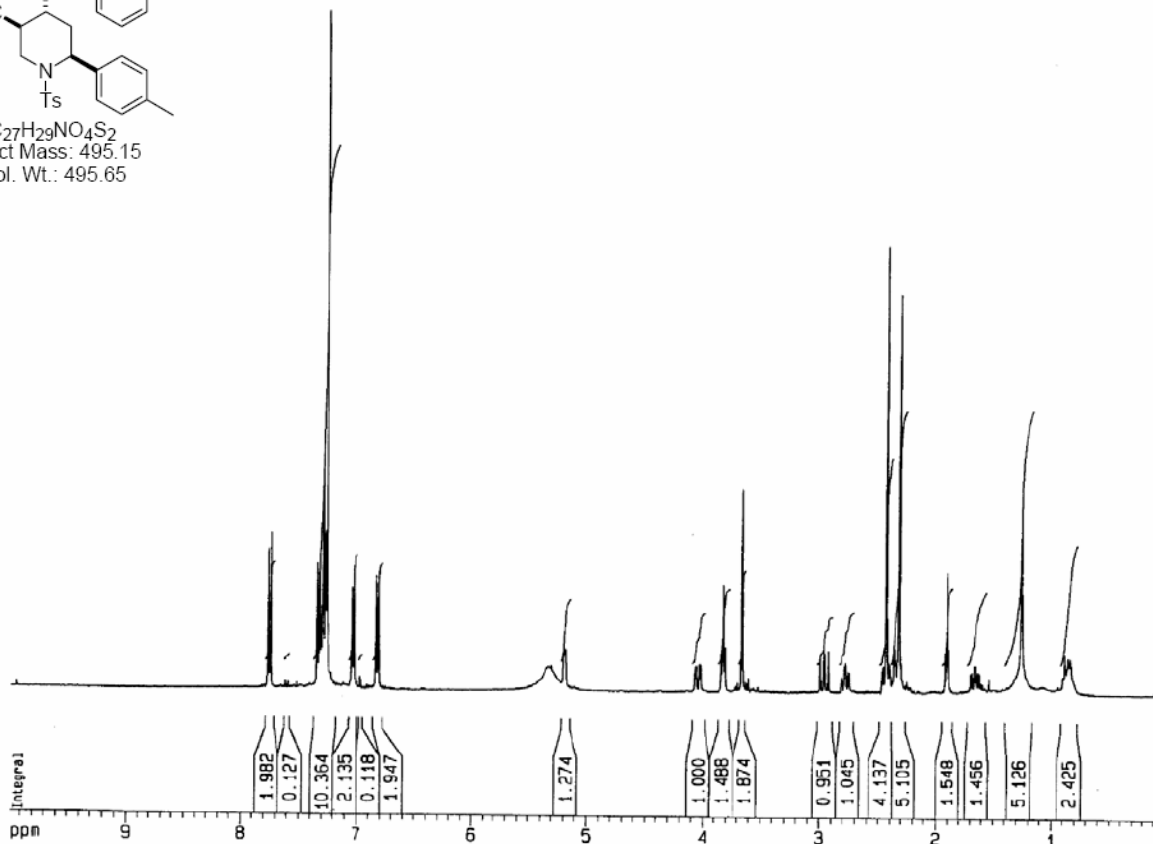
4-(4-Chlorophenylsulfanyl)-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C02E05)



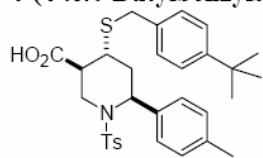
4-Benzylsulfanyl-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C02E06)



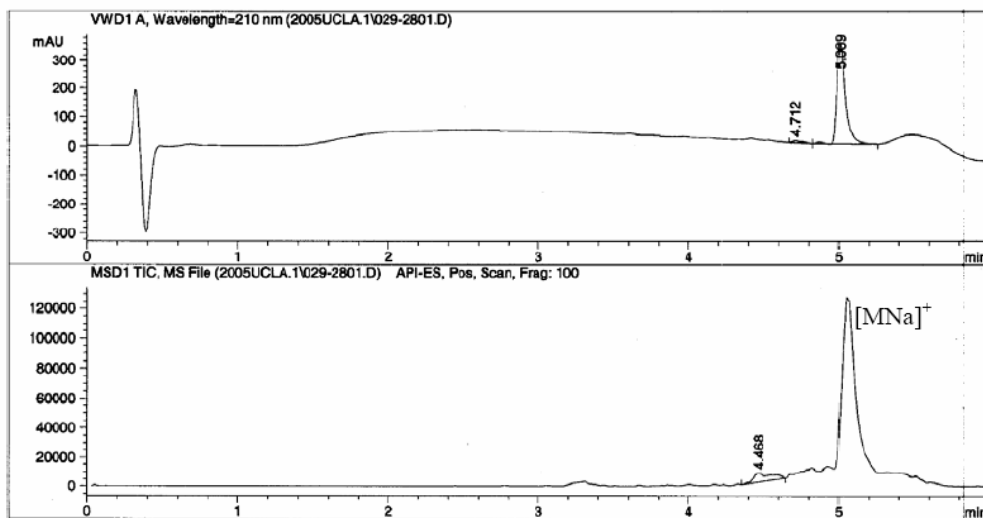
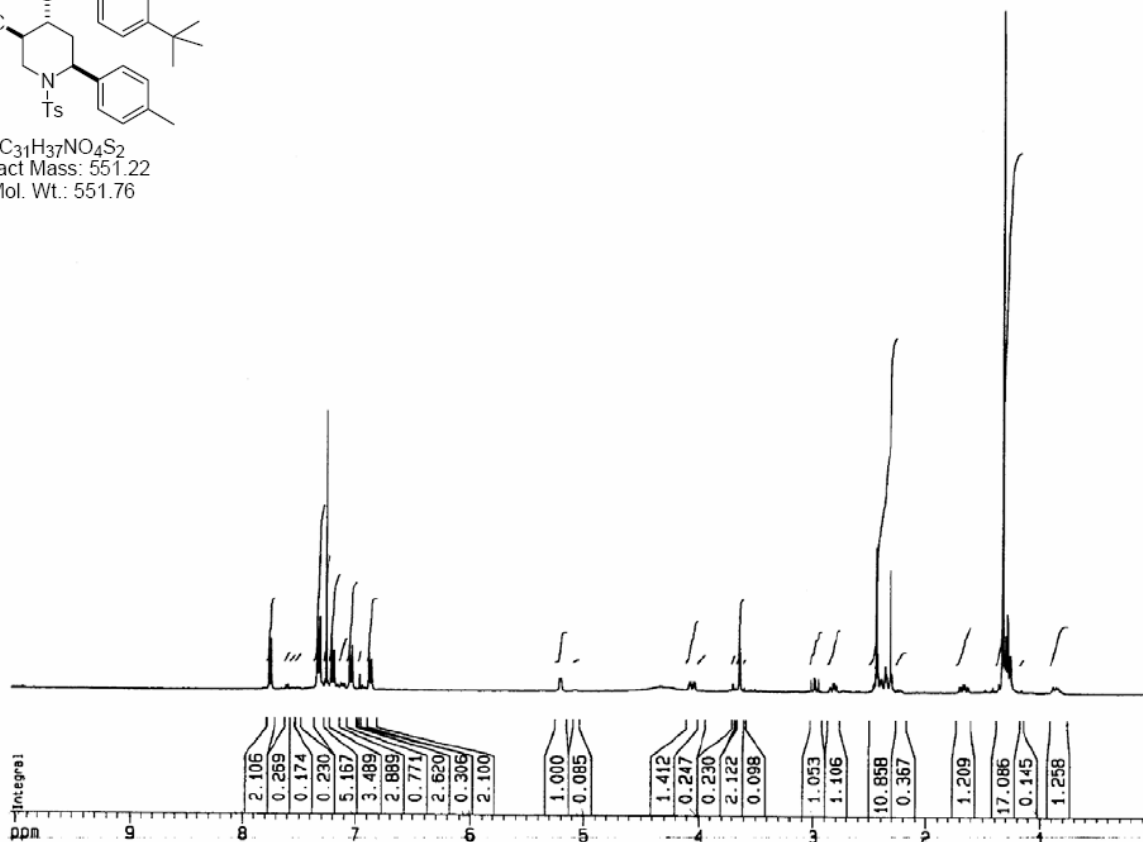
C₂₇H₂₉NO₄S₂
 Exact Mass: 495.15
 Mol. Wt.: 495.65



4-(4-*tert*-Butylbenzylsulfanyl)-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C02E07)



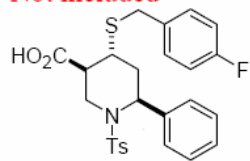
C₃₁H₃₇NO₄S₂
 Exact Mass: 551.22
 Mol. Wt.: 551.76



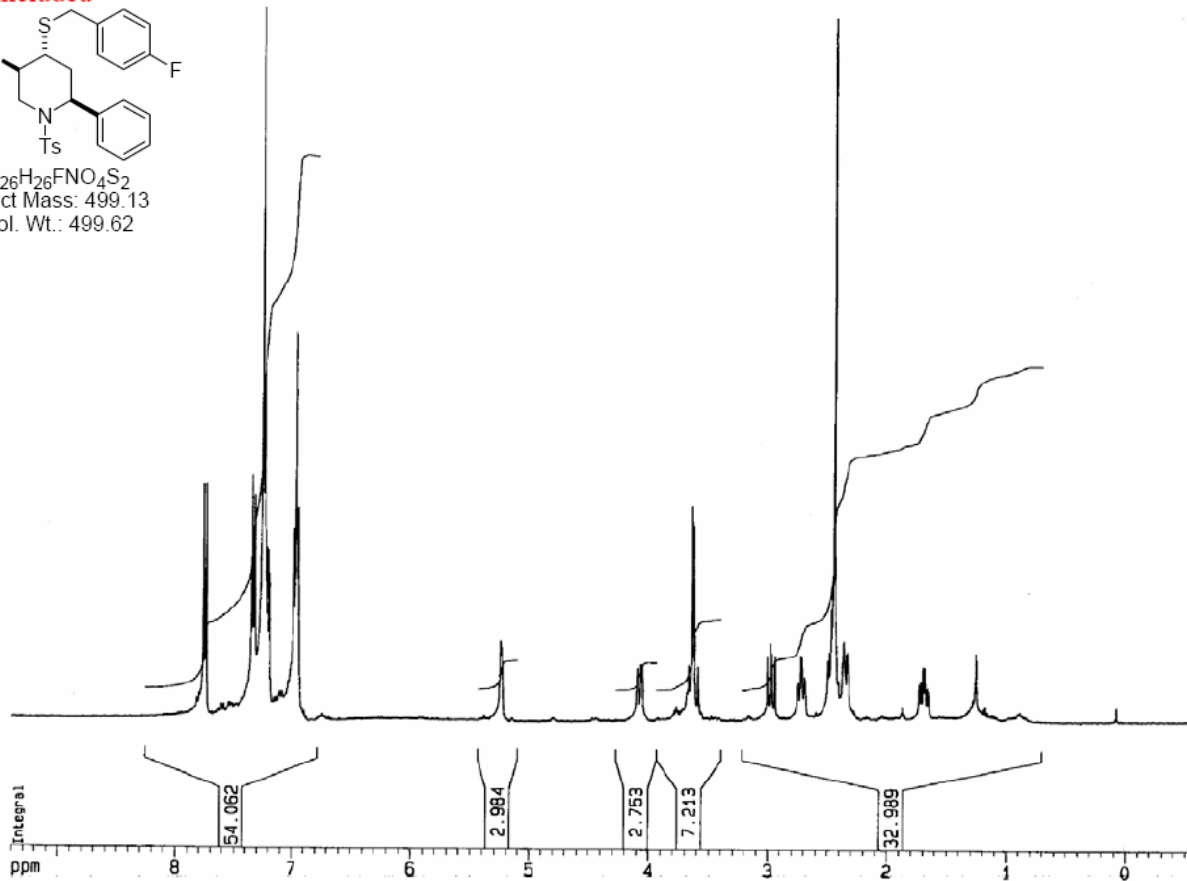
Since the automatic analysis took place up to 5 min retention time, the sample was analyzed independently and we detected (M+Na)⁺ at m/z 574.0.

4-(4-Fluorobenzylsulfanyl)-6-phenyl-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C01E08)

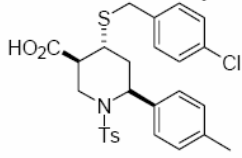
Not included



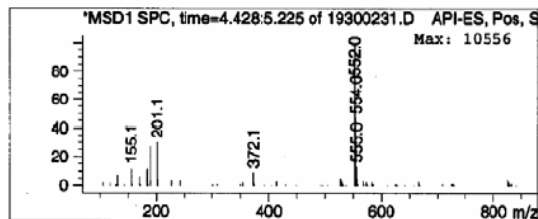
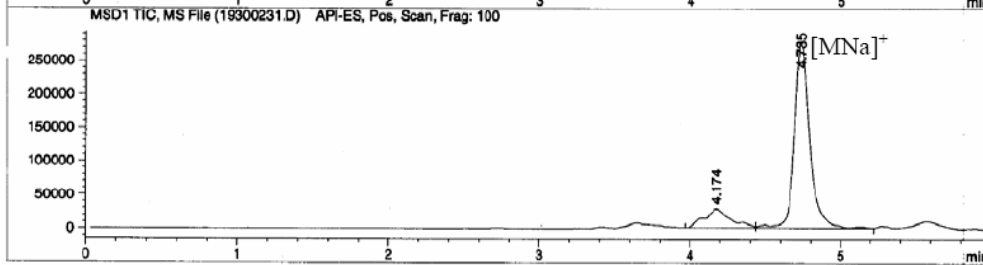
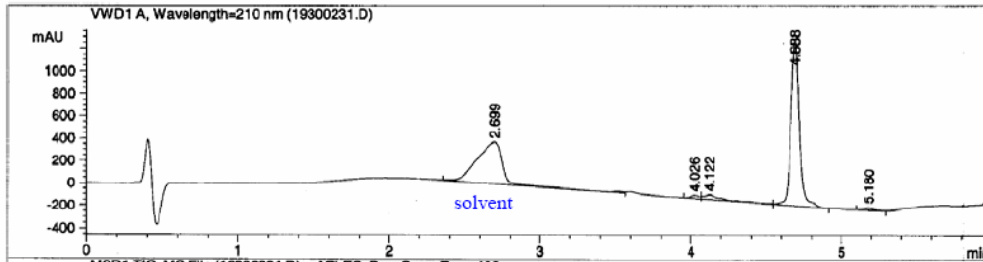
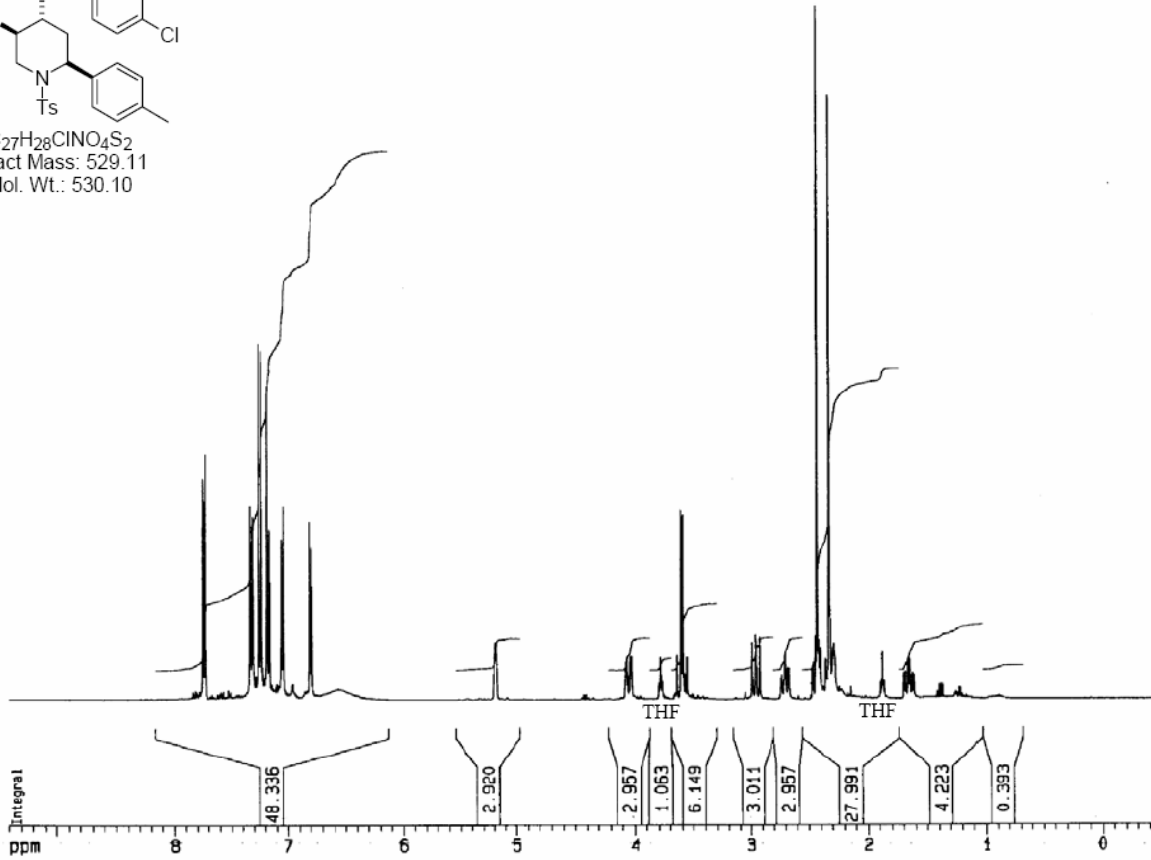
$C_{26}H_{26}FNO_4S_2$
Exact Mass: 499.13
Mol. Wt.: 499.62



4-(4-Chlorobenzylsulfanyl)-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C02E09)

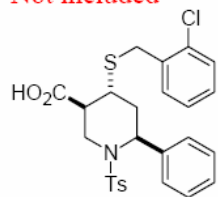


C₂₇H₂₈ClNO₄S₂
 Exact Mass: 529.11
 Mol. Wt.: 530.10

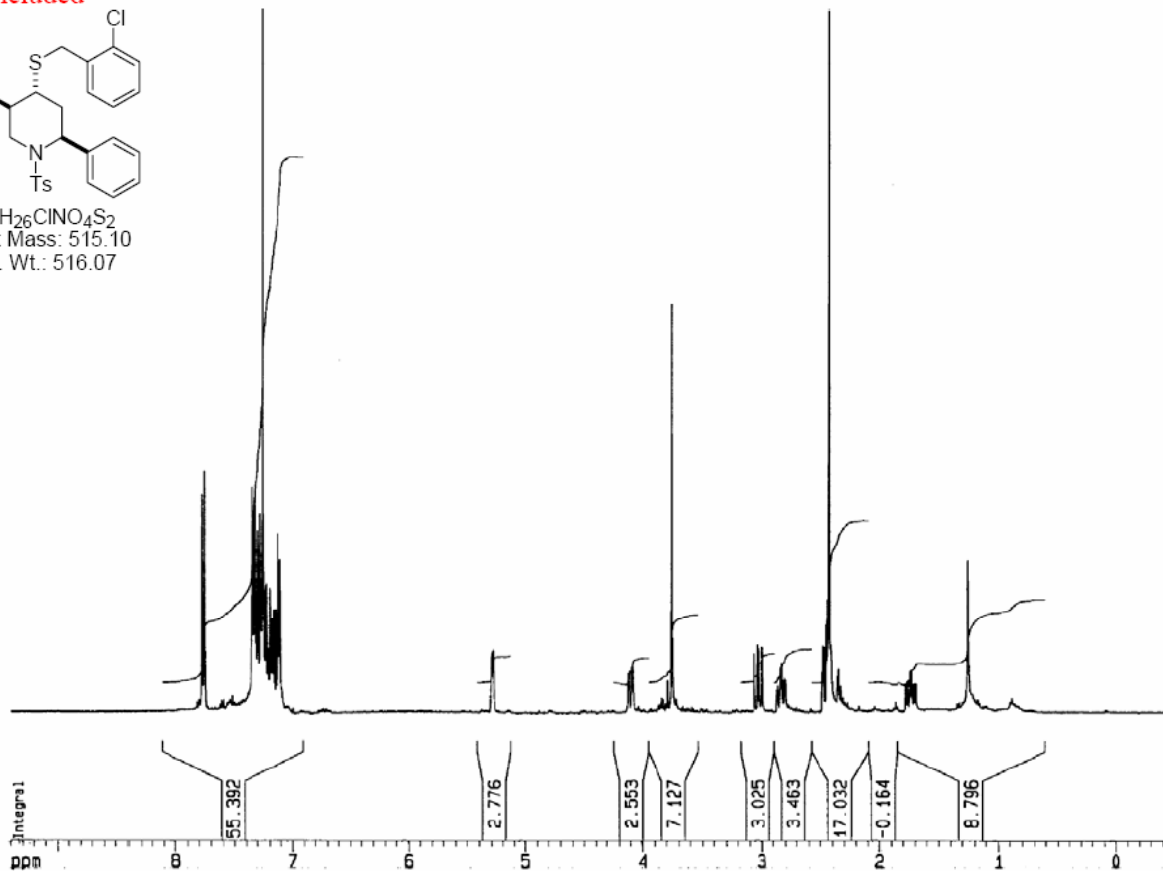


4-(2-Chlorobenzylsulfanyl)-6-phenyl-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C01E10)

Not included

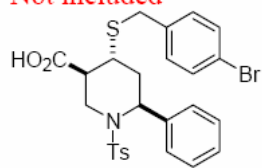


C₂₆H₂₆ClNO₄S₂
Exact Mass: 515.10
Mol. Wt.: 516.07

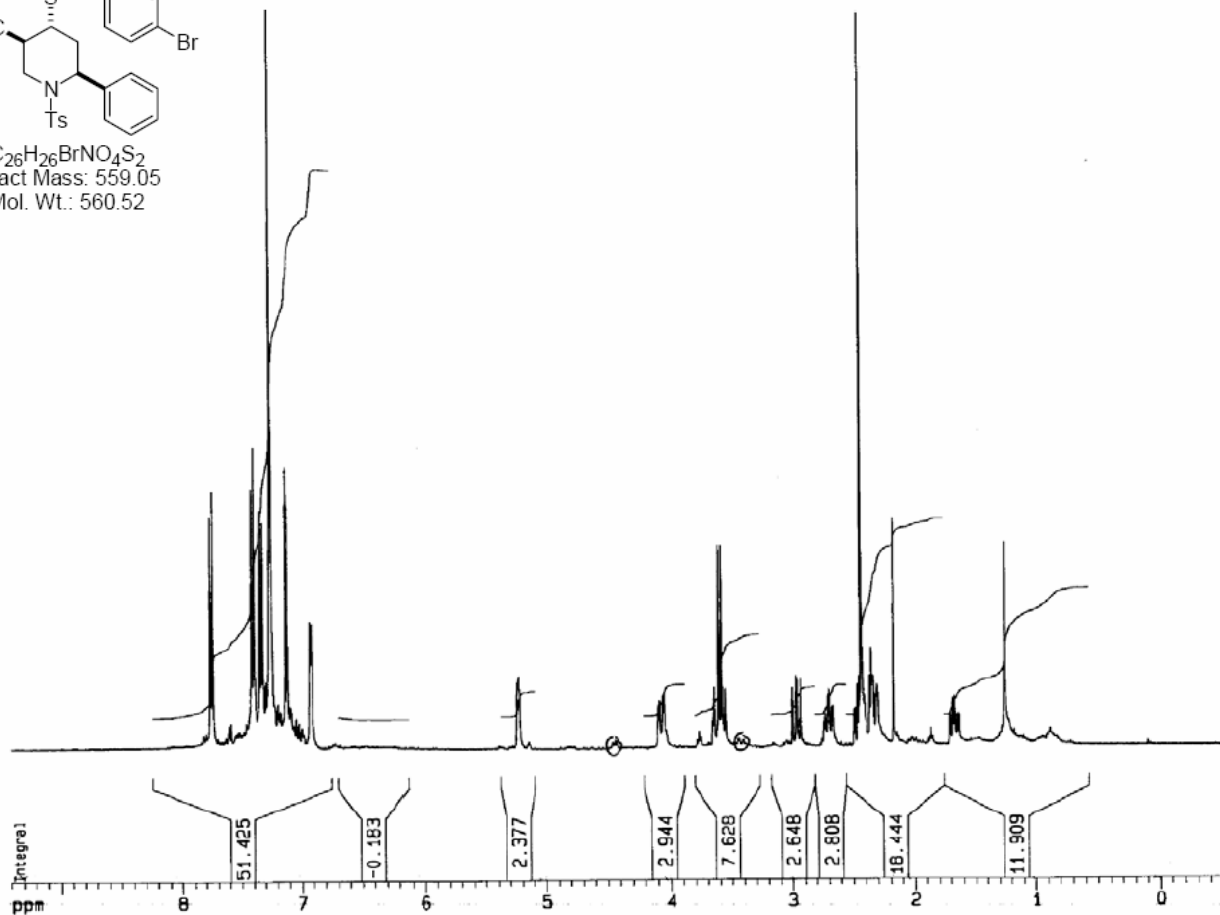


4-(4-Bromobenzylsulfanyl)-6-phenyl-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C01E11)

Not included

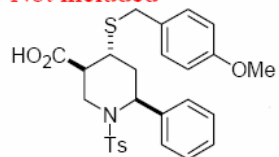


C₂₆H₂₆BrNO₄S₂
Exact Mass: 559.05
Mol. Wt.: 560.52

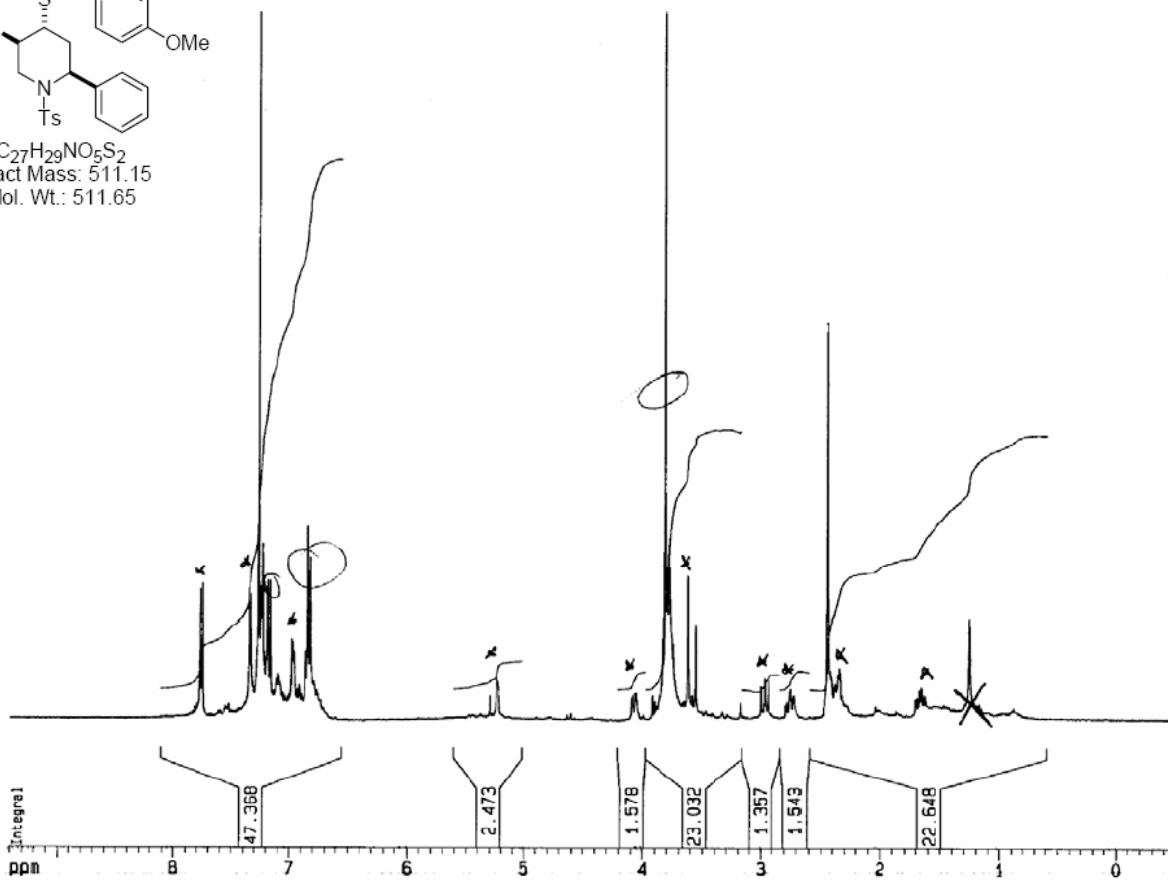


4-(4-Methoxybenzylsulfanyl)-6-phenyl-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C01E12)

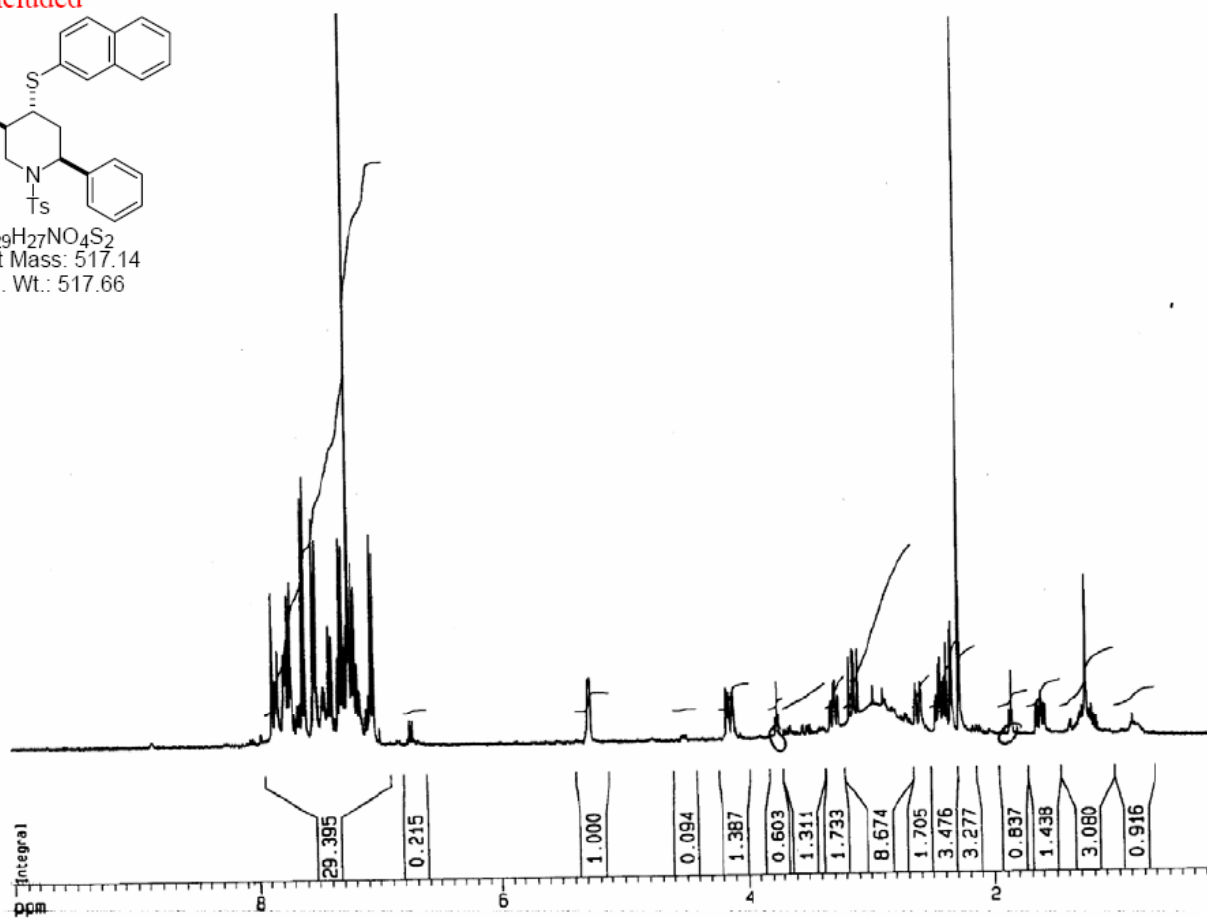
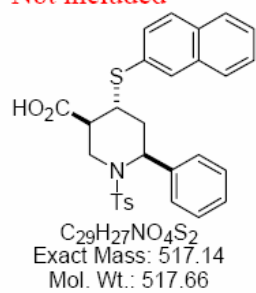
Not included



C₂₇H₂₉NO₅S₂
Exact Mass: 511.15
Mol. Wt.: 511.65

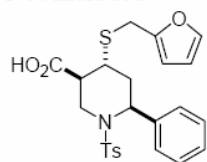


4-(Naphthalen-2-ylsulfanyl)-6-phenyl-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C01E13)
Not included

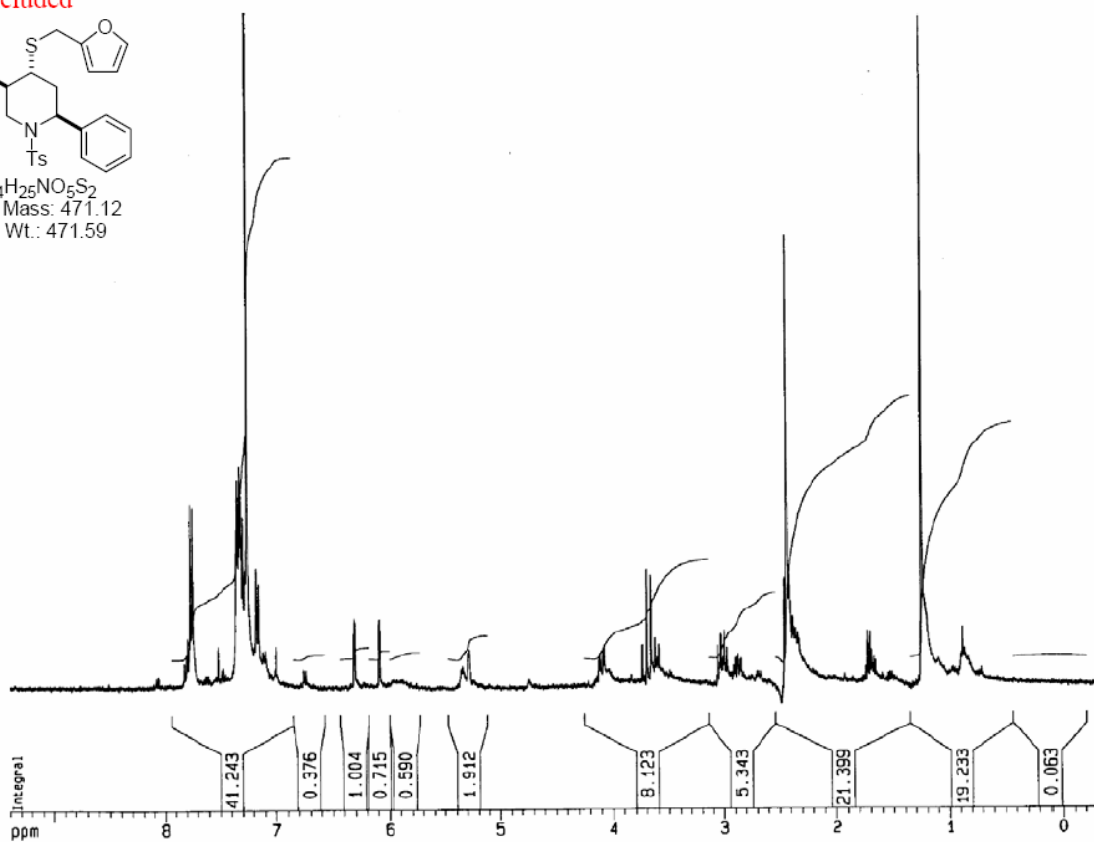


4-(Furan-2-ylmethylsulfanyl)-6-phenyl-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C01E14)

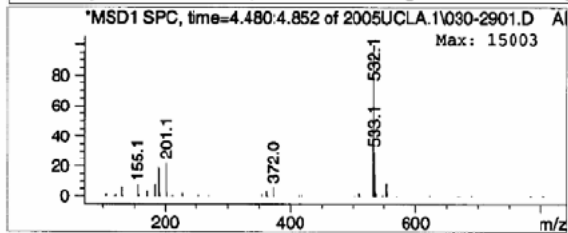
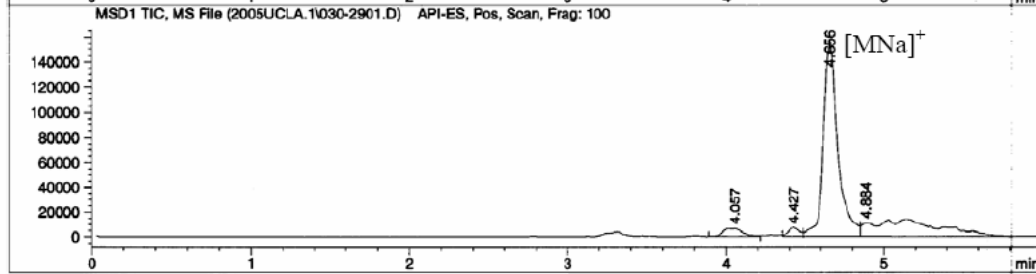
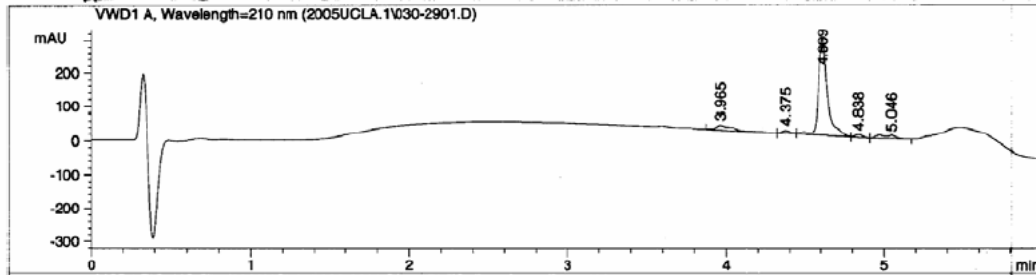
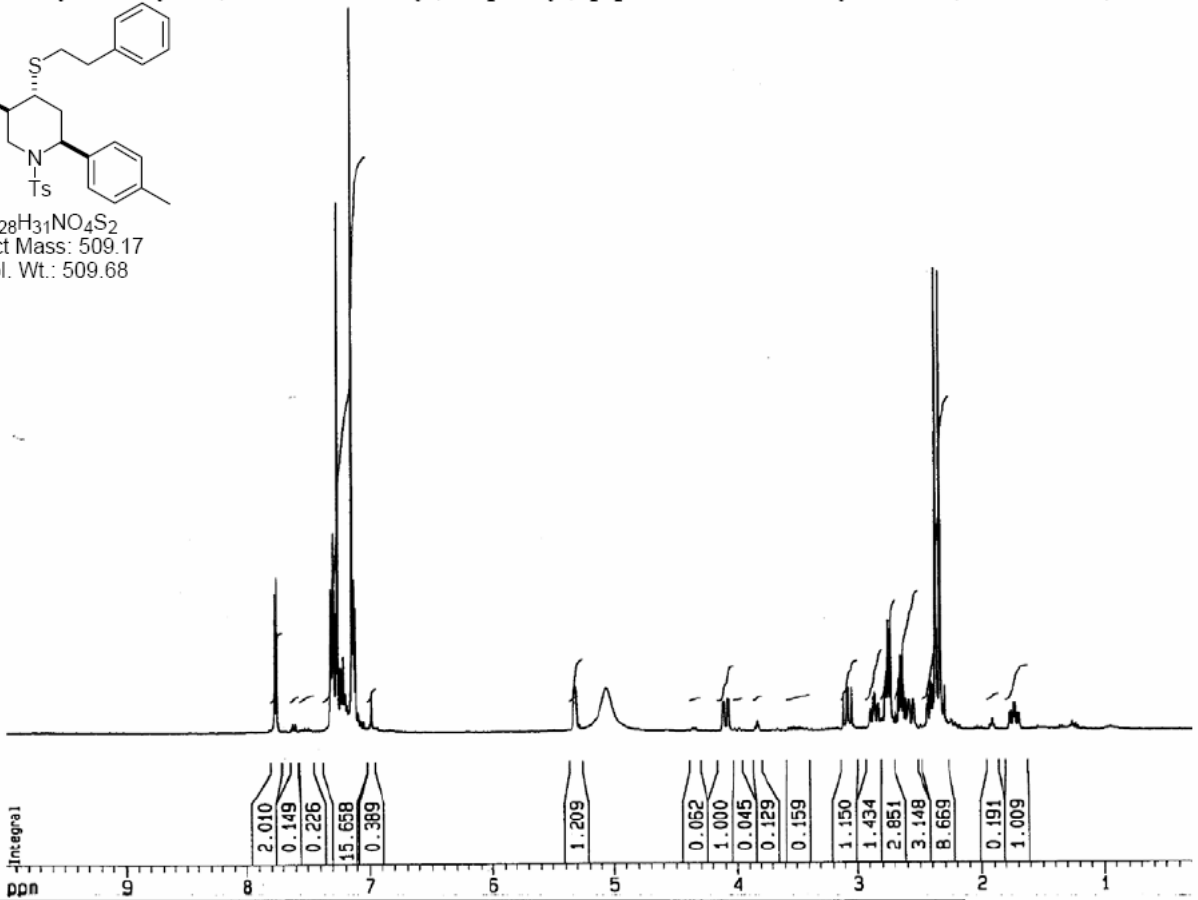
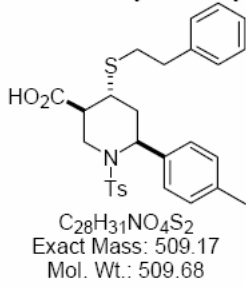
Not included



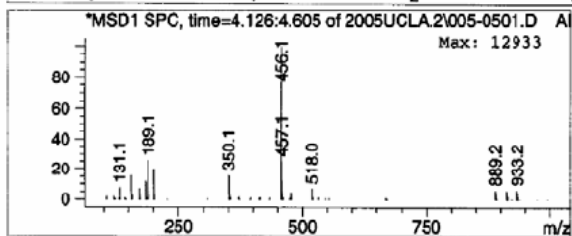
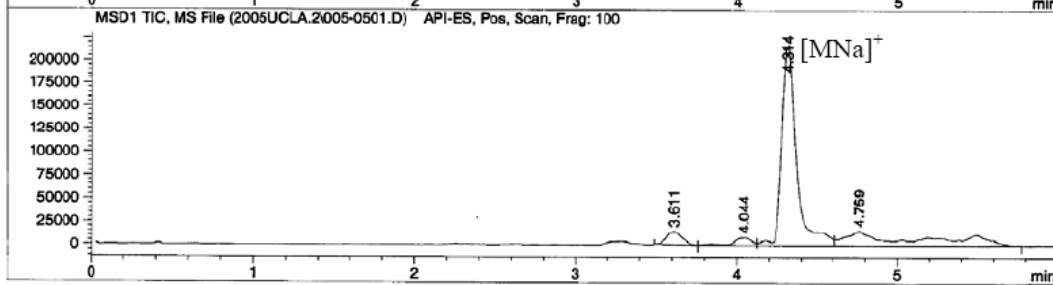
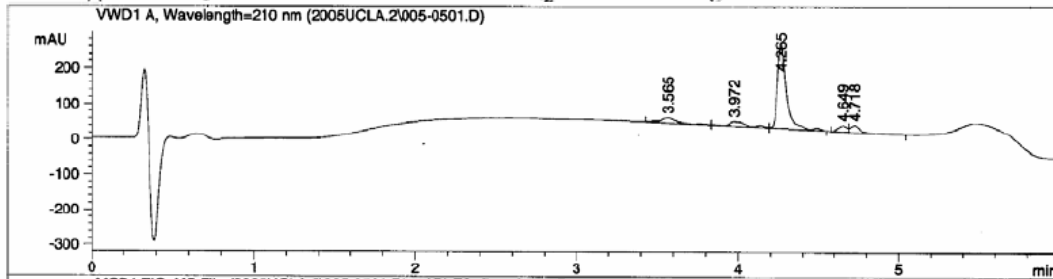
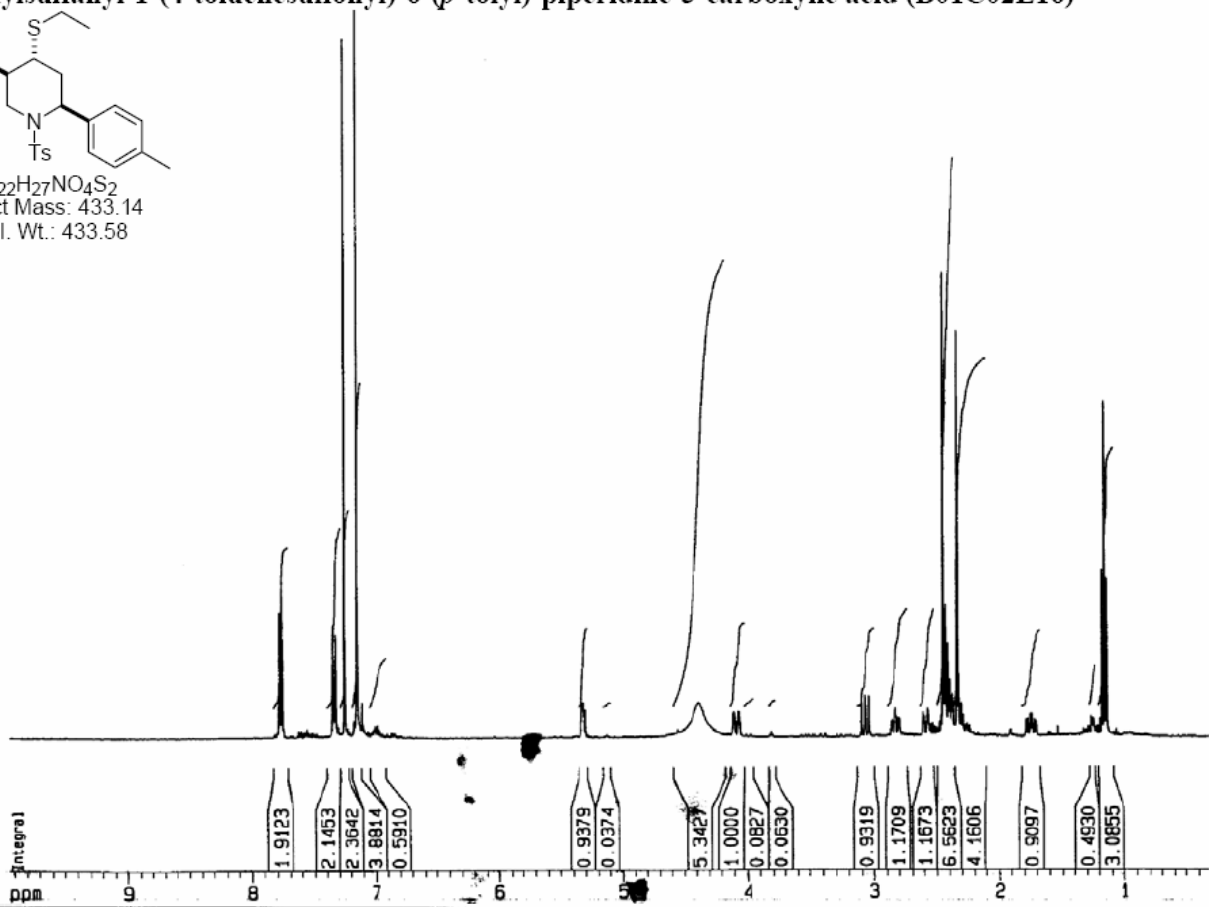
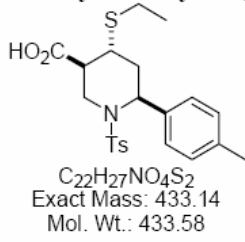
C₂₄H₂₅NO₅S₂
Exact Mass: 471.12
Mol. Wt.: 471.59



4-Phenethylsulfanyl-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C02E15)

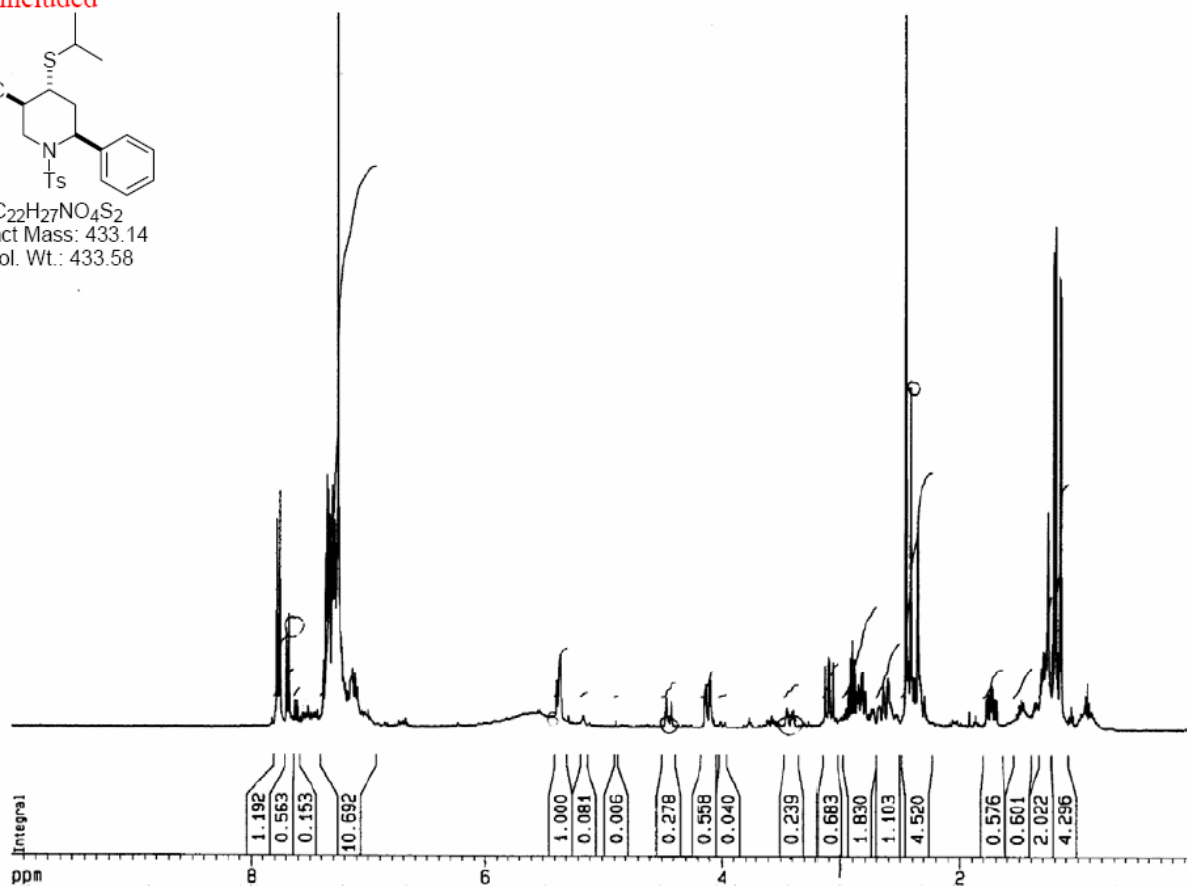
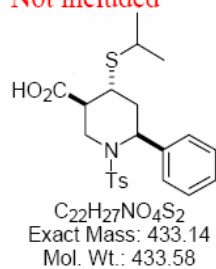


4-Ethylsulfanyl-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C02E16)

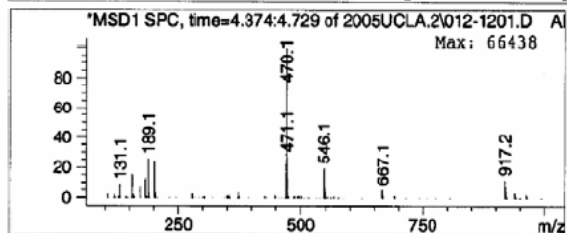
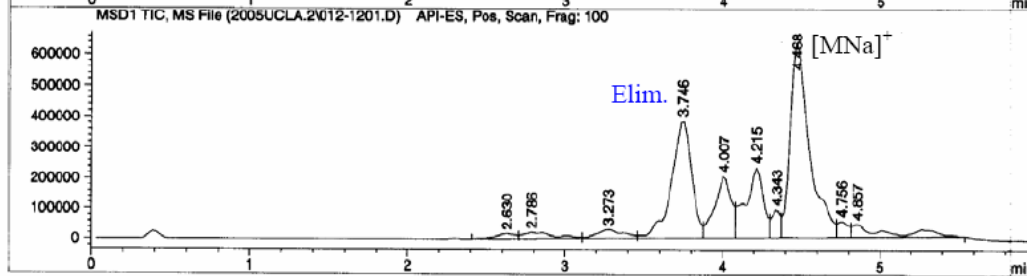
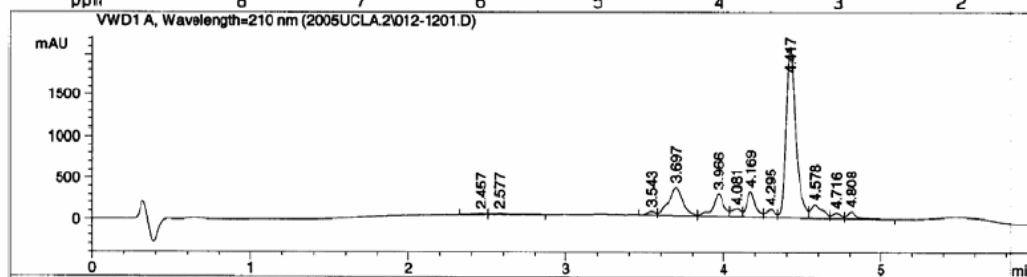
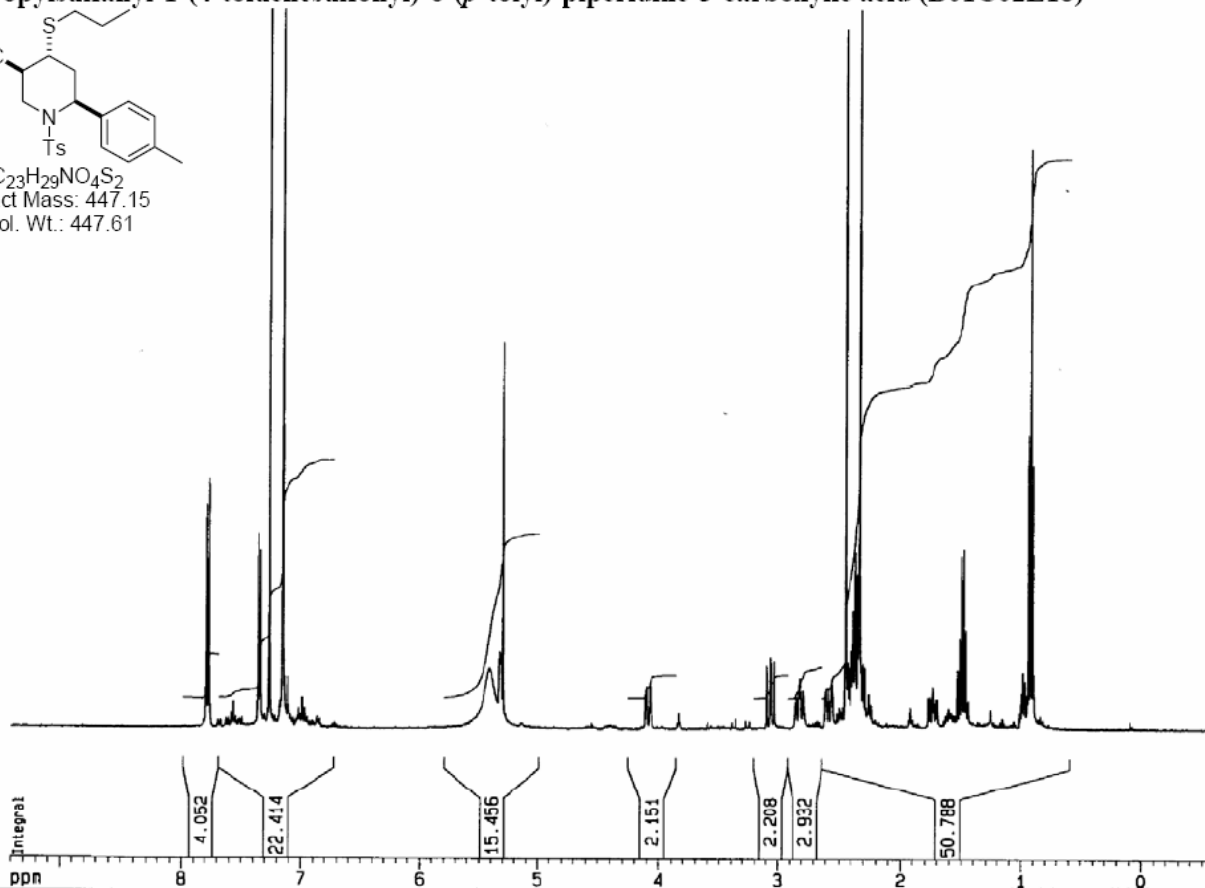
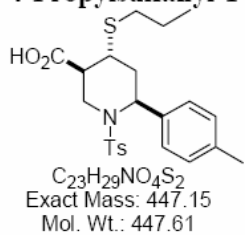


4-Isopropylsulfanyl-6-phenyl-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C01E17)

Not included

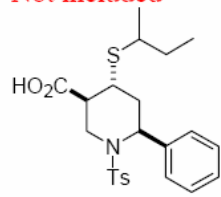


4-Propylsulfanyl-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C02E18)

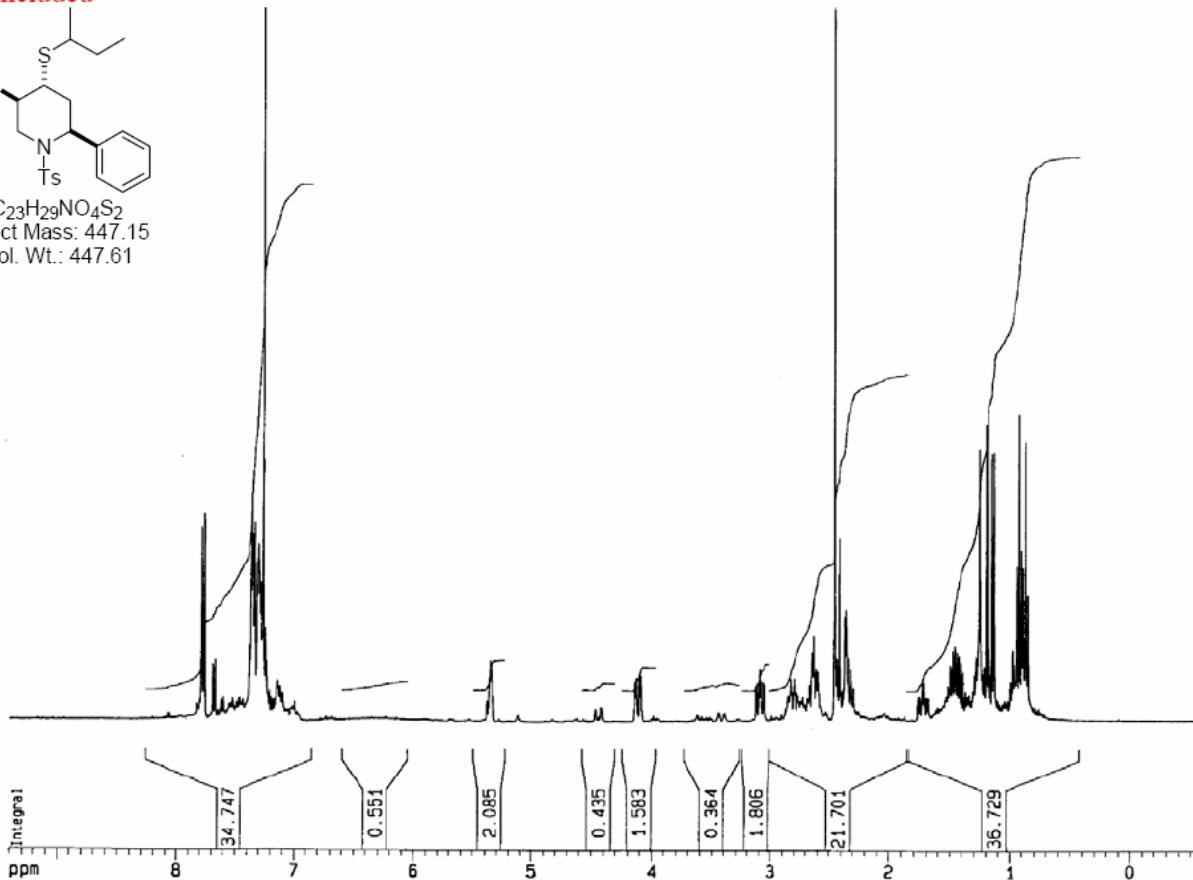


4-sec-Butylsulfanyl-1-(4-toluenesulfonyl)-6-(p-tolyl)-piperidine-3-carboxylic acid (B01C01E20)

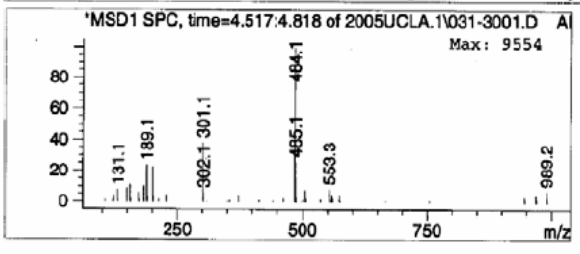
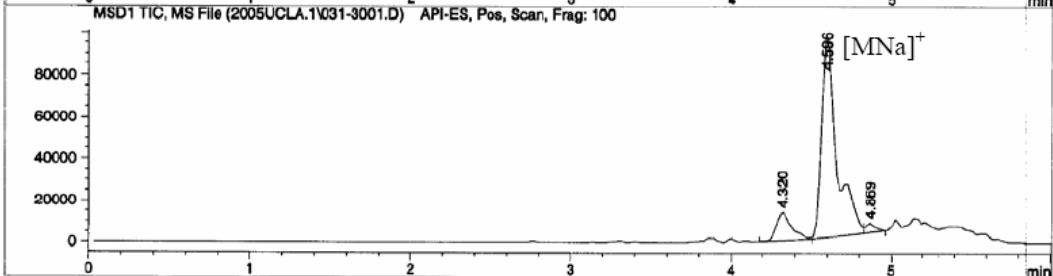
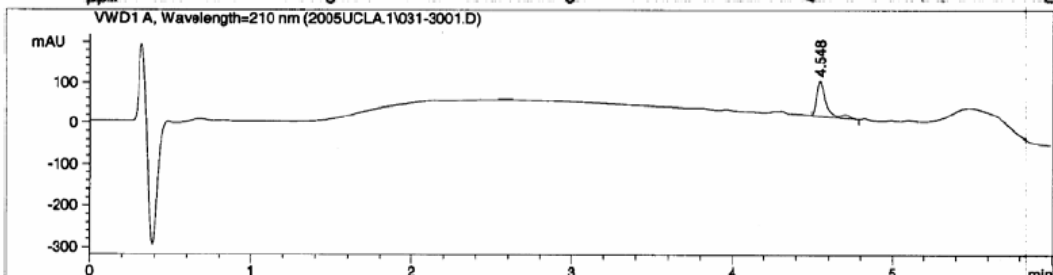
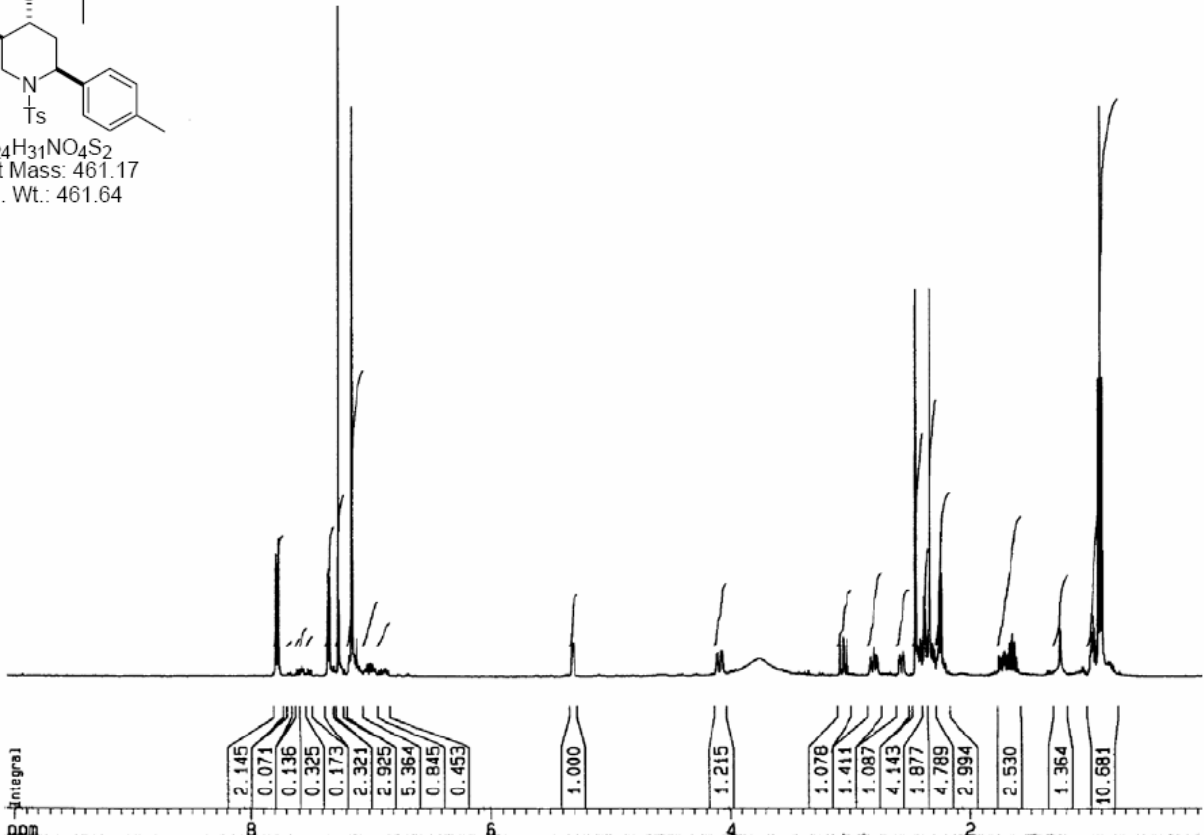
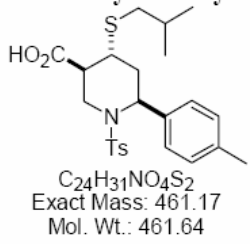
Not included



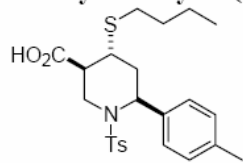
C₂₃H₂₉NO₄S₂
Exact Mass: 447.15
Mol. Wt.: 447.61



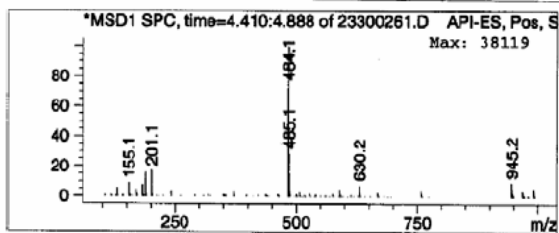
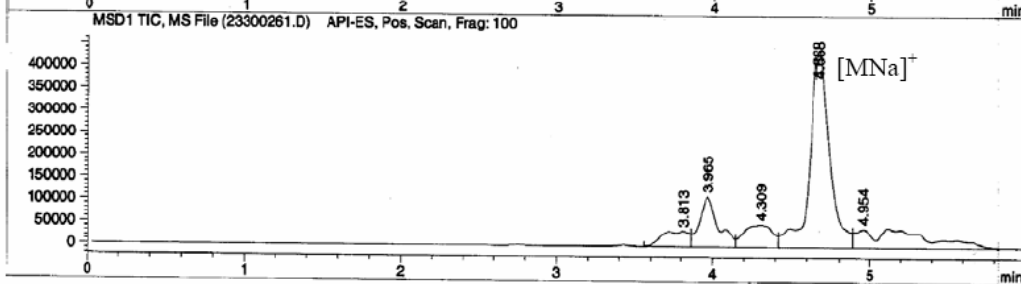
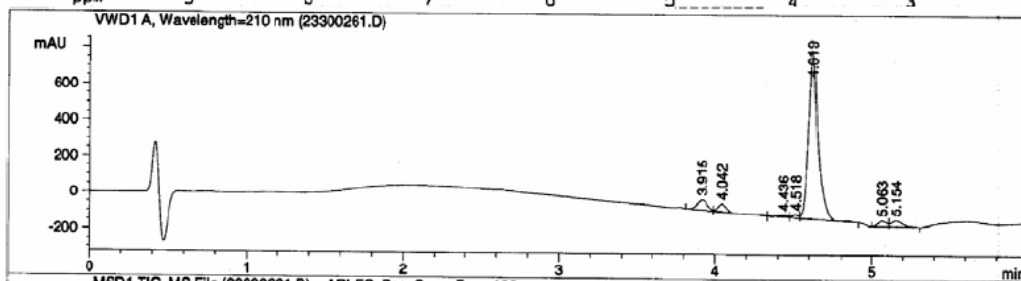
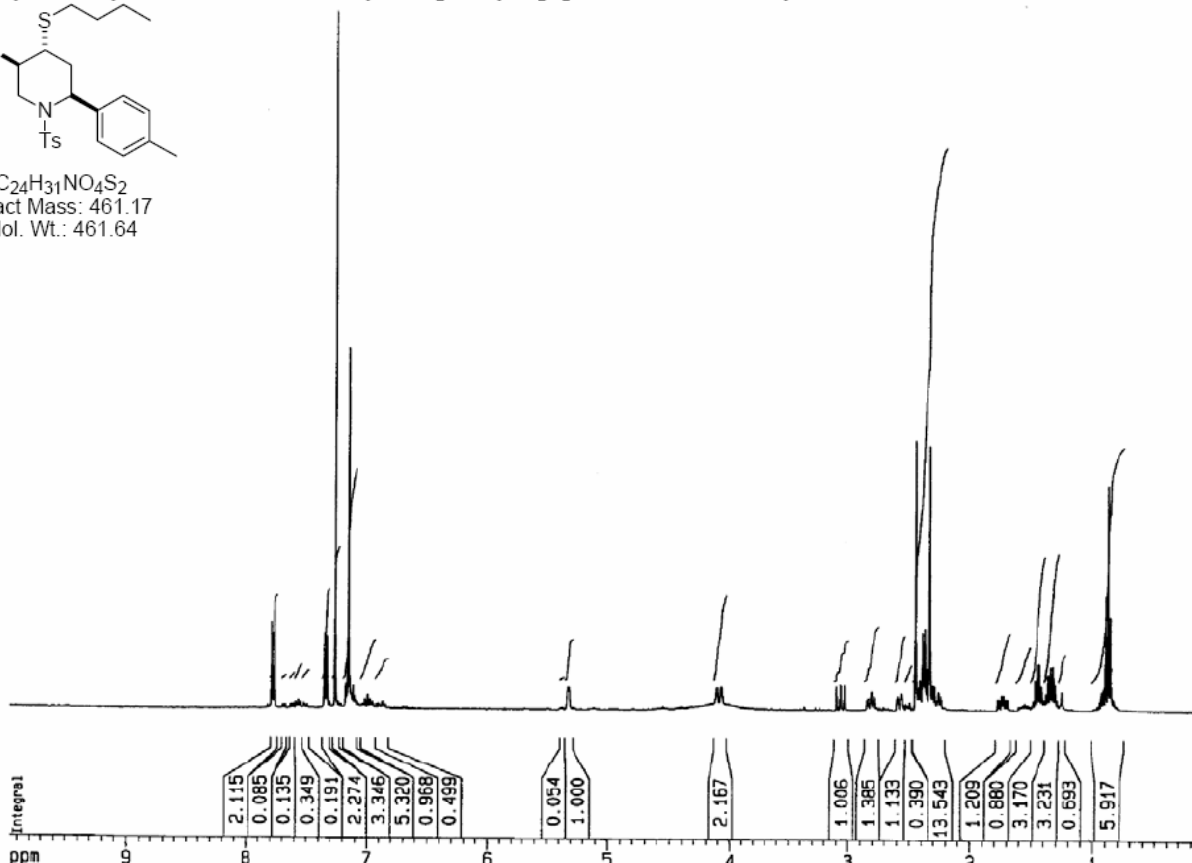
4-Isobutylsulfanyl-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C02E21)



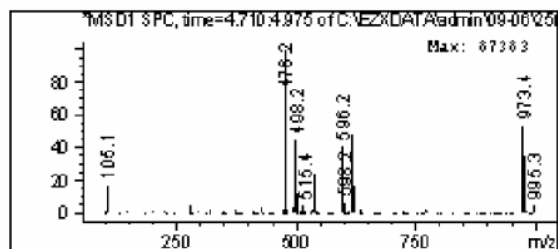
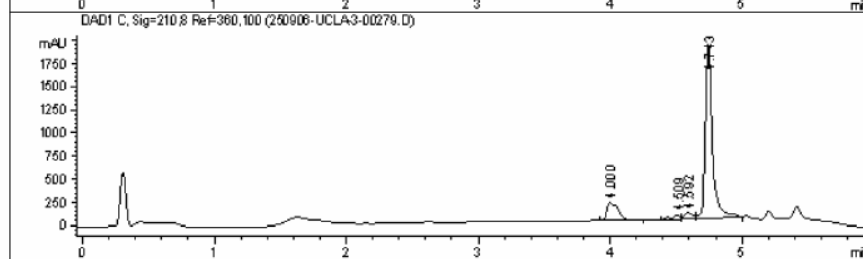
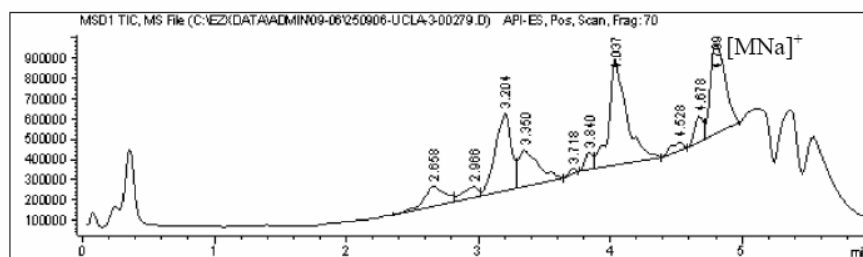
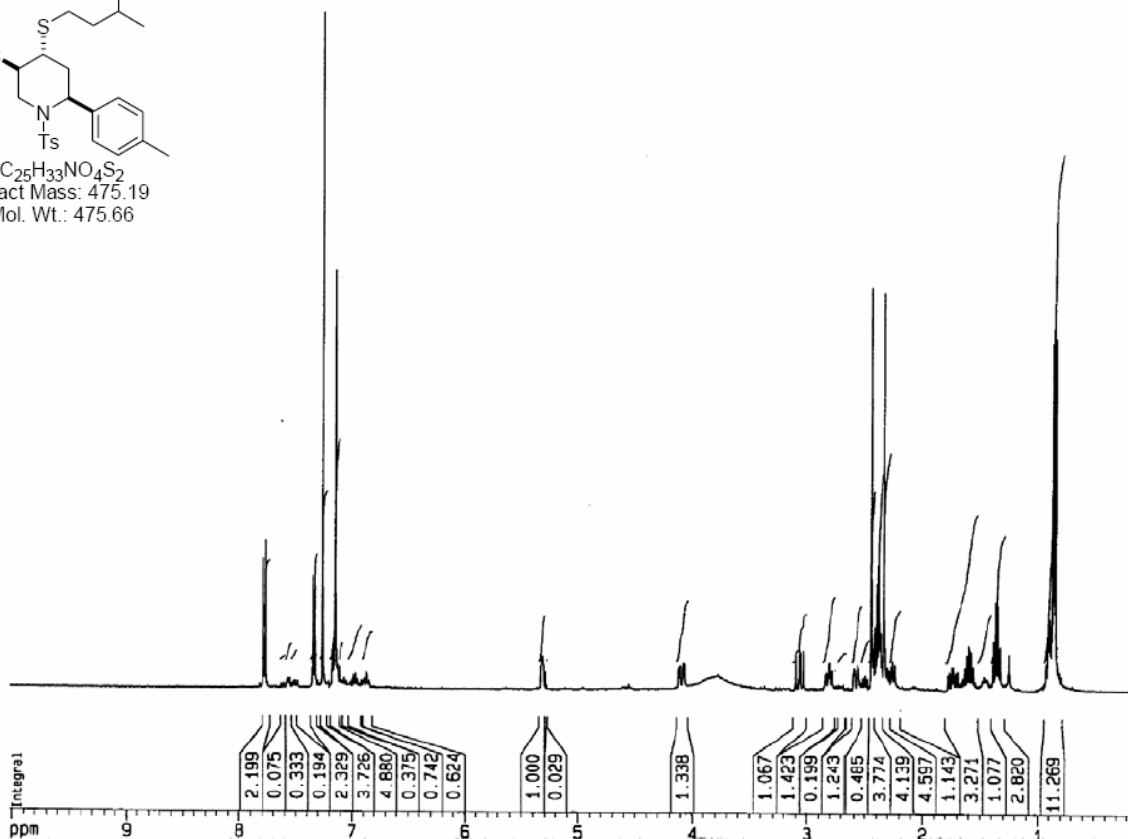
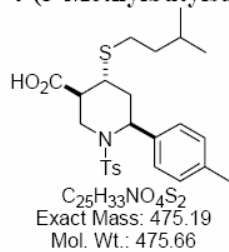
4-Butylsulfanyl-1-(4-toluenesulfonyl)-6-(p-tolyl)-piperidine-3-carboxylic acid (B01C02E22)



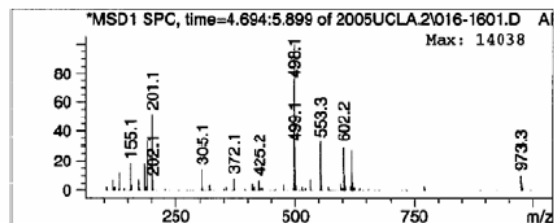
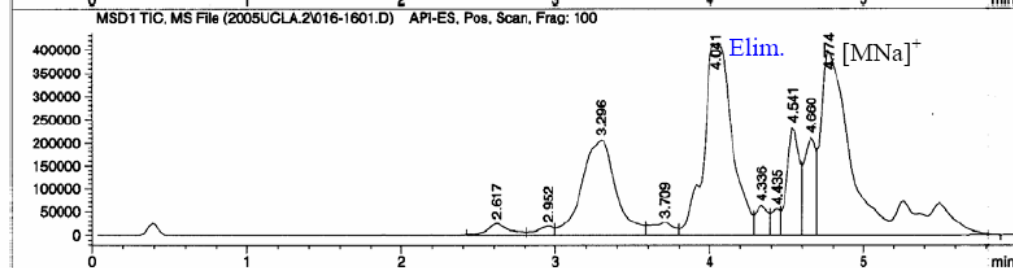
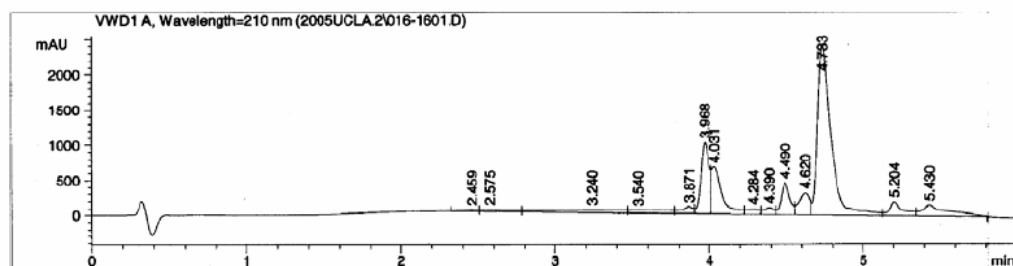
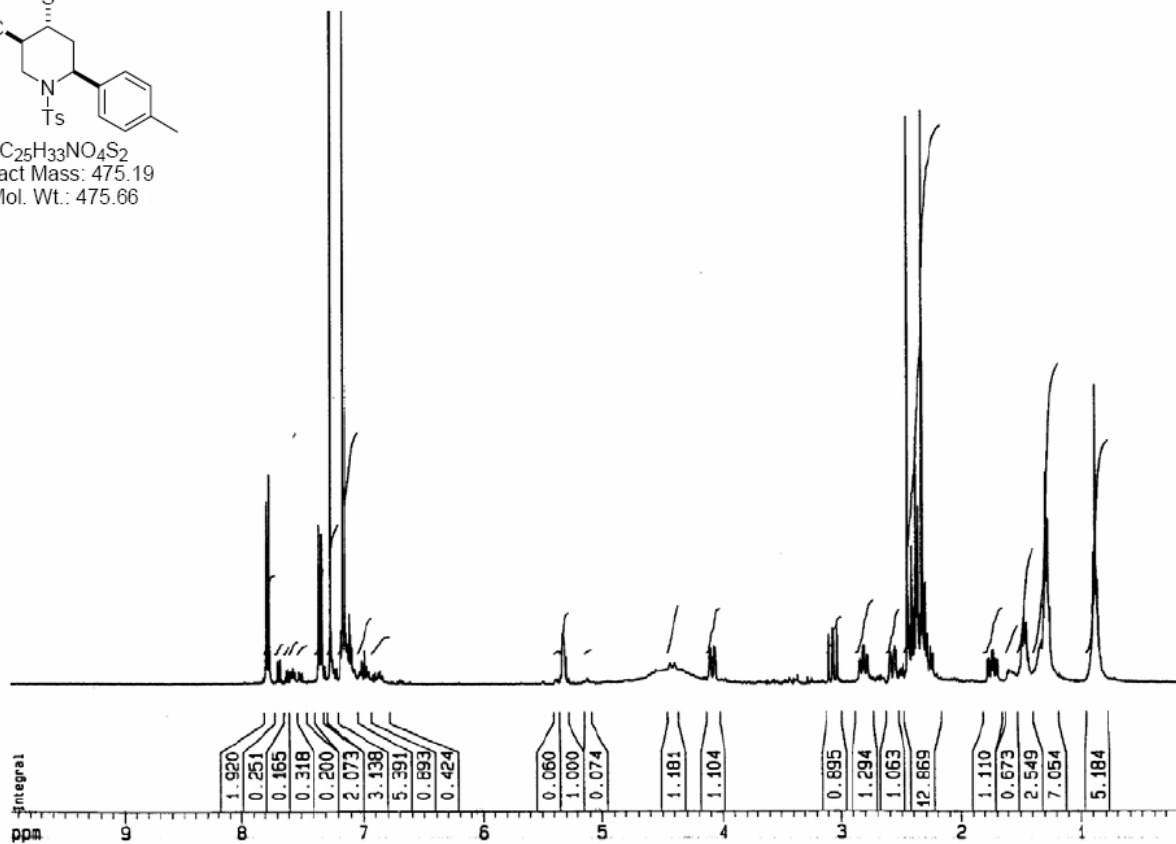
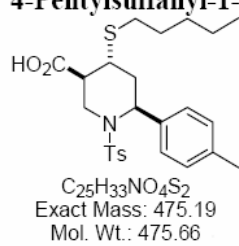
C₂₄H₃₁NO₄S₂
 Exact Mass: 461.17
 Mol. Wt.: 461.64



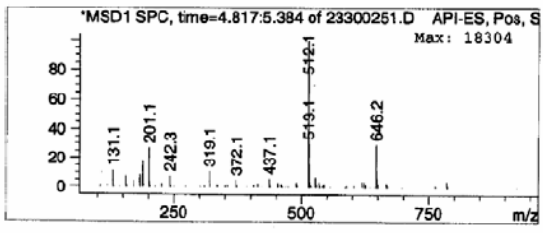
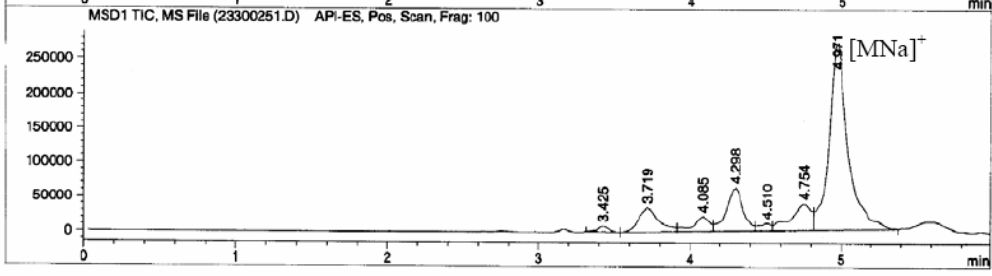
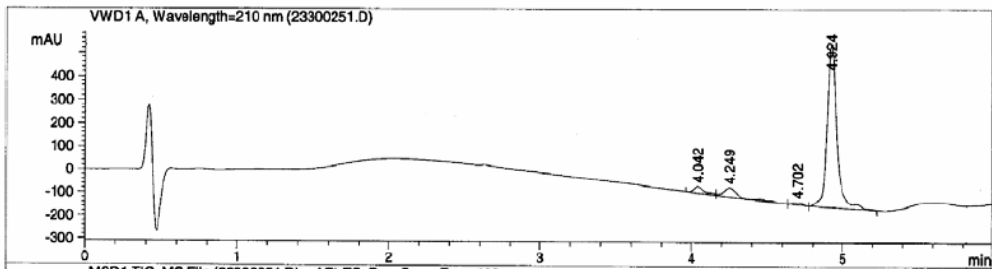
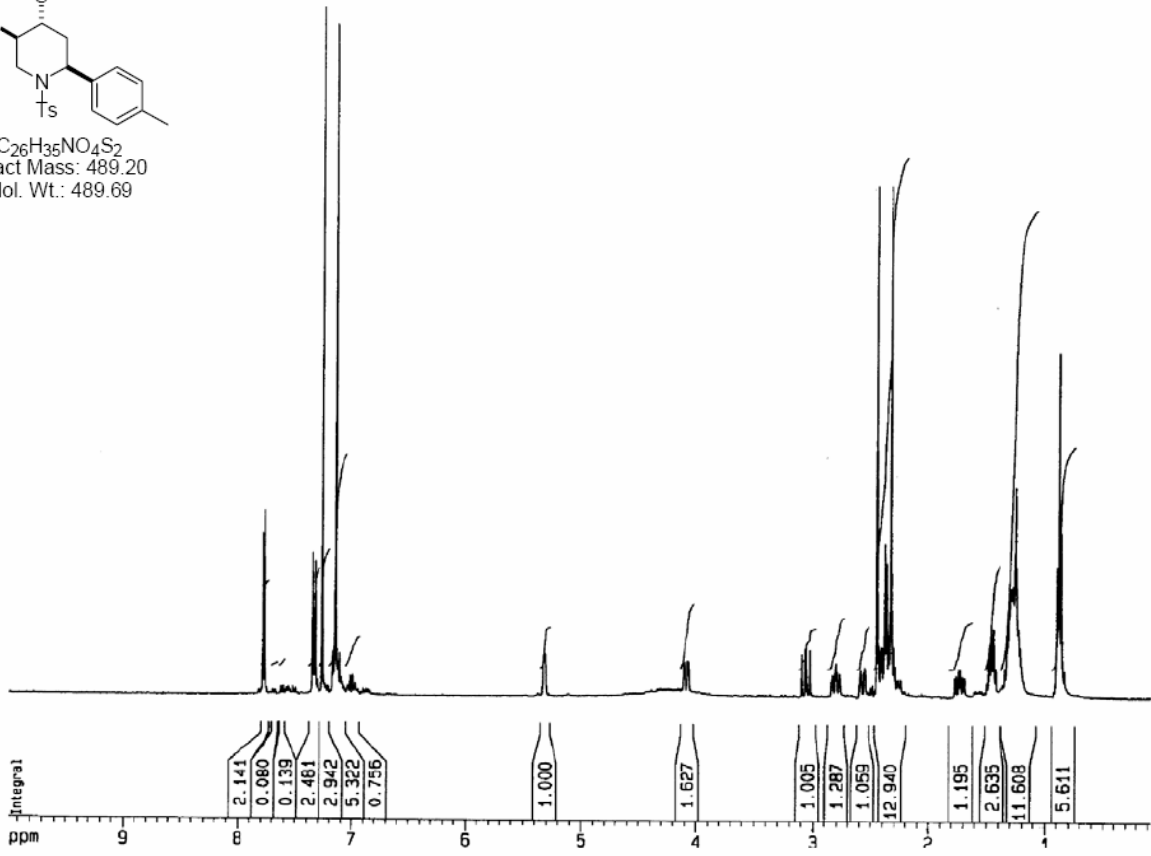
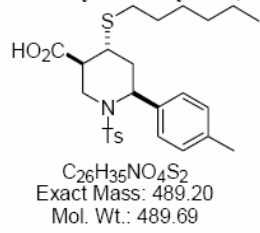
4-(3-Methylbutylsulfanyl)-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C02E23)



4-Pentylsulfanyl-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C02E24)

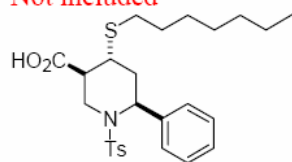


4-Hexylsulfanyl-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C02E25)

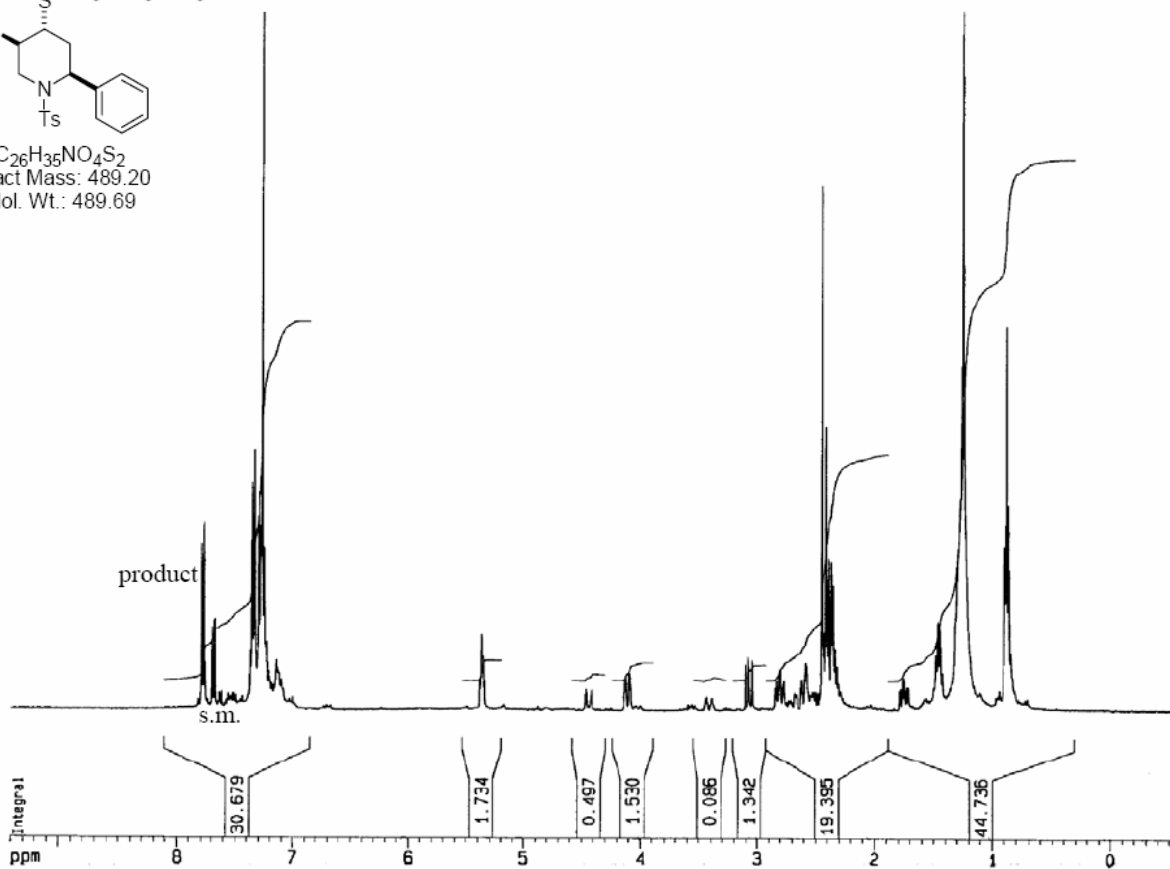


4-Heptylsulfanyl-6-phenyl-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C01E26)

Not included

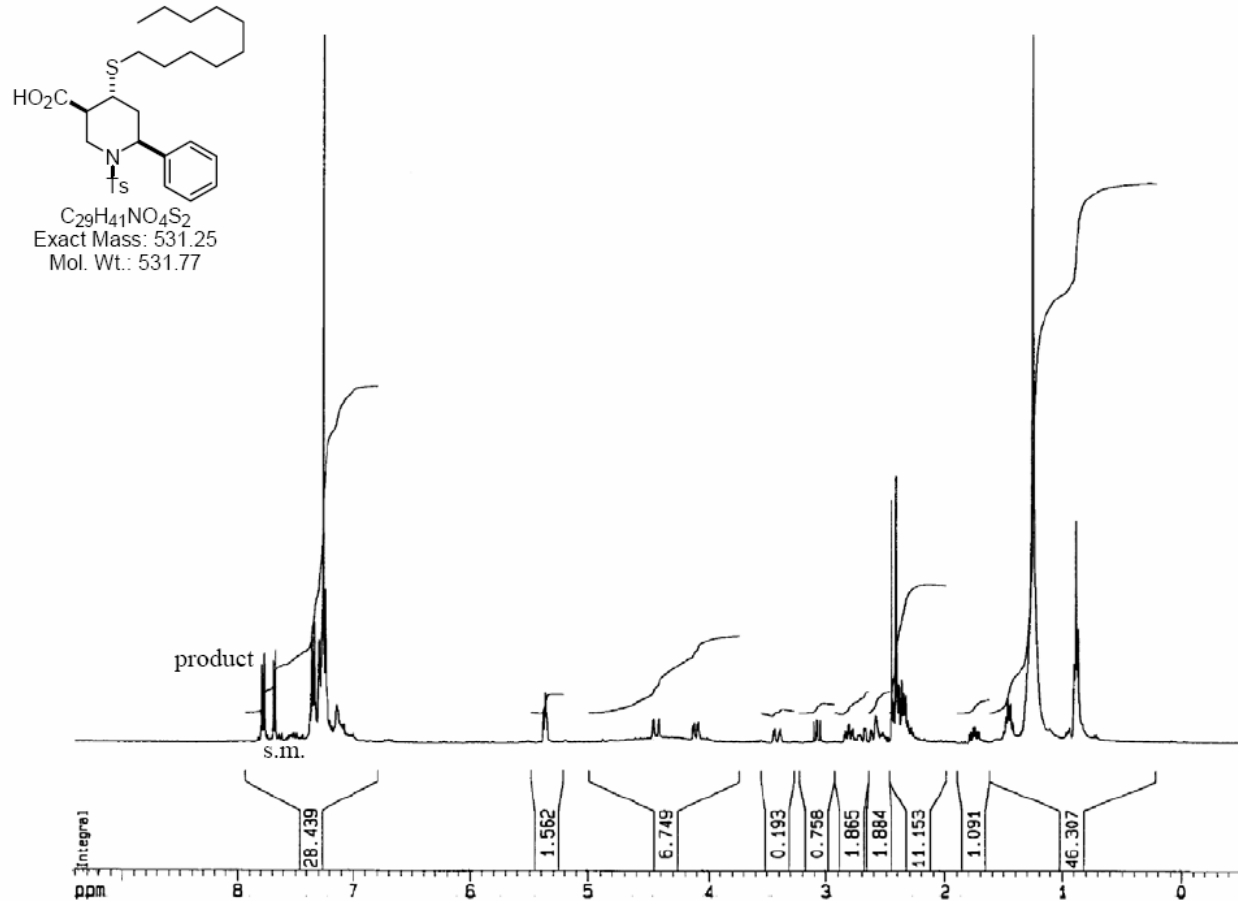


C₂₆H₃₅NO₄S₂
Exact Mass: 489.20
Mol. Wt.: 489.69

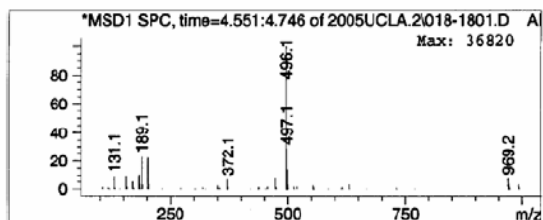
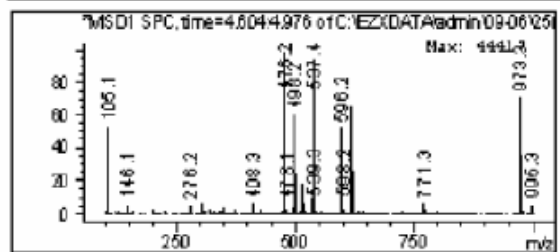
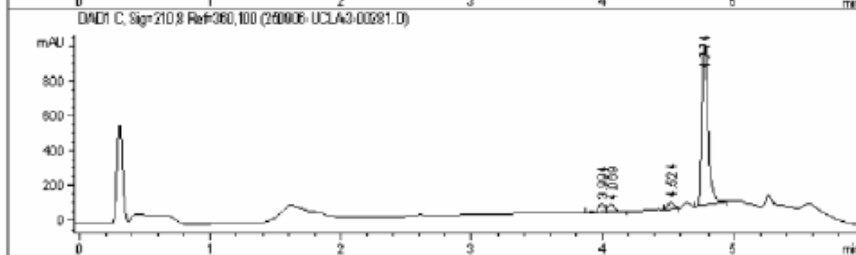
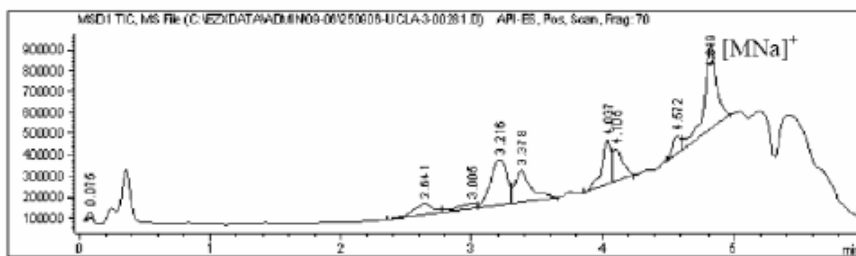
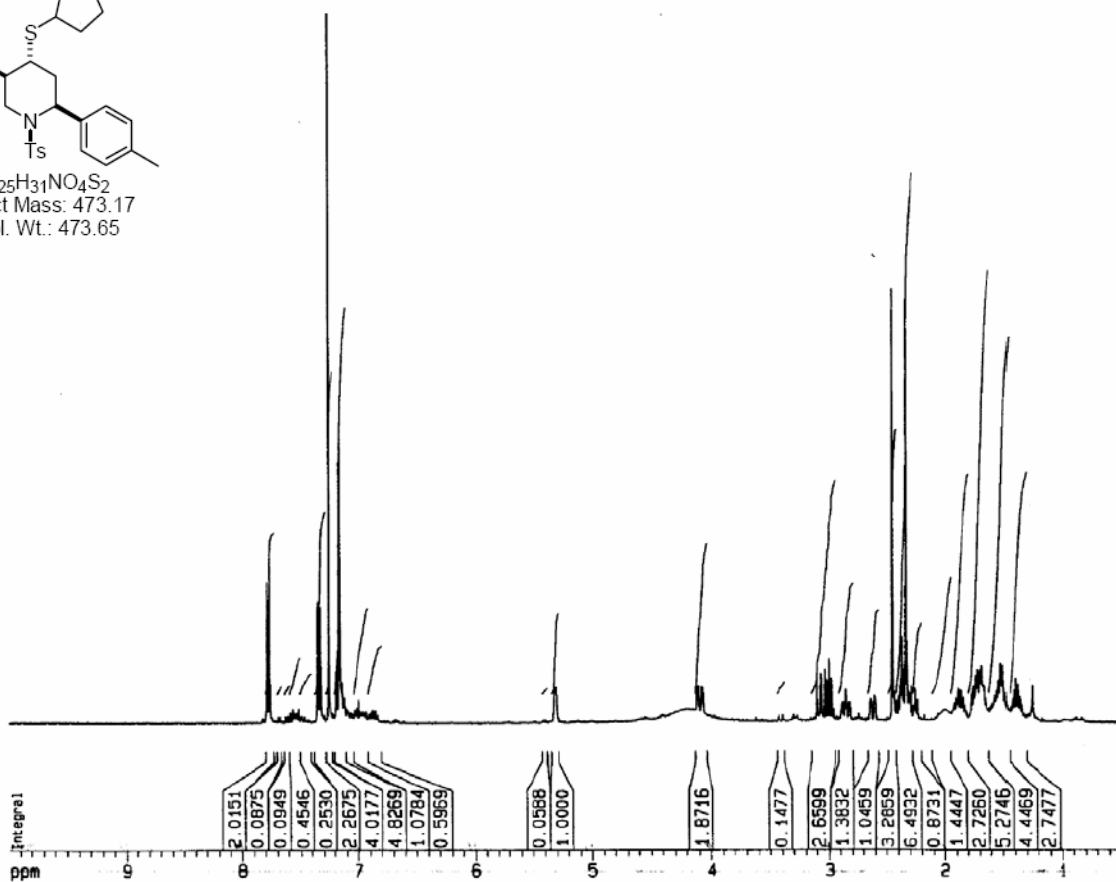
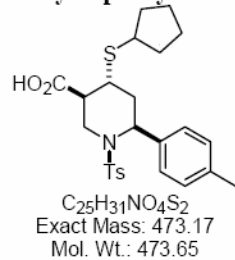


4-Decylsulfanyl-6-phenyl-1-(4-toluenesulfonyl)-piperidine-3-carboxylic acid (B01C01E27)

Not included

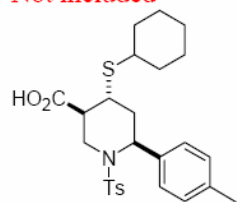


4-Cyclopentylsulfanyl-1-(toluene-4-sulfonyl)-6-*p*-tolylpiperidine-3-carboxylic acid (B01C02E28)

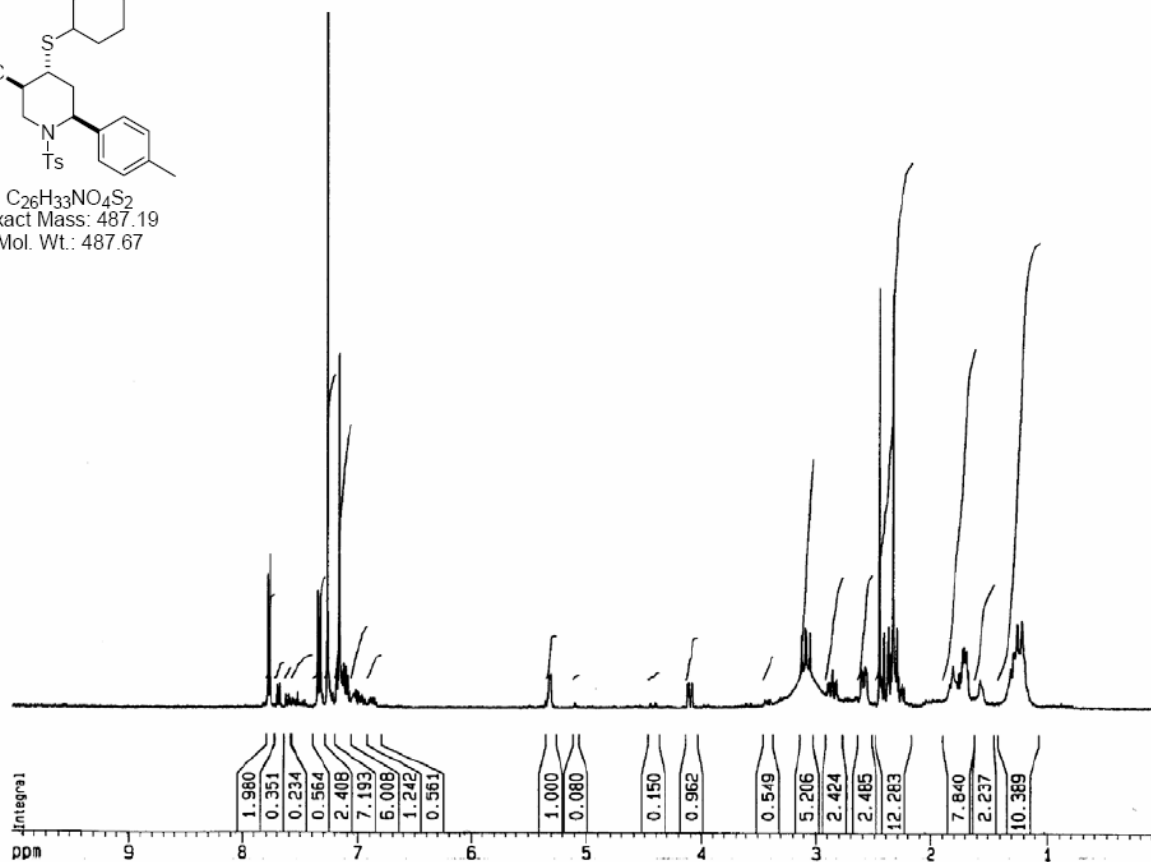


4-Cyclohexylsulfanyl-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C02E29)

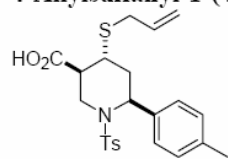
Not included



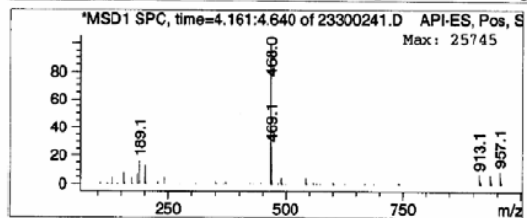
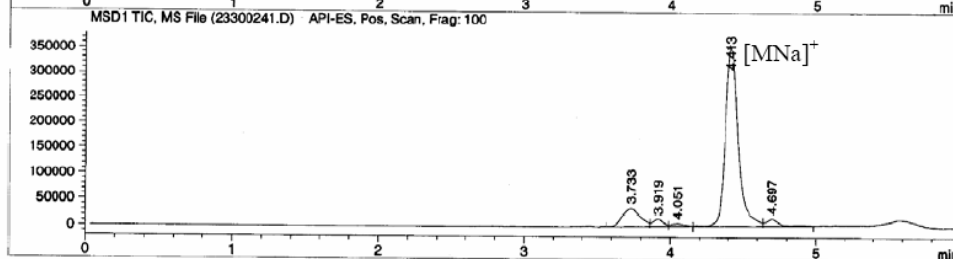
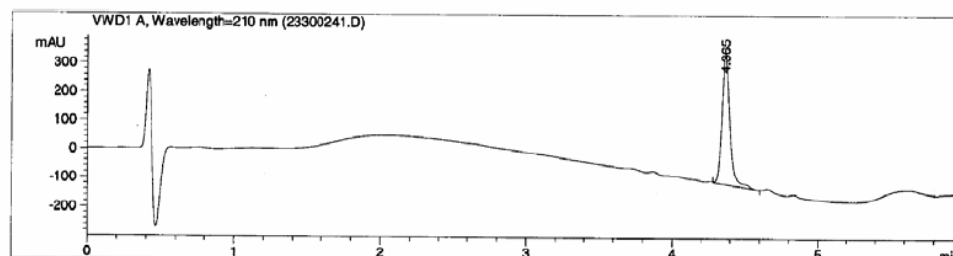
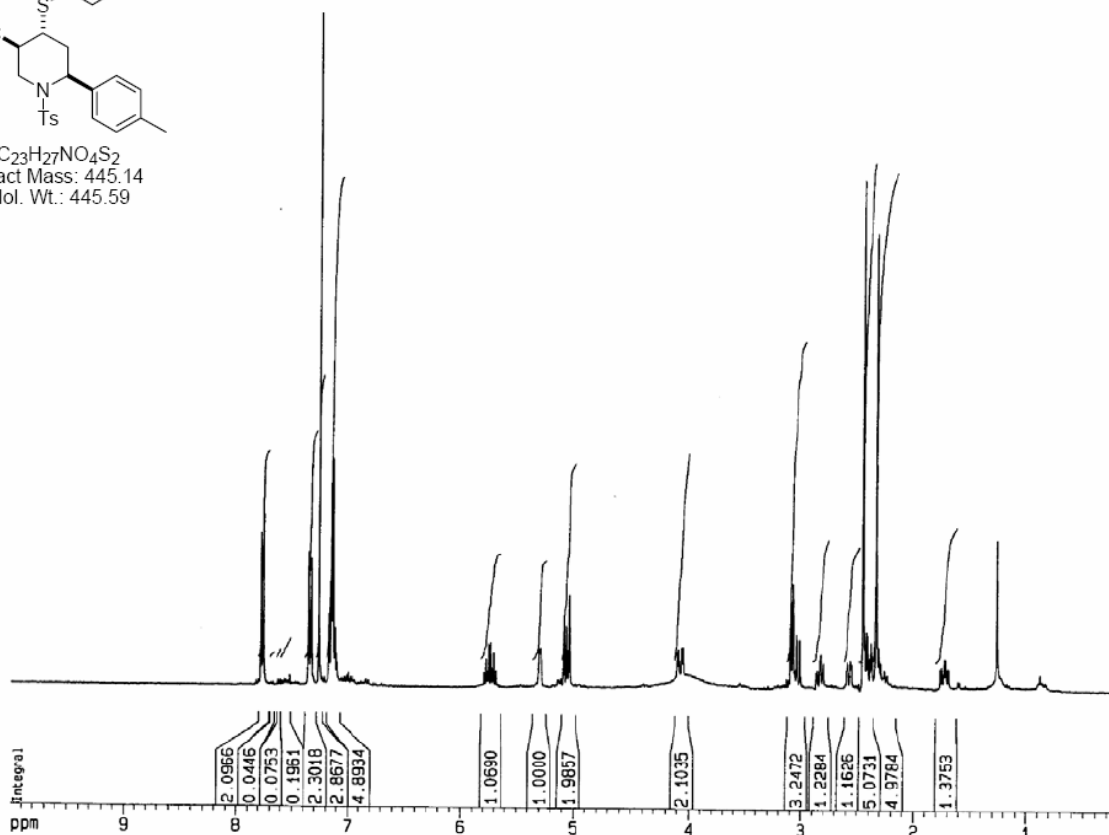
C₂₆H₃₃NO₄S₂
Exact Mass: 487.19
Mol. Wt.: 487.67



4-Allylsulfanyl-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid (B01C02E30)



C₂₃H₂₇NO₄S₂
 Exact Mass: 445.14
 Mol. Wt.: 445.59

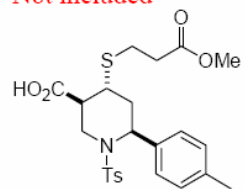


4-(2-Methoxycarbonylethylsulfanyl)-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid

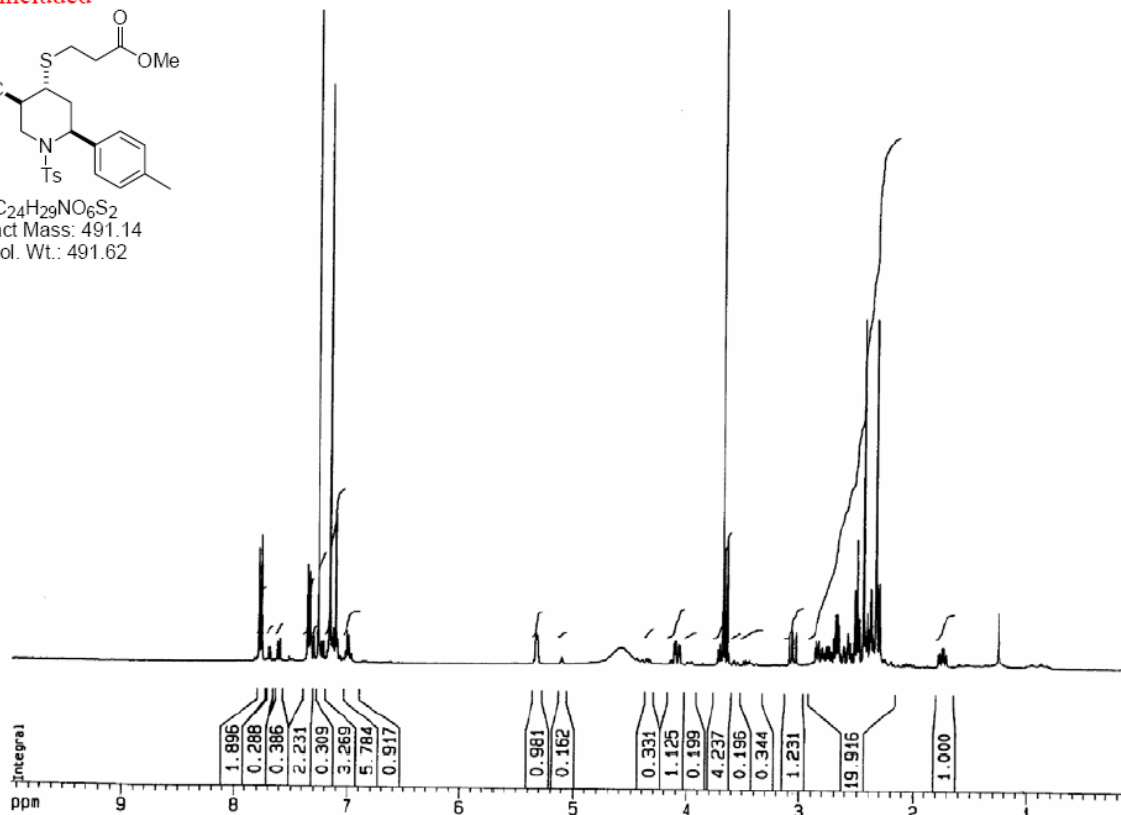
acid

(B01C02E31)

Not included



C₂₄H₂₉NO₆S₂
Exact Mass: 491.14
Mol. Wt.: 491.62



4-(2-*tert*-Butoxycarbonylethylsulfanyl)-1-(4-toluenesulfonyl)-6-(*p*-tolyl)-piperidine-3-carboxylic acid
(B01C02E32)
Not included

