

Supporting Information, Part E

**Small-Molecule Inhibitors of Protein Geranylgeranyltransferase Type I**

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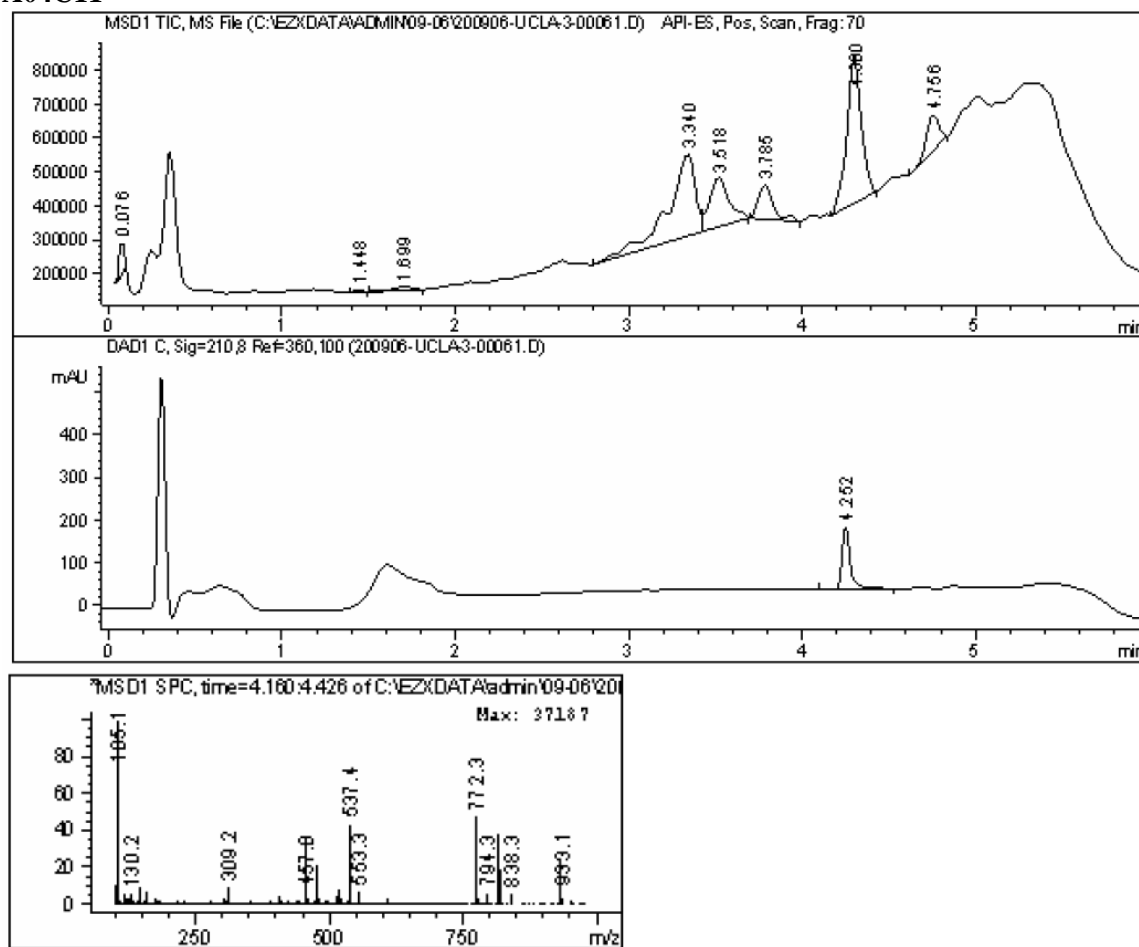
Spectral Data for Table 17

S382

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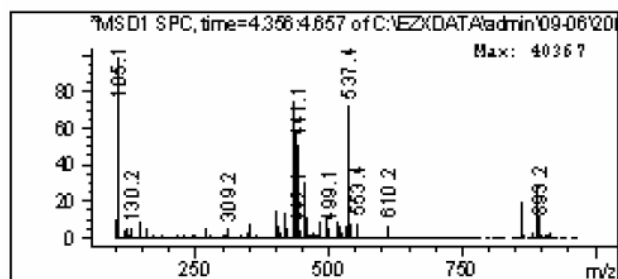
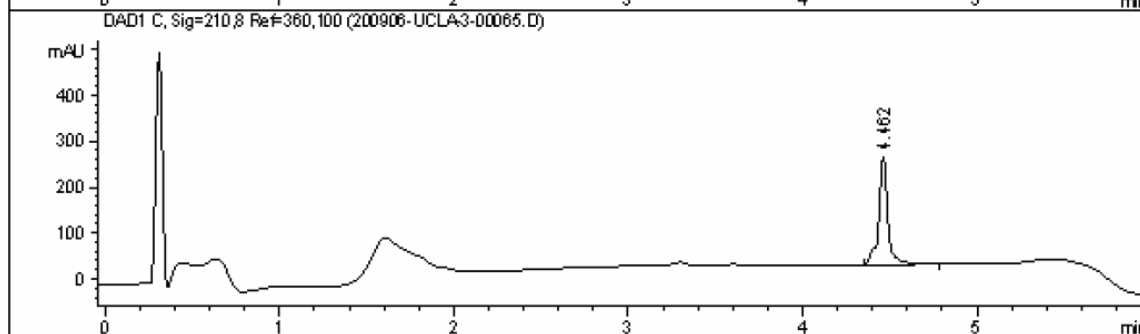
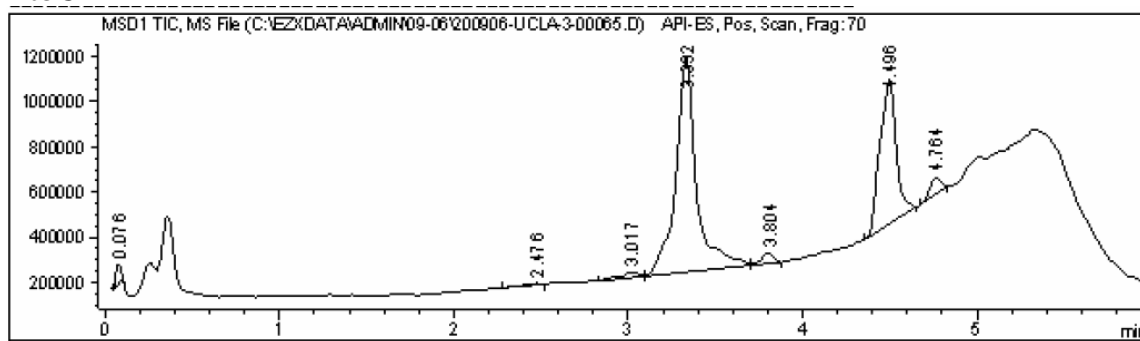
<sup>1</sup> Department of Microbiology, Immunology and Molecular Genetics

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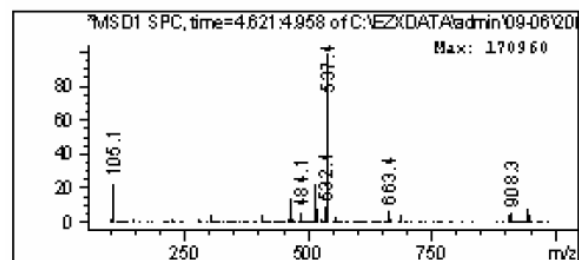
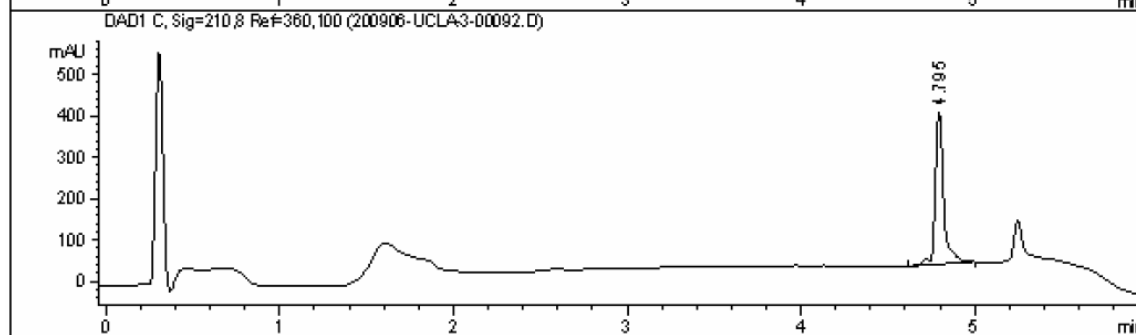
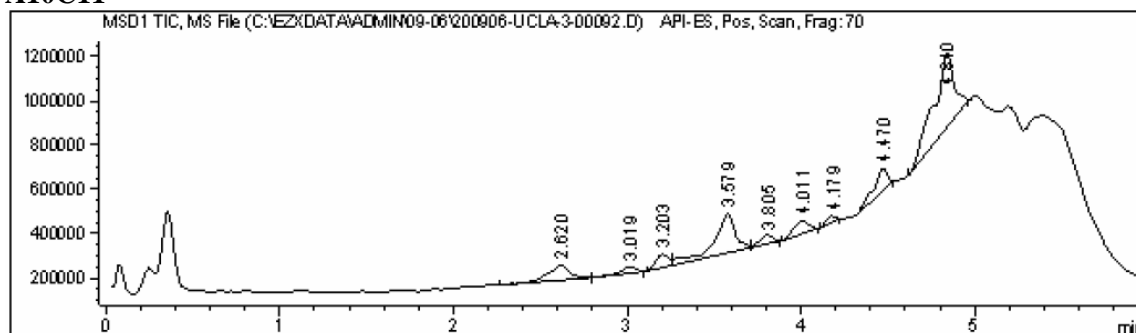
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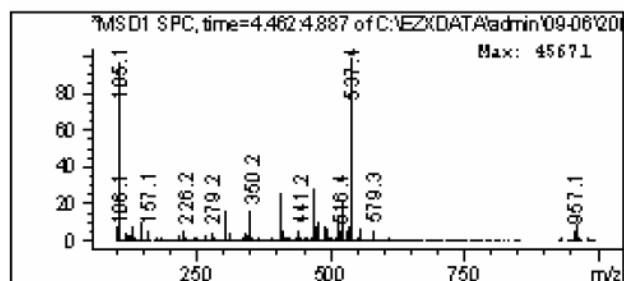
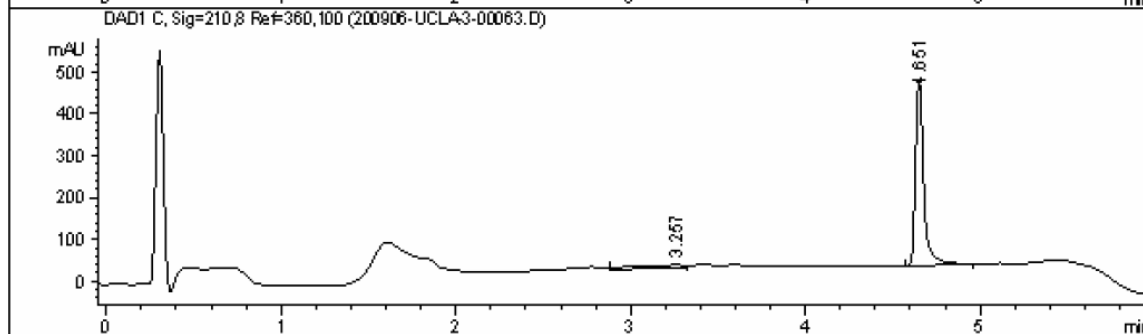
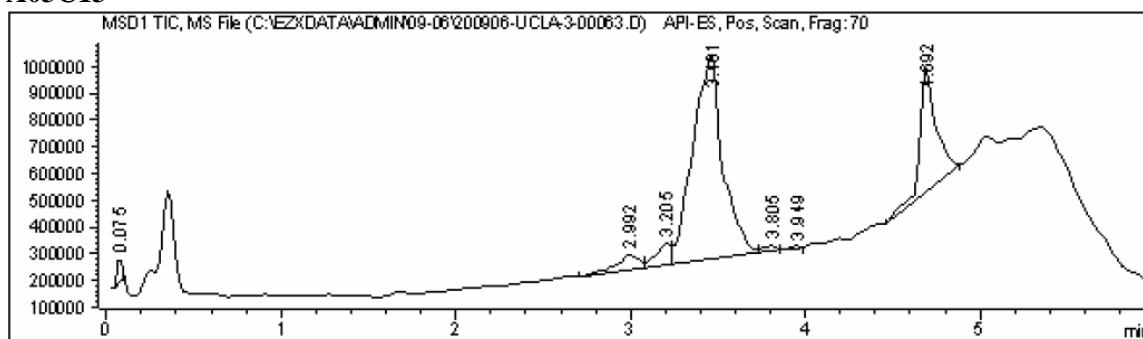
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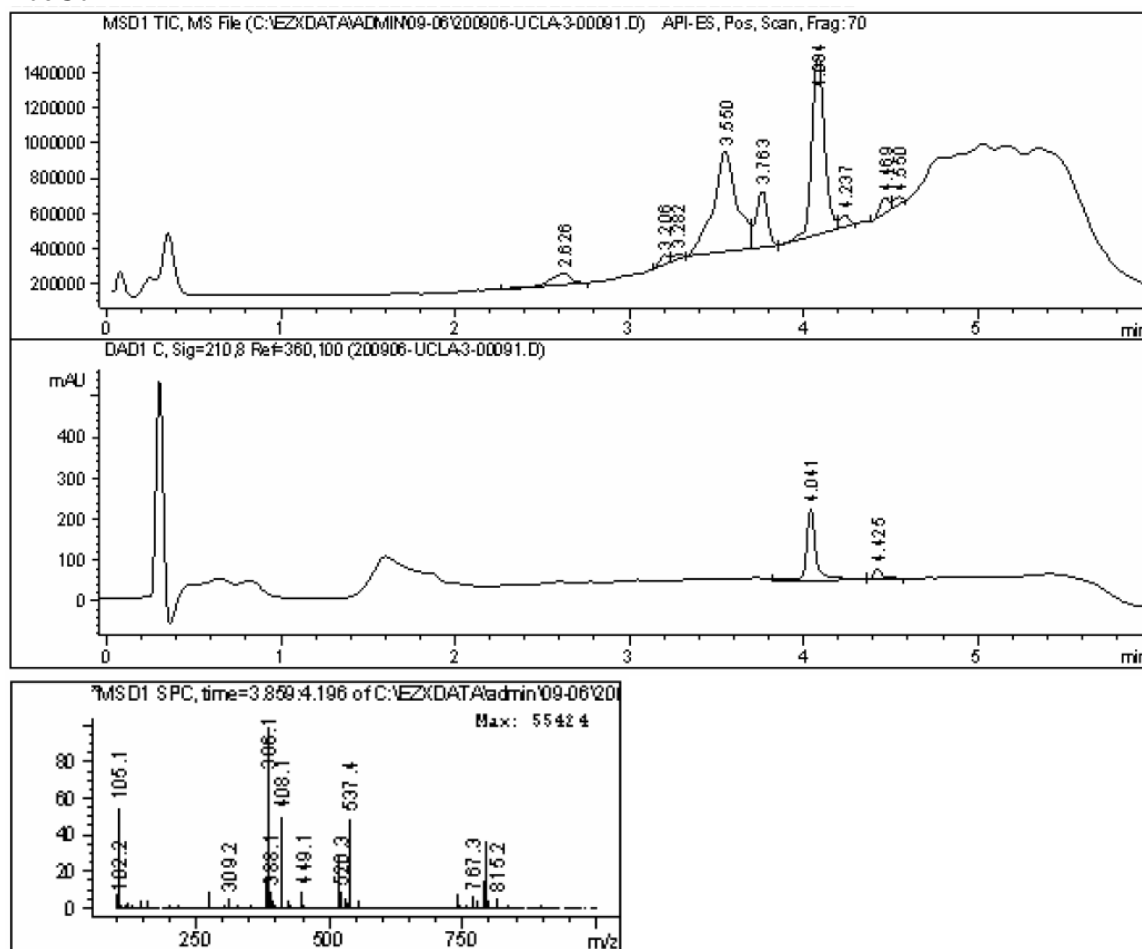
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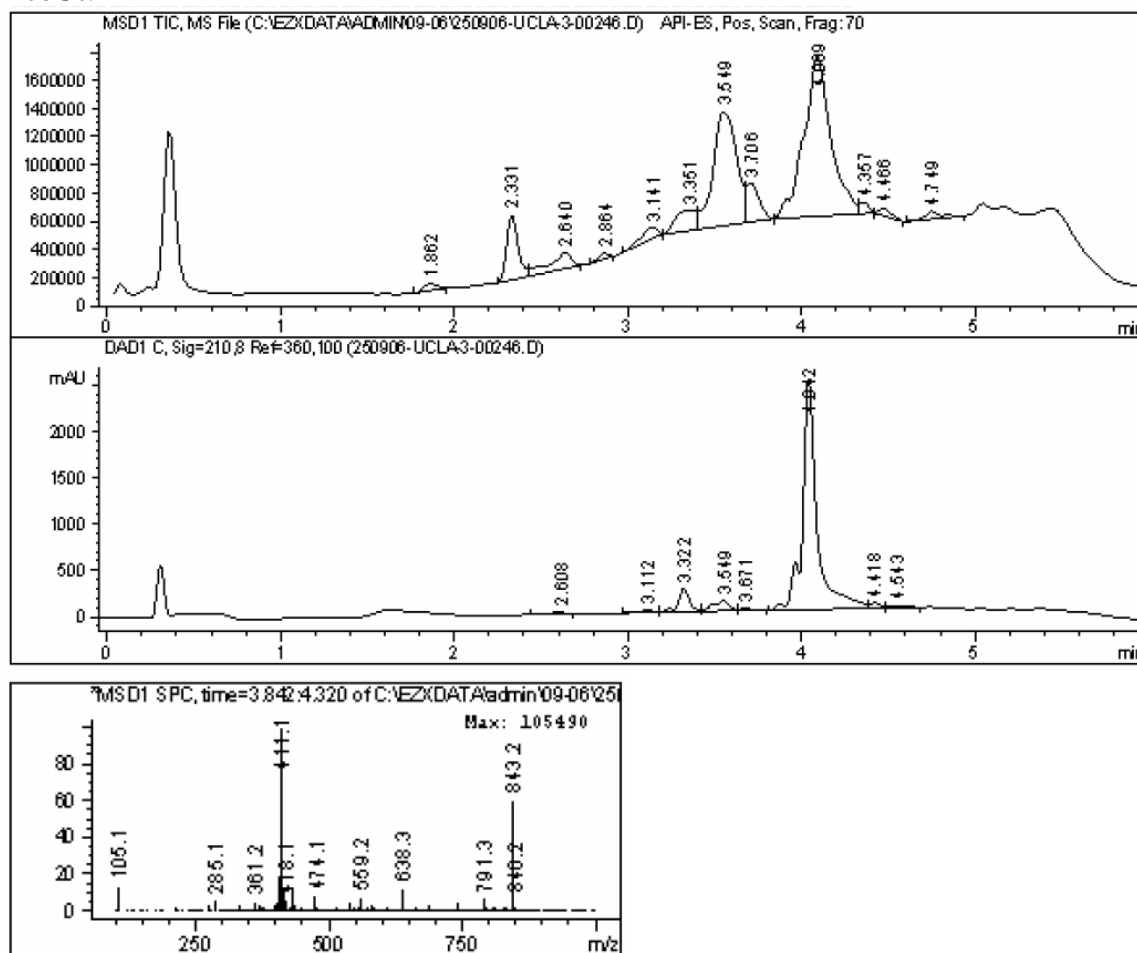


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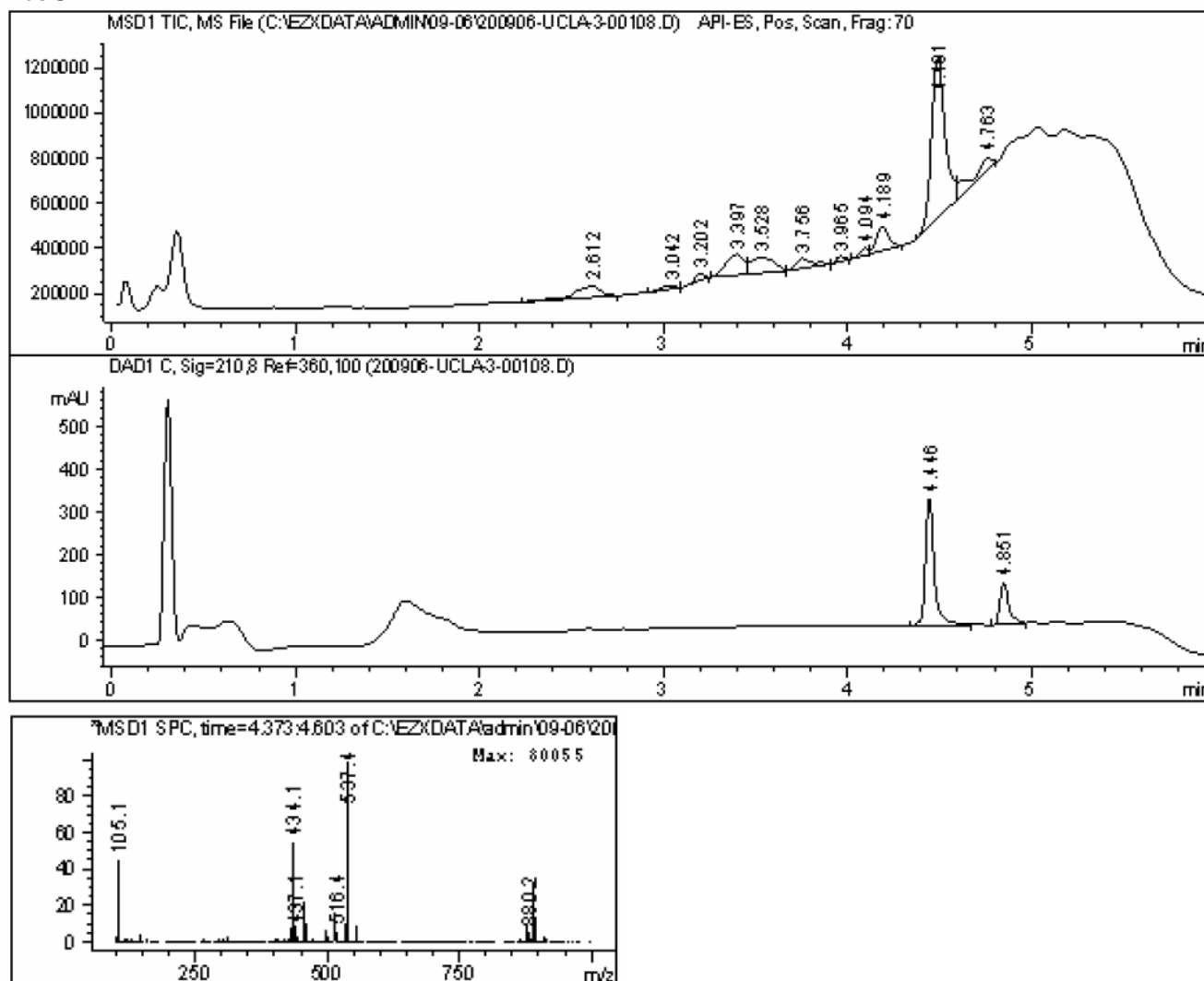
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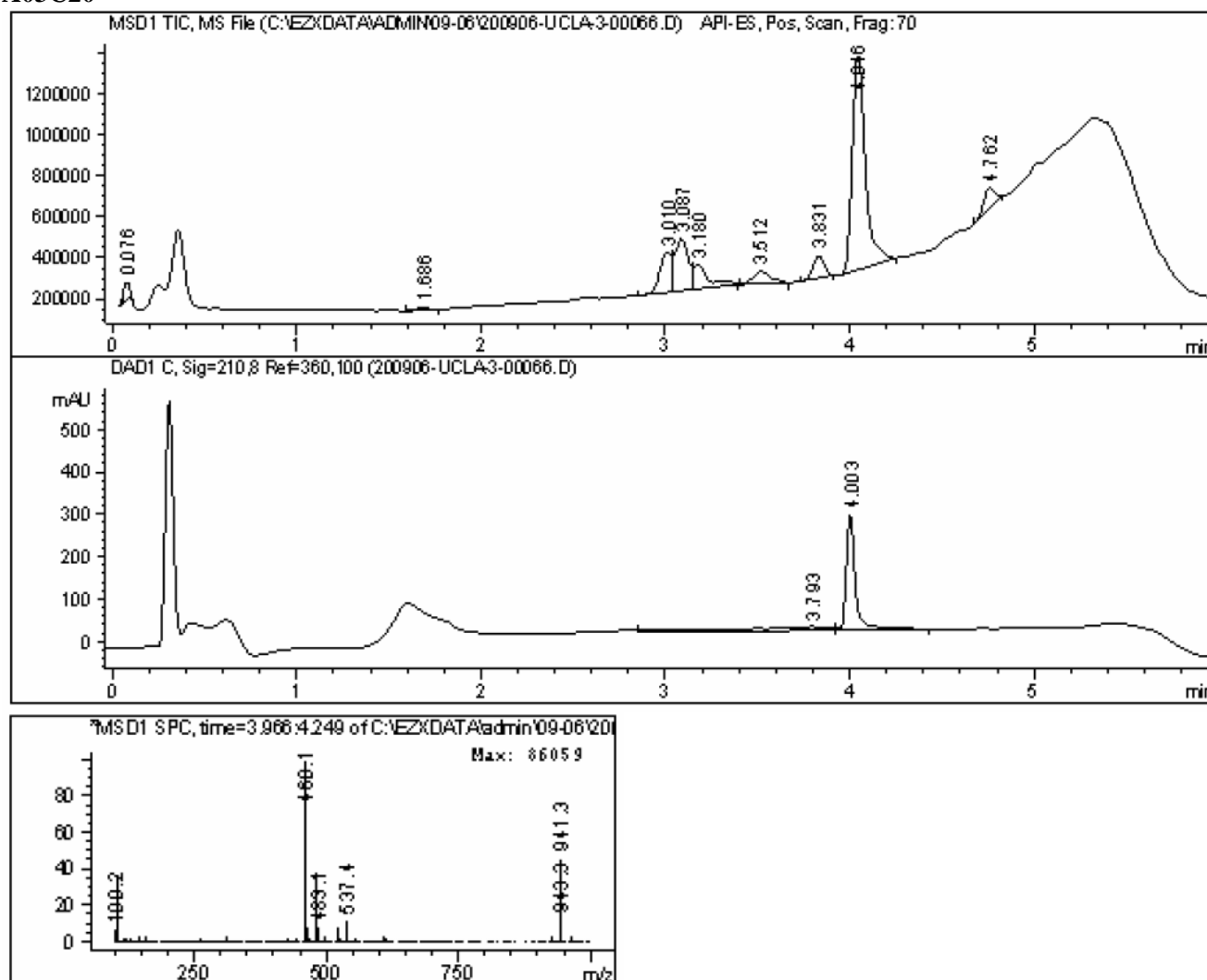


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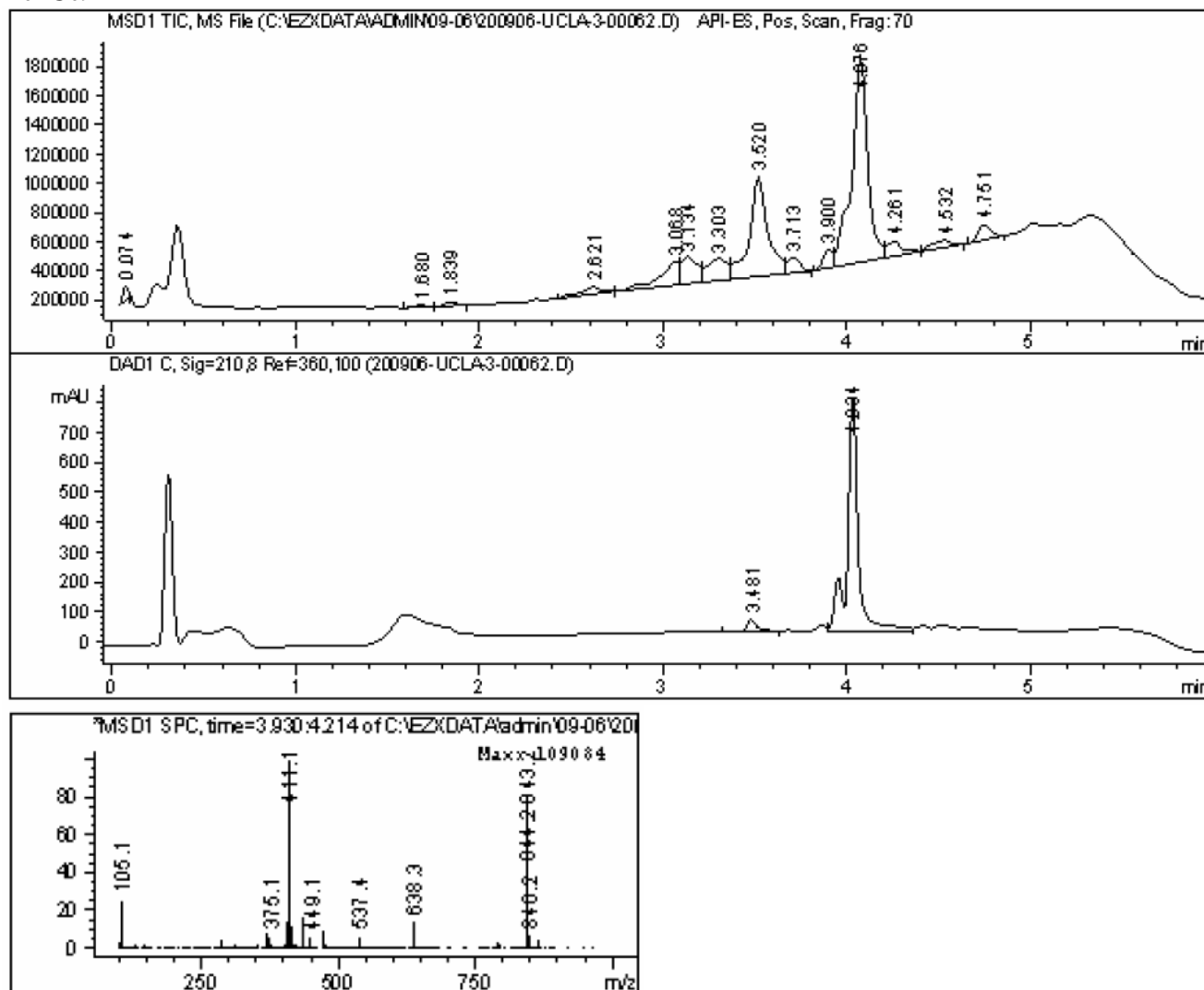




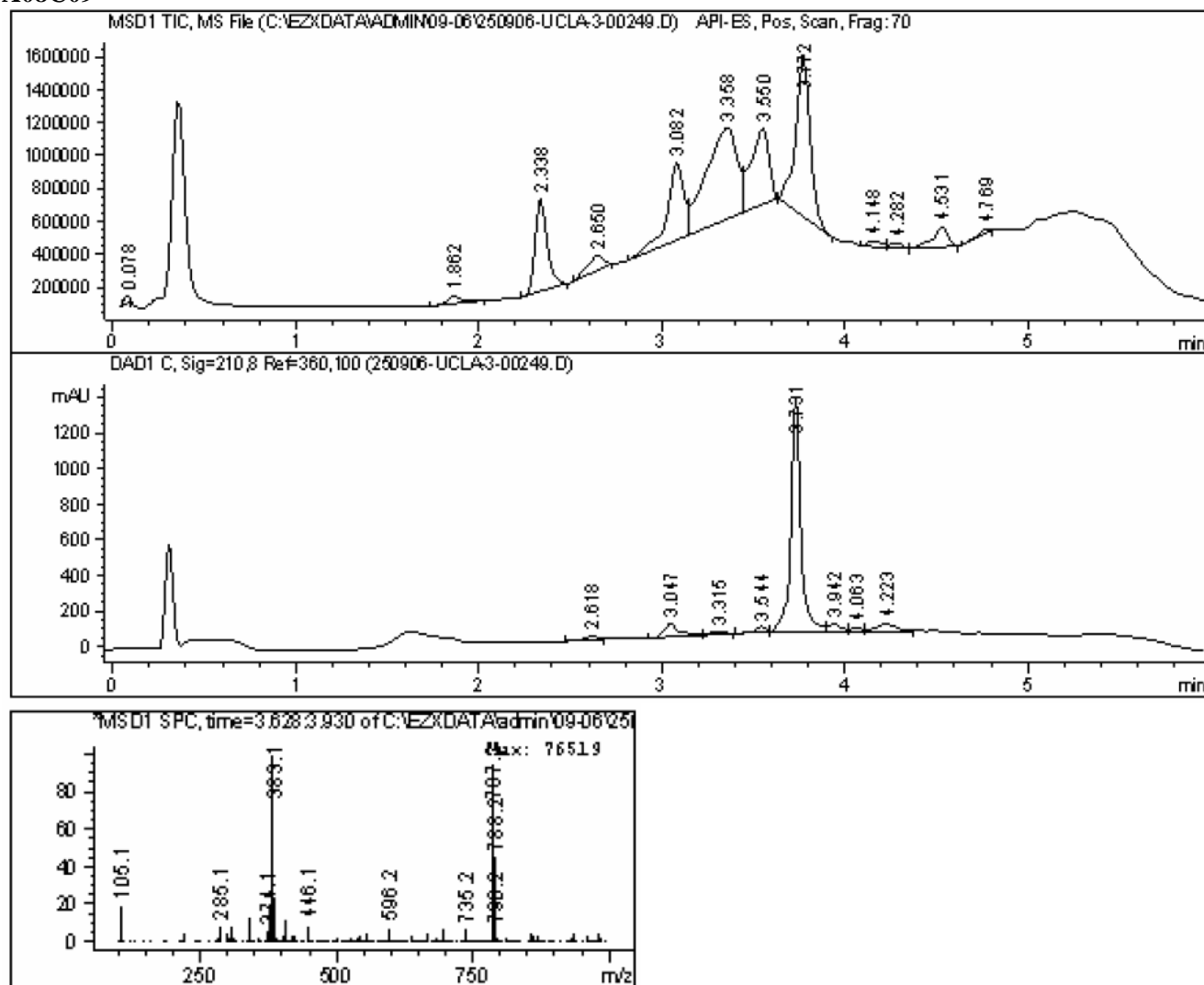
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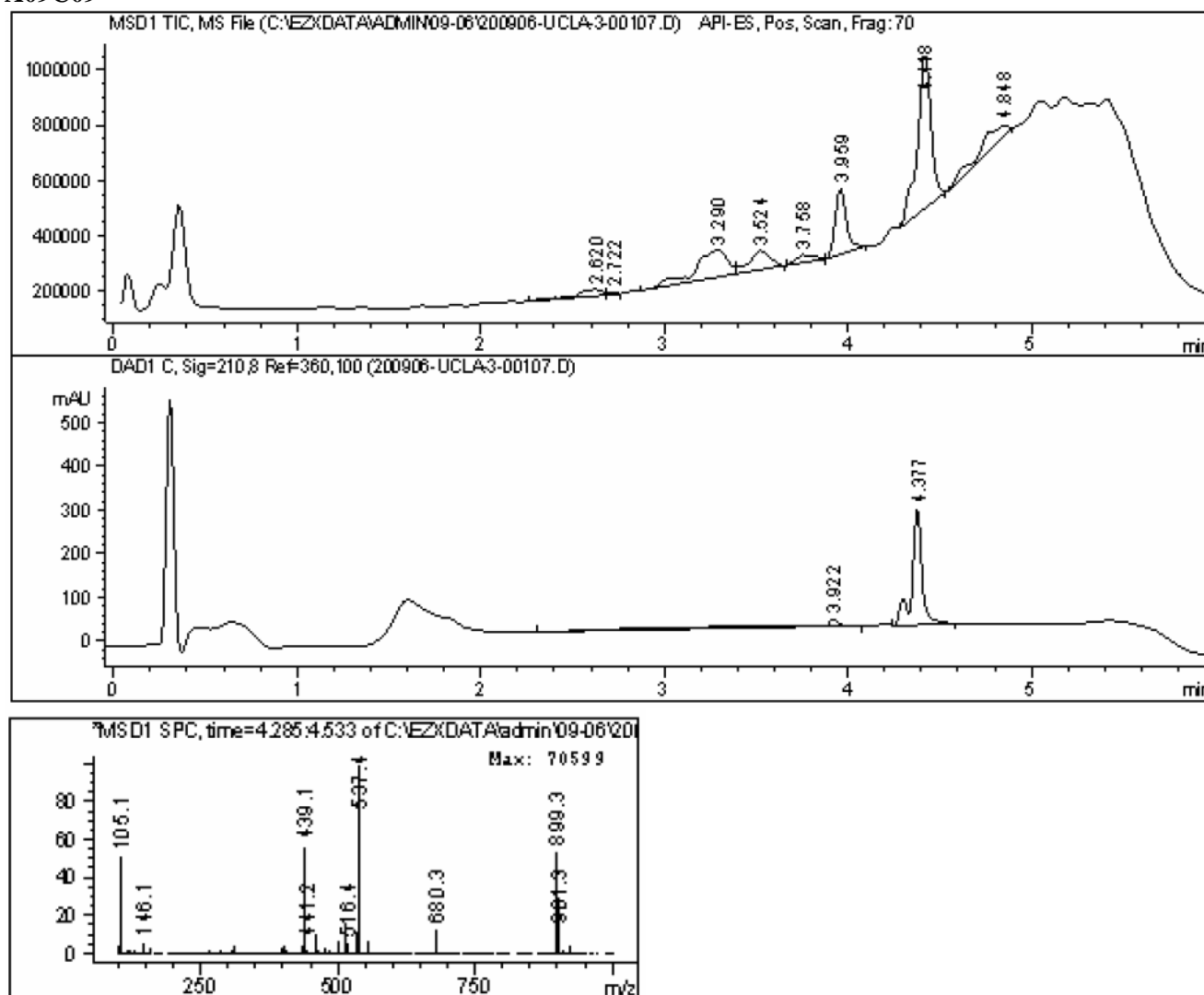
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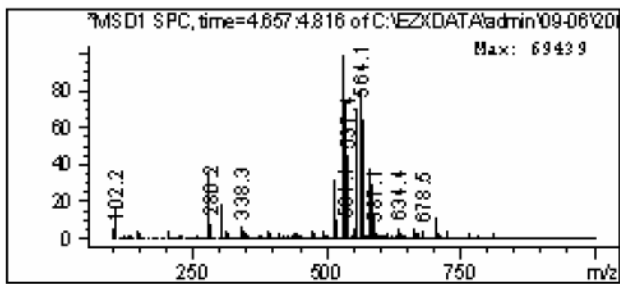
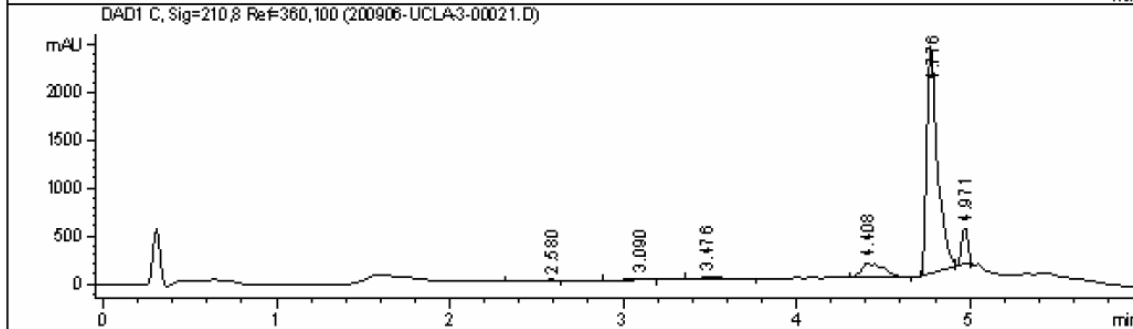
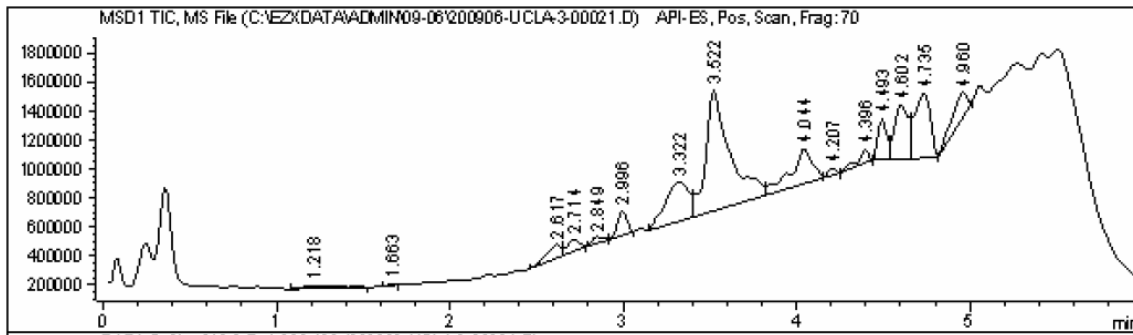
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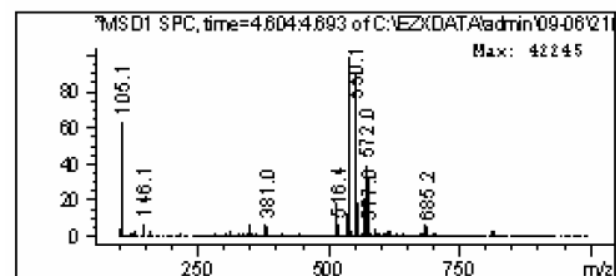
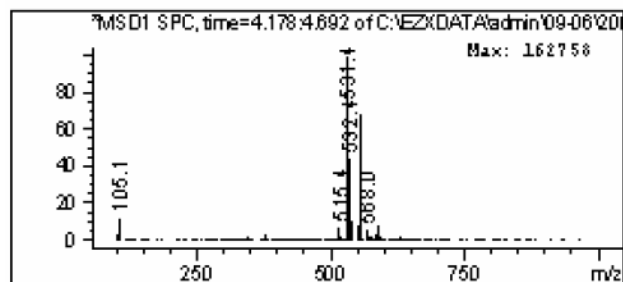
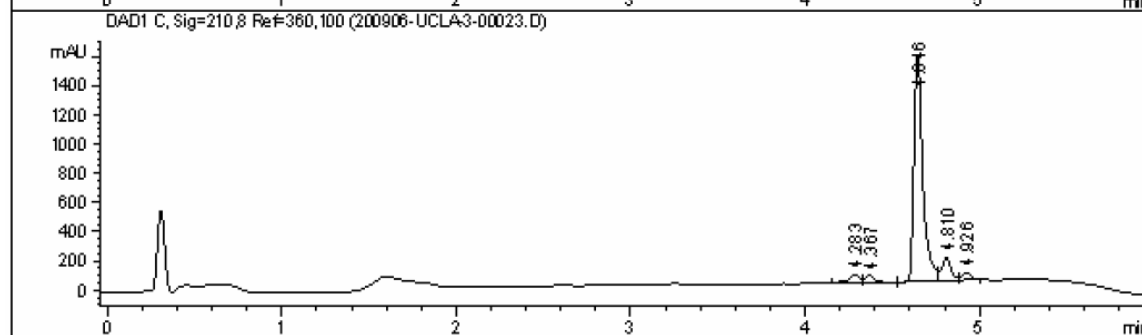
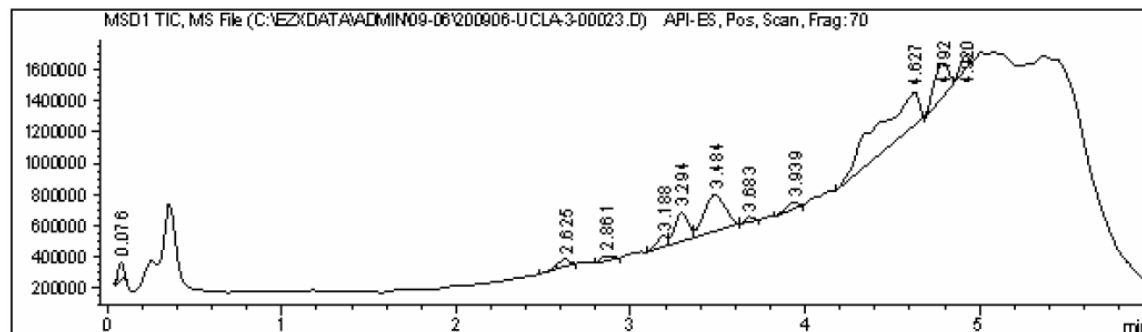
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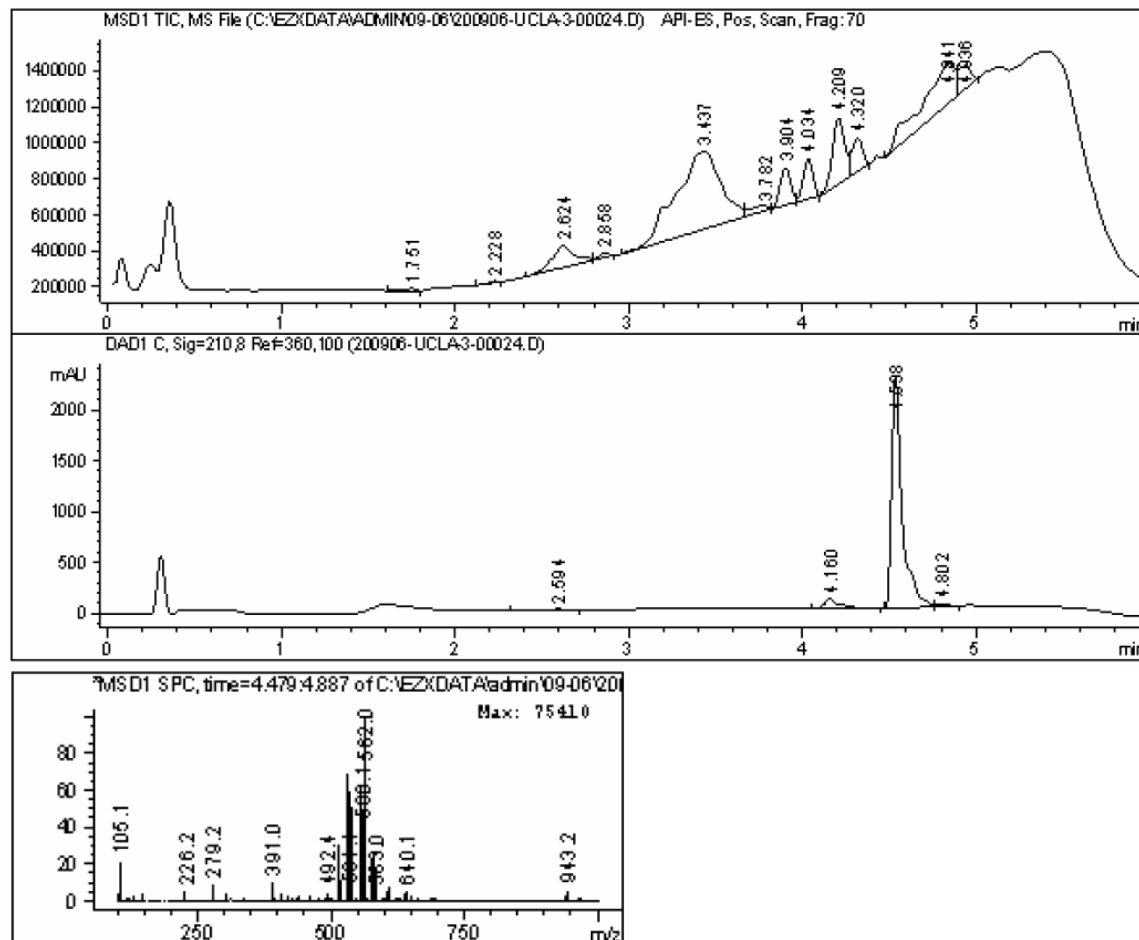
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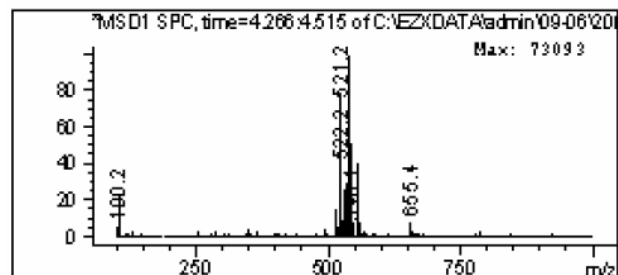
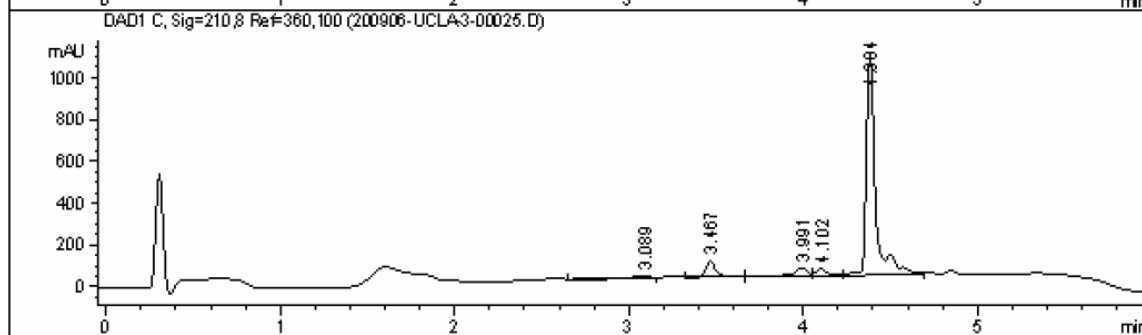
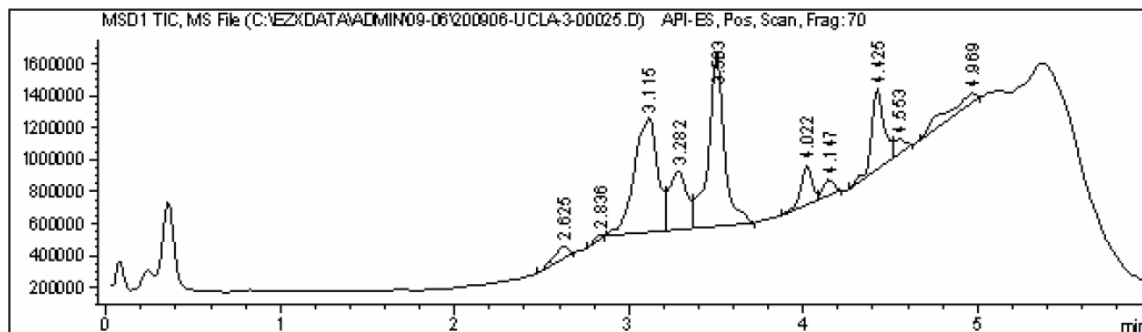


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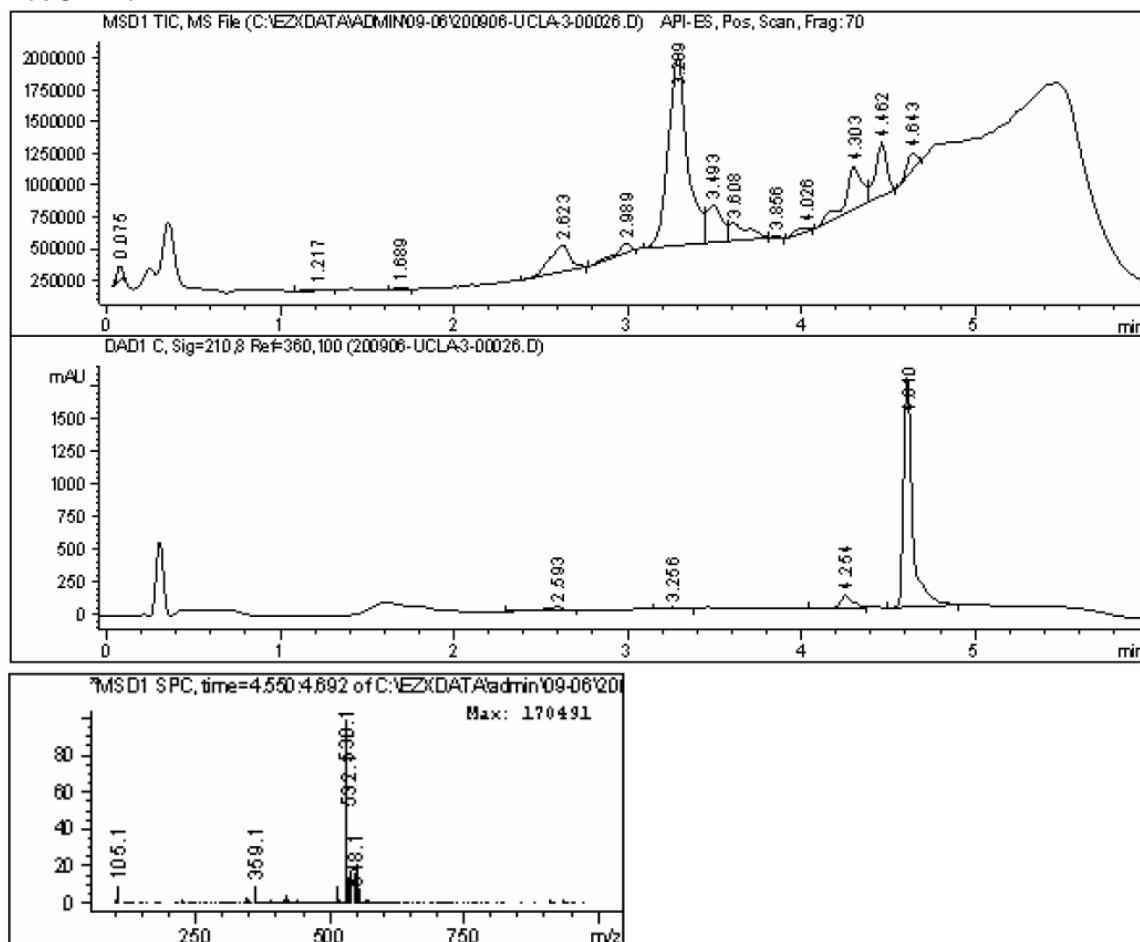
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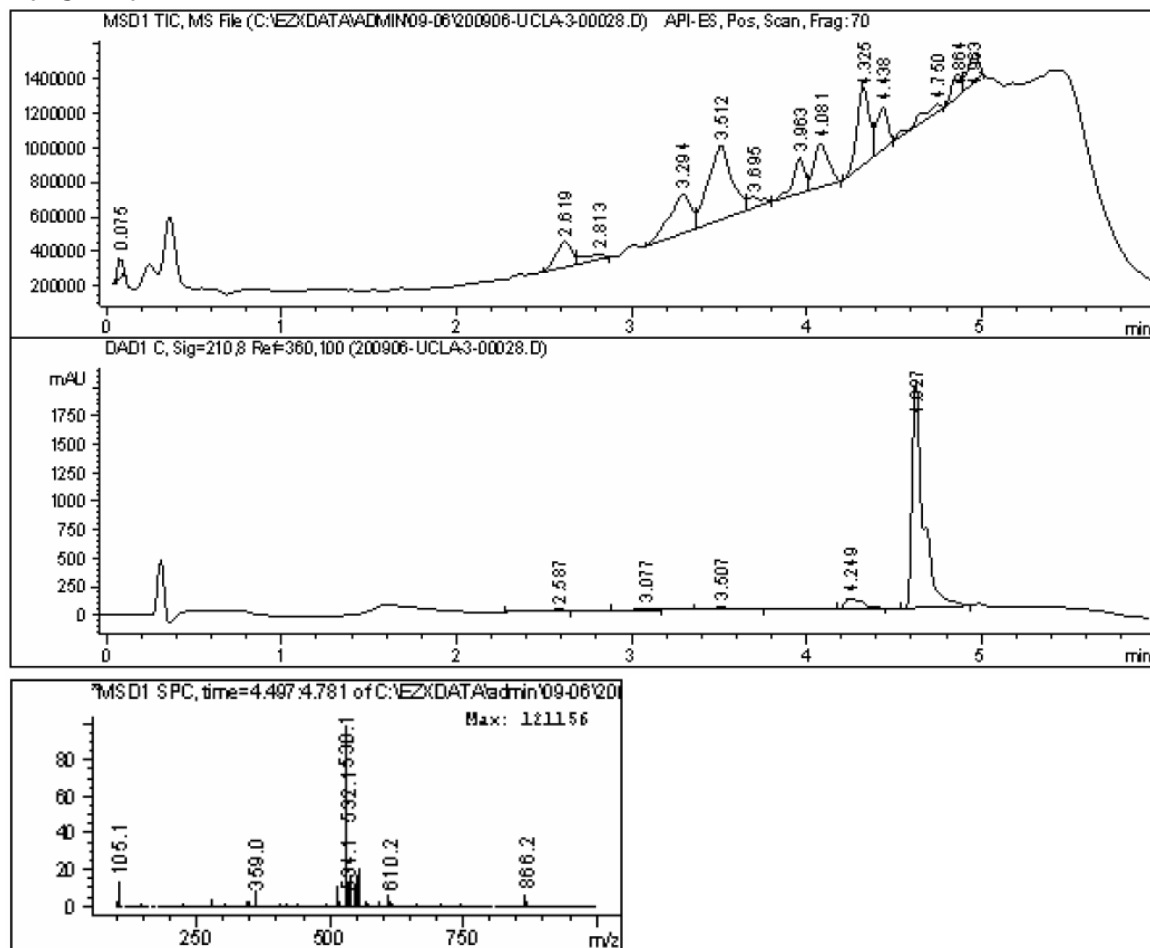




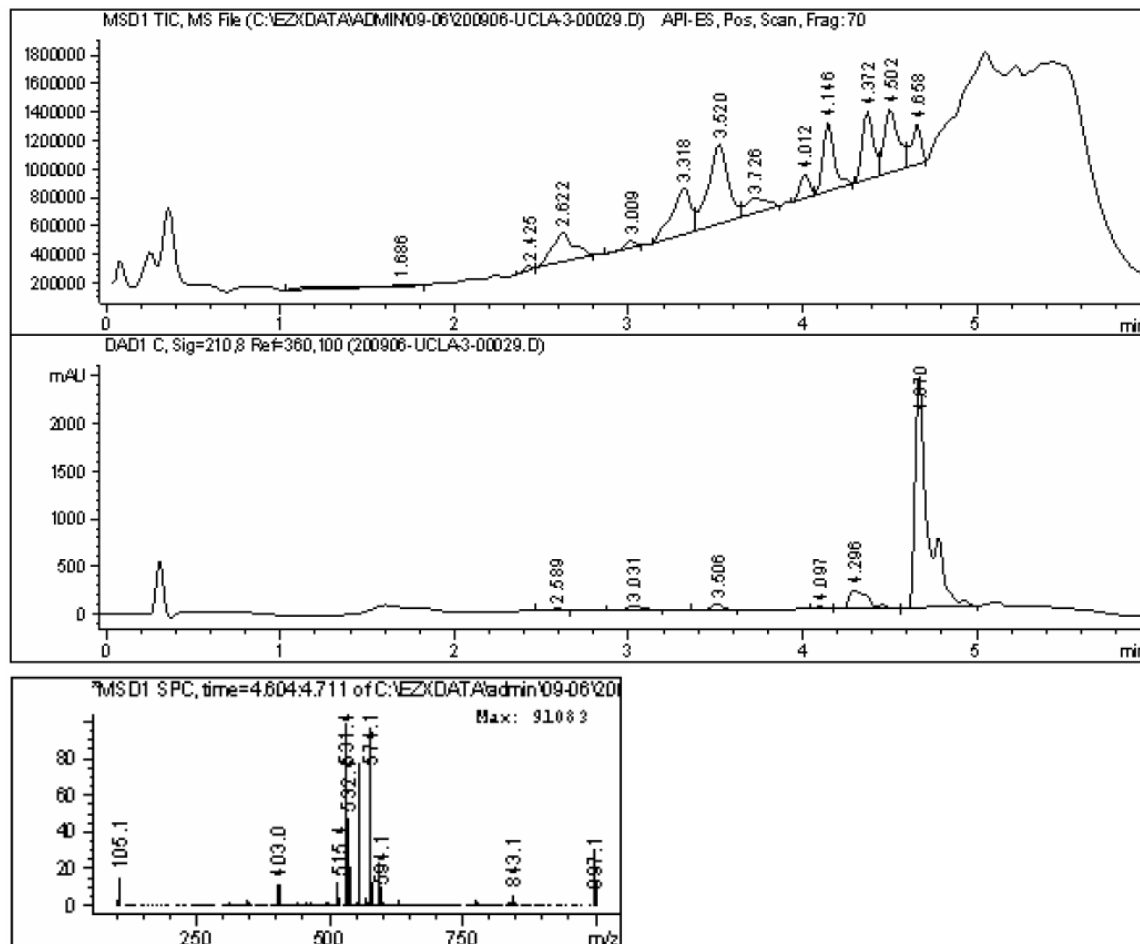
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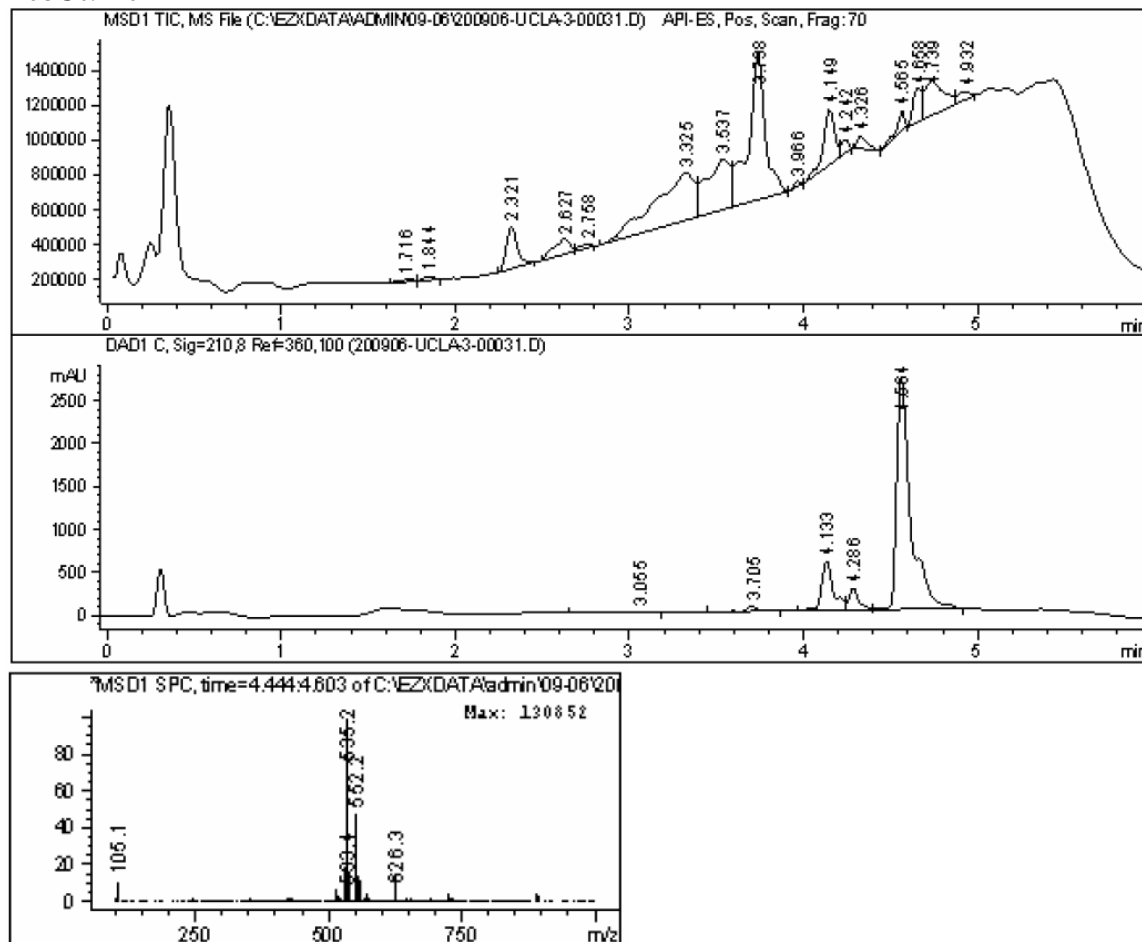
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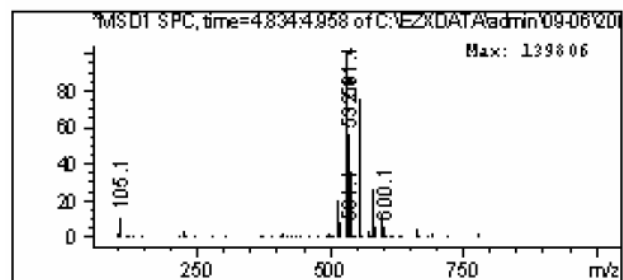
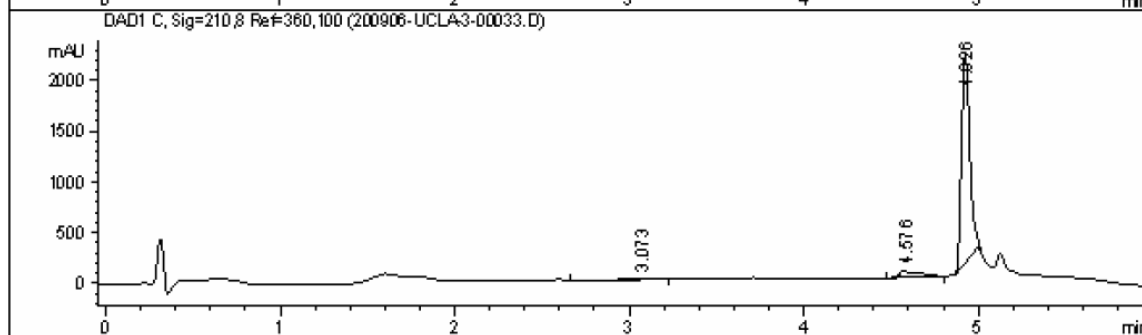
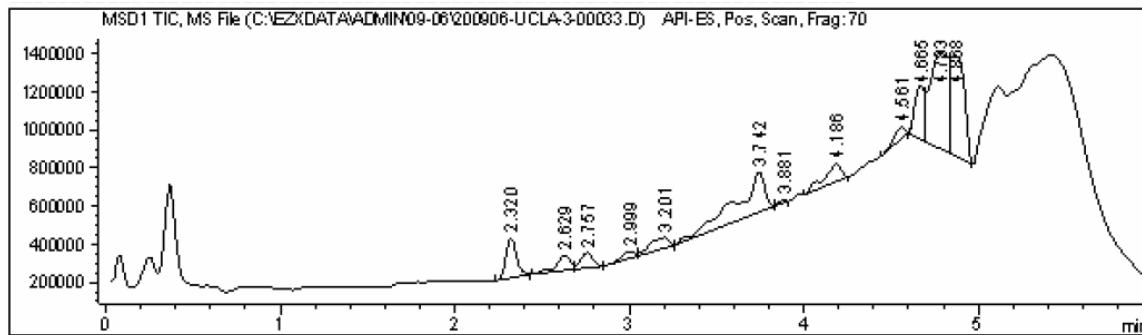
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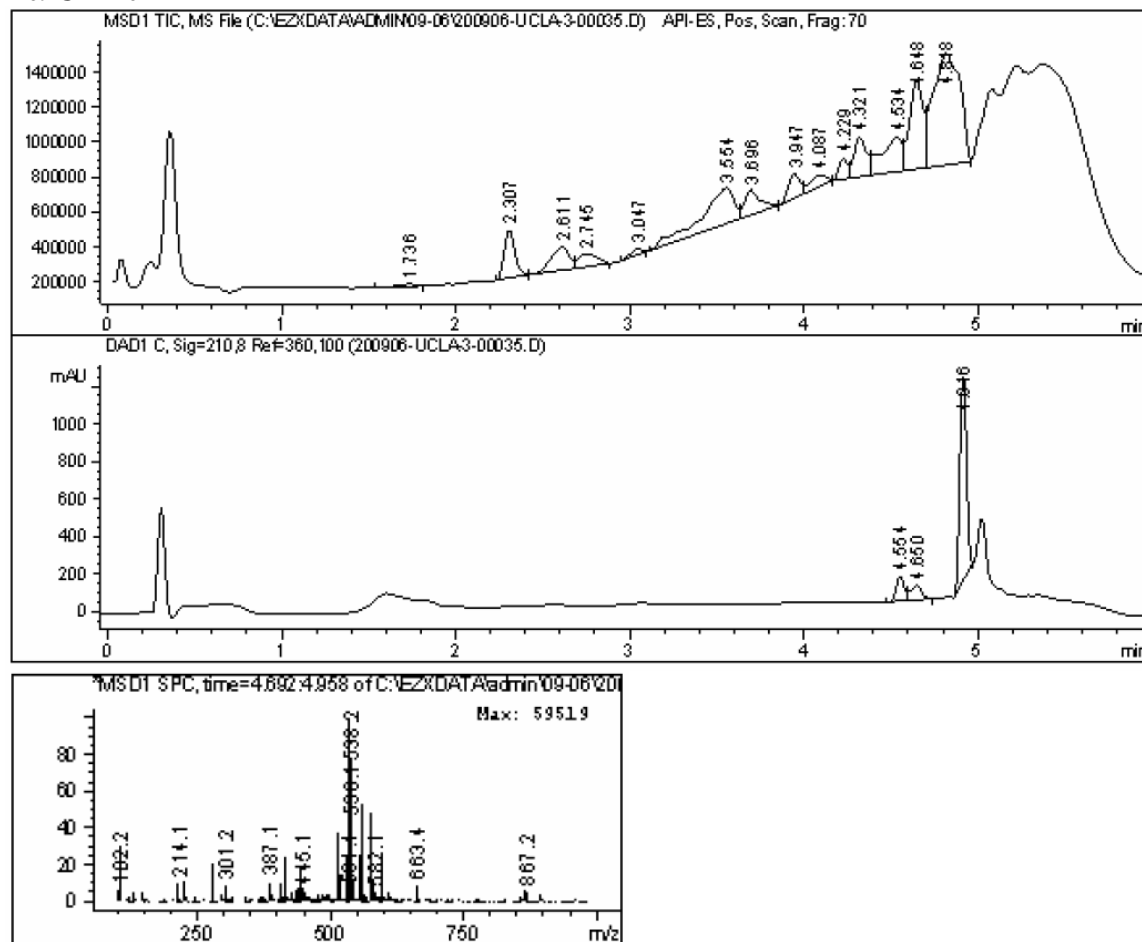
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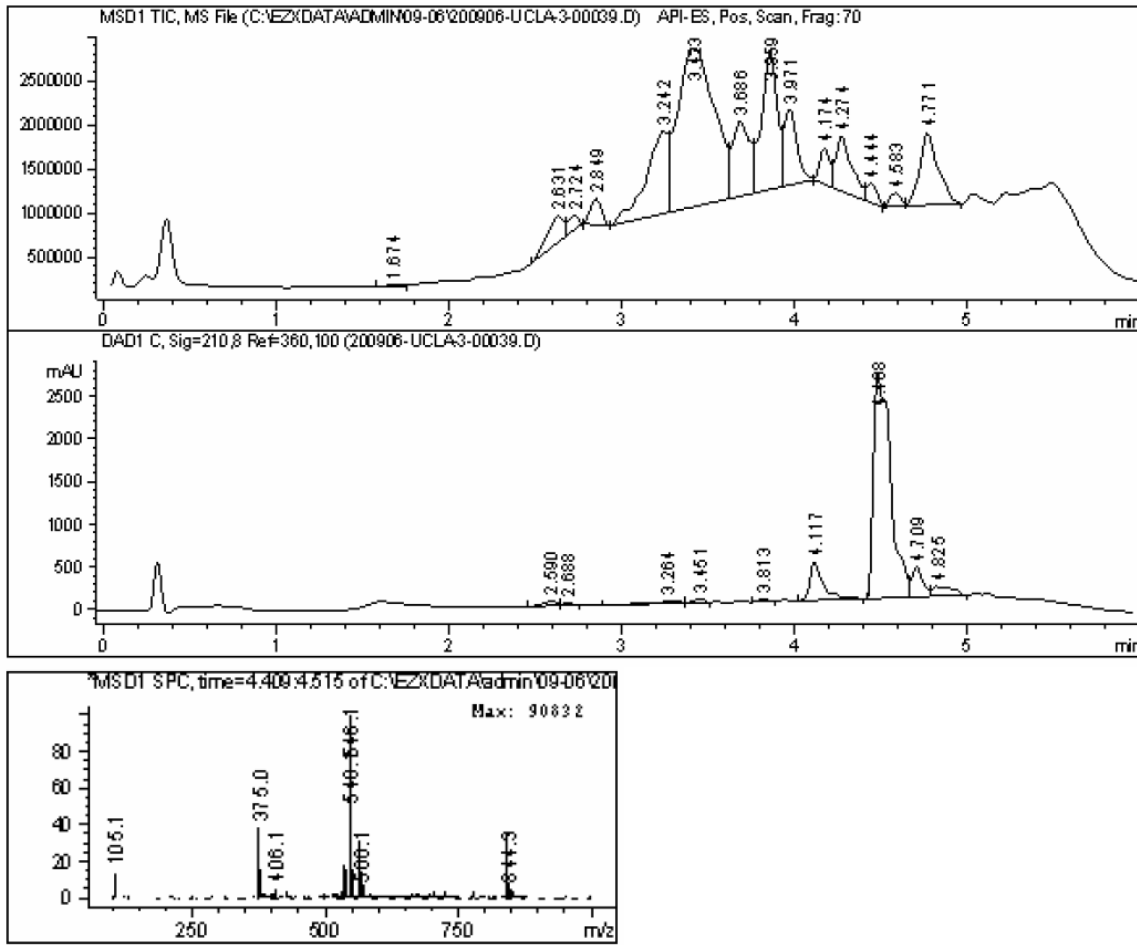
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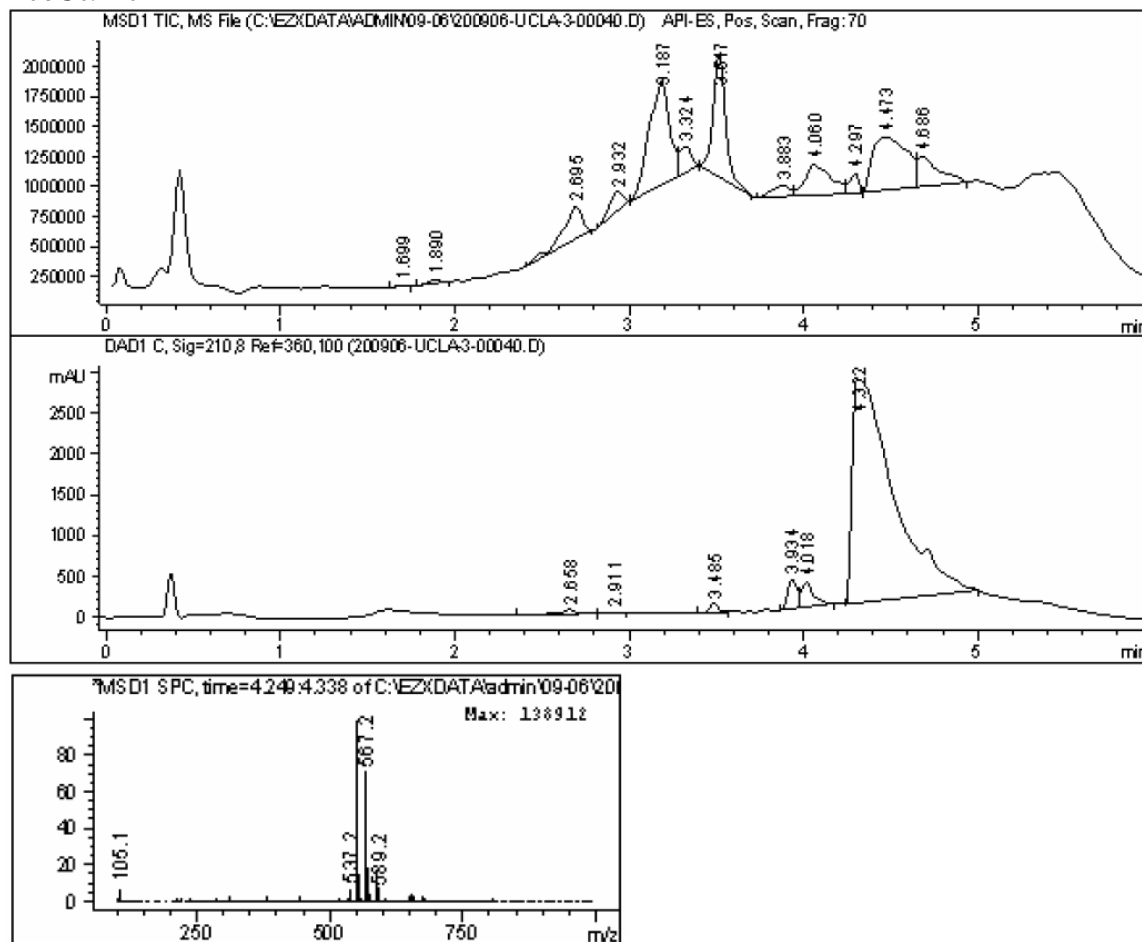
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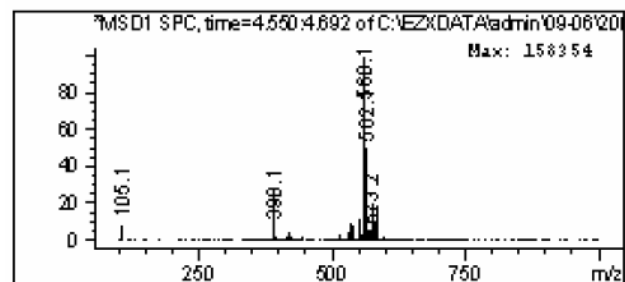
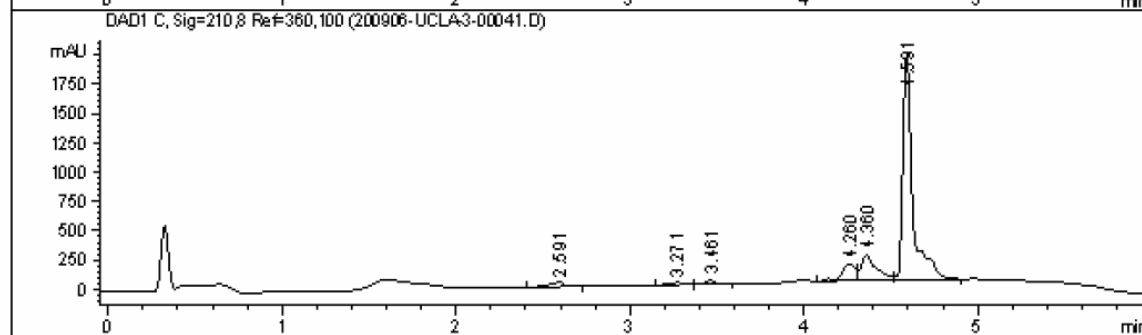
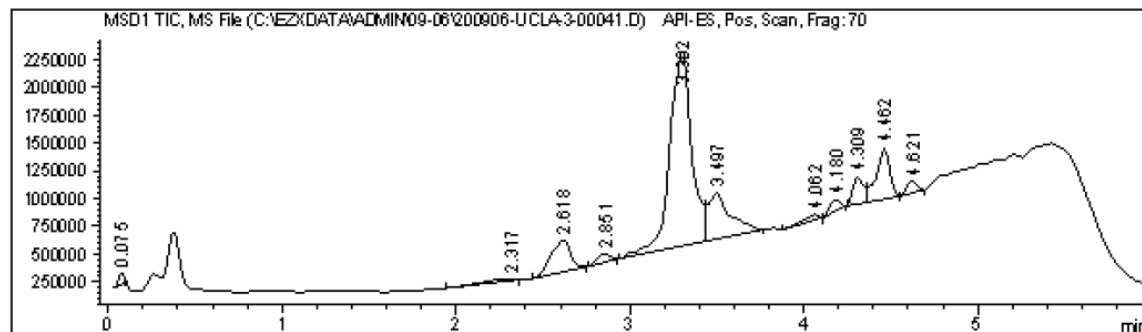


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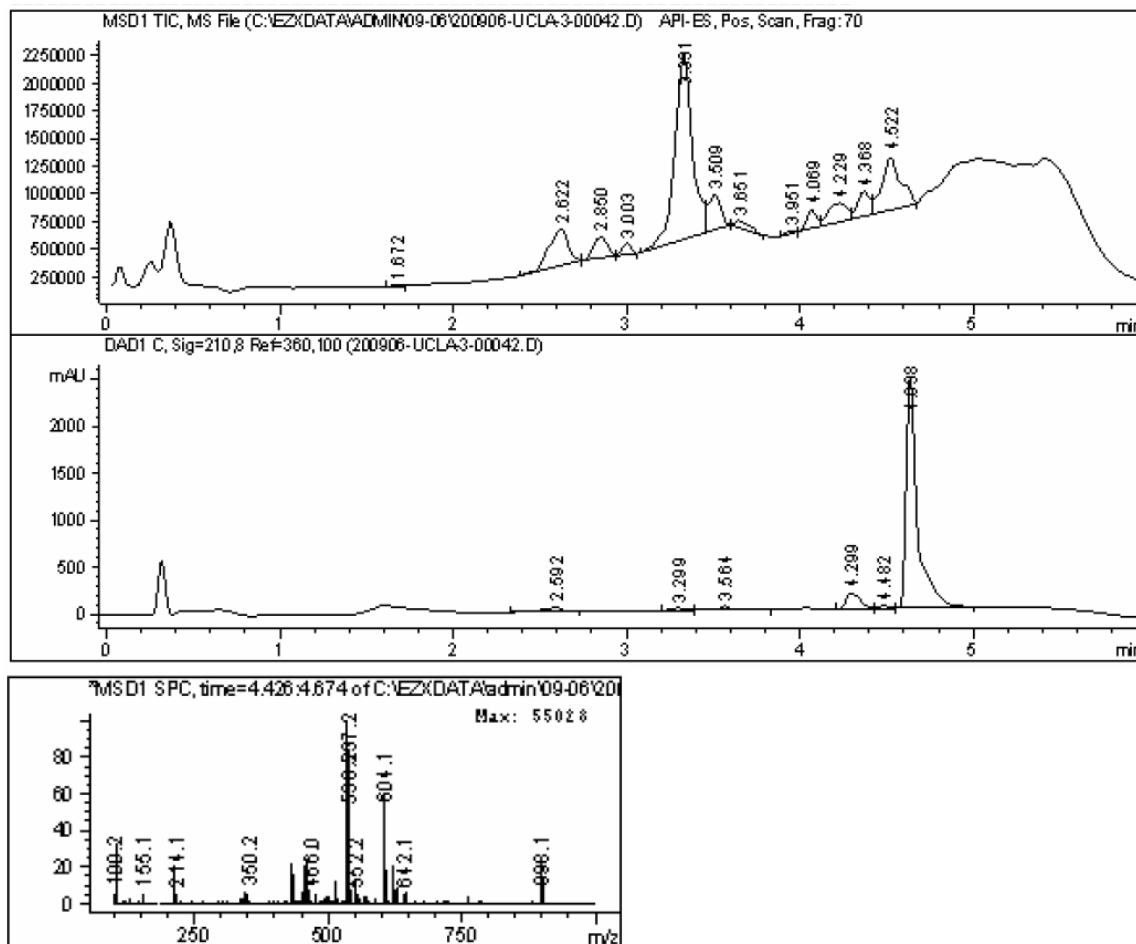




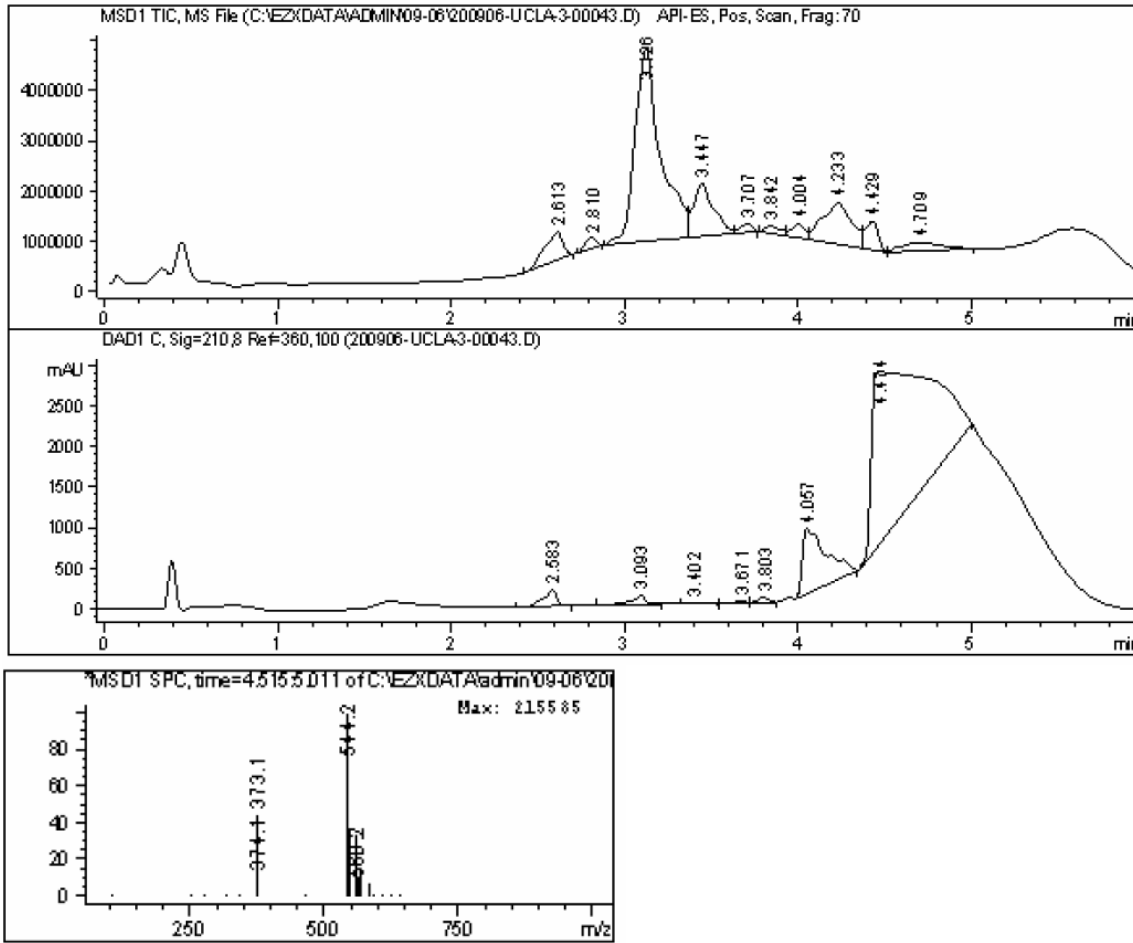
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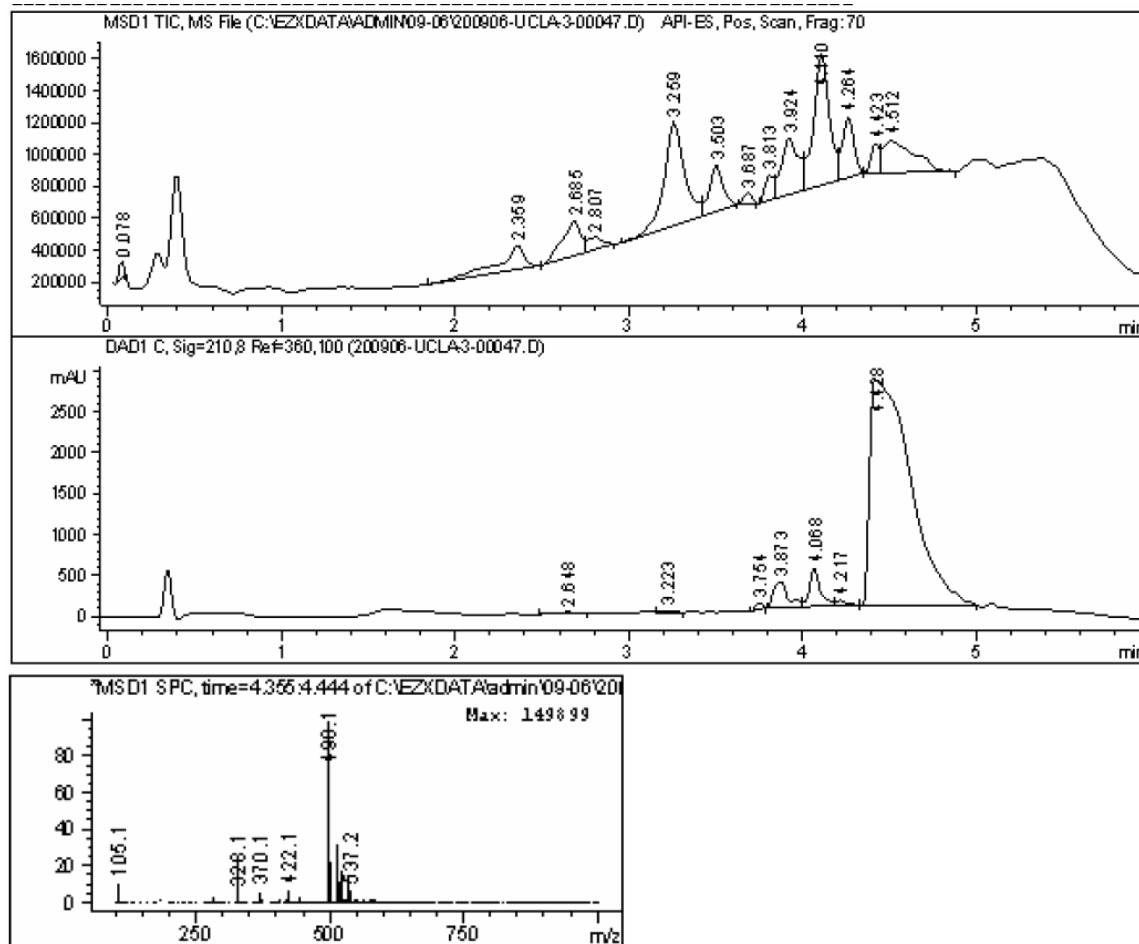
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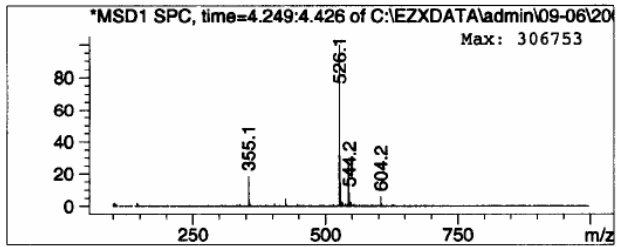
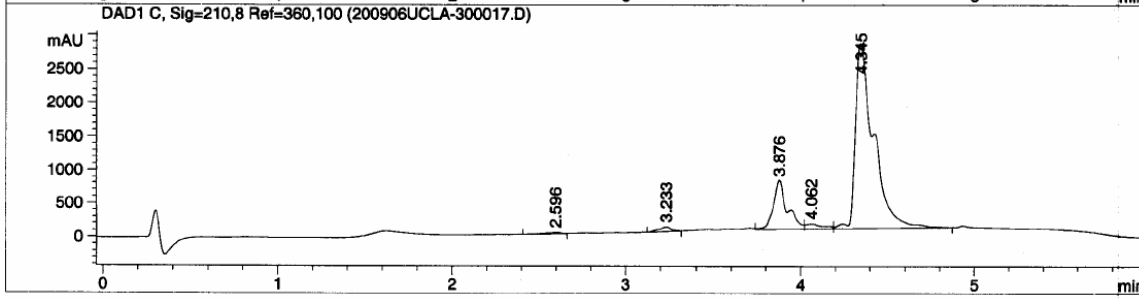
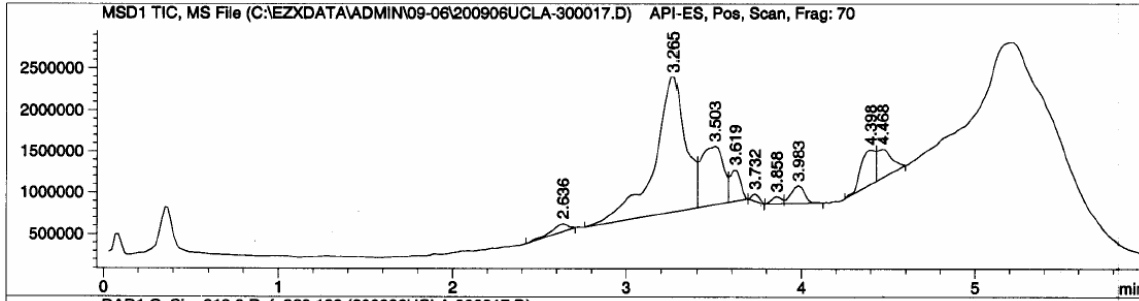
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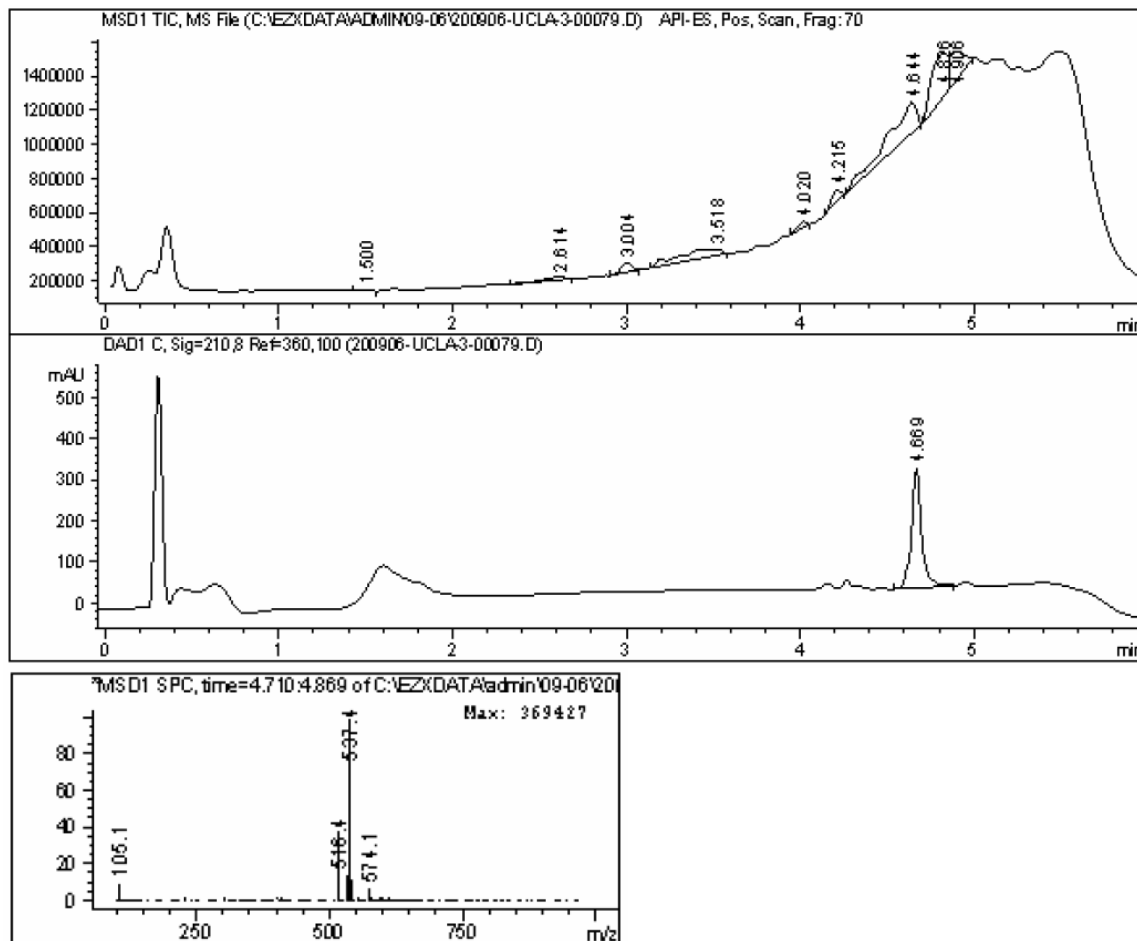
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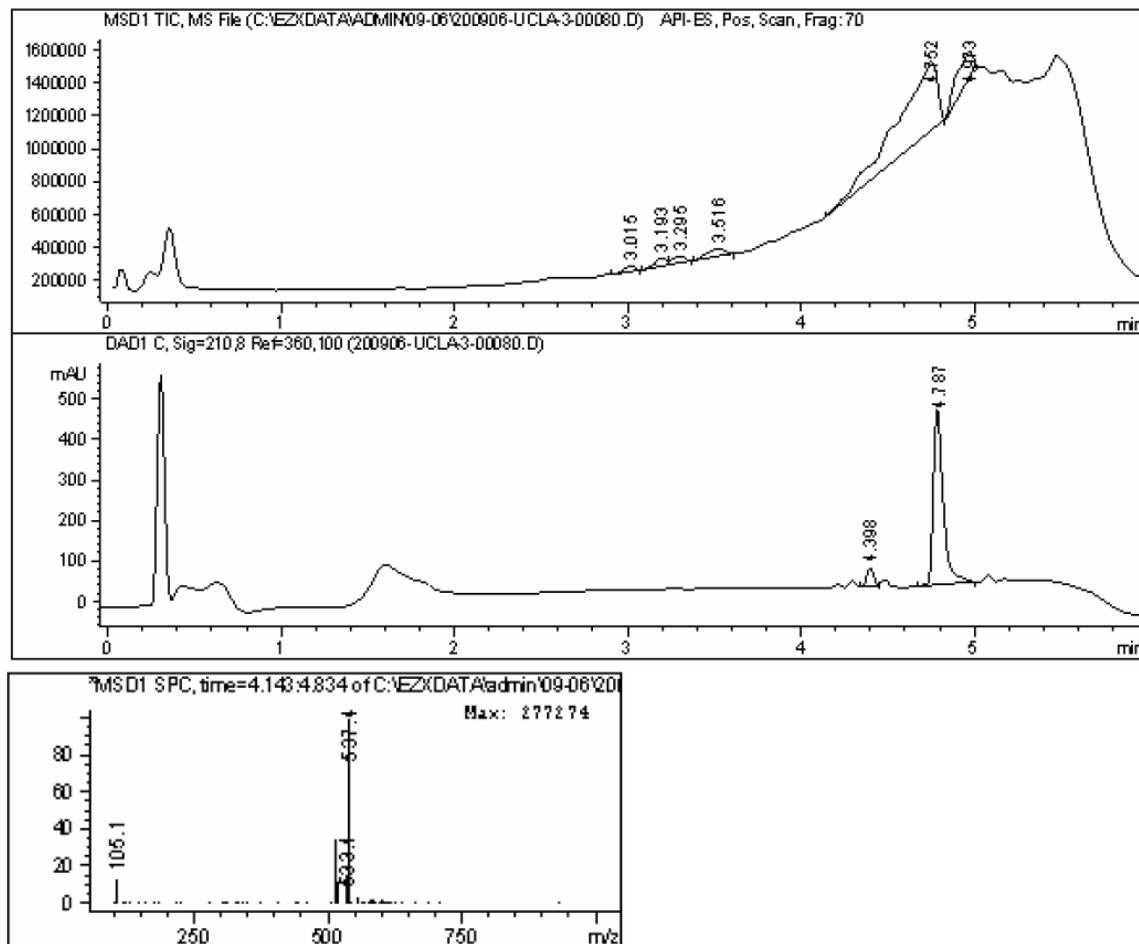
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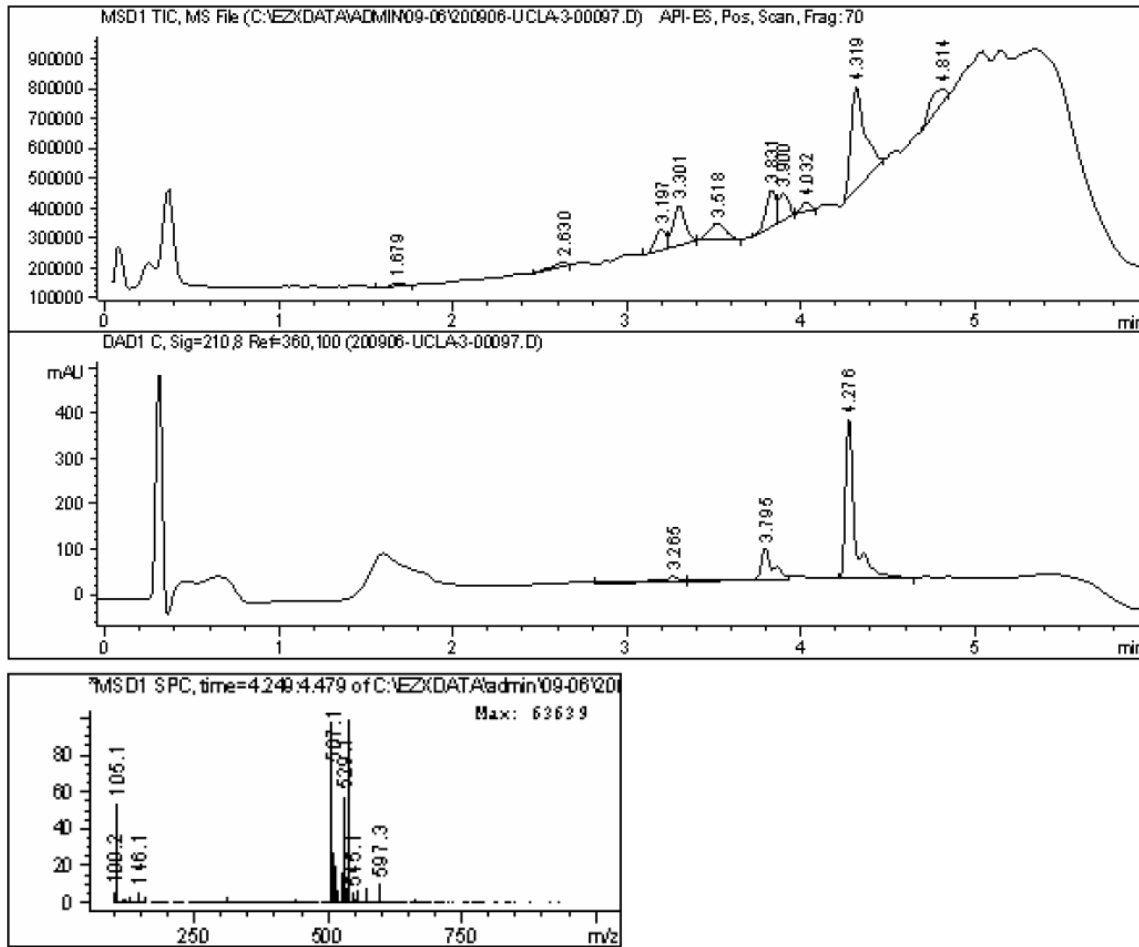
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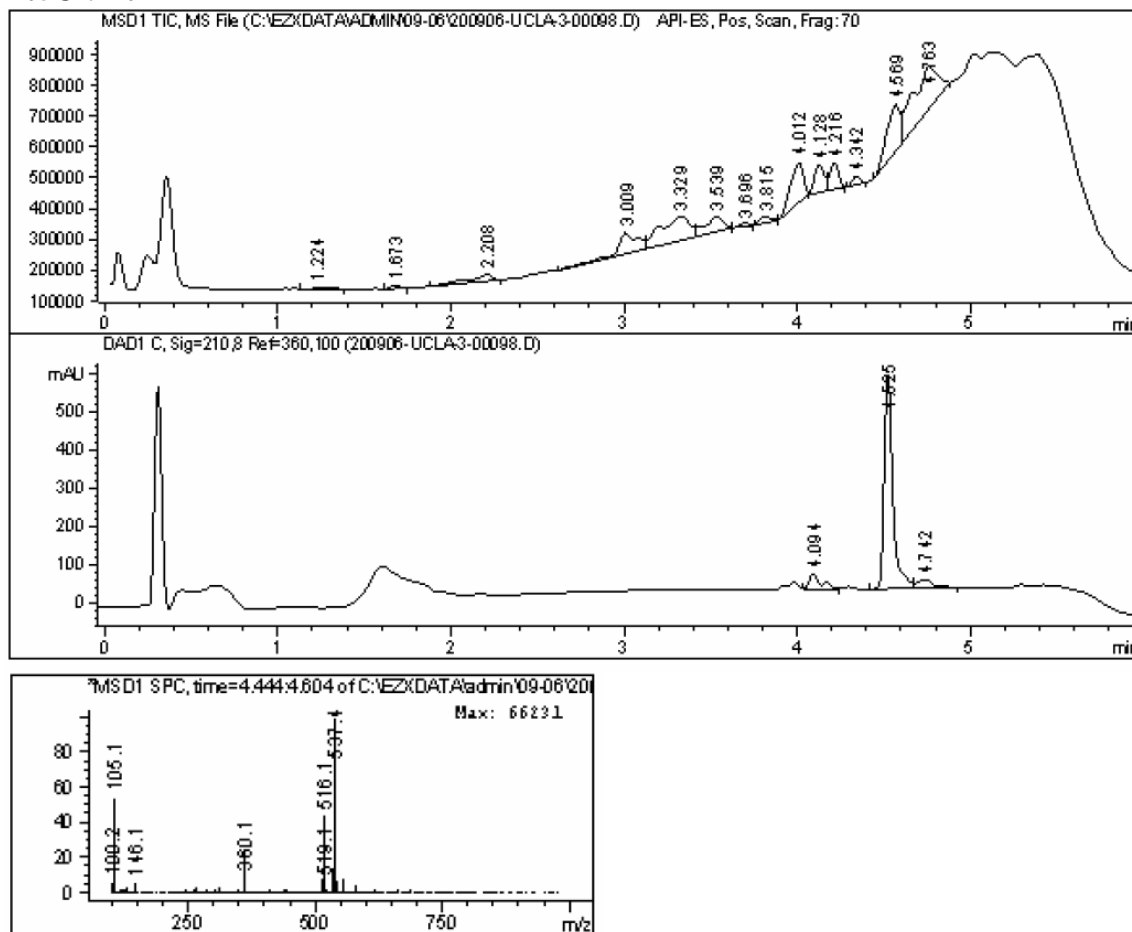


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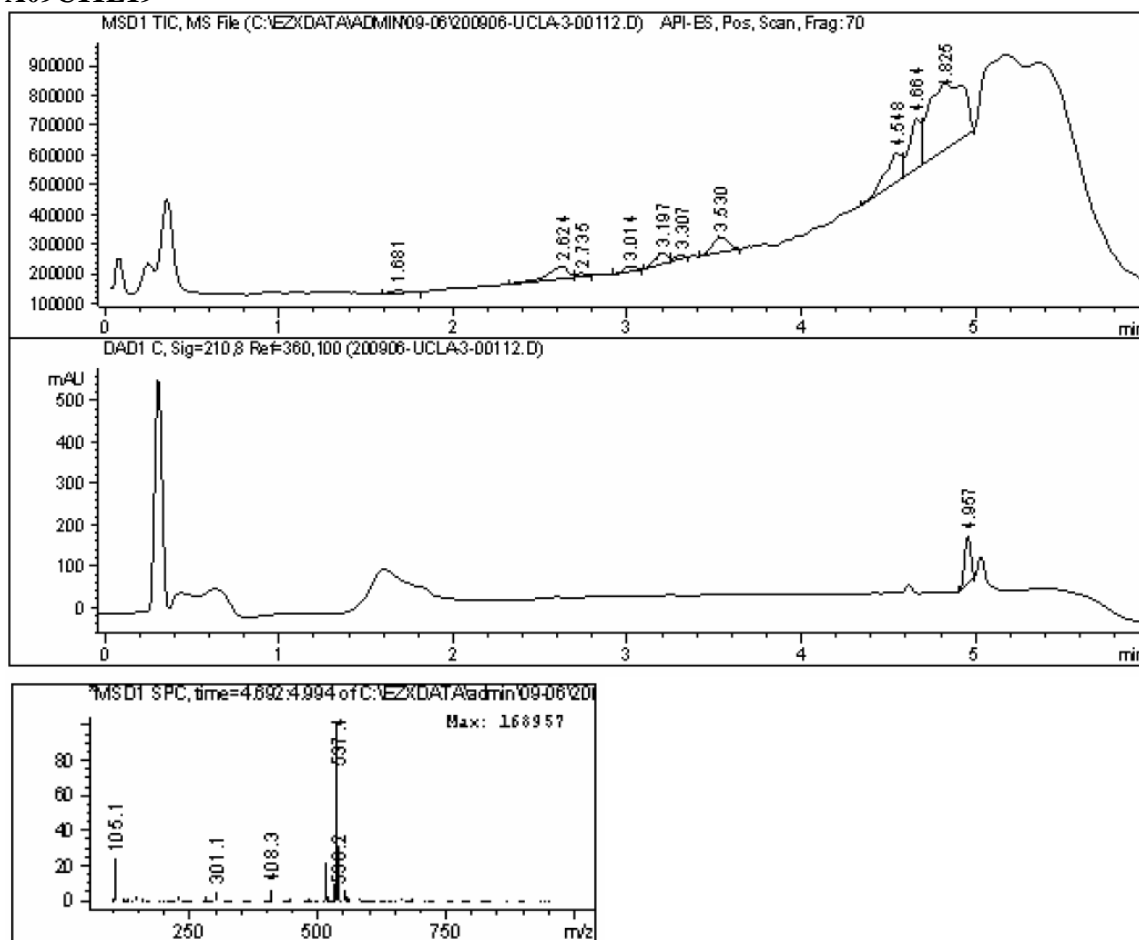




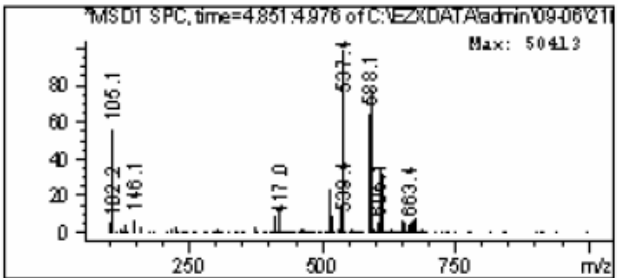
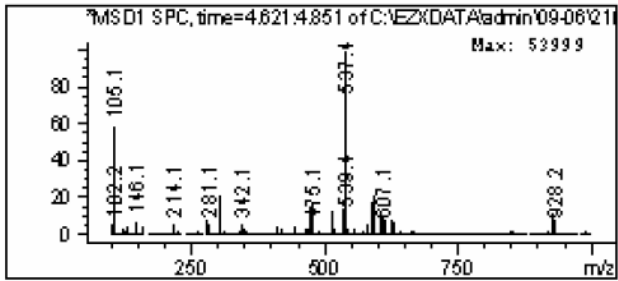
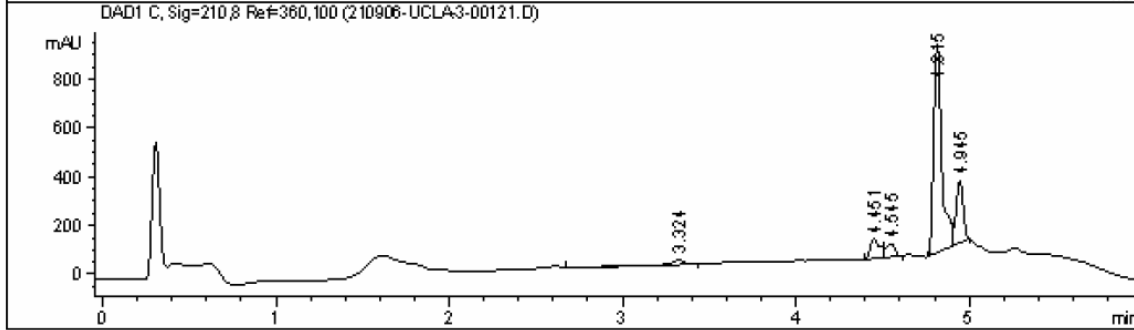
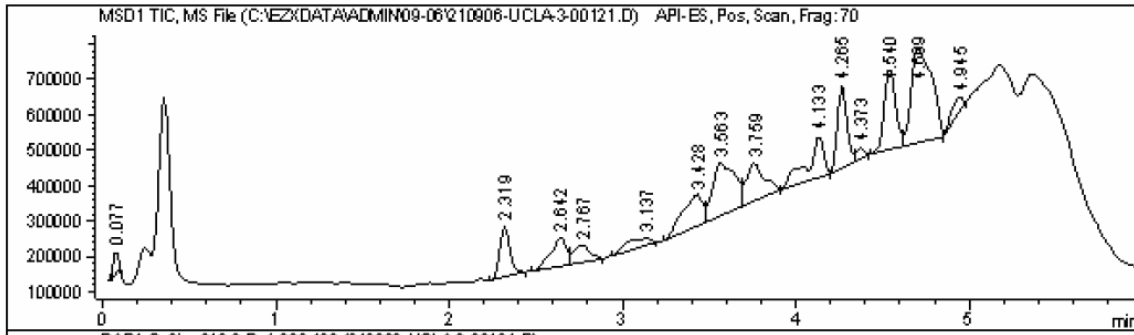
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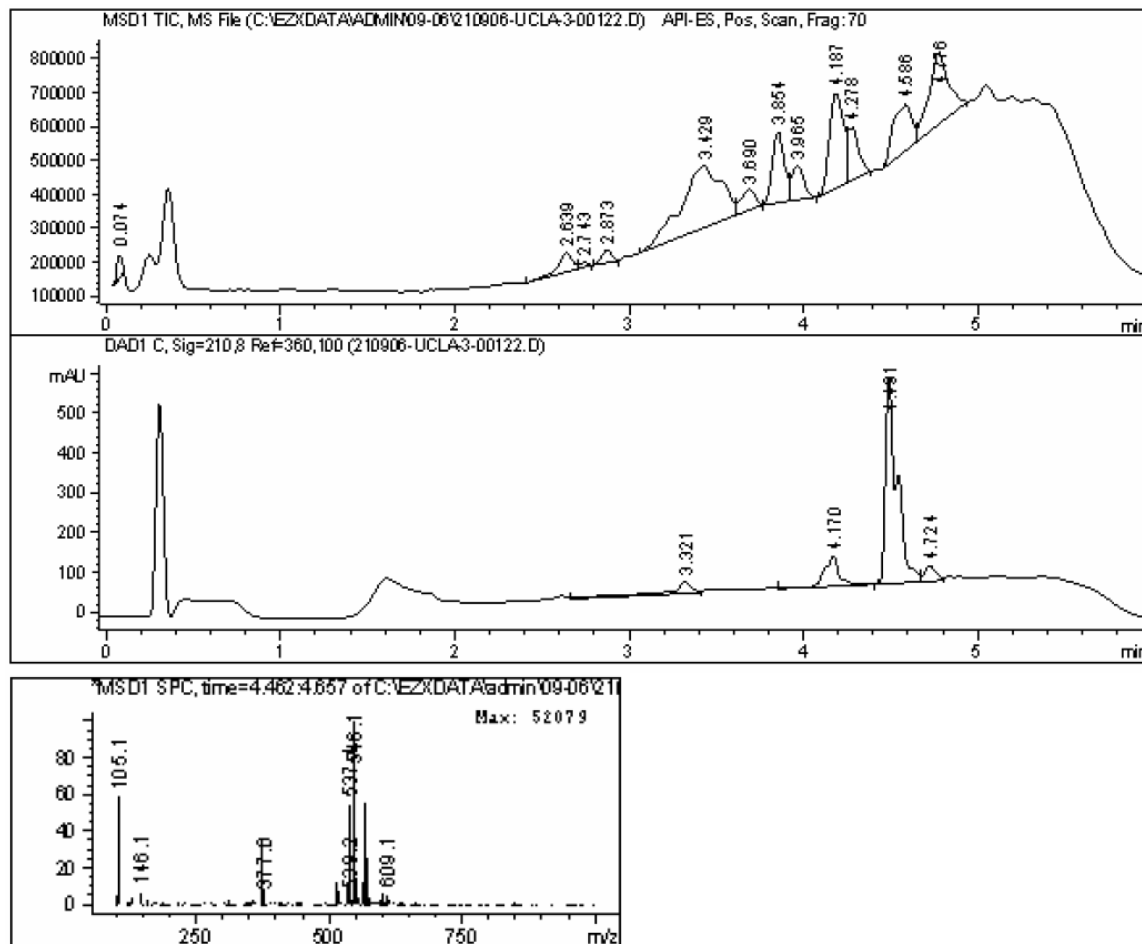
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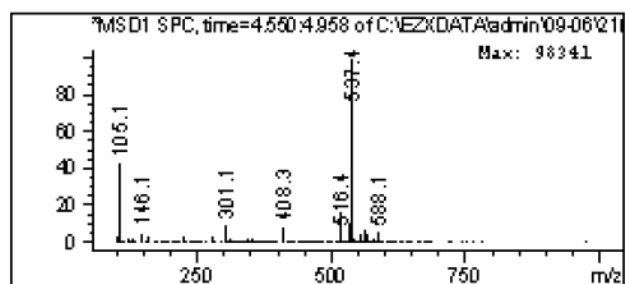
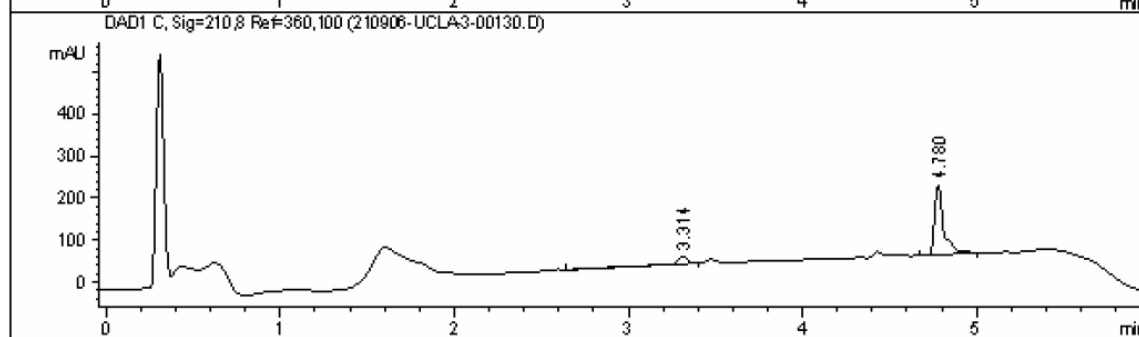
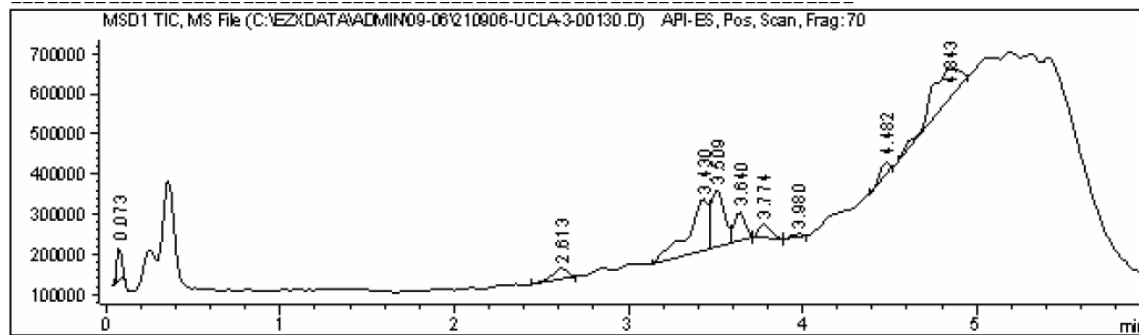
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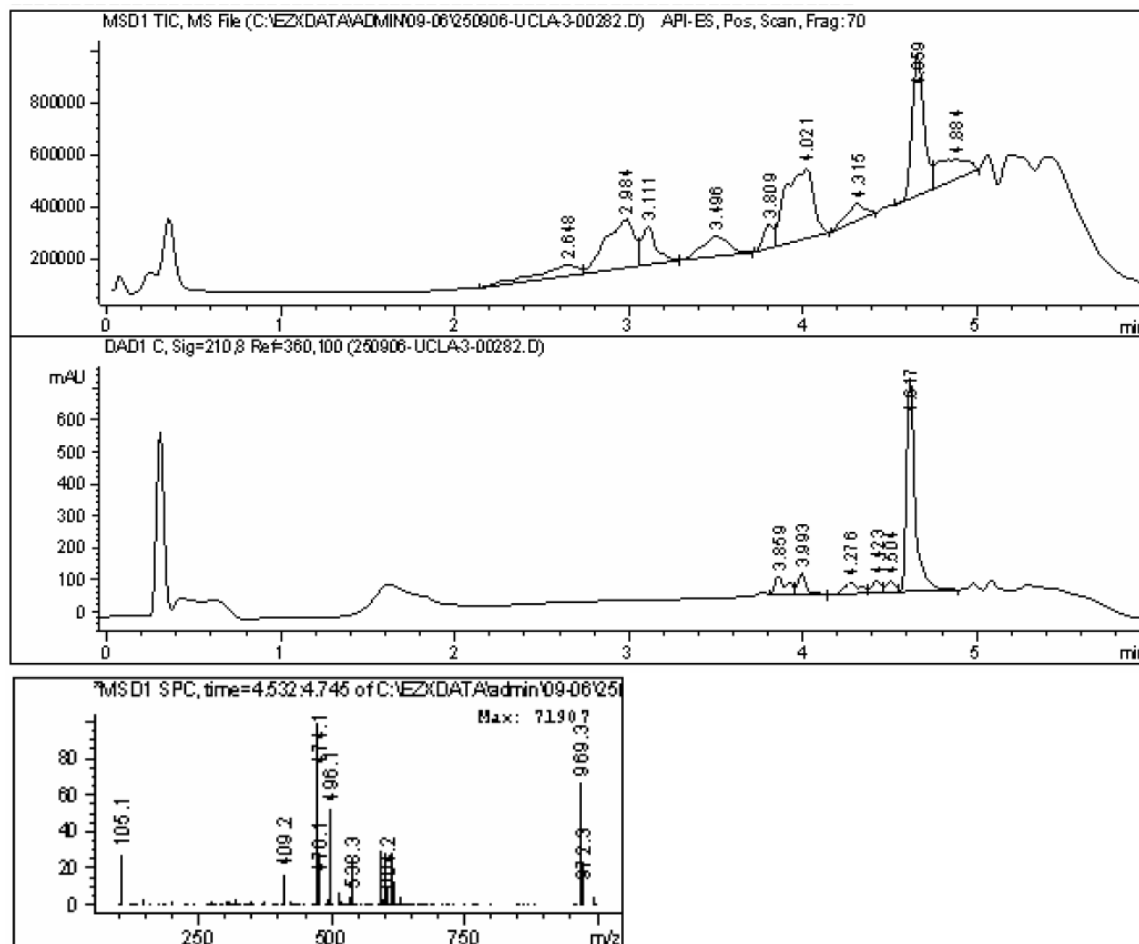


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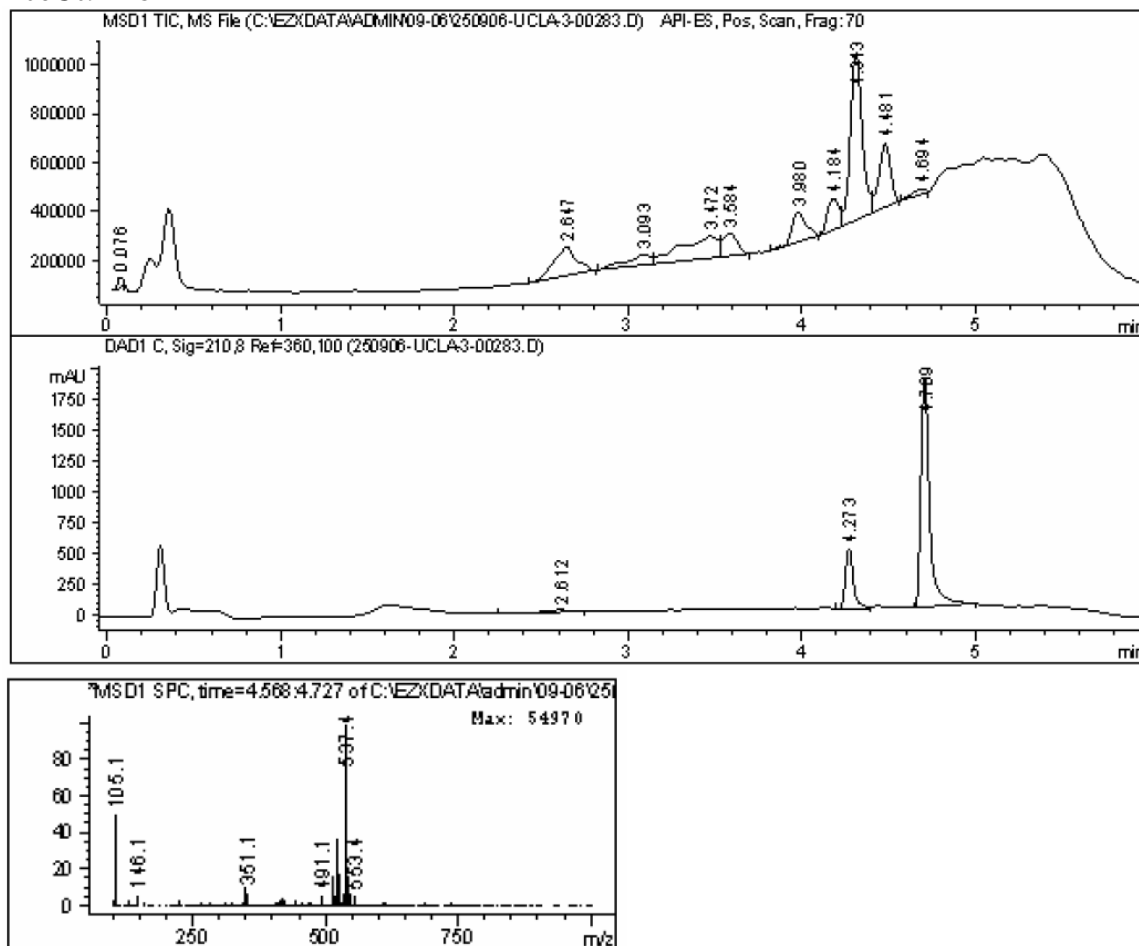


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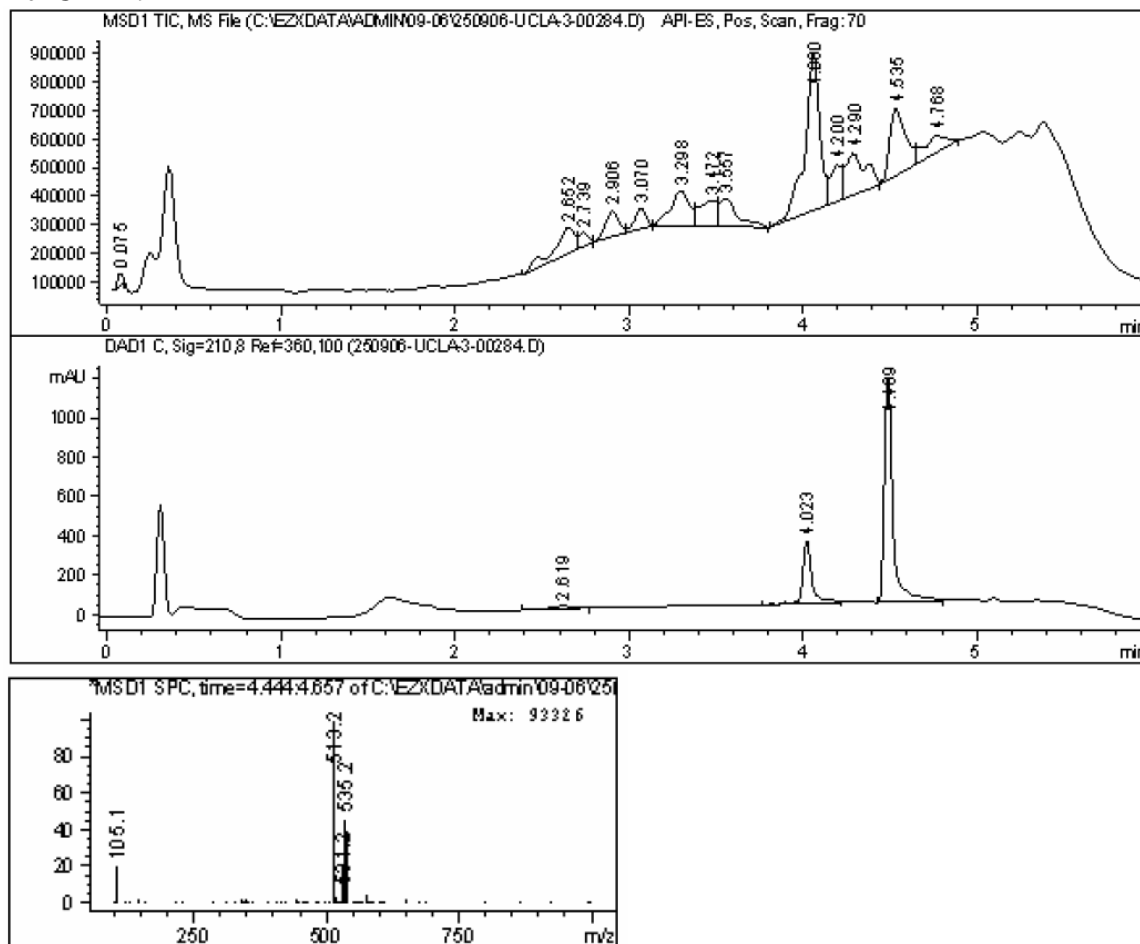
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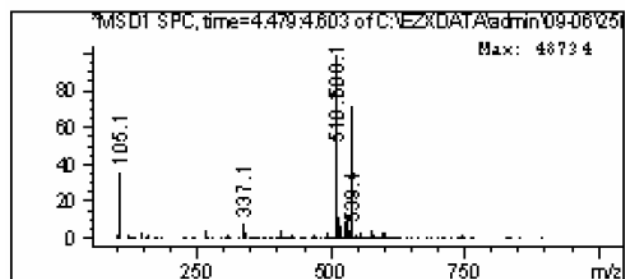
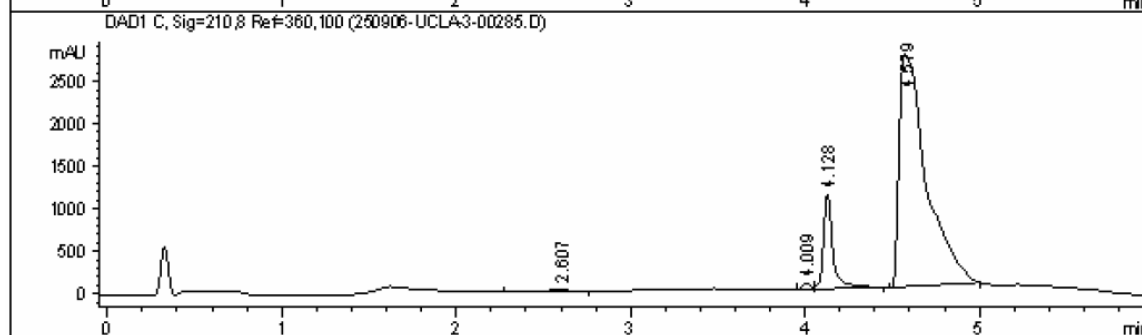
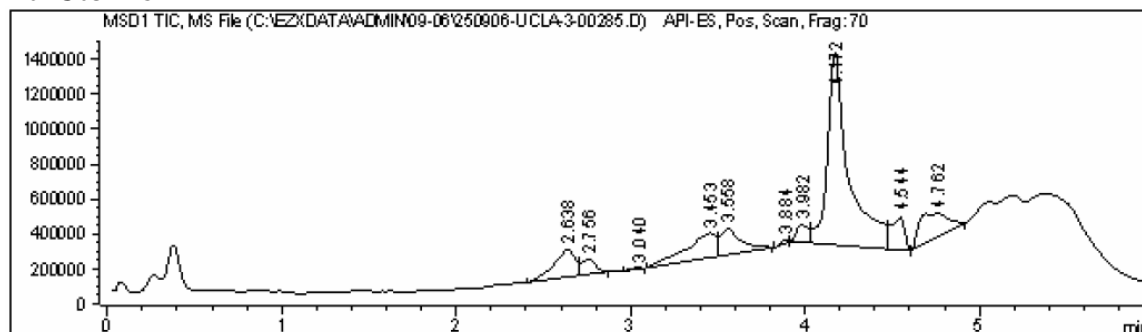


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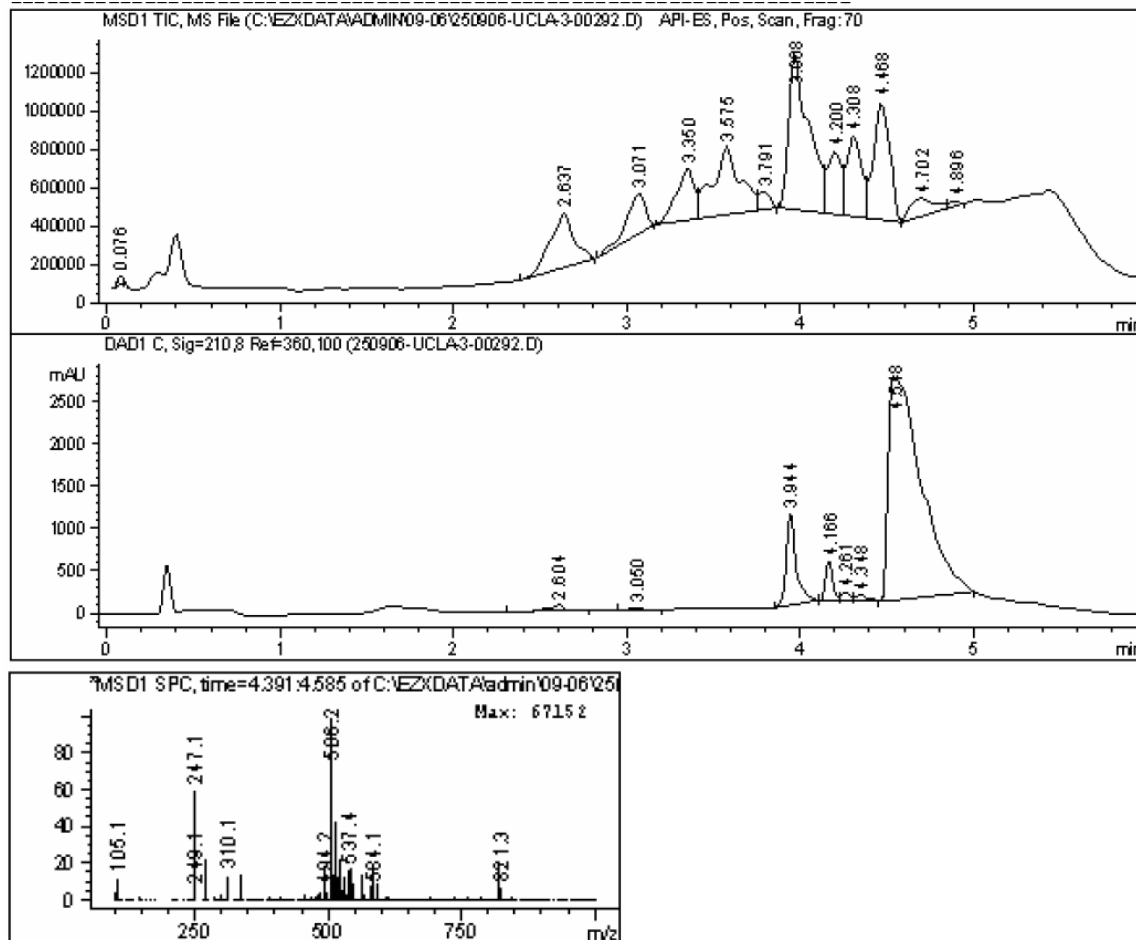


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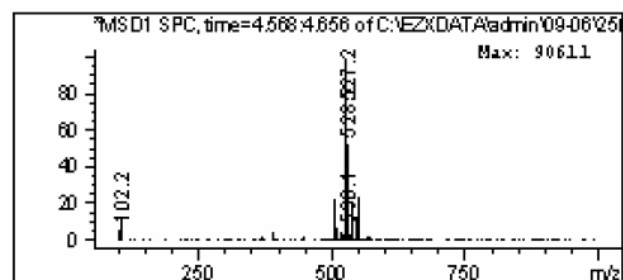
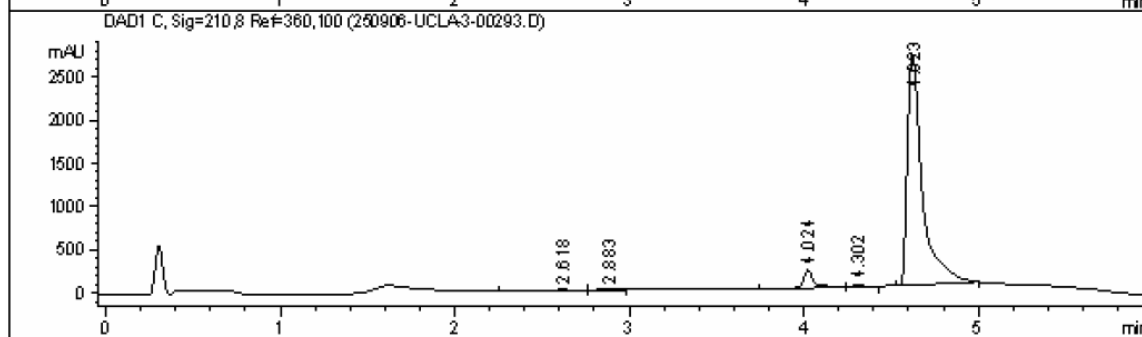
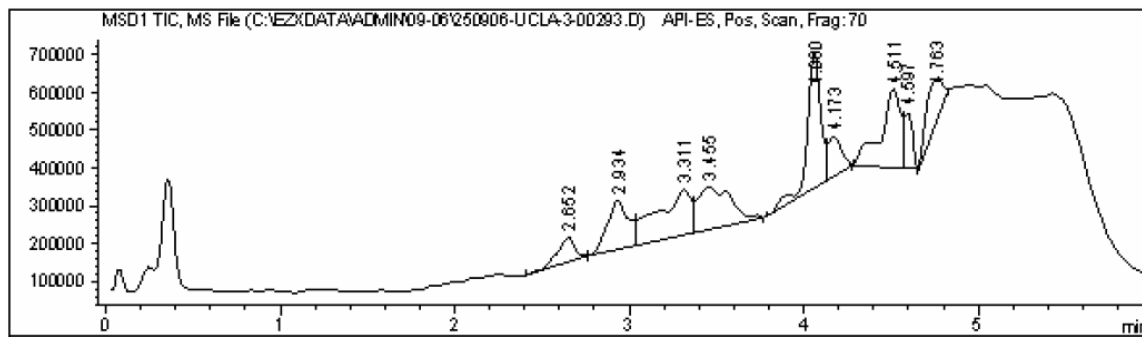


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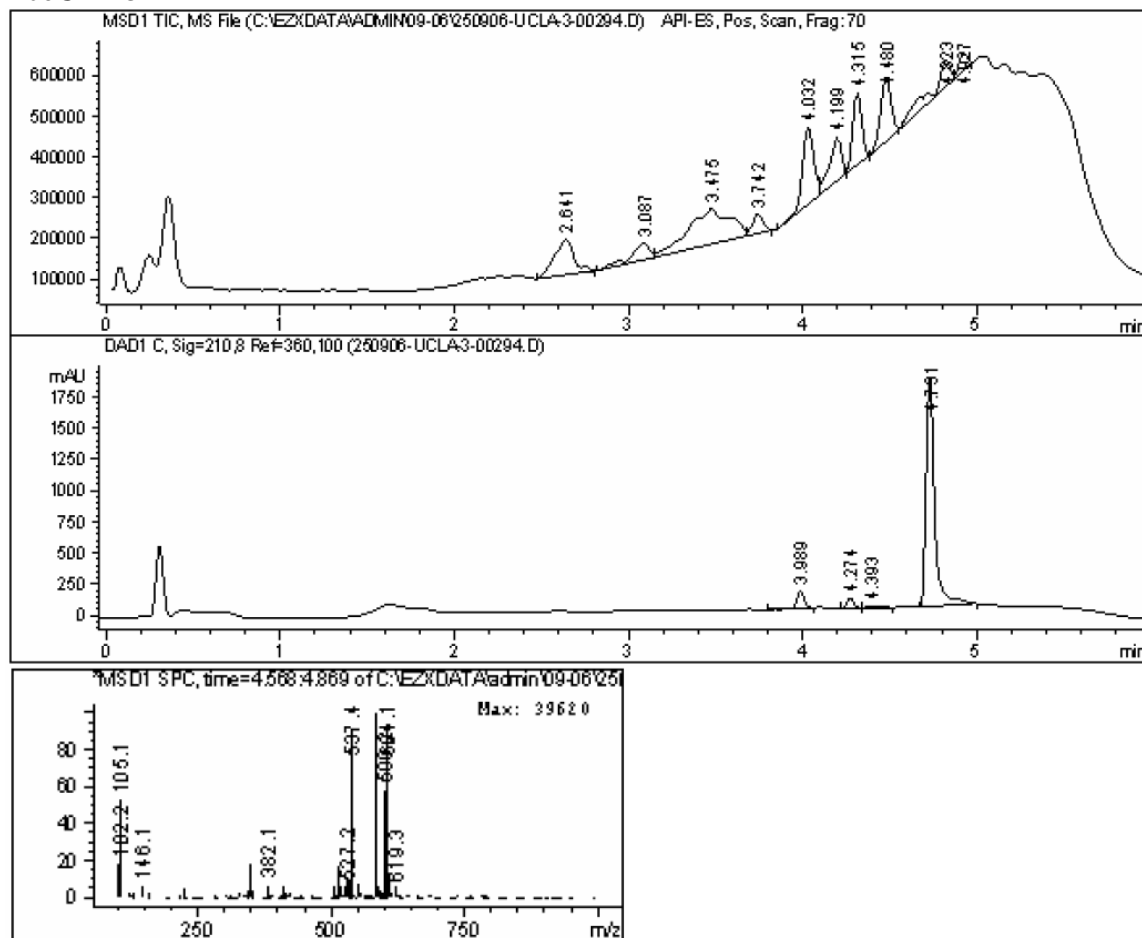
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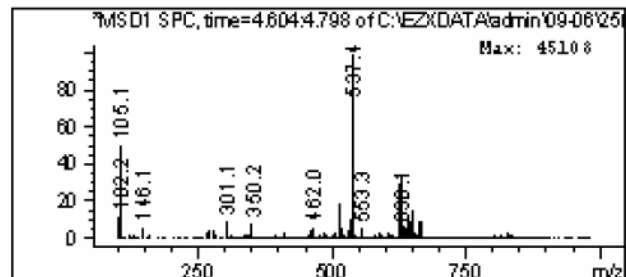
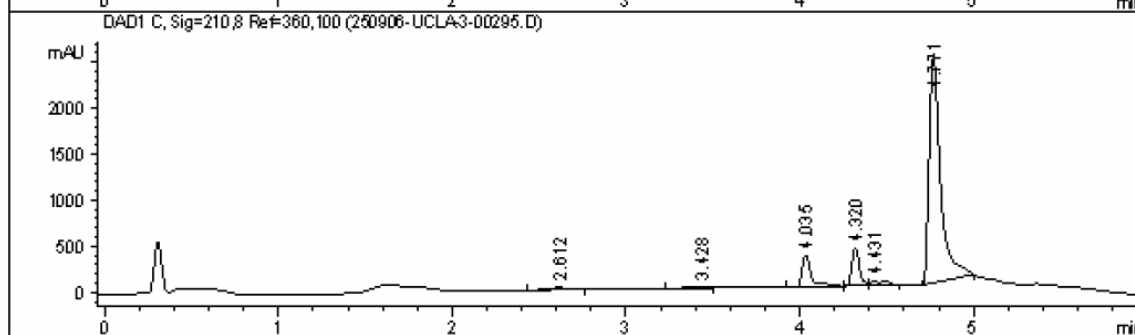
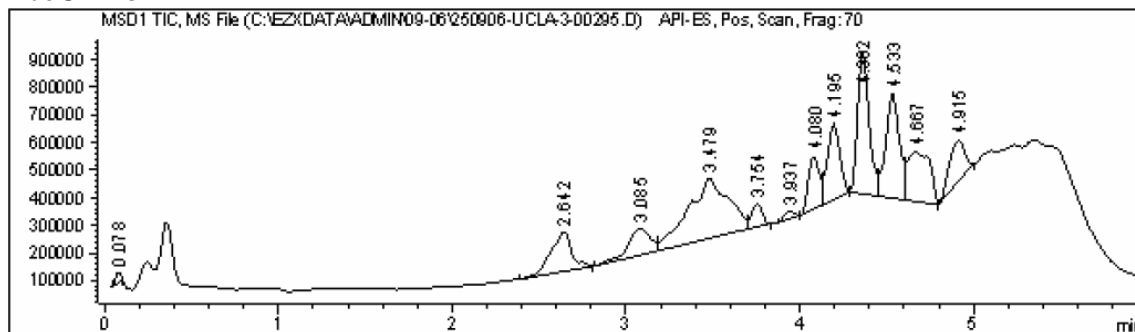
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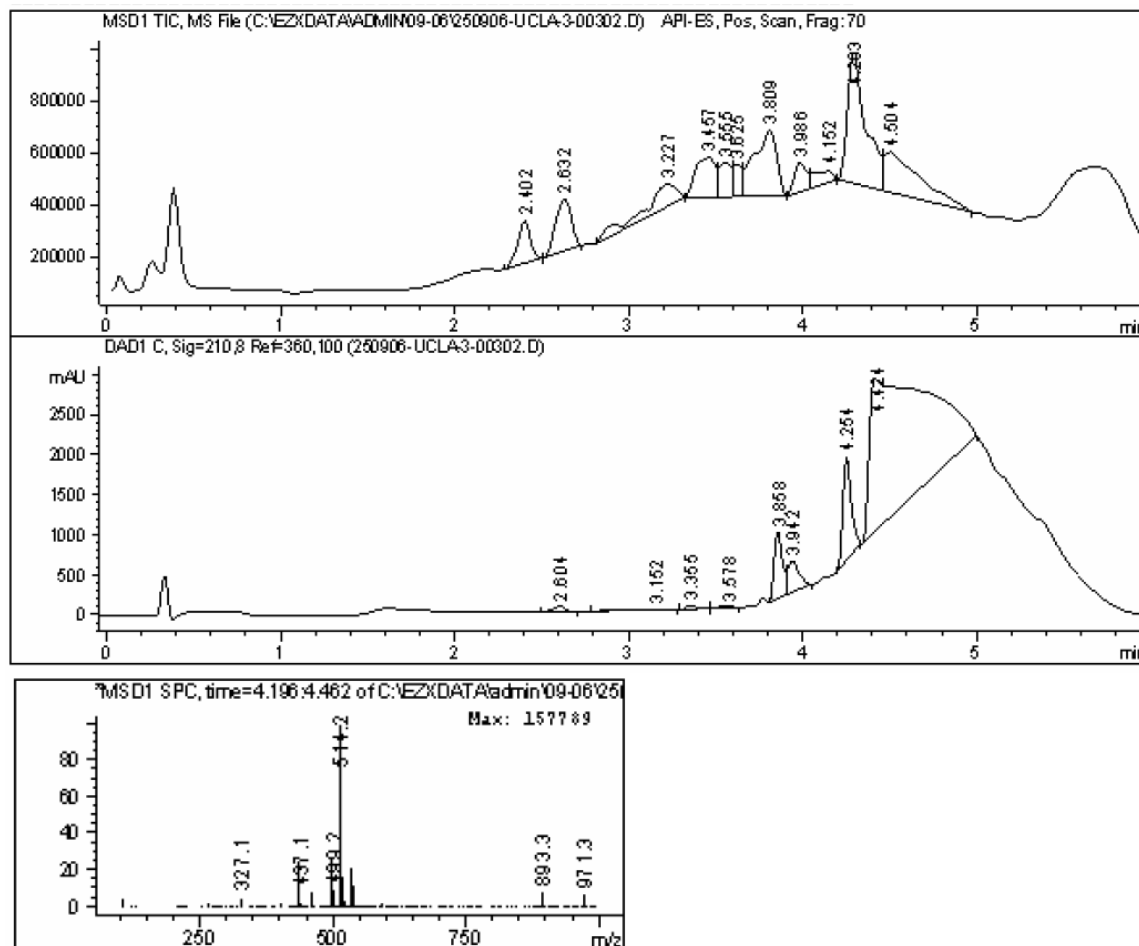


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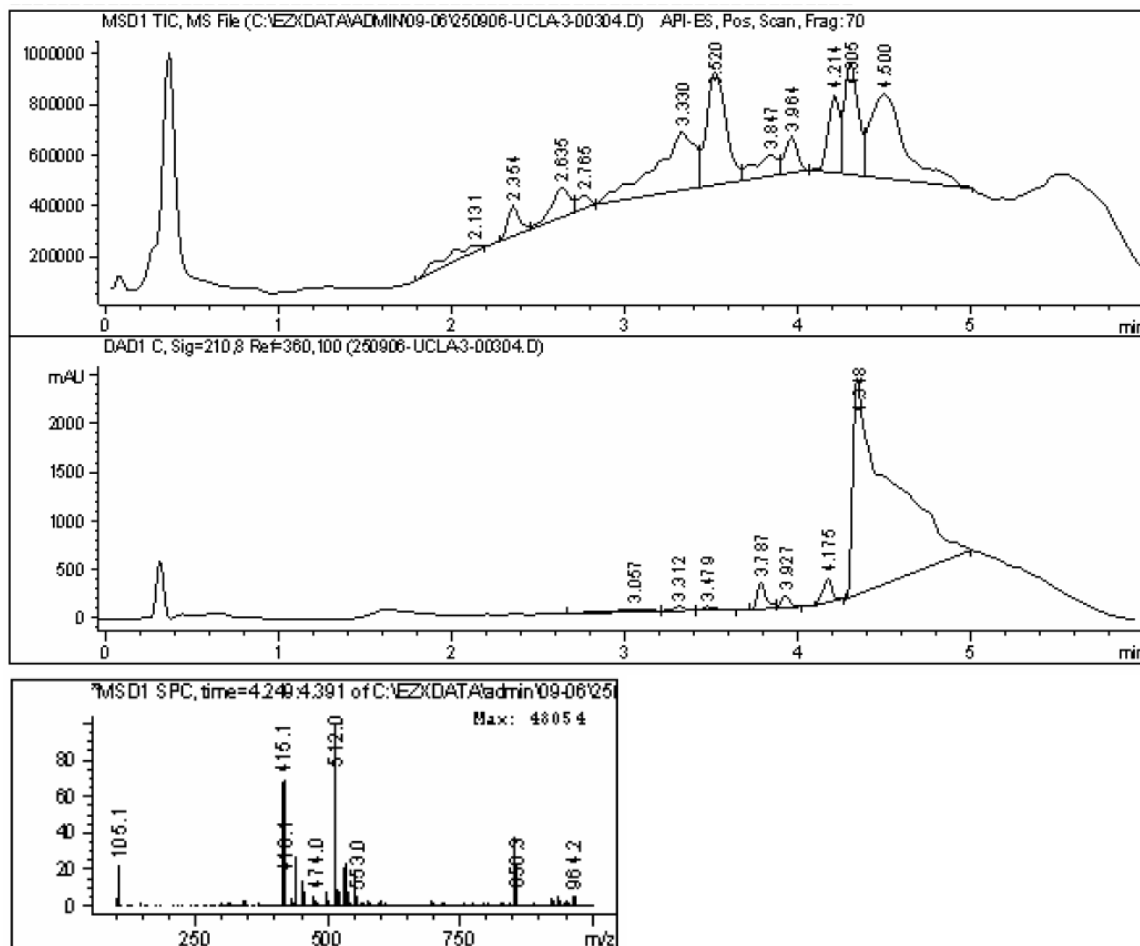


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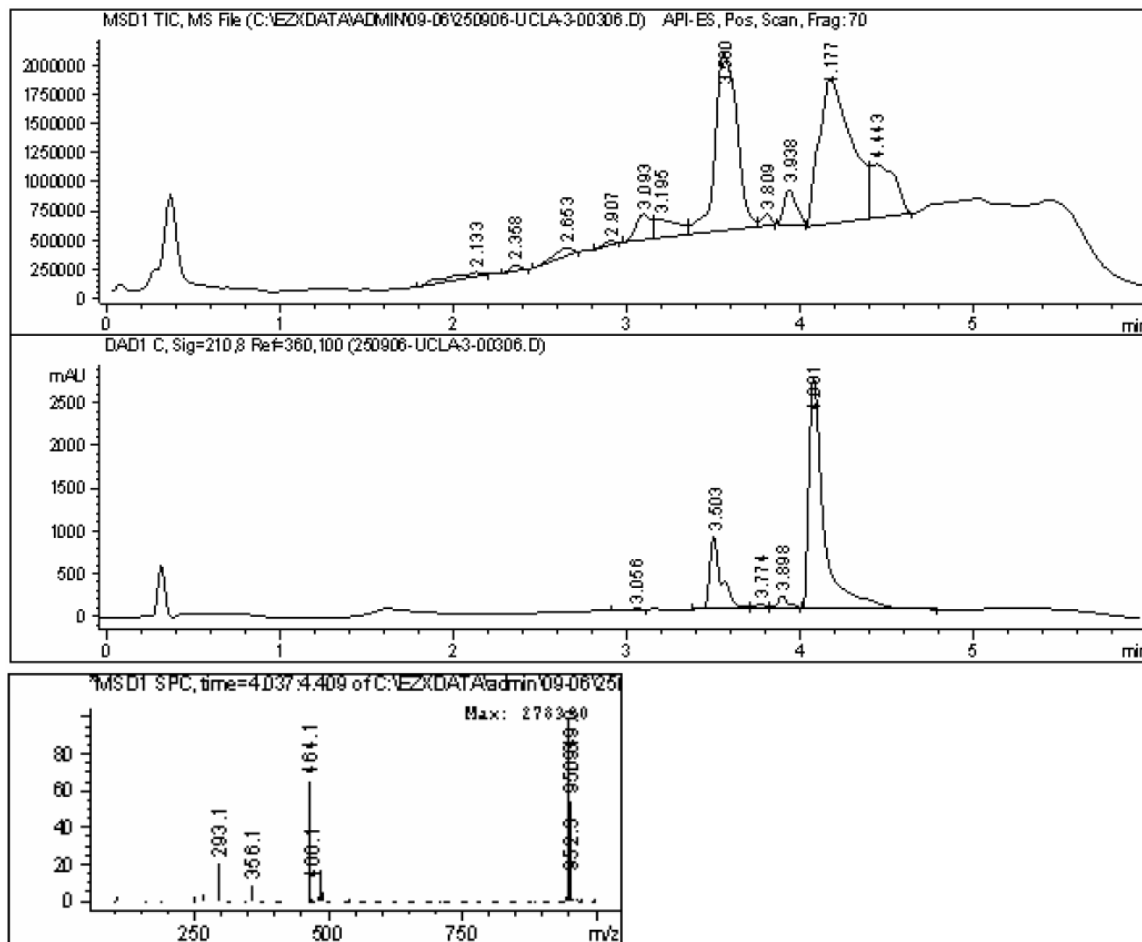
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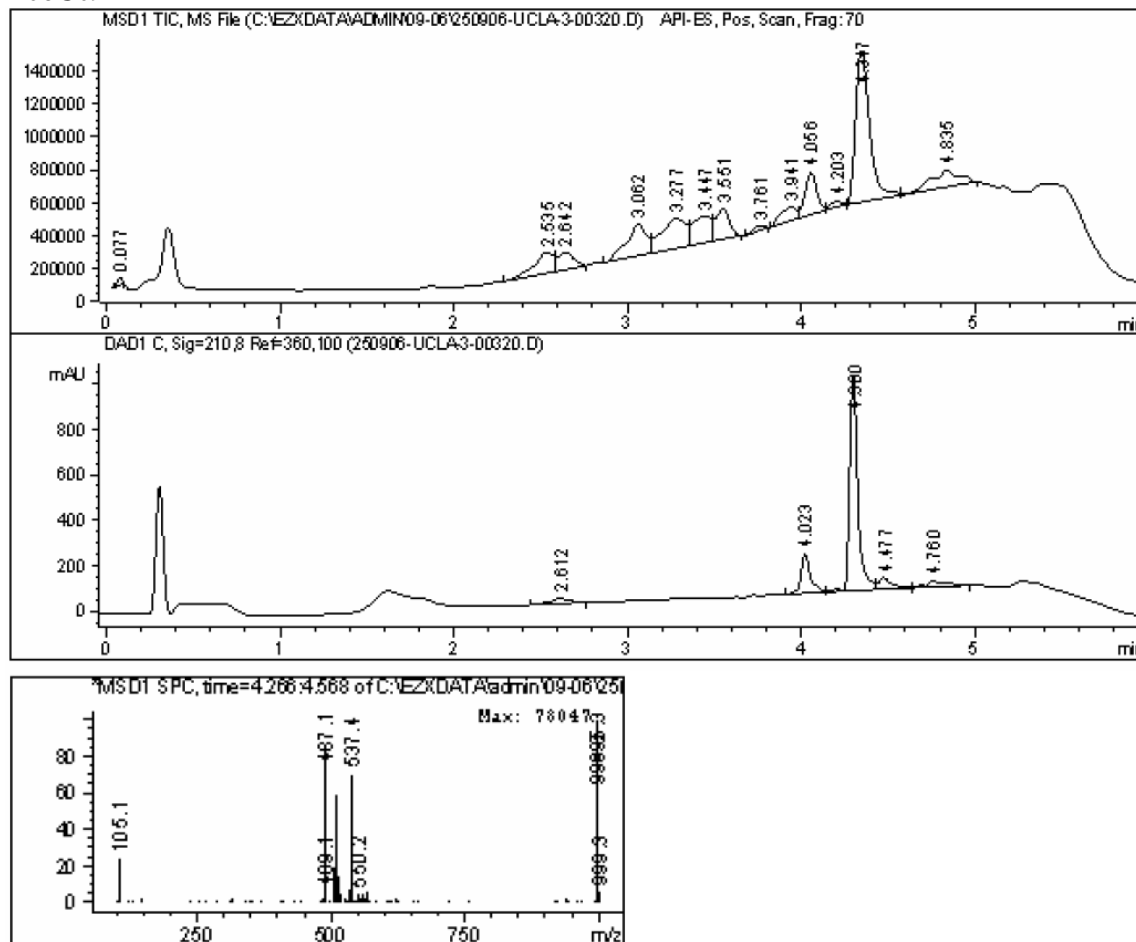


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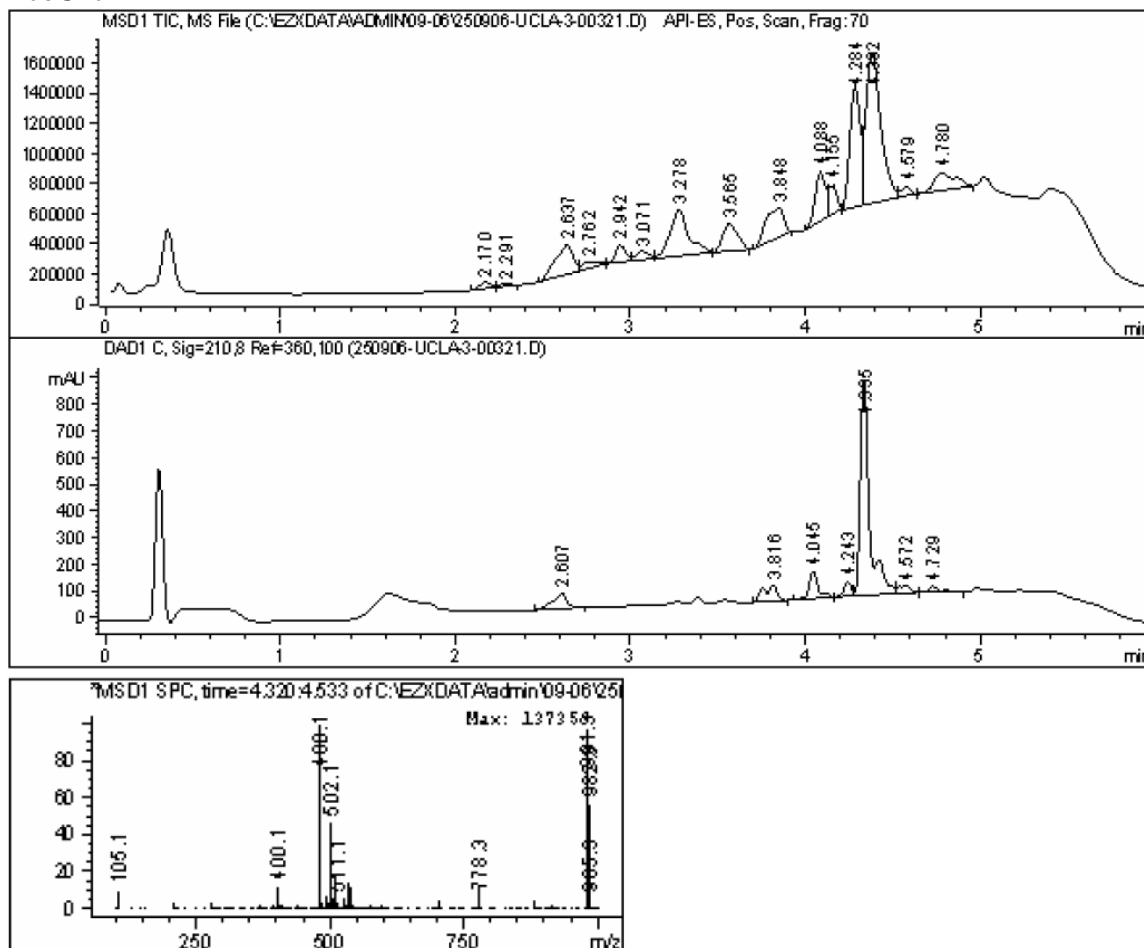




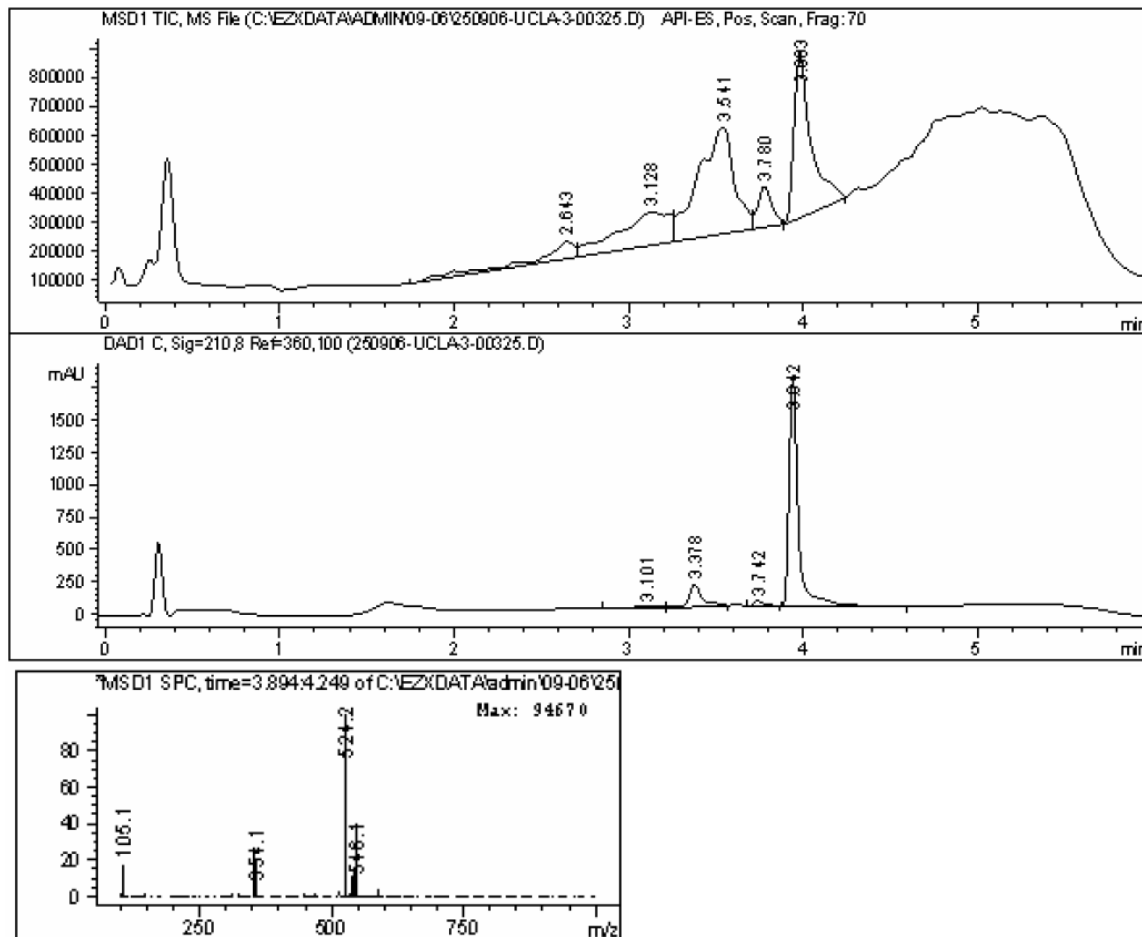
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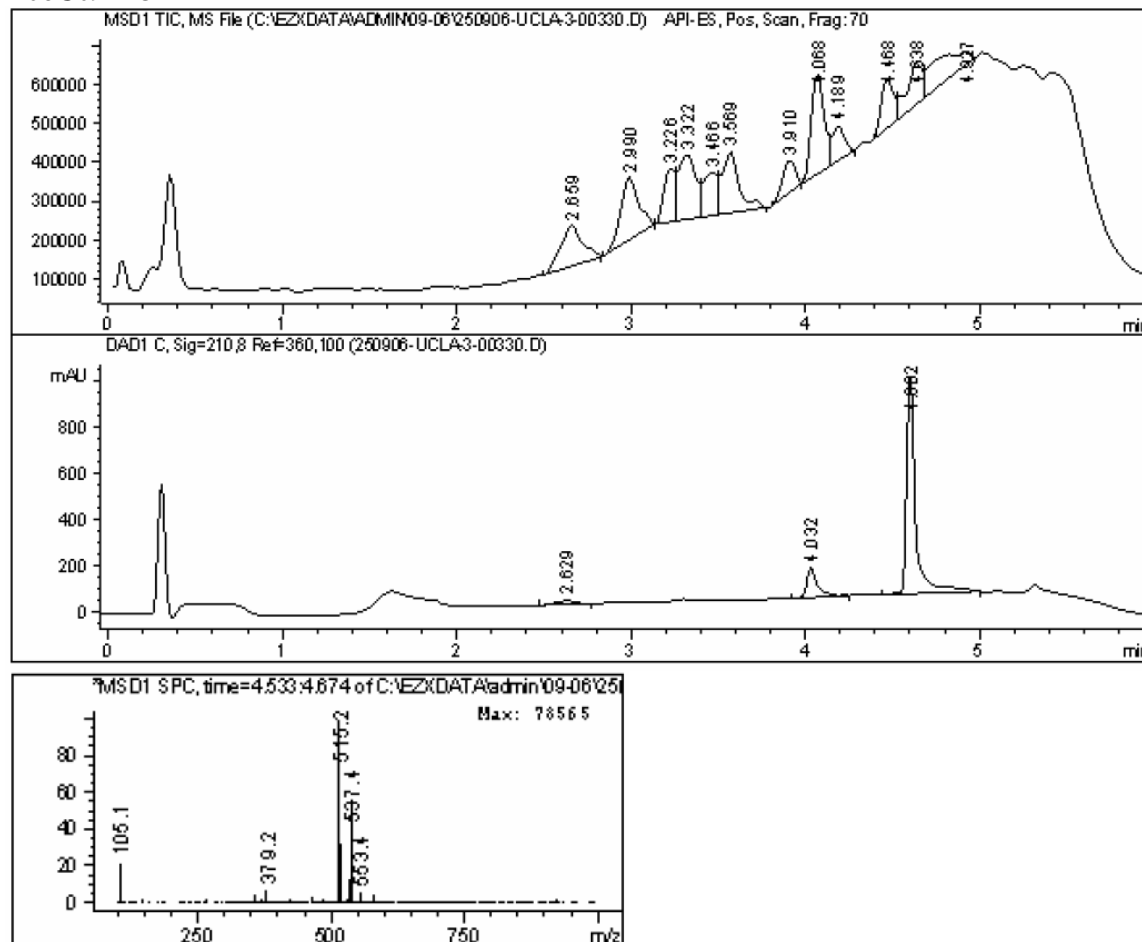
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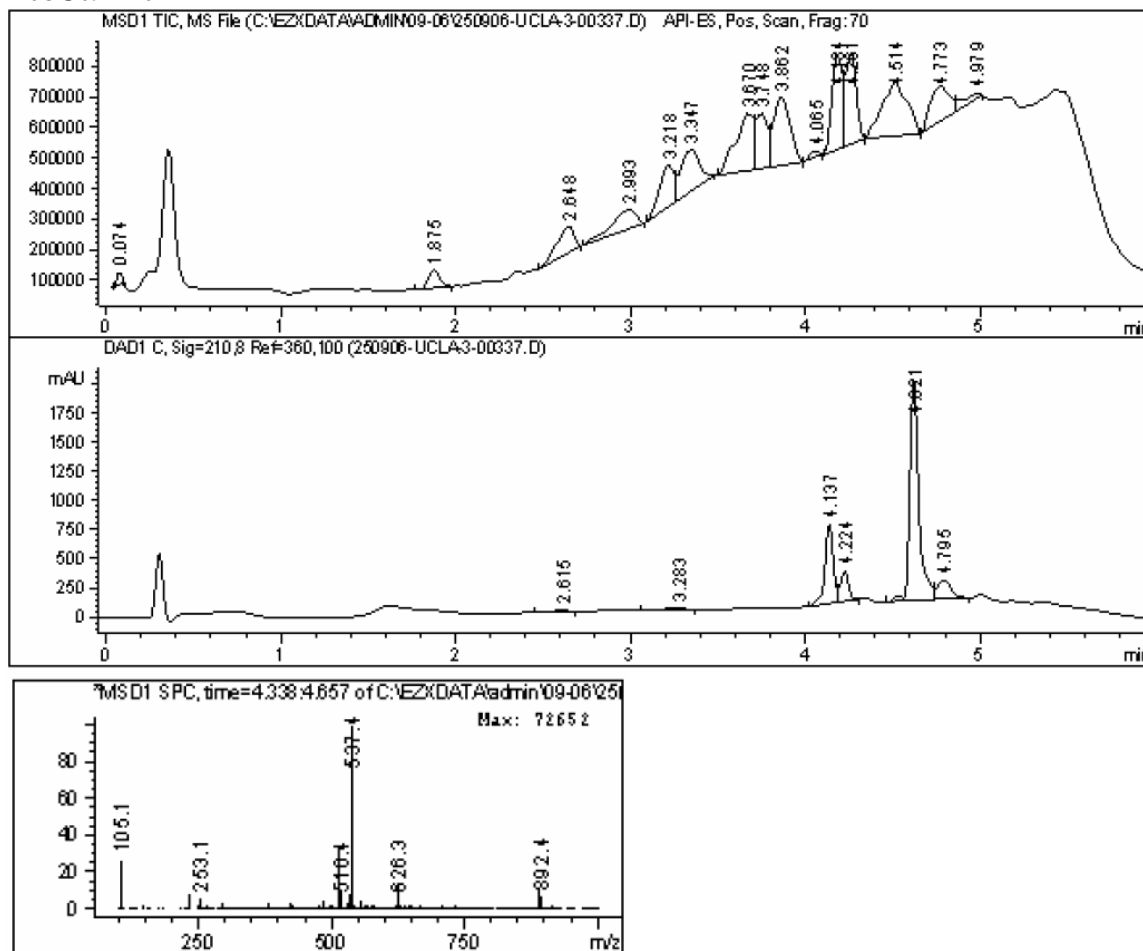
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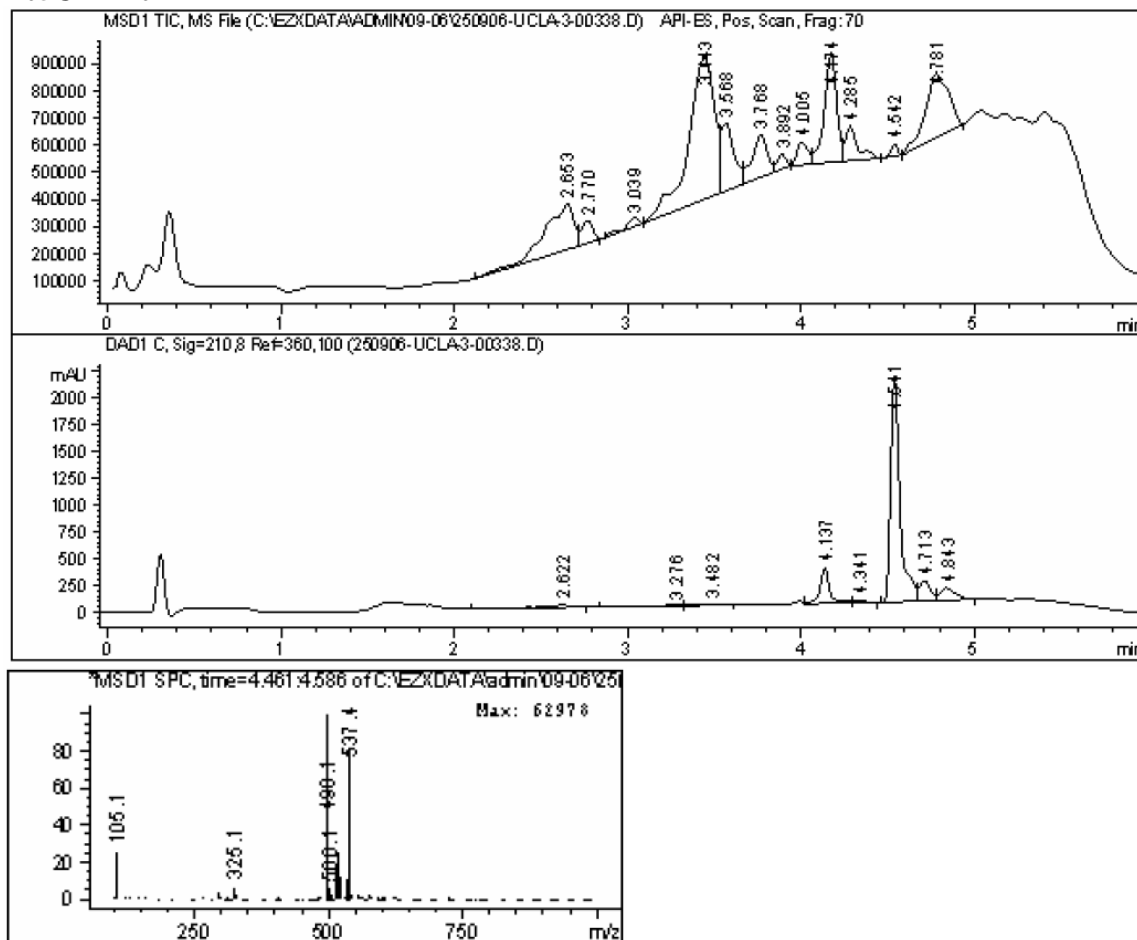
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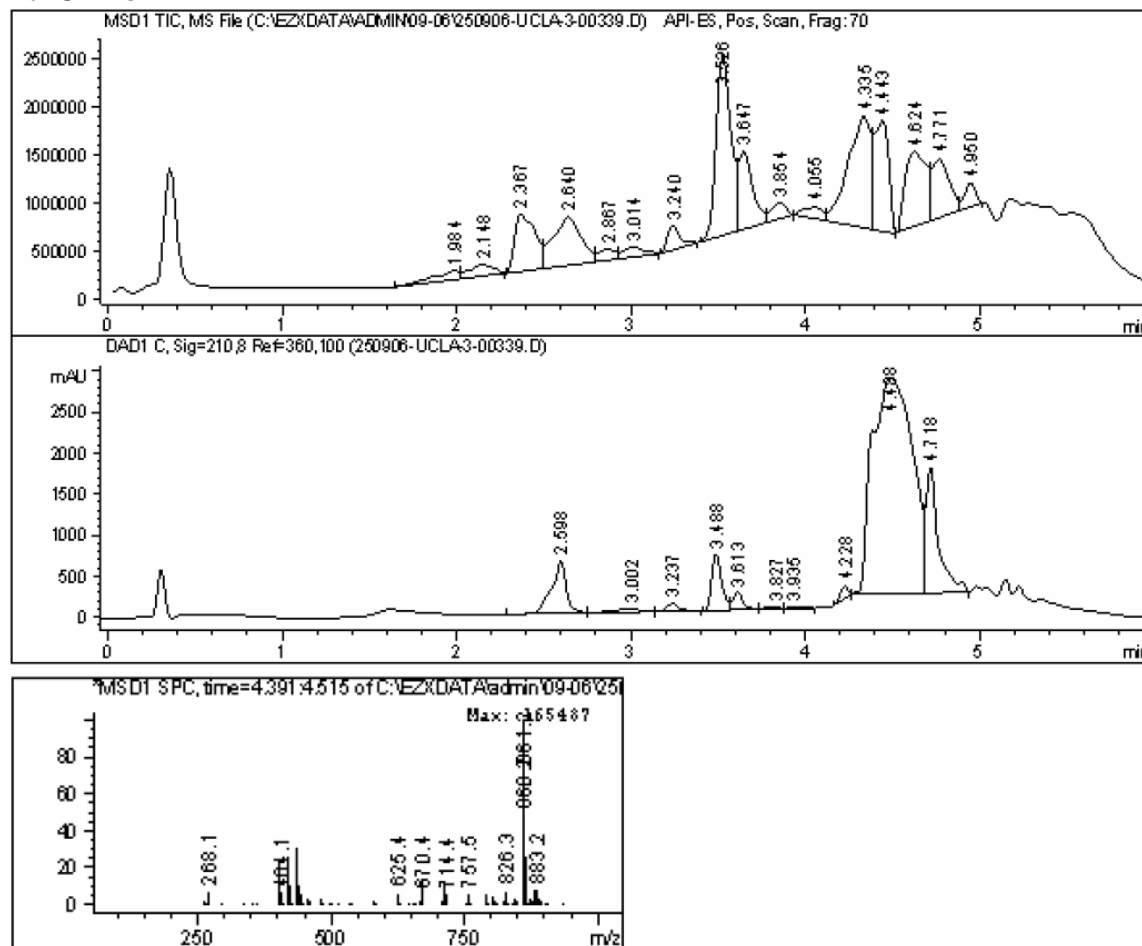
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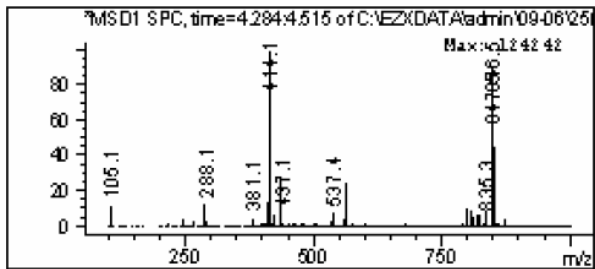
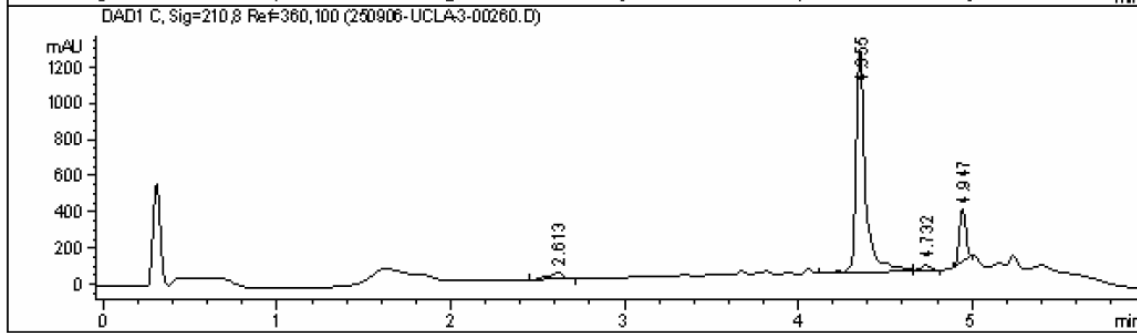
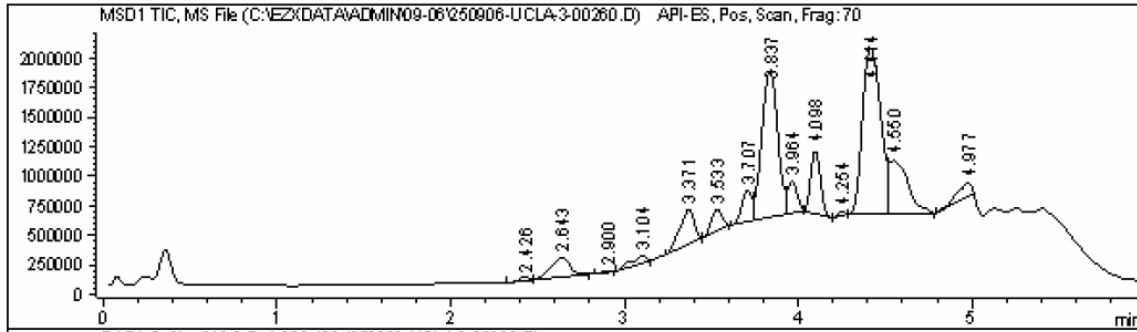
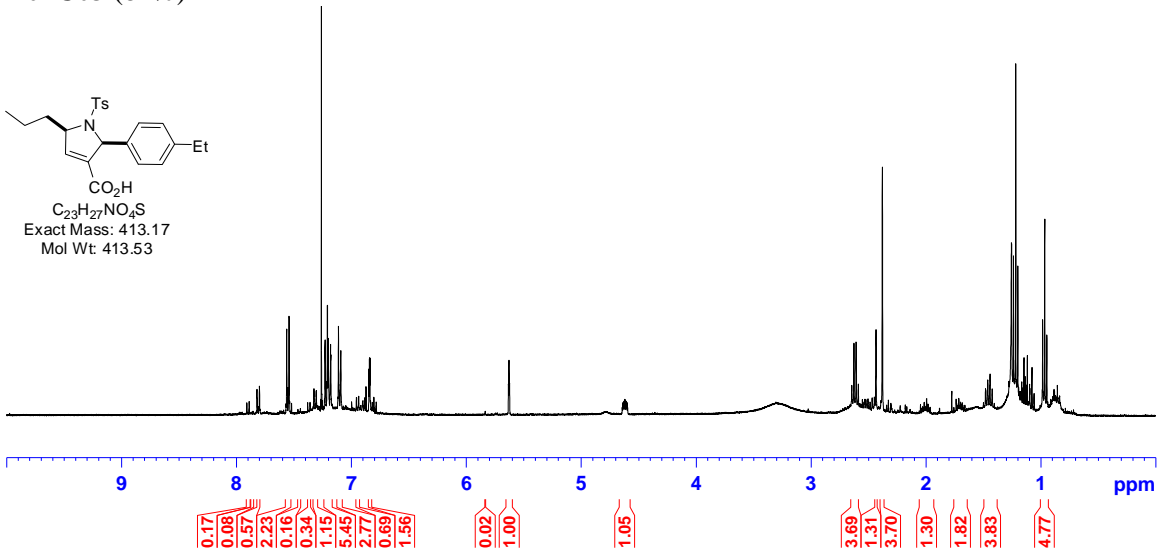
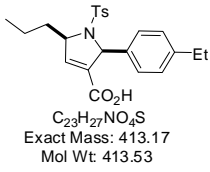
**A05C11E20**



A07C14E32

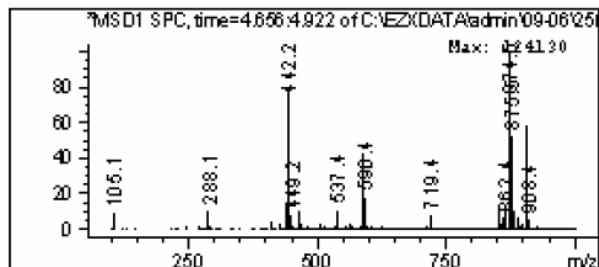
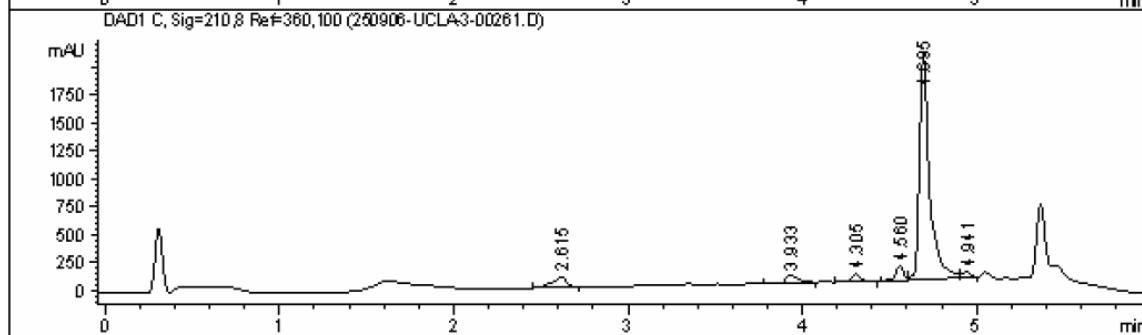
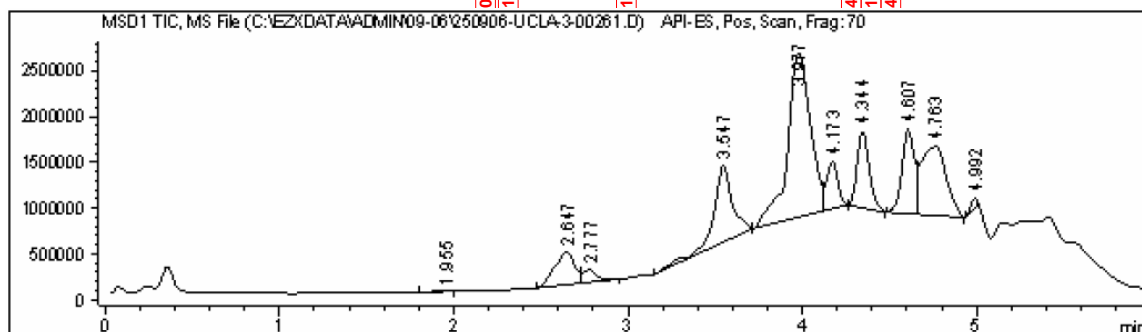
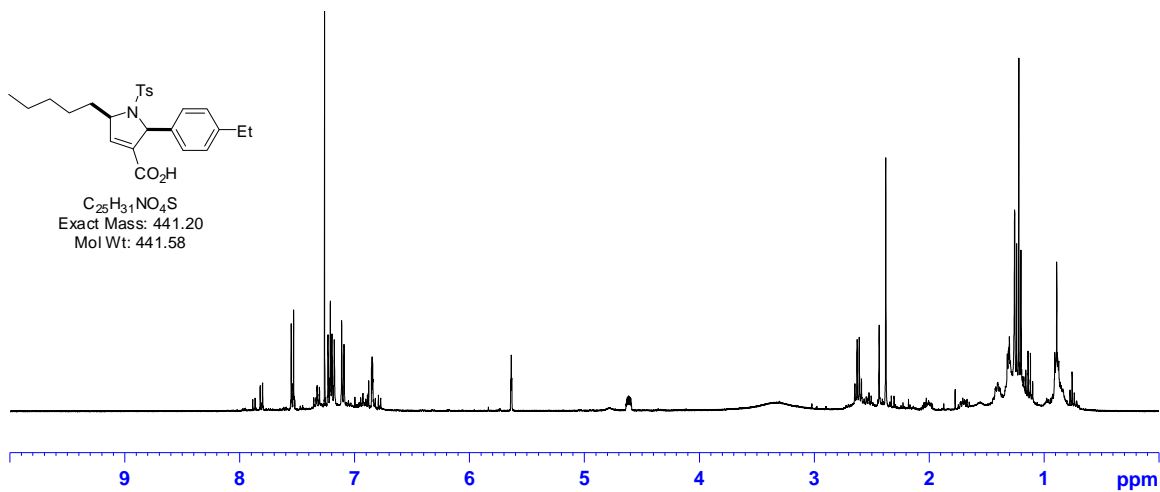


**A07C03 (81%)**

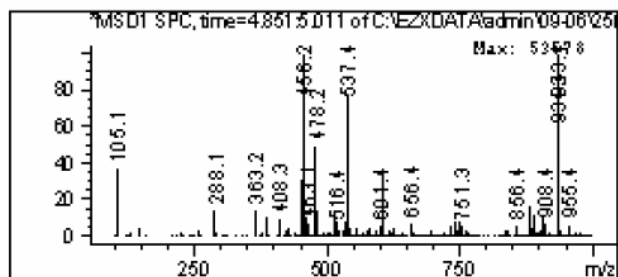
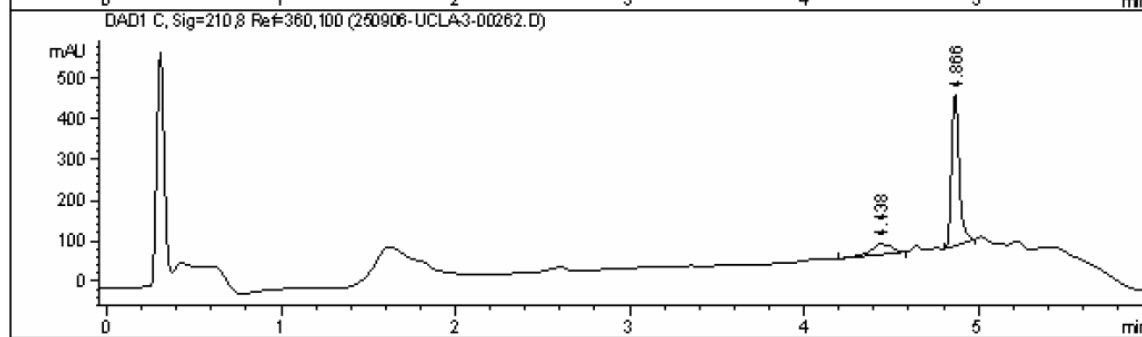
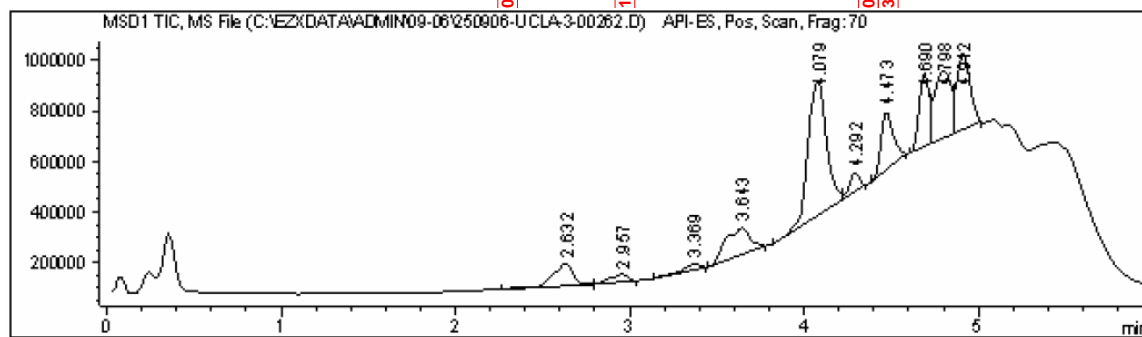
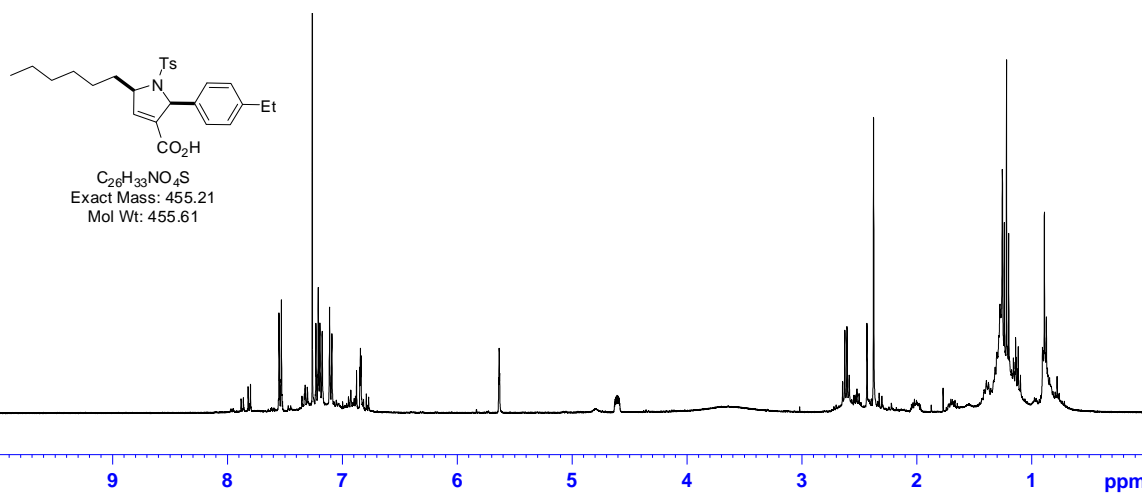




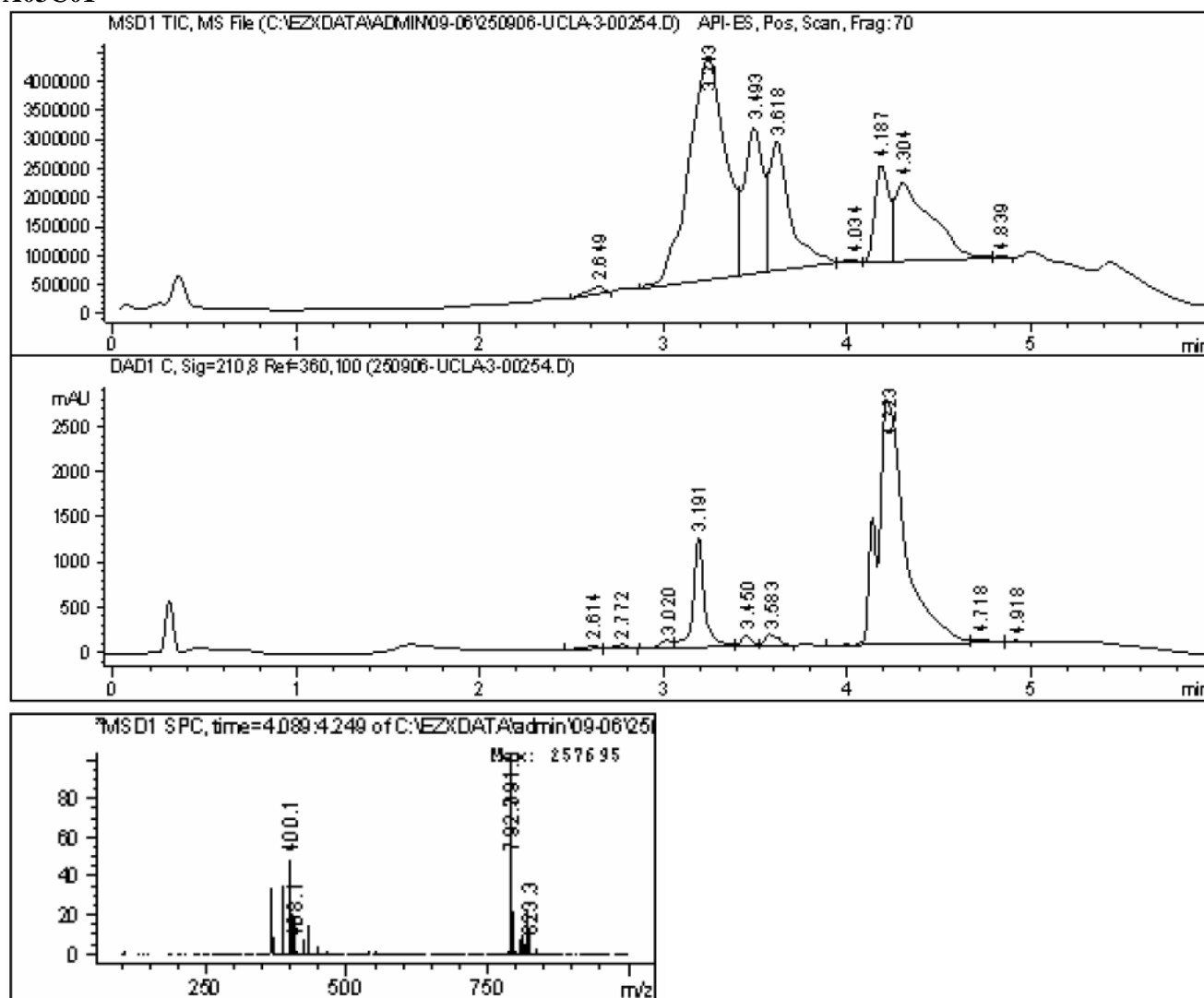
A09C03 (82%)



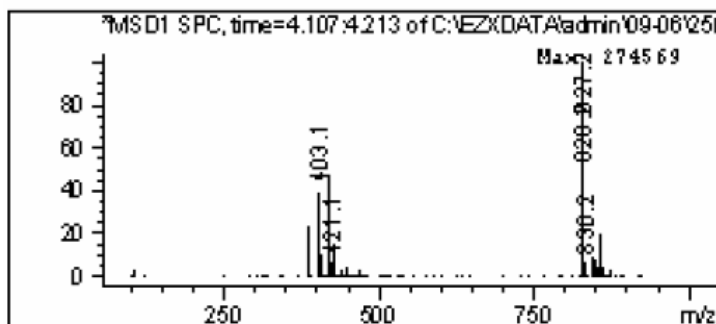
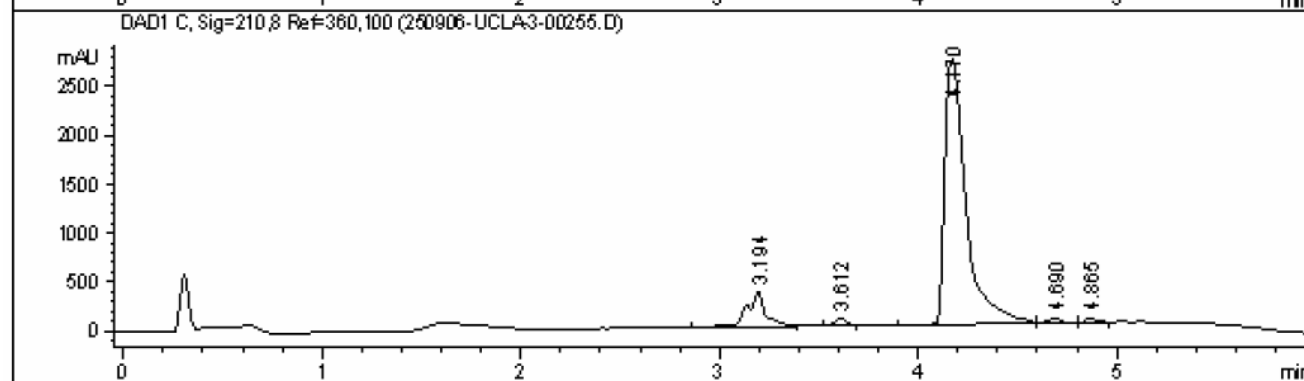
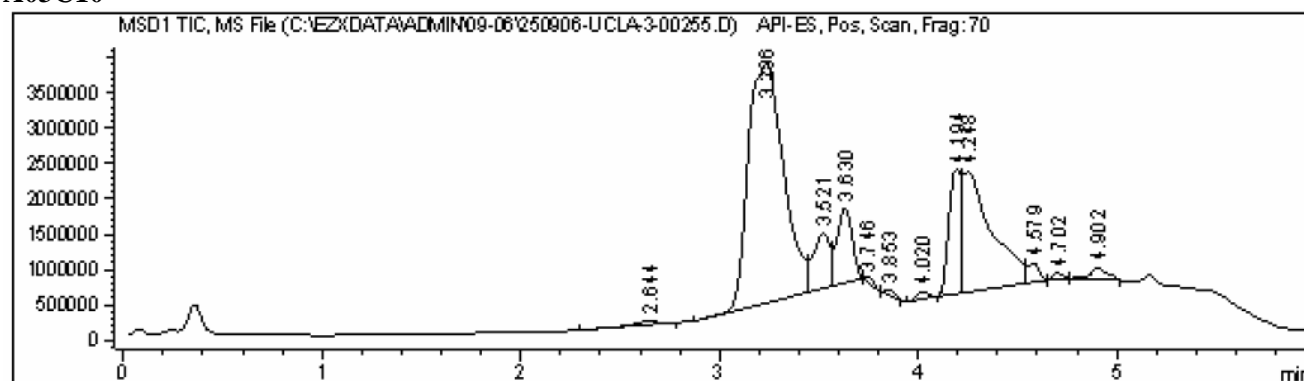
**A10C03 (84%)**



A03C01

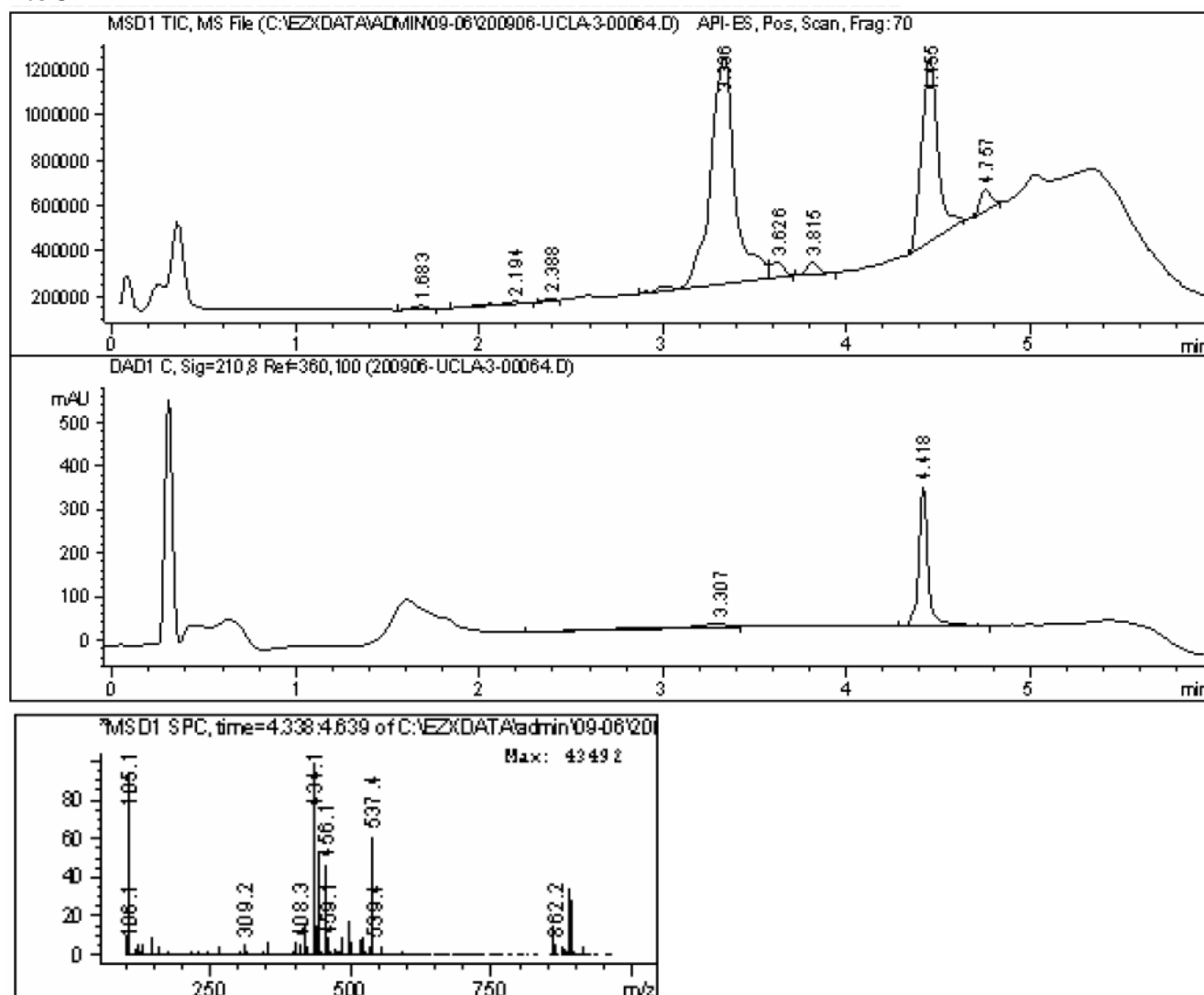


A03C10

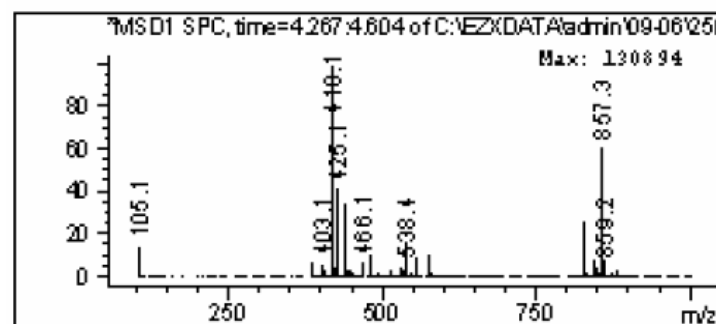
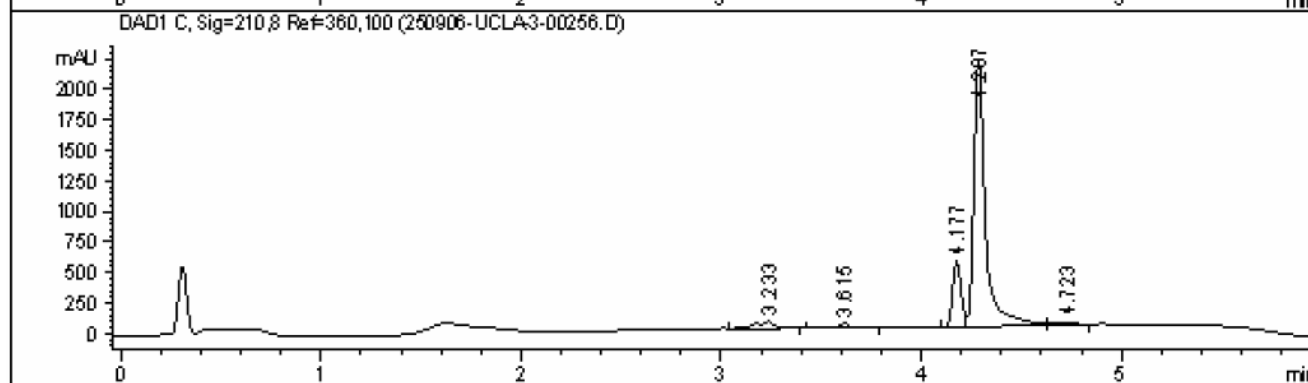
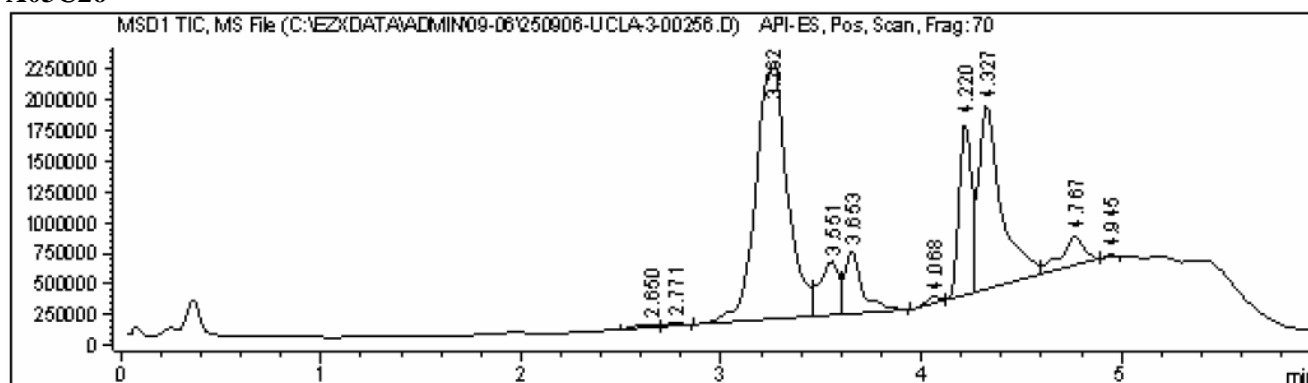


Component 1: Peak at Scan 237.9. Top ions are 418 857 842

A03C12

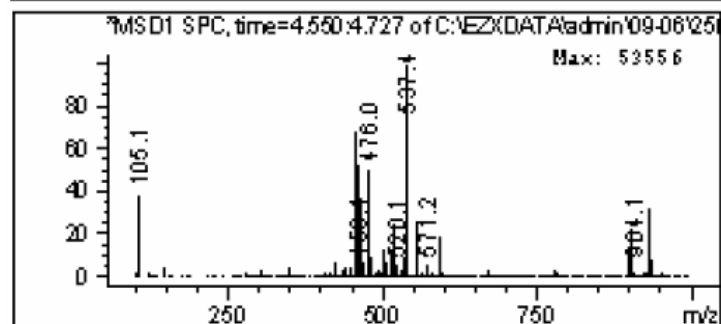
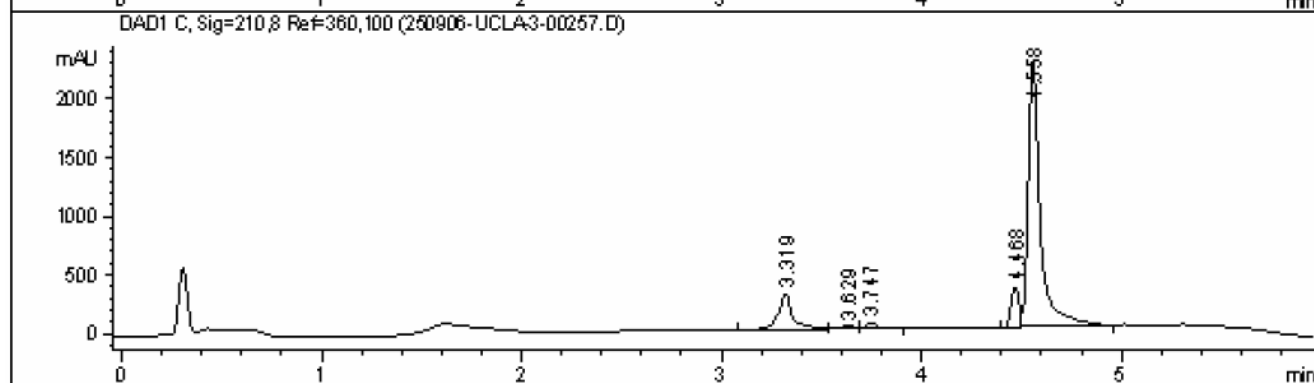
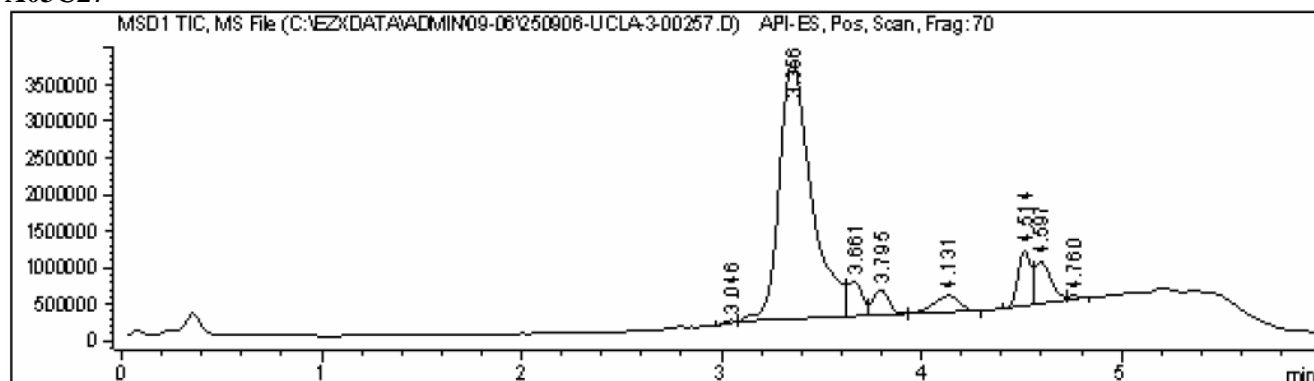


A03C26



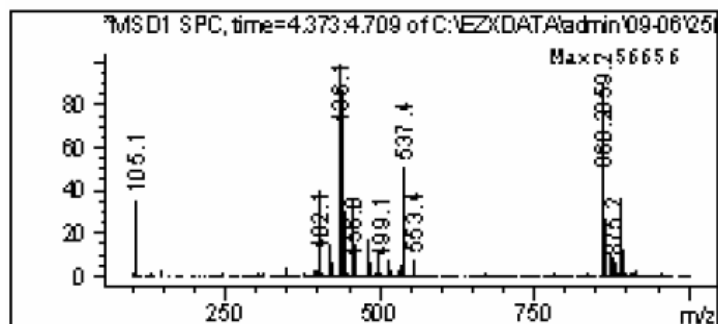
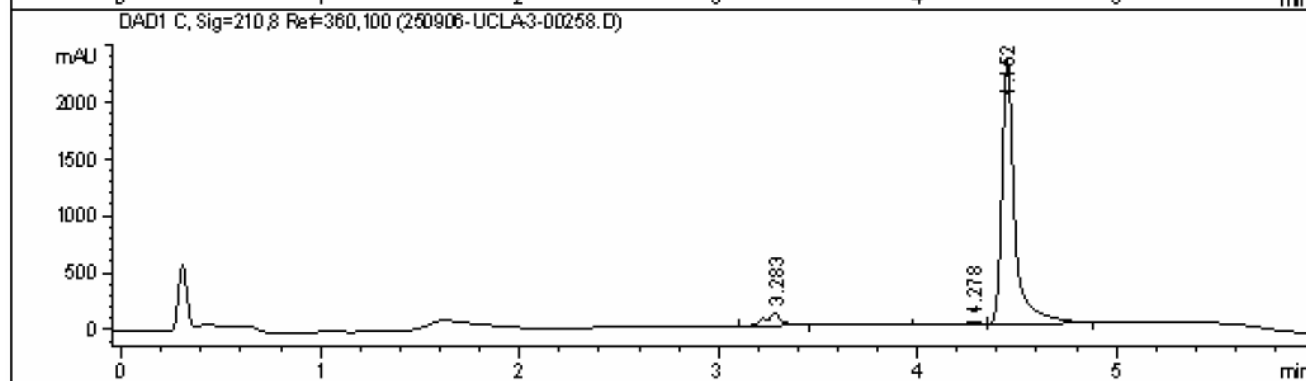
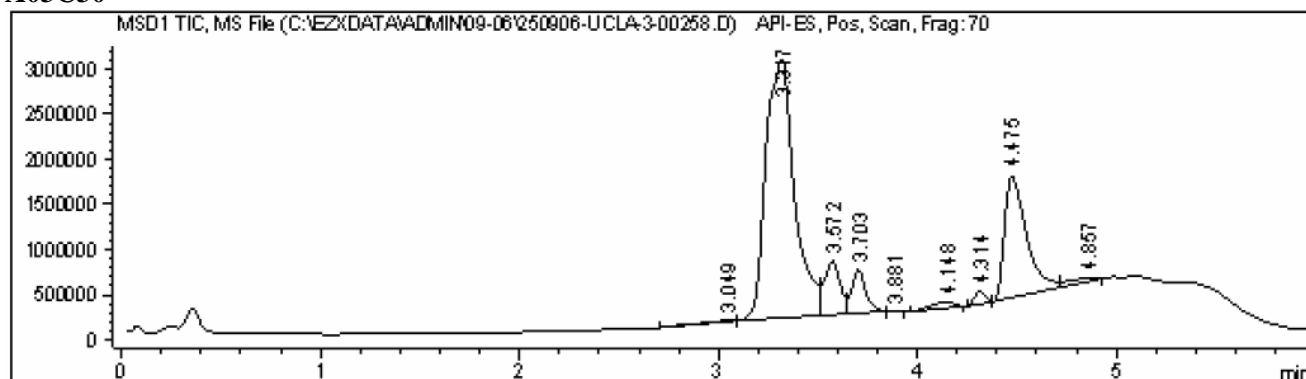
Component 2: Peak at Scan 243.8. Top ions are 418 857 858

A03C27



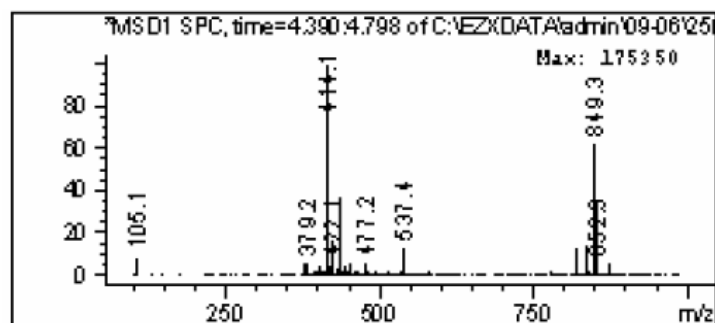
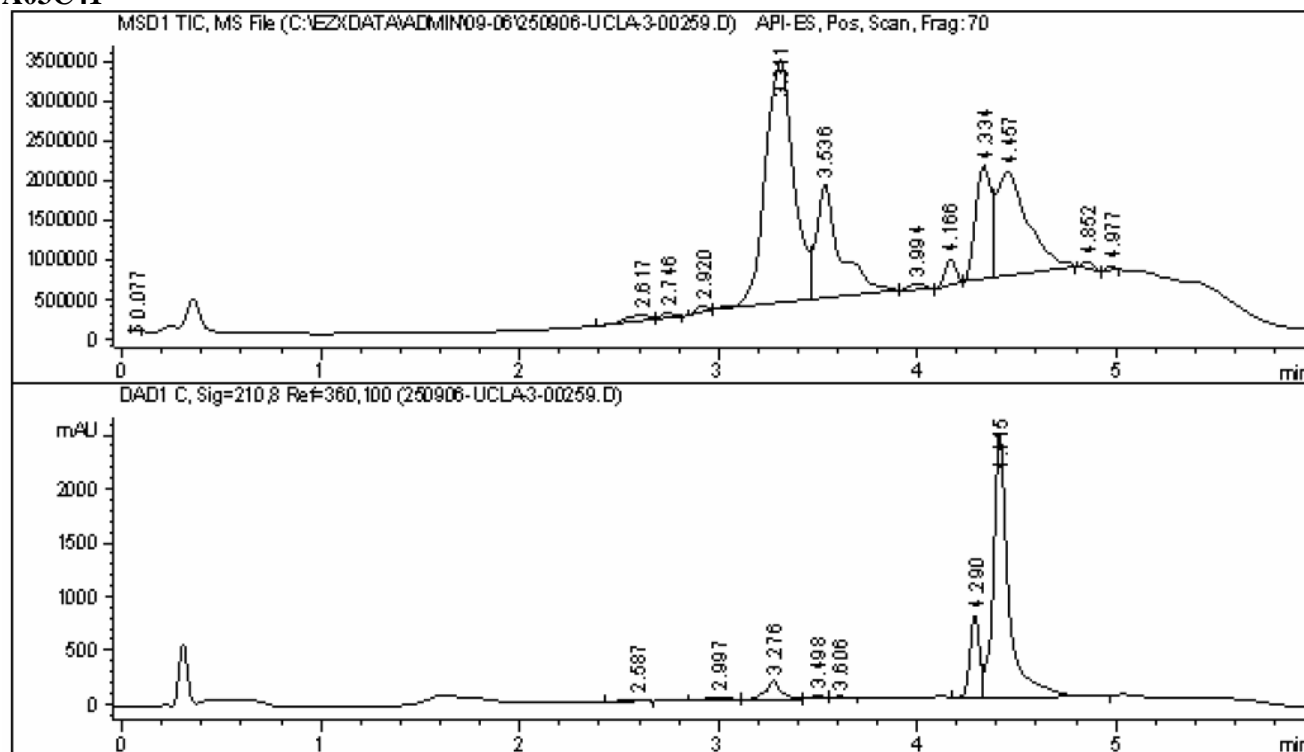
Component 2: Peak at Scan 258.8. Top ions are 454 476 931

A03C30

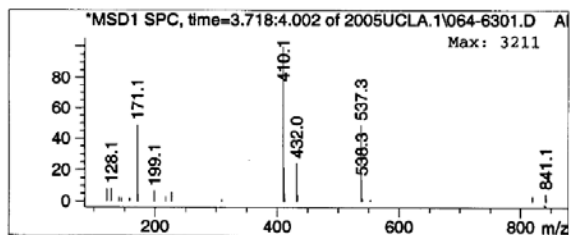
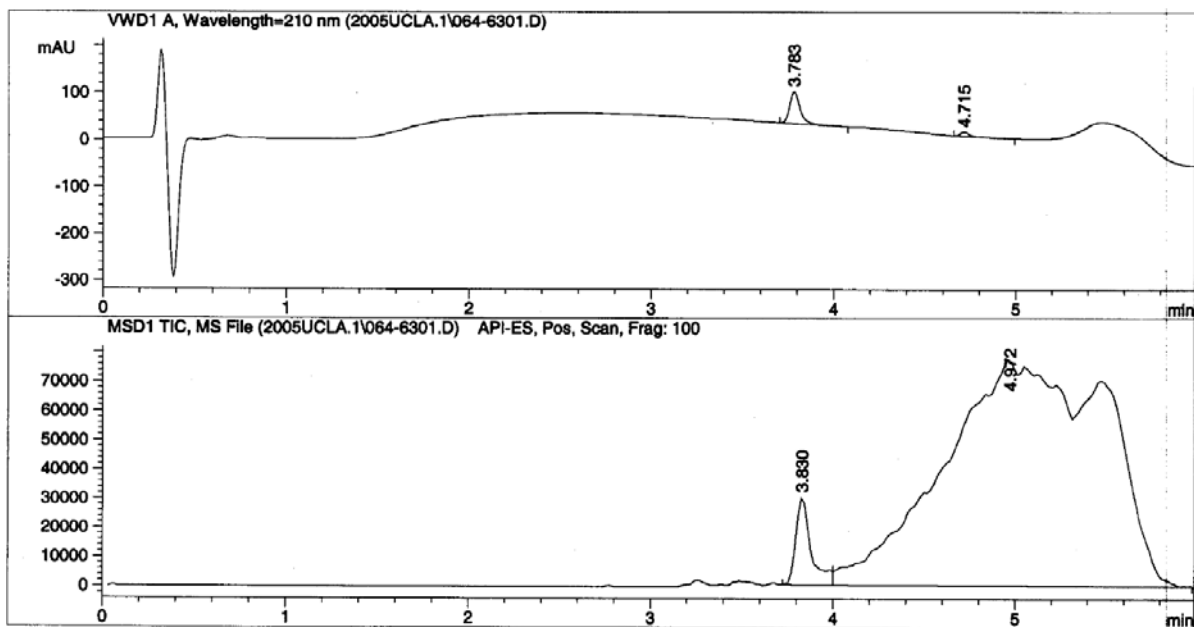
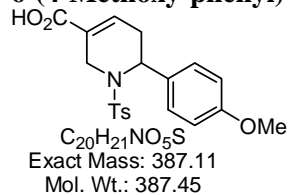




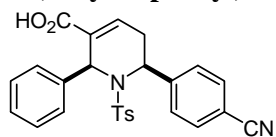
A03C41



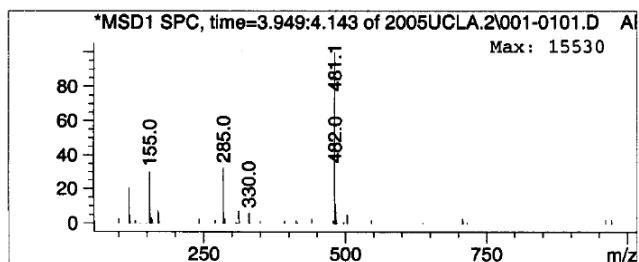
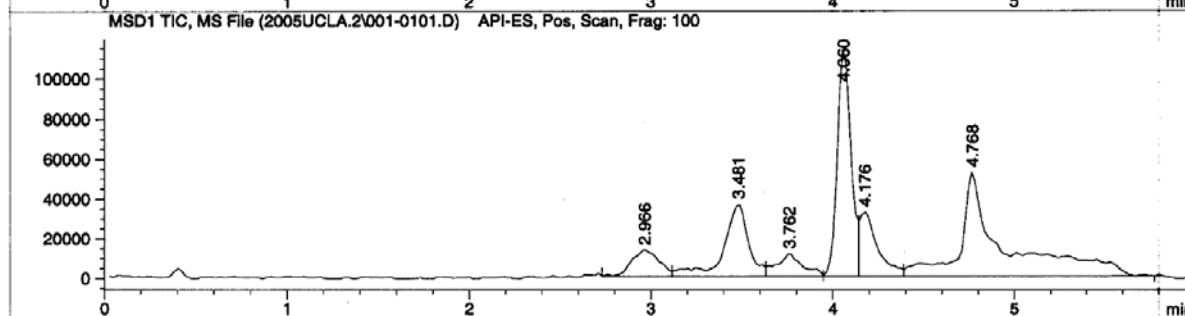
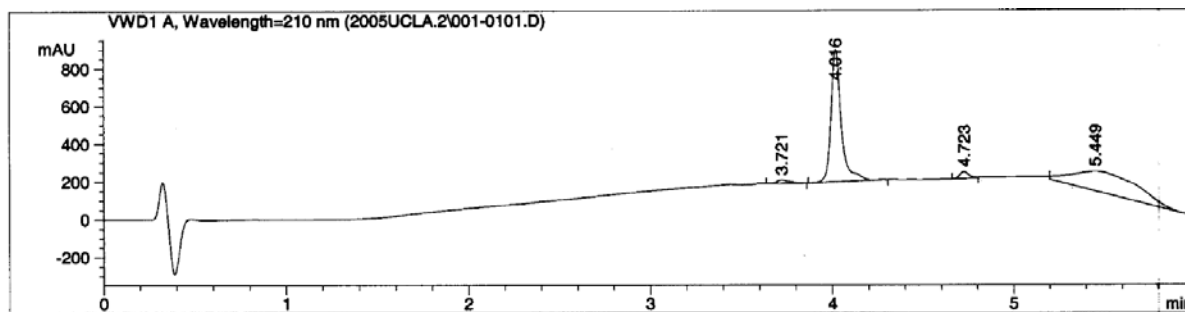
**6-(4-Methoxy-phenyl)-1-(toluene-4-sulfonyl)-1,2,5,6-tetrahydro-pyridine-3-carboxylic acid (B01C04)**



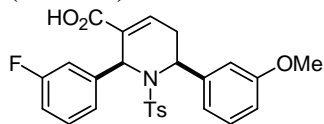
**6-(4-Cyanophenyl)-2-phenyl-1-(toluene-4-sulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B02C09)**



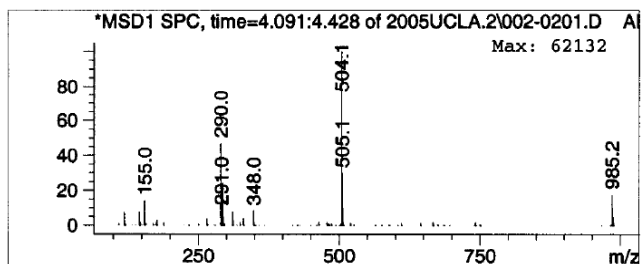
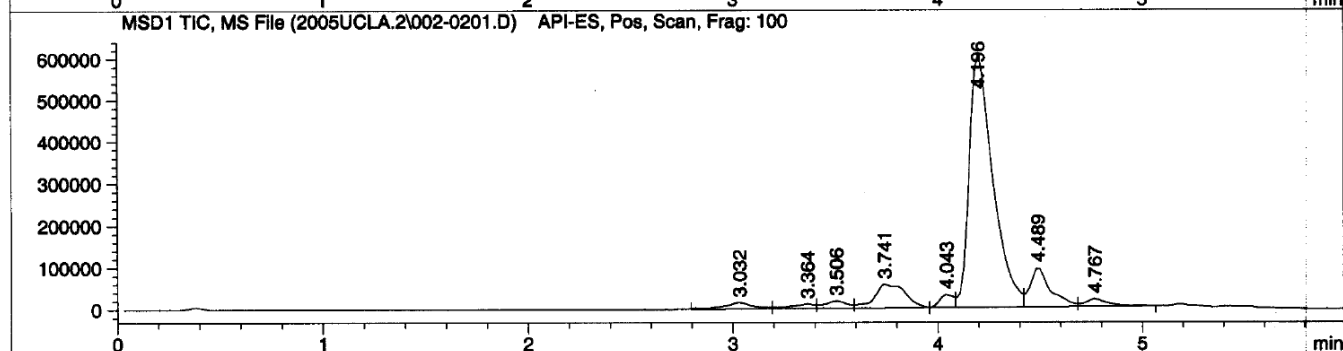
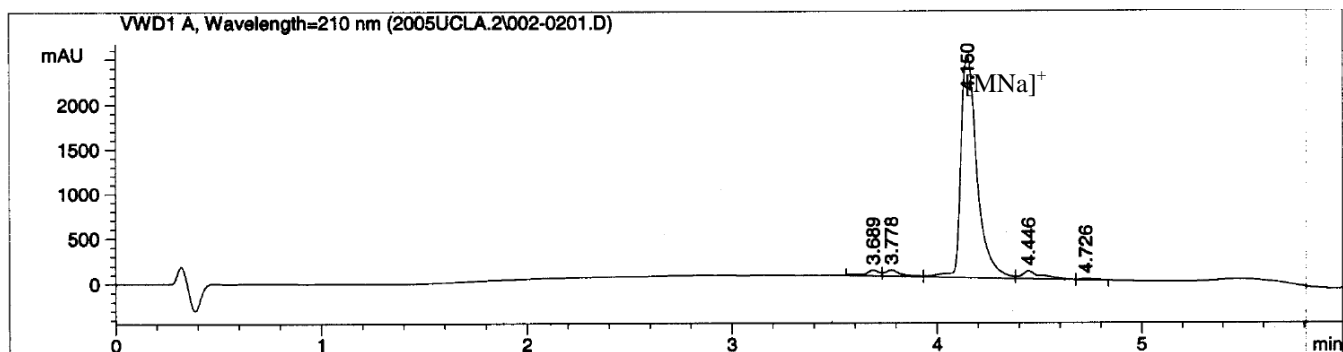
C<sub>26</sub>H<sub>22</sub>N<sub>2</sub>O<sub>4</sub>S  
Exact Mass: 458.13  
Mol. Wt.: 458.53



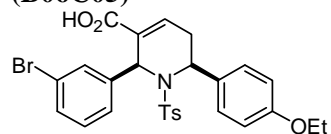
**2-(3-Fluorophenyl)-6-(3-methoxyphenyl)-1-(toluene-4-sulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B04C39)**



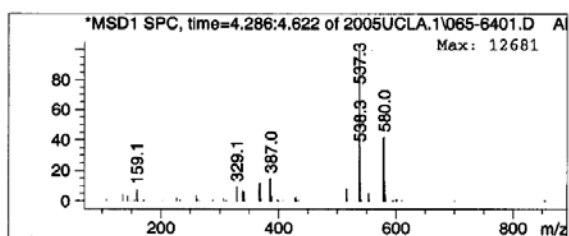
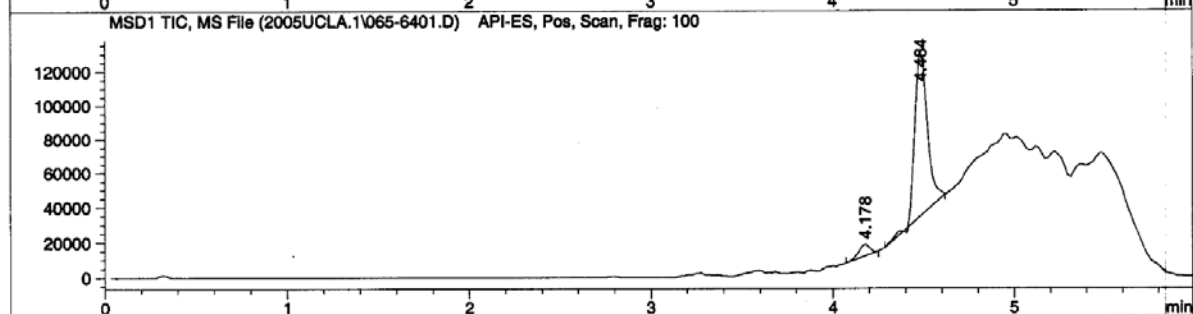
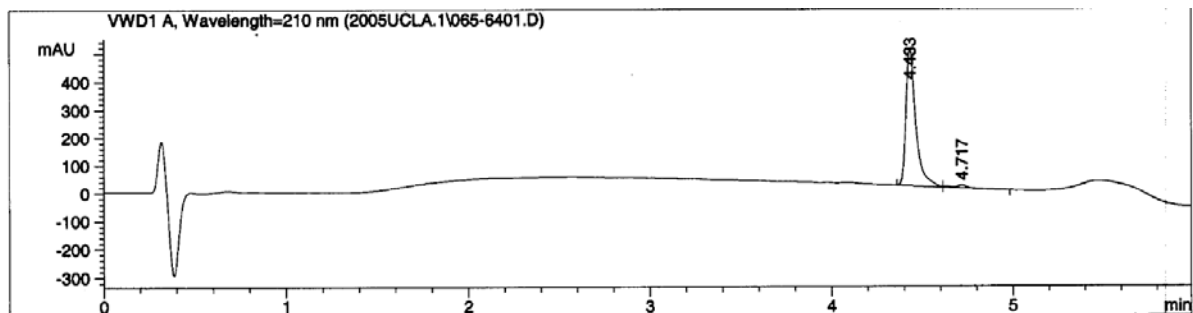
C<sub>26</sub>H<sub>24</sub>FNO<sub>5</sub>S  
Exact Mass: 481.14  
Mol. Wt.: 481.54



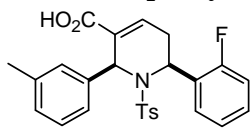
**2-(3-Bromophenyl)-6-(4-ethoxyphenyl)-1-(toluene-4-sulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B06C05)**



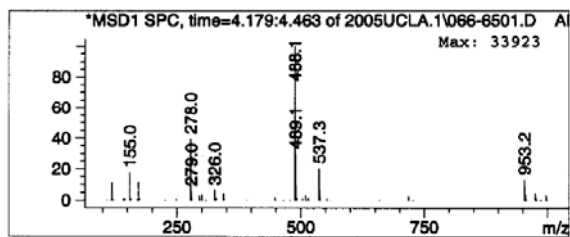
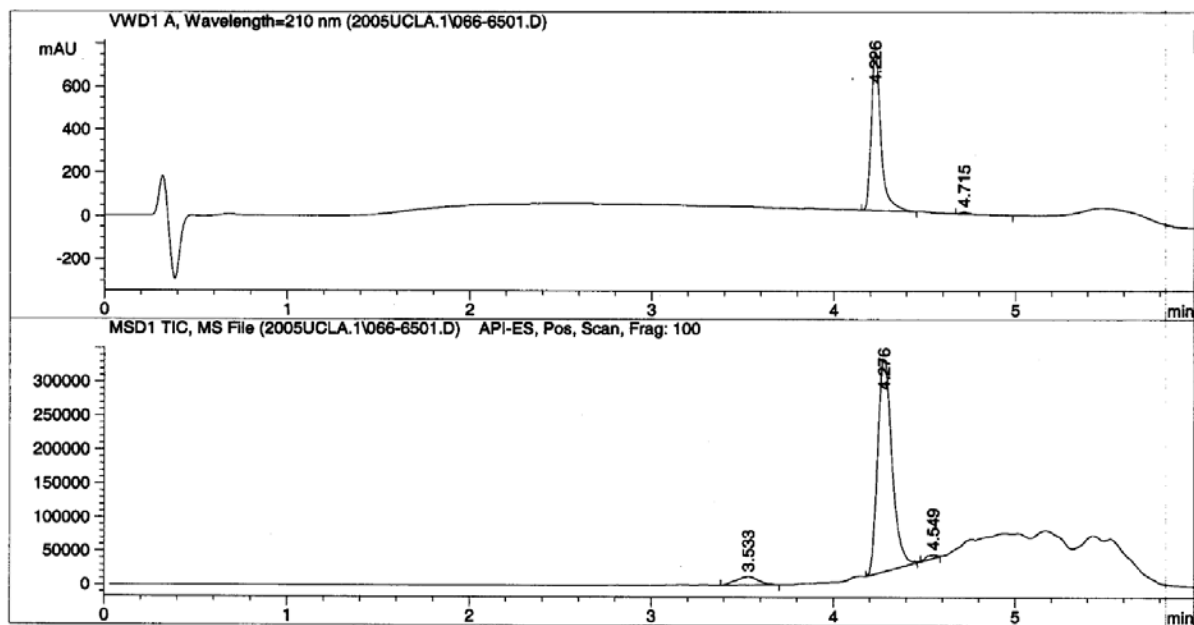
$C_{27}H_{26}BrNO_5S$   
Exact Mass: 555.07  
Mol. Wt.: 556.47



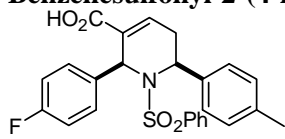
6-(2-Fluorophenyl)-1-(toluene-4-sulfonyl)-2-*m*-tolyl-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B07C10)



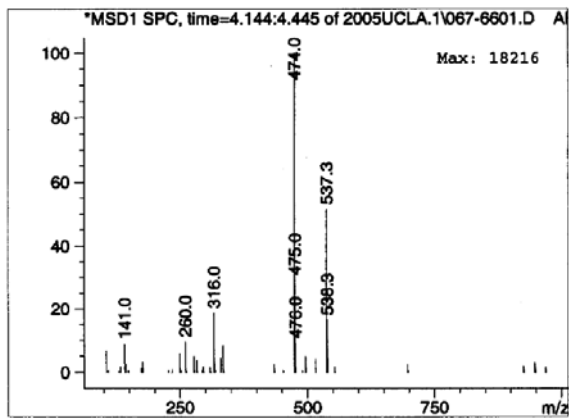
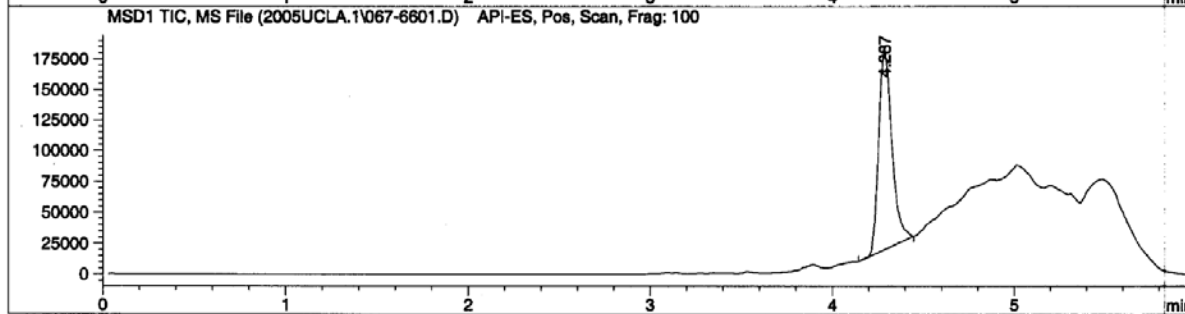
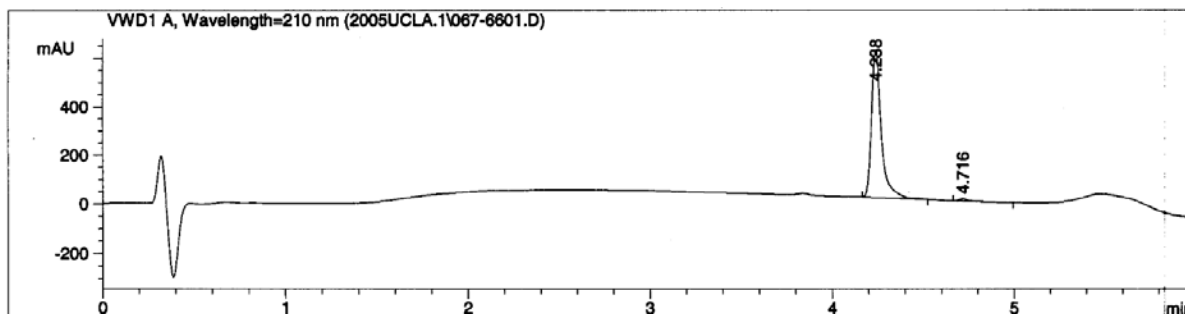
C<sub>26</sub>H<sub>24</sub>FNO<sub>4</sub>S  
Exact Mass: 465.14  
Mol. Wt.: 465.54



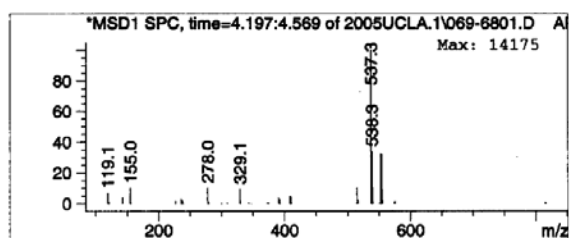
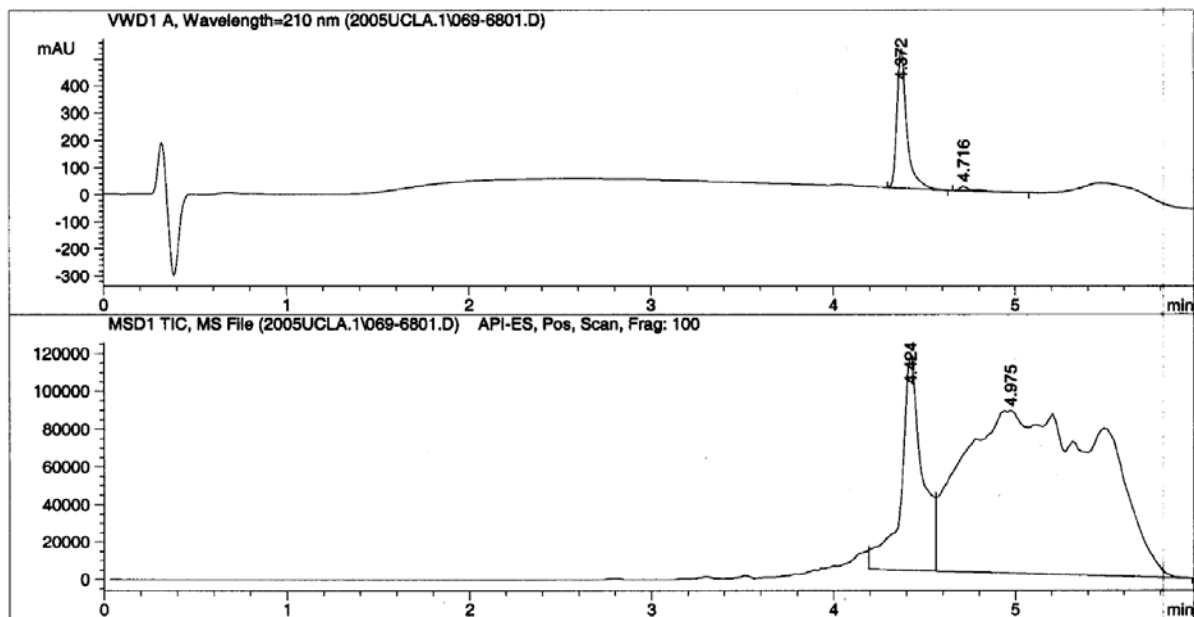
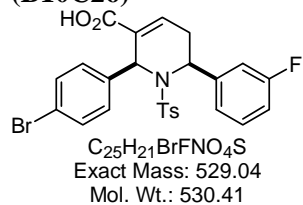
**Benzenesulfonyl-2-(4-fluorophenyl)-6-*p*-tolyl-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B08C43)**



C<sub>25</sub>H<sub>22</sub>FNO<sub>4</sub>S  
Exact Mass: 451.13  
Mol. Wt.: 451.51



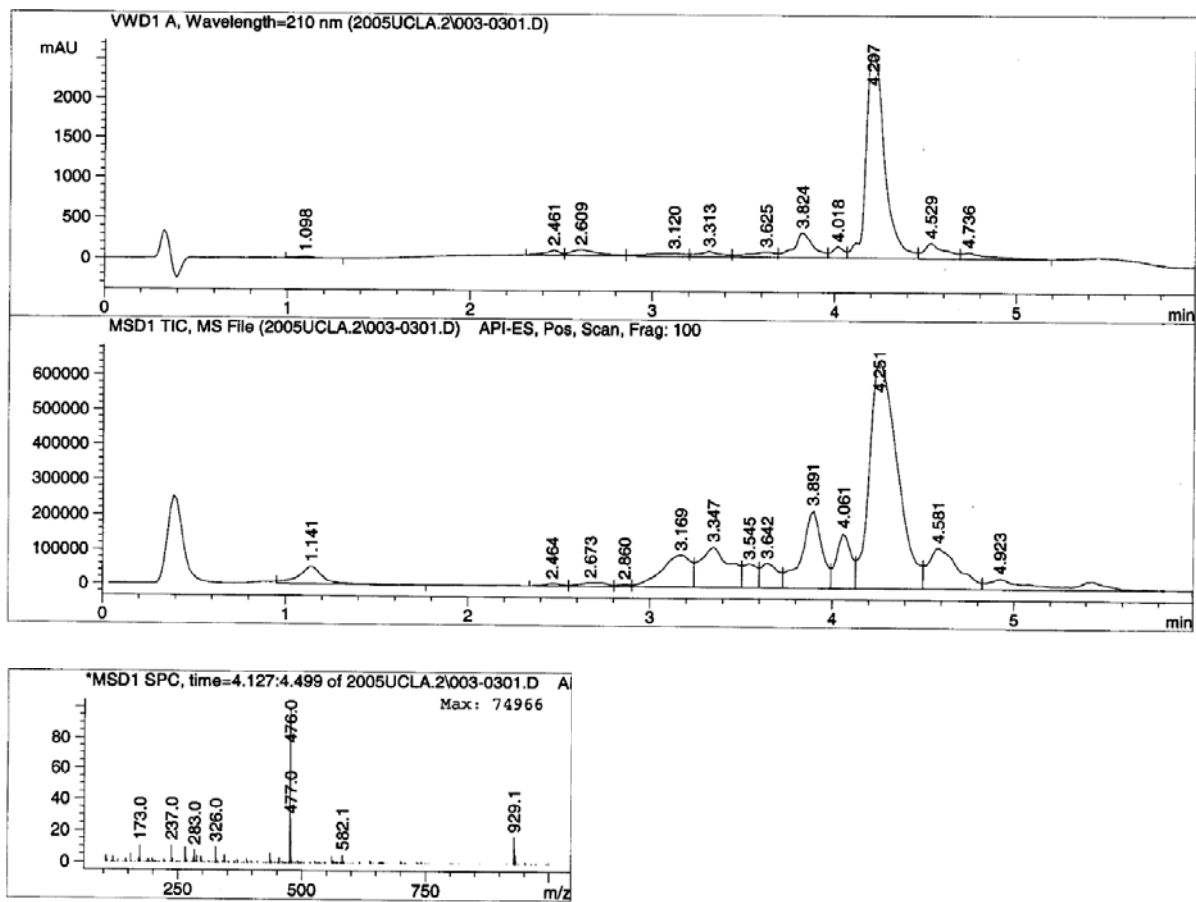
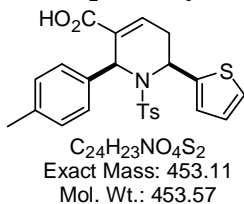
**2-(4-Bromophenyl)-6-(3-fluorophenyl)-1-(toluene-4-sulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B10C26)**



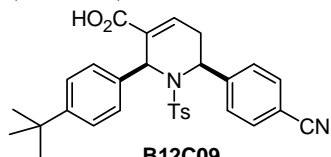
Component 3: Peak at Scan 248.4. Top ions are 552 554 278



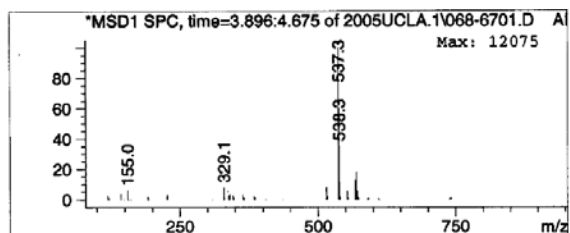
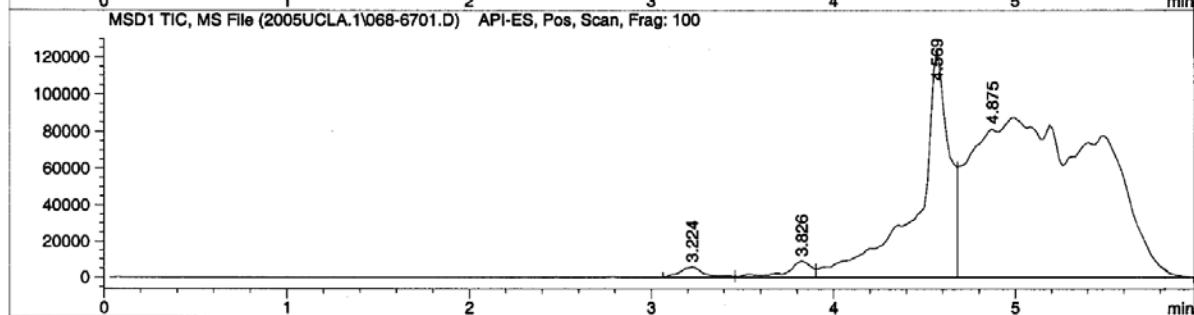
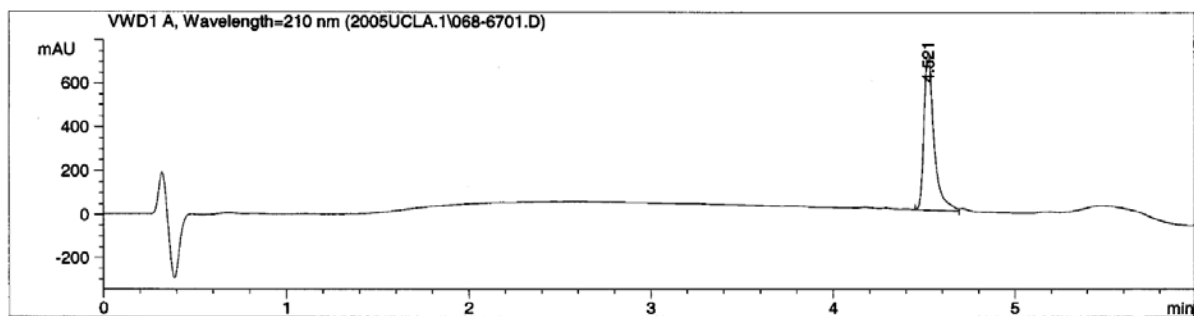
# 6-Thiophen-2-yl-1-(toluene-4-sulfonyl)-2-*p*-tolyl-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B11C21)



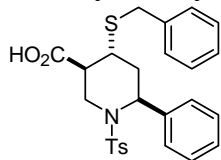
**2-(4-*tert*-Butylphenyl)-6-(4-cyanophenyl)-1-(toluene-4-sulfonyl)-1,2,5,6-tetrahydropyridine-3-carboxylic acid (B12C09)**



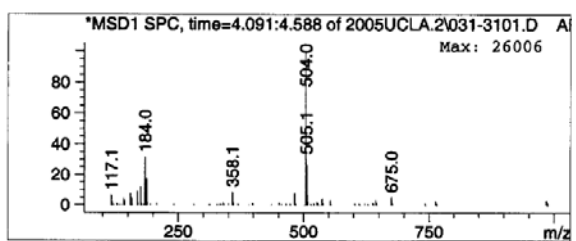
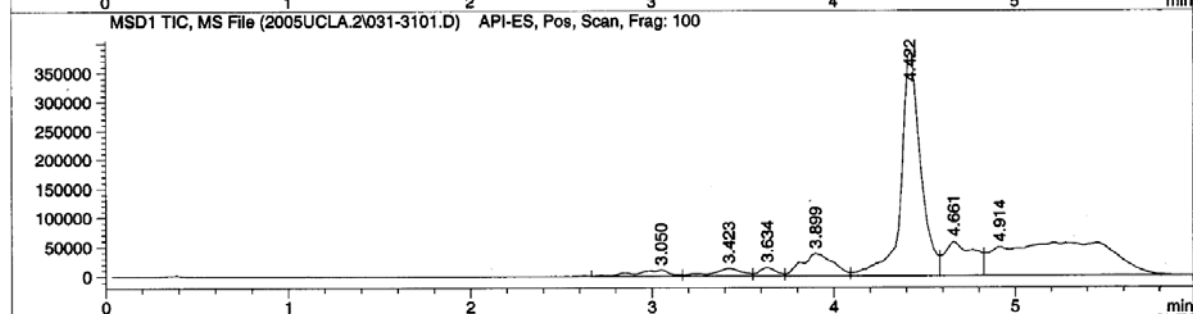
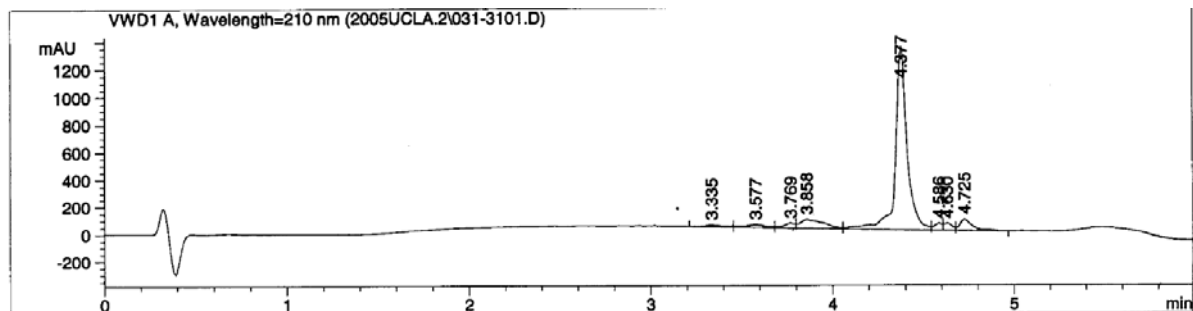
**B12C09**  
C<sub>30</sub>H<sub>30</sub>N<sub>2</sub>O<sub>4</sub>S  
Exact Mass: 514.19  
Mol. Wt.: 514.64



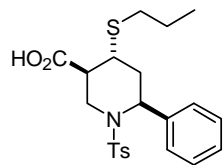
### 4-Benzylsulfanyl-6-phenyl-1-(toluene-4-sulfonyl)-piperidine-3-carboxylic acid (B01C01E06)



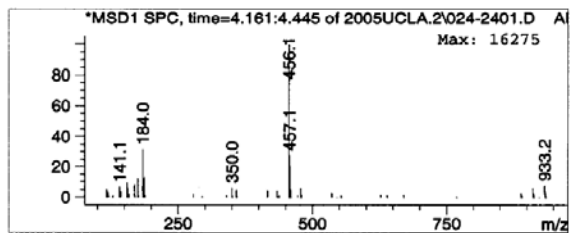
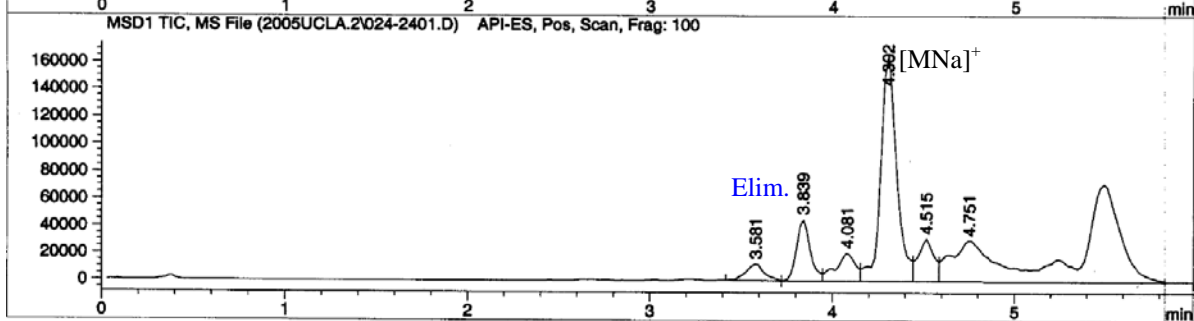
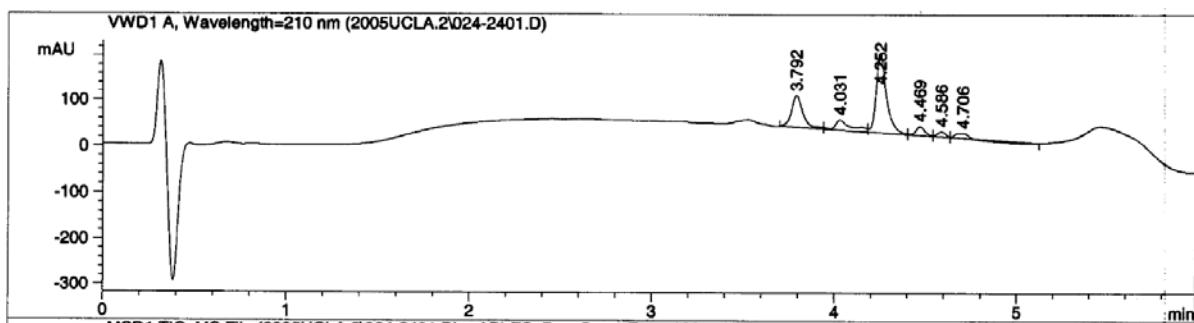
$C_{26}H_{27}NO_4S_2$   
Exact Mass: 481.14  
Mol. Wt.: 481.63



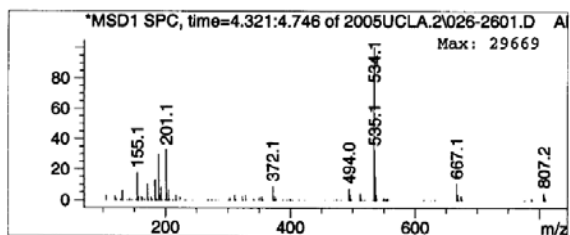
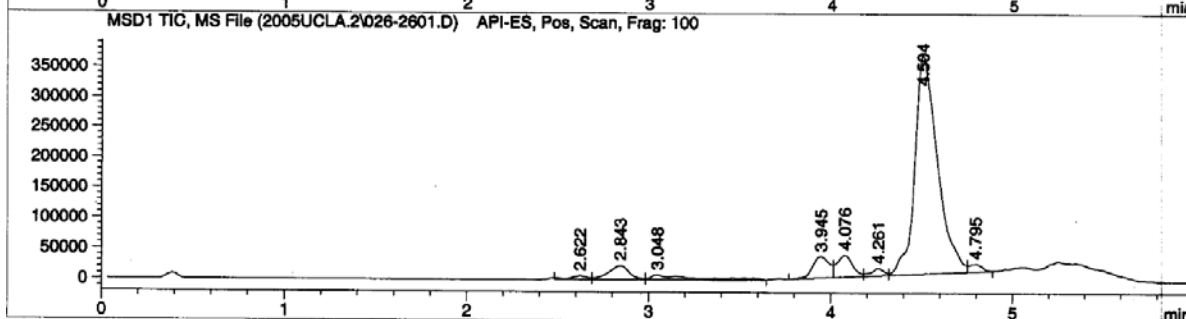
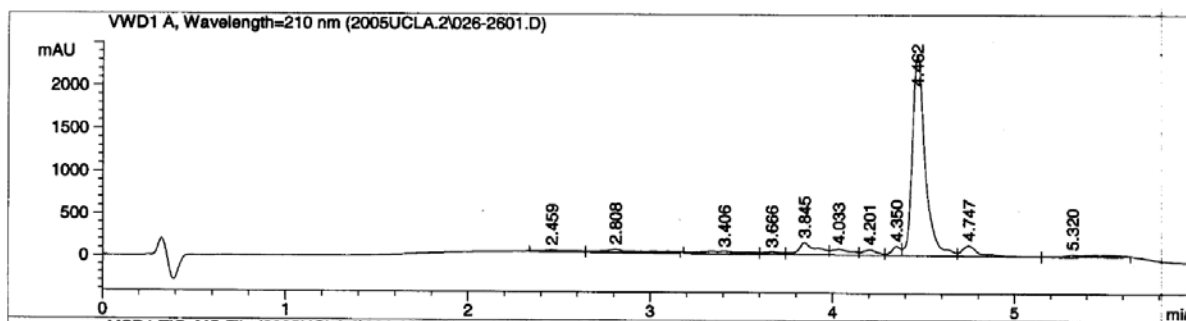
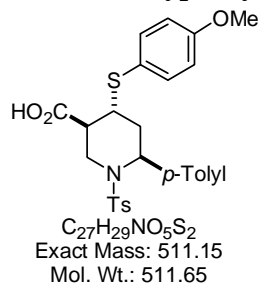
### 6-Phenyl-4-propylsulfanyl-1-(toluene-4-sulfonyl)-piperidine-3-carboxylic acid (B01C01E18)



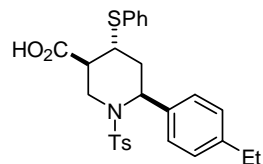
$C_{22}H_{27}NO_4S_2$   
Exact Mass: 433.14  
Mol. Wt.: 433.58



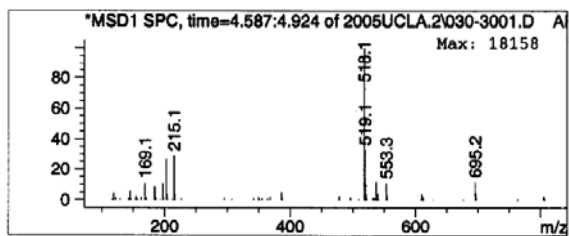
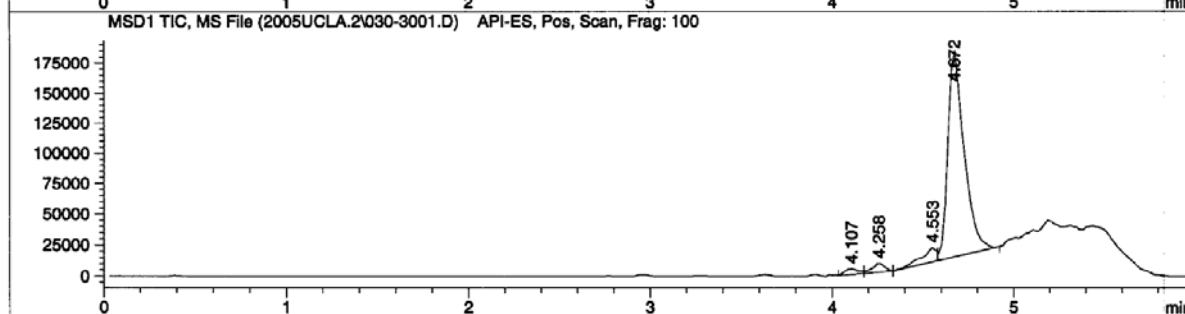
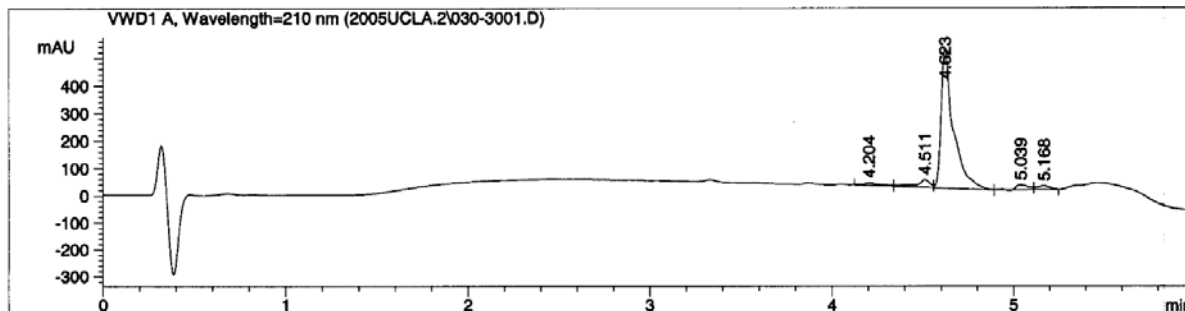
**4-(4-Methoxyphenylsulfanyl)-1-(toluene-4-sulfonyl)-6-*p*-tolylpiperidine-3-carboxylic acid (B01C02E04)**



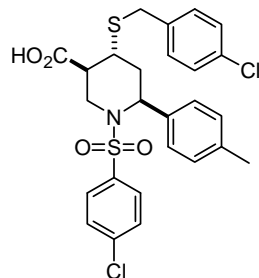
**6-(4-Ethylphenyl)-4-phenylsulfanyl-1-(toluene-4-sulfonyl)-piperidine-3-carboxylic acid (B01C03E01)**



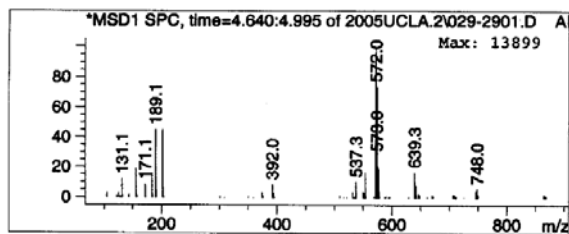
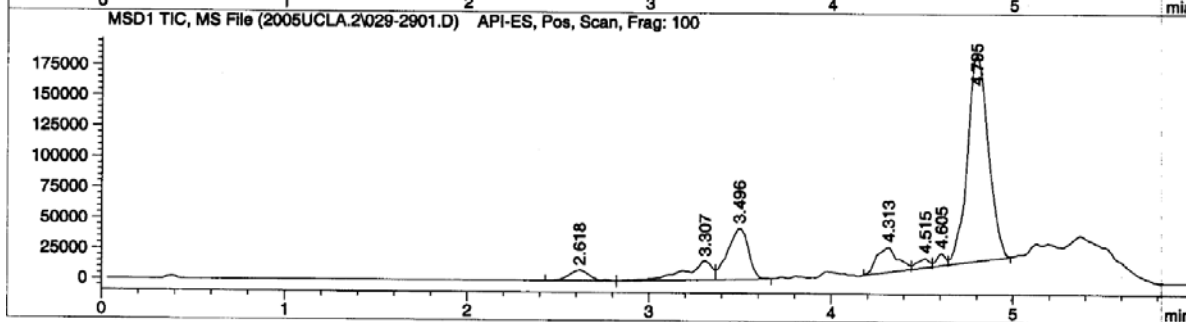
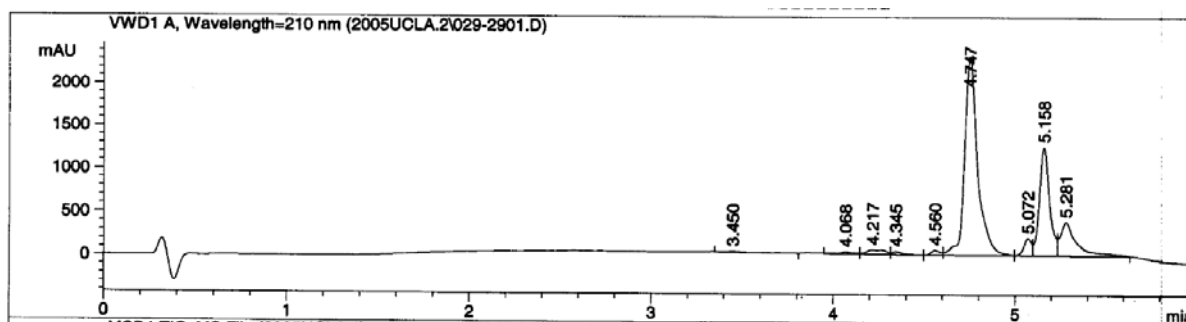
C<sub>27</sub>H<sub>29</sub>NO<sub>4</sub>S<sub>2</sub>  
Exact Mass: 495.15  
Mol. Wt.: 495.65



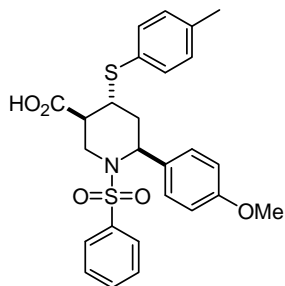
1-(4-Chlorobenzenesulfonyl)-4-(4-chlorobenzylsulfanyl)-6-*p*-tolyl-piperidine-3-carboxylic acid (B01C30E09)



C<sub>26</sub>H<sub>25</sub>Cl<sub>2</sub>NO<sub>4</sub>S<sub>2</sub>  
Exact Mass: 549.06  
Mol. Wt.: 550.52



**Benzenesulfonyl-6-(4-methoxyphenyl)-4-*p*-tolylsulfanyl-piperidine-3-carboxylic acid (B01C35E02)**



C<sub>26</sub>H<sub>27</sub>NO<sub>5</sub>S<sub>2</sub>  
Exact Mass: 497.13  
Mol. Wt.: 497.63

