

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF073120\  
 Data File : BF121156.D  
 Acq On : 31 Jul 2020 14:20  
 Operator : JU/CG  
 Sample : L3518-22  
 Misc :  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TP-8

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF071620.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 5.004       | 492           | 496         | 503          | rVB      | 33073          | 44842         | 1.57%           | 0.219%        |
| 2         | 5.416       | 562           | 566         | 580          | rBV      | 2379775        | 2264440       | 79.12%          | 11.064%       |
| 3         | 6.434       | 734           | 739         | 742          | rBV      | 2182961        | 2243666       | 78.39%          | 10.963%       |
| 4         | 6.628       | 769           | 772         | 778          | rBV      | 40874          | 45184         | 1.58%           | 0.221%        |
| 5         | 6.793       | 797           | 800         | 804          | rBV      | 798225         | 704898        | 24.63%          | 3.444%        |
| 6         | 7.357       | 891           | 896         | 899          | rBV      | 1593488        | 1611804       | 56.32%          | 7.875%        |
| 7         | 8.081       | 1014          | 1019        | 1027         | rBV      | 977890         | 931339        | 32.54%          | 4.551%        |
| 8         | 9.157       | 1197          | 1202        | 1205         | rBV      | 2999189        | 2862059       | 100.00%         | 13.984%       |
| 9         | 9.551       | 1265          | 1269        | 1273         | rBV      | 284482         | 237898        | 8.31%           | 1.162%        |
| 10        | 9.775       | 1300          | 1307        | 1313         | rBV      | 56317          | 134418        | 4.70%           | 0.657%        |
| 11        | 9.833       | 1313          | 1317        | 1321         | rVB      | 1143235        | 1049090       | 36.66%          | 5.126%        |
| 12        | 10.628      | 1447          | 1452        | 1463         | rBV      | 1799902        | 1742561       | 60.88%          | 8.514%        |
| 13        | 11.322      | 1566          | 1570        | 1574         | rBV      | 1234566        | 1086412       | 37.96%          | 5.308%        |
| 14        | 12.910      | 1835          | 1840        | 1844         | rBV      | 2819325        | 2796404       | 97.71%          | 13.663%       |
| 15        | 13.480      | 1933          | 1937        | 1941         | rBV2     | 29891          | 29246         | 1.02%           | 0.143%        |
| 16        | 13.810      | 1989          | 1993        | 2004         | rVB      | 366645         | 496332        | 17.34%          | 2.425%        |
| 17        | 13.963      | 2015          | 2019        | 2023         | rBV      | 1002989        | 862657        | 30.14%          | 4.215%        |
| 18        | 14.127      | 2044          | 2047        | 2052         | rBV      | 53165          | 55512         | 1.94%           | 0.271%        |
| 19        | 14.445      | 2096          | 2101        | 2107         | rBV2     | 87781          | 156064        | 5.45%           | 0.763%        |
| 20        | 14.733      | 2148          | 2150        | 2154         | rVB      | 43287          | 37447         | 1.31%           | 0.183%        |
| 21        | 15.068      | 2203          | 2207        | 2209         | rBV      | 59145          | 70158         | 2.45%           | 0.343%        |
| 22        | 15.098      | 2210          | 2212        | 2218         | rVB5     | 28987          | 44967         | 1.57%           | 0.220%        |
| 23        | 15.415      | 2261          | 2266        | 2276         | rVB      | 596906         | 824822        | 28.82%          | 4.030%        |
| 24        | 15.863      | 2339          | 2342        | 2347         | rVB3     | 40237          | 54888         | 1.92%           | 0.268%        |
| 25        | 15.927      | 2349          | 2353        | 2359         | rVV4     | 35615          | 79592         | 2.78%           | 0.389%        |

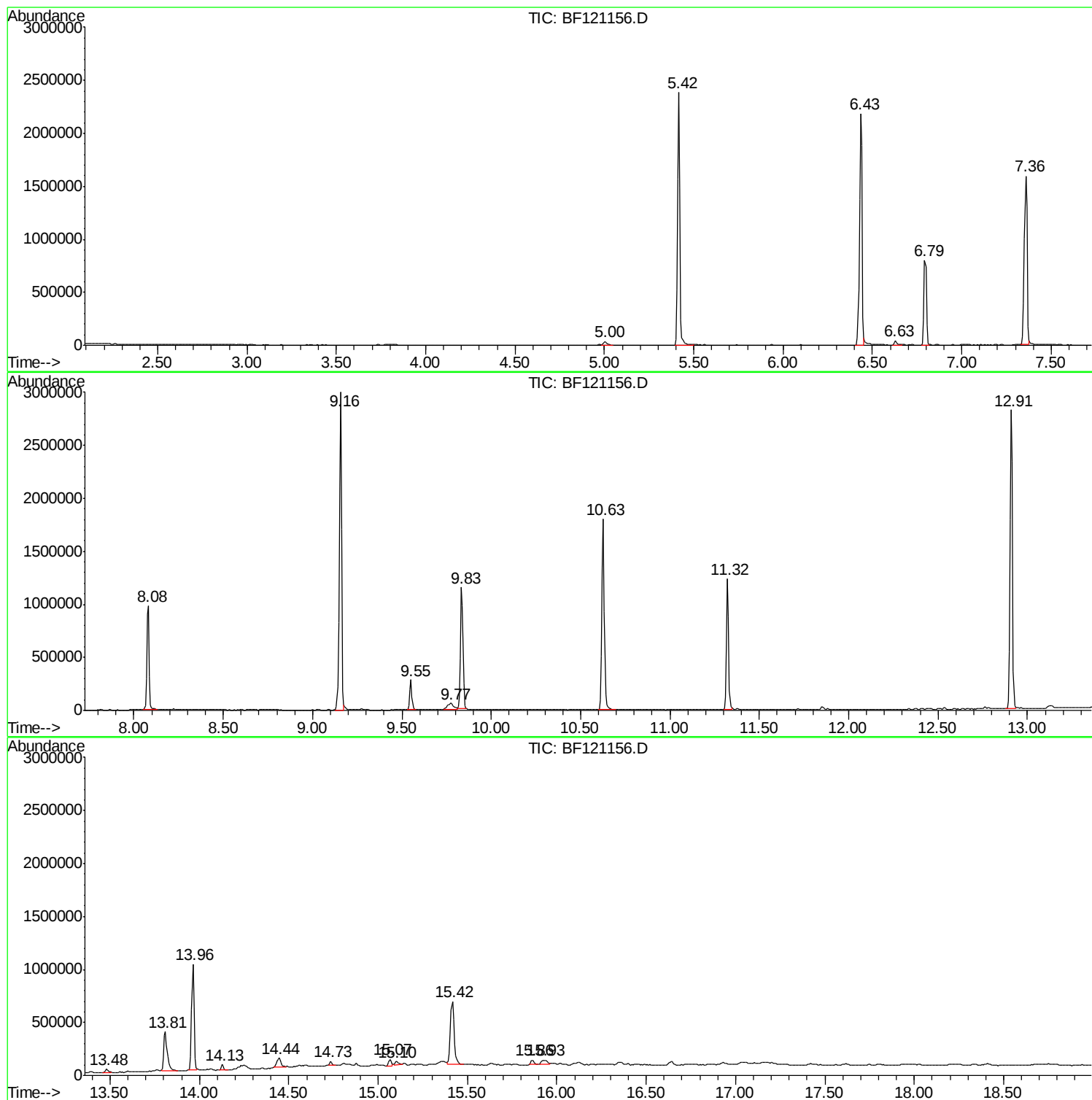
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Misc :  
ALS Vial : 10 Sample Multiplier: 1

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ClientSampleId :  
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF071620.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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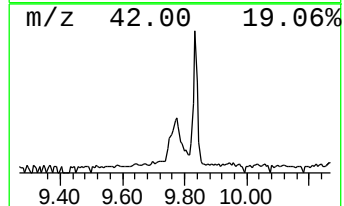
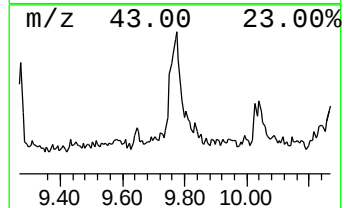
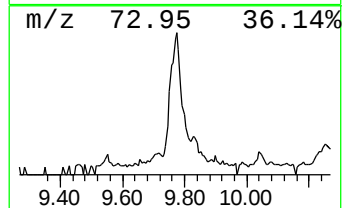
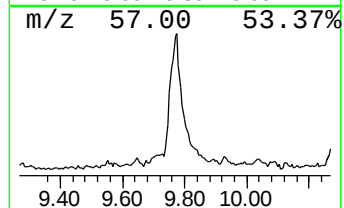
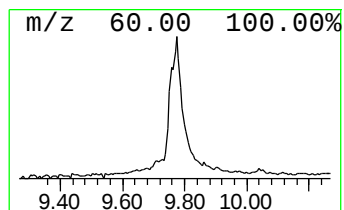
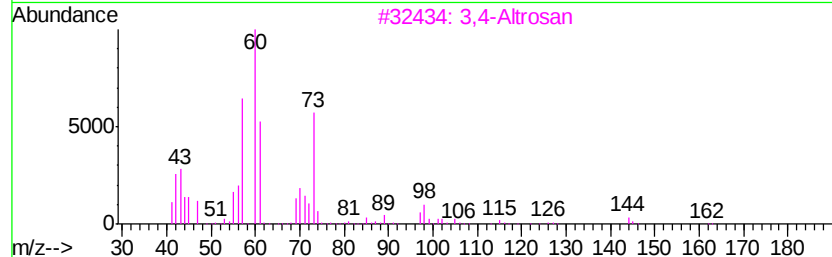
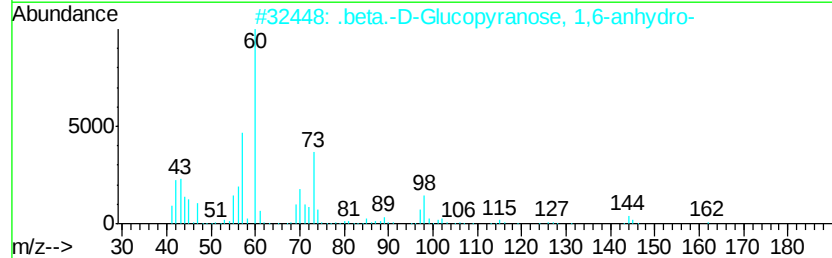
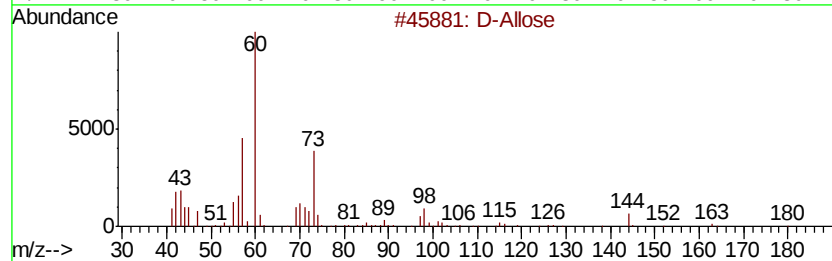
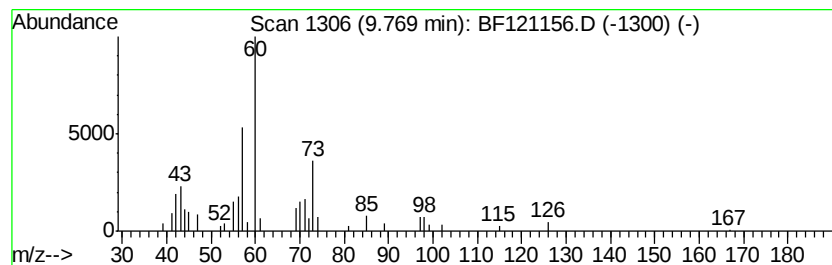
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 D-Allose Concentration Rank 3

| R.T. | EstConc | Area   | Relative to ISTD | R.T. |
|------|---------|--------|------------------|------|
| 9.77 | 2.56 ng | 134418 | Acenaphthene-d10 | 9.83 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|-------------------------------------|-----|---------|--------------|------|
| 1    | 5  | D-Allose                            | 180 | C6H12O6 | 002595-97-3  | 90   |
| 2    |    | .beta.-D-Glucopyranose, 1,6-anhy... | 162 | C6H10O5 | 000498-07-7  | 86   |
| 3    |    | 3,4-Altrosan                        | 162 | C6H10O5 | 1000129-76-4 | 53   |
| 4    |    | 1,6-Anhydro-.beta.-d-talopyranose   | 162 | C6H10O5 | 1000133-05-8 | 50   |
| 5    |    | Pentanoic acid                      | 102 | C5H10O2 | 000109-52-4  | 47   |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

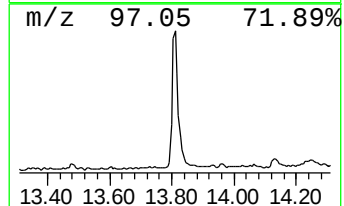
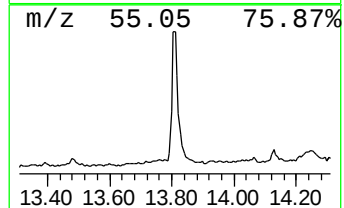
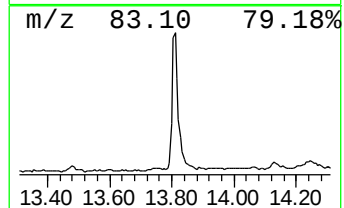
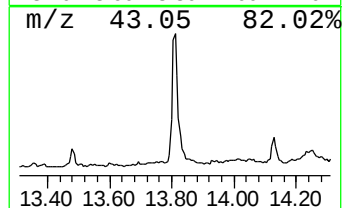
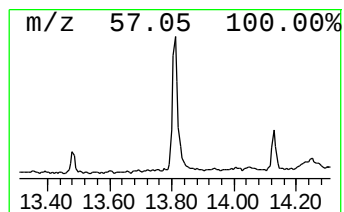
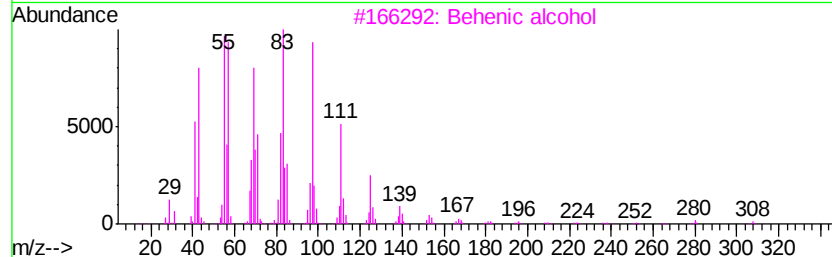
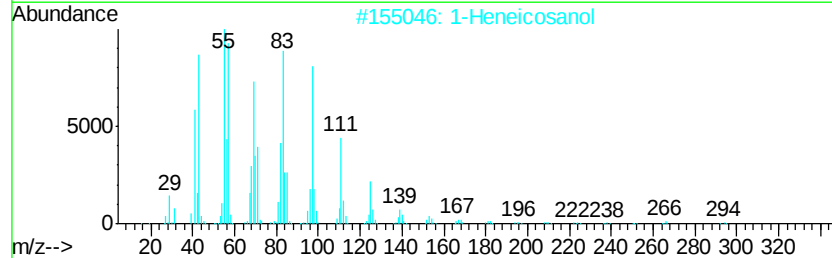
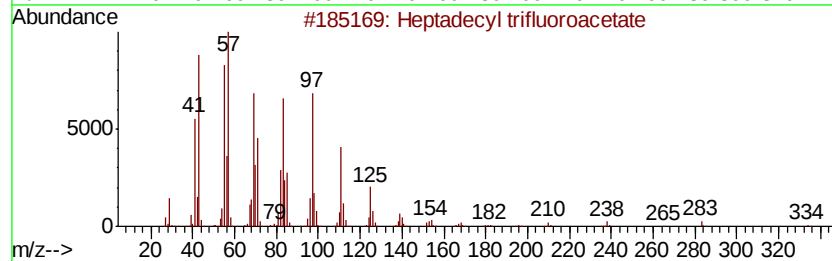
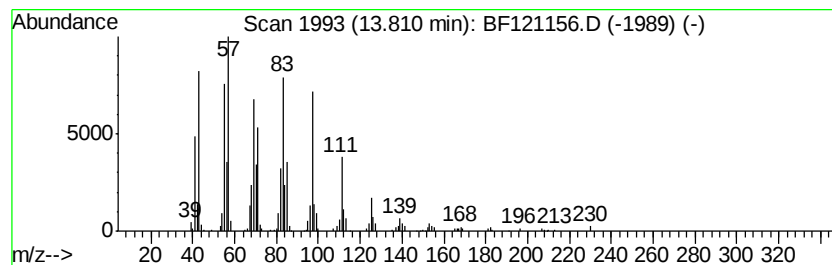
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Peak Number 2 Heptadecyl trifluoroacetate Concentration Rank 1

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 13.81 | 11.51 ng | 496332 | Chrysene-d12     | 13.96 |

| Hit# | of | Tentative ID                    | MW  | MolForm    | CAS#         | Qual |
|------|----|---------------------------------|-----|------------|--------------|------|
| 1    | 5  | Heptadecyl trifluoroacetate     | 352 | C19H35F3O2 | 1000351-87-0 | 94   |
| 2    |    | 1-Heneicosanol                  | 312 | C21H44O    | 015594-90-8  | 93   |
| 3    |    | Behenic alcohol                 | 326 | C22H46O    | 000661-19-8  | 93   |
| 4    |    | n-Tetracosanol-1                | 354 | C24H50O    | 000506-51-4  | 93   |
| 5    |    | Nonadecyl pentafluoropropionate | 430 | C22H39F5O2 | 1000351-88-8 | 91   |



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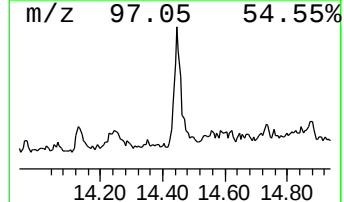
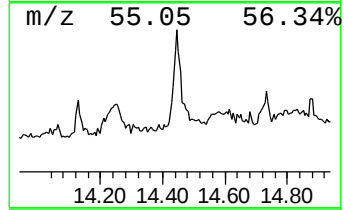
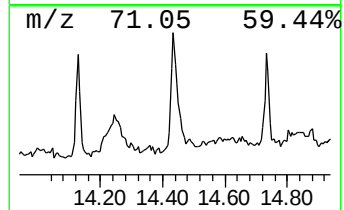
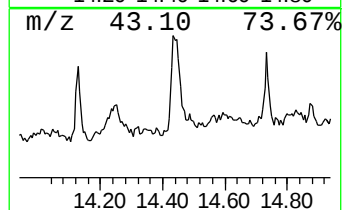
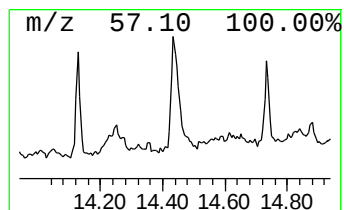
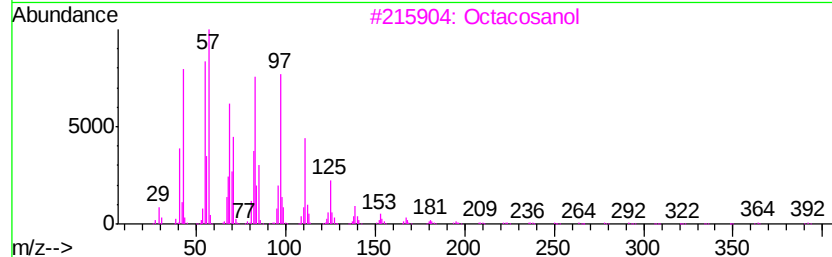
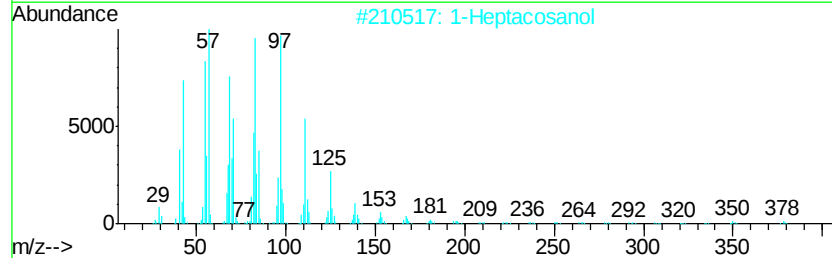
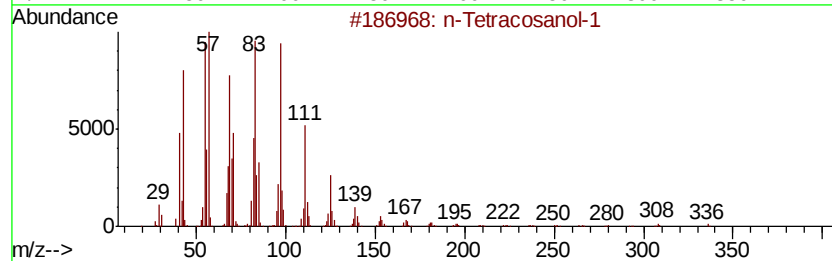
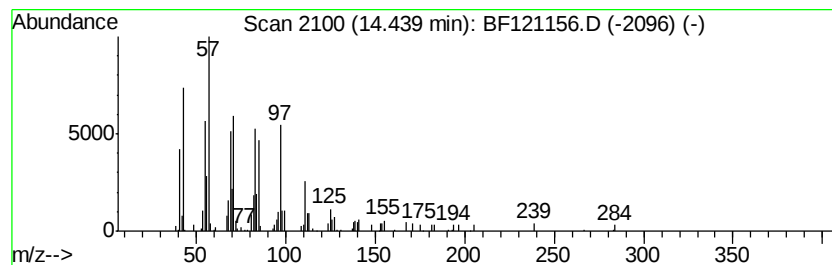
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 n-Tetracosanol-1 Concentration Rank 2

| R.T.      | EstConc                             | Area   | Relative to ISTD |             | R.T.  |
|-----------|-------------------------------------|--------|------------------|-------------|-------|
| 14.44     | 3.62 ng                             | 156064 | Chrysene-d12     |             | 13.96 |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#        | Qual  |
| 1         | n-Tetracosanol-1                    | 354    | C24H50O          | 000506-51-4 | 94    |
| 2         | 1-Heptacosanol                      | 396    | C27H56O          | 002004-39-9 | 91    |
| 3         | Octacosanol                         | 410    | C28H58O          | 000557-61-9 | 90    |
| 4         | n-Nonadecanol-1                     | 284    | C19H40O          | 001454-84-8 | 90    |
| 5         | Heptafluorobutyric acid, n-octad... | 466    | C22H37F7O2       | 000400-57-7 | 90    |



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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| D-Allose             | 9.77  | 2.6     | ng    | 134418   | 3                     | 9.83  | 1049090 | 20.0 |
| Heptadecyl triflu... | 13.81 | 11.5    | ng    | 496332   | 5                     | 13.96 | 862657  | 20.0 |
| n-Tetracosanol-1     | 14.44 | 3.6     | ng    | 156064   | 5                     | 13.96 | 862657  | 20.0 |