

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF021317\  
 Data File : BF092931.D  
 Acq On : 13 Feb 2017 21:13  
 Operator : SJ/MA  
 Sample : I1790-01  
 Misc :  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 38-FB021017

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON Filtering: 5  
 Sampling : 1 Min Area: 3 % of largest Peak  
 Start Thrs: 0.2 Max Peaks: 100  
 Stop Thrs : 0 Peak Location: TOP

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

Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF013017.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         | 5.047       | 258           | 259         | 273          | rVB      | 437191         | 562123        | 12.41%          | 1.765%        |
| 2         | 5.482       | 294           | 297         | 299          | rBV      | 1847115        | 1685953       | 37.21%          | 5.294%        |
| 3         | 6.510       | 385           | 387         | 390          | rBV      | 1224862        | 1011377       | 22.32%          | 3.176%        |
| 4         | 6.647       | 397           | 399         | 402          | rBV      | 3266642        | 2974849       | 65.65%          | 9.342%        |
| 5         | 6.876       | 417           | 419         | 422          | rBV      | 797119         | 801004        | 17.68%          | 2.515%        |
| 6         | 7.036       | 430           | 433         | 436          | rBV      | 3171123        | 2895152       | 63.89%          | 9.092%        |
| 7         | 7.447       | 466           | 469         | 471          | rBV      | 2633852        | 2569380       | 56.70%          | 8.069%        |
| 8         | 8.168       | 529           | 532         | 534          | rBV      | 1159023        | 1102066       | 24.32%          | 3.461%        |
| 9         | 9.242       | 623           | 626         | 628          | rBV      | 4550398        | 4500476       | 99.32%          | 14.133%       |
| 10        | 9.916       | 682           | 685         | 687          | rBV      | 1518703        | 1285211       | 28.36%          | 4.036%        |
| 11        | 10.705      | 751           | 754         | 757          | rBV      | 2307429        | 2351920       | 51.90%          | 7.386%        |
| 12        | 11.402      | 812           | 815         | 817          | rBV      | 1326983        | 1273664       | 28.11%          | 4.000%        |
| 13        | 12.991      | 951           | 954         | 956          | rBV      | 4163582        | 4531373       | 100.00%         | 14.230%       |
| 14        | 13.459      | 991           | 995         | 1001         | rBV      | 666858         | 1440381       | 31.79%          | 4.523%        |
| 15        | 13.539      | 1001          | 1002        | 1012         | rVB      | 53126          | 73570         | 1.62%           | 0.231%        |
| 16        | 14.031      | 1043          | 1045        | 1048         | rBV      | 893959         | 1186974       | 26.19%          | 3.727%        |
| 17        | 14.145      | 1053          | 1055        | 1059         | rBV      | 50932          | 67479         | 1.49%           | 0.212%        |
| 18        | 14.785      | 1108          | 1111        | 1126         | rBV      | 382785         | 443726        | 9.79%           | 1.393%        |
| 19        | 15.471      | 1168          | 1171        | 1174         | rBV      | 738877         | 1087548       | 24.00%          | 3.415%        |

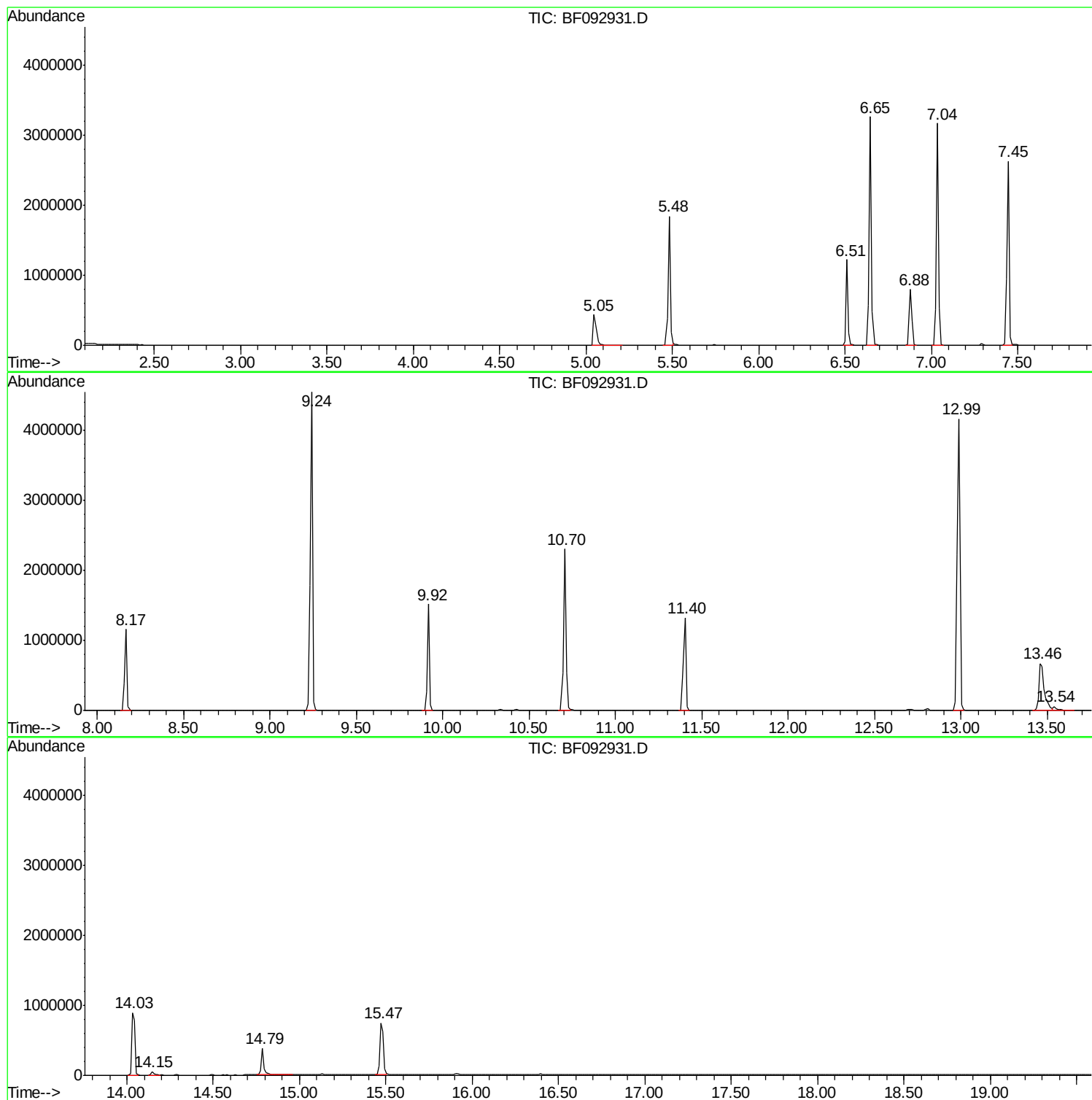
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF013017.M  
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TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



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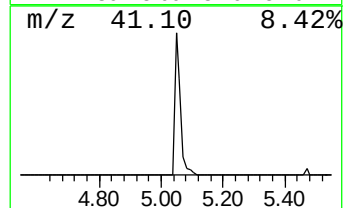
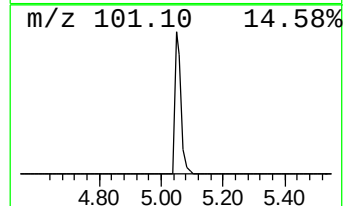
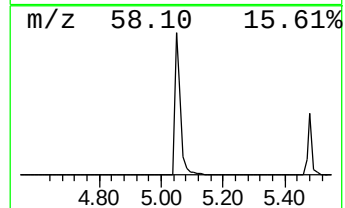
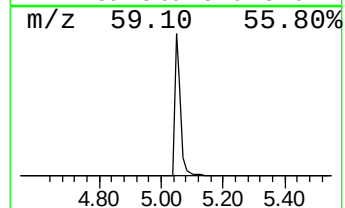
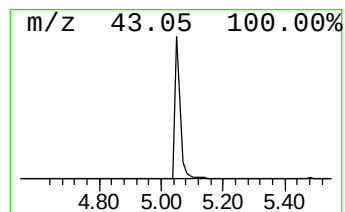
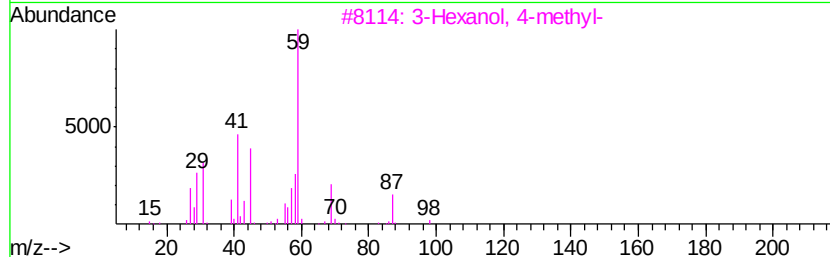
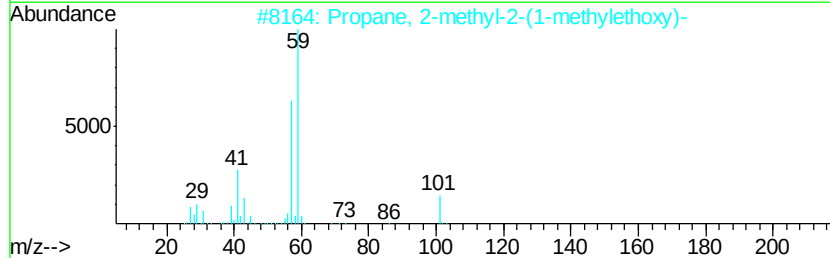
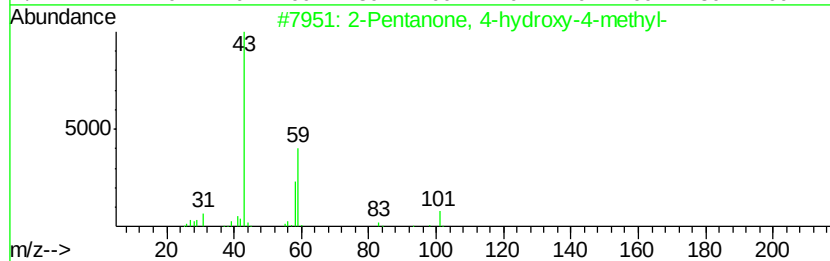
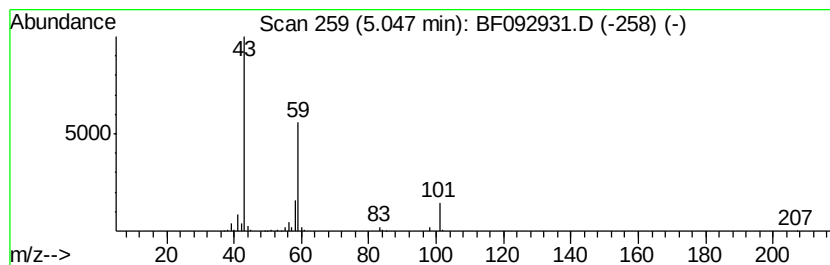
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF013017.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

| R.T.    | EstConc                             | Area         | Relative to ISTD       | R.T.        |      |      |
|---------|-------------------------------------|--------------|------------------------|-------------|------|------|
| 5.05    | 14.04 ng                            | 562123       | 1,4-Dichlorobenzene-d4 | 6.88        |      |      |
| Hit# of | 5                                   | Tentative ID | MW                     | MolForm     | CAS# | Qual |
| 1       | 2-Pentanone, 4-hydroxy-4-methyl-    | 116          | C6H12O2                | 000123-42-2 | 50   |      |
| 2       | Propane, 2-methyl-2-(1-methyleth... | 116          | C7H16O                 | 017348-59-3 | 36   |      |
| 3       | 3-Hexanol, 4-methyl-                | 116          | C7H16O                 | 000615-29-2 | 33   |      |
| 4       | 2-Hexanol, 2-methyl-                | 116          | C7H16O                 | 000625-23-0 | 28   |      |
| 5       | Acetic acid, cyano-, 1,1-dimethy... | 141          | C7H11NO2               | 001116-98-9 | 23   |      |



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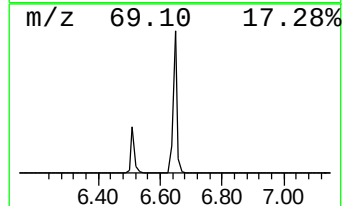
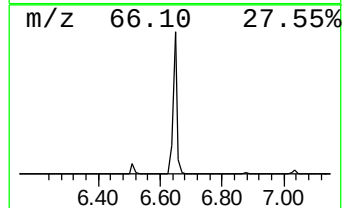
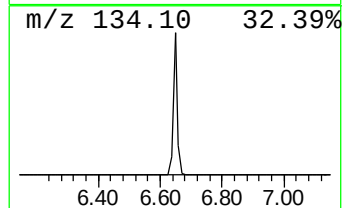
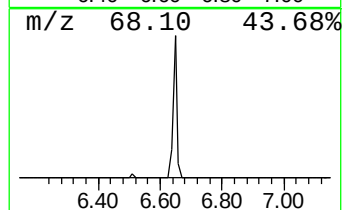
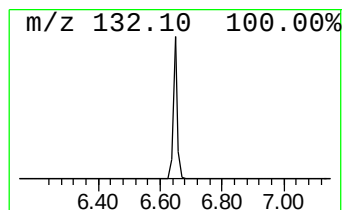
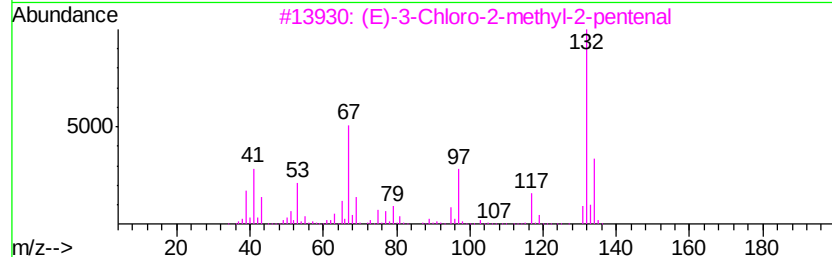
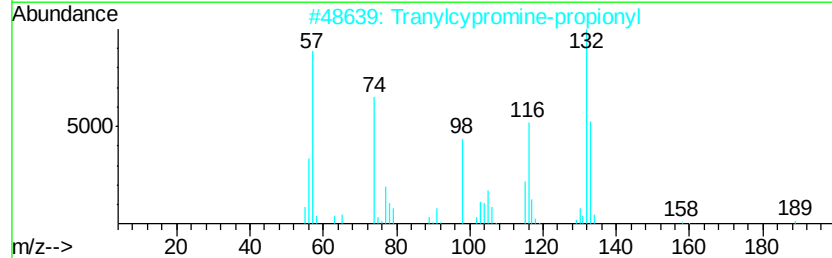
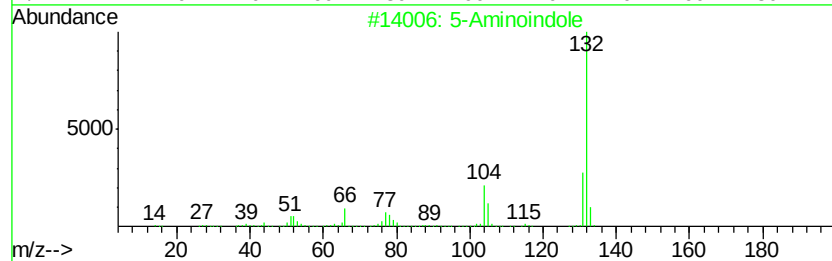
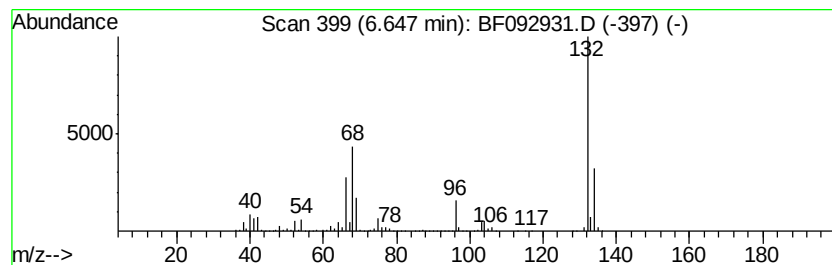
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\*\*\*\*\*  
Peak Number 2 unknown6.65 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.65 | 74.28 ng | 2974850 | 1,4-Dichlorobenzene-d4 | 6.88 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | 5-Aminoindole                       | 132 | C8H8N2    | 005192-03-0  | 12   |
| 2    |    |   | Tranylcypromine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 3    |    |   | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 9    |
| 4    |    |   | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 5    |    |   | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 9    |



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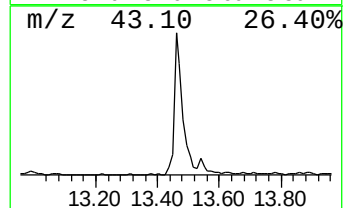
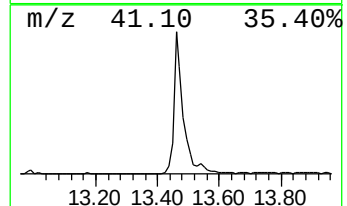
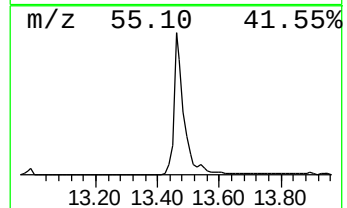
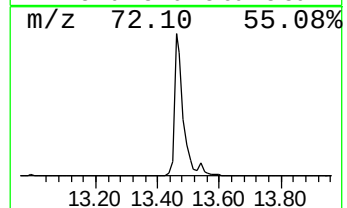
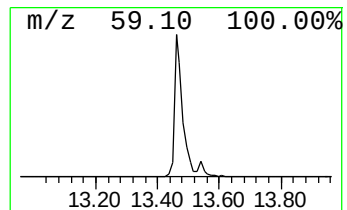
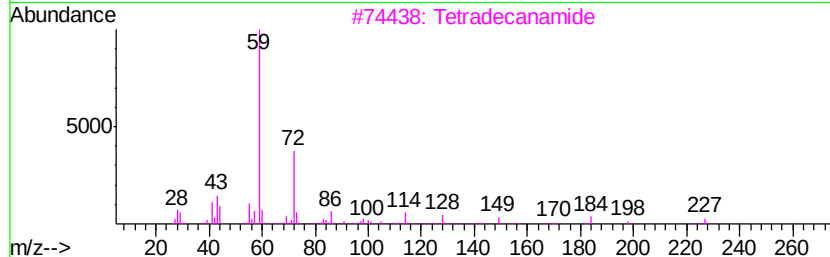
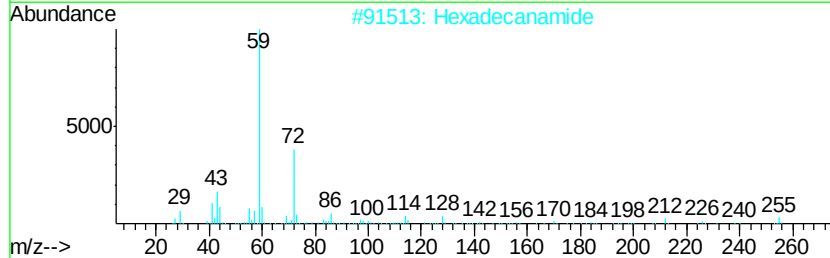
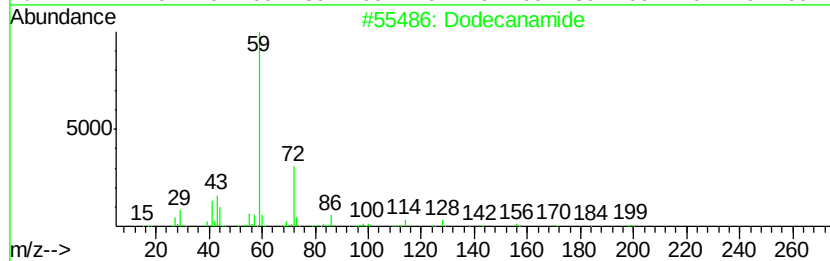
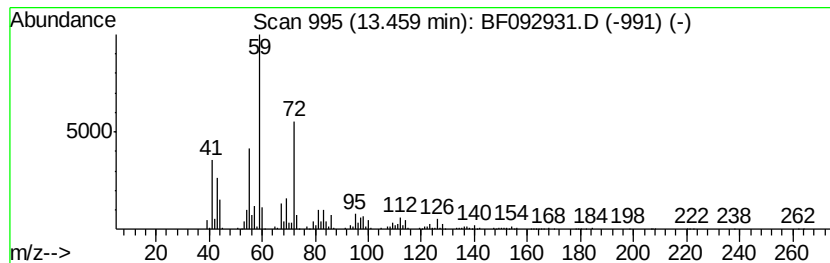
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Dodecanamide Concentration Rank 3

| R.T.  | EstConc  | Area    | Relative to ISTD | R.T.  |
|-------|----------|---------|------------------|-------|
| 13.46 | 24.27 ng | 1440380 | Chrysene-d12     | 14.04 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|-------------------------------------|-----|----------|--------------|------|
| 1    | 5  | Dodecanamide                        | 199 | C12H25NO | 001120-16-7  | 59   |
| 2    |    | Hexadecanamide                      | 255 | C16H33NO | 000629-54-9  | 56   |
| 3    |    | Tetradecanamide                     | 227 | C14H29NO | 000638-58-4  | 50   |
| 4    |    | Pentanamide, 4-methyl-              | 115 | C6H13NO  | 001119-29-5  | 47   |
| 5    |    | Methyl 17-methoxy-10-methoxycarb... | 386 | C22H42O5 | 1000110-20-7 | 47   |



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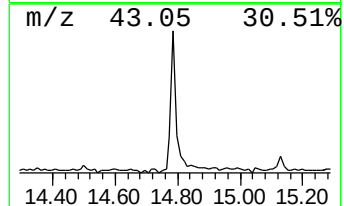
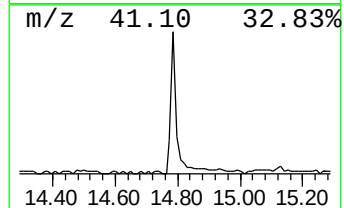
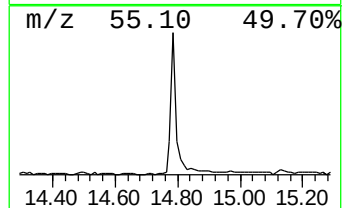
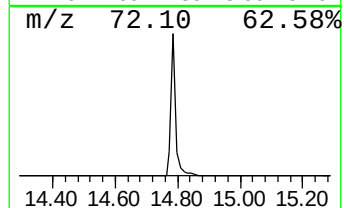
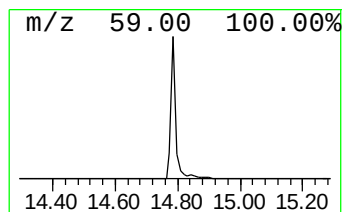
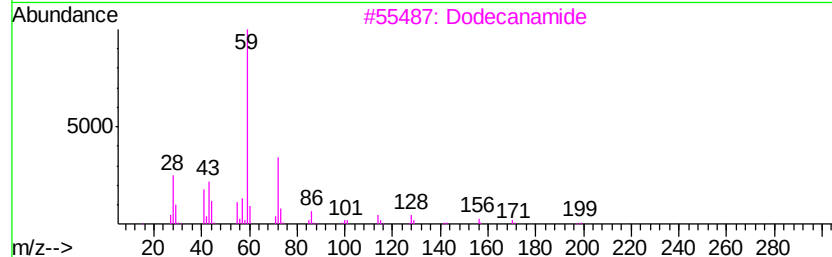
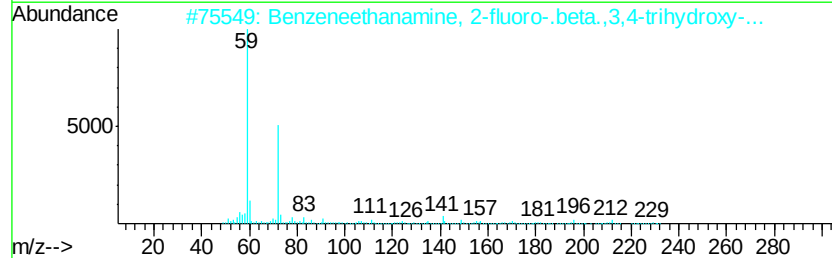
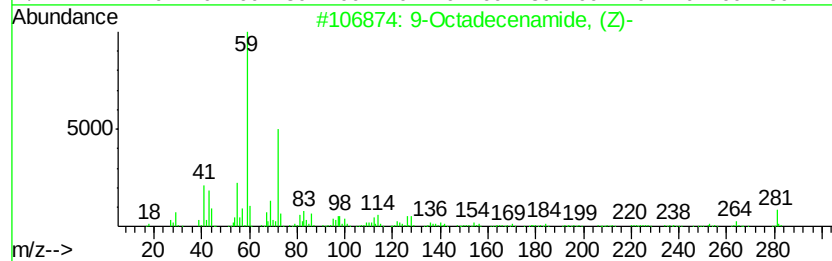
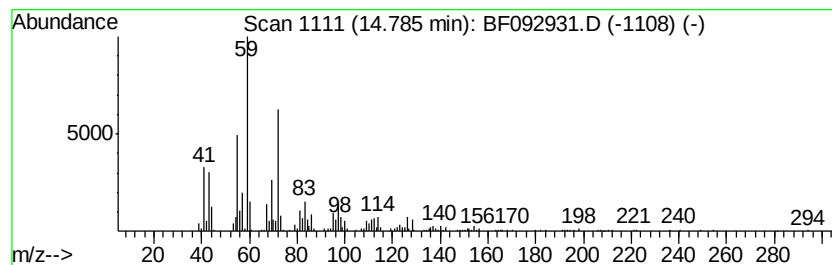
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TIC Integration Parameters: LSCINT.P

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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.79 | 8.16 ng | 443726 | Perylene-d12     | 15.47 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|-------------------------------------|-----|------------|--------------|------|
| 1    | 5  | 9-Octadecenamide, (Z)-              | 281 | C18H35NO   | 000301-02-0  | 90   |
| 2    |    | Benzeneethanamine, 2-fluoro-.bet... | 229 | C11H16FN03 | 061338-98-5  | 59   |
| 3    |    | Dodecanamide                        | 199 | C12H25NO   | 001120-16-7  | 53   |
| 4    |    | Methyl 17-methoxy-10-methoxycarb... | 386 | C22H42O5   | 1000110-20-7 | 43   |
| 5    |    | 1,7-Octanediol, 3,7-dimethyl-       | 174 | C10H22O2   | 000107-74-4  | 43   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 5.05  | 14.0    | ng    | 562123   | 1                     | 6.88  | 801004  | 20.0 |
| unknown6.65          | 6.65  | 74.3    | ng    | 2974850  | 1                     | 6.88  | 801004  | 20.0 |
| Dodecanamide         | 13.46 | 24.3    | ng    | 1440380  | 5                     | 14.04 | 1186970 | 20.0 |
| 9-Octadecenamide,... | 14.79 | 8.2     | ng    | 443726   | 6                     | 15.47 | 1087550 | 20.0 |