LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102416\
Data File : BF090798.D
Acq On : 24 Oct 2016 20:09
Operator : UM/SJ
Sample : H5393-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** END-WEST-UL

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-BF102116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.023 | 233 | 235 | 248 | rBV | 752264 | 1395524 | 21.22% | 2.615% |
| 2 | 5.446 | 269 | 272 | 274 | rBV | 4853190 | 5525005 | 84.01% | 10.352% |
| 3 | 6.474 | 359 | 362 | 365 | rBV | 3859147 | 5629464 | 85.60% | 10.548% |
| 4 | 6.600 | 371 | 373 | 376 | rBV | 4192268 | 5873198 | 89.31% | 11.004% |
| 5 | 6.829 | 391 | 393 | 404 | rBV | 906905 | 1194986 | 18.17% | 2.239% |
| 6 | 6.989 | 404 | 407 | 410 | rBV | 4504143 | 4500509 | 68.43% | 8.432% |
| 7 | 7.400 | 440 | 443 | 450 | rBV | 3213931 | 3803282 | 57.83% | 7.126% |
| 8 | 7.503 | 450 | 452 | 460 | rVB | 78211 | 164208 | 2.50% | 0.308% |
| 9 | 8.120 | 503 | 506 | 508 | rBV | 1792949 | 1680733 | 25.56% | 3.149% |
| 10 | 9.195 | 597 | 600 | 603 | rBV | 4928259 | 6576556 | 100.00% | 12.322% |
| 11 | 9.595 | 632 | 635 | 637 | rBV | 1234510 | 1138778 | 17.32% | 2.134% |
| 12 | 9.869 | 657 | 659 | 662 | rBV | 1627418 | 1664515 | 25.31% | 3.119% |
| 13 | 10.315 | 693 | 698 | 699 | rBV2 | 56382 | 93214 | 1.42% | 0.175% |
| 14 | 10.669 | 726 | 729 | 731 | rBV2 | 3159746 | 3960476 | 60.22% | 7.421% |
| 15 | 10.783 | 737 | 739 | 745 | rVB | 122943 | 165662 | 2.52% | 0.310% |
| 16 | 11.229 | 776 | 778 | 780 | rBV | 87357 | 85351 | 1.30% | 0.160% |
| 17 | 11.355 | 787 | 789 | 793 | rBV | 1620050 | 1525634 | 23.20% | 2.859% |
| 18 | 12.943 | 926 | 928 | 931 | rBV | 4415434 | 5230080 | 79.53% | 9.799% |
| 19 | 13.435 | 968 | 971 | 976 | rBV2 | 127860 | 388519 | 5.91% | 0.728% |
| 20 | 13.846 | 1005 | 1007 | 1017 | rBV | 221726 | 304923 | 4.64% | 0.571% |
| 21 | 13.995 | 1017 | 1020 | 1027 | rBV | 1103709 | 1149120 | 17.47% | 2.153% |
| 22 | 14.109 | 1027 | 1030 | 1034 | rVV2 | 25886 | 67159 | 1.02% | 0.126% |
| 23 | 14.486 | 1060 | 1063 | 1068 | rBV3 | 51036 | 108703 | 1.65% | 0.204% |
| 24 | 14.841 | 1092 | 1094 | 1097 | rVB | 105359 | 110887 | 1.69% | 0.208% |
| 25 | 15.424 | 1142 | 1145 | 1153 | rVB | 781033 | 1034756 | 15.73% | 1.939% |

Sum of corrected areas: 53371242

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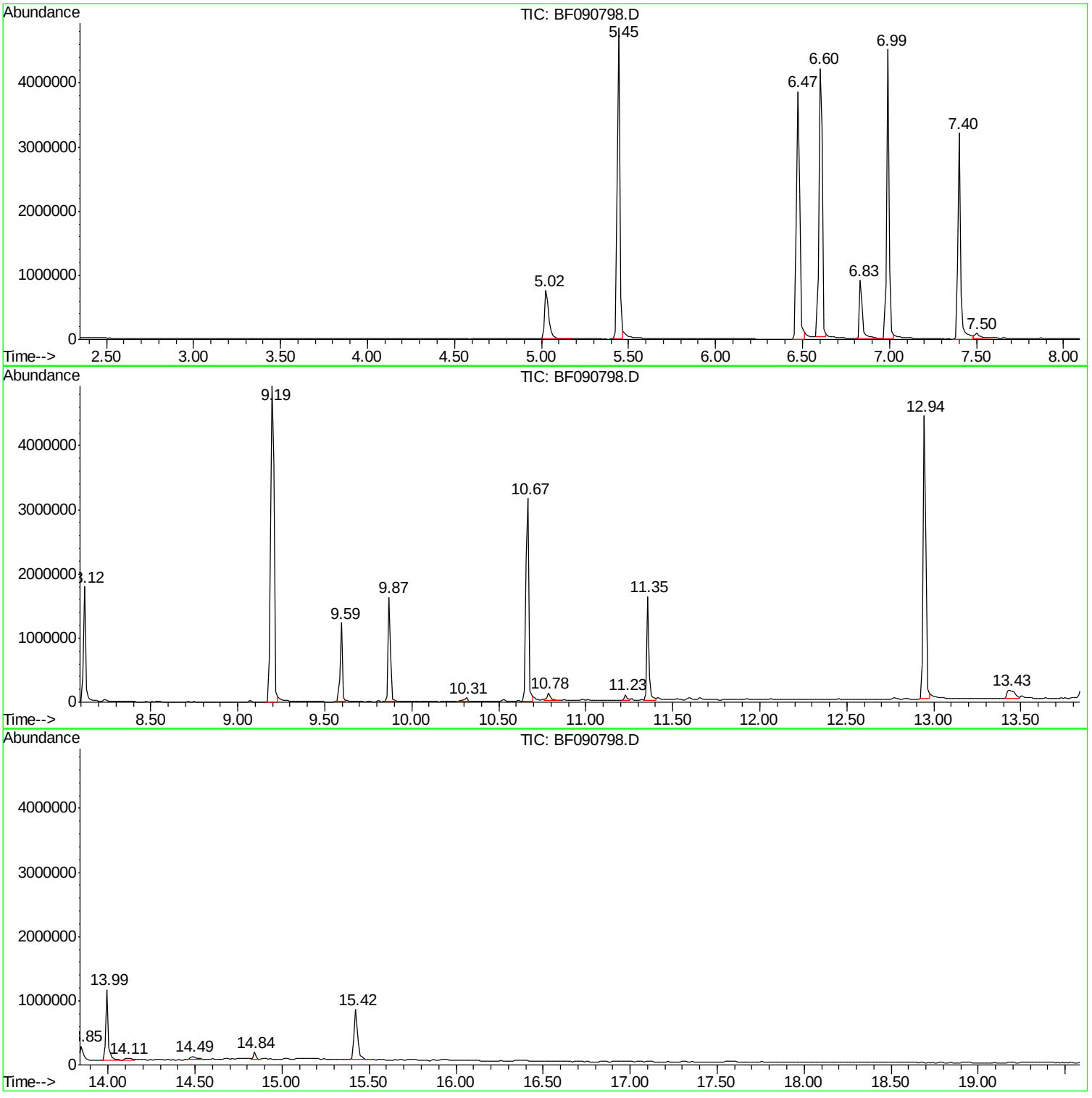
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
END-WEST-UL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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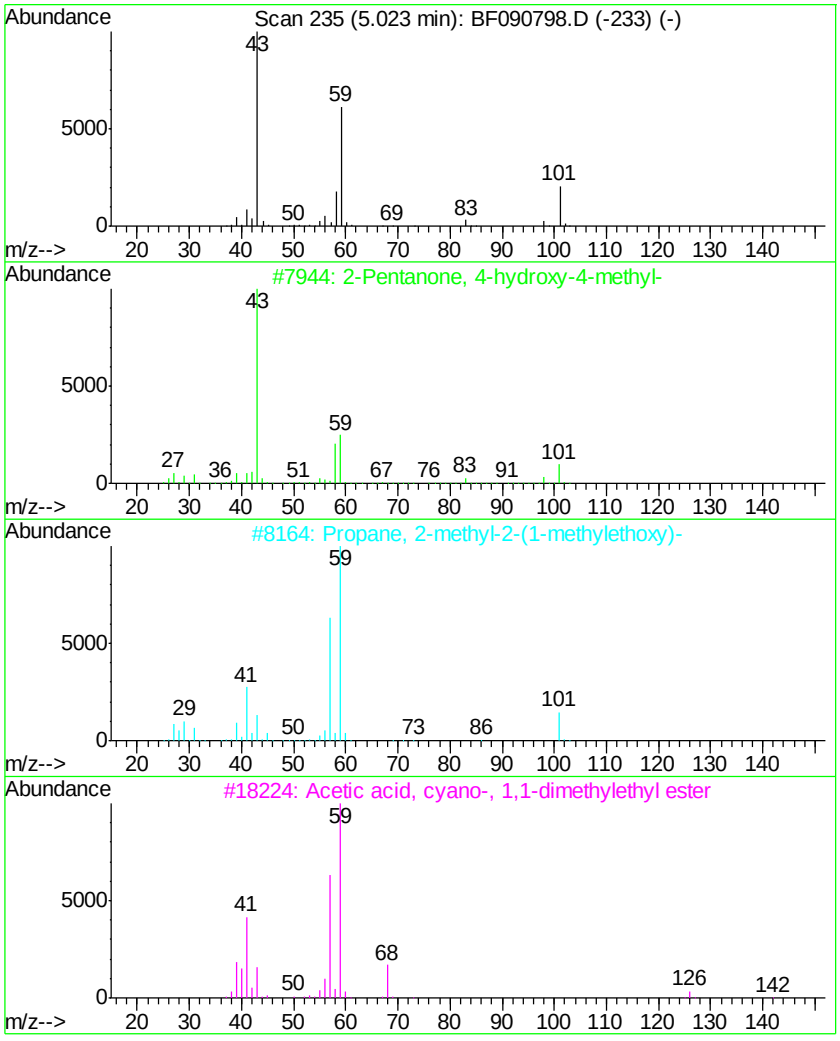
TIC Integration Parameters: LSCINT.P

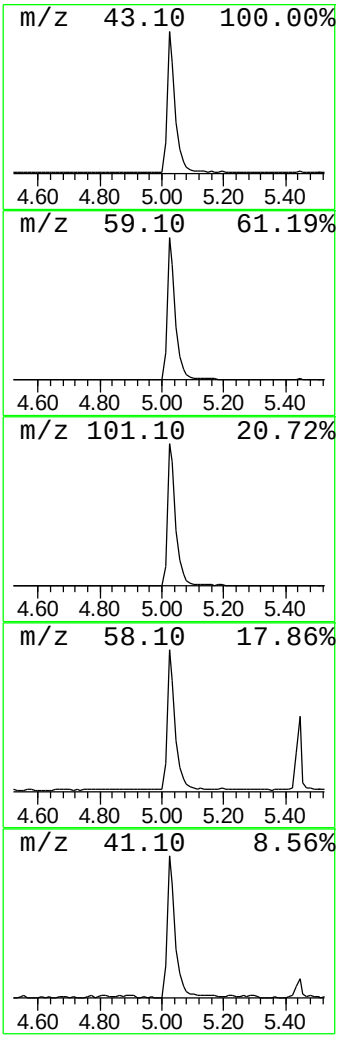
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.02 | 23.36 ng | 1395520 | 1,4-Dichlorobenzene-d4 | 6.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 53 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 4 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |
| 5 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102416\
Data File : BF090798.D
Acq On : 24 Oct 2016 20:09
Operator : UM/SJ
Sample : H5393-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** END-WEST-UL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

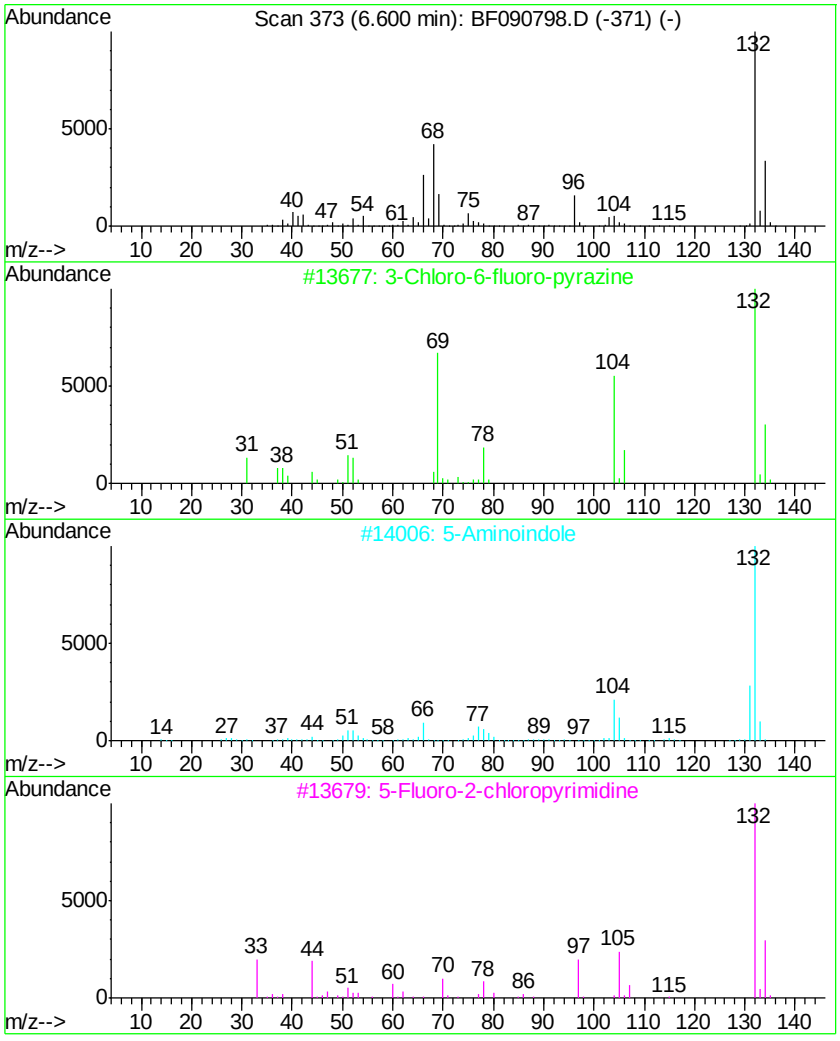
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

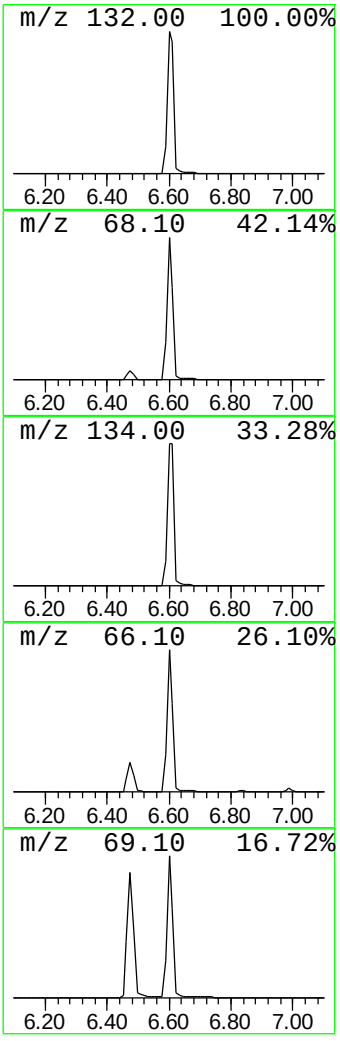
**********

Peak Number 2 unknown6.60 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.60 | 98.30 ng | 5873200 | 1,4-Dichlorobenzene-d4 | 6.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 16 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 3 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |
| 4 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |
| 5 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |



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Operator : UM/SJ
Sample : H5393-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** END-WEST-UL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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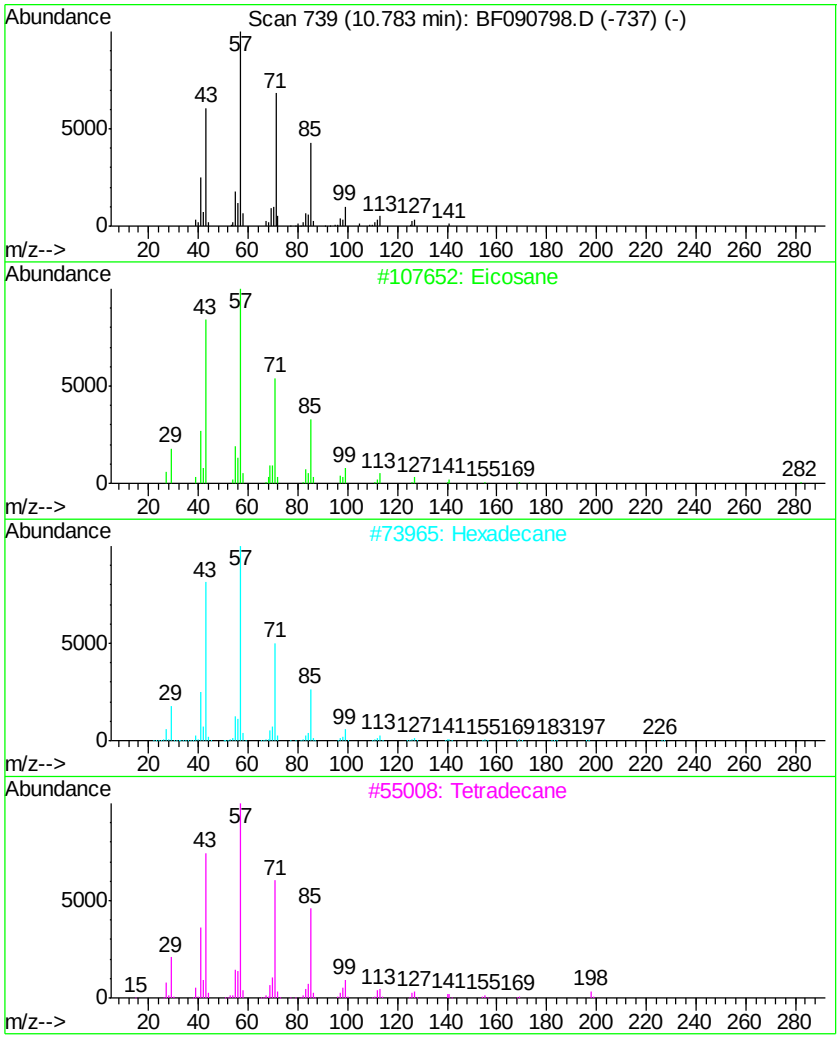
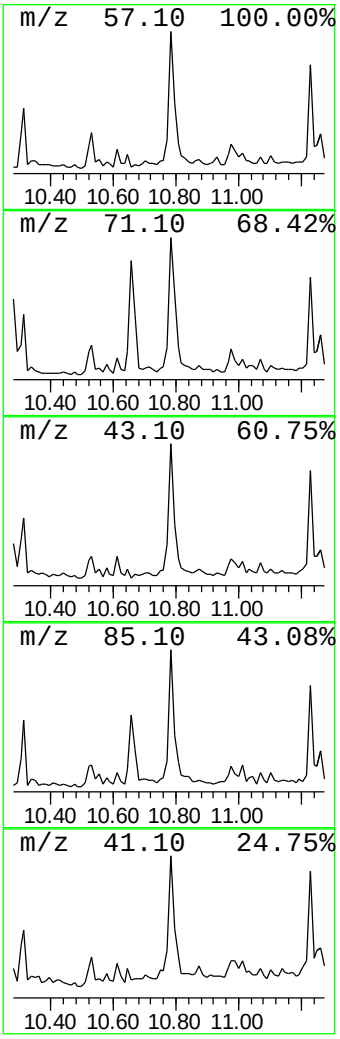
Peak Number 4 Eicosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.78 | 2.17 ng | 165662 | Phenanthrene-d10 | 11.35 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 91 |
| 2 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 3 | Tetradecane | 198 | C14H30 | 000629-59-4 | 86 |
| 4 | Octacosane | 394 | C28H58 | 000630-02-4 | 64 |
| 5 | Pentadecane | 212 | C15H32 | 000629-62-9 | 64 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102416\
Data File : BF090798.D
Acq On : 24 Oct 2016 20:09
Operator : UM/SJ
Sample : H5393-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** END-WEST-UL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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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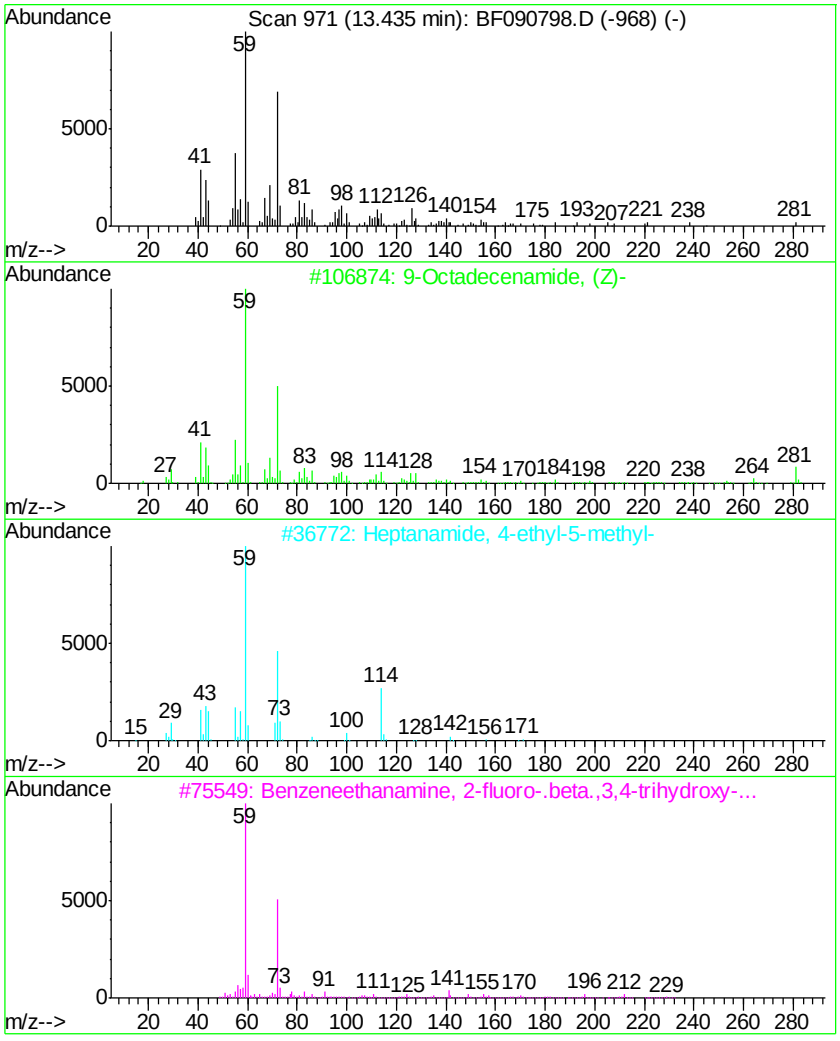
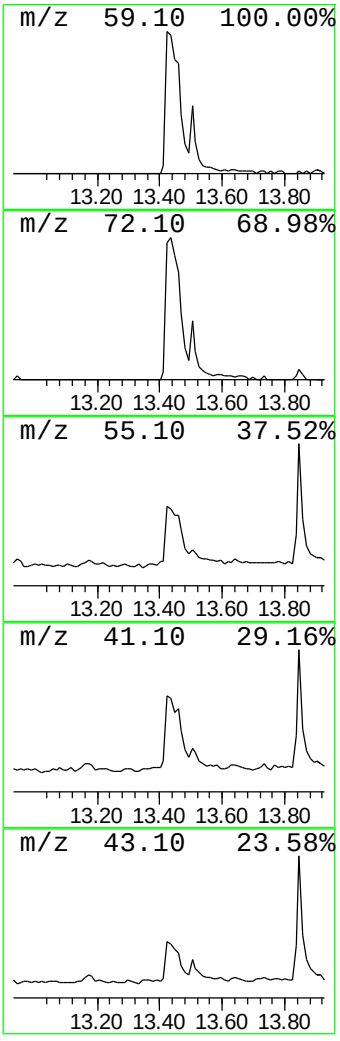
Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.43 | 6.76 ng | 388519 | Chrysene-d12 | 13.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 91 |
| 2 | Heptanamide, 4-ethyl-5-methyl- | 171 | C10H21NO | 054789-40-1 | 64 |
| 3 | Benzeneethanamine, 2-fluoro-.bet... | 229 | C11H16FNO3 | 061338-98-5 | 64 |
| 4 | Hexadecanamide | 255 | C16H33NO | 000629-54-9 | 53 |
| 5 | Octanamide | 143 | C8H17NO | 000629-01-6 | 50 |



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Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** END-WEST-UL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

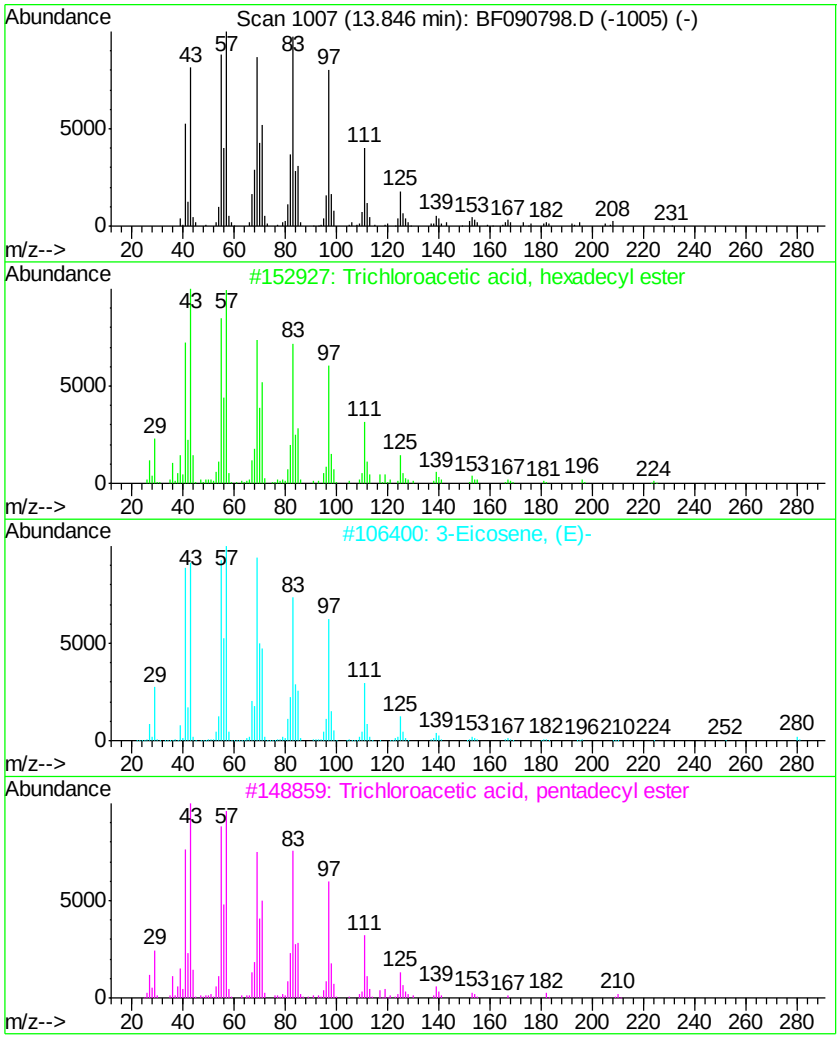
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

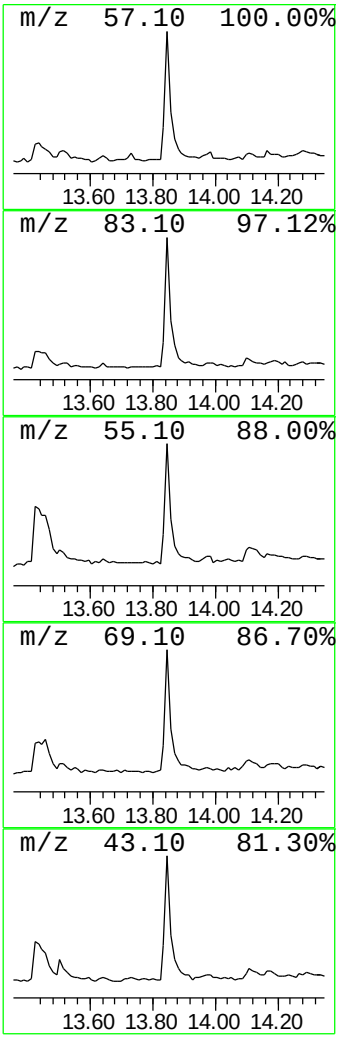
**********

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.85 | 5.31 ng | 304923 | Chrysene-d12 | 13.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94 |
| 2 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 91 |
| 3 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 91 |
| 4 | 3-Chloropropionic acid, heptadec... | 346 | C20H39ClO2 | 1000283-05-1 | 91 |
| 5 | 9-Eicosene, (E)- | 280 | C20H40 | 074685-29-3 | 91 |



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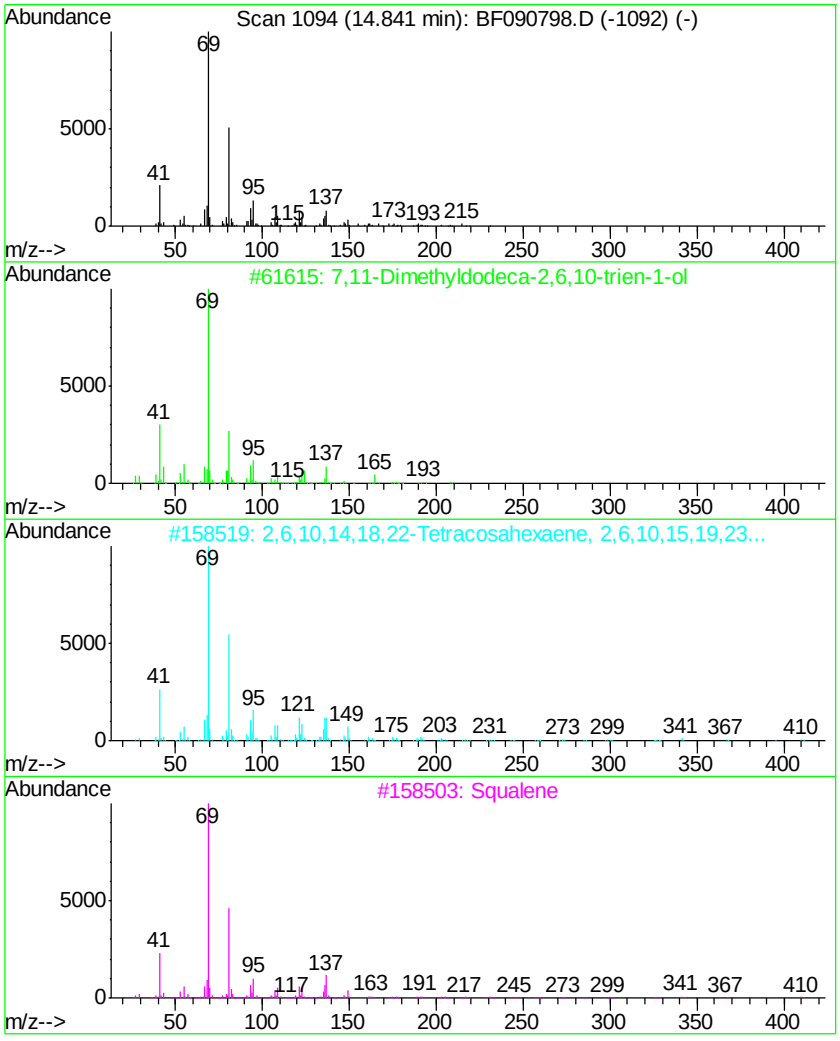
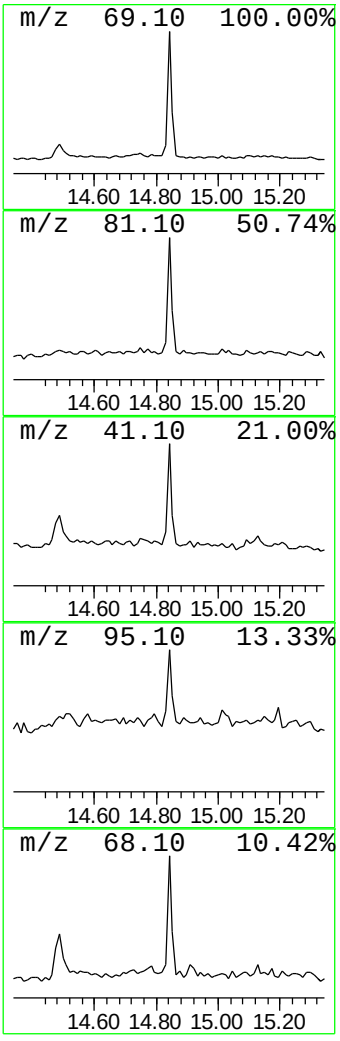
Peak Number 7 7,11-Dimethyldodeca-2,6,10-... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.84 | 2.14 ng | 110887 | Perylene-d12 | 15.42 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 90 |
| 2 | 2,6,10,14,18,22-Tetracosahexaene... | 410 | C30H50 | 000111-02-4 | 90 |
| 3 | Squalene | 410 | C30H50 | 007683-64-9 | 90 |
| 4 | 2,6,10,14,18-Pentamethyl-2,6,10,... | 342 | C25H42 | 075581-03-2 | 83 |
| 5 | 2,6,10-Dodecatrien-1-ol, 3,7,11-... | 222 | C15H26O | 000106-28-5 | 83 |



Tentatively Identified Compound (LSC) summary

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 5.02 | 23.4 | ng | 1395520 | 1 | 6.83 | 1194990 | 20.0 |
| unknown6.60 | 6.60 | 98.3 | ng | 5873200 | 1 | 6.83 | 1194990 | 20.0 |
| Eicosane | 10.78 | 2.2 | ng | 165662 | 4 | 11.35 | 1525630 | 20.0 |
| 9-Octadecenamide,... | 13.43 | 6.8 | ng | 388519 | 5 | 13.99 | 1149120 | 20.0 |
| Trichloroacetic a... | 13.85 | 5.3 | ng | 304923 | 5 | 13.99 | 1149120 | 20.0 |
| 7,11-Dimethyldode... | 14.84 | 2.1 | ng | 110887 | 6 | 15.42 | 1034760 | 20.0 |