LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101715\
Data File : BF082344.D
Acq On : 17 Oct 2015 1:05
Operator : UM/IZ
Sample : G4016-03 10X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CS-3

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-BF101015.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 | 5.154 | 262 | 264 | 268 | rBV | 56557 | 61159 | 9.72% | 1.397% |
| 2 | 5.577 | 299 | 301 | 313 | rVB | 66441 | 74262 | 11.80% | 1.696% |
| 3 | 6.606 | 389 | 391 | 399 | rBV | 46337 | 76775 | 12.20% | 1.753% |
| 4 | 6.731 | 400 | 402 | 410 | rVB | 94872 | 97262 | 15.46% | 2.221% |
| 5 | 6.960 | 420 | 422 | 425 | rBV | 335818 | 298158 | 47.38% | 6.809% |
| 6 | 7.120 | 433 | 436 | 438 | rBV | 66888 | 78190 | 12.42% | 1.786% |
| 7 | 7.520 | 469 | 471 | 481 | rBV3 | 28675 | 46447 | 7.38% | 1.061% |
| 8 | 8.240 | 532 | 534 | 537 | rBV | 518933 | 440857 | 70.05% | 10.068% |
| 9 | 9.315 | 626 | 628 | 630 | rBV | 91470 | 126793 | 20.15% | 2.896% |
| 10 | 9.703 | 660 | 662 | 664 | rBV | 22582 | 17917 | 2.85% | 0.409% |
| 11 | 9.989 | 685 | 687 | 690 | rBV | 640379 | 560082 | 89.00% | 12.791% |
| 12 | 10.778 | 754 | 756 | 762 | rBV | 87826 | 89361 | 14.20% | 2.041% |
| 13 | 11.475 | 815 | 817 | 822 | rBV | 676838 | 629312 | 100.00% | 14.372% |
| 14 | 11.703 | 832 | 837 | 840 | rBV5 | 7561 | 23503 | 3.73% | 0.537% |
| 15 | 11.749 | 840 | 841 | 845 | rVB4 | 5085 | 8520 | 1.35% | 0.195% |
| 16 | 11.818 | 845 | 847 | 848 | rBV2 | 4919 | 7898 | 1.26% | 0.180% |
| 17 | 11.932 | 856 | 857 | 859 | rBV2 | 6623 | 8815 | 1.40% | 0.201% |
| 18 | 11.989 | 859 | 862 | 864 | rBV3 | 12847 | 28563 | 4.54% | 0.652% |
| 19 | 12.686 | 922 | 923 | 925 | rBV | 27192 | 31592 | 5.02% | 0.722% |
| 20 | 12.869 | 937 | 939 | 940 | rVB | 22197 | 16876 | 2.68% | 0.385% |
| 21 | 12.915 | 941 | 943 | 946 | rBV2 | 26426 | 51734 | 8.22% | 1.182% |
| 22 | 13.052 | 953 | 955 | 959 | rVB | 167333 | 192548 | 30.60% | 4.397% |
| 23 | 14.138 | 1048 | 1050 | 1053 | rBV | 515705 | 557496 | 88.59% | 12.732% |
| 24 | 14.938 | 1118 | 1120 | 1123 | rBV | 84005 | 104137 | 16.55% | 2.378% |
| 25 | 15.669 | 1181 | 1184 | 1187 | rBV | 391030 | 499674 | 79.40% | 11.412% |
| 26 | 16.367 | 1243 | 1245 | 1253 | rVB | 57488 | 140634 | 22.35% | 3.212% |
| 27 | 16.812 | 1281 | 1284 | 1289 | rVB | 48812 | 110046 | 17.49% | 2.513% |

Sum of corrected areas: 4378611

LSC Report - Integrated Chromatogram

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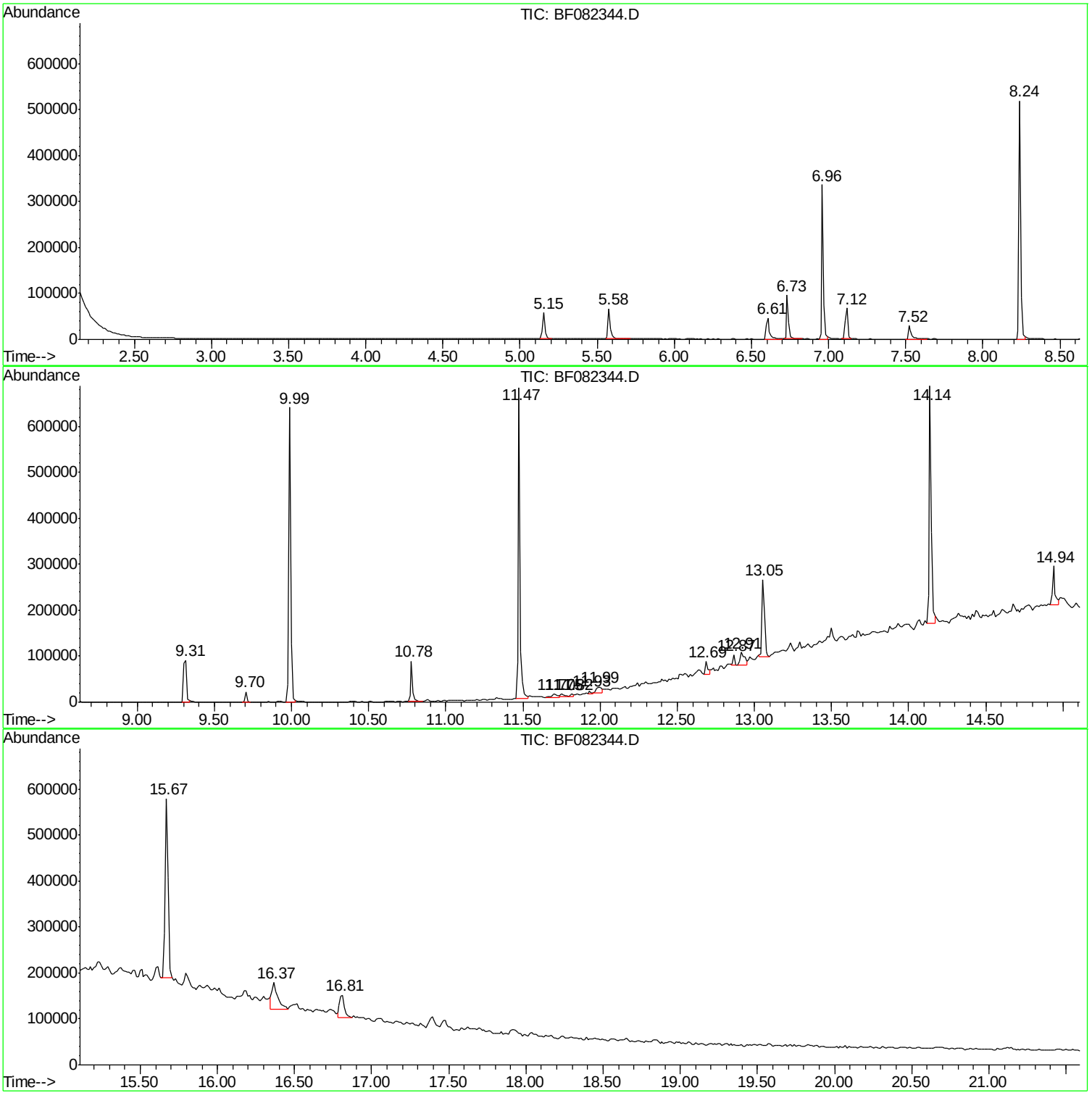
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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Data File : BF082344.D
Acq On : 17 Oct 2015 1:05
Operator : UM/IZ
Sample : G4016-03 10X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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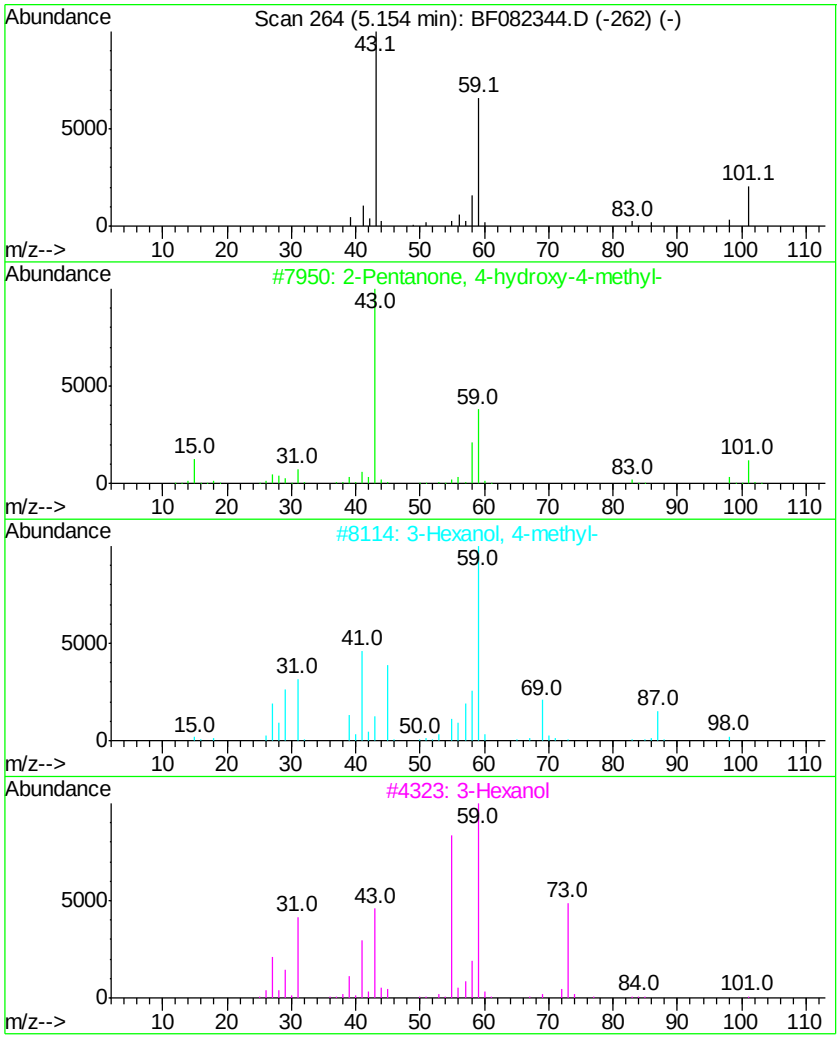
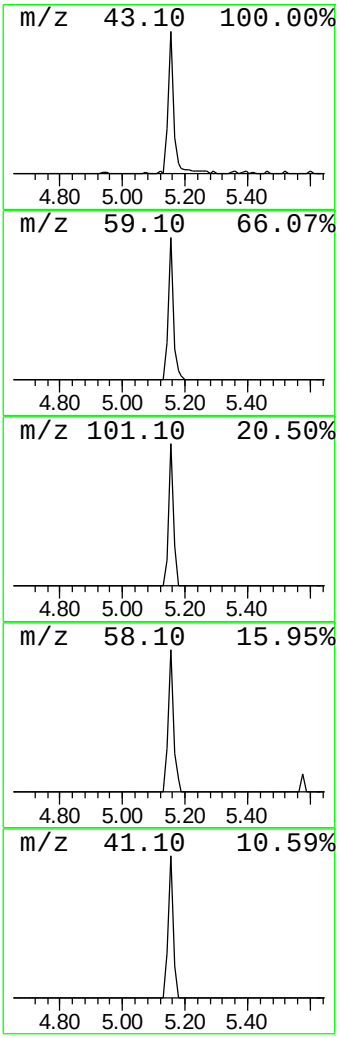
Peak Number 1 unknown5.15 Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.15 | 4.10 ng | 61159 | 1,4-Dichlorobenzene-d4 | 6.96 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 40 |
| 2 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 28 |
| 3 | 3-Hexanol | 102 | C6H14O | 000623-37-0 | 28 |
| 4 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 9 |
| 5 | 3-Heptanol | 116 | C7H16O | 000589-82-2 | 9 |



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Acq On : 17 Oct 2015 1:05
Operator : UM/IZ
Sample : G4016-03 10X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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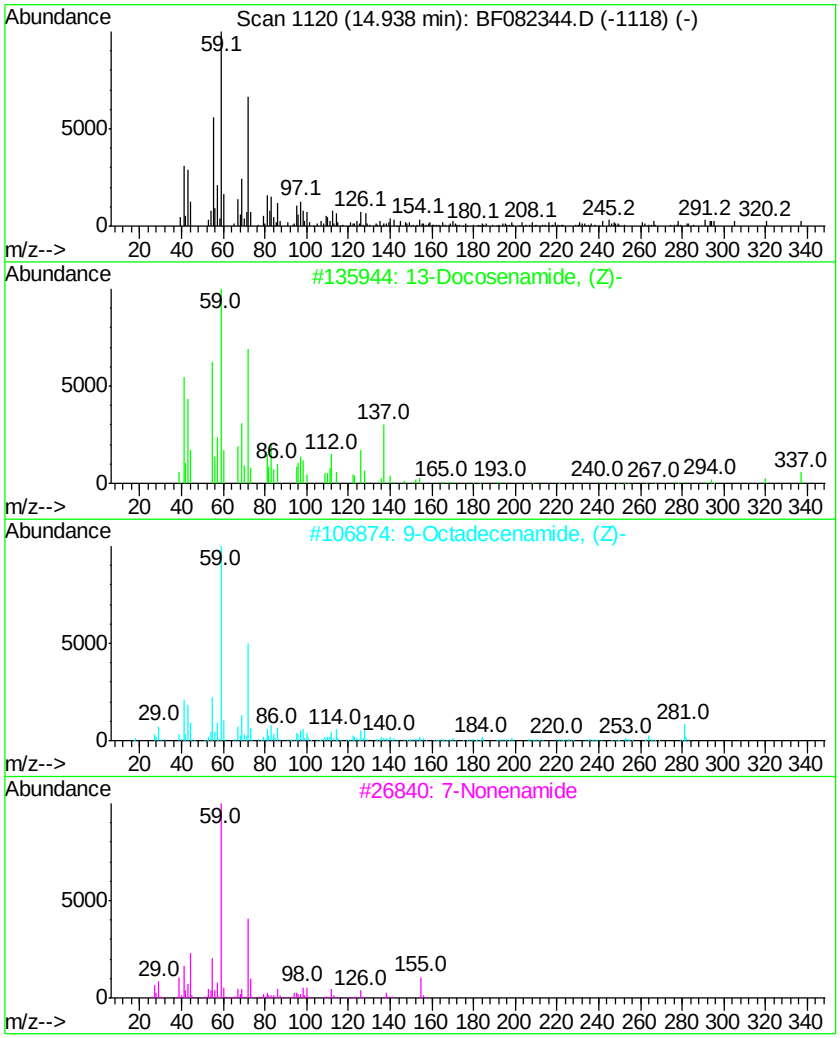
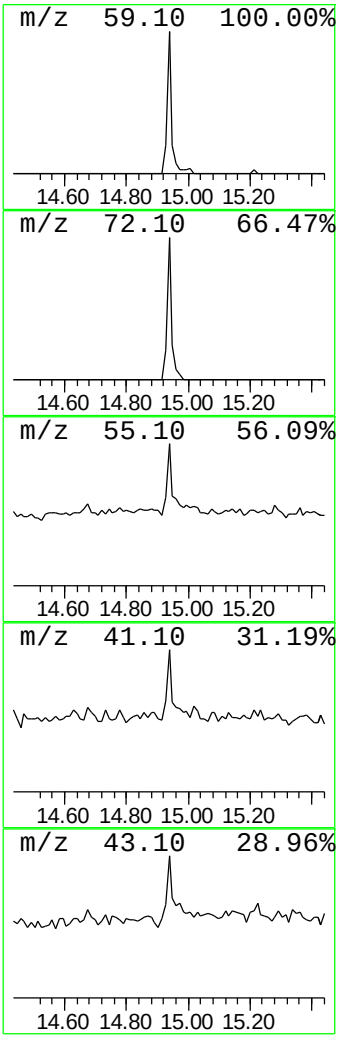
Peak Number 4 13-Docosenamide, (Z)- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.94 | 4.17 ng | 104137 | Perylene-d12 | 15.67 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 13-Docosenamide, (Z)- | 337 | C22H43NO | 000112-84-5 | 93 |
| 2 | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 86 |
| 3 | 7-Nonenamide | 155 | C9H17NO | 090949-53-4 | 68 |
| 4 | Benzeneethanamine, 2-fluoro-.bet... | 229 | C11H16FNO3 | 061338-98-5 | 64 |
| 5 | Pentanamide, 4-methyl- | 115 | C6H13NO | 001119-29-5 | 59 |



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Data File : BF082344.D
Acq On : 17 Oct 2015 1:05
Operator : UM/IZ
Sample : G4016-03 10X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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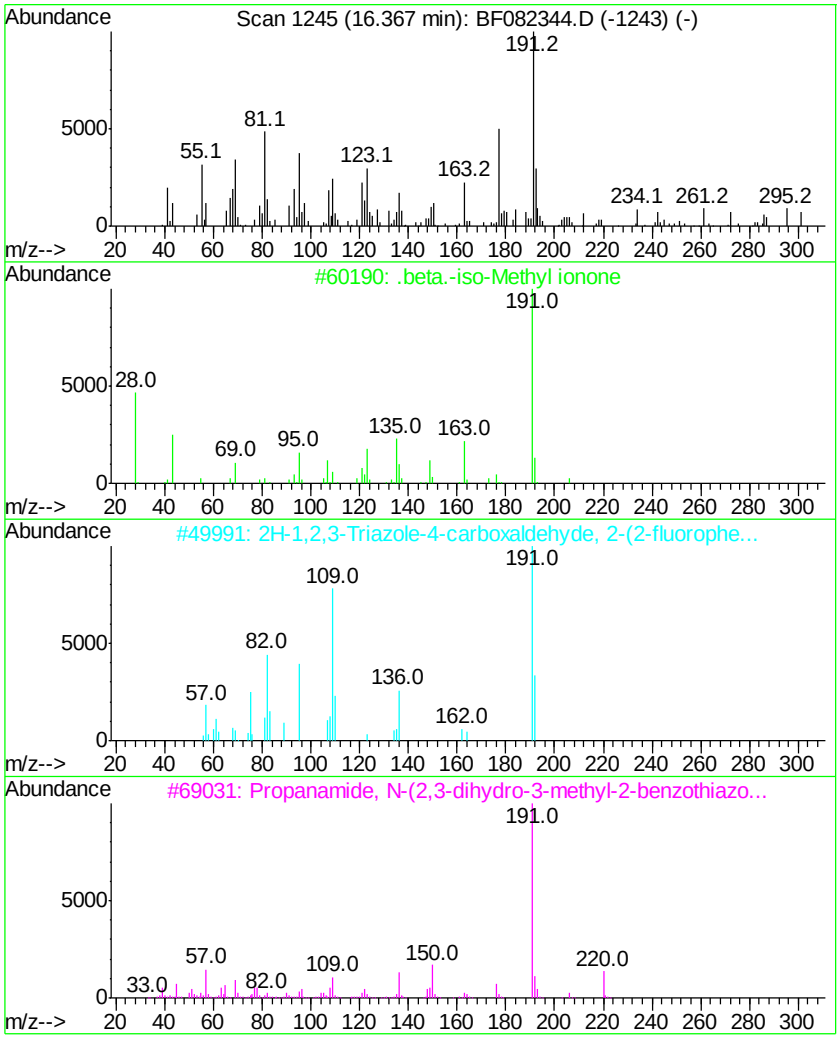
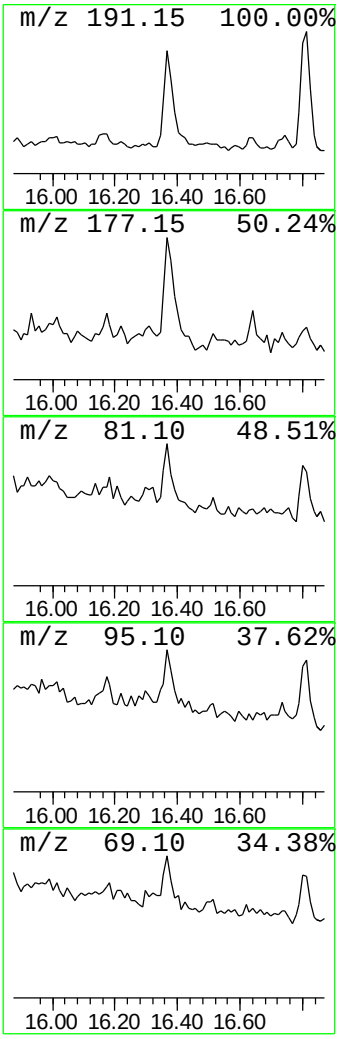
Peak Number 5 .beta.-iso-Methyl ionone Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.37 | 5.63 ng | 140634 | Perylene-d12 | 15.67 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | .beta.-iso-Methyl ionone | 206 | C14H22O | 1000285-40-2 | 58 |
| 2 | 2H-1,2,3-Triazole-4-carboxaldehy... | 191 | C9H6FN3O | 051306-43-5 | 43 |
| 3 | Propanamide, N-(2,3-dihydro-3-me... | 220 | C11H12N2OS | 332413-15-7 | 35 |
| 4 | N-(3,4,5,6-Tetrahydro-1,3-thiazi... | 192 | C10H12N2S | 003420-40-4 | 27 |
| 5 | 3-Buten-2-one, 4-(2,5,6,6-tetram... | 206 | C14H22O | 000079-70-9 | 27 |



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Operator : UM/IZ
Sample : G4016-03 10X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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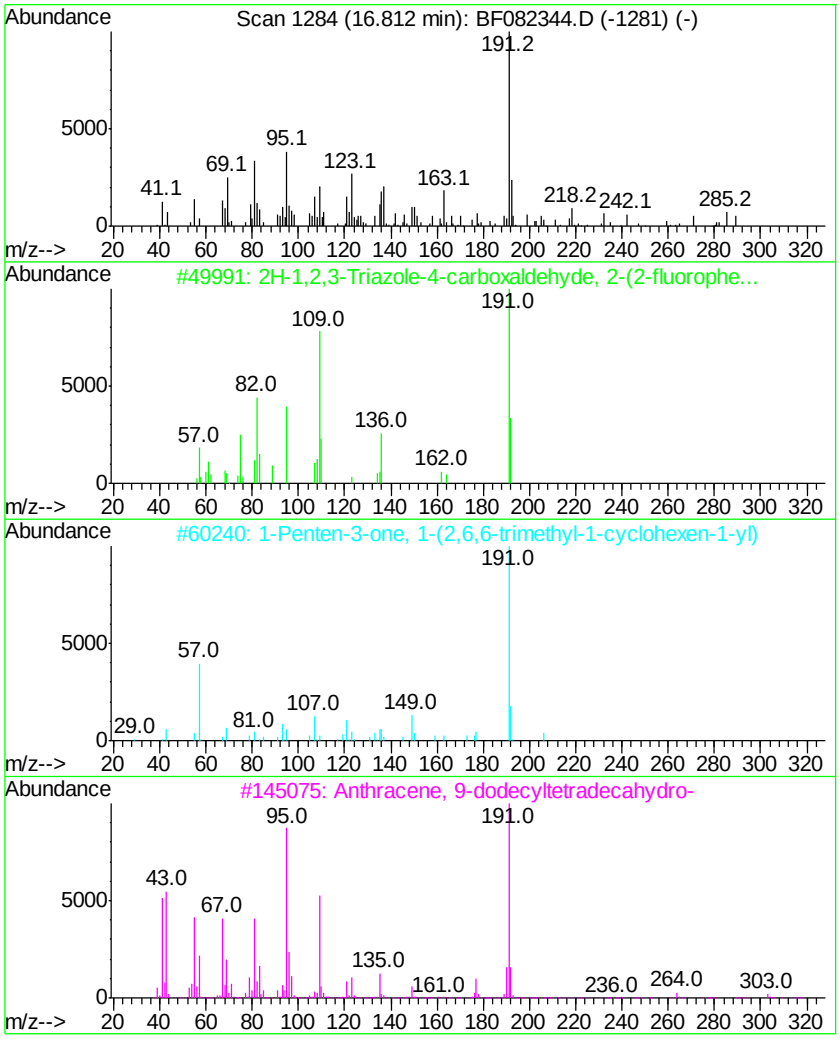
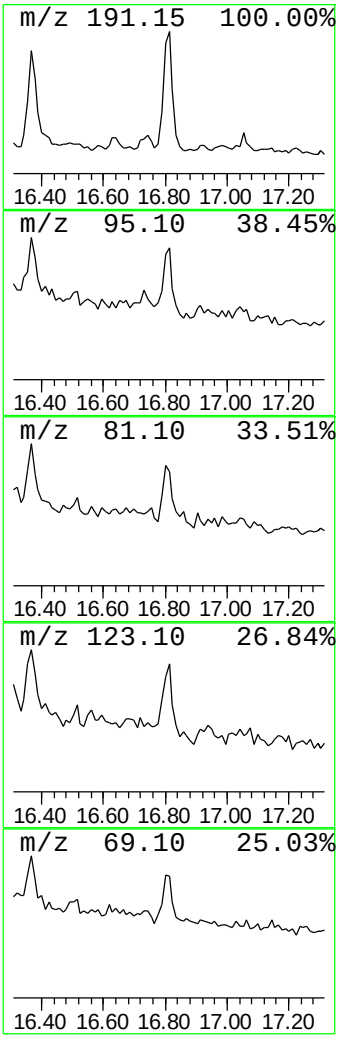
Peak Number 6 unknown16.81 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.81 | 4.40 ng | 110046 | Perylene-d12 | 15.67 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2H-1,2,3-Triazole-4-carboxaldehv... | 191 | C9H6FN3O | 051306-43-5 | 47 |
| 2 | 1-Penten-3-one, 1-(2,6,6-trimeth... | 206 | C14H22O | 000127-43-5 | 43 |
| 3 | Anthracene, 9-dodecyltetradecahv... | 360 | C26H48 | 055401-75-7 | 40 |
| 4 | 1-Cyclohexene, 1,3,3-trimethyl-2... | 206 | C14H22O | 1000197-08-4 | 38 |
| 5 | 3-Buten-2-one, 4-(2,5,6,6-tetram... | 206 | C14H22O | 000079-70-9 | 38 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101715\
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Operator : UM/IZ
Sample : G4016-03 10X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| unknown5.15 | 5.15 | 4.1 | ng | 61159 | 1 | 6.96 | 298158 | 20.0 |
| 13-Docosenamide, ... | 14.94 | 4.2 | ng | 104137 | 6 | 15.67 | 499674 | 20.0 |
| .beta.-iso-Methyl... | 16.37 | 5.6 | ng | 140634 | 6 | 15.67 | 499674 | 20.0 |
| unknown16.81 | 16.81 | 4.4 | ng | 110046 | 6 | 15.67 | 499674 | 20.0 |