LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106613.D
Acq On : 20 Jun 2018 5:52
Operator : JU/SJ
Sample : J3548-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 061318-DBRI-E-D-S

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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 | 5.195 | 482 | 486 | 495 | rBV | 63101 | 71471 | 2.72% | 0.408% |
| 2 | 5.601 | 552 | 555 | 567 | rBB | 1004001 | 961677 | 36.56% | 5.493% |
| 3 | 6.595 | 721 | 724 | 733 | rBV | 782841 | 685414 | 26.05% | 3.915% |
| 4 | 6.737 | 744 | 748 | 751 | rBV | 1801430 | 1578093 | 59.99% | 9.015% |
| 5 | 6.960 | 782 | 786 | 790 | rBB | 732040 | 602636 | 22.91% | 3.443% |
| 6 | 7.119 | 809 | 813 | 816 | rBV | 2255467 | 2065084 | 78.50% | 11.797% |
| 7 | 7.531 | 877 | 883 | 885 | rBV | 1607177 | 1734884 | 65.95% | 9.910% |
| 8 | 8.242 | 1000 | 1004 | 1008 | rBV | 808104 | 679527 | 25.83% | 3.882% |
| 9 | 8.795 | 1095 | 1098 | 1102 | rBV | 39494 | 32463 | 1.23% | 0.185% |
| 10 | 9.319 | 1182 | 1187 | 1190 | rBV | 2801886 | 2630714 | 100.00% | 15.028% |
| 11 | 9.707 | 1250 | 1253 | 1262 | rBV | 120007 | 101201 | 3.85% | 0.578% |
| 12 | 10.001 | 1300 | 1303 | 1314 | rVB2 | 679992 | 620679 | 23.59% | 3.546% |
| 13 | 10.666 | 1413 | 1416 | 1419 | rBV | 36584 | 27660 | 1.05% | 0.158% |
| 14 | 10.713 | 1421 | 1424 | 1428 | rVB | 106176 | 82883 | 3.15% | 0.473% |
| 15 | 10.795 | 1434 | 1438 | 1447 | rBV | 1068969 | 899332 | 34.19% | 5.137% |
| 16 | 11.495 | 1553 | 1557 | 1561 | rBV | 649443 | 532374 | 20.24% | 3.041% |
| 17 | 13.083 | 1822 | 1827 | 1830 | rBV | 2608552 | 2434974 | 92.56% | 13.910% |
| 18 | 13.965 | 1974 | 1977 | 1982 | rBV | 58605 | 64998 | 2.47% | 0.371% |
| 19 | 14.142 | 2004 | 2007 | 2011 | rBV | 690817 | 682096 | 25.93% | 3.896% |
| 20 | 14.289 | 2028 | 2032 | 2037 | rVB | 37898 | 37102 | 1.41% | 0.212% |
| 21 | 14.601 | 2082 | 2085 | 2091 | rBV | 74835 | 81555 | 3.10% | 0.466% |
| 22 | 14.918 | 2136 | 2139 | 2144 | rVB | 92776 | 91473 | 3.48% | 0.523% |
| 23 | 15.271 | 2196 | 2199 | 2203 | rBV | 84621 | 92834 | 3.53% | 0.530% |
| 24 | 15.677 | 2263 | 2268 | 2276 | rBV | 428642 | 591717 | 22.49% | 3.380% |
| 25 | 16.142 | 2342 | 2347 | 2351 | rBV | 52407 | 78948 | 3.00% | 0.451% |
| 26 | 16.677 | 2434 | 2438 | 2446 | rVB4 | 26154 | 43937 | 1.67% | 0.251% |

Sum of corrected areas: 17505726

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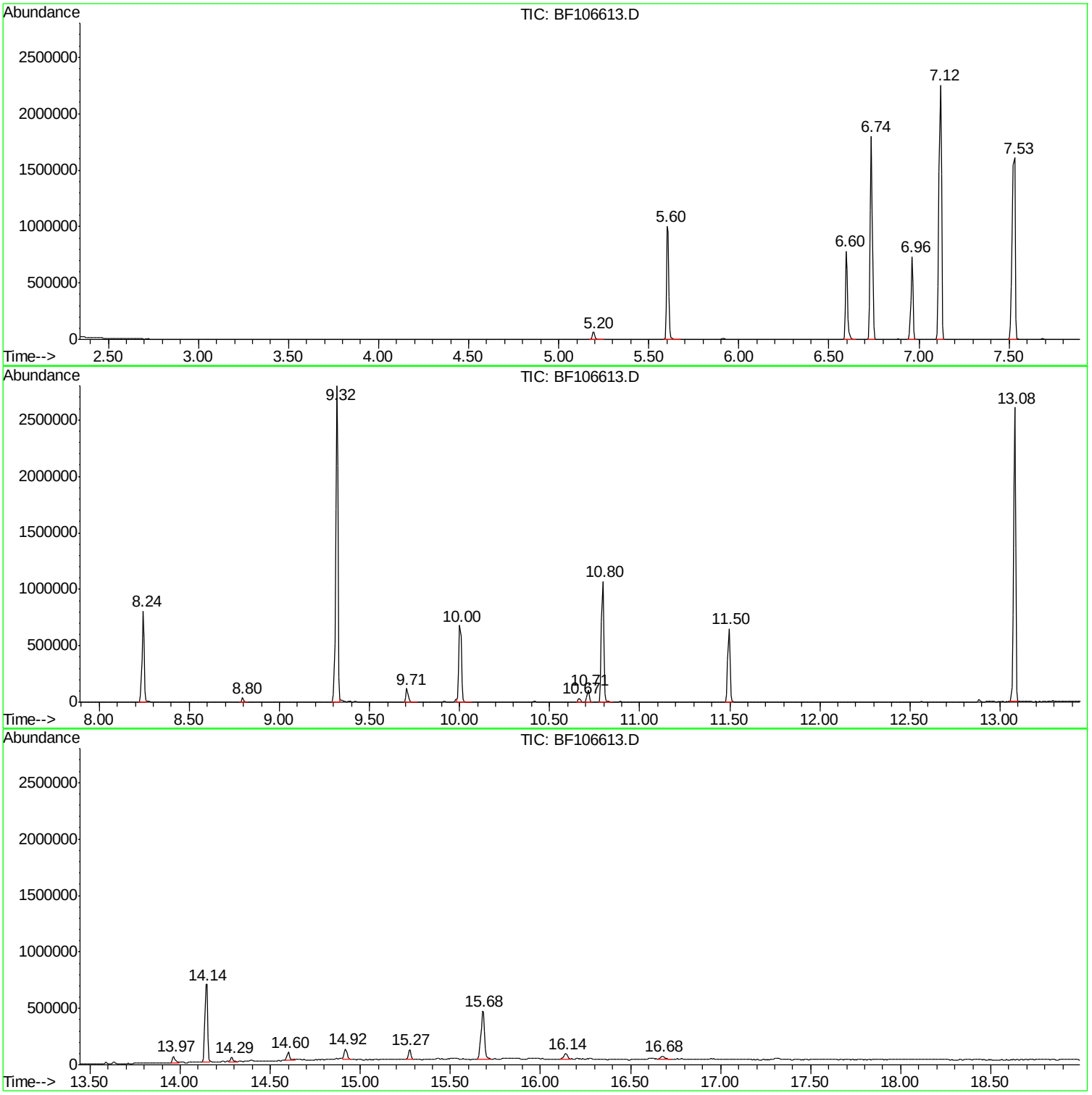
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
061318-DBRI-E-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106613.D
Acq On : 20 Jun 2018 5:52
Operator : JU/SJ
Sample : J3548-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 061318-DBRI-E-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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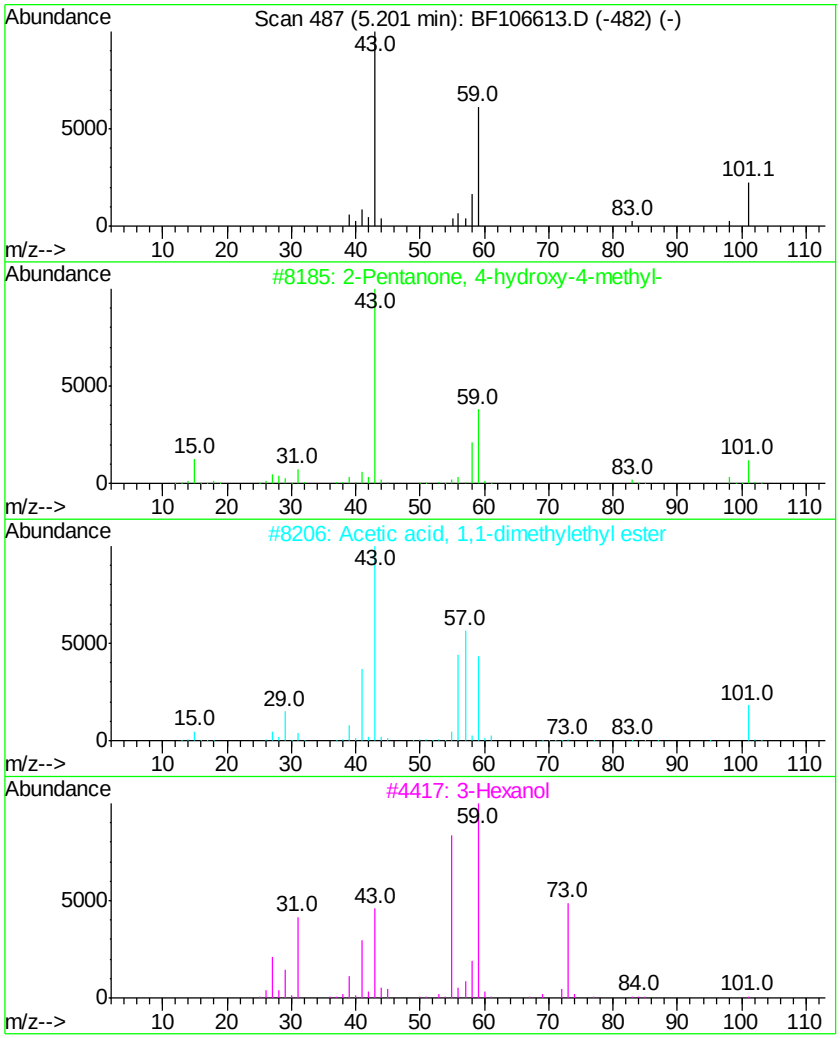
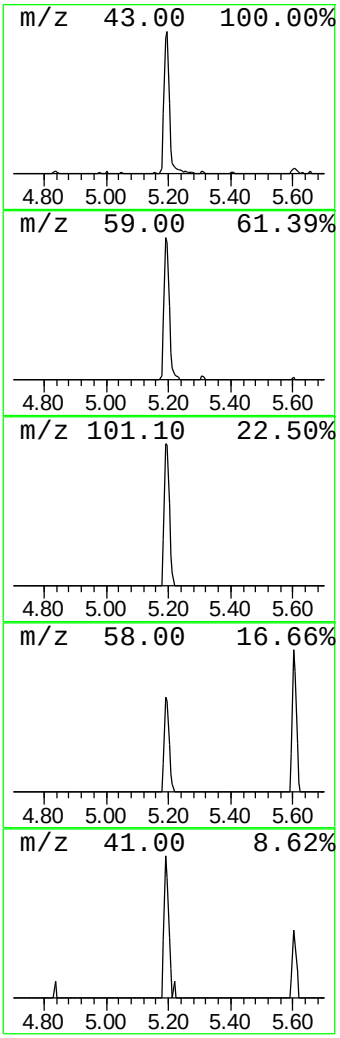
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.20 | 2.37 ng | 71471 | 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 | 59 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 3 | 3-Hexanol | 102 | C6H14O | 000623-37-0 | 33 |
| 4 | Butyl aldoxime, 3-methyl-, syn- | 101 | C5H11NO | 005780-40-5 | 23 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106613.D
Acq On : 20 Jun 2018 5:52
Operator : JU/SJ
Sample : J3548-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 061318-DBRI-E-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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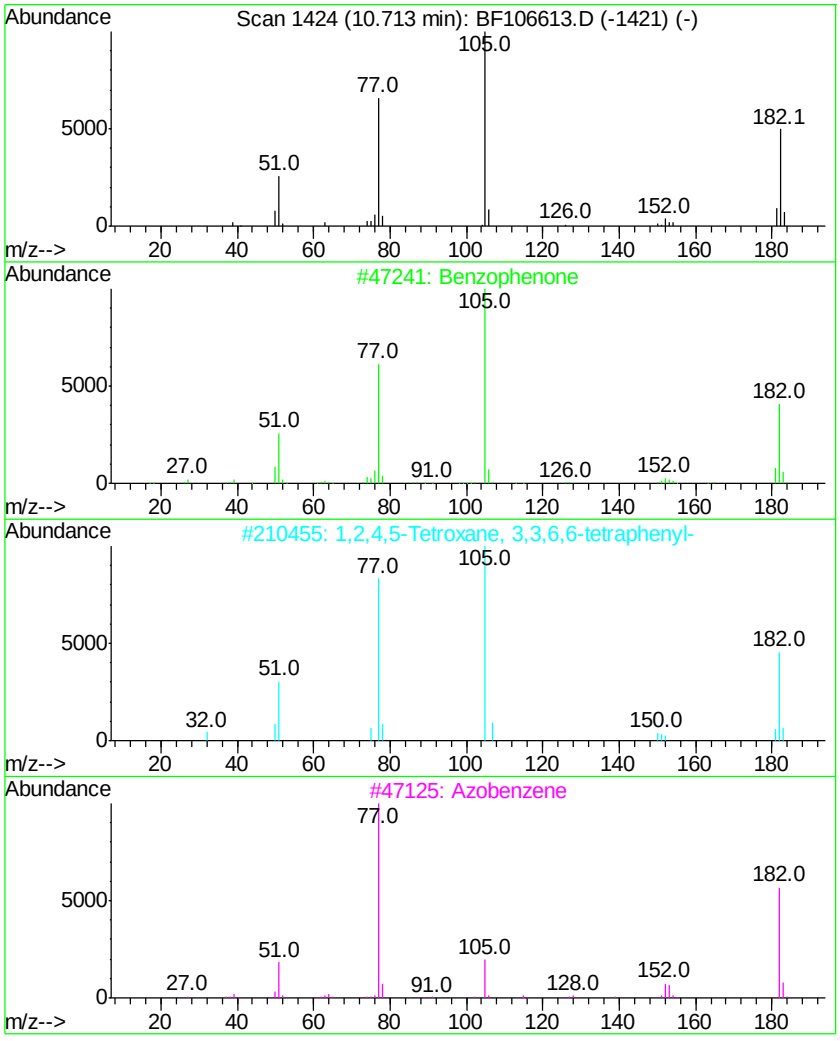
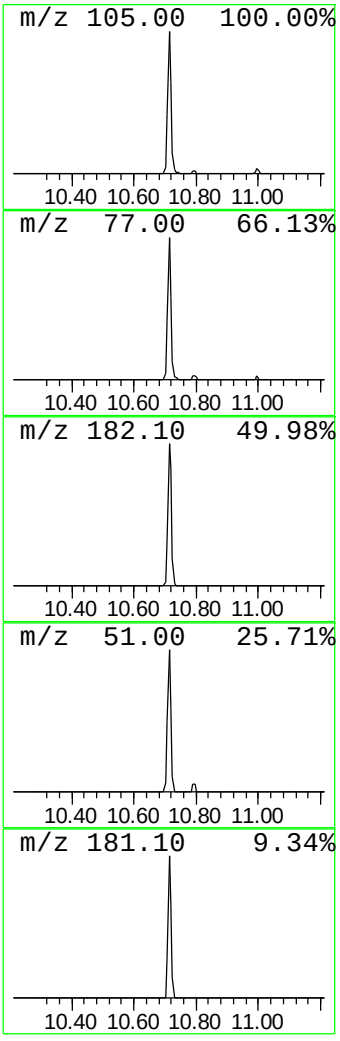
Peak Number 4 Benzophenone Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.71 | 2.67 ng | 82883 | Acenaphthene-d10 | 10.00 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 94 |
| 2 | 1,2,4,5-Tetroxane, 3,3,6,6-tetra... | 396 | C26H20O4 | 016204-36-7 | 78 |
| 3 | Azobenzene | 182 | C12H10N2 | 000103-33-3 | 59 |
| 4 | Benzoic acid, pentafluorophenyl ... | 288 | C13H5F5O2 | 1000360-67-9 | 47 |
| 5 | N-(1-Cyanovinyl)benzamide | 172 | C10H8N2O | 1000186-19-1 | 47 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106613.D
Acq On : 20 Jun 2018 5:52
Operator : JU/SJ
Sample : J3548-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 061318-DBRI-E-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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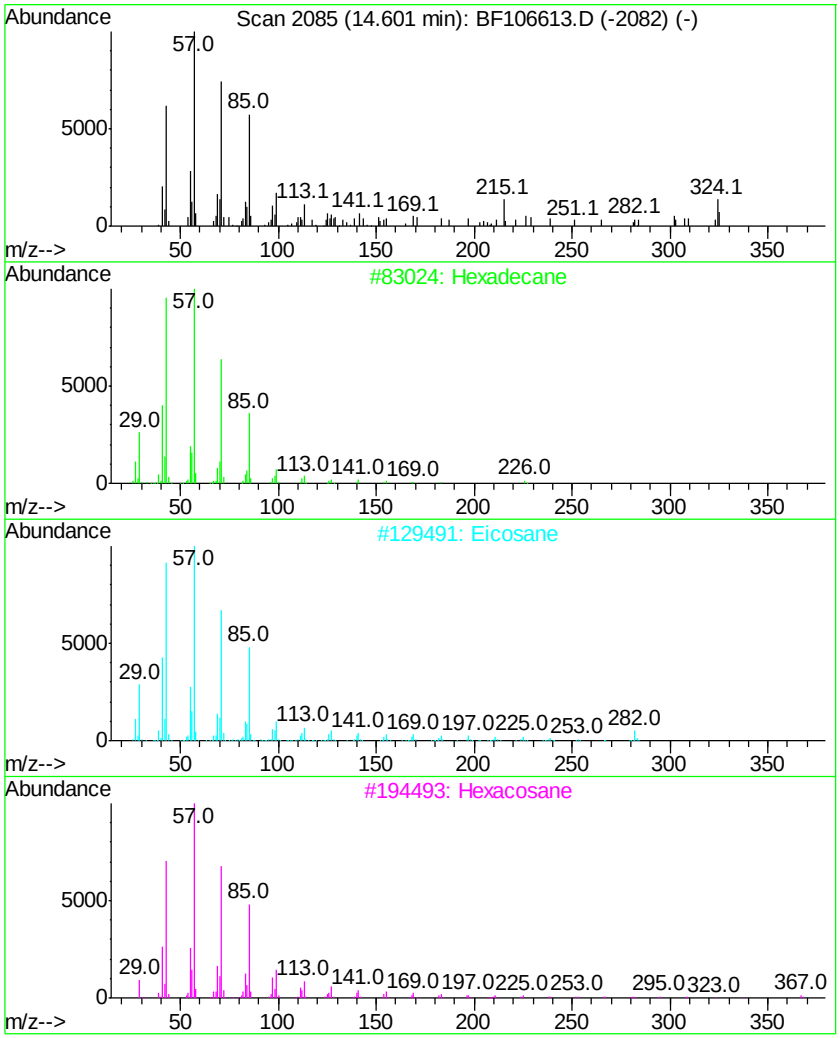
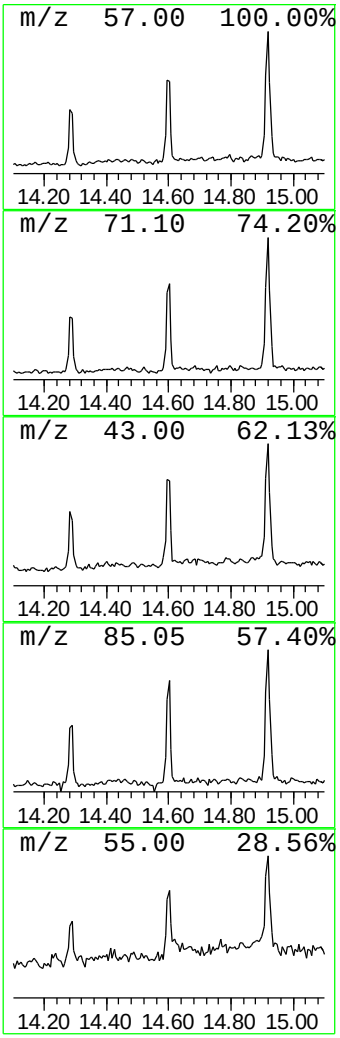
Peak Number 5 Hexadecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.60 | 2.39 ng | 81555 | Chrysene-d12 | 14.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 95 |
| 2 | Eicosane | 282 | C20H42 | 000112-95-8 | 80 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 76 |
| 4 | Octacosane | 394 | C28H58 | 000630-02-4 | 76 |
| 5 | Dodecane, 1-iodo- | 296 | C12H25I | 004292-19-7 | 68 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106613.D
Acq On : 20 Jun 2018 5:52
Operator : JU/SJ
Sample : J3548-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 061318-DBRI-E-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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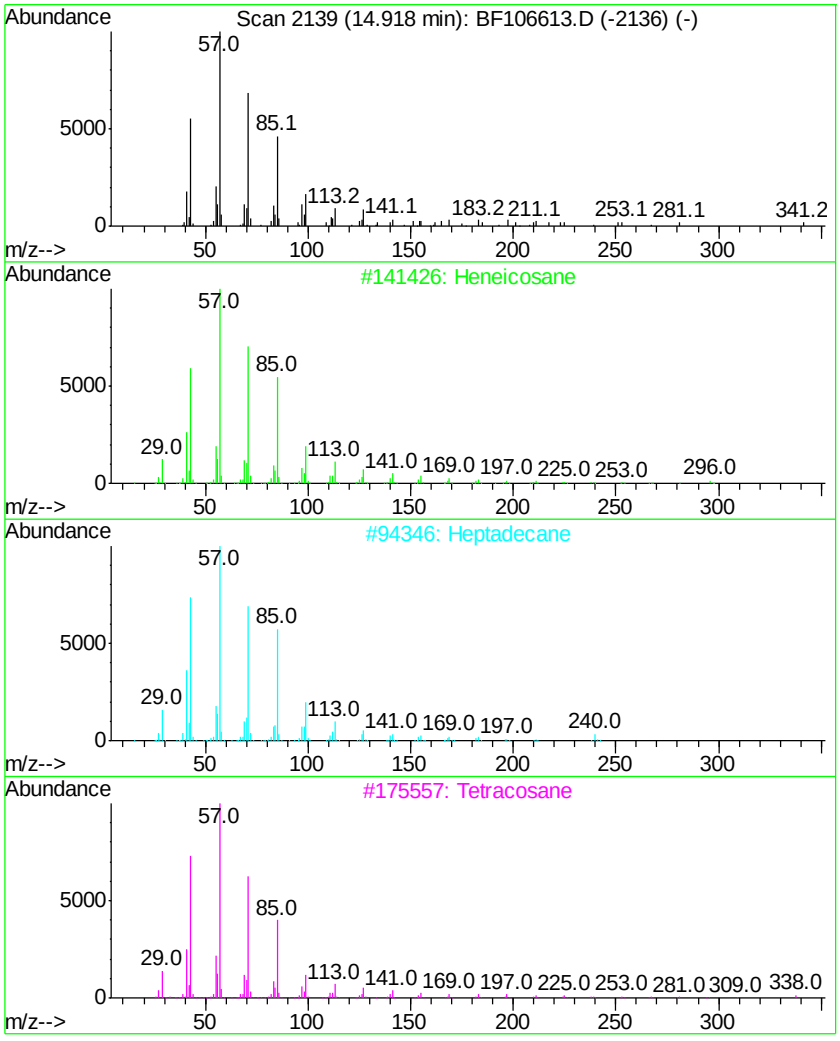
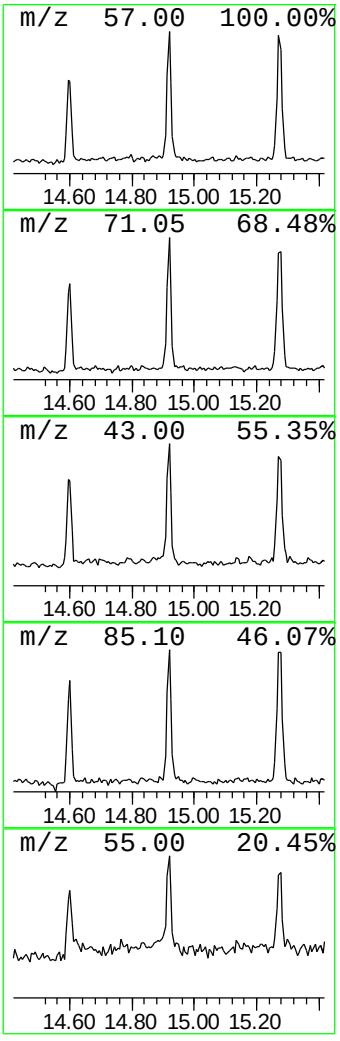
Peak Number 6 Heneicosane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.92 | 3.09 ng | 91473 | Perylene-d12 | 15.68 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 90 |
| 2 | Heptadecane | 240 | C17H36 | 000629-78-7 | 90 |
| 3 | Tetracosane | 338 | C24H50 | 000646-31-1 | 87 |
| 4 | Nonadecane | 268 | C19H40 | 000629-92-5 | 87 |
| 5 | Octacosane | 394 | C28H58 | 000630-02-4 | 87 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106613.D
Acq On : 20 Jun 2018 5:52
Operator : JU/SJ
Sample : J3548-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 061318-DBRI-E-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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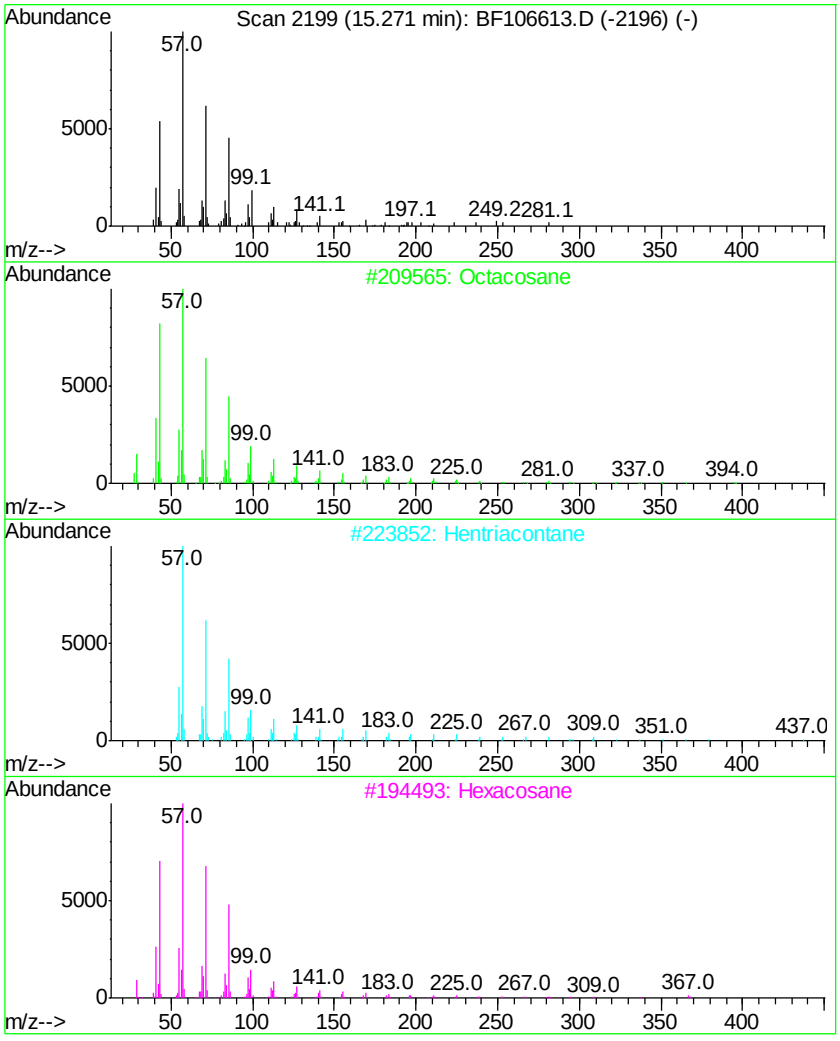
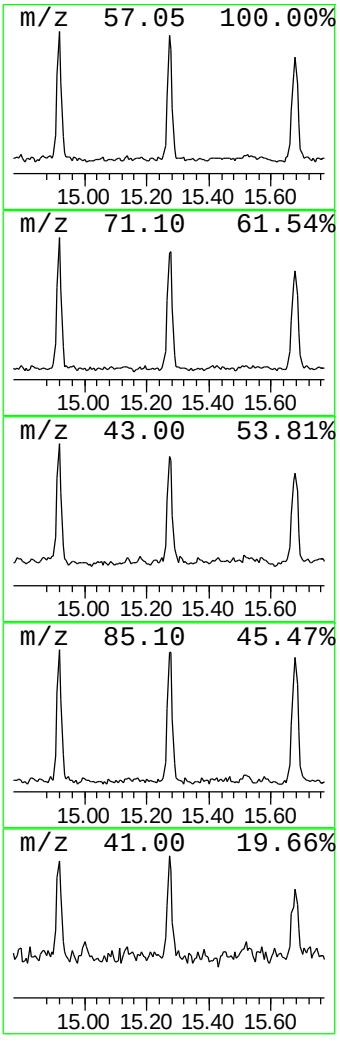
Peak Number 7 Octacosane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.27 | 3.14 ng | 92834 | Perylene-d12 | 15.68 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 2 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 91 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 4 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 90 |
| 5 | Heneicosane | 296 | C21H44 | 000629-94-7 | 90 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061918\
Data File : BF106613.D
Acq On : 20 Jun 2018 5:52
Operator : JU/SJ
Sample : J3548-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 061318-DBRI-E-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 5.20 | 2.4 | ng | 71471 | 1 | 6.96 | 602636 | 20.0 |
| Benzophenone | 10.71 | 2.7 | ng | 82883 | 3 | 10.00 | 620679 | 20.0 |
| Hexadecane | 14.60 | 2.4 | ng | 81555 | 5 | 14.15 | 682096 | 20.0 |
| Heneicosane | 14.92 | 3.1 | ng | 91473 | 6 | 15.68 | 591717 | 20.0 |
| Octacosane | 15.27 | 3.1 | ng | 92834 | 6 | 15.68 | 591717 | 20.0 |