LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102299.D
Acq On : 22 Jan 2018 15:09
Operator : SJ/JU
Sample : PB105837BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PB105837BL

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-BF012218.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 | 4.922 | 476 | 482 | 494 | rBV | 162358 | 239248 | 5.94% | 0.726% |
| 2 | 5.328 | 546 | 551 | 554 | rBV | 3030083 | 3251966 | 80.75% | 9.870% |
| 3 | 6.357 | 720 | 726 | 729 | rBV | 2973389 | 3170388 | 78.72% | 9.623% |
| 4 | 6.487 | 743 | 748 | 751 | rBV | 3154500 | 3355003 | 83.31% | 10.183% |
| 5 | 6.710 | 783 | 786 | 795 | rBV | 914821 | 786772 | 19.54% | 2.388% |
| 6 | 6.869 | 808 | 813 | 816 | rBV | 2878250 | 2616006 | 64.96% | 7.940% |
| 7 | 7.281 | 877 | 883 | 886 | rBV | 2035958 | 2120891 | 52.66% | 6.437% |
| 8 | 7.992 | 1000 | 1004 | 1022 | rVB | 1141456 | 1088425 | 27.03% | 3.304% |
| 9 | 9.075 | 1182 | 1188 | 1191 | rBV | 3536723 | 3908329 | 97.05% | 11.862% |
| 10 | 9.745 | 1297 | 1302 | 1311 | rBV2 | 1279338 | 1202787 | 29.87% | 3.651% |
| 11 | 10.539 | 1431 | 1437 | 1440 | rBV | 2243459 | 2242209 | 55.68% | 6.805% |
| 12 | 11.233 | 1550 | 1555 | 1558 | rBV | 1273199 | 1232834 | 30.61% | 3.742% |
| 13 | 12.821 | 1820 | 1825 | 1828 | rBV | 3858496 | 4027241 | 100.00% | 12.223% |
| 14 | 13.868 | 1998 | 2003 | 2006 | rBV | 1442540 | 1317772 | 32.72% | 4.000% |
| 15 | 14.633 | 2130 | 2133 | 2137 | rVB | 57129 | 53281 | 1.32% | 0.162% |
| 16 | 14.951 | 2183 | 2187 | 2192 | rBV | 99908 | 113777 | 2.83% | 0.345% |
| 17 | 15.292 | 2239 | 2245 | 2254 | rBV | 1045745 | 1451999 | 36.05% | 4.407% |
| 18 | 15.721 | 2313 | 2318 | 2324 | rVB | 144262 | 212907 | 5.29% | 0.646% |
| 19 | 16.192 | 2392 | 2398 | 2405 | rVB | 126567 | 222630 | 5.53% | 0.676% |
| 20 | 16.739 | 2485 | 2491 | 2502 | rVB | 76351 | 155822 | 3.87% | 0.473% |
| 21 | 17.392 | 2595 | 2602 | 2612 | rBV2 | 46237 | 115411 | 2.87% | 0.350% |
| 22 | 18.162 | 2726 | 2733 | 2742 | rVB5 | 22432 | 61891 | 1.54% | 0.188% |

Sum of corrected areas: 32947589

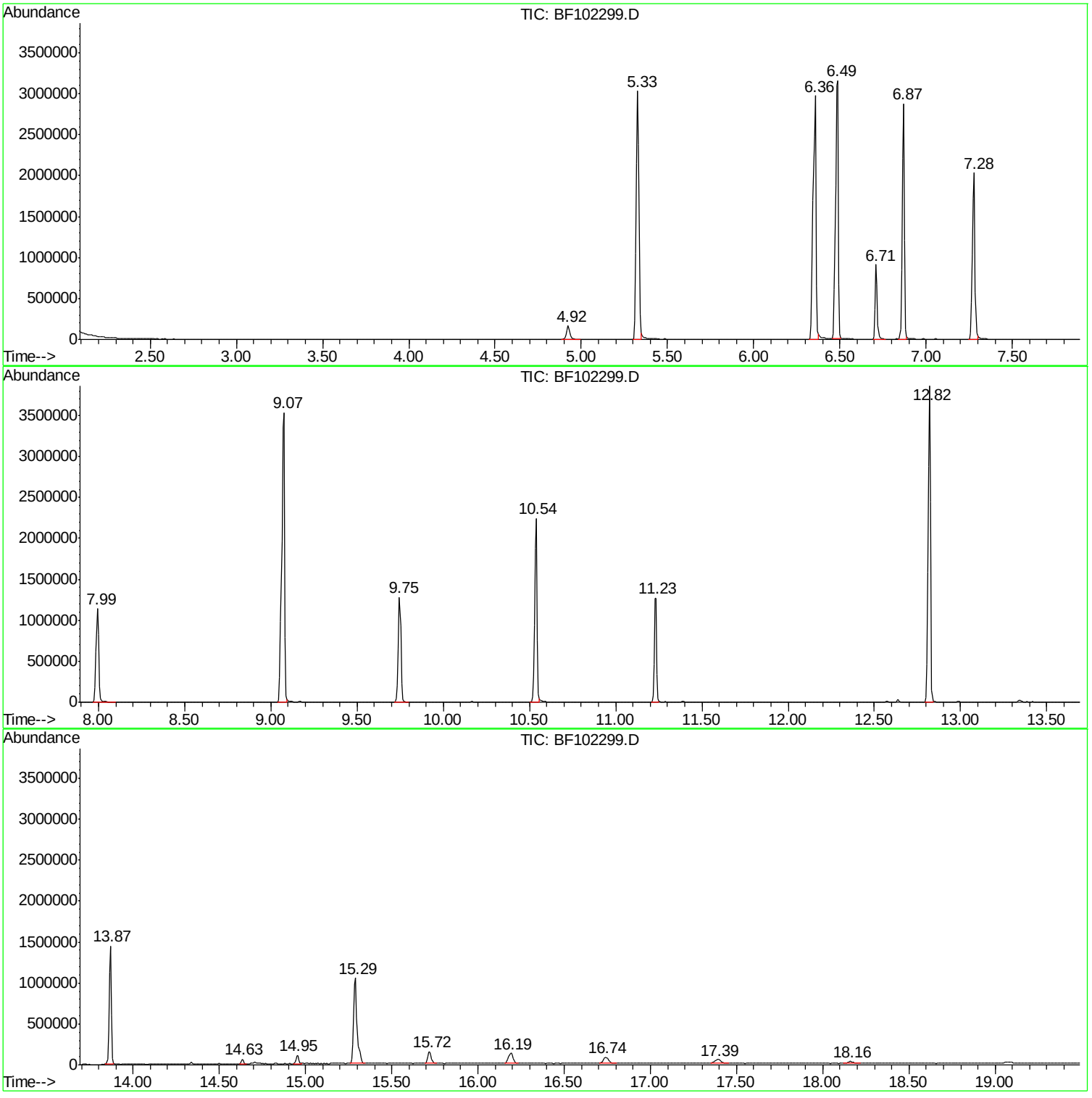
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102299.D
Acq On : 22 Jan 2018 15:09
Operator : SJ/JU
Sample : PB105837BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PB105837BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102299.D
Acq On : 22 Jan 2018 15:09
Operator : SJ/JU
Sample : PB105837BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PB105837BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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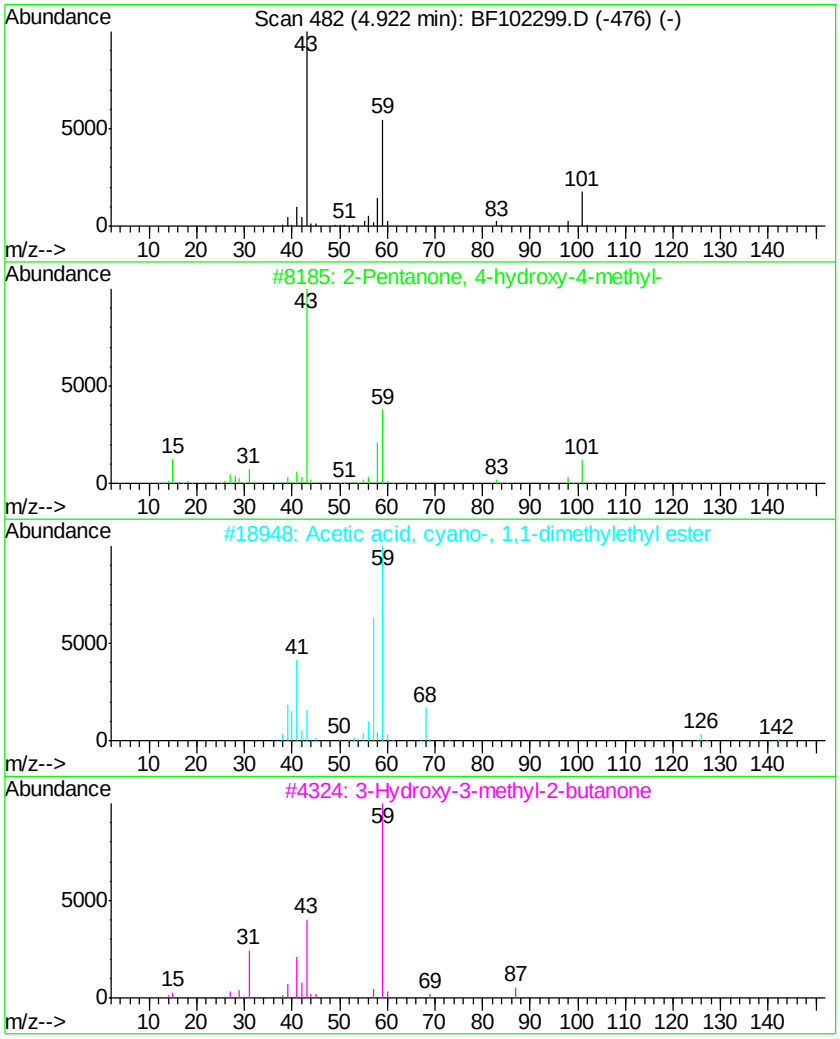
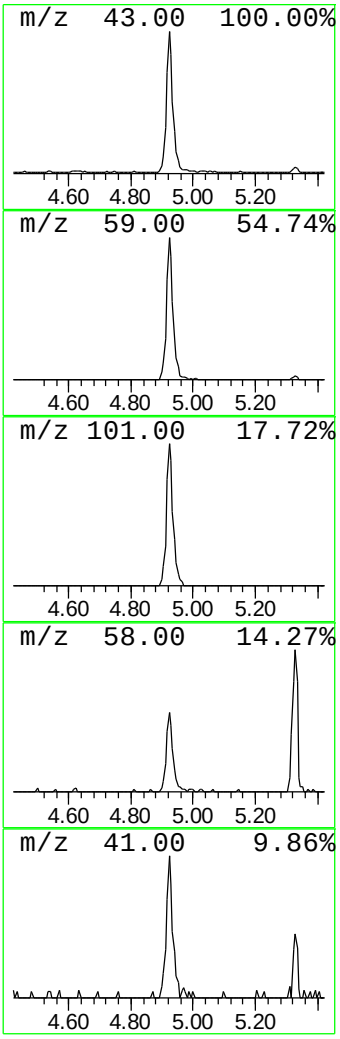
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.92 | 6.08 ng | 239248 | 1,4-Dichlorobenzene-d4 | 6.71 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 32 |
| 3 | 3-Hydroxy-3-methyl-2-butanone | 102 | C5H10O2 | 000115-22-0 | 23 |
| 4 | Propane, 1-ethoxy-2-methyl- | 102 | C6H14O | 000627-02-1 | 23 |
| 5 | Ethanone, 1-(2-methylcyclopropyl)- | 98 | C6H10O | 000930-56-3 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102299.D
Acq On : 22 Jan 2018 15:09
Operator : SJ/JU
Sample : PB105837BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PB105837BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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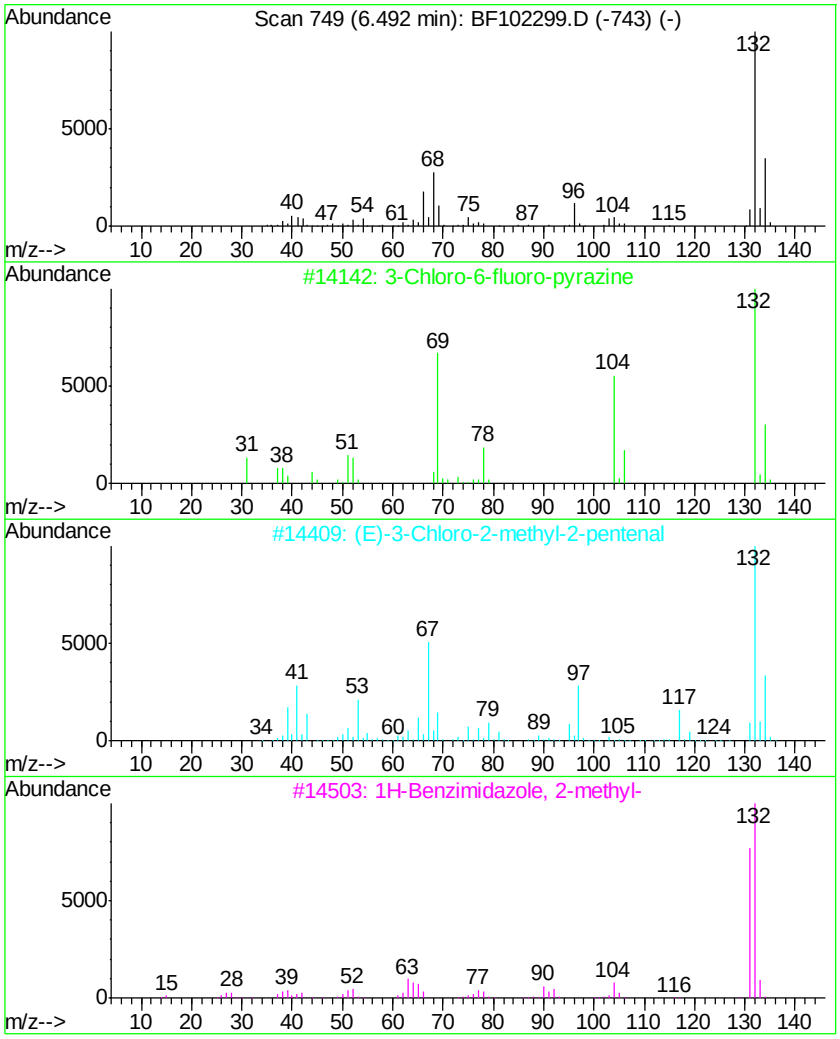
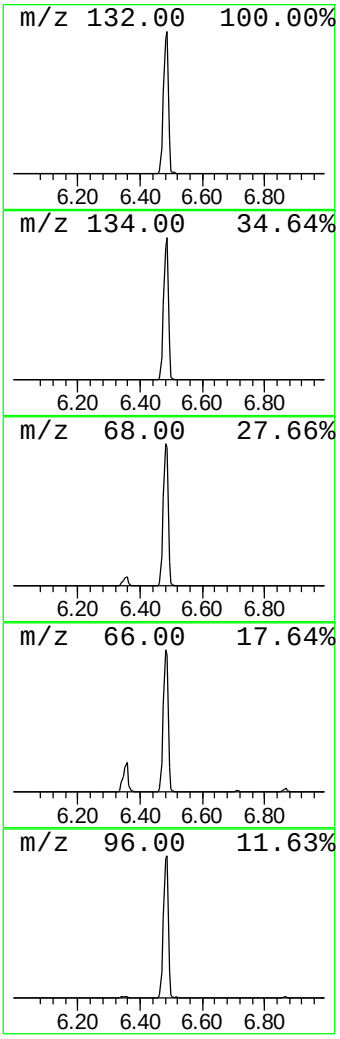
Peak Number 2 unknown6.49 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.49 | 85.29 ng | 3355000 | 1,4-Dichlorobenzene-d4 | 6.71 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 35 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 10 |
| 4 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 9 |
| 5 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102299.D
Acq On : 22 Jan 2018 15:09
Operator : SJ/JU
Sample : PB105837BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PB105837BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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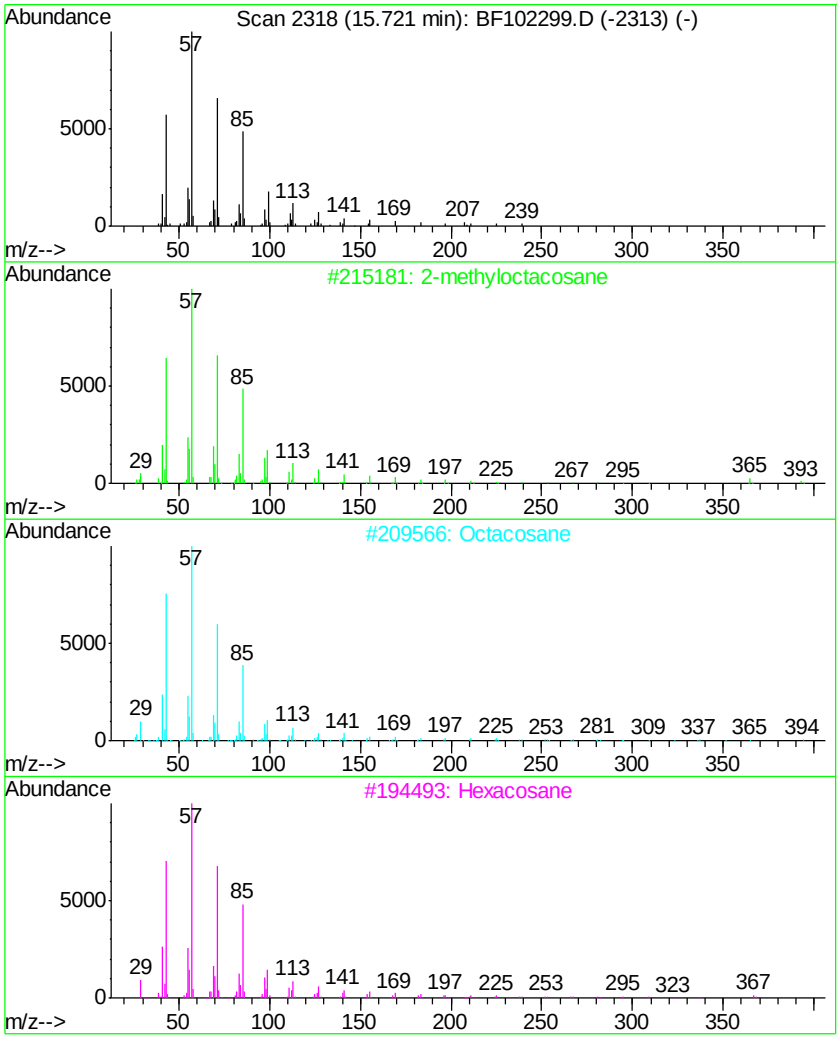
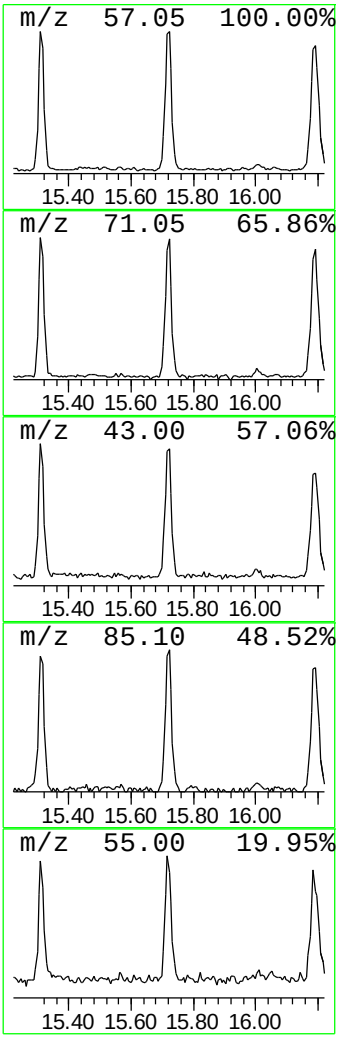
Peak Number 4 2-methyloctacosane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.72 | 2.93 ng | 212907 | Perylene-d12 | 15.29 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 91 |
| 2 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 4 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 5 | Triacontane | 422 | C30H62 | 000638-68-6 | 91 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102299.D
Acq On : 22 Jan 2018 15:09
Operator : SJ/JU
Sample : PB105837BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PB105837BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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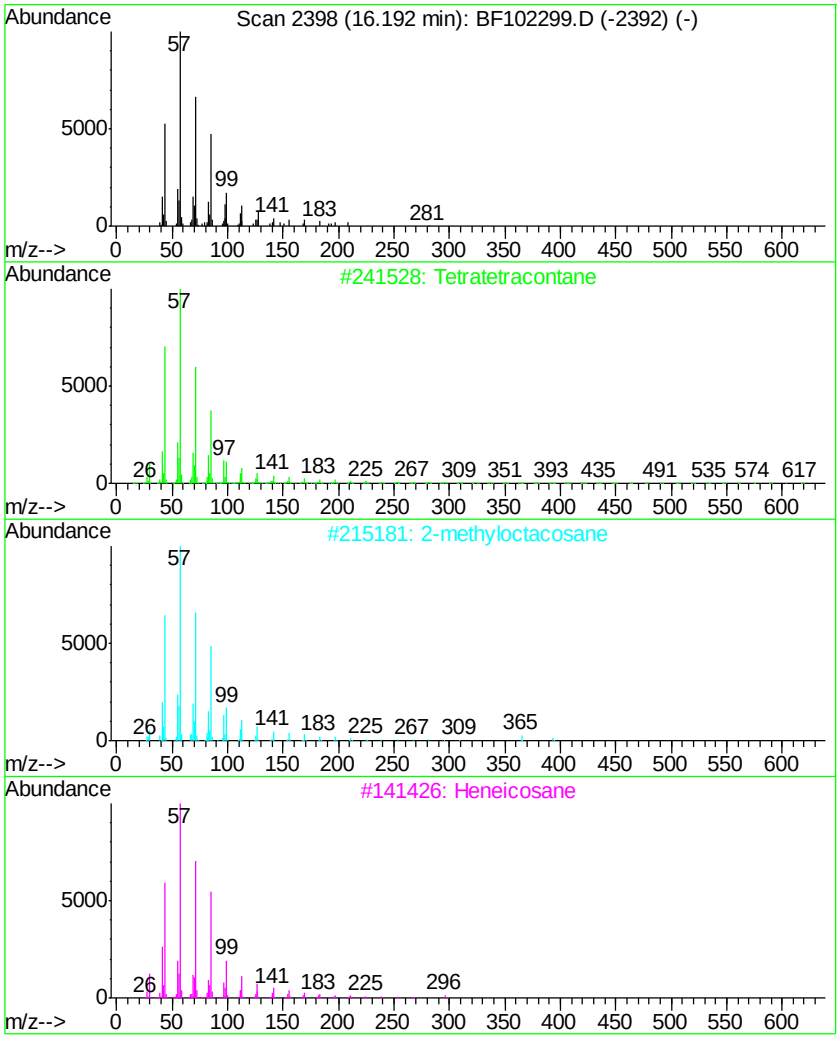
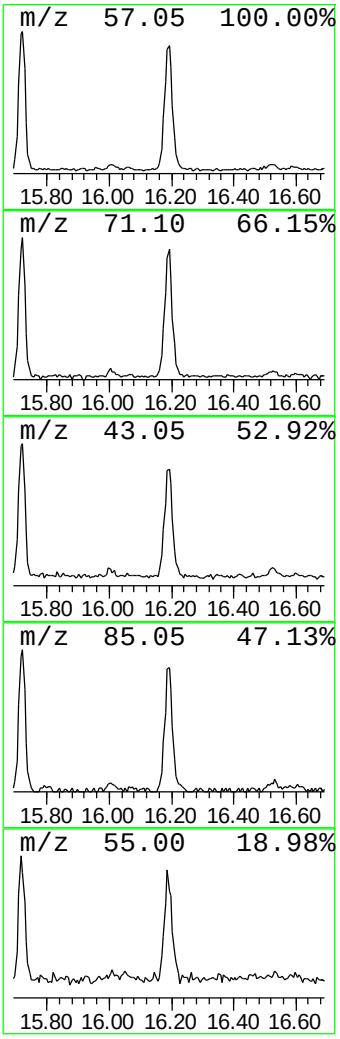
Peak Number 5 Tetratetracontane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.19 | 3.07 ng | 222630 | Perylene-d12 | 15.29 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 91 |
| 2 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 91 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 4 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 5 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102299.D
Acq On : 22 Jan 2018 15:09
Operator : SJ/JU
Sample : PB105837BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PB105837BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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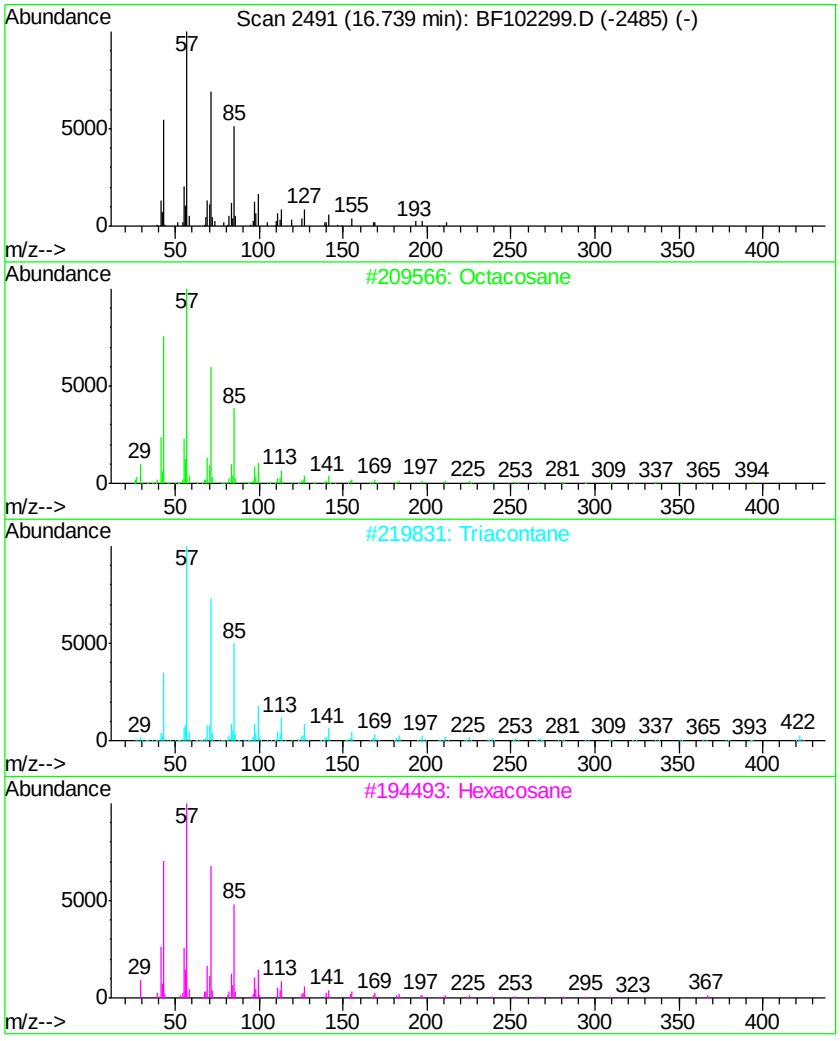
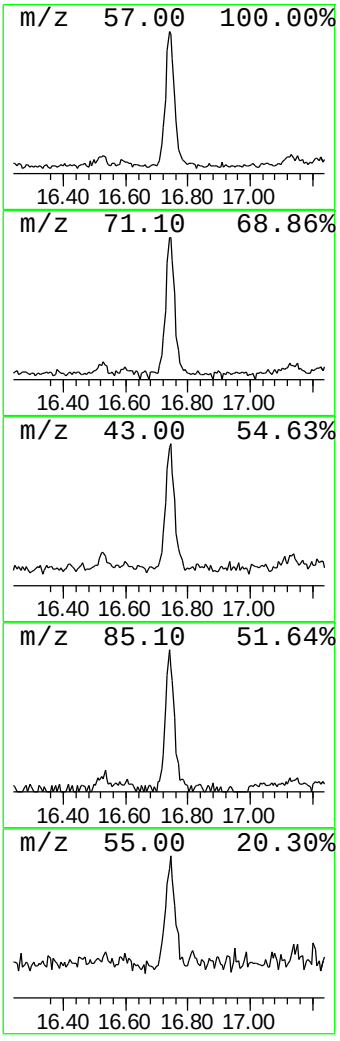
Peak Number 6 Octacosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.74 | 2.15 ng | 155822 | Perylene-d12 | 15.29 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 2 | Triacontane | 422 | C30H62 | 000638-68-6 | 90 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 86 |
| 4 | Docosane | 310 | C22H46 | 000629-97-0 | 86 |
| 5 | 10-Methylnonadecane | 282 | C20H42 | 056862-62-5 | 86 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012218\
Data File : BF102299.D
Acq On : 22 Jan 2018 15:09
Operator : SJ/JU
Sample : PB105837BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PB105837BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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... | 4.92 | 6.1 | ng | 239248 | 1 | 6.71 | 786772 | 20.0 |
| unknown6.49 | 6.49 | 85.3 | ng | 3355000 | 1 | 6.71 | 786772 | 20.0 |
| 2-methyloctacosane | 15.72 | 2.9 | ng | 212907 | 6 | 15.29 | 1452000 | 20.0 |
| Tetratetracontane | 16.19 | 3.1 | ng | 222630 | 6 | 15.29 | 1452000 | 20.0 |
| Octacosane | 16.74 | 2.1 | ng | 155822 | 6 | 15.29 | 1452000 | 20.0 |