LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040518\
Data File : BF104282.D
Acq On : 5 Apr 2018 21:00
Operator : JU/SJ
Sample : J2183-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** ES-4-DWS-2-NW@5

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-BF032818.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 | 2.281 | 29 | 33 | 47 | rVB | 142359 | 236115 | 6.05% | 0.743% |
| 2 | 5.198 | 525 | 529 | 539 | rBV | 50334 | 102182 | 2.62% | 0.321% |
| 3 | 5.581 | 591 | 594 | 629 | rBV | 1321909 | 2852465 | 73.04% | 8.974% |
| 4 | 6.581 | 761 | 764 | 784 | rBV | 1435704 | 3075126 | 78.74% | 9.675% |
| 5 | 6.716 | 784 | 787 | 823 | rVV | 2148068 | 3841317 | 98.36% | 12.086% |
| 6 | 6.951 | 823 | 827 | 848 | rVV | 204040 | 698499 | 17.89% | 2.198% |
| 7 | 7.098 | 848 | 852 | 881 | rVB | 1629180 | 2523081 | 64.60% | 7.938% |
| 8 | 7.510 | 919 | 922 | 945 | rBV | 881217 | 1977303 | 50.63% | 6.221% |
| 9 | 8.228 | 1040 | 1044 | 1070 | rBV | 438293 | 948477 | 24.29% | 2.984% |
| 10 | 9.298 | 1221 | 1226 | 1259 | rBV | 2609353 | 3905411 | 100.00% | 12.287% |
| 11 | 9.686 | 1287 | 1292 | 1299 | rBV | 232891 | 303623 | 7.77% | 0.955% |
| 12 | 9.886 | 1323 | 1326 | 1330 | rBV | 67104 | 58160 | 1.49% | 0.183% |
| 13 | 9.980 | 1338 | 1342 | 1362 | rBV | 887283 | 1112977 | 28.50% | 3.502% |
| 14 | 10.386 | 1409 | 1411 | 1414 | rVB | 91981 | 67034 | 1.72% | 0.211% |
| 15 | 10.780 | 1474 | 1478 | 1489 | rBV | 1590040 | 2401461 | 61.49% | 7.555% |
| 16 | 10.857 | 1489 | 1491 | 1501 | rVB | 121101 | 202347 | 5.18% | 0.637% |
| 17 | 11.310 | 1564 | 1568 | 1570 | rBV | 46614 | 42008 | 1.08% | 0.132% |
| 18 | 11.480 | 1593 | 1597 | 1618 | rBV | 653819 | 1143414 | 29.28% | 3.597% |
| 19 | 11.980 | 1679 | 1682 | 1693 | rBV4 | 56595 | 93677 | 2.40% | 0.295% |
| 20 | 13.063 | 1861 | 1866 | 1888 | rBV | 2776897 | 3576194 | 91.57% | 11.251% |
| 21 | 13.927 | 2010 | 2013 | 2028 | rBV | 411308 | 495935 | 12.70% | 1.560% |
| 22 | 14.133 | 2044 | 2048 | 2064 | rBV | 706499 | 1037327 | 26.56% | 3.264% |
| 23 | 14.574 | 2118 | 2123 | 2126 | rBV4 | 31044 | 43156 | 1.11% | 0.136% |
| 24 | 14.868 | 2169 | 2173 | 2185 | rBV | 173837 | 238877 | 6.12% | 0.752% |
| 25 | 15.662 | 2303 | 2308 | 2323 | rBV | 359395 | 739490 | 18.94% | 2.327% |
| 26 | 16.145 | 2384 | 2390 | 2396 | rBV6 | 31228 | 68624 | 1.76% | 0.216% |

Sum of corrected areas: 31784280

LSC Report - Integrated Chromatogram

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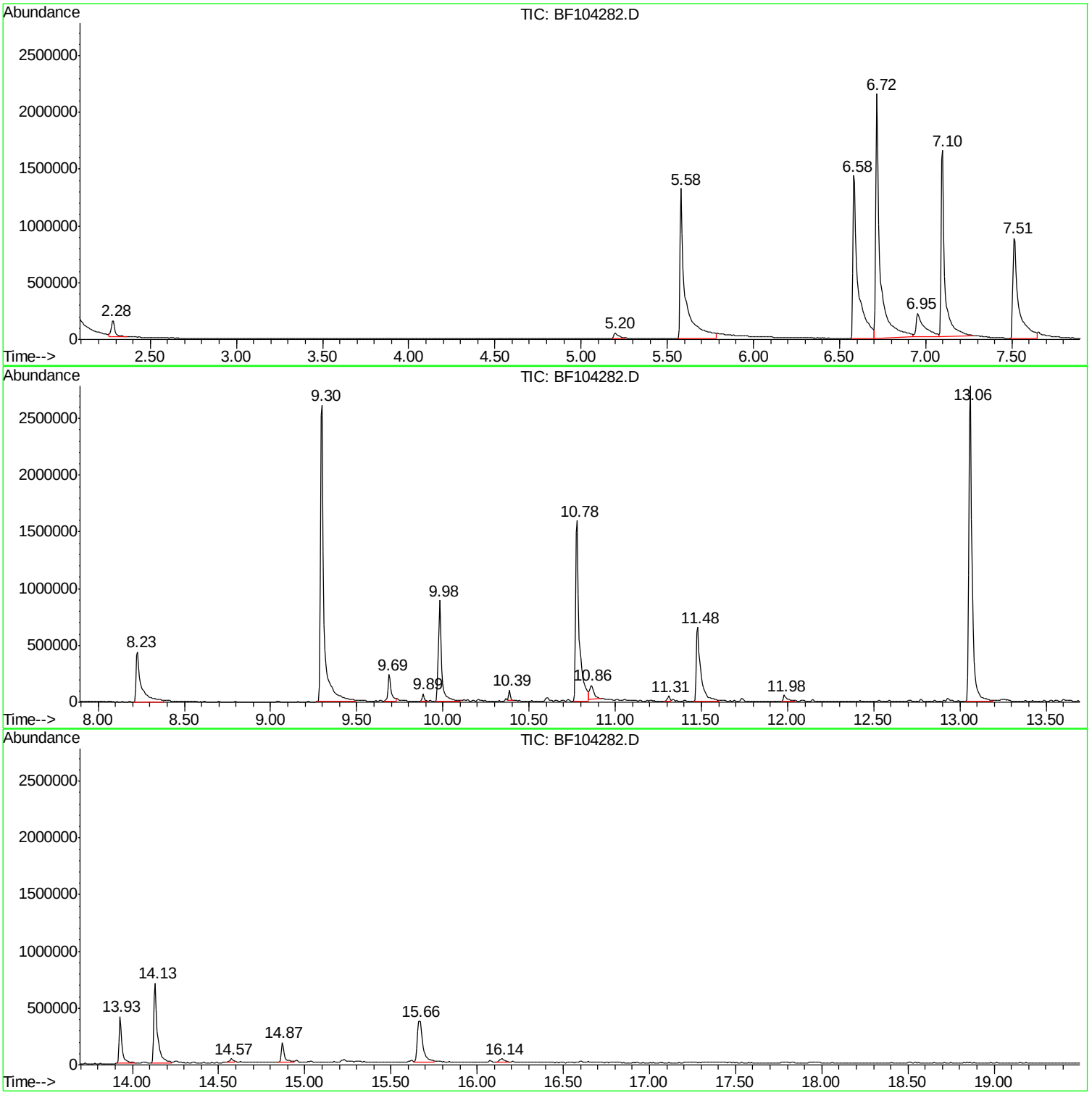
Data File : BF104282.D
Acq On : 5 Apr 2018 21:00
Operator : JU/SJ
Sample : J2183-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** ES-4-DWS-2-NW@5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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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Data File : BF104282.D
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Operator : JU/SJ
Sample : J2183-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** ES-4-DWS-2-NW@5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

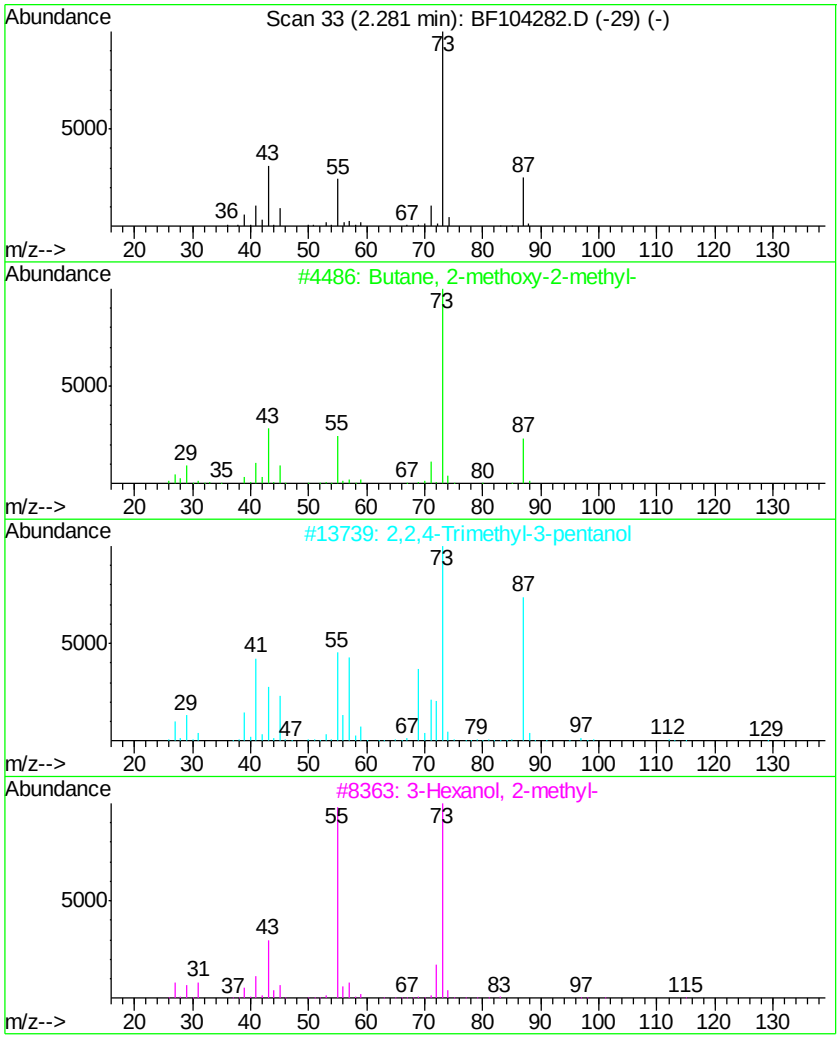
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

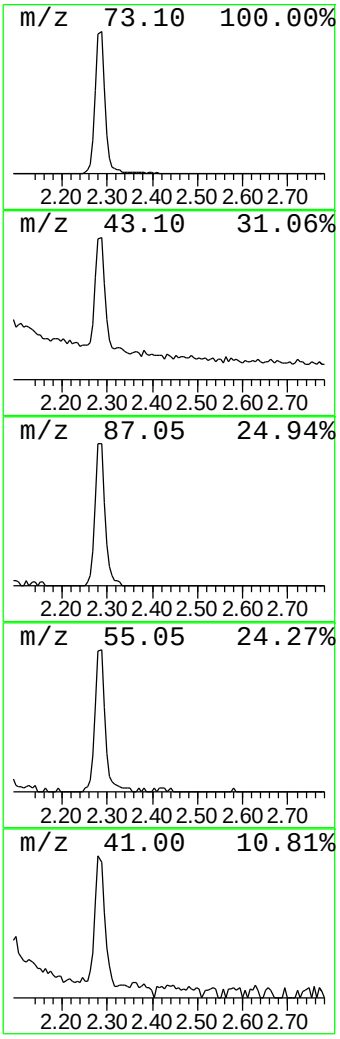
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.28 | 6.76 ng | 236115 | 1,4-Dichlorobenzene-d4 | 6.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 86 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 40 |
| 3 | 3-Hexanol, 2-methyl- | 116 | C7H16O | 000617-29-8 | 17 |
| 4 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 17 |
| 5 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 12 |



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Data File : BF104282.D
Acq On : 5 Apr 2018 21:00
Operator : JU/SJ
Sample : J2183-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** ES-4-DWS-2-NW@5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

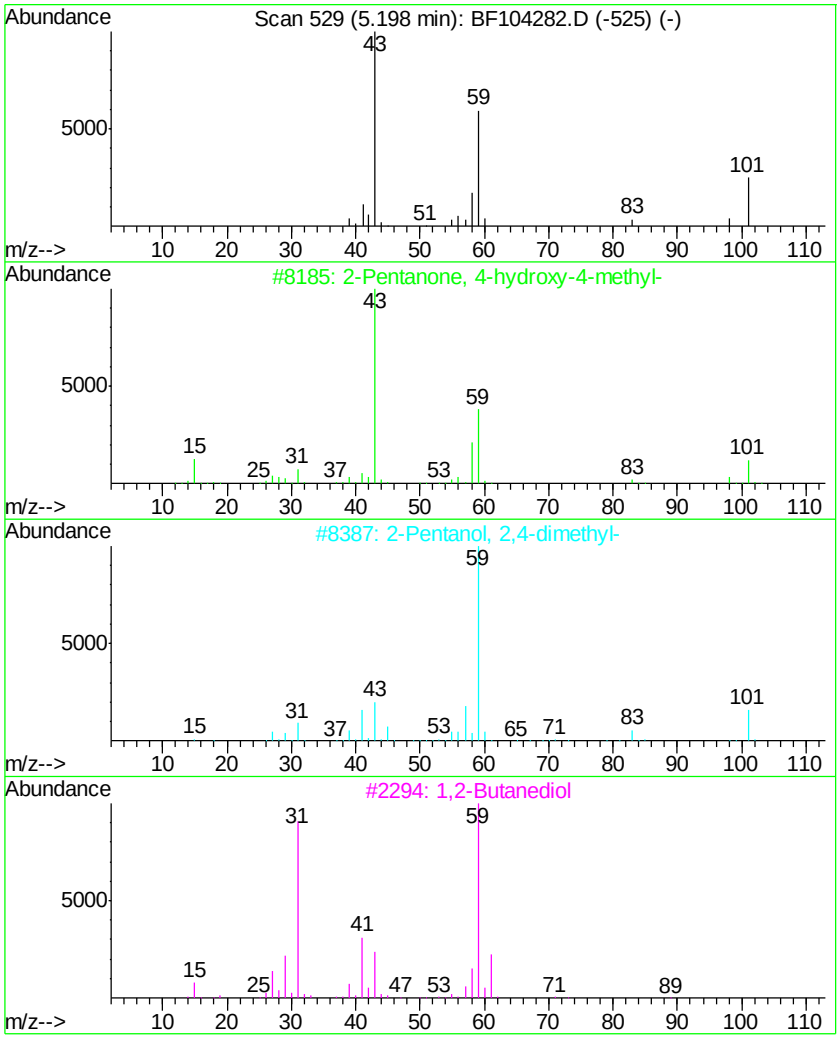
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

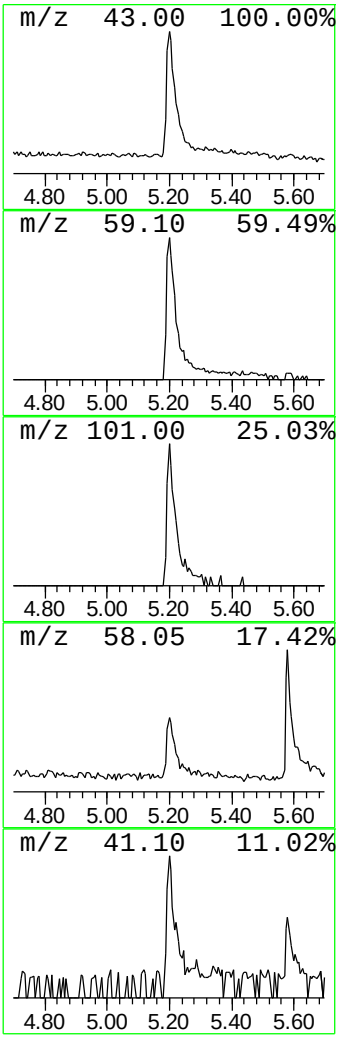
**********

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.20 | 2.93 ng | 102182 | 1,4-Dichlorobenzene-d4 | 6.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | 2-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000625-06-9 | 42 |
| 3 | 1,2-Butanediol | 90 | C4H10O2 | 000584-03-2 | 25 |
| 4 | Acetone | 58 | C3H6O | 000067-64-1 | 9 |
| 5 | 1-Butanol, 3-methoxy- | 104 | C5H12O2 | 002517-43-3 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040518\
Data File : BF104282.D
Acq On : 5 Apr 2018 21:00
Operator : JU/SJ
Sample : J2183-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** ES-4-DWS-2-NW@5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

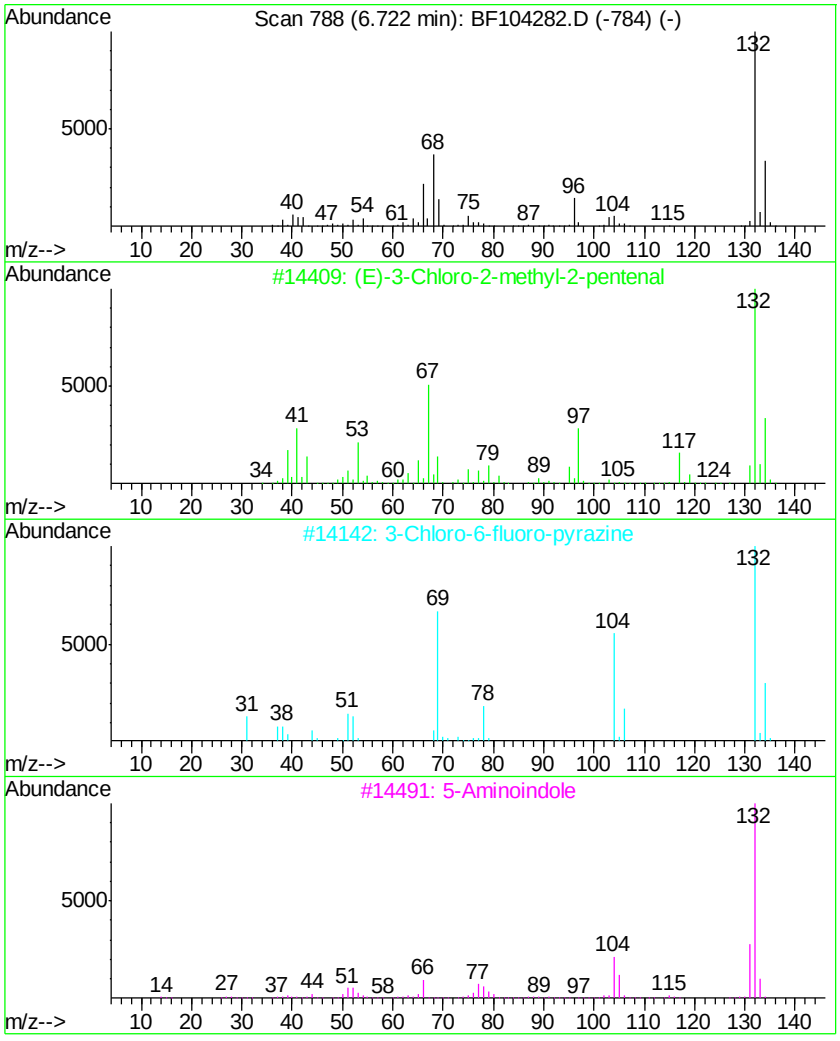
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

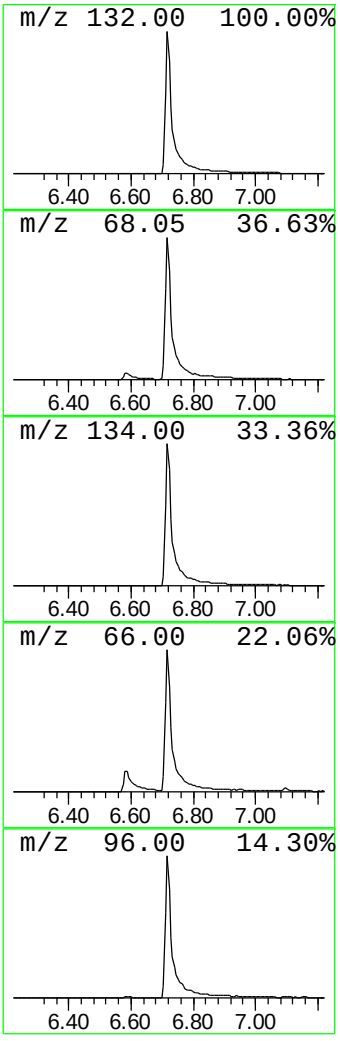
**********

Peak Number 3 unknown6.72 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.72 | 109.99 ng | 3841320 | 1,4-Dichlorobenzene-d4 | 6.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 2 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 16 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 10 |
| 5 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040518\
Data File : BF104282.D
Acq On : 5 Apr 2018 21:00
Operator : JU/SJ
Sample : J2183-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** ES-4-DWS-2-NW@5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

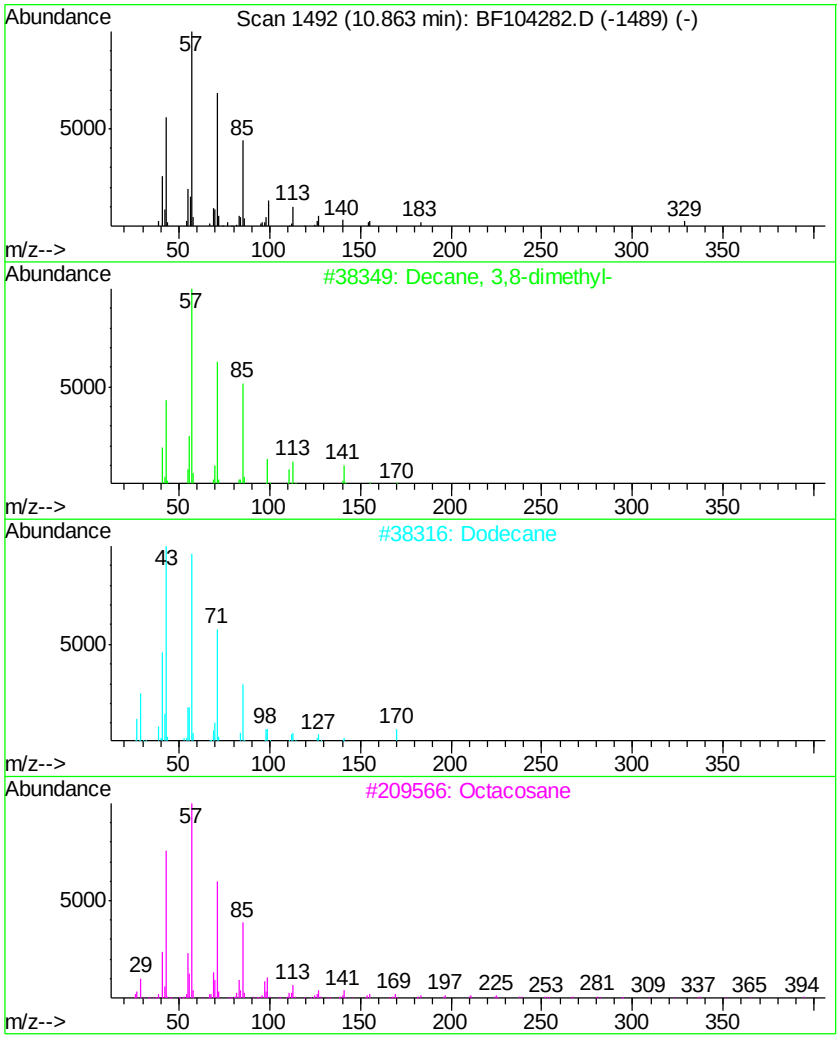
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

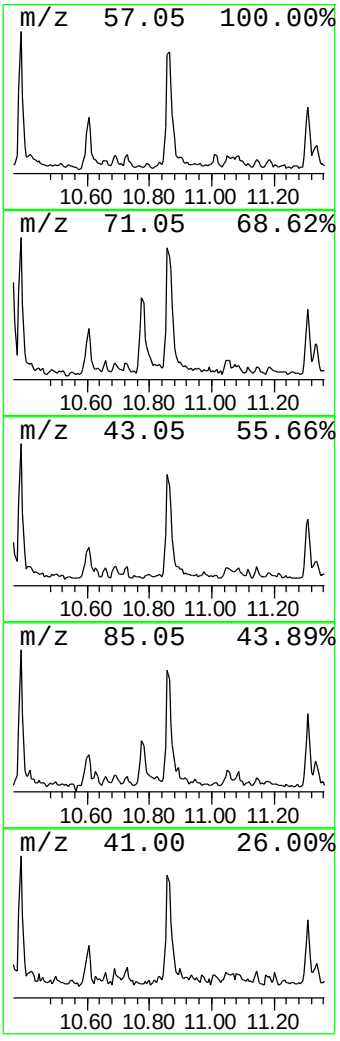
**********

Peak Number 5 Decane, 3,8-dimethyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.86 | 3.54 ng | 202347 | Phenanthrene-d10 | 11.48 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Decane, 3,8-dimethyl- | 170 | C12H26 | 017312-55-9 | 87 |
| 2 | Dodecane | 170 | C12H26 | 000112-40-3 | 87 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 86 |
| 4 | Dodecane, 1-iodo- | 296 | C12H25I | 004292-19-7 | 86 |
| 5 | Undecane, 5-methyl- | 170 | C12H26 | 001632-70-8 | 83 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040518\
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Acq On : 5 Apr 2018 21:00
Operator : JU/SJ
Sample : J2183-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** ES-4-DWS-2-NW@5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

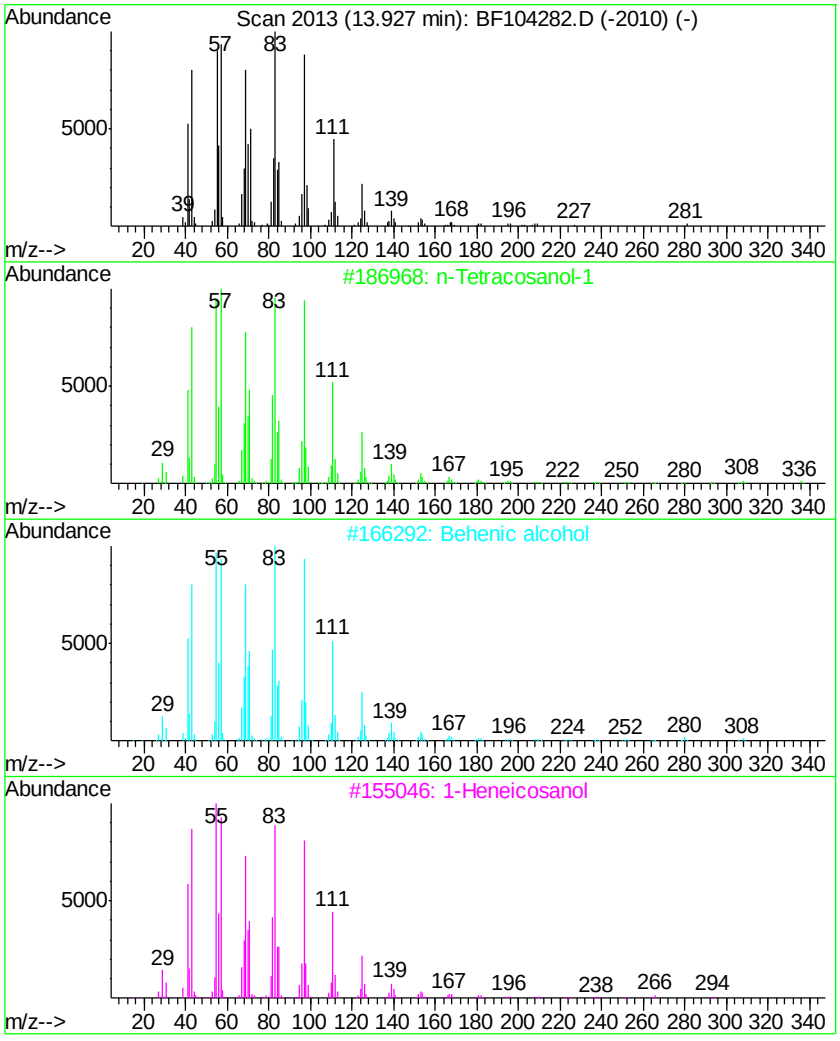
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

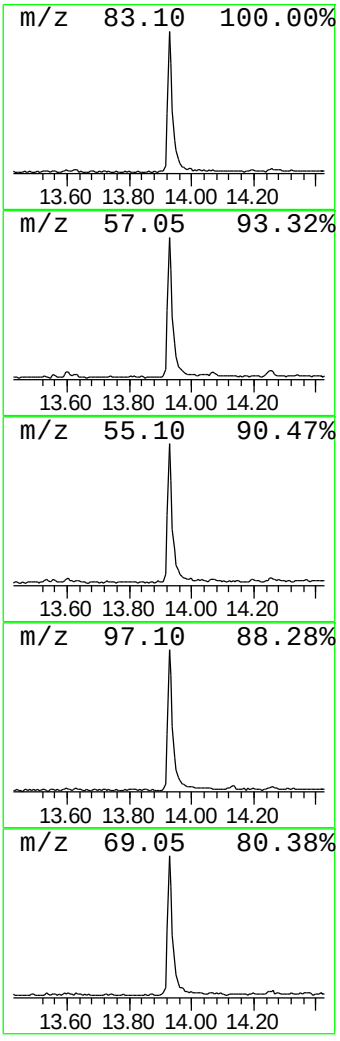
**********

Peak Number 6 n-Tetracosanol-1 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.93 | 9.56 ng | 495935 | Chrysene-d12 | 14.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 95 |
| 2 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 95 |
| 3 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 95 |
| 4 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 95 |
| 5 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 94 |



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Sample : J2183-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** ES-4-DWS-2-NW@5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

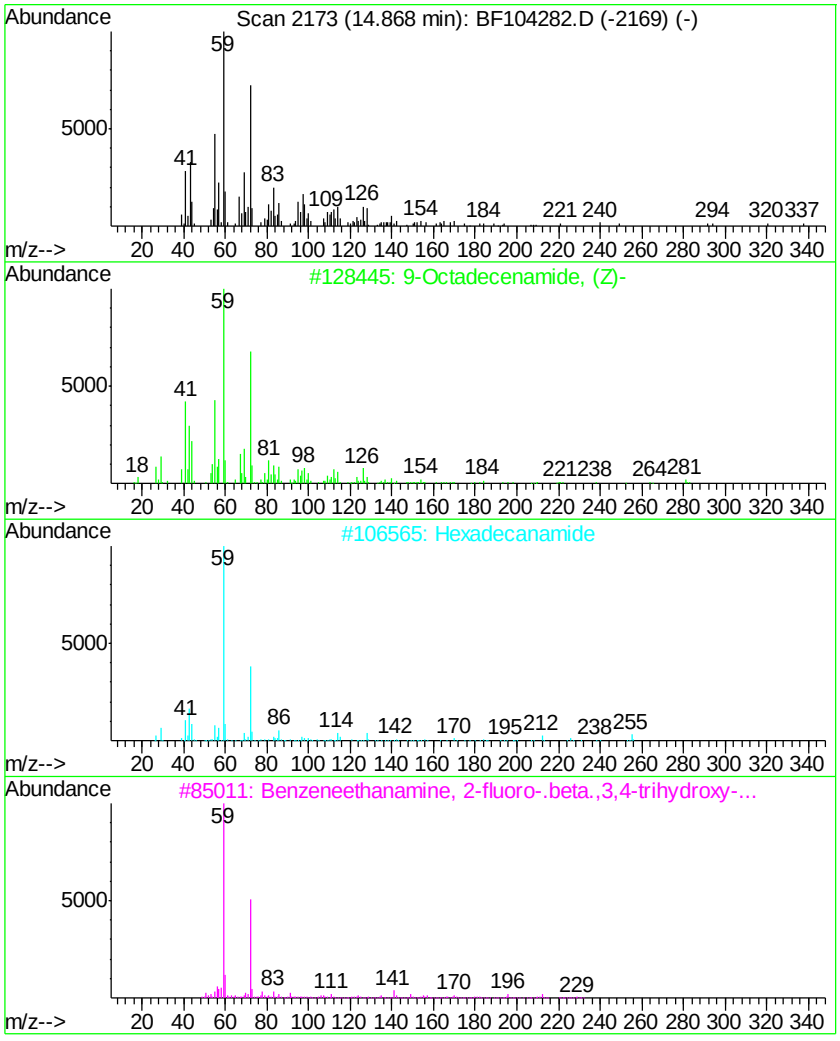
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

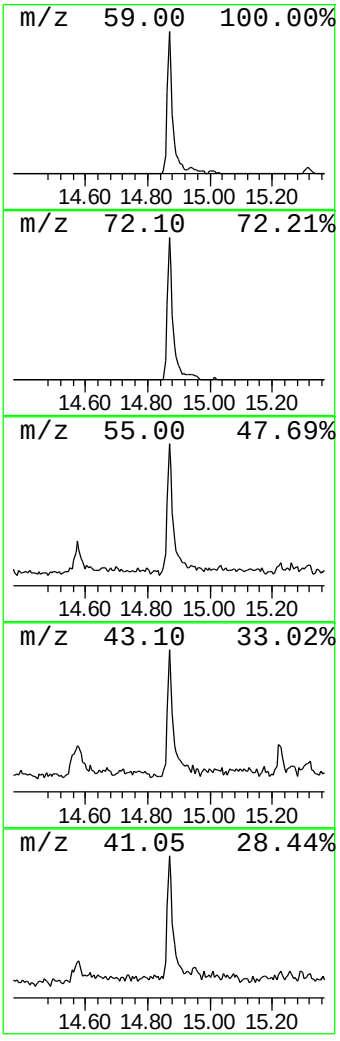
**********

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.87 | 4.61 ng | 238877 | Chrysene-d12 | 14.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 83 |
| 2 | Hexadecanamide | 255 | C16H33NO | 000629-54-9 | 53 |
| 3 | Benzeneethanamine, 2-fluoro-.bet... | 229 | C11H16FNO3 | 061338-98-5 | 47 |
| 4 | Octadecanamide | 283 | C18H37NO | 000124-26-5 | 43 |
| 5 | 1,1,2-Trimethyl-1-silacyclobutane | 114 | C6H14Si | 030681-90-4 | 30 |



# Tentatively Identified Compound (LSC) summary

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Misc :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.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 |
| Butane, 2-methoxy... | 2.28 | 6.8 | ng | 236115 | 1 | 6.95 | 698499 | 20.0 |
| 2-Pentanone, 4-hy... | 5.20 | 2.9 | ng | 102182 | 1 | 6.95 | 698499 | 20.0 |
| unknown6.72 | 6.72 | 110.0 | ng | 3841320 | 1 | 6.95 | 698499 | 20.0 |
| Decane, 3,8-dimet... | 10.86 | 3.5 | ng | 202347 | 4 | 11.48 | 1143410 | 20.0 |
| n-Tetracosanol-1 | 13.93 | 9.6 | ng | 495935 | 5 | 14.13 | 1037330 | 20.0 |
| 9-Octadecenamide,... | 14.87 | 4.6 | ng | 238877 | 5 | 14.13 | 1037330 | 20.0 |