LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030918\
Data File : BF103567.D
Acq On : 9 Mar 2018 19:47
Operator : SJ/JU
Sample : J1821-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-4-5-20180205

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-BF022218.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 | 5.098 | 509 | 512 | 528 | rBV | 73180 | 129648 | 4.11% | 0.468% |
| 2 | 5.493 | 576 | 579 | 614 | rBV | 1913207 | 3057788 | 96.96% | 11.040% |
| 3 | 6.151 | 686 | 691 | 694 | rBV3 | 36468 | 70687 | 2.24% | 0.255% |
| 4 | 6.504 | 748 | 751 | 770 | rBV | 1947235 | 3153768 | 100.00% | 11.386% |
| 5 | 6.640 | 770 | 774 | 784 | rVV | 2616191 | 2957290 | 93.77% | 10.677% |
| 6 | 6.716 | 784 | 787 | 797 | rVV | 81471 | 269794 | 8.55% | 0.974% |
| 7 | 6.787 | 797 | 799 | 809 | rVV2 | 45289 | 118150 | 3.75% | 0.427% |
| 8 | 6.863 | 809 | 812 | 831 | rVV | 753801 | 914128 | 28.99% | 3.300% |
| 9 | 7.022 | 835 | 839 | 854 | rBV | 1518408 | 1720118 | 54.54% | 6.210% |
| 10 | 7.434 | 905 | 909 | 933 | rBV | 1152604 | 1836084 | 58.22% | 6.629% |
| 11 | 7.587 | 933 | 935 | 945 | rVB | 32682 | 45224 | 1.43% | 0.163% |
| 12 | 8.151 | 1027 | 1031 | 1056 | rVV | 726446 | 1166452 | 36.99% | 4.211% |
| 13 | 8.522 | 1088 | 1094 | 1102 | rBV3 | 16838 | 48568 | 1.54% | 0.175% |
| 14 | 9.028 | 1176 | 1180 | 1182 | rBV | 37666 | 45200 | 1.43% | 0.163% |
| 15 | 9.086 | 1186 | 1190 | 1199 | rVB | 233082 | 254608 | 8.07% | 0.919% |
| 16 | 9.222 | 1206 | 1213 | 1223 | rBV | 1983620 | 2410929 | 76.45% | 8.704% |
| 17 | 9.398 | 1239 | 1243 | 1254 | rBV | 71383 | 155196 | 4.92% | 0.560% |
| 18 | 9.622 | 1274 | 1281 | 1287 | rBV5 | 16449 | 39034 | 1.24% | 0.141% |
| 19 | 9.704 | 1291 | 1295 | 1302 | rBV | 56895 | 77667 | 2.46% | 0.280% |
| 20 | 9.816 | 1311 | 1314 | 1318 | rVB | 36339 | 33111 | 1.05% | 0.120% |
| 21 | 9.904 | 1326 | 1329 | 1342 | rBV | 945803 | 1077741 | 34.17% | 3.891% |
| 22 | 10.292 | 1392 | 1395 | 1397 | rBV | 92055 | 77535 | 2.46% | 0.280% |
| 23 | 10.316 | 1397 | 1399 | 1402 | rVB | 120186 | 94462 | 3.00% | 0.341% |
| 24 | 10.704 | 1461 | 1465 | 1477 | rBV | 925105 | 1233434 | 39.11% | 4.453% |
| 25 | 10.792 | 1477 | 1480 | 1488 | rVB2 | 51127 | 74817 | 2.37% | 0.270% |
| 26 | 10.898 | 1495 | 1498 | 1503 | rVB | 49527 | 44967 | 1.43% | 0.162% |
| 27 | 11.239 | 1552 | 1556 | 1558 | rBV2 | 36923 | 39391 | 1.25% | 0.142% |
| 28 | 11.404 | 1580 | 1584 | 1596 | rBV | 701091 | 897208 | 28.45% | 3.239% |
| 29 | 11.545 | 1605 | 1608 | 1612 | rBV | 360961 | 317402 | 10.06% | 1.146% |
| 30 | 11.610 | 1615 | 1619 | 1623 | rVB5 | 25658 | 36935 | 1.17% | 0.133% |
| 31 | 11.945 | 1672 | 1676 | 1680 | rBV | 2184487 | 2089977 | 66.27% | 7.546% |
| 32 | 12.074 | 1695 | 1698 | 1700 | rBV | 40206 | 33792 | 1.07% | 0.122% |
| 33 | 12.157 | 1710 | 1712 | 1719 | rVB3 | 36714 | 31861 | 1.01% | 0.115% |
| 34 | 12.463 | 1761 | 1764 | 1768 | rVB | 47841 | 38087 | 1.21% | 0.138% |

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030918\
Data File : BF103567.D
Acq On : 9 Mar 2018 19:47
Operator : SJ/JU
Sample : J1821-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-4-5-20180205

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-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 12.839 | 1825 | 1828 | 1830 | rBV | 45533 | 44178 | 1.40% | 0.159% |
| 36 | 12.863 | 1830 | 1832 | 1840 | rVB3 | 33597 | 38618 | 1.22% | 0.139% |
| 37 | 12.986 | 1849 | 1853 | 1864 | rBV | 1427803 | 1449056 | 45.95% | 5.232% |
| 38 | 13.192 | 1884 | 1888 | 1892 | rVB | 48243 | 43234 | 1.37% | 0.156% |
| 39 | 13.533 | 1943 | 1946 | 1949 | rBV | 36591 | 35522 | 1.13% | 0.128% |
| 40 | 13.868 | 1999 | 2003 | 2013 | rBV | 85583 | 130347 | 4.13% | 0.471% |
| 41 | 14.004 | 2023 | 2026 | 2031 | rBV | 58690 | 50363 | 1.60% | 0.182% |
| 42 | 14.063 | 2032 | 2036 | 2045 | rBV | 595653 | 729887 | 23.14% | 2.635% |
| 43 | 14.492 | 2106 | 2109 | 2115 | rBV4 | 26958 | 39400 | 1.25% | 0.142% |
| 44 | 15.574 | 2288 | 2293 | 2304 | rVB | 320448 | 546237 | 17.32% | 1.972% |

Sum of corrected areas: 27697895

LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030918\
Data File : BF103567.D
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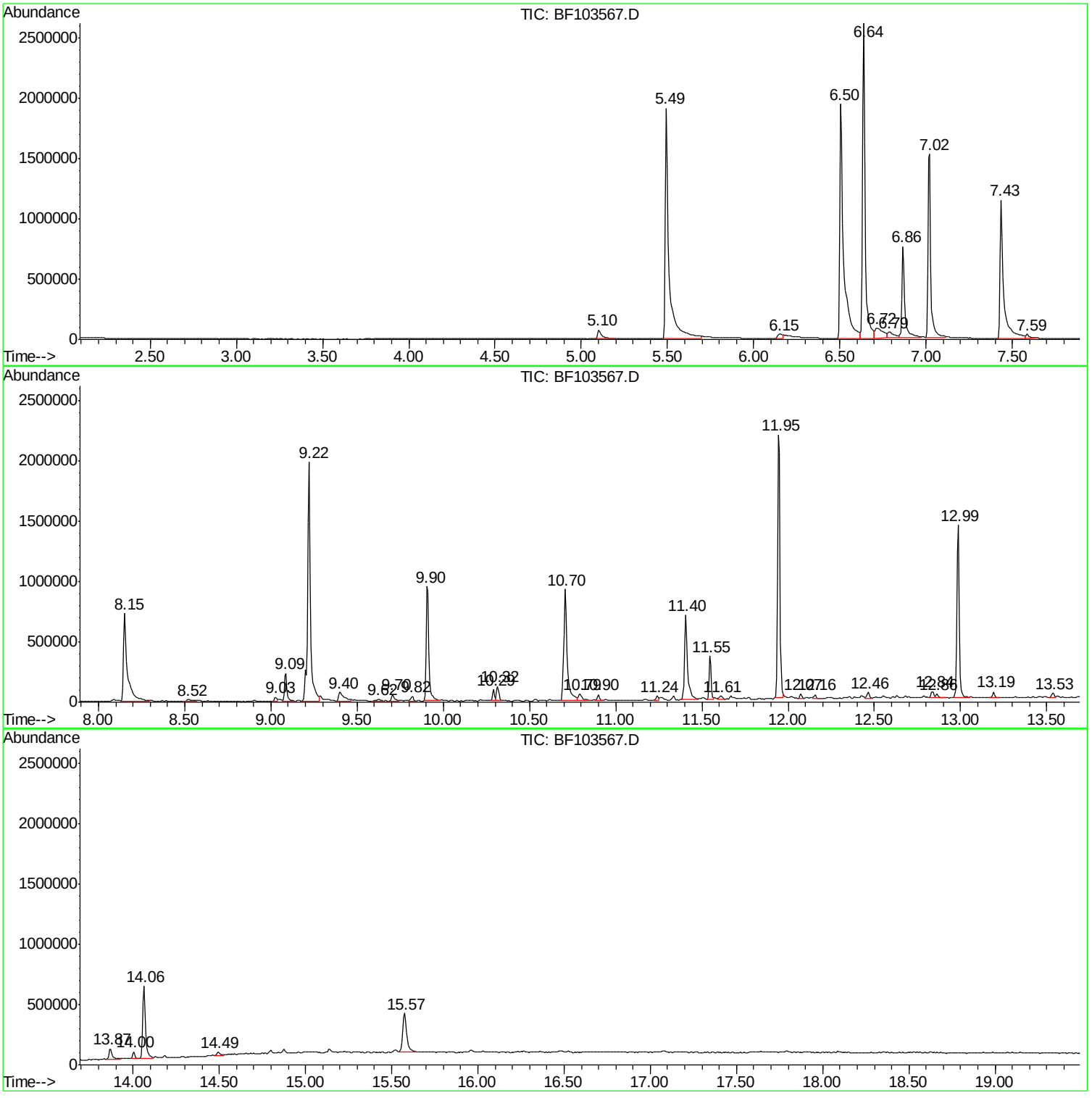
Operator : SJ/JU
Sample : J1821-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
COMPOSITE-4-5-20180205

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030918\
Data File : BF103567.D
Acq On : 9 Mar 2018 19:47
Operator : SJ/JU
Sample : J1821-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-4-5-20180205

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

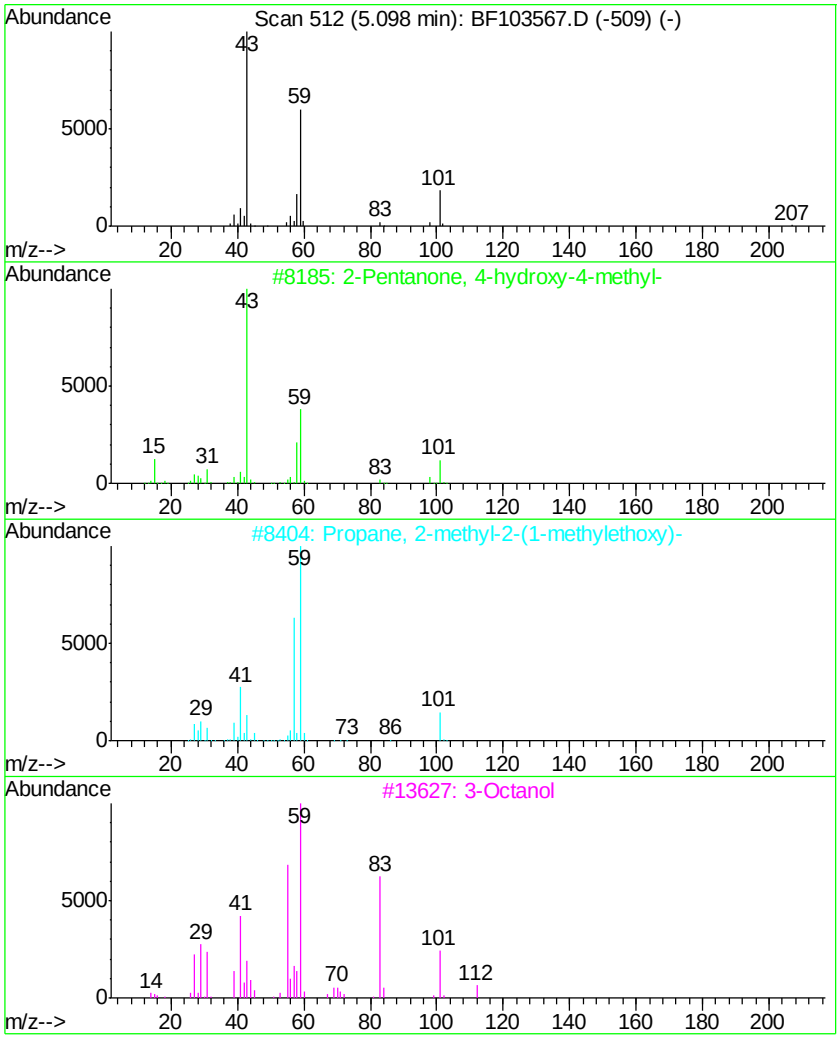
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

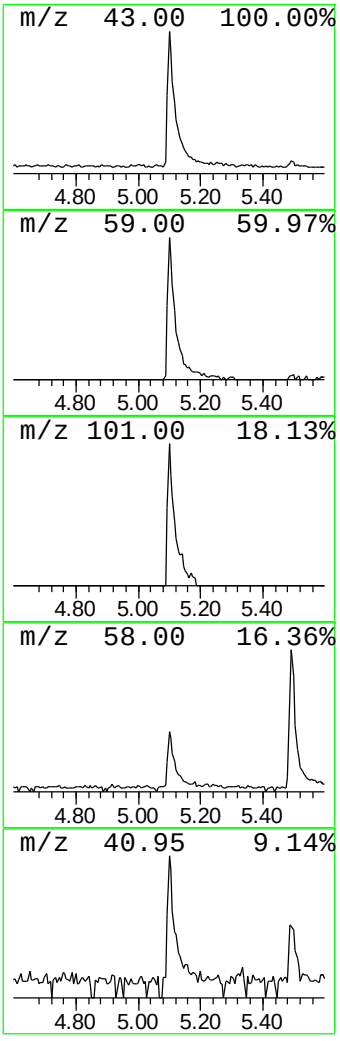
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.10 | 2.84 ng | 129648 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 36 |
| 3 | 3-Octanol | 130 | C8H18O | 000589-98-0 | 33 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030918\
Data File : BF103567.D
Acq On : 9 Mar 2018 19:47
Operator : SJ/JU
Sample : J1821-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-4-5-20180205

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

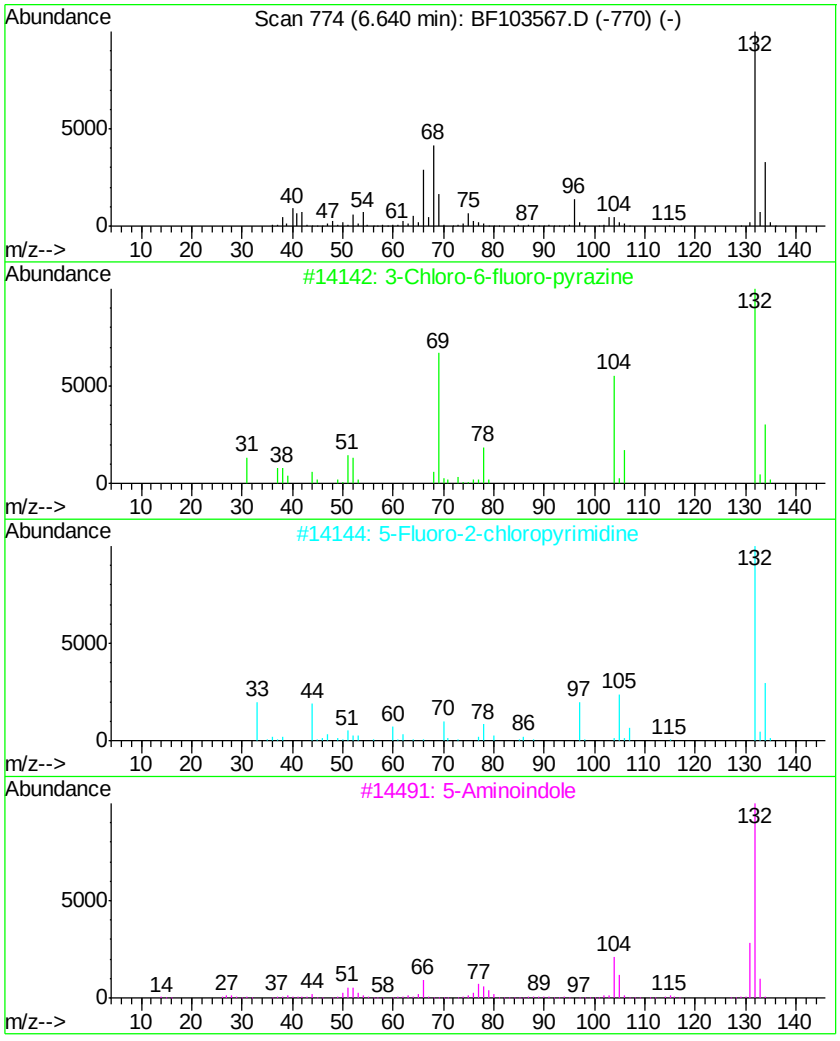
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

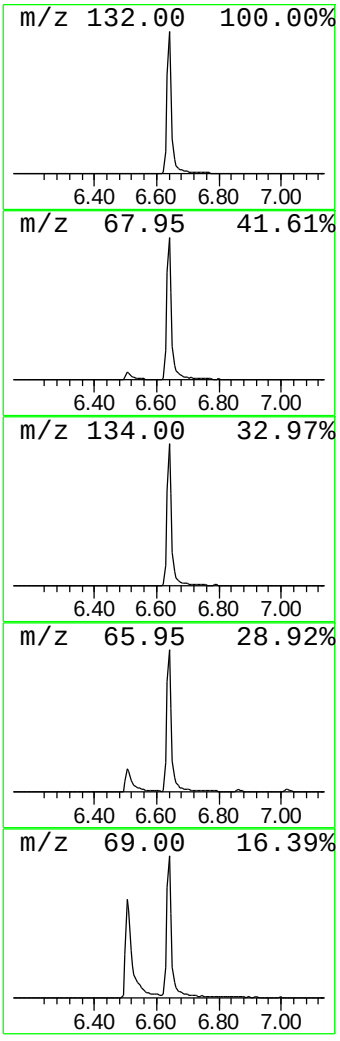
**********

Peak Number 2 unknown6.64 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.64 | 64.70 ng | 2957290 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



# Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030918\
Data File : BF103567.D
Acq On : 9 Mar 2018 19:47
Operator : SJ/JU
Sample : J1821-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-4-5-20180205

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

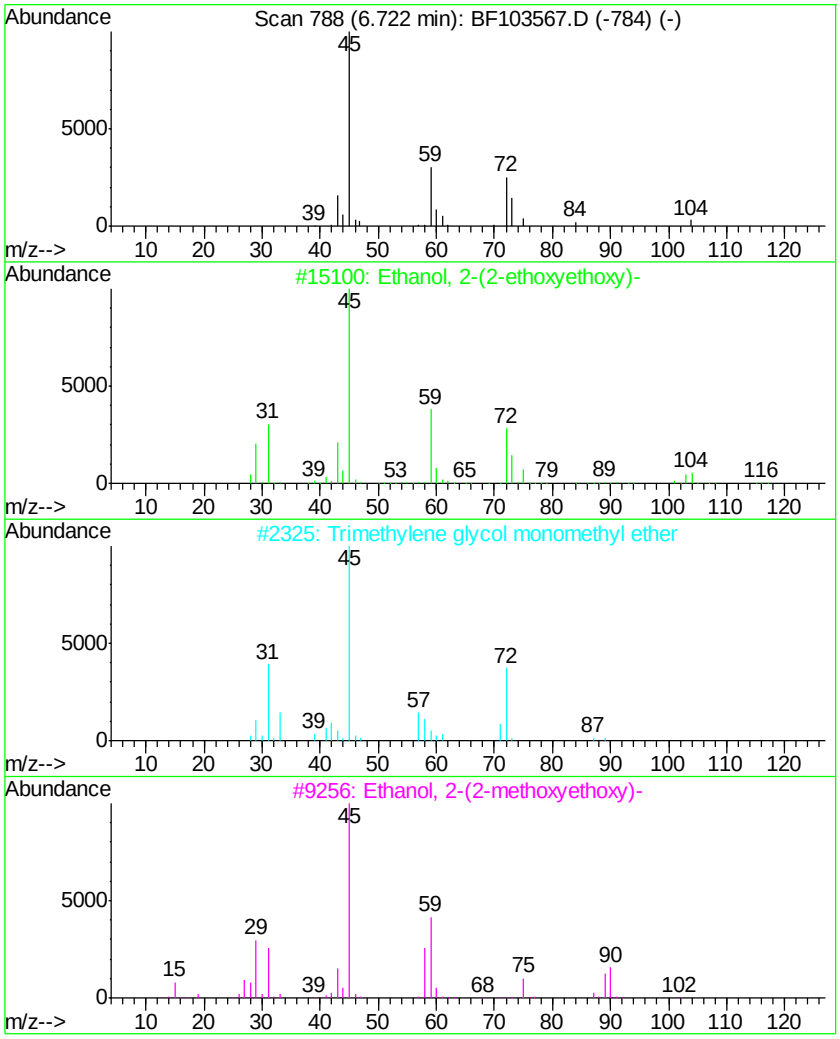
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

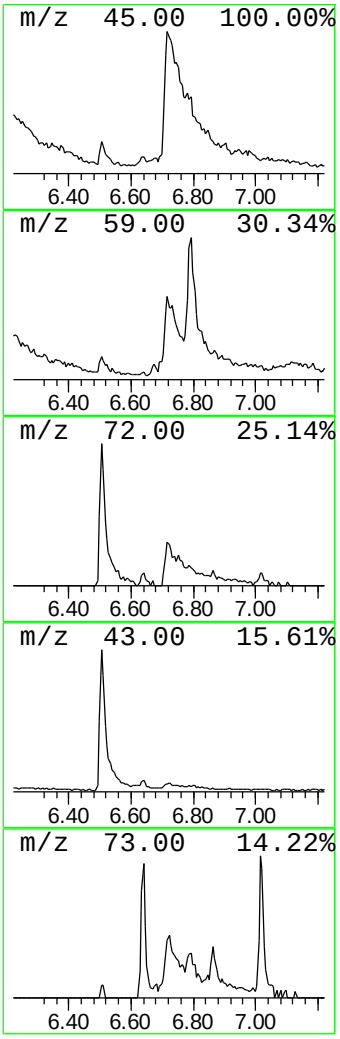
**********

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.72 | 5.90 ng | 269794 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(2-ethoxyethoxy)- | 134 | C6H14O3 | 000111-90-0 | 83 |
| 2 | Trimethylene glycol monomethyl e... | 90 | C4H10O2 | 001589-49-7 | 45 |
| 3 | Ethanol, 2-(2-methoxyethoxy)- | 120 | C5H12O3 | 000111-77-3 | 36 |
| 4 | 2-Butanol, 3-methyl- | 88 | C5H12O | 000598-75-4 | 28 |
| 5 | Ethyl ether | 74 | C4H10O | 000060-29-7 | 28 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF030918\
Data File : BF103567.D
Acq On : 9 Mar 2018 19:47
Operator : SJ/JU
Sample : J1821-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-4-5-20180205

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

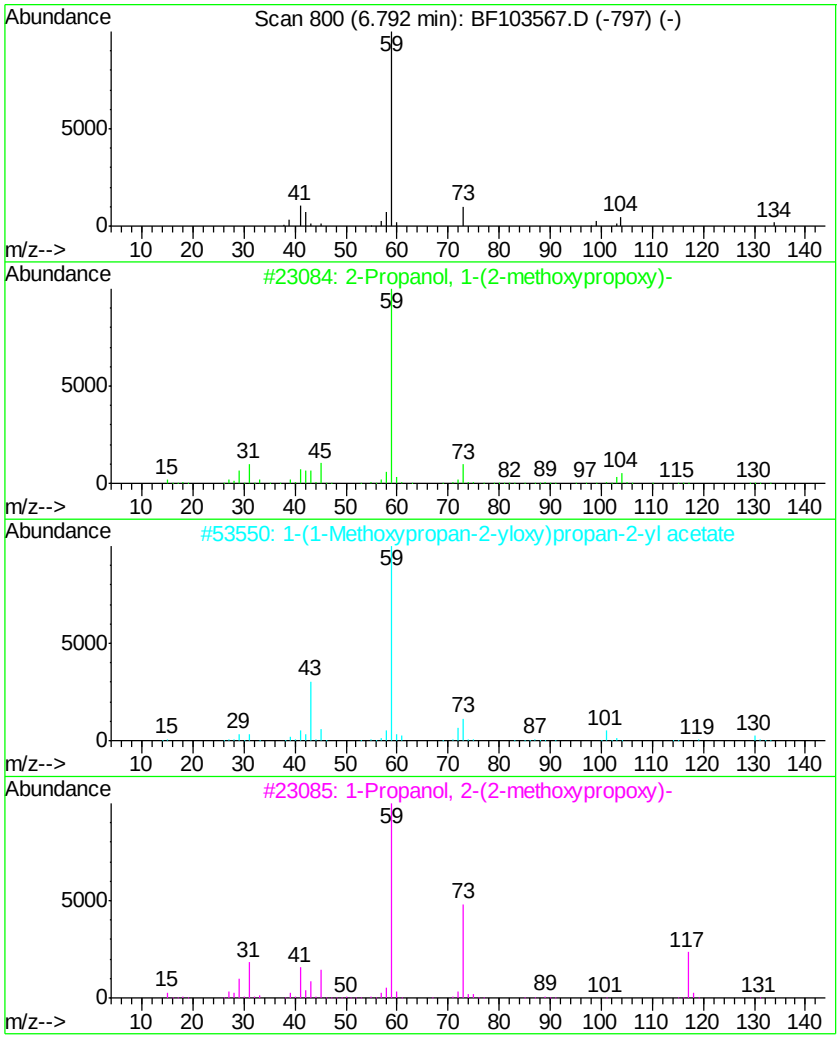
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

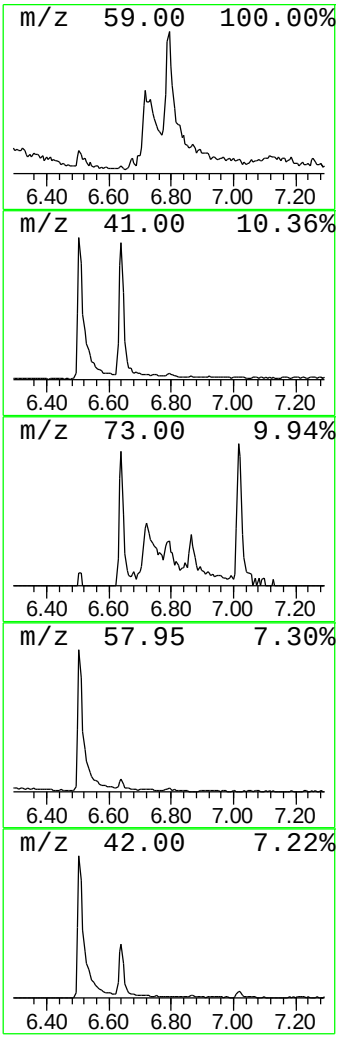
**********

Peak Number 4 2-Propanol, 1-(2-methoxypro... Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.79 | 2.58 ng | 118150 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Propanol, 1-(2-methoxypropoxy)- | 148 | C7H16O3 | 013429-07-7 | 64 |
| 2 | 1-(1-Methoxypropan-2-yloxy)propa... | 190 | C9H18O4 | 1000367-08-6 | 39 |
| 3 | 1-Propanol, 2-(2-methoxypropoxy)- | 148 | C7H16O3 | 013588-28-8 | 38 |
| 4 | 2-Propanol, 1-(2-methoxy-1-methy... | 148 | C7H16O3 | 020324-32-7 | 9 |
| 5 | 1-(1-Methoxypropan-2-yloxy)propa... | 244 | C9H15F3O4 | 1000367-08-7 | 9 |



Library Search Compound Report

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Data File : BF103567.D
Acq On : 9 Mar 2018 19:47
Operator : SJ/JU
Sample : J1821-02
Misc :
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**Instrument :** BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

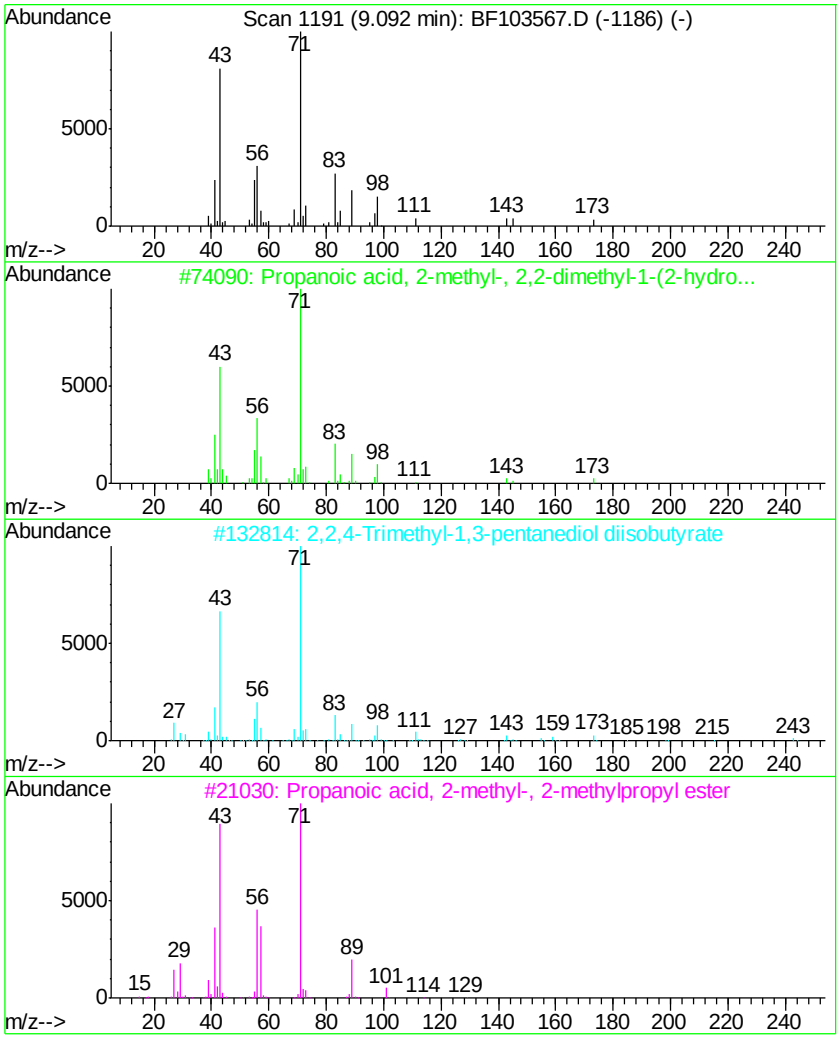
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

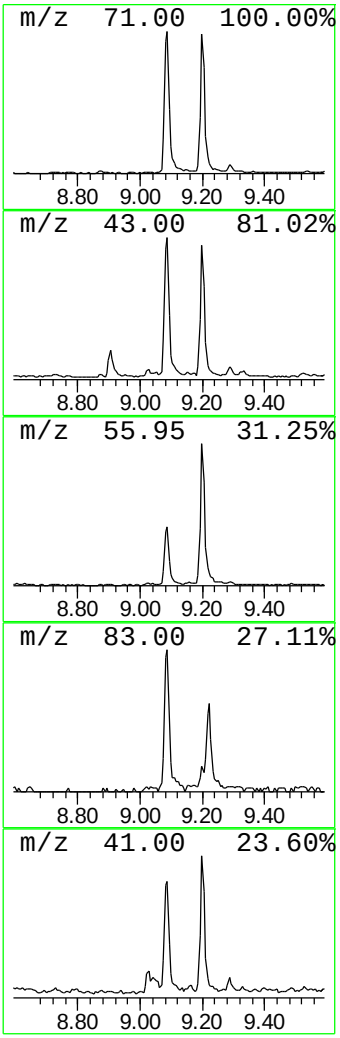
**********

Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.09 | 4.72 ng | 254608 | Acenaphthene-d10 | 9.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propanoic acid, 2-methyl-, 2,2-d... | 216 | C12H24O3 | 074367-33-2 | 90 |
| 2 | 2,2,4-Trimethyl-1,3-pentanediol ... | 286 | C16H30O4 | 006846-50-0 | 72 |
| 3 | Propanoic acid, 2-methyl-, 2-met... | 144 | C8H16O2 | 000097-85-8 | 50 |
| 4 | Butanoic acid, decyl ester | 228 | C14H28O2 | 005454-09-1 | 45 |
| 5 | Butanoic acid, 2-methylpropyl ester | 144 | C8H16O2 | 000539-90-2 | 42 |



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Acq On : 9 Mar 2018 19:47
Operator : SJ/JU
Sample : J1821-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-4-5-20180205

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

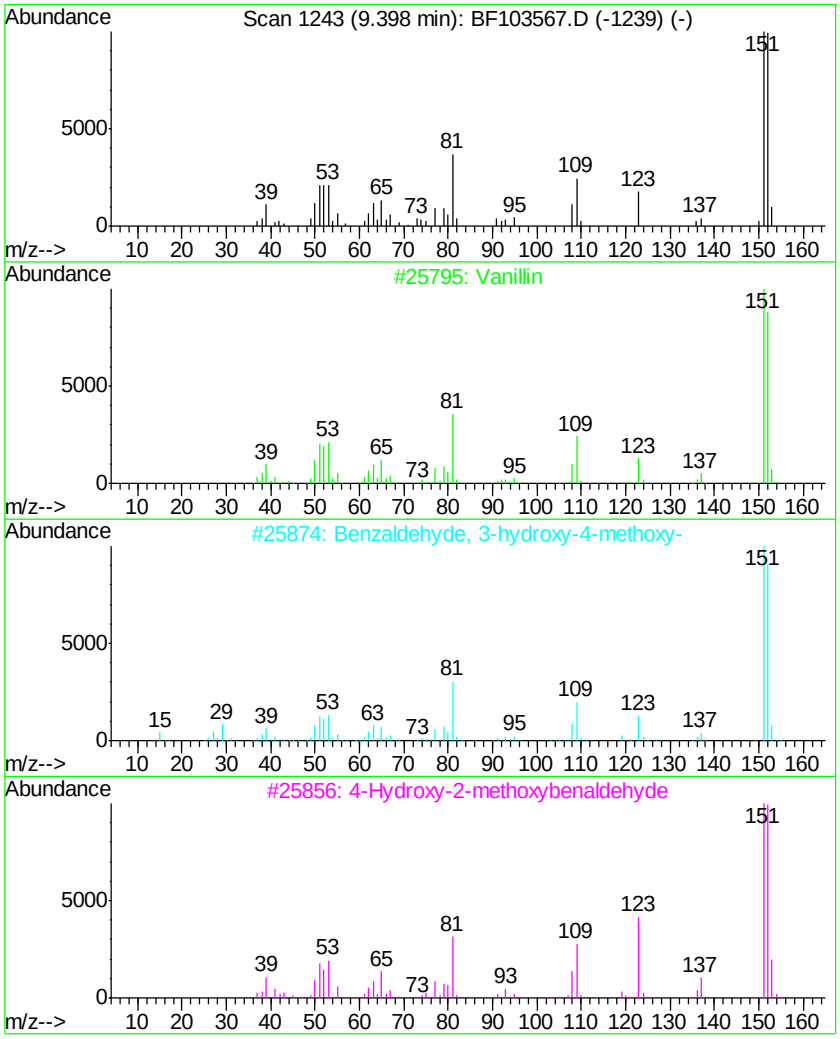
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

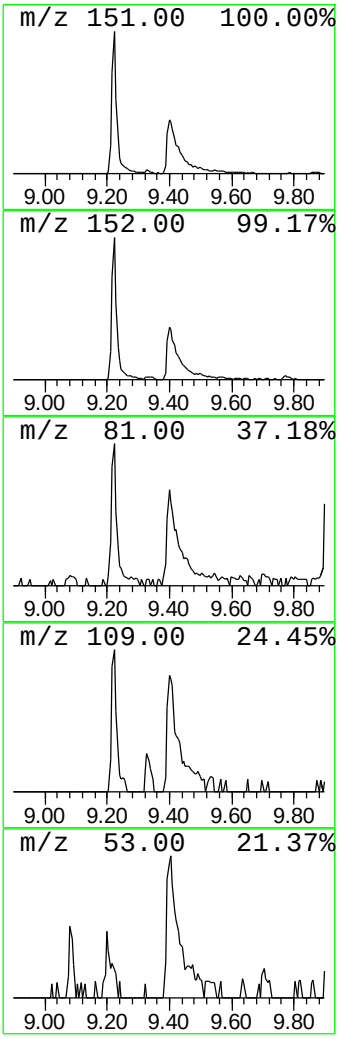
**********

Peak Number 7 Vanillin Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.40 | 2.88 ng | 155196 | Acenaphthene-d10 | 9.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Vanillin | 152 | C8H8O3 | 000121-33-5 | 97 |
| 2 | Benzaldehyde, 3-hydroxy-4-methoxy- | 152 | C8H8O3 | 000621-59-0 | 95 |
| 3 | 4-Hydroxy-2-methoxybenaldehyde | 152 | C8H8O3 | 018278-34-7 | 86 |
| 4 | Benzaldehyde, 2-hydroxy-4-methoxy- | 152 | C8H8O3 | 000673-22-3 | 46 |
| 5 | Benzaldehyde, 2,4-dihydroxy-6-me... | 152 | C8H8O3 | 000487-69-4 | 43 |



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Data File : BF103567.D
Acq On : 9 Mar 2018 19:47
Operator : SJ/JU
Sample : J1821-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-4-5-20180205

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

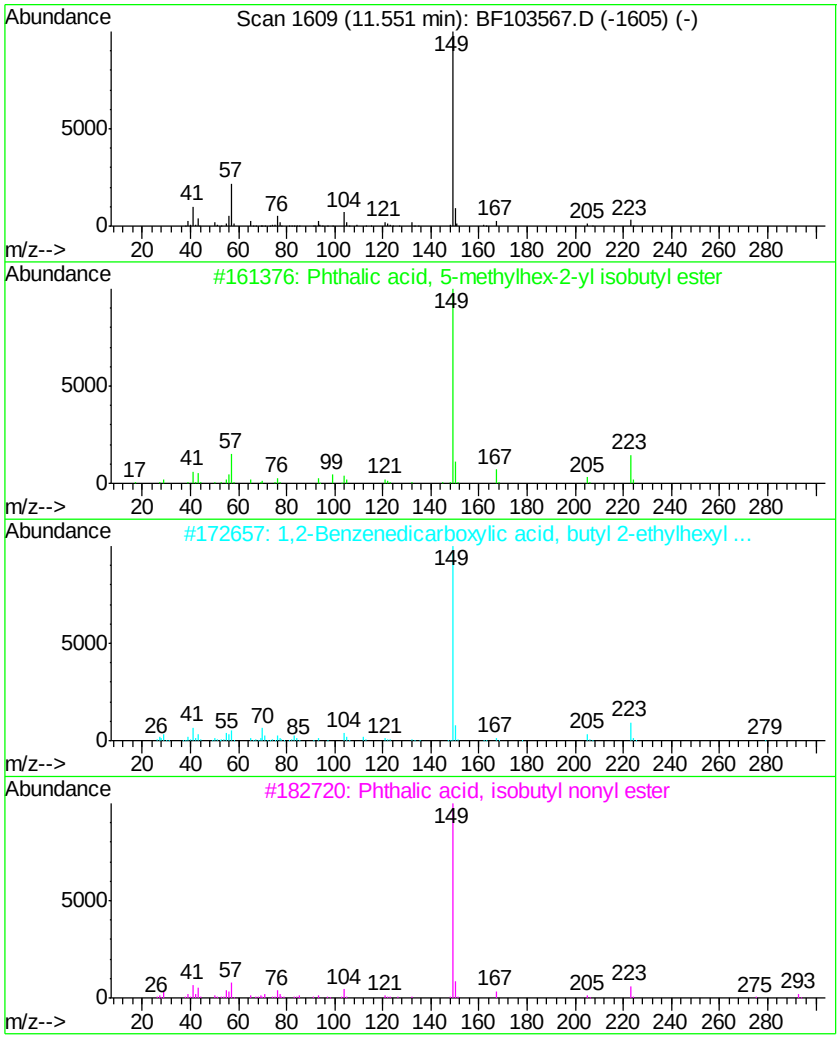
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

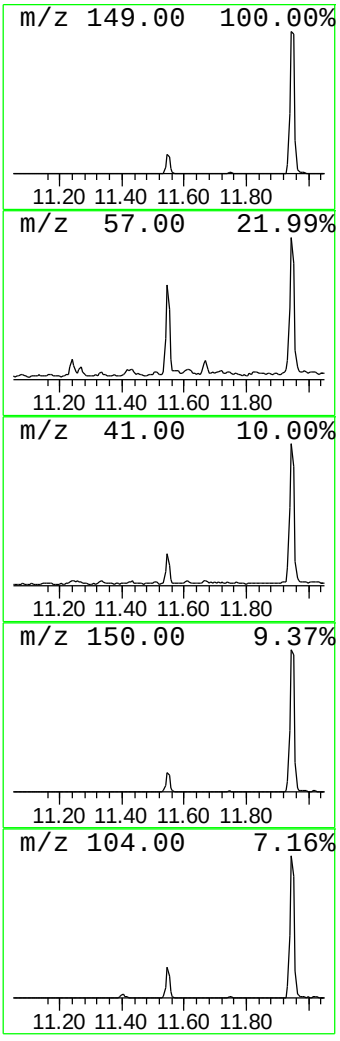
**********

Peak Number 8 Phthalic acid, 5-methylhex-... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.55 | 7.08 ng | 317402 | Phenanthrene-d10 | 11.40 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phthalic acid, 5-methylhex-2-yl ... | 320 | C19H28O4 | 1000371-09-1 | 83 |
| 2 | 1,2-Benzenedicarboxylic acid, bu... | 334 | C20H30O4 | 000085-69-8 | 83 |
| 3 | Phthalic acid, isobutyl nonyl ester | 348 | C21H32O4 | 1000309-04-4 | 83 |
| 4 | 1,2-Benzenedicarboxylic acid, bu... | 304 | C18H24O4 | 000084-64-0 | 78 |
| 5 | Phthalic acid, 2-ethylhexyl isob... | 334 | C20H30O4 | 1000308-98-0 | 78 |



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Data File : BF103567.D
Acq On : 9 Mar 2018 19:47
Operator : SJ/JU
Sample : J1821-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-4-5-20180205

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

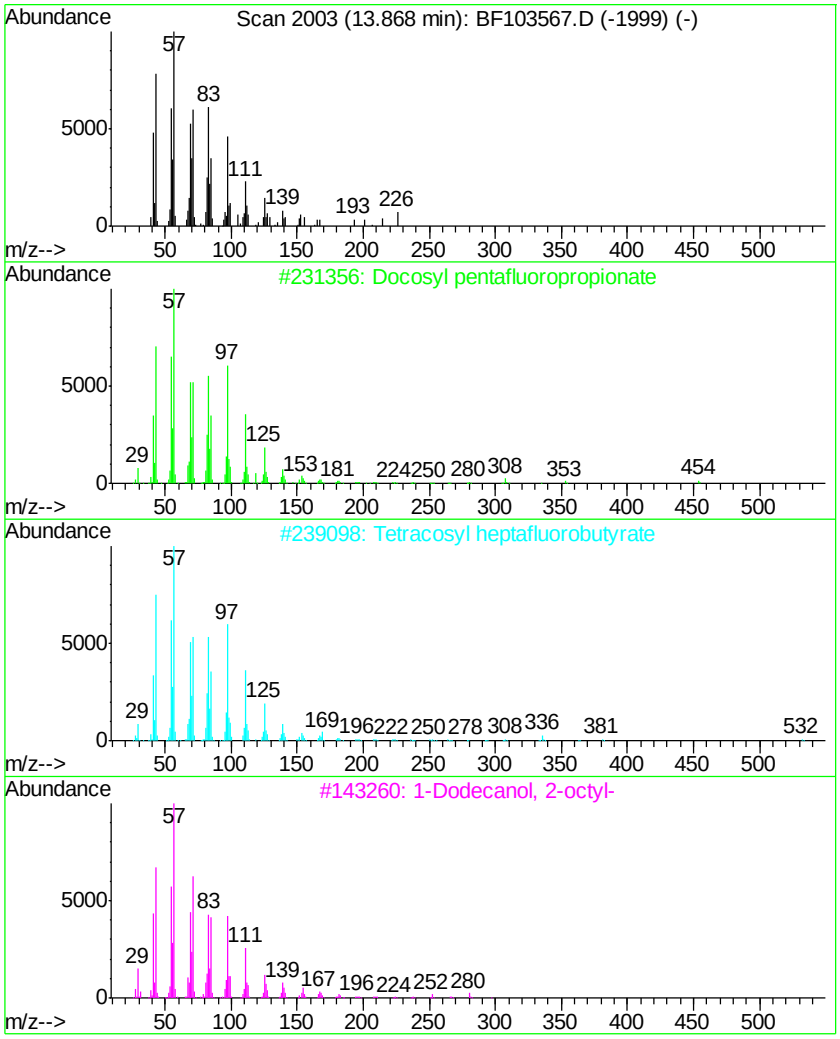
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

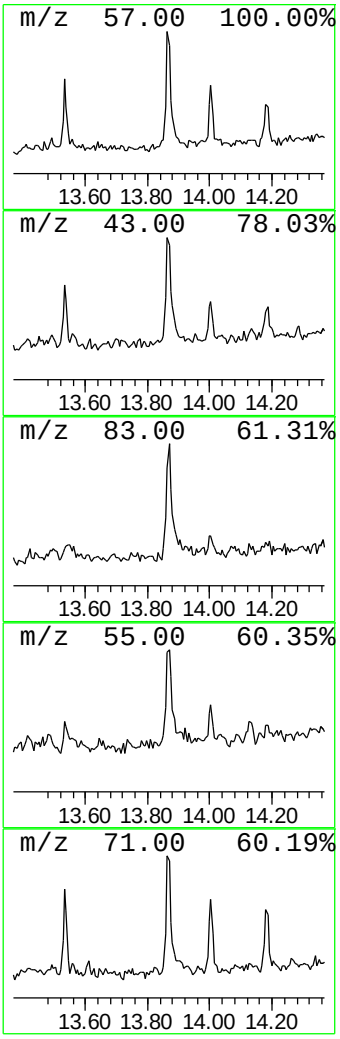
**********

Peak Number 9 Docosyl pentafluoropropionate Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.87 | 3.57 ng | 130347 | Chrysene-d12 | 14.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Docosyl pentafluoropropionate | 472 | C25H45F5O2 | 1000351-80-9 | 87 |
| 2 | Tetracosyl heptafluorobutyrate | 550 | C28H49F7O2 | 1000351-83-7 | 87 |
| 3 | 1-Dodecanol, 2-octyl- | 298 | C20H42O | 005333-42-6 | 83 |
| 4 | Acetic acid, chloro-, hexadecyl ... | 318 | C18H35ClO2 | 052132-58-8 | 83 |
| 5 | 1-Decanol, 2-hexyl- | 242 | C16H34O | 002425-77-6 | 83 |



Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF030918\
Data File : BF103567.D
Acq On : 9 Mar 2018 19:47
Operator : SJ/JU
Sample : J1821-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-4-5-20180205

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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... | 5.10 | 2.8 | ng | 129648 | 1 | 6.86 | 914128 | 20.0 |
| unknown6.64 | 6.64 | 64.7 | ng | 2957290 | 1 | 6.86 | 914128 | 20.0 |
| Ethanol, 2-(2-eth... | 6.72 | 5.9 | ng | 269794 | 1 | 6.86 | 914128 | 20.0 |
| 2-Propanol, 1-(2-... | 6.79 | 2.6 | ng | 118150 | 1 | 6.86 | 914128 | 20.0 |
| Propanoic acid, 2... | 9.09 | 4.7 | ng | 254608 | 3 | 9.90 | 1077740 | 20.0 |
| Vanillin | 9.40 | 2.9 | ng | 155196 | 3 | 9.90 | 1077740 | 20.0 |
| Phthalic acid, 5-... | 11.55 | 7.1 | ng | 317402 | 4 | 11.40 | 897208 | 20.0 |
| Docosyl pentafluo... | 13.87 | 3.6 | ng | 130347 | 5 | 14.06 | 729887 | 20.0 |