LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
Data File : BF093755.D
Acq On : 18 Mar 2017 15:49
Operator : SJ/MA
Sample : I2207-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 41D-9-11

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-BF031817.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 | 2.115 | 18 | 20 | 27 | rVB | 95150 | 132978 | 2.21% | 0.263% |
| 2 | 3.144 | 109 | 110 | 119 | rBV3 | 22717 | 73389 | 1.22% | 0.145% |
| 3 | 5.030 | 272 | 275 | 282 | rBV | 746241 | 1186499 | 19.69% | 2.350% |
| 4 | 5.453 | 308 | 312 | 314 | rBV | 3804950 | 4975818 | 82.59% | 9.854% |
| 5 | 6.482 | 398 | 402 | 404 | rBV | 4082519 | 5457900 | 90.59% | 10.809% |
| 6 | 6.619 | 410 | 414 | 416 | rBV | 3818481 | 5099879 | 84.65% | 10.100% |
| 7 | 6.847 | 431 | 434 | 436 | rBV | 1416299 | 1234454 | 20.49% | 2.445% |
| 8 | 7.007 | 445 | 448 | 450 | rVB | 3677296 | 3945838 | 65.49% | 7.814% |
| 9 | 7.407 | 480 | 483 | 485 | rBV | 3142255 | 3264662 | 54.19% | 6.465% |
| 10 | 8.127 | 544 | 546 | 549 | rBV | 1712912 | 1587331 | 26.35% | 3.144% |
| 11 | 9.213 | 638 | 641 | 643 | rVB | 4992000 | 6024700 | 100.00% | 11.931% |
| 12 | 9.602 | 672 | 675 | 677 | rBV | 972698 | 936663 | 15.55% | 1.855% |
| 13 | 9.830 | 693 | 695 | 697 | rBV | 69219 | 65130 | 1.08% | 0.129% |
| 14 | 9.876 | 697 | 699 | 702 | rVB | 1301065 | 1731638 | 28.74% | 3.429% |
| 15 | 10.322 | 737 | 738 | 740 | rVB | 88398 | 106050 | 1.76% | 0.210% |
| 16 | 10.551 | 756 | 758 | 760 | rBV | 51512 | 60539 | 1.00% | 0.120% |
| 17 | 10.665 | 765 | 768 | 770 | rVV | 2781944 | 2971809 | 49.33% | 5.885% |
| 18 | 10.699 | 770 | 771 | 775 | rVV | 64139 | 62583 | 1.04% | 0.124% |
| 19 | 10.768 | 775 | 777 | 778 | rVV | 104126 | 121169 | 2.01% | 0.240% |
| 20 | 10.802 | 778 | 780 | 785 | rVB | 152728 | 226169 | 3.75% | 0.448% |
| 21 | 11.248 | 816 | 819 | 820 | rBV2 | 165587 | 146893 | 2.44% | 0.291% |
| 22 | 11.362 | 826 | 829 | 831 | rVV | 1719298 | 1789436 | 29.70% | 3.544% |
| 23 | 11.671 | 854 | 856 | 858 | rBV | 135770 | 108791 | 1.81% | 0.215% |
| 24 | 11.899 | 874 | 876 | 878 | rBV | 82287 | 101635 | 1.69% | 0.201% |
| 25 | 12.082 | 889 | 892 | 894 | rBV | 55127 | 65449 | 1.09% | 0.130% |
| 26 | 12.951 | 965 | 968 | 970 | rBV | 4720179 | 5203940 | 86.38% | 10.306% |
| 27 | 13.854 | 1044 | 1047 | 1052 | rBV | 166166 | 298607 | 4.96% | 0.591% |
| 28 | 13.991 | 1056 | 1059 | 1061 | rBV | 1277014 | 1681064 | 27.90% | 3.329% |
| 29 | 14.574 | 1107 | 1110 | 1113 | rBV | 69833 | 167939 | 2.79% | 0.333% |
| 30 | 14.631 | 1113 | 1115 | 1117 | rVV | 145400 | 181870 | 3.02% | 0.360% |
| 31 | 14.677 | 1117 | 1119 | 1122 | rVV2 | 52056 | 130692 | 2.17% | 0.259% |
| 32 | 14.757 | 1124 | 1126 | 1129 | rVB | 54630 | 124720 | 2.07% | 0.247% |
| 33 | 15.397 | 1179 | 1182 | 1185 | rBV | 957451 | 1228986 | 20.40% | 2.434% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
Data File : BF093755.D
Acq On : 18 Mar 2017 15:49
Operator : SJ/MA
Sample : I2207-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 41D-9-11

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-BF031817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

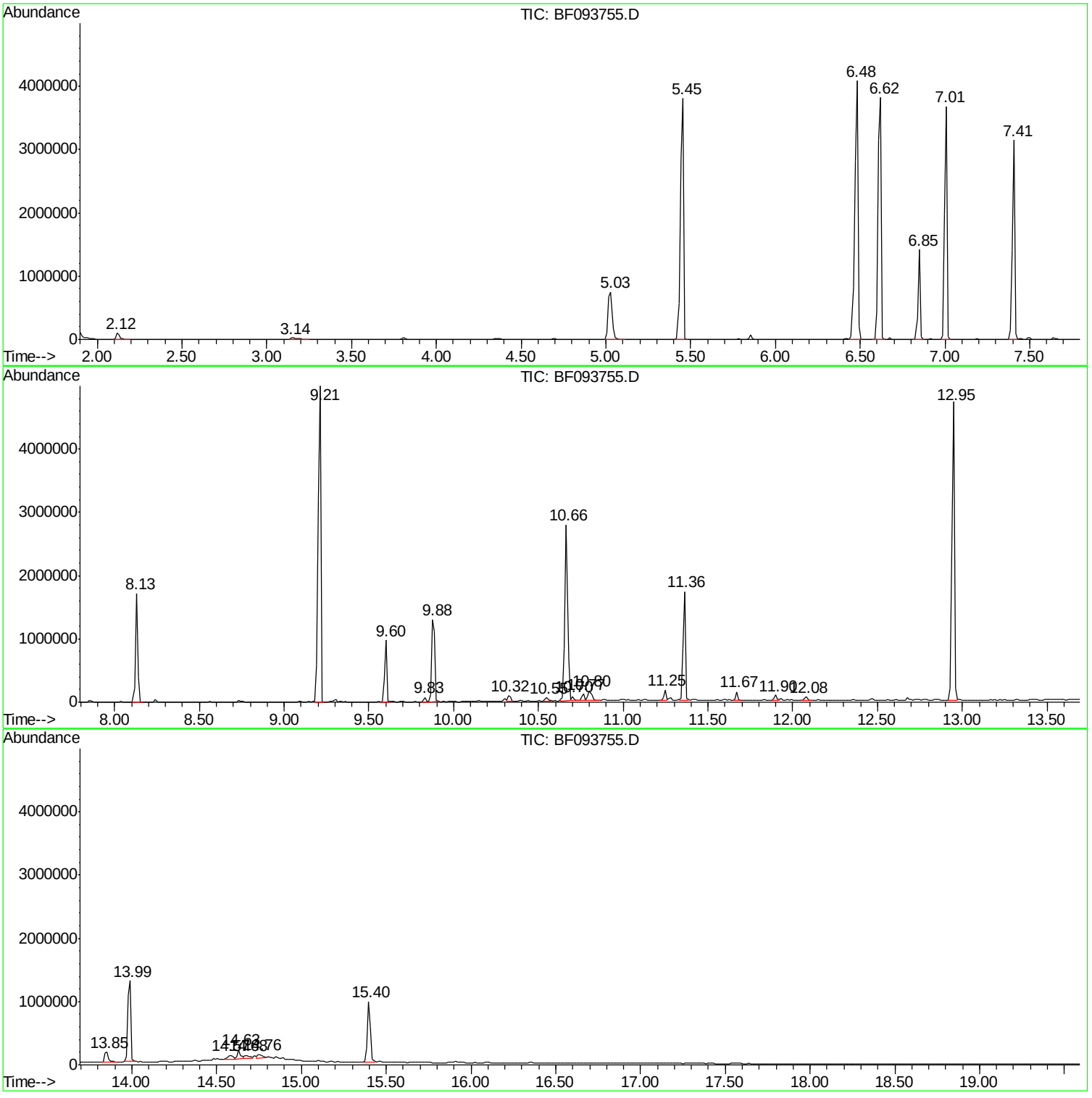
Sum of corrected areas: 50495220

Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
Data File : BF093755.D
Acq On : 18 Mar 2017 15:49
Operator : SJ/MA
Sample : I2207-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
41D-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
Data File : BF093755.D
Acq On : 18 Mar 2017 15:49
Operator : SJ/MA
Sample : I2207-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 41D-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

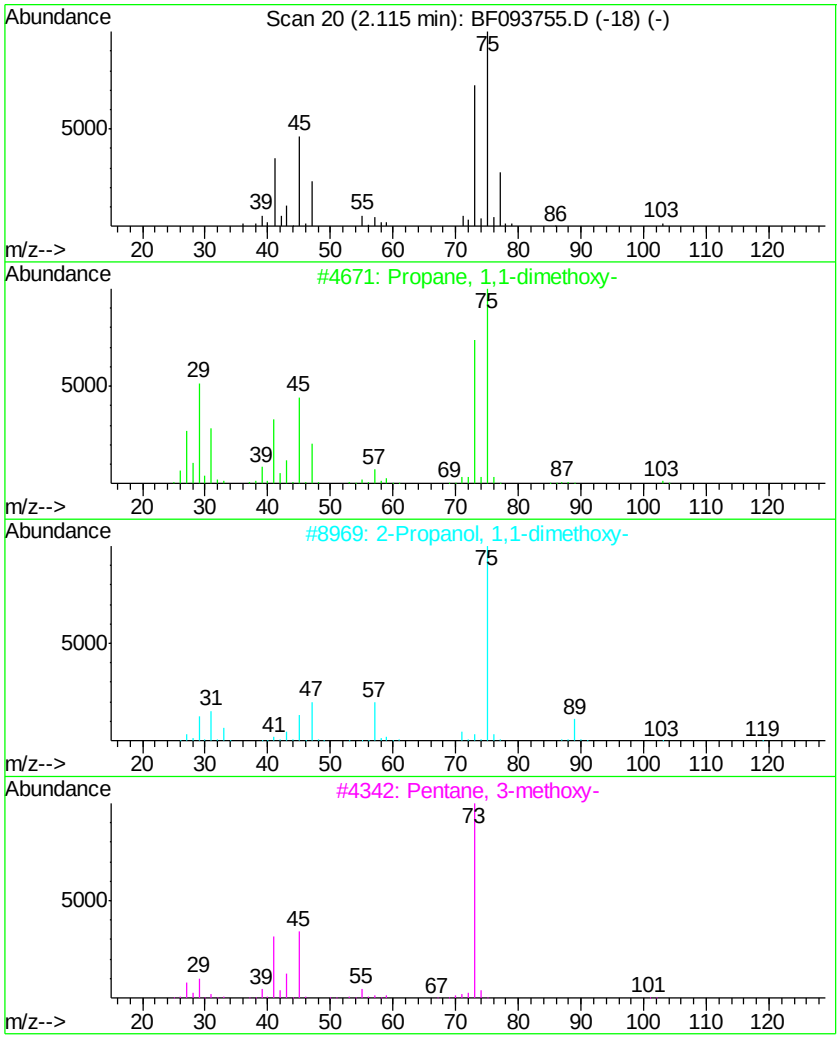
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

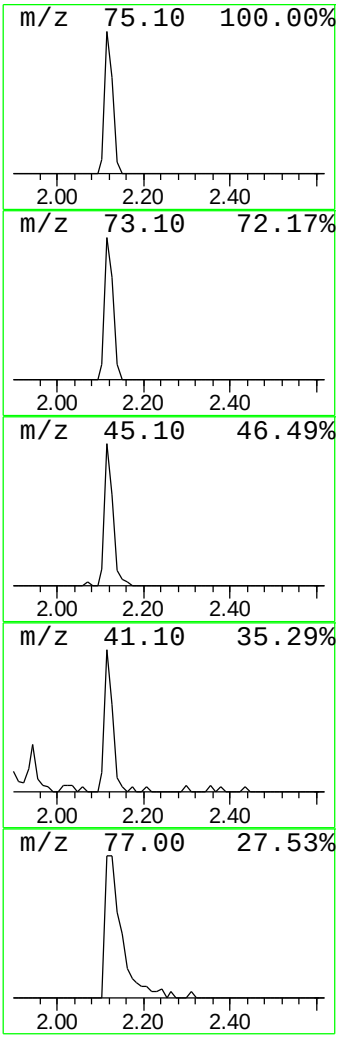
**********

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.12 | 2.15 ng | 132978 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 1,1-dimethoxy- | 104 | C5H12O2 | 004744-10-9 | 72 |
| 2 | 2-Propanol, 1,1-dimethoxy- | 120 | C5H12O3 | 042919-42-6 | 38 |
| 3 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 14 |
| 4 | 2,2'-Trimethylenebis-1,3-dioxolane | 188 | C9H16O4 | 006543-04-0 | 9 |
| 5 | Ethane, 1,1,2-trimethoxy- | 120 | C5H12O3 | 024332-20-5 | 9 |



Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
Data File : BF093755.D
Acq On : 18 Mar 2017 15:49
Operator : SJ/MA
Sample : I2207-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 41D-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

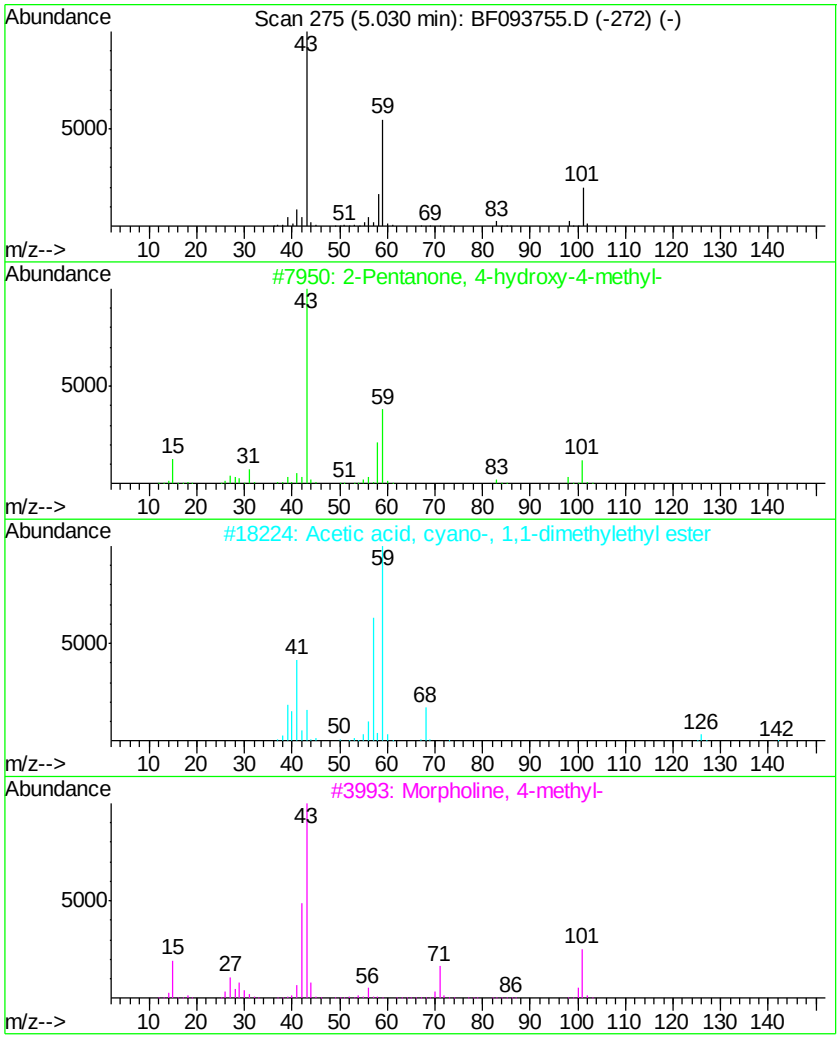
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

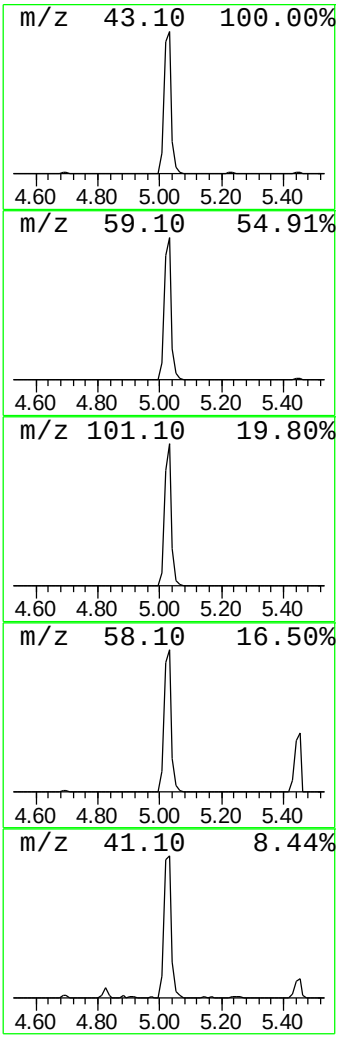
**********

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.03 | 19.22 ng | 1186500 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 53 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 3 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 4 | 3-Hydroxy-3-methyl-2-butanone | 102 | C5H10O2 | 000115-22-0 | 9 |
| 5 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 9 |



Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
Data File : BF093755.D
Acq On : 18 Mar 2017 15:49
Operator : SJ/MA
Sample : I2207-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 41D-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

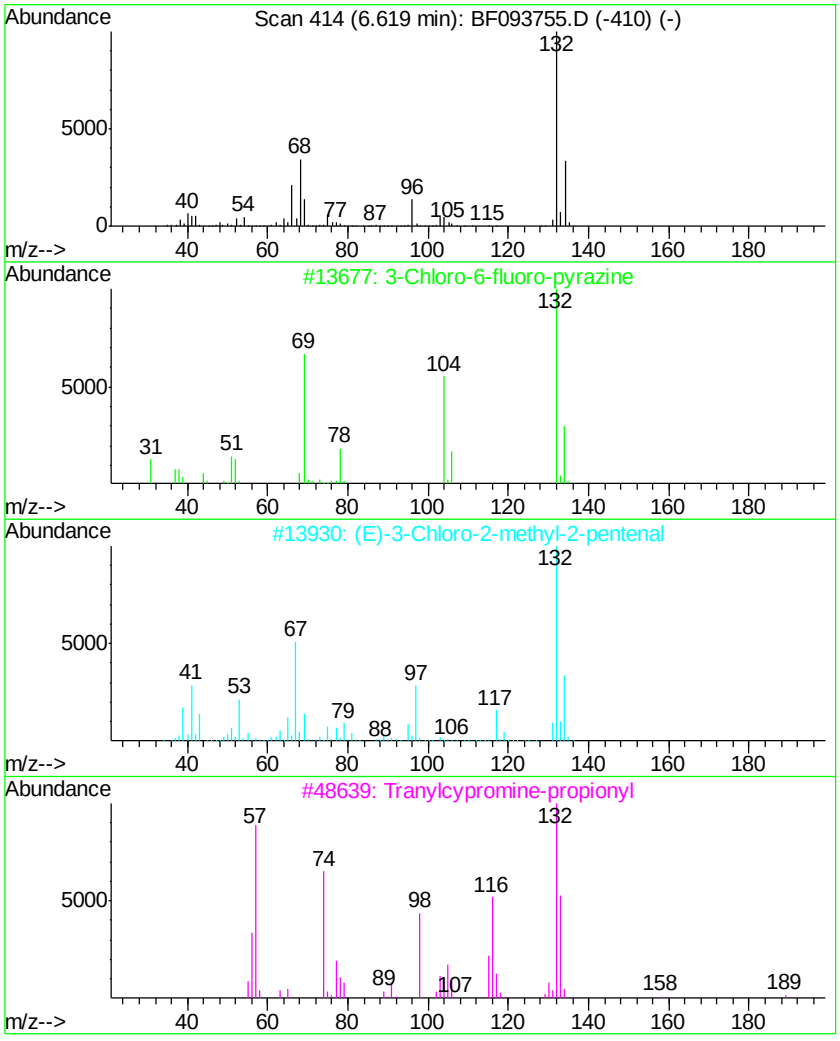
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

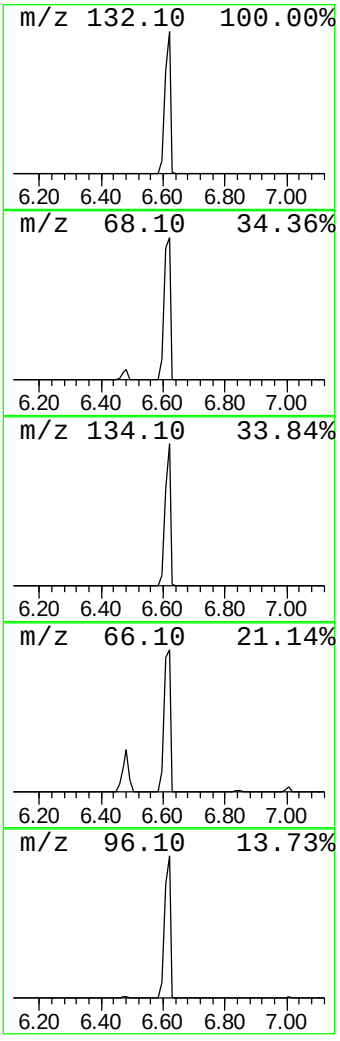
**********

Peak Number 3 unknown6.62 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.62 | 82.63 ng | 5099880 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 38 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 16 |
| 4 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |
| 5 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 9 |



Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
Data File : BF093755.D
Acq On : 18 Mar 2017 15:49
Operator : SJ/MA
Sample : I2207-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 41D-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

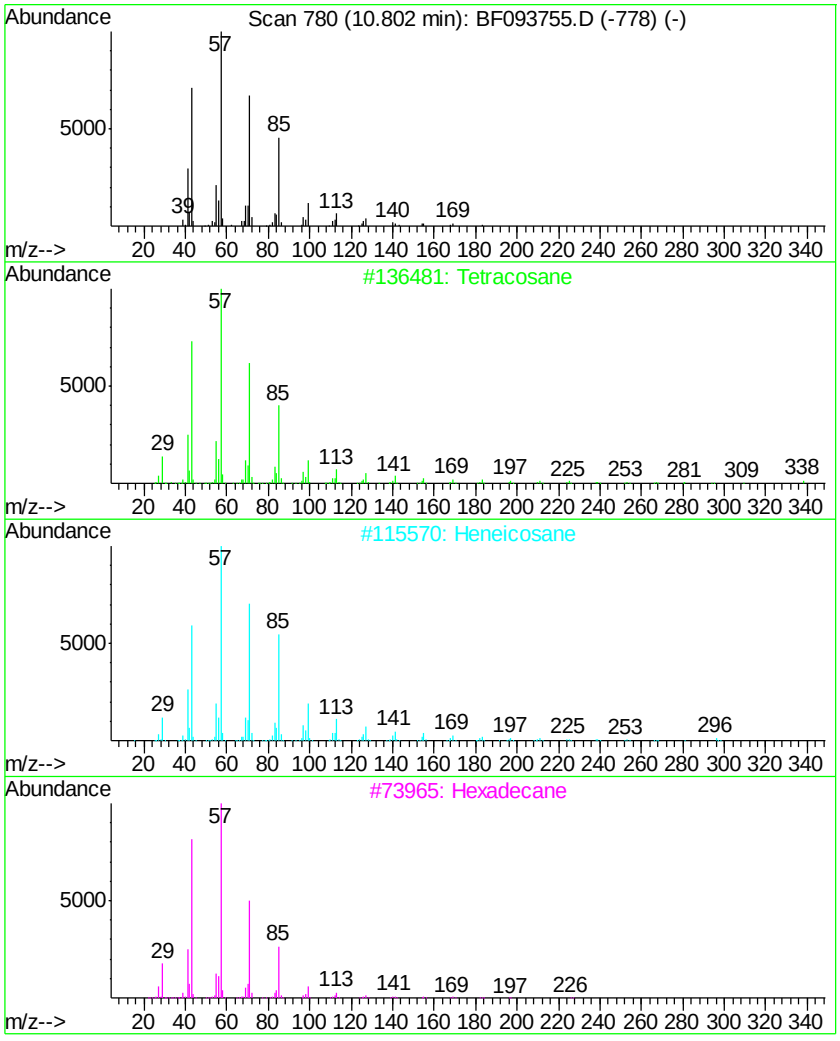
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

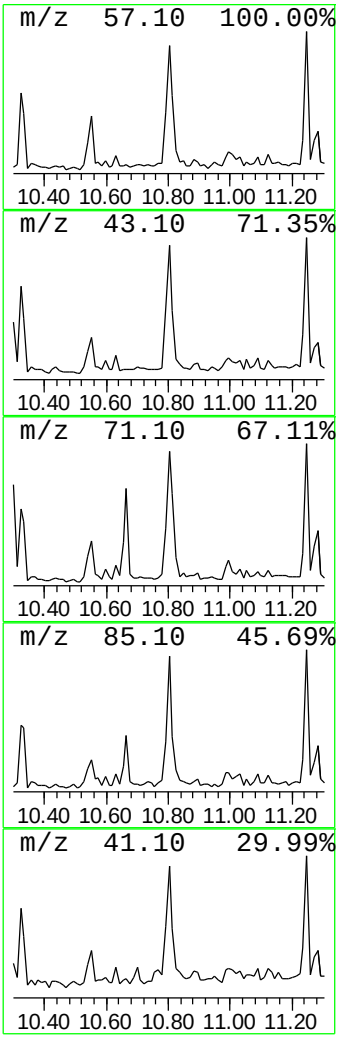
**********

Peak Number 5 Tetracosane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.80 | 2.53 ng | 226169 | Phenanthrene-d10 | 11.36 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetracosane | 338 | C24H50 | 000646-31-1 | 91 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 3 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 4 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |
| 5 | Octadecane | 254 | C18H38 | 000593-45-3 | 90 |



Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
Data File : BF093755.D
Acq On : 18 Mar 2017 15:49
Operator : SJ/MA
Sample : I2207-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 41D-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

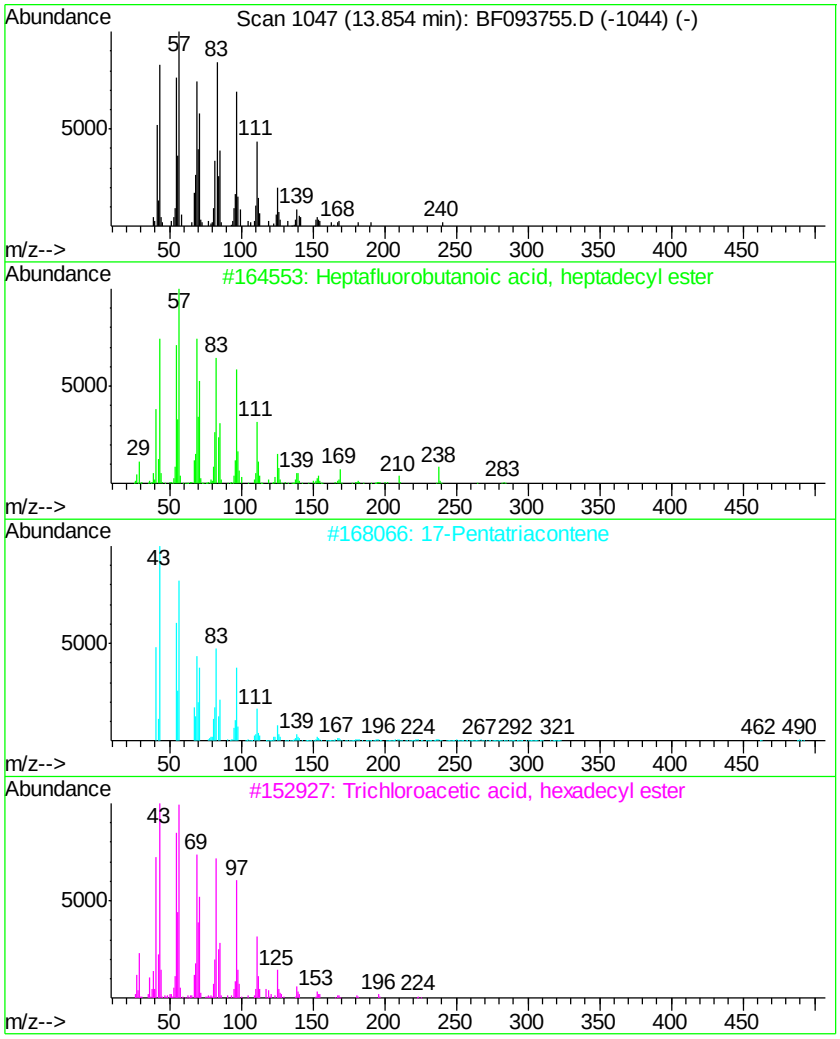
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

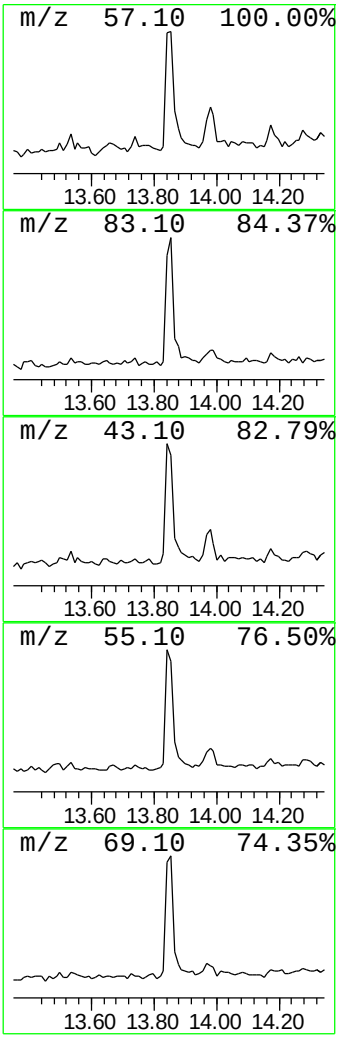
**********

Peak Number 6 Heptafluorobutanoic acid, h... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.85 | 3.55 ng | 298607 | Chrysene-d12 | 13.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptafluorobutanoic acid, heptad... | 452 | C21H35F7O2 | 1000282-97-3 | 95 |
| 2 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 91 |
| 3 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 91 |
| 4 | Pentafluoropropionic acid, octad... | 416 | C21H37F5O2 | 1000280-07-7 | 91 |
| 5 | Heptafluorobutyric acid, n-penta... | 424 | C19H31F7O2 | 1000216-79-3 | 90 |



Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
Data File : BF093755.D
Acq On : 18 Mar 2017 15:49
Operator : SJ/MA
Sample : I2207-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 41D-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

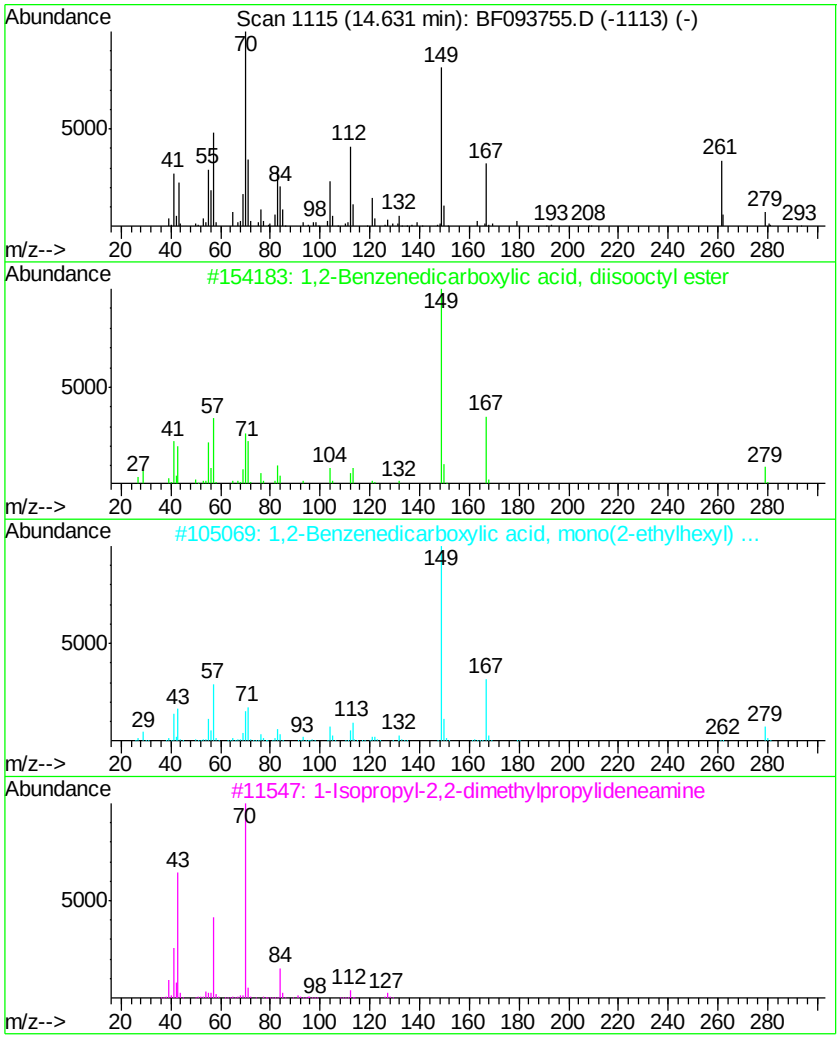
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

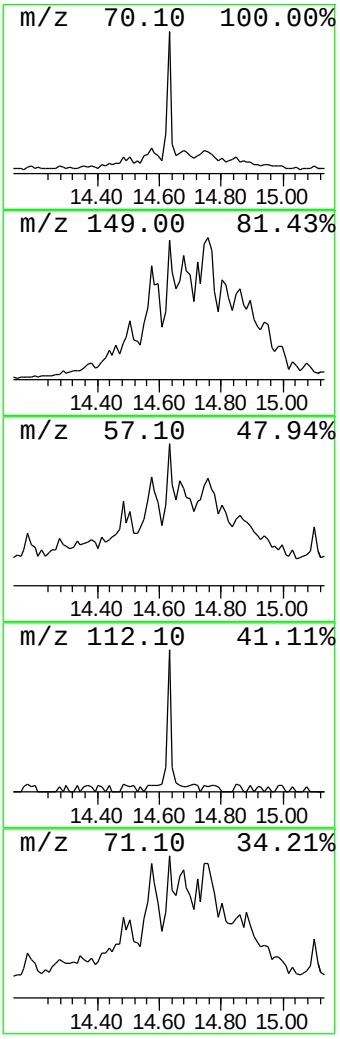
**********

Peak Number 7 unknown14.63 Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.63 | 2.16 ng | 181870 | Chrysene-d12 | 13.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,2-Benzenedicarboxylic acid, di... | 390 | C24H38O4 | 027554-26-3 | 38 |
| 2 | 1,2-Benzenedicarboxylic acid, mo... | 278 | C16H22O4 | 004376-20-9 | 35 |
| 3 | 1-Isopropyl-2,2-dimethylpropylid... | 127 | C8H17N | 1000210-05-3 | 22 |
| 4 | Benzoic acid, 3-(4-nitro-1-pyraz... | 261 | C12H11N3O4 | 1000273-84-4 | 22 |
| 5 | Cyclohexaneamine, N-but-2-enylid... | 167 | C10H17NO | 068048-01-1 | 16 |



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Sample : I2207-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

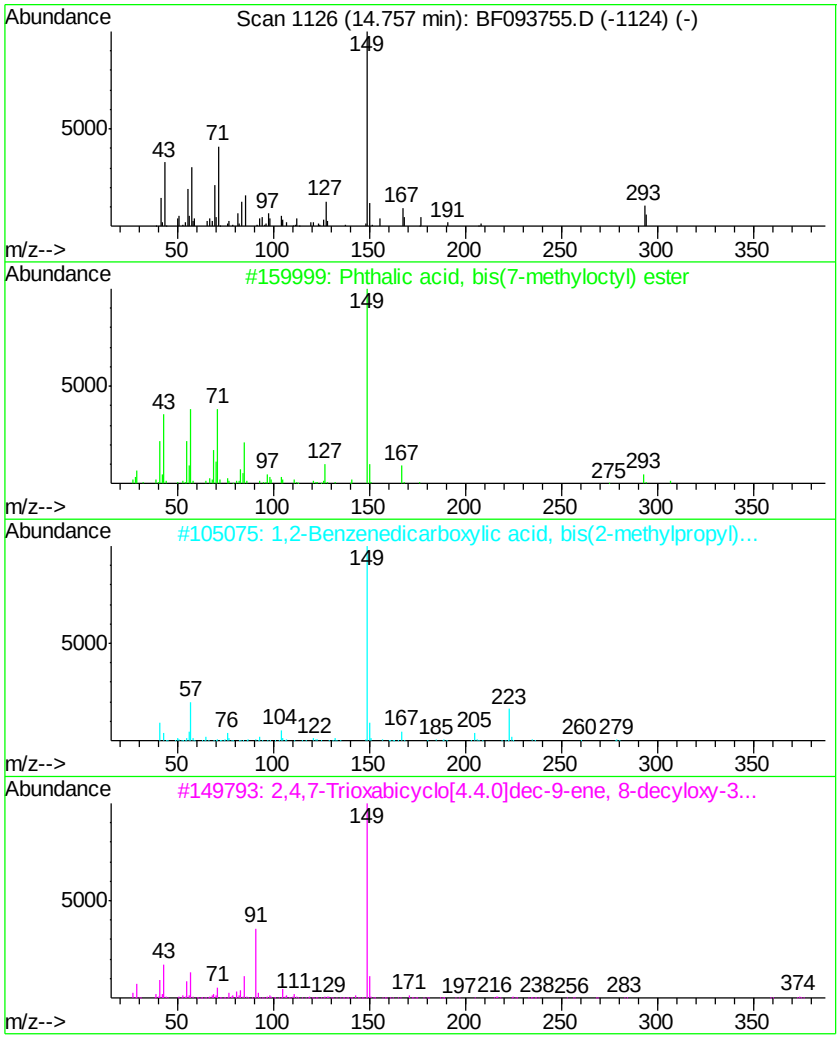
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

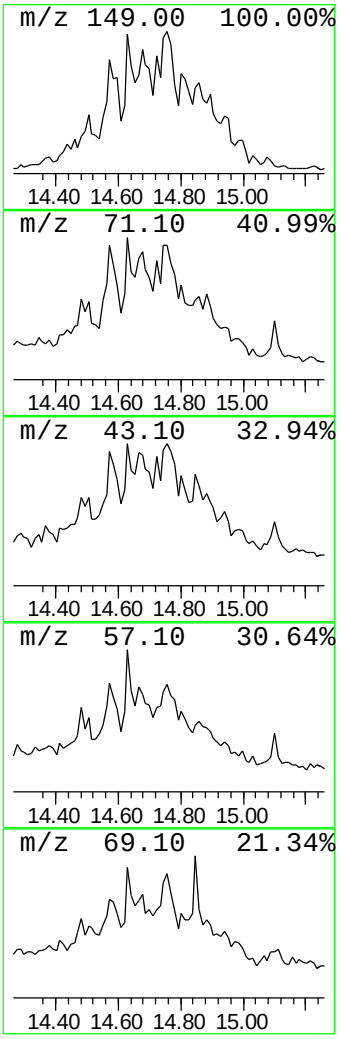
**********

Peak Number 8 Phthalic acid, bis(7-methyl... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.76 | 2.03 ng | 124720 | Perylene-d12 | 15.40 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phthalic acid, bis(7-methyloctyl... | 418 | C26H42O4 | 020548-62-3 | 72 |
| 2 | 1,2-Benzenedicarboxylic acid, bi... | 278 | C16H22O4 | 000084-69-5 | 43 |
| 3 | 2,4,7-Trioxabicyclo[4.4.0]dec-9-... | 374 | C23H34O4 | 1000161-14-6 | 43 |
| 4 | 1,2-Benzenedicarboxylic acid, is... | 418 | C26H42O4 | 001330-96-7 | 43 |
| 5 | 1,2-Benzenedicarboxylic acid, di... | 362 | C22H34O4 | 003648-21-3 | 38 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\Data\BF031817\
Data File : BF093755.D
Acq On : 18 Mar 2017 15:49
Operator : SJ/MA
Sample : I2207-02
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 41D-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031817.M
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 |
| Propane, 1,1-dime... | 2.12 | 2.1 | ng | 132978 | 1 | 6.85 | 1234450 | 20.0 |
| 2-Pentanone, 4-hy... | 5.03 | 19.2 | ng | 1186500 | 1 | 6.85 | 1234450 | 20.0 |
| unknown6.62 | 6.62 | 82.6 | ng | 5099880 | 1 | 6.85 | 1234450 | 20.0 |
| Tetracosane | 10.80 | 2.5 | ng | 226169 | 4 | 11.36 | 1789440 | 20.0 |
| Heptafluorobutano... | 13.85 | 3.5 | ng | 298607 | 5 | 13.99 | 1681060 | 20.0 |
| unknown14.63 | 14.63 | 2.2 | ng | 181870 | 5 | 13.99 | 1681060 | 20.0 |
| Phthalic acid, bi... | 14.76 | 2.0 | ng | 124720 | 6 | 15.40 | 1228990 | 20.0 |