LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088137.D
Acq On : 18 Jun 2016 16:41
Operator : UM/SJ
Sample : H3501-17
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB8-4-6

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-BF060716.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 | 1.667 | 5 | 7 | 12 | rVV | 73897 | 104555 | 4.31% | 0.505% |
| 2 | 1.781 | 15 | 17 | 25 | rVV | 570921 | 815348 | 33.61% | 3.936% |
| 3 | 1.884 | 25 | 26 | 46 | rVB3 | 70459 | 182001 | 7.50% | 0.879% |
| 4 | 2.913 | 114 | 116 | 124 | rBV | 28882 | 70452 | 2.90% | 0.340% |
| 5 | 4.856 | 284 | 286 | 295 | rBV | 103341 | 156964 | 6.47% | 0.758% |
| 6 | 5.290 | 321 | 324 | 327 | rBV | 1564551 | 1984918 | 81.83% | 9.581% |
| 7 | 6.353 | 413 | 417 | 419 | rBV2 | 1781011 | 2425643 | 100.00% | 11.708% |
| 8 | 6.467 | 424 | 427 | 429 | rBV | 1560855 | 2171143 | 89.51% | 10.480% |
| 9 | 6.684 | 444 | 446 | 449 | rBV | 623715 | 550953 | 22.71% | 2.659% |
| 10 | 6.844 | 457 | 460 | 462 | rBV | 2021571 | 1855393 | 76.49% | 8.956% |
| 11 | 7.256 | 493 | 496 | 498 | rBV | 1168340 | 1150656 | 47.44% | 5.554% |
| 12 | 7.382 | 502 | 507 | 512 | rVB3 | 16056 | 33680 | 1.39% | 0.163% |
| 13 | 7.976 | 556 | 559 | 561 | rBV | 699675 | 697371 | 28.75% | 3.366% |
| 14 | 9.050 | 650 | 653 | 656 | rBV | 2104235 | 2244299 | 92.52% | 10.833% |
| 15 | 9.450 | 685 | 688 | 690 | rBV | 910068 | 774620 | 31.93% | 3.739% |
| 16 | 9.542 | 692 | 696 | 701 | rVB | 18553 | 37461 | 1.54% | 0.181% |
| 17 | 9.725 | 709 | 712 | 714 | rBV | 747865 | 679703 | 28.02% | 3.281% |
| 18 | 10.513 | 778 | 781 | 783 | rBV | 876067 | 885146 | 36.49% | 4.273% |
| 19 | 10.548 | 783 | 784 | 790 | rVV | 23628 | 28051 | 1.16% | 0.135% |
| 20 | 10.639 | 790 | 792 | 796 | rVB | 24586 | 39680 | 1.64% | 0.192% |
| 21 | 10.730 | 798 | 800 | 802 | rBV | 28741 | 25238 | 1.04% | 0.122% |
| 22 | 11.085 | 829 | 831 | 832 | rBV | 30728 | 34505 | 1.42% | 0.167% |
| 23 | 11.199 | 839 | 841 | 844 | rVB | 626662 | 558471 | 23.02% | 2.696% |
| 24 | 11.451 | 859 | 863 | 866 | rBV | 62029 | 93694 | 3.86% | 0.452% |
| 25 | 11.508 | 866 | 868 | 870 | rVB | 50144 | 44277 | 1.83% | 0.214% |
| 26 | 11.702 | 878 | 885 | 887 | rBV3 | 23366 | 55928 | 2.31% | 0.270% |
| 27 | 11.748 | 887 | 889 | 892 | rVB2 | 20957 | 38092 | 1.57% | 0.184% |
| 28 | 11.908 | 902 | 903 | 905 | rVB | 29447 | 26043 | 1.07% | 0.126% |
| 29 | 12.788 | 977 | 980 | 982 | rBV | 1926159 | 1854829 | 76.47% | 8.953% |
| 30 | 13.702 | 1057 | 1060 | 1063 | rBV2 | 34641 | 56622 | 2.33% | 0.273% |
| 31 | 13.828 | 1069 | 1071 | 1074 | rBV | 580602 | 570708 | 23.53% | 2.755% |
| 32 | 13.931 | 1078 | 1080 | 1082 | rVV | 38820 | 44603 | 1.84% | 0.215% |
| 33 | 15.211 | 1190 | 1192 | 1200 | rBV | 339514 | 426055 | 17.56% | 2.057% |

LSC Area Percent Report

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Data File : BF088137.D
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Operator : UM/SJ
Sample : H3501-17
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SB8-4-6

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

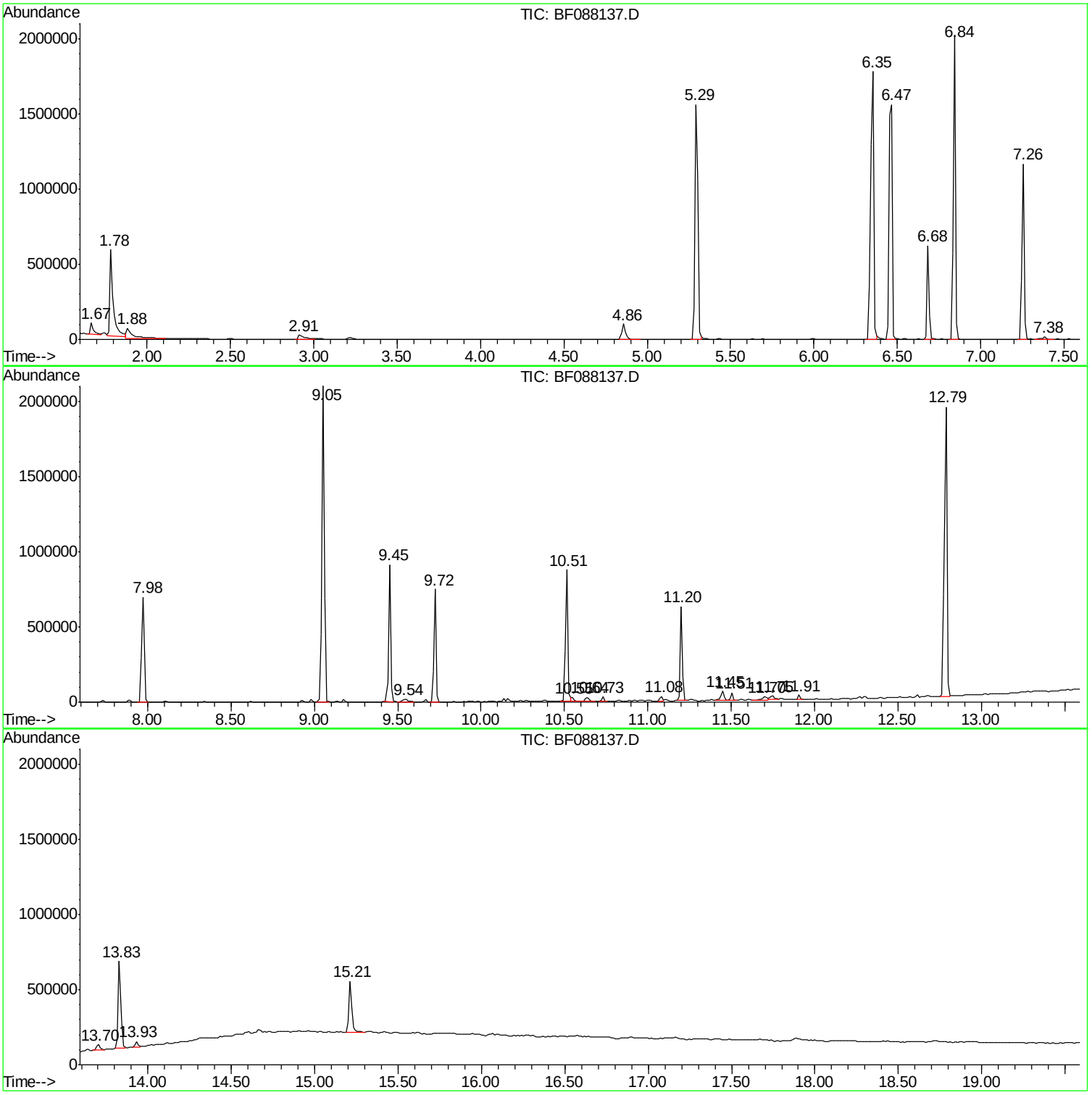
Sum of corrected areas: 20717102

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088137.D
Acq On : 18 Jun 2016 16:41
Operator : UM/SJ
Sample : H3501-17
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB8-4-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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\BF061816\
Data File : BF088137.D
Acq On : 18 Jun 2016 16:41
Operator : UM/SJ
Sample : H3501-17
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB8-4-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

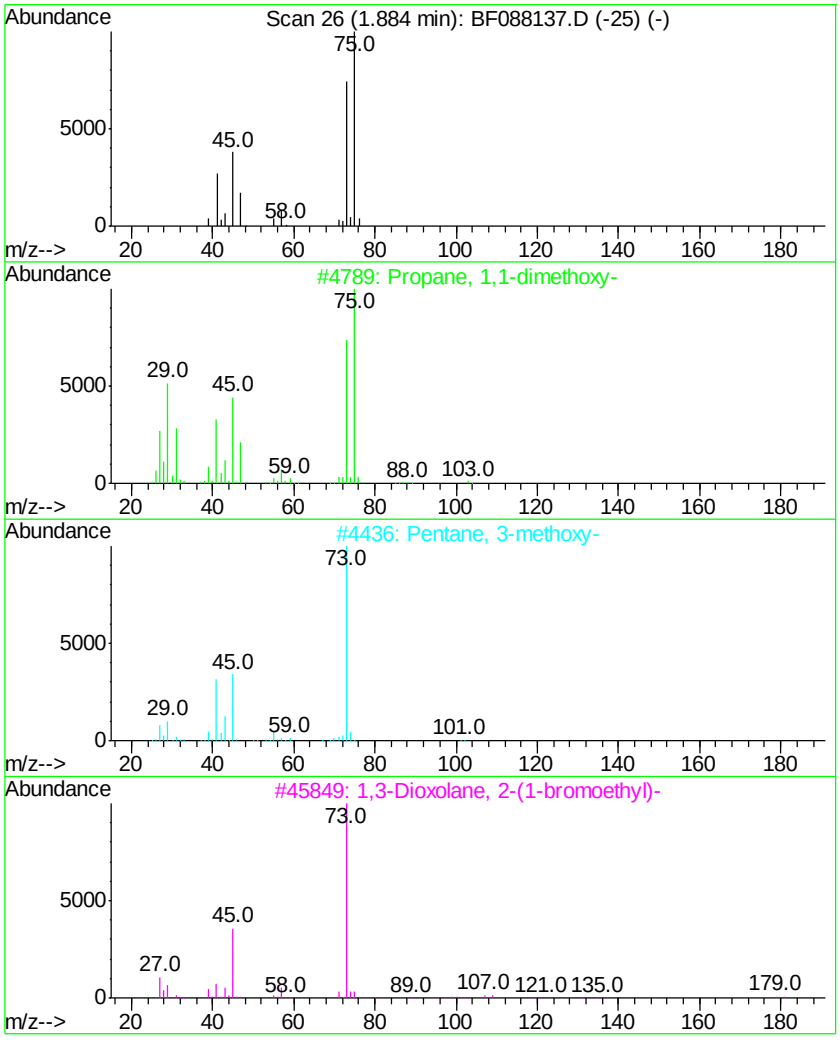
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

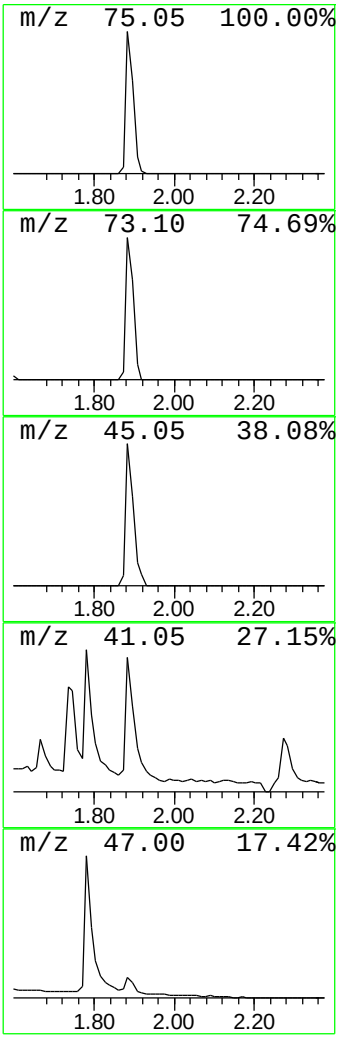
**********

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.88 | 6.61 ng | 182001 | 1,4-Dichlorobenzene-d4 | 6.68 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 1,1-dimethoxy- | 104 | C5H12O2 | 004744-10-9 | 74 |
| 2 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 35 |
| 3 | 1,3-Dioxolane, 2-(1-bromoethyl)- | 180 | C5H9BrO2 | 005267-73-2 | 12 |
| 4 | Thiocyanic acid, methyl ester | 73 | C2H3NS | 000556-64-9 | 9 |
| 5 | Glycine | 75 | C2H5NO2 | 000056-40-6 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088137.D
Acq On : 18 Jun 2016 16:41
Operator : UM/SJ
Sample : H3501-17
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB8-4-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

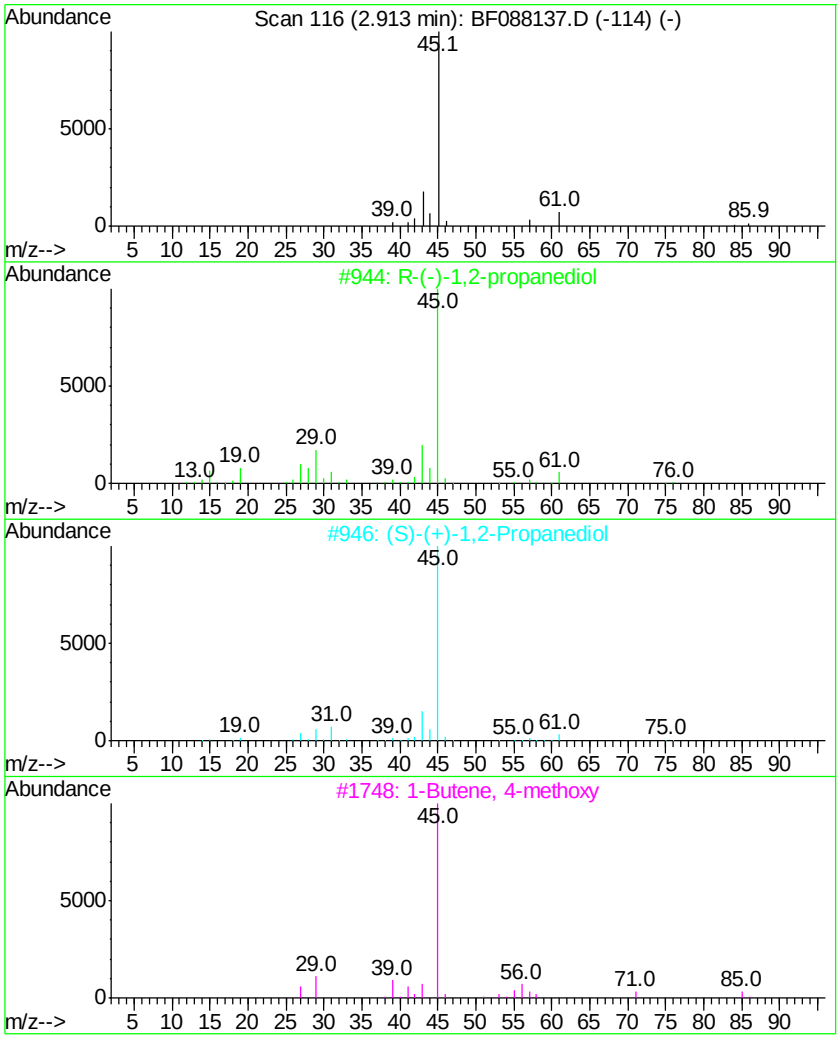
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

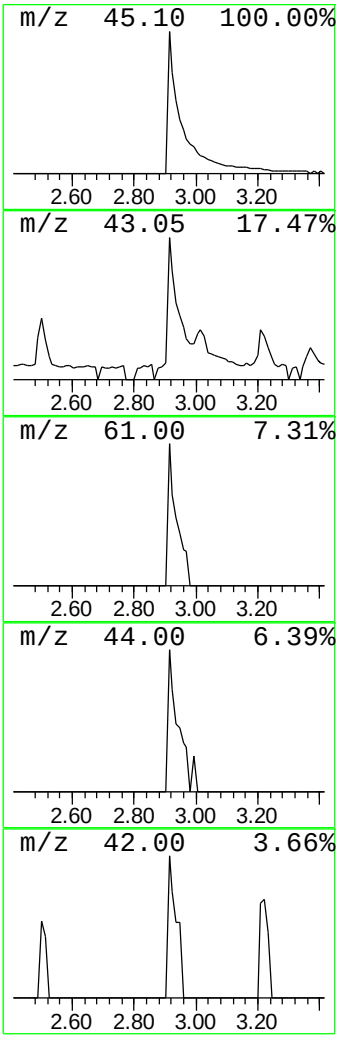
**********

Peak Number 4 R-(-)-1,2-propanediol Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.91 | 2.56 ng | 70452 | 1,4-Dichlorobenzene-d4 | 6.68 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | R-(-)-1,2-propanediol | 76 | C3H8O2 | 004254-14-2 | 64 |
| 2 | (S)-(+)-1,2-Propanediol | 76 | C3H8O2 | 004254-15-3 | 43 |
| 3 | 1-Butene, 4-methoxy | 86 | C5H10O | 004696-30-4 | 9 |
| 4 | Propylene Glycol | 76 | C3H8O2 | 000057-55-6 | 9 |
| 5 | Isopropyl Alcohol | 60 | C3H8O | 000067-63-0 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088137.D
Acq On : 18 Jun 2016 16:41
Operator : UM/SJ
Sample : H3501-17
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB8-4-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

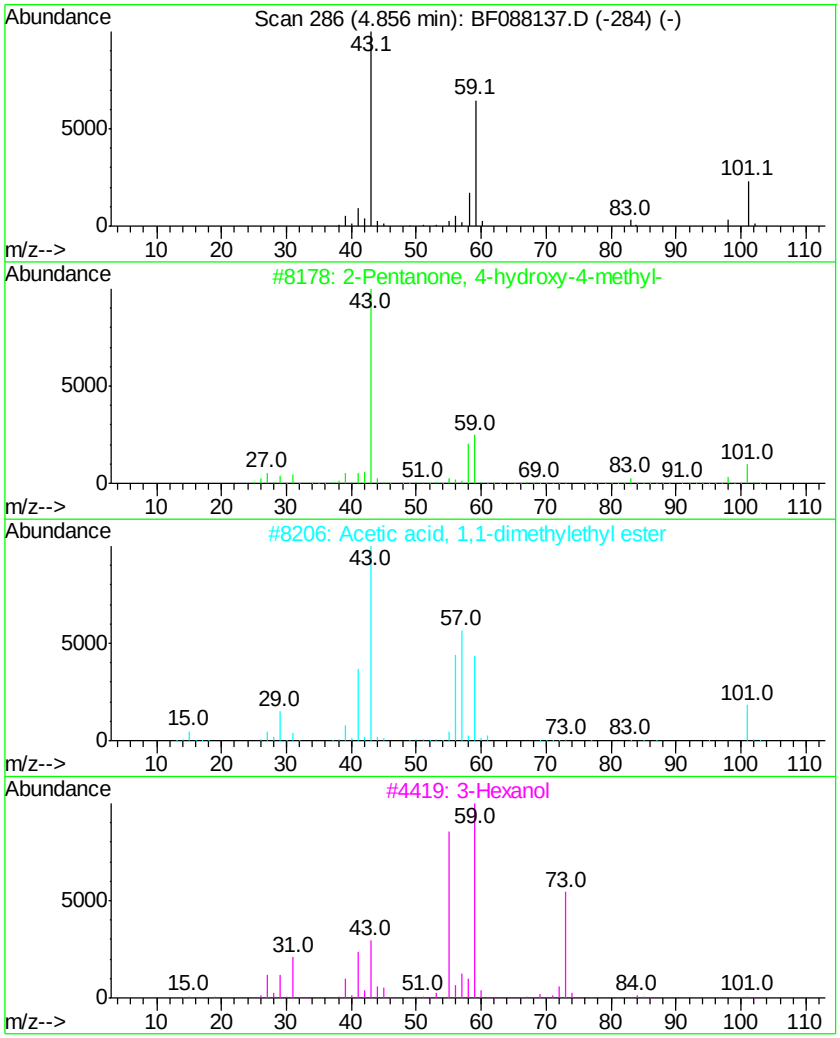
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

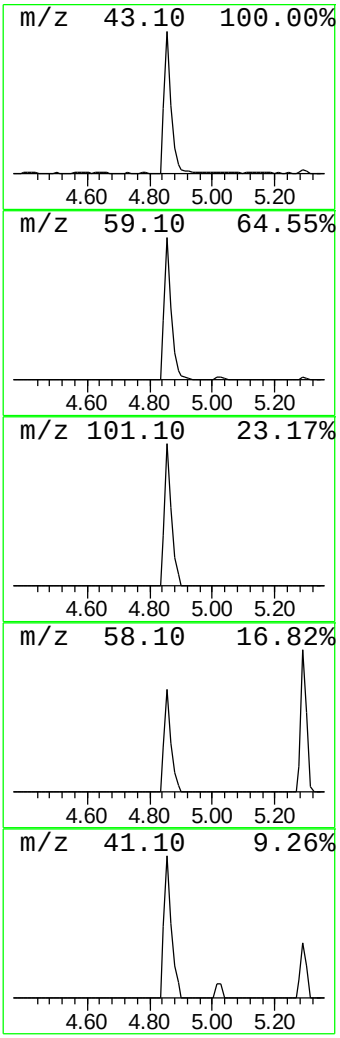
**********

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.86 | 5.70 ng | 156964 | 1,4-Dichlorobenzene-d4 | 6.68 |

| 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, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 3 | 3-Hexanol | 102 | C6H14O | 000623-37-0 | 25 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 5 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088137.D
Acq On : 18 Jun 2016 16:41
Operator : UM/SJ
Sample : H3501-17
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB8-4-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

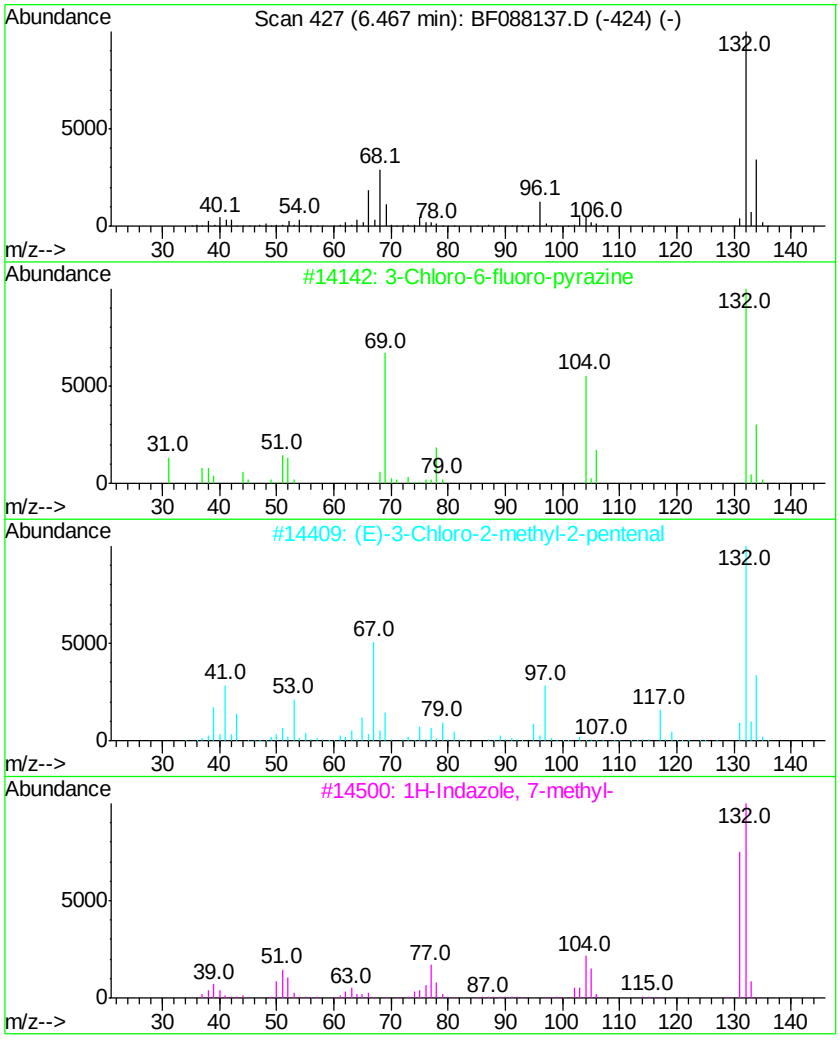
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

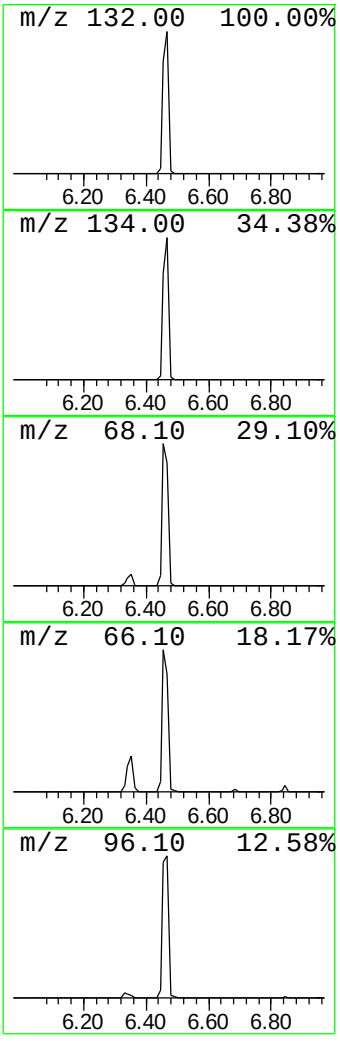
**********

Peak Number 6 3-Chloro-6-fluoro-pyrazine Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.47 | 78.81 ng | 2171140 | 1,4-Dichlorobenzene-d4 | 6.68 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 52 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 33 |
| 3 | 1H-Indazole, 7-methyl- | 132 | C8H8N2 | 1000316-00-7 | 25 |
| 4 | Xenon | 132 | Xe | 007440-63-3 | 9 |
| 5 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 9 |



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Data File : BF088137.D
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Operator : UM/SJ
Sample : H3501-17
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB8-4-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

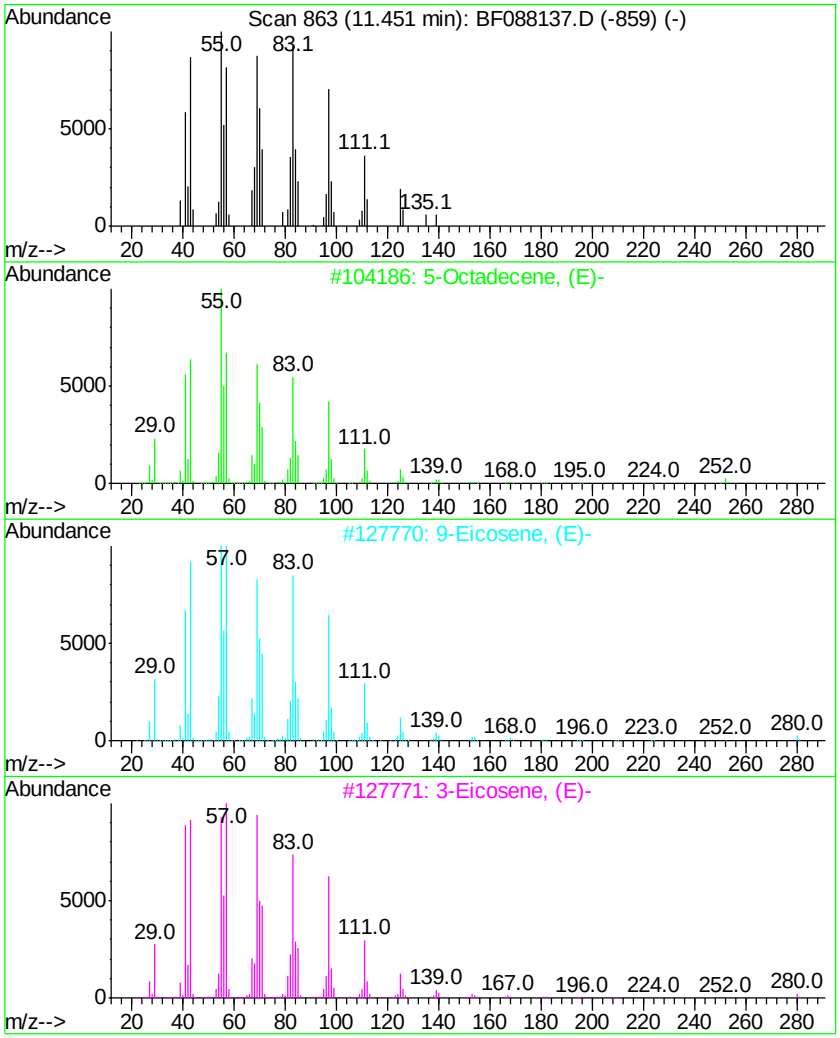
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

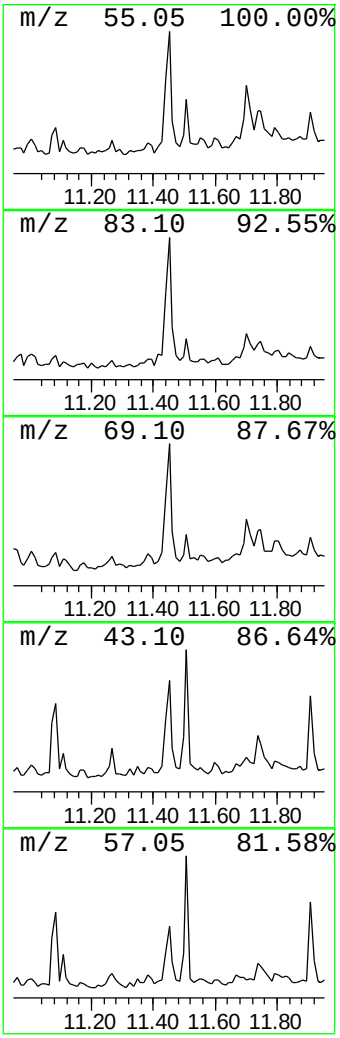
**********

Peak Number 8 5-Octadecene, (E)- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.45 | 3.36 ng | 93694 | Phenanthrene-d10 | 11.20 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Octadecene, (E)- | 252 | C18H36 | 007206-21-5 | 91 |
| 2 | 9-Eicosene, (E)- | 280 | C20H40 | 074685-29-3 | 87 |
| 3 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 74 |
| 4 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 68 |
| 5 | 1-Hexadecanol | 242 | C16H34O | 036653-82-4 | 64 |



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Acq On : 18 Jun 2016 16:41
Operator : UM/SJ
Sample : H3501-17
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB8-4-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

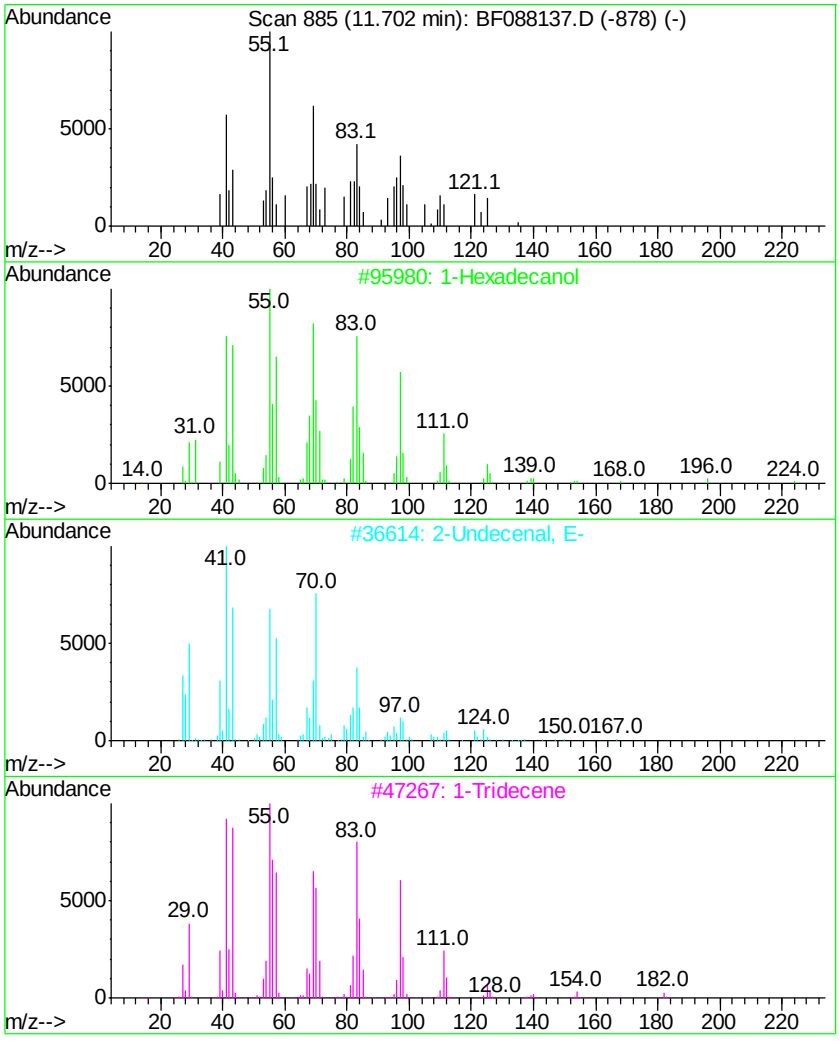
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

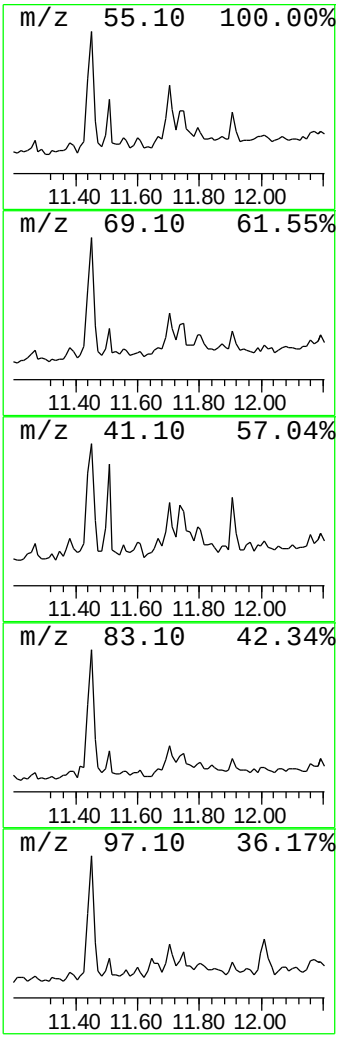
**********

Peak Number 9 unknown11.70 Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.70 | 2.00 ng | 55928 | Phenanthrene-d10 | 11.20 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Hexadecanol | 242 | C16H34O | 036653-82-4 | 43 |
| 2 | 2-Undecenal, E- | 168 | C11H20O | 053448-07-0 | 42 |
| 3 | 1-Tridecene | 182 | C13H26 | 002437-56-1 | 38 |
| 4 | 2-Tridecenal, (E)- | 196 | C13H24O | 007069-41-2 | 35 |
| 5 | 1,14-Tetradecanediol | 230 | C14H30O2 | 019812-64-7 | 32 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088137.D
Acq On : 18 Jun 2016 16:41
Operator : UM/SJ
Sample : H3501-17
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB8-4-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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 |
| Propane, 1,1-dime... | 1.88 | 6.6 | ng | 182001 | 1 | 6.68 | 550953 | 20.0 |
| R-(-)-1,2-propane... | 2.91 | 2.6 | ng | 70452 | 1 | 6.68 | 550953 | 20.0 |
| 2-Pentanone, 4-hy... | 4.86 | 5.7 | ng | 156964 | 1 | 6.68 | 550953 | 20.0 |
| 3-Chloro-6-fluoro... | 6.47 | 78.8 | ng | 2171140 | 1 | 6.68 | 550953 | 20.0 |
| 5-Octadecene, (E)- | 11.45 | 3.4 | ng | 93694 | 4 | 11.20 | 558471 | 20.0 |
| unknown11.70 | 11.70 | 2.0 | ng | 55928 | 4 | 11.20 | 558471 | 20.0 |