LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061115\
Data File : BF079922.D
Acq On : 12 Jun 2015 5:48
Operator : TP/IZ
Sample : G2573-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4

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-BF061115.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 | 2.170 | 85 | 86 | 92 | rVV | 131433 | 167299 | 2.83% | 0.741% |
| 2 | 2.273 | 92 | 95 | 98 | rVB | 4374244 | 5905547 | 100.00% | 26.160% |
| 3 | 2.353 | 100 | 102 | 110 | rBV | 522064 | 903227 | 15.29% | 4.001% |
| 4 | 2.707 | 130 | 133 | 137 | rVB | 272125 | 376037 | 6.37% | 1.666% |
| 5 | 5.622 | 384 | 388 | 391 | rBV | 98883 | 164137 | 2.78% | 0.727% |
| 6 | 6.010 | 419 | 422 | 424 | rBV | 1200278 | 1402232 | 23.74% | 6.212% |
| 7 | 6.993 | 506 | 508 | 510 | rBV | 1801149 | 1564969 | 26.50% | 6.932% |
| 8 | 7.165 | 520 | 523 | 525 | rBV | 1149994 | 1487114 | 25.18% | 6.588% |
| 9 | 7.393 | 541 | 543 | 545 | rVB | 346022 | 278172 | 4.71% | 1.232% |
| 10 | 7.553 | 555 | 557 | 559 | rBV | 1477006 | 1186837 | 20.10% | 5.257% |
| 11 | 7.953 | 589 | 592 | 594 | rBV | 674666 | 795653 | 13.47% | 3.525% |
| 12 | 8.685 | 654 | 656 | 658 | rVB | 486959 | 381096 | 6.45% | 1.688% |
| 13 | 9.759 | 748 | 750 | 753 | rVB | 2245609 | 1841390 | 31.18% | 8.157% |
| 14 | 10.456 | 809 | 811 | 814 | rBV | 493064 | 450632 | 7.63% | 1.996% |
| 15 | 11.256 | 878 | 881 | 883 | rBV | 927770 | 1079980 | 18.29% | 4.784% |
| 16 | 11.965 | 941 | 943 | 947 | rVB | 574670 | 516762 | 8.75% | 2.289% |
| 17 | 12.502 | 985 | 990 | 997 | rBV2 | 135820 | 194834 | 3.30% | 0.863% |
| 18 | 12.925 | 1025 | 1027 | 1032 | rBV | 249915 | 265858 | 4.50% | 1.178% |
| 19 | 13.657 | 1088 | 1091 | 1094 | rBV | 2490872 | 2361081 | 39.98% | 10.459% |
| 20 | 14.708 | 1181 | 1183 | 1187 | rBV2 | 104520 | 165543 | 2.80% | 0.733% |
| 21 | 14.937 | 1201 | 1203 | 1205 | rBV | 539029 | 560258 | 9.49% | 2.482% |
| 22 | 16.857 | 1367 | 1371 | 1374 | rBV | 301910 | 525984 | 8.91% | 2.330% |

Sum of corrected areas: 22574642

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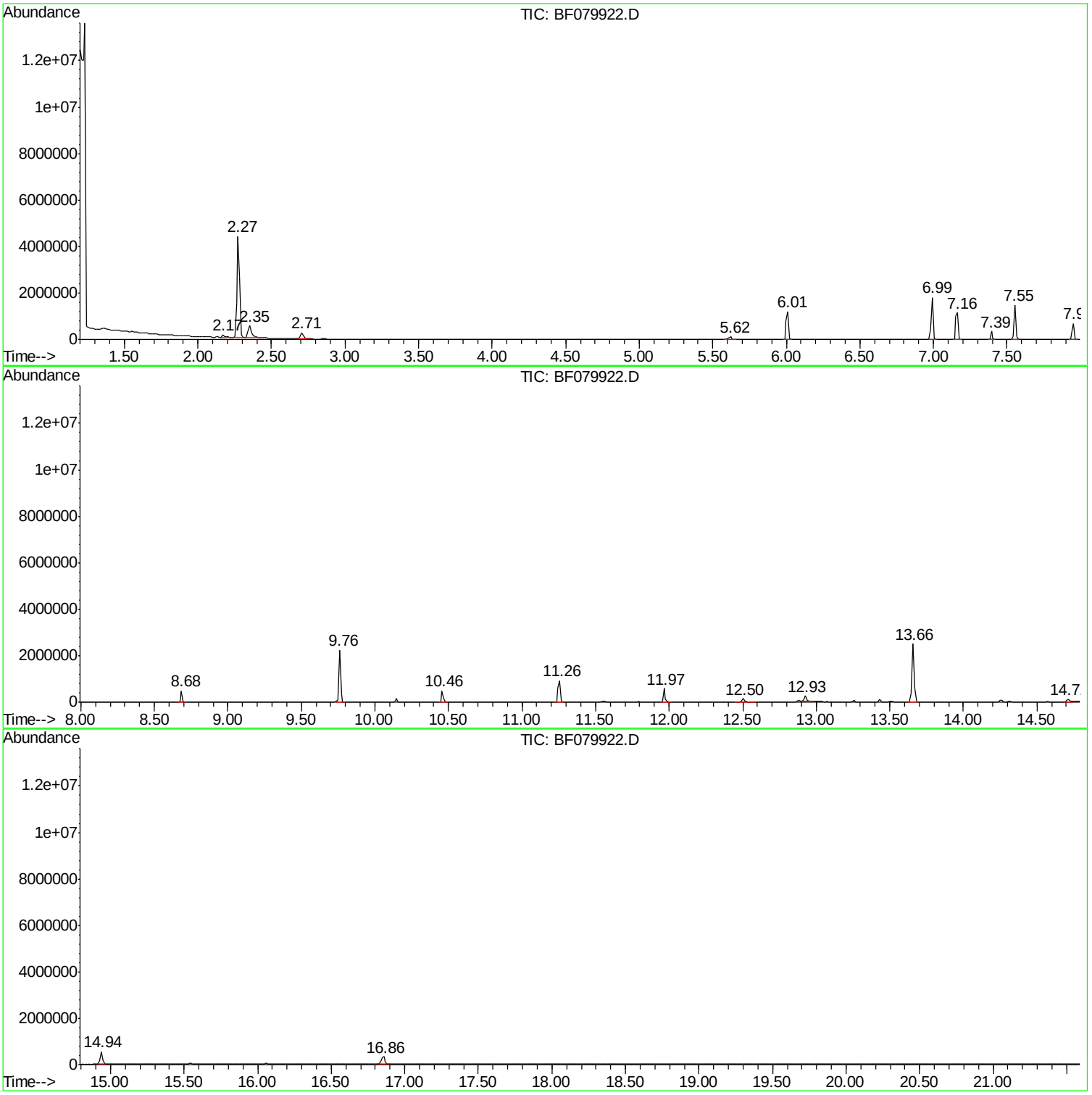
ALS Vial : 33 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
S4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF079922.D
Acq On : 12 Jun 2015 5:48
Operator : TP/IZ
Sample : G2573-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

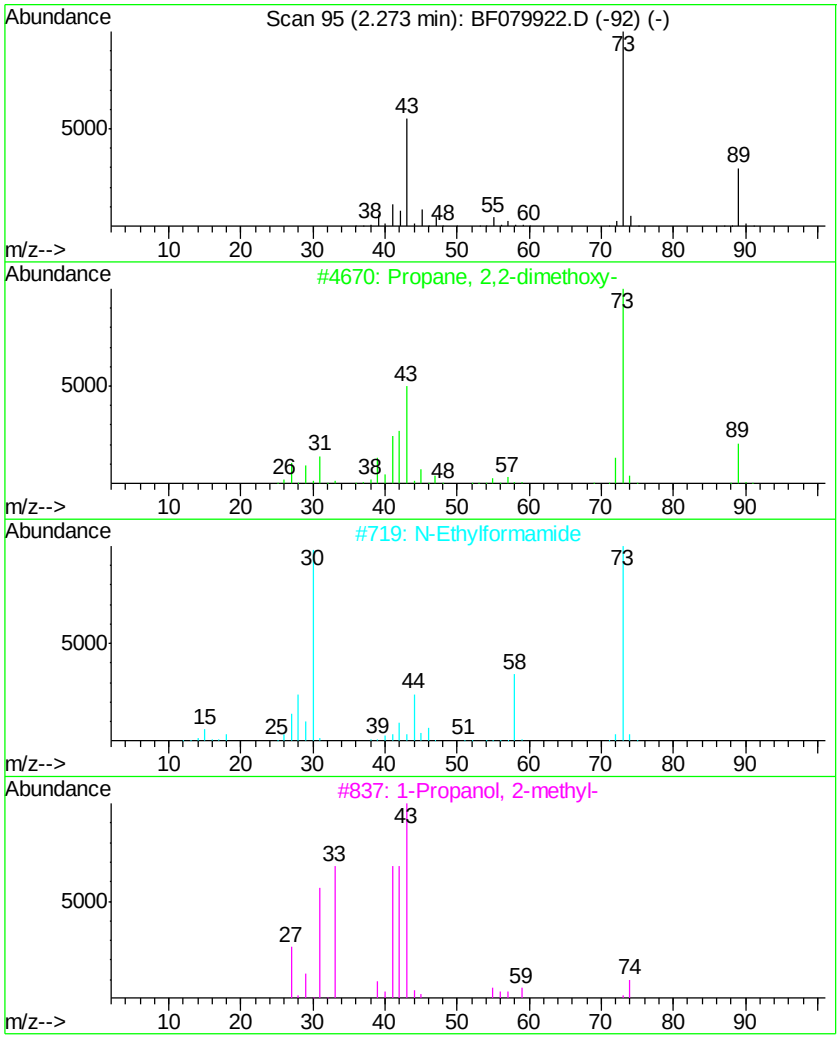
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

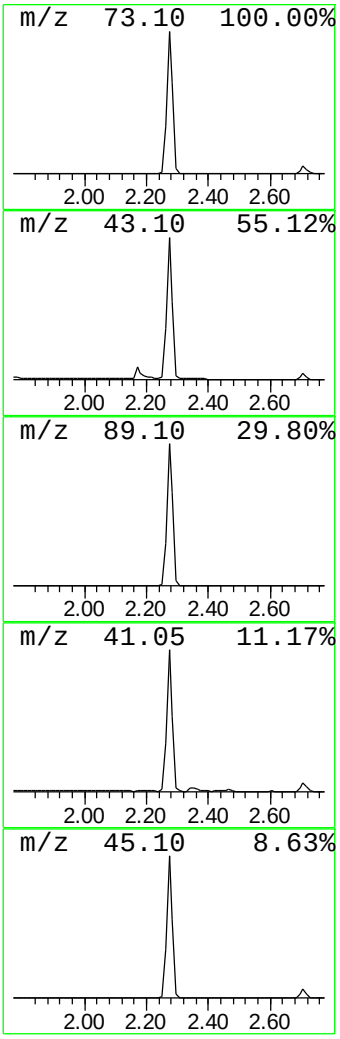
**********

Peak Number 2 Propane, 2,2-dimethoxy- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.27 | 424.60 ng | 5905550 | 1,4-Dichlorobenzene-d4 | 7.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 2,2-dimethoxy- | 104 | C5H12O2 | 000077-76-9 | 72 |
| 2 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |
| 3 | 1-Propanol, 2-methyl- | 74 | C4H10O | 000078-83-1 | 9 |
| 4 | Propanoic acid, 2-methyl-, propy... | 130 | C7H14O2 | 000644-49-5 | 9 |
| 5 | 1-Hexen-4-ol, 1-chloro-3,5-dimet... | 162 | C8H15ClO | 100244-09-5 | 9 |



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Data File : BF079922.D
Acq On : 12 Jun 2015 5:48
Operator : TP/IZ
Sample : G2573-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

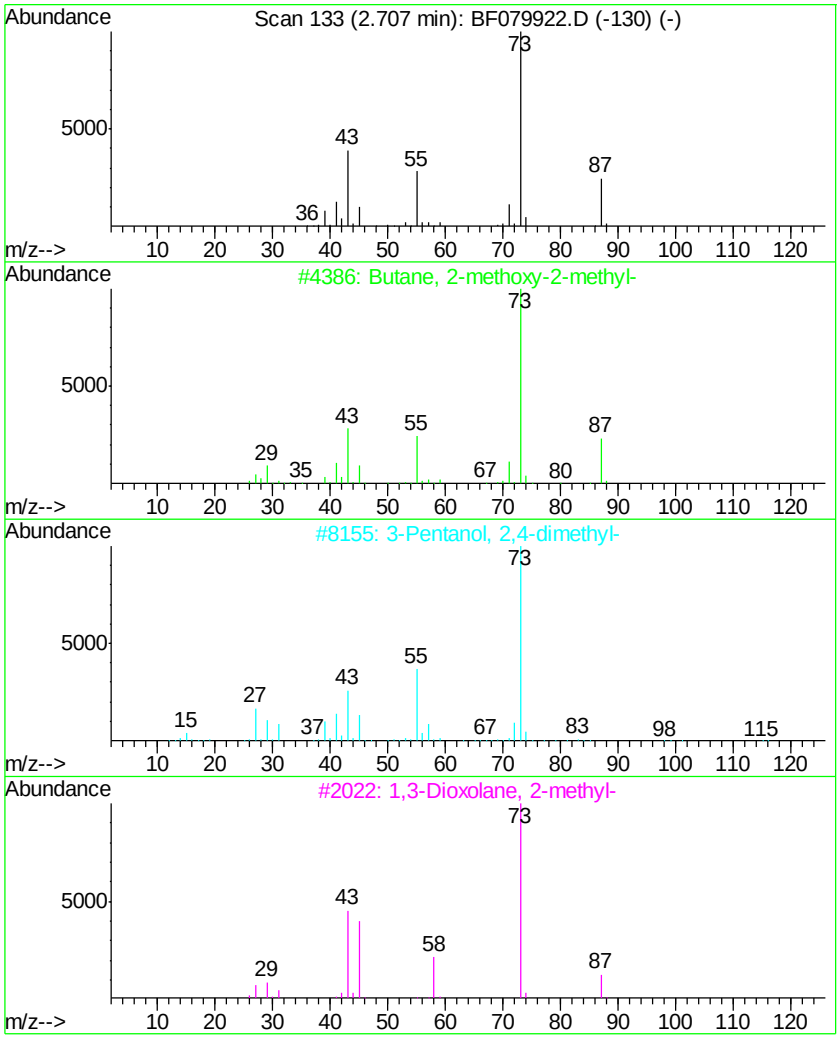
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

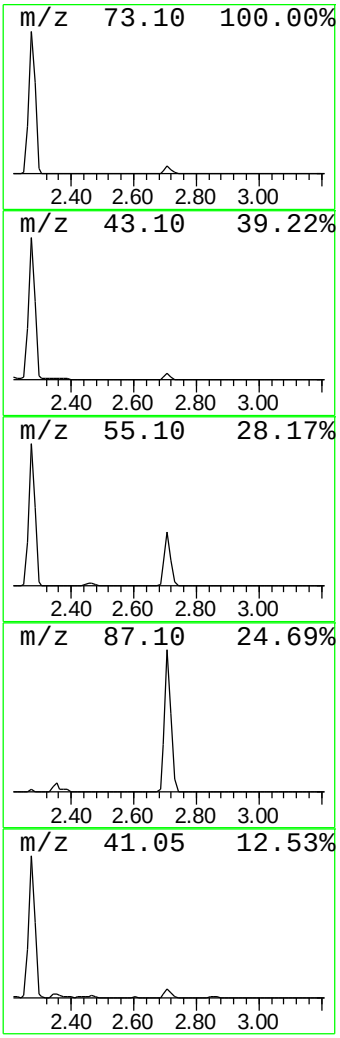
**********

Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.71 | 27.04 ng | 376037 | 1,4-Dichlorobenzene-d4 | 7.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 3-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000600-36-2 | 37 |
| 3 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 25 |
| 4 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 12 |
| 5 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 10 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061115\
Data File : BF079922.D
Acq On : 12 Jun 2015 5:48
Operator : TP/IZ
Sample : G2573-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

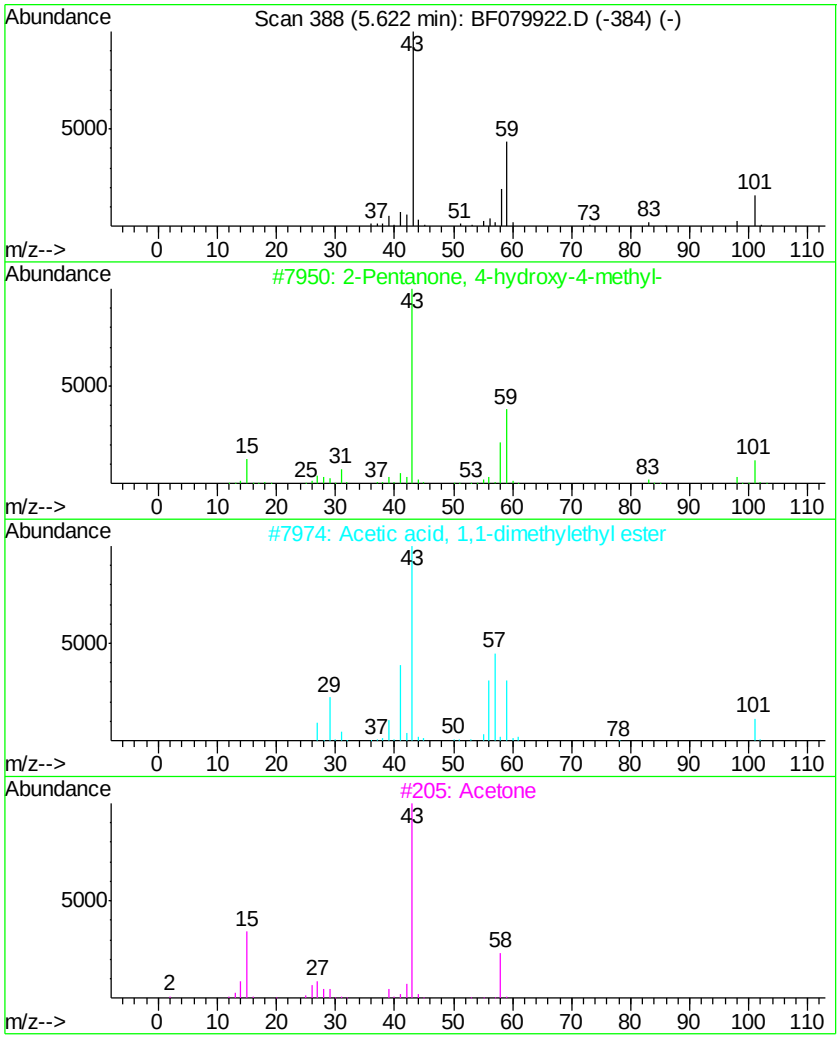
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

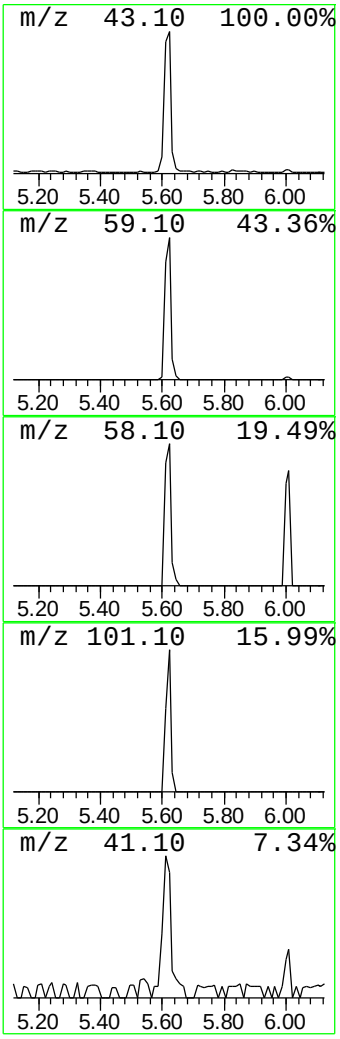
**********

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.62 | 11.80 ng | 164137 | 1,4-Dichlorobenzene-d4 | 7.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 78 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 36 |
| 3 | Acetone | 58 | C3H6O | 000067-64-1 | 16 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 12 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061115\
Data File : BF079922.D
Acq On : 12 Jun 2015 5:48
Operator : TP/IZ
Sample : G2573-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

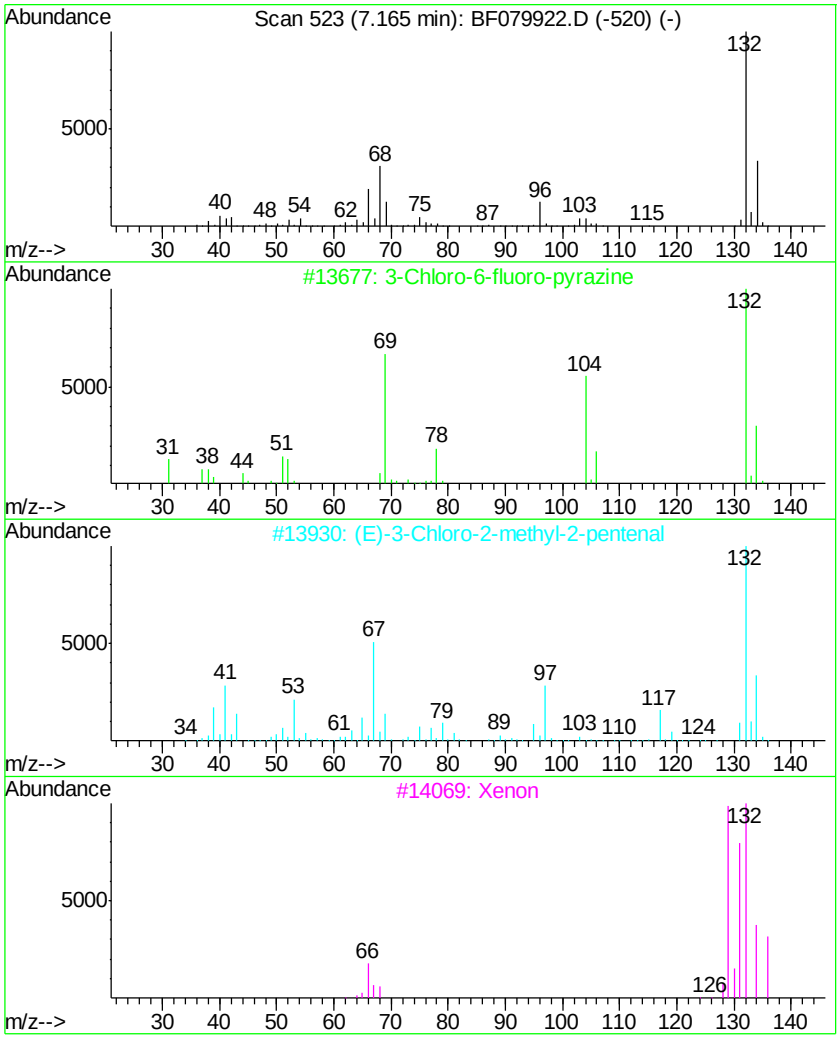
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

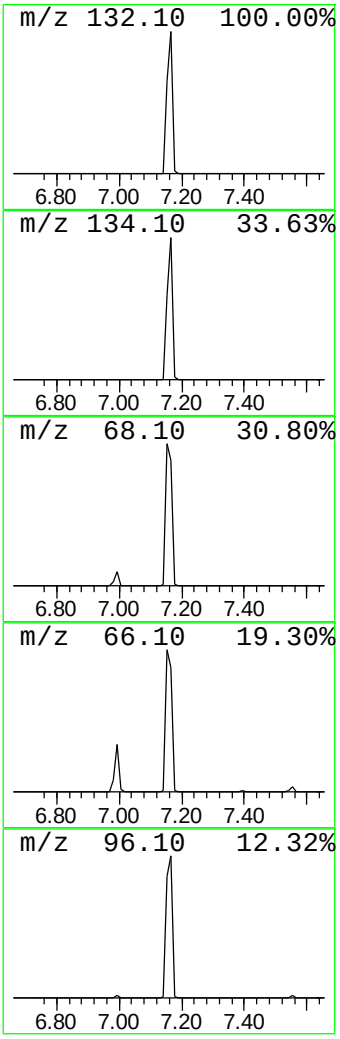
**********

Peak Number 6 unknown7.16 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.16 | 106.92 ng | 1487110 | 1,4-Dichlorobenzene-d4 | 7.39 |

| 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 | 25 |
| 3 | Xenon | 132 | Xe | 007440-63-3 | 9 |
| 4 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 9 |
| 5 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 9 |



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Data File : BF079922.D
Acq On : 12 Jun 2015 5:48
Operator : TP/IZ
Sample : G2573-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

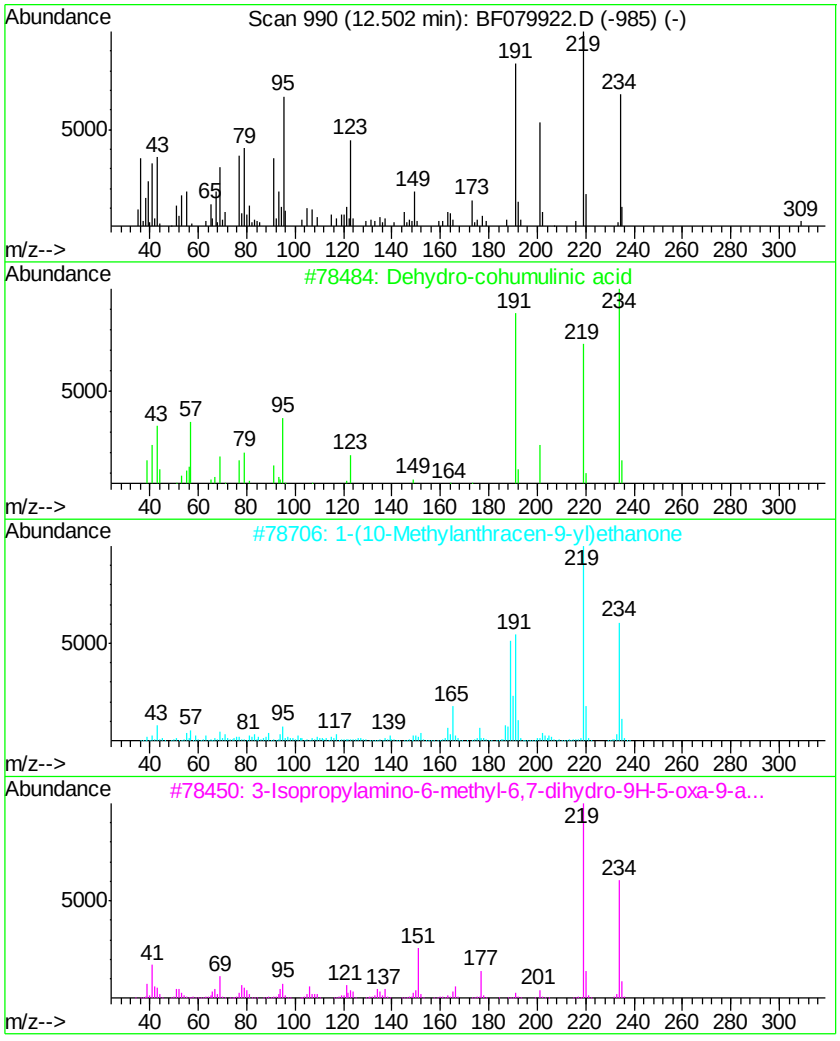
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

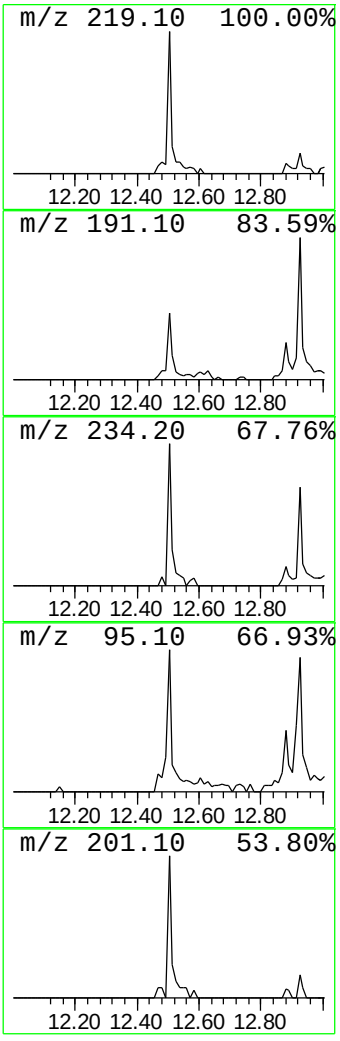
**********

Peak Number 8 Dehydro-cohumulinic acid Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.50 | 7.54 ng | 194834 | Phenanthrene-d10 | 11.97 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dehydro-cohumulinic acid | 234 | C14H18O3 | 1000041-27-1 | 95 |
| 2 | 1-(10-Methylanthracen-9-yl)ethanone | 234 | C17H14O | 036778-18-4 | 49 |
| 3 | 3-Isopropylamino-6-methyl-6,7-di... | 234 | C13H18N2O2 | 145220-69-5 | 46 |
| 4 | Ethanone, 1-(4,6-dihydroxy-2,3,5... | 234 | C13H14O4 | 021987-07-5 | 35 |
| 5 | 2-Propanone, 1-(5-phenyl-3H-1,2-... | 234 | C12H10OS2 | 027315-83-9 | 30 |



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Data File : BF079922.D
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Operator : TP/IZ
Sample : G2573-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

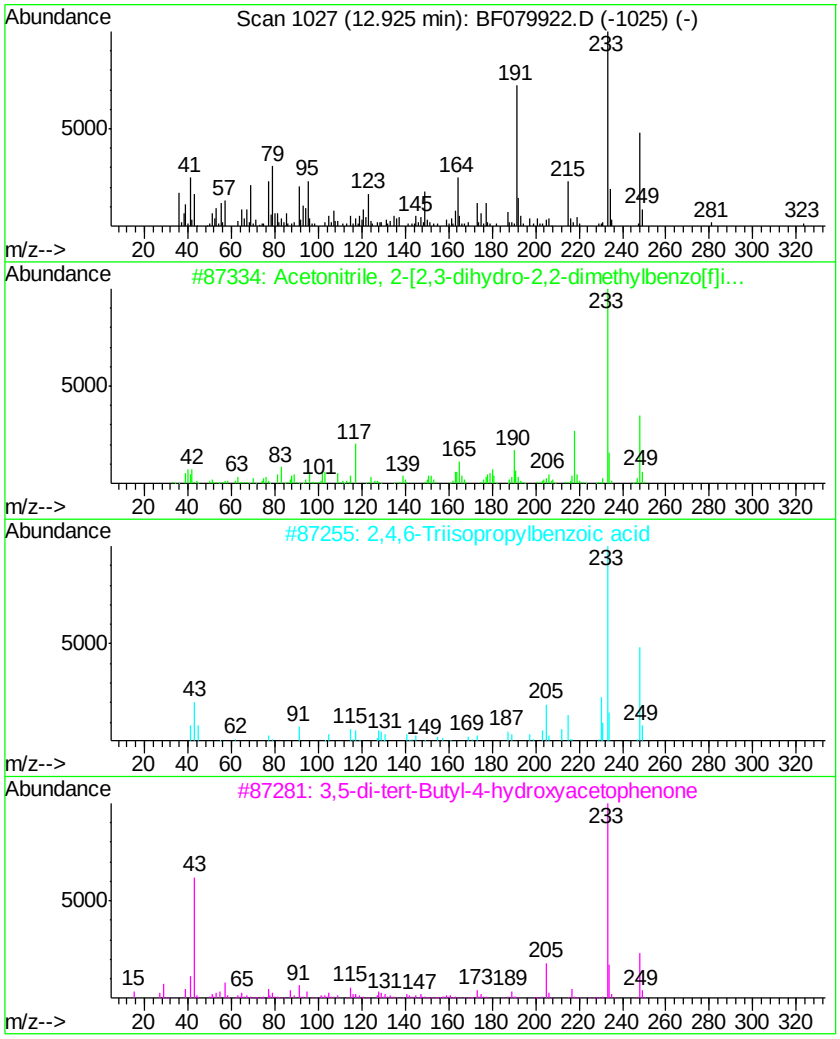
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

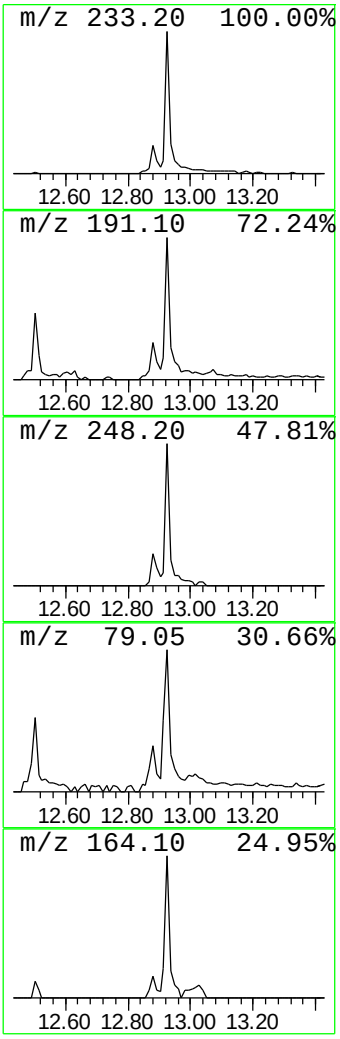
**********

Peak Number 9 unknown12.93 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.93 | 10.29 ng | 265858 | Phenanthrene-d10 | 11.97 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Acetonitrile, 2-[2,3-dihydro-2,2... | 248 | C17H16N2 | 144498-83-9 | 49 |
| 2 | 2,4,6-Triisopropylbenzoic acid | 248 | C16H24O2 | 049623-71-4 | 46 |
| 3 | 3,5-di-tert-Butyl-4-hydroxyaceto... | 248 | C16H24O2 | 014035-33-7 | 43 |
| 4 | Phenanthro[9,10-d]oxazole, 2-met... | 233 | C16H11NO | 021639-88-3 | 38 |
| 5 | 2(1H)-Pyrimidinethione, 3,4-dihy... | 248 | C13H16N2OS | 063704-47-2 | 38 |



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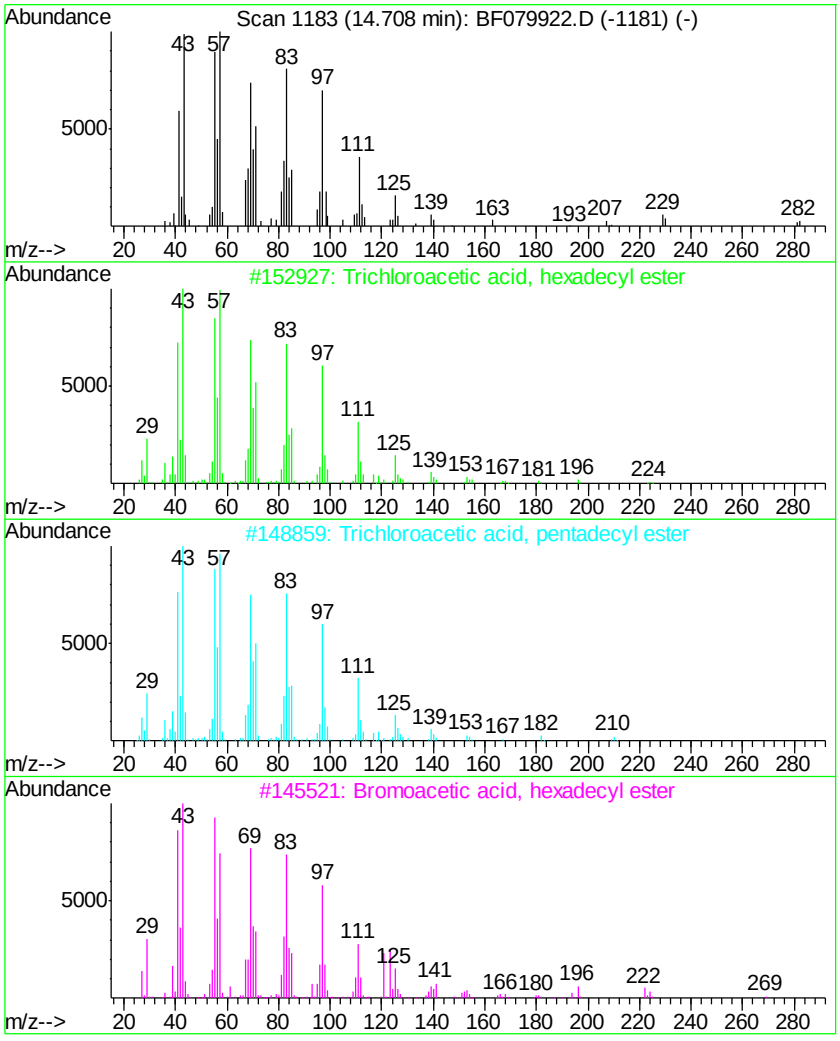
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

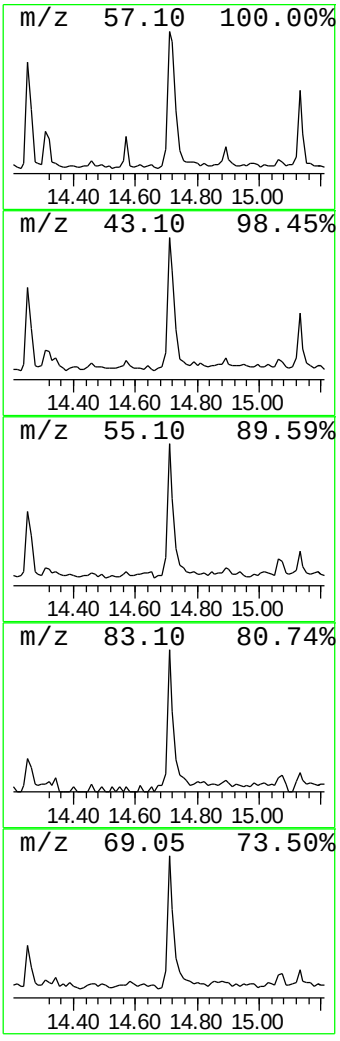
**********

Peak Number 10 Trichloroacetic acid, hexad... Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.71 | 5.91 ng | 165543 | Chrysene-d12 | 14.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94 |
| 2 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 94 |
| 3 | Bromoacetic acid, hexadecyl ester | 362 | C18H35BrO2 | 005454-48-8 | 93 |
| 4 | 2- Chloropropionic acid, pentade... | 318 | C18H35ClO2 | 1000292-44-1 | 91 |
| 5 | 1-Tetracosanol | 354 | C24H50O | 000506-51-4 | 91 |



Tentatively Identified Compound (LSC) summary

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Sample : G2573-04
Misc :
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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, 2,2-dime... | 2.27 | 424.6 | ng | 5905550 | 1 | 7.39 | 278172 | 20.0 |
| Butane, 2-methoxy... | 2.71 | 27.0 | ng | 376037 | 1 | 7.39 | 278172 | 20.0 |
| 2-Pentanone, 4-hy... | 5.62 | 11.8 | ng | 164137 | 1 | 7.39 | 278172 | 20.0 |
| unknown7.16 | 7.16 | 106.9 | ng | 1487110 | 1 | 7.39 | 278172 | 20.0 |
| Dehydro-cohumulin... | 12.50 | 7.5 | ng | 194834 | 4 | 11.97 | 516762 | 20.0 |
| unknown12.93 | 12.93 | 10.3 | ng | 265858 | 4 | 11.97 | 516762 | 20.0 |
| Trichloroacetic a... | 14.71 | 5.9 | ng | 165543 | 5 | 14.94 | 560258 | 20.0 |