LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
Data File : BF085475.D
Acq On : 16 Mar 2016 21:33
Operator : UM/SJ
Sample : H1788-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2(8-9)

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-BF031516.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 | 244 | 246 | 253 | rBV | 90879 | 125979 | 3.59% | 0.415% |
| 2 | 5.510 | 279 | 282 | 284 | rBV | 2170761 | 3140223 | 89.50% | 10.338% |
| 3 | 6.527 | 368 | 371 | 374 | rBV | 2447555 | 2960517 | 84.38% | 9.746% |
| 4 | 6.664 | 381 | 383 | 386 | rBV | 2760060 | 3099106 | 88.33% | 10.202% |
| 5 | 6.904 | 401 | 404 | 406 | rBV | 569871 | 694601 | 19.80% | 2.287% |
| 6 | 7.053 | 415 | 417 | 420 | rBV | 2222569 | 2462679 | 70.19% | 8.107% |
| 7 | 7.464 | 450 | 453 | 455 | rBV | 2197521 | 2106605 | 60.04% | 6.935% |
| 8 | 8.184 | 514 | 516 | 518 | rBV | 1173704 | 974229 | 27.77% | 3.207% |
| 9 | 9.259 | 608 | 610 | 613 | rBV | 2765373 | 3508723 | 100.00% | 11.551% |
| 10 | 9.659 | 643 | 645 | 647 | rBV | 610004 | 587781 | 16.75% | 1.935% |
| 11 | 9.876 | 662 | 664 | 666 | rVB | 74873 | 79480 | 2.27% | 0.262% |
| 12 | 9.945 | 667 | 670 | 672 | rVB | 1041098 | 1065594 | 30.37% | 3.508% |
| 13 | 10.368 | 706 | 707 | 709 | rVB | 121449 | 113291 | 3.23% | 0.373% |
| 14 | 10.585 | 723 | 726 | 730 | rBV | 39727 | 75428 | 2.15% | 0.248% |
| 15 | 10.733 | 736 | 739 | 741 | rBV | 2135479 | 2340564 | 66.71% | 7.705% |
| 16 | 10.848 | 747 | 749 | 756 | rBV | 112097 | 162742 | 4.64% | 0.536% |
| 17 | 11.042 | 764 | 766 | 770 | rBV4 | 14234 | 36894 | 1.05% | 0.121% |
| 18 | 11.293 | 786 | 788 | 789 | rBV | 60449 | 54592 | 1.56% | 0.180% |
| 19 | 11.431 | 797 | 800 | 802 | rBV | 762056 | 1062309 | 30.28% | 3.497% |
| 20 | 11.945 | 843 | 845 | 858 | rBV3 | 107906 | 172379 | 4.91% | 0.567% |
| 21 | 12.734 | 912 | 914 | 918 | rBV | 40767 | 43653 | 1.24% | 0.144% |
| 22 | 13.008 | 935 | 938 | 941 | rBV | 2904137 | 3280565 | 93.50% | 10.800% |
| 23 | 13.579 | 985 | 988 | 992 | rVB | 37352 | 41198 | 1.17% | 0.136% |
| 24 | 13.899 | 1014 | 1016 | 1024 | rBV | 205070 | 299723 | 8.54% | 0.987% |
| 25 | 14.059 | 1026 | 1030 | 1033 | rBV | 1003210 | 925858 | 26.39% | 3.048% |
| 26 | 14.219 | 1043 | 1044 | 1047 | rBV | 46235 | 58716 | 1.67% | 0.193% |
| 27 | 14.528 | 1069 | 1071 | 1074 | rBV | 73281 | 82731 | 2.36% | 0.272% |
| 28 | 14.825 | 1095 | 1097 | 1100 | rVB | 36435 | 49363 | 1.41% | 0.163% |
| 29 | 15.157 | 1124 | 1126 | 1129 | rBV | 40752 | 54405 | 1.55% | 0.179% |
| 30 | 15.511 | 1154 | 1157 | 1162 | rBV | 392464 | 617495 | 17.60% | 2.033% |
| 31 | 16.014 | 1198 | 1201 | 1213 | rVB6 | 17421 | 59652 | 1.70% | 0.196% |
| 32 | 16.448 | 1236 | 1239 | 1248 | rBV7 | 15161 | 39649 | 1.13% | 0.131% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
Data File : BF085475.D
Acq On : 16 Mar 2016 21:33
Operator : UM/SJ
Sample : H1788-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2(8-9)

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-BF031516.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

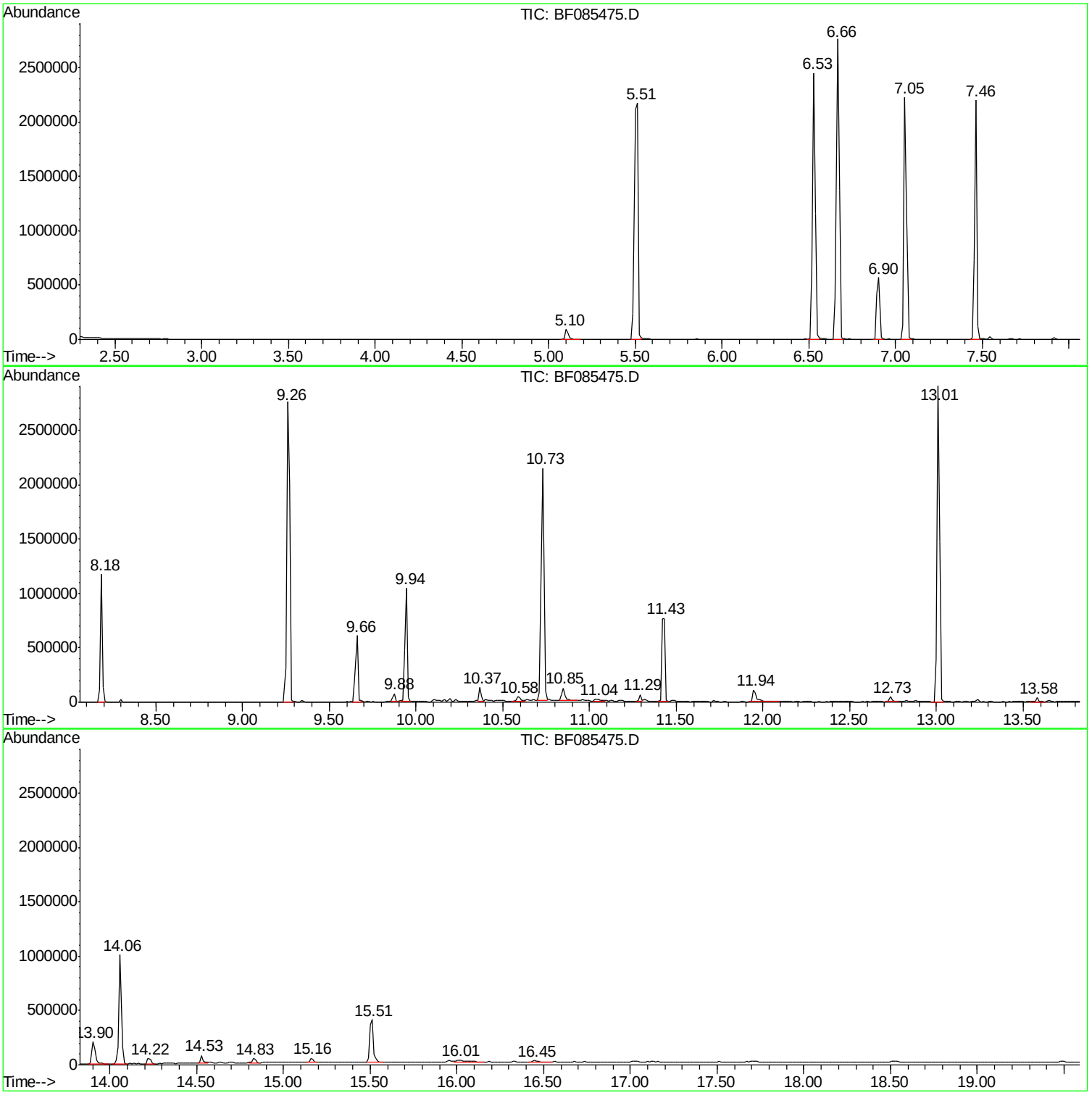
Sum of corrected areas: 30376724

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
Data File : BF085475.D
Acq On : 16 Mar 2016 21:33
Operator : UM/SJ
Sample : H1788-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2(8-9)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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\BF031616\
Data File : BF085475.D
Acq On : 16 Mar 2016 21:33
Operator : UM/SJ
Sample : H1788-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2(8-9)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

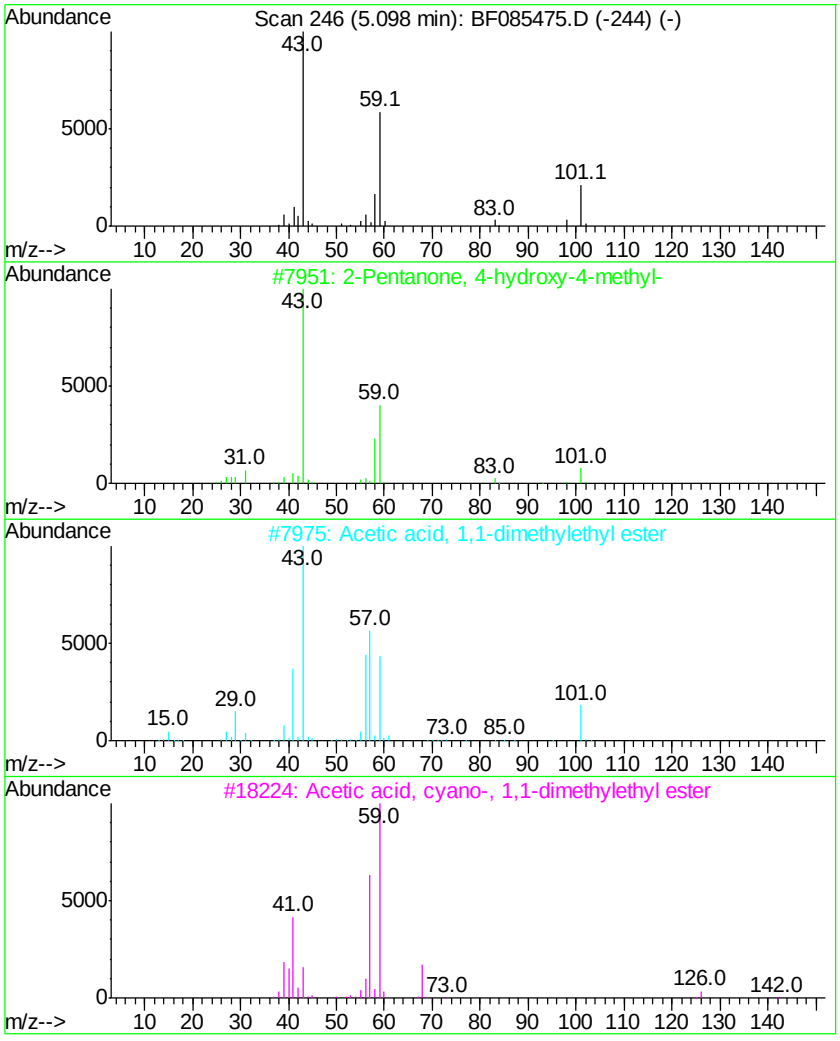
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

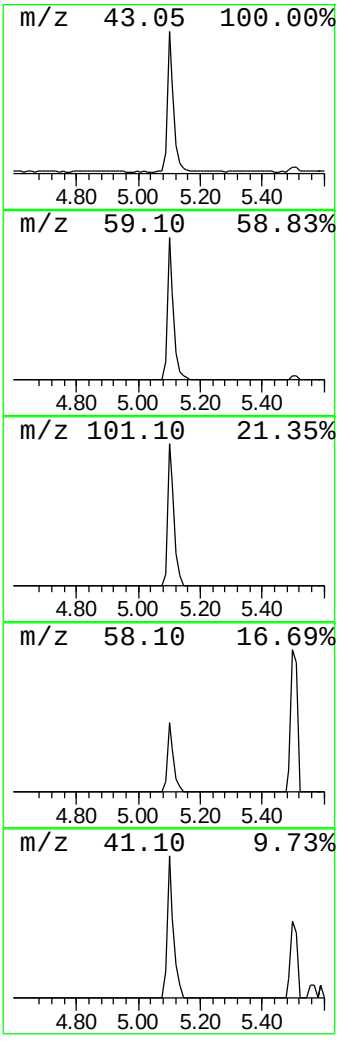
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.10 | 3.63 ng | 125979 | 1,4-Dichlorobenzene-d4 | 6.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 42 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 4 | Acetone | 58 | C3H6O | 000067-64-1 | 10 |
| 5 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
Data File : BF085475.D
Acq On : 16 Mar 2016 21:33
Operator : UM/SJ
Sample : H1788-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SB-2(8-9)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

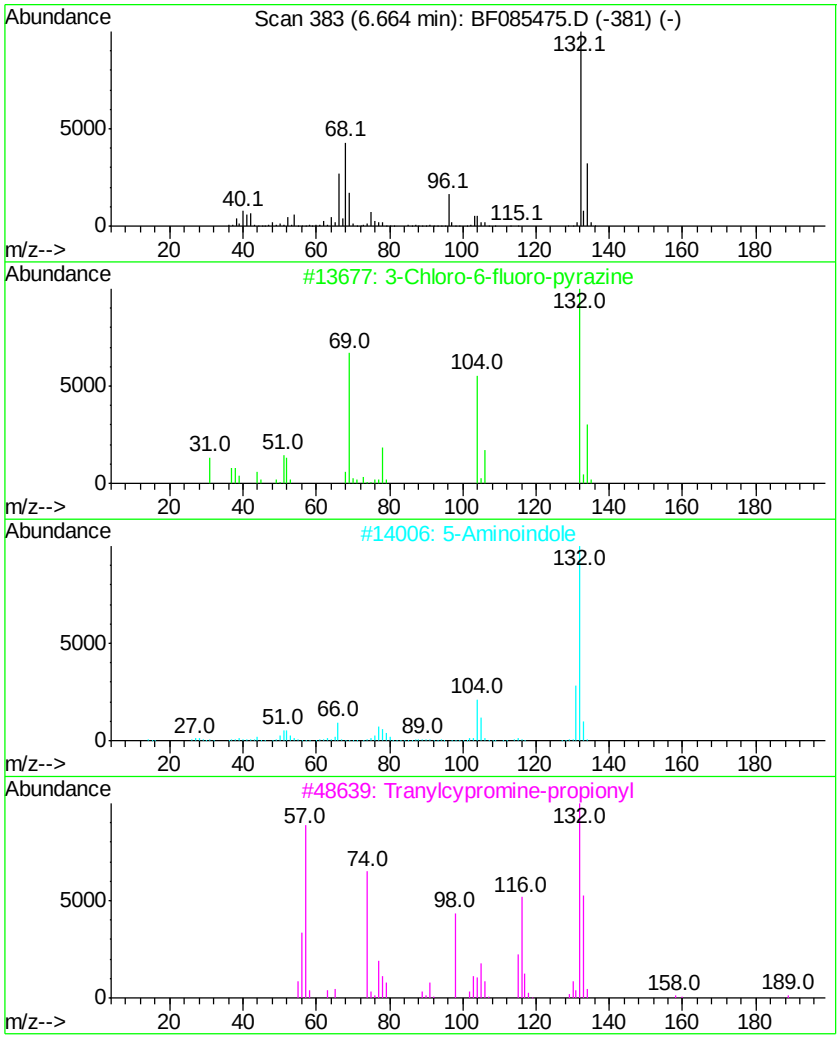
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

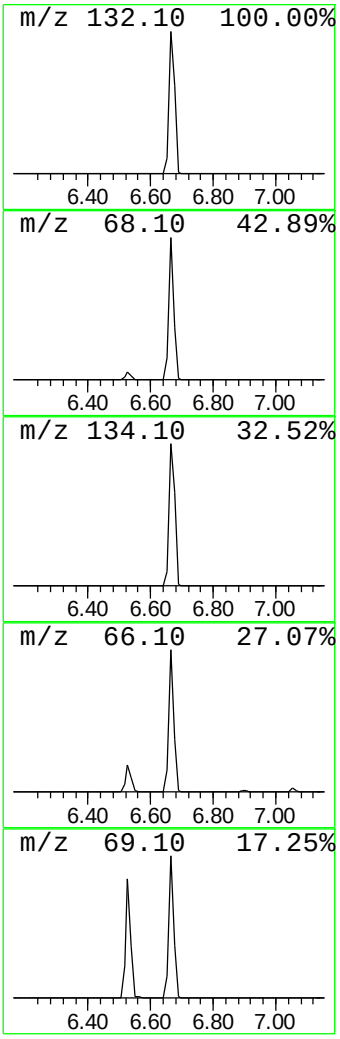
**********

Peak Number 2 unknown6.66 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.66 | 89.23 ng | 3099110 | 1,4-Dichlorobenzene-d4 | 6.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 9 |
| 5 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
Data File : BF085475.D
Acq On : 16 Mar 2016 21:33
Operator : UM/SJ
Sample : H1788-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2(8-9)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

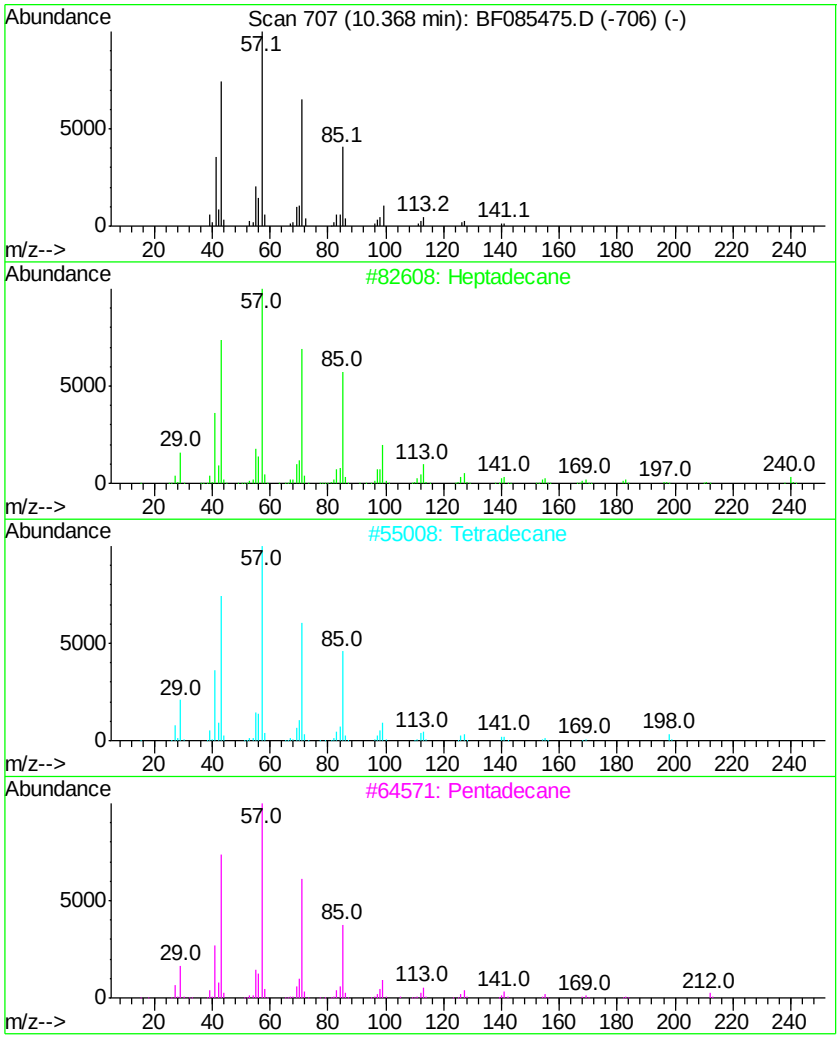
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

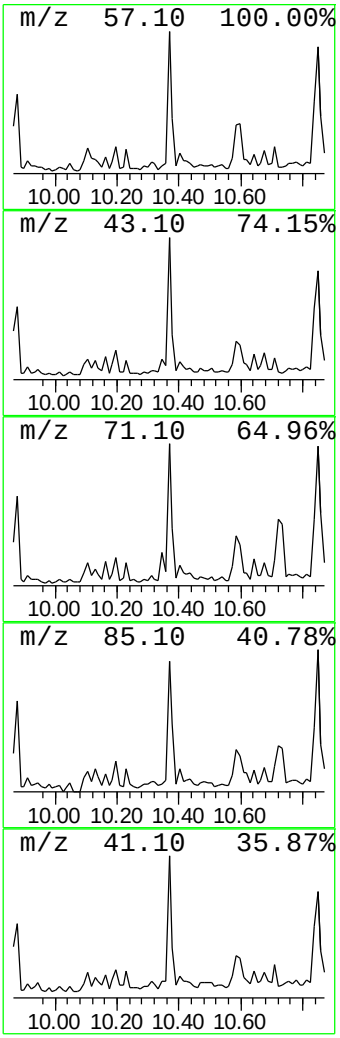
**********

Peak Number 4 Heptadecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.37 | 2.13 ng | 113291 | Acenaphthene-d10 | 9.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 90 |
| 2 | Tetradecane | 198 | C14H30 | 000629-59-4 | 86 |
| 3 | Pentadecane | 212 | C15H32 | 000629-62-9 | 86 |
| 4 | Eicosane | 282 | C20H42 | 000112-95-8 | 83 |
| 5 | Decane, 2,3,5-trimethyl- | 184 | C13H28 | 062238-11-3 | 83 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
Data File : BF085475.D
Acq On : 16 Mar 2016 21:33
Operator : UM/SJ
Sample : H1788-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2(8-9)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

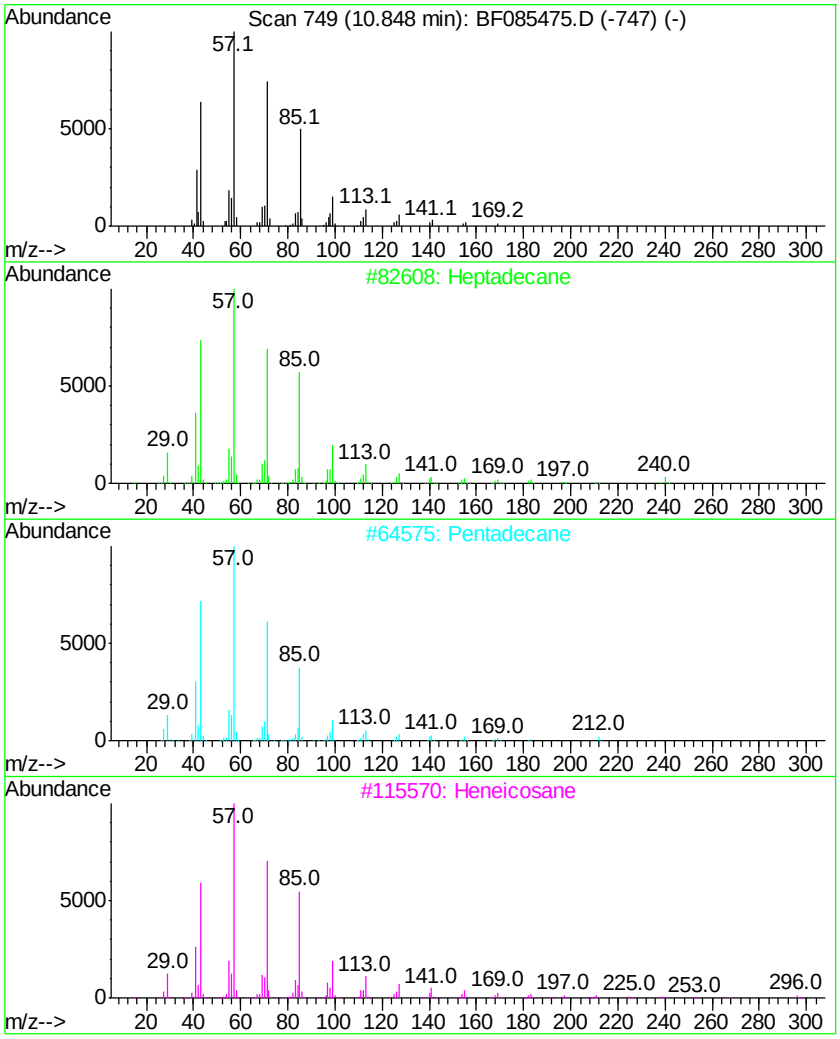
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

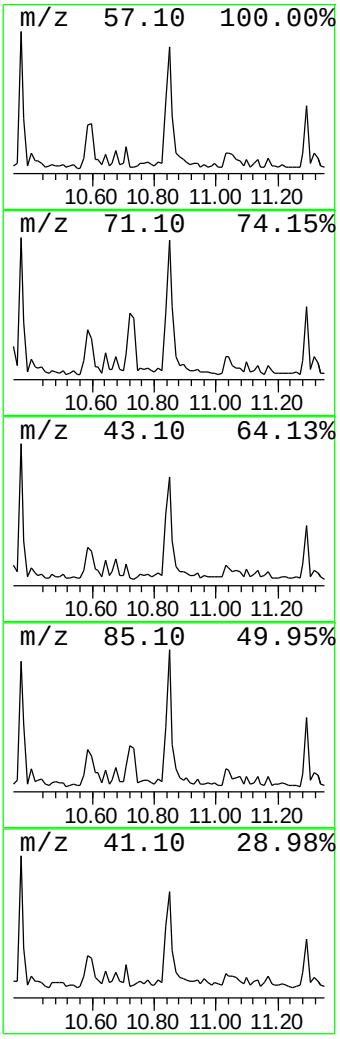
**********

Peak Number 5 Pentadecane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.85 | 3.06 ng | 162742 | Phenanthrene-d10 | 11.43 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 91 |
| 2 | Pentadecane | 212 | C15H32 | 000629-62-9 | 91 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 90 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 5 | 2-Bromo dodecane | 248 | C12H25Br | 013187-99-0 | 90 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
Data File : BF085475.D
Acq On : 16 Mar 2016 21:33
Operator : UM/SJ
Sample : H1788-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2(8-9)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

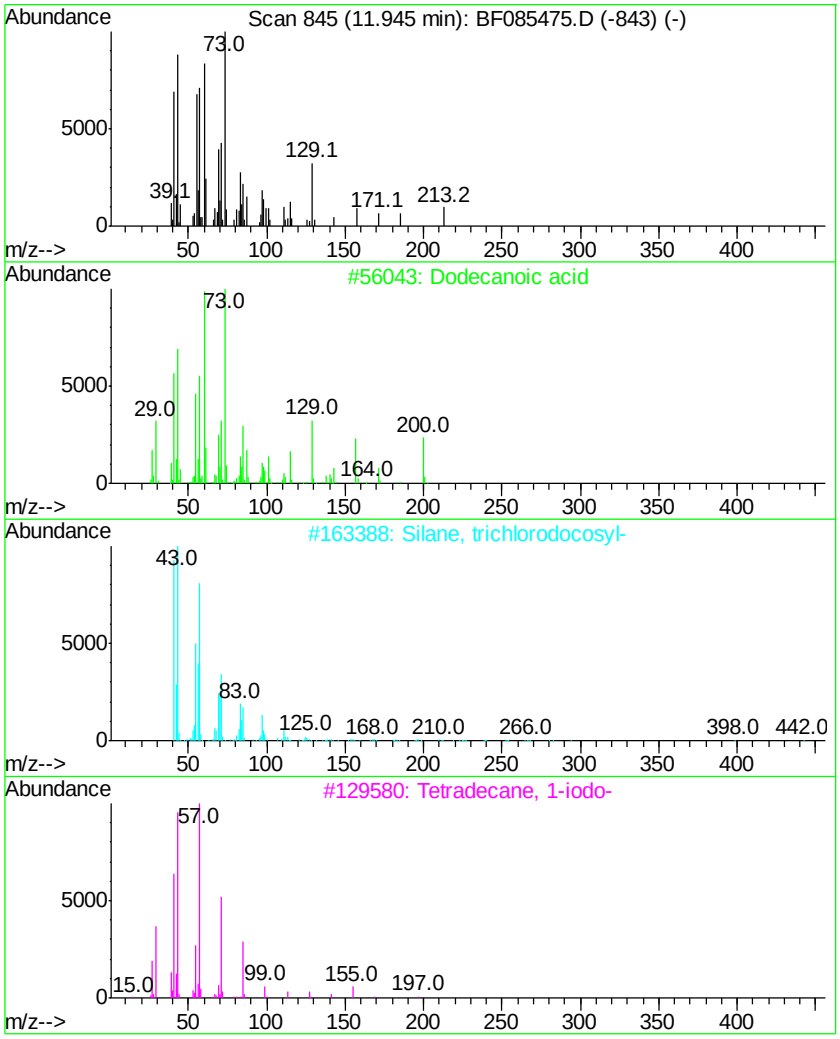
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

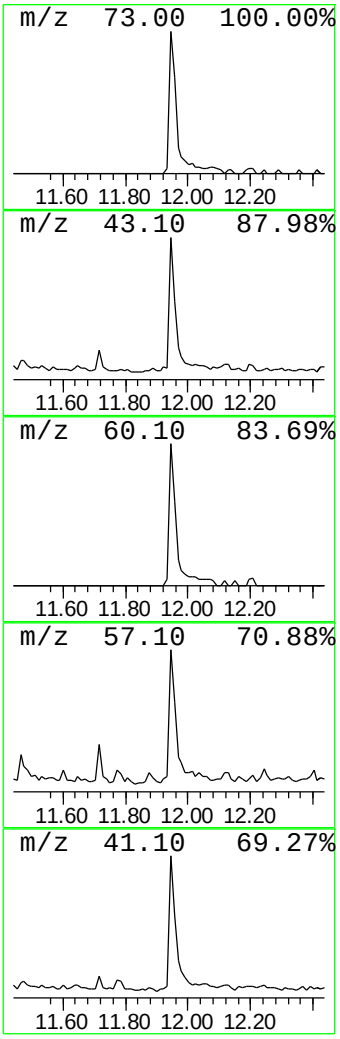
**********

Peak Number 6 Dodecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.94 | 3.25 ng | 172379 | Phenanthrene-d10 | 11.43 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 53 |
| 2 | Silane, trichlorodocosyl- | 442 | C22H45Cl3Si | 007325-84-0 | 18 |
| 3 | Tetradecane, 1-iodo- | 324 | C14H29I | 019218-94-1 | 11 |
| 4 | Undecane | 156 | C11H24 | 001120-21-4 | 11 |
| 5 | 1-Iodo-2-methylundecane | 296 | C12H25I | 073105-67-6 | 10 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
Data File : BF085475.D
Acq On : 16 Mar 2016 21:33
Operator : UM/SJ
Sample : H1788-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2(8-9)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

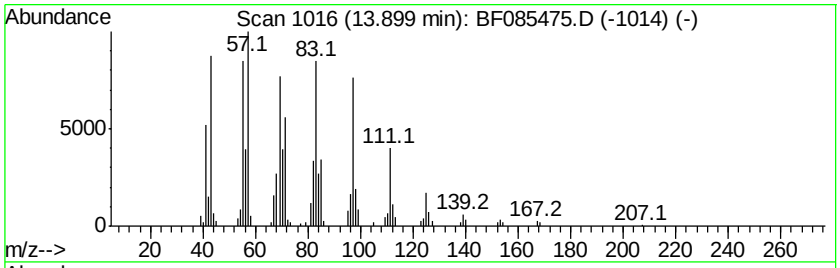
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

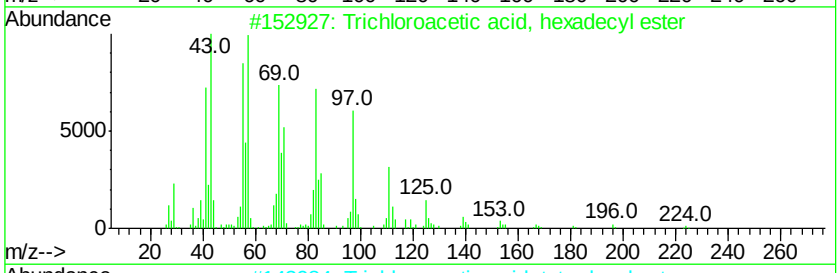
**********

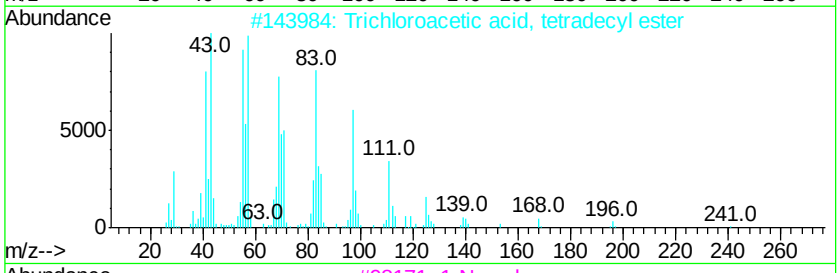
Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 3

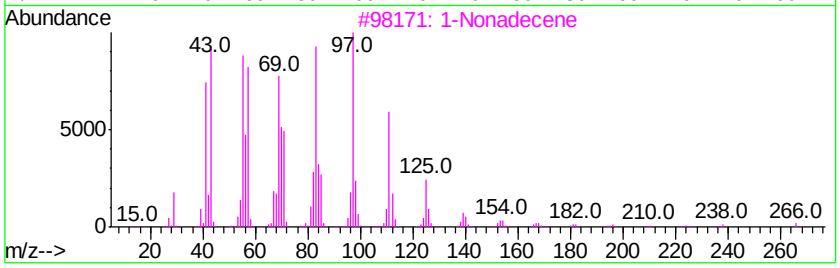
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.90 | 6.47 ng | 299723 | Chrysene-d12 | 14.06 |

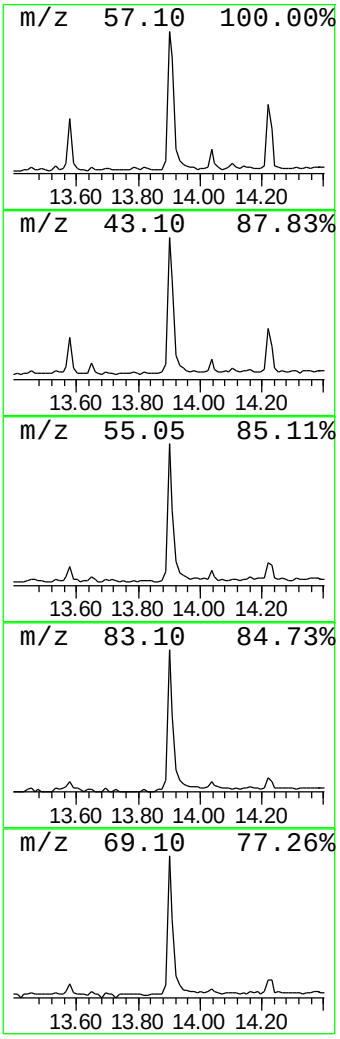
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94 |
| 2 | Trichloroacetic acid, tetradecyl... | 358 | C16H29Cl3O2 | 074339-52-9 | 91 |
| 3 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 91 |
| 4 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 91 |
| 5 | Pentafluoropropionic acid, octad... | 416 | C21H37F5O2 | 1000280-07-7 | 91 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
Data File : BF085475.D
Acq On : 16 Mar 2016 21:33
Operator : UM/SJ
Sample : H1788-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2(8-9)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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 |
| 2-Pentanone, 4-hy... | 5.10 | 3.6 | ng | 125979 | 1 | 6.90 | 694601 | 20.0 |
| unknown6.66 | 6.66 | 89.2 | ng | 3099110 | 1 | 6.90 | 694601 | 20.0 |
| Heptadecane | 10.37 | 2.1 | ng | 113291 | 3 | 9.94 | 1065590 | 20.0 |
| Pentadecane | 10.85 | 3.1 | ng | 162742 | 4 | 11.43 | 1062310 | 20.0 |
| Dodecanoic acid | 11.94 | 3.3 | ng | 172379 | 4 | 11.43 | 1062310 | 20.0 |
| Trichloroacetic a... | 13.90 | 6.5 | ng | 299723 | 5 | 14.06 | 925858 | 20.0 |