LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
Data File : BF107902.D
Acq On : 1 Aug 2018 21:11
Operator : JU/SJ
Sample : J4252-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FM-1026

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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 | 5.190 | 482 | 485 | 499 | rBV | 255027 | 305528 | 6.11% | 0.930% |
| 2 | 5.601 | 551 | 555 | 585 | rBV | 889321 | 1725597 | 34.48% | 5.250% |
| 3 | 6.607 | 723 | 726 | 744 | rBV | 455190 | 1096274 | 21.91% | 3.336% |
| 4 | 6.737 | 744 | 748 | 773 | rVV | 2770271 | 3594695 | 71.83% | 10.937% |
| 5 | 6.960 | 783 | 786 | 794 | rBV | 490905 | 745412 | 14.90% | 2.268% |
| 6 | 7.119 | 808 | 813 | 832 | rBV | 2758846 | 3370830 | 67.36% | 10.256% |
| 7 | 7.531 | 879 | 883 | 905 | rBV | 1823416 | 2915871 | 58.27% | 8.872% |
| 8 | 8.242 | 1000 | 1004 | 1018 | rBV | 824023 | 1127650 | 22.53% | 3.431% |
| 9 | 9.319 | 1182 | 1187 | 1202 | rBV | 3975199 | 5004262 | 100.00% | 15.226% |
| 10 | 9.707 | 1250 | 1253 | 1261 | rBV | 915566 | 963449 | 19.25% | 2.931% |
| 11 | 10.001 | 1299 | 1303 | 1314 | rBV | 1190563 | 1282595 | 25.63% | 3.902% |
| 12 | 10.619 | 1405 | 1408 | 1411 | rBV | 60004 | 53514 | 1.07% | 0.163% |
| 13 | 10.801 | 1435 | 1439 | 1450 | rBV | 2345316 | 3038572 | 60.72% | 9.245% |
| 14 | 11.342 | 1527 | 1531 | 1535 | rBV2 | 117542 | 143685 | 2.87% | 0.437% |
| 15 | 11.501 | 1554 | 1558 | 1566 | rBV | 838676 | 1116129 | 22.30% | 3.396% |
| 16 | 12.007 | 1641 | 1644 | 1654 | rBV2 | 288532 | 345787 | 6.91% | 1.052% |
| 17 | 12.742 | 1767 | 1769 | 1774 | rBV2 | 62481 | 68208 | 1.36% | 0.208% |
| 18 | 12.789 | 1774 | 1777 | 1784 | rBV5 | 56498 | 86687 | 1.73% | 0.264% |
| 19 | 13.083 | 1823 | 1827 | 1846 | rBV | 3174599 | 3627330 | 72.48% | 11.037% |
| 20 | 13.954 | 1972 | 1975 | 1982 | rBV | 266319 | 292283 | 5.84% | 0.889% |
| 21 | 14.154 | 2005 | 2009 | 2019 | rBV | 682463 | 941965 | 18.82% | 2.866% |
| 22 | 15.689 | 2265 | 2270 | 2288 | rVB | 588481 | 1019790 | 20.38% | 3.103% |

Sum of corrected areas: 32866113

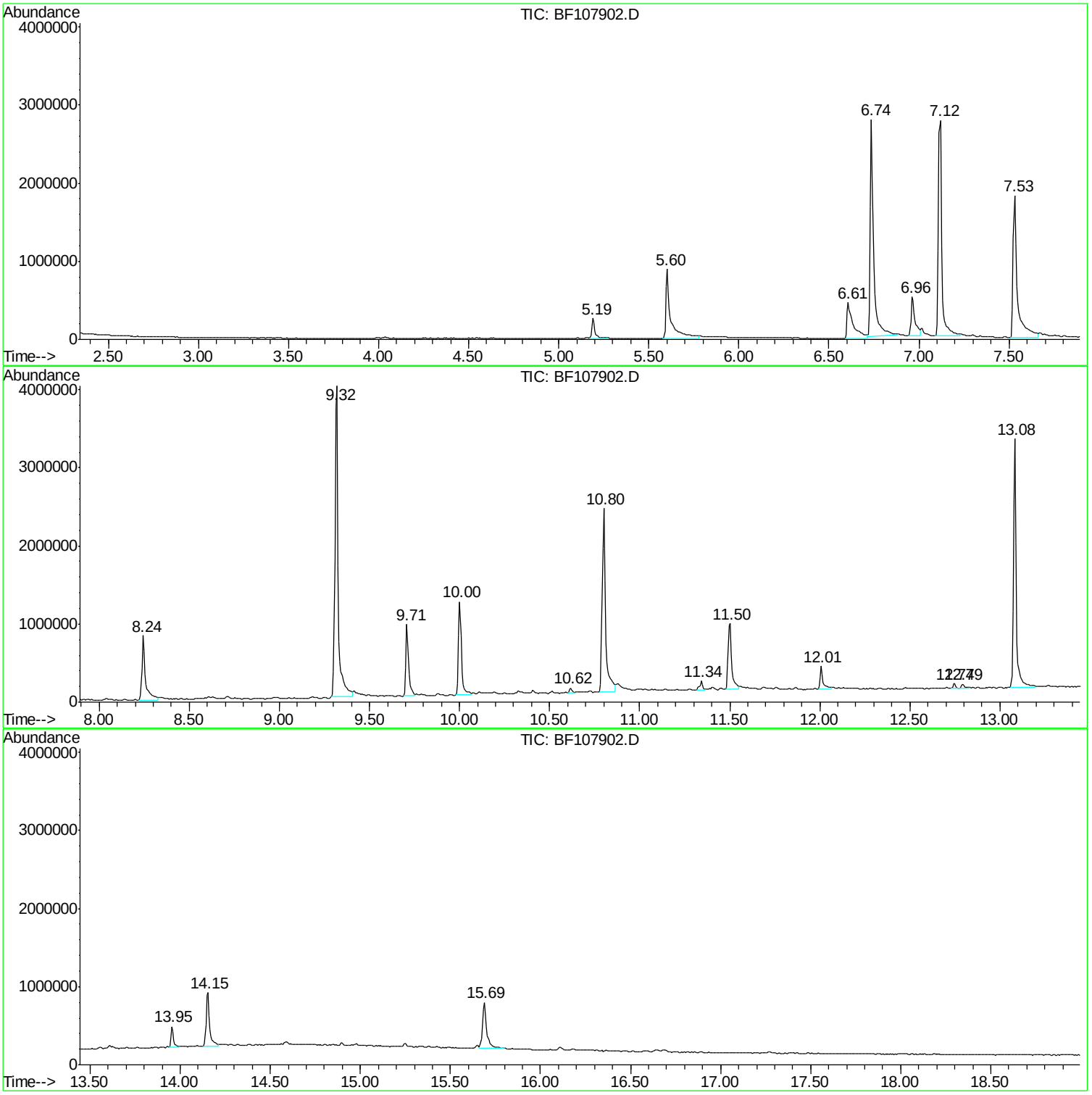
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
Data File : BF107902.D
Acq On : 1 Aug 2018 21:11
Operator : JU/SJ
Sample : J4252-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FM-1026

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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 : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
Data File : BF107902.D
Acq On : 1 Aug 2018 21:11
Operator : JU/SJ
Sample : J4252-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FM-1026

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

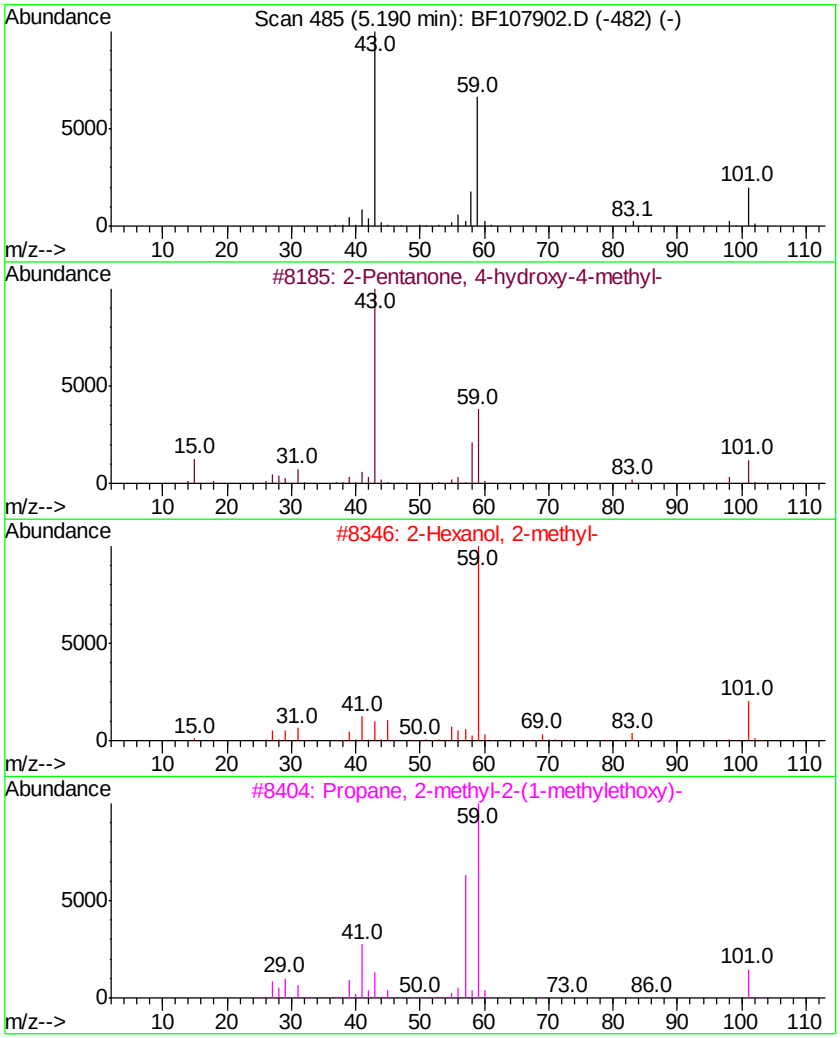
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

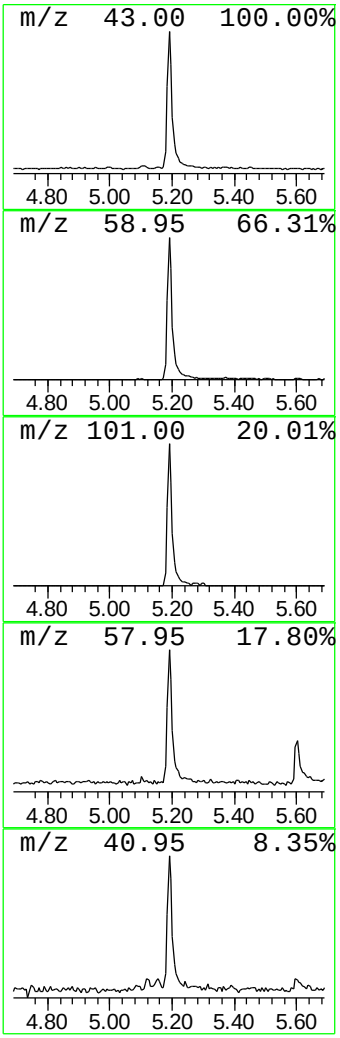
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.19 | 8.20 ng | 305528 | 1,4-Dichlorobenzene-d4 | 6.96 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 33 |
| 3 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 28 |
| 4 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 28 |
| 5 | 1,8-Nonanediol, 8-methyl- | 174 | C10H22O2 | 054725-73-4 | 23 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
Data File : BF107902.D
Acq On : 1 Aug 2018 21:11
Operator : JU/SJ
Sample : J4252-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FM-1026

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

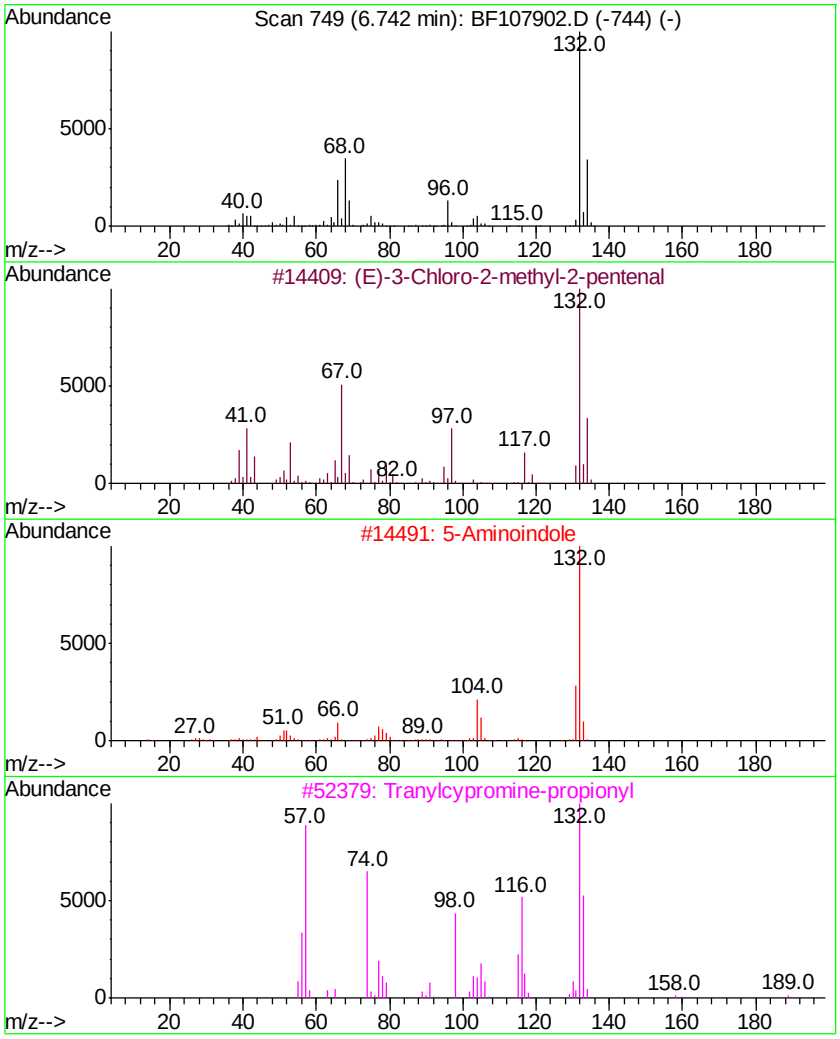
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

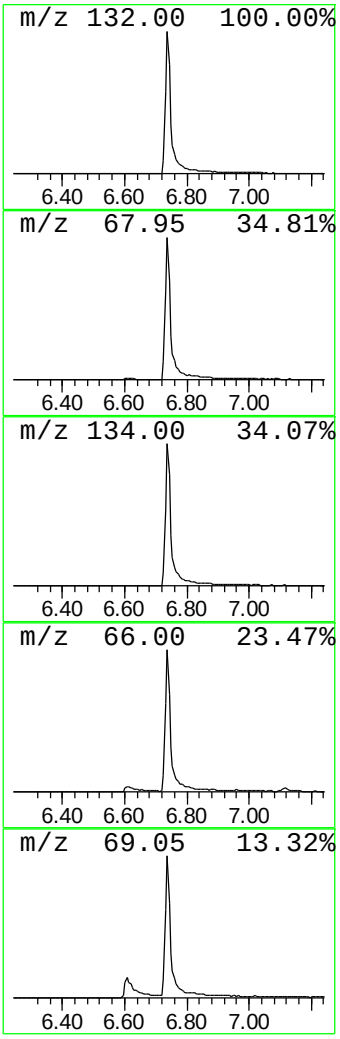
**********

Peak Number 2 unknown6.74 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.74 | 96.45 ng | 3594700 | 1,4-Dichlorobenzene-d4 | 6.96 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |
| 5 | 4-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-60-2 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
Data File : BF107902.D
Acq On : 1 Aug 2018 21:11
Operator : JU/SJ
Sample : J4252-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FM-1026

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

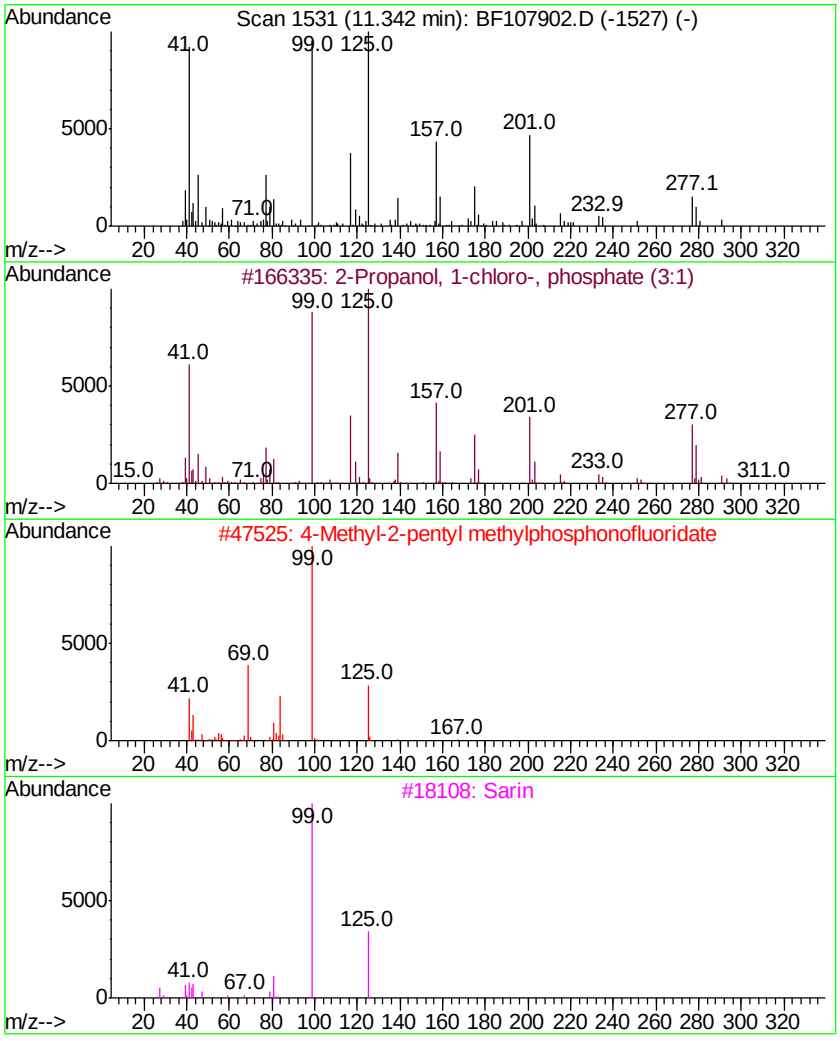
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

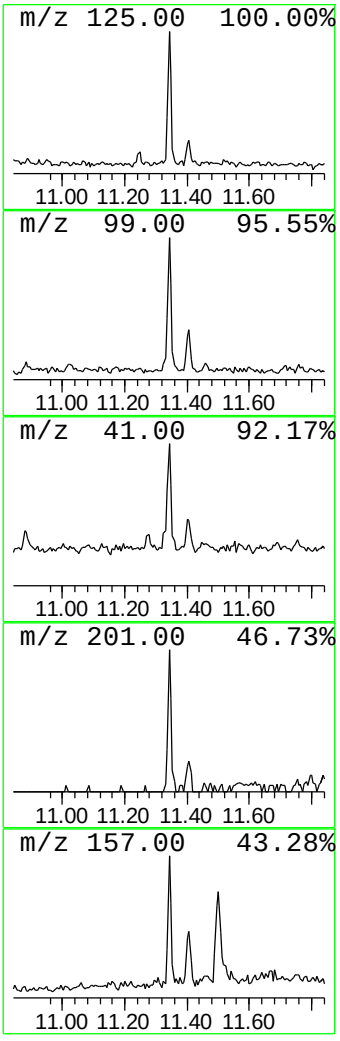
**********

Peak Number 4 2-Propanol, 1-chloro-, phos... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.34 | 2.57 ng | 143685 | Phenanthrene-d10 | 11.50 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Propanol, 1-chloro-, phosphate... | 326 | C9H18Cl3O4P | 013674-84-5 | 90 |
| 2 | 4-Methyl-2-pentyl methylphosphon... | 182 | C7H16FO2P | 000352-53-4 | 32 |
| 3 | Sarin | 140 | C4H10FO2P | 000107-44-8 | 23 |
| 4 | Cyclopropanecarbohydrazide, 2,2,... | 277 | C14H19N3O3 | 329069-29-6 | 10 |
| 5 | 3-Ureidopropionic acid, N-dimeth... | 215 | C9H17N3O3 | 1000375-52-1 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
Data File : BF107902.D
Acq On : 1 Aug 2018 21:11
Operator : JU/SJ
Sample : J4252-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FM-1026

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

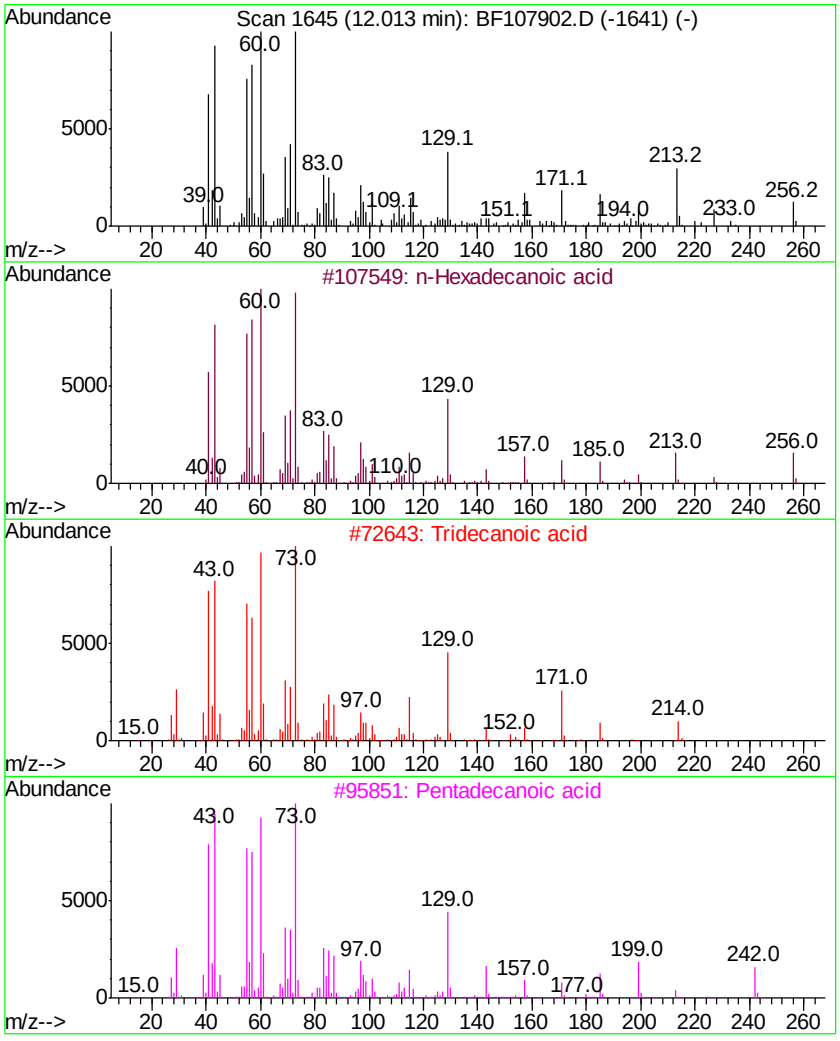
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

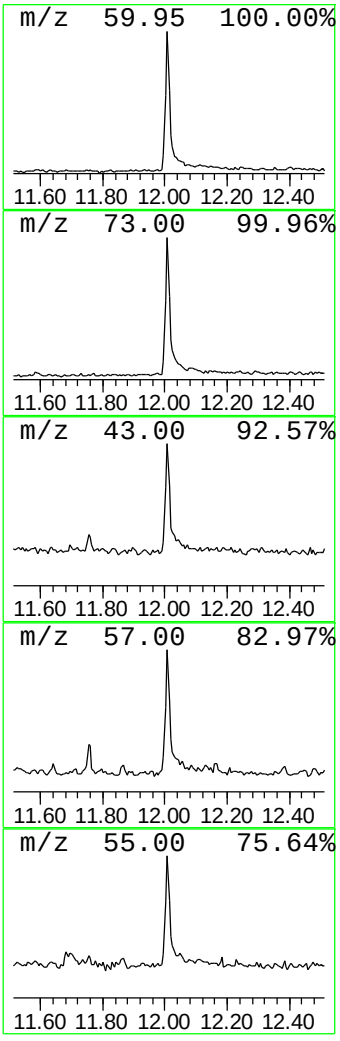
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.01 | 6.20 ng | 345787 | Phenanthrene-d10 | 11.50 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 94 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 93 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 59 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080118\
Data File : BF107902.D
Acq On : 1 Aug 2018 21:11
Operator : JU/SJ
Sample : J4252-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FM-1026

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

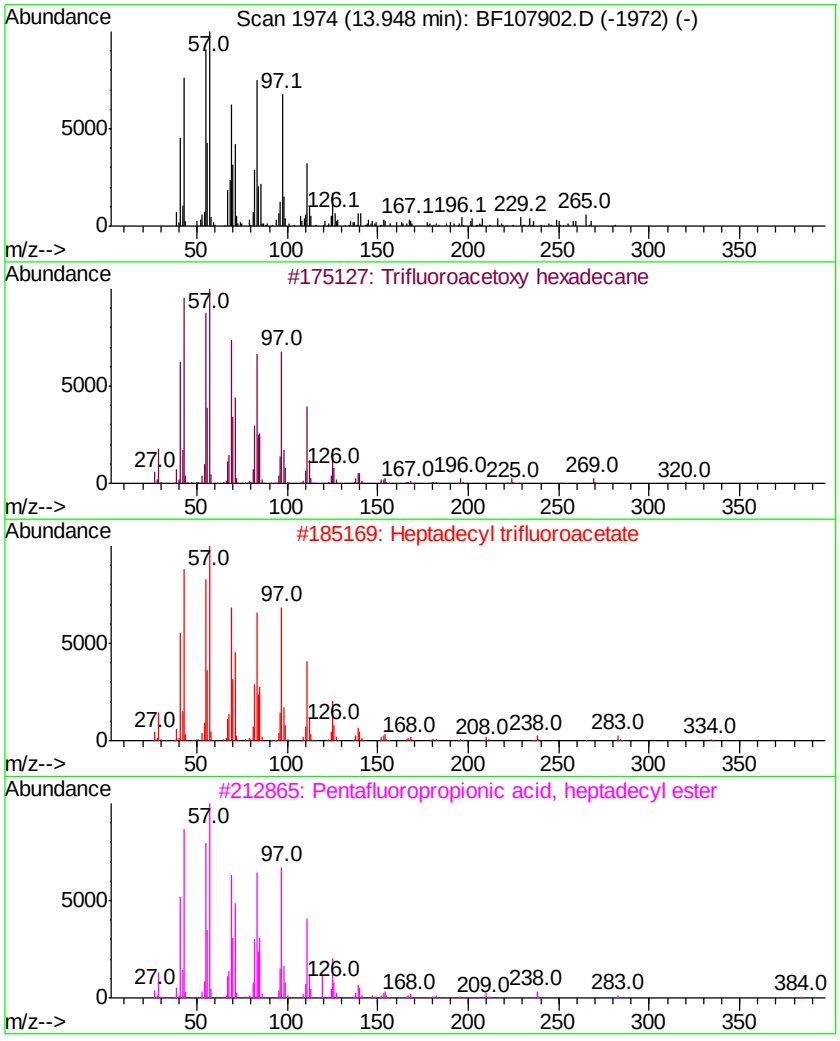
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

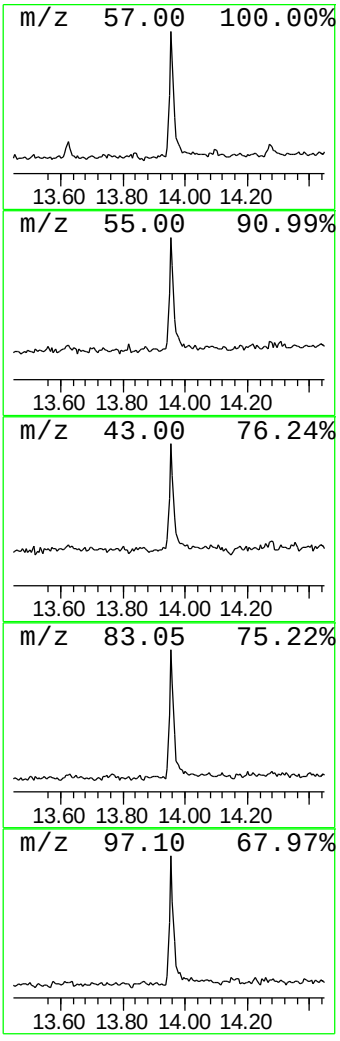
**********

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.95 | 6.21 ng | 292283 | Chrysene-d12 | 14.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 95 |
| 2 | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1000351-87-0 | 94 |
| 3 | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1 | 94 |
| 4 | Heptafluorobutyric acid, hexadec... | 438 | C20H33F7O2 | 006385-15-5 | 94 |
| 5 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 93 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080118\
Data File : BF107902.D
Acq On : 1 Aug 2018 21:11
Operator : JU/SJ
Sample : J4252-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FM-1026

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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... | 5.19 | 8.2 | ng | 305528 | 1 | 6.96 | 745412 | 20.0 |
| unknown6.74 | 6.74 | 96.5 | ng | 3594700 | 1 | 6.96 | 745412 | 20.0 |
| 2-Propanol, 1-chl... | 11.34 | 2.6 | ng | 143685 | 4 | 11.50 | 1116130 | 20.0 |
| n-Hexadecanoic acid | 12.01 | 6.2 | ng | 345787 | 4 | 11.50 | 1116130 | 20.0 |
| Trifluoroacetoxy ... | 13.95 | 6.2 | ng | 292283 | 5 | 14.15 | 941965 | 20.0 |