LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070918\
Data File : BF107256.D
Acq On : 10 Jul 2018 4:16
Operator : JU/SJ
Sample : J3876-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 070318-TIPC-E-U-M

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-BF061918.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 | 5.172 | 479 | 482 | 490 | rBB | 9319 | 10283 | 1.08% | 0.190% |
| 2 | 5.590 | 550 | 553 | 571 | rBV | 240457 | 258281 | 27.10% | 4.772% |
| 3 | 6.595 | 721 | 724 | 736 | rBV | 150846 | 178874 | 18.77% | 3.305% |
| 4 | 6.725 | 742 | 746 | 753 | rBV | 477854 | 446619 | 46.87% | 8.252% |
| 5 | 6.942 | 780 | 783 | 787 | rBV | 187420 | 166967 | 17.52% | 3.085% |
| 6 | 7.101 | 806 | 810 | 814 | rBV | 689778 | 628131 | 65.92% | 11.606% |
| 7 | 7.513 | 875 | 880 | 895 | rBV | 473269 | 451627 | 47.39% | 8.344% |
| 8 | 8.231 | 998 | 1002 | 1021 | rBB | 189158 | 182631 | 19.17% | 3.374% |
| 9 | 9.301 | 1180 | 1184 | 1195 | rBV | 917531 | 833758 | 87.49% | 15.405% |
| 10 | 9.695 | 1248 | 1251 | 1259 | rBB | 74176 | 61048 | 6.41% | 1.128% |
| 11 | 9.989 | 1298 | 1301 | 1308 | rVB | 238500 | 200498 | 21.04% | 3.704% |
| 12 | 10.642 | 1409 | 1412 | 1419 | rBB | 66361 | 59538 | 6.25% | 1.100% |
| 13 | 10.789 | 1433 | 1437 | 1449 | rBV | 368595 | 349678 | 36.70% | 6.461% |
| 14 | 11.489 | 1552 | 1556 | 1565 | rBV | 258066 | 232697 | 24.42% | 4.299% |
| 15 | 13.071 | 1820 | 1825 | 1828 | rBV | 1064084 | 952922 | 100.00% | 17.607% |
| 16 | 13.954 | 1971 | 1975 | 1984 | rBV4 | 20064 | 37693 | 3.96% | 0.696% |
| 17 | 14.142 | 2003 | 2007 | 2011 | rBV | 203198 | 184612 | 19.37% | 3.411% |
| 18 | 14.883 | 2130 | 2133 | 2137 | rVB2 | 16011 | 14848 | 1.56% | 0.274% |
| 19 | 15.230 | 2189 | 2192 | 2195 | rVB2 | 12163 | 13094 | 1.37% | 0.242% |
| 20 | 15.636 | 2257 | 2261 | 2264 | rVB | 12227 | 14567 | 1.53% | 0.269% |
| 21 | 15.683 | 2264 | 2269 | 2276 | rBV | 101305 | 133944 | 14.06% | 2.475% |

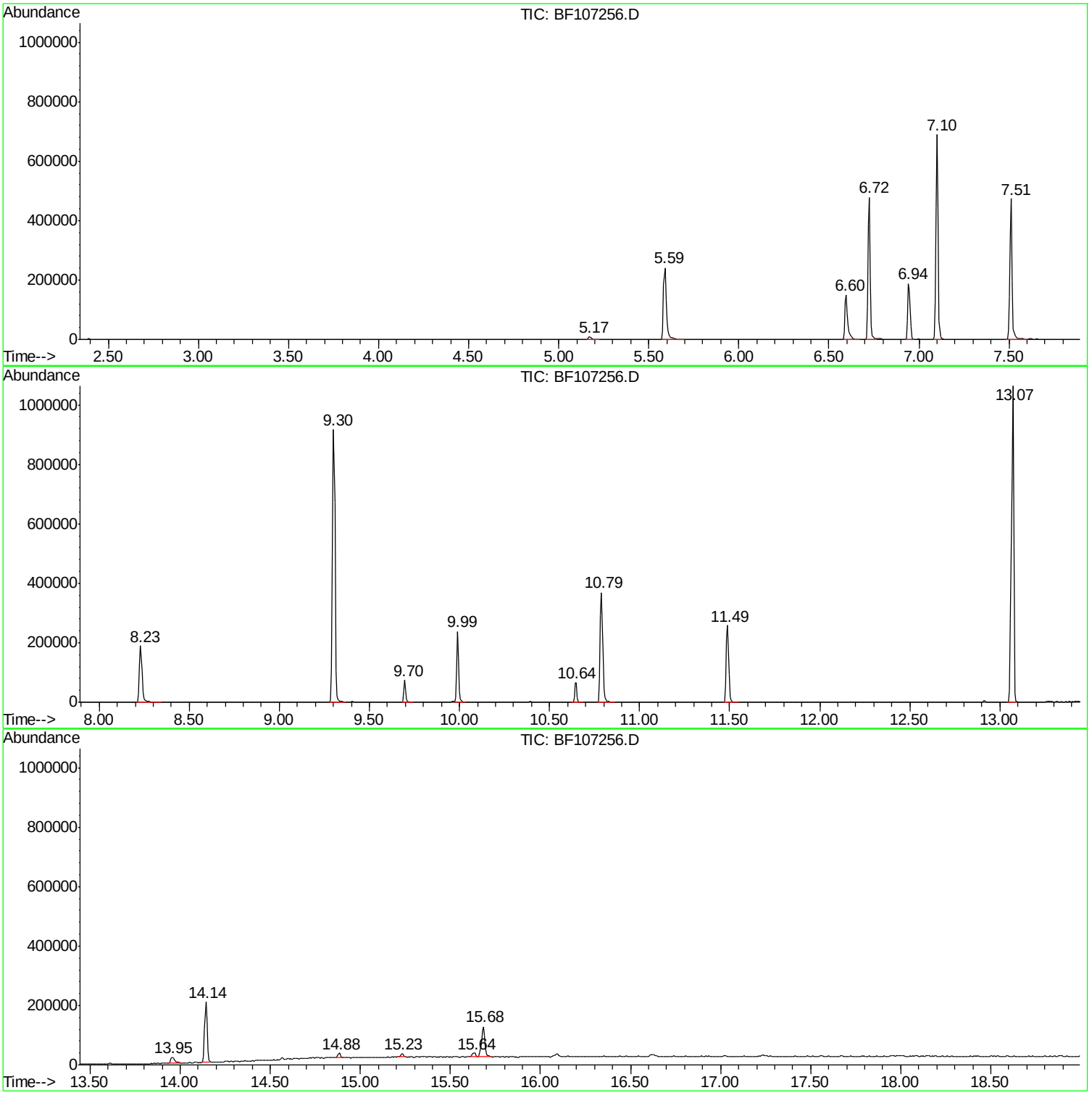
Sum of corrected areas: 5412310

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070918\
Data File : BF107256.D
Acq On : 10 Jul 2018 4:16
Operator : JU/SJ
Sample : J3876-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
070318-TIPC-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070918\
Data File : BF107256.D
Acq On : 10 Jul 2018 4:16
Operator : JU/SJ
Sample : J3876-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 070318-TIPC-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

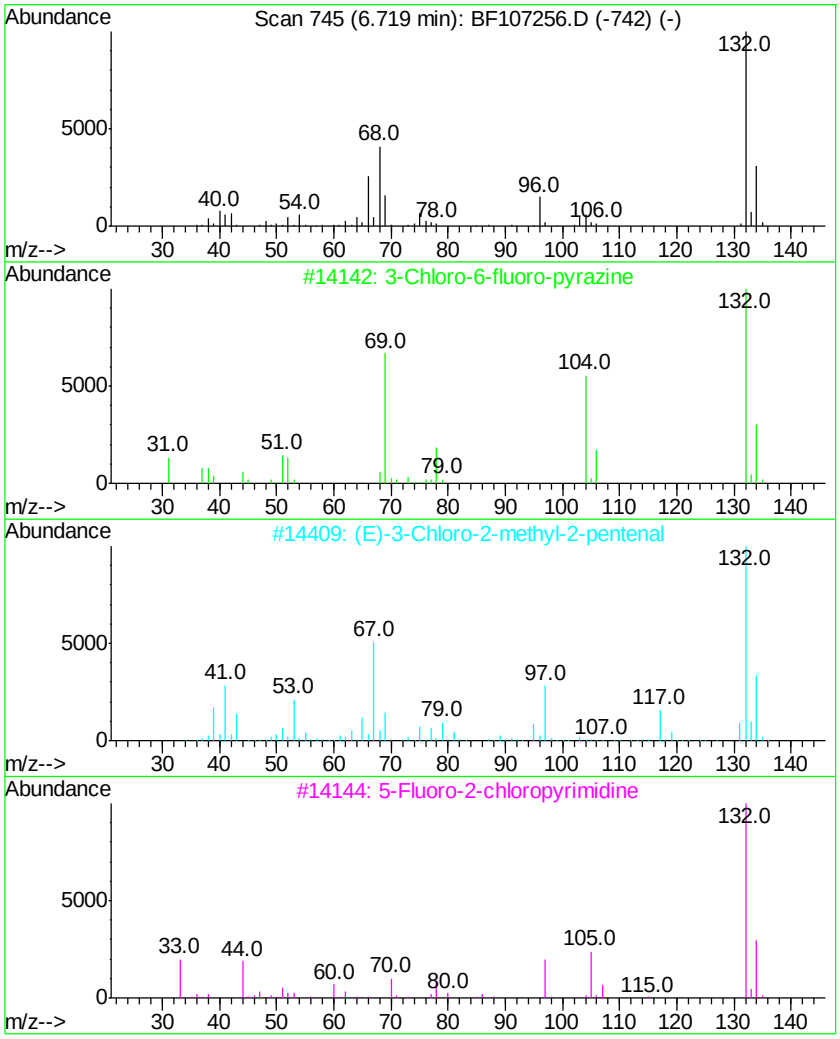
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

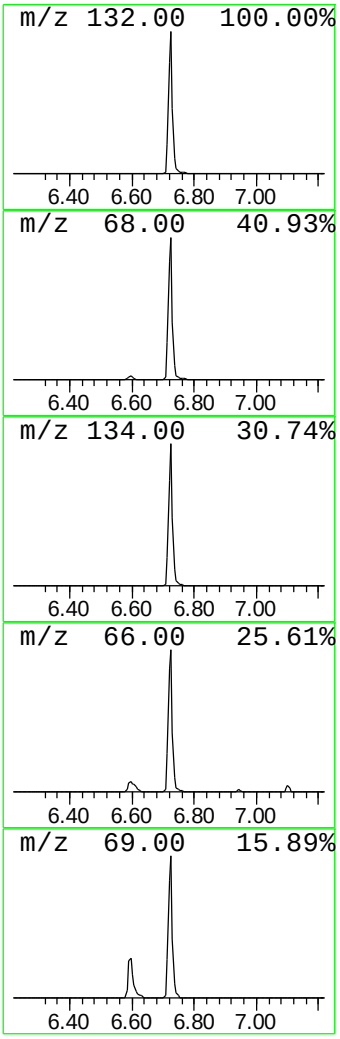
**********

Peak Number 1 unknown6.72 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.72 | 53.50 ng | 446619 | 1,4-Dichlorobenzene-d4 | 6.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 16 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 12 |
| 3 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |
| 4 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 9 |
| 5 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070918\
Data File : BF107256.D
Acq On : 10 Jul 2018 4:16
Operator : JU/SJ
Sample : J3876-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 070318-TIPC-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

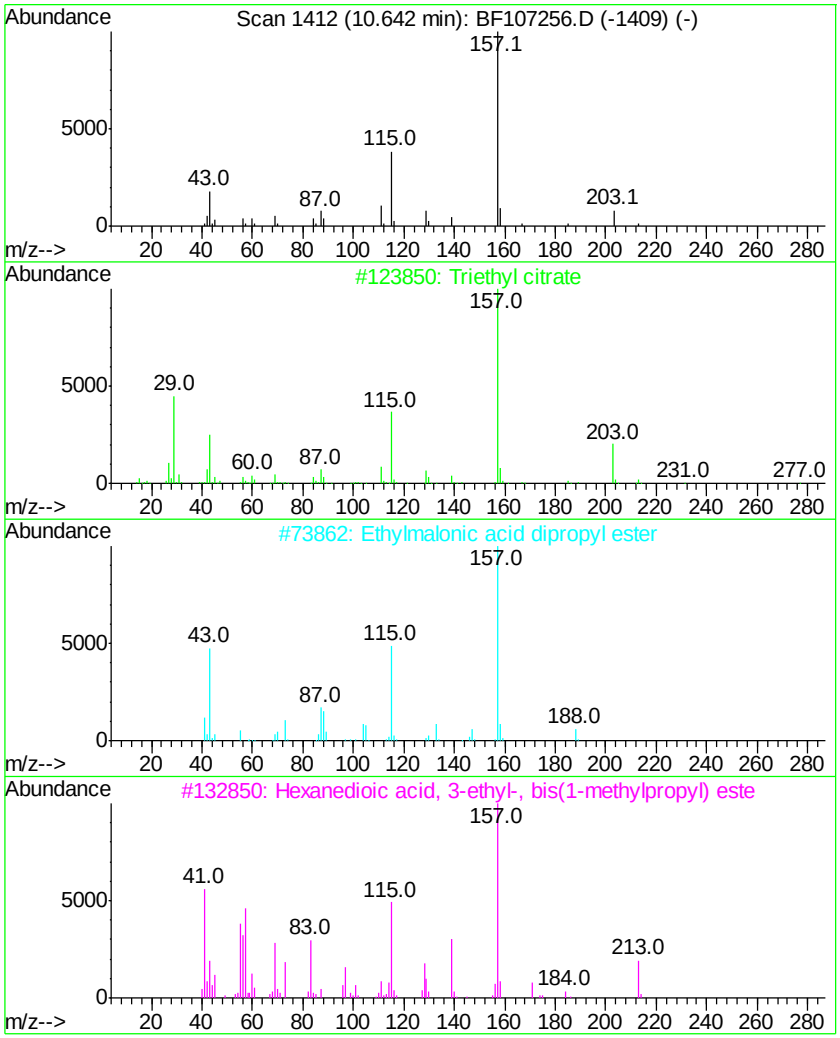
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

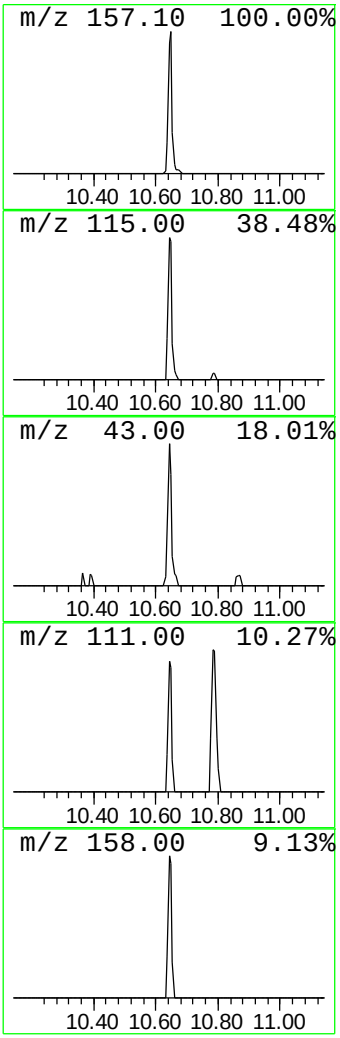
**********

Peak Number 3 Triethyl citrate Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.64 | 5.94 ng | 59538 | Acenaphthene-d10 | 9.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Triethyl citrate | 276 | C12H20O7 | 000077-93-0 | 90 |
| 2 | Ethylmalonic acid dipropyl ester | 216 | C11H20O4 | 001113-91-3 | 50 |
| 3 | Hexanedioic acid, 3-ethyl-, bis(... | 286 | C16H30O4 | 057983-54-7 | 40 |
| 4 | 1-Amino-2-methylnaphthalene | 157 | C11H11N | 002246-44-8 | 37 |
| 5 | Piperazine-1-carboxylic acid, 4-... | 362 | C14H19ClN2O5S | 1000303-79-9 | 33 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070918\
Data File : BF107256.D
Acq On : 10 Jul 2018 4:16
Operator : JU/SJ
Sample : J3876-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 070318-TIPC-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

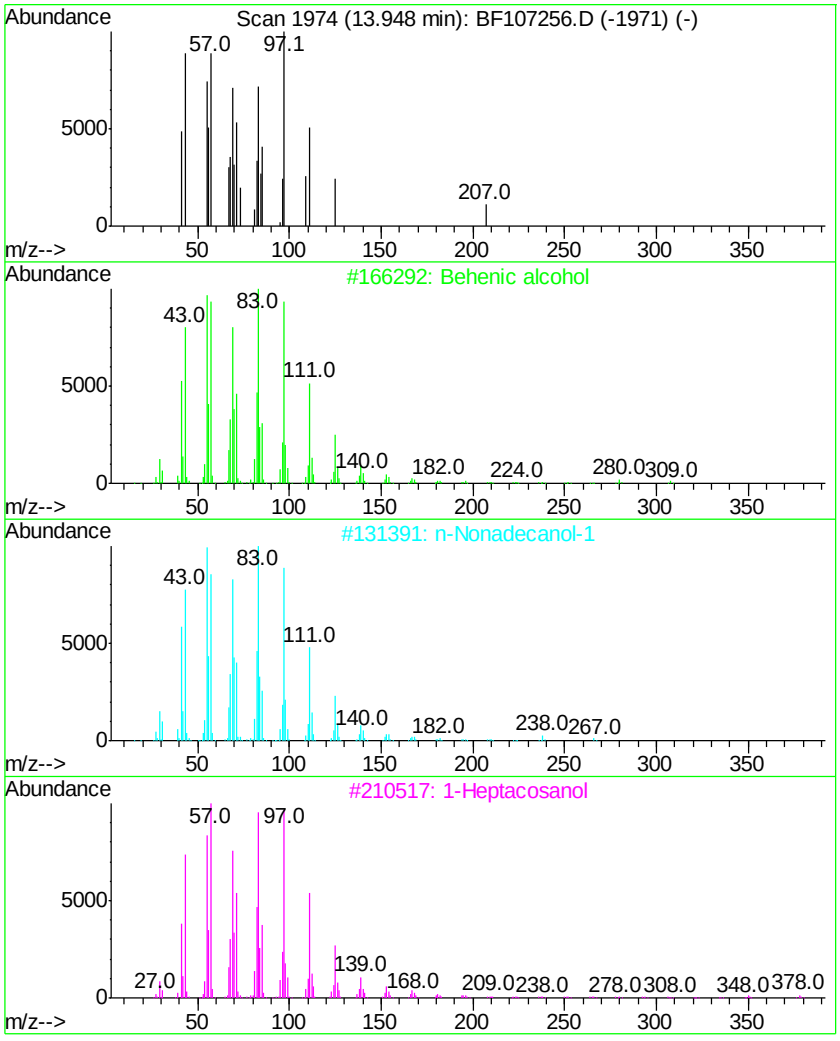
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

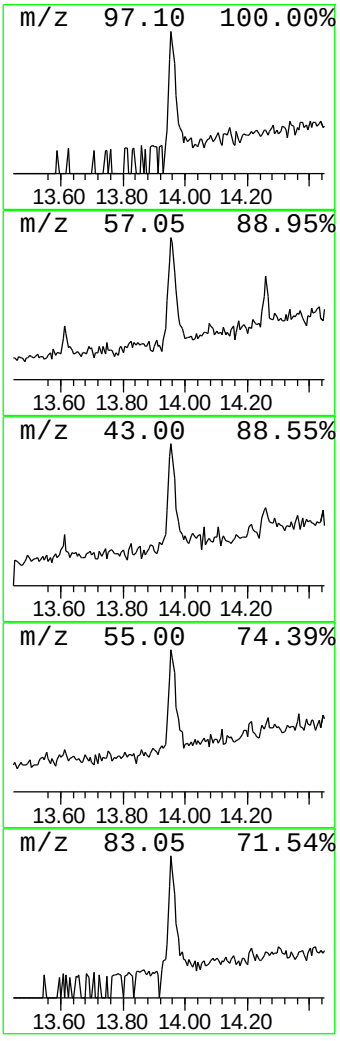
**********

Peak Number 4 Behenic alcohol Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.95 | 4.08 ng | 37693 | Chrysene-d12 | 14.14 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 91 |
| 2 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 91 |
| 3 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 91 |
| 4 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 91 |
| 5 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 91 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF070918\
Data File : BF107256.D
Acq On : 10 Jul 2018 4:16
Operator : JU/SJ
Sample : J3876-04
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 070318-TIPC-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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 |
| unknown6.72 | 6.72 | 53.5 | ng | 446619 | 1 | 6.94 | 166967 | 20.0 |
| Triethyl citrate | 10.64 | 5.9 | ng | 59538 | 3 | 9.99 | 200498 | 20.0 |
| Behenic alcohol | 13.95 | 4.1 | ng | 37693 | 5 | 14.14 | 184612 | 20.0 |