LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087574.D
Acq On : 31 May 2016 5:03
Operator : UM/SJ
Sample : H3316-04
Misc :
ALS Vial : 92 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-06-COMP

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-BF052316.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 | 4.730 | 272 | 275 | 293 | rBV | 82877 | 379057 | 10.98% | 1.409% |
| 2 | 5.381 | 330 | 332 | 374 | rBV6 | 956983 | 2886545 | 83.63% | 10.727% |
| 3 | 7.039 | 475 | 477 | 483 | rBV | 1729121 | 2502961 | 72.51% | 9.301% |
| 4 | 7.130 | 483 | 485 | 510 | rVV | 1779544 | 3451668 | 100.00% | 12.827% |
| 5 | 7.473 | 513 | 515 | 527 | rVV | 475977 | 823210 | 23.85% | 3.059% |
| 6 | 7.702 | 533 | 535 | 551 | rVV | 1497063 | 2234139 | 64.73% | 8.302% |
| 7 | 8.399 | 594 | 596 | 627 | rBV | 732481 | 1961595 | 56.83% | 7.290% |
| 8 | 9.507 | 691 | 693 | 708 | rBV | 515007 | 1016817 | 29.46% | 3.779% |
| 9 | 11.279 | 845 | 848 | 864 | rBV | 2385185 | 3098347 | 89.76% | 11.514% |
| 10 | 12.011 | 909 | 912 | 922 | rBV | 40610 | 118370 | 3.43% | 0.440% |
| 11 | 12.331 | 938 | 940 | 958 | rVB | 624991 | 1029395 | 29.82% | 3.825% |
| 12 | 13.165 | 1010 | 1013 | 1015 | rVB | 29490 | 43912 | 1.27% | 0.163% |
| 13 | 13.634 | 1052 | 1054 | 1075 | rBV | 619483 | 1338635 | 38.78% | 4.975% |
| 14 | 13.931 | 1078 | 1080 | 1085 | rVV | 42328 | 84680 | 2.45% | 0.315% |
| 15 | 14.662 | 1142 | 1144 | 1146 | rBV | 26813 | 34800 | 1.01% | 0.129% |
| 16 | 14.754 | 1150 | 1152 | 1165 | rBV | 375079 | 824568 | 23.89% | 3.064% |
| 17 | 16.640 | 1314 | 1317 | 1321 | rBV2 | 25738 | 69508 | 2.01% | 0.258% |
| 18 | 16.925 | 1340 | 1342 | 1344 | rBV2 | 122056 | 152656 | 4.42% | 0.567% |
| 19 | 17.085 | 1354 | 1356 | 1366 | rBV | 1569728 | 2259526 | 65.46% | 8.397% |
| 20 | 17.268 | 1370 | 1372 | 1375 | rVV3 | 22793 | 44262 | 1.28% | 0.164% |
| 21 | 17.851 | 1421 | 1423 | 1426 | rBV | 60611 | 86575 | 2.51% | 0.322% |
| 22 | 18.468 | 1475 | 1477 | 1489 | rBV | 315649 | 919058 | 26.63% | 3.415% |
| 23 | 19.554 | 1570 | 1572 | 1575 | rVB | 251119 | 275597 | 7.98% | 1.024% |
| 24 | 20.171 | 1623 | 1626 | 1634 | rBV2 | 224876 | 609849 | 17.67% | 2.266% |
| 25 | 20.629 | 1664 | 1666 | 1672 | rVB2 | 165548 | 313573 | 9.08% | 1.165% |
| 26 | 20.971 | 1693 | 1696 | 1700 | rVB | 109983 | 214082 | 6.20% | 0.796% |
| 27 | 21.417 | 1732 | 1735 | 1737 | rVB | 75669 | 135855 | 3.94% | 0.505% |

Sum of corrected areas: 26909240

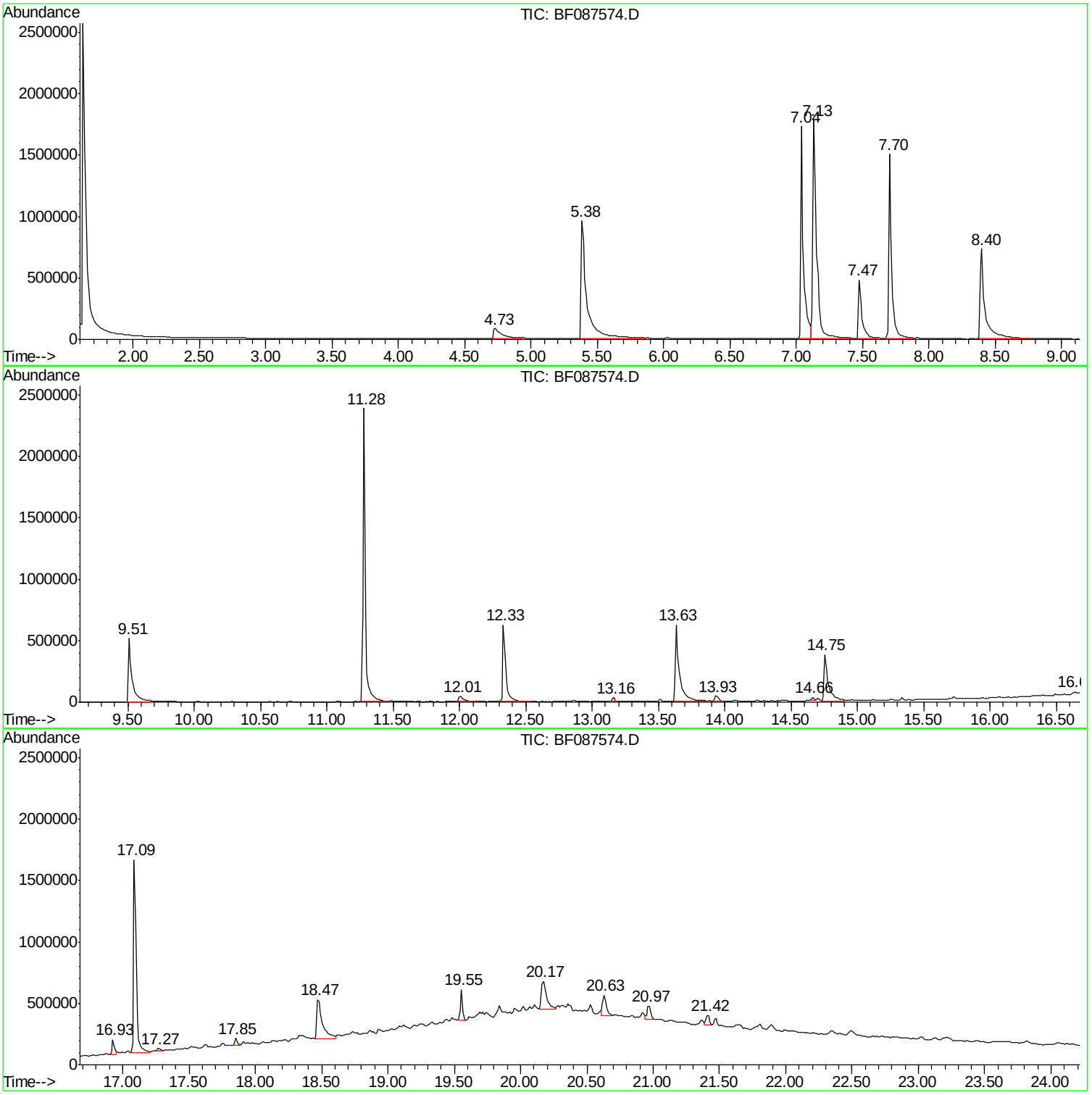
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087574.D
Acq On : 31 May 2016 5:03
Operator : UM/SJ
Sample : H3316-04
Misc :
ALS Vial : 92 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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\BF052916\
Data File : BF087574.D
Acq On : 31 May 2016 5:03
Operator : UM/SJ
Sample : H3316-04
Misc :
ALS Vial : 92 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

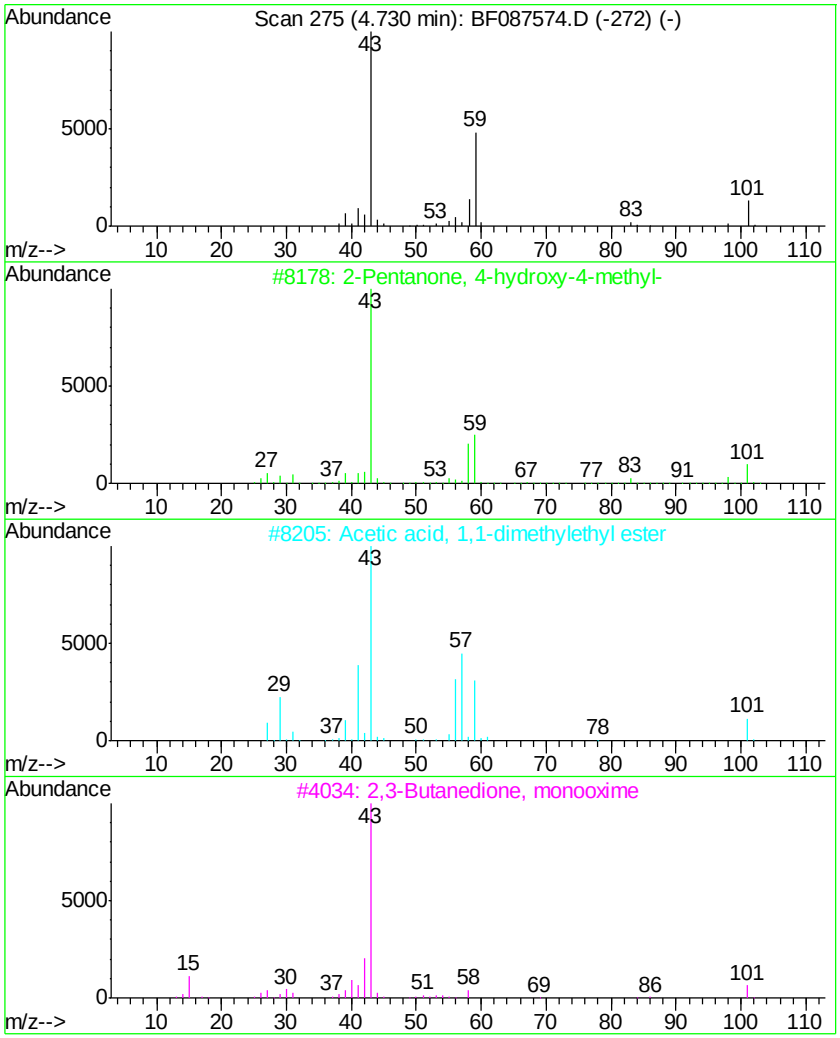
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

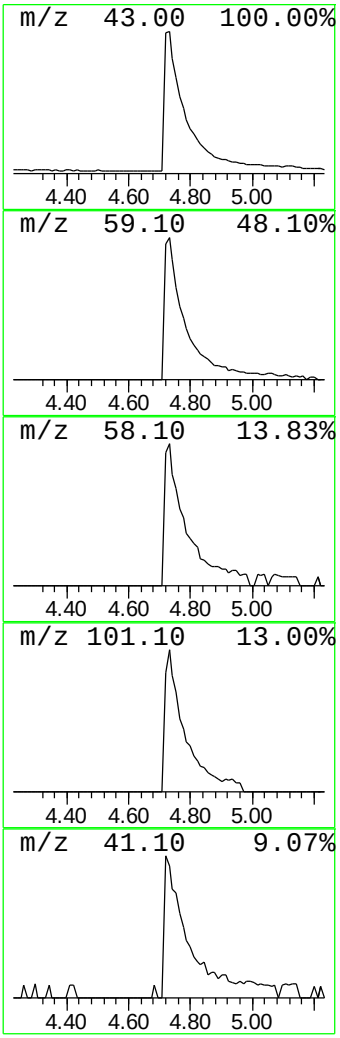
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.73 | 9.21 ng | 379057 | 1,4-Dichlorobenzene-d4 | 7.47 |

| 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 | 28 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | Diacetamide | 101 | C4H7NO2 | 000625-77-4 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087574.D
Acq On : 31 May 2016 5:03
Operator : UM/SJ
Sample : H3316-04
Misc :
ALS Vial : 92 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

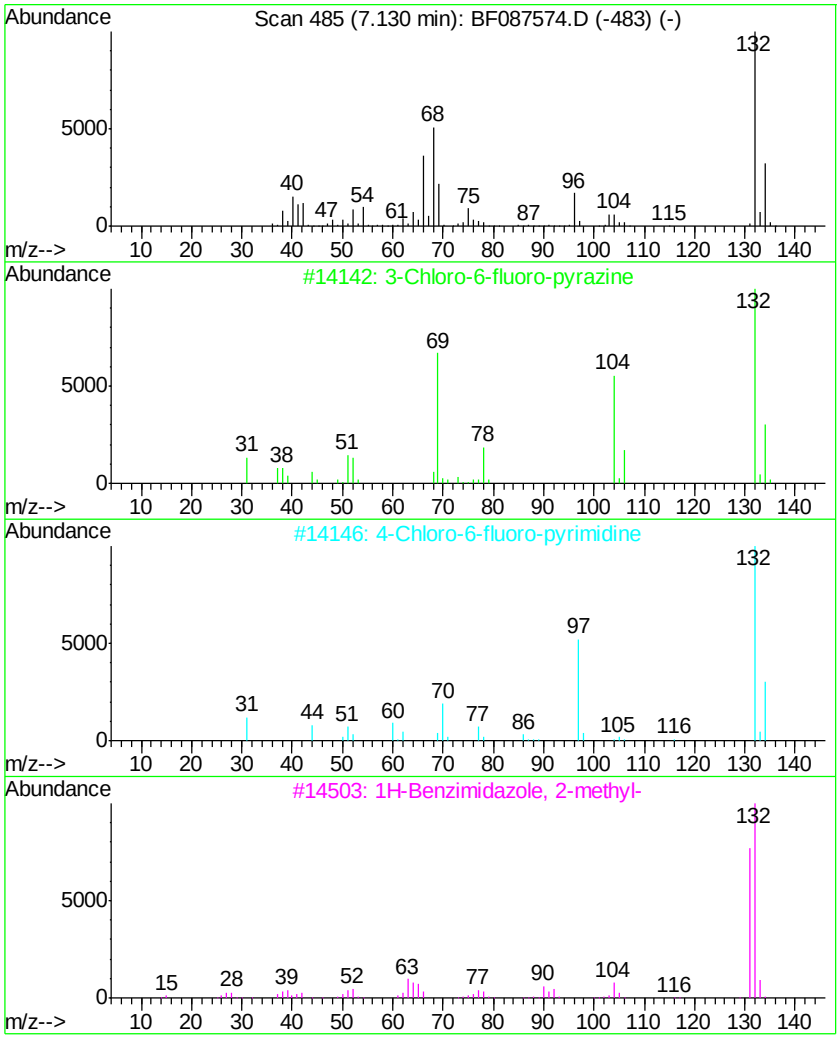
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

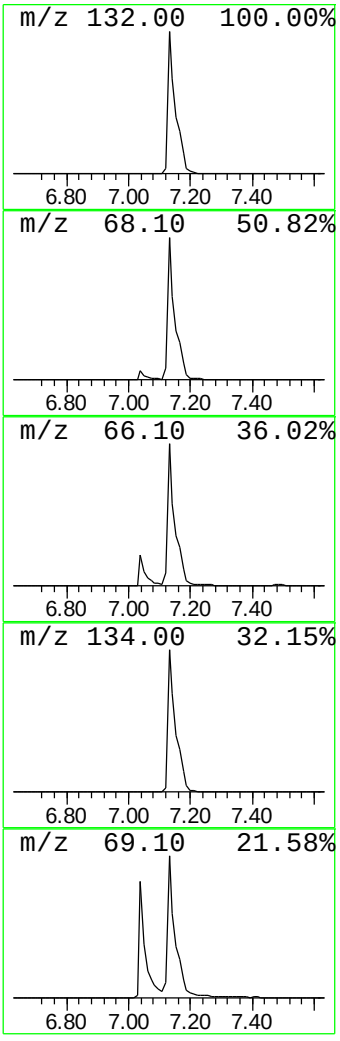
**********

Peak Number 2 unknown7.13 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.13 | 83.86 ng | 3451670 | 1,4-Dichlorobenzene-d4 | 7.47 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 3 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 22 |
| 5 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087574.D
Acq On : 31 May 2016 5:03
Operator : UM/SJ
Sample : H3316-04
Misc :
ALS Vial : 92 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

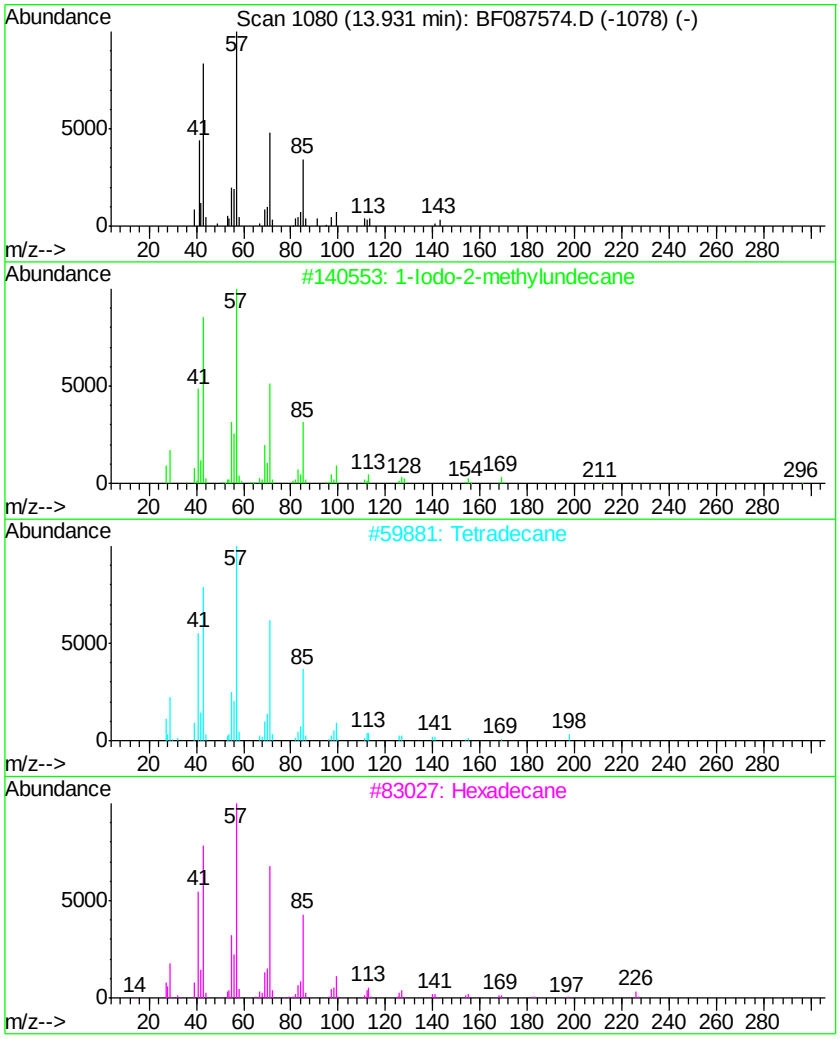
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

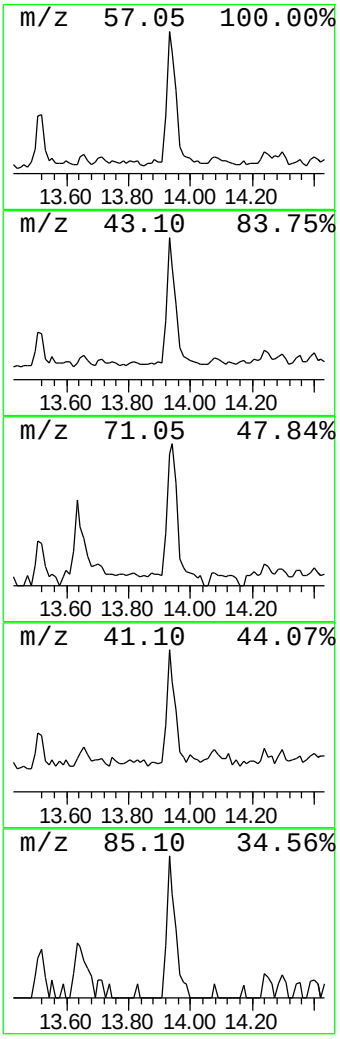
**********

Peak Number 4 1-Iodo-2-methylundecane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.93 | 2.05 ng | 84680 | Phenanthrene-d10 | 14.75 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Iodo-2-methylundecane | 296 | C12H25I | 073105-67-6 | 86 |
| 2 | Tetradecane | 198 | C14H30 | 000629-59-4 | 80 |
| 3 | Hexadecane | 226 | C16H34 | 000544-76-3 | 72 |
| 4 | Octadecane | 254 | C18H38 | 000593-45-3 | 72 |
| 5 | Tridecane | 184 | C13H28 | 000629-50-5 | 72 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087574.D
Acq On : 31 May 2016 5:03
Operator : UM/SJ
Sample : H3316-04
Misc :
ALS Vial : 92 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

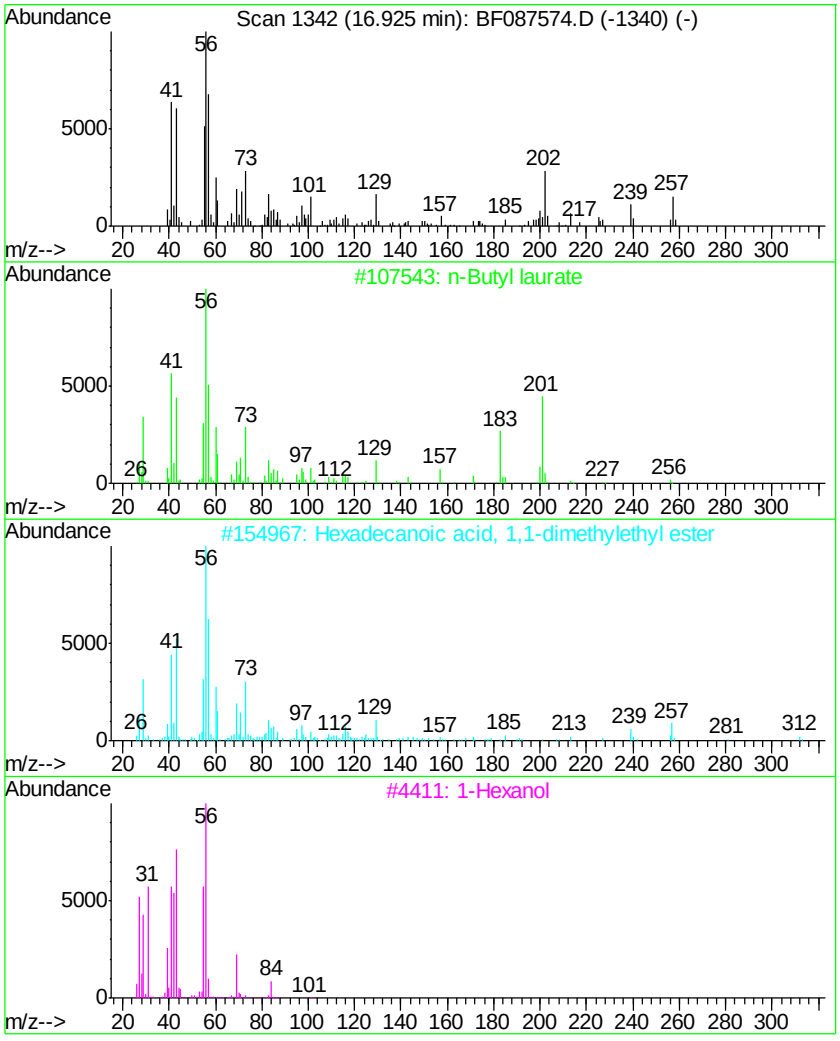
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

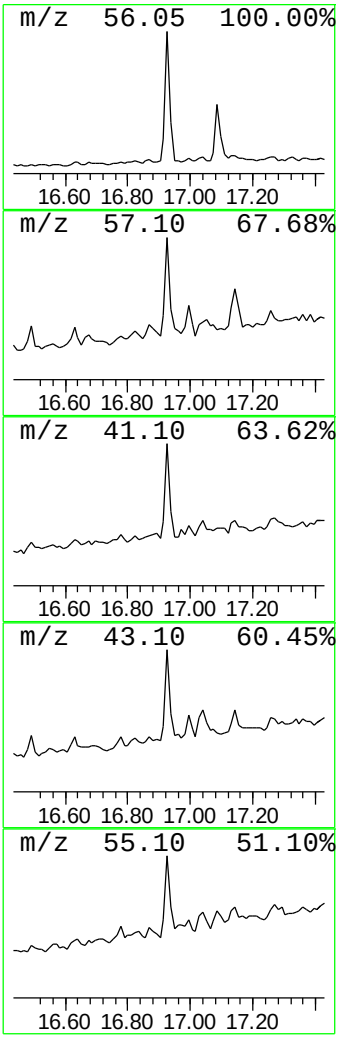
**********

Peak Number 5 n-Butyl laurate Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.93 | 3.32 ng | 152656 | Chrysene-d12 | 18.47 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Butyl laurate | 256 | C16H32O2 | 000106-18-3 | 86 |
| 2 | Hexadecanoic acid, 1,1-dimethyle... | 312 | C20H40O2 | 031158-91-5 | 81 |
| 3 | 1-Hexanol | 102 | C6H14O | 000111-27-3 | 35 |
| 4 | 3-Bromopropyl isocyanate | 163 | C4H6BrNO | 056017-72-2 | 27 |
| 5 | Cyclobutanone, 3,3-dimethyl- | 98 | C6H10O | 001192-33-2 | 27 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087574.D
Acq On : 31 May 2016 5:03
Operator : UM/SJ
Sample : H3316-04
Misc :
ALS Vial : 92 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

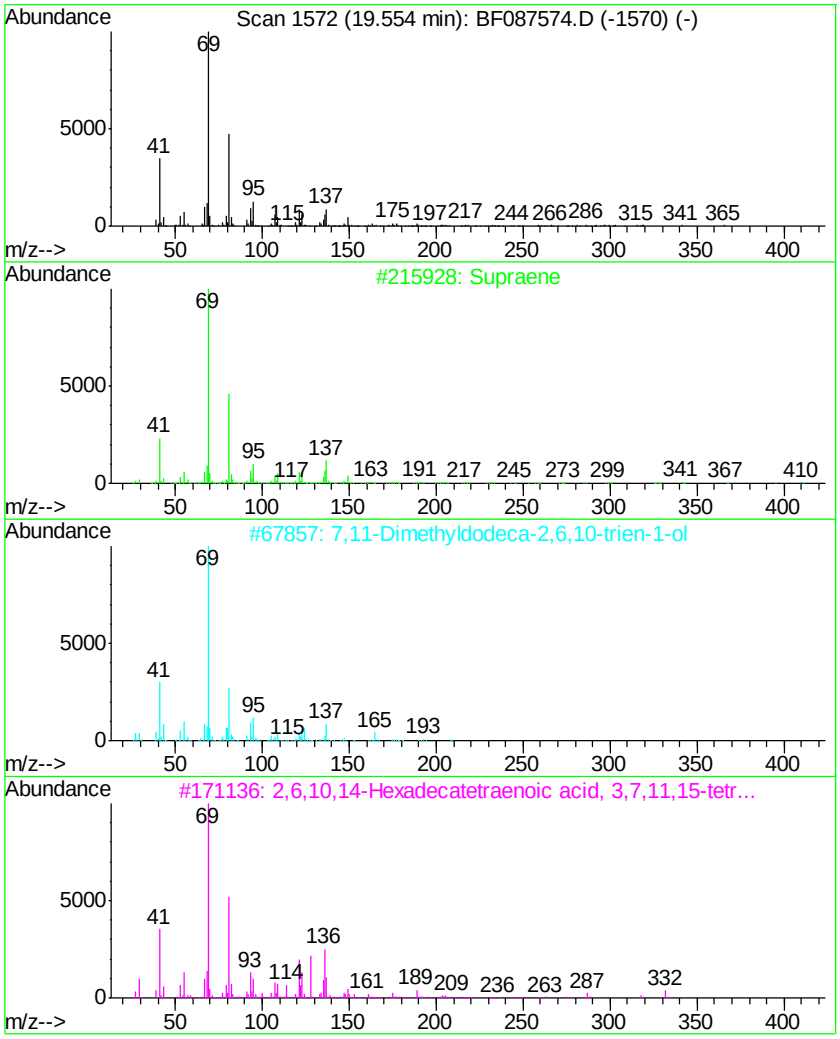
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

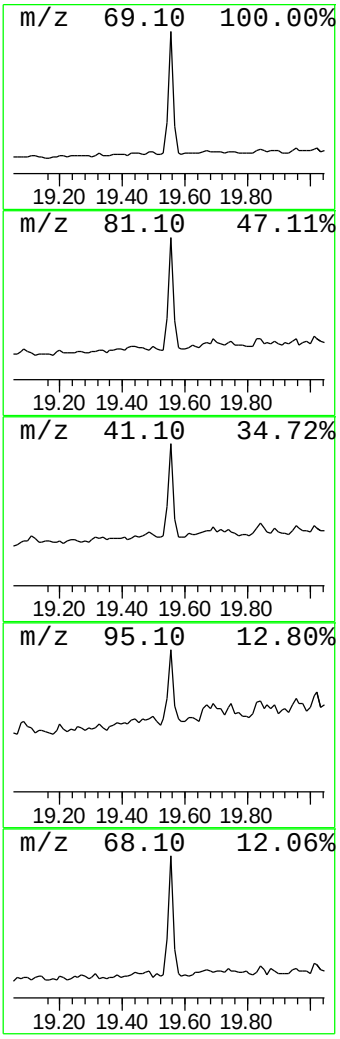
**********

Peak Number 6 Supraene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.55 | 9.04 ng | 275597 | Perylene-d12 | 20.16 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Supraene | 410 | C30H50 | 007683-64-9 | 91 |
| 2 | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 83 |
| 3 | 2,6,10,14-Hexadecatetraenoic aci... | 332 | C22H36O2 | 024035-35-6 | 78 |
| 4 | trans-Farnesol | 222 | C15H26O | 000106-28-5 | 78 |
| 5 | 4,8,12-Tetradecatrienal, 5,9,13-... | 248 | C17H28O | 066408-55-7 | 64 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087574.D
Acq On : 31 May 2016 5:03
Operator : UM/SJ
Sample : H3316-04
Misc :
ALS Vial : 92 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

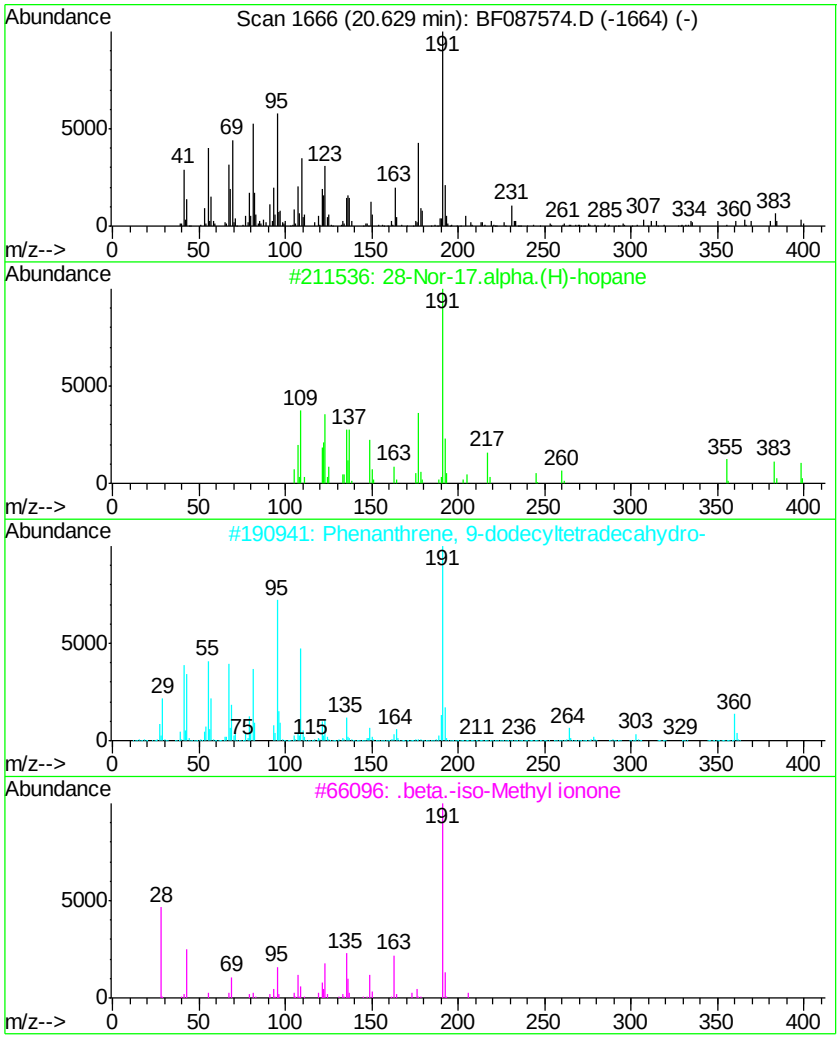
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

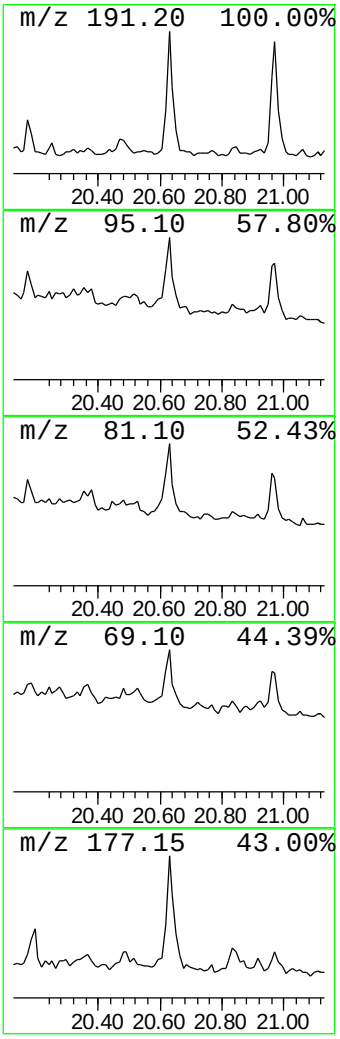
**********

Peak Number 7 28-Nor-17.alpha.(H)-hopane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.63 | 10.28 ng | 313573 | Perylene-d12 | 20.16 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 28-Nor-17.alpha.(H)-hopane | 398 | C29H50 | 053584-60-4 | 78 |
| 2 | Phenanthrene, 9-dodecyltetradeca... | 360 | C26H48 | 055334-01-5 | 46 |
| 3 | .beta.-iso-Methyl ionone | 206 | C14H22O | 1000285-40-2 | 40 |
| 4 | 2-(2-((2-Chloro-6-fluorobenzyl)s... | 334 | C17H16ClFN2S | 1000298-18-2 | 38 |
| 5 | Anthracene, 9-dodecyltetradecahy... | 360 | C26H48 | 055401-75-7 | 38 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087574.D
Acq On : 31 May 2016 5:03
Operator : UM/SJ
Sample : H3316-04
Misc :
ALS Vial : 92 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

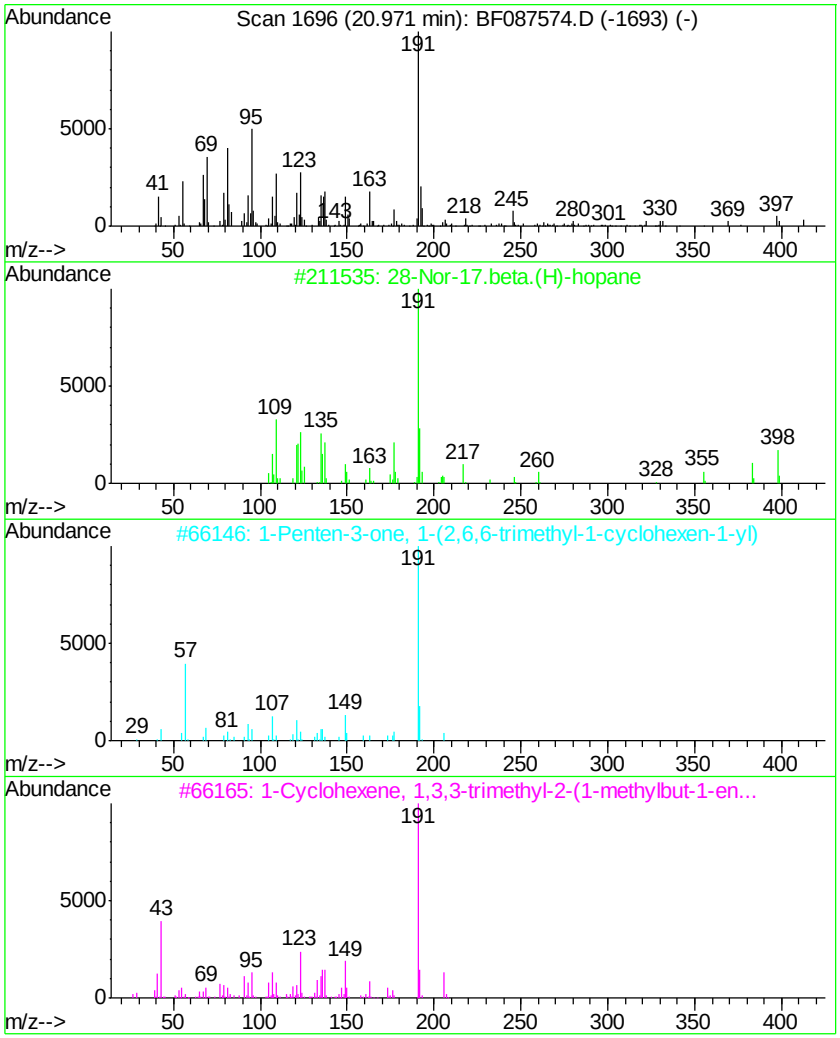
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

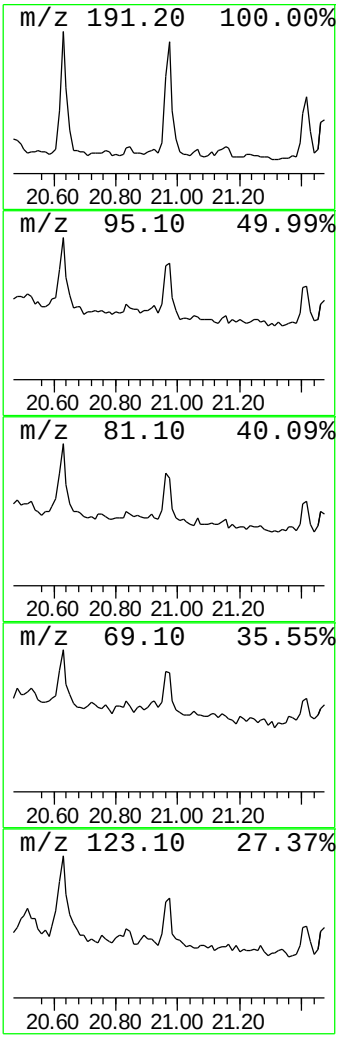
**********

Peak Number 8 28-Nor-17.beta.(H)-hopane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.97 | 7.02 ng | 214082 | Perylene-d12 | 20.16 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 28-Nor-17.beta.(H)-hopane | 398 | C29H50 | 036728-72-0 | 64 |
| 2 | 1-Penten-3-one, 1-(2,6,6-trimeth... | 206 | C14H22O | 000127-43-5 | 50 |
| 3 | 1-Cyclohexene, 1,3,3-trimethyl-2... | 206 | C14H22O | 1000197-08-4 | 40 |
| 4 | 2,4,5,5,8a-Pentamethyl-6,7,8,8a-... | 206 | C14H22O | 1000195-40-9 | 38 |
| 5 | 5-(p-Aminophenyl)-2-thiazolamine | 191 | C9H9N3S | 090349-87-4 | 38 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087574.D
Acq On : 31 May 2016 5:03
Operator : UM/SJ
Sample : H3316-04
Misc :
ALS Vial : 92 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SB-06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

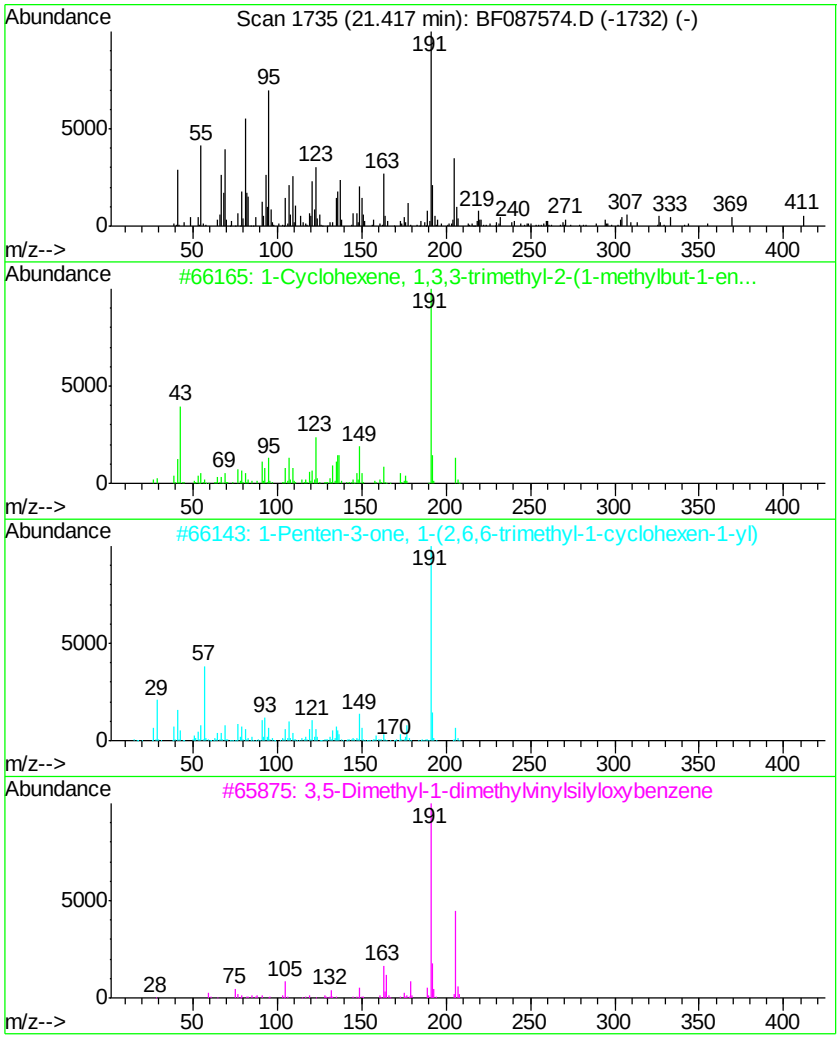
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

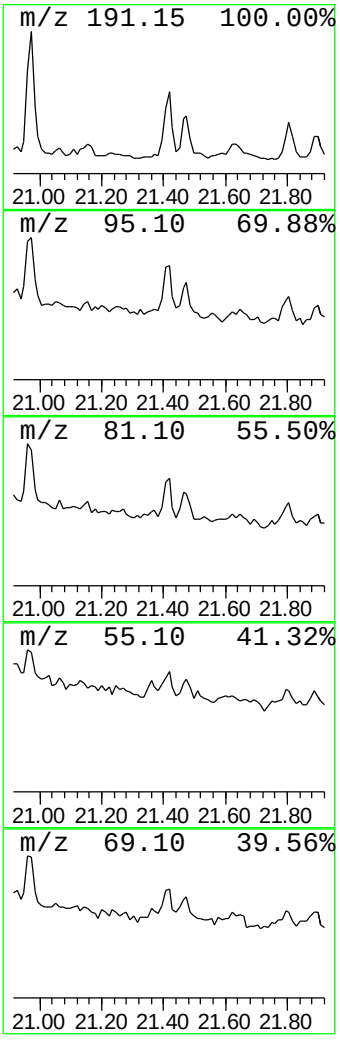
**********

Peak Number 9 1-Cyclohexene, 1,3,3-trimet... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.42 | 4.46 ng | 135855 | Perylene-d12 | 20.16 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Cyclohexene, 1,3,3-trimethyl-2... | 206 | C14H22O | 1000197-08-4 | 53 |
| 2 | 1-Penten-3-one, 1-(2,6,6-trimeth... | 206 | C14H22O | 000127-43-5 | 46 |
| 3 | 3,5-Dimethyl-1-dimethylvinylsilv... | 206 | C12H18OSi | 1000307-91-8 | 38 |
| 4 | Phenol, 2,6-bis(1,1-dimethylethyl)- | 206 | C14H22O | 000128-39-2 | 35 |
| 5 | Phenol, 2,5-bis(1,1-dimethylethyl)- | 206 | C14H22O | 005875-45-6 | 35 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052916\
Data File : BF087574.D
Acq On : 31 May 2016 5:03
Operator : UM/SJ
Sample : H3316-04
Misc :
ALS Vial : 92 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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... | 4.73 | 9.2 | ng | 379057 | 1 | 7.47 | 823210 | 20.0 |
| unknown7.13 | 7.13 | 83.9 | ng | 3451670 | 1 | 7.47 | 823210 | 20.0 |
| 1-Iodo-2-methylun... | 13.93 | 2.0 | ng | 84680 | 4 | 14.75 | 824568 | 20.0 |
| n-Butyl laurate | 16.93 | 3.3 | ng | 152656 | 5 | 18.47 | 919058 | 20.0 |
| Supraene | 19.55 | 9.0 | ng | 275597 | 6 | 20.16 | 609849 | 20.0 |
| 28-Nor-17.alpha.(... | 20.63 | 10.3 | ng | 313573 | 6 | 20.16 | 609849 | 20.0 |
| 28-Nor-17.beta.(H... | 20.97 | 7.0 | ng | 214082 | 6 | 20.16 | 609849 | 20.0 |
| 1-Cyclohexene, 1,... | 21.42 | 4.5 | ng | 135855 | 6 | 20.16 | 609849 | 20.0 |