LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102257.D
Acq On : 20 Jan 2018 11:22
Operator : SJ/JU
Sample : J1114-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-21-2.0-2.5

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-BF010918.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 | 4.922 | 477 | 482 | 490 | rVB | 152282 | 209558 | 6.56% | 0.773% |
| 2 | 5.334 | 547 | 552 | 555 | rBV | 2933840 | 2861414 | 89.63% | 10.553% |
| 3 | 6.363 | 722 | 727 | 737 | rVB | 2837064 | 2926038 | 91.66% | 10.792% |
| 4 | 6.492 | 744 | 749 | 752 | rBV | 3239007 | 2918476 | 91.42% | 10.764% |
| 5 | 6.722 | 784 | 788 | 791 | rBV | 918280 | 819291 | 25.66% | 3.022% |
| 6 | 6.875 | 810 | 814 | 817 | rBV | 2714029 | 2295512 | 71.91% | 8.466% |
| 7 | 7.286 | 879 | 884 | 887 | rBV | 1986488 | 1812159 | 56.77% | 6.683% |
| 8 | 8.004 | 1001 | 1006 | 1009 | rBV | 1186951 | 1066065 | 33.39% | 3.932% |
| 9 | 9.080 | 1184 | 1189 | 1192 | rBV | 3477601 | 3192306 | 100.00% | 11.774% |
| 10 | 9.474 | 1252 | 1256 | 1258 | rBV | 315049 | 266657 | 8.35% | 0.983% |
| 11 | 9.686 | 1288 | 1292 | 1295 | rVB | 124814 | 98296 | 3.08% | 0.363% |
| 12 | 9.757 | 1300 | 1304 | 1307 | rVV | 1203826 | 1075748 | 33.70% | 3.967% |
| 13 | 10.186 | 1369 | 1377 | 1380 | rVB2 | 151509 | 141499 | 4.43% | 0.522% |
| 14 | 10.404 | 1408 | 1414 | 1416 | rBV | 41323 | 49168 | 1.54% | 0.181% |
| 15 | 10.545 | 1432 | 1438 | 1441 | rBV | 1803036 | 1638515 | 51.33% | 6.043% |
| 16 | 10.657 | 1454 | 1457 | 1466 | rBV | 132573 | 126371 | 3.96% | 0.466% |
| 17 | 11.104 | 1530 | 1533 | 1536 | rBV | 43143 | 34395 | 1.08% | 0.127% |
| 18 | 11.239 | 1552 | 1556 | 1559 | rBV | 1131729 | 950617 | 29.78% | 3.506% |
| 19 | 12.645 | 1792 | 1795 | 1798 | rBV | 156612 | 122070 | 3.82% | 0.450% |
| 20 | 12.721 | 1805 | 1808 | 1811 | rVB | 41690 | 33486 | 1.05% | 0.123% |
| 21 | 12.827 | 1821 | 1826 | 1829 | rBV | 2332275 | 2319559 | 72.66% | 8.555% |
| 22 | 13.304 | 1902 | 1907 | 1910 | rBV | 39318 | 43784 | 1.37% | 0.161% |
| 23 | 13.351 | 1912 | 1915 | 1918 | rBV | 99263 | 88582 | 2.77% | 0.327% |
| 24 | 13.715 | 1973 | 1977 | 1981 | rBV | 404139 | 402788 | 12.62% | 1.486% |
| 25 | 13.874 | 2000 | 2004 | 2007 | rBV | 821616 | 728879 | 22.83% | 2.688% |
| 26 | 14.351 | 2082 | 2085 | 2089 | rVB | 47487 | 49037 | 1.54% | 0.181% |
| 27 | 15.298 | 2241 | 2246 | 2255 | rVB | 565653 | 761189 | 23.84% | 2.807% |
| 28 | 17.209 | 2567 | 2571 | 2578 | rVB9 | 42899 | 82724 | 2.59% | 0.305% |

Sum of corrected areas: 27114183

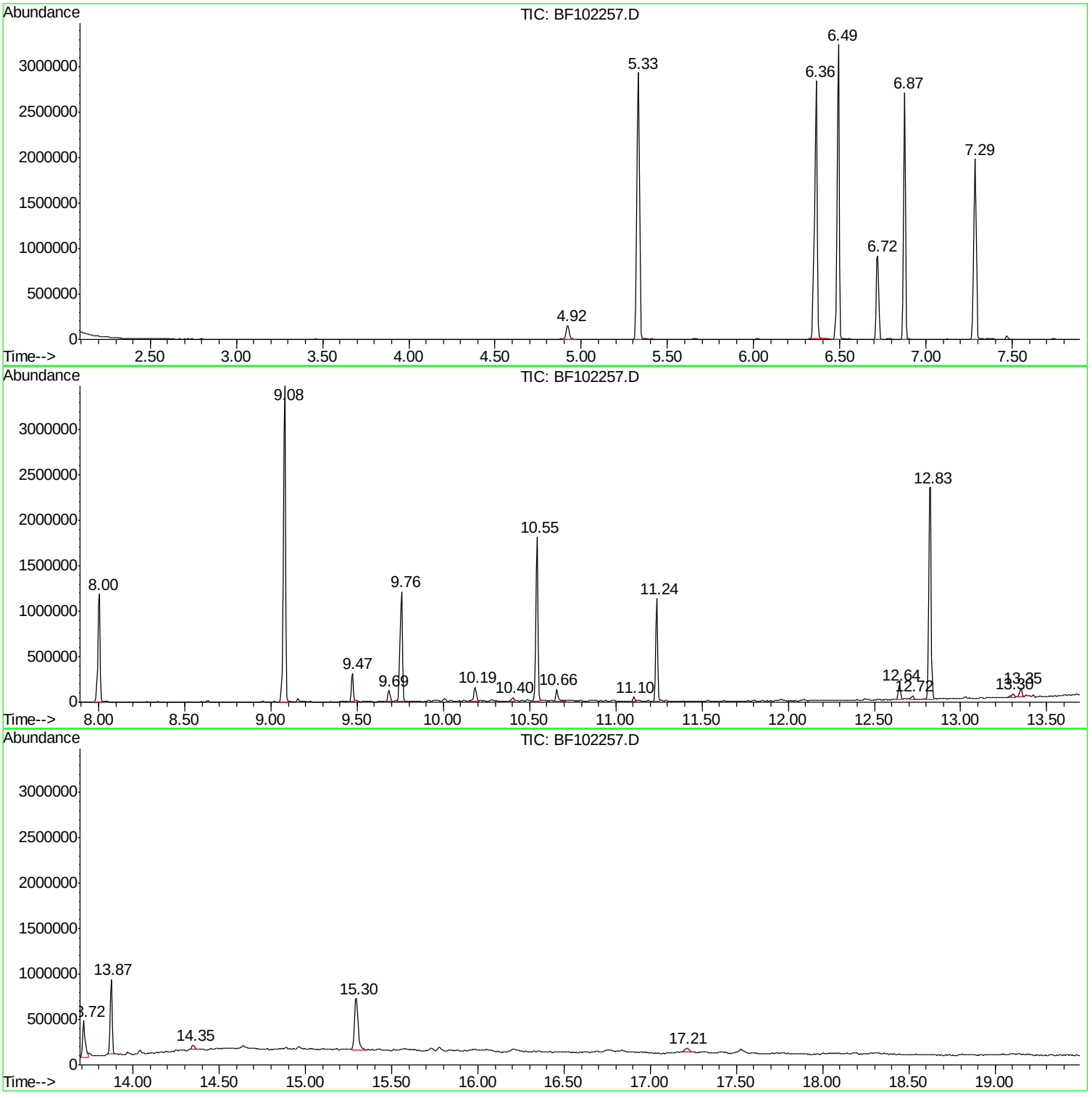
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102257.D
Acq On : 20 Jan 2018 11:22
Operator : SJ/JU
Sample : J1114-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-21-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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\BF012018\
Data File : BF102257.D
Acq On : 20 Jan 2018 11:22
Operator : SJ/JU
Sample : J1114-01
Misc :
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**Instrument :** BNA_F
**ClientSampleId :** SB-21-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

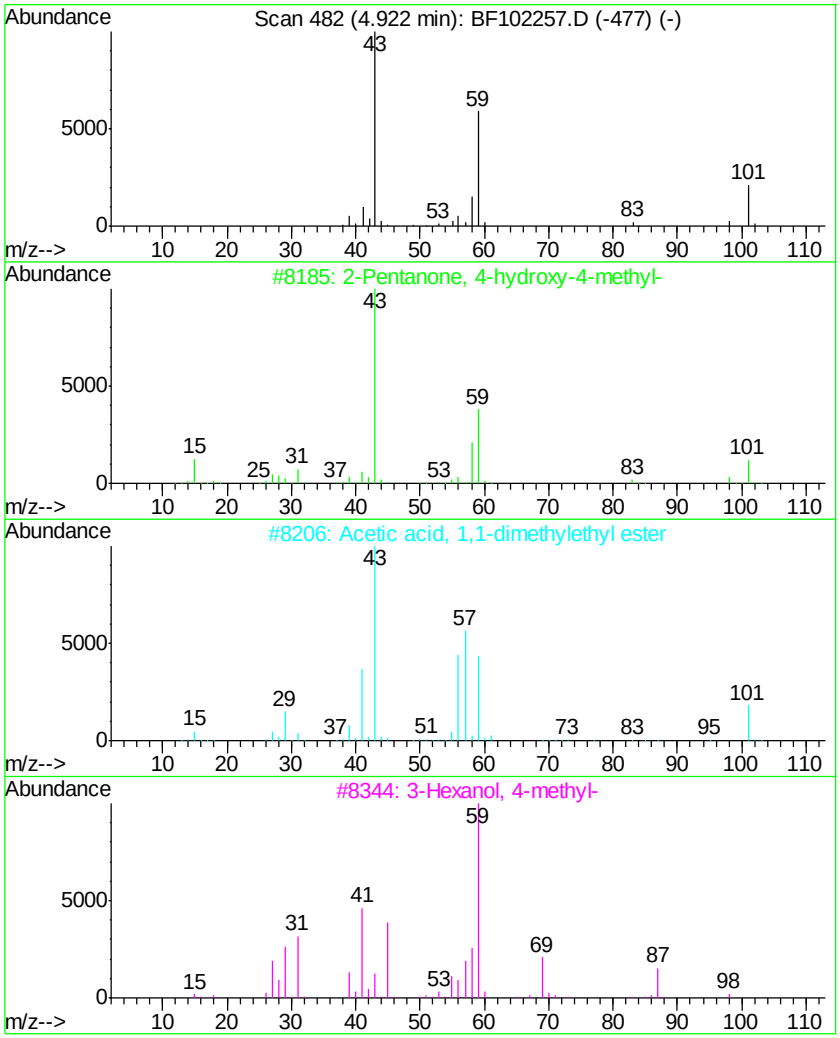
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

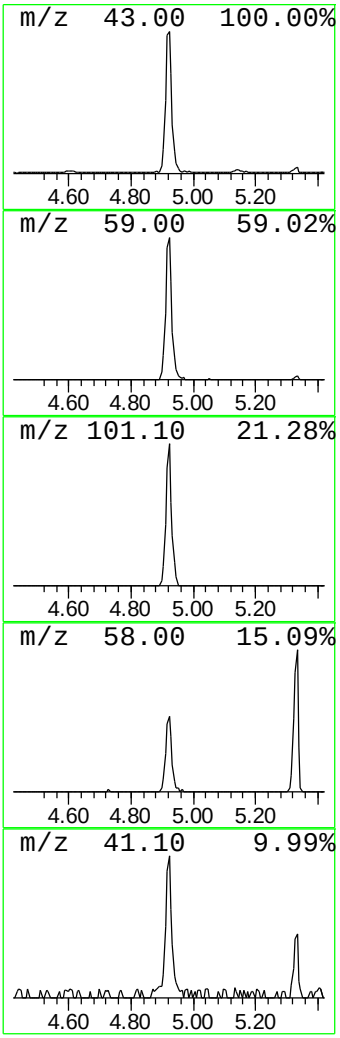
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.92 | 5.12 ng | 209558 | 1,4-Dichlorobenzene-d4 | 6.72 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 40 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 3 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 28 |
| 4 | 3-Hexanol | 102 | C6H14O | 000623-37-0 | 28 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102257.D
Acq On : 20 Jan 2018 11:22
Operator : SJ/JU
Sample : J1114-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-21-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

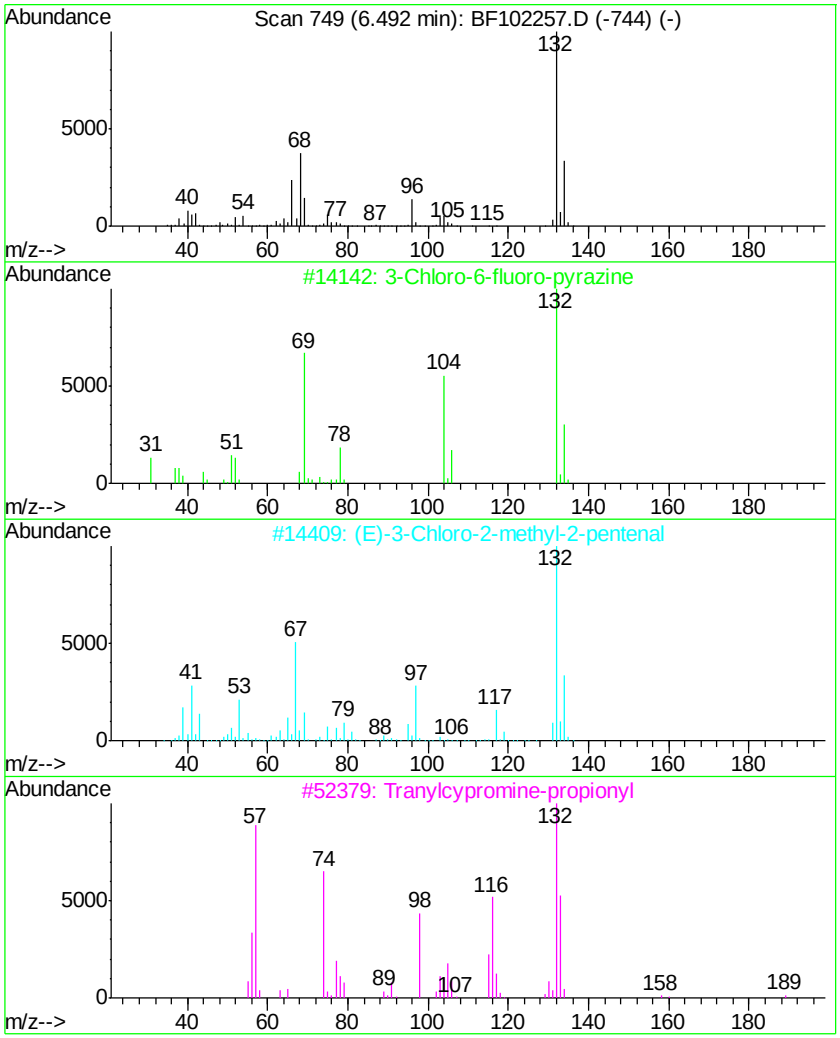
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

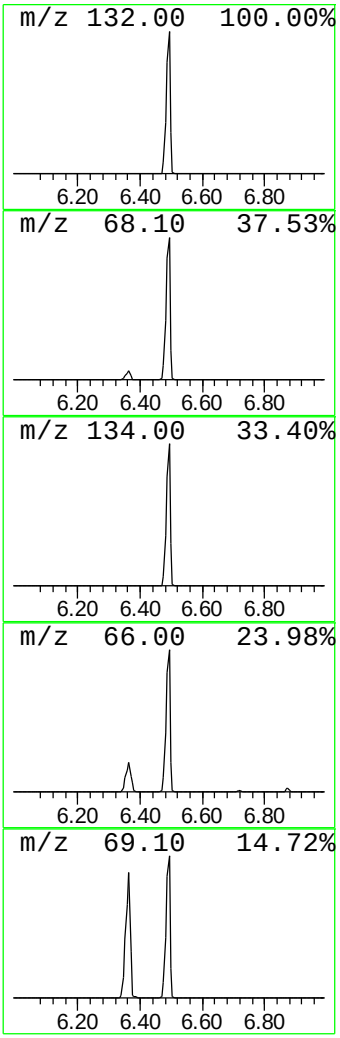
**********

Peak Number 2 unknown6.49 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.49 | 71.24 ng | 2918480 | 1,4-Dichlorobenzene-d4 | 6.72 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 35 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 5 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102257.D
Acq On : 20 Jan 2018 11:22
Operator : SJ/JU
Sample : J1114-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-21-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

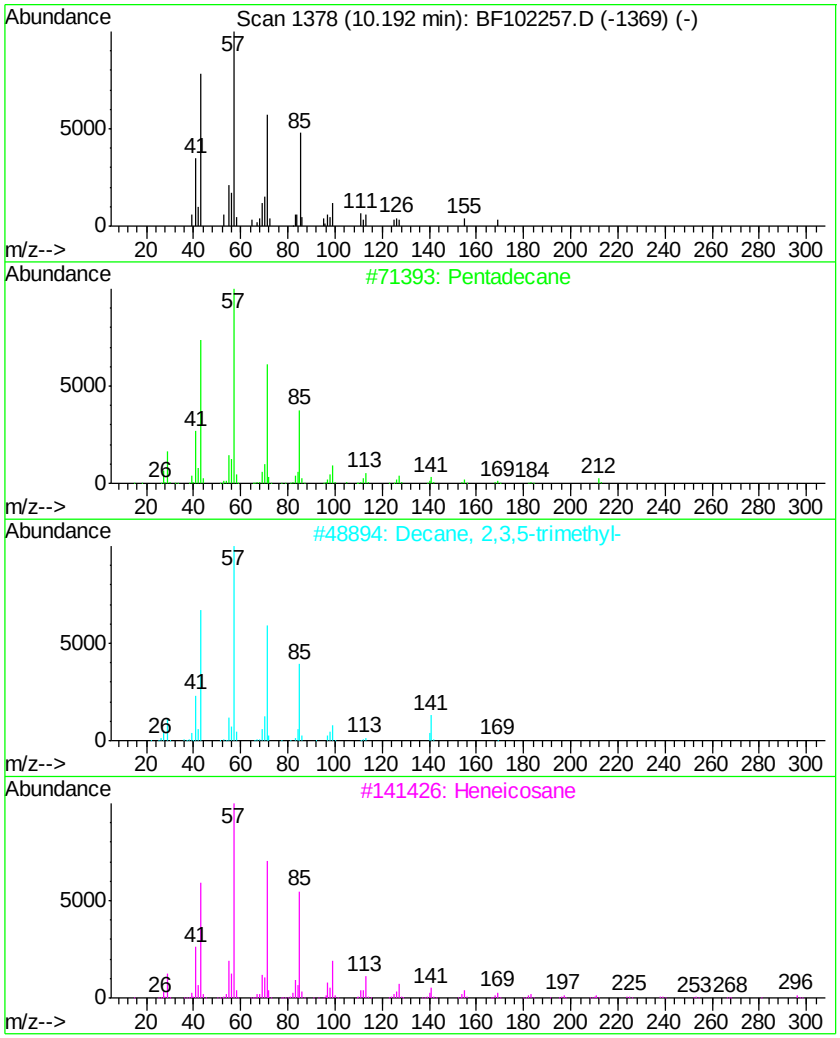
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

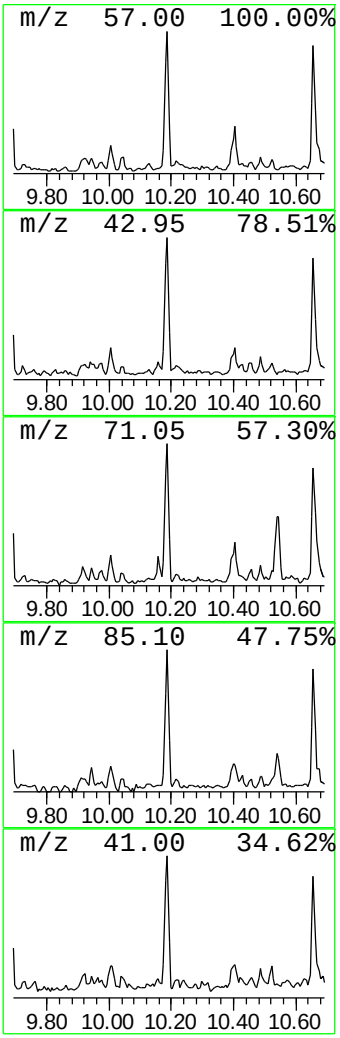
**********

Peak Number 4 Pentadecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.19 | 2.63 ng | 141499 | Acenaphthene-d10 | 9.76 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentadecane | 212 | C15H32 | 000629-62-9 | 86 |
| 2 | Decane, 2,3,5-trimethyl- | 184 | C13H28 | 062238-11-3 | 83 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 83 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 78 |
| 5 | Tetradecane | 198 | C14H30 | 000629-59-4 | 72 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102257.D
Acq On : 20 Jan 2018 11:22
Operator : SJ/JU
Sample : J1114-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-21-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

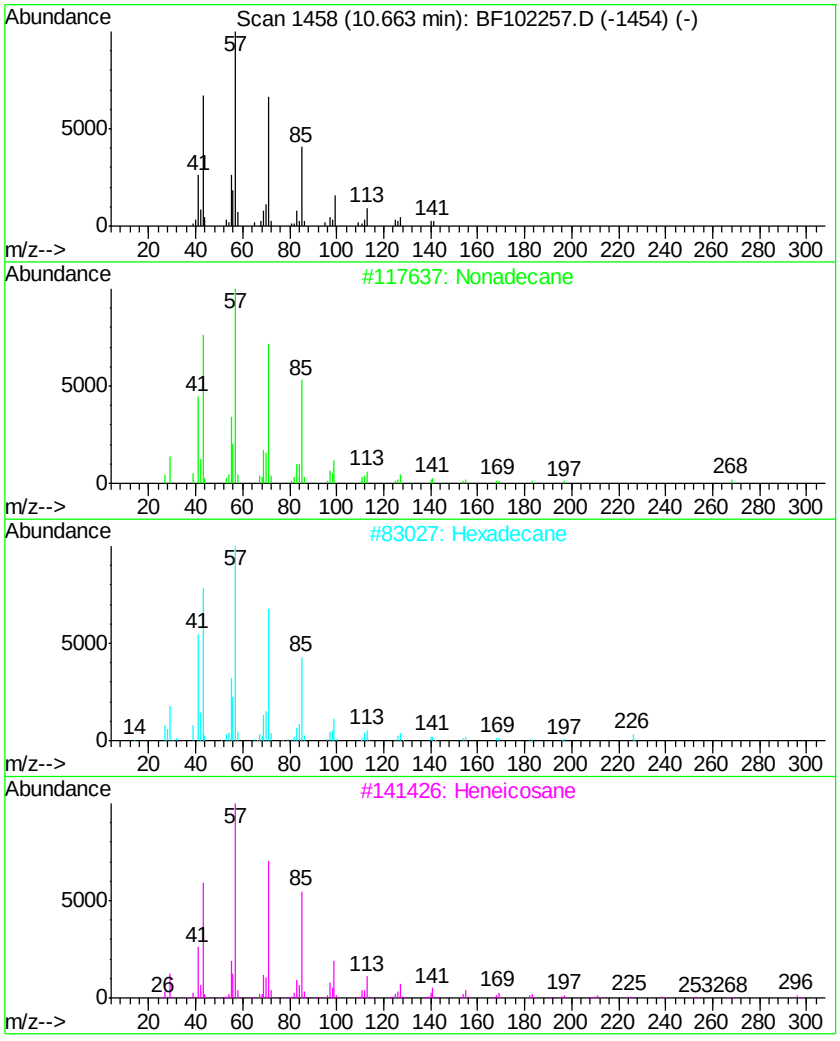
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

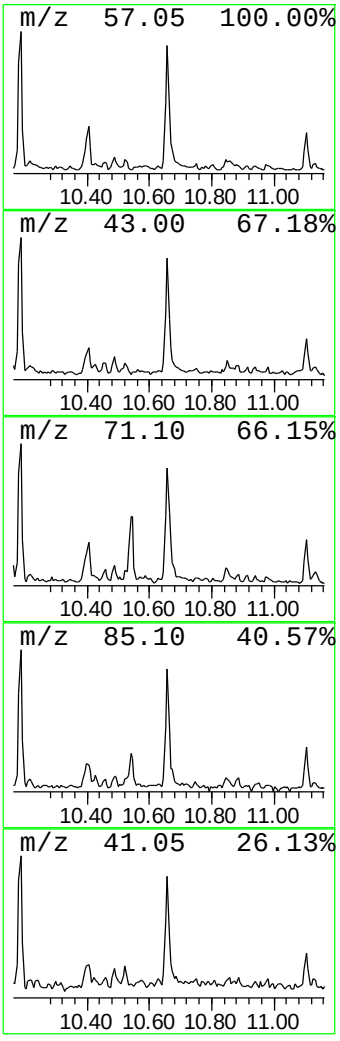
**********

Peak Number 5 Nonadecane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.66 | 2.66 ng | 126371 | Phenanthrene-d10 | 11.24 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Nonadecane | 268 | C19H40 | 000629-92-5 | 87 |
| 2 | Hexadecane | 226 | C16H34 | 000544-76-3 | 87 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 83 |
| 4 | Nonane, 5-butyl- | 184 | C13H28 | 017312-63-9 | 80 |
| 5 | Tetradecane | 198 | C14H30 | 000629-59-4 | 72 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102257.D
Acq On : 20 Jan 2018 11:22
Operator : SJ/JU
Sample : J1114-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-21-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

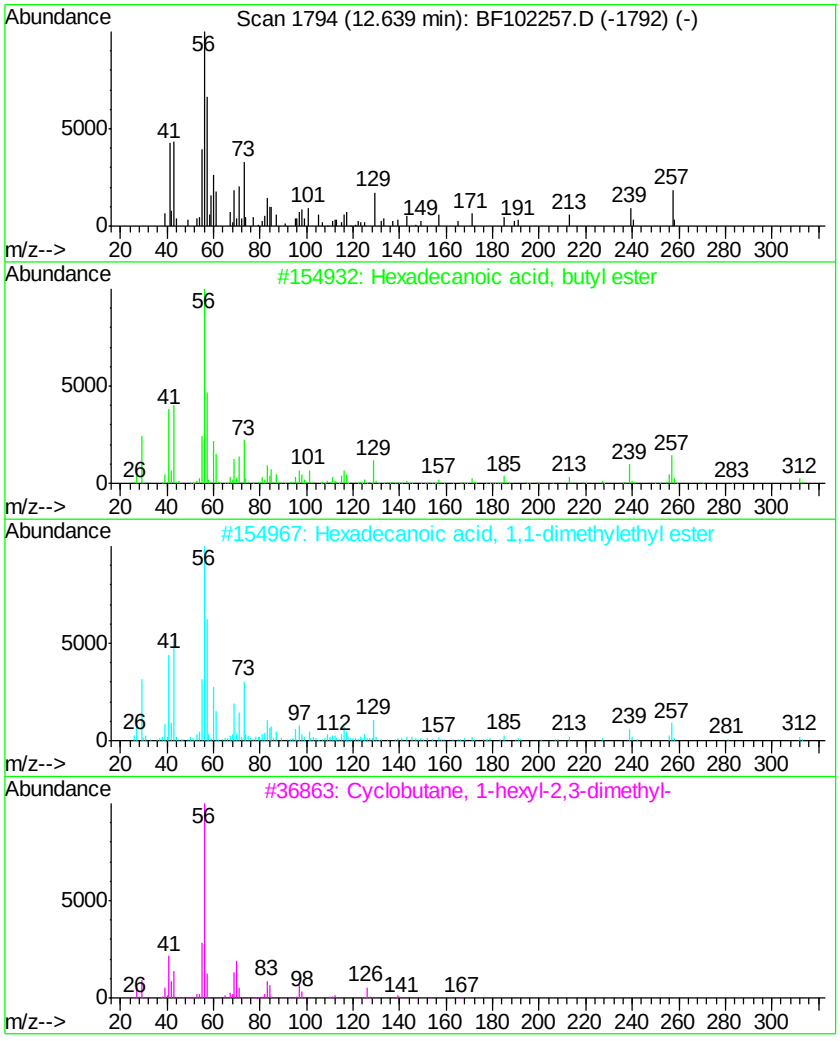
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

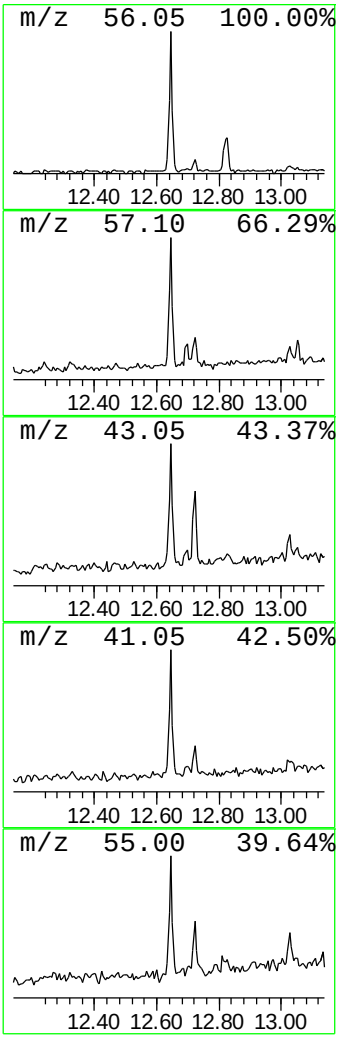
**********

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.64 | 3.35 ng | 122070 | Chrysene-d12 | 13.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, butyl ester | 312 | C20H40O2 | 000111-06-8 | 87 |
| 2 | Hexadecanoic acid, 1,1-dimethyle... | 312 | C20H40O2 | 031158-91-5 | 74 |
| 3 | Cyclobutane, 1-hexyl-2,3-dimethyl- | 168 | C12H24 | 055170-84-8 | 38 |
| 4 | 2-Methyl-n-1-tridecene | 196 | C14H28 | 018094-01-4 | 38 |
| 5 | 1-Heptene, 2-methyl- | 112 | C8H16 | 015870-10-7 | 35 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102257.D
Acq On : 20 Jan 2018 11:22
Operator : SJ/JU
Sample : J1114-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-21-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

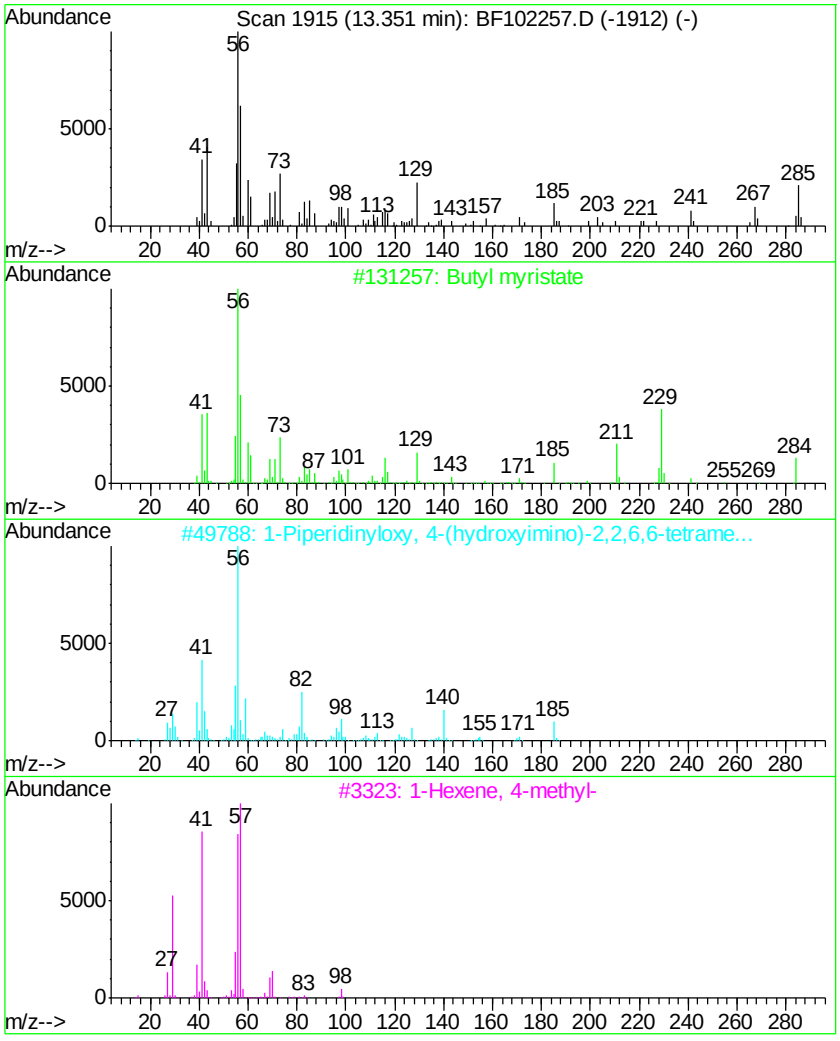
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

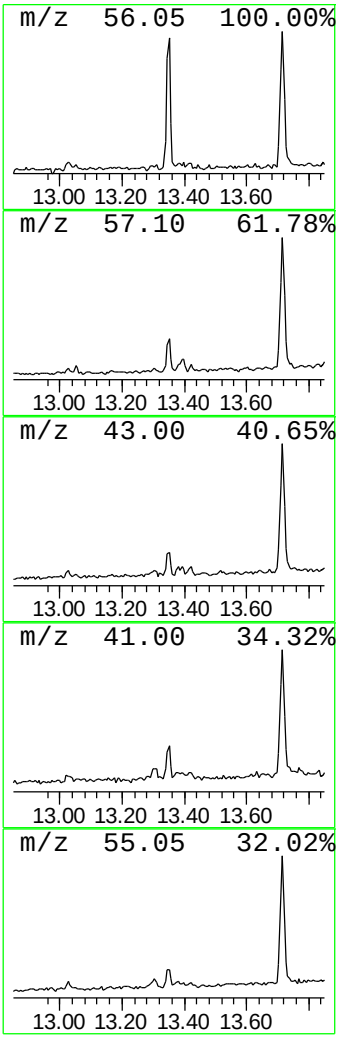
**********

Peak Number 7 Butyl myristate Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.35 | 2.43 ng | 88582 | Chrysene-d12 | 13.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butyl myristate | 284 | C18H36O2 | 000110-36-1 | 53 |
| 2 | 1-Piperidinyloxy, 4-(hydroxyimin... | 185 | C9H17N2O2 | 003229-75-2 | 35 |
| 3 | 1-Hexene, 4-methyl- | 98 | C7H14 | 003769-23-1 | 30 |
| 4 | 1-Pentene, 2,4-dimethyl- | 98 | C7H14 | 002213-32-3 | 27 |
| 5 | Dodecane, 2,2,11,11-tetramethyl- | 226 | C16H34 | 127204-12-0 | 27 |



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Data File : BF102257.D
Acq On : 20 Jan 2018 11:22
Operator : SJ/JU
Sample : J1114-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-21-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

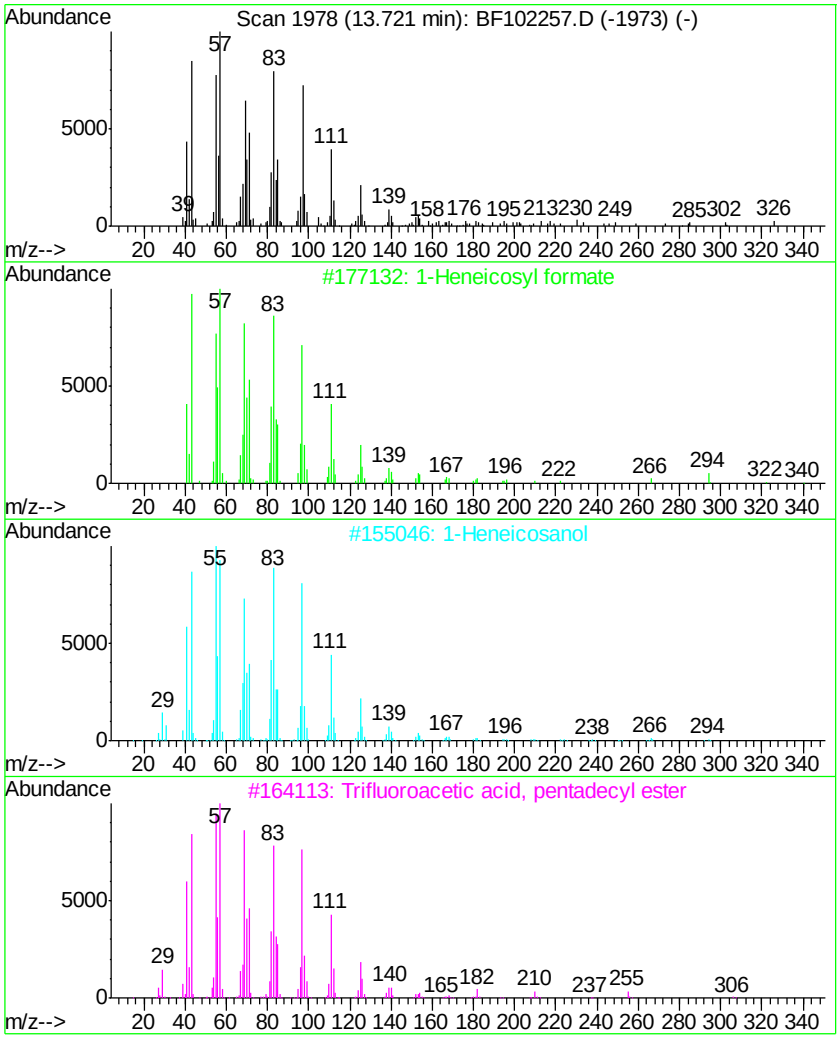
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

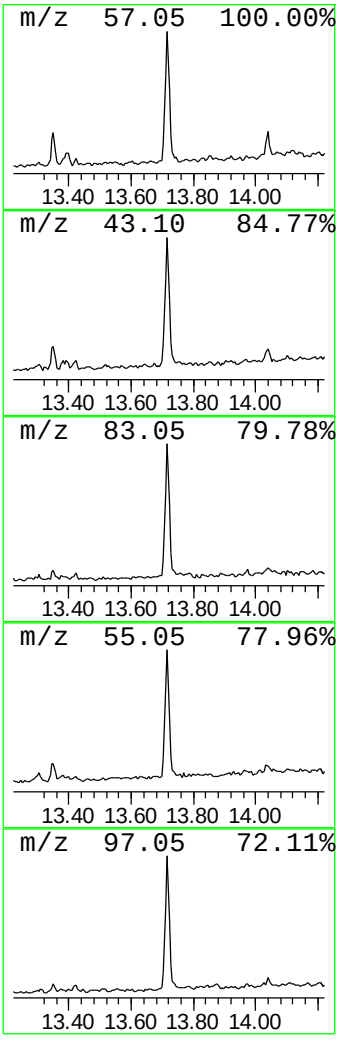
**********

Peak Number 8 1-Heneicosyl formate Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.72 | 11.05 ng | 402788 | Chrysene-d12 | 13.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosyl formate | 340 | C22H44O2 | 077899-03-7 | 95 |
| 2 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 95 |
| 3 | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 94 |
| 4 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 94 |
| 5 | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1 | 94 |



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Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-21-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

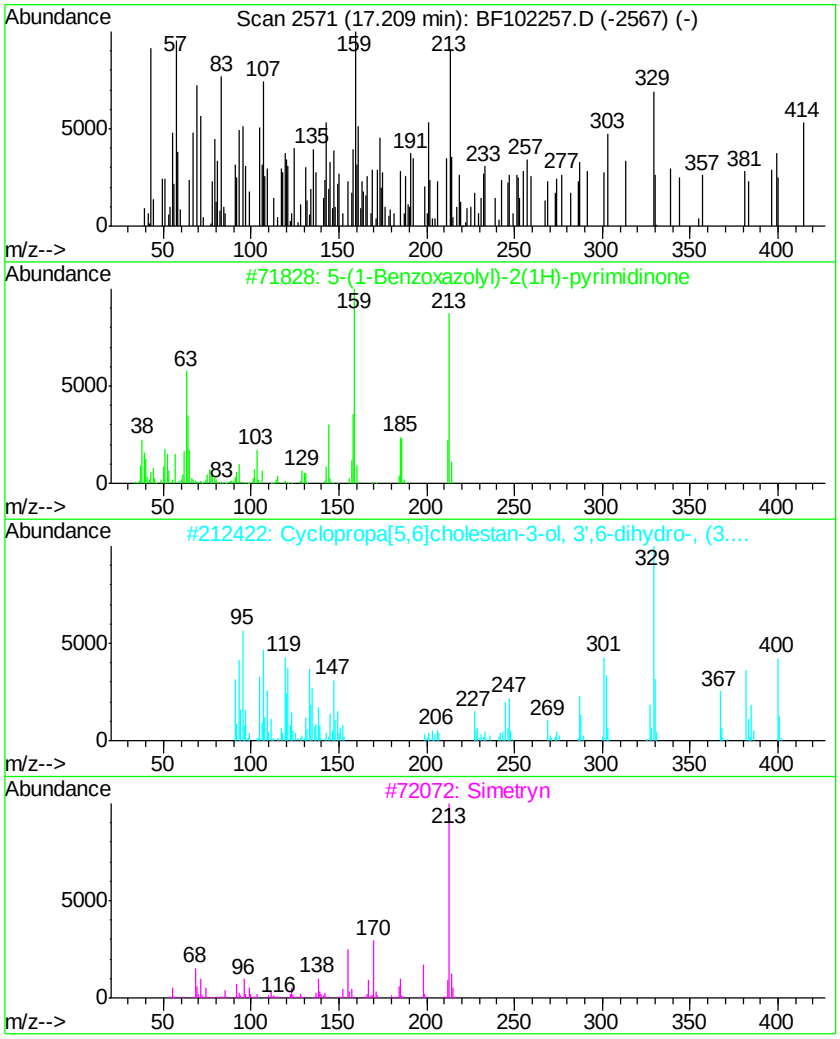
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

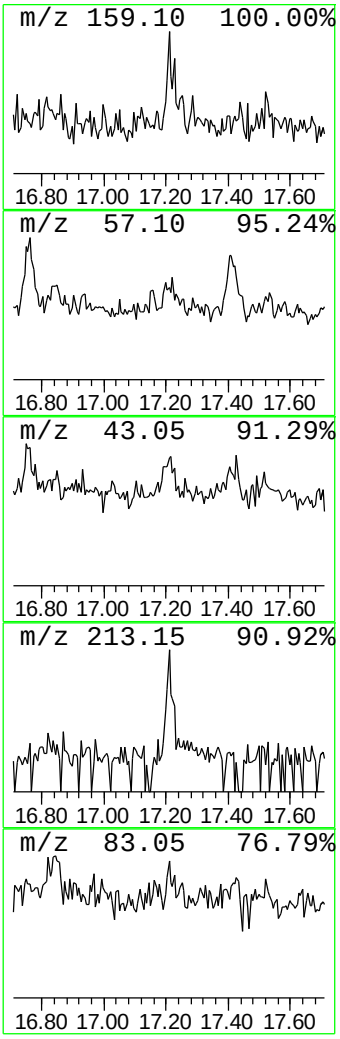
**********

Peak Number 9 unknown17.21 Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.21 | 2.17 ng | 82724 | Perylene-d12 | 15.30 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-(1-Benzoxazolyl)-2(1H)-pyrimid... | 213 | C11H7N3O2 | 349488-95-5 | 14 |
| 2 | Cyclopropa[5,6]cholestan-3-ol, 3... | 400 | C28H48O | 035339-47-0 | 11 |
| 3 | Simetryn | 213 | C8H15N5S | 001014-70-6 | 10 |
| 4 | 1-Nitro-2,4,6-trimethoxybenzene | 213 | C9H11NO5 | 014227-18-0 | 10 |
| 5 | Bufa-20,22-dienolide, 14,15-epox... | 400 | C24H32O5 | 004026-95-3 | 10 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102257.D
Acq On : 20 Jan 2018 11:22
Operator : SJ/JU
Sample : J1114-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-21-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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... | 4.92 | 5.1 | ng | 209558 | 1 | 6.72 | 819291 | 20.0 |
| unknown6.49 | 6.49 | 71.2 | ng | 2918480 | 1 | 6.72 | 819291 | 20.0 |
| Pentadecane | 10.19 | 2.6 | ng | 141499 | 3 | 9.76 | 1075750 | 20.0 |
| Nonadecane | 10.66 | 2.7 | ng | 126371 | 4 | 11.24 | 950617 | 20.0 |
| Hexadecanoic acid... | 12.64 | 3.4 | ng | 122070 | 5 | 13.87 | 728879 | 20.0 |
| Butyl myristate | 13.35 | 2.4 | ng | 88582 | 5 | 13.87 | 728879 | 20.0 |
| 1-Heneicosyl formate | 13.72 | 11.1 | ng | 402788 | 5 | 13.87 | 728879 | 20.0 |
| unknown17.21 | 17.21 | 2.2 | ng | 82724 | 6 | 15.30 | 761189 | 20.0 |