LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030419\
Data File : BF112829.D
Acq On : 4 Mar 2019 17:29
Operator : JU/SJ
Sample : K1712-07 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Z-2-1

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-BF022719.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 | 5.351 | 551 | 555 | 571 | rBV | 2107368 | 2016418 | 92.52% | 8.725% |
| 2 | 6.375 | 725 | 729 | 741 | rBV | 2261405 | 2071528 | 95.05% | 8.963% |
| 3 | 6.516 | 748 | 753 | 756 | rBV | 2203640 | 2120225 | 97.28% | 9.174% |
| 4 | 6.745 | 788 | 792 | 802 | rBV | 1161025 | 953865 | 43.77% | 4.127% |
| 5 | 6.904 | 815 | 819 | 822 | rBV | 2017823 | 1675818 | 76.89% | 7.251% |
| 6 | 7.304 | 882 | 887 | 895 | rBV | 1272443 | 1247829 | 57.26% | 5.399% |
| 7 | 8.028 | 1006 | 1010 | 1030 | rBV | 1174339 | 1132222 | 51.95% | 4.899% |
| 8 | 9.098 | 1189 | 1192 | 1203 | rBV | 2110960 | 2045863 | 93.87% | 8.852% |
| 9 | 9.492 | 1256 | 1259 | 1270 | rVB | 83084 | 82842 | 3.80% | 0.358% |
| 10 | 9.775 | 1303 | 1307 | 1320 | rVB2 | 1302228 | 1158371 | 53.15% | 5.012% |
| 11 | 10.557 | 1436 | 1440 | 1455 | rBV | 1407013 | 1378984 | 63.27% | 5.967% |
| 12 | 11.139 | 1535 | 1539 | 1542 | rBV | 19508 | 24848 | 1.14% | 0.108% |
| 13 | 11.251 | 1555 | 1558 | 1562 | rBV | 1260786 | 1298925 | 59.60% | 5.620% |
| 14 | 11.786 | 1646 | 1649 | 1659 | rBV2 | 295150 | 339045 | 15.56% | 1.467% |
| 15 | 11.863 | 1659 | 1662 | 1665 | rBV4 | 17911 | 25243 | 1.16% | 0.109% |
| 16 | 12.463 | 1760 | 1764 | 1767 | rBV | 113257 | 127073 | 5.83% | 0.550% |
| 17 | 12.574 | 1779 | 1783 | 1793 | rBV3 | 108907 | 169195 | 7.76% | 0.732% |
| 18 | 12.686 | 1799 | 1802 | 1806 | rVB | 89153 | 78831 | 3.62% | 0.341% |
| 19 | 12.833 | 1823 | 1827 | 1831 | rBV | 2376286 | 2179416 | 100.00% | 9.430% |
| 20 | 13.080 | 1867 | 1869 | 1872 | rVB | 46715 | 37360 | 1.71% | 0.162% |
| 21 | 13.421 | 1925 | 1927 | 1930 | rVB | 54042 | 43796 | 2.01% | 0.190% |
| 22 | 13.739 | 1978 | 1981 | 1988 | rBV2 | 298403 | 348133 | 15.97% | 1.506% |
| 23 | 13.880 | 2001 | 2005 | 2008 | rBV | 1473971 | 1377114 | 63.19% | 5.959% |
| 24 | 14.063 | 2034 | 2036 | 2040 | rVB | 103839 | 93005 | 4.27% | 0.402% |
| 25 | 14.368 | 2086 | 2088 | 2091 | rBV | 149598 | 123133 | 5.65% | 0.533% |
| 26 | 14.663 | 2136 | 2138 | 2145 | rVB | 166641 | 183842 | 8.44% | 0.795% |
| 27 | 15.298 | 2242 | 2246 | 2250 | rVB | 660890 | 777944 | 35.70% | 3.366% |

Sum of corrected areas: 23110868

LSC Report - Integrated Chromatogram

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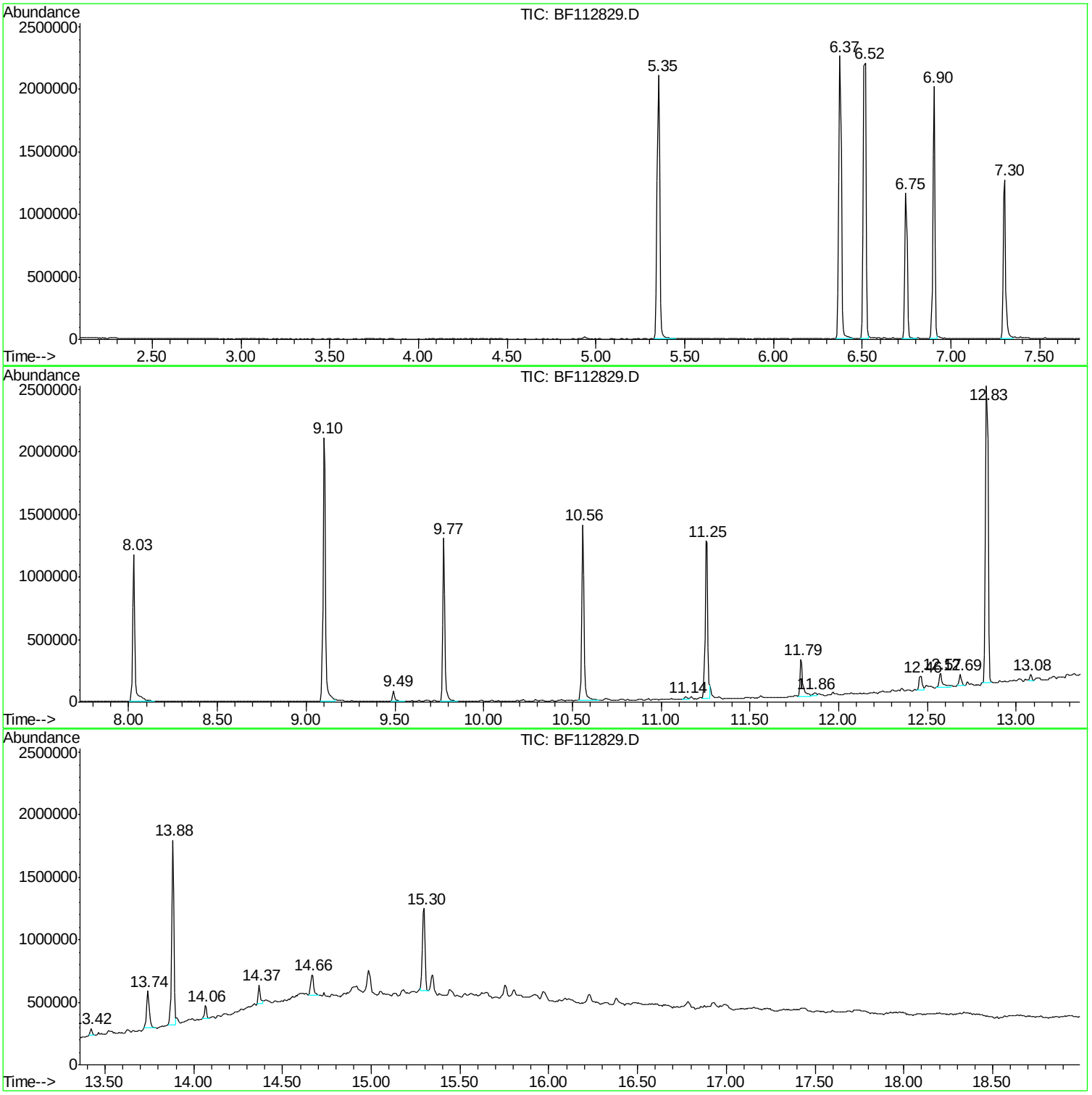
Acq On : 4 Mar 2019 17:29
Operator : JU/SJ
Sample : K1712-07 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Z-2-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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\BF030419\
Data File : BF112829.D
Acq On : 4 Mar 2019 17:29
Operator : JU/SJ
Sample : K1712-07 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Z-2-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

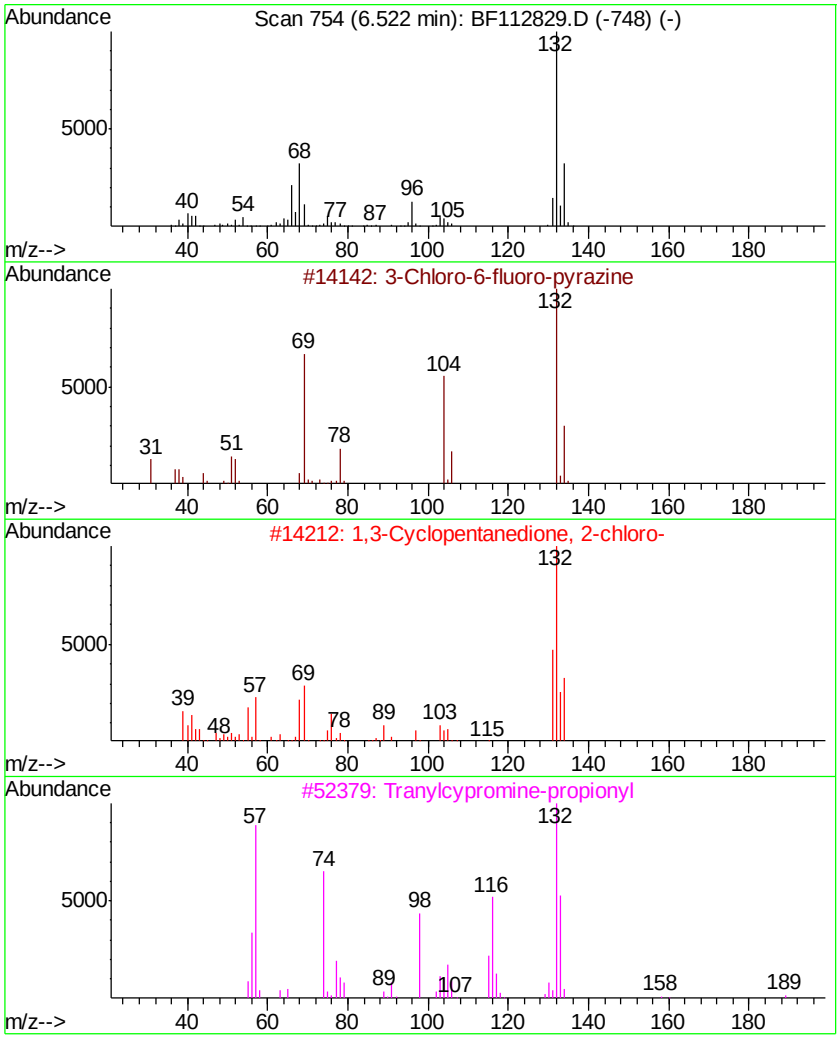
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

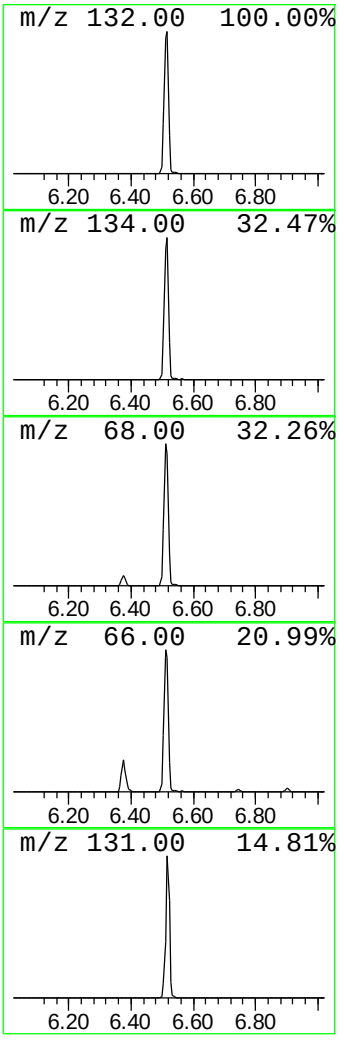
**********

Peak Number 1 unknown6.52 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.52 | 44.46 ng | 2120230 | 1,4-Dichlorobenzene-d4 | 6.75 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 35 |
| 2 | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2 | 014203-19-1 | 23 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 16 |
| 4 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 16 |
| 5 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030419\
Data File : BF112829.D
Acq On : 4 Mar 2019 17:29
Operator : JU/SJ
Sample : K1712-07 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Z-2-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

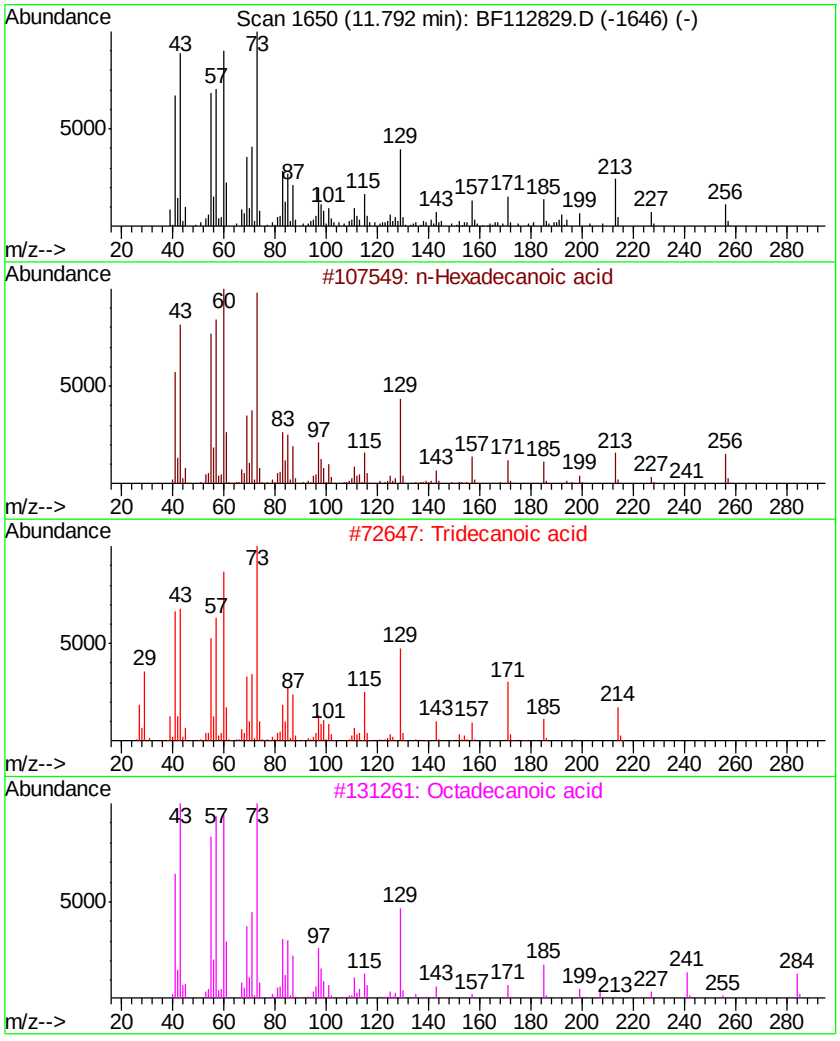
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

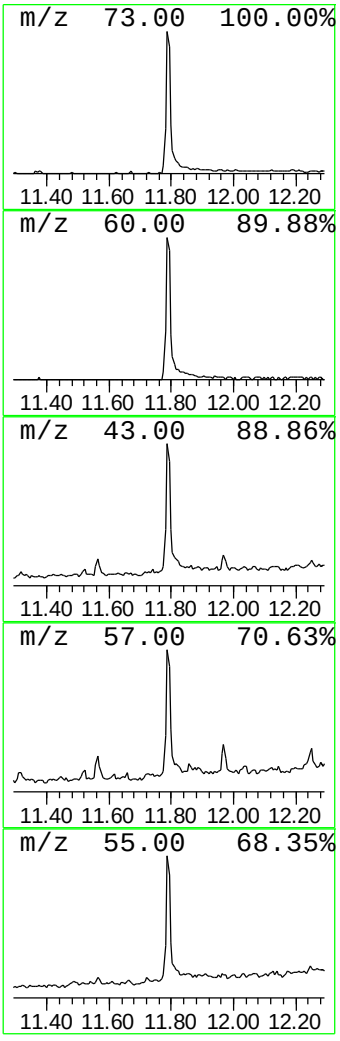
**********

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.79 | 5.22 ng | 339045 | Phenanthrene-d10 | 11.26 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 94 |
| 3 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 90 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 80 |



# Library Search Compound Report

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Data File : BF112829.D
Acq On : 4 Mar 2019 17:29
Operator : JU/SJ
Sample : K1712-07 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Z-2-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

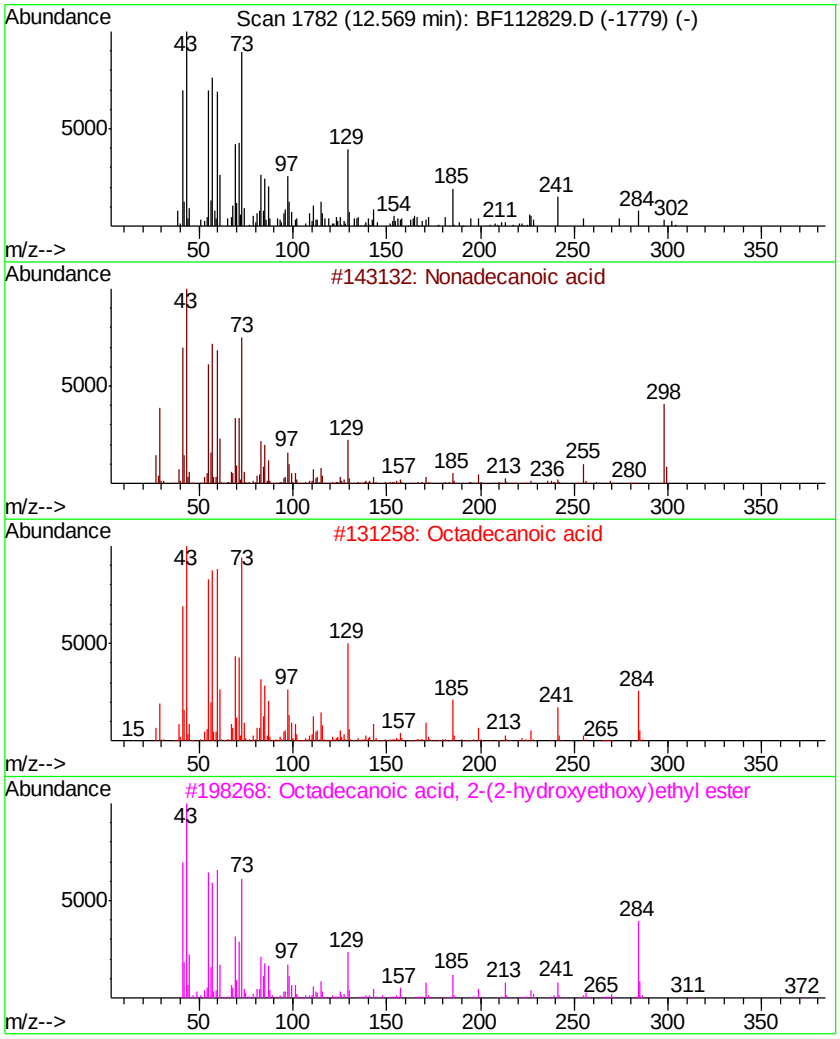
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

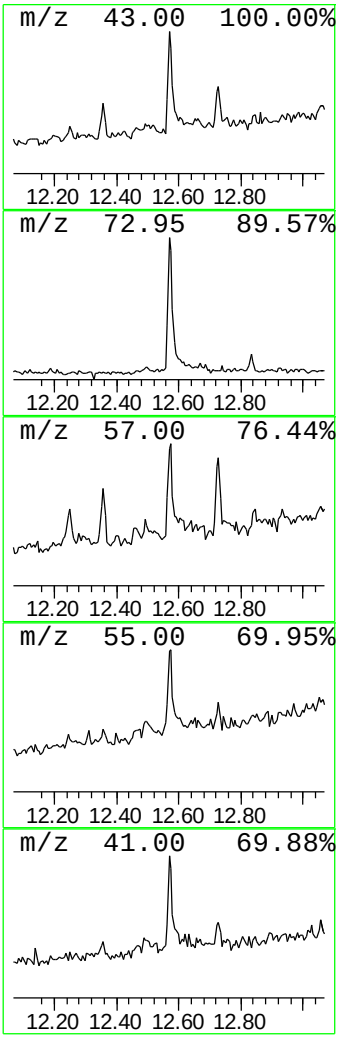
**********

Peak Number 4 Nonadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.57 | 2.46 ng | 169195 | Chrysene-d12 | 13.88 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Nonadecanoic acid | 298 | C19H38O2 | 000646-30-0 | 94 |
| 2 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 94 |
| 3 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 64 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 59 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 58 |



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Operator : JU/SJ
Sample : K1712-07 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Z-2-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

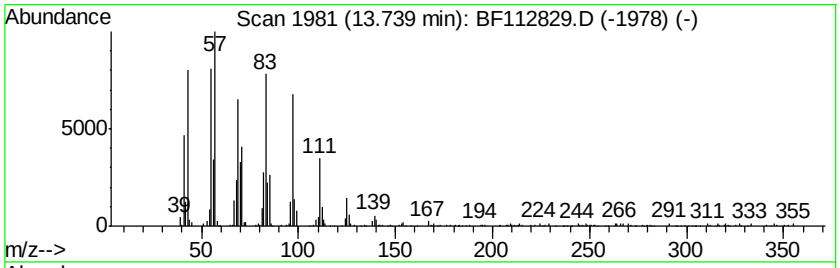
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

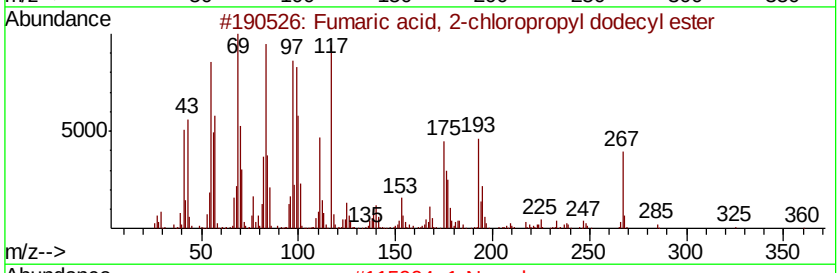
**********

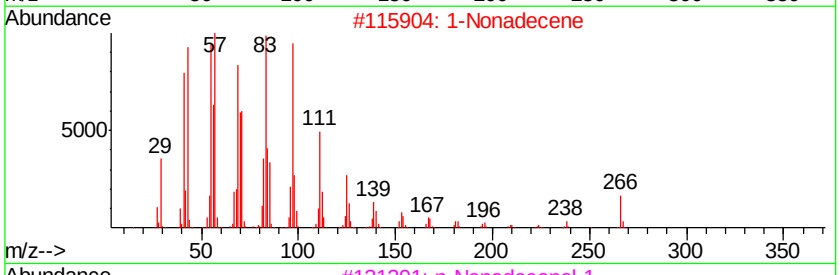
Peak Number 5 Fumaric acid, 2-chloropropy... Concentration Rank 4

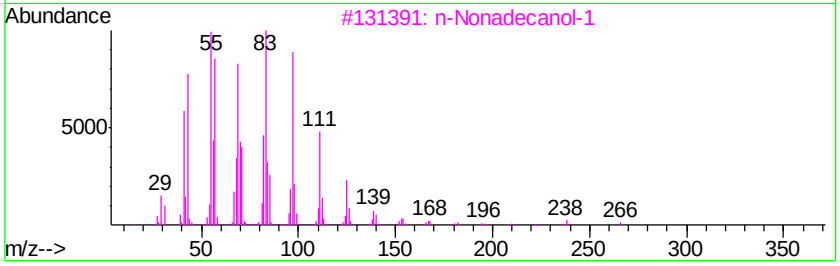
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.74 | 5.06 ng | 348133 | Chrysene-d12 | 13.88 |

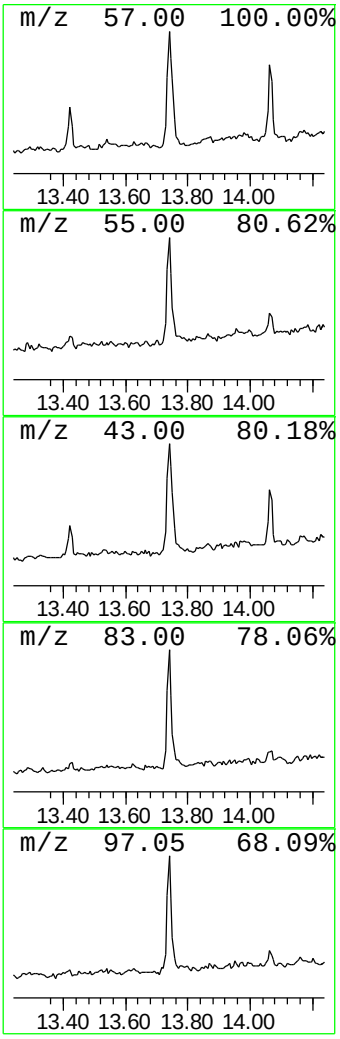
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Fumaric acid, 2-chloropropyl dod... | 360 | C19H33ClO4 | 1000348-57-0 | 96 |
| 2 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 94 |
| 3 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 93 |
| 4 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 93 |
| 5 | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1 | 91 |



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**Instrument :** BNA_F
**ClientSampleId :** Z-2-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

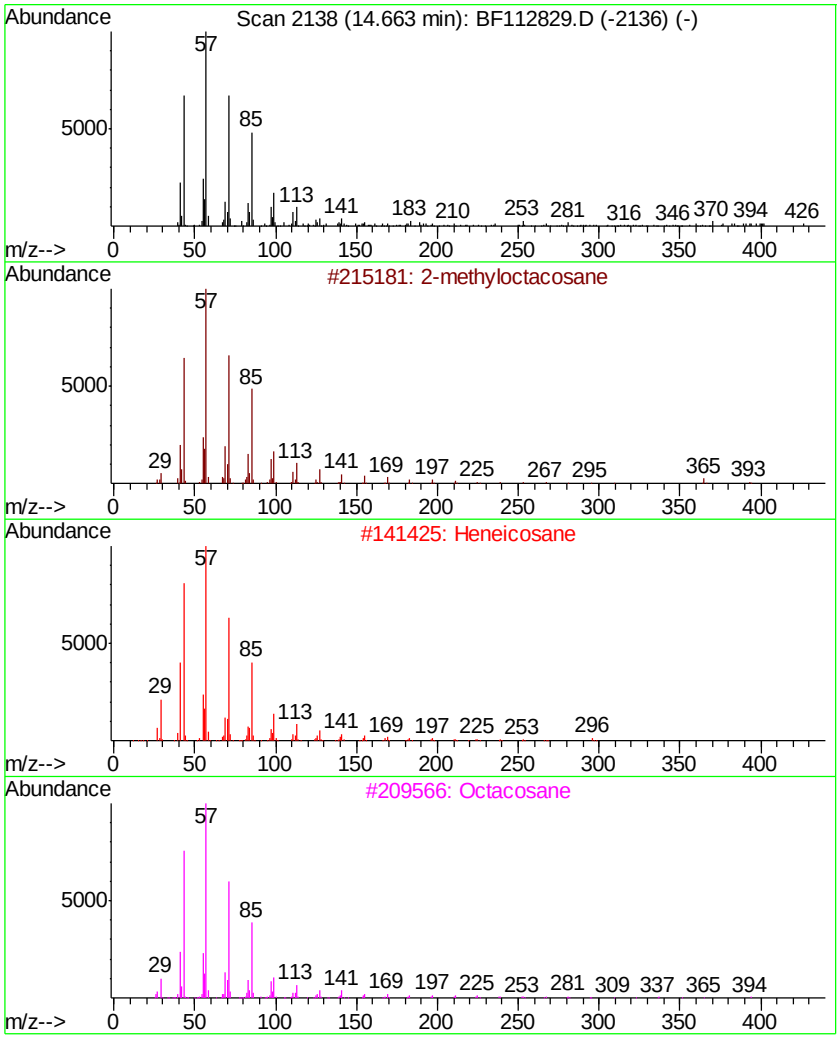
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

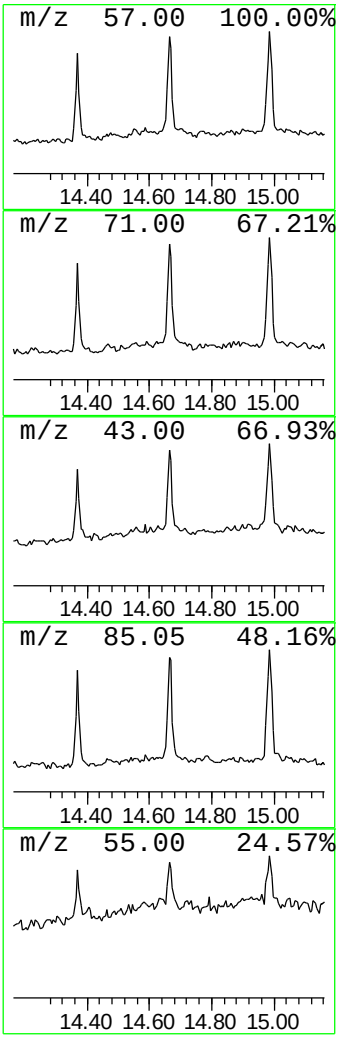
**********

Peak Number 6 2-methyloctacosane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.66 | 4.73 ng | 183842 | Perylene-d12 | 15.30 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 87 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 87 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 87 |
| 4 | Eicosane, 10-methyl- | 296 | C21H44 | 054833-23-7 | 86 |
| 5 | Heptacosane | 380 | C27H56 | 000593-49-7 | 86 |



# Tentatively Identified Compound (LSC) summary

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Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Z-2-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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 |
| unknown6.52 | 6.52 | 44.5 | ng | 2120230 | 1 | 6.75 | 953865 | 20.0 |
| n-Hexadecanoic acid | 11.79 | 5.2 | ng | 339045 | 4 | 11.26 | 1298930 | 20.0 |
| Nonadecanoic acid | 12.57 | 2.5 | ng | 169195 | 5 | 13.88 | 1377110 | 20.0 |
| Fumaric acid, 2-c... | 13.74 | 5.1 | ng | 348133 | 5 | 13.88 | 1377110 | 20.0 |
| 2-methyloctacosane | 14.66 | 4.7 | ng | 183842 | 6 | 15.30 | 777944 | 20.0 |