LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

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-BF070117.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 | 5.287 | 540 | 544 | 553 | rVB | 465683 | 411109 | 2.76% | 0.683% |
| 2 | 6.316 | 716 | 719 | 725 | rVB | 437775 | 390507 | 2.62% | 0.649% |
| 3 | 6.451 | 735 | 742 | 747 | rBV | 521259 | 472082 | 3.17% | 0.784% |
| 4 | 6.539 | 754 | 757 | 763 | rVB | 210963 | 197962 | 1.33% | 0.329% |
| 5 | 6.686 | 777 | 782 | 785 | rBV | 680790 | 568990 | 3.82% | 0.945% |
| 6 | 6.839 | 805 | 808 | 813 | rVB | 417161 | 367509 | 2.47% | 0.610% |
| 7 | 7.086 | 847 | 850 | 853 | rBV | 216257 | 186147 | 1.25% | 0.309% |
| 8 | 7.239 | 870 | 876 | 881 | rBV3 | 296706 | 403070 | 2.71% | 0.669% |
| 9 | 7.298 | 884 | 886 | 889 | rVV | 565479 | 444084 | 2.98% | 0.738% |
| 10 | 7.486 | 916 | 918 | 924 | rVB3 | 157275 | 229764 | 1.54% | 0.382% |
| 11 | 7.604 | 931 | 938 | 941 | rBV6 | 109176 | 226325 | 1.52% | 0.376% |
| 12 | 7.663 | 946 | 948 | 952 | rVV2 | 143109 | 179085 | 1.20% | 0.297% |
| 13 | 7.704 | 952 | 955 | 958 | rVV3 | 228515 | 301122 | 2.02% | 0.500% |
| 14 | 7.739 | 958 | 961 | 964 | rVV2 | 251991 | 282901 | 1.90% | 0.470% |
| 15 | 7.781 | 965 | 968 | 970 | rVV2 | 214765 | 194664 | 1.31% | 0.323% |
| 16 | 7.810 | 970 | 973 | 976 | rVB3 | 169520 | 191622 | 1.29% | 0.318% |
| 17 | 7.969 | 996 | 1000 | 1003 | rBV | 1535858 | 1265037 | 8.50% | 2.101% |
| 18 | 8.045 | 1011 | 1013 | 1016 | rVB | 253625 | 185319 | 1.24% | 0.308% |
| 19 | 8.269 | 1046 | 1051 | 1054 | rVV4 | 208561 | 320769 | 2.15% | 0.533% |
| 20 | 8.328 | 1059 | 1061 | 1064 | rVV2 | 243970 | 190558 | 1.28% | 0.317% |
| 21 | 8.363 | 1064 | 1067 | 1070 | rVV3 | 258731 | 266903 | 1.79% | 0.443% |
| 22 | 8.404 | 1072 | 1074 | 1079 | rVV3 | 414776 | 482960 | 3.24% | 0.802% |
| 23 | 8.475 | 1083 | 1086 | 1090 | rBV2 | 274552 | 241134 | 1.62% | 0.401% |
| 24 | 8.575 | 1099 | 1103 | 1108 | rVV | 1081453 | 987032 | 6.63% | 1.639% |
| 25 | 8.633 | 1110 | 1113 | 1115 | rVV2 | 227378 | 264821 | 1.78% | 0.440% |
| 26 | 8.669 | 1116 | 1119 | 1123 | rVB3 | 186952 | 237308 | 1.59% | 0.394% |
| 27 | 8.792 | 1138 | 1140 | 1142 | rVB | 204927 | 155030 | 1.04% | 0.257% |
| 28 | 8.857 | 1148 | 1151 | 1153 | rBV2 | 180762 | 157303 | 1.06% | 0.261% |
| 29 | 8.875 | 1153 | 1154 | 1158 | rVV4 | 139300 | 171371 | 1.15% | 0.285% |
| 30 | 8.904 | 1158 | 1159 | 1163 | rVV4 | 147765 | 168543 | 1.13% | 0.280% |
| 31 | 8.939 | 1163 | 1165 | 1168 | rVB2 | 245162 | 192077 | 1.29% | 0.319% |
| 32 | 8.980 | 1169 | 1172 | 1174 | rVV2 | 205361 | 188763 | 1.27% | 0.314% |
| 33 | 9.004 | 1174 | 1176 | 1179 | rVV2 | 397158 | 353307 | 2.37% | 0.587% |
| 34 | 9.039 | 1179 | 1182 | 1188 | rVB | 402273 | 368630 | 2.48% | 0.612% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

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-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 9.139 | 1195 | 1199 | 1203 | rBV | 1061171 | 918780 | 6.17% | 1.526% |
| 36 | 9.198 | 1204 | 1209 | 1211 | rVV3 | 187977 | 290377 | 1.95% | 0.482% |
| 37 | 9.310 | 1222 | 1228 | 1233 | rBV5 | 224096 | 339911 | 2.28% | 0.565% |
| 38 | 9.398 | 1239 | 1243 | 1245 | rVV3 | 167146 | 282217 | 1.90% | 0.469% |
| 39 | 9.457 | 1247 | 1253 | 1255 | rVV3 | 364663 | 575360 | 3.87% | 0.956% |
| 40 | 9.480 | 1255 | 1257 | 1260 | rVV | 240354 | 230732 | 1.55% | 0.383% |
| 41 | 9.669 | 1286 | 1289 | 1292 | rBV | 861344 | 689782 | 4.63% | 1.146% |
| 42 | 9.716 | 1292 | 1297 | 1301 | rVV | 688479 | 717734 | 4.82% | 1.192% |
| 43 | 9.904 | 1324 | 1329 | 1331 | rBV3 | 129752 | 209928 | 1.41% | 0.349% |
| 44 | 9.986 | 1340 | 1343 | 1347 | rVB2 | 184078 | 198238 | 1.33% | 0.329% |
| 45 | 10.163 | 1370 | 1373 | 1376 | rVB | 704062 | 590768 | 3.97% | 0.981% |
| 46 | 10.386 | 1406 | 1411 | 1413 | rBV | 269868 | 297370 | 2.00% | 0.494% |
| 47 | 10.498 | 1428 | 1430 | 1434 | rVB2 | 275619 | 243745 | 1.64% | 0.405% |
| 48 | 10.633 | 1450 | 1453 | 1461 | rBV | 702139 | 872676 | 5.86% | 1.449% |
| 49 | 11.080 | 1526 | 1529 | 1532 | rBV | 656708 | 571830 | 3.84% | 0.950% |
| 50 | 11.116 | 1532 | 1535 | 1540 | rVB | 251229 | 254590 | 1.71% | 0.423% |
| 51 | 11.192 | 1545 | 1548 | 1551 | rVB | 574887 | 510097 | 3.43% | 0.847% |
| 52 | 11.510 | 1598 | 1602 | 1604 | rBV | 540193 | 469455 | 3.15% | 0.780% |
| 53 | 11.616 | 1614 | 1620 | 1623 | rVB | 5204857 | 6033121 | 40.53% | 10.021% |
| 54 | 11.751 | 1639 | 1643 | 1649 | rVB | 301965 | 337652 | 2.27% | 0.561% |
| 55 | 11.916 | 1668 | 1671 | 1676 | rVB | 471793 | 463279 | 3.11% | 0.769% |
| 56 | 12.321 | 1730 | 1740 | 1741 | rBV2 | 5962215 | 14886232 | 100.00% | 24.725% |
| 57 | 12.404 | 1750 | 1754 | 1757 | rVB | 3704122 | 3490249 | 23.45% | 5.797% |
| 58 | 12.474 | 1757 | 1766 | 1774 | rBV2 | 2149391 | 4359084 | 29.28% | 7.240% |
| 59 | 12.633 | 1790 | 1793 | 1797 | rVB2 | 470339 | 434544 | 2.92% | 0.722% |
| 60 | 12.674 | 1797 | 1800 | 1810 | rVB2 | 365056 | 387543 | 2.60% | 0.644% |
| 61 | 12.786 | 1816 | 1819 | 1821 | rVV | 348031 | 341793 | 2.30% | 0.568% |
| 62 | 12.833 | 1824 | 1827 | 1830 | rVV | 279702 | 302597 | 2.03% | 0.503% |
| 63 | 12.880 | 1830 | 1835 | 1840 | rVB3 | 280862 | 531581 | 3.57% | 0.883% |
| 64 | 12.957 | 1845 | 1848 | 1849 | rVV | 292448 | 300082 | 2.02% | 0.498% |
| 65 | 12.992 | 1849 | 1854 | 1857 | rVV3 | 581226 | 1054145 | 7.08% | 1.751% |
| 66 | 13.045 | 1857 | 1863 | 1868 | rVB2 | 452456 | 859757 | 5.78% | 1.428% |
| 67 | 13.121 | 1873 | 1876 | 1879 | rVB | 545664 | 472143 | 3.17% | 0.784% |
| 68 | 13.227 | 1891 | 1894 | 1898 | rBV2 | 151574 | 174926 | 1.18% | 0.291% |
| 69 | 13.274 | 1900 | 1902 | 1906 | rVB2 | 242689 | 261987 | 1.76% | 0.435% |
| 70 | 13.368 | 1916 | 1918 | 1923 | rVB | 167044 | 158165 | 1.06% | 0.263% |
| 71 | 13.545 | 1944 | 1948 | 1951 | rVB2 | 367510 | 453833 | 3.05% | 0.754% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

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-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 72 | 13.786 | 1986 | 1989 | 1993 | rBV | 531768 | 522306 | 3.51% | 0.868% |
| 73 | 13.827 | 1993 | 1996 | 1999 | rBV | 611613 | 564018 | 3.79% | 0.937% |
| 74 | 14.168 | 2051 | 2054 | 2059 | rVB | 173137 | 177244 | 1.19% | 0.294% |
| 75 | 14.298 | 2071 | 2076 | 2078 | rBV2 | 495373 | 718262 | 4.83% | 1.193% |
| 76 | 14.404 | 2092 | 2094 | 2099 | rBV3 | 227470 | 285088 | 1.92% | 0.474% |
| 77 | 14.615 | 2127 | 2130 | 2134 | rBV2 | 251000 | 252962 | 1.70% | 0.420% |
| 78 | 14.721 | 2142 | 2148 | 2158 | rVB | 1654886 | 2539058 | 17.06% | 4.217% |
| 79 | 15.233 | 2232 | 2235 | 2239 | rVB | 323226 | 338445 | 2.27% | 0.562% |

Sum of corrected areas: 60207494

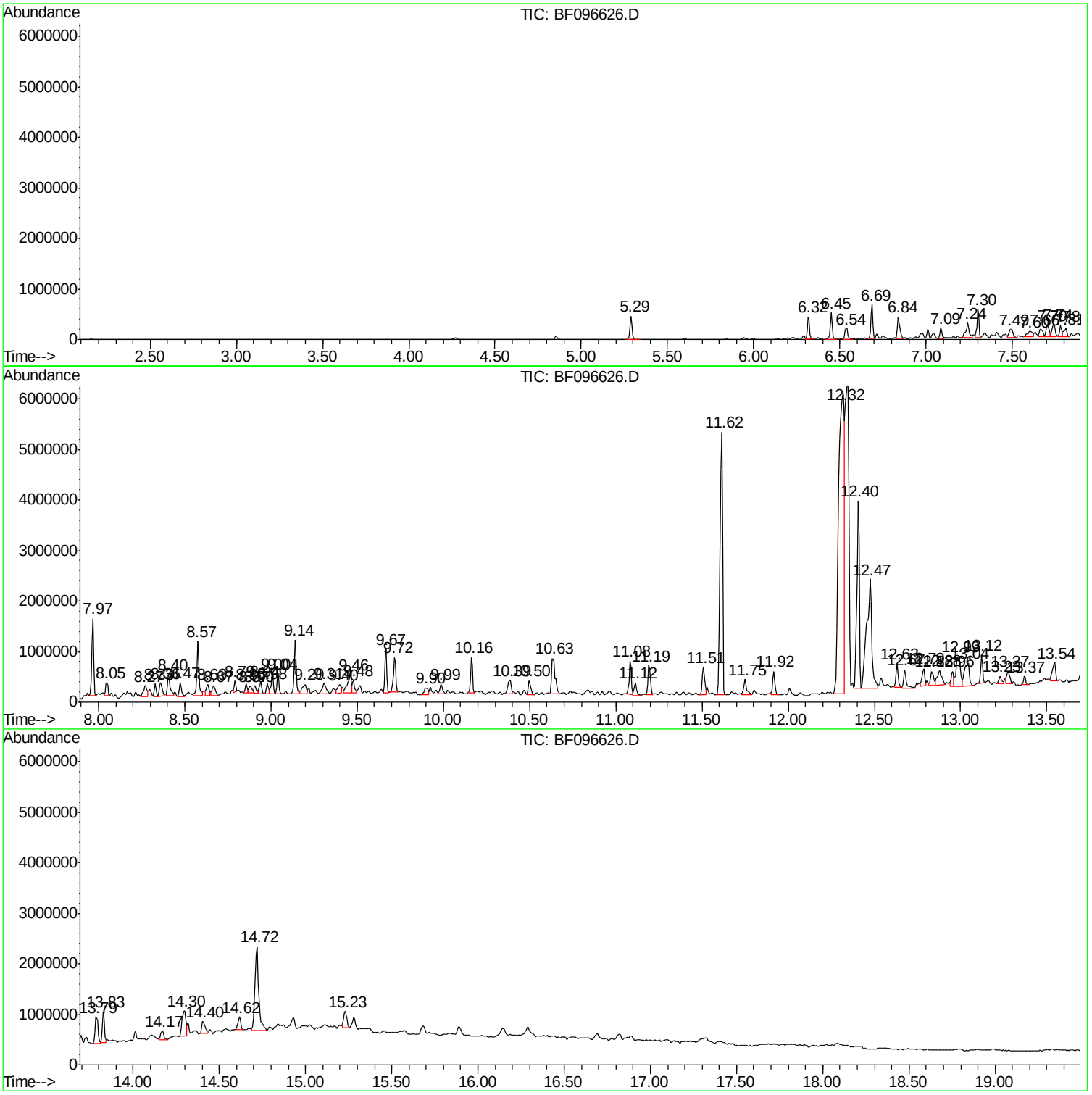
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

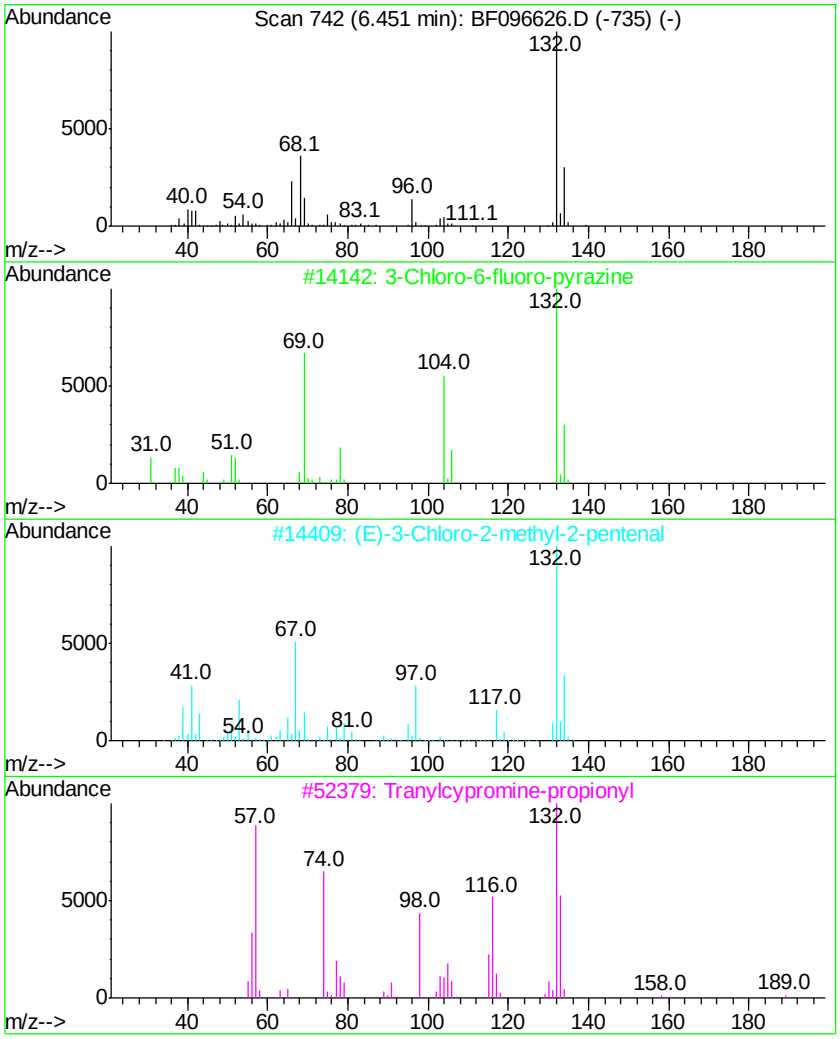
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

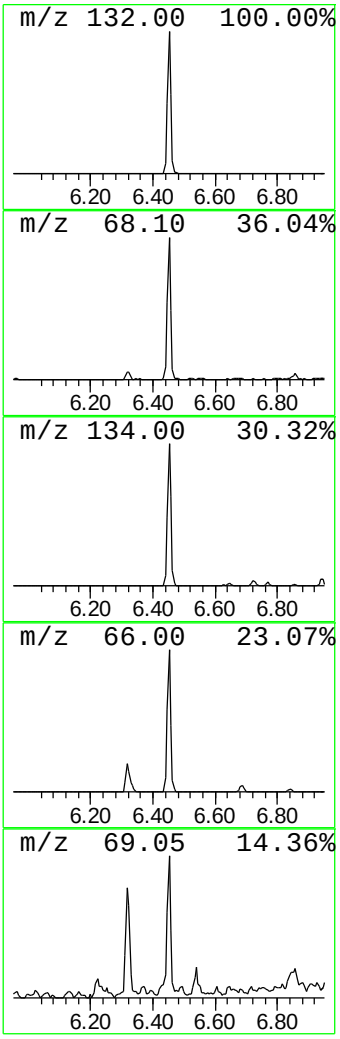
**********

Peak Number 1 unknown6.45 Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.45 | 16.59 ng | 472082 | 1,4-Dichlorobenzene-d4 | 6.69 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 25 |
| 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-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |
| 5 | 4-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-60-2 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

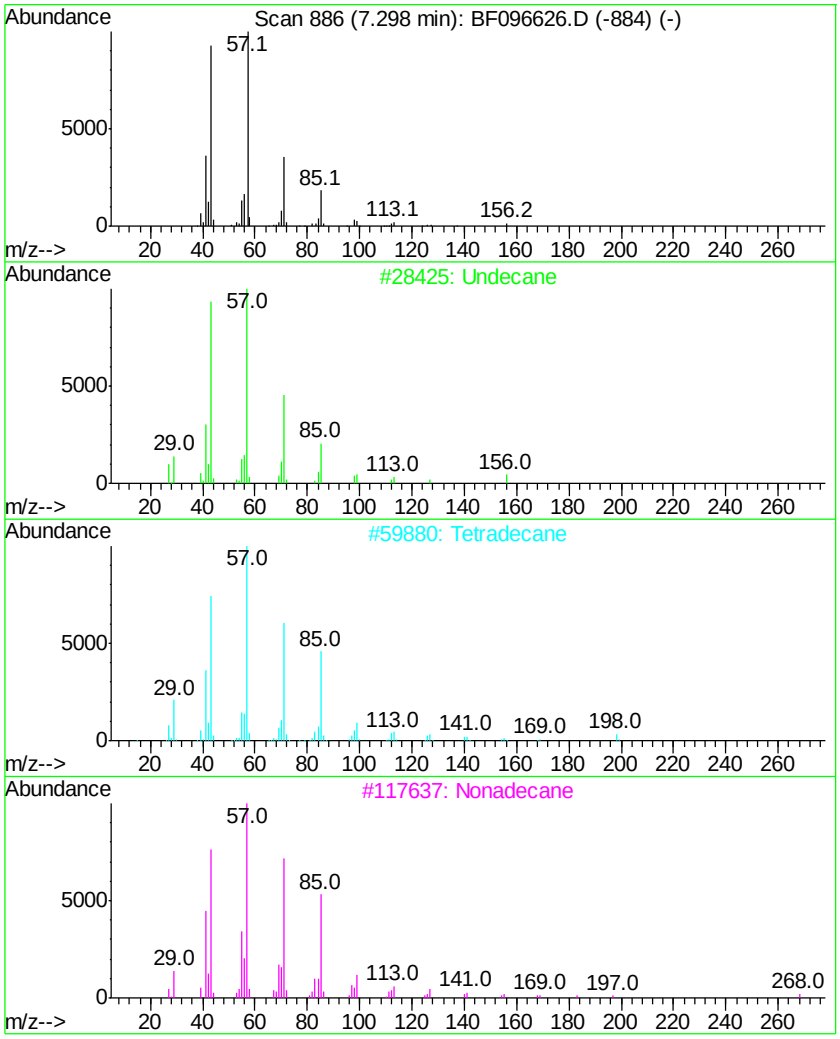
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

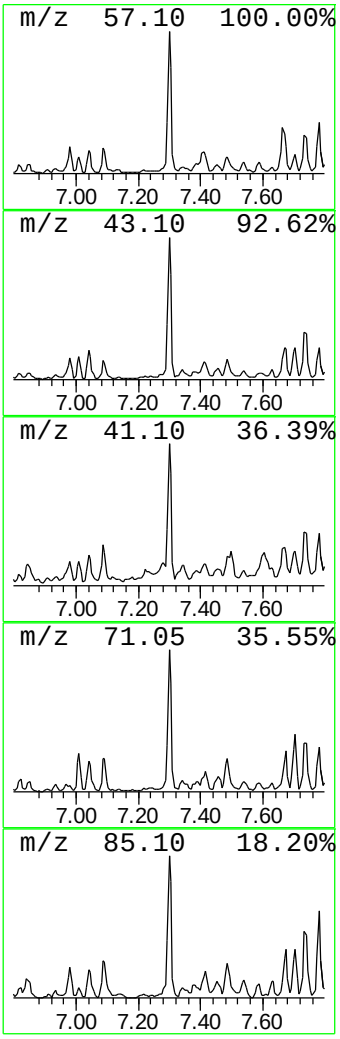
**********

Peak Number 2 Undecane Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.30 | 15.61 ng | 444084 | 1,4-Dichlorobenzene-d4 | 6.69 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Undecane | 156 | C11H24 | 001120-21-4 | 83 |
| 2 | Tetradecane | 198 | C14H30 | 000629-59-4 | 78 |
| 3 | Nonadecane | 268 | C19H40 | 000629-92-5 | 78 |
| 4 | Heptadecane, 2,6-dimethyl- | 268 | C19H40 | 054105-67-8 | 78 |
| 5 | Tridecane | 184 | C13H28 | 000629-50-5 | 78 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

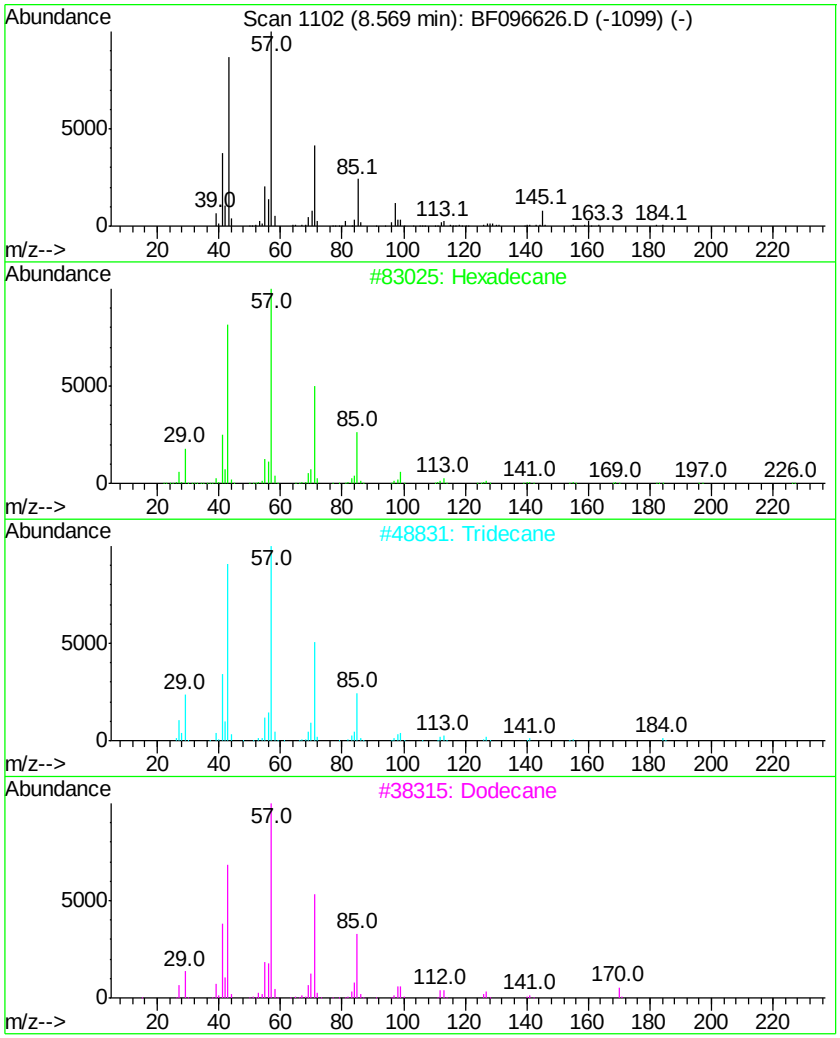
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

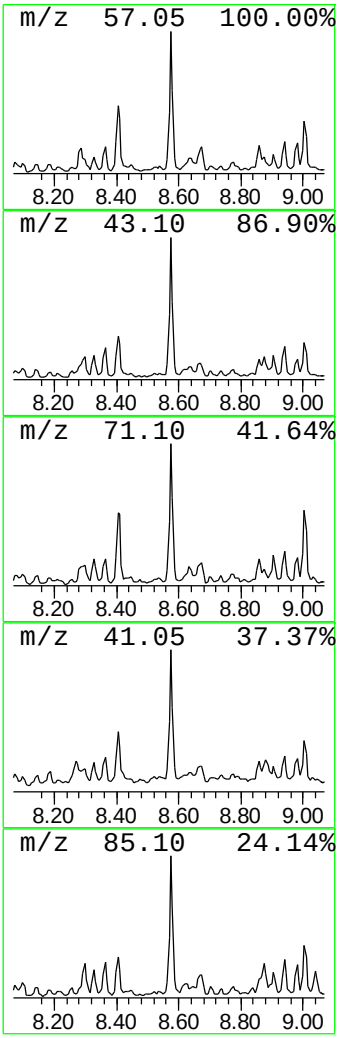
**********

Peak Number 3 Hexadecane Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.57 | 15.60 ng | 987032 | Naphthalene-d8 | 7.97 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 2 | Tridecane | 184 | C13H28 | 000629-50-5 | 86 |
| 3 | Dodecane | 170 | C12H26 | 000112-40-3 | 64 |
| 4 | Decane, 2,3,6-trimethyl- | 184 | C13H28 | 062238-12-4 | 59 |
| 5 | Tetradecane | 198 | C14H30 | 000629-59-4 | 53 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

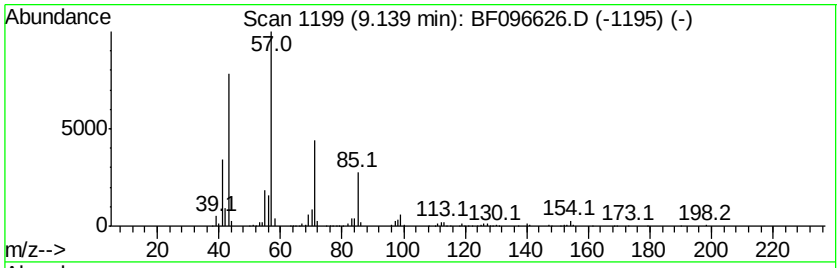
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

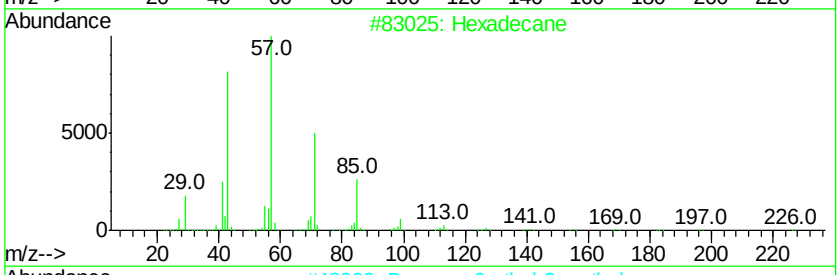
**********

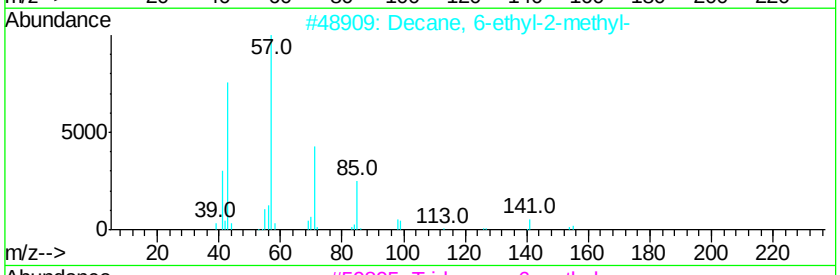
Peak Number 4 Decane, 6-ethyl-2-methyl- Concentration Rank 9

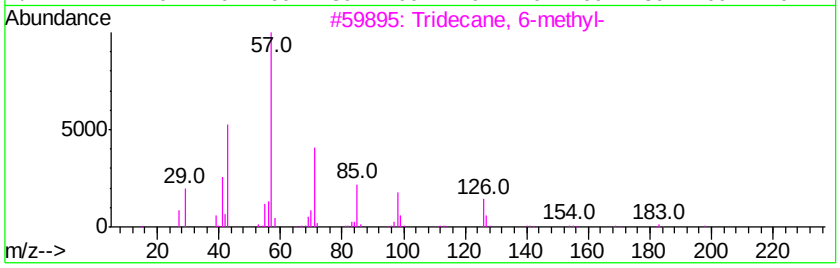
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.14 | 25.60 ng | 918780 | Acenaphthene-d10 | 9.72 |

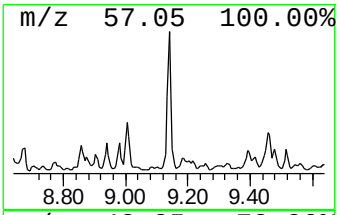
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 91 |
| 2 | Decane, 6-ethyl-2-methyl- | 184 | C13H28 | 062108-21-8 | 83 |
| 3 | Tridecane, 6-methyl- | 198 | C14H30 | 013287-21-3 | 76 |
| 4 | Tetradecane | 198 | C14H30 | 000629-59-4 | 72 |
| 5 | Tridecane | 184 | C13H28 | 000629-50-5 | 72 |

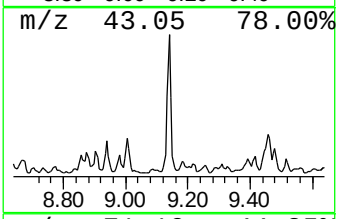


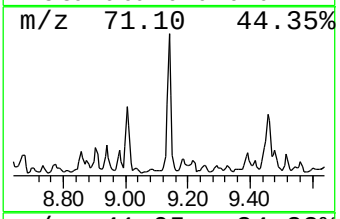



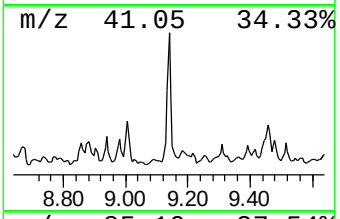



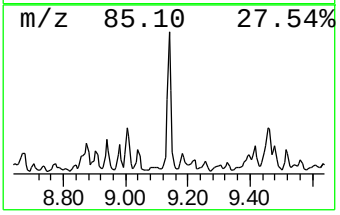



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

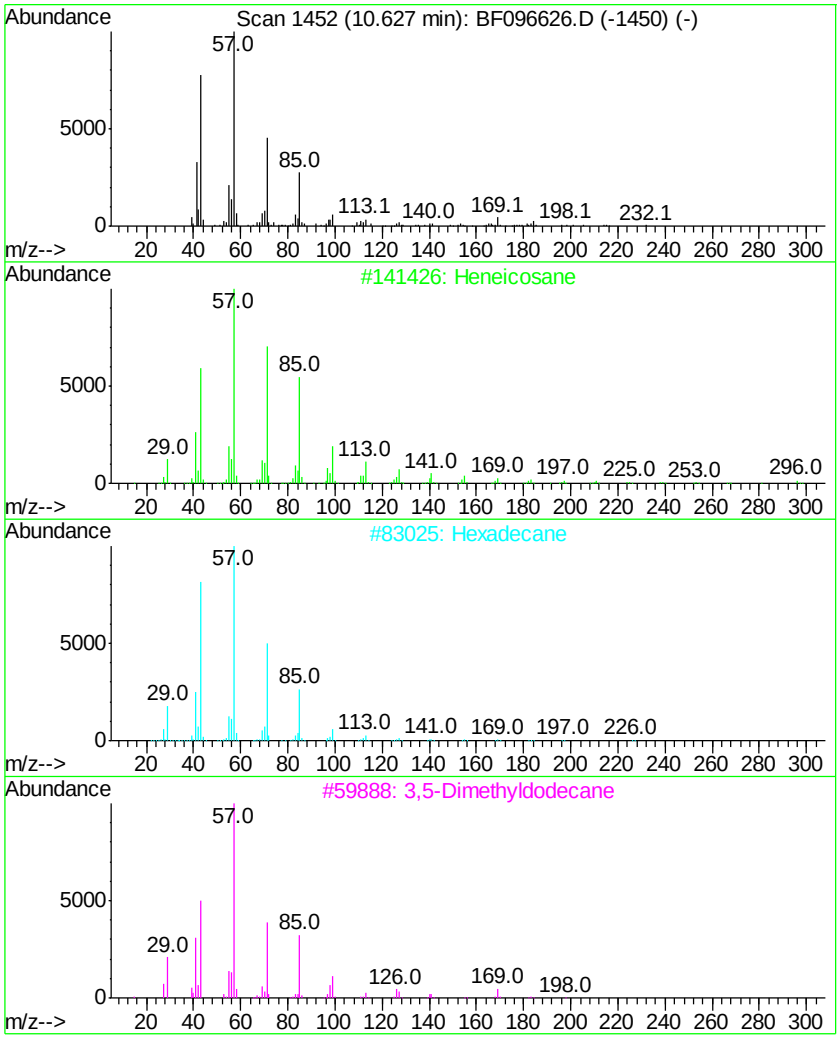
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

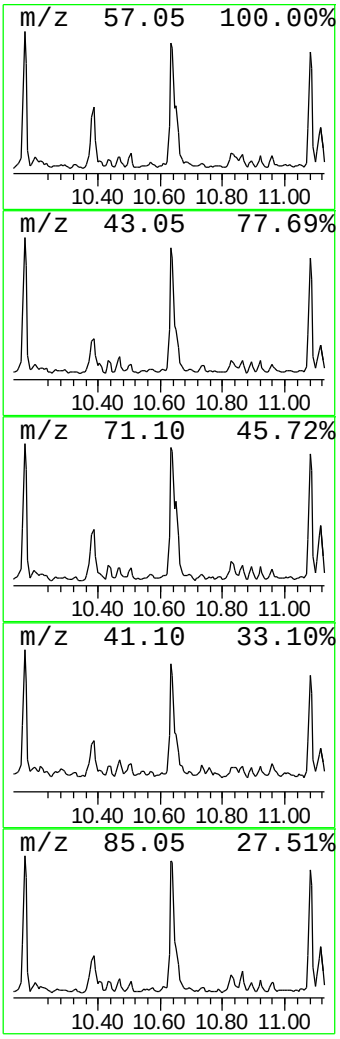
**********

Peak Number 6 Heneicosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.63 | 34.22 ng | 872676 | Phenanthrene-d10 | 11.19 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 90 |
| 2 | Hexadecane | 226 | C16H34 | 000544-76-3 | 87 |
| 3 | 3,5-Dimethyldodecane | 198 | C14H30 | 107770-99-0 | 86 |
| 4 | Dodecane, 2-methyl- | 184 | C13H28 | 001560-97-0 | 86 |
| 5 | Tridecane | 184 | C13H28 | 000629-50-5 | 86 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

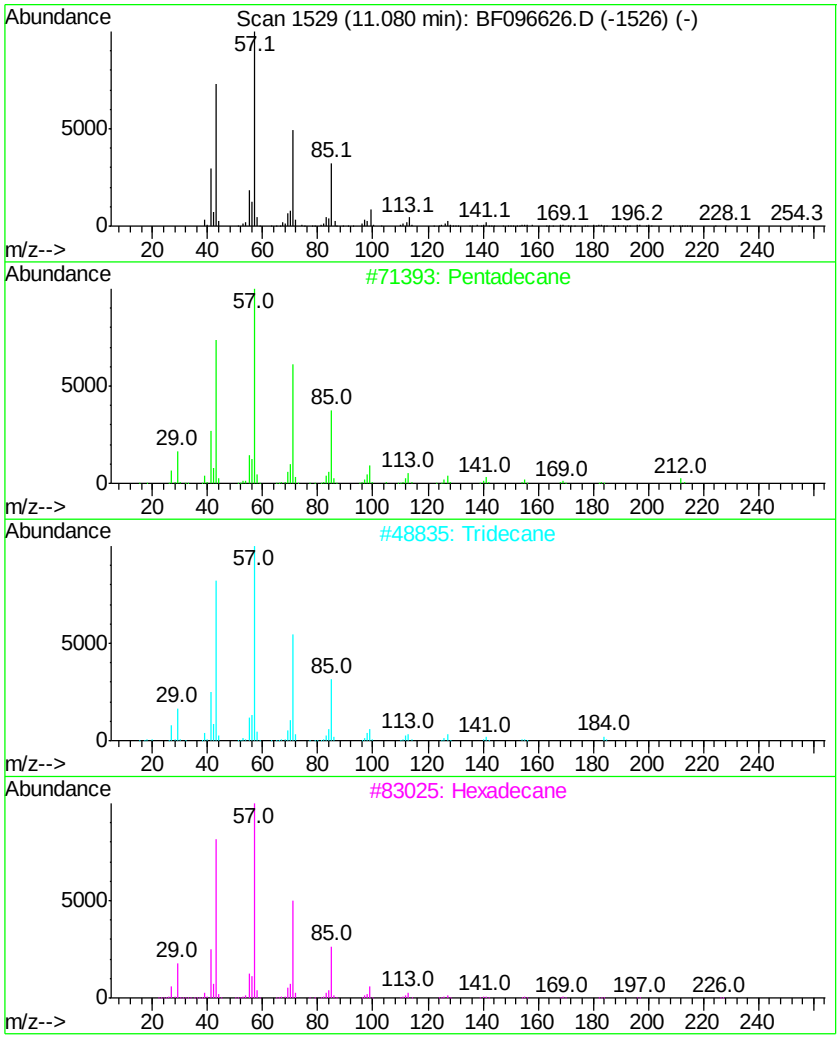
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

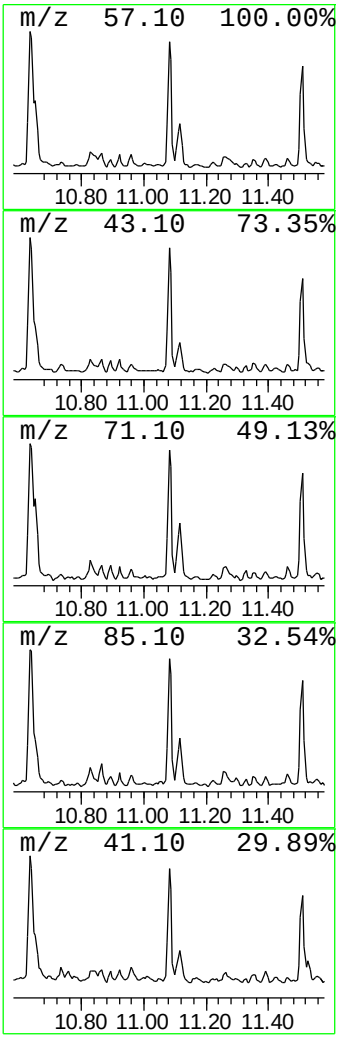
**********

Peak Number 7 Pentadecane Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.08 | 22.42 ng | 571830 | Phenanthrene-d10 | 11.19 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentadecane | 212 | C15H32 | 000629-62-9 | 97 |
| 2 | Tridecane | 184 | C13H28 | 000629-50-5 | 91 |
| 3 | Hexadecane | 226 | C16H34 | 000544-76-3 | 91 |
| 4 | Tetradecane | 198 | C14H30 | 000629-59-4 | 90 |
| 5 | Octadecane | 254 | C18H38 | 000593-45-3 | 86 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

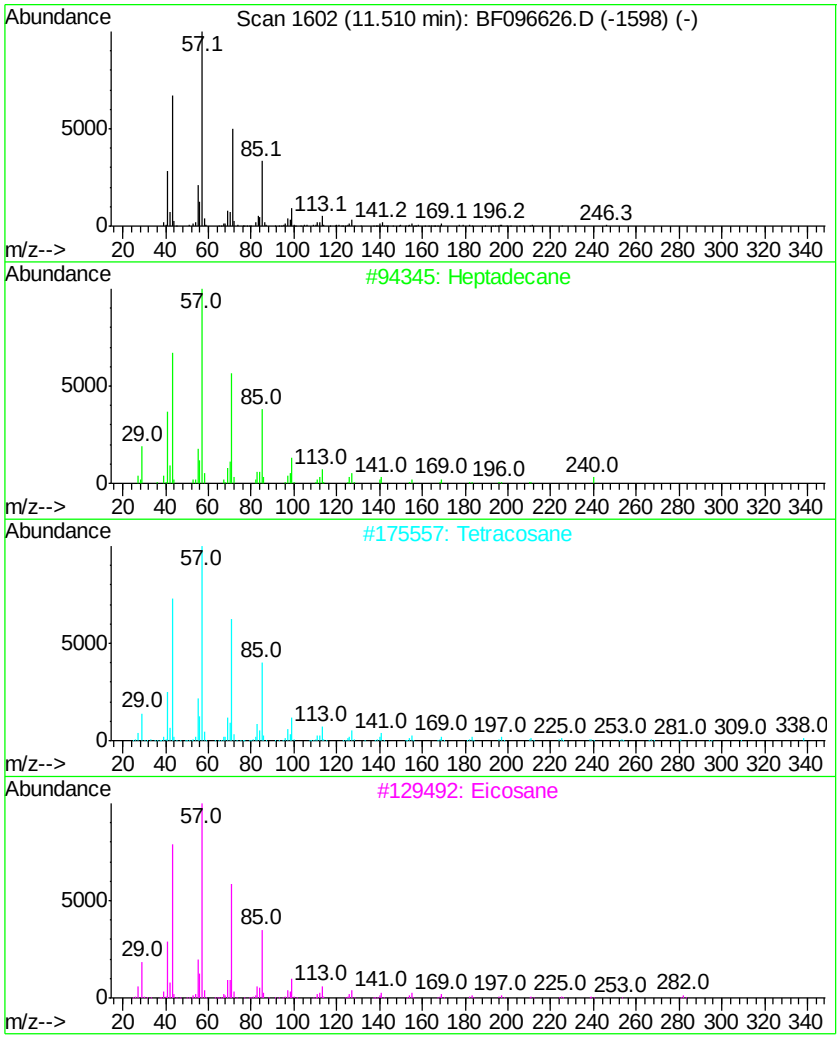
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

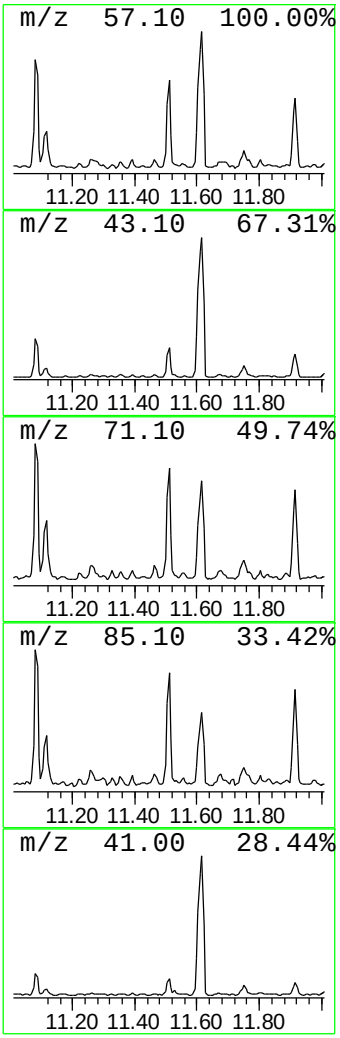
**********

Peak Number 8 Heptadecane Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.51 | 18.41 ng | 469455 | Phenanthrene-d10 | 11.19 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 90 |
| 2 | Tetracosane | 338 | C24H50 | 000646-31-1 | 90 |
| 3 | Eicosane | 282 | C20H42 | 000112-95-8 | 90 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 86 |
| 5 | Dodecane, 2-methyl-6-propyl- | 226 | C16H34 | 055045-08-4 | 86 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

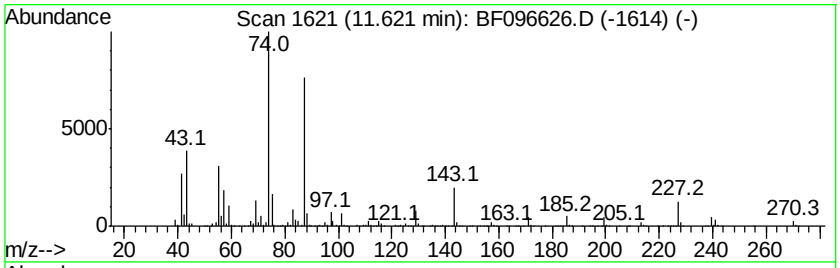
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

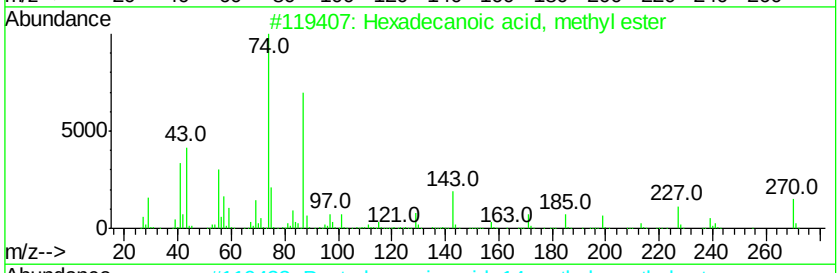
**********

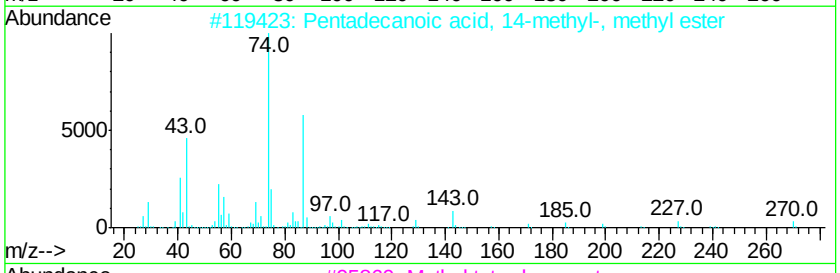
Peak Number 9 Hexadecanoic acid, methyl e... Concentration Rank 2

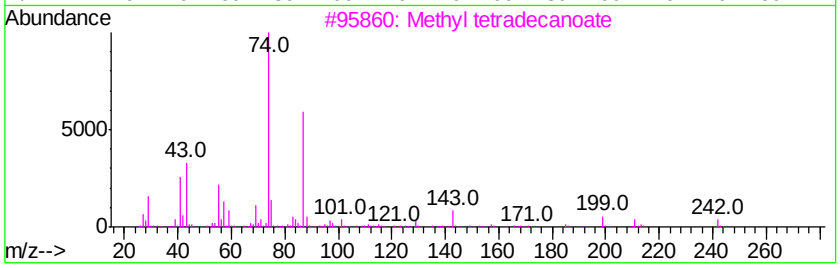
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.62 | 236.55 ng | 6033120 | Phenanthrene-d10 | 11.19 |

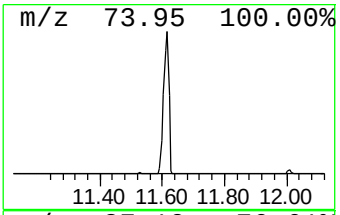
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, methyl ester | 270 | C17H34O2 | 000112-39-0 | 94 |
| 2 | Pentadecanoic acid, 14-methyl-, ... | 270 | C17H34O2 | 005129-60-2 | 91 |
| 3 | Methyl tetradecanoate | 242 | C15H30O2 | 000124-10-7 | 90 |
| 4 | Pentadecanoic acid, methyl ester | 256 | C16H32O2 | 007132-64-1 | 90 |
| 5 | Dodecanoic acid, methyl ester | 214 | C13H26O2 | 000111-82-0 | 90 |

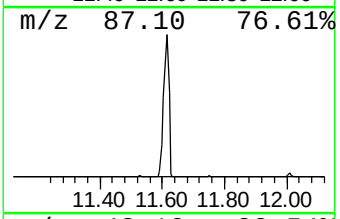


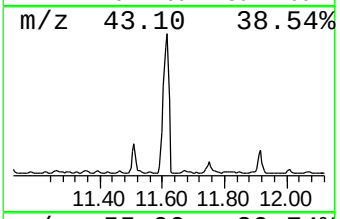



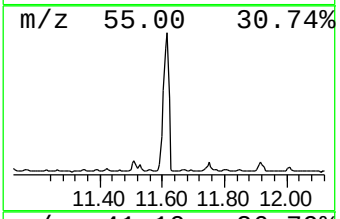



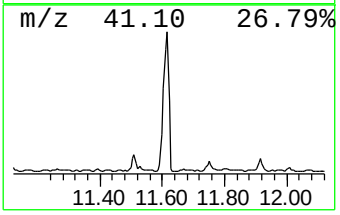



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

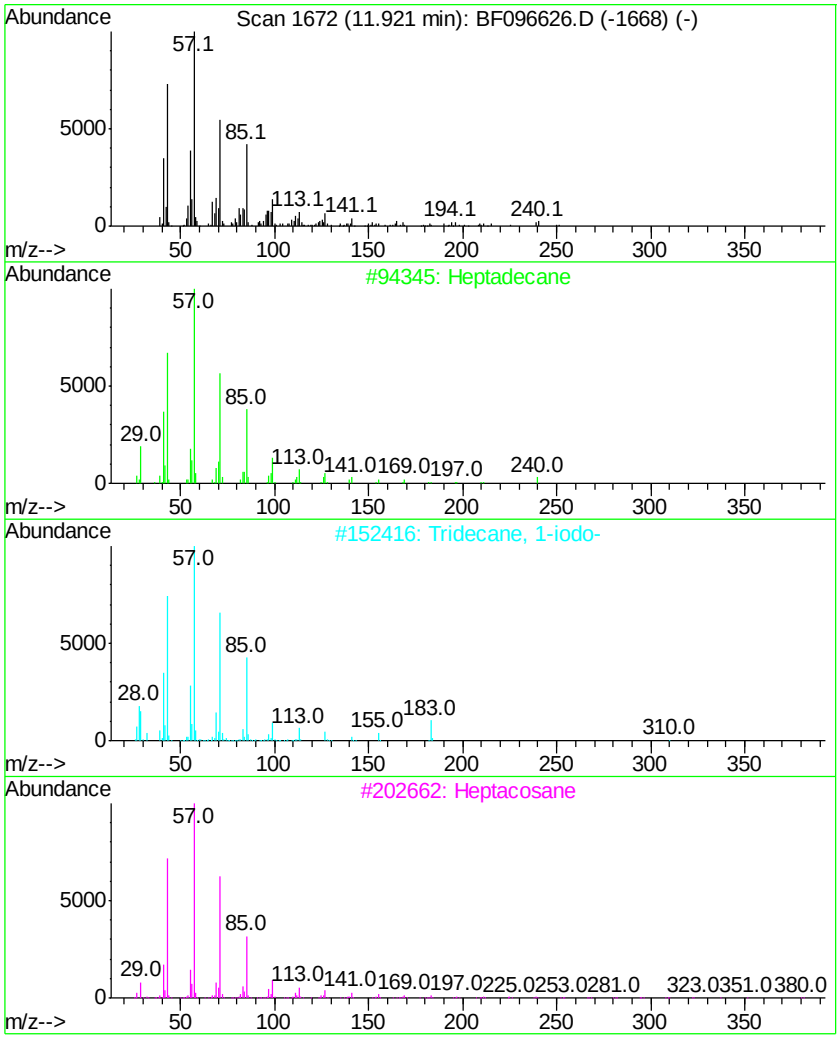
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

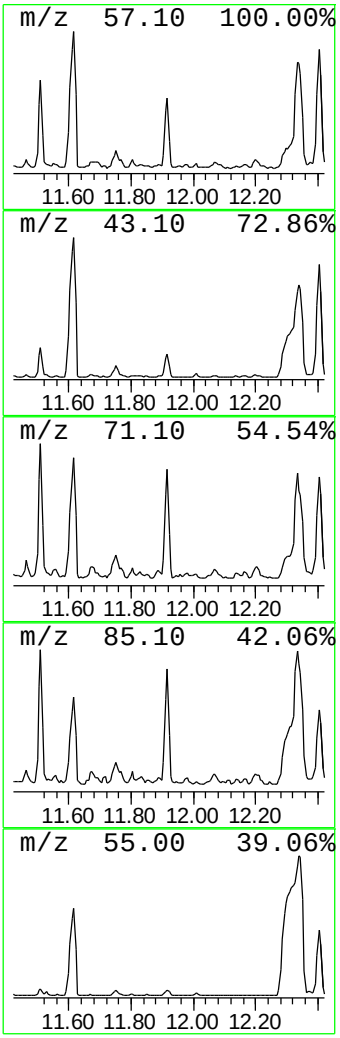
**********

Peak Number 10 Tridecane, 1-iodo- Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.92 | 18.16 ng | 463279 | Phenanthrene-d10 | 11.19 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 95 |
| 2 | Tridecane, 1-iodo- | 310 | C13H27I | 035599-77-0 | 90 |
| 3 | Heptacosane | 380 | C27H56 | 000593-49-7 | 87 |
| 4 | Dodecane, 2-methyl-6-propyl- | 226 | C16H34 | 055045-08-4 | 86 |
| 5 | Tetracosane | 338 | C24H50 | 000646-31-1 | 86 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

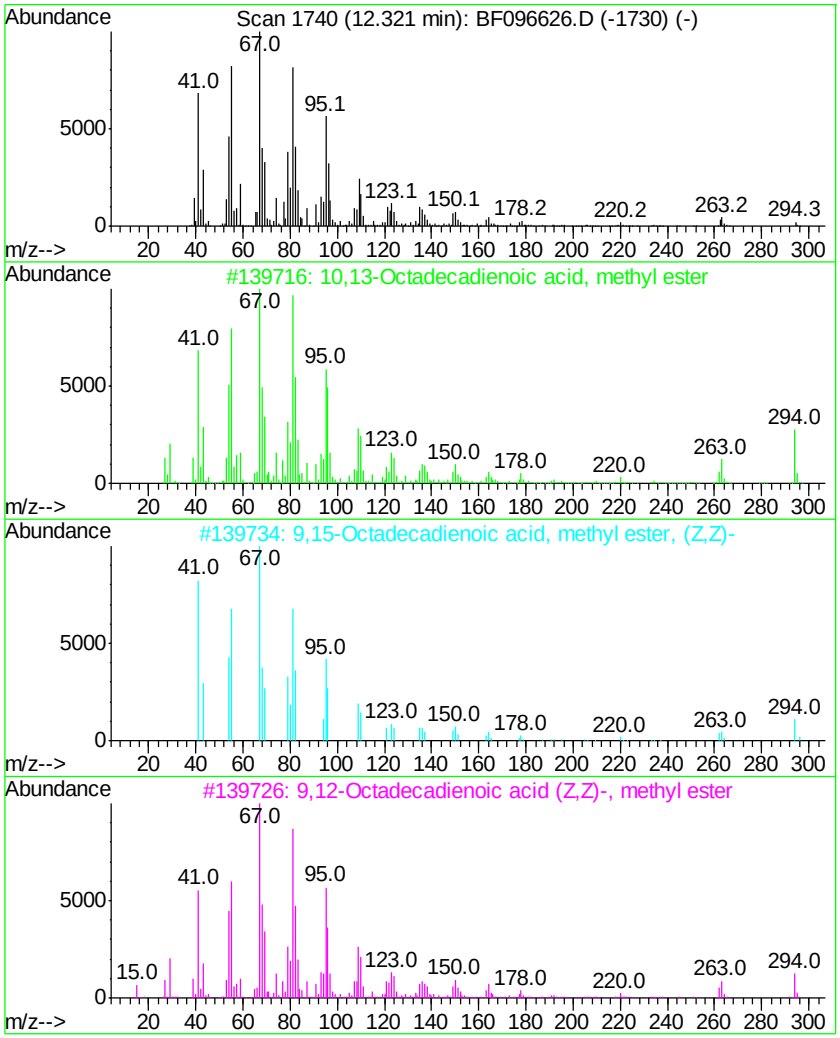
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

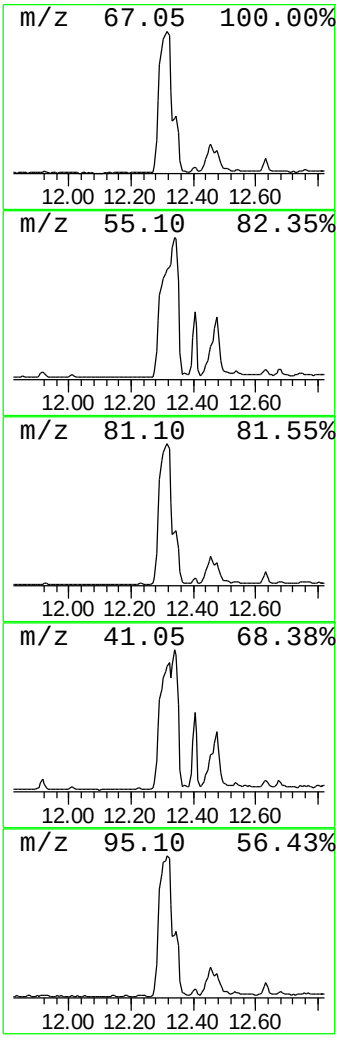
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 11 10,13-Octadecadienoic acid,... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.32 | 583.66 ng | 14886200 | Phenanthrene-d10 | 11.19 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 10,13-Octadecadienoic acid, meth... | 294 | C19H34O2 | 056554-62-2 | 99 |
| 2 | 9,15-Octadecadienoic acid, methy... | 294 | C19H34O2 | 017309-05-6 | 99 |
| 3 | 9,12-Octadecadienoic acid (Z,Z)-... | 294 | C19H34O2 | 000112-63-0 | 99 |
| 4 | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002566-97-4 | 99 |
| 5 | Methyl 10-trans,12-cis-octadecad... | 294 | C19H34O2 | 1000336-44-2 | 98 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

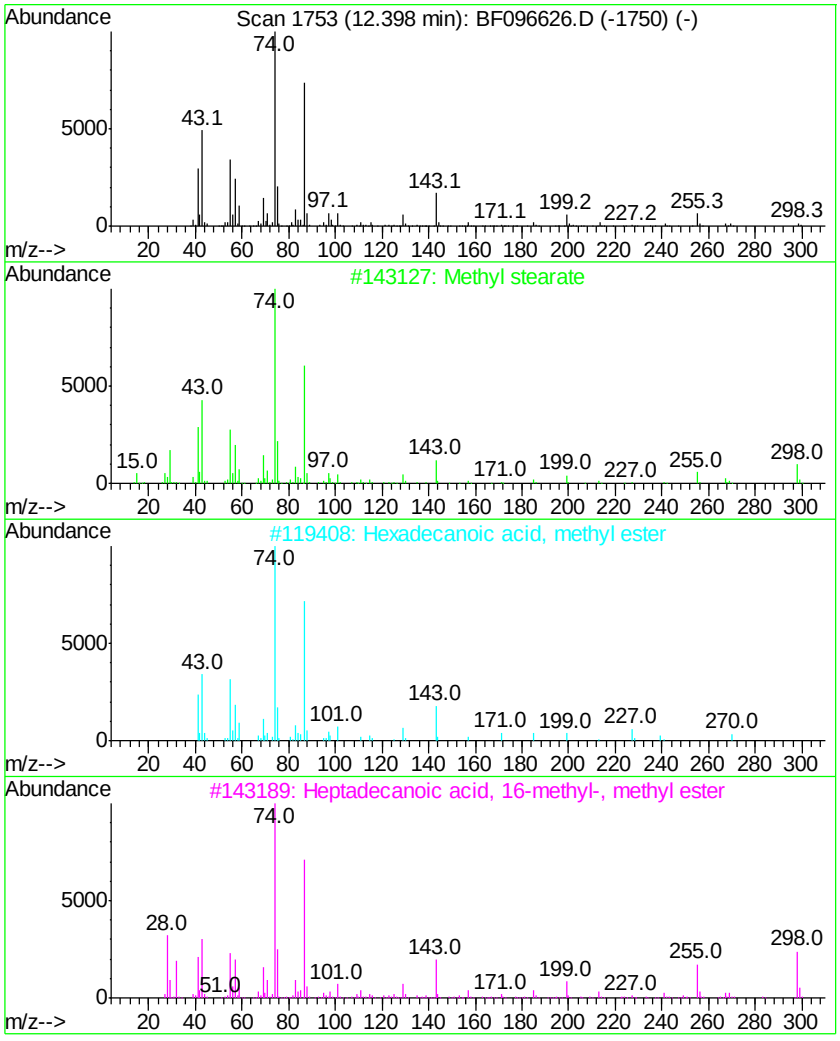
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

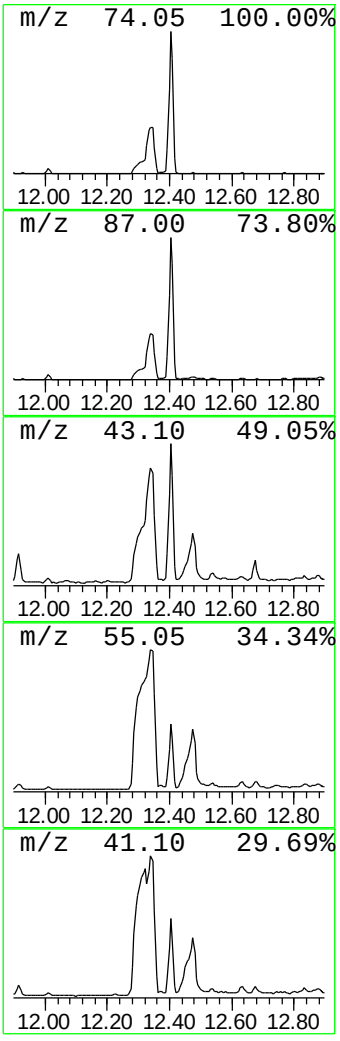
**********

Peak Number 12 Methyl stearate Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.40 | 136.85 ng | 3490250 | Phenanthrene-d10 | 11.19 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl stearate | 298 | C19H38O2 | 000112-61-8 | 97 |
| 2 | Hexadecanoic acid, methyl ester | 270 | C17H34O2 | 000112-39-0 | 94 |
| 3 | Heptadecanoic acid, 16-methyl-, ... | 298 | C19H38O2 | 005129-61-3 | 94 |
| 4 | Pentadecanoic acid, methyl ester | 256 | C16H32O2 | 007132-64-1 | 91 |
| 5 | Methyl tetradecanoate | 242 | C15H30O2 | 000124-10-7 | 91 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

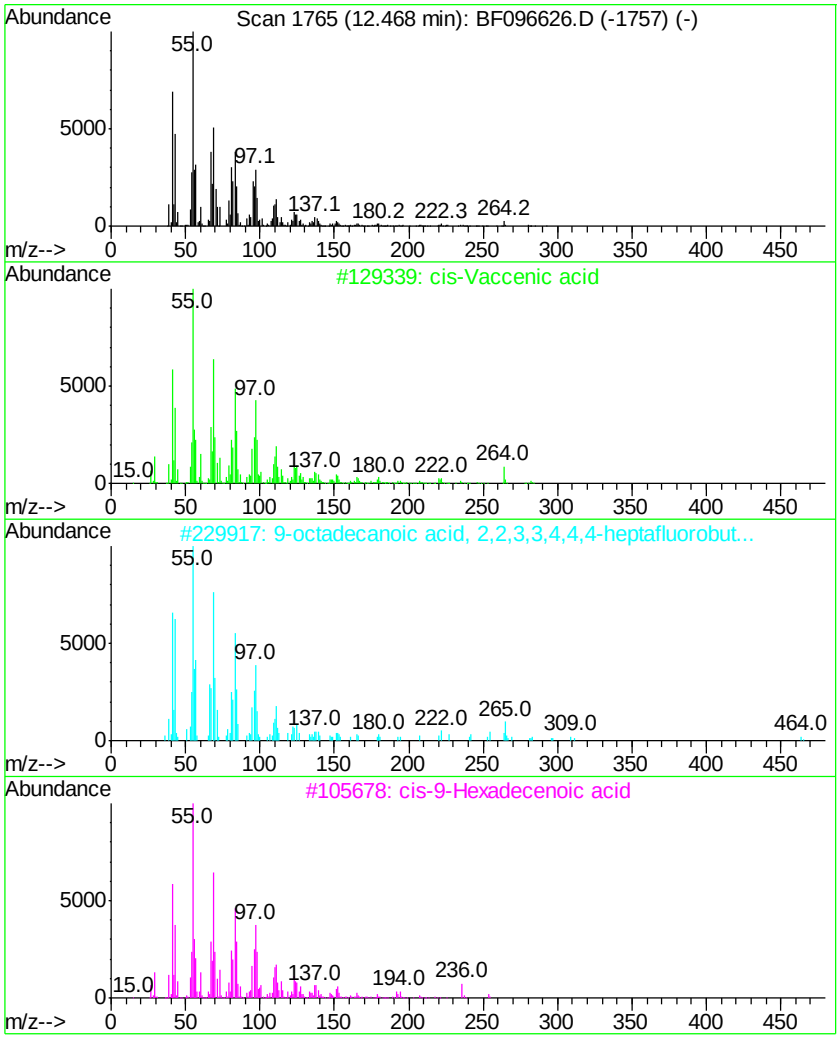
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

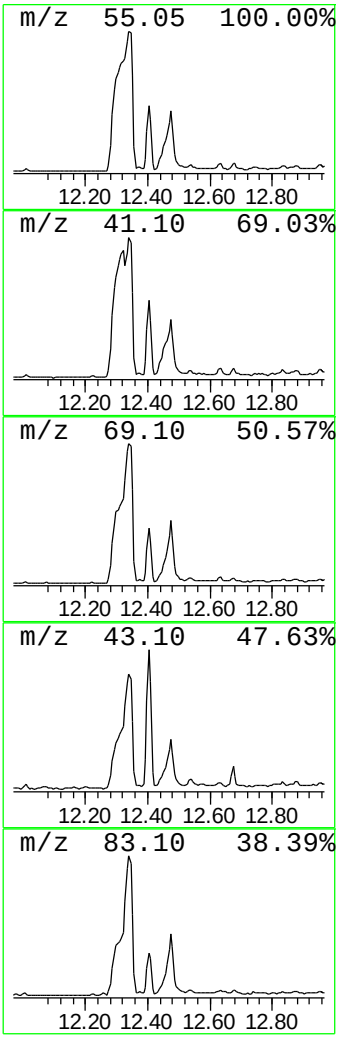
**********

Peak Number 13 cis-Vaccenic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.47 | 170.91 ng | 4359080 | Phenanthrene-d10 | 11.19 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | cis-Vaccenic acid | 282 | C18H34O2 | 000506-17-2 | 90 |
| 2 | 9-octadecanoic acid, 2,2,3,3,4,4... | 464 | C22H35F7O2 | 1000376-61-4 | 87 |
| 3 | cis-9-Hexadecenoic acid | 254 | C16H30O2 | 1000333-19-5 | 87 |
| 4 | cis-13-Octadecenoic acid | 282 | C18H34O2 | 013126-39-1 | 83 |
| 5 | Aspidospermidin-17-ol, 1-acetyl-... | 414 | C23H30N2O5 | 002122-26-1 | 83 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

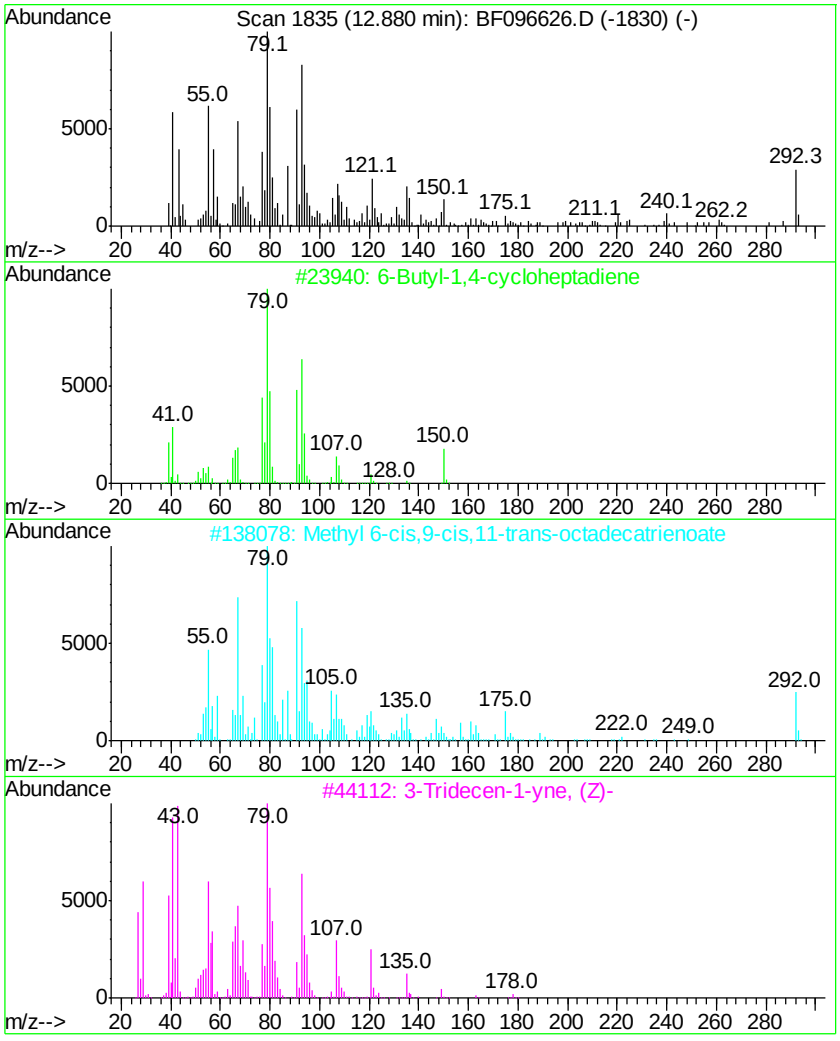
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

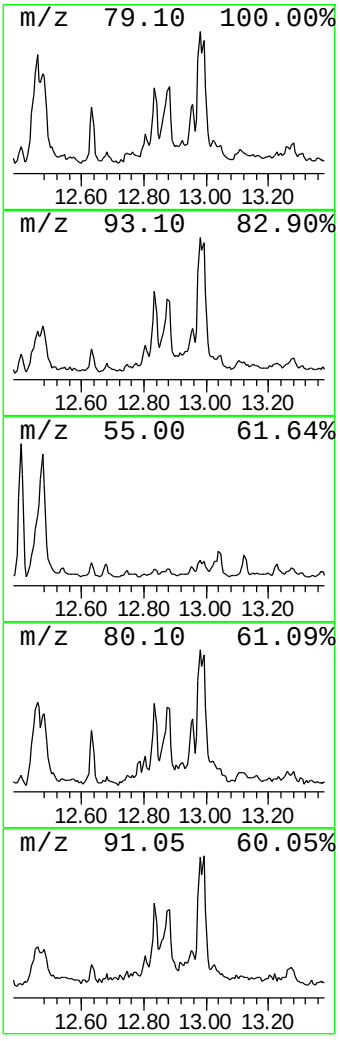
**********

Peak Number 14 6-Butyl-1,4-cycloheptadiene Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.88 | 18.85 ng | 531581 | Chrysene-d12 | 13.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 6-Butyl-1,4-cycloheptadiene | 150 | C11H18 | 022735-58-6 | 93 |
| 2 | Methyl 6-cis,9-cis,11-trans-octa... | 292 | C19H32O2 | 1000336-37-7 | 81 |
| 3 | 3-Tridecen-1-yne, (Z)- | 178 | C13H22 | 037981-62-7 | 68 |
| 4 | Cyclohexene, 3-methyl-6-(1-methy... | 136 | C10H16 | 005113-87-1 | 60 |
| 5 | Bicyclo[3.3.1]non-2-en-9-one | 136 | C9H12O | 004844-11-5 | 58 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

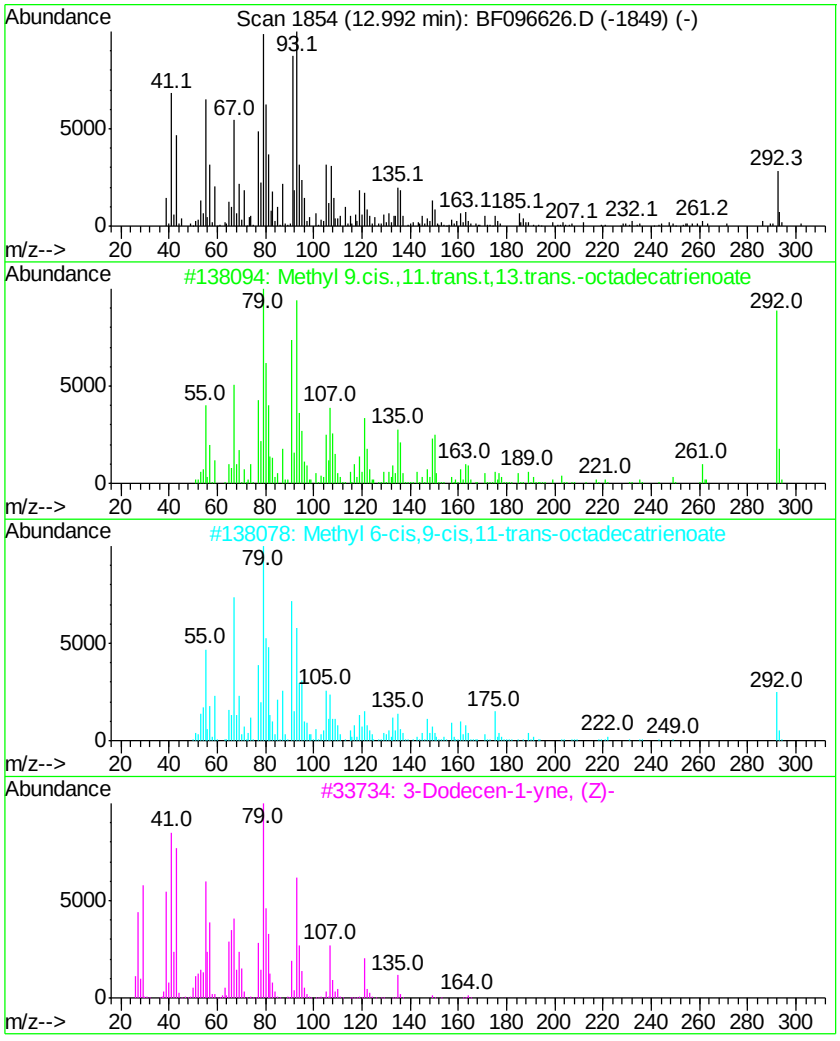
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

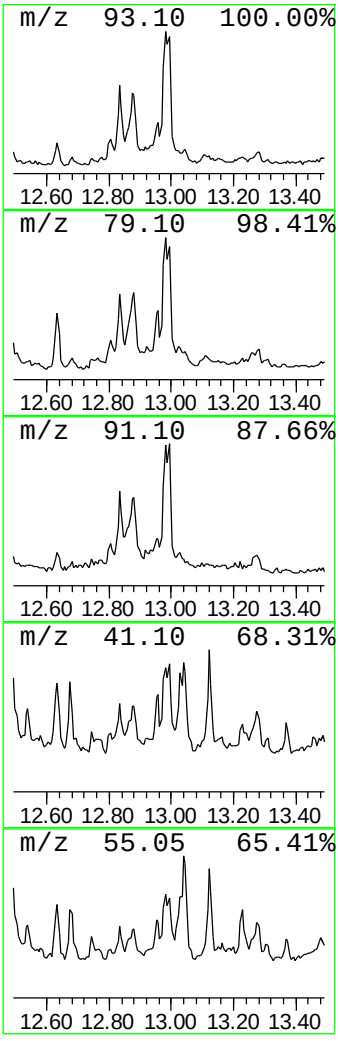
**********

Peak Number 15 Methyl 9.cis.,11.trans.t,13... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.99 | 37.38 ng | 1054150 | Chrysene-d12 | 13.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl 9.cis.,11.trans.t,13.tran... | 292 | C19H32O2 | 1000336-42-6 | 91 |
| 2 | Methyl 6-cis,9-cis,11-trans-octa... | 292 | C19H32O2 | 1000336-37-7 | 89 |
| 3 | 3-Dodecen-1-yne, (Z)- | 164 | C12H20 | 025091-24-1 | 83 |
| 4 | Bicyclo[2.2.1]heptane, 7,7-dimet... | 136 | C10H16 | 000471-84-1 | 81 |
| 5 | cis-3-Butyl-4-vinyl-cyclopentene | 150 | C11H18 | 093779-52-3 | 76 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

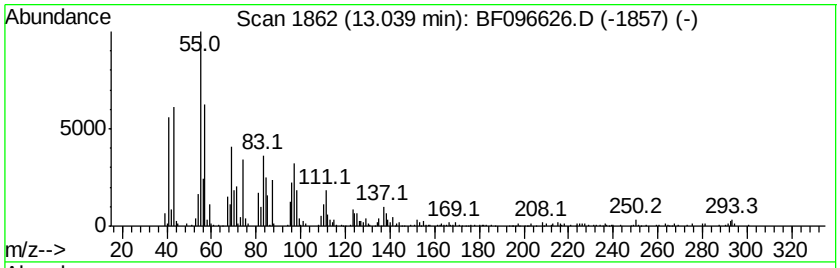
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

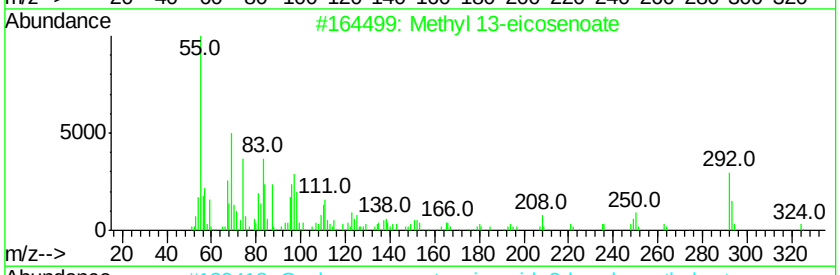
**********

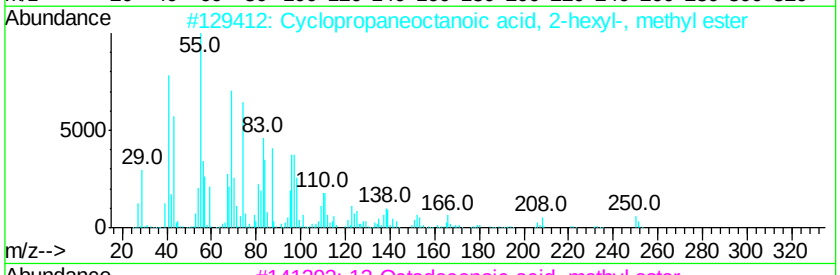
Peak Number 16 Methyl 13-eicosenoate Concentration Rank 8

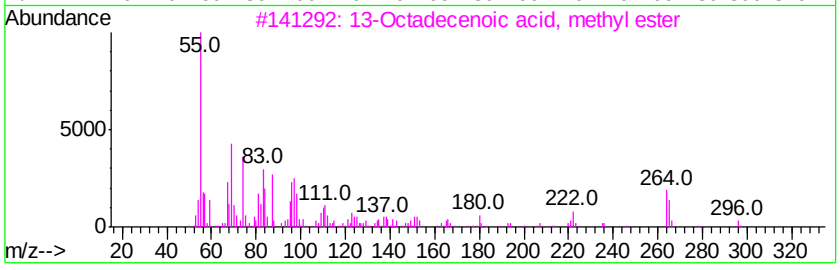
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.04 | 30.49 ng | 859757 | Chrysene-d12 | 13.83 |

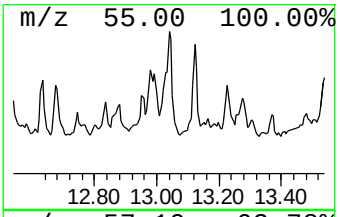
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl 13-eicosenoate | 324 | C21H40O2 | 1000336-48-4 | 90 |
| 2 | Cyclopropaneoctanoic acid, 2-hex... | 282 | C18H34O2 | 010152-61-1 | 72 |
| 3 | 13-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 056554-47-3 | 72 |
| 4 | Cyclopentadecanone, 2-hydroxy- | 240 | C15H28O2 | 004727-18-8 | 70 |
| 5 | 9-Octadecenoic acid (Z)-, methyl... | 296 | C19H36O2 | 000112-62-9 | 58 |

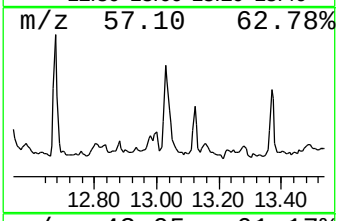


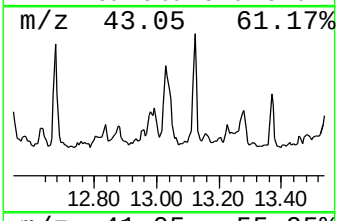



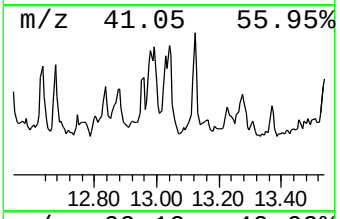



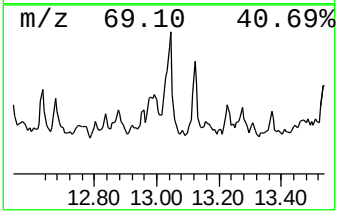



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

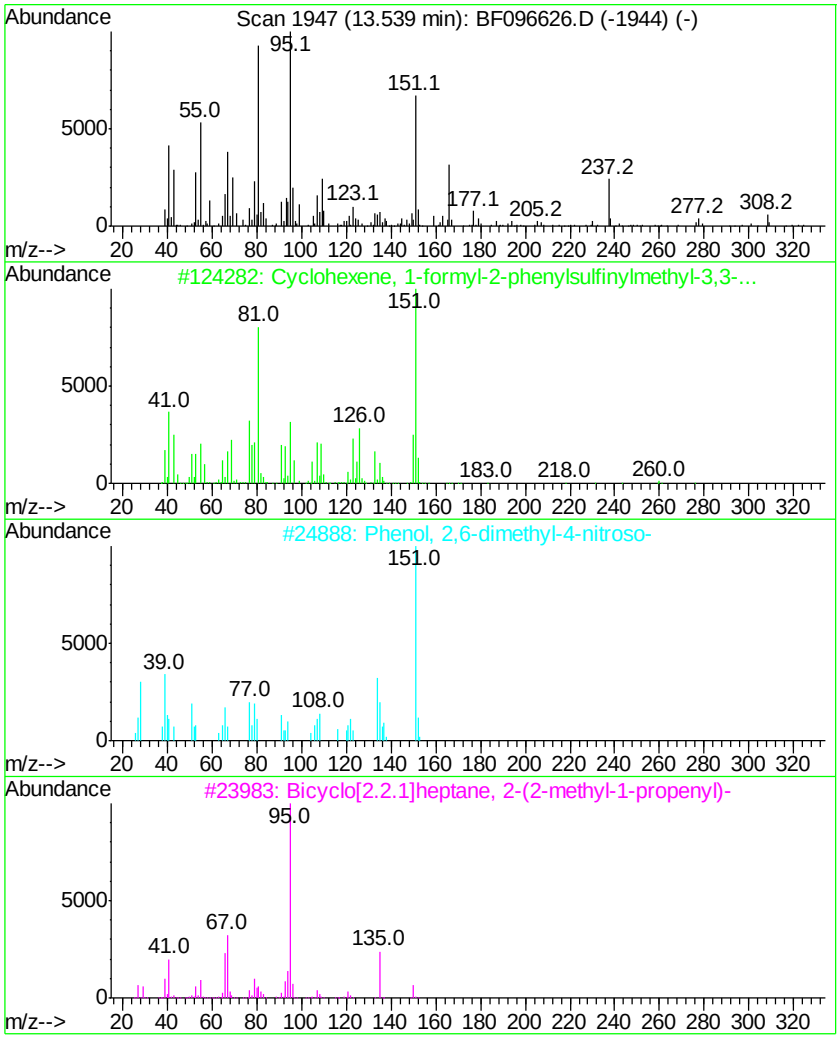
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

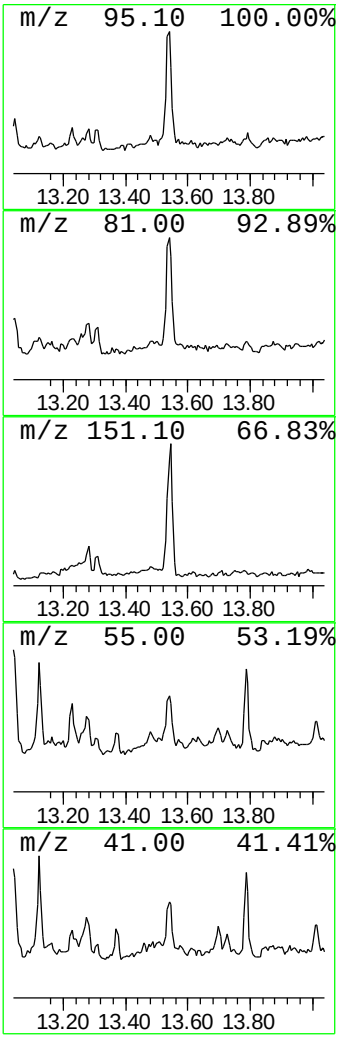
**********

Peak Number 18 unknown13.54 Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.54 | 16.09 ng | 453833 | Chrysene-d12 | 13.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexene, 1-formyl-2-phenylsu... | 276 | C16H20O2S | 081054-00-4 | 45 |
| 2 | Phenol, 2,6-dimethyl-4-nitroso- | 151 | C8H9NO2 | 013331-93-6 | 38 |
| 3 | Bicyclo[2.2.1]heptane, 2-(2-meth... | 150 | C11H18 | 061142-27-6 | 35 |
| 4 | Endo-tricyclo[5.2.1.0(2.6)]decane | 136 | C10H16 | 1000215-28-8 | 30 |
| 5 | 4-Cyclopropylnorcarane | 136 | C10H16 | 1000222-73-9 | 25 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

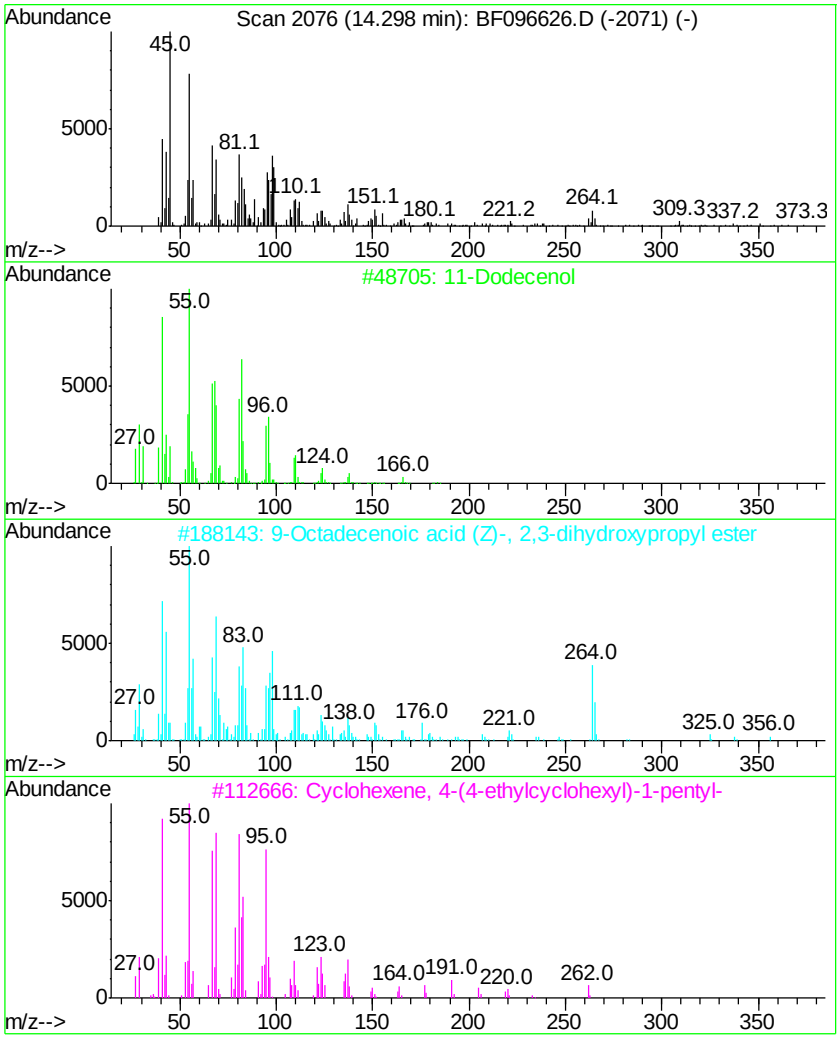
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

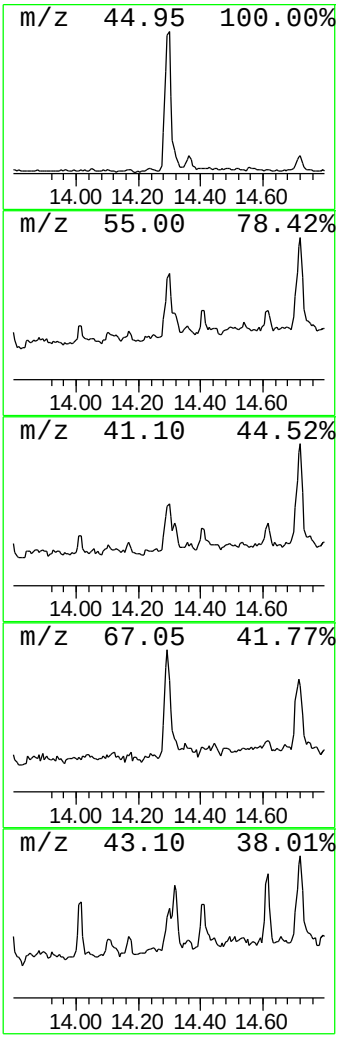
**********

Peak Number 19 11-Dodecenol Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.30 | 25.47 ng | 718262 | Chrysene-d12 | 13.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 11-Dodecenol | 184 | C12H24O | 035289-31-7 | 50 |
| 2 | 9-Octadecenoic acid (Z)-, 2,3-di... | 356 | C21H40O4 | 000111-03-5 | 46 |
| 3 | Cyclohexene, 4-(4-ethylcyclohexy... | 262 | C19H34 | 301643-32-3 | 44 |
| 4 | 1,11-Dodecadiene | 166 | C12H22 | 005876-87-9 | 43 |
| 5 | cis-9-Hexadecenal | 238 | C16H30O | 056219-04-6 | 41 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

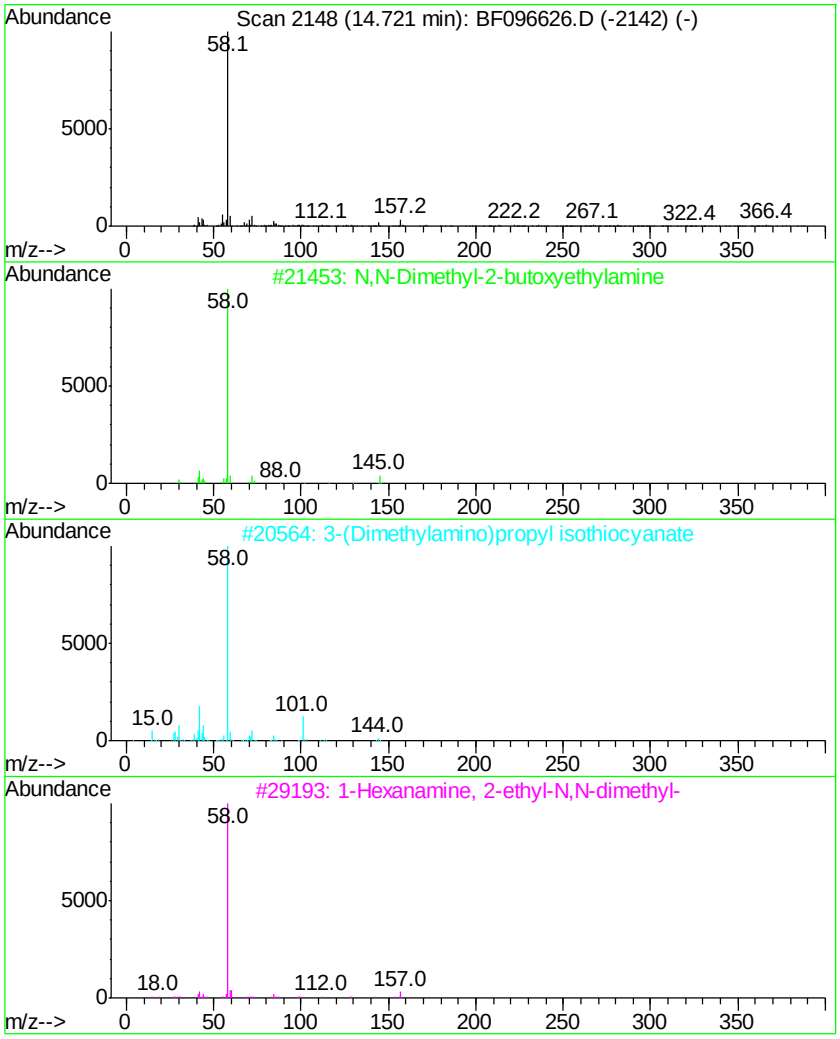
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

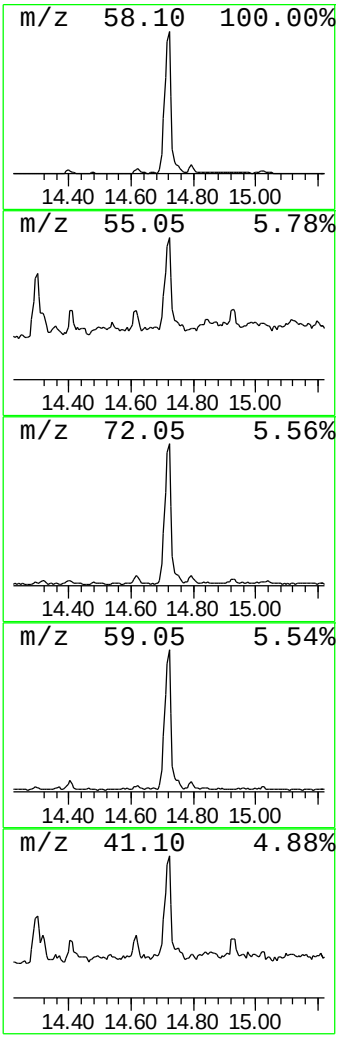
**********

Peak Number 20 N,N-Dimethyl-2-butoxyethyla... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.72 | 150.04 ng | 2539060 | Perylene-d12 | 15.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | N,N-Dimethyl-2-butoxyethylamine | 145 | C8H19NO | 071126-58-4 | 64 |
| 2 | 3-(Dimethylamino)propyl isothioc... | 144 | C6H12N2S | 027421-70-1 | 64 |
| 3 | 1-Hexanamine, 2-ethyl-N,N-dimethyl- | 157 | C10H23N | 028056-87-3 | 64 |
| 4 | Trifluomeprazine | 366 | C19H21F3N2S | 002622-37-9 | 64 |
| 5 | 1-Pentadecanamine, N,N-dimethyl- | 255 | C17H37N | 017678-60-3 | 59 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071017\
Data File : BF096626.D
Acq On : 11 Jul 2017 2:52
Operator : SJ/JU
Sample : I4071-04 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-06-070617-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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 |
| unknown6.45 | 6.45 | 16.6 | ng | 472082 | 1 | 6.69 | 568990 | 20.0 |
| Undecane | 7.30 | 15.6 | ng | 444084 | 1 | 6.69 | 568990 | 20.0 |
| Hexadecane | 8.57 | 15.6 | ng | 987032 | 2 | 7.97 | 1265040 | 20.0 |
| Decane, 6-ethyl-2... | 9.14 | 25.6 | ng | 918780 | 3 | 9.72 | 717734 | 20.0 |
| Heneicosane | 10.63 | 34.2 | ng | 872676 | 4 | 11.19 | 510097 | 20.0 |
| Pentadecane | 11.08 | 22.4 | ng | 571830 | 4 | 11.19 | 510097 | 20.0 |
| Heptadecane | 11.51 | 18.4 | ng | 469455 | 4 | 11.19 | 510097 | 20.0 |
| Hexadecanoic acid... | 11.62 | 236.6 | ng | 6033120 | 4 | 11.19 | 510097 | 20.0 |
| Tridecane, 1-iodo- | 11.92 | 18.2 | ng | 463279 | 4 | 11.19 | 510097 | 20.0 |
| 10,13-Octadecadie... | 12.32 | 583.7 | ng | 14886200 | 4 | 11.19 | 510097 | 20.0 |
| Methyl stearate | 12.40 | 136.8 | ng | 3490250 | 4 | 11.19 | 510097 | 20.0 |
| cis-Vaccenic acid | 12.47 | 170.9 | ng | 4359080 | 4 | 11.19 | 510097 | 20.0 |
| 6-Butyl-1,4-cyclo... | 12.88 | 18.9 | ng | 531581 | 5 | 13.83 | 564018 | 20.0 |
| Methyl 9.cis.,11.... | 12.99 | 37.4 | ng | 1054150 | 5 | 13.83 | 564018 | 20.0 |
| Methyl 13-eicosen... | 13.04 | 30.5 | ng | 859757 | 5 | 13.83 | 564018 | 20.0 |
| unknown13.54 | 13.54 | 16.1 | ng | 453833 | 5 | 13.83 | 564018 | 20.0 |
| 11-Dodecenol | 14.30 | 25.5 | ng | 718262 | 5 | 13.83 | 564018 | 20.0 |
| N,N-Dimethyl-2-bu... | 14.72 | 150.0 | ng | 2539060 | 6 | 15.23 | 338445 | 20.0 |