LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121516\
Data File : BF091631.D
Acq On : 15 Dec 2016 16:33
Operator : UM/SJ
Sample : H6012-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2-3-4

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-BF120916.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 | 4.956 | 248 | 251 | 258 | rBV | 2018523 | 2823566 | 34.58% | 3.625% |
| 2 | 5.390 | 286 | 289 | 291 | rBV | 6690417 | 7396970 | 90.58% | 9.498% |
| 3 | 6.430 | 377 | 380 | 382 | rBV | 6811167 | 8166087 | 100.00% | 10.485% |
| 4 | 6.556 | 388 | 391 | 393 | rBV | 7105038 | 7489155 | 91.71% | 9.616% |
| 5 | 6.784 | 408 | 411 | 413 | rBV | 2132891 | 1897293 | 23.23% | 2.436% |
| 6 | 6.944 | 422 | 425 | 427 | rBV | 5052742 | 5821264 | 71.29% | 7.474% |
| 7 | 7.345 | 457 | 460 | 463 | rBV | 3784435 | 4637670 | 56.79% | 5.955% |
| 8 | 8.065 | 521 | 523 | 526 | rBV | 2367812 | 2419646 | 29.63% | 3.107% |
| 9 | 9.150 | 615 | 618 | 620 | rBV | 8060745 | 7814014 | 95.69% | 10.033% |
| 10 | 9.539 | 650 | 652 | 655 | rBV | 739271 | 720458 | 8.82% | 0.925% |
| 11 | 9.745 | 666 | 670 | 674 | rVB2 | 90019 | 263684 | 3.23% | 0.339% |
| 12 | 9.825 | 674 | 677 | 679 | rBV | 2884822 | 2819877 | 34.53% | 3.621% |
| 13 | 10.236 | 711 | 713 | 714 | rBV | 96117 | 85477 | 1.05% | 0.110% |
| 14 | 10.259 | 714 | 715 | 717 | rVB | 147400 | 146637 | 1.80% | 0.188% |
| 15 | 10.488 | 731 | 735 | 737 | rBV2 | 56816 | 108233 | 1.33% | 0.139% |
| 16 | 10.613 | 743 | 746 | 748 | rBV | 4549221 | 4908793 | 60.11% | 6.303% |
| 17 | 10.739 | 755 | 757 | 761 | rVB | 188100 | 284573 | 3.48% | 0.365% |
| 18 | 11.185 | 791 | 796 | 797 | rBV | 223307 | 252954 | 3.10% | 0.325% |
| 19 | 11.299 | 804 | 806 | 810 | rBV2 | 2493373 | 3025632 | 37.05% | 3.885% |
| 20 | 11.379 | 810 | 813 | 814 | rVB | 131574 | 168773 | 2.07% | 0.217% |
| 21 | 11.482 | 819 | 822 | 824 | rVB | 60232 | 83950 | 1.03% | 0.108% |
| 22 | 11.608 | 831 | 833 | 834 | rBV | 204940 | 169808 | 2.08% | 0.218% |
| 23 | 11.836 | 851 | 853 | 855 | rBV2 | 185166 | 277958 | 3.40% | 0.357% |
| 24 | 11.916 | 858 | 860 | 865 | rVB2 | 135136 | 208306 | 2.55% | 0.267% |
| 25 | 12.099 | 872 | 876 | 880 | rVB2 | 66878 | 122645 | 1.50% | 0.157% |
| 26 | 12.511 | 910 | 912 | 914 | rBV | 887623 | 766054 | 9.38% | 0.984% |
| 27 | 12.739 | 929 | 932 | 934 | rBV | 641977 | 765117 | 9.37% | 0.982% |
| 28 | 12.797 | 934 | 937 | 939 | rVB3 | 49276 | 87173 | 1.07% | 0.112% |
| 29 | 12.888 | 942 | 945 | 948 | rVV | 5492647 | 5903970 | 72.30% | 7.581% |
| 30 | 12.957 | 948 | 951 | 955 | rVB2 | 42202 | 85915 | 1.05% | 0.110% |
| 31 | 13.071 | 957 | 961 | 962 | rVB | 81695 | 137605 | 1.69% | 0.177% |
| 32 | 13.128 | 965 | 966 | 968 | rVB | 79793 | 84123 | 1.03% | 0.108% |
| 33 | 13.174 | 968 | 970 | 974 | rBV2 | 51506 | 89147 | 1.09% | 0.114% |
| 34 | 13.471 | 992 | 996 | 999 | rBV3 | 52151 | 104460 | 1.28% | 0.134% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121516\
Data File : BF091631.D
Acq On : 15 Dec 2016 16:33
Operator : UM/SJ
Sample : H6012-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2-3-4

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-BF120916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 13.791 | 1021 | 1024 | 1027 | rVB3 | 269022 | 350704 | 4.29% | 0.450% |
| 36 | 13.928 | 1033 | 1036 | 1042 | rVB3 | 2269080 | 2976197 | 36.45% | 3.821% |
| 37 | 14.317 | 1066 | 1070 | 1072 | rBV | 54981 | 102664 | 1.26% | 0.132% |
| 38 | 14.420 | 1075 | 1079 | 1082 | rBV3 | 116544 | 232239 | 2.84% | 0.298% |
| 39 | 14.785 | 1109 | 1111 | 1115 | rBV3 | 81936 | 105643 | 1.29% | 0.136% |
| 40 | 14.854 | 1115 | 1117 | 1119 | rVB | 130363 | 146622 | 1.80% | 0.188% |
| 41 | 14.945 | 1122 | 1125 | 1130 | rBV | 225497 | 451974 | 5.53% | 0.580% |
| 42 | 15.048 | 1130 | 1134 | 1138 | rBV3 | 143912 | 366883 | 4.49% | 0.471% |
| 43 | 15.220 | 1147 | 1149 | 1152 | rVB | 144268 | 180653 | 2.21% | 0.232% |
| 44 | 15.277 | 1152 | 1154 | 1157 | rBV | 199064 | 246424 | 3.02% | 0.316% |
| 45 | 15.345 | 1157 | 1160 | 1162 | rBV | 1250789 | 1708652 | 20.92% | 2.194% |
| 46 | 15.791 | 1196 | 1199 | 1202 | rBV | 117877 | 217572 | 2.66% | 0.279% |
| 47 | 16.683 | 1274 | 1277 | 1283 | rVB2 | 99460 | 241912 | 2.96% | 0.311% |
| 48 | 16.808 | 1285 | 1288 | 1291 | rBV | 53981 | 125554 | 1.54% | 0.161% |
| 49 | 17.094 | 1309 | 1313 | 1322 | rBV | 81375 | 198528 | 2.43% | 0.255% |
| 50 | 17.311 | 1329 | 1332 | 1339 | rVB2 | 33493 | 94053 | 1.15% | 0.121% |

Sum of corrected areas: 77883261

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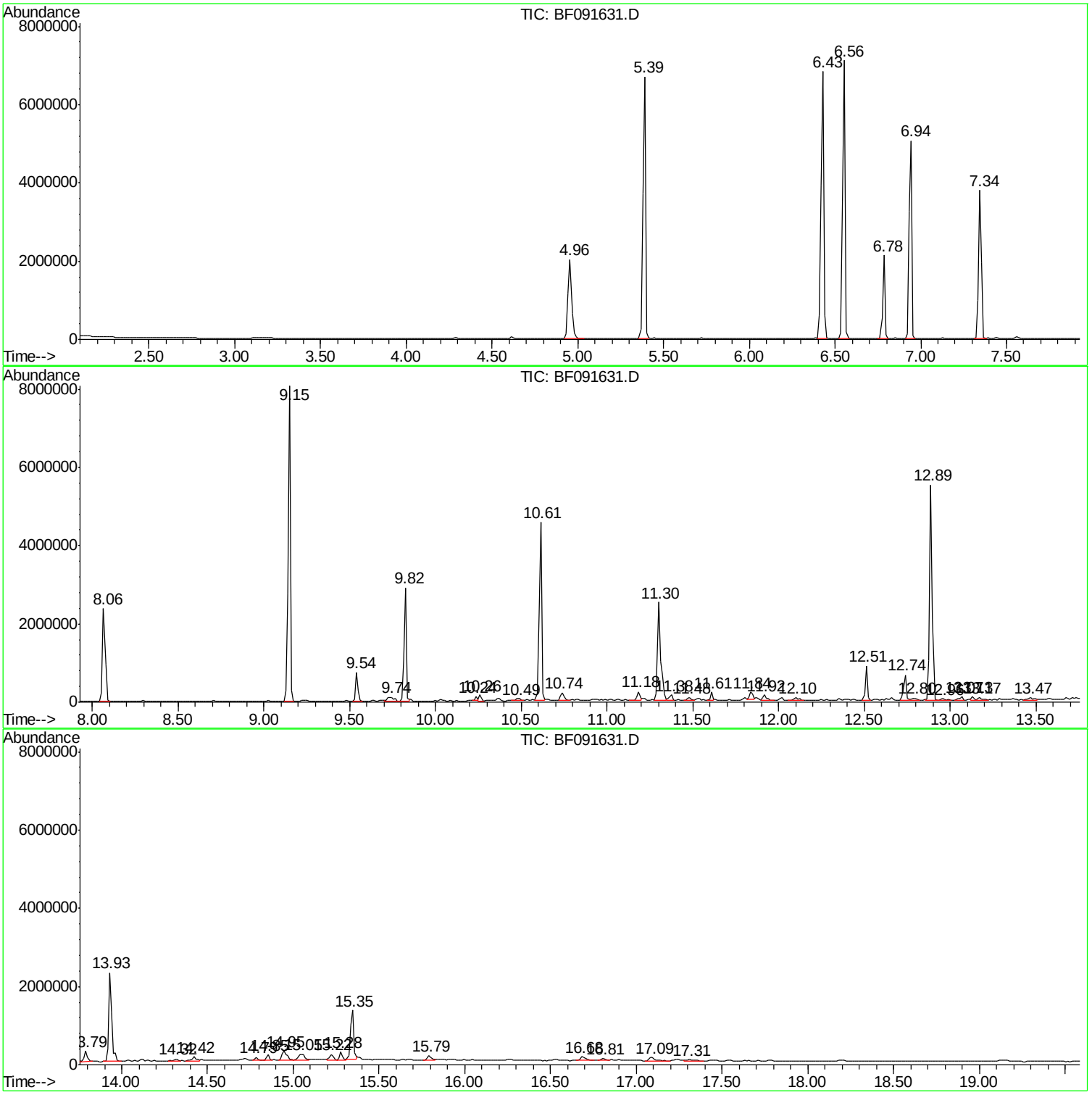
Acq On : 15 Dec 2016 16:33
Operator : UM/SJ
Sample : H6012-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2-3-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121516\
Data File : BF091631.D
Acq On : 15 Dec 2016 16:33
Operator : UM/SJ
Sample : H6012-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2-3-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

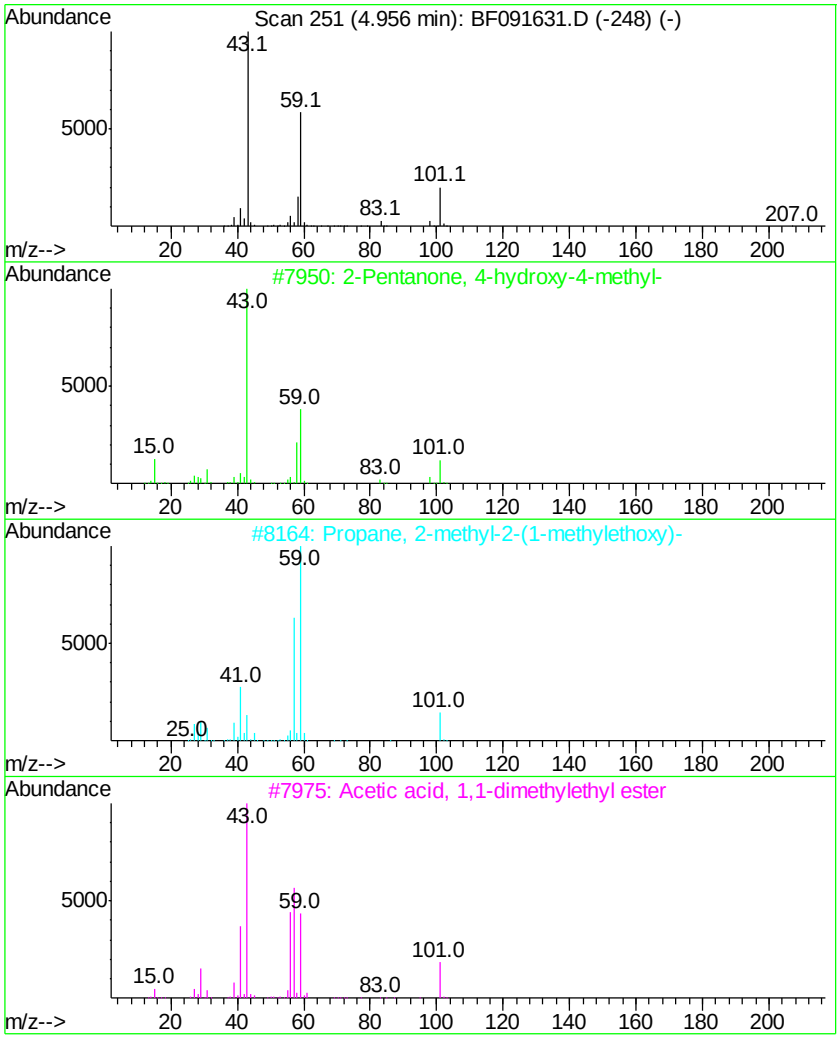
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

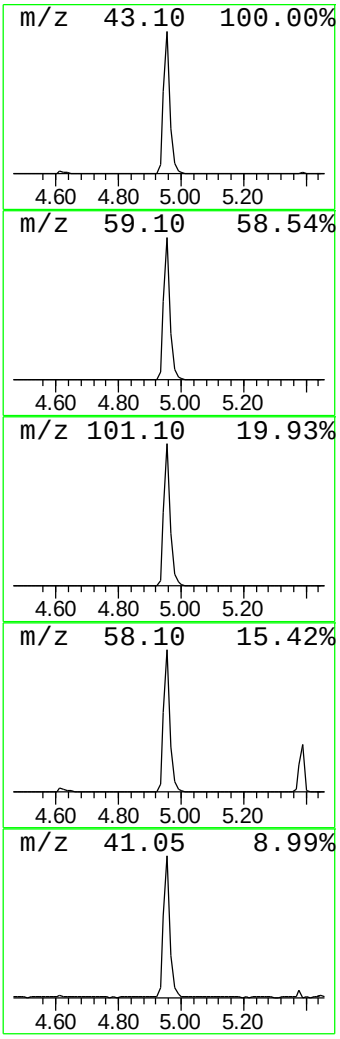
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.96 | 29.76 ng | 2823570 | 1,4-Dichlorobenzene-d4 | 6.78 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 53 |
| 3 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 5 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121516\
Data File : BF091631.D
Acq On : 15 Dec 2016 16:33
Operator : UM/SJ
Sample : H6012-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2-3-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

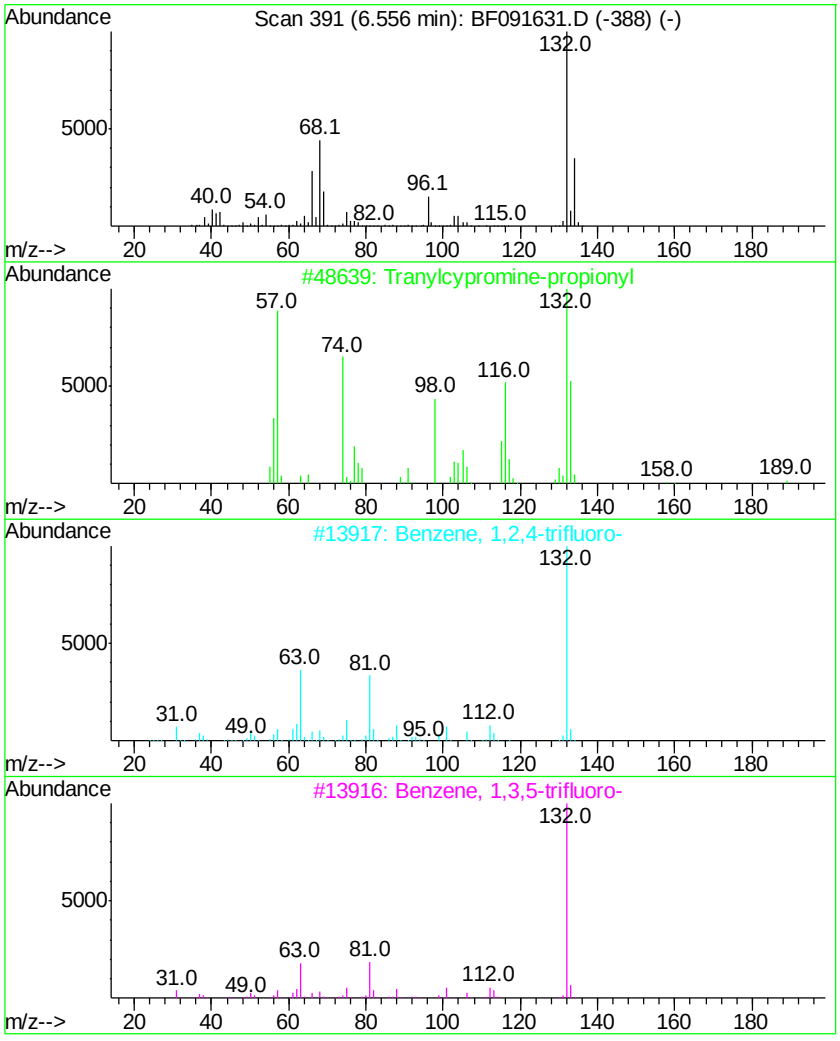
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

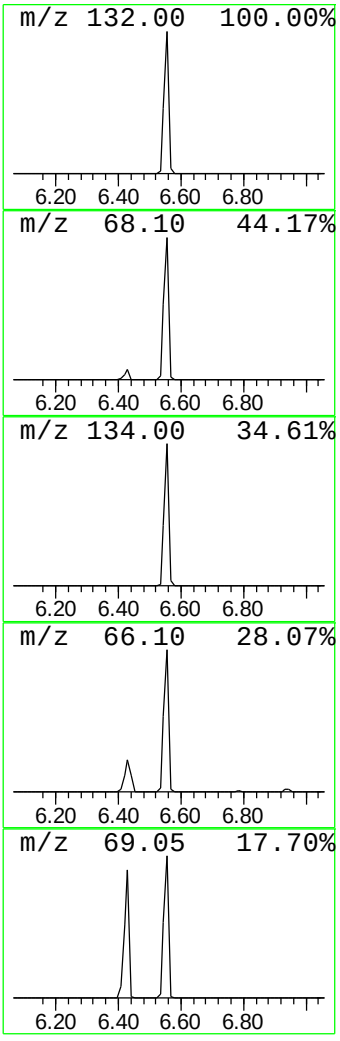
**********

Peak Number 2 unknown6.56 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.56 | 78.95 ng | 7489160 | 1,4-Dichlorobenzene-d4 | 6.78 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 2 | Benzene, 1,2,4-trifluoro- | 132 | C6H3F3 | 000367-23-7 | 9 |
| 3 | Benzene, 1,3,5-trifluoro- | 132 | C6H3F3 | 000372-38-3 | 9 |
| 4 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 5 | Benzene, 1-ethenyl-3,5-dimethyl- | 132 | C10H12 | 005379-20-4 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121516\
Data File : BF091631.D
Acq On : 15 Dec 2016 16:33
Operator : UM/SJ
Sample : H6012-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2-3-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

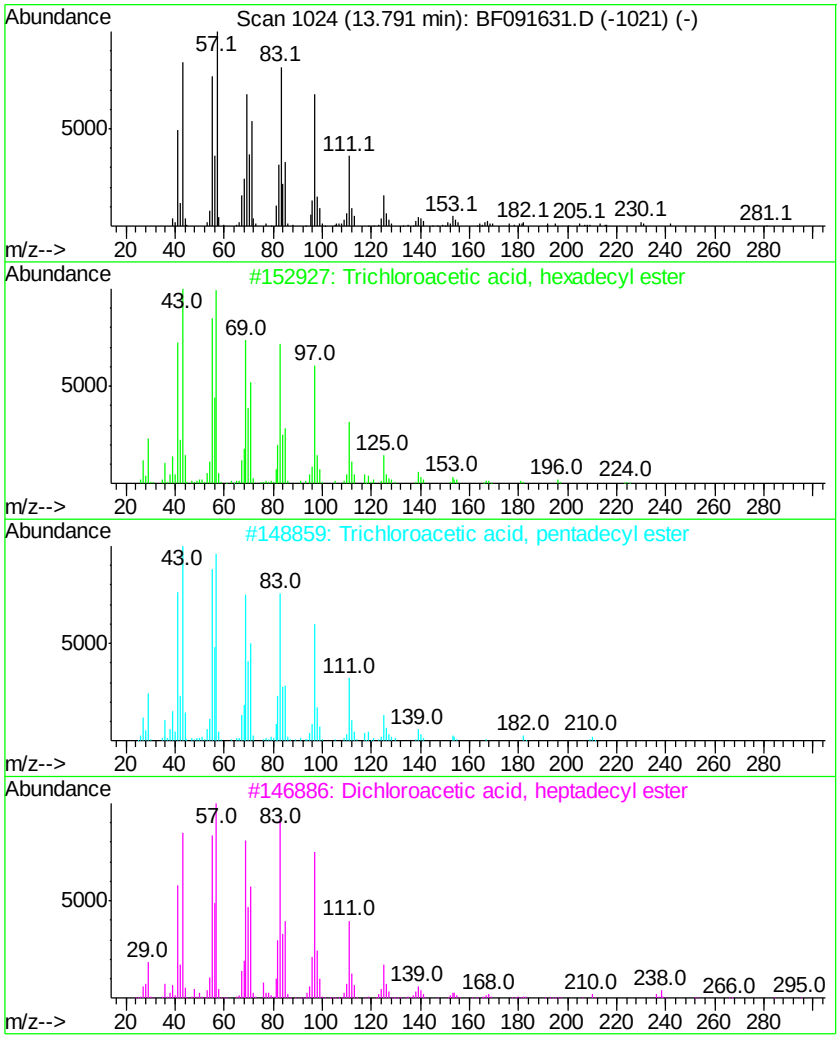
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

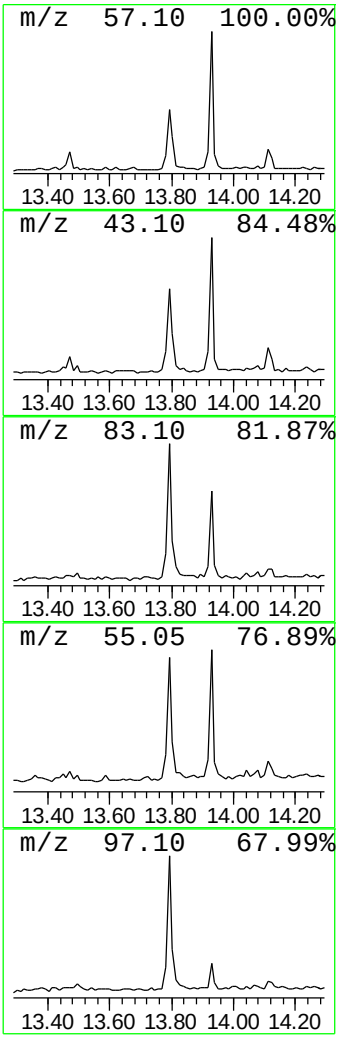
**********

Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.79 | 2.36 ng | 350704 | Chrysene-d12 | 13.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 93 |
| 2 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 90 |
| 3 | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 90 |
| 4 | 1-Octadecanol | 270 | C18H38O | 000112-92-5 | 87 |
| 5 | 1-Heptadecanol | 256 | C17H36O | 001454-85-9 | 87 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121516\
Data File : BF091631.D
Acq On : 15 Dec 2016 16:33
Operator : UM/SJ
Sample : H6012-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2-3-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

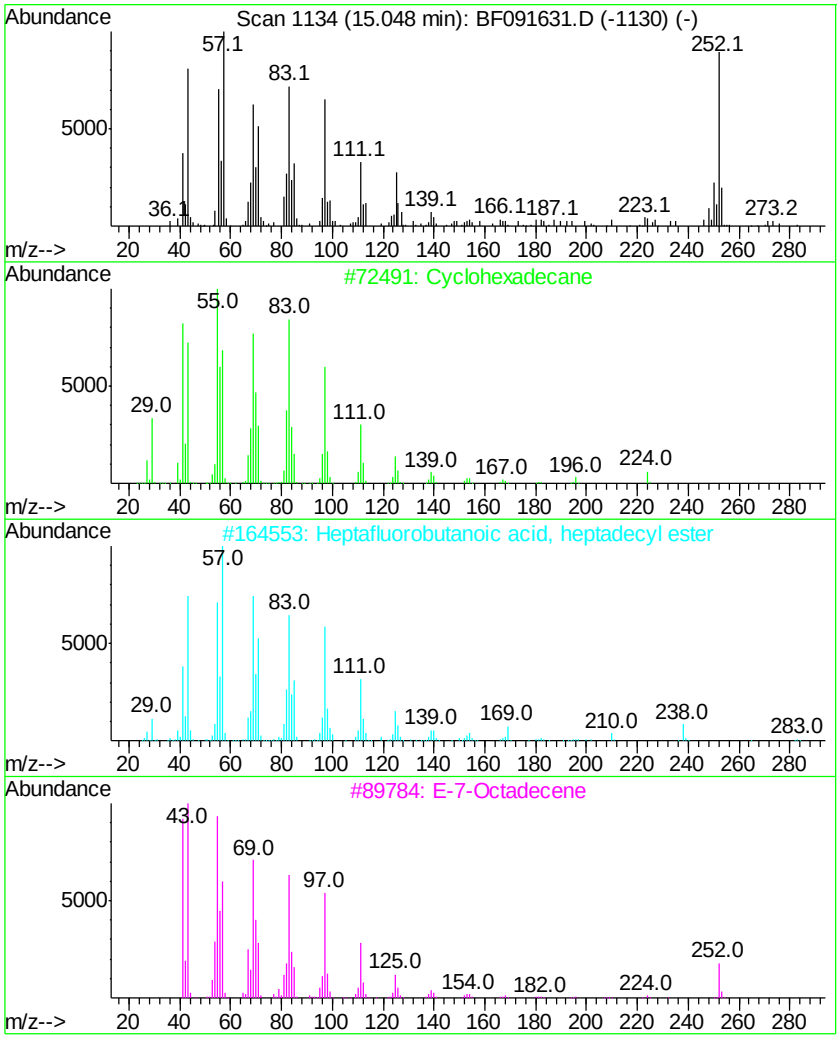
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

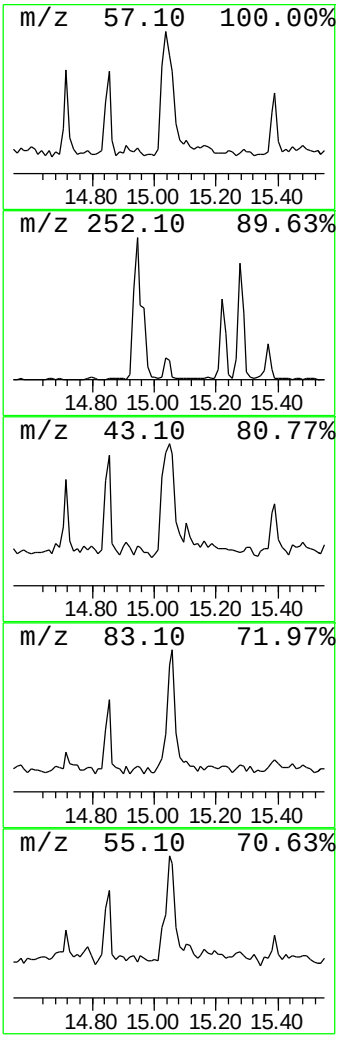
**********

Peak Number 5 Cyclohexadecane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.05 | 4.29 ng | 366883 | Perylene-d12 | 15.35 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexadecane | 224 | C16H32 | 000295-65-8 | 93 |
| 2 | Heptafluorobutanoic acid, heptad... | 452 | C21H35F7O2 | 1000282-97-3 | 81 |
| 3 | E-7-Octadecene | 252 | C18H36 | 1000130-92-0 | 62 |
| 4 | Benz[e]acephenanthrylene | 252 | C20H12 | 000205-99-2 | 50 |
| 5 | Benzo[k]fluoranthene | 252 | C20H12 | 000207-08-9 | 46 |



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Sample : H6012-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2-3-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

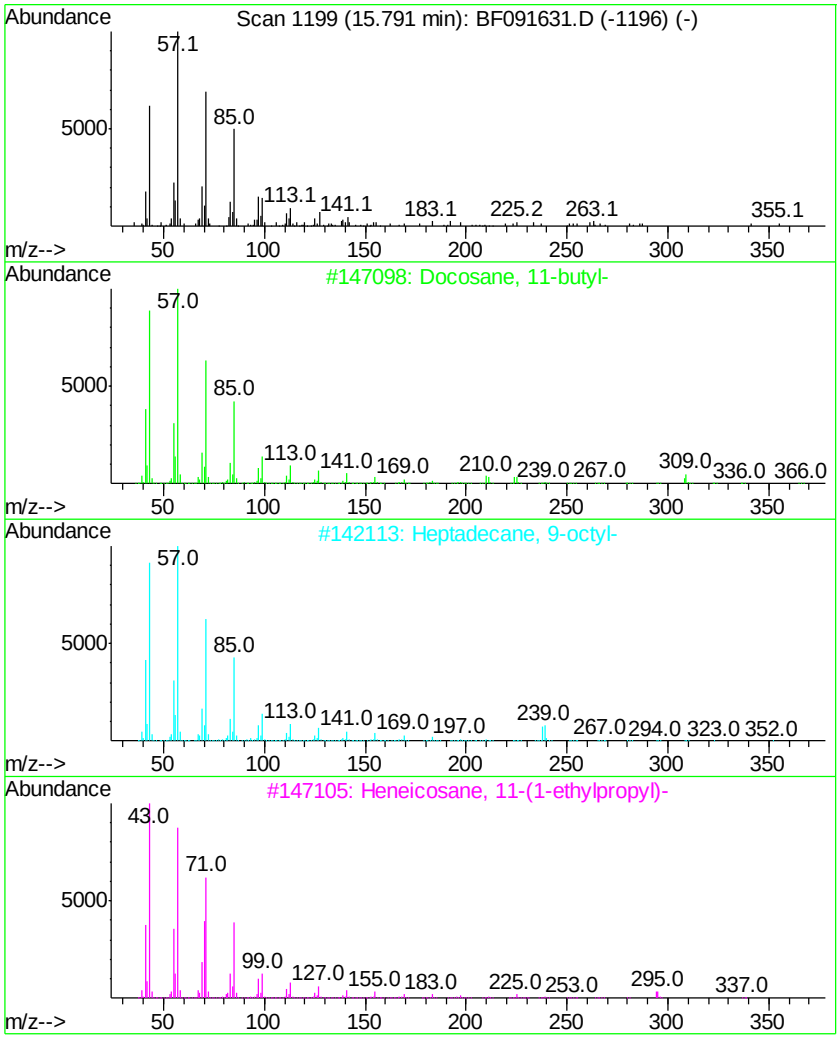
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

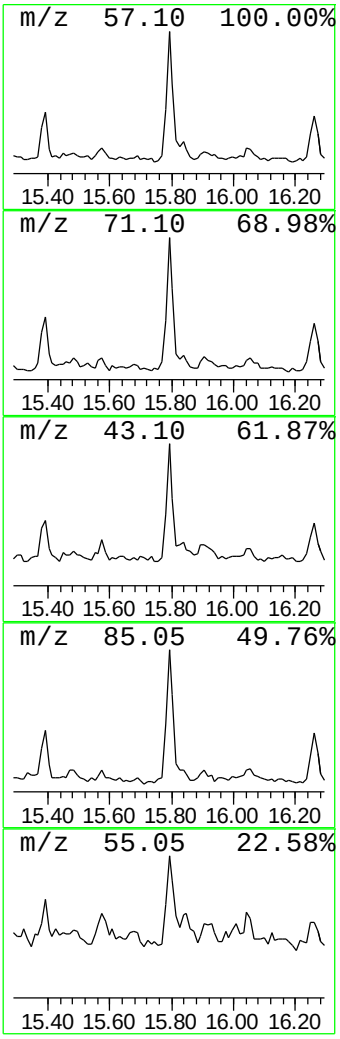
**********

Peak Number 7 Docosane, 11-butyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.79 | 2.55 ng | 217572 | Perylene-d12 | 15.35 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Docosane, 11-butyl- | 366 | C26H54 | 013475-76-8 | 91 |
| 2 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 91 |
| 3 | Heneicosane, 11-(1-ethylpropyl)- | 366 | C26H54 | 055282-11-6 | 91 |
| 4 | Docosane, 9-butyl- | 366 | C26H54 | 055282-14-9 | 91 |
| 5 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121516\
Data File : BF091631.D
Acq On : 15 Dec 2016 16:33
Operator : UM/SJ
Sample : H6012-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-2-3-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 4.96 | 29.8 | ng | 2823570 | 1 | 6.78 | 1897290 | 20.0 |
| unknown6.56 | 6.56 | 79.0 | ng | 7489160 | 1 | 6.78 | 1897290 | 20.0 |
| Trichloroacetic a... | 13.79 | 2.4 | ng | 350704 | 5 | 13.93 | 2976200 | 20.0 |
| Cyclohexadecane | 15.05 | 4.3 | ng | 366883 | 6 | 15.35 | 1708650 | 20.0 |
| Docosane, 11-butyl- | 15.79 | 2.5 | ng | 217572 | 6 | 15.35 | 1708650 | 20.0 |