LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG062716\
Data File : BG022646.D
Acq On : 27 Jun 2016 17:01
Operator : UM/SJ
Sample : H3630-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B1409-TPGW04-0616

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_G\METHODS\8270-BG062516.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 | 4.629 | 299 | 305 | 315 | rVB | 1179992 | 1790393 | 17.03% | 3.206% |
| 2 | 4.747 | 320 | 325 | 330 | rBV | 74135 | 118097 | 1.12% | 0.211% |
| 3 | 5.234 | 403 | 408 | 414 | rBV | 173006 | 260467 | 2.48% | 0.466% |
| 4 | 5.704 | 482 | 488 | 499 | rBV | 1067983 | 1714802 | 16.31% | 3.071% |
| 5 | 7.261 | 747 | 753 | 756 | rBV | 122414 | 195356 | 1.86% | 0.350% |
| 6 | 7.309 | 756 | 761 | 770 | rVB | 742825 | 1289518 | 12.27% | 2.309% |
| 7 | 7.690 | 818 | 826 | 834 | rBV | 1836875 | 3201770 | 30.45% | 5.733% |
| 8 | 8.160 | 899 | 906 | 913 | rVB | 555332 | 970294 | 9.23% | 1.737% |
| 9 | 8.489 | 954 | 962 | 969 | rBV | 1607086 | 2843620 | 27.05% | 5.092% |
| 10 | 9.330 | 1098 | 1105 | 1113 | rBV | 1522211 | 2705356 | 25.73% | 4.844% |
| 11 | 10.987 | 1378 | 1387 | 1394 | rBV | 788257 | 1484667 | 14.12% | 2.658% |
| 12 | 12.749 | 1683 | 1687 | 1696 | rBV6 | 45241 | 107110 | 1.02% | 0.192% |
| 13 | 13.419 | 1794 | 1801 | 1808 | rBV | 3958666 | 6162500 | 58.61% | 11.035% |
| 14 | 13.930 | 1883 | 1888 | 1892 | rBV7 | 75905 | 128376 | 1.22% | 0.230% |
| 15 | 13.995 | 1892 | 1899 | 1904 | rVV10 | 45554 | 106603 | 1.01% | 0.191% |
| 16 | 14.242 | 1936 | 1941 | 1950 | rVB | 220231 | 384629 | 3.66% | 0.689% |
| 17 | 14.794 | 2029 | 2035 | 2043 | rBV2 | 1307849 | 2205736 | 20.98% | 3.950% |
| 18 | 16.286 | 2283 | 2289 | 2299 | rBV | 3917007 | 6136270 | 58.36% | 10.988% |
| 19 | 17.555 | 2499 | 2505 | 2511 | rBV2 | 1862685 | 2870394 | 27.30% | 5.140% |
| 20 | 18.207 | 2613 | 2616 | 2620 | rVB2 | 118491 | 151271 | 1.44% | 0.271% |
| 21 | 18.431 | 2650 | 2654 | 2662 | rBV | 983259 | 1309253 | 12.45% | 2.344% |
| 22 | 19.500 | 2833 | 2836 | 2840 | rVB | 240206 | 279920 | 2.66% | 0.501% |
| 23 | 19.553 | 2841 | 2845 | 2847 | rBV4 | 165316 | 226460 | 2.15% | 0.405% |
| 24 | 19.694 | 2865 | 2869 | 2880 | rBV2 | 1373185 | 1923733 | 18.30% | 3.445% |
| 25 | 20.158 | 2942 | 2948 | 2955 | rVB | 7449573 | 10513627 | 100.00% | 18.826% |
| 26 | 21.844 | 3230 | 3235 | 3244 | rVB | 2069794 | 3574919 | 34.00% | 6.401% |
| 27 | 25.205 | 3799 | 3807 | 3822 | rVB3 | 1030165 | 3192141 | 30.36% | 5.716% |

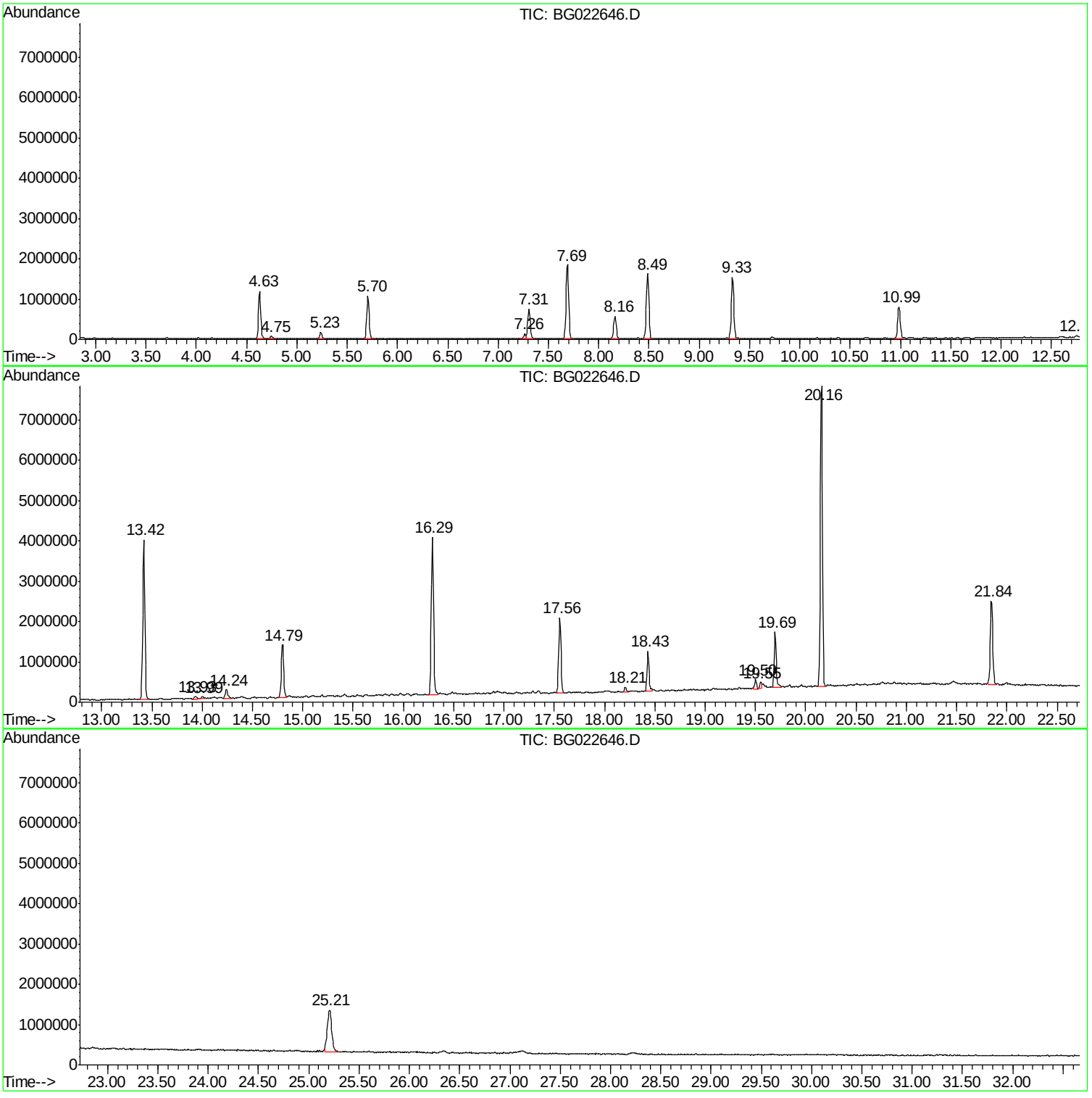
Sum of corrected areas: 55847282

Data Path : Z:\HPCHEM1\BNA G\DATA\BG062716\
Data File : BG022646.D
Acq On : 27 Jun 2016 17:01
Operator : UM/SJ
Sample : H3630-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
B1409-TPGW04-0616

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.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 G\DATA\BG062716\
Data File : BG022646.D
Acq On : 27 Jun 2016 17:01
Operator : UM/SJ
Sample : H3630-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B1409-TPGW04-0616

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

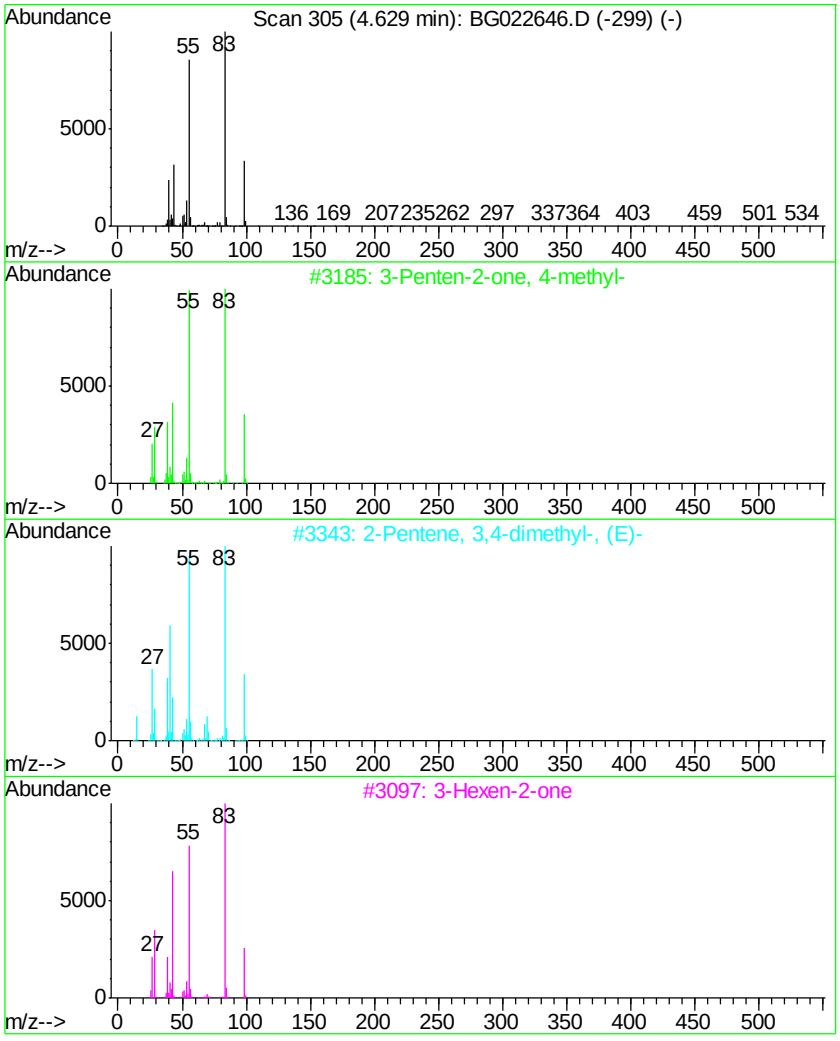
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

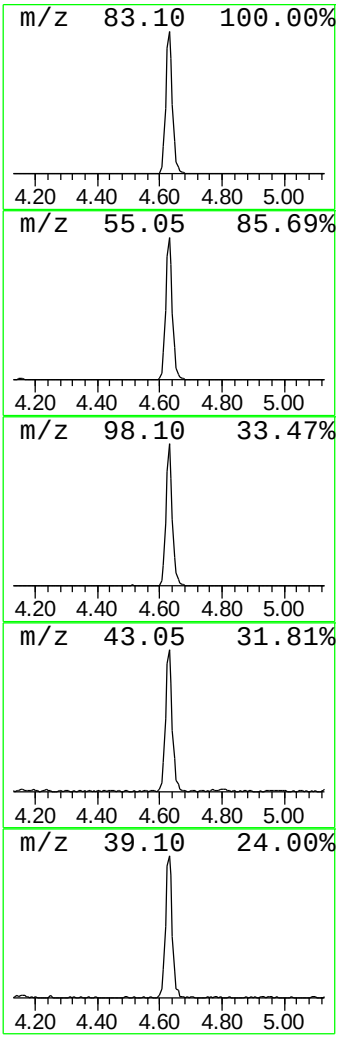
**********

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.63 | 36.90 ng | 1790390 | 1,4-Dichlorobenzene-d4 | 8.16 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Penten-2-one, 4-methyl- | 98 | C6H10O | 000141-79-7 | 91 |
| 2 | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14 | 004914-92-5 | 90 |
| 3 | 3-Hexen-2-one | 98 | C6H10O | 000763-93-9 | 90 |
| 4 | Furan, 2-methoxy- | 98 | C5H6O2 | 025414-22-6 | 86 |
| 5 | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14 | 004914-91-4 | 86 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG062716\
Data File : BG022646.D
Acq On : 27 Jun 2016 17:01
Operator : UM/SJ
Sample : H3630-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B1409-TPGW04-0616

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

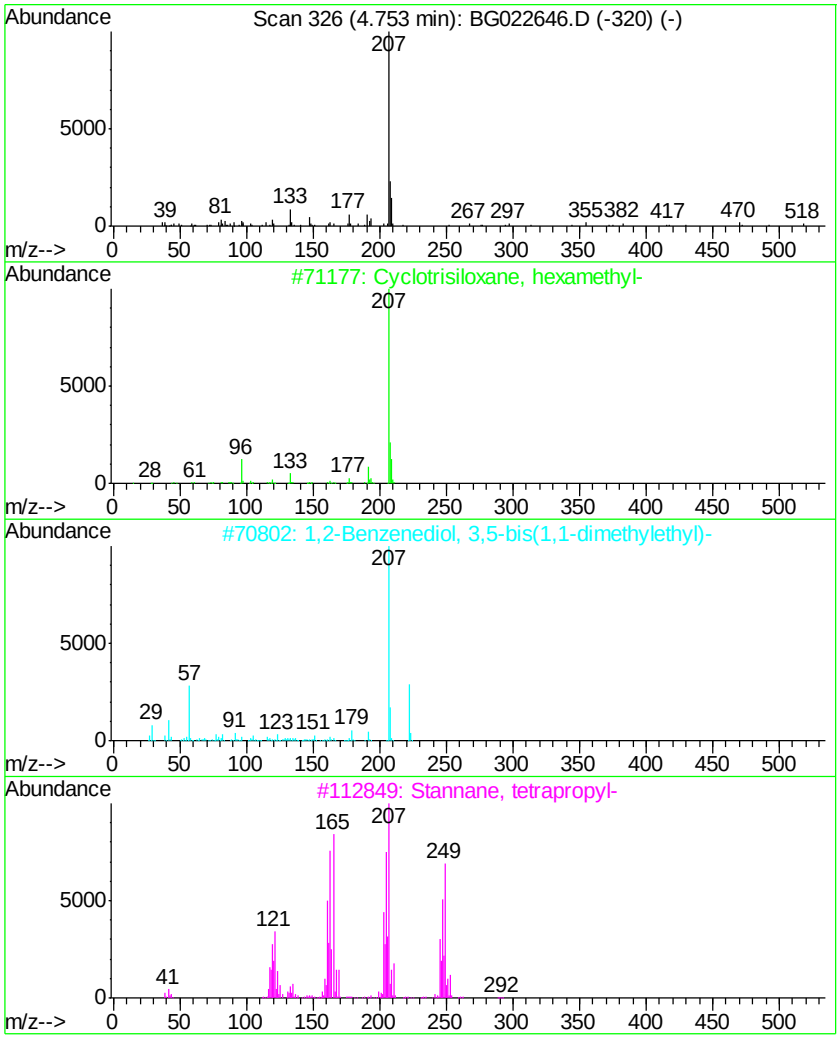
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

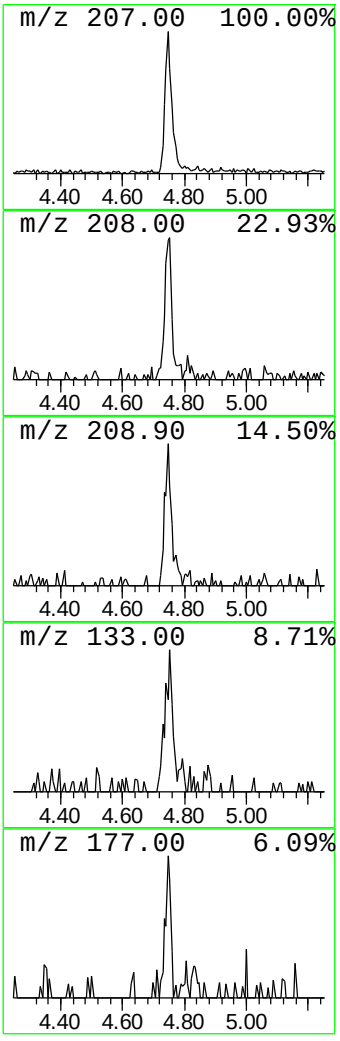
**********

Peak Number 2 Cyclotrisiloxane, hexamethyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.75 | 2.43 ng | 118097 | 1,4-Dichlorobenzene-d4 | 8.16 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclotrisiloxane, hexamethyl- | 222 | C6H18O3Si3 | 000541-05-9 | 56 |
| 2 | 1,2-Benzenediol, 3,5-bis(1,1-dim... | 222 | C14H22O2 | 001020-31-1 | 45 |
| 3 | Stannane, tetrapropyl- | 292 | C12H28Sn | 002176-98-9 | 40 |
| 4 | 2,4,6-Cycloheptatrien-1-one, 3,5... | 250 | C13H22OSi2 | 1000161-21-8 | 39 |
| 5 | Acetic acid, [4-(1,1-dimethyleth... | 222 | C13H18O3 | 088530-52-3 | 38 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG062716\
Data File : BG022646.D
Acq On : 27 Jun 2016 17:01
Operator : UM/SJ
Sample : H3630-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B1409-TPGW04-0616

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

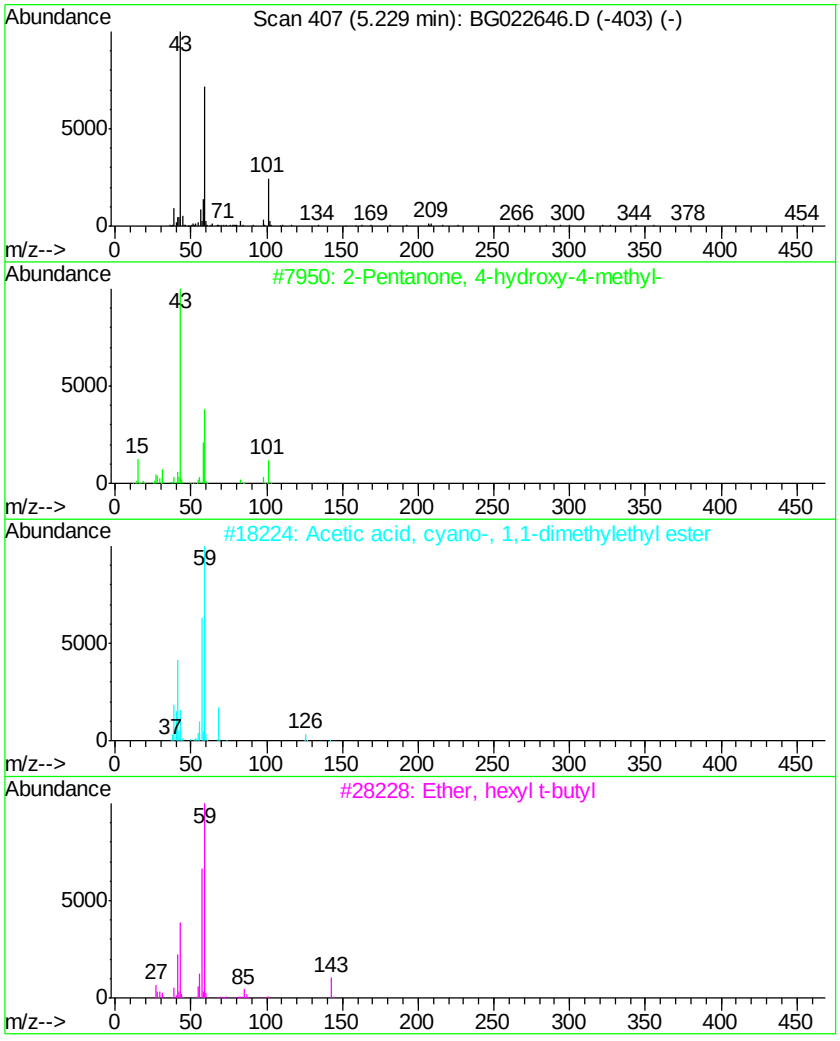
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

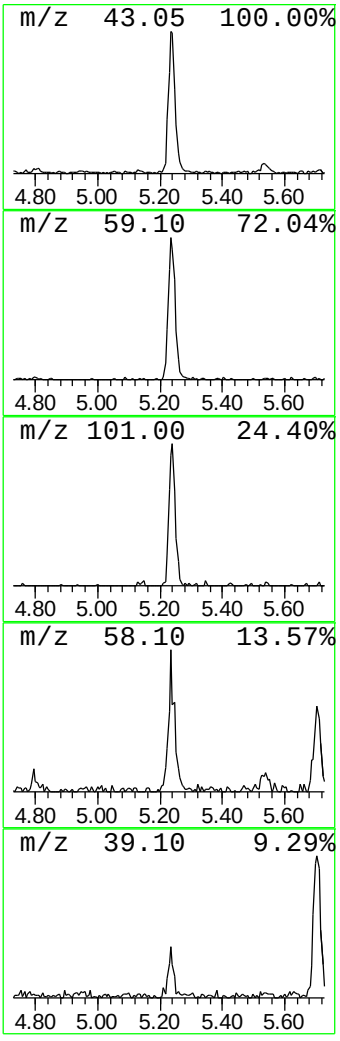
**********

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.23 | 5.37 ng | 260467 | 1,4-Dichlorobenzene-d4 | 8.16 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 38 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 27 |
| 3 | Ether, hexyl t-butyl | 158 | C10H22O | 069775-79-7 | 17 |
| 4 | 3-Hydroxy-3-methyl-2-butanone | 102 | C5H10O2 | 000115-22-0 | 12 |
| 5 | Oxirane, tetramethyl- | 100 | C6H12O | 005076-20-0 | 9 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG062716\
Data File : BG022646.D
Acq On : 27 Jun 2016 17:01
Operator : UM/SJ
Sample : H3630-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B1409-TPGW04-0616

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

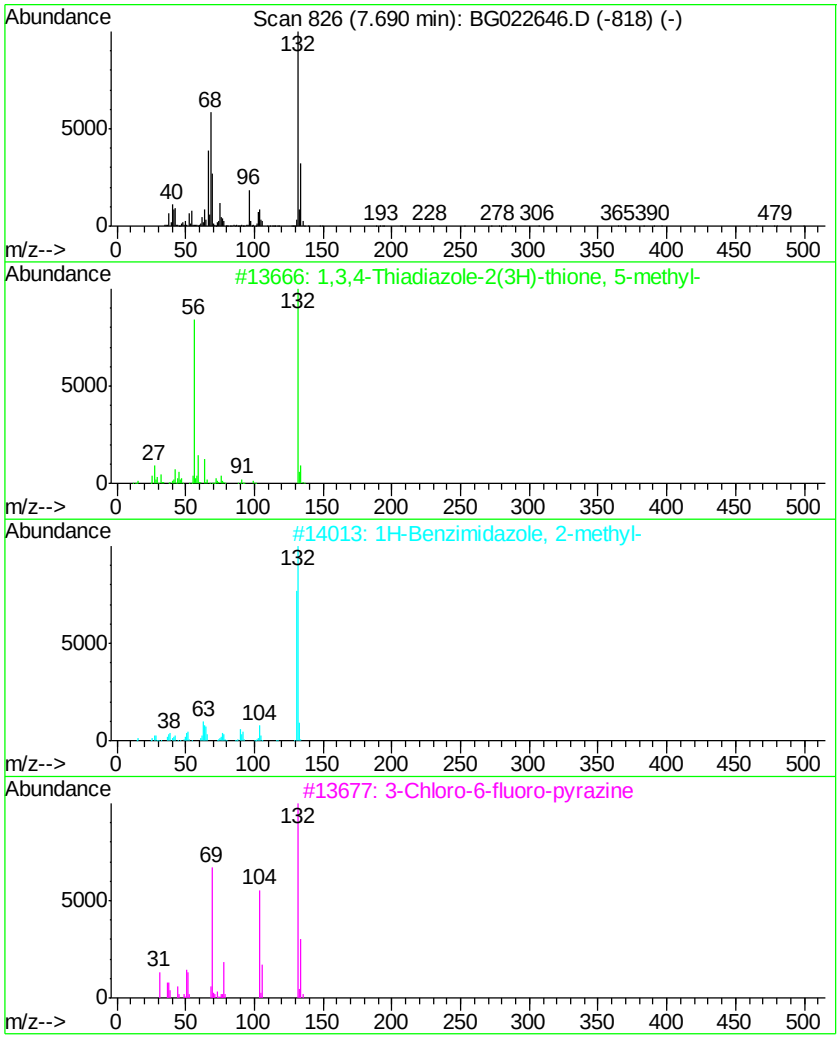
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

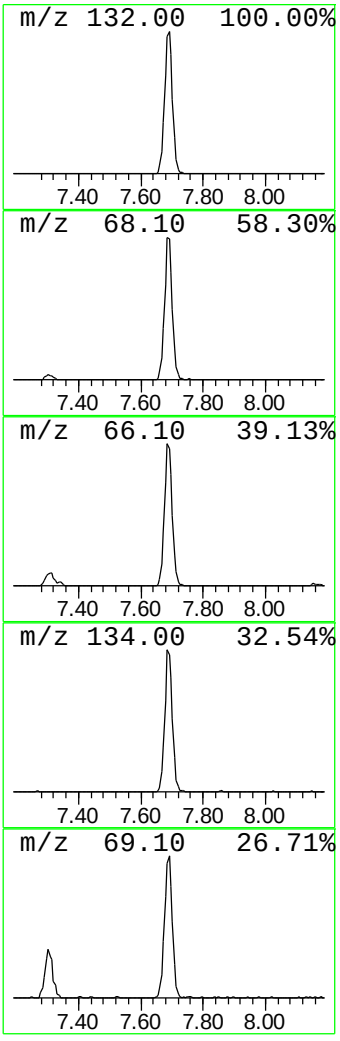
**********

Peak Number 4 unknown7.69 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.69 | 66.00 ng | 3201770 | 1,4-Dichlorobenzene-d4 | 8.16 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2 | 029490-19-5 | 14 |
| 2 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 14 |
| 3 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 14 |
| 4 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 14 |
| 5 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 14 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG062716\
Data File : BG022646.D
Acq On : 27 Jun 2016 17:01
Operator : UM/SJ
Sample : H3630-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B1409-TPGW04-0616

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

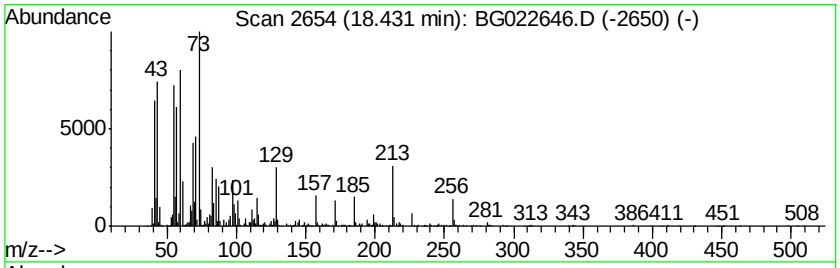
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

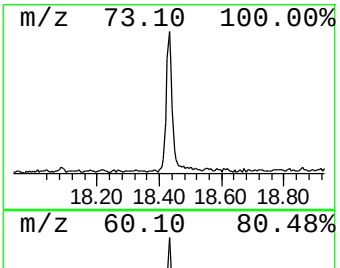
**********

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.43 | 9.12 ng | 1309250 | Phenanthrene-d10 | 17.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 86 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 76 |
| 4 | l-(+)-Ascorbic acid 2,6-dihexade... | 652 | C38H68O8 | 028474-90-0 | 64 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 50 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG062716\
Data File : BG022646.D
Acq On : 27 Jun 2016 17:01
Operator : UM/SJ
Sample : H3630-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B1409-TPGW04-0616

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

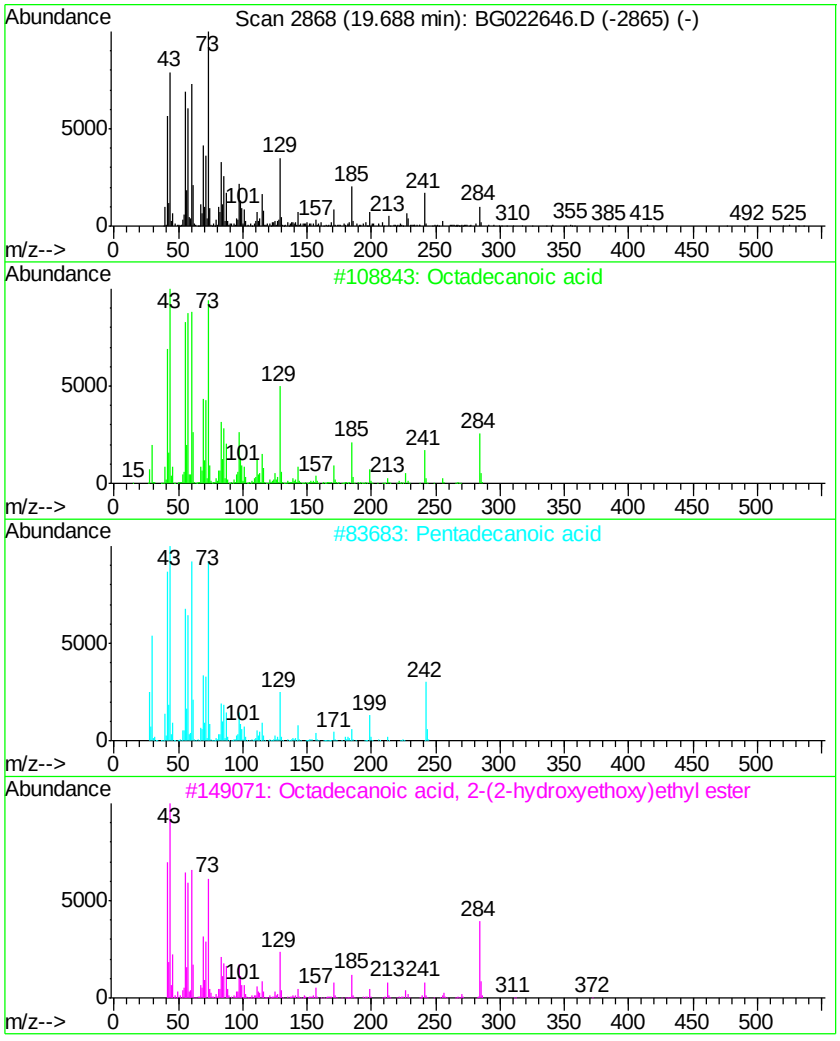
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

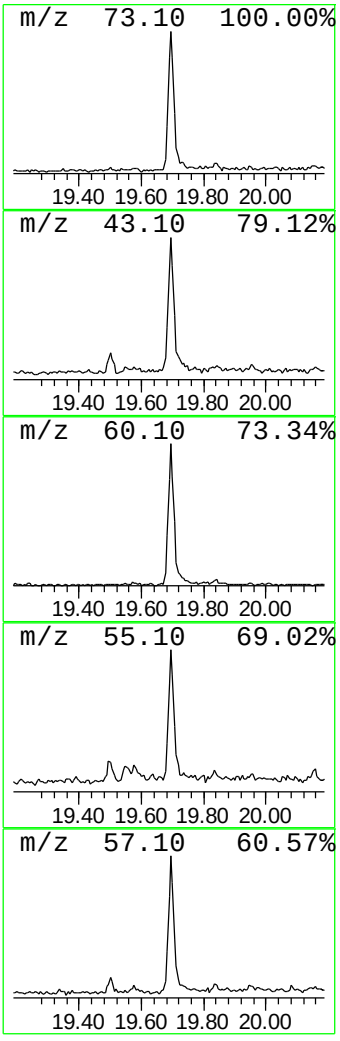
**********

Peak Number 7 Octadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.69 | 13.40 ng | 1923730 | Phenanthrene-d10 | 17.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 91 |
| 3 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 86 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 83 |
| 5 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 74 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062716\
Data File : BG022646.D
Acq On : 27 Jun 2016 17:01
Operator : UM/SJ
Sample : H3630-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B1409-TPGW04-0616

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.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 |
| 3-Penten-2-one, 4... | 4.63 | 36.9 | ng | 1790390 | 1 | 8.16 | 970294 | 20.0 |
| Cyclotrisiloxane,... | 4.75 | 2.4 | ng | 118097 | 1 | 8.16 | 970294 | 20.0 |
| 2-Pentanone, 4-hy... | 5.23 | 5.4 | ng | 260467 | 1 | 8.16 | 970294 | 20.0 |
| unknown7.69 | 7.69 | 66.0 | ng | 3201770 | 1 | 8.16 | 970294 | 20.0 |
| n-Hexadecanoic acid | 18.43 | 9.1 | ng | 1309250 | 4 | 17.56 | 2870390 | 20.0 |
| Octadecanoic acid | 19.69 | 13.4 | ng | 1923730 | 4 | 17.56 | 2870390 | 20.0 |