LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011623\
Data File : BG056300.D
Acq On : 16 Jan 2023 17:28
Operator : CG/JU
Sample : 01133-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** COMPOSITE-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_G\Methods\8270-BG122722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056300.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.334 | 3 | 8 | 22 | rVB | 154924 | 234313 | 8.39% | 1.834% |
| 2 | 5.355 | 346 | 352 | 362 | rVB | 129975 | 193071 | 6.91% | 1.511% |
| 3 | 5.831 | 426 | 433 | 447 | rBV | 526045 | 836562 | 29.94% | 6.547% |
| 4 | 7.447 | 699 | 708 | 718 | rBV | 511993 | 894808 | 32.03% | 7.002% |
| 5 | 8.316 | 848 | 856 | 866 | rBB | 124479 | 212379 | 7.60% | 1.662% |
| 6 | 9.486 | 1045 | 1055 | 1066 | rBB | 300667 | 533921 | 19.11% | 4.178% |
| 7 | 11.148 | 1331 | 1338 | 1345 | rBV | 161923 | 287717 | 10.30% | 2.252% |
| 8 | 13.551 | 1738 | 1747 | 1754 | rBV | 1000909 | 1561715 | 55.90% | 12.221% |
| 9 | 14.926 | 1974 | 1981 | 1988 | rVB | 306068 | 484254 | 17.33% | 3.790% |
| 10 | 16.266 | 2203 | 2209 | 2215 | rBV | 249977 | 348956 | 12.49% | 2.731% |
| 11 | 16.401 | 2226 | 2232 | 2245 | rBV | 829921 | 1287973 | 46.10% | 10.079% |
| 12 | 17.664 | 2440 | 2447 | 2458 | rVB | 441938 | 675171 | 24.17% | 5.284% |
| 13 | 18.510 | 2582 | 2591 | 2599 | rBV | 103359 | 153438 | 5.49% | 1.201% |
| 14 | 18.928 | 2658 | 2662 | 2666 | rVB4 | 22833 | 30038 | 1.08% | 0.235% |
| 15 | 19.762 | 2800 | 2804 | 2811 | rBV6 | 26197 | 36920 | 1.32% | 0.289% |
| 16 | 20.050 | 2845 | 2853 | 2859 | rBV3 | 21961 | 47030 | 1.68% | 0.368% |
| 17 | 20.238 | 2879 | 2885 | 2892 | rVB | 2205578 | 2793765 | 100.00% | 21.863% |
| 18 | 20.678 | 2957 | 2960 | 2965 | rVB2 | 20053 | 29022 | 1.04% | 0.227% |
| 19 | 21.542 | 3102 | 3107 | 3115 | rBV2 | 74924 | 129808 | 4.65% | 1.016% |
| 20 | 21.959 | 3171 | 3178 | 3184 | rVB2 | 434619 | 768306 | 27.50% | 6.012% |
| 21 | 23.164 | 3379 | 3383 | 3389 | rVB6 | 24786 | 44892 | 1.61% | 0.351% |
| 22 | 23.710 | 3469 | 3476 | 3483 | rVB | 131183 | 257210 | 9.21% | 2.013% |
| 23 | 25.396 | 3754 | 3763 | 3776 | rVB2 | 261000 | 825869 | 29.56% | 6.463% |
| 24 | 27.835 | 4171 | 4178 | 4188 | rVB2 | 32208 | 111524 | 3.99% | 0.873% |

Sum of corrected areas: 12778662

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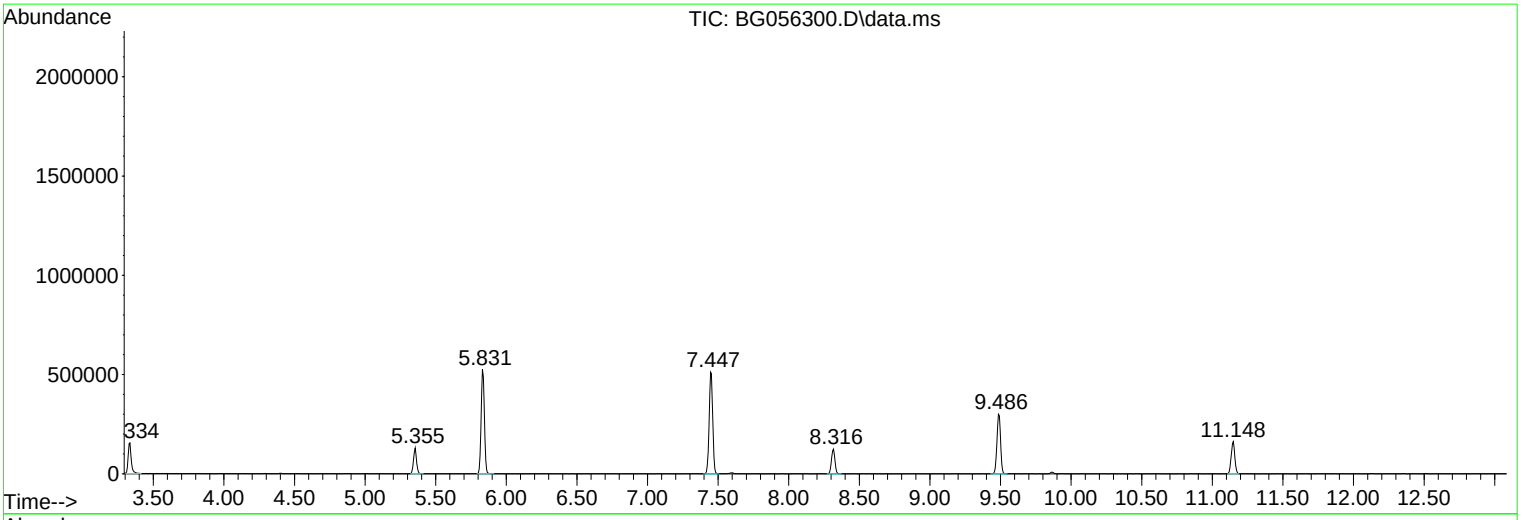
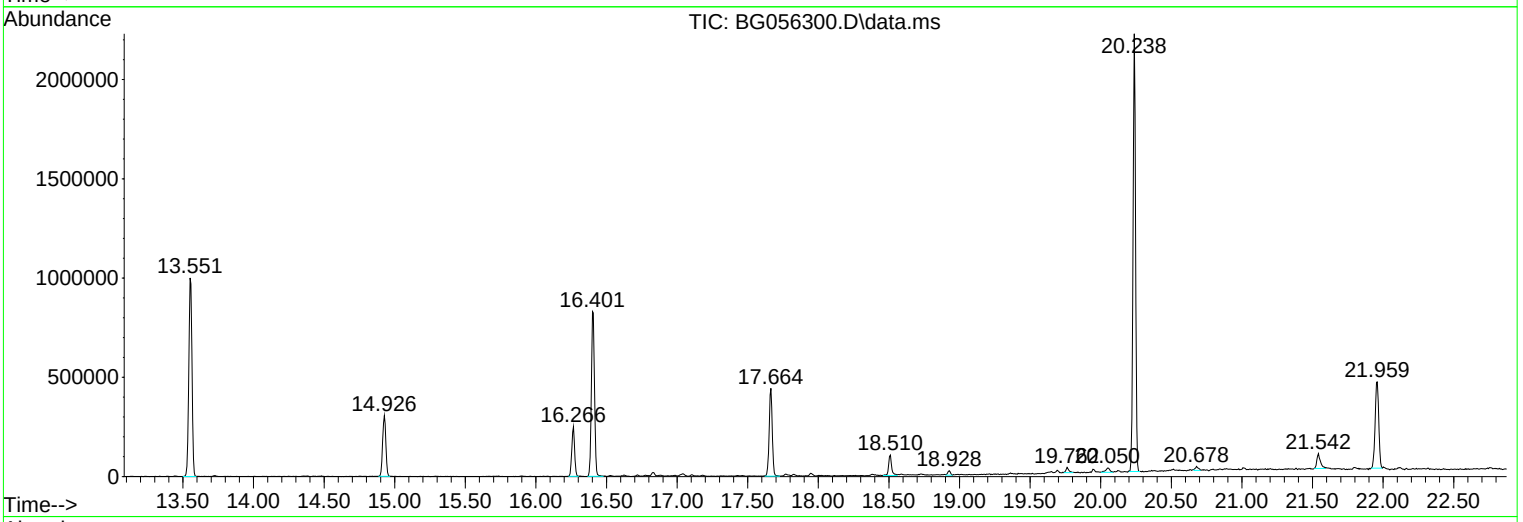
Sample : 01133-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

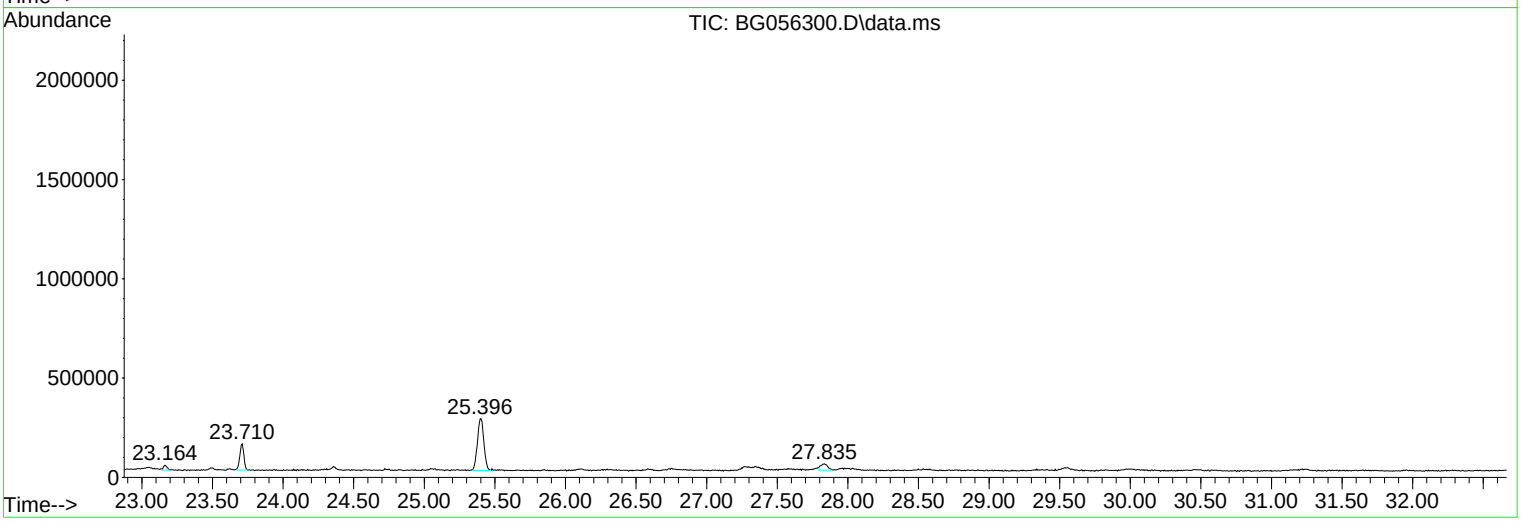
**Instrument :**
BNA_G
**ClientSampleId :**
COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011623\
Data File : BG056300.D
Acq On : 16 Jan 2023 17:28
Operator : CG/JU
Sample : 01133-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
COMPOSITE-1

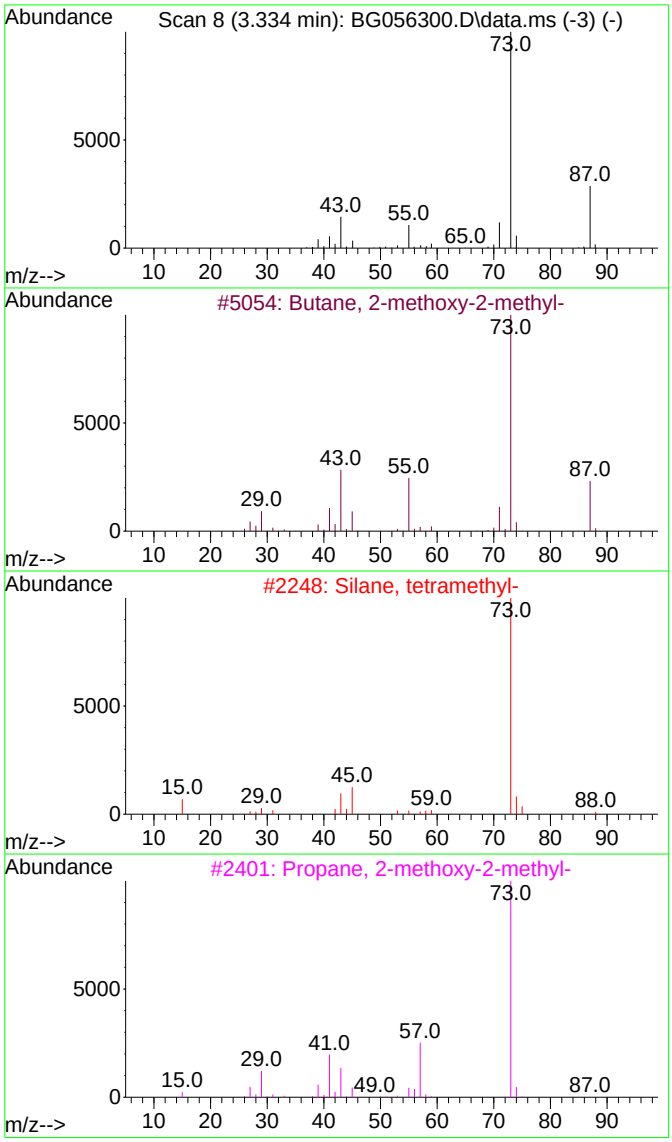
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

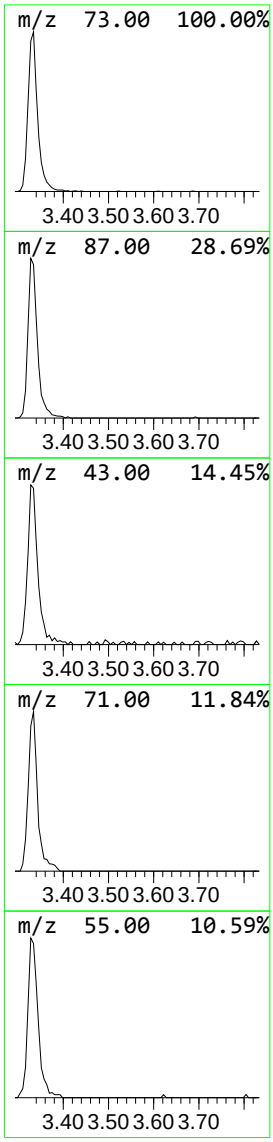
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.334 | 22.07 ng | 234313 | 1,4-Dichlorobenzene-d4 | 8.316 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 78 |
| 2 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 9 |
| 3 | Propane, 2-methoxy-2-methyl- | 88 | C5H12O | 001634-04-4 | 9 |
| 4 | 1,3-Dioxolane, 2-propyl- | 116 | C6H12O2 | 003390-13-4 | 9 |
| 5 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011623\
Data File : BG056300.D
Acq On : 16 Jan 2023 17:28
Operator : CG/JU
Sample : 01133-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
COMPOSITE-1

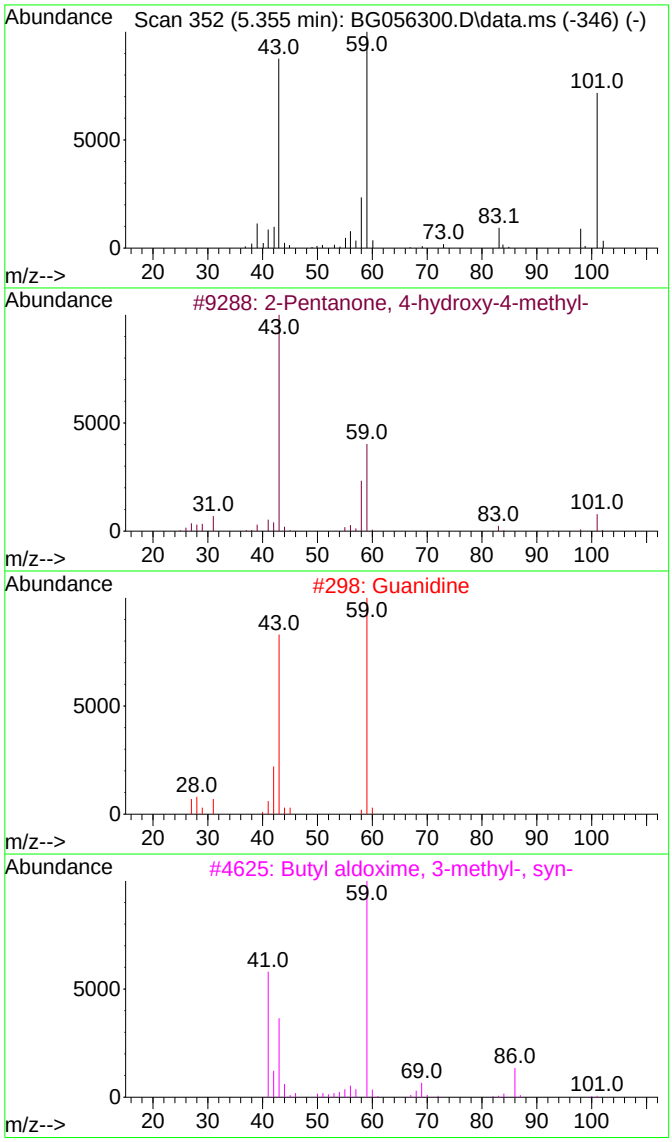
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

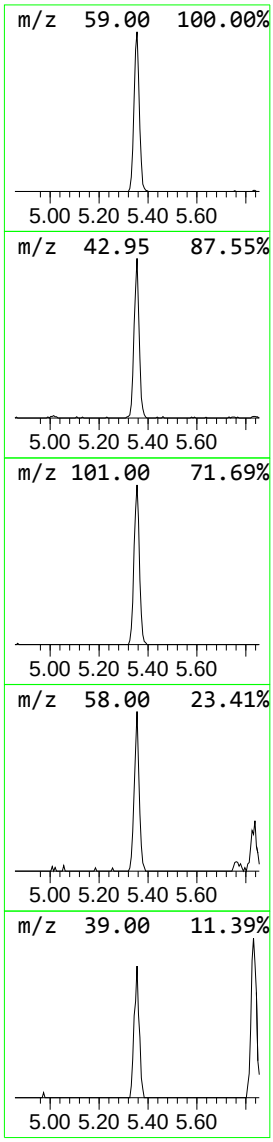
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.355 | 18.18 ng | 193071 | 1,4-Dichlorobenzene-d4 | 8.316 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 45 |
| 2 | Guanidine | 59 | CH5N3 | 000113-00-8 | 37 |
| 3 | Butyl aldoxime, 3-methyl-, syn- | 101 | C5H11NO | 005780-40-5 | 35 |
| 4 | 3-Heptanol, 4-methyl- | 130 | C8H18O | 014979-39-6 | 33 |
| 5 | Oxirane, tetramethyl- | 100 | C6H12O | 005076-20-0 | 25 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011623\
Data File : BG056300.D
Acq On : 16 Jan 2023 17:28
Operator : CG/JU
Sample : 01133-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

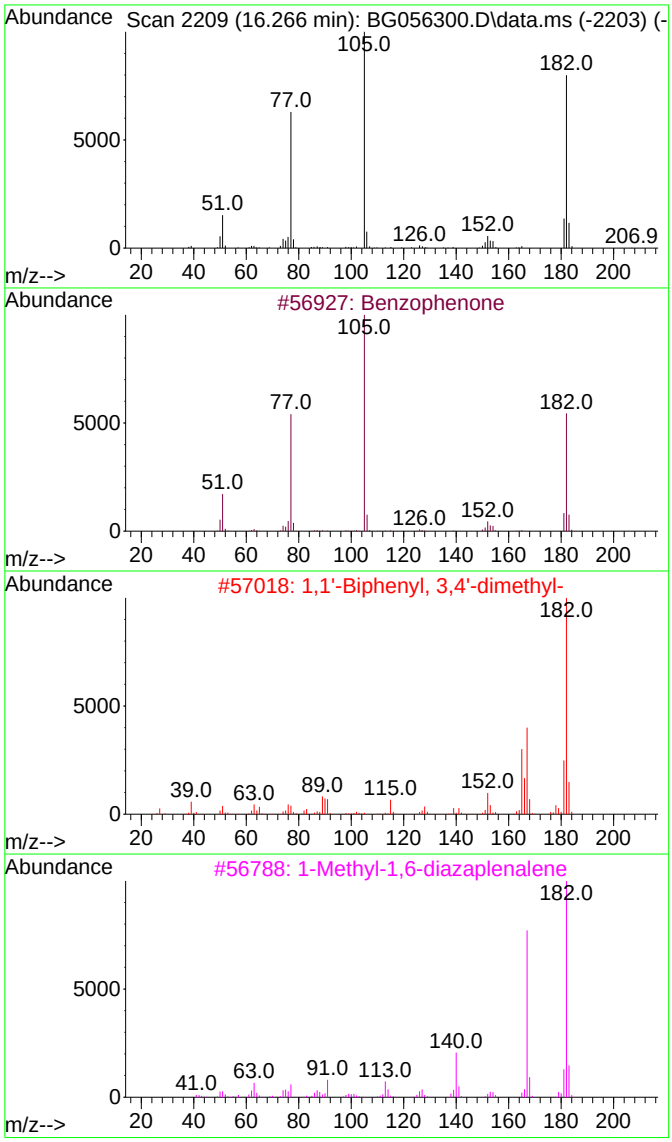
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

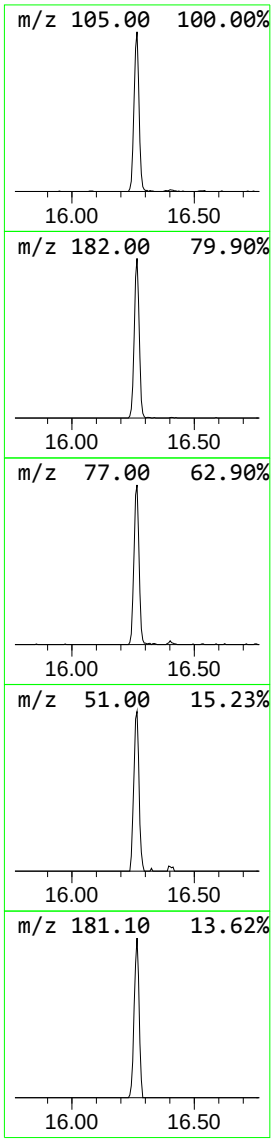
**********

Peak Number 3 Benzophenone Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.266 | 14.41 ng | 348956 | Acenaphthene-d10 | 14.926 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 94 |
| 2 | 1,1'-Biphenyl, 3,4'-dimethyl- | 182 | C14H14 | 007383-90-6 | 49 |
| 3 | 1-Methyl-1,6-diazaplenalene | 182 | C12H10N2 | 079691-99-9 | 43 |
| 4 | 2-Methyl-1H-perimidine | 182 | C12H10N2 | 005157-10-8 | 43 |
| 5 | 3,4-Dimethoxy-5-hydroxybenzaldehyde | 182 | C9H10O4 | 029865-90-5 | 43 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011623\
Data File : BG056300.D
Acq On : 16 Jan 2023 17:28
Operator : CG/JU
Sample : 01133-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

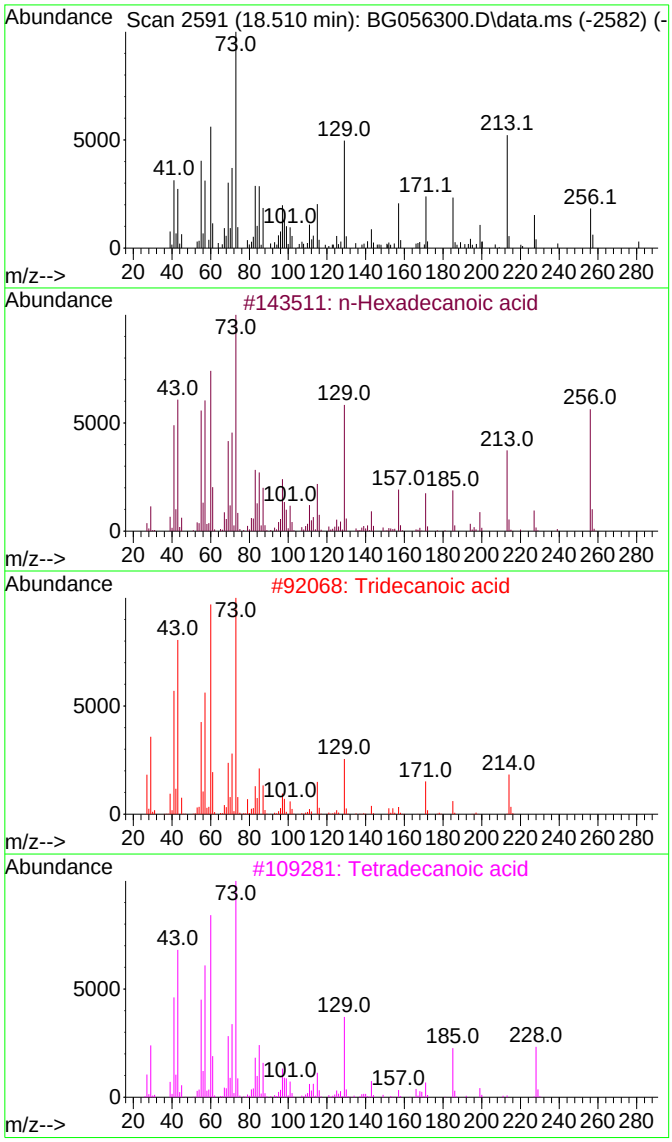
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

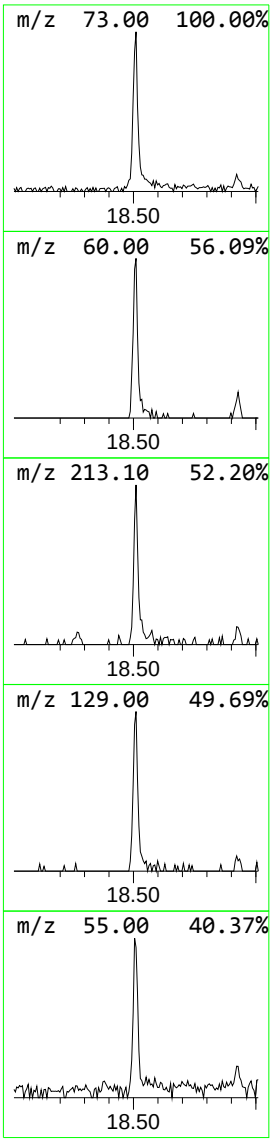
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.510 | 4.55 ng | 153438 | Phenanthrene-d10 | 17.664 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 95 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 92 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 91 |
| 4 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 45 |
| 5 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 38 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011623\
Data File : BG056300.D
Acq On : 16 Jan 2023 17:28
Operator : CG/JU
Sample : 01133-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

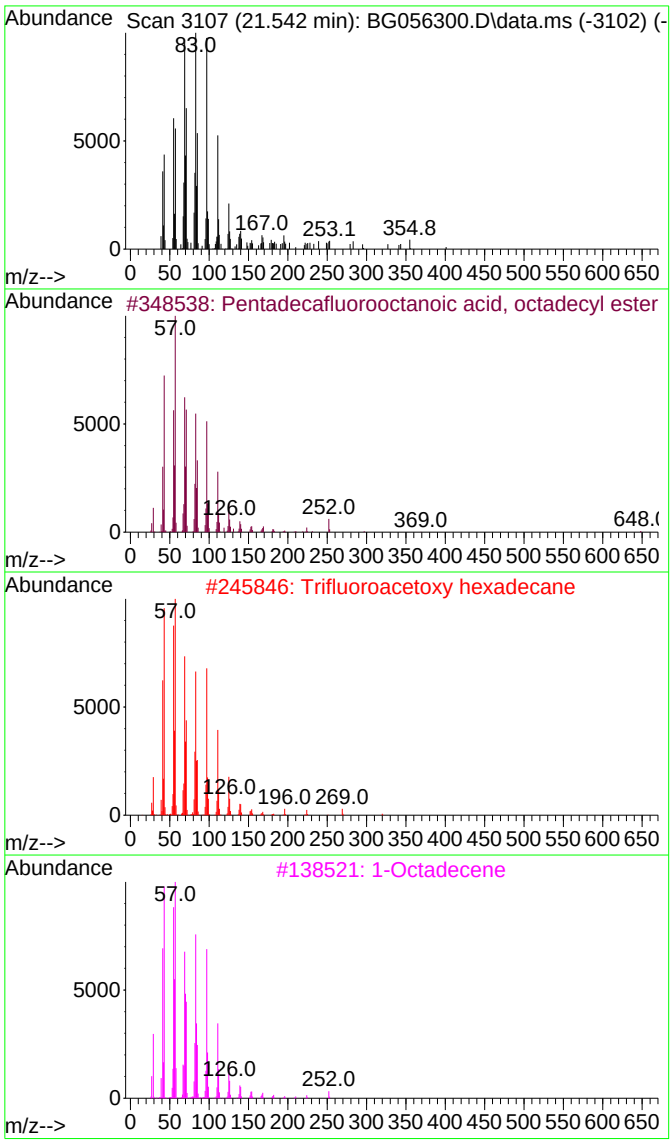
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

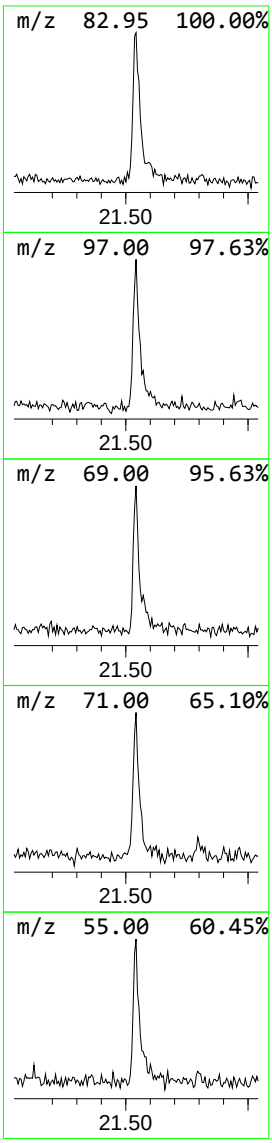
**********

Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.542 | 3.38 ng | 129808 | Chrysene-d12 | 21.959 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentadecafluorooctanoic acid, oc... | 666 | C26H37F15O2 | 1000406-04-8 | 87 |
| 2 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 87 |
| 3 | 1-Octadecene | 252 | C18H36 | 000112-88-9 | 78 |
| 4 | Cyclooctacosane | 392 | C28H56 | 000297-24-5 | 74 |
| 5 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 74 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011623\
Data File : BG056300.D
Acq On : 16 Jan 2023 17:28
Operator : CG/JU
Sample : 01133-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

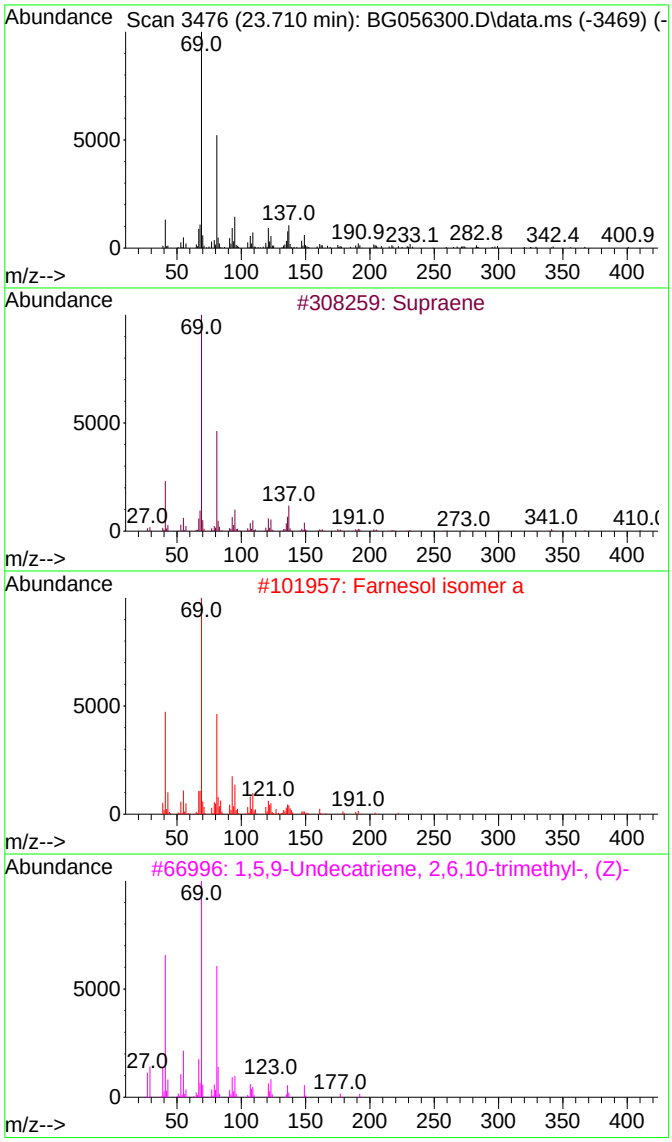
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

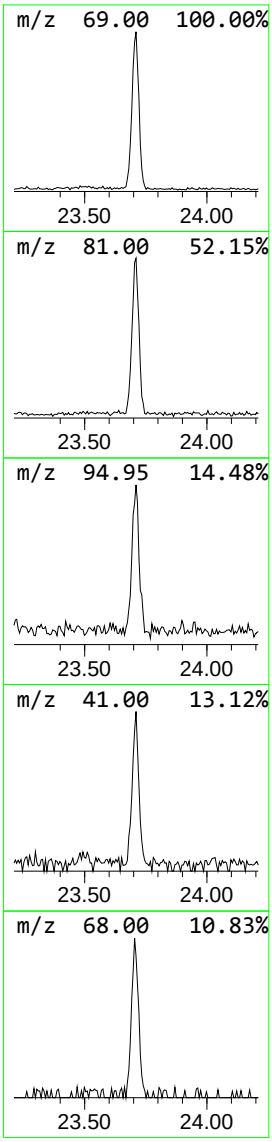
**********

Peak Number 6 Supraene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.710 | 6.23 ng | 257210 | Perylene-d12 | 25.402 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Supraene | 410 | C30H50 | 007683-64-9 | 91 |
| 2 | Farnesol isomer a | 222 | C15H26O | 1000108-92-4 | 83 |
| 3 | 1,5,9-Undecatriene, 2,6,10-trime... | 192 | C14H24 | 062951-96-6 | 80 |
| 4 | 1,5,9-Decatriene, 2,3,5,8-tetram... | 192 | C14H24 | 230646-72-7 | 74 |
| 5 | 2,6,10,14-Hexadecatetraenoic aci... | 332 | C22H36O2 | 024035-35-6 | 64 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011623\
Data File : BG056300.D
Acq On : 16 Jan 2023 17:28
Operator : CG/JU
Sample : 01133-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

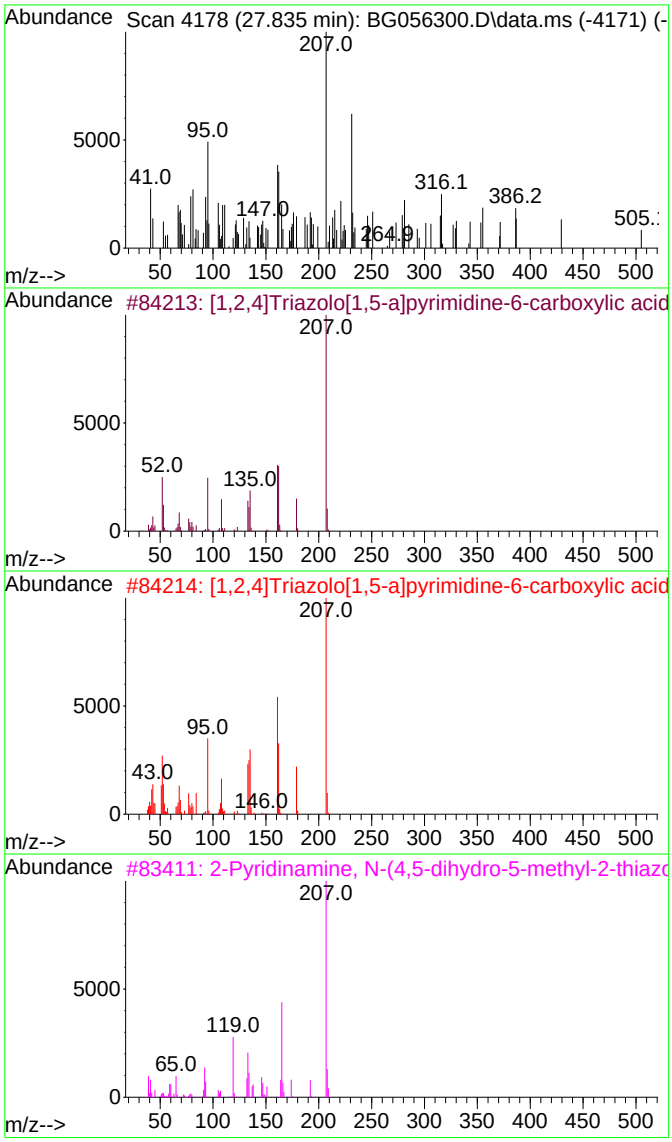
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

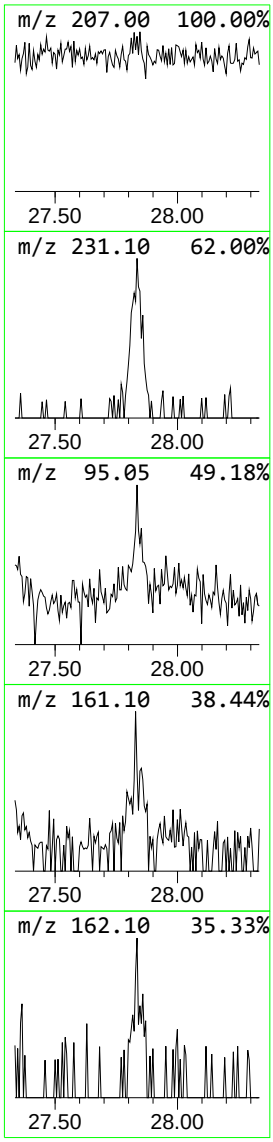
**********

Peak Number 7 unknown27.835 Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 27.835 | 2.70 ng | 111524 | Perylene-d12 | 25.402 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | [1,2,4]Triazolo[1,5-a]pyrimidine... | 207 | C8H9N5O2 | 092673-40-0 | 43 |
| 2 | [1,2,4]Triazolo[1,5-a]pyrimidine... | 207 | C8H9N5O2 | 1000351-62-2 | 38 |
| 3 | 2-Pyridinamine, N-(4,5-dihydro-5... | 207 | C10H13N3S | 1000362-45-9 | 18 |
| 4 | 2,3,4-Trimethoxyphenylacetonitrile | 207 | C11H13NO3 | 068913-85-9 | 18 |
| 5 | Phenol, 6-methyl-2-[(4-morpholin... | 207 | C12H17NO2 | 060460-71-1 | 14 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011623\
Data File : BG056300.D
Acq On : 16 Jan 2023 17:28
Operator : CG/JU
Sample : 01133-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-metho... | 3.334 | 22.1 | ng | 234313 | 1 | 8.316 | 212379 | 20.0 |
| 2-Pentanone, 4-... | 5.355 | 18.2 | ng | 193071 | 1 | 8.316 | 212379 | 20.0 |
| Benzophenone | 16.266 | 14.4 | ng | 348956 | 3 | 14.926 | 484254 | 20.0 |
| n-Hexadecanoic ... | 18.510 | 4.5 | ng | 153438 | 4 | 17.664 | 675171 | 20.0 |
| Pentadecafluoro... | 21.542 | 3.4 | ng | 129808 | 5 | 21.959 | 768306 | 20.0 |
| Supraene | 23.710 | 6.2 | ng | 257210 | 6 | 25.402 | 825869 | 20.0 |
| unknown27.835 | 27.835 | 2.7 | ng | 111524 | 6 | 25.402 | 825869 | 20.0 |