LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
Data File : BF140271.D
Acq On : 07 Nov 2024 13:33
Operator : RC/JU
Sample : P4718-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
WB-307-SB02

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-BF110524.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140271.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.152 | 4 | 10 | 24 | rVB | 1870938 | 3034273 | 78.12% | 10.047% |
| 2 | 2.263 | 24 | 29 | 45 | rVB | 52128 | 106866 | 2.75% | 0.354% |
| 3 | 5.093 | 499 | 510 | 525 | rBV | 429344 | 693416 | 17.85% | 2.296% |
| 4 | 5.493 | 572 | 578 | 583 | rBV | 2420566 | 3262416 | 83.99% | 10.802% |
| 5 | 5.893 | 641 | 646 | 654 | rVB | 41202 | 52420 | 1.35% | 0.174% |
| 6 | 6.498 | 742 | 749 | 754 | rBV | 2400763 | 3383033 | 87.10% | 11.201% |
| 7 | 6.875 | 808 | 813 | 818 | rBV | 621523 | 747533 | 19.25% | 2.475% |
| 8 | 7.434 | 902 | 908 | 913 | rBV | 1669482 | 2161700 | 55.65% | 7.158% |
| 9 | 8.157 | 1025 | 1031 | 1046 | rVB | 746699 | 970018 | 24.97% | 3.212% |
| 10 | 8.369 | 1063 | 1067 | 1070 | rBV | 31261 | 44488 | 1.15% | 0.147% |
| 11 | 9.233 | 1207 | 1214 | 1219 | rBV | 2979779 | 3884222 | 100.00% | 12.861% |
| 12 | 9.910 | 1324 | 1329 | 1342 | rVB | 860195 | 1115525 | 28.72% | 3.694% |
| 13 | 10.322 | 1375 | 1399 | 1401 | rBV2 | 21139 | 106099 | 2.73% | 0.351% |
| 14 | 10.628 | 1446 | 1451 | 1458 | rBV | 386506 | 472958 | 12.18% | 1.566% |
| 15 | 10.704 | 1458 | 1464 | 1479 | rBV | 2067895 | 2676150 | 68.90% | 8.861% |
| 16 | 11.404 | 1577 | 1583 | 1589 | rBV | 916856 | 1170394 | 30.13% | 3.875% |
| 17 | 11.469 | 1590 | 1594 | 1598 | rVB3 | 47286 | 57221 | 1.47% | 0.189% |
| 18 | 11.933 | 1667 | 1673 | 1696 | rBV | 374933 | 633879 | 16.32% | 2.099% |
| 19 | 12.716 | 1802 | 1806 | 1817 | rBV2 | 39006 | 75230 | 1.94% | 0.249% |
| 20 | 12.992 | 1847 | 1853 | 1858 | rBV | 2946491 | 3836198 | 98.76% | 12.702% |
| 21 | 13.904 | 2002 | 2008 | 2027 | rBV | 73524 | 193068 | 4.97% | 0.639% |
| 22 | 14.051 | 2028 | 2033 | 2042 | rVB | 606825 | 802585 | 20.66% | 2.657% |
| 23 | 15.557 | 2283 | 2289 | 2300 | rBV | 451949 | 722116 | 18.59% | 2.391% |

Sum of corrected areas: 30201808

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**ClientSampleId :**
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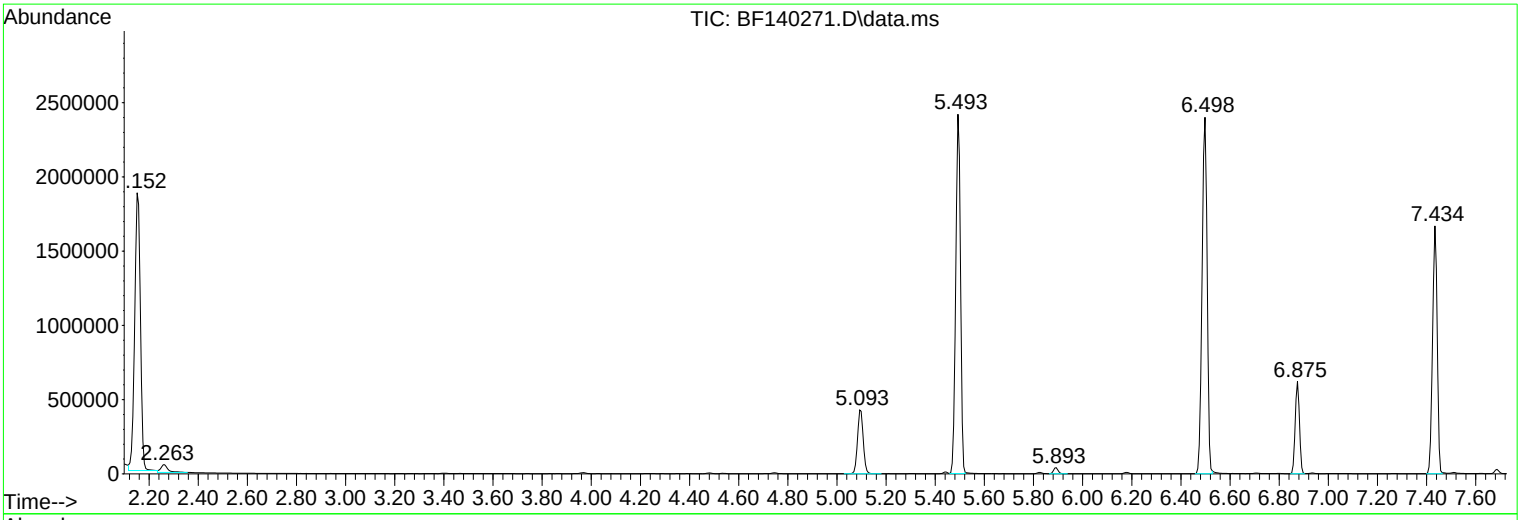
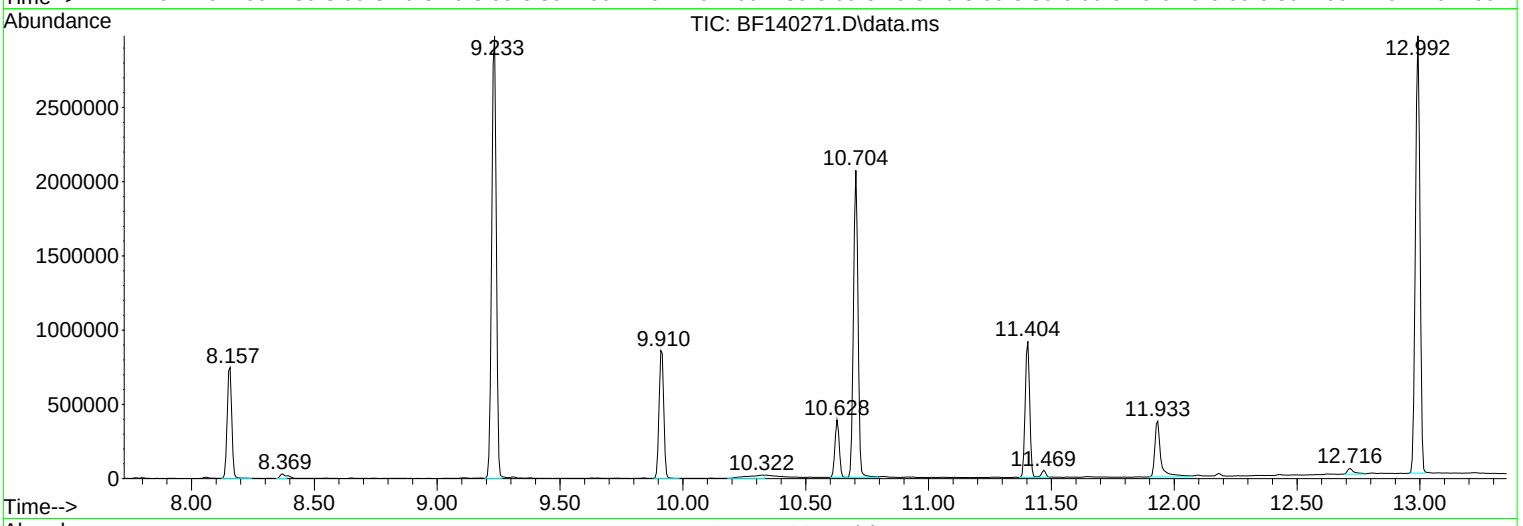
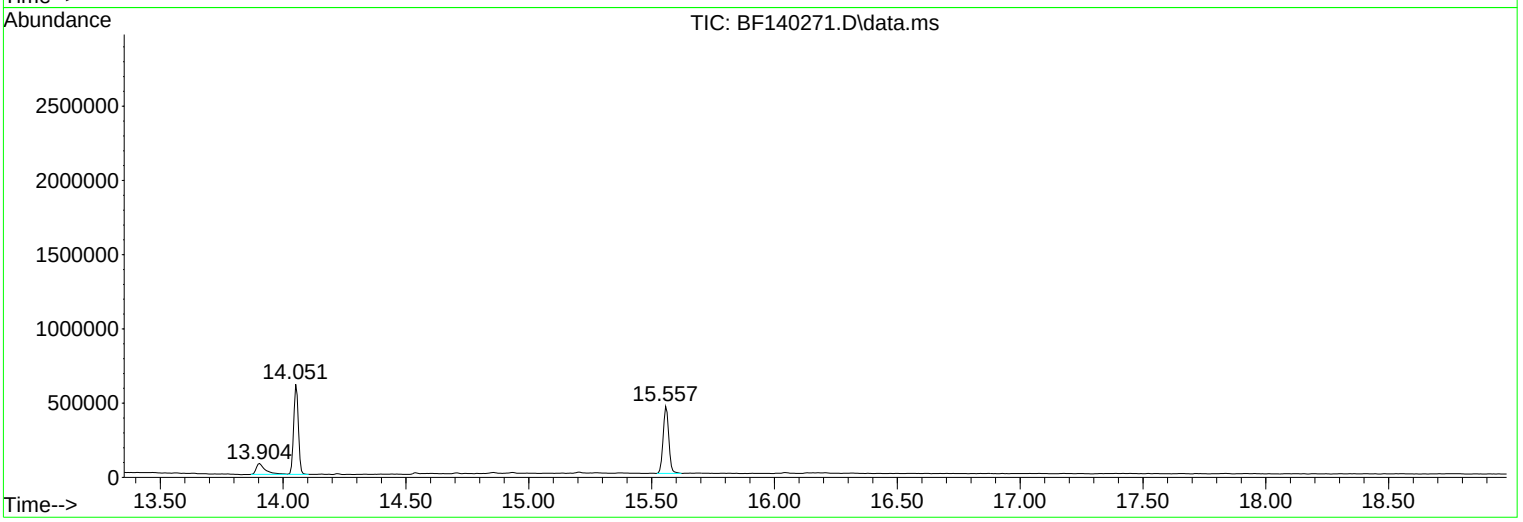
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

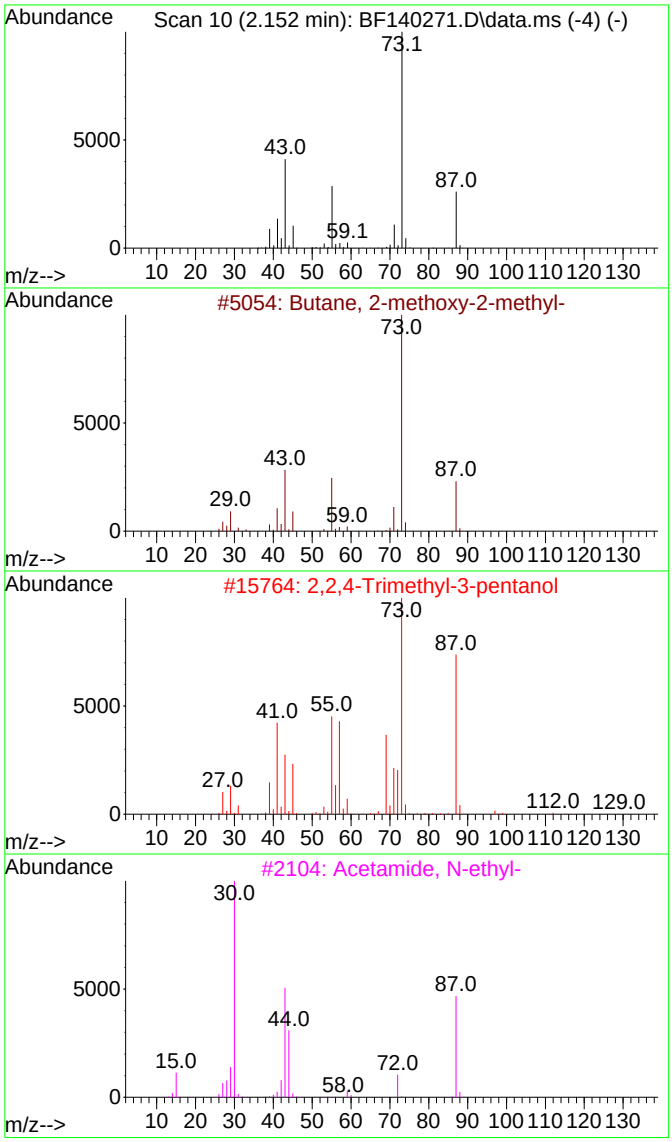
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

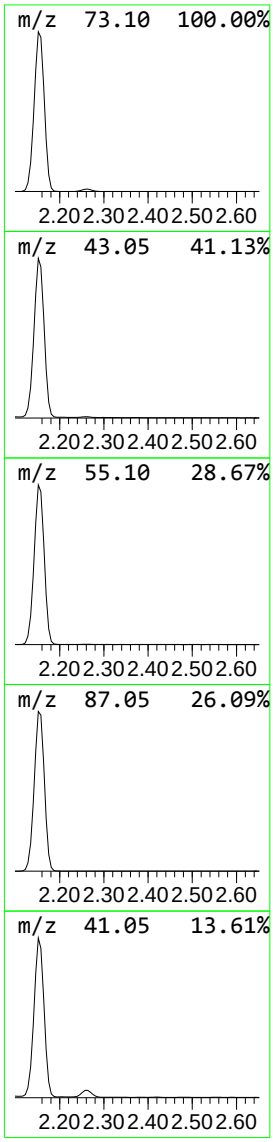
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.152 | 81.18 ng | 3034270 | 1,4-Dichlorobenzene-d4 | 6.875 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 39 |
| 3 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 27 |
| 4 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 25 |
| 5 | Octanal, 7-methoxy-3,7-dimethyl- | 186 | C11H22O2 | 003613-30-7 | 17 |



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Data File : BF140271.D
Acq On : 07 Nov 2024 13:33
Operator : RC/JU
Sample : P4718-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
WB-307-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

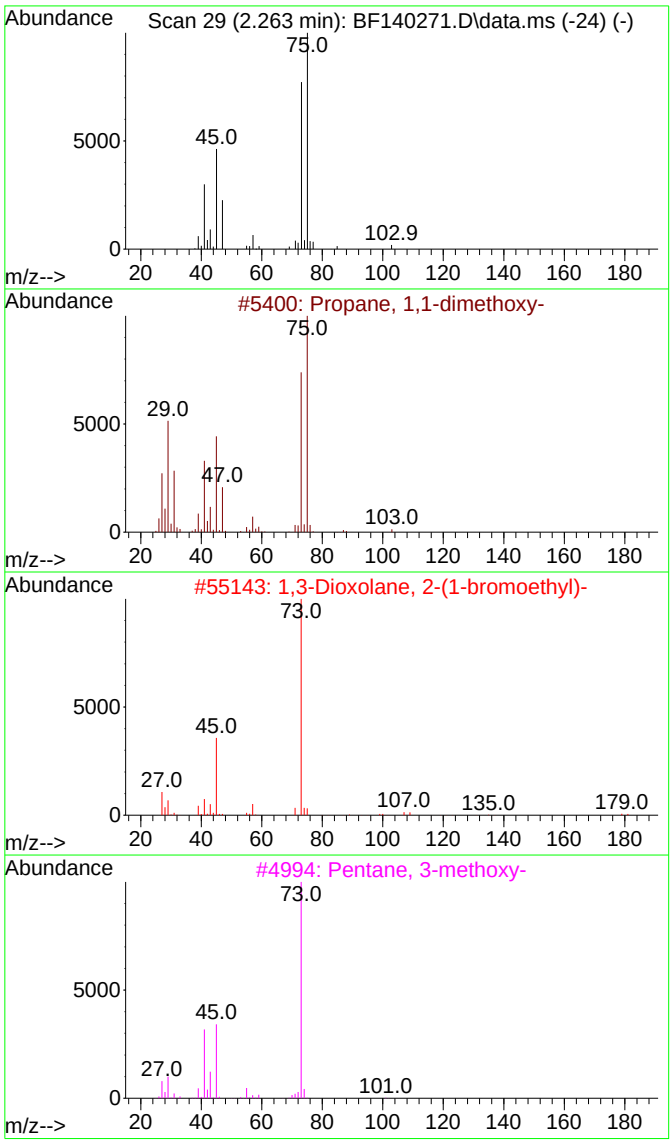
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

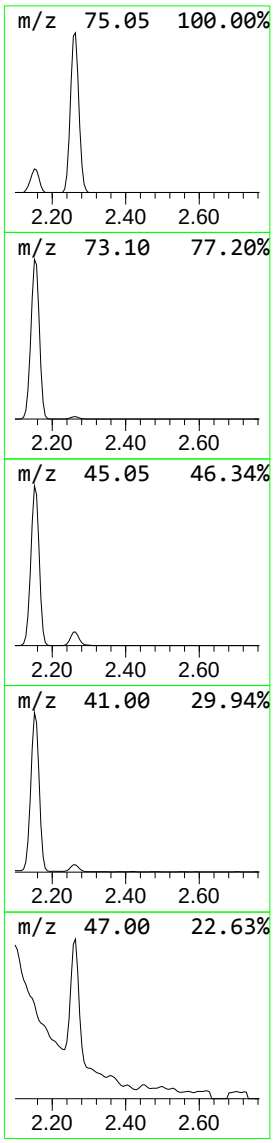
**********

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.263 | 2.86 ng | 106866 | 1,4-Dichlorobenzene-d4 | 6.875 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 1,1-dimethoxy- | 104 | C5H12O2 | 004744-10-9 | 83 |
| 2 | 1,3-Dioxolane, 2-(1-bromoethyl)- | 180 | C5H9BrO2 | 005267-73-2 | 27 |
| 3 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 27 |
| 4 | Methane, isothiocyanato- | 73 | C2H3NS | 000556-61-6 | 9 |
| 5 | 1-Cyclohexyl-3-ethoxy-butan-2-one | 198 | C12H22O2 | 074897-69-1 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
Data File : BF140271.D
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Operator : RC/JU
Sample : P4718-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
WB-307-SB02

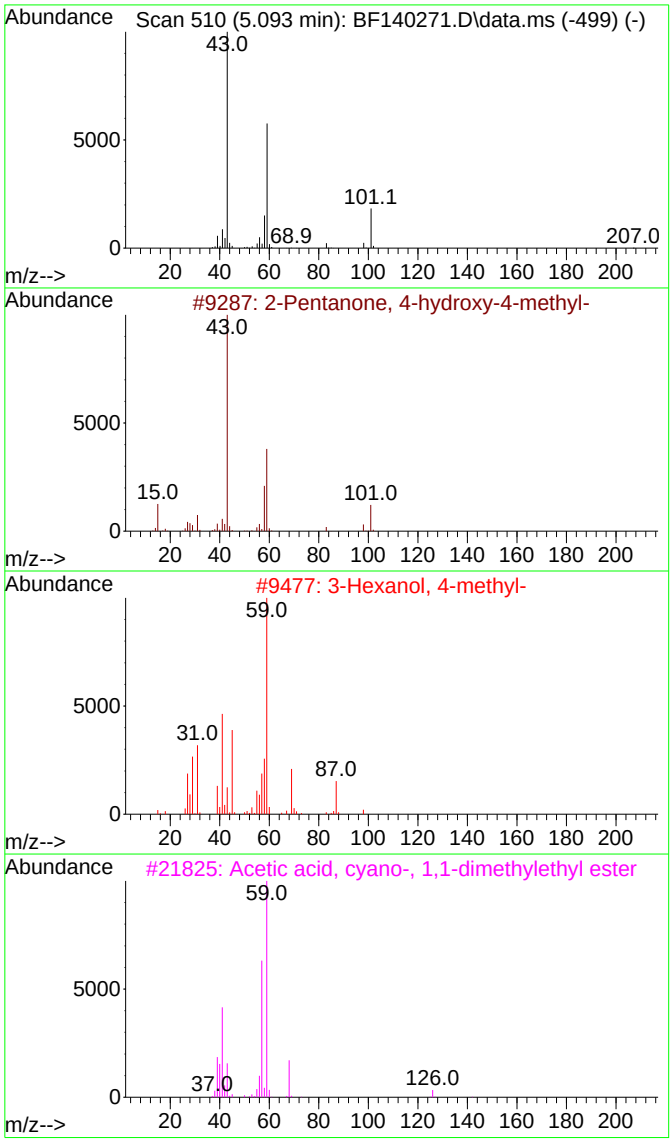
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

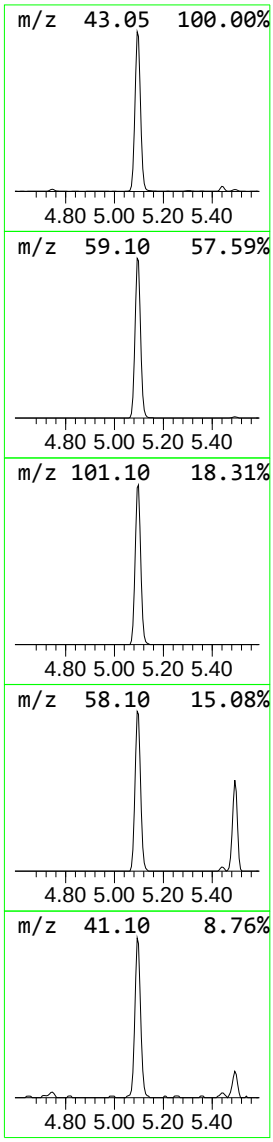
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.093 | 18.55 ng | 693416 | 1,4-Dichlorobenzene-d4 | 6.875 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 4 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 12 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |



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Operator : RC/JU
Sample : P4718-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
WB-307-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

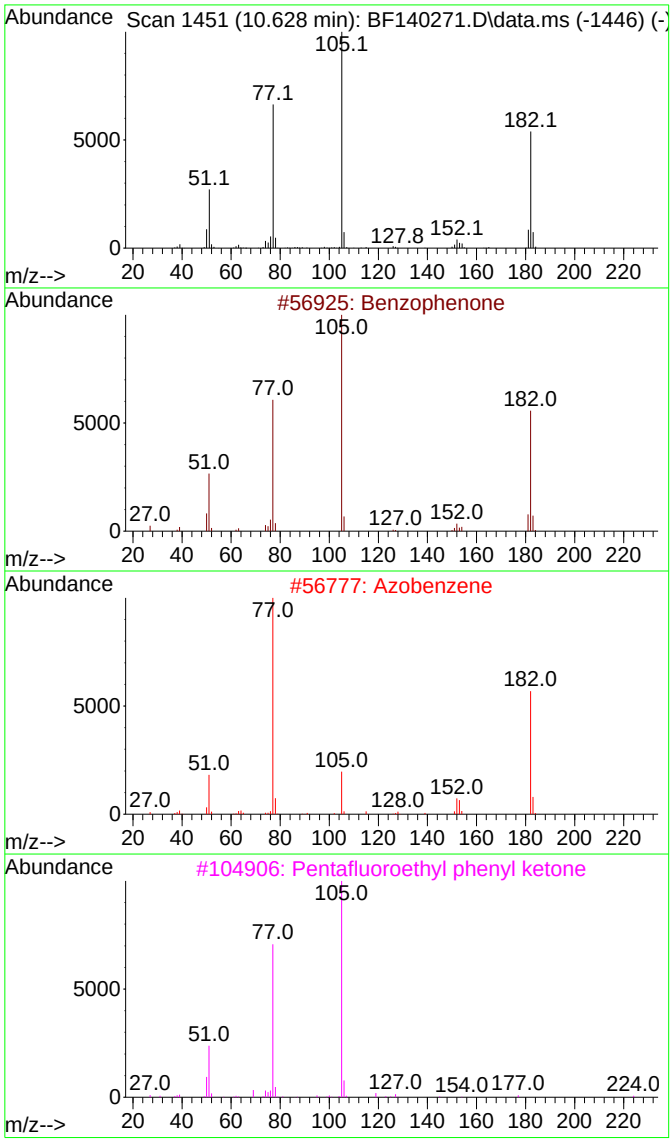
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

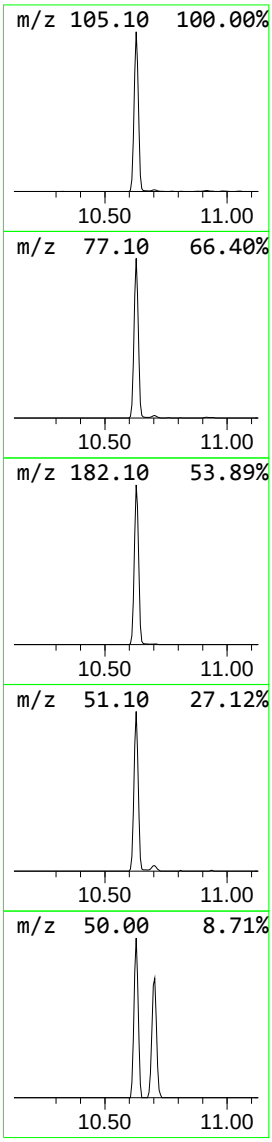
**********

Peak Number 4 Benzophenone Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.628 | 8.48 ng | 472958 | Acenaphthene-d10 | 9.910 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 96 |
| 2 | Azobenzene | 182 | C12H10N2 | 000103-33-3 | 64 |
| 3 | Pentafluoroethyl phenyl ketone | 224 | C9H5F5O | 000394-52-5 | 47 |
| 4 | Benzilamide | 227 | C14H13NO2 | 004746-87-6 | 47 |
| 5 | Benzenebutanoic acid, .gamma.-oxo- | 178 | C10H10O3 | 002051-95-8 | 47 |



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Operator : RC/JU
Sample : P4718-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
WB-307-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

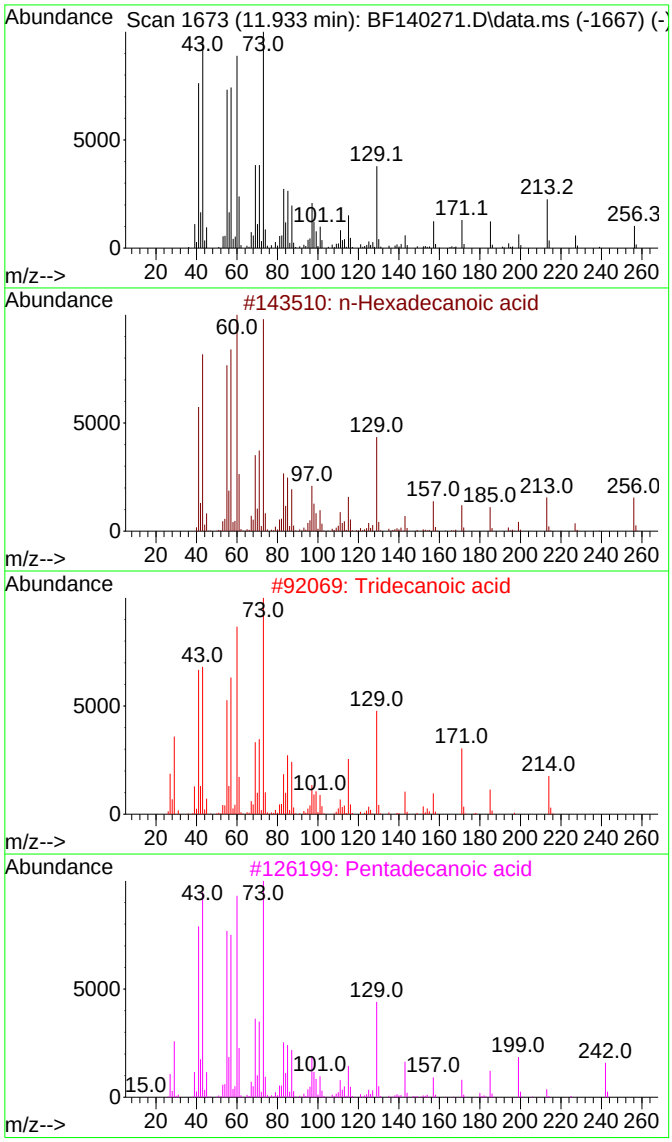
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

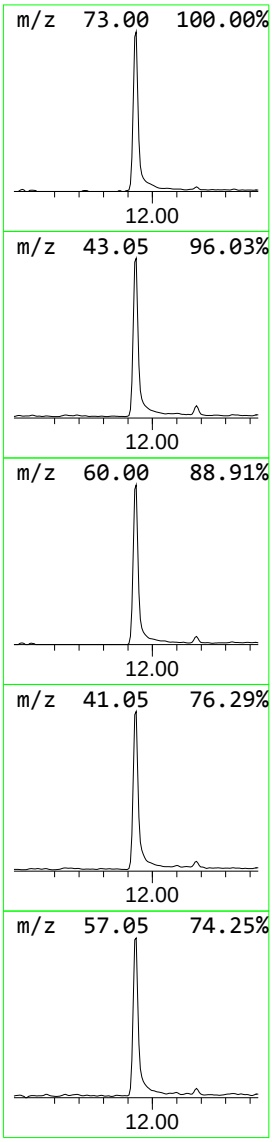
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.933 | 10.83 ng | 633879 | Phenanthrene-d10 | 11.404 |

| 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 | 95 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 91 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 74 |



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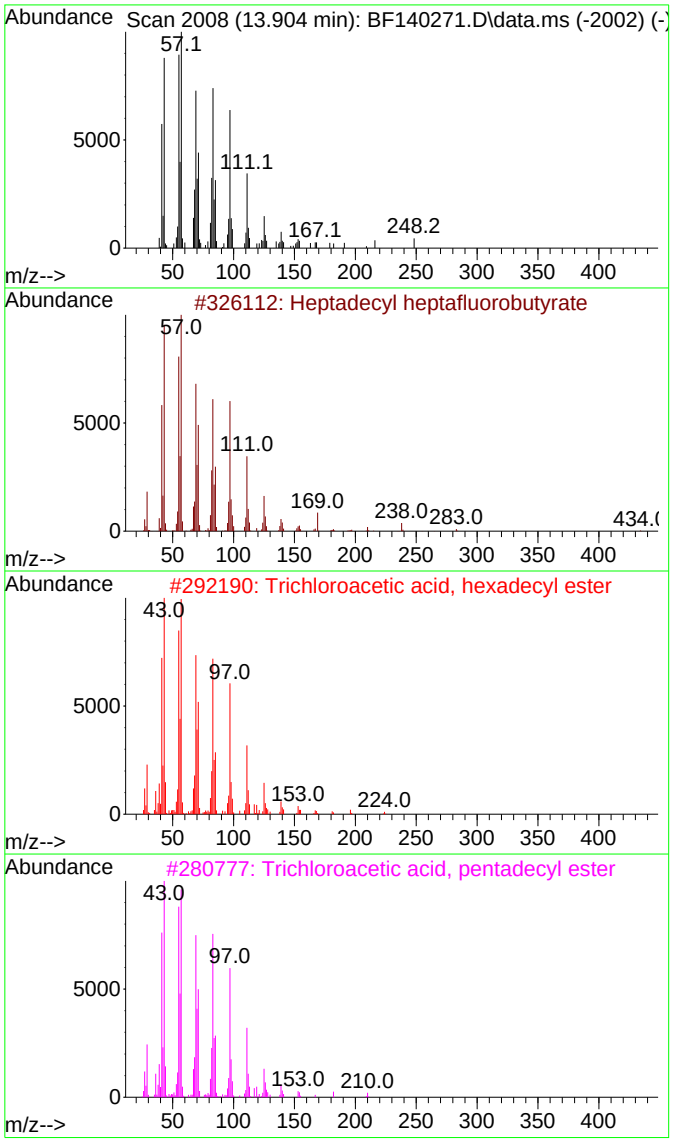
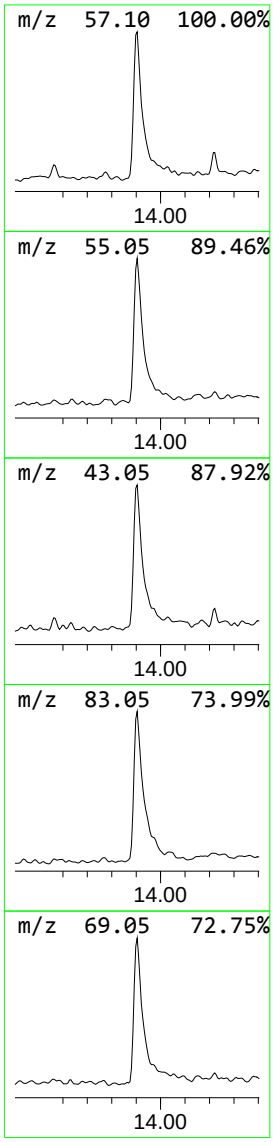
**********
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.904 | 4.81 ng | 193068 | Chrysene-d12 | 14.051 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 95 |
| 2 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94 |
| 3 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 94 |
| 4 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 93 |
| 5 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 93 |



Tentatively Identified Compound (LSC) summary

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| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-metho... | 2.152 | 81.2 | ng | 3034270 | 1 | 6.875 | 747533 | 20.0 |
| Propane, 1,1-di... | 2.263 | 2.9 | ng | 106866 | 1 | 6.875 | 747533 | 20.0 |
| 2-Pentanone, 4-... | 5.093 | 18.6 | ng | 693416 | 1 | 6.875 | 747533 | 20.0 |
| Benzophenone | 10.628 | 8.5 | ng | 472958 | 3 | 9.910 | 1115530 | 20.0 |
| n-Hexadecanoic ... | 11.933 | 10.8 | ng | 633879 | 4 | 11.404 | 1170390 | 20.0 |
| Heptadecyl hept... | 13.904 | 4.8 | ng | 193068 | 5 | 14.051 | 802585 | 20.0 |