LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
Data File : BF133929.D
Acq On : 23 Jun 2023 06:18
Operator : CG\JU
Sample : 03320-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
WC-10

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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133929.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.163 | 6 | 13 | 19 | rVB | 168944 | 221777 | 8.55% | 1.198% |
| 2 | 4.487 | 404 | 408 | 413 | rBV | 33337 | 38770 | 1.50% | 0.209% |
| 3 | 5.098 | 507 | 512 | 523 | rBV | 810394 | 1056789 | 40.76% | 5.707% |
| 4 | 5.498 | 575 | 580 | 583 | rBV | 2470400 | 2238347 | 86.34% | 12.088% |
| 5 | 5.881 | 642 | 645 | 651 | rVB | 52177 | 43779 | 1.69% | 0.236% |
| 6 | 6.498 | 745 | 750 | 767 | rBV | 2207957 | 2321832 | 89.56% | 12.539% |
| 7 | 6.857 | 808 | 811 | 815 | rBV | 799370 | 638866 | 24.64% | 3.450% |
| 8 | 7.422 | 902 | 907 | 910 | rBV | 1704837 | 1497759 | 57.77% | 8.088% |
| 9 | 8.139 | 1025 | 1029 | 1032 | rBV | 900558 | 776235 | 29.94% | 4.192% |
| 10 | 9.216 | 1208 | 1212 | 1215 | rBV | 3217643 | 2592564 | 100.00% | 14.001% |
| 11 | 9.898 | 1324 | 1328 | 1331 | rBV | 891751 | 764952 | 29.51% | 4.131% |
| 12 | 10.610 | 1446 | 1449 | 1453 | rBV | 366210 | 329654 | 12.72% | 1.780% |
| 13 | 10.686 | 1458 | 1462 | 1473 | rBV | 1527372 | 1443723 | 55.69% | 7.797% |
| 14 | 10.922 | 1499 | 1502 | 1507 | rVB | 99362 | 79750 | 3.08% | 0.431% |
| 15 | 11.392 | 1578 | 1582 | 1585 | rBV | 751514 | 694518 | 26.79% | 3.751% |
| 16 | 11.916 | 1668 | 1671 | 1681 | rBV2 | 155467 | 174835 | 6.74% | 0.944% |
| 17 | 12.710 | 1803 | 1806 | 1810 | rBV2 | 41766 | 45964 | 1.77% | 0.248% |
| 18 | 12.869 | 1827 | 1833 | 1846 | rVB | 125656 | 257052 | 9.91% | 1.388% |
| 19 | 12.986 | 1849 | 1853 | 1857 | rBV | 2442745 | 2159603 | 83.30% | 11.662% |
| 20 | 13.898 | 2005 | 2008 | 2015 | rBV3 | 88711 | 184923 | 7.13% | 0.999% |
| 21 | 14.051 | 2030 | 2034 | 2038 | rVB | 590772 | 586493 | 22.62% | 3.167% |
| 22 | 15.557 | 2286 | 2290 | 2295 | rVB | 295020 | 369384 | 14.25% | 1.995% |

Sum of corrected areas: 18517569

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**ClientSampleId :**
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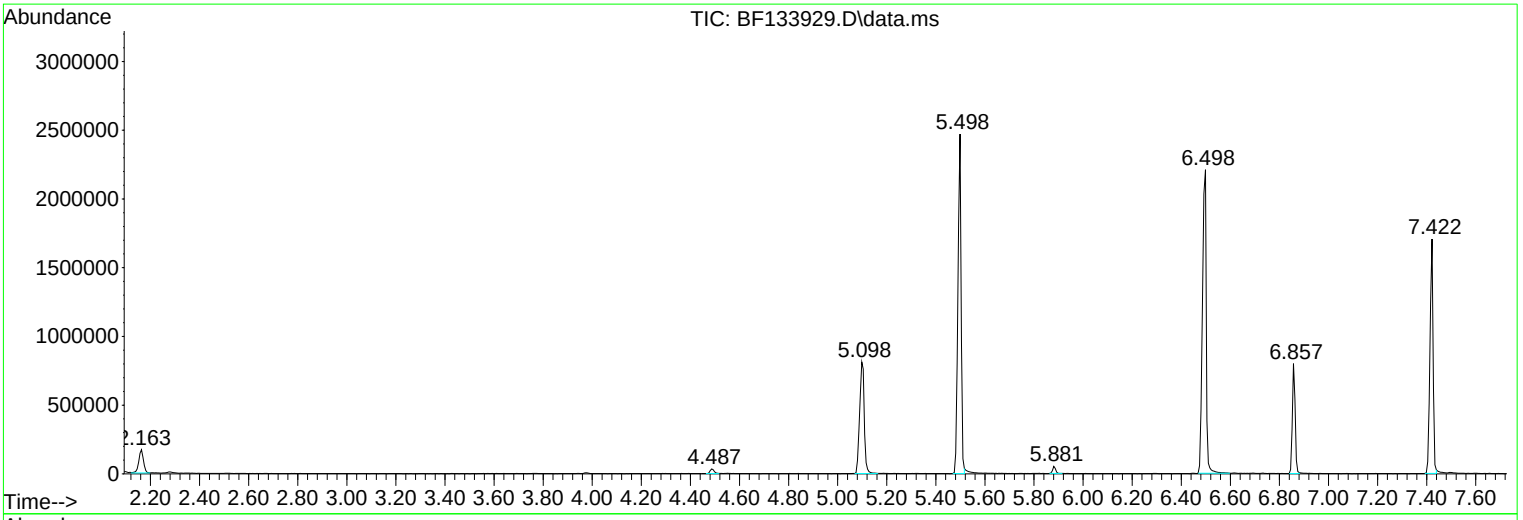
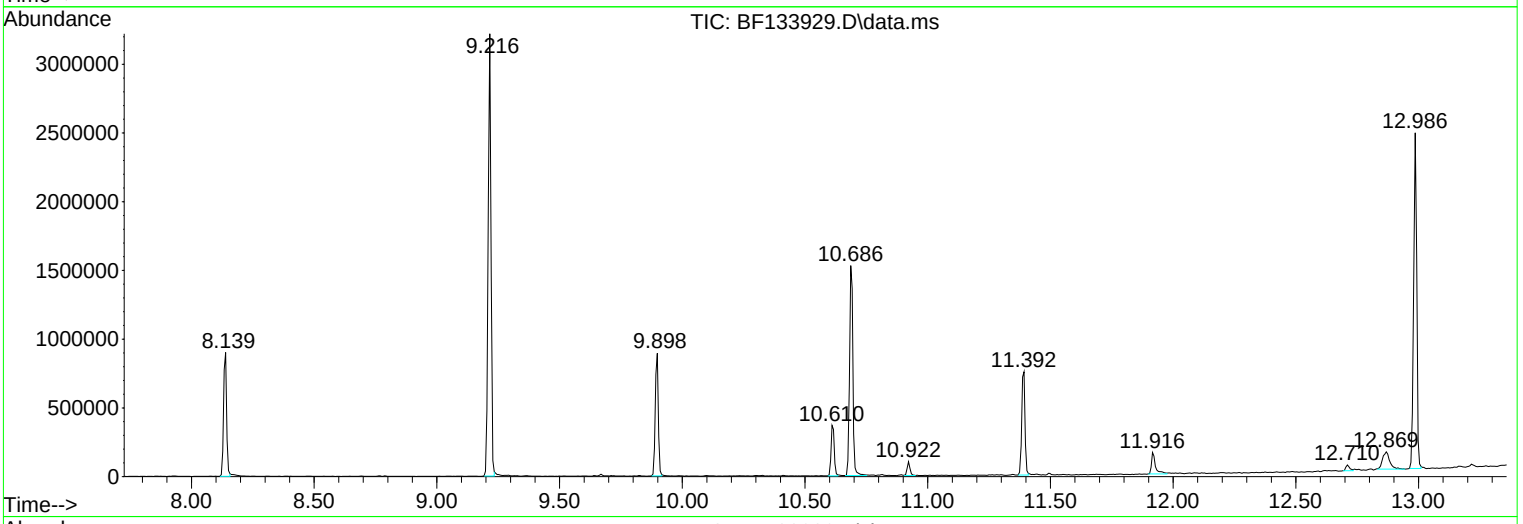
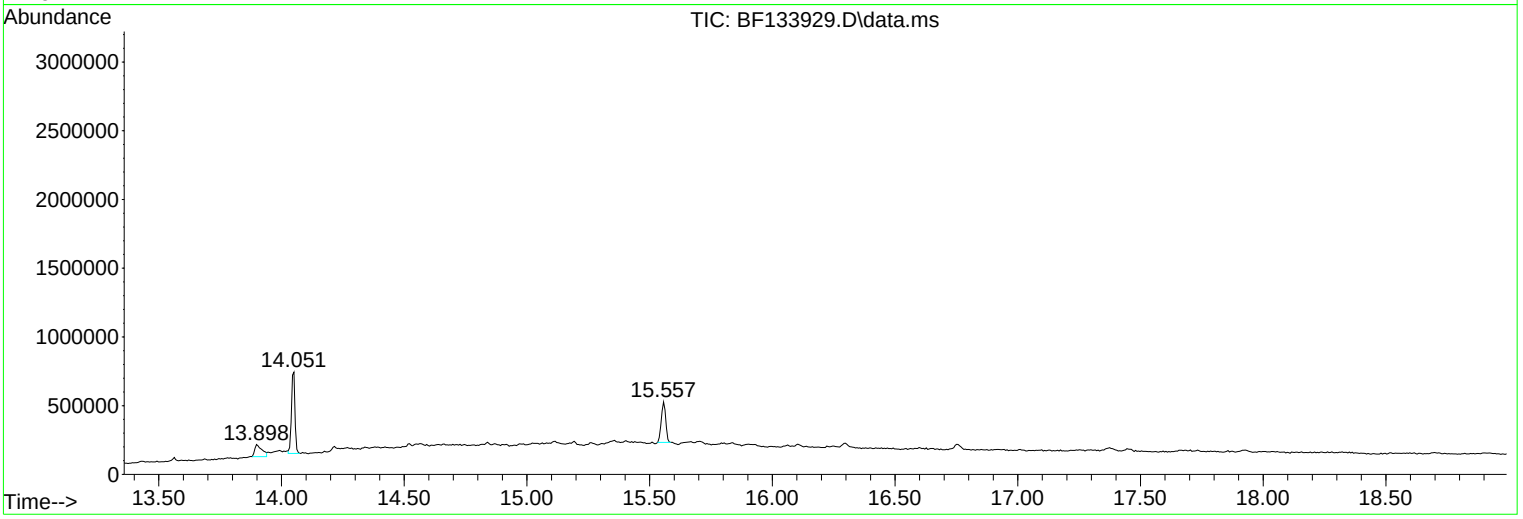
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

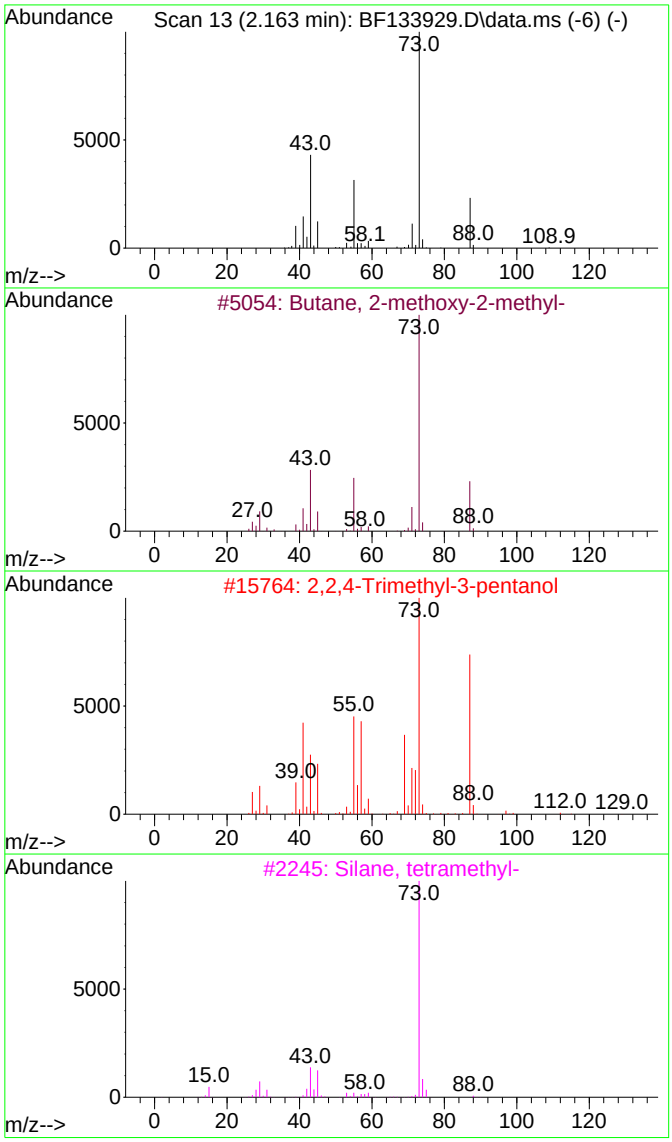
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

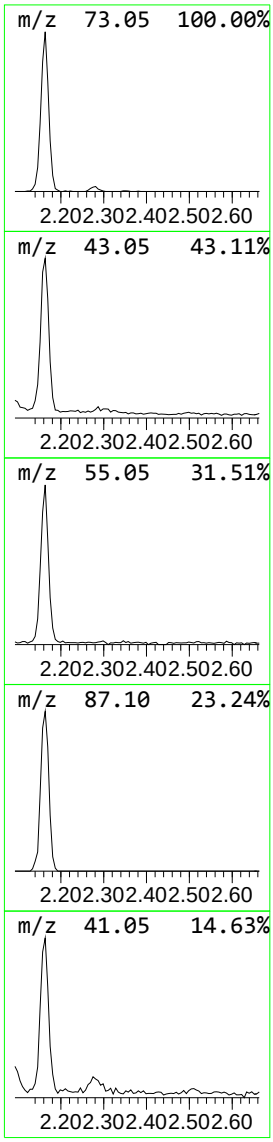
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.163 | 6.94 ng | 221777 | 1,4-Dichlorobenzene-d4 | 6.857 |

| 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 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 35 |
| 4 | 2,5-Dimethyl-4-hydroxy-3-hexanone | 144 | C8H16O2 | 000815-77-0 | 28 |
| 5 | Butanoic acid, 2-hydroxy-2-methy... | 132 | C6H12O3 | 032793-34-3 | 28 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
Data File : BF133929.D
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Operator : CG\JU
Sample : 03320-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
WC-10

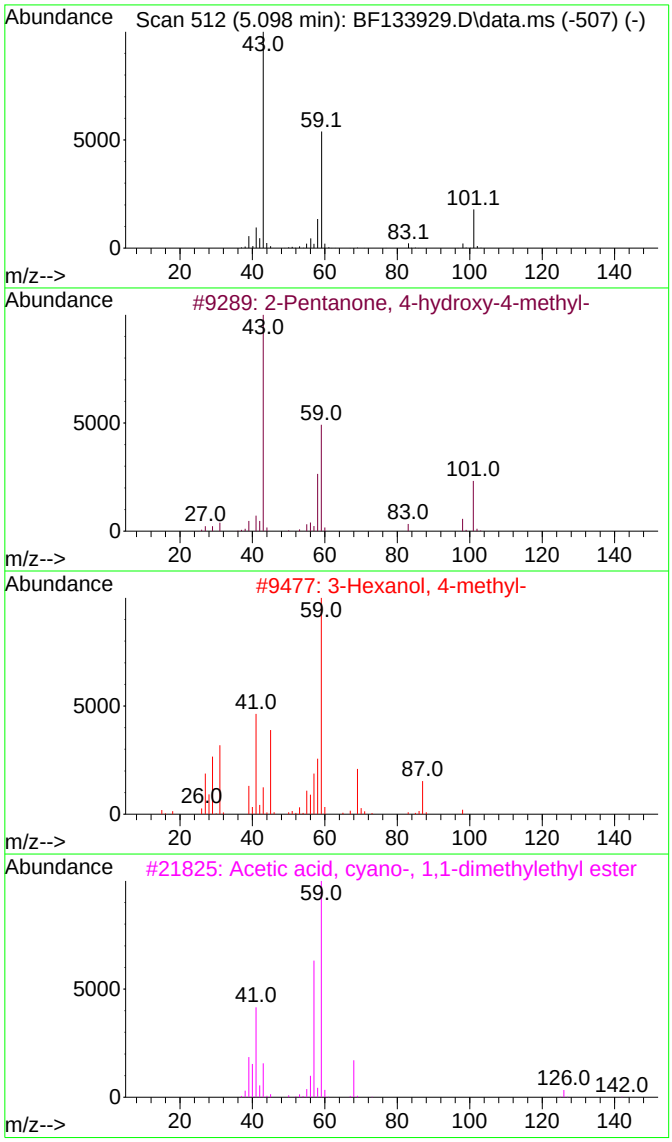
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

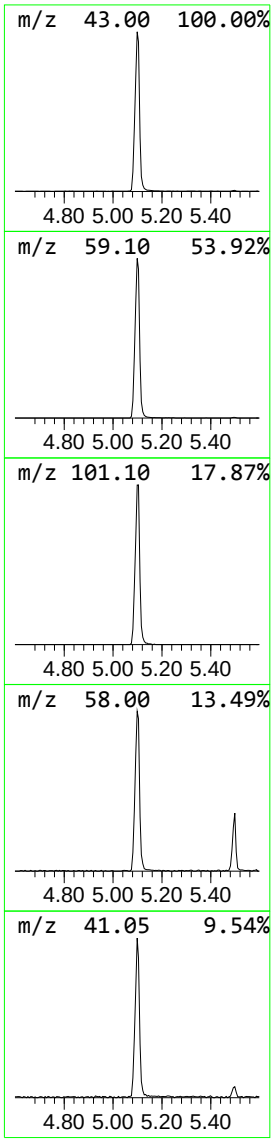
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.098 | 33.08 ng | 1056790 | 1,4-Dichlorobenzene-d4 | 6.857 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 72 |
| 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 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
Data File : BF133929.D
Acq On : 23 Jun 2023 06:18
Operator : CG\JU
Sample : 03320-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
WC-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

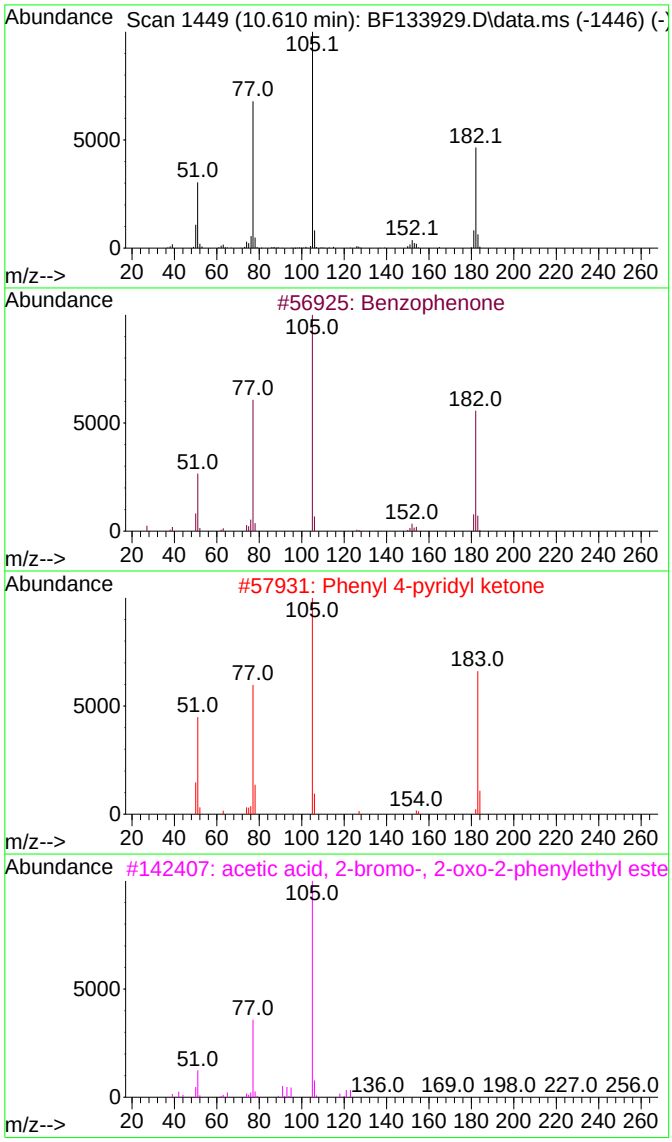
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

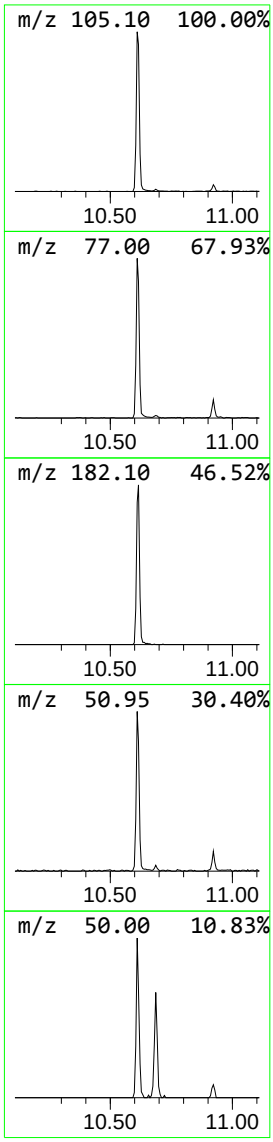
**********

Peak Number 3 Benzophenone Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.610 | 8.62 ng | 329654 | Acenaphthene-d10 | 9.898 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 96 |
| 2 | Phenyl 4-pyridyl ketone | 183 | C12H9NO | 014548-46-0 | 52 |
| 3 | acetic acid, 2-bromo-, 2-oxo-2-p... | 256 | C10H9BrO3 | 1000401-50-0 | 50 |
| 4 | Methyl 2-benzoyl-4-cyanobutanoate | 231 | C13H13NO3 | 1010486-83-8 | 50 |
| 5 | N-cyanobenzamide | 146 | C8H6N2O | 015150-25-1 | 50 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
Data File : BF133929.D
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Operator : CG\JU
Sample : 03320-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
WC-10

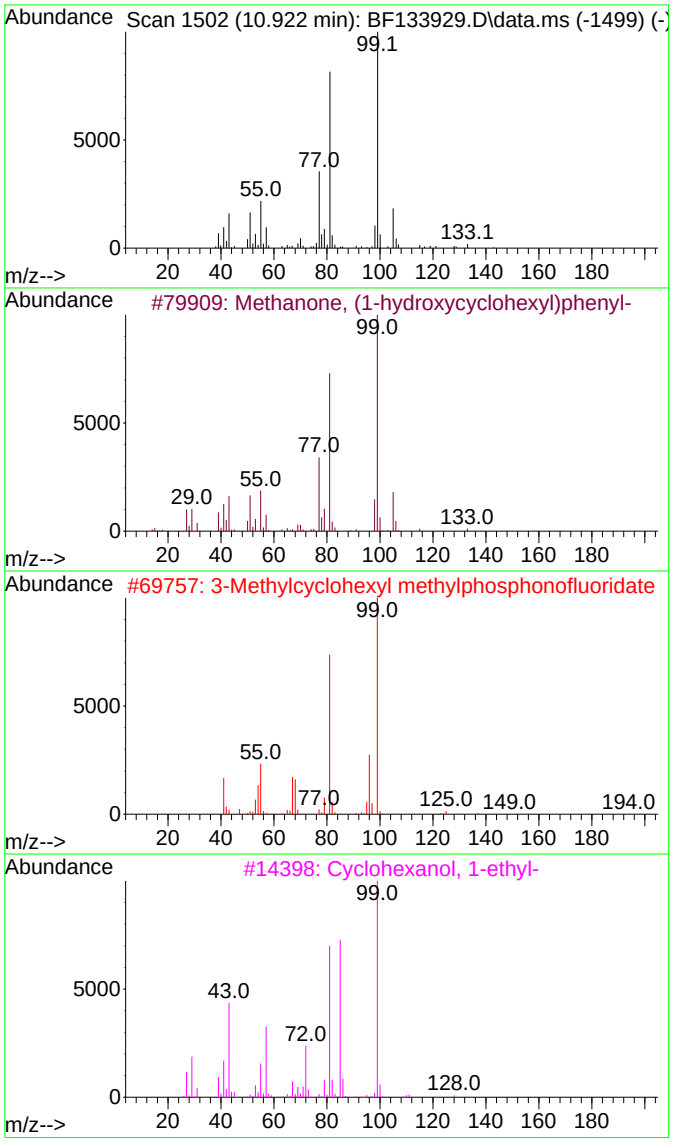
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

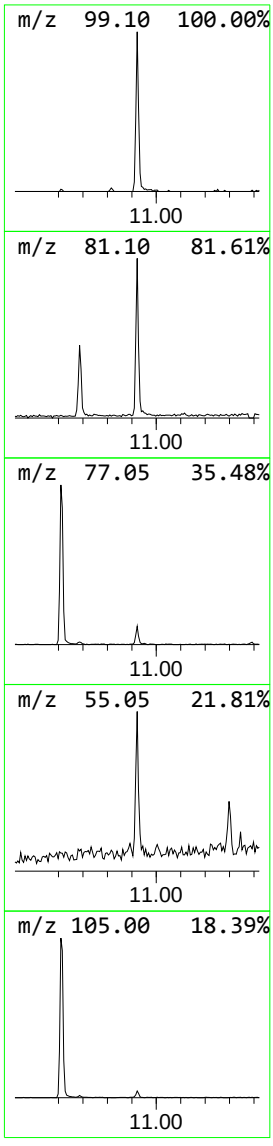
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 Methanone, (1-hydroxycycloh... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.922 | 2.30 ng | 79750 | Phenanthrene-d10 | 11.392 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methanone, (1-hydroxycyclohexyl)... | 204 | C13H16O2 | 000947-19-3 | 83 |
| 2 | 3-Methylcyclohexyl methylphospho... | 194 | C8H16FO2P | 113548-86-0 | 53 |
| 3 | Cyclohexanol, 1-ethyl- | 128 | C8H16O | 001940-18-7 | 53 |
| 4 | Cyclohexanol, 1-(aminomethyl)- | 129 | C7H15NO | 004000-72-0 | 50 |
| 5 | 1-Hydroxycyclohexanecarboxylic acid | 144 | C7H12O3 | 001123-28-0 | 45 |



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Data File : BF133929.D
Acq On : 23 Jun 2023 06:18
Operator : CG\JU
Sample : 03320-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
WC-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

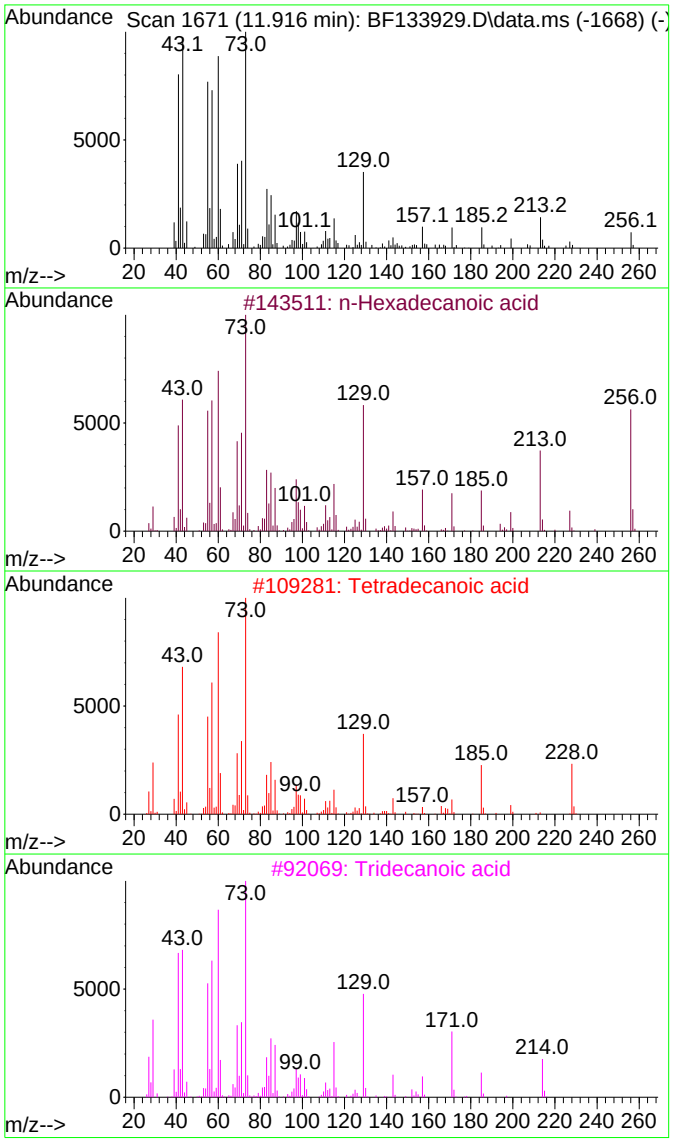
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

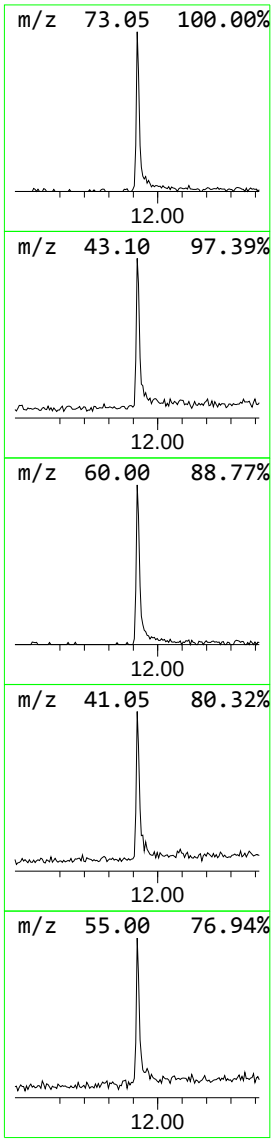
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.916 | 5.03 ng | 174835 | Phenanthrene-d10 | 11.392 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 94 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 90 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 81 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 58 |



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Sample : 03320-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

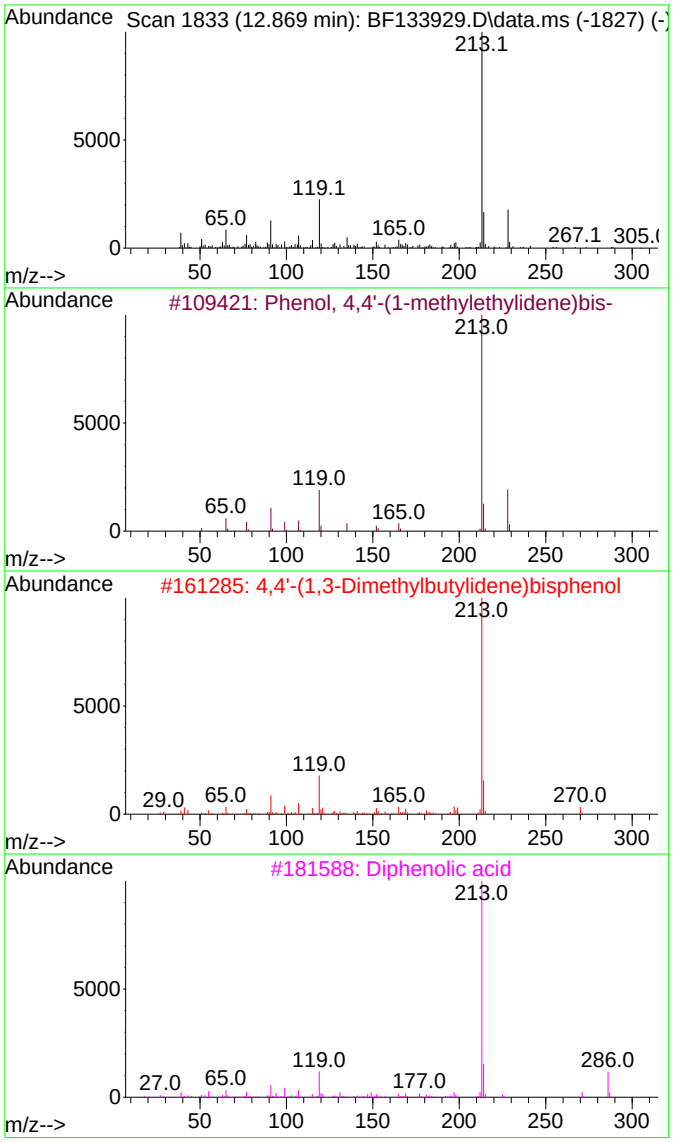
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

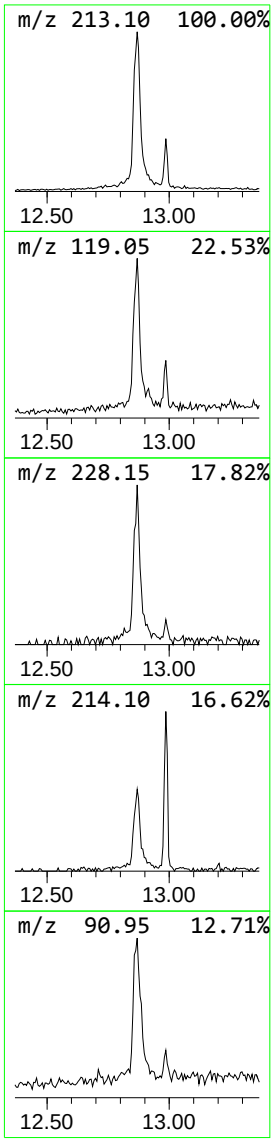
**********

Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.868 | 8.77 ng | 257052 | Chrysene-d12 | 14.051 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 4,4'-(1-methylethylidene... | 228 | C15H16O2 | 000080-05-7 | 95 |
| 2 | 4,4'-(1,3-Dimethylbutylidene)bis... | 270 | C18H22O2 | 006807-17-6 | 80 |
| 3 | Diphenolic acid | 286 | C17H18O4 | 000126-00-1 | 72 |
| 4 | 5-Fluoro-2-nitrophenylamine, TMS... | 228 | C9H13FN2O2Si | 1000484-54-5 | 58 |
| 5 | 2H,8H-Benzo[1,2-b:3,4-b']dipyran... | 228 | C14H12O3 | 000523-59-1 | 58 |



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Sample : 03320-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
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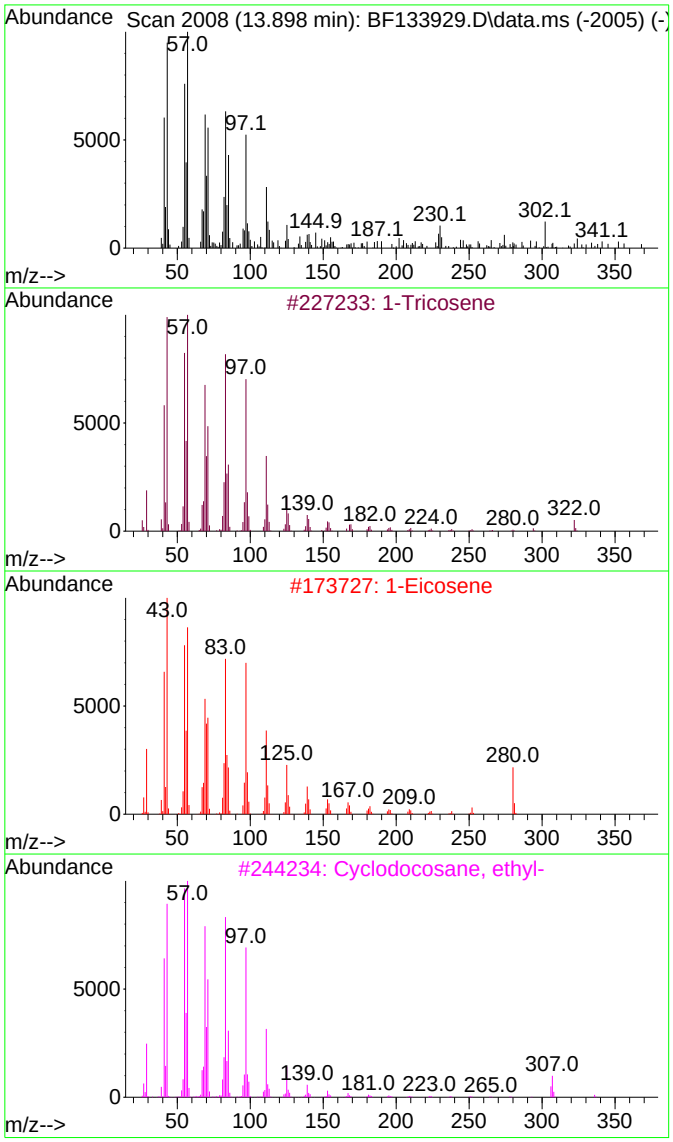
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

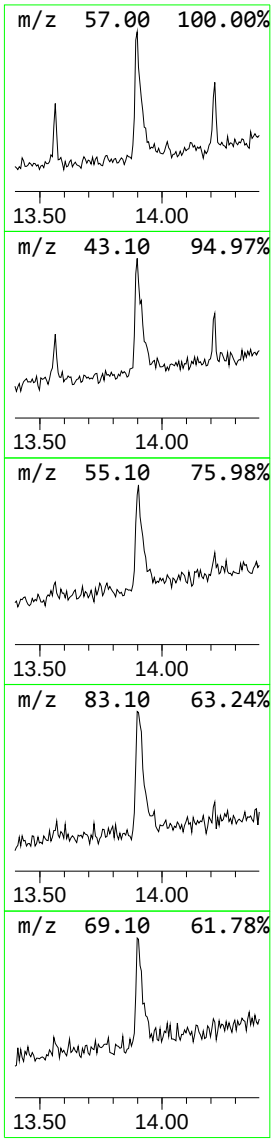
**********

Peak Number 7 1-Tricosene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.898 | 6.31 ng | 184923 | Chrysene-d12 | 14.051 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Tricosene | 322 | C23H46 | 018835-32-0 | 95 |
| 2 | 1-Eicosene | 280 | C20H40 | 003452-07-1 | 95 |
| 3 | Cyclodocosane, ethyl- | 336 | C24H48 | 1000151-22-6 | 94 |
| 4 | Cycloeicosane | 280 | C20H40 | 000296-56-0 | 92 |
| 5 | Cyclohexadecane, 1,2-diethyl- | 280 | C20H40 | 1000155-85-3 | 91 |



Tentatively Identified Compound (LSC) summary

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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... | 2.163 | 6.9 | ng | 221777 | 1 | 6.857 | 638866 | 20.0 |
| 2-Pentanone, 4-... | 5.098 | 33.1 | ng | 1056790 | 1 | 6.857 | 638866 | 20.0 |
| Benzophenone | 10.610 | 8.6 | ng | 329654 | 3 | 9.898 | 764952 | 20.0 |
| Methanone, (1-h... | 10.922 | 2.3 | ng | 79750 | 4 | 11.392 | 694518 | 20.0 |
| n-Hexadecanoic ... | 11.916 | 5.0 | ng | 174835 | 4 | 11.392 | 694518 | 20.0 |
| Phenol, 4,4'-(1... | 12.868 | 8.8 | ng | 257052 | 5 | 14.051 | 586493 | 20.0 |
| 1-Tricosene | 13.898 | 6.3 | ng | 184923 | 5 | 14.051 | 586493 | 20.0 |