LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042424\
Data File : BF137717.D
Acq On : 24 Apr 2024 14:17
Operator : CG\JU
Sample : PB160462BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB160462BL

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-BF042324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137717.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.157 | 7 | 12 | 18 | rVB | 247290 | 294215 | 2.67% | 0.428% |
| 2 | 2.581 | 52 | 84 | 91 | rBV | 2367390 | 9265896 | 83.96% | 13.474% |
| 3 | 4.463 | 402 | 404 | 419 | rBV | 77484 | 176055 | 1.60% | 0.256% |
| 4 | 5.322 | 543 | 550 | 553 | rBV | 3083424 | 3765167 | 34.12% | 5.475% |
| 5 | 5.693 | 608 | 613 | 616 | rBV | 5332125 | 5341752 | 48.40% | 7.767% |
| 6 | 5.881 | 641 | 645 | 647 | rBV | 284285 | 279361 | 2.53% | 0.406% |
| 7 | 6.322 | 716 | 720 | 723 | rBV | 457641 | 420958 | 3.81% | 0.612% |
| 8 | 6.669 | 773 | 779 | 782 | rBV | 5263487 | 5468292 | 49.55% | 7.951% |
| 9 | 7.063 | 842 | 846 | 849 | rBV | 2000361 | 1681550 | 15.24% | 2.445% |
| 10 | 7.198 | 865 | 869 | 870 | rVV | 142530 | 121286 | 1.10% | 0.176% |
| 11 | 7.216 | 870 | 872 | 882 | rVB | 466429 | 394856 | 3.58% | 0.574% |
| 12 | 7.622 | 935 | 941 | 944 | rBV | 4949875 | 5140995 | 46.58% | 7.476% |
| 13 | 8.345 | 1059 | 1064 | 1067 | rBV | 2644606 | 2300221 | 20.84% | 3.345% |
| 14 | 9.422 | 1241 | 1247 | 1250 | rBV | 9732878 | 9820577 | 88.98% | 14.280% |
| 15 | 10.110 | 1358 | 1364 | 1367 | rBV | 2820459 | 2618584 | 23.73% | 3.808% |
| 16 | 10.898 | 1492 | 1498 | 1501 | rBV | 4329303 | 3766441 | 34.13% | 5.477% |
| 17 | 11.604 | 1614 | 1618 | 1621 | rBV | 3356591 | 2750386 | 24.92% | 3.999% |
| 18 | 13.198 | 1883 | 1889 | 1892 | rBV | 10509521 | 11036406 | 100.00% | 16.048% |
| 19 | 14.251 | 2064 | 2068 | 2072 | rBV | 2664282 | 2374578 | 21.52% | 3.453% |
| 20 | 15.827 | 2329 | 2336 | 2349 | rBV | 1313351 | 1753366 | 15.89% | 2.550% |

Sum of corrected areas: 68770942

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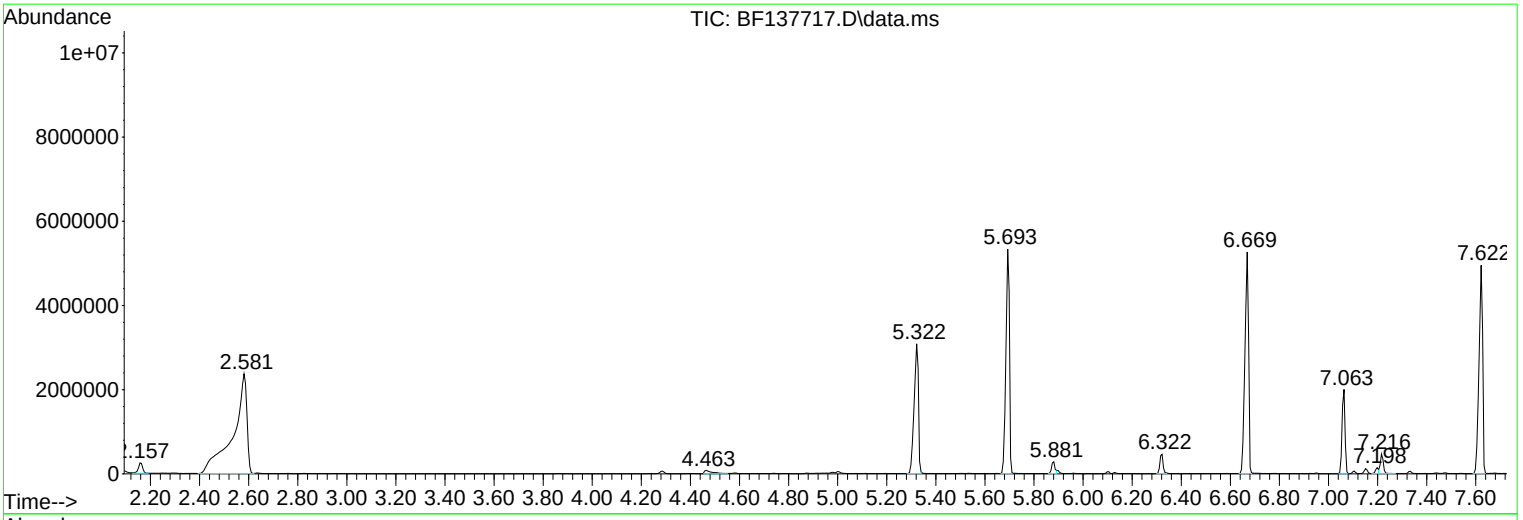
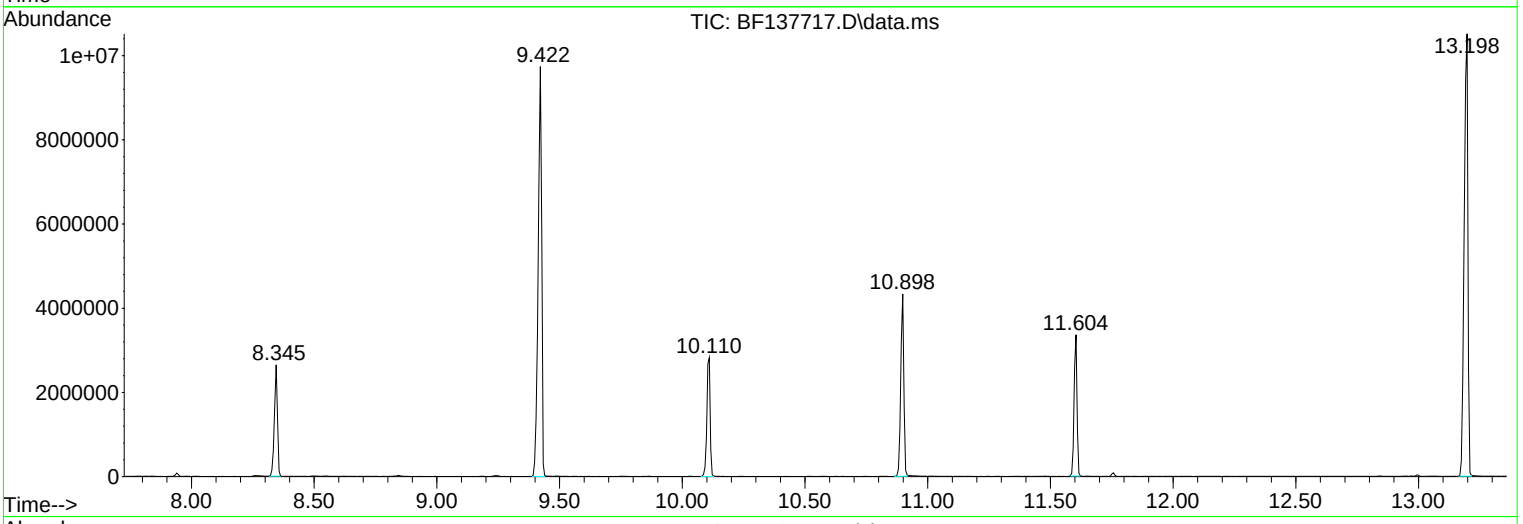
Operator : CG\JU
Sample : PB160462BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

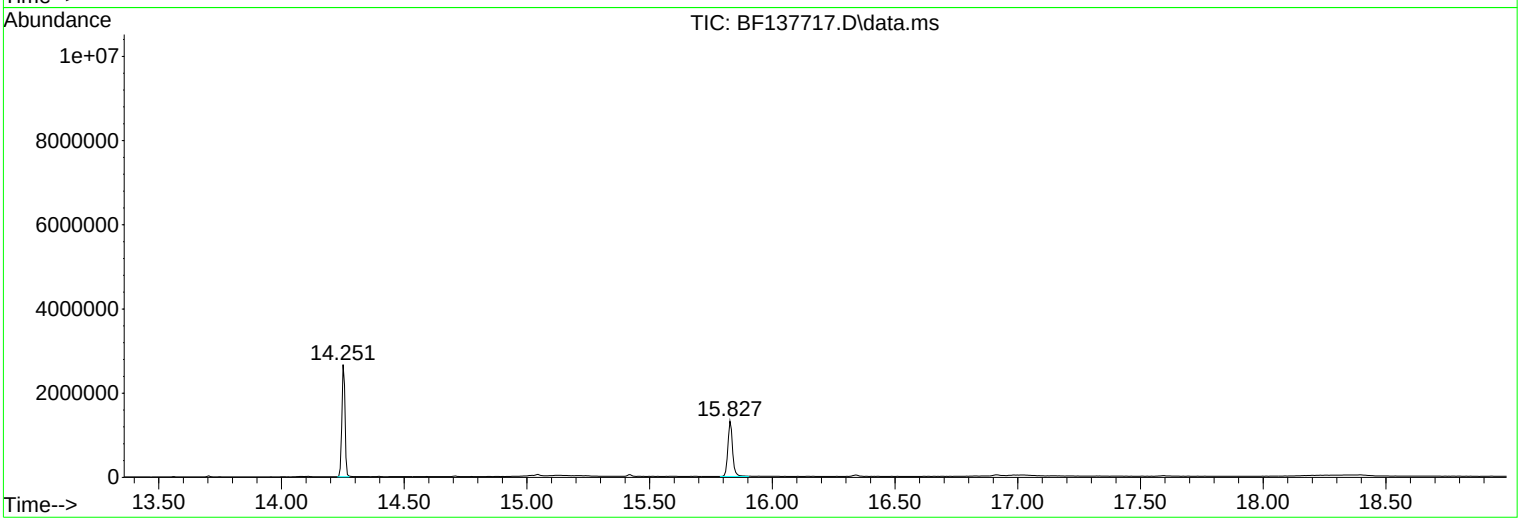
**Instrument :**
BNA_F
**ClientSampleId :**
PB160462BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.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_F\Data\BF042424\
Data File : BF137717.D
Acq On : 24 Apr 2024 14:17
Operator : CG\JU
Sample : PB160462BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB160462BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

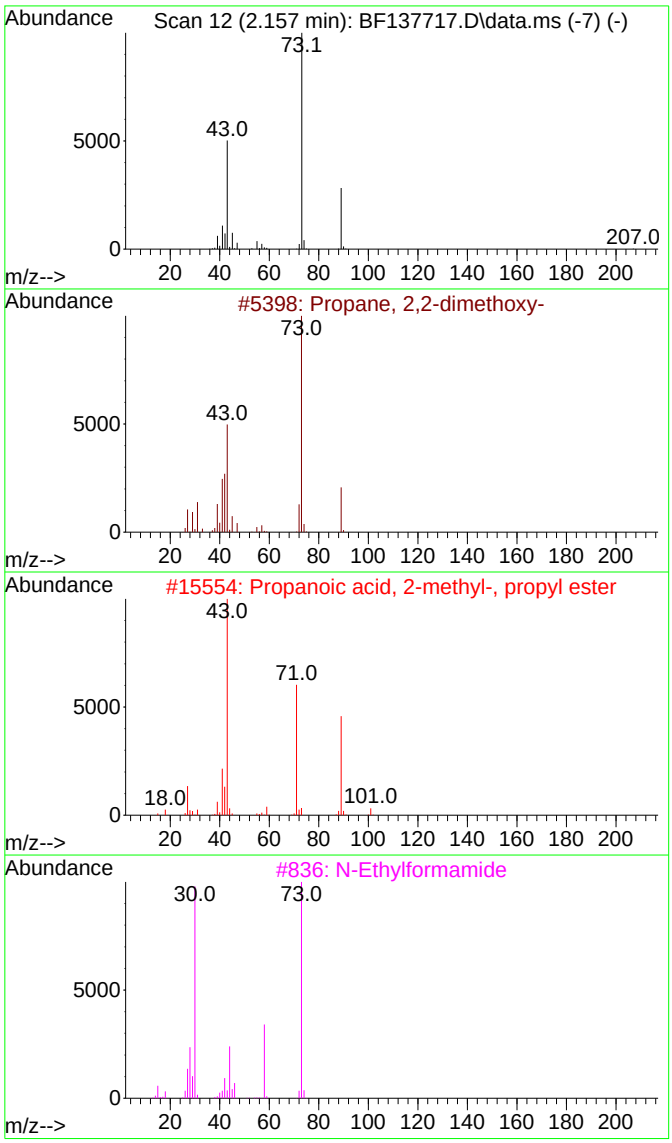
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

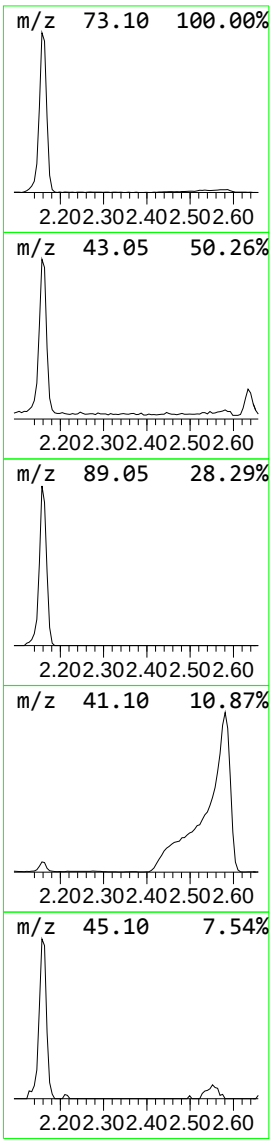
**********

Peak Number 1 unknown2.157 Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.157 | 3.50 ng | 294215 | 1,4-Dichlorobenzene-d4 | 7.063 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 2,2-dimethoxy- | 104 | C5H12O2 | 000077-76-9 | 40 |
| 2 | Propanoic acid, 2-methyl-, propy... | 130 | C7H14O2 | 000644-49-5 | 23 |
| 3 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |
| 4 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 9 |
| 5 | 1-Hexen-4-ol, 1-chloro-3,5-dimet... | 162 | C8H15ClO | 100244-09-5 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042424\
Data File : BF137717.D
Acq On : 24 Apr 2024 14:17
Operator : CG\JU
Sample : PB160462BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB160462BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

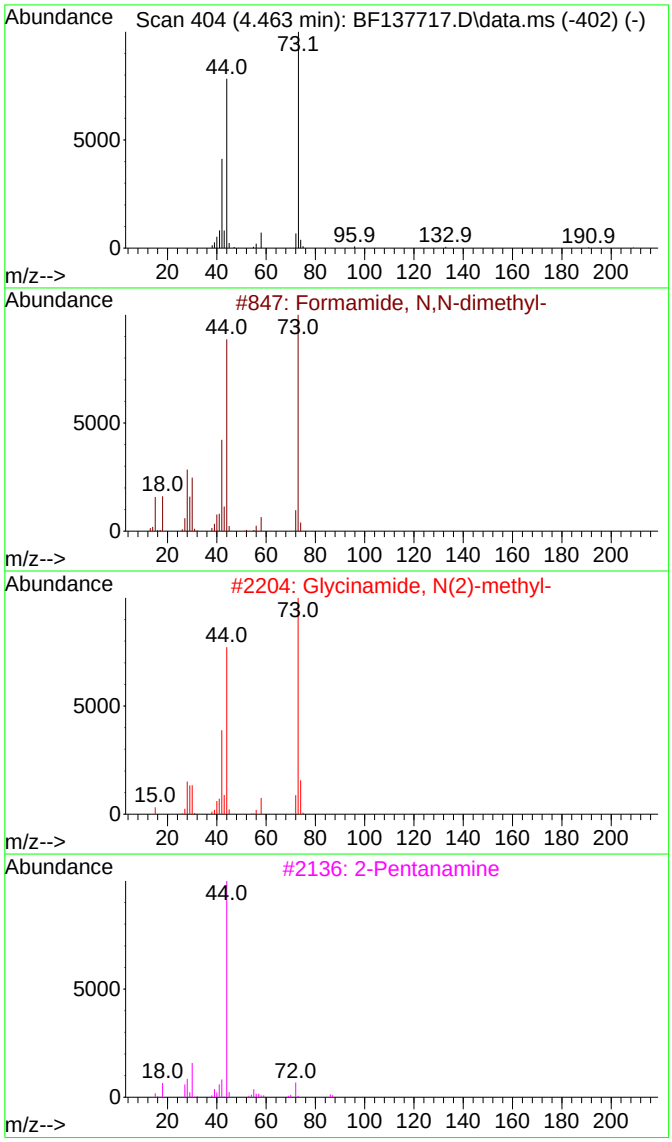
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

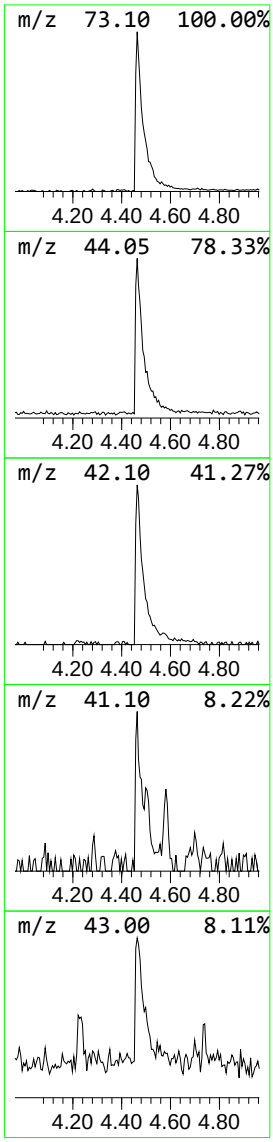
**********

Peak Number 3 Formamide, N,N-dimethyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.463 | 2.09 ng | 176055 | 1,4-Dichlorobenzene-d4 | 7.063 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Formamide, N,N-dimethyl- | 73 | C3H7NO | 000068-12-2 | 87 |
| 2 | Glycinamide, N(2)-methyl- | 88 | C3H8N2O | 1000452-55-9 | 78 |
| 3 | 2-Pentanamine | 87 | C5H13N | 063493-28-7 | 9 |
| 4 | 3-METHYL-CYCLOBUTANE-1,1-DICARBO... | 158 | C7H10O4 | 057252-84-3 | 9 |
| 5 | Acetonitrile-d3 | 44 | C2D3N | 002206-26-0 | 7 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042424\
Data File : BF137717.D
Acq On : 24 Apr 2024 14:17
Operator : CG\JU
Sample : PB160462BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB160462BL

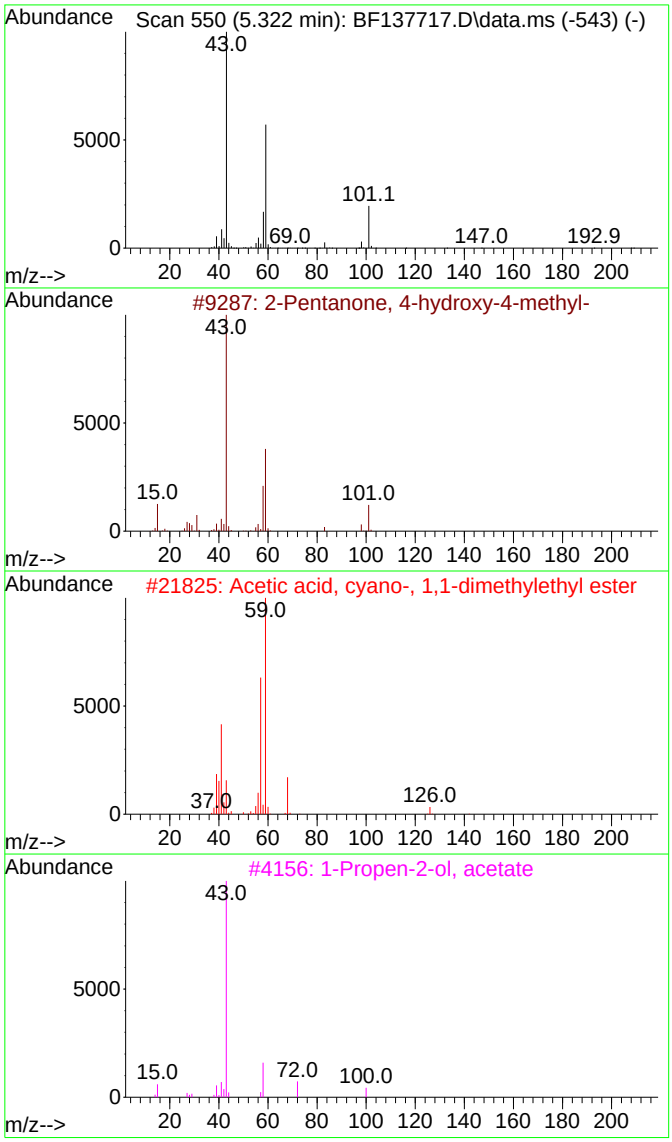
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

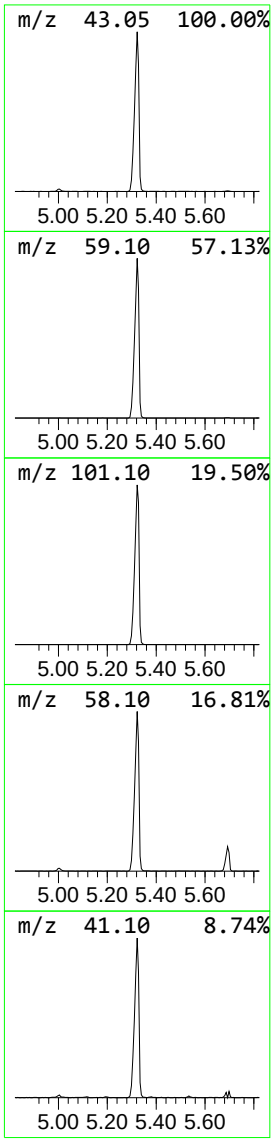
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.322 | 44.78 ng | 3765170 | 1,4-Dichlorobenzene-d4 | 7.063 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 3 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |
| 4 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042424\
Data File : BF137717.D
Acq On : 24 Apr 2024 14:17
Operator : CG\JU
Sample : PB160462BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB160462BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.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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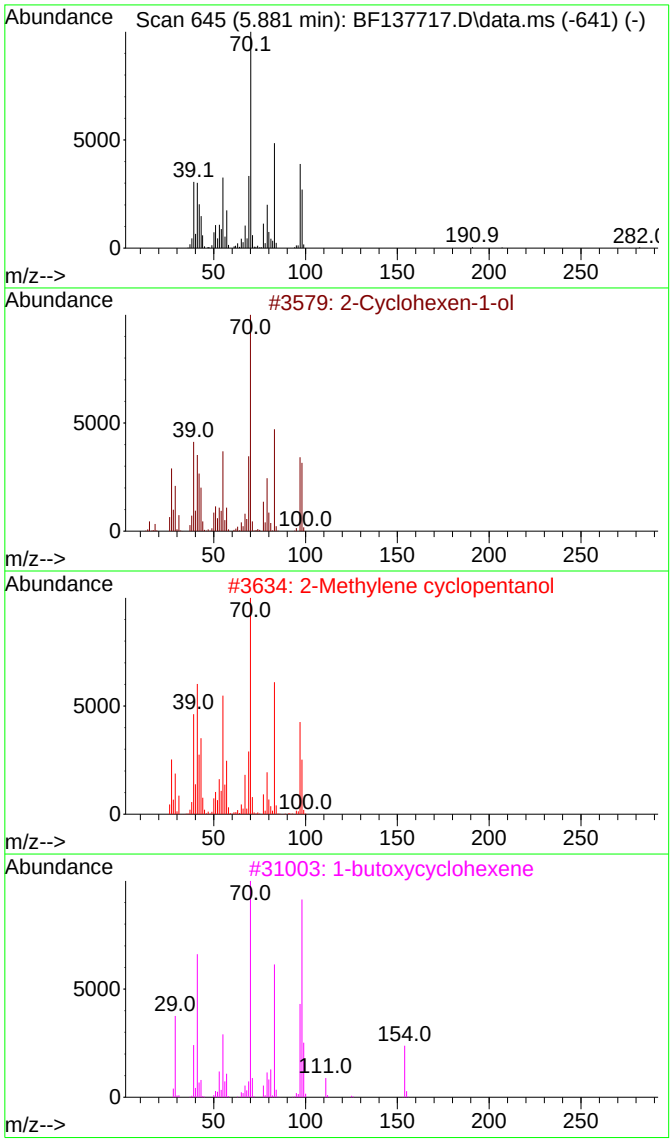
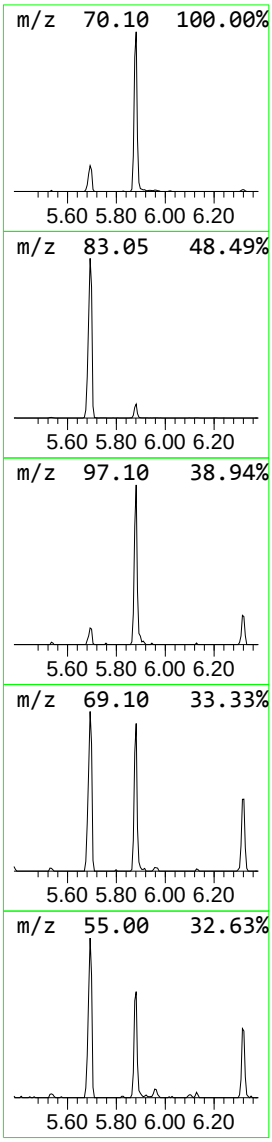
Peak Number 5 2-Cyclohexen-1-ol Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.881 | 3.32 ng | 279361 | 1,4-Dichlorobenzene-d4 | 7.063 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Cyclohexen-1-ol | 98 | C6H10O | 000822-67-3 | 95 |
| 2 | 2-Methylene cyclopentanol | 98 | C6H10O | 020461-31-8 | 42 |
| 3 | 1-butoxycyclohexene | 154 | C10H18O | 024159-57-7 | 40 |
| 4 | Cyclopentane, 1,3-dimethyl- | 98 | C7H14 | 002453-00-1 | 38 |
| 5 | Cyclopentane, 1,3-dimethyl-, cis- | 98 | C7H14 | 002532-58-3 | 32 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042424\
Data File : BF137717.D
Acq On : 24 Apr 2024 14:17
Operator : CG\JU
Sample : PB160462BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB160462BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

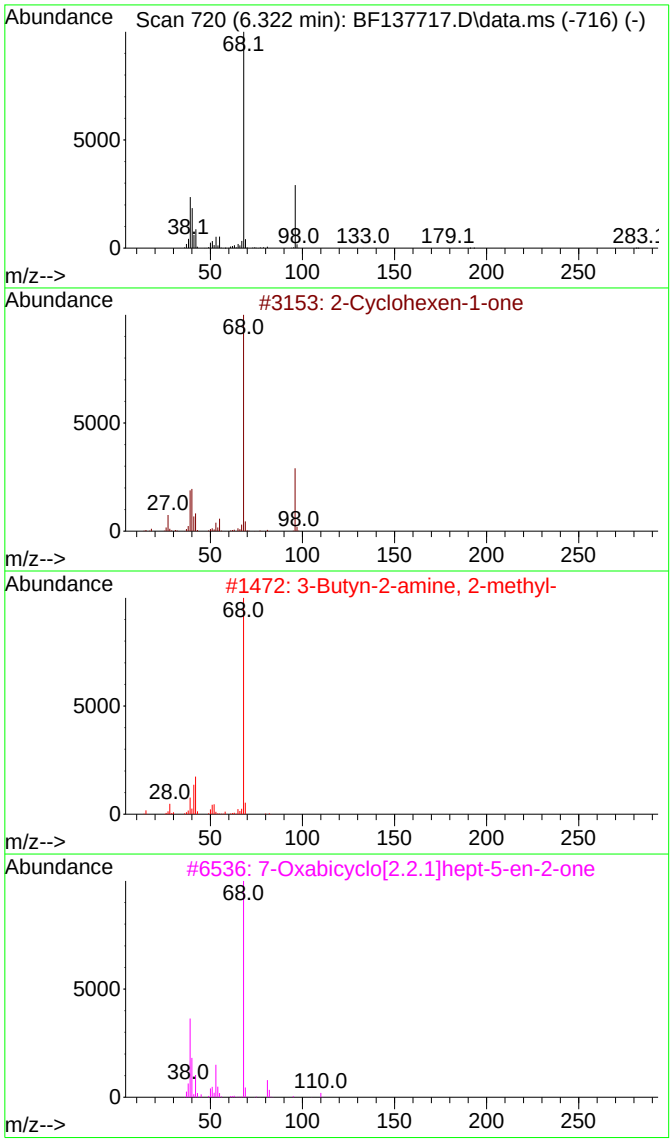
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

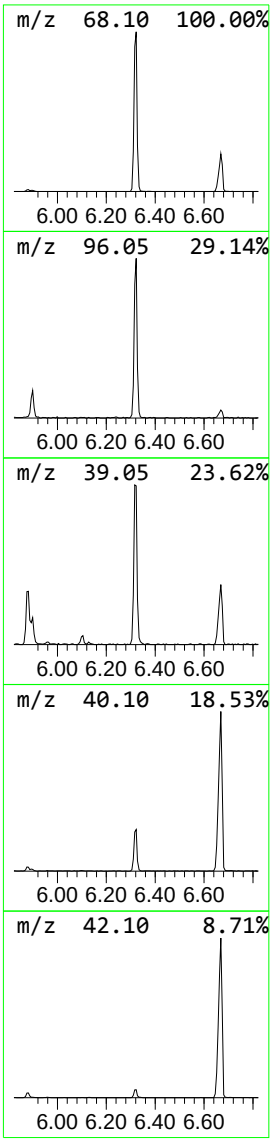
**********

Peak Number 6 2-Cyclohexen-1-one Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.322 | 5.01 ng | 420958 | 1,4-Dichlorobenzene-d4 | 7.063 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Cyclohexen-1-one | 96 | C6H8O | 000930-68-7 | 91 |
| 2 | 3-Butyn-2-amine, 2-methyl- | 83 | C5H9N | 002978-58-7 | 53 |
| 3 | 7-Oxabicyclo[2.2.1]hept-5-en-2-one | 110 | C6H6O2 | 095530-78-2 | 17 |
| 4 | 2,5-Dihydro-3-methyl-thiophene 1... | 132 | C5H8O2S | 001193-10-8 | 12 |
| 5 | But-1-ene-3-yne, 1-ethoxy- | 96 | C6H8O | 002806-41-9 | 10 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042424\
Data File : BF137717.D
Acq On : 24 Apr 2024 14:17
Operator : CG\JU
Sample : PB160462BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB160462BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

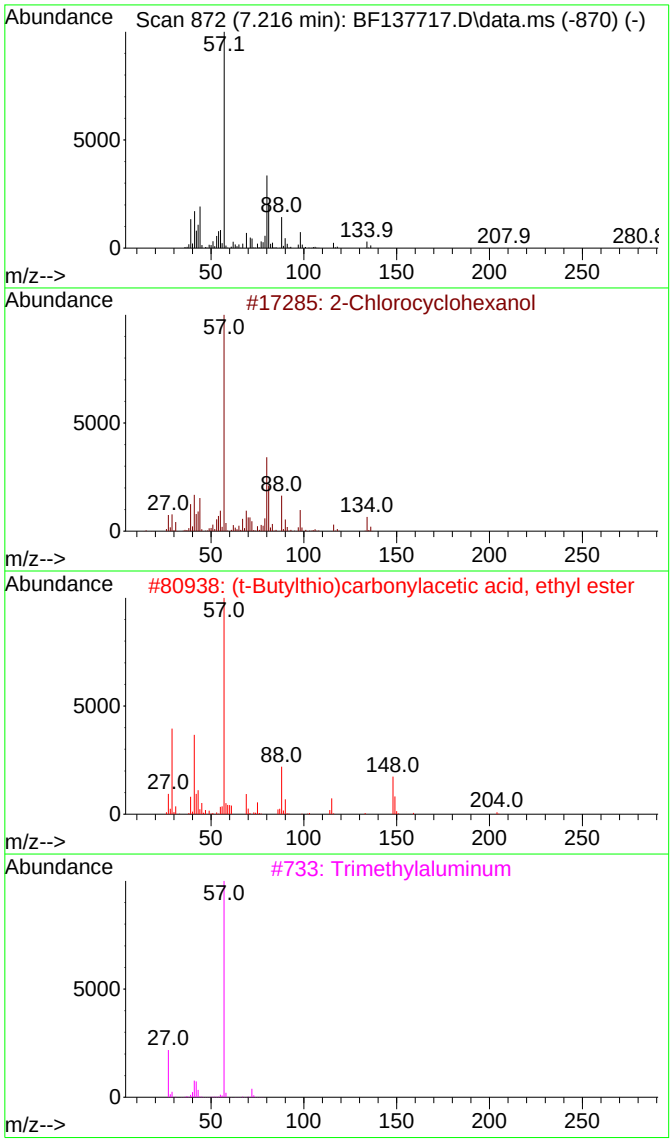
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

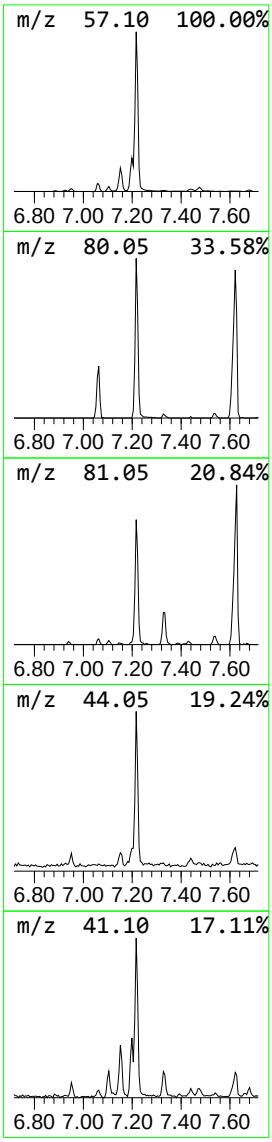
**********

Peak Number 7 2-Chlorocyclohexanol Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.216 | 4.70 ng | 394856 | 1,4-Dichlorobenzene-d4 | 7.063 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Chlorocyclohexanol | 134 | C6H11ClO | 001561-86-0 | 95 |
| 2 | (t-Butylthio)carbonylacetic acid... | 204 | C9H16O3S | 1000192-52-7 | 16 |
| 3 | Trimethylaluminum | 72 | C3H9Al | 000075-24-1 | 9 |
| 4 | 1,3-Propanediol, 2-methyl-, dipr... | 202 | C10H18O4 | 054932-83-1 | 9 |
| 5 | 1-Decanamine | 157 | C10H23N | 002016-57-1 | 9 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042424\
Data File : BF137717.D
Acq On : 24 Apr 2024 14:17
Operator : CG\JU
Sample : PB160462BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB160462BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.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 |
| unknown2.157 | 2.157 | 3.5 | ng | 294215 | 1 | 7.063 | 1681550 | 20.0 |
| Formamide, N,N-... | 4.463 | 2.1 | ng | 176055 | 1 | 7.063 | 1681550 | 20.0 |
| 2-Pentanone, 4-... | 5.322 | 44.8 | ng | 3765170 | 1 | 7.063 | 1681550 | 20.0 |
| 2-Cyclohexen-1-ol | 5.881 | 3.3 | ng | 279361 | 1 | 7.063 | 1681550 | 20.0 |
| 2-Cyclohexen-1-one | 6.322 | 5.0 | ng | 420958 | 1 | 7.063 | 1681550 | 20.0 |
| 2-Chlorocyclohe... | 7.216 | 4.7 | ng | 394856 | 1 | 7.063 | 1681550 | 20.0 |