LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021122\
Data File : BF126858.D
Acq On : 11 Feb 2022 15:35
Operator : CG\JU
Sample : N1477-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220087-AMENDED-BERKELEY-7-COMP

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-BF020922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126858.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.181 | 488 | 492 | 500 | rVB | 162271 | 202013 | 4.53% | 0.678% |
| 2 | 5.563 | 551 | 557 | 560 | rBV | 3643981 | 3697565 | 82.87% | 12.414% |
| 3 | 6.475 | 708 | 712 | 720 | rBV | 67425 | 79223 | 1.78% | 0.266% |
| 4 | 6.563 | 720 | 727 | 730 | rBV | 3289764 | 4089420 | 91.65% | 13.730% |
| 5 | 6.940 | 787 | 791 | 794 | rBV | 915631 | 740926 | 16.61% | 2.488% |
| 6 | 7.504 | 881 | 887 | 890 | rBV | 2670261 | 2606046 | 58.41% | 8.749% |
| 7 | 7.657 | 910 | 913 | 918 | rBV2 | 118673 | 127793 | 2.86% | 0.429% |
| 8 | 8.116 | 987 | 991 | 1002 | rBV | 82144 | 95837 | 2.15% | 0.322% |
| 9 | 8.222 | 1005 | 1009 | 1012 | rBV | 1211098 | 1018901 | 22.84% | 3.421% |
| 10 | 8.351 | 1029 | 1031 | 1038 | rBV2 | 30934 | 57028 | 1.28% | 0.191% |
| 11 | 9.298 | 1186 | 1192 | 1195 | rBV | 4758805 | 4174531 | 93.56% | 14.015% |
| 12 | 9.375 | 1200 | 1205 | 1208 | rBV2 | 74510 | 83107 | 1.86% | 0.279% |
| 13 | 9.786 | 1270 | 1275 | 1282 | rBV4 | 28310 | 55609 | 1.25% | 0.187% |
| 14 | 9.981 | 1304 | 1308 | 1311 | rVB | 1254761 | 1132953 | 25.39% | 3.804% |
| 15 | 10.769 | 1437 | 1442 | 1445 | rBV | 3050026 | 2863860 | 64.18% | 9.615% |
| 16 | 10.904 | 1462 | 1465 | 1472 | rVB | 210944 | 192246 | 4.31% | 0.645% |
| 17 | 11.345 | 1537 | 1540 | 1547 | rVB | 154936 | 146324 | 3.28% | 0.491% |
| 18 | 11.469 | 1557 | 1561 | 1564 | rBV | 1543677 | 1249867 | 28.01% | 4.196% |
| 19 | 11.980 | 1645 | 1648 | 1652 | rBV | 89531 | 80448 | 1.80% | 0.270% |
| 20 | 13.063 | 1826 | 1832 | 1835 | rBV | 4303557 | 4461968 | 100.00% | 14.980% |
| 21 | 13.951 | 1978 | 1983 | 1998 | rBV3 | 173968 | 420056 | 9.41% | 1.410% |
| 22 | 14.110 | 2007 | 2010 | 2014 | rBV | 1004828 | 892407 | 20.00% | 2.996% |
| 23 | 14.263 | 2033 | 2036 | 2039 | rBV | 57219 | 49242 | 1.10% | 0.165% |
| 24 | 14.569 | 2085 | 2088 | 2090 | rBV | 70583 | 59797 | 1.34% | 0.201% |
| 25 | 14.598 | 2090 | 2093 | 2097 | rVV3 | 33623 | 57692 | 1.29% | 0.194% |
| 26 | 14.886 | 2138 | 2142 | 2147 | rBV | 49581 | 49316 | 1.11% | 0.166% |
| 27 | 14.968 | 2152 | 2156 | 2160 | rVB | 108670 | 103839 | 2.33% | 0.349% |
| 28 | 15.239 | 2198 | 2202 | 2207 | rBV | 66260 | 72842 | 1.63% | 0.245% |
| 29 | 15.621 | 2261 | 2267 | 2279 | rBV | 551505 | 734225 | 16.46% | 2.465% |
| 30 | 15.845 | 2293 | 2305 | 2314 | rVB8 | 24119 | 81901 | 1.84% | 0.275% |
| 31 | 16.098 | 2343 | 2348 | 2352 | rBV2 | 32175 | 46035 | 1.03% | 0.155% |
| 32 | 17.868 | 2643 | 2649 | 2657 | rVB8 | 28704 | 62502 | 1.40% | 0.210% |

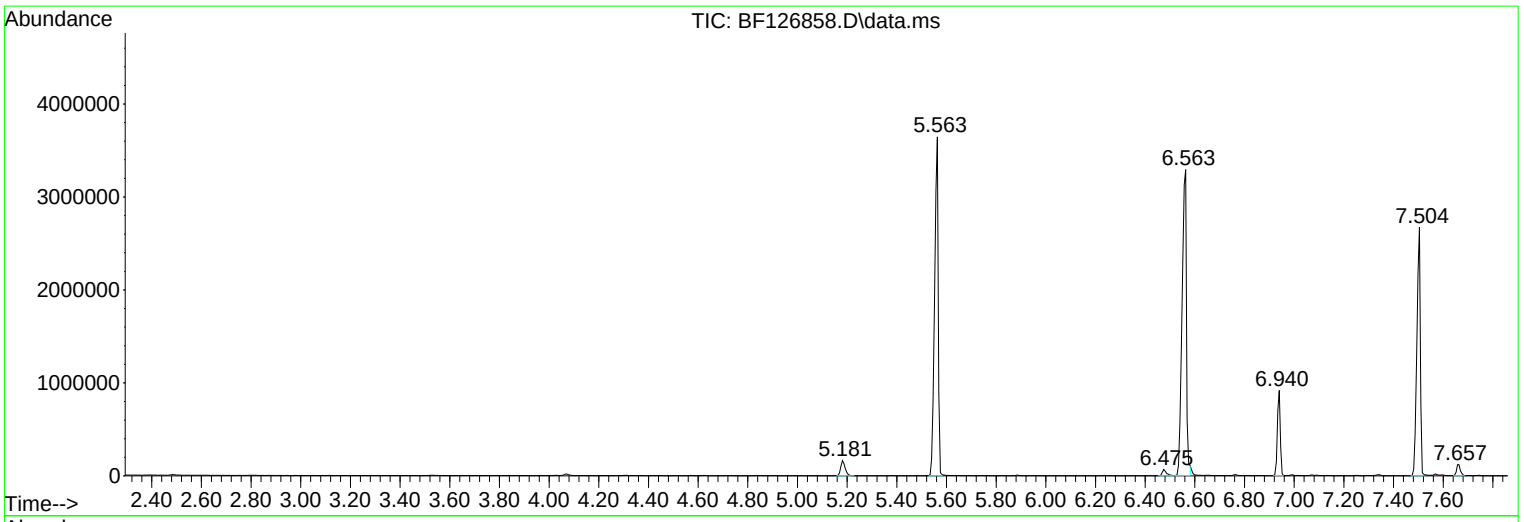
Sum of corrected areas: 29785519

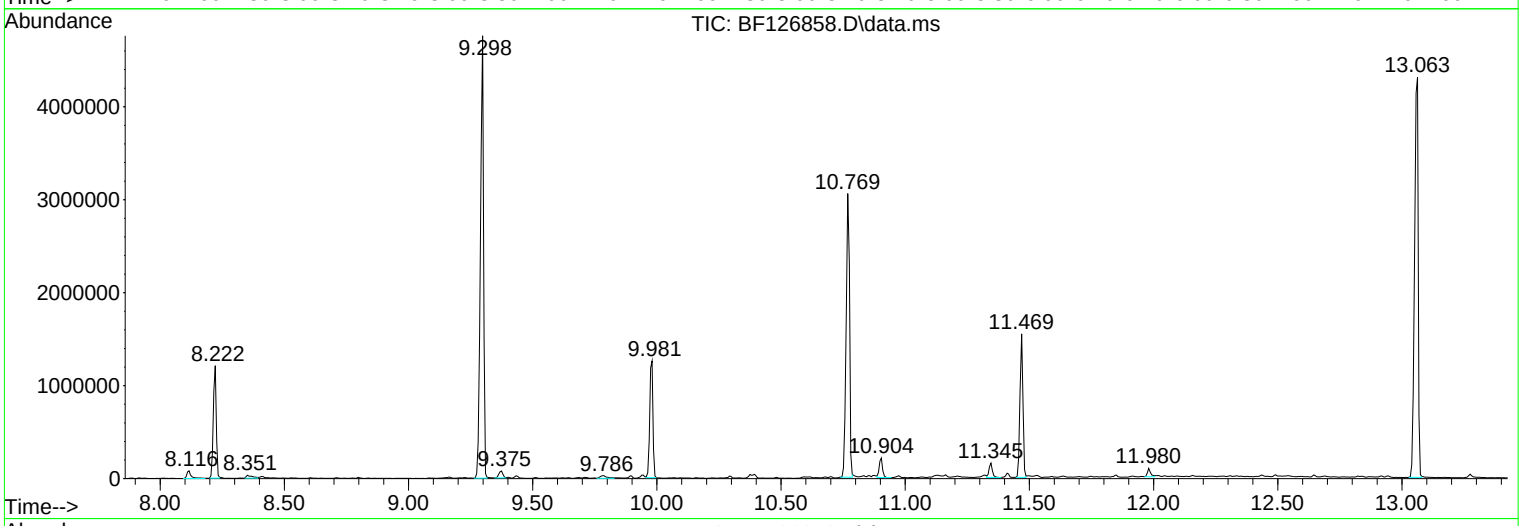
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021122\
Data File : BF126858.D
Acq On : 11 Feb 2022 15:35
Operator : CG\JU
Sample : N1477-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

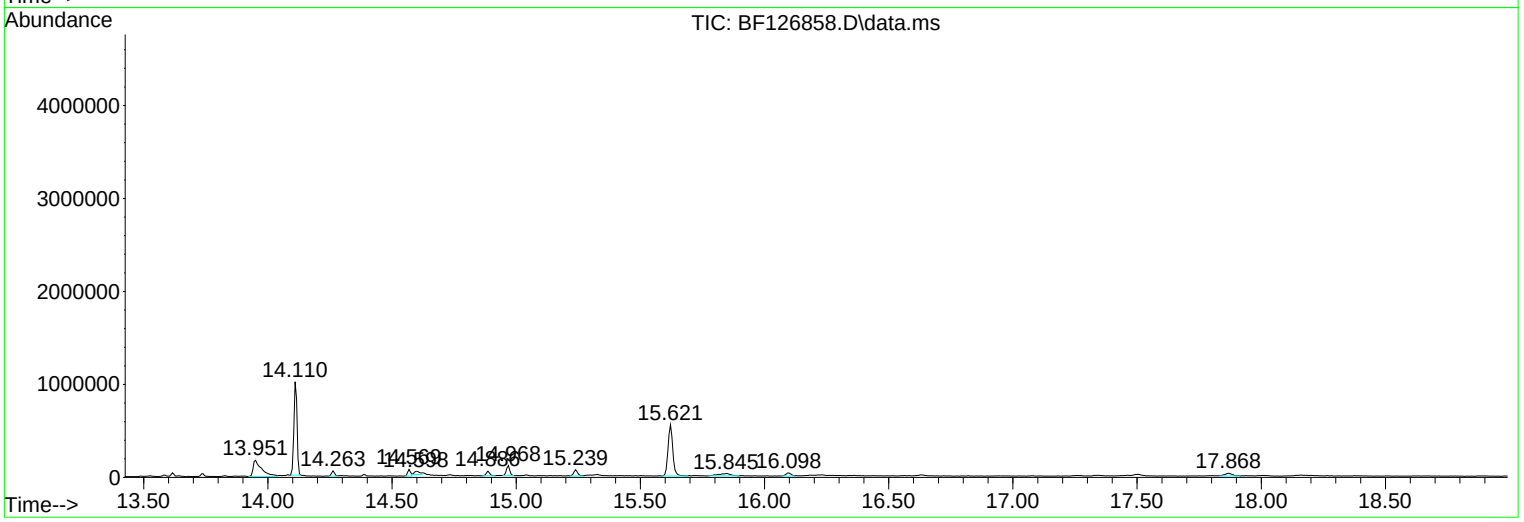
**Instrument :**
BNA_F
**ClientSampleId :**
20220087-AMENDED-BERKELEY-7-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.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\BF021122\
Data File : BF126858.D
Acq On : 11 Feb 2022 15:35
Operator : CG\JU
Sample : N1477-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220087-AMENDED-BERKELEY-7-COMP

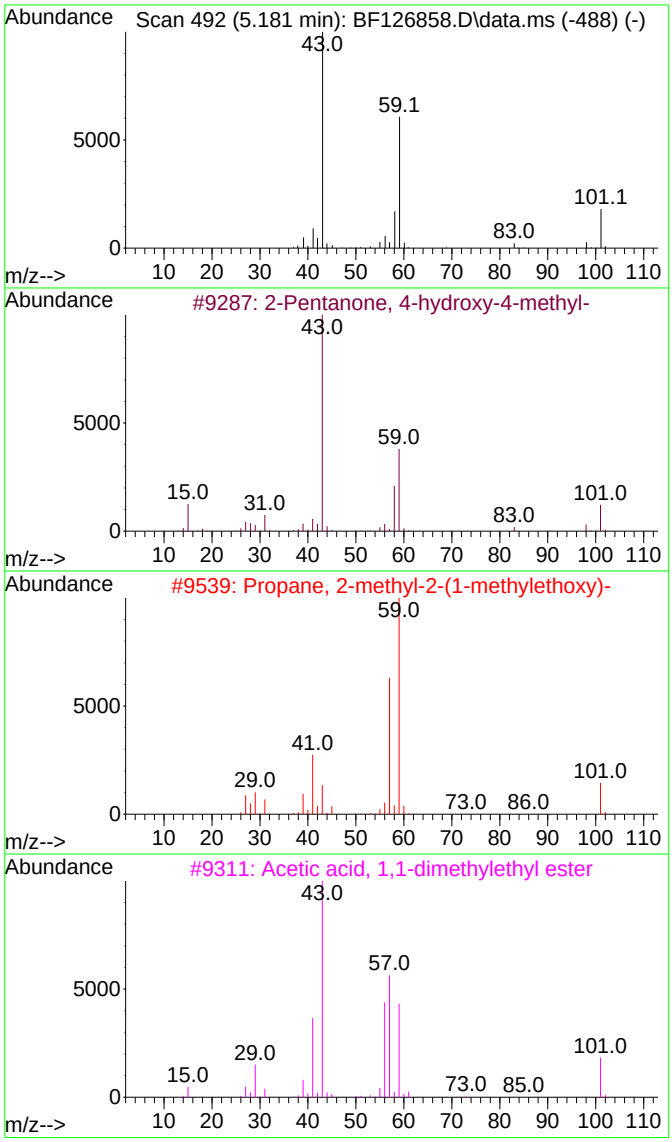
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

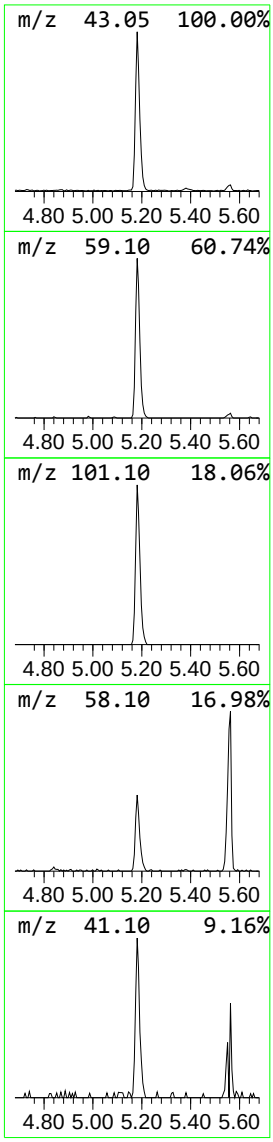
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.181 | 5.45 ng | 202013 | 1,4-Dichlorobenzene-d4 | 6.940 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 45 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 42 |
| 3 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 38 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 37 |
| 5 | 3-Octanol | 130 | C8H18O | 000589-98-0 | 36 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021122\
Data File : BF126858.D
Acq On : 11 Feb 2022 15:35
Operator : CG\JU
Sample : N1477-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220087-AMENDED-BERKELEY-7-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

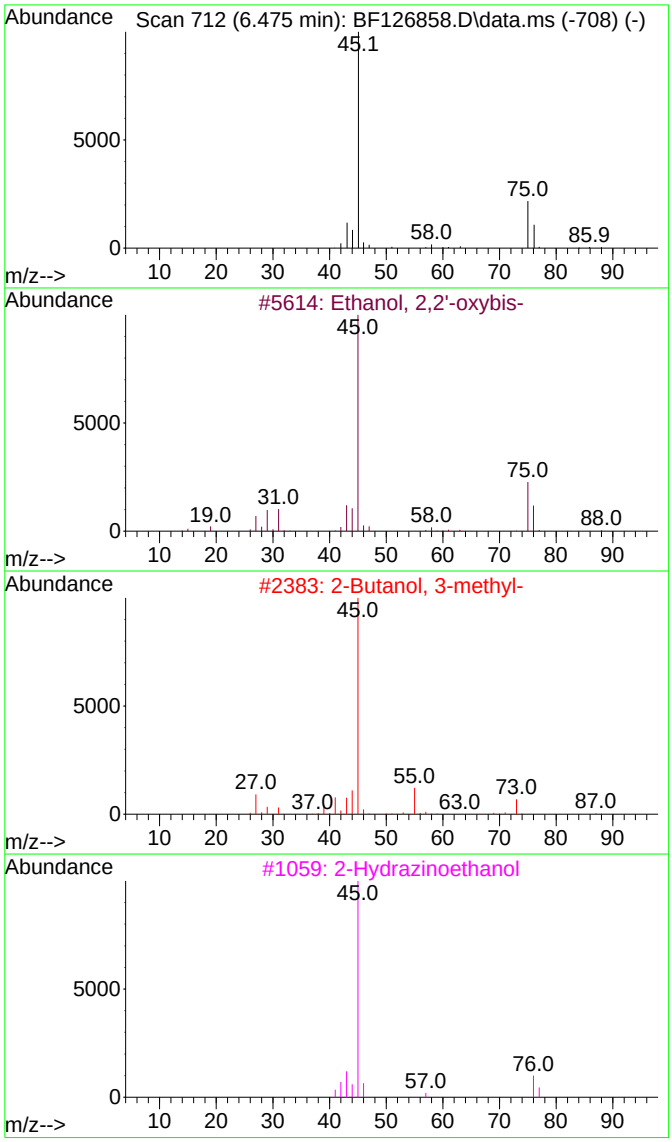
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

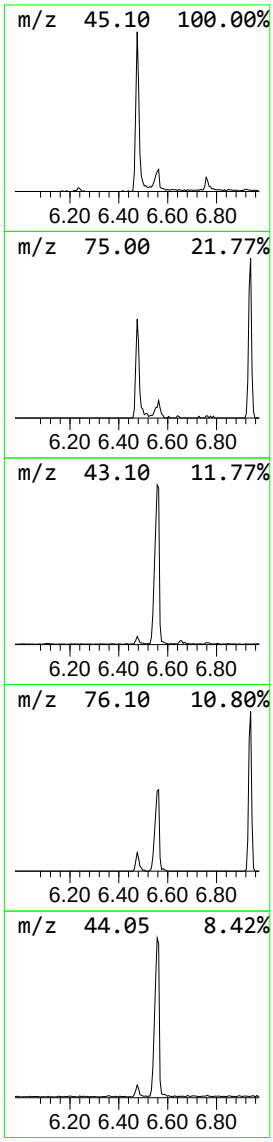
**********

Peak Number 2 Ethanol, 2,2'-oxybis- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.475 | 2.14 ng | 79223 | 1,4-Dichlorobenzene-d4 | 6.940 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2,2'-oxybis- | 106 | C4H10O3 | 000111-46-6 | 83 |
| 2 | 2-Butanol, 3-methyl- | 88 | C5H12O | 000598-75-4 | 42 |
| 3 | 2-Hydrazinoethanol | 76 | C2H8N2O | 000109-84-2 | 9 |
| 4 | Isopropyl Alcohol | 60 | C3H8O | 000067-63-0 | 9 |
| 5 | Ethanol, 2-methoxy- | 76 | C3H8O2 | 000109-86-4 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021122\
Data File : BF126858.D
Acq On : 11 Feb 2022 15:35
Operator : CG\JU
Sample : N1477-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220087-AMENDED-BERKELEY-7-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

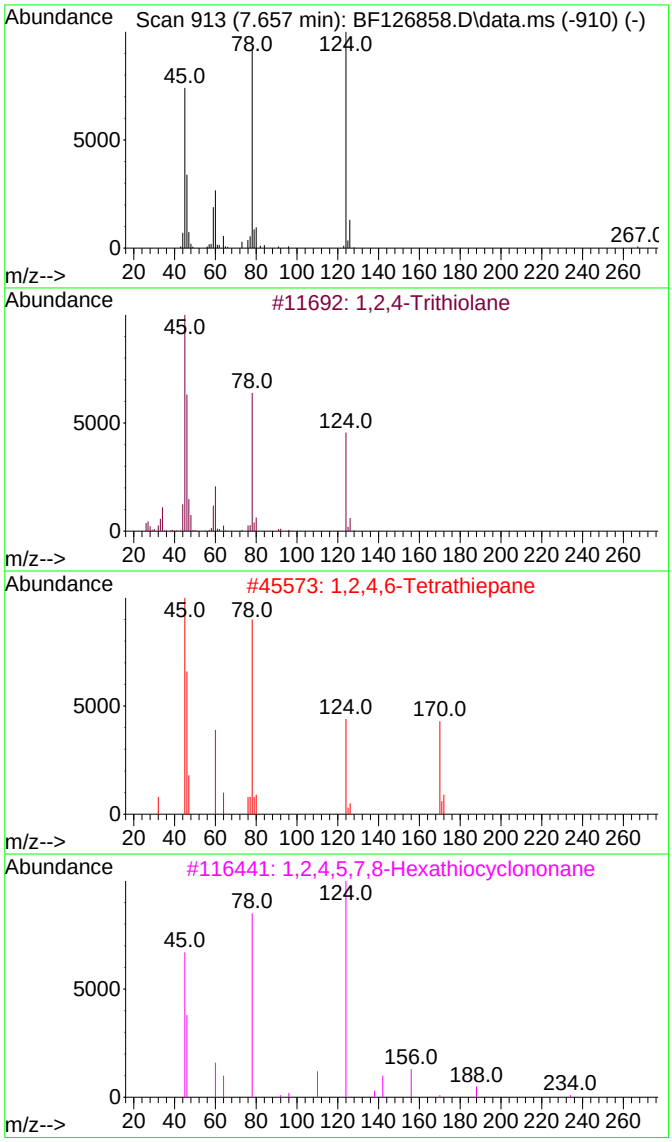
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

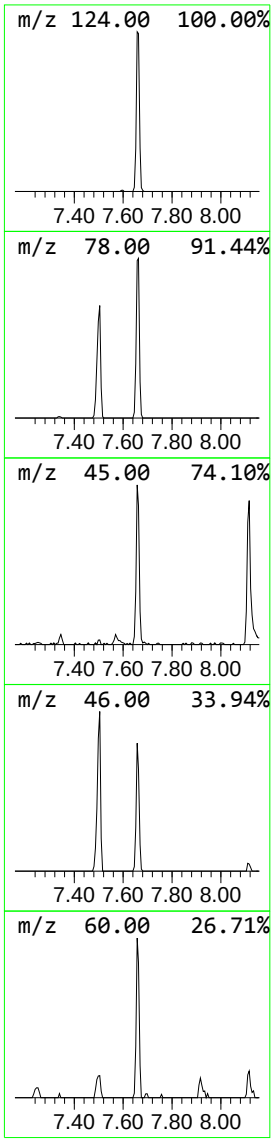
**********

Peak Number 3 1,2,4-Trithiolane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.657 | 2.51 ng | 127793 | Naphthalene-d8 | 8.222 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,2,4-Trithiolane | 124 | C2H4S3 | 000289-16-7 | 86 |
| 2 | 1,2,4,6-Tetrathiepane | 170 | C3H6S4 | 000292-45-5 | 45 |
| 3 | 1,2,4,5,7,8-Hexathiocyclononane | 234 | C3H6S6 | 081531-38-6 | 43 |
| 4 | 1,2-Benzenediol, 4-methyl- | 124 | C7H8O2 | 000452-86-8 | 36 |
| 5 | Benzene | 78 | C6H6 | 000071-43-2 | 25 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021122\
Data File : BF126858.D
Acq On : 11 Feb 2022 15:35
Operator : CG\JU
Sample : N1477-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220087-AMENDED-BERKELEY-7-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

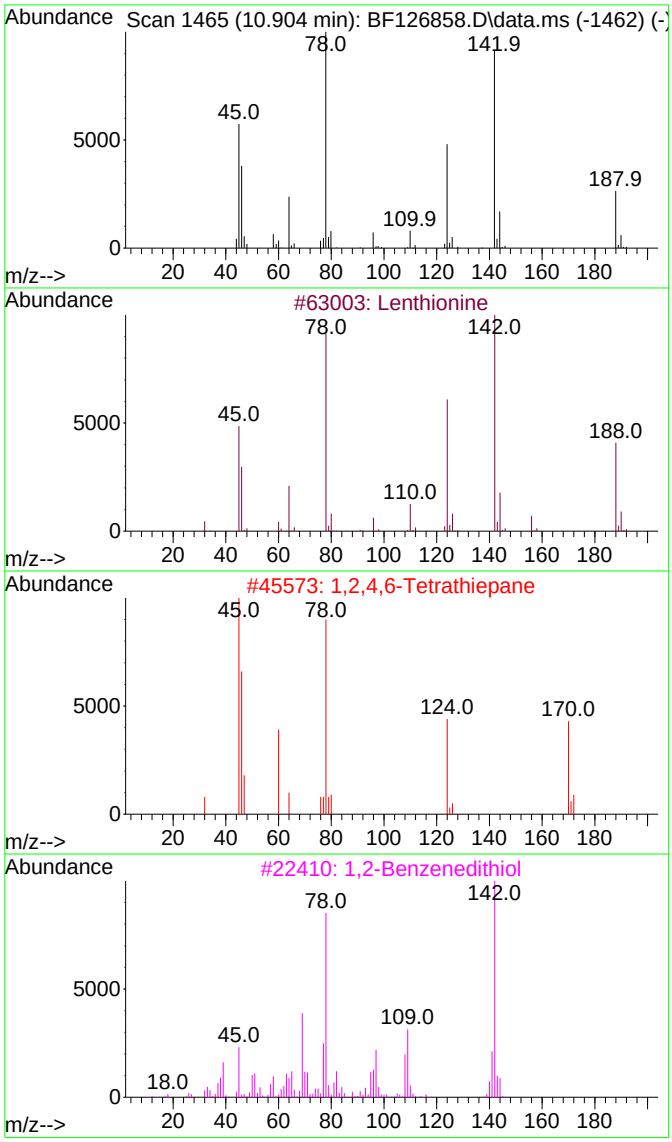
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

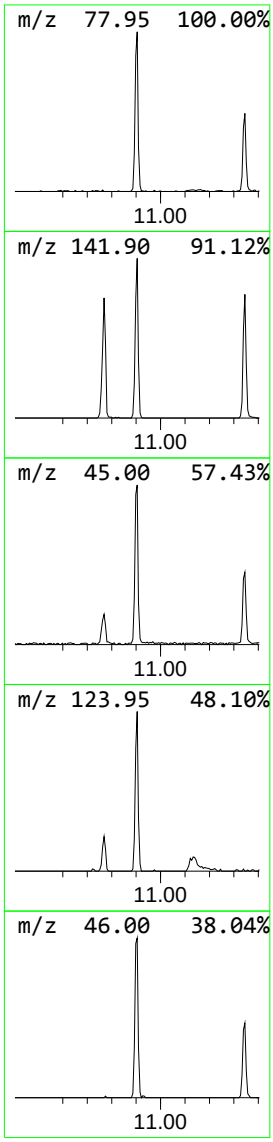
**********

Peak Number 4 Lenthionine Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.904 | 3.08 ng | 192246 | Phenanthrene-d10 | 11.469 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Lenthionine | 188 | C2H4S5 | 000292-46-6 | 94 |
| 2 | 1,2,4,6-Tetrathiepane | 170 | C3H6S4 | 000292-45-5 | 45 |
| 3 | 1,2-Benzenedithiol | 142 | C6H6S2 | 017534-15-5 | 9 |
| 4 | 1,2,4-Trithiolane | 124 | C2H4S3 | 000289-16-7 | 9 |
| 5 | 1,3-Benzenedithiol | 142 | C6H6S2 | 000626-04-0 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021122\
Data File : BF126858.D
Acq On : 11 Feb 2022 15:35
Operator : CG\JU
Sample : N1477-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220087-AMENDED-BERKELEY-7-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

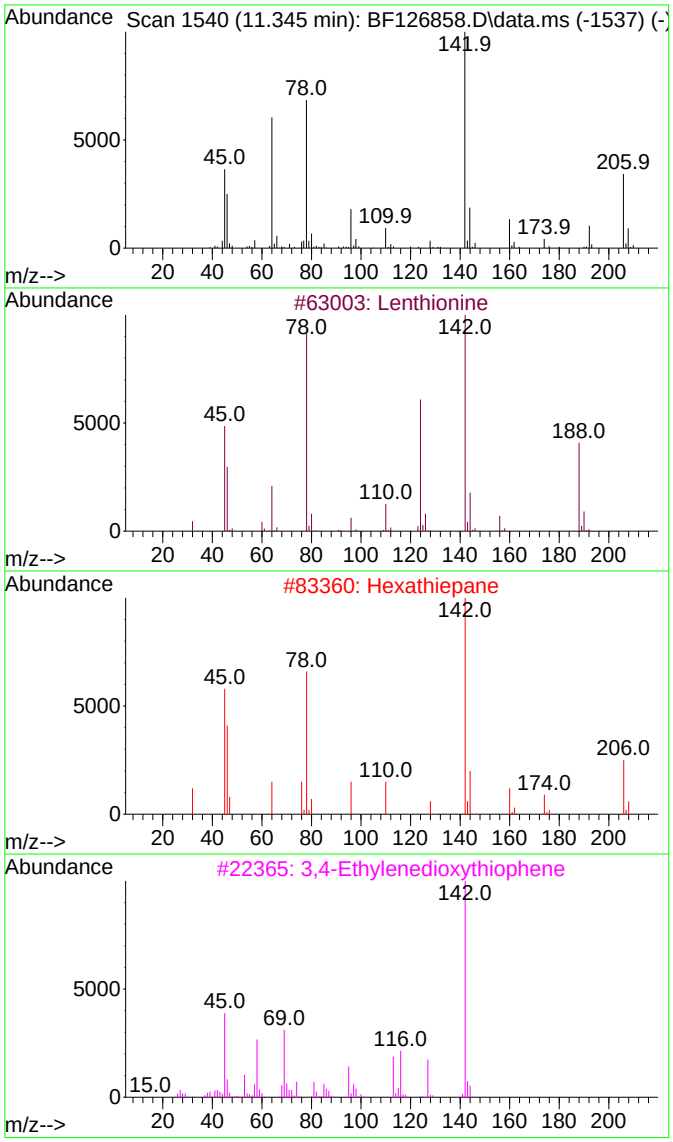
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

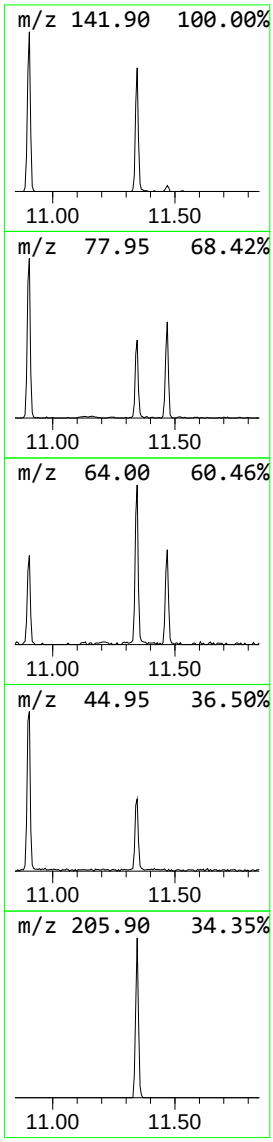
**********

Peak Number 5 unknown11.345 Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.345 | 2.34 ng | 146324 | Phenanthrene-d10 | 11.469 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Lenthionine | 188 | C2H4S5 | 000292-46-6 | 38 |
| 2 | Hexathiepane | 206 | CH2S6 | 017233-71-5 | 35 |
| 3 | 3,4-Ethylenedioxythiophene | 142 | C6H6O2S | 126213-50-1 | 9 |
| 4 | 4(1H)-Pyrimidinone, 2-(methylthio)- | 142 | C5H6N2OS | 005751-20-2 | 9 |
| 5 | 1,3-Benzenedithiol | 142 | C6H6S2 | 000626-04-0 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021122\
Data File : BF126858.D
Acq On : 11 Feb 2022 15:35
Operator : CG\JU
Sample : N1477-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220087-AMENDED-BERKELEY-7-COMP

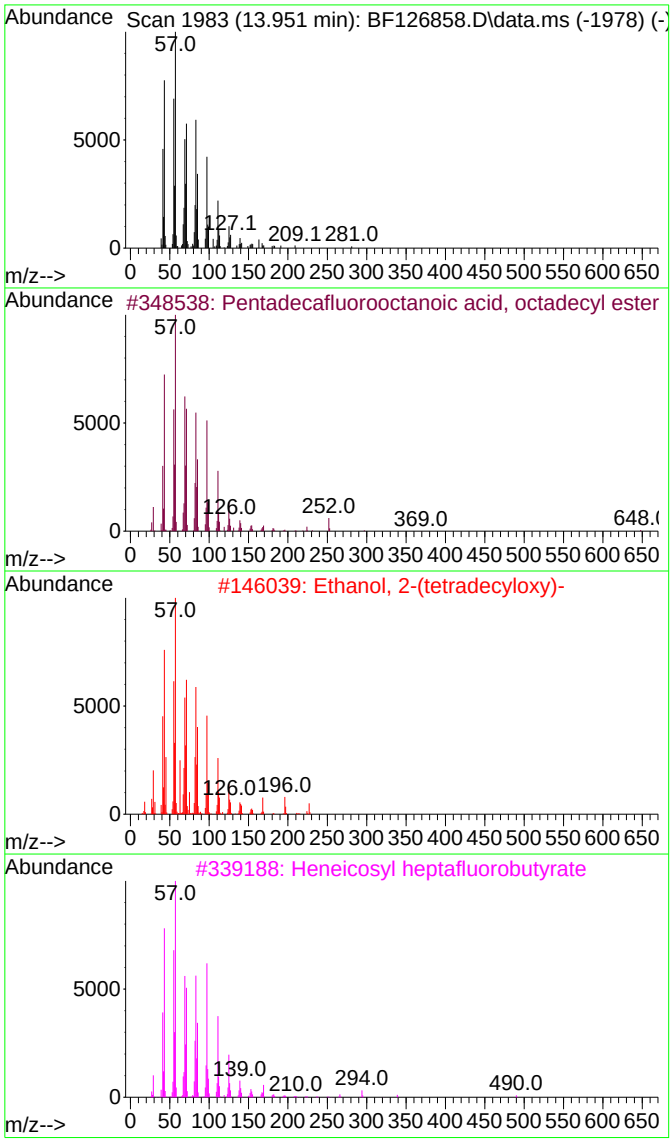
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

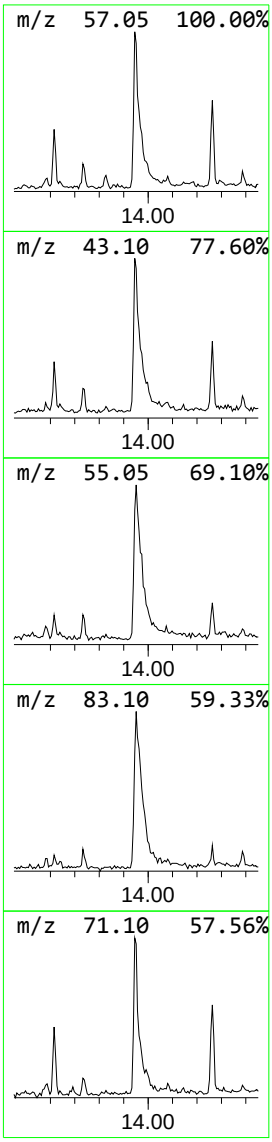
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.951 | 9.41 ng | 420056 | Chrysene-d12 | 14.110 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentadecafluorooctanoic acid, oc... | 666 | C26H37F15O2 | 1000406-04-8 | 91 |
| 2 | Ethanol, 2-(tetradecyloxy)- | 258 | C16H34O2 | 002136-70-1 | 91 |
| 3 | Heneicosyl heptafluorobutyrate | 508 | C25H43F7O2 | 1000351-83-8 | 91 |
| 4 | Oxalic acid, isobutyl hexadecyl ... | 370 | C22H42O4 | 1000309-38-1 | 87 |
| 5 | Octacosyl trifluoroacetate | 506 | C30H57F3O2 | 1000351-74-9 | 87 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021122\
Data File : BF126858.D
Acq On : 11 Feb 2022 15:35
Operator : CG\JU
Sample : N1477-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220087-AMENDED-BERKELEY-7-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

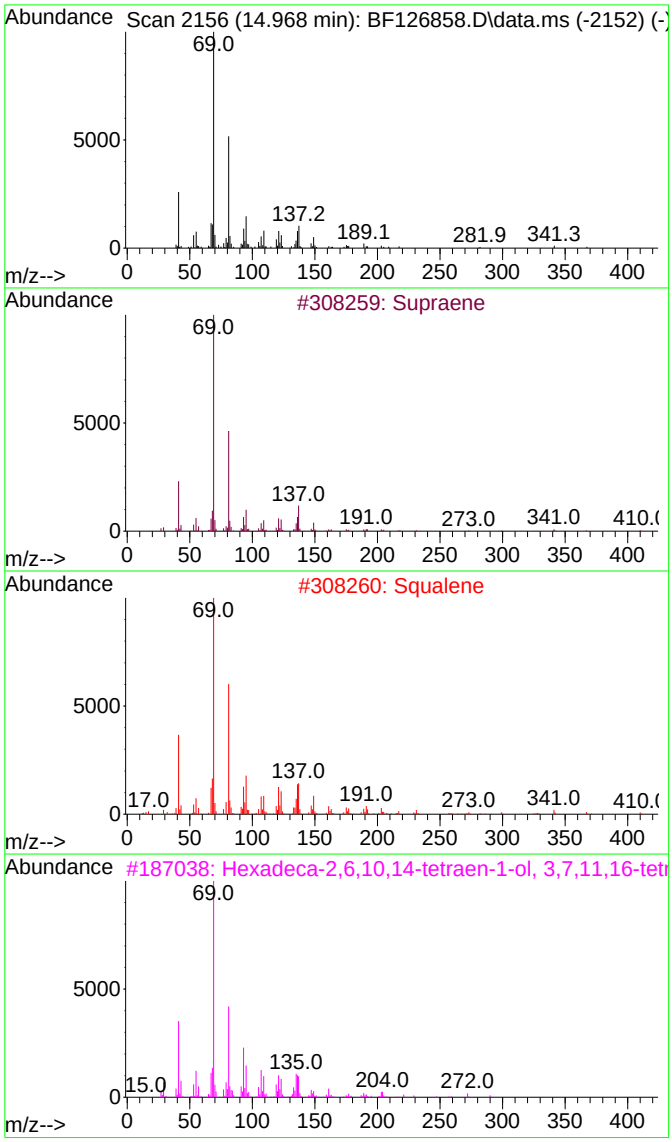
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

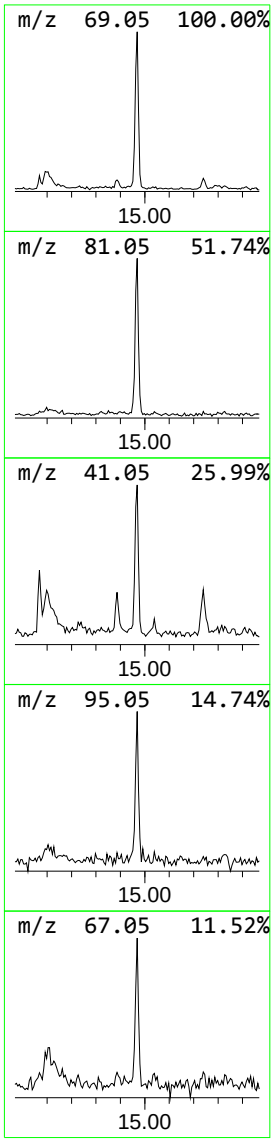
**********

Peak Number 7 Supraene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.969 | 2.83 ng | 103839 | Perylene-d12 | 15.621 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Supraene | 410 | C30H50 | 007683-64-9 | 91 |
| 2 | Squalene | 410 | C30H50 | 000111-02-4 | 90 |
| 3 | Hexadeca-2,6,10,14-tetraen-1-ol,... | 290 | C20H34O | 007614-21-3 | 86 |
| 4 | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 72 |
| 5 | 2,6,10,14-Hexadecatetraenoic aci... | 332 | C22H36O2 | 024035-35-6 | 64 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021122\
Data File : BF126858.D
Acq On : 11 Feb 2022 15:35
Operator : CG\JU
Sample : N1477-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220087-AMENDED-BERKELEY-7-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

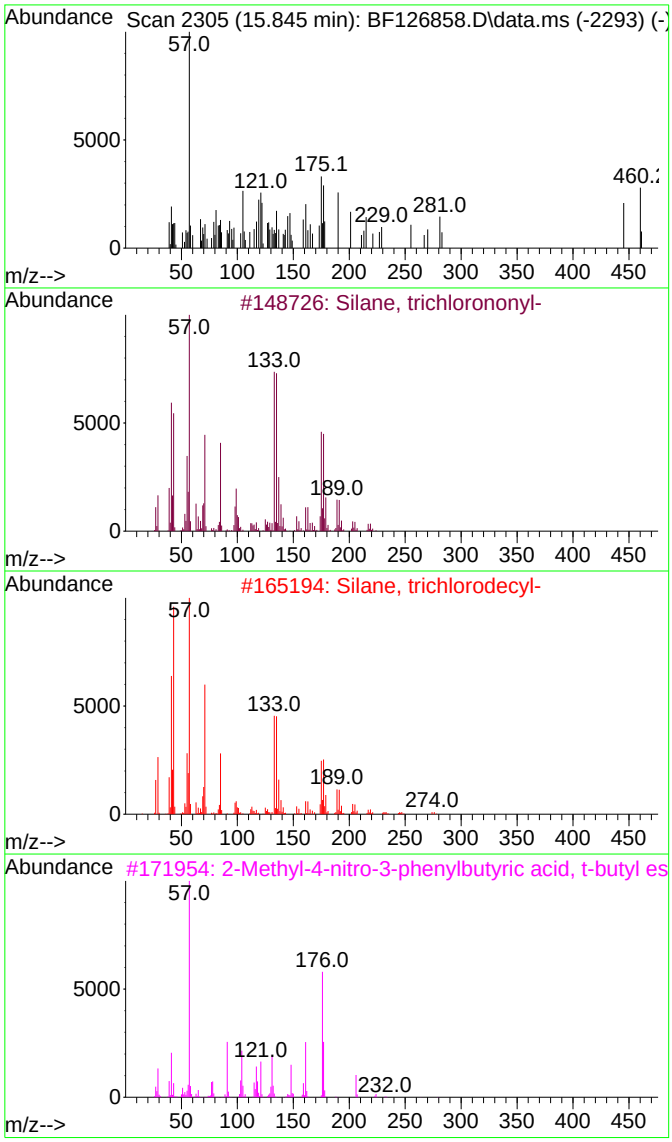
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

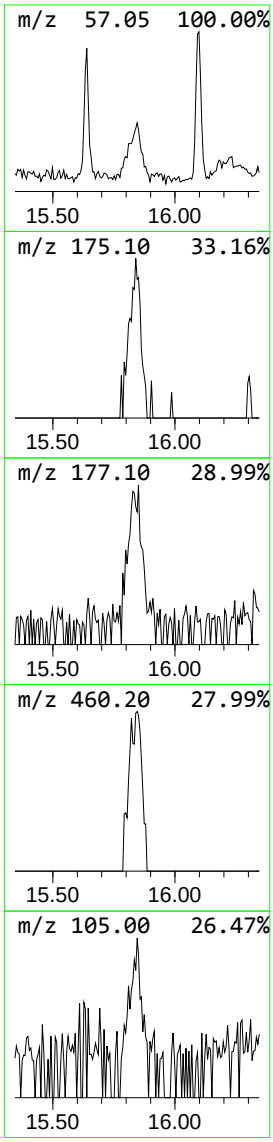
**********

Peak Number 8 unknown15.845 Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.845 | 2.23 ng | 81901 | Perylene-d12 | 15.621 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Silane, trichlorononyl- | 260 | C9H19Cl3Si | 005283-67-0 | 9 |
| 2 | Silane, trichlorodecyl- | 274 | C10H21Cl3Si | 013829-21-5 | 9 |
| 3 | 2-Methyl-4-nitro-3-phenylbutyric... | 279 | C15H21NO4 | 1000186-56-8 | 9 |
| 4 | Propanehydrazide, N2-(3-trifluor... | 232 | C10H11F3N2O | 120773-99-1 | 7 |
| 5 | Silane, tert-butyldichlorophenyl- | 232 | C10H14Cl2Si | 017887-41-1 | 4 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021122\
Data File : BF126858.D
Acq On : 11 Feb 2022 15:35
Operator : CG\JU
Sample : N1477-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220087-AMENDED-BERKELEY-7-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.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 |
| 2-Pentanone, 4-... | 5.181 | 5.5 | ng | 202013 | 1 | 6.940 | 740926 | 20.0 |
| Ethanol, 2,2'-o... | 6.475 | 2.1 | ng | 79223 | 1 | 6.940 | 740926 | 20.0 |
| 1,2,4-Trithiolane | 7.657 | 2.5 | ng | 127793 | 2 | 8.222 | 1018900 | 20.0 |
| Lenthionine | 10.904 | 3.1 | ng | 192246 | 4 | 11.469 | 1249870 | 20.0 |
| unknown11.345 | 11.345 | 2.3 | ng | 146324 | 4 | 11.469 | 1249870 | 20.0 |
| Pentadecafluoro... | 13.951 | 9.4 | ng | 420056 | 5 | 14.110 | 892407 | 20.0 |
| Supraene | 14.969 | 2.8 | ng | 103839 | 6 | 15.621 | 734225 | 20.0 |
| unknown15.845 | 15.845 | 2.2 | ng | 81901 | 6 | 15.621 | 734225 | 20.0 |