LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051045.D
Acq On : 15 Nov 2021 17:21
Operator : CG/JU
Sample : M4595-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
CMC-OF4-001-002

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-BG111321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051045.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.297 | 300 | 308 | 315 | rBV | 53197 | 83669 | 3.74% | 0.664% |
| 2 | 5.762 | 380 | 387 | 398 | rBV | 675454 | 1118744 | 49.98% | 8.872% |
| 3 | 7.377 | 653 | 662 | 671 | rBV | 680261 | 1228589 | 54.89% | 9.744% |
| 4 | 8.223 | 798 | 806 | 819 | rBV | 156398 | 281387 | 12.57% | 2.232% |
| 5 | 9.404 | 998 | 1007 | 1015 | rBV | 414021 | 773631 | 34.56% | 6.135% |
| 6 | 10.803 | 1237 | 1245 | 1258 | rBV | 155078 | 291221 | 13.01% | 2.310% |
| 7 | 11.055 | 1280 | 1288 | 1296 | rBV | 222297 | 411090 | 18.37% | 3.260% |
| 8 | 13.476 | 1692 | 1700 | 1712 | rVB | 1097578 | 1766029 | 78.90% | 14.006% |
| 9 | 13.717 | 1737 | 1741 | 1748 | rVB2 | 14798 | 23519 | 1.05% | 0.187% |
| 10 | 14.851 | 1926 | 1934 | 1943 | rBV | 372876 | 595118 | 26.59% | 4.720% |
| 11 | 16.337 | 2181 | 2187 | 2196 | rBV | 826607 | 1284060 | 57.37% | 10.184% |
| 12 | 17.307 | 2348 | 2352 | 2356 | rBV3 | 16522 | 23962 | 1.07% | 0.190% |
| 13 | 17.360 | 2357 | 2361 | 2366 | rVV4 | 15454 | 23465 | 1.05% | 0.186% |
| 14 | 17.601 | 2395 | 2402 | 2408 | rBV | 445601 | 703718 | 31.44% | 5.581% |
| 15 | 17.706 | 2416 | 2420 | 2424 | rBV5 | 16821 | 24573 | 1.10% | 0.195% |
| 16 | 18.047 | 2475 | 2478 | 2482 | rBV4 | 15083 | 25334 | 1.13% | 0.201% |
| 17 | 18.224 | 2505 | 2508 | 2513 | rVB2 | 40681 | 52397 | 2.34% | 0.416% |
| 18 | 18.447 | 2543 | 2546 | 2551 | rBV2 | 40333 | 58810 | 2.63% | 0.466% |
| 19 | 19.363 | 2699 | 2702 | 2703 | rBV3 | 25565 | 26630 | 1.19% | 0.211% |
| 20 | 19.387 | 2703 | 2706 | 2709 | rVB4 | 50518 | 61539 | 2.75% | 0.488% |
| 21 | 20.186 | 2837 | 2842 | 2848 | rVB | 1641758 | 2238273 | 100.00% | 17.751% |
| 22 | 21.490 | 3061 | 3064 | 3076 | rVB3 | 102464 | 201922 | 9.02% | 1.601% |
| 23 | 21.902 | 3128 | 3134 | 3144 | rVB | 354930 | 663223 | 29.63% | 5.260% |
| 24 | 25.309 | 3707 | 3714 | 3727 | rVB3 | 209503 | 648216 | 28.96% | 5.141% |

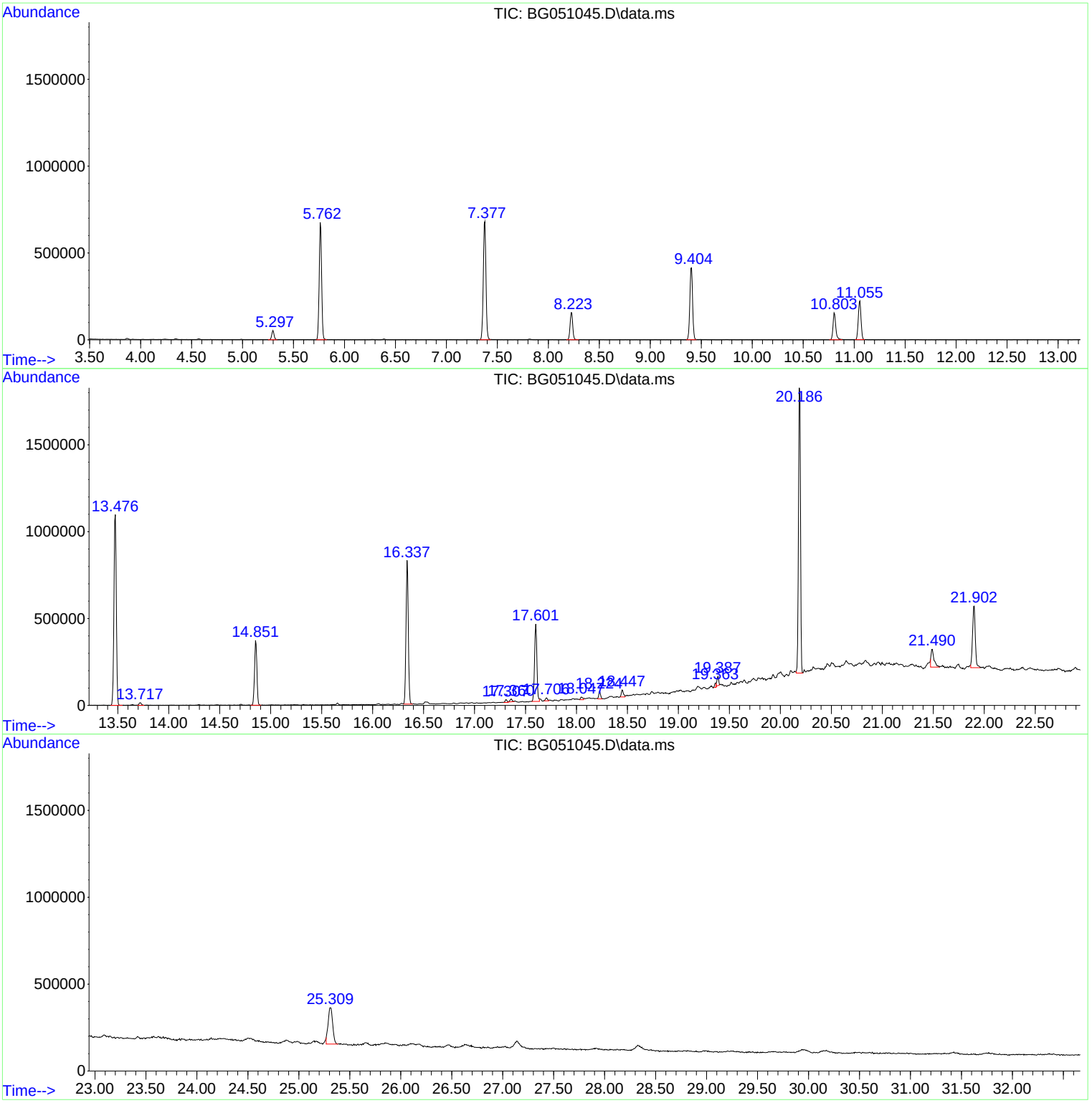
Sum of corrected areas: 12609119

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051045.D
Acq On : 15 Nov 2021 17:21
Operator : CG/JU
Sample : M4595-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
CMC-OF4-001-002

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.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\BG111621\
Data File : BG051045.D
Acq On : 15 Nov 2021 17:21
Operator : CG/JU
Sample : M4595-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
CMC-OF4-001-002

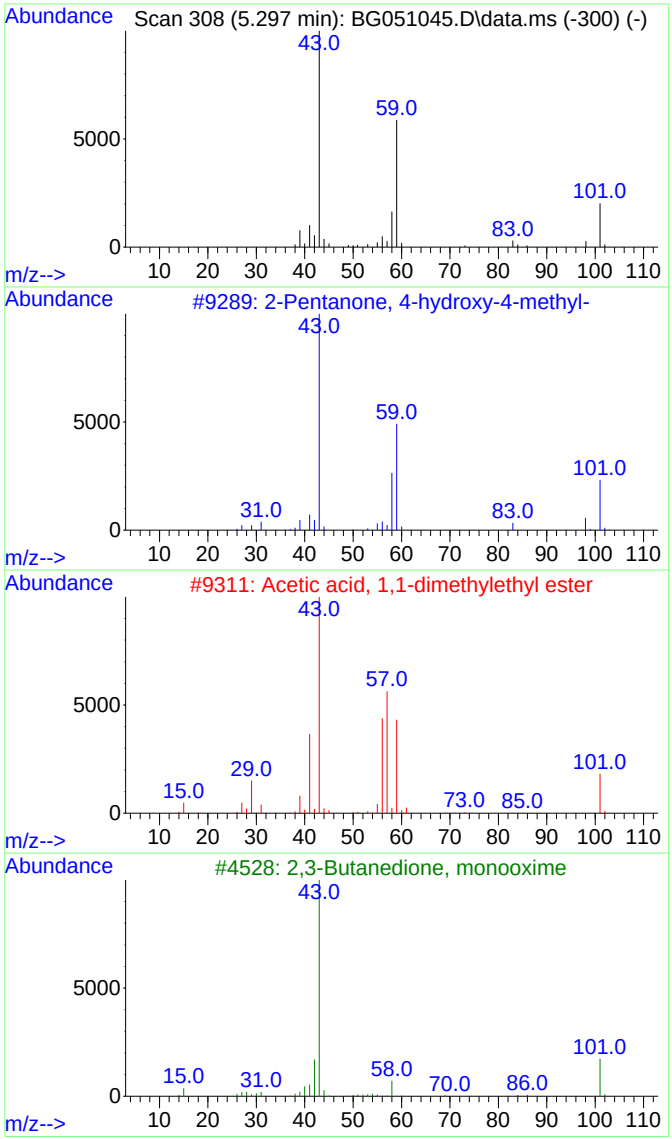
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

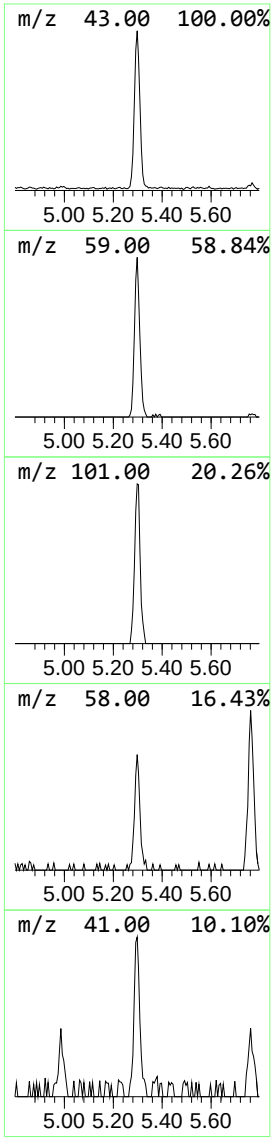
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.297 | 5.95 ng | 83669 | 1,4-Dichlorobenzene-d4 | 8.229 |

| 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, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 35 |
| 4 | 3-Octanol | 130 | C8H18O | 000589-98-0 | 28 |
| 5 | Butyl aldoxime, 3-methyl-, syn- | 101 | C5H11NO | 005780-40-5 | 25 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051045.D
Acq On : 15 Nov 2021 17:21
Operator : CG/JU
Sample : M4595-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
CMC-OF4-001-002

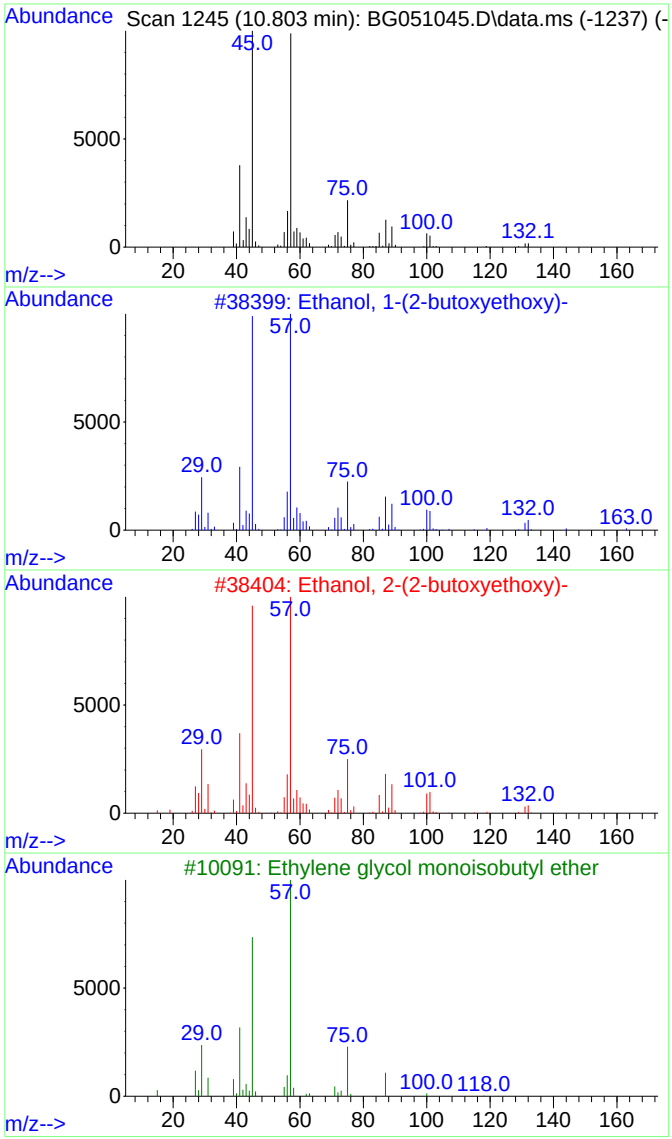
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

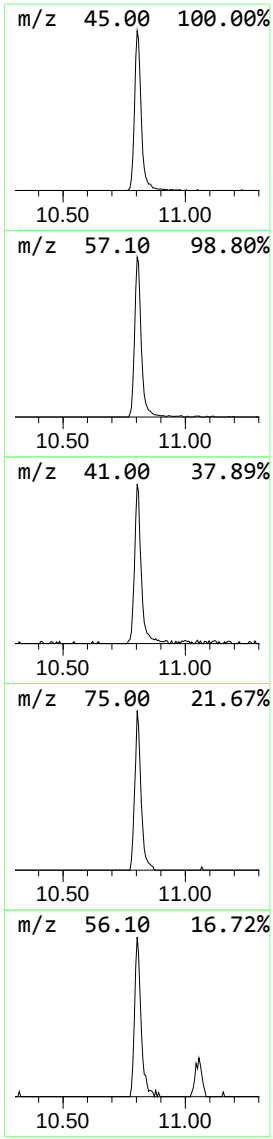
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.803 | 14.17 ng | 291221 | Naphthalene-d8 | 11.055 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 1-(2-butoxyethoxy)- | 162 | C8H18O3 | 054446-78-5 | 90 |
| 2 | Ethanol, 2-(2-butoxyethoxy)- | 162 | C8H18O3 | 000112-34-5 | 90 |
| 3 | Ethylene glycol monoisobutyl ether | 118 | C6H14O2 | 004439-24-1 | 72 |
| 4 | Methoxyacetic acid, 2-butyl ester | 146 | C7H14O3 | 070159-90-9 | 50 |
| 5 | Di-sec-Butyl ether | 130 | C8H18O | 006863-58-7 | 50 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051045.D
Acq On : 15 Nov 2021 17:21
Operator : CG/JU
Sample : M4595-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
CMC-OF4-001-002

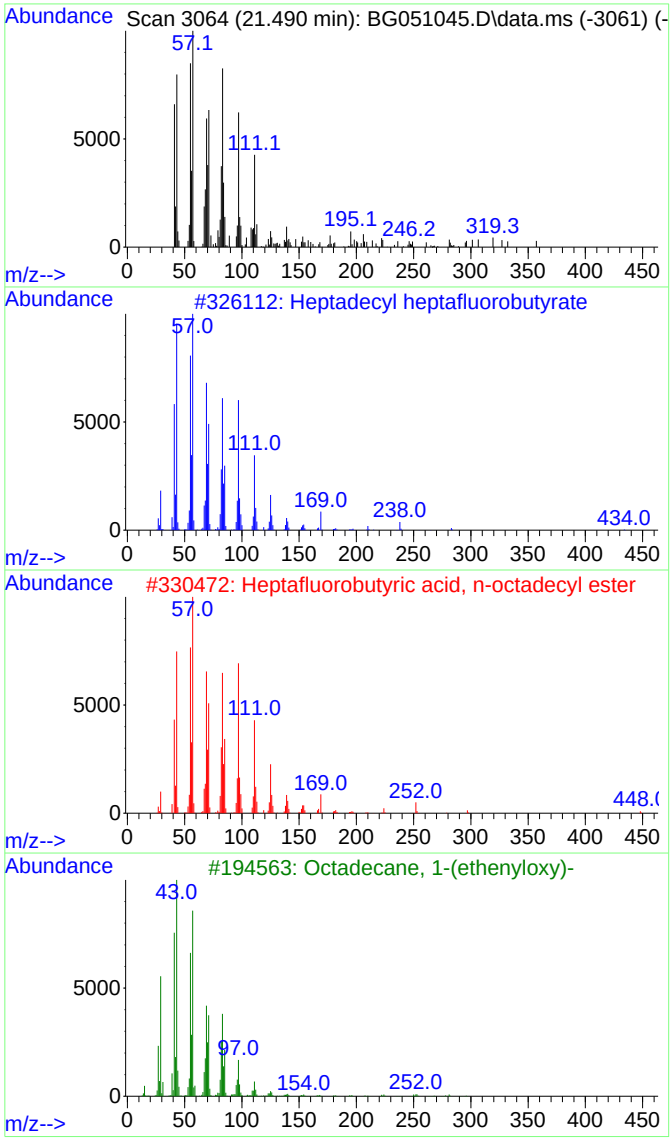
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

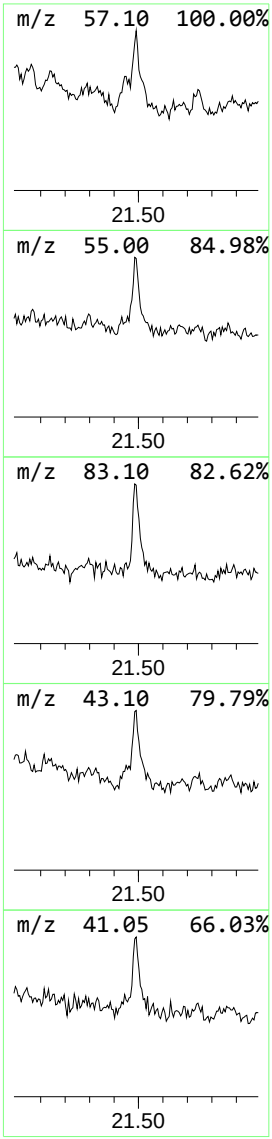
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 Heptadecyl heptafluorobutyrate Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.490 | 6.09 ng | 201922 | Chrysene-d12 | 21.902 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 86 |
| 2 | Heptafluorobutyric acid, n-octad... | 466 | C22H37F7O2 | 000400-57-7 | 86 |
| 3 | Octadecane, 1-(ethenyloxy)- | 296 | C20H40O | 000930-02-9 | 86 |
| 4 | Pentafluoropropionic acid, octad... | 416 | C21H37F5O2 | 959261-25-7 | 86 |
| 5 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 80 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051045.D
Acq On : 15 Nov 2021 17:21
Operator : CG/JU
Sample : M4595-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
CMC-OF4-001-002

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.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-... | 5.297 | 6.0 | ng | 83669 | 1 | 8.229 | 281387 | 20.0 |
| Ethanol, 1-(2-b... | 10.803 | 14.2 | ng | 291221 | 2 | 11.055 | 411090 | 20.0 |
| Heptadecyl hept... | 21.490 | 6.1 | ng | 201922 | 5 | 21.902 | 663223 | 20.0 |