LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP072220\
Data File : BP002831.D
Acq On : 22 Jul 2020 18:40
Operator : CG/JU
Sample : L3189-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** BU-02-072120

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_P\METHODS\8270-BP071020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 4.705 | 304 | 309 | 319 | rBV | 91912 | 130464 | 4.21% | 0.536% |
| 2 | 5.175 | 383 | 389 | 416 | rBV | 1337015 | 2063876 | 66.55% | 8.475% |
| 3 | 6.758 | 651 | 658 | 670 | rBV | 1211612 | 2138872 | 68.97% | 8.783% |
| 4 | 6.852 | 670 | 674 | 684 | rVB | 31692 | 60869 | 1.96% | 0.250% |
| 5 | 7.546 | 784 | 792 | 802 | rBV | 626949 | 974979 | 31.44% | 4.004% |
| 6 | 8.693 | 980 | 987 | 1006 | rBV | 804739 | 1405415 | 45.32% | 5.771% |
| 7 | 10.316 | 1255 | 1263 | 1280 | rBV | 777321 | 1372856 | 44.27% | 5.638% |
| 8 | 12.810 | 1680 | 1687 | 1705 | rBV | 1927006 | 3034180 | 97.83% | 12.460% |
| 9 | 13.663 | 1827 | 1832 | 1845 | rBV | 237383 | 354750 | 11.44% | 1.457% |
| 10 | 13.916 | 1871 | 1875 | 1885 | rVB | 45564 | 74745 | 2.41% | 0.307% |
| 11 | 14.198 | 1916 | 1923 | 1932 | rBV2 | 1106147 | 1672575 | 53.93% | 6.869% |
| 12 | 15.704 | 2173 | 2179 | 2190 | rBV | 1128647 | 1788159 | 57.66% | 7.343% |
| 13 | 16.534 | 2316 | 2320 | 2326 | rBV2 | 29000 | 40893 | 1.32% | 0.168% |
| 14 | 16.957 | 2387 | 2392 | 2398 | rBV | 1164067 | 1753346 | 56.53% | 7.200% |
| 15 | 17.098 | 2412 | 2416 | 2422 | rVB | 48423 | 79474 | 2.56% | 0.326% |
| 16 | 18.616 | 2670 | 2674 | 2679 | rBV | 235495 | 286989 | 9.25% | 1.179% |
| 17 | 18.710 | 2686 | 2690 | 2692 | rBV2 | 47238 | 71831 | 2.32% | 0.295% |
| 18 | 18.992 | 2734 | 2738 | 2744 | rBV2 | 110379 | 178150 | 5.74% | 0.732% |
| 19 | 19.339 | 2794 | 2797 | 2802 | rVB | 128043 | 161887 | 5.22% | 0.665% |
| 20 | 19.545 | 2827 | 2832 | 2844 | rVB | 2355964 | 3101387 | 100.00% | 12.736% |
| 21 | 20.227 | 2945 | 2948 | 2953 | rVB3 | 71994 | 97654 | 3.15% | 0.401% |
| 22 | 20.433 | 2979 | 2983 | 2988 | rBV | 207377 | 260074 | 8.39% | 1.068% |
| 23 | 20.798 | 3042 | 3045 | 3053 | rBV | 353034 | 475862 | 15.34% | 1.954% |
| 24 | 21.069 | 3086 | 3091 | 3096 | rBV | 1172108 | 1506098 | 48.56% | 6.185% |
| 25 | 23.257 | 3458 | 3463 | 3470 | rVB2 | 718647 | 1265958 | 40.82% | 5.199% |

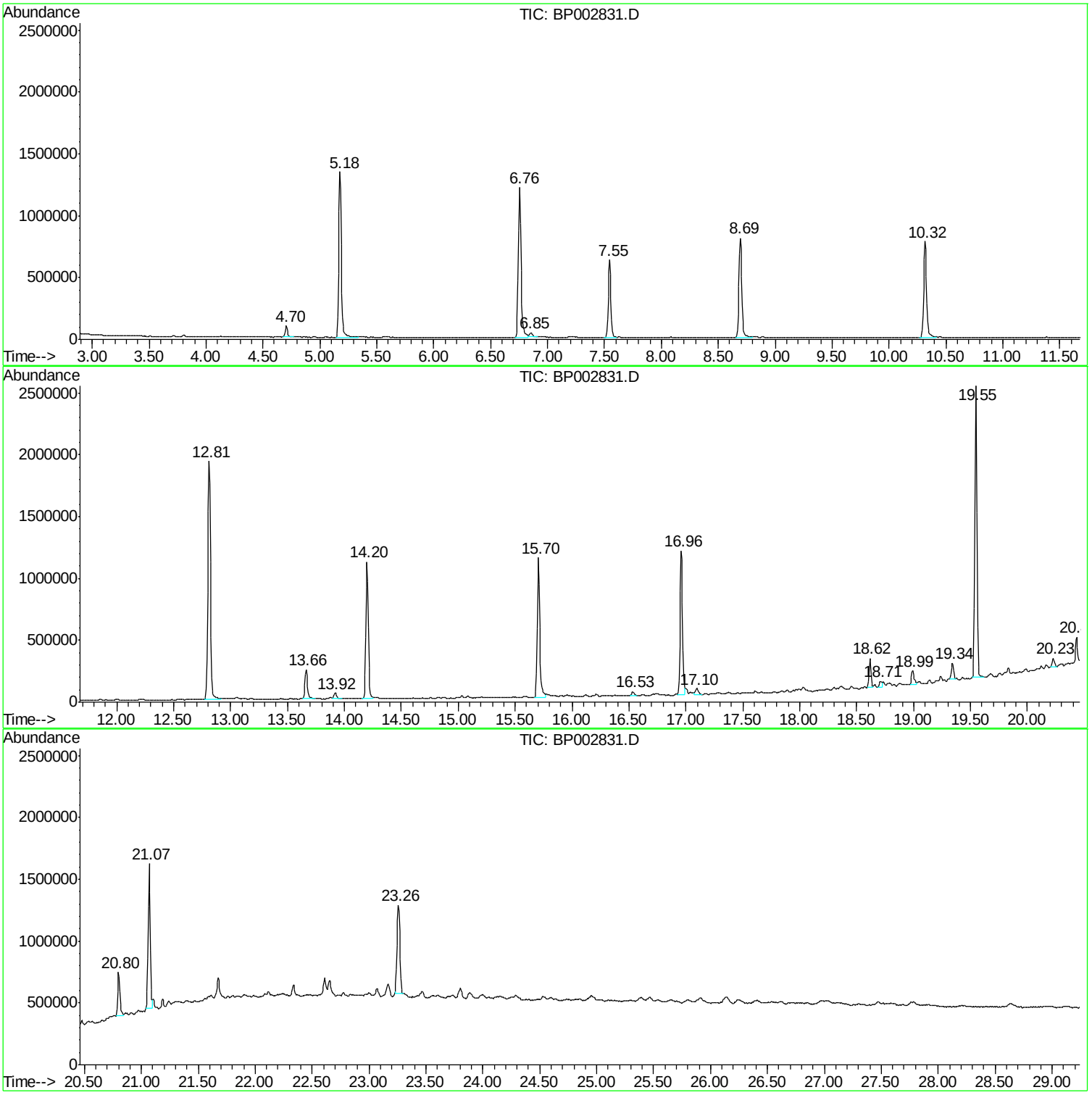
Sum of corrected areas: 24351343

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP072220\
Data File : BP002831.D
Acq On : 22 Jul 2020 18:40
Operator : CG/JU
Sample : L3189-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
BU-02-072120

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP071020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP072220\
Data File : BP002831.D
Acq On : 22 Jul 2020 18:40
Operator : CG/JU
Sample : L3189-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** BU-02-072120

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP071020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

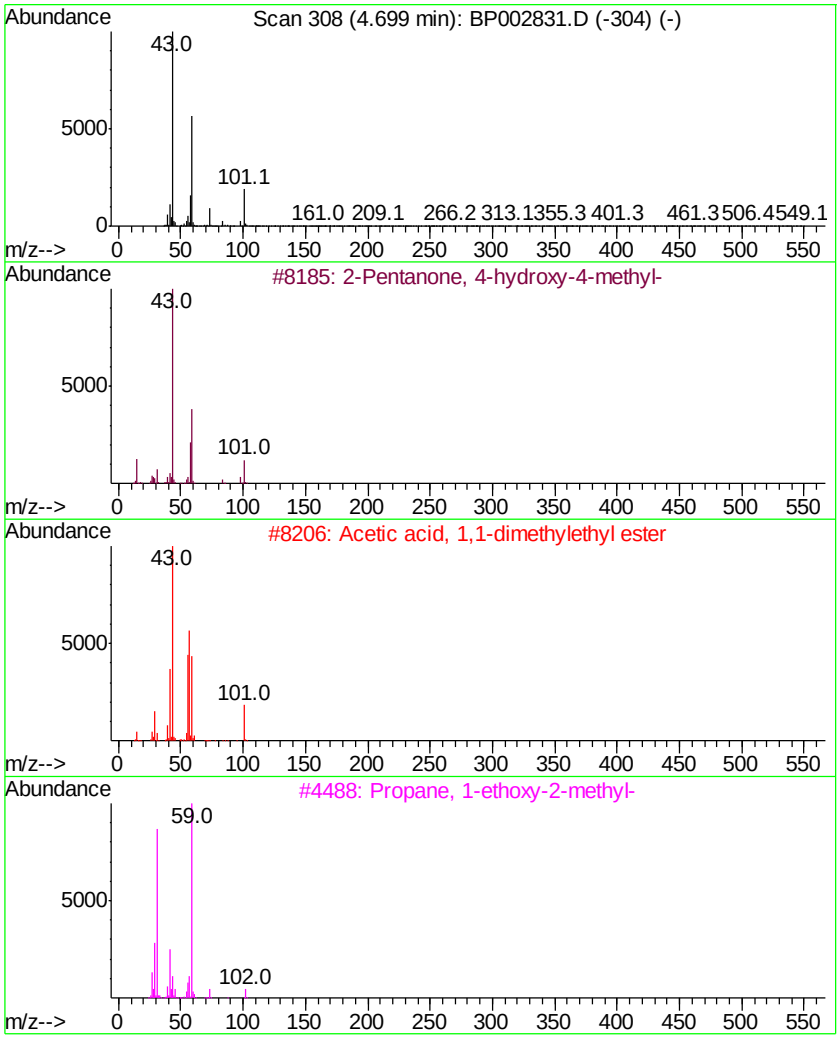
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

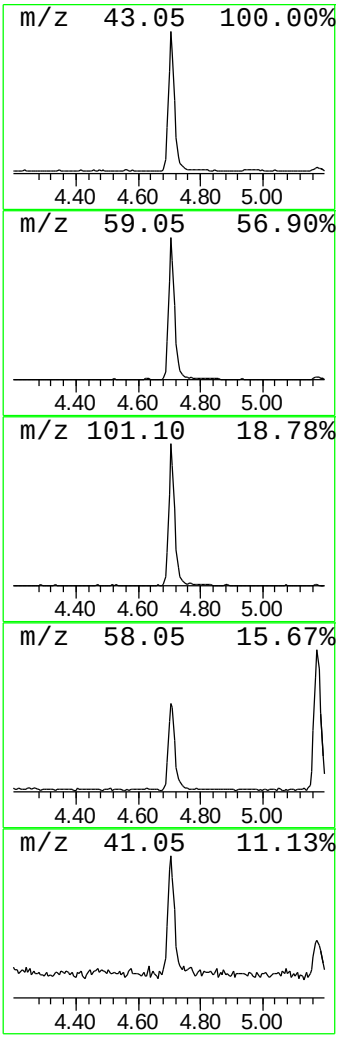
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.70 | 2.68 ng | 130464 | 1,4-Dichlorobenzene-d4 | 7.55 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 50 |
| 3 | Propane, 1-ethoxy-2-methyl- | 102 | C6H14O | 000627-02-1 | 32 |
| 4 | Guanidine | 59 | CH5N3 | 000113-00-8 | 9 |
| 5 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP072220\
Data File : BP002831.D
Acq On : 22 Jul 2020 18:40
Operator : CG/JU
Sample : L3189-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** BU-02-072120

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP071020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

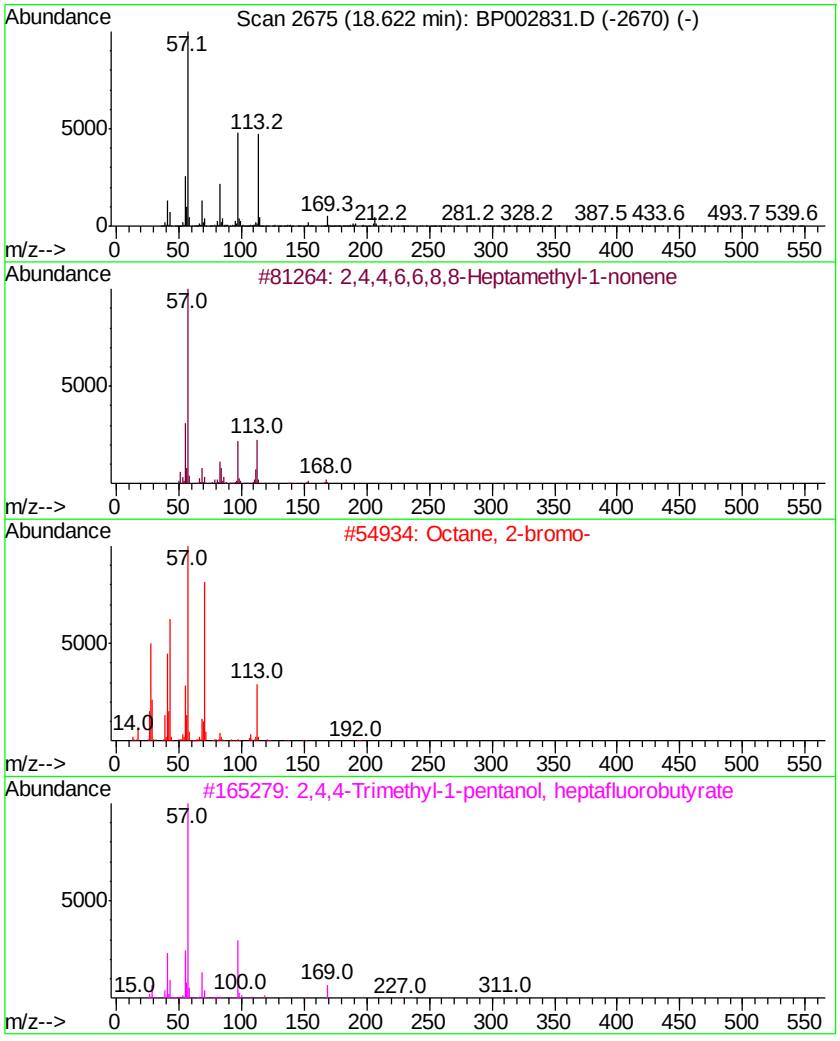
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

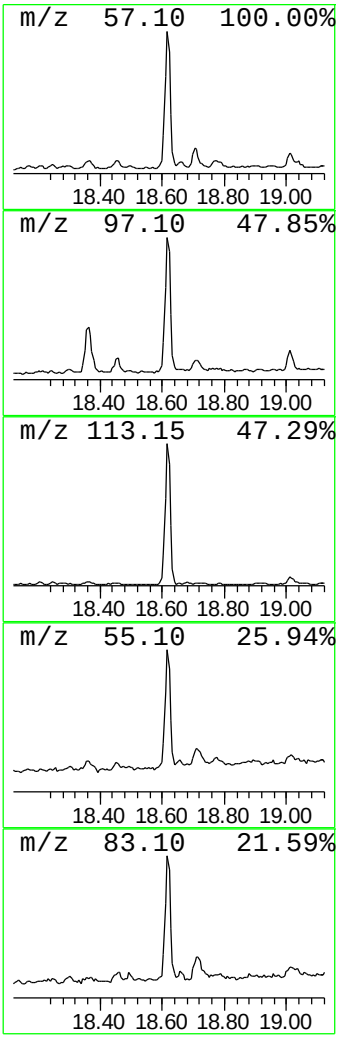
**********

Peak Number 2 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.62 | 3.27 ng | 286989 | Phenanthrene-d10 | 16.96 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,4,4,6,6,8,8-Heptamethyl-1-nonene | 224 | C16H32 | 015796-04-0 | 56 |
| 2 | Octane, 2-bromo- | 192 | C8H17Br | 000557-35-7 | 37 |
| 3 | 2,4,4-Trimethyl-1-pentanol, hept... | 326 | C12H17F7O2 | 1000365-01-4 | 35 |
| 4 | 1-Pentanol, 3-methyl-2-propyl- | 144 | C9H20O | 054004-40-9 | 28 |
| 5 | 2,4,4-Trimethyl-1-pentanol, trif... | 226 | C10H17F3O2 | 1000365-19-5 | 25 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP072220\
Data File : BP002831.D
Acq On : 22 Jul 2020 18:40
Operator : CG/JU
Sample : L3189-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** BU-02-072120

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP071020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

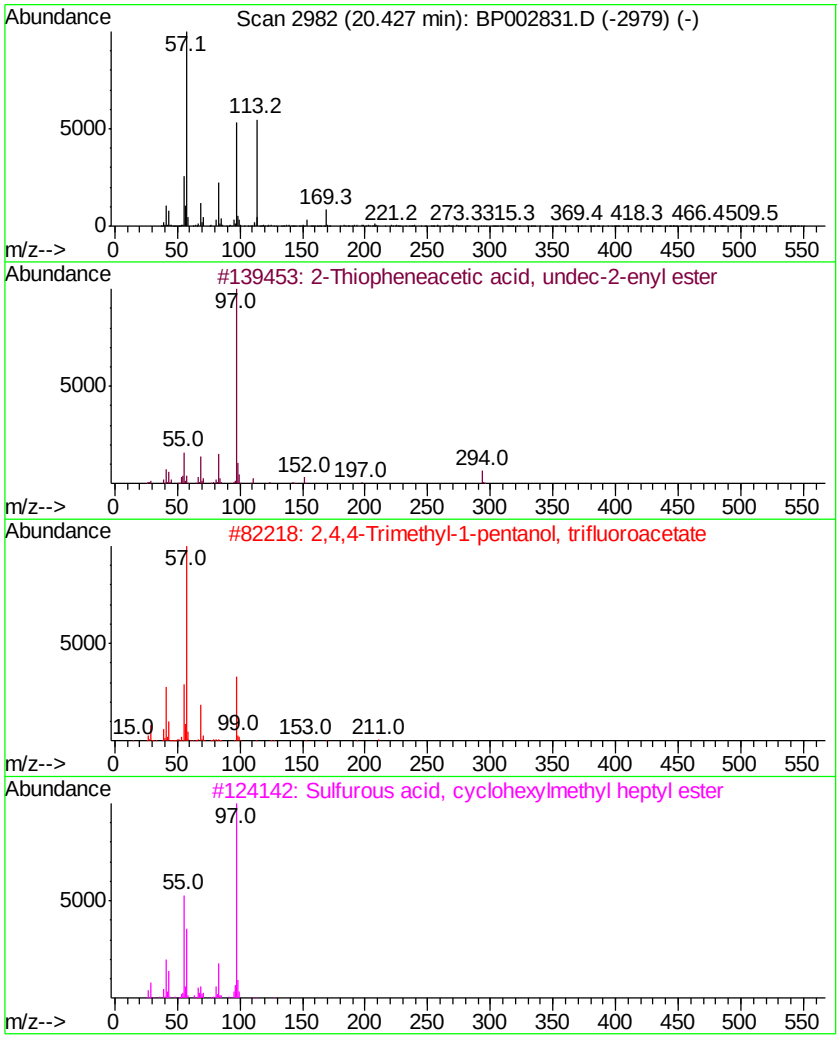
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

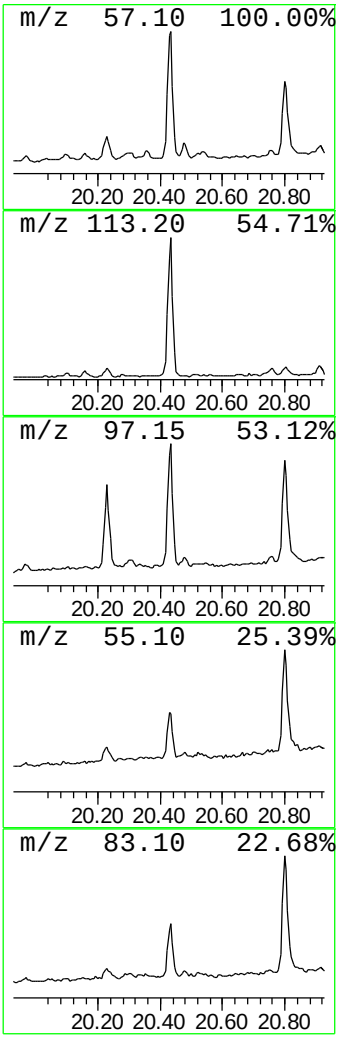
**********

Peak Number 4 unknown20.43 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.43 | 3.45 ng | 260074 | Chrysene-d12 | 21.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Thiopheneacetic acid, undec-2-... | 294 | C17H26O2S | 1000299-39-0 | 32 |
| 2 | 2,4,4-Trimethyl-1-pentanol, trif... | 226 | C10H17F3O2 | 1000365-19-5 | 25 |
| 3 | Sulfurous acid, cyclohexylmethyl... | 276 | C14H28O3S | 1000309-21-7 | 25 |
| 4 | 3-Cyclopent-1-enyl-3-hydroxy-2-m... | 170 | C9H14O3 | 1000191-19-7 | 22 |
| 5 | 6H-Pyrido[2,3-b][1,4]benzodiazep... | 351 | C19H21N5O2 | 028797-61-7 | 22 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP072220\
Data File : BP002831.D
Acq On : 22 Jul 2020 18:40
Operator : CG/JU
Sample : L3189-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** BU-02-072120

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP071020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

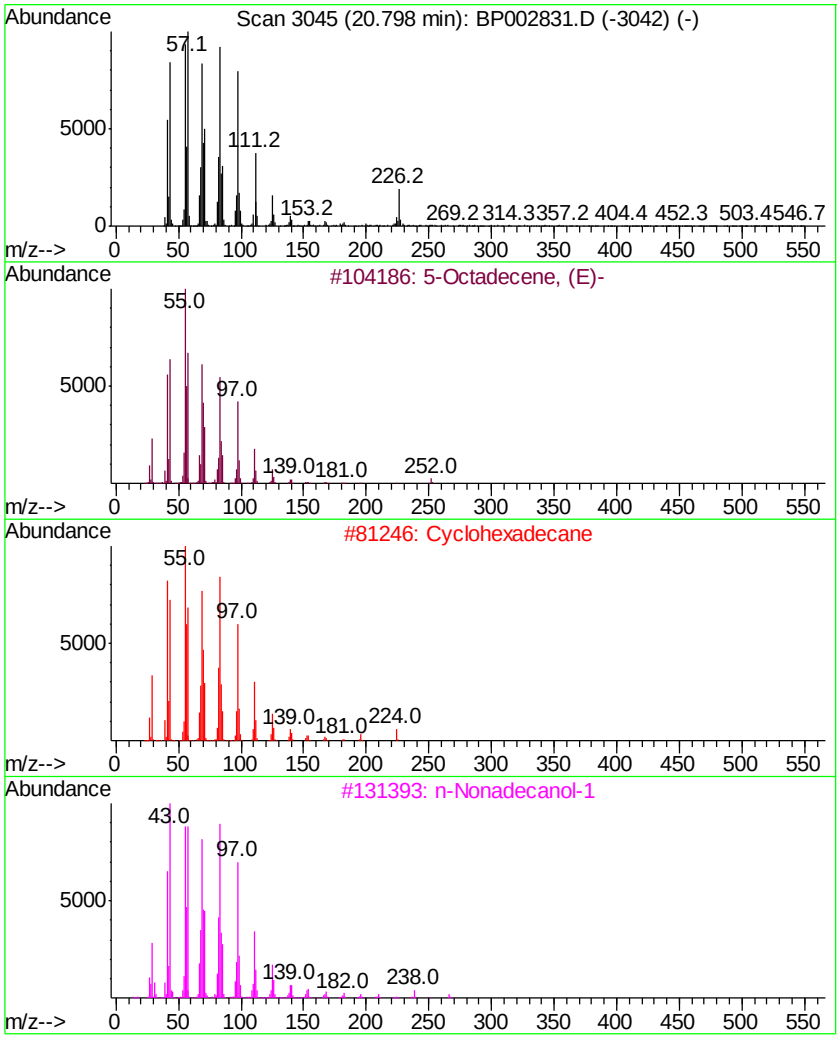
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

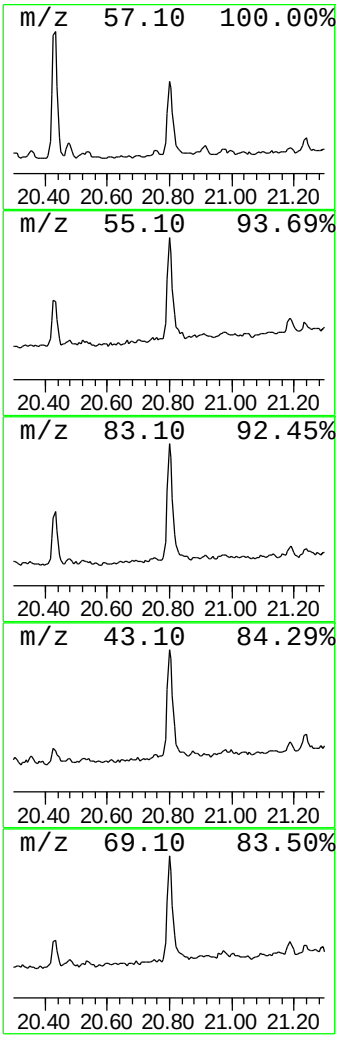
**********

Peak Number 5 5-Octadecene, (E)- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.80 | 6.32 ng | 475862 | Chrysene-d12 | 21.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Octadecene, (E)- | 252 | C18H36 | 007206-21-5 | 94 |
| 2 | Cyclohexadecane | 224 | C16H32 | 000295-65-8 | 94 |
| 3 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 94 |
| 4 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 94 |
| 5 | 1-Heneicosyl formate | 340 | C22H44O2 | 077899-03-7 | 94 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP072220\
Data File : BP002831.D
Acq On : 22 Jul 2020 18:40
Operator : CG/JU
Sample : L3189-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** BU-02-072120

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP071020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 4.70 | 2.7 | ng | 130464 | 1 | 7.55 | 974979 | 20.0 |
| 2,4,4,6,6,8,8-Hep... | 18.62 | 3.3 | ng | 286989 | 4 | 16.96 | 1753350 | 20.0 |
| unknown20.43 | 20.43 | 3.5 | ng | 260074 | 5 | 21.07 | 1506100 | 20.0 |
| 5-Octadecene, (E)- | 20.80 | 6.3 | ng | 475862 | 5 | 21.07 | 1506100 | 20.0 |