LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121087.D
Acq On : 29 Jul 2020 00:28
Operator : JU/CG
Sample : L3457-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SHB-MOTOR-ROOM

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-BF071620.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 | 5.010 | 494 | 497 | 505 | rVB | 67840 | 81311 | 2.01% | 0.347% |
| 2 | 5.422 | 563 | 567 | 576 | rBV | 1695482 | 1725546 | 42.75% | 7.354% |
| 3 | 6.445 | 737 | 741 | 756 | rVB | 1022965 | 1066063 | 26.41% | 4.544% |
| 4 | 6.645 | 772 | 775 | 779 | rBV | 71673 | 70492 | 1.75% | 0.300% |
| 5 | 6.810 | 800 | 803 | 811 | rBV | 1139744 | 899355 | 22.28% | 3.833% |
| 6 | 6.875 | 811 | 814 | 826 | rVV | 415848 | 410998 | 10.18% | 1.752% |
| 7 | 7.375 | 894 | 899 | 902 | rBV | 2278386 | 2228673 | 55.21% | 9.499% |
| 8 | 7.834 | 968 | 977 | 983 | rBV2 | 126689 | 226930 | 5.62% | 0.967% |
| 9 | 8.092 | 1017 | 1021 | 1025 | rBV | 1252000 | 1119558 | 27.74% | 4.772% |
| 10 | 9.016 | 1174 | 1178 | 1181 | rBV | 112374 | 105057 | 2.60% | 0.448% |
| 11 | 9.175 | 1199 | 1205 | 1208 | rBV | 3621777 | 4036516 | 100.00% | 17.204% |
| 12 | 9.292 | 1220 | 1225 | 1229 | rVB | 600256 | 568749 | 14.09% | 2.424% |
| 13 | 9.510 | 1259 | 1262 | 1265 | rBV2 | 48401 | 63041 | 1.56% | 0.269% |
| 14 | 9.563 | 1267 | 1271 | 1275 | rVV2 | 250858 | 264510 | 6.55% | 1.127% |
| 15 | 9.851 | 1315 | 1320 | 1323 | rBV | 1340310 | 1304835 | 32.33% | 5.561% |
| 16 | 10.086 | 1354 | 1360 | 1363 | rBV | 1076395 | 1341714 | 33.24% | 5.718% |
| 17 | 10.439 | 1418 | 1420 | 1425 | rBV | 170342 | 192462 | 4.77% | 0.820% |
| 18 | 10.645 | 1451 | 1455 | 1458 | rBV | 1928600 | 2008288 | 49.75% | 8.559% |
| 19 | 11.033 | 1519 | 1521 | 1524 | rVB | 505347 | 417611 | 10.35% | 1.780% |
| 20 | 11.339 | 1570 | 1573 | 1576 | rBV | 1106288 | 1045069 | 25.89% | 4.454% |
| 21 | 12.939 | 1842 | 1845 | 1851 | rVB2 | 1423335 | 1754148 | 43.46% | 7.476% |
| 22 | 13.992 | 2021 | 2024 | 2029 | rVB | 838291 | 873808 | 21.65% | 3.724% |
| 23 | 15.439 | 2266 | 2270 | 2276 | rVB | 770532 | 1084991 | 26.88% | 4.624% |
| 24 | 16.539 | 2453 | 2457 | 2462 | rVB | 367084 | 573382 | 14.20% | 2.444% |

Sum of corrected areas: 23463107

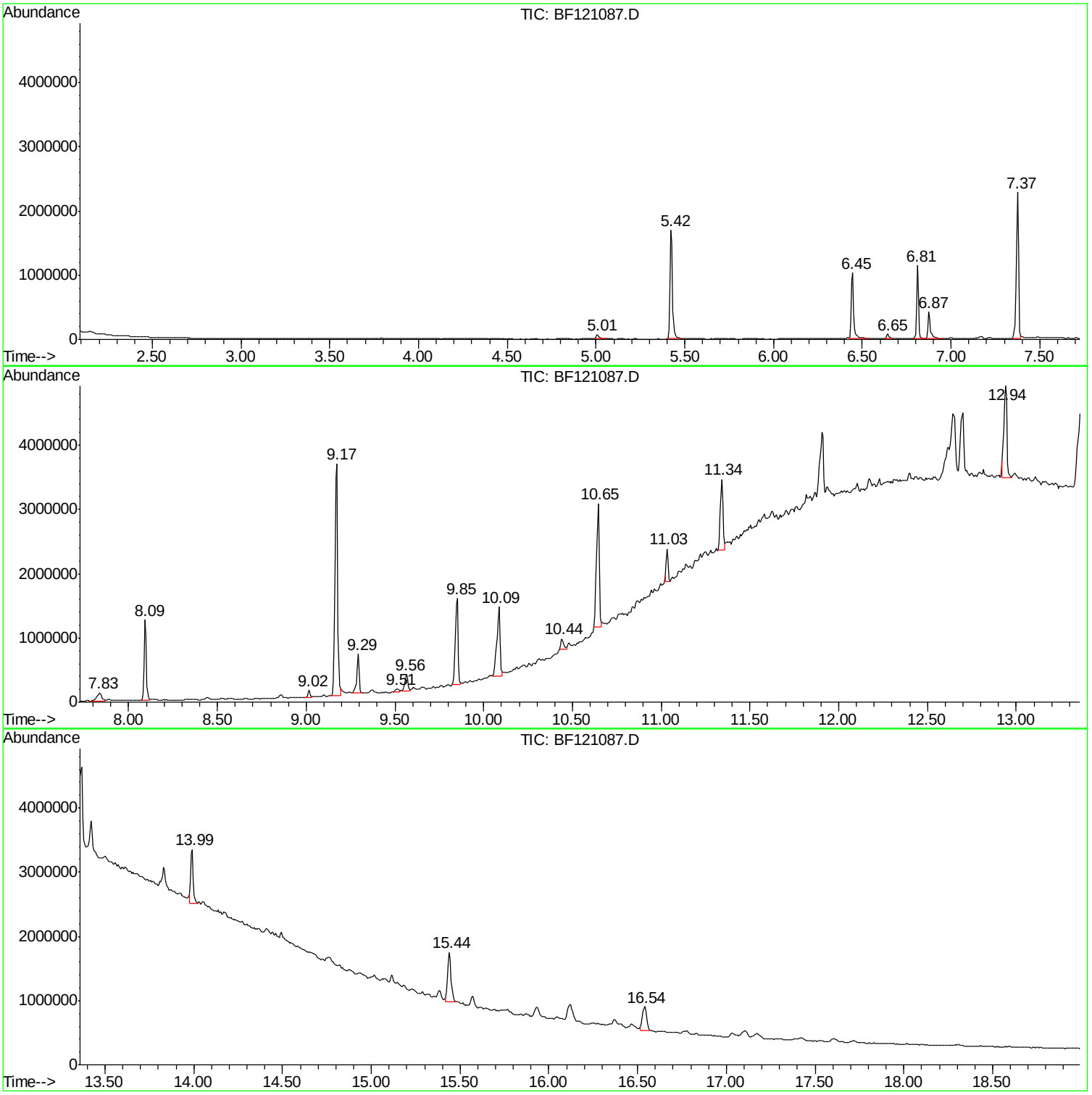
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121087.D
Acq On : 29 Jul 2020 00:28
Operator : JU/CG
Sample : L3457-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SHB-MOTOR-ROOM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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 F\DATA\BF072820\
Data File : BF121087.D
Acq On : 29 Jul 2020 00:28
Operator : JU/CG
Sample : L3457-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SHB-MOTOR-ROOM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

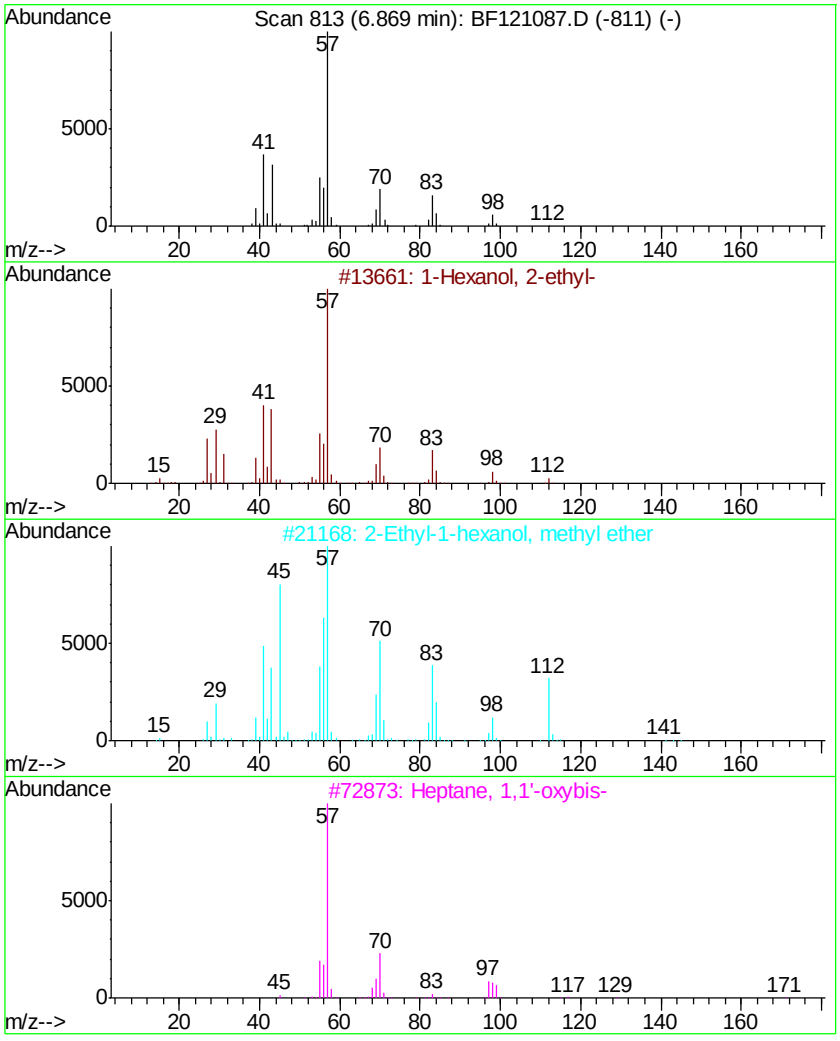
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

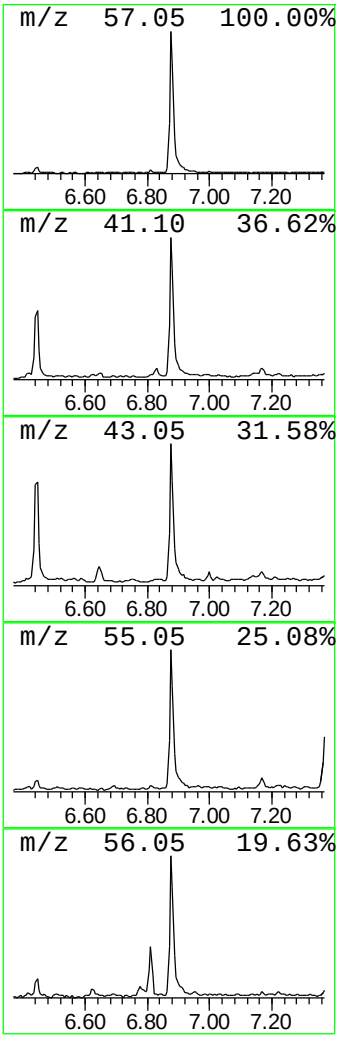
**********

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.87 | 9.14 ng | 410998 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 83 |
| 2 | 2-Ethyl-1-hexanol, methyl ether | 144 | C9H20O | 1000365-10-2 | 59 |
| 3 | Heptane, 1,1'-oxybis- | 214 | C14H30O | 000629-64-1 | 56 |
| 4 | Oxalic acid, isobutyl octyl ester | 258 | C14H26O4 | 1000309-37-3 | 47 |
| 5 | 2-Propyl-1-pentanol | 130 | C8H18O | 058175-57-8 | 45 |



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Data File : BF121087.D
Acq On : 29 Jul 2020 00:28
Operator : JU/CG
Sample : L3457-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SHB-MOTOR-ROOM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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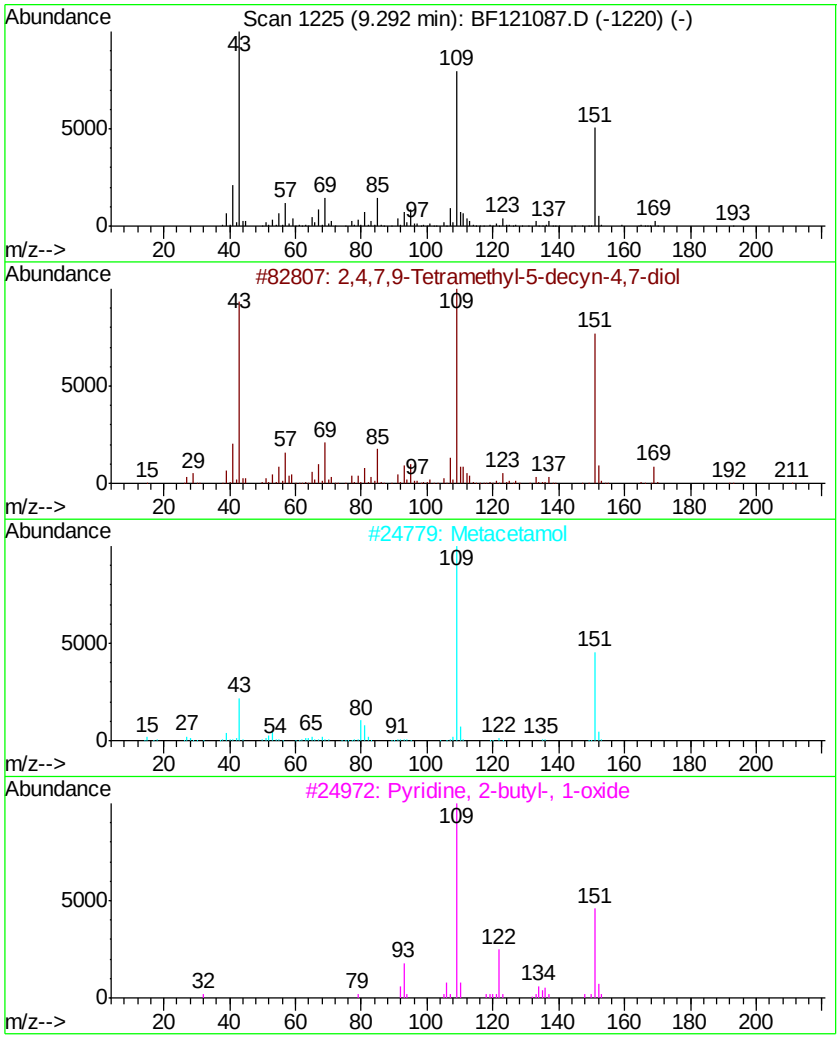
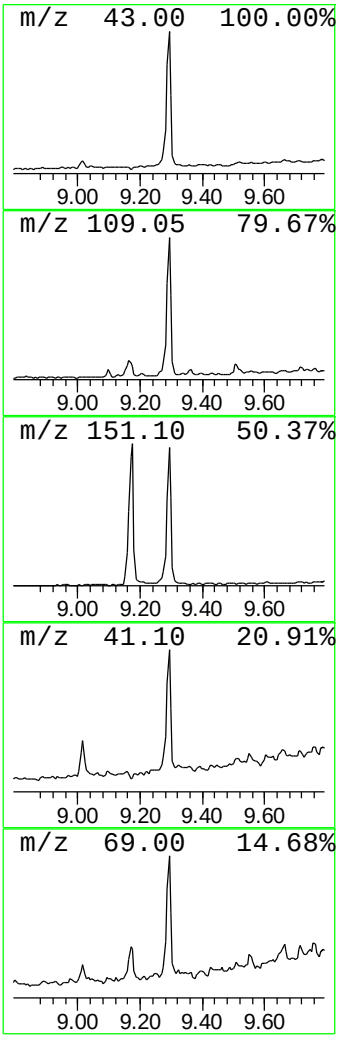
Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.29 | 8.72 ng | 568749 | Acenaphthene-d10 | 9.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,4,7,9-Tetramethyl-5-decyn-4,7-... | 226 | C14H26O2 | 000126-86-3 | 91 |
| 2 | Metacetamol | 151 | C8H9NO2 | 000621-42-1 | 64 |
| 3 | Pyridine, 2-butyl-, 1-oxide | 151 | C9H13NO | 031396-32-4 | 59 |
| 4 | Acetaminophen | 151 | C8H9NO2 | 000103-90-2 | 59 |
| 5 | 1-(1,2,3-Trimethyl-cyclopent-2-e... | 152 | C10H16O | 070987-81-4 | 46 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121087.D
Acq On : 29 Jul 2020 00:28
Operator : JU/CG
Sample : L3457-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SHB-MOTOR-ROOM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

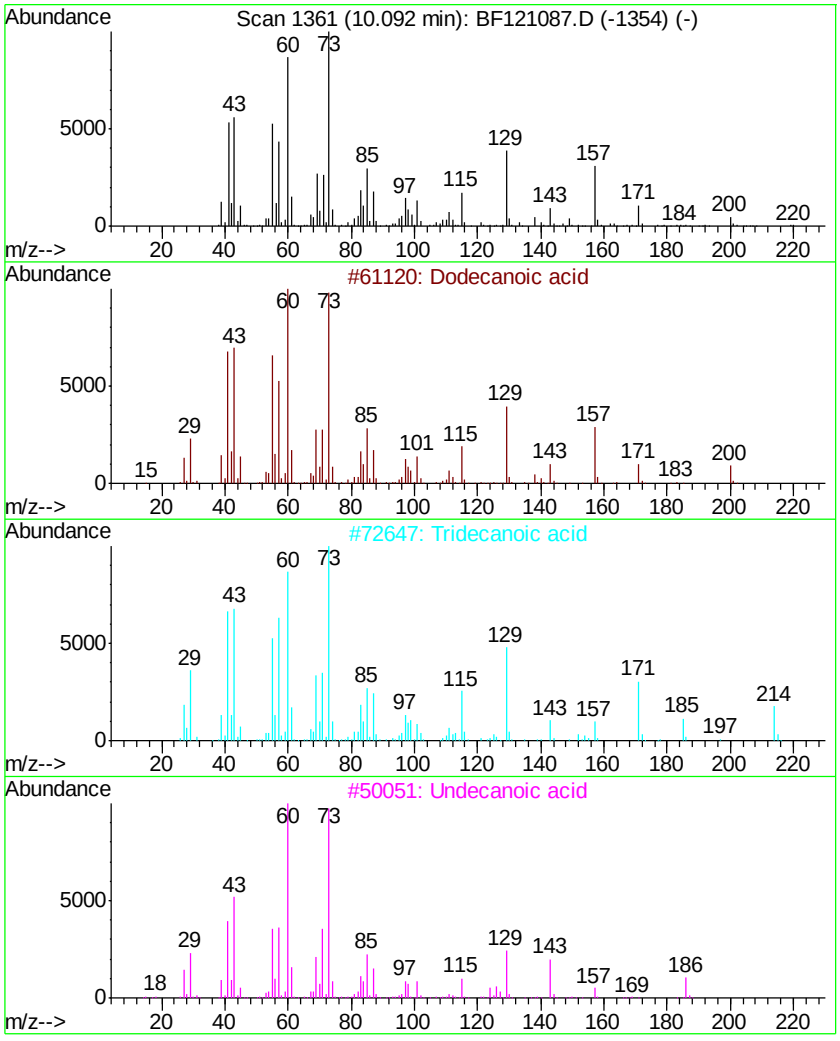
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

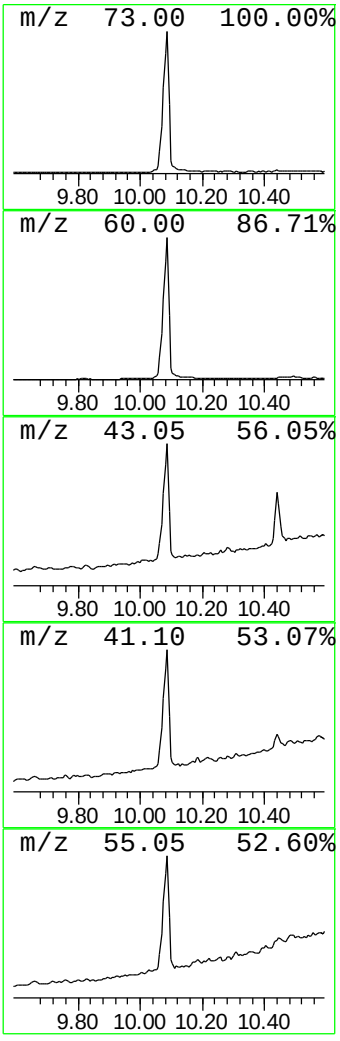
**********

Peak Number 3 Dodecanoic acid Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.09 | 20.57 ng | 1341710 | Acenaphthene-d10 | 9.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 97 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 74 |
| 3 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 72 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 70 |
| 5 | Nonanoic acid | 158 | C9H18O2 | 000112-05-0 | 46 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121087.D
Acq On : 29 Jul 2020 00:28
Operator : JU/CG
Sample : L3457-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SHB-MOTOR-ROOM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

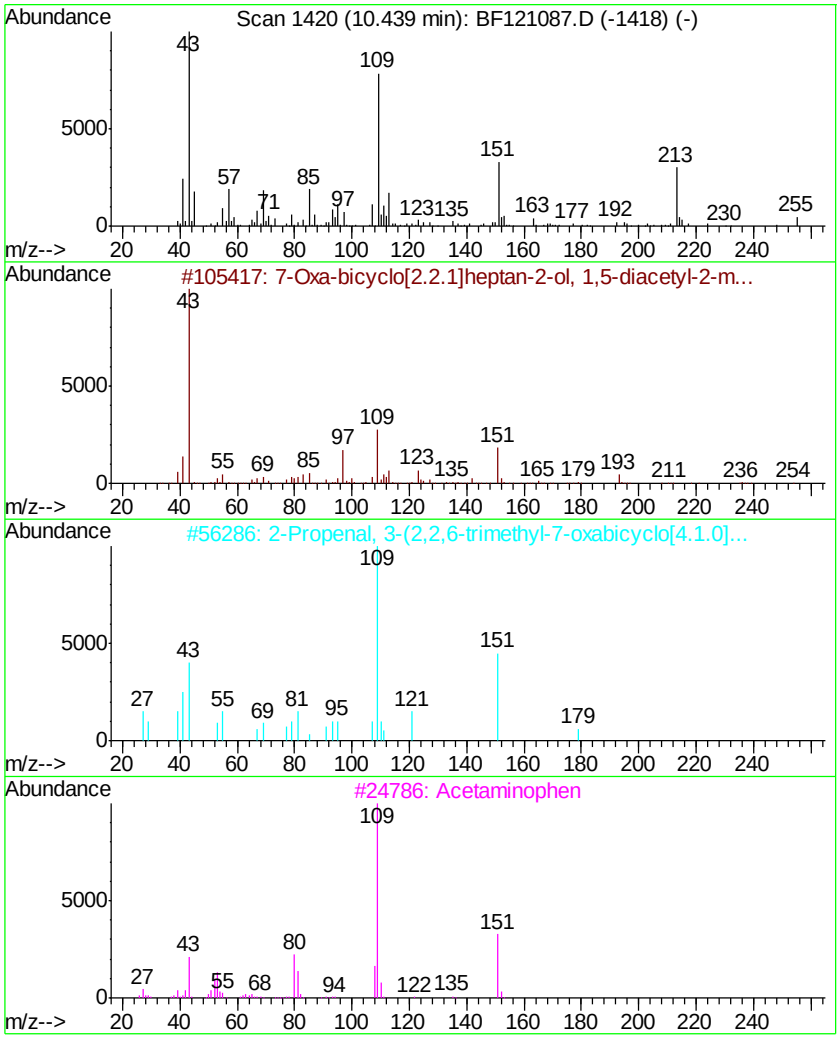
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

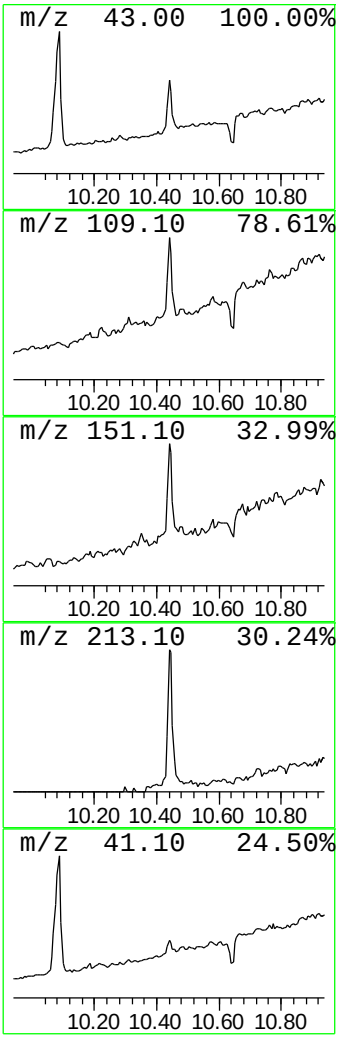
**********

Peak Number 4 7-Oxa-bicyclo[2.2.1]heptan-... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.44 | 2.95 ng | 192462 | Acenaphthene-d10 | 9.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 7-Oxa-bicyclo[2.2.1]heptan-2-ol,... | 254 | C14H22O4 | 329362-13-2 | 53 |
| 2 | 2-Propenal, 3-(2,2,6-trimethyl-7... | 194 | C12H18O2 | 055759-91-6 | 40 |
| 3 | Acetaminophen | 151 | C8H9NO2 | 000103-90-2 | 38 |
| 4 | Cyclopentanol, 1-(methylenecyclo... | 138 | C9H14O | 086951-58-8 | 38 |
| 5 | Metacetamol | 151 | C8H9NO2 | 000621-42-1 | 38 |



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Data File : BF121087.D
Acq On : 29 Jul 2020 00:28
Operator : JU/CG
Sample : L3457-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SHB-MOTOR-ROOM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

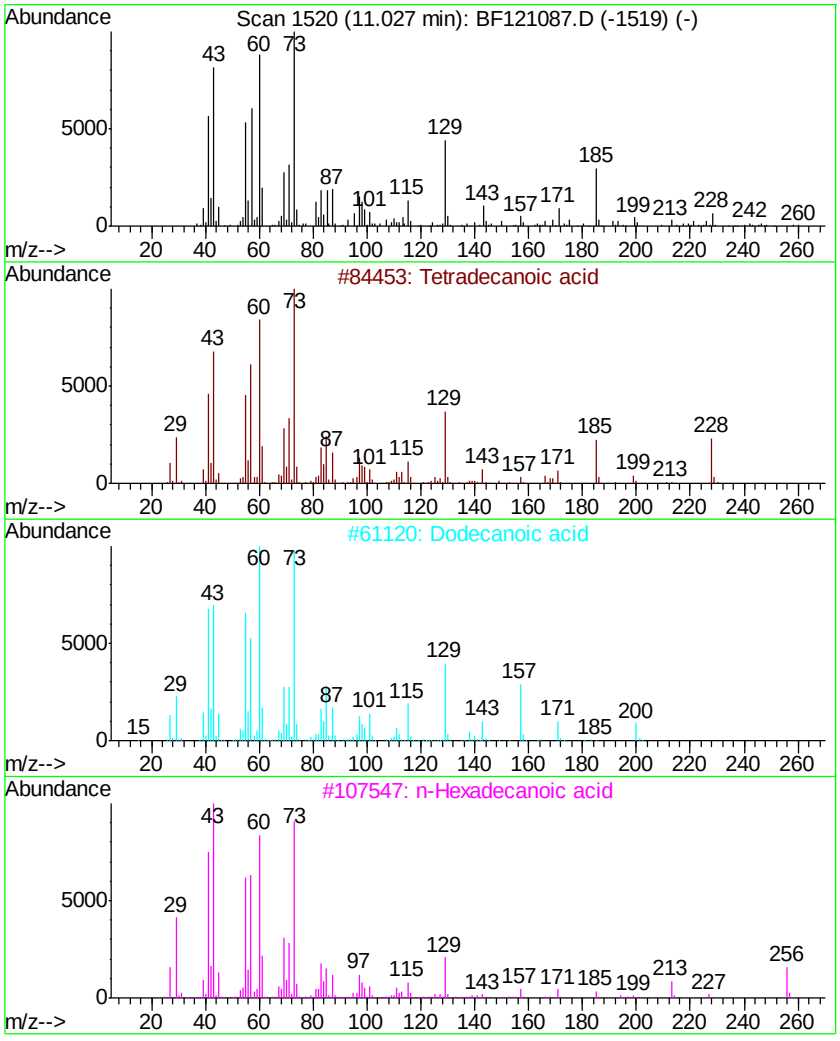
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

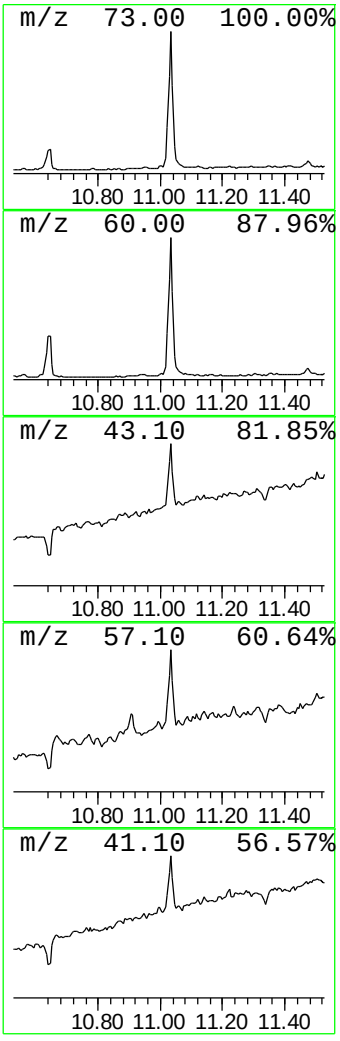
**********

Peak Number 5 Tetradecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.03 | 7.99 ng | 417611 | Phenanthrene-d10 | 11.34 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 87 |
| 2 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 72 |
| 3 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 59 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 58 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 58 |



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Sample : L3457-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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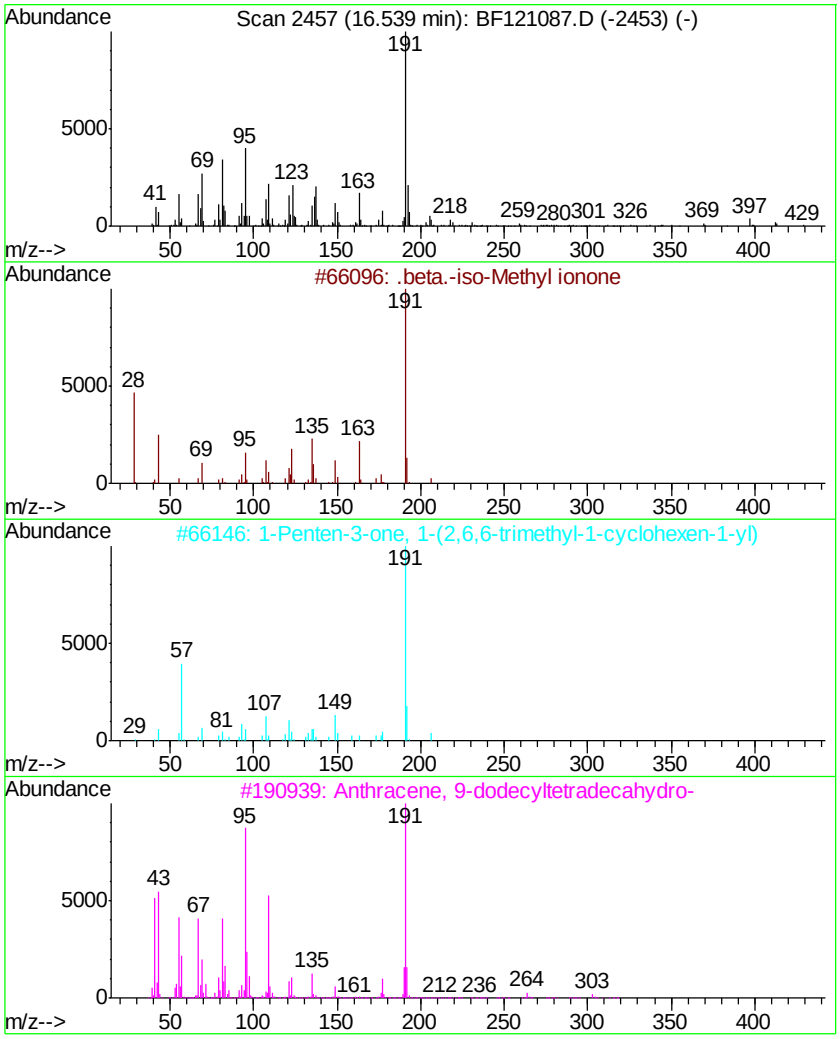
TIC Integration Parameters: LSCINT.P

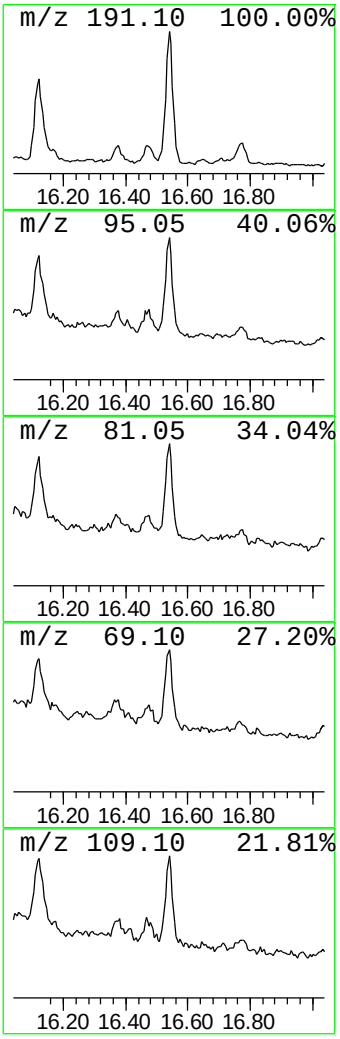
**********

Peak Number 6 unknown16.54 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.54 | 10.57 ng | 573382 | Perylene-d12 | 15.44 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | .beta.-iso-Methyl ionone | 206 | C14H22O | 1000285-40-2 | 49 |
| 2 | 1-Penten-3-one, 1-(2,6,6-trimeth... | 206 | C14H22O | 000127-43-5 | 45 |
| 3 | Anthracene, 9-dodecyltetradecahy... | 360 | C26H48 | 055401-75-7 | 42 |
| 4 | 9H-Fluorene-9-carbonitrile | 191 | C14H9N | 001529-40-4 | 38 |
| 5 | 5-(p-Aminophenyl)-2-thiazolamine | 191 | C9H9N3S | 090349-87-4 | 38 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072820\
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**Instrument :** BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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 |
| 1-Hexanol, 2-ethyl- | 6.87 | 9.1 | ng | 410998 | 1 | 6.81 | 899355 | 20.0 |
| 2,4,7,9-Tetrameth... | 9.29 | 8.7 | ng | 568749 | 3 | 9.85 | 1304840 | 20.0 |
| Dodecanoic acid | 10.09 | 20.6 | ng | 1341710 | 3 | 9.85 | 1304840 | 20.0 |
| 7-Oxa-bicyclo[2.2... | 10.44 | 3.0 | ng | 192462 | 3 | 9.85 | 1304840 | 20.0 |
| Tetradecanoic acid | 11.03 | 8.0 | ng | 417611 | 4 | 11.34 | 1045070 | 20.0 |
| unknown16.54 | 16.54 | 10.6 | ng | 573382 | 6 | 15.44 | 1084990 | 20.0 |