LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140164.D
Acq On : 30 Oct 2024 18:13
Operator : RC/JU
Sample : P4611-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-2

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140164.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.163 | 5 | 12 | 22 | rVB | 1268754 | 2022592 | 95.90% | 12.056% |
| 2 | 5.498 | 573 | 579 | 584 | rBV | 1491657 | 1956224 | 92.76% | 11.661% |
| 3 | 6.504 | 743 | 750 | 755 | rBV | 1437492 | 1963286 | 93.09% | 11.703% |
| 4 | 6.881 | 809 | 814 | 820 | rVB | 429821 | 527196 | 25.00% | 3.143% |
| 5 | 7.439 | 903 | 909 | 914 | rBV | 1027119 | 1314766 | 62.34% | 7.837% |
| 6 | 7.692 | 948 | 952 | 957 | rVB | 32729 | 38503 | 1.83% | 0.230% |
| 7 | 8.163 | 1022 | 1032 | 1039 | rBV | 526253 | 673144 | 31.92% | 4.013% |
| 8 | 9.239 | 1209 | 1215 | 1220 | rBV | 1699677 | 2109017 | 100.00% | 12.572% |
| 9 | 9.922 | 1326 | 1331 | 1336 | rBV | 513356 | 631226 | 29.93% | 3.763% |
| 10 | 10.639 | 1448 | 1453 | 1460 | rBV | 167126 | 211110 | 10.01% | 1.258% |
| 11 | 10.710 | 1460 | 1465 | 1477 | rVV | 794375 | 1053291 | 49.94% | 6.278% |
| 12 | 11.416 | 1580 | 1585 | 1593 | rBV | 428229 | 551462 | 26.15% | 3.287% |
| 13 | 11.945 | 1667 | 1675 | 1687 | rBV | 204908 | 342014 | 16.22% | 2.039% |
| 14 | 12.198 | 1714 | 1718 | 1723 | rBV2 | 15810 | 25378 | 1.20% | 0.151% |
| 15 | 12.633 | 1788 | 1792 | 1798 | rBV | 29216 | 39109 | 1.85% | 0.233% |
| 16 | 12.733 | 1804 | 1809 | 1816 | rBV2 | 38531 | 67326 | 3.19% | 0.401% |
| 17 | 12.863 | 1827 | 1831 | 1837 | rVB | 25466 | 38398 | 1.82% | 0.229% |
| 18 | 13.010 | 1850 | 1856 | 1863 | rVB | 1215570 | 1585000 | 75.15% | 9.448% |
| 19 | 13.551 | 1944 | 1948 | 1953 | rBV | 118266 | 161276 | 7.65% | 0.961% |
| 20 | 13.927 | 2007 | 2012 | 2021 | rBV3 | 62598 | 182955 | 8.67% | 1.091% |
| 21 | 14.080 | 2033 | 2038 | 2054 | rVB | 418943 | 678890 | 32.19% | 4.047% |
| 22 | 15.168 | 2219 | 2223 | 2233 | rVB | 48000 | 110681 | 5.25% | 0.660% |
| 23 | 15.615 | 2293 | 2299 | 2304 | rBV | 304498 | 493330 | 23.39% | 2.941% |

Sum of corrected areas: 16776174

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ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
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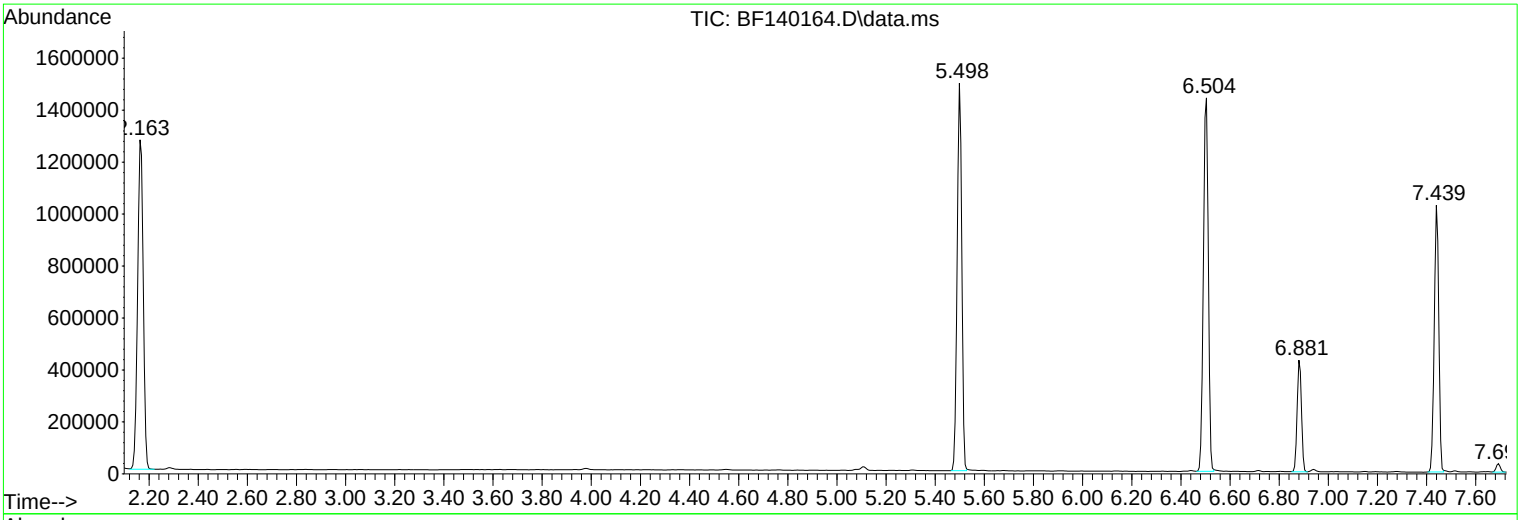
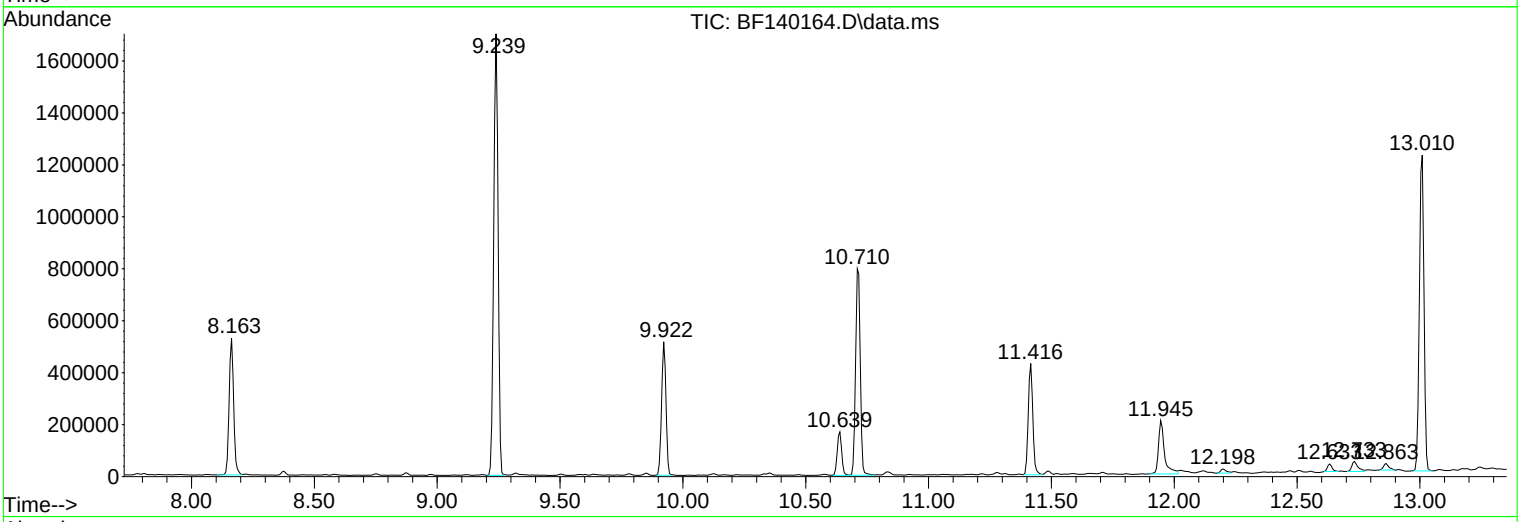
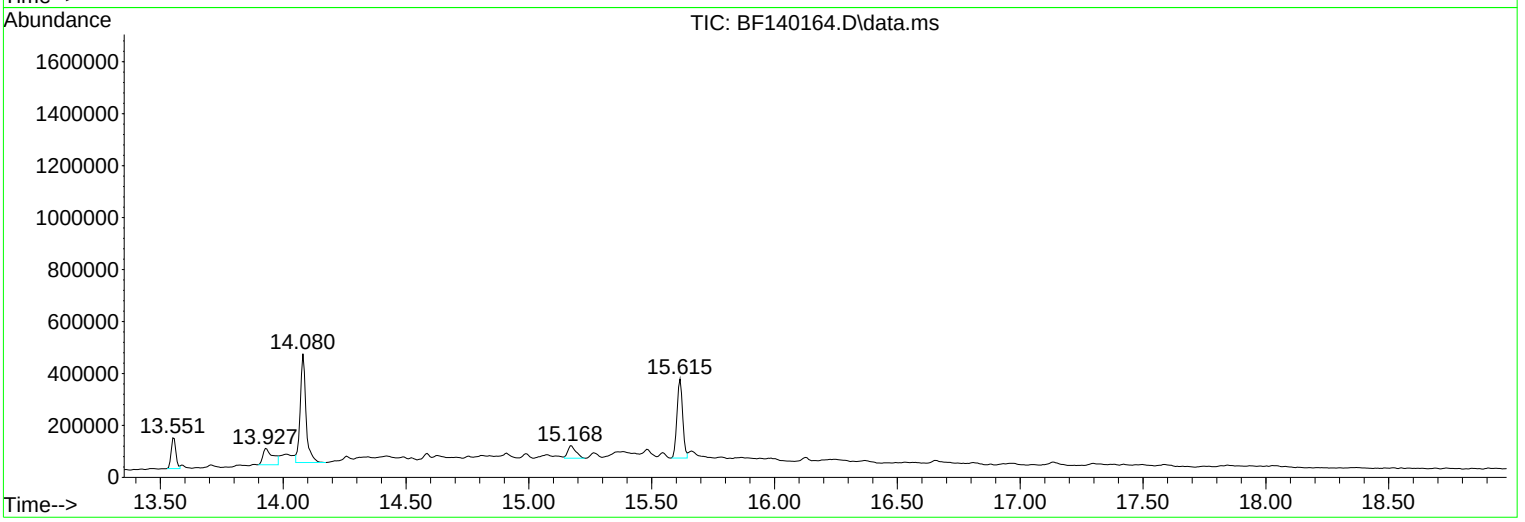
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF140164.D
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**Instrument :**
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

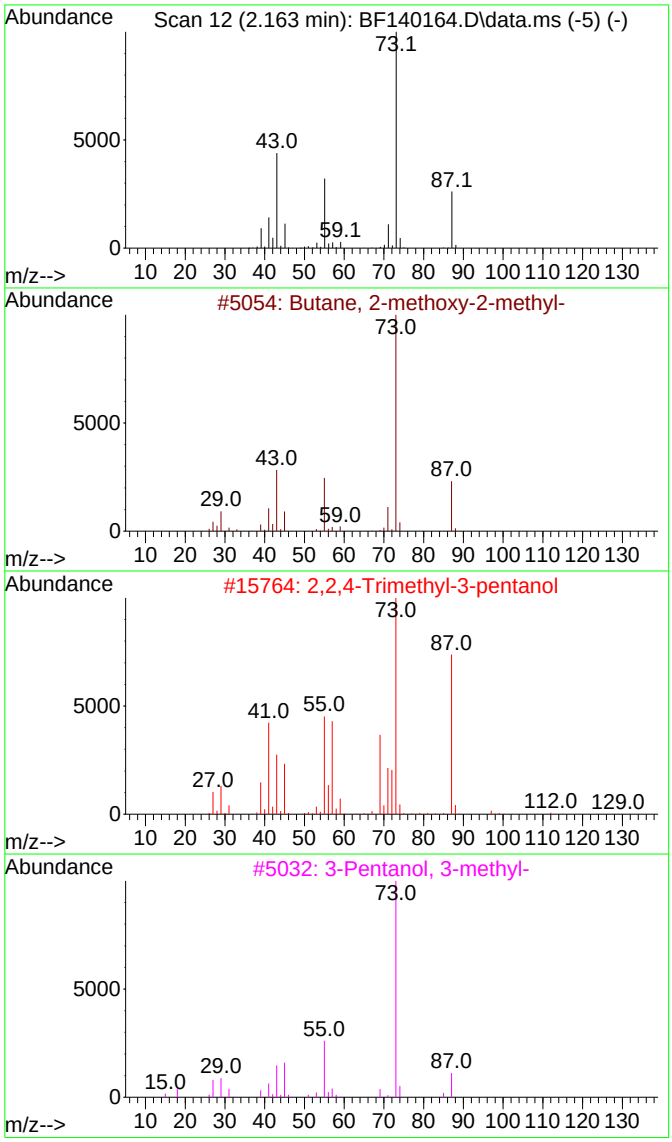
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

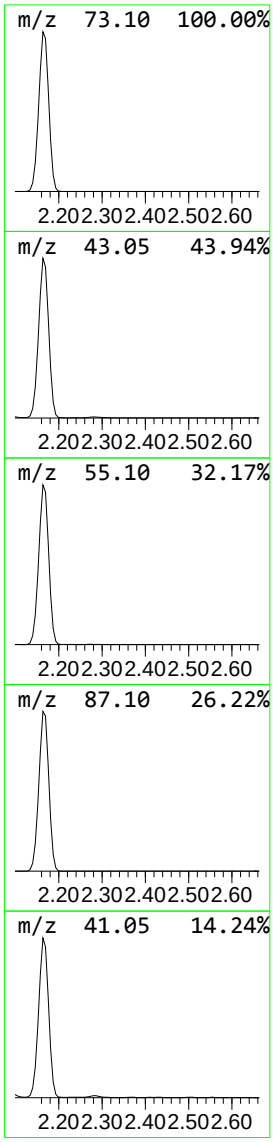
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.163 | 76.73 ng | 2022590 | 1,4-Dichlorobenzene-d4 | 6.881 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 40 |
| 3 | 3-Pentanol, 3-methyl- | 102 | C6H14O | 000077-74-7 | 38 |
| 4 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 23 |
| 5 | Octanal, 7-methoxy-3,7-dimethyl- | 186 | C11H22O2 | 003613-30-7 | 17 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140164.D
Acq On : 30 Oct 2024 18:13
Operator : RC/JU
Sample : P4611-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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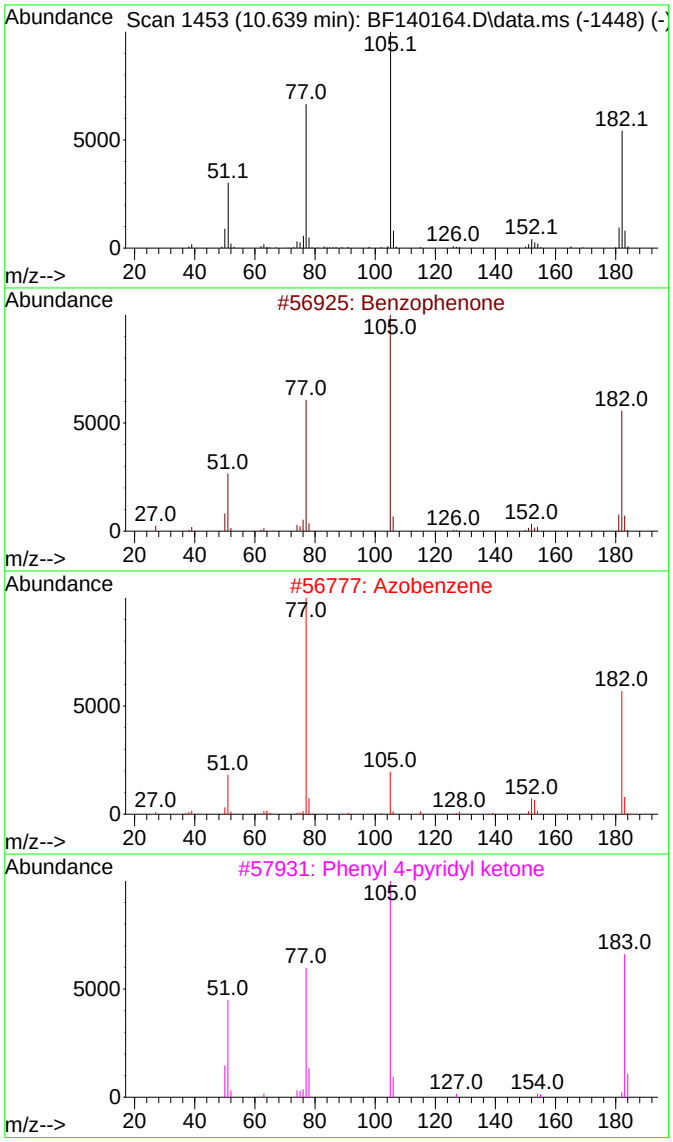
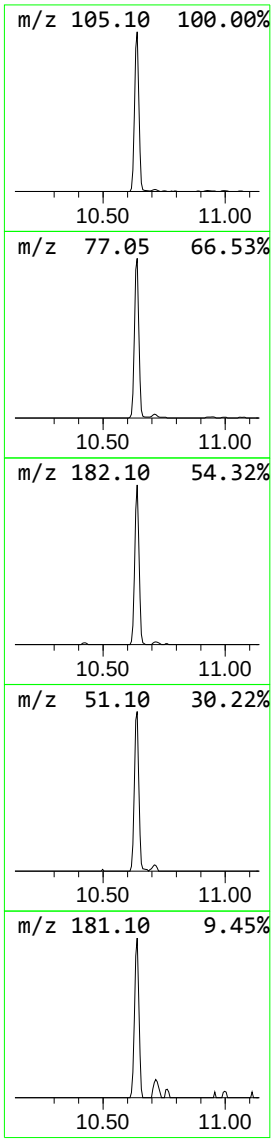
Peak Number 2 Benzophenone Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.639 | 6.69 ng | 211110 | Acenaphthene-d10 | 9.922 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 96 |
| 2 | Azobenzene | 182 | C12H10N2 | 000103-33-3 | 58 |
| 3 | Phenyl 4-pyridyl ketone | 183 | C12H9NO | 014548-46-0 | 49 |
| 4 | 1-Butanone, 1-phenyl- | 148 | C10H12O | 000495-40-9 | 47 |
| 5 | Pentafluoroethyl phenyl ketone | 224 | C9H5F5O | 000394-52-5 | 47 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140164.D
Acq On : 30 Oct 2024 18:13
Operator : RC/JU
Sample : P4611-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

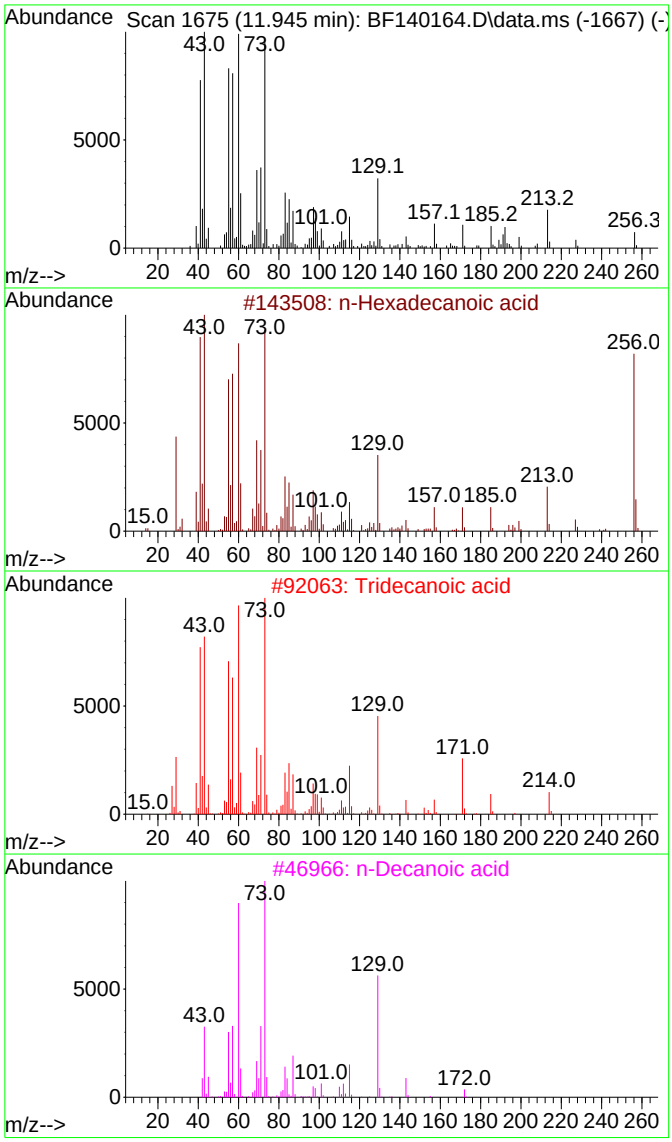
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

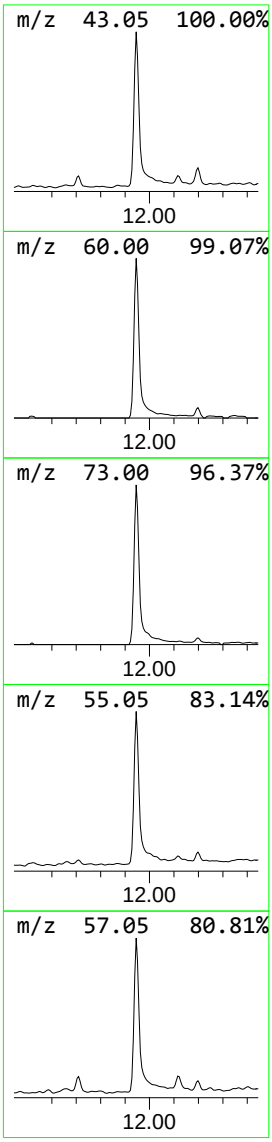
**********

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.945 | 12.40 ng | 342014 | Phenanthrene-d10 | 11.416 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 94 |
| 3 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 90 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 83 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |



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Acq On : 30 Oct 2024 18:13
Operator : RC/JU
Sample : P4611-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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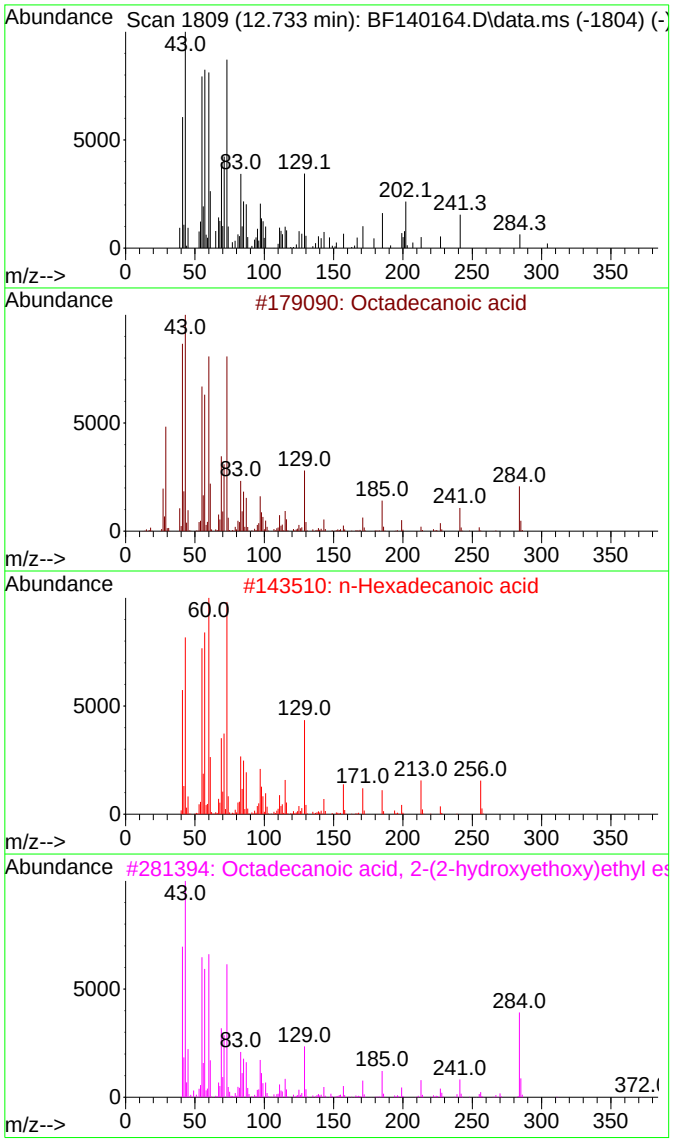
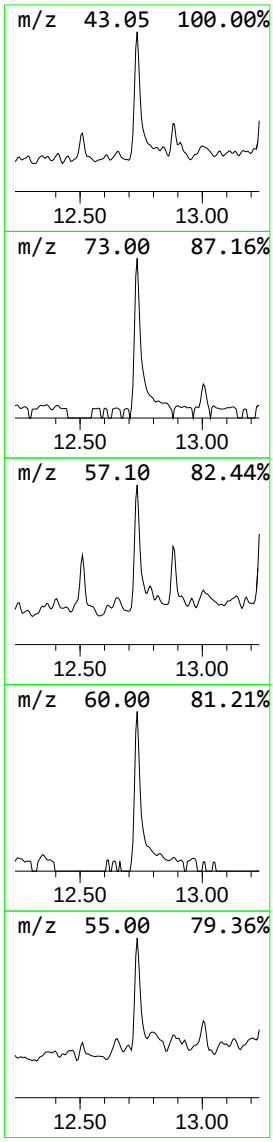
Peak Number 4 Octadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.733 | 2.44 ng | 67326 | Phenanthrene-d10 | 11.416 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 97 |
| 2 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 90 |
| 3 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 80 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 72 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |



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Data File : BF140164.D
Acq On : 30 Oct 2024 18:13
Operator : RC/JU
Sample : P4611-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

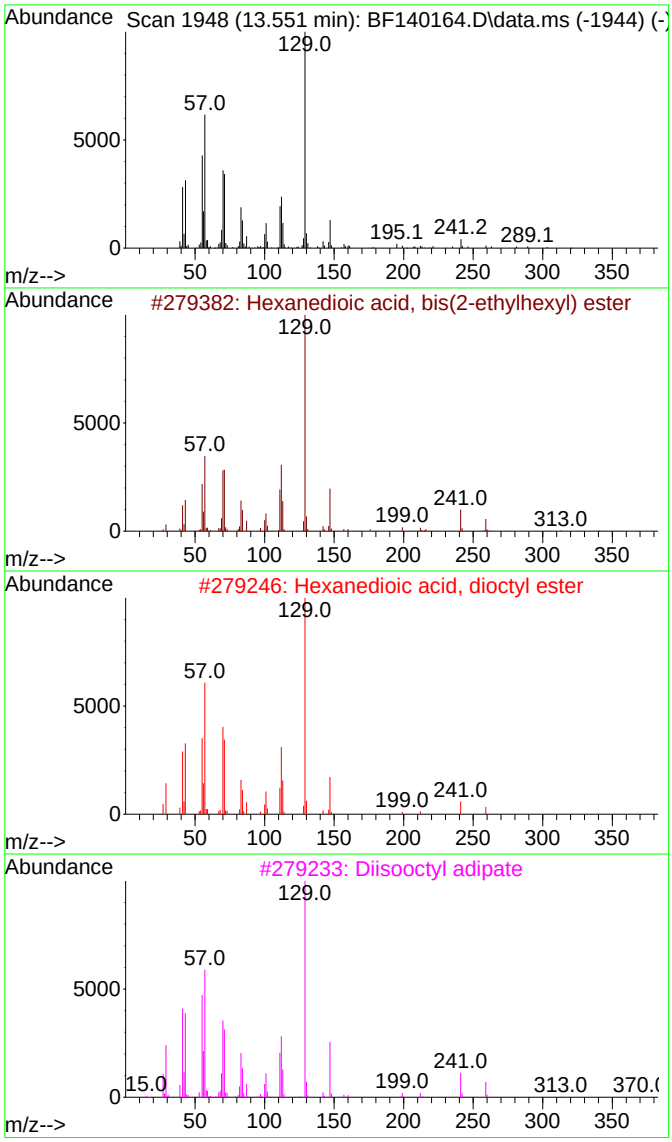
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

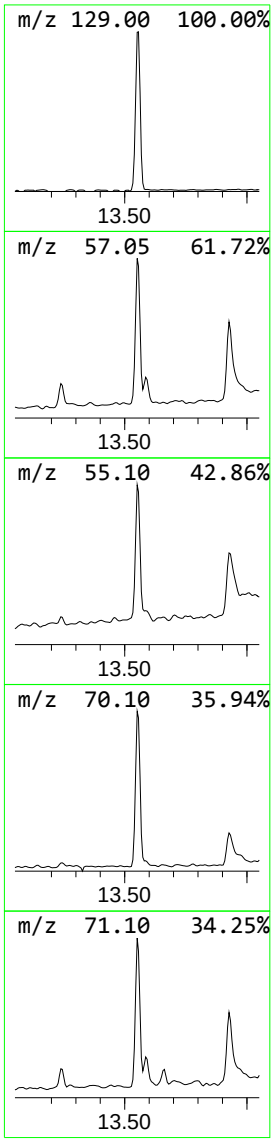
**********

Peak Number 5 Hexanedioic acid, bis(2-eth... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.551 | 4.75 ng | 161276 | Chrysene-d12 | 14.080 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexanedioic acid, bis(2-ethylhex... | 370 | C22H42O4 | 000103-23-1 | 91 |
| 2 | Hexanedioic acid, dioctyl ester | 370 | C22H42O4 | 000123-79-5 | 90 |
| 3 | Diisooctyl adipate | 370 | C22H42O4 | 001330-86-5 | 86 |
| 4 | Adipic acid, 2-ethylhexyl octyl ... | 370 | C22H42O4 | 1000324-48-6 | 83 |
| 5 | Hexanedioic acid, mono(2-ethylhe... | 258 | C14H26O4 | 004337-65-9 | 64 |



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Sample : P4611-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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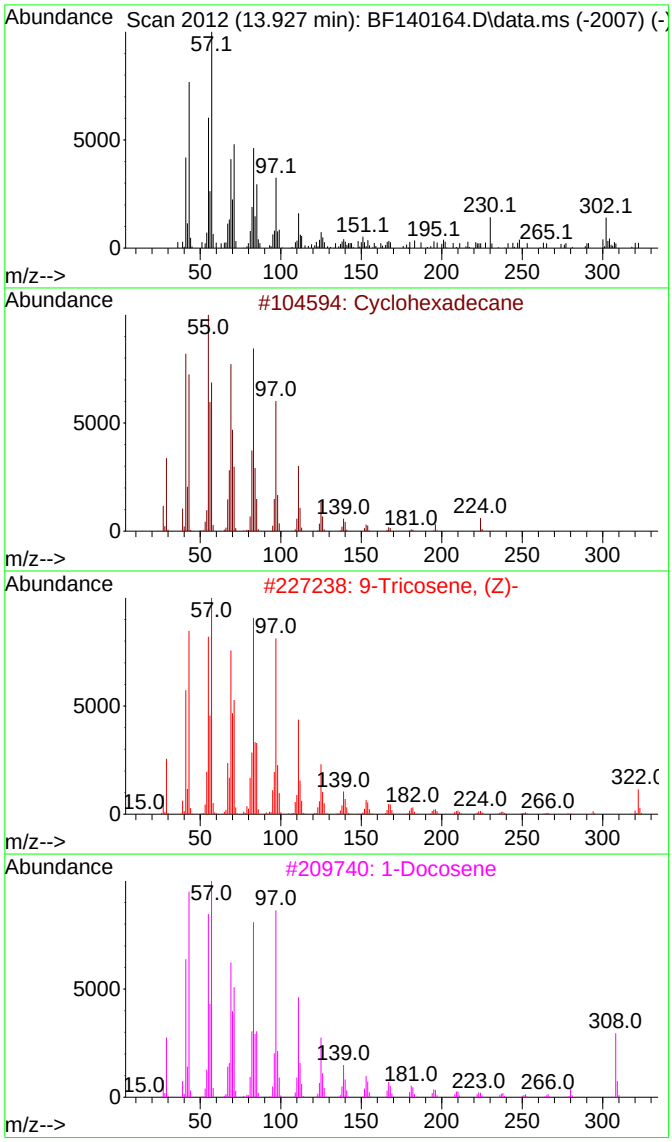
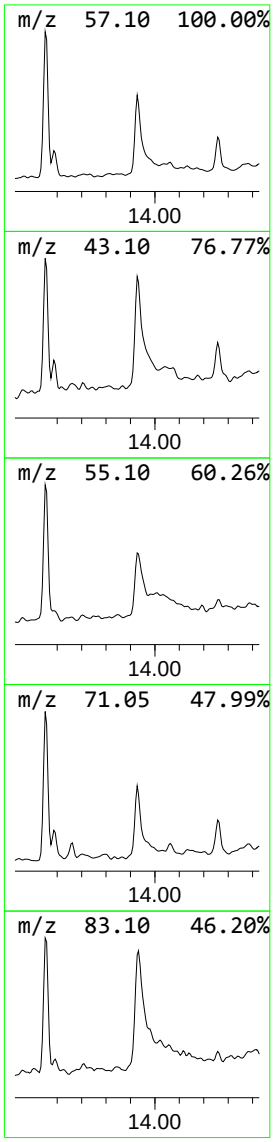
Peak Number 6 Cyclohexadecane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.927 | 5.39 ng | 182955 | Chrysene-d12 | 14.080 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexadecane | 224 | C16H32 | 000295-65-8 | 95 |
| 2 | 9-Tricosene, (Z)- | 322 | C23H46 | 027519-02-4 | 95 |
| 3 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 92 |
| 4 | 1-Tricosene | 322 | C23H46 | 018835-32-0 | 78 |
| 5 | Ethanol, 2-(tetradecyloxy)- | 258 | C16H34O2 | 002136-70-1 | 76 |



Tentatively Identified Compound (LSC) summary

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Sample : P4611-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-metho... | 2.163 | 76.7 | ng | 2022590 | 1 | 6.881 | 527196 | 20.0 |
| Benzophenone | 10.639 | 6.7 | ng | 211110 | 3 | 9.922 | 631226 | 20.0 |
| n-Hexadecanoic ... | 11.945 | 12.4 | ng | 342014 | 4 | 11.416 | 551462 | 20.0 |
| Octadecanoic acid | 12.733 | 2.4 | ng | 67326 | 4 | 11.416 | 551462 | 20.0 |
| Hexanedioic aci... | 13.551 | 4.8 | ng | 161276 | 5 | 14.080 | 678890 | 20.0 |
| Cyclohexadecane | 13.927 | 5.4 | ng | 182955 | 5 | 14.080 | 678890 | 20.0 |