LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138652.D
Acq On : 25 Jul 2024 14:49
Operator : RC/JU
Sample : P3357-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
S-853-J-SO-3-3.5-072024

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-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138652.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.146 | 3 | 9 | 16 | rVB | 1007760 | 1565773 | 48.16% | 9.008% |
| 2 | 3.375 | 212 | 218 | 236 | rBV | 62654 | 147058 | 4.52% | 0.846% |
| 3 | 5.075 | 501 | 507 | 514 | rVB | 80364 | 119751 | 3.68% | 0.689% |
| 4 | 5.481 | 570 | 576 | 594 | rBV | 1265495 | 1628216 | 50.08% | 9.367% |
| 5 | 6.487 | 741 | 747 | 768 | rBV | 1278875 | 1711523 | 52.64% | 9.847% |
| 6 | 6.681 | 773 | 780 | 793 | rBV | 49399 | 75477 | 2.32% | 0.434% |
| 7 | 6.851 | 804 | 809 | 814 | rBV | 359167 | 431525 | 13.27% | 2.483% |
| 8 | 7.416 | 898 | 905 | 910 | rBV | 829299 | 1090360 | 33.54% | 6.273% |
| 9 | 8.134 | 1021 | 1027 | 1032 | rBV | 472025 | 583177 | 17.94% | 3.355% |
| 10 | 8.445 | 1075 | 1080 | 1095 | rBV | 97540 | 155457 | 4.78% | 0.894% |
| 11 | 9.210 | 1203 | 1210 | 1219 | rBV | 1422831 | 1862805 | 57.30% | 10.717% |
| 12 | 9.886 | 1320 | 1325 | 1334 | rBV | 531665 | 651213 | 20.03% | 3.747% |
| 13 | 9.987 | 1334 | 1342 | 1366 | rBV | 1963235 | 3251205 | 100.00% | 18.705% |
| 14 | 10.675 | 1454 | 1459 | 1475 | rBV | 838084 | 1122259 | 34.52% | 6.457% |
| 15 | 11.375 | 1572 | 1578 | 1583 | rBV | 489451 | 619063 | 19.04% | 3.562% |
| 16 | 11.898 | 1659 | 1667 | 1681 | rBV2 | 48313 | 90879 | 2.80% | 0.523% |
| 17 | 12.463 | 1751 | 1763 | 1774 | rBV4 | 28658 | 70089 | 2.16% | 0.403% |
| 18 | 12.957 | 1842 | 1847 | 1852 | rBV | 1085809 | 1351265 | 41.56% | 7.774% |
| 19 | 13.869 | 1995 | 2002 | 2015 | rBV4 | 36818 | 109525 | 3.37% | 0.630% |
| 20 | 14.010 | 2021 | 2026 | 2034 | rVB | 261552 | 334280 | 10.28% | 1.923% |
| 21 | 14.851 | 2164 | 2169 | 2177 | rVB | 30559 | 44084 | 1.36% | 0.254% |
| 22 | 15.474 | 2269 | 2275 | 2286 | rVB | 234220 | 366850 | 11.28% | 2.111% |

Sum of corrected areas: 17381834

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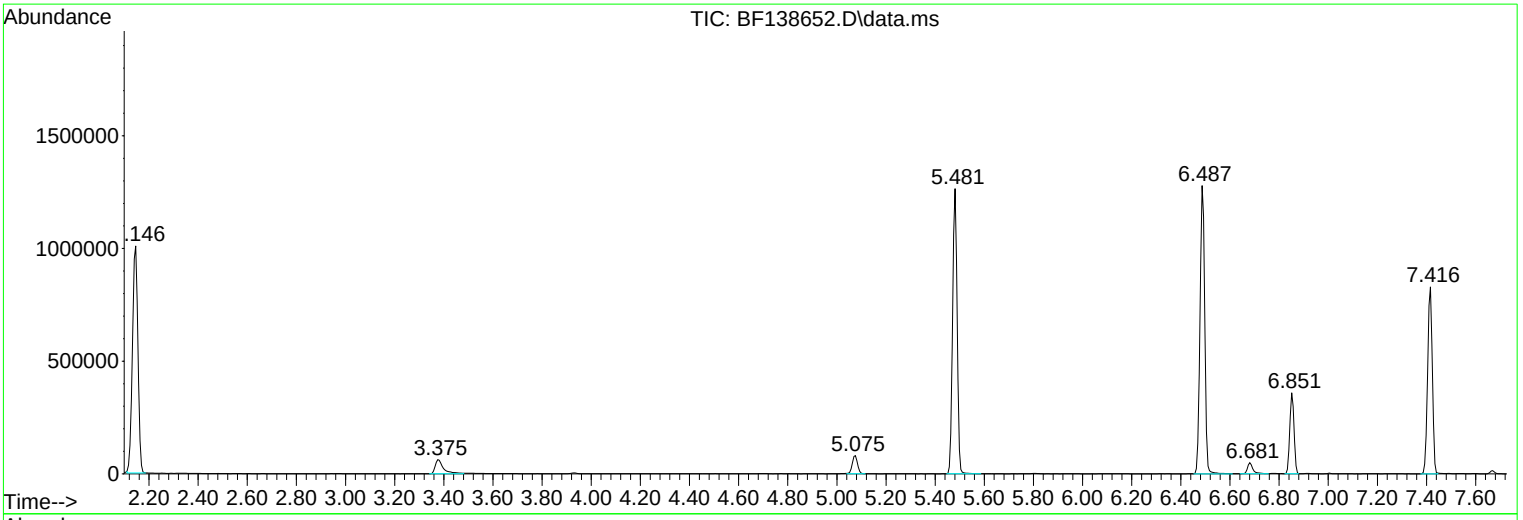
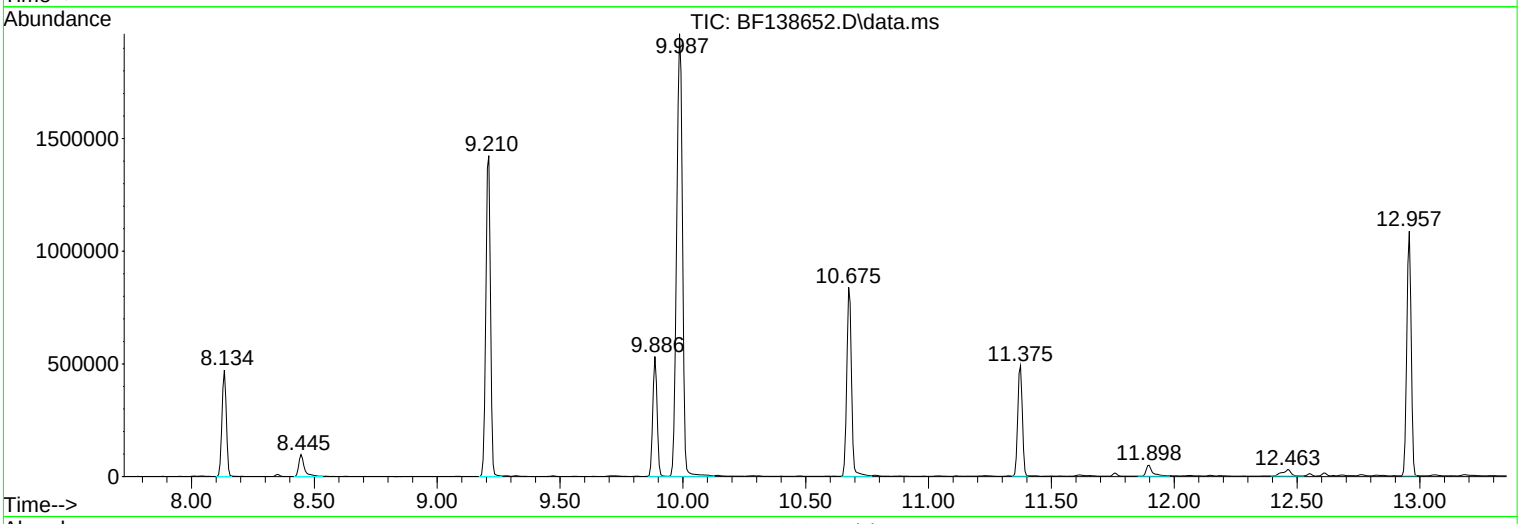
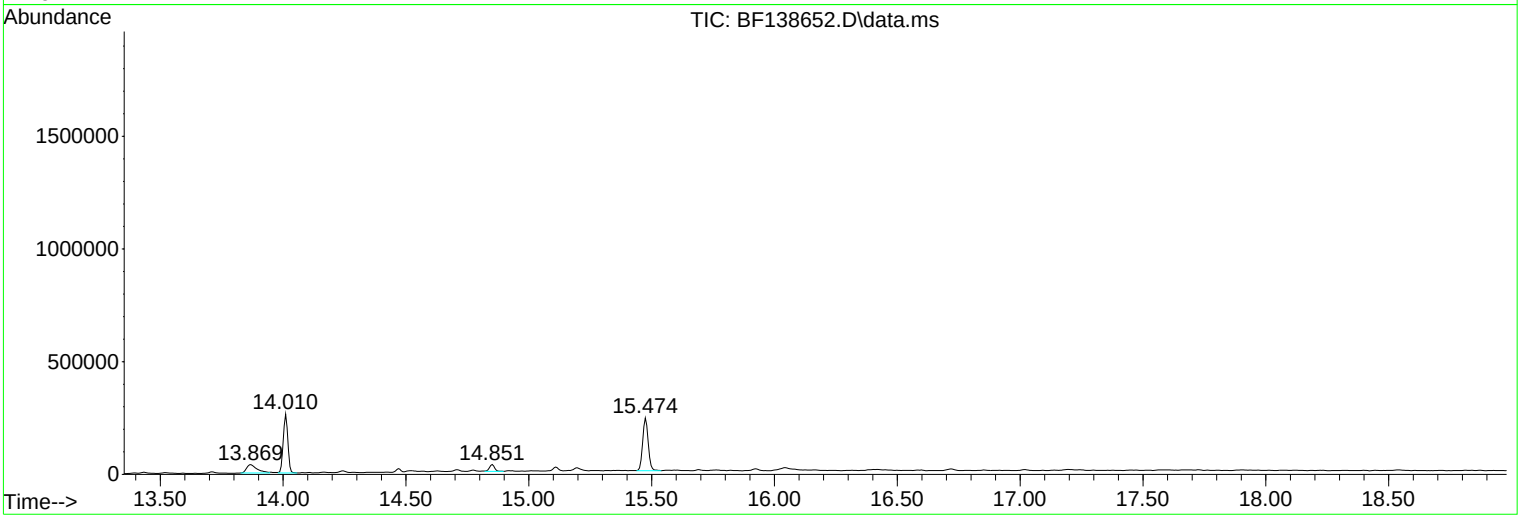
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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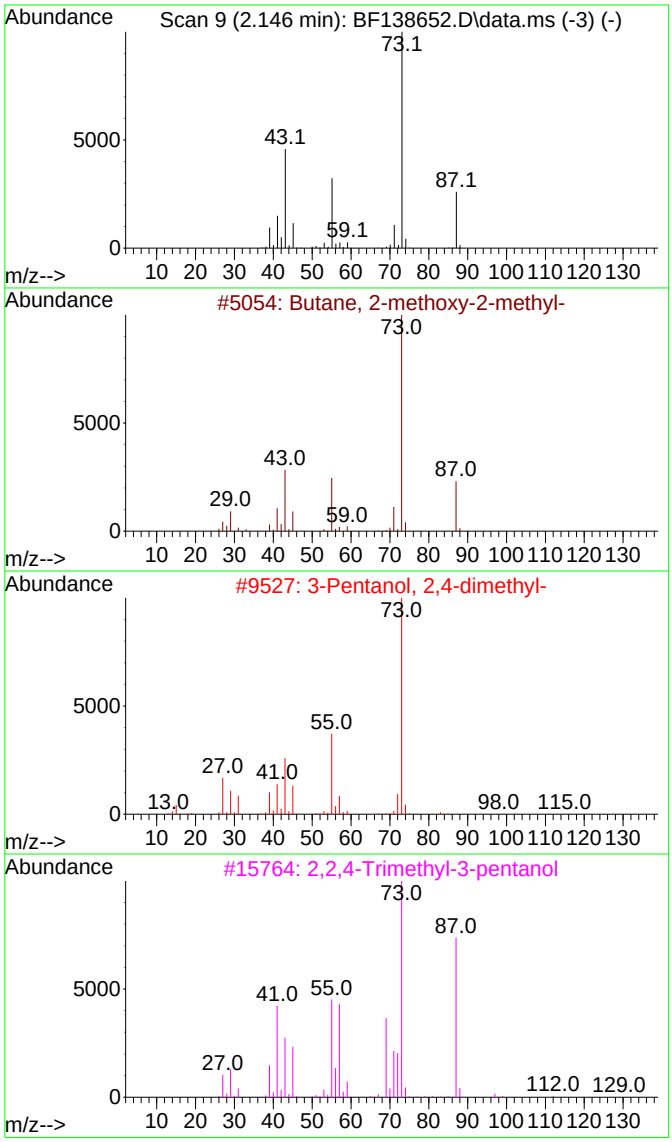
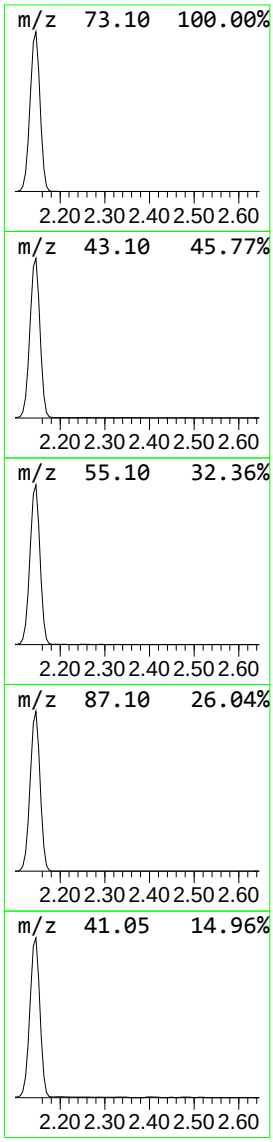
**********
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.146 | 72.57 ng | 1565770 | 1,4-Dichlorobenzene-d4 | 6.851 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 3-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000600-36-2 | 43 |
| 3 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 40 |
| 4 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 23 |
| 5 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 17 |



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**Instrument :**
BNA_F
**ClientSampleId :**
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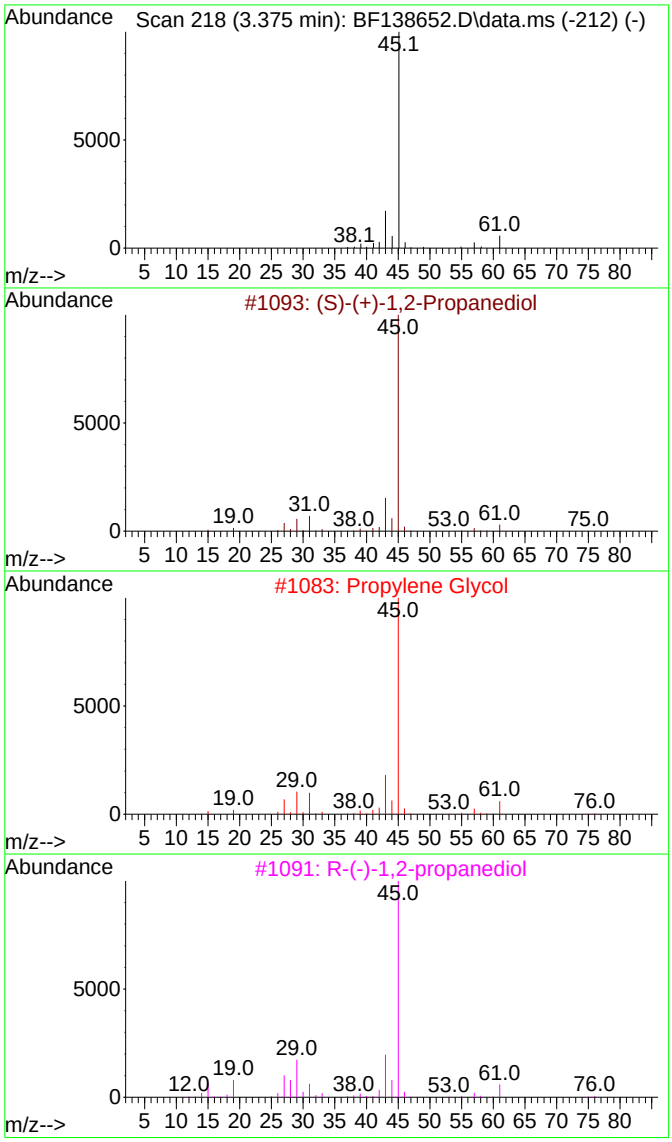
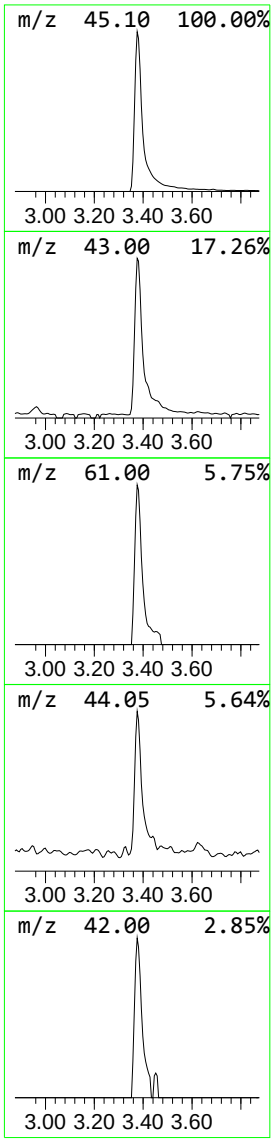
**********

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.375 | 6.82 ng | 147058 | 1,4-Dichlorobenzene-d4 | 6.851 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (S)-(+)-1,2-Propanediol | 76 | C3H8O2 | 004254-15-3 | 64 |
| 2 | Propylene Glycol | 76 | C3H8O2 | 000057-55-6 | 43 |
| 3 | R-(-)-1,2-propanediol | 76 | C3H8O2 | 004254-14-2 | 43 |
| 4 | Propanoic acid, 2-hydroxy-, meth... | 104 | C4H8O3 | 000547-64-8 | 9 |
| 5 | 2-Butanol | 74 | C4H10O | 000078-92-2 | 9 |



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Sample : P3357-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

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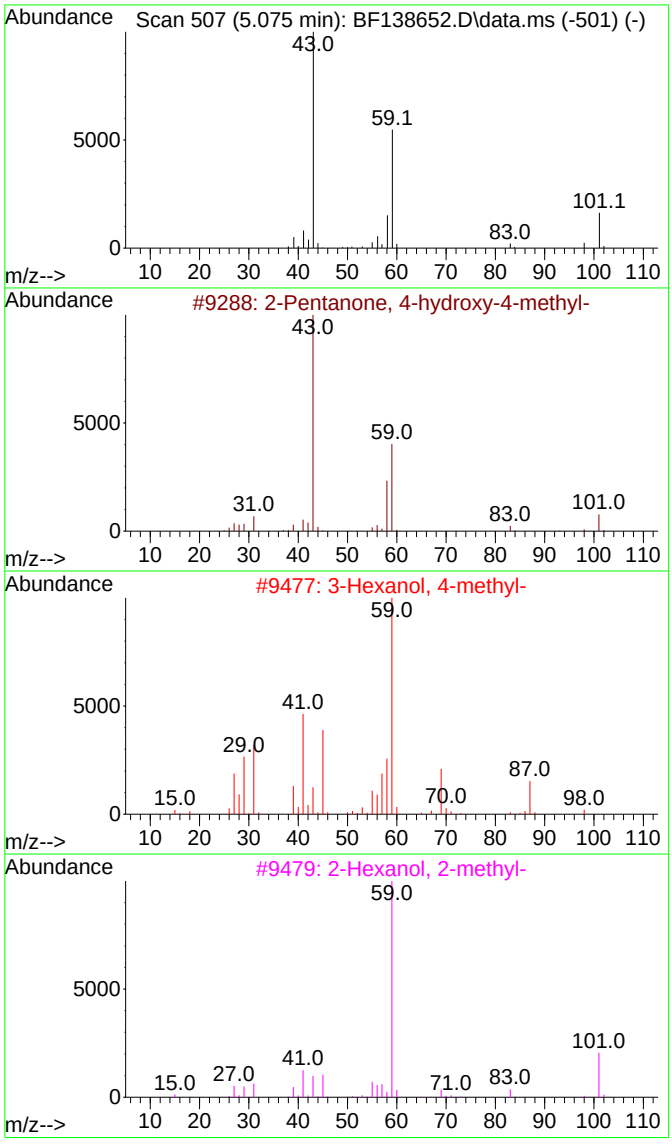
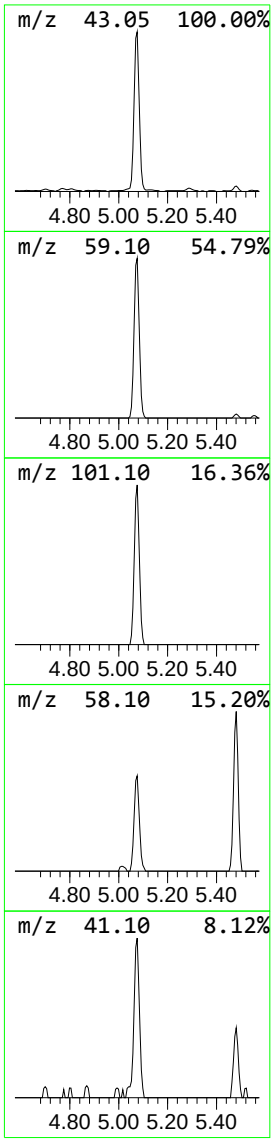
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.075 | 5.55 ng | 119751 | 1,4-Dichlorobenzene-d4 | 6.851 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 3 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 28 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 27 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |



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**Instrument :**
BNA_F
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S-853-J-SO-3-3.5-072024

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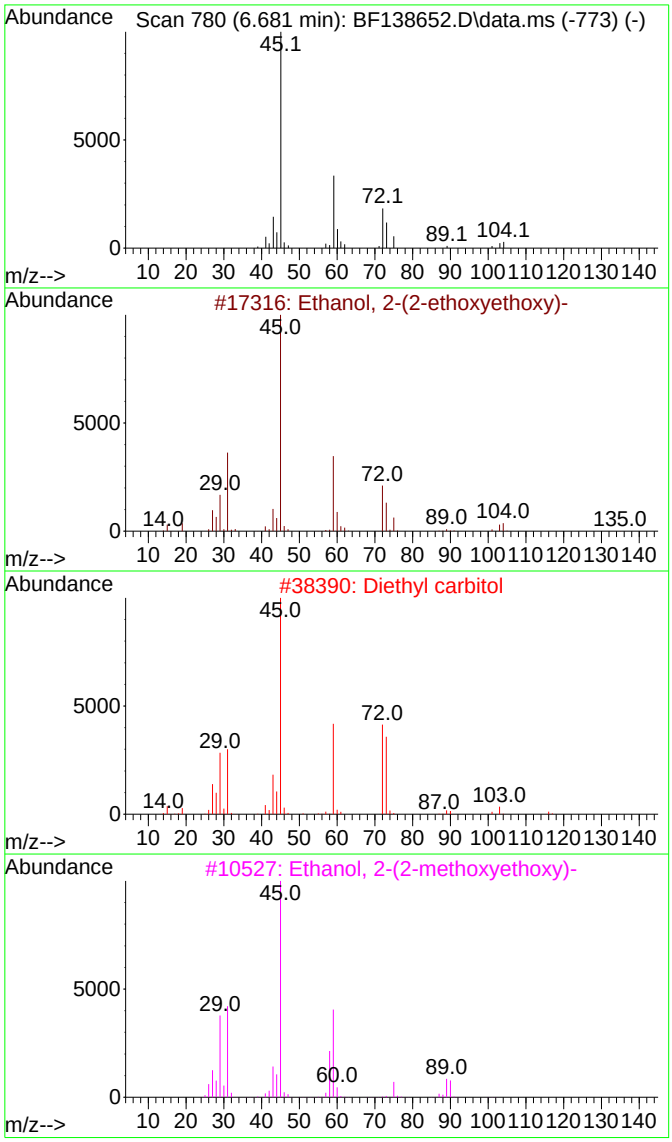
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

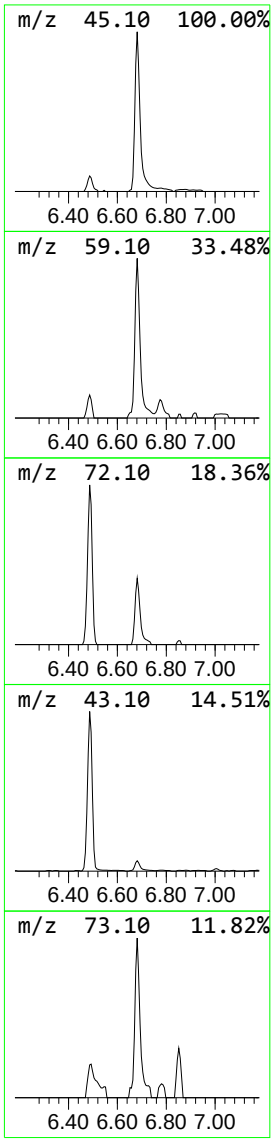
**********

Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.681 | 3.50 ng | 75477 | 1,4-Dichlorobenzene-d4 | 6.851 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(2-ethoxyethoxy)- | 134 | C6H14O3 | 000111-90-0 | 83 |
| 2 | Diethyl carbitol | 162 | C8H18O3 | 000112-36-7 | 78 |
| 3 | Ethanol, 2-(2-methoxyethoxy)- | 120 | C5H12O3 | 000111-77-3 | 50 |
| 4 | 2-Propanol, 1-propoxy- | 118 | C6H14O2 | 001569-01-3 | 39 |
| 5 | Ethanol, 2,2'-oxybis- | 106 | C4H10O3 | 000111-46-6 | 38 |



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Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
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S-853-J-SO-3-3.5-072024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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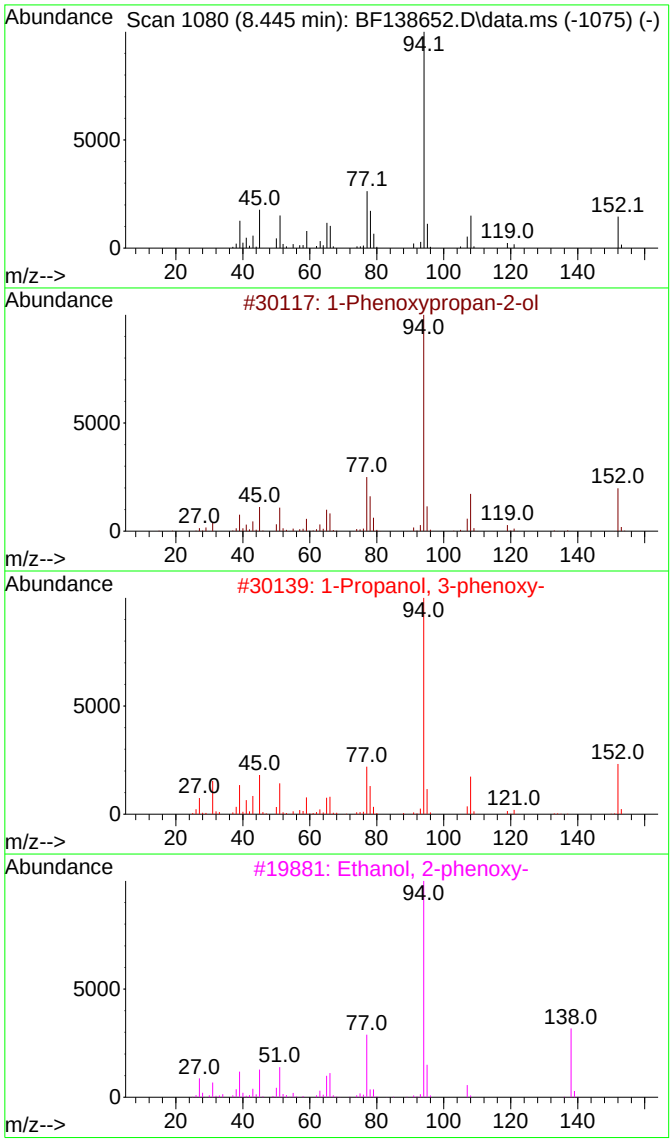
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

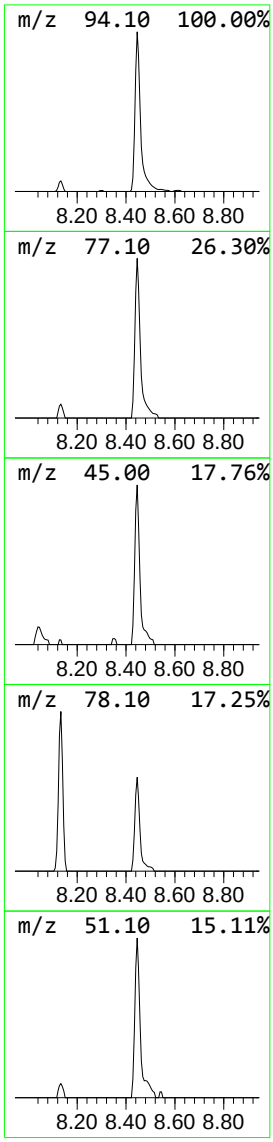
**********

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.445 | 5.33 ng | 155457 | Naphthalene-d8 | 8.134 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Phenoxypropan-2-ol | 152 | C9H12O2 | 000770-35-4 | 96 |
| 2 | 1-Propanol, 3-phenoxy- | 152 | C9H12O2 | 006180-61-6 | 91 |
| 3 | Ethanol, 2-phenoxy- | 138 | C8H10O2 | 000122-99-6 | 64 |
| 4 | 1-Propanol, 2-phenoxy- | 152 | C9H12O2 | 004169-04-4 | 59 |
| 5 | Benzene, (1-methylpropoxy)- | 150 | C10H14O | 010574-17-1 | 53 |



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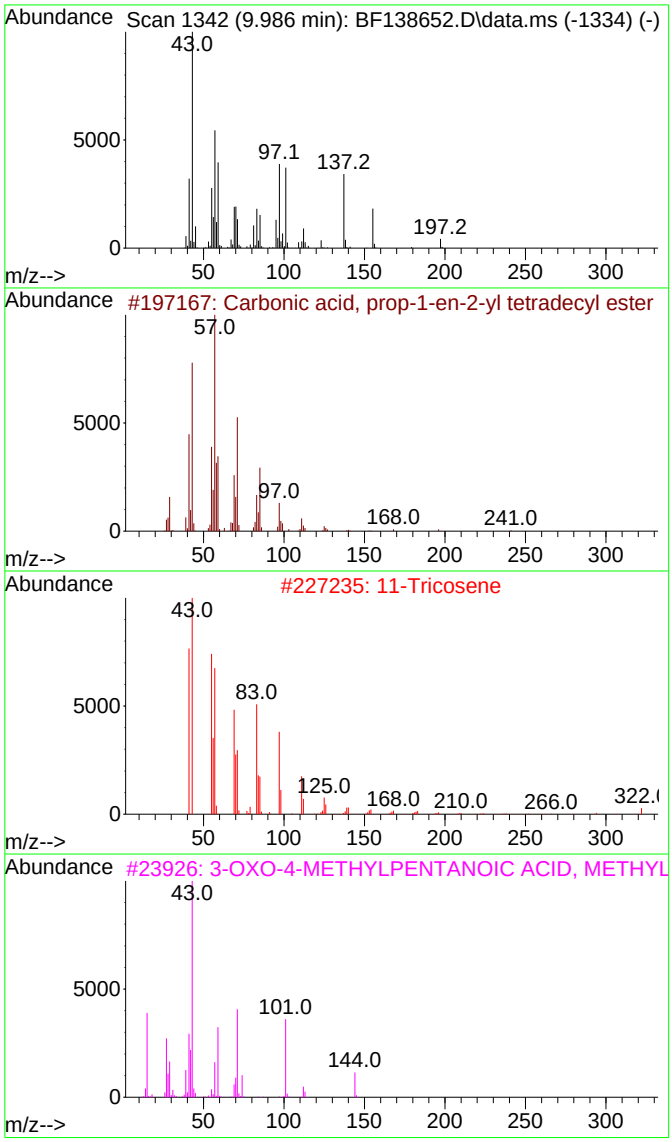
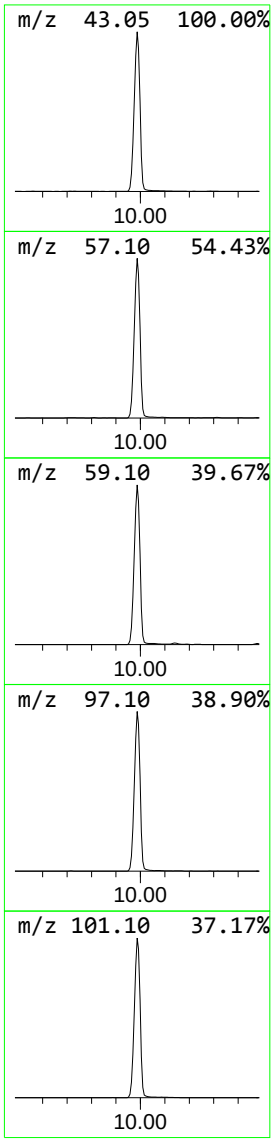
**********

Peak Number 6 unknown9.986 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.986 | 99.85 ng | 3251210 | Acenaphthene-d10 | 9.886 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Carbonic acid, prop-1-en-2-yl te... | 298 | C18H34O3 | 1000382-90-9 | 16 |
| 2 | 11-Tricosene | 322 | C23H46 | 052078-56-5 | 16 |
| 3 | 3-OXO-4-METHYLPENTANOIC ACID, ME... | 144 | C7H12O3 | 042558-54-3 | 12 |
| 4 | Decyl heptyl ether | 256 | C17H36O | 1000406-39-1 | 10 |
| 5 | 2-Propionyloxytetradecane | 270 | C17H34O2 | 1000245-62-7 | 10 |



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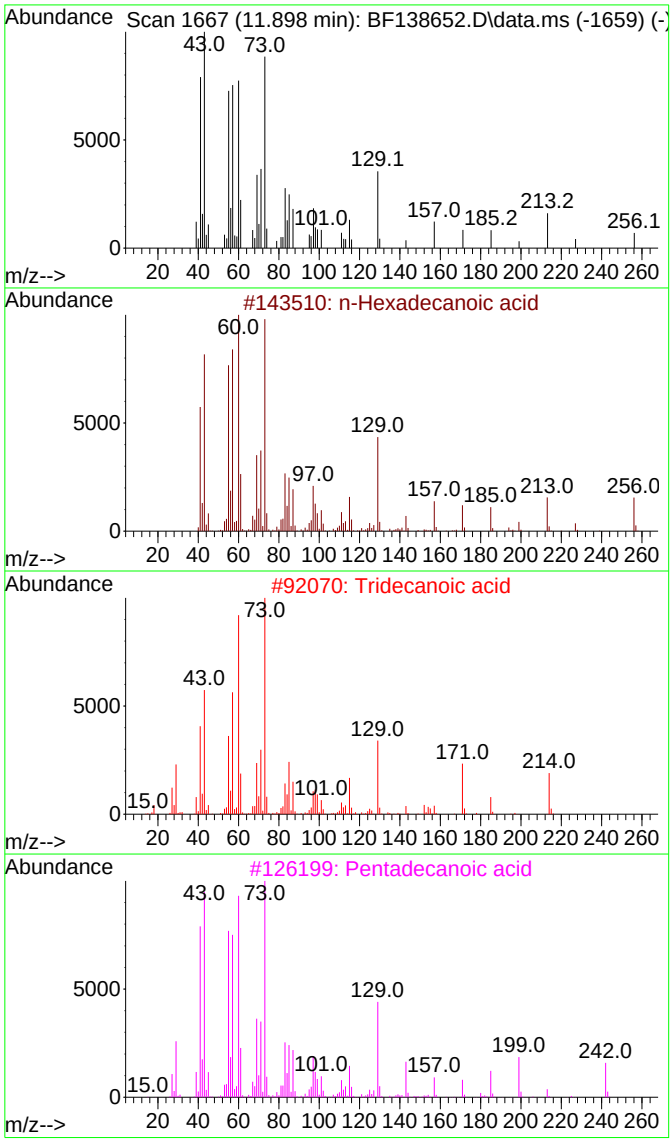
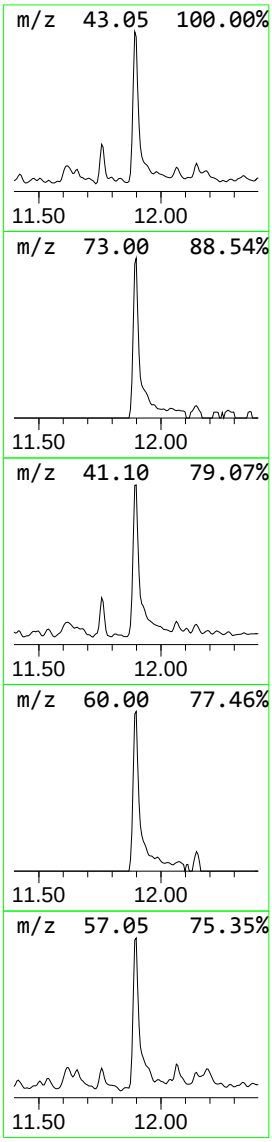
**********

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.898 | 2.94 ng | 90879 | Phenanthrene-d10 | 11.375 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 87 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 4 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 64 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 59 |



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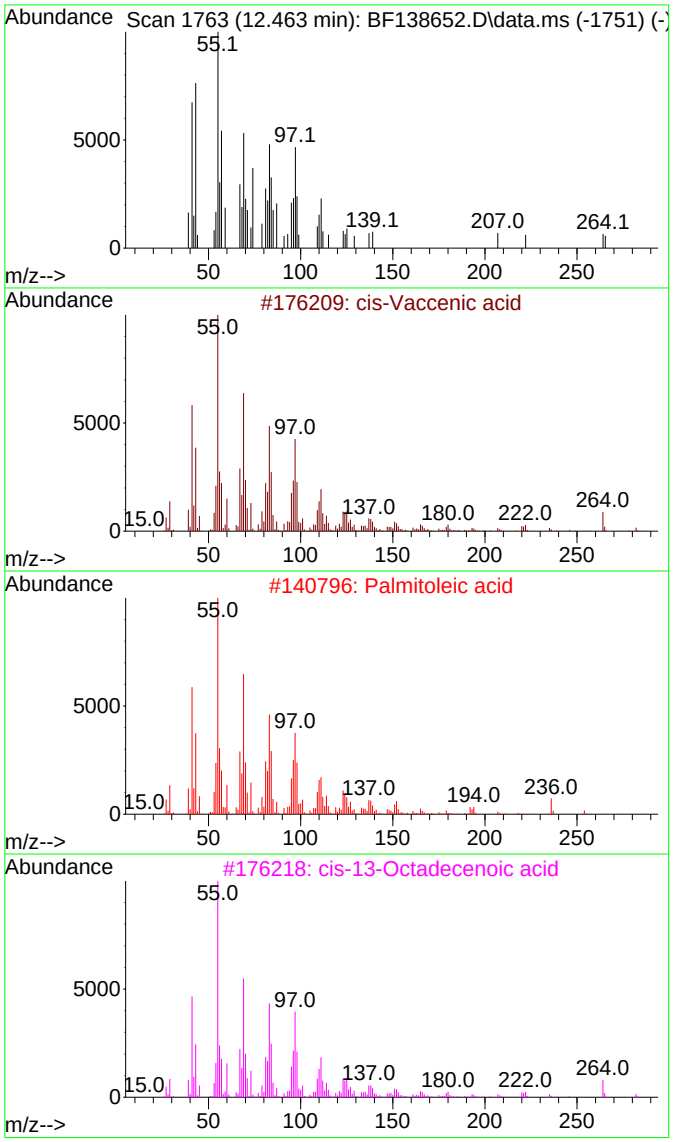
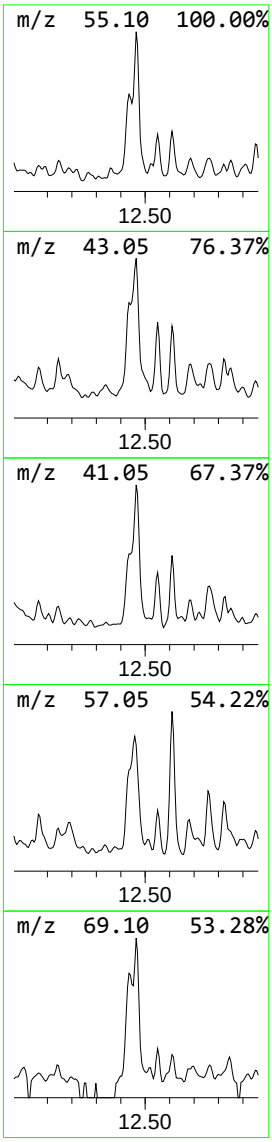
**********

Peak Number 8 cis-Vaccenic acid Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.463 | 2.26 ng | 70089 | Phenanthrene-d10 | 11.375 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | cis-Vaccenic acid | 282 | C18H34O2 | 000506-17-2 | 87 |
| 2 | Palmitoleic acid | 254 | C16H30O2 | 000373-49-9 | 83 |
| 3 | cis-13-Octadecenoic acid | 282 | C18H34O2 | 013126-39-1 | 83 |
| 4 | 10-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 013481-95-3 | 68 |
| 5 | 9-Octadecenoic acid (Z)-, methyl... | 296 | C19H36O2 | 000112-62-9 | 58 |



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**Instrument :**
BNA_F
**ClientSampleId :**
S-853-J-SO-3-3.5-072024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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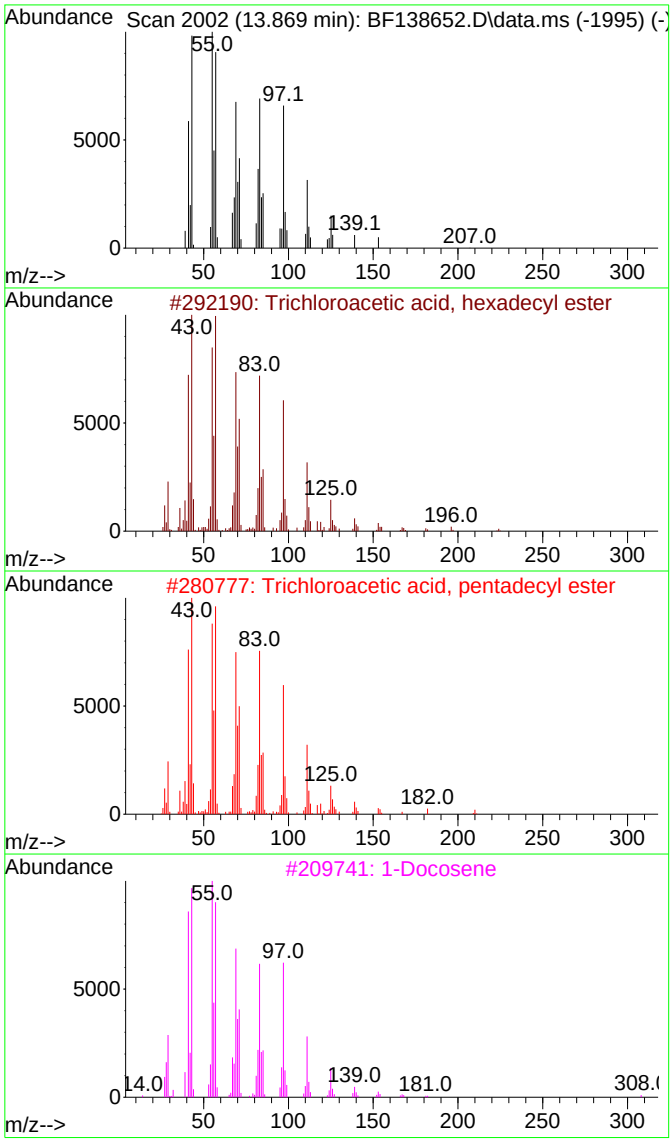
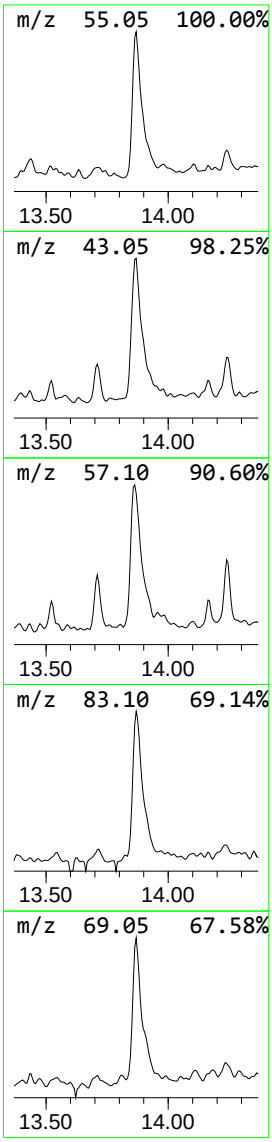
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.869 | 6.55 ng | 109525 | Chrysene-d12 | 14.010 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 95 |
| 2 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 91 |
| 3 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 91 |
| 4 | Octadecyl trifluoroacetate | 366 | C20H37F3O2 | 079392-43-1 | 91 |
| 5 | 1-Tetracosene | 336 | C24H48 | 010192-32-2 | 91 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138652.D
Acq On : 25 Jul 2024 14:49
Operator : RC/JU
Sample : P3357-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
S-853-J-SO-3-3.5-072024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

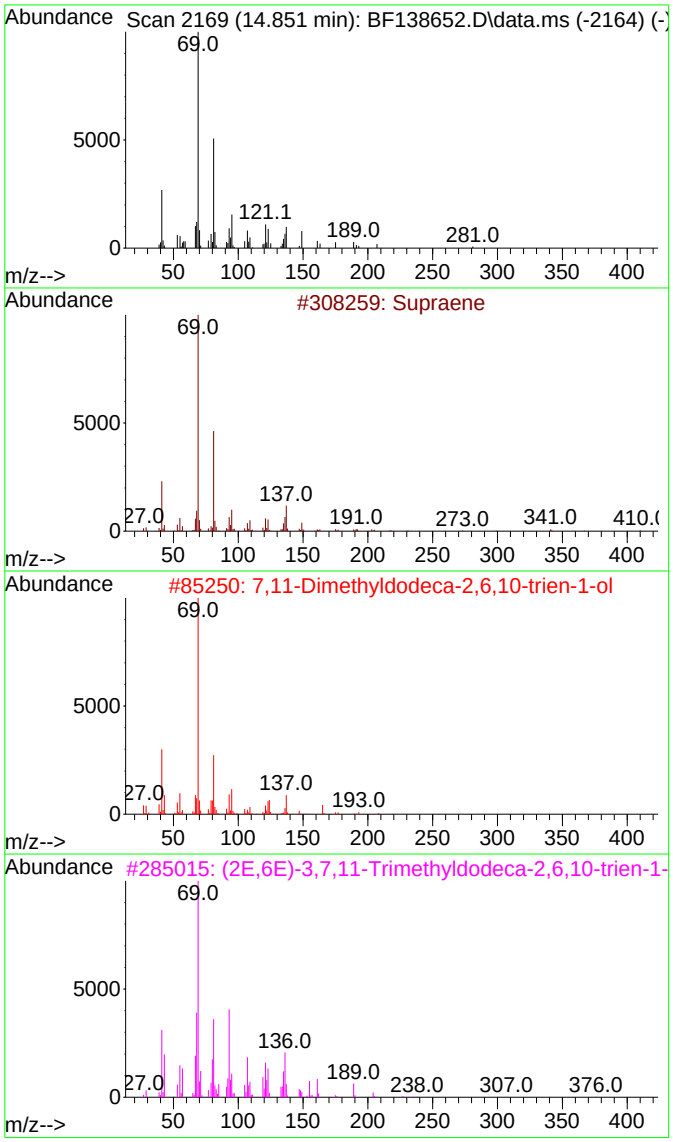
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

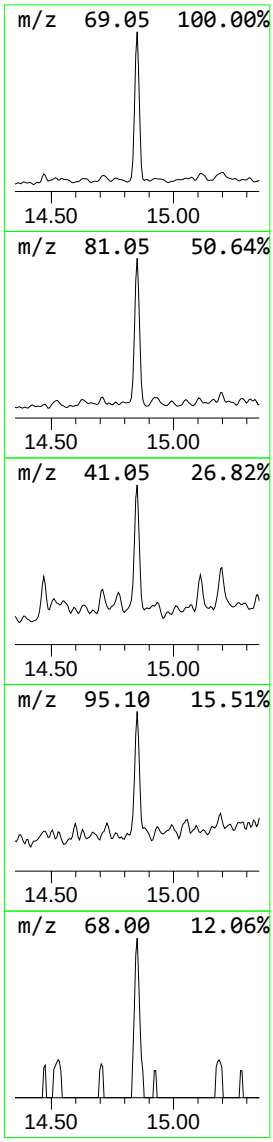
**********

Peak Number 10 Supraene Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.851 | 2.40 ng | 44084 | Perylene-d12 | 15.474 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Supraene | 410 | C30H50 | 007683-64-9 | 86 |
| 2 | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 72 |
| 3 | (2E,6E)-3,7,11-Trimethyldodeca-2... | 376 | C25H44O2 | 078368-57-7 | 72 |
| 4 | .psi.,.psi.-Carotene, 7,7',8,8',... | 547 | C40H66 | 000502-62-5 | 64 |
| 5 | 2,6-Octadiene, 2,6-dimethyl- | 138 | C10H18 | 002792-39-4 | 50 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072524\
Data File : BF138652.D
Acq On : 25 Jul 2024 14:49
Operator : RC/JU
Sample : P3357-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
S-853-J-SO-3-3.5-072024

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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 |
| Butane, 2-metho... | 2.146 | 72.6 | ng | 1565770 | 1 | 6.851 | 431525 | 20.0 |
| (S)-(+)-1,2-Pro... | 3.375 | 6.8 | ng | 147058 | 1 | 6.851 | 431525 | 20.0 |
| 2-Pentanone, 4-... | 5.075 | 5.5 | ng | 119751 | 1 | 6.851 | 431525 | 20.0 |
| Ethanol, 2-(2-e... | 6.681 | 3.5 | ng | 75477 | 1 | 6.851 | 431525 | 20.0 |
| 1-Phenoxypropan... | 8.445 | 5.3 | ng | 155457 | 2 | 8.134 | 583177 | 20.0 |
| unknown9.986 | 9.986 | 99.8 | ng | 3251210 | 3 | 9.886 | 651213 | 20.0 |
| n-Hexadecanoic ... | 11.898 | 2.9 | ng | 90879 | 4 | 11.375 | 619063 | 20.0 |
| cis-Vaccenic acid | 12.463 | 2.3 | ng | 70089 | 4 | 11.375 | 619063 | 20.0 |
| Trichloroacetic... | 13.869 | 6.5 | ng | 109525 | 5 | 14.010 | 334280 | 20.0 |
| Supraene | 14.851 | 2.4 | ng | 44084 | 6 | 15.474 | 366850 | 20.0 |