LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091924\
Data File : BF139488.D
Acq On : 20 Sep 2024 02:59
Operator : RC/JU
Sample : P4027-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** DN-B-49

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-BF091324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139488.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.210 | 11 | 20 | 27 | rVB | 951399 | 1491946 | 100.00% | 16.284% |
| 2 | 5.093 | 502 | 510 | 519 | rVB | 37692 | 52442 | 3.52% | 0.572% |
| 3 | 5.498 | 573 | 579 | 590 | rBV | 591956 | 758970 | 50.87% | 8.284% |
| 4 | 6.504 | 744 | 750 | 763 | rBV | 582117 | 780867 | 52.34% | 8.523% |
| 5 | 6.875 | 808 | 813 | 818 | rBV | 388765 | 470854 | 31.56% | 5.139% |
| 6 | 7.434 | 902 | 908 | 913 | rBV | 398738 | 493792 | 33.10% | 5.389% |
| 7 | 7.692 | 947 | 952 | 956 | rBV | 18367 | 23313 | 1.56% | 0.254% |
| 8 | 8.157 | 1025 | 1031 | 1036 | rBV | 483401 | 595564 | 39.92% | 6.500% |
| 9 | 9.228 | 1208 | 1213 | 1223 | rBV | 736060 | 927360 | 62.16% | 10.122% |
| 10 | 9.910 | 1324 | 1329 | 1344 | rVB | 515343 | 639617 | 42.87% | 6.981% |
| 11 | 10.622 | 1445 | 1450 | 1458 | rBV | 126405 | 154608 | 10.36% | 1.687% |
| 12 | 10.698 | 1458 | 1463 | 1475 | rVV | 345570 | 453895 | 30.42% | 4.954% |
| 13 | 11.392 | 1576 | 1581 | 1592 | rBV | 430566 | 565169 | 37.88% | 6.168% |
| 14 | 11.921 | 1663 | 1671 | 1681 | rBV3 | 29551 | 72190 | 4.84% | 0.788% |
| 15 | 12.604 | 1783 | 1787 | 1795 | rBV | 22614 | 27731 | 1.86% | 0.303% |
| 16 | 12.792 | 1814 | 1819 | 1822 | rBV3 | 20179 | 28474 | 1.91% | 0.311% |
| 17 | 12.833 | 1822 | 1826 | 1830 | rVB | 19560 | 26167 | 1.75% | 0.286% |
| 18 | 12.974 | 1845 | 1850 | 1859 | rBV | 452325 | 587330 | 39.37% | 6.410% |
| 19 | 13.457 | 1925 | 1932 | 1938 | rBV | 174977 | 253215 | 16.97% | 2.764% |
| 20 | 13.510 | 1938 | 1941 | 1950 | rVB | 39941 | 58157 | 3.90% | 0.635% |
| 21 | 14.027 | 2024 | 2029 | 2038 | rVB | 261260 | 352725 | 23.64% | 3.850% |
| 22 | 15.068 | 2202 | 2206 | 2215 | rVB | 10656 | 23348 | 1.56% | 0.255% |
| 23 | 15.498 | 2273 | 2279 | 2291 | rVB | 205523 | 324482 | 21.75% | 3.542% |

Sum of corrected areas: 9162216

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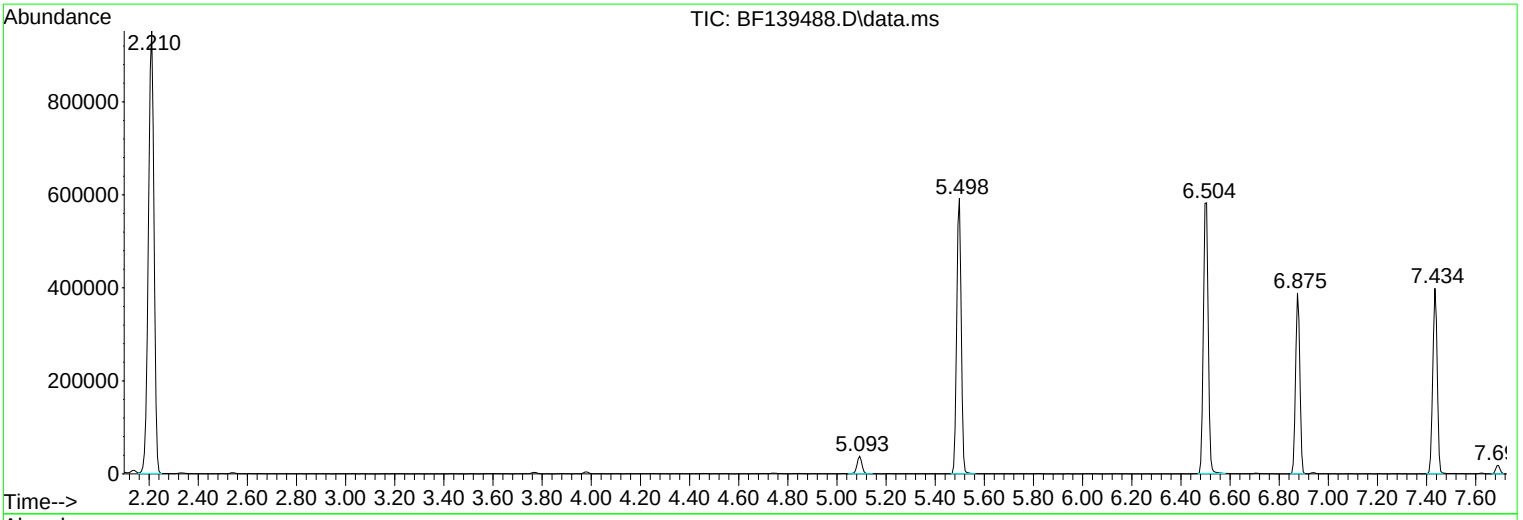
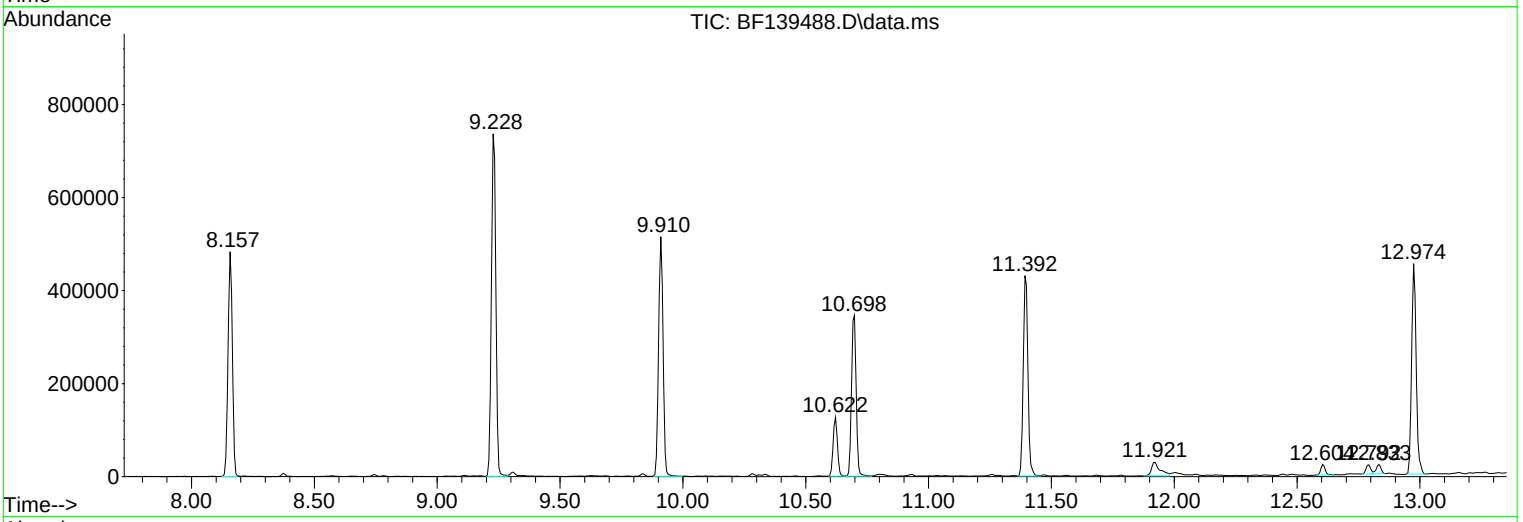
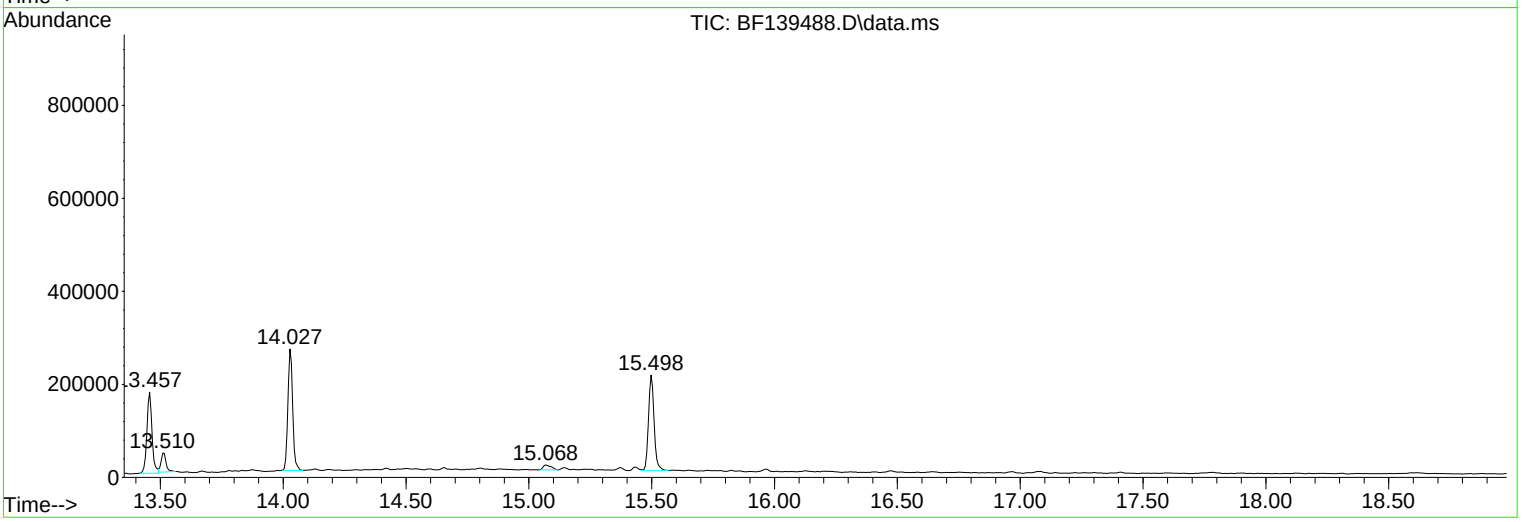
**Instrument :**
BNA_F
**ClientSampleId :**
DN-B-49

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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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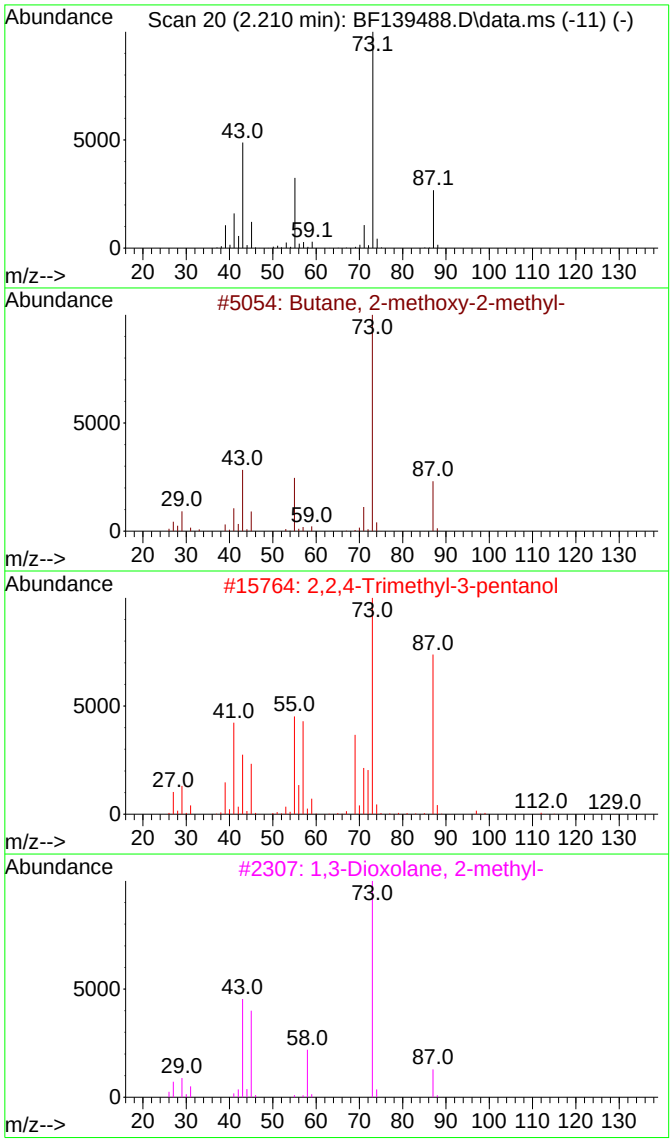
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

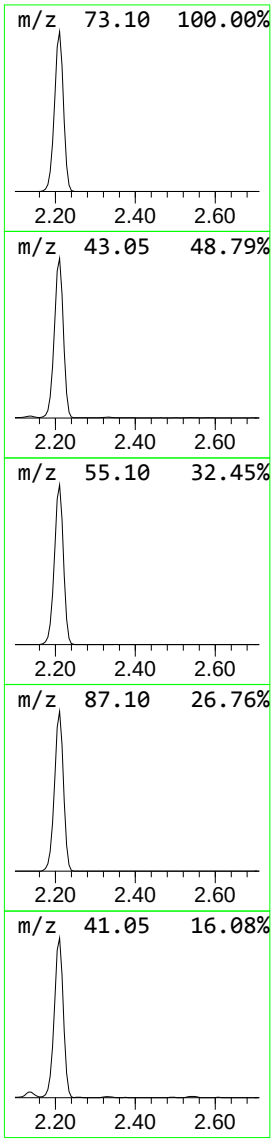
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.210 | 63.37 ng | 1491950 | 1,4-Dichlorobenzene-d4 | 6.875 |

| 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 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 23 |
| 4 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 17 |
| 5 | Borane, dimethoxy- | 74 | C2H7BO2 | 004542-61-4 | 9 |



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Acq On : 20 Sep 2024 02:59
Operator : RC/JU
Sample : P4027-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
DN-B-49

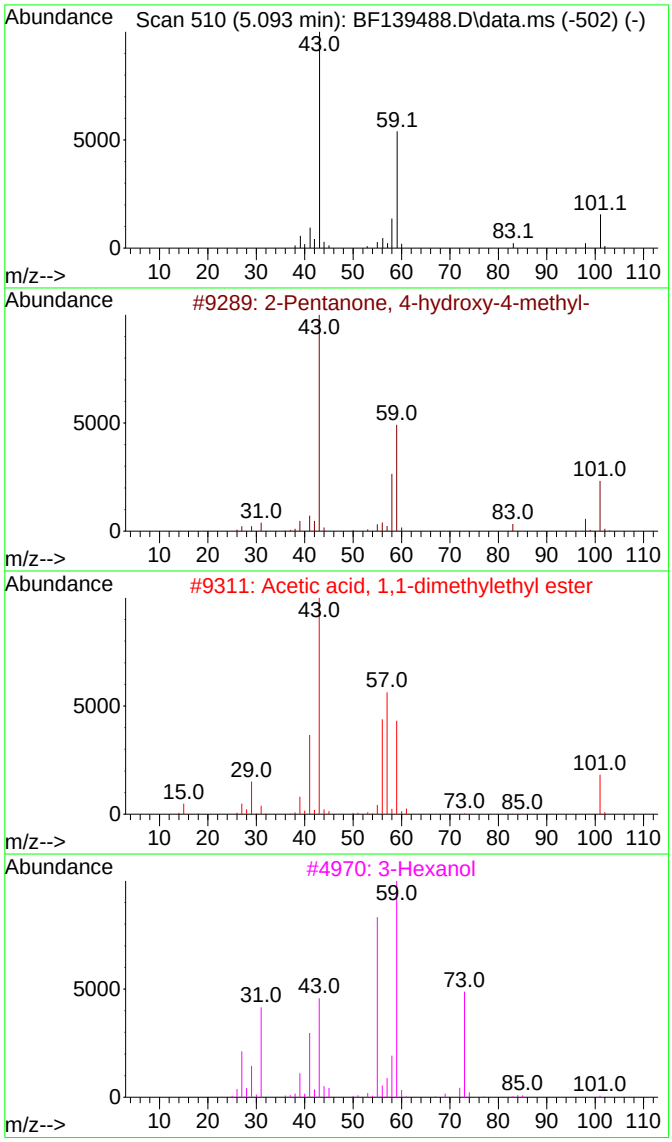
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

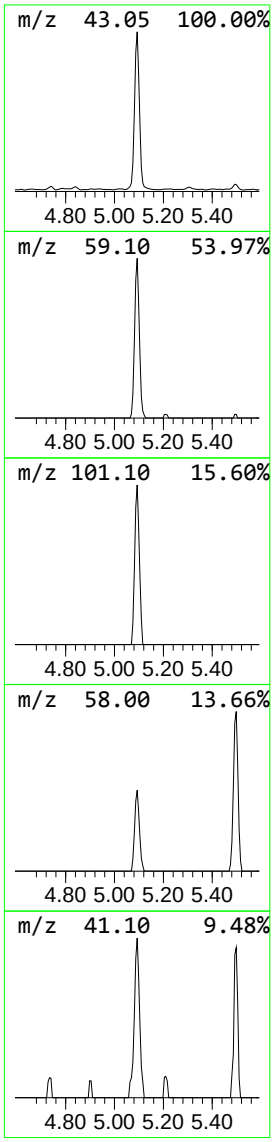
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.093 | 2.23 ng | 52442 | 1,4-Dichlorobenzene-d4 | 6.875 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 38 |
| 3 | 3-Hexanol | 102 | C6H14O | 000623-37-0 | 33 |
| 4 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 5 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 28 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091924\
Data File : BF139488.D
Acq On : 20 Sep 2024 02:59
Operator : RC/JU
Sample : P4027-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
DN-B-49

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

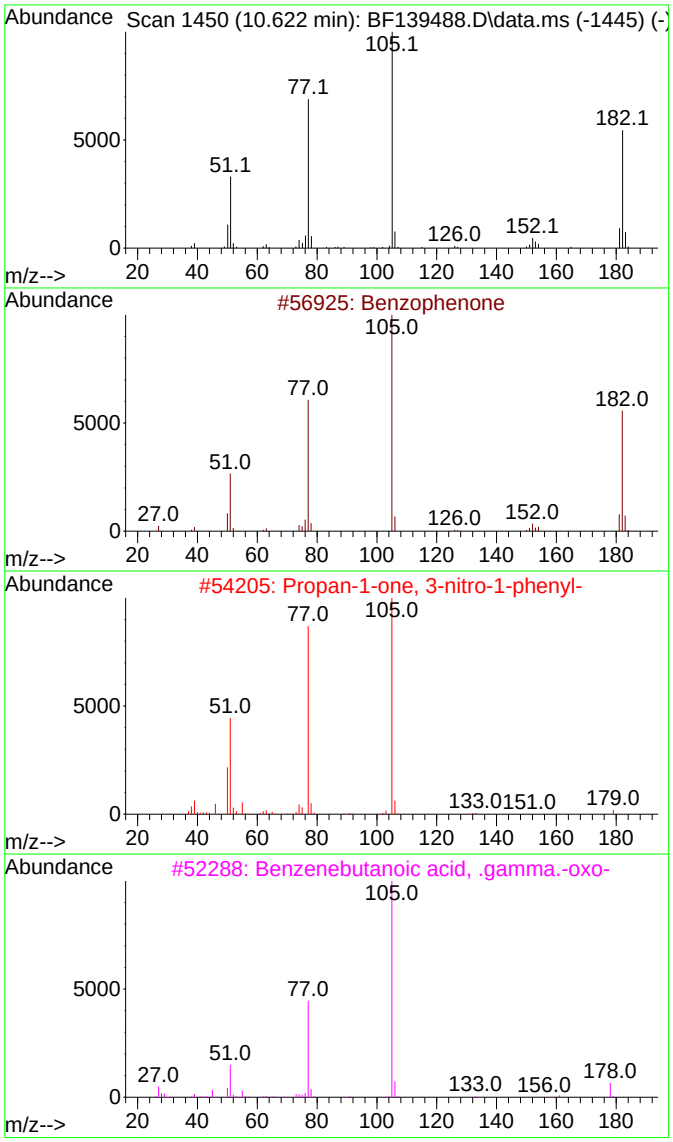
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

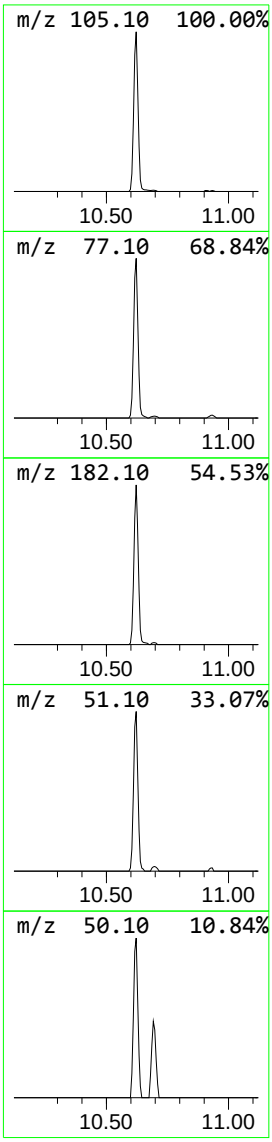
**********

Peak Number 3 Benzophenone Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.622 | 4.83 ng | 154608 | Acenaphthene-d10 | 9.910 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 96 |
| 2 | Propan-1-one, 3-nitro-1-phenyl- | 179 | C9H9NO3 | 062847-52-3 | 47 |
| 3 | Benzenebutanoic acid, .gamma.-oxo- | 178 | C10H10O3 | 002051-95-8 | 47 |
| 4 | Ethanedione, diphenyl- | 210 | C14H10O2 | 000134-81-6 | 47 |
| 5 | Benzoic acid, (4-pyridylmethylen... | 225 | C13H11N3O | 001507-93-3 | 47 |



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Operator : RC/JU
Sample : P4027-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
DN-B-49

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

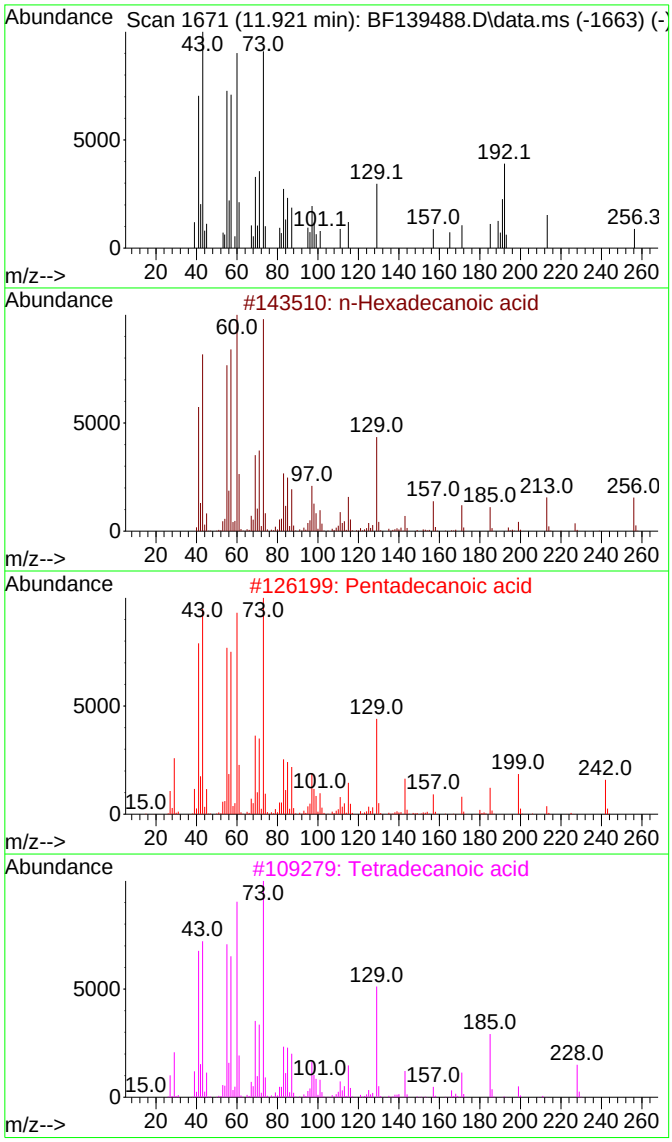
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

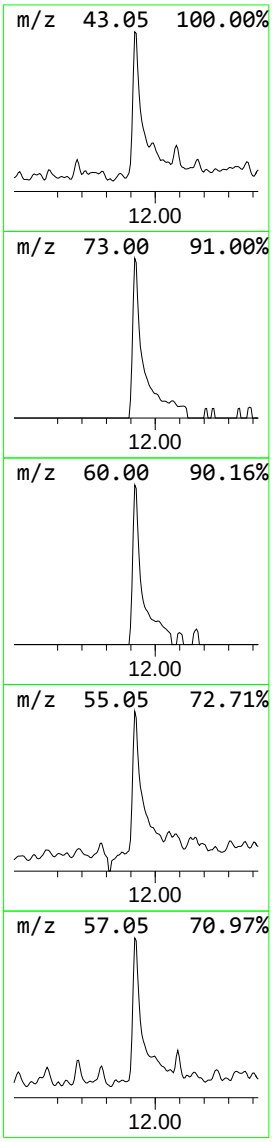
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.922 | 2.55 ng | 72190 | Phenanthrene-d10 | 11.392 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 70 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 53 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 52 |
| 5 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 49 |



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Sample : P4027-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
DN-B-49

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

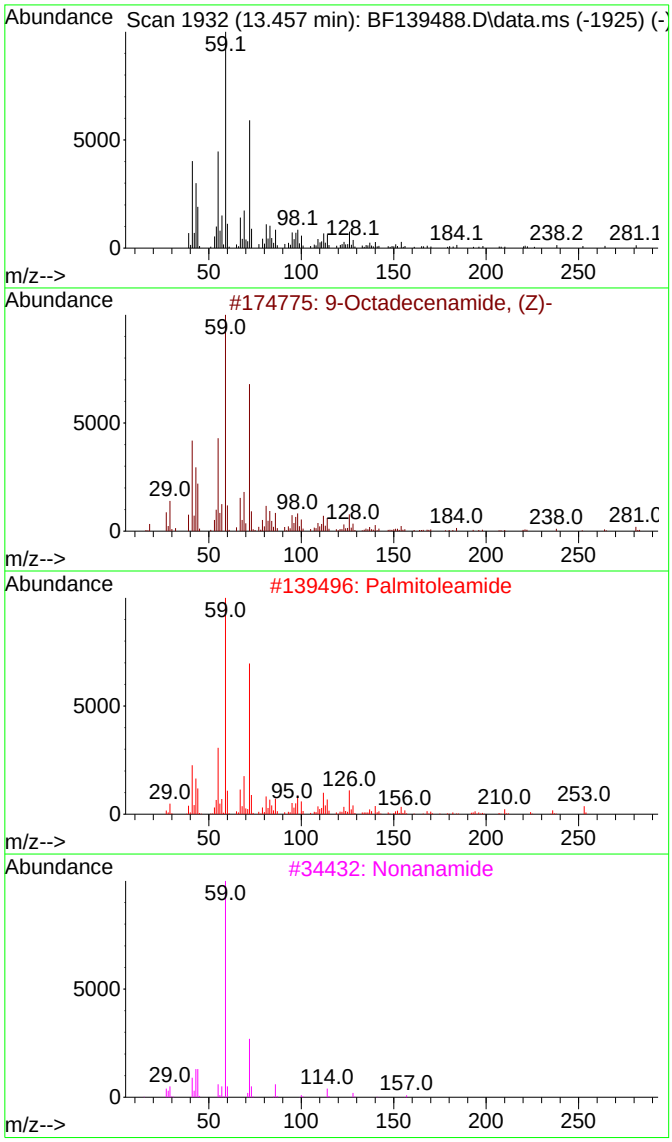
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

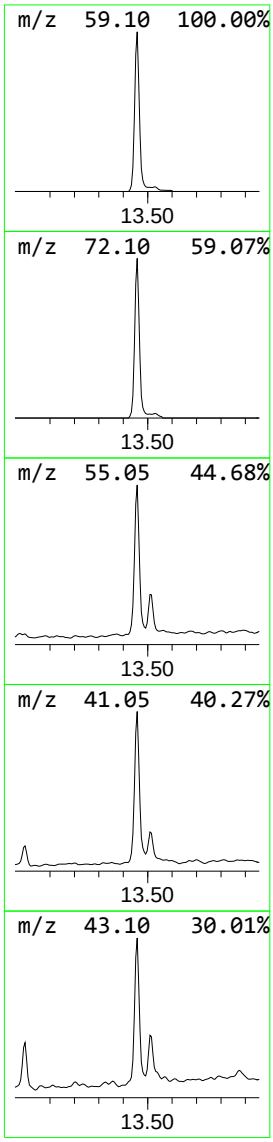
**********

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.457 | 14.36 ng | 253215 | Chrysene-d12 | 14.027 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 99 |
| 2 | Palmitoleamide | 253 | C16H31NO | 106010-22-4 | 72 |
| 3 | Nonanamide | 157 | C9H19NO | 001120-07-6 | 64 |
| 4 | Octanamide | 143 | C8H17NO | 000629-01-6 | 64 |
| 5 | Hexadecanamide | 255 | C16H33NO | 000629-54-9 | 59 |



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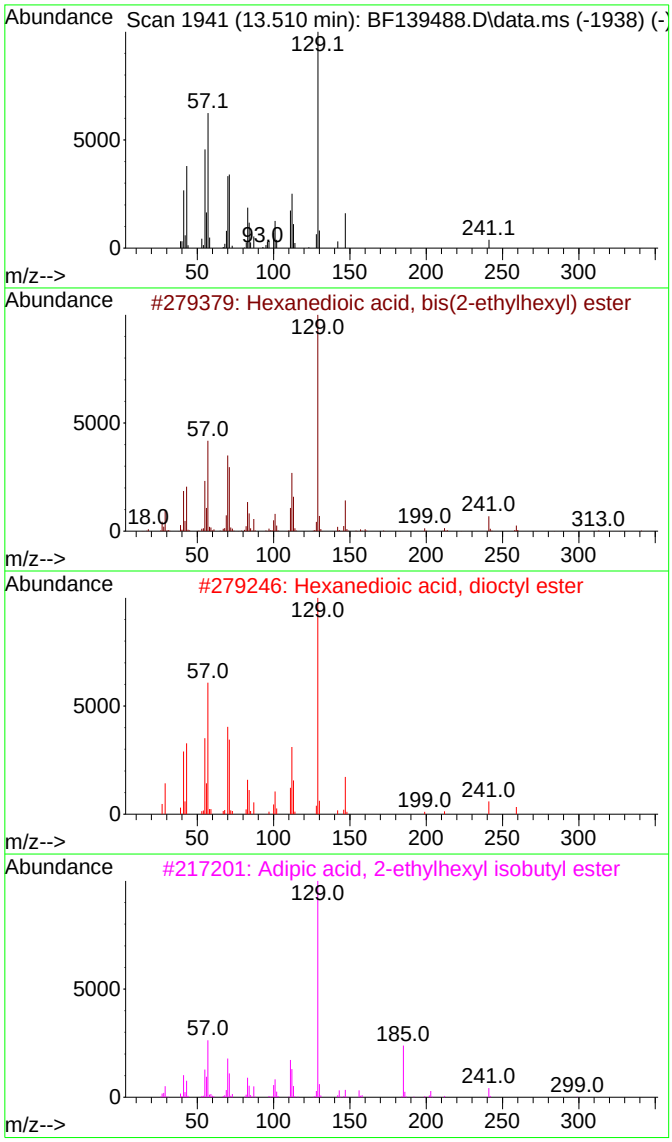
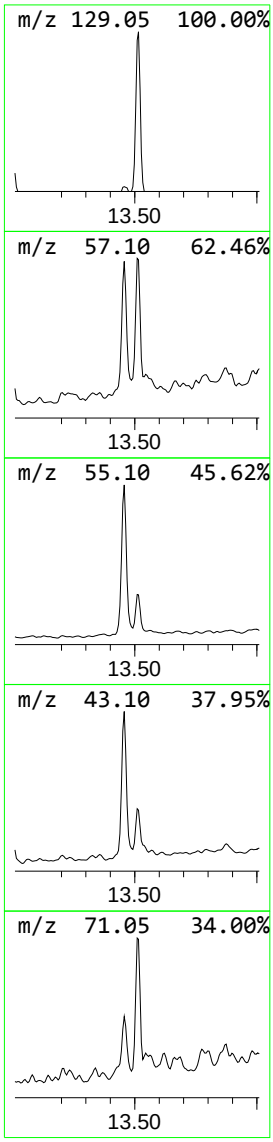
**********
Peak Number 6 Hexanedioic acid, bis(2-eth... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.510 | 3.30 ng | 58157 | Chrysene-d12 | 14.027 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexanedioic acid, bis(2-ethylhex... | 370 | C22H42O4 | 000103-23-1 | 86 |
| 2 | Hexanedioic acid, dioctyl ester | 370 | C22H42O4 | 000123-79-5 | 83 |
| 3 | Adipic acid, 2-ethylhexyl isobut... | 314 | C18H34O4 | 1010324-48-0 | 59 |
| 4 | Adipic acid, isohexyl 3-pentyl e... | 300 | C17H32O4 | 1000324-60-7 | 47 |
| 5 | Adipic acid, isobutyl 3-pentyl e... | 272 | C15H28O4 | 1000324-60-4 | 43 |



Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-metho... | 2.210 | 63.4 | ng | 1491950 | 1 | 6.875 | 470854 | 20.0 |
| 2-Pentanone, 4-... | 5.093 | 2.2 | ng | 52442 | 1 | 6.875 | 470854 | 20.0 |
| Benzophenone | 10.622 | 4.8 | ng | 154608 | 3 | 9.910 | 639617 | 20.0 |
| n-Hexadecanoic ... | 11.922 | 2.5 | ng | 72190 | 4 | 11.392 | 565169 | 20.0 |
| 9-Octadecenamid... | 13.457 | 14.4 | ng | 253215 | 5 | 14.027 | 352725 | 20.0 |
| Hexanedioic aci... | 13.510 | 3.3 | ng | 58157 | 5 | 14.027 | 352725 | 20.0 |