LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042325\
Data File : BM050012.D
Acq On : 23 Apr 2025 13:58
Operator : RC/JU
Sample : Q1852-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
72-12013

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_M\Methods\8270-BM040825.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM050012.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 4.881 | 317 | 322 | 335 | rVB | 718928 | 1002059 | 7.41% | 1.413% |
| 2 | 5.357 | 395 | 403 | 419 | rBV | 3826165 | 5875628 | 43.43% | 8.286% |
| 3 | 6.951 | 667 | 674 | 698 | rBV | 3502994 | 6005467 | 44.39% | 8.469% |
| 4 | 7.763 | 805 | 812 | 820 | rBV | 948817 | 1464594 | 10.83% | 2.065% |
| 5 | 8.922 | 998 | 1009 | 1028 | rBV | 2189093 | 3804991 | 28.13% | 5.366% |
| 6 | 10.557 | 1278 | 1287 | 1301 | rBV | 1054574 | 1837970 | 13.59% | 2.592% |
| 7 | 13.027 | 1699 | 1707 | 1727 | rBV | 6079213 | 9063726 | 67.00% | 12.782% |
| 8 | 14.410 | 1935 | 1942 | 1954 | rBV | 1647436 | 2473875 | 18.29% | 3.489% |
| 9 | 15.227 | 2073 | 2081 | 2095 | rBV | 266580 | 504991 | 3.73% | 0.712% |
| 10 | 15.768 | 2167 | 2173 | 2188 | rBV | 1140726 | 1674662 | 12.38% | 2.362% |
| 11 | 15.904 | 2189 | 2196 | 2211 | rBV | 5324901 | 8038744 | 59.42% | 11.336% |
| 12 | 16.333 | 2264 | 2269 | 2274 | rVB | 126324 | 174126 | 1.29% | 0.246% |
| 13 | 17.157 | 2403 | 2409 | 2420 | rBV2 | 1968138 | 2851431 | 21.08% | 4.021% |
| 14 | 18.057 | 2557 | 2562 | 2569 | rBV | 1393486 | 2083217 | 15.40% | 2.938% |
| 15 | 18.121 | 2569 | 2573 | 2584 | rVB | 325332 | 591756 | 4.37% | 0.834% |
| 16 | 18.474 | 2629 | 2633 | 2640 | rBV2 | 265606 | 370279 | 2.74% | 0.522% |
| 17 | 19.262 | 2761 | 2767 | 2775 | rBV2 | 477903 | 1002366 | 7.41% | 1.414% |
| 18 | 19.333 | 2775 | 2779 | 2794 | rVB | 752723 | 1262120 | 9.33% | 1.780% |
| 19 | 19.780 | 2850 | 2855 | 2862 | rBV | 11634316 | 13528021 | 100.00% | 19.077% |
| 20 | 21.074 | 3071 | 3075 | 3083 | rBV2 | 300667 | 460737 | 3.41% | 0.650% |
| 21 | 21.397 | 3125 | 3130 | 3136 | rBV | 2200988 | 3251700 | 24.04% | 4.585% |
| 22 | 24.397 | 3633 | 3640 | 3661 | rVB | 1307660 | 3590327 | 26.54% | 5.063% |

Sum of corrected areas: 70912787

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**Instrument :**
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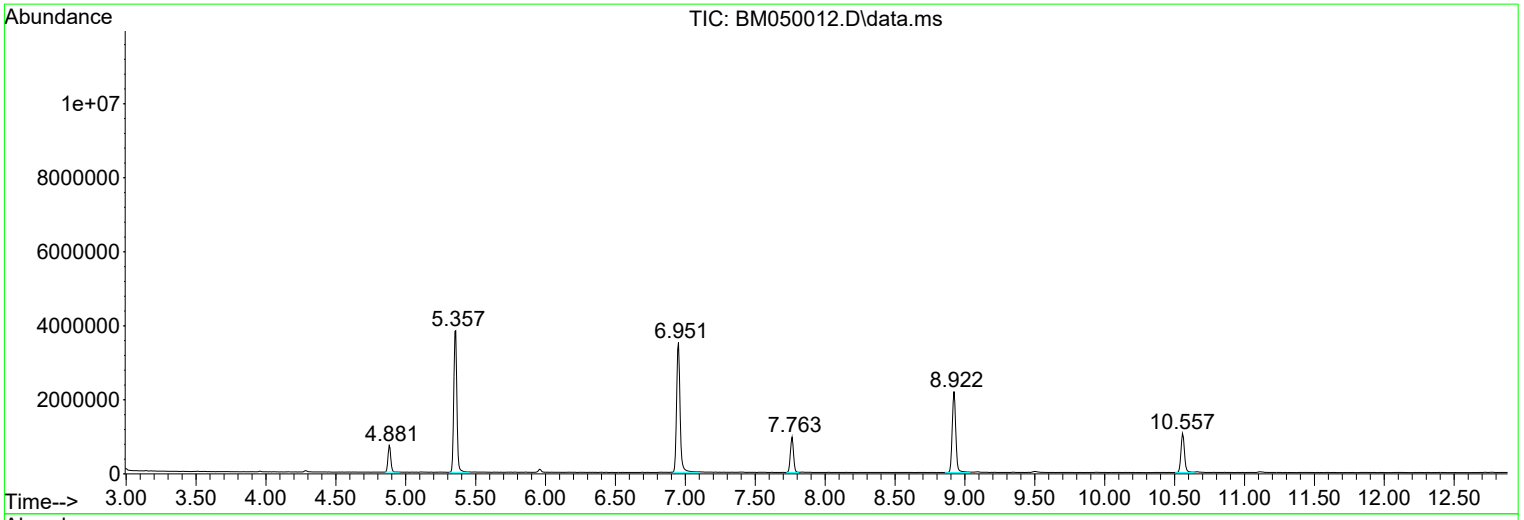
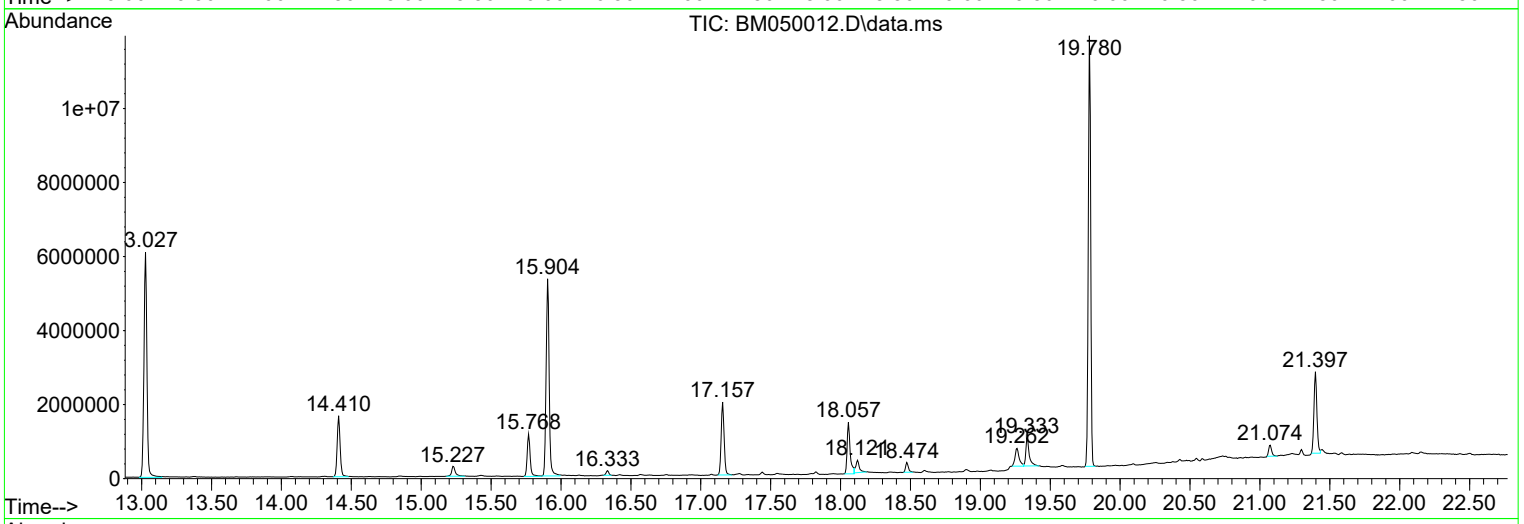
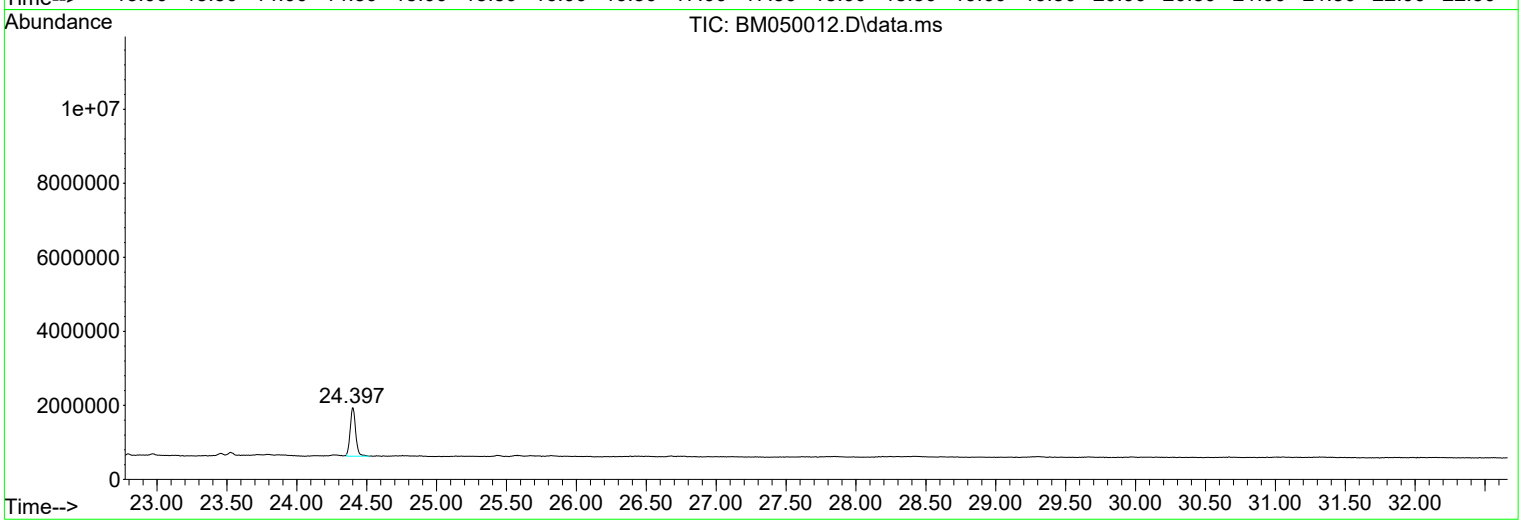
**ClientSampleId :**
72-12013

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.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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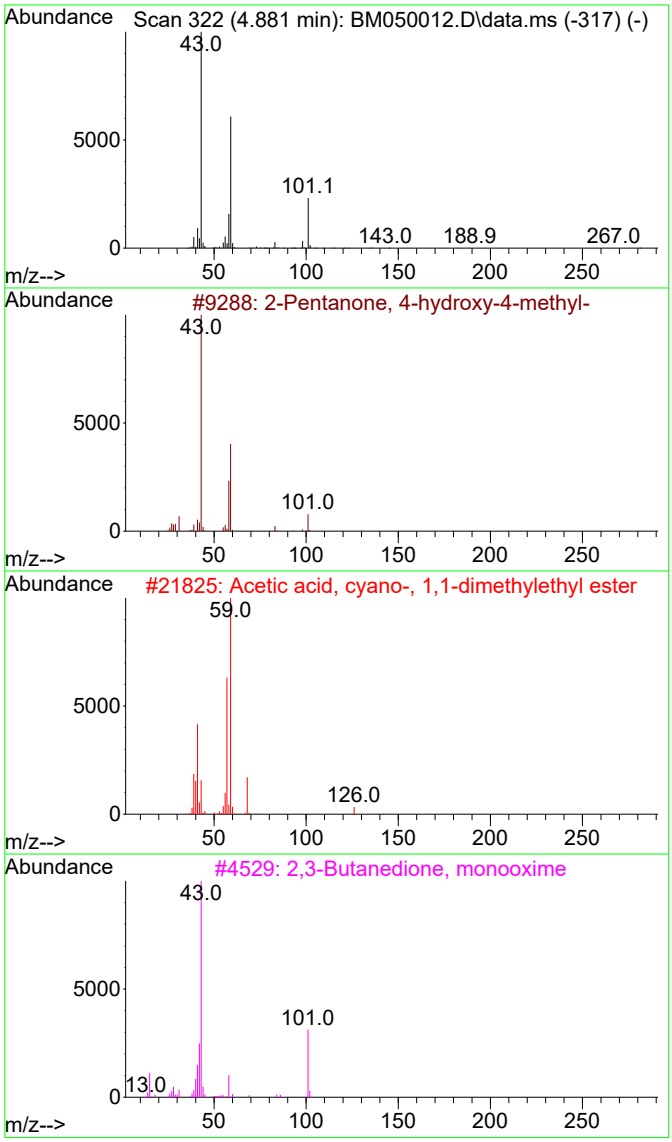
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

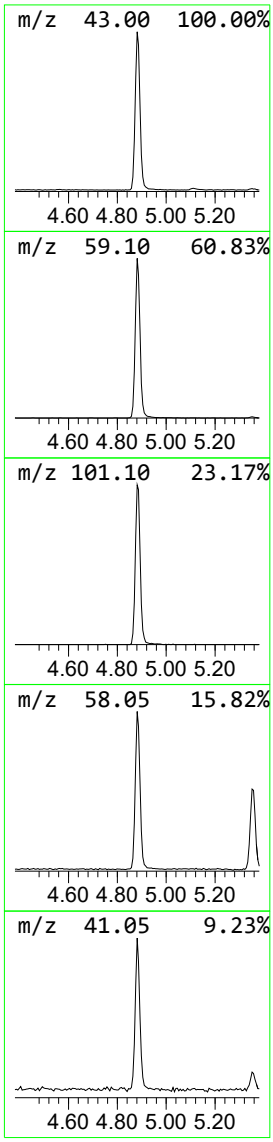
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.881 | 13.68 ng | 1002060 | 1,4-Dichlorobenzene-d4 | 7.763 |

| 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, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 17 |
| 4 | Formamide, N,N-diethyl- | 101 | C5H11NO | 000617-84-5 | 9 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042325\
Data File : BM050012.D
Acq On : 23 Apr 2025 13:58
Operator : RC/JU
Sample : Q1852-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
72-12013

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

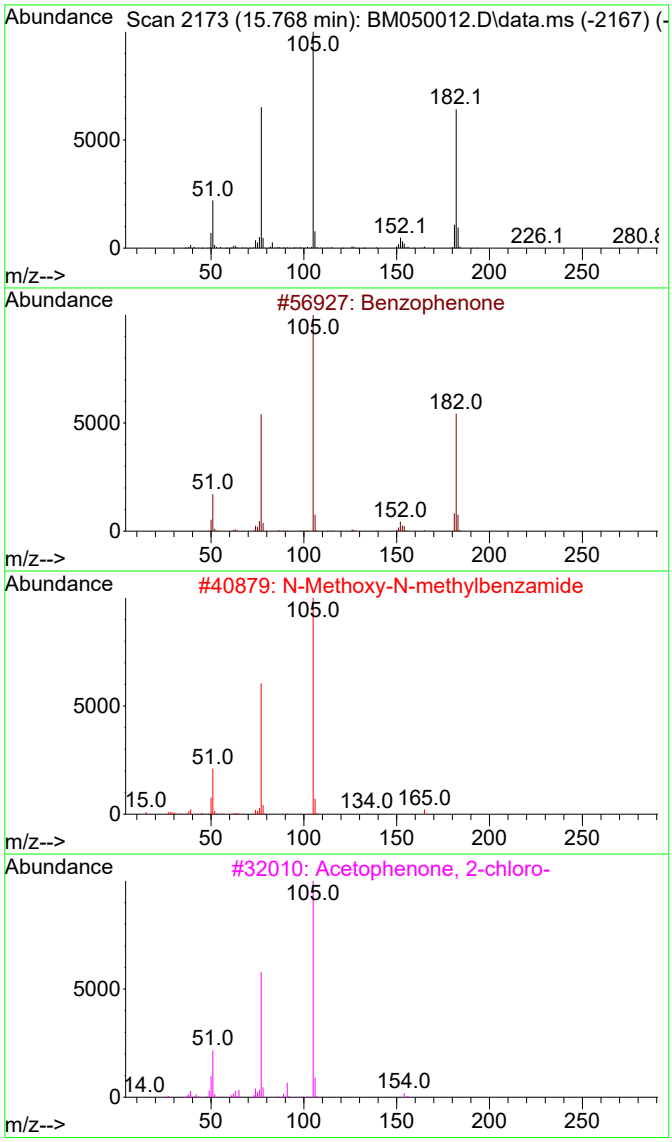
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

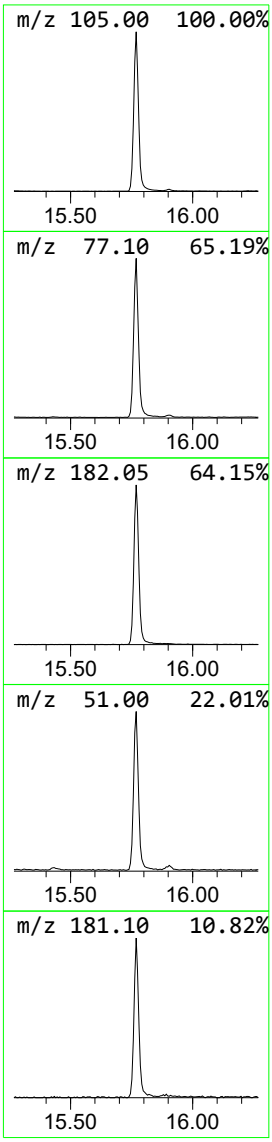
**********

Peak Number 2 Benzophenone Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.768 | 13.54 ng | 1674660 | Acenaphthene-d10 | 14.410 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 96 |
| 2 | N-Methoxy-N-methylbenzamide | 165 | C9H11NO2 | 006919-61-5 | 46 |
| 3 | Acetophenone, 2-chloro- | 154 | C8H7ClO | 000532-27-4 | 46 |
| 4 | Benzenecarbothioic acid, S-methy... | 152 | C8H8OS | 005925-68-8 | 46 |
| 5 | Benzeneacetic acid, .alpha.-oxo-... | 164 | C9H8O3 | 015206-55-0 | 43 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042325\
Data File : BM050012.D
Acq On : 23 Apr 2025 13:58
Operator : RC/JU
Sample : Q1852-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
72-12013

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

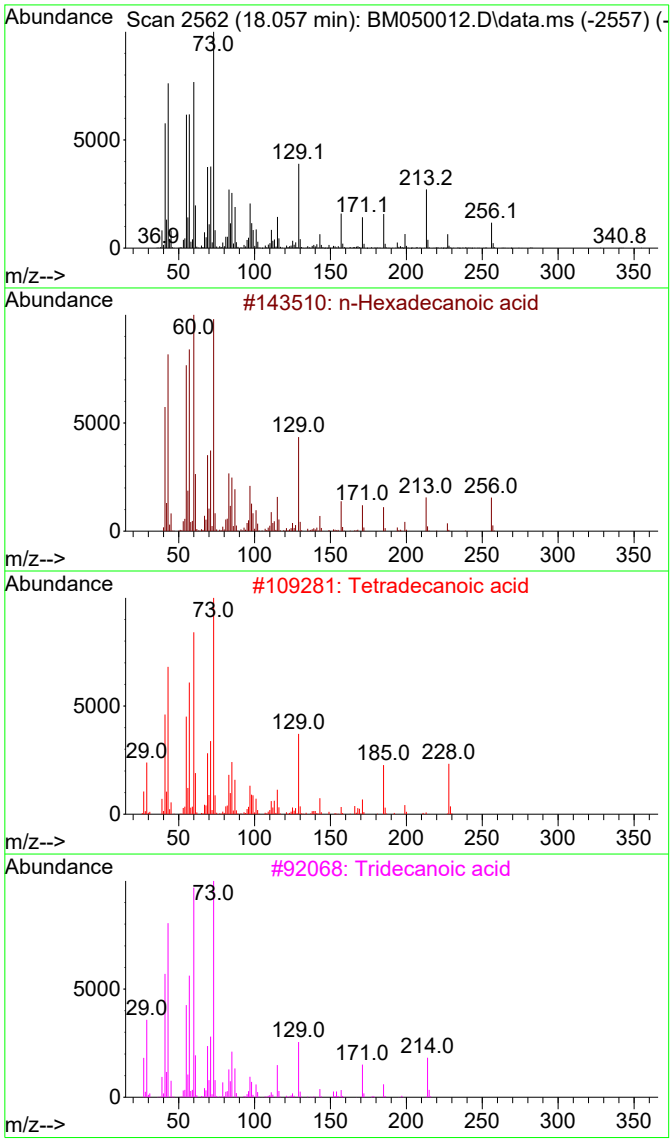
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

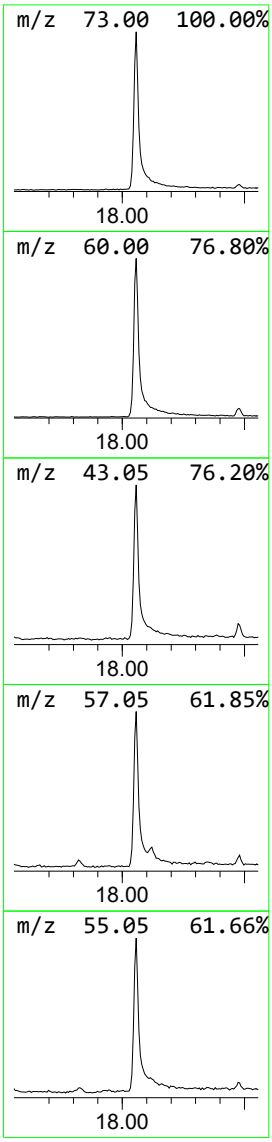
**********

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.057 | 14.61 ng | 2083220 | Phenanthrene-d10 | 17.157 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 94 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 90 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 64 |



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Data File : BM050012.D
Acq On : 23 Apr 2025 13:58
Operator : RC/JU
Sample : Q1852-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
72-12013

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

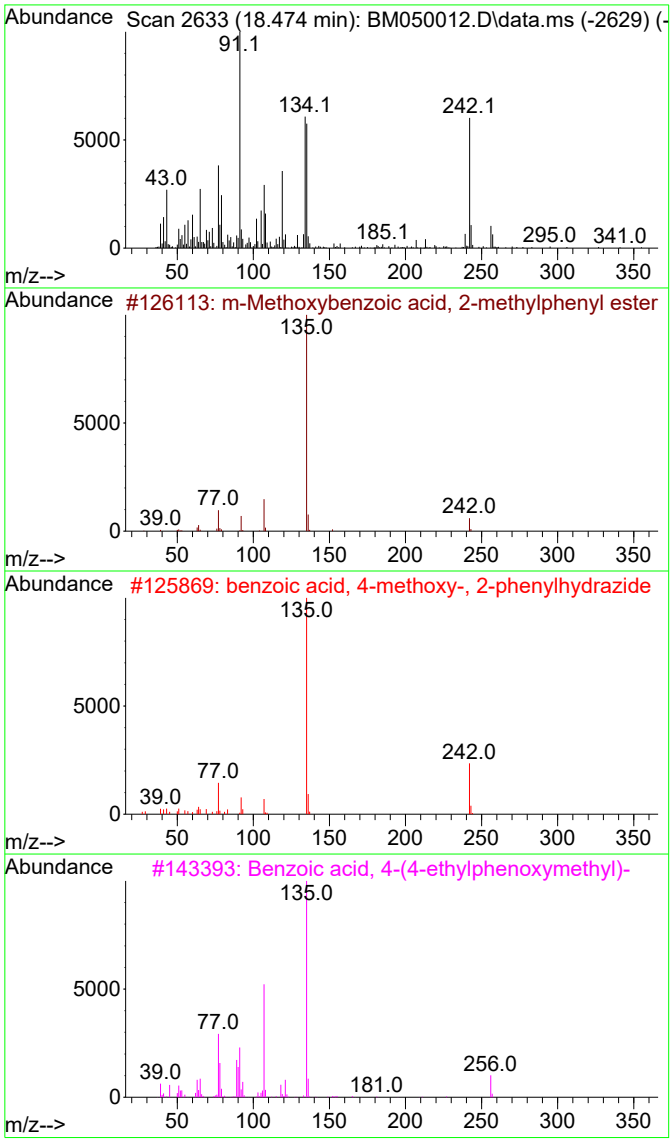
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

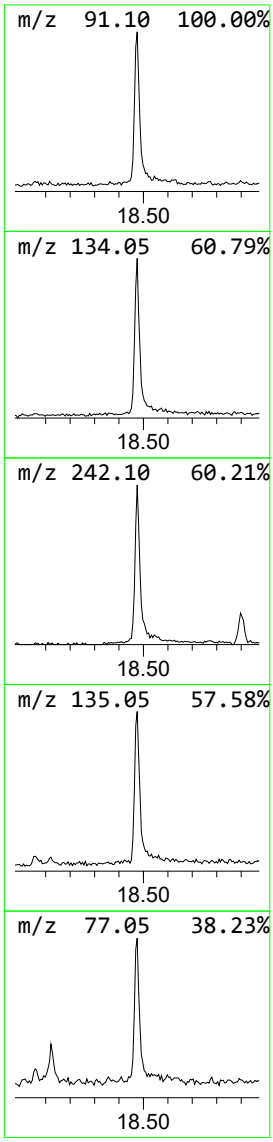
**********

Peak Number 4 unknown18.474 Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.474 | 2.60 ng | 370279 | Phenanthrene-d10 | 17.157 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | m-Methoxybenzoic acid, 2-methylp... | 242 | C15H14O3 | 1000292-62-8 | 49 |
| 2 | benzoic acid, 4-methoxy-, 2-phen... | 242 | C14H14N2O2 | 1000401-23-1 | 30 |
| 3 | Benzoic acid, 4-(4-ethylphenoxym... | 256 | C16H16O3 | 1000272-90-4 | 25 |
| 4 | Cyclopentanecarboxylic acid, 2-a... | 248 | C16H24O2 | 1000282-77-0 | 25 |
| 5 | Benzenamine, N,N,2-trimethyl- | 135 | C9H13N | 000609-72-3 | 25 |



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Sample : Q1852-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
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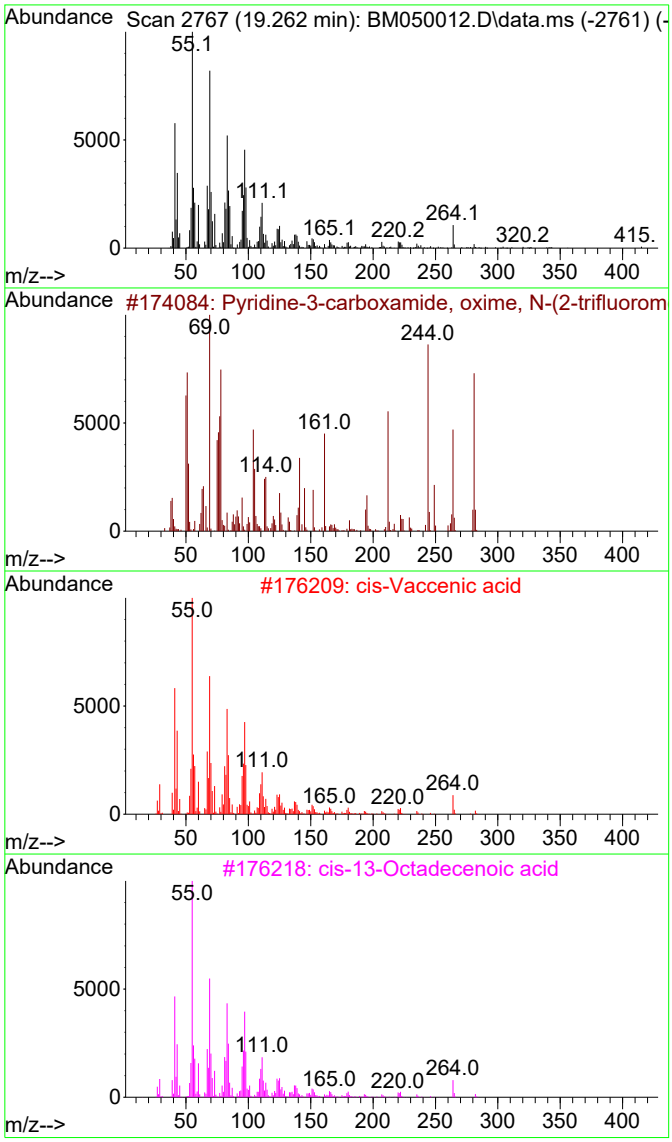
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

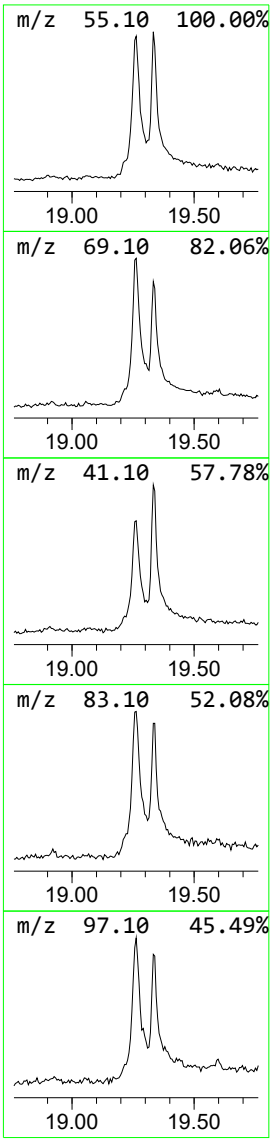
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 Pyridine-3-carboxamide, oxi... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.262 | 7.03 ng | 1002370 | Phenanthrene-d10 | 17.157 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pyridine-3-carboxamide, oxime, N... | 281 | C13H10F3N3O | 288246-53-7 | 91 |
| 2 | cis-Vaccenic acid | 282 | C18H34O2 | 000506-17-2 | 83 |
| 3 | cis-13-Octadecenoic acid | 282 | C18H34O2 | 013126-39-1 | 83 |
| 4 | 9-Octadecenoic acid, (E)- | 282 | C18H34O2 | 000112-79-8 | 78 |
| 5 | trans-13-Octadecenoic acid | 282 | C18H34O2 | 000693-71-0 | 55 |



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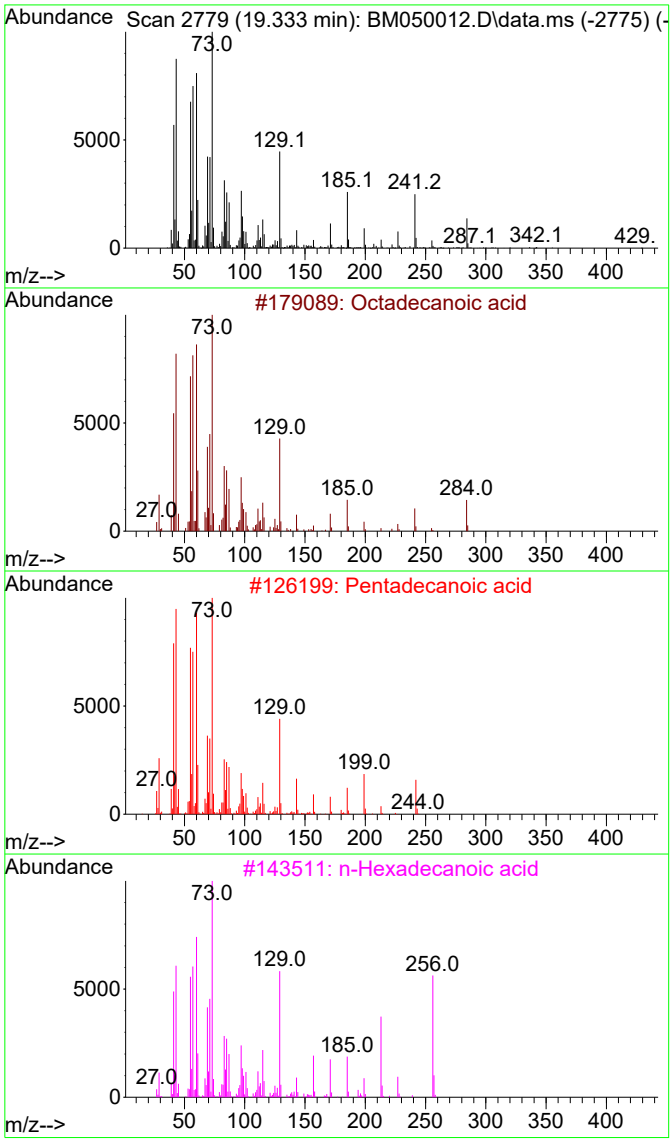
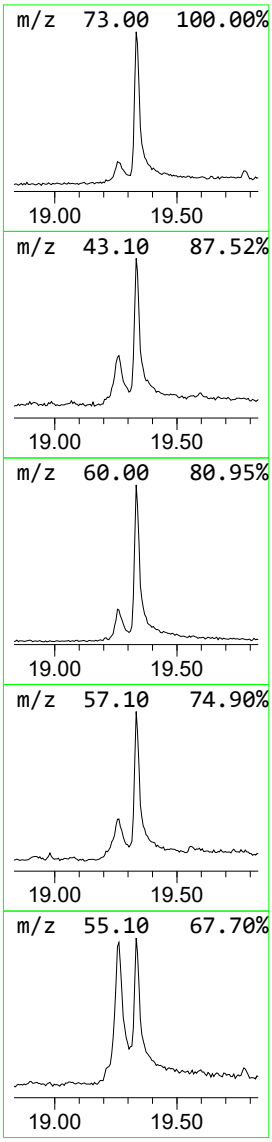
**********

Peak Number 6 Octadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.333 | 7.76 ng | 1262120 | Chrysene-d12 | 21.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 93 |
| 3 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 91 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 83 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 70 |



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Misc :
ALS Vial : 7 Sample Multiplier: 1

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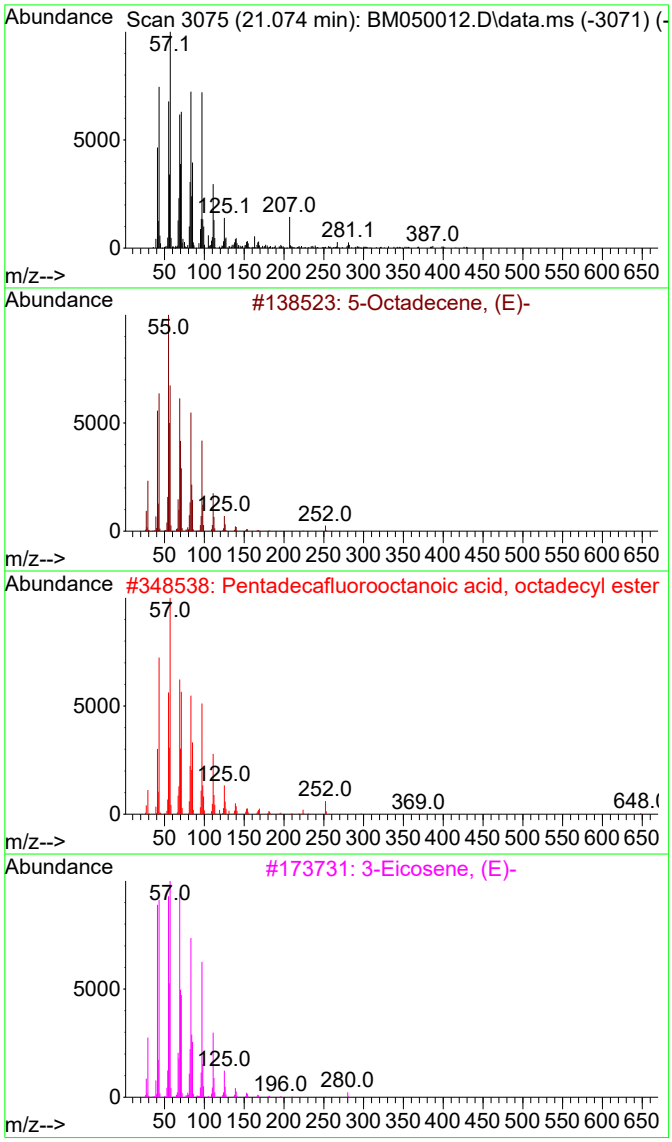
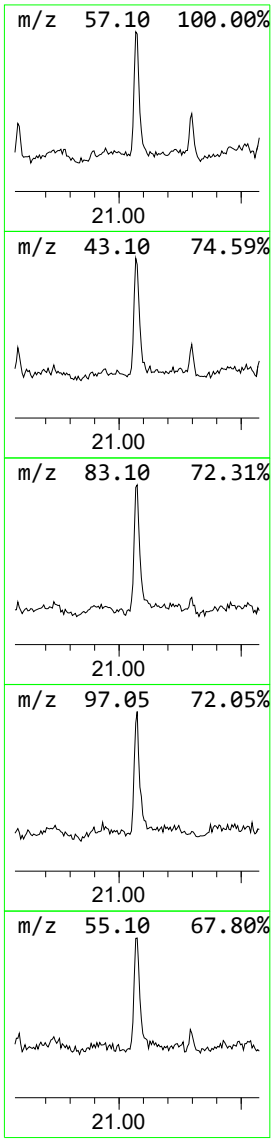
**********

Peak Number 7 5-Octadecene, (E)- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.074 | 2.83 ng | 460737 | Chrysene-d12 | 21.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Octadecene, (E)- | 252 | C18H36 | 007206-21-5 | 95 |
| 2 | Pentadecafluorooctanoic acid, oc... | 666 | C26H37F15O2 | 1000406-04-8 | 94 |
| 3 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 93 |
| 4 | Ethanol, 2-(tetradecyloxy)- | 258 | C16H34O2 | 002136-70-1 | 91 |
| 5 | 9-Eicosene, (E)- | 280 | C20H40 | 074685-29-3 | 89 |



Tentatively Identified Compound (LSC) summary

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| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-... | 4.881 | 13.7 | ng | 1002060 | 1 | 7.763 | 1464590 | 20.0 |
| Benzophenone | 15.768 | 13.5 | ng | 1674660 | 3 | 14.410 | 2473880 | 20.0 |
| n-Hexadecanoic ... | 18.057 | 14.6 | ng | 2083220 | 4 | 17.157 | 2851430 | 20.0 |
| unknown18.474 | 18.474 | 2.6 | ng | 370279 | 4 | 17.157 | 2851430 | 20.0 |
| Pyridine-3-carb... | 19.262 | 7.0 | ng | 1002370 | 4 | 17.157 | 2851430 | 20.0 |
| Octadecanoic acid | 19.333 | 7.8 | ng | 1262120 | 5 | 21.398 | 3251700 | 20.0 |
| 5-Octadecene, (E)- | 21.074 | 2.8 | ng | 460737 | 5 | 21.398 | 3251700 | 20.0 |