

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM081924\  
 Data File : BM047258.D  
 Acq On : 19 Aug 2024 18:49  
 Operator : RC/JU  
 Sample : P3619-01  
 Misc :  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 917-J-WS-081424

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-BM081024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047258.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 4.569       | 278           | 286         | 292          | rBV2     | 95759          | 150411        | 1.05%           | 0.254%        |
| 2         | 5.016       | 356           | 362         | 375          | rBV      | 1972881        | 2885063       | 20.14%          | 4.870%        |
| 3         | 6.575       | 621           | 627         | 638          | rBV      | 1250280        | 1945907       | 13.58%          | 3.284%        |
| 4         | 7.363       | 754           | 761         | 768          | rBV      | 768864         | 1159912       | 8.10%           | 1.958%        |
| 5         | 8.510       | 945           | 956         | 971          | rBV      | 2439858        | 3947059       | 27.55%          | 6.662%        |
| 6         | 10.116      | 1223          | 1229        | 1237         | rBV      | 919549         | 1540507       | 10.75%          | 2.600%        |
| 7         | 10.880      | 1351          | 1359        | 1368         | rBV      | 93793          | 190624        | 1.33%           | 0.322%        |
| 8         | 11.839      | 1516          | 1522        | 1535         | rBV      | 64951          | 203764        | 1.42%           | 0.344%        |
| 9         | 12.633      | 1649          | 1657        | 1664         | rBV      | 5940069        | 8932116       | 62.34%          | 15.076%       |
| 10        | 13.898      | 1861          | 1872        | 1887         | rBV3     | 57394          | 194704        | 1.36%           | 0.329%        |
| 11        | 14.021      | 1887          | 1893        | 1903         | rVV      | 1451103        | 2120253       | 14.80%          | 3.579%        |
| 12        | 14.263      | 1928          | 1934        | 1935         | rBV2     | 321293         | 445998        | 3.11%           | 0.753%        |
| 13        | 14.280      | 1935          | 1937        | 1946         | rVB      | 360724         | 407380        | 2.84%           | 0.688%        |
| 14        | 15.533      | 2143          | 2150        | 2162         | rBV      | 5542860        | 8016210       | 55.95%          | 13.530%       |
| 15        | 16.233      | 2264          | 2269        | 2278         | rBV2     | 100865         | 197290        | 1.38%           | 0.333%        |
| 16        | 16.786      | 2358          | 2363        | 2372         | rBV      | 1834663        | 2623032       | 18.31%          | 4.427%        |
| 17        | 16.868      | 2372          | 2377        | 2381         | rBV2     | 250252         | 305365        | 2.13%           | 0.515%        |
| 18        | 17.727      | 2517          | 2523        | 2531         | rBV      | 1087526        | 1721296       | 12.01%          | 2.905%        |
| 19        | 18.903      | 2720          | 2723        | 2735         | rVB3     | 148142         | 303462        | 2.12%           | 0.512%        |
| 20        | 19.027      | 2739          | 2744        | 2756         | rBV      | 505413         | 844472        | 5.89%           | 1.425%        |
| 21        | 19.456      | 2811          | 2817        | 2822         | rBV      | 11756271       | 14326950      | 100.00%         | 24.182%       |
| 22        | 19.797      | 2872          | 2875        | 2879         | rBV      | 152999         | 175481        | 1.22%           | 0.296%        |
| 23        | 20.762      | 3036          | 3039        | 3047         | rBV2     | 172282         | 260106        | 1.82%           | 0.439%        |
| 24        | 21.027      | 3079          | 3084        | 3090         | rBV      | 2516748        | 3215714       | 22.45%          | 5.428%        |
| 25        | 23.727      | 3536          | 3543        | 3558         | rVB      | 1315311        | 3134127       | 21.88%          | 5.290%        |

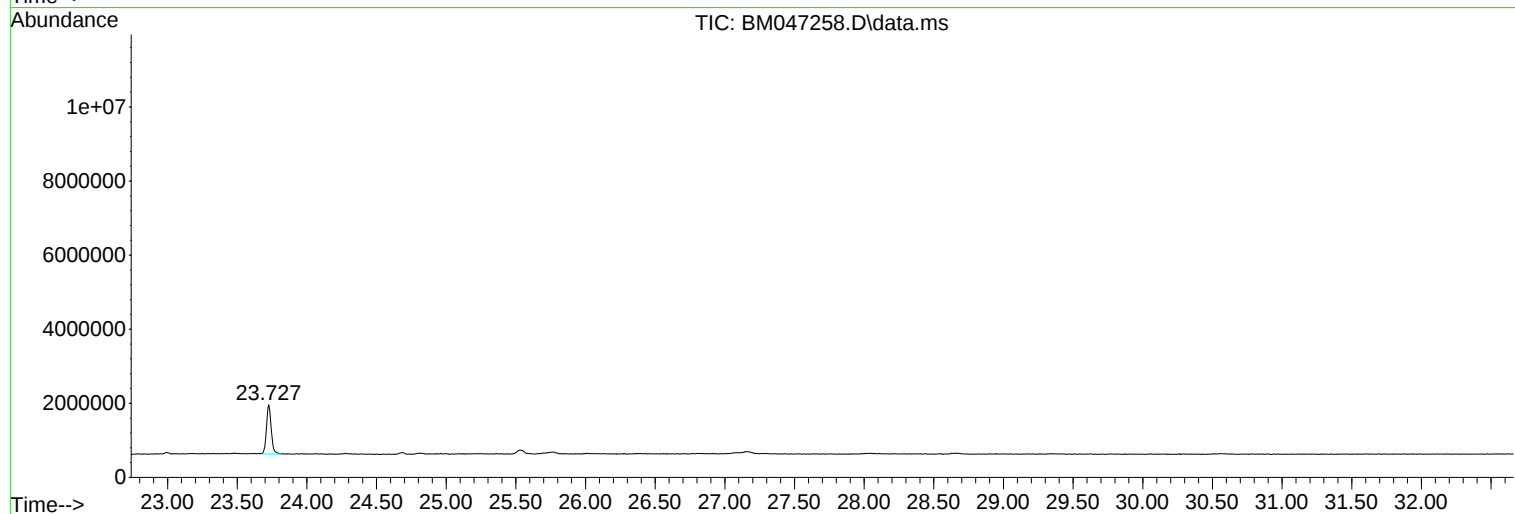
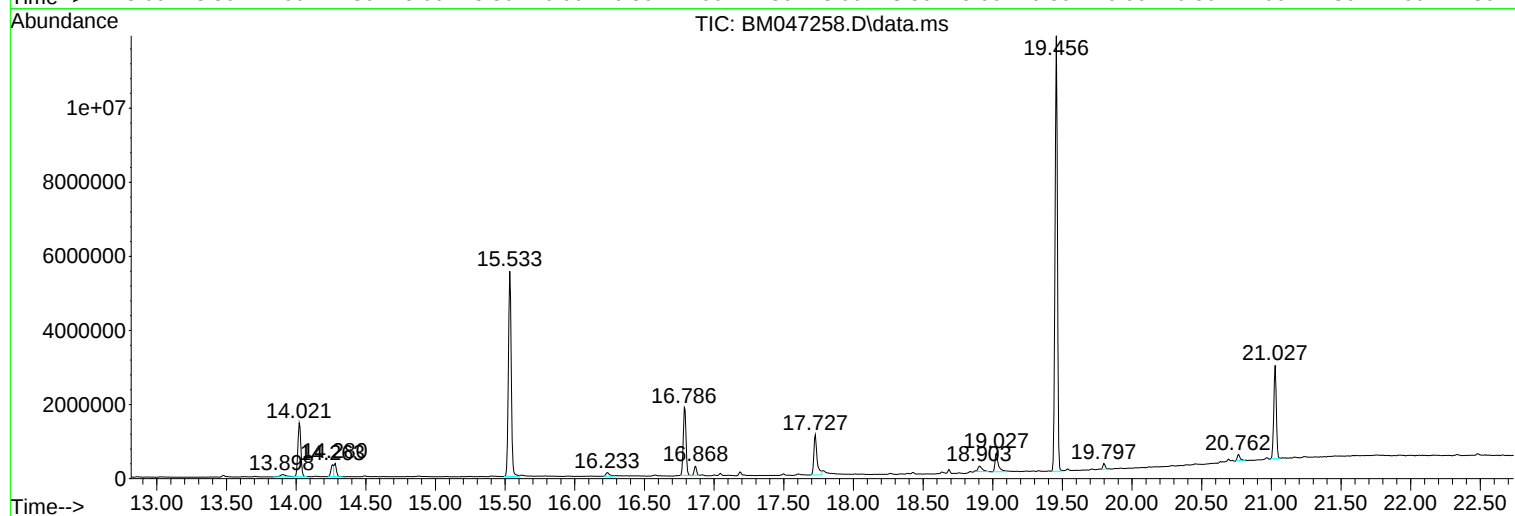
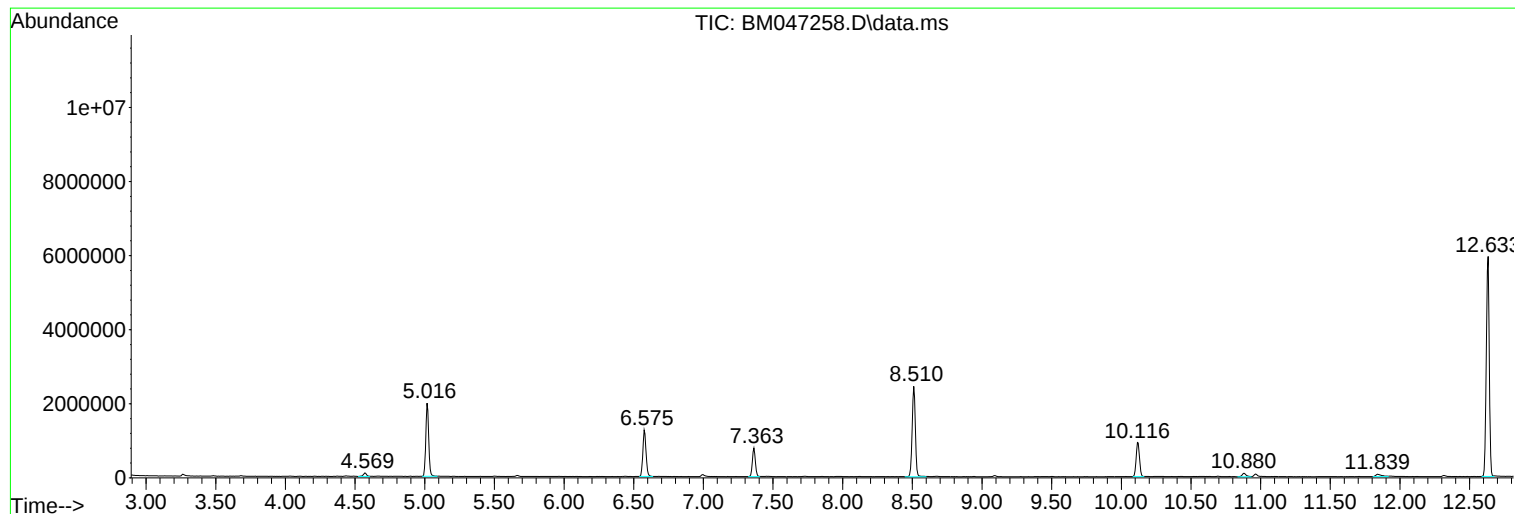
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM081024.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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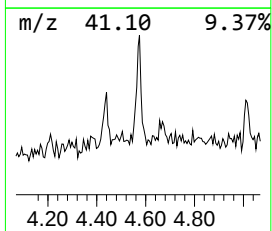
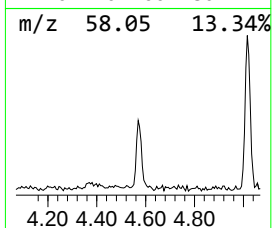
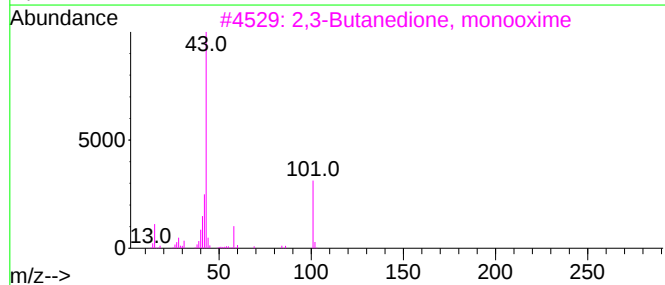
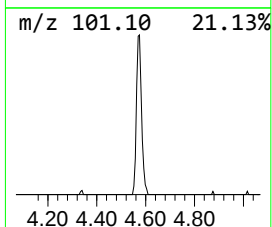
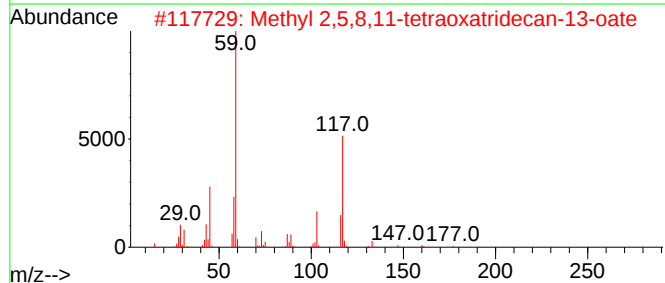
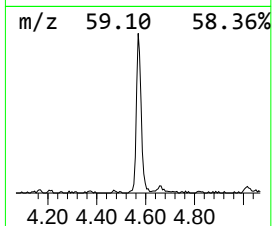
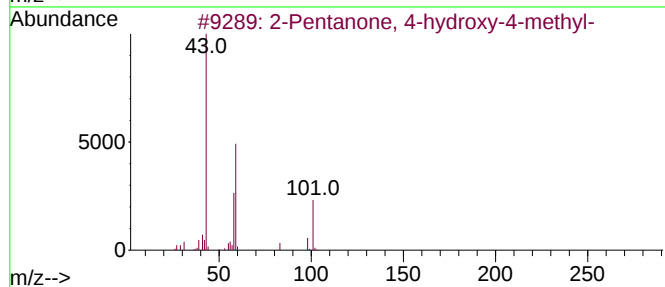
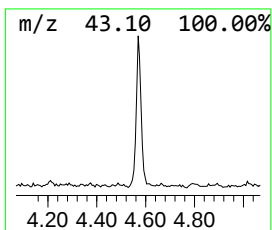
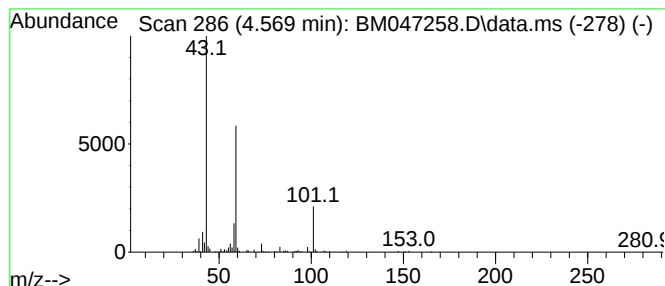
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 4.569 | 2.59 ng | 150411 | 1,4-Dichlorobenzene-d4 | 7.363 |

| Hit# | of                                  | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2  | 64      |      |      |
| 2    | Methyl 2,5,8,11-tetraoxatridecan... | 236 | C10H20O6     | 1000366-78-2 | 37      |      |      |
| 3    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2      | 000057-71-6  | 35      |      |      |
| 4    | Propane, 1-ethoxy-2-methyl-         | 102 | C6H14O       | 000627-02-1  | 32      |      |      |
| 5    | 2-Butanol, 1-methoxy-               | 104 | C5H12O2      | 053778-73-7  | 25      |      |      |



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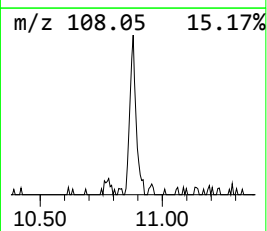
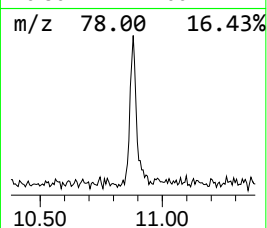
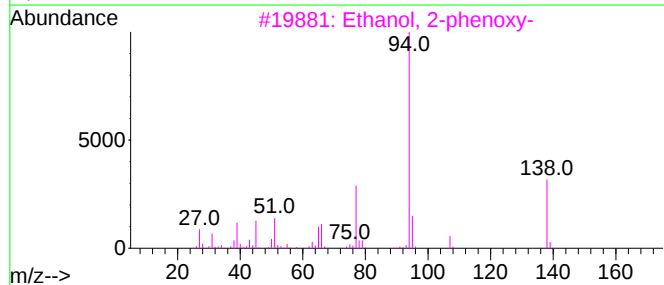
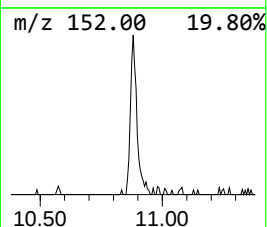
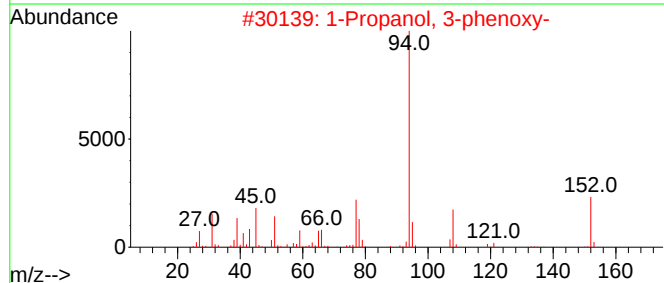
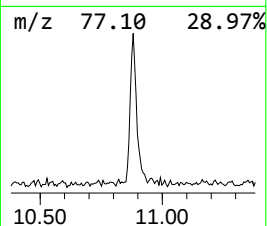
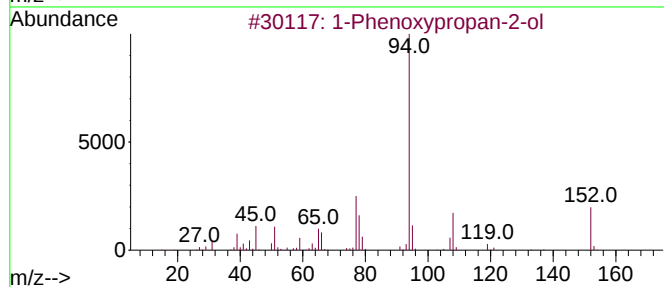
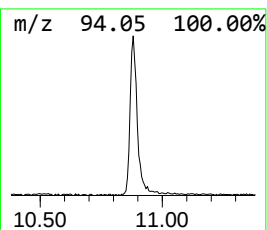
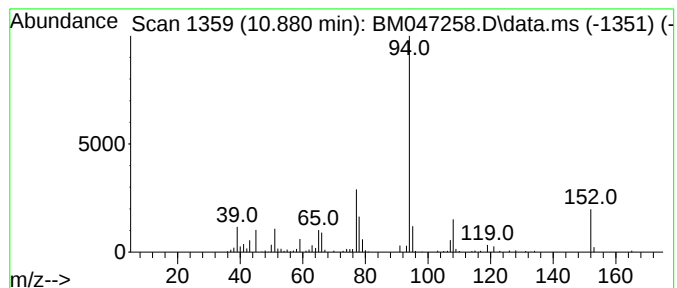
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM081024.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 7

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 10.880 | 2.47 ng | 190624 | Naphthalene-d8   | 10.116 |

| 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 | 87   |
| 3    |    |   | Ethanol, 2-phenoxy-                 | 138 | C8H10O2  | 000122-99-6 | 59   |
| 4    |    |   | 1-Propanol, 2-phenoxy-              | 152 | C9H12O2  | 004169-04-4 | 59   |
| 5    |    |   | Carbonic acid, neopentyl phenyl ... | 208 | C12H16O3 | 013183-19-2 | 53   |



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ALS Vial : 15 Sample Multiplier: 1

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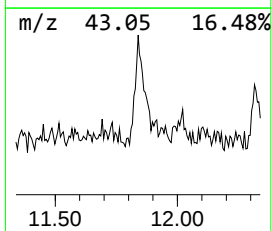
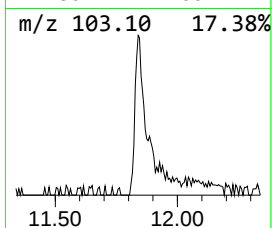
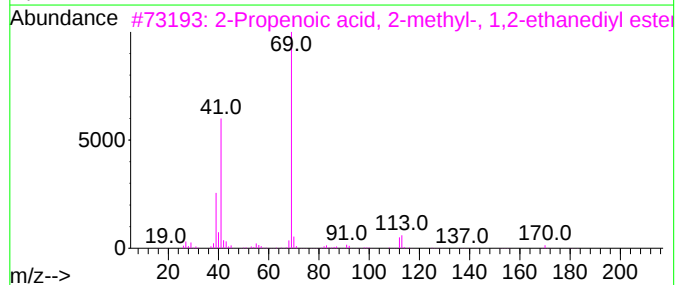
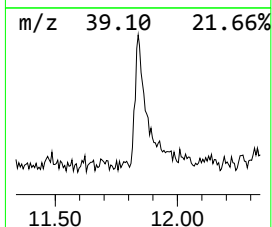
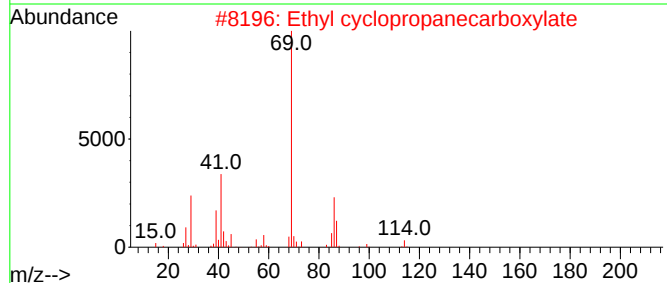
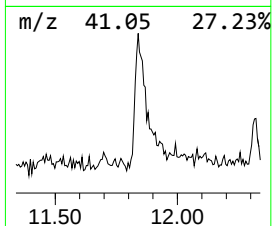
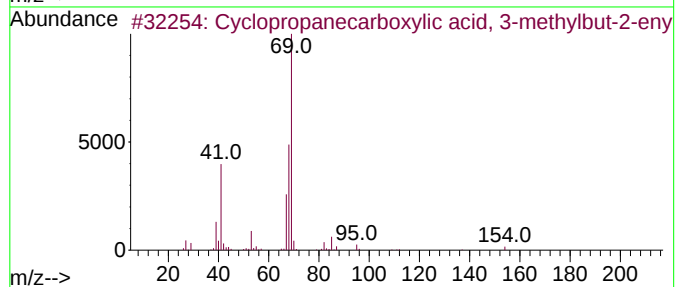
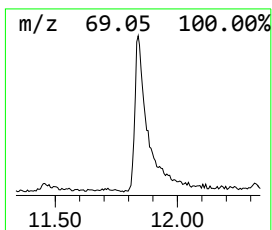
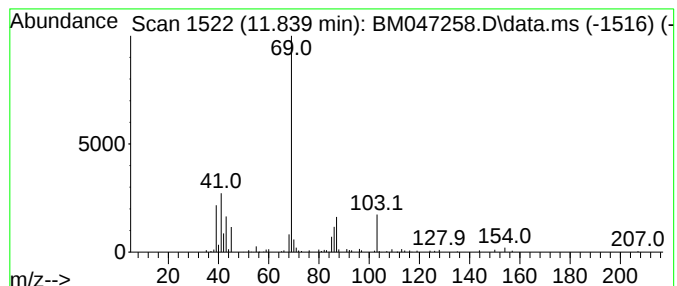
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM081024.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Cyclopropanecarboxylic acid... Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.839 | 2.65 ng | 203764 | Naphthalene-d8   | 10.116 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Cyclopropanecarboxylic acid, 3-m... | 154 | C9H14O2  | 1000299-37-4 | 50   |
| 2    |    |   | Ethyl cyclopropanecarboxylate       | 114 | C6H10O2  | 004606-07-9  | 45   |
| 3    |    |   | 2-Propenoic acid, 2-methyl-, 1,2... | 198 | C10H14O4 | 000097-90-5  | 38   |
| 4    |    |   | 2-Butenoic acid, 2-propenylidene... | 210 | C11H14O4 | 055030-70-1  | 36   |
| 5    |    |   | Cyclopentanecarboxylic acid, iso... | 156 | C9H16O2  | 106083-73-2  | 33   |



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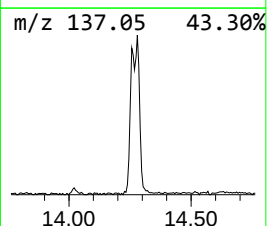
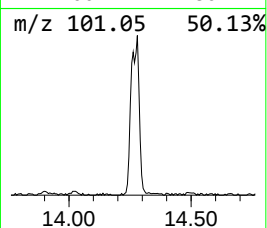
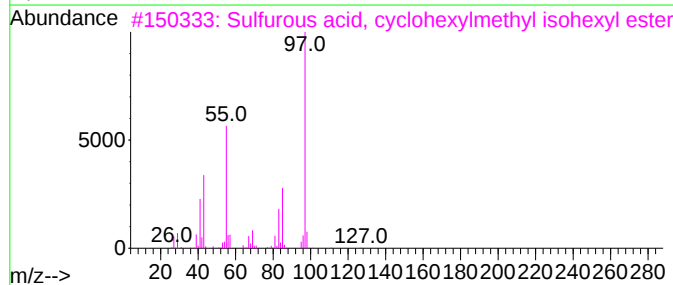
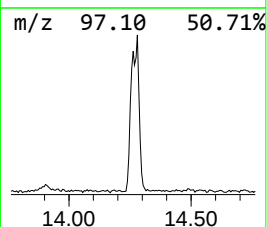
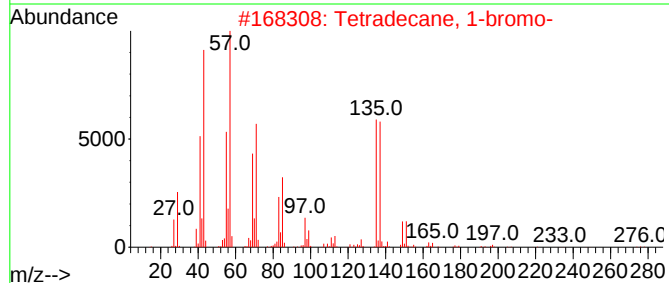
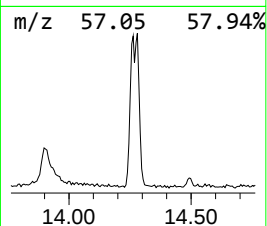
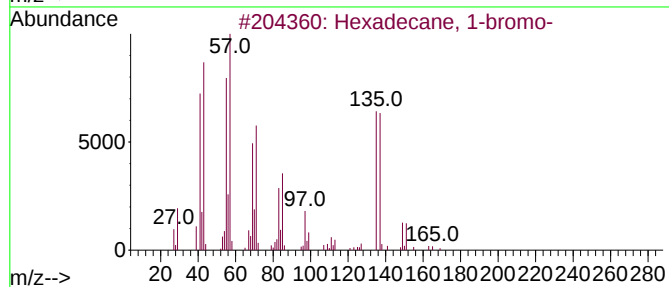
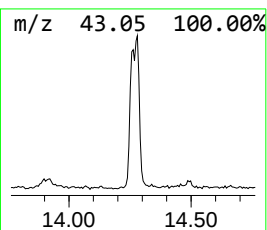
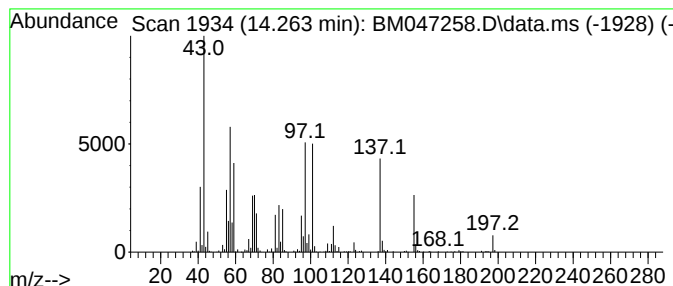
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Peak Number 4 unknown14.263 Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.263 | 4.21 ng | 445998 | Acenaphthene-d10 | 14.021 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Hexadecane, 1-bromo-                | 304 | C16H33Br  | 000112-82-3  | 22   |
| 2    |    |   | Tetradecane, 1-bromo-               | 276 | C14H29Br  | 000112-71-0  | 14   |
| 3    |    |   | Sulfurous acid, cyclohexylmethyl... | 262 | C13H26O3S | 1000309-21-5 | 14   |
| 4    |    |   | Sulfurous acid, cyclohexylmethyl... | 402 | C23H46O3S | 1000309-22-4 | 10   |
| 5    |    |   | 17-Pentatriacontene                 | 491 | C35H70    | 006971-40-0  | 10   |



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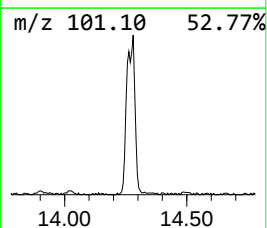
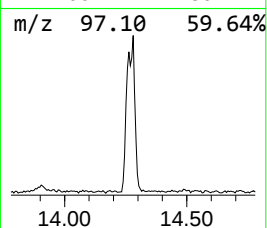
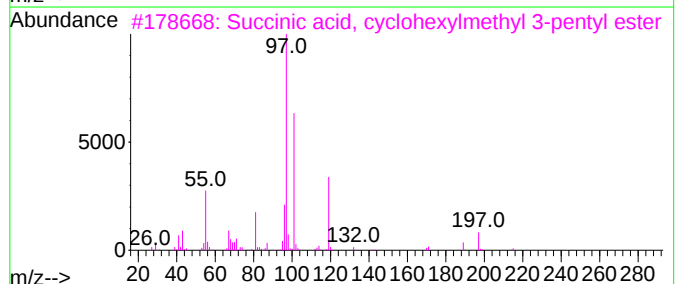
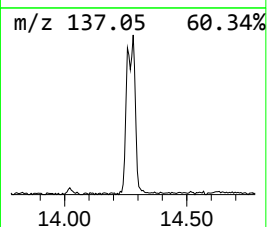
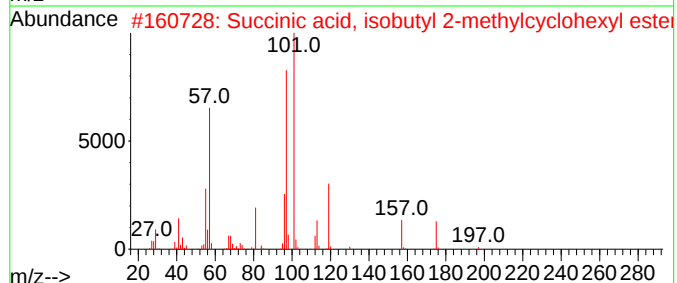
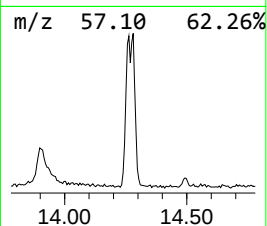
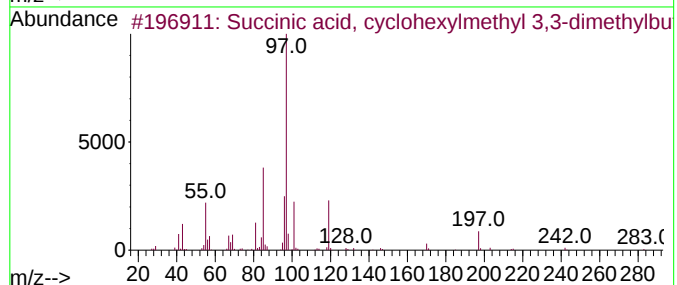
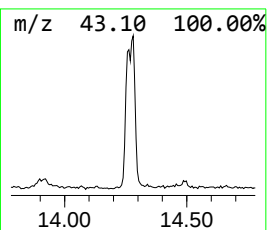
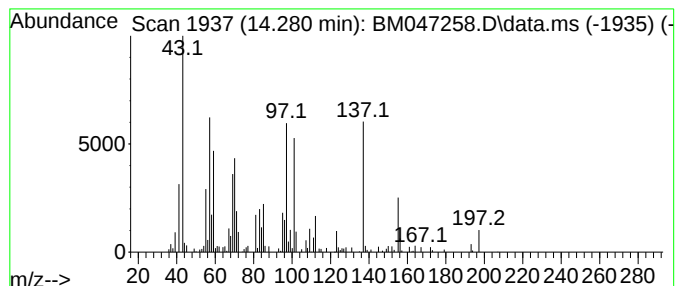
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 unknown14.280 Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.280 | 3.84 ng | 407380 | Acenaphthene-d10 | 14.021 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Succinic acid, cyclohexylmethyl ... | 298 | C17H30O4 | 1000390-62-6 | 14   |
| 2    |    |   | Succinic acid, isobutyl 2-methyl... | 270 | C15H26O4 | 1000329-81-7 | 14   |
| 3    |    |   | Succinic acid, cyclohexylmethyl ... | 284 | C16H28O4 | 1000370-91-3 | 12   |
| 4    |    |   | Propanoic acid, 2,2-dimethyl-, 2... | 214 | C13H26O2 | 016387-18-1  | 10   |
| 5    |    |   | Carbonic acid, eicosyl prop-1-en... | 382 | C24H46O3 | 1000383-10-8 | 10   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM081924\  
Data File : BM047258.D  
Acq On : 19 Aug 2024 18:49  
Operator : RC/JU  
Sample : P3619-01  
Misc :  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
917-J-WS-081424

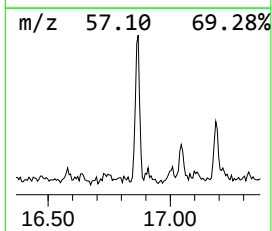
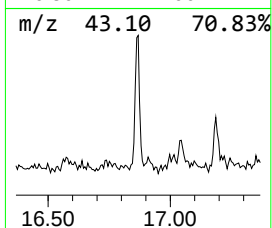
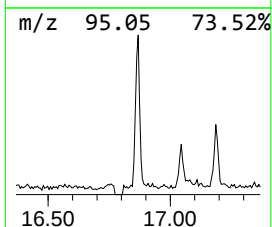
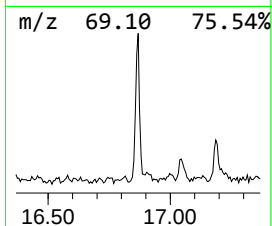
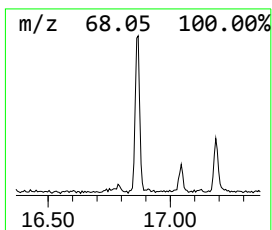
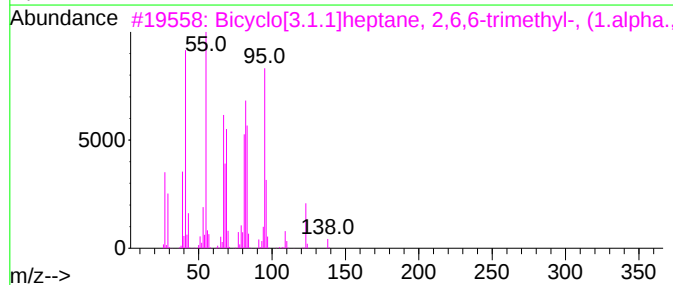
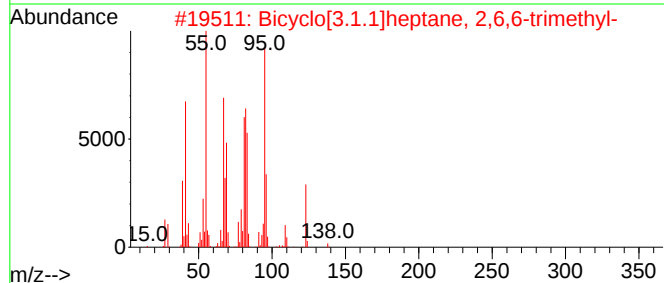
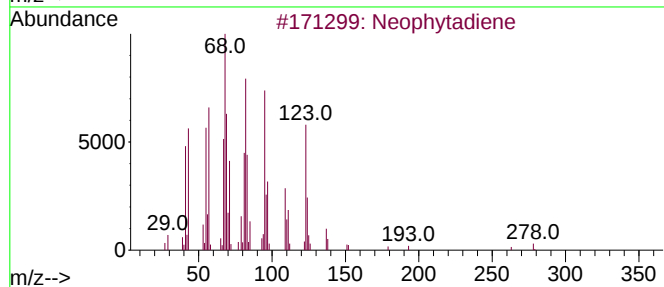
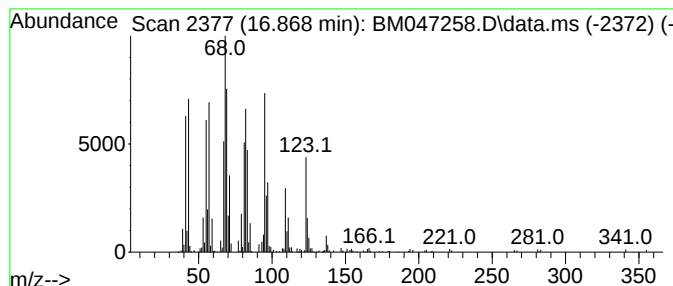
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Neophytadiene Concentration Rank 8

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 16.868 | 2.33 ng | 305365 | Phenanthrene-d10 | 16.786 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Neophytadiene                       | 278 | C20H38   | 000504-96-1  | 81   |
| 2    |    |   | Bicyclo[3.1.1]heptane, 2,6,6-tri... | 138 | C10H18   | 000473-55-2  | 60   |
| 3    |    |   | Bicyclo[3.1.1]heptane, 2,6,6-tri... | 138 | C10H18   | 006876-13-7  | 55   |
| 4    |    |   | 11,13-Dimethyl-12-tetradecen-1-o... | 282 | C18H34O2 | 1000130-81-0 | 43   |
| 5    |    |   | Bicyclo[3.1.1]heptane, 2,6,6-tri... | 138 | C10H18   | 004795-86-2  | 41   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM081924\  
Data File : BM047258.D  
Acq On : 19 Aug 2024 18:49  
Operator : RC/JU  
Sample : P3619-01  
Misc :  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
917-J-WS-081424

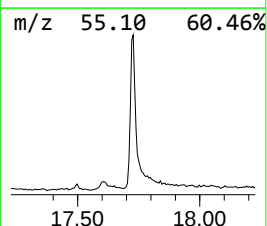
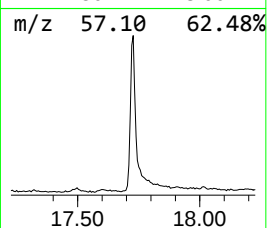
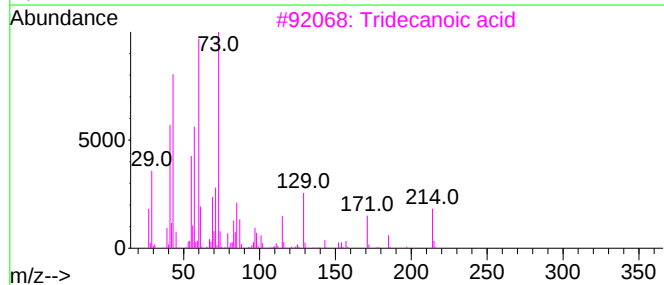
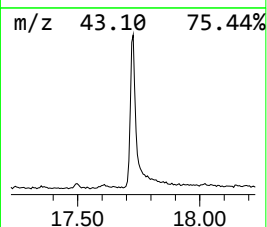
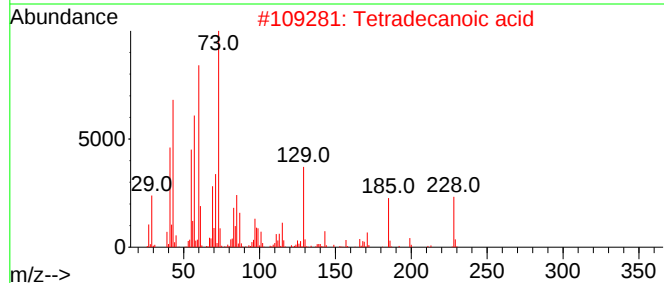
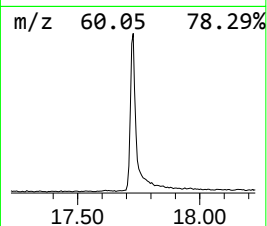
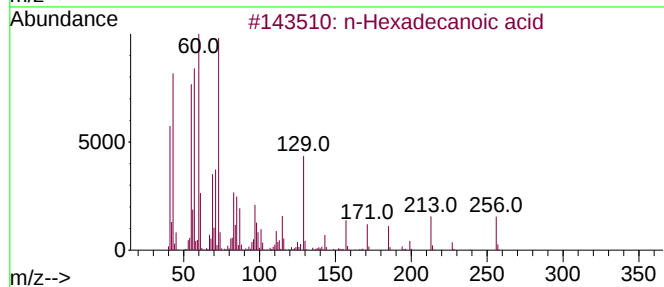
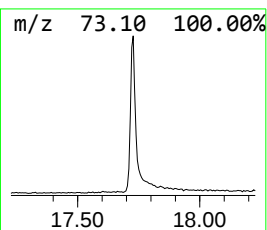
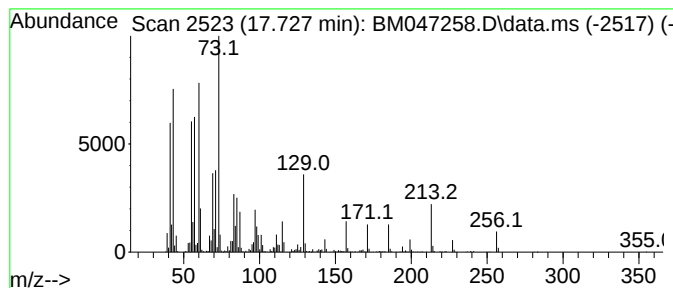
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 7 n-Hexadecanoic acid Concentration Rank 1

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 17.727 | 13.12 ng | 1721300 | Phenanthrene-d10 | 16.786 |

| 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 | 86   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 81   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 47   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM081924\  
Data File : BM047258.D  
Acq On : 19 Aug 2024 18:49  
Operator : RC/JU  
Sample : P3619-01  
Misc :  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
917-J-WS-081424

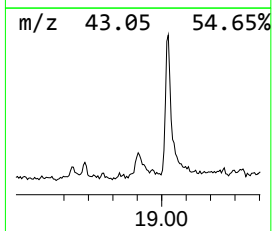
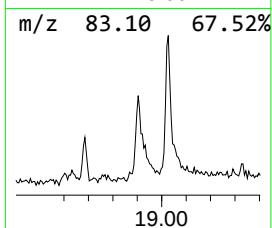
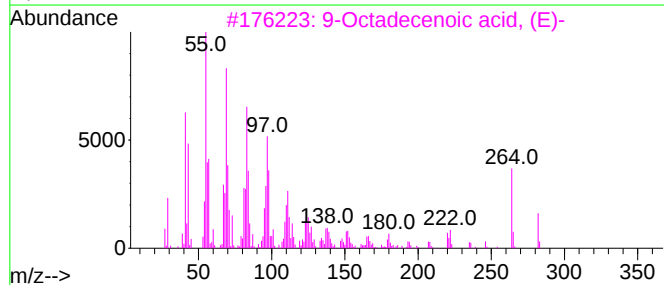
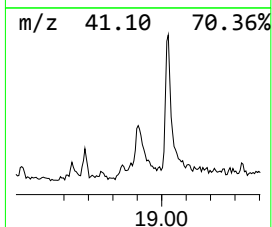
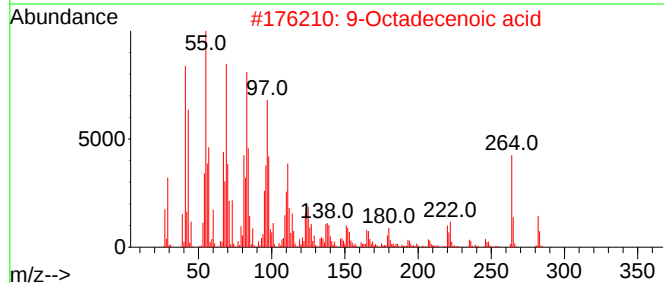
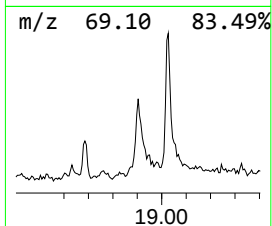
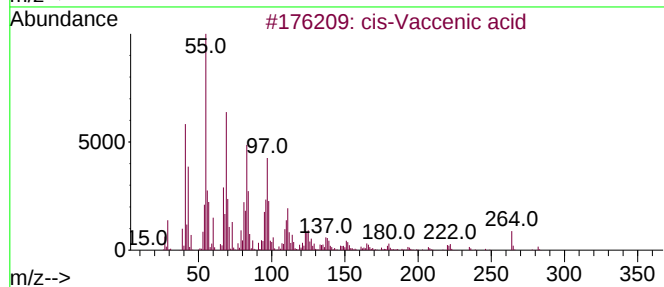
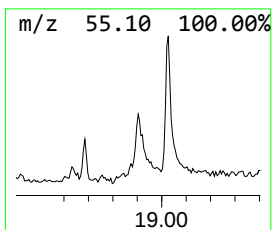
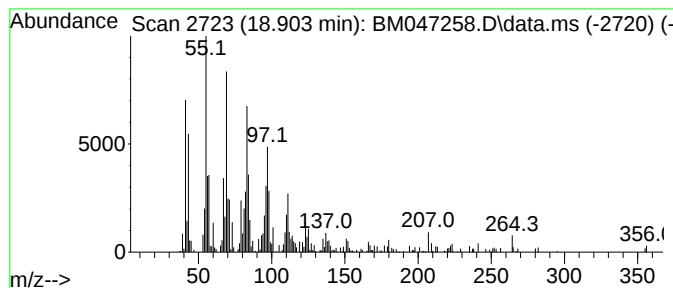
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 8 cis-Vaccenic acid Concentration Rank 9

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.903 | 2.31 ng | 303462 | Phenanthrene-d10 | 16.786 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm  | CAS#         | Qual |
|------|----|---|---------------------------|-----|----------|--------------|------|
| 1    |    |   | cis-Vaccenic acid         | 282 | C18H34O2 | 000506-17-2  | 98   |
| 2    |    |   | 9-Octadecenoic acid       | 282 | C18H34O2 | 002027-47-6  | 96   |
| 3    |    |   | 9-Octadecenoic acid, (E)- | 282 | C18H34O2 | 000112-79-8  | 93   |
| 4    |    |   | 6-Octadecenoic acid       | 282 | C18H34O2 | 1000336-66-8 | 92   |
| 5    |    |   | cis-13-Octadecenoic acid  | 282 | C18H34O2 | 013126-39-1  | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM081924\  
Data File : BM047258.D  
Acq On : 19 Aug 2024 18:49  
Operator : RC/JU  
Sample : P3619-01  
Misc :  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
917-J-WS-081424

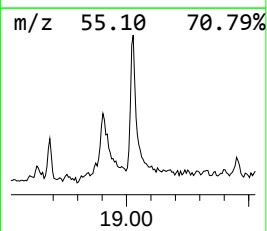
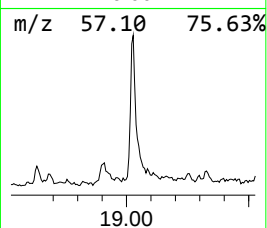
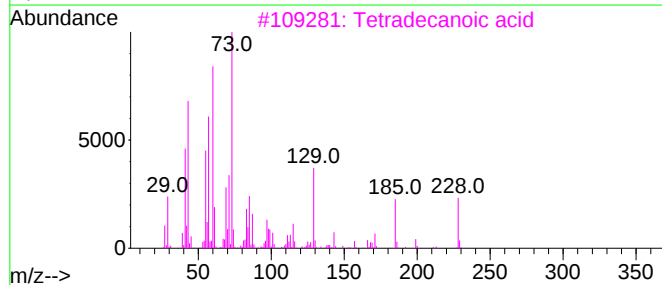
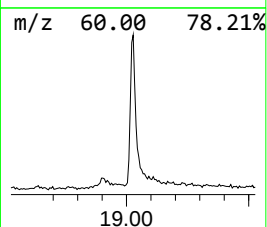
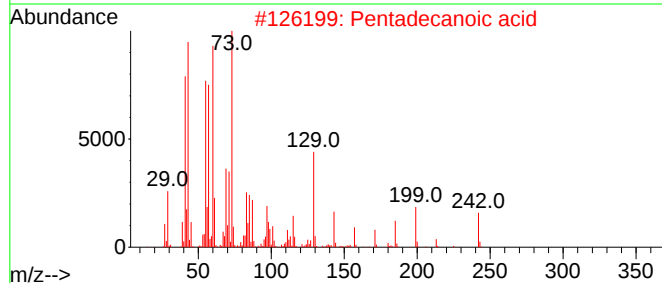
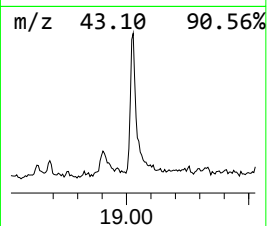
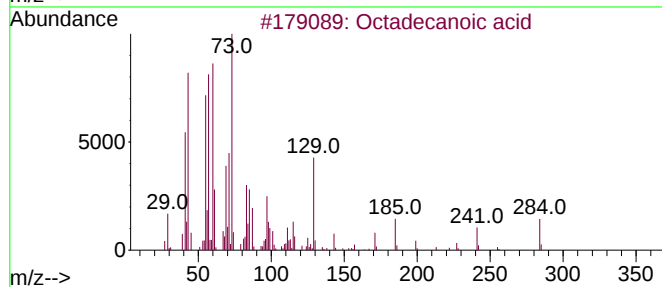
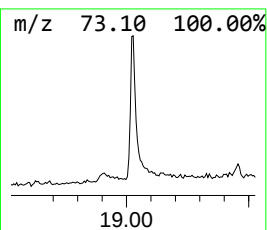
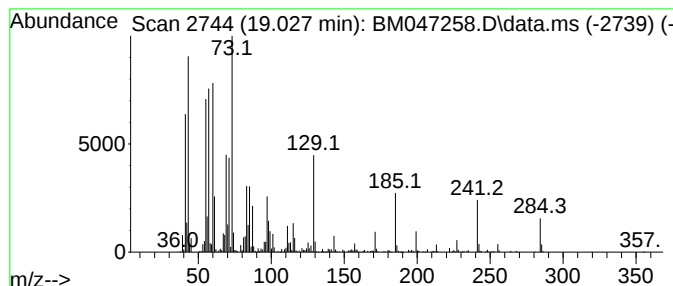
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 9 Octadecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.027 | 5.25 ng | 844472 | Chrysene-d12     | 21.027 |

| 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    |    |   | Tetradecanoic acid                  | 228 | C14H28O2 | 000544-63-8 | 83   |
| 4    |    |   | n-Hexadecanoic acid                 | 256 | C16H32O2 | 000057-10-3 | 72   |
| 5    |    |   | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 64   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM081924\  
Data File : BM047258.D  
Acq On : 19 Aug 2024 18:49  
Operator : RC/JU  
Sample : P3619-01  
Misc :  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
917-J-WS-081424

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM081024.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| 2-Pentanone, 4-... | 4.569  | 2.6     | ng    | 150411   | 1                     | 7.363  | 1159910 | 20.0 |
| 1-Phenoxypropan... | 10.880 | 2.5     | ng    | 190624   | 2                     | 10.116 | 1540510 | 20.0 |
| Cyclopropanecar... | 11.839 | 2.6     | ng    | 203764   | 2                     | 10.116 | 1540510 | 20.0 |
| unknown14.263      | 14.263 | 4.2     | ng    | 445998   | 3                     | 14.021 | 2120250 | 20.0 |
| unknown14.280      | 14.280 | 3.8     | ng    | 407380   | 3                     | 14.021 | 2120250 | 20.0 |
| Neophytadiene      | 16.868 | 2.3     | ng    | 305365   | 4                     | 16.786 | 2623030 | 20.0 |
| n-Hexadecanoic ... | 17.727 | 13.1    | ng    | 1721300  | 4                     | 16.786 | 2623030 | 20.0 |
| cis-Vaccenic acid  | 18.903 | 2.3     | ng    | 303462   | 4                     | 16.786 | 2623030 | 20.0 |
| Octadecanoic acid  | 19.027 | 5.3     | ng    | 844472   | 5                     | 21.027 | 3215710 | 20.0 |