

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM032823\  
 Data File : BM039189.D  
 Acq On : 28 Mar 2023 20:59  
 Operator : CG/JU  
 Sample : 02111-03  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 APCS-NORTH

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-BM030823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039189.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         | 5.028       | 289           | 296         | 307          | rVB      | 1739362        | 2347063       | 31.78%          | 3.855%        |
| 2         | 5.492       | 369           | 375         | 385          | rBV      | 3821461        | 5483232       | 74.24%          | 9.005%        |
| 3         | 7.104       | 639           | 649         | 662          | rBV      | 3439137        | 5353801       | 72.48%          | 8.793%        |
| 4         | 7.934       | 783           | 790         | 797          | rBV      | 1051733        | 1613368       | 21.84%          | 2.650%        |
| 5         | 9.104       | 981           | 989         | 997          | rBV      | 2165023        | 3523642       | 47.71%          | 5.787%        |
| 6         | 10.745      | 1259          | 1268        | 1277         | rBV      | 1229414        | 2058688       | 27.87%          | 3.381%        |
| 7         | 12.380      | 1541          | 1546        | 1559         | rBV2     | 26934          | 87544         | 1.19%           | 0.144%        |
| 8         | 13.204      | 1679          | 1686        | 1699         | rBV      | 4784560        | 6757282       | 91.49%          | 11.098%       |
| 9         | 14.580      | 1913          | 1920        | 1930         | rBV      | 1561816        | 2300165       | 31.14%          | 3.778%        |
| 10        | 15.939      | 2145          | 2151        | 2163         | rVB      | 107188         | 165297        | 2.24%           | 0.271%        |
| 11        | 16.068      | 2166          | 2173        | 2187         | rBV      | 2889339        | 4239400       | 57.40%          | 6.963%        |
| 12        | 16.721      | 2280          | 2284        | 2292         | rBV2     | 68080          | 121738        | 1.65%           | 0.200%        |
| 13        | 17.215      | 2365          | 2368        | 2374         | rBV2     | 71041          | 106761        | 1.45%           | 0.175%        |
| 14        | 17.286      | 2376          | 2380        | 2382         | rBV4     | 56795          | 81627         | 1.11%           | 0.134%        |
| 15        | 17.327      | 2382          | 2387        | 2392         | rVV      | 1648470        | 2284192       | 30.93%          | 3.751%        |
| 16        | 18.103      | 2514          | 2519        | 2524         | rBV3     | 82411          | 150346        | 2.04%           | 0.247%        |
| 17        | 18.162      | 2526          | 2529        | 2534         | rBV      | 77169          | 96760         | 1.31%           | 0.159%        |
| 18        | 18.221      | 2534          | 2539        | 2549         | rBV      | 1244644        | 1893524       | 25.64%          | 3.110%        |
| 19        | 18.515      | 2585          | 2589        | 2594         | rBV2     | 83974          | 148936        | 2.02%           | 0.245%        |
| 20        | 19.380      | 2732          | 2736        | 2738         | rBV      | 228749         | 305603        | 4.14%           | 0.502%        |
| 21        | 19.497      | 2752          | 2756        | 2765         | rBV      | 525879         | 838883        | 11.36%          | 1.378%        |
| 22        | 19.945      | 2827          | 2832        | 2839         | rBV      | 6079516        | 7386155       | 100.00%         | 12.131%       |
| 23        | 21.209      | 3043          | 3047        | 3055         | rBV      | 1307132        | 1590780       | 21.54%          | 2.613%        |
| 24        | 21.415      | 3080          | 3082        | 3088         | rVB      | 272367         | 248949        | 3.37%           | 0.409%        |
| 25        | 21.509      | 3093          | 3098        | 3107         | rVV      | 2261254        | 3157782       | 42.75%          | 5.186%        |
| 26        | 22.144      | 3202          | 3206        | 3216         | rVB3     | 850942         | 1677875       | 22.72%          | 2.756%        |
| 27        | 22.297      | 3228          | 3232        | 3239         | rVB      | 1019063        | 1492372       | 20.20%          | 2.451%        |
| 28        | 23.174      | 3378          | 3381        | 3386         | rVV      | 641639         | 874879        | 11.84%          | 1.437%        |
| 29        | 23.227      | 3386          | 3390        | 3401         | rVB      | 889790         | 1594835       | 21.59%          | 2.619%        |
| 30        | 23.927      | 3504          | 3509        | 3516         | rVB2     | 1470187        | 2907351       | 39.36%          | 4.775%        |

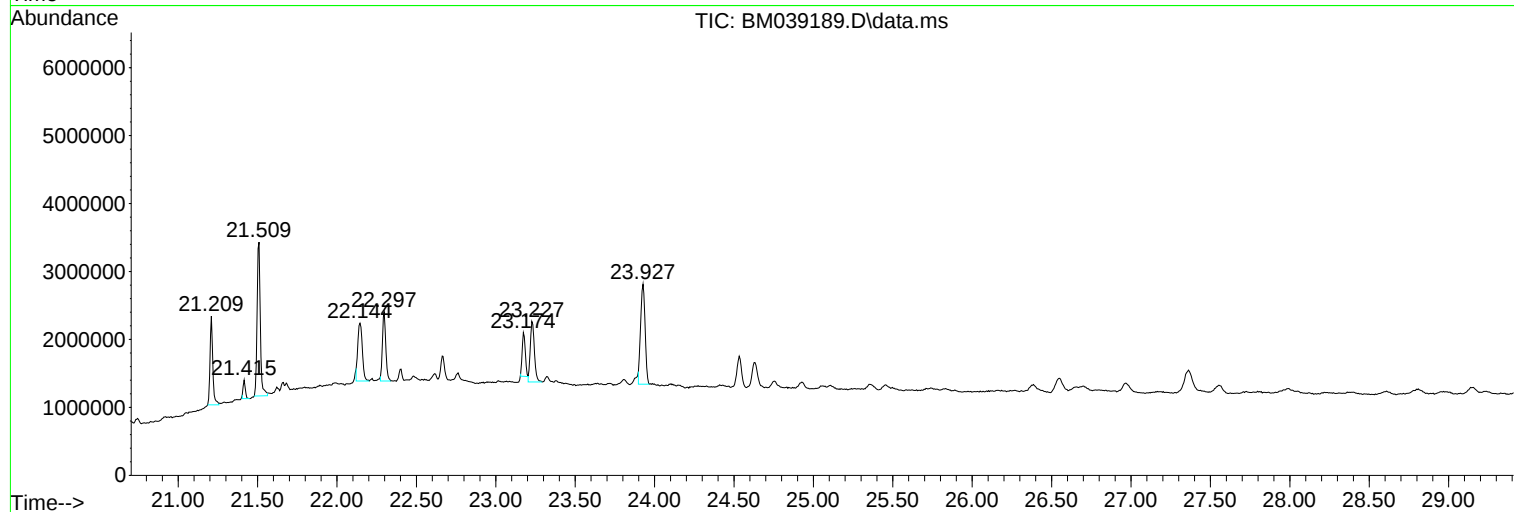
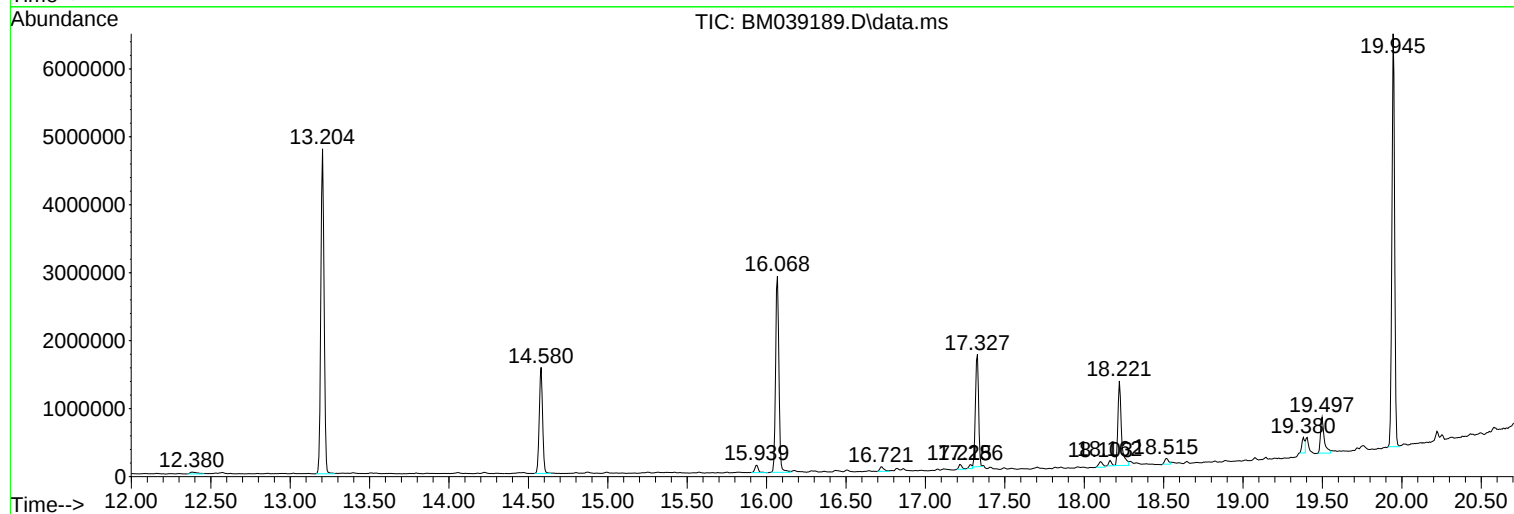
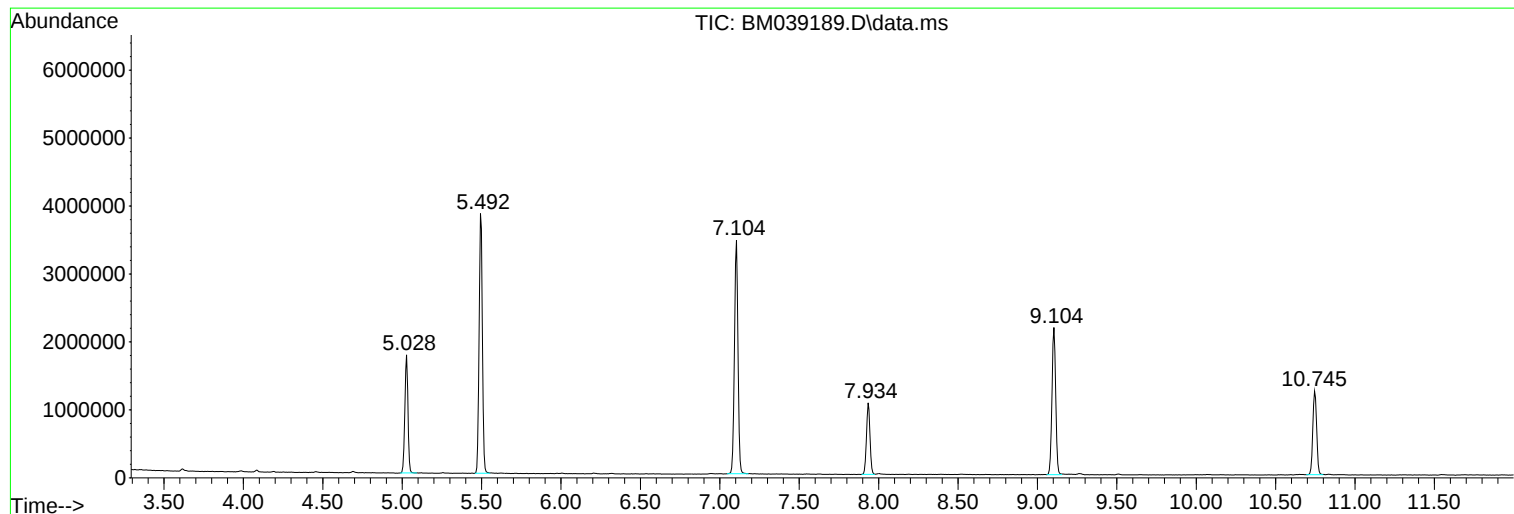
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ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
APCS-NORTH

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM030823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM032823\  
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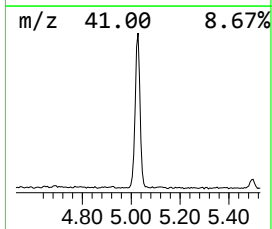
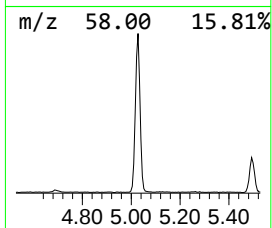
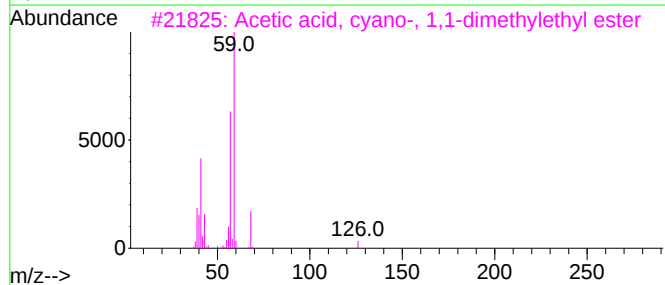
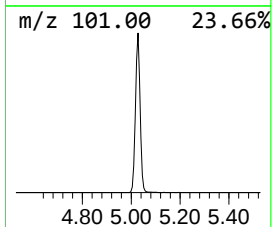
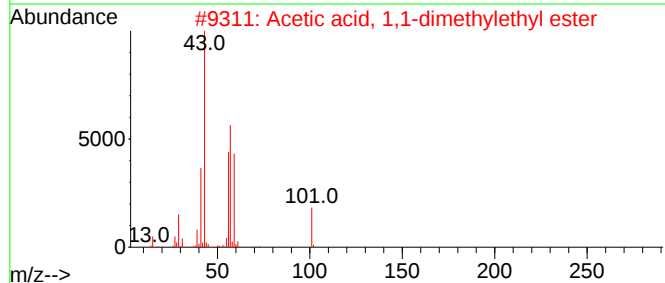
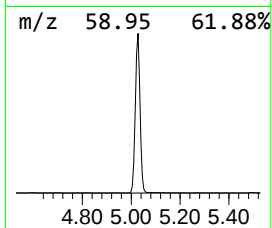
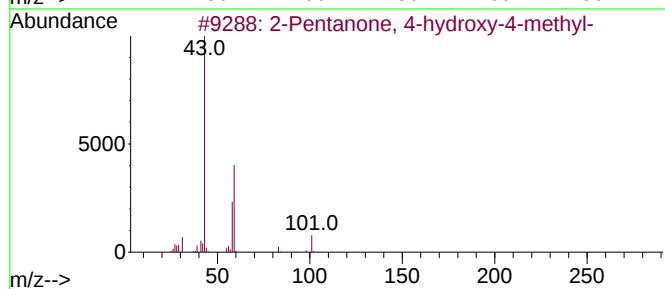
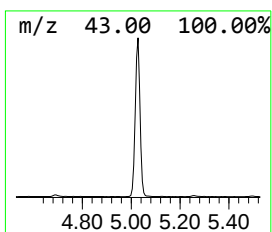
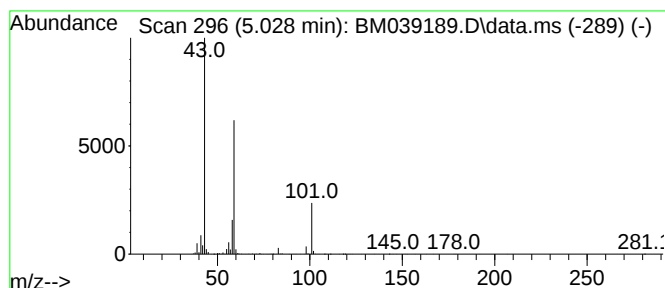
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc  | Area    | Relative to ISTD       | R.T.  |
|-------|----------|---------|------------------------|-------|
| 5.028 | 29.10 ng | 2347060 | 1,4-Dichlorobenzene-d4 | 7.934 |

| 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, 1,1-dimethylethyl e... | 116 | C6H12O2      | 000540-88-5 | 39      |      |      |
| 3    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 17      |      |      |
| 4    | Morpholine, 4-methyl-               | 101 | C5H11NO      | 000109-02-4 | 9       |      |      |
| 5    | 5-Hexen-2-one                       | 98  | C6H10O       | 000109-49-9 | 9       |      |      |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM030823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

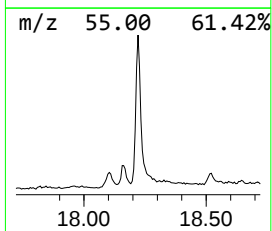
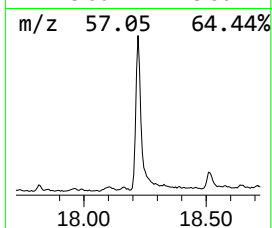
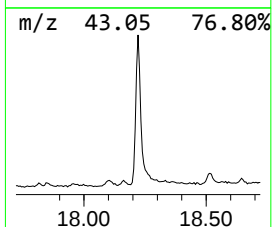
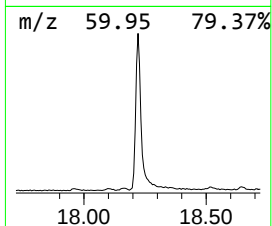
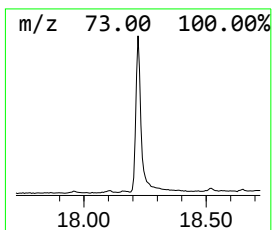
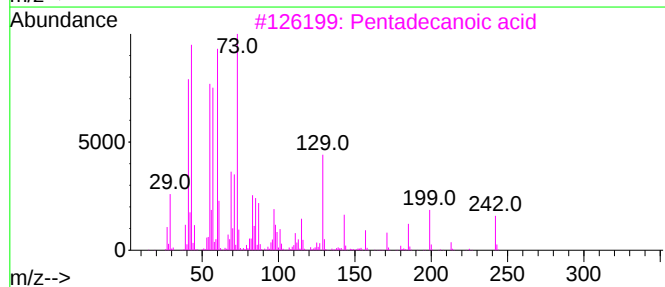
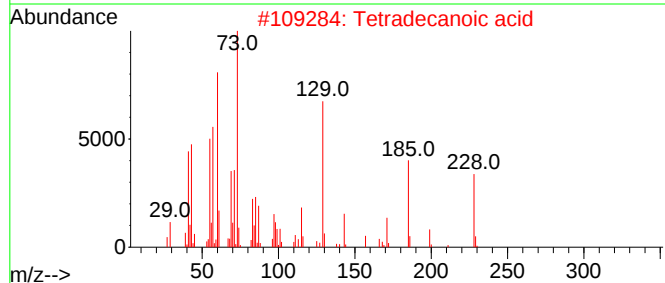
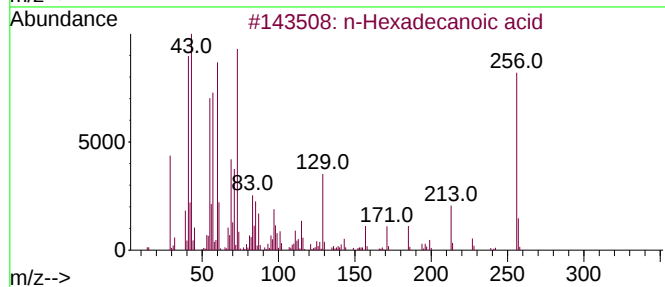
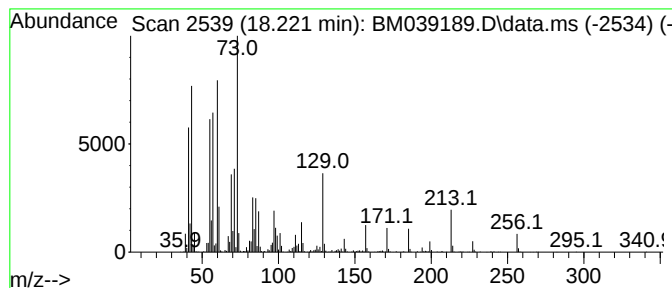
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 18.221 | 16.58 ng | 1893520 | Phenanthrene-d10 | 17.327 |

| 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 | 89   |
| 3    |    |   | Pentadecanoic acid    | 242 | C15H30O2 | 001002-84-2 | 87   |
| 4    |    |   | Tridecanoic acid      | 214 | C13H26O2 | 000638-53-9 | 64   |
| 5    |    |   | 8-Methylnonanoic acid | 172 | C10H20O2 | 005963-14-4 | 55   |



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Sample : 02111-03  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
APCS-NORTH

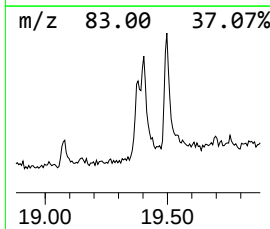
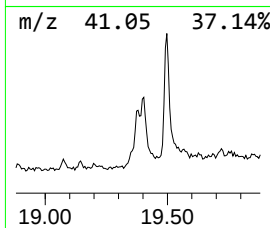
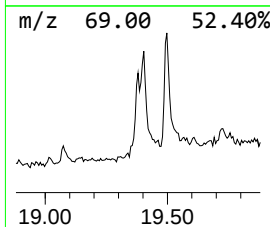
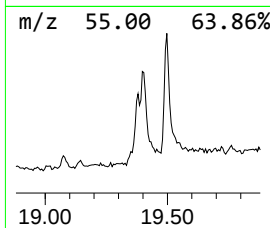
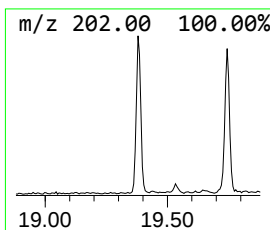
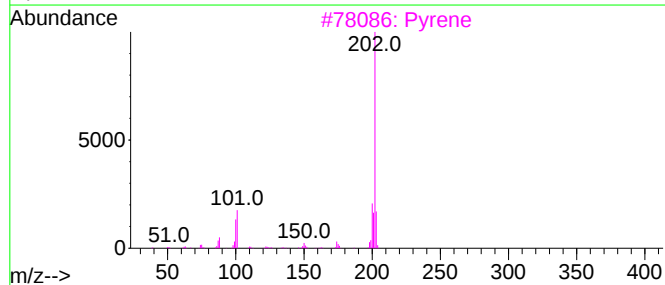
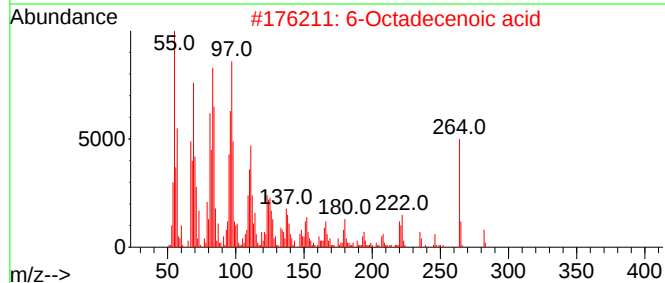
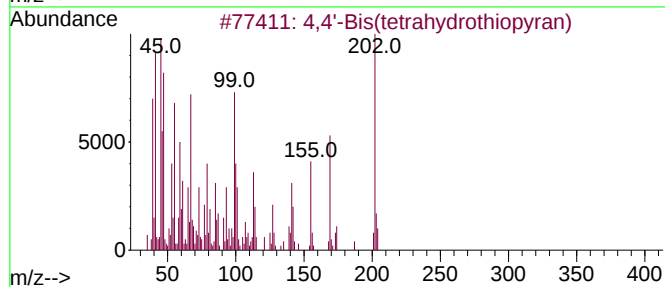
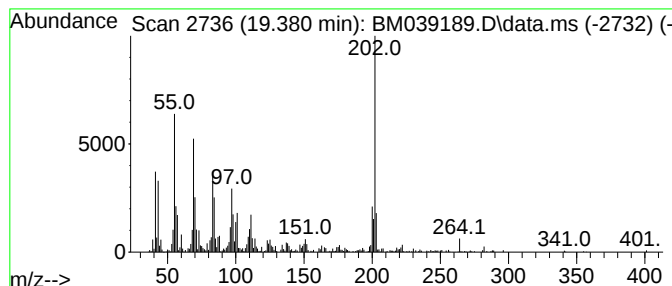
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM030823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 9

| R.T.      | EstConc                       | Area   | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------|--------|------------------|--------------|------|
| 19.380    | 2.68 ng                       | 305603 | Phenanthrene-d10 | 17.327       |      |
| Hit# of 5 | Tentative ID                  | MW     | MolForm          | CAS#         | Qual |
| 1         | 4,4'-Bis(tetrahydrothiopyran) | 202    | C10H18S2         | 116196-83-9  | 95   |
| 2         | 6-Octadecenoic acid           | 282    | C18H34O2         | 1000336-66-8 | 70   |
| 3         | Pyrene                        | 202    | C16H10           | 000129-00-0  | 64   |
| 4         | 9-Octadecenoic acid, (E)-     | 282    | C18H34O2         | 000112-79-8  | 52   |
| 5         | 1-Dodecanethiol               | 202    | C12H26S          | 000112-55-0  | 52   |



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BNA\_M  
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APCS-NORTH

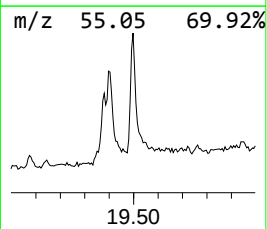
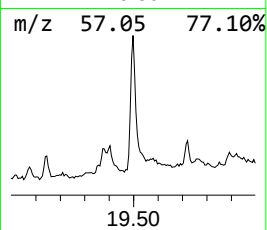
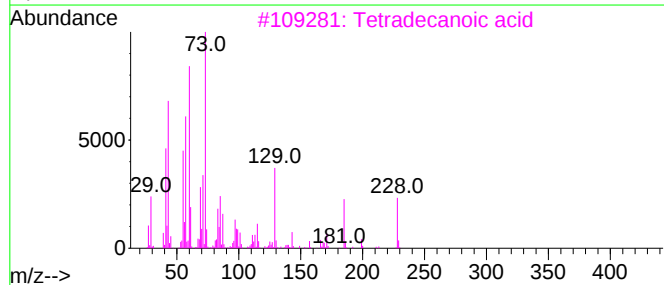
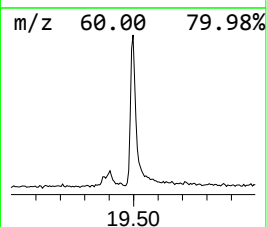
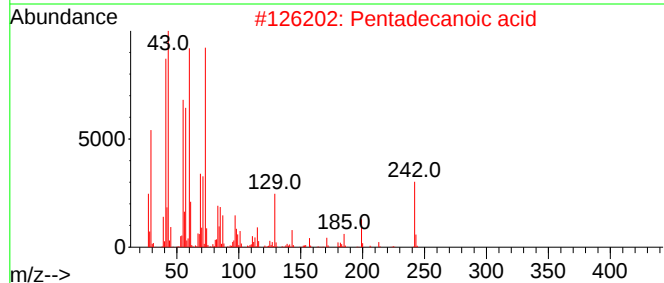
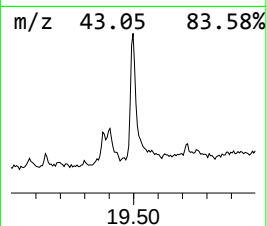
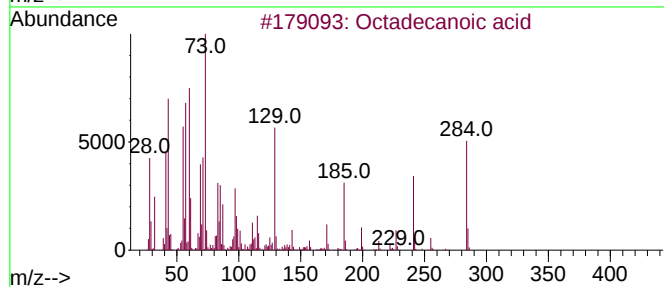
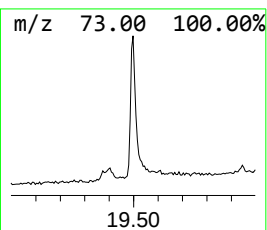
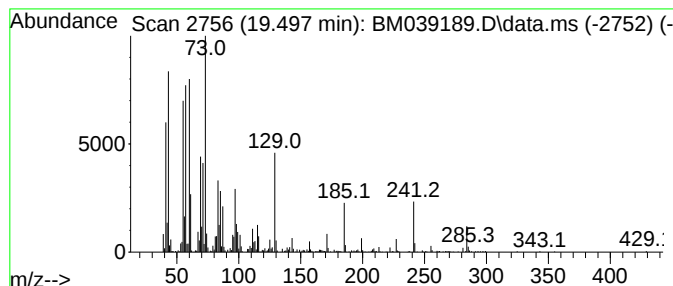
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TIC Library : C:\Database\NIST20.L  
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Peak Number 4 Octadecanoic acid Concentration Rank 8

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.497 | 5.31 ng | 838883 | Chrysene-d12     | 21.509 |

| 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 | 81   |
| 3    |    |   | Tetradecanoic acid    | 228 | C14H28O2 | 000544-63-8 | 74   |
| 4    |    |   | 8-Methylnonanoic acid | 172 | C10H20O2 | 005963-14-4 | 70   |
| 5    |    |   | n-Decanoic acid       | 172 | C10H20O2 | 000334-48-5 | 70   |



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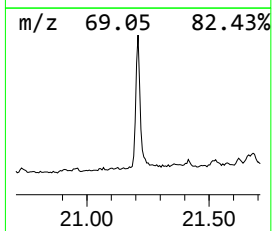
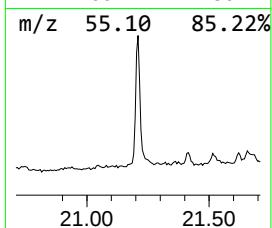
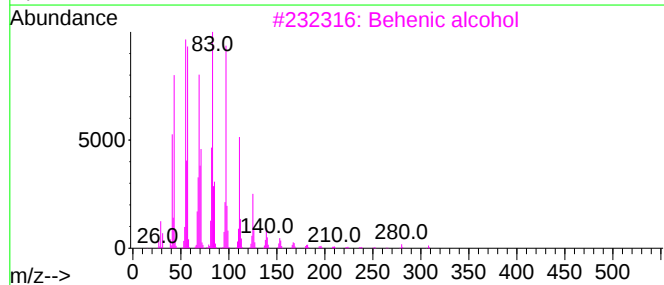
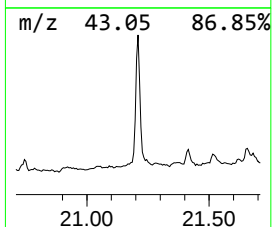
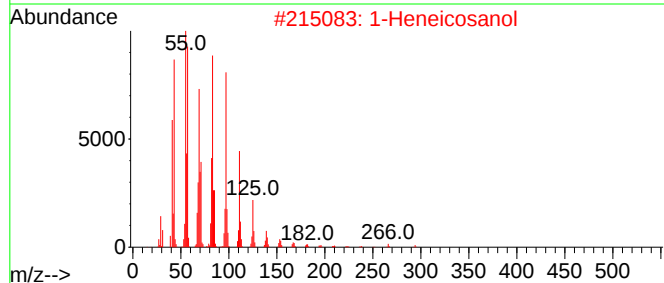
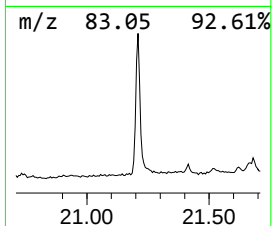
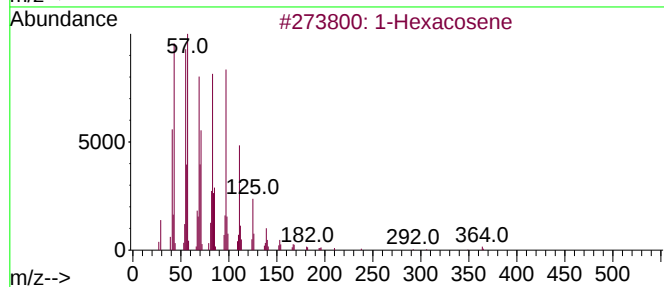
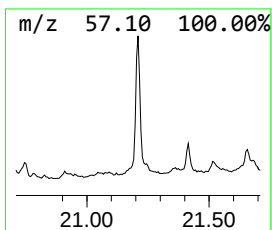
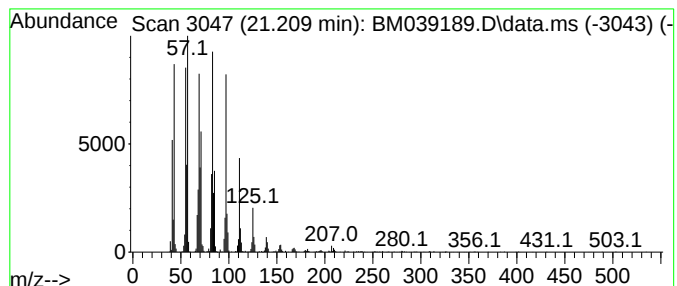
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TIC Integration Parameters: LSCINT.P

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Peak Number 5 1-Hexacosene Concentration Rank 5

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 21.209 | 10.08 ng | 1590780 | Chrysene-d12     | 21.509 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | 1-Hexacosene                        | 364 | C26H52     | 018835-33-1 | 94   |
| 2    |    |   | 1-Heneicosanol                      | 312 | C21H44O    | 015594-90-8 | 94   |
| 3    |    |   | Behenic alcohol                     | 326 | C22H46O    | 000661-19-8 | 94   |
| 4    |    |   | 1-Tetracosene                       | 336 | C24H48     | 010192-32-2 | 94   |
| 5    |    |   | 2- Chloropropionic acid, hexadec... | 332 | C19H37ClO2 | 086711-81-1 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM032823\  
Data File : BM039189.D  
Acq On : 28 Mar 2023 20:59  
Operator : CG/JU  
Sample : 02111-03  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
APCS-NORTH

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM030823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

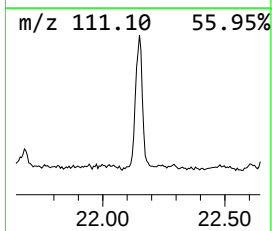
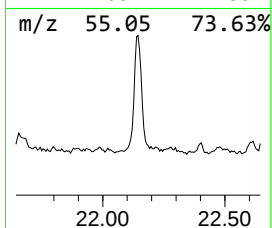
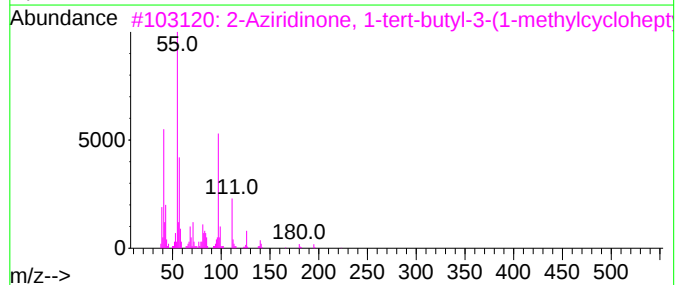
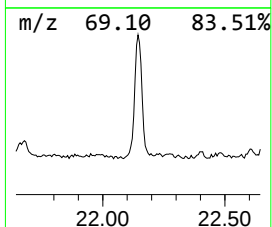
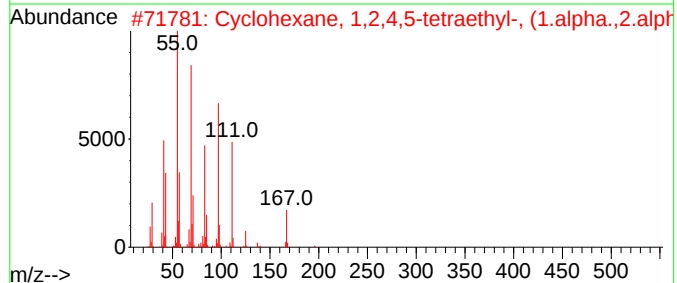
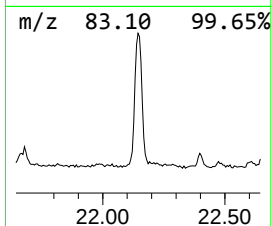
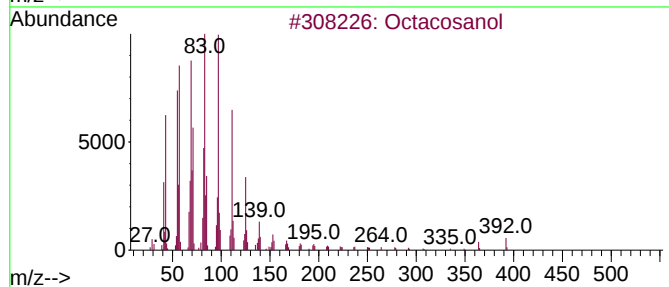
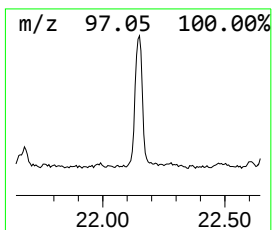
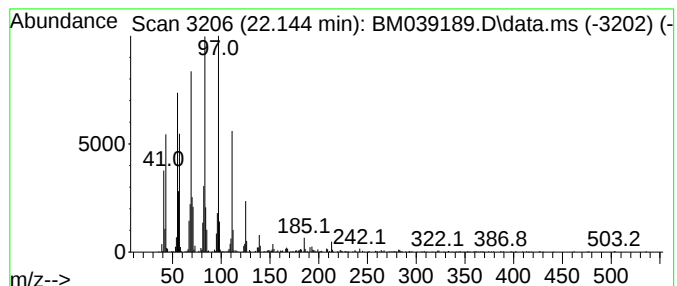
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 unknown22.144 Concentration Rank 4

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 22.144 | 10.63 ng | 1677880 | Chrysene-d12     | 21.509 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Octacosanol                         | 410 | C28H58O    | 000557-61-9  | 43   |
| 2    |    |   | Cyclohexane, 1,2,4,5-tetraethyl-... | 196 | C14H28     | 061142-24-3  | 43   |
| 3    |    |   | 2-Aziridinone, 1-tert-butyl-3-(1... | 223 | C14H25NO   | 026944-18-3  | 42   |
| 4    |    |   | n-Heptadecanol-1                    | 256 | C17H36O    | 001454-85-9  | 41   |
| 5    |    |   | Docosyl pentafluoropropionate       | 472 | C25H45F5O2 | 1000351-80-9 | 38   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM032823\  
Data File : BM039189.D  
Acq On : 28 Mar 2023 20:59  
Operator : CG/JU  
Sample : 02111-03  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
APCS-NORTH

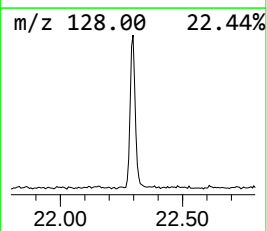
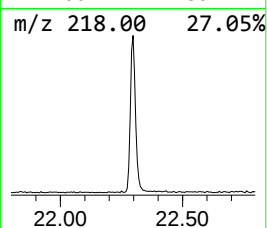
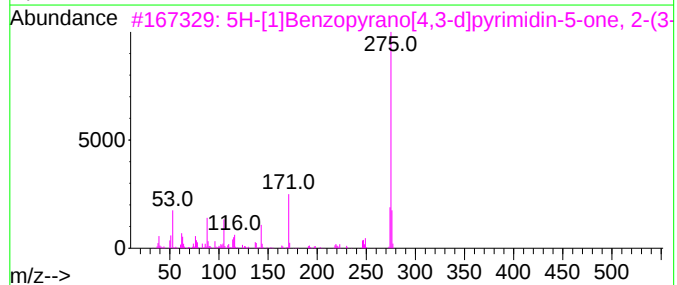
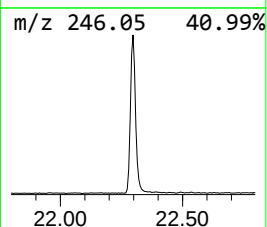
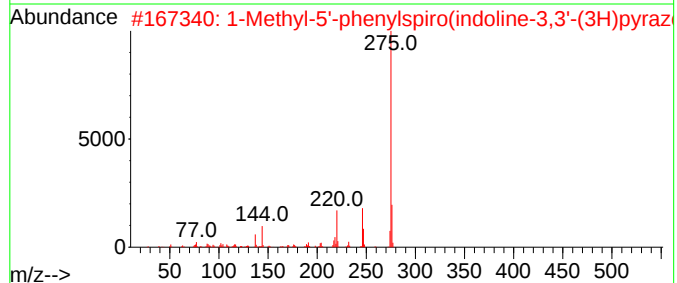
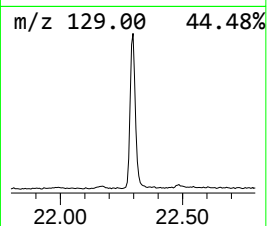
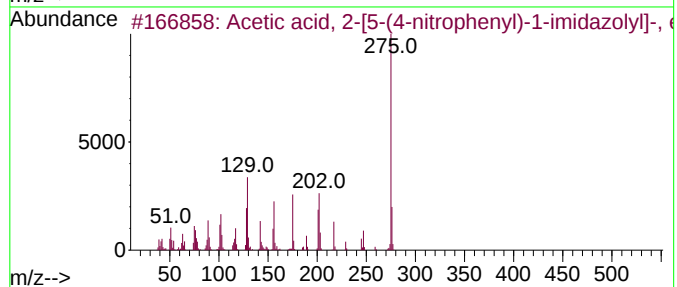
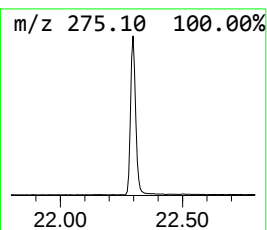
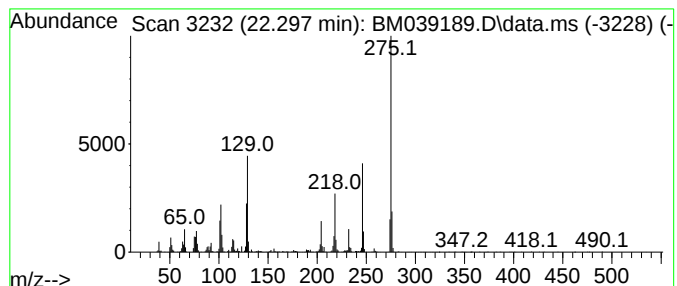
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 7 Acetic acid, 2-[5-(4-nitrop... Concentration Rank 6

| R.T.   | EstConc | Area    | Relative to ISTD | R.T.   |
|--------|---------|---------|------------------|--------|
| 22.297 | 9.45 ng | 1492370 | Chrysene-d12     | 21.509 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm     | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Acetic acid, 2-[5-(4-nitrophenyl)... | 275 | C13H13N3O4  | 351064-45-4  | 58   |
| 2    |    |   | 1-Methyl-5'-phenylspiro(indoline...) | 275 | C17H13N3O   | 015970-21-5  | 43   |
| 3    |    |   | 5H-[1]Benzopyrano[4,3-d]pyrimidi...  | 275 | C16H9N3O2   | 1000337-49-1 | 42   |
| 4    |    |   | 3,5-Diamino-6-[3,4-diethoxypheny...  | 275 | C13H17N5O2  | 058848-69-4  | 32   |
| 5    |    |   | 5-[4-(Dimethylamino)benzylidene]...  | 275 | C13H13N3O2S | 027430-15-5  | 30   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM032823\  
Data File : BM039189.D  
Acq On : 28 Mar 2023 20:59  
Operator : CG/JU  
Sample : 02111-03  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
APCS-NORTH

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM030823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

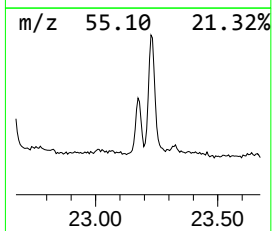
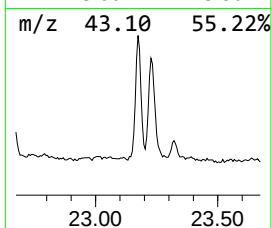
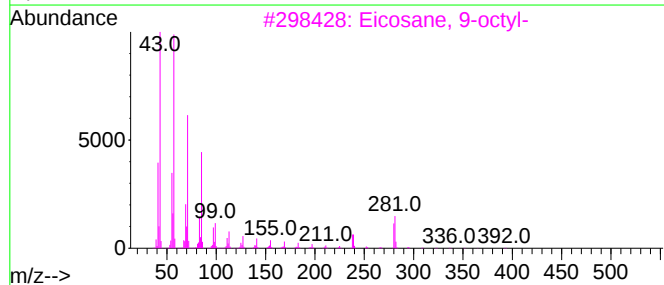
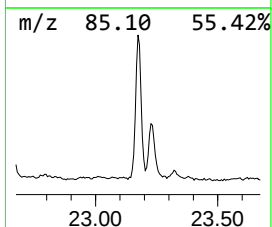
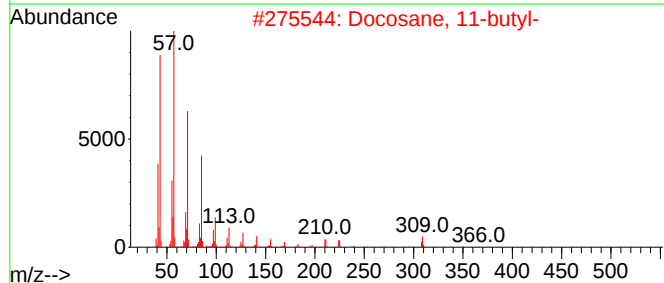
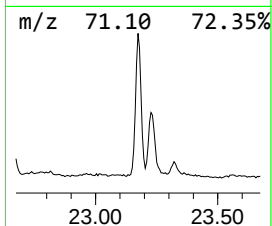
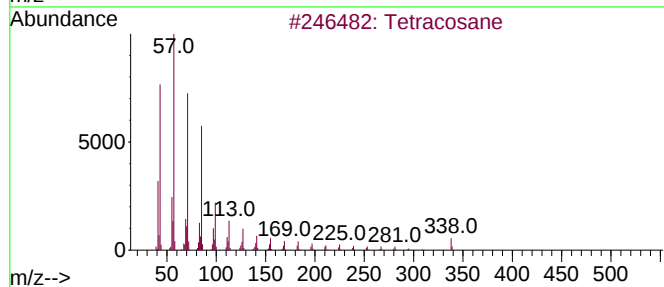
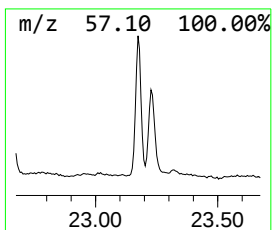
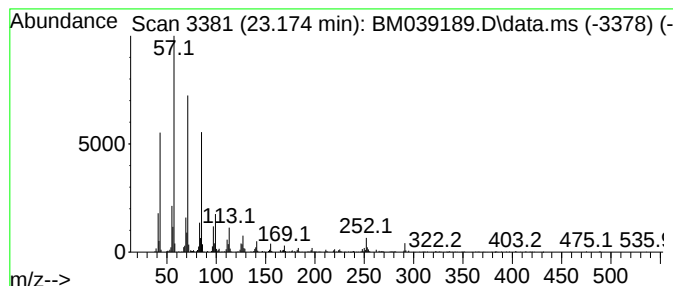
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 8 Tetracosane Concentration Rank 7

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 23.174 | 6.02 ng | 874879 | Perylene-d12     | 23.927 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------|-----|---------|-------------|------|
| 1    |    |   | Tetracosane         | 338 | C24H50  | 000646-31-1 | 98   |
| 2    |    |   | Docosane, 11-butyl- | 366 | C26H54  | 013475-76-8 | 93   |
| 3    |    |   | Eicosane, 9-octyl-  | 394 | C28H58  | 013475-77-9 | 93   |
| 4    |    |   | Heneicosane         | 296 | C21H44  | 000629-94-7 | 90   |
| 5    |    |   | Octacosane          | 394 | C28H58  | 000630-02-4 | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM032823\  
Data File : BM039189.D  
Acq On : 28 Mar 2023 20:59  
Operator : CG/JU  
Sample : 02111-03  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
APCS-NORTH

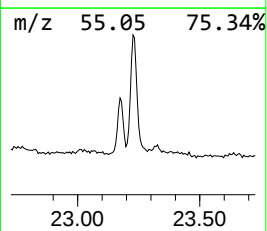
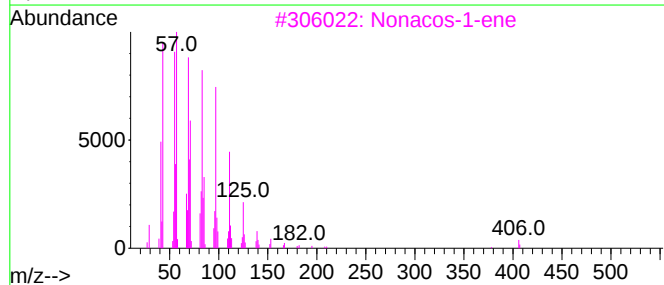
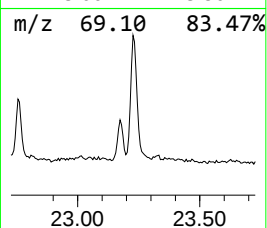
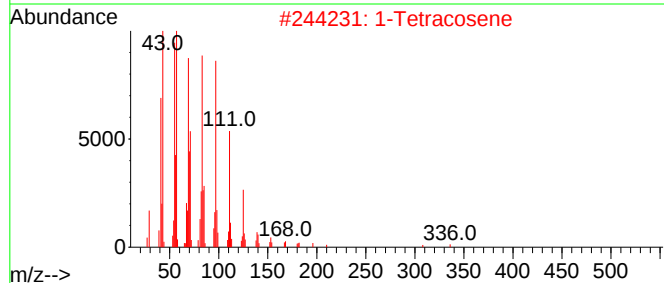
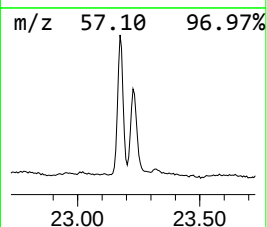
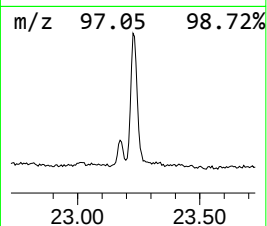
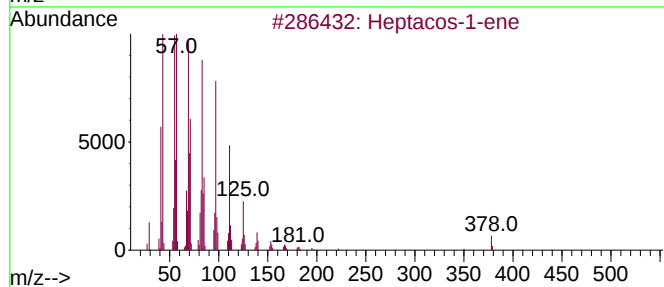
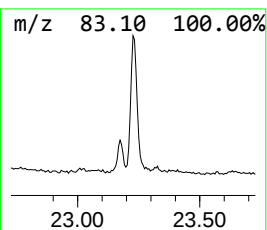
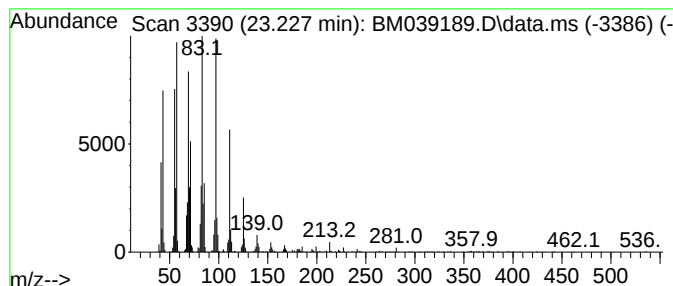
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM030823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 9 Heptacos-1-ene Concentration Rank 3

| R.T.      | EstConc                             | Area    | Relative to ISTD |             | R.T.         |      |
|-----------|-------------------------------------|---------|------------------|-------------|--------------|------|
| 23.227    | 10.97 ng                            | 1594840 | Perylene-d12     |             | 23.927       |      |
| Hit# of 5 | Tentative ID                        |         | MW               | MolForm     | CAS#         | Qual |
| 1         | Heptacos-1-ene                      |         | 378              | C27H54      | 015306-27-1  | 93   |
| 2         | 1-Tetracosene                       |         | 336              | C24H48      | 010192-32-2  | 87   |
| 3         | Nonacos-1-ene                       |         | 406              | C29H58      | 018835-35-3  | 76   |
| 4         | Pentadecafluorooctanoic acid, oc... |         | 666              | C26H37F15O2 | 1000406-04-8 | 70   |
| 5         | Triacontyl acetate                  |         | 480              | C32H64O2    | 041755-58-2  | 68   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM032823\  
Data File : BM039189.D  
Acq On : 28 Mar 2023 20:59  
Operator : CG/JU  
Sample : 02111-03  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
APCS-NORTH

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM030823.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-... | 5.028  | 29.1    | ng    | 2347060  | 1                     | 7.934  | 1613370 | 20.0 |
| n-Hexadecanoic ... | 18.221 | 16.6    | ng    | 1893520  | 4                     | 17.327 | 2284190 | 20.0 |
| 4,4'-Bis(tetra...  | 19.380 | 2.7     | ng    | 305603   | 4                     | 17.327 | 2284190 | 20.0 |
| Octadecanoic acid  | 19.497 | 5.3     | ng    | 838883   | 5                     | 21.509 | 3157780 | 20.0 |
| 1-Hexacosene       | 21.209 | 10.1    | ng    | 1590780  | 5                     | 21.509 | 3157780 | 20.0 |
| unknown22.144      | 22.144 | 10.6    | ng    | 1677880  | 5                     | 21.509 | 3157780 | 20.0 |
| Acetic acid, 2-... | 22.297 | 9.4     | ng    | 1492370  | 5                     | 21.509 | 3157780 | 20.0 |
| Tetracosane        | 23.174 | 6.0     | ng    | 874879   | 6                     | 23.927 | 2907350 | 20.0 |
| Heptacos-1-ene     | 23.227 | 11.0    | ng    | 1594840  | 6                     | 23.927 | 2907350 | 20.0 |