

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM052522\  
 Data File : BM035260.D  
 Acq On : 26 May 2022 02:22  
 Operator : CG/JU  
 Sample : N2895-15  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 P030-SS003-0006-01

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-BM042722.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035260.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         | 5.463       | 398           | 404         | 417          | rBV      | 906204         | 1384986       | 33.94%          | 5.080%        |
| 2         | 7.057       | 667           | 675         | 691          | rBV      | 900657         | 1435496       | 35.17%          | 5.265%        |
| 3         | 7.887       | 809           | 816         | 825          | rBV      | 291349         | 470641        | 11.53%          | 1.726%        |
| 4         | 9.045       | 1006          | 1013        | 1027         | rBV      | 546635         | 937437        | 22.97%          | 3.438%        |
| 5         | 10.686      | 1285          | 1292        | 1304         | rBV      | 373339         | 629250        | 15.42%          | 2.308%        |
| 6         | 13.145      | 1703          | 1710        | 1723         | rBV      | 1679797        | 2502809       | 61.32%          | 9.180%        |
| 7         | 14.521      | 1938          | 1944        | 1952         | rBV      | 606594         | 892262        | 21.86%          | 3.273%        |
| 8         | 16.009      | 2191          | 2197        | 2210         | rBV      | 1435167        | 2057282       | 50.41%          | 7.546%        |
| 9         | 17.268      | 2402          | 2411        | 2416         | rBV      | 770102         | 1118842       | 27.41%          | 4.104%        |
| 10        | 17.321      | 2416          | 2420        | 2425         | rVV2     | 65412          | 78120         | 1.91%           | 0.287%        |
| 11        | 18.174      | 2559          | 2565        | 2575         | rBV      | 320899         | 479099        | 11.74%          | 1.757%        |
| 12        | 18.468      | 2610          | 2615        | 2625         | rBV5     | 24076          | 51000         | 1.25%           | 0.187%        |
| 13        | 19.298      | 2752          | 2756        | 2758         | rBV      | 52922          | 66428         | 1.63%           | 0.244%        |
| 14        | 19.327      | 2758          | 2761        | 2777         | rVB      | 126320         | 228663        | 5.60%           | 0.839%        |
| 15        | 19.445      | 2777          | 2781        | 2791         | rBV2     | 241451         | 385122        | 9.44%           | 1.413%        |
| 16        | 19.686      | 2818          | 2822        | 2831         | rVB      | 49990          | 87618         | 2.15%           | 0.321%        |
| 17        | 19.892      | 2851          | 2857        | 2867         | rBV      | 3466063        | 4081250       | 100.00%         | 14.970%       |
| 18        | 21.174      | 3071          | 3075        | 3080         | rBV      | 184538         | 286625        | 7.02%           | 1.051%        |
| 19        | 21.450      | 3117          | 3122        | 3136         | rVB      | 1212605        | 1856304       | 45.48%          | 6.809%        |
| 20        | 23.821      | 3519          | 3525        | 3541         | rVB2     | 811541         | 1628277       | 39.90%          | 5.972%        |
| 21        | 24.538      | 3641          | 3647        | 3662         | rVB      | 492426         | 1329379       | 32.57%          | 4.876%        |
| 22        | 25.762      | 3848          | 3855        | 3871         | rVB      | 577961         | 1497414       | 36.69%          | 5.492%        |
| 23        | 26.421      | 3960          | 3967        | 3976         | rBV2     | 257744         | 761809        | 18.67%          | 2.794%        |
| 24        | 26.832      | 4028          | 4037        | 4051         | rVB2     | 970105         | 3017439       | 73.93%          | 11.068%       |

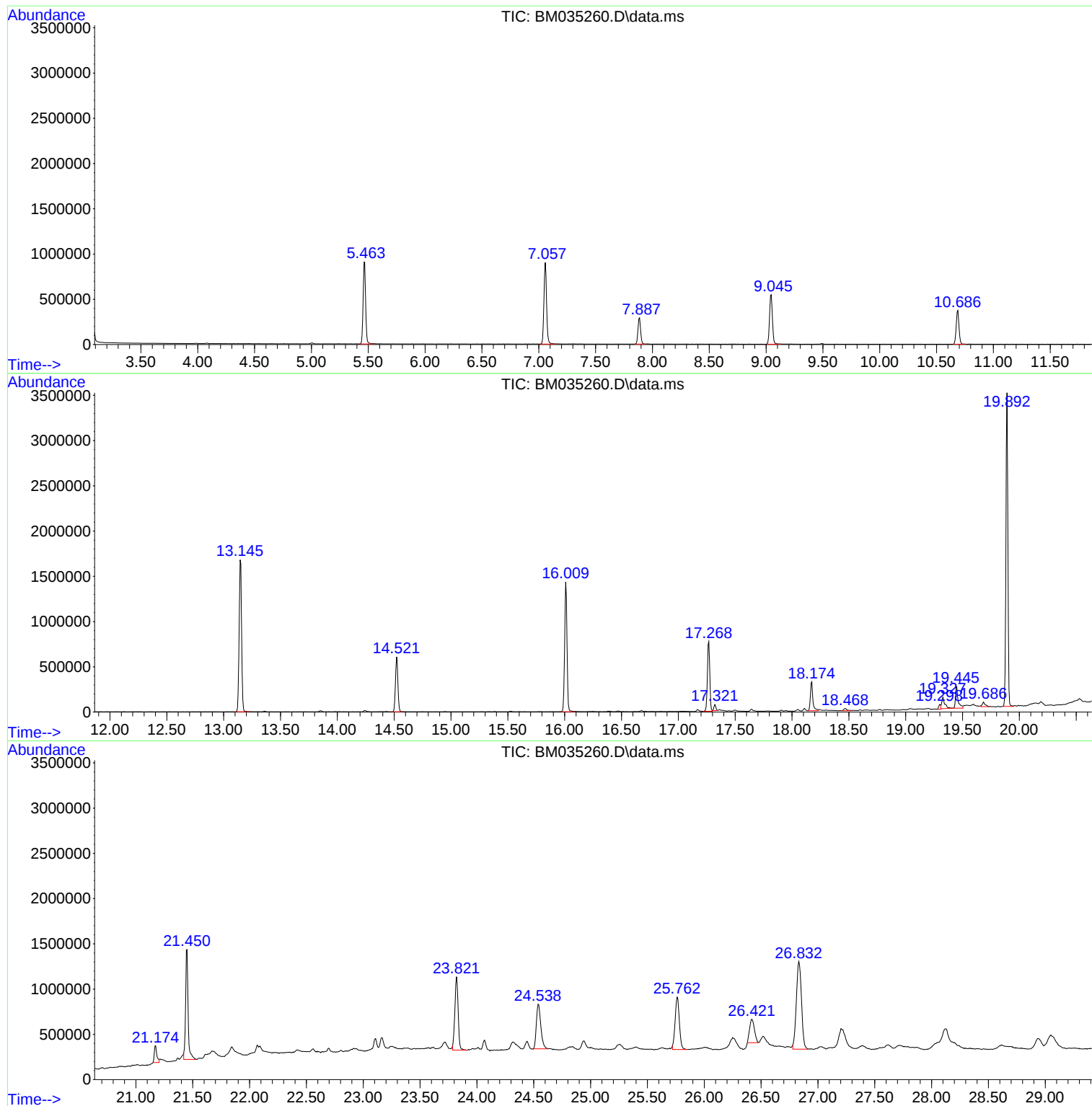
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Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM052522\  
Data File : BM035260.D  
Acq On : 26 May 2022 02:22  
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Sample : N2895-15  
Misc :  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
P030-SS003-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM042722.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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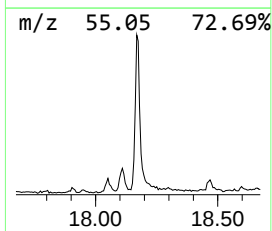
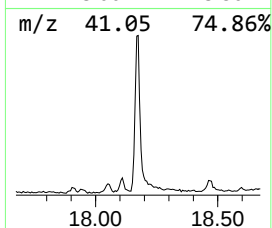
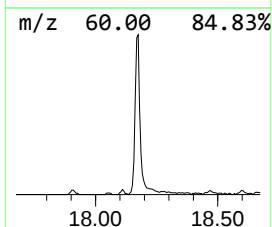
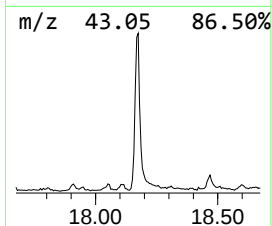
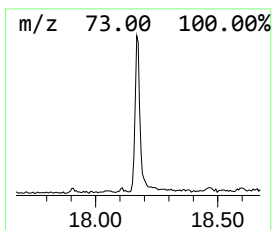
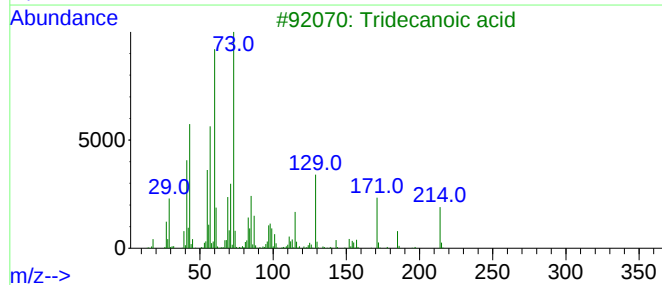
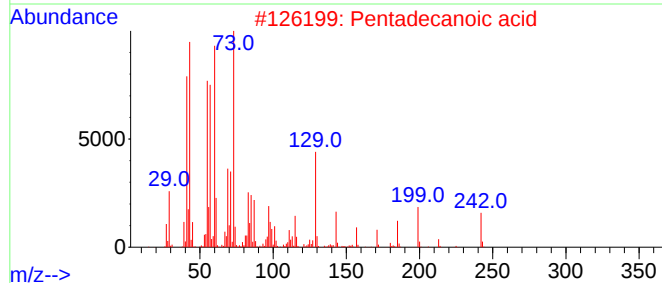
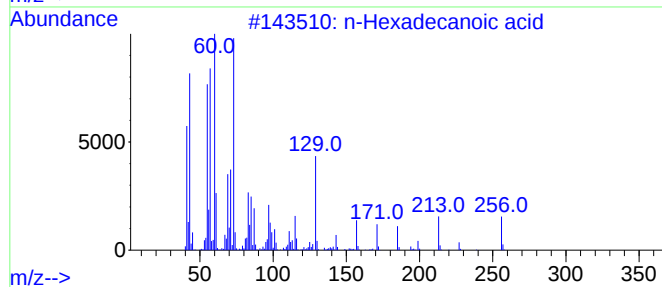
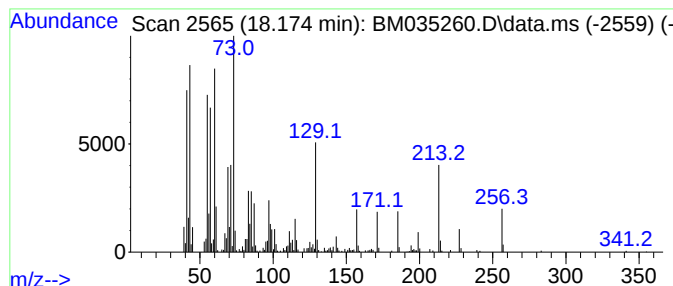
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 n-Hexadecanoic acid Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.174 | 8.56 ng | 479099 | Phenanthrene-d10 | 17.268 |

| 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 | 76   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 70   |
| 4    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 58   |
| 5    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 58   |



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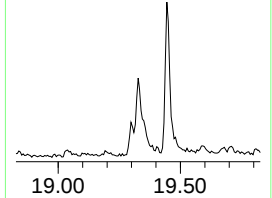
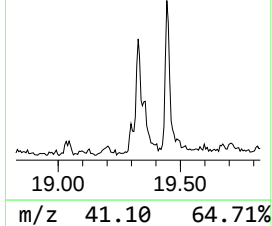
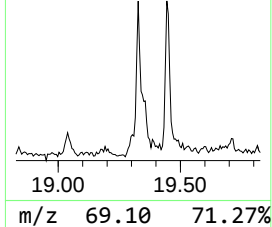
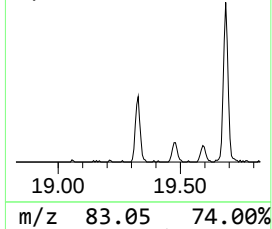
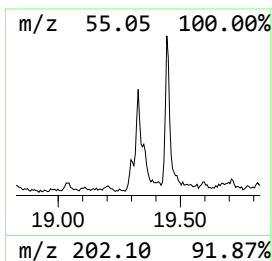
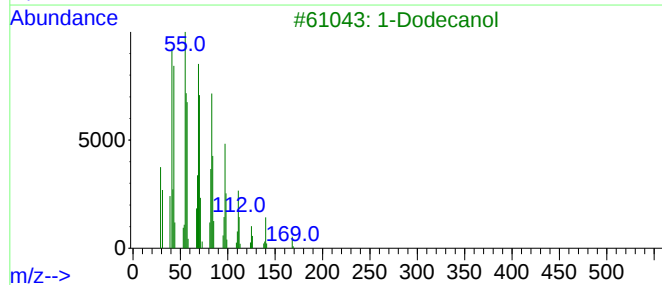
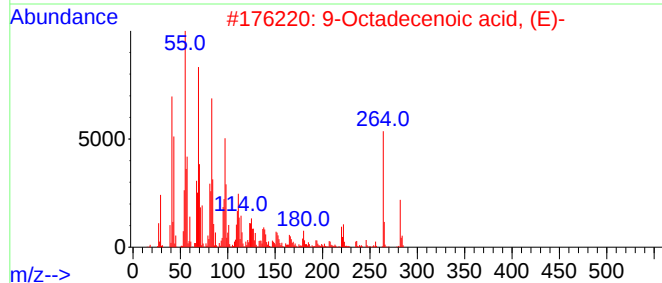
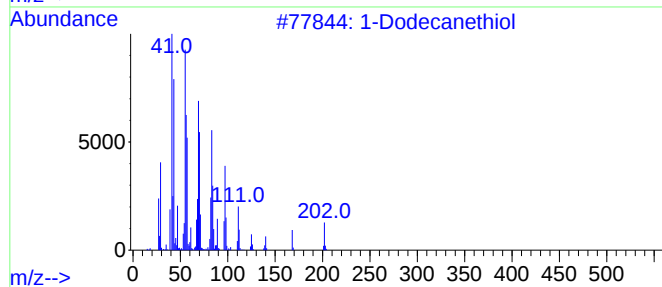
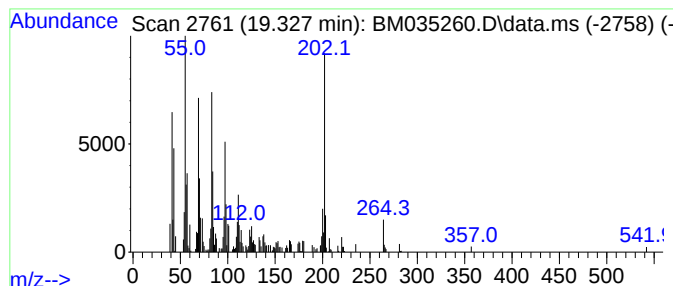
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM042722.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 1-Dodecanethiol Concentration Rank 7

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.327 | 4.09 ng | 228663 | Phenanthrene-d10 | 17.268 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|------|-------------------------------------|-----|------------|-------------|------|
| 1    |      | 1-Dodecanethiol                     | 202 | C12H26S    | 000112-55-0 | 70   |
| 2    |      | 9-Octadecenoic acid, (E)-           | 282 | C18H34O2   | 000112-79-8 | 60   |
| 3    |      | 1-Dodecanol                         | 186 | C12H26O    | 000112-53-8 | 53   |
| 4    |      | Cyclotetradecane                    | 196 | C14H28     | 000295-17-0 | 53   |
| 5    |      | Acetic acid, trifluoro-, dodecyl... | 282 | C14H25F3O2 | 006222-00-0 | 53   |



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ClientSampleId :  
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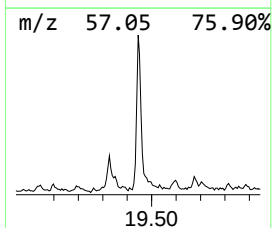
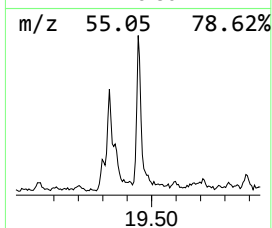
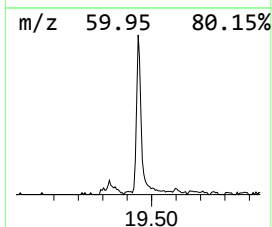
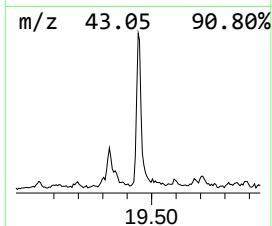
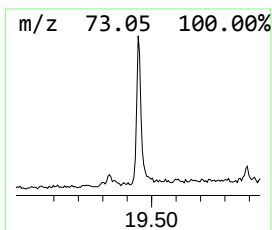
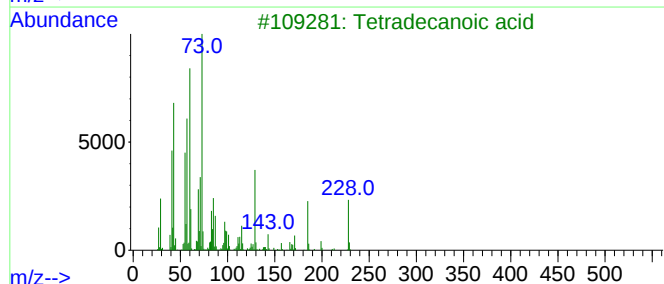
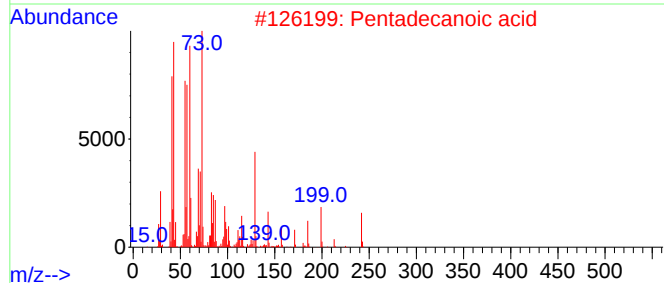
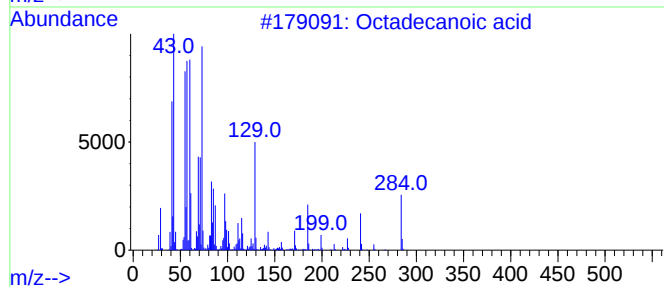
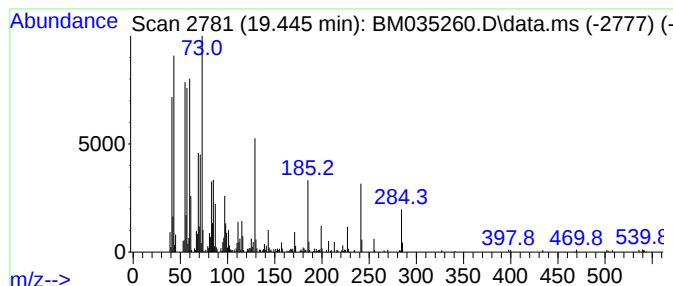
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM042722.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Octadecanoic acid Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.445 | 4.15 ng | 385122 | Chrysene-d12     | 21.450 |

| 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 | 94   |
| 3    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 68   |
| 4    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 60   |
| 5    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 53   |



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ALS Vial : 18 Sample Multiplier: 1

Instrument :  
BNA\_M  
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P030-SS003-0006-01

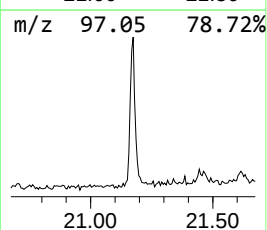
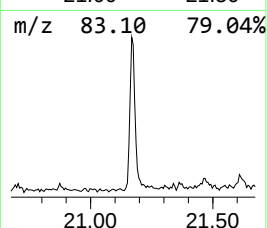
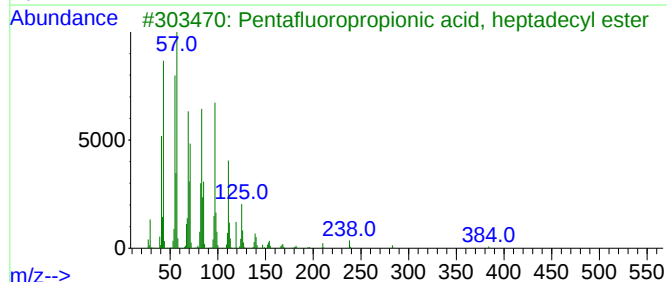
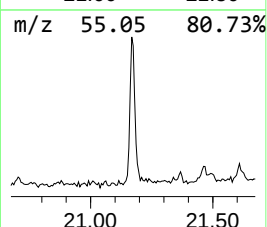
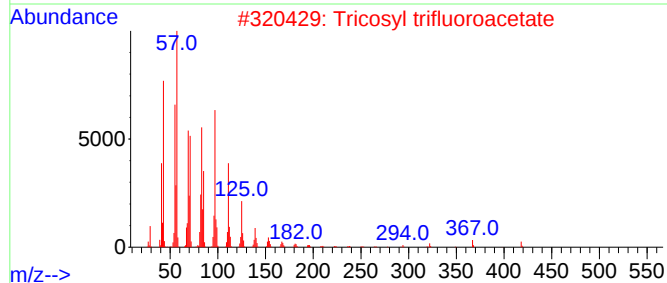
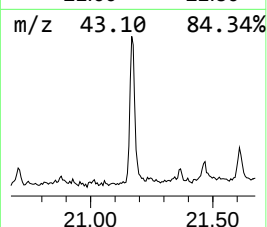
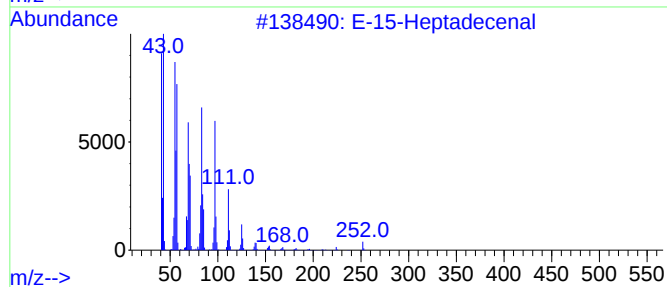
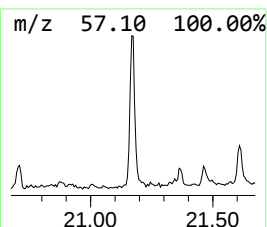
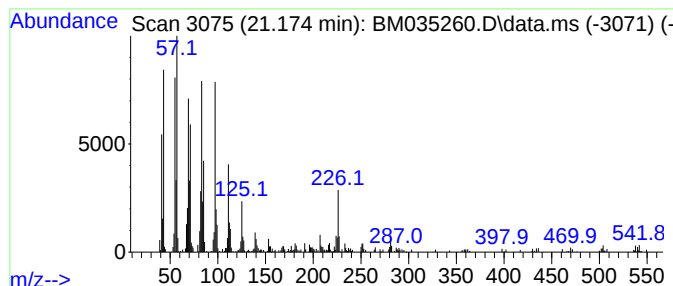
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM042722.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 E-15-Heptadecenal Concentration Rank 8

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.174 | 3.09 ng | 286625 | Chrysene-d12     | 21.450 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | E-15-Heptadecenal                   | 252 | C17H32O    | 1000130-97-9 | 94   |
| 2    |    |   | Tricosyl trifluoroacetate           | 436 | C25H47F3O2 | 1000351-75-1 | 94   |
| 3    |    |   | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1  | 94   |
| 4    |    |   | Heptadecyl heptafluorobutyrate      | 452 | C21H35F7O2 | 959085-66-6  | 94   |
| 5    |    |   | Pentafluoropropionic acid, octad... | 416 | C21H37F5O2 | 959261-25-7  | 94   |



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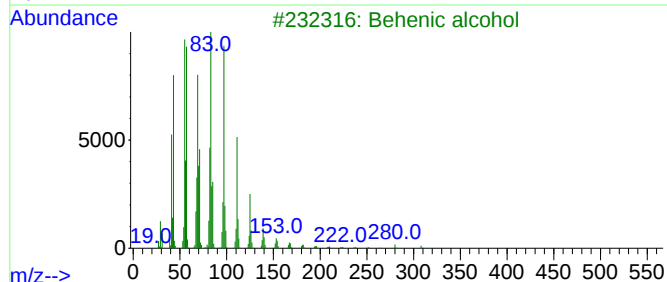
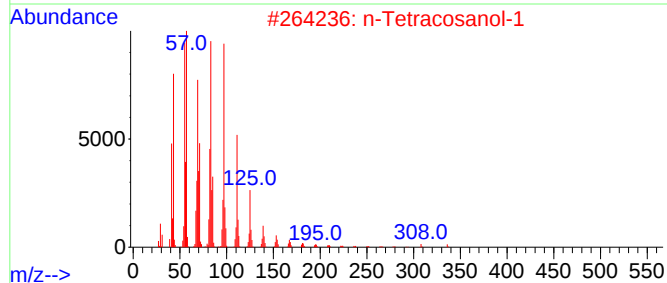
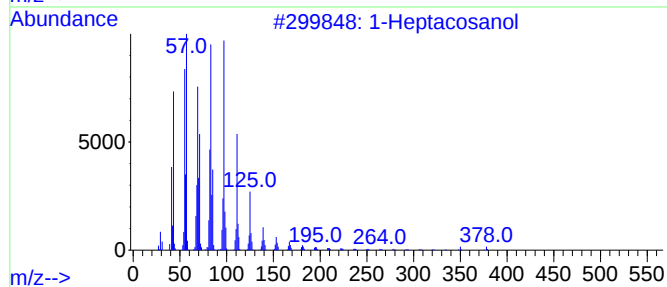
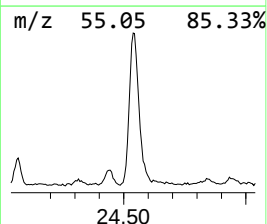
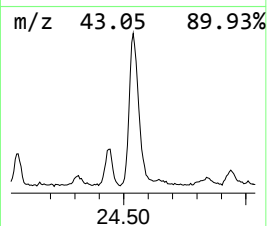
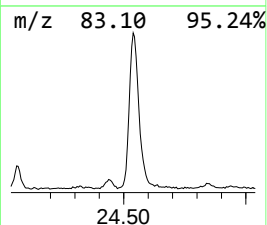
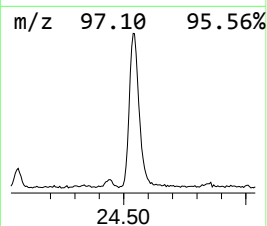
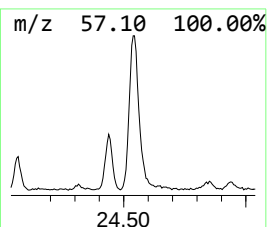
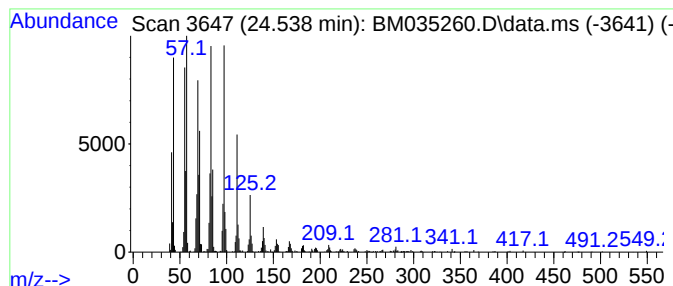
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Peak Number 5 1-Heptacosanol Concentration Rank 3

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 24.538 | 16.33 ng | 1329380 | Perylene-d12     | 23.821 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm | CAS#         | Qual |
|------|----|---|---------------------------|-----|---------|--------------|------|
| 1    |    |   | 1-Heptacosanol            | 396 | C27H56O | 002004-39-9  | 95   |
| 2    |    |   | n-Tetracosanol-1          | 354 | C24H50O | 000506-51-4  | 94   |
| 3    |    |   | Behenic alcohol           | 326 | C22H46O | 000661-19-8  | 94   |
| 4    |    |   | 1-Methoxyhexacosane       | 396 | C27H56O | 237742-59-5  | 94   |
| 5    |    |   | 1-Docosanol, methyl ether | 340 | C23H48O | 1000333-91-9 | 94   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM052522\  
Data File : BM035260.D  
Acq On : 26 May 2022 02:22  
Operator : CG/JU  
Sample : N2895-15  
Misc :  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
P030-SS003-0006-01

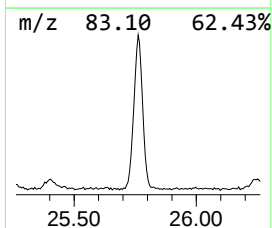
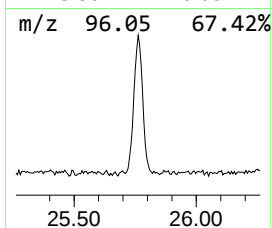
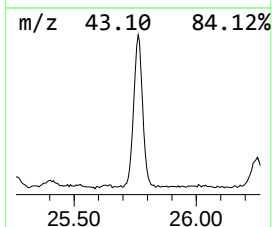
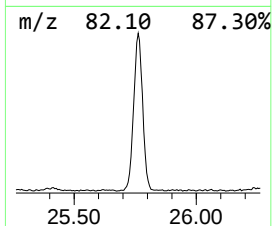
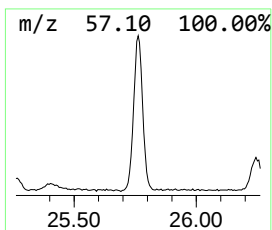
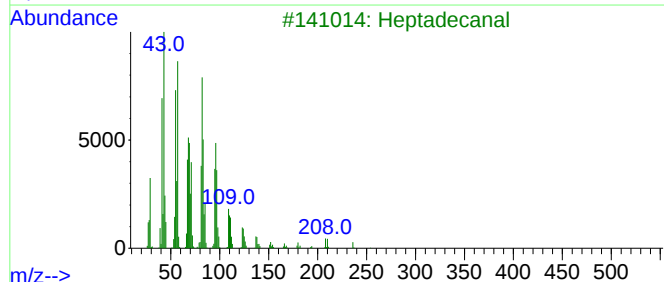
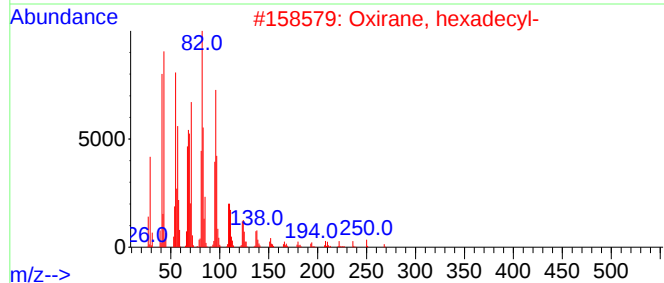
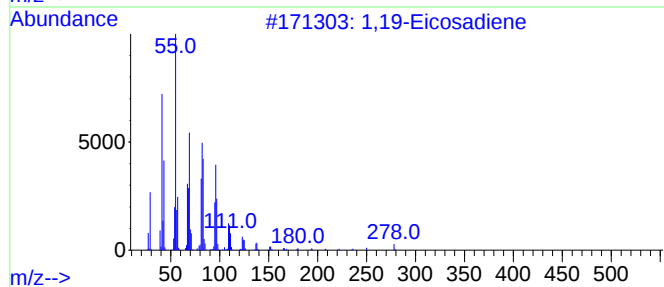
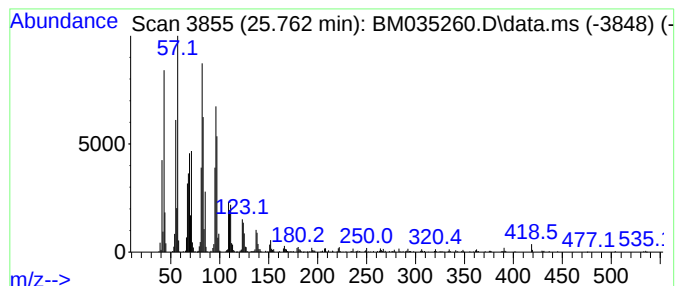
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 1,19-Eicosadiene Concentration Rank 2

| R.T.      | EstConc             | Area    | Relative to ISTD |          | R.T.         |      |
|-----------|---------------------|---------|------------------|----------|--------------|------|
| 25.762    | 18.39 ng            | 1497410 | Perylene-d12     |          | 23.821       |      |
| Hit# of 5 | Tentative ID        |         | MW               | MolForm  | CAS#         | Qual |
| 1         | 1,19-Eicosadiene    |         | 278              | C20H38   | 014811-95-1  | 97   |
| 2         | Oxirane, hexadecyl- |         | 268              | C18H36O  | 007390-81-0  | 96   |
| 3         | Heptadecanal        |         | 254              | C17H34O  | 1000376-70-0 | 95   |
| 4         | 1,22-Docosanediol   |         | 342              | C22H46O2 | 022513-81-1  | 94   |
| 5         | Hexadecanal         |         | 240              | C16H32O  | 000629-80-1  | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM052522\  
Data File : BM035260.D  
Acq On : 26 May 2022 02:22  
Operator : CG/JU  
Sample : N2895-15  
Misc :  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
P030-SS003-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM042722.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

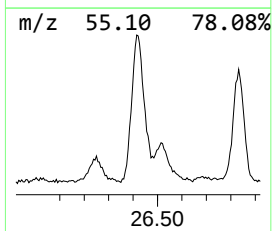
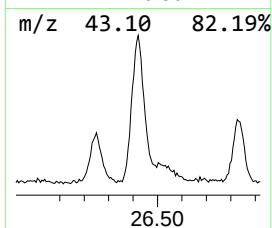
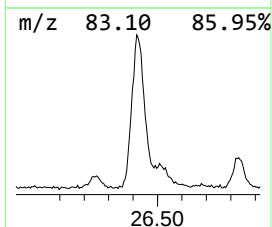
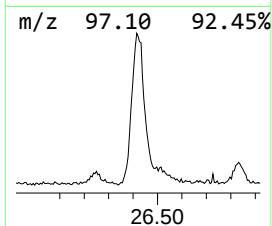
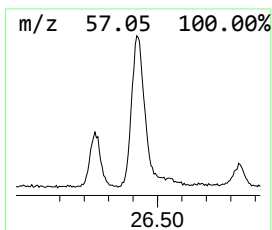
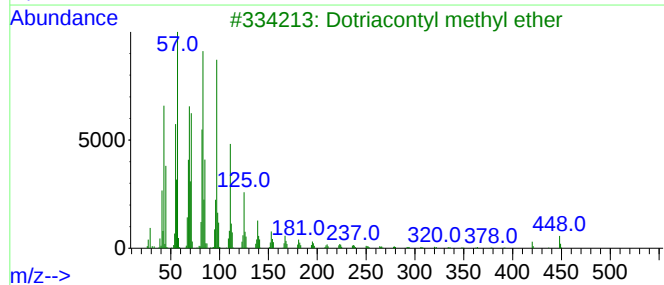
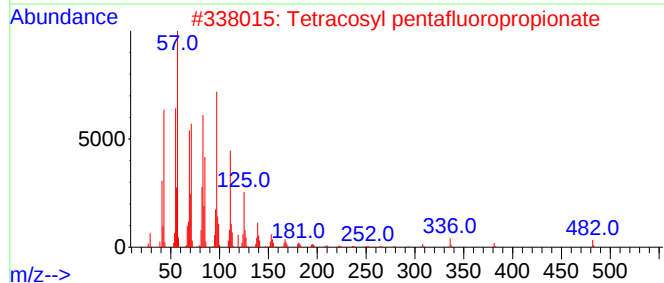
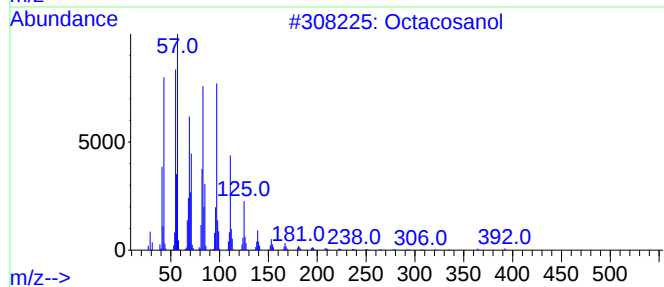
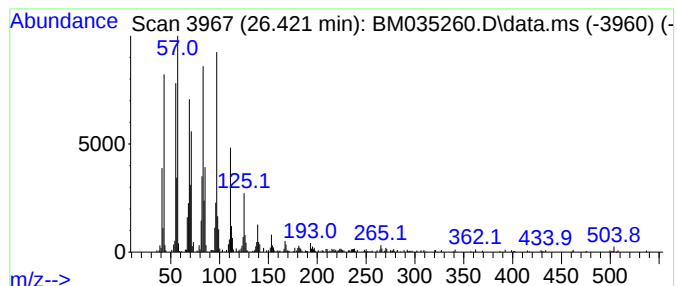
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Octacosanol Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 26.421 | 9.36 ng | 761809 | Perylene-d12     | 23.821 |

| Hit# | of | 5 | Tentative ID                     | MW  | MolForm    | CAS#         | Qual |
|------|----|---|----------------------------------|-----|------------|--------------|------|
| 1    |    |   | Octacosanol                      | 410 | C28H58O    | 000557-61-9  | 95   |
| 2    |    |   | Tetracosyl pentafluoropropionate | 500 | C27H49F5O2 | 1000351-81-3 | 95   |
| 3    |    |   | Dotriacontyl methyl ether        | 481 | C33H68O    | 1000406-30-0 | 94   |
| 4    |    |   | Heneicosyl trifluoroacetate      | 408 | C23H43F3O2 | 1000351-76-5 | 94   |
| 5    |    |   | Docosyl trifluoroacetate         | 422 | C24H45F3O2 | 1000351-75-5 | 94   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM052522\  
Data File : BM035260.D  
Acq On : 26 May 2022 02:22  
Operator : CG/JU  
Sample : N2895-15  
Misc :  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
P030-SS003-0006-01

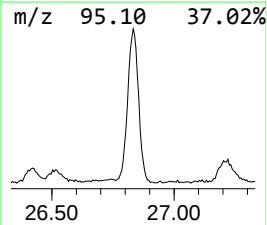
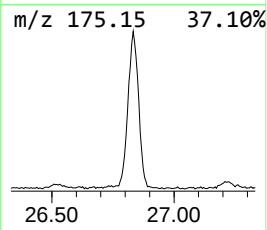
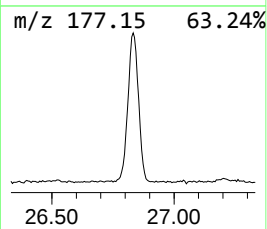
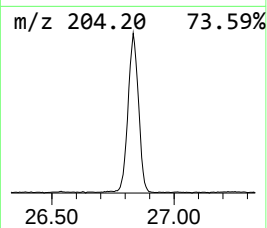
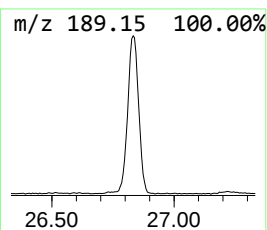
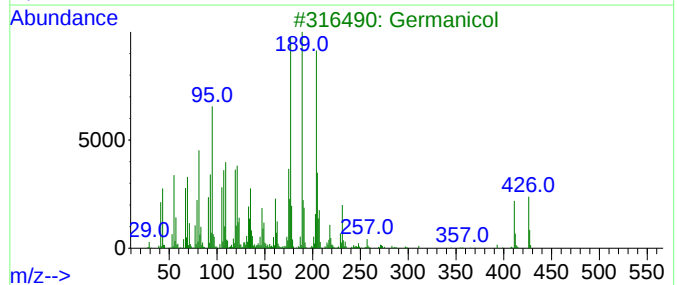
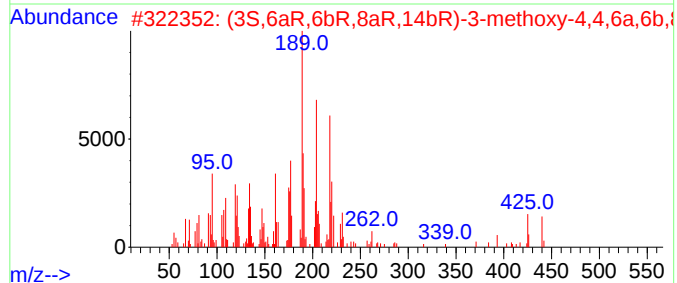
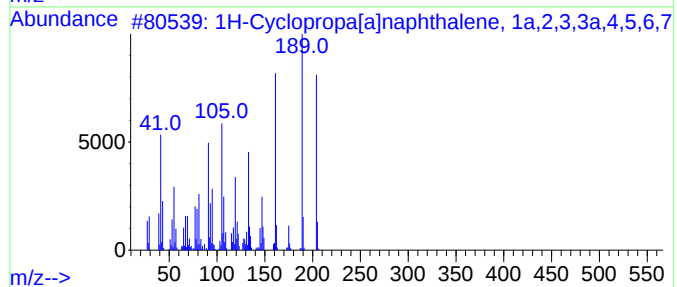
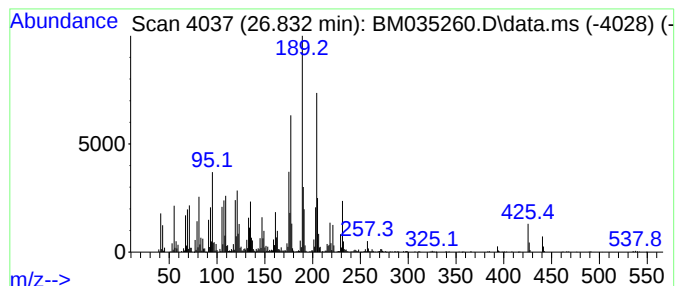
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 8 1H-Cyclopropa[a]naphthalene... Concentration Rank 1

| R.T.      | EstConc                             | Area    | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|---------|------------------|--------------|------|
| 26.832    | 37.06 ng                            | 3017440 | Perylene-d12     | 23.821       |      |
| Hit# of 5 | Tentative ID                        | MW      | MolForm          | CAS#         | Qual |
| 1         | 1H-Cyclopropa[a]naphthalene, 1a,... | 204     | C15H24           | 000489-29-2  | 55   |
| 2         | (3S,6aR,6bR,8aR,14bR)-3-methoxy-... | 440     | C31H52O          | 1000441-97-8 | 50   |
| 3         | Germanicol                          | 426     | C30H50O          | 000465-02-1  | 50   |
| 4         | Naphthalene, 2,3,4,4a,5,6-hexahy... | 204     | C15H24           | 000473-14-3  | 46   |
| 5         | 4a,8-Dimethyl-2-(prop-1-en-2-yl)... | 204     | C15H24           | 103827-22-1  | 46   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM052522\  
Data File : BM035260.D  
Acq On : 26 May 2022 02:22  
Operator : CG/JU  
Sample : N2895-15  
Misc :  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
P030-SS003-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM042722.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 |
| n-Hexadecanoic ...  | 18.174 | 8.6     | ng    | 479099   | 4                     | 17.268 | 1118840 | 20.0 |
| 1-Dodecanethiol     | 19.327 | 4.1     | ng    | 228663   | 4                     | 17.268 | 1118840 | 20.0 |
| Octadecanoic acid   | 19.445 | 4.2     | ng    | 385122   | 5                     | 21.450 | 1856300 | 20.0 |
| E-15-Heptadecenal   | 21.174 | 3.1     | ng    | 286625   | 5                     | 21.450 | 1856300 | 20.0 |
| 1-Heptacosanol      | 24.538 | 16.3    | ng    | 1329380  | 6                     | 23.821 | 1628280 | 20.0 |
| 1,19-Eicosadiene    | 25.762 | 18.4    | ng    | 1497410  | 6                     | 23.821 | 1628280 | 20.0 |
| Octacosanol         | 26.421 | 9.4     | ng    | 761809   | 6                     | 23.821 | 1628280 | 20.0 |
| 1H-Cyclopropa[a]... | 26.832 | 37.1    | ng    | 3017440  | 6                     | 23.821 | 1628280 | 20.0 |