

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM100422\  
 Data File : BM036828.D  
 Acq On : 04 Oct 2022 14:43  
 Operator : CG/JU  
 Sample : N4785-03  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 PT-BN-WP

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-BM100322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036828.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         | 4.446       | 226           | 231         | 249          | rVB      | 775376         | 1111863       | 3.82%           | 0.200%        |
| 2         | 5.063       | 330           | 336         | 350          | rVB      | 2396921        | 3385278       | 11.63%          | 0.609%        |
| 3         | 5.528       | 408           | 415         | 432          | rBV      | 7206212        | 10769196      | 36.98%          | 1.939%        |
| 4         | 7.134       | 679           | 688         | 707          | rBV      | 7339488        | 11506241      | 39.52%          | 2.071%        |
| 5         | 7.392       | 725           | 732         | 743          | rBV      | 6764778        | 9921249       | 34.07%          | 1.786%        |
| 6         | 7.857       | 803           | 811         | 821          | rBV      | 4301156        | 6629819       | 22.77%          | 1.193%        |
| 7         | 7.969       | 823           | 830         | 832          | rVV      | 1439223        | 2315405       | 7.95%           | 0.417%        |
| 8         | 8.004       | 832           | 836         | 848          | rVB      | 9320468        | 14532612      | 49.91%          | 2.616%        |
| 9         | 9.051       | 1005          | 1014        | 1021         | rBV      | 7004613        | 11264914      | 38.69%          | 2.028%        |
| 10        | 9.139       | 1021          | 1029        | 1032         | rVV      | 4235113        | 7104052       | 24.40%          | 1.279%        |
| 11        | 9.181       | 1032          | 1036        | 1052         | rVB      | 5449137        | 8877356       | 30.49%          | 1.598%        |
| 12        | 10.192      | 1200          | 1208        | 1221         | rBV      | 7518109        | 11308999      | 38.84%          | 2.036%        |
| 13        | 10.780      | 1300          | 1308        | 1311         | rBV      | 1909354        | 3231749       | 11.10%          | 0.582%        |
| 14        | 10.833      | 1311          | 1317        | 1332         | rVB      | 12771090       | 21555827      | 74.03%          | 3.880%        |
| 15        | 12.651      | 1615          | 1626        | 1640         | rVB      | 2250979        | 3444824       | 11.83%          | 0.620%        |
| 16        | 12.774      | 1640          | 1647        | 1655         | rBV2     | 4011591        | 5846816       | 20.08%          | 1.052%        |
| 17        | 13.227      | 1717          | 1724        | 1734         | rBV      | 10844230       | 15627552      | 53.67%          | 2.813%        |
| 18        | 13.480      | 1759          | 1767        | 1778         | rBV      | 7989482        | 11395074      | 39.13%          | 2.051%        |
| 19        | 14.063      | 1859          | 1866        | 1880         | rBV      | 12084345       | 17148566      | 58.89%          | 3.087%        |
| 20        | 14.180      | 1880          | 1886        | 1896         | rVV      | 4424290        | 5883987       | 20.21%          | 1.059%        |
| 21        | 14.327      | 1903          | 1911        | 1922         | rBV      | 11929885       | 17843719      | 61.28%          | 3.212%        |
| 22        | 14.598      | 1950          | 1957        | 1962         | rBV      | 2681035        | 3856229       | 13.24%          | 0.694%        |
| 23        | 14.663      | 1962          | 1968        | 1975         | rVB      | 5854532        | 8164868       | 28.04%          | 1.470%        |
| 24        | 14.998      | 2014          | 2025        | 2041         | rBV      | 11150179       | 15781470      | 54.20%          | 2.841%        |
| 25        | 15.415      | 2090          | 2096        | 2100         | rBV      | 4717547        | 6408317       | 22.01%          | 1.154%        |
| 26        | 15.457      | 2100          | 2103        | 2115         | rVB      | 736084         | 991328        | 3.40%           | 0.178%        |
| 27        | 15.639      | 2127          | 2134        | 2138         | rBV2     | 14153848       | 22583759      | 77.56%          | 4.065%        |
| 28        | 15.668      | 2138          | 2139        | 2155         | rVB      | 4807007        | 4890386       | 16.79%          | 0.880%        |
| 29        | 15.851      | 2164          | 2170        | 2175         | rBV      | 3975487        | 5170190       | 17.76%          | 0.931%        |
| 30        | 16.080      | 2202          | 2209        | 2224         | rBV      | 7064806        | 9959844       | 34.20%          | 1.793%        |
| 31        | 16.527      | 2279          | 2285        | 2293         | rBV      | 5871531        | 7498396       | 25.75%          | 1.350%        |
| 32        | 16.639      | 2298          | 2304        | 2311         | rBV      | 4731553        | 6425139       | 22.07%          | 1.157%        |
| 33        | 17.339      | 2414          | 2423        | 2426         | rBV      | 2774214        | 4113444       | 14.13%          | 0.740%        |
| 34        | 17.380      | 2426          | 2430        | 2439         | rVV      | 8780271        | 12066271      | 41.44%          | 2.172%        |
| 35        | 17.474      | 2439          | 2446        | 2466         | rVB      | 18828639       | 27628977      | 94.88%          | 4.973%        |
| 36        | 17.745      | 2485          | 2492        | 2504         | rBV      | 10278264       | 14278008      | 49.03%          | 2.570%        |

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 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 PT-BN-WP

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-BM100322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |          |          |         |        |
|----|--------|------|------|------|------|----------|----------|---------|--------|
| 37 | 19.386 | 2765 | 2771 | 2780 | rBV  | 6149961  | 8158413  | 28.02%  | 1.469% |
| 38 | 19.950 | 2862 | 2867 | 2880 | rBV  | 14181836 | 17630879 | 60.55%  | 3.174% |
| 39 | 21.421 | 3113 | 3117 | 3124 | rBV  | 21741046 | 24424957 | 83.88%  | 4.397% |
| 40 | 21.497 | 3124 | 3130 | 3135 | rVV2 | 14384318 | 22493873 | 77.25%  | 4.049% |
| 41 | 21.556 | 3135 | 3140 | 3155 | rVB  | 20680558 | 27856611 | 95.67%  | 5.014% |
| 42 | 22.356 | 3270 | 3276 | 3290 | rVB  | 13262802 | 17797493 | 61.12%  | 3.204% |
| 43 | 23.180 | 3413 | 3416 | 3419 | rBV2 | 265589   | 373038   | 1.28%   | 0.067% |
| 44 | 23.250 | 3419 | 3428 | 3442 | rVB  | 14954637 | 28273959 | 97.10%  | 5.090% |
| 45 | 23.827 | 3517 | 3526 | 3535 | rBV  | 9565125  | 19485791 | 66.92%  | 3.508% |
| 46 | 23.927 | 3537 | 3543 | 3560 | rVB2 | 1733037  | 3561250  | 12.23%  | 0.641% |
| 47 | 24.544 | 3644 | 3648 | 3654 | rVB  | 409667   | 763786   | 2.62%   | 0.137% |
| 48 | 26.462 | 3959 | 3974 | 3992 | rVB2 | 9001447  | 29118504 | 100.00% | 5.242% |
| 49 | 27.203 | 4091 | 4100 | 4116 | rVB  | 1603233  | 5071252  | 17.42%  | 0.913% |

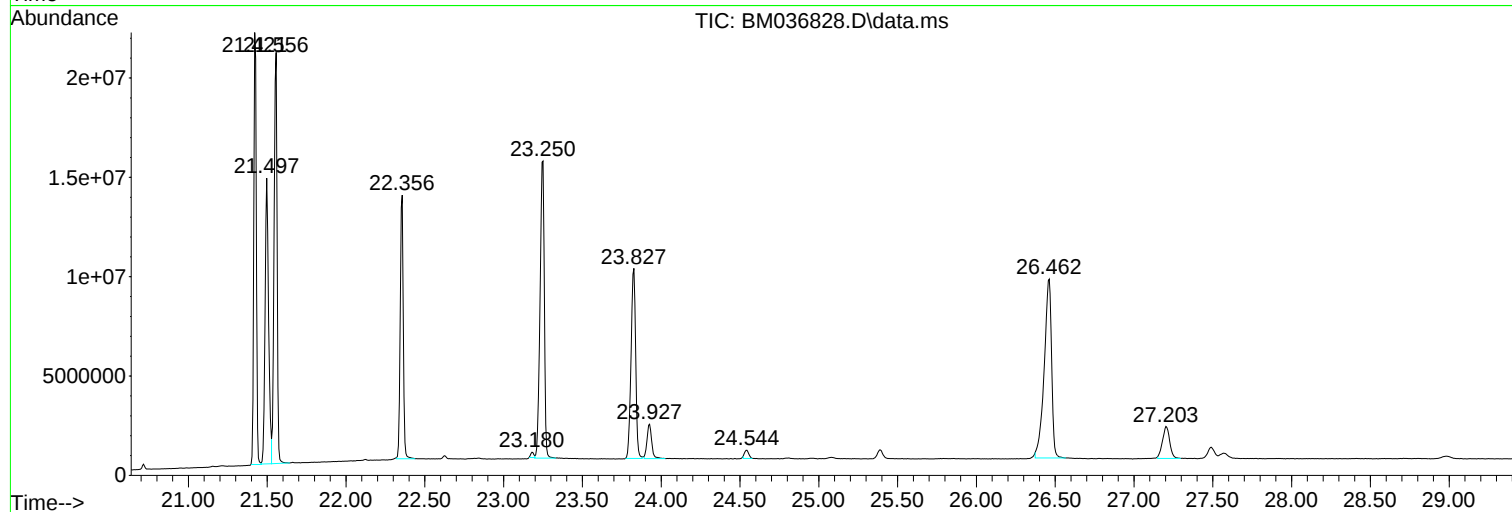
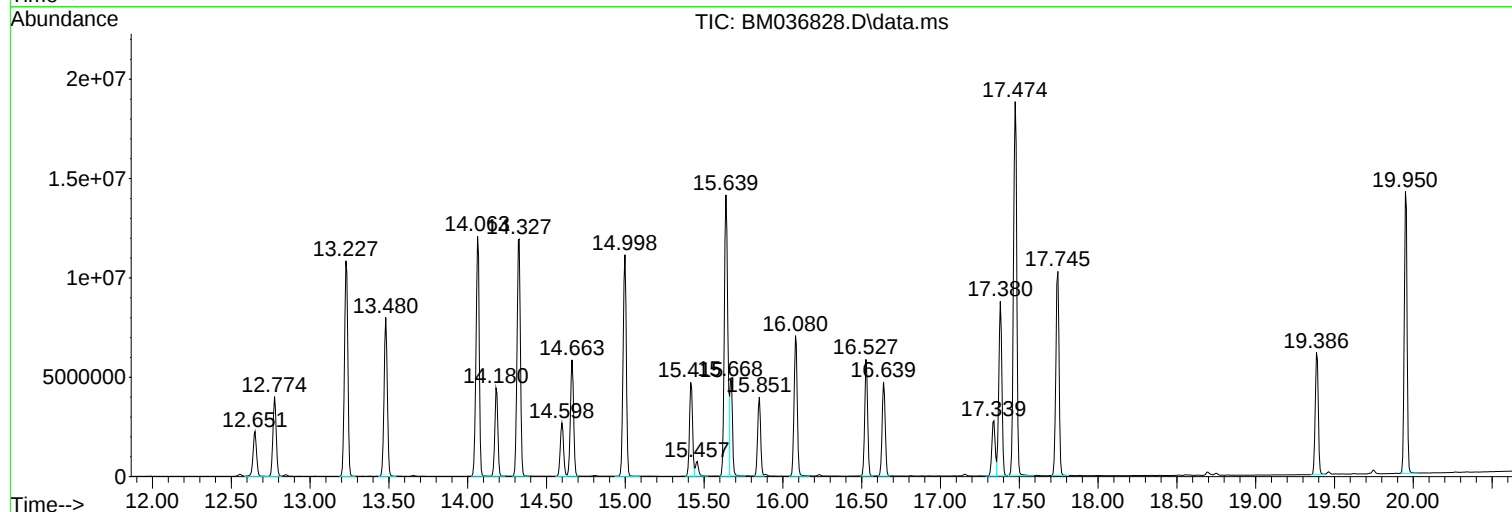
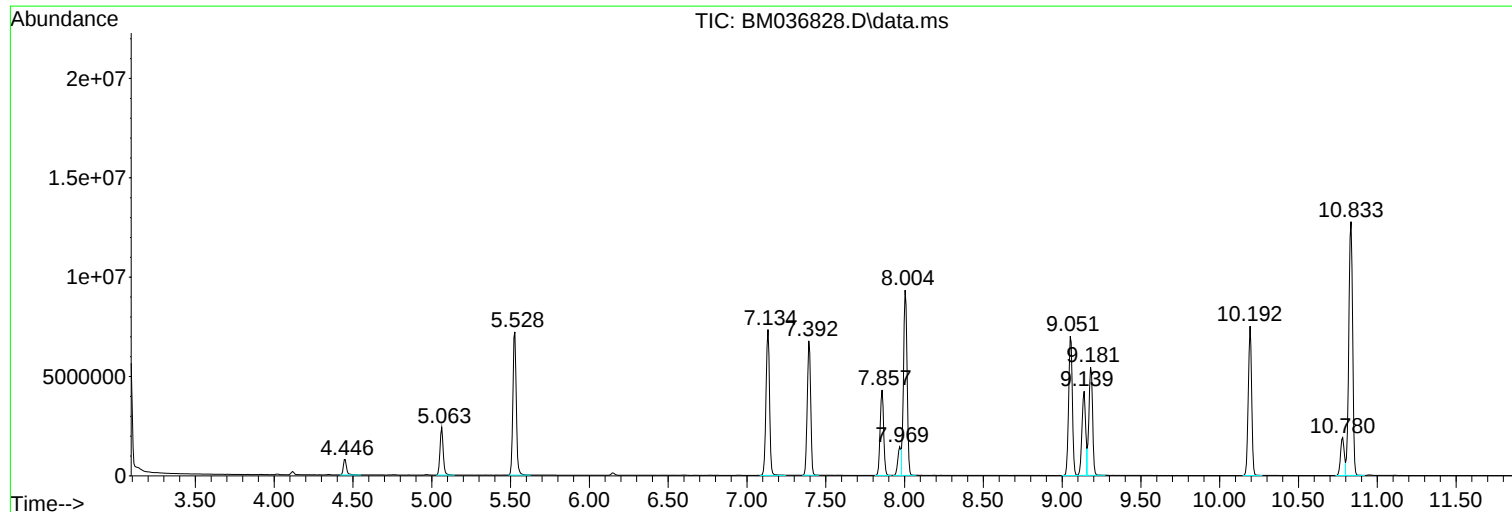
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Data File : BM036828.D  
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Sample : N4785-03  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
PT-BN-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM100322.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\BM100422\  
Data File : BM036828.D  
Acq On : 04 Oct 2022 14:43  
Operator : CG/JU  
Sample : N4785-03  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
PT-BN-WP

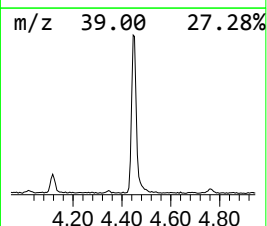
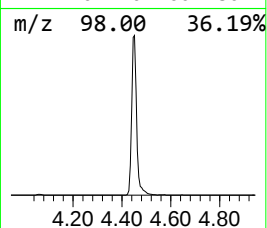
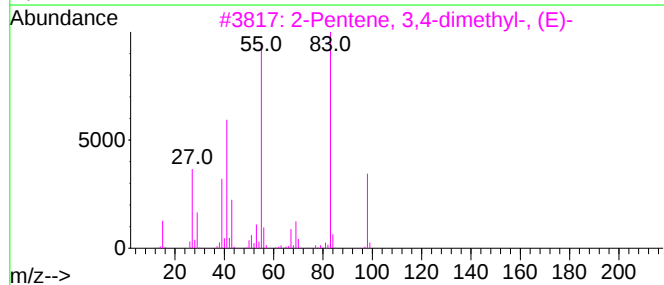
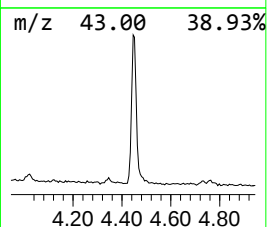
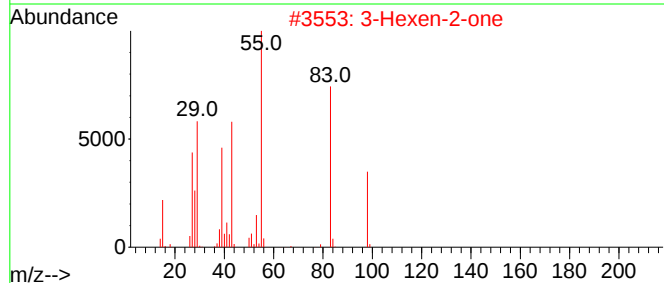
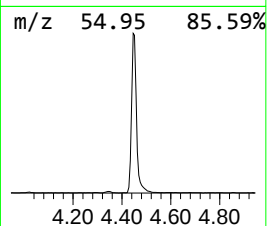
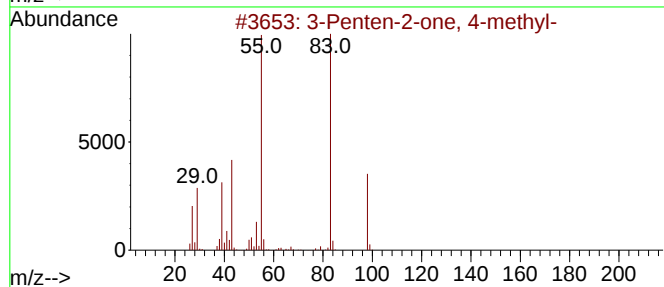
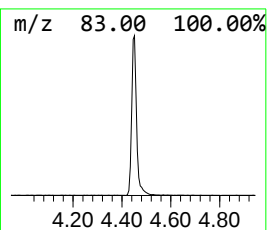
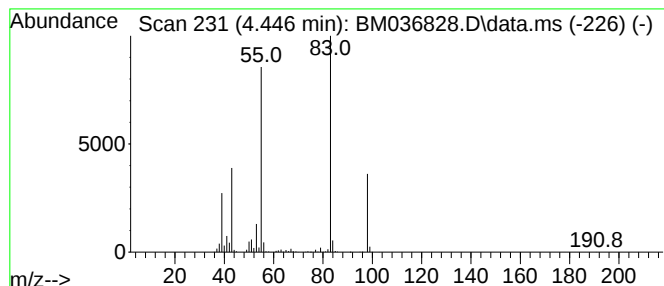
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM100322.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

| R.T.  | EstConc | Area    | Relative to ISTD       | R.T.  |
|-------|---------|---------|------------------------|-------|
| 4.446 | 9.60 ng | 1111860 | 1,4-Dichlorobenzene-d4 | 7.969 |

| Hit# | of | 5 | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|----|---------|-------------|------|
| 1    |    |   | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 95   |
| 2    |    |   | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 91   |
| 3    |    |   | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 90   |
| 4    |    |   | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14   | 004914-91-4 | 86   |
| 5    |    |   | 2-Pentene, 4,4-dimethyl-, (Z)- | 98 | C7H14   | 000762-63-0 | 80   |



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Instrument :  
BNA\_M  
ClientSampleId :  
PT-BN-WP

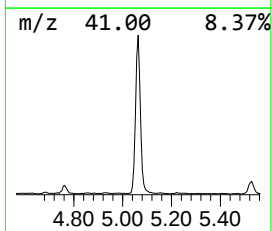
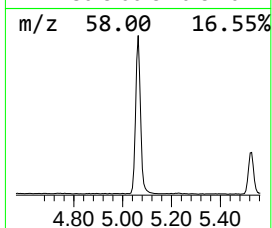
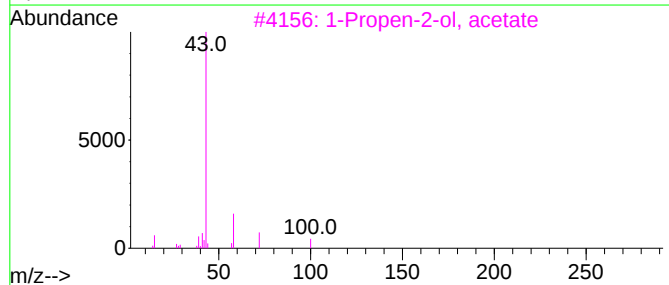
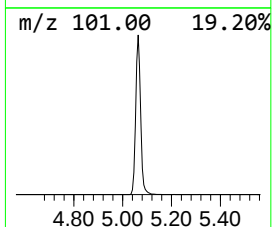
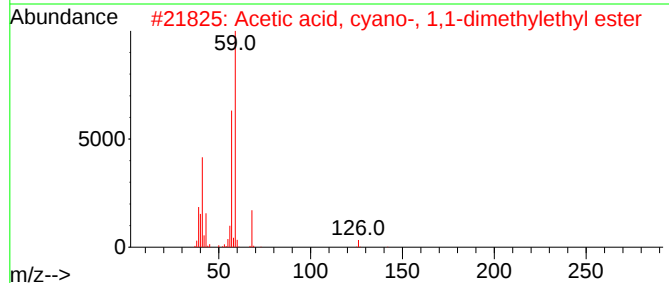
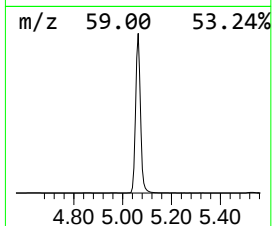
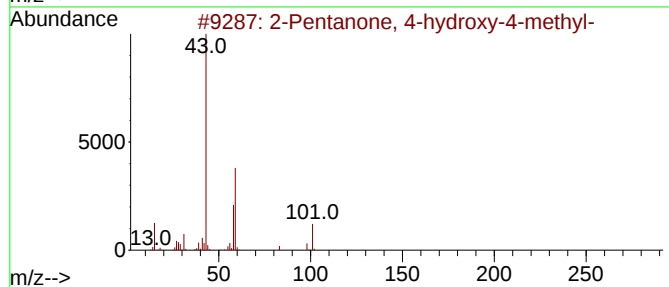
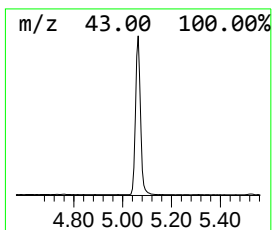
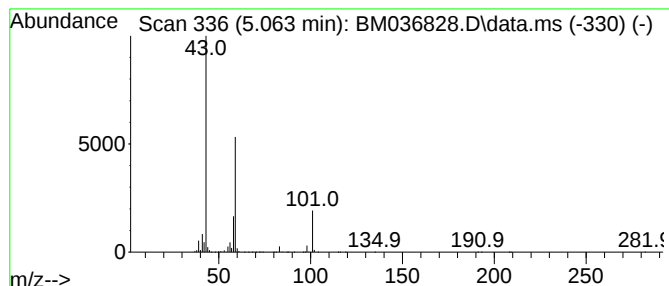
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM100322.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.      | EstConc                             | Area    | Relative to ISTD       | R.T.        |      |
|-----------|-------------------------------------|---------|------------------------|-------------|------|
| 5.063     | 29.24 ng                            | 3385280 | 1,4-Dichlorobenzene-d4 | 7.969       |      |
| Hit# of 5 | Tentative ID                        | MW      | MolForm                | CAS#        | Qual |
| 1         | 2-Pentanone, 4-hydroxy-4-methyl-    | 116     | C6H12O2                | 000123-42-2 | 50   |
| 2         | Acetic acid, cyano-, 1,1-dimethy... | 141     | C7H11NO2               | 001116-98-9 | 23   |
| 3         | 1-Propen-2-ol, acetate              | 100     | C5H8O2                 | 000108-22-5 | 10   |
| 4         | 5-Hexen-2-one                       | 98      | C6H10O                 | 000109-49-9 | 9    |
| 5         | Morpholine, 4-methyl-               | 101     | C5H11NO                | 000109-02-4 | 9    |



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ClientSampleId :  
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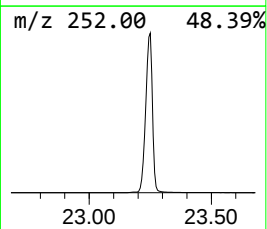
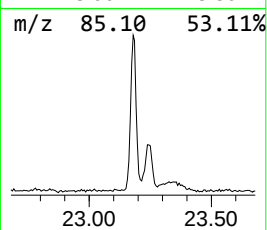
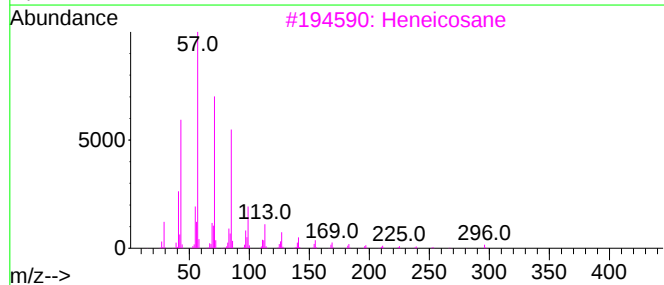
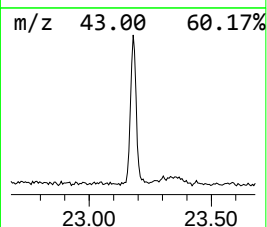
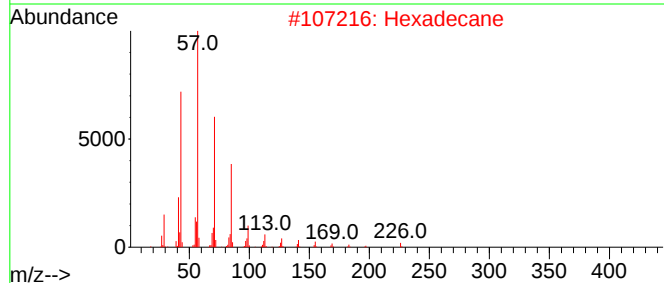
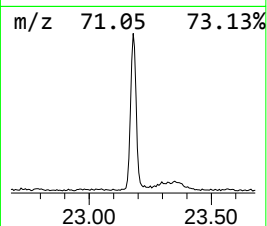
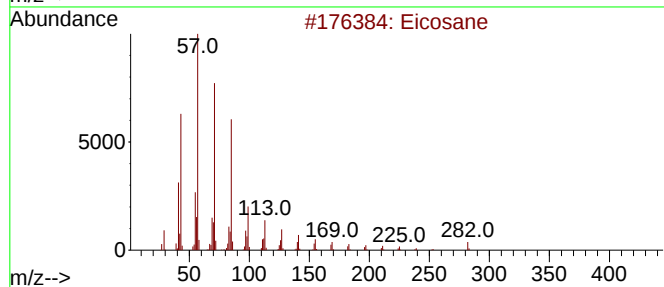
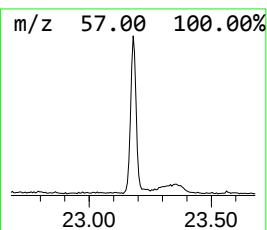
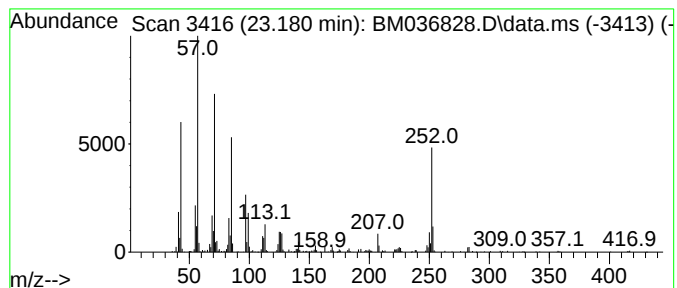
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM100322.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Eicosane Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 23.180 | 2.09 ng | 373038 | Perylene-d12     | 23.927 |

| Hit# | of                     | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|------------------------|---|--------------|-----|---------|-------------|------|
| 1    | Eicosane               |   |              | 282 | C20H42  | 000112-95-8 | 70   |
| 2    | Hexadecane             |   |              | 226 | C16H34  | 000544-76-3 | 55   |
| 3    | Heneicosane            |   |              | 296 | C21H44  | 000629-94-7 | 49   |
| 4    | Heptadecane, 8-methyl- |   |              | 254 | C18H38  | 013287-23-5 | 49   |
| 5    | Heptacosane            |   |              | 380 | C27H56  | 000593-49-7 | 49   |



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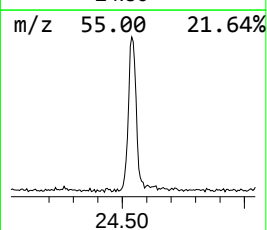
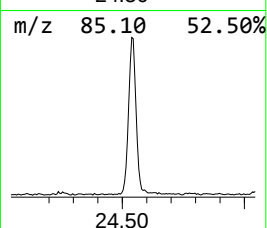
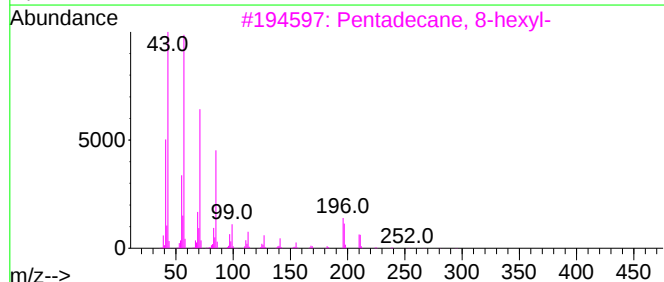
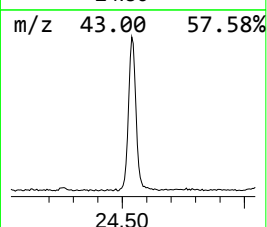
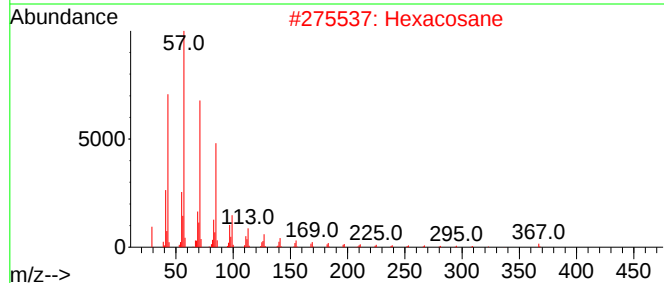
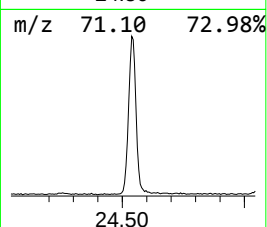
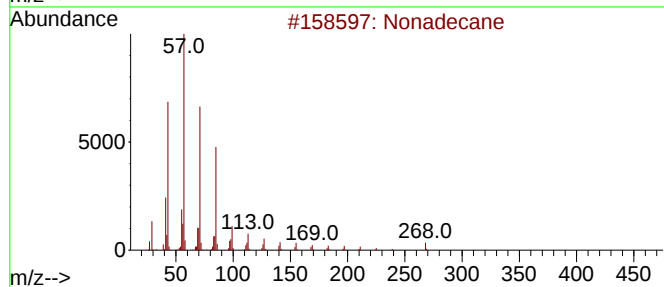
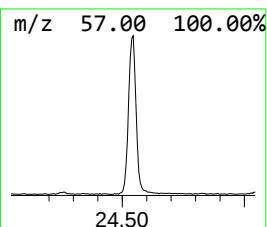
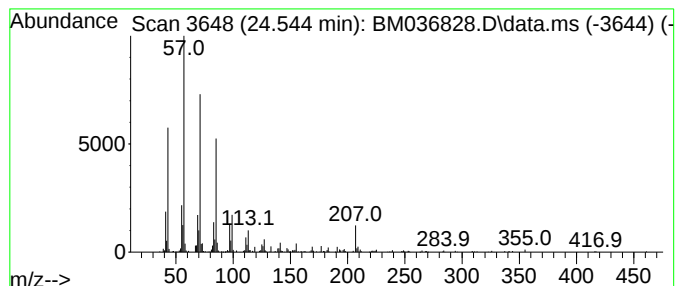
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM100322.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 4 Nonadecane Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 24.544 | 4.29 ng | 763786 | Perylene-d12     | 23.927 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Nonadecane            | 268 | C19H40  | 000629-92-5 | 94   |
| 2    |    |   | Hexacosane            | 366 | C26H54  | 000630-01-3 | 93   |
| 3    |    |   | Pentadecane, 8-hexyl- | 296 | C21H44  | 013475-75-7 | 91   |
| 4    |    |   | Eicosane, 10-methyl-  | 296 | C21H44  | 054833-23-7 | 91   |
| 5    |    |   | Tetracosane           | 338 | C24H50  | 000646-31-1 | 87   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM100422\  
Data File : BM036828.D  
Acq On : 04 Oct 2022 14:43  
Operator : CG/JU  
Sample : N4785-03  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
PT-BN-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM100322.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| 3-Penten-2-one,... | 4.446  | 9.6     | ng    | 1111860  | 1                     | 7.969  | 2315410 | 20.0 |
| 2-Pentanone, 4-... | 5.063  | 29.2    | ng    | 3385280  | 1                     | 7.969  | 2315410 | 20.0 |
| Eicosane           | 23.180 | 2.1     | ng    | 373038   | 6                     | 23.927 | 3561250 | 20.0 |
| Nonadecane         | 24.544 | 4.3     | ng    | 763786   | 6                     | 23.927 | 3561250 | 20.0 |