

Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP041221\  
 Data File : BP005266.D  
 Acq On : 12 Apr 2021 15:08  
 Operator : CG/JU  
 Sample : M1967-05  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_P  
 ClientSampleId :  
 SED-1C

Integration Parameters: rteint.p

Integrator: RTE

Smothing : 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\_P\Methods\8270E-BP040921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005266.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         | 5.275       | 367           | 372         | 384          | rVB      | 718744         | 1061894       | 84.05%          | 11.236%       |
| 2         | 6.863       | 635           | 642         | 652          | rBV      | 590606         | 924320        | 73.16%          | 9.780%        |
| 3         | 7.675       | 774           | 780         | 789          | rVB      | 121562         | 185892        | 14.71%          | 1.967%        |
| 4         | 8.840       | 971           | 978         | 992          | rVB      | 324109         | 525918        | 41.63%          | 5.565%        |
| 5         | 10.469      | 1248          | 1255        | 1261         | rBV      | 125610         | 209191        | 16.56%          | 2.213%        |
| 6         | 12.951      | 1670          | 1677        | 1687         | rBV      | 607478         | 820624        | 64.95%          | 8.683%        |
| 7         | 13.798      | 1815          | 1821        | 1829         | rBV2     | 17462          | 28294         | 2.24%           | 0.299%        |
| 8         | 14.339      | 1904          | 1913        | 1920         | rBV      | 189594         | 264138        | 20.91%          | 2.795%        |
| 9         | 15.839      | 2160          | 2168        | 2184         | rBV      | 542078         | 741415        | 58.68%          | 7.845%        |
| 10        | 17.104      | 2376          | 2383        | 2387         | rBV      | 234721         | 324394        | 25.68%          | 3.432%        |
| 11        | 17.145      | 2387          | 2390        | 2396         | rVV      | 51403          | 66645         | 5.27%           | 0.705%        |
| 12        | 17.239      | 2399          | 2406        | 2412         | rVB      | 37623          | 56353         | 4.46%           | 0.596%        |
| 13        | 17.886      | 2510          | 2516        | 2523         | rBV9     | 8470           | 15842         | 1.25%           | 0.168%        |
| 14        | 18.004      | 2532          | 2536        | 2545         | rBV3     | 46314          | 69356         | 5.49%           | 0.734%        |
| 15        | 18.169      | 2559          | 2564        | 2568         | rBV2     | 13337          | 20244         | 1.60%           | 0.214%        |
| 16        | 19.127      | 2720          | 2727        | 2733         | rBV      | 167432         | 212718        | 16.84%          | 2.251%        |
| 17        | 19.245      | 2741          | 2747        | 2749         | rBV4     | 18622          | 27479         | 2.17%           | 0.291%        |
| 18        | 19.274      | 2749          | 2752        | 2757         | rVB      | 15050          | 21166         | 1.68%           | 0.224%        |
| 19        | 19.480      | 2776          | 2787        | 2796         | rBV      | 125915         | 241186        | 19.09%          | 2.552%        |
| 20        | 19.680      | 2814          | 2821        | 2832         | rVB      | 1098598        | 1263422       | 100.00%         | 13.368%       |
| 21        | 19.963      | 2865          | 2869        | 2878         | rVB      | 29311          | 45919         | 3.63%           | 0.486%        |
| 22        | 20.063      | 2882          | 2886        | 2890         | rBV      | 32572          | 38886         | 3.08%           | 0.411%        |
| 23        | 20.886      | 3020          | 3026        | 3029         | rBV2     | 59634          | 108950        | 8.62%           | 1.153%        |
| 24        | 20.933      | 3029          | 3034        | 3039         | rVV2     | 131707         | 242853        | 19.22%          | 2.570%        |
| 25        | 20.986      | 3039          | 3043        | 3051         | rVV      | 283343         | 365457        | 28.93%          | 3.867%        |
| 26        | 21.051      | 3052          | 3054        | 3059         | rVB      | 15740          | 18879         | 1.49%           | 0.200%        |
| 27        | 21.204      | 3073          | 3080        | 3084         | rBV2     | 411215         | 620972        | 49.15%          | 6.571%        |
| 28        | 21.239      | 3084          | 3086        | 3093         | rVB      | 119052         | 129915        | 10.28%          | 1.375%        |
| 29        | 22.792      | 3344          | 3350        | 3354         | rBV      | 71213          | 163357        | 12.93%          | 1.728%        |
| 30        | 23.280      | 3429          | 3433        | 3441         | rVB2     | 43204          | 86857         | 6.87%           | 0.919%        |
| 31        | 23.374      | 3445          | 3449        | 3455         | rVB      | 73806          | 136228        | 10.78%          | 1.441%        |
| 32        | 23.480      | 3461          | 3467        | 3474         | rBV      | 225601         | 412063        | 32.61%          | 4.360%        |

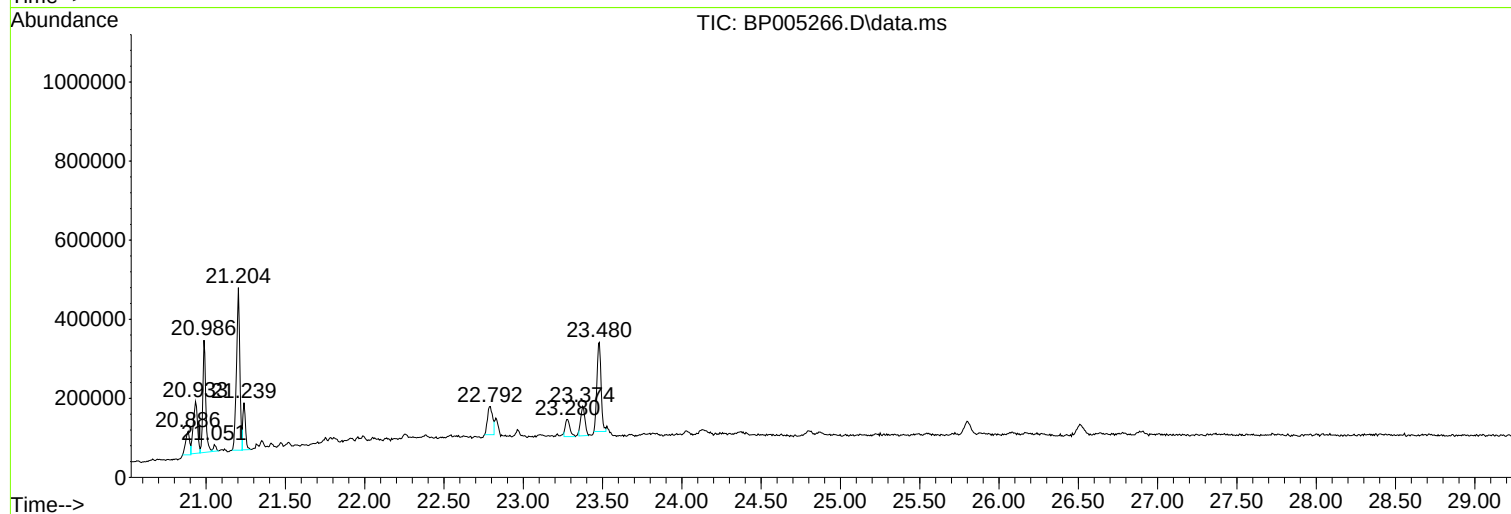
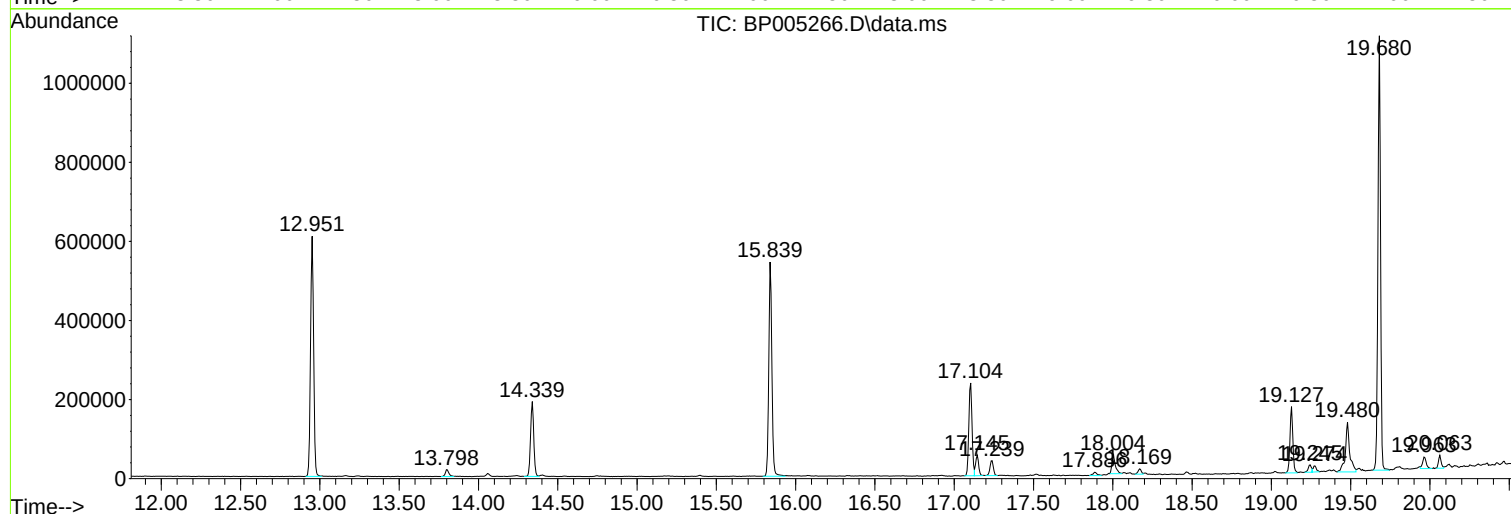
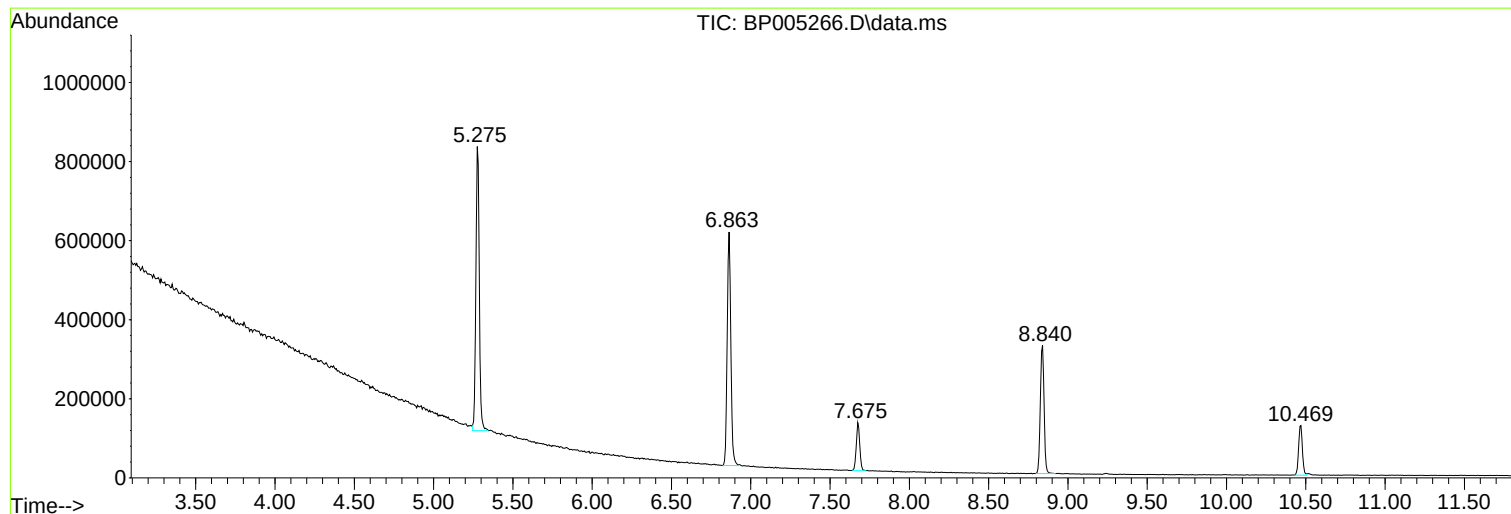
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Sample : M1967-05  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
SED-1C

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP040921.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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Acq On : 12 Apr 2021 15:08  
Operator : CG/JU  
Sample : M1967-05  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
SED-1C

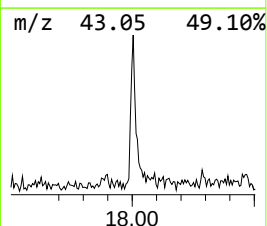
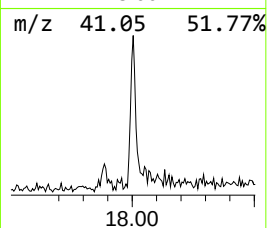
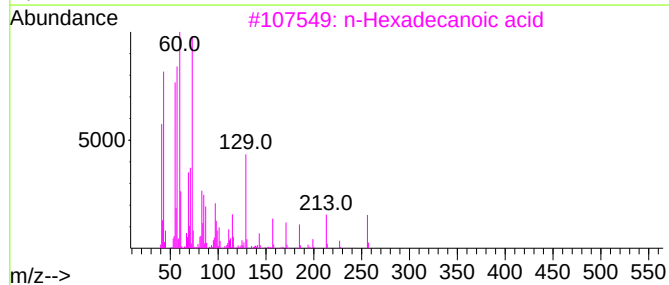
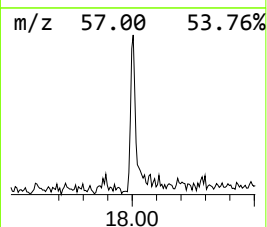
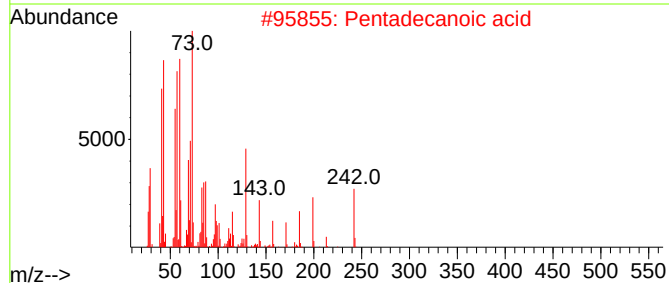
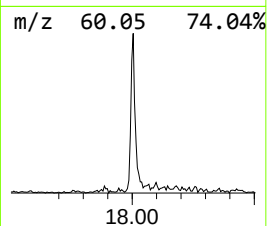
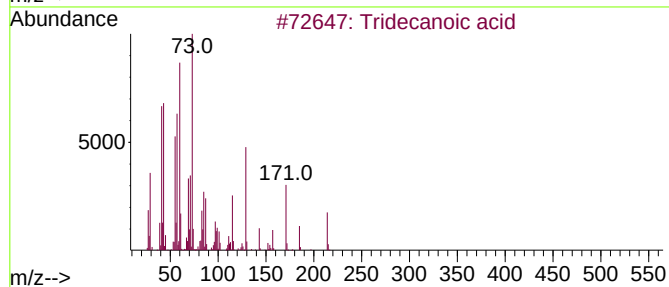
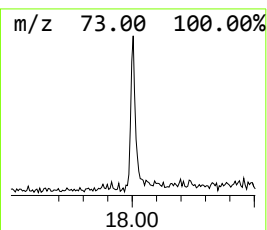
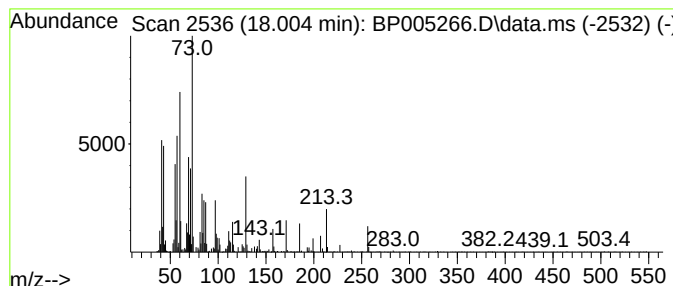
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP040921.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Tridecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 18.004 | 4.28 ng | 69356 | Phenanthrene-d10 | 17.104 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 87   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 72   |
| 3    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 64   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 64   |
| 5    |    |   | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 59   |



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Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
SED-1C

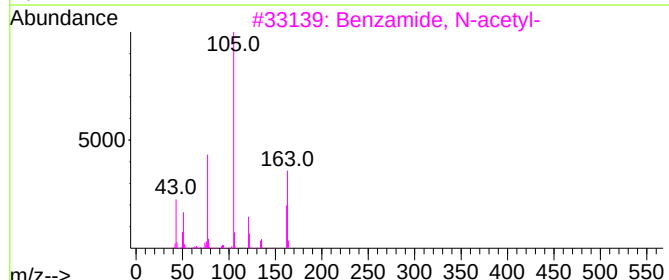
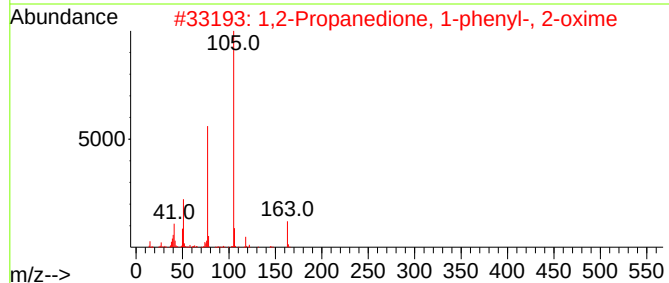
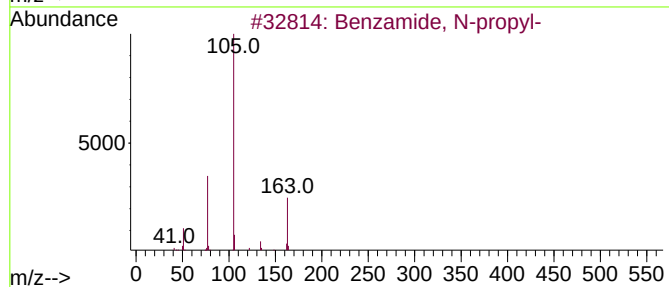
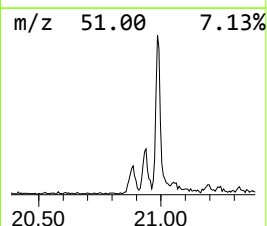
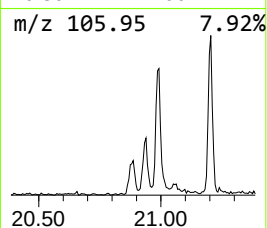
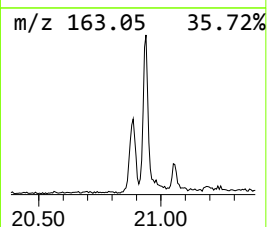
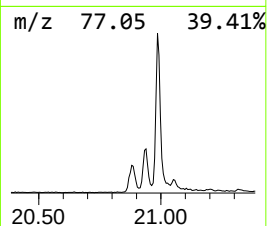
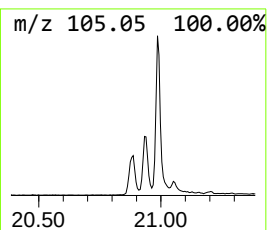
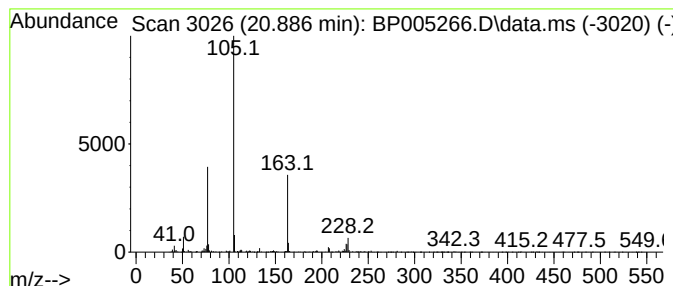
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Benzamide, N-propyl- Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 20.886 | 3.51 ng | 108950 | Chrysene-d12     | 21.204 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm      | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|--------------|-------------|------|
| 1    |    |   | Benzamide, N-propyl-                | 163 | C10H13NO     | 010546-70-0 | 64   |
| 2    |    |   | 1,2-Propanedione, 1-phenyl-, 2-o... | 163 | C9H9NO2      | 000119-51-7 | 64   |
| 3    |    |   | Benzamide, N-acetyl-                | 163 | C9H9NO2      | 001575-95-7 | 64   |
| 4    |    |   | Benzhydrazide, N2-benzoyl-2-brom... | 439 | C20H14BrN3O4 | 145933-17-1 | 47   |
| 5    |    |   | 2,6-Dimethylphenyl benzoate         | 226 | C15H14O2     | 001871-36-9 | 47   |



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Sample : M1967-05  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
SED-1C

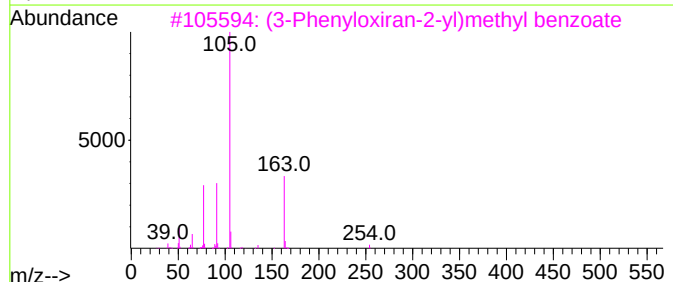
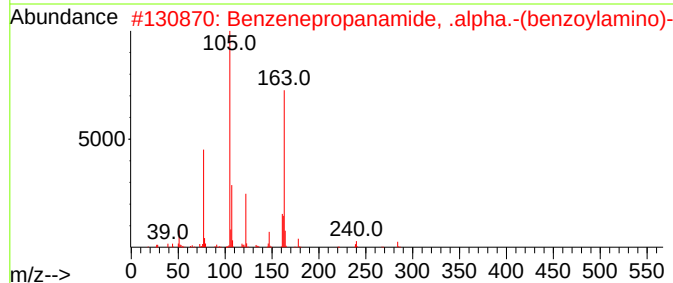
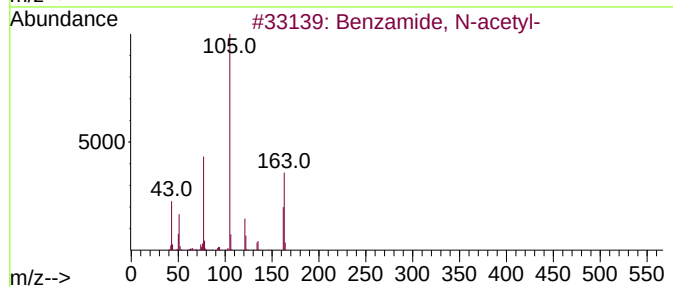
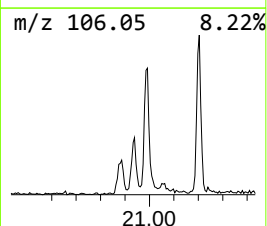
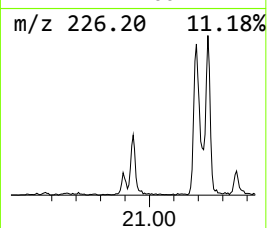
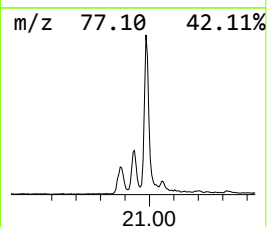
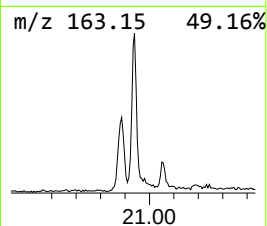
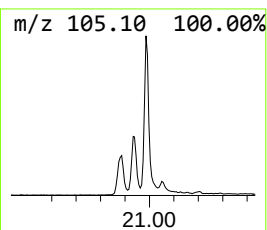
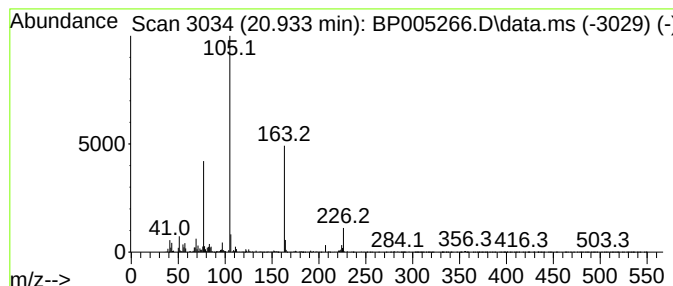
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP040921.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Benzamide, N-acetyl- Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 20.933 | 7.82 ng | 242853 | Chrysene-d12     | 21.204 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Benzamide, N-acetyl-                | 163 | C9H9NO2    | 001575-95-7  | 64   |
| 2    |    |   | Benzenepropanamide, .alpha.-(ben... | 284 | C16H16N2O3 | 058690-81-6  | 64   |
| 3    |    |   | (3-Phenyloxiran-2-yl)methyl benz... | 254 | C16H14O3   | 1000366-96-1 | 50   |
| 4    |    |   | N-(.alpha.-Methoxybenzyl)benzamide  | 241 | C15H15NO2  | 010387-93-6  | 43   |
| 5    |    |   | 2-Pyrrolidinone, 3-hydroxy-4-met... | 191 | C11H13NO2  | 104194-17-4  | 39   |



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ClientSampleId :  
SED-1C

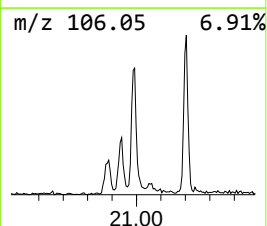
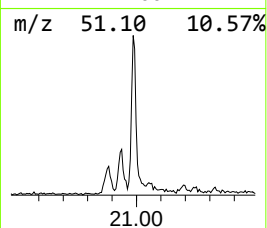
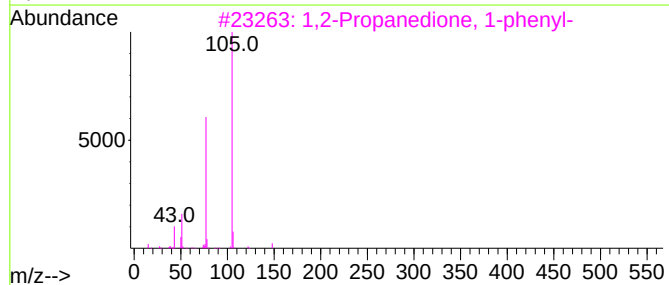
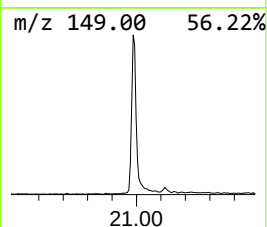
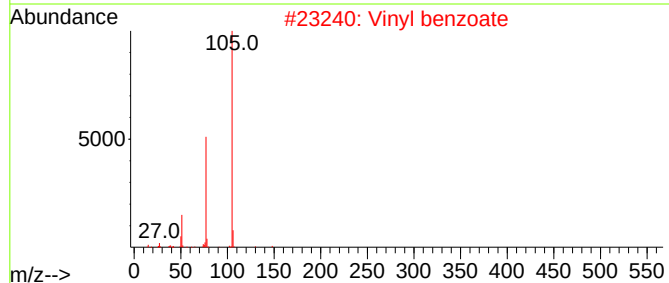
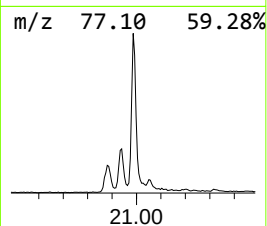
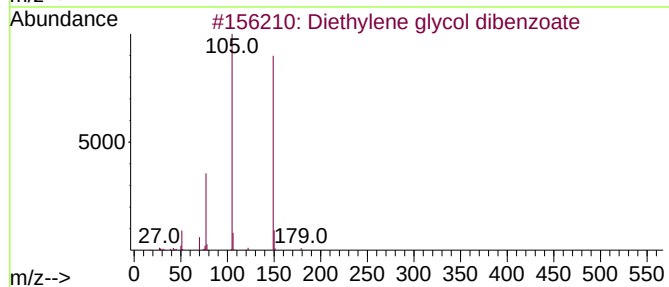
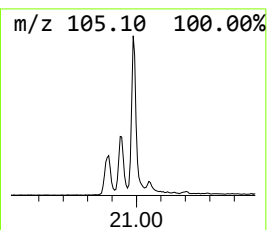
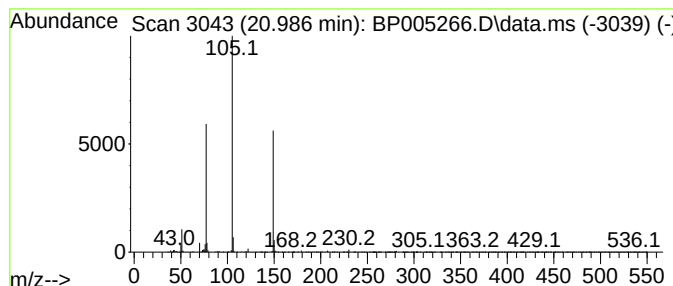
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 1

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 20.986 | 11.77 ng | 365457 | Chrysene-d12     | 21.204 |

| Hit# | of | 5 | Tentative ID                 | MW  | MolForm    | CAS#        | Qual |
|------|----|---|------------------------------|-----|------------|-------------|------|
| 1    |    |   | Diethylene glycol dibenzoate | 314 | C18H18O5   | 000120-55-8 | 53   |
| 2    |    |   | Vinyl benzoate               | 148 | C9H8O2     | 000769-78-8 | 47   |
| 3    |    |   | 1,2-Propanedione, 1-phenyl-  | 148 | C9H8O2     | 000579-07-7 | 47   |
| 4    |    |   | 4'-Nitrobenzanilide          | 242 | C13H10N2O3 | 003393-96-2 | 47   |
| 5    |    |   | Benzoyl isothiocyanate       | 163 | C8H5NOS    | 000532-55-8 | 47   |



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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Tridecanoic acid   | 18.004 | 4.3     | ng    | 69356    | 4                     | 17.104 | 324394 | 20.0 |
| Benzamide, N-pr... | 20.886 | 3.5     | ng    | 108950   | 5                     | 21.204 | 620972 | 20.0 |
| Benzamide, N-ac... | 20.933 | 7.8     | ng    | 242853   | 5                     | 21.204 | 620972 | 20.0 |
| Diethylene glyc... | 20.986 | 11.8    | ng    | 365457   | 5                     | 21.204 | 620972 | 20.0 |