

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF110422\  
 Data File : BF131003.D  
 Acq On : 04 Nov 2022 21:58  
 Operator : CG\JU  
 Sample : N5340-05  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 MW-9-102722

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\_F\Methods\8270-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131003.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         | 2.193       | 11            | 18          | 28           | rVB      | 1191377        | 1579860       | 65.27%          | 15.301%       |
| 2         | 5.122       | 513           | 516         | 521          | rBV      | 142503         | 143468        | 5.93%           | 1.389%        |
| 3         | 5.522       | 581           | 584         | 591          | rVB      | 94671          | 83110         | 3.43%           | 0.805%        |
| 4         | 6.528       | 751           | 755         | 761          | rBV      | 370622         | 318809        | 13.17%          | 3.088%        |
| 5         | 6.910       | 816           | 820         | 823          | rBV      | 469803         | 365544        | 15.10%          | 3.540%        |
| 6         | 7.475       | 907           | 916         | 919          | rBV      | 1293223        | 1315721       | 54.36%          | 12.743%       |
| 7         | 8.192       | 1035          | 1038        | 1042         | rBV      | 560907         | 500220        | 20.67%          | 4.845%        |
| 8         | 9.275       | 1217          | 1222        | 1225         | rBV      | 2846960        | 2420533       | 100.00%         | 23.443%       |
| 9         | 9.957       | 1334          | 1338        | 1341         | rBV      | 564523         | 464402        | 19.19%          | 4.498%        |
| 10        | 10.575      | 1440          | 1443        | 1446         | rBV      | 35855          | 27901         | 1.15%           | 0.270%        |
| 11        | 11.445      | 1588          | 1591        | 1595         | rVB      | 508521         | 463930        | 19.17%          | 4.493%        |
| 12        | 13.039      | 1858          | 1862        | 1865         | rBV      | 2026099        | 1751891       | 72.38%          | 16.967%       |
| 13        | 14.010      | 2019          | 2027        | 2034         | rBV      | 15381          | 53200         | 2.20%           | 0.515%        |
| 14        | 14.098      | 2038          | 2042        | 2048         | rVB      | 470871         | 398406        | 16.46%          | 3.859%        |
| 15        | 14.192      | 2053          | 2058        | 2061         | rBV      | 105324         | 103215        | 4.26%           | 1.000%        |
| 16        | 15.604      | 2293          | 2298        | 2305         | rBV      | 264722         | 335189        | 13.85%          | 3.246%        |

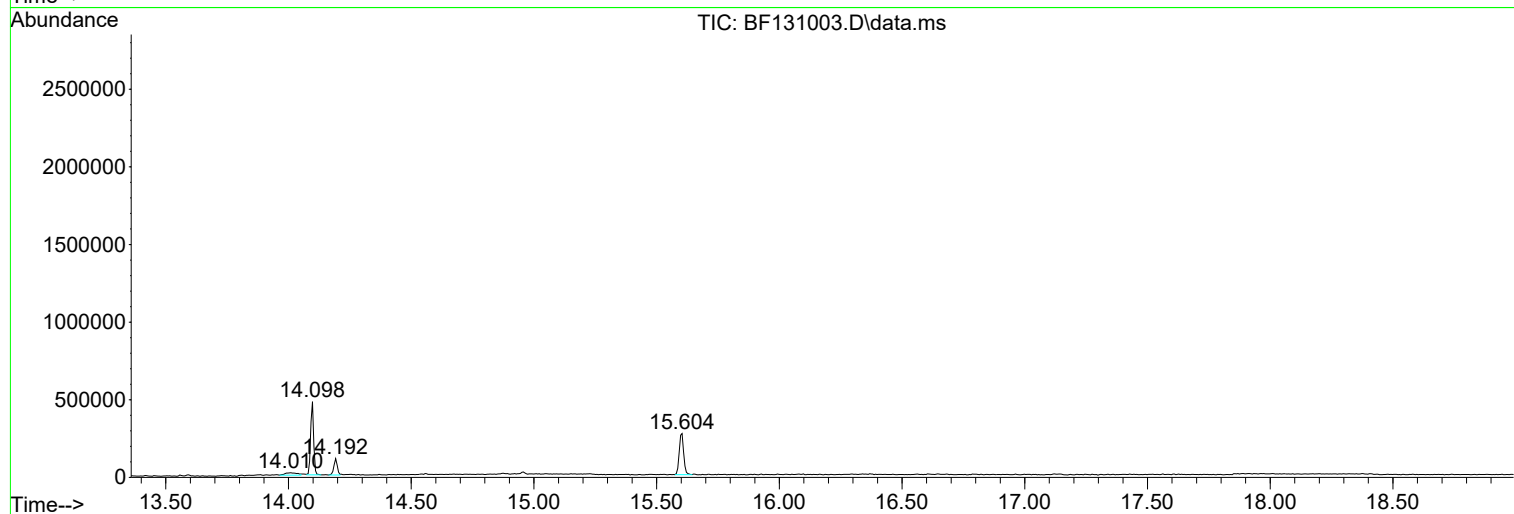
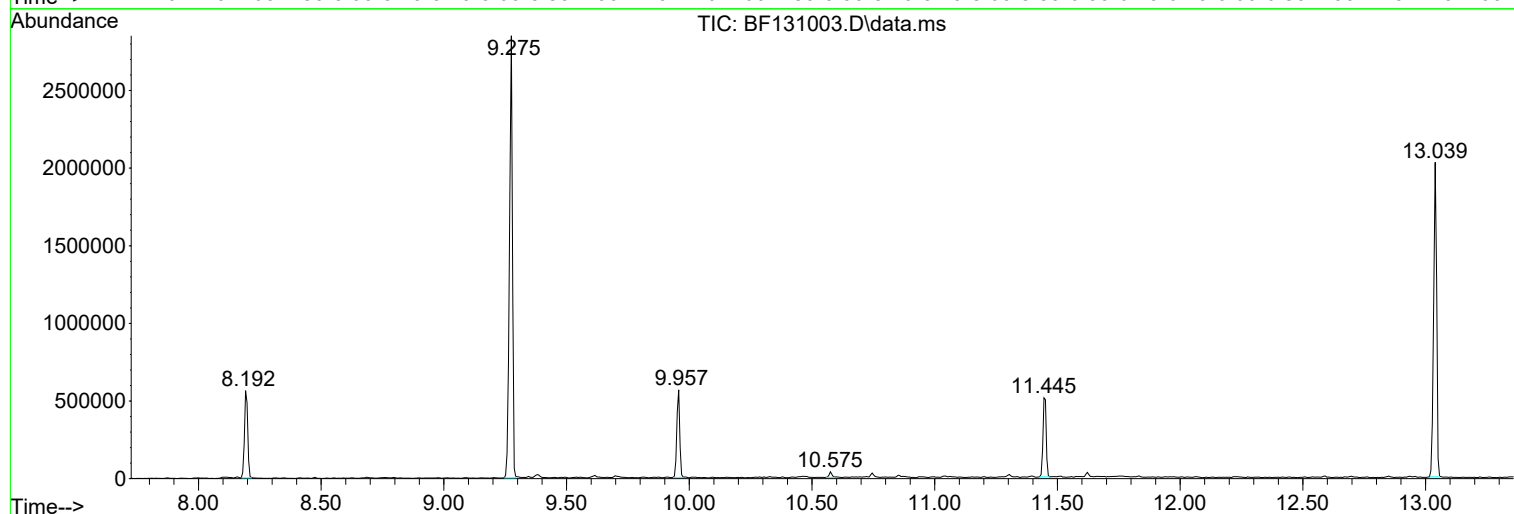
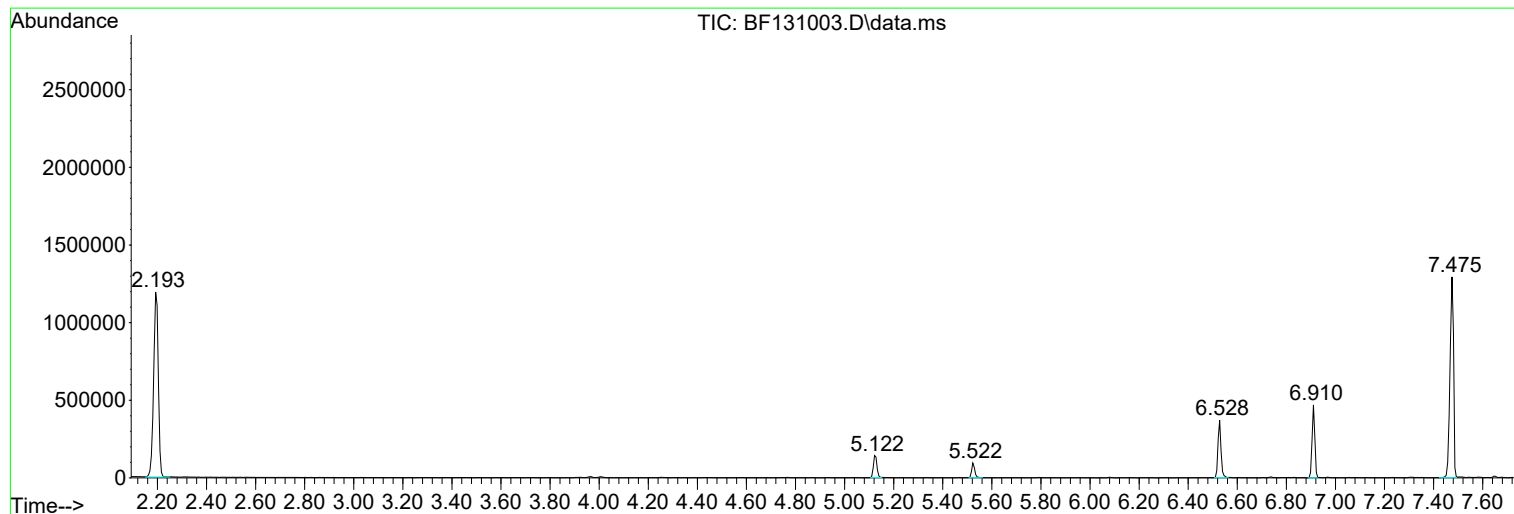
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ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF102722.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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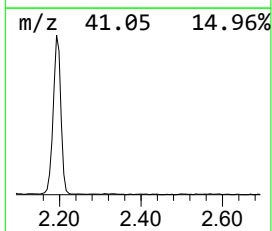
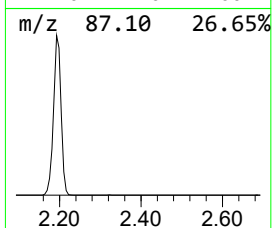
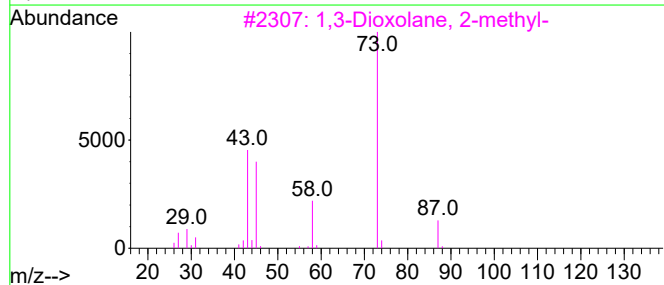
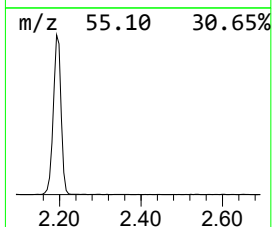
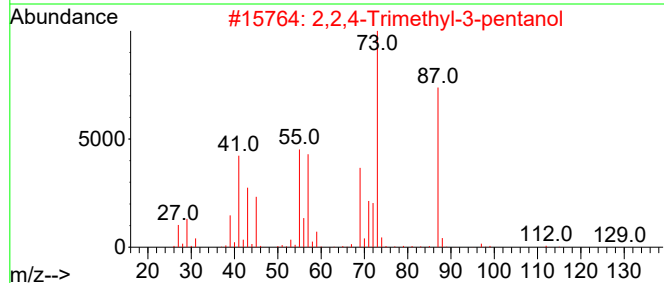
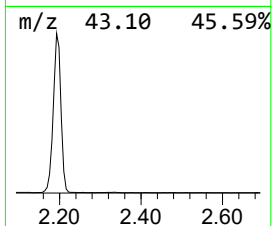
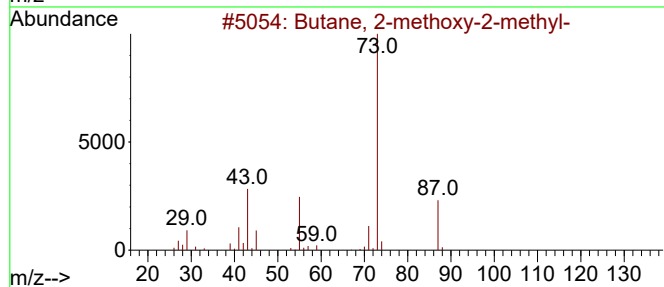
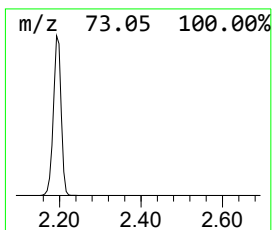
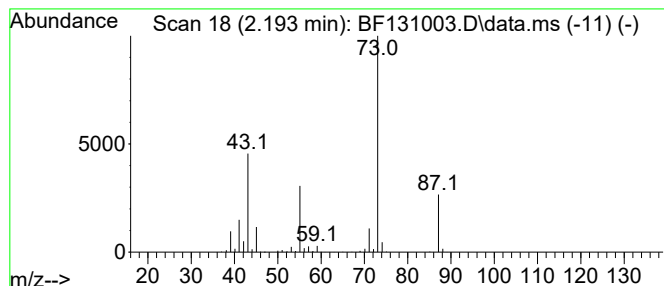
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF102722.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T.  | EstConc  | Area    | Relative to ISTD       | R.T.  |
|-------|----------|---------|------------------------|-------|
| 2.193 | 86.44 ng | 1579860 | 1,4-Dichlorobenzene-d4 | 6.910 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 83   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 39   |
| 3    |    |   | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 37   |
| 4    |    |   | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 12   |
| 5    |    |   | N-Ethylformamide            | 73  | C3H7NO  | 000627-45-2 | 9    |



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ClientSampleId :  
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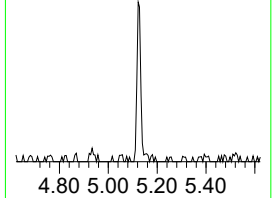
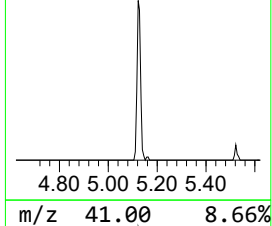
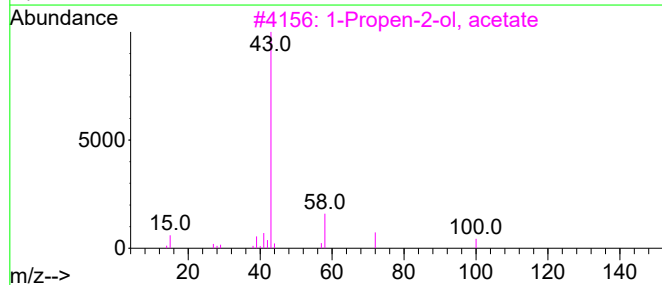
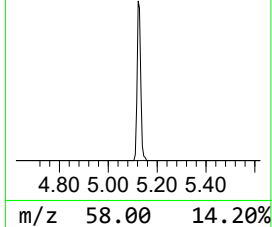
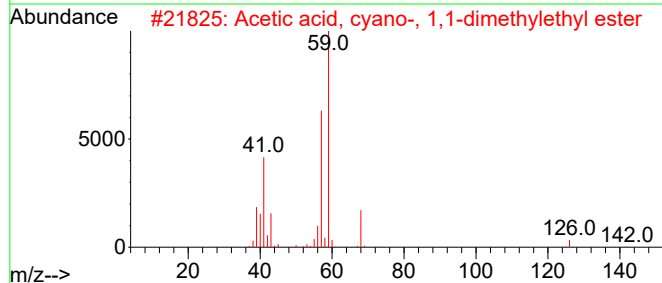
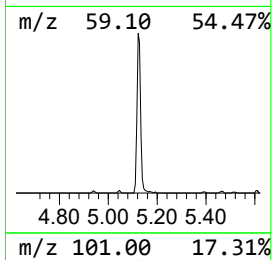
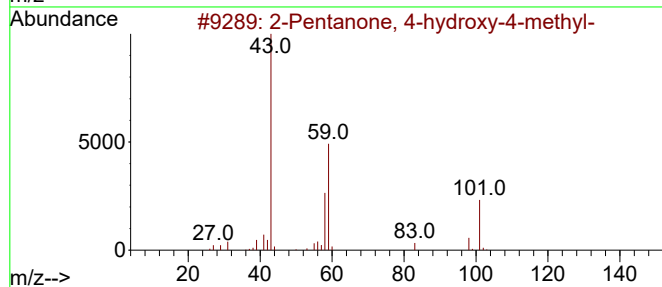
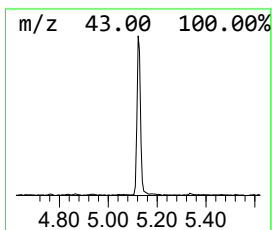
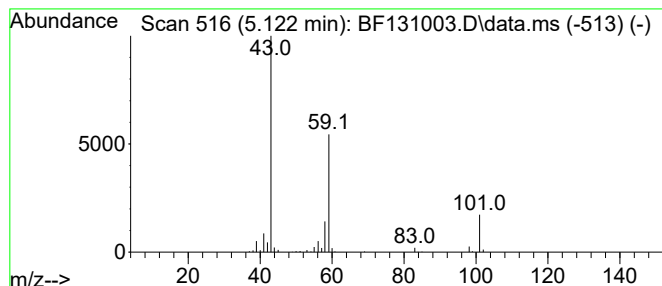
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.122 | 7.85 ng | 143468 | 1,4-Dichlorobenzene-d4 | 6.910 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 64   |
| 2    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 3    |    |   | 1-Propen-2-ol, acetate              | 100 | C5H8O2   | 000108-22-5 | 12   |
| 4    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 9    |
| 5    |    |   | Butane, 1-ethoxy-                   | 102 | C6H14O   | 000628-81-9 | 9    |



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Sample : N5340-05  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MW-9-102722

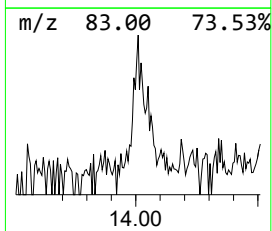
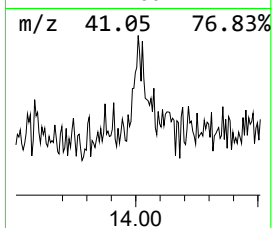
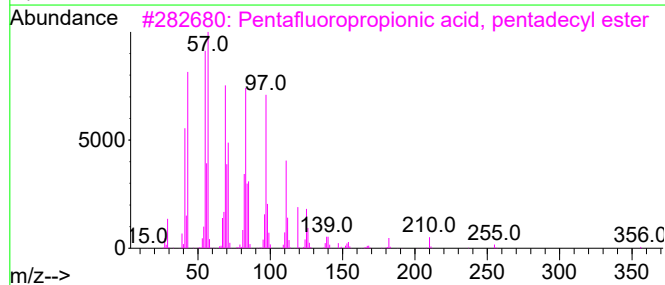
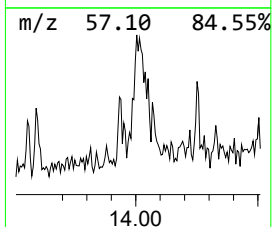
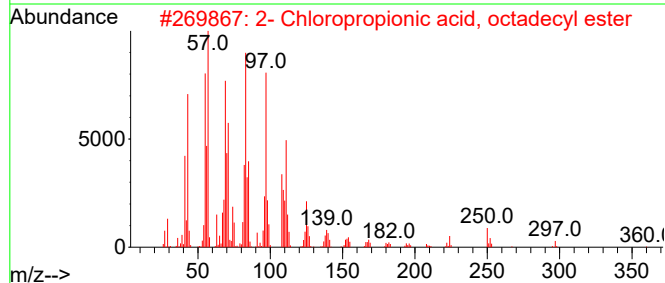
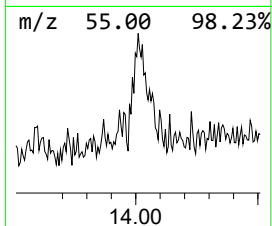
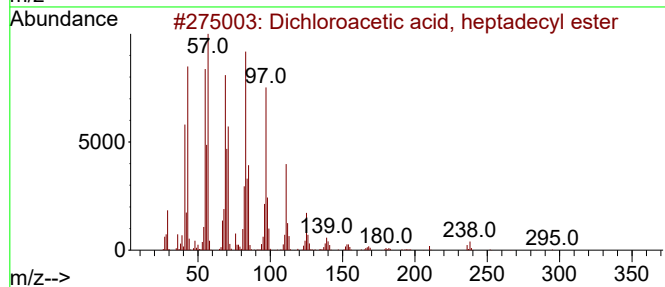
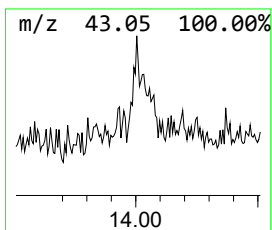
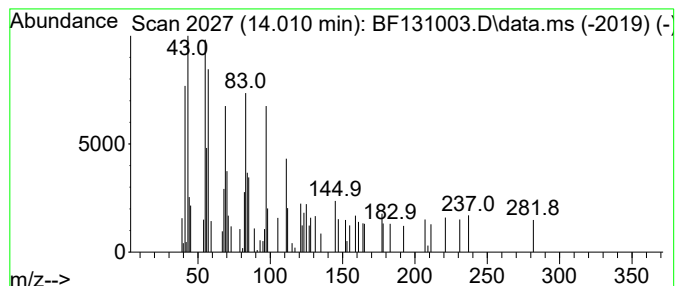
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF102722.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Dichloroacetic acid, heptad... Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 14.010 | 2.67 ng | 53200 | Chrysene-d12     | 14.098 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 76   |
| 2    |    |   | 2- Chloropropionic acid, octadec... | 360 | C21H41ClO2  | 088104-31-8  | 68   |
| 3    |    |   | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2  | 959092-08-1  | 68   |
| 4    |    |   | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2  | 959261-23-5  | 68   |
| 5    |    |   | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0  | 68   |



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ALS Vial : 11 Sample Multiplier: 1

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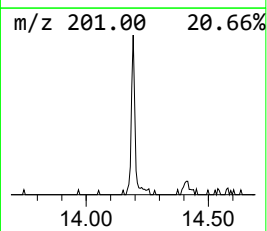
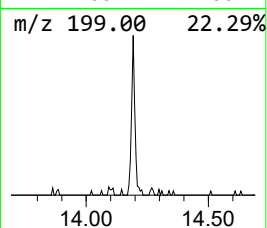
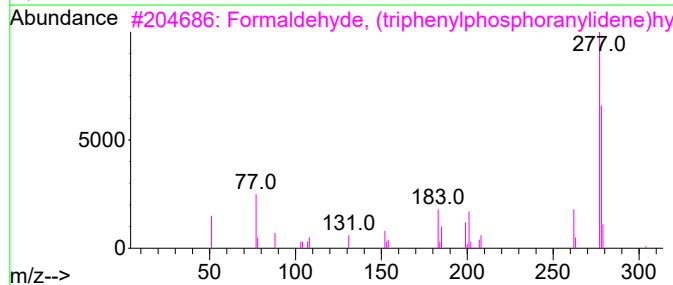
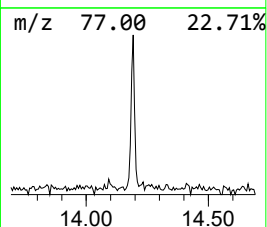
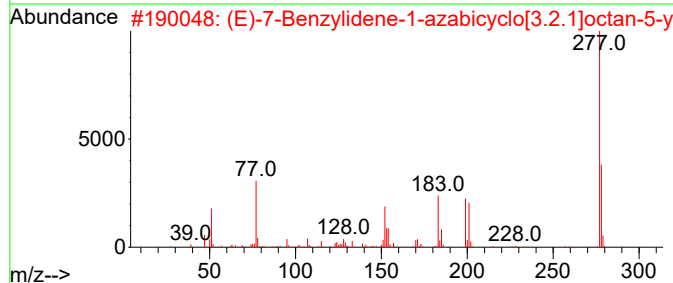
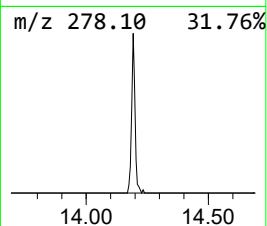
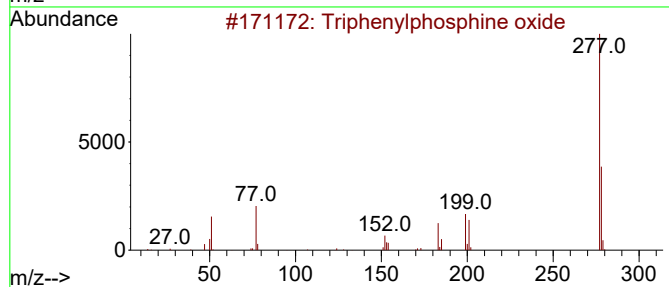
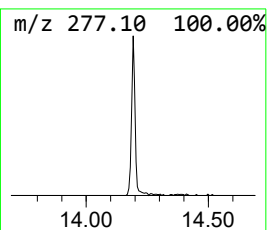
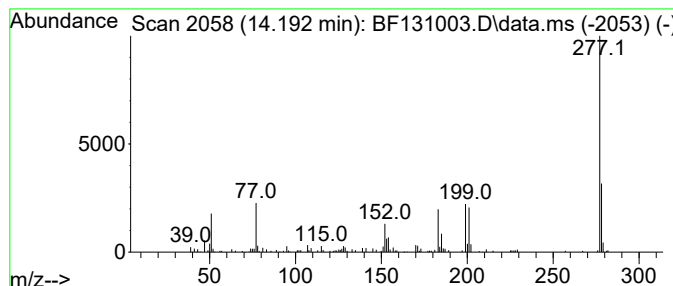
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TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Triphenylphosphine oxide Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.192 | 5.18 ng | 103215 | Chrysene-d12     | 14.098 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm    | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide             | 278 | C18H15OP   | 000791-28-6  | 96   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3...] | 293 | C15H19NO3S | 1000483-83-4 | 91   |
| 3    |    |   | Formaldehyde, (triphenylphosphor...] | 304 | C19H17N2P  | 015990-54-2  | 45   |
| 4    |    |   | Cobalt,(.eta.<5>-2,4-cyclopentad...  | 277 | C16H15BCo  | 036682-12-9  | 38   |
| 5    |    |   | 2-Phenyl-6-(trifluoromethyl)-1H-...  | 277 | C15H10F3NO | 1000387-59-3 | 23   |



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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Butane, 2-metho... | 2.193  | 86.4    | ng    | 1579860  | 1                     | 6.910  | 365544 | 20.0 |
| 2-Pentanone, 4-... | 5.122  | 7.8     | ng    | 143468   | 1                     | 6.910  | 365544 | 20.0 |
| Dichloroacetic ... | 14.010 | 2.7     | ng    | 53200    | 5                     | 14.098 | 398406 | 20.0 |
| Triphenylphosph... | 14.192 | 5.2     | ng    | 103215   | 5                     | 14.098 | 398406 | 20.0 |