

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG030521\  
 Data File : BG048353.D  
 Acq On : 6 Mar 2021 1:11  
 Operator : CG/JU  
 Sample : M1556-01 2X  
 Misc :  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 TR-04-030321

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\_G\METHODS\8270-BG021021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048353.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         | 5.841       | 419           | 426         | 441          | rBV      | 260919         | 532530        | 54.88%          | 5.653%        |
| 2         | 7.568       | 712           | 720         | 735          | rBV      | 259552         | 620355        | 63.93%          | 6.586%        |
| 3         | 8.079       | 800           | 807         | 815          | rVB      | 186314         | 323174        | 33.31%          | 3.431%        |
| 4         | 9.266       | 1000          | 1009        | 1017         | rBV      | 201810         | 384302        | 39.61%          | 4.080%        |
| 5         | 10.899      | 1279          | 1287        | 1297         | rBV      | 241689         | 443792        | 45.74%          | 4.711%        |
| 6         | 12.503      | 1555          | 1560        | 1564         | rBV6     | 5058           | 11854         | 1.22%           | 0.126%        |
| 7         | 12.550      | 1564          | 1568        | 1577         | rVB5     | 10744          | 18630         | 1.92%           | 0.198%        |
| 8         | 13.338      | 1695          | 1702        | 1709         | rBV      | 499885         | 773159        | 79.68%          | 8.208%        |
| 9         | 13.502      | 1726          | 1730        | 1735         | rBV7     | 9144           | 13896         | 1.43%           | 0.148%        |
| 10        | 13.637      | 1746          | 1753        | 1762         | rBV      | 88557          | 168446        | 17.36%          | 1.788%        |
| 11        | 14.166      | 1839          | 1843        | 1848         | rVB      | 21891          | 33984         | 3.50%           | 0.361%        |
| 12        | 14.712      | 1928          | 1936        | 1943         | rBV2     | 346140         | 580932        | 59.87%          | 6.167%        |
| 13        | 14.777      | 1943          | 1947        | 1953         | rVB2     | 26382          | 44560         | 4.59%           | 0.473%        |
| 14        | 15.112      | 2000          | 2004        | 2012         | rVB3     | 16299          | 31006         | 3.20%           | 0.329%        |
| 15        | 15.517      | 2071          | 2073        | 2077         | rVB5     | 7776           | 10099         | 1.04%           | 0.107%        |
| 16        | 15.764      | 2111          | 2115        | 2120         | rVB2     | 31971          | 45466         | 4.69%           | 0.483%        |
| 17        | 15.829      | 2123          | 2126        | 2133         | rBV4     | 20285          | 33624         | 3.47%           | 0.357%        |
| 18        | 15.923      | 2140          | 2142        | 2147         | rVB6     | 8096           | 10028         | 1.03%           | 0.106%        |
| 19        | 16.052      | 2161          | 2164        | 2167         | rBV5     | 8617           | 13422         | 1.38%           | 0.142%        |
| 20        | 16.205      | 2184          | 2190        | 2192         | rBV6     | 10157          | 17894         | 1.84%           | 0.190%        |
| 21        | 16.252      | 2192          | 2198        | 2210         | rVV      | 272098         | 451383        | 46.52%          | 4.792%        |
| 22        | 17.027      | 2327          | 2330        | 2332         | rBV4     | 8735           | 11219         | 1.16%           | 0.119%        |
| 23        | 17.116      | 2343          | 2345        | 2351         | rVB7     | 7471           | 10515         | 1.08%           | 0.112%        |
| 24        | 17.468      | 2398          | 2405        | 2408         | rBV      | 403775         | 641834        | 66.15%          | 6.814%        |
| 25        | 17.509      | 2408          | 2412        | 2417         | rVB      | 215672         | 327270        | 33.73%          | 3.474%        |
| 26        | 17.597      | 2423          | 2427        | 2431         | rVB      | 65338          | 86708         | 8.94%           | 0.920%        |
| 27        | 18.091      | 2509          | 2511        | 2515         | rVB4     | 22499          | 29585         | 3.05%           | 0.314%        |
| 28        | 18.338      | 2550          | 2553        | 2557         | rVB2     | 25371          | 28904         | 2.98%           | 0.307%        |
| 29        | 18.385      | 2558          | 2561        | 2567         | rVV      | 40161          | 48550         | 5.00%           | 0.515%        |
| 30        | 18.532      | 2581          | 2586        | 2591         | rBV2     | 62903          | 119867        | 12.35%          | 1.272%        |
| 31        | 19.072      | 2676          | 2678        | 2683         | rVB2     | 33888          | 42360         | 4.37%           | 0.450%        |
| 32        | 19.231      | 2701          | 2705        | 2707         | rBV      | 137132         | 175857        | 18.12%          | 1.867%        |
| 33        | 19.260      | 2708          | 2710        | 2721         | rVB5     | 102087         | 145520        | 15.00%          | 1.545%        |
| 34        | 19.513      | 2748          | 2753        | 2759         | rVB      | 493225         | 673411        | 69.40%          | 7.149%        |
| 35        | 19.836      | 2805          | 2808        | 2810         | rBV2     | 73294          | 100076        | 10.31%          | 1.062%        |
| 36        | 19.871      | 2810          | 2814        | 2820         | rVB      | 379762         | 543672        | 56.03%          | 5.772%        |

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Misc :  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TR-04-030321

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\_G\METHODS\8270-BG021021.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |        |        |         |         |
|----|--------|------|------|------|------|--------|--------|---------|---------|
| 37 | 20.059 | 2841 | 2846 | 2851 | rVB  | 757533 | 970296 | 100.00% | 10.300% |
| 38 | 21.740 | 3125 | 3132 | 3136 | rBV3 | 418746 | 901756 | 92.94%  | 9.573%  |

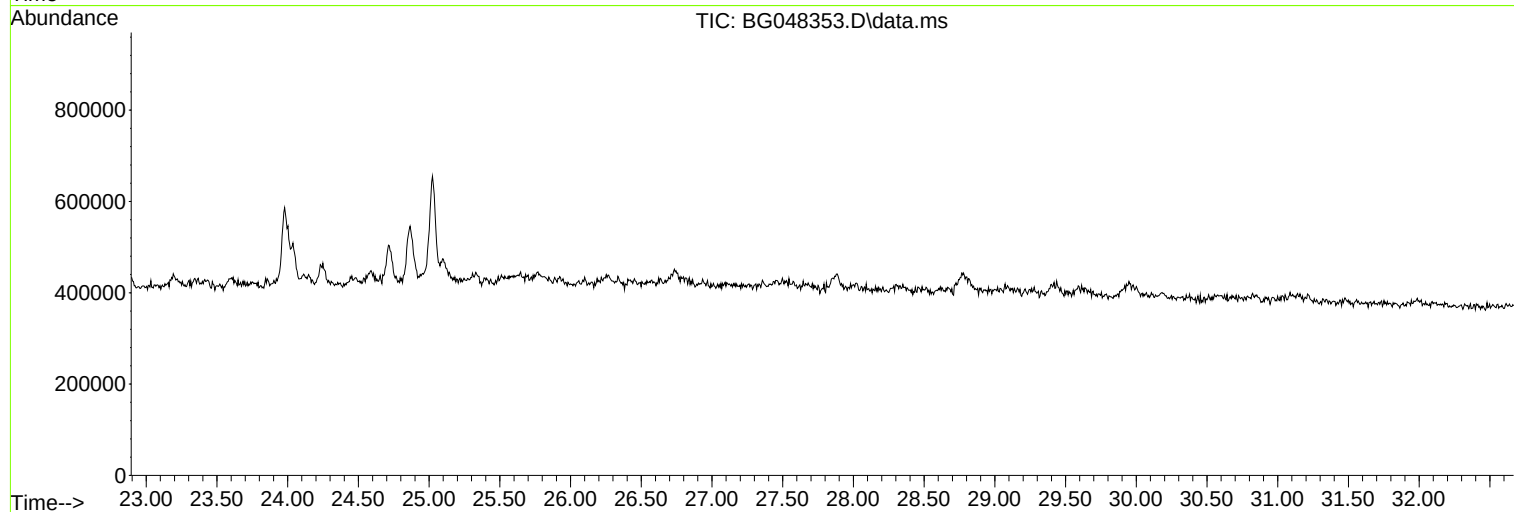
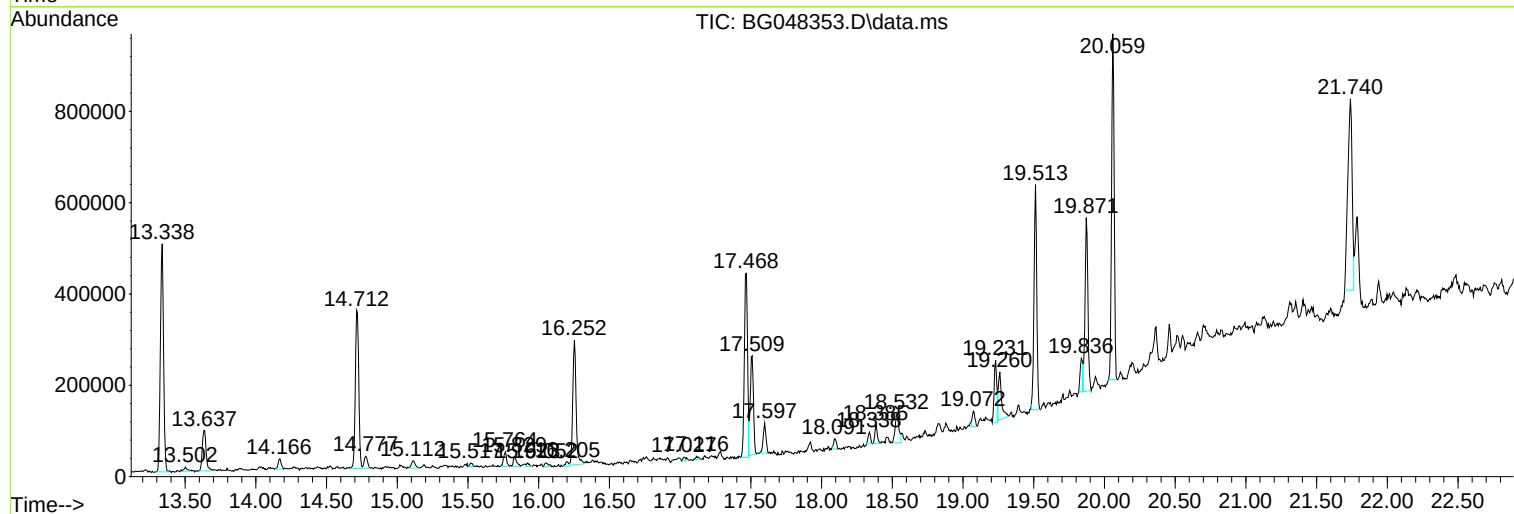
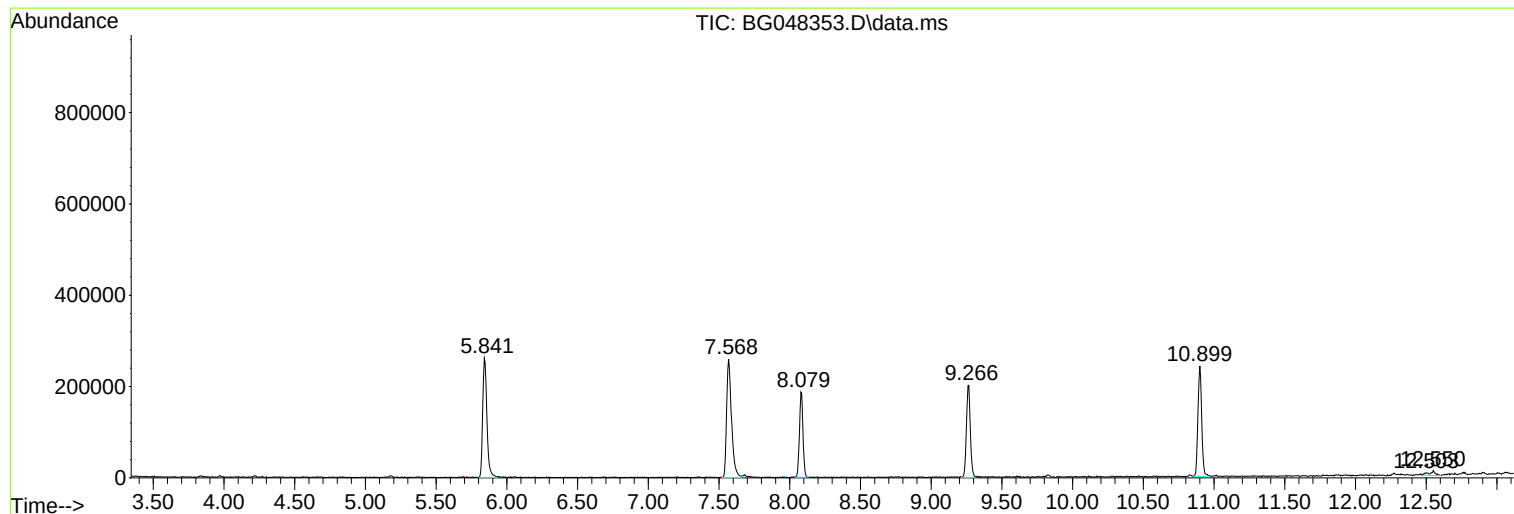
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG021021.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :  
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG021021.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

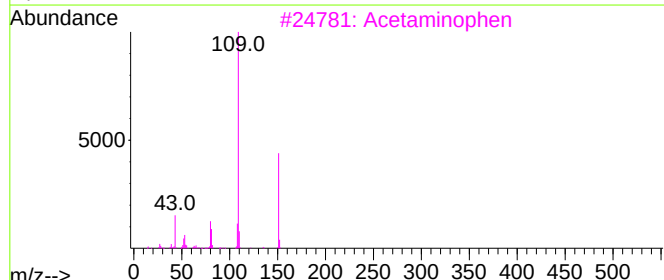
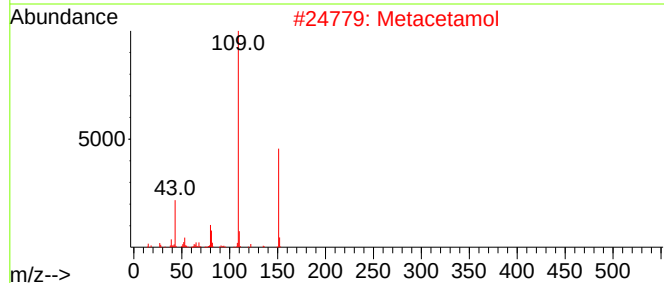
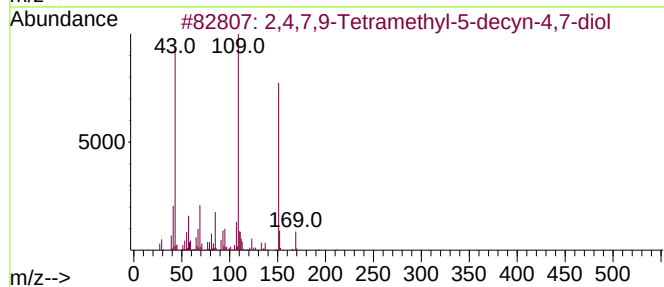
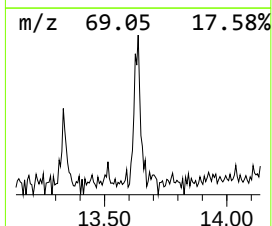
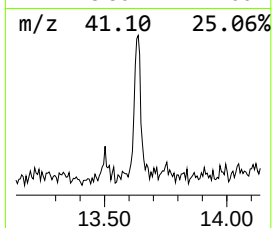
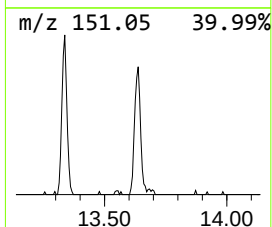
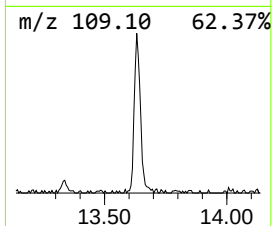
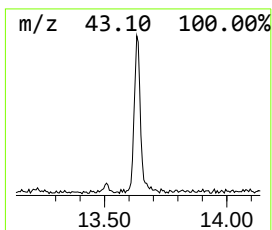
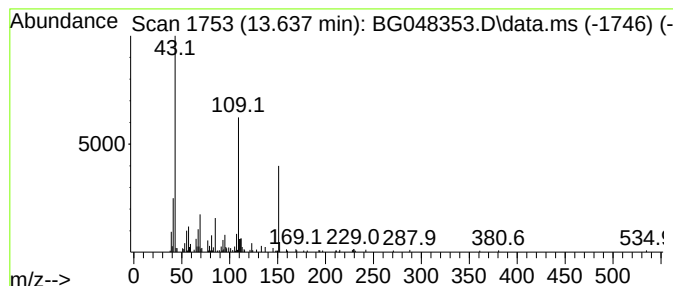
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.637 | 5.80 ng | 168446 | Acenaphthene-d10 | 14.713 |

| Hit# | of                                  | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | 2,4,7,9-Tetramethyl-5-decyn-4,7-... | 226 | C14H26O2     | 000126-86-3  | 83      |      |      |
| 2    | Metacetamol                         | 151 | C8H9NO2      | 000621-42-1  | 59      |      |      |
| 3    | Acetaminophen                       | 151 | C8H9NO2      | 000103-90-2  | 59      |      |      |
| 4    | Butanamide, N-acetyl-N-(4-hydrox... | 221 | C12H15NO3    | 1000107-08-7 | 45      |      |      |
| 5    | Ethanone, 1-(4,5-diethyl-2-methy... | 180 | C12H20O      | 062338-24-3  | 38      |      |      |



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ALS Vial : 16 Sample Multiplier: 1

Instrument :  
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TR-04-030321

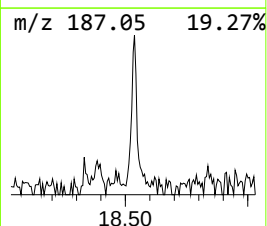
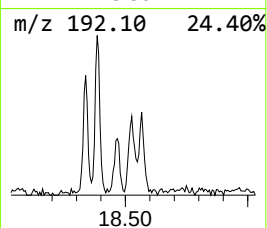
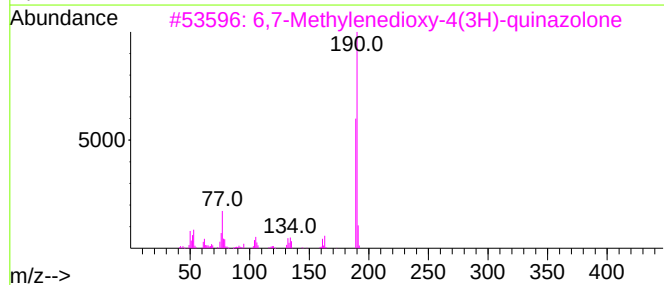
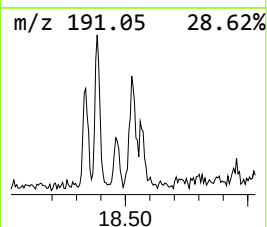
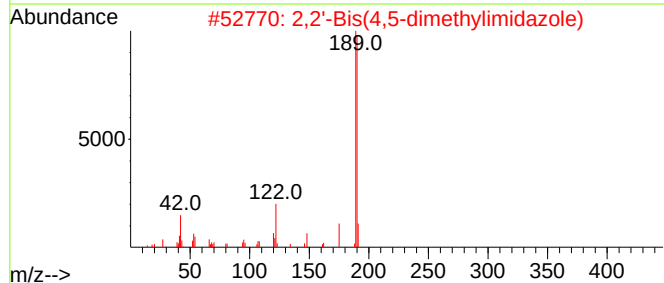
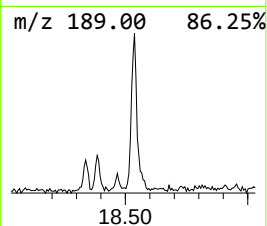
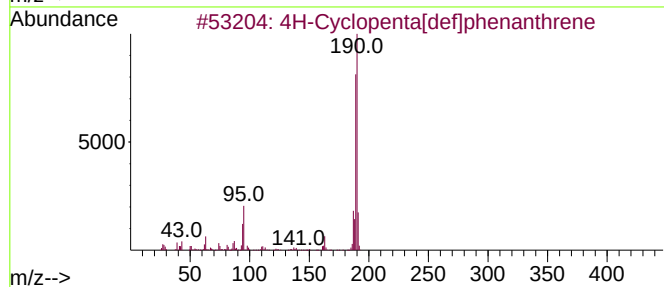
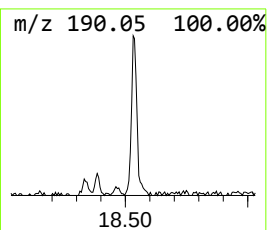
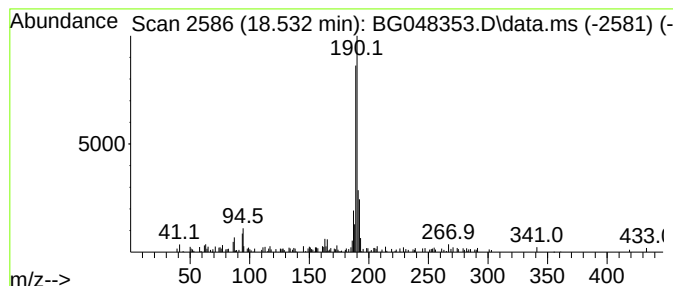
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG021021.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.532 | 3.74 ng | 119867 | Phenanthrene-d10 | 17.468 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 4H-Cyclopenta[def]phenanthrene      | 190 | C15H10   | 000203-64-5 | 76   |
| 2    |    |   | 2,2'-Bis(4,5-dimethylimidazole)     | 190 | C10H14N4 | 069286-06-2 | 50   |
| 3    |    |   | 6,7-Methylenedioxy-4(3H)-quinazo... | 190 | C9H6N2O3 | 028310-11-4 | 50   |
| 4    |    |   | 4-(4-Methyl-piperidin-1-yl)-phen... | 190 | C12H18N2 | 342013-25-6 | 40   |
| 5    |    |   | 1,1'-Biphenyl, 4,4'-difluoro-       | 190 | C12H8F2  | 000398-23-2 | 35   |



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ALS Vial : 16 Sample Multiplier: 1

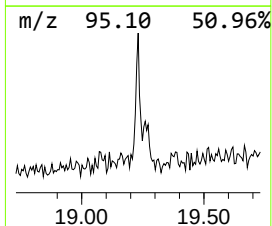
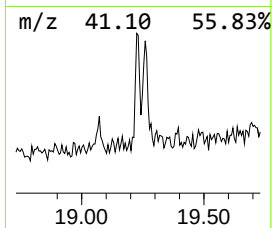
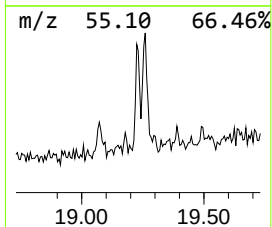
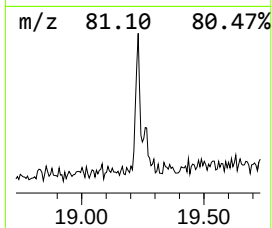
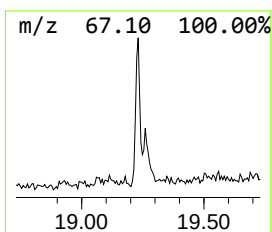
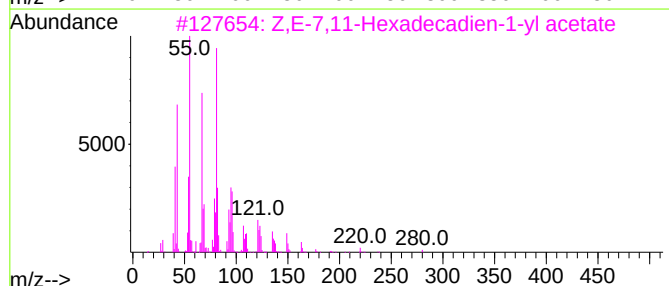
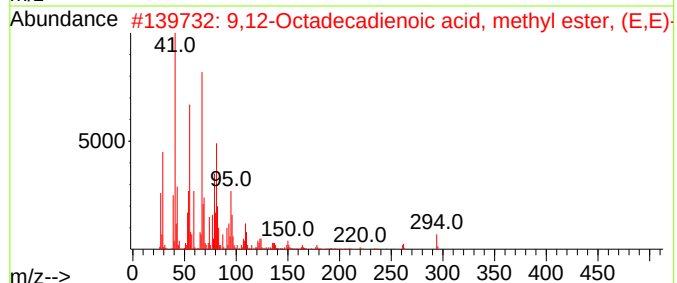
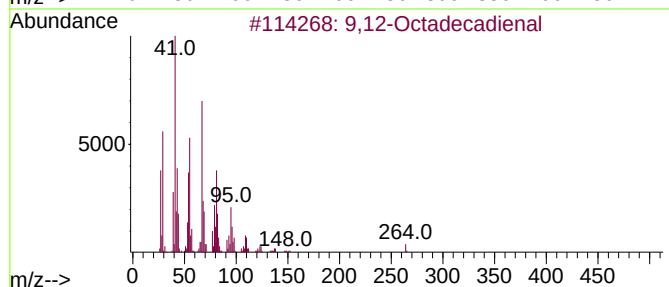
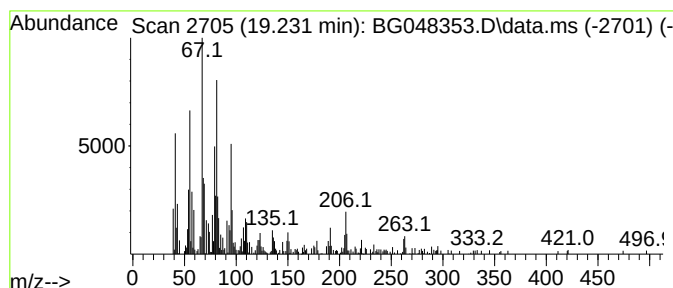
Instrument :  
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG021021.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 9,12-Octadecadienal Concentration Rank 2

| R.T.      | EstConc                                 | Area   | Relative to ISTD | R.T.        |      |
|-----------|-----------------------------------------|--------|------------------|-------------|------|
| 19.231    | 5.48 ng                                 | 175857 | Phenanthrene-d10 | 17.468      |      |
| Hit# of 5 | Tentative ID                            | MW     | MolForm          | CAS#        | Qual |
| 1         | 9,12-Octadecadienal                     | 264    | C18H32O          | 026537-70-2 | 64   |
| 2         | 9,12-Octadecadienoic acid, methyl ester | 294    | C19H34O2         | 002566-97-4 | 55   |
| 3         | Z,E-7,11-Hexadecadien-1-yl acetate      | 280    | C18H32O2         | 051607-94-4 | 55   |
| 4         | 1,E-8,Z-10-Tridecatriene                | 178    | C13H22           | 080625-30-5 | 53   |
| 5         | 4,5-Nonadiene, 2-methyl-                | 138    | C10H18           | 055956-32-6 | 49   |



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Misc :  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TR-04-030321

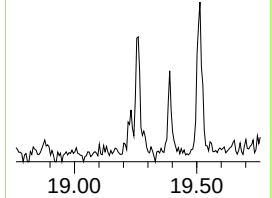
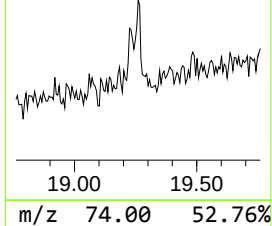
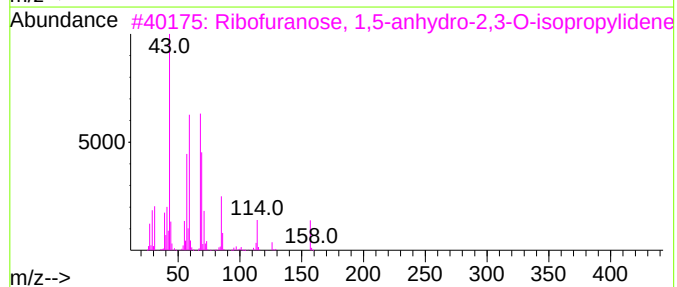
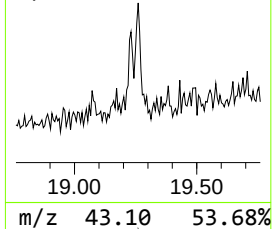
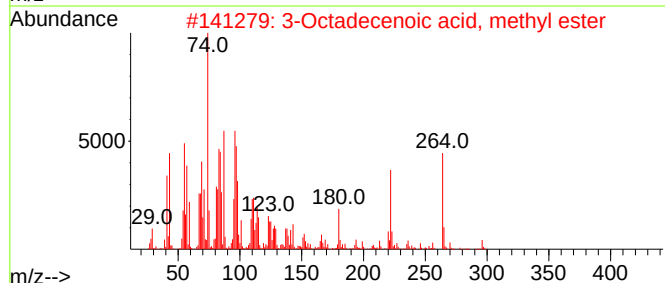
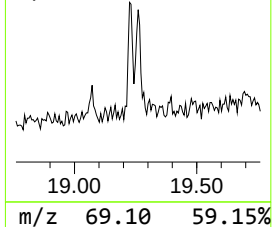
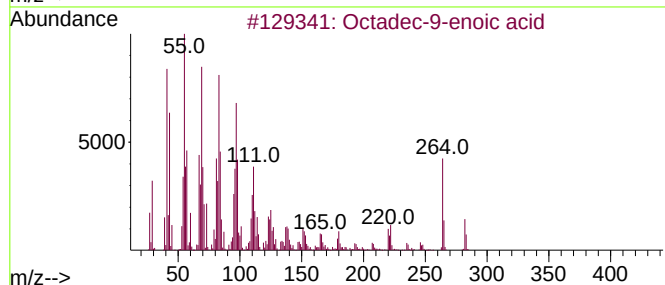
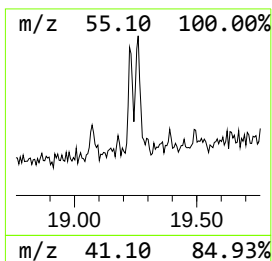
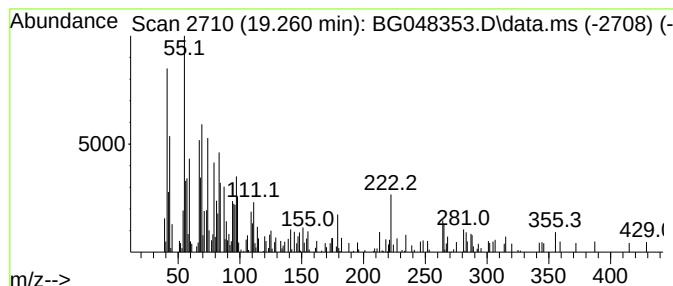
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG021021.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 unknown19.260 Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.260 | 4.53 ng | 145520 | Phenanthrene-d10 | 17.468 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Octadec-9-enoic acid                | 282 | C18H34O2 | 1000190-13-7 | 30   |
| 2    |    |   | 3-Octadecenoic acid, methyl ester   | 296 | C19H36O2 | 056599-33-8  | 22   |
| 3    |    |   | Ribofuranose, 1,5-anhydro-2,3-O-... | 172 | C8H12O4  | 004625-13-2  | 22   |
| 4    |    |   | 10-Octadecenoic acid, methyl ester  | 296 | C19H36O2 | 013481-95-3  | 20   |
| 5    |    |   | 11-Octadecenoic acid, methyl est... | 296 | C19H36O2 | 001937-63-9  | 18   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG030521\  
Data File : BG048353.D  
Acq On : 6 Mar 2021 1:11  
Operator : CG/JU  
Sample : M1556-01 2X  
Misc :  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TR-04-030321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG021021.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2,4,7,9-Tetrame... | 13.637 | 5.8     | ng    | 168446   | 3                     | 14.713 | 580932 | 20.0 |
| 4H-Cyclopenta[d... | 18.532 | 3.7     | ng    | 119867   | 4                     | 17.468 | 641834 | 20.0 |
| 9,12-Octadecadi... | 19.231 | 5.5     | ng    | 175857   | 4                     | 17.468 | 641834 | 20.0 |
| unknown19.260      | 19.260 | 4.5     | ng    | 145520   | 4                     | 17.468 | 641834 | 20.0 |