

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG032219\
 Data File : BG040084.D
 Acq On : 22 Mar 2019 15:34
 Operator : JU/SJ
 Sample : K2040-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 S4B(12-20)

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-BG030419.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|--------|----------|------------|----------|-----------|-------|-------------|------------|--------------|------------|
| 1 | 3.188 | 12 | 17 | 27 | rBV2 | 81816 | 240148 | 8.48% | 1.273% |
| 2 | 3.270 | 27 | 31 | 42 | rVV | 158293 | 304084 | 10.73% | 1.612% |
| 3 | 3.370 | 42 | 48 | 54 | rVB | 136984 | 251404 | 8.87% | 1.333% |
| 4 | 5.691 | 436 | 443 | 459 | rBV | 928163 | 1543384 | 54.47% | 8.182% |
| 5 | 7.294 | 708 | 716 | 729 | rBV | 941943 | 1689626 | 59.63% | 8.957% |
| 6 | 7.676 | 772 | 781 | 793 | rBV | 899463 | 1611311 | 56.87% | 8.542% |
| 7 | 8.146 | 853 | 861 | 871 | rVB | 177651 | 316102 | 11.16% | 1.676% |
| 8 | 8.469 | 907 | 916 | 924 | rBV | 644371 | 1173819 | 41.43% | 6.223% |
| 9 | 9.321 | 1052 | 1061 | 1070 | rBV | 558516 | 1012944 | 35.75% | 5.370% |
| 10 | 10.966 | 1332 | 1341 | 1350 | rBV | 234941 | 422751 | 14.92% | 2.241% |
| 11 | 13.392 | 1745 | 1754 | 1765 | rBV | 1367257 | 2100279 | 74.13% | 11.134% |
| 12 | 14.208 | 1888 | 1893 | 1900 | rVB | 103393 | 151004 | 5.33% | 0.800% |
| 13 | 14.772 | 1982 | 1989 | 1996 | rVB2 | 364375 | 595976 | 21.03% | 3.159% |
| 14 | 16.259 | 2235 | 2242 | 2252 | rBV | 1188752 | 1842263 | 65.02% | 9.766% |
| 15 | 17.516 | 2449 | 2456 | 2467 | rBV2 | 510193 | 778052 | 27.46% | 4.125% |
| 16 | 18.368 | 2594 | 2601 | 2608 | rBV2 | 47541 | 78219 | 2.76% | 0.415% |
| 17 | 19.766 | 2835 | 2839 | 2844 | rBV | 28750 | 33986 | 1.20% | 0.180% |
| 18 | 20.106 | 2892 | 2897 | 2903 | rVB | 2171995 | 2833363 | 100.00% | 15.020% |
| 19 | 21.393 | 3110 | 3116 | 3123 | rBV5 | 42041 | 122309 | 4.32% | 0.648% |
| 20 | 21.804 | 3179 | 3186 | 3195 | rVB2 | 442621 | 766937 | 27.07% | 4.066% |
| 21 | 22.568 | 3311 | 3316 | 3322 | rVB3 | 21816 | 38258 | 1.35% | 0.203% |
| 22 | 23.279 | 3432 | 3437 | 3444 | rVB2 | 28382 | 52025 | 1.84% | 0.276% |
| 23 | 24.113 | 3571 | 3579 | 3587 | rVB3 | 31307 | 71649 | 2.53% | 0.380% |
| 24 | 25.100 | 3740 | 3747 | 3749 | rBV4 | 25706 | 55712 | 1.97% | 0.295% |
| 25 | 25.164 | 3750 | 3758 | 3773 | rVB | 248345 | 725782 | 25.62% | 3.847% |
| 26 | 26.269 | 3940 | 3946 | 3955 | rVB4 | 17847 | 52478 | 1.85% | 0.278% |

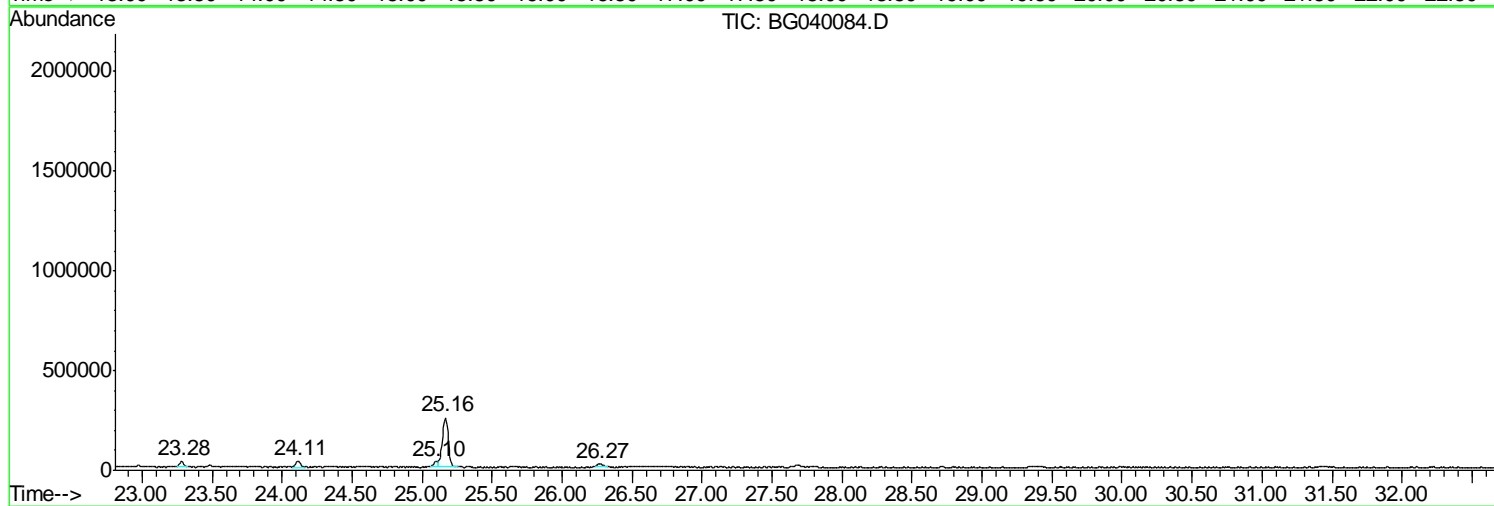
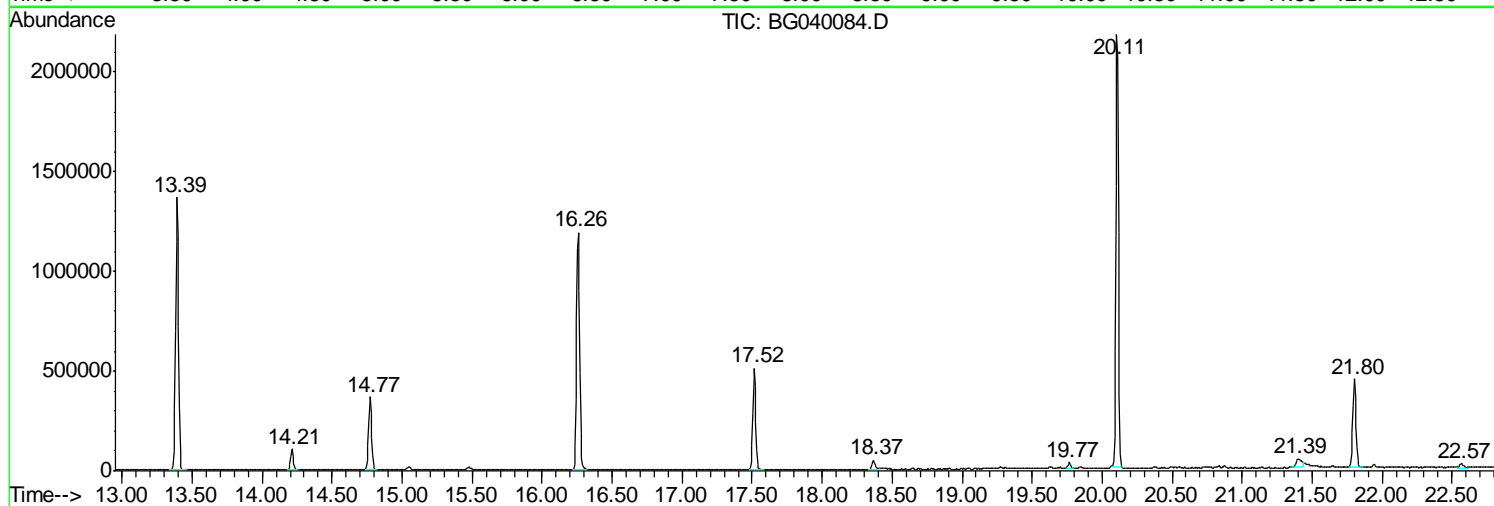
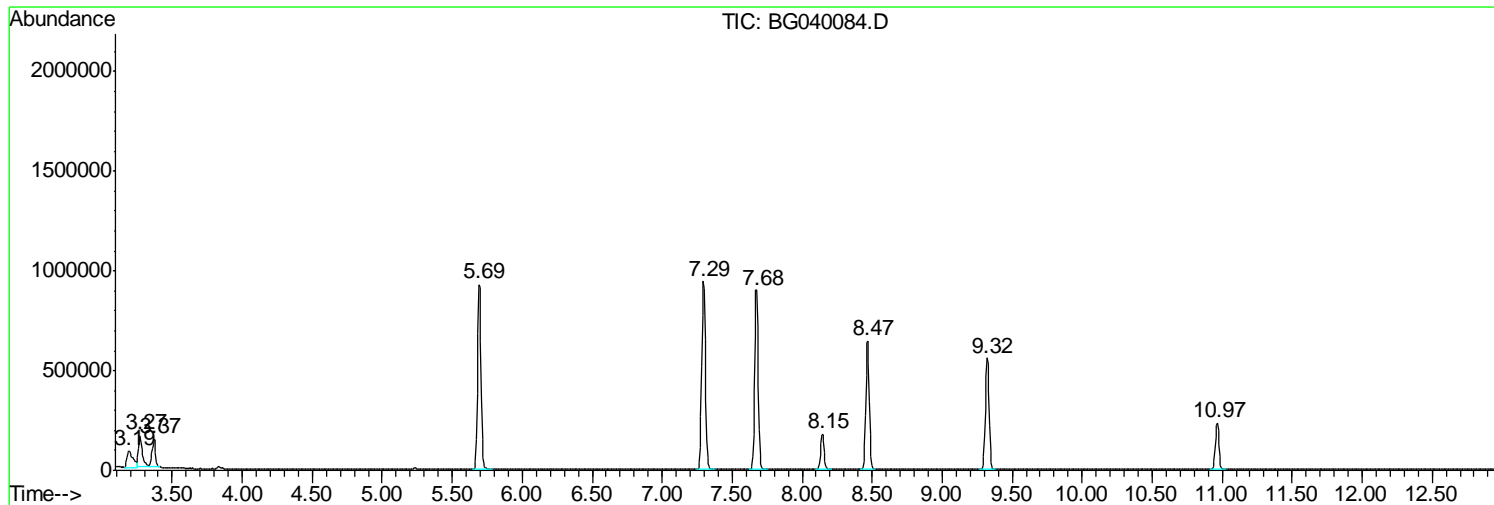
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S4B(12-20)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG030419.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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 Sample : K2040-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampled :
 S4B(12-20)

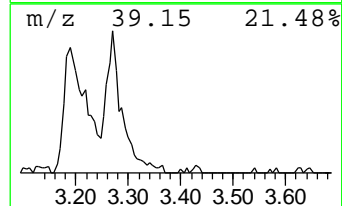
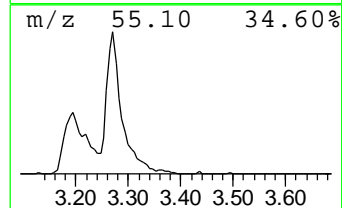
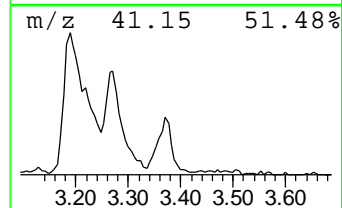
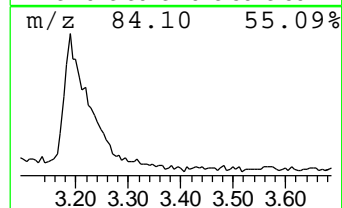
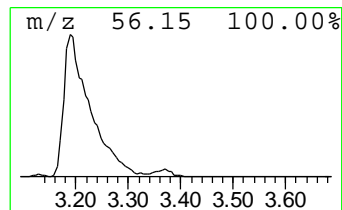
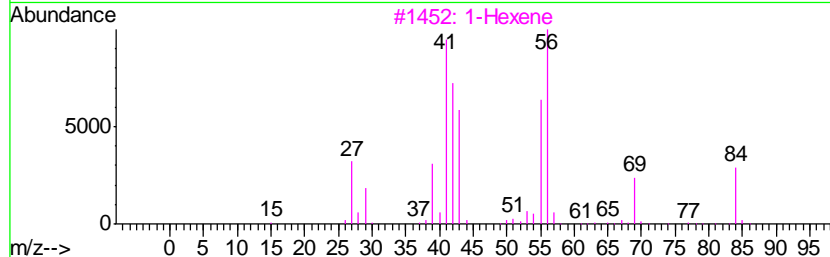
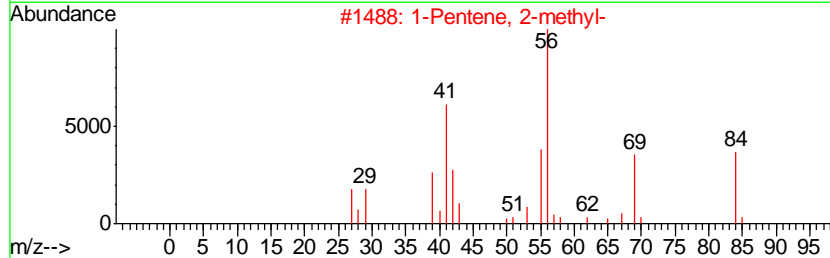
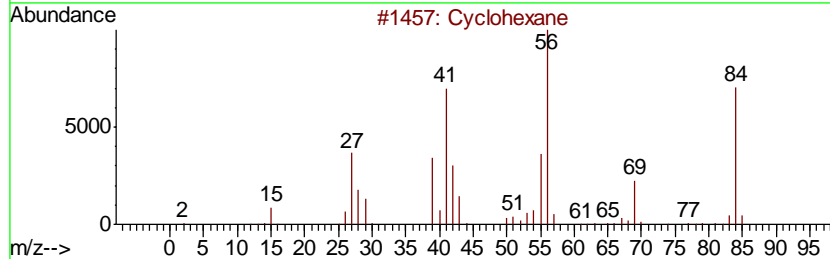
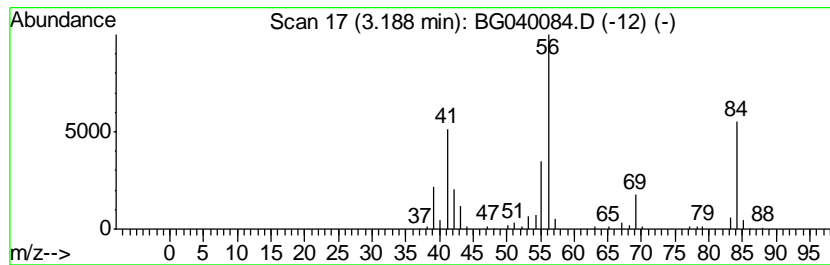
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG030419.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|------|----------|--------|------------------------|------|
| 3.19 | 15.19 ng | 240148 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# | of | Tentative ID | MW | MolForm | CAS# | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1 | 5 | Cyclohexane | 84 | C6H12 | 000110-82-7 | 91 |
| 2 | | 1-Pentene, 2-methyl- | 84 | C6H12 | 000763-29-1 | 72 |
| 3 | | 1-Hexene | 84 | C6H12 | 000592-41-6 | 59 |
| 4 | | Cyclobutane, ethyl- | 84 | C6H12 | 004806-61-5 | 53 |
| 5 | | 2H-Pyran-2,6(3H)-dione, dihydro-... | 142 | C7H10O3 | 004160-82-1 | 50 |



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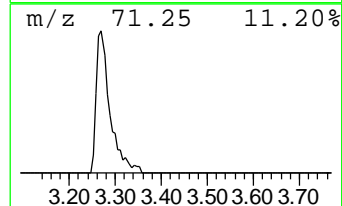
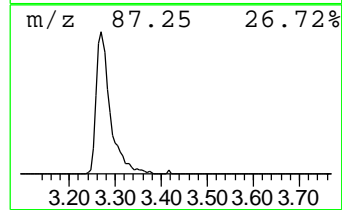
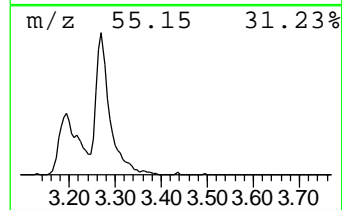
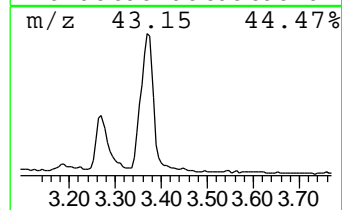
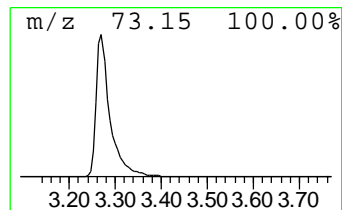
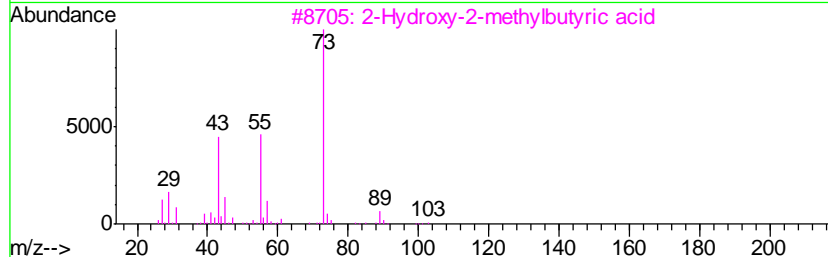
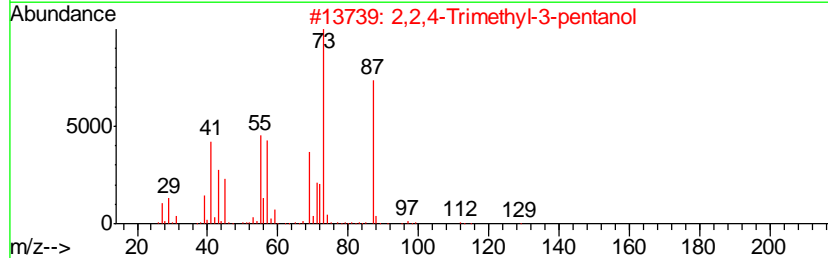
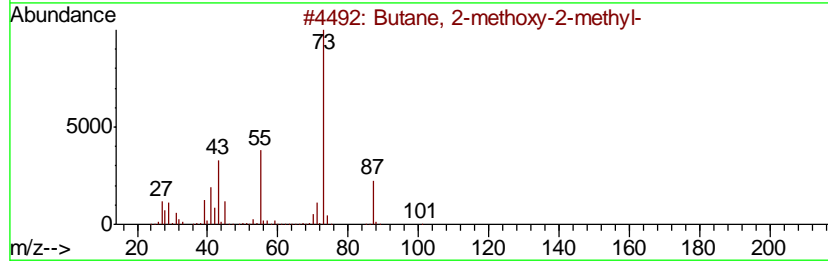
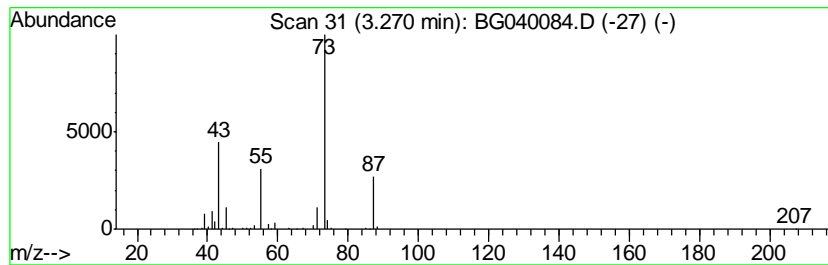
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG030419.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|------|----------|--------|------------------------|------|
| 3.27 | 19.24 ng | 304084 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# | of | Tentative ID | MW | MolForm | CAS# | Qual |
|------|----|--------------------------------|-----|---------|-------------|------|
| 1 | 5 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 78 |
| 2 | | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 42 |
| 3 | | 2-Hydroxy-2-methylbutyric acid | 118 | C5H10O3 | 003739-30-8 | 23 |
| 4 | | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 17 |
| 5 | | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 9 |



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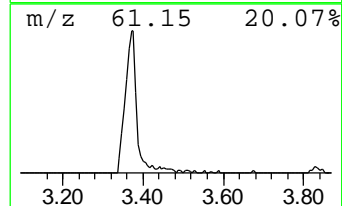
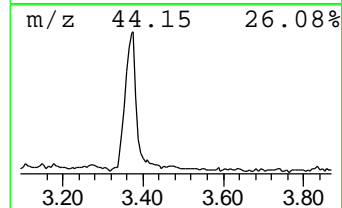
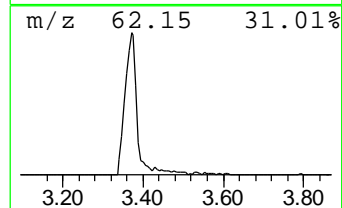
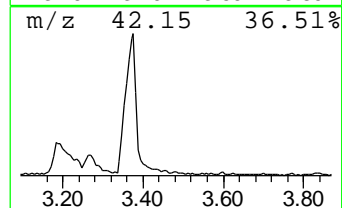
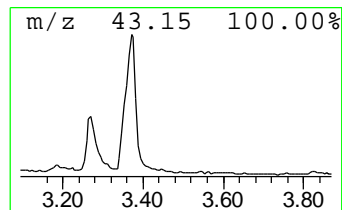
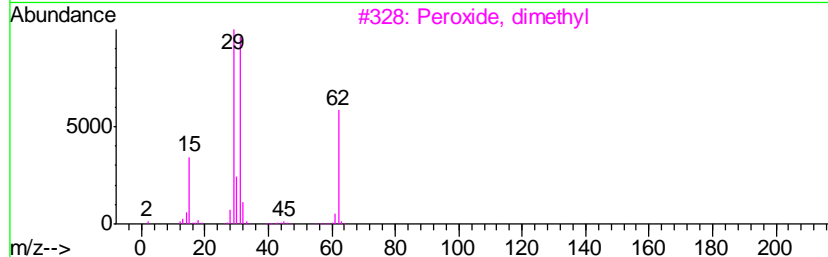
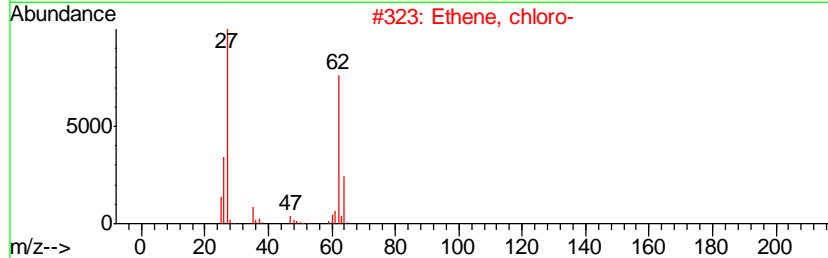
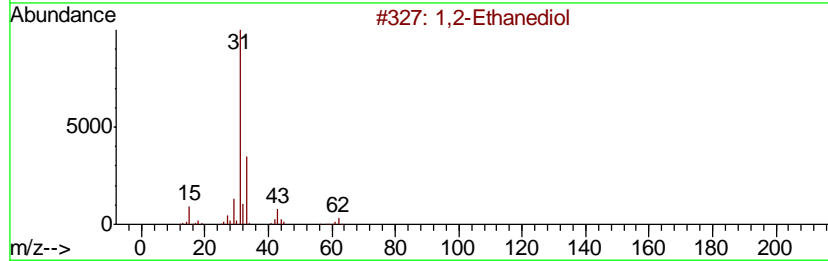
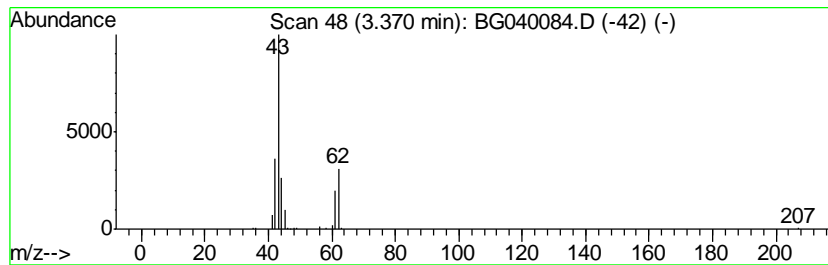
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG030419.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 3 unknown3.37 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|------|----------|--------|------------------------|------|
| 3.37 | 15.91 ng | 251404 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# | of | Tentative ID | MW | MolForm | CAS# | Qual |
|------|----|-------------------------------------|-----|------------|--------------|------|
| 1 | 5 | 1,2-Ethanediol | 62 | C2H6O2 | 000107-21-1 | 9 |
| 2 | | Ethene, chloro- | 62 | C2H3Cl | 000075-01-4 | 7 |
| 3 | | Peroxide, dimethyl | 62 | C2H6O2 | 000690-02-8 | 5 |
| 4 | | Ethanethiol | 62 | C2H6S | 000075-08-1 | 4 |
| 5 | | Adenosine, 4'-de(hydroxymethyl)-... | 442 | C20H22N6O6 | 1000129-52-5 | 4 |



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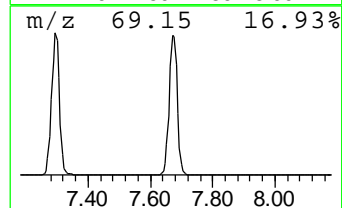
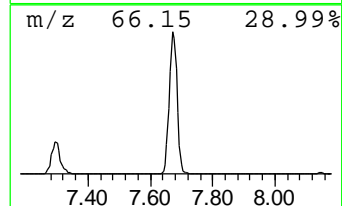
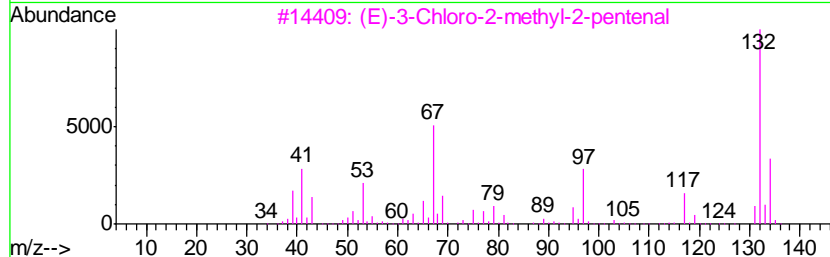
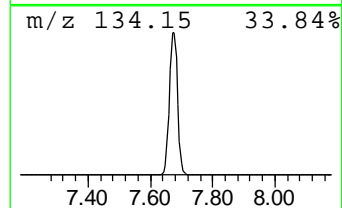
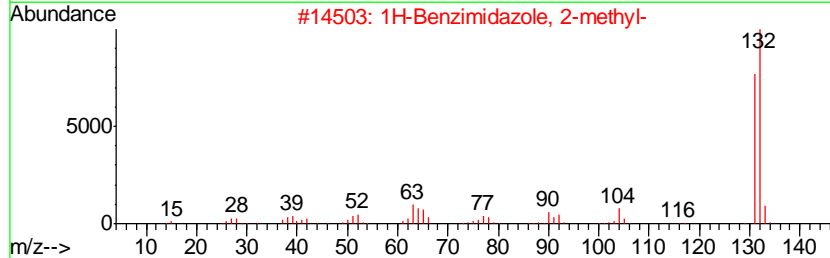
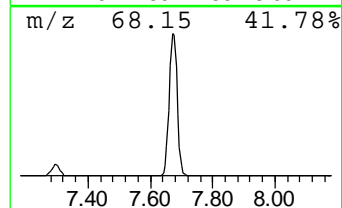
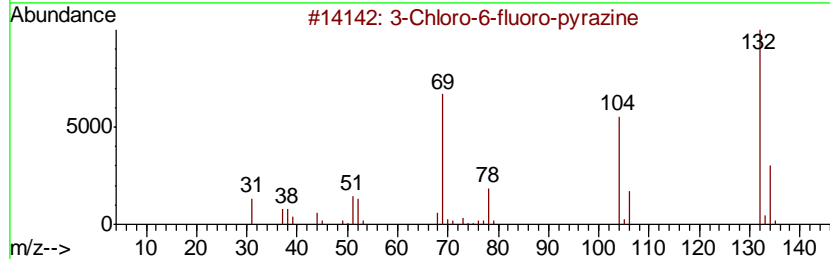
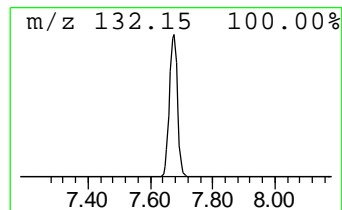
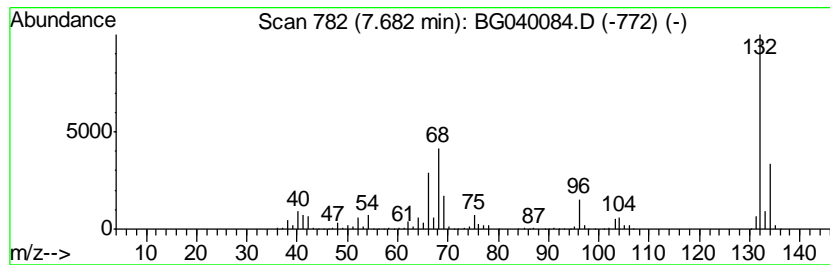
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TIC Library : C:\Database\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 4 unknown7.68 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|------|-----------|---------|------------------------|------|
| 7.68 | 101.95 ng | 1611310 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# | of | Tentative ID | MW | MolForm | CAS# | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1 | 5 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 25 |
| 3 | | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 4 | | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 5 | | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |



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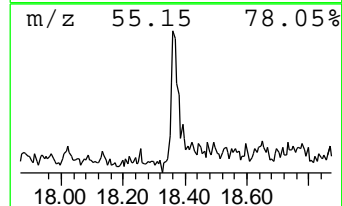
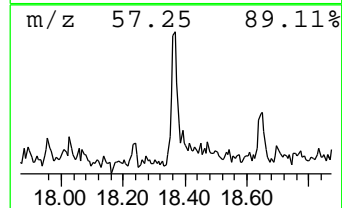
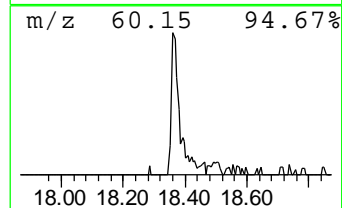
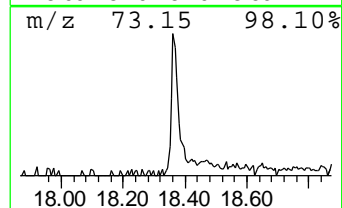
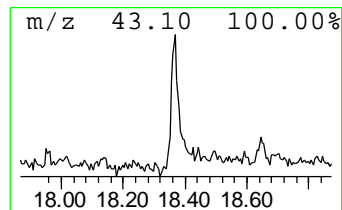
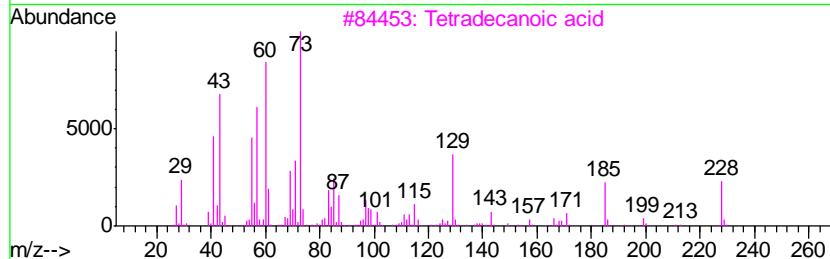
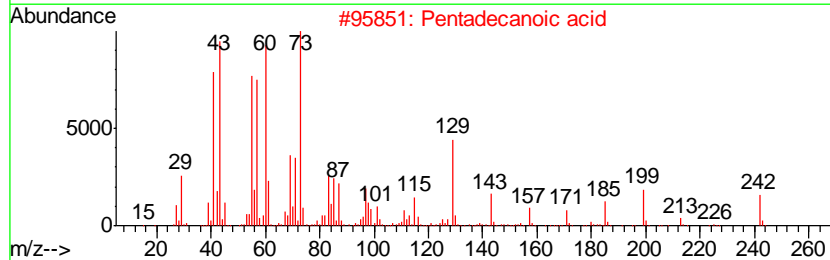
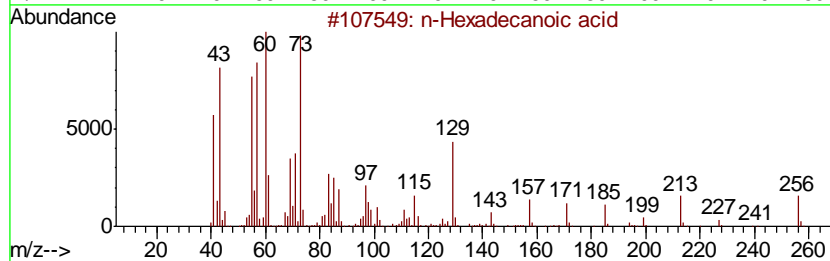
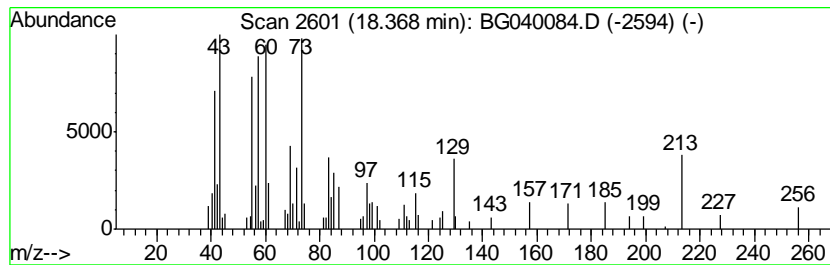
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|-------|---------|-------|------------------|-------|
| 18.37 | 2.01 ng | 78219 | Phenanthrene-d10 | 17.52 |

| Hit# | of | Tentative ID | MW | MolForm | CAS# | Qual |
|------|----|---------------------|-----|----------|-------------|------|
| 1 | 5 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 68 |
| 3 | | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 59 |
| 4 | | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 59 |
| 5 | | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 53 |



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 ClientSampleID :
 S4B(12-20)

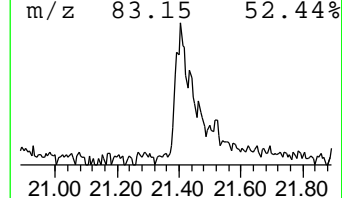
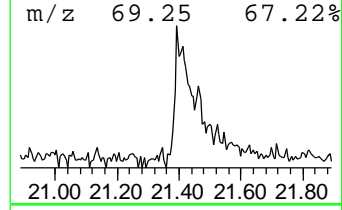
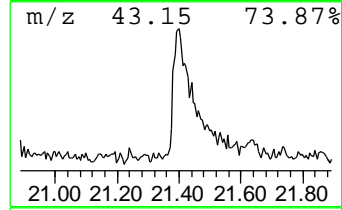
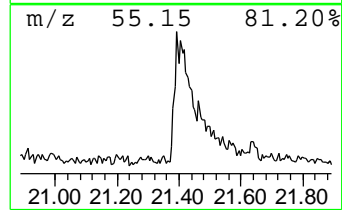
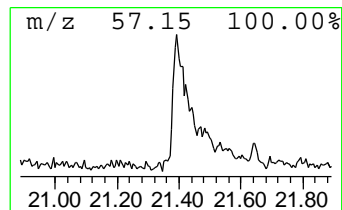
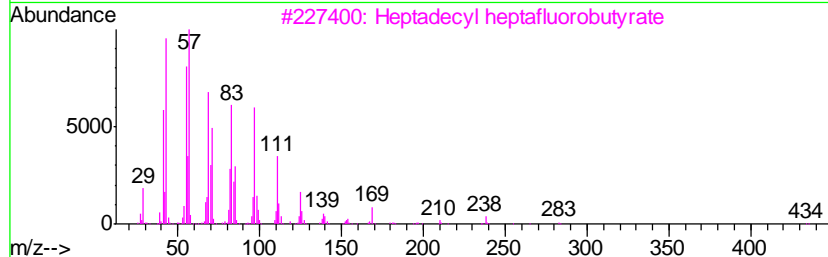
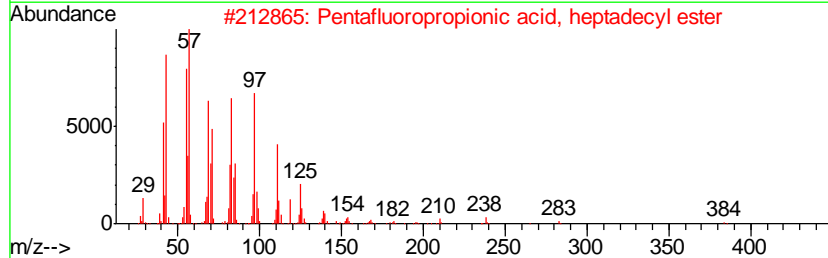
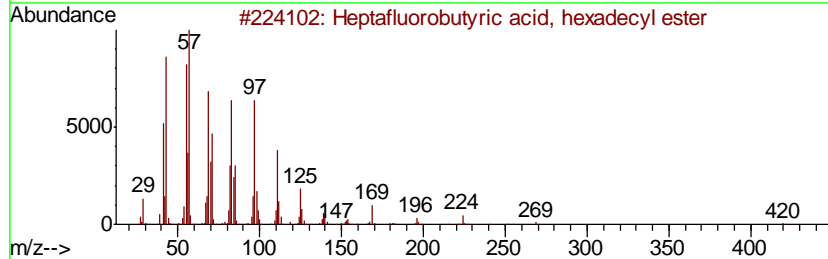
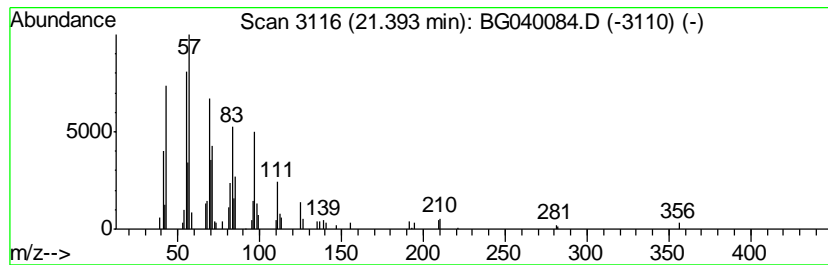
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG030419.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Heptafluorobutyric acid, he... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|-------|---------|--------|------------------|-------|
| 21.39 | 3.19 ng | 122309 | Chrysene-d12 | 21.80 |

| Hit# | of | Tentative ID | MW | MolForm | CAS# | Qual |
|------|----|-------------------------------------|-----|------------|--------------|------|
| 1 | 5 | Heptafluorobutyric acid, hexadec... | 438 | C20H33F7O2 | 006385-15-5 | 91 |
| 2 | | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1 | 91 |
| 3 | | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 91 |
| 4 | | Tricosyl trifluoroacetate | 436 | C25H47F3O2 | 1000351-75-1 | 91 |
| 5 | | Pentafluoropropionic acid, octad... | 416 | C21H37F5O2 | 959261-25-7 | 91 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG032219\
Data File : BG040084.D
Acq On : 22 Mar 2019 15:34
Operator : JU/SJ
Sample : K2040-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S4B(12-20)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.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 |
| 1-Pentene, 2-methyl- | 3.19 | 15.2 | ng | 240148 | 1 | 8.15 | 316102 | 20.0 |
| Butane, 2-methoxy... | 3.27 | 19.2 | ng | 304084 | 1 | 8.15 | 316102 | 20.0 |
| unknown3.37 | 3.37 | 15.9 | ng | 251404 | 1 | 8.15 | 316102 | 20.0 |
| unknown7.68 | 7.68 | 102.0 | ng | 1611310 | 1 | 8.15 | 316102 | 20.0 |
| n-Hexadecanoic acid | 18.37 | 2.0 | ng | 78219 | 4 | 17.52 | 778052 | 20.0 |
| Heptafluorobutyri... | 21.39 | 3.2 | ng | 122309 | 5 | 21.80 | 766937 | 20.0 |