LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112021\
Data File : BP008071.D
Acq On : 20 Nov 2021 22:46
Operator : CG/JU
Sample : M4762-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** RBR-251674

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_P\Methods\8270E-BP111921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008071.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.416 | 355 | 362 | 369 | rBV | 2204606 | 3350115 | 57.94% | 9.150% |
| 2 | 7.005 | 622 | 632 | 646 | rBV | 2149711 | 3595255 | 62.18% | 9.820% |
| 3 | 7.475 | 705 | 712 | 718 | rBV | 54375 | 88165 | 1.52% | 0.241% |
| 4 | 7.822 | 761 | 771 | 779 | rBV | 514633 | 801171 | 13.86% | 2.188% |
| 5 | 8.981 | 961 | 968 | 978 | rBV | 1377929 | 2251384 | 38.93% | 6.149% |
| 6 | 10.410 | 1204 | 1211 | 1219 | rBV2 | 37567 | 72134 | 1.25% | 0.197% |
| 7 | 10.616 | 1236 | 1246 | 1262 | rBV | 649352 | 1127311 | 19.50% | 3.079% |
| 8 | 13.087 | 1659 | 1666 | 1677 | rBV | 3296142 | 4980882 | 86.14% | 13.604% |
| 9 | 13.251 | 1689 | 1694 | 1698 | rBV2 | 67150 | 107916 | 1.87% | 0.295% |
| 10 | 13.887 | 1798 | 1802 | 1806 | rBV | 127232 | 180058 | 3.11% | 0.492% |
| 11 | 14.116 | 1838 | 1841 | 1846 | rVB4 | 91609 | 129983 | 2.25% | 0.355% |
| 12 | 14.210 | 1852 | 1857 | 1862 | rBV6 | 136656 | 309633 | 5.35% | 0.846% |
| 13 | 14.298 | 1868 | 1872 | 1879 | rVB4 | 232534 | 401744 | 6.95% | 1.097% |
| 14 | 14.369 | 1880 | 1884 | 1889 | rBV2 | 162125 | 270806 | 4.68% | 0.740% |
| 15 | 14.463 | 1890 | 1900 | 1906 | rBV | 1084534 | 1949630 | 33.72% | 5.325% |
| 16 | 15.251 | 2031 | 2034 | 2038 | rBV3 | 200180 | 317054 | 5.48% | 0.866% |
| 17 | 15.957 | 2149 | 2154 | 2162 | rBV | 2350090 | 3716734 | 64.28% | 10.152% |
| 18 | 17.222 | 2366 | 2369 | 2374 | rBV | 777206 | 1100865 | 19.04% | 3.007% |
| 19 | 19.792 | 2801 | 2806 | 2811 | rVB | 4525670 | 5782421 | 100.00% | 15.794% |
| 20 | 21.310 | 3060 | 3064 | 3069 | rBV2 | 1277630 | 1831194 | 31.67% | 5.002% |
| 21 | 21.986 | 3175 | 3179 | 3185 | rVB | 1198096 | 1570330 | 27.16% | 4.289% |
| 22 | 22.980 | 3344 | 3348 | 3353 | rBV | 459232 | 788435 | 13.64% | 2.153% |
| 23 | 23.704 | 3465 | 3471 | 3478 | rBV2 | 926429 | 1888865 | 32.67% | 5.159% |

Sum of corrected areas: 36612085

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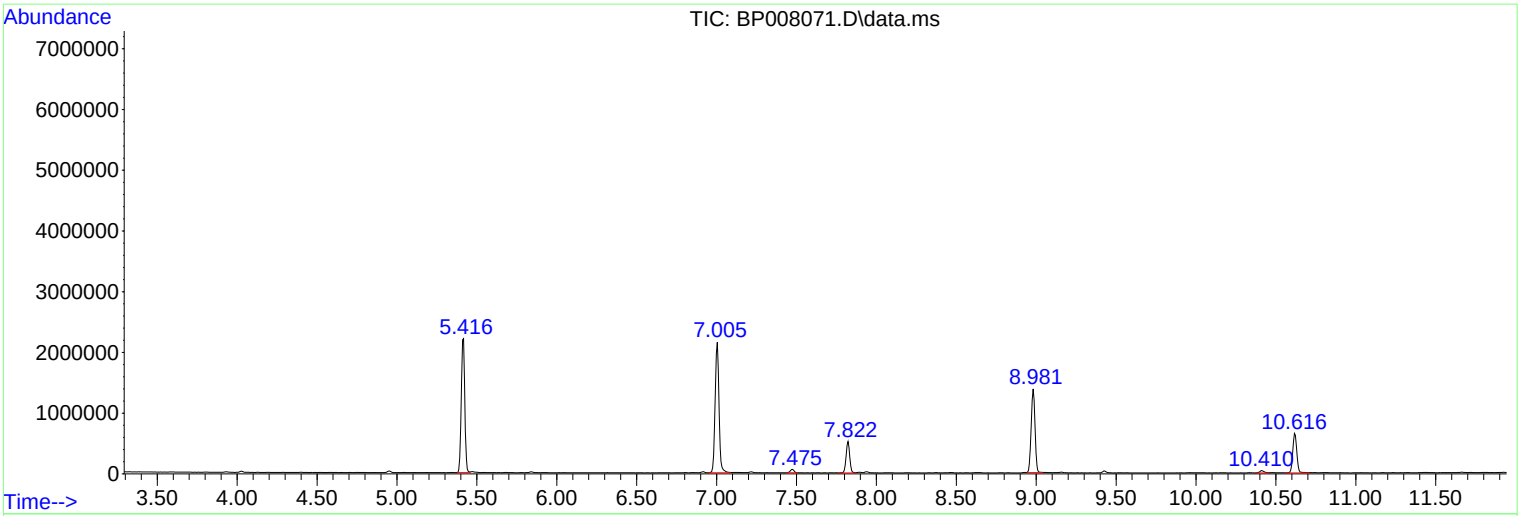
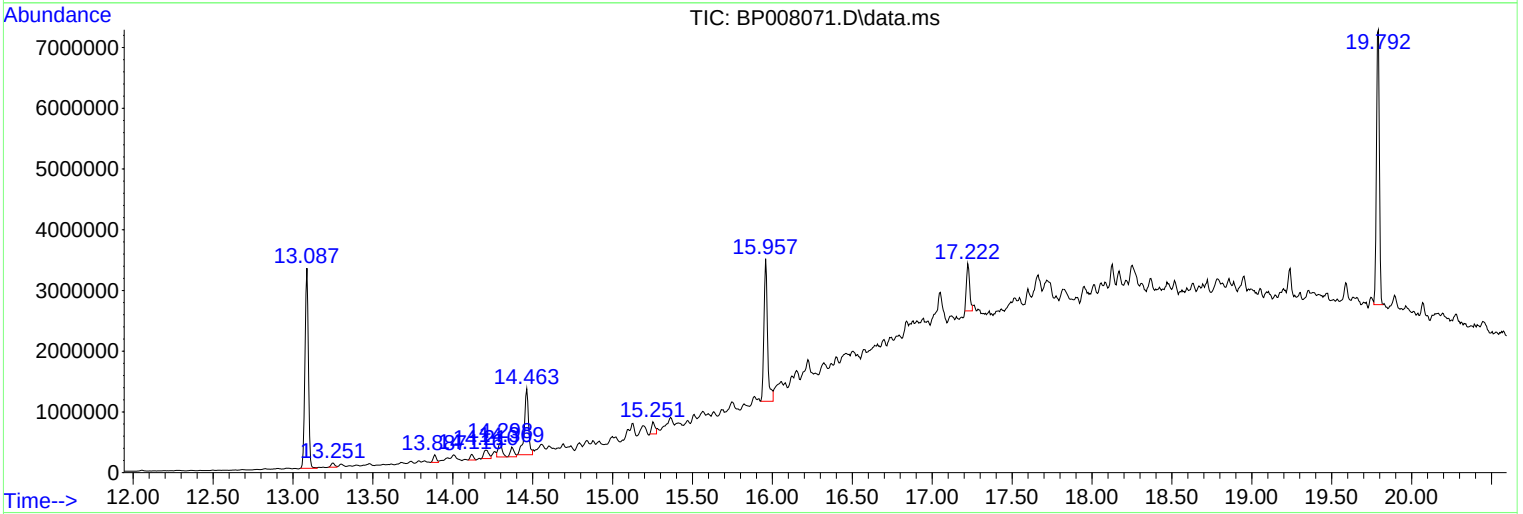
Misc :
ALS Vial : 19 Sample Multiplier: 1

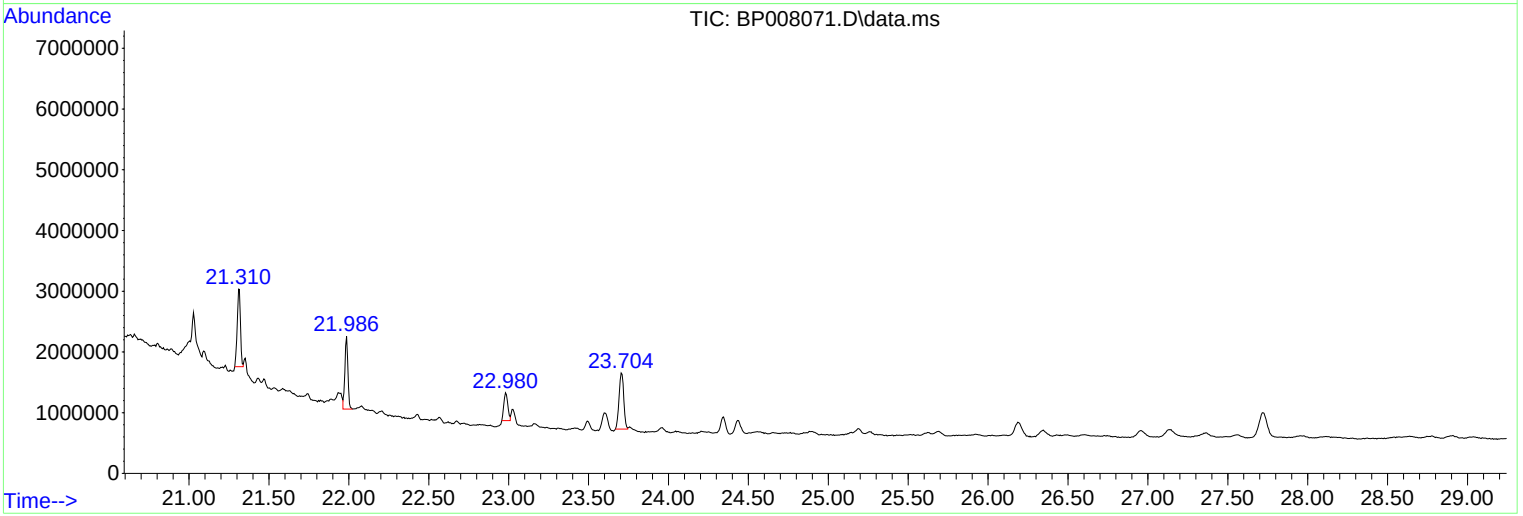
**Instrument :**
BNA_P
**ClientSampleId :**
RBR-251674

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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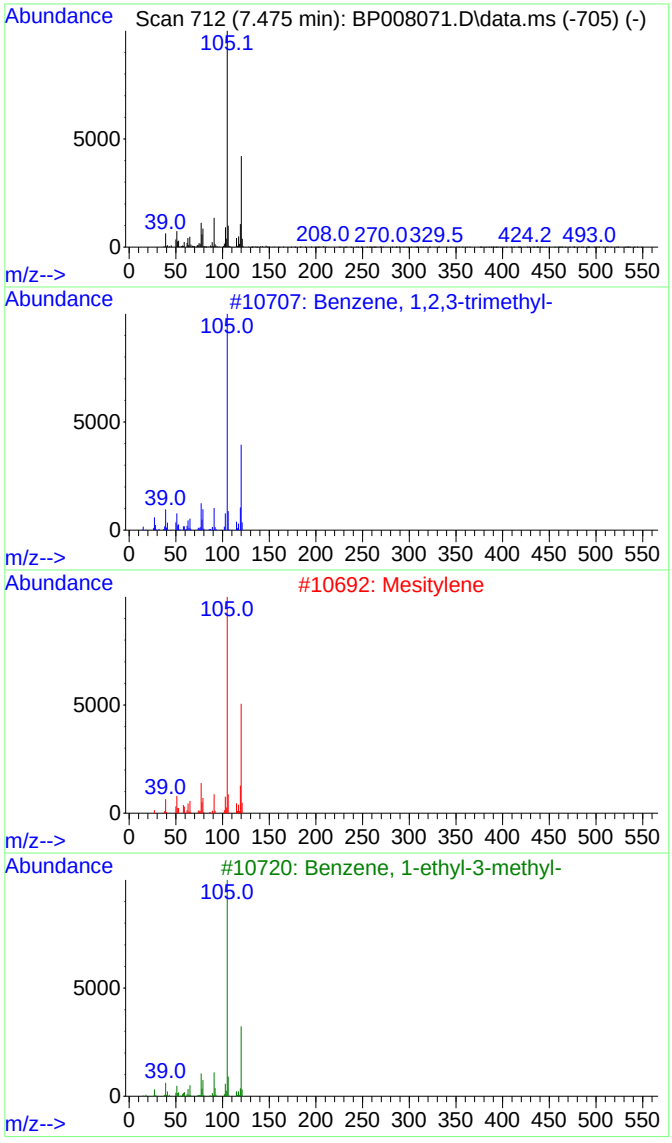
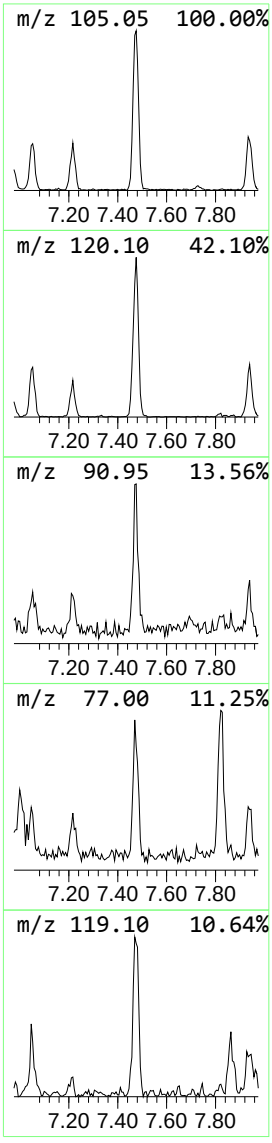
**********

Peak Number 1 Benzene, 1,2,3-trimethyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.475 | 2.20 ng | 88165 | 1,4-Dichlorobenzene-d4 | 7.822 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, 1,2,3-trimethyl- | 120 | C9H12 | 000526-73-8 | 95 |
| 2 | Mesitylene | 120 | C9H12 | 000108-67-8 | 95 |
| 3 | Benzene, 1-ethyl-3-methyl- | 120 | C9H12 | 000620-14-4 | 91 |
| 4 | Benzene, 1,2,4-trimethyl- | 120 | C9H12 | 000095-63-6 | 91 |
| 5 | Benzene, 1-ethyl-4-methyl- | 120 | C9H12 | 000622-96-8 | 90 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112021\
Data File : BP008071.D
Acq On : 20 Nov 2021 22:46
Operator : CG/JU
Sample : M4762-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
RBR-251674

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

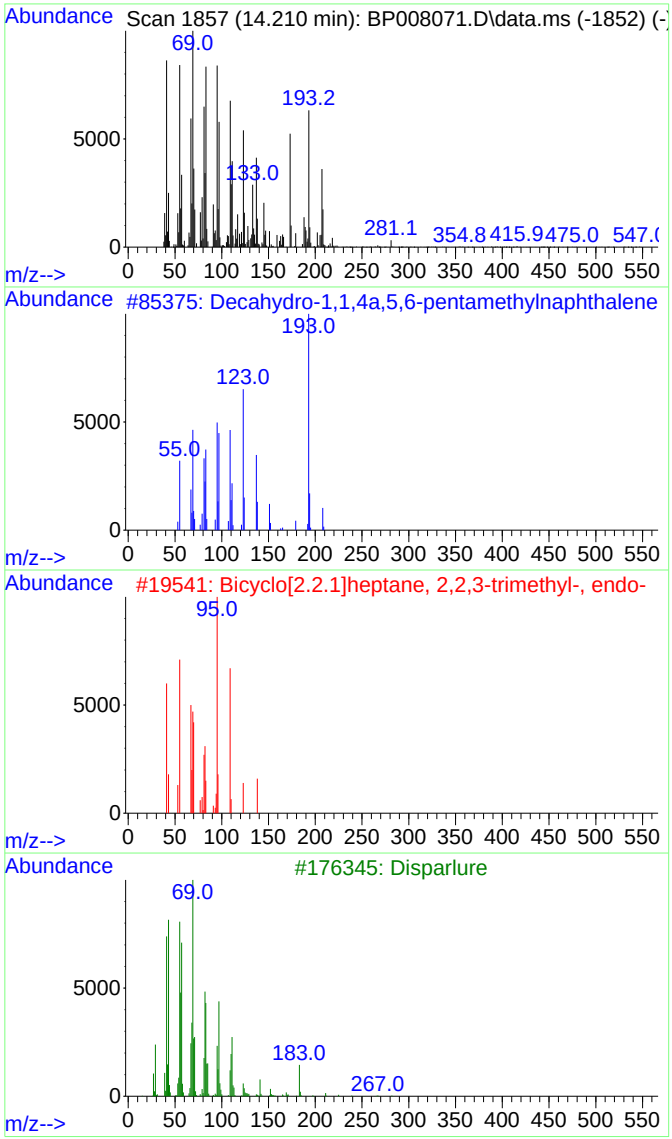
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

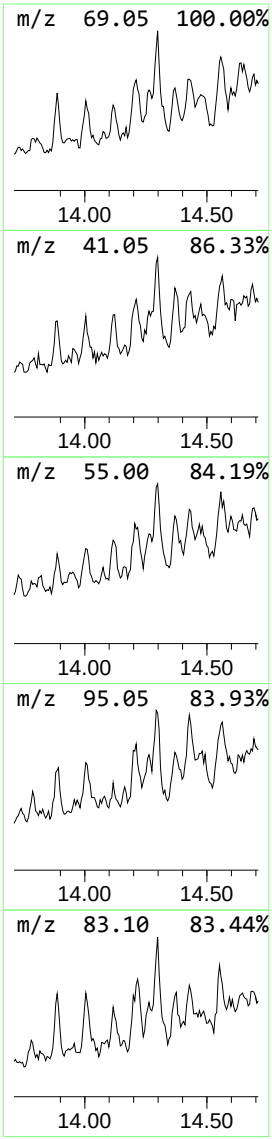
**********

Peak Number 2 unknown14.210 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.210 | 3.18 ng | 309633 | Acenaphthene-d10 | 14.463 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Decahydro-1,1,4a,5,6-pentamethyl... | 208 | C15H28 | 080655-44-3 | 45 |
| 2 | Bicyclo[2.2.1]heptane, 2,2,3-tri... | 138 | C10H18 | 020536-40-7 | 44 |
| 3 | Disparlure | 282 | C19H38O | 029804-22-6 | 38 |
| 4 | 2,6-Heptadienal, 2,4-dimethyl- | 138 | C9H14O | 085136-08-9 | 38 |
| 5 | 1-(2-Furyl)-4,4,4-trifluoro-1,3-... | 206 | C8H5F3O3 | 000326-90-9 | 25 |



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Data File : BP008071.D
Acq On : 20 Nov 2021 22:46
Operator : CG/JU
Sample : M4762-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
RBR-251674

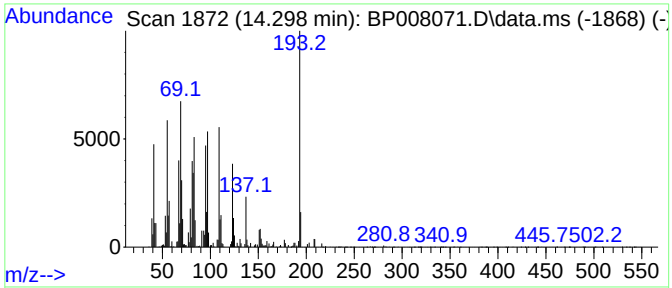
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

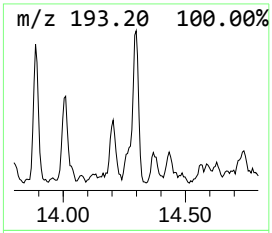
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

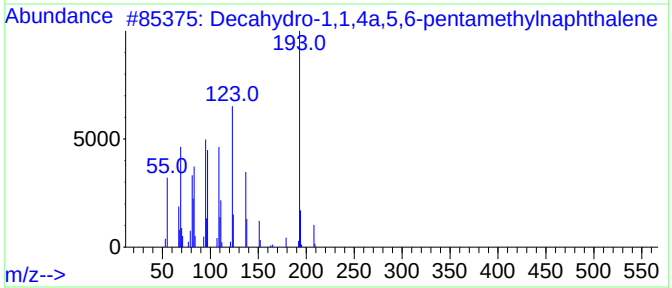
**********
Peak Number 3 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 2

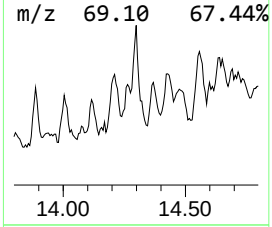
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.298 | 4.12 ng | 401744 | Acenaphthene-d10 | 14.463 |

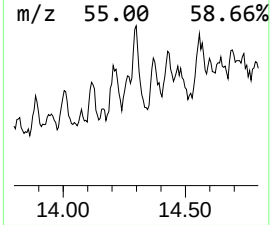
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Decahydro-1,1,4a,5,6-pentamethyl... | 208 | C15H28 | 080655-44-3 | 72 |
| 2 | Toxoflavin | 193 | C7H7N5O2 | 000084-82-2 | 22 |
| 3 | 4-Amino-N-hydroxypyrazolo[3,2-c]... | 193 | C6H7N7O | 1000443-50-2 | 16 |
| 4 | 3-((2R,5S)-7-(Cyclohexylsulfonyl... | 340 | C17H28N2O3S | 1000483-82-6 | 14 |
| 5 | Cyclohexane, 1,1',1''-(1-ethanyl... | 276 | C20H36 | 055682-86-5 | 12 |

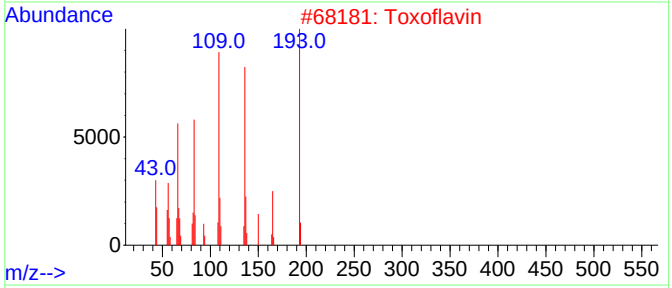


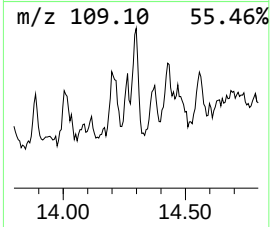



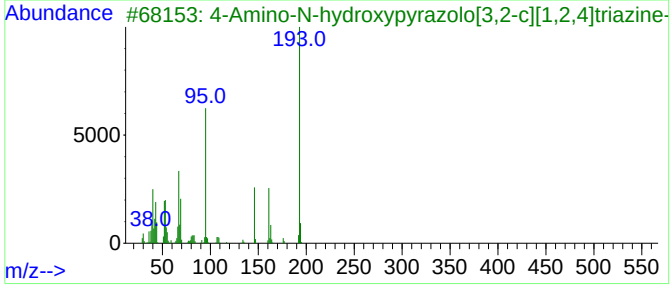



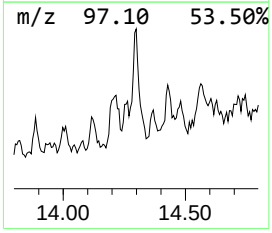



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ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
RBR-251674

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

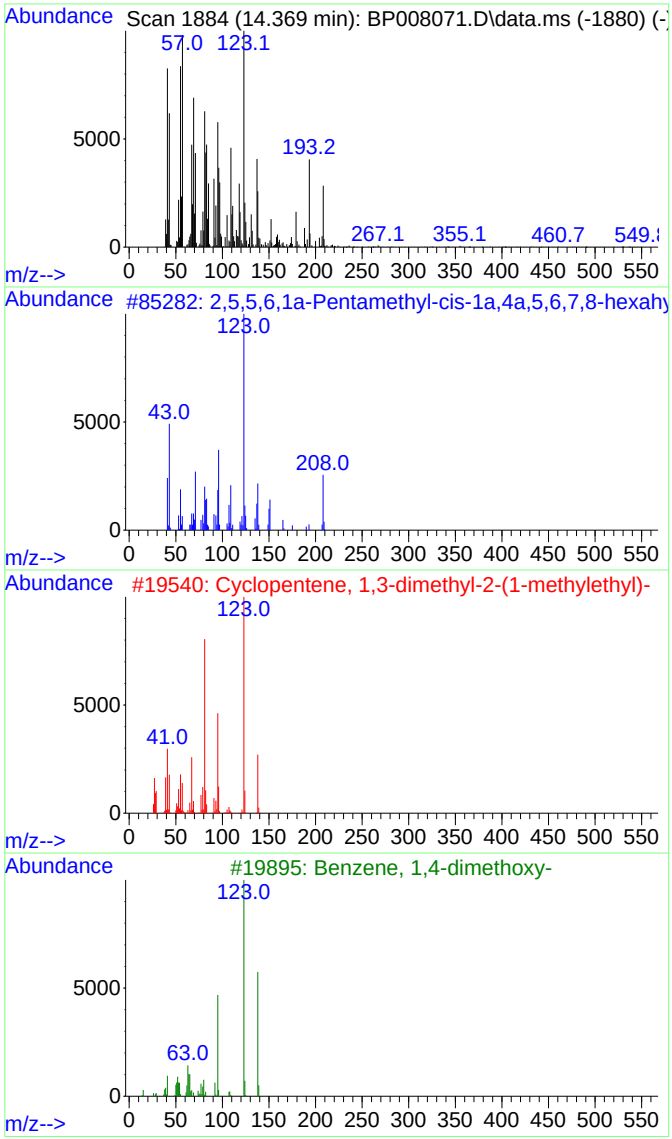
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

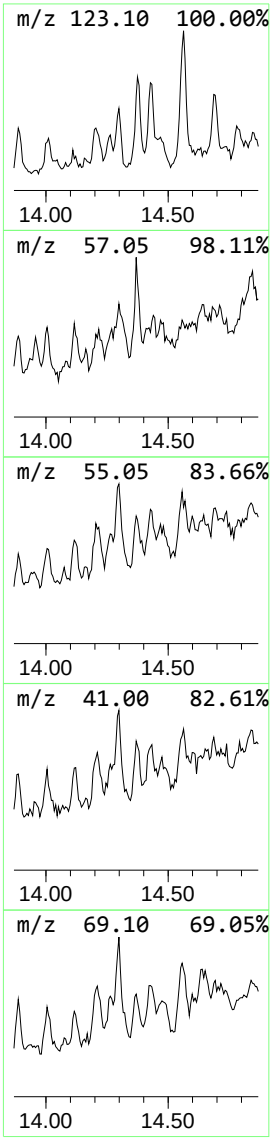
**********

Peak Number 4 unknown14.369 Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.369 | 2.78 ng | 270806 | Acenaphthene-d10 | 14.463 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,5,5,6,1a-Pentamethyl-cis-1a,4a... | 208 | C14H24O | 1010215-77-9 | 43 |
| 2 | Cyclopentene, 1,3-dimethyl-2-(1-... | 138 | C10H18 | 061142-32-3 | 38 |
| 3 | Benzene, 1,4-dimethoxy- | 138 | C8H10O2 | 000150-78-7 | 30 |
| 4 | Citronellyl butyrate | 226 | C14H26O2 | 000141-16-2 | 25 |
| 5 | Citronellyl isobutyrate | 226 | C14H26O2 | 000097-89-2 | 22 |



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**Instrument :**
BNA_P
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RBR-251674

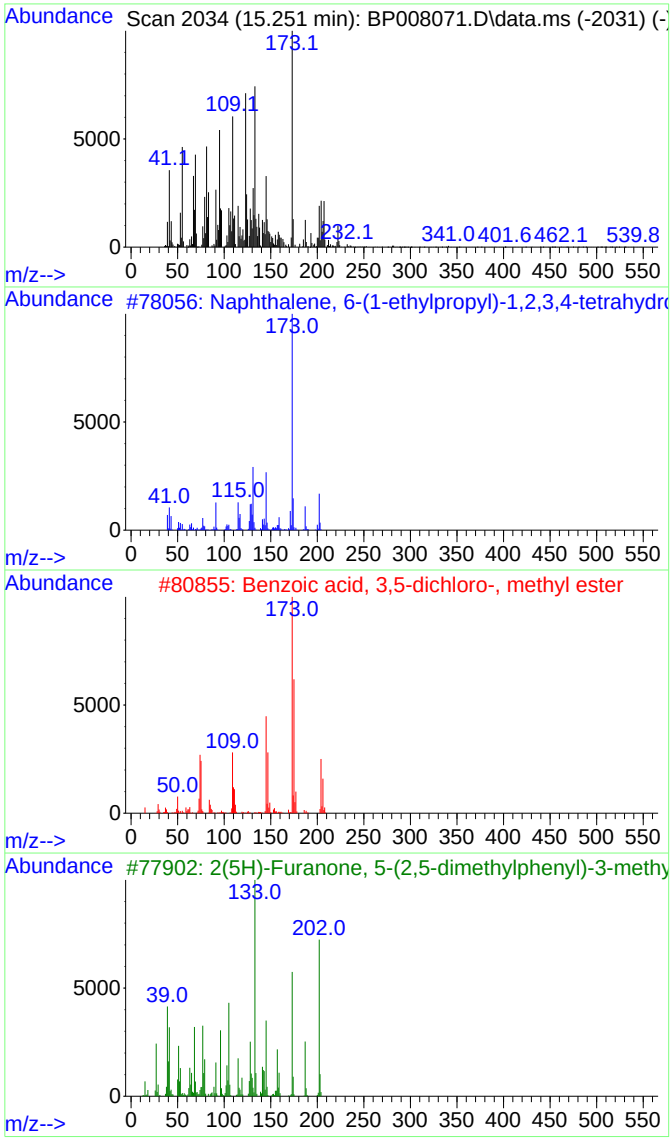
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

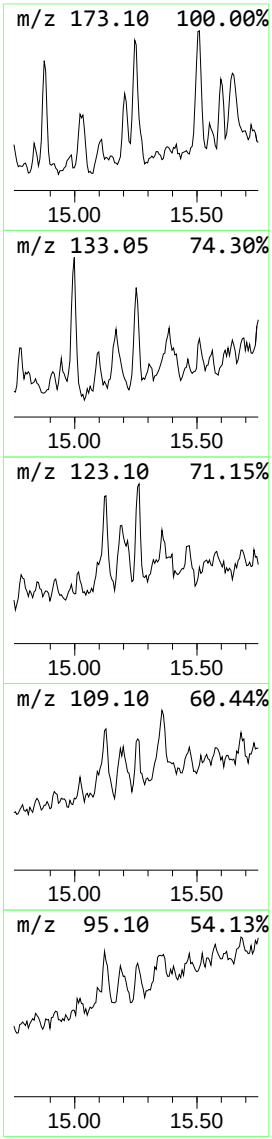
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 Naphthalene, 6-(1-ethylprop... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.251 | 3.25 ng | 317054 | Acenaphthene-d10 | 14.463 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Naphthalene, 6-(1-ethylpropyl)-1... | 202 | C15H22 | 054889-56-4 | 53 |
| 2 | Benzoic acid, 3,5-dichloro-, met... | 204 | C8H6Cl2O2 | 002905-67-1 | 38 |
| 3 | 2(5H)-Furanone, 5-(2,5-dimethylp... | 202 | C13H14O2 | 055591-07-6 | 35 |
| 4 | 2-Cyclohexen-1-one, 5-bromo-4,4-... | 202 | C8H11BrO | 1000327-26-6 | 35 |
| 5 | Butanoic acid, 4-(3-ethylphenyl)... | 206 | C12H14O3 | 017503-46-7 | 25 |



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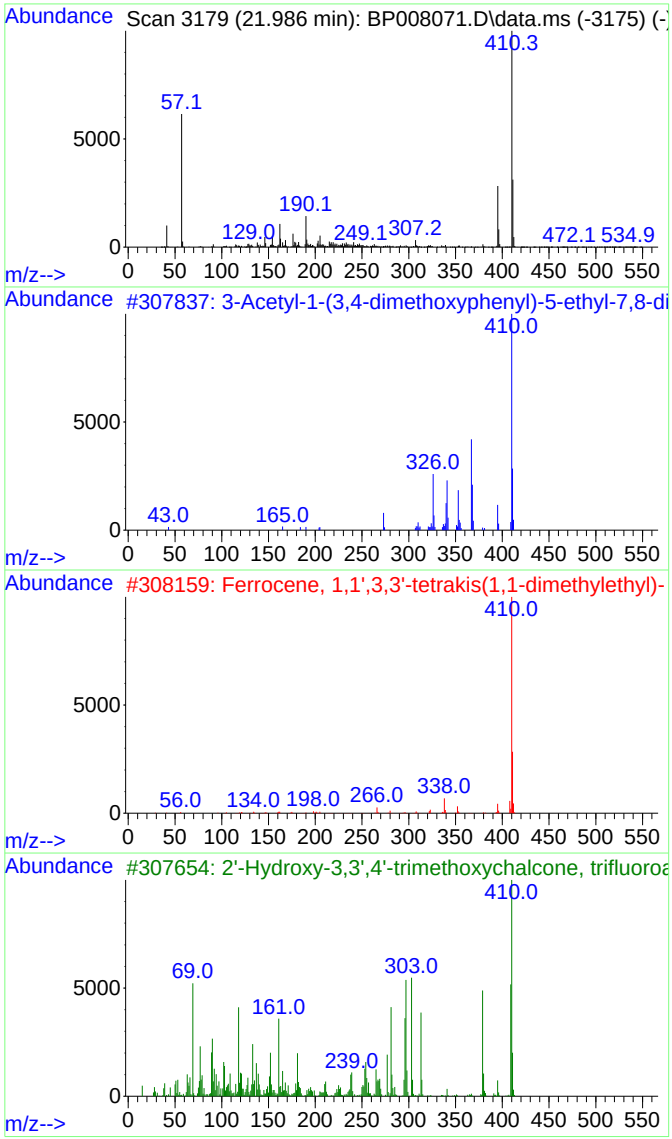
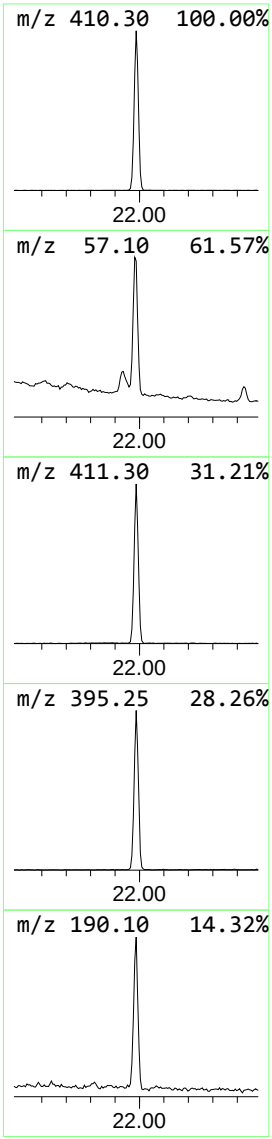
**********
Peak Number 6 3-Acetyl-1-(3,4-dimethoxyph... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.986 | 17.15 ng | 1570330 | Chrysene-d12 | 21.316 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Acetyl-1-(3,4-dimethoxyphenyl)... | 410 | C23H26N2O5 | 090140-65-1 | 59 |
| 2 | Ferrocene, 1,1',3,3'-tetrakis(1,... | 410 | C26H42Fe | 001317-17-5 | 58 |
| 3 | 2'-Hydroxy-3,3',4'-trimethoxycha... | 410 | C20H17F3O6 | 1010453-84-8 | 50 |
| 4 | 9-Chloro-4,5-dihydro-4-[3,4,5-tr... | 410 | C22H19ClN2O4 | 1000212-48-1 | 42 |
| 5 | 2'-Hydroxy-3,4,5-trimethoxychalc... | 410 | C20H17F3O6 | 1000449-43-8 | 38 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112021\
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BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Benzene, 1,2,3-... | 7.475 | 2.2 | ng | 88165 | 1 | 7.822 | 801171 | 20.0 |
| unknown14.210 | 14.210 | 3.2 | ng | 309633 | 3 | 14.463 | 1949630 | 20.0 |
| Decahydro-1,1,4... | 14.298 | 4.1 | ng | 401744 | 3 | 14.463 | 1949630 | 20.0 |
| unknown14.369 | 14.369 | 2.8 | ng | 270806 | 3 | 14.463 | 1949630 | 20.0 |
| Naphthalene, 6-... | 15.251 | 3.3 | ng | 317054 | 3 | 14.463 | 1949630 | 20.0 |
| 3-Acetyl-1-(3,4... | 21.986 | 17.1 | ng | 1570330 | 5 | 21.316 | 1831190 | 20.0 |