LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053055.D
Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

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-BG031522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053055.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.690 | 386 | 392 | 400 | rBV | 253920 | 419807 | 15.58% | 3.005% |
| 2 | 7.135 | 631 | 638 | 645 | rBV3 | 15667 | 30869 | 1.15% | 0.221% |
| 3 | 7.282 | 655 | 663 | 679 | rVB | 174847 | 322361 | 11.96% | 2.308% |
| 4 | 8.128 | 800 | 807 | 814 | rBV | 123293 | 216746 | 8.04% | 1.552% |
| 5 | 9.291 | 997 | 1005 | 1014 | rVB | 413053 | 760677 | 28.23% | 5.445% |
| 6 | 9.420 | 1022 | 1027 | 1038 | rVB3 | 18668 | 42550 | 1.58% | 0.305% |
| 7 | 10.254 | 1163 | 1169 | 1176 | rVB3 | 18714 | 35862 | 1.33% | 0.257% |
| 8 | 10.942 | 1278 | 1286 | 1292 | rBV | 173829 | 312186 | 11.59% | 2.235% |
| 9 | 11.206 | 1325 | 1331 | 1334 | rBV4 | 14778 | 27667 | 1.03% | 0.198% |
| 10 | 11.370 | 1348 | 1359 | 1365 | rVB7 | 14081 | 35251 | 1.31% | 0.252% |
| 11 | 11.741 | 1413 | 1422 | 1435 | rVB8 | 22788 | 67209 | 2.49% | 0.481% |
| 12 | 13.027 | 1637 | 1641 | 1647 | rBV4 | 17855 | 29234 | 1.08% | 0.209% |
| 13 | 13.203 | 1664 | 1671 | 1680 | rVB8 | 10859 | 29889 | 1.11% | 0.214% |
| 14 | 13.374 | 1693 | 1700 | 1709 | rVB | 1108635 | 1740002 | 64.57% | 12.455% |
| 15 | 13.661 | 1742 | 1749 | 1759 | rBV3 | 51326 | 99848 | 3.71% | 0.715% |
| 16 | 14.155 | 1831 | 1833 | 1844 | rVB7 | 17491 | 27201 | 1.01% | 0.195% |
| 17 | 14.590 | 1900 | 1907 | 1912 | rVB5 | 13970 | 31785 | 1.18% | 0.228% |
| 18 | 14.701 | 1921 | 1926 | 1927 | rBV | 31130 | 38845 | 1.44% | 0.278% |
| 19 | 14.748 | 1927 | 1934 | 1940 | rVB | 298425 | 506053 | 18.78% | 3.622% |
| 20 | 14.819 | 1940 | 1946 | 1952 | rBV4 | 36405 | 72117 | 2.68% | 0.516% |
| 21 | 15.159 | 1996 | 2004 | 2015 | rBV3 | 163074 | 293717 | 10.90% | 2.102% |
| 22 | 15.676 | 2088 | 2092 | 2098 | rBV | 24902 | 31371 | 1.16% | 0.225% |
| 23 | 15.941 | 2129 | 2137 | 2142 | rBV | 78054 | 104789 | 3.89% | 0.750% |
| 24 | 16.052 | 2149 | 2156 | 2159 | rBV4 | 20037 | 31918 | 1.18% | 0.228% |
| 25 | 16.093 | 2159 | 2163 | 2171 | rVV | 103931 | 161380 | 5.99% | 1.155% |
| 26 | 16.170 | 2171 | 2176 | 2180 | rVV2 | 31390 | 45055 | 1.67% | 0.323% |
| 27 | 16.234 | 2180 | 2187 | 2193 | rVV | 993462 | 1482083 | 55.00% | 10.609% |
| 28 | 16.505 | 2229 | 2233 | 2239 | rVB | 24190 | 39720 | 1.47% | 0.284% |
| 29 | 16.869 | 2290 | 2295 | 2304 | rBV4 | 108033 | 238406 | 8.85% | 1.707% |
| 30 | 16.975 | 2309 | 2313 | 2320 | rVB | 25326 | 41732 | 1.55% | 0.299% |
| 31 | 17.133 | 2333 | 2340 | 2345 | rVB | 30279 | 57963 | 2.15% | 0.415% |
| 32 | 17.257 | 2355 | 2361 | 2370 | rBV4 | 44215 | 81740 | 3.03% | 0.585% |
| 33 | 17.492 | 2395 | 2401 | 2406 | rBV | 367621 | 563786 | 20.92% | 4.036% |
| 34 | 17.533 | 2406 | 2408 | 2414 | rVB2 | 26035 | 28163 | 1.05% | 0.202% |
| 35 | 17.785 | 2447 | 2451 | 2456 | rVB2 | 24862 | 38395 | 1.42% | 0.275% |
| 36 | 17.891 | 2465 | 2469 | 2475 | rVB3 | 34346 | 69254 | 2.57% | 0.496% |

LSC Area Percent Report

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Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

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-BG031522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 18.044 | 2491 | 2495 | 2502 | rBV | 38114 | 70451 | 2.61% | 0.504% |
| 38 | 18.255 | 2526 | 2531 | 2538 | rBV5 | 41806 | 77987 | 2.89% | 0.558% |
| 39 | 18.373 | 2547 | 2551 | 2555 | rBV5 | 37412 | 55325 | 2.05% | 0.396% |
| 40 | 18.449 | 2560 | 2564 | 2569 | rVV | 61462 | 91259 | 3.39% | 0.653% |
| 41 | 18.508 | 2571 | 2574 | 2578 | rVB2 | 30769 | 35494 | 1.32% | 0.254% |
| 42 | 18.696 | 2602 | 2606 | 2613 | rBV8 | 31931 | 70325 | 2.61% | 0.503% |
| 43 | 20.094 | 2838 | 2844 | 2849 | rBV | 2046688 | 2694579 | 100.00% | 19.288% |
| 44 | 20.141 | 2849 | 2852 | 2859 | rVB | 123110 | 173724 | 6.45% | 1.244% |
| 45 | 20.629 | 2931 | 2935 | 2940 | rVB | 65076 | 84645 | 3.14% | 0.606% |
| 46 | 21.134 | 3019 | 3021 | 3027 | rVB | 37073 | 50062 | 1.86% | 0.358% |
| 47 | 21.774 | 3125 | 3130 | 3138 | rVB2 | 328502 | 565630 | 20.99% | 4.049% |
| 48 | 24.741 | 3628 | 3635 | 3637 | rBV4 | 45310 | 99076 | 3.68% | 0.709% |
| 49 | 24.805 | 3638 | 3646 | 3656 | rVB | 451396 | 1130723 | 41.96% | 8.094% |
| 50 | 25.081 | 3684 | 3693 | 3706 | rVB2 | 205551 | 615010 | 22.82% | 4.402% |

Sum of corrected areas: 13969921

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053055.D
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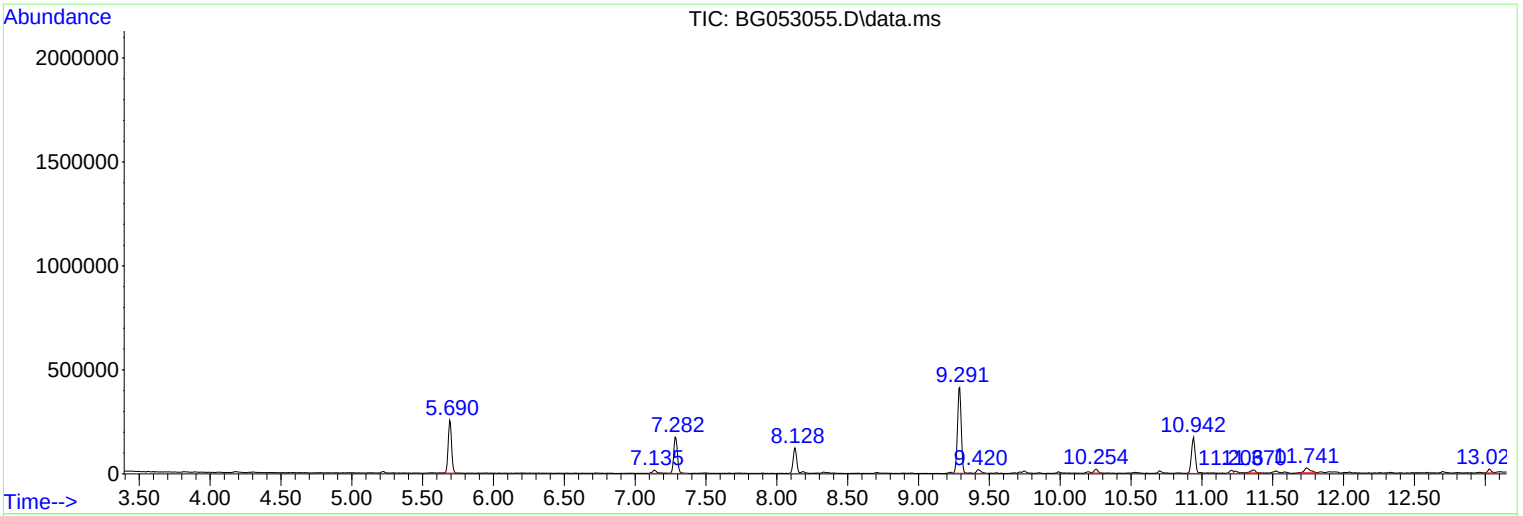
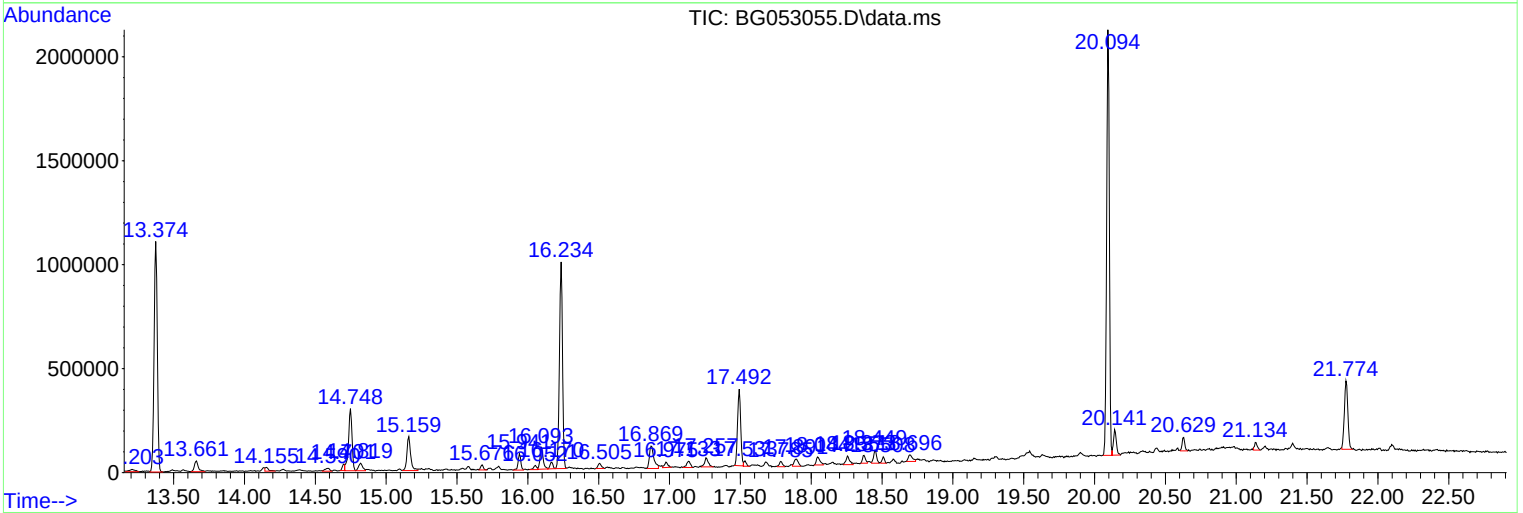
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

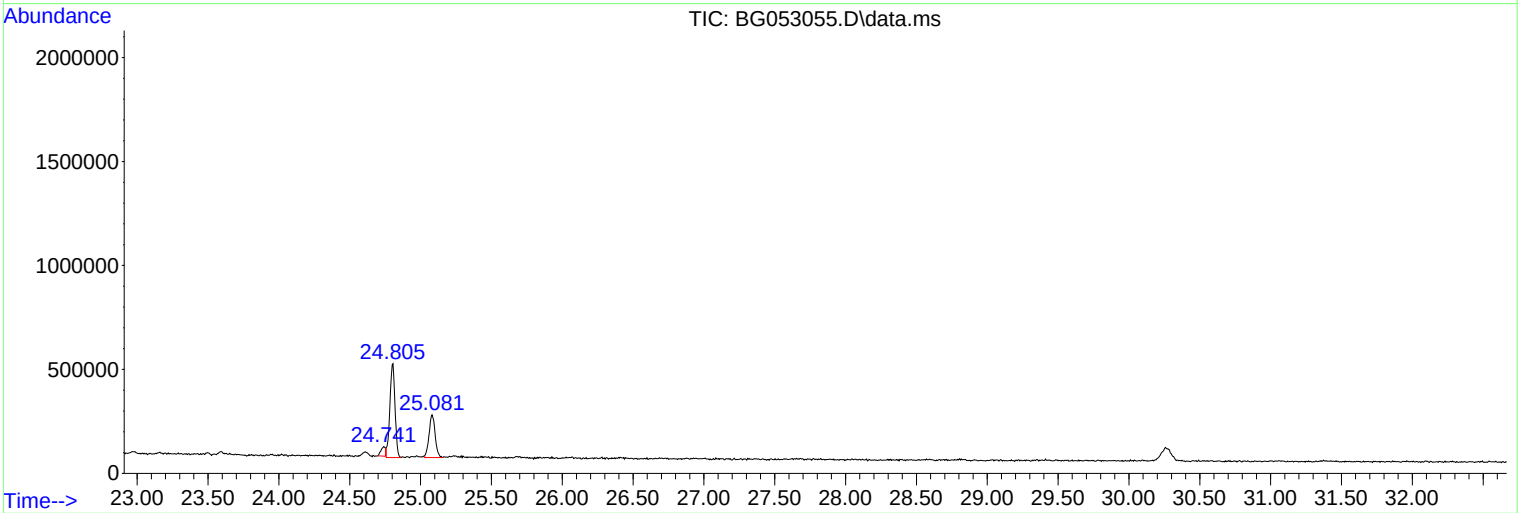
**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053055.D
Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

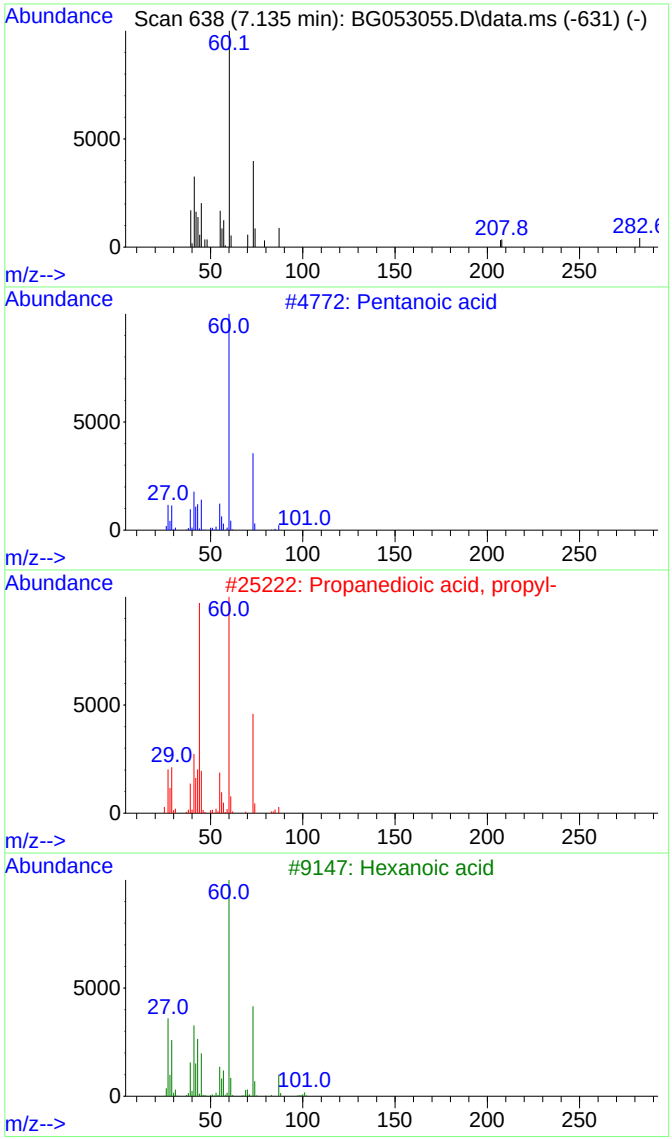
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

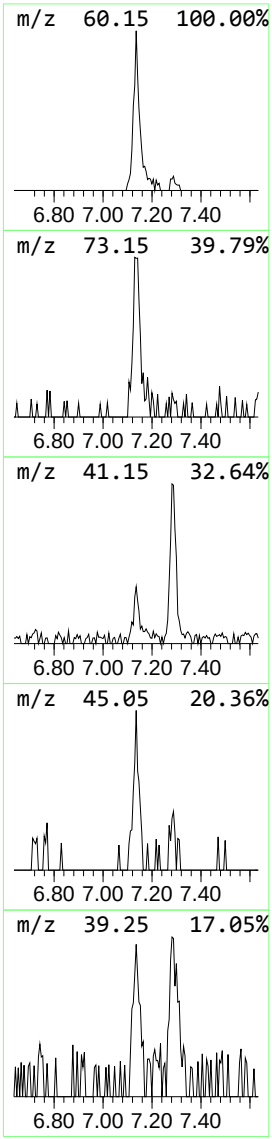
**********

Peak Number 1 Pentanoic acid Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.135 | 2.85 ng | 30869 | 1,4-Dichlorobenzene-d4 | 8.128 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentanoic acid | 102 | C5H10O2 | 000109-52-4 | 64 |
| 2 | Propanedioic acid, propyl- | 146 | C6H10O4 | 000616-62-6 | 64 |
| 3 | Hexanoic acid | 116 | C6H12O2 | 000142-62-1 | 64 |
| 4 | Butanoic acid, 4-chloro- | 122 | C4H7ClO2 | 000627-00-9 | 45 |
| 5 | Thiirane | 60 | C2H4S | 000420-12-2 | 40 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053055.D
Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

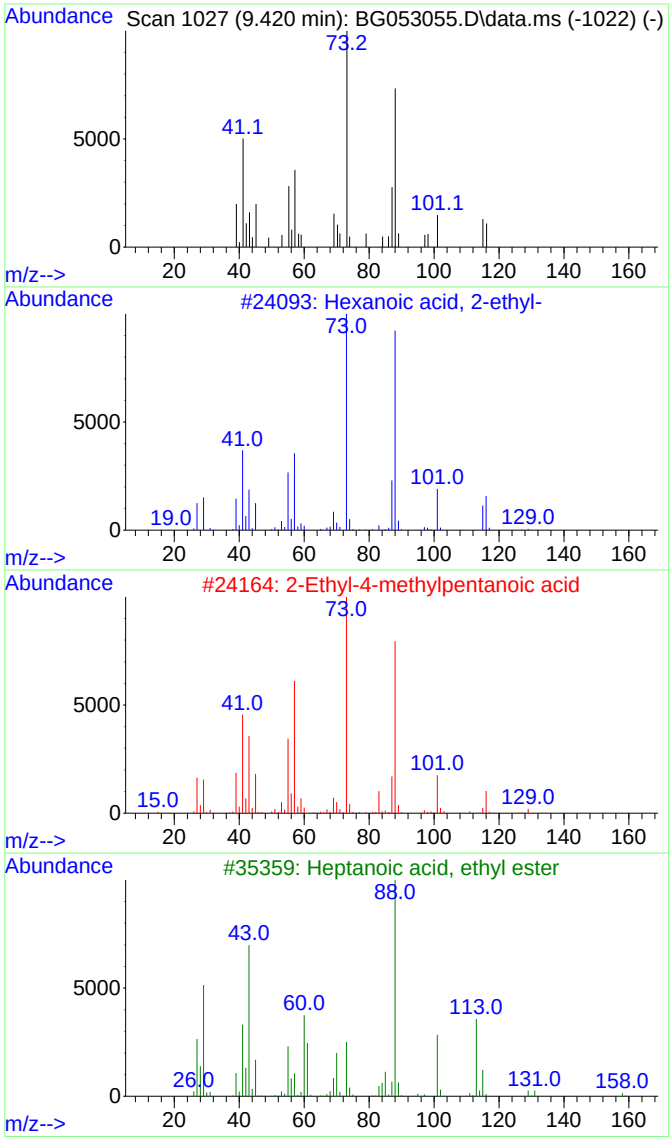
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

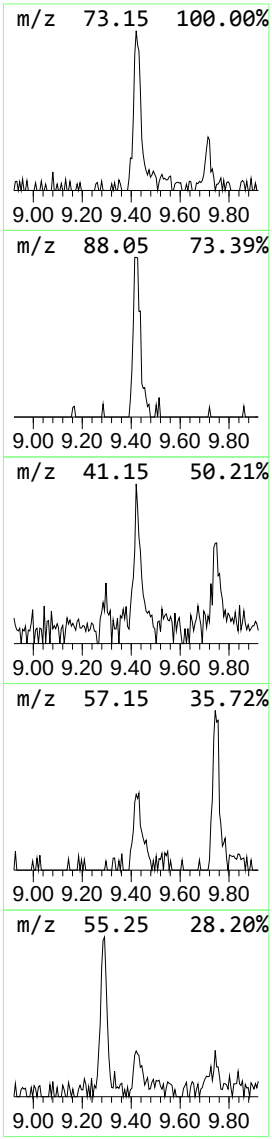
**********

Peak Number 2 Hexanoic acid, 2-ethyl- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.420 | 3.93 ng | 42550 | 1,4-Dichlorobenzene-d4 | 8.128 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexanoic acid, 2-ethyl- | 144 | C8H16O2 | 000149-57-5 | 64 |
| 2 | 2-Ethyl-4-methylpentanoic acid | 144 | C8H16O2 | 000108-81-6 | 59 |
| 3 | Heptanoic acid, ethyl ester | 158 | C9H18O2 | 000106-30-9 | 47 |
| 4 | Ethyl 5-methylhexanoate | 158 | C9H18O2 | 010236-10-9 | 47 |
| 5 | Hydrazine, 1,2-diethyl- | 88 | C4H12N2 | 001615-80-1 | 38 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053055.D
Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

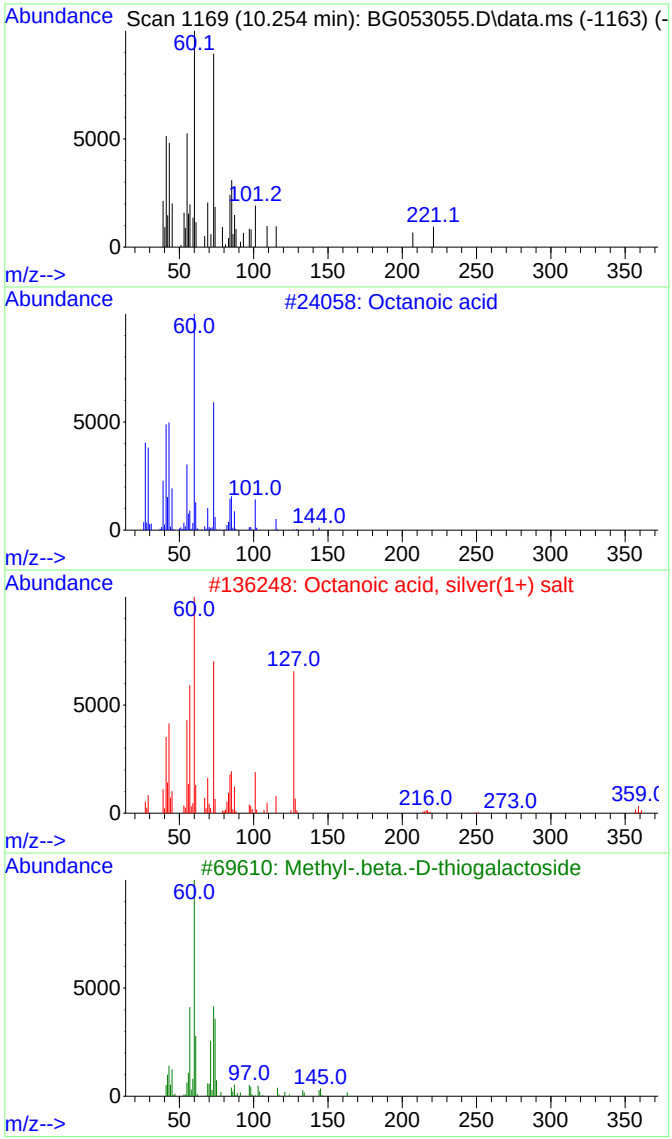
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

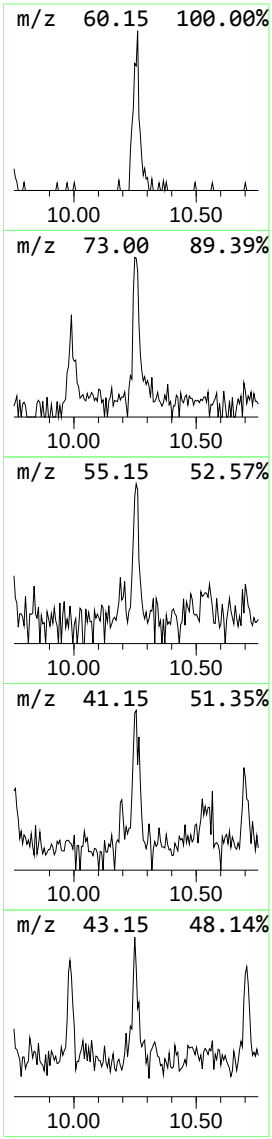
**********

Peak Number 3 Octanoic acid Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.254 | 2.30 ng | 35862 | Naphthalene-d8 | 10.942 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octanoic acid | 144 | C8H16O2 | 000124-07-2 | 64 |
| 2 | Octanoic acid, silver(1+) salt | 250 | C8H15AgO2 | 024927-67-1 | 50 |
| 3 | Methyl-.beta.-D-thiogalactoside | 194 | C7H14O6 | 001824-94-8 | 47 |
| 4 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 40 |
| 5 | .alpha.-d-Riboside, 1-O-dodecyl- | 318 | C17H34O5 | 1000154-76-8 | 40 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053055.D
Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

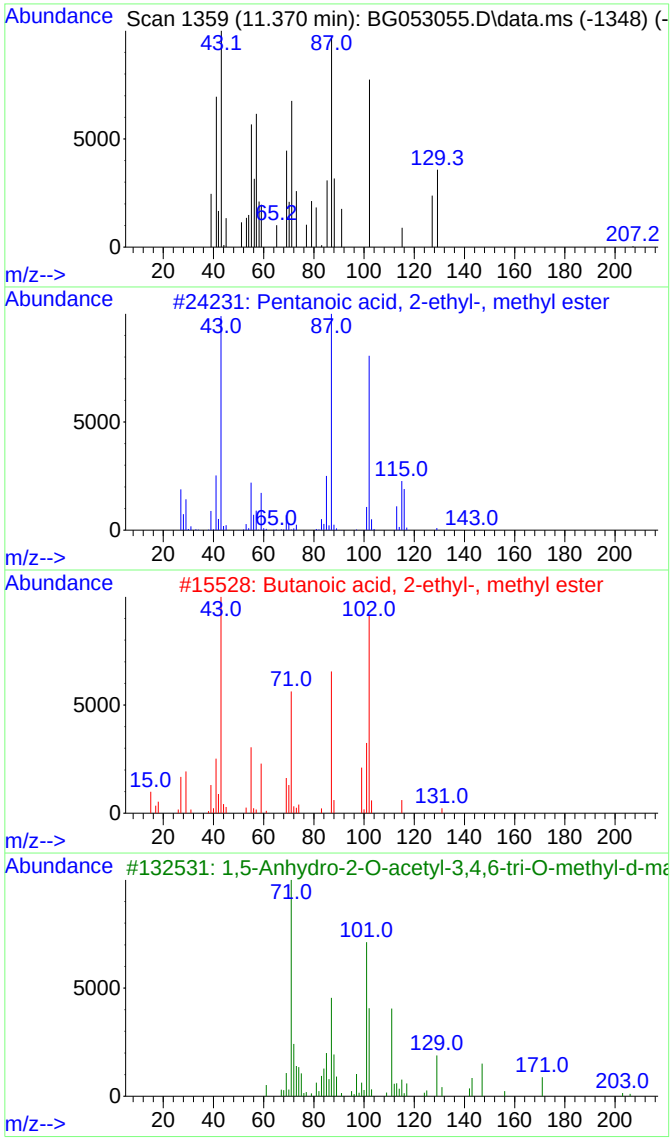
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

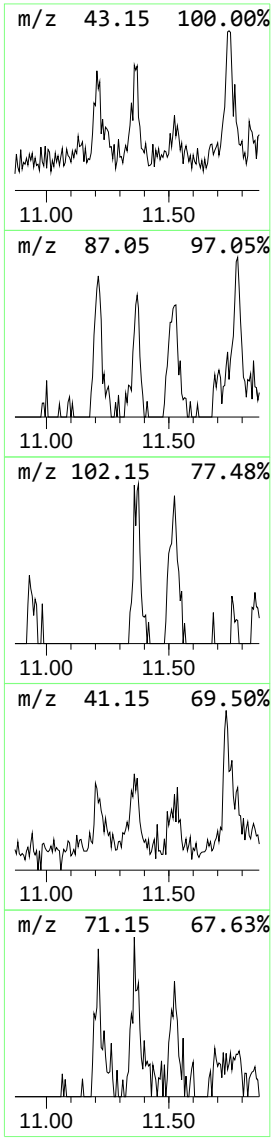
**********

Peak Number 4 unknown11.371 Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.371 | 2.26 ng | 35251 | Naphthalene-d8 | 10.942 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentanoic acid, 2-ethyl-, methyl... | 144 | C8H16O2 | 000816-16-0 | 38 |
| 2 | Butanoic acid, 2-ethyl-, methyl ... | 130 | C7H14O2 | 000816-11-5 | 37 |
| 3 | 1,5-Anhydro-2-O-acetyl-3,4,6-tri... | 248 | C11H20O6 | 093635-82-6 | 36 |
| 4 | 2-Butanone, 4-methoxy- | 102 | C5H10O2 | 006975-85-5 | 33 |
| 5 | 4-Isopropoxy-2-butanone | 130 | C7H14O2 | 032541-58-5 | 17 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053055.D
Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

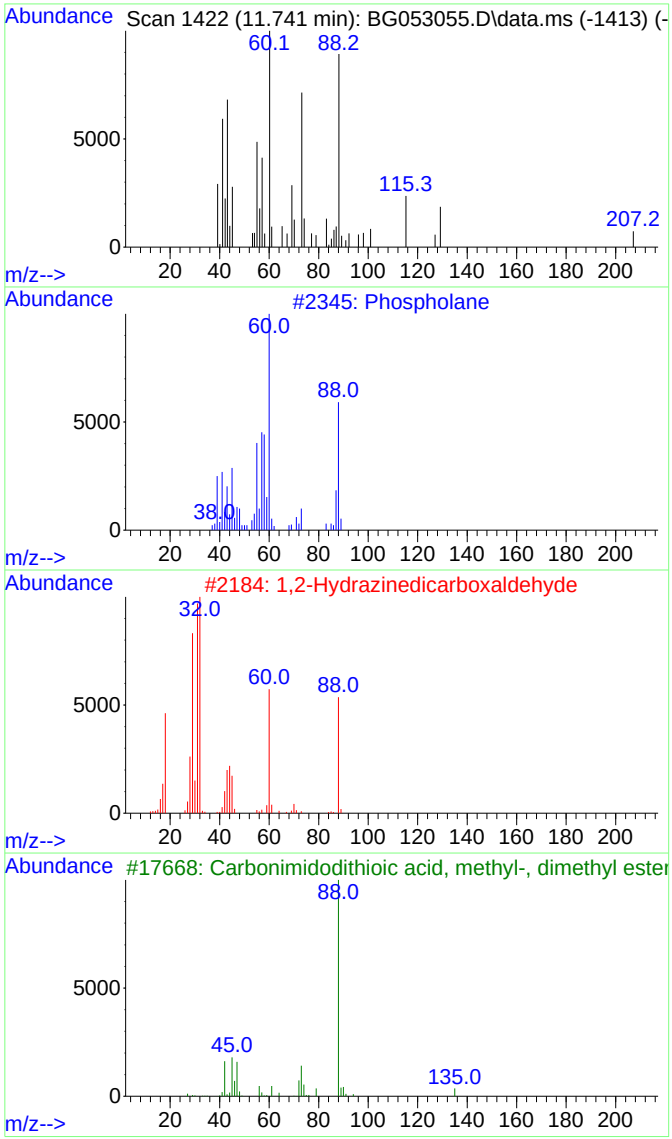
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

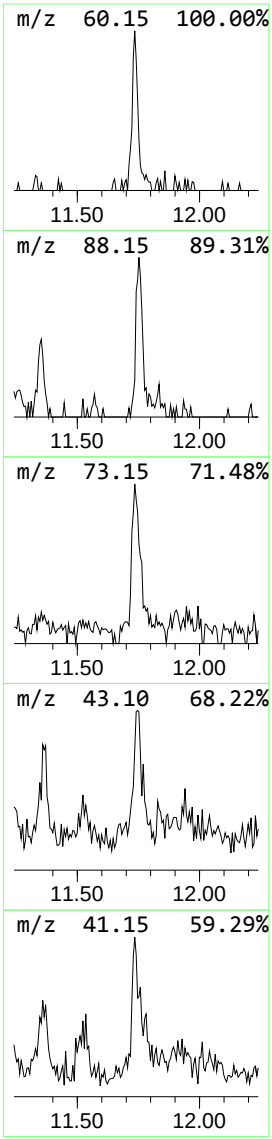
**********

Peak Number 5 Phospholane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.741 | 4.31 ng | 67209 | Naphthalene-d8 | 10.942 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phospholane | 88 | C4H9P | 003466-00-0 | 59 |
| 2 | 1,2-Hydrazinedicarboxaldehyde | 88 | C2H4N2O2 | 000628-36-4 | 50 |
| 3 | Carbonimidodithioic acid, methyl... | 135 | C4H9NS2 | 018805-25-9 | 43 |
| 4 | Serine, methyl ester | 119 | C4H9NO3 | 002104-89-4 | 42 |
| 5 | 1,5-Anhydro-l-rhamnitol | 148 | C6H12O4 | 1000129-02-4 | 38 |



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Data File : BG053055.D
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Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

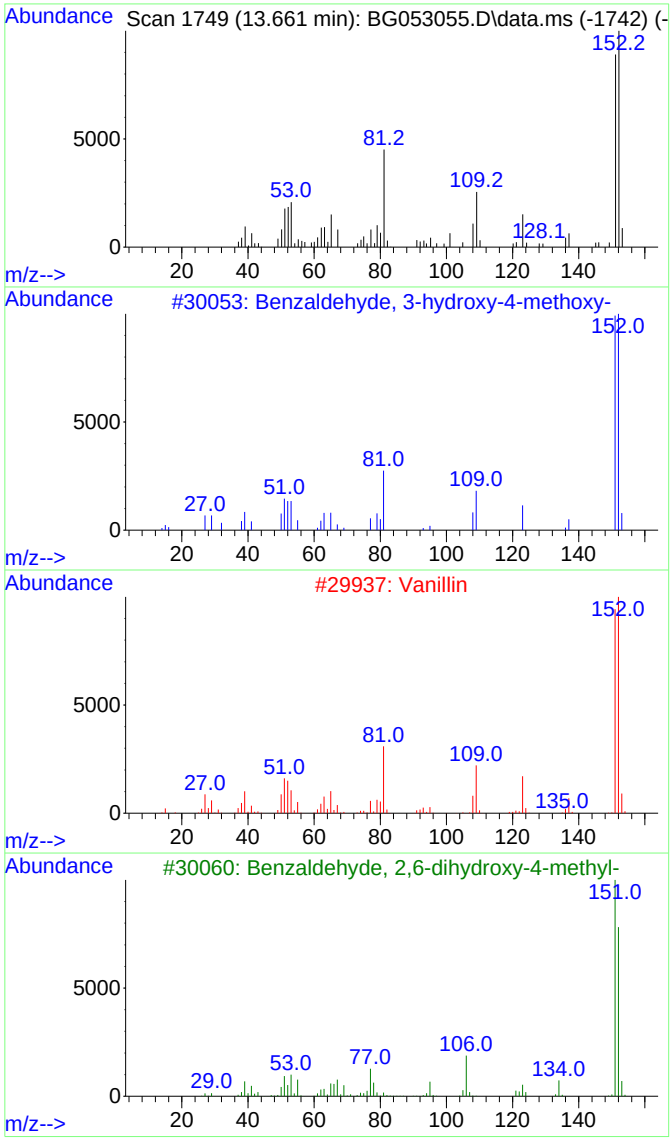
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

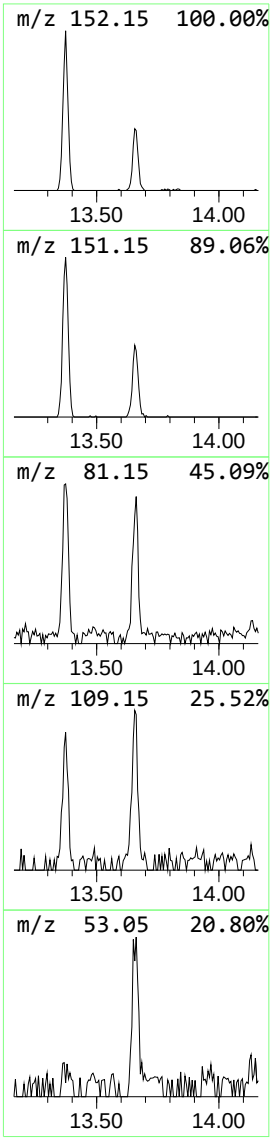
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 6 Benzaldehyde, 3-hydroxy-4-m... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.662 | 3.95 ng | 99848 | Acenaphthene-d10 | 14.748 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzaldehyde, 3-hydroxy-4-methoxy- | 152 | C8H8O3 | 000621-59-0 | 96 |
| 2 | Vanillin | 152 | C8H8O3 | 000121-33-5 | 96 |
| 3 | Benzaldehyde, 2,6-dihydroxy-4-me... | 152 | C8H8O3 | 000526-37-4 | 50 |
| 4 | 2,4-Dihydroxy-3-methylbenzaldehyde | 152 | C8H8O3 | 006248-20-0 | 47 |
| 5 | Benzaldehyde, 2-hydroxy-5-methoxy- | 152 | C8H8O3 | 000672-13-9 | 47 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053055.D
Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

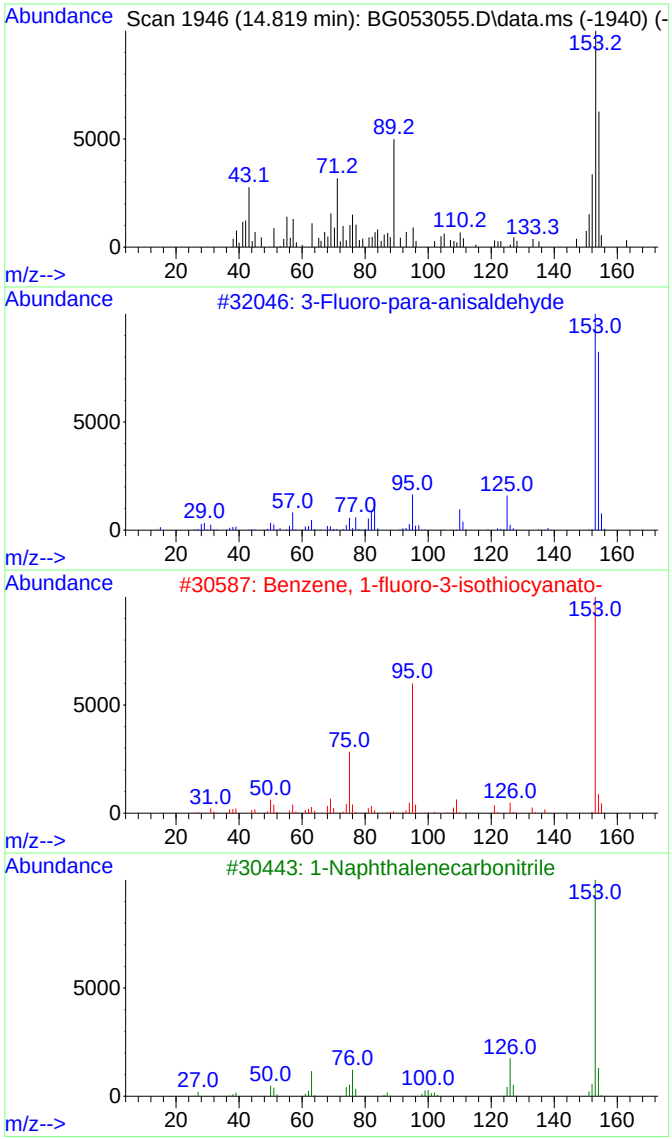
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

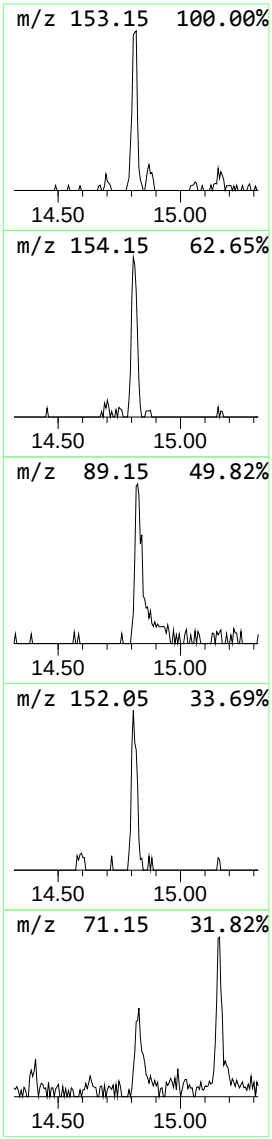
**********

Peak Number 7 unknown14.819 Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.819 | 2.85 ng | 72117 | Acenaphthene-d10 | 14.748 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Fluoro-para-anisaldehyde | 154 | C8H7FO2 | 000351-54-2 | 38 |
| 2 | Benzene, 1-fluoro-3-isothiocyanato- | 153 | C7H4FNS | 000404-72-8 | 30 |
| 3 | 1-Naphthalenecarbonitrile | 153 | C11H7N | 000086-53-3 | 27 |
| 4 | Acenaphthene | 154 | C12H10 | 000083-32-9 | 27 |
| 5 | 2,4,6-Trihydroxybenzaldehyde | 154 | C7H6O4 | 000487-70-7 | 25 |



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Data File : BG053055.D
Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

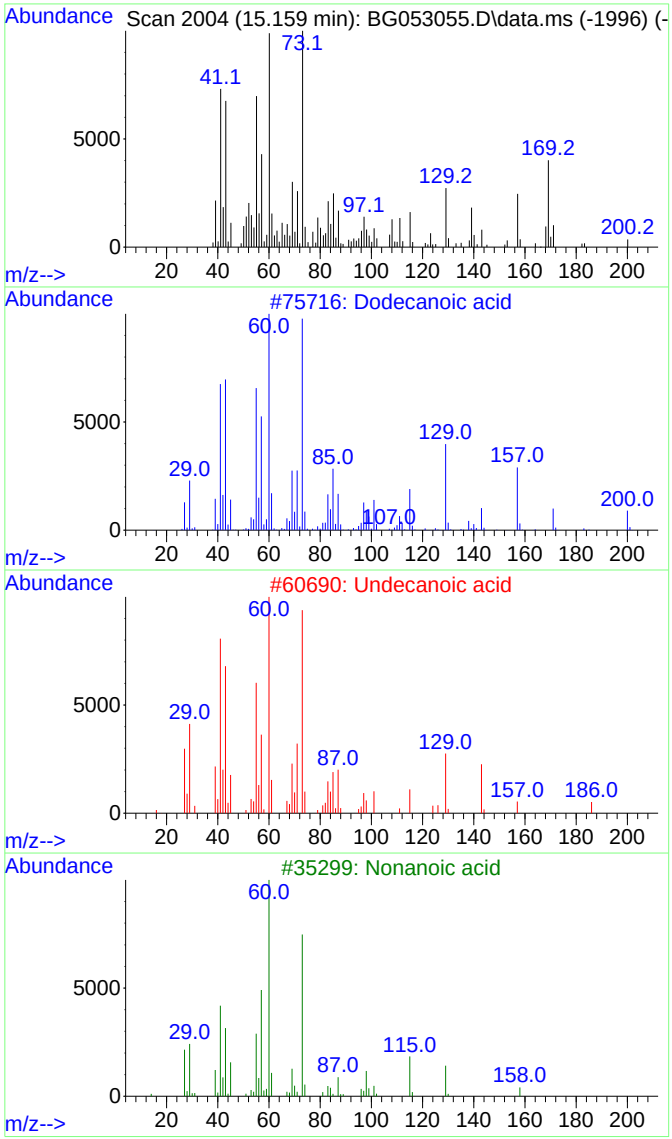
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

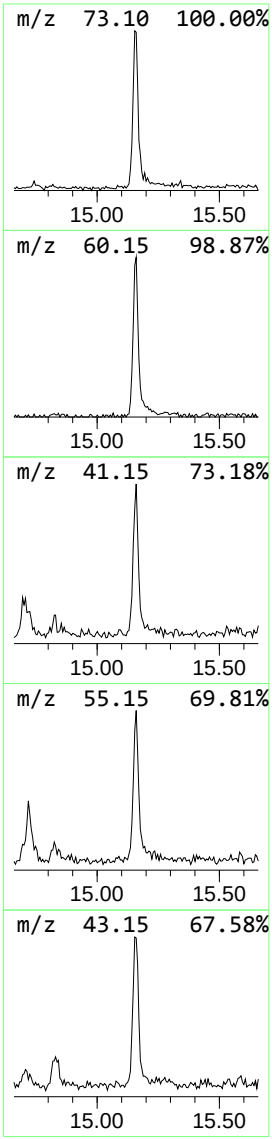
**********

Peak Number 8 Dodecanoic acid Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.160 | 11.61 ng | 293717 | Acenaphthene-d10 | 14.748 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 83 |
| 2 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 35 |
| 3 | Nonanoic acid | 158 | C9H18O2 | 000112-05-0 | 30 |
| 4 | Octanoic acid, silver(1+) salt | 250 | C8H15AgO2 | 024927-67-1 | 27 |
| 5 | Octanoic acid | 144 | C8H16O2 | 000124-07-2 | 27 |



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Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

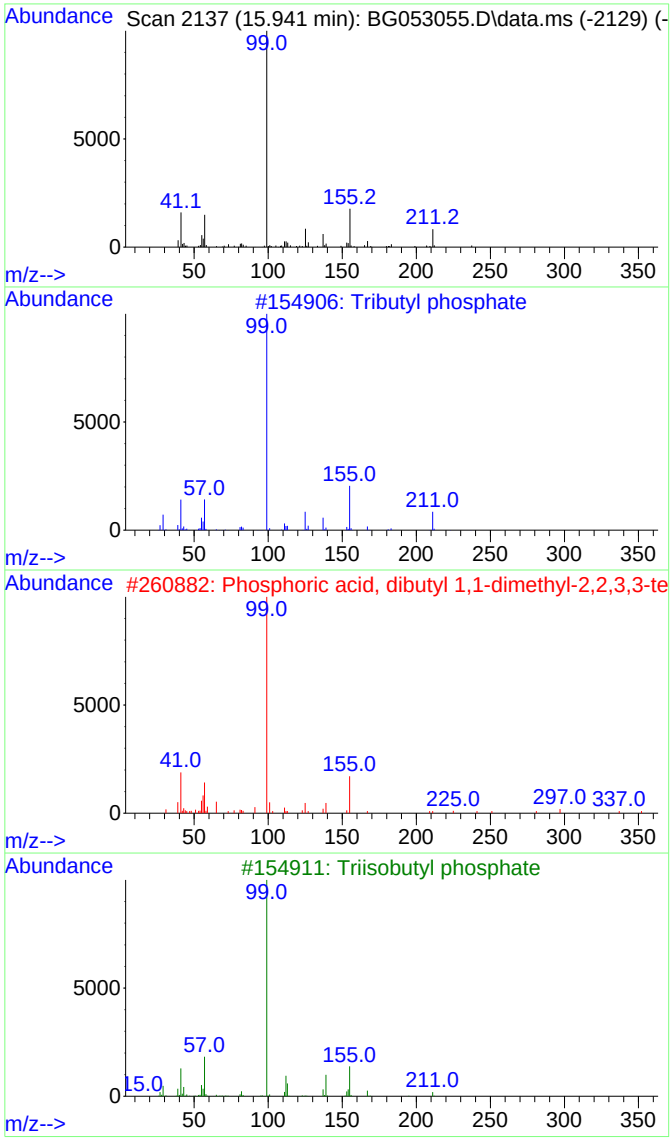
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

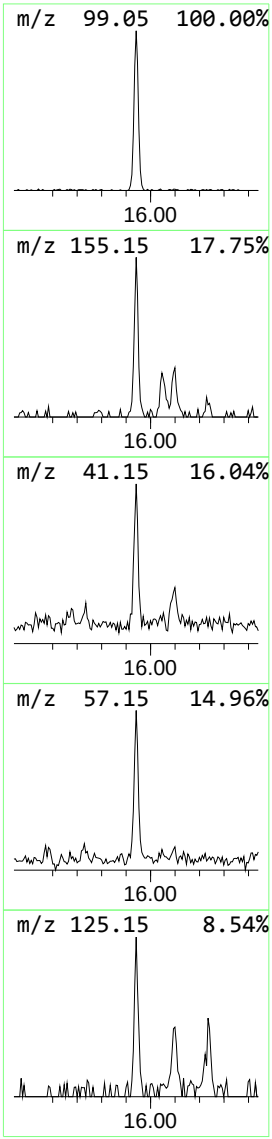
**********

Peak Number 9 Tributyl phosphate Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.941 | 4.14 ng | 104789 | Acenaphthene-d10 | 14.748 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tributyl phosphate | 266 | C12H27O4P | 000126-73-8 | 91 |
| 2 | Phosphoric acid, dibutyl 1,1-dim... | 352 | C13H25F4O4P | 1000298-93-9 | 56 |
| 3 | Triisobutyl phosphate | 266 | C12H27O4P | 000126-71-6 | 56 |
| 4 | 1,4-Dioxaspiro[4.6]undec-7-ene | 154 | C9H14O2 | 007140-60-5 | 52 |
| 5 | Phosphoric acid, tris(2-ethylhex... | 434 | C24H51O4P | 000078-42-2 | 45 |



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Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

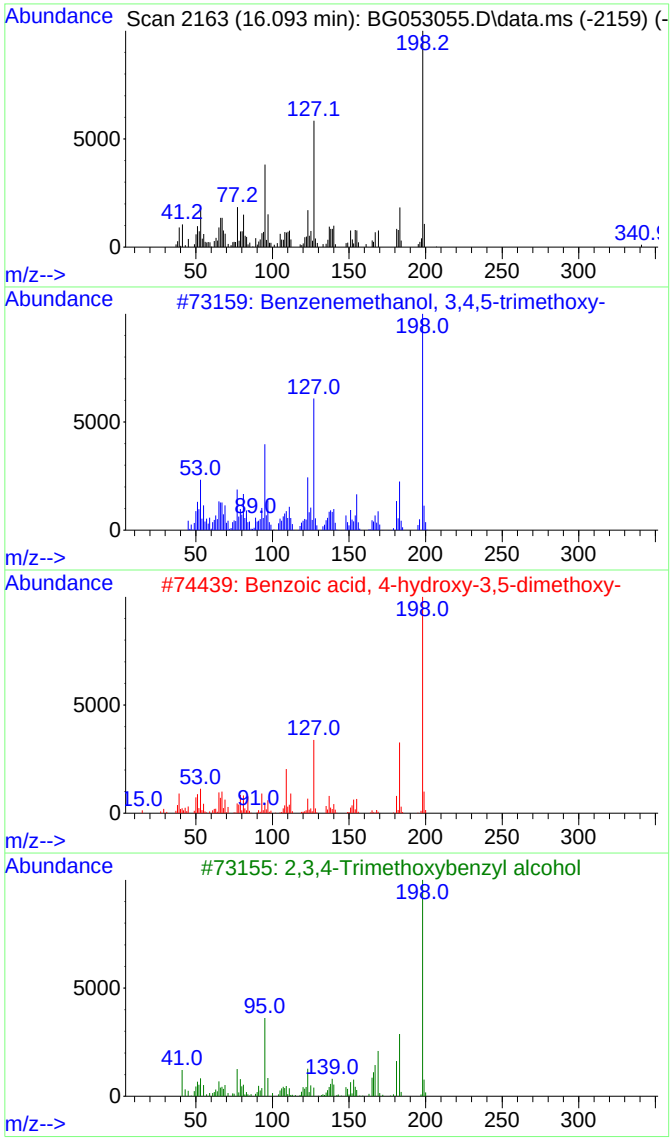
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

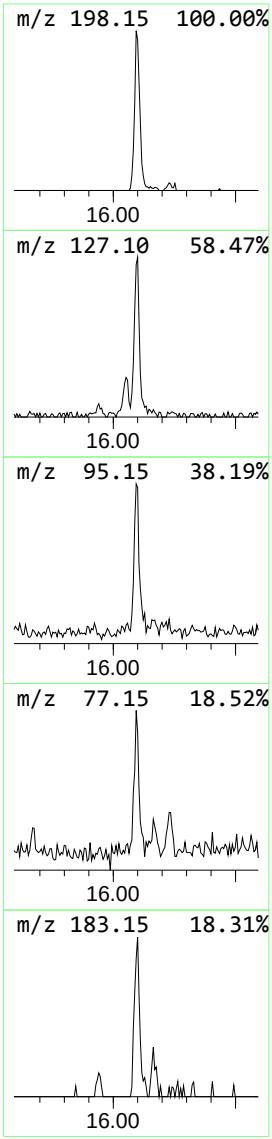
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 10 Benzenemethanol, 3,4,5-trim... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.093 | 6.38 ng | 161380 | Acenaphthene-d10 | 14.748 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzenemethanol, 3,4,5-trimethoxy- | 198 | C10H14O4 | 003840-31-1 | 91 |
| 2 | Benzoic acid, 4-hydroxy-3,5-dime... | 198 | C9H10O5 | 000530-57-4 | 70 |
| 3 | 2,3,4-Trimethoxybenzyl alcohol | 198 | C10H14O4 | 071989-96-3 | 58 |
| 4 | 1,2,3,4-Tetramethoxybenzene | 198 | C10H14O4 | 021450-56-6 | 49 |
| 5 | 3-Hydroxy-4,5-dimethoxybenzoic acid | 198 | C9H10O5 | 001916-08-1 | 49 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053055.D
Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

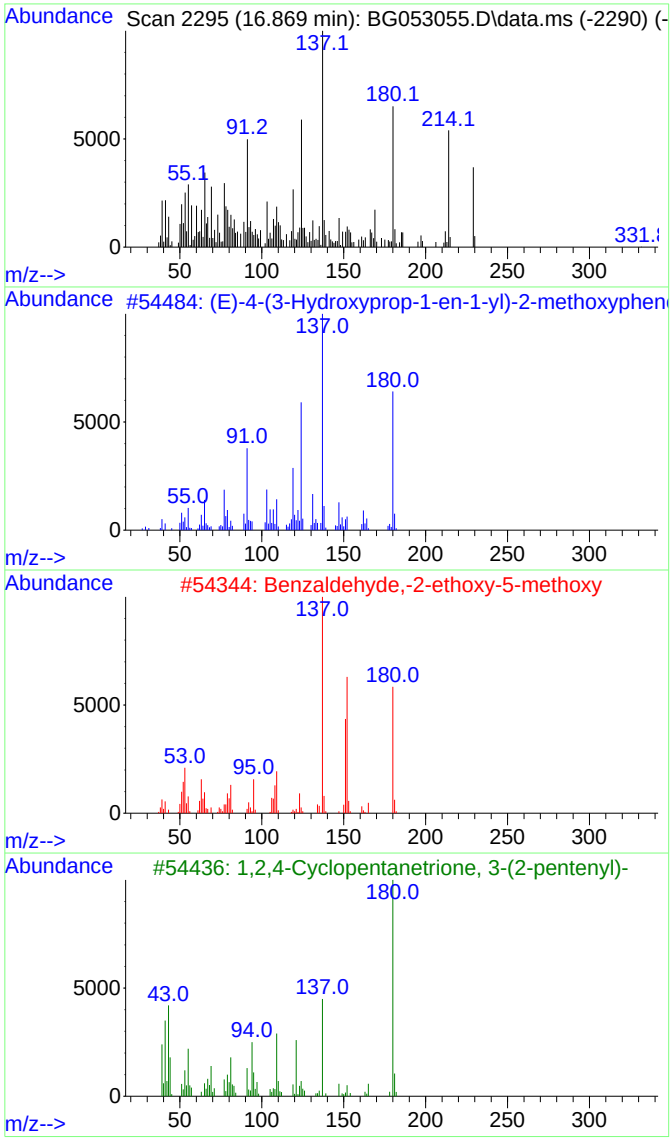
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

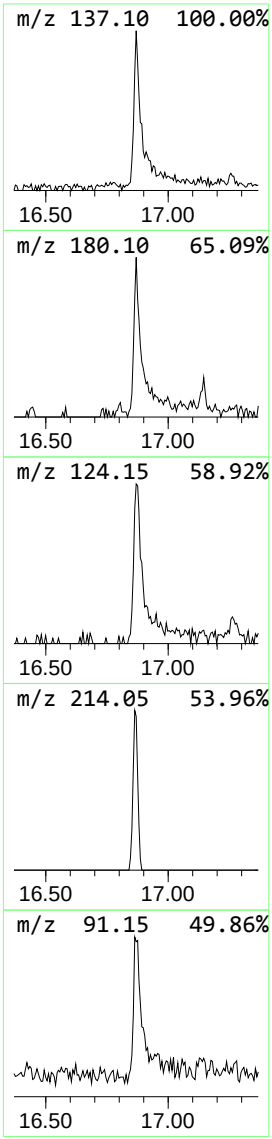
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 11 (E)-4-(3-Hydroxyprop-1-en-1... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.869 | 8.46 ng | 238406 | Phenanthrene-d10 | 17.492 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (E)-4-(3-Hydroxyprop-1-en-1-yl)-... | 180 | C10H12O3 | 032811-40-8 | 91 |
| 2 | Benzaldehyde,-2-ethoxy-5-methoxy | 180 | C10H12O3 | 039206-04-7 | 42 |
| 3 | 1,2,4-Cyclopentanetrione, 3-(2-p... | 180 | C10H12O3 | 054644-27-8 | 41 |
| 4 | Benzenecarbothioamide | 137 | C7H7NS | 002227-79-4 | 38 |
| 5 | (4-Methylphenylthio)acetone | 180 | C10H12OS | 001200-13-1 | 30 |



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Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

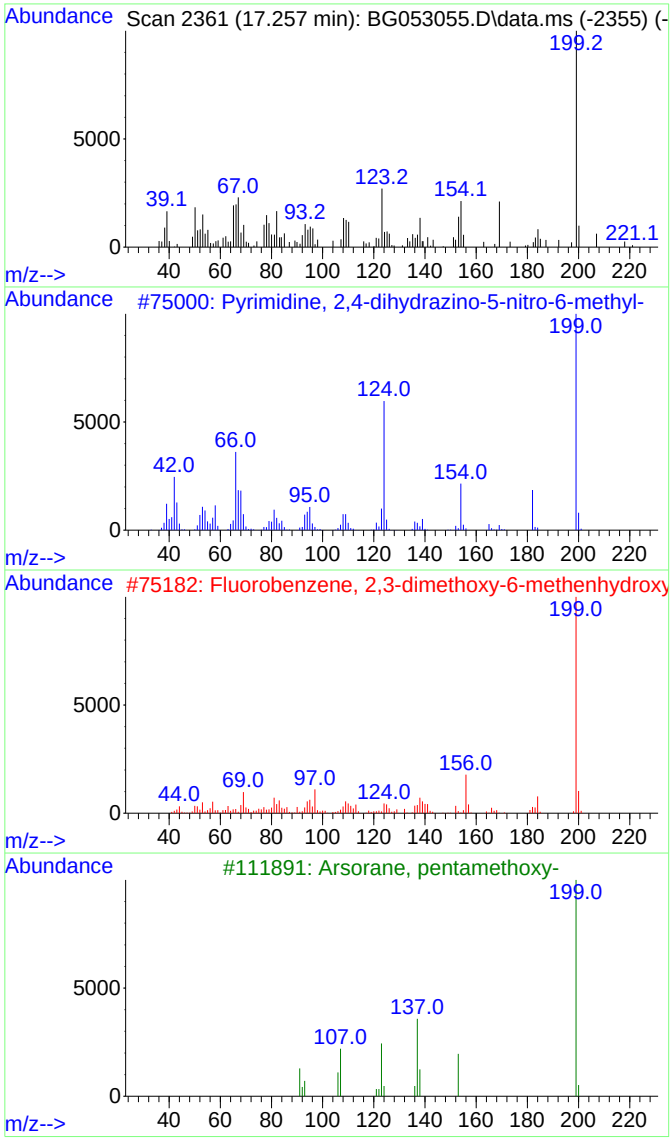
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

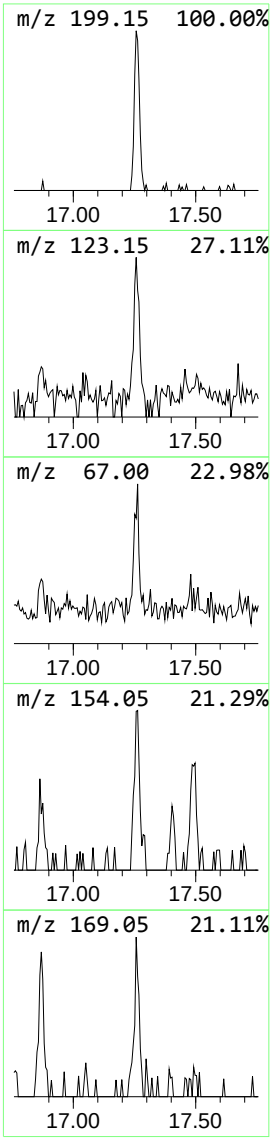
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 12 Pyrimidine, 2,4-dihydrazino... Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.257 | 2.90 ng | 81740 | Phenanthrene-d10 | 17.492 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pyrimidine, 2,4-dihydrazino-5-ni... | 199 | C5H9N7O2 | 030561-02-5 | 60 |
| 2 | Fluorobenzene, 2,3-dimethoxy-6-m... | 199 | C9H10FNO3 | 1000116-17-6 | 42 |
| 3 | Arsorane, pentamethoxy- | 230 | C5H15AsO5 | 002087-23-2 | 40 |
| 4 | Fluorobenzene, 4,5-dimethoxy-2-m... | 199 | C9H10FNO3 | 1000116-17-4 | 27 |
| 5 | 3,4-Dihydroxy-5-nitrobenzoic acid | 199 | C7H5NO6 | 084211-30-3 | 25 |



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Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

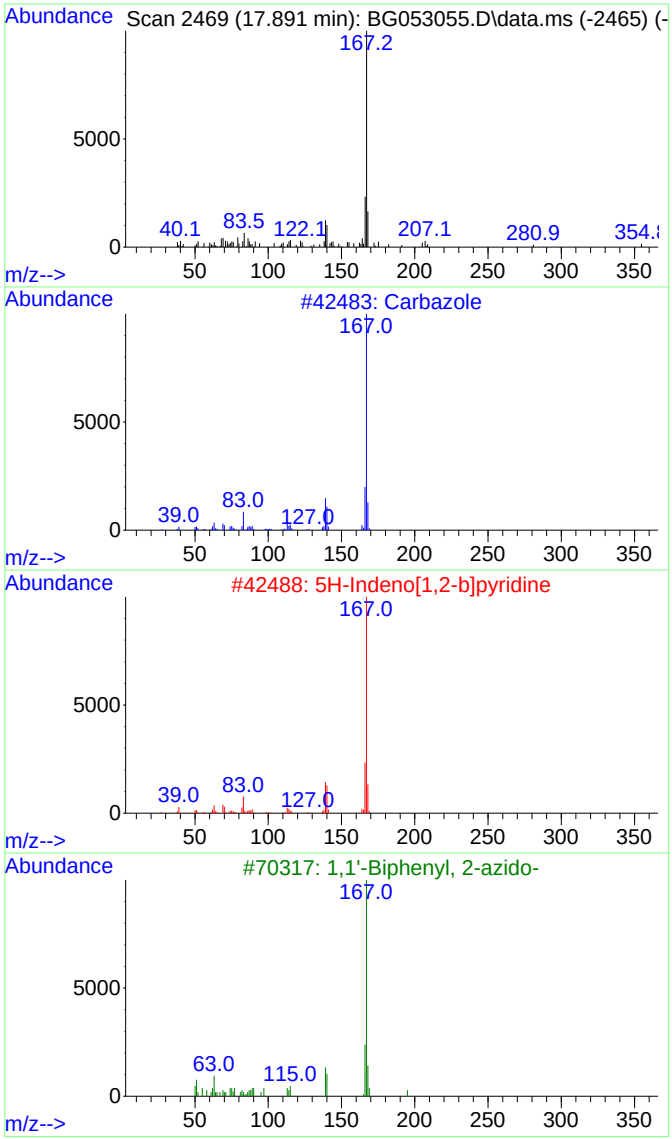
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

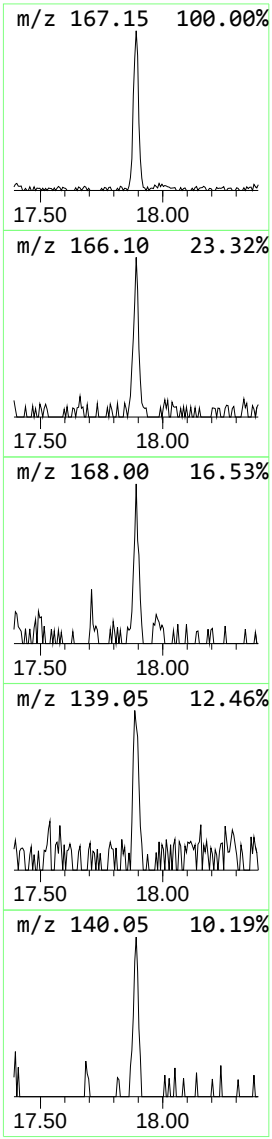
**********

Peak Number 13 5H-Indeno[1,2-b]pyridine Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.891 | 2.46 ng | 69254 | Phenanthrene-d10 | 17.492 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Carbazole | 167 | C12H9N | 000086-74-8 | 91 |
| 2 | 5H-Indeno[1,2-b]pyridine | 167 | C12H9N | 000244-99-5 | 80 |
| 3 | 1,1'-Biphenyl, 2-azido- | 195 | C12H9N3 | 007599-23-7 | 78 |
| 4 | 9H-Carbazole, 9-nitroso- | 196 | C12H8N2O | 002788-23-0 | 74 |
| 5 | 9H-Carbazole-9-methanol | 197 | C13H11NO | 002409-36-1 | 74 |



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Data File : BG053055.D
Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

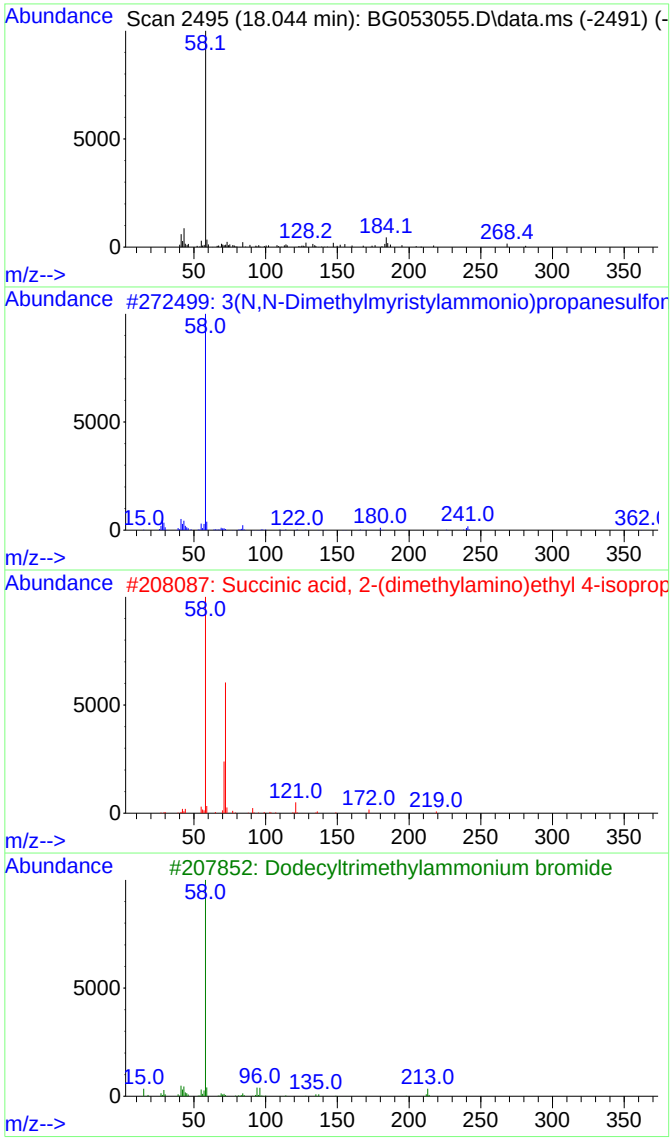
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

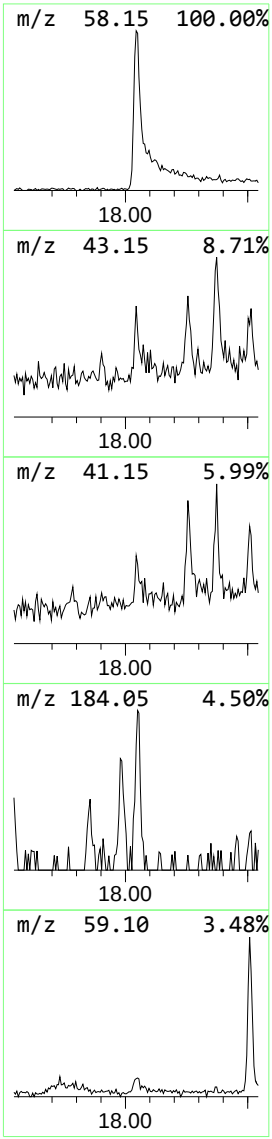
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 14 3(N,N-Dimethylmyristylammon... Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.044 | 2.50 ng | 70451 | Phenanthrene-d10 | 17.492 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3(N,N-Dimethylmyristylammonio)pr... | 363 | C19H41NO3S | 014933-09-6 | 64 |
| 2 | Succinic acid, 2-(dimethylamino)... | 307 | C17H25NO4 | 1000360-71-8 | 64 |
| 3 | Dodecyltrimethylammonium bromide | 307 | C15H34BrN | 001119-94-4 | 64 |
| 4 | Cetrimonium Bromide | 363 | C19H42BrN | 000057-09-0 | 64 |
| 5 | Tetradonium Bromide | 335 | C17H38BrN | 001119-97-7 | 64 |



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Data File : BG053055.D
Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

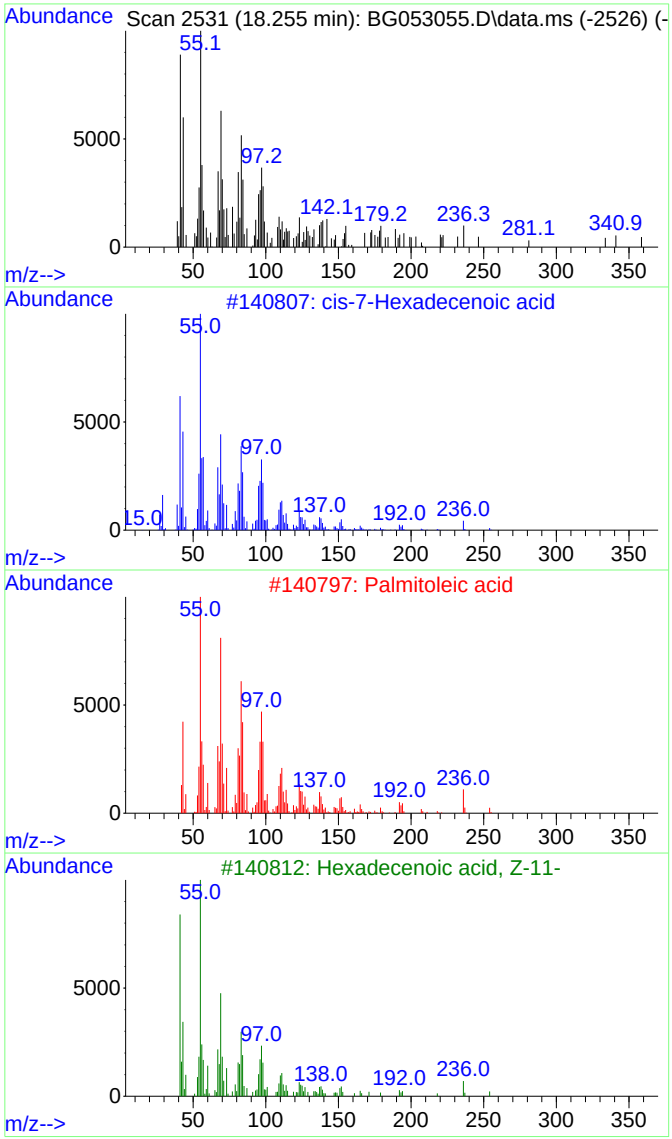
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

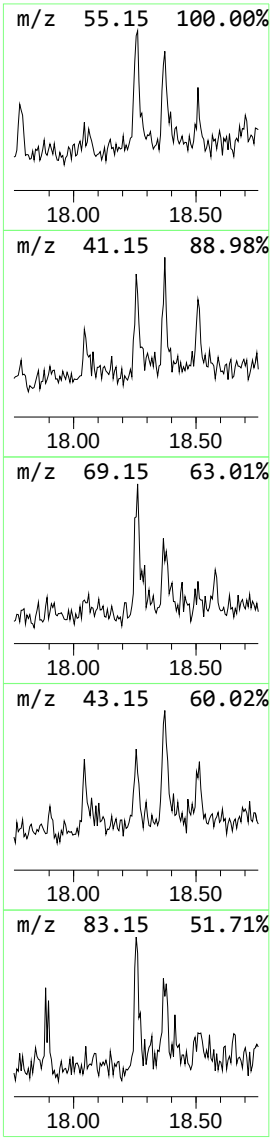
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 15 cis-7-Hexadecenoic acid Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.255 | 2.77 ng | 77987 | Phenanthrene-d10 | 17.492 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | cis-7-Hexadecenoic acid | 254 | C16H30O2 | 002416-19-5 | 87 |
| 2 | Palmitoleic acid | 254 | C16H30O2 | 000373-49-9 | 83 |
| 3 | Hexadecenoic acid, Z-11- | 254 | C16H30O2 | 002416-20-8 | 80 |
| 4 | (E)-Hexadec-9-enoic acid | 254 | C16H30O2 | 010030-73-6 | 74 |
| 5 | 6-Pentadecenoic acid, 13-methyl-... | 254 | C16H30O2 | 682751-34-4 | 58 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053055.D
Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

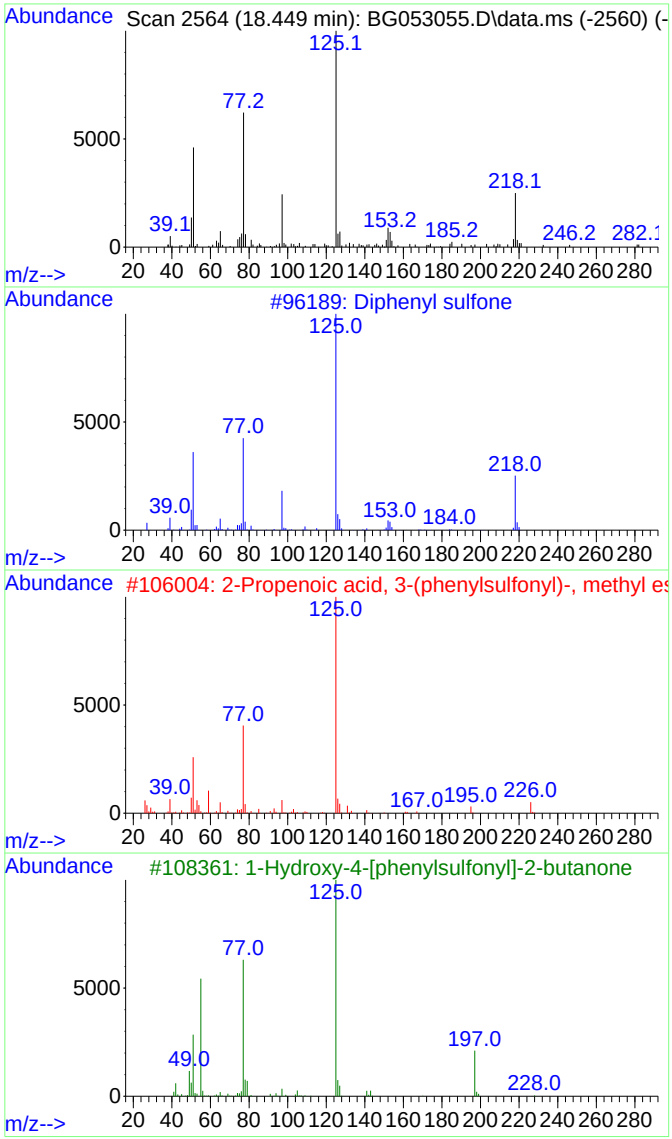
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

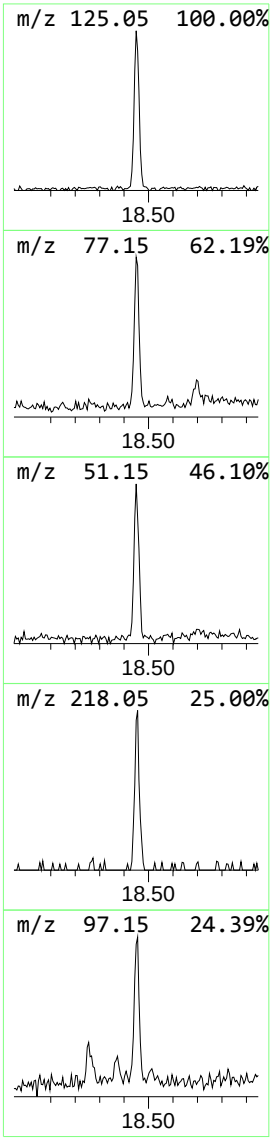
**********

Peak Number 16 Diphenyl sulfone Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.449 | 3.24 ng | 91259 | Phenanthrene-d10 | 17.492 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Diphenyl sulfone | 218 | C12H10O2S | 000127-63-9 | 91 |
| 2 | 2-Propenoic acid, 3-(phenylsulfo... | 226 | C10H10O4S | 063068-63-3 | 59 |
| 3 | 1-Hydroxy-4-[phenylsulfonyl]-2-b... | 228 | C10H12O4S | 160956-37-6 | 40 |
| 4 | Benzene, (1-propenylsulfonyl)-, ... | 182 | C9H10O2S | 028691-72-7 | 39 |
| 5 | 2-Propenenitrile, 3-(phenylsulfo... | 193 | C9H7NO2S | 001424-51-7 | 38 |



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Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

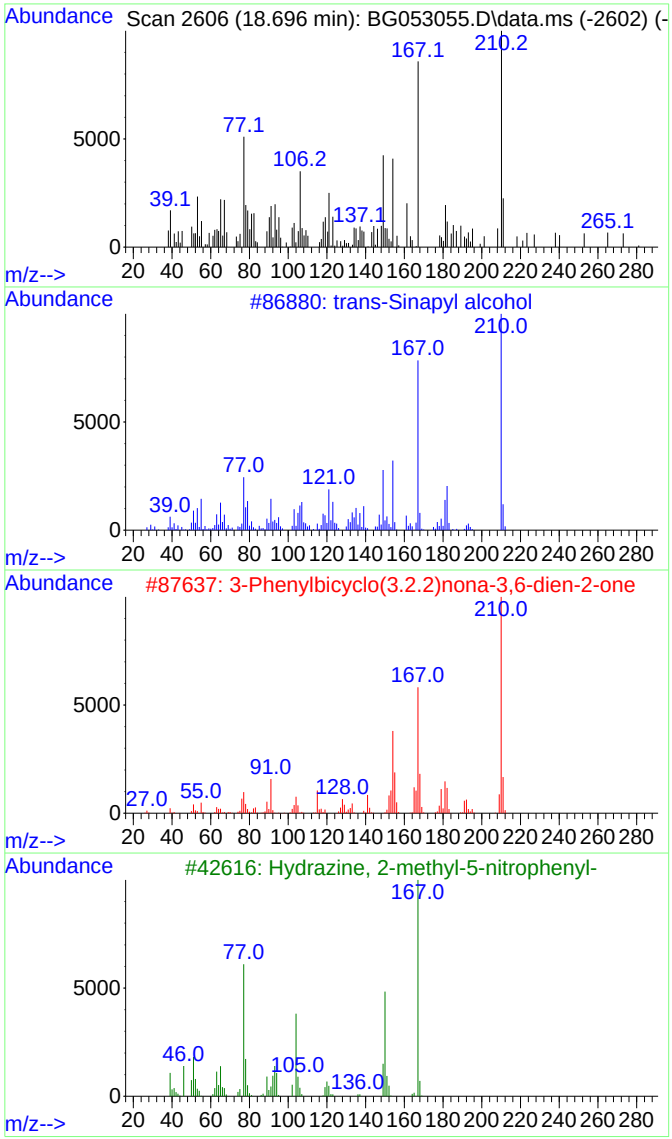
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

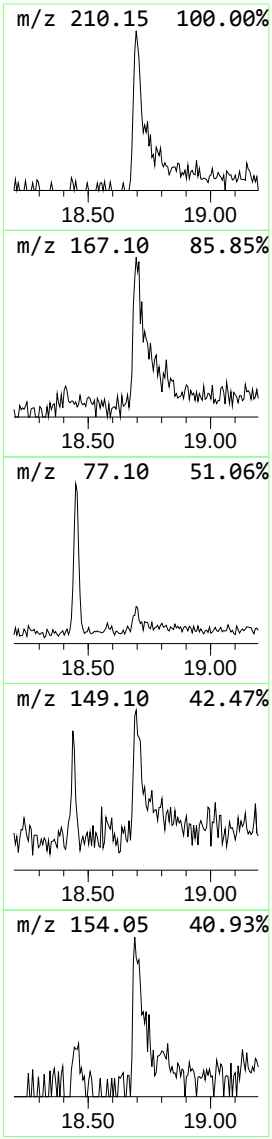
**********

Peak Number 17 trans-Sinapyl alcohol Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.696 | 2.49 ng | 70325 | Phenanthrene-d10 | 17.492 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | trans-Sinapyl alcohol | 210 | C11H14O4 | 020675-96-1 | 64 |
| 2 | 3-Phenylbicyclo(3.2.2)nona-3,6-d... | 210 | C15H14O | 073830-83-8 | 58 |
| 3 | Hydrazine, 2-methyl-5-nitrophenyl- | 167 | C7H9N3O2 | 005089-08-7 | 25 |
| 4 | Altretamine | 210 | C9H18N6 | 000645-05-6 | 25 |
| 5 | Benzaldehydrazine, N-methyl-N-ph... | 210 | C14H14N2 | 1000128-92-5 | 22 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053055.D
Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

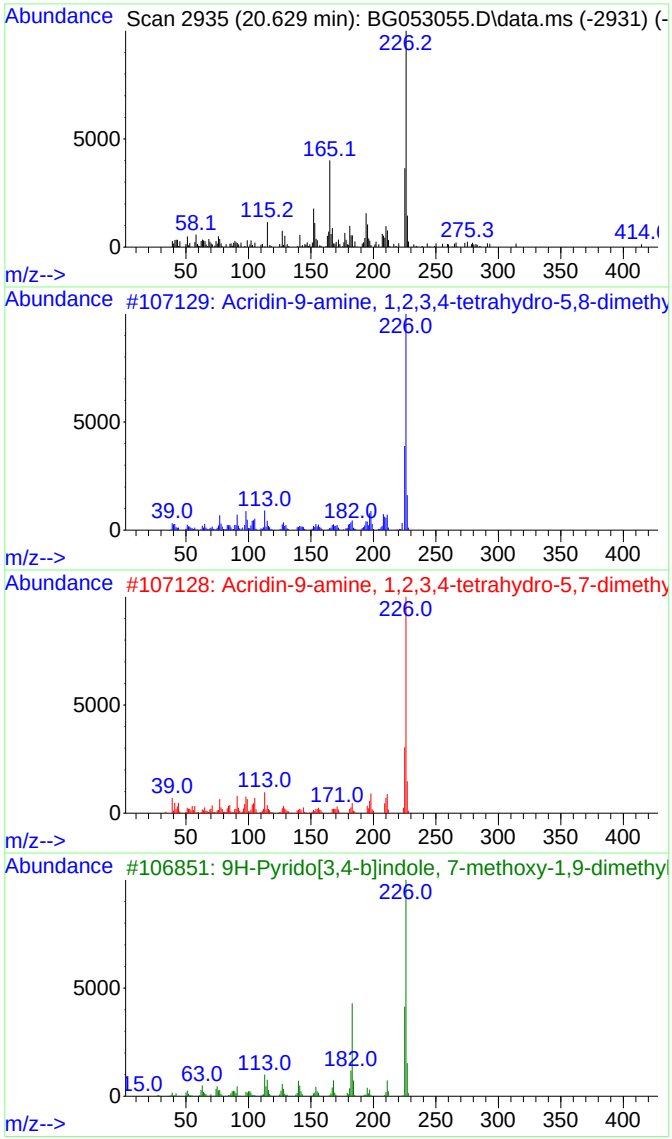
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

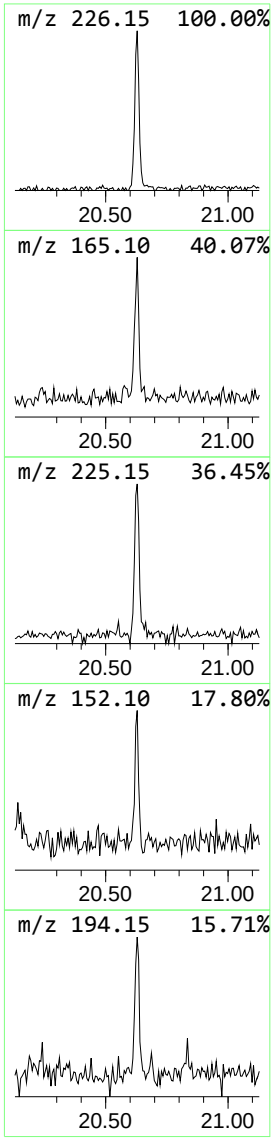
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 18 Acridin-9-amine, 1,2,3,4-te... Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.628 | 2.99 ng | 84645 | Chrysene-d12 | 21.774 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Acridin-9-amine, 1,2,3,4-tetrahy... | 226 | C15H18N2 | 297758-19-1 | 70 |
| 2 | Acridin-9-amine, 1,2,3,4-tetrahy... | 226 | C15H18N2 | 1000300-57-6 | 58 |
| 3 | 9H-Pyrido[3,4-b]indole, 7-methox... | 226 | C14H14N2O | 143502-37-8 | 49 |
| 4 | 1,2,10-Trihydroxyanthracene | 226 | C14H10O3 | 000577-33-3 | 49 |
| 5 | 4'-Methoxy-2-hydroxystilbene | 226 | C15H14O2 | 1000147-93-1 | 49 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053055.D
Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

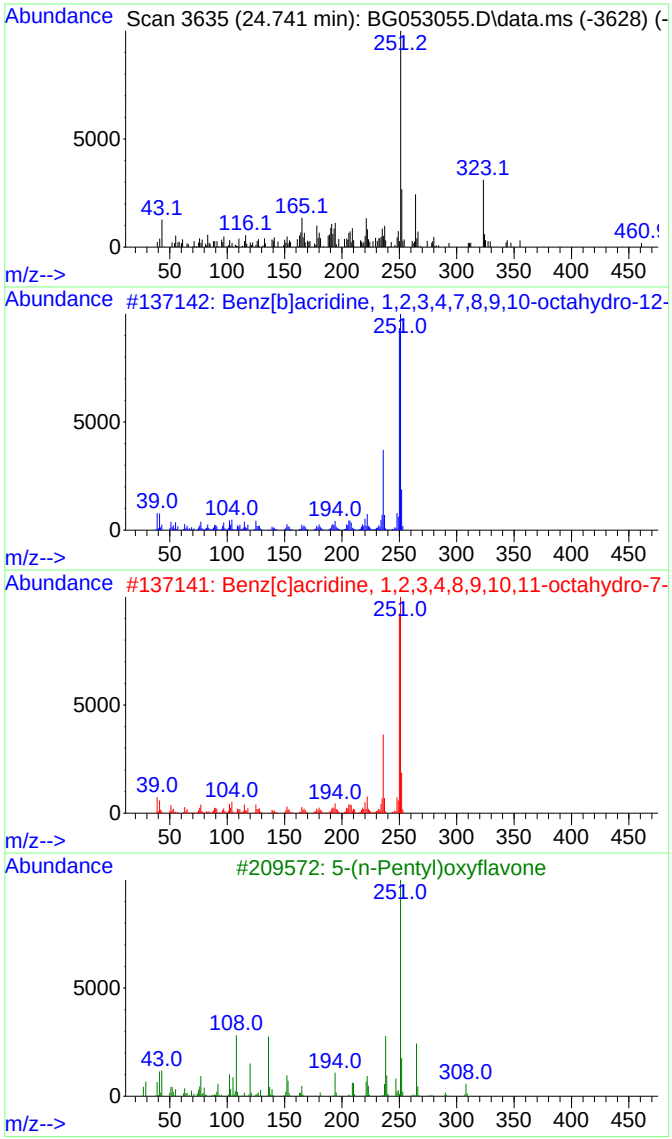
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

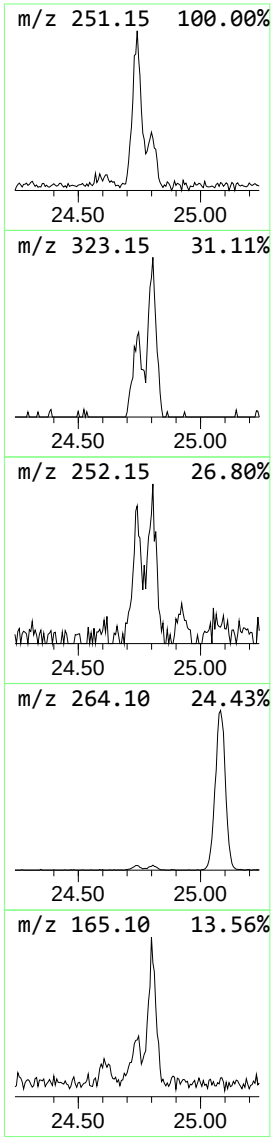
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 19 Benz[b]acridine, 1,2,3,4,7,... Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 24.741 | 3.22 ng | 99076 | Perylene-d12 | 25.081 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benz[b]acridine, 1,2,3,4,7,8,9,1... | 251 | C18H21N | 055044-74-1 | 83 |
| 2 | Benz[c]acridine, 1,2,3,4,8,9,10,... | 251 | C18H21N | 055044-73-0 | 83 |
| 3 | 5-(n-Pentyl)oxyflavone | 308 | C20H20O3 | 1000454-53-1 | 50 |
| 4 | 9-(4-Chlorobenzyl)-9-hydroxy-3,6... | 376 | C25H25ClO | 142728-02-7 | 50 |
| 5 | 2-Benzo[1,3]dioxol-5-yl-7-methyl... | 251 | C16H13NO2 | 1000274-75-9 | 49 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053055.D
Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

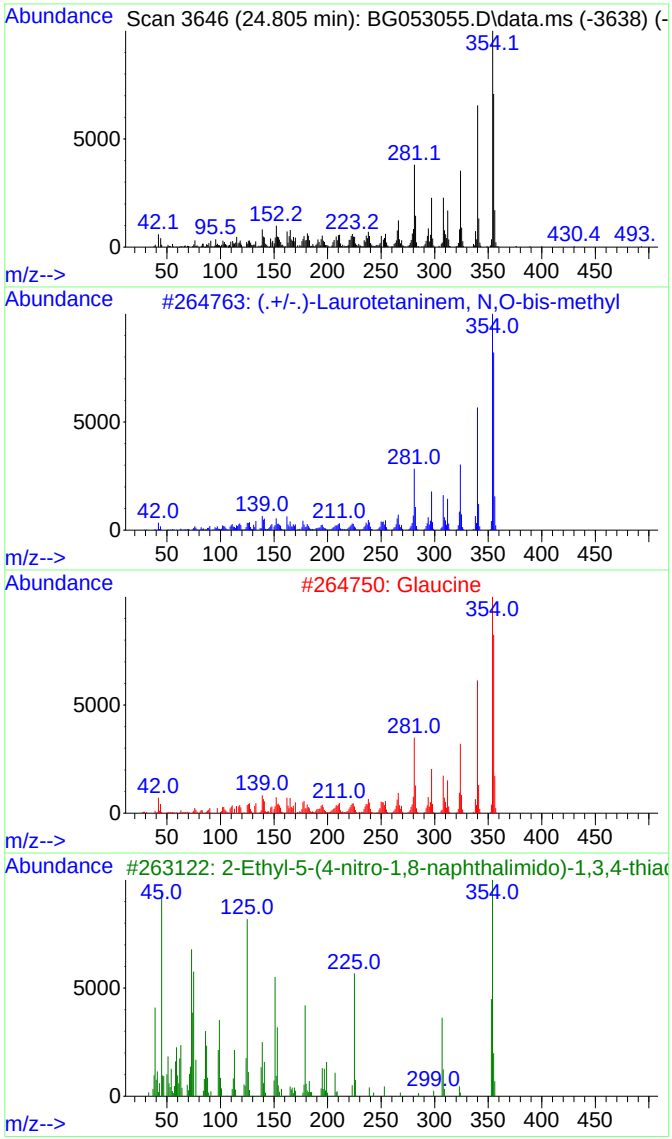
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

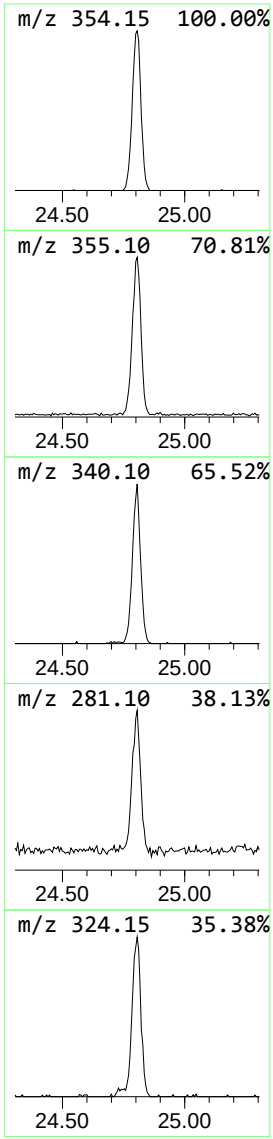
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 20 (.+/-.)-Laurotetaninem, N,O... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 24.805 | 36.77 ng | 1130720 | Perylene-d12 | 25.081 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (.+/-.)-Laurotetaninem, N,O-bis-... | 355 | C21H25NO4 | 005630-11-5 | 99 |
| 2 | Glaucine | 355 | C21H25NO4 | 000475-81-0 | 99 |
| 3 | 2-Ethyl-5-(4-nitro-1,8-naphthali... | 354 | C16H10N4O4S | 302955-08-4 | 83 |
| 4 | 3-Pyrrol5-[2-(1H-benzoimidazol-2... | 355 | C21H13N3O3 | 1000311-47-5 | 41 |
| 5 | Pregna-5,16-dien-20-one, 3,21-bi... | 414 | C25H34O5 | 037413-93-7 | 38 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040622\
Data File : BG053055.D
Acq On : 6 Apr 2022 15:11
Operator : CG/JU
Sample : N2269-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.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 |
| Pentanoic acid | 7.135 | 2.9 | ng | 30869 | 1 | 8.128 | 216746 | 20.0 |
| Hexanoic acid, ... | 9.420 | 3.9 | ng | 42550 | 1 | 8.128 | 216746 | 20.0 |
| Octanoic acid | 10.254 | 2.3 | ng | 35862 | 2 | 10.942 | 312186 | 20.0 |
| unknown11.371 | 11.371 | 2.3 | ng | 35251 | 2 | 10.942 | 312186 | 20.0 |
| Phospholane | 11.741 | 4.3 | ng | 67209 | 2 | 10.942 | 312186 | 20.0 |
| Benzaldehyde, 3... | 13.662 | 4.0 | ng | 99848 | 3 | 14.748 | 506053 | 20.0 |
| unknown14.819 | 14.819 | 2.9 | ng | 72117 | 3 | 14.748 | 506053 | 20.0 |
| Dodecanoic acid | 15.160 | 11.6 | ng | 293717 | 3 | 14.748 | 506053 | 20.0 |
| Tributyl phosphate | 15.941 | 4.1 | ng | 104789 | 3 | 14.748 | 506053 | 20.0 |
| Benzenemethanol... | 16.093 | 6.4 | ng | 161380 | 3 | 14.748 | 506053 | 20.0 |
| (E)-4-(3-Hydrox... | 16.869 | 8.5 | ng | 238406 | 4 | 17.492 | 563786 | 20.0 |
| Pyrimidine, 2,4... | 17.257 | 2.9 | ng | 81740 | 4 | 17.492 | 563786 | 20.0 |
| 5H-Indeno[1,2-b... | 17.891 | 2.5 | ng | 69254 | 4 | 17.492 | 563786 | 20.0 |
| 3(N,N-Dimethylm... | 18.044 | 2.5 | ng | 70451 | 4 | 17.492 | 563786 | 20.0 |
| cis-7-Hexadecen... | 18.255 | 2.8 | ng | 77987 | 4 | 17.492 | 563786 | 20.0 |
| Diphenyl sulfone | 18.449 | 3.2 | ng | 91259 | 4 | 17.492 | 563786 | 20.0 |
| trans-Sinapyl a... | 18.696 | 2.5 | ng | 70325 | 4 | 17.492 | 563786 | 20.0 |
| Acridin-9-amine... | 20.628 | 3.0 | ng | 84645 | 5 | 21.774 | 565630 | 20.0 |
| Benz[b]acridine... | 24.741 | 3.2 | ng | 99076 | 6 | 25.081 | 615010 | 20.0 |
| (.+/-.)-Laurote... | 24.805 | 36.8 | ng | 1130720 | 6 | 25.081 | 615010 | 20.0 |