LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070821\
Data File : BP006142.D
Acq On : 08 Jul 2021 16:27
Operator : CG/JU
Sample : M2963-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** MH-2B-COMP

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-BP070721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006142.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 4.987 | 318 | 323 | 334 | rBV | 80715 | 128546 | 1.23% | 0.226% |
| 2 | 5.452 | 396 | 402 | 422 | rBV | 3990286 | 6104490 | 58.25% | 10.727% |
| 3 | 7.063 | 668 | 676 | 698 | rBV | 3558894 | 6058807 | 57.82% | 10.646% |
| 4 | 7.875 | 804 | 814 | 826 | rBV | 736060 | 1205492 | 11.50% | 2.118% |
| 5 | 9.046 | 1006 | 1013 | 1036 | rBV | 2174669 | 3806796 | 36.33% | 6.689% |
| 6 | 10.493 | 1250 | 1259 | 1271 | rBV2 | 70512 | 217821 | 2.08% | 0.383% |
| 7 | 10.681 | 1284 | 1291 | 1306 | rBV | 849396 | 1575271 | 15.03% | 2.768% |
| 8 | 13.140 | 1701 | 1709 | 1724 | rBV | 5287949 | 8116005 | 77.45% | 14.261% |
| 9 | 14.510 | 1936 | 1942 | 1959 | rVB | 1253057 | 1957363 | 18.68% | 3.439% |
| 10 | 16.004 | 2187 | 2196 | 2215 | rBV | 4052340 | 6192789 | 59.09% | 10.882% |
| 11 | 17.263 | 2404 | 2410 | 2427 | rBV | 1407061 | 2199851 | 20.99% | 3.866% |
| 12 | 18.151 | 2556 | 2561 | 2567 | rBV | 126079 | 214169 | 2.04% | 0.376% |
| 13 | 19.816 | 2838 | 2844 | 2854 | rBV | 8854855 | 10479508 | 100.00% | 18.414% |
| 14 | 21.010 | 3043 | 3047 | 3050 | rBV | 150861 | 238552 | 2.28% | 0.419% |
| 15 | 21.051 | 3050 | 3054 | 3061 | rVV2 | 515754 | 987380 | 9.42% | 1.735% |
| 16 | 21.116 | 3061 | 3065 | 3072 | rVV | 640037 | 851654 | 8.13% | 1.497% |
| 17 | 21.345 | 3099 | 3104 | 3112 | rBV | 1791679 | 2374433 | 22.66% | 4.172% |
| 18 | 22.427 | 3283 | 3288 | 3301 | rVB | 1035865 | 1534666 | 14.64% | 2.697% |
| 19 | 23.739 | 3505 | 3511 | 3521 | rVB2 | 1277526 | 2666097 | 25.44% | 4.685% |

Sum of corrected areas: 56909690

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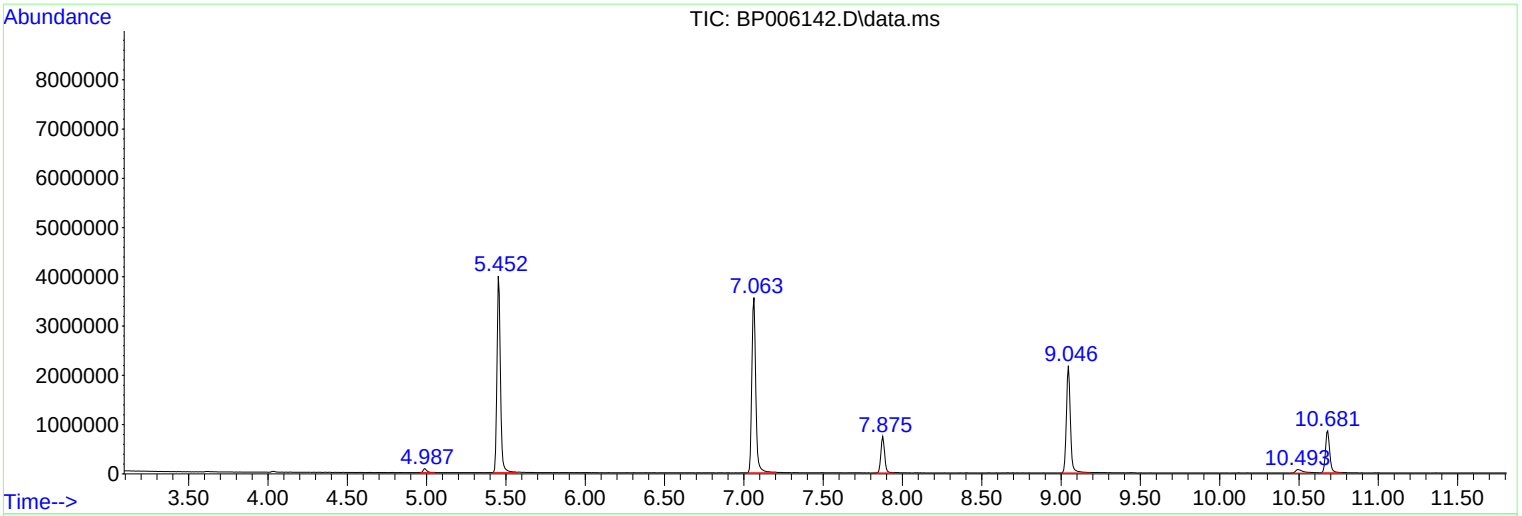
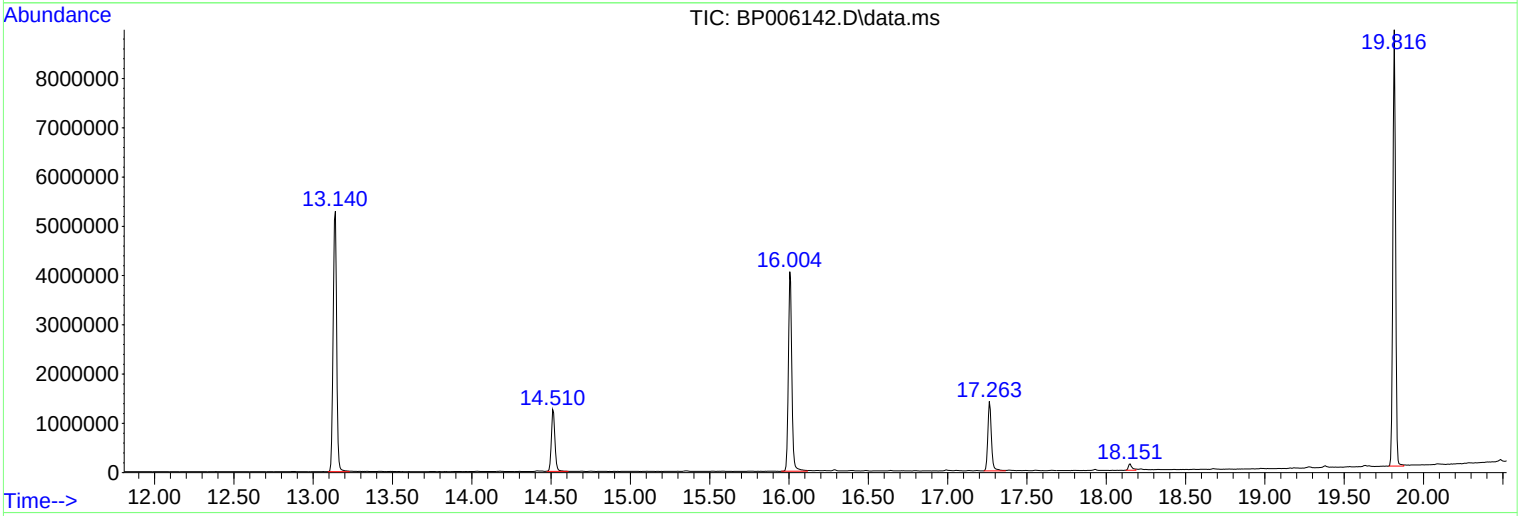
Misc :
ALS Vial : 7 Sample Multiplier: 1

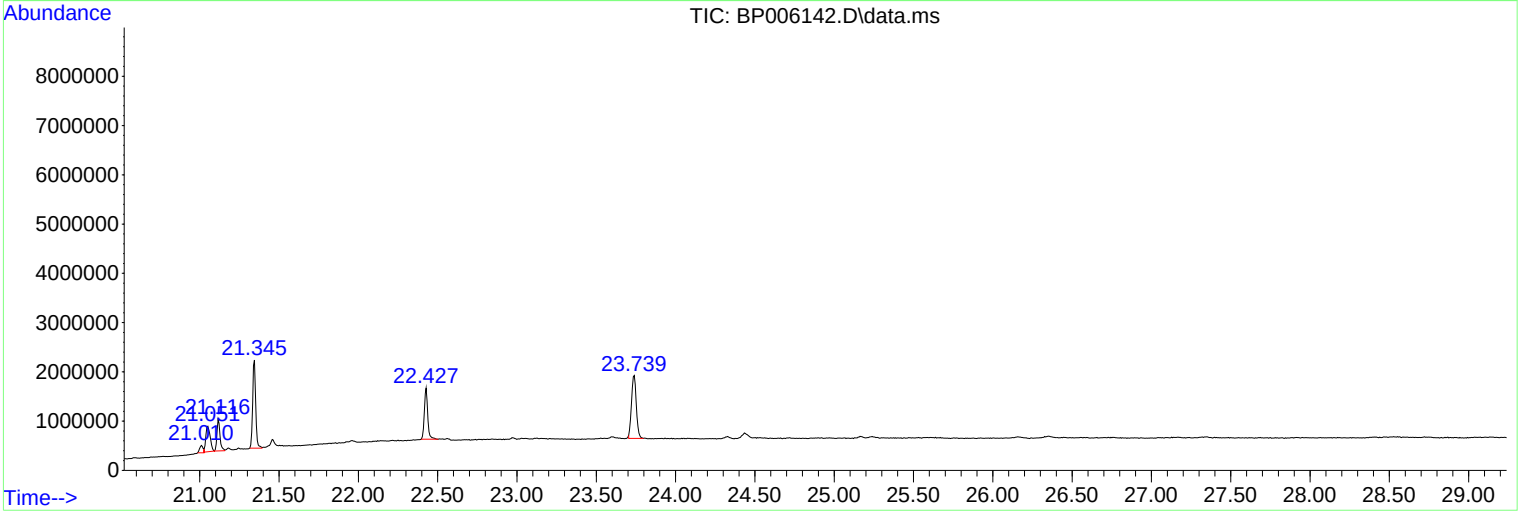
**Instrument :**
BNA_P
**ClientSampleId :**
MH-2B-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.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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ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_P
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MH-2B-COMP

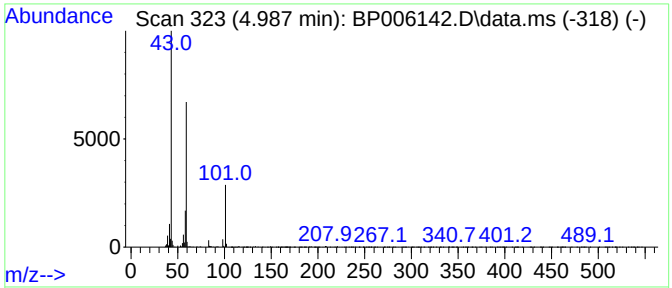
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

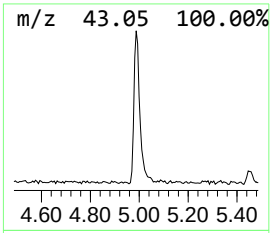
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

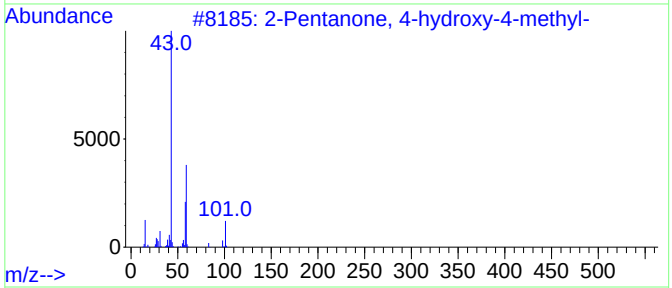
**********
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

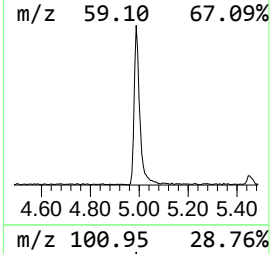
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.987 | 2.13 ng | 128546 | 1,4-Dichlorobenzene-d4 | 7.875 |

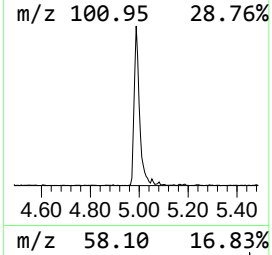
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Succinic acid, heptyl 2-methoxye... | 274 | C14H26O5 | 1000325-80-7 | 33 |
| 3 | Dimethadione | 129 | C5H7NO3 | 000695-53-4 | 33 |
| 4 | 3-Hexanol | 102 | C6H14O | 000623-37-0 | 28 |
| 5 | Hydrazine, 1,1-bis(1-methylethyl)- | 116 | C6H16N2 | 000921-14-2 | 28 |

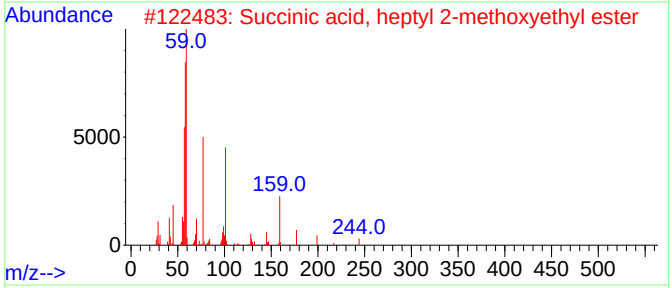


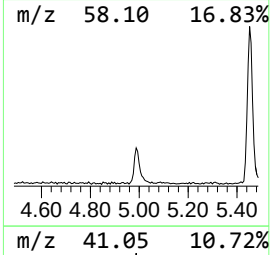



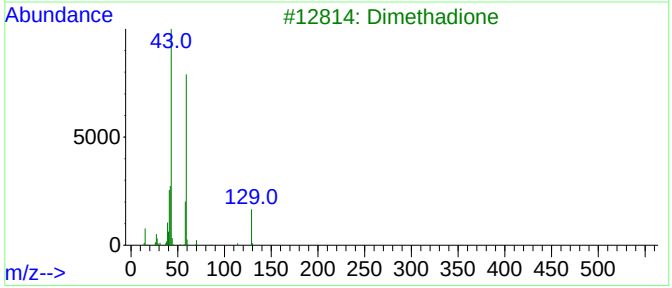



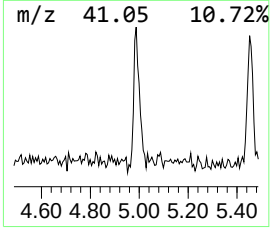



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Data File : BP006142.D
Acq On : 08 Jul 2021 16:27
Operator : CG/JU
Sample : M2963-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
MH-2B-COMP

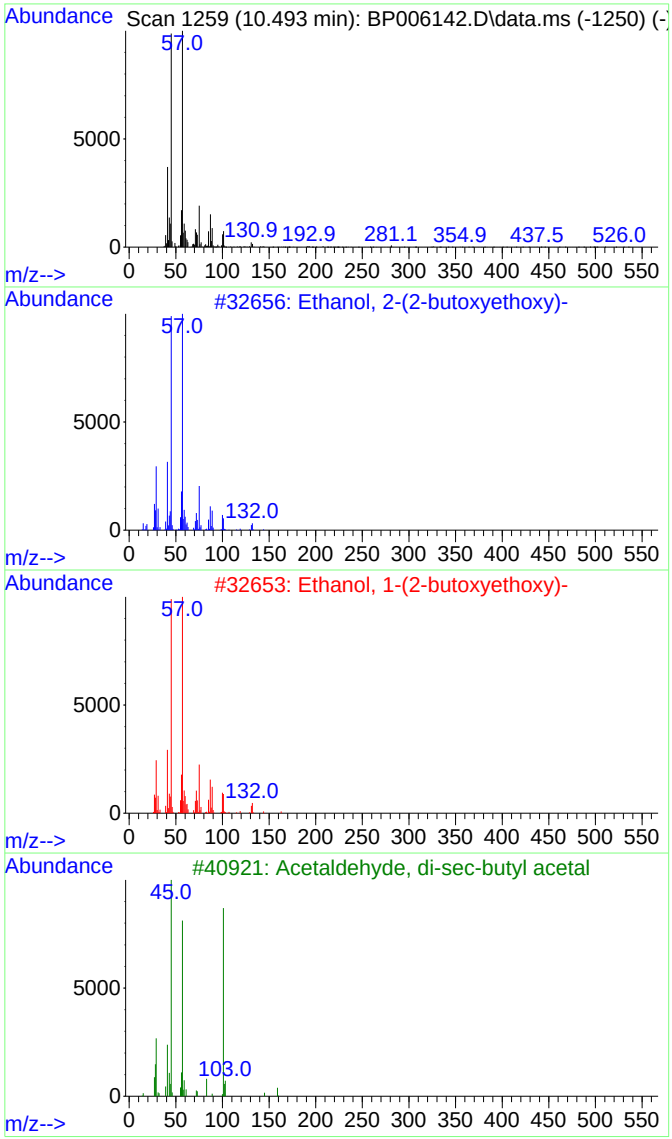
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

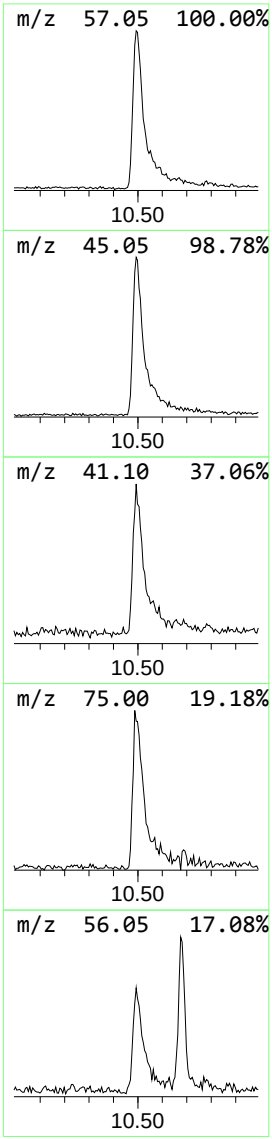
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.493 | 2.77 ng | 217821 | Naphthalene-d8 | 10.681 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(2-butoxyethoxy)- | 162 | C8H18O3 | 000112-34-5 | 90 |
| 2 | Ethanol, 1-(2-butoxyethoxy)- | 162 | C8H18O3 | 054446-78-5 | 83 |
| 3 | Acetaldehyde, di-sec-butyl acetal | 174 | C10H22O2 | 005314-41-0 | 50 |
| 4 | Di-sec-butyl ether | 130 | C8H18O | 006863-58-7 | 50 |
| 5 | 3,3-Dimethylbutane-2-ol | 102 | C6H14O | 000464-07-3 | 50 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070821\
Data File : BP006142.D
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Operator : CG/JU
Sample : M2963-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** MH-2B-COMP

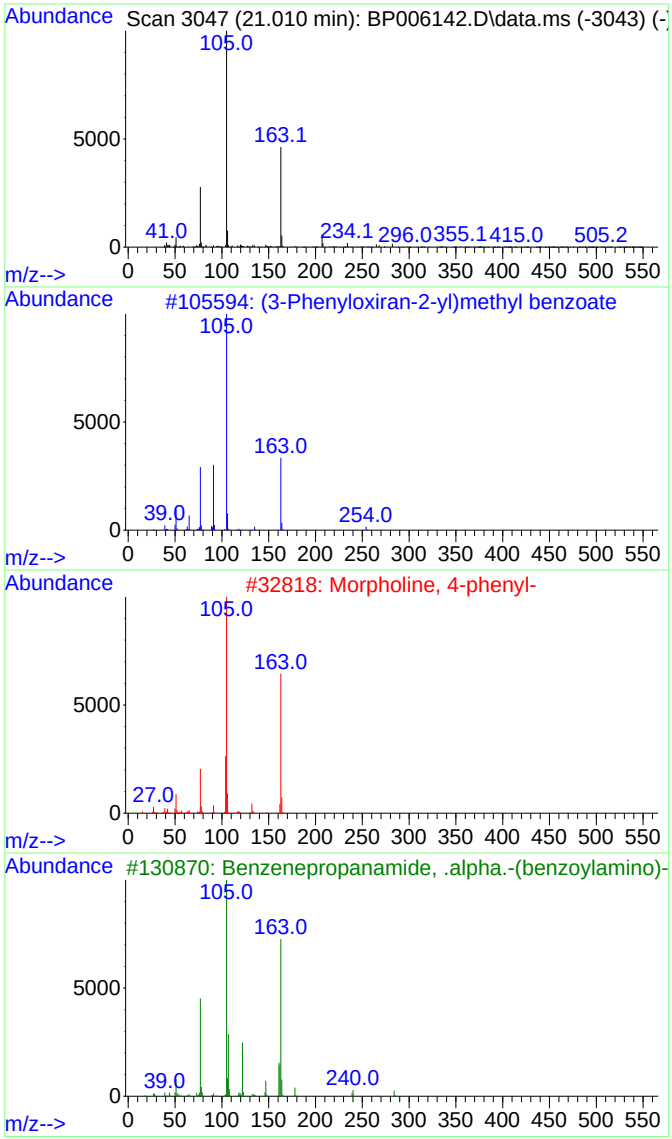
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

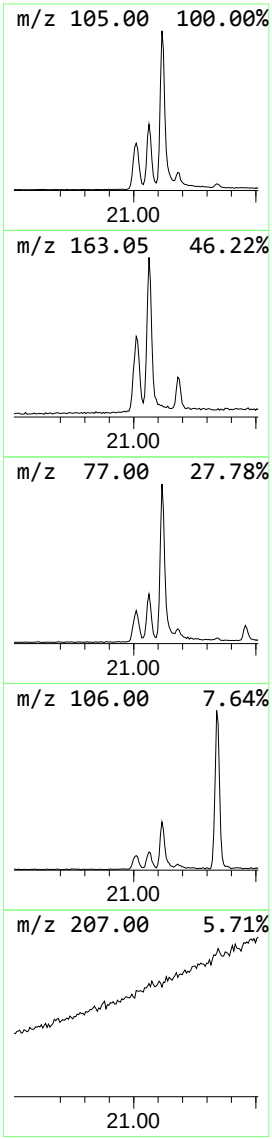
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 (3-Phenyloxiran-2-yl)methyl... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.010 | 2.01 ng | 238552 | Chrysene-d12 | 21.345 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (3-Phenyloxiran-2-yl)methyl benz... | 254 | C16H14O3 | 1000366-96-1 | 50 |
| 2 | Morpholine, 4-phenyl- | 163 | C10H13NO | 000092-53-5 | 47 |
| 3 | Benzenepropanamide, .alpha.-(ben... | 284 | C16H16N2O3 | 058690-81-6 | 42 |
| 4 | 1-Propanol, 2-[2-(benzoyloxy)pro... | 342 | C20H22O5 | 020109-39-1 | 40 |
| 5 | N-(4-Oxo-4H-chromen-3-yl)benzamide | 265 | C16H11NO3 | 1000243-49-5 | 27 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070821\
Data File : BP006142.D
Acq On : 08 Jul 2021 16:27
Operator : CG/JU
Sample : M2963-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** MH-2B-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

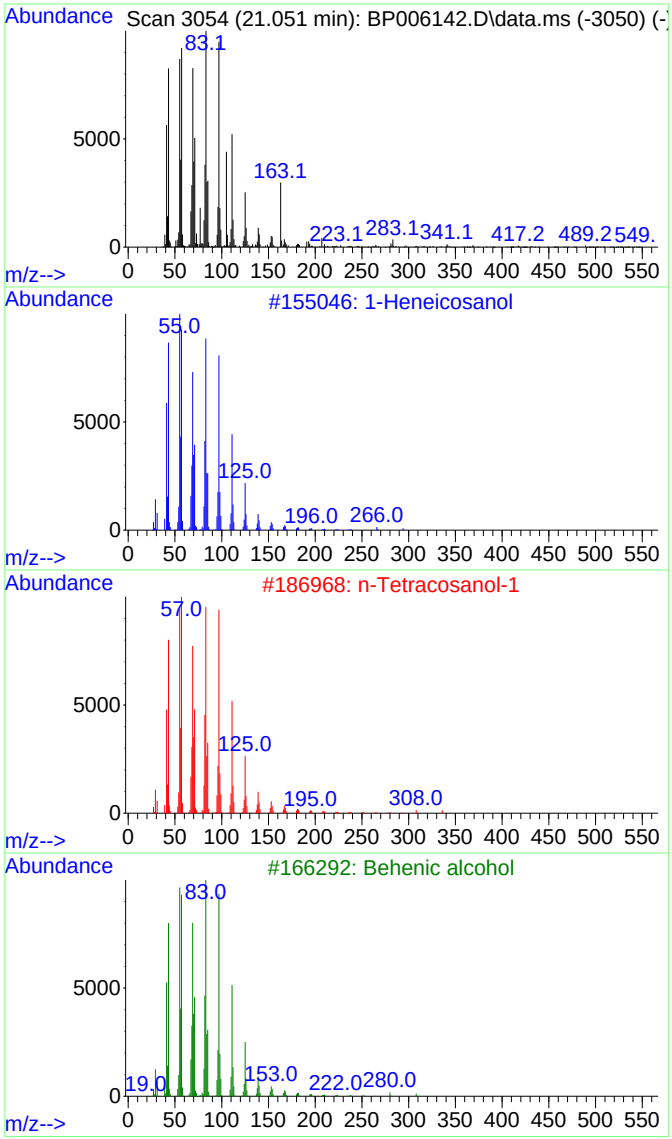
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

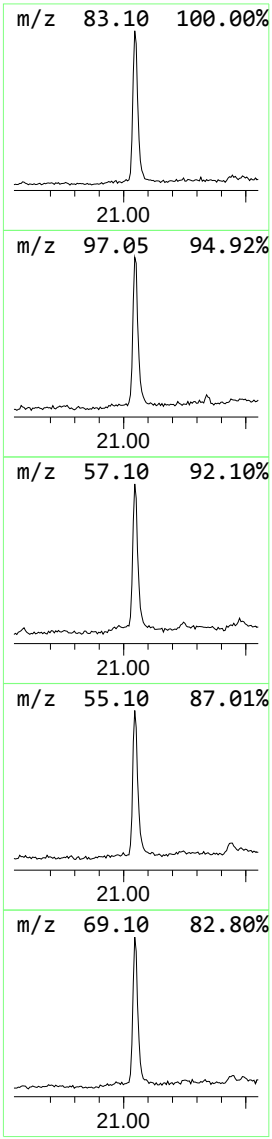
**********

Peak Number 4 1-Heneicosanol Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.051 | 8.32 ng | 987380 | Chrysene-d12 | 21.345 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 94 |
| 2 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 94 |
| 3 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 94 |
| 4 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 93 |
| 5 | 1-Heneicosyl formate | 340 | C22H44O2 | 077899-03-7 | 91 |



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Sample : M2963-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** MH-2B-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

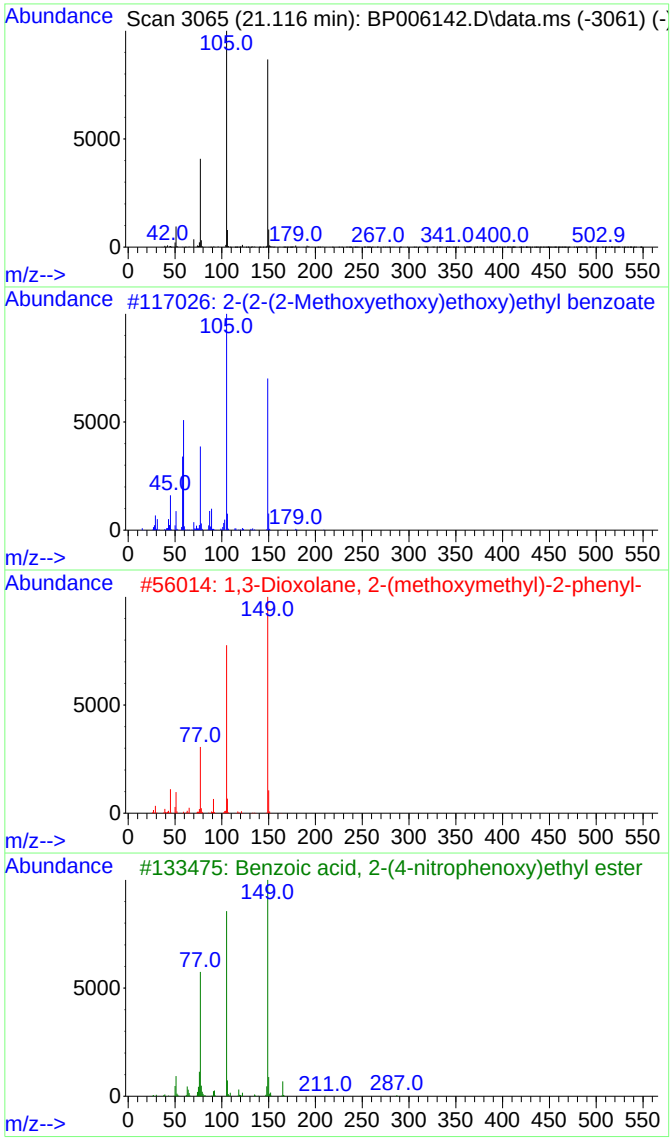
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

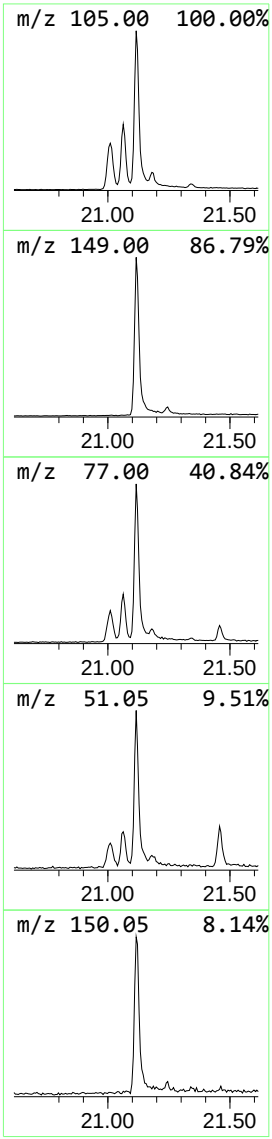
**********

Peak Number 5 2-(2-(2-Methoxyethoxy)ethox... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.116 | 7.17 ng | 851654 | Chrysene-d12 | 21.345 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-(2-(2-Methoxyethoxy)ethoxy)eth... | 268 | C14H20O5 | 1000366-99-1 | 74 |
| 2 | 1,3-Dioxolane, 2-(methoxymethyl)... | 194 | C11H14O3 | 1000156-71-2 | 72 |
| 3 | Benzoic acid, 2-(4-nitrophenoxy)... | 287 | C15H13NO5 | 1000368-92-7 | 72 |
| 4 | 3,6,9,12-Tetraoxatetradecane-1,1... | 446 | C24H30O8 | 1000366-97-0 | 64 |
| 5 | Benzoic acid, 2-(3-nitrophenyl)e... | 271 | C15H13NO4 | 1000368-22-4 | 56 |



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Operator : CG/JU
Sample : M2963-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** MH-2B-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
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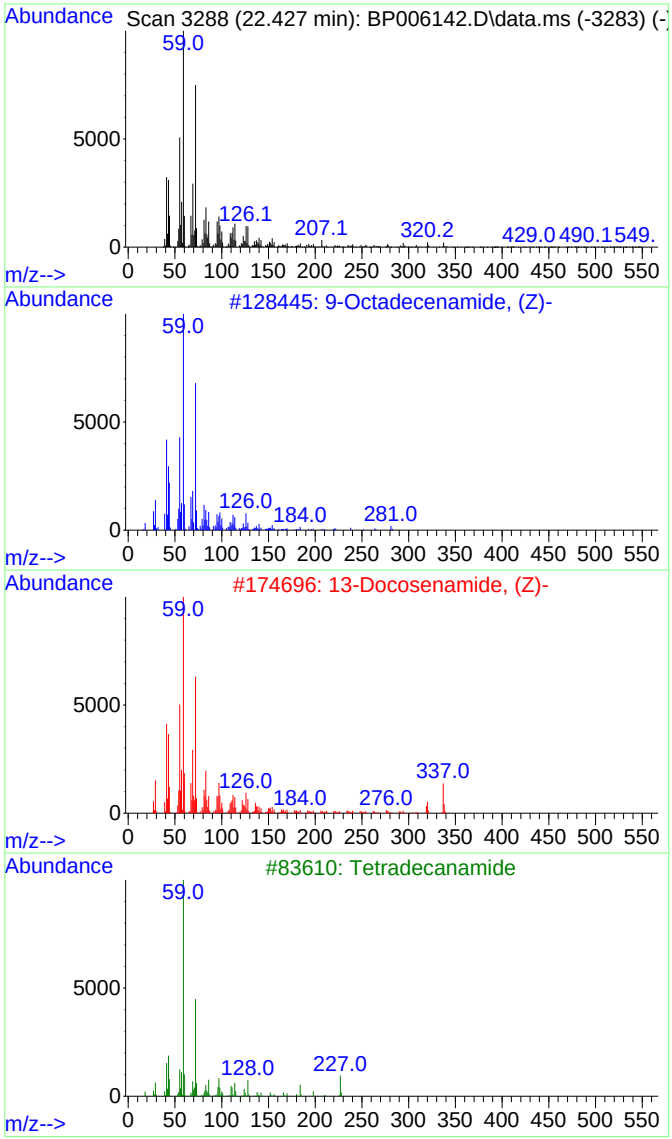
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

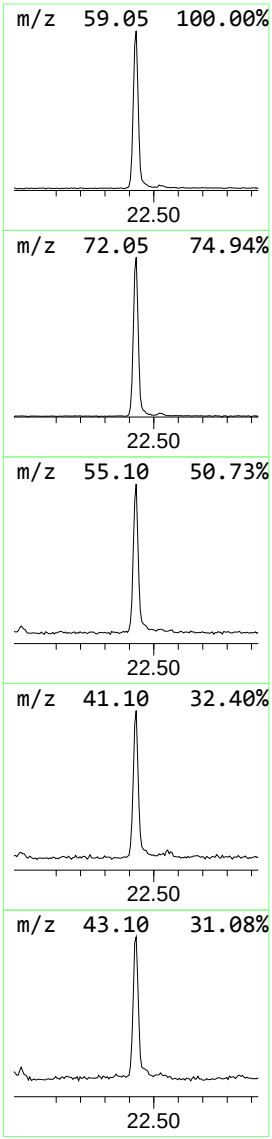
**********

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.427 | 12.93 ng | 1534670 | Chrysene-d12 | 21.345 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 91 |
| 2 | 13-Docosenamide, (Z)- | 337 | C22H43NO | 000112-84-5 | 81 |
| 3 | Tetradecanamide | 227 | C14H29NO | 000638-58-4 | 43 |
| 4 | Octadecanamide | 283 | C18H37NO | 000124-26-5 | 43 |
| 5 | 2,11-Dimethyl-2,11-dodecanediol | 230 | C14H30O2 | 022092-59-7 | 35 |



Tentatively Identified Compound (LSC) summary

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**Instrument :** BNA_P
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-... | 4.987 | 2.1 | ng | 128546 | 1 | 7.875 | 1205490 | 20.0 |
| Ethanol, 2-(2-b... | 10.493 | 2.8 | ng | 217821 | 2 | 10.681 | 1575270 | 20.0 |
| (3-Phenyloxiran... | 21.010 | 2.0 | ng | 238552 | 5 | 21.345 | 2374430 | 20.0 |
| 1-Heneicosanol | 21.051 | 8.3 | ng | 987380 | 5 | 21.345 | 2374430 | 20.0 |
| 2-(2-(2-Methoxy... | 21.116 | 7.2 | ng | 851654 | 5 | 21.345 | 2374430 | 20.0 |
| 9-Octadecenamid... | 22.427 | 12.9 | ng | 1534670 | 5 | 21.345 | 2374430 | 20.0 |