LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081721\
Data File : BP006697.D
Acq On : 16 Aug 2021 23:11
Operator : CG/JU
Sample : M3425-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 22S

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-BP080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006697.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 4.858 | 298 | 301 | 308 | rVB | 75977 | 104455 | 1.43% | 0.186% |
| 2 | 5.305 | 371 | 377 | 394 | rVB | 3067637 | 4375299 | 59.71% | 7.801% |
| 3 | 6.887 | 637 | 646 | 665 | rVB | 2965733 | 4836770 | 66.01% | 8.624% |
| 4 | 7.705 | 779 | 785 | 791 | rVB | 706397 | 1079559 | 14.73% | 1.925% |
| 5 | 8.863 | 975 | 982 | 993 | rBV | 1917484 | 3054745 | 41.69% | 5.447% |
| 6 | 10.287 | 1218 | 1224 | 1238 | rBV | 131073 | 243950 | 3.33% | 0.435% |
| 7 | 10.487 | 1251 | 1258 | 1265 | rBV | 977654 | 1567101 | 21.39% | 2.794% |
| 8 | 12.969 | 1672 | 1680 | 1688 | rBV | 4059705 | 5790022 | 79.02% | 10.324% |
| 9 | 14.346 | 1905 | 1914 | 1921 | rBV | 1378556 | 1928891 | 26.32% | 3.439% |
| 10 | 15.840 | 2159 | 2168 | 2178 | rBV | 3357920 | 4580372 | 62.51% | 8.167% |
| 11 | 16.510 | 2275 | 2282 | 2291 | rBV2 | 57823 | 116109 | 1.58% | 0.207% |
| 12 | 17.104 | 2376 | 2383 | 2387 | rBV | 1517052 | 2184639 | 29.81% | 3.895% |
| 13 | 17.145 | 2387 | 2390 | 2395 | rVB | 173165 | 221793 | 3.03% | 0.395% |
| 14 | 18.010 | 2533 | 2537 | 2545 | rBV2 | 195439 | 271805 | 3.71% | 0.485% |
| 15 | 18.916 | 2686 | 2691 | 2701 | rBV | 327729 | 431000 | 5.88% | 0.768% |
| 16 | 19.122 | 2721 | 2726 | 2735 | rBV | 195826 | 328645 | 4.49% | 0.586% |
| 17 | 19.251 | 2744 | 2748 | 2755 | rBV | 101669 | 136657 | 1.86% | 0.244% |
| 18 | 19.475 | 2782 | 2786 | 2788 | rBV | 111008 | 124573 | 1.70% | 0.222% |
| 19 | 19.504 | 2788 | 2791 | 2796 | rVB | 104358 | 127388 | 1.74% | 0.227% |
| 20 | 19.681 | 2816 | 2821 | 2832 | rVB | 6074641 | 7327500 | 100.00% | 13.065% |
| 21 | 19.839 | 2844 | 2848 | 2853 | rVB | 273038 | 317194 | 4.33% | 0.566% |
| 22 | 20.222 | 2907 | 2913 | 2923 | rBV | 3747531 | 4636208 | 63.27% | 8.267% |
| 23 | 20.751 | 2998 | 3003 | 3010 | rBV | 1666384 | 1963238 | 26.79% | 3.501% |
| 24 | 20.822 | 3011 | 3015 | 3024 | rVV | 239938 | 362106 | 4.94% | 0.646% |
| 25 | 20.939 | 3030 | 3035 | 3040 | rBV3 | 313026 | 467904 | 6.39% | 0.834% |
| 26 | 21.122 | 3062 | 3066 | 3073 | rBV | 500556 | 706625 | 9.64% | 1.260% |
| 27 | 21.204 | 3073 | 3080 | 3085 | rBV | 2097903 | 3416033 | 46.62% | 6.091% |
| 28 | 21.298 | 3093 | 3096 | 3099 | rBV2 | 117402 | 136129 | 1.86% | 0.243% |
| 29 | 21.333 | 3099 | 3102 | 3107 | rVV | 191269 | 250811 | 3.42% | 0.447% |
| 30 | 21.392 | 3108 | 3112 | 3119 | rVB | 469772 | 620619 | 8.47% | 1.107% |
| 31 | 21.498 | 3127 | 3130 | 3139 | rVB2 | 217562 | 324512 | 4.43% | 0.579% |
| 32 | 21.675 | 3155 | 3160 | 3172 | rBV | 1122839 | 1524779 | 20.81% | 2.719% |
| 33 | 23.522 | 3467 | 3474 | 3483 | rVB2 | 1277976 | 2526732 | 34.48% | 4.505% |

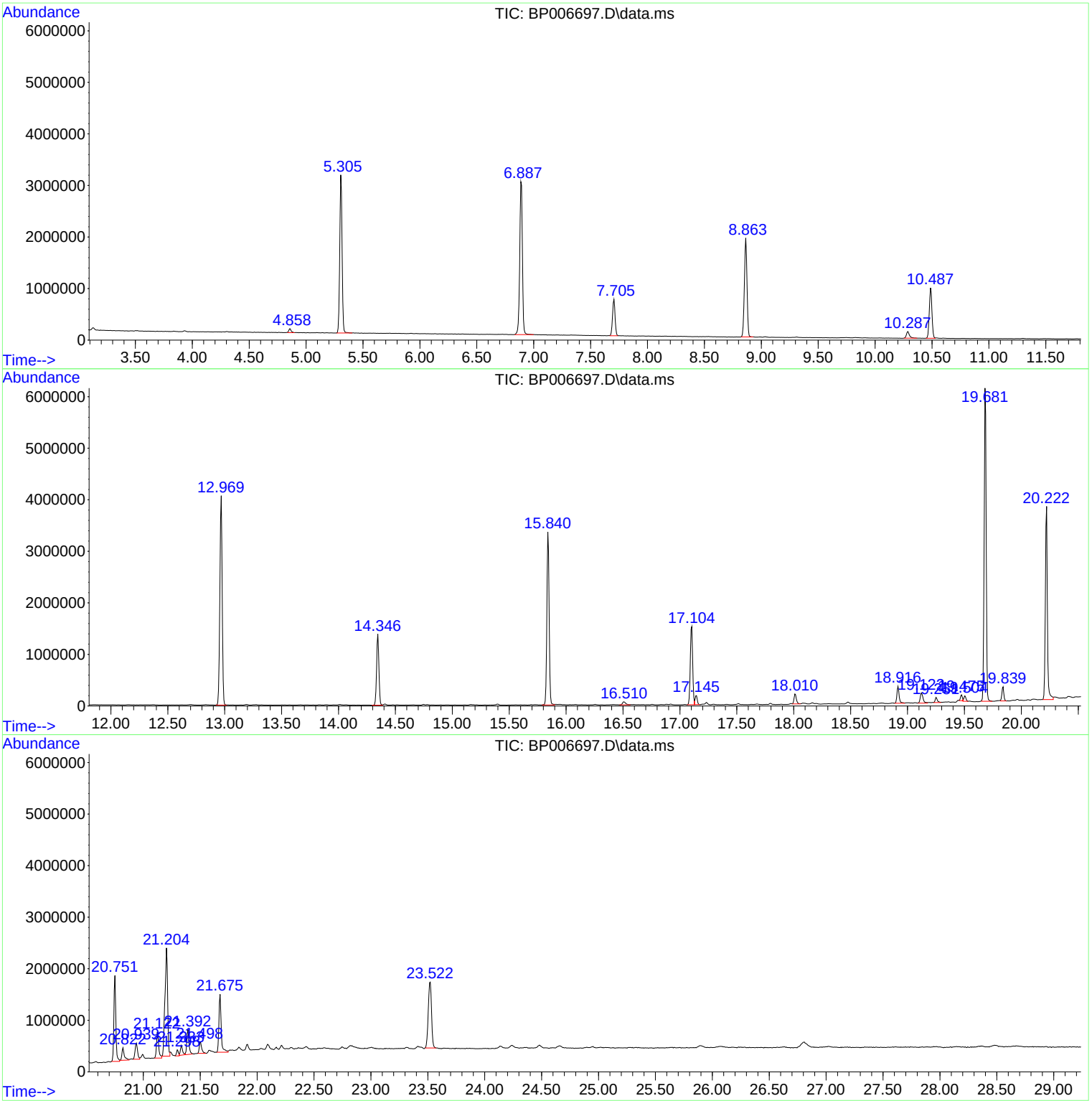
Sum of corrected areas: 56084163

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081721\
Data File : BP006697.D
Acq On : 16 Aug 2021 23:11
Operator : CG/JU
Sample : M3425-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
22S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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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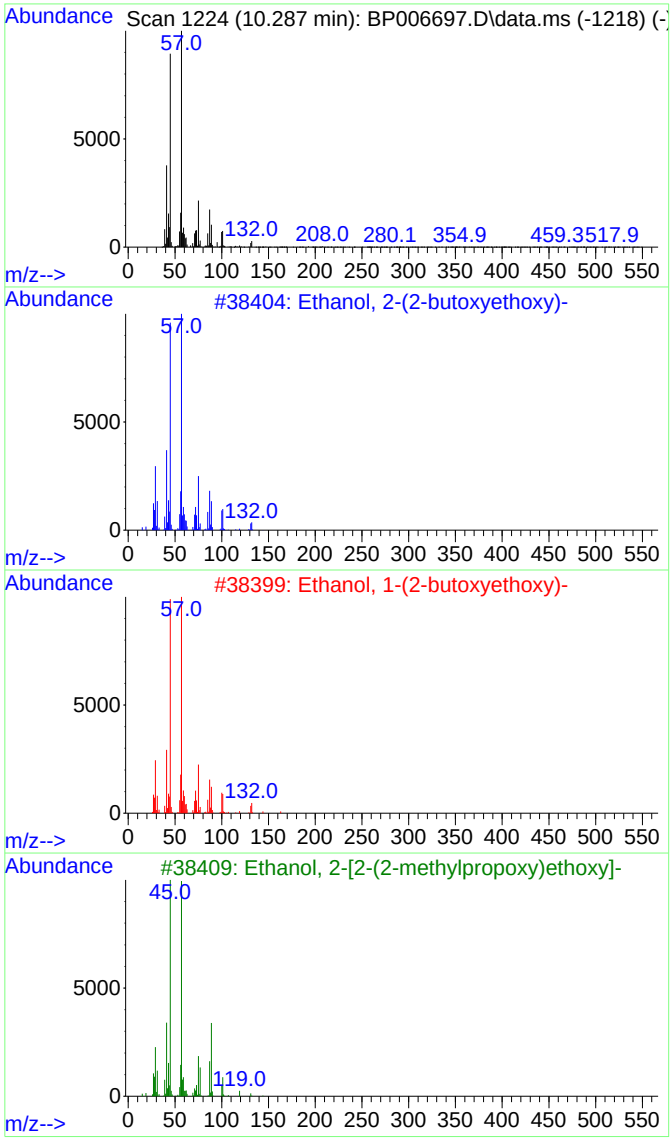
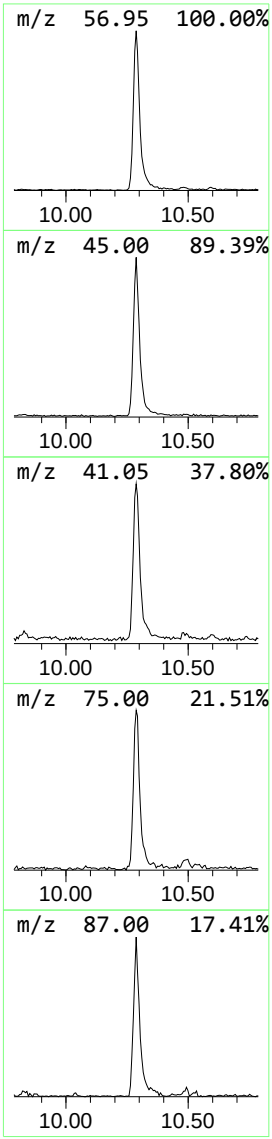
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.287 | 3.11 ng | 243950 | Naphthalene-d8 | 10.487 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(2-butoxyethoxy)- | 162 | C8H18O3 | 000112-34-5 | 91 |
| 2 | Ethanol, 1-(2-butoxyethoxy)- | 162 | C8H18O3 | 054446-78-5 | 83 |
| 3 | Ethanol, 2-[2-(2-methylpropoxy)e... | 162 | C8H18O3 | 018912-80-6 | 72 |
| 4 | Ethylene glycol monoisobutyl ether | 118 | C6H14O2 | 004439-24-1 | 64 |
| 5 | 3,3-Dimethylbutane-2-ol | 102 | C6H14O | 000464-07-3 | 52 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081721\
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ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
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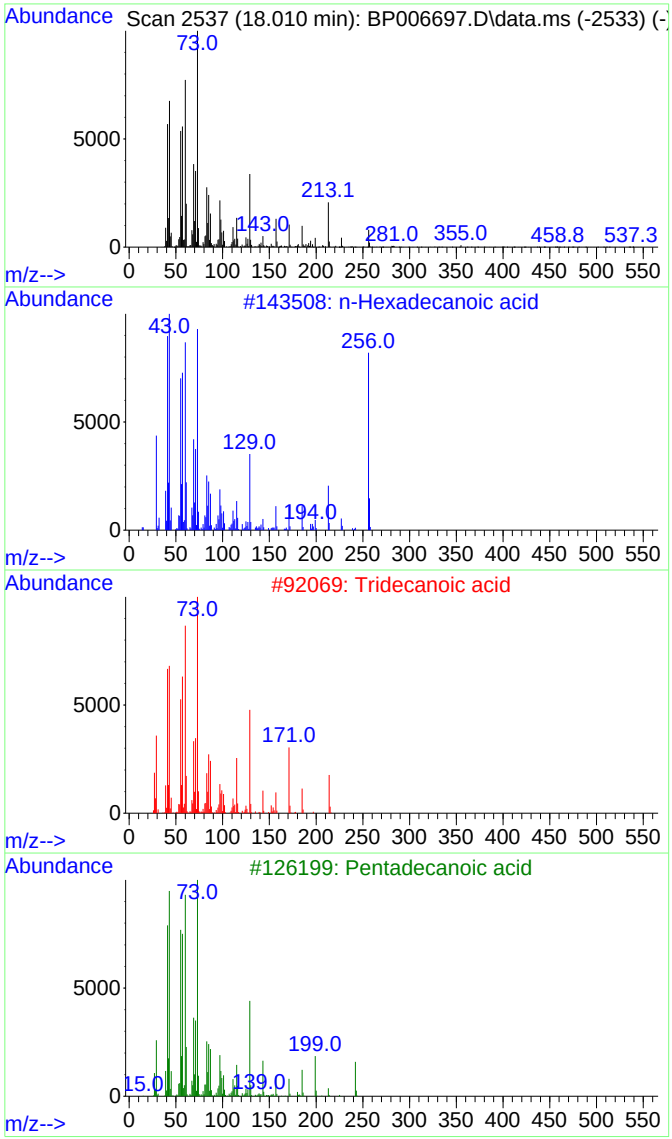
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

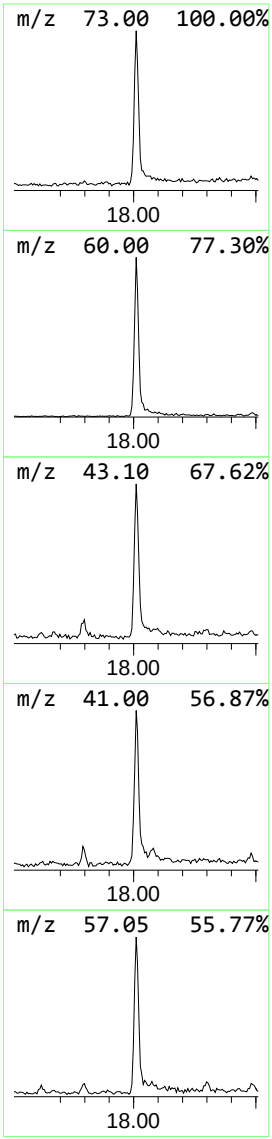
**********

Peak Number 2 n-Hexadecanoic acid Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.010 | 2.49 ng | 271805 | Phenanthrene-d10 | 17.104 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 92 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 81 |
| 4 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 64 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |



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Operator : CG/JU
Sample : M3425-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 22S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
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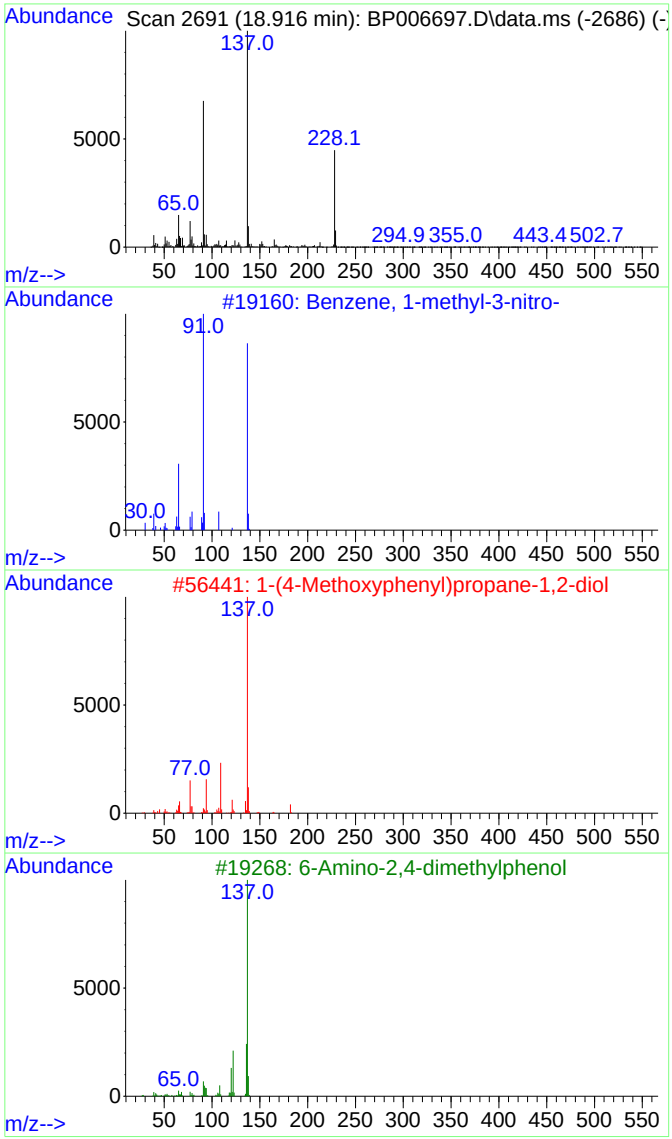
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

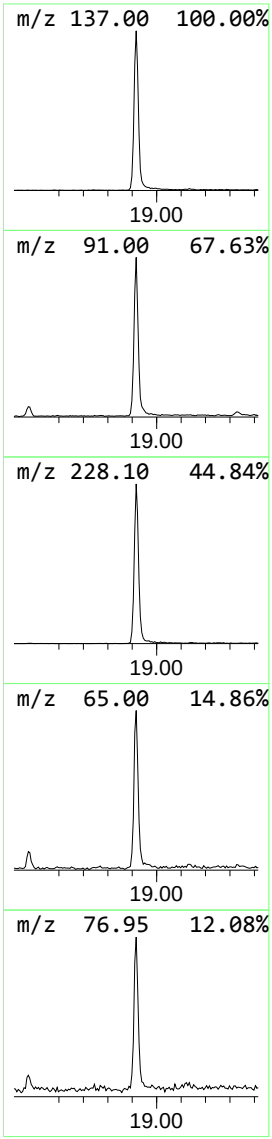
**********

Peak Number 3 unknown18.916 Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.916 | 3.95 ng | 431000 | Phenanthrene-d10 | 17.104 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, 1-methyl-3-nitro- | 137 | C7H7NO2 | 000099-08-1 | 47 |
| 2 | 1-(4-Methoxyphenyl)propane-1,2-diol | 182 | C10H14O3 | 051410-48-1 | 47 |
| 3 | 6-Amino-2,4-dimethylphenol | 137 | C8H11NO | 041458-65-5 | 43 |
| 4 | 3-Pyridineacetic acid | 137 | C7H7NO2 | 000501-81-5 | 43 |
| 5 | Homovanillyl alcohol | 168 | C9H12O3 | 002380-78-1 | 43 |



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Sample : M3425-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 22S

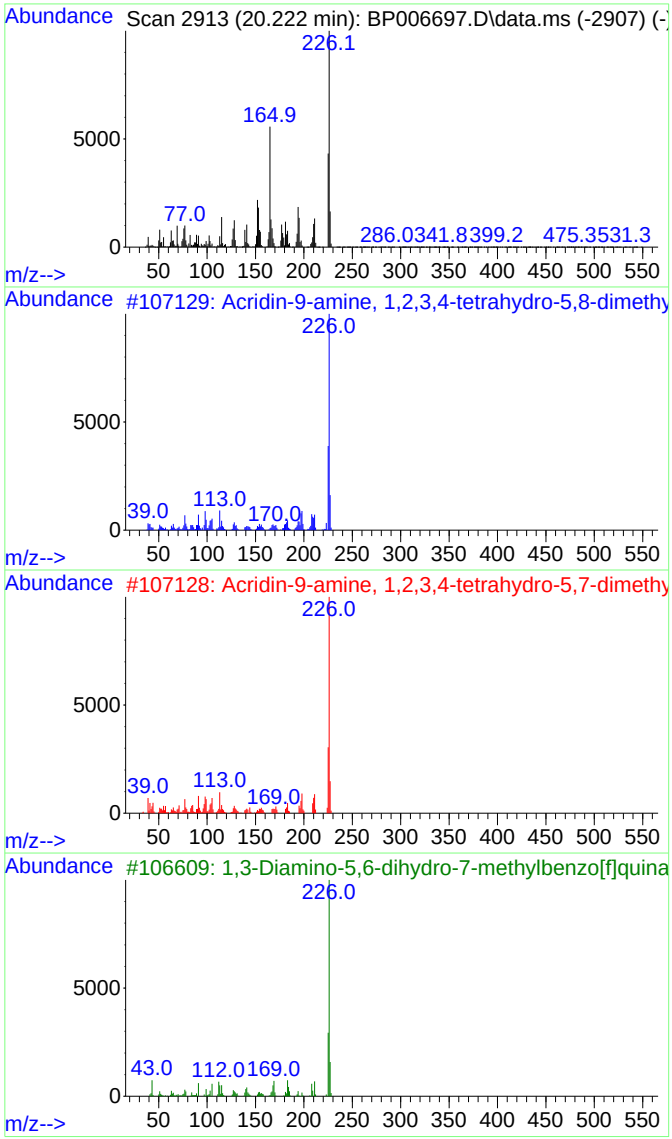
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

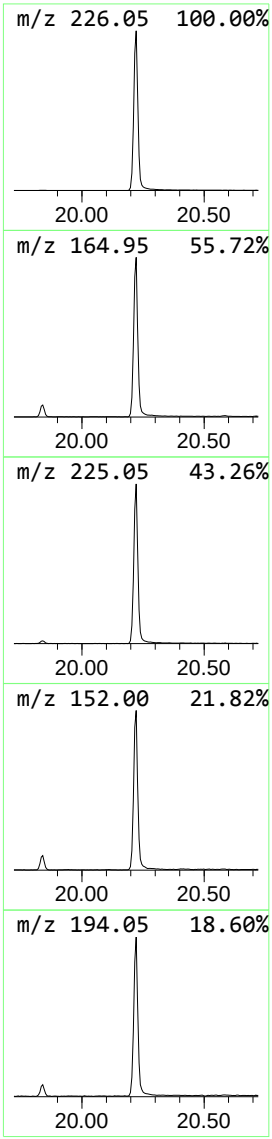
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 Acridin-9-amine, 1,2,3,4-te... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.222 | 27.14 ng | 4636210 | Chrysene-d12 | 21.204 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Acridin-9-amine, 1,2,3,4-tetrahy... | 226 | C15H18N2 | 297758-19-1 | 64 |
| 2 | Acridin-9-amine, 1,2,3,4-tetrahy... | 226 | C15H18N2 | 1000300-57-6 | 58 |
| 3 | 1,3-Diamino-5,6-dihydro-7-methyl... | 226 | C13H14N4 | 037436-37-6 | 53 |
| 4 | Anthralin | 226 | C14H10O3 | 001143-38-0 | 50 |
| 5 | N,N-Dimethylindoaniline | 226 | C14H14N2O | 002150-58-5 | 50 |



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Data File : BP006697.D
Acq On : 16 Aug 2021 23:11
Operator : CG/JU
Sample : M3425-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 22S

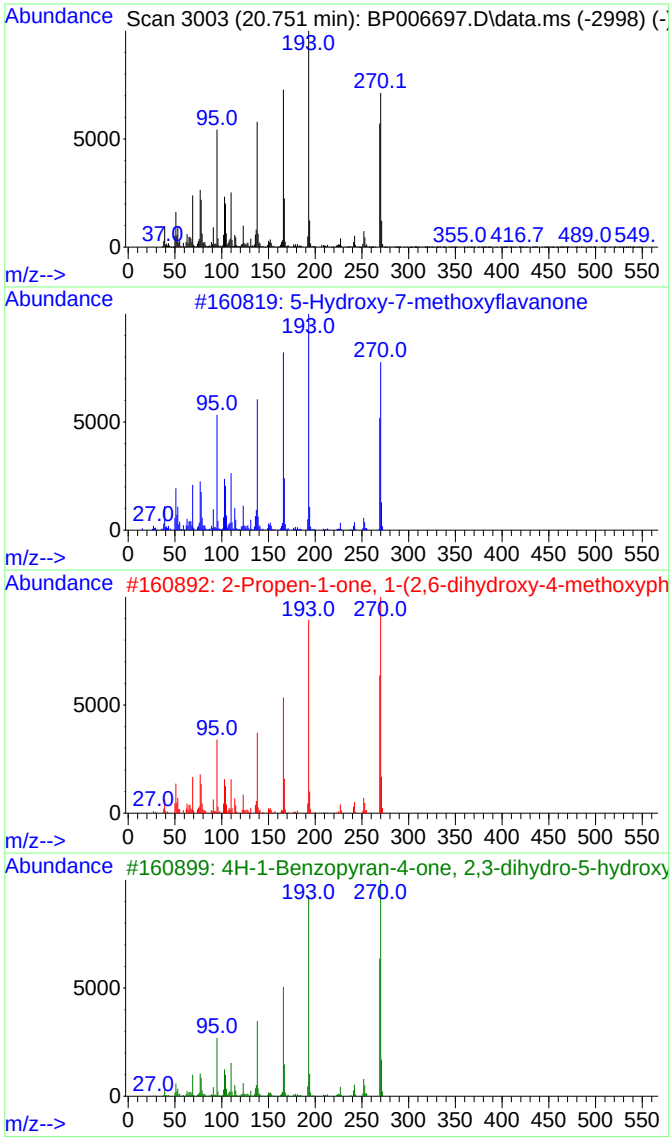
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

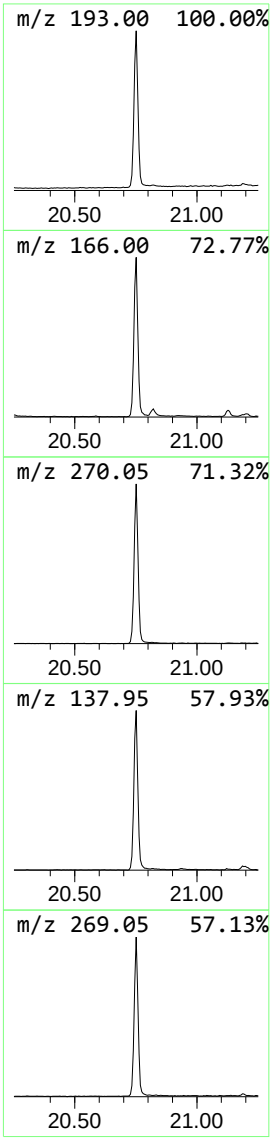
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 6 5-Hydroxy-7-methoxyflavanone Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.751 | 11.49 ng | 1963240 | Chrysene-d12 | 21.204 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Hydroxy-7-methoxyflavanone | 270 | C16H14O4 | 075291-74-6 | 97 |
| 2 | 2-Propen-1-one, 1-(2,6-dihydroxy... | 270 | C16H14O4 | 018956-15-5 | 96 |
| 3 | 4H-1-Benzopyran-4-one, 2,3-dihyd... | 270 | C16H14O4 | 000480-37-5 | 94 |
| 4 | Cryptostrobin | 270 | C16H14O4 | 1010497-72-2 | 50 |
| 5 | Cardamonin | 270 | C16H14O4 | 019309-14-9 | 46 |



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Data File : BP006697.D
Acq On : 16 Aug 2021 23:11
Operator : CG/JU
Sample : M3425-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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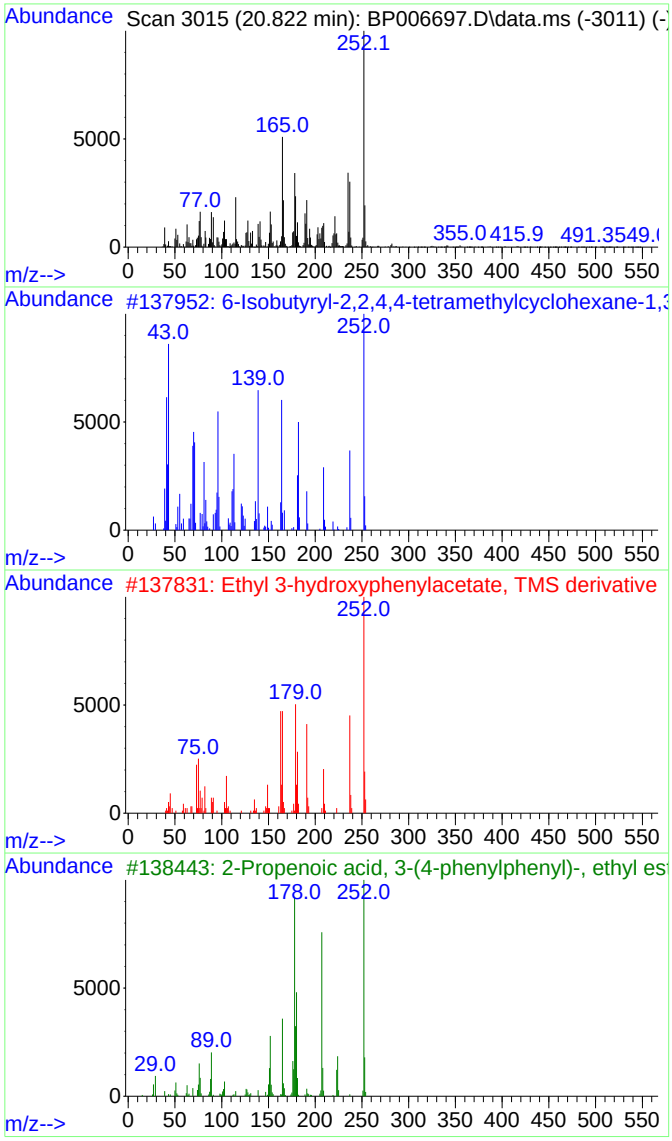
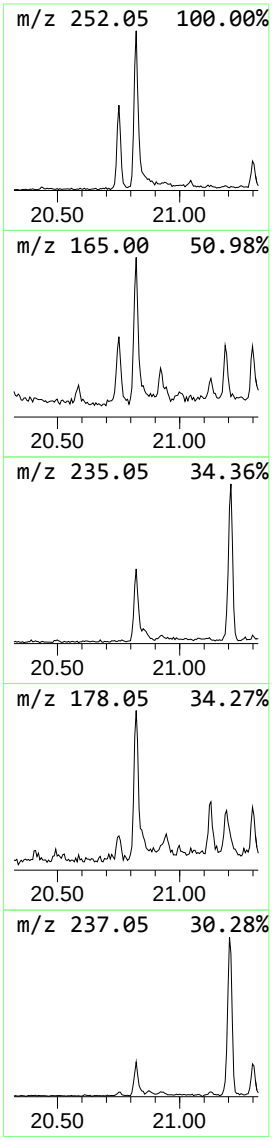
**********
Peak Number 7 6-Isobutyryl-2,2,4,4-tetram... Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.822 | 2.12 ng | 362106 | Chrysene-d12 | 21.204 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 6-Isobutyryl-2,2,4,4-tetramethyl... | 252 | C14H20O4 | 022595-45-5 | 90 |
| 2 | Ethyl 3-hydroxyphenylacetate, TM... | 252 | C13H20O3Si | 067903-48-4 | 78 |
| 3 | 2-Propenoic acid, 3-(4-phenylphe... | 252 | C17H16O2 | 040795-99-1 | 55 |
| 4 | Benzo[b]furan, 3-(4-methoxypheny... | 252 | C17H16O2 | 074228-98-1 | 53 |
| 5 | benzene, 1,1'-(1-cyclopropene-1,... | 252 | C17H16O2 | 1000396-66-7 | 46 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081721\
Data File : BP006697.D
Acq On : 16 Aug 2021 23:11
Operator : CG/JU
Sample : M3425-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 22S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
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TIC Library : C:\Database\NIST20.L
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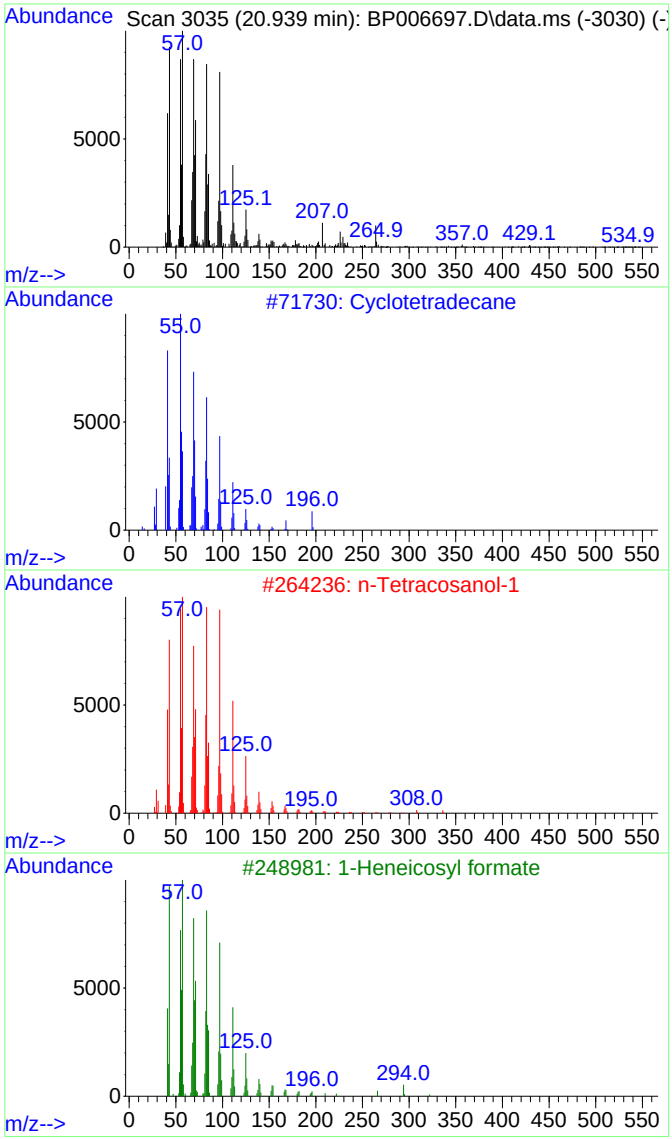
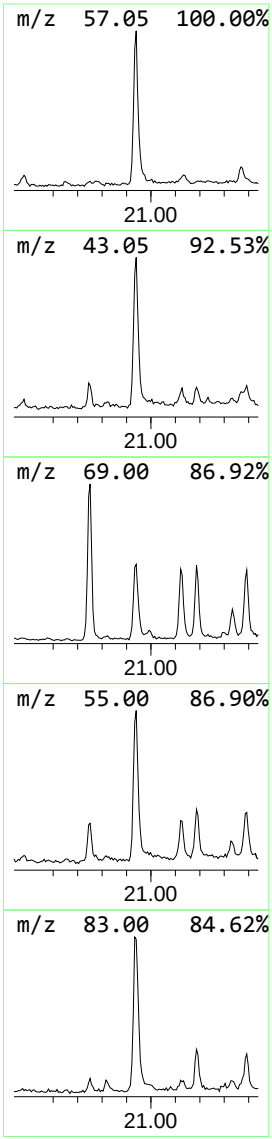
**********

Peak Number 8 Cyclotetradecane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.939 | 2.74 ng | 467904 | Chrysene-d12 | 21.204 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclotetradecane | 196 | C14H28 | 000295-17-0 | 94 |
| 2 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 94 |
| 3 | 1-Heneicosyl formate | 340 | C22H44O2 | 077899-03-7 | 94 |
| 4 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 94 |
| 5 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 94 |



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Operator : CG/JU
Sample : M3425-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 22S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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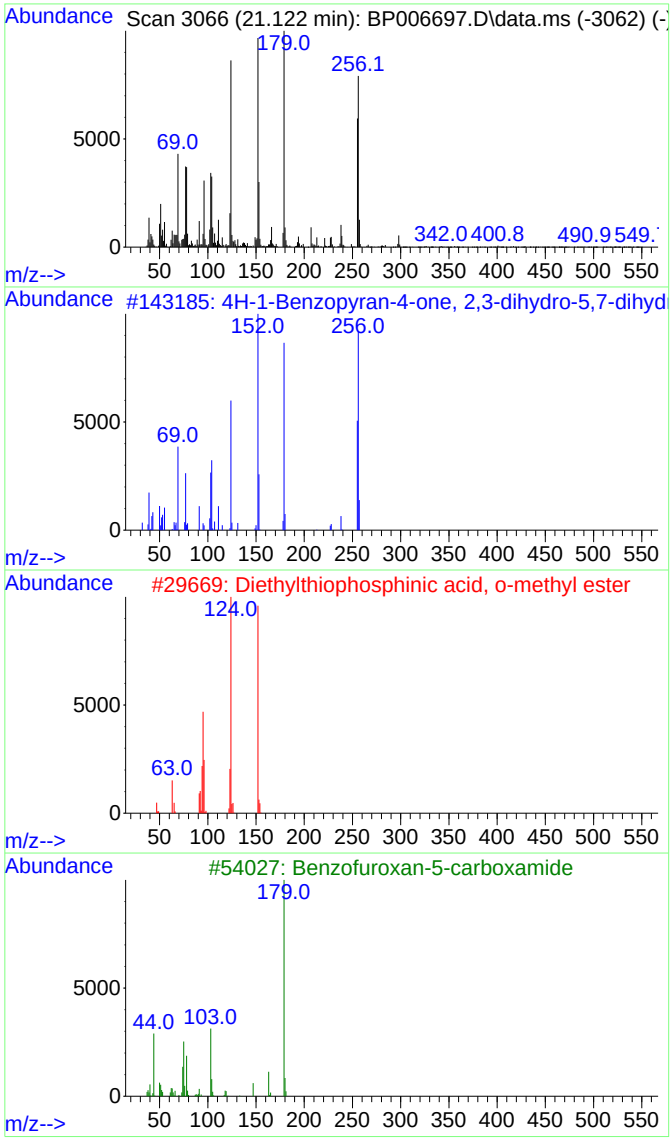
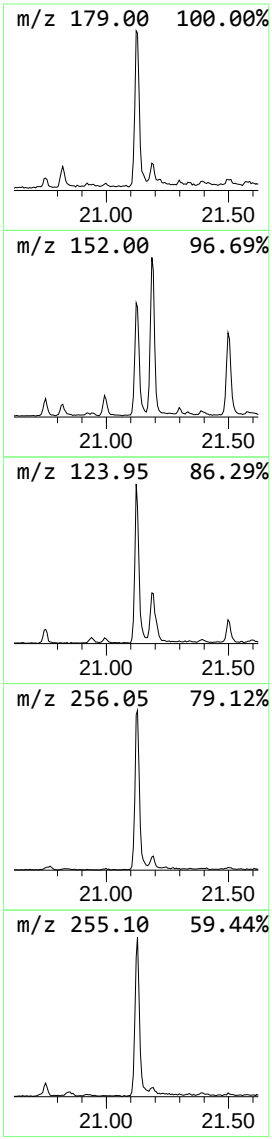
**********
Peak Number 9 4H-1-Benzopyran-4-one, 2,3-... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.122 | 4.14 ng | 706625 | Chrysene-d12 | 21.204 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4H-1-Benzopyran-4-one, 2,3-dihyd... | 256 | C15H12O4 | 000480-39-7 | 99 |
| 2 | Diethylthiophosphinic acid, o-me... | 152 | C5H13OPS | 1000306-04-1 | 22 |
| 3 | Benzofuroxan-5-carboxamide | 179 | C7H5N3O3 | 036389-09-0 | 11 |
| 4 | 2-Methylaminomethyl-5-nitrobenzo... | 256 | C14H12N2O3 | 004958-56-9 | 10 |
| 5 | 3-Phenyl-1-(6,7,8,9-tetrahydro-5... | 375 | C22H25N5O | 1000297-09-0 | 10 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081721\
Data File : BP006697.D
Acq On : 16 Aug 2021 23:11
Operator : CG/JU
Sample : M3425-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 22S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

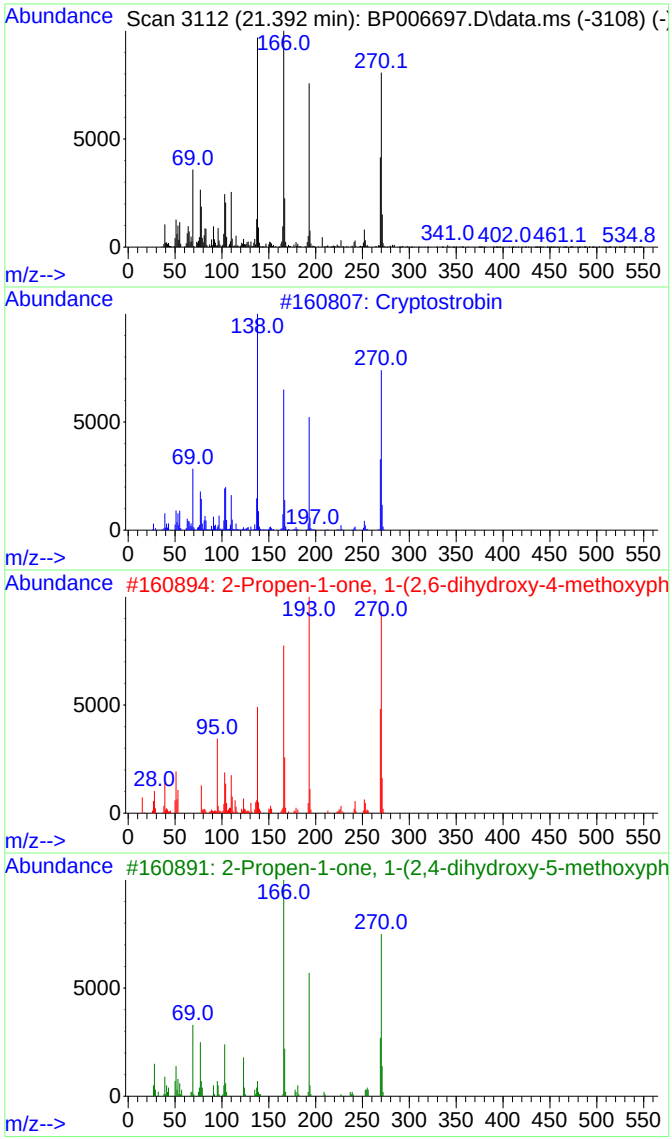
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

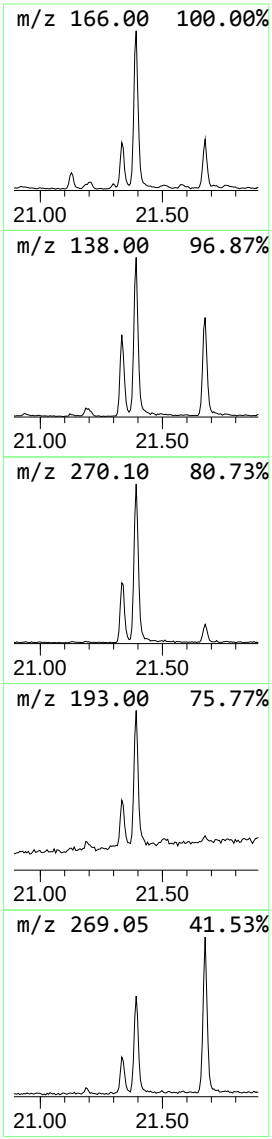
**********

Peak Number 10 Cryptostrobin Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.392 | 3.63 ng | 620619 | Chrysene-d12 | 21.204 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cryptostrobin | 270 | C16H14O4 | 1010497-72-2 | 95 |
| 2 | 2-Propen-1-one, 1-(2,6-dihydroxy... | 270 | C16H14O4 | 018956-15-5 | 86 |
| 3 | 2-Propen-1-one, 1-(2,4-dihydroxy... | 270 | C16H14O4 | 028143-82-0 | 62 |
| 4 | 4H-1-Benzopyran-4-one, 2,3-dihyd... | 270 | C16H14O4 | 000480-37-5 | 60 |
| 5 | 5-Hydroxy-7-methoxyflavanone | 270 | C16H14O4 | 075291-74-6 | 58 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081721\
Data File : BP006697.D
Acq On : 16 Aug 2021 23:11
Operator : CG/JU
Sample : M3425-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 22S

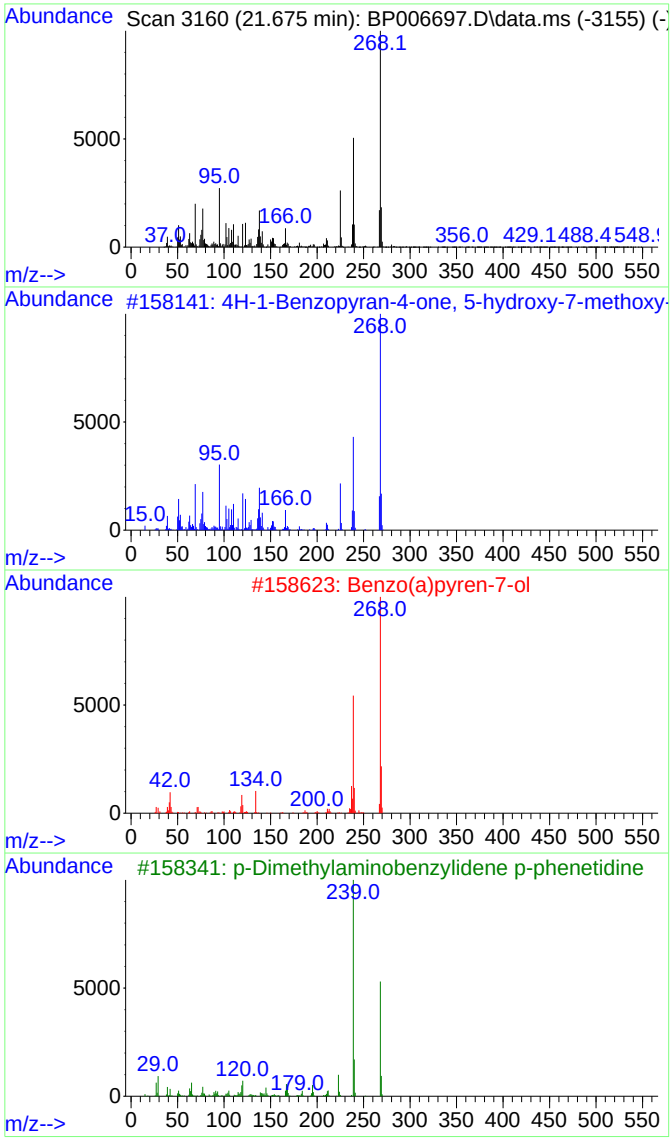
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

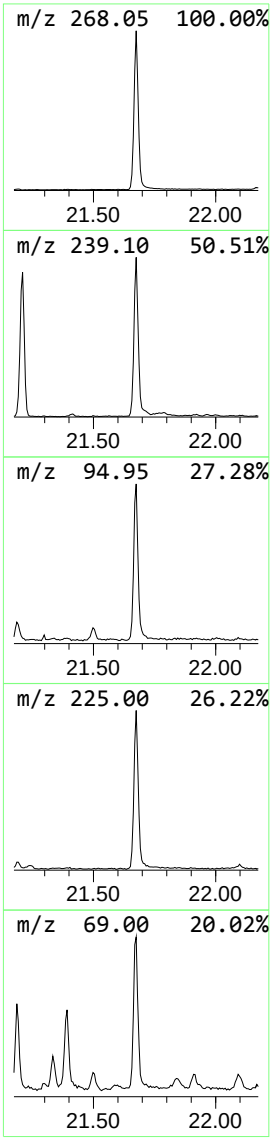
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 11 4H-1-Benzopyran-4-one, 5-hy... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.675 | 8.93 ng | 1524780 | Chrysene-d12 | 21.204 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4H-1-Benzopyran-4-one, 5-hydroxy... | 268 | C16H12O4 | 000520-28-5 | 98 |
| 2 | Benzo(a)pyren-7-ol | 268 | C20H12O | 037994-82-4 | 70 |
| 3 | p-Dimethylaminobenzylidene p-phe... | 268 | C17H20N2O | 015484-93-2 | 50 |
| 4 | 9,10-anthracenedione, 2,3,6,7-te... | 268 | C14H12N4O2 | 1000401-68-7 | 43 |
| 5 | Dinaphtho[1,2-b:1',2'-d]furan | 268 | C20H12O | 000207-93-2 | 43 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081721\
Data File : BP006697.D
Acq On : 16 Aug 2021 23:11
Operator : CG/JU
Sample : M3425-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 22S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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 |
| Ethanol, 2-(2-b... | 10.287 | 3.1 | ng | 243950 | 2 | 10.487 | 1567100 | 20.0 |
| n-Hexadecanoic ... | 18.010 | 2.5 | ng | 271805 | 4 | 17.104 | 2184640 | 20.0 |
| unknown18.916 | 18.916 | 4.0 | ng | 431000 | 4 | 17.104 | 2184640 | 20.0 |
| Acridin-9-amine... | 20.222 | 27.1 | ng | 4636210 | 5 | 21.204 | 3416030 | 20.0 |
| 5-Hydroxy-7-met... | 20.751 | 11.5 | ng | 1963240 | 5 | 21.204 | 3416030 | 20.0 |
| 6-Isobutyryl-2,... | 20.822 | 2.1 | ng | 362106 | 5 | 21.204 | 3416030 | 20.0 |
| Cyclotetradecane | 20.939 | 2.7 | ng | 467904 | 5 | 21.204 | 3416030 | 20.0 |
| 4H-1-Benzopyran... | 21.122 | 4.1 | ng | 706625 | 5 | 21.204 | 3416030 | 20.0 |
| Cryptostrobin | 21.392 | 3.6 | ng | 620619 | 5 | 21.204 | 3416030 | 20.0 |
| 4H-1-Benzopyran... | 21.675 | 8.9 | ng | 1524780 | 5 | 21.204 | 3416030 | 20.0 |