LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082418\
Data File : BM016593.D
Acq On : 24 Aug 2018 18:03
Operator : SJ/JU
Sample : J4612-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** TOTE

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_M\METHODS\8270-BM082118.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 | 4.452 | 194 | 198 | 207 | rBV | 128859 | 213236 | 1.90% | 0.526% |
| 2 | 5.552 | 380 | 385 | 398 | rBV | 639704 | 1122833 | 9.98% | 2.768% |
| 3 | 7.187 | 655 | 663 | 677 | rBV | 507088 | 995655 | 8.85% | 2.454% |
| 4 | 7.534 | 716 | 722 | 738 | rBV | 1113463 | 1912463 | 17.00% | 4.714% |
| 5 | 8.004 | 797 | 802 | 821 | rVB2 | 420092 | 753614 | 6.70% | 1.858% |
| 6 | 8.322 | 850 | 856 | 872 | rBV | 1187541 | 2006916 | 17.84% | 4.947% |
| 7 | 9.192 | 998 | 1004 | 1021 | rBV | 675262 | 1306180 | 11.61% | 3.220% |
| 8 | 10.810 | 1272 | 1279 | 1296 | rBV | 459105 | 898674 | 7.99% | 2.215% |
| 9 | 13.263 | 1687 | 1696 | 1710 | rBV | 3032798 | 4283587 | 38.09% | 10.559% |
| 10 | 14.110 | 1835 | 1840 | 1849 | rBV | 335959 | 491939 | 4.37% | 1.213% |
| 11 | 14.645 | 1924 | 1931 | 1940 | rBV2 | 858101 | 1339732 | 11.91% | 3.302% |
| 12 | 16.139 | 2179 | 2185 | 2199 | rBV | 2848143 | 4287861 | 38.12% | 10.569% |
| 13 | 17.392 | 2392 | 2398 | 2407 | rBV | 1407988 | 2124210 | 18.89% | 5.236% |
| 14 | 18.245 | 2536 | 2543 | 2549 | rBV | 416468 | 585713 | 5.21% | 1.444% |
| 15 | 19.509 | 2754 | 2758 | 2764 | rBV3 | 195687 | 254924 | 2.27% | 0.628% |
| 16 | 19.980 | 2832 | 2838 | 2844 | rBV | 9944481 | 11247191 | 100.00% | 27.723% |
| 17 | 21.215 | 3045 | 3048 | 3057 | rVB9 | 131585 | 230025 | 2.05% | 0.567% |
| 18 | 21.533 | 3097 | 3102 | 3110 | rBV | 2558262 | 3375998 | 30.02% | 8.321% |
| 19 | 23.815 | 3484 | 3490 | 3499 | rBV | 1559310 | 3139128 | 27.91% | 7.738% |

Sum of corrected areas: 40569879

LSC Report - Integrated Chromatogram

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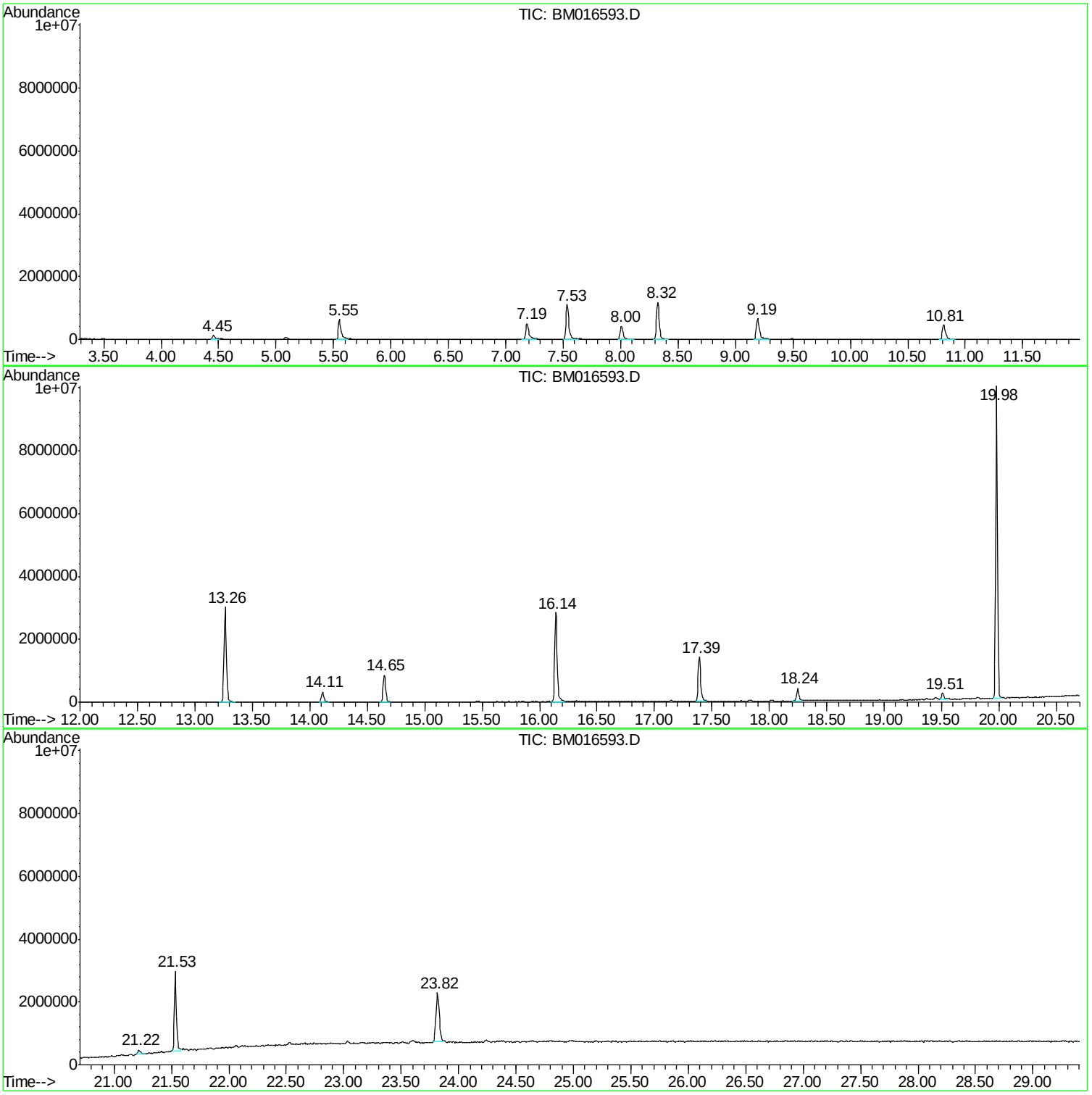
Sample : J4612-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** TOTE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082418\
Data File : BM016593.D
Acq On : 24 Aug 2018 18:03
Operator : SJ/JU
Sample : J4612-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** TOTE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

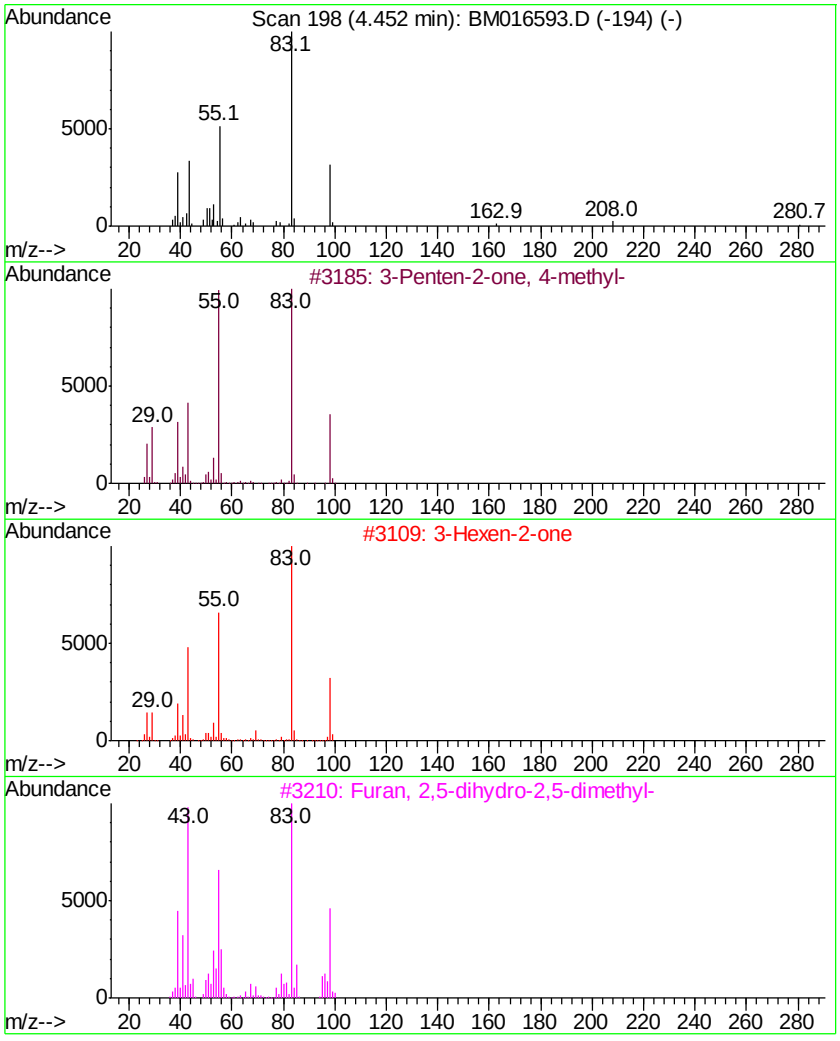
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

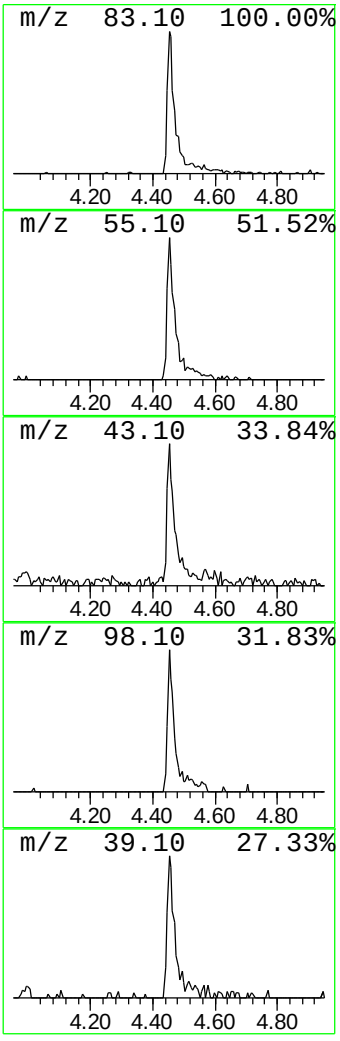
**********

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.45 | 5.66 ng | 213236 | 1,4-Dichlorobenzene-d4 | 8.00 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Penten-2-one, 4-methyl- | 98 | C6H10O | 000141-79-7 | 83 |
| 2 | 3-Hexen-2-one | 98 | C6H10O | 000763-93-9 | 80 |
| 3 | Furan, 2,5-dihydro-2,5-dimethyl- | 98 | C6H10O | 059242-27-2 | 78 |
| 4 | 2-Pentene, 2,4-dimethyl- | 98 | C7H14 | 000625-65-0 | 59 |
| 5 | 3,4-Dimethyl-2-pentene(c,t) | 98 | C7H14 | 1000118-16-5 | 59 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082418\
Data File : BM016593.D
Acq On : 24 Aug 2018 18:03
Operator : SJ/JU
Sample : J4612-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** TOTE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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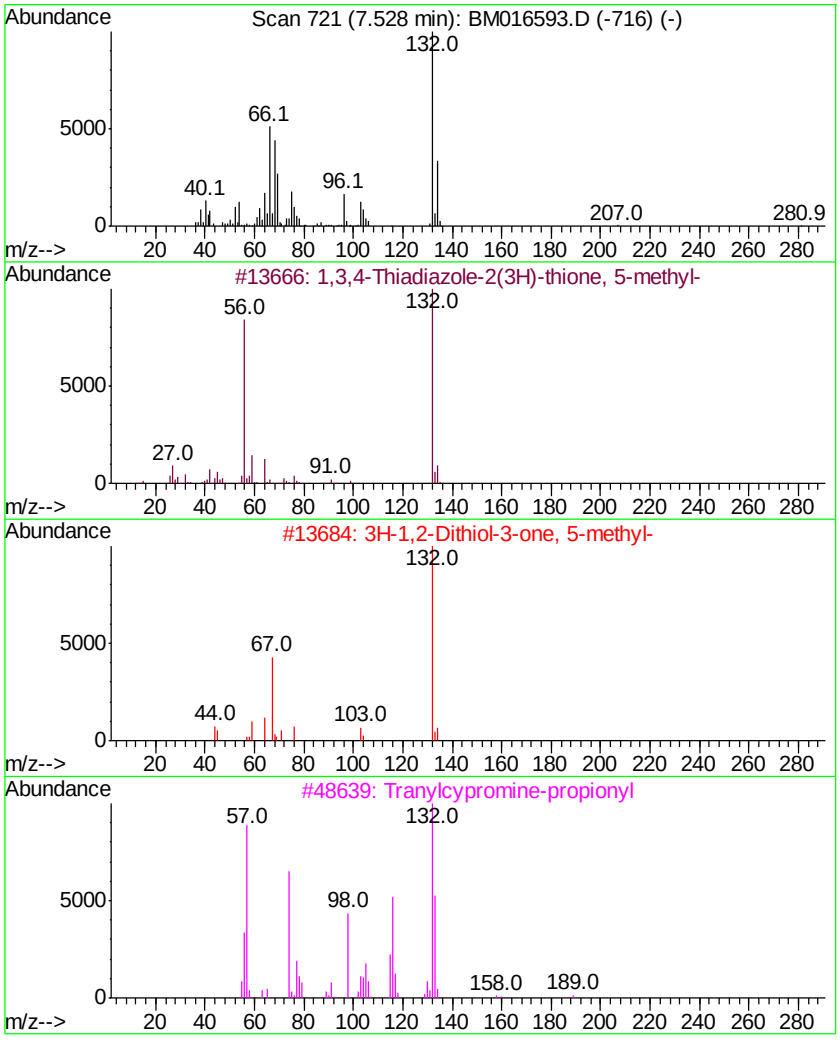
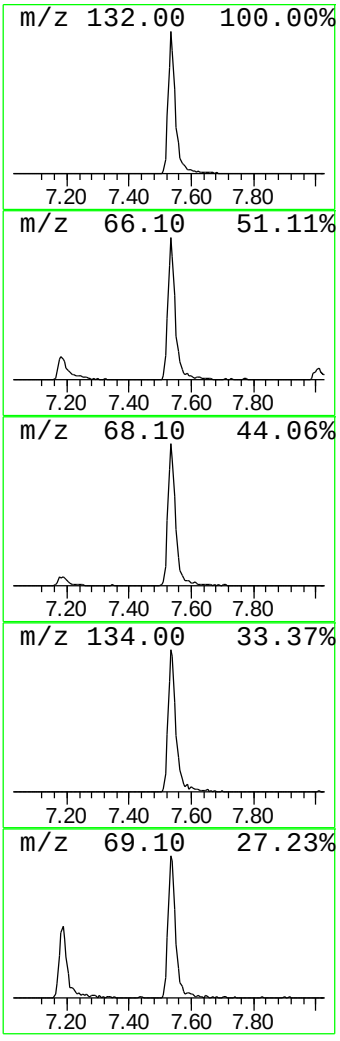
Peak Number 2 unknown7.53 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.53 | 50.75 ng | 1912460 | 1,4-Dichlorobenzene-d4 | 8.00 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2 | 029490-19-5 | 14 |
| 2 | 3H-1,2-Dithiol-3-one, 5-methyl- | 132 | C4H4OS2 | 003620-08-4 | 14 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 11 |
| 4 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 10 |
| 5 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 10 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082418\
Data File : BM016593.D
Acq On : 24 Aug 2018 18:03
Operator : SJ/JU
Sample : J4612-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** TOTE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

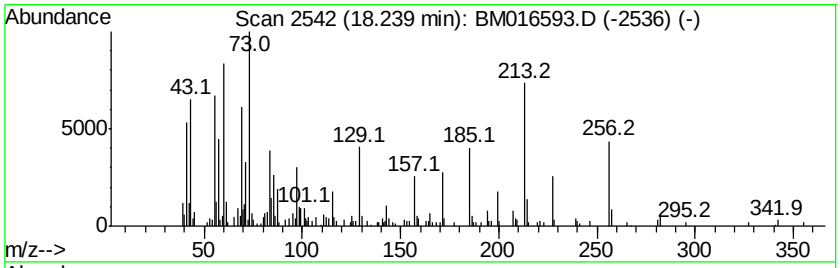
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

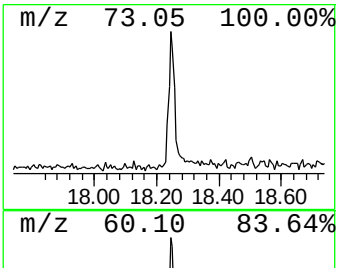
**********

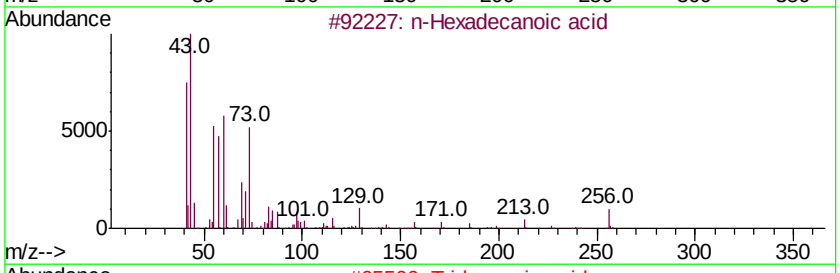
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

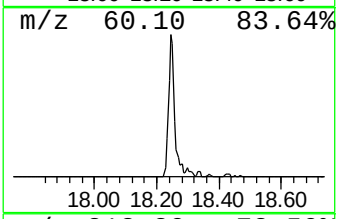
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.24 | 5.51 ng | 585713 | Phenanthrene-d10 | 17.39 |

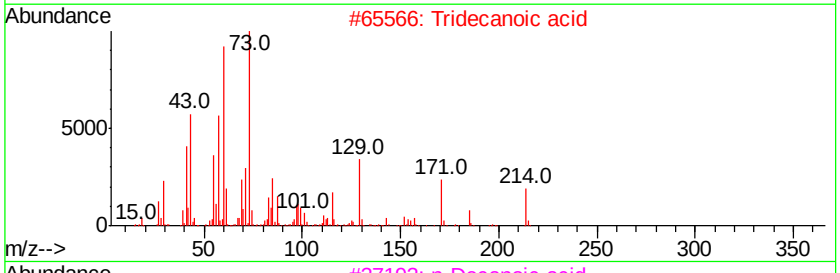
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 95 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 59 |
| 3 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 59 |
| 4 | 6-Isopropyl-3-phenoxytropolone | 256 | C16H16O3 | 002904-79-2 | 38 |
| 5 | Pyrido[3,4-c]coumarine, 3,4-dihy... | 213 | C12H7NO3 | 040547-98-6 | 35 |

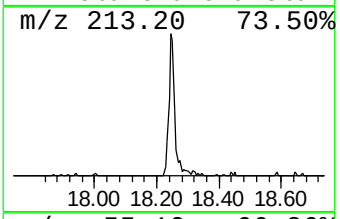


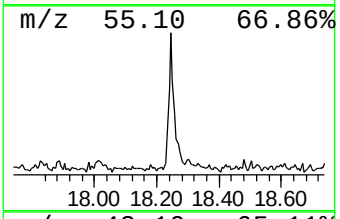



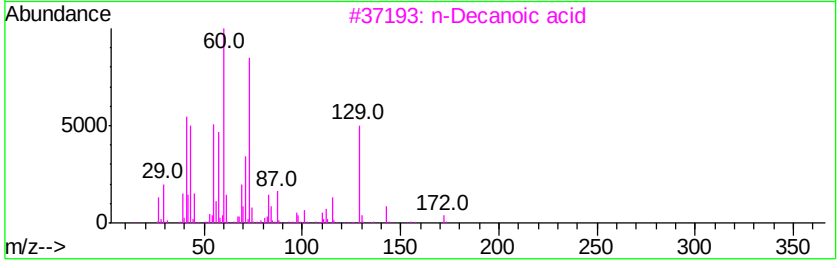



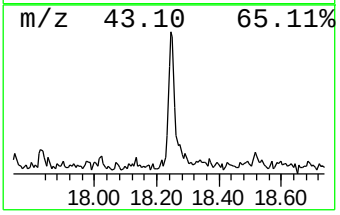



Tentatively Identified Compound (LSC) summary

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Data File : BM016593.D
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Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_M
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 3-Penten-2-one, 4... | 4.45 | 5.7 | ng | 213236 | 1 | 8.00 | 753614 | 20.0 |
| unknown7.53 | 7.53 | 50.8 | ng | 1912460 | 1 | 8.00 | 753614 | 20.0 |
| n-Hexadecanoic acid | 18.24 | 5.5 | ng | 585713 | 4 | 17.39 | 2124210 | 20.0 |