LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
Data File : BF108322.D
Acq On : 21 Aug 2018 6:48
Operator : JU/SJ
Sample : J4521-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT2286

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_F\METHODS\8270-BF080818.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 | 3.201 | 142 | 147 | 153 | rVB | 47748 | 71848 | 1.39% | 0.182% |
| 2 | 4.695 | 396 | 401 | 407 | rBV | 157234 | 173291 | 3.36% | 0.439% |
| 3 | 5.284 | 496 | 501 | 515 | rVB | 657359 | 941741 | 18.26% | 2.388% |
| 4 | 5.666 | 560 | 566 | 569 | rBV | 4345537 | 4506597 | 87.39% | 11.425% |
| 5 | 6.648 | 727 | 733 | 735 | rBV | 3646237 | 4171096 | 80.89% | 10.575% |
| 6 | 6.666 | 735 | 736 | 746 | rVB | 108286 | 90617 | 1.76% | 0.230% |
| 7 | 6.795 | 752 | 758 | 761 | rBV | 4816415 | 4874146 | 94.52% | 12.357% |
| 8 | 7.019 | 792 | 796 | 799 | rBV | 1169030 | 930321 | 18.04% | 2.359% |
| 9 | 7.178 | 818 | 823 | 826 | rBV | 4416760 | 3876969 | 75.18% | 9.829% |
| 10 | 7.583 | 886 | 892 | 895 | rBV | 3031315 | 3113228 | 60.37% | 7.893% |
| 11 | 8.301 | 1009 | 1014 | 1017 | rBV | 1145835 | 1021482 | 19.81% | 2.590% |
| 12 | 9.377 | 1191 | 1197 | 1200 | rBV | 4969247 | 5156712 | 100.00% | 13.074% |
| 13 | 10.060 | 1309 | 1313 | 1323 | rBV | 992748 | 982608 | 19.05% | 2.491% |
| 14 | 10.860 | 1444 | 1449 | 1465 | rBV | 2636645 | 2735402 | 53.05% | 6.935% |
| 15 | 11.560 | 1564 | 1568 | 1576 | rBV | 1053937 | 926834 | 17.97% | 2.350% |
| 16 | 12.942 | 1800 | 1803 | 1806 | rBV | 114862 | 90625 | 1.76% | 0.230% |
| 17 | 13.148 | 1833 | 1838 | 1841 | rBV | 4876621 | 4481832 | 86.91% | 11.363% |
| 18 | 14.212 | 2015 | 2019 | 2028 | rBV | 820148 | 746588 | 14.48% | 1.893% |
| 19 | 15.777 | 2279 | 2285 | 2291 | rBV | 377413 | 551724 | 10.70% | 1.399% |

Sum of corrected areas: 39443661

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
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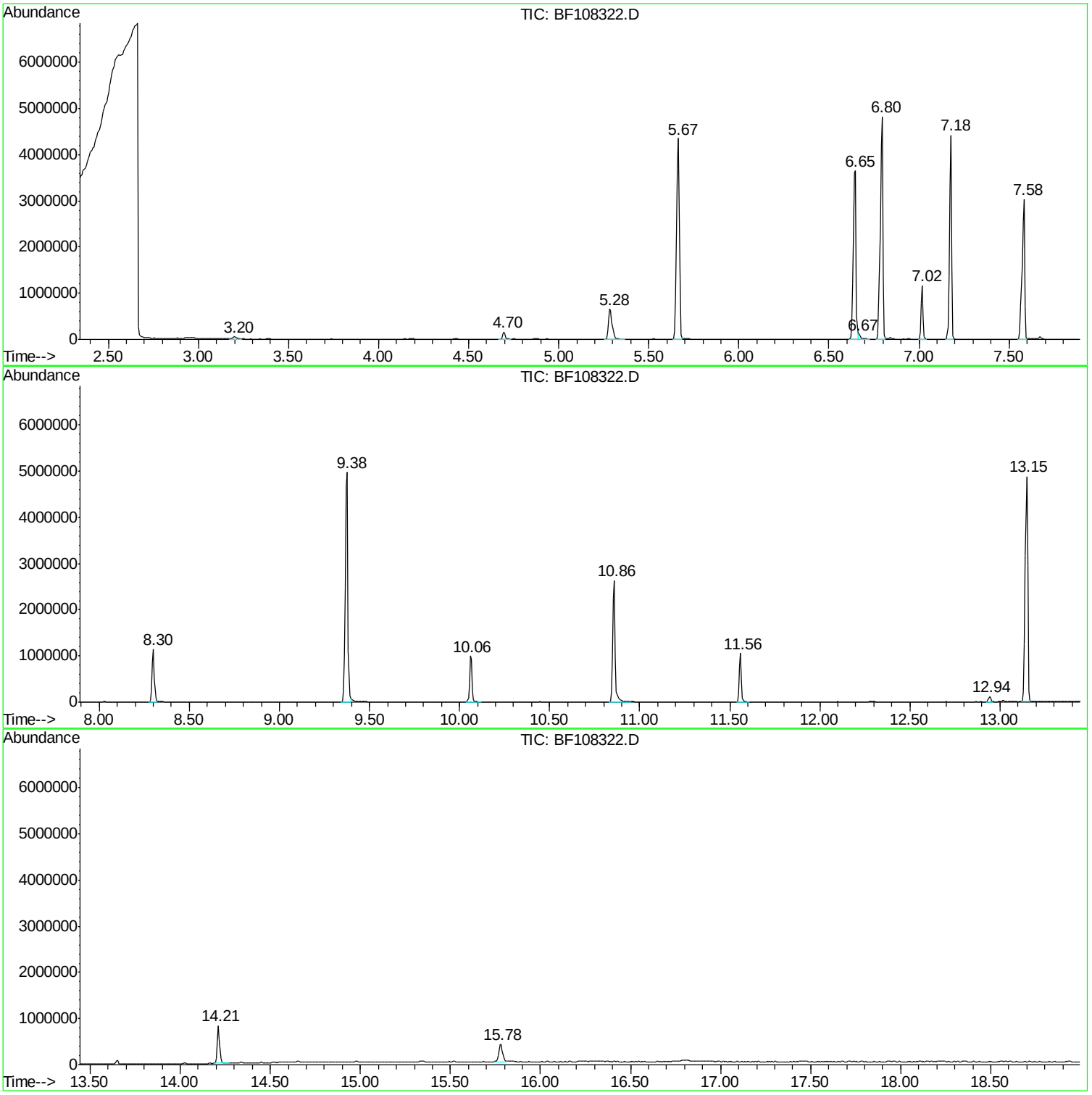
Operator : JU/SJ
Sample : J4521-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT2286

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
Data File : BF108322.D
Acq On : 21 Aug 2018 6:48
Operator : JU/SJ
Sample : J4521-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT2286

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

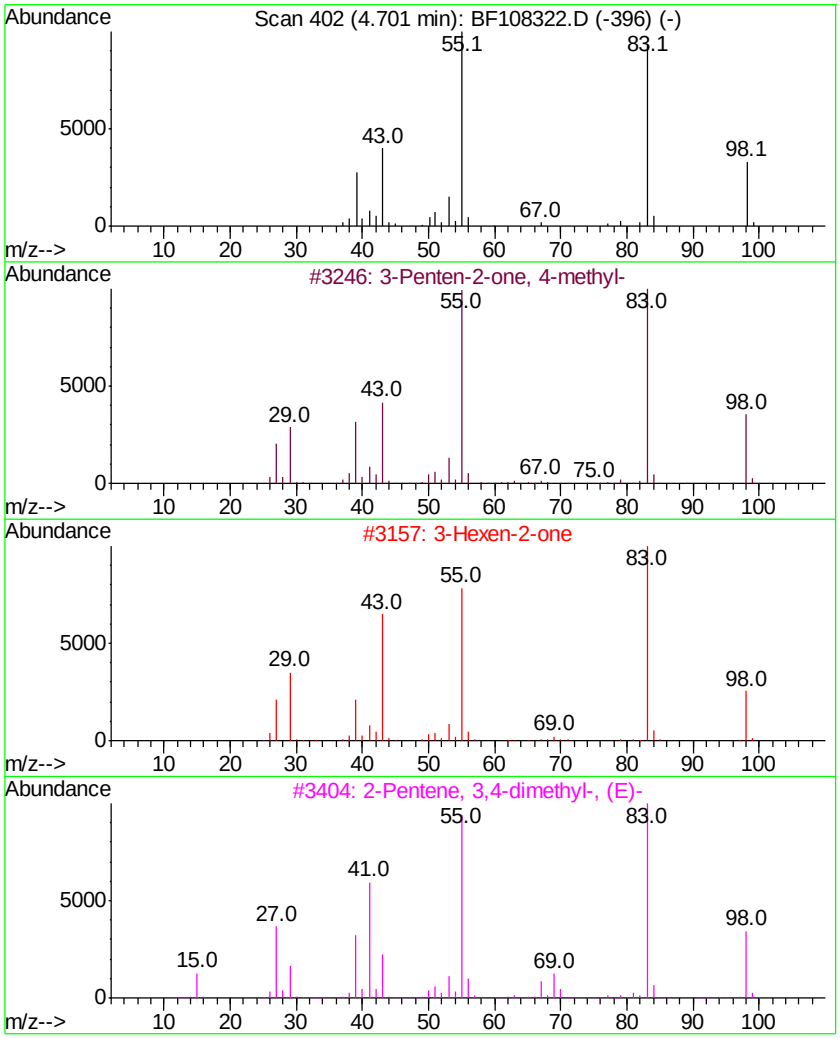
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

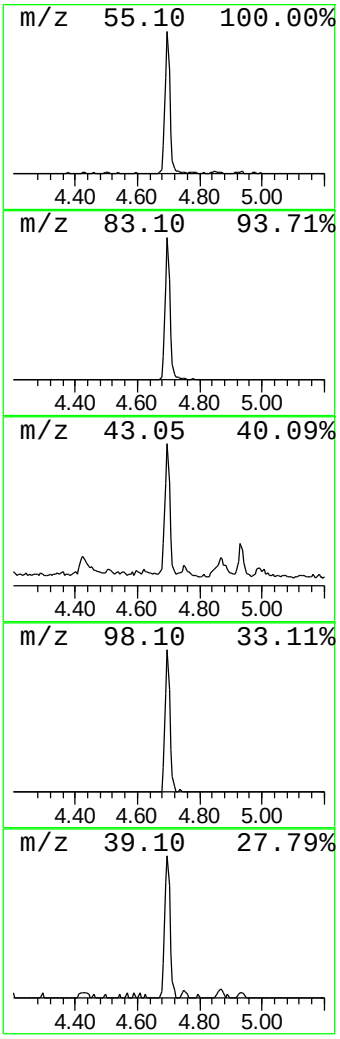
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.70 | 3.73 ng | 173291 | 1,4-Dichlorobenzene-d4 | 7.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Penten-2-one, 4-methyl- | 98 | C6H10O | 000141-79-7 | 91 |
| 2 | 3-Hexen-2-one | 98 | C6H10O | 000763-93-9 | 91 |
| 3 | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14 | 004914-92-5 | 90 |
| 4 | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14 | 004914-91-4 | 86 |
| 5 | 2-Pentene, 4,4-dimethyl-, (E)- | 98 | C7H14 | 000690-08-4 | 86 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
Data File : BF108322.D
Acq On : 21 Aug 2018 6:48
Operator : JU/SJ
Sample : J4521-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT2286

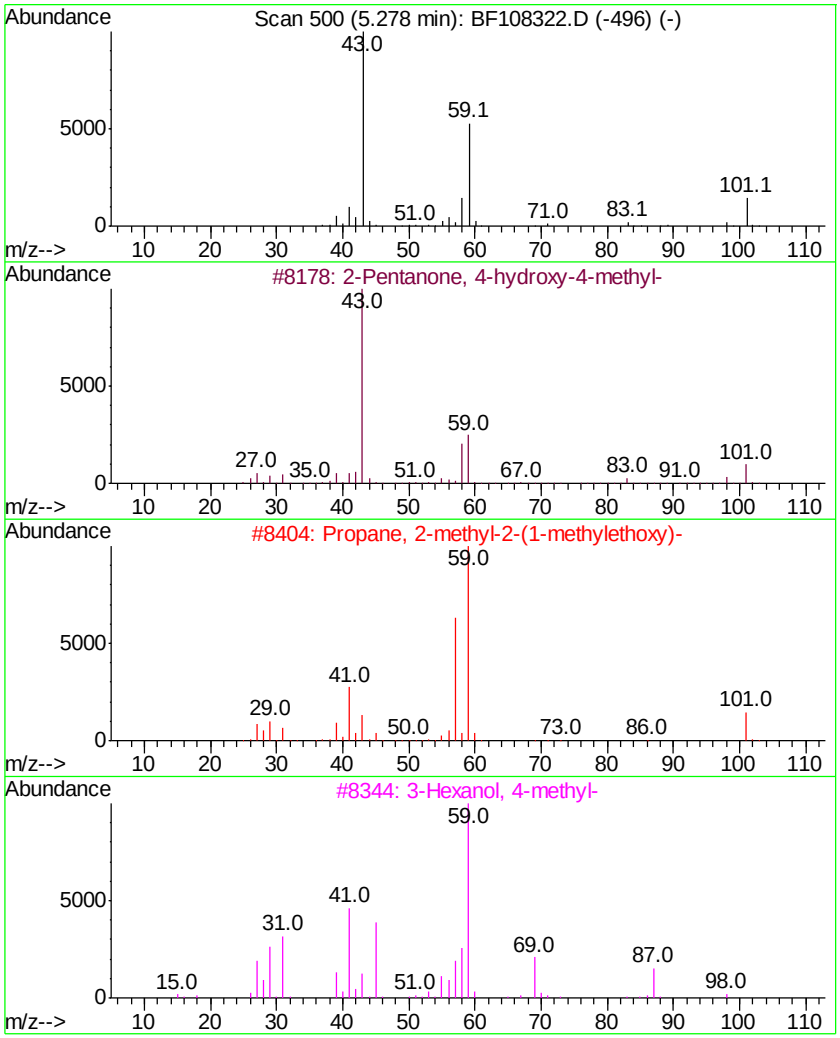
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

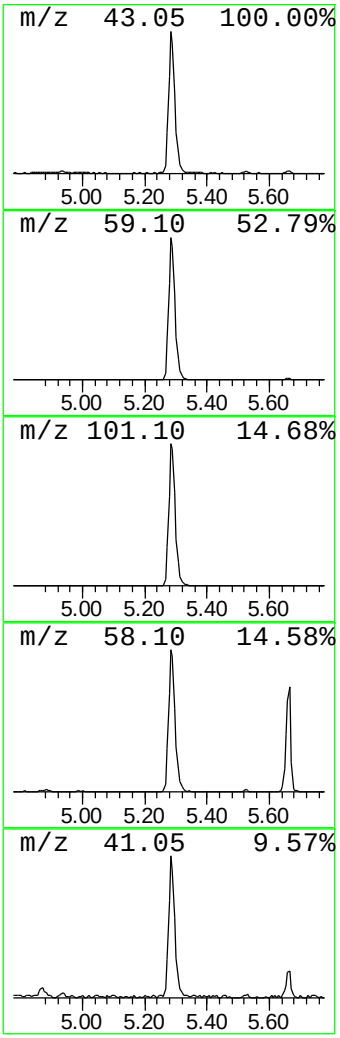
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.28 | 20.25 ng | 941741 | 1,4-Dichlorobenzene-d4 | 7.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 53 |
| 3 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 32 |
| 5 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 28 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
Data File : BF108322.D
Acq On : 21 Aug 2018 6:48
Operator : JU/SJ
Sample : J4521-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT2286

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

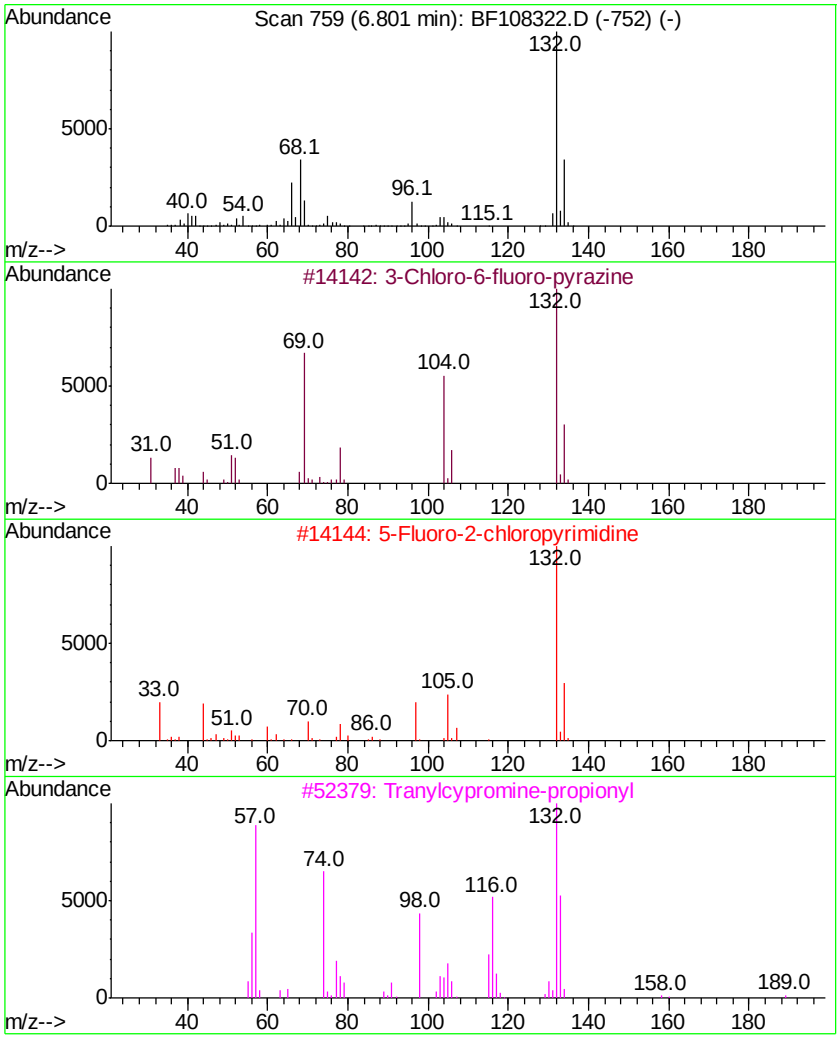
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

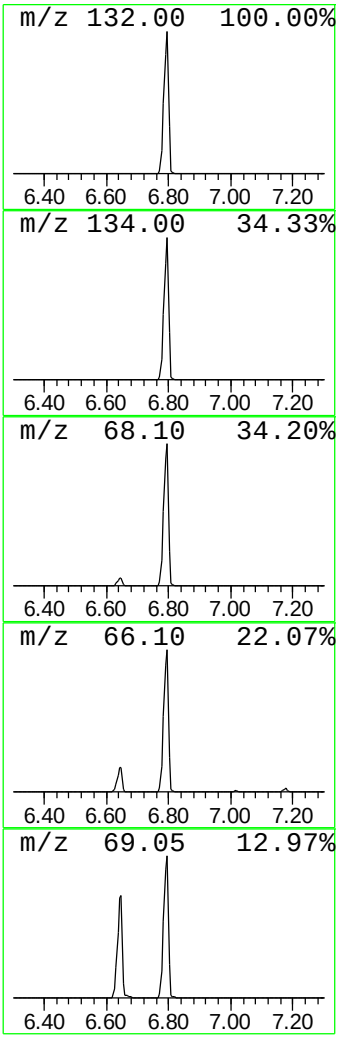
**********

Peak Number 3 unknown6.80 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.80 | 104.78 ng | 4874150 | 1,4-Dichlorobenzene-d4 | 7.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | (5-Methyl-2-pyridyl)acetonitrile | 132 | C8H8N2 | 1000241-93-9 | 10 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082018\
Data File : BF108322.D
Acq On : 21 Aug 2018 6:48
Operator : JU/SJ
Sample : J4521-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT2286

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

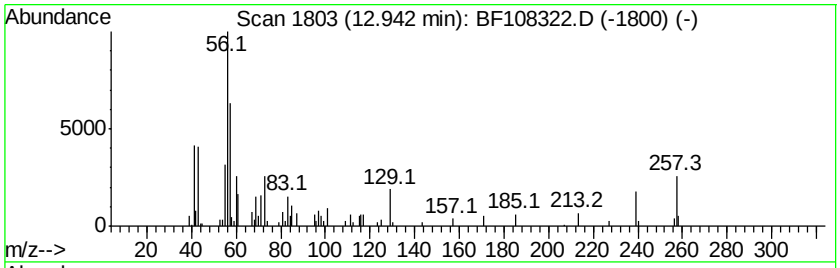
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

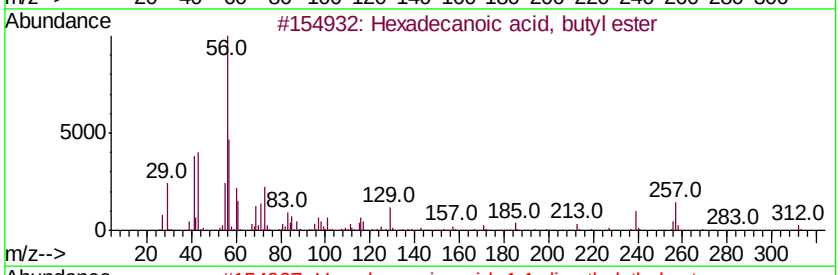
**********

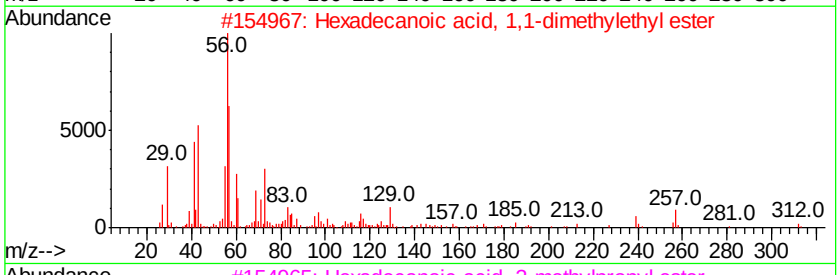
Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

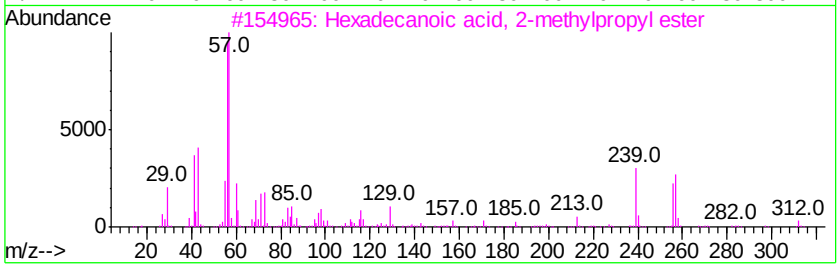
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.94 | 2.43 ng | 90625 | Chrysene-d12 | 14.21 |

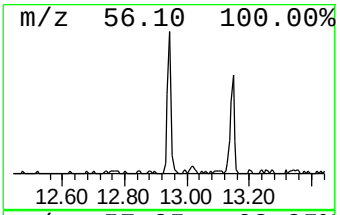
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, butyl ester | 312 | C20H40O2 | 000111-06-8 | 90 |
| 2 | Hexadecanoic acid, 1,1-dimethyle... | 312 | C20H40O2 | 031158-91-5 | 74 |
| 3 | Hexadecanoic acid, 2-methylpropy... | 312 | C20H40O2 | 000110-34-9 | 72 |
| 4 | Hexane, 3,4-dimethyl- | 114 | C8H18 | 000583-48-2 | 35 |
| 5 | Urea, N,N'-di-2-propenyl- | 140 | C7H12N2O | 001801-72-5 | 35 |

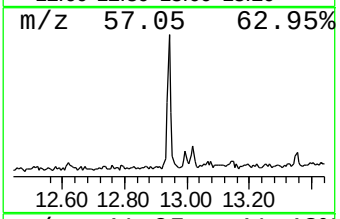


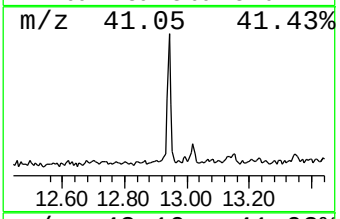



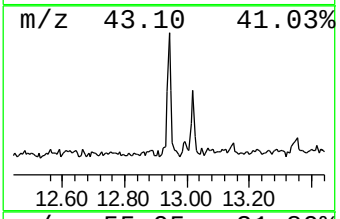



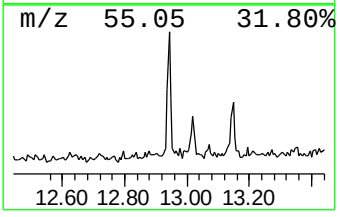



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082018\
Data File : BF108322.D
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Operator : JU/SJ
Sample : J4521-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT2286

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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 |
| 3-Penten-2-one, 4... | 4.70 | 3.7 | ng | 173291 | 1 | 7.02 | 930321 | 20.0 |
| 2-Pentanone, 4-hy... | 5.28 | 20.3 | ng | 941741 | 1 | 7.02 | 930321 | 20.0 |
| unknown6.80 | 6.80 | 104.8 | ng | 4874150 | 1 | 7.02 | 930321 | 20.0 |
| Hexadecanoic acid... | 12.94 | 2.4 | ng | 90625 | 5 | 14.21 | 746588 | 20.0 |