LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061416\
Data File : BF088031.D
Acq On : 15 Jun 2016 7:14
Operator : UM/SJ
Sample : H3473-09
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** STA-1065-(0-4)

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:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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 | 1.724 | 10 | 12 | 13 | rBV | 272381 | 361555 | 10.67% | 1.396% |
| 2 | 1.850 | 21 | 23 | 26 | rBV | 684335 | 1292592 | 38.13% | 4.992% |
| 3 | 2.547 | 82 | 84 | 88 | rVB | 51046 | 65327 | 1.93% | 0.252% |
| 4 | 3.278 | 145 | 148 | 153 | rVB | 42171 | 74730 | 2.20% | 0.289% |
| 5 | 4.307 | 233 | 238 | 241 | rBV | 1885401 | 3389673 | 100.00% | 13.090% |
| 6 | 4.959 | 293 | 295 | 306 | rVB | 218975 | 408245 | 12.04% | 1.577% |
| 7 | 5.393 | 330 | 333 | 335 | rBV | 1695806 | 2277966 | 67.20% | 8.797% |
| 8 | 6.422 | 420 | 423 | 426 | rBV | 1619919 | 1907101 | 56.26% | 7.365% |
| 9 | 6.547 | 432 | 434 | 437 | rBV | 1674932 | 2336231 | 68.92% | 9.022% |
| 10 | 6.776 | 452 | 454 | 457 | rBV | 418247 | 550621 | 16.24% | 2.126% |
| 11 | 6.936 | 466 | 468 | 471 | rVB | 1857463 | 1755616 | 51.79% | 6.780% |
| 12 | 7.347 | 501 | 504 | 506 | rBV | 1469296 | 1407307 | 41.52% | 5.435% |
| 13 | 8.067 | 565 | 567 | 569 | rBV | 918584 | 775077 | 22.87% | 2.993% |
| 14 | 9.153 | 659 | 662 | 664 | rBV | 2315312 | 2884796 | 85.11% | 11.141% |
| 15 | 9.816 | 718 | 720 | 723 | rBV | 589565 | 747004 | 22.04% | 2.885% |
| 16 | 10.605 | 787 | 789 | 792 | rBV2 | 1054409 | 1332909 | 39.32% | 5.148% |
| 17 | 11.302 | 848 | 850 | 852 | rBV | 823489 | 671725 | 19.82% | 2.594% |
| 18 | 12.011 | 910 | 912 | 916 | rBV | 58522 | 67757 | 2.00% | 0.262% |
| 19 | 12.719 | 971 | 974 | 976 | rBV | 230435 | 186874 | 5.51% | 0.722% |
| 20 | 12.799 | 976 | 981 | 982 | rVB2 | 25738 | 38157 | 1.13% | 0.147% |
| 21 | 12.891 | 986 | 989 | 991 | rBV | 2176217 | 2099115 | 61.93% | 8.106% |
| 22 | 13.417 | 1033 | 1035 | 1037 | rBV | 91283 | 126120 | 3.72% | 0.487% |
| 23 | 13.931 | 1078 | 1080 | 1083 | rBV | 592572 | 625954 | 18.47% | 2.417% |
| 24 | 15.337 | 1201 | 1203 | 1206 | rBV | 315307 | 470884 | 13.89% | 1.818% |
| 25 | 16.022 | 1259 | 1263 | 1266 | rVB | 25997 | 40895 | 1.21% | 0.158% |

Sum of corrected areas: 25894231

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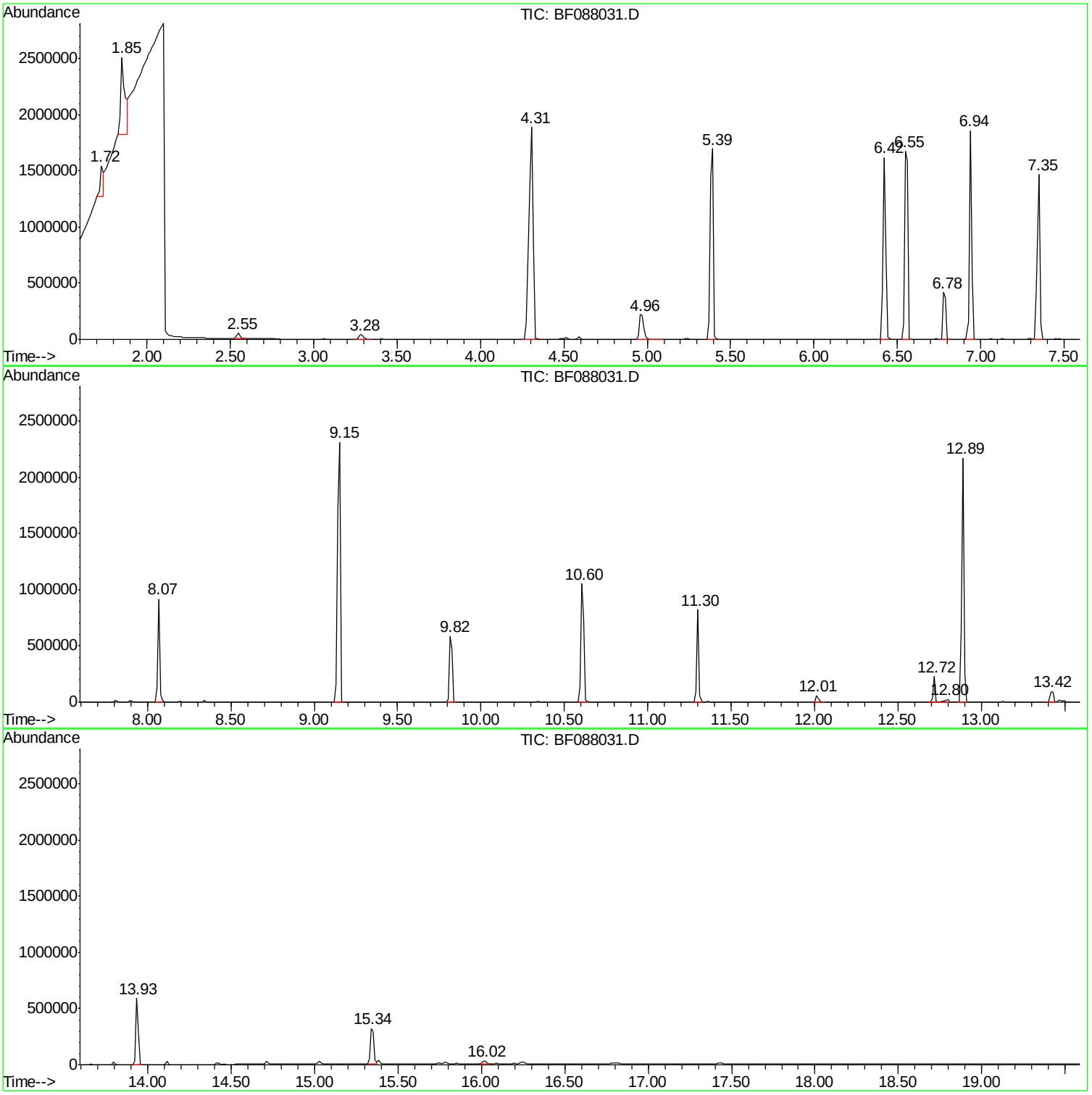
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
STA-1065-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061416\
Data File : BF088031.D
Acq On : 15 Jun 2016 7:14
Operator : UM/SJ
Sample : H3473-09
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** STA-1065-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

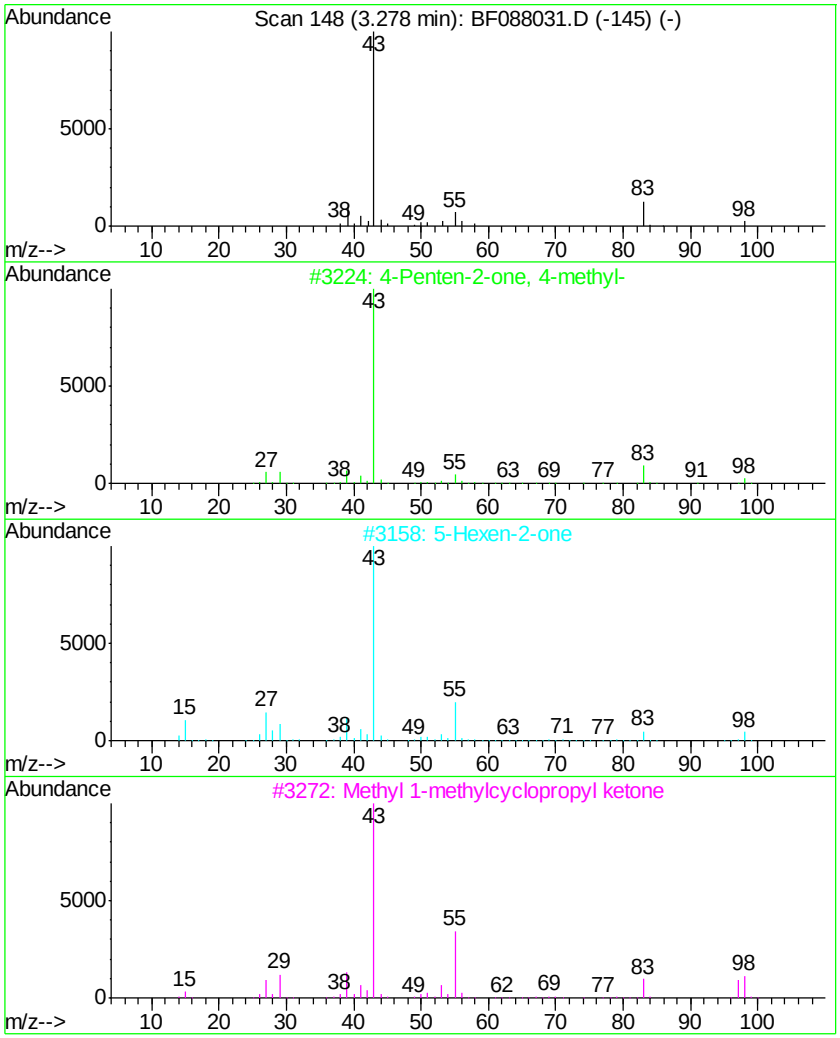
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

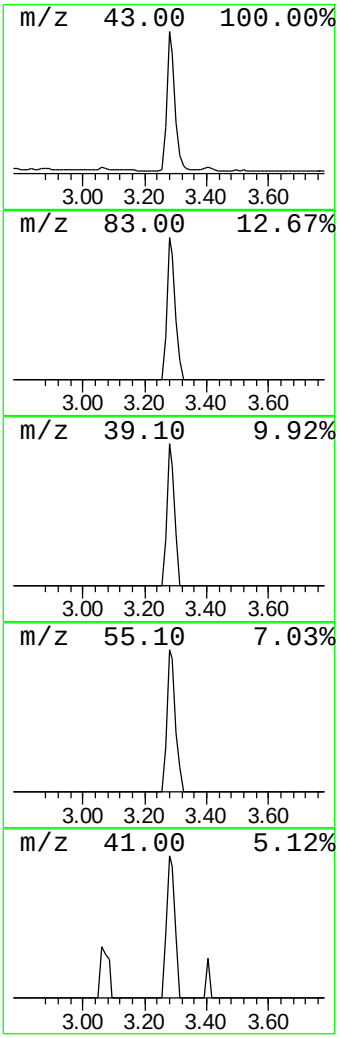
**********

Peak Number 4 4-Penten-2-one, 4-methyl- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.28 | 2.71 ng | 74730 | 1,4-Dichlorobenzene-d4 | 6.79 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Penten-2-one, 4-methyl- | 98 | C6H10O | 003744-02-3 | 86 |
| 2 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 50 |
| 3 | Methyl 1-methylcyclopropyl ketone | 98 | C6H10O | 001567-75-5 | 30 |
| 4 | 4-Penten-2-one, 3-methyl- | 98 | C6H10O | 000758-87-2 | 28 |
| 5 | 2-Pentanone, 3-methylene- | 98 | C6H10O | 004359-77-7 | 17 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061416\
Data File : BF088031.D
Acq On : 15 Jun 2016 7:14
Operator : UM/SJ
Sample : H3473-09
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** STA-1065-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

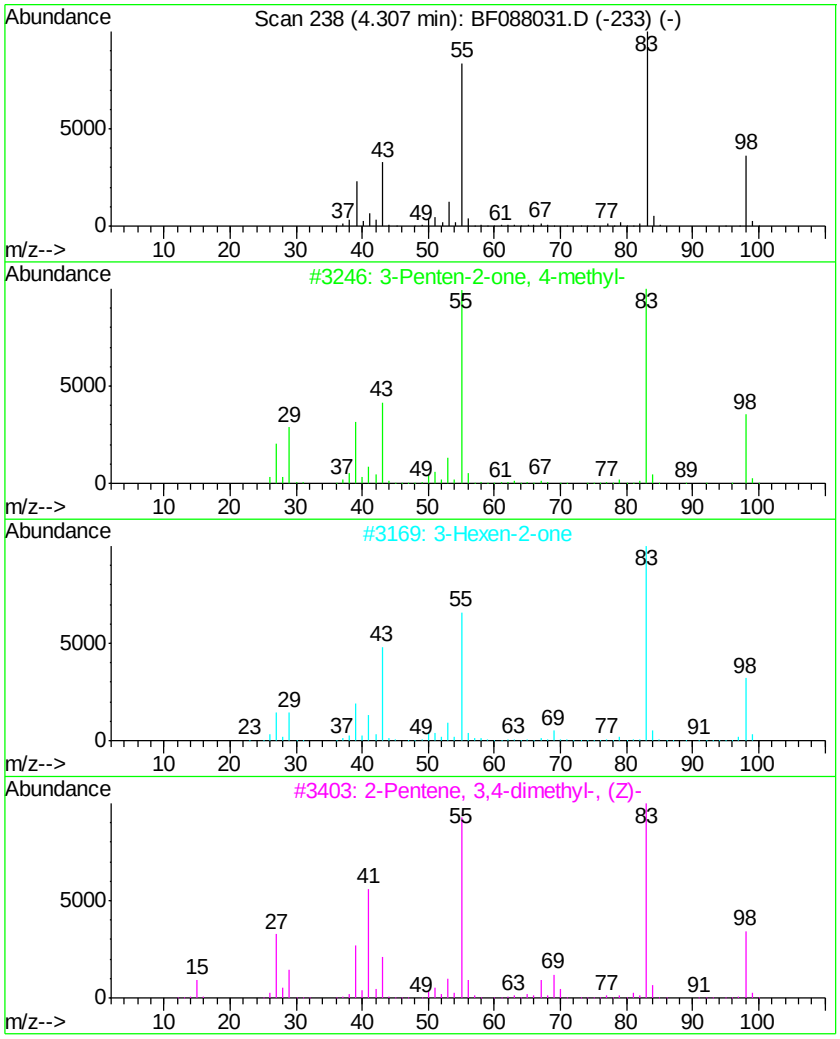
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

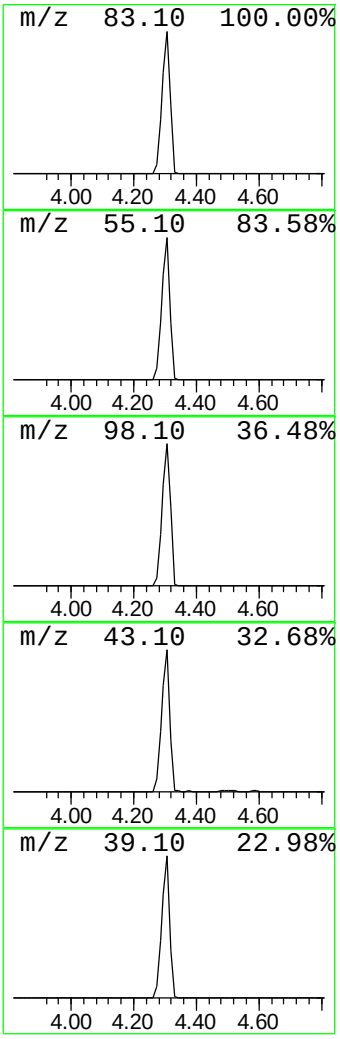
**********

Peak Number 5 3-Penten-2-one, 4-methyl- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.31 | 123.12 ng | 3389670 | 1,4-Dichlorobenzene-d4 | 6.79 |

| 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 | 87 |
| 3 | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14 | 004914-91-4 | 86 |
| 4 | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14 | 004914-92-5 | 86 |
| 5 | Furan, 2-methoxy- | 98 | C5H6O2 | 025414-22-6 | 78 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061416\
Data File : BF088031.D
Acq On : 15 Jun 2016 7:14
Operator : UM/SJ
Sample : H3473-09
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** STA-1065-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

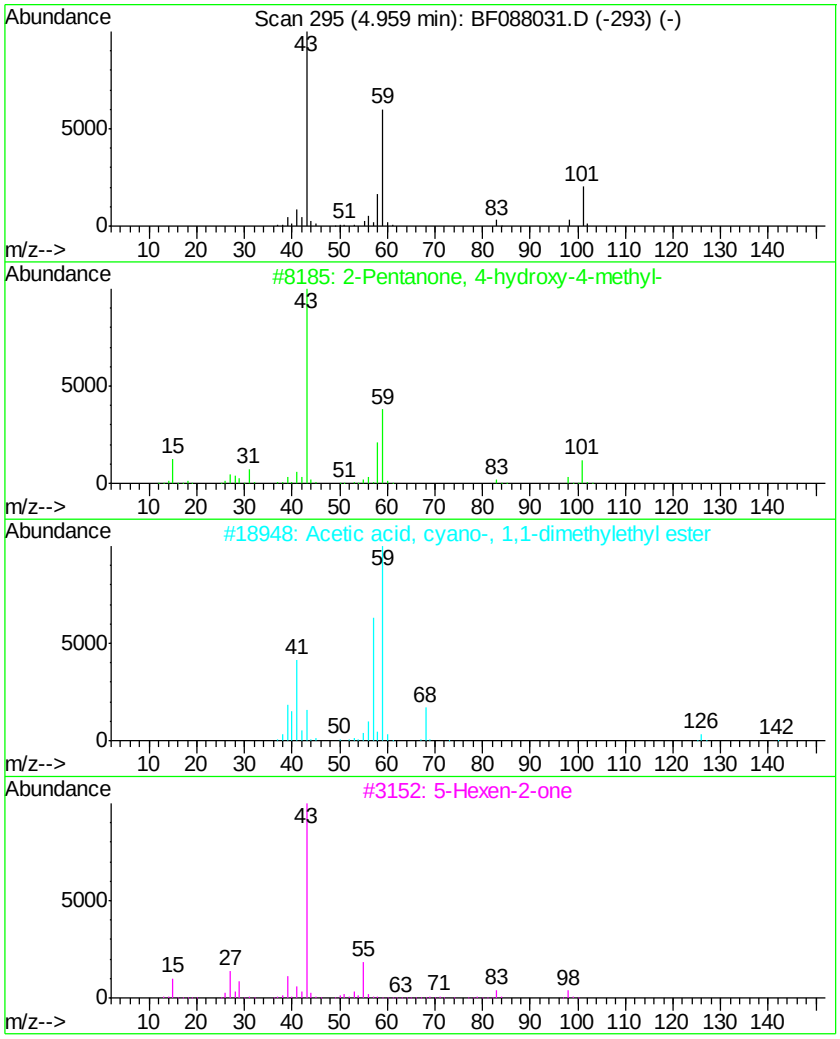
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

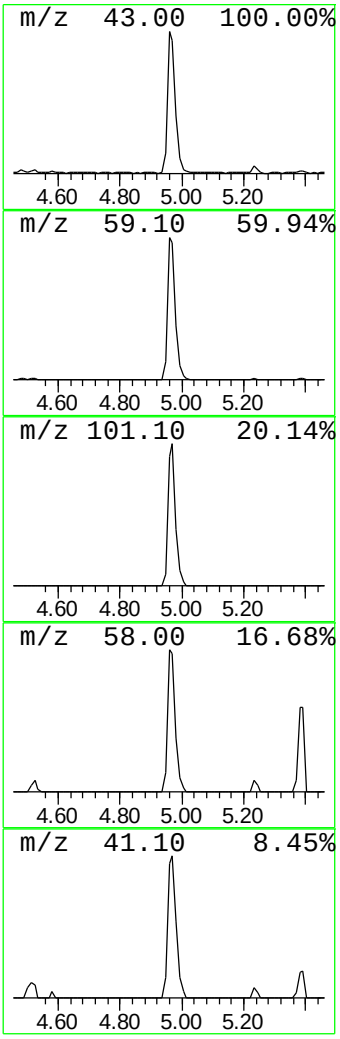
**********

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.96 | 14.83 ng | 408245 | 1,4-Dichlorobenzene-d4 | 6.79 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 3 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061416\
Data File : BF088031.D
Acq On : 15 Jun 2016 7:14
Operator : UM/SJ
Sample : H3473-09
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** STA-1065-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

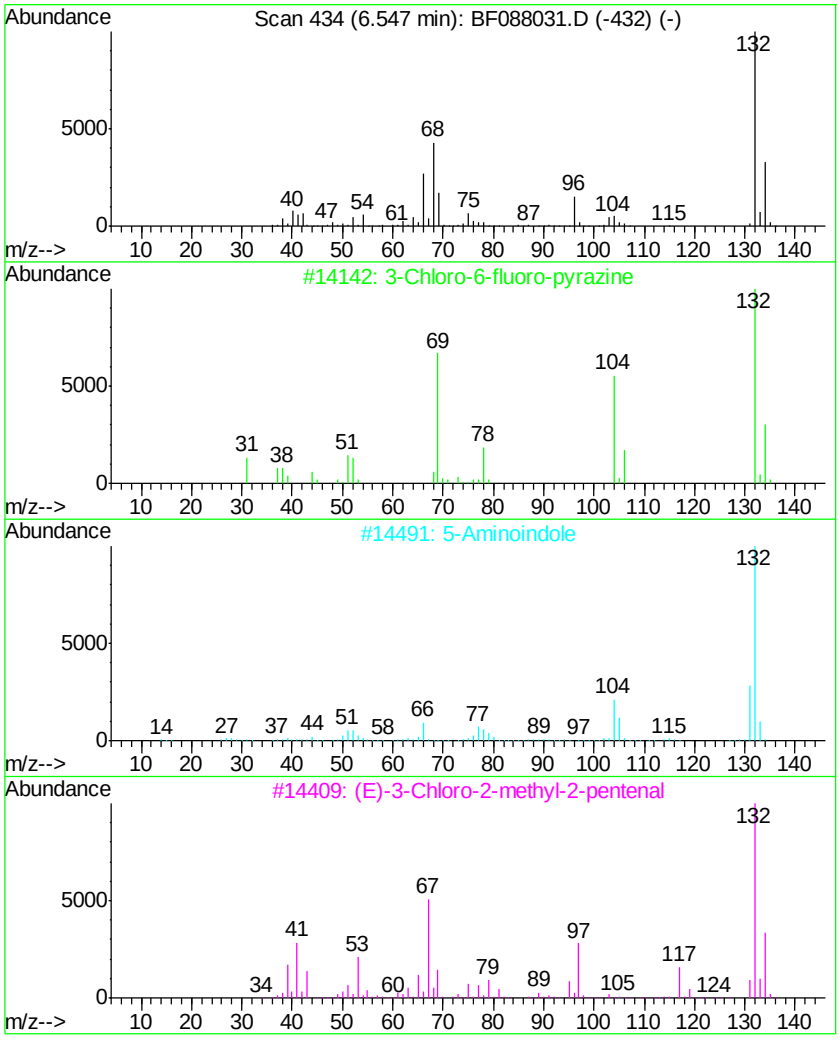
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

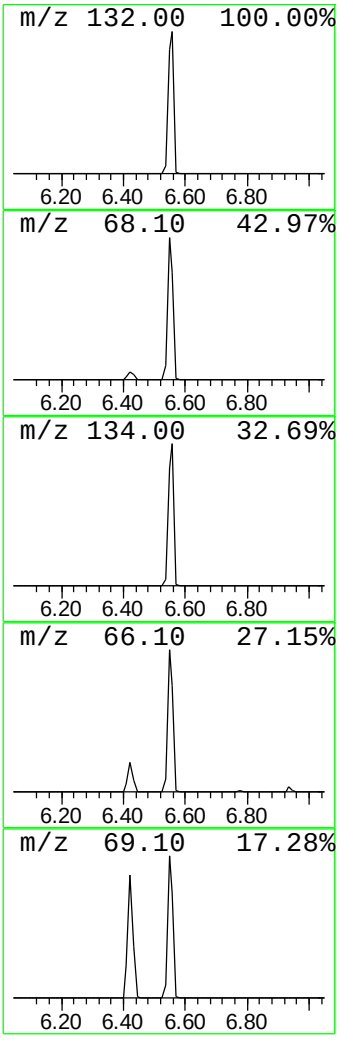
**********

Peak Number 7 unknown6.55 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.55 | 84.86 ng | 2336230 | 1,4-Dichlorobenzene-d4 | 6.79 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 3 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 9 |
| 4 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |
| 5 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061416\
Data File : BF088031.D
Acq On : 15 Jun 2016 7:14
Operator : UM/SJ
Sample : H3473-09
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** STA-1065-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

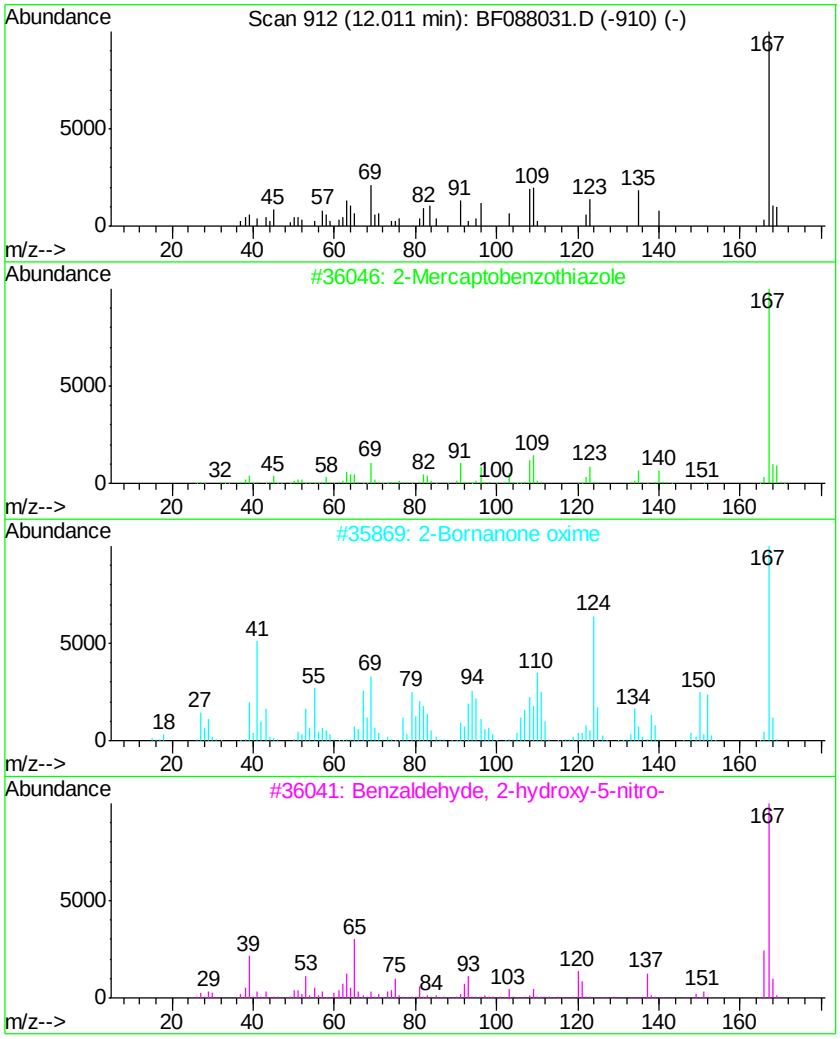
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

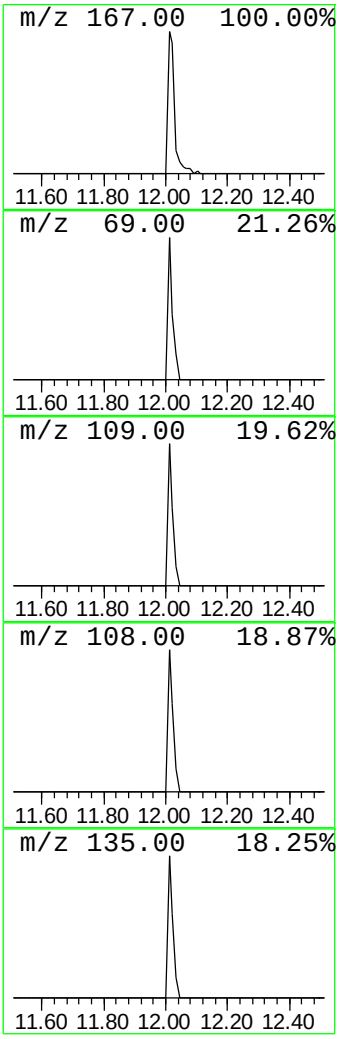
**********

Peak Number 9 2-Mercaptobenzothiazole Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.01 | 2.02 ng | 67757 | Phenanthrene-d10 | 11.30 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Mercaptobenzothiazole | 167 | C7H5NS2 | 000149-30-4 | 97 |
| 2 | 2-Bornanone oxime | 167 | C10H17NO | 013559-66-5 | 50 |
| 3 | Benzaldehyde, 2-hydroxy-5-nitro- | 167 | C7H5NO4 | 000097-51-8 | 47 |
| 4 | 3-Hydroxy-4-nitrobenzaldehyde | 167 | C7H5NO4 | 000704-13-2 | 47 |
| 5 | 6H-Purine-6-thione, 9-amino-1,9-... | 167 | C5H5N5S | 020914-56-1 | 43 |



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Data File : BF088031.D
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Operator : UM/SJ
Sample : H3473-09
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** STA-1065-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

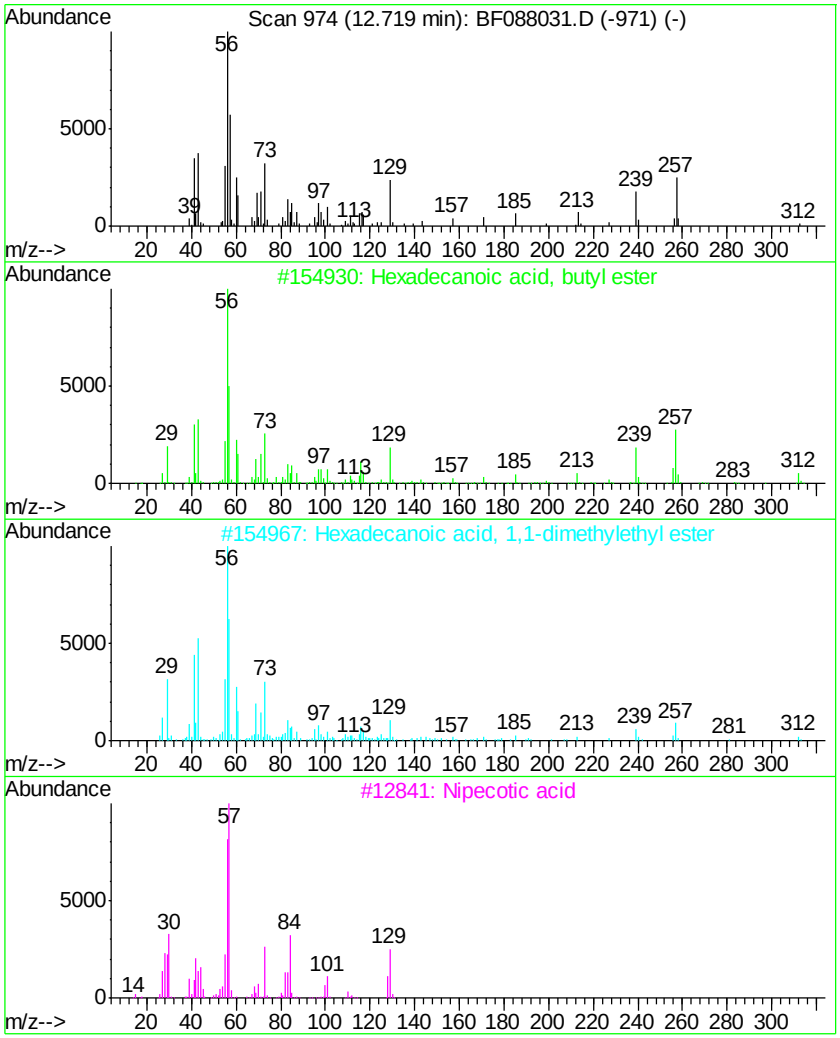
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

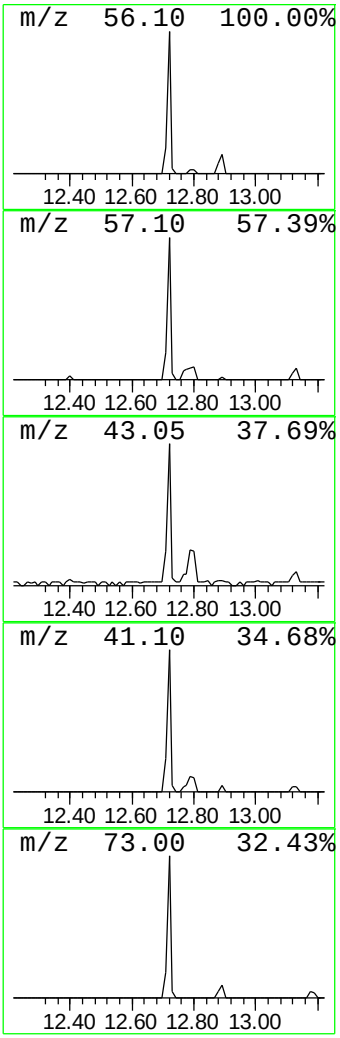
**********

Peak Number 10 Hexadecanoic acid, butyl ester Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.72 | 5.97 ng | 186874 | Chrysene-d12 | 13.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, butyl ester | 312 | C20H40O2 | 000111-06-8 | 91 |
| 2 | Hexadecanoic acid, 1,1-dimethyle... | 312 | C20H40O2 | 031158-91-5 | 72 |
| 3 | Nipecotic acid | 129 | C6H11NO2 | 000498-95-3 | 47 |
| 4 | Cyclopropane, 1-(1-methylethyl)-... | 210 | C15H30 | 041977-39-3 | 35 |
| 5 | 1-Hexene, 2,5-dimethyl- | 112 | C8H16 | 006975-92-4 | 27 |



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Sample : H3473-09
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** STA-1065-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

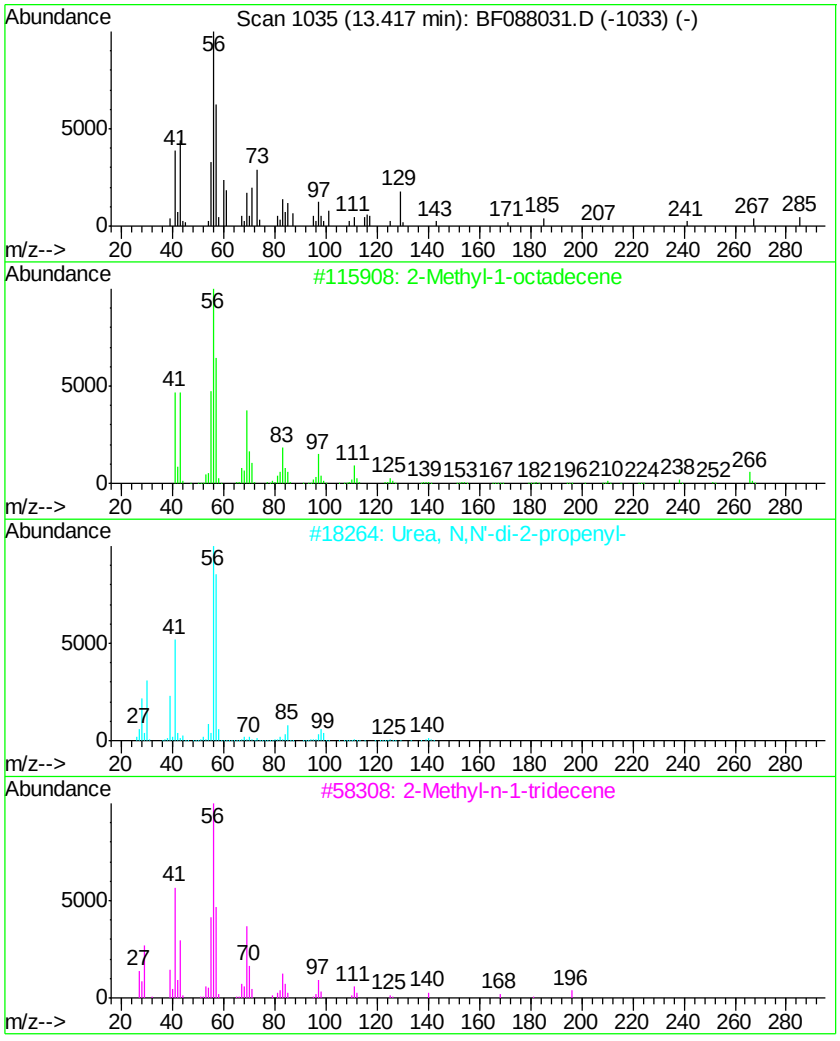
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

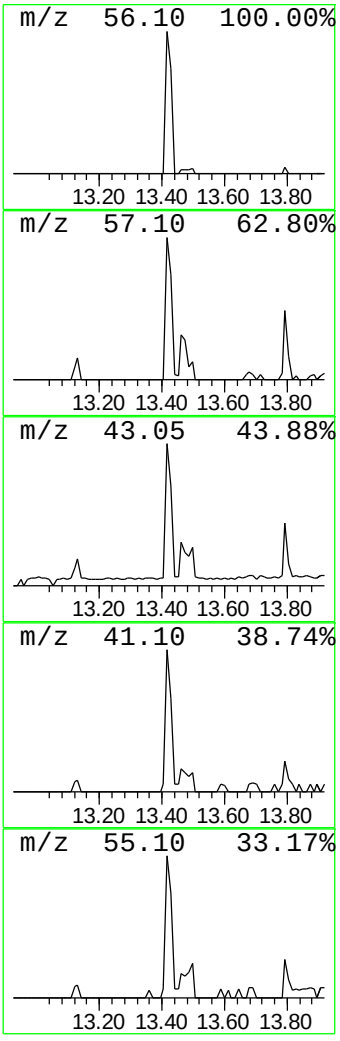
**********

Peak Number 11 unknown13.42 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.42 | 4.03 ng | 126120 | Chrysene-d12 | 13.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Methyl-1-octadecene | 266 | C19H38 | 061868-20-0 | 38 |
| 2 | Urea, N,N'-di-2-propenyl- | 140 | C7H12N2O | 001801-72-5 | 38 |
| 3 | 2-Methyl-n-1-tridecene | 196 | C14H28 | 018094-01-4 | 35 |
| 4 | Cyclobutane, 1-hexyl-2,3-dimethyl- | 168 | C12H24 | 055170-84-8 | 32 |
| 5 | Trifluoroacetic acid, 4-methylpe... | 198 | C8H13F3O2 | 000327-71-9 | 32 |



# Tentatively Identified Compound (LSC) summary

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 4-Penten-2-one, 4... | 3.28 | 2.7 | ng | 74730 | 1 | 6.79 | 550621 | 20.0 |
| 3-Penten-2-one, 4... | 4.31 | 123.1 | ng | 3389670 | 1 | 6.79 | 550621 | 20.0 |
| 2-Pentanone, 4-hy... | 4.96 | 14.8 | ng | 408245 | 1 | 6.79 | 550621 | 20.0 |
| unknown6.55 | 6.55 | 84.9 | ng | 2336230 | 1 | 6.79 | 550621 | 20.0 |
| 2-Mercaptobenzoth... | 12.01 | 2.0 | ng | 67757 | 4 | 11.30 | 671725 | 20.0 |
| Hexadecanoic acid... | 12.72 | 6.0 | ng | 186874 | 5 | 13.93 | 625954 | 20.0 |
| unknown13.42 | 13.42 | 4.0 | ng | 126120 | 5 | 13.93 | 625954 | 20.0 |