LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020416\
Data File : BF084847.D
Acq On : 4 Feb 2016 23:56
Operator : SJ/IZ
Sample : H1320-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4-B017(10-12)

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-BF020116.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 | 4.110 | 175 | 177 | 183 | rBV | 44253 | 72008 | 1.48% | 0.182% |
| 2 | 4.830 | 236 | 240 | 247 | rVB | 1049006 | 1831719 | 37.66% | 4.625% |
| 3 | 5.276 | 276 | 279 | 281 | rBV | 3409447 | 4863347 | 100.00% | 12.279% |
| 4 | 5.676 | 312 | 314 | 317 | rBV | 59009 | 59761 | 1.23% | 0.151% |
| 5 | 6.327 | 368 | 371 | 374 | rBV | 3797145 | 4216843 | 86.71% | 10.646% |
| 6 | 6.442 | 378 | 381 | 384 | rBV | 4056392 | 4362613 | 89.70% | 11.014% |
| 7 | 6.670 | 399 | 401 | 403 | rBV | 946361 | 822939 | 16.92% | 2.078% |
| 8 | 6.830 | 412 | 415 | 417 | rBV | 4058688 | 3542768 | 72.85% | 8.944% |
| 9 | 7.242 | 448 | 451 | 454 | rBV | 2410354 | 2830841 | 58.21% | 7.147% |
| 10 | 7.367 | 457 | 462 | 468 | rVB | 66530 | 95089 | 1.96% | 0.240% |
| 11 | 7.962 | 512 | 514 | 516 | rBV | 1287276 | 1122978 | 23.09% | 2.835% |
| 12 | 9.036 | 606 | 608 | 611 | rBV | 3546227 | 4767571 | 98.03% | 12.037% |
| 13 | 9.436 | 641 | 643 | 646 | rBV | 743690 | 670083 | 13.78% | 1.692% |
| 14 | 9.711 | 664 | 667 | 669 | rBV | 1299595 | 1103853 | 22.70% | 2.787% |
| 15 | 10.156 | 705 | 706 | 708 | rVB | 106705 | 75975 | 1.56% | 0.192% |
| 16 | 10.499 | 733 | 736 | 738 | rBV | 2872563 | 2680499 | 55.12% | 6.767% |
| 17 | 10.625 | 745 | 747 | 754 | rVB | 114284 | 140652 | 2.89% | 0.355% |
| 18 | 11.071 | 785 | 786 | 792 | rVB | 62772 | 94635 | 1.95% | 0.239% |
| 19 | 11.185 | 794 | 796 | 800 | rVB | 890991 | 931449 | 19.15% | 2.352% |
| 20 | 12.397 | 900 | 902 | 904 | rBV | 75364 | 70426 | 1.45% | 0.178% |
| 21 | 12.625 | 918 | 922 | 923 | rBV | 55511 | 100204 | 2.06% | 0.253% |
| 22 | 12.774 | 933 | 935 | 938 | rVB | 2879822 | 2925961 | 60.16% | 7.387% |
| 23 | 13.688 | 1012 | 1015 | 1021 | rVB | 99662 | 162932 | 3.35% | 0.411% |
| 24 | 13.814 | 1024 | 1026 | 1028 | rVV | 758835 | 820338 | 16.87% | 2.071% |
| 25 | 15.185 | 1144 | 1146 | 1149 | rBV | 533098 | 784103 | 16.12% | 1.980% |
| 26 | 18.454 | 1422 | 1432 | 1442 | rBV3 | 64899 | 459012 | 9.44% | 1.159% |

Sum of corrected areas: 39608599

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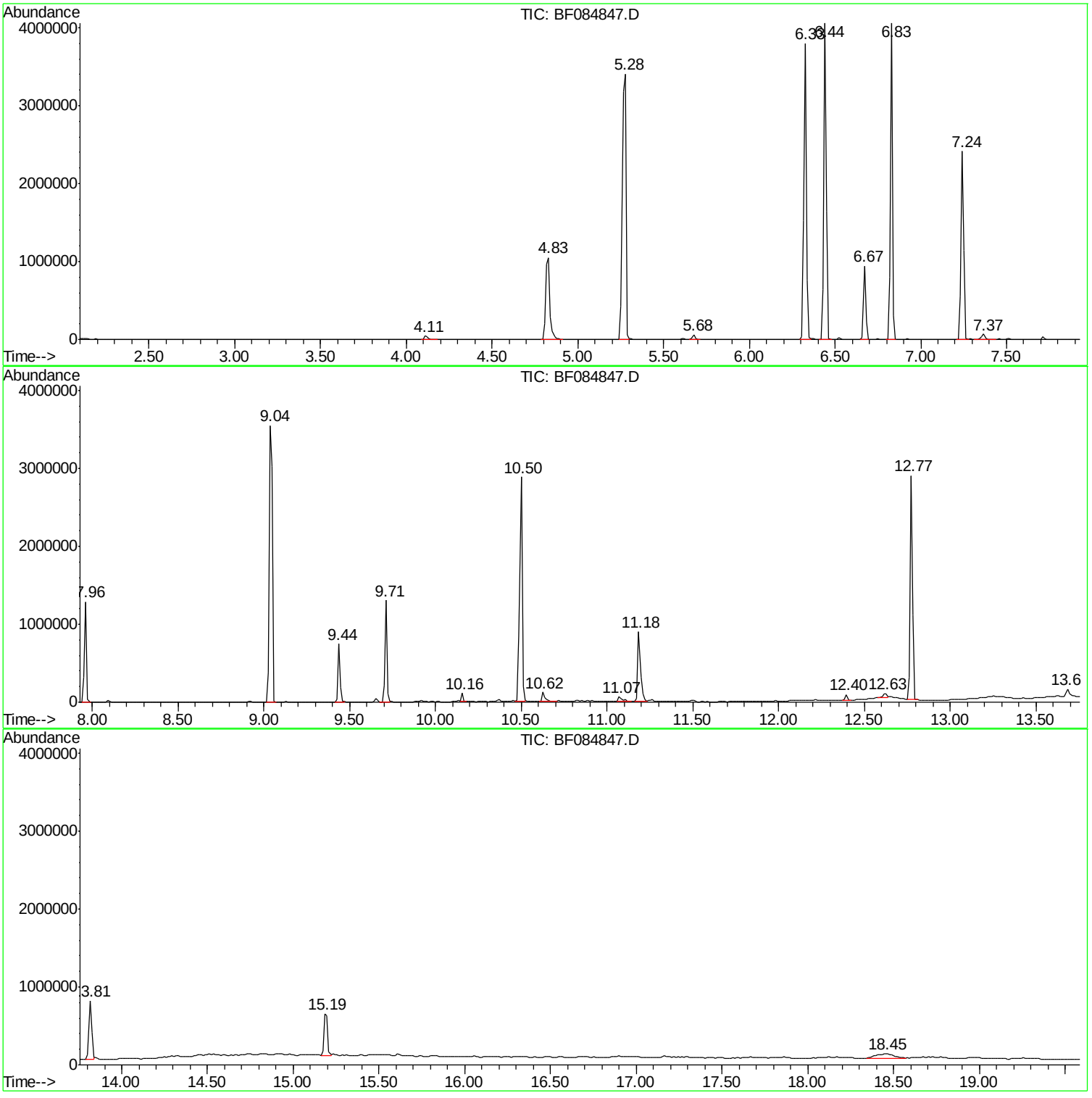
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
S4-B017(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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:\HPCHEM1\BNA F\DATA\BF020416\
Data File : BF084847.D
Acq On : 4 Feb 2016 23:56
Operator : SJ/IZ
Sample : H1320-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4-B017(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

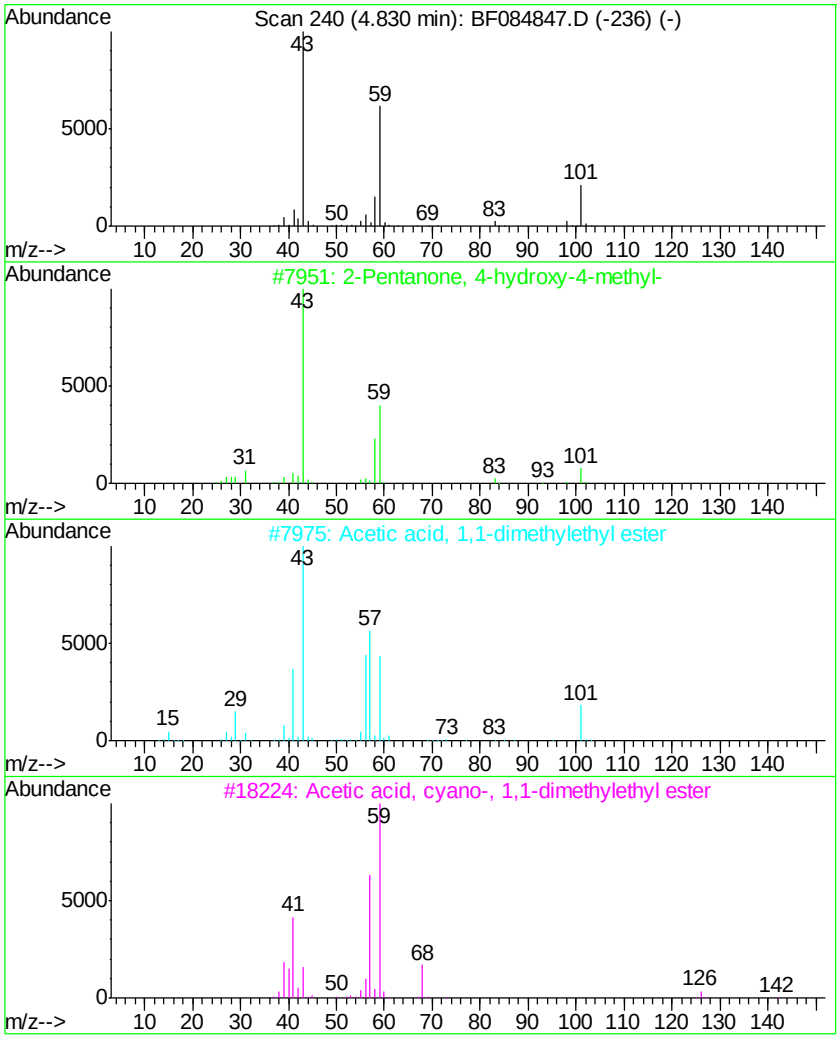
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

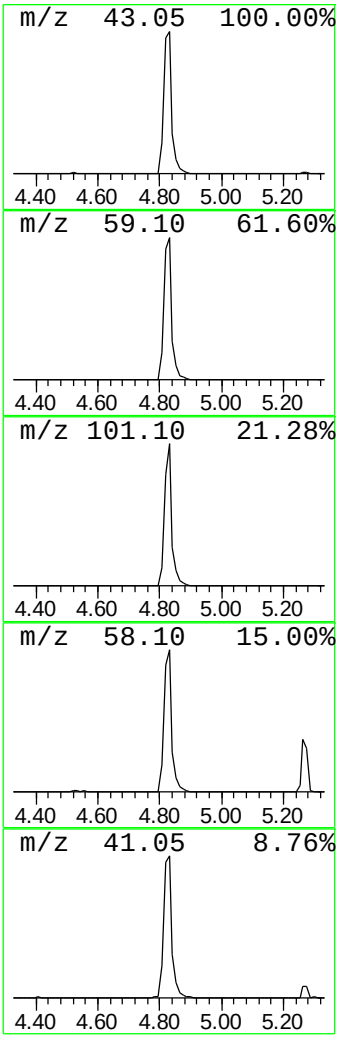
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.83 | 44.52 ng | 1831720 | 1,4-Dichlorobenzene-d4 | 6.67 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |



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Operator : SJ/IZ
Sample : H1320-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4-B017(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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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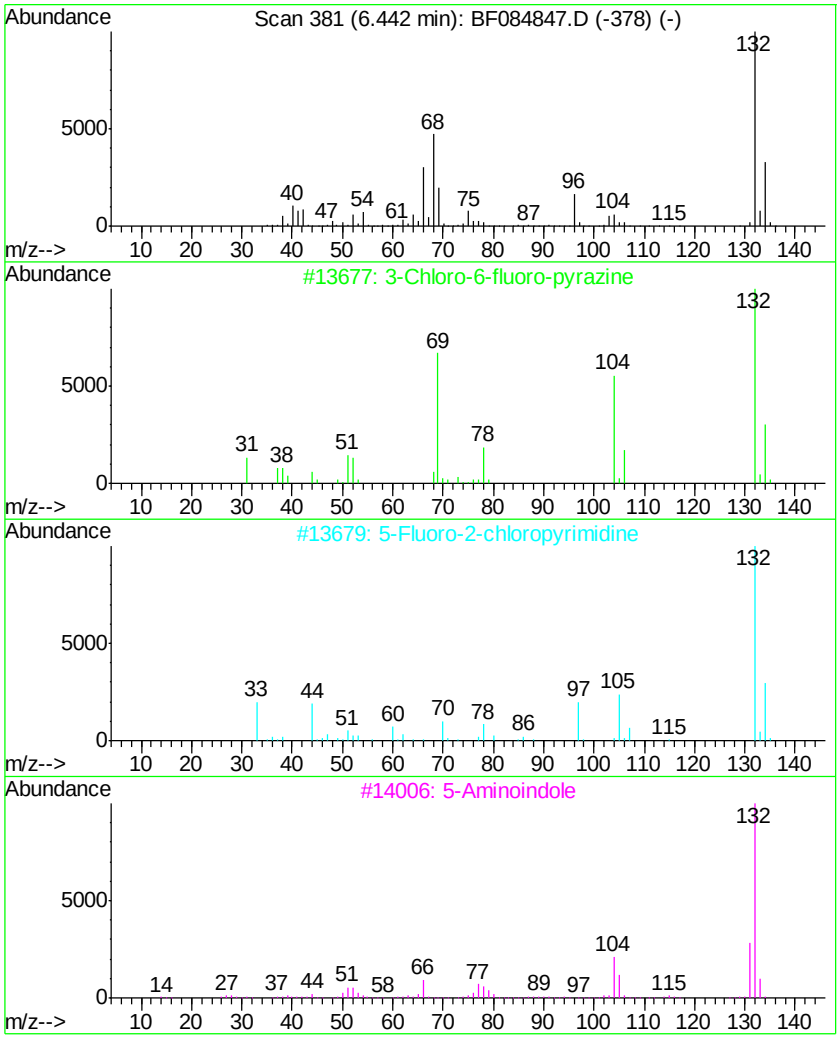
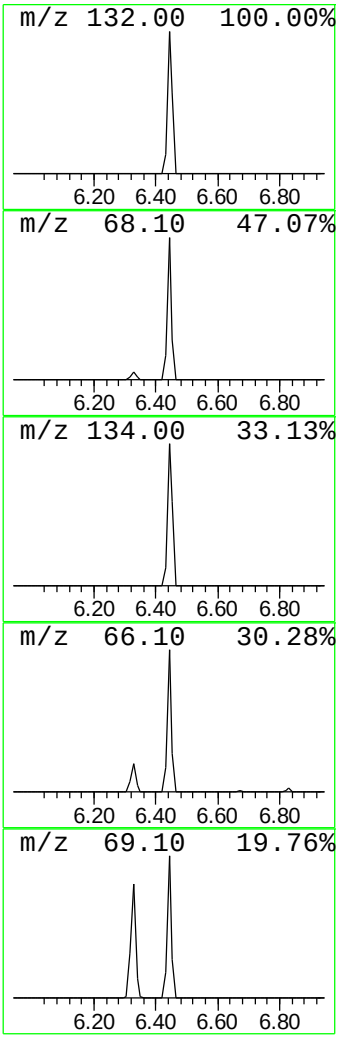
Peak Number 2 unknown6.44 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.44 | 106.03 ng | 4362610 | 1,4-Dichlorobenzene-d4 | 6.67 |

| 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 | 12 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 5 | (5-METHYL-2-PYRIDYL)ACETONITRILE | 132 | C8H8N2 | 1000241-93-9 | 10 |



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Data File : BF084847.D
Acq On : 4 Feb 2016 23:56
Operator : SJ/IZ
Sample : H1320-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4-B017(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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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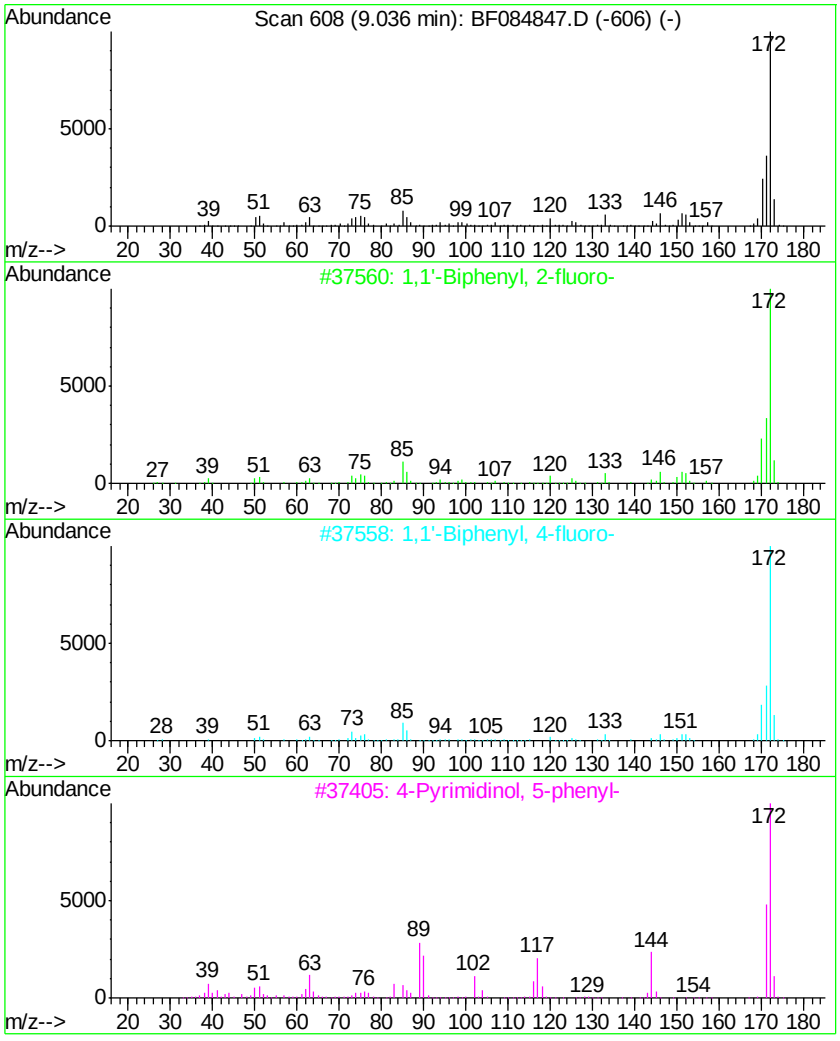
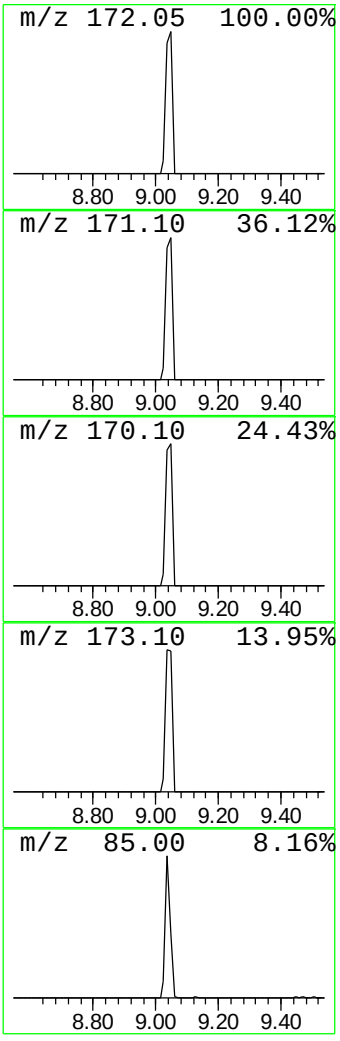
Peak Number 4 1,1'-Biphenyl, 2-fluoro- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.04 | 86.38 ng | 4767570 | Acenaphthene-d10 | 9.71 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,1'-Biphenyl, 2-fluoro- | 172 | C12H9F | 000321-60-8 | 96 |
| 2 | 1,1'-Biphenyl, 4-fluoro- | 172 | C12H9F | 000324-74-3 | 93 |
| 3 | 4-Pyrimidinol, 5-phenyl- | 172 | C10H8N2O | 022433-69-8 | 50 |
| 4 | 4-Amino-6-hydroxy-2-mercapto-5-n... | 172 | C4H4N4O2S | 001672-48-6 | 43 |
| 5 | 5-Hydroxy-2-phenylpyrimidine | 172 | C10H8N2O | 066739-85-3 | 43 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020416\
Data File : BF084847.D
Acq On : 4 Feb 2016 23:56
Operator : SJ/IZ
Sample : H1320-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4-B017(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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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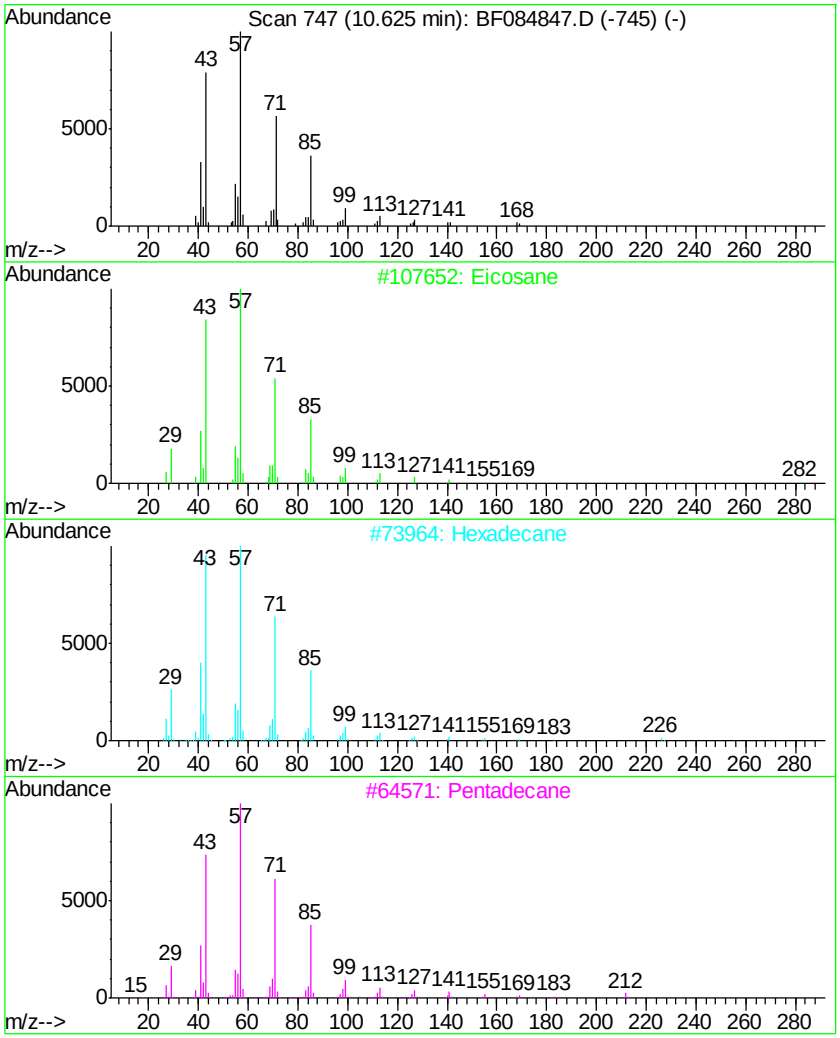
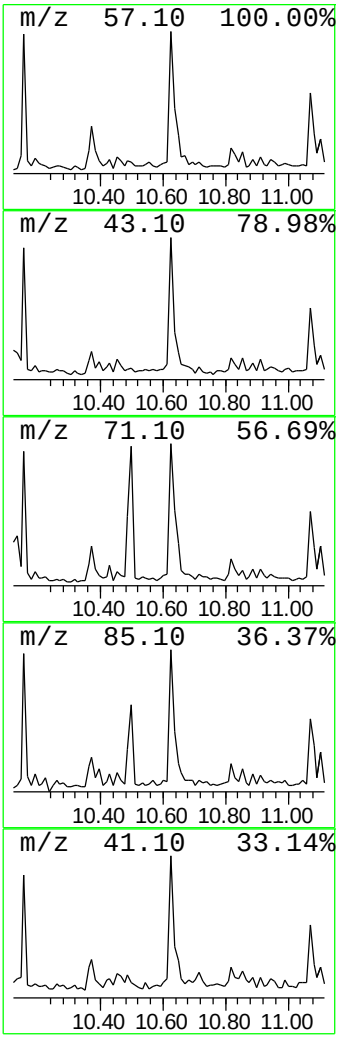
Peak Number 5 Eicosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.62 | 3.02 ng | 140652 | Phenanthrene-d10 | 11.19 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 91 |
| 2 | Hexadecane | 226 | C16H34 | 000544-76-3 | 91 |
| 3 | Pentadecane | 212 | C15H32 | 000629-62-9 | 90 |
| 4 | Tridecane | 184 | C13H28 | 000629-50-5 | 86 |
| 5 | Heptacosane | 380 | C27H56 | 000593-49-7 | 83 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020416\
Data File : BF084847.D
Acq On : 4 Feb 2016 23:56
Operator : SJ/IZ
Sample : H1320-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4-B017(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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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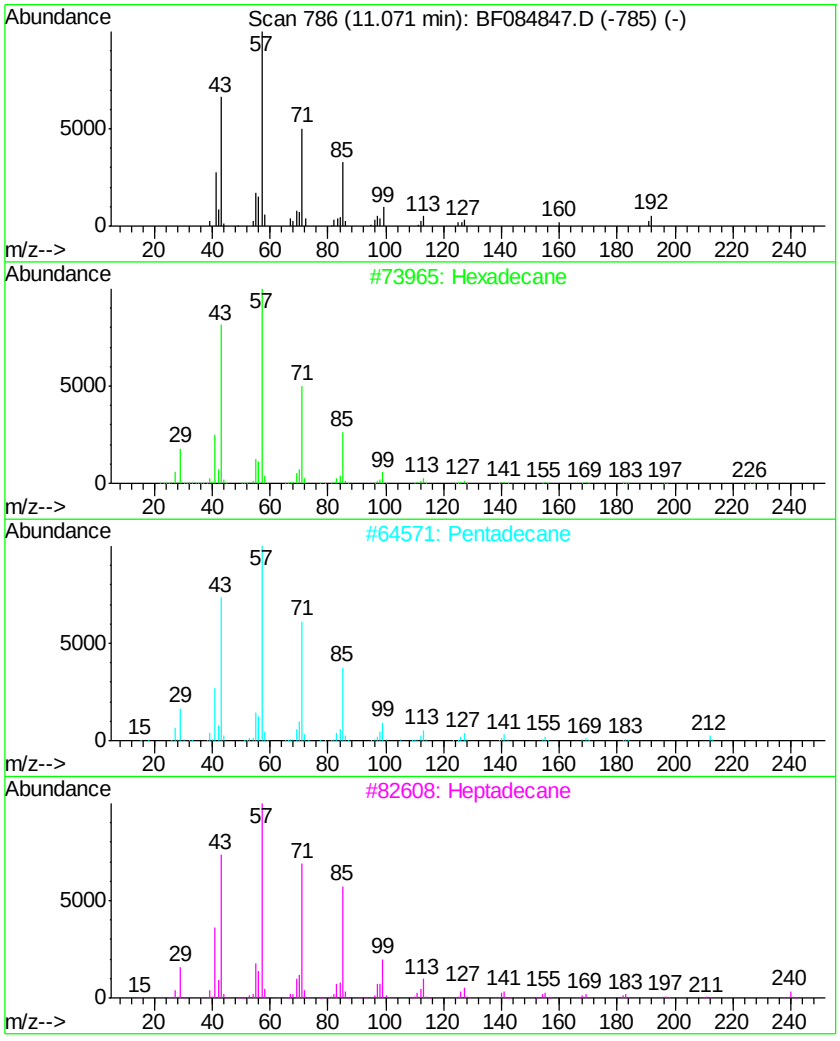
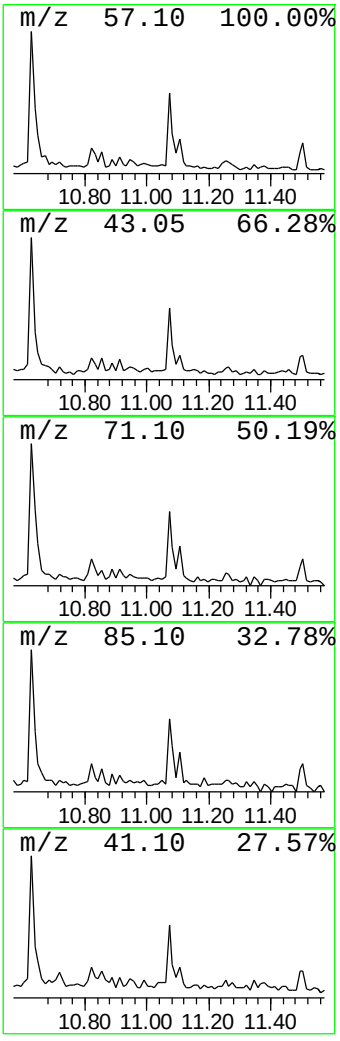
Peak Number 6 Hexadecane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.07 | 2.03 ng | 94635 | Phenanthrene-d10 | 11.19 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 86 |
| 2 | Pentadecane | 212 | C15H32 | 000629-62-9 | 86 |
| 3 | Heptadecane | 240 | C17H36 | 000629-78-7 | 80 |
| 4 | Eicosane | 282 | C20H42 | 000112-95-8 | 80 |
| 5 | Dodecane, 2-methyl-6-propyl- | 226 | C16H34 | 055045-08-4 | 80 |



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Sample : H1320-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4-B017(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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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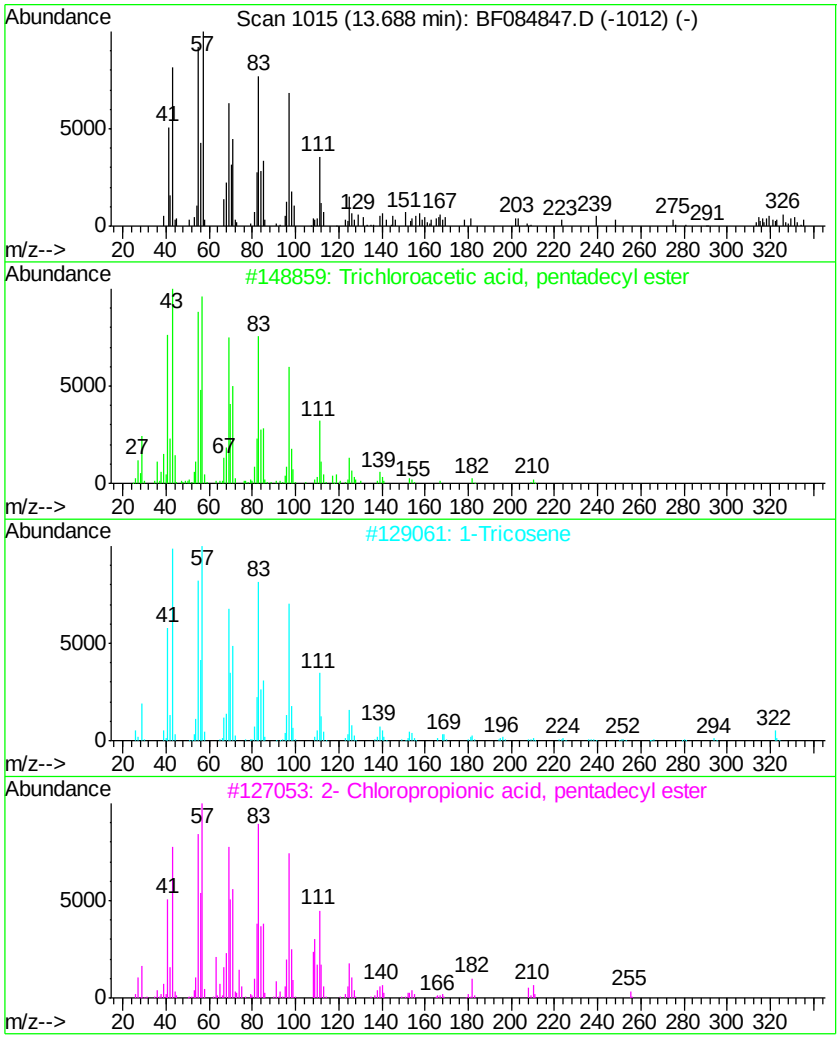
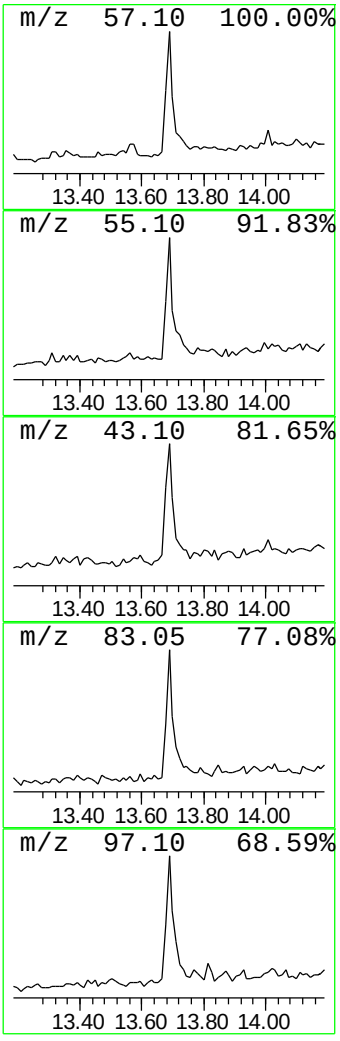
Peak Number 8 Trichloroacetic acid, penta... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.69 | 3.97 ng | 162932 | Chrysene-d12 | 13.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 91 |
| 2 | 1-Tricosene | 322 | C23H46 | 018835-32-0 | 91 |
| 3 | 2- Chloropropionic acid, pentade... | 318 | C18H35ClO2 | 1000292-44-1 | 91 |
| 4 | 9-Tricosene, (Z)- | 322 | C23H46 | 027519-02-4 | 91 |
| 5 | 11-Tricosene | 322 | C23H46 | 052078-56-5 | 91 |



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Operator : SJ/IZ
Sample : H1320-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4-B017(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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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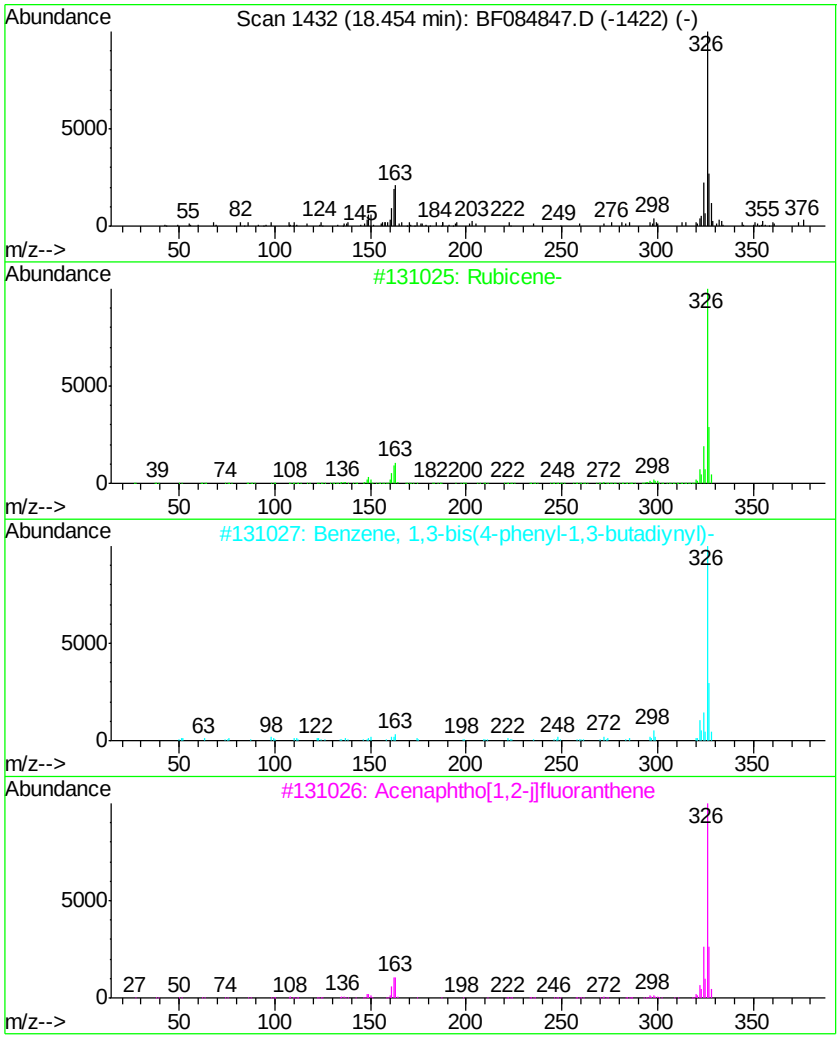
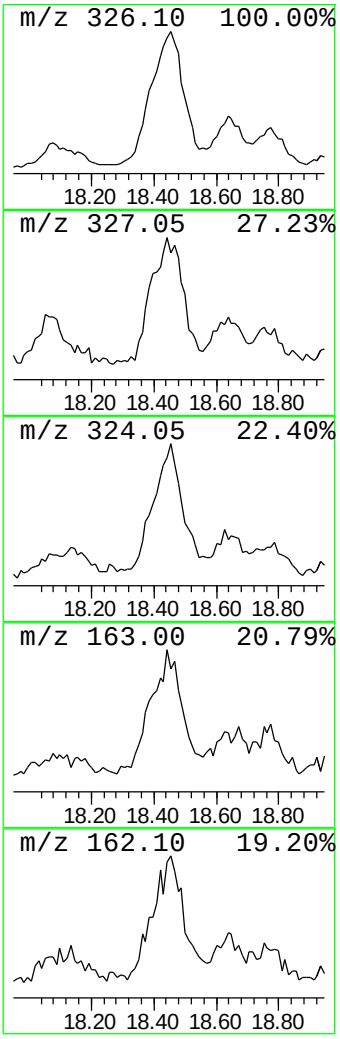
Peak Number 9 Rubicene- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.45 | 11.71 ng | 459012 | Perylene-d12 | 15.20 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Rubicene- | 326 | C26H14 | 000197-61-5 | 93 |
| 2 | Benzene, 1,3-bis(4-phenyl-1,3-bu... | 326 | C26H14 | 037902-13-9 | 90 |
| 3 | Acenaphtho[1,2-j]fluoranthene | 326 | C26H14 | 000193-21-5 | 70 |
| 4 | 2-(4-Biphenylyl)imidazo[2,1-b]be... | 326 | C21H14N2S | 038956-29-5 | 52 |
| 5 | Bis(pentamethylcyclopentadienyl)... | 326 | C20H30Fe | 012126-50-0 | 47 |



Tentatively Identified Compound (LSC) summary

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Misc :
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**Instrument :** BNA_F
**ClientSampleId :** S4-B017(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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 |
| 2-Pentanone, 4-hy... | 4.83 | 44.5 | ng | 1831720 | 1 | 6.67 | 822939 | 20.0 |
| unknown6.44 | 6.44 | 106.0 | ng | 4362610 | 1 | 6.67 | 822939 | 20.0 |
| 1,1'-Biphenyl, 2-... | 9.04 | 86.4 | ng | 4767570 | 3 | 9.71 | 1103850 | 20.0 |
| Eicosane | 10.62 | 3.0 | ng | 140652 | 4 | 11.19 | 931449 | 20.0 |
| Hexadecane | 11.07 | 2.0 | ng | 94635 | 4 | 11.19 | 931449 | 20.0 |
| Trichloroacetic a... | 13.69 | 4.0 | ng | 162932 | 5 | 13.81 | 820338 | 20.0 |
| Rubicene- | 18.45 | 11.7 | ng | 459012 | 6 | 15.20 | 784103 | 20.0 |