LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

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-BF122116.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 | 4.633 | 246 | 249 | 264 | rBV | 509437 | 764880 | 13.41% | 1.905% |
| 2 | 5.124 | 290 | 292 | 307 | rBV | 1969287 | 2764415 | 48.45% | 6.885% |
| 3 | 6.176 | 383 | 384 | 385 | rBV | 64379 | 75166 | 1.32% | 0.187% |
| 4 | 6.210 | 385 | 387 | 393 | rVV | 1072750 | 1662870 | 29.14% | 4.142% |
| 5 | 6.302 | 393 | 395 | 398 | rVB | 4725825 | 4628689 | 81.12% | 11.528% |
| 6 | 6.519 | 412 | 414 | 417 | rBV | 1044508 | 1074221 | 18.83% | 2.675% |
| 7 | 6.679 | 426 | 428 | 431 | rBV | 4301072 | 4201556 | 73.64% | 10.464% |
| 8 | 7.102 | 462 | 465 | 467 | rBV | 3235868 | 3301284 | 57.86% | 8.222% |
| 9 | 7.307 | 480 | 483 | 488 | rVB2 | 36785 | 76847 | 1.35% | 0.191% |
| 10 | 7.559 | 502 | 505 | 507 | rBV | 76632 | 82085 | 1.44% | 0.204% |
| 11 | 7.628 | 509 | 511 | 512 | rBV | 74759 | 85705 | 1.50% | 0.213% |
| 12 | 7.810 | 525 | 527 | 531 | rBV | 1609280 | 1467997 | 25.73% | 3.656% |
| 13 | 8.210 | 558 | 562 | 565 | rBV3 | 32100 | 58009 | 1.02% | 0.144% |
| 14 | 8.473 | 583 | 585 | 587 | rBV2 | 64322 | 70433 | 1.23% | 0.175% |
| 15 | 8.622 | 596 | 598 | 600 | rVB | 69641 | 66544 | 1.17% | 0.166% |
| 16 | 8.759 | 609 | 610 | 612 | rBV2 | 201093 | 240703 | 4.22% | 0.599% |
| 17 | 8.793 | 612 | 613 | 616 | rVV | 564166 | 557928 | 9.78% | 1.390% |
| 18 | 8.896 | 619 | 622 | 624 | rVV | 5854776 | 5705729 | 100.00% | 14.211% |
| 19 | 9.011 | 627 | 632 | 633 | rVV4 | 37748 | 84315 | 1.48% | 0.210% |
| 20 | 9.045 | 633 | 635 | 637 | rVB | 216432 | 201567 | 3.53% | 0.502% |
| 21 | 9.113 | 637 | 641 | 643 | rBV | 252823 | 368536 | 6.46% | 0.918% |
| 22 | 9.296 | 655 | 657 | 658 | rBV | 68669 | 59608 | 1.04% | 0.148% |
| 23 | 9.331 | 658 | 660 | 661 | rVV | 409325 | 436997 | 7.66% | 1.088% |
| 24 | 9.365 | 661 | 663 | 665 | rVV | 319395 | 291279 | 5.11% | 0.725% |
| 25 | 9.433 | 666 | 669 | 674 | rVB | 31105 | 57934 | 1.02% | 0.144% |
| 26 | 9.559 | 677 | 680 | 682 | rBV2 | 1026163 | 1136356 | 19.92% | 2.830% |
| 27 | 9.811 | 700 | 702 | 706 | rBV | 202327 | 225464 | 3.95% | 0.562% |
| 28 | 9.993 | 712 | 718 | 724 | rBV2 | 213569 | 452610 | 7.93% | 1.127% |
| 29 | 10.348 | 747 | 749 | 752 | rBV2 | 1505219 | 2008998 | 35.21% | 5.004% |
| 30 | 10.485 | 759 | 761 | 764 | rVB2 | 49441 | 74692 | 1.31% | 0.186% |
| 31 | 10.919 | 795 | 799 | 805 | rBV3 | 26659 | 75288 | 1.32% | 0.188% |
| 32 | 11.034 | 807 | 809 | 812 | rVB | 841188 | 768882 | 13.48% | 1.915% |
| 33 | 11.216 | 819 | 825 | 827 | rBV | 87921 | 273318 | 4.79% | 0.681% |
| 34 | 11.262 | 827 | 829 | 831 | rVB | 176608 | 258285 | 4.53% | 0.643% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 11.594 | 856 | 858 | 862 | rBV2 | 63381 | 86140 | 1.51% | 0.215% |
| 36 | 12.302 | 913 | 920 | 925 | rBV | 101174 | 465695 | 8.16% | 1.160% |
| 37 | 12.405 | 927 | 929 | 932 | rVB | 211773 | 234954 | 4.12% | 0.585% |
| 38 | 12.462 | 932 | 934 | 936 | rBV | 69423 | 61950 | 1.09% | 0.154% |
| 39 | 12.622 | 945 | 948 | 950 | rBV | 2941438 | 2931115 | 51.37% | 7.300% |
| 40 | 13.251 | 994 | 1003 | 1013 | rVB | 105353 | 653793 | 11.46% | 1.628% |
| 41 | 13.411 | 1015 | 1017 | 1020 | rVV | 94859 | 92206 | 1.62% | 0.230% |
| 42 | 13.537 | 1025 | 1028 | 1031 | rVB2 | 56831 | 69881 | 1.22% | 0.174% |
| 43 | 13.662 | 1037 | 1039 | 1042 | rBV | 594822 | 645687 | 11.32% | 1.608% |
| 44 | 14.085 | 1070 | 1076 | 1079 | rBV | 40204 | 165096 | 2.89% | 0.411% |
| 45 | 14.291 | 1090 | 1094 | 1097 | rBV2 | 96998 | 272772 | 4.78% | 0.679% |
| 46 | 15.023 | 1155 | 1158 | 1160 | rBV | 421258 | 661625 | 11.60% | 1.648% |
| 47 | 15.400 | 1189 | 1191 | 1194 | rBV | 48134 | 69668 | 1.22% | 0.174% |
| 48 | 15.811 | 1224 | 1227 | 1230 | rVB2 | 50602 | 81017 | 1.42% | 0.202% |

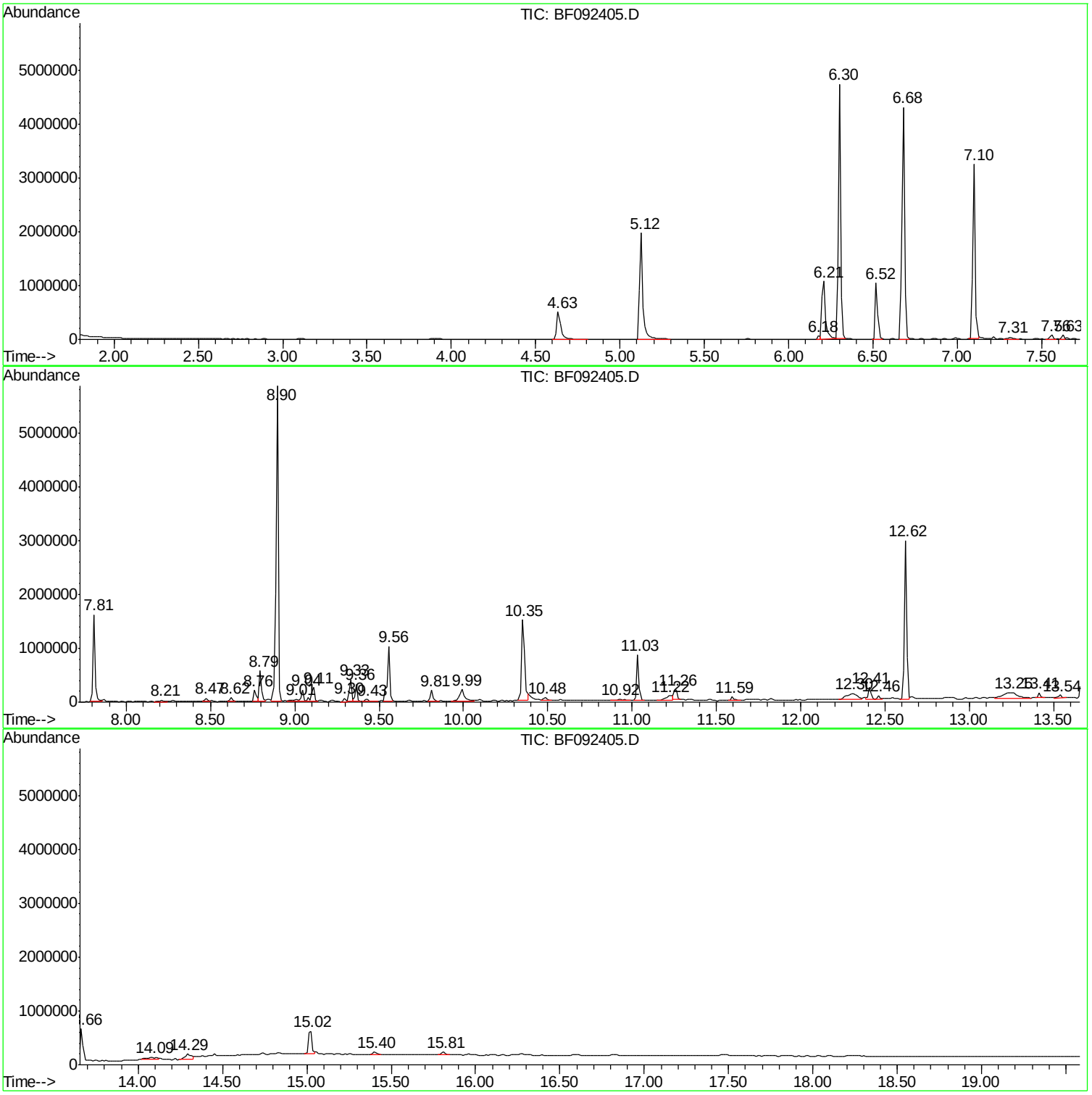
Sum of corrected areas: 40150789

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

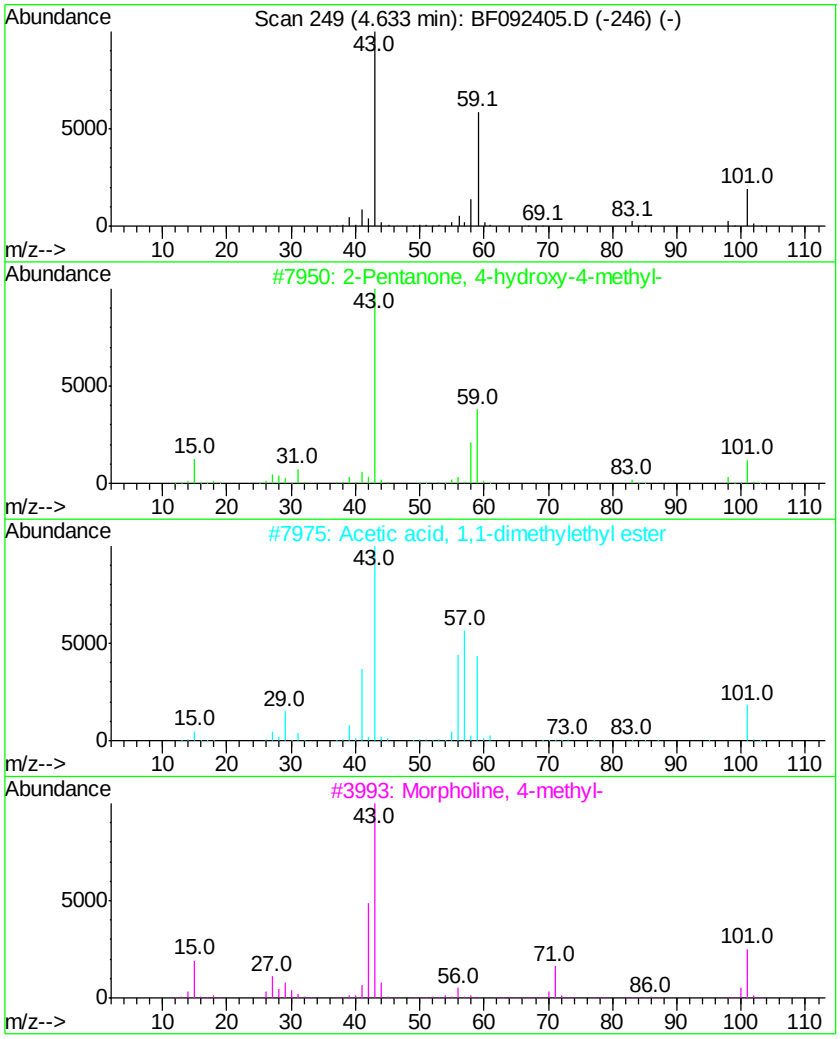
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

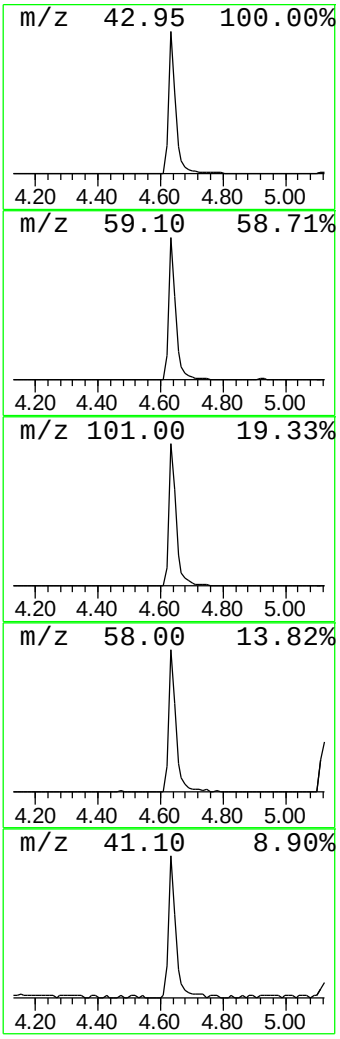
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.63 | 14.24 ng | 764880 | 1,4-Dichlorobenzene-d4 | 6.52 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 72 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 3 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | 4-Hydroxy-3-hexanone | 116 | C6H12O2 | 004984-85-4 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

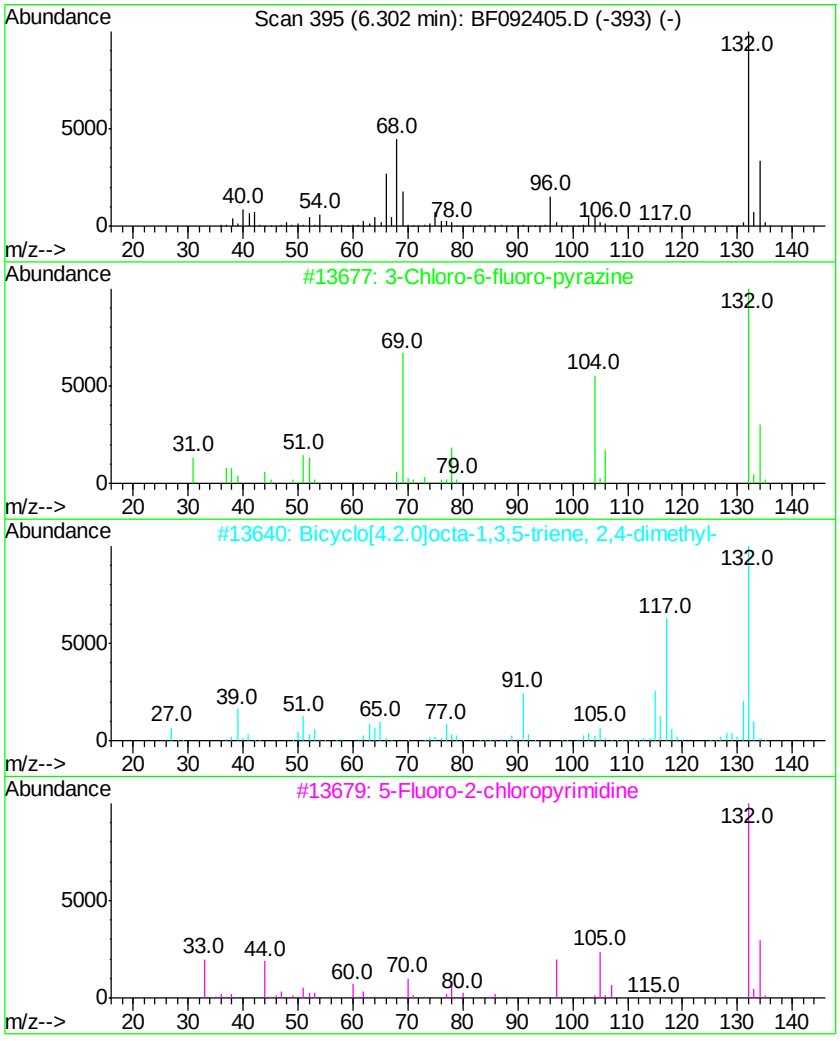
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

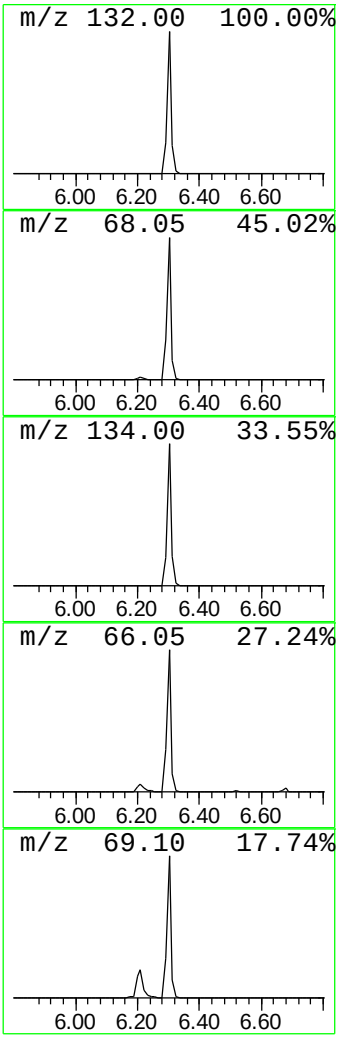
**********

Peak Number 2 unknown6.30 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.30 | 86.18 ng | 4628690 | 1,4-Dichlorobenzene-d4 | 6.52 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 3 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |
| 4 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |
| 5 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

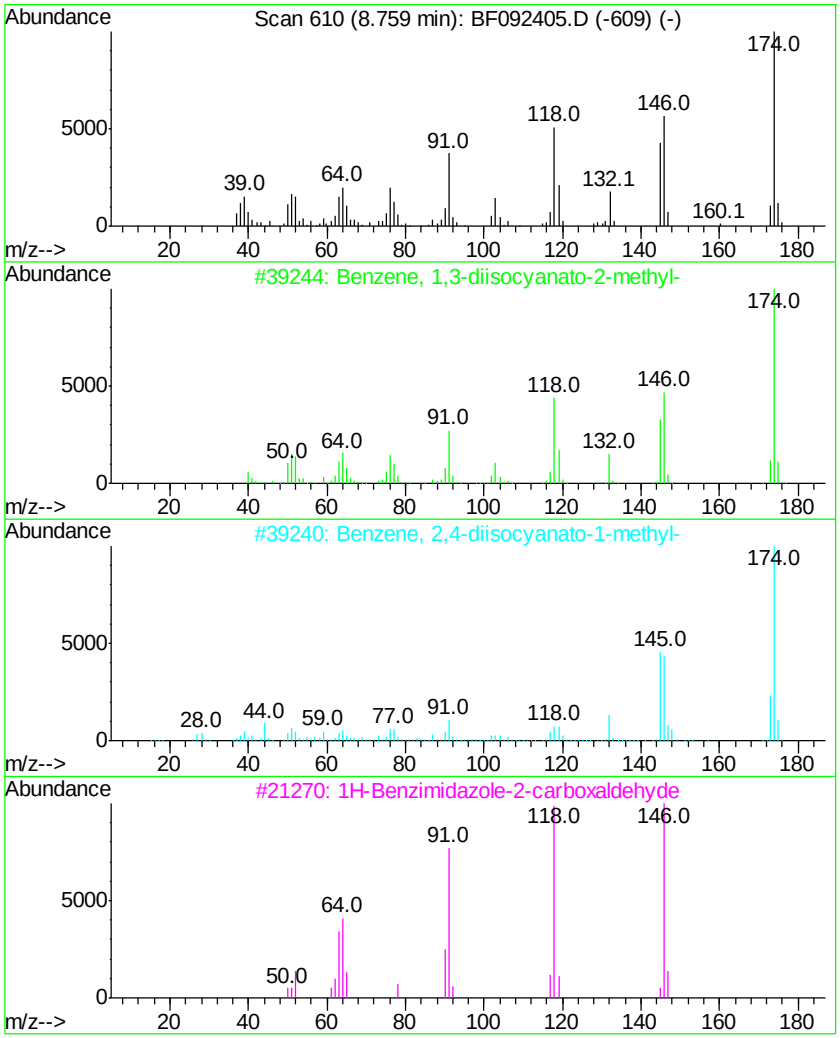
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

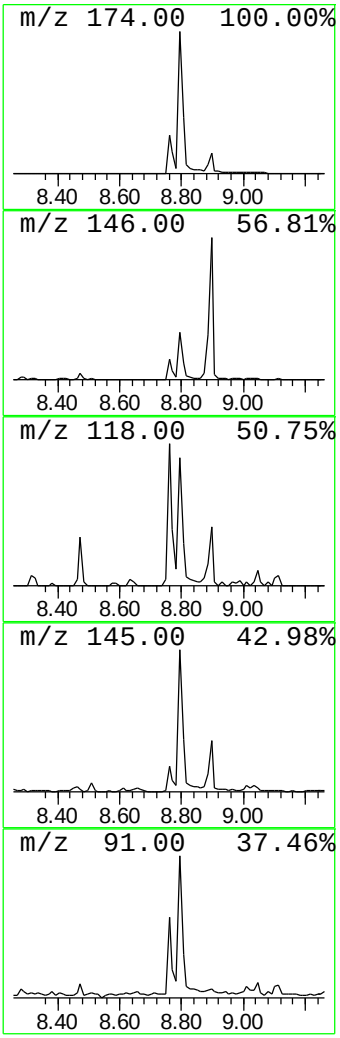
**********

Peak Number 4 Benzene, 1,3-diisocyanato-2... Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.76 | 4.24 ng | 240703 | Acenaphthene-d10 | 9.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, 1,3-diisocyanato-2-methyl- | 174 | C9H6N2O2 | 000091-08-7 | 97 |
| 2 | Benzene, 2,4-diisocyanato-1-methyl- | 174 | C9H6N2O2 | 000584-84-9 | 81 |
| 3 | 1H-Benzimidazole-2-carboxaldehyde | 146 | C8H6N2O | 003314-30-5 | 74 |
| 4 | 2H-Pyrido[1,2-a]pyrimidin-2-one,... | 174 | C10H10N2O | 022365-23-7 | 53 |
| 5 | 2H-1-Benzopyran-2-one, 4,6-dimet... | 174 | C11H10O2 | 014002-89-2 | 49 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

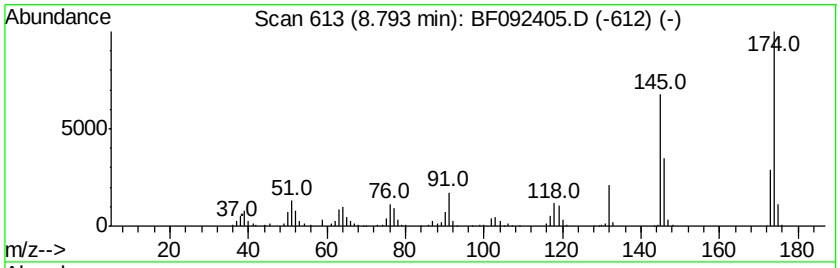
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

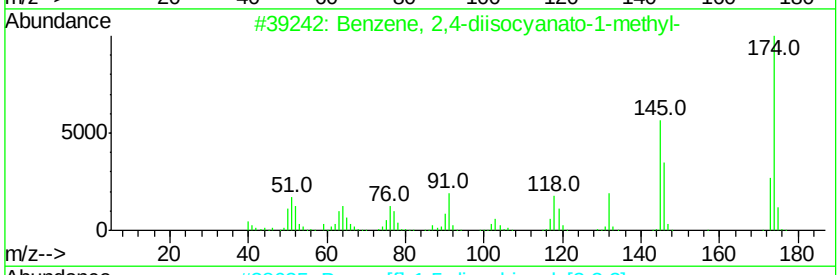
**********

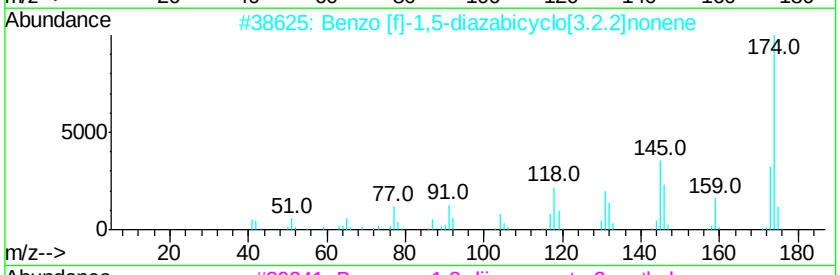
Peak Number 5 Benzene, 2,4-diisocyanato-1... Concentration Rank 6

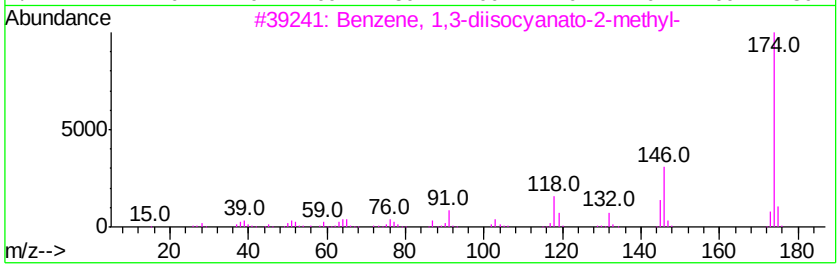
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.79 | 9.82 ng | 557928 | Acenaphthene-d10 | 9.56 |

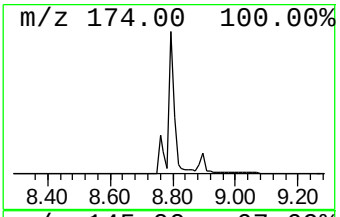
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, 2,4-diisocyanato-1-methyl- | 174 | C9H6N2O2 | 000584-84-9 | 93 |
| 2 | Benzo [f]-1,5-diazabicyclo[3.2.2... | 174 | C11H14N2 | 007092-76-4 | 59 |
| 3 | Benzene, 1,3-diisocyanato-2-methyl- | 174 | C9H6N2O2 | 000091-08-7 | 52 |
| 4 | 1,2-Dihydro-1,3-dimethyl-2-oxoqu... | 174 | C10H10N2O | 003149-25-5 | 49 |
| 5 | 2-Fluoro-5-phenylpyrimidine | 174 | C10H7FN2 | 062850-13-9 | 43 |

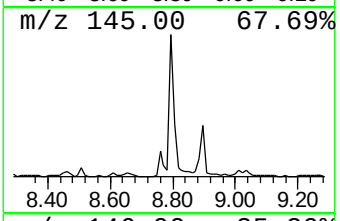


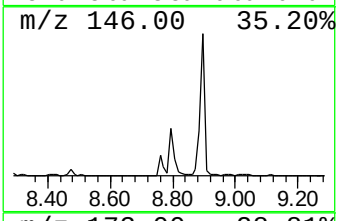



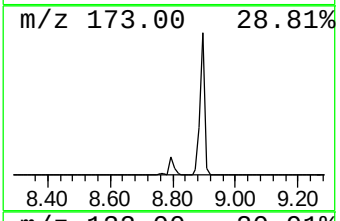



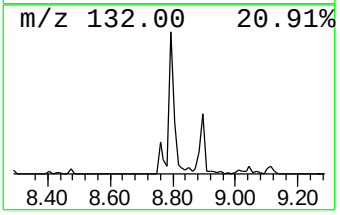



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Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

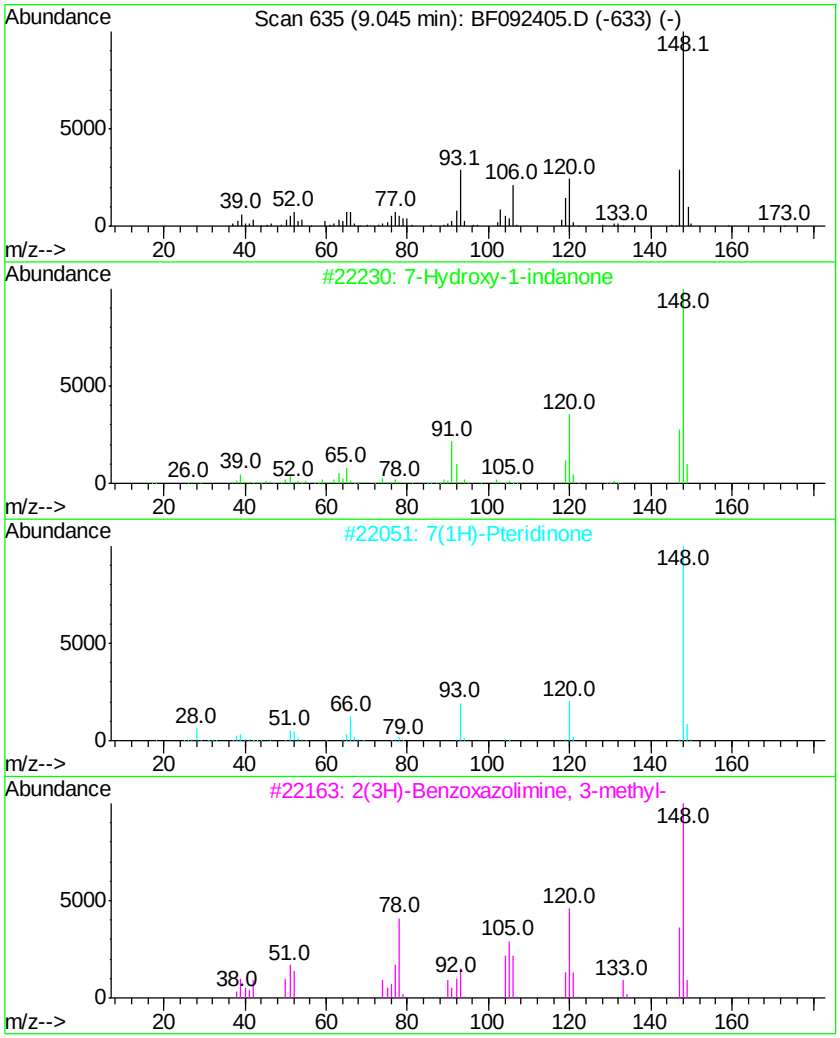
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

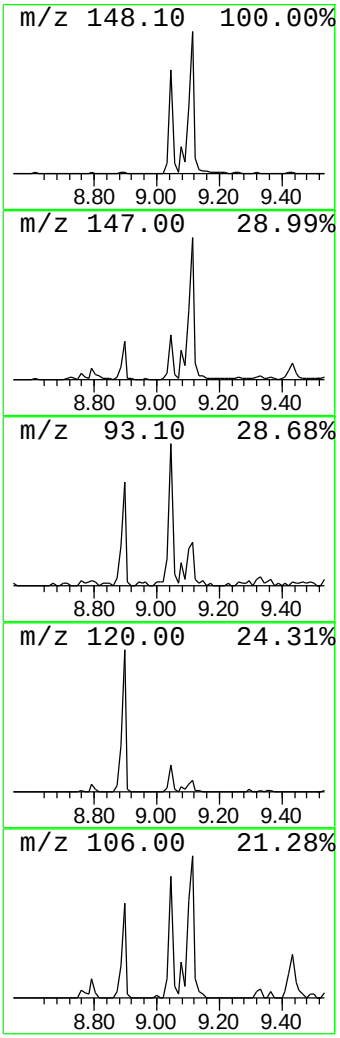
**********

Peak Number 6 7-Hydroxy-1-indanone Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.04 | 3.55 ng | 201567 | Acenaphthene-d10 | 9.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 7-Hydroxy-1-indanone | 148 | C9H8O2 | 006968-35-0 | 76 |
| 2 | 7(1H)-Pteridinone | 148 | C6H4N4O | 002432-27-1 | 64 |
| 3 | 2(3H)-Benzoxazolimine, 3-methyl- | 148 | C8H8N2O | 018034-93-0 | 64 |
| 4 | 2-Hydroxymethylbenzimidazole | 148 | C8H8N2O | 022128-99-0 | 59 |
| 5 | 2H-Benzimidazol-2-one, 1,3-dihyd... | 148 | C8H8N2O | 001849-01-0 | 50 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

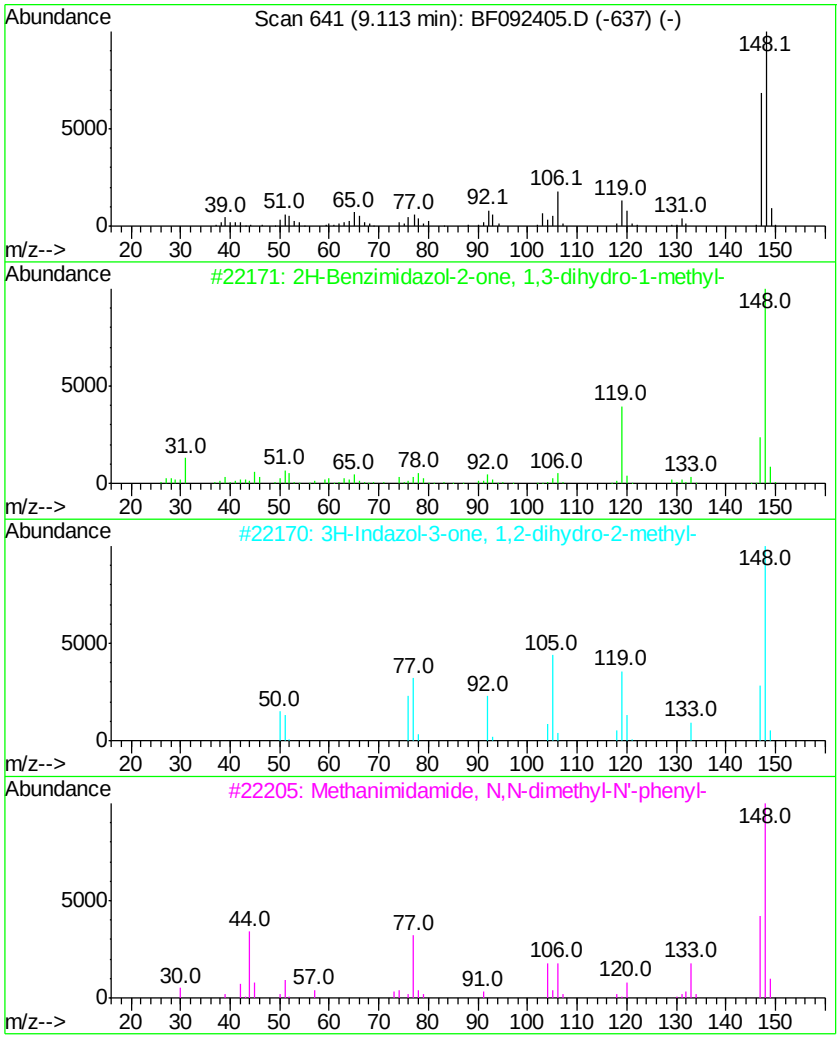
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

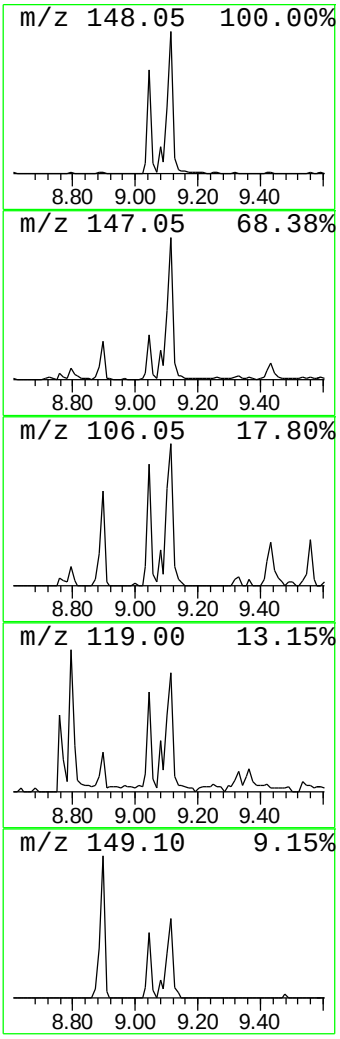
**********

Peak Number 7 2H-Benzimidazol-2-one, 1,3-... Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.11 | 6.49 ng | 368536 | Acenaphthene-d10 | 9.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2H-Benzimidazol-2-one, 1,3-dihyd... | 148 | C8H8N2O | 001849-01-0 | 59 |
| 2 | 3H-Indazol-3-one, 1,2-dihydro-2-... | 148 | C8H8N2O | 001848-40-4 | 59 |
| 3 | Methanimidamide, N,N-dimethyl-N'... | 148 | C9H12N2 | 001783-25-1 | 53 |
| 4 | Indole-2-one, 2,3-dihydro-6-amino- | 148 | C8H8N2O | 150544-04-0 | 50 |
| 5 | 1H-Benzotriazole, 6-amino-1-methyl- | 148 | C7H8N4 | 026861-23-4 | 47 |



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Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

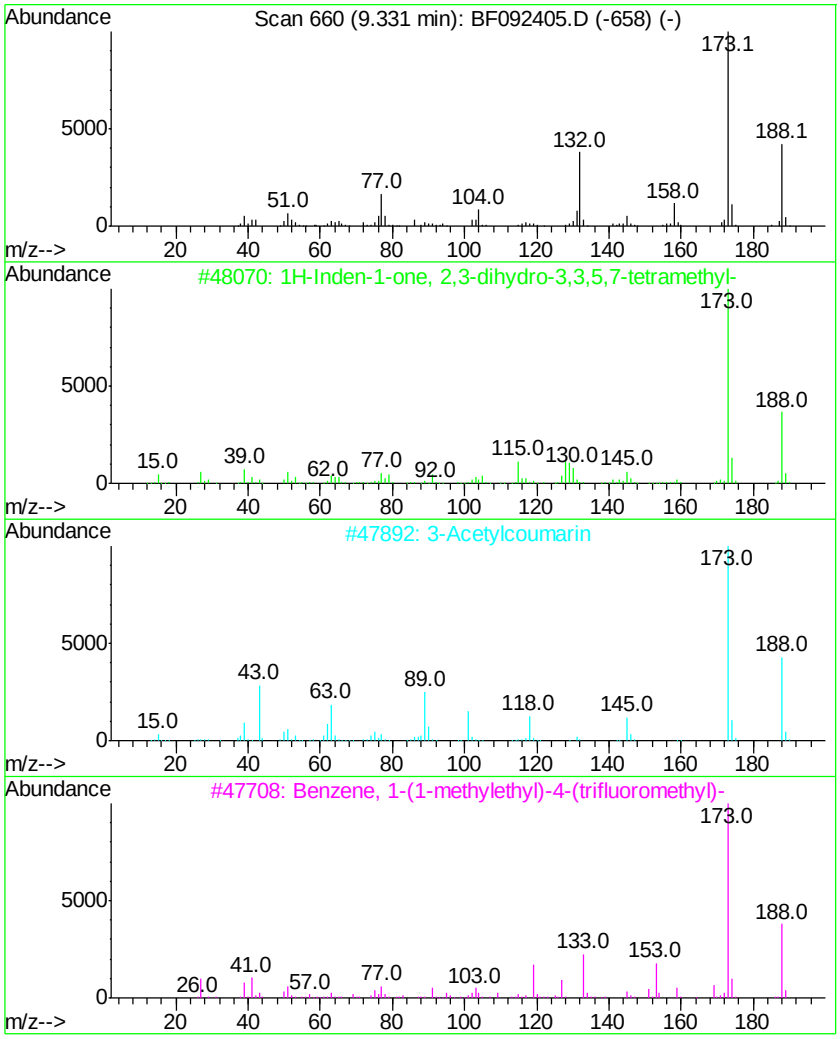
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

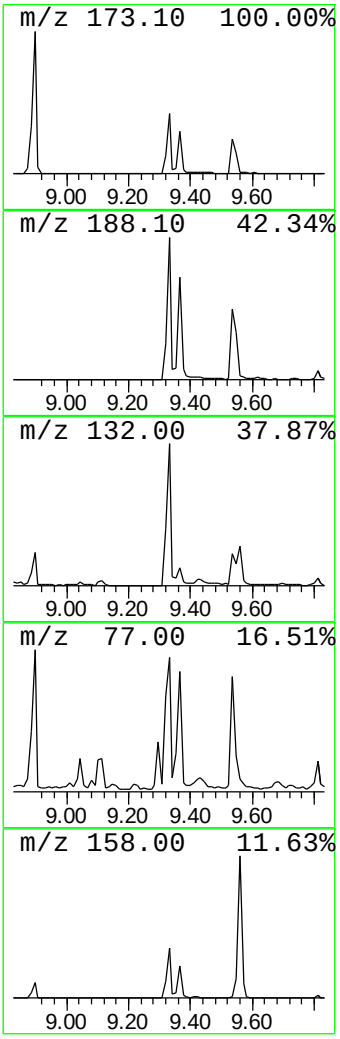
**********

Peak Number 8 1H-Inden-1-one, 2,3-dihydro... Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.33 | 7.69 ng | 436997 | Acenaphthene-d10 | 9.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1H-Inden-1-one, 2,3-dihydro-3,3,... | 188 | C13H16O | 054789-23-0 | 72 |
| 2 | 3-Acetylcoumarin | 188 | C11H8O3 | 003949-36-8 | 64 |
| 3 | Benzene, 1-(1-methylethyl)-4-(tr... | 188 | C10H11F3 | 032445-99-1 | 59 |
| 4 | 1,3-Indandione, 2-acetyl- | 188 | C11H8O3 | 001133-72-8 | 59 |
| 5 | 1H-Inden-1-one, 2,3-dihydro-3,3,... | 188 | C13H16O | 054789-22-9 | 53 |



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Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

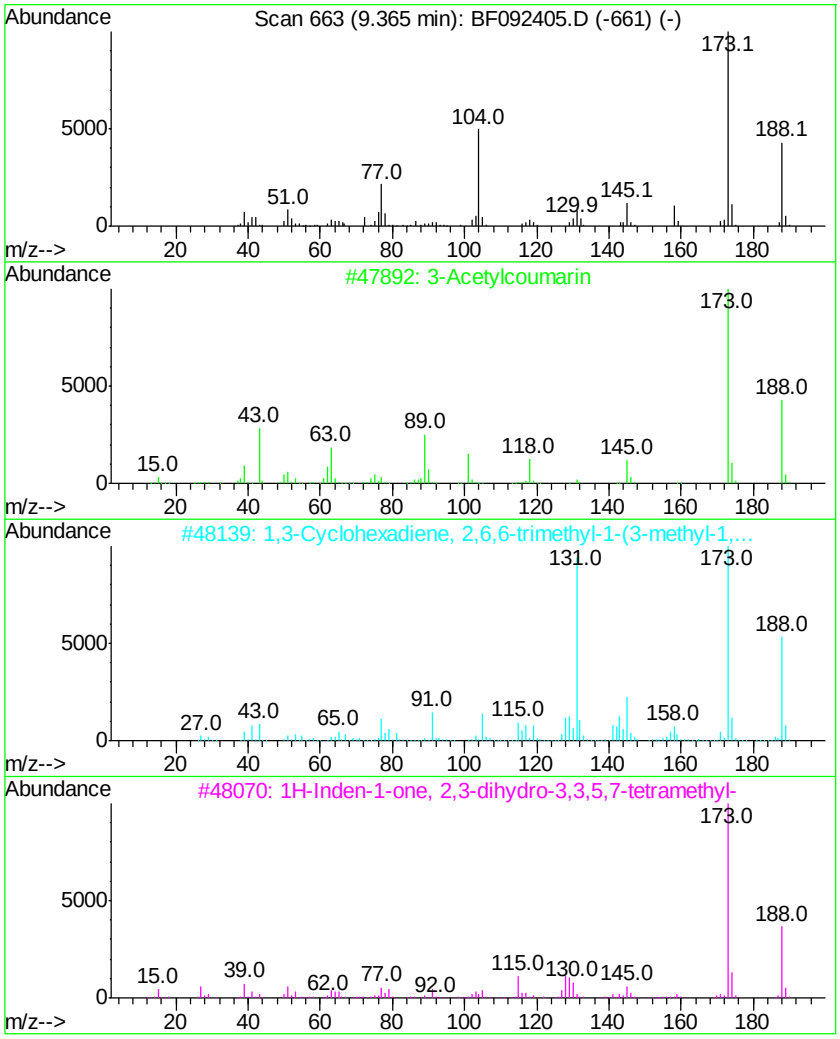
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

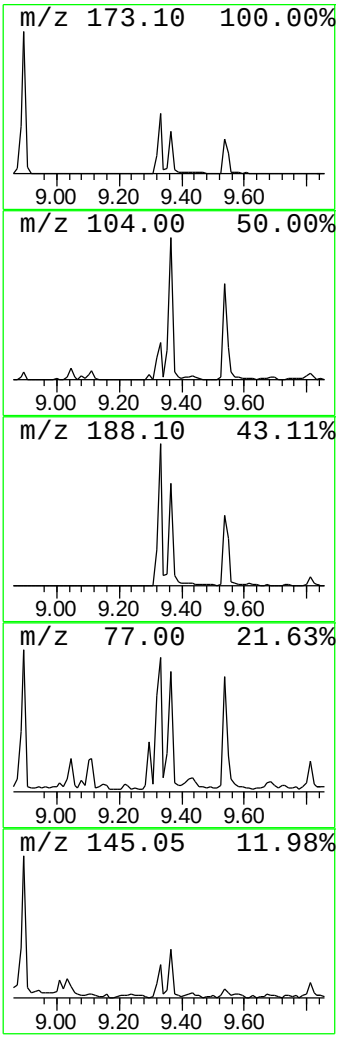
**********

Peak Number 9 3-Acetylcoumarin Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.36 | 5.13 ng | 291279 | Acenaphthene-d10 | 9.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Acetylcoumarin | 188 | C11H8O3 | 003949-36-8 | 58 |
| 2 | 1,3-Cyclohexadiene, 2,6,6-trimet... | 188 | C14H20 | 052260-01-2 | 53 |
| 3 | 1H-Inden-1-one, 2,3-dihydro-3,3,... | 188 | C13H16O | 054789-23-0 | 52 |
| 4 | 1H-Inden-1-one, 2,3-dihydro-3,3,... | 188 | C13H16O | 055255-42-0 | 50 |
| 5 | Benzene, 1-(1-methylethyl)-4-(tr... | 188 | C10H11F3 | 032445-99-1 | 49 |



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Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

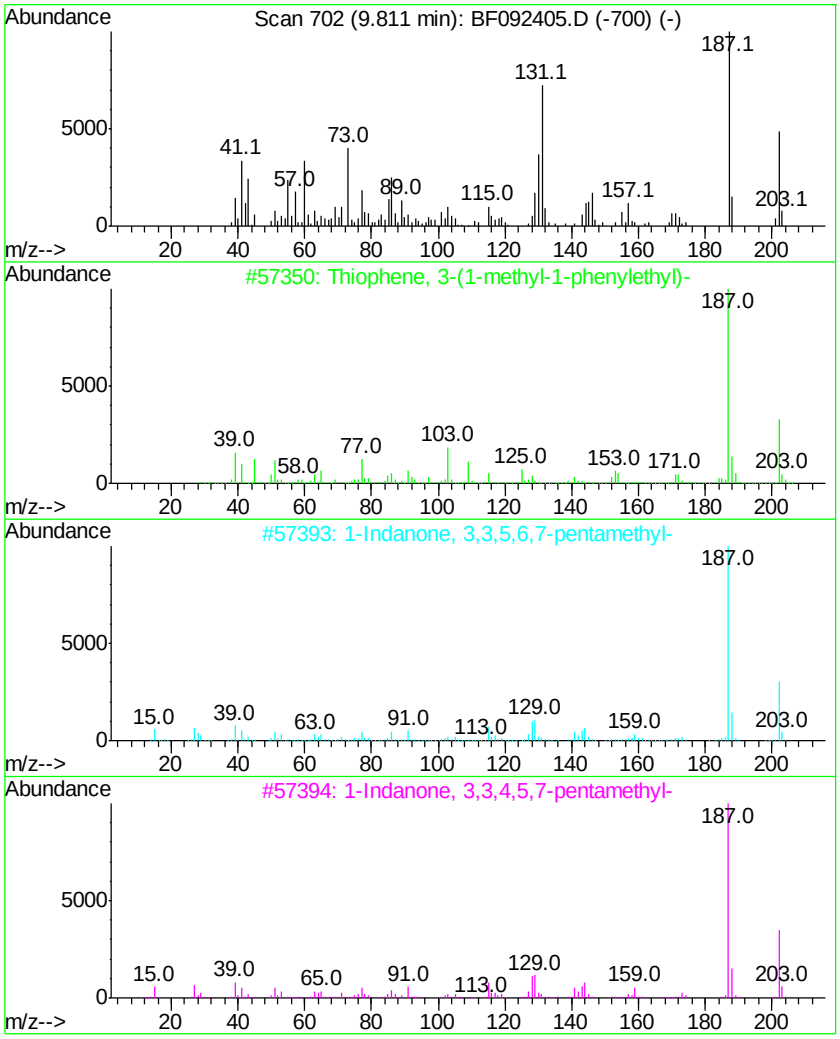
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

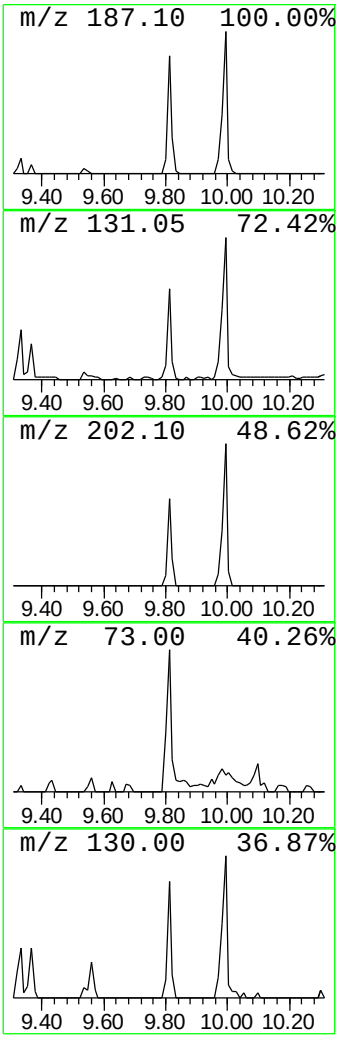
**********

Peak Number 10 Thiophene, 3-(1-methyl-1-ph... Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.81 | 3.97 ng | 225464 | Acenaphthene-d10 | 9.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Thiophene, 3-(1-methyl-1-phenyle... | 202 | C13H14S | 054889-45-1 | 55 |
| 2 | 1-Indanone, 3,3,5,6,7-pentamethyl- | 202 | C14H18O | 016204-69-6 | 49 |
| 3 | 1-Indanone, 3,3,4,5,7-pentamethyl- | 202 | C14H18O | 010425-83-9 | 49 |
| 4 | Quinoxaline, 2-tert-butyl-, 4-oxide | 202 | C12H14N2O | 016007-51-5 | 49 |
| 5 | Silane, trimethyl(3-phenyl-1-but... | 202 | C13H18Si | 028129-04-6 | 49 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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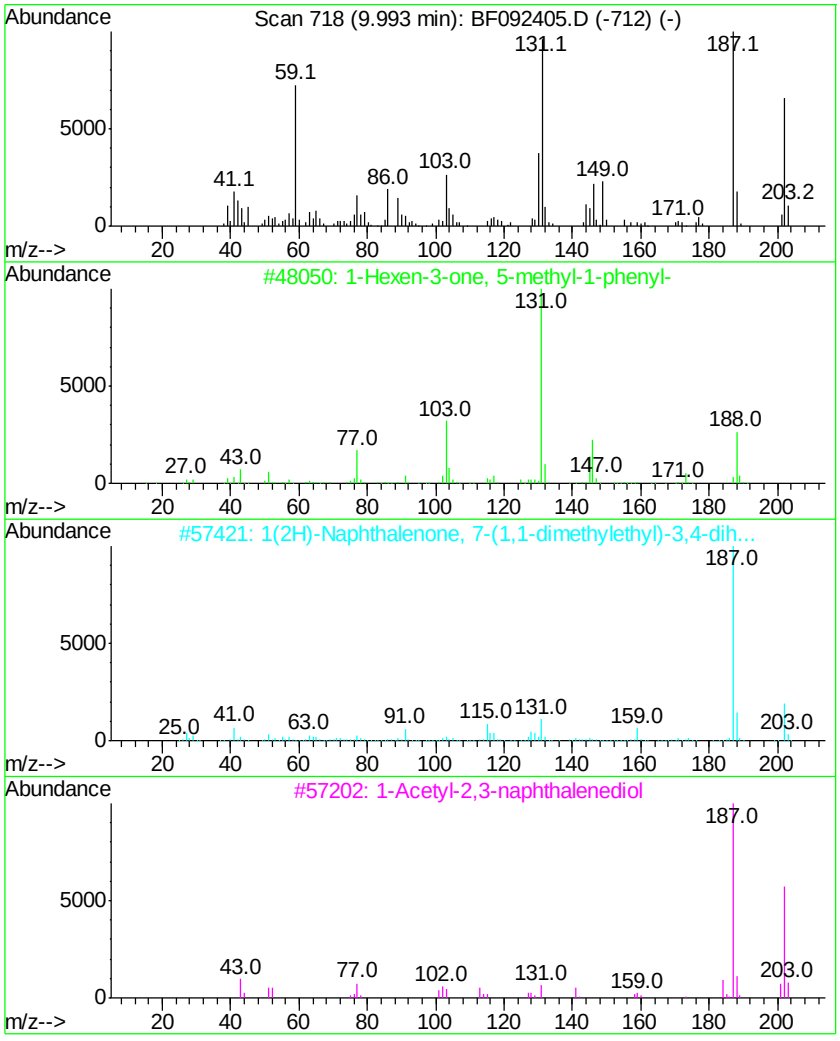
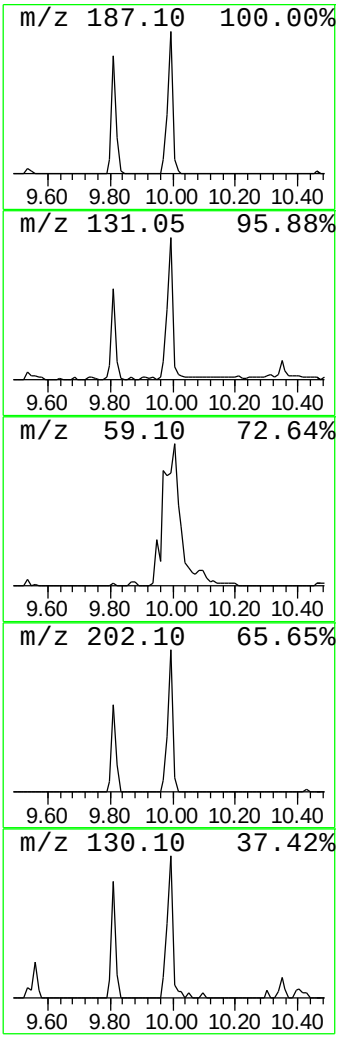
Peak Number 11 1-Hexen-3-one, 5-methyl-1-p... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.99 | 7.97 ng | 452610 | Acenaphthene-d10 | 9.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Hexen-3-one, 5-methyl-1-phenyl- | 188 | C13H16O | 002892-18-4 | 51 |
| 2 | 1(2H)-Naphthalenone, 7-(1,1-dime... | 202 | C14H18O | 022583-68-2 | 32 |
| 3 | 1-Acetyl-2,3-naphthalenediol | 202 | C12H10O3 | 091368-52-4 | 30 |
| 4 | Benzimidazole, 5-tert-butyl-2-et... | 202 | C13H18N2 | 005805-63-0 | 30 |
| 5 | 1-Acetyl-2,7-naphthalenediol | 202 | C12H10O3 | 086358-83-0 | 27 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
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Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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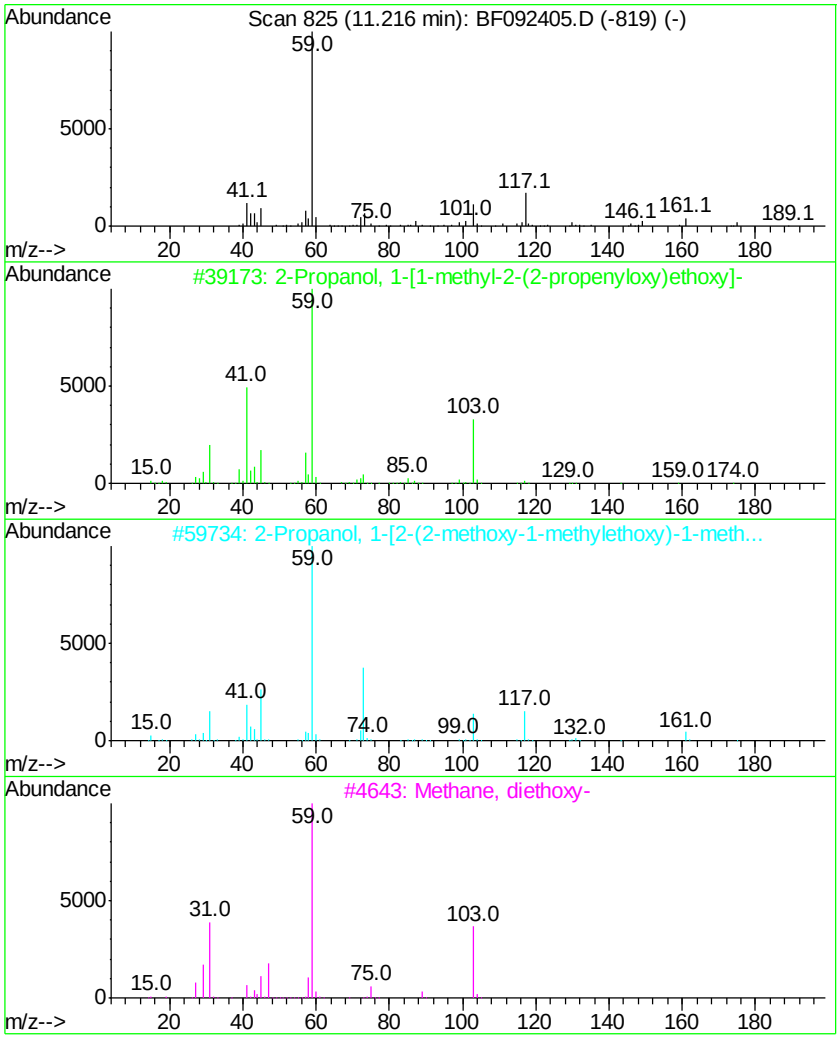
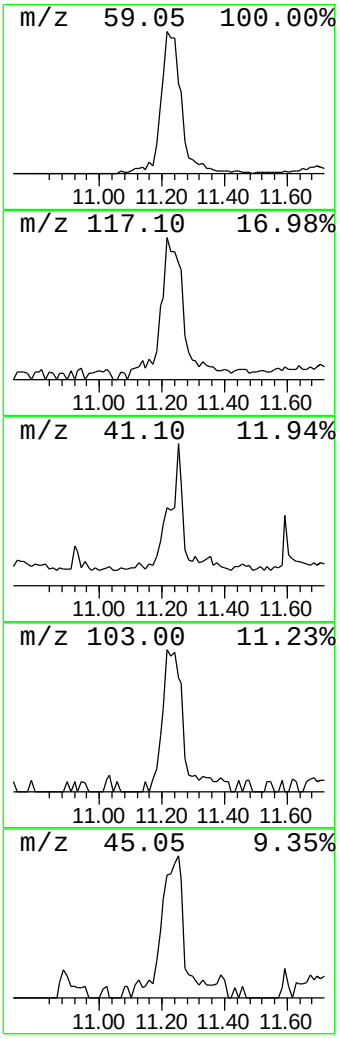
Peak Number 12 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.22 | 7.11 ng | 273318 | Phenanthrene-d10 | 11.03 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Propanol, 1-[1-methyl-2-(2-pro... | 174 | C9H18O3 | 055956-25-7 | 72 |
| 2 | 2-Propanol, 1-[2-(2-methoxy-1-me... | 206 | C10H22O4 | 020324-33-8 | 56 |
| 3 | Methane, diethoxy- | 104 | C5H12O2 | 000462-95-3 | 53 |
| 4 | 1-Propanol, 2-(2-hydroxypropoxy)- | 134 | C6H14O3 | 000106-62-7 | 53 |
| 5 | Dipropylene glycol | 134 | C6H14O3 | 025265-71-8 | 53 |



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Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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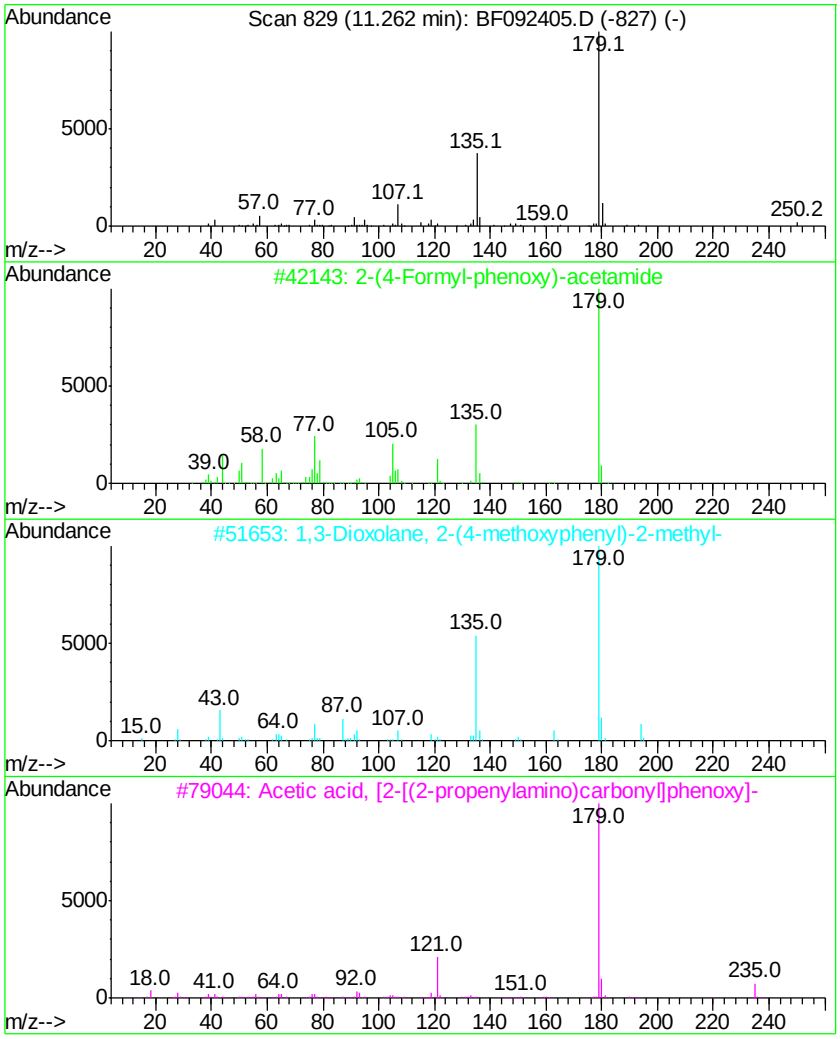
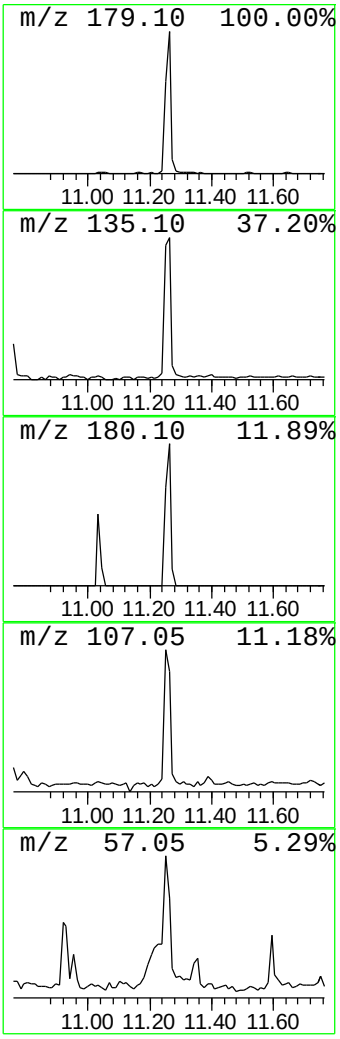
Peak Number 13 2-(4-Formyl-phenoxy)-acetamide Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.26 | 6.72 ng | 258285 | Phenanthrene-d10 | 11.03 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-(4-Formyl-phenoxy)-acetamide | 179 | C9H9NO3 | 135857-20-4 | 72 |
| 2 | 1,3-Dioxolane, 2-(4-methoxyphenyl... | 194 | C11H14O3 | 036881-00-2 | 72 |
| 3 | Acetic acid, [2-[(2-propenylamin... | 235 | C12H13NO4 | 000119-45-9 | 40 |
| 4 | 4,2-Cresotic acid, 6-methoxy-, b... | 538 | C29H30O10 | 019314-74-0 | 38 |
| 5 | Ethanol, 2-[4-(1,1-dimethylethyl... | 194 | C12H18O2 | 000713-46-2 | 38 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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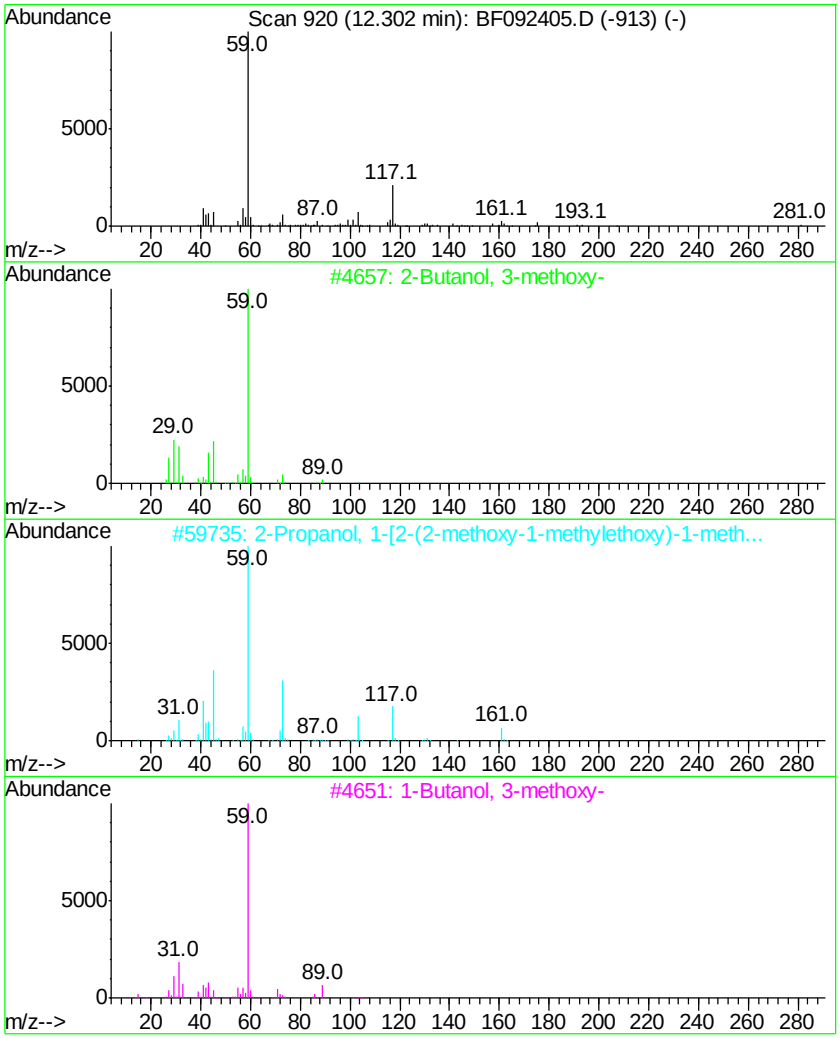
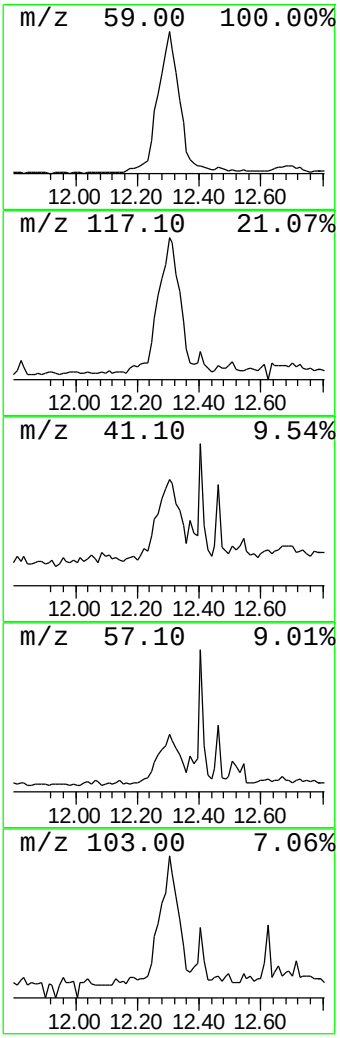
Peak Number 14 2-Butanol, 3-methoxy- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.30 | 12.11 ng | 465695 | Phenanthrene-d10 | 11.03 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Butanol, 3-methoxy- | 104 | C5H12O2 | 053778-72-6 | 53 |
| 2 | 2-Propanol, 1-[2-(2-methoxy-1-me... | 206 | C10H22O4 | 020324-33-8 | 50 |
| 3 | 1-Butanol, 3-methoxy- | 104 | C5H12O2 | 002517-43-3 | 40 |
| 4 | 2,5,8,11-Tetraoxatetradecan-13-o... | 264 | C13H28O5 | 020324-34-9 | 39 |
| 5 | 2-Propanol, 1-[1-methyl-2-(2-pro... | 174 | C9H18O3 | 055956-25-7 | 39 |



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Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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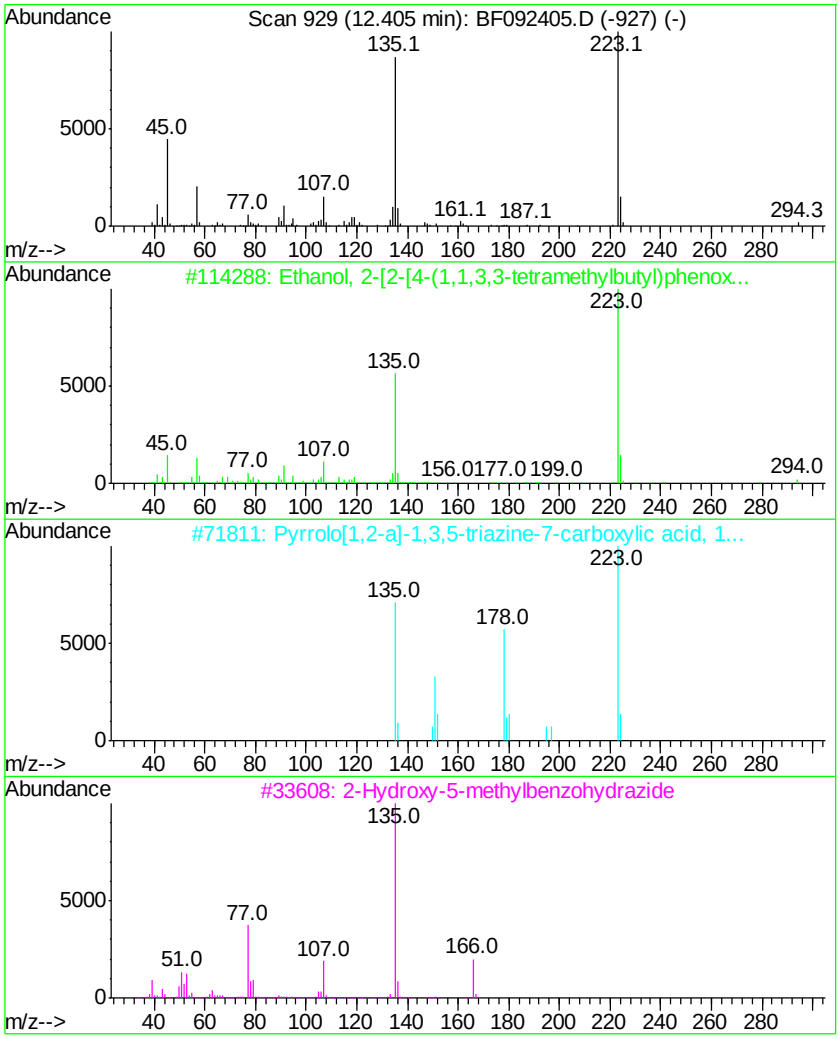
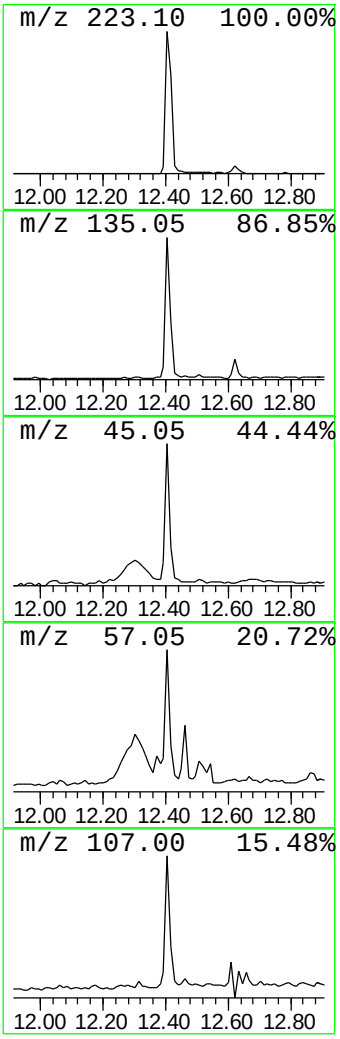
Peak Number 15 Ethanol, 2-[2-[4-(1,1,3,3-t... Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.41 | 7.28 ng | 234954 | Chrysene-d12 | 13.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-[2-[4-(1,1,3,3-tetram... | 294 | C18H30O3 | 002315-61-9 | 91 |
| 2 | Pyrrolo[1,2-a]-1,3,5-triazine-7-... | 223 | C9H9N3O4 | 054449-89-7 | 90 |
| 3 | 2-Hydroxy-5-methylbenzohydrazide | 166 | C8H10N2O2 | 028397-43-5 | 27 |
| 4 | 5-(4-Trifluormethylsulfonylphenyl... | 372 | C17H19F3N2O2S | 187338-96-1 | 27 |
| 5 | 4-Cyanobenzoic acid, 2-(1-adaman... | 309 | C20H23NO2 | 1000292-45-1 | 27 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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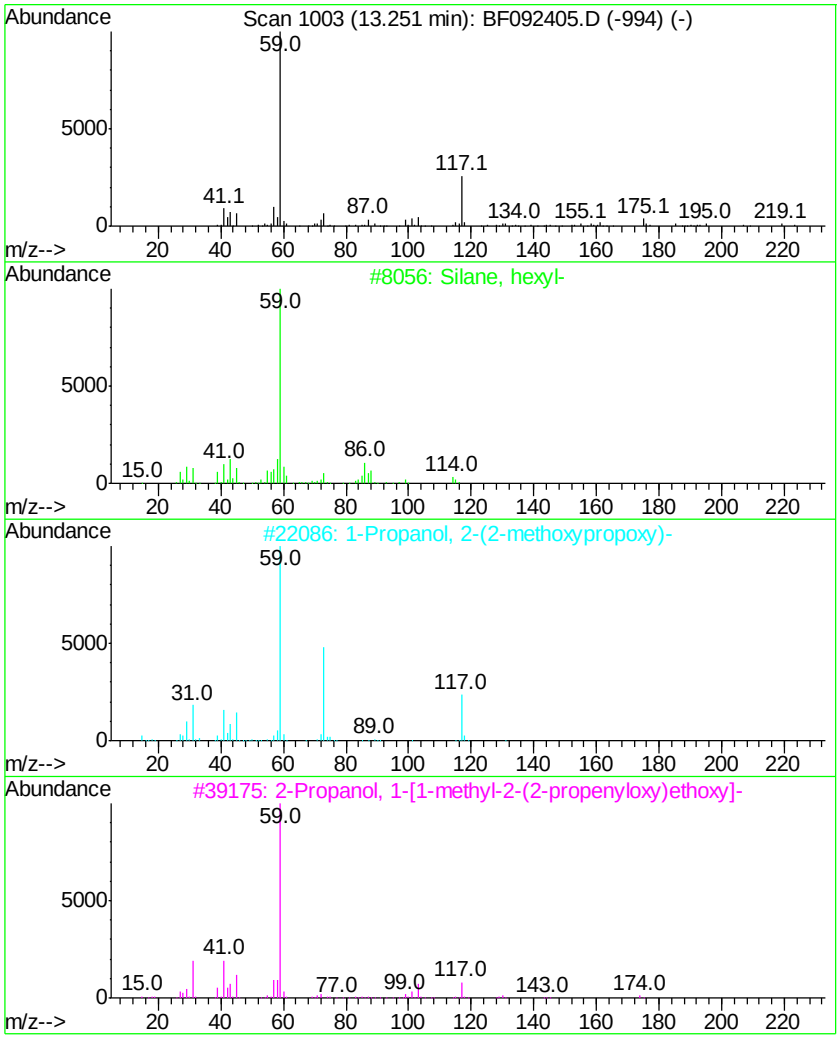
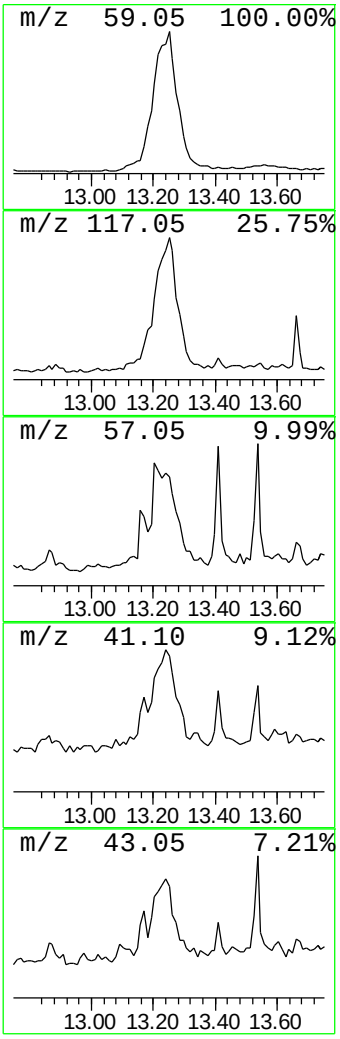
Peak Number 16 Silane, hexyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.25 | 20.25 ng | 653793 | Chrysene-d12 | 13.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Silane, hexyl- | 116 | C6H16Si | 001072-14-6 | 53 |
| 2 | 1-Propanol, 2-(2-methoxypropoxy)- | 148 | C7H16O3 | 013588-28-8 | 45 |
| 3 | 2-Propanol, 1-[1-methyl-2-(2-pro... | 174 | C9H18O3 | 055956-25-7 | 42 |
| 4 | Propane, 1-ethoxy-2-methyl- | 102 | C6H14O | 000627-02-1 | 40 |
| 5 | 3-Pentanol, 2-methyl- | 102 | C6H14O | 000565-67-3 | 40 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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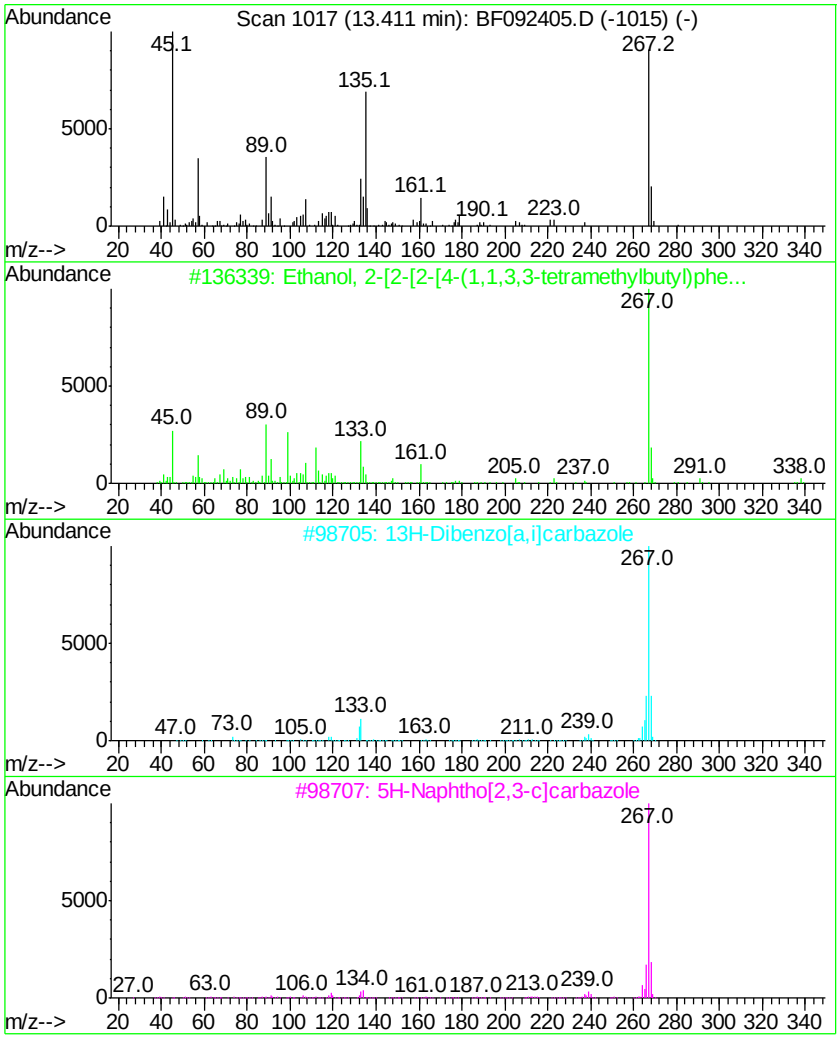
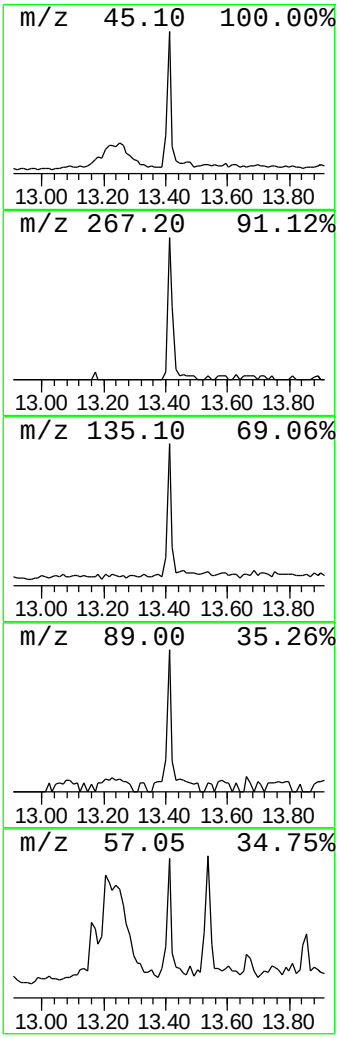
Peak Number 17 Ethanol, 2-[2-[2-[4-(1,1,3,... Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.41 | 2.86 ng | 92206 | Chrysene-d12 | 13.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-[2-[2-[4-(1,1,3,3-tet... | 338 | C20H34O4 | 002315-62-0 | 58 |
| 2 | 13H-Dibenzo[a,i]carbazole | 267 | C20H13N | 000239-64-5 | 35 |
| 3 | 5H-Naphtho[2,3-c]carbazole | 267 | C20H13N | 000198-96-9 | 27 |
| 4 | 7H-Dibenzo(a,g)carbazole | 267 | C20H13N | 000207-84-1 | 25 |
| 5 | Hexaethylene glycol monododecyl ... | 450 | C24H50O7 | 003055-96-7 | 22 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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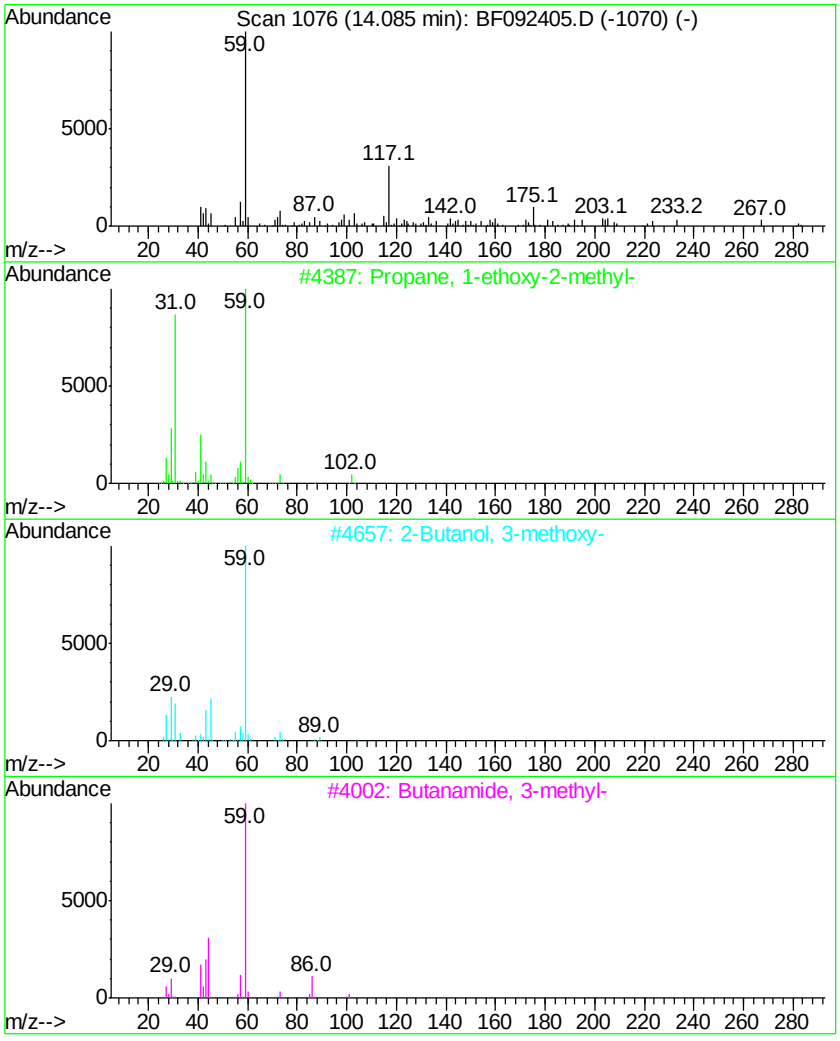
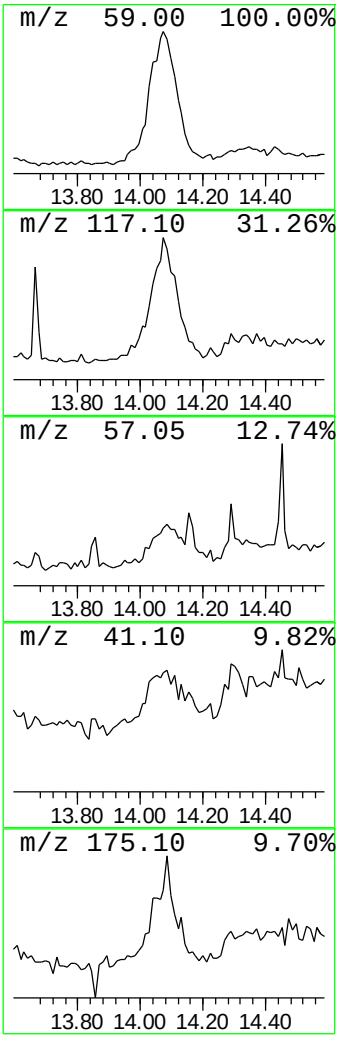
Peak Number 18 unknown14.09 Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.09 | 5.11 ng | 165096 | Chrysene-d12 | 13.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 1-ethoxy-2-methyl- | 102 | C6H14O | 000627-02-1 | 43 |
| 2 | 2-Butanol, 3-methoxy- | 104 | C5H12O2 | 053778-72-6 | 43 |
| 3 | Butanamide, 3-methyl- | 101 | C5H11NO | 000541-46-8 | 43 |
| 4 | 2-Propanol, 1-[1-methyl-2-(2-pro... | 174 | C9H18O3 | 055956-25-7 | 42 |
| 5 | 2-[5-(1-Hydroxy-1-methylethyl)-2... | 218 | C11H22O4 | 1000190-33-6 | 38 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

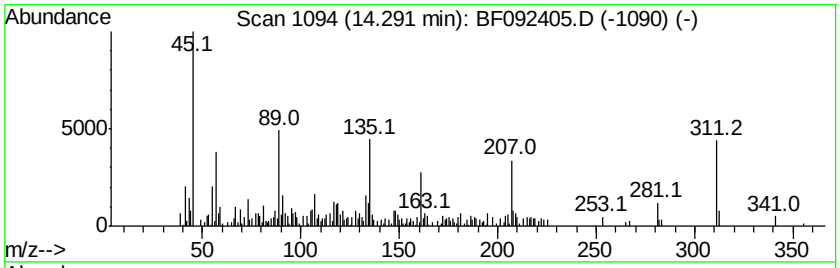
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

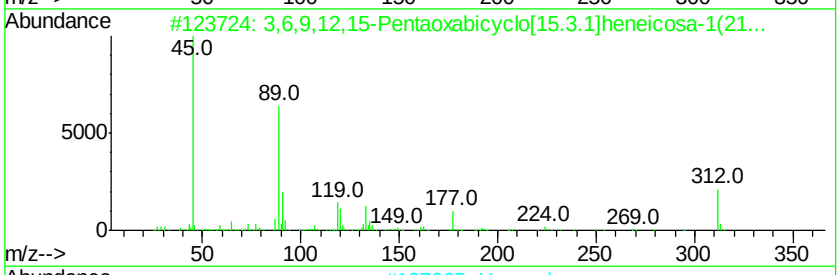
**********

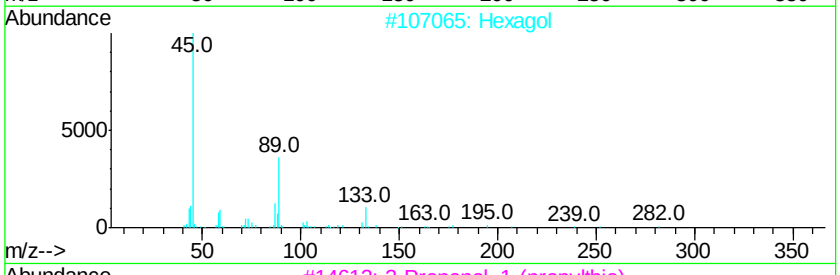
Peak Number 19 unknown14.29 Concentration Rank 7

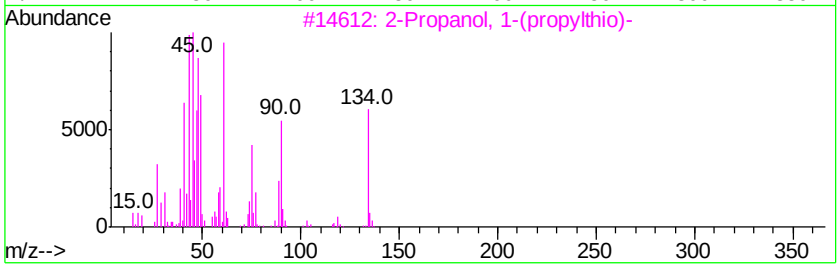
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.29 | 8.45 ng | 272772 | Chrysene-d12 | 13.66 |

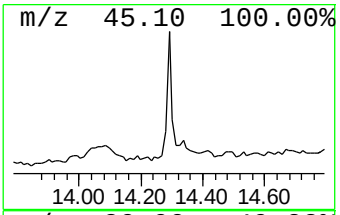
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3,6,9,12,15-Pentaoxabicyclo[15.3... | 312 | C16H24O6 | 065112-36-9 | 38 |
| 2 | Hexagol | 282 | C12H26O7 | 002615-15-8 | 35 |
| 3 | 2-Propanol, 1-(propylthio)- | 134 | C6H14OS | 053957-22-5 | 27 |
| 4 | 3,6,9,12,15-Pentaoxabicyclo[15.3... | 326 | C17H26O6 | 071128-99-9 | 25 |
| 5 | Triethylene glycol | 150 | C6H14O4 | 000112-27-6 | 25 |

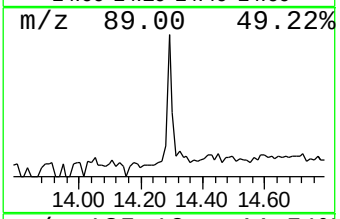


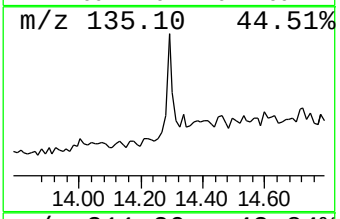



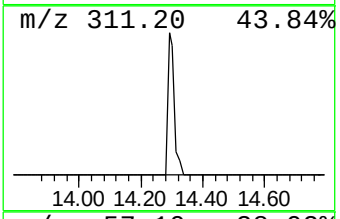



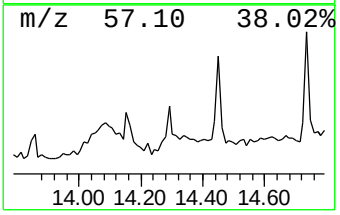



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

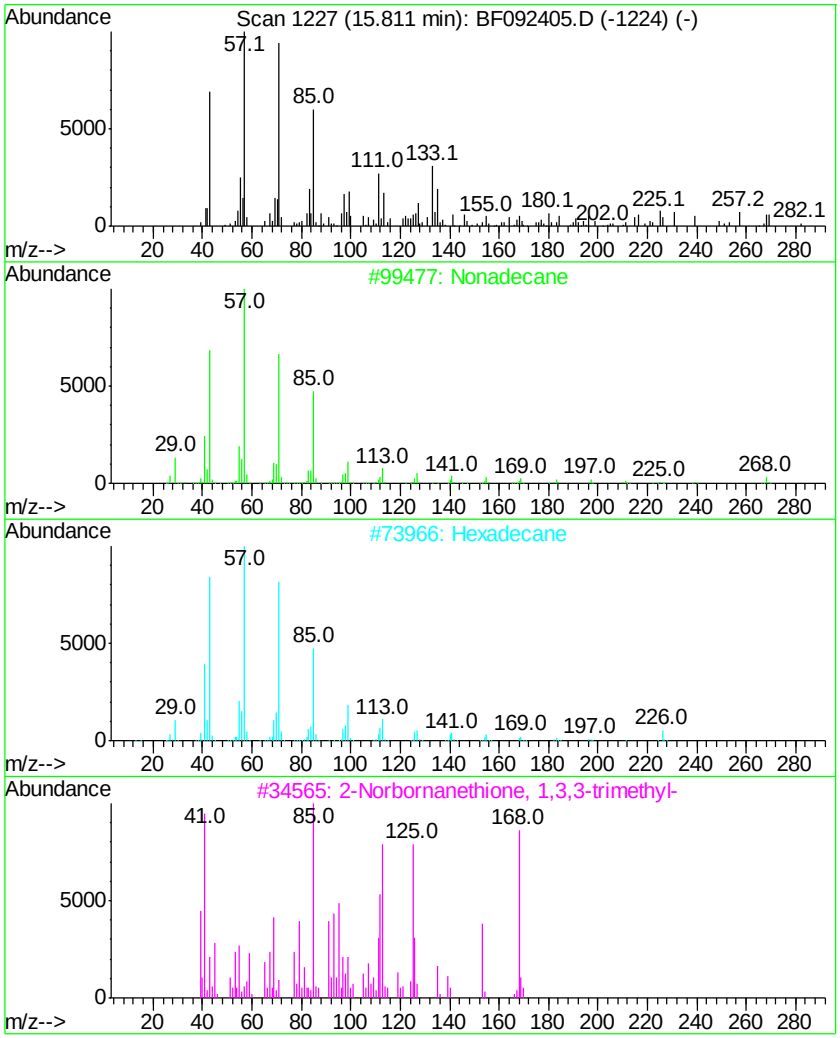
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

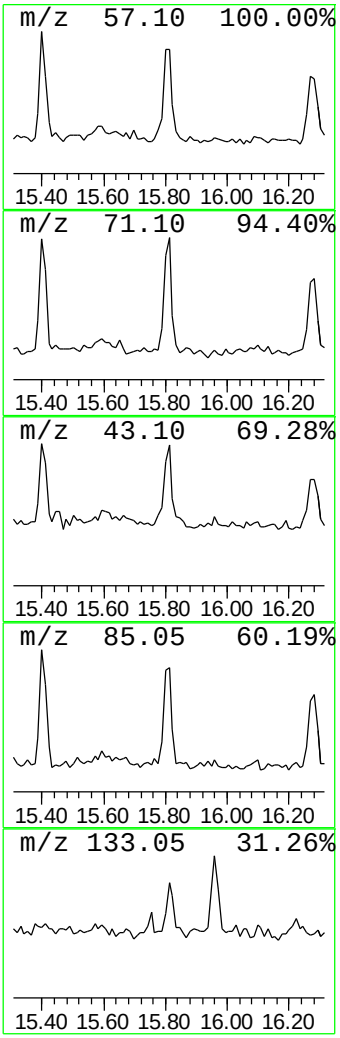
**********

Peak Number 20 Nonadecane Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.81 | 2.45 ng | 81017 | Perylene-d12 | 15.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Nonadecane | 268 | C19H40 | 000629-92-5 | 92 |
| 2 | Hexadecane | 226 | C16H34 | 000544-76-3 | 83 |
| 3 | 2-Norbornanethione, 1,3,3-trimet... | 168 | C10H16S | 000875-06-9 | 60 |
| 4 | Decane, 3-methyl- | 156 | C11H24 | 013151-34-3 | 58 |
| 5 | Heneicosane | 296 | C21H44 | 000629-94-7 | 58 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012017\
Data File : BF092405.D
Acq On : 21 Jan 2017 8:48
Operator : UM/SJ
Sample : I1267-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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... | 4.63 | 14.2 | ng | 764880 | 1 | 6.52 | 1074220 | 20.0 |
| unknown6.30 | 6.30 | 86.2 | ng | 4628690 | 1 | 6.52 | 1074220 | 20.0 |
| Benzene, 1,3-diis... | 8.76 | 4.2 | ng | 240703 | 3 | 9.56 | 1136360 | 20.0 |
| Benzene, 2,4-diis... | 8.79 | 9.8 | ng | 557928 | 3 | 9.56 | 1136360 | 20.0 |
| 7-Hydroxy-1-indanone | 9.04 | 3.5 | ng | 201567 | 3 | 9.56 | 1136360 | 20.0 |
| 2H-Benzimidazol-2... | 9.11 | 6.5 | ng | 368536 | 3 | 9.56 | 1136360 | 20.0 |
| 1H-Inden-1-one, 2... | 9.33 | 7.7 | ng | 436997 | 3 | 9.56 | 1136360 | 20.0 |
| 3-Acetylcoumarin | 9.36 | 5.1 | ng | 291279 | 3 | 9.56 | 1136360 | 20.0 |
| Thiophene, 3-(1-m... | 9.81 | 4.0 | ng | 225464 | 3 | 9.56 | 1136360 | 20.0 |
| 1-Hexen-3-one, 5-... | 9.99 | 8.0 | ng | 452610 | 3 | 9.56 | 1136360 | 20.0 |
| 2-Propanol, 1-[1-... | 11.22 | 7.1 | ng | 273318 | 4 | 11.03 | 768882 | 20.0 |
| 2-(4-Formyl-pheno... | 11.26 | 6.7 | ng | 258285 | 4 | 11.03 | 768882 | 20.0 |
| 2-Butanol, 3-meth... | 12.30 | 12.1 | ng | 465695 | 4 | 11.03 | 768882 | 20.0 |
| Ethanol, 2-[2-[4-... | 12.41 | 7.3 | ng | 234954 | 5 | 13.66 | 645687 | 20.0 |
| Silane, hexyl- | 13.25 | 20.3 | ng | 653793 | 5 | 13.66 | 645687 | 20.0 |
| Ethanol, 2-[2-[2-... | 13.41 | 2.9 | ng | 92206 | 5 | 13.66 | 645687 | 20.0 |
| unknown14.09 | 14.09 | 5.1 | ng | 165096 | 5 | 13.66 | 645687 | 20.0 |
| unknown14.29 | 14.29 | 8.4 | ng | 272772 | 5 | 13.66 | 645687 | 20.0 |
| Nonadecane | 15.81 | 2.5 | ng | 81017 | 6 | 15.02 | 661625 | 20.0 |