LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092206.D
Acq On : 12 Jan 2017 14:20
Operator : UM/SJ
Sample : I1029-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-002

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 | 3.990 | 182 | 184 | 189 | rBV | 93798 | 183444 | 2.88% | 0.315% |
| 2 | 4.733 | 246 | 249 | 261 | rVB | 1876563 | 3253304 | 51.02% | 5.589% |
| 3 | 5.201 | 287 | 290 | 292 | rBV | 5557111 | 6376324 | 100.00% | 10.954% |
| 4 | 6.264 | 380 | 383 | 386 | rBV | 4924977 | 6202146 | 97.27% | 10.655% |
| 5 | 6.367 | 390 | 392 | 395 | rVB | 5357129 | 5920741 | 92.86% | 10.171% |
| 6 | 6.596 | 410 | 412 | 414 | rBV | 1230923 | 1175594 | 18.44% | 2.020% |
| 7 | 6.756 | 423 | 426 | 428 | rBV | 3951657 | 5013581 | 78.63% | 8.613% |
| 8 | 7.167 | 459 | 462 | 464 | rBV | 3678842 | 3963051 | 62.15% | 6.808% |
| 9 | 7.876 | 522 | 524 | 527 | rBV | 1409152 | 1620938 | 25.42% | 2.785% |
| 10 | 8.962 | 616 | 619 | 622 | rBV | 5914656 | 6345424 | 99.52% | 10.901% |
| 11 | 9.362 | 652 | 654 | 656 | rBV | 645237 | 563353 | 8.84% | 0.968% |
| 12 | 9.625 | 675 | 677 | 680 | rVB | 1493418 | 1538304 | 24.13% | 2.643% |
| 13 | 10.082 | 713 | 717 | 718 | rBV | 69587 | 91178 | 1.43% | 0.157% |
| 14 | 10.425 | 744 | 747 | 749 | rBV | 3055048 | 3707017 | 58.14% | 6.368% |
| 15 | 10.551 | 756 | 758 | 764 | rVB | 150063 | 182176 | 2.86% | 0.313% |
| 16 | 10.996 | 792 | 797 | 798 | rBV2 | 125285 | 129902 | 2.04% | 0.223% |
| 17 | 11.099 | 804 | 806 | 809 | rVB | 1099702 | 1503120 | 23.57% | 2.582% |
| 18 | 11.659 | 853 | 855 | 862 | rVB | 677565 | 674273 | 10.57% | 1.158% |
| 19 | 12.436 | 921 | 923 | 929 | rBV2 | 207096 | 278329 | 4.37% | 0.478% |
| 20 | 12.699 | 943 | 946 | 948 | rVB | 5089689 | 5920494 | 92.85% | 10.171% |
| 21 | 13.602 | 1022 | 1025 | 1034 | rBV | 302439 | 421629 | 6.61% | 0.724% |
| 22 | 13.728 | 1034 | 1036 | 1039 | rBV | 1077031 | 1233080 | 19.34% | 2.118% |
| 23 | 14.242 | 1075 | 1081 | 1086 | rBV | 42480 | 111162 | 1.74% | 0.191% |
| 24 | 14.814 | 1128 | 1131 | 1132 | rBV | 55827 | 65078 | 1.02% | 0.112% |
| 25 | 15.088 | 1152 | 1155 | 1157 | rBV | 789747 | 897994 | 14.08% | 1.543% |
| 26 | 15.134 | 1157 | 1159 | 1162 | rVB | 57768 | 71645 | 1.12% | 0.123% |
| 27 | 15.500 | 1188 | 1191 | 1193 | rBV | 77155 | 105438 | 1.65% | 0.181% |
| 28 | 15.911 | 1224 | 1227 | 1233 | rVB2 | 48165 | 98294 | 1.54% | 0.169% |
| 29 | 16.448 | 1271 | 1274 | 1278 | rVB | 199948 | 361919 | 5.68% | 0.622% |
| 30 | 16.585 | 1284 | 1286 | 1290 | rVB4 | 29656 | 64040 | 1.00% | 0.110% |
| 31 | 16.974 | 1317 | 1320 | 1324 | rVB | 29426 | 69023 | 1.08% | 0.119% |
| 32 | 17.648 | 1375 | 1379 | 1384 | rBV2 | 26232 | 69155 | 1.08% | 0.119% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092206.D
Acq On : 12 Jan 2017 14:20
Operator : UM/SJ
Sample : I1029-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-002

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

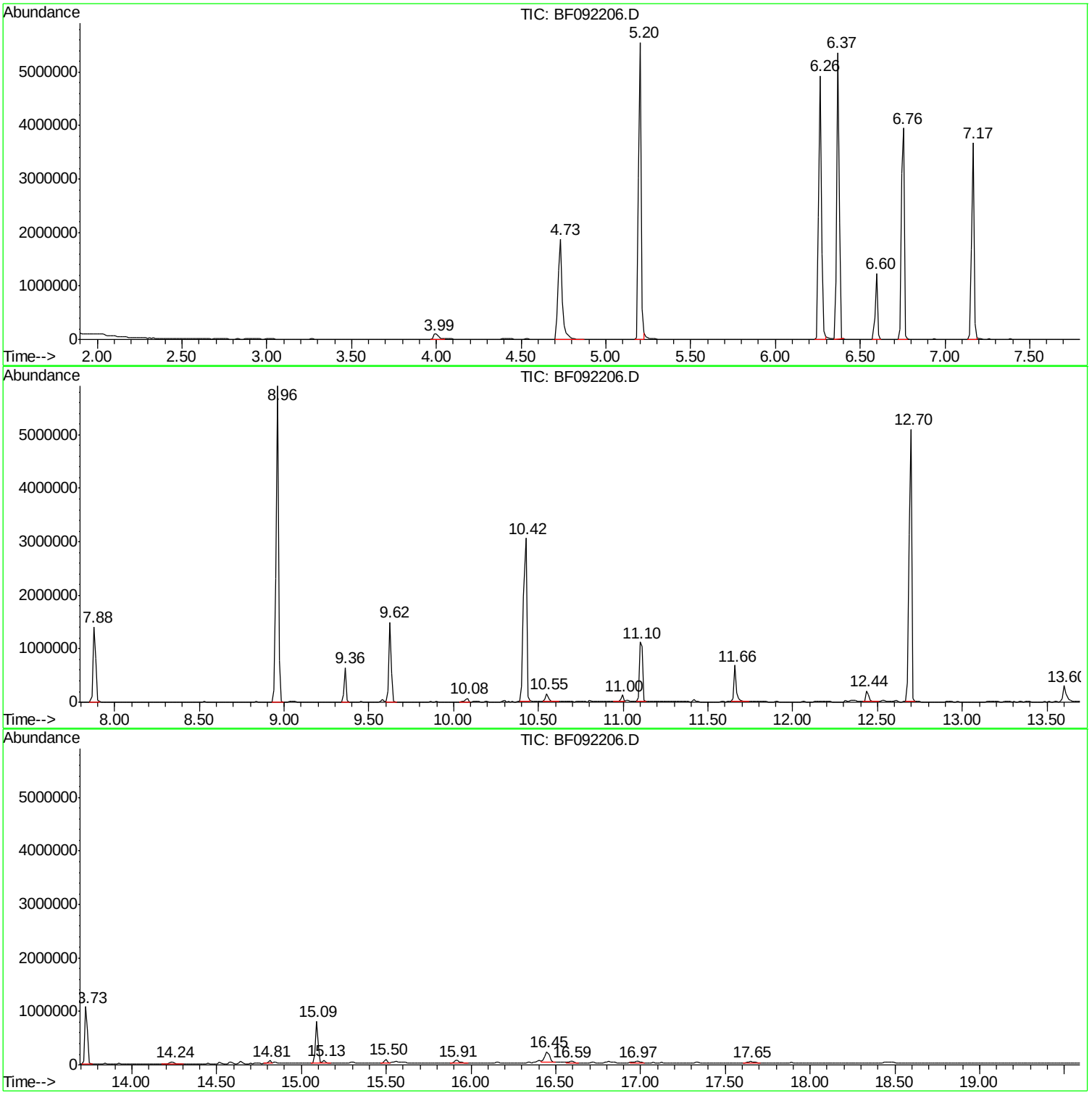
Sum of corrected areas: 58211150

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092206.D
Acq On : 12 Jan 2017 14:20
Operator : UM/SJ
Sample : I1029-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-002

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092206.D
Acq On : 12 Jan 2017 14:20
Operator : UM/SJ
Sample : I1029-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-002

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

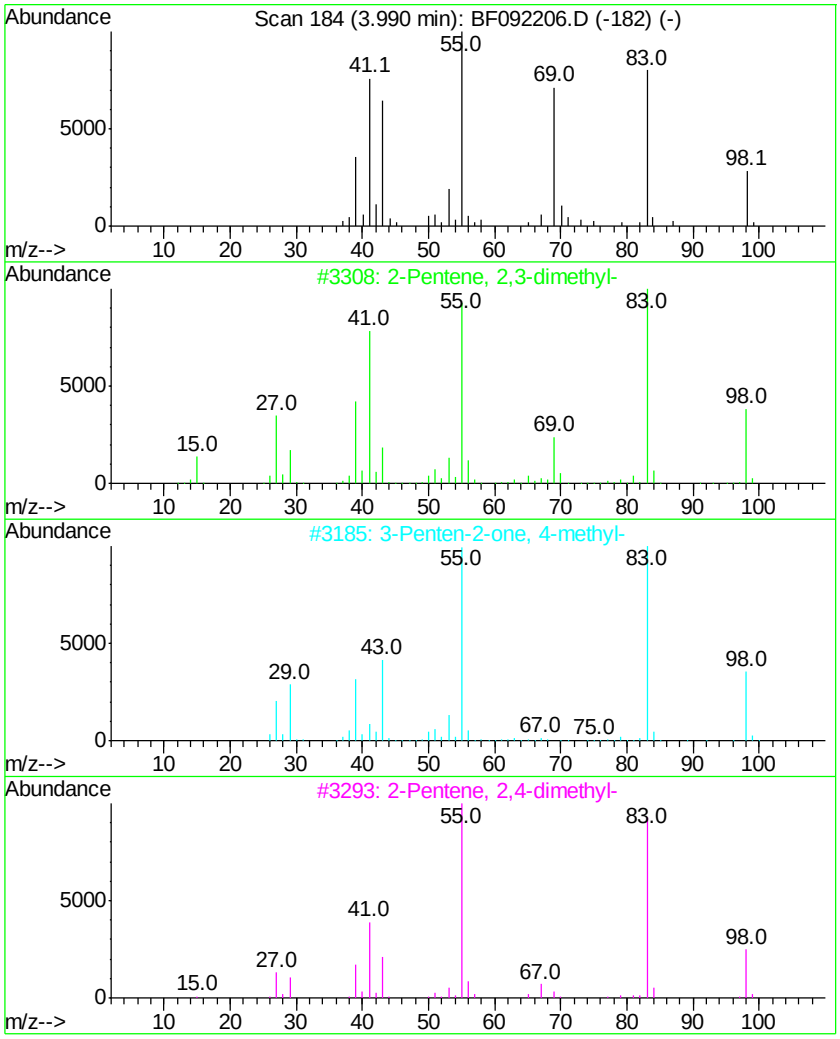
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

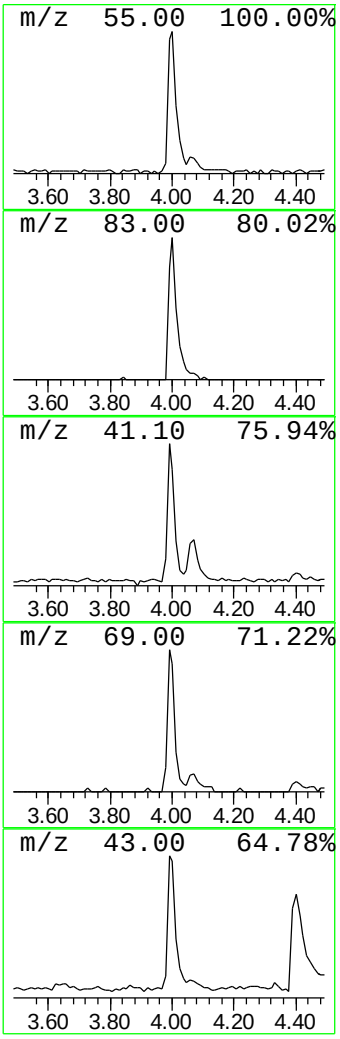
**********

Peak Number 1 2-Pentene, 2,3-dimethyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.99 | 3.12 ng | 183444 | 1,4-Dichlorobenzene-d4 | 6.60 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentene, 2,3-dimethyl- | 98 | C7H14 | 010574-37-5 | 86 |
| 2 | 3-Penten-2-one, 4-methyl- | 98 | C6H10O | 000141-79-7 | 68 |
| 3 | 2-Pentene, 2,4-dimethyl- | 98 | C7H14 | 000625-65-0 | 64 |
| 4 | 3-Hexen-2-one | 98 | C6H10O | 000763-93-9 | 58 |
| 5 | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14 | 004914-92-5 | 58 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092206.D
Acq On : 12 Jan 2017 14:20
Operator : UM/SJ
Sample : I1029-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-002

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

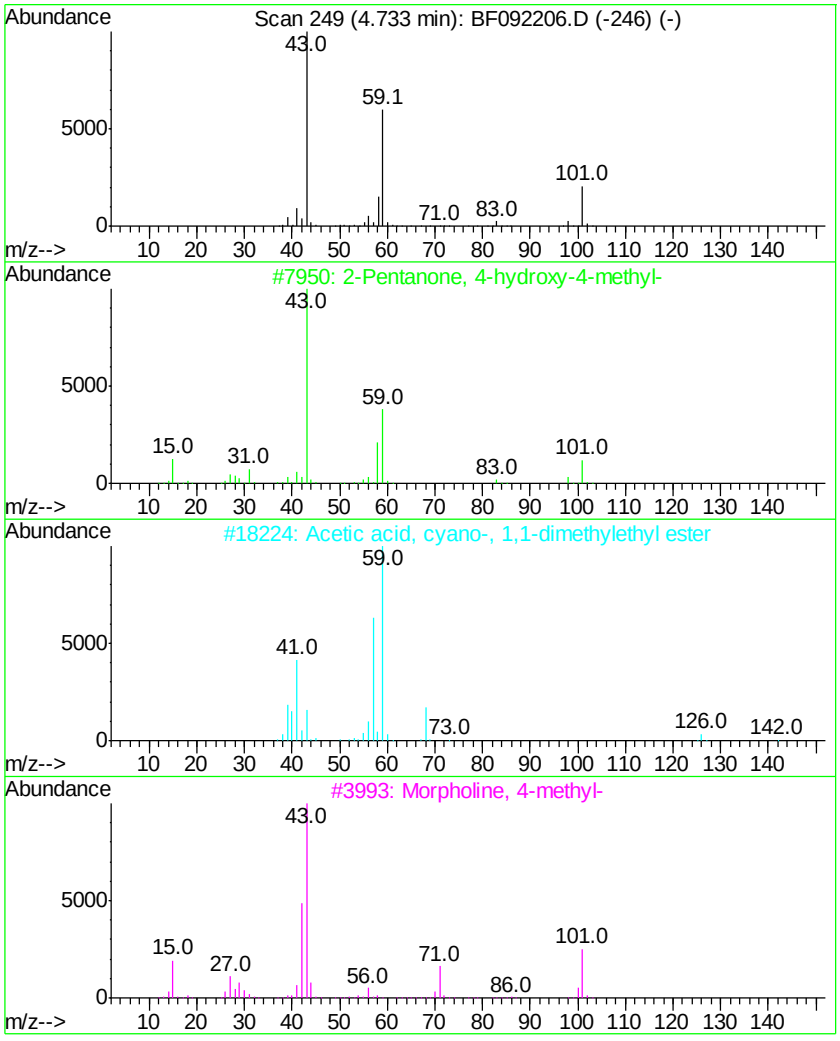
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

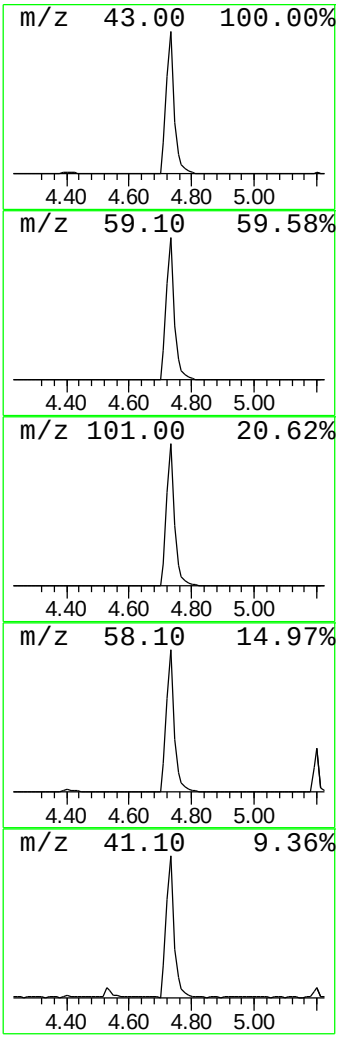
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.73 | 55.35 ng | 3253300 | 1,4-Dichlorobenzene-d4 | 6.60 |

| 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, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 3 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | 1,2-Butanediol, (.+/-.)- | 90 | C4H10O2 | 026171-83-5 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092206.D
Acq On : 12 Jan 2017 14:20
Operator : UM/SJ
Sample : I1029-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-002

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

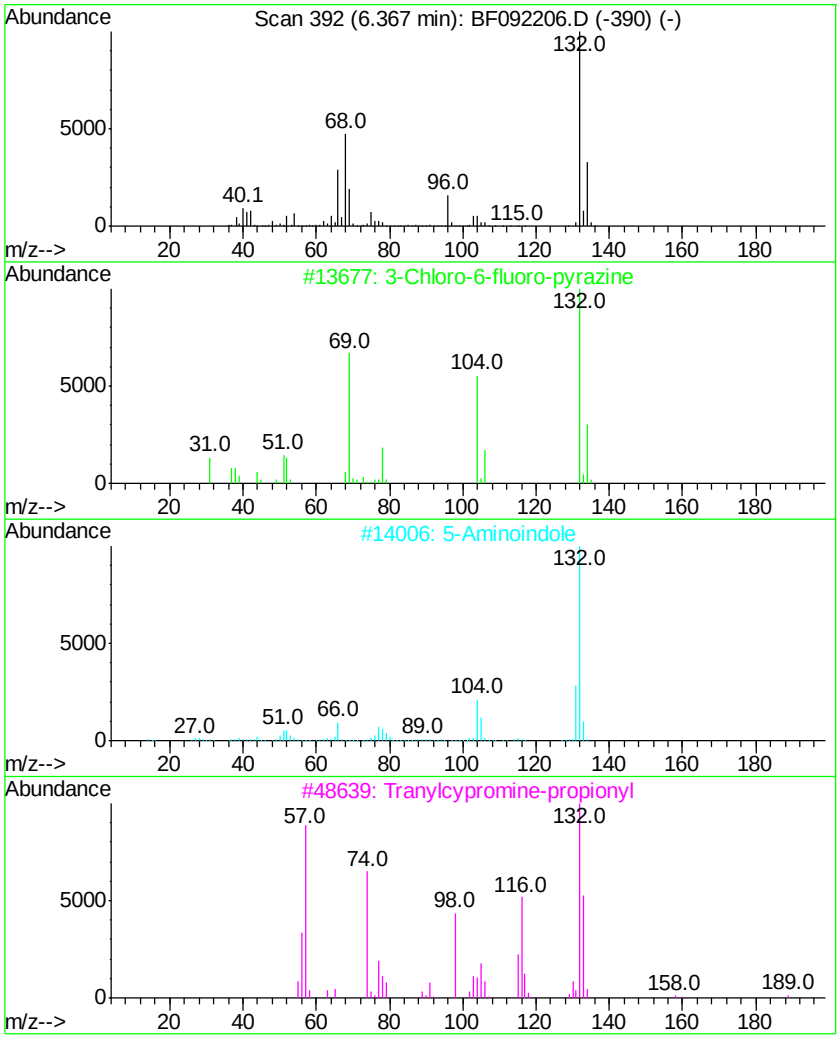
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

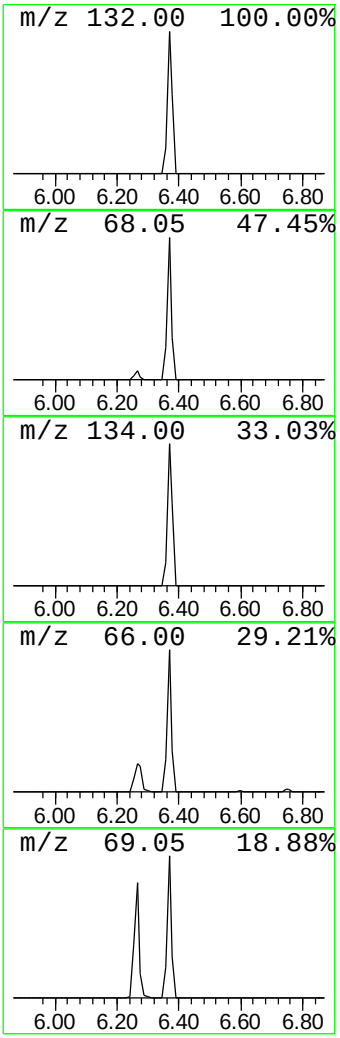
**********

Peak Number 3 unknown6.37 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.37 | 100.73 ng | 5920740 | 1,4-Dichlorobenzene-d4 | 6.60 |

| 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 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 9 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092206.D
Acq On : 12 Jan 2017 14:20
Operator : UM/SJ
Sample : I1029-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-002

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

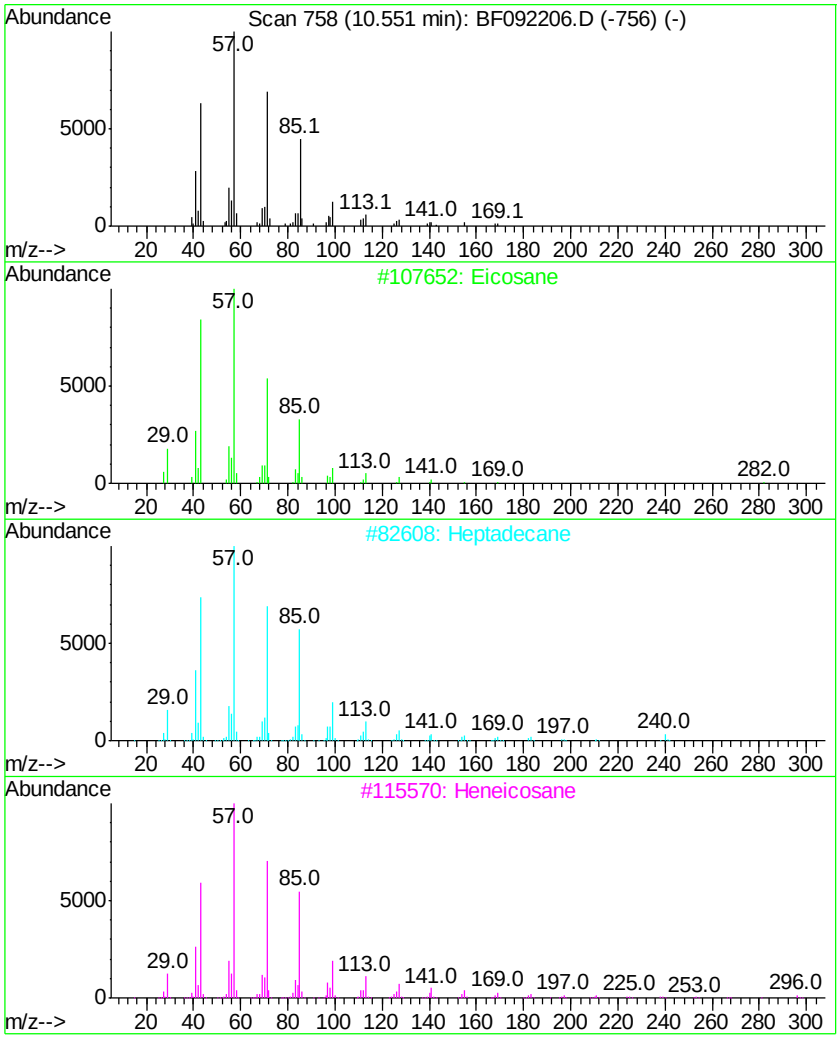
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

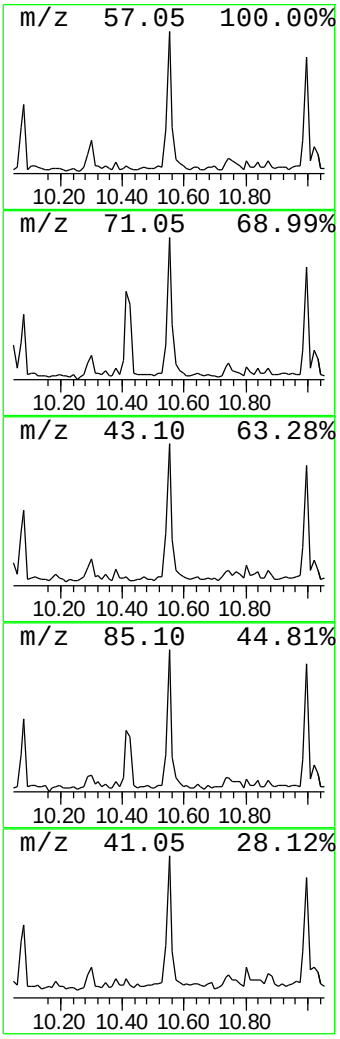
**********

Peak Number 4 Eicosane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.55 | 2.42 ng | 182176 | Phenanthrene-d10 | 11.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 91 |
| 2 | Heptadecane | 240 | C17H36 | 000629-78-7 | 91 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 5 | Tetradecane | 198 | C14H30 | 000629-59-4 | 87 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092206.D
Acq On : 12 Jan 2017 14:20
Operator : UM/SJ
Sample : I1029-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-002

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

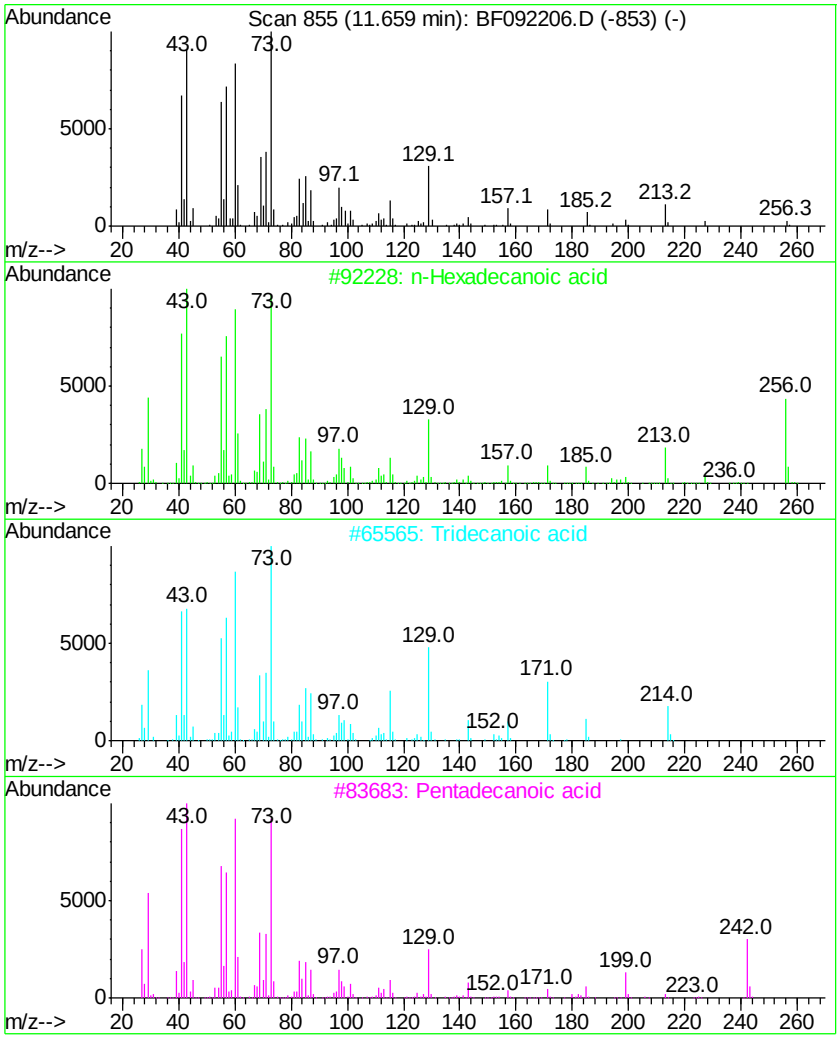
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

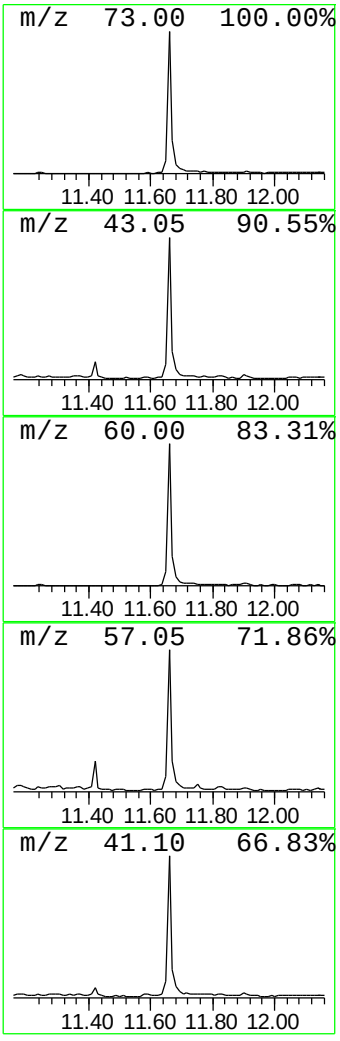
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.66 | 8.97 ng | 674273 | Phenanthrene-d10 | 11.11 |

| 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 | 93 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 72 |
| 4 | Undecane | 156 | C11H24 | 001120-21-4 | 11 |
| 5 | Hexadecane | 226 | C16H34 | 000544-76-3 | 11 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092206.D
Acq On : 12 Jan 2017 14:20
Operator : UM/SJ
Sample : I1029-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-002

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

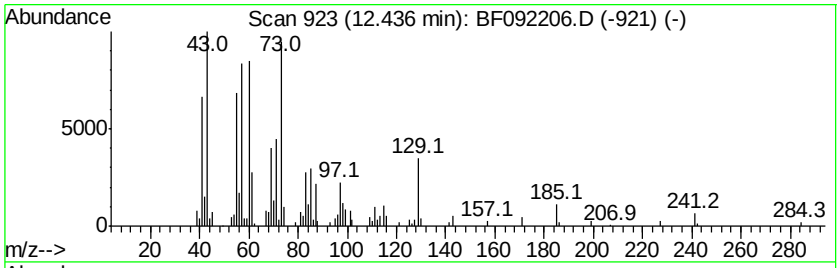
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

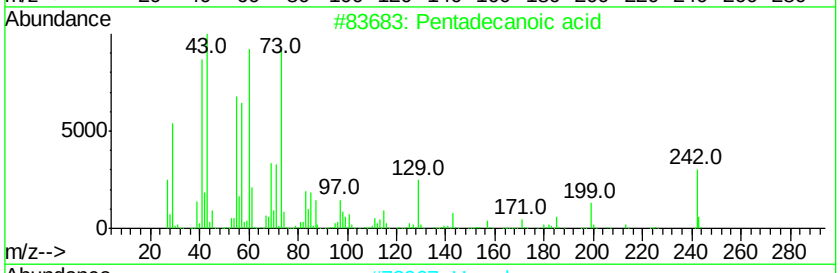
**********

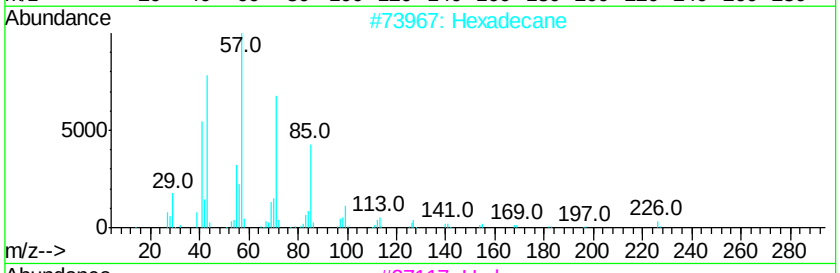
Peak Number 6 Pentadecanoic acid Concentration Rank 6

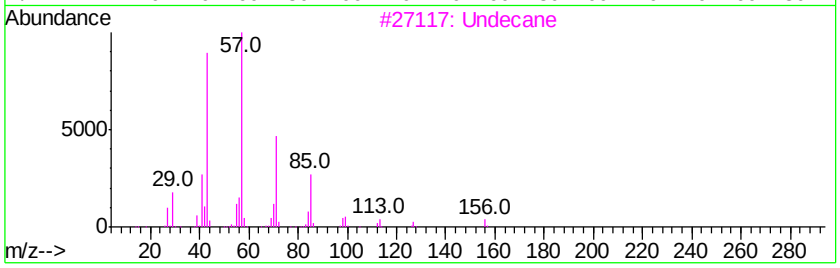
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.44 | 4.51 ng | 278329 | Chrysene-d12 | 13.73 |

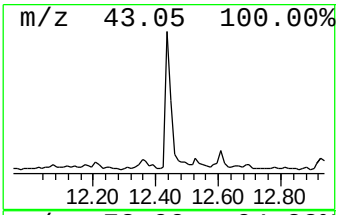
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 91 |
| 2 | Hexadecane | 226 | C16H34 | 000544-76-3 | 11 |
| 3 | Undecane | 156 | C11H24 | 001120-21-4 | 11 |
| 4 | Dodecane | 170 | C12H26 | 000112-40-3 | 11 |
| 5 | Tetradecane | 198 | C14H30 | 000629-59-4 | 11 |

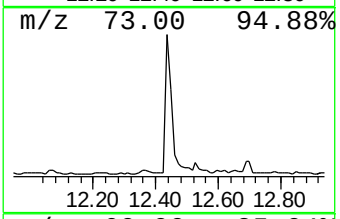


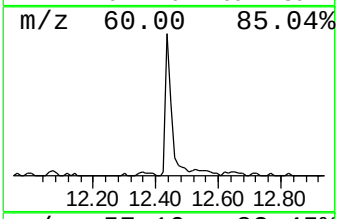



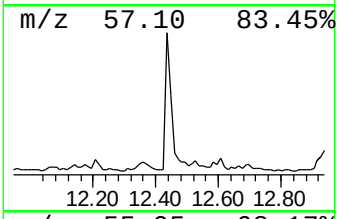



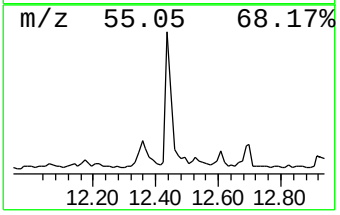



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092206.D
Acq On : 12 Jan 2017 14:20
Operator : UM/SJ
Sample : I1029-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-002

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

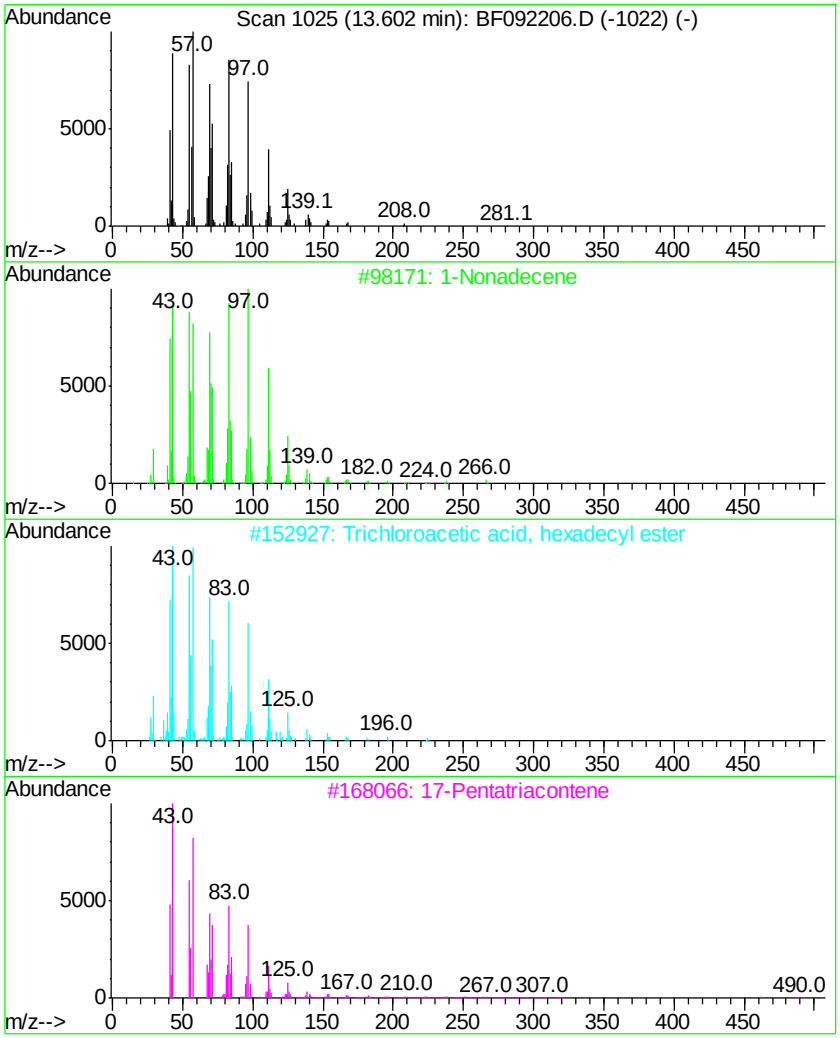
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

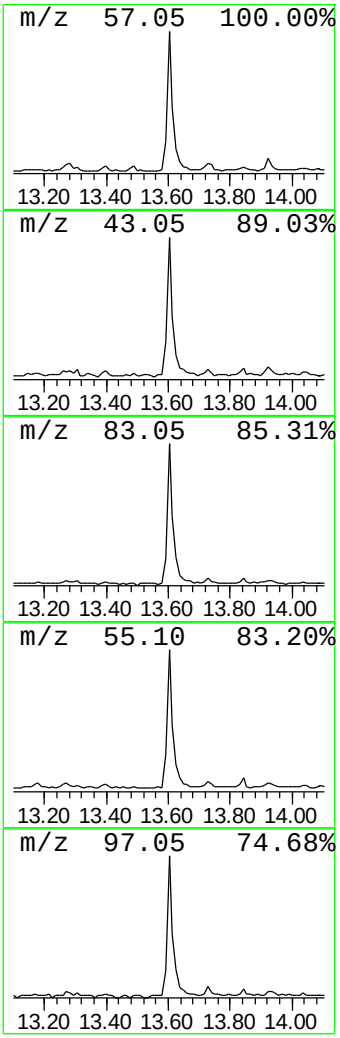
**********

Peak Number 7 1-Nonadecene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.60 | 6.84 ng | 421629 | Chrysene-d12 | 13.73 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 91 |
| 2 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 91 |
| 3 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 87 |
| 4 | Trichloroacetic acid, tetradecyl... | 358 | C16H29Cl3O2 | 074339-52-9 | 87 |
| 5 | Pentafluoropropionic acid, hexad... | 388 | C19H33F5O2 | 006222-07-7 | 87 |



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Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092206.D
Acq On : 12 Jan 2017 14:20
Operator : UM/SJ
Sample : I1029-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-002

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

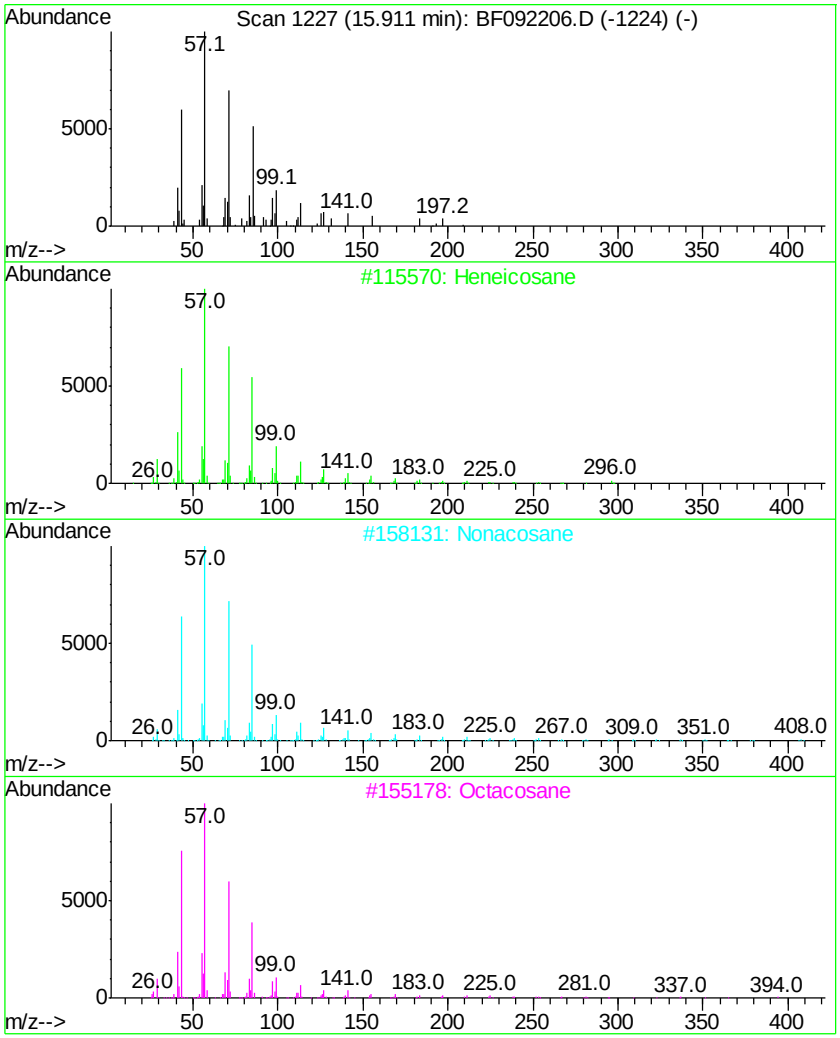
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

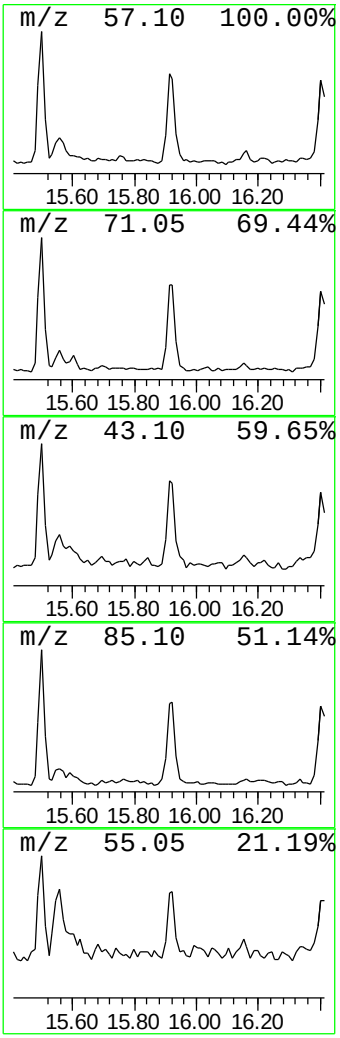
**********

Peak Number 9 Heneicosane Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.91 | 2.19 ng | 98294 | Perylene-d12 | 15.09 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 90 |
| 2 | Nonacosane | 408 | C29H60 | 000630-03-5 | 90 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |
| 4 | Tetratriacontane | 479 | C34H70 | 014167-59-0 | 86 |
| 5 | Heptadecane, 2,6,10,15-tetramethyl- | 296 | C21H44 | 054833-48-6 | 86 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092206.D
Acq On : 12 Jan 2017 14:20
Operator : UM/SJ
Sample : I1029-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-002

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

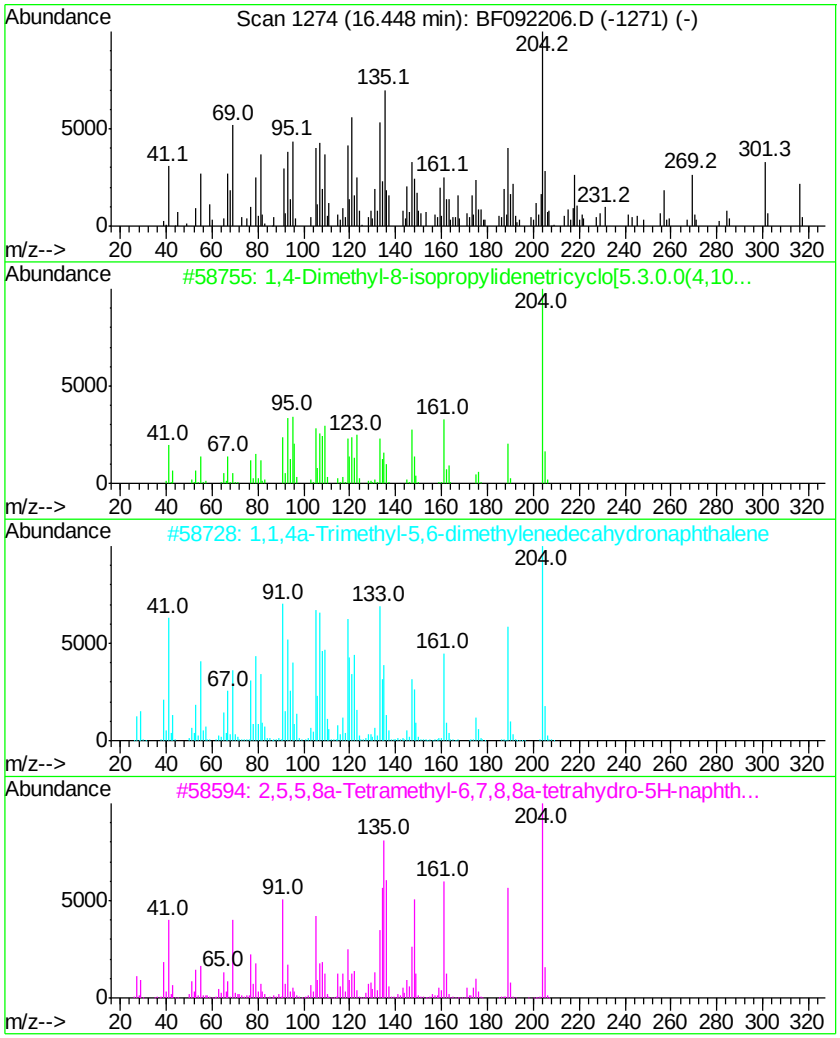
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

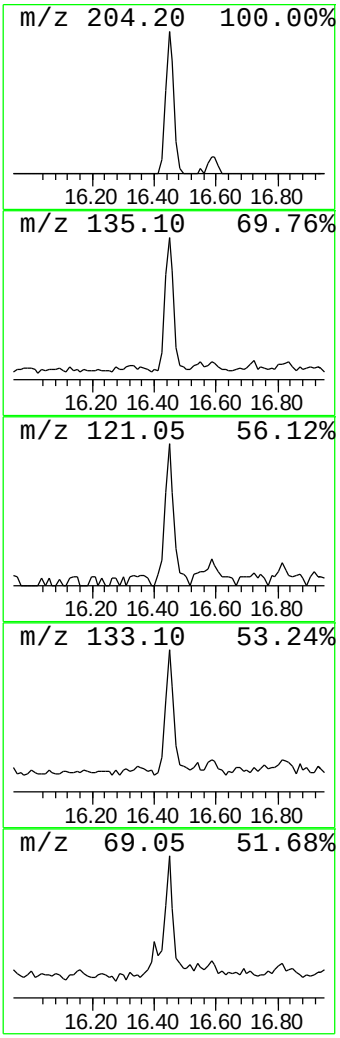
**********

Peak Number 10 1,4-Dimethyl-8-isopropylide... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.45 | 8.06 ng | 361919 | Perylene-d12 | 15.09 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,4-Dimethyl-8-isopropylidenetri... | 204 | C15H24 | 1000140-07-7 | 64 |
| 2 | 1,1,4a-Trimethyl-5,6-dimethylene... | 204 | C15H24 | 1000193-60-8 | 47 |
| 3 | 2,5,5,8a-Tetramethyl-6,7,8,8a-te... | 204 | C14H20O | 124957-09-1 | 46 |
| 4 | Farnesyl bromide | 284 | C15H25Br | 006874-67-5 | 45 |
| 5 | 1H-3a,7-Methanoazulene, 2,3,6,7,... | 204 | C15H24 | 000560-32-7 | 43 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011217\
Data File : BF092206.D
Acq On : 12 Jan 2017 14:20
Operator : UM/SJ
Sample : I1029-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-002

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-Pentene, 2,3-di... | 3.99 | 3.1 | ng | 183444 | 1 | 6.60 | 1175590 | 20.0 |
| 2-Pentanone, 4-hy... | 4.73 | 55.4 | ng | 3253300 | 1 | 6.60 | 1175590 | 20.0 |
| unknown6.37 | 6.37 | 100.7 | ng | 5920740 | 1 | 6.60 | 1175590 | 20.0 |
| Eicosane | 10.55 | 2.4 | ng | 182176 | 4 | 11.11 | 1503120 | 20.0 |
| n-Hexadecanoic acid | 11.66 | 9.0 | ng | 674273 | 4 | 11.11 | 1503120 | 20.0 |
| Pentadecanoic acid | 12.44 | 4.5 | ng | 278329 | 5 | 13.73 | 1233080 | 20.0 |
| 1-Nonadecene | 13.60 | 6.8 | ng | 421629 | 5 | 13.73 | 1233080 | 20.0 |
| Heneicosane | 15.91 | 2.2 | ng | 98294 | 6 | 15.09 | 897994 | 20.0 |
| 1,4-Dimethyl-8-is... | 16.45 | 8.1 | ng | 361919 | 6 | 15.09 | 897994 | 20.0 |