LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM020119\
Data File : BM018713.D
Acq On : 01 Feb 2019 19:25
Operator : JU/SJ
Sample : K1308-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** SB-18(34.5-35)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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 | 4.869 | 298 | 303 | 313 | rBV | 247772 | 351115 | 2.86% | 0.421% |
| 2 | 5.310 | 371 | 378 | 393 | rBV | 5107605 | 7234106 | 58.87% | 8.675% |
| 3 | 6.898 | 640 | 648 | 661 | rBV | 4836907 | 7637420 | 62.15% | 9.159% |
| 4 | 7.257 | 701 | 709 | 718 | rBV | 5209931 | 8207487 | 66.79% | 9.842% |
| 5 | 7.722 | 781 | 788 | 794 | rBV | 925738 | 1456917 | 11.86% | 1.747% |
| 6 | 8.040 | 834 | 842 | 853 | rBV | 3978783 | 6395084 | 52.04% | 7.669% |
| 7 | 8.887 | 978 | 986 | 1002 | rBV | 2897099 | 4745116 | 38.61% | 5.690% |
| 8 | 10.510 | 1254 | 1262 | 1274 | rBV | 1093118 | 1859196 | 15.13% | 2.229% |
| 9 | 12.986 | 1675 | 1683 | 1700 | rBV | 6847680 | 9871006 | 80.33% | 11.837% |
| 10 | 13.833 | 1821 | 1827 | 1836 | rBV | 357158 | 525255 | 4.27% | 0.630% |
| 11 | 14.369 | 1910 | 1918 | 1933 | rBV2 | 1455101 | 2202059 | 17.92% | 2.641% |
| 12 | 15.868 | 2163 | 2173 | 2192 | rBV | 4957190 | 7538401 | 61.34% | 9.040% |
| 13 | 17.121 | 2380 | 2386 | 2399 | rBV | 1746173 | 2472253 | 20.12% | 2.965% |
| 14 | 18.009 | 2531 | 2537 | 2547 | rBV | 739547 | 1056192 | 8.59% | 1.267% |
| 15 | 19.292 | 2751 | 2755 | 2764 | rBV2 | 231482 | 347048 | 2.82% | 0.416% |
| 16 | 19.751 | 2827 | 2833 | 2840 | rBV | 9451117 | 12288804 | 100.00% | 14.736% |
| 17 | 21.015 | 3043 | 3048 | 3057 | rBV | 1048554 | 1358390 | 11.05% | 1.629% |
| 18 | 21.315 | 3094 | 3099 | 3104 | rBV | 2242059 | 2915239 | 23.72% | 3.496% |
| 19 | 21.450 | 3119 | 3122 | 3127 | rBV | 171656 | 190628 | 1.55% | 0.229% |
| 20 | 21.886 | 3193 | 3196 | 3211 | rVB2 | 209700 | 395337 | 3.22% | 0.474% |
| 21 | 22.350 | 3272 | 3275 | 3282 | rVB | 296161 | 355145 | 2.89% | 0.426% |
| 22 | 22.862 | 3358 | 3362 | 3367 | rVB | 291500 | 402156 | 3.27% | 0.482% |
| 23 | 23.433 | 3456 | 3459 | 3465 | rVB2 | 290472 | 420244 | 3.42% | 0.504% |
| 24 | 23.574 | 3477 | 3483 | 3494 | rVB | 1675083 | 3166509 | 25.77% | 3.797% |

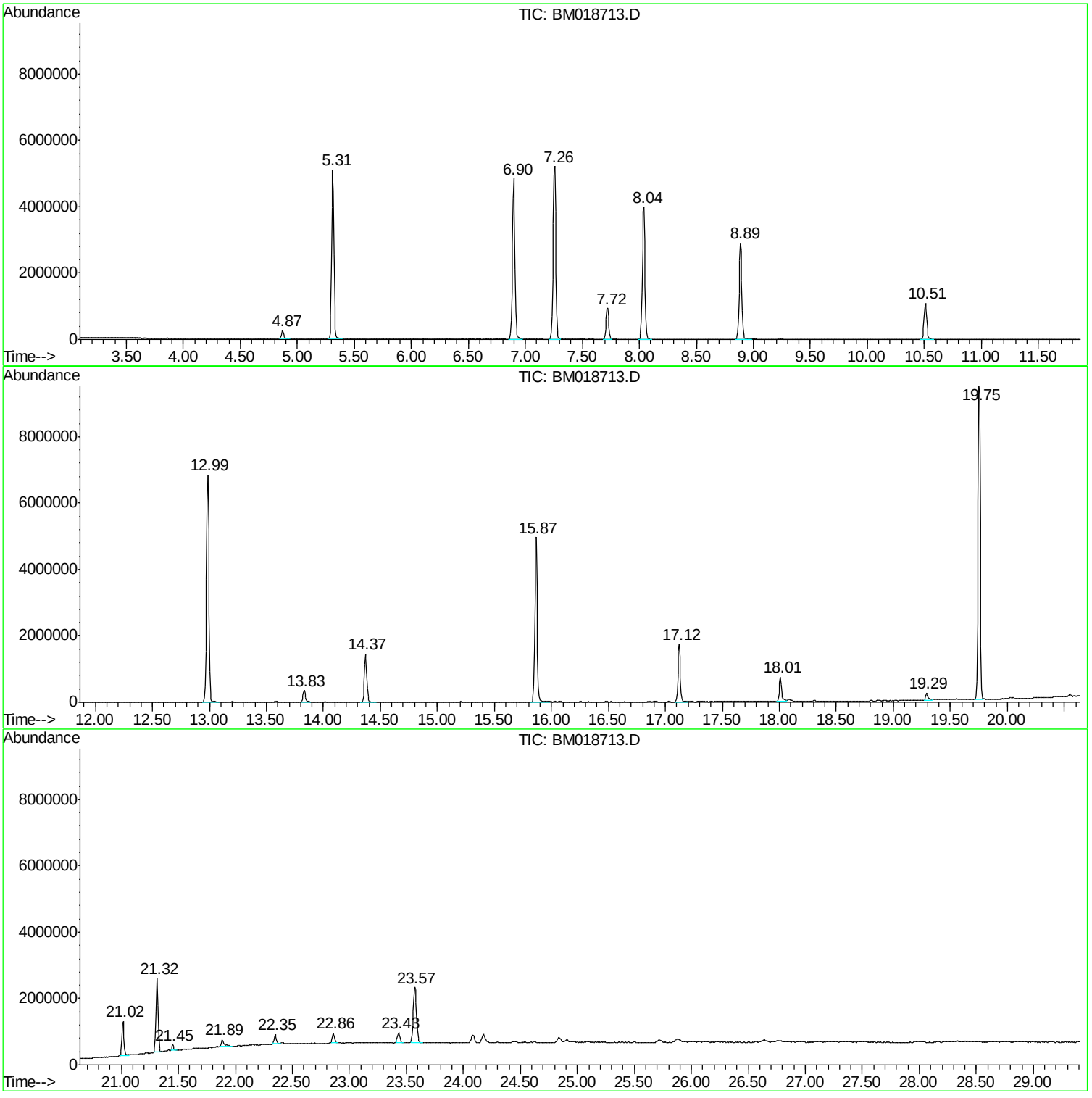
Sum of corrected areas: 83391107

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM020119\
Data File : BM018713.D
Acq On : 01 Feb 2019 19:25
Operator : JU/SJ
Sample : K1308-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
SB-18(34.5-35)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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:\SVOASRV\HPCHEM1\BNA M\DATA\BM020119\
Data File : BM018713.D
Acq On : 01 Feb 2019 19:25
Operator : JU/SJ
Sample : K1308-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** SB-18(34.5-35)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

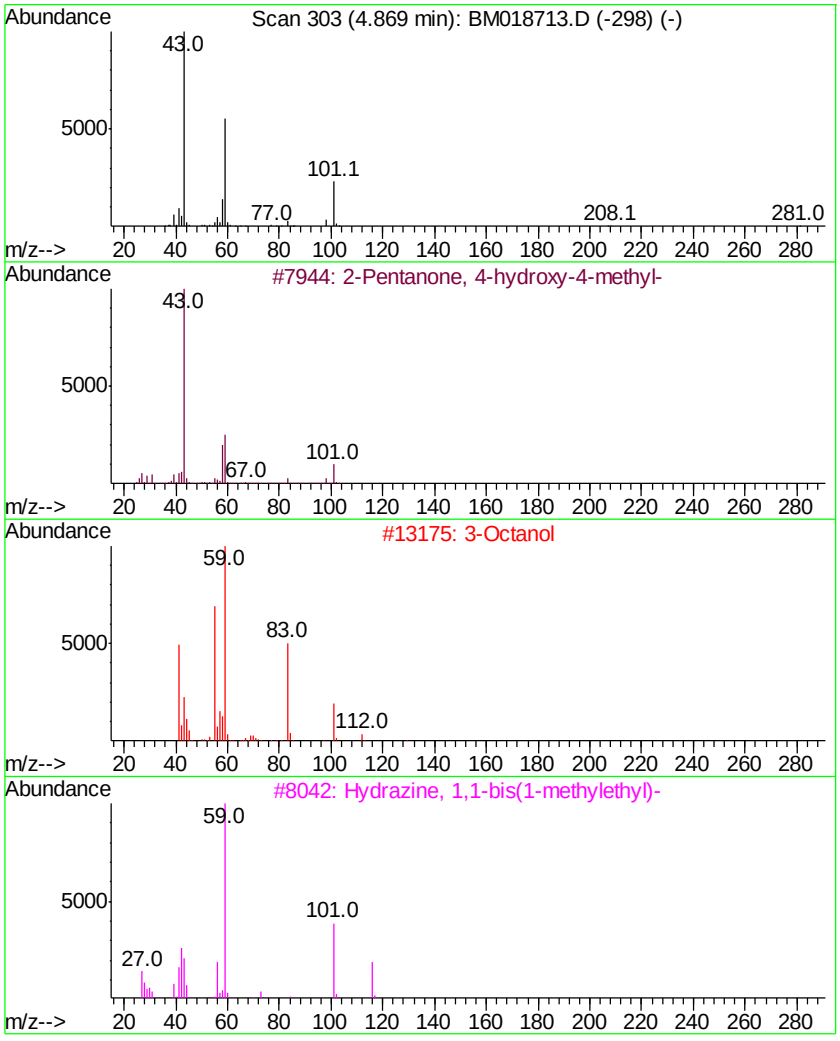
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

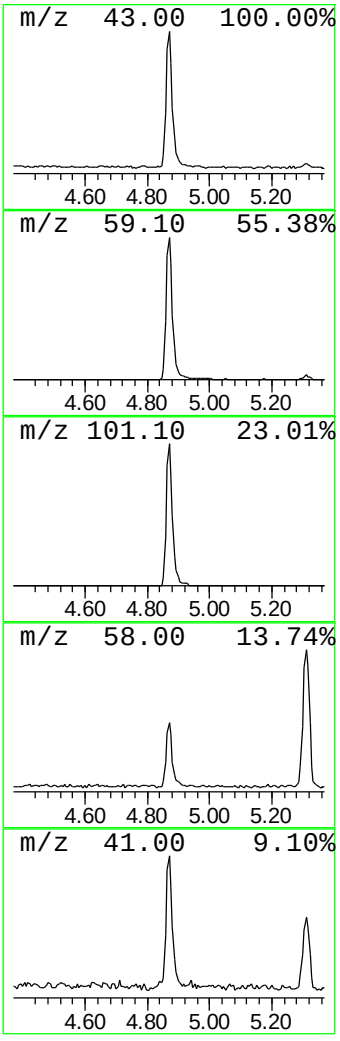
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.87 | 4.82 ng | 351115 | 1,4-Dichlorobenzene-d4 | 7.72 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | 3-Octanol | 130 | C8H18O | 020296-29-1 | 28 |
| 3 | Hydrazine, 1,1-bis(1-methylethyl)- | 116 | C6H16N2 | 000921-14-2 | 28 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 5 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM020119\
Data File : BM018713.D
Acq On : 01 Feb 2019 19:25
Operator : JU/SJ
Sample : K1308-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** SB-18(34.5-35)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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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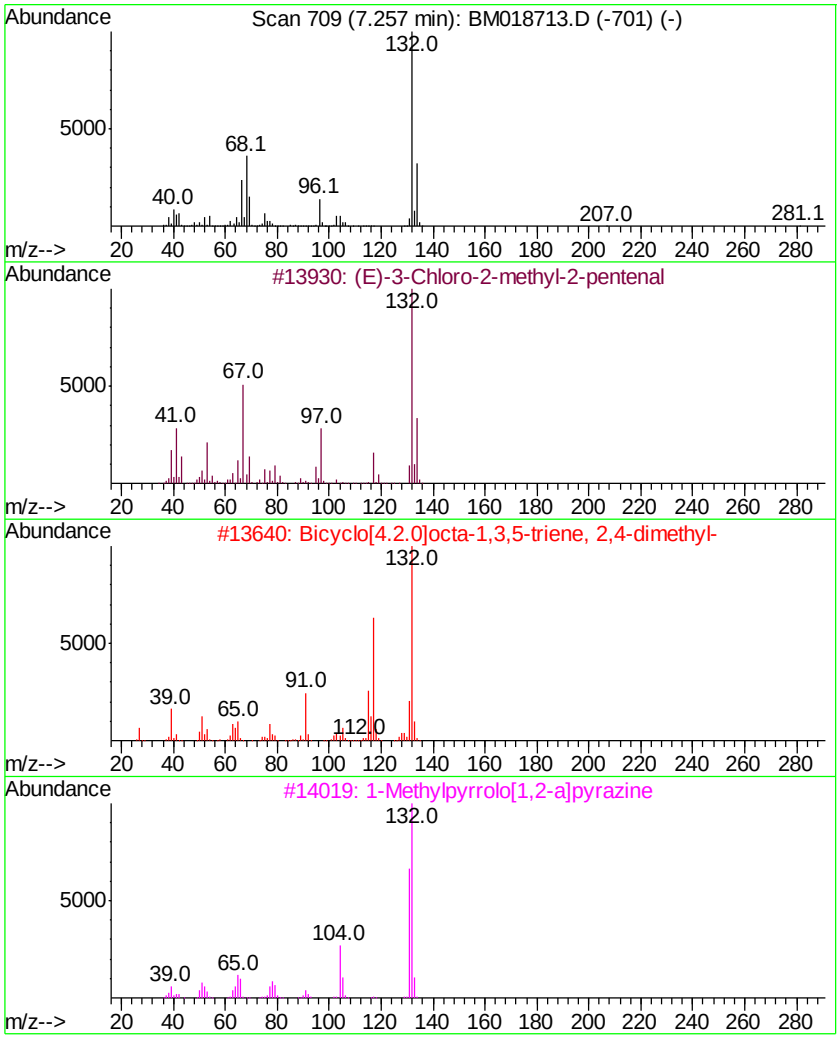
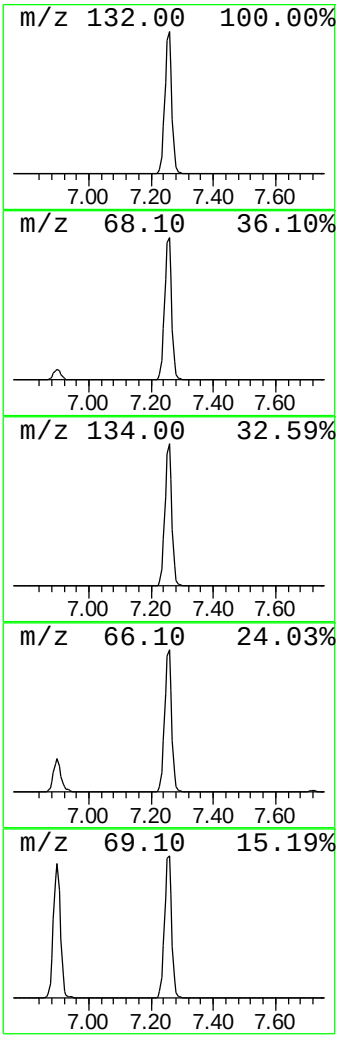
Peak Number 2 unknown7.26 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.26 | 112.67 ng | 8207490 | 1,4-Dichlorobenzene-d4 | 7.72 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 2 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 3 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |
| 4 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |
| 5 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM020119\
Data File : BM018713.D
Acq On : 01 Feb 2019 19:25
Operator : JU/SJ
Sample : K1308-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** SB-18(34.5-35)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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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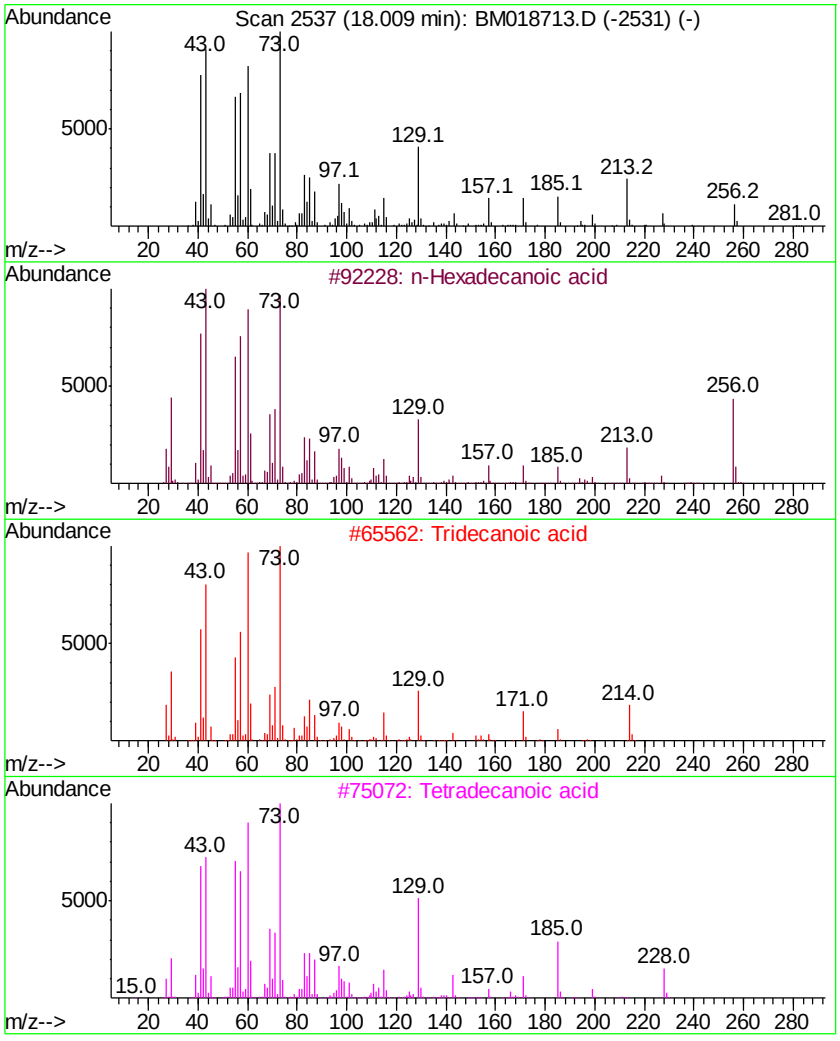
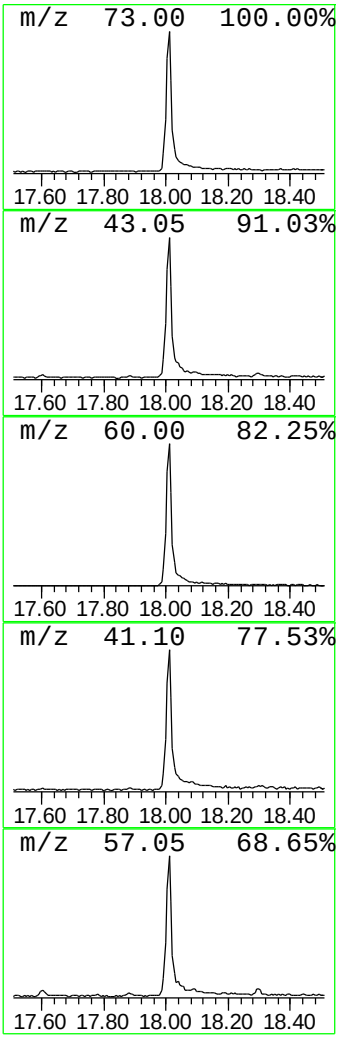
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.01 | 8.54 ng | 1056190 | Phenanthrene-d10 | 17.12 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 90 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 70 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 53 |
| 5 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 50 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM020119\
Data File : BM018713.D
Acq On : 01 Feb 2019 19:25
Operator : JU/SJ
Sample : K1308-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** SB-18(34.5-35)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

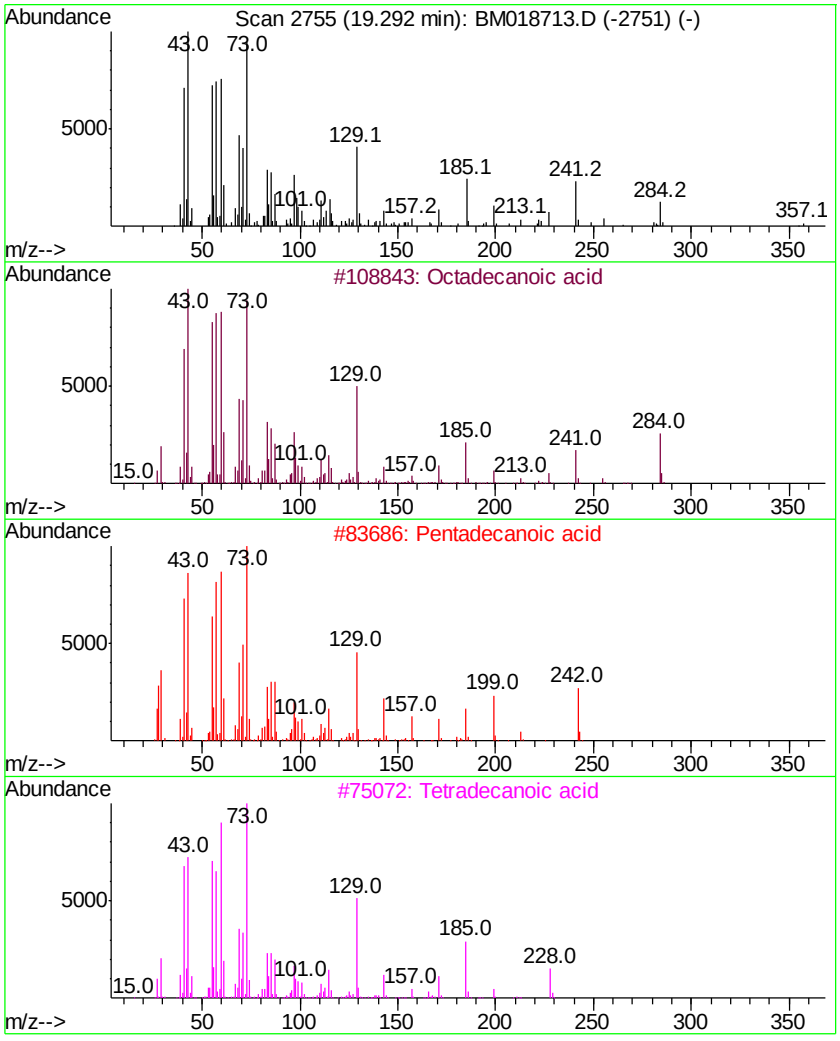
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

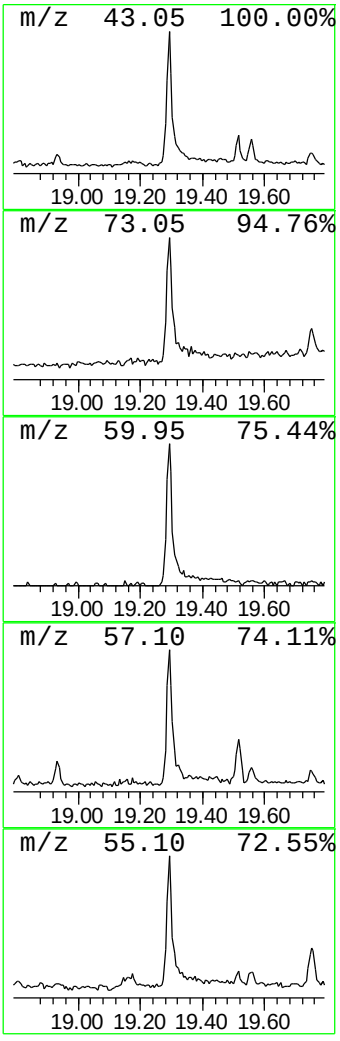
**********

Peak Number 5 Octadecanoic acid Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.29 | 2.38 ng | 347048 | Chrysene-d12 | 21.32 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 97 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 83 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 58 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 58 |
| 5 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 38 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM020119\
Data File : BM018713.D
Acq On : 01 Feb 2019 19:25
Operator : JU/SJ
Sample : K1308-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** SB-18(34.5-35)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

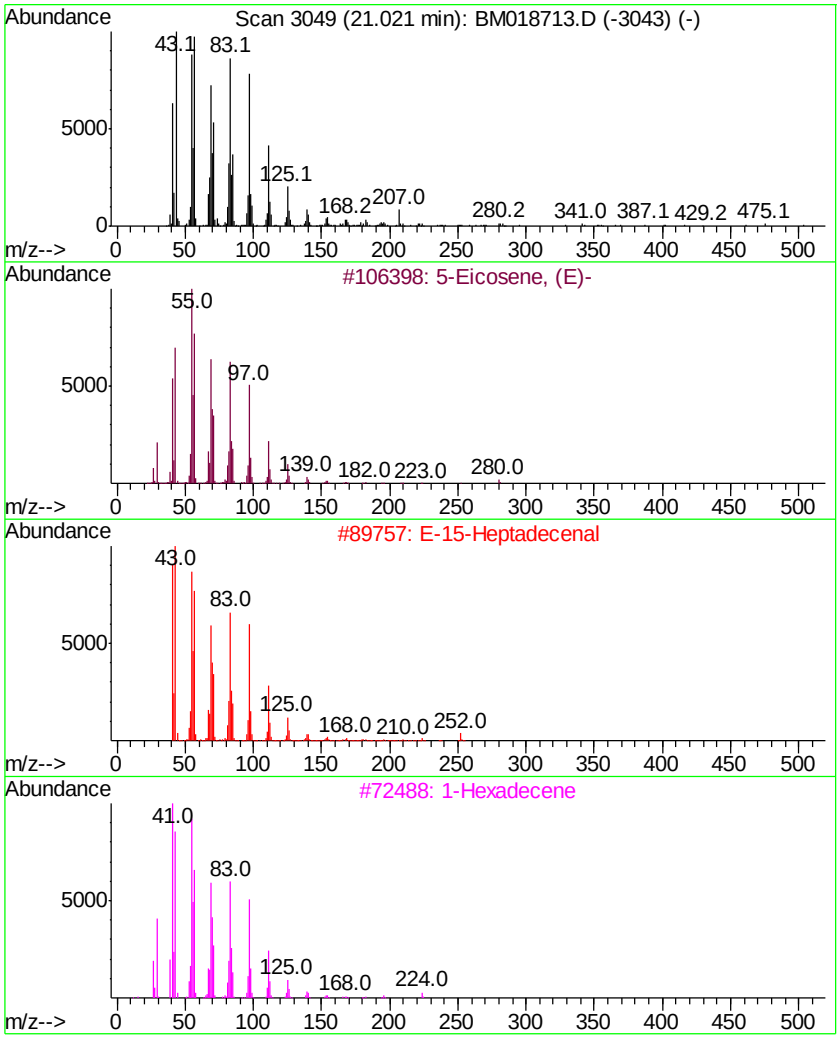
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

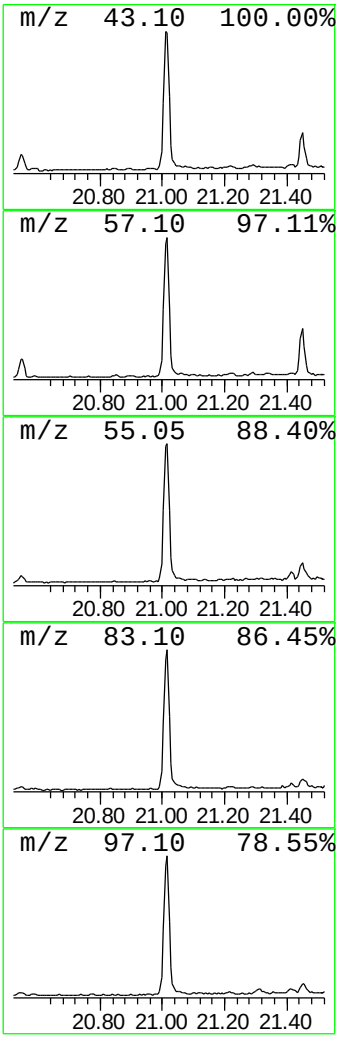
**********

Peak Number 6 5-Eicosene, (E)- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.02 | 9.32 ng | 1358390 | Chrysene-d12 | 21.32 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Eicosene, (E)- | 280 | C20H40 | 074685-30-6 | 97 |
| 2 | E-15-Heptadecenal | 252 | C17H32O | 1000130-97-9 | 97 |
| 3 | 1-Hexadecene | 224 | C16H32 | 000629-73-2 | 95 |
| 4 | Heptafluorobutanoic acid, heptad... | 452 | C21H35F7O2 | 1000282-97-3 | 94 |
| 5 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 93 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM020119\
Data File : BM018713.D
Acq On : 01 Feb 2019 19:25
Operator : JU/SJ
Sample : K1308-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** SB-18(34.5-35)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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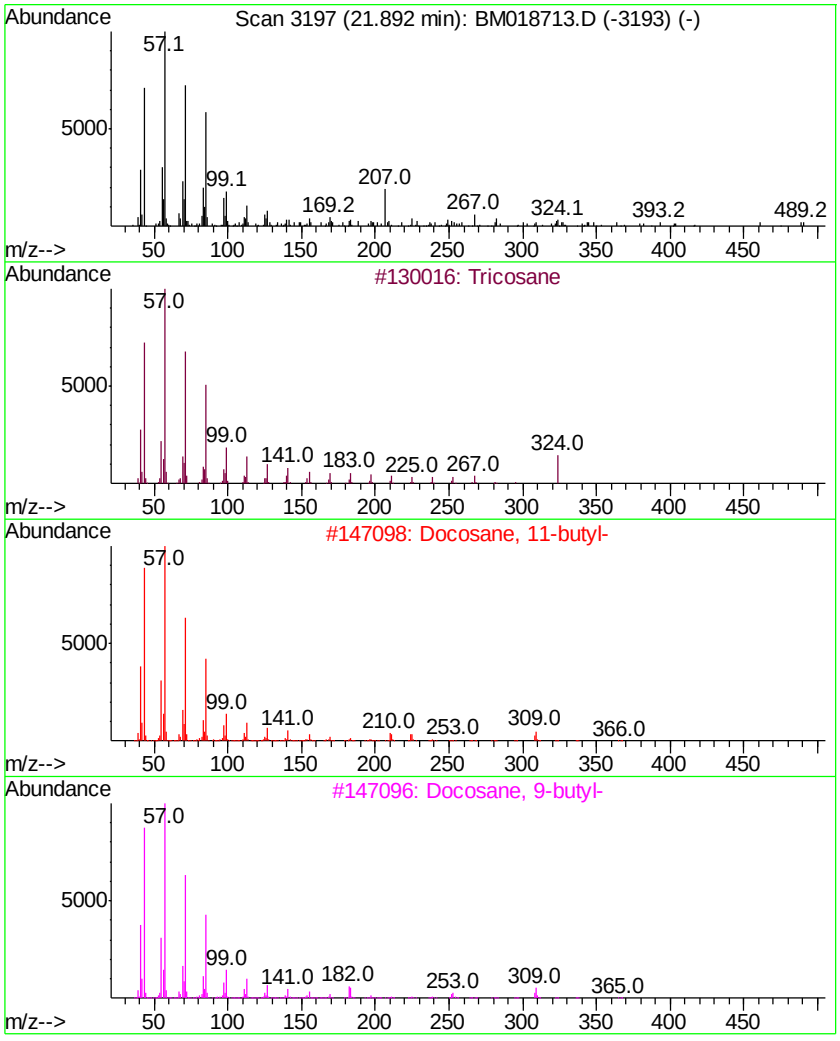
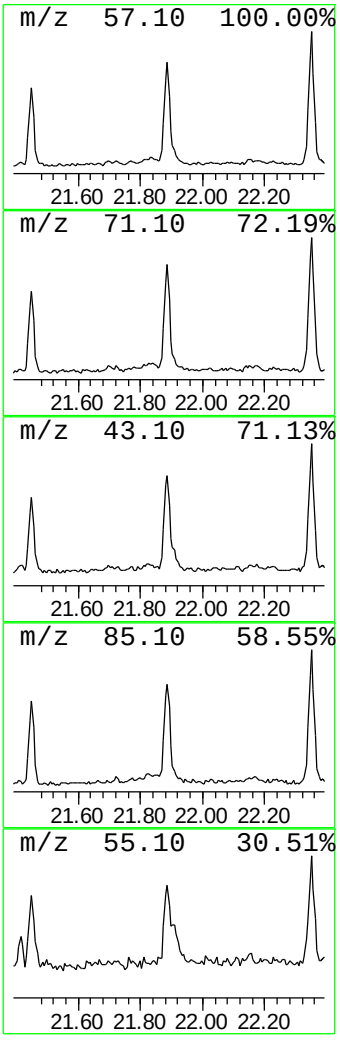
**********

Peak Number 7 Tricosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.89 | 2.71 ng | 395337 | Chrysene-d12 | 21.32 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tricosane | 324 | C23H48 | 000638-67-5 | 95 |
| 2 | Docosane, 11-butyl- | 366 | C26H54 | 013475-76-8 | 94 |
| 3 | Docosane, 9-butyl- | 366 | C26H54 | 055282-14-9 | 93 |
| 4 | Heptadecane, 2,6,10,15-tetramethyl- | 296 | C21H44 | 054833-48-6 | 93 |
| 5 | Eicosane | 282 | C20H42 | 000112-95-8 | 92 |



# Library Search Compound Report

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Data File : BM018713.D
Acq On : 01 Feb 2019 19:25
Operator : JU/SJ
Sample : K1308-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** SB-18(34.5-35)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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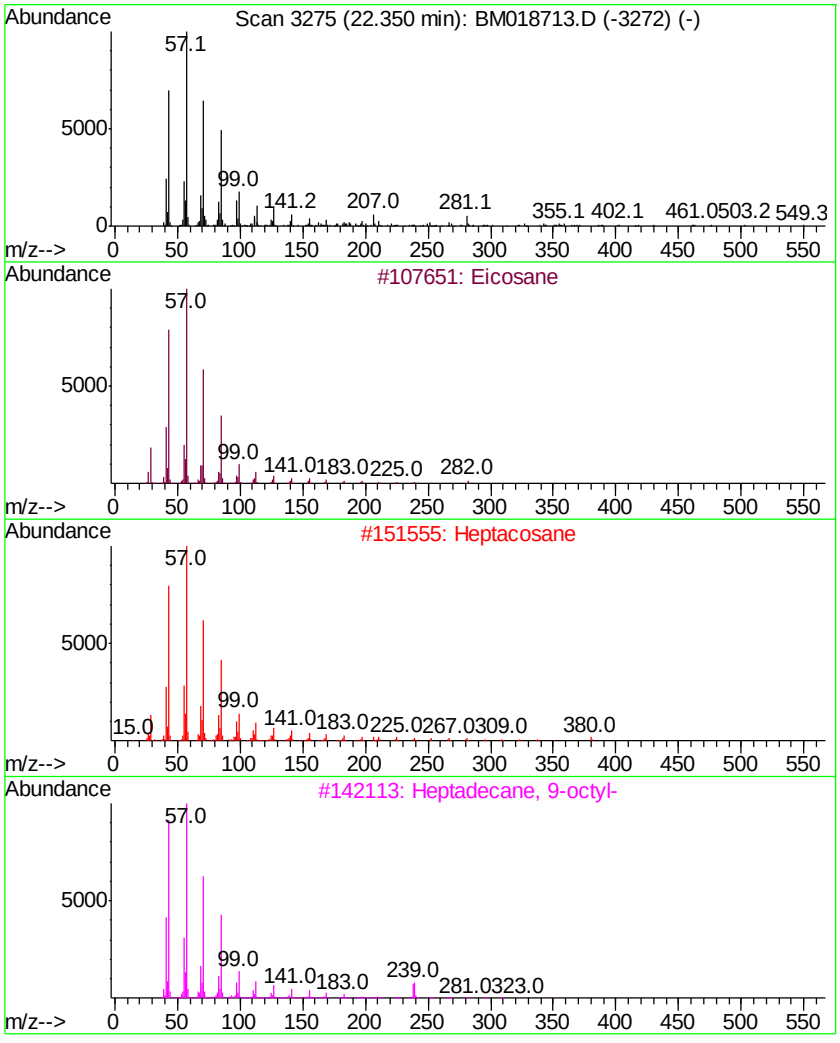
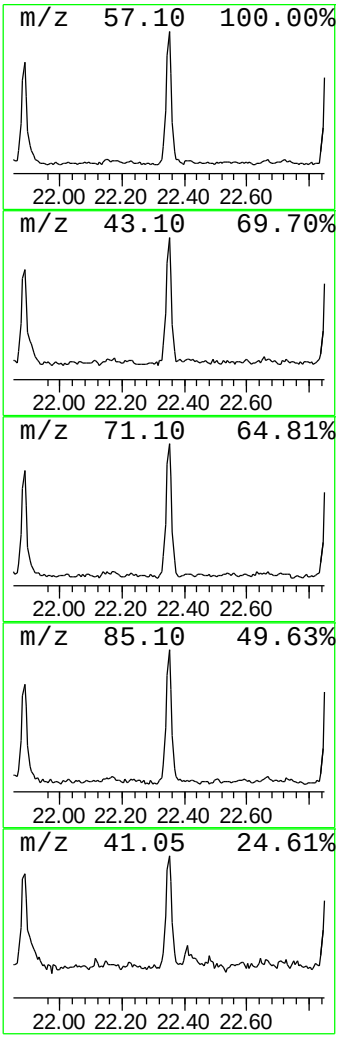
**********

Peak Number 8 Eicosane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.35 | 2.44 ng | 355145 | Chrysene-d12 | 21.32 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 95 |
| 2 | Heptacosane | 380 | C27H56 | 000593-49-7 | 91 |
| 3 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 90 |
| 4 | Heneicosane | 296 | C21H44 | 000629-94-7 | 90 |
| 5 | Triacontane | 422 | C30H62 | 000638-68-6 | 90 |



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Sample : K1308-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** SB-18(34.5-35)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
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TIC Library : C:\DATABASE\NIST02.L
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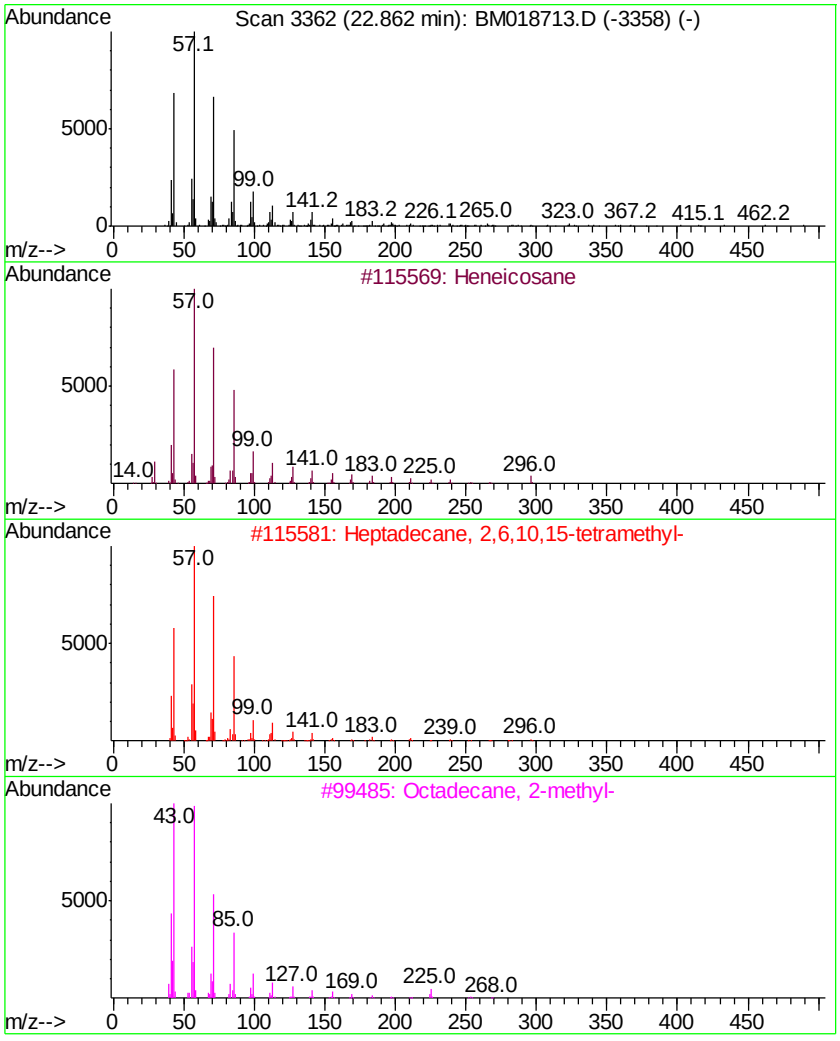
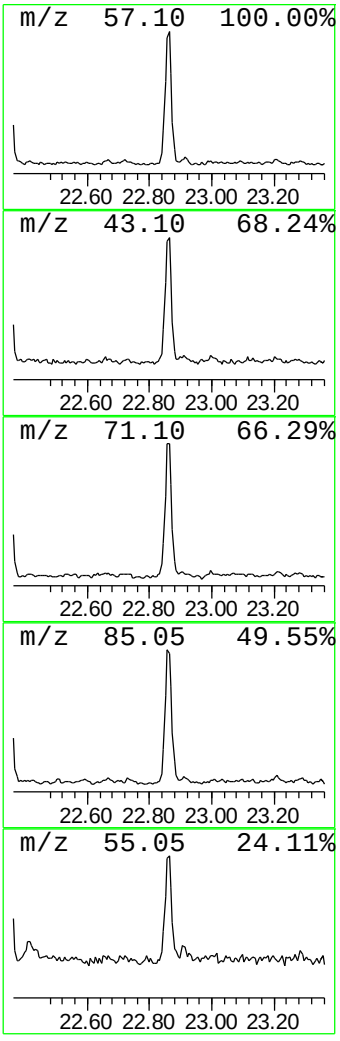
**********

Peak Number 9 Heneicosane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.86 | 2.54 ng | 402156 | Perylene-d12 | 23.57 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 96 |
| 2 | Heptadecane, 2,6,10,15-tetramethyl- | 296 | C21H44 | 054833-48-6 | 93 |
| 3 | Octadecane, 2-methyl- | 268 | C19H40 | 001560-88-9 | 93 |
| 4 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |
| 5 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM020119\
Data File : BM018713.D
Acq On : 01 Feb 2019 19:25
Operator : JU/SJ
Sample : K1308-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** SB-18(34.5-35)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

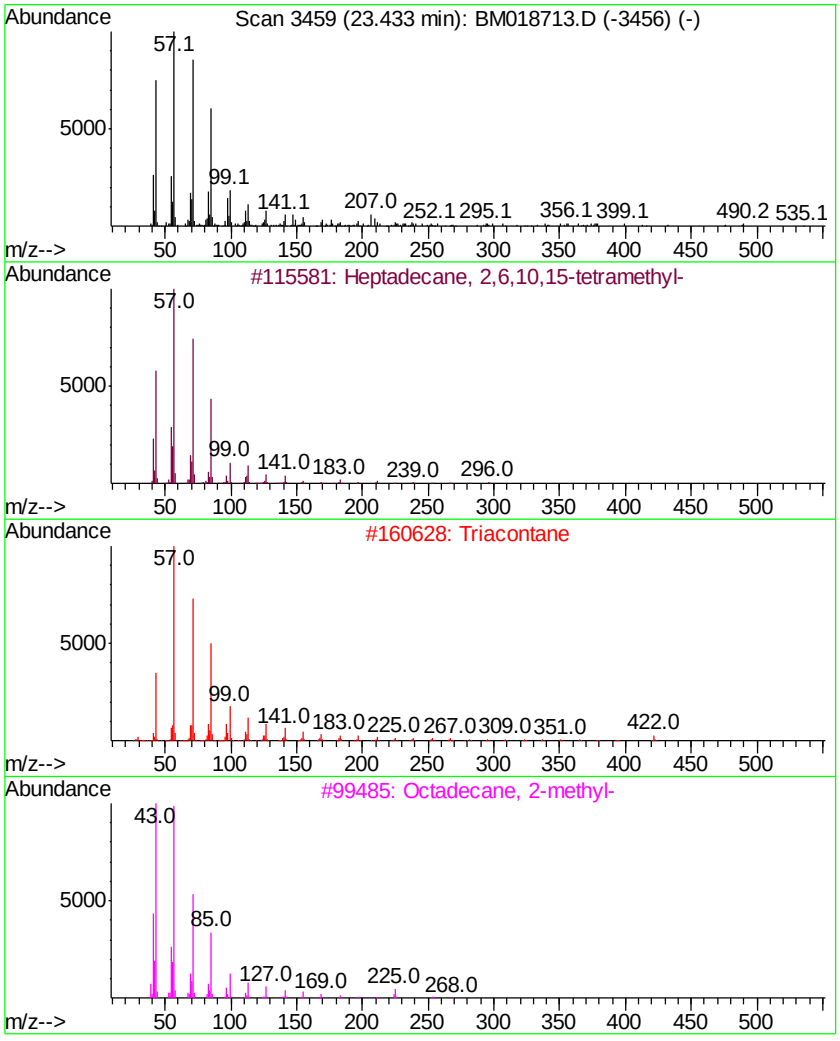
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

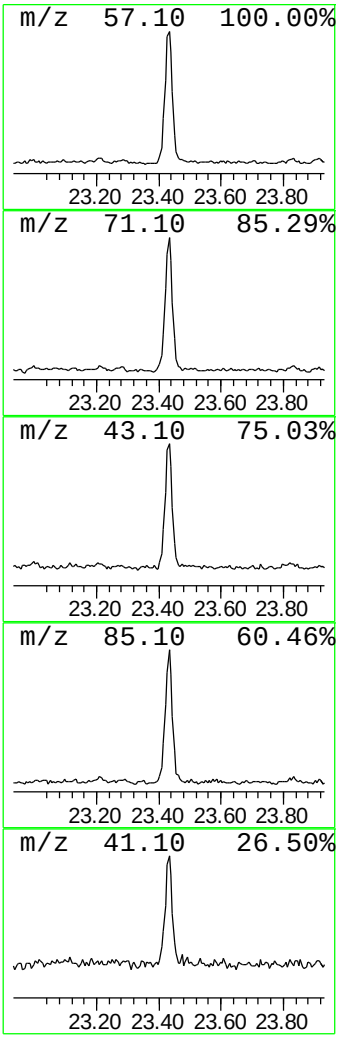
**********

Peak Number 10 Heptadecane, 2,6,10,15-tetr... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.43 | 2.65 ng | 420244 | Perylene-d12 | 23.57 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane, 2,6,10,15-tetramethyl- | 296 | C21H44 | 054833-48-6 | 93 |
| 2 | Triacontane | 422 | C30H62 | 000638-68-6 | 90 |
| 3 | Octadecane, 2-methyl- | 268 | C19H40 | 001560-88-9 | 90 |
| 4 | Docosane | 310 | C22H46 | 000629-97-0 | 87 |
| 5 | Pentadecane, 8-heptyl- | 310 | C22H46 | 071005-15-7 | 87 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM020119\
Data File : BM018713.D
Acq On : 01 Feb 2019 19:25
Operator : JU/SJ
Sample : K1308-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** SB-18(34.5-35)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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... | 4.87 | 4.8 | ng | 351115 | 1 | 7.72 | 1456920 | 20.0 |
| unknown7.26 | 7.26 | 112.7 | ng | 8207490 | 1 | 7.72 | 1456920 | 20.0 |
| n-Hexadecanoic acid | 18.01 | 8.5 | ng | 1056190 | 4 | 17.12 | 2472250 | 20.0 |
| Octadecanoic acid | 19.29 | 2.4 | ng | 347048 | 5 | 21.32 | 2915240 | 20.0 |
| 5-Eicosene, (E)- | 21.02 | 9.3 | ng | 1358390 | 5 | 21.32 | 2915240 | 20.0 |
| Tricosane | 21.89 | 2.7 | ng | 395337 | 5 | 21.32 | 2915240 | 20.0 |
| Eicosane | 22.35 | 2.4 | ng | 355145 | 5 | 21.32 | 2915240 | 20.0 |
| Heneicosane | 22.86 | 2.5 | ng | 402156 | 6 | 23.57 | 3166510 | 20.0 |
| Heptadecane, 2,6,... | 23.43 | 2.6 | ng | 420244 | 6 | 23.57 | 3166510 | 20.0 |