LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073124\
Data File : BF138696.D
Acq On : 31 Jul 2024 11:31
Operator : RC/JU
Sample : PB162317BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB162317BL

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_F\Methods\8270-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138696.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.216 | 15 | 21 | 29 | rVB | 703628 | 1579062 | 56.81% | 8.993% |
| 2 | 5.069 | 499 | 506 | 528 | rVB | 779353 | 1235621 | 44.45% | 7.037% |
| 3 | 5.475 | 570 | 575 | 593 | rBV | 1184756 | 1544568 | 55.56% | 8.797% |
| 4 | 5.651 | 600 | 605 | 614 | rVB2 | 56230 | 87559 | 3.15% | 0.499% |
| 5 | 6.098 | 676 | 681 | 688 | rBV | 102188 | 137203 | 4.94% | 0.781% |
| 6 | 6.481 | 740 | 746 | 759 | rBV | 1211264 | 1616865 | 58.17% | 9.209% |
| 7 | 6.840 | 802 | 807 | 812 | rBV | 352288 | 450835 | 16.22% | 2.568% |
| 8 | 6.998 | 829 | 834 | 850 | rVB | 111205 | 145006 | 5.22% | 0.826% |
| 9 | 7.404 | 897 | 903 | 909 | rBV | 1134139 | 1582057 | 56.91% | 9.010% |
| 10 | 8.122 | 1020 | 1025 | 1030 | rVB | 479504 | 609657 | 21.93% | 3.472% |
| 11 | 9.198 | 1201 | 1208 | 1213 | rBV | 2100726 | 2779785 | 100.00% | 15.832% |
| 12 | 9.875 | 1318 | 1323 | 1336 | rVB | 552031 | 686664 | 24.70% | 3.911% |
| 13 | 10.663 | 1452 | 1457 | 1470 | rBV | 707791 | 938735 | 33.77% | 5.346% |
| 14 | 11.363 | 1571 | 1576 | 1581 | rBV | 579663 | 706745 | 25.42% | 4.025% |
| 15 | 12.951 | 1840 | 1846 | 1851 | rBV | 1848520 | 2462450 | 88.58% | 14.024% |
| 16 | 13.998 | 2019 | 2024 | 2035 | rBV | 311084 | 409269 | 14.72% | 2.331% |
| 17 | 15.463 | 2267 | 2273 | 2286 | rVB | 247125 | 403856 | 14.53% | 2.300% |
| 18 | 15.910 | 2343 | 2349 | 2357 | rBV | 28770 | 48744 | 1.75% | 0.278% |
| 19 | 16.410 | 2428 | 2434 | 2442 | rVB | 29574 | 52790 | 1.90% | 0.301% |
| 20 | 16.998 | 2527 | 2534 | 2543 | rVB | 20651 | 45600 | 1.64% | 0.260% |
| 21 | 17.698 | 2646 | 2653 | 2660 | rVB2 | 14969 | 35269 | 1.27% | 0.201% |

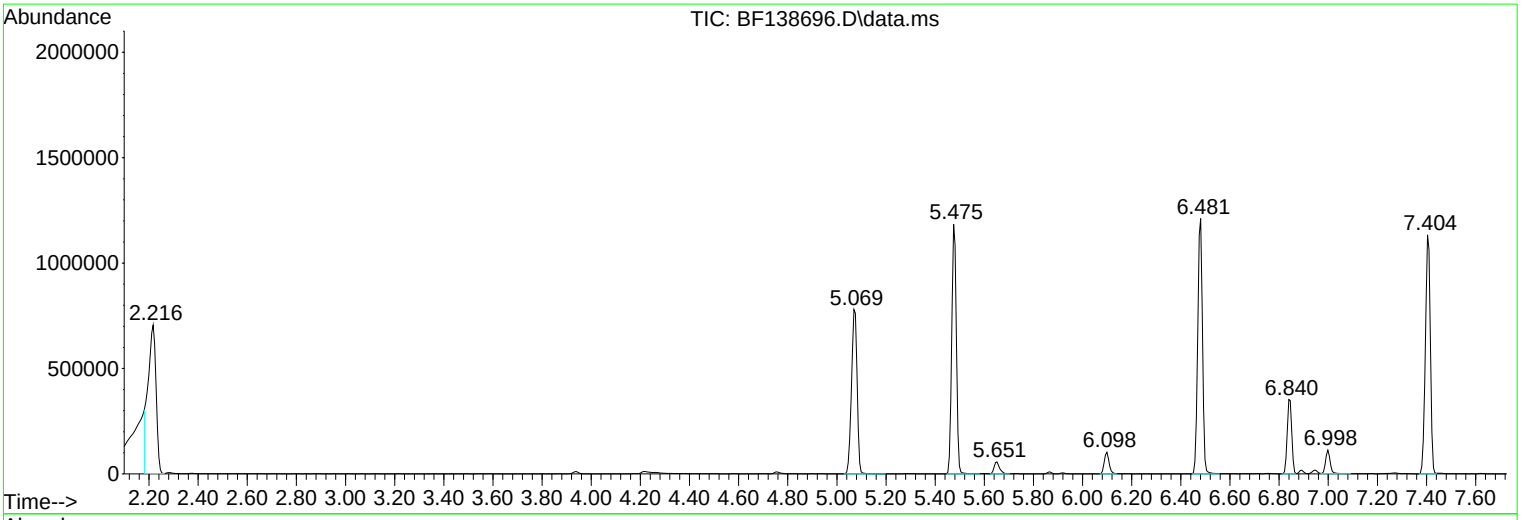
Sum of corrected areas: 17558340

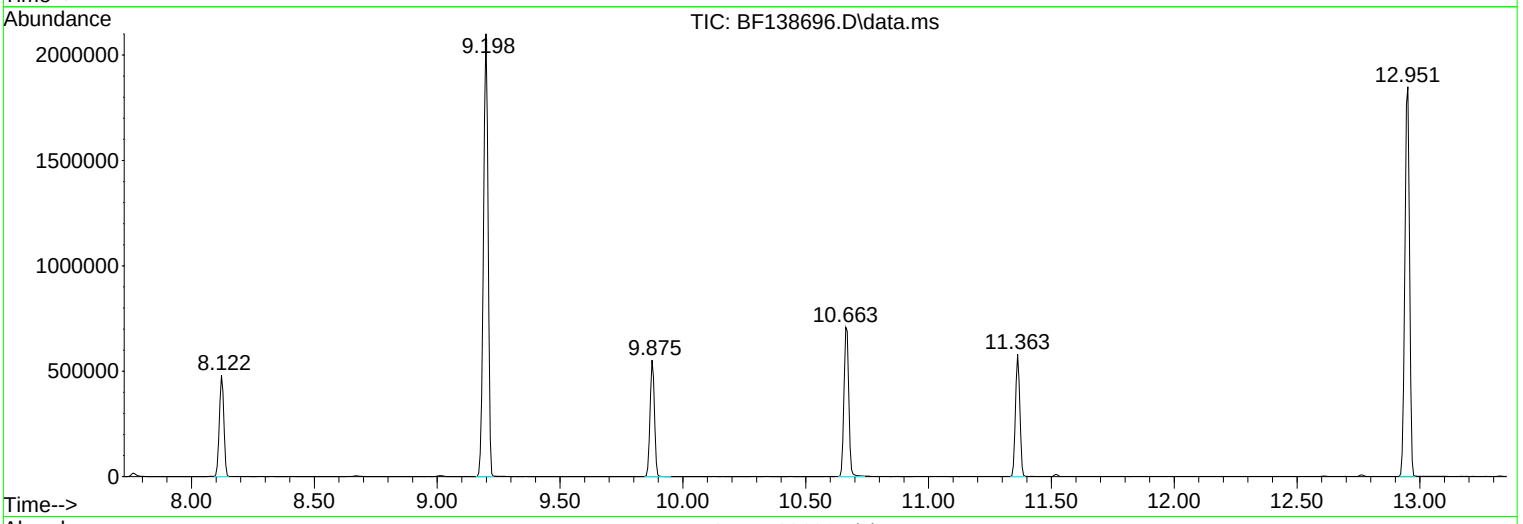
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073124\
Data File : BF138696.D
Acq On : 31 Jul 2024 11:31
Operator : RC/JU
Sample : PB162317BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

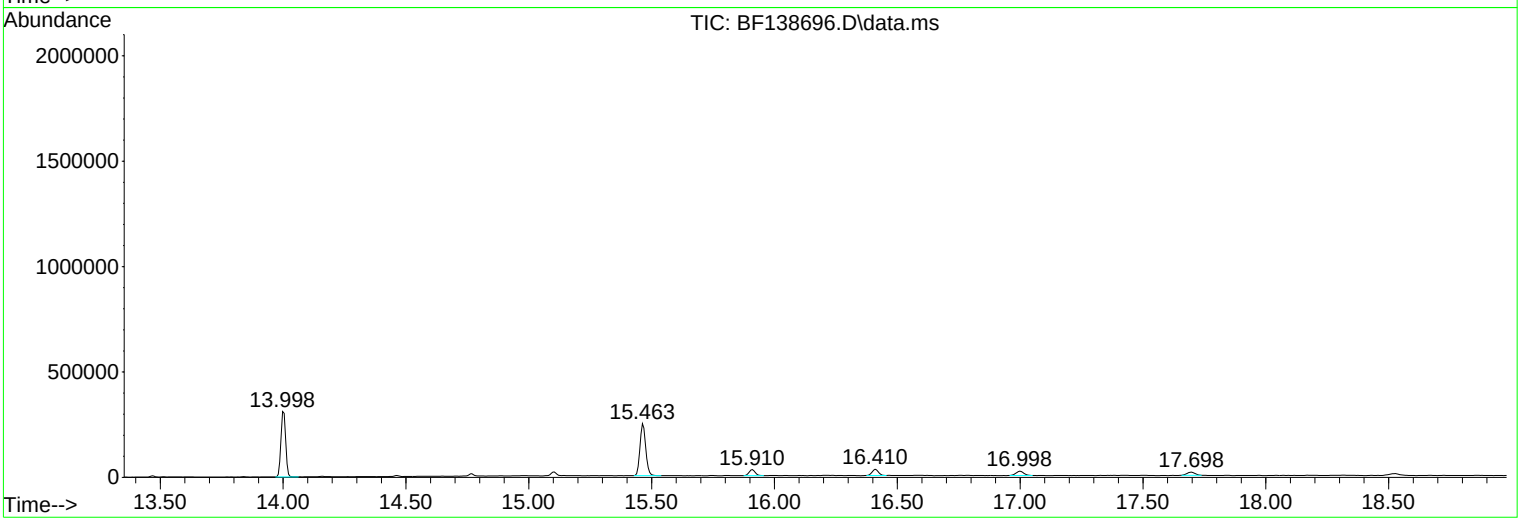
**Instrument :**
BNA_F
**ClientSampleId :**
PB162317BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073124\
Data File : BF138696.D
Acq On : 31 Jul 2024 11:31
Operator : RC/JU
Sample : PB162317BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB162317BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

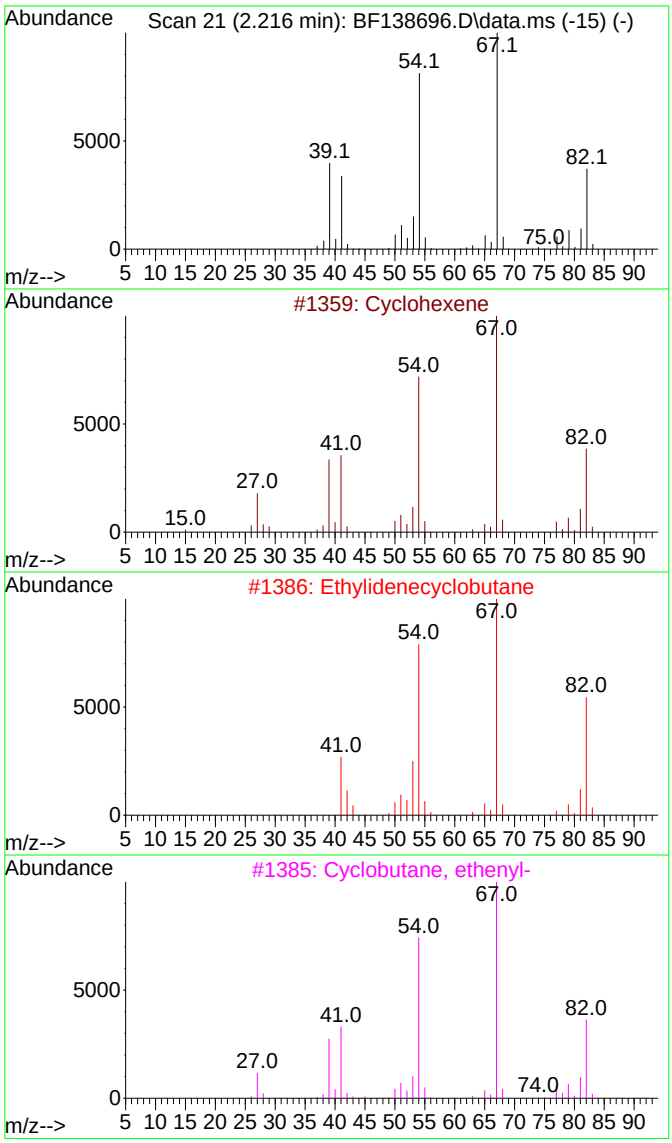
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

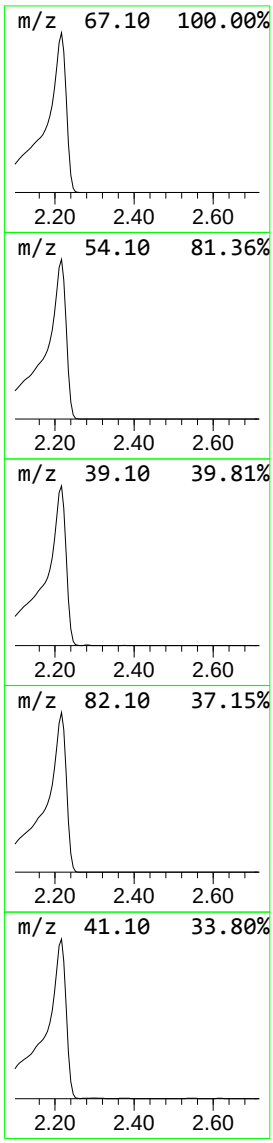
**********

Peak Number 1 Cyclohexene Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.216 | 70.05 ng | 1579060 | 1,4-Dichlorobenzene-d4 | 6.845 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexene | 82 | C6H10 | 000110-83-8 | 94 |
| 2 | Ethylidenecyclobutane | 82 | C6H10 | 001528-21-8 | 91 |
| 3 | Cyclobutane, ethenyl- | 82 | C6H10 | 002597-49-1 | 90 |
| 4 | C2H5CH=CHCH=CH2 | 82 | C6H10 | 000592-48-3 | 38 |
| 5 | 1,3-Pentadiene, 2-methyl-, (E)- | 82 | C6H10 | 000926-54-5 | 38 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073124\
Data File : BF138696.D
Acq On : 31 Jul 2024 11:31
Operator : RC/JU
Sample : PB162317BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB162317BL

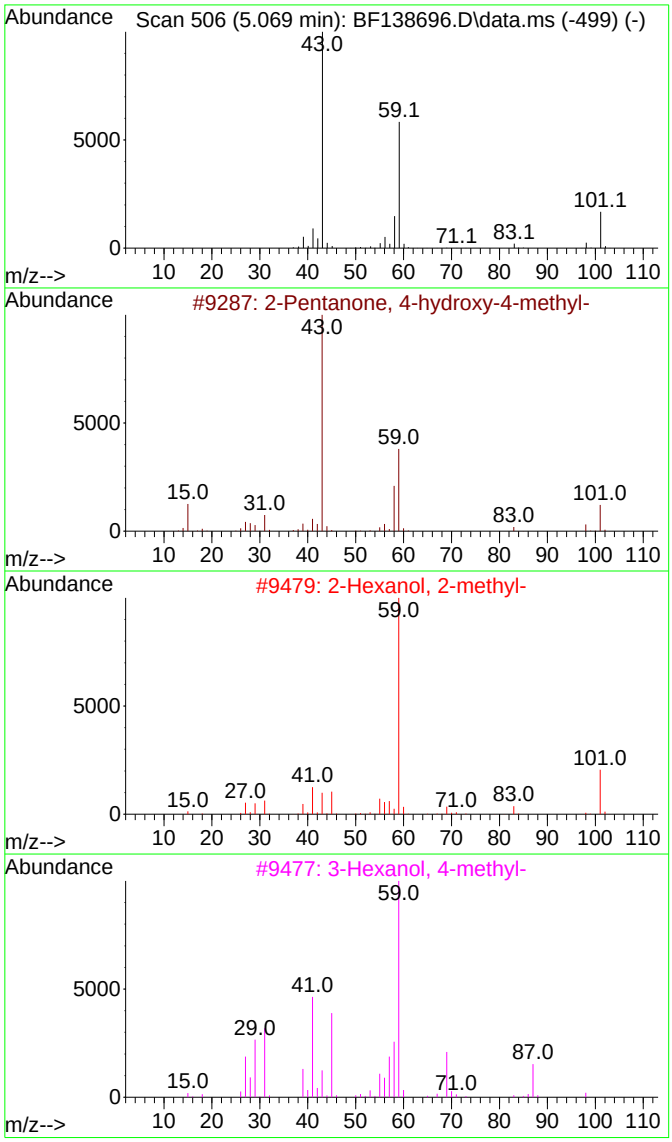
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

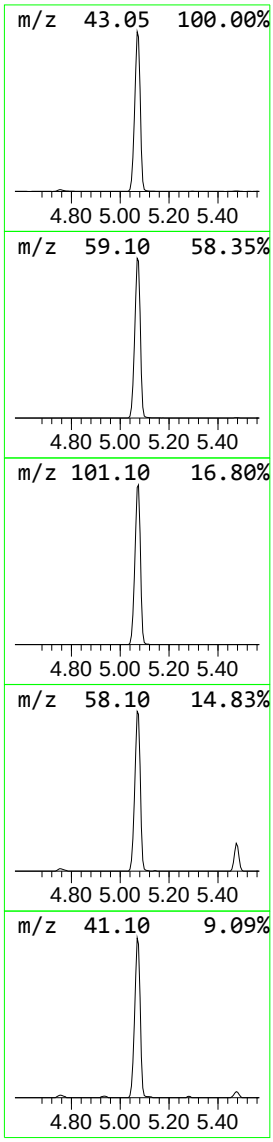
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.069 | 54.81 ng | 1235620 | 1,4-Dichlorobenzene-d4 | 6.845 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 33 |
| 3 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 32 |
| 5 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 12 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073124\
Data File : BF138696.D
Acq On : 31 Jul 2024 11:31
Operator : RC/JU
Sample : PB162317BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB162317BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

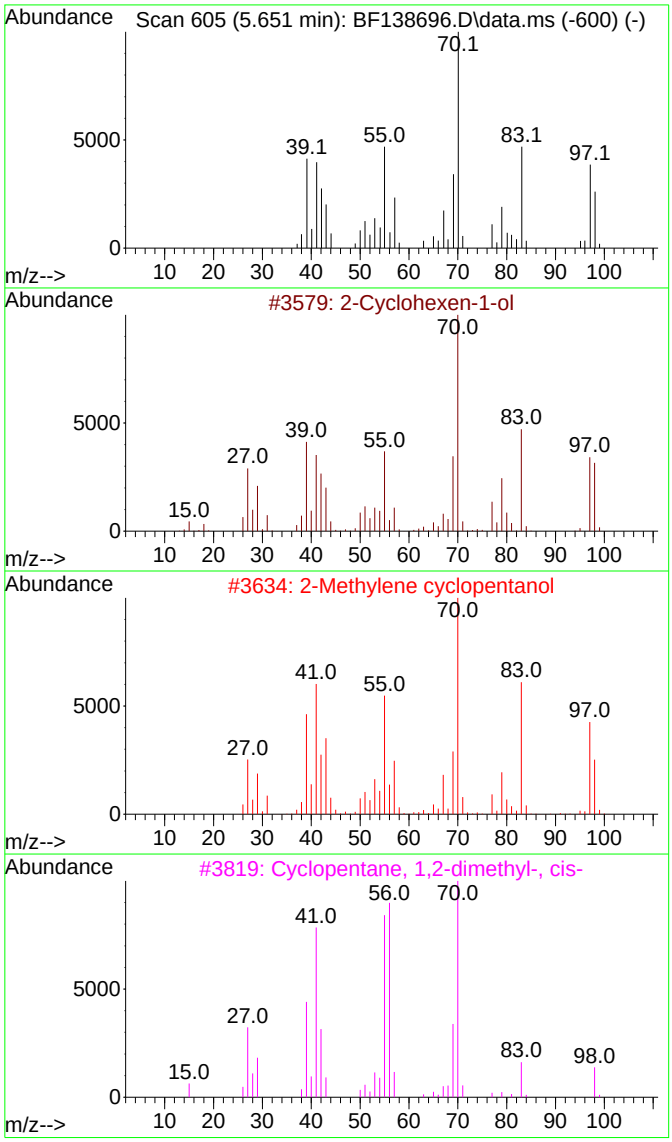
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

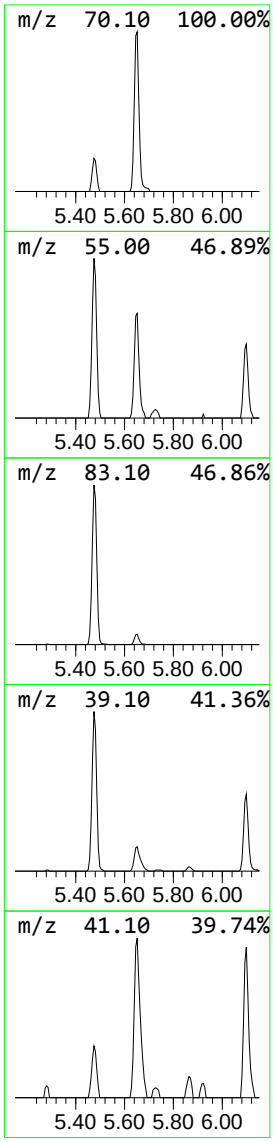
**********

Peak Number 3 2-Cyclohexen-1-ol Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.651 | 3.88 ng | 87559 | 1,4-Dichlorobenzene-d4 | 6.845 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Cyclohexen-1-ol | 98 | C6H10O | 000822-67-3 | 96 |
| 2 | 2-Methylene cyclopentanol | 98 | C6H10O | 020461-31-8 | 90 |
| 3 | Cyclopentane, 1,2-dimethyl-, cis- | 98 | C7H14 | 001192-18-3 | 37 |
| 4 | 2-Butenal, (Z)- | 70 | C4H6O | 015798-64-8 | 35 |
| 5 | Cyclopentane, 1,3-dimethyl-, cis- | 98 | C7H14 | 002532-58-3 | 35 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073124\
Data File : BF138696.D
Acq On : 31 Jul 2024 11:31
Operator : RC/JU
Sample : PB162317BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB162317BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

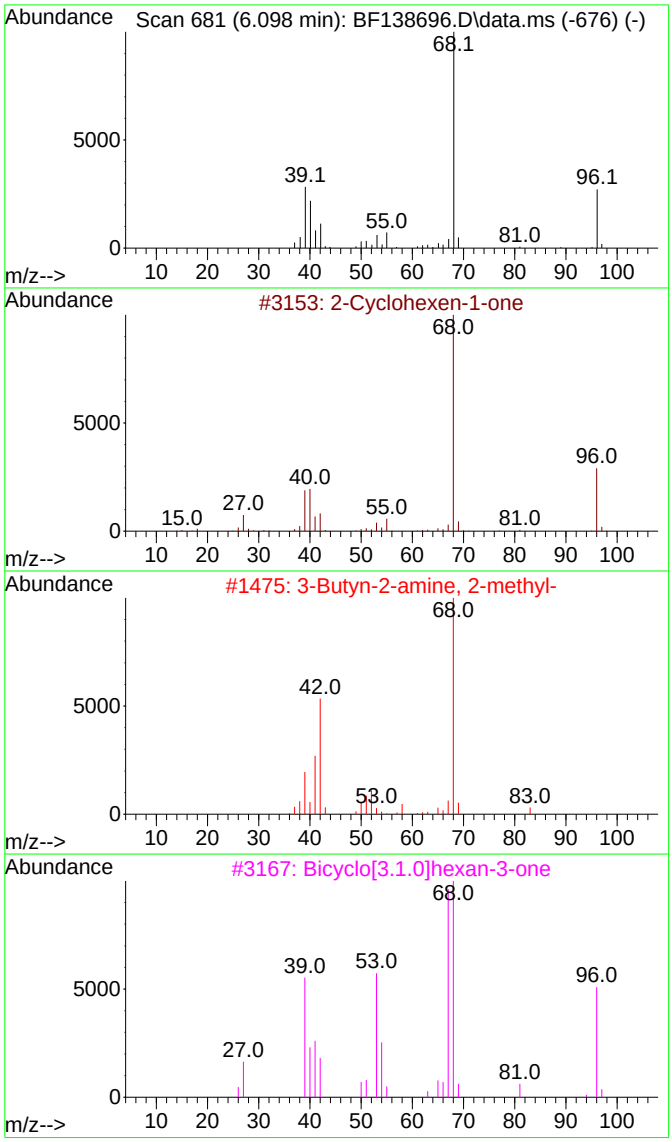
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

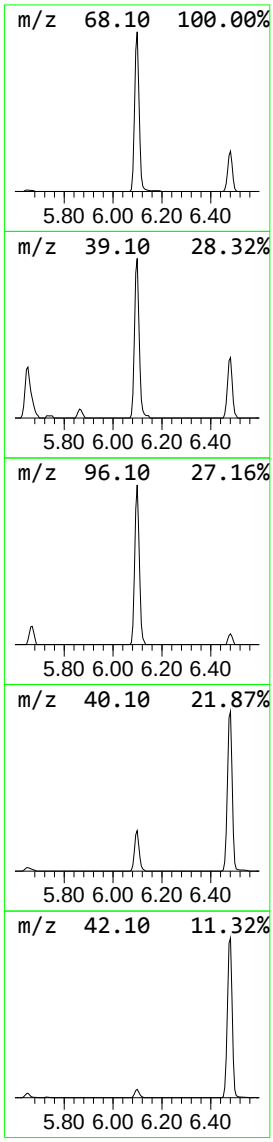
**********

Peak Number 4 2-Cyclohexen-1-one Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.098 | 6.09 ng | 137203 | 1,4-Dichlorobenzene-d4 | 6.845 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Cyclohexen-1-one | 96 | C6H8O | 000930-68-7 | 91 |
| 2 | 3-Butyn-2-amine, 2-methyl- | 83 | C5H9N | 002978-58-7 | 45 |
| 3 | Bicyclo[3.1.0]hexan-3-one | 96 | C6H8O | 001755-04-0 | 43 |
| 4 | 7-Oxabicyclo[2.2.1]hept-5-en-2-one | 110 | C6H6O2 | 095530-78-2 | 42 |
| 5 | 1H-Pyrazole | 68 | C3H4N2 | 000288-13-1 | 36 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073124\
Data File : BF138696.D
Acq On : 31 Jul 2024 11:31
Operator : RC/JU
Sample : PB162317BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB162317BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

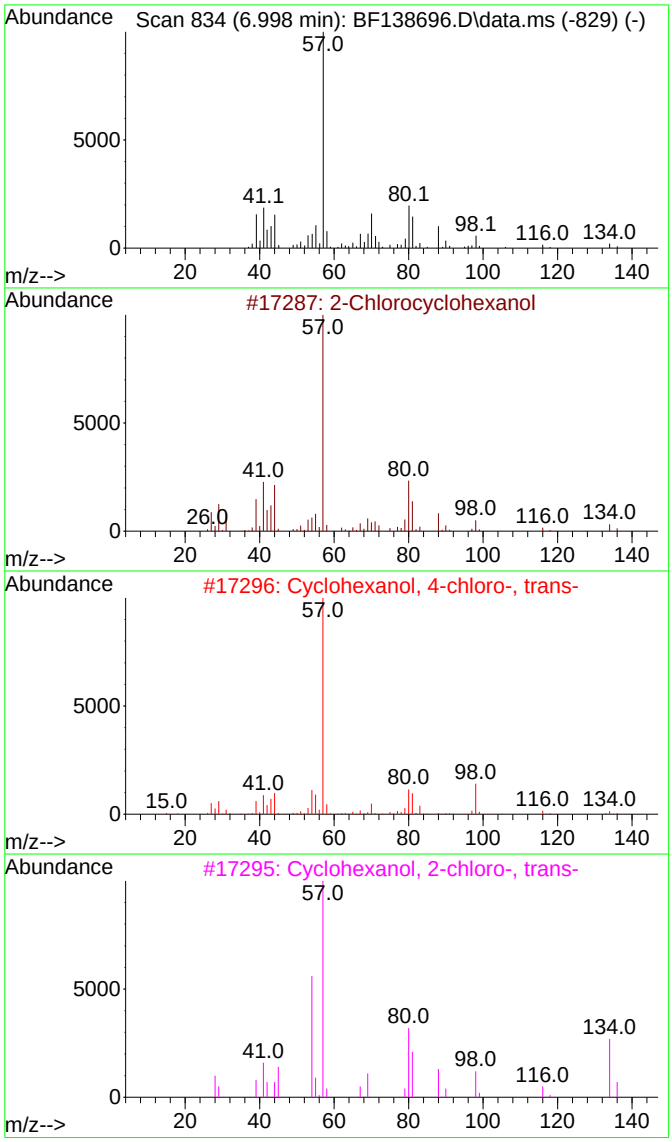
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

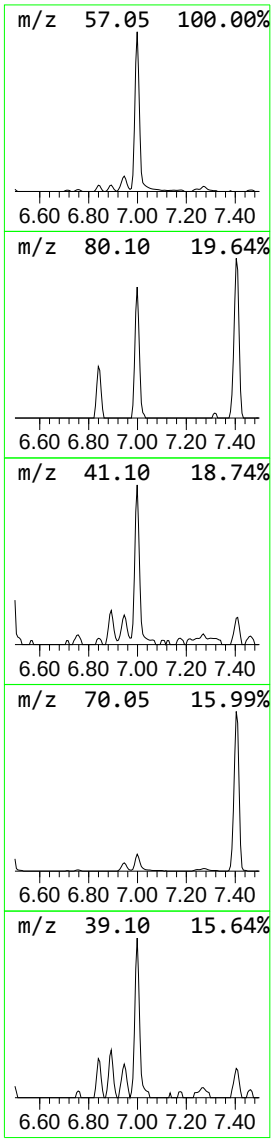
**********

Peak Number 5 2-Chlorocyclohexanol Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.998 | 6.43 ng | 145006 | 1,4-Dichlorobenzene-d4 | 6.845 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Chlorocyclohexanol | 134 | C6H11ClO | 001561-86-0 | 93 |
| 2 | Cyclohexanol, 4-chloro-, trans- | 134 | C6H11ClO | 029538-77-0 | 47 |
| 3 | Cyclohexanol, 2-chloro-, trans- | 134 | C6H11ClO | 006628-80-4 | 47 |
| 4 | 3-Furanol, tetrahydro- | 88 | C4H8O2 | 000453-20-3 | 32 |
| 5 | Oxalic acid, isobutyl heptyl ester | 244 | C13H24O4 | 1000309-37-2 | 22 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073124\
Data File : BF138696.D
Acq On : 31 Jul 2024 11:31
Operator : RC/JU
Sample : PB162317BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB162317BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

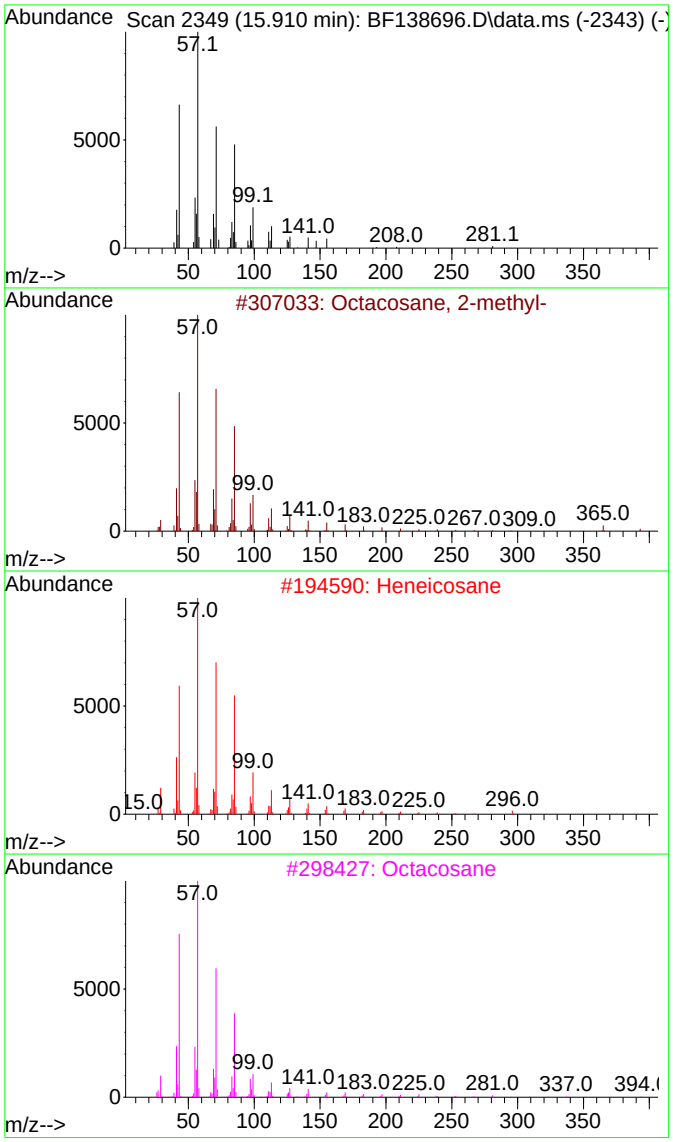
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

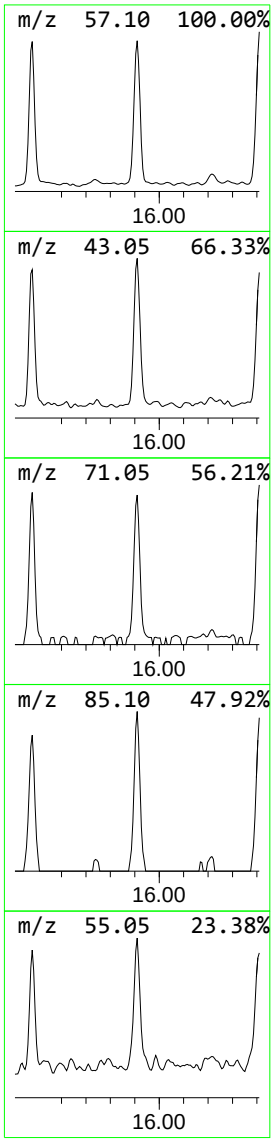
**********

Peak Number 6 Octacosane, 2-methyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.910 | 2.41 ng | 48744 | Perylene-d12 | 15.463 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane, 2-methyl- | 408 | C29H60 | 001560-98-1 | 91 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 4 | Eicosane, 9-octyl- | 394 | C28H58 | 013475-77-9 | 90 |
| 5 | Hexacosane | 366 | C26H54 | 000630-01-3 | 87 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073124\
Data File : BF138696.D
Acq On : 31 Jul 2024 11:31
Operator : RC/JU
Sample : PB162317BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB162317BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

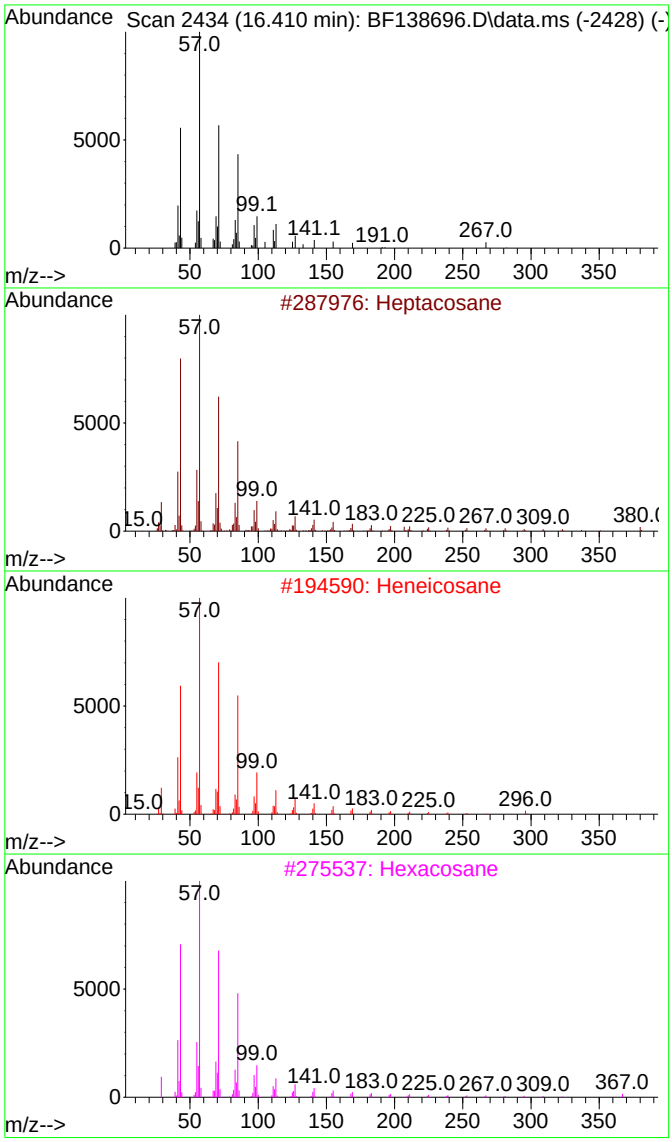
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

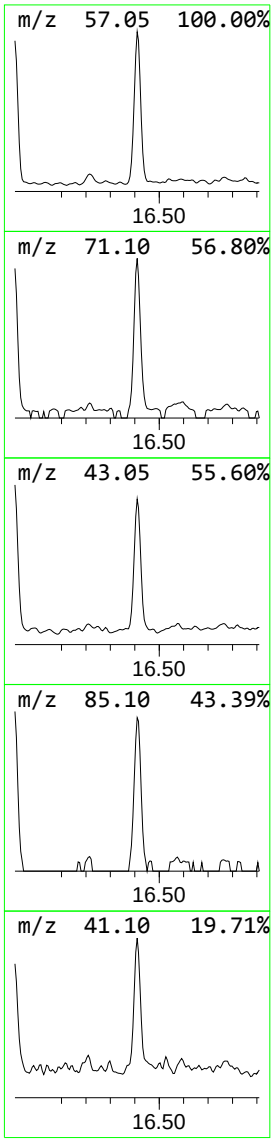
**********

Peak Number 7 Heptacosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.410 | 2.61 ng | 52790 | Perylene-d12 | 15.463 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptacosane | 380 | C27H56 | 000593-49-7 | 91 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 4 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 91 |
| 5 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073124\
Data File : BF138696.D
Acq On : 31 Jul 2024 11:31
Operator : RC/JU
Sample : PB162317BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB162317BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

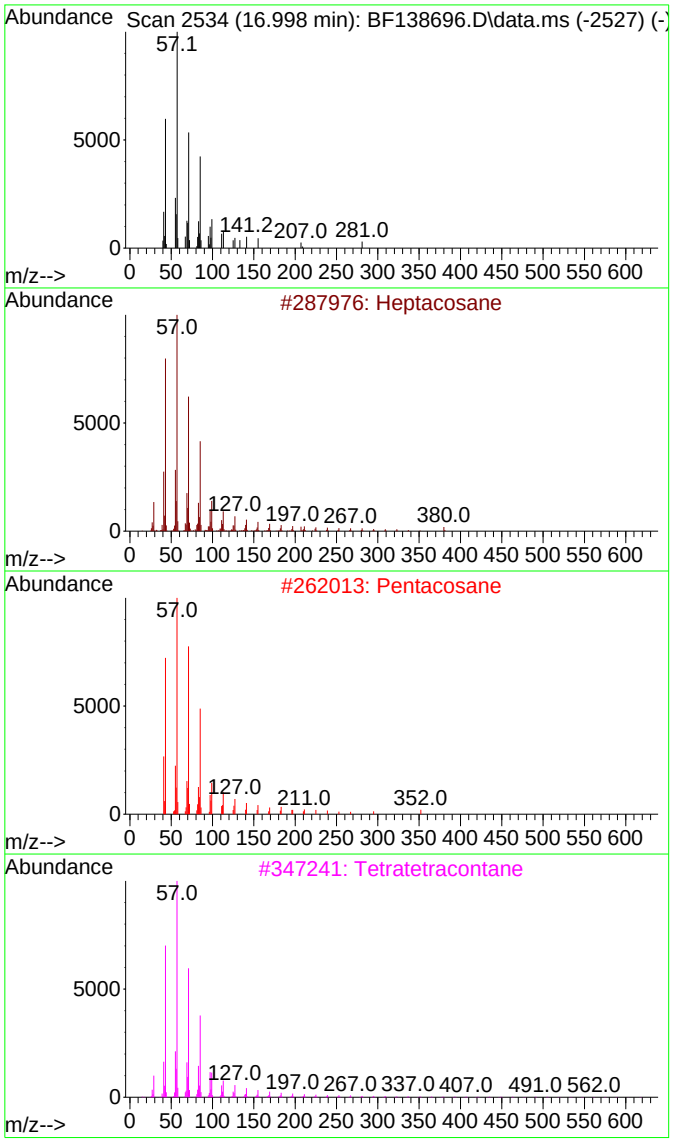
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

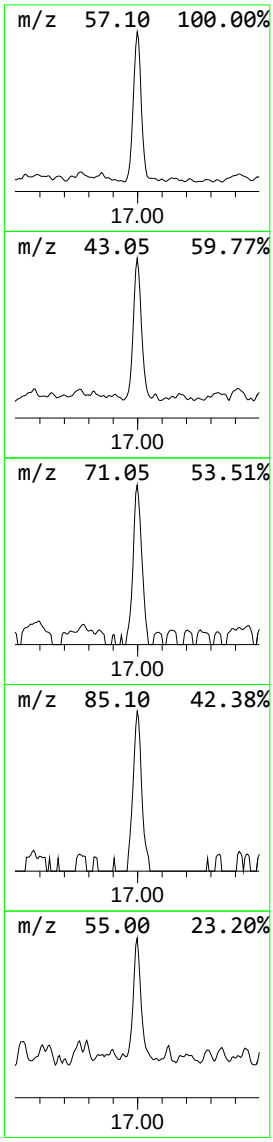
**********

Peak Number 8 Pentacosane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.998 | 2.26 ng | 45600 | Perylene-d12 | 15.463 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptacosane | 380 | C27H56 | 000593-49-7 | 91 |
| 2 | Pentacosane | 352 | C25H52 | 000629-99-2 | 91 |
| 3 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 91 |
| 4 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 5 | Tetracosane | 338 | C24H50 | 000646-31-1 | 87 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073124\
Data File : BF138696.D
Acq On : 31 Jul 2024 11:31
Operator : RC/JU
Sample : PB162317BL
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB162317BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Cyclohexene | 2.216 | 70.0 | ng | 1579060 | 1 | 6.845 | 450835 | 20.0 |
| 2-Pentanone, 4-... | 5.069 | 54.8 | ng | 1235620 | 1 | 6.845 | 450835 | 20.0 |
| 2-Cyclohexen-1-ol | 5.651 | 3.9 | ng | 87559 | 1 | 6.845 | 450835 | 20.0 |
| 2-Cyclohexen-1-one | 6.098 | 6.1 | ng | 137203 | 1 | 6.845 | 450835 | 20.0 |
| 2-Chlorocyclohe... | 6.998 | 6.4 | ng | 145006 | 1 | 6.845 | 450835 | 20.0 |
| Octacosane, 2-m... | 15.910 | 2.4 | ng | 48744 | 6 | 15.463 | 403856 | 20.0 |
| Heptacosane | 16.410 | 2.6 | ng | 52790 | 6 | 15.463 | 403856 | 20.0 |
| Pentacosane | 16.998 | 2.3 | ng | 45600 | 6 | 15.463 | 403856 | 20.0 |