LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131160.D
Acq On : 11 Nov 2022 18:44
Operator : CG\JU
Sample : N5506-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-8

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-BF110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131160.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.210 | 14 | 21 | 27 | rVB | 595851 | 783063 | 34.72% | 4.564% |
| 2 | 2.322 | 35 | 40 | 45 | rBV | 44409 | 60110 | 2.67% | 0.350% |
| 3 | 3.446 | 225 | 231 | 243 | rBV2 | 12130 | 28552 | 1.27% | 0.166% |
| 4 | 4.487 | 404 | 408 | 416 | rBV | 81425 | 89067 | 3.95% | 0.519% |
| 5 | 5.104 | 508 | 513 | 525 | rVB | 509369 | 674036 | 29.88% | 3.929% |
| 6 | 5.498 | 575 | 580 | 583 | rBV | 2115758 | 2088962 | 92.62% | 12.176% |
| 7 | 6.504 | 745 | 751 | 754 | rBV | 2056298 | 2135402 | 94.68% | 12.446% |
| 8 | 6.869 | 809 | 813 | 817 | rBV | 754417 | 624270 | 27.68% | 3.639% |
| 9 | 7.439 | 904 | 910 | 913 | rBV | 1639483 | 1605999 | 71.21% | 9.361% |
| 10 | 8.157 | 1026 | 1032 | 1035 | rBV | 889041 | 791605 | 35.10% | 4.614% |
| 11 | 9.233 | 1209 | 1215 | 1218 | rBV | 2762725 | 2255433 | 100.00% | 13.146% |
| 12 | 9.916 | 1325 | 1331 | 1334 | rVB | 1007232 | 818223 | 36.28% | 4.769% |
| 13 | 10.704 | 1461 | 1465 | 1469 | rBV | 1322856 | 1261008 | 55.91% | 7.350% |
| 14 | 11.404 | 1580 | 1584 | 1588 | rBV | 724789 | 606114 | 26.87% | 3.533% |
| 15 | 11.786 | 1645 | 1649 | 1652 | rBV2 | 46948 | 42505 | 1.88% | 0.248% |
| 16 | 11.927 | 1669 | 1673 | 1682 | rBV2 | 32874 | 38300 | 1.70% | 0.223% |
| 17 | 12.498 | 1764 | 1770 | 1776 | rBV | 65701 | 65014 | 2.88% | 0.379% |
| 18 | 12.992 | 1850 | 1854 | 1858 | rBV | 1592173 | 1386232 | 61.46% | 8.080% |
| 19 | 13.557 | 1946 | 1950 | 1953 | rVB2 | 35788 | 30506 | 1.35% | 0.178% |
| 20 | 13.886 | 2003 | 2006 | 2010 | rBV | 45921 | 42230 | 1.87% | 0.246% |
| 21 | 13.939 | 2010 | 2015 | 2024 | rBV5 | 79843 | 208628 | 9.25% | 1.216% |
| 22 | 14.051 | 2031 | 2034 | 2039 | rVB | 565081 | 484067 | 21.46% | 2.821% |
| 23 | 14.145 | 2045 | 2050 | 2055 | rVB | 125627 | 139579 | 6.19% | 0.814% |
| 24 | 14.204 | 2057 | 2060 | 2064 | rBV | 42581 | 38822 | 1.72% | 0.226% |
| 25 | 14.509 | 2109 | 2112 | 2115 | rBV | 38839 | 30609 | 1.36% | 0.178% |
| 26 | 14.809 | 2159 | 2163 | 2168 | rBV3 | 57804 | 99300 | 4.40% | 0.579% |
| 27 | 14.898 | 2175 | 2178 | 2182 | rVB | 152142 | 138779 | 6.15% | 0.809% |
| 28 | 15.168 | 2221 | 2224 | 2230 | rVB2 | 36640 | 42341 | 1.88% | 0.247% |
| 29 | 15.545 | 2283 | 2288 | 2297 | rVB | 317364 | 405227 | 17.97% | 2.362% |
| 30 | 16.168 | 2391 | 2394 | 2401 | rBV8 | 25222 | 48196 | 2.14% | 0.281% |
| 31 | 16.515 | 2450 | 2453 | 2458 | rBV7 | 21090 | 33797 | 1.50% | 0.197% |
| 32 | 16.815 | 2501 | 2504 | 2509 | rVB6 | 20672 | 30433 | 1.35% | 0.177% |
| 33 | 18.162 | 2730 | 2733 | 2736 | rBV5 | 16479 | 30542 | 1.35% | 0.178% |

Sum of corrected areas: 17156951

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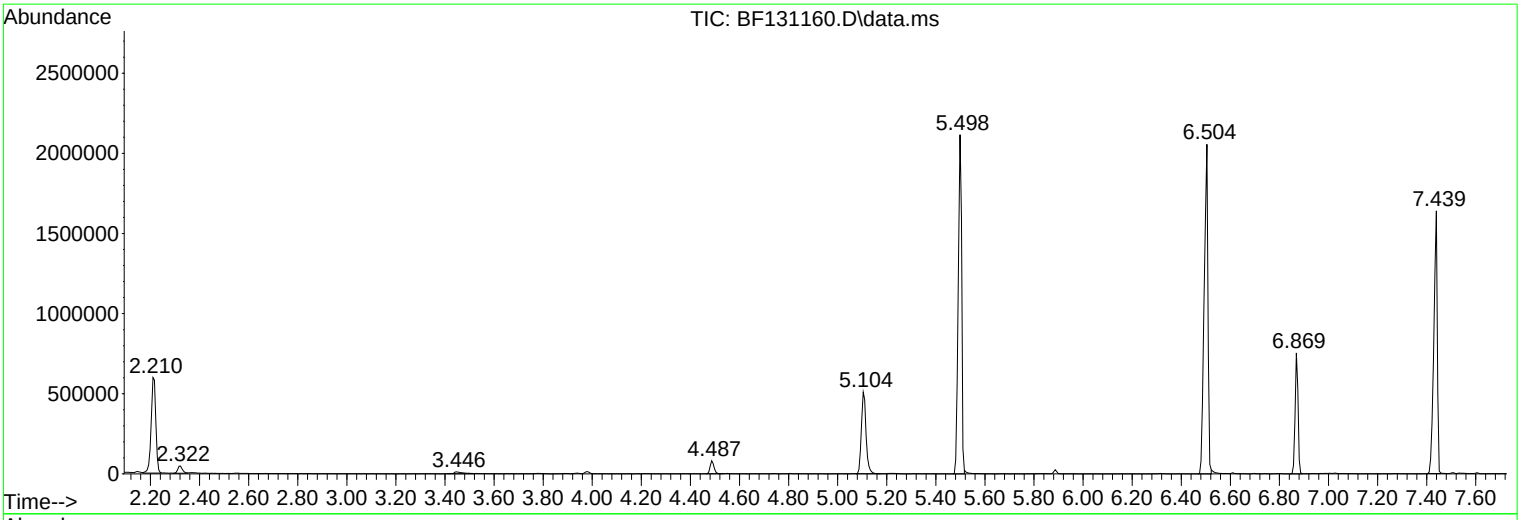
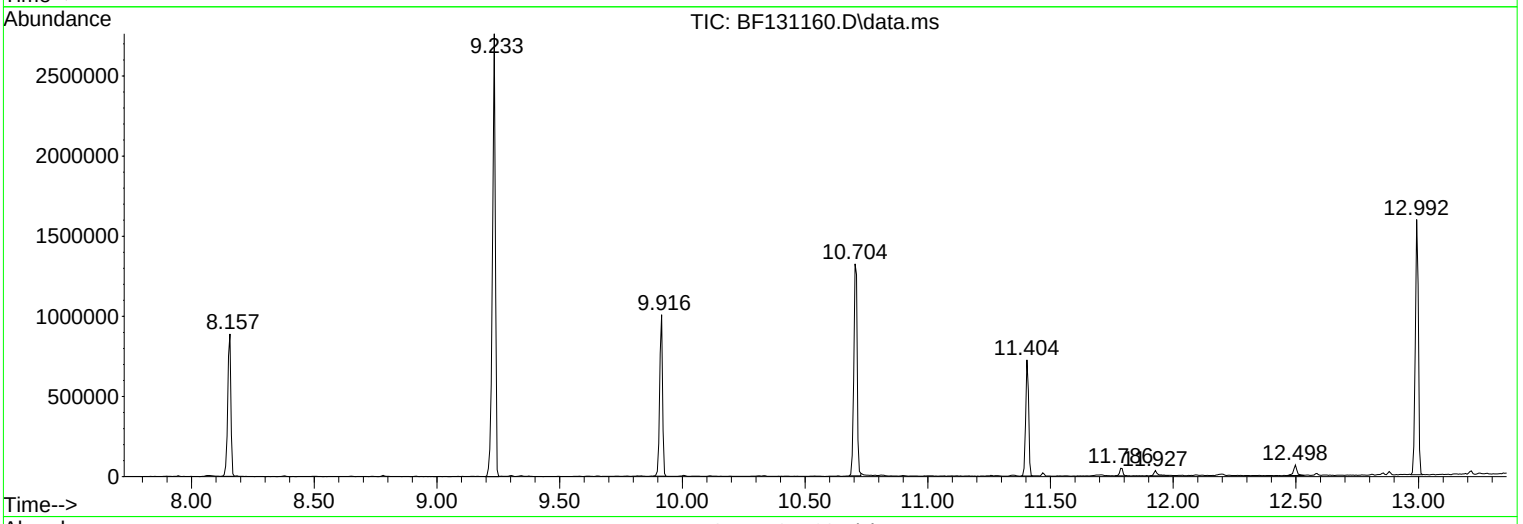
Misc :
ALS Vial : 5 Sample Multiplier: 1

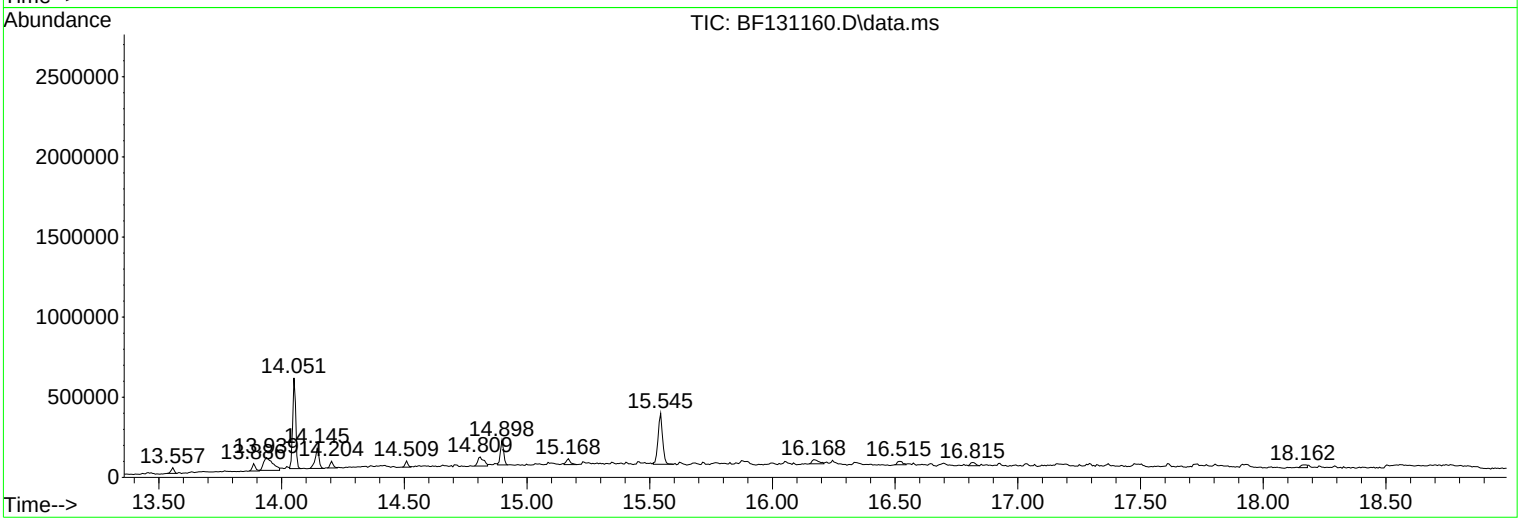
**Instrument :**
BNA_F
**ClientSampleId :**
TP-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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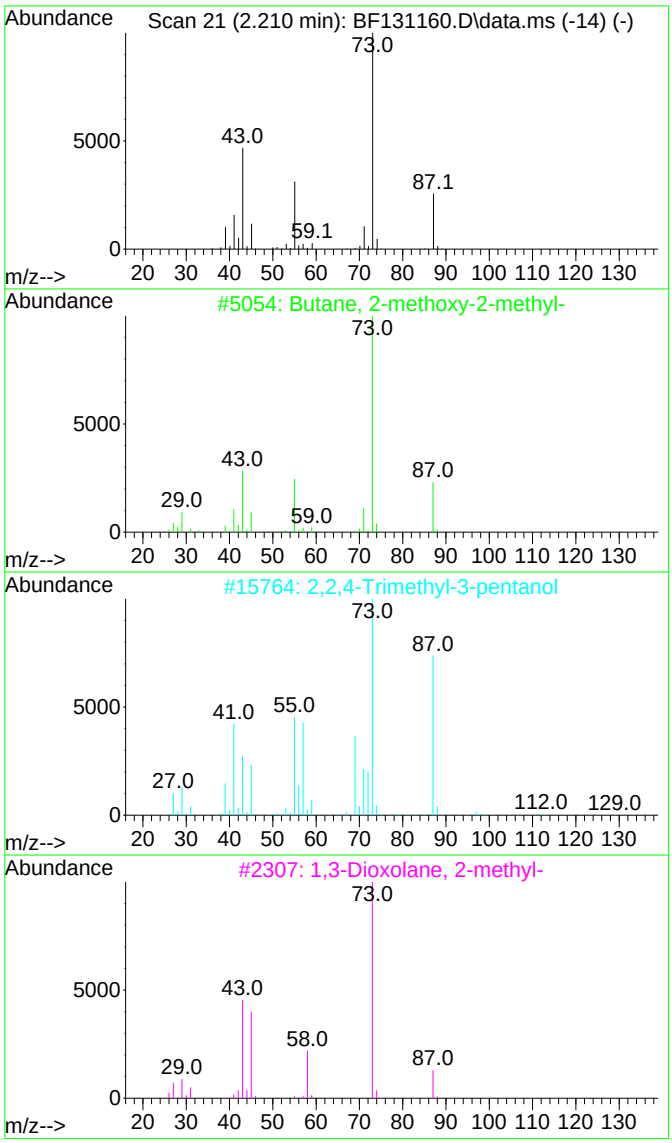
TIC Integration Parameters: LSCINT.P

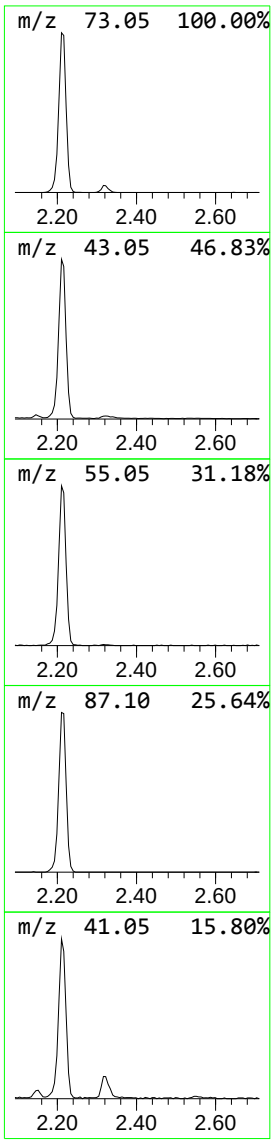
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.210 | 25.09 ng | 783063 | 1,4-Dichlorobenzene-d4 | 6.869 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 39 |
| 3 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 37 |
| 4 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 35 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131160.D
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Operator : CG\JU
Sample : N5506-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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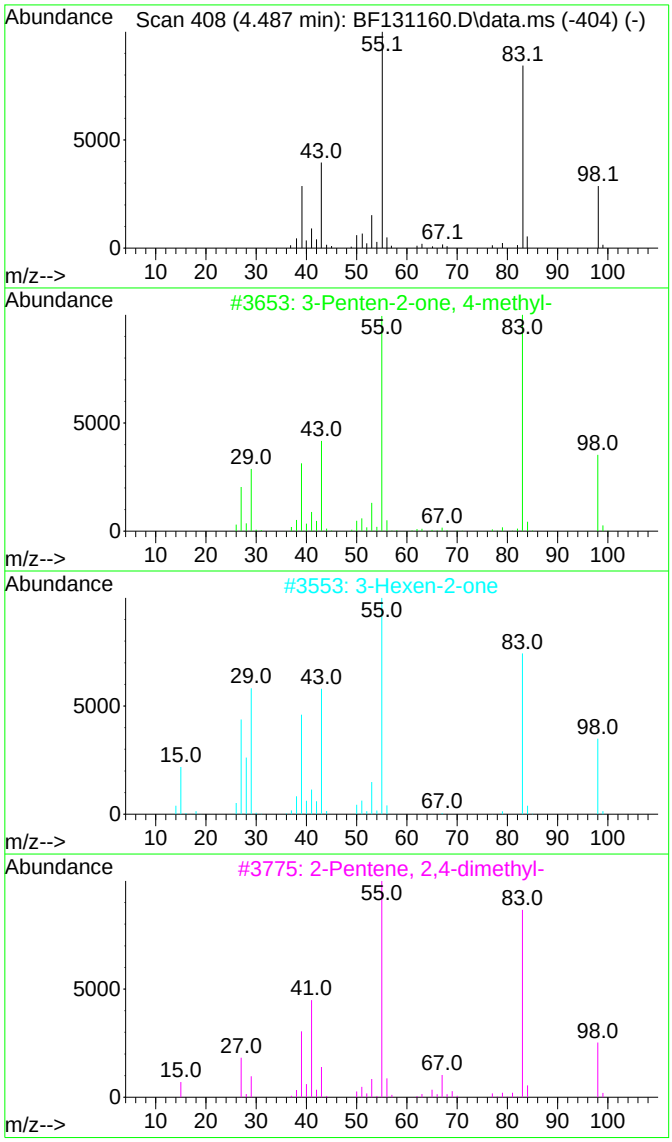
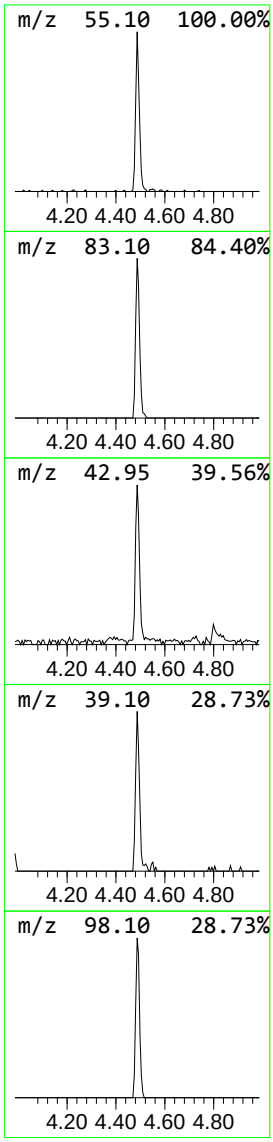
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.487 | 2.85 ng | 89067 | 1,4-Dichlorobenzene-d4 | 6.869 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Penten-2-one, 4-methyl- | 98 | C6H10O | 000141-79-7 | 91 |
| 2 | 3-Hexen-2-one | 98 | C6H10O | 000763-93-9 | 91 |
| 3 | 2-Pentene, 2,4-dimethyl- | 98 | C7H14 | 000625-65-0 | 78 |
| 4 | 2-Pentene, 3,4-dimethyl- | 98 | C7H14 | 024910-63-2 | 78 |
| 5 | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14 | 004914-91-4 | 78 |



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Operator : CG\JU
Sample : N5506-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
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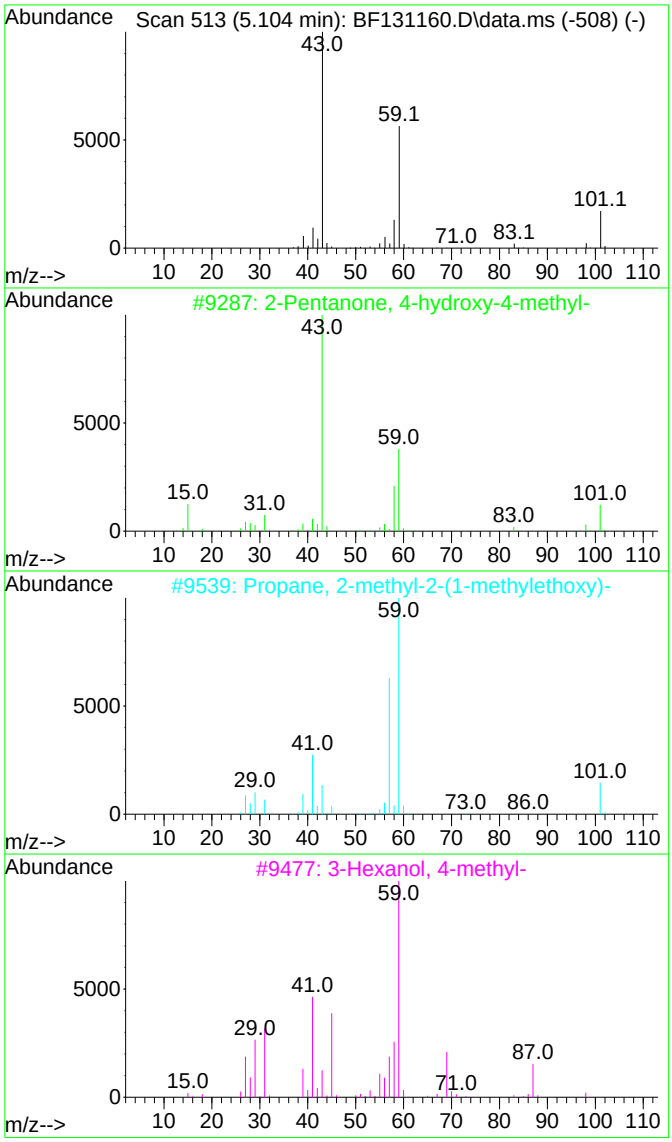
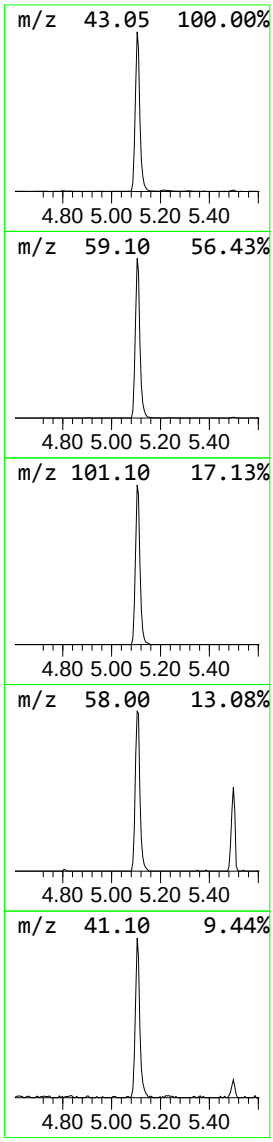
**********
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.104 | 21.59 ng | 674036 | 1,4-Dichlorobenzene-d4 | 6.869 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 36 |
| 3 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 4 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 33 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 32 |



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TIC Library : C:\Database\NIST20.L
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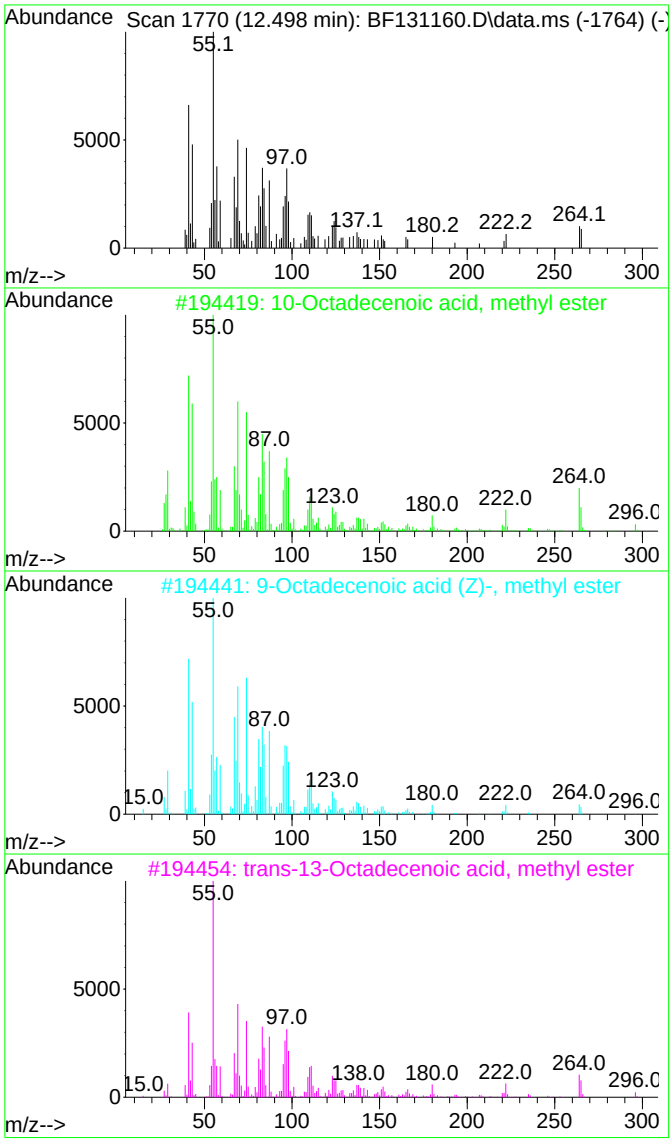
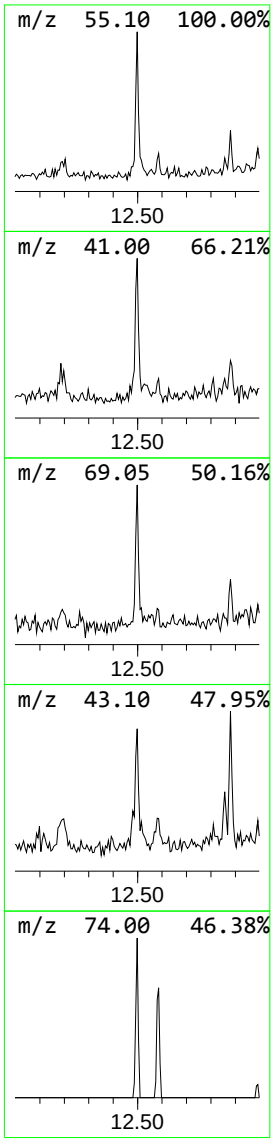
**********
Peak Number 4 10-Octadecenoic acid, methy... Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.498 | 2.15 ng | 65014 | Phenanthrene-d10 | 11.404 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 10-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 013481-95-3 | 94 |
| 2 | 9-Octadecenoic acid (Z)-, methyl... | 296 | C19H36O2 | 000112-62-9 | 93 |
| 3 | trans-13-Octadecenoic acid, meth... | 296 | C19H36O2 | 1000333-61-3 | 91 |
| 4 | 11-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 052380-33-3 | 91 |
| 5 | 7-Hexadecenoic acid, methyl este... | 268 | C17H32O2 | 056875-67-3 | 90 |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
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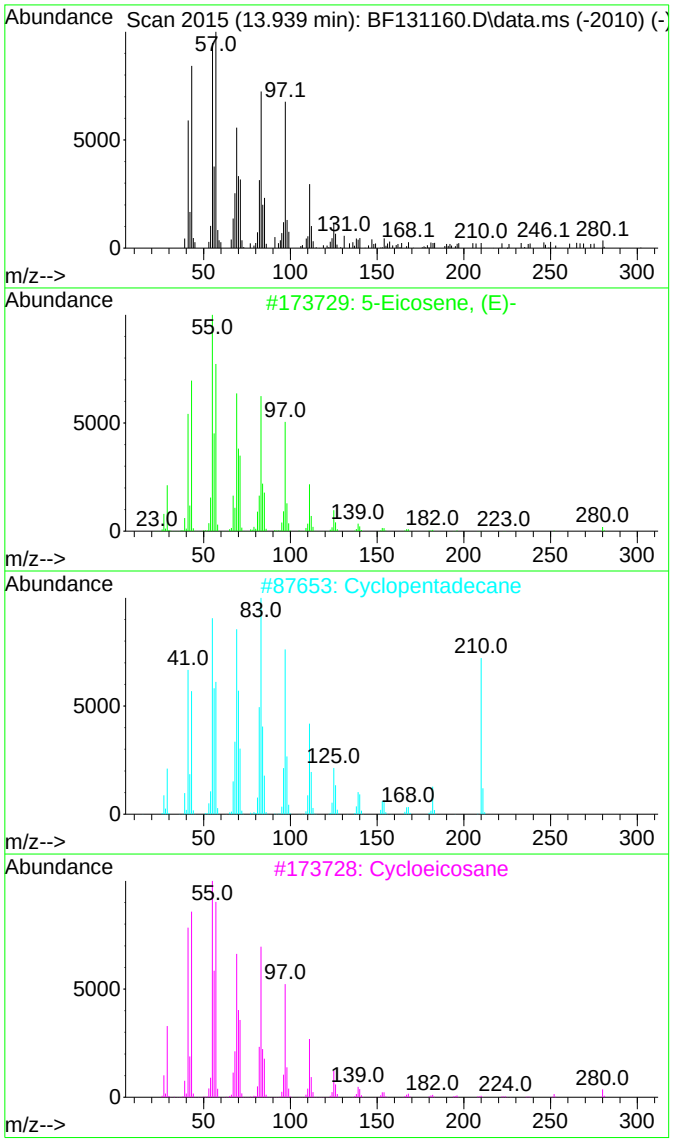
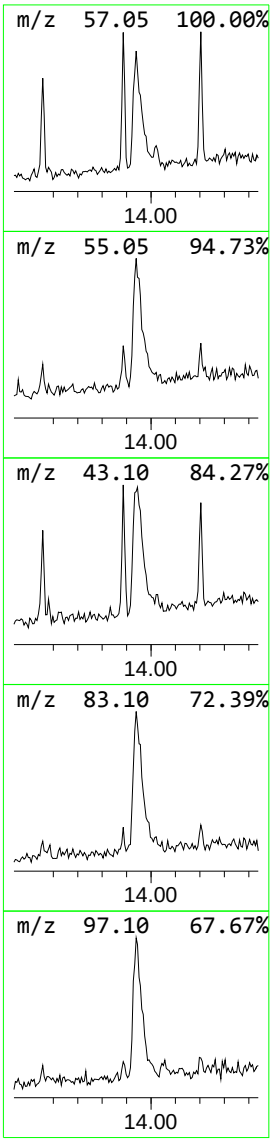
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.939 | 8.62 ng | 208628 | Chrysene-d12 | 14.051 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Eicosene, (E)- | 280 | C20H40 | 074685-30-6 | 97 |
| 2 | Cyclopentadecane | 210 | C15H30 | 000295-48-7 | 96 |
| 3 | Cycloeicosane | 280 | C20H40 | 000296-56-0 | 96 |
| 4 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 95 |
| 5 | 1-Heptadecene | 238 | C17H34 | 006765-39-5 | 93 |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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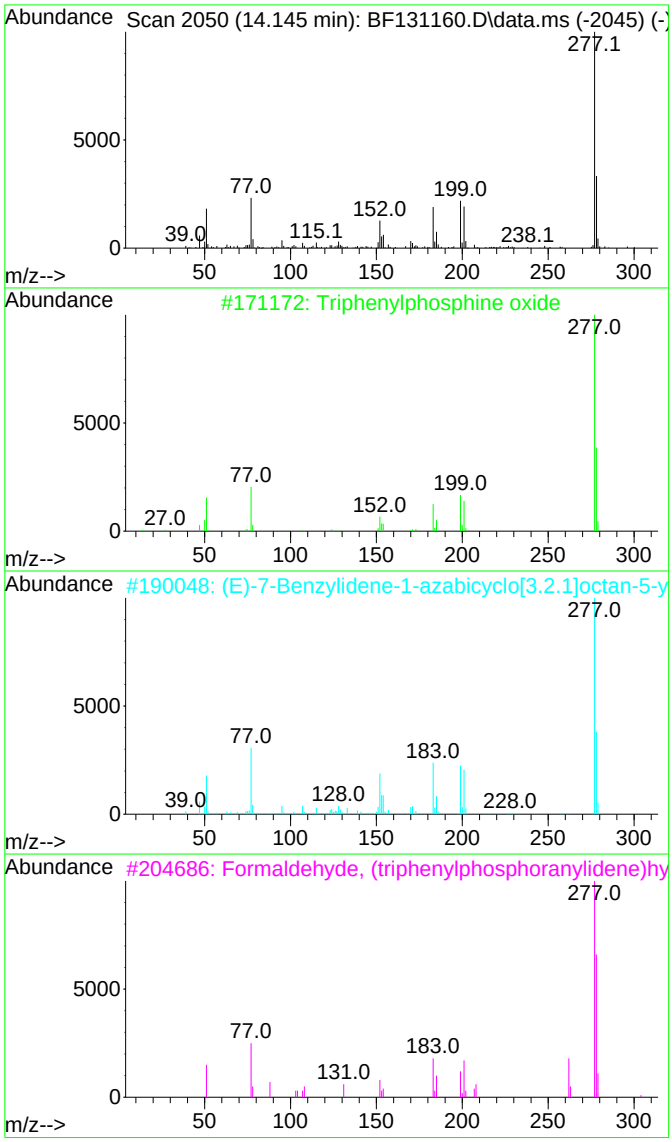
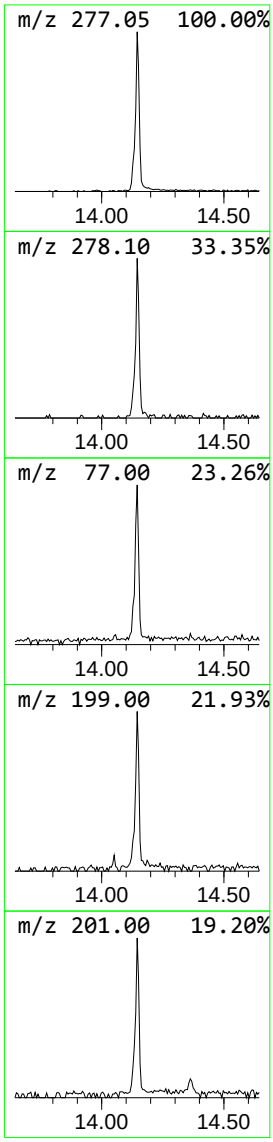
**********

Peak Number 6 Triphenylphosphine oxide Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.145 | 5.77 ng | 139579 | Chrysene-d12 | 14.051 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Triphenylphosphine oxide | 278 | C18H15OP | 000791-28-6 | 94 |
| 2 | (E)-7-Benzylidene-1-azabicyclo[3... | 293 | C15H19NO3S | 1000483-83-4 | 87 |
| 3 | Formaldehyde, (triphenylphosphor... | 304 | C19H17N2P | 015990-54-2 | 64 |
| 4 | 2-Phenyl-6-(trifluoromethyl)-1H-... | 277 | C15H10F3NO | 1000387-59-3 | 37 |
| 5 | Thiophene-3-carbonitrile, 4-(4-m... | 277 | C13H11NO2S2 | 1000268-75-0 | 9 |



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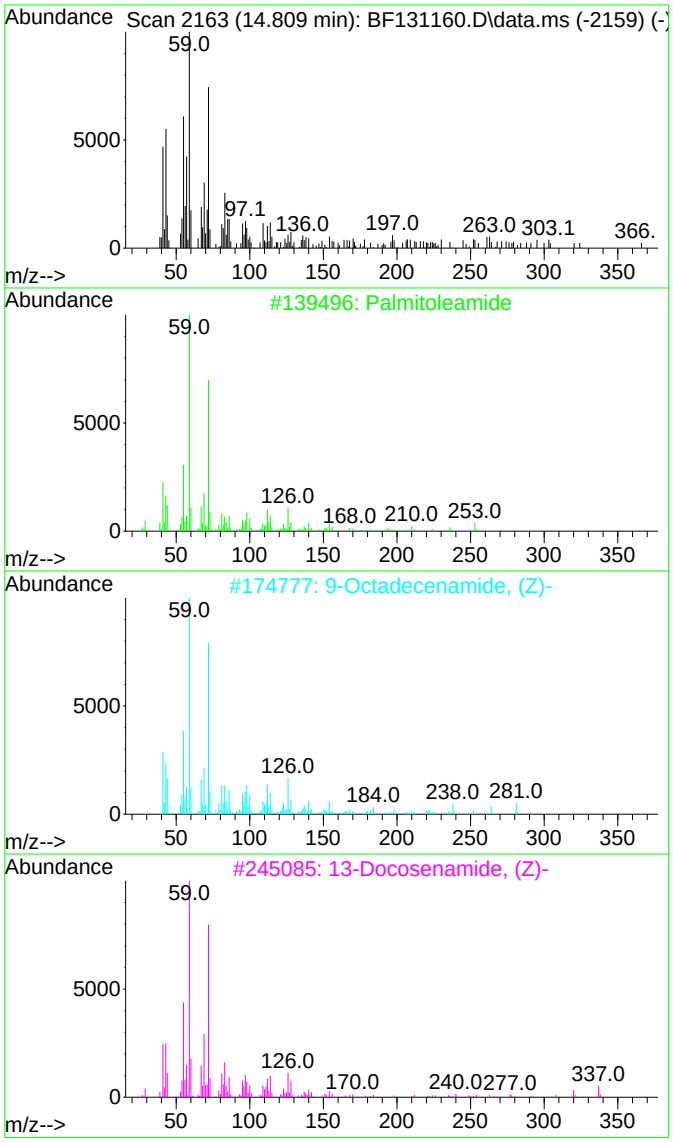
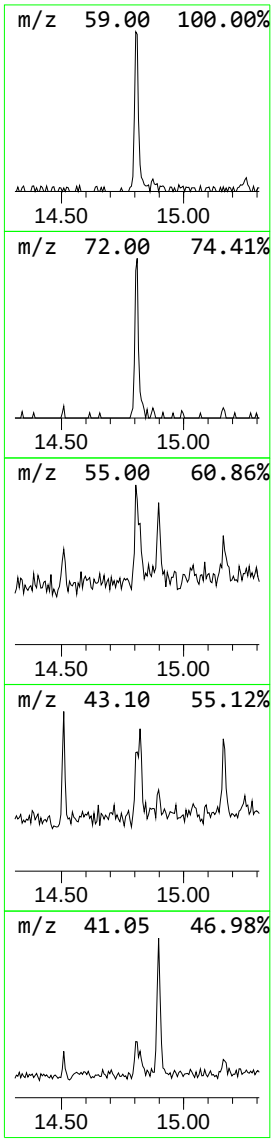
Peak Number 7 Palmitoleamide Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.810 | 4.90 ng | 99300 | Perylene-d12 | 15.545 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Palmitoleamide | 253 | C16H31NO | 106010-22-4 | 81 |
| 2 | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 80 |
| 3 | 13-Docosenamide, (Z)- | 337 | C22H43NO | 000112-84-5 | 72 |
| 4 | Hexanamide, N-hexanoyl- | 213 | C12H23NO2 | 004430-07-3 | 43 |
| 5 | N,N'-Di-n-propyl-1,4-butanediamine | 172 | C10H24N2 | 1010342-33-5 | 38 |



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**Instrument :**
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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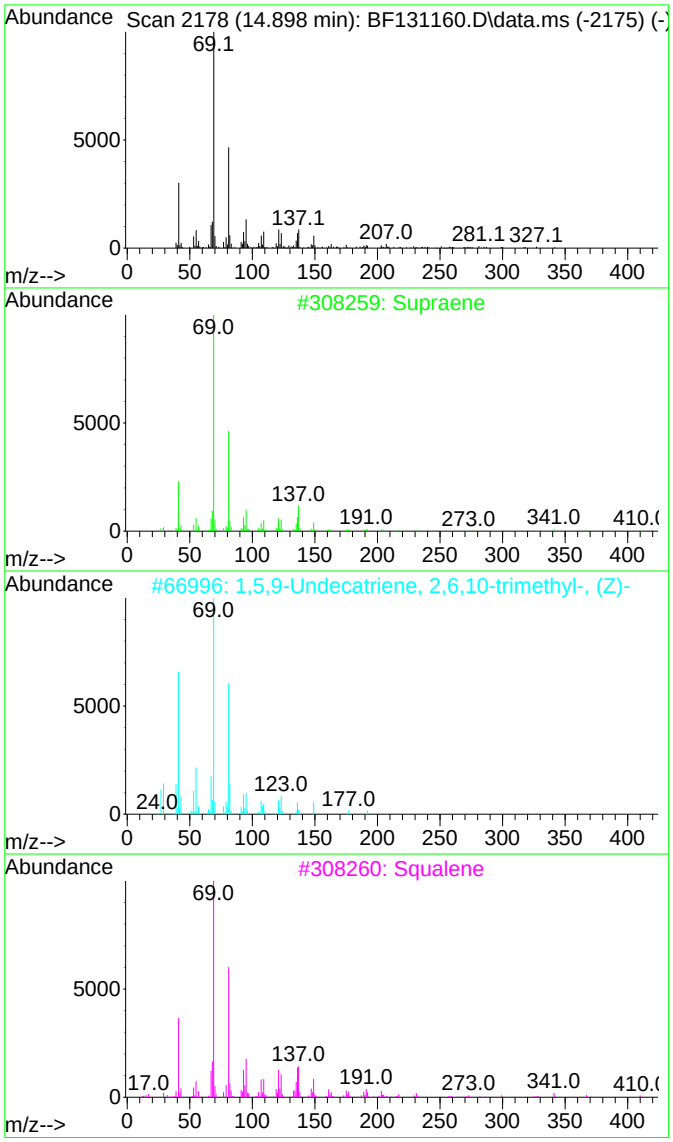
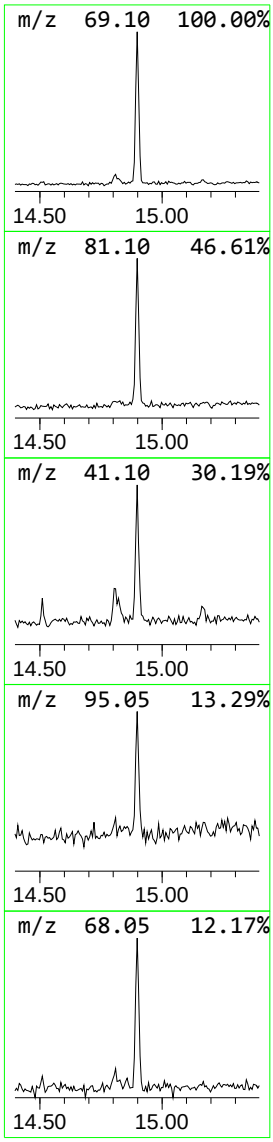
**********

Peak Number 8 Supraene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.898 | 6.85 ng | 138779 | Perylene-d12 | 15.545 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Supraene | 410 | C30H50 | 007683-64-9 | 91 |
| 2 | 1,5,9-Undecatriene, 2,6,10-trime... | 192 | C14H24 | 062951-96-6 | 86 |
| 3 | Squalene | 410 | C30H50 | 000111-02-4 | 83 |
| 4 | 4,9,13,17-Tetramethyl-4,8,12,16-... | 316 | C22H36O | 056882-09-8 | 83 |
| 5 | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 80 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131160.D
Acq On : 11 Nov 2022 18:44
Operator : CG\JU
Sample : N5506-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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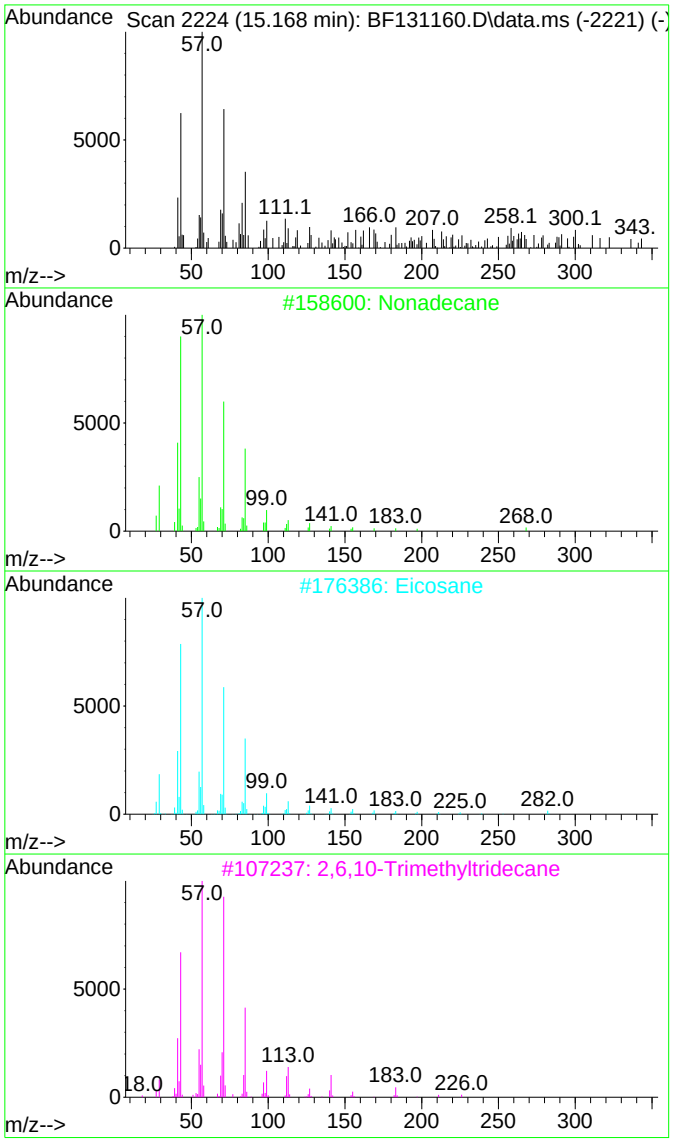
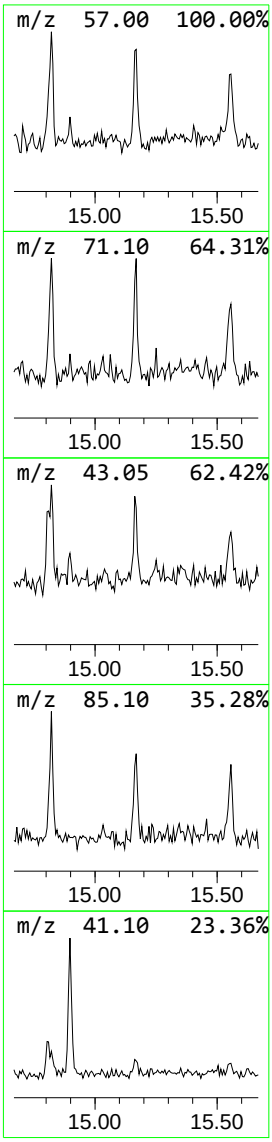
Peak Number 9 Nonadecane Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.168 | 2.09 ng | 42341 | Perylene-d12 | 15.545 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Nonadecane | 268 | C19H40 | 000629-92-5 | 89 |
| 2 | Eicosane | 282 | C20H42 | 000112-95-8 | 55 |
| 3 | 2,6,10-Trimethyltridecane | 226 | C16H34 | 003891-99-4 | 55 |
| 4 | Heptadecane, 2,6,10,14-tetramethyl- | 296 | C21H44 | 018344-37-1 | 55 |
| 5 | Tetradecane | 198 | C14H30 | 000629-59-4 | 55 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131160.D
Acq On : 11 Nov 2022 18:44
Operator : CG\JU
Sample : N5506-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

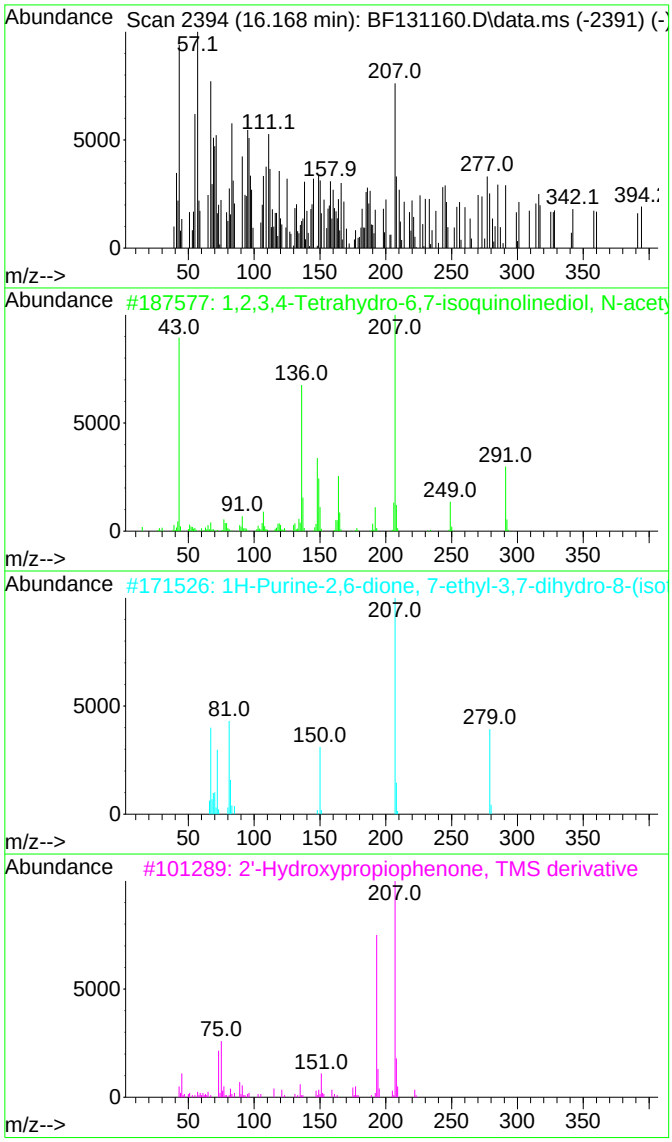
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

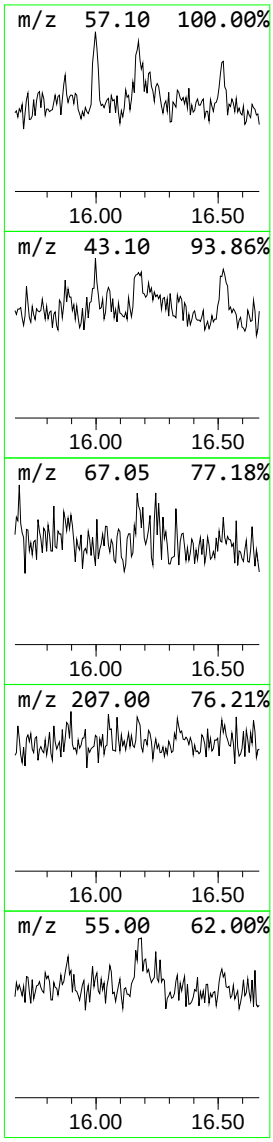
**********

Peak Number 10 unknown16.168 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.168 | 2.38 ng | 48196 | Perylene-d12 | 15.545 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,2,3,4-Tetrahydro-6,7-isoquinol... | 291 | C15H17NO5 | 1000511-71-3 | 30 |
| 2 | 1H-Purine-2,6-dione, 7-ethyl-3,7... | 279 | C11H13N5O2S | 027042-75-7 | 30 |
| 3 | 2'-Hydroxypropiophenone, TMS der... | 222 | C12H18O2Si | 033342-87-9 | 18 |
| 4 | Methyl 3-(1-pyrrolo)thiophene-2-... | 207 | C10H9NO2S | 074772-16-0 | 18 |
| 5 | (3R,5aR,9S,9aS)-2,2,5a,9-Tetrame... | 222 | C15H26O | 765307-45-7 | 18 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131160.D
Acq On : 11 Nov 2022 18:44
Operator : CG\JU
Sample : N5506-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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 |
| Butane, 2-metho... | 2.210 | 25.1 | ng | 783063 | 1 | 6.869 | 624270 | 20.0 |
| 3-Penten-2-one,... | 4.487 | 2.9 | ng | 89067 | 1 | 6.869 | 624270 | 20.0 |
| 2-Pentanone, 4-... | 5.104 | 21.6 | ng | 674036 | 1 | 6.869 | 624270 | 20.0 |
| 10-Octadecenoic... | 12.498 | 2.1 | ng | 65014 | 4 | 11.404 | 606114 | 20.0 |
| 5-Eicosene, (E)- | 13.939 | 8.6 | ng | 208628 | 5 | 14.051 | 484067 | 20.0 |
| Triphenylphosph... | 14.145 | 5.8 | ng | 139579 | 5 | 14.051 | 484067 | 20.0 |
| Palmitoleamide | 14.810 | 4.9 | ng | 99300 | 6 | 15.545 | 405227 | 20.0 |
| Supraene | 14.898 | 6.8 | ng | 138779 | 6 | 15.545 | 405227 | 20.0 |
| Nonadecane | 15.168 | 2.1 | ng | 42341 | 6 | 15.545 | 405227 | 20.0 |
| unknown16.168 | 16.168 | 2.4 | ng | 48196 | 6 | 15.545 | 405227 | 20.0 |