LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090222\
Data File : BG054841.D
Acq On : 2 Sep 2022 15:30
Operator : CG/JU
Sample : N4453-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SASP2-T-5-(5-10)

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_G\Methods\8270-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054841.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.209 | 319 | 327 | 333 | rBV | 88724 | 138294 | 6.19% | 1.385% |
| 2 | 5.685 | 401 | 408 | 421 | rVB | 425267 | 679567 | 30.42% | 6.806% |
| 3 | 7.295 | 673 | 682 | 696 | rBV | 420763 | 749834 | 33.57% | 7.510% |
| 4 | 8.147 | 820 | 827 | 833 | rBV | 107266 | 178878 | 8.01% | 1.792% |
| 5 | 9.322 | 1019 | 1027 | 1039 | rBV | 252894 | 464078 | 20.77% | 4.648% |
| 6 | 10.973 | 1301 | 1308 | 1317 | rBV | 146965 | 266609 | 11.93% | 2.670% |
| 7 | 13.406 | 1714 | 1722 | 1738 | rBV | 803152 | 1246995 | 55.82% | 12.489% |
| 8 | 14.780 | 1949 | 1956 | 1966 | rBV | 257391 | 418515 | 18.73% | 4.192% |
| 9 | 16.267 | 2202 | 2209 | 2228 | rBV | 595004 | 950558 | 42.55% | 9.520% |
| 10 | 17.530 | 2417 | 2424 | 2430 | rBV | 349924 | 556170 | 24.90% | 5.570% |
| 11 | 19.575 | 2768 | 2772 | 2780 | rVB | 16619 | 25380 | 1.14% | 0.254% |
| 12 | 19.939 | 2827 | 2834 | 2841 | rVB | 18202 | 32946 | 1.47% | 0.330% |
| 13 | 20.127 | 2860 | 2866 | 2881 | rBV | 1675372 | 2233975 | 100.00% | 22.374% |
| 14 | 20.409 | 2906 | 2914 | 2921 | rBV2 | 16578 | 33295 | 1.49% | 0.333% |
| 15 | 20.909 | 2995 | 2999 | 3004 | rVB2 | 28716 | 33768 | 1.51% | 0.338% |
| 16 | 21.426 | 3082 | 3087 | 3094 | rBV | 111104 | 159662 | 7.15% | 1.599% |
| 17 | 21.678 | 3126 | 3130 | 3136 | rVB | 20145 | 29279 | 1.31% | 0.293% |
| 18 | 21.819 | 3144 | 3154 | 3162 | rBV | 363579 | 670589 | 30.02% | 6.716% |
| 19 | 21.990 | 3178 | 3183 | 3189 | rBV | 38668 | 60914 | 2.73% | 0.610% |
| 20 | 22.624 | 3286 | 3291 | 3306 | rVB | 36377 | 76970 | 3.45% | 0.771% |
| 21 | 23.018 | 3353 | 3358 | 3364 | rVB3 | 26628 | 48505 | 2.17% | 0.486% |
| 22 | 23.347 | 3408 | 3414 | 3421 | rBV2 | 32427 | 66040 | 2.96% | 0.661% |
| 23 | 24.193 | 3552 | 3558 | 3567 | rVB4 | 32841 | 73895 | 3.31% | 0.740% |
| 24 | 25.192 | 3717 | 3728 | 3744 | rBV2 | 234481 | 720682 | 32.26% | 7.218% |
| 25 | 26.390 | 3923 | 3932 | 3942 | rVB5 | 22500 | 69106 | 3.09% | 0.692% |

Sum of corrected areas: 9984504

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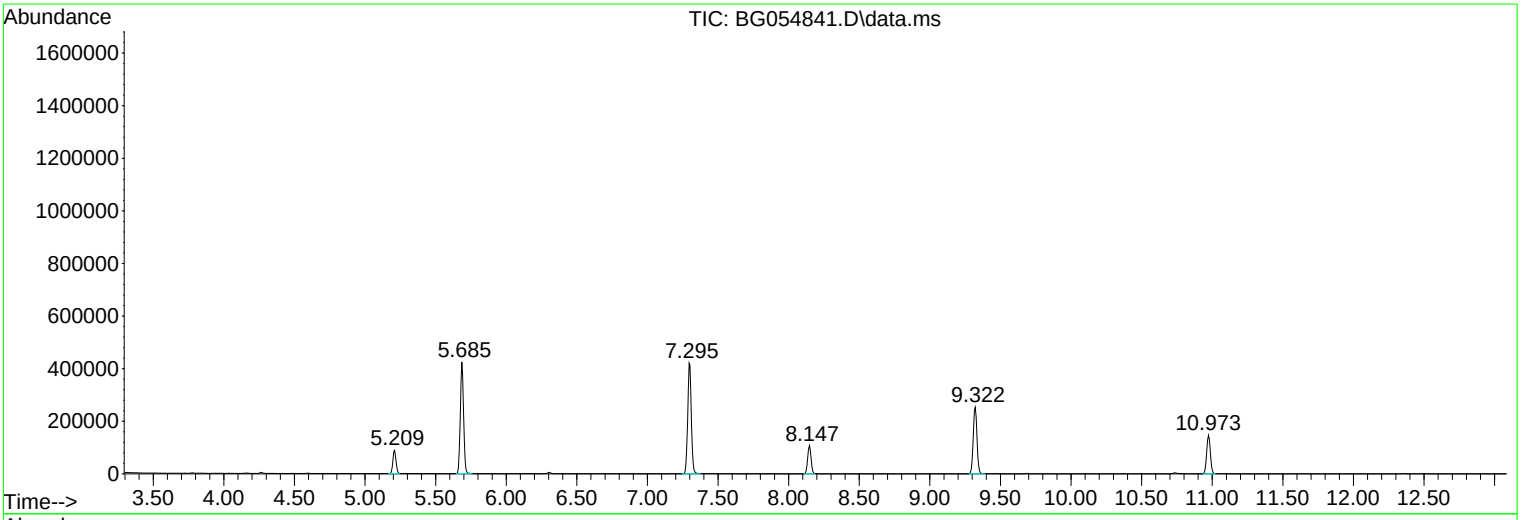
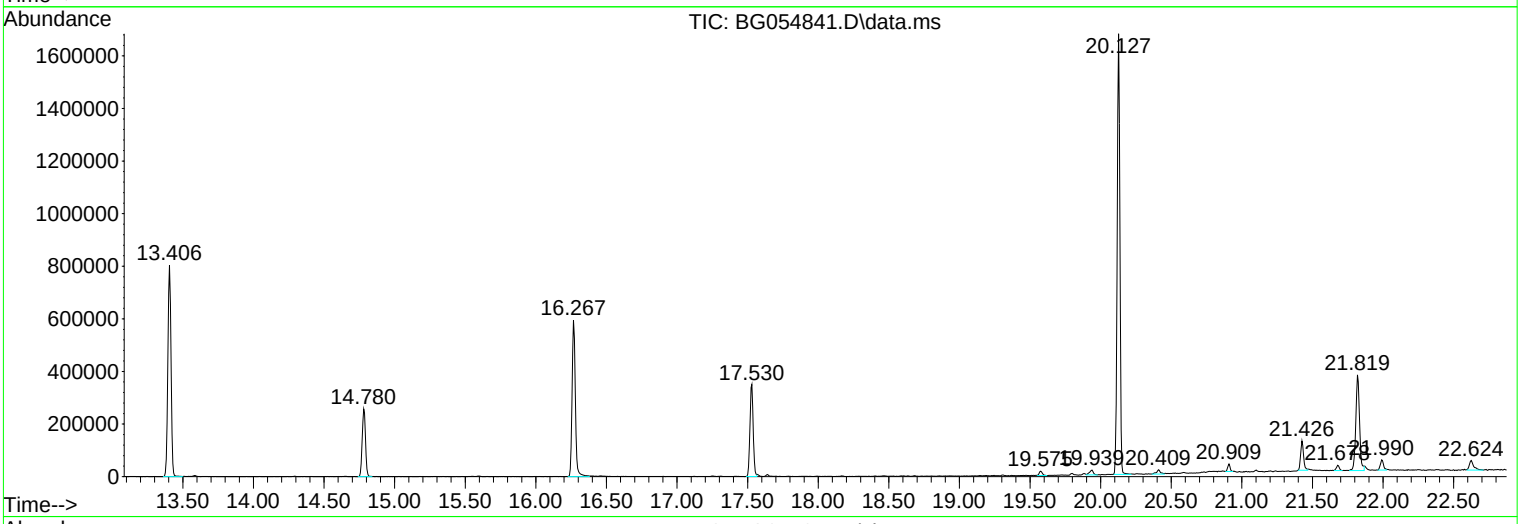
ALS Vial : 9 Sample Multiplier: 1

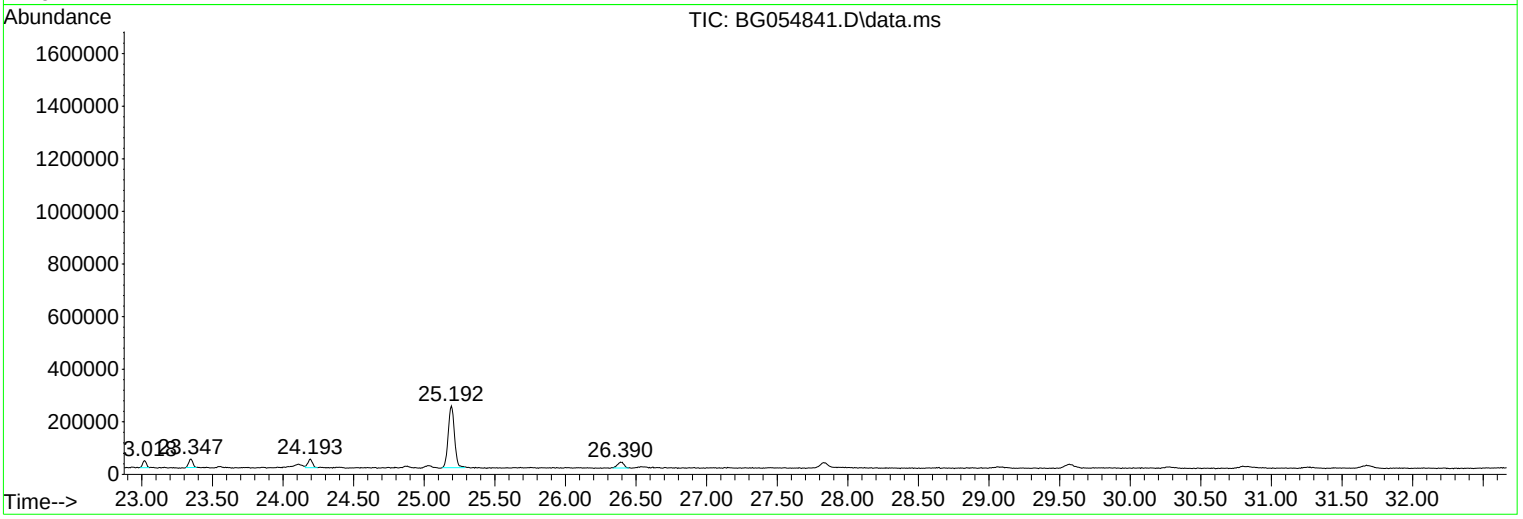
**Instrument :**
BNA_G
**ClientSampleId :**
SASP2-T-5-(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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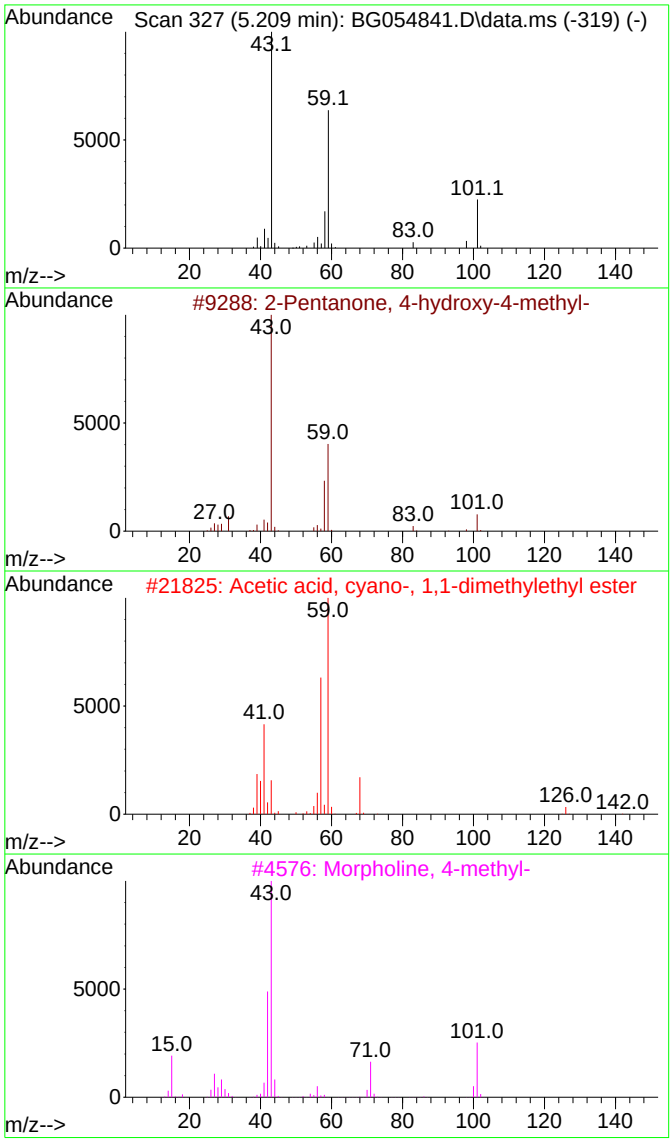
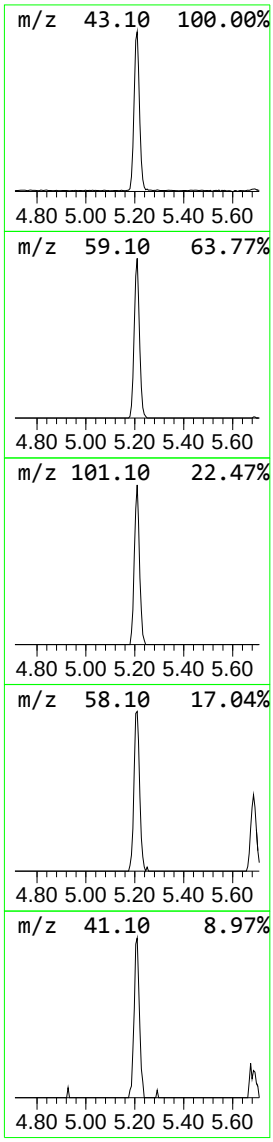
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.209 | 15.46 ng | 138294 | 1,4-Dichlorobenzene-d4 | 8.147 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 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 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090222\
Data File : BG054841.D
Acq On : 2 Sep 2022 15:30
Operator : CG/JU
Sample : N4453-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
SASP2-T-5-(5-10)

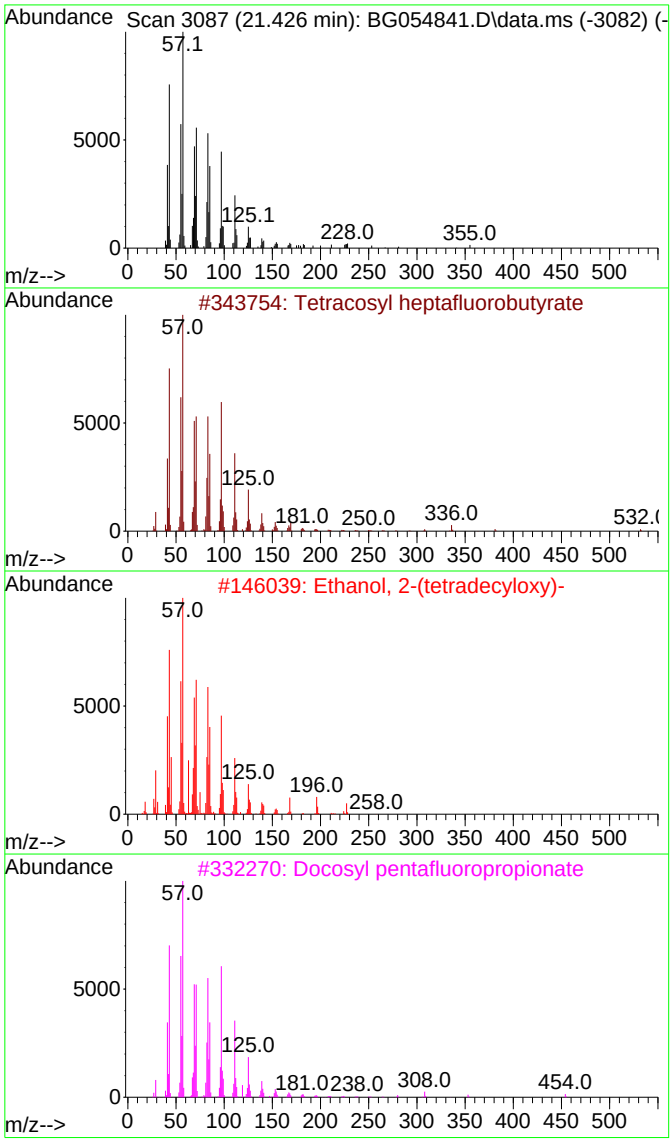
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

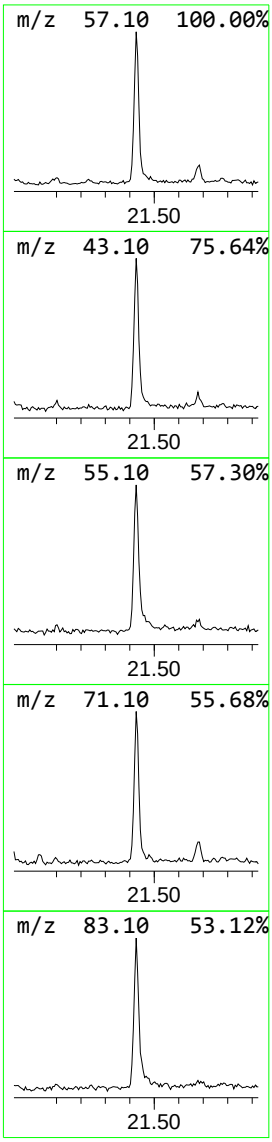
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 Tetracosyl heptafluorobutyrate Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.426 | 4.76 ng | 159662 | Chrysene-d12 | 21.819 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetracosyl heptafluorobutyrate | 550 | C28H49F7O2 | 1000351-83-7 | 91 |
| 2 | Ethanol, 2-(tetradecyloxy)- | 258 | C16H34O2 | 002136-70-1 | 91 |
| 3 | Docosyl pentafluoropropionate | 472 | C25H45F5O2 | 1000351-80-9 | 91 |
| 4 | Heneicosyl heptafluorobutyrate | 508 | C25H43F7O2 | 1000351-83-8 | 91 |
| 5 | Tricosyl pentafluoropropionate | 486 | C26H47F5O2 | 1000351-81-0 | 91 |



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Data File : BG054841.D
Acq On : 2 Sep 2022 15:30
Operator : CG/JU
Sample : N4453-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
SASP2-T-5-(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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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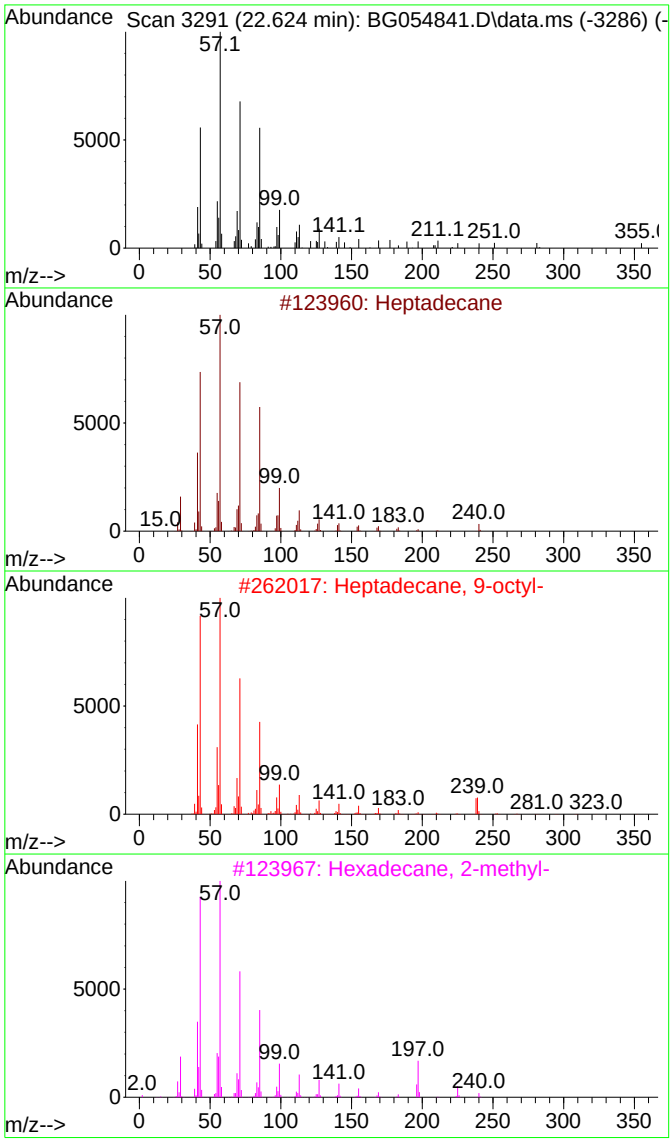
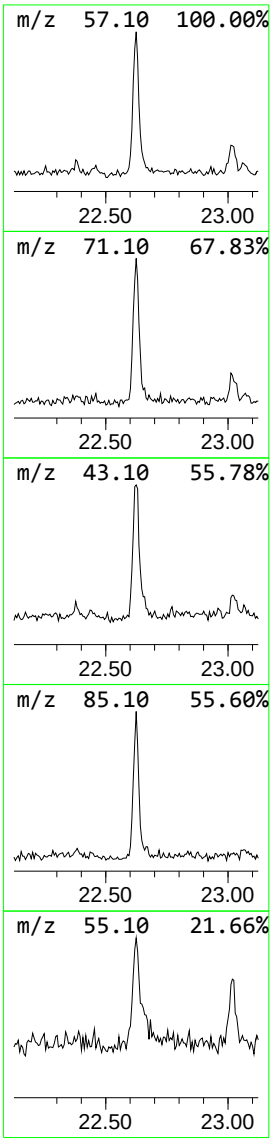
Peak Number 3 Heptadecane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.624 | 2.30 ng | 76970 | Chrysene-d12 | 21.819 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 97 |
| 2 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 91 |
| 3 | Hexadecane, 2-methyl- | 240 | C17H36 | 001560-92-5 | 91 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 91 |
| 5 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |



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Sample : N4453-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
SASP2-T-5-(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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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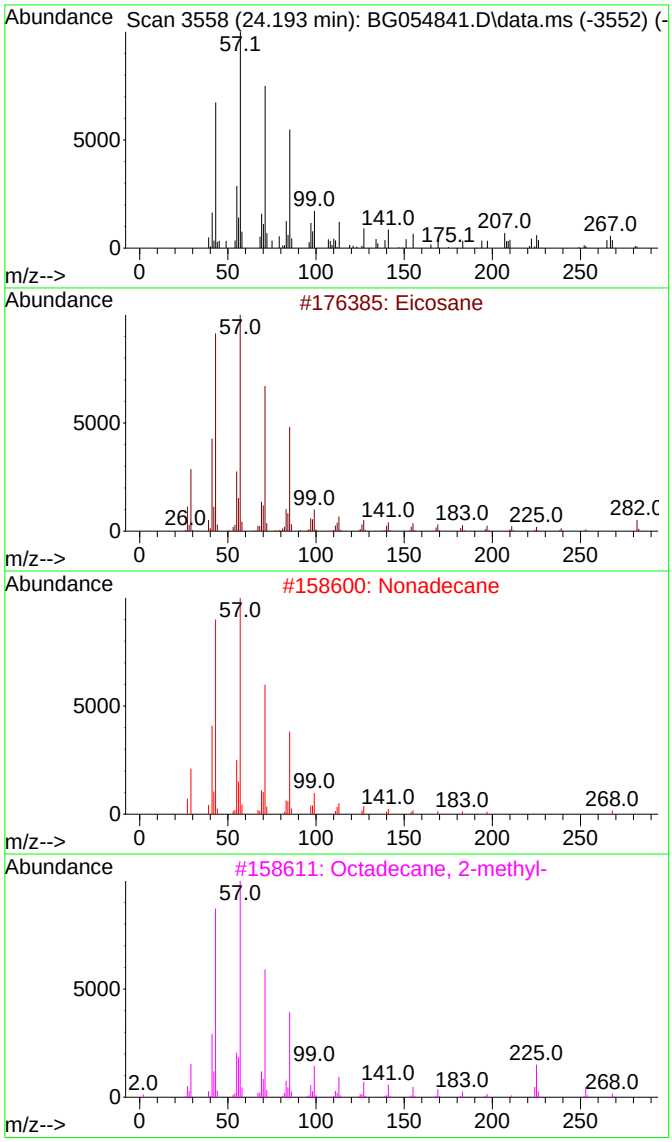
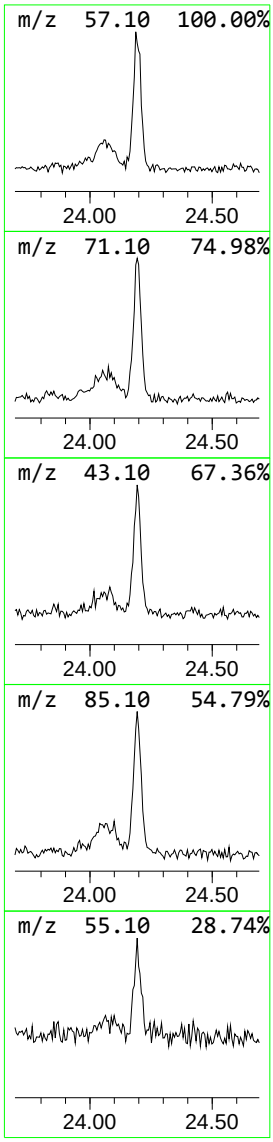
Peak Number 4 Eicosane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 24.193 | 2.05 ng | 73895 | Perylene-d12 | 25.192 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 93 |
| 2 | Nonadecane | 268 | C19H40 | 000629-92-5 | 93 |
| 3 | Octadecane, 2-methyl- | 268 | C19H40 | 001560-88-9 | 93 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 91 |
| 5 | Heneicosane | 296 | C21H44 | 000629-94-7 | 87 |



Tentatively Identified Compound (LSC) summary

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Sample : N4453-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
SASP2-T-5-(5-10)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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 |
| 2-Pentanone, 4-... | 5.209 | 15.5 | ng | 138294 | 1 | 8.147 | 178878 | 20.0 |
| Tetracosyl hept... | 21.426 | 4.8 | ng | 159662 | 5 | 21.819 | 670589 | 20.0 |
| Heptadecane | 22.624 | 2.3 | ng | 76970 | 5 | 21.819 | 670589 | 20.0 |
| Eicosane | 24.193 | 2.0 | ng | 73895 | 6 | 25.192 | 720682 | 20.0 |