LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102518\
Data File : BG037565.D
Acq On : 26 Oct 2018 4:46
Operator : JU/SJ
Sample : J5649-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TWP-01

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-BG101818.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	5.644	394	401	410	rBV	456144	748474	18.04%	3.261%
2	7.248	664	674	686	rBV2	297571	739577	17.83%	3.222%
3	7.629	731	739	751	rBV	796721	1425426	34.36%	6.210%
4	8.105	812	820	830	rBV	206726	372968	8.99%	1.625%
5	8.423	866	874	883	rBV	706837	1283528	30.94%	5.592%
6	9.280	1010	1020	1028	rBV	628647	1165883	28.10%	5.080%
7	10.920	1292	1299	1310	rVB	297802	564377	13.60%	2.459%
8	13.358	1705	1714	1723	rBV	1827460	2929733	70.62%	12.764%
9	14.181	1848	1854	1859	rBV	91366	137522	3.32%	0.599%
10	14.733	1941	1948	1957	rBV2	524737	887149	21.39%	3.865%
11	16.219	2194	2201	2213	rBV	1450385	2295441	55.33%	10.001%
12	17.483	2409	2416	2428	rVB2	727006	1109597	26.75%	4.834%
13	18.340	2556	2562	2574	rBV	383699	626677	15.11%	2.730%
14	19.610	2772	2778	2796	rBV	374315	625623	15.08%	2.726%
15	20.080	2852	2858	2869	rBV	2910289	4148396	100.00%	18.074%
16	21.184	3042	3046	3050	rBV	66917	85247	2.05%	0.371%
17	21.366	3073	3077	3091	rVB	128087	242389	5.84%	1.056%
18	21.766	3138	3145	3157	rBV2	635068	1123313	27.08%	4.894%
19	21.919	3167	3171	3178	rVB	37446	56983	1.37%	0.248%
20	22.506	3266	3271	3273	rBV3	28241	43917	1.06%	0.191%
21	22.541	3273	3277	3286	rVB	54564	101442	2.45%	0.442%
22	22.788	3314	3319	3324	rBV8	26632	61758	1.49%	0.269%
23	23.252	3392	3398	3405	rBV2	83515	158548	3.82%	0.691%
24	23.458	3427	3433	3444	rVB	52262	105191	2.54%	0.458%
25	24.081	3533	3539	3549	rVB	91464	217750	5.25%	0.949%
26	25.097	3698	3712	3724	rBV4	360841	1325270	31.95%	5.774%
27	26.237	3898	3906	3918	rVB4	70889	228320	5.50%	0.995%
28	27.635	4136	4144	4158	rVB4	39528	142210	3.43%	0.620%

Sum of corrected areas: 22952709

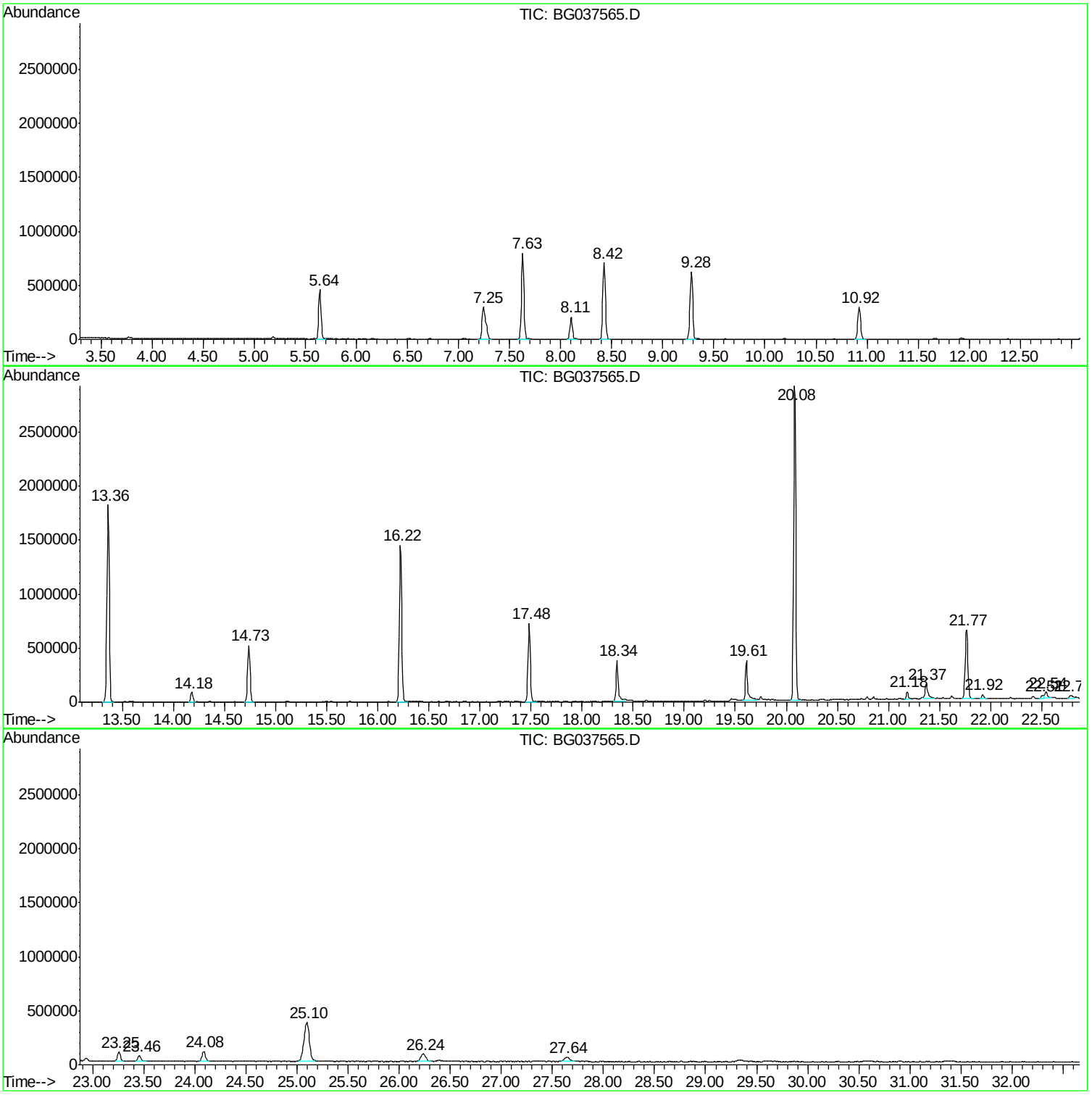
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102518\
Data File : BG037565.D
Acq On : 26 Oct 2018 4:46
Operator : JU/SJ
Sample : J5649-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TWP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102518\
Data File : BG037565.D
Acq On : 26 Oct 2018 4:46
Operator : JU/SJ
Sample : J5649-14
Misc :
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ClientSampleId : TWP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

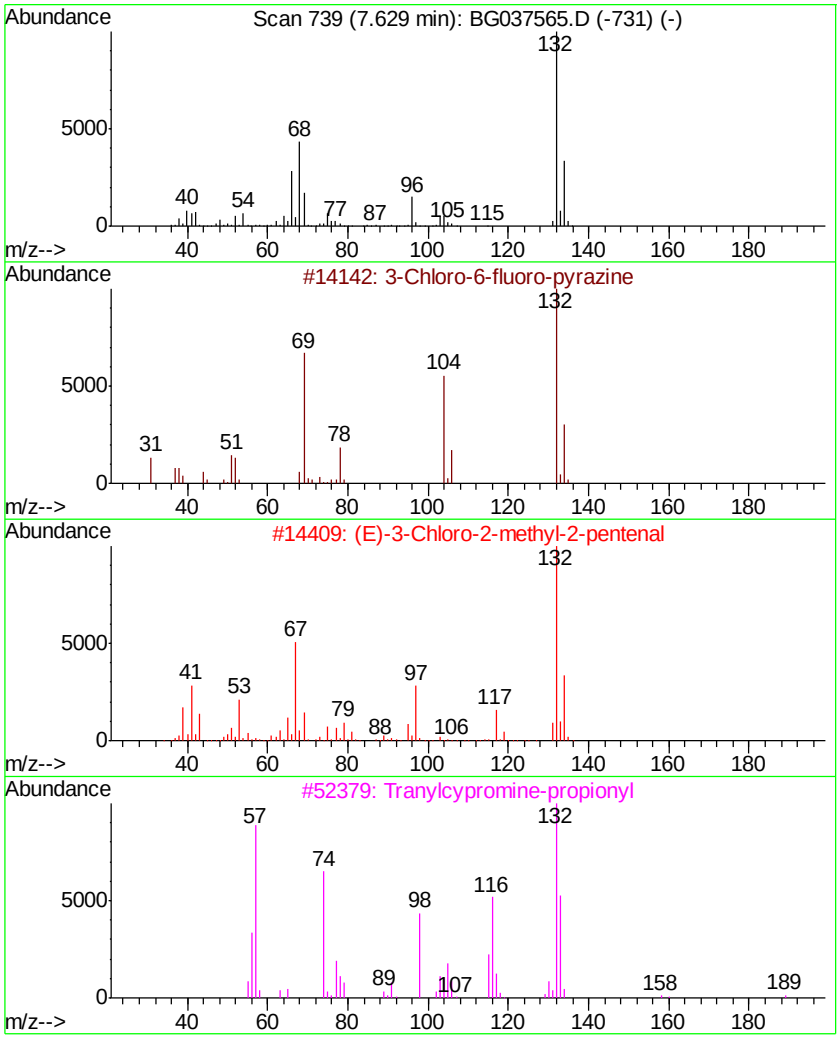
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

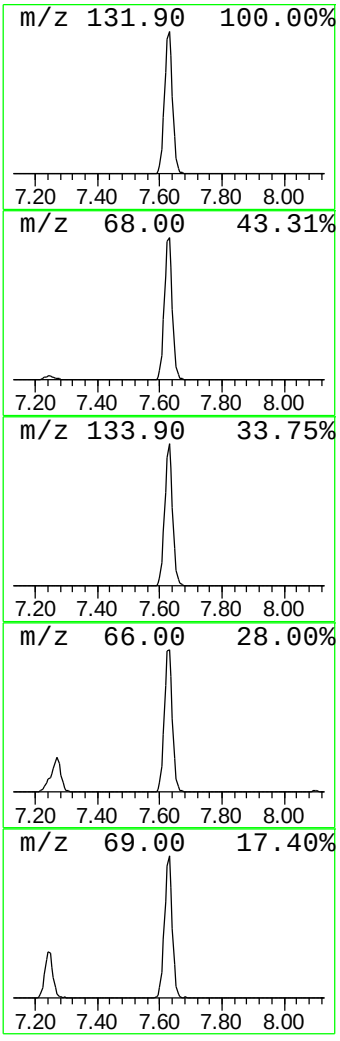
****

Peak Number 1 unknown7.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	76.44 ng	1425430	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102518\
Data File : BG037565.D
Acq On : 26 Oct 2018 4:46
Operator : JU/SJ
Sample : J5649-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TWP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

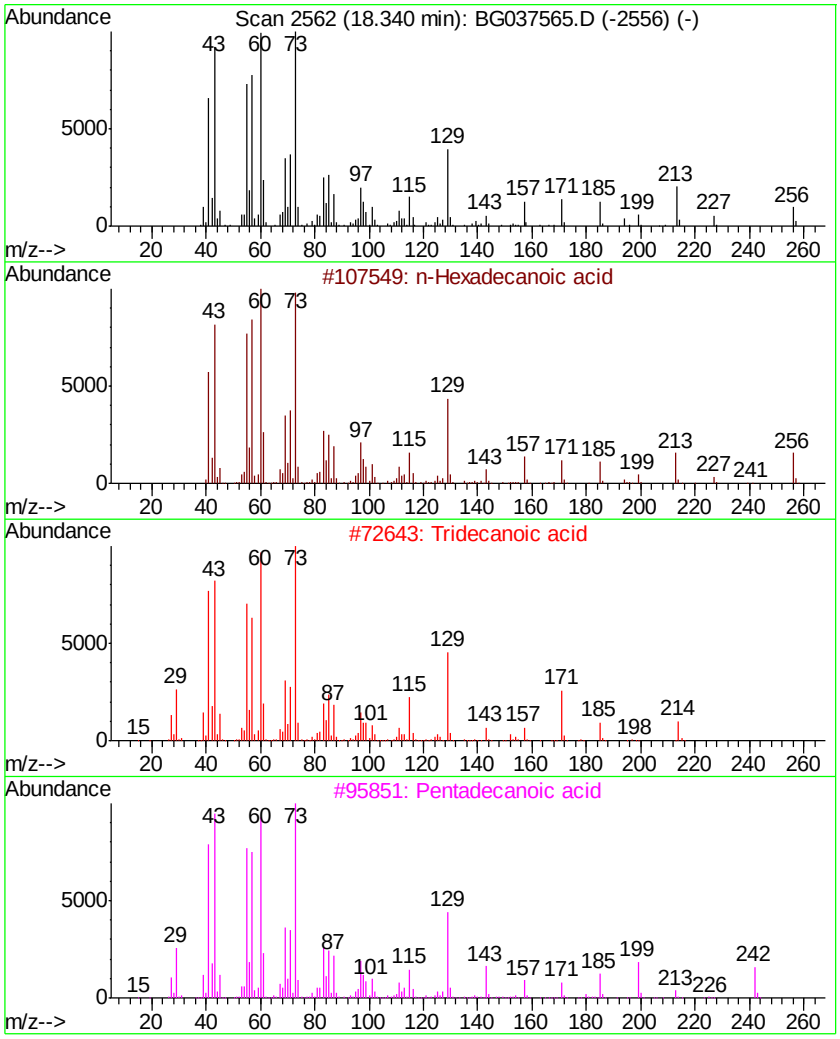
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

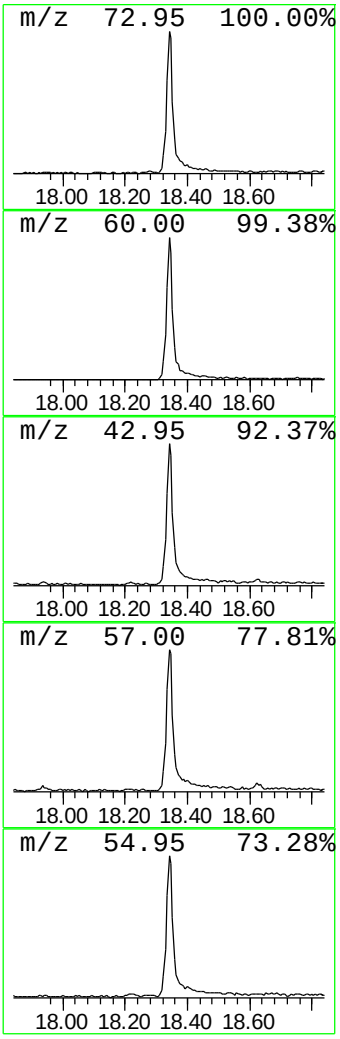
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	11.30 ng	626677	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102518\
Data File : BG037565.D
Acq On : 26 Oct 2018 4:46
Operator : JU/SJ
Sample : J5649-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TWP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

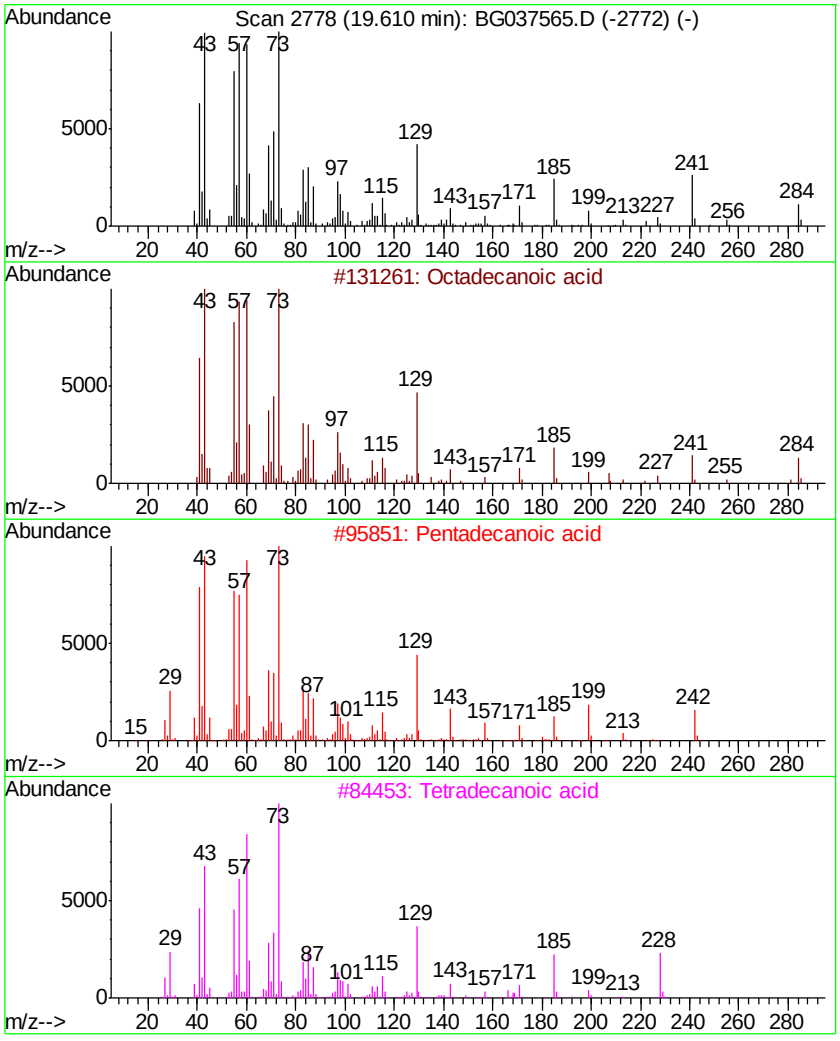
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

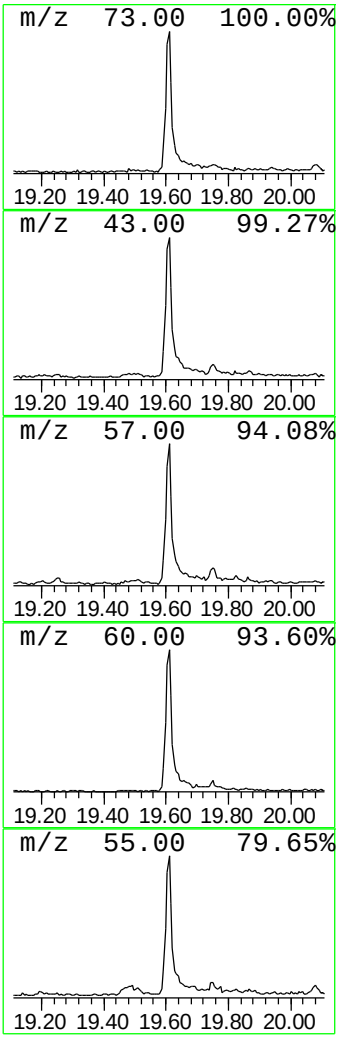
****

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.61	11.28 ng	625623	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102518\
Data File : BG037565.D
Acq On : 26 Oct 2018 4:46
Operator : JU/SJ
Sample : J5649-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TWP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

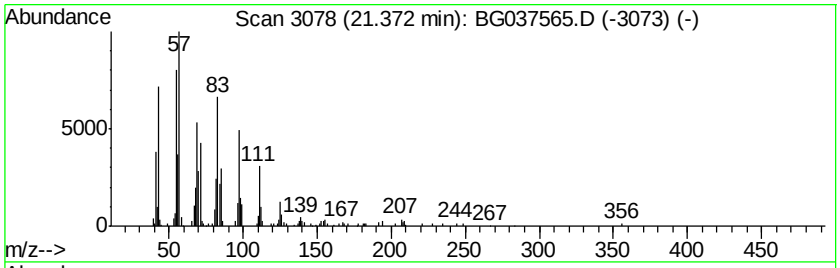
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

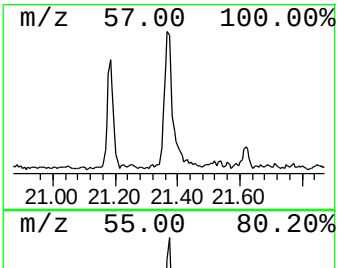
****

Peak Number 5 Tricosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.37	4.32 ng	242389	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102518\
Data File : BG037565.D
Acq On : 26 Oct 2018 4:46
Operator : JU/SJ
Sample : J5649-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TWP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

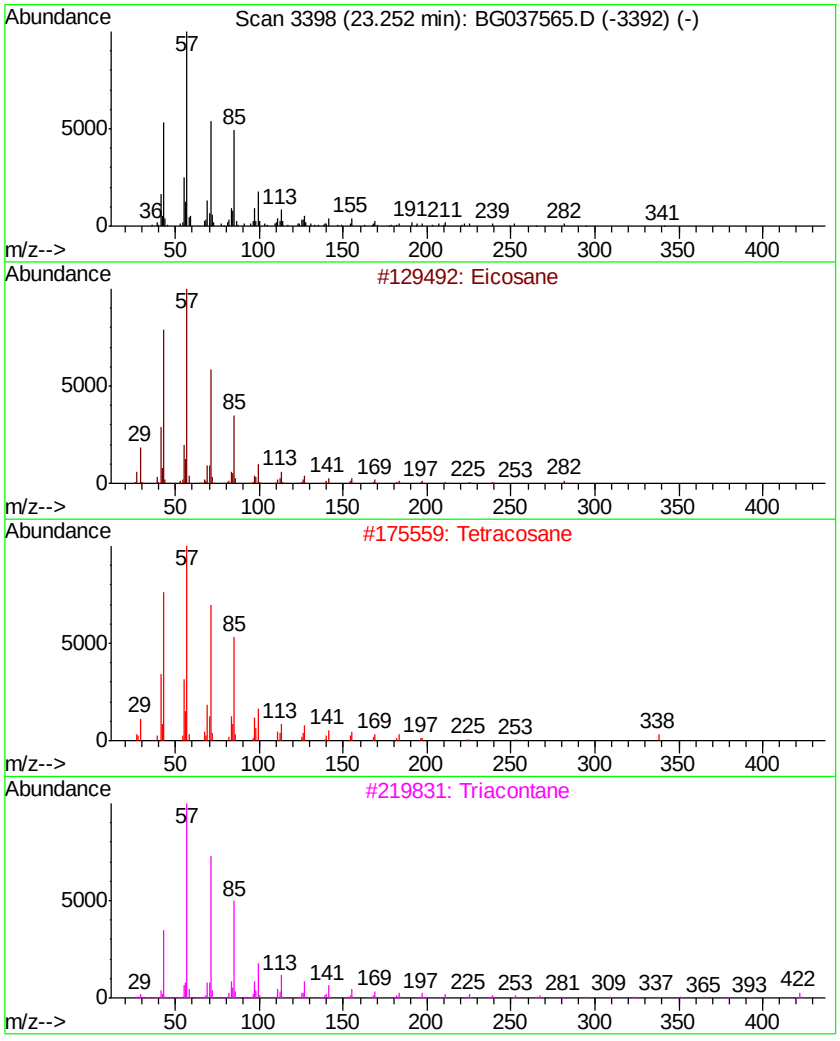
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

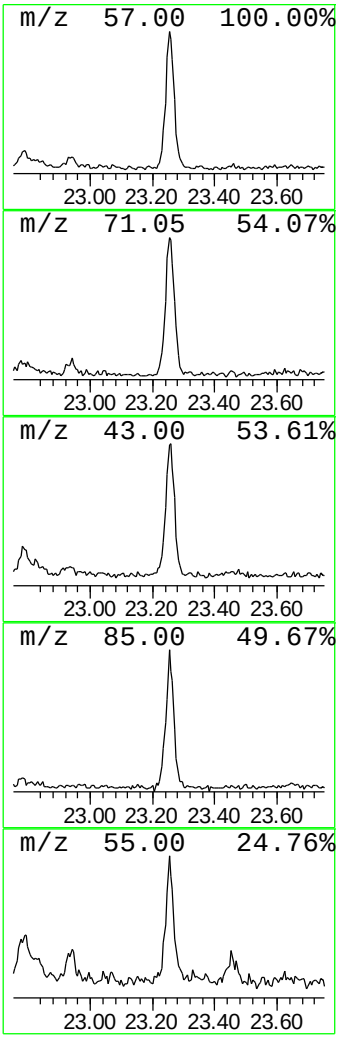
****

Peak Number 6 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.25	2.82 ng	158548	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Tetracosane	338	C24H50	000646-31-1	86
3	Triacontane	422	C30H62	000638-68-6	86
4	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	86
5	Hexatriacontane	507	C36H74	000630-06-8	62





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102518\
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Acq On : 26 Oct 2018 4:46
Operator : JU/SJ
Sample : J5649-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TWP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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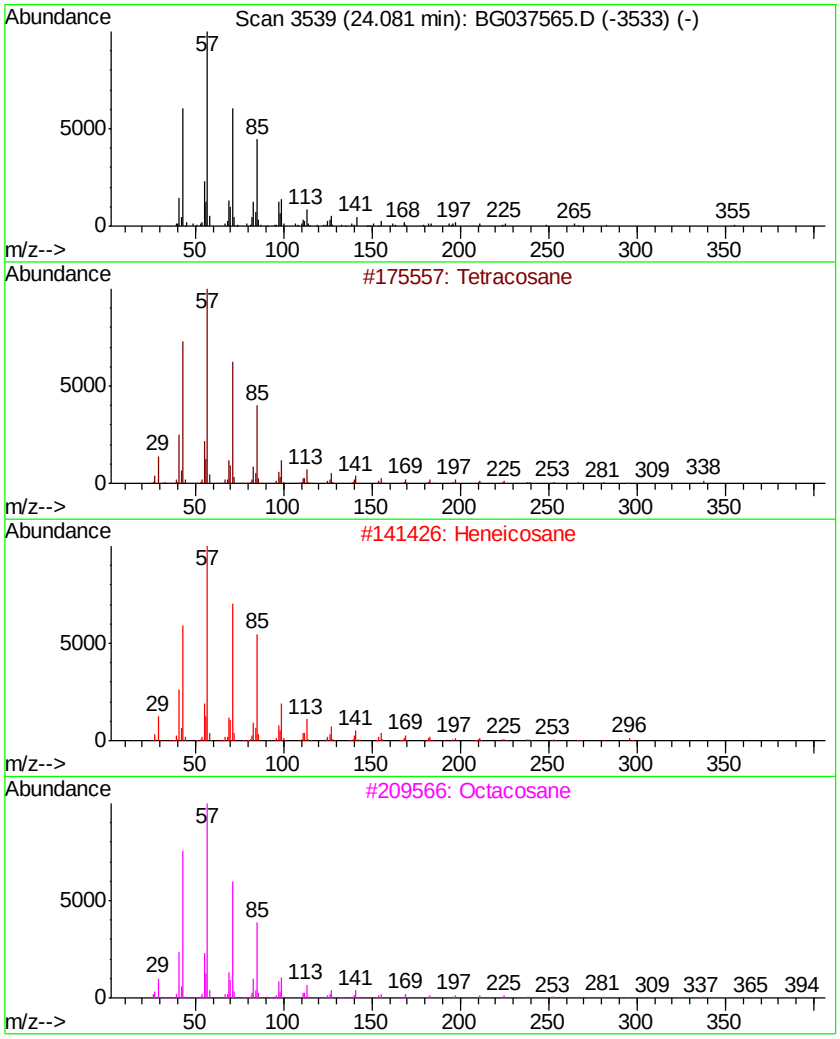
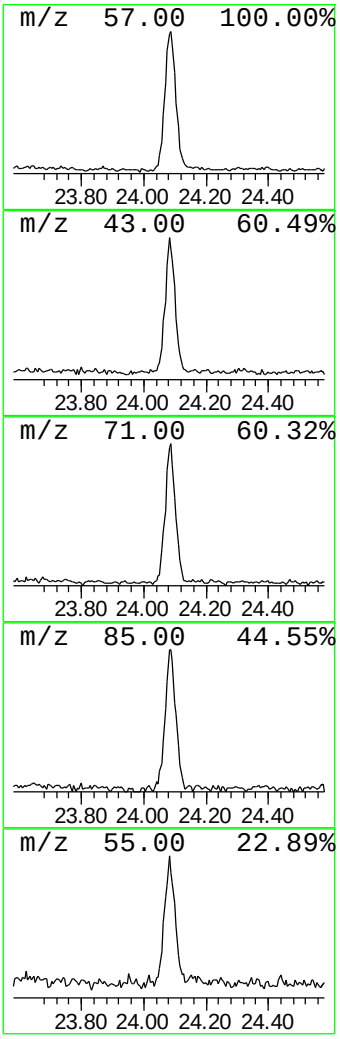
Peak Number 7 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.08	3.29 ng	217750	Perylene-d12	25.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tritetracontane	605	C43H88	007098-21-7	91
5	Hexacosane	366	C26H54	000630-01-3	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102518\
Data File : BG037565.D
Acq On : 26 Oct 2018 4:46
Operator : JU/SJ
Sample : J5649-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TWP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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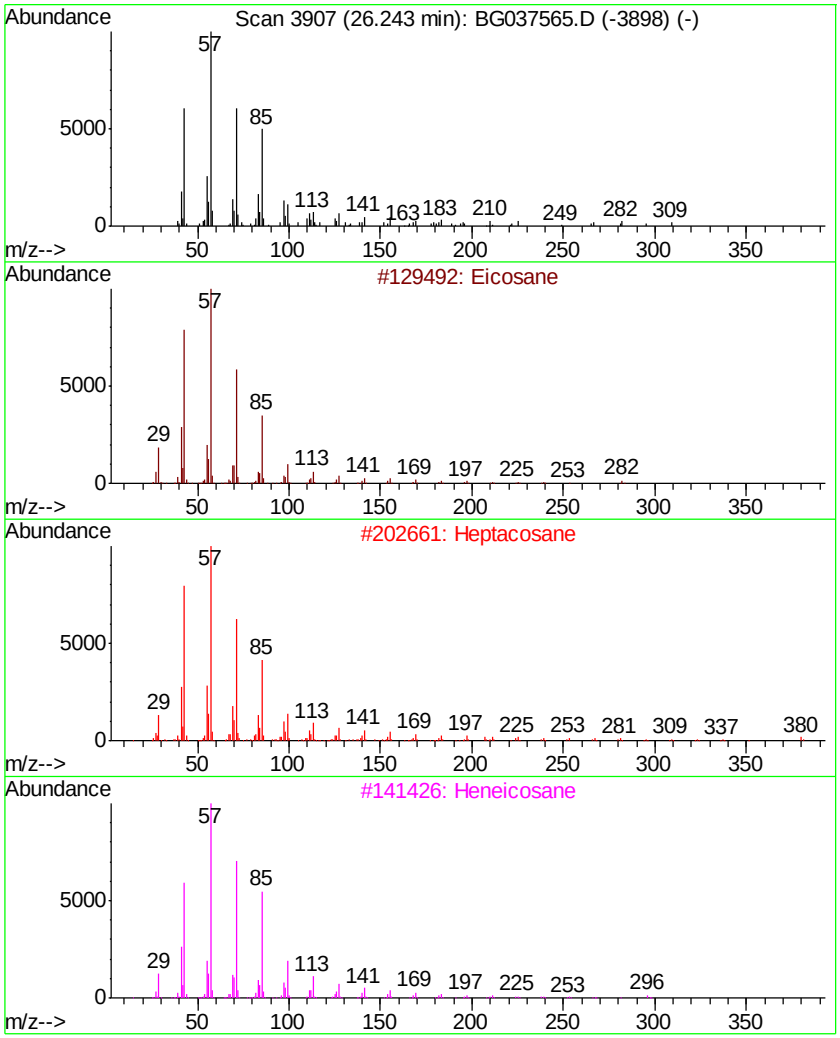
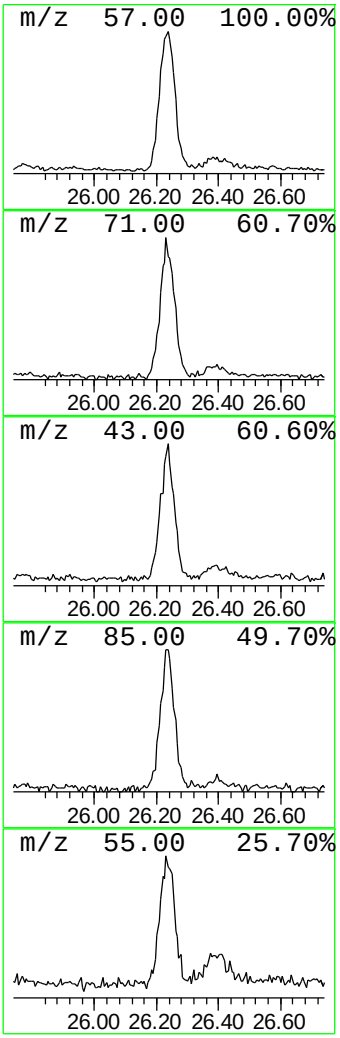
Peak Number 8 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.24	3.45 ng	228320	Perylene-d12	25.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Heptacosane	380	C27H56	000593-49-7	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Octacosane	394	C28H58	000630-02-4	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102518\
Data File : BG037565.D
Acq On : 26 Oct 2018 4:46
Operator : JU/SJ
Sample : J5649-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TWP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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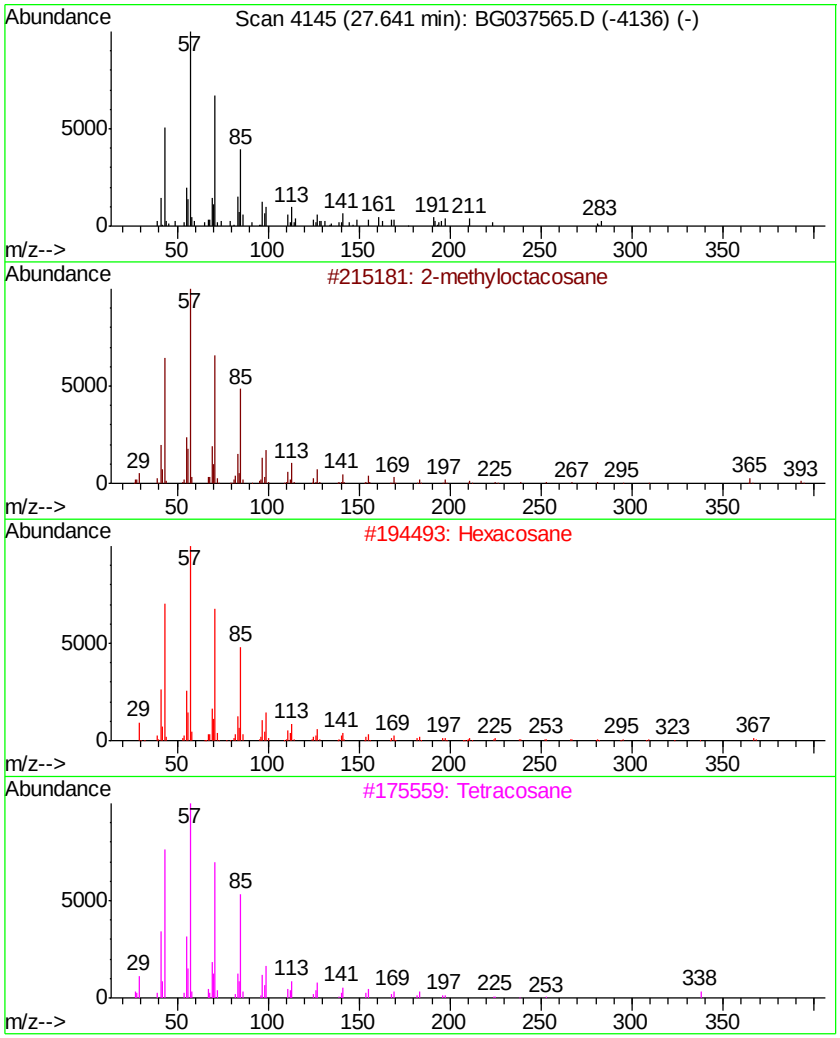
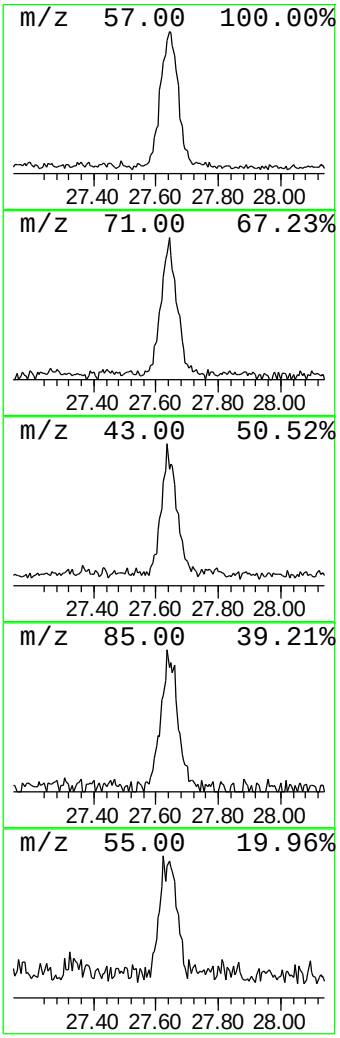
Peak Number 9 2-methyloctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.64	2.15 ng	142210	Perylene-d12	25.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Heneicosane	296	C21H44	000629-94-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG102518\
Data File : BG037565.D
Acq On : 26 Oct 2018 4:46
Operator : JU/SJ
Sample : J5649-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TWP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.63	7.63	76.4	ng	1425430	1	8.11	372968	20.0
n-Hexadecanoic acid	18.34	11.3	ng	626677	4	17.48	1109600	20.0
Octadecanoic acid	19.61	11.3	ng	625623	4	17.48	1109600	20.0
Tricosyl trifluor...	21.37	4.3	ng	242389	5	21.77	1123310	20.0
Eicosane	23.25	2.8	ng	158548	5	21.77	1123310	20.0
Tetracosane	24.08	3.3	ng	217750	6	25.10	1325270	20.0
Heptacosane	26.24	3.5	ng	228320	6	25.10	1325270	20.0
2-methyloctacosane	27.64	2.1	ng	142210	6	25.10	1325270	20.0