LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103018\
Data File : BG037657.D
Acq On : 30 Oct 2018 17:19
Operator : JU/SJ
Sample : J5692-20
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CAL-IDW-20181025

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	5.638	394	400	412	rBV	281842	479433	16.31%	2.713%
2	7.242	666	673	675	rBV	203583	337038	11.47%	1.907%
3	7.624	730	738	749	rBV	542046	978847	33.30%	5.539%
4	8.100	812	819	832	rBV	199320	351534	11.96%	1.989%
5	8.423	866	874	884	rBV	491353	891240	30.32%	5.043%
6	9.275	1011	1019	1031	rBV	457692	839183	28.55%	4.749%
7	10.920	1292	1299	1308	rBV	303482	557132	18.96%	3.153%
8	13.352	1706	1713	1724	rBV	1276934	2089411	71.09%	11.824%
9	14.175	1848	1853	1860	rBV	98197	147112	5.01%	0.832%
10	14.733	1941	1948	1967	rBV2	519254	976341	33.22%	5.525%
11	16.220	2192	2201	2214	rBV	963501	1530902	52.09%	8.663%
12	17.483	2409	2416	2424	rBV2	666722	1085628	36.94%	6.143%
13	18.341	2555	2562	2572	rBV	193530	321882	10.95%	1.822%
14	19.604	2772	2777	2784	rBV2	97044	157085	5.34%	0.889%
15	20.080	2852	2858	2870	rBV	2214714	2939055	100.00%	16.632%
16	20.849	2984	2989	2993	rBV4	22387	36233	1.23%	0.205%
17	21.372	3072	3078	3089	rBV6	66693	191631	6.52%	1.084%
18	21.766	3138	3145	3157	rBV2	603139	1089113	37.06%	6.163%
19	21.919	3166	3171	3178	rVB	48440	73133	2.49%	0.414%
20	22.542	3271	3277	3285	rBV2	79745	138274	4.70%	0.782%
21	23.253	3391	3398	3408	rVB2	123683	245135	8.34%	1.387%
22	24.081	3532	3539	3553	rVB2	139783	320440	10.90%	1.813%
23	25.097	3696	3712	3730	rBV4	330614	1392612	47.38%	7.881%
24	26.231	3894	3905	3916	rVB2	95475	304195	10.35%	1.721%
25	27.624	4133	4142	4159	rVB4	48388	198642	6.76%	1.124%

Sum of corrected areas: 17671231

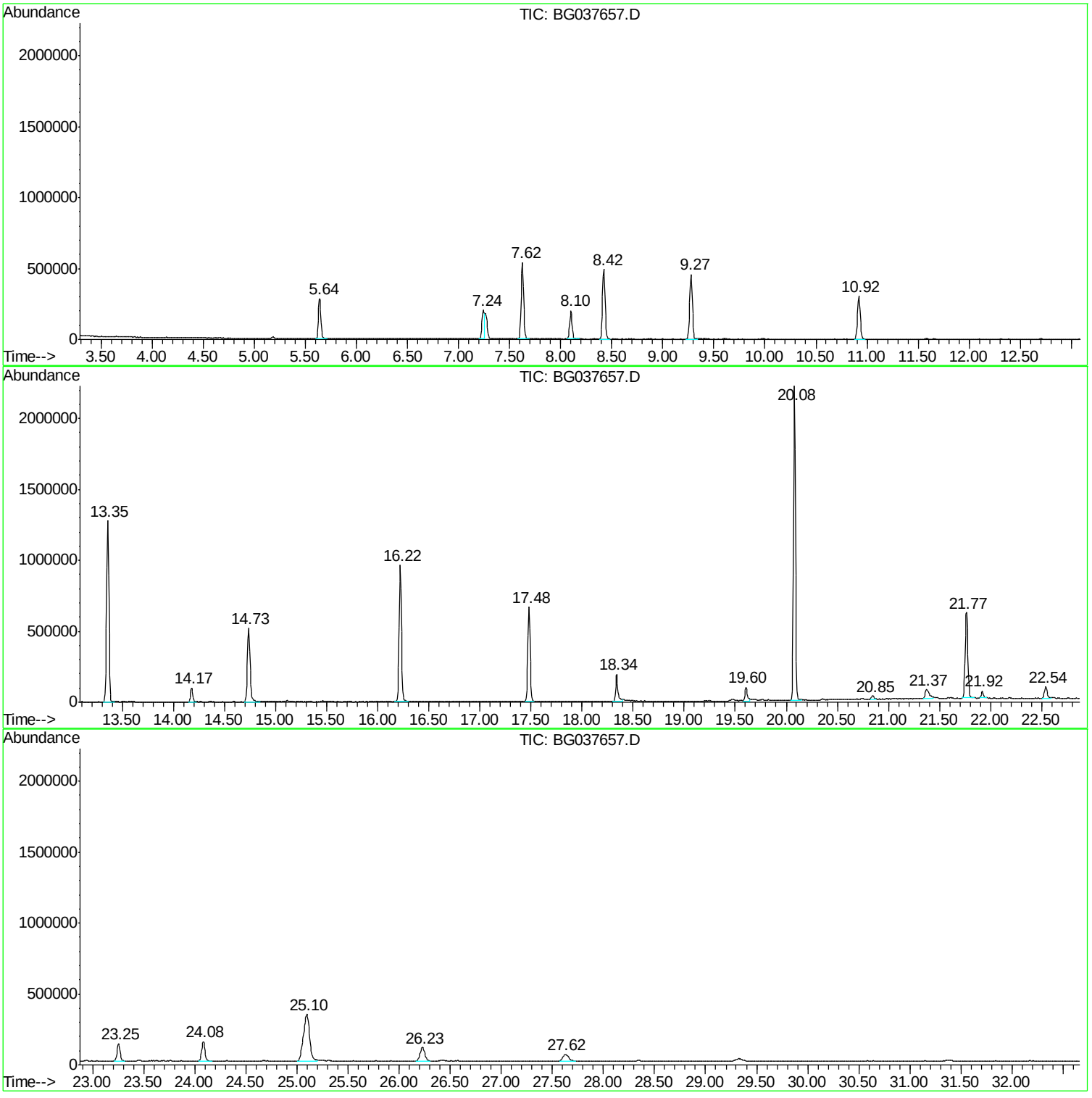
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103018\
Data File : BG037657.D
Acq On : 30 Oct 2018 17:19
Operator : JU/SJ
Sample : J5692-20
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CAL-IDW-20181025

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\BG103018\
Data File : BG037657.D
Acq On : 30 Oct 2018 17:19
Operator : JU/SJ
Sample : J5692-20
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CAL-IDW-20181025

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

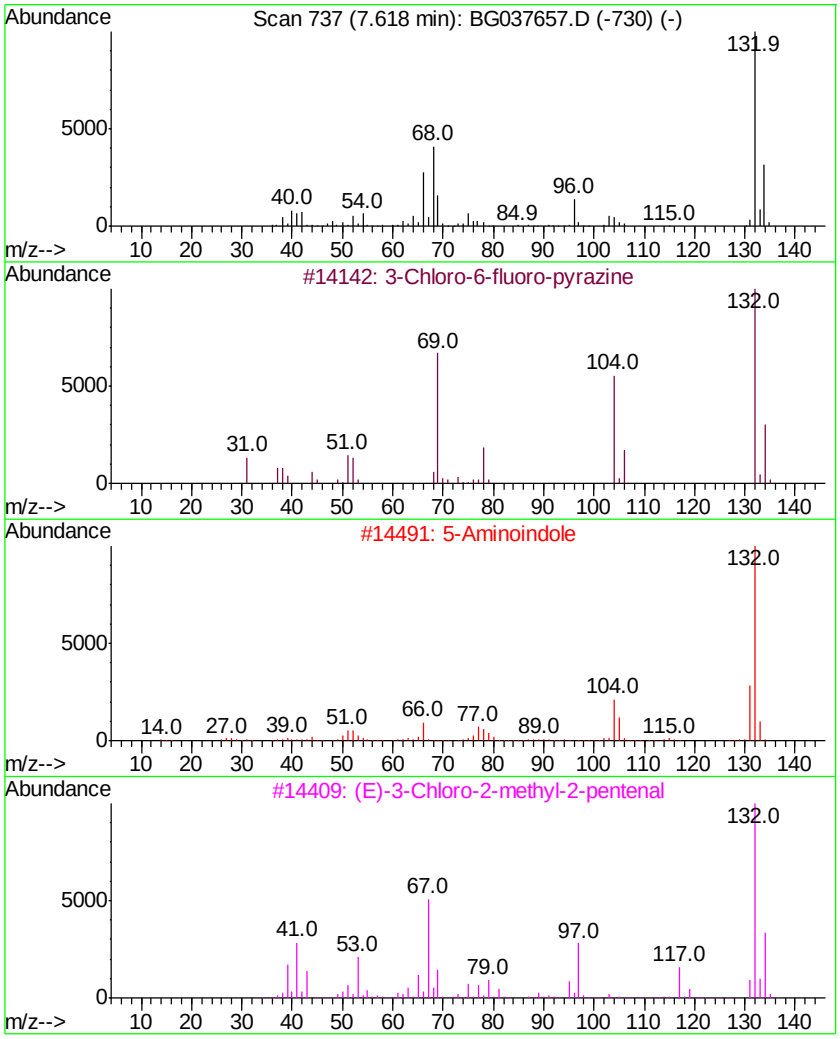
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

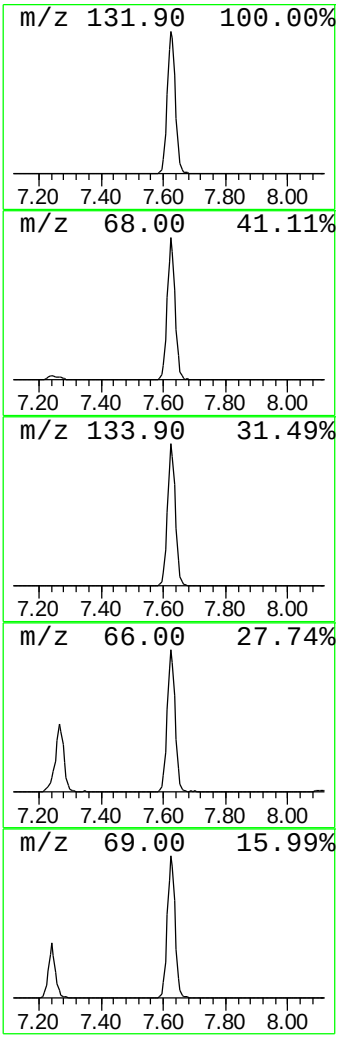
****

Peak Number 1 unknown7.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	55.69 ng	978847	1,4-Dichlorobenzene-d4	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	22
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4	Amphetaminil	250	C17H18N2	017590-01-1	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12





Library Search Compound Report

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Operator : JU/SJ
Sample : J5692-20
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CAL-IDW-20181025

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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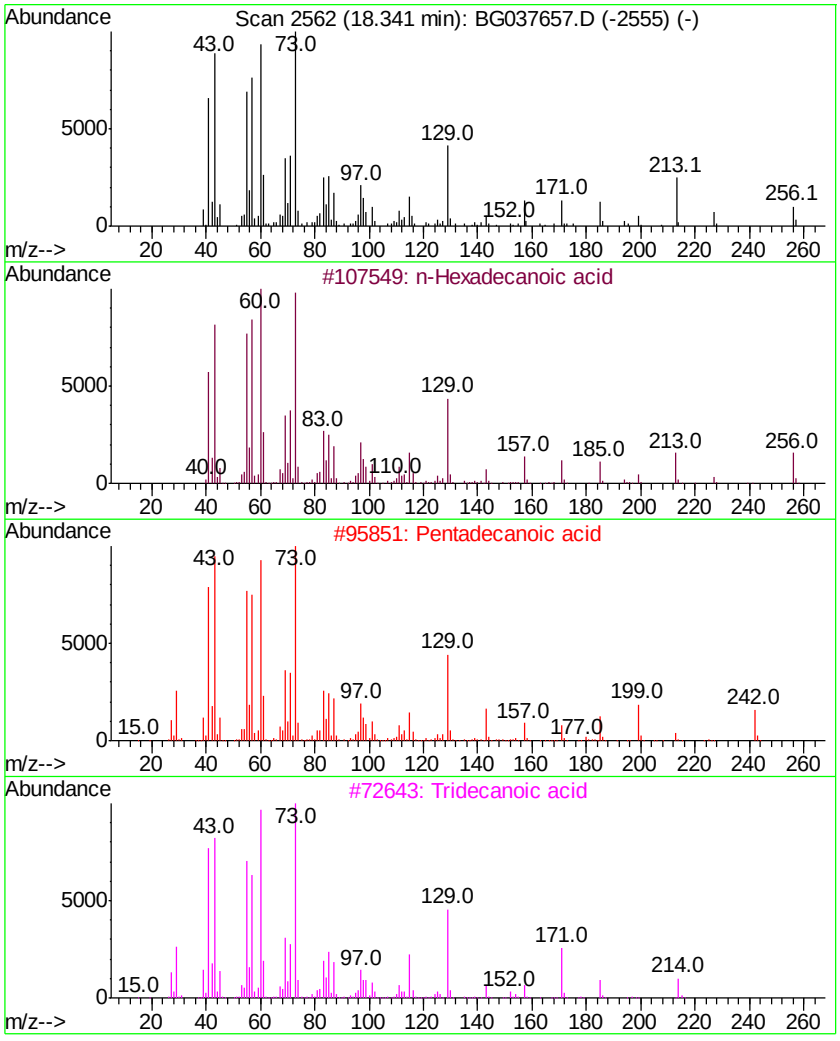
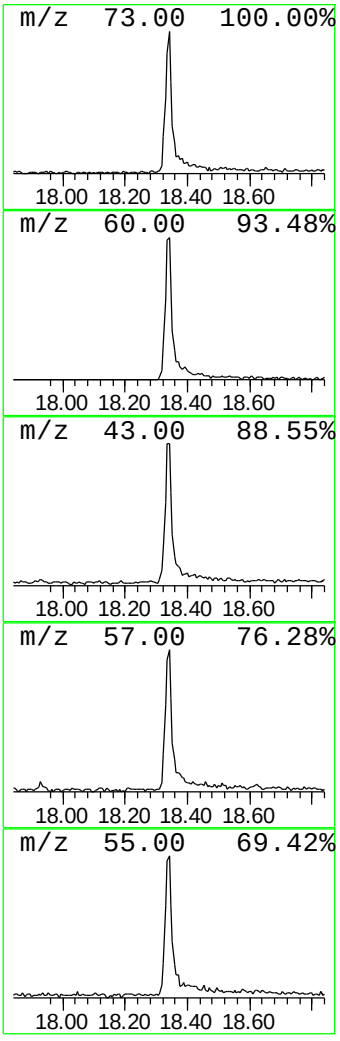
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	5.93 ng	321882	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103018\
Data File : BG037657.D
Acq On : 30 Oct 2018 17:19
Operator : JU/SJ
Sample : J5692-20
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CAL-IDW-20181025

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

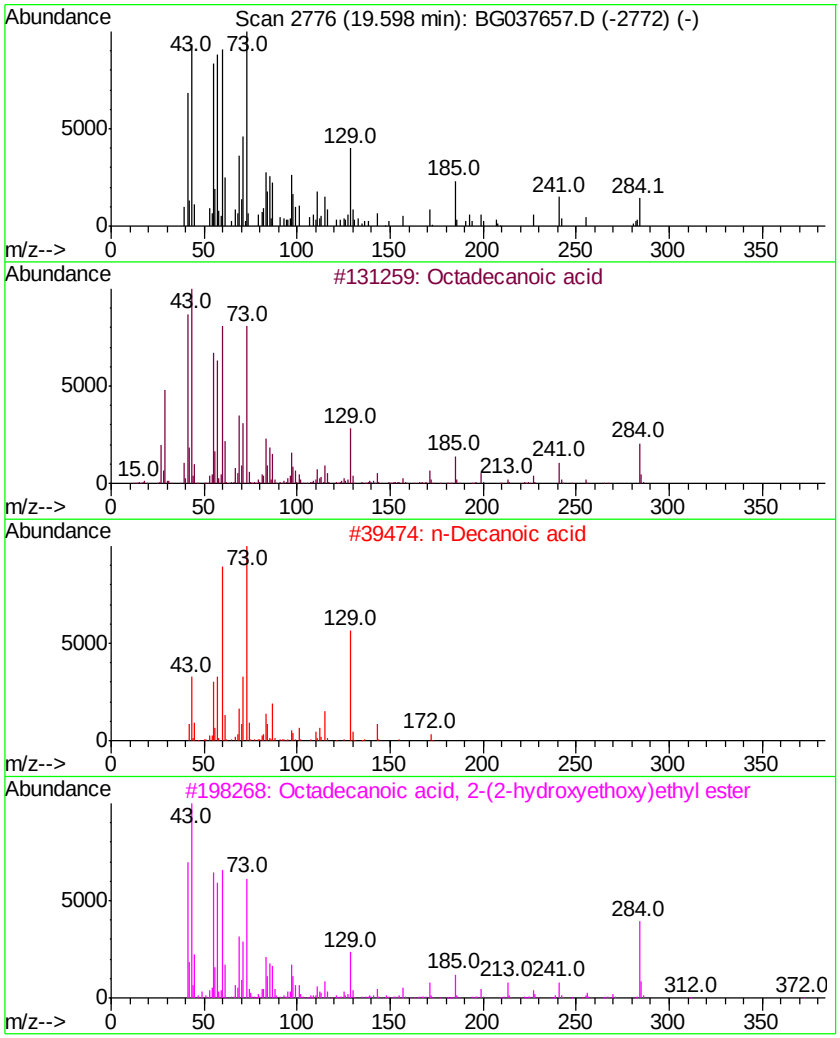
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

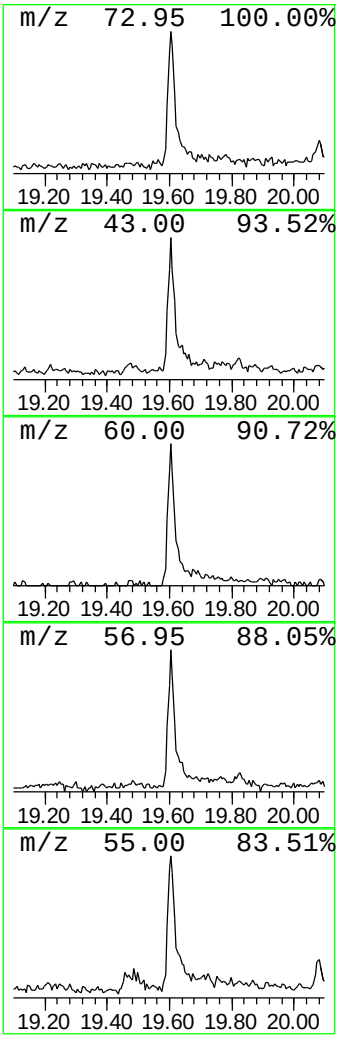
****

Peak Number 4 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.60	2.89 ng	157085	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Decanoic acid	172	C10H20O2	000334-48-5	90
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	81





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103018\
Data File : BG037657.D
Acq On : 30 Oct 2018 17:19
Operator : JU/SJ
Sample : J5692-20
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CAL-IDW-20181025

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

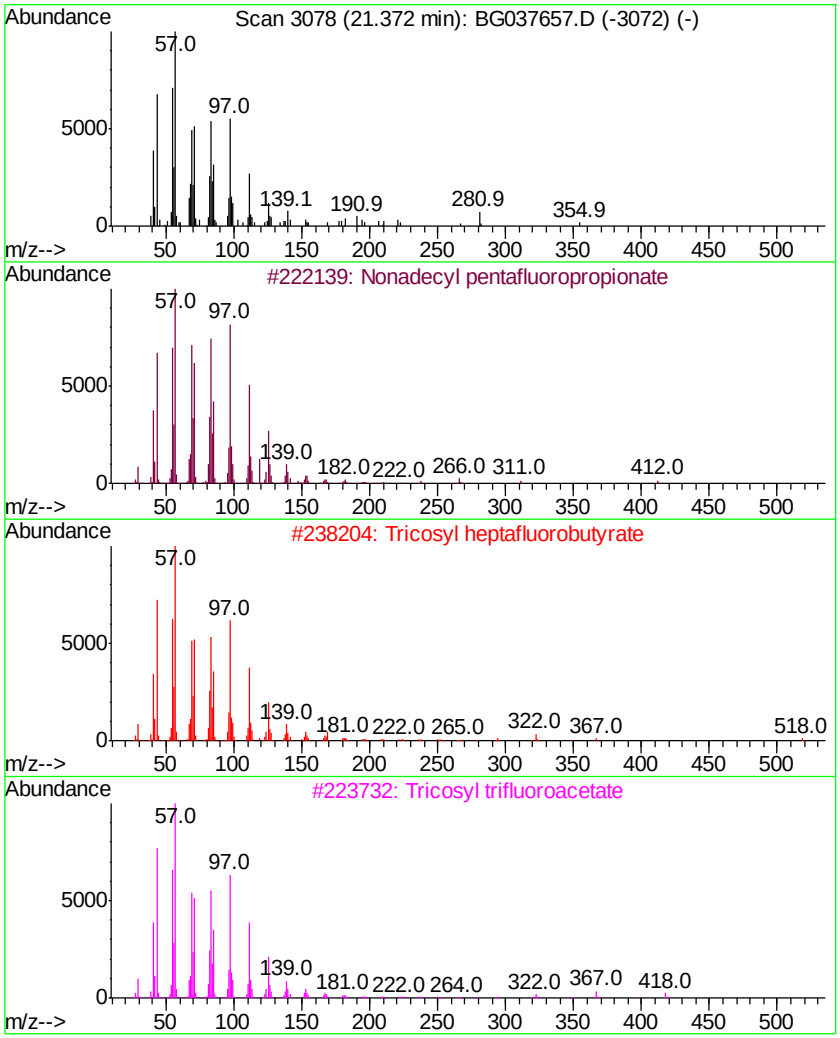
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

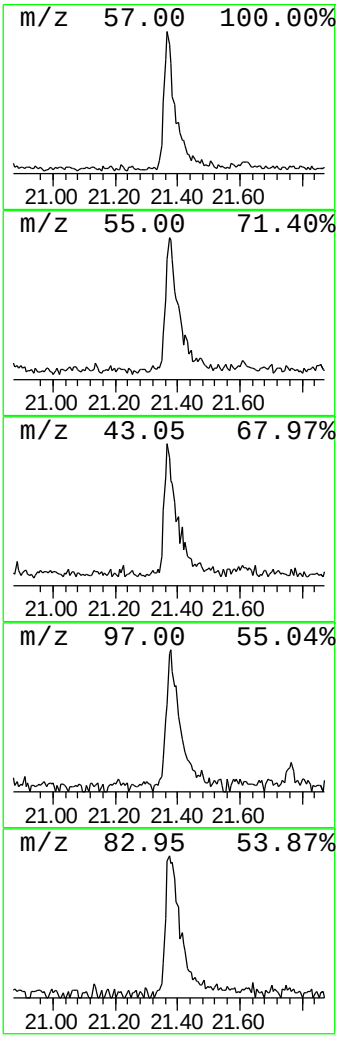
****

Peak Number 5 Nonadecyl pentafluoropropio... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.37	3.52 ng	191631	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	90
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	87
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87





Library Search Compound Report

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Operator : JU/SJ
Sample : J5692-20
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CAL-IDW-20181025

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
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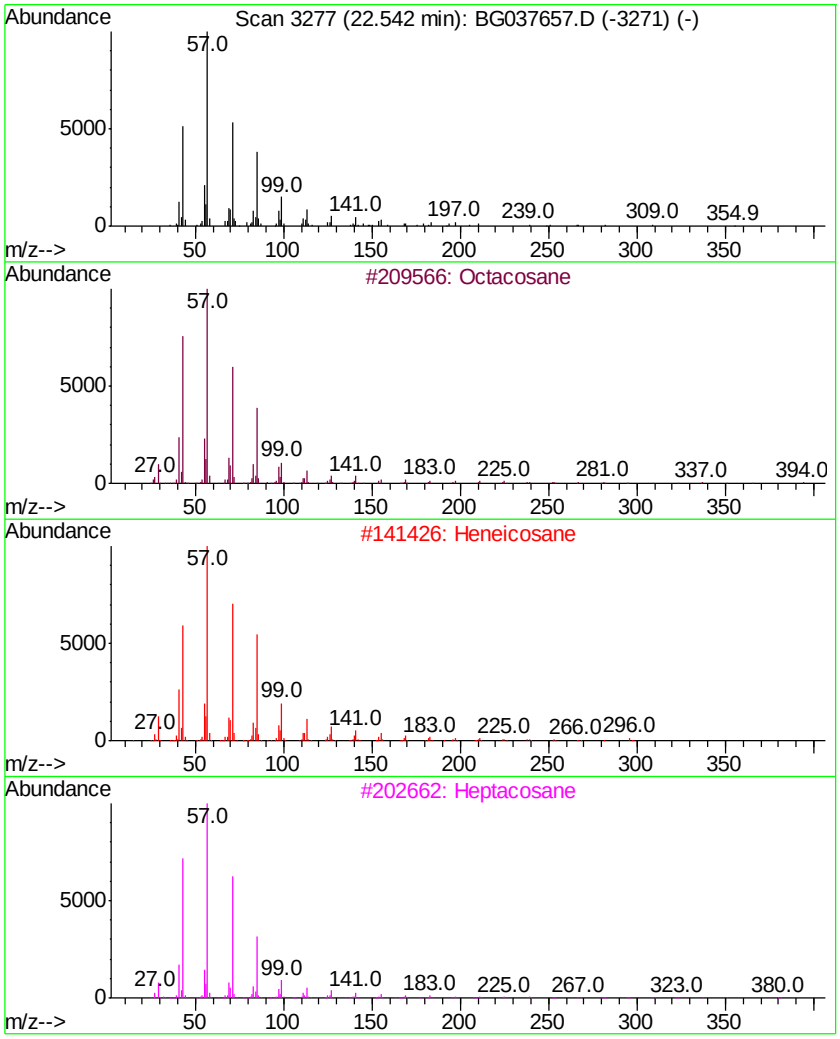
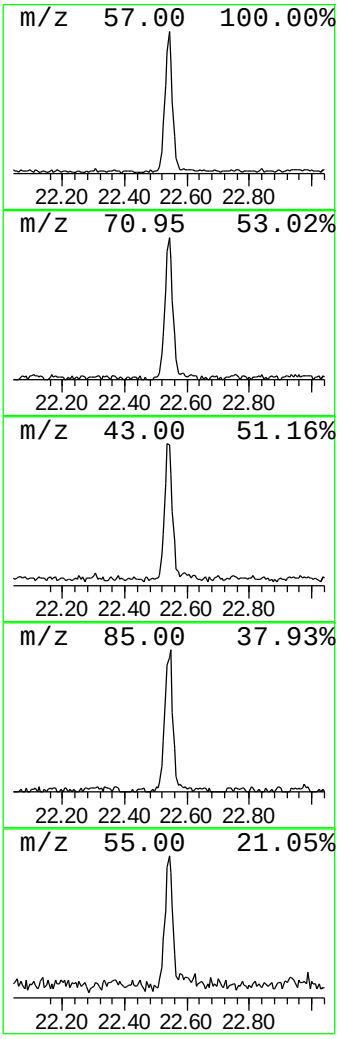
****

Peak Number 6 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.54	2.54 ng	138274	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Heptacosane	380	C27H56	000593-49-7	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Docosane	310	C22H46	000629-97-0	86





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CAL-IDW-20181025

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

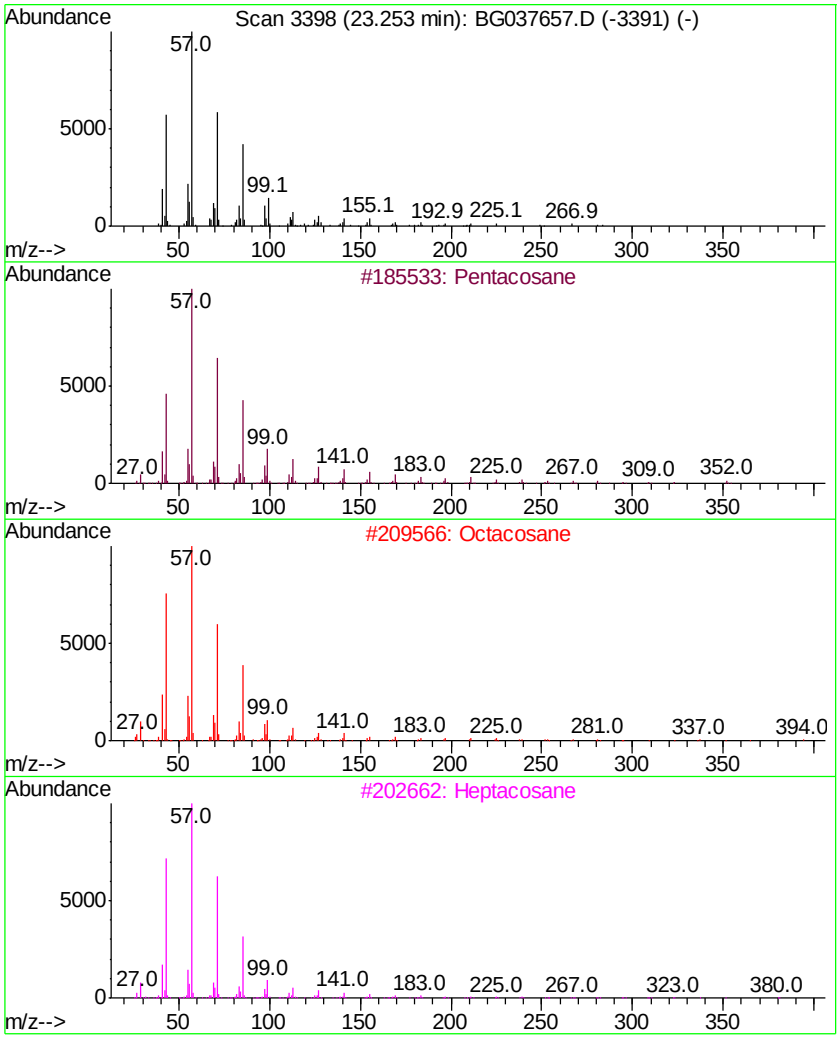
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

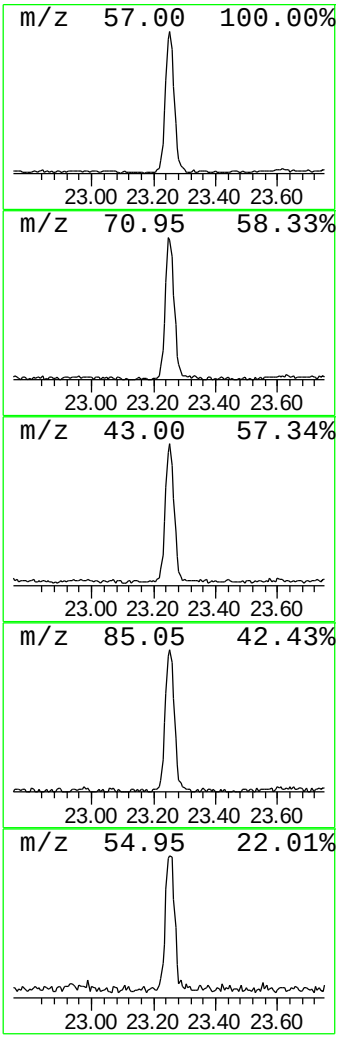
****

Peak Number 7 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.25	4.50 ng	245135	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Octadecane	254	C18H38	000593-45-3	90





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Instrument : BNA_G
ClientSampleId : CAL-IDW-20181025

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

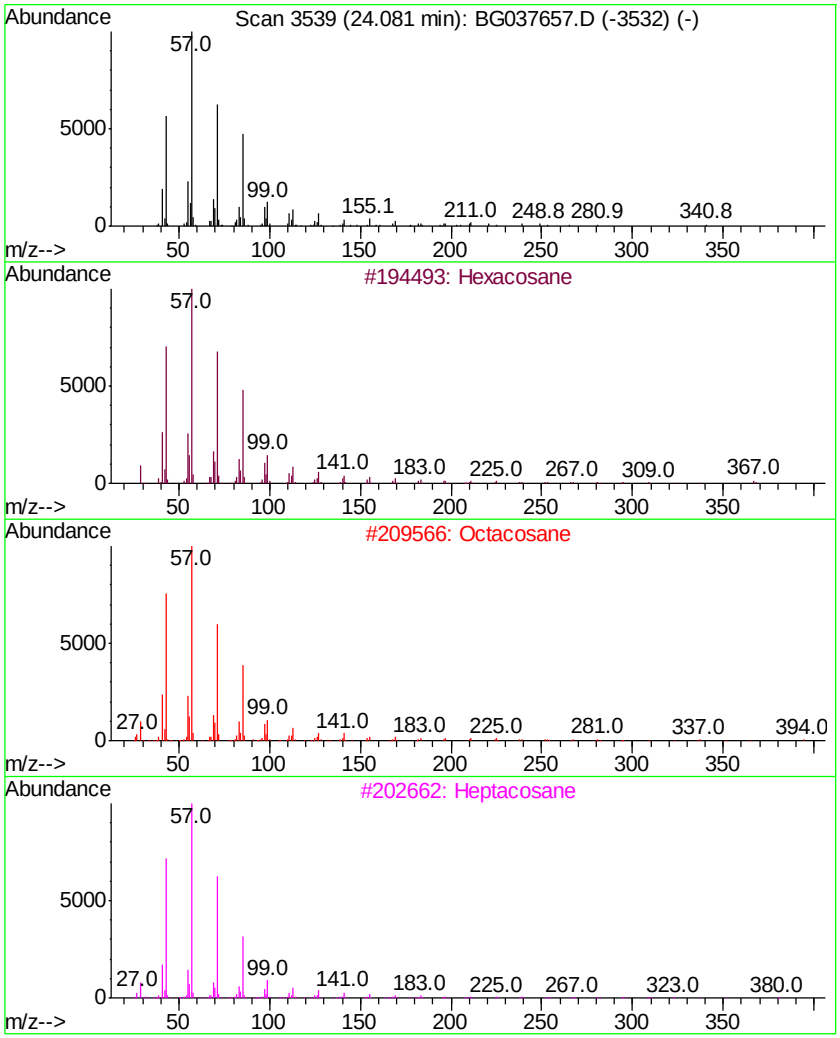
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

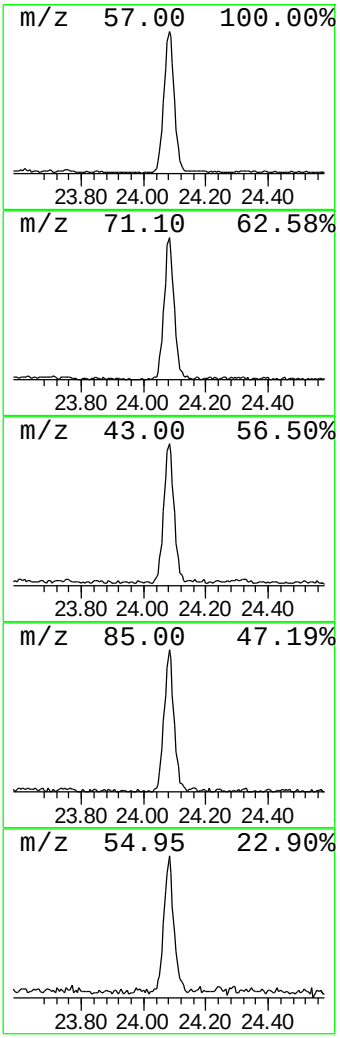
****

Peak Number 8 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.08	4.60 ng	320440	Perylene-d12	25.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	93
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptacosane	380	C27H56	000593-49-7	87
4	Eicosane	282	C20H42	000112-95-8	87
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87





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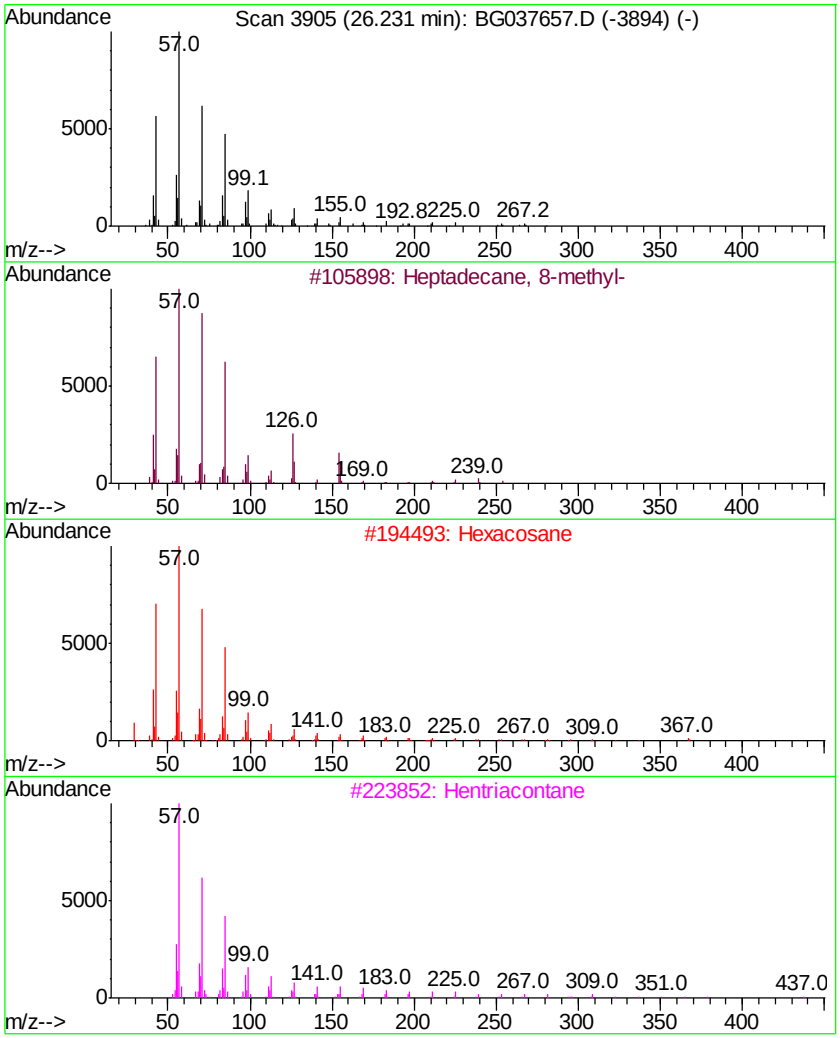
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

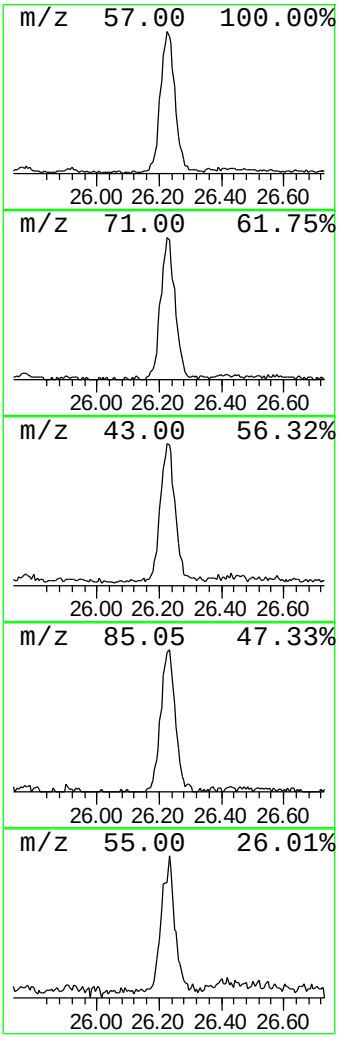
****

Peak Number 9 Heptadecane, 8-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.23	4.37 ng	304195	Perylene-d12	25.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	93
2	Hexacosane	366	C26H54	000630-01-3	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heneicosane	296	C21H44	000629-94-7	91





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_G
ClientSampleId : CAL-IDW-20181025

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
unknown7.62	7.62	55.7	ng	978847	1	8.10	351534	20.0
n-Hexadecanoic acid	18.34	5.9	ng	321882	4	17.48	1085630	20.0
Octadecanoic acid	19.60	2.9	ng	157085	4	17.48	1085630	20.0
Nonadecyl pentafl...	21.37	3.5	ng	191631	5	21.77	1089110	20.0
Octacosane	22.54	2.5	ng	138274	5	21.77	1089110	20.0
Pentacosane	23.25	4.5	ng	245135	5	21.77	1089110	20.0
Hexacosane	24.08	4.6	ng	320440	6	25.10	1392610	20.0
Heptadecane, 8-me...	26.23	4.4	ng	304195	6	25.10	1392610	20.0