LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG083119\
Data File : BG042637.D
Acq On : 31 Aug 2019 16:29
Operator : HP/JU
Sample : K4577-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-1

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-BG082219.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	3.117	3	5	23	rVB	1415524	1779083	66.32%	13.229%
2	5.549	413	419	430	rBV	178573	305713	11.40%	2.273%
3	7.159	684	693	710	rBV	108937	222754	8.30%	1.656%
4	7.529	746	756	767	rBV	384993	692401	25.81%	5.149%
5	7.993	829	835	844	rBV	104135	177604	6.62%	1.321%
6	8.322	883	891	903	rBV	398935	691452	25.78%	5.142%
7	9.162	1026	1034	1049	rBV	274100	509542	18.99%	3.789%
8	10.819	1309	1316	1332	rBV	123335	237696	8.86%	1.767%
9	13.275	1727	1734	1752	rBV	951025	1540194	57.41%	11.453%
10	14.104	1868	1875	1885	rBV	72736	116468	4.34%	0.866%
11	14.656	1961	1969	1981	rBV2	238149	387783	14.46%	2.884%
12	16.148	2216	2223	2244	rBV	803929	1288090	48.02%	9.578%
13	17.406	2431	2437	2447	rBV2	327932	507946	18.94%	3.777%
14	18.299	2584	2589	2597	rBV2	65865	95179	3.55%	0.708%
15	19.162	2731	2736	2741	rBV5	12890	30047	1.12%	0.223%
16	20.020	2876	2882	2890	rBV	2077825	2682571	100.00%	19.947%
17	20.819	3015	3018	3021	rVB2	21780	26828	1.00%	0.199%
18	21.325	3099	3104	3114	rBV	102562	195479	7.29%	1.454%
19	21.683	3158	3165	3178	rVB2	377796	644620	24.03%	4.793%
20	21.871	3193	3197	3201	rBV2	37954	48756	1.82%	0.363%
21	22.482	3296	3301	3306	rBV	44957	72039	2.69%	0.536%
22	23.181	3410	3420	3427	rBV	54197	106164	3.96%	0.789%
23	23.369	3444	3452	3461	rBV	69002	141105	5.26%	1.049%
24	23.992	3551	3558	3565	rBV2	49387	104707	3.90%	0.779%
25	24.920	3706	3716	3732	rBV2	245670	776062	28.93%	5.771%
26	26.090	3906	3915	3923	rBV4	22450	67969	2.53%	0.505%

Sum of corrected areas: 13448252

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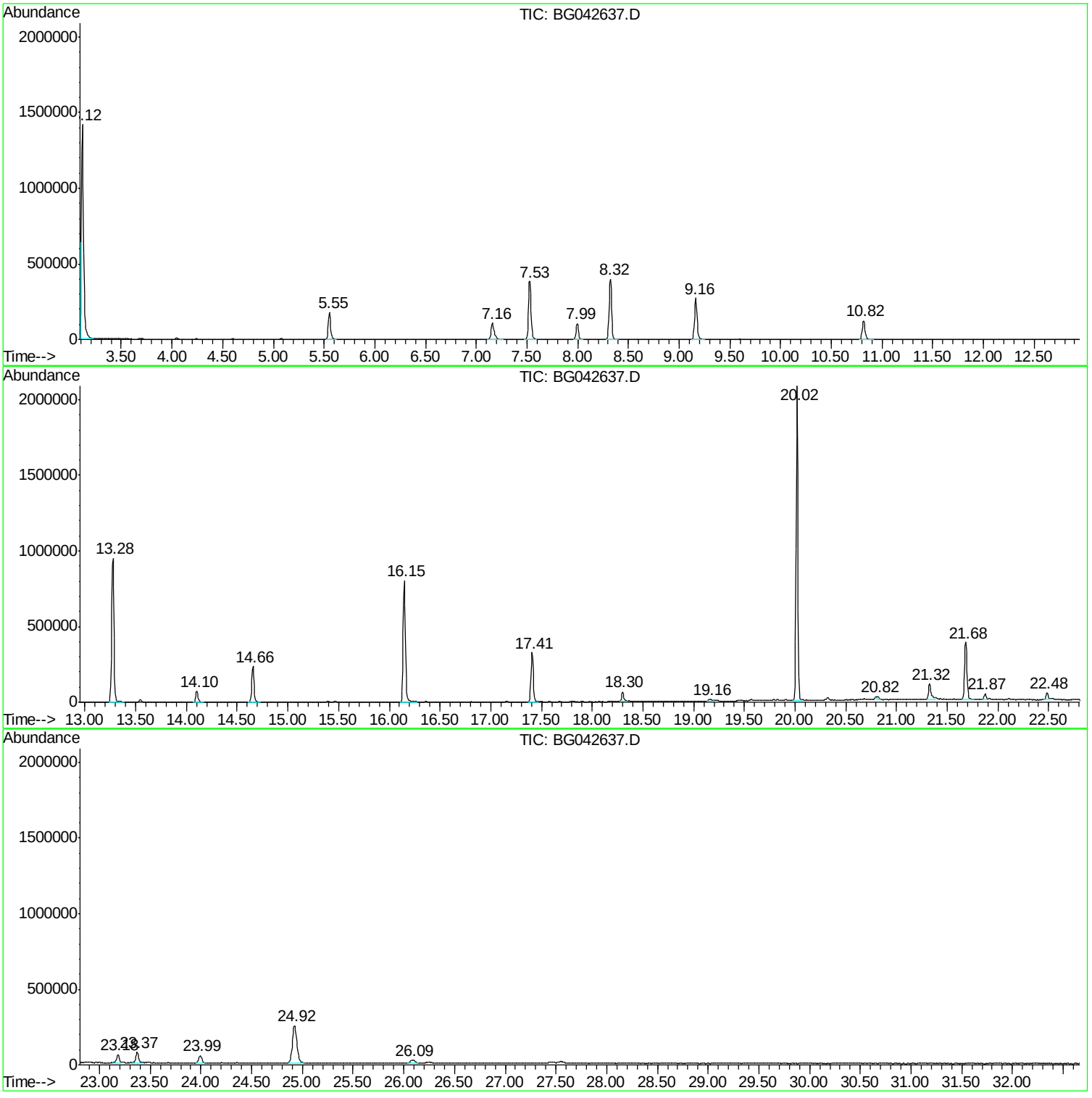
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG083119\
Data File : BG042637.D
Acq On : 31 Aug 2019 16:29
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Sample : K4577-07
Misc :
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Instrument : BNA_G
ClientSampleId : GW-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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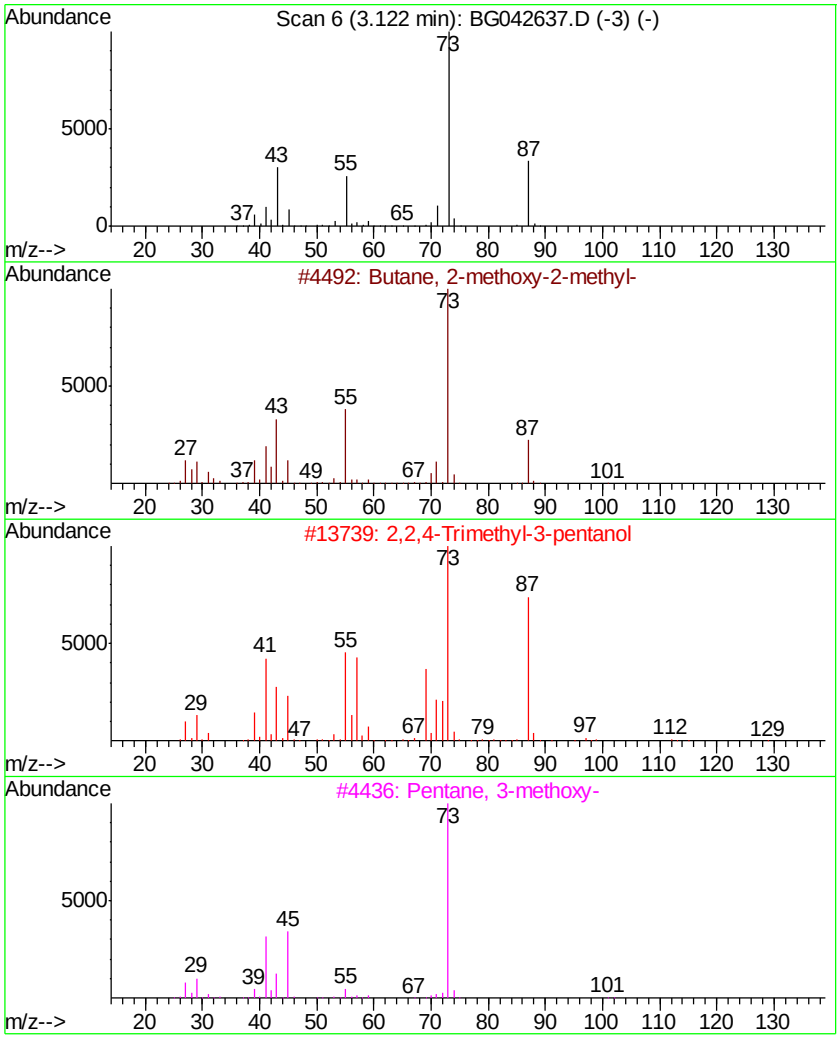
TIC Integration Parameters: LSCINT.P

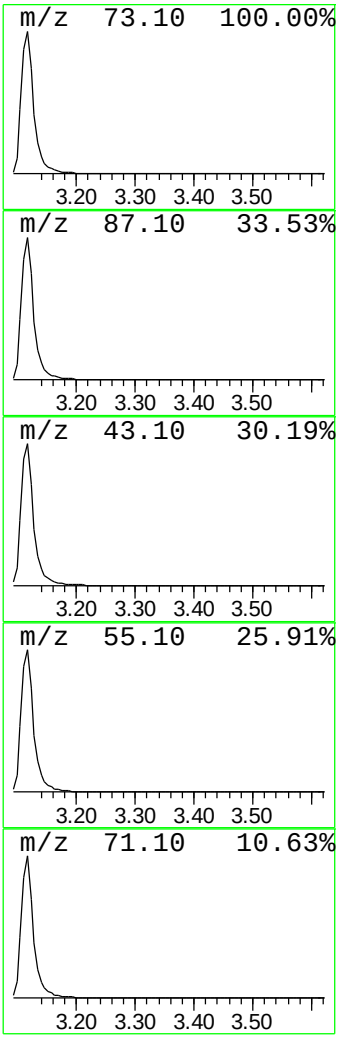
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	200.34 ng	1779080	1,4-Dichlorobenzene-d4	8.00

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	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG083119\
Data File : BG042637.D
Acq On : 31 Aug 2019 16:29
Operator : HP/JU
Sample : K4577-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

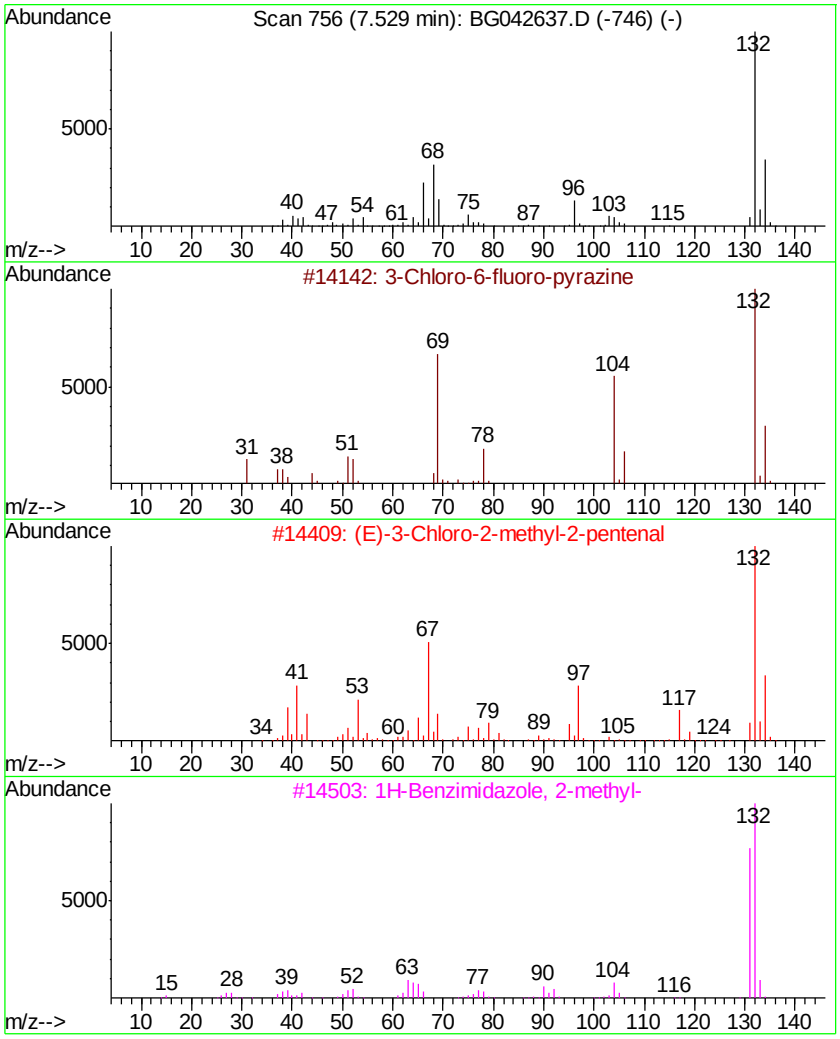
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

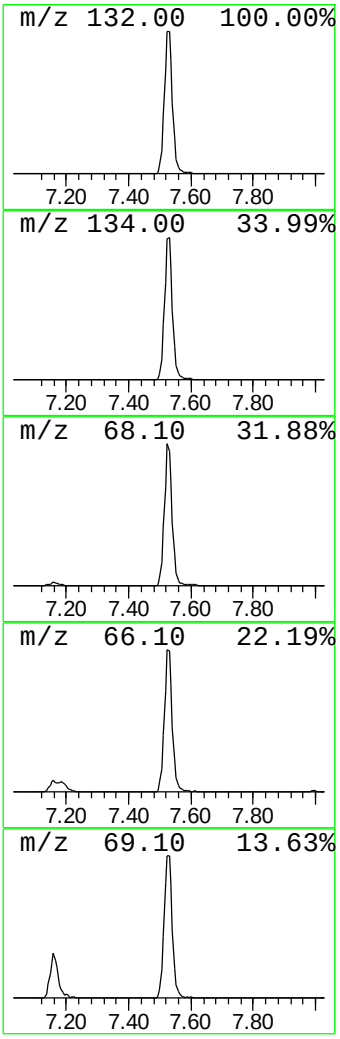
****

Peak Number 2 unknown7.53 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	77.97 ng	692401	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG083119\
Data File : BG042637.D
Acq On : 31 Aug 2019 16:29
Operator : HP/JU
Sample : K4577-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

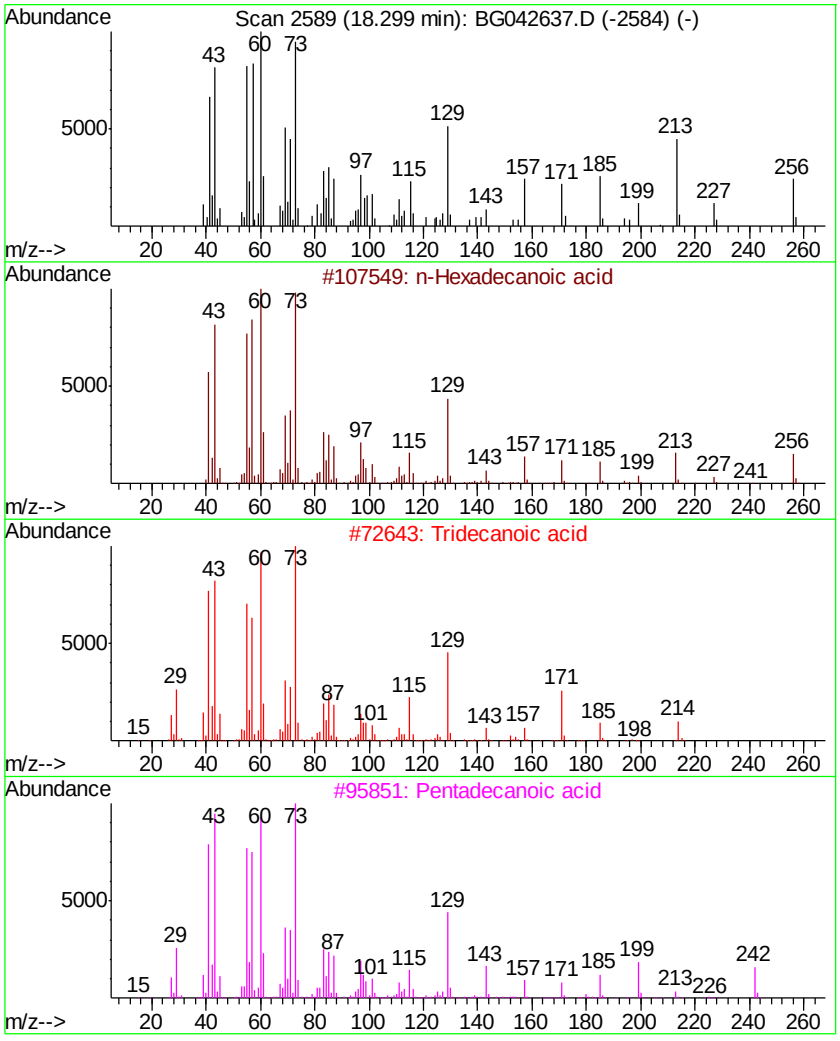
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

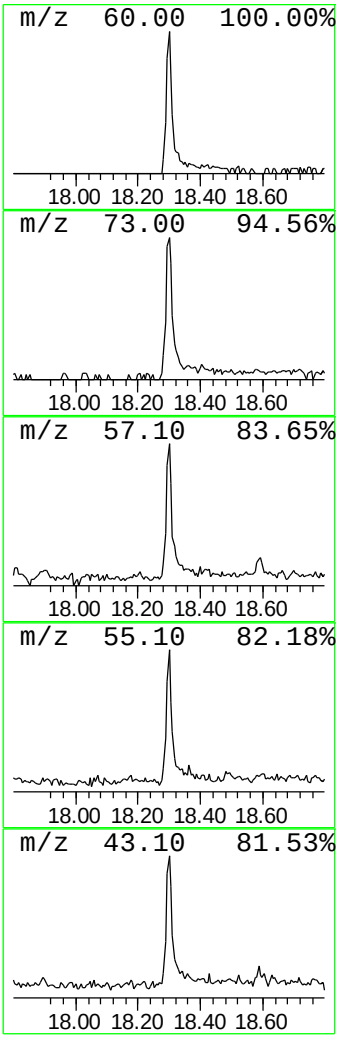
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	3.75 ng	95179	Phenanthrene-d10	17.41

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	58
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5	Dodecanoic acid	200	C12H24O2	000143-07-7	49





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG083119\
Data File : BG042637.D
Acq On : 31 Aug 2019 16:29
Operator : HP/JU
Sample : K4577-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.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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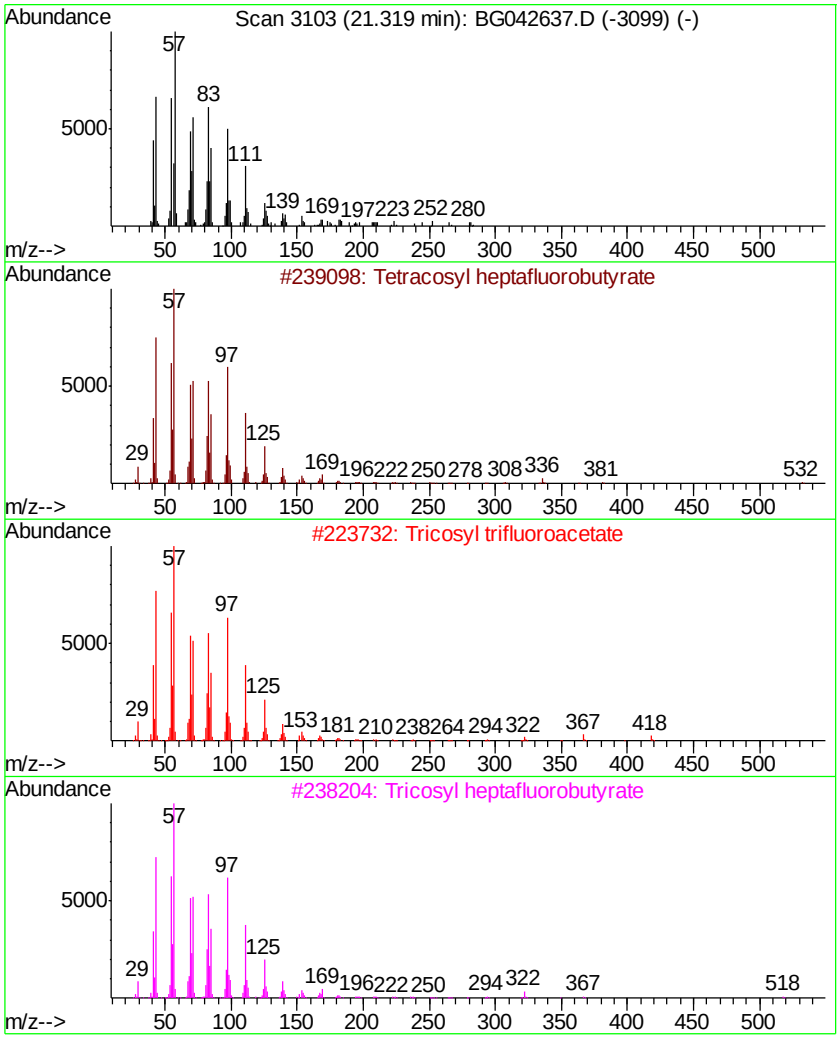
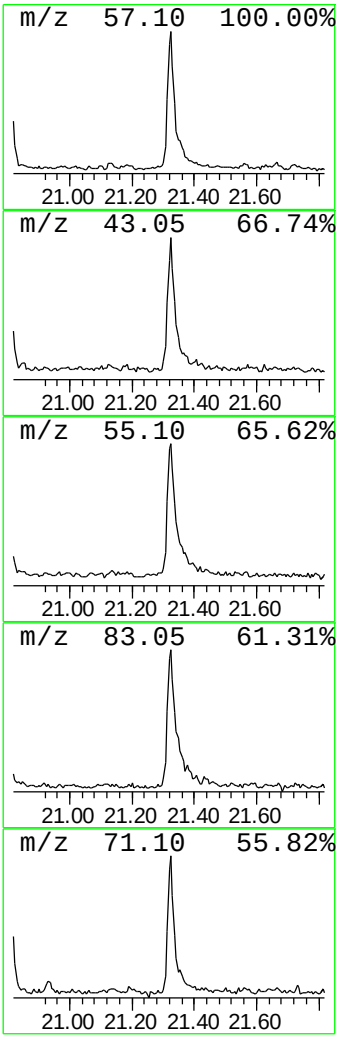
Peak Number 5 Tetracosyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	6.06 ng	195479	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	93
2	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
3	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG083119\
Data File : BG042637.D
Acq On : 31 Aug 2019 16:29
Operator : HP/JU
Sample : K4577-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

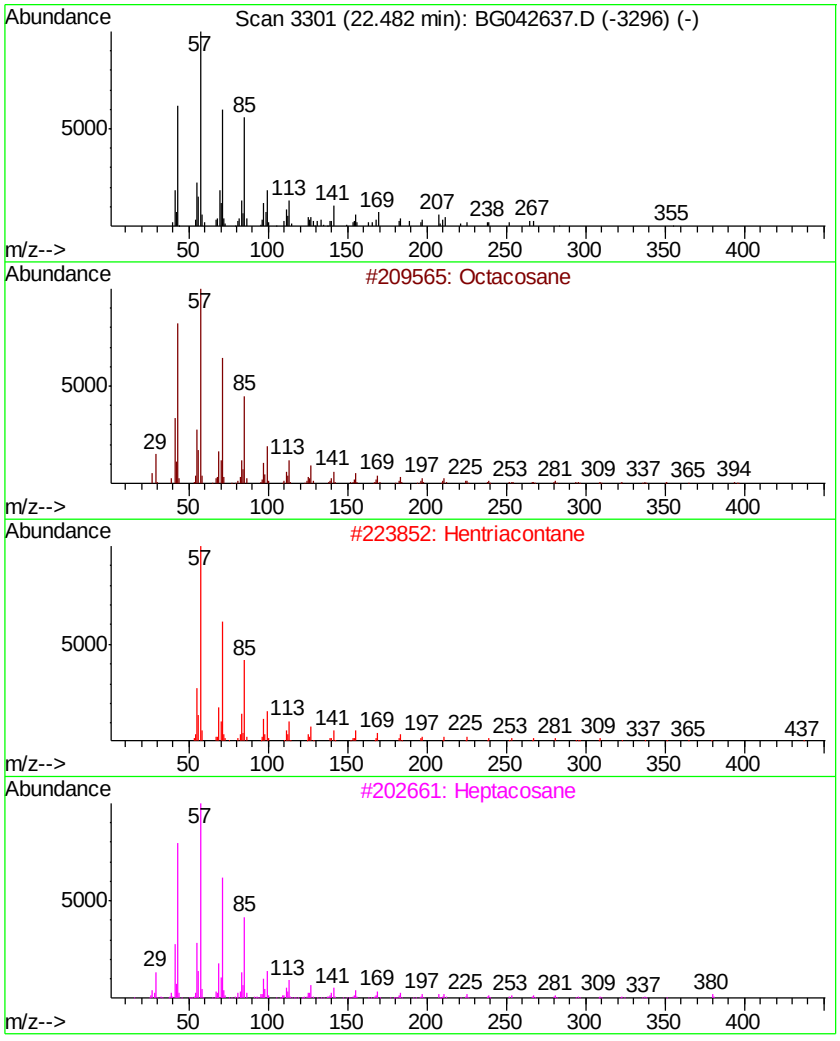
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

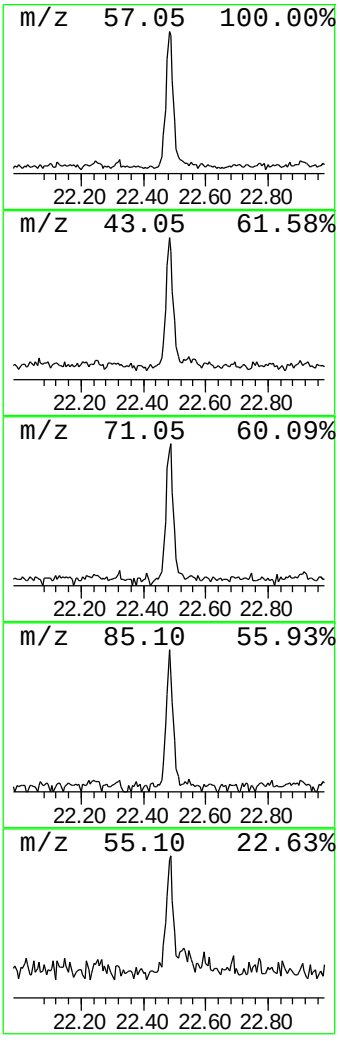
****

Peak Number 6 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.48	2.24 ng	72039	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG083119\
Data File : BG042637.D
Acq On : 31 Aug 2019 16:29
Operator : HP/JU
Sample : K4577-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

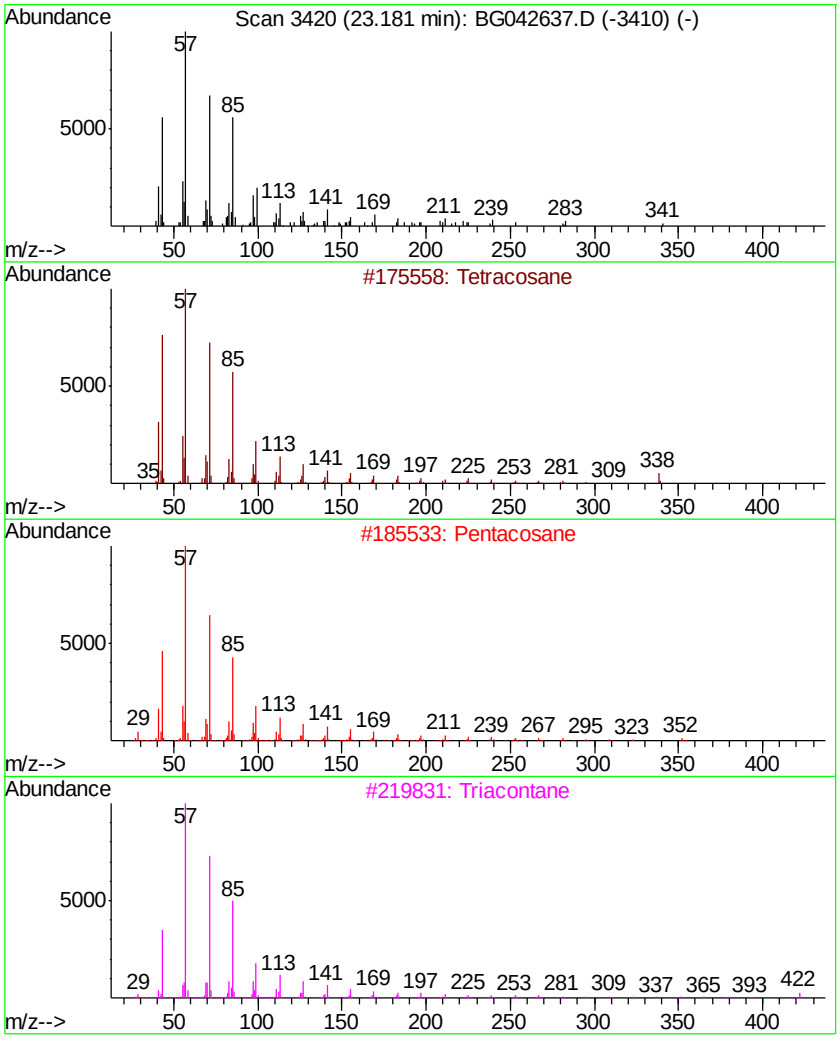
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

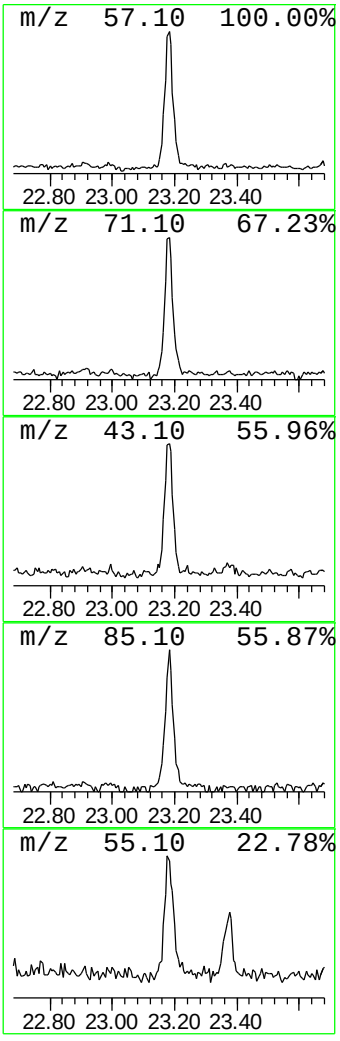
****

Peak Number 7 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	3.29 ng	106164	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Triacontane	422	C30H62	000638-68-6	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Docosane	310	C22H46	000629-97-0	87





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Data File : BG042637.D
Acq On : 31 Aug 2019 16:29
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Sample : K4577-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.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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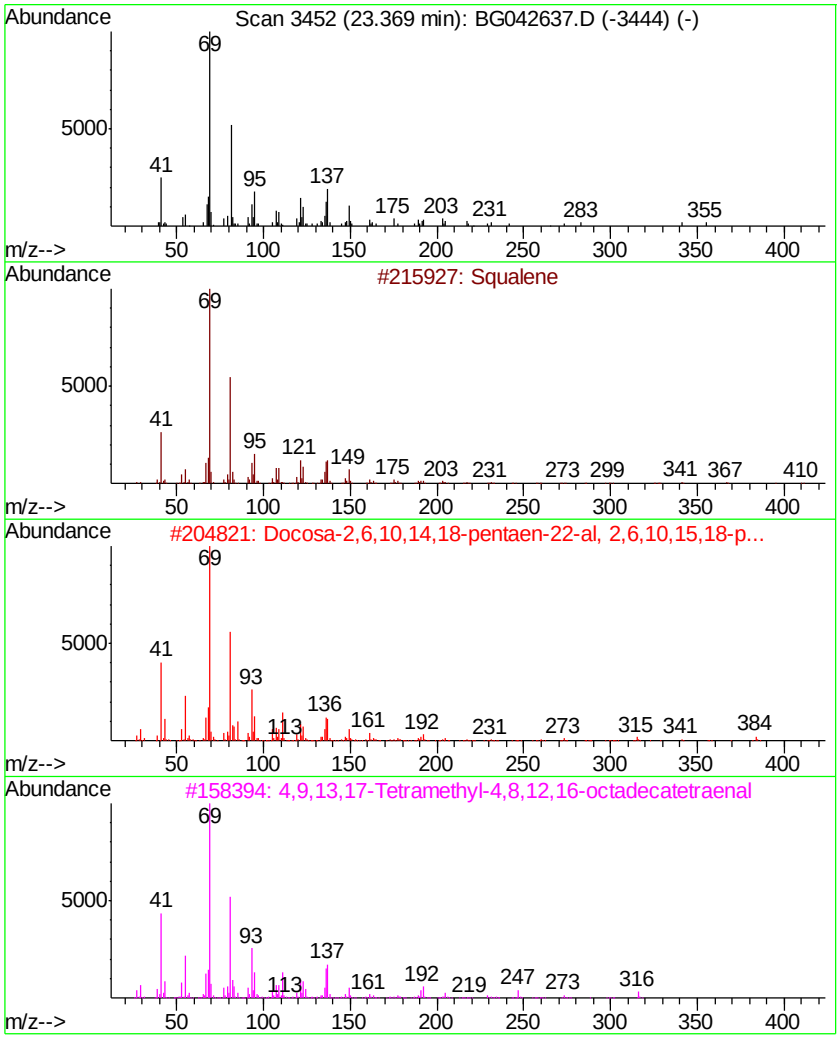
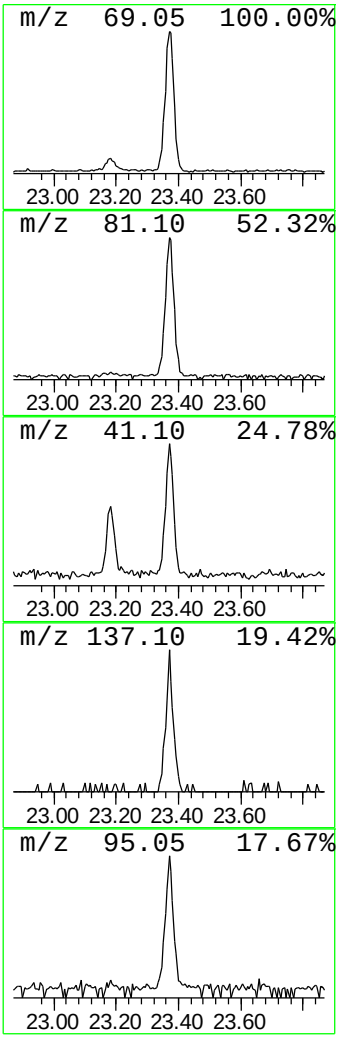
Peak Number 8 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.37	3.64 ng	141105	Perylene-d12	24.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	87
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59
5	trans-Farnesol	222	C15H26O	000106-28-5	53





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ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

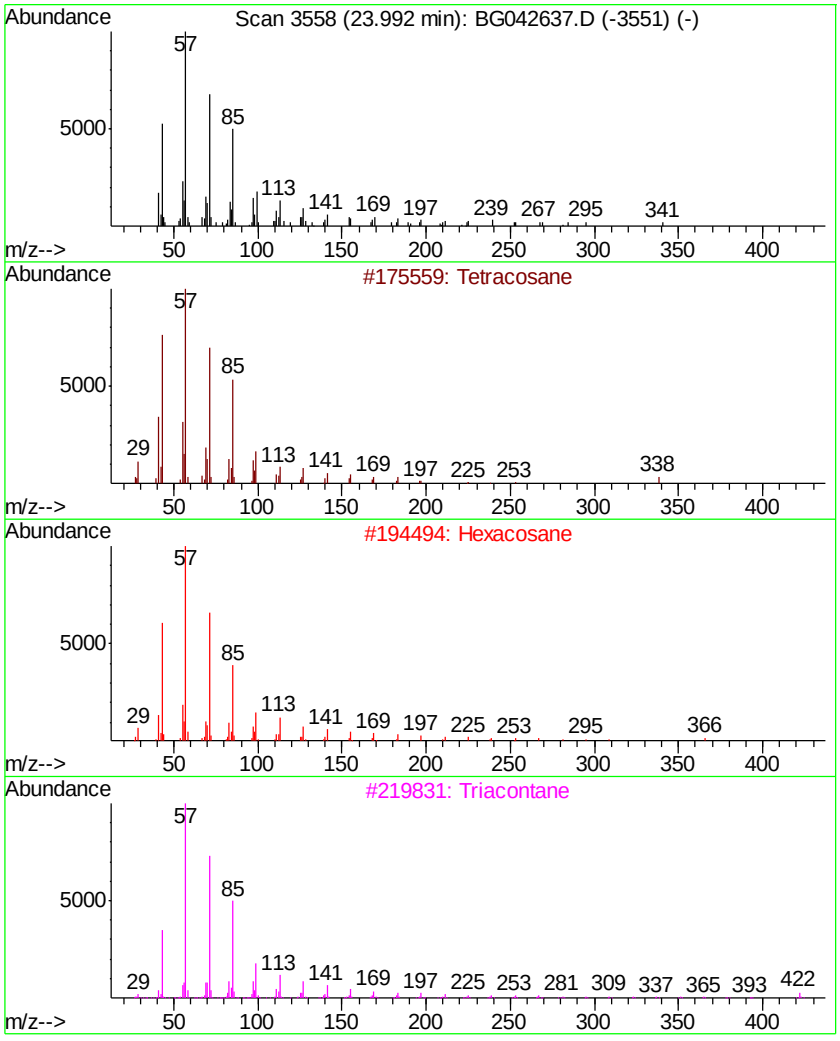
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

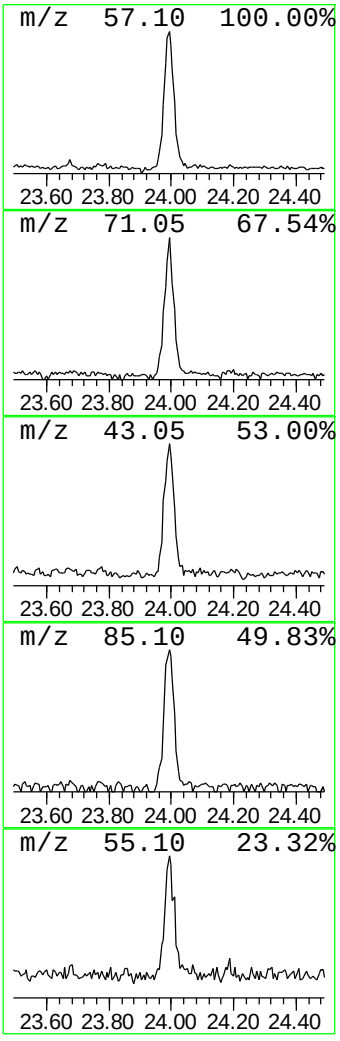
****

Peak Number 9 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	2.70 ng	104707	Perylene-d12	24.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	93
2	Hexacosane	366	C26H54	000630-01-3	91
3	Triacontane	422	C30H62	000638-68-6	90
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Heneicosane	296	C21H44	000629-94-7	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG083119\
Data File : BG042637.D
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Operator : HP/JU
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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
Butane, 2-methoxy...	3.12	200.3	ng	1779080	1	8.00	177604	20.0
unknown7.53	7.53	78.0	ng	692401	1	8.00	177604	20.0
n-Hexadecanoic acid	18.30	3.8	ng	95179	4	17.41	507946	20.0
Tetracosyl heptaf...	21.32	6.1	ng	195479	5	21.68	644620	20.0
Octacosane	22.48	2.2	ng	72039	5	21.68	644620	20.0
Pentacosane	23.18	3.3	ng	106164	5	21.68	644620	20.0
Squalene	23.37	3.6	ng	141105	6	24.92	776062	20.0
Hexacosane	23.99	2.7	ng	104707	6	24.92	776062	20.0