LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092718\
Data File : BG037044.D
Acq On : 28 Sep 2018 10:50
Operator : JU/SJ
Sample : J5090-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-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-BG092018.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	5.147	311	316	322	rBV	40979	61404	1.60%	0.401%
2	5.611	390	395	411	rBV	214672	420405	10.98%	2.748%
3	7.204	660	666	684	rBV	120510	312553	8.16%	2.043%
4	7.574	722	729	747	rBV	403243	814312	21.26%	5.322%
5	8.044	802	809	823	rBV	119111	256565	6.70%	1.677%
6	8.361	856	863	880	rBV	585855	1104972	28.85%	7.222%
7	9.201	999	1006	1027	rBV	474890	1005703	26.26%	6.573%
8	10.846	1278	1286	1299	rBV	162967	345952	9.03%	2.261%
9	13.291	1694	1702	1723	rBV	1192052	2149278	56.11%	14.047%
10	14.666	1929	1936	1951	rBV2	286000	494939	12.92%	3.235%
11	16.152	2182	2189	2209	rBV	710645	1213506	31.68%	7.931%
12	17.409	2397	2403	2415	rBV	382969	676669	17.67%	4.422%
13	18.291	2548	2553	2561	rBV5	25412	47112	1.23%	0.308%
14	20.018	2841	2847	2863	rBV	2733245	3830183	100.00%	25.033%
15	20.700	2958	2963	2968	rBV	28953	39608	1.03%	0.259%
16	21.317	3064	3068	3077	rBV4	26376	60615	1.58%	0.396%
17	21.675	3122	3129	3140	rBV2	470468	820796	21.43%	5.364%
18	22.468	3259	3264	3269	rBV	31777	50049	1.31%	0.327%
19	23.150	3372	3380	3390	rVB4	59475	132979	3.47%	0.869%
20	23.344	3406	3413	3420	rVB	92421	187865	4.90%	1.228%
21	23.949	3509	3516	3523	rBV	62767	135381	3.53%	0.885%
22	24.877	3664	3674	3688	rBV	308828	921423	24.06%	6.022%
23	26.005	3858	3866	3878	rVB4	41164	127530	3.33%	0.833%
24	27.351	4085	4095	4109	rBV4	23649	90905	2.37%	0.594%

Sum of corrected areas: 15300704

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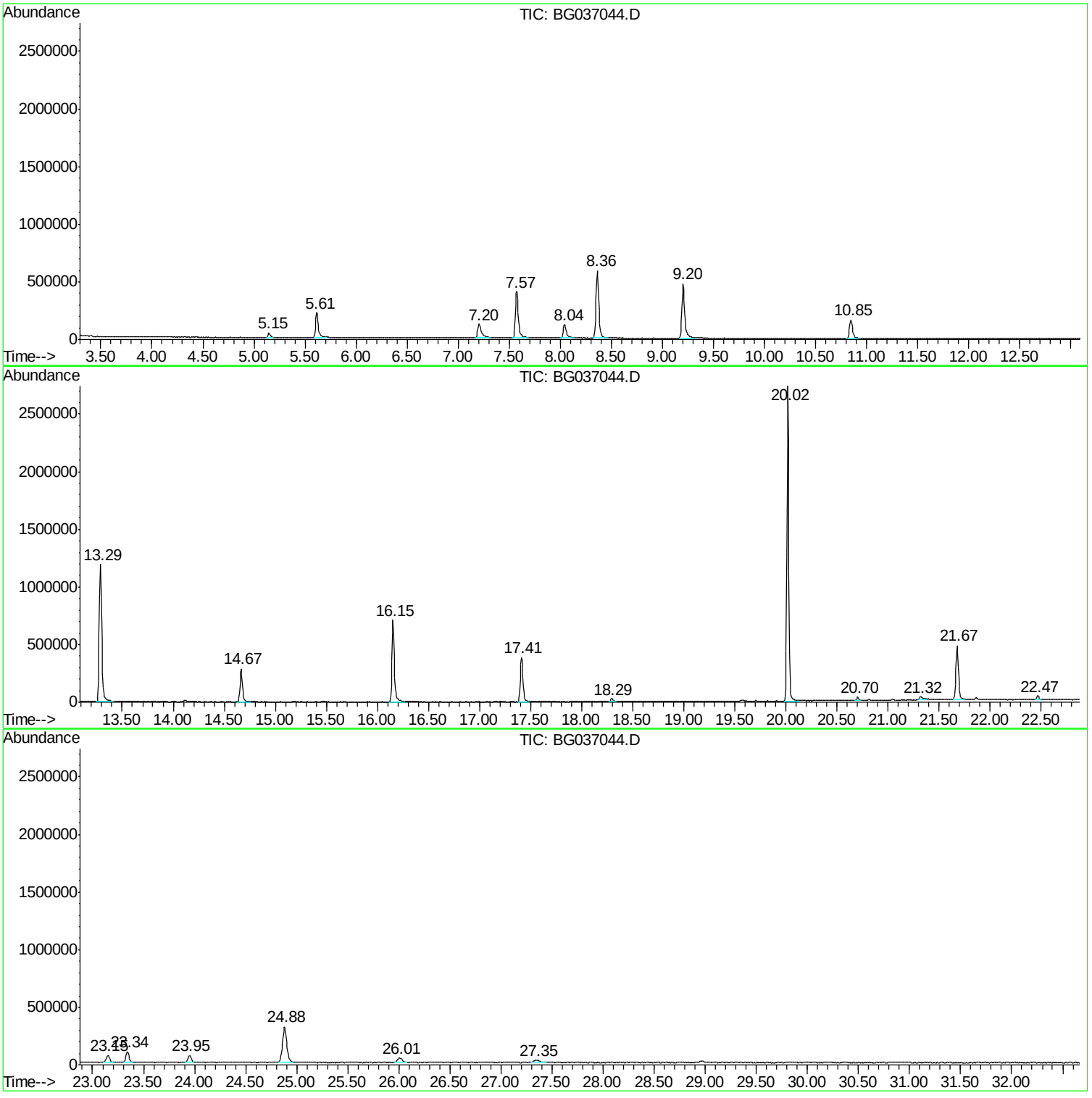
Instrument :
BNA_G
ClientSampleId :
MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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

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Instrument : BNA_G
ClientSampleId : MW-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

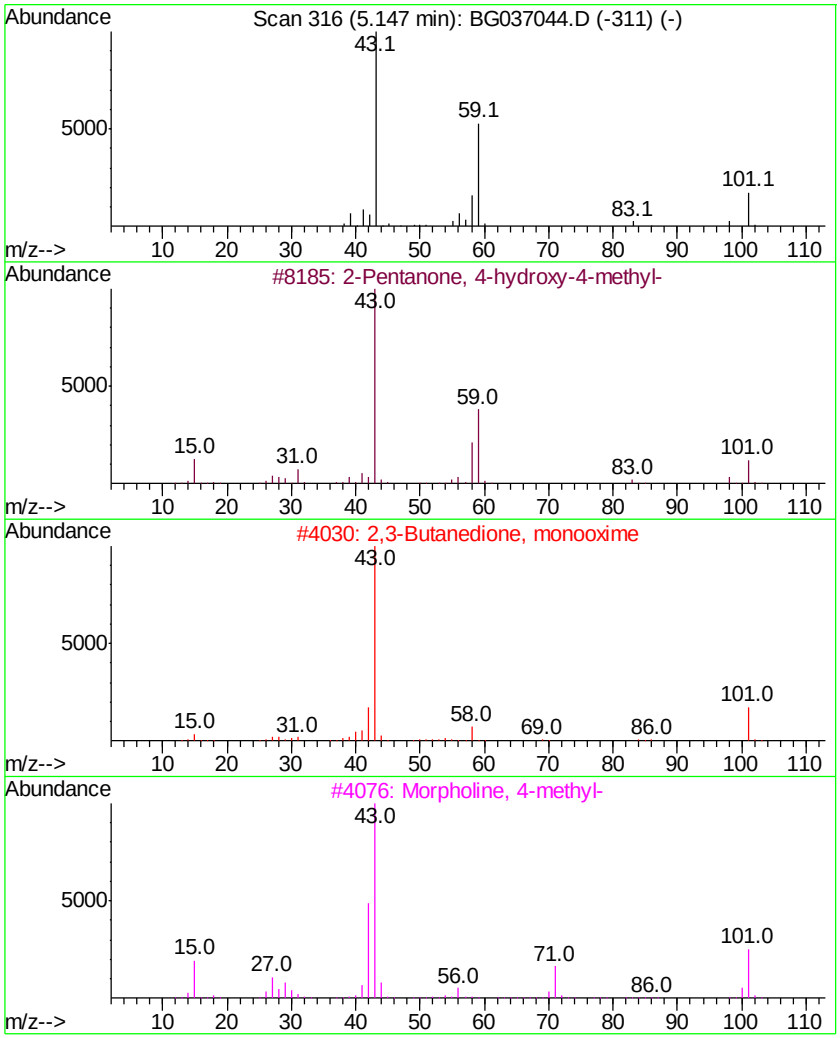
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

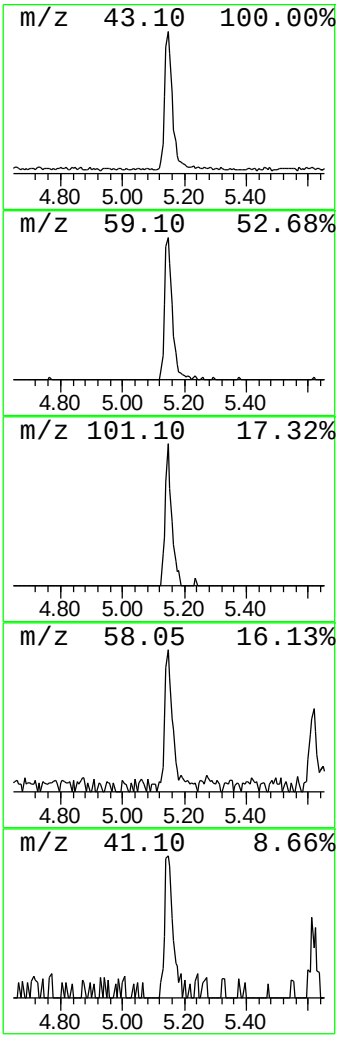
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	4.79 ng	61404	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	9
5	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9





Library Search Compound Report

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Operator : JU/SJ
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Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.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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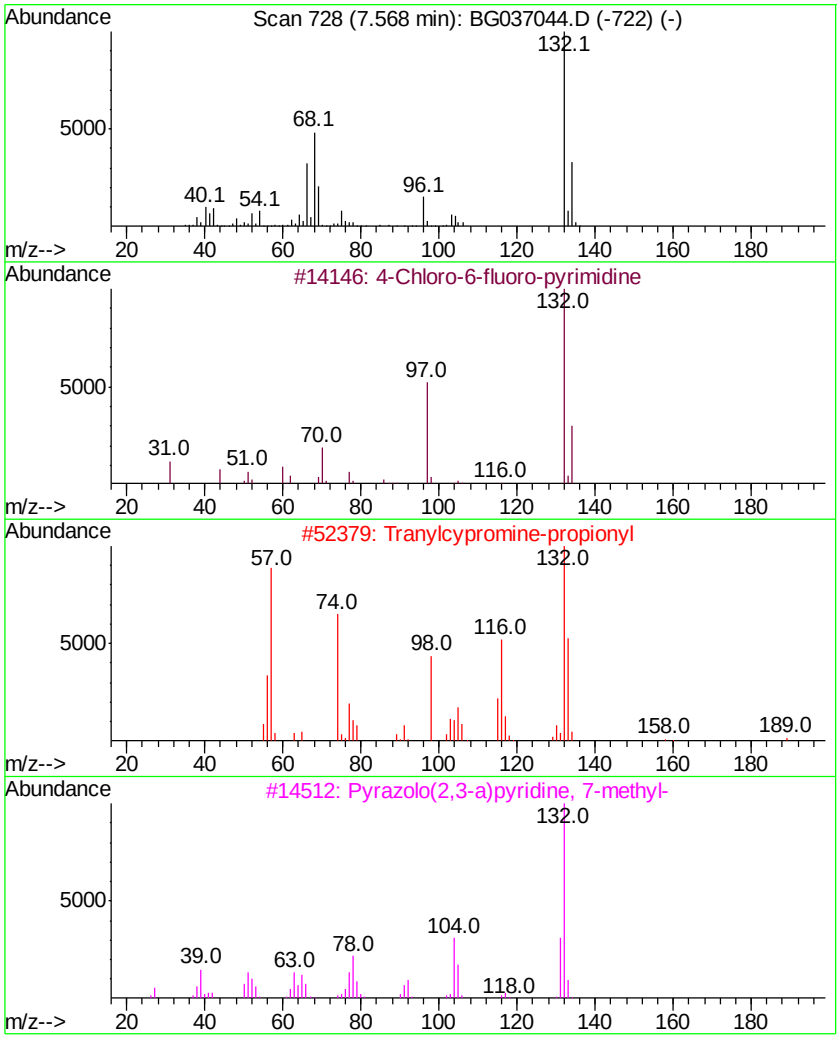
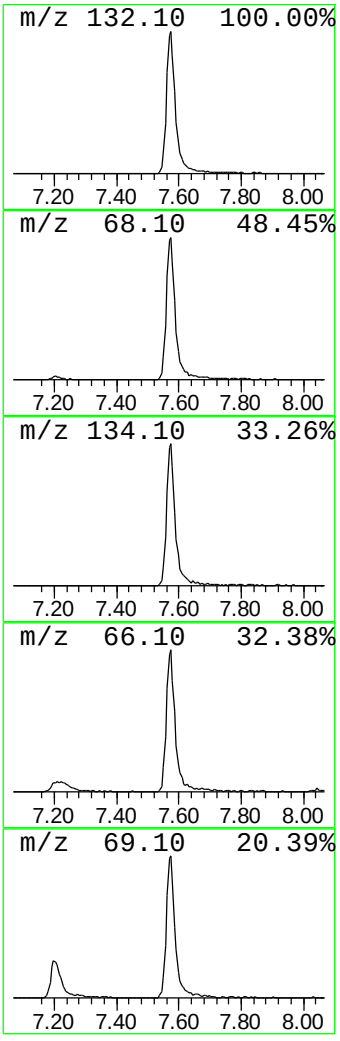
Peak Number 2 unknown7.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	63.48 ng	814312	1,4-Dichlorobenzene-d4	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
3	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092718\
Data File : BG037044.D
Acq On : 28 Sep 2018 10:50
Operator : JU/SJ
Sample : J5090-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
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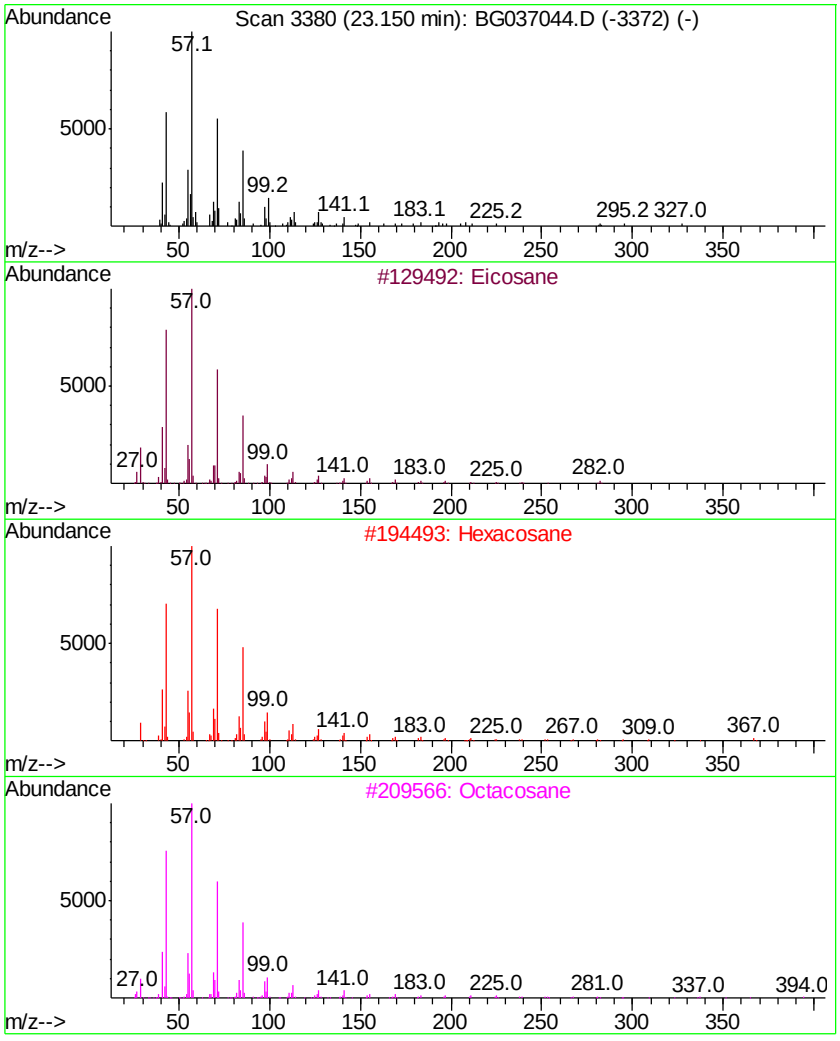
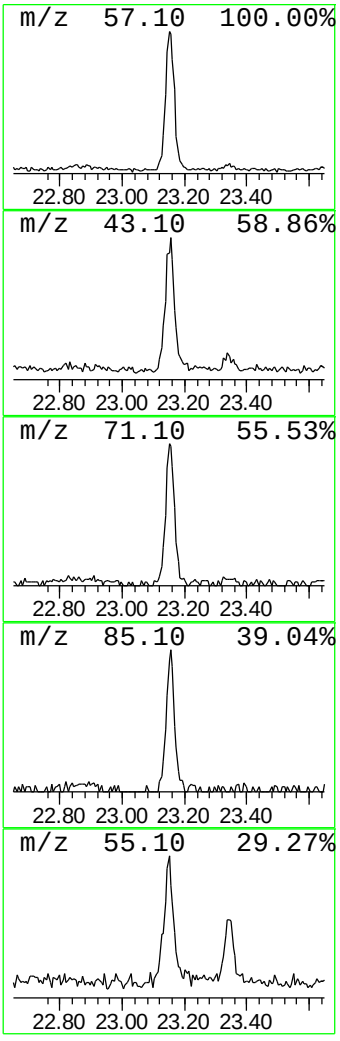
Peak Number 4 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.15	3.24 ng	132979	Chrysene-d12	21.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Hexacosane	366	C26H54	000630-01-3	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	87
5	Tetratetracontane	619	C44H90	007098-22-8	83





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Sample : J5090-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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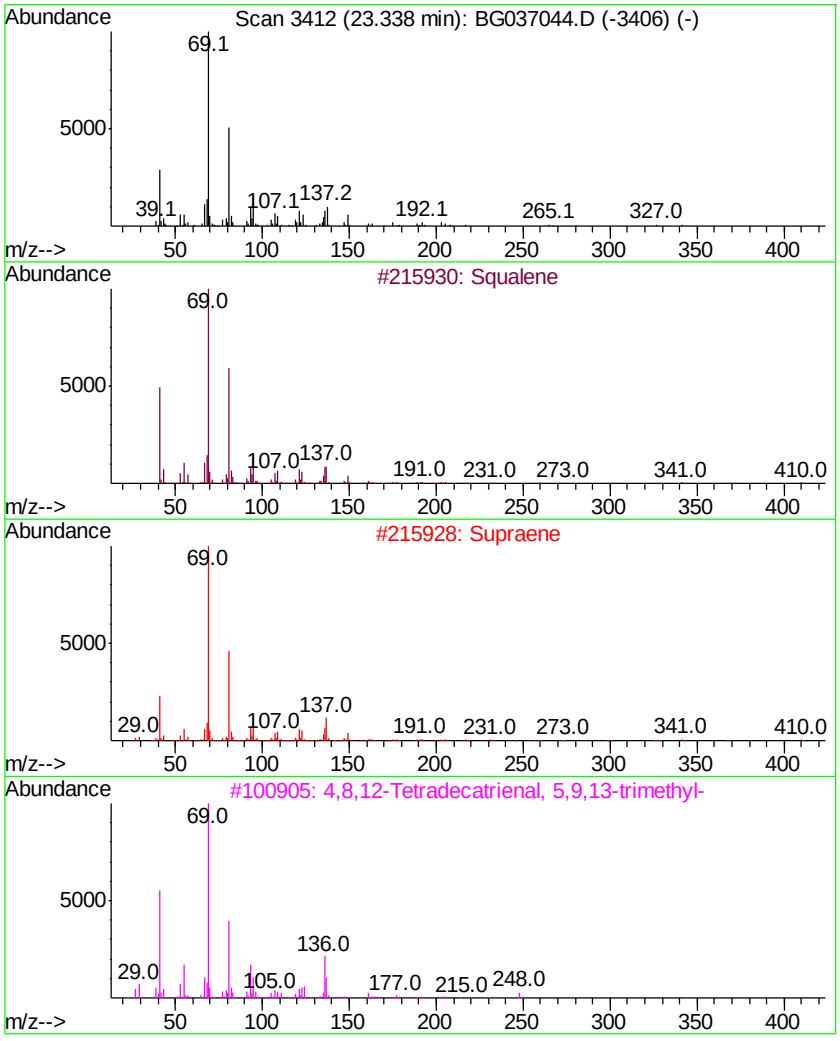
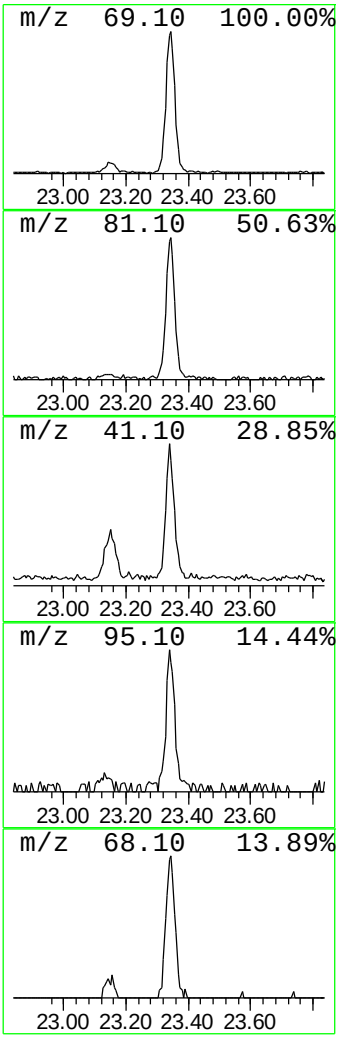
Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.34	4.08 ng	187865	Perylene-d12	24.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	80
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72





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Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
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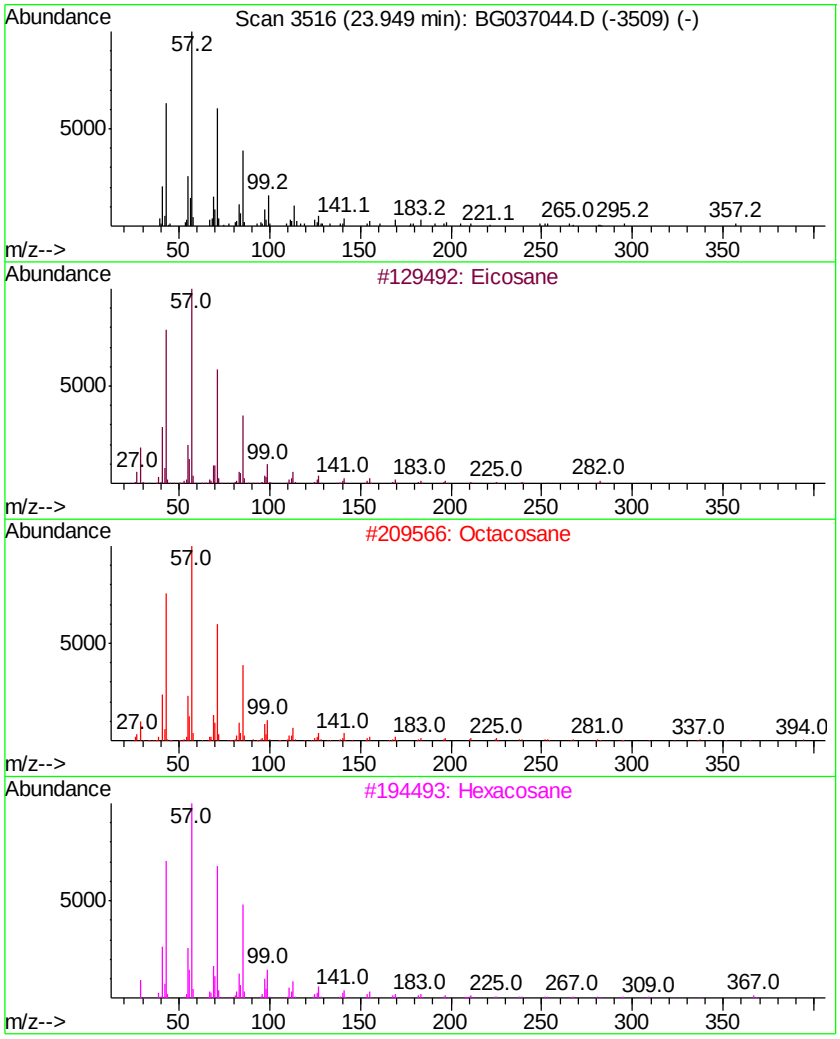
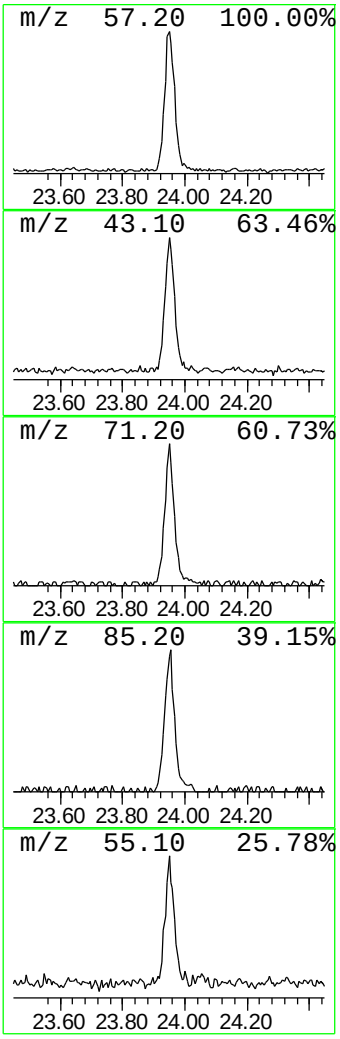
Peak Number 6 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.95	2.94 ng	135381	Perylene-d12	24.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Octacosane	394	C28H58	000630-02-4	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Hentriacontane	437	C31H64	000630-04-6	90
5	Heneicosane	296	C21H44	000629-94-7	90





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Misc :
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Instrument : BNA_G
ClientSampleId : MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092018.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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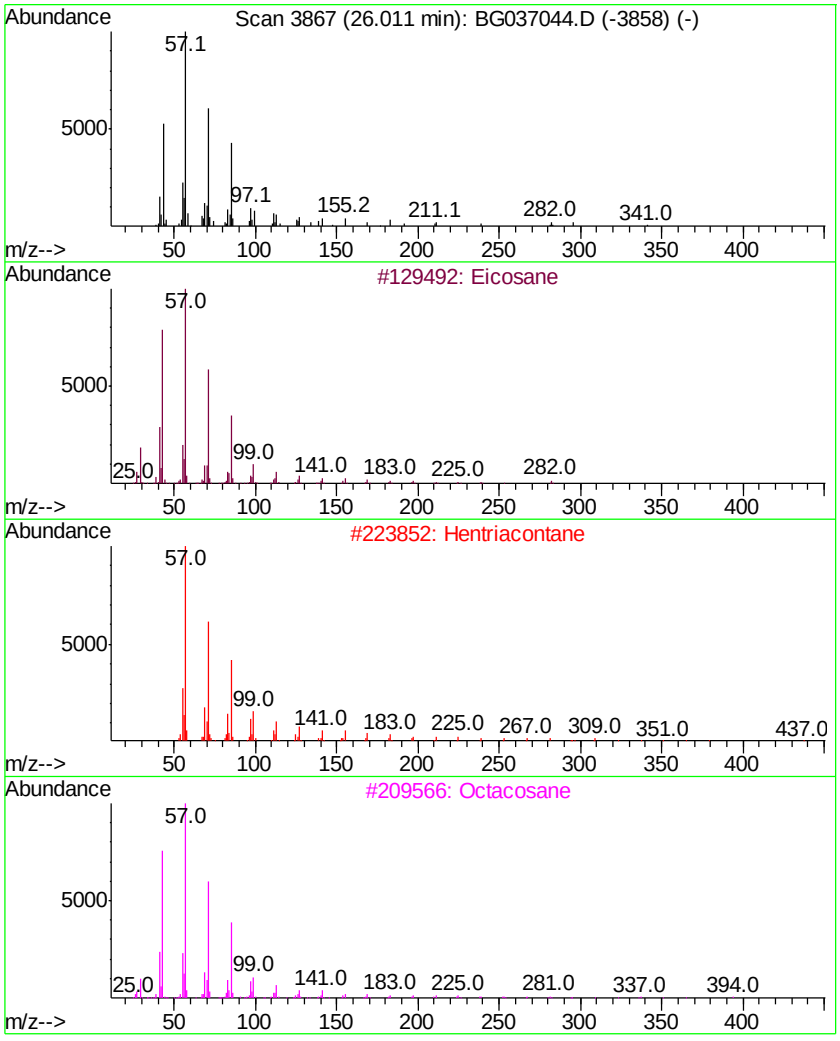
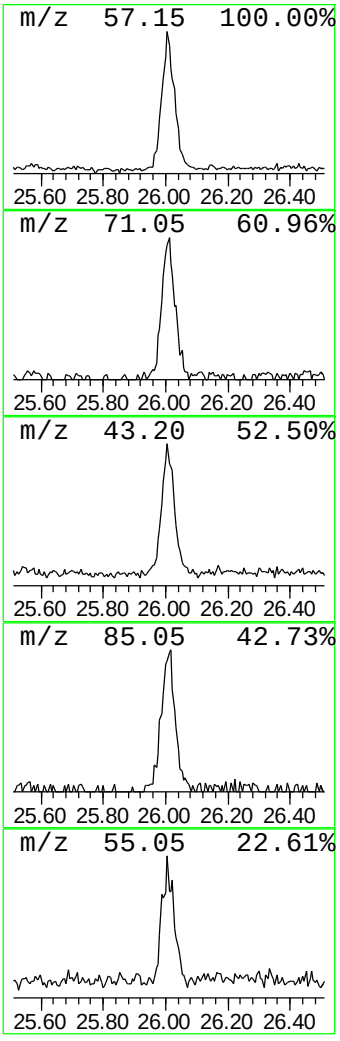
Peak Number 7 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.01	2.77 ng	127530	Perylene-d12	24.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Hentriacontane	437	C31H64	000630-04-6	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Hexatriacontane	507	C36H74	000630-06-8	87
5	Tetracosane	338	C24H50	000646-31-1	83





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	5.15	4.8	ng	61404	1	8.04	256565	20.0
unknown7.57	7.57	63.5	ng	814312	1	8.04	256565	20.0
Eicosane	23.15	3.2	ng	132979	5	21.67	820796	20.0
Squalene	23.34	4.1	ng	187865	6	24.88	921423	20.0
Octacosane	23.95	2.9	ng	135381	6	24.88	921423	20.0
Hentriacontane	26.01	2.8	ng	127530	6	24.88	921423	20.0