LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110819\
Data File : BG043573.D
Acq On : 8 Nov 2019 17:23
Operator : JU
Sample : K5746-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-1A-COMP

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-BG102119.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	3.163	9	13	23	rVB	116882	178696	6.82%	1.475%
2	5.108	338	344	351	rBV	139957	218573	8.35%	1.804%
3	5.602	421	428	447	rBV	452611	786816	30.04%	6.494%
4	7.206	692	701	719	rBV	484297	904830	34.55%	7.468%
5	7.552	752	760	771	rBV	496174	884809	33.78%	7.303%
6	8.005	829	837	845	rBV	85877	151069	5.77%	1.247%
7	8.328	884	892	904	rBV	380850	668505	25.53%	5.518%
8	9.168	1025	1035	1052	rBV	253952	517665	19.77%	4.273%
9	10.807	1307	1314	1324	rBV2	85896	183023	6.99%	1.511%
10	13.257	1724	1731	1747	rBV	759369	1257210	48.00%	10.377%
11	14.086	1867	1872	1882	rBV	57754	105927	4.04%	0.874%
12	14.632	1959	1965	1980	rBV2	178675	316953	12.10%	2.616%
13	16.125	2212	2219	2244	rBV	695019	1281112	48.92%	10.574%
14	17.382	2426	2433	2449	rBV	250846	446341	17.04%	3.684%
15	19.991	2871	2877	2893	rBV	1901555	2618941	100.00%	21.616%
16	21.295	3093	3099	3108	rBV7	36742	109473	4.18%	0.904%
17	21.648	3152	3159	3177	rBV2	272810	558904	21.34%	4.613%
18	22.429	3286	3292	3299	rBV7	12768	27508	1.05%	0.227%
19	23.099	3400	3406	3413	rBV6	35685	84793	3.24%	0.700%
20	23.304	3434	3441	3448	rVB	87476	165044	6.30%	1.362%
21	23.904	3538	3543	3550	rVB5	20117	37270	1.42%	0.308%
22	24.838	3691	3702	3720	rBV	204983	612161	23.37%	5.053%

Sum of corrected areas: 12115623

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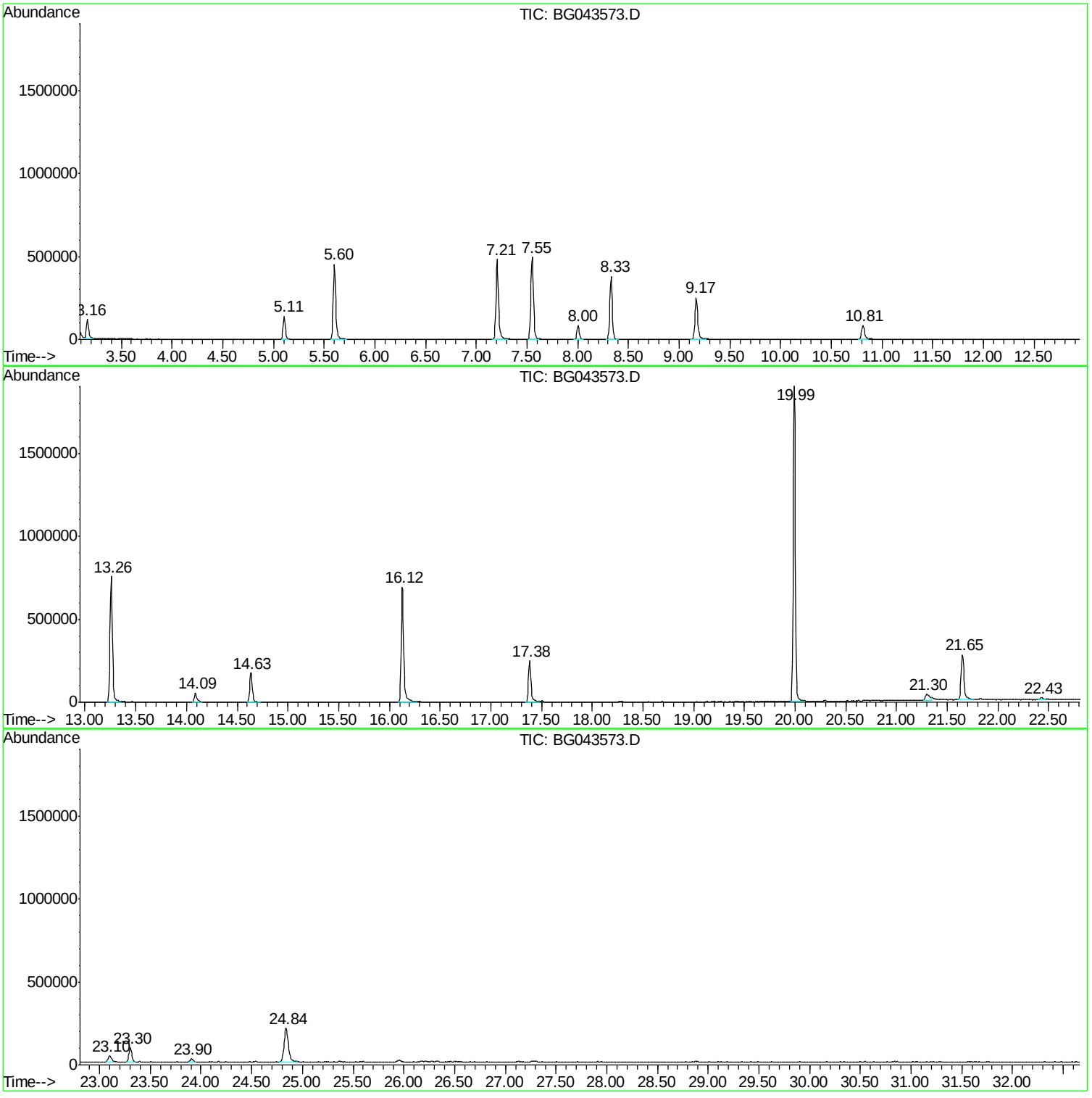
Instrument :
BNA_G
ClientSampleId :
TP-1A-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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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Data File : BG043573.D
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Operator : JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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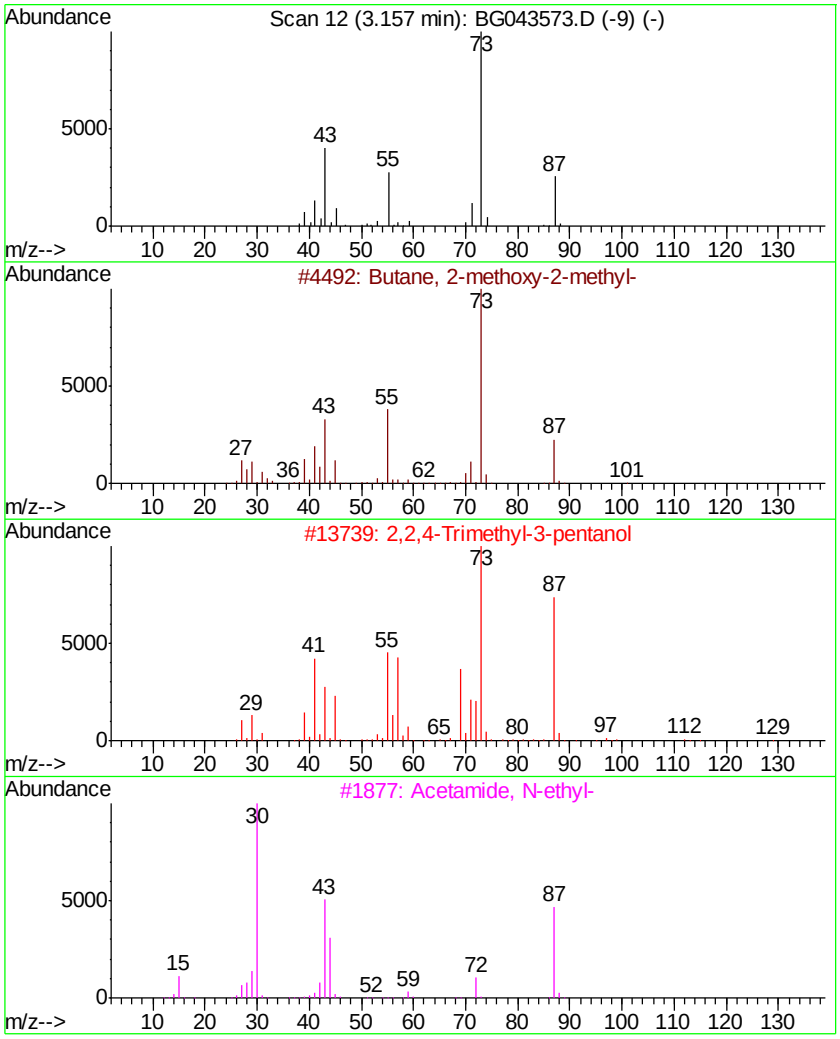
TIC Integration Parameters: LSCINT.P

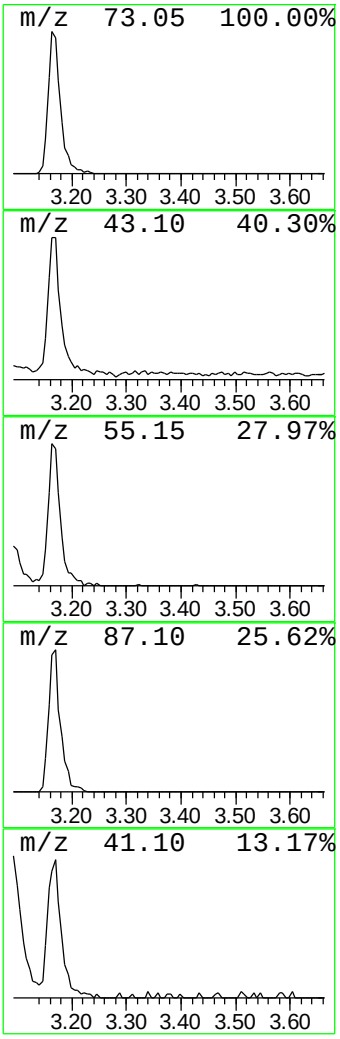
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.16	23.66 ng	178696	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	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
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

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Data File : BG043573.D
Acq On : 8 Nov 2019 17:23
Operator : JU
Sample : K5746-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-1A-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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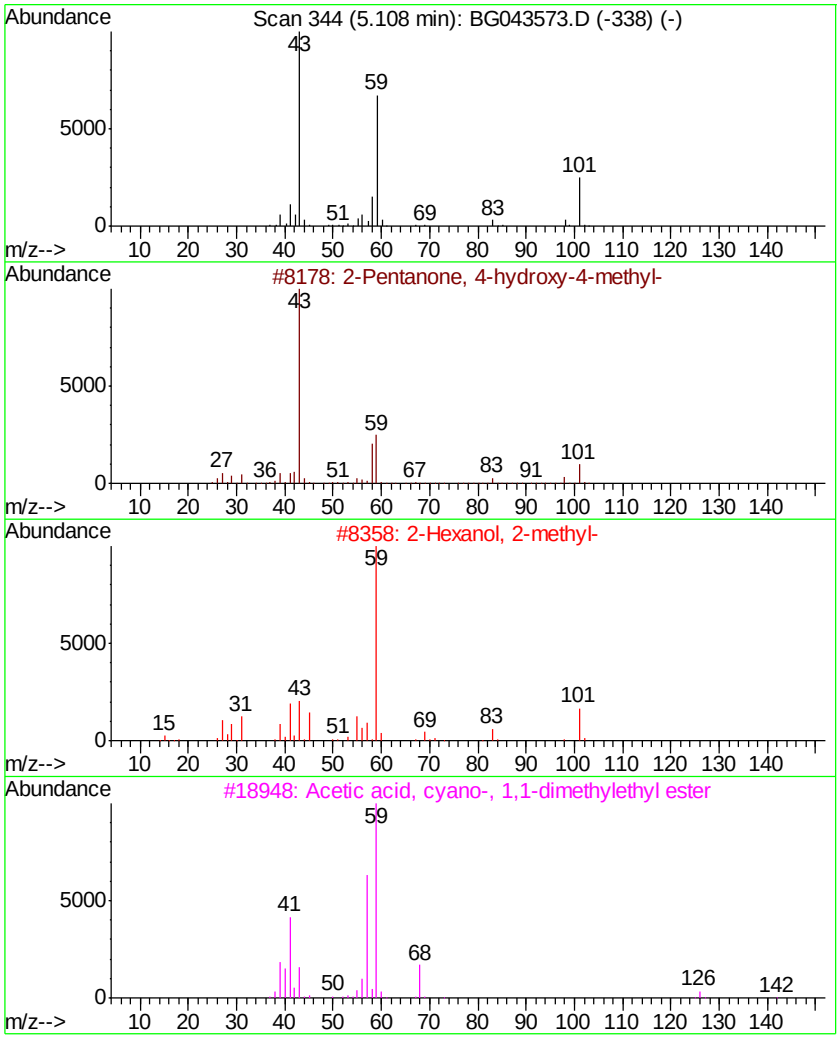
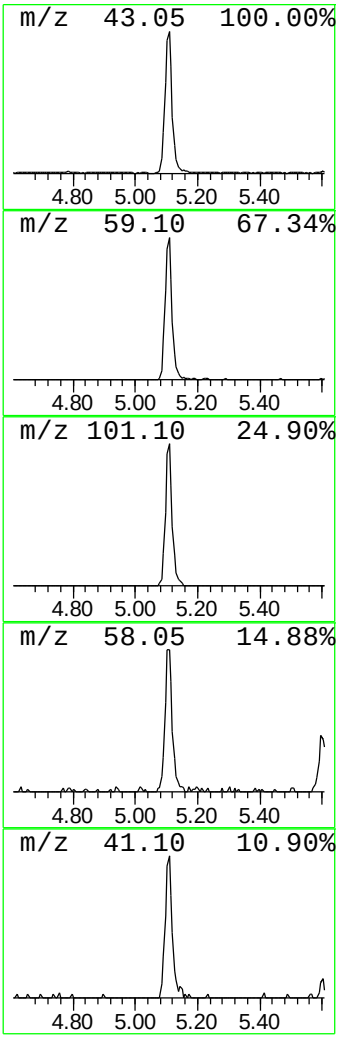
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	28.94 ng	218573	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	37
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25





Library Search Compound Report

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Data File : BG043573.D
Acq On : 8 Nov 2019 17:23
Operator : JU
Sample : K5746-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-1A-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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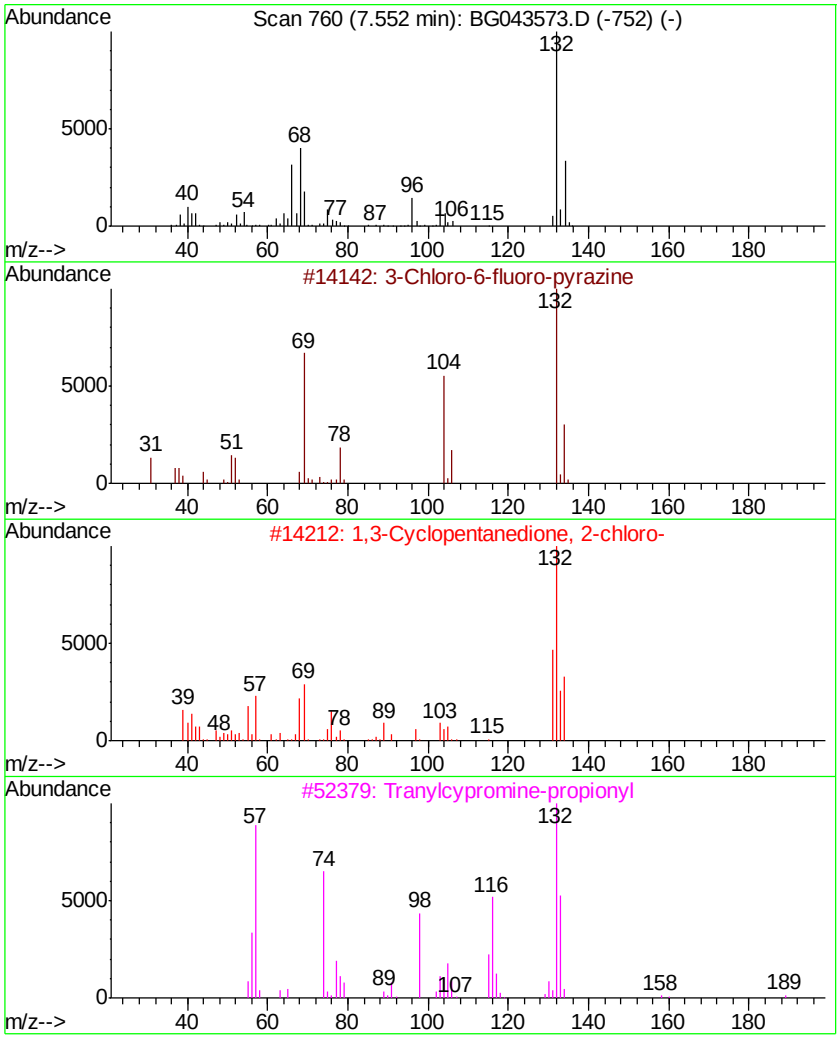
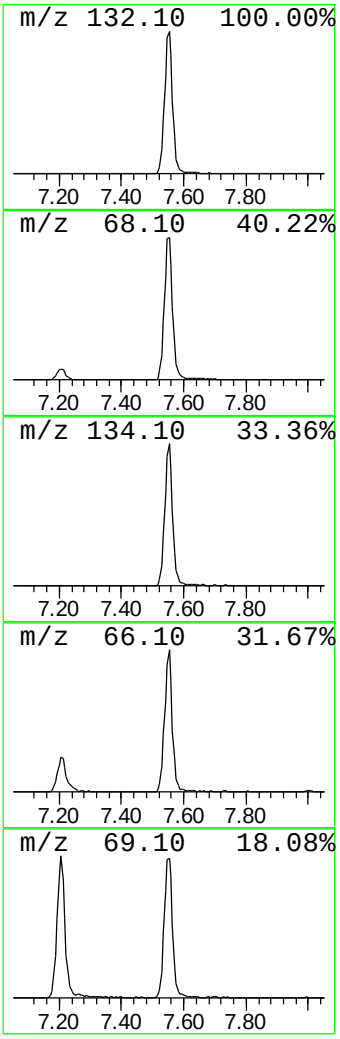
****

Peak Number 3 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	117.14 ng	884809	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	27
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10





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Operator : JU
Sample : K5746-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-1A-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
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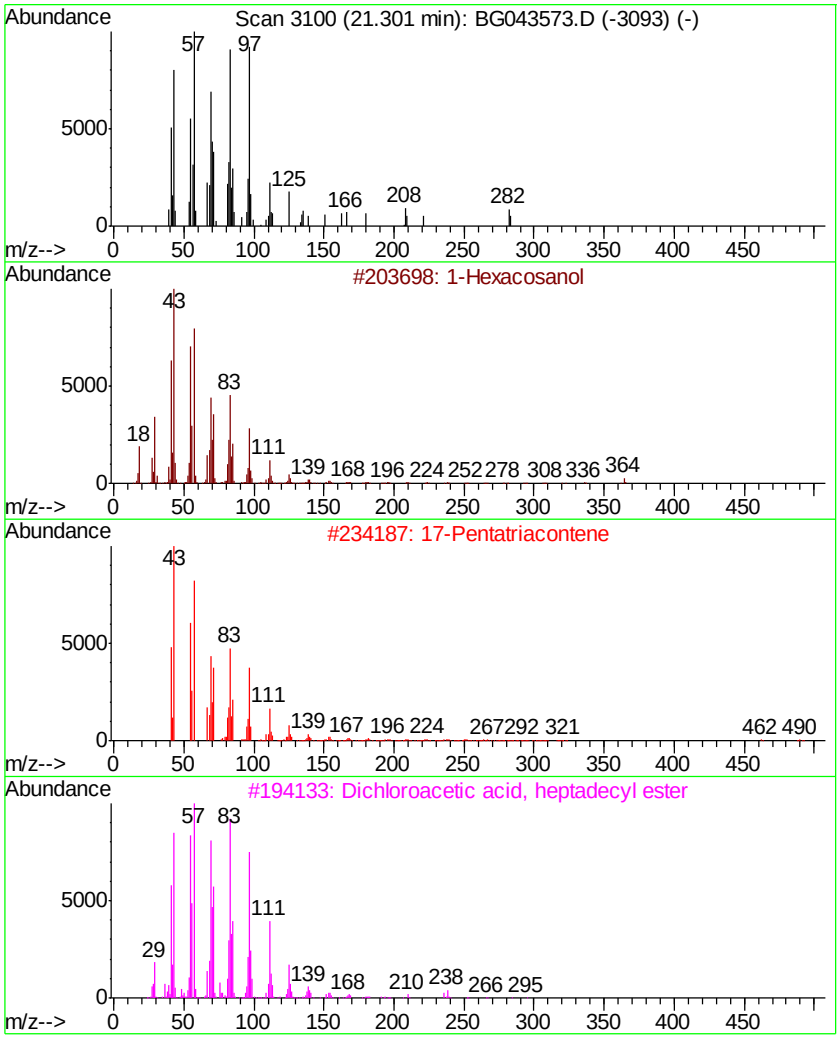
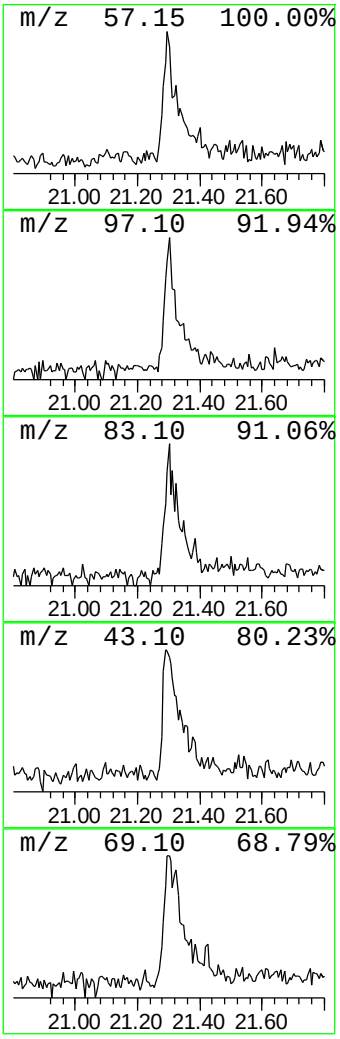
****

Peak Number 5 1-Hexacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	3.92 ng	109473	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	87
2	17-Pentatriacontene	491	C35H70	006971-40-0	87
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	70
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	70
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	70





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Sample : K5746-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-1A-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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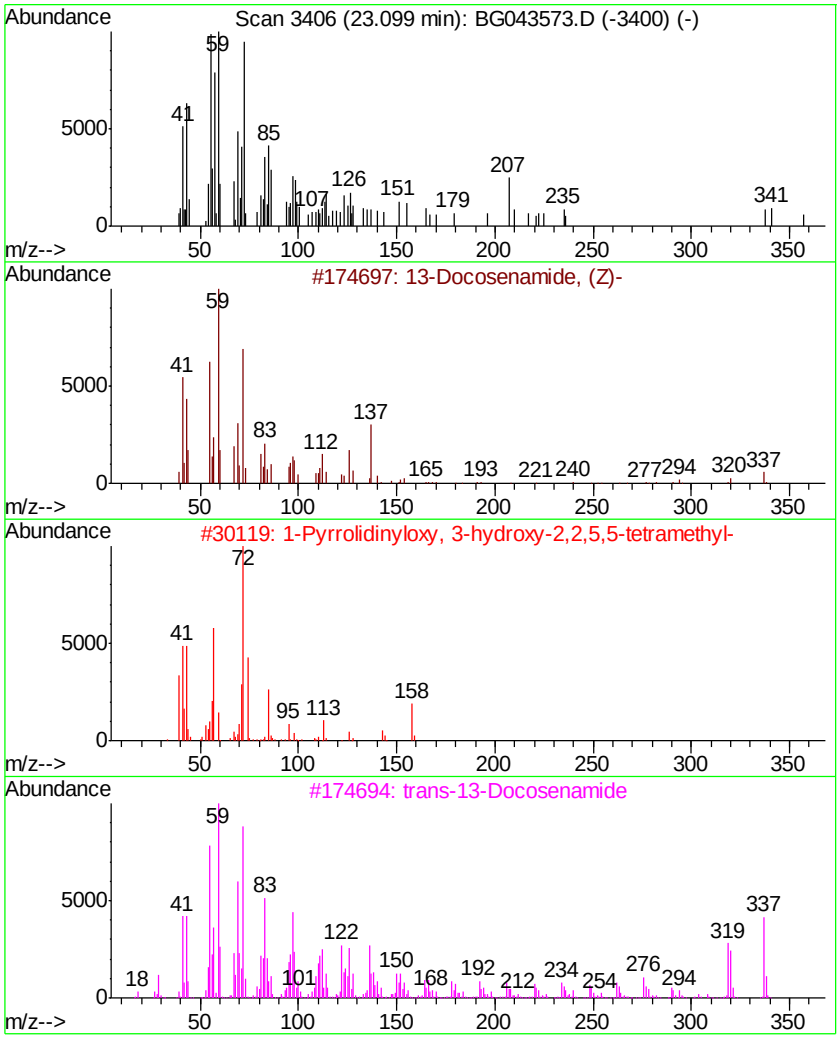
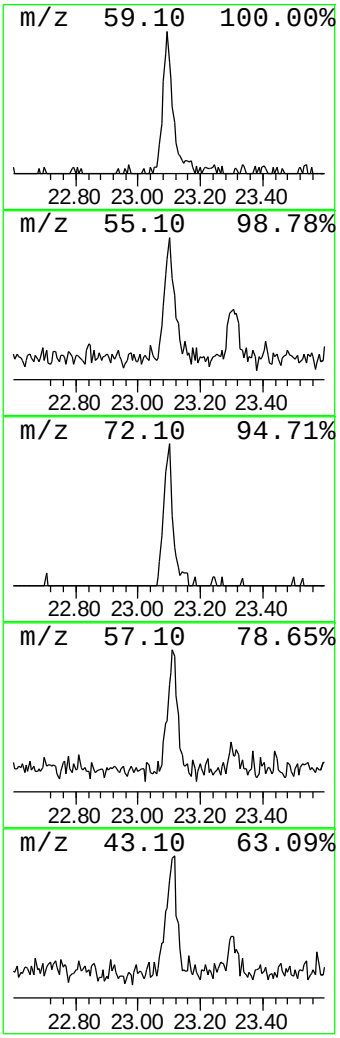
****

Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.10	3.03 ng	84793	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	55
2	1-Pyrrolidinyloxy, 3-hydroxy-2,2...	158	C8H16NO2	002154-37-2	35
3	trans-13-Docosenamide	337	C22H43NO	010436-09-6	27
4	Hydrazinecarboxamide, 2-(1-methy...	115	C4H9N3O	000110-20-3	18
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	14





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ClientSampleId : TP-1A-COMP

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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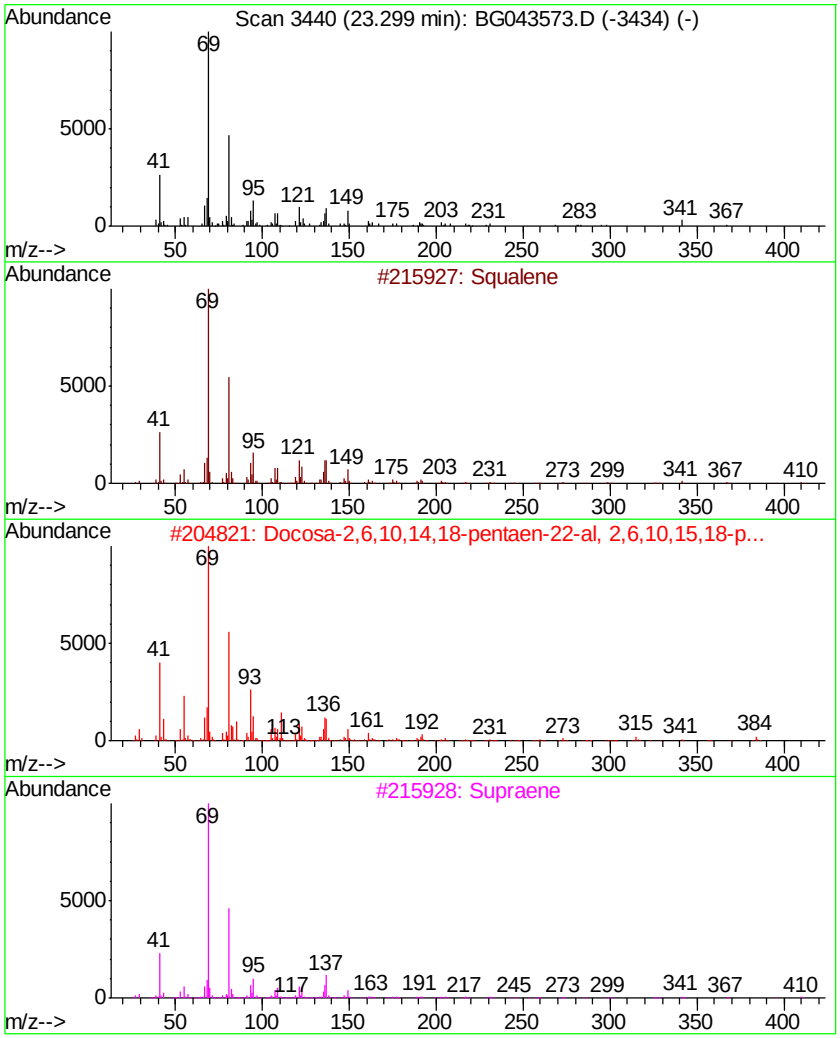
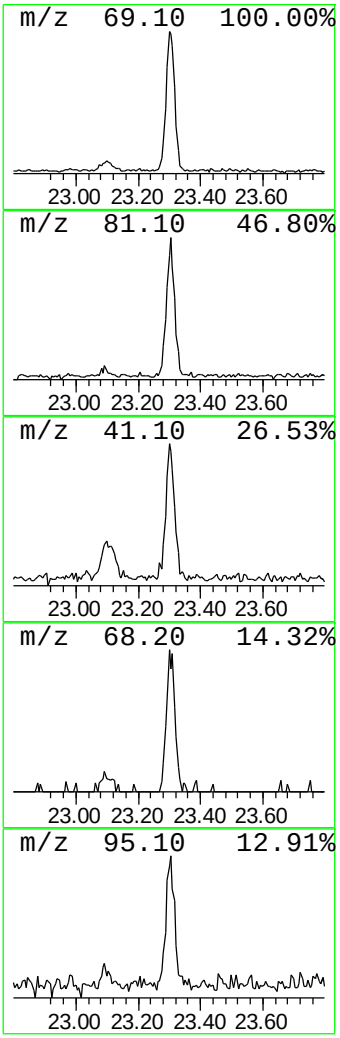
Peak Number 7 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.30	5.39 ng	165044	Perylene-d12	24.84

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	86
3	Supraene	410	C30H50	007683-64-9	83
4	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	78
5	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72





Tentatively Identified Compound (LSC) summary

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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...	3.16	23.7	ng	178696	1	8.00	151069	20.0
2-Pentanone, 4-hy...	5.11	28.9	ng	218573	1	8.00	151069	20.0
unknown7.55	7.55	117.1	ng	884809	1	8.00	151069	20.0
1-Hexacosanol	21.30	3.9	ng	109473	5	21.65	558904	20.0
13-Docosenamide, ...	23.10	3.0	ng	84793	5	21.65	558904	20.0
Squalene	23.30	5.4	ng	165044	6	24.84	612161	20.0