LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043554.D
Acq On : 8 Nov 2019 00:40
Operator : JU
Sample : K5722-12
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 1-B

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	3.171	10	14	26	rVB	59389	98945	5.84%	1.006%
2	5.109	338	344	353	rBV	61731	97622	5.76%	0.992%
3	5.603	422	428	442	rBV	266001	491102	28.98%	4.991%
4	7.213	694	702	715	rBV	280071	553994	32.69%	5.630%
5	7.554	753	760	775	rBV	311763	571566	33.73%	5.809%
6	8.006	830	837	846	rBV	103947	181113	10.69%	1.841%
7	8.329	885	892	903	rBV	257443	465677	27.48%	4.733%
8	9.169	1027	1035	1053	rBV	159924	348671	20.58%	3.544%
9	10.815	1304	1315	1321	rBV	120434	234362	13.83%	2.382%
10	10.862	1321	1323	1334	rVB	18080	33283	1.96%	0.338%
11	12.471	1590	1597	1606	rBV	21963	46403	2.74%	0.472%
12	13.259	1724	1731	1742	rBV	553811	939304	55.43%	9.546%
13	14.093	1868	1873	1881	rVB4	12594	24274	1.43%	0.247%
14	14.640	1957	1966	1973	rBV	228944	386334	22.80%	3.926%
15	14.704	1973	1977	1984	rVB2	14785	25951	1.53%	0.264%
16	16.132	2211	2220	2236	rBV	486402	867581	51.20%	8.817%
17	16.361	2252	2259	2264	rBV6	18872	41580	2.45%	0.423%
18	17.383	2428	2433	2438	rBV	303475	481453	28.41%	4.893%
19	19.240	2745	2749	2753	rVB3	59814	76993	4.54%	0.783%
20	19.440	2779	2783	2788	rVB	87911	137040	8.09%	1.393%
21	19.998	2873	2878	2887	rVB	1284388	1694533	100.00%	17.222%
22	21.655	3154	3160	3166	rBV2	340722	604306	35.66%	6.142%
23	23.312	3436	3442	3450	rVB2	166073	316643	18.69%	3.218%
24	24.845	3696	3703	3714	rVB	218266	600612	35.44%	6.104%
25	27.025	4065	4074	4093	rBV10	126994	519990	30.69%	5.285%

Sum of corrected areas: 9839332

LSC Report - Integrated Chromatogram

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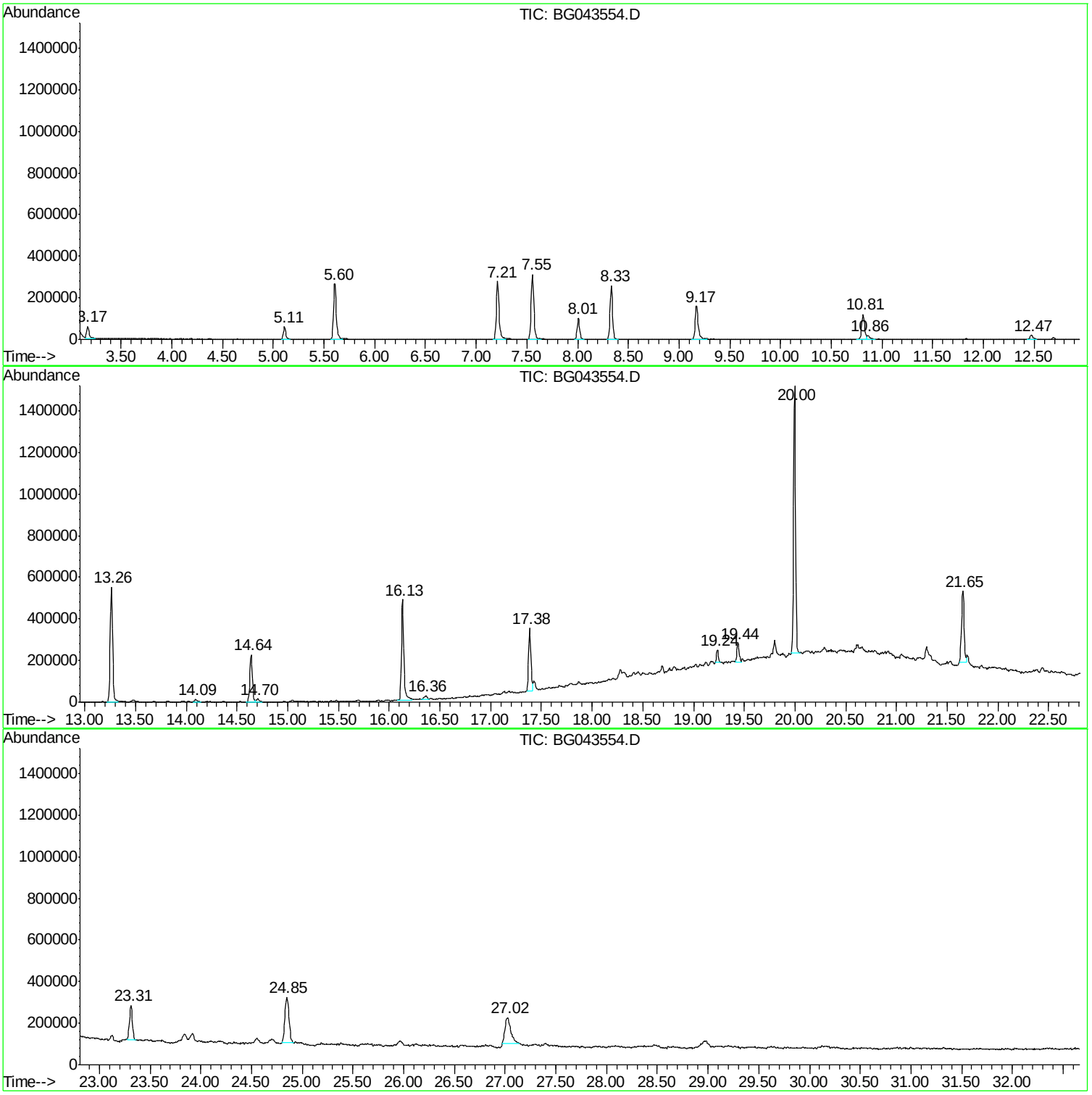
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 1-B

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043554.D
Acq On : 8 Nov 2019 00:40
Operator : JU
Sample : K5722-12
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 1-B

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

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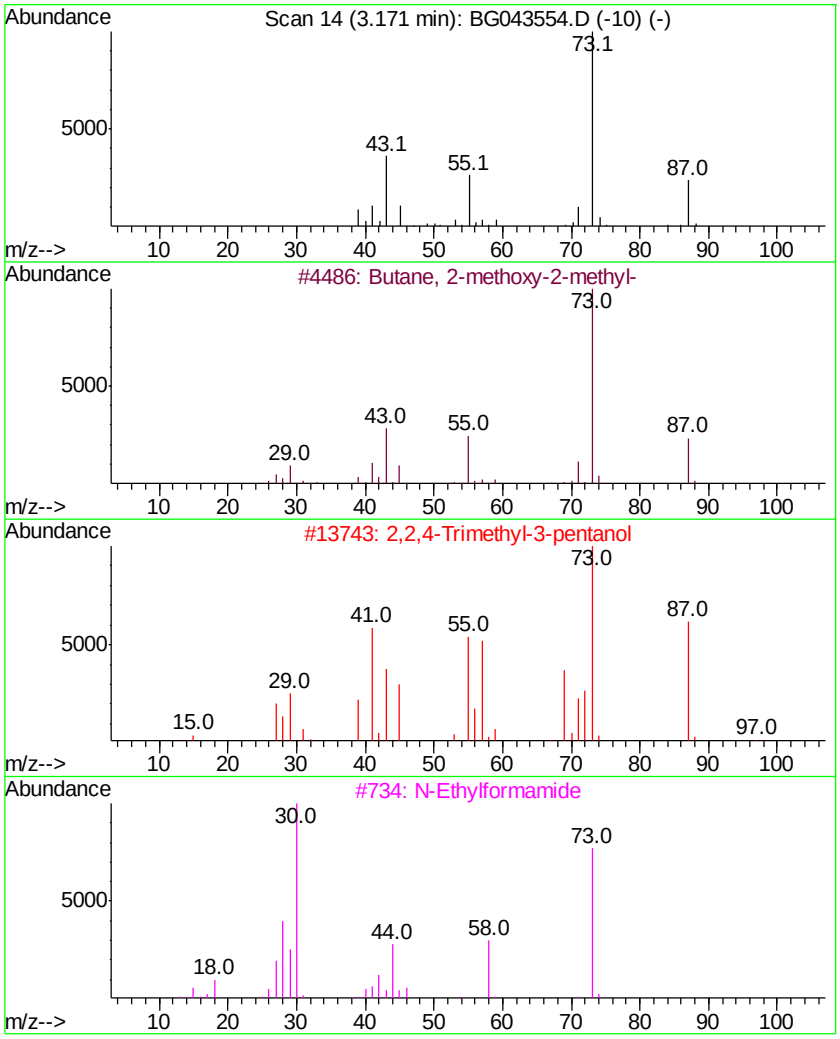
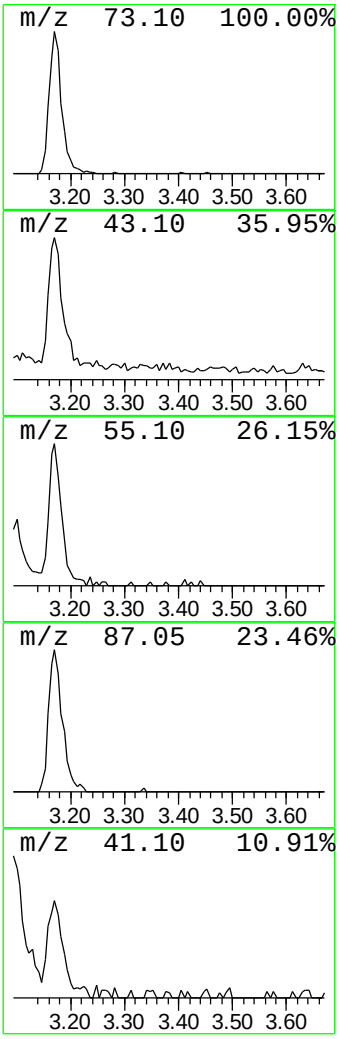
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	10.93 ng	98945	1,4-Dichlorobenzene-d4	8.01

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	43
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043554.D
Acq On : 8 Nov 2019 00:40
Operator : JU
Sample : K5722-12
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 1-B

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

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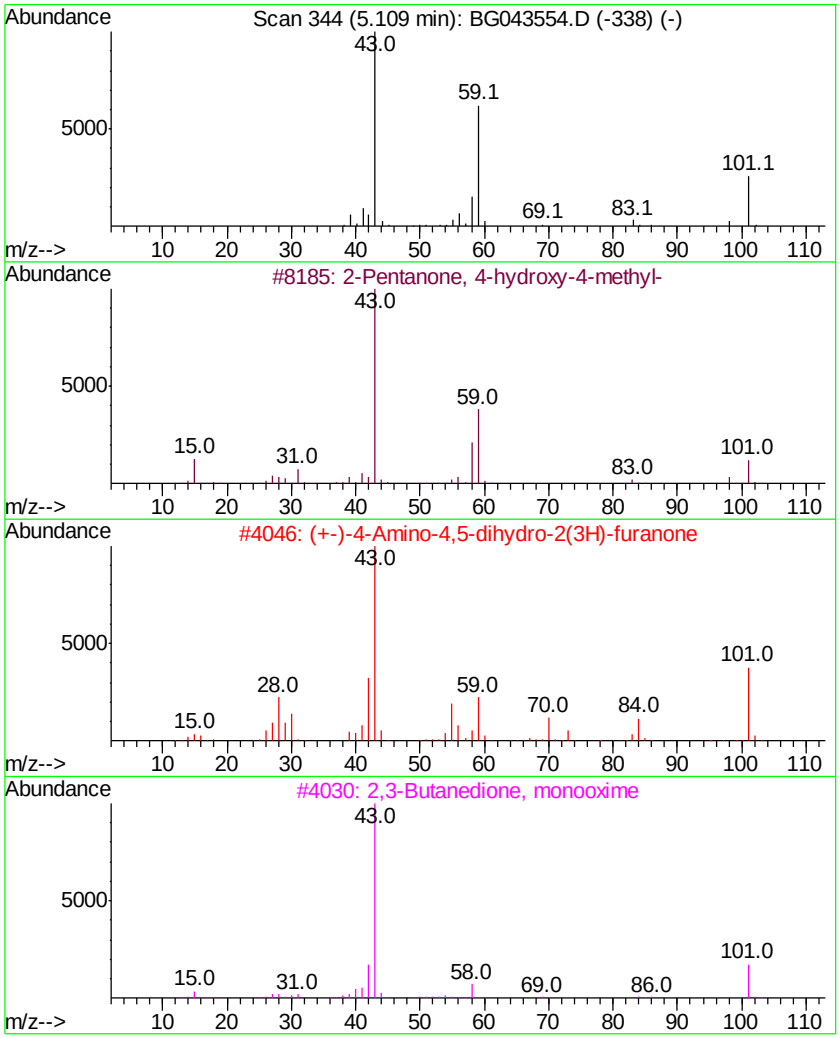
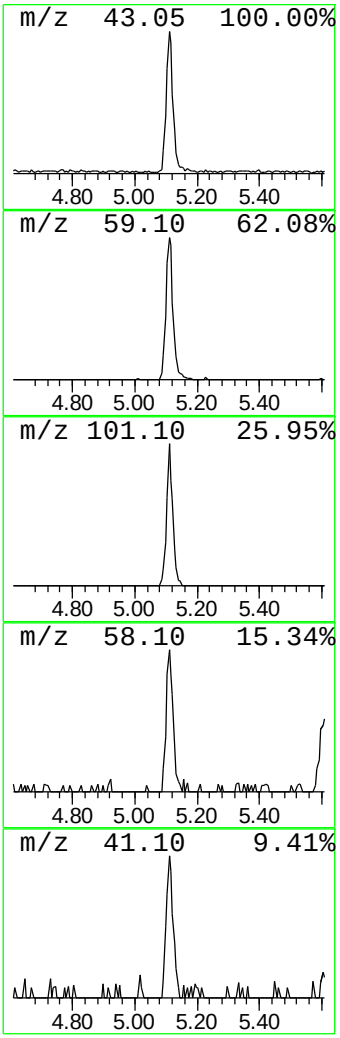
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	10.78 ng	97622	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	37
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043554.D
Acq On : 8 Nov 2019 00:40
Operator : JU
Sample : K5722-12
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 1-B

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

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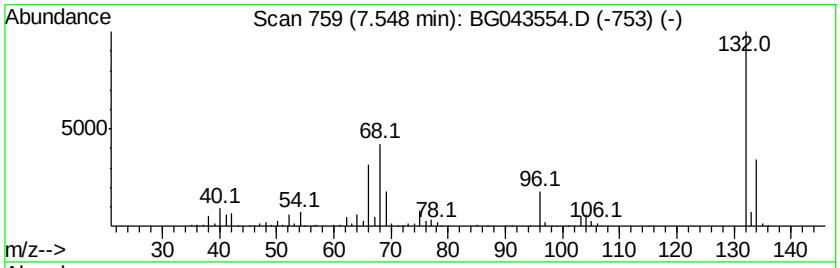
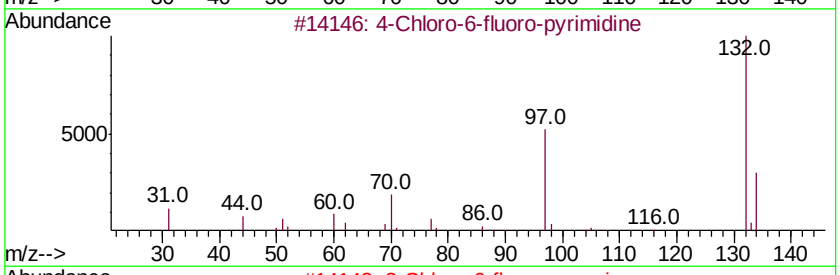
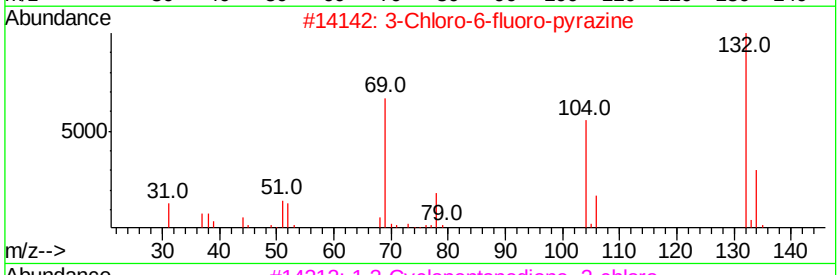
Peak Number 3 unknown7.55 Concentration Rank 1

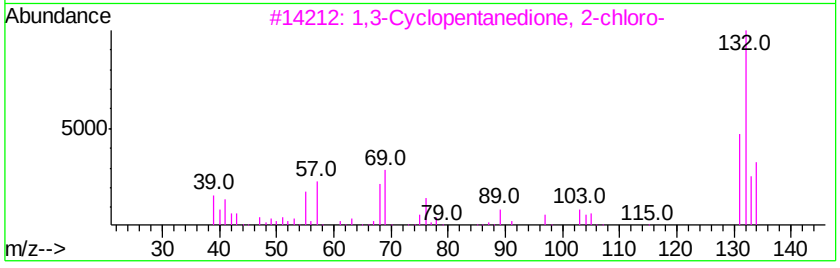
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	63.12 ng	571566	1,4-Dichlorobenzene-d4	8.01

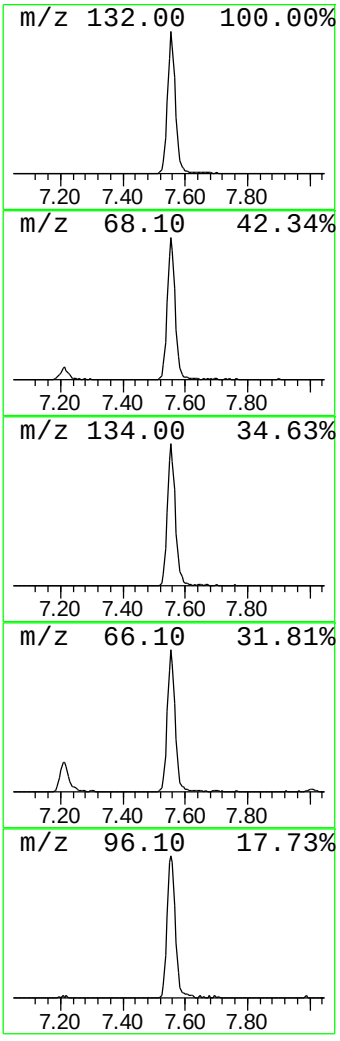
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12











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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 1-B

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

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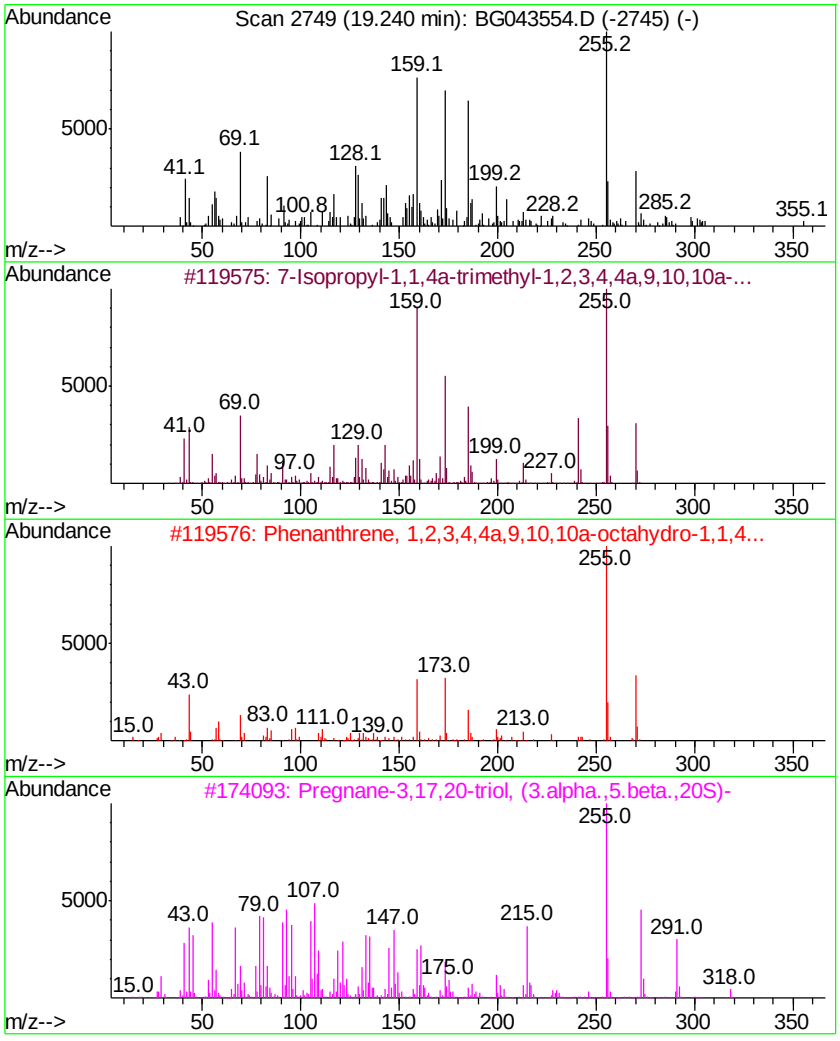
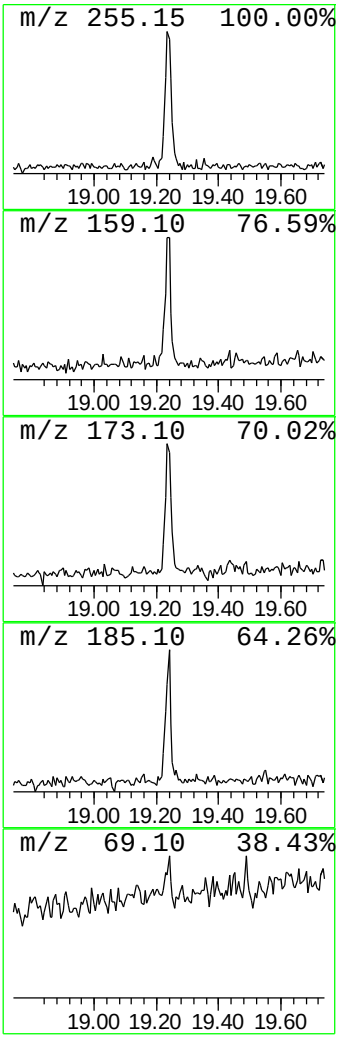
Peak Number 5 7-Isopropyl-1,1,4a-trimethy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.24	3.20 ng	76993	Phenanthrene-d10	17.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Isopropyl-1,1,4a-trimethyl-1,2...	270	C20H30	1000210-28-9	89
2	Phenanthrene, 1,2,3,4,4a,9,10,10...	270	C20H30	019407-28-4	43
3	Pregnane-3,17,20-triol, (3.alpha...	336	C21H36O3	001098-45-9	25
4	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	25
5	S-Indacene-1,7-dione, 2,3,5,6-te...	270	C18H22O2	055591-16-7	25





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Instrument : BNA_G
ClientSampleId : 1-B

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TIC Library : C:\Database\NIST11.L
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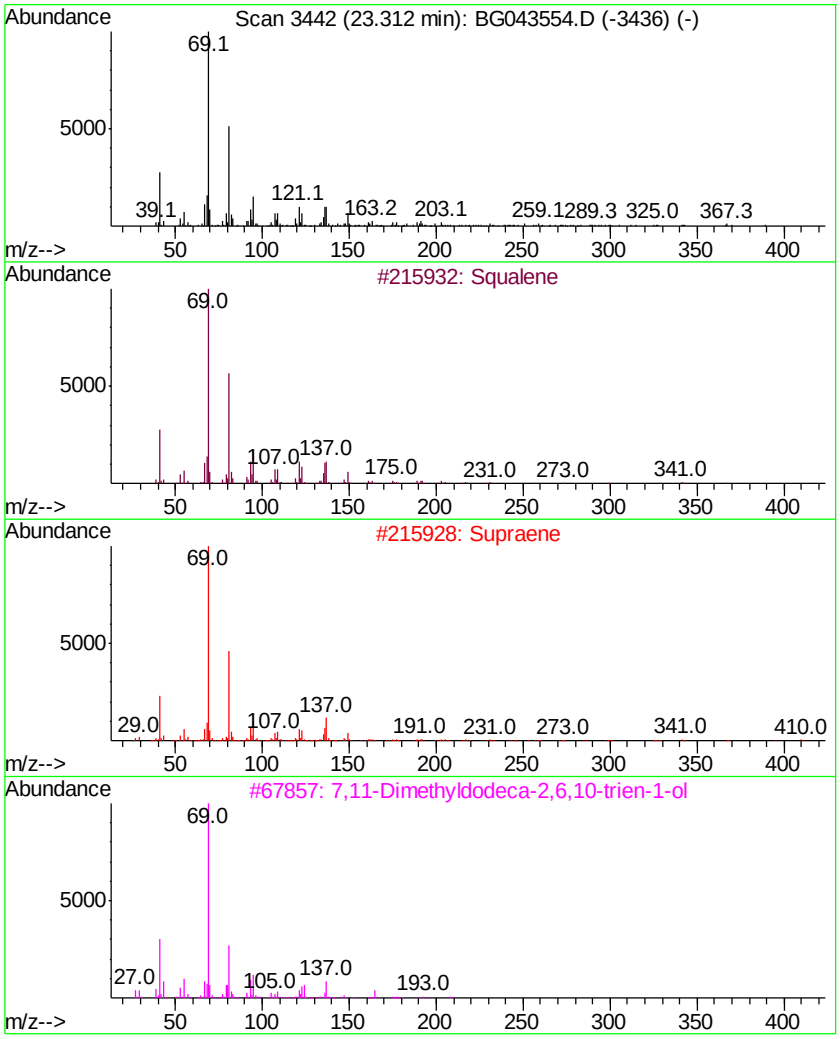
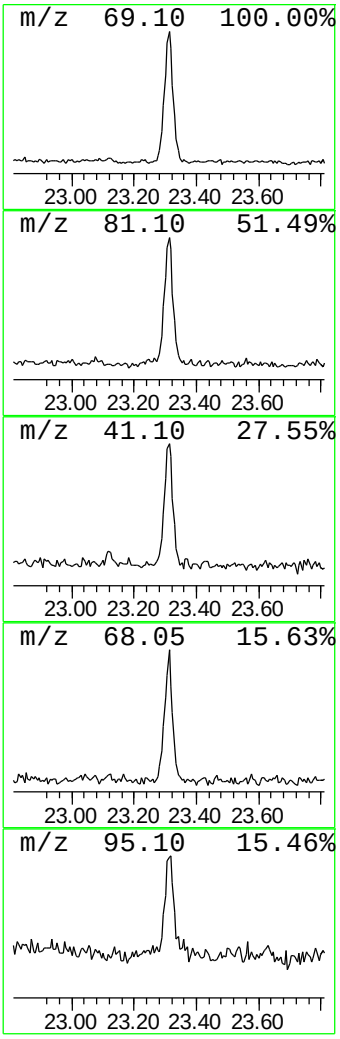
Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.31	10.54 ng	316643	Perylene-d12	24.85

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	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	68
4	1,6,10,14-Hexadecatetraen-3-ol, ...	290	C20H34O	001113-21-9	53
5	3-Ethyl-1,5-octadiene	138	C10H18	1000114-87-7	50





Library Search Compound Report

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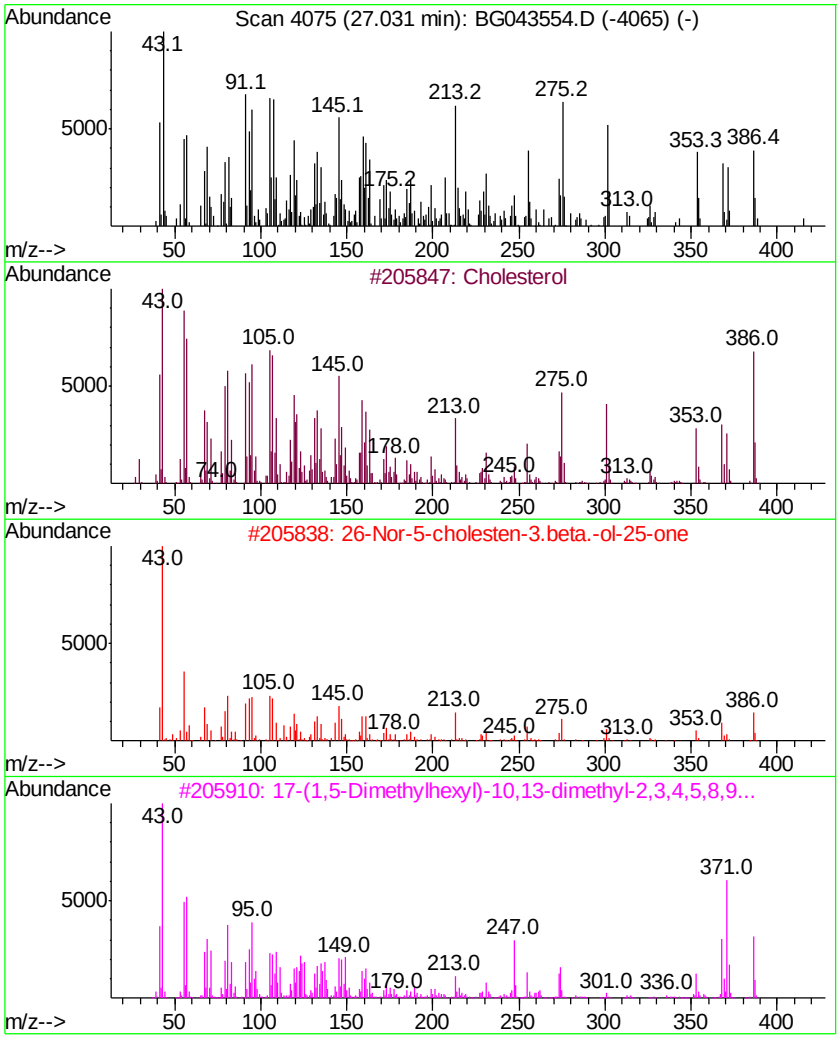
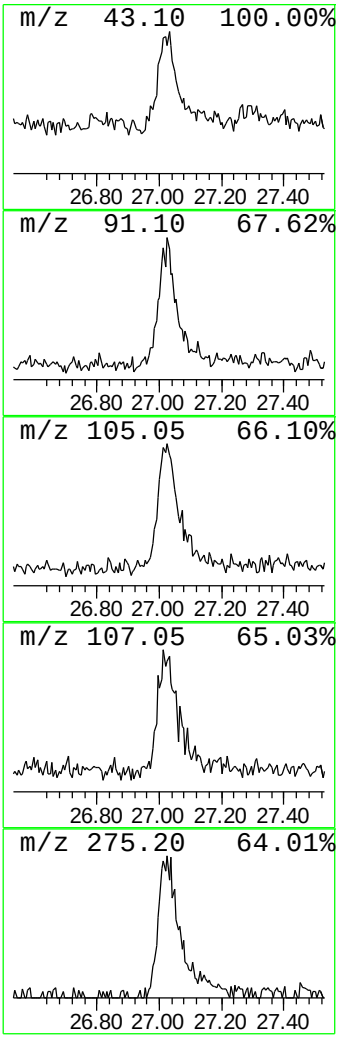
Peak Number 7 Cholesterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.03	17.32 ng	519990	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholesterol	386	C27H46O	000057-88-5	90
2	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	46
3	17-(1,5-Dimethylhexyl)-10,13-dim...	386	C27H46O	1000210-50-0	44
4	21-Acetoxypregnenolone	374	C23H34O4	000566-78-9	35
5	Propanoic acid, 3,3,3-trifluoro-...	386	C17H17F3N2O5	1000362-46-1	25





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.17	10.9	ng	98945	1	8.01	181113	20.0
2-Pentanone, 4-hy...	5.11	10.8	ng	97622	1	8.01	181113	20.0
unknown7.55	7.55	63.1	ng	571566	1	8.01	181113	20.0
7-Isopropyl-1,1,4...	19.24	3.2	ng	76993	4	17.38	481453	20.0
Squalene	23.31	10.5	ng	316643	6	24.85	600612	20.0
Cholesterol	27.03	17.3	ng	519990	6	24.85	600612	20.0