

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
 Data File : BG060142.D
 Acq On : 22 Dec 2023 17:32
 Operator : MA/JU
 Sample : 05900-23
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GHL-SS-65a

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-BG122123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060142.D\data.ms

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	10	rVB	245173	305420	2.47%	0.401%
2	5.045	328	333	339	rBV2	94077	162576	1.32%	0.214%
3	5.515	406	413	429	rBV	3493165	5793576	46.93%	7.615%
4	7.107	674	684	695	rBV	4131781	7388386	59.85%	9.711%
5	7.941	819	826	835	rBV	850318	1448409	11.73%	1.904%
6	9.105	1015	1024	1040	rBV	2349795	4284955	34.71%	5.632%
7	10.744	1293	1303	1310	rBV	1397159	2444318	19.80%	3.213%
8	12.430	1582	1590	1600	rVB2	227616	401748	3.25%	0.528%
9	13.200	1714	1721	1731	rBV	7286109	11326097	91.74%	14.887%
10	14.575	1944	1955	1965	rBV	2591063	4080510	33.05%	5.363%
11	16.067	2202	2209	2219	rBV	5380623	8317043	67.37%	10.932%
12	17.324	2415	2423	2434	rBV	3262884	4905598	39.74%	6.448%
13	18.212	2570	2574	2583	rBV	666828	1002758	8.12%	1.318%
14	19.134	2727	2731	2737	rBV6	104467	166076	1.35%	0.218%
15	19.486	2788	2791	2800	rVB3	118805	179885	1.46%	0.236%
16	19.945	2863	2869	2876	rBV	9151983	12345749	100.00%	16.227%
17	20.415	2944	2949	2955	rBV10	86466	181130	1.47%	0.238%
18	20.556	2970	2973	2980	rBV2	102378	167169	1.35%	0.220%
19	21.237	3082	3089	3103	rVB2	1012564	1963489	15.90%	2.581%
20	21.590	3143	3149	3158	rBV	2263801	3693917	29.92%	4.855%
21	23.253	3428	3432	3437	rVB	152761	281332	2.28%	0.370%
22	23.858	3531	3535	3541	rBV2	115997	206348	1.67%	0.271%
23	24.763	3680	3689	3702	rVB2	1301250	3685740	29.85%	4.844%
24	30.009	4573	4582	4598	rVB9	303147	1350095	10.94%	1.775%

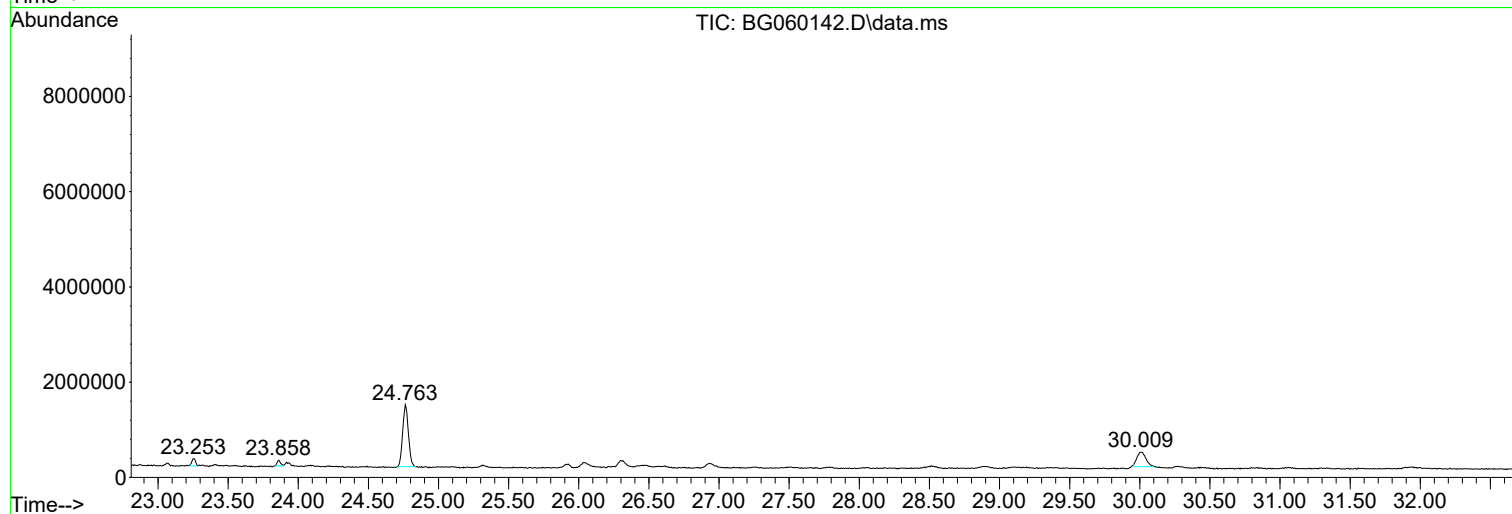
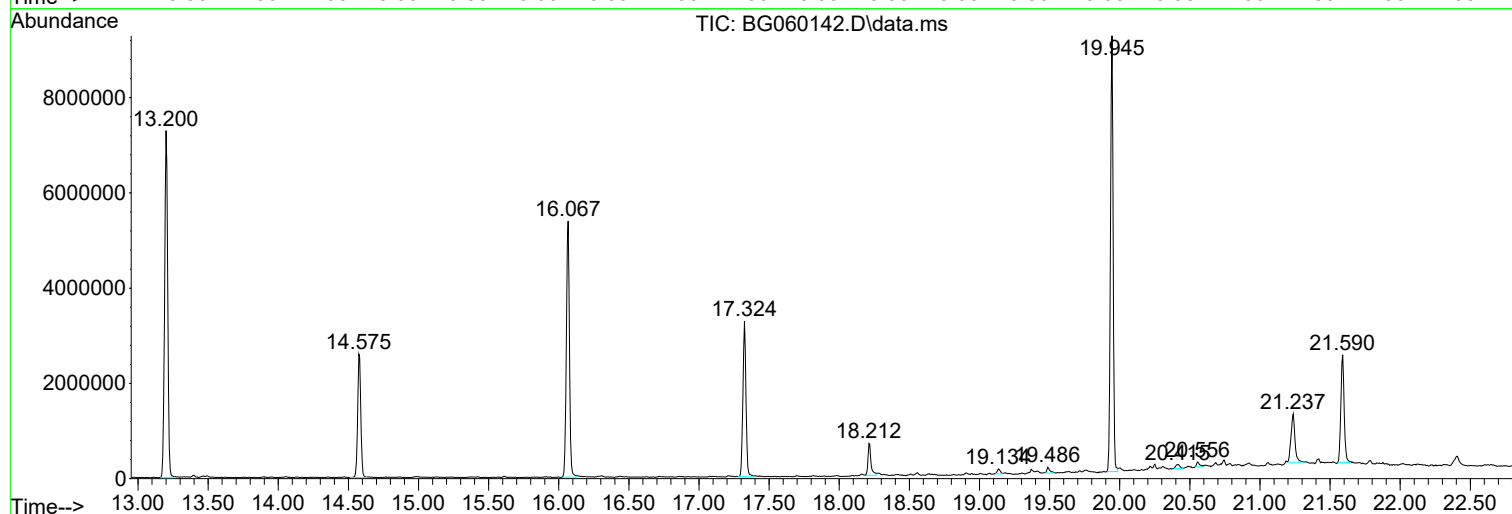
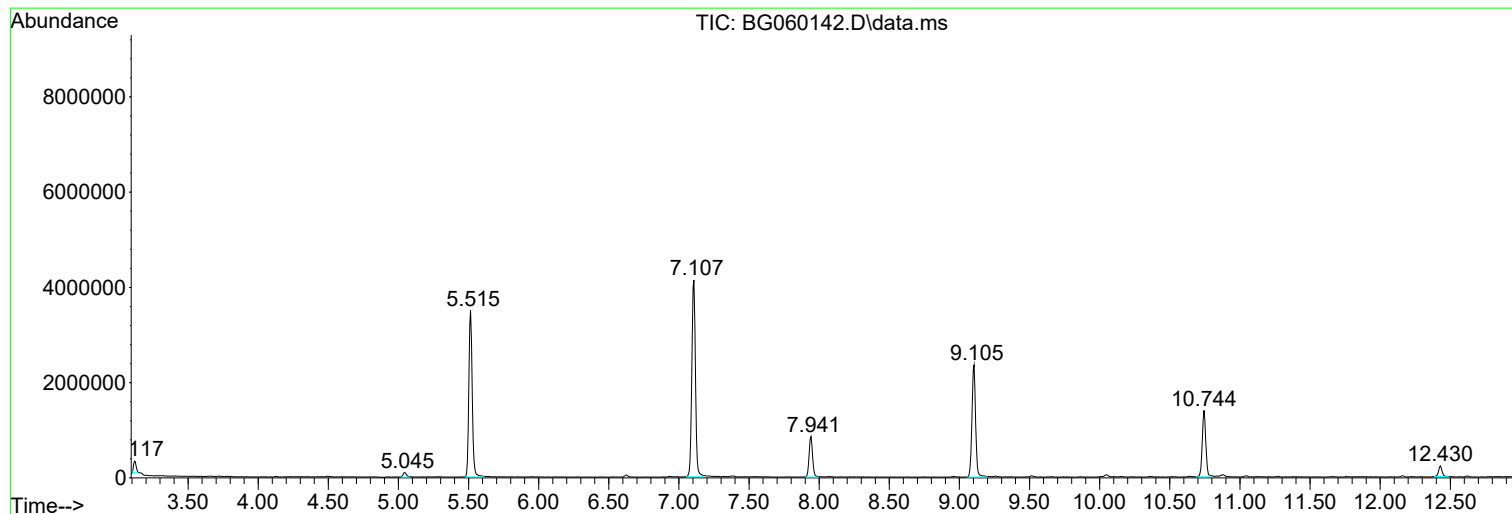
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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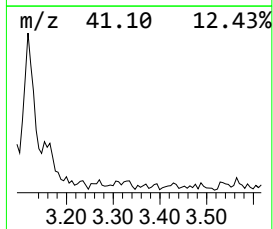
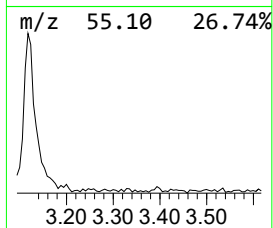
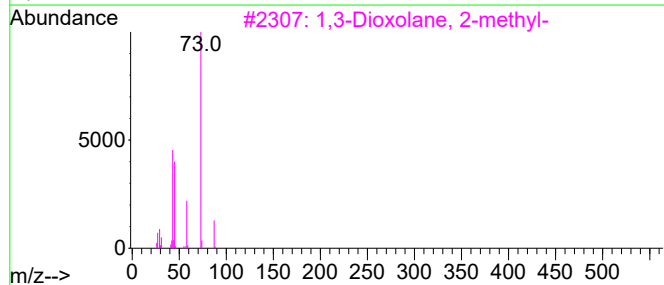
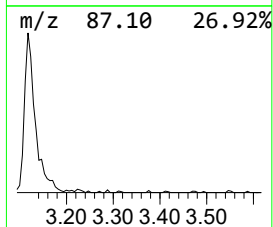
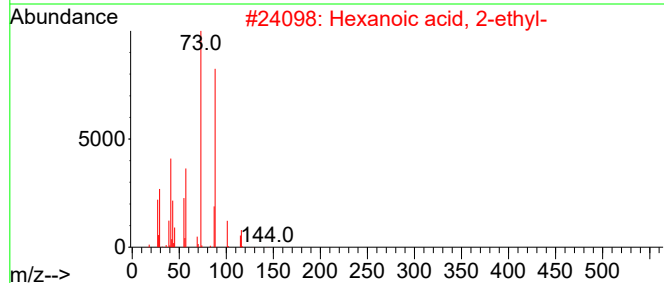
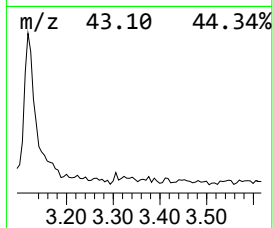
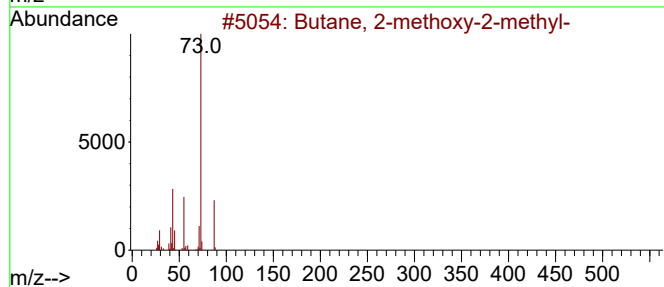
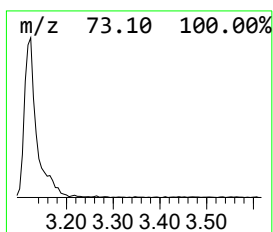
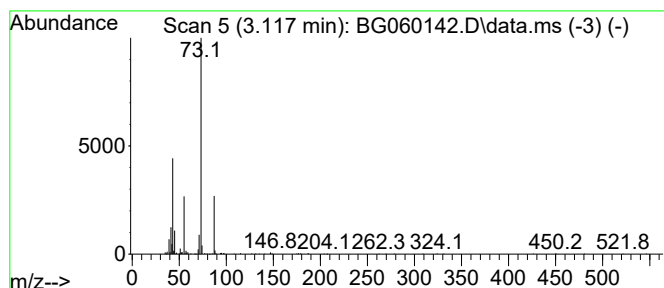
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.117	4.22 ng	305420	1,4-Dichlorobenzene-d4	7.941

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	33
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4			Myo-Inositol, 2-C-methyl-	194	C7H14O6	000472-96-8	9
5			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9



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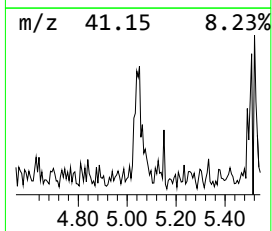
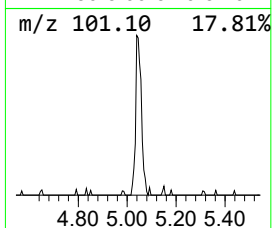
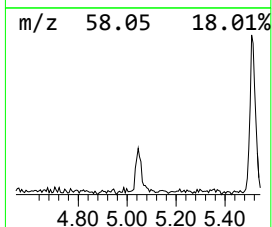
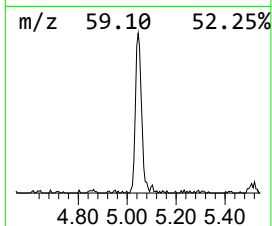
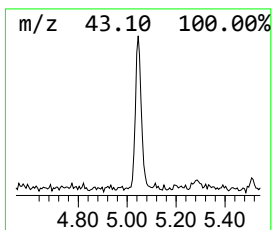
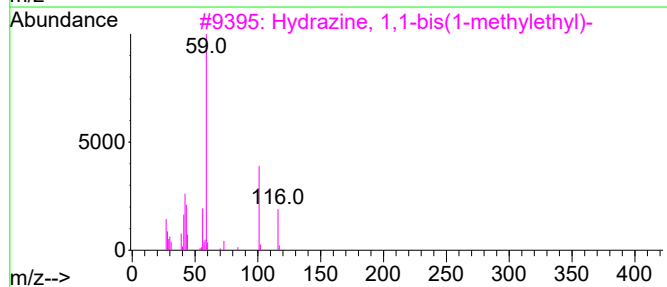
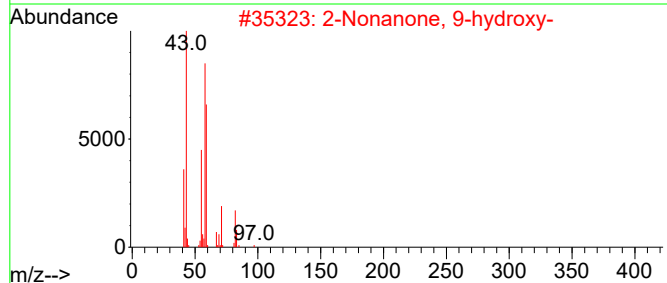
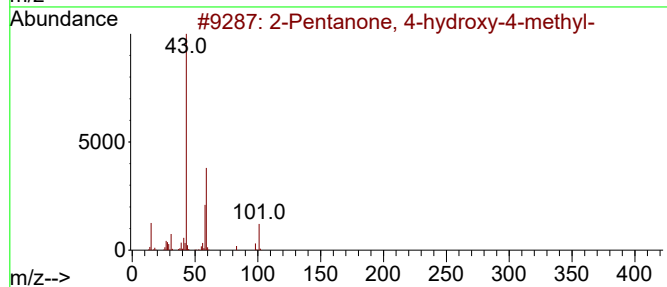
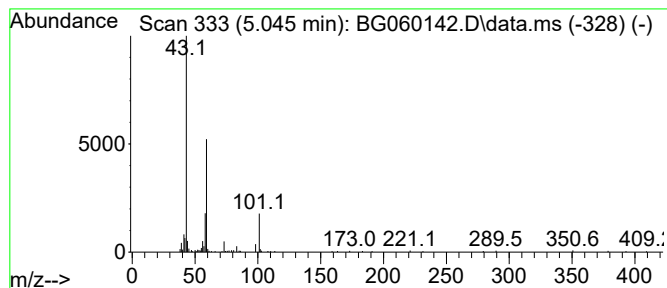
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown5.045 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	2.24 ng	162576	1,4-Dichlorobenzene-d4	7.941

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
3		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25
4		1,3-Dioxolane-4-methanol, 2,2-di...	132	C6H12O3	000100-79-8	25
5		2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	25



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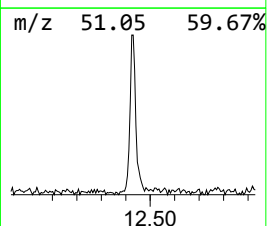
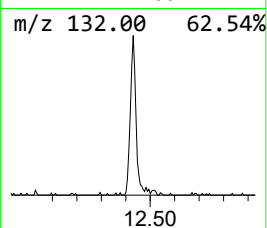
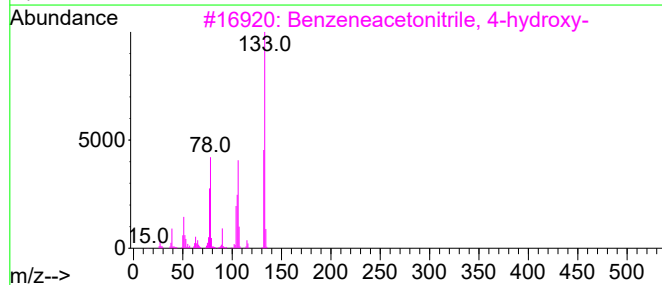
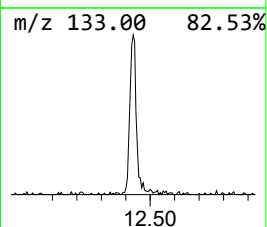
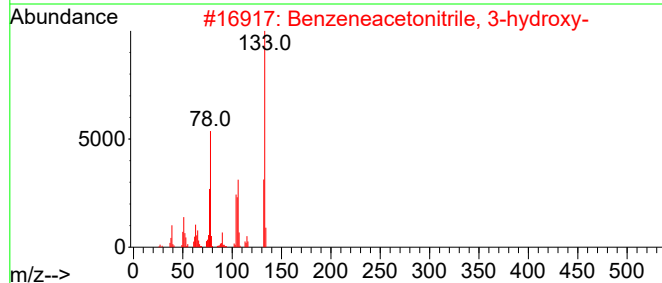
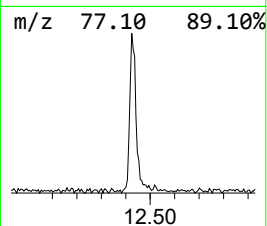
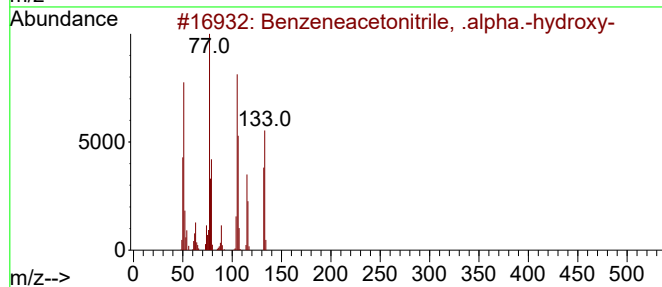
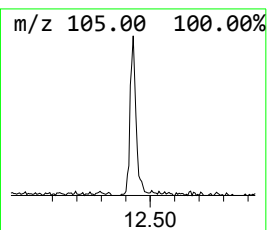
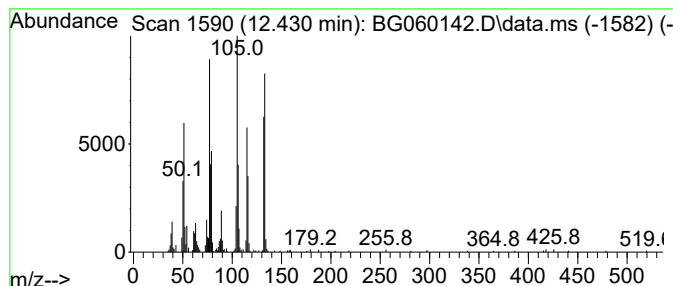
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzeneacetonitrile, .alpha... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.430	3.29 ng	401748	Naphthalene-d8	10.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetonitrile, .alpha.-hyd...	133	C8H7NO	000532-28-5	87
2			Benzeneacetonitrile, 3-hydroxy-	133	C8H7NO	025263-44-9	38
3			Benzeneacetonitrile, 4-hydroxy-	133	C8H7NO	014191-95-8	27
4			1H-Benzimidazol-2-amine	133	C7H7N3	000934-32-7	18
5			Benzene, 1-isocyanato-4-methyl-	133	C8H7NO	000622-58-2	14



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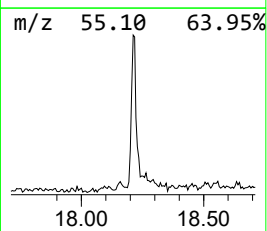
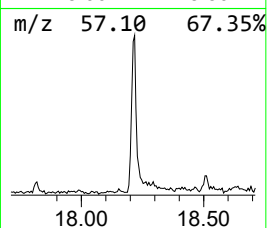
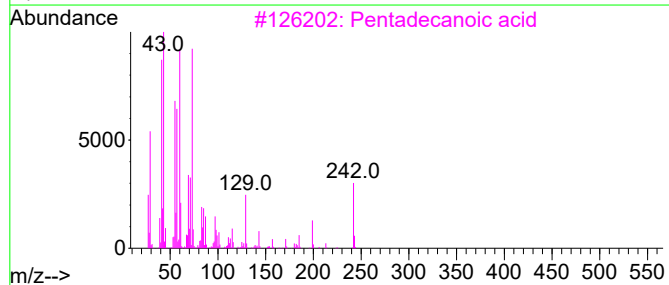
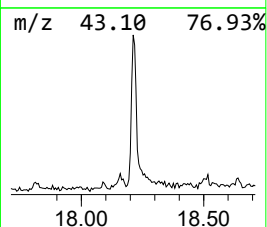
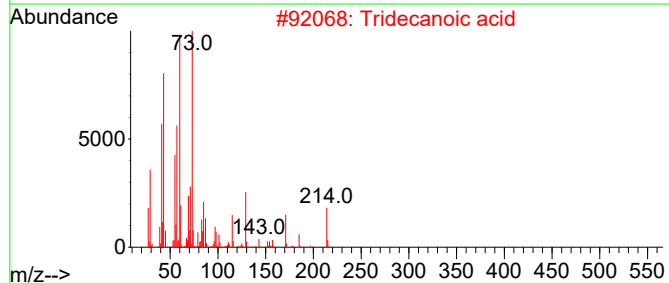
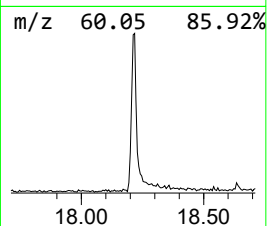
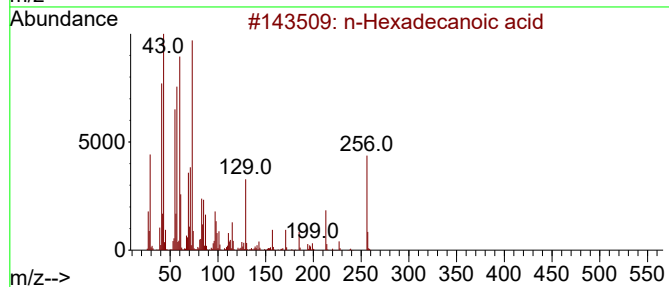
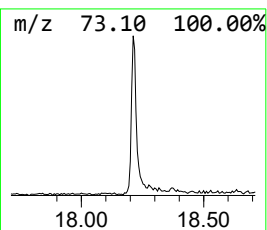
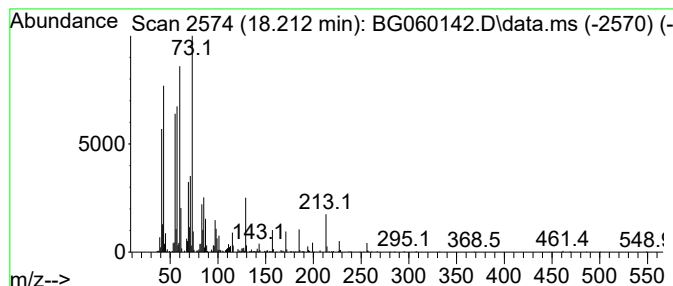
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.212	4.09 ng	1002760	Phenanthrene-d10	17.324

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5			Undecanoic acid	186	C11H22O2	000112-37-8	72



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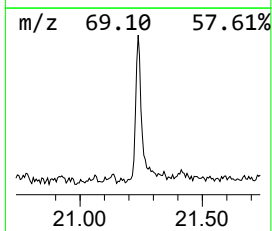
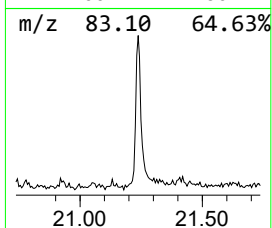
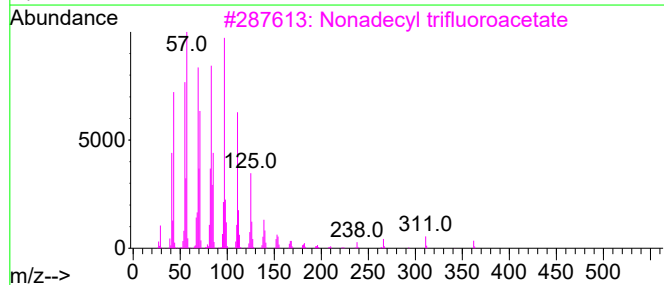
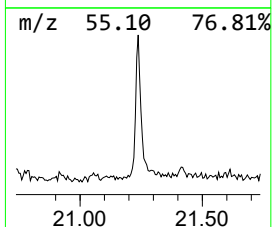
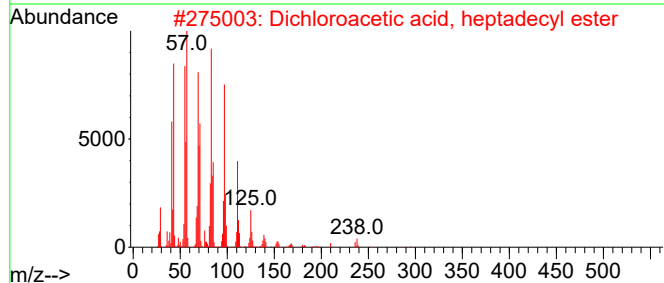
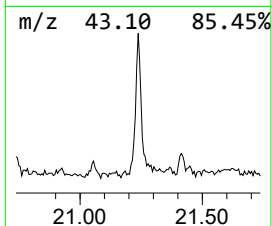
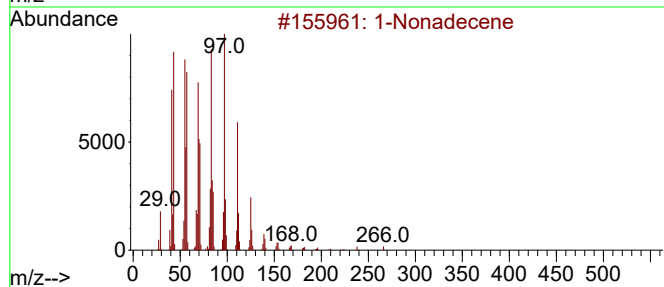
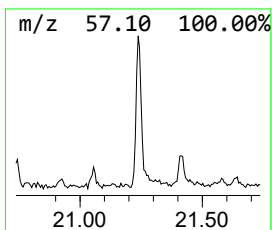
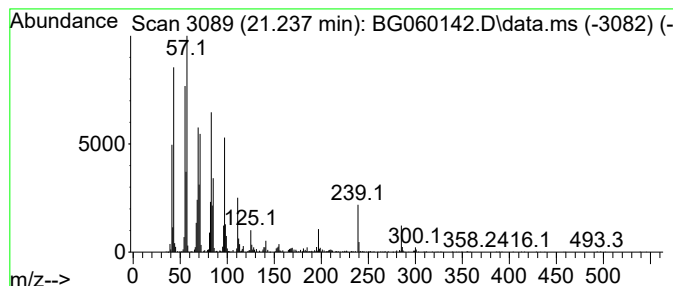
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Nonadecene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.237	10.63 ng	1963490	Chrysene-d12	21.590

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonadecene	266	C19H38	018435-45-5	91
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81
3			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	81
4			17-Pentatriacontene	491	C35H70	006971-40-0	76
5			1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	74



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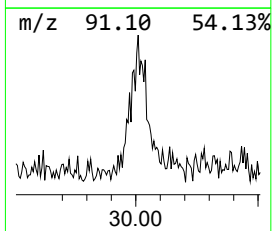
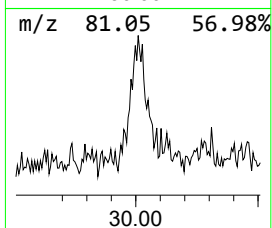
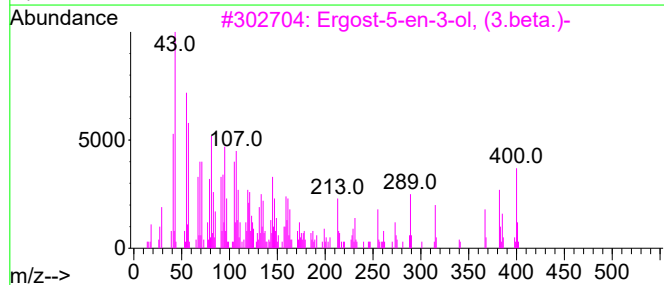
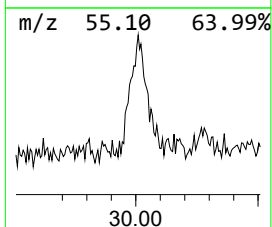
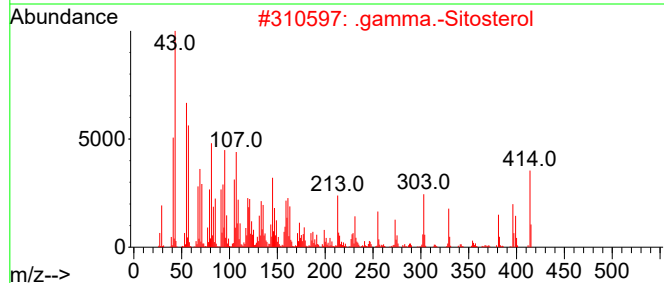
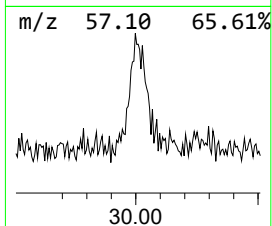
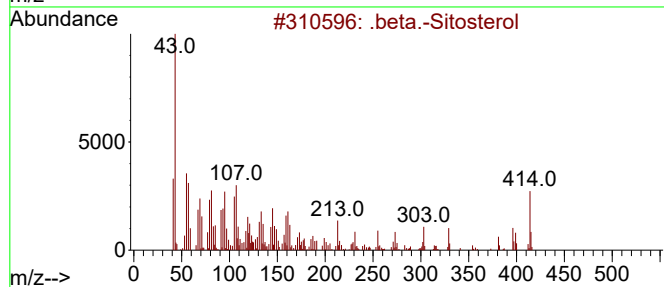
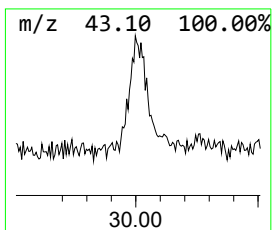
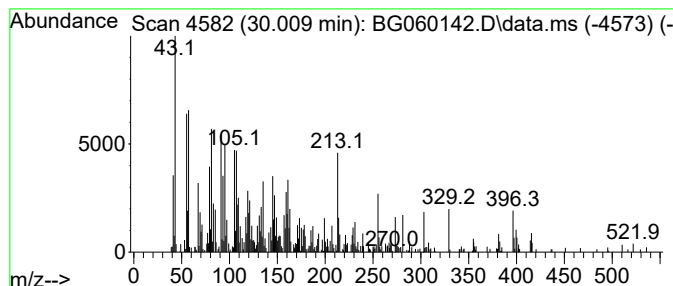
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 .beta.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.009	7.33 ng	1350100	Perylene-d12	24.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Sitosterol	414	C29H50O	000083-46-5	74
2		.gamma.-Sitosterol	414	C29H50O	000083-47-6	64
3		Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	46
4		Ergost-7-en-3-ol	400	C28H48O	116179-22-7	46
5		Campesterol	400	C28H48O	000474-62-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
Data File : BG060142.D
Acq On : 22 Dec 2023 17:32
Operator : MA/JU
Sample : 05900-23
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-65a

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.117	4.2	ng	305420	1	7.941	1448410	20.0
unknown5.045	5.045	2.2	ng	162576	1	7.941	1448410	20.0
Benzeneacetone...	12.430	3.3	ng	401748	2	10.744	2444320	20.0
n-Hexadecanoic ...	18.212	4.1	ng	1002760	4	17.324	4905600	20.0
1-Nonadecene	21.237	10.6	ng	1963490	5	21.590	3693920	20.0
.beta.-Sitosterol	30.009	7.3	ng	1350100	6	24.763	3685740	20.0