

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
 Data File : BG059887.D
 Acq On : 25 Nov 2023 11:56
 Operator : MA/JU
 Sample : 05466-04
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RB200018

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-BG111623.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059887.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.349	329	334	339	rBV2	26009	40281	1.86%	0.320%
2	5.814	403	413	420	rBV	555714	887397	40.87%	7.052%
3	7.441	681	690	699	rBV2	608009	1020663	47.01%	8.111%
4	8.316	832	839	846	rBV2	141453	236435	10.89%	1.879%
5	9.521	1035	1044	1051	rVB2	392291	703035	32.38%	5.587%
6	11.166	1316	1324	1330	rBV	177368	328441	15.13%	2.610%
7	13.569	1726	1733	1740	rBV	1120030	1663340	76.61%	13.218%
8	13.775	1761	1768	1777	rVB	347010	512910	23.62%	4.076%
9	14.944	1961	1967	1976	rBV2	330757	535636	24.67%	4.256%
10	16.436	2214	2221	2228	rBV	933942	1396000	64.30%	11.093%
11	16.906	2297	2301	2305	rBV3	16054	24938	1.15%	0.198%
12	17.700	2429	2436	2441	rBV	385883	582590	26.83%	4.630%
13	17.741	2441	2443	2448	rVB	54995	70564	3.25%	0.561%
14	18.510	2569	2574	2581	rBV2	177505	243655	11.22%	1.936%
15	18.610	2588	2591	2596	rVB3	18430	25168	1.16%	0.200%
16	18.751	2608	2615	2619	rBV7	12952	27354	1.26%	0.217%
17	19.110	2673	2676	2682	rVB7	12851	24707	1.14%	0.196%
18	19.450	2730	2734	2738	rBV7	29840	41422	1.91%	0.329%
19	19.668	2768	2771	2776	rVB2	36962	44113	2.03%	0.351%
20	19.733	2776	2782	2785	rBV2	110003	159349	7.34%	1.266%
21	19.768	2785	2788	2793	rVB4	77040	92291	4.25%	0.733%
22	20.050	2832	2836	2840	rVV4	25332	45961	2.12%	0.365%
23	20.097	2840	2844	2850	rVB	100574	145040	6.68%	1.153%
24	20.273	2868	2874	2879	rBV	1690469	2171048	100.00%	17.252%
25	21.007	2996	2999	3003	rBV5	14773	24725	1.14%	0.196%
26	21.372	3055	3061	3068	rVB5	18286	42821	1.97%	0.340%
27	21.554	3086	3092	3098	rBV5	56349	127076	5.85%	1.010%
28	21.701	3114	3117	3120	rVV2	19816	25080	1.16%	0.199%
29	21.824	3132	3138	3143	rVB3	37556	61995	2.86%	0.493%
30	22.018	3163	3171	3177	rBV4	273840	544972	25.10%	4.331%
31	22.065	3177	3179	3186	rVB2	51777	95285	4.39%	0.757%
32	22.118	3186	3188	3193	rBV6	15336	24386	1.12%	0.194%
33	24.421	3576	3580	3586	rBV6	28645	64257	2.96%	0.511%
34	25.255	3715	3722	3725	rBV4	17001	37444	1.72%	0.298%
35	25.408	3743	3748	3754	rVB4	26786	67632	3.12%	0.537%
36	25.590	3769	3779	3788	rVB2	141899	445958	20.54%	3.544%

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Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

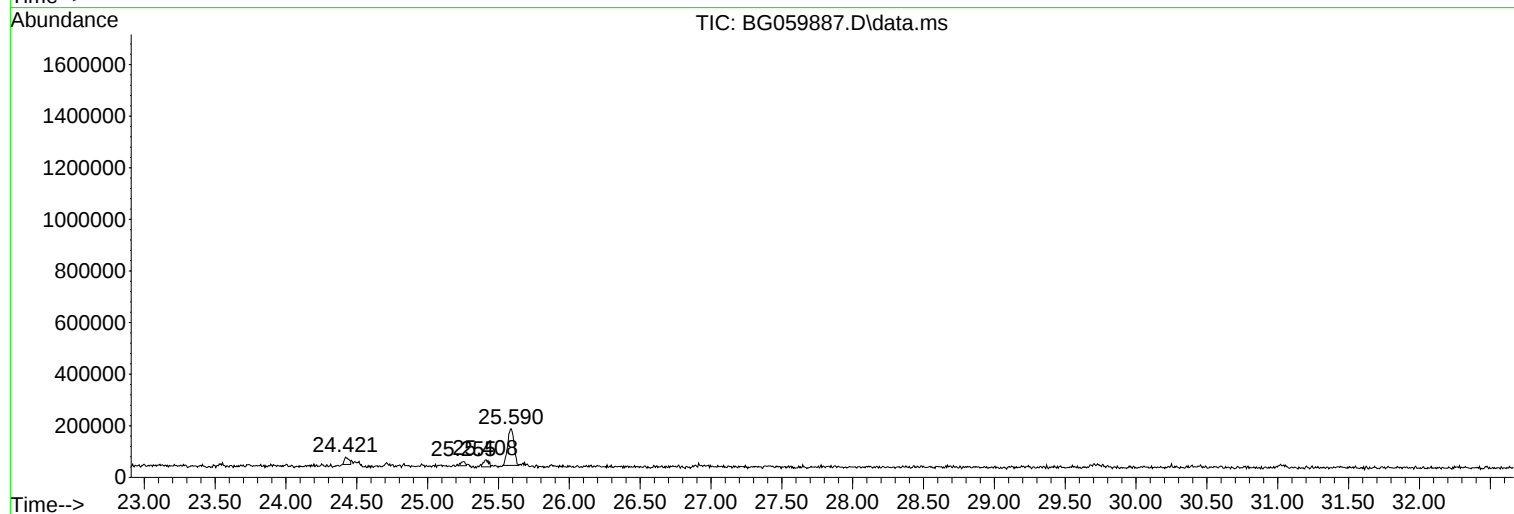
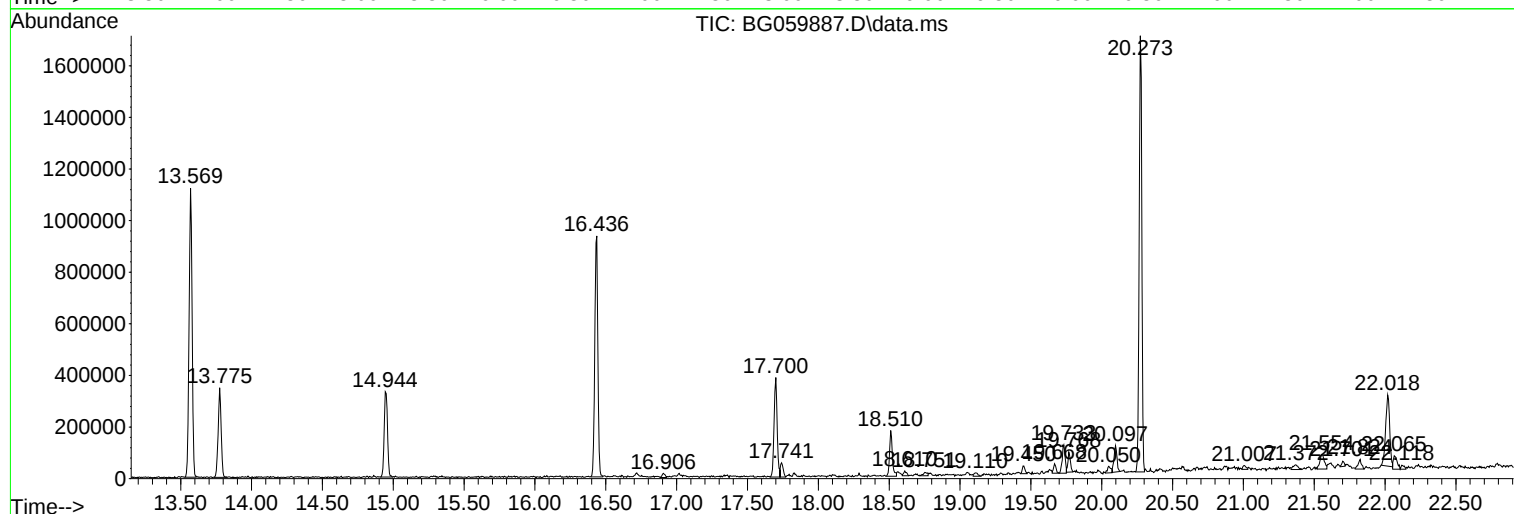
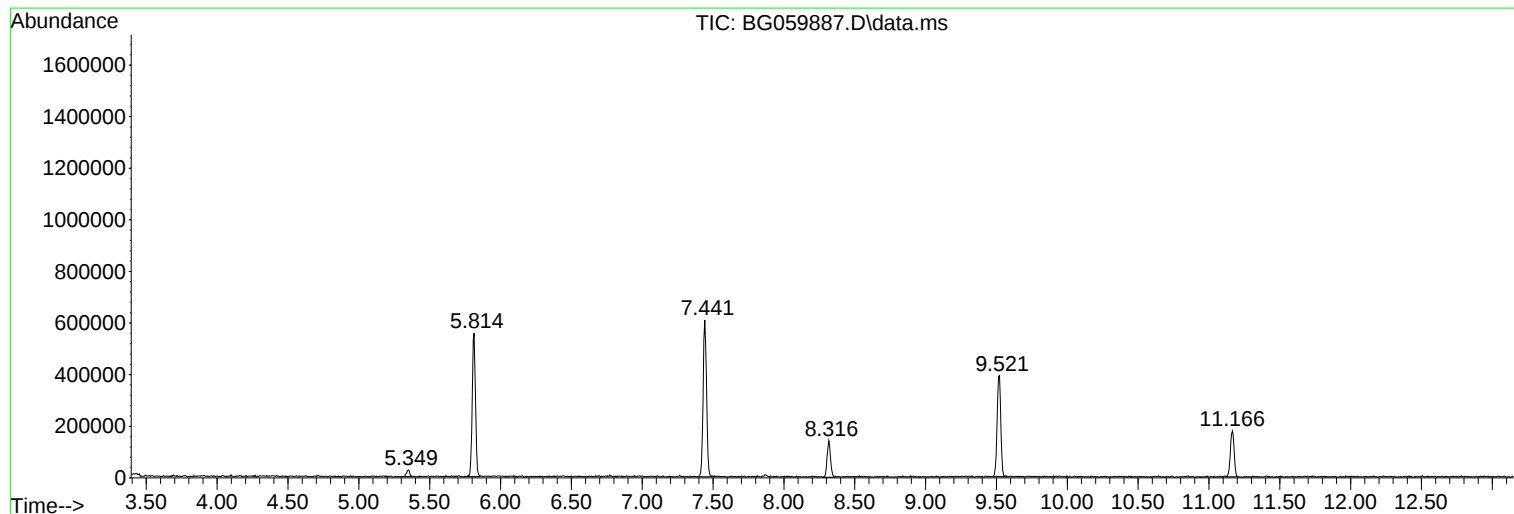
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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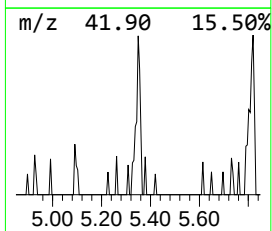
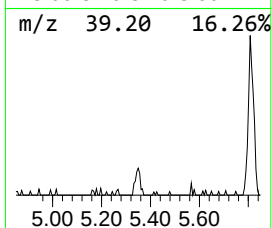
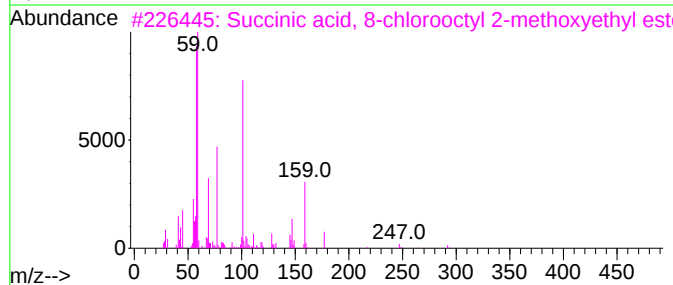
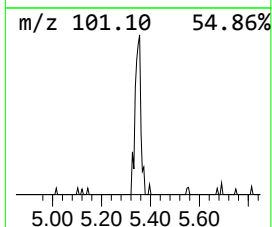
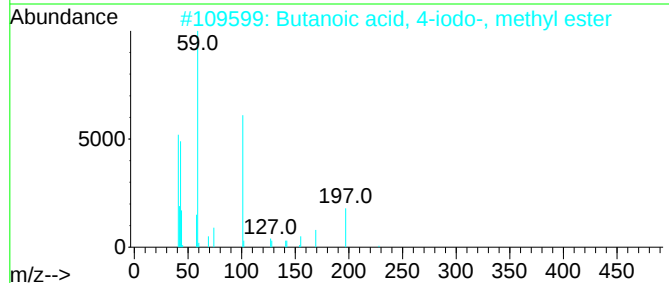
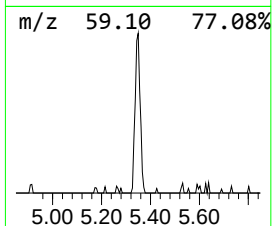
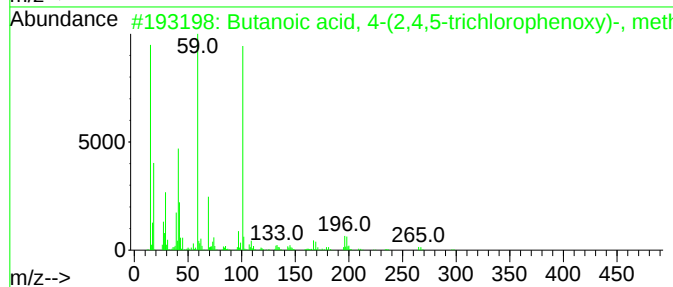
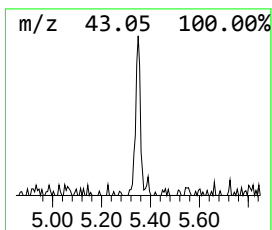
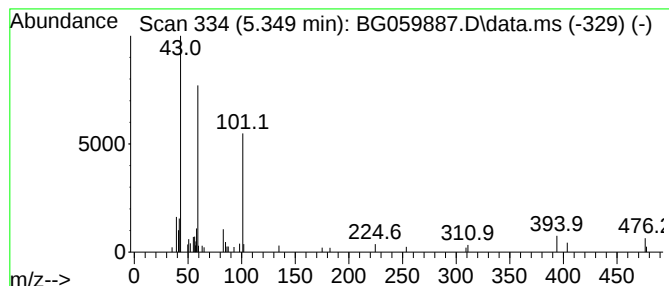
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butanoic acid, 4-(2,4,5-tri... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.349	3.41 ng	40281	1,4-Dichlorobenzene-d4	8.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 4-(2,4,5-trichlor...	296	C11H11Cl3O3	025333-21-5	50
2			Butanoic acid, 4-iodo-, methyl e...	228	C5H9IO2	014273-85-9	50
3			Succinic acid, 8-chlorooctyl 2-m...	322	C15H27ClO5	1010390-74-8	50
4			3-Heptanol	116	C7H16O	000589-82-2	38
5			Butanamide	87	C4H9NO	000541-35-5	32



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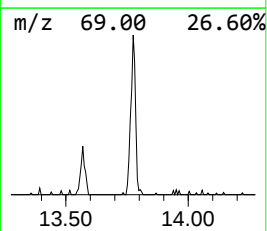
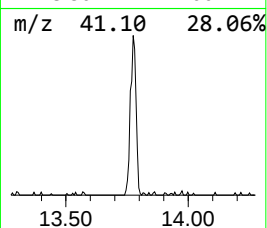
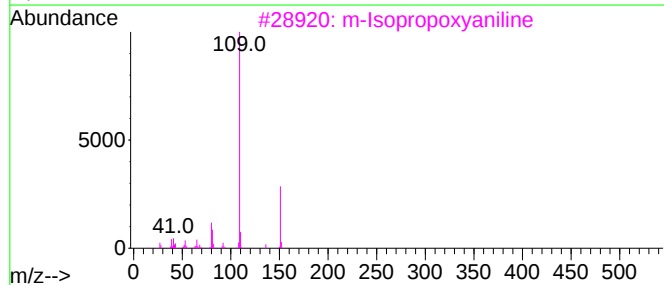
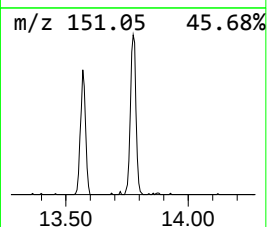
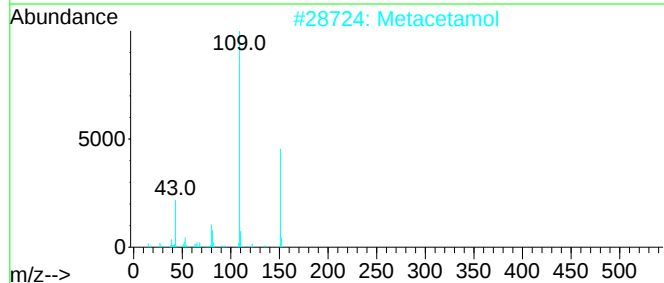
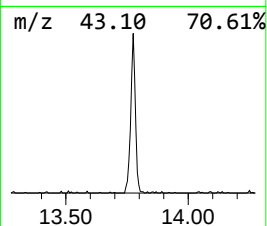
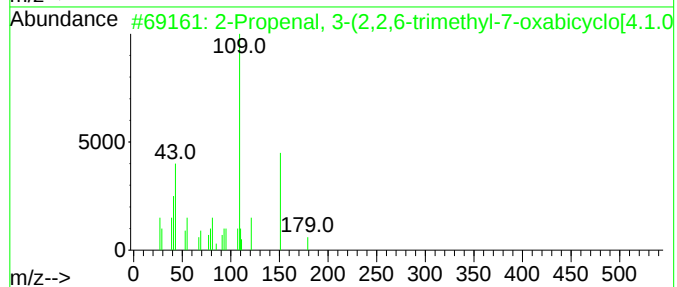
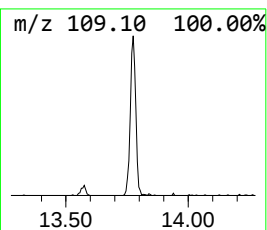
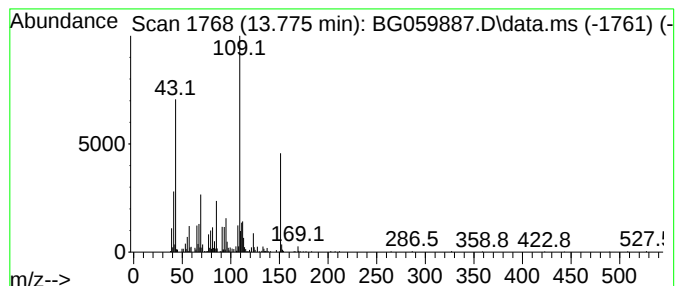
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Peak Number 2 2-Propenal, 3-(2,2,6-trimet... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.775	19.15 ng	512910	Acenaphthene-d10	14.950

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	64		
2	Metacetamol	151	C8H9NO2	000621-42-1	58		
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	58		
4	Diacetamate	193	C10H11NO3	002623-33-8	50		
5	2-Amino-4-methylpyrimidine	109	C5H7N3	000108-52-1	38		



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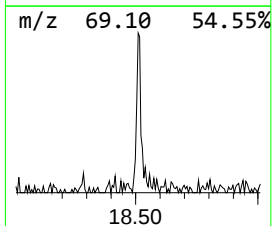
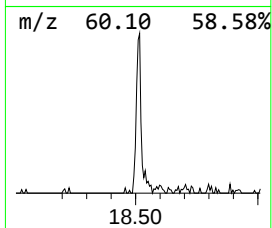
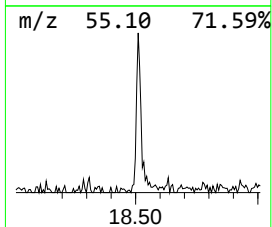
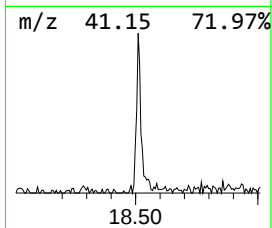
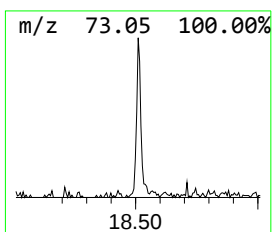
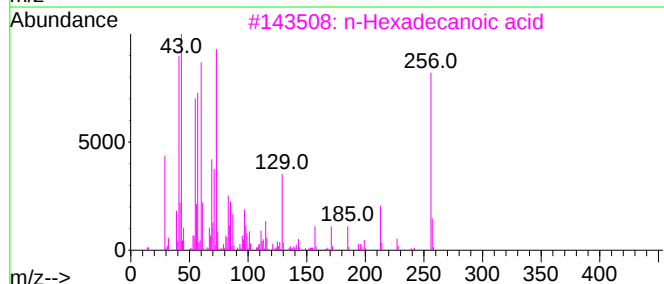
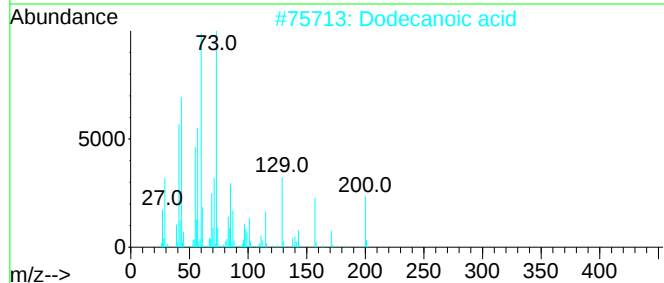
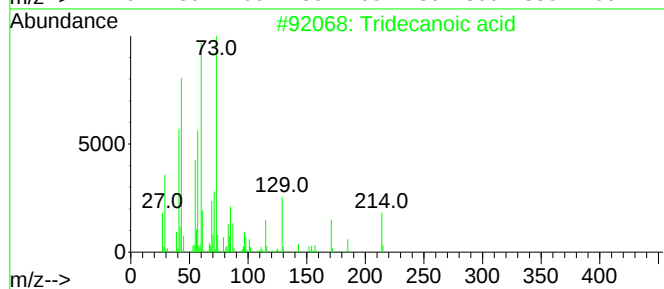
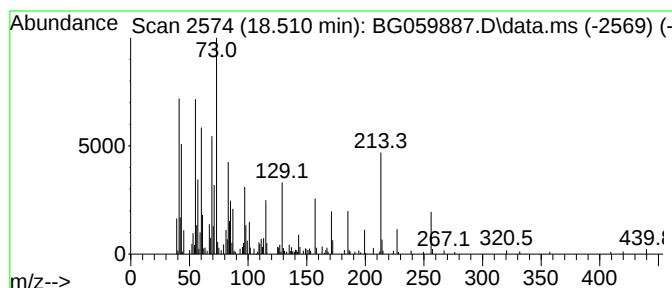
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Tridecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.510	8.36 ng	243655	Phenanthrene-d10	17.700

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	60
2			Dodecanoic acid	200	C12H24O2	000143-07-7	49
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	45
5			Undecanoic acid	186	C11H22O2	000112-37-8	35



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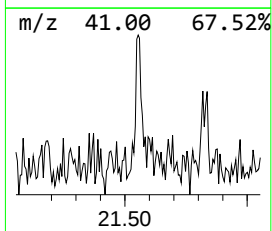
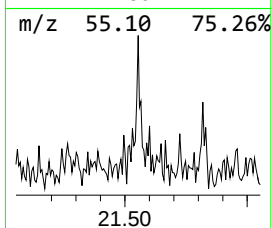
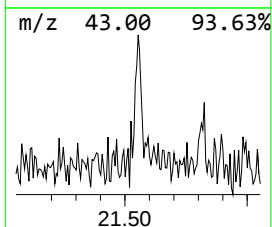
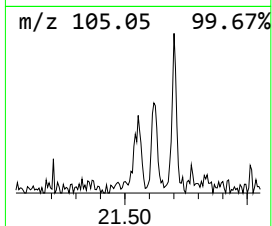
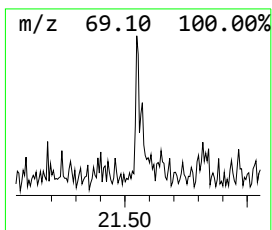
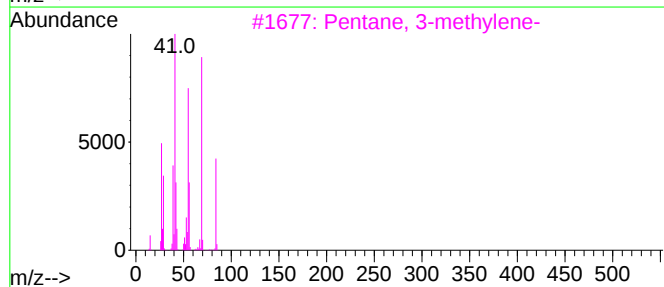
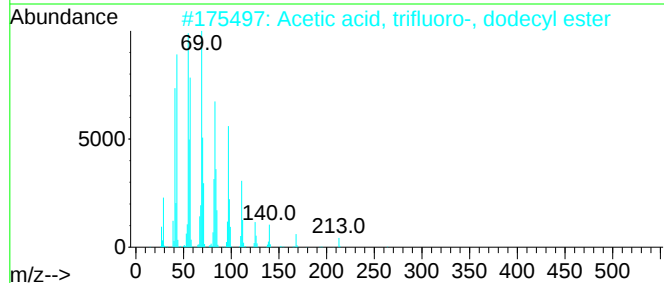
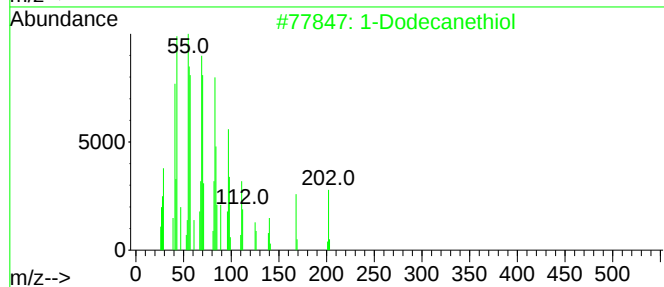
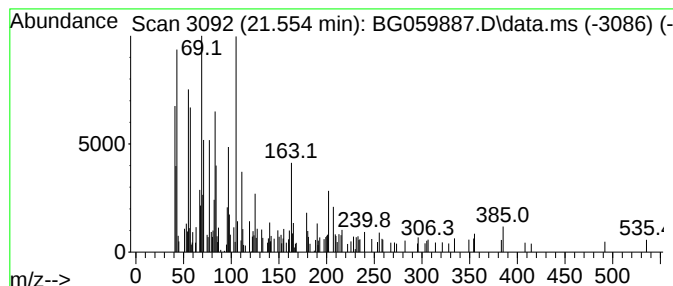
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Peak Number 4 1-Dodecanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.554	4.66 ng	127076	Chrysene-d12	22.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Dodecanethiol	202	C12H26S	000112-55-0	52
2			Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	52
3			Pentane, 3-methylene-	84	C6H12	000760-21-4	43
4			1-Pentadecene	210	C15H30	013360-61-7	38
5			1-Tridecene	182	C13H26	002437-56-1	30



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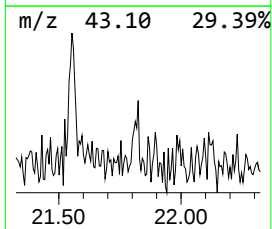
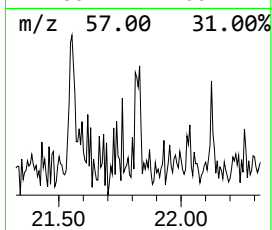
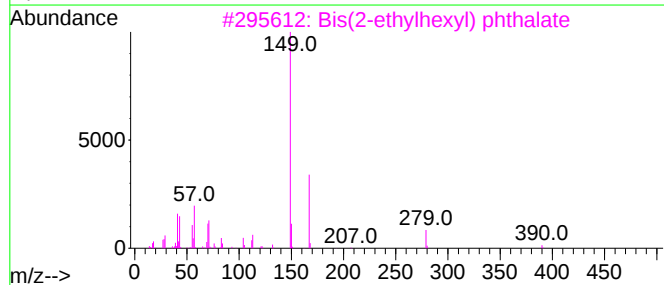
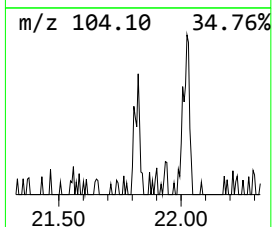
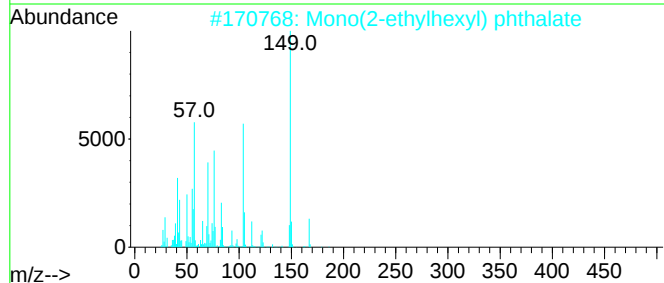
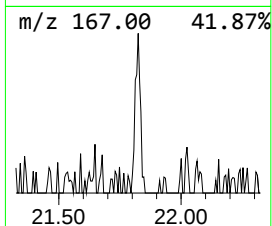
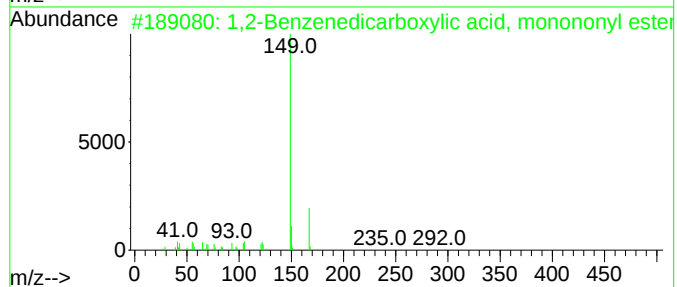
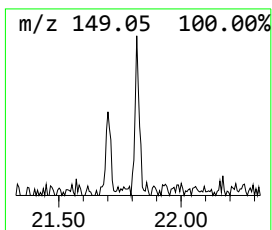
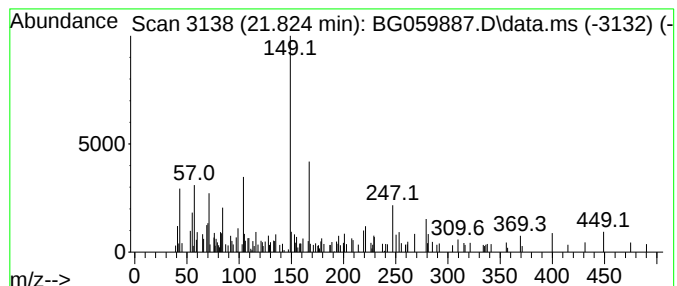
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1,2-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.824	2.28 ng	61995	Chrysene-d12	22.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, mo...	292	C17H24O4	024539-59-1	60
2			Mono(2-ethylhexyl) phthalate	278	C16H22O4	004376-20-9	43
3			Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	43
4			Phthalic acid, monodecyl ester	306	C18H26O4	024539-60-4	38
5			Phthalic acid, heptadecyl 6-meth...	516	C33H56O4	1000377-97-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059887.D
Acq On : 25 Nov 2023 11:56
Operator : MA/JU
Sample : 05466-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB200018

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanoic acid, ...	5.349	3.4	ng	40281	1	8.316	236435	20.0
2-Propenal, 3-(...	13.775	19.1	ng	512910	3	14.950	535636	20.0
Tridecanoic acid	18.510	8.4	ng	243655	4	17.700	582590	20.0
1-Dodecanethiol	21.554	4.7	ng	127076	5	22.018	544972	20.0
1,2-Benzenedica...	21.824	2.3	ng	61995	5	22.018	544972	20.0