

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
 Data File : BG055845.D
 Acq On : 30 Nov 2022 17:06
 Operator : CG/JU
 Sample : N5795-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-10

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-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055845.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.268	330	337	347	rBV	351450	549079	25.33%	4.147%
2	5.750	413	419	431	rBV	521706	861298	39.73%	6.505%
3	6.367	518	524	531	rVB	21646	33685	1.55%	0.254%
4	7.371	687	695	707	rBV	534396	940212	43.37%	7.101%
5	8.217	829	839	849	rBV	142319	238105	10.98%	1.798%
6	9.392	1028	1039	1053	rBV	331780	595402	27.46%	4.497%
7	10.791	1270	1277	1305	rBV2	65895	183575	8.47%	1.386%
8	11.049	1313	1321	1328	rBV	207869	364963	16.83%	2.756%
9	13.470	1724	1733	1741	rBV	920389	1485776	68.53%	11.222%
10	13.717	1767	1775	1783	rBV	19158	33833	1.56%	0.256%
11	14.845	1960	1967	1975	rVB	349730	549420	25.34%	4.150%
12	16.184	2189	2195	2202	rBV	23951	35811	1.65%	0.270%
13	16.325	2213	2219	2232	rBV	757122	1186310	54.72%	8.960%
14	17.583	2427	2433	2438	rBV	433397	672930	31.04%	5.082%
15	17.624	2438	2440	2447	rVB	46778	62057	2.86%	0.469%
16	18.211	2536	2540	2544	rVB	23356	28646	1.32%	0.216%
17	18.441	2574	2579	2585	rBV4	63420	118689	5.47%	0.896%
18	18.505	2586	2590	2596	rVB2	20795	36835	1.70%	0.278%
19	18.646	2609	2614	2619	rBV3	15832	33745	1.56%	0.255%
20	18.852	2645	2649	2654	rVB	71353	84275	3.89%	0.637%
21	19.375	2730	2738	2741	rBV5	61913	106442	4.91%	0.804%
22	19.504	2754	2760	2767	rVB4	28453	43703	2.02%	0.330%
23	19.622	2767	2780	2786	rBV	170542	271259	12.51%	2.049%
24	19.704	2790	2794	2801	rVV4	28603	51747	2.39%	0.391%
25	19.986	2838	2842	2848	rVB	134905	191795	8.85%	1.449%
26	20.168	2867	2873	2879	rBV	1631369	2167936	100.00%	16.374%
27	20.309	2889	2897	2903	rBV7	17965	49438	2.28%	0.373%
28	20.468	2922	2924	2928	rVB2	24525	29104	1.34%	0.220%
29	20.626	2949	2951	2957	rVB2	22599	28066	1.29%	0.212%
30	21.243	3052	3056	3063	rBV	28082	46158	2.13%	0.349%
31	21.872	3155	3163	3169	rBV2	432323	890177	41.06%	6.723%
32	21.919	3169	3171	3182	rVB	75332	124069	5.72%	0.937%
33	23.587	3450	3455	3466	rVB2	49729	107091	4.94%	0.809%
34	24.175	3548	3555	3561	rBV	65285	194314	8.96%	1.468%
35	25.092	3706	3711	3722	rVB	52333	147765	6.82%	1.116%
36	25.262	3730	3740	3750	rBV3	236858	696553	32.13%	5.261%

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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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

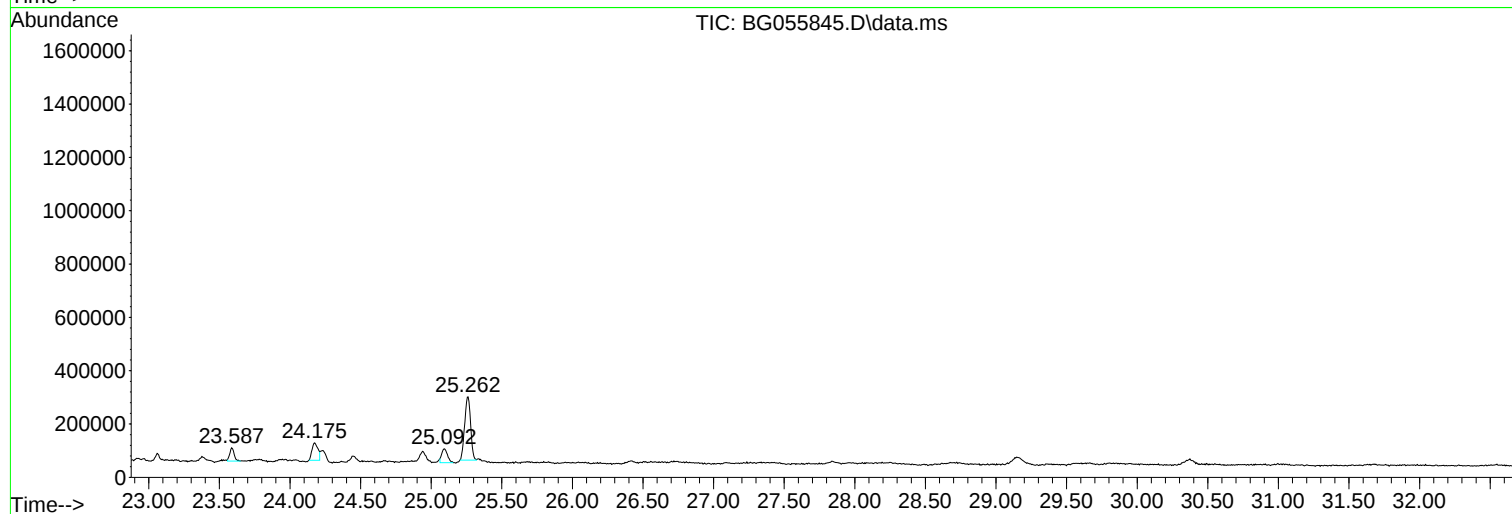
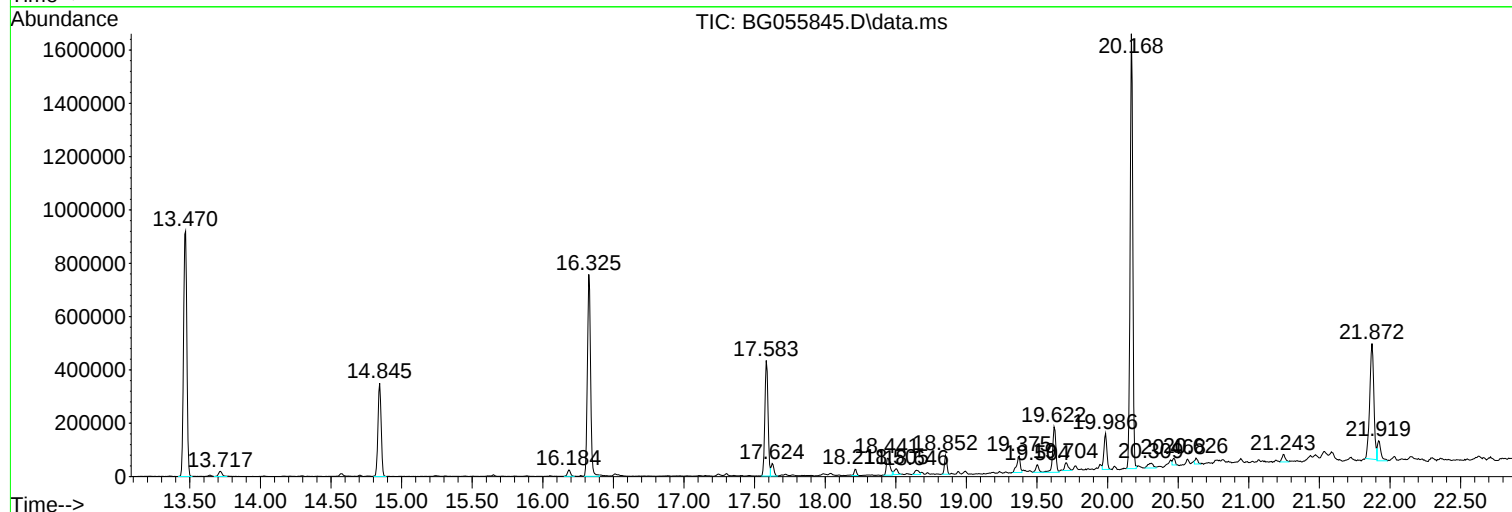
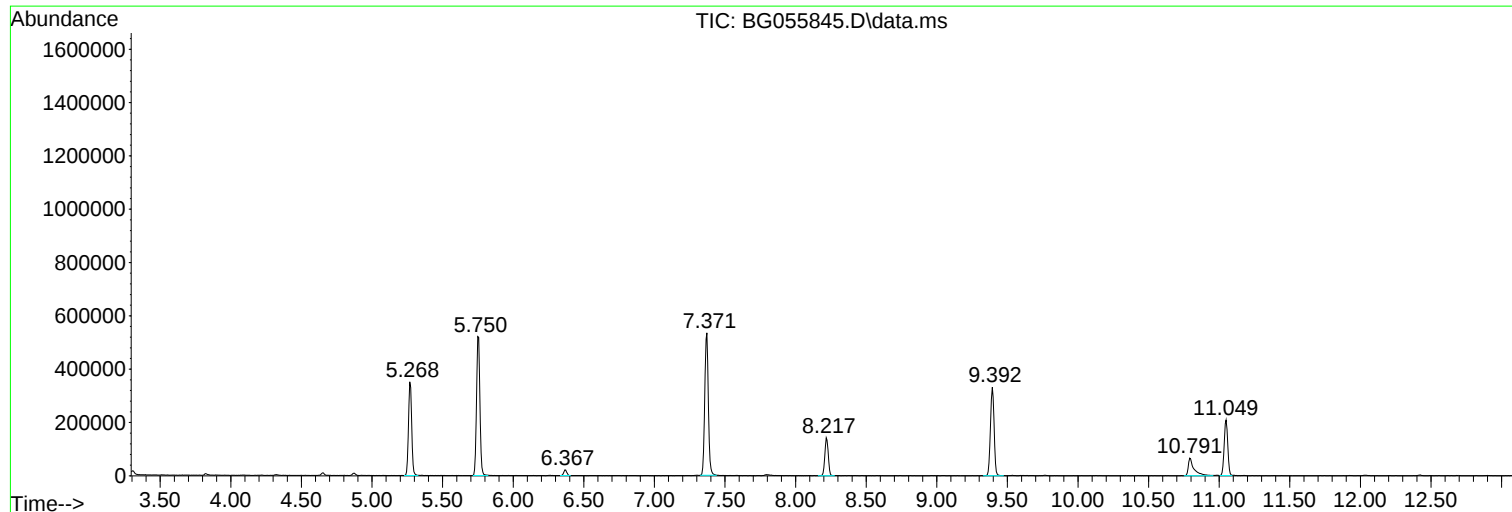
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG/JU
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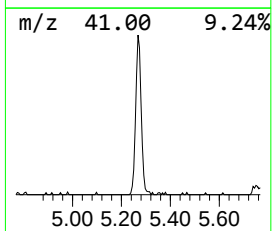
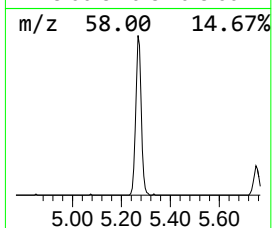
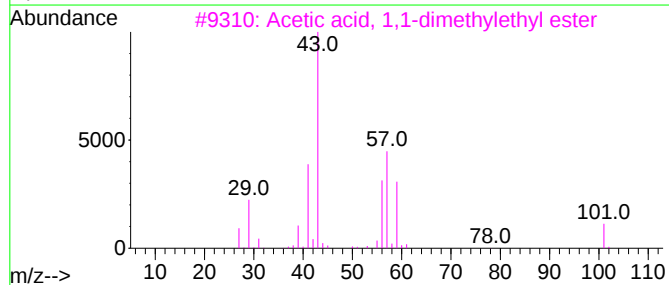
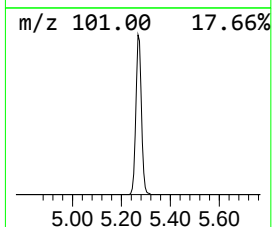
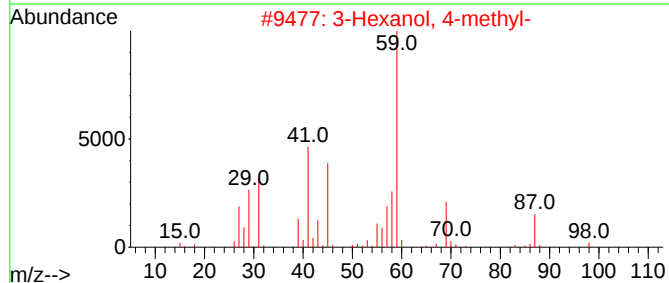
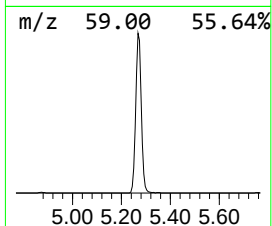
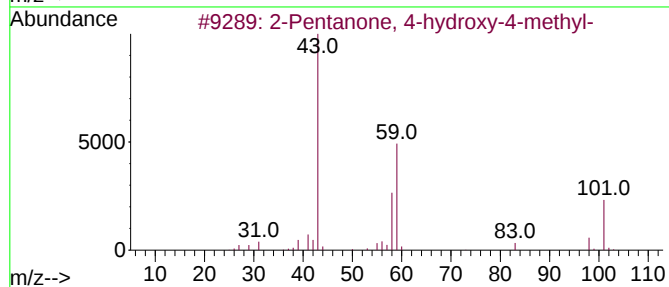
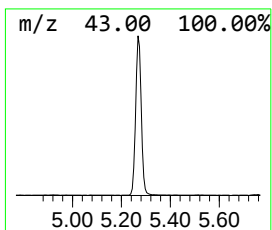
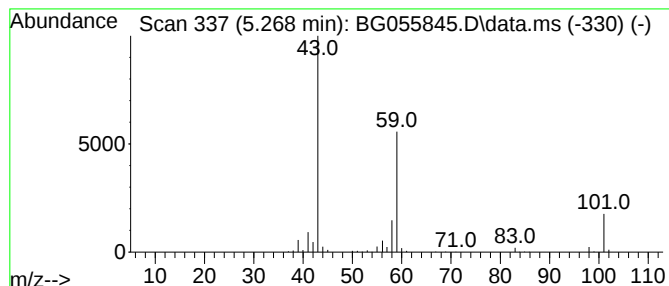
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.268	46.12 ng	549079	1,4-Dichlorobenzene-d4	8.217

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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Instrument :
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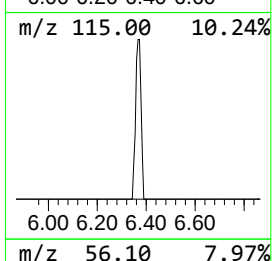
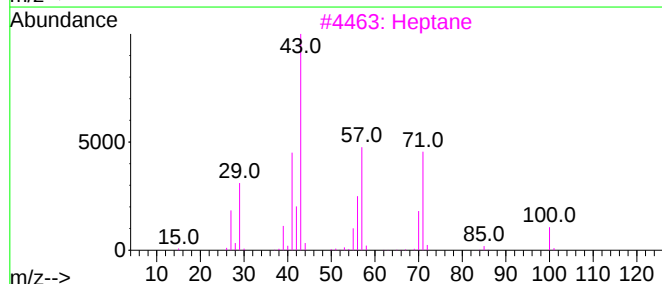
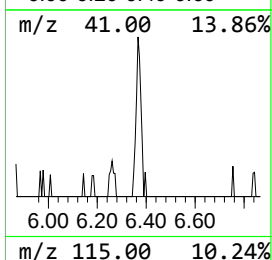
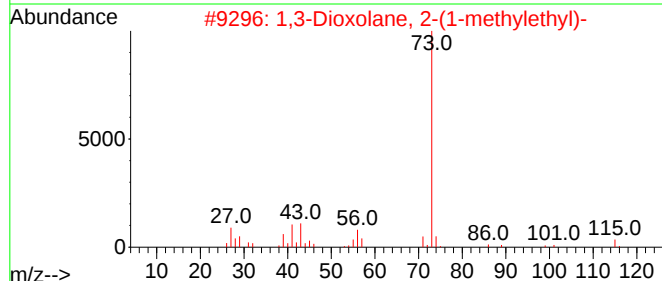
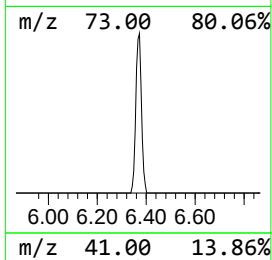
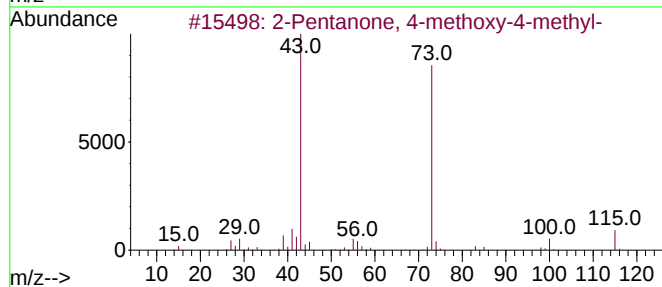
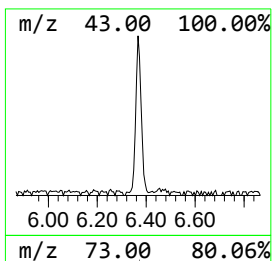
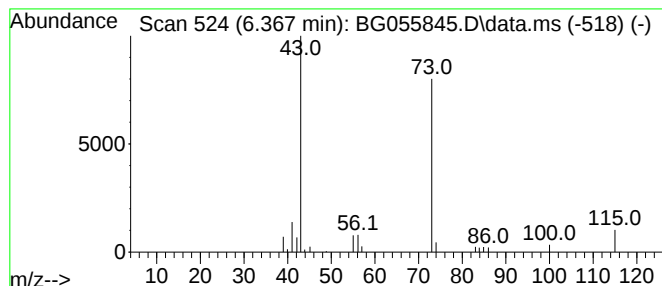
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.367	2.83 ng	33685	1,4-Dichlorobenzene-d4	8.217

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	28
3			Heptane	100	C7H16	000142-82-5	9
4			Octane, 4-methyl-	128	C9H20	002216-34-4	9
5			Pentane, 2-methoxy-2,4,4-trimethyl-	144	C9H20O	062108-41-2	9



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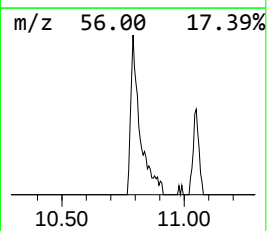
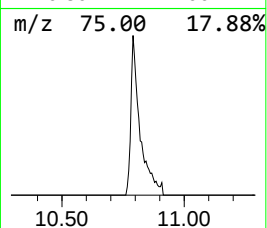
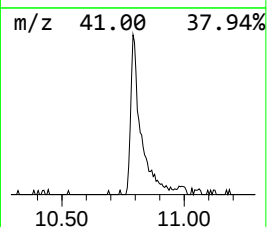
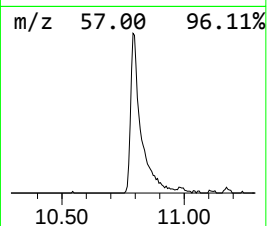
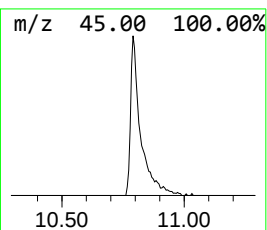
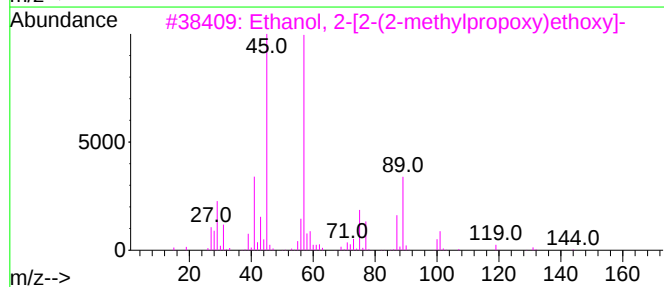
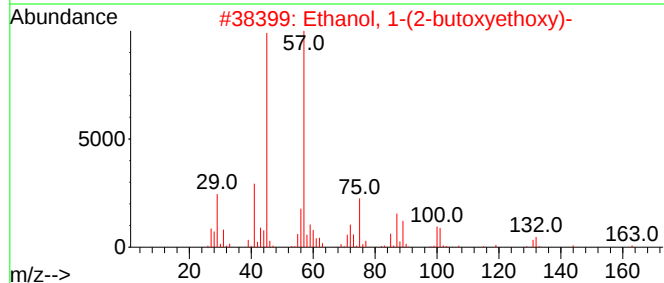
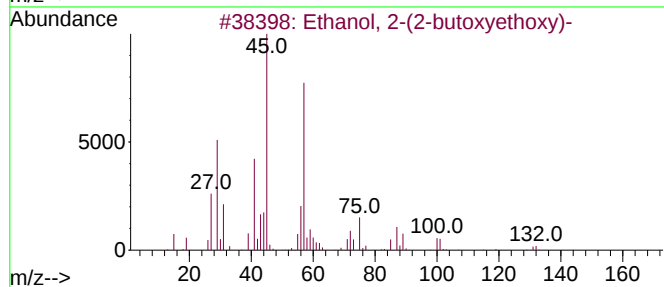
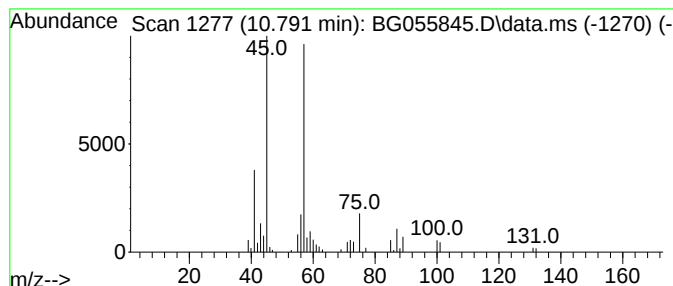
Instrument :
BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.791	10.06 ng	183575	Naphthalene-d8	11.049	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53



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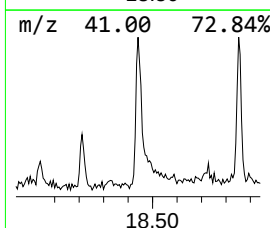
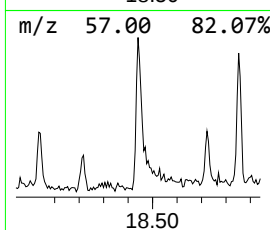
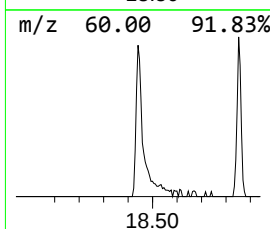
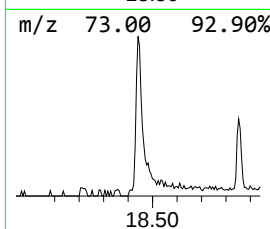
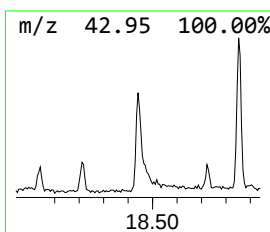
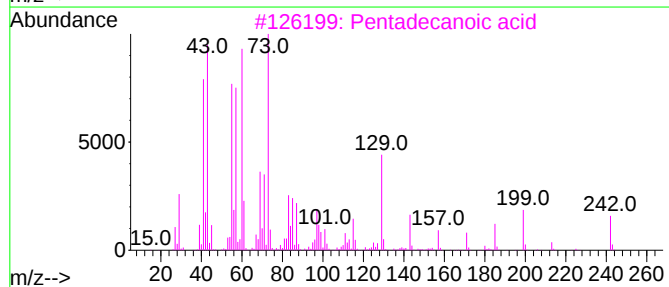
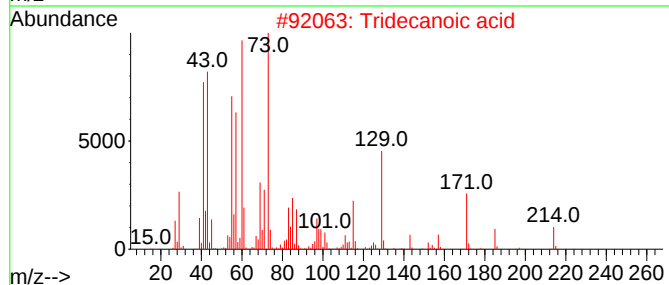
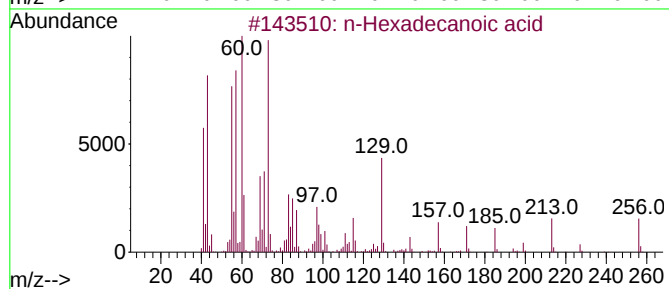
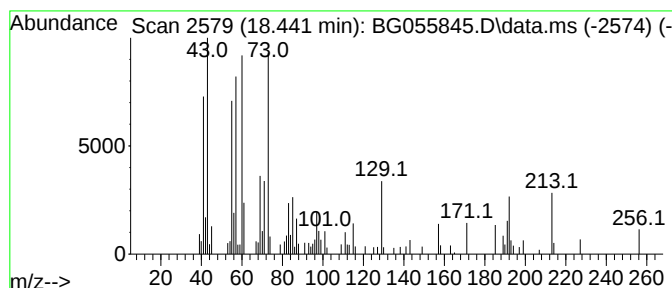
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.441	3.53 ng	118689	Phenanthrene-d10	17.583

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5		Dodecanoic acid	200	C12H24O2	000143-07-7	50



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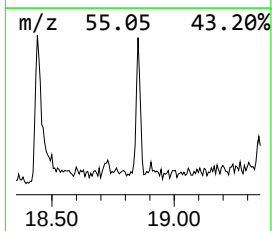
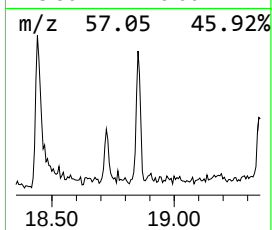
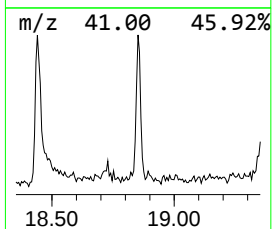
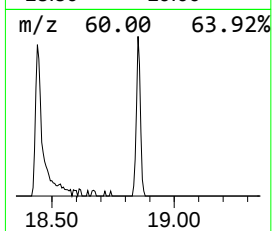
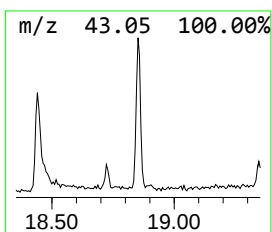
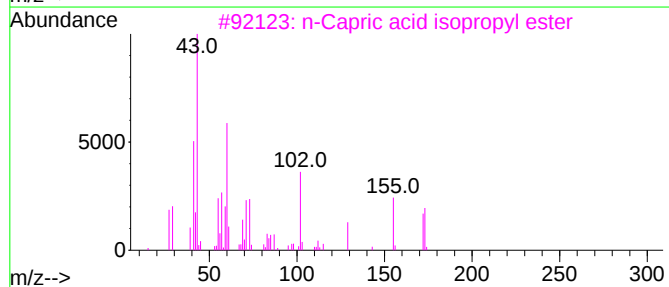
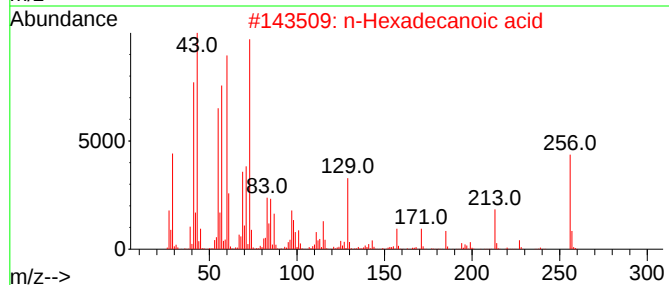
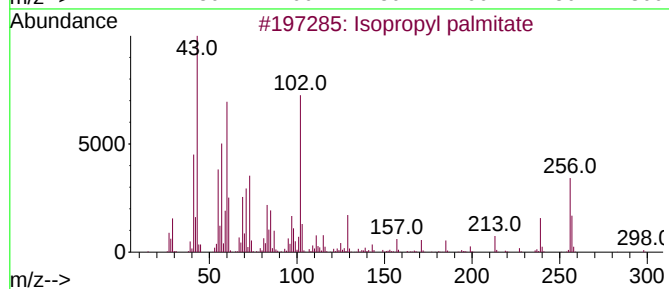
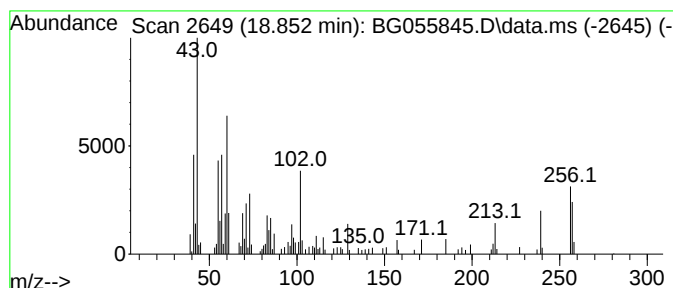
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Isopropyl palmitate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.852	2.50 ng	84275	Phenanthrene-d10	17.583

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl palmitate	298	C19H38O2	000142-91-6	72
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
3			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	46
4			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	46
5			Nonanoic acid, 1-methylethyl ester	200	C12H24O2	028267-32-5	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
Data File : BG055845.D
Acq On : 30 Nov 2022 17:06
Operator : CG/JU
Sample : N5795-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-10

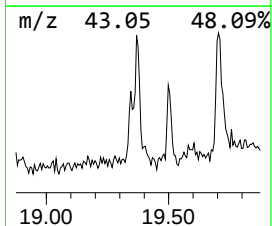
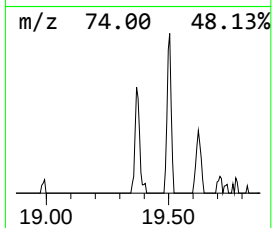
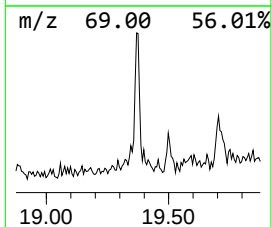
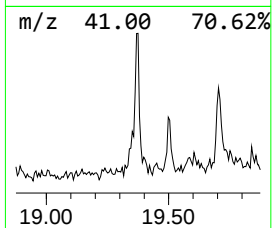
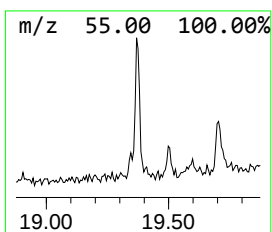
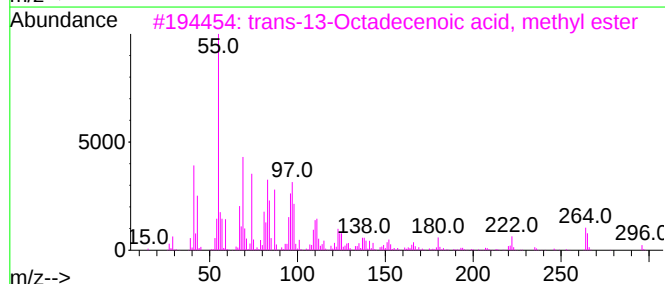
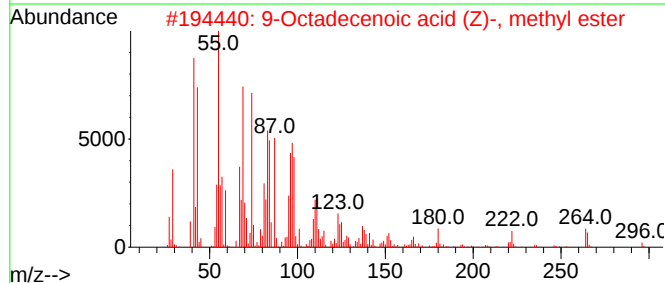
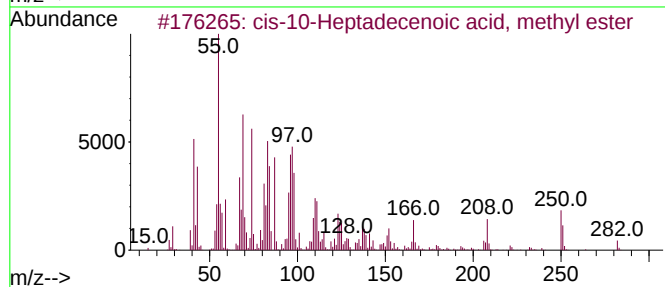
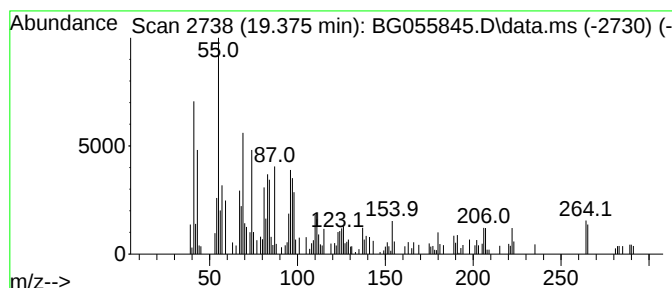
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 cis-10-Heptadecenoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.375	3.16 ng	106442	Phenanthrene-d10	17.583

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	94
2			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
3			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
4			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
5			6-Octadecenoic acid	282	C18H34O2	1000336-66-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
Data File : BG055845.D
Acq On : 30 Nov 2022 17:06
Operator : CG/JU
Sample : N5795-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

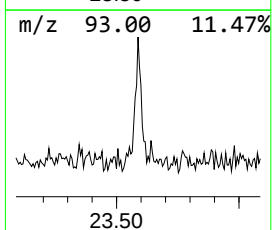
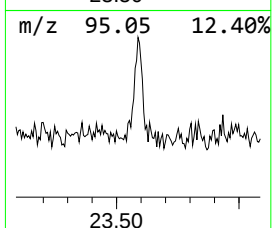
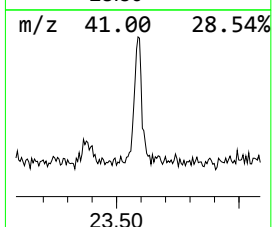
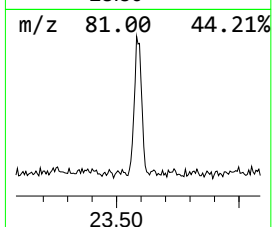
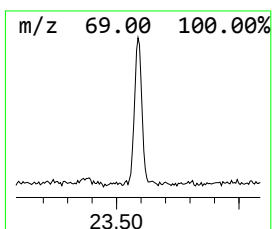
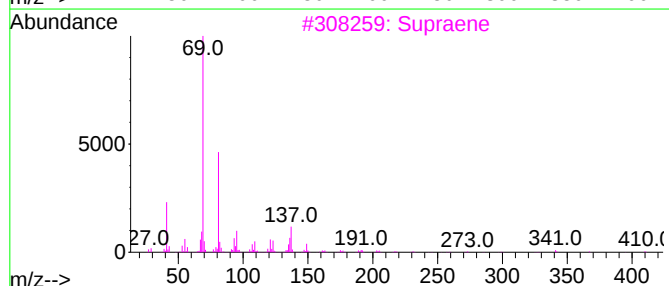
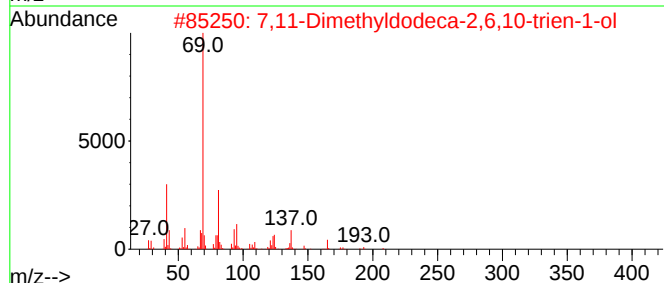
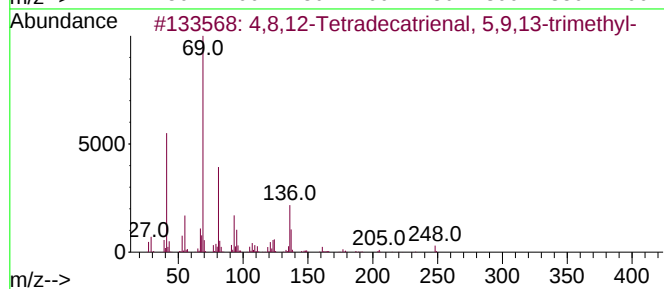
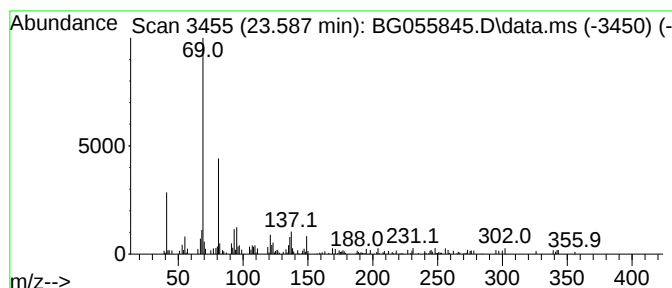
Instrument :
BNA_G
ClientSampleId :
TP-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4,8,12-Tetradecatrienal, 5,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
23.587	3.07 ng	107091	Perylene-d12		25.256	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4,8,12-Tetradecatrienal, 5,9,13-...		248	C17H28O	066408-55-7	87
2	7,11-Dimethyldodeca-2,6,10-trien...		208	C14H24O	125529-10-4	80
3	Supraene		410	C30H50	007683-64-9	80
4	3,7,11-Tridecatrienenitrile, 4,8...		231	C16H25N	006006-01-5	80
5	2,6,10,14-Hexadecatetraenoic aci...		332	C22H36O2	024035-35-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
Data File : BG055845.D
Acq On : 30 Nov 2022 17:06
Operator : CG/JU
Sample : N5795-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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
2-Pentanone, 4-...	5.268	46.1	ng	549079	1	8.217	238105	20.0
2-Pentanone, 4-...	6.367	2.8	ng	33685	1	8.217	238105	20.0
Ethanol, 2-(2-b...	10.791	10.1	ng	183575	2	11.049	364963	20.0
n-Hexadecanoic ...	18.441	3.5	ng	118689	4	17.583	672930	20.0
Isopropyl palmi...	18.852	2.5	ng	84275	4	17.583	672930	20.0
cis-10-Heptadec...	19.375	3.2	ng	106442	4	17.583	672930	20.0
4,8,12-Tetradec...	23.587	3.1	ng	107091	6	25.256	696553	20.0