

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
 Data File : BG060034.D
 Acq On : 15 Dec 2023 13:48
 Operator : MA/JU
 Sample : 05791-11
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-1B-EE-NN

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-BG121323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060034.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.144	4	9	21	rVB	691544	1129665	24.17%	4.879%
2	5.059	329	335	340	rBV	100637	153641	3.29%	0.664%
3	5.523	408	414	426	rBV	710429	1120113	23.96%	4.837%
4	6.029	491	500	505	rVB	34743	50095	1.07%	0.216%
5	7.110	677	684	693	rBV	469049	774779	16.57%	3.346%
6	7.956	821	828	834	rBV	261180	436144	9.33%	1.884%
7	8.009	834	837	845	rVB3	29050	49280	1.05%	0.213%
8	8.191	860	868	873	rBV	190167	314252	6.72%	1.357%
9	9.113	1018	1025	1032	rVB	417952	732231	15.66%	3.162%
10	10.764	1298	1306	1313	rBV	355574	643190	13.76%	2.778%
11	11.499	1423	1431	1435	rBV3	37363	72730	1.56%	0.314%
12	13.214	1716	1723	1731	rBV	1525127	2360646	50.50%	10.195%
13	13.432	1751	1760	1766	rBV3	56149	101304	2.17%	0.438%
14	14.595	1945	1958	1968	rBV	662718	1058765	22.65%	4.572%
15	16.082	2204	2211	2218	rBV	3048030	4512489	96.53%	19.488%
16	17.339	2419	2425	2432	rBV	961091	1401138	29.97%	6.051%
17	18.232	2568	2577	2584	rBV4	270148	558003	11.94%	2.410%
18	18.449	2609	2614	2620	rBV2	61815	87335	1.87%	0.377%
19	18.661	2646	2650	2656	rVB4	65764	80123	1.71%	0.346%
20	18.784	2666	2671	2676	rBV8	25777	54736	1.17%	0.236%
21	19.166	2733	2736	2740	rBV5	32824	46979	1.01%	0.203%
22	19.390	2770	2774	2776	rBV3	62048	81578	1.75%	0.352%
23	19.507	2790	2794	2797	rBV4	122880	170799	3.65%	0.738%
24	19.959	2865	2871	2878	rBV	3522608	4674478	100.00%	20.188%
25	20.453	2953	2955	2962	rBV3	88337	137739	2.95%	0.595%
26	21.264	3090	3093	3097	rVB	269321	347177	7.43%	1.499%
27	21.610	3147	3152	3160	rBV2	1158655	2005707	42.91%	8.662%

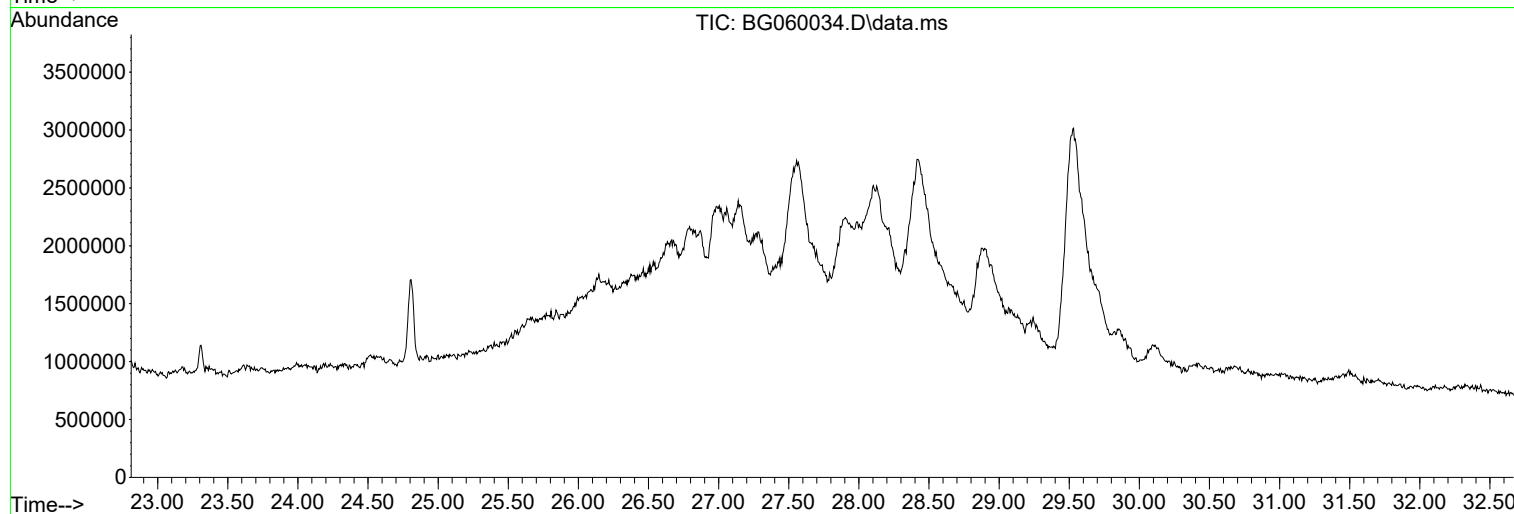
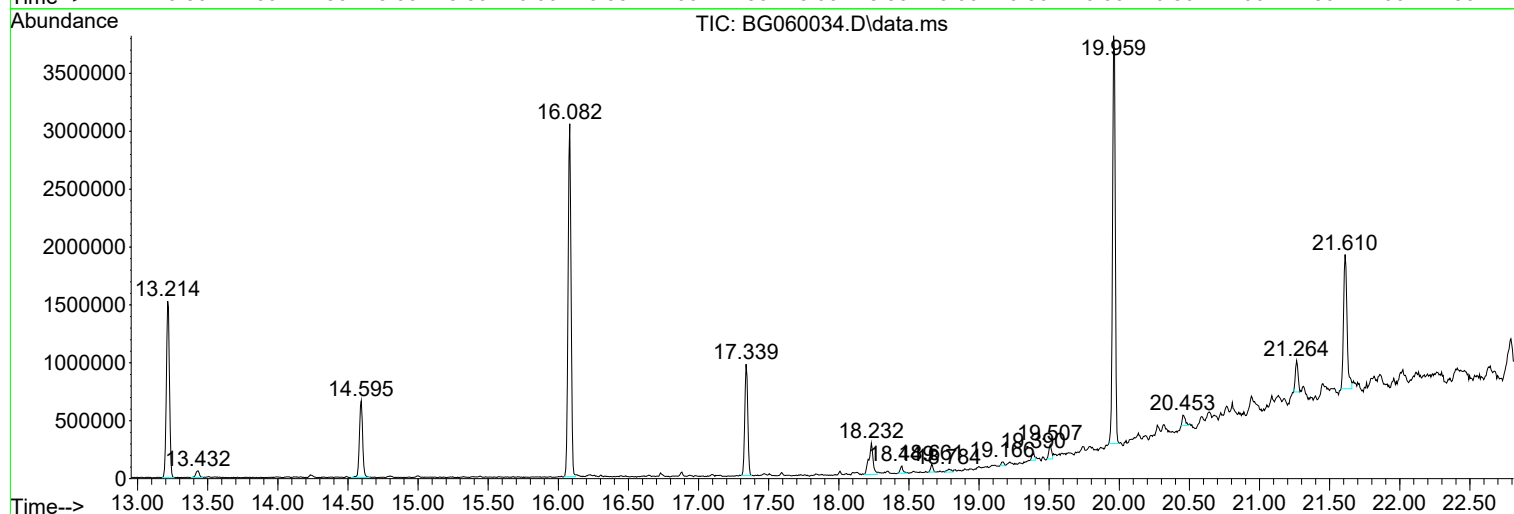
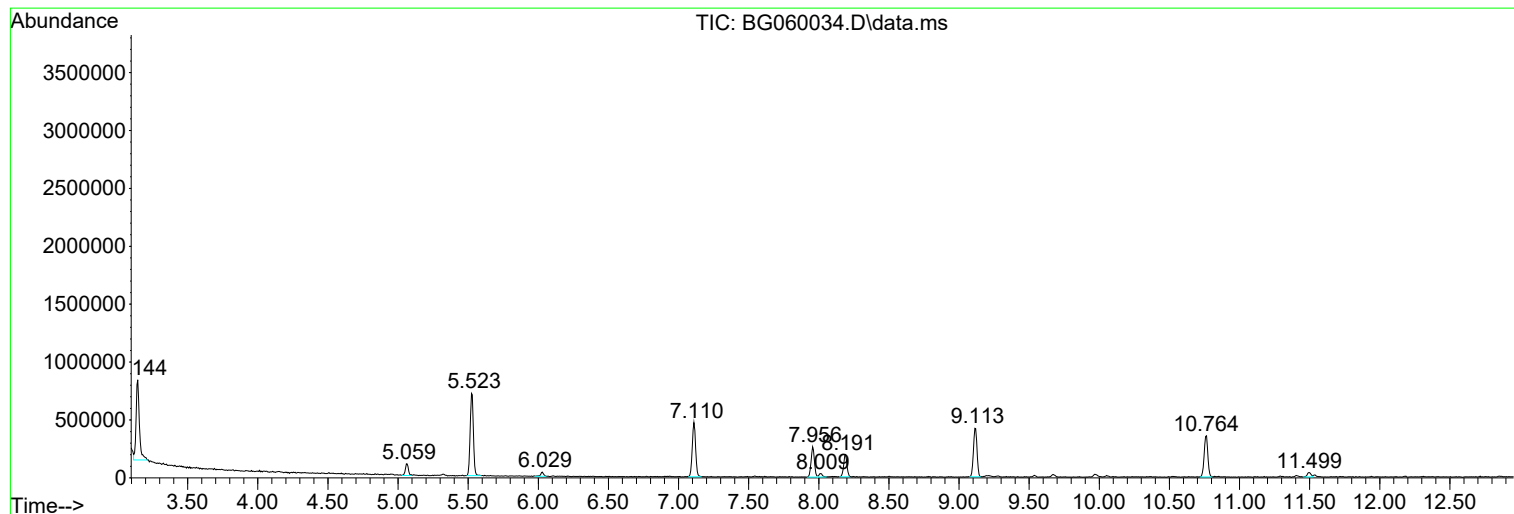
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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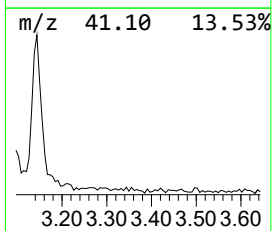
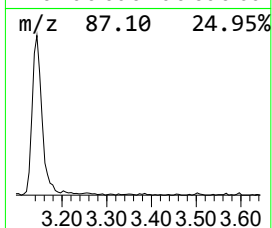
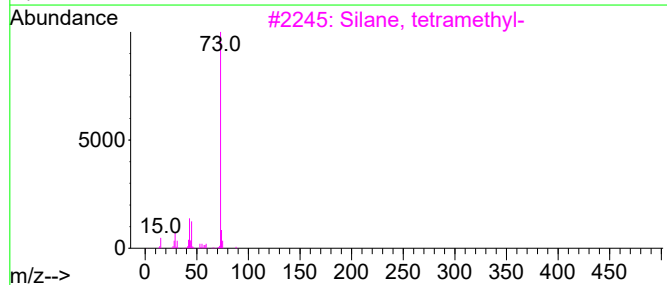
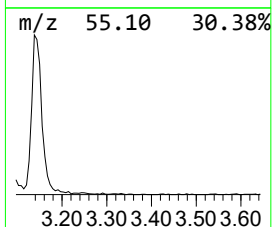
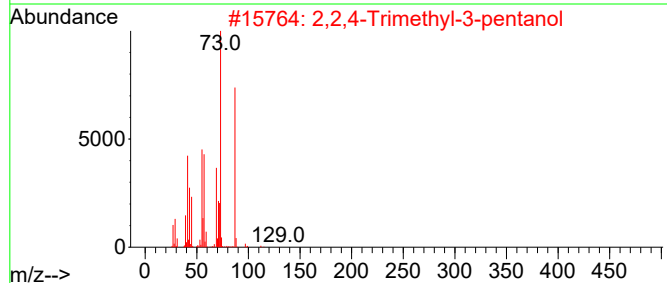
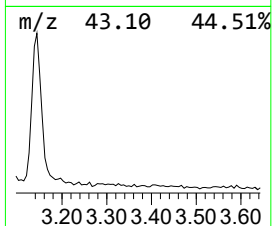
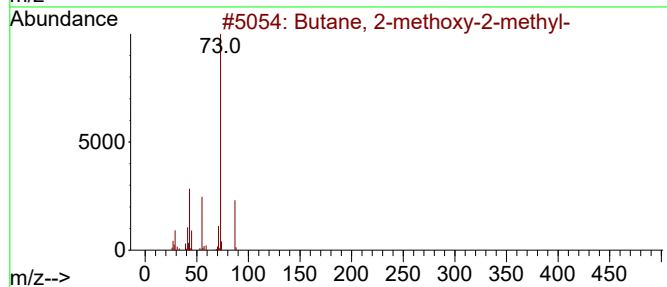
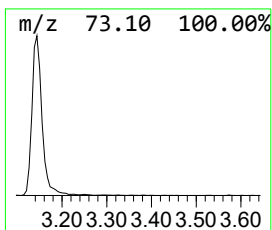
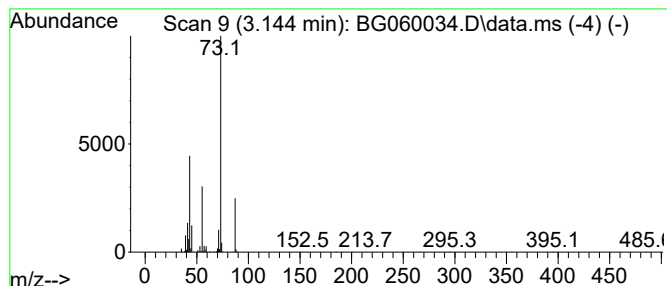
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.144	51.80 ng	1129670	1,4-Dichlorobenzene-d4	7.956

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
5			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	28



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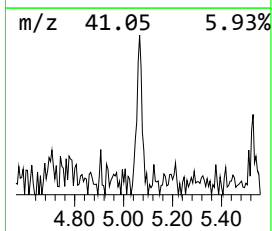
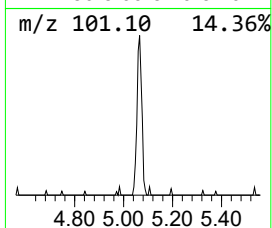
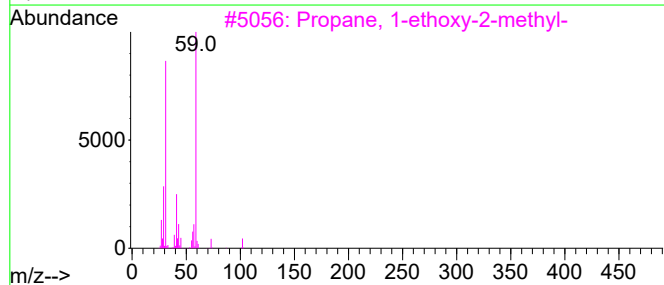
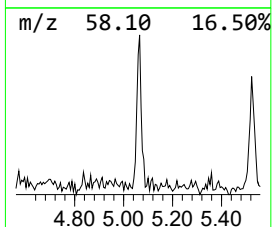
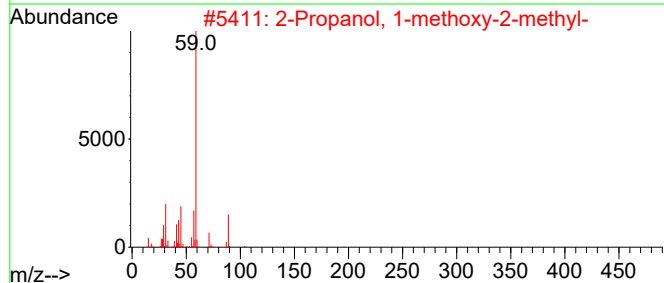
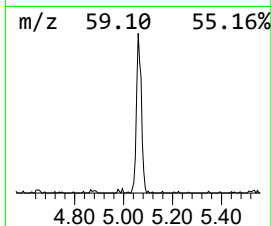
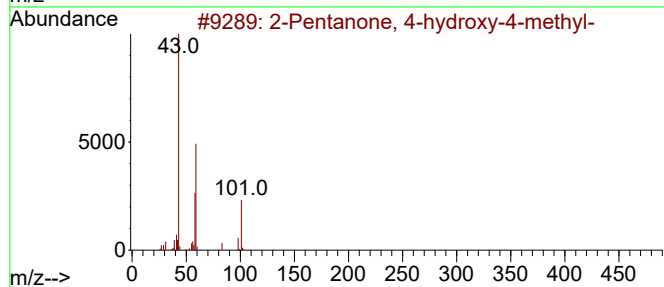
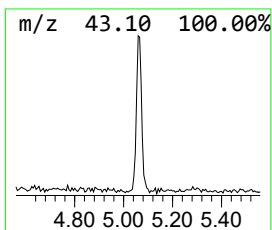
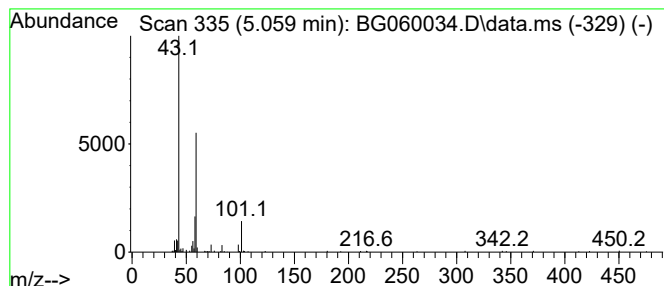
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.059	7.05 ng	153641	1,4-Dichlorobenzene-d4	7.956

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	43
2		2-Propanol, 1-methoxy-2-methyl-	104	C5H12O2	003587-64-2	37
3		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	37
4		3-[2-Ethoxycarbonyl-2-methyl)pro...	290	C14H26O4S	021153-32-2	36
5		Tetraglyme	222	C10H22O5	000143-24-8	33



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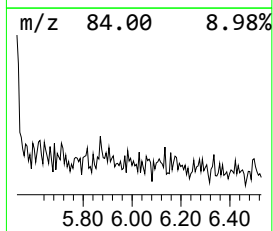
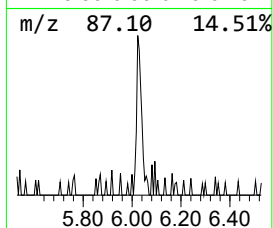
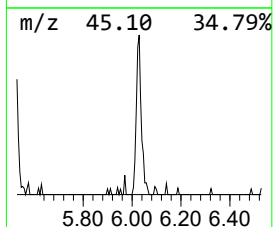
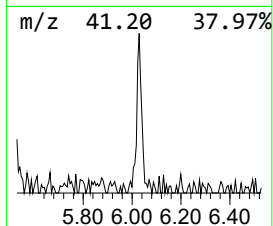
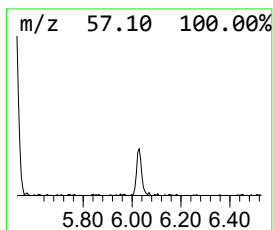
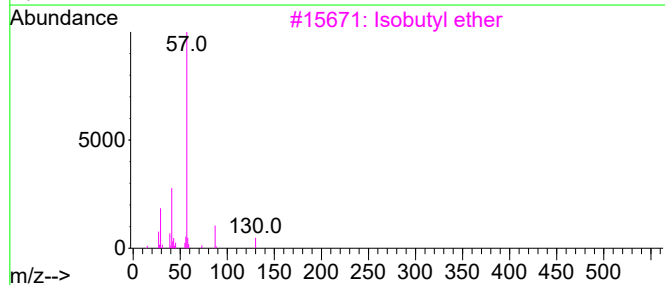
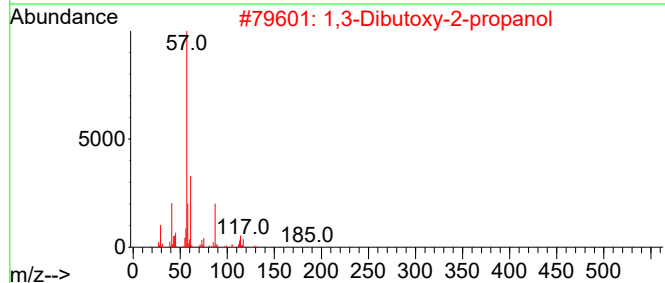
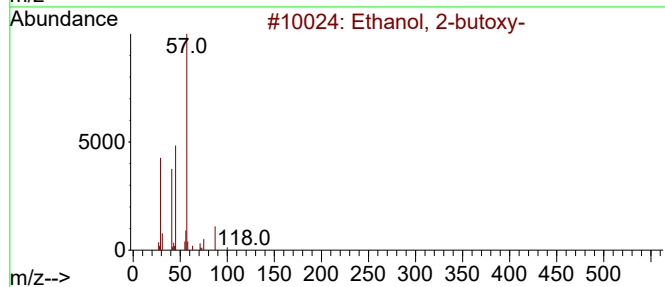
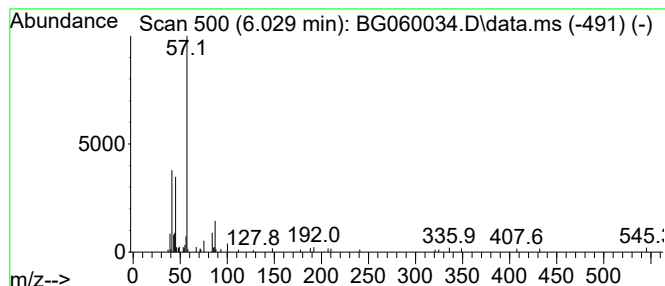
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.029 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.029	2.30 ng	50095	1,4-Dichlorobenzene-d4	7.956

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	42
2		1,3-Dibutoxy-2-propanol	204	C11H24O3	002216-77-5	38
3		Isobutyl ether	130	C8H18O	000628-55-7	25
4		1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	17
5		1-Penten-3-ol	86	C5H10O	000616-25-1	14



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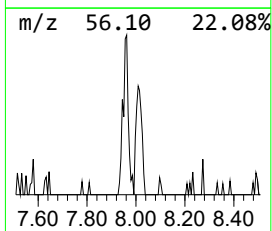
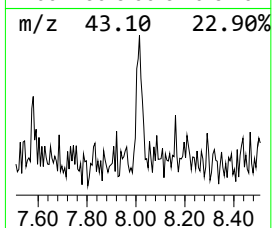
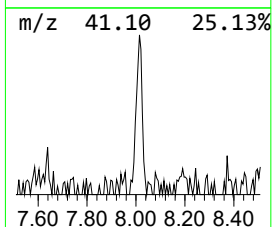
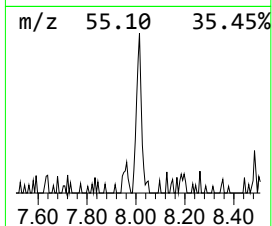
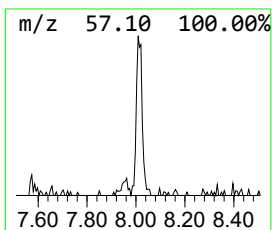
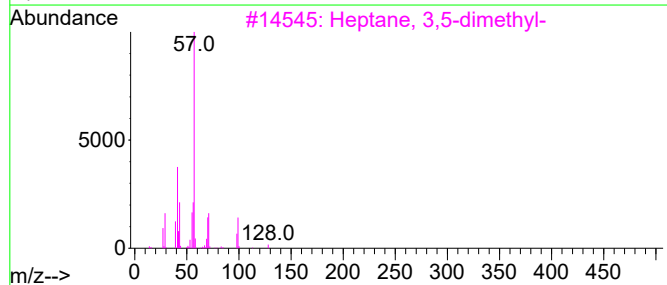
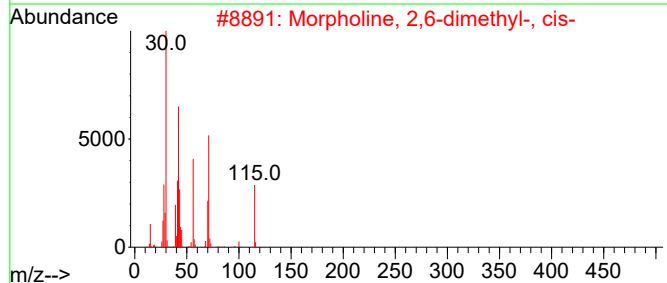
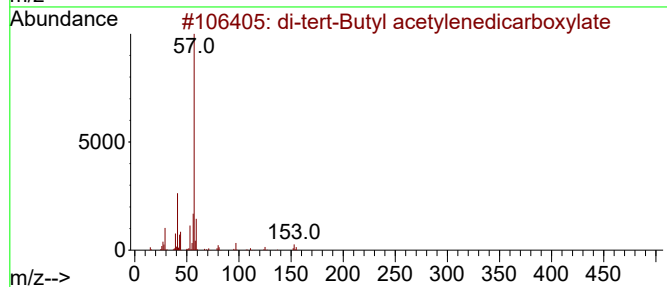
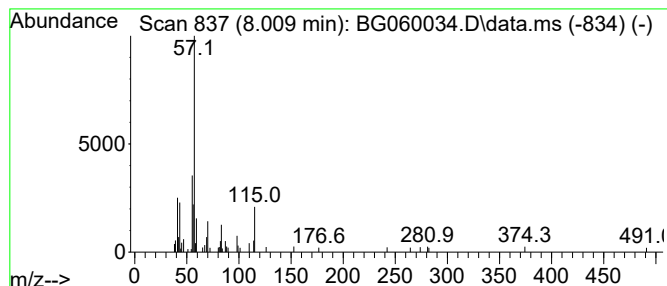
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Peak Number 4 unknown8.009 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.009	2.26 ng	49280	1,4-Dichlorobenzene-d4	7.956

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			di-tert-Butyl acetylenedicarboxy...	226	C12H18O4	066086-33-7	43
2			Morpholine, 2,6-dimethyl-, cis-	115	C6H13NO	006485-55-8	35
3			Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	35
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	35
5			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	35



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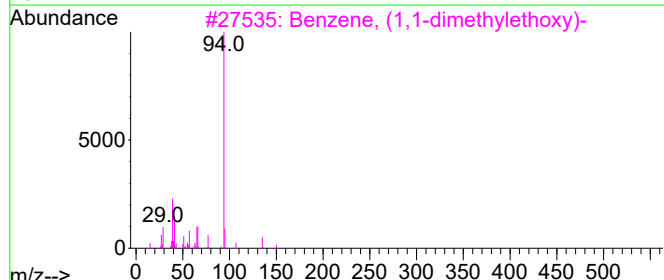
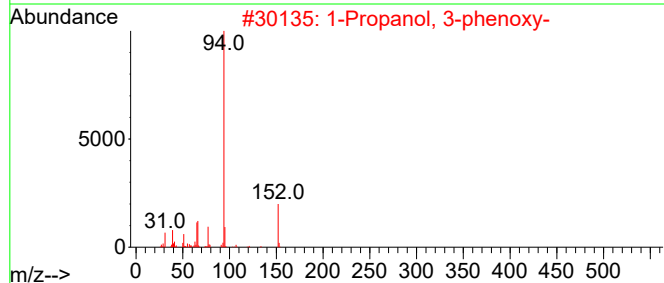
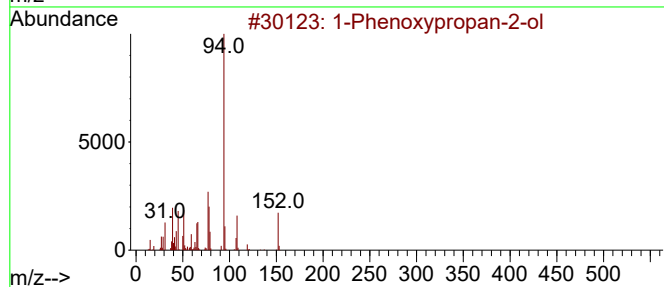
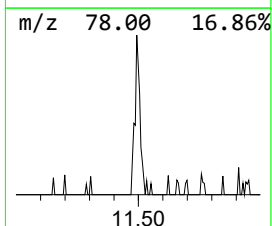
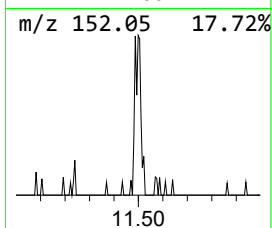
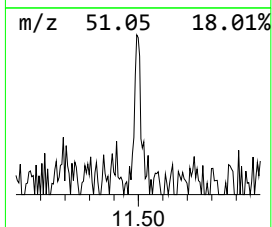
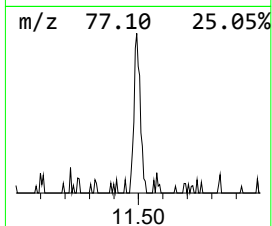
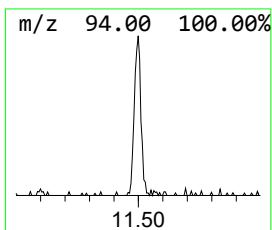
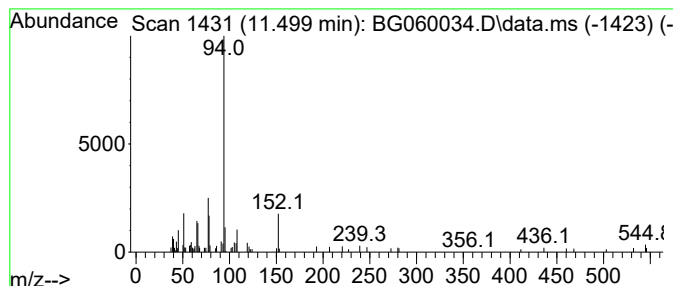
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Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.499	2.26 ng	72730	Naphthalene-d8	10.764

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	72
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	64
3			Benzene, (1,1-dimethylethoxy)-	150	C10H14O	006669-13-2	58
4			Benzene, (3-bromopropoxy)-	214	C9H11BrO	000588-63-6	53
5			Methane, isopropoxyphenoxy-	166	C10H14O2	000828-12-6	53



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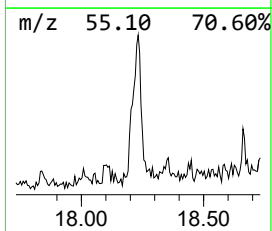
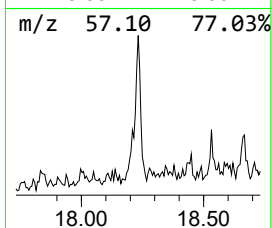
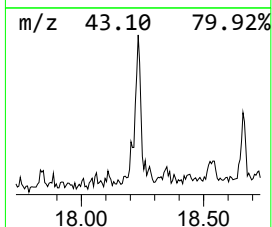
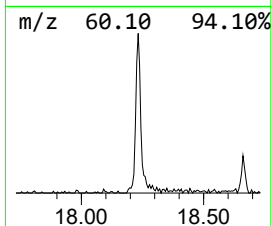
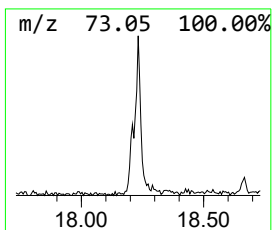
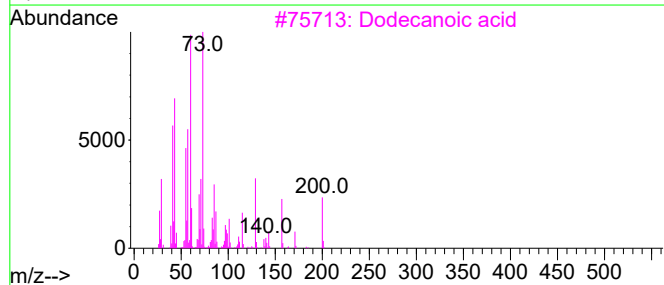
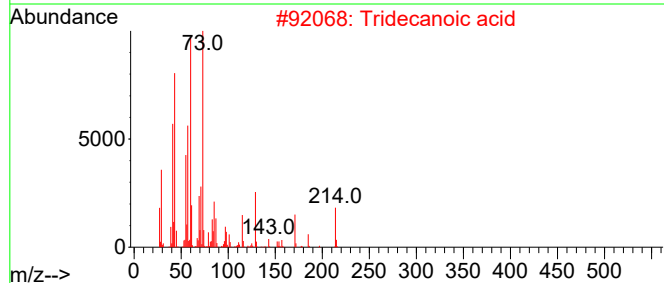
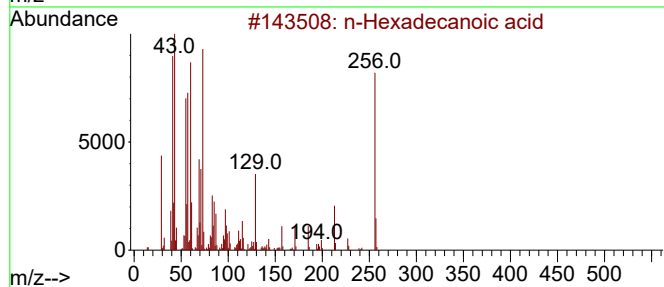
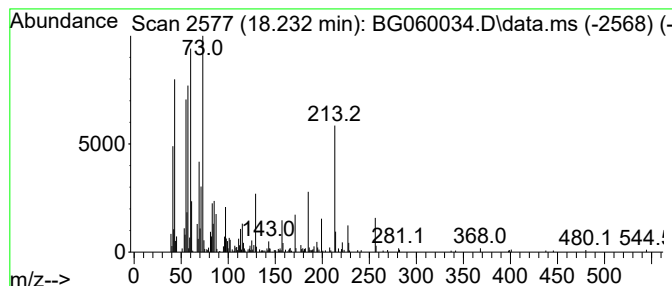
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.232	7.96 ng	558003	Phenanthrene-d10	17.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Dodecanoic acid	200	C12H24O2	000143-07-7	60
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	52
5			Tetracosanoic acid	368	C24H48O2	000557-59-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060034.D
Acq On : 15 Dec 2023 13:48
Operator : MA/JU
Sample : 05791-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

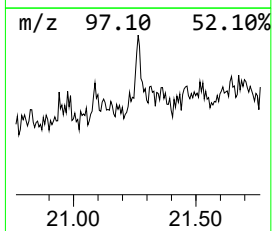
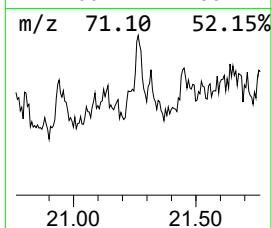
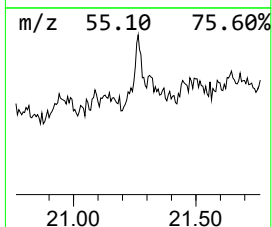
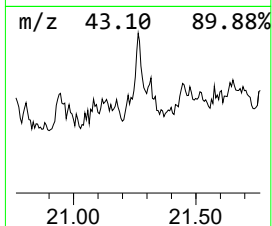
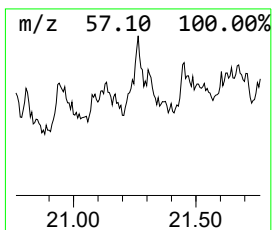
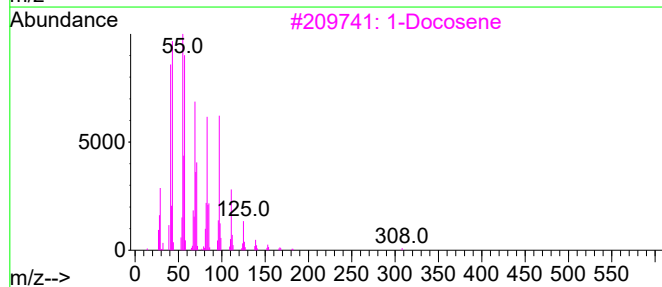
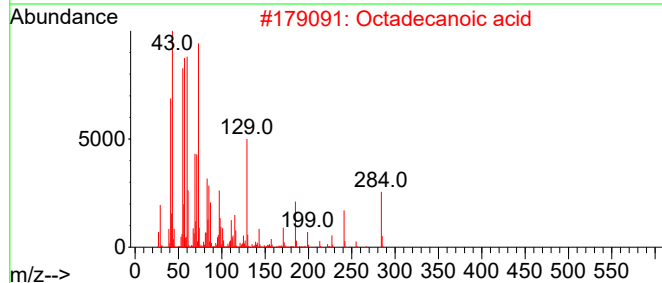
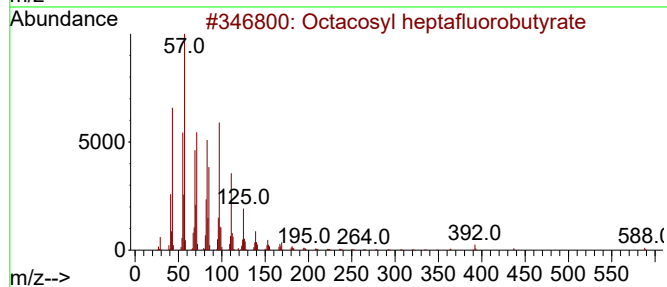
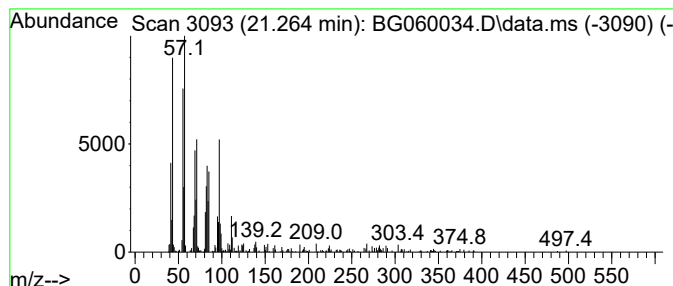
Instrument :
BNA_G
ClientSampleId :
MW-1B-EE-NN

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.264	3.46 ng	347177	Chrysene-d12	21.610	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	80
2	Octadecanoic acid	284	C18H36O2	000057-11-4	64
3	1-Docosene	308	C22H44	001599-67-3	64
4	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	60
5	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
Data File : BG060034.D
Acq On : 15 Dec 2023 13:48
Operator : MA/JU
Sample : 05791-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1B-EE-NN

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.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...	3.144	51.8	ng	1129670	1	7.956	436144	20.0
2-Pentanone, 4-...	5.059	7.0	ng	153641	1	7.956	436144	20.0
unknown6.029	6.029	2.3	ng	50095	1	7.956	436144	20.0
unknown8.009	8.009	2.3	ng	49280	1	7.956	436144	20.0
1-Phenoxypropan...	11.499	2.3	ng	72730	2	10.764	643190	20.0
n-Hexadecanoic ...	18.232	8.0	ng	558003	4	17.339	1401140	20.0
Octacosyl hepta...	21.264	3.5	ng	347177	5	21.610	2005710	20.0