

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
 Data File : BG053728.D
 Acq On : 26 May 2022 22:21
 Operator : CG/JU
 Sample : N3032-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SU-406-ROLL-OFF

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-BG050522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053728.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.096	12	18	31	rVB	143785	307845	26.98%	4.272%
2	3.531	85	92	104	rBV	104111	186972	16.39%	2.595%
3	3.654	108	113	125	rBV	42236	82988	7.27%	1.152%
4	5.558	430	437	449	rBV	343984	591958	51.88%	8.214%
5	6.239	545	553	564	rBV7	5995	16560	1.45%	0.230%
6	6.527	598	602	607	rBV3	12324	17506	1.53%	0.243%
7	7.120	698	703	705	rBV2	9660	13714	1.20%	0.190%
8	7.167	705	711	724	rVB	364806	653260	57.25%	9.065%
9	7.296	729	733	740	rVB8	5744	12751	1.12%	0.177%
10	7.367	740	745	749	rBV2	7916	14160	1.24%	0.196%
11	7.984	840	850	856	rVB	118873	221058	19.37%	3.068%
12	8.236	885	893	900	rVB8	8192	17460	1.53%	0.242%
13	9.088	1028	1038	1042	rBV6	9649	23073	2.02%	0.320%
14	9.147	1042	1048	1064	rVB	231749	437034	38.30%	6.065%
15	9.464	1098	1102	1107	rVB7	7002	12947	1.13%	0.180%
16	9.629	1125	1130	1137	rBV7	9465	15802	1.38%	0.219%
17	9.963	1183	1187	1194	rVB7	7207	14248	1.25%	0.198%
18	10.792	1317	1328	1336	rBV	151908	286764	25.13%	3.979%
19	10.944	1351	1354	1361	rVB3	12641	19165	1.68%	0.266%
20	11.814	1494	1502	1505	rBV4	5394	11427	1.00%	0.159%
21	13.241	1739	1745	1752	rVB	627938	965726	84.64%	13.401%
22	14.622	1974	1980	1988	rBV	244437	382319	33.51%	5.305%
23	16.114	2225	2234	2245	rBV	459079	711542	62.36%	9.874%
24	17.165	2408	2413	2423	rVB6	16140	33843	2.97%	0.470%
25	17.371	2441	2448	2455	rBV	285945	444149	38.93%	6.163%
26	17.776	2513	2517	2523	rVB8	8054	12018	1.05%	0.167%
27	18.023	2555	2559	2564	rVB4	16662	23994	2.10%	0.333%
28	18.258	2595	2599	2611	rBV4	67020	161372	14.14%	2.239%
29	19.979	2887	2892	2897	rVB	908760	1141017	100.00%	15.833%
30	21.636	3172	3174	3181	rVB2	257582	373689	32.75%	5.186%

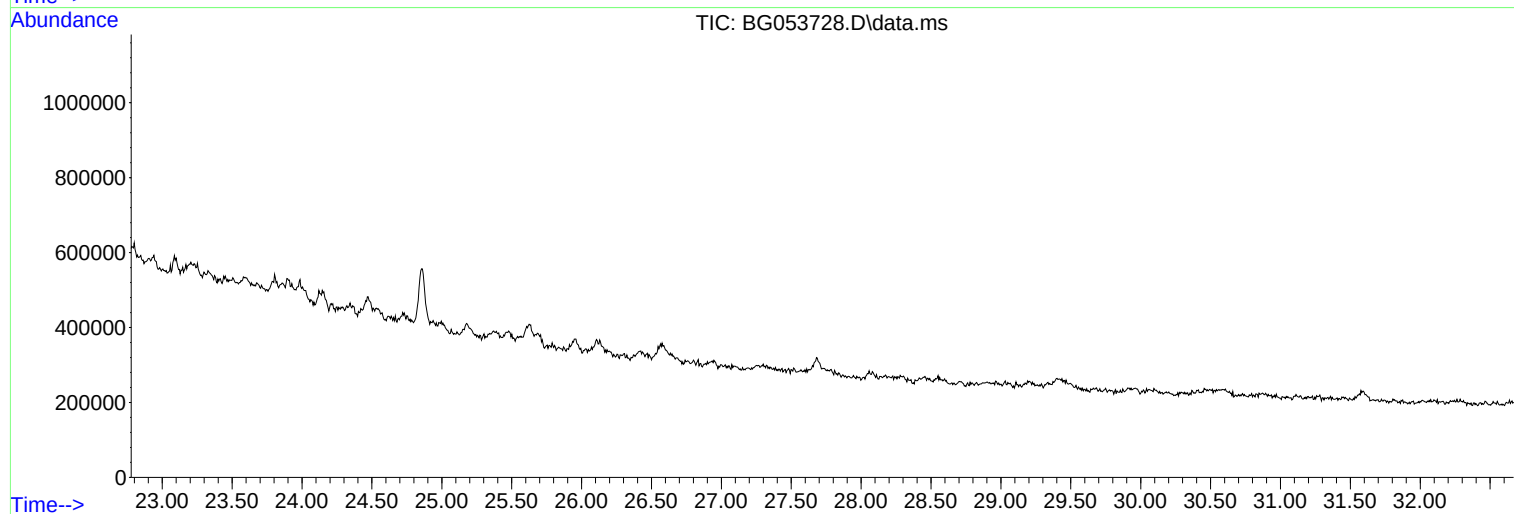
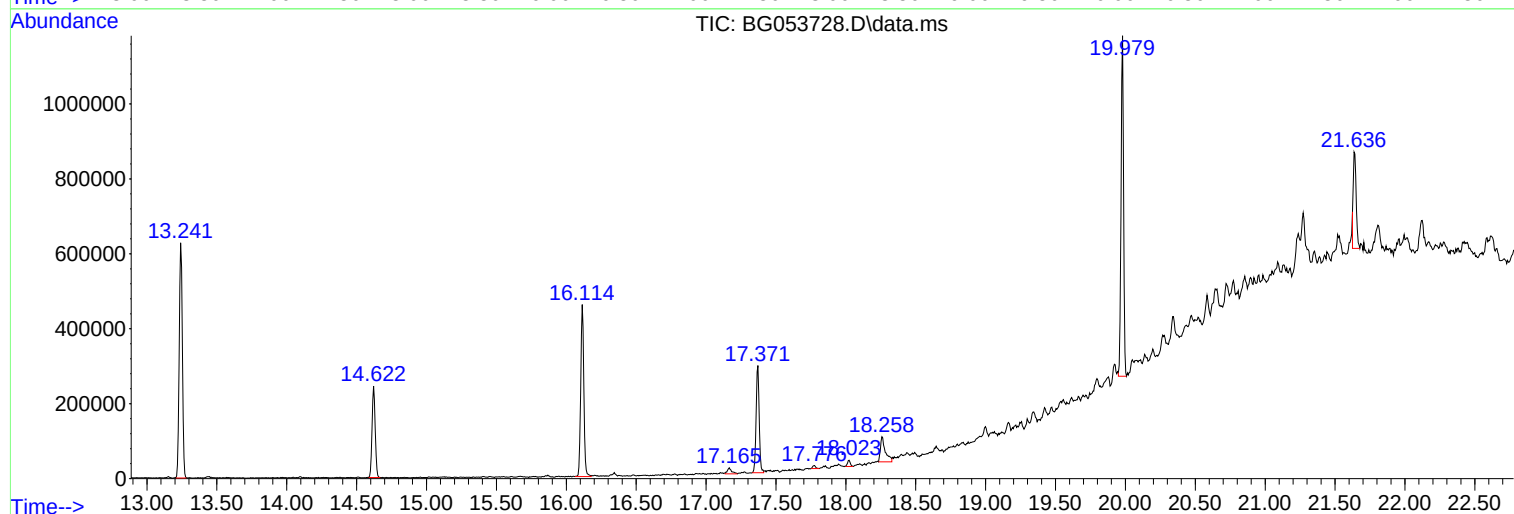
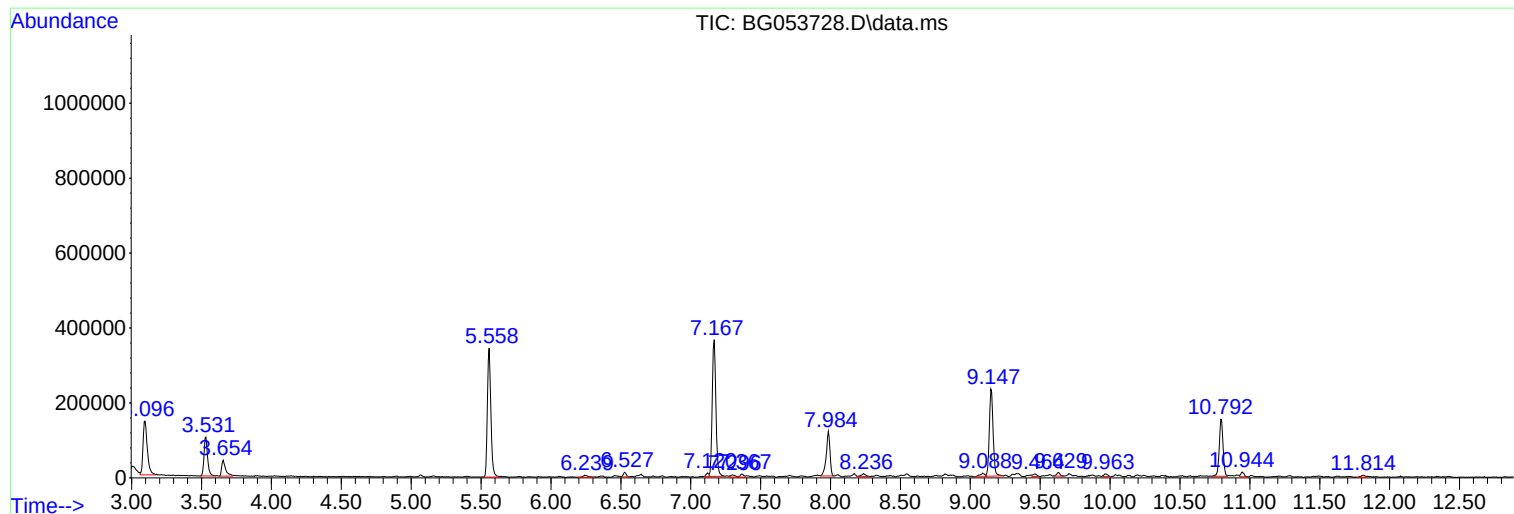
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-406-ROLL-OFF

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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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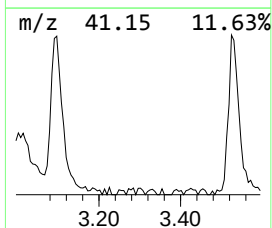
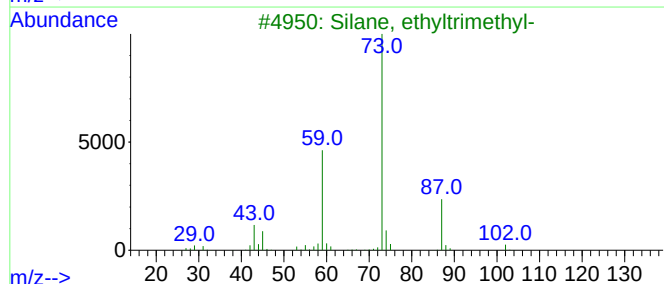
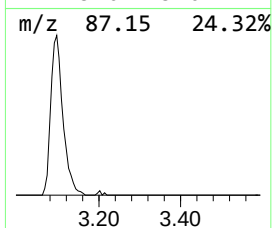
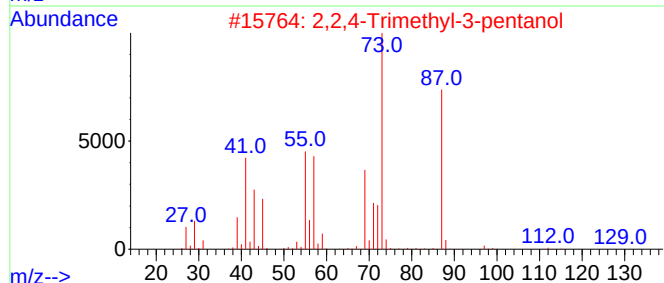
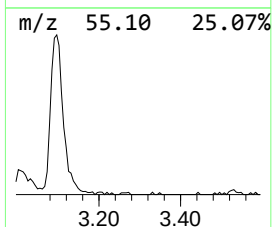
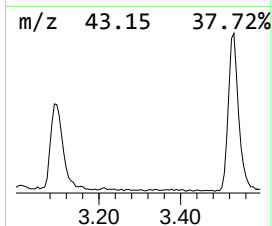
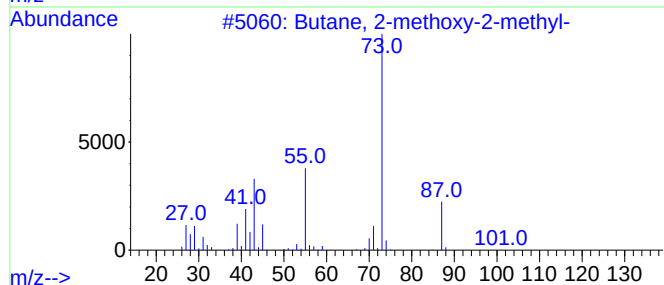
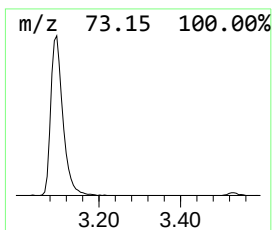
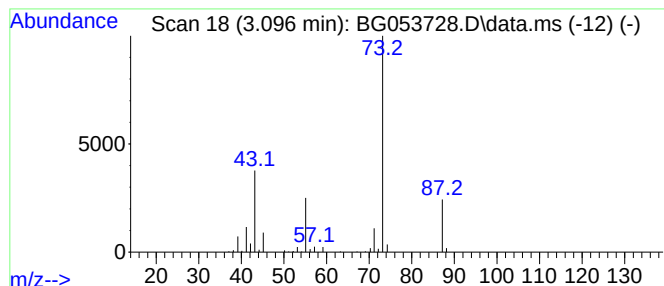
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.096	27.85 ng	307845	1,4-Dichlorobenzene-d4	7.984

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, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10



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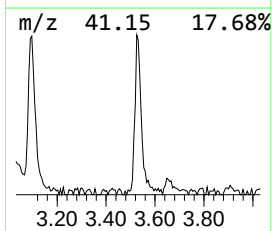
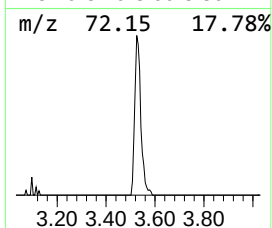
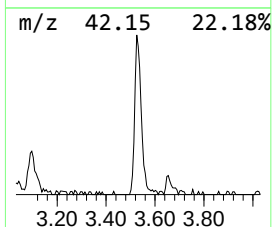
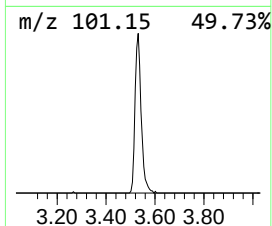
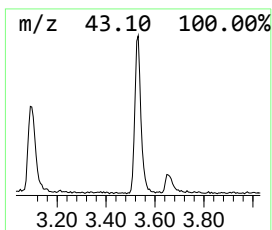
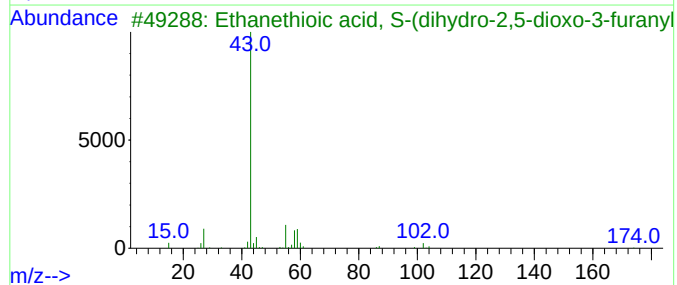
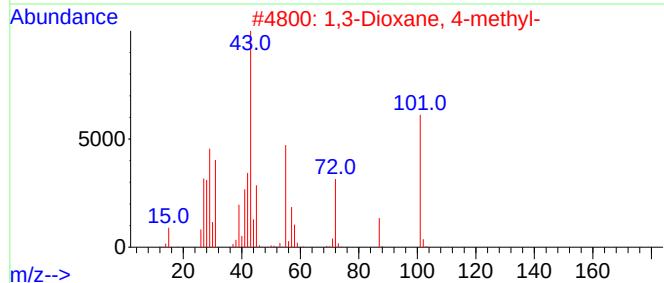
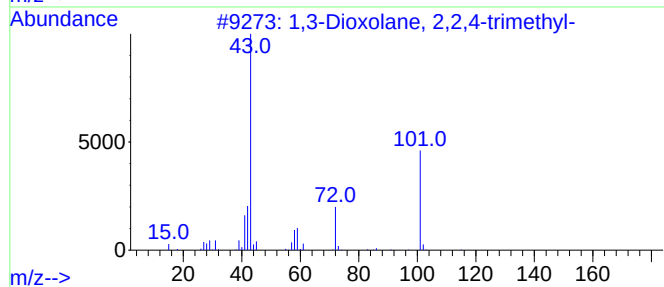
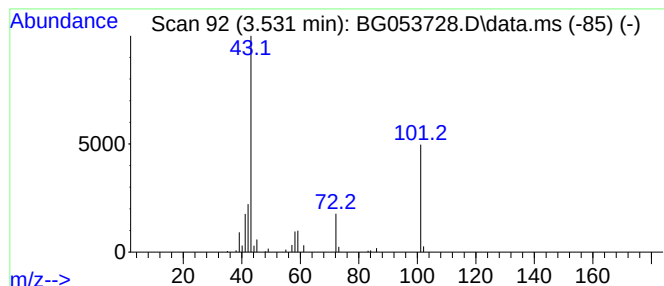
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.531	16.92 ng	186972	1,4-Dichlorobenzene-d4	7.984

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	86
2			1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	45
3			Ethanethioic acid, S-(dihydro-2,...	174	C6H6O4S	006953-60-2	10
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9



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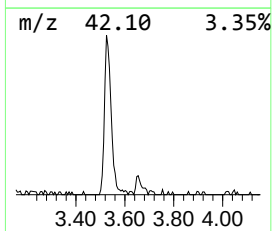
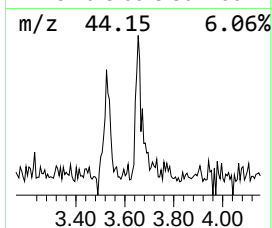
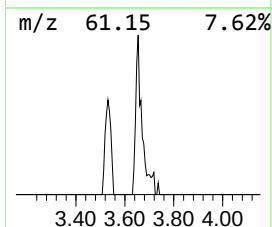
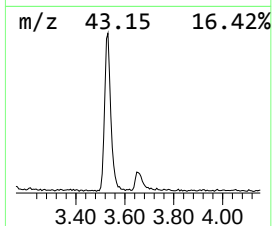
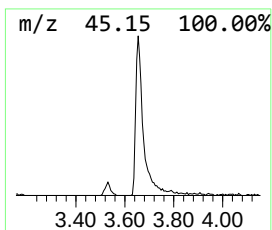
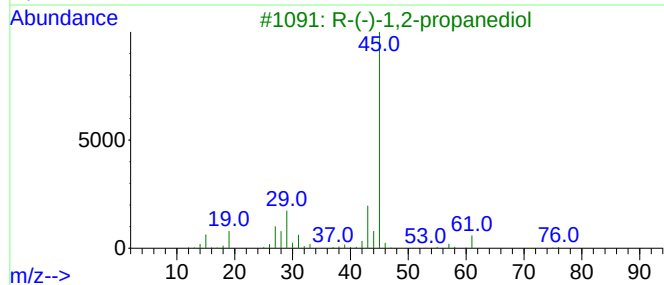
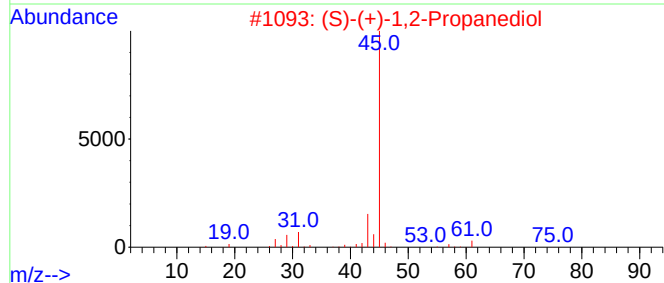
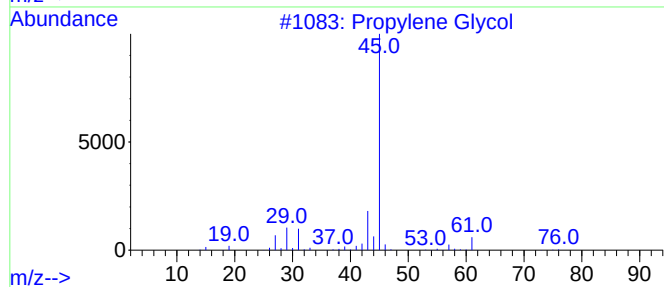
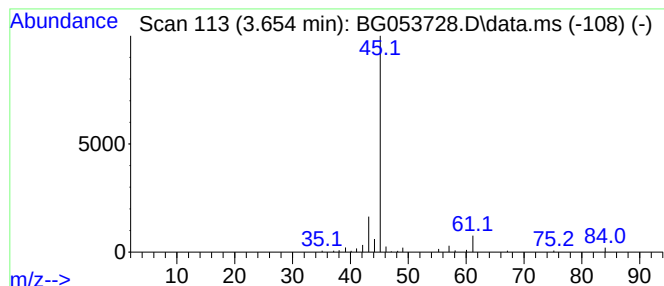
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Propylene Glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.654	7.51 ng	82988	1,4-Dichlorobenzene-d4	7.984

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	56
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
3			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	39
5			Isopropyl Alcohol	60	C3H8O	000067-63-0	9



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ALS Vial : 18 Sample Multiplier: 1

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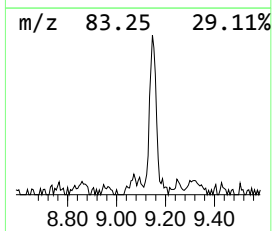
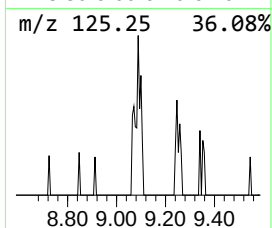
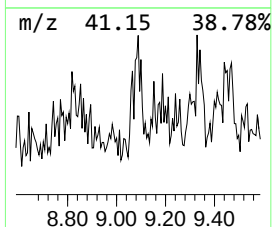
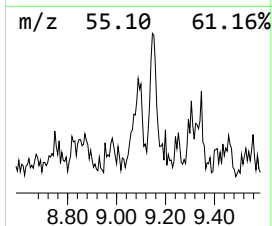
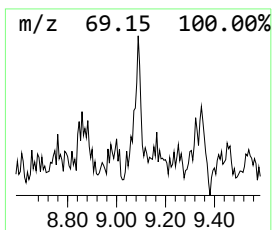
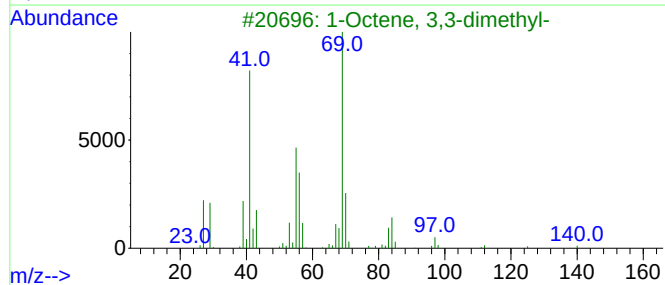
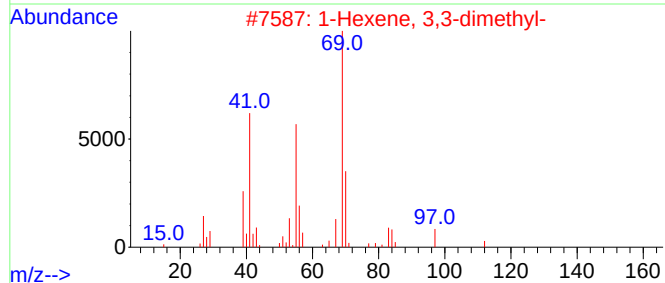
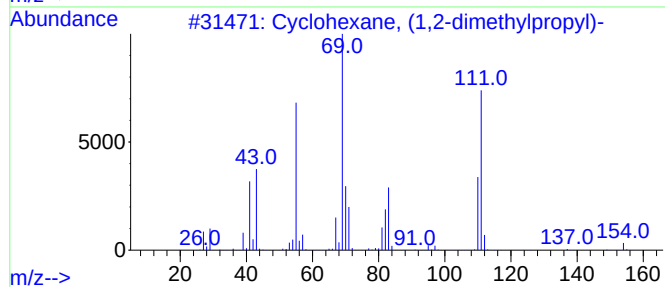
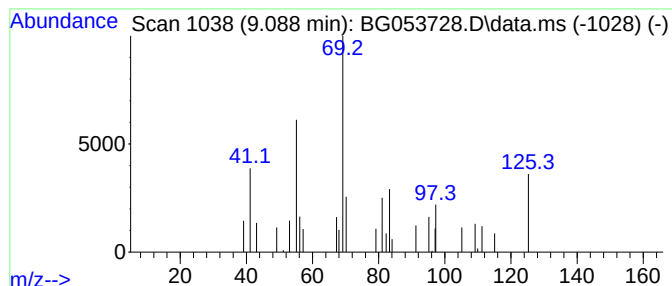
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclohexane, (1,2-dimethylp... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.088	2.09 ng	23073	1,4-Dichlorobenzene-d4	7.984

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, (1,2-dimethylpropyl)-	154	C11H22	051284-29-8	50
2		1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	38
3		1-Octene, 3,3-dimethyl-	140	C10H20	074511-51-6	37
4		Cyclopentane, (2-methylbutyl)-	140	C10H20	053366-38-4	37
5		Cyclopentaneethanol, .beta.,2,3-...	156	C10H20O	021721-18-6	36



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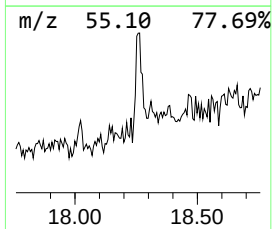
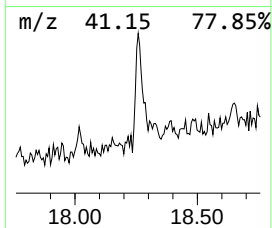
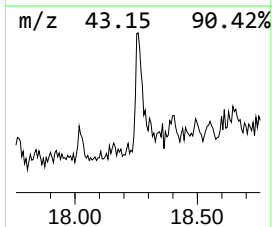
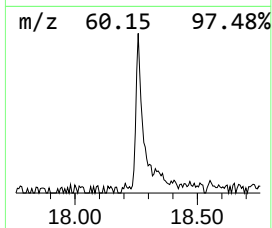
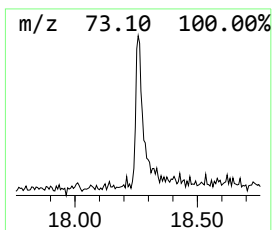
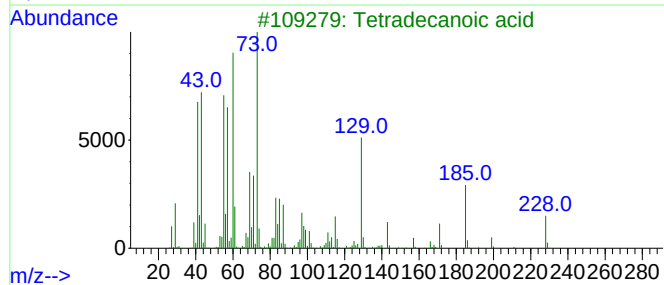
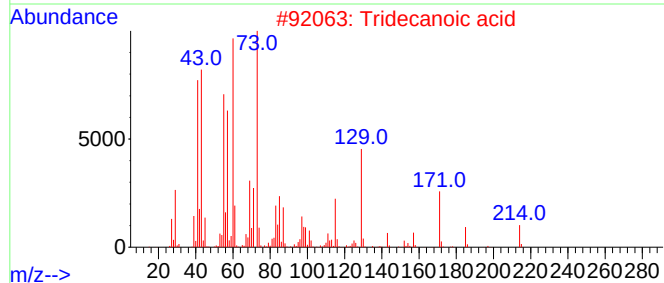
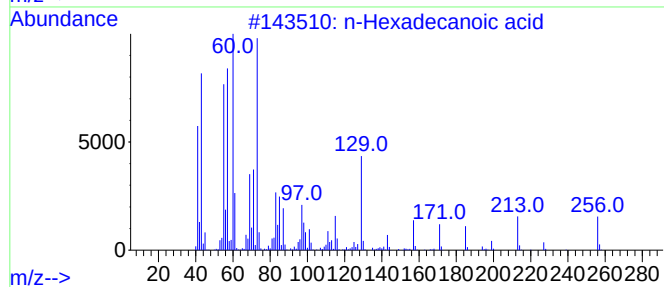
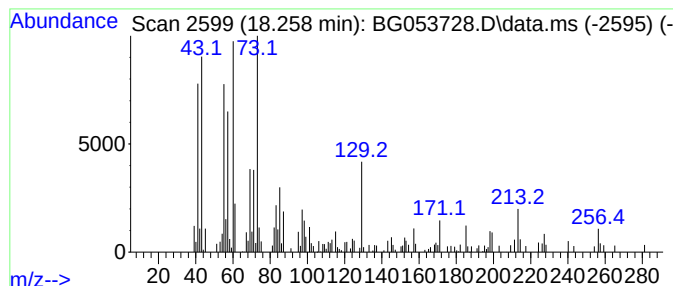
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.258	7.27 ng	161372	Phenanthrene-d10	17.371

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	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Undecanoic acid	186	C11H22O2	000112-37-8	60



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.096	27.9	ng	307845	1	7.984	221058	20.0
1,3-Dioxolane, ...	3.531	16.9	ng	186972	1	7.984	221058	20.0
Propylene Glycol	3.654	7.5	ng	82988	1	7.984	221058	20.0
Cyclohexane, (1...	9.088	2.1	ng	23073	1	7.984	221058	20.0
n-Hexadecanoic ...	18.258	7.3	ng	161372	4	17.371	444149	20.0