

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
 Data File : BG055551.D
 Acq On : 10 Nov 2022 23:02
 Operator : CG/JU
 Sample : N5495-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-32B

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-BG110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055551.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.329	3	7	24	rVB	277246	473468	15.77%	3.206%
2	3.875	96	100	113	rBV	16994	30067	1.00%	0.204%
3	5.327	340	347	356	rBV	140805	221088	7.37%	1.497%
4	5.797	419	427	437	rBV	779928	1276944	42.54%	8.647%
5	7.401	692	700	711	rBV	772240	1328461	44.26%	8.996%
6	8.270	840	848	854	rBV	169856	293240	9.77%	1.986%
7	9.439	1039	1047	1056	rBV	435737	787619	26.24%	5.333%
8	11.096	1321	1329	1339	rVB	236088	416212	13.87%	2.818%
9	13.517	1733	1741	1748	rBV	1153557	1825954	60.83%	12.364%
10	14.886	1966	1974	1982	rVB	368461	583775	19.45%	3.953%
11	16.361	2219	2225	2237	rBV	956559	1451807	48.37%	9.831%
12	17.624	2433	2440	2446	rBV	515253	756628	25.21%	5.124%
13	17.736	2454	2459	2465	rVB4	24327	31005	1.03%	0.210%
14	18.488	2582	2587	2595	rBV	70276	115546	3.85%	0.782%
15	19.745	2798	2801	2808	rBV3	32839	48686	1.62%	0.330%
16	20.209	2875	2880	2886	rVB	2228071	3001515	100.00%	20.325%
17	21.531	3100	3105	3111	rBV2	138328	216812	7.22%	1.468%
18	21.919	3165	3171	3178	rBV2	534252	888959	29.62%	6.020%
19	22.119	3201	3205	3211	rVB2	30190	46248	1.54%	0.313%
20	22.759	3312	3314	3326	rVB5	27491	52414	1.75%	0.355%
21	25.333	3743	3752	3771	rVB2	293250	921287	30.69%	6.239%

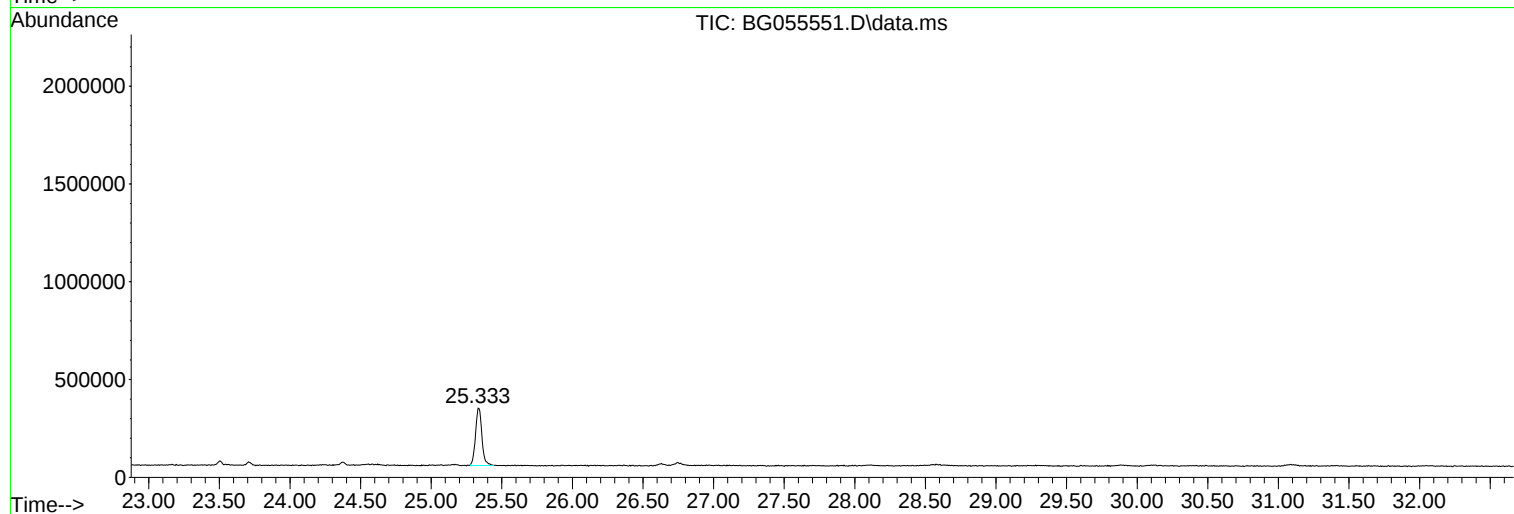
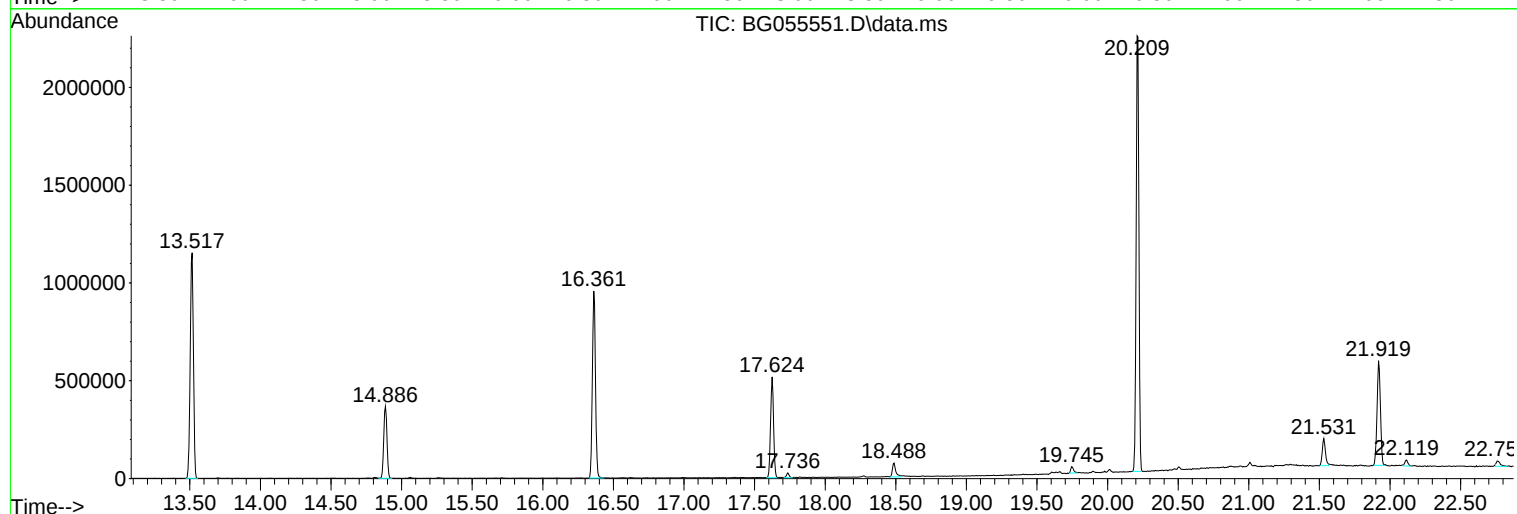
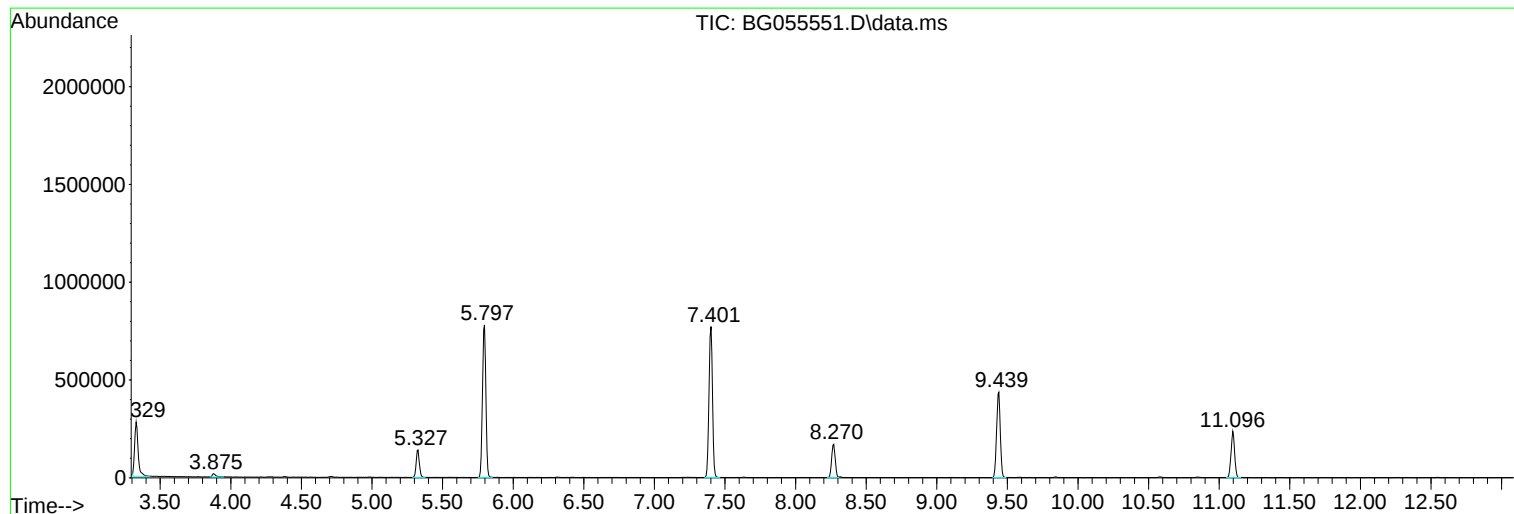
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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ClientSampleId :
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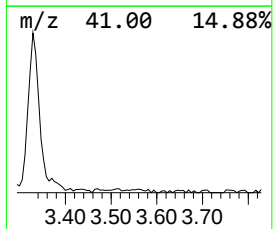
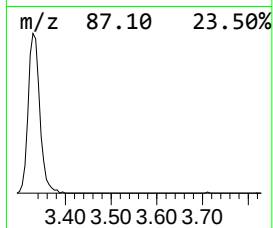
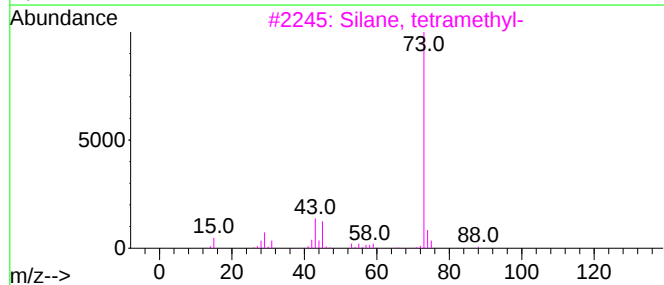
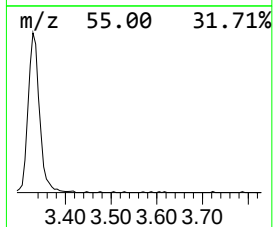
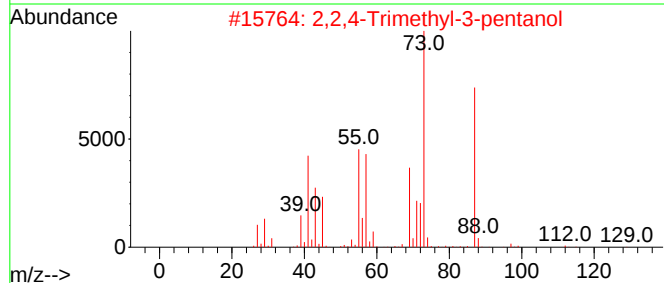
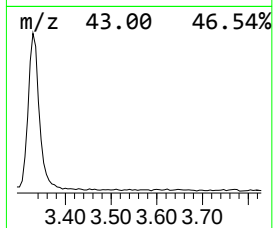
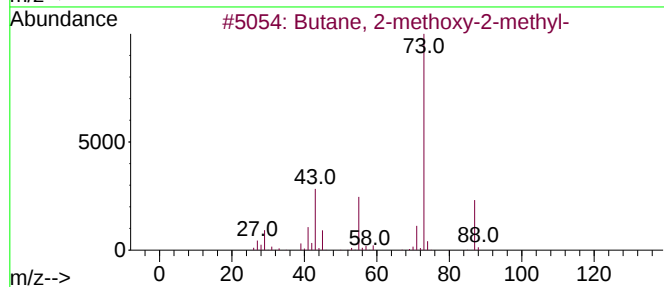
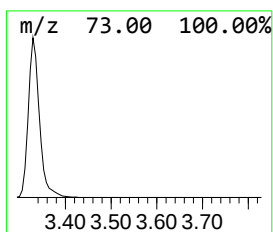
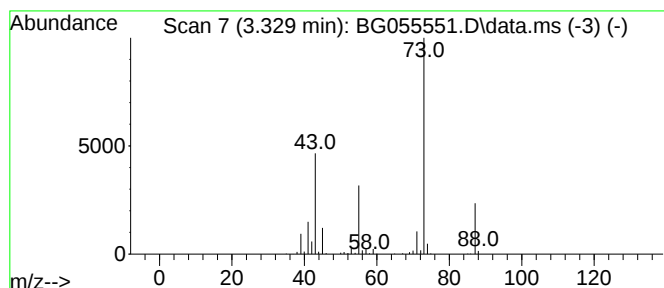
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.329	32.29 ng	473468	1,4-Dichlorobenzene-d4	8.270

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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



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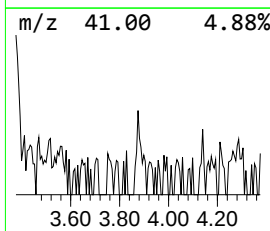
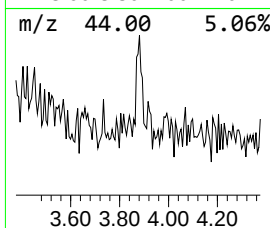
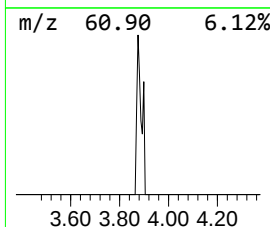
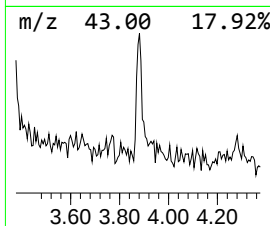
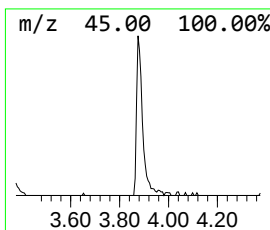
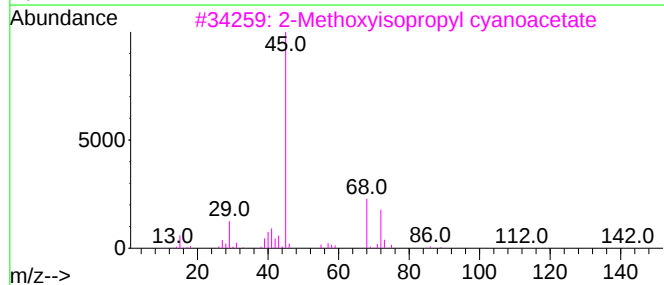
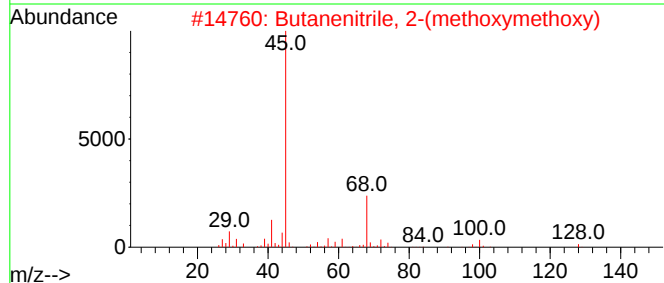
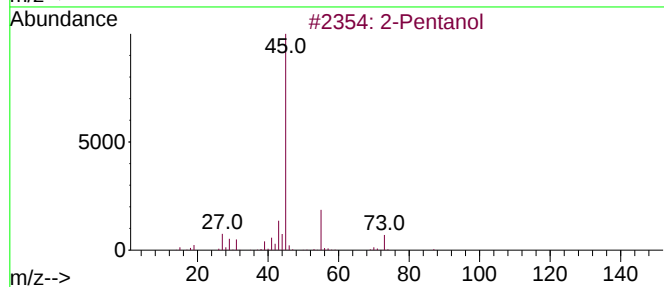
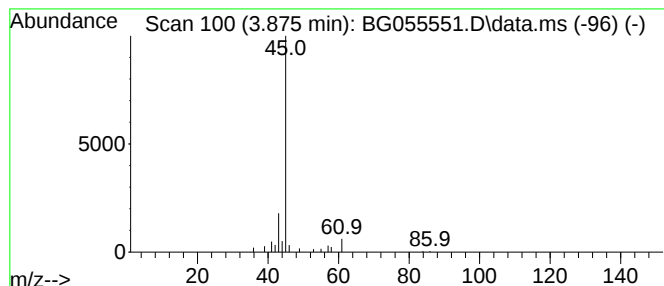
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown3.875 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.875	2.05 ng	30067	1,4-Dichlorobenzene-d4	8.270

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanol	88	C5H12O	006032-29-7	9
2			Butanenitrile, 2-(methoxymethoxy)	129	C6H11NO2	1000196-86-5	9
3			2-Methoxyisopropyl cyanoacetate	157	C7H11NO3	032804-79-8	9
4			2,3-Butanediol	90	C4H10O2	000513-85-9	9
5			Propylene Glycol	76	C3H8O2	000057-55-6	9



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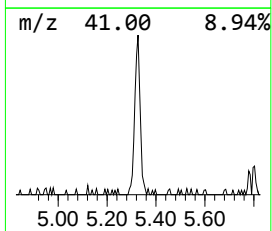
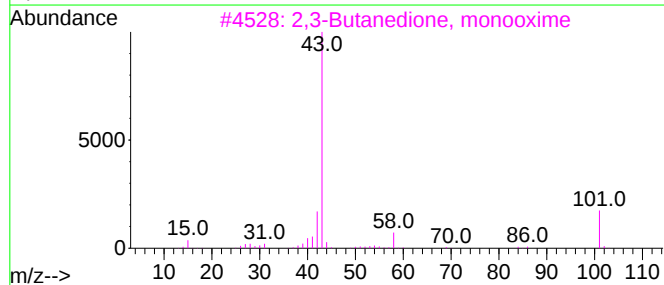
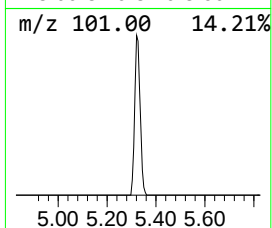
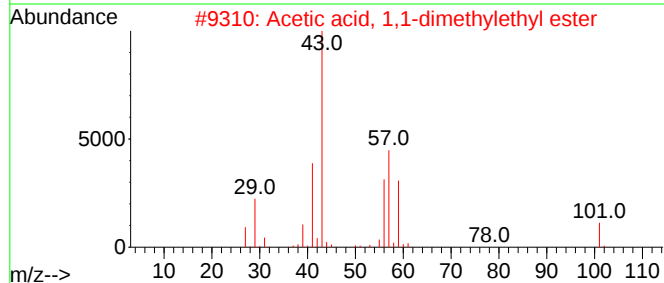
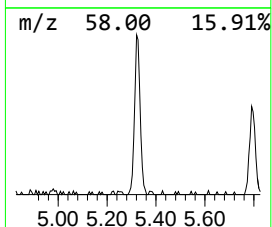
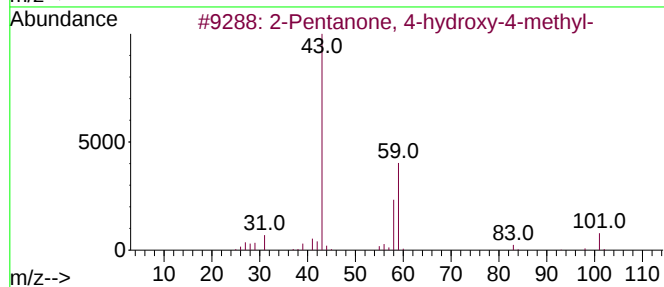
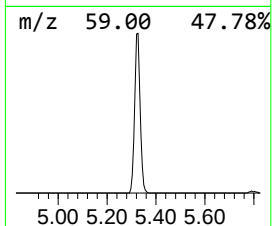
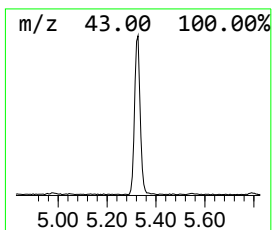
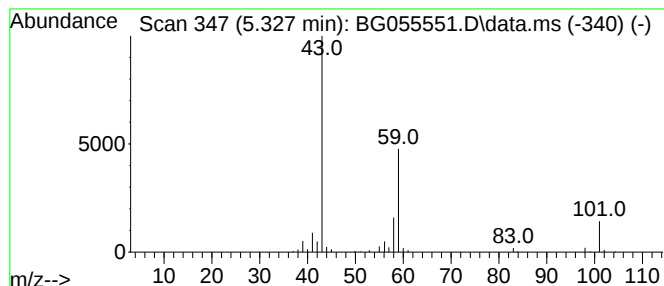
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.327	15.08 ng	221088	1,4-Dichlorobenzene-d4	8.270

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9



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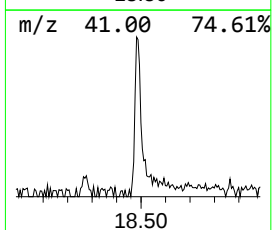
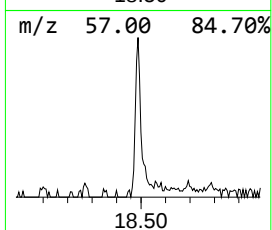
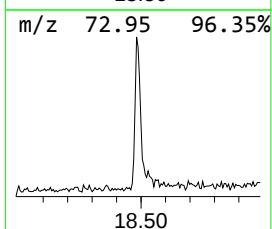
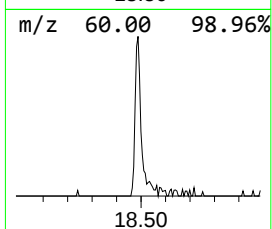
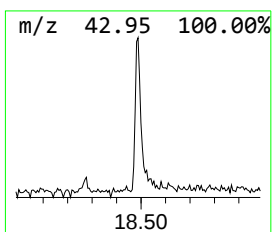
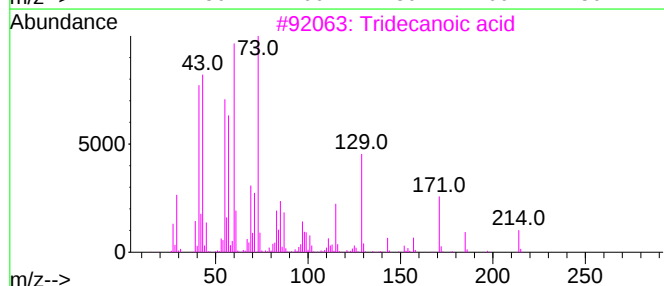
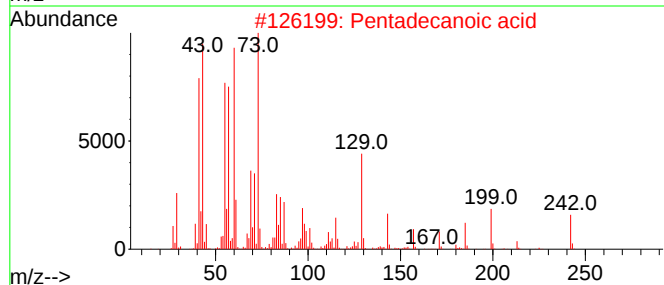
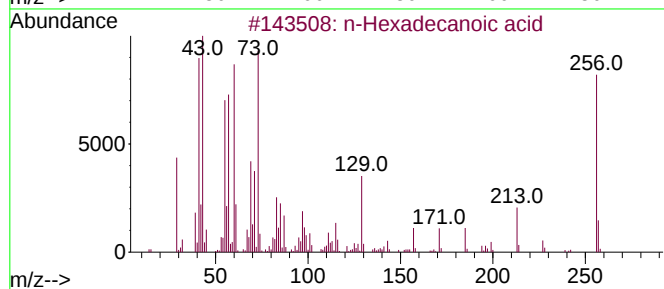
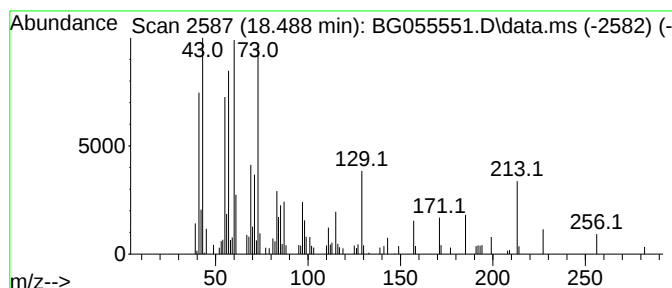
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.488	3.05 ng	115546	Phenanthrene-d10	17.624

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3			Tridecanoic acid	214	C13H26O2	000638-53-9	58
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5			Nonanoic acid	158	C9H18O2	000112-05-0	43



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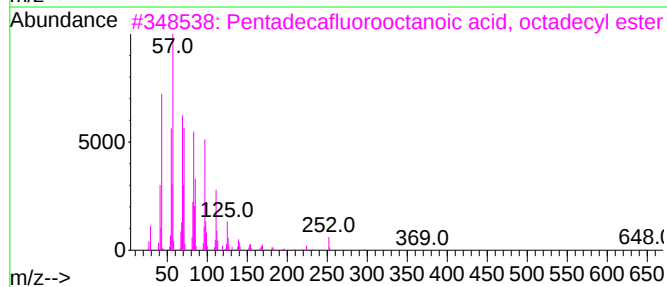
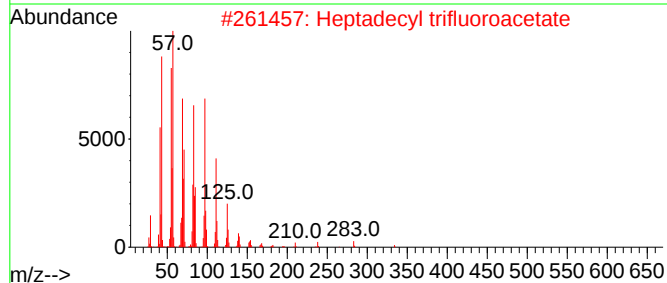
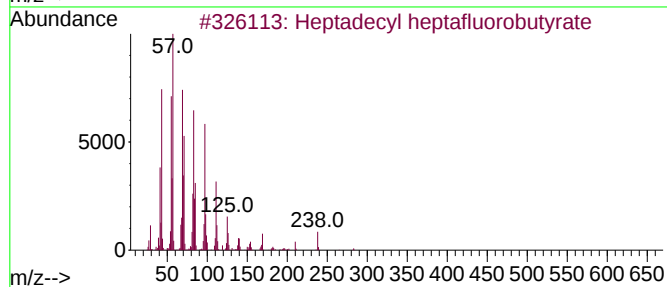
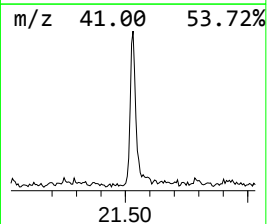
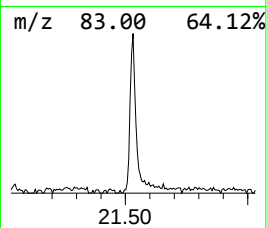
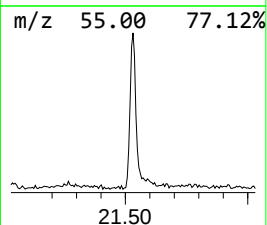
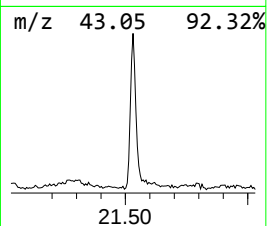
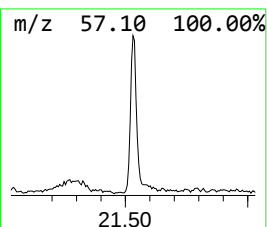
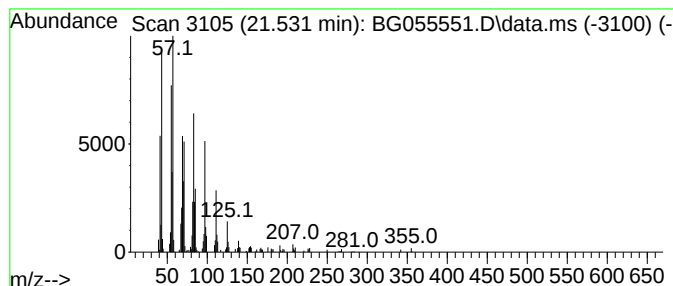
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.531	4.88 ng	216812	Chrysene-d12	21.919

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4			17-Pentatriacontene	491	C35H70	006971-40-0	91
5			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.329	32.3	ng	473468	1	8.270	293240	20.0
unknown3.875	3.875	2.0	ng	30067	1	8.270	293240	20.0
2-Pentanone, 4-...	5.327	15.1	ng	221088	1	8.270	293240	20.0
n-Hexadecanoic ...	18.488	3.0	ng	115546	4	17.624	756628	20.0
Heptadecyl hept...	21.531	4.9	ng	216812	5	21.919	888959	20.0