

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111822\
 Data File : BG055700.D
 Acq On : 18 Nov 2022 21:39
 Operator : CG/JU
 Sample : N5613-01 2X
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-COMP-1

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: BG055700.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.853	92	96	103	rBV	8948	15020	1.04%	0.139%
2	5.299	337	342	351	rVB	56505	94151	6.53%	0.871%
3	5.780	417	424	435	rVB	424700	690342	47.88%	6.388%
4	7.396	691	699	710	rBV	434209	768488	53.30%	7.111%
5	8.248	837	844	852	rBV	181942	308026	21.36%	2.850%
6	9.417	1034	1043	1053	rBV	266697	478658	33.20%	4.429%
7	10.821	1274	1282	1296	rBV	128598	227395	15.77%	2.104%
8	11.080	1318	1326	1332	rBV	263216	468814	32.51%	4.338%
9	13.495	1729	1737	1745	rVB	768546	1178381	81.72%	10.904%
10	13.747	1772	1780	1788	rBV	52710	87814	6.09%	0.813%
11	14.870	1964	1971	1978	rBV	403466	637861	44.24%	5.902%
12	14.934	1978	1982	1988	rVB	16406	26780	1.86%	0.248%
13	15.263	2034	2038	2045	rVB3	12321	24885	1.73%	0.230%
14	15.798	2125	2129	2134	rVB5	10567	15056	1.04%	0.139%
15	15.910	2144	2148	2154	rBV	16144	24911	1.73%	0.231%
16	16.292	2207	2213	2217	rBV9	8997	21307	1.48%	0.197%
17	16.350	2217	2223	2230	rBV	561659	862585	59.82%	7.982%
18	17.302	2382	2385	2389	rBV	13546	19611	1.36%	0.181%
19	17.614	2432	2438	2442	rBV	466462	714480	49.55%	6.611%
20	17.655	2442	2445	2451	rVB	134231	193786	13.44%	1.793%
21	17.743	2456	2460	2465	rVB	39459	59265	4.11%	0.548%
22	18.013	2502	2506	2509	rVB	14765	21122	1.46%	0.195%
23	18.248	2543	2546	2553	rVB2	20764	26024	1.80%	0.241%
24	18.471	2579	2584	2591	rBV2	135083	227347	15.77%	2.104%
25	18.683	2616	2620	2624	rBV	20929	34664	2.40%	0.321%
26	19.652	2781	2785	2791	rVB	209082	297024	20.60%	2.748%
27	19.729	2796	2798	2806	rVB3	54290	88207	6.12%	0.816%
28	20.011	2842	2846	2854	rVB2	253076	417606	28.96%	3.864%
29	20.199	2873	2878	2883	rBV	1130455	1441911	100.00%	13.342%
30	21.908	3163	3169	3175	rVB2	409046	728380	50.51%	6.740%
31	25.328	3745	3751	3762	rVB	227206	607126	42.11%	5.618%

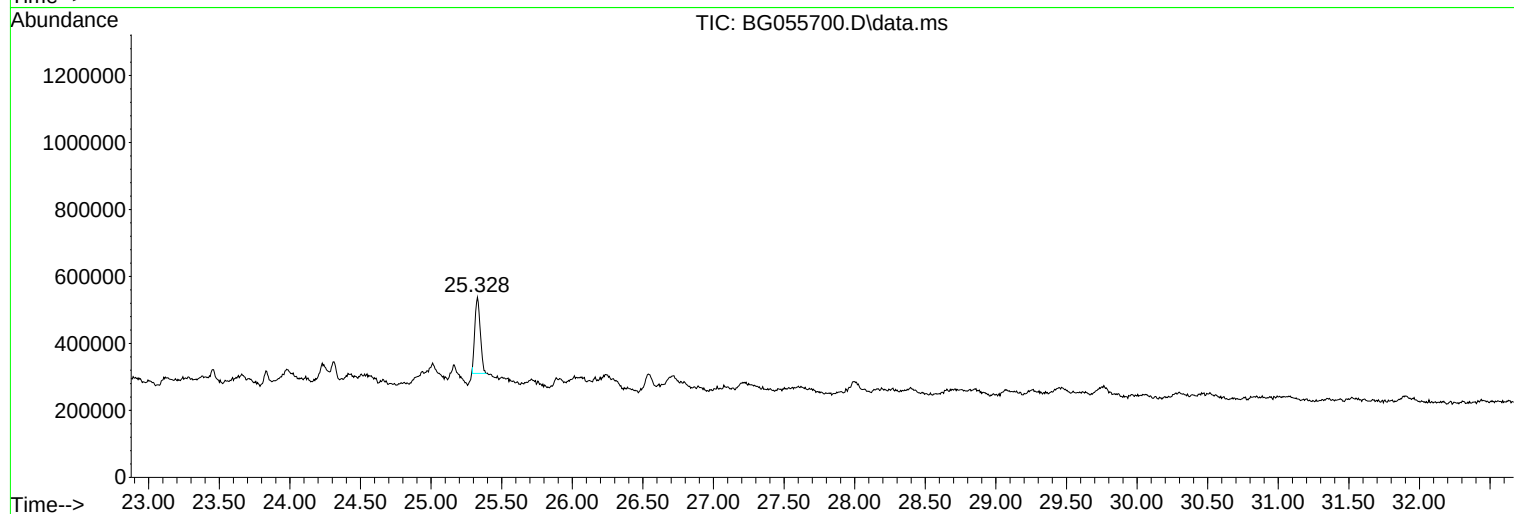
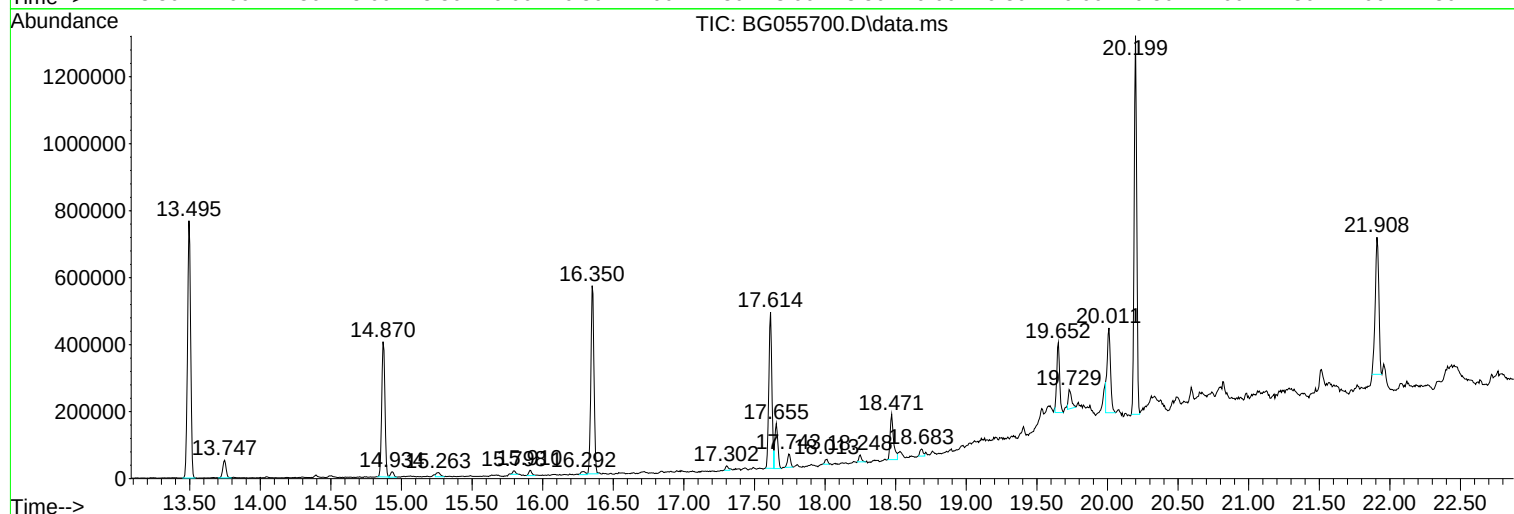
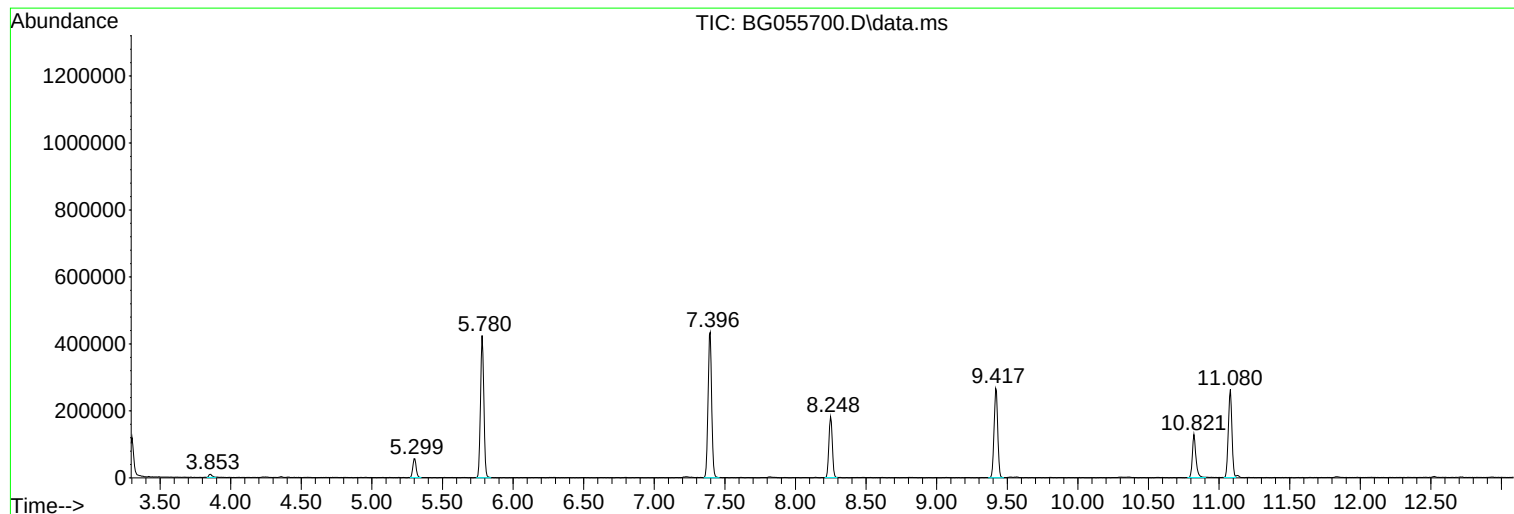
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BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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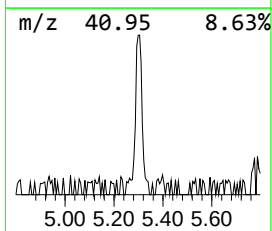
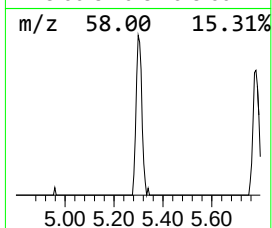
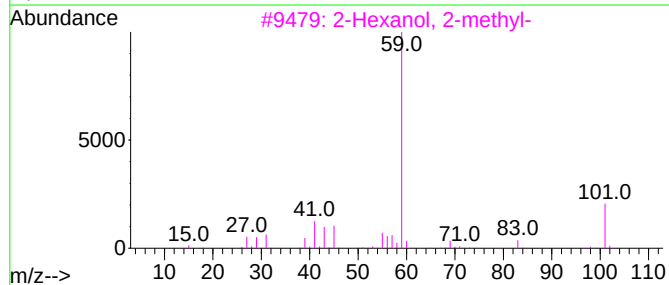
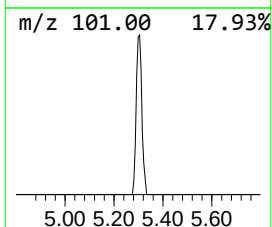
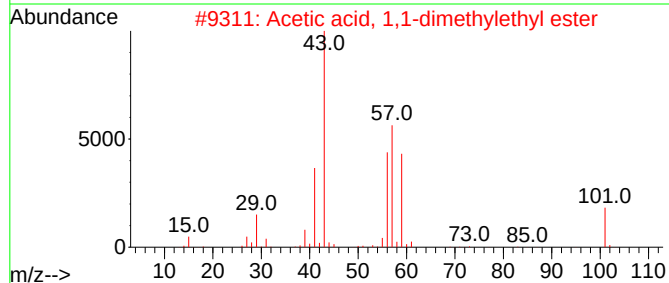
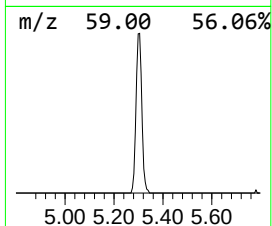
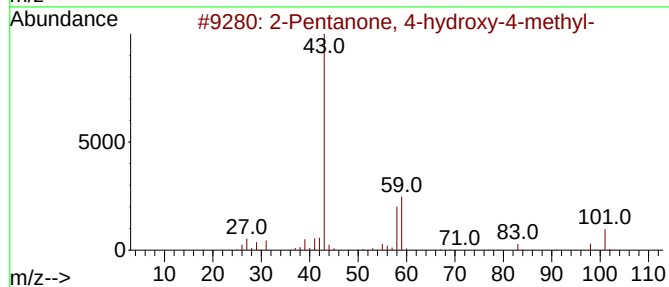
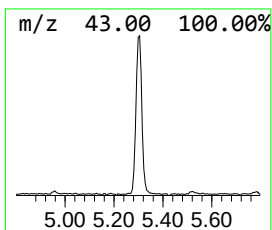
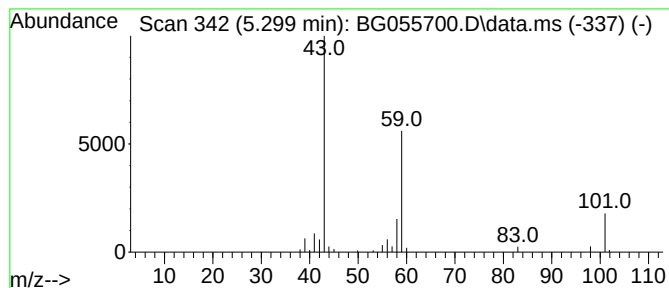
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.299	6.11 ng	94151	1,4-Dichlorobenzene-d4	8.248

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	38	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10	



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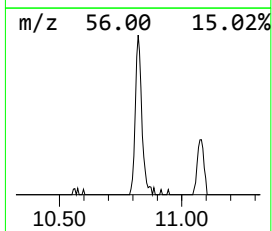
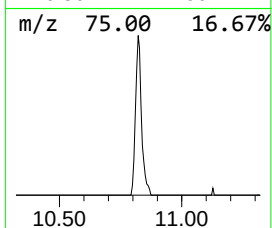
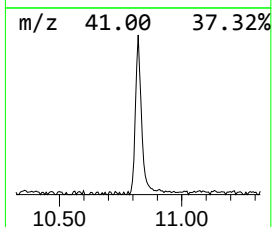
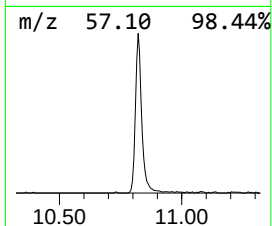
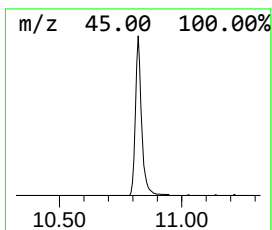
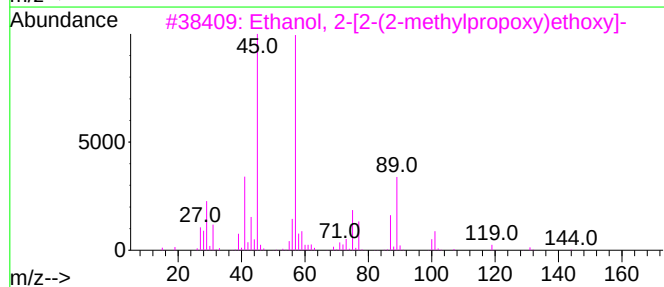
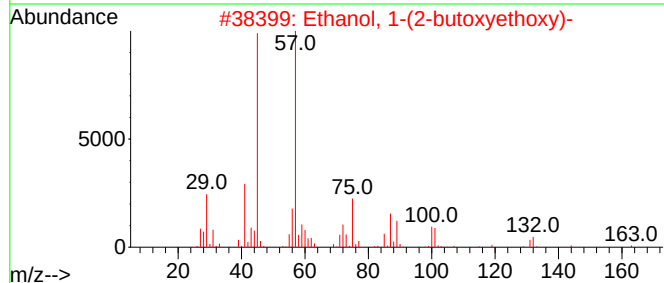
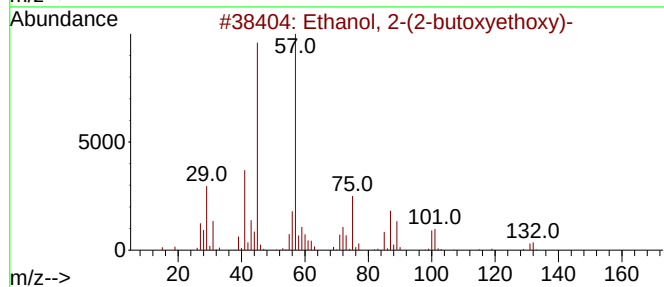
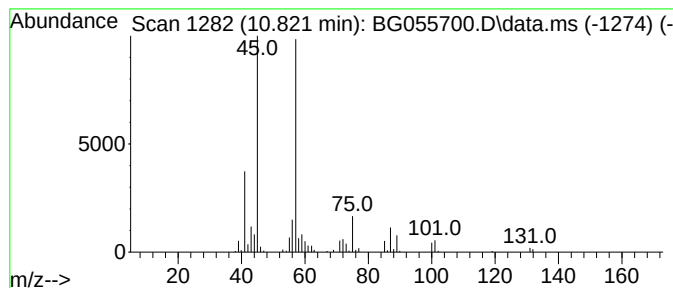
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.822	9.70 ng	227395	Naphthalene-d8	11.080

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)ethoxy]-	162	C8H18O3	018912-80-6	50
4			Butyl lactate	146	C7H14O3	000138-22-7	47
5			1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	47



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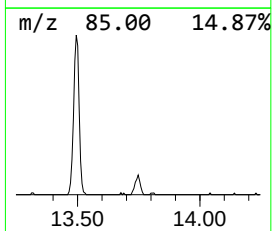
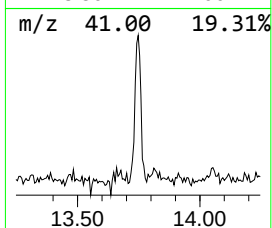
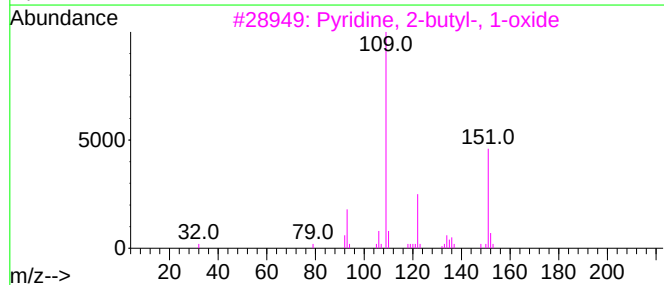
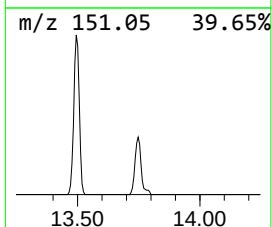
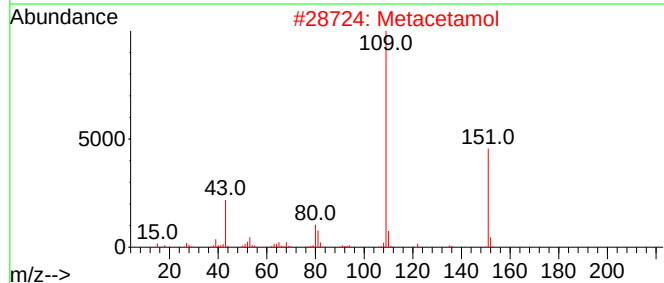
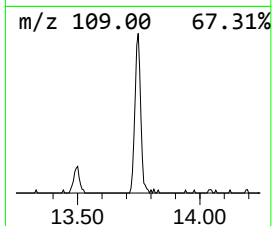
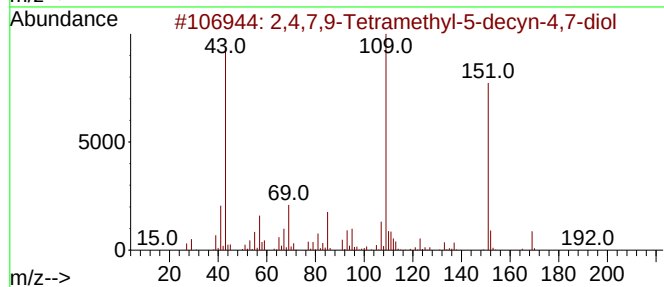
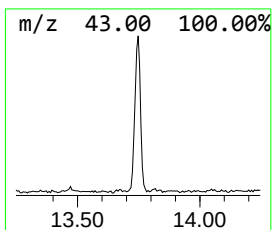
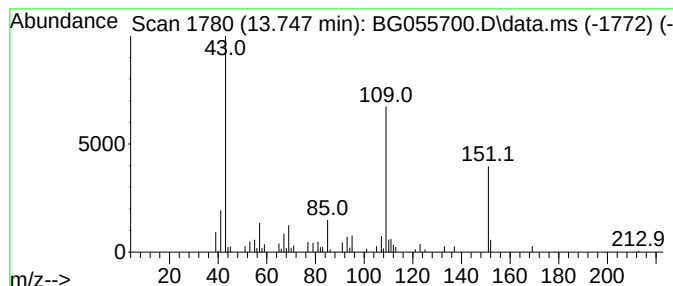
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.748	2.75 ng	87814	Acenaphthene-d10	14.870

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	91
2	Metacetamol	151	C8H9NO2		000621-42-1	58
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO		031396-32-4	53
4	m-Isopropoxyaniline	151	C9H13NO		041406-00-2	53
5	Ethanone, 1-(4,5-diethyl-2-methy...	180	C12H20O		062338-24-3	40



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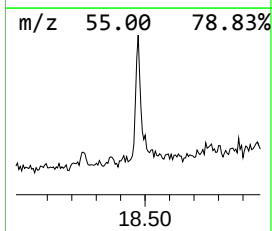
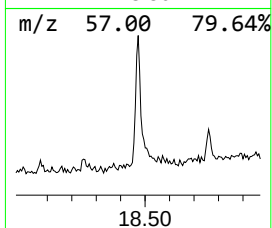
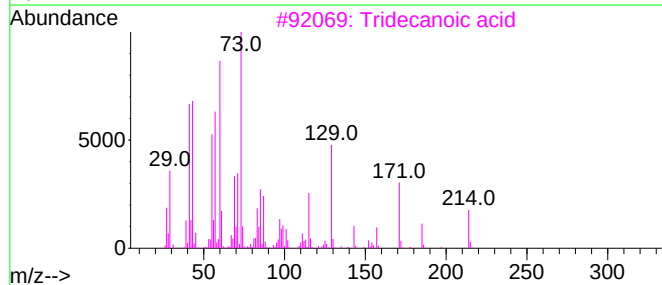
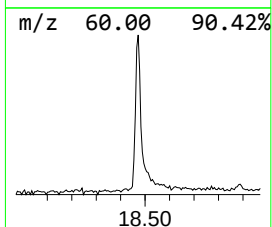
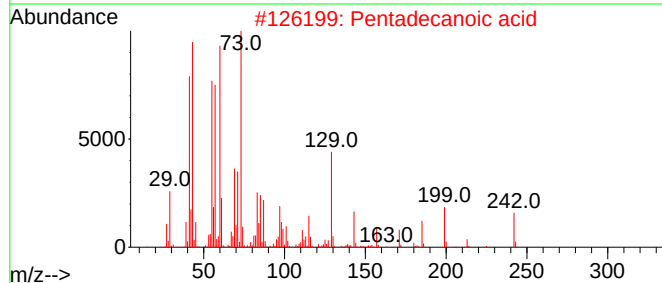
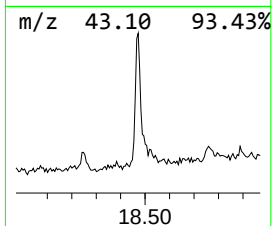
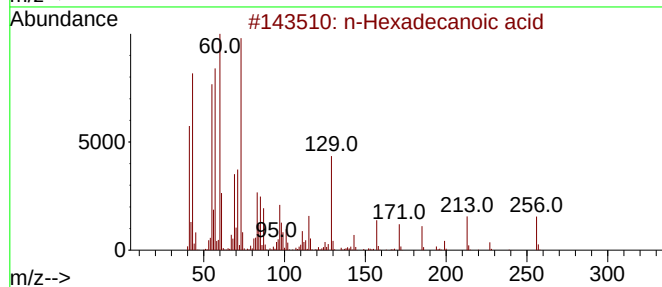
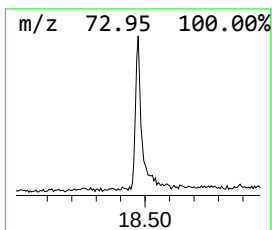
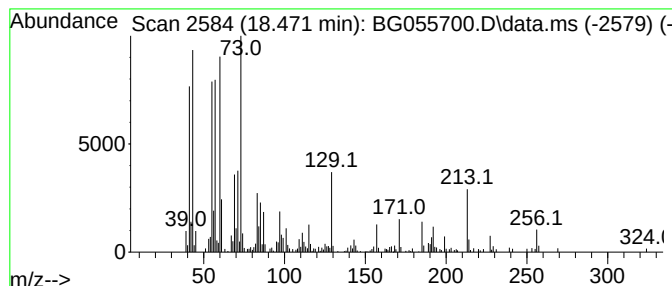
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.471	6.36 ng	227347	Phenanthrene-d10		17.613	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	81
3	Tridecanoic acid		214	C13H26O2	000638-53-9	70
4	Undecanoic acid		186	C11H22O2	000112-37-8	70
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	64



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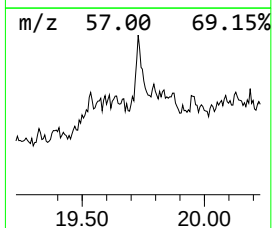
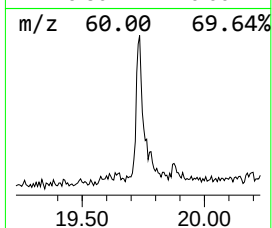
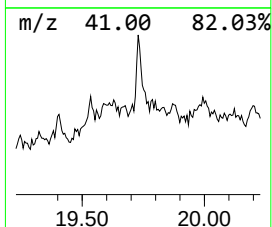
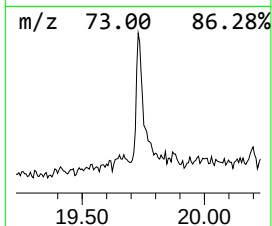
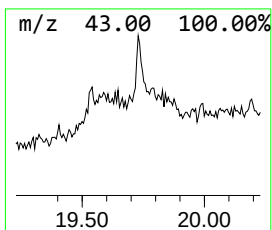
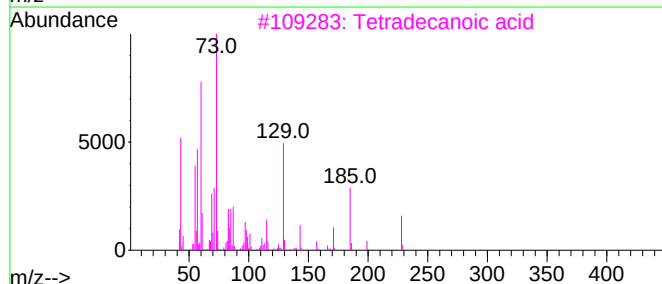
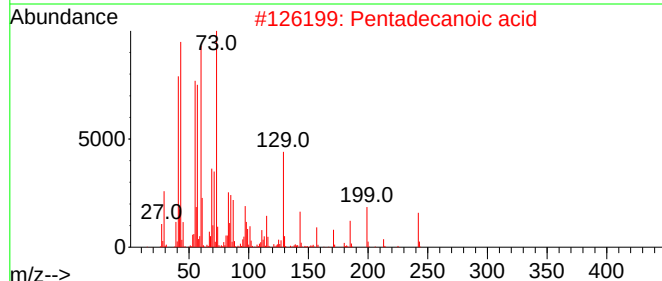
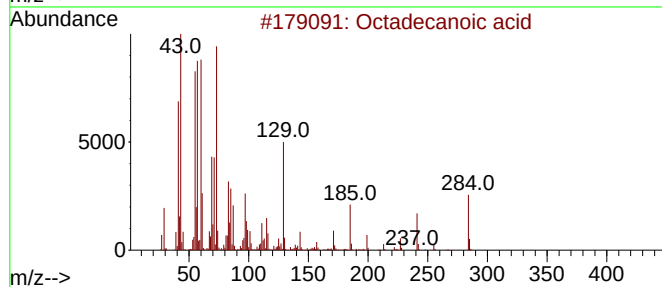
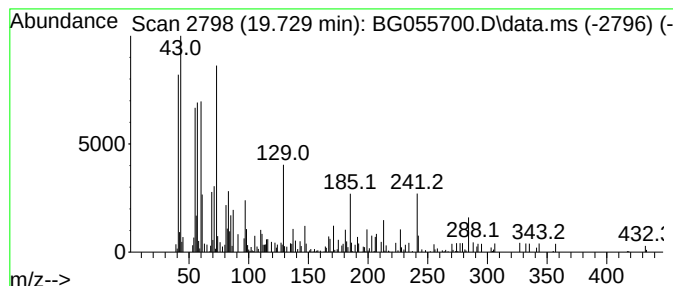
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.729	2.47 ng	88207	Phenanthrene-d10	17.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4			Heptadecanoic acid	270	C17H34O2	000506-12-7	64
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62



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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
2-Pentanone, 4-...	5.299	6.1	ng	94151	1	8.248	308026	20.0
Ethanol, 2-(2-b...	10.822	9.7	ng	227395	2	11.080	468814	20.0
2,4,7,9-Tetrame...	13.748	2.8	ng	87814	3	14.870	637861	20.0
n-Hexadecanoic ...	18.471	6.4	ng	227347	4	17.613	714480	20.0
Octadecanoic acid	19.729	2.5	ng	88207	4	17.613	714480	20.0