

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
 Data File : BG060145.D
 Acq On : 22 Dec 2023 19:33
 Operator : MA/JU
 Sample : 05899-06
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GHL-SS-12

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-BG122123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060145.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.116	3	5	10	rVB	246532	282264	1.80%	0.398%
2	5.043	328	333	340	rVB	120914	185891	1.19%	0.262%
3	5.513	406	413	431	rBV	3018752	5105445	32.58%	7.198%
4	7.106	676	684	698	rBV	3497373	6115103	39.02%	8.621%
5	7.940	818	826	834	rBV	659106	1150480	7.34%	1.622%
6	9.103	1015	1024	1033	rBV	1923523	3452090	22.03%	4.867%
7	10.743	1295	1303	1313	rBV	1013700	1911047	12.20%	2.694%
8	13.199	1711	1721	1731	rBV	6440082	10281902	65.62%	14.495%
9	14.579	1948	1956	1964	rBV	2271021	3551125	22.66%	5.006%
10	16.066	2200	2209	2219	rBV	5707306	8671446	55.34%	12.225%
11	17.323	2416	2423	2436	rBV	3178004	4935888	31.50%	6.959%
12	17.446	2438	2444	2451	rVB6	107123	204521	1.31%	0.288%
13	18.216	2570	2575	2592	rBV	536769	882366	5.63%	1.244%
14	19.944	2863	2869	2883	rBV	11392451	15669991	100.00%	22.092%
15	21.236	3084	3089	3099	rBV	397031	641113	4.09%	0.904%
16	21.589	3142	3149	3159	rBV	2446116	3914511	24.98%	5.519%
17	24.761	3679	3689	3703	rBV2	1394665	3976719	25.38%	5.606%

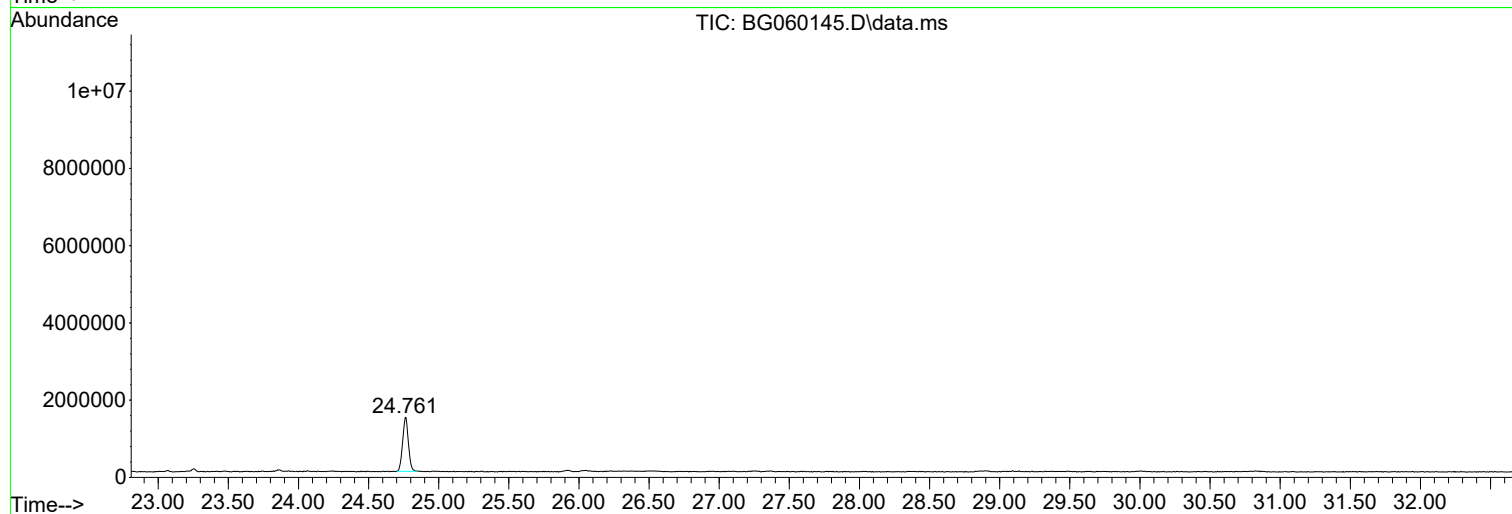
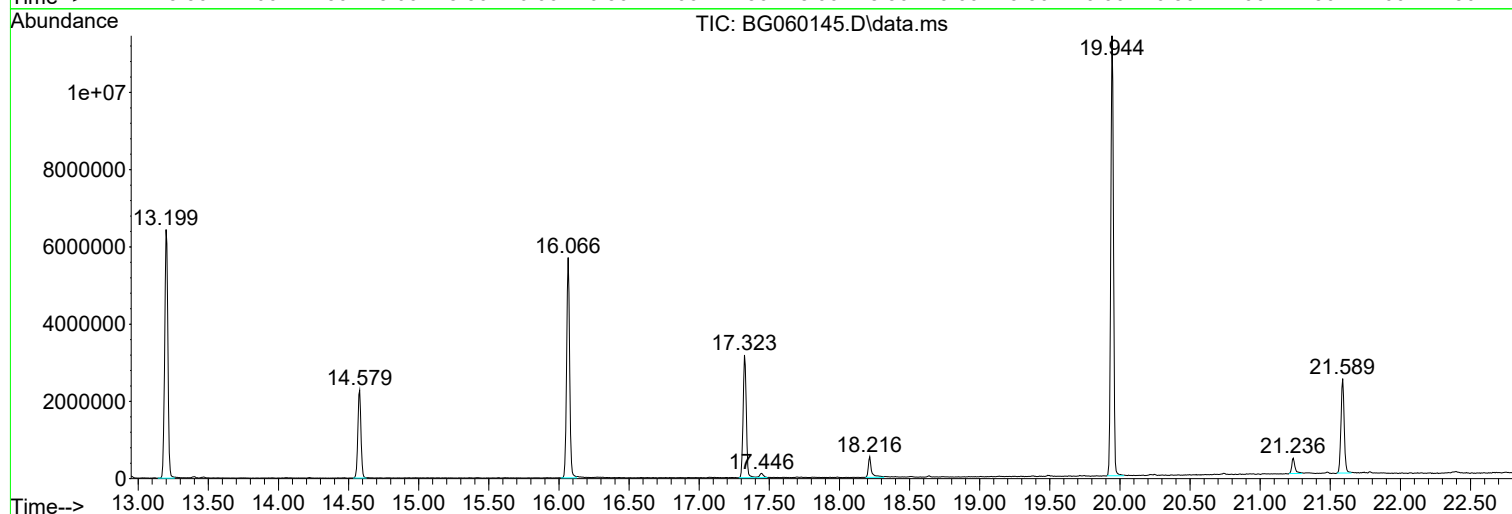
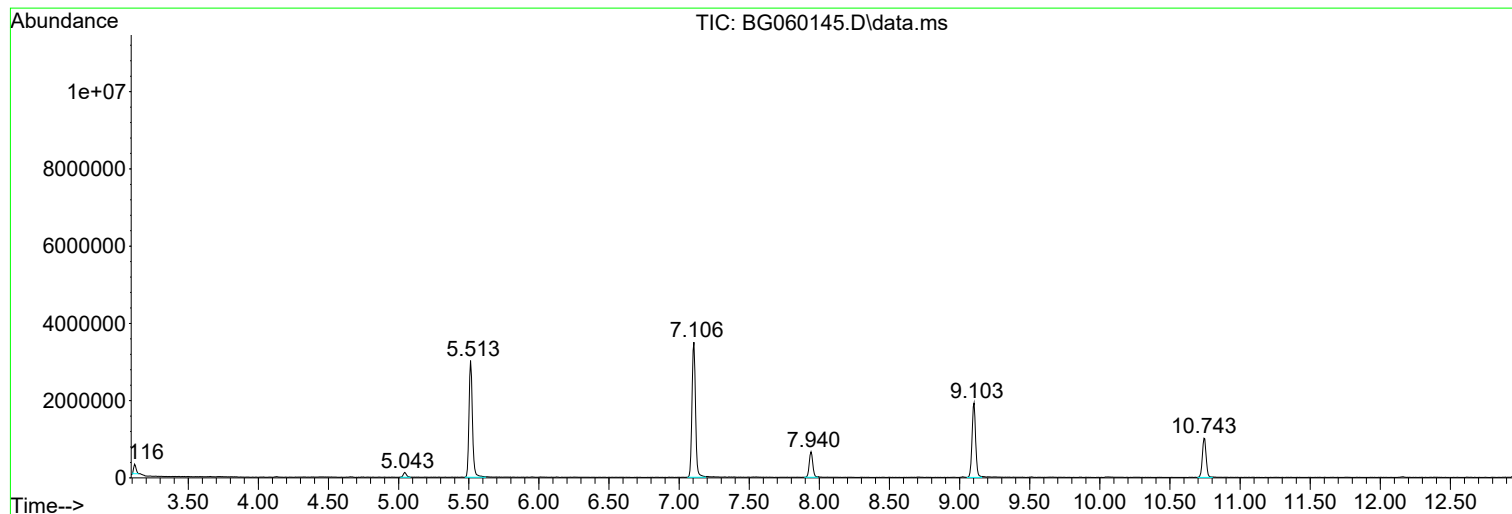
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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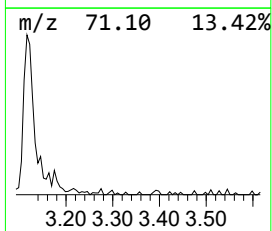
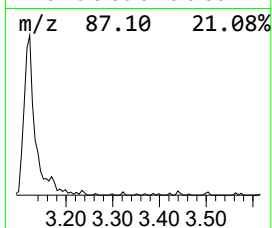
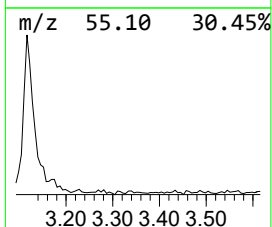
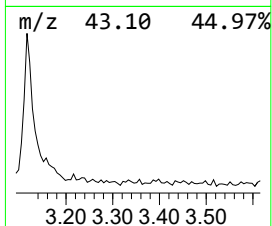
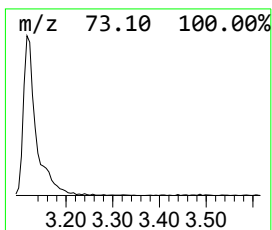
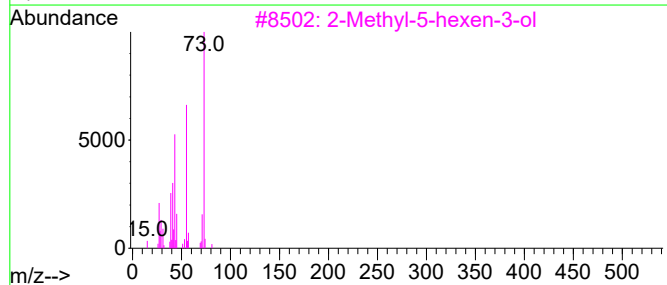
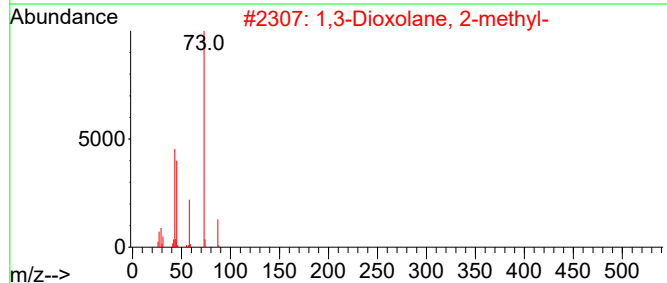
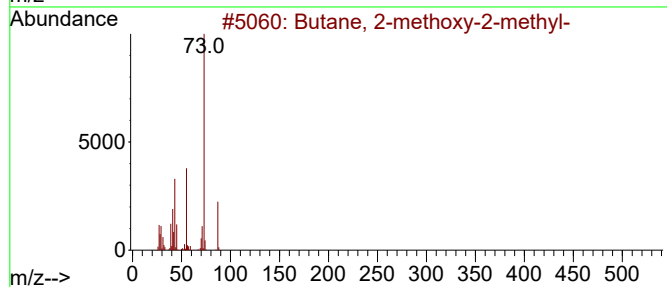
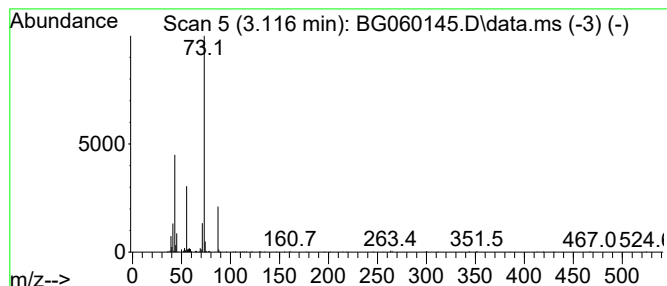
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.116	4.91 ng	282264	1,4-Dichlorobenzene-d4	7.940

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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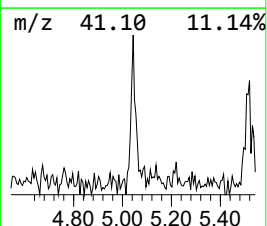
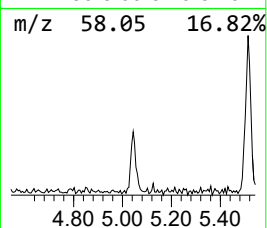
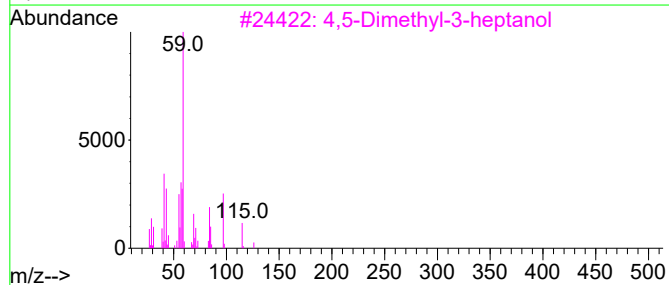
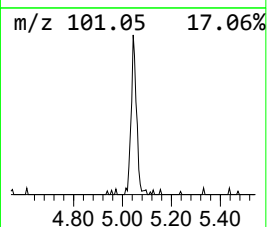
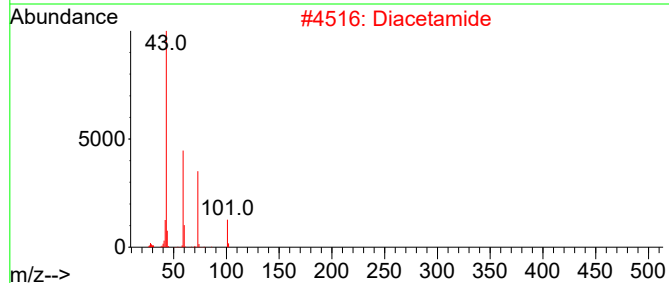
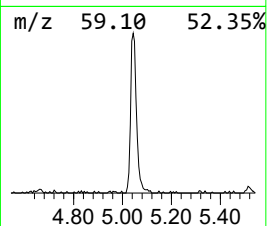
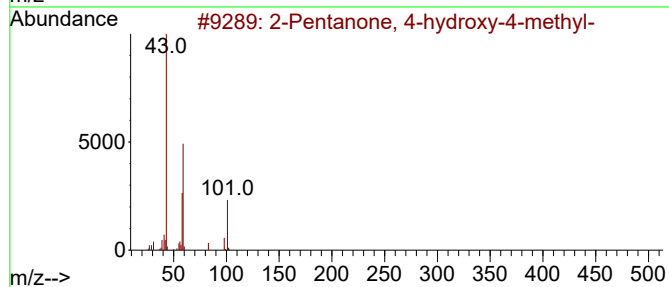
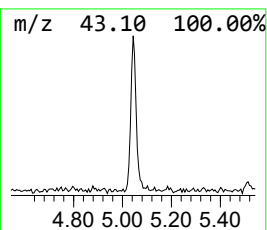
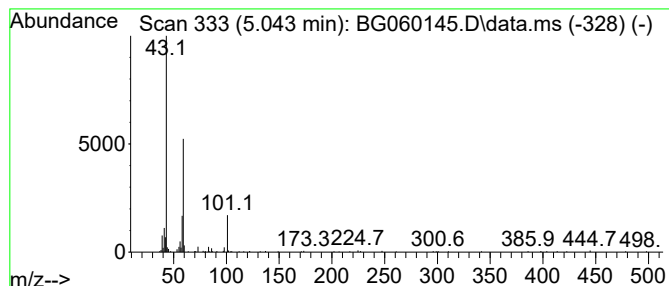
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown5.043 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.043	3.23 ng	185891	1,4-Dichlorobenzene-d4	7.940

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2		Diacetamide	101	C4H7NO2	000625-77-4	36
3		4,5-Dimethyl-3-heptanol	144	C9H20O	019549-76-9	32
4		2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	17
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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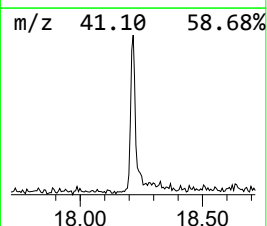
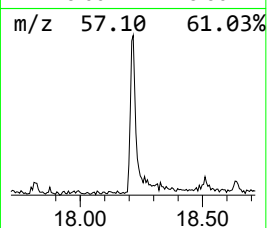
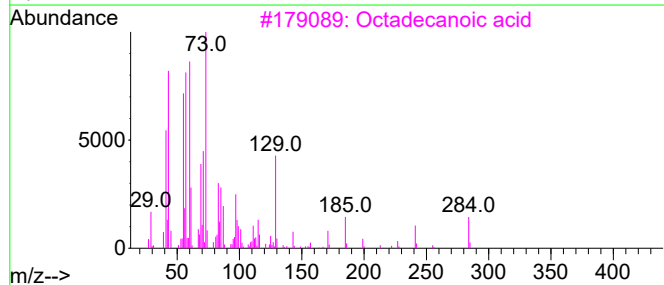
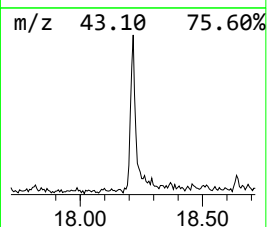
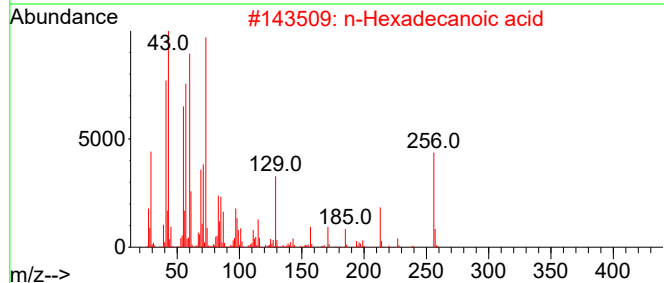
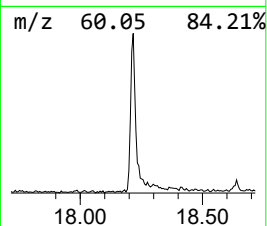
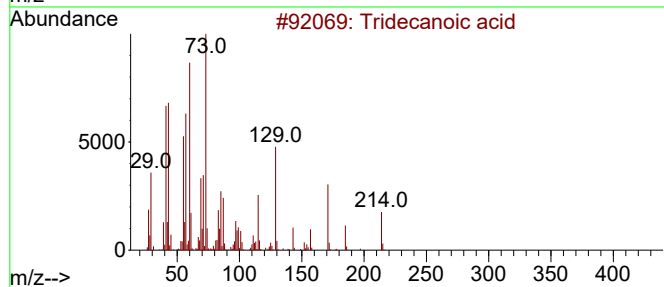
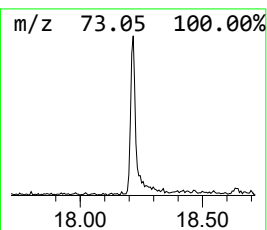
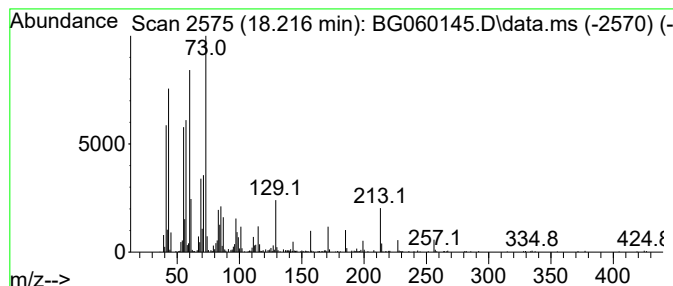
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tridecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	3.58 ng	882366	Phenanthrene-d10	17.323

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	95
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Octadecanoic acid	284	C18H36O2	000057-11-4	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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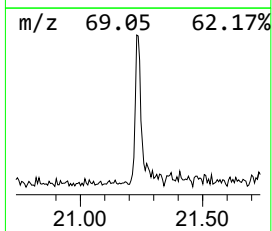
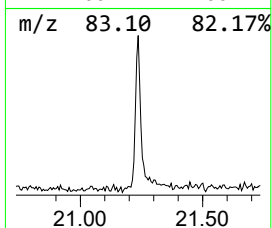
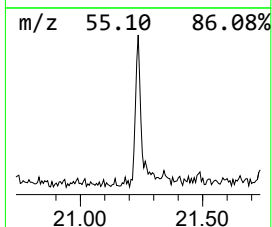
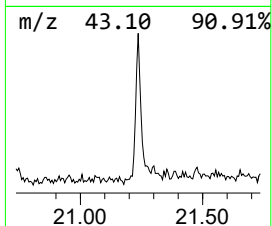
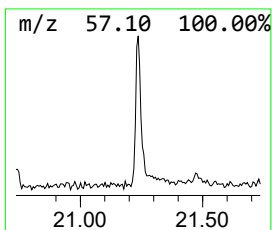
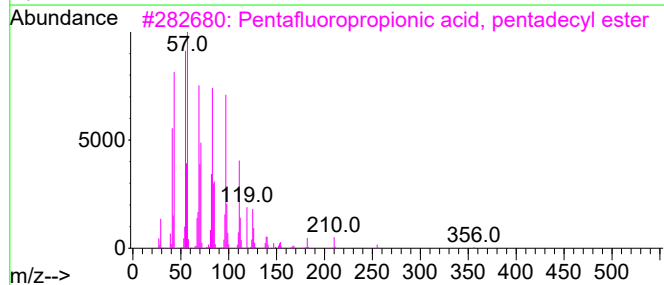
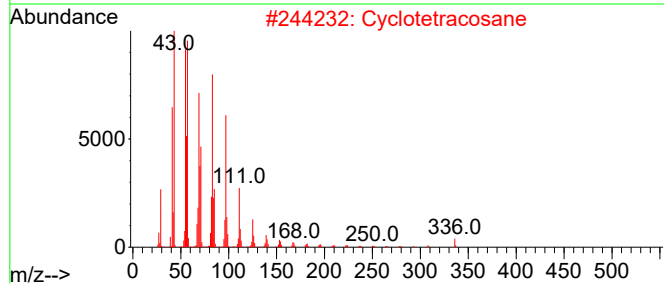
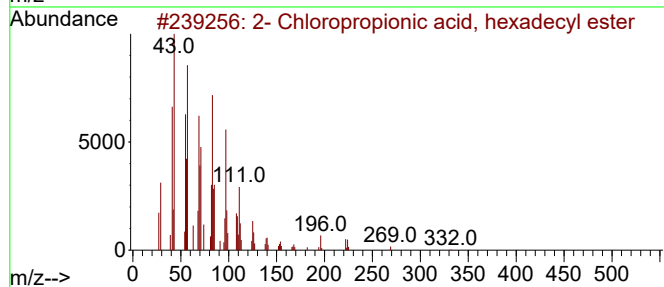
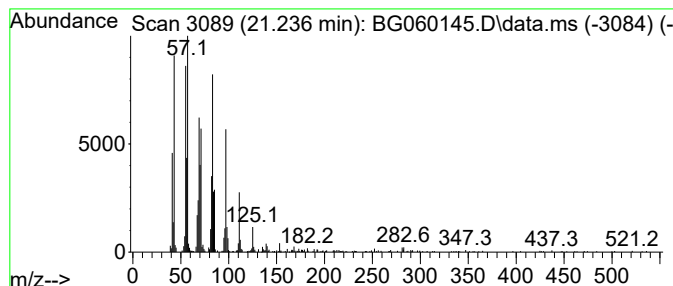
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 2- Chloropropionic acid, he... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.236	3.28 ng	641113	Chrysene-d12	21.589

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	95
2			Cyclotetracosane	336	C24H48	000297-03-0	91
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
4			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5			Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	87



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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...	3.116	4.9	ng	282264	1	7.940	1150480	20.0
unknown5.043	5.043	3.2	ng	185891	1	7.940	1150480	20.0
Tridecanoic acid	18.216	3.6	ng	882366	4	17.323	4935890	20.0
2- Chloropropio...	21.236	3.3	ng	641113	5	21.589	3914510	20.0