

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012023\
 Data File : BG056373.D
 Acq On : 20 Jan 2023 18:47
 Operator : CG/JU
 Sample : 01232-05
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B-P-18B

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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056373.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.339	341	349	357	rBV	122386	197731	5.33%	1.309%
2	5.827	424	432	440	rBV	691072	1119498	30.16%	7.409%
3	7.449	699	708	722	rBV	692118	1202205	32.39%	7.957%
4	8.301	846	853	861	rVB	131322	219695	5.92%	1.454%
5	9.476	1045	1053	1061	rBV	402921	715553	19.28%	4.736%
6	11.133	1326	1335	1348	rBB	182367	324287	8.74%	2.146%
7	13.542	1738	1745	1757	rVB	1649686	2440704	65.76%	16.154%
8	14.916	1970	1979	1986	rBV	337418	518847	13.98%	3.434%
9	16.250	2201	2206	2212	rBV	34978	51329	1.38%	0.340%
10	16.397	2224	2231	2242	rBV	1177608	1741128	46.91%	11.524%
11	17.654	2438	2445	2449	rBV	417531	649343	17.50%	4.298%
12	17.696	2449	2452	2457	rVB2	39885	54487	1.47%	0.361%
13	18.495	2584	2588	2596	rBV2	98277	161418	4.35%	1.068%
14	19.687	2786	2791	2796	rVB	73941	108188	2.92%	0.716%
15	19.752	2798	2802	2811	rBV5	38829	63918	1.72%	0.423%
16	19.887	2821	2825	2830	rBV	135113	148721	4.01%	0.984%
17	20.046	2848	2852	2858	rVB	79999	120050	3.23%	0.795%
18	20.193	2873	2877	2878	rBV	61175	59040	1.59%	0.391%
19	20.228	2878	2883	2889	rVB	2898793	3711391	100.00%	24.564%
20	21.526	3100	3104	3114	rVB3	69784	132957	3.58%	0.880%
21	21.944	3168	3175	3181	rBV2	403301	735362	19.81%	4.867%
22	25.387	3754	3761	3772	rVB2	213370	633117	17.06%	4.190%

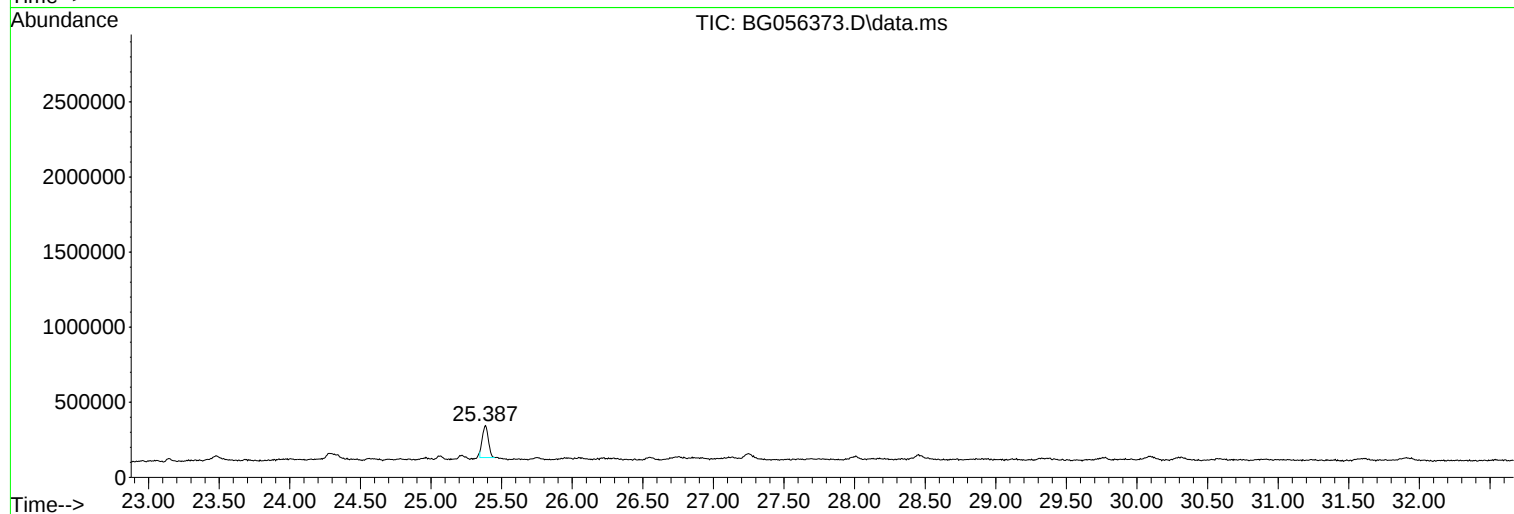
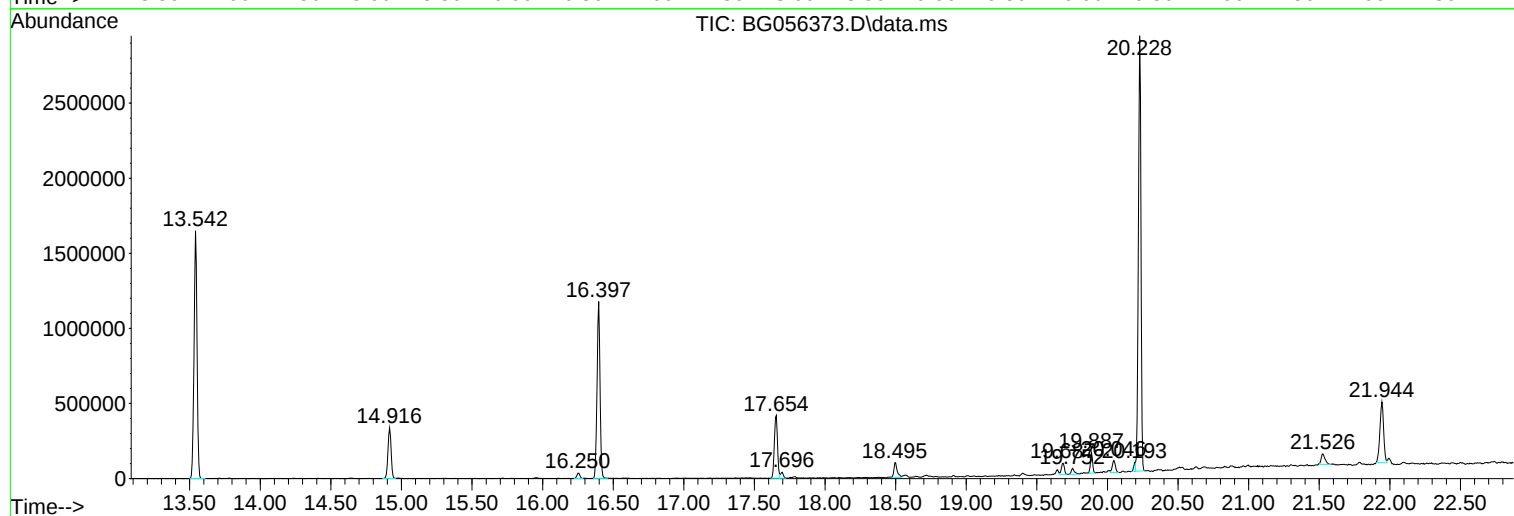
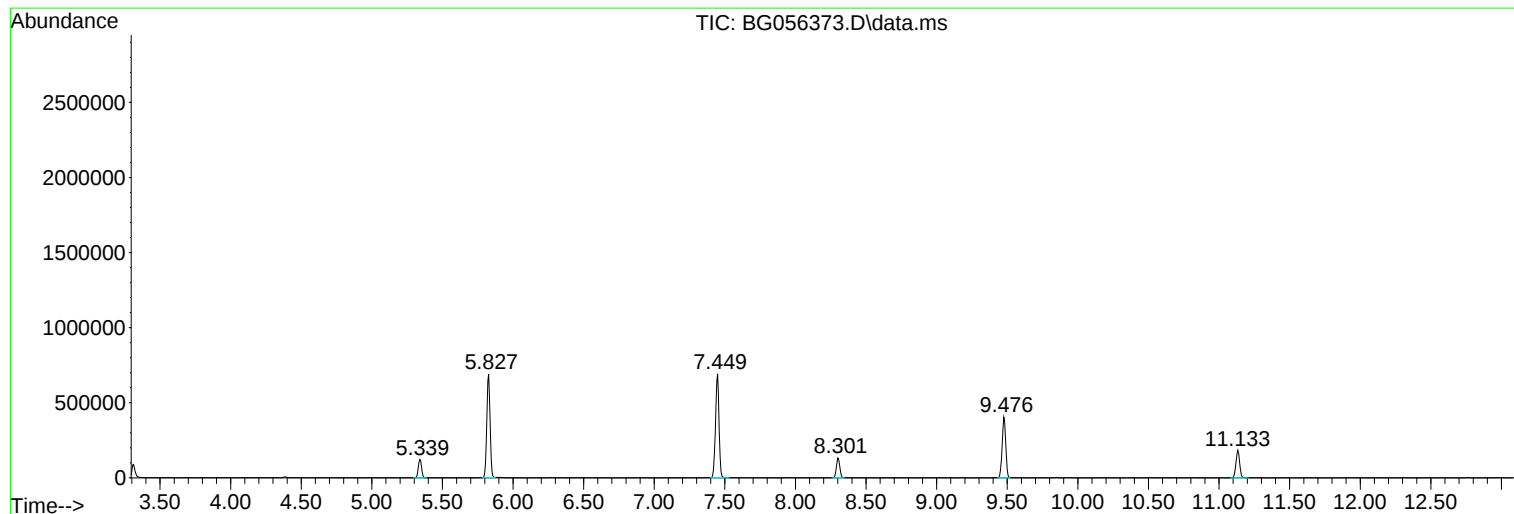
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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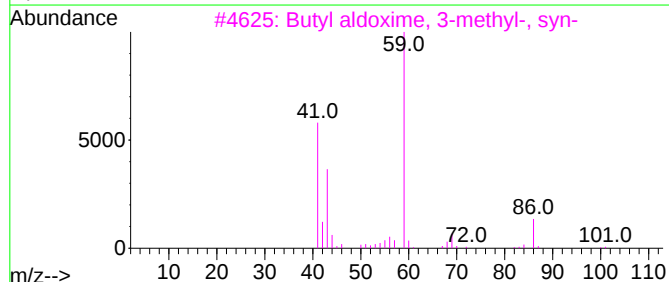
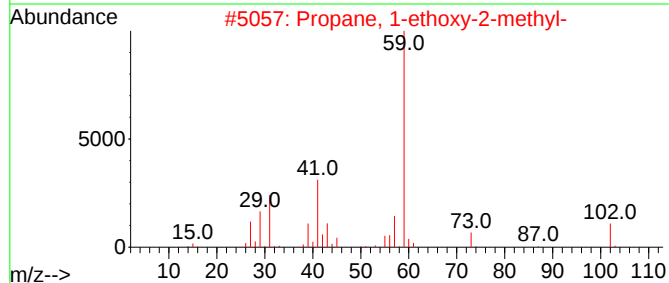
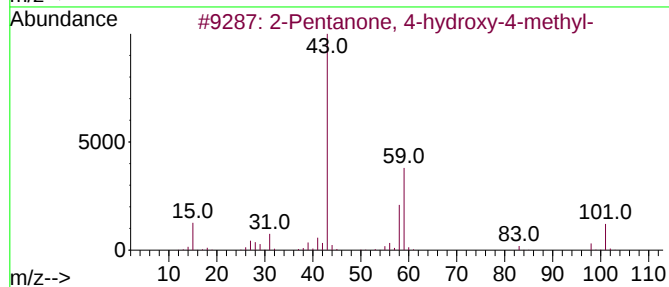
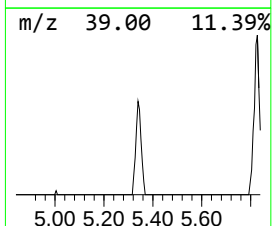
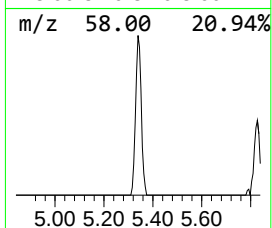
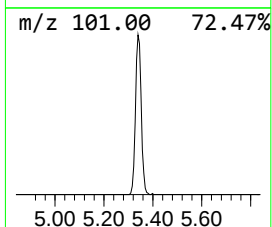
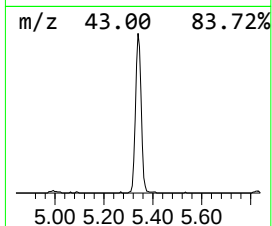
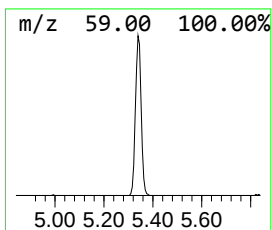
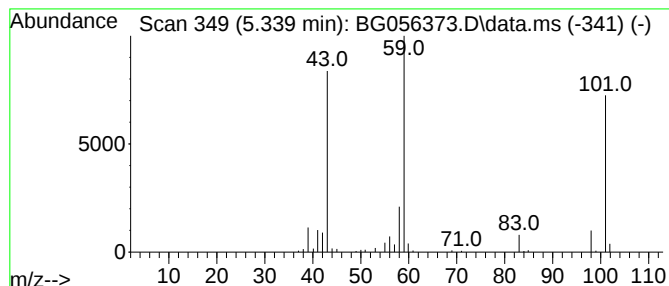
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.339	18.00 ng	197731	1,4-Dichlorobenzene-d4	8.301

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38	
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25	
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25	
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	17	



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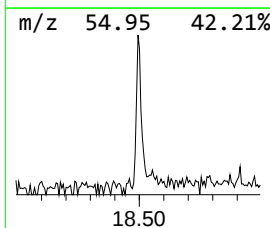
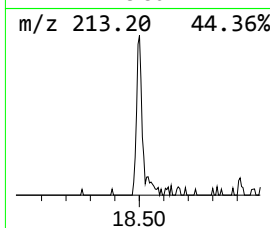
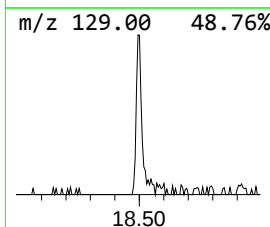
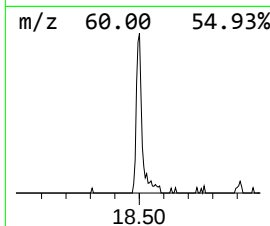
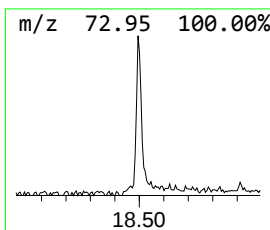
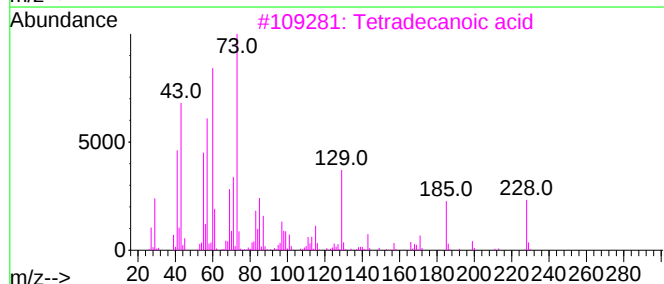
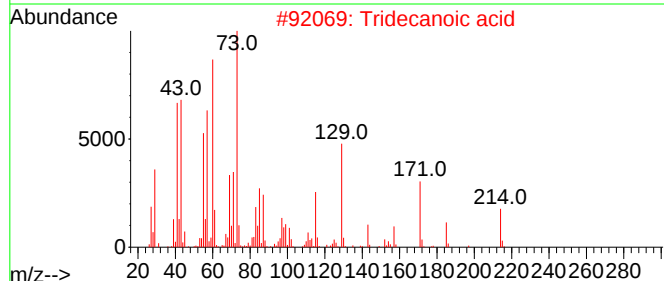
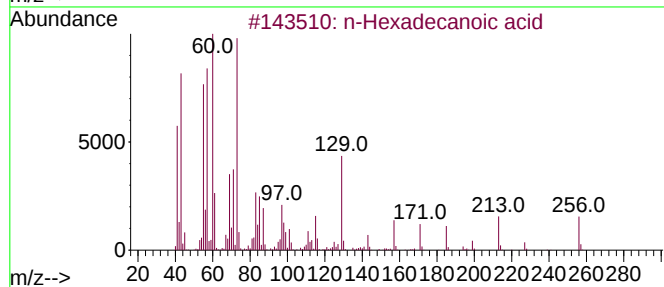
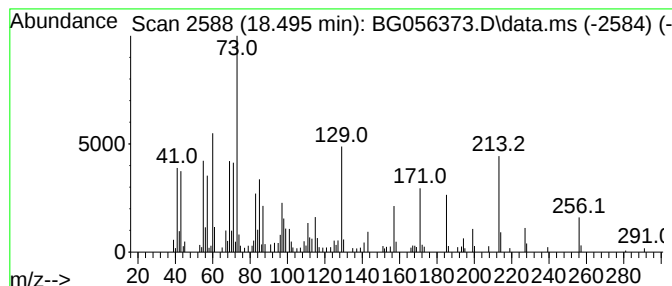
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.495	4.97 ng	161418	Phenanthrene-d10	17.654

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Tridecanoic acid	214	C13H26O2	000638-53-9	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	78
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	43
5			Dodecanoic acid	200	C12H24O2	000143-07-7	43



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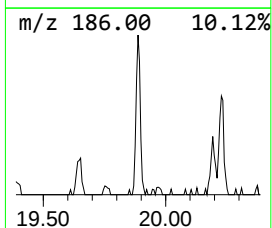
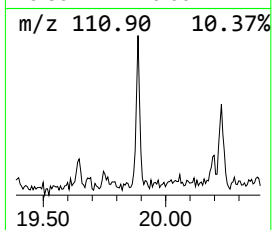
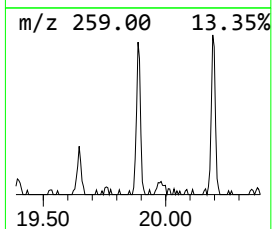
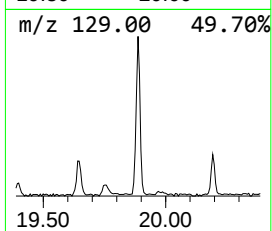
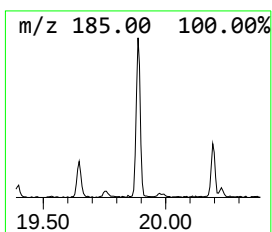
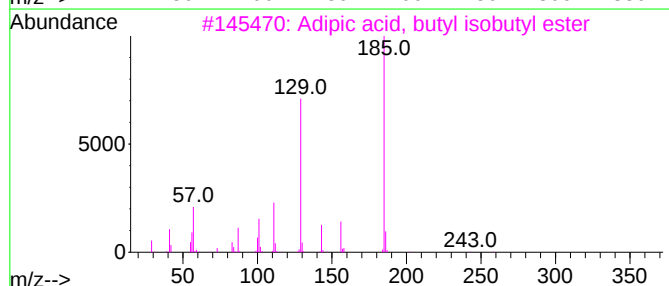
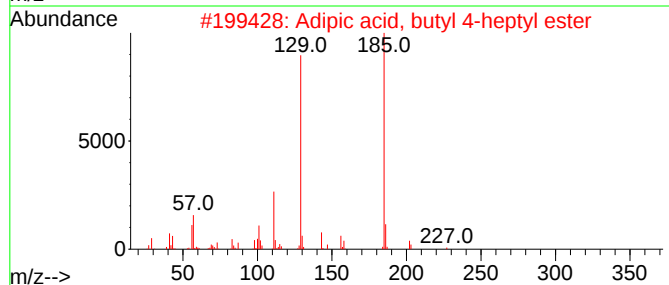
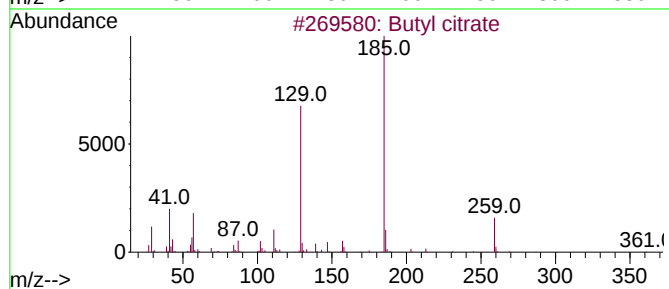
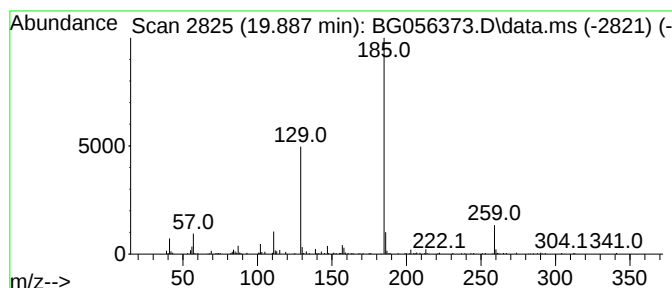
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Peak Number 3 Butyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.887	4.04 ng	148721	Chrysene-d12	21.944

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	91
2			Adipic acid, butyl 4-heptyl ester	300	C17H32O4	1000349-73-7	56
3			Adipic acid, butyl isobutyl ester	258	C14H26O4	1010324-09-3	56
4			2-((Dimethylamino)methylene)ami...	382	C20H31ClN2O3	1000378-74-1	47
5			Adipic acid, 4-bromophenyl butyl...	356	C16H21BrO4	1000324-37-9	45



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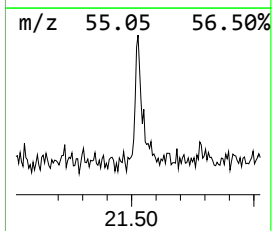
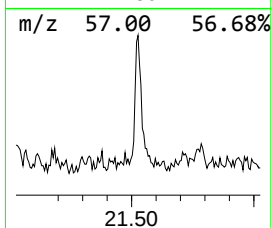
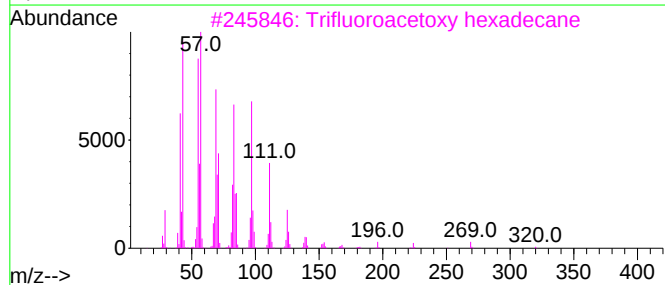
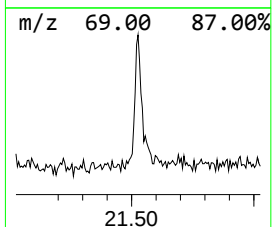
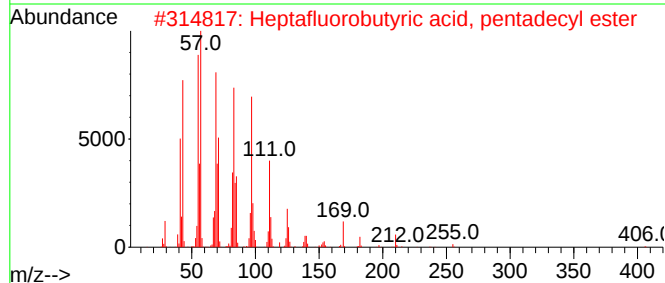
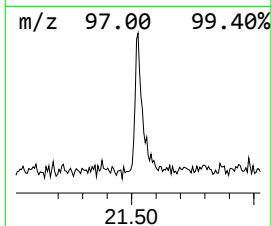
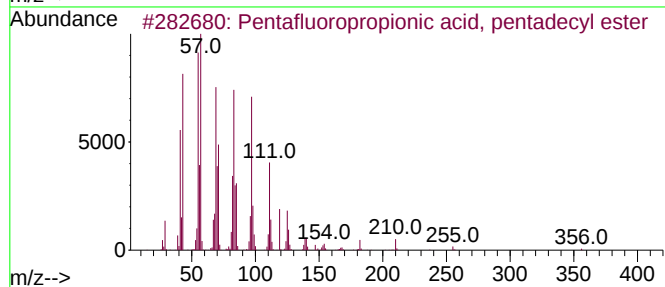
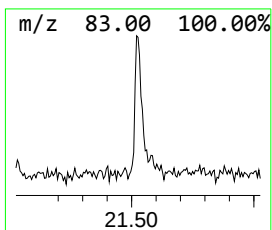
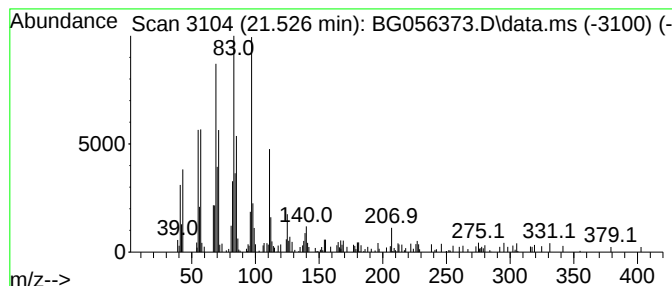
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Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.526	3.62 ng	132957	Chrysene-d12	21.944

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4			1-Nonadecene	266	C19H38	018435-45-5	91
5			1-Heptadecene	238	C17H34	006765-39-5	89



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.339	18.0	ng	197731	1	8.301	219695	20.0
n-Hexadecanoic ...	18.495	5.0	ng	161418	4	17.654	649343	20.0
Butyl citrate	19.887	4.0	ng	148721	5	21.944	735362	20.0
Pentafluoroprop...	21.526	3.6	ng	132957	5	21.944	735362	20.0