

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011923\
 Data File : BG056353.D
 Acq On : 19 Jan 2023 19:06
 Operator : CG/JU
 Sample : 01217-14
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BORING-2

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: BG056353.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.315	3	4	16	rVB	112882	132911	5.55%	1.373%
2	5.342	342	349	356	rBV	96014	141121	5.89%	1.458%
3	5.824	424	431	440	rBV	365930	592063	24.72%	6.118%
4	7.445	699	707	718	rBV	361803	620830	25.92%	6.415%
5	8.303	846	853	861	rBB	109639	185394	7.74%	1.916%
6	9.478	1045	1053	1060	rBV	208333	368189	15.37%	3.805%
7	11.135	1327	1335	1344	rBB	141350	244414	10.21%	2.526%
8	13.544	1738	1745	1754	rBB	795484	1179669	49.26%	12.190%
9	14.919	1971	1979	1987	rBB	261910	409411	17.10%	4.231%
10	16.258	2197	2207	2212	rBV	15884	24215	1.01%	0.250%
11	16.394	2223	2230	2238	rBV	607021	956583	39.94%	9.885%
12	17.657	2436	2445	2451	rBV	381381	593755	24.79%	6.136%
13	18.497	2584	2588	2598	rBV	72930	110854	4.63%	1.146%
14	19.754	2799	2802	2805	rBV4	21268	25545	1.07%	0.264%
15	20.048	2848	2852	2859	rVB	18286	24970	1.04%	0.258%
16	20.230	2877	2883	2891	rBV	1851719	2394873	100.00%	24.748%
17	21.523	3099	3103	3112	rVB3	81756	132364	5.53%	1.368%
18	21.946	3168	3175	3182	rBV2	443809	760392	31.75%	7.858%
19	25.389	3750	3761	3774	rVB2	252577	779571	32.55%	8.056%

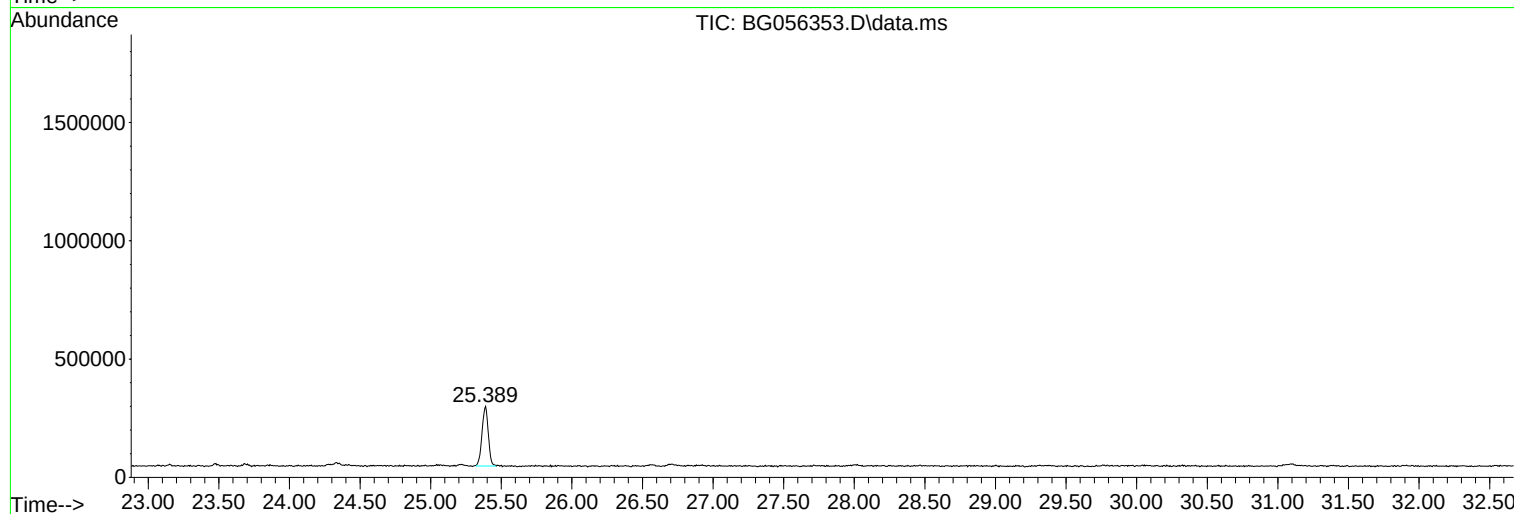
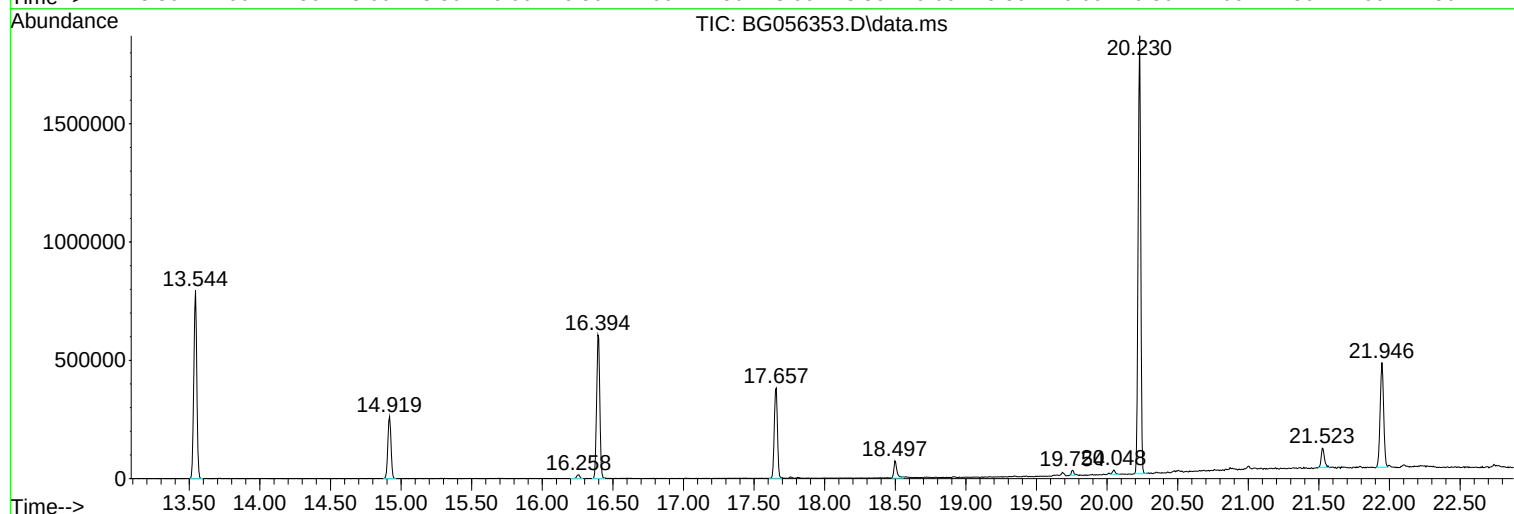
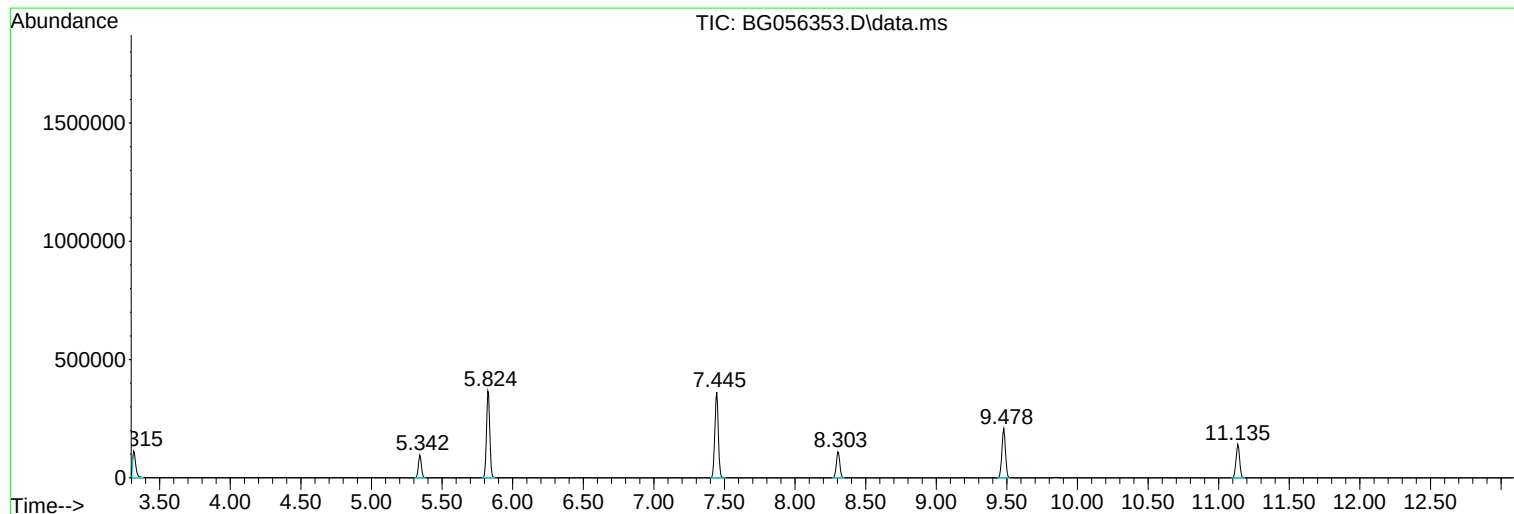
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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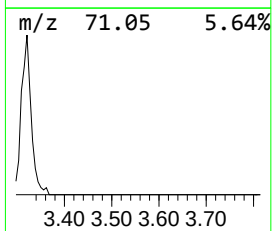
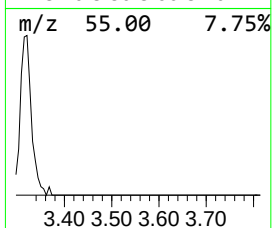
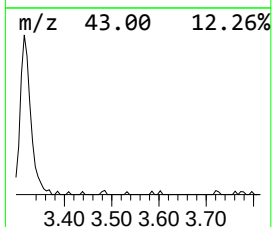
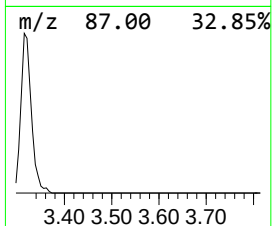
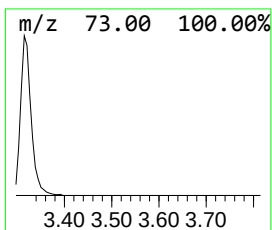
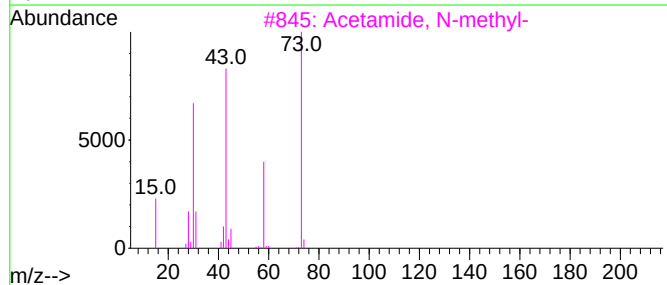
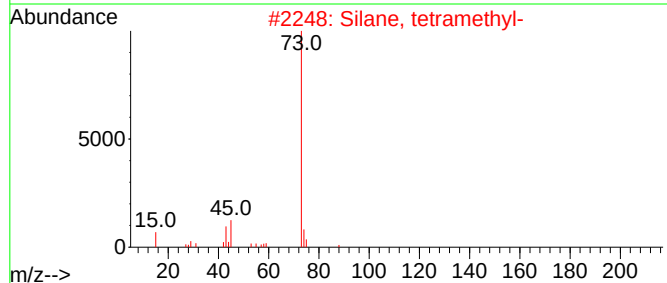
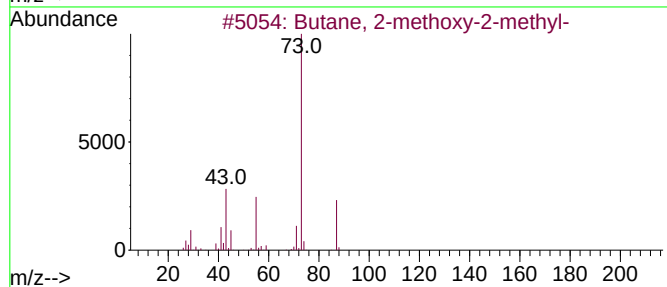
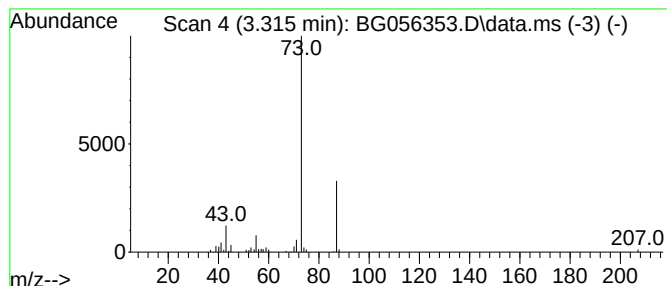
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.315 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.315	14.34 ng	132911	1,4-Dichlorobenzene-d4	8.309

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	33
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
3			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	5
4			2-Propanone, oxime	73	C3H7NO	000127-06-0	4
5			N-Ethylformamide	73	C3H7NO	000627-45-2	4



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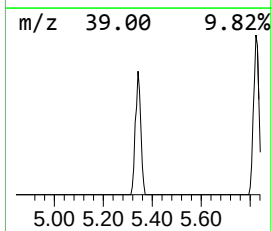
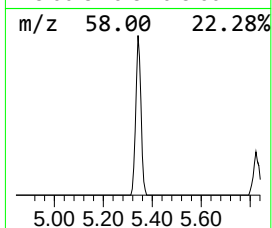
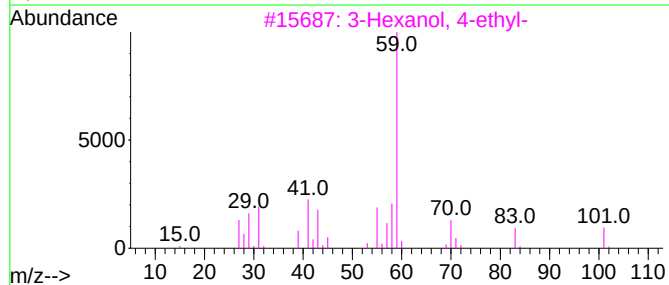
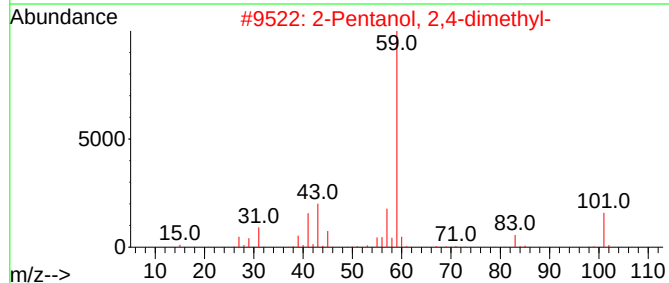
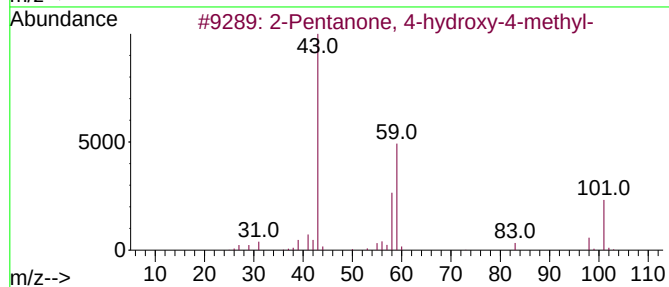
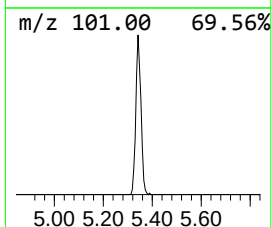
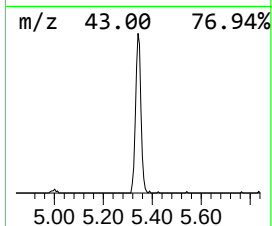
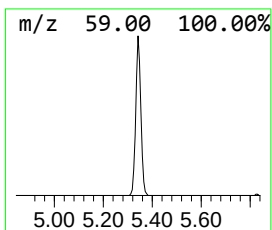
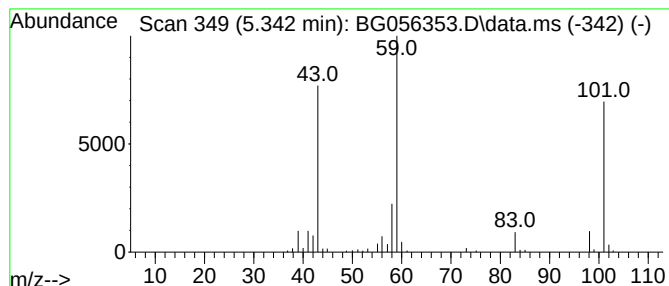
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.342	15.22 ng	141121	1,4-Dichlorobenzene-d4	8.309

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	45
3		3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	38
4		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25



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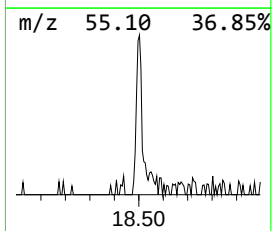
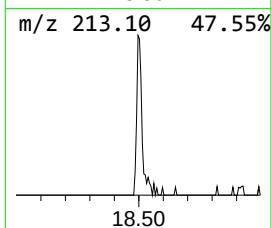
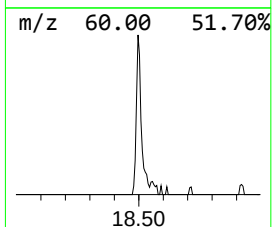
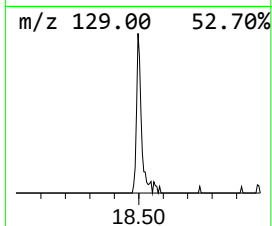
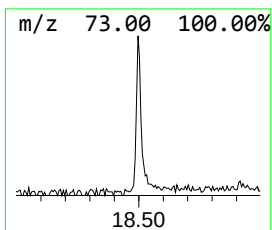
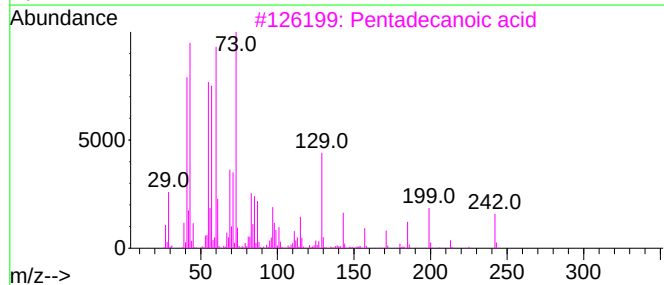
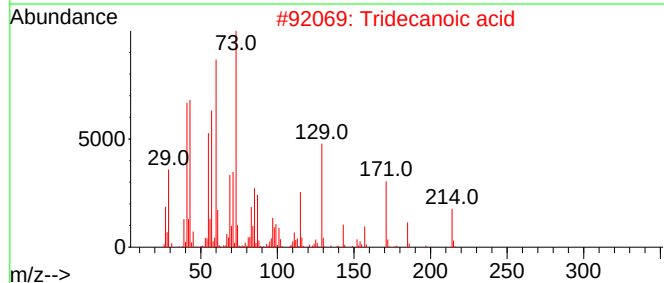
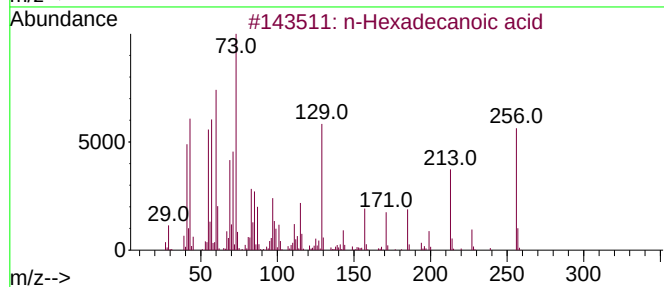
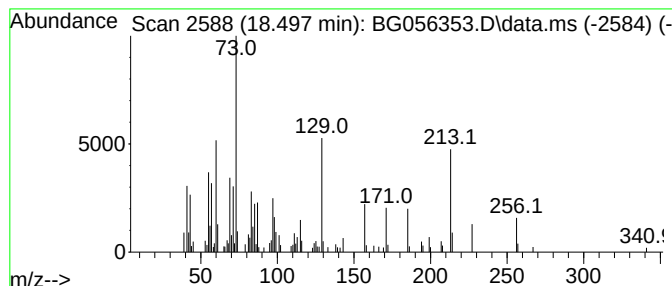
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.497	3.73 ng	110854	Phenanthrene-d10	17.657

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2			Tridecanoic acid	214	C13H26O2	000638-53-9	60
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4			Dodecanoic acid	200	C12H24O2	000143-07-7	52
5			Undecanoic acid	186	C11H22O2	000112-37-8	45



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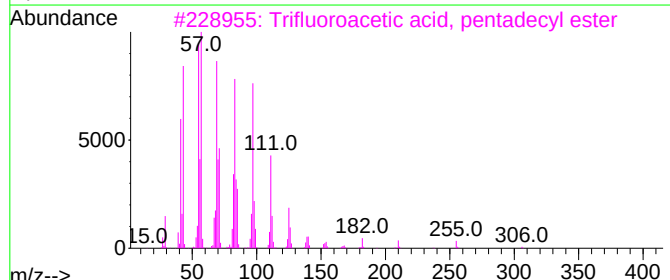
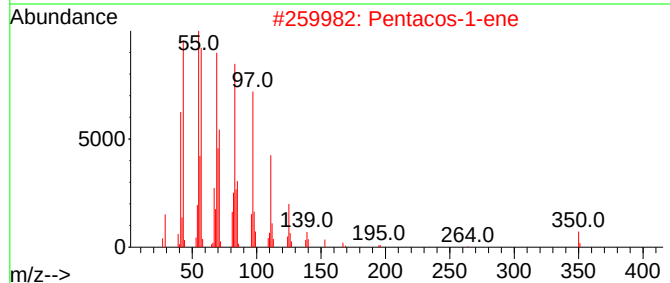
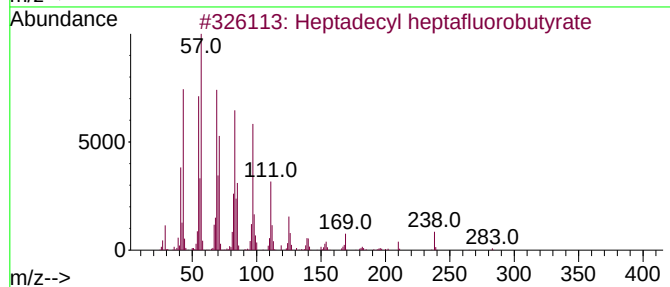
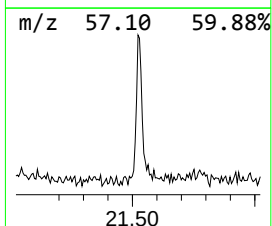
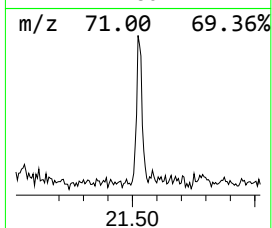
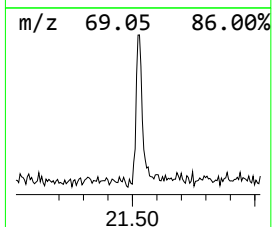
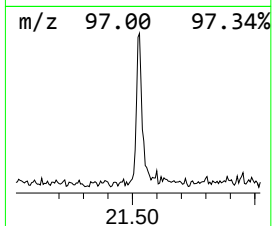
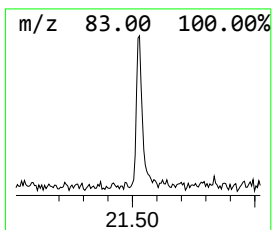
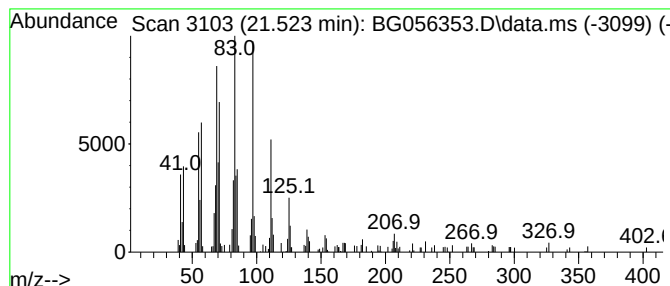
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Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.523	3.48 ng	132364	Chrysene-d12	21.946

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Pentacos-1-ene	350	C25H50	016980-85-1	91
3			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
4			1-Hexacosene	364	C26H52	018835-33-1	91
5			Heptacos-1-ene	378	C27H54	015306-27-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.315	3.315	14.3	ng	132911	1	8.309	185394	20.0
2-Pentanone, 4-...	5.342	15.2	ng	141121	1	8.309	185394	20.0
n-Hexadecanoic ...	18.497	3.7	ng	110854	4	17.657	593755	20.0
Heptadecyl hept...	21.523	3.5	ng	132364	5	21.946	760392	20.0