

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032123\
 Data File : BM039071.D
 Acq On : 21 Mar 2023 16:24
 Operator : CG/JU
 Sample : 02020-21
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP-3

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_M\Methods\8270-BM030823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039071.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.058	295	301	311	rVB	1893925	2520377	27.01%	4.317%
2	5.522	374	380	395	rVB	3748588	5308730	56.90%	9.093%
3	6.640	565	570	576	rBV	80690	126475	1.36%	0.217%
4	7.128	645	653	664	rBV	3653665	5597320	59.99%	9.587%
5	7.969	788	796	803	rBV	1145451	1774479	19.02%	3.039%
6	9.134	986	994	1003	rBV	2133720	3446363	36.94%	5.903%
7	10.781	1264	1274	1281	rBV	1434429	2339725	25.08%	4.007%
8	13.233	1682	1691	1700	rBV	5218256	7255471	77.76%	12.427%
9	14.610	1918	1925	1935	rVB	1887894	2796676	29.97%	4.790%
10	15.963	2145	2155	2161	rBV	80000	122197	1.31%	0.209%
11	16.092	2167	2177	2186	rBV	3542776	4881880	52.32%	8.362%
12	17.351	2385	2391	2403	rBV	2323616	3226500	34.58%	5.526%
13	18.245	2538	2543	2552	rBV	472498	749784	8.04%	1.284%
14	19.515	2755	2759	2770	rBV	254233	474412	5.08%	0.813%
15	19.968	2831	2836	2843	rBV	7511363	9330434	100.00%	15.981%
16	21.233	3045	3051	3061	rBV3	588091	915270	9.81%	1.568%
17	21.527	3096	3101	3114	rBV	2813553	3749866	40.19%	6.423%
18	23.962	3509	3515	3524	rVB2	1869789	3768049	40.38%	6.454%

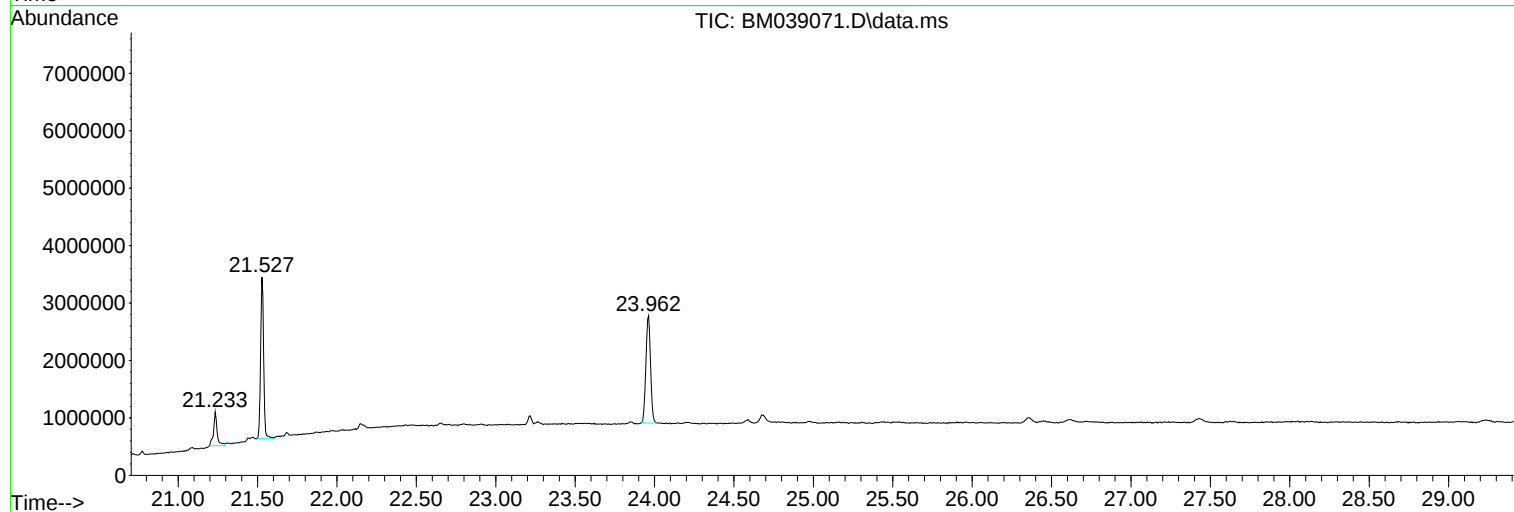
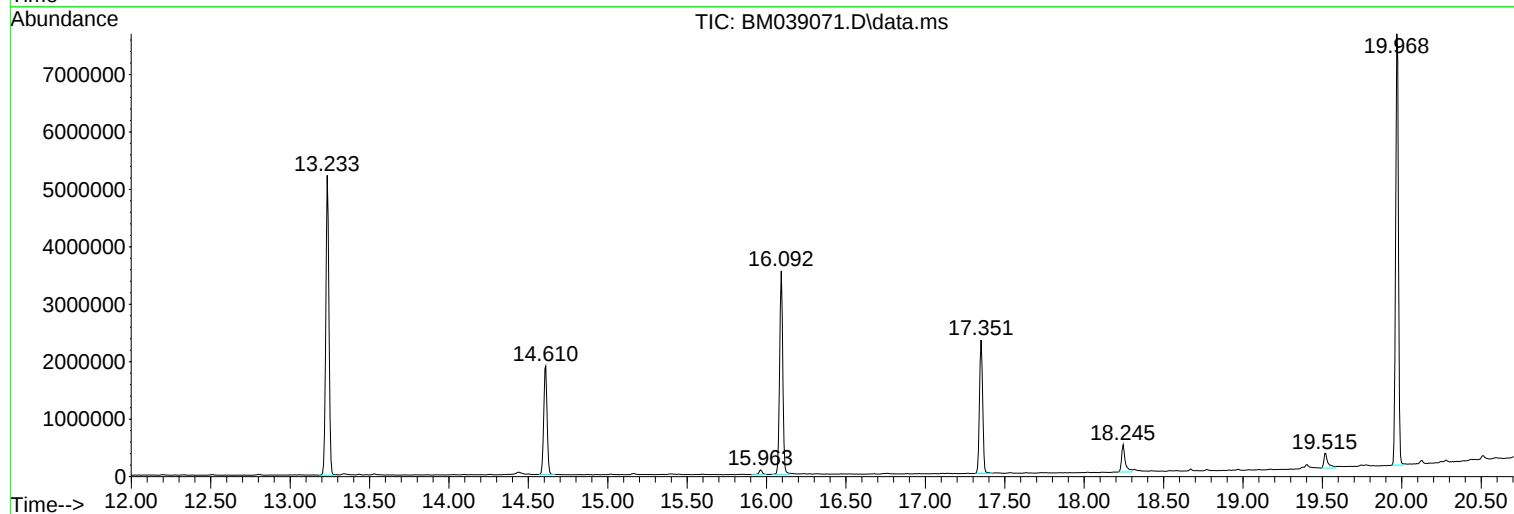
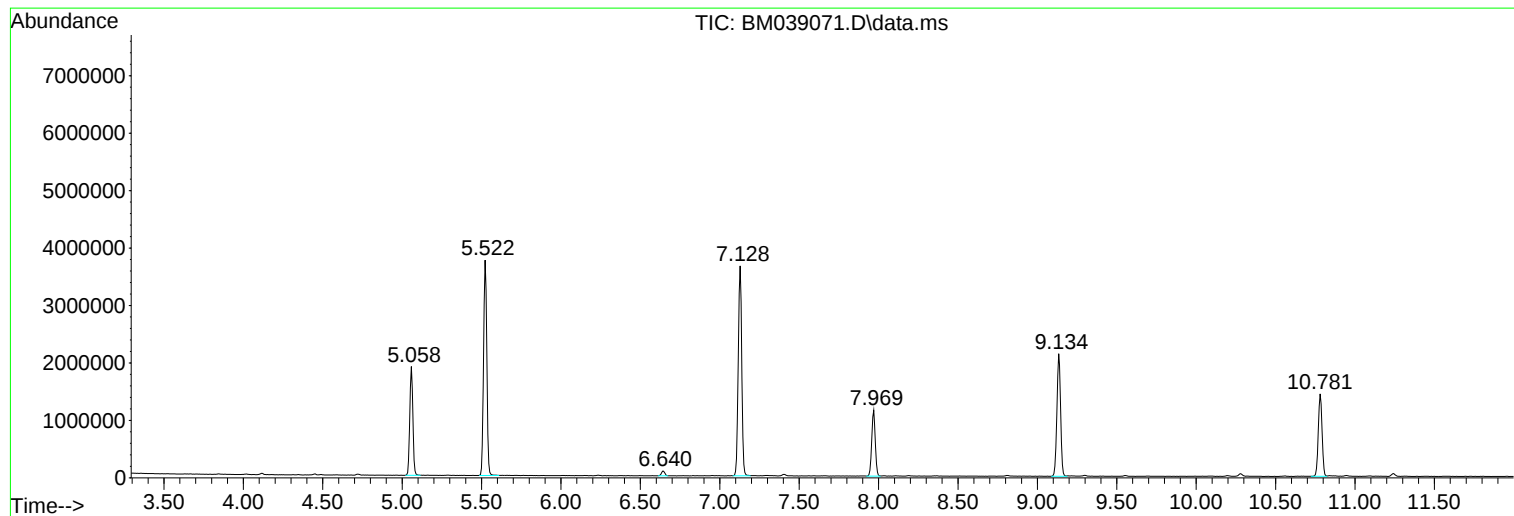
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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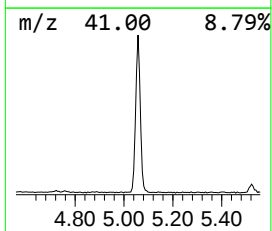
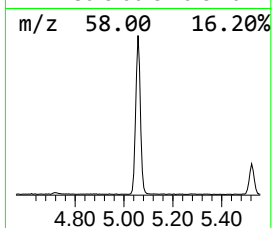
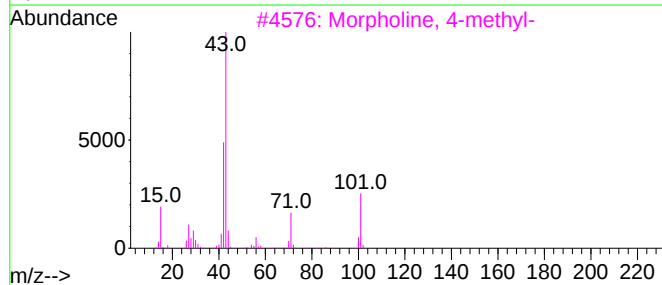
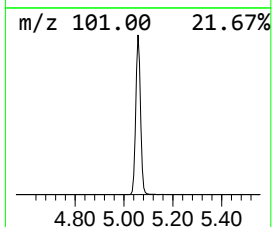
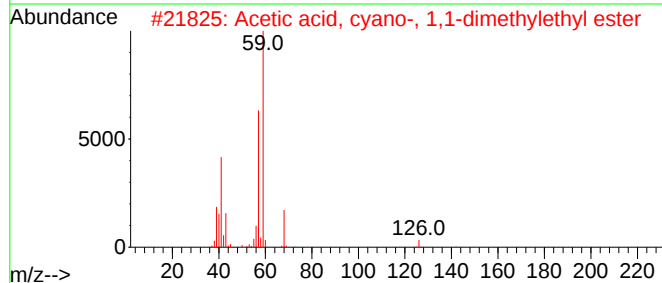
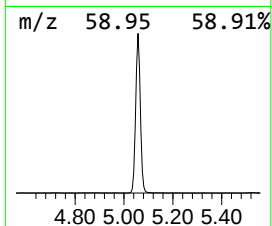
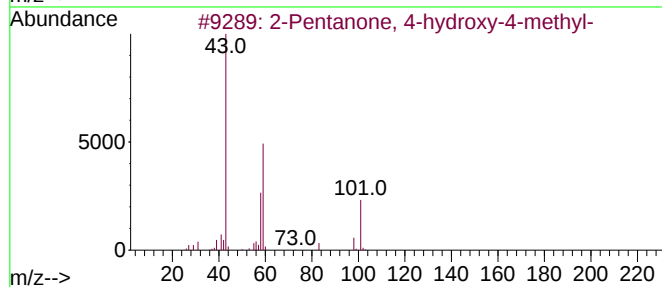
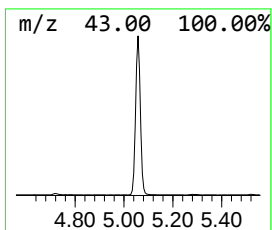
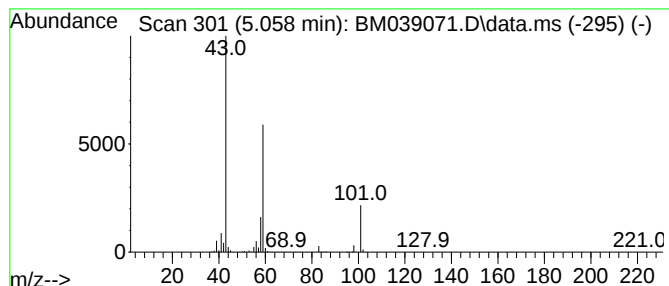
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.058	28.41 ng	2520380	1,4-Dichlorobenzene-d4	7.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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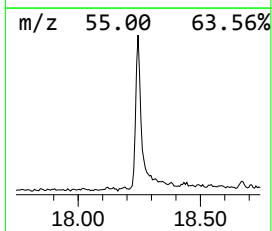
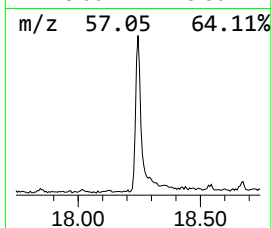
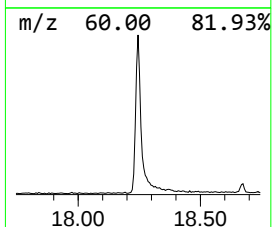
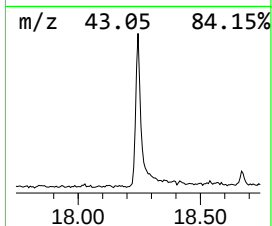
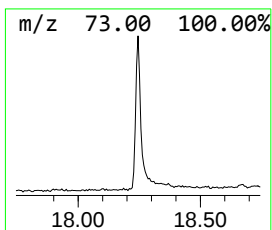
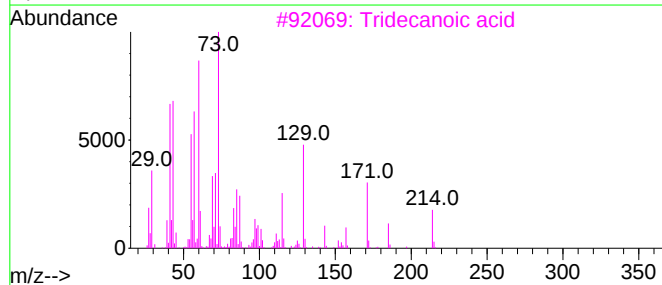
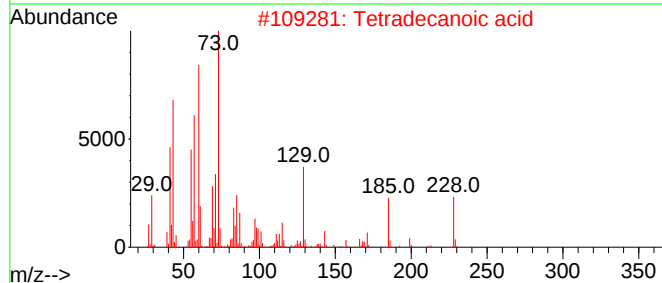
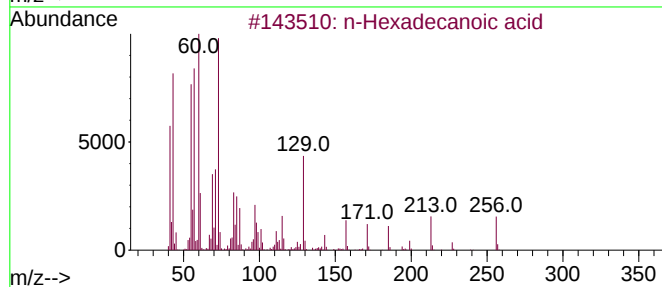
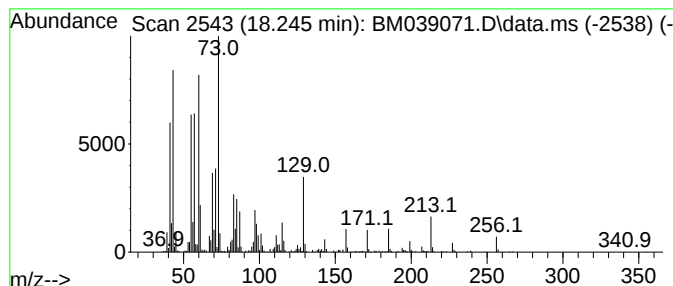
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.245	4.65 ng	749784	Phenanthrene-d10	17.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	92
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	46



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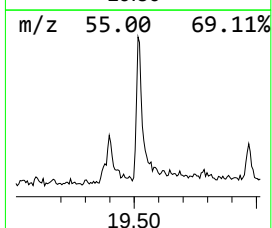
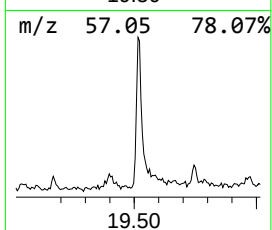
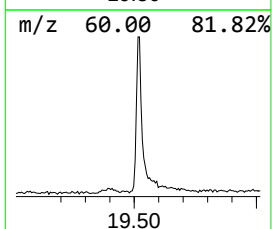
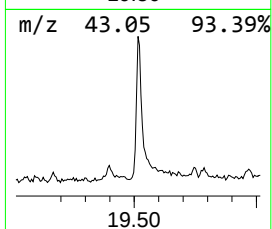
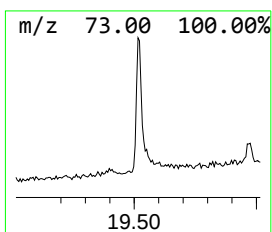
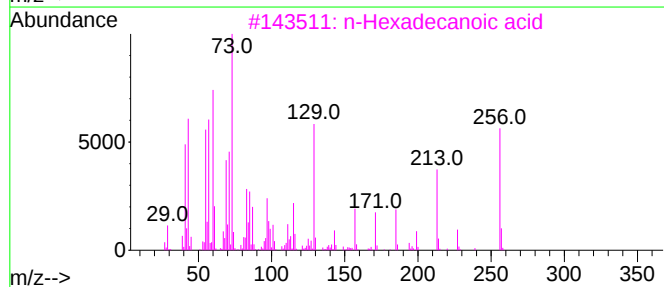
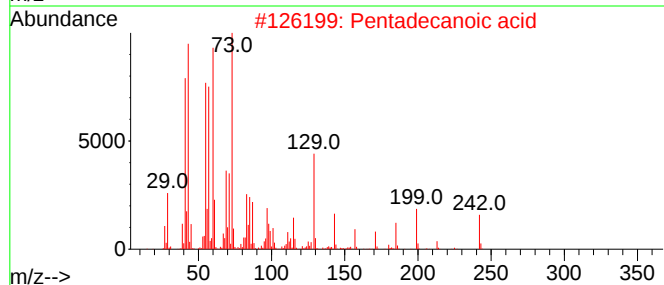
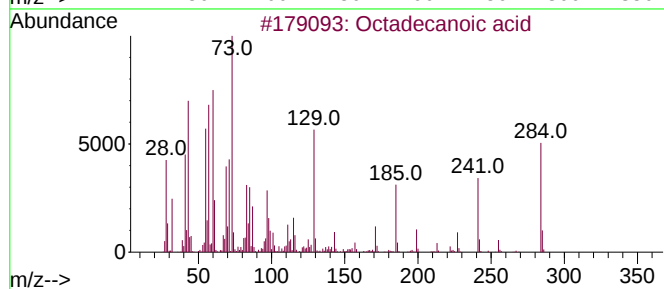
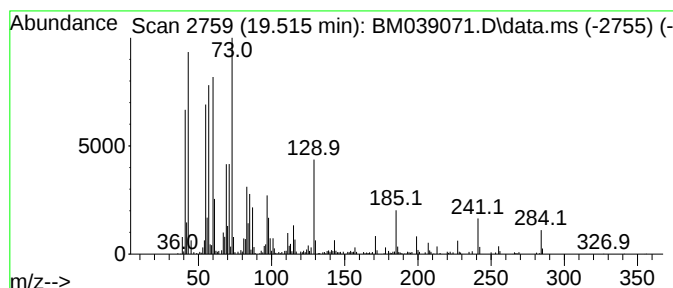
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Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.515	2.53 ng	474412	Chrysene-d12	21.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91



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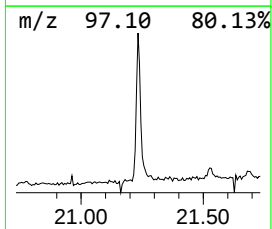
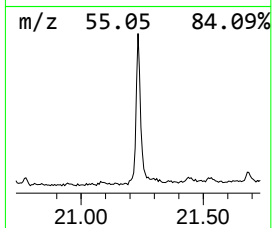
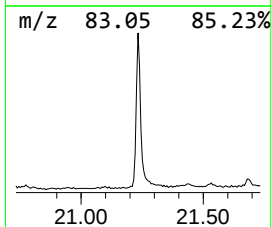
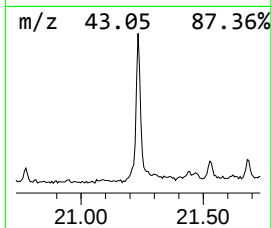
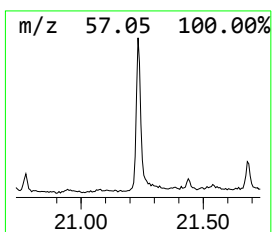
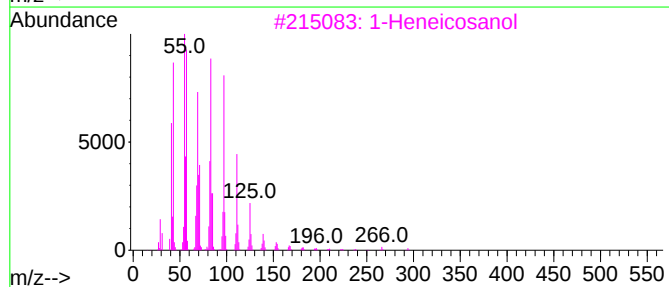
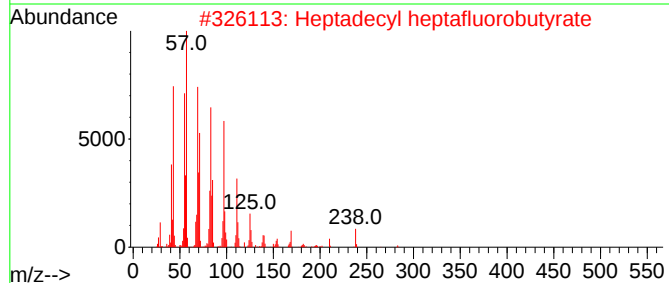
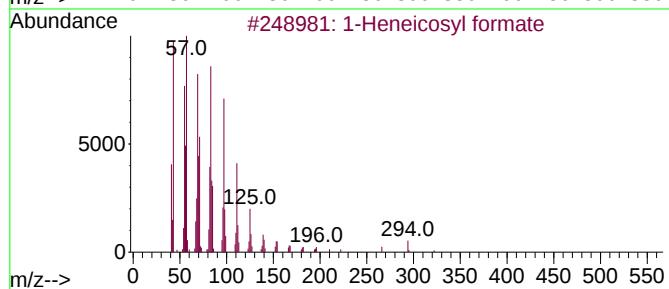
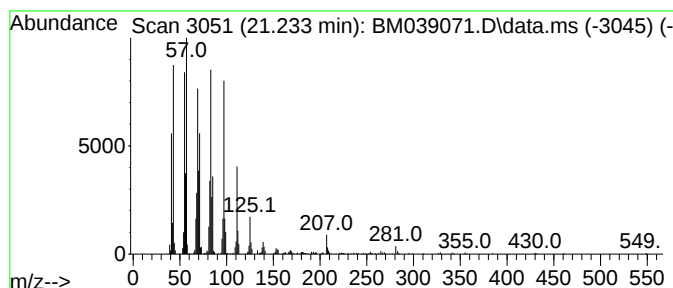
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Peak Number 4 1-Heneicosyl formate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.233	4.88 ng	915270	Chrysene-d12	21.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			1-Heptacosanol	396	C27H56O	002004-39-9	93
5			1-Tetracosene	336	C24H48	010192-32-2	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.058	28.4	ng	2520380	1	7.969	1774480	20.0
n-Hexadecanoic ...	18.245	4.7	ng	749784	4	17.351	3226500	20.0
Octadecanoic acid	19.515	2.5	ng	474412	5	21.527	3749870	20.0
1-Heneicosyl fo...	21.233	4.9	ng	915270	5	21.527	3749870	20.0