

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080322\
 Data File : BM036083.D
 Acq On : 03 Aug 2022 18:16
 Operator : CG/JU
 Sample : N3998-05
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-5

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-BM080122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036083.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.428	391	398	410	rBV	3321430	4861793	36.49%	7.565%
2	7.034	664	671	689	rVB	3423894	5341055	40.08%	8.311%
3	7.863	806	812	819	rBV	714032	1117821	8.39%	1.739%
4	9.034	1003	1011	1020	rBV	2026591	3286447	24.66%	5.114%
5	10.669	1282	1289	1302	rBV	1103261	1801297	13.52%	2.803%
6	13.133	1700	1708	1720	rBV	5623443	8104950	60.83%	12.612%
7	13.727	1802	1809	1817	rBV	460630	614505	4.61%	0.956%
8	14.504	1934	1941	1957	rVB	1856366	2634417	19.77%	4.099%
9	15.992	2187	2194	2202	rBV	5188793	7336047	55.06%	11.416%
10	17.245	2400	2407	2413	rBV	2452436	3358108	25.20%	5.226%
11	18.145	2554	2560	2570	rBV	843096	1251056	9.39%	1.947%
12	19.303	2749	2757	2761	rBV	106602	210764	1.58%	0.328%
13	19.421	2773	2777	2789	rBV	309881	468768	3.52%	0.729%
14	19.868	2848	2853	2861	rBV	11169505	13324833	100.00%	20.735%
15	21.145	3065	3070	3080	rBV	1008322	1485367	11.15%	2.311%
16	21.427	3113	3118	3123	rBV	3508479	4324521	32.45%	6.729%
17	23.791	3513	3520	3530	rVB2	2413910	4741510	35.58%	7.378%

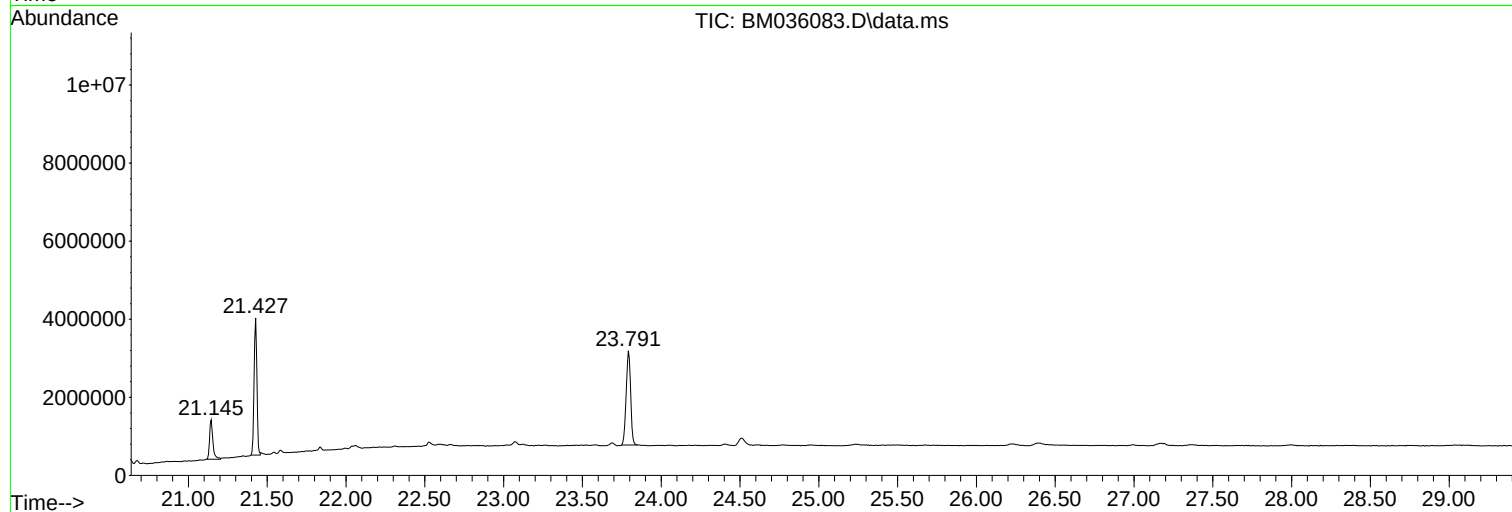
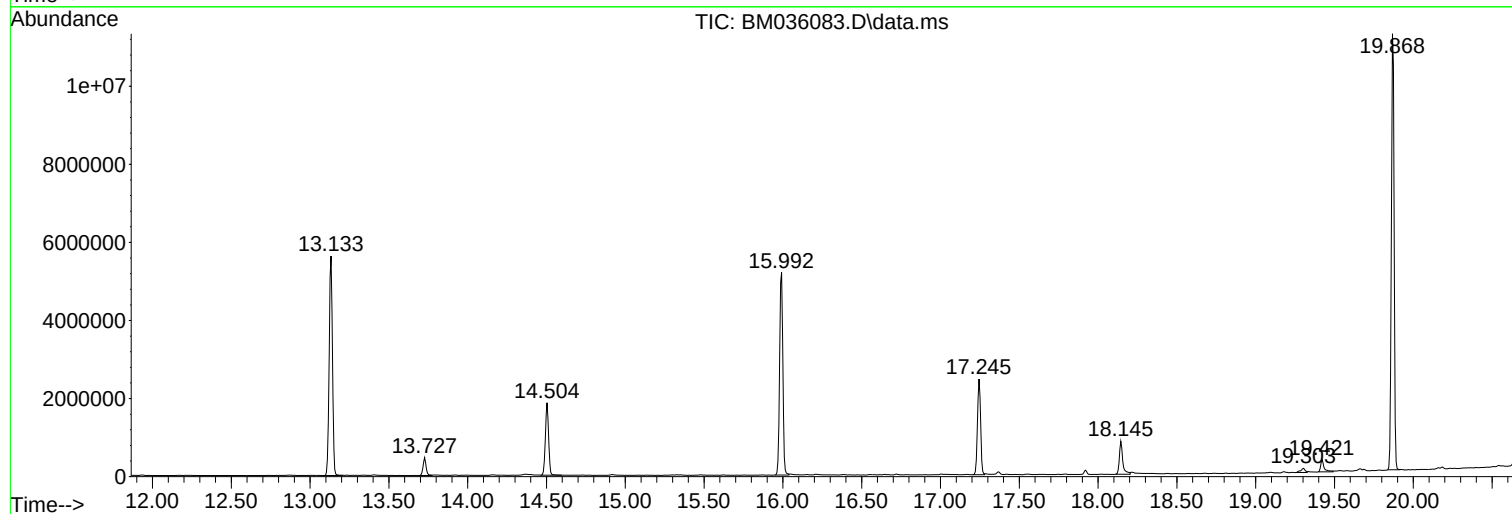
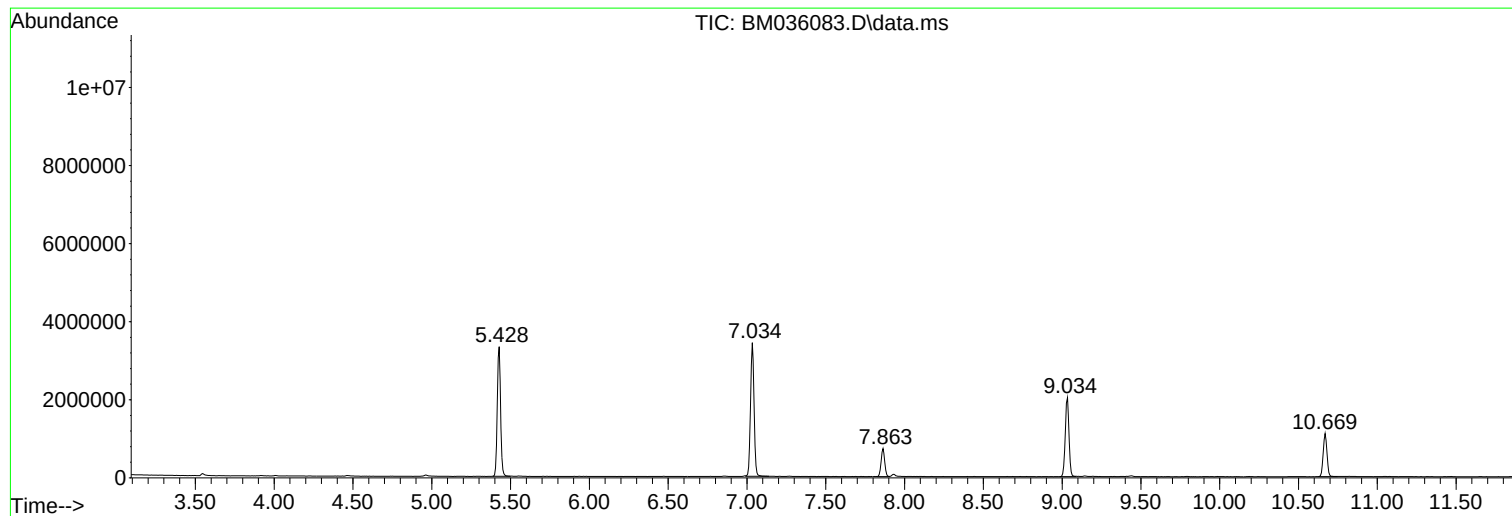
Sum of corrected areas: 64263259

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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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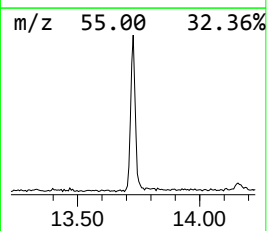
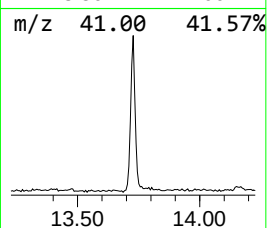
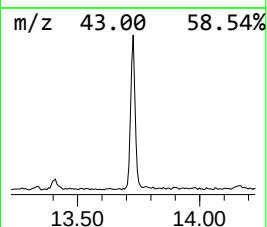
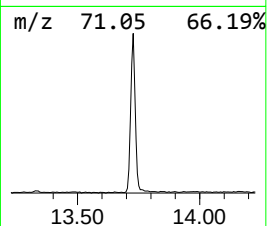
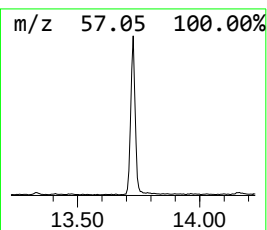
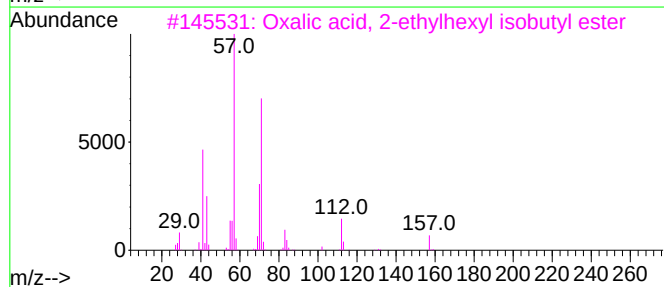
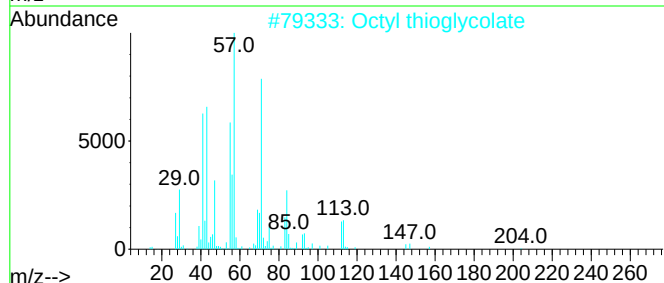
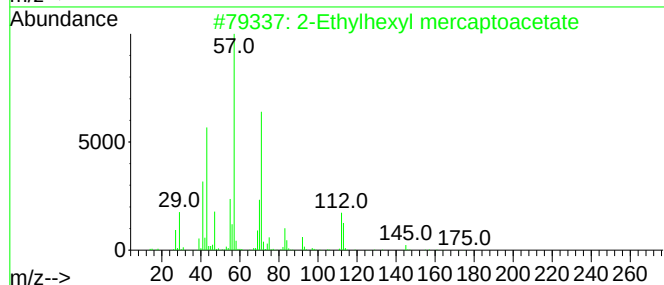
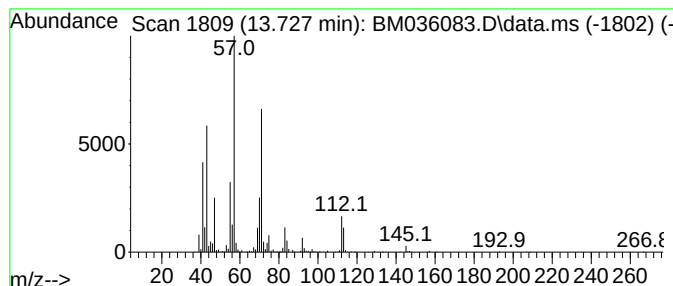
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Ethylhexyl mercaptoacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	4.67 ng	614505	Acenaphthene-d10	14.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	87
2			Octyl thioglycolate	204	C10H20O2S	007664-80-4	64
3			Oxalic acid, 2-ethylhexyl isobut...	258	C14H26O4	1010309-38-5	64
4			Oxalic acid, 2-ethylhexyl octyl ...	314	C18H34O4	1000309-39-1	59
5			Oxalic acid, bis(2-ethylhexyl) e...	314	C18H34O4	1000309-39-0	58



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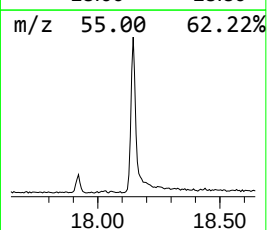
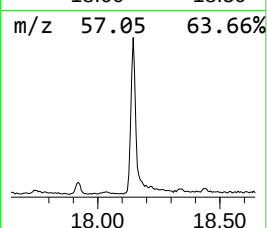
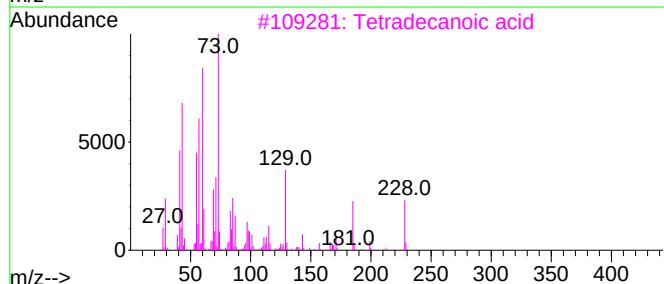
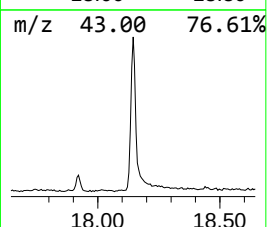
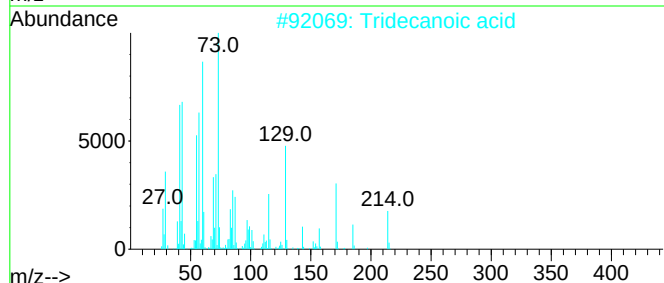
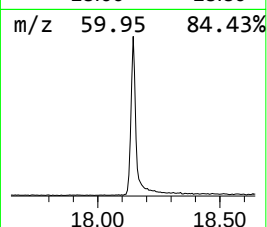
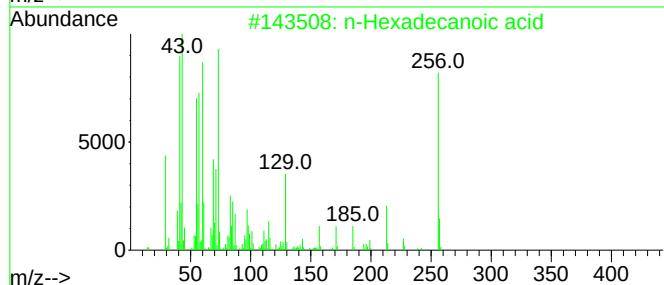
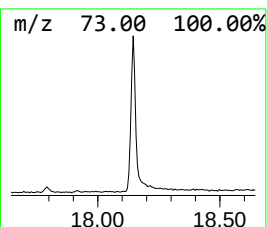
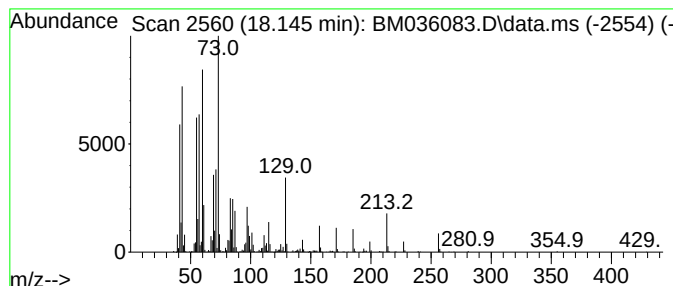
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	7.45 ng	1251060	Phenanthrene-d10	17.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5		Octadecanoic acid	284	C18H36O2	000057-11-4	91



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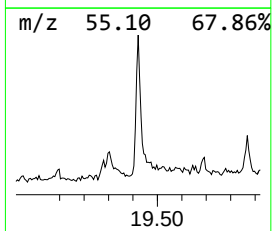
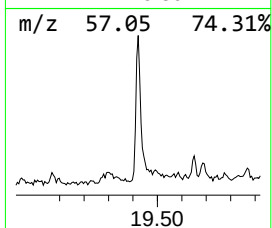
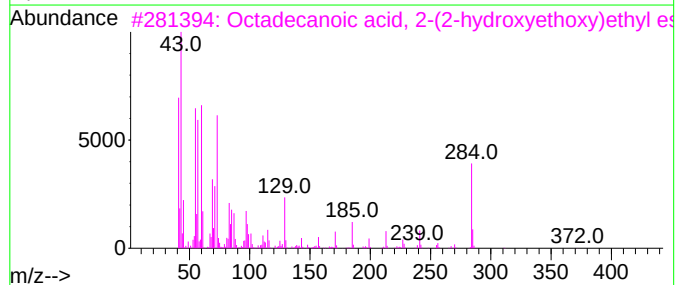
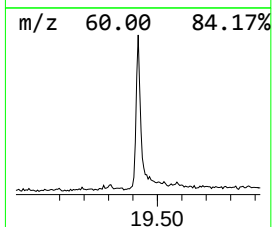
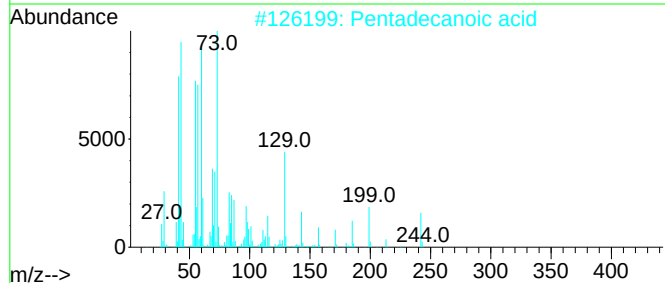
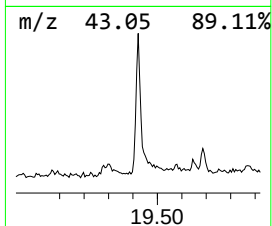
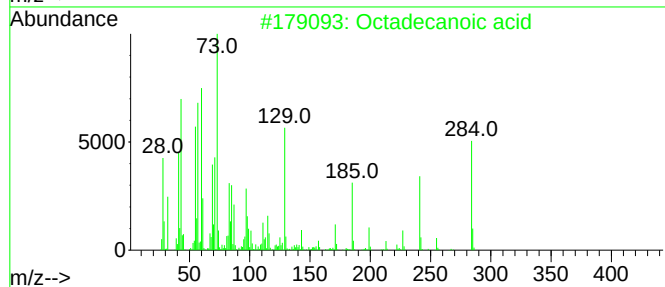
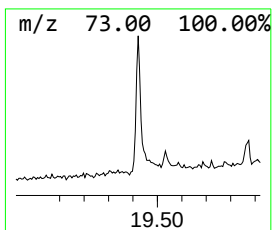
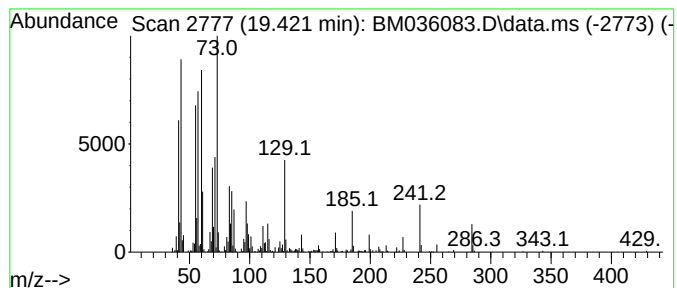
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Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.421	2.17 ng	468768	Chrysene-d12	21.427

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			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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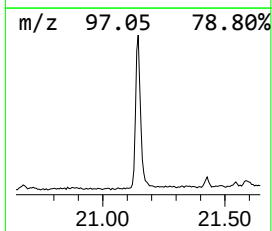
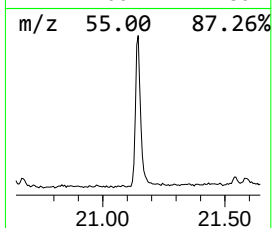
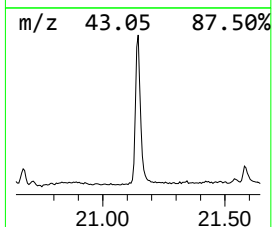
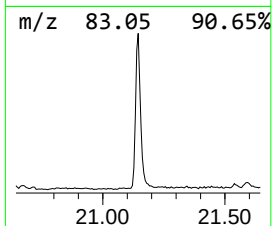
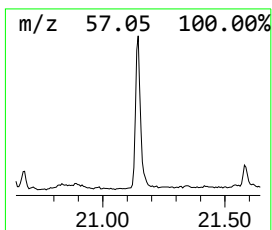
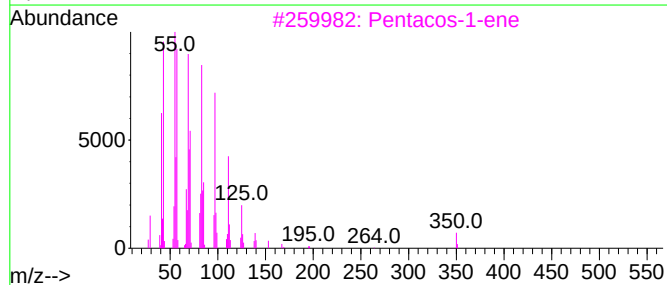
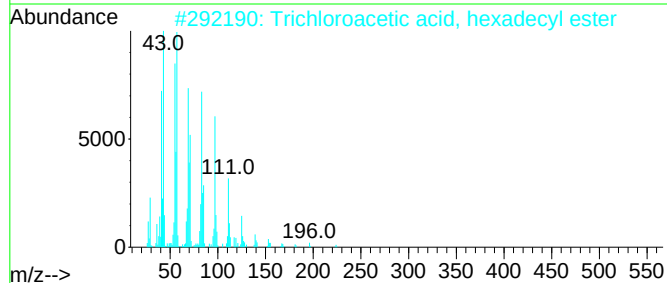
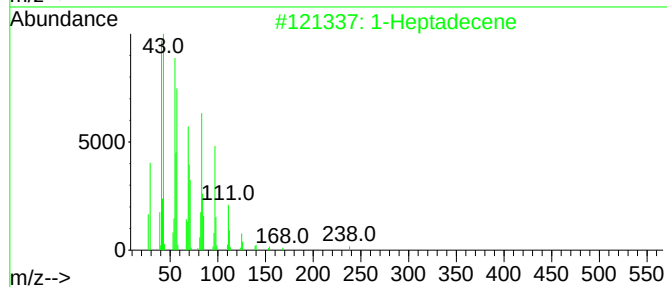
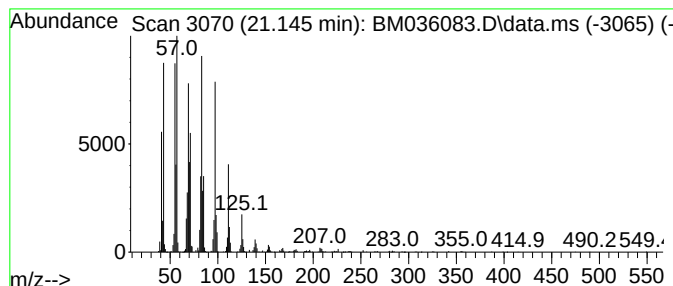
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Peak Number 4 1-Heptadecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.145	6.87 ng	1485370	Chrysene-d12	21.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptadecene	238	C17H34	006765-39-5	95
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			Pentacos-1-ene	350	C25H50	016980-85-1	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Ethylhexyl me...	13.727	4.7	ng	614505	3	14.504	2634420	20.0
n-Hexadecanoic ...	18.145	7.5	ng	1251060	4	17.245	3358110	20.0
Octadecanoic acid	19.421	2.2	ng	468768	5	21.427	4324520	20.0
1-Heptadecene	21.145	6.9	ng	1485370	5	21.427	4324520	20.0