

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092021\
 Data File : BP007050.D
 Acq On : 20 Sep 2021 13:57
 Operator : CG/JU
 Sample : M3687-28
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 A004015

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_P\Methods\8270E-BP091621.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007050.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	323	329	341	rVB	633919	913419	8.18%	1.520%
2	5.481	400	407	417	rBV	3550196	5160151	46.23%	8.585%
3	7.075	670	678	691	rBV	3314497	5277355	47.28%	8.780%
4	7.910	810	820	828	rBV	1008289	1548776	13.88%	2.577%
5	9.069	1009	1017	1030	rBV	2084287	3459731	31.00%	5.756%
6	10.487	1249	1258	1270	rBV	320764	596965	5.35%	0.993%
7	10.710	1289	1296	1305	rBV	1230729	2060083	18.46%	3.428%
8	13.163	1706	1713	1726	rBV	5205271	7683103	68.83%	12.783%
9	14.534	1940	1946	1955	rVB	1869393	2754481	24.68%	4.583%
10	16.022	2193	2199	2221	rVB	4383465	6134787	54.96%	10.207%
11	17.286	2407	2414	2426	rBV	2211600	3304512	29.61%	5.498%
12	18.169	2559	2564	2574	rBV	483735	777268	6.96%	1.293%
13	19.398	2769	2773	2784	rBV2	192071	358098	3.21%	0.596%
14	19.839	2843	2848	2854	rBV	9289043	11161698	100.00%	18.571%
15	21.074	3054	3058	3067	rBV2	462906	675000	6.05%	1.123%
16	21.363	3102	3107	3113	rBV	2967161	3968572	35.56%	6.603%
17	23.786	3512	3519	3530	rVB2	2083521	4269594	38.25%	7.104%

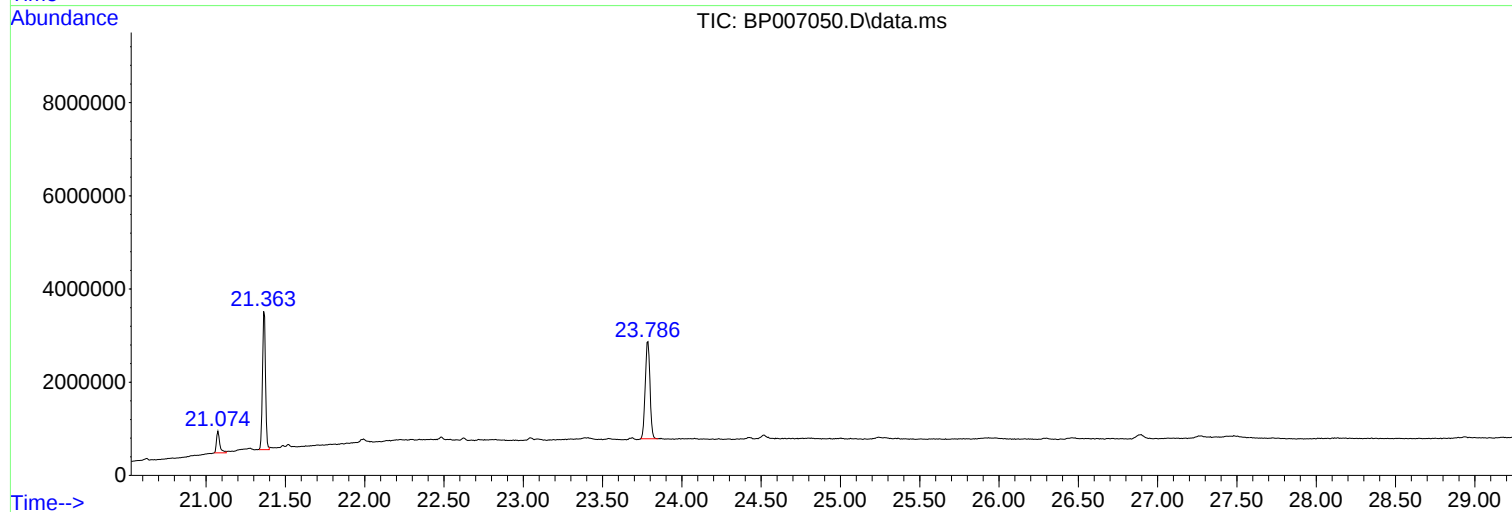
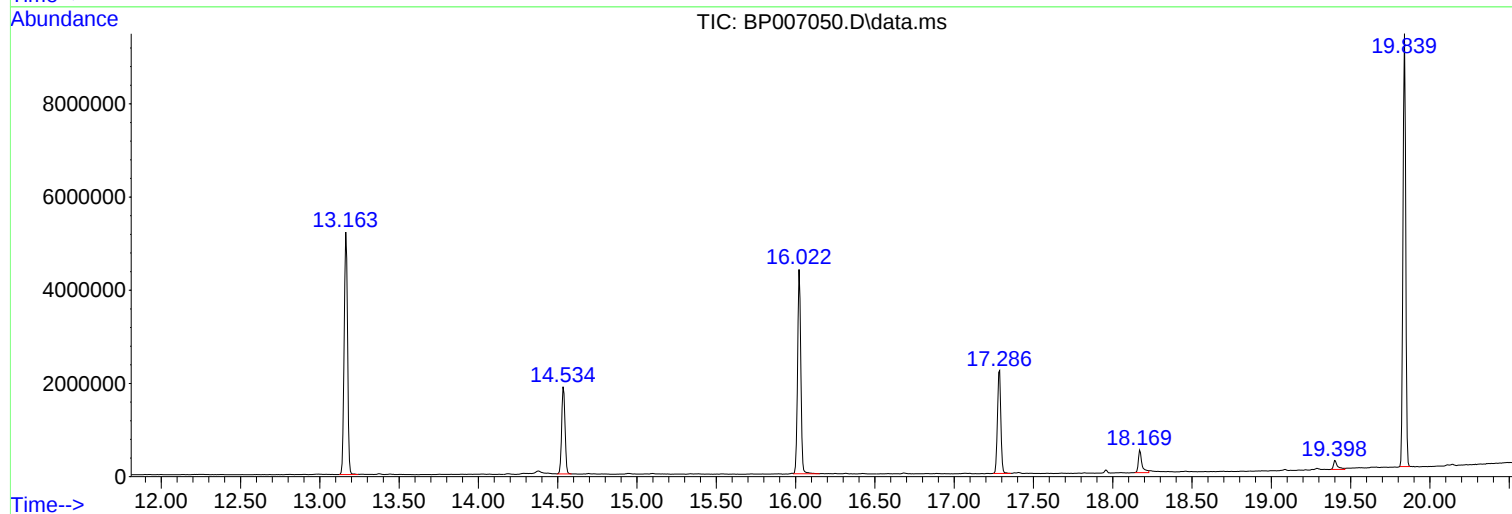
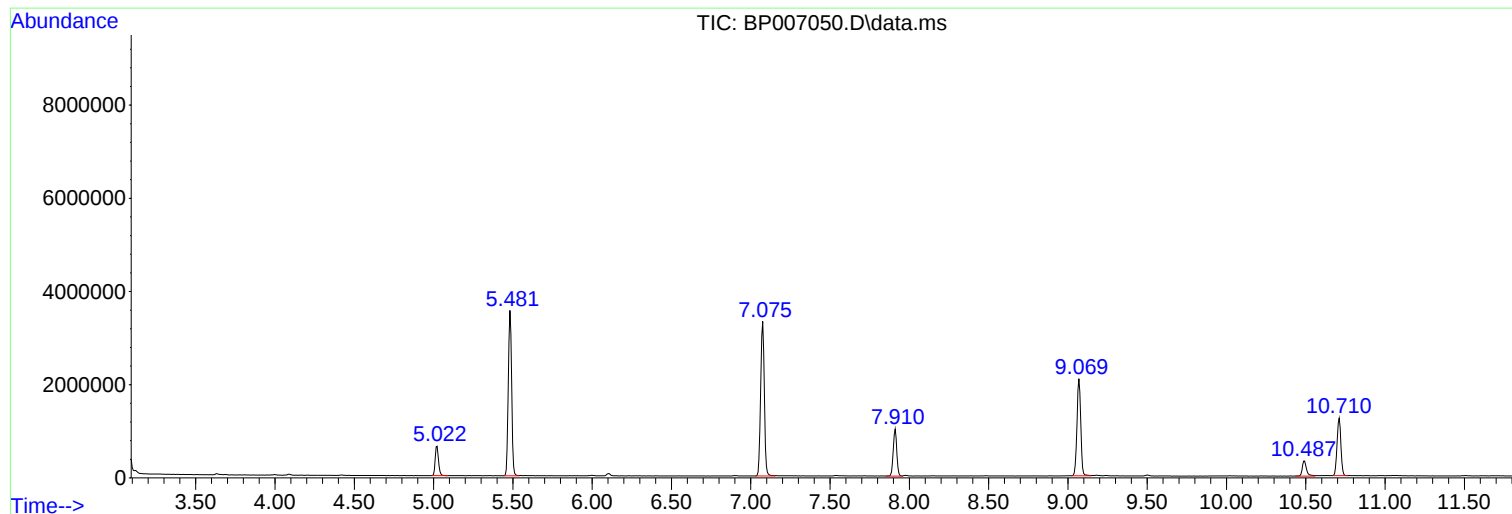
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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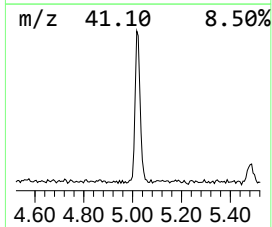
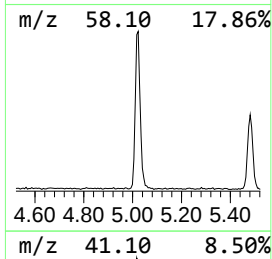
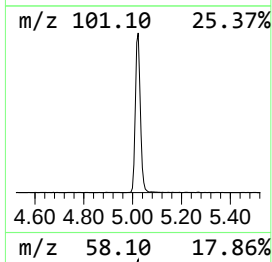
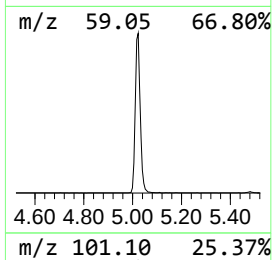
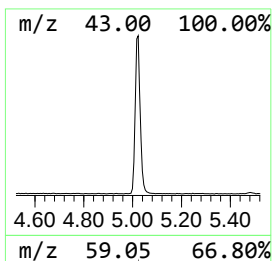
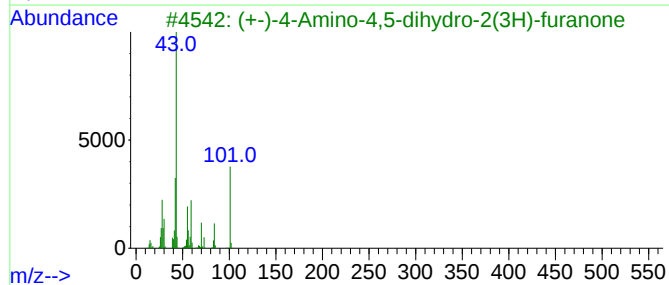
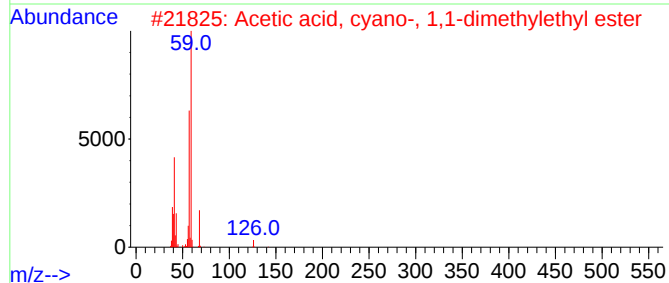
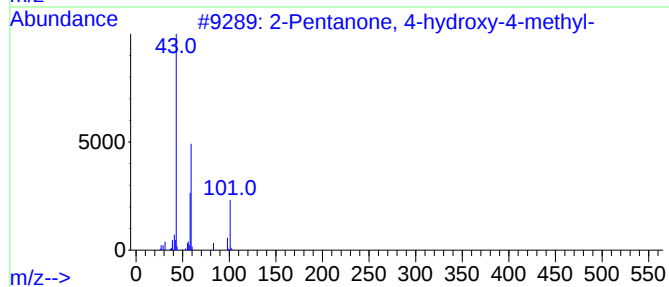
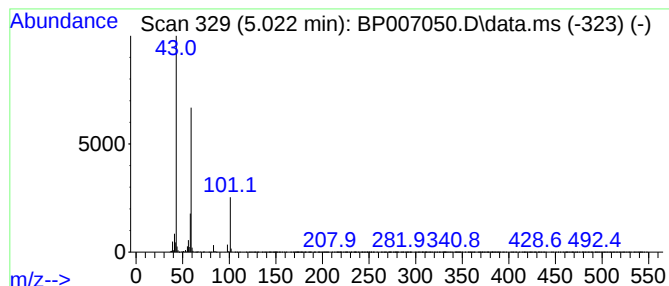
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	11.80 ng	913419	1,4-Dichlorobenzene-d4	7.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		
4	Acetone	58	C3H6O	000067-64-1	9		
5	Guanidine	59	CH5N3	000113-00-8	9		



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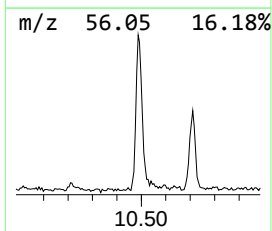
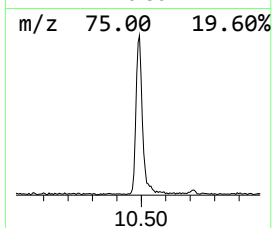
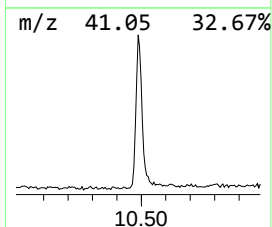
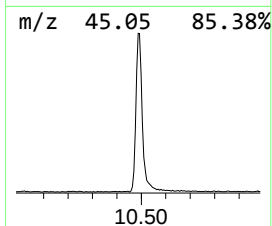
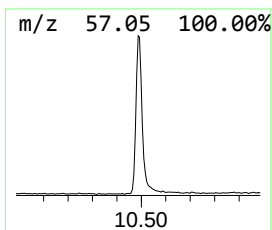
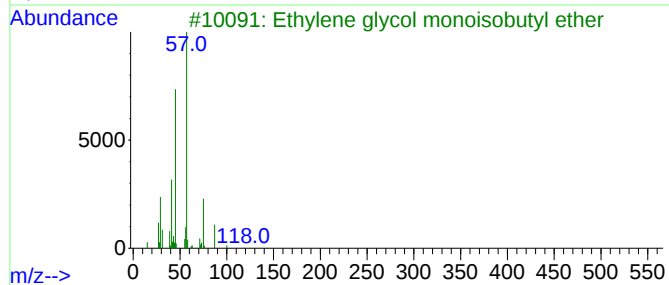
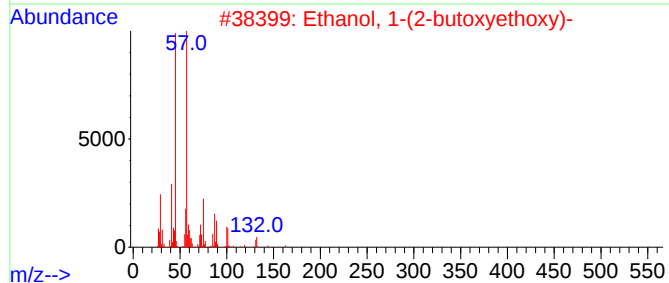
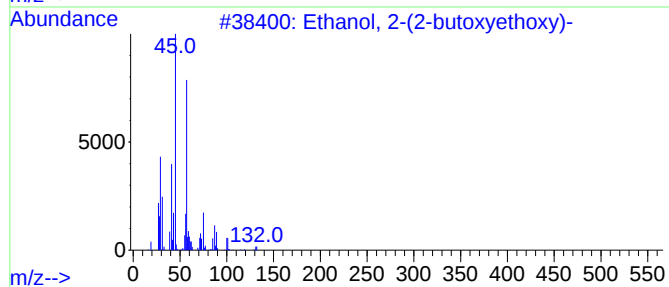
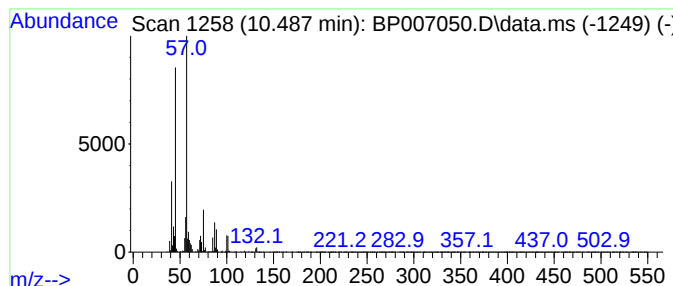
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.487	5.80 ng	596965	Naphthalene-d8	10.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5			2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	38



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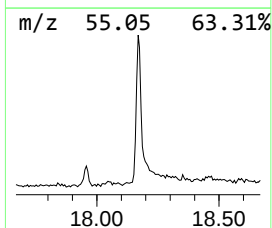
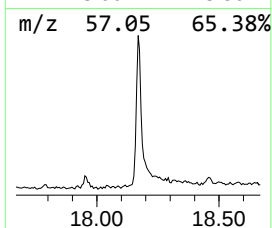
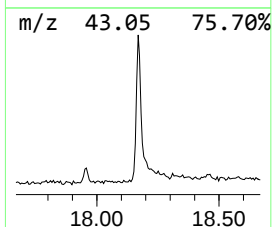
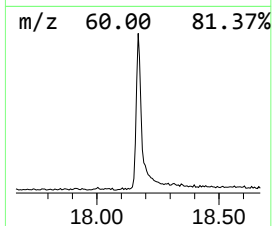
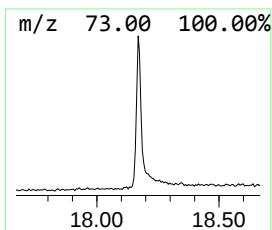
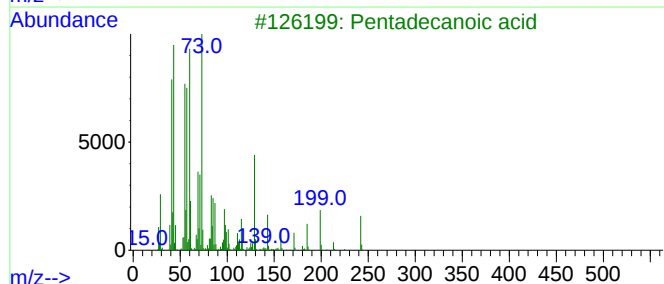
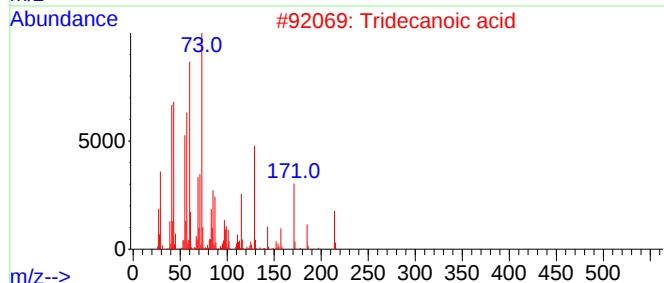
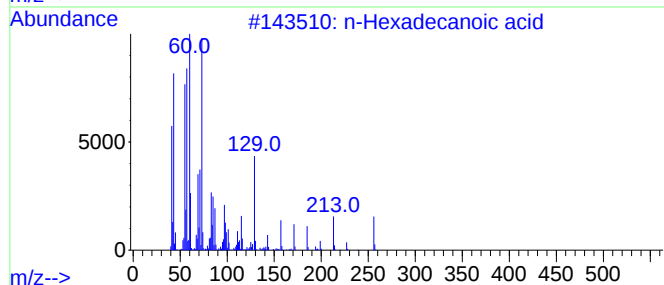
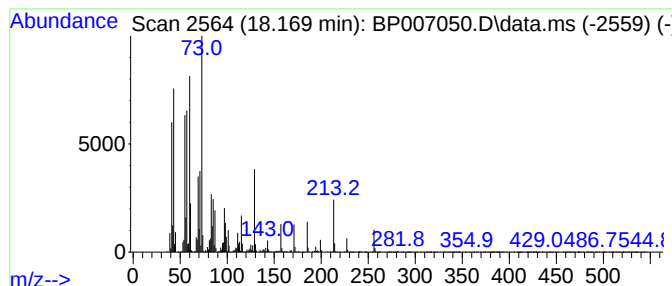
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.169	4.70 ng	777268	Phenanthrene-d10	17.286

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			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	76



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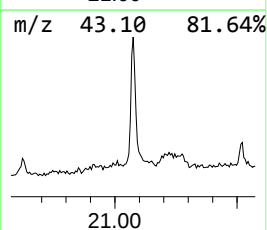
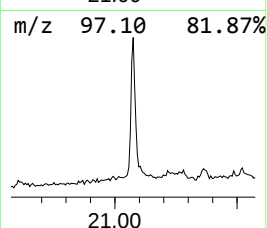
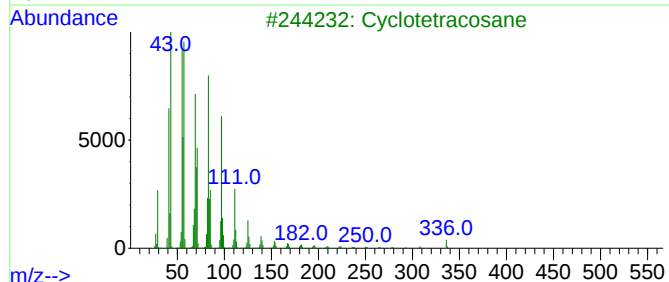
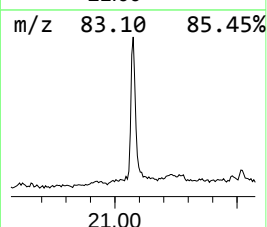
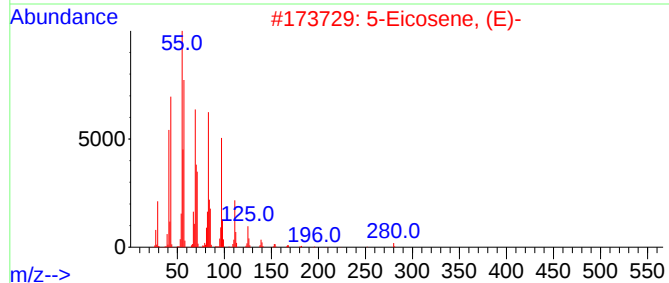
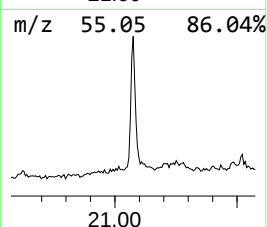
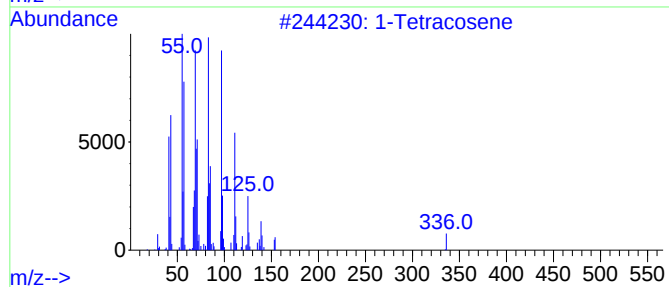
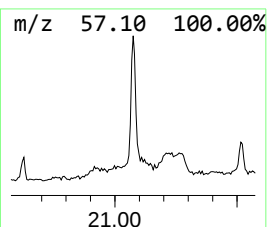
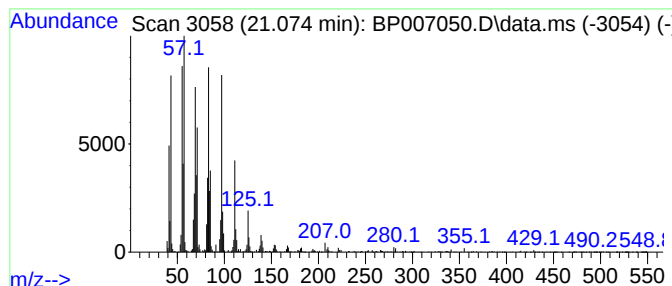
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Peak Number 4 1-Tetracosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	3.40 ng	675000	Chrysene-d12	21.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetracosene	336	C24H48	010192-32-2	99
2			5-Eicosene, (E)-	280	C20H40	074685-30-6	98
3			Cyclotetracosane	336	C24H48	000297-03-0	95
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5			Behenic alcohol	326	C22H46O	000661-19-8	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.022	11.8	ng	913419	1	7.910	1548780	20.0
Ethanol, 2-(2-b...	10.487	5.8	ng	596965	2	10.710	2060080	20.0
n-Hexadecanoic ...	18.169	4.7	ng	777268	4	17.286	3304510	20.0
1-Tetracosene	21.074	3.4	ng	675000	5	21.363	3968570	20.0