

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031221\
 Data File : BM029119.D
 Acq On : 12 Mar 2021 19:59
 Operator : CG/JU
 Sample : M1649-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP-1-1

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-BM022321.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029119.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.199	370	376	394	rBB	208434	299050	61.34%	12.014%
2	6.822	645	652	671	rBB	192704	310365	63.66%	12.468%
3	7.616	783	787	795	rBB	30127	45822	9.40%	1.841%
4	8.792	981	987	999	rBB	119196	191802	39.34%	7.705%
5	10.410	1256	1262	1269	rBV	37850	60634	12.44%	2.436%
6	12.904	1679	1686	1694	rBB	265825	380841	78.11%	15.300%
7	14.292	1916	1922	1927	rBB	52114	72567	14.88%	2.915%
8	15.792	2172	2177	2185	rBB	208325	271116	55.61%	10.892%
9	17.039	2384	2389	2395	rBV	57799	77972	15.99%	3.132%
10	17.939	2537	2542	2551	rBV2	16670	26368	5.41%	1.059%
11	18.674	2662	2667	2673	rBV	14476	17040	3.49%	0.685%
12	19.221	2754	2760	2767	rBV	22862	33275	6.82%	1.337%
13	19.668	2831	2836	2841	rBV	425105	487561	100.00%	19.587%
14	20.945	3048	3053	3059	rBV2	20616	34536	7.08%	1.387%
15	21.221	3095	3100	3104	rBV	75023	87811	18.01%	3.528%
16	23.356	3457	3463	3470	rBV2	51707	92440	18.96%	3.714%

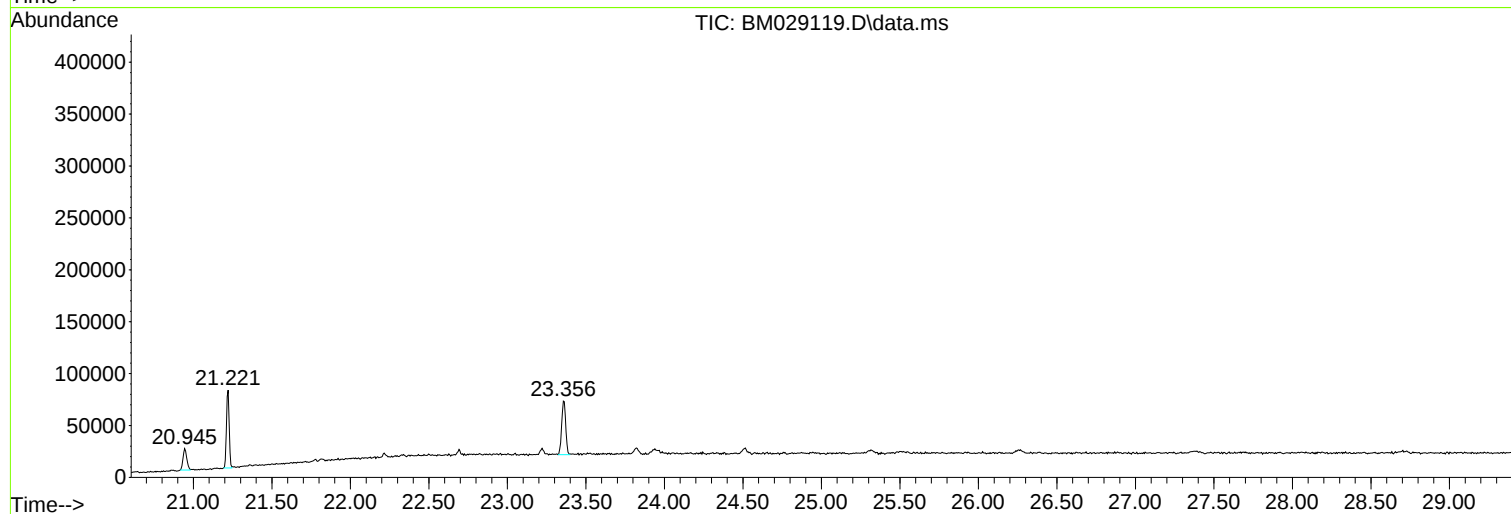
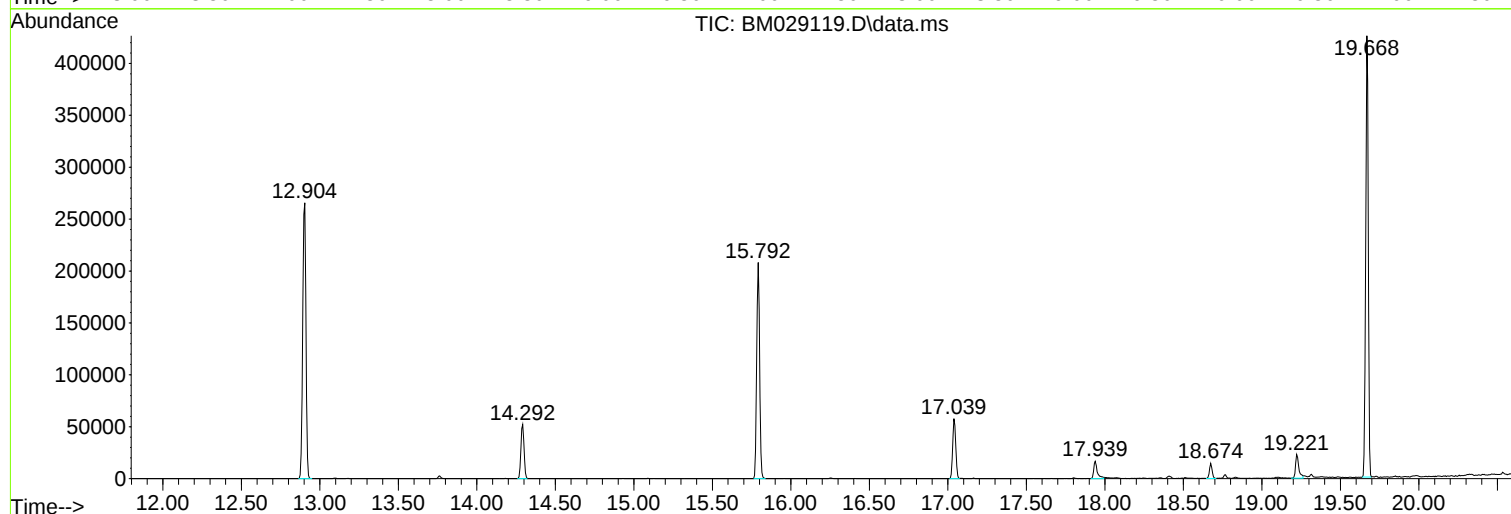
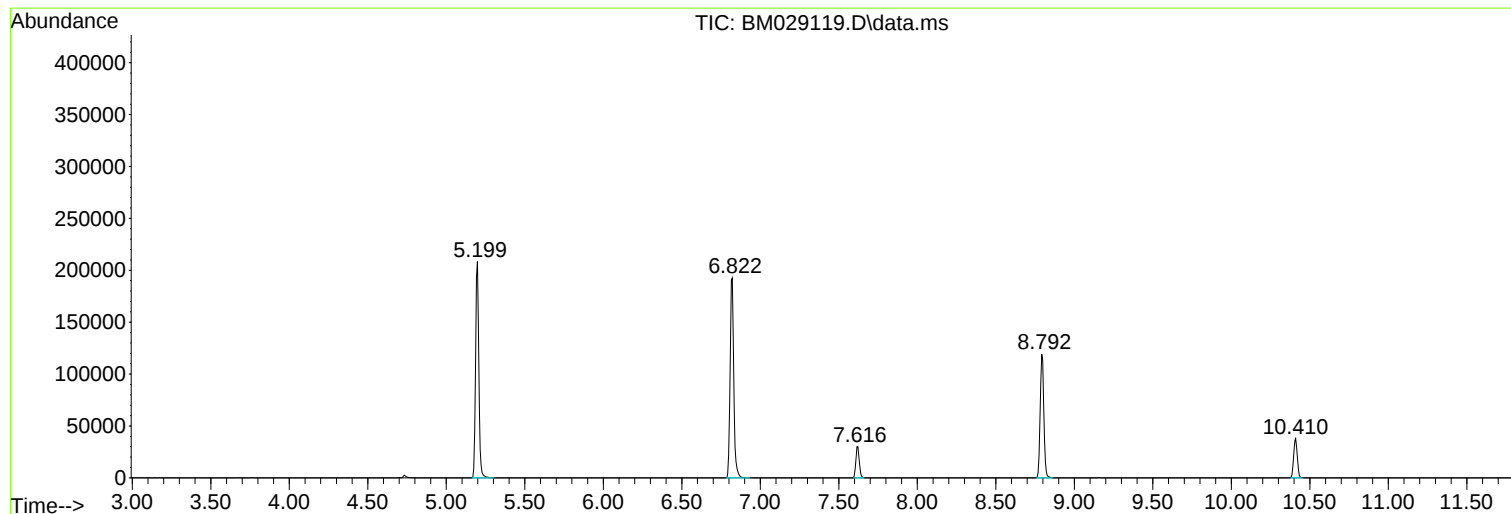
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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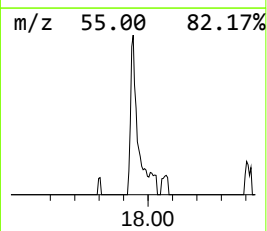
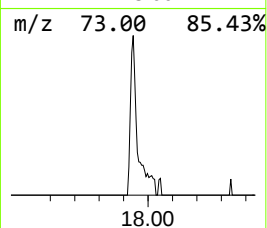
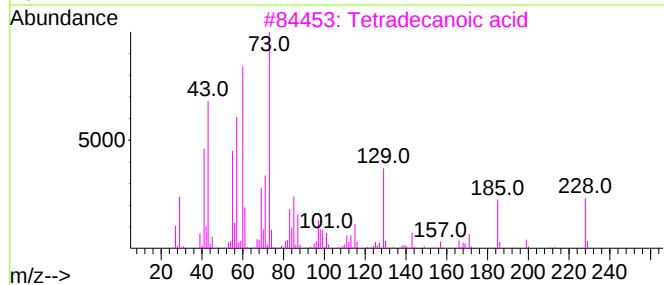
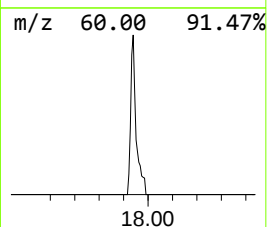
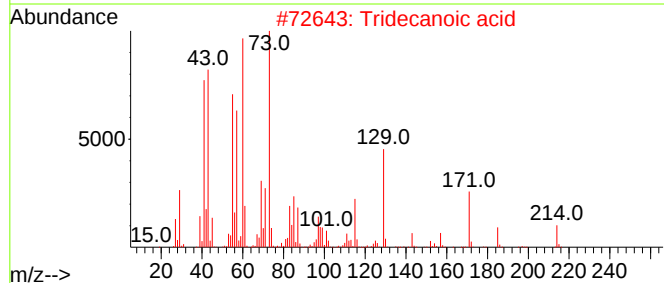
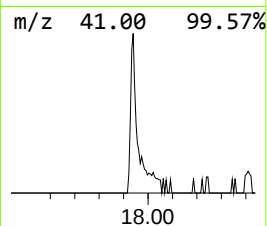
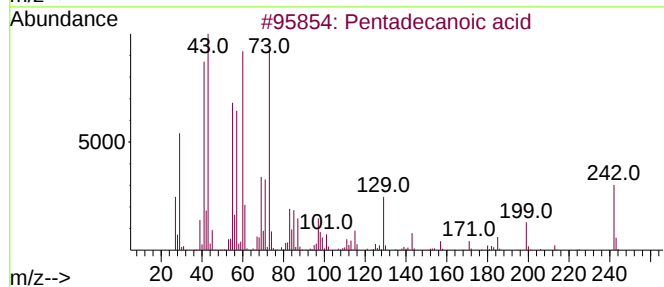
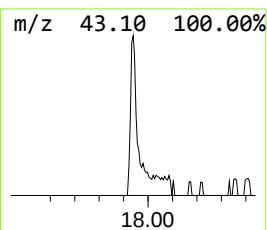
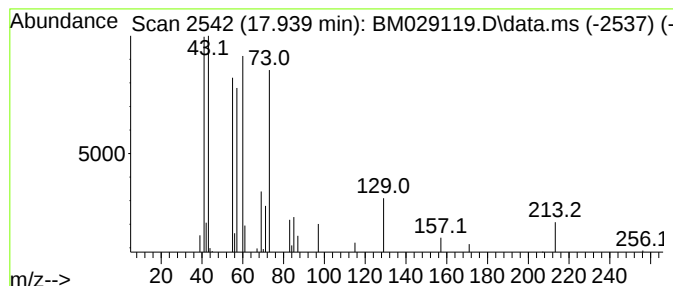
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Pentadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.939	6.76 ng	26368	Phenanthrene-d10	17.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
2			Tridecanoic acid	214	C13H26O2	000638-53-9	72
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Dodecanoic acid	200	C12H24O2	000143-07-7	72
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60



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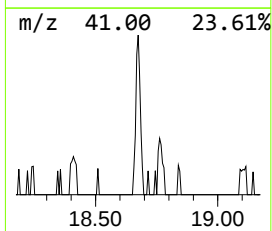
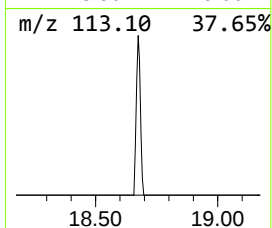
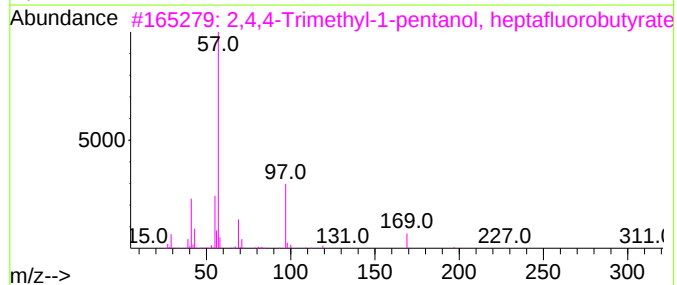
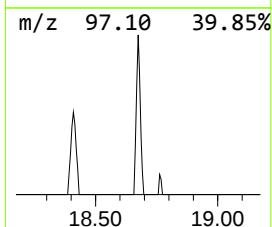
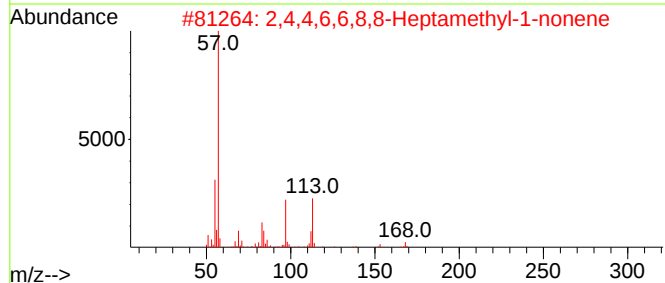
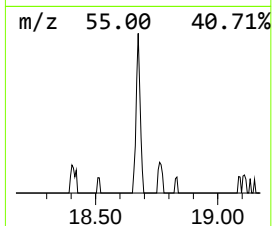
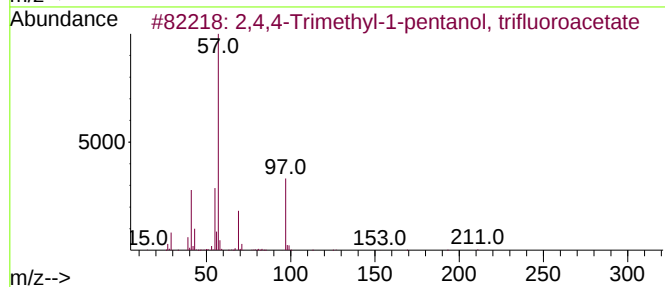
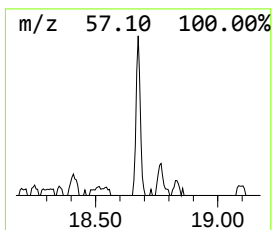
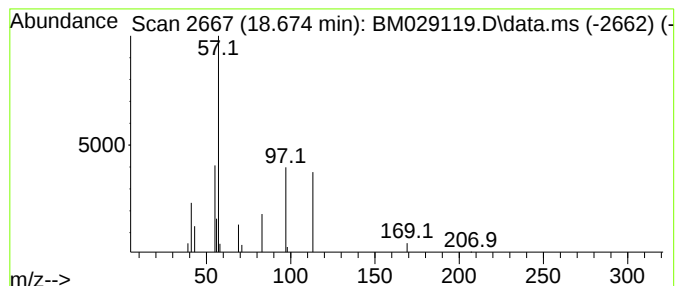
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2,4,4-Trimethyl-1-pentanol,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.674	4.37 ng	17040	Phenanthrene-d10	17.039	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	50
2	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	50
3	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	50
4	Pentane, 2,2,4-trimethyl-4-nitro-	159	C8H17NO2	005342-78-9	42
5	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	40



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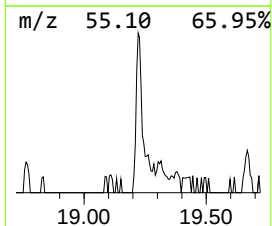
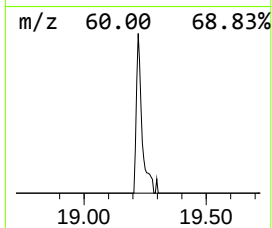
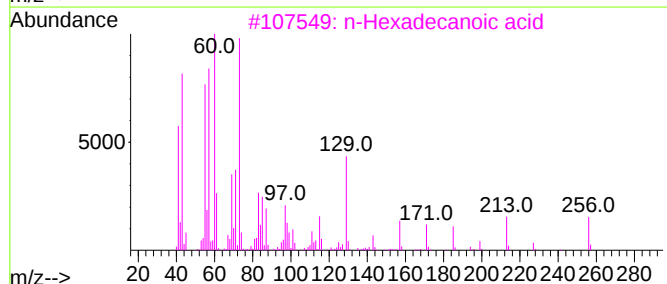
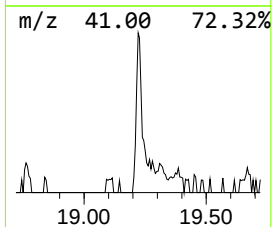
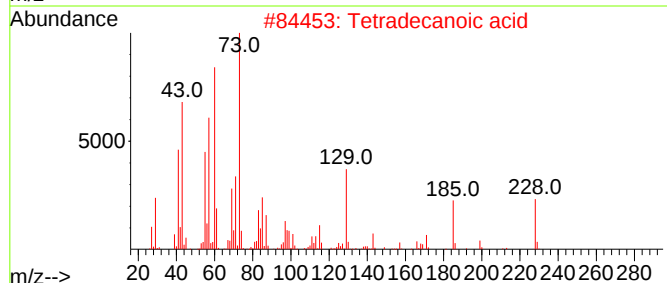
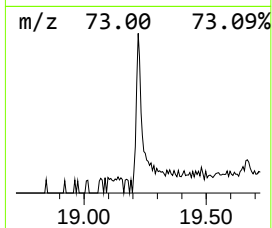
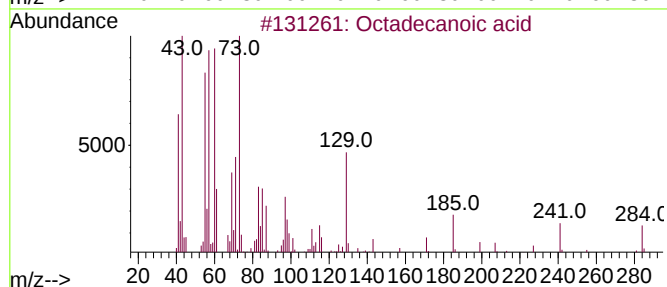
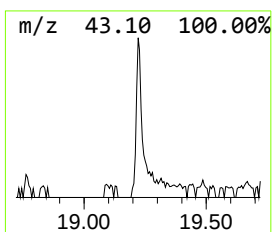
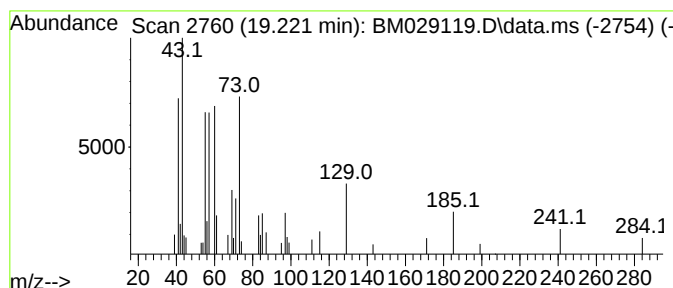
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Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.221	7.58 ng	33275	Chrysene-d12	21.221

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
4			Tridecanoic acid	214	C13H26O2	000638-53-9	58
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



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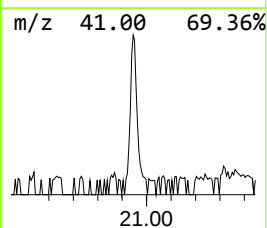
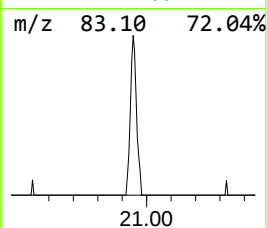
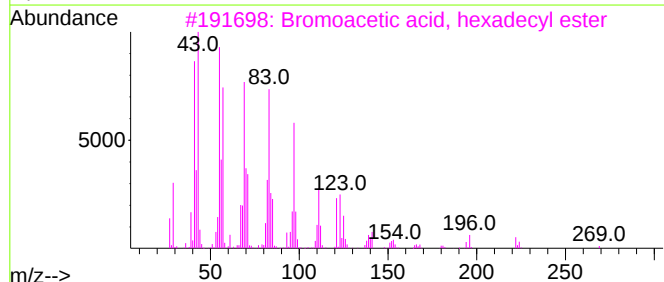
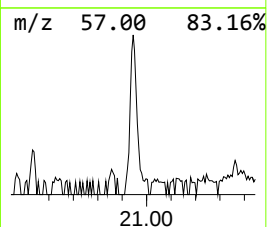
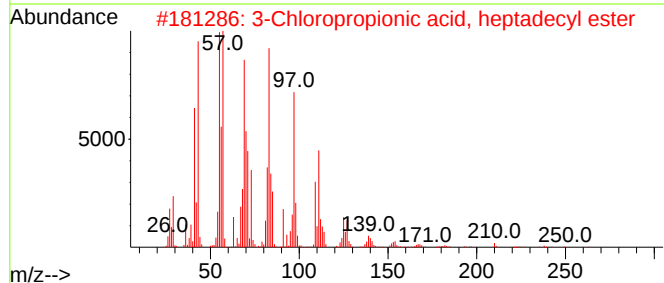
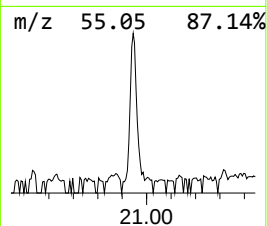
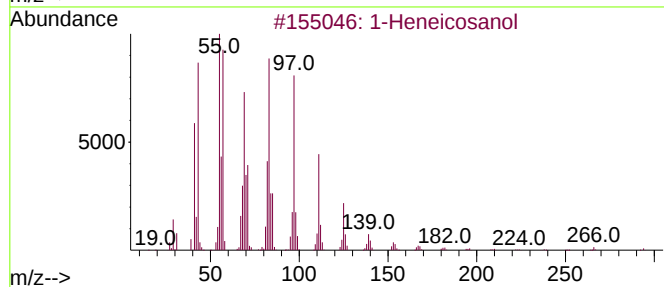
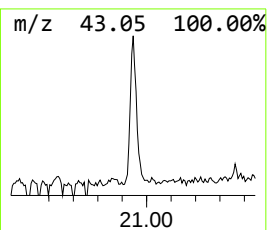
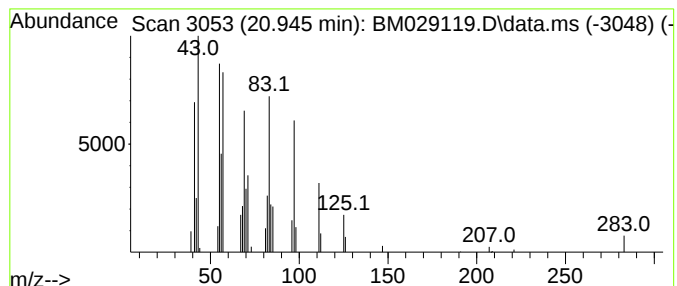
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Peak Number 4 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.945	7.87 ng	34536	Chrysene-d12	21.221

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	93
2			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
3			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
4			1-Docosene	308	C22H44	001599-67-3	91
5			Cycloeicosane	280	C20H40	000296-56-0	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentadecanoic acid	17.939	6.8	ng	26368	4	17.039	77972	20.0
2,4,4-Trimethyl...	18.674	4.4	ng	17040	4	17.039	77972	20.0
Octadecanoic acid	19.221	7.6	ng	33275	5	21.221	87811	20.0
1-Heneicosanol	20.945	7.9	ng	34536	5	21.221	87811	20.0