

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031221\
 Data File : BM029120.D
 Acq On : 12 Mar 2021 20:36
 Operator : CG/JU
 Sample : M1649-04
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP-1-2

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_M\Methods\8270-BM022321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029120.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.192	370	375	390	rBV	146962	216016	61.01%	10.784%
2	6.816	645	651	665	rBV	144809	225272	63.63%	11.246%
3	7.616	782	787	795	rBB	30795	48142	13.60%	2.403%
4	8.792	981	987	1000	rBV	88768	141492	39.96%	7.064%
5	10.410	1256	1262	1269	rBV	41002	64432	18.20%	3.217%
6	12.898	1679	1685	1692	rBV	203940	286330	80.87%	14.294%
7	14.292	1916	1922	1927	rBB	54880	76965	21.74%	3.842%
8	15.792	2172	2177	2185	rBB	150889	196543	55.51%	9.812%
9	17.039	2384	2389	2395	rBV	64180	83427	23.56%	4.165%
10	17.939	2537	2542	2554	rBV2	17799	29017	8.20%	1.449%
11	18.674	2661	2667	2672	rBV	10584	12456	3.52%	0.622%
12	19.221	2756	2760	2772	rBV	19423	29496	8.33%	1.473%
13	19.668	2831	2836	2842	rVB	317208	354053	100.00%	17.675%
14	20.944	3046	3053	3062	rBV2	27902	54996	15.53%	2.746%
15	21.221	3095	3100	3106	rBV	74604	89336	25.23%	4.460%
16	23.356	3457	3463	3470	rVB	56452	95116	26.86%	4.748%

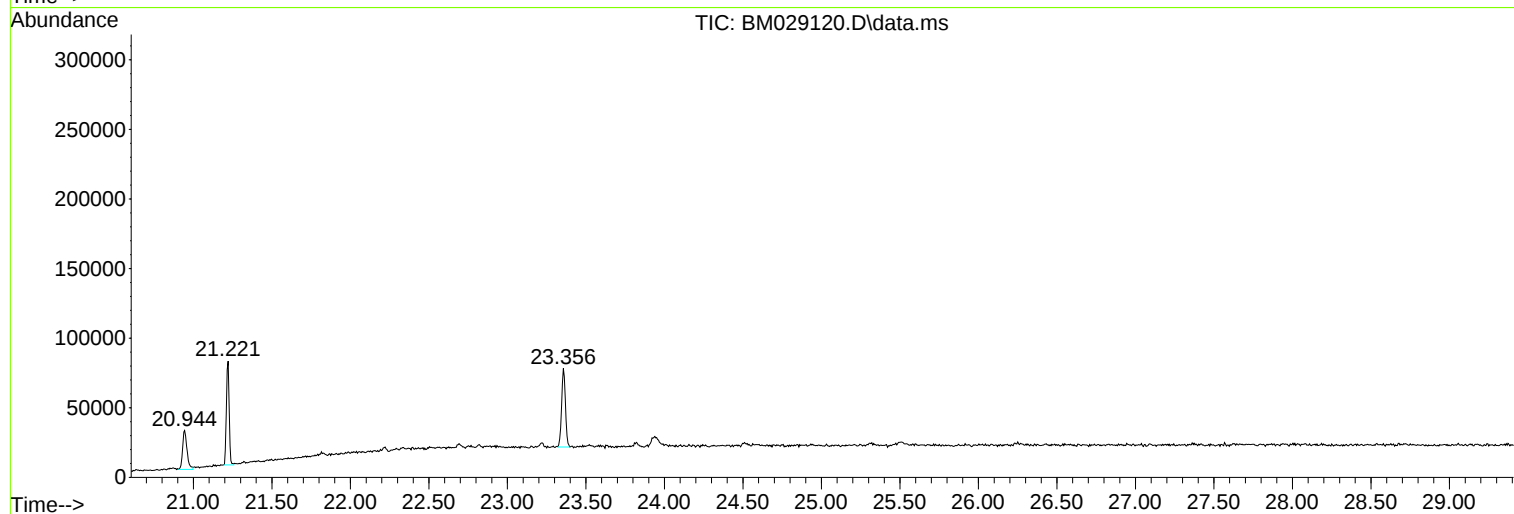
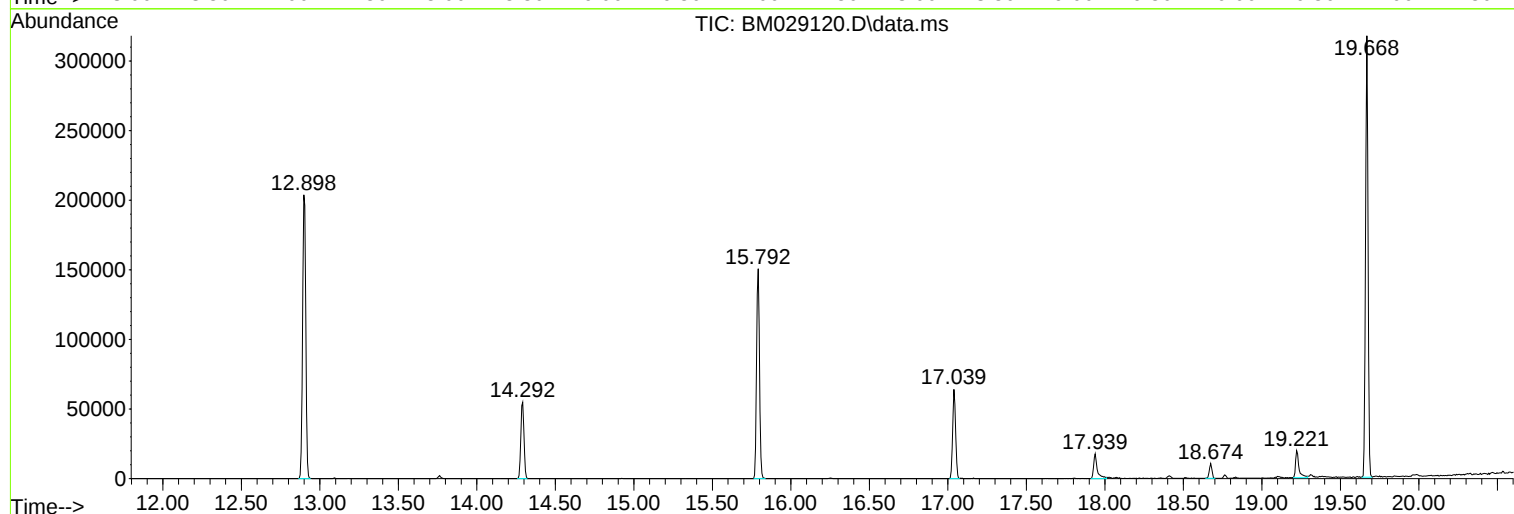
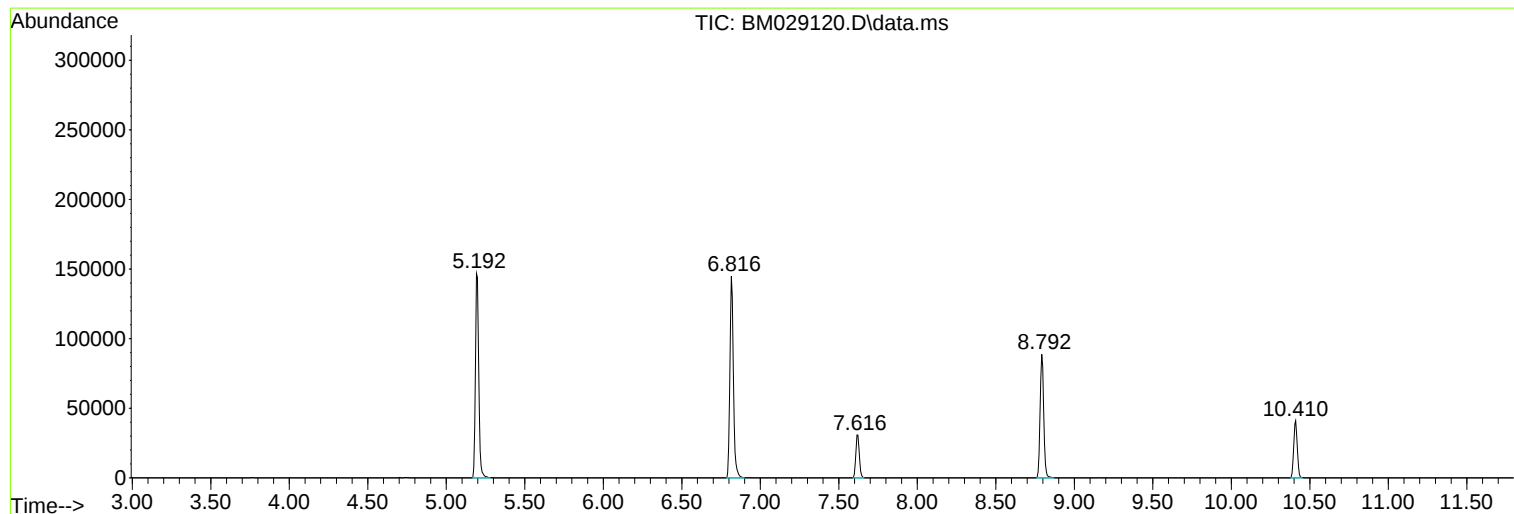
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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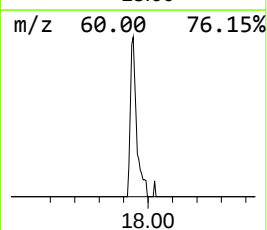
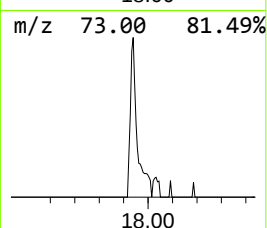
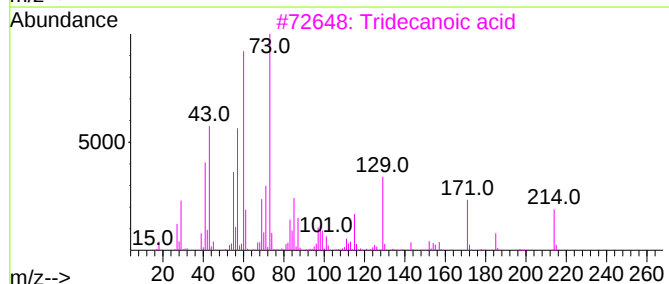
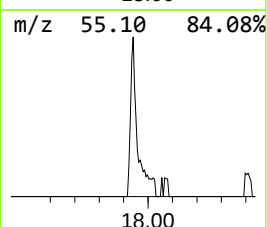
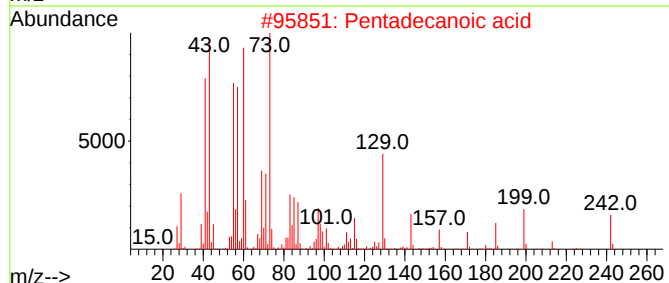
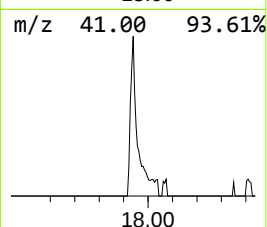
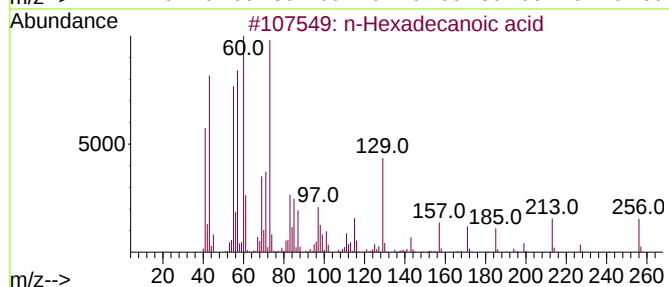
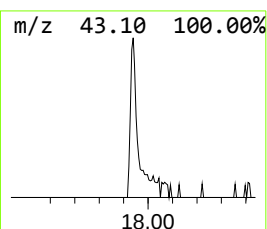
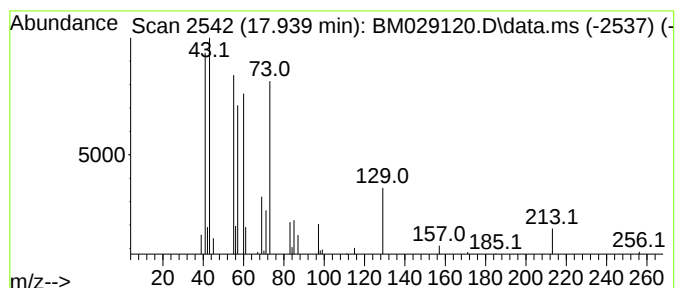
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.939	6.96 ng	29017	Phenanthrene-d10	17.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tridecanoic acid	214	C13H26O2	000638-53-9	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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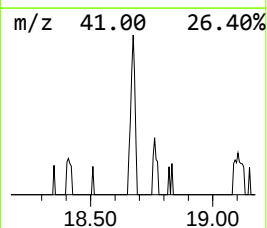
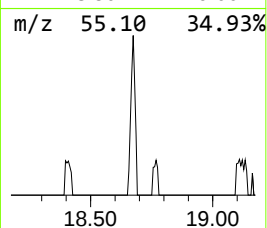
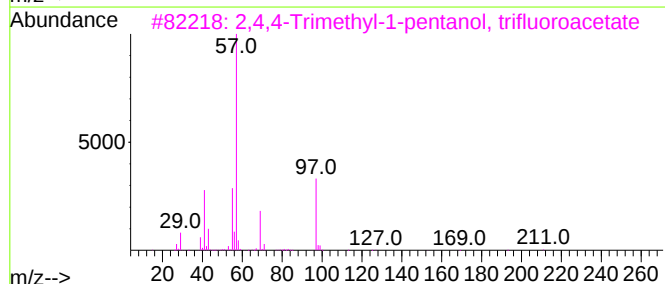
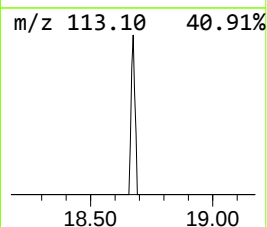
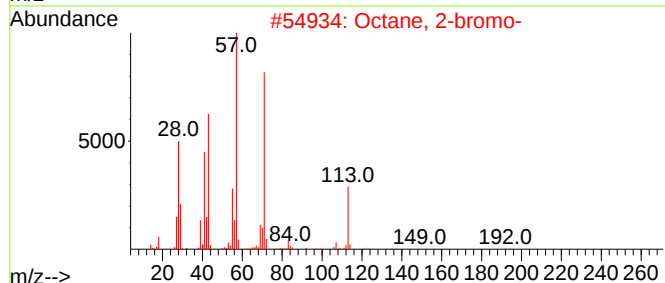
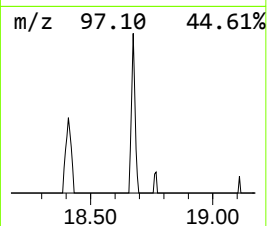
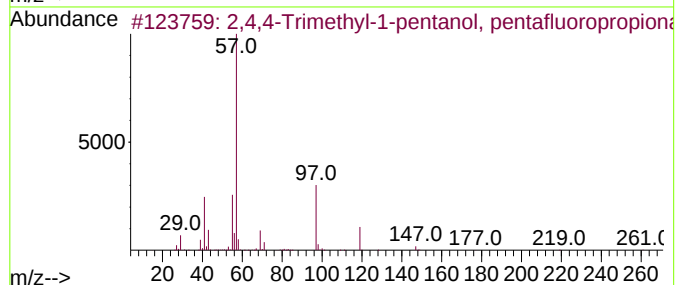
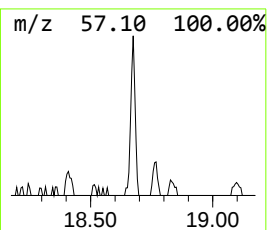
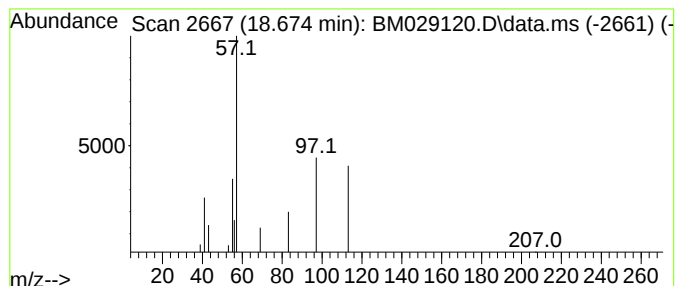
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Peak Number 2 unknown18.674 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.674	2.99 ng	12456	Phenanthrene-d10	17.039

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	37
2		Octane, 2-bromo-	192	C8H17Br	000557-35-7	28
3		2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	23
4		2,2-Dimethyl-3-pentanol, chlorod...	228	C9H15ClF2O2	1000376-26-4	16
5		Pentane, 2,2,4-trimethyl-4-nitro-	159	C8H17NO2	005342-78-9	9



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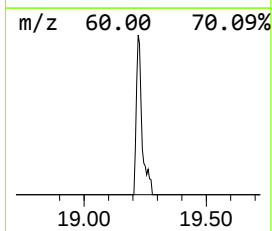
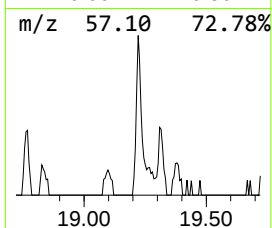
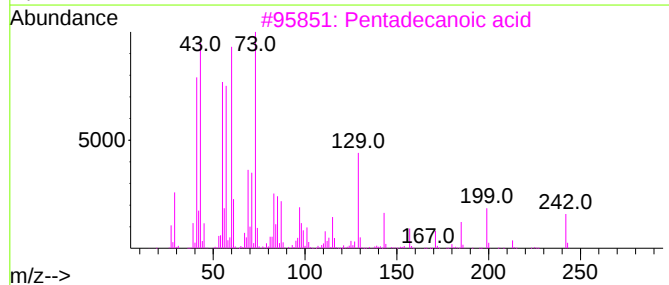
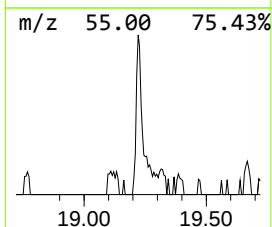
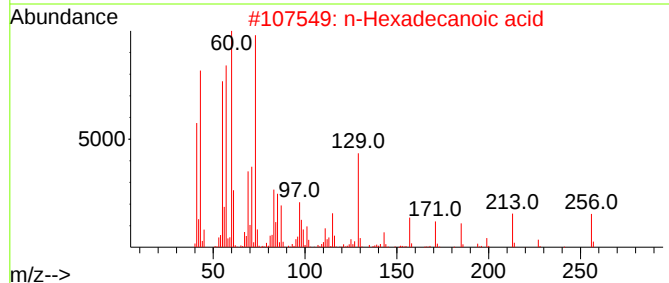
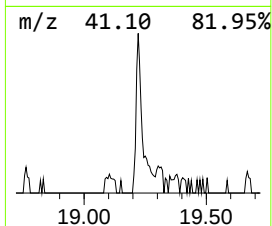
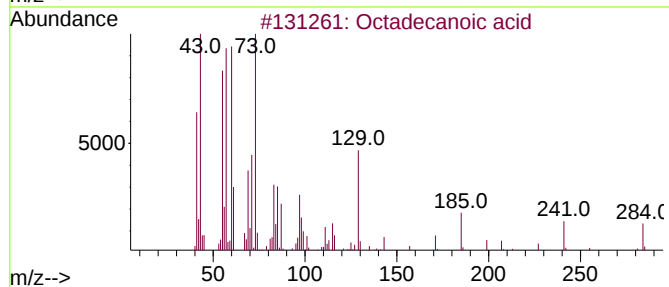
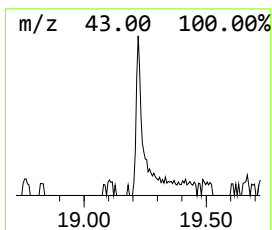
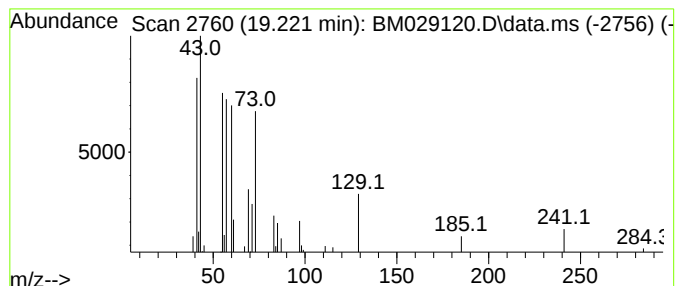
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Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.221	6.60 ng	29496	Chrysene-d12	21.221

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5			Tridecanoic acid	214	C13H26O2	000638-53-9	53



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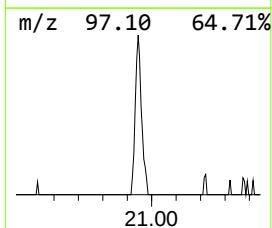
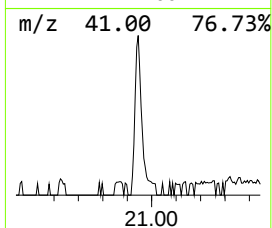
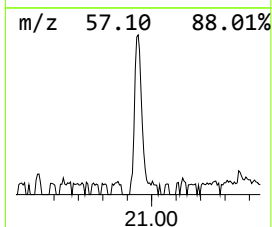
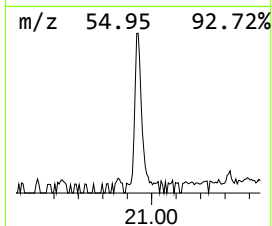
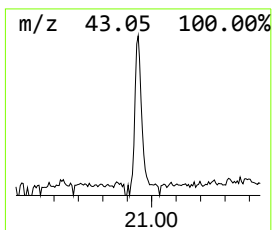
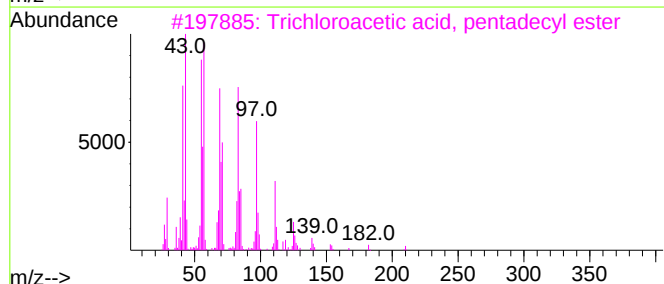
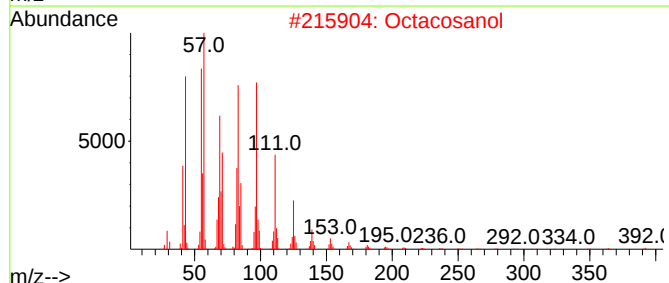
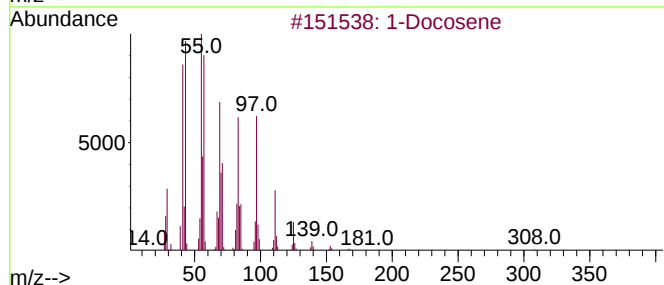
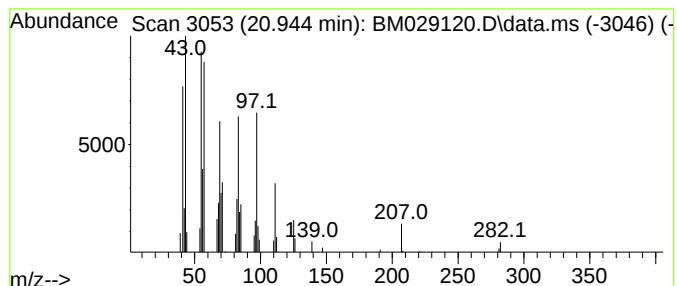
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Peak Number 4 1-Docosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.944	12.31 ng	54996	Chrysene-d12	21.221

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	93
2			Octacosanol	410	C28H58O	000557-61-9	90
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
5			1-Heneicosanol	312	C21H44O	015594-90-8	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	17.939	7.0	ng	29017	4	17.039	83427	20.0
unknown18.674	18.674	3.0	ng	12456	4	17.039	83427	20.0
Octadecanoic acid	19.221	6.6	ng	29496	5	21.221	89336	20.0
1-Docosene	20.944	12.3	ng	54996	5	21.221	89336	20.0