

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103122\
 Data File : BM037294.D
 Acq On : 31 Oct 2022 17:45
 Operator : CG/JU
 Sample : N5341-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WC-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-BM102822.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM037294.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.975	315	321	332	rBV	644383	862028	10.57%	1.633%
2	5.440	393	400	414	rBV	4329465	6170489	75.65%	11.689%
3	7.040	665	672	689	rBV	3819526	6111139	74.93%	11.577%
4	7.869	806	813	821	rBV	963854	1503813	18.44%	2.849%
5	9.040	1002	1012	1022	rBV	2290466	3772768	46.26%	7.147%
6	10.457	1247	1253	1263	rBV	76899	177458	2.18%	0.336%
7	10.669	1281	1289	1303	rBV	1174794	1943710	23.83%	3.682%
8	13.128	1698	1707	1720	rBV	4977616	7233032	88.68%	13.702%
9	14.504	1935	1941	1958	rVB	1403272	2128732	26.10%	4.033%
10	15.992	2183	2194	2216	rBV	3449610	5156116	63.22%	9.768%
11	17.245	2400	2407	2420	rBV	1544590	2221815	27.24%	4.209%
12	18.139	2553	2559	2569	rBV	315221	578189	7.09%	1.095%
13	19.416	2771	2776	2788	rBV	245435	461955	5.66%	0.875%
14	19.863	2847	2852	2867	rBV	6859185	8156199	100.00%	15.451%
15	20.663	2985	2988	2992	rBV2	91086	96746	1.19%	0.183%
16	21.127	3063	3067	3076	rBV	332532	593573	7.28%	1.124%
17	21.421	3112	3117	3124	rBV	1946339	2592132	31.78%	4.911%
18	23.780	3512	3518	3527	rVB2	1519320	3027231	37.12%	5.735%

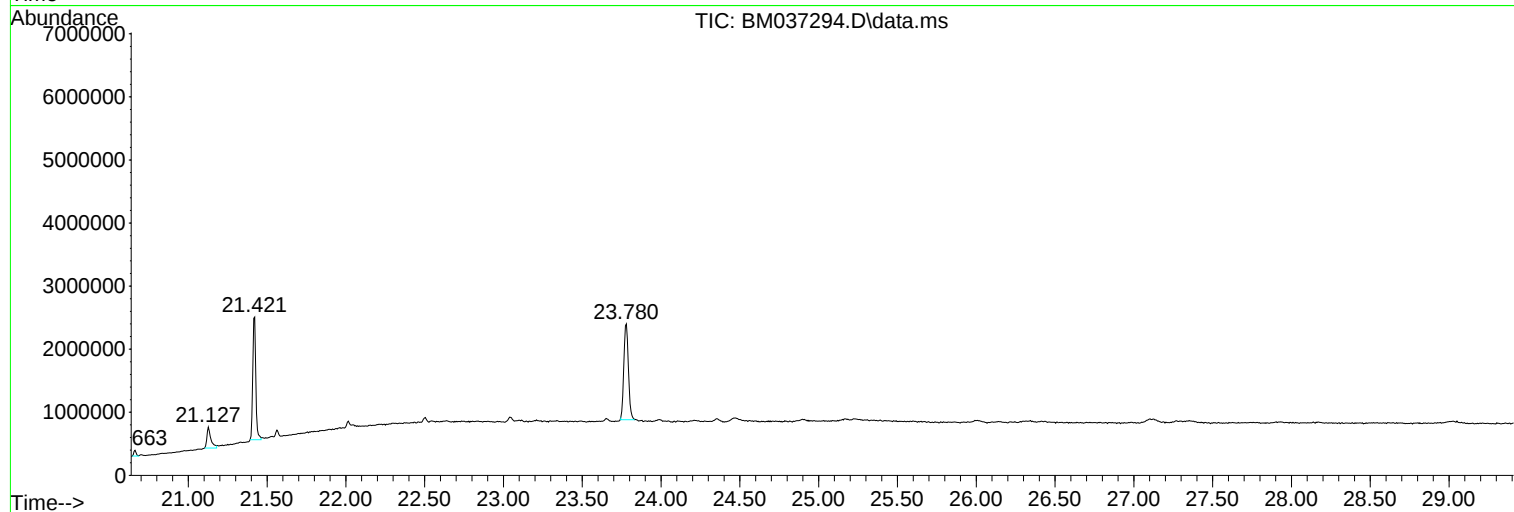
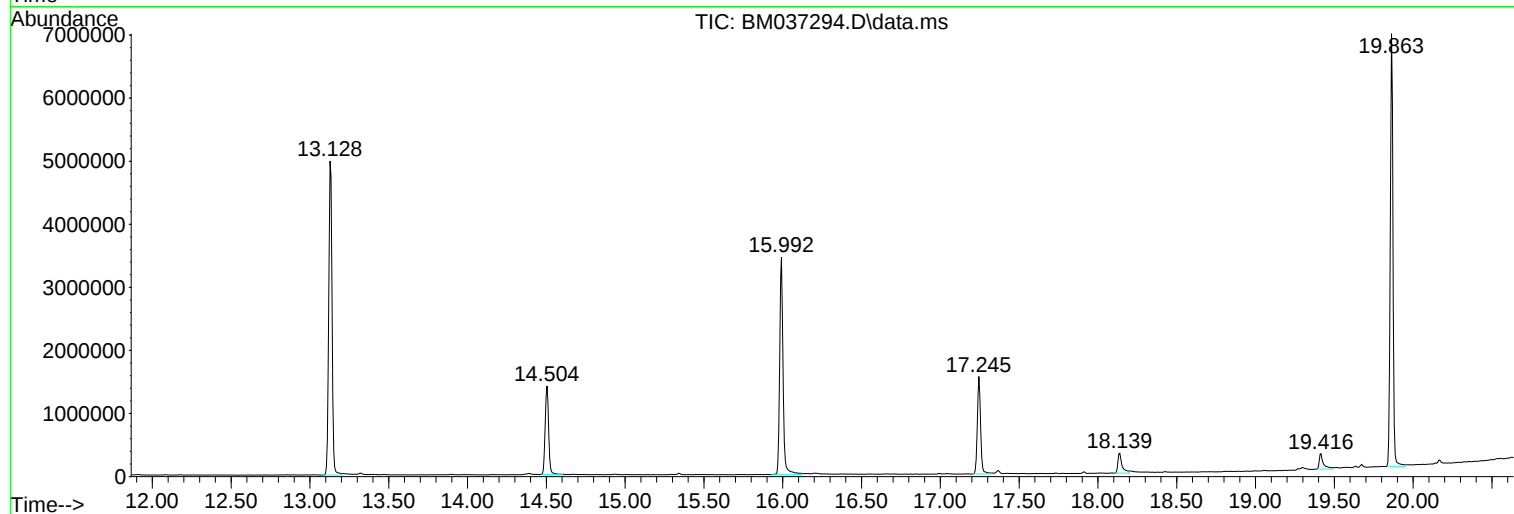
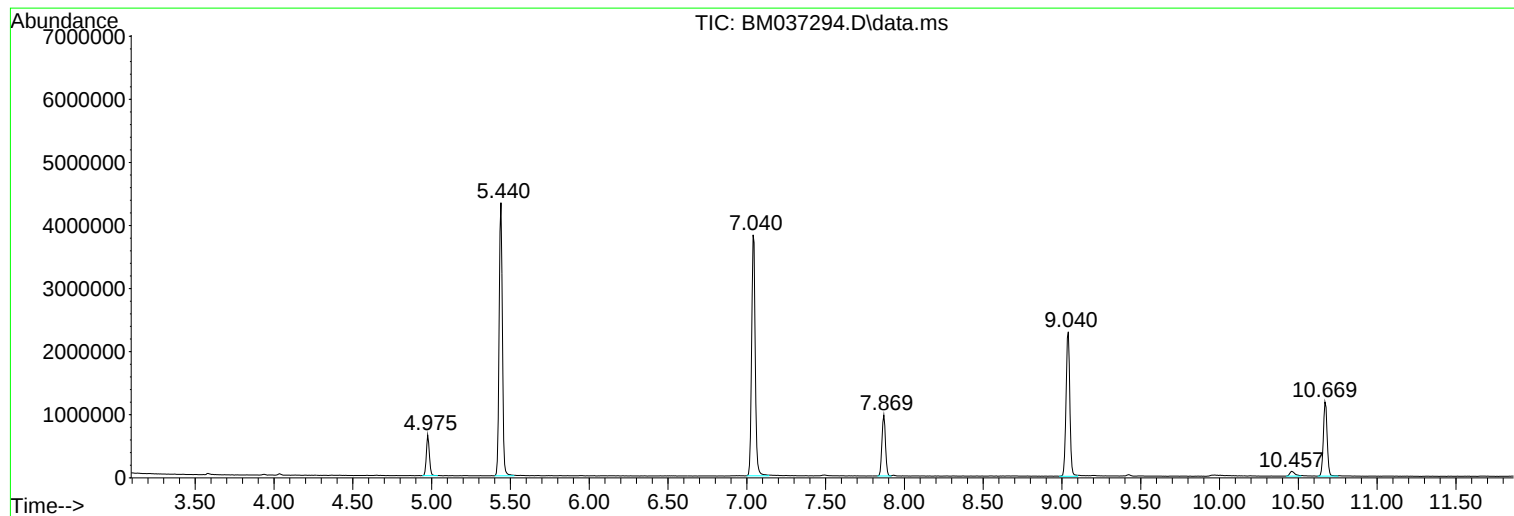
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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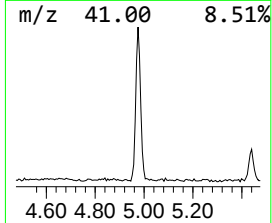
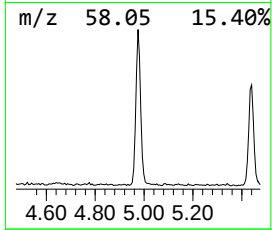
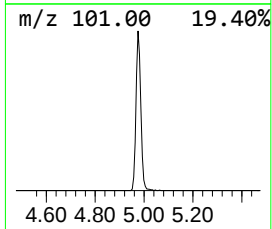
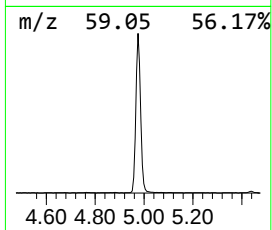
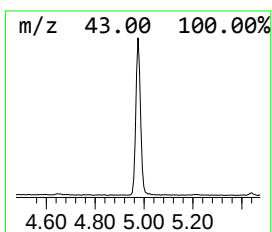
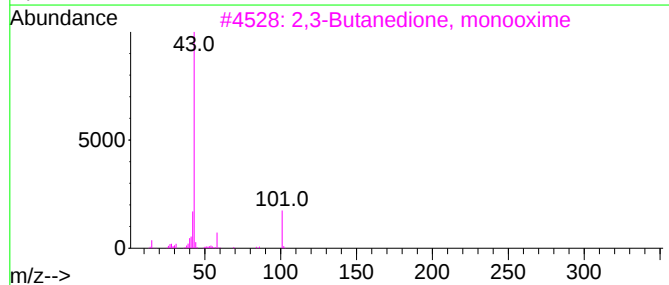
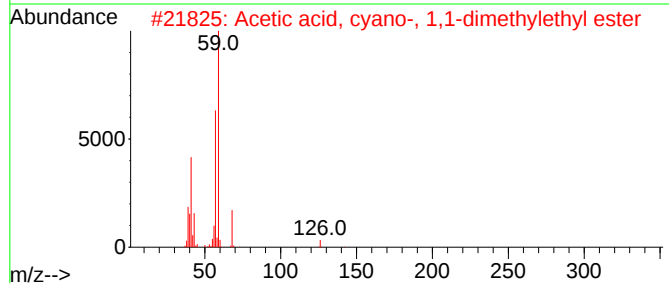
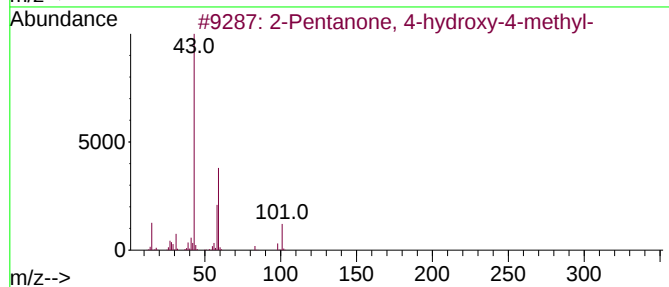
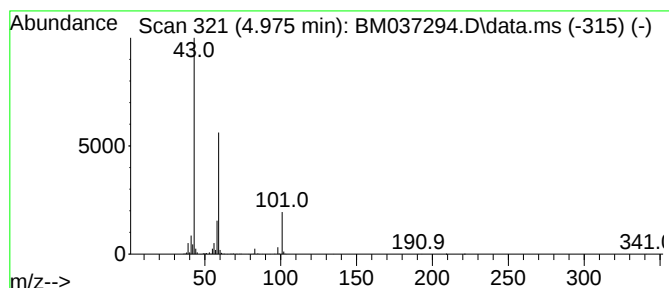
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown4.975 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.975	11.46 ng	862028	1,4-Dichlorobenzene-d4	7.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9		



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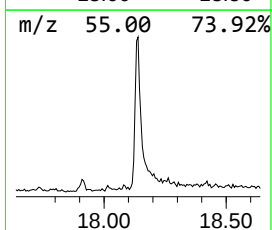
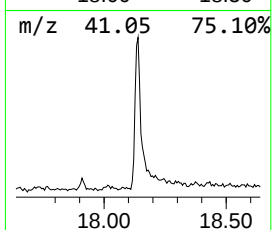
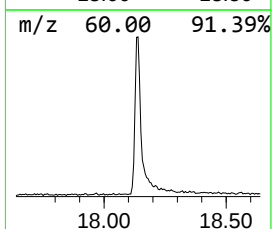
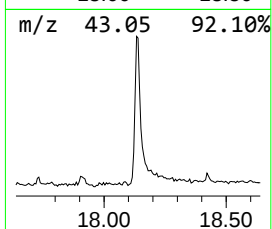
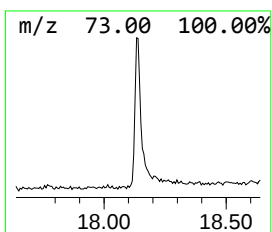
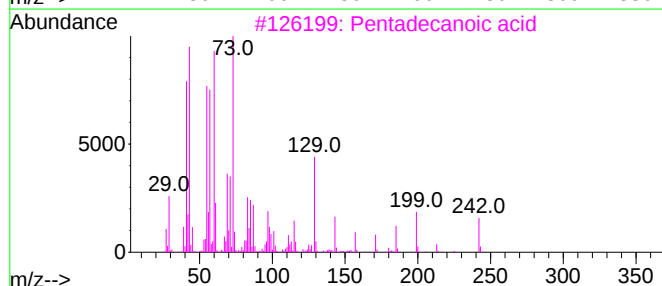
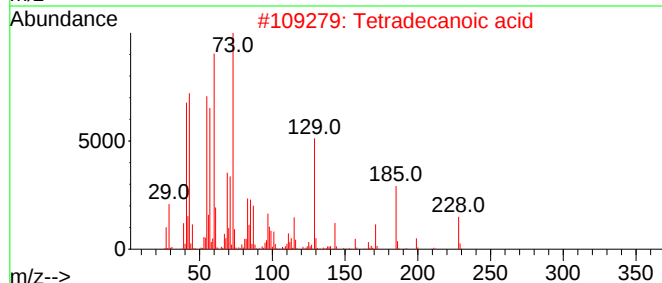
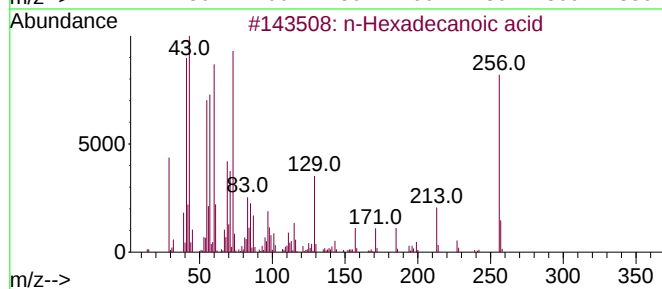
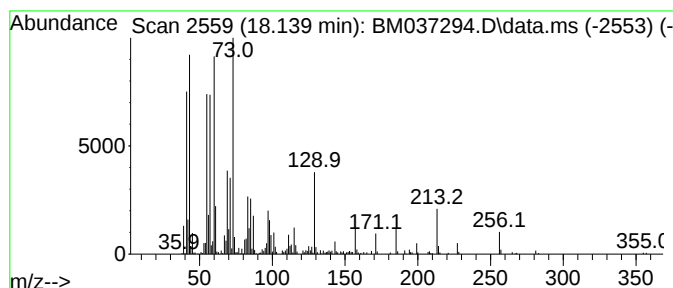
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.139	5.20 ng	578189	Phenanthrene-d10	17.245

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Octadecanoic acid	284	C18H36O2	000057-11-4	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	81



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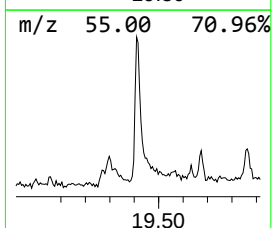
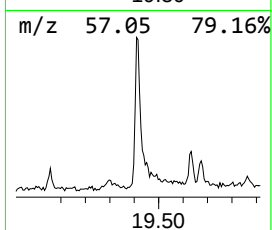
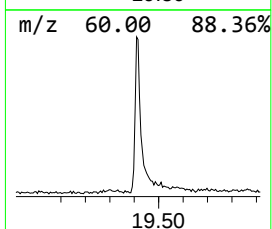
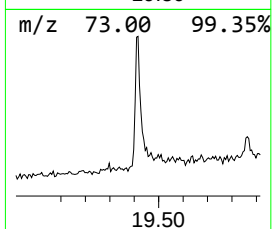
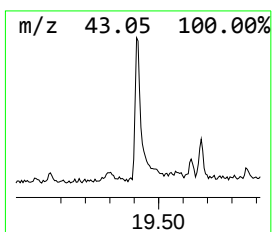
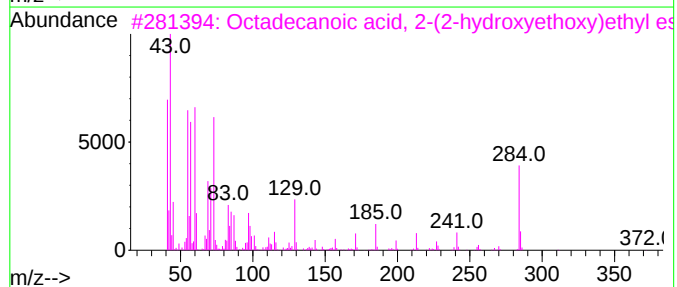
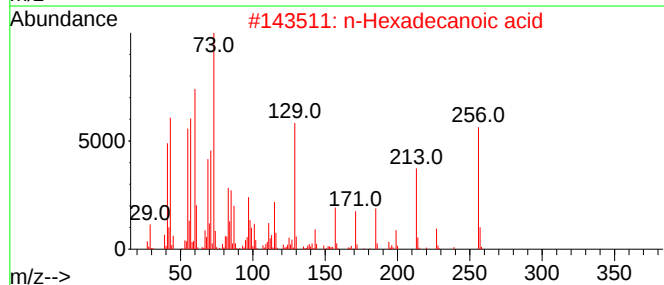
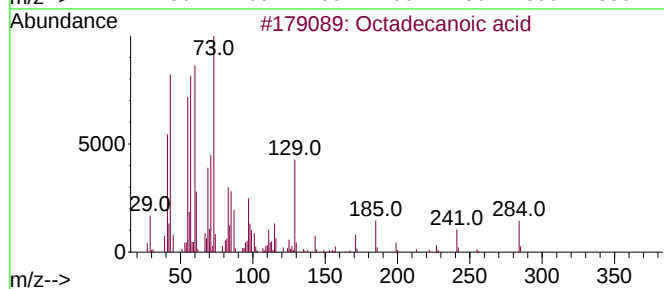
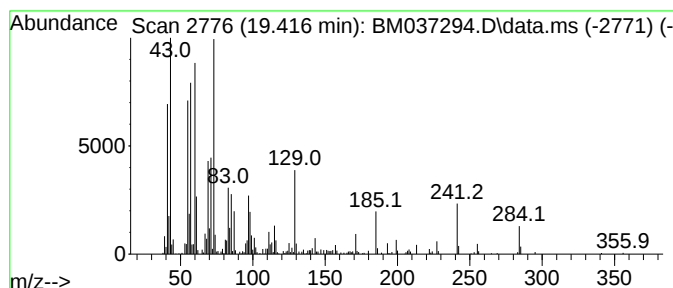
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Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.416	3.56 ng	461955	Chrysene-d12	21.421

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	89
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	58



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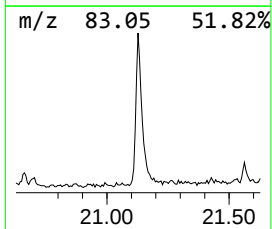
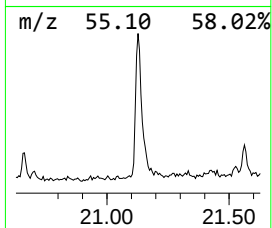
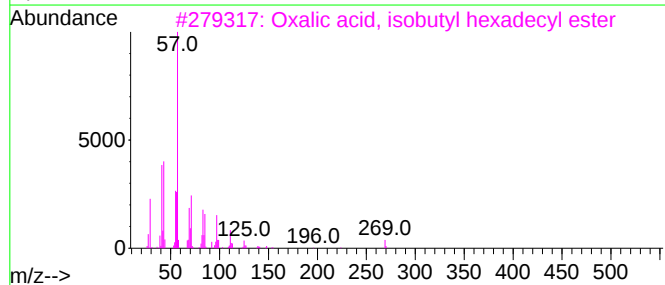
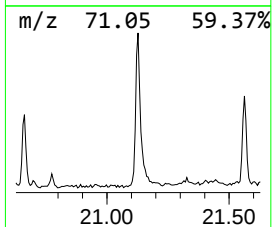
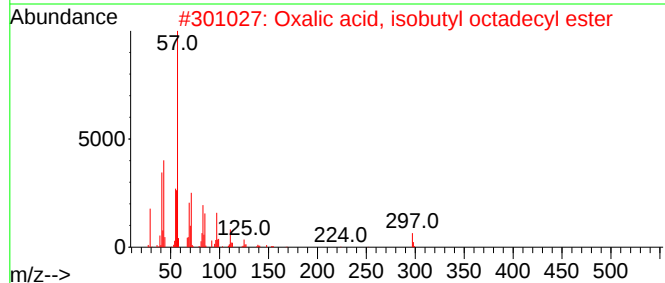
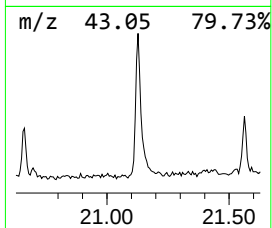
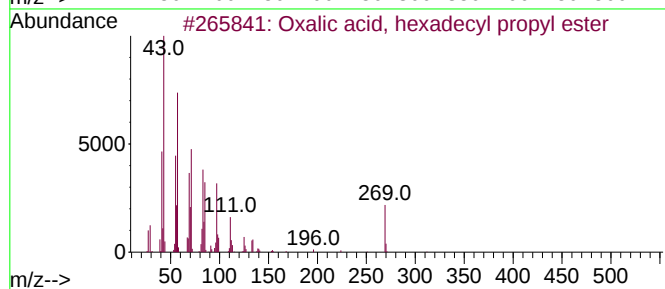
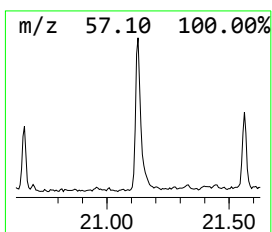
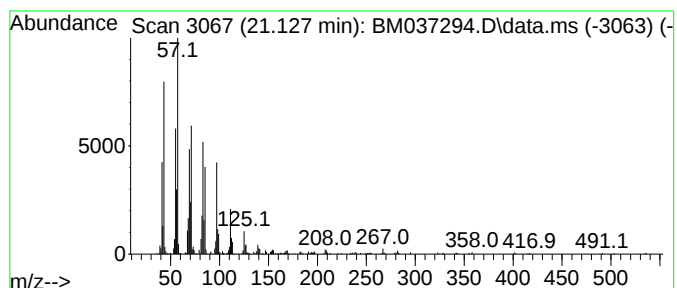
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Peak Number 4 Oxalic acid, hexadecyl prop... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	4.58 ng	593573	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	91
2			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
3			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
4			Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	91
5			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown4.975	4.975	11.5	ng	862028	1	7.869	1503810	20.0
n-Hexadecanoic ...	18.139	5.2	ng	578189	4	17.245	2221820	20.0
Octadecanoic acid	19.416	3.6	ng	461955	5	21.421	2592130	20.0
Oxalic acid, he...	21.127	4.6	ng	593573	5	21.421	2592130	20.0