

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
 Data File : BM041217.D
 Acq On : 01 Aug 2023 10:10
 Operator : MA/JU
 Sample : PB154495BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB154495BL

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-BM072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041217.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.910	288	293	299	rVB	89138	119096	1.21%	0.248%
2	5.369	364	371	383	rBV	3599921	5105057	52.00%	10.637%
3	6.981	637	645	658	rBV	3330072	5196372	52.93%	10.827%
4	7.798	777	784	792	rBV	652406	971224	9.89%	2.024%
5	8.975	975	984	995	rBV	2110106	3384124	34.47%	7.051%
6	10.604	1254	1261	1273	rBV	828113	1345975	13.71%	2.804%
7	13.080	1675	1682	1698	rBV	5343164	7635560	77.78%	15.909%
8	14.345	1884	1897	1910	rBV	93125	296301	3.02%	0.617%
9	14.463	1911	1917	1929	rVB	1169365	1706701	17.39%	3.556%
10	15.963	2165	2172	2189	rBV	4140413	5837834	59.47%	12.163%
11	17.221	2380	2386	2397	rBV	1428371	1931464	19.68%	4.024%
12	18.121	2534	2539	2549	rBV	298239	549423	5.60%	1.145%
13	19.404	2753	2757	2771	rBV	234557	478739	4.88%	0.997%
14	19.862	2829	2835	2840	rBV	8415264	9816742	100.00%	20.454%
15	21.333	3082	3085	3090	rBV	154795	170204	1.73%	0.355%
16	21.427	3096	3101	3110	rBV	1385410	1747835	17.80%	3.642%
17	23.797	3498	3504	3511	rVB	909790	1702733	17.35%	3.548%

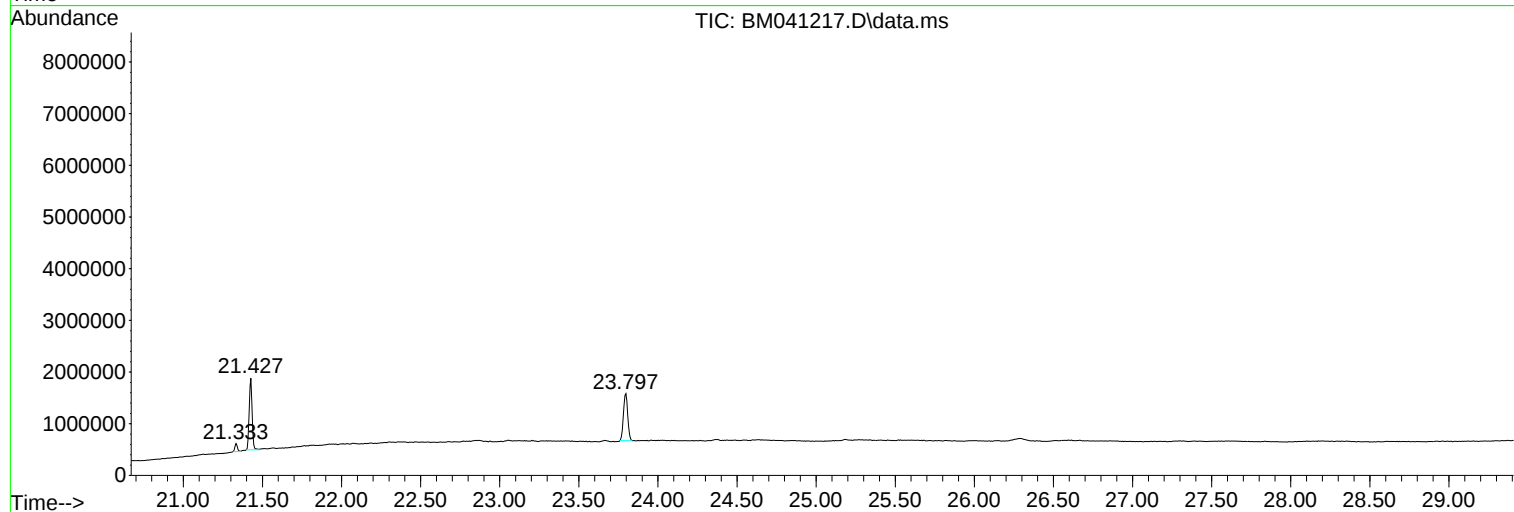
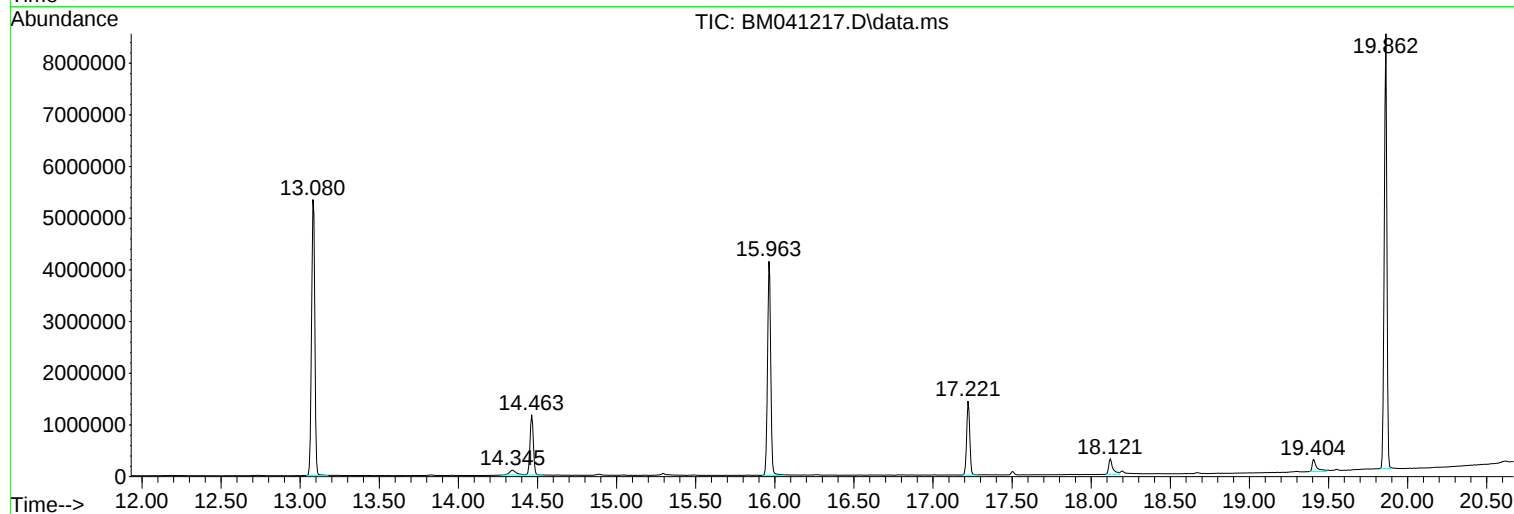
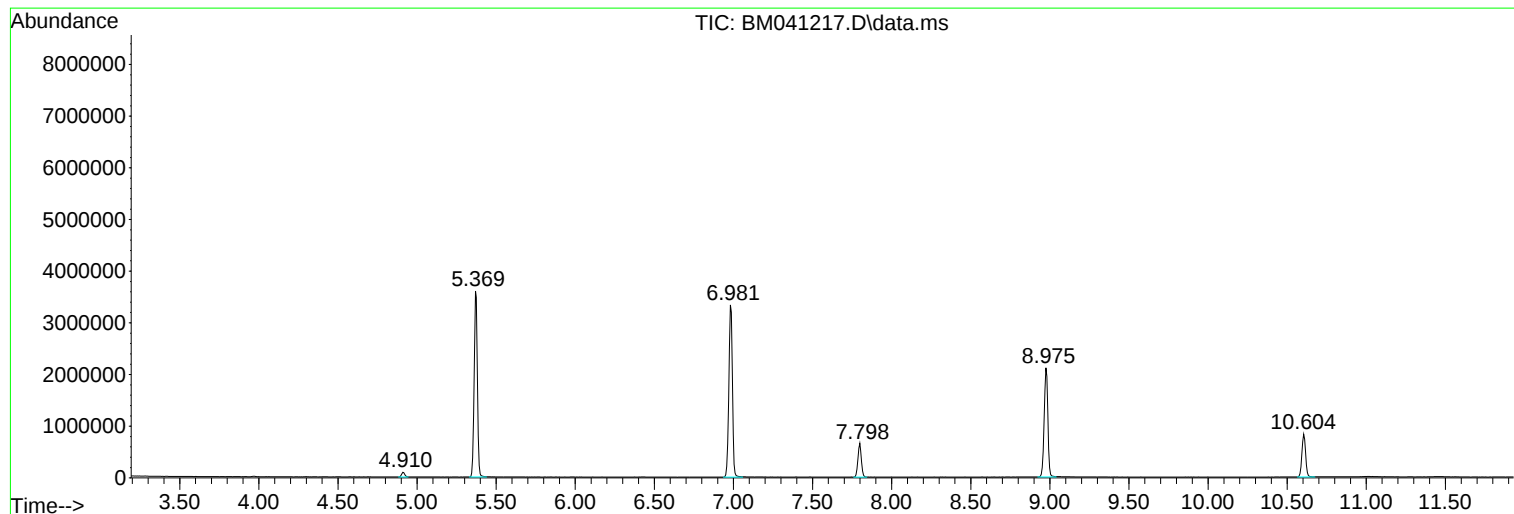
Sum of corrected areas: 47995384

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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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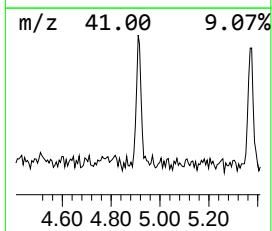
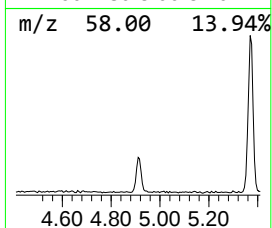
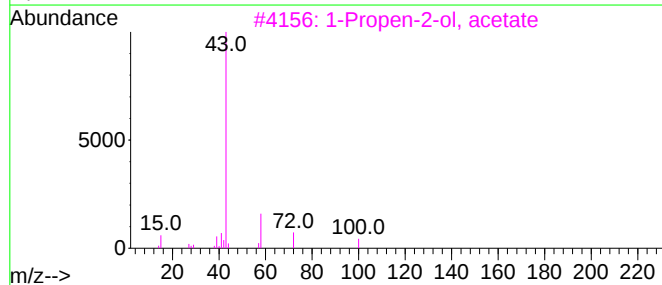
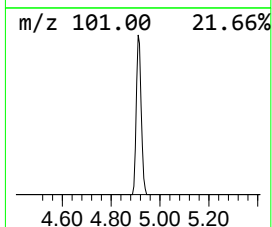
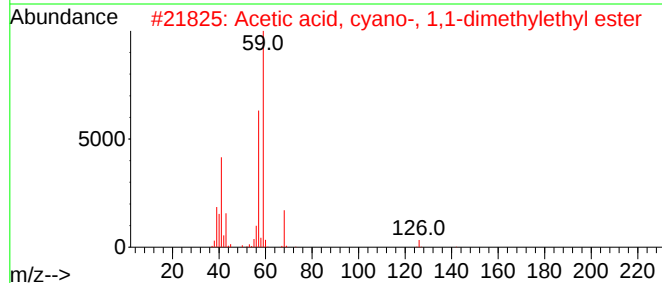
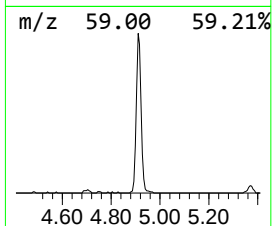
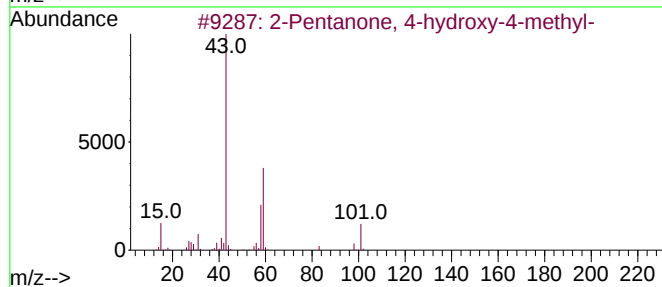
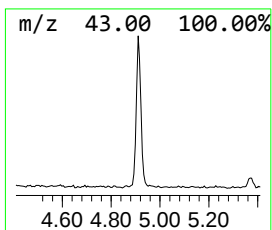
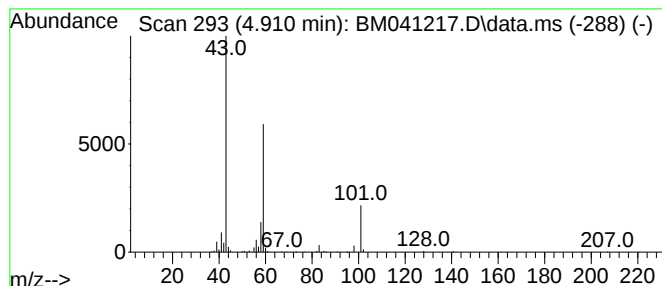
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.910	2.45 ng	119096	1,4-Dichlorobenzene-d4	7.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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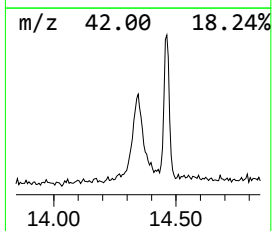
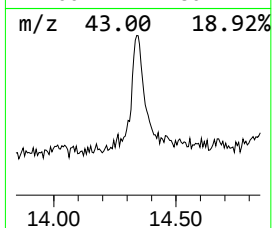
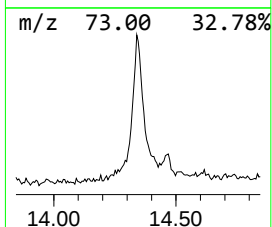
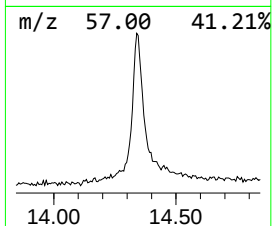
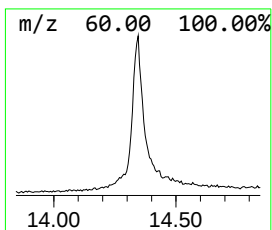
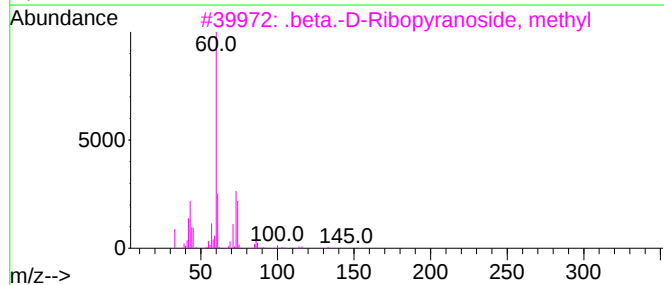
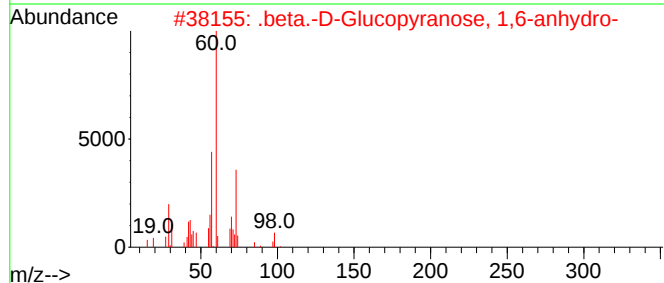
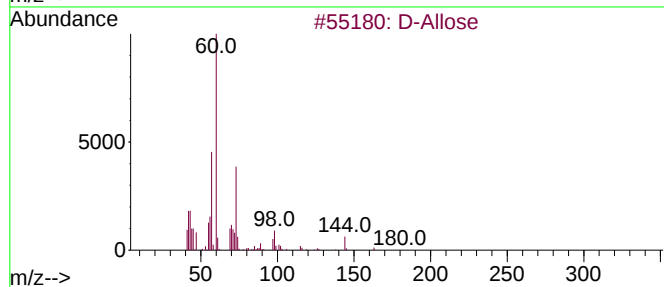
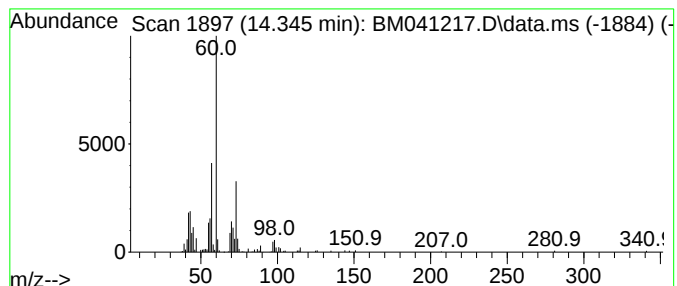
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 D-Allose Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.345	3.47 ng	296301	Acenaphthene-d10	14.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Allose	180	C6H12O6	002595-97-3	90
2			.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	78
3			.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	59
4			Heptanoic acid	130	C7H14O2	000111-14-8	59
5			3,4-Altrosan	162	C6H10O5	1000129-76-4	53



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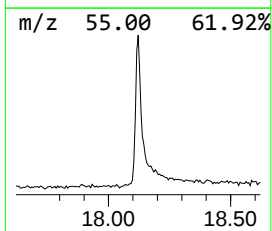
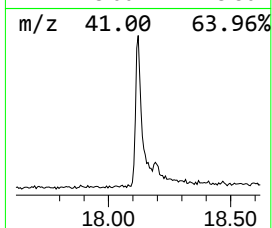
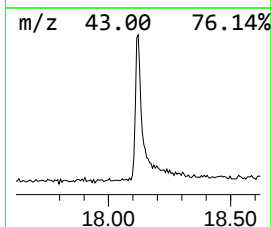
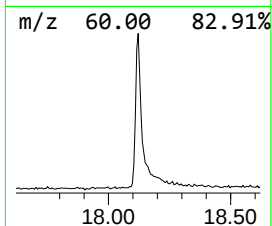
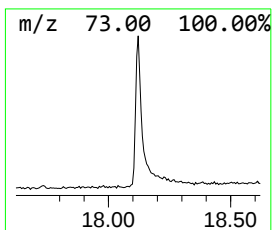
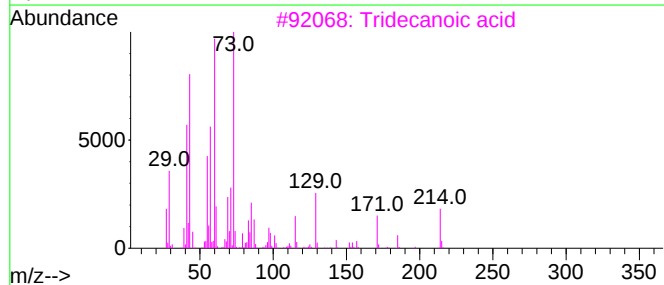
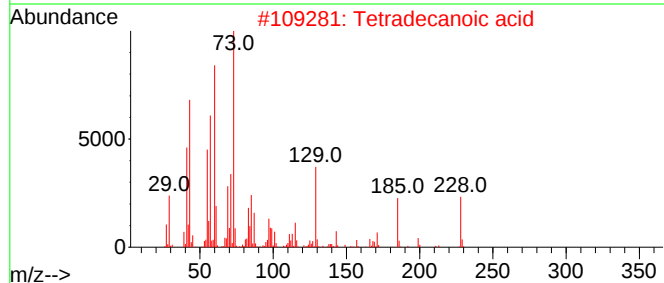
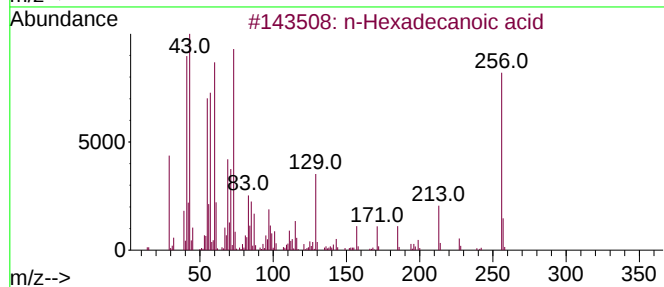
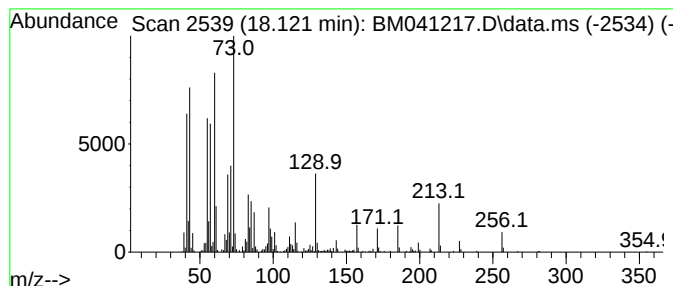
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.121	5.69 ng	549423	Phenanthrene-d10	17.221	
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	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Octadecanoic acid	284	C18H36O2	000057-11-4	87



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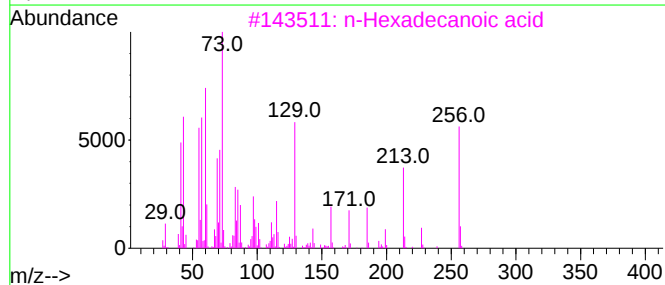
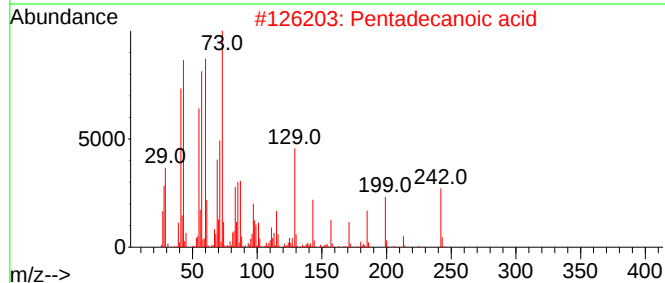
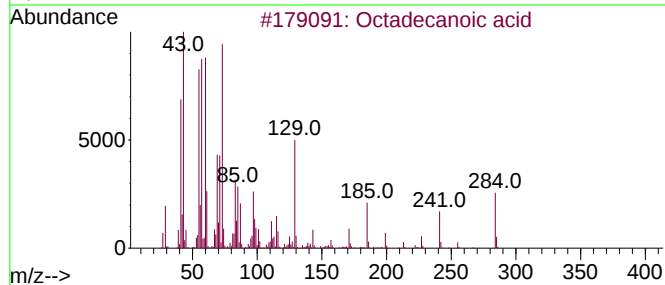
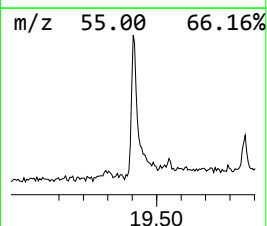
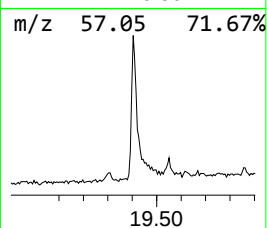
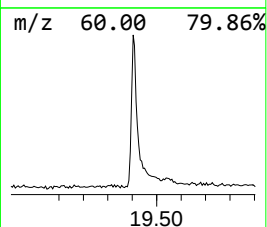
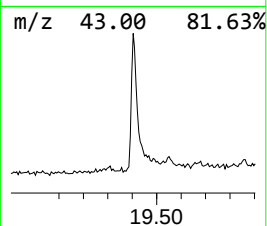
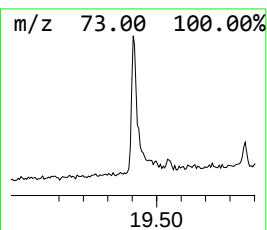
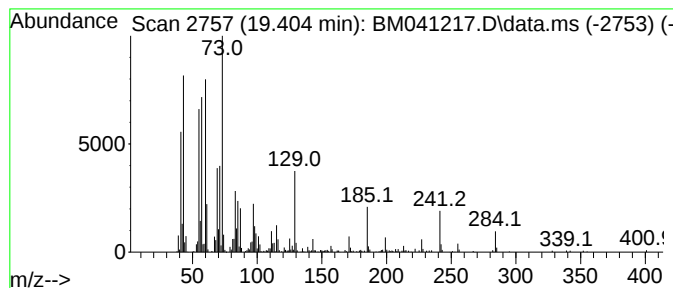
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Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.404	5.48 ng	478739	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			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.910	2.5	ng	119096	1	7.798	971224	20.0
D-Allose	14.345	3.5	ng	296301	3	14.463	1706700	20.0
n-Hexadecanoic ...	18.121	5.7	ng	549423	4	17.221	1931460	20.0
Octadecanoic acid	19.404	5.5	ng	478739	5	21.427	1747840	20.0