

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM081924\
 Data File : BM047256.D
 Acq On : 19 Aug 2024 17:28
 Operator : RC/JU
 Sample : P3609-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 915-J-WS-081424

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-BM081024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047256.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	356	362	375	rBV	1391424	2064552	15.69%	4.093%
2	6.575	621	627	638	rBV	877728	1413600	10.74%	2.802%
3	7.363	754	761	770	rBV	713062	1098402	8.35%	2.177%
4	8.510	947	956	967	rBV	1751678	2794708	21.24%	5.540%
5	10.122	1220	1230	1241	rBV	889380	1480726	11.25%	2.935%
6	10.881	1353	1359	1367	rBV	84259	156040	1.19%	0.309%
7	12.633	1648	1657	1664	rBV	4239907	6399604	48.63%	12.686%
8	13.904	1861	1873	1884	rBV2	65818	217149	1.65%	0.430%
9	14.027	1887	1894	1901	rVB	1418025	2092432	15.90%	4.148%
10	15.533	2144	2150	2161	rBV	5001105	7004150	53.23%	13.885%
11	16.786	2358	2363	2372	rVB	1879619	2702205	20.54%	5.357%
12	17.727	2517	2523	2530	rBV	797514	1272280	9.67%	2.522%
13	17.786	2531	2533	2543	rVB	95875	155509	1.18%	0.308%
14	19.027	2739	2744	2763	rBV	834538	1473117	11.20%	2.920%
15	19.456	2811	2817	2822	rBV	11350835	13158585	100.00%	26.085%
16	20.762	3036	3039	3046	rBV2	178377	303725	2.31%	0.602%
17	21.027	3079	3084	3091	rBV	2658343	3409347	25.91%	6.759%
18	23.733	3537	3544	3557	rVB	1388962	3248893	24.69%	6.440%

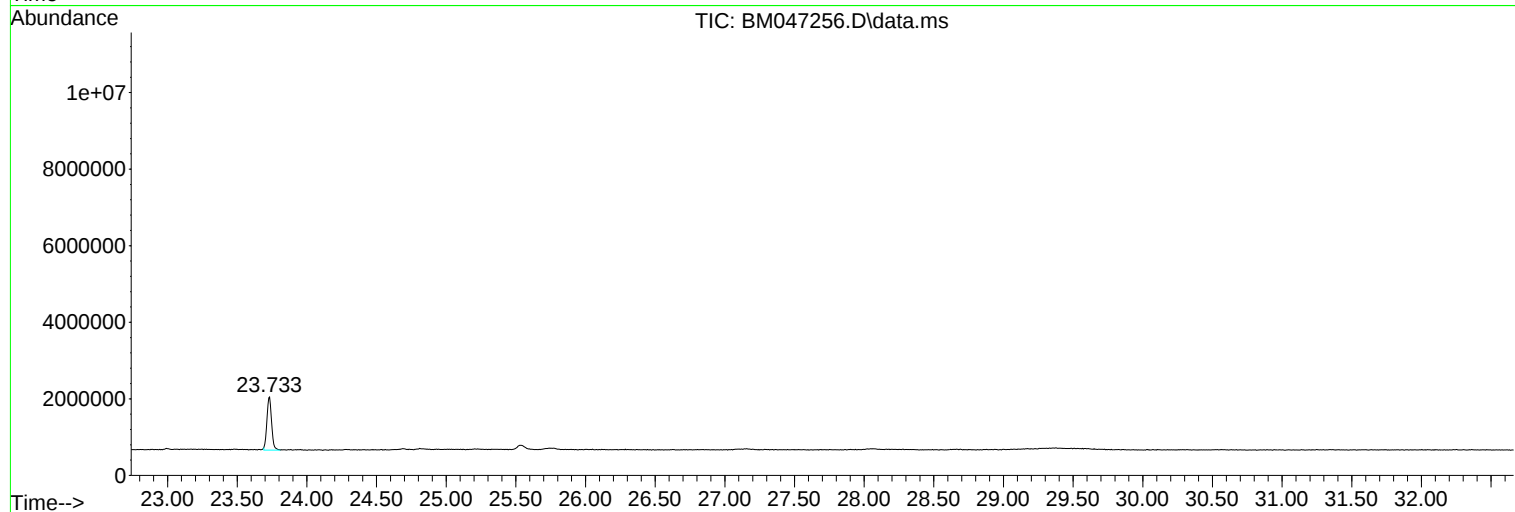
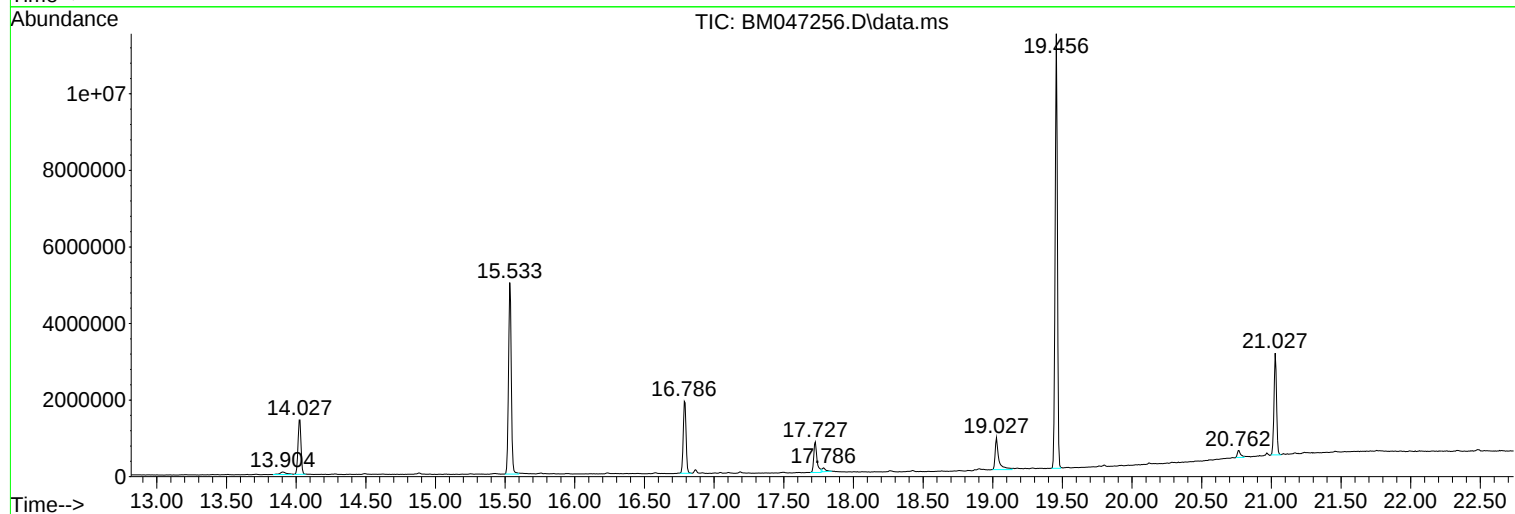
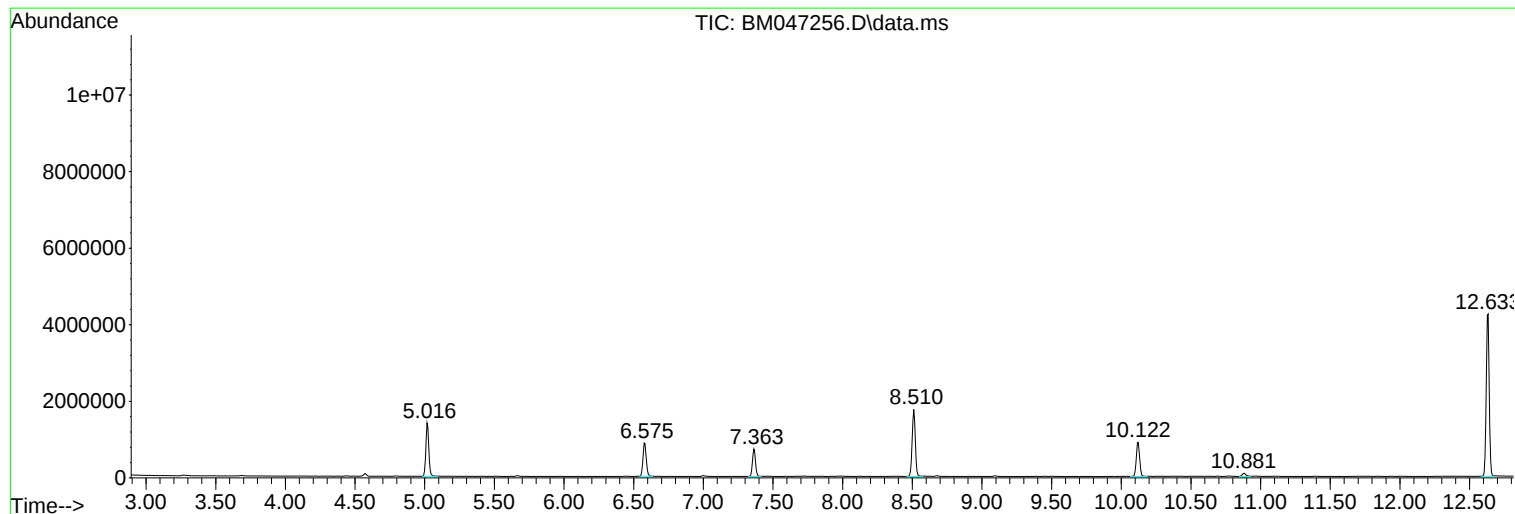
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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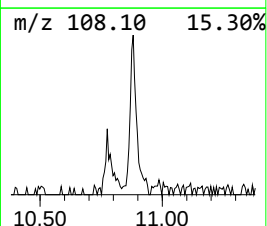
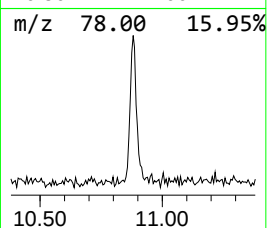
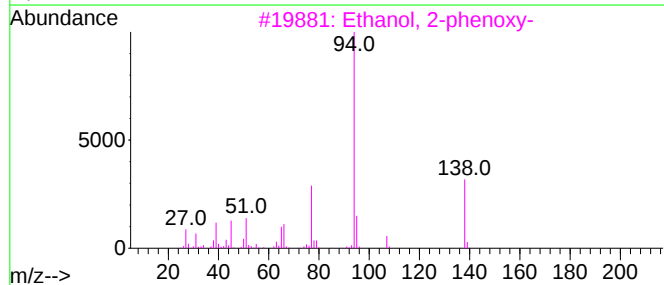
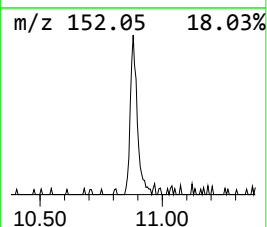
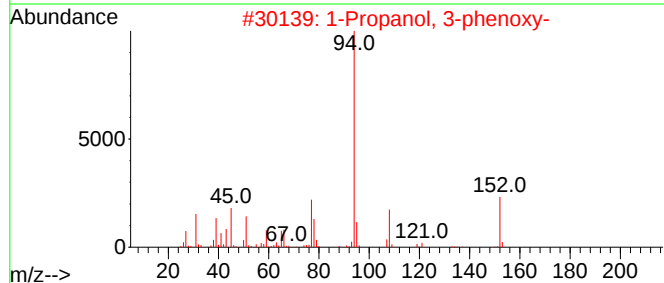
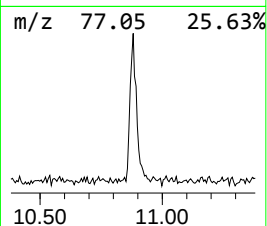
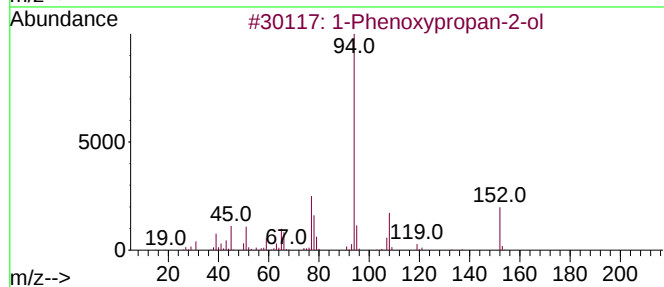
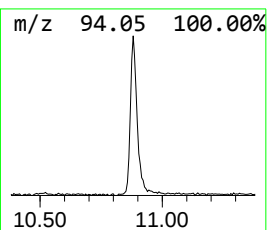
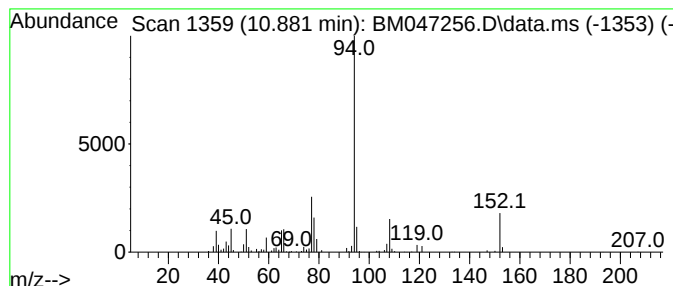
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.881	2.11 ng	156040	Naphthalene-d8	10.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	59
5			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59



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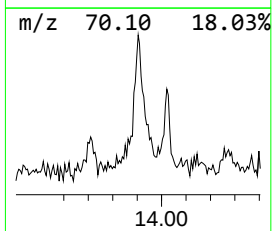
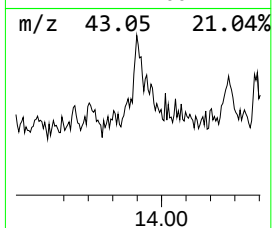
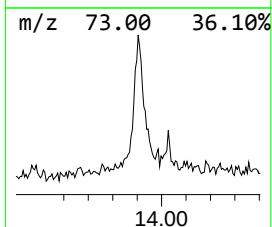
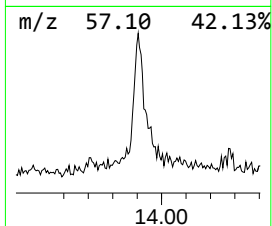
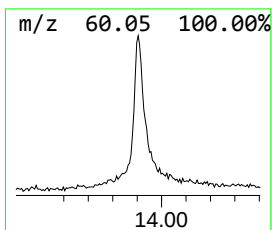
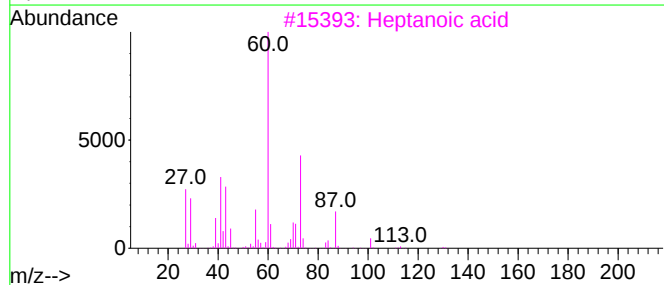
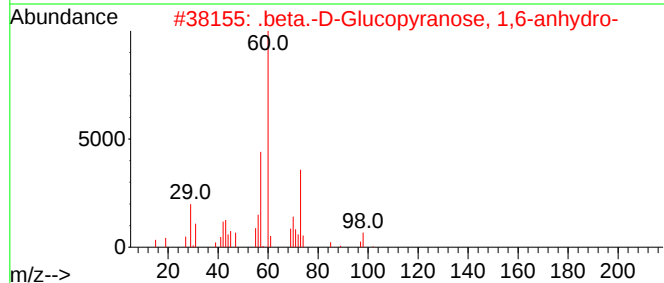
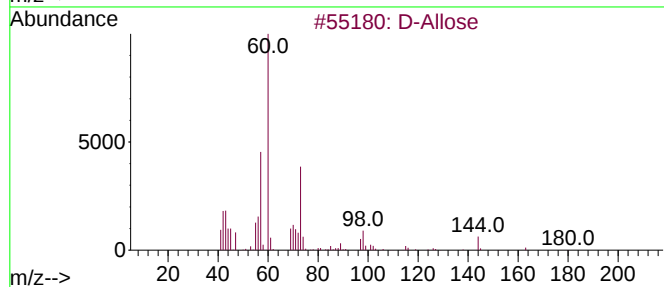
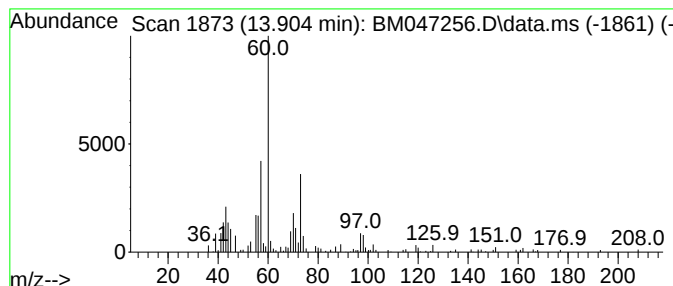
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Peak Number 2 D-Allose Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	2.08 ng	217149	Acenaphthene-d10	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Allose	180	C6H12O6	002595-97-3	80
2			.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	72
3			Heptanoic acid	130	C7H14O2	000111-14-8	59
4			Pentanoic acid	102	C5H10O2	000109-52-4	59
5			Butanoic acid	88	C4H8O2	000107-92-6	59



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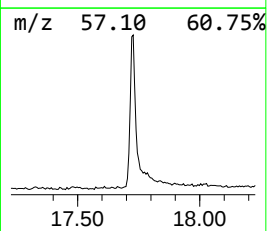
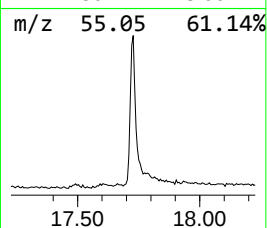
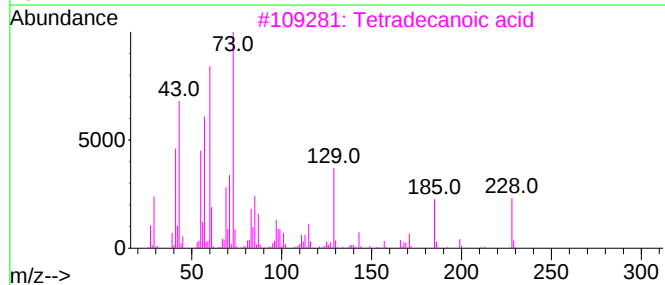
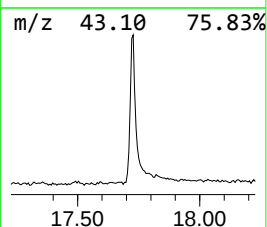
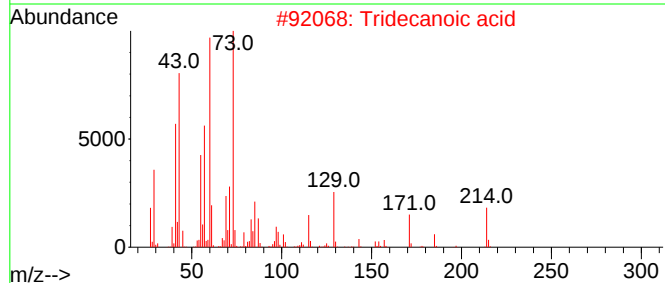
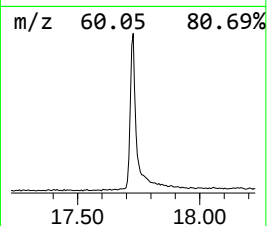
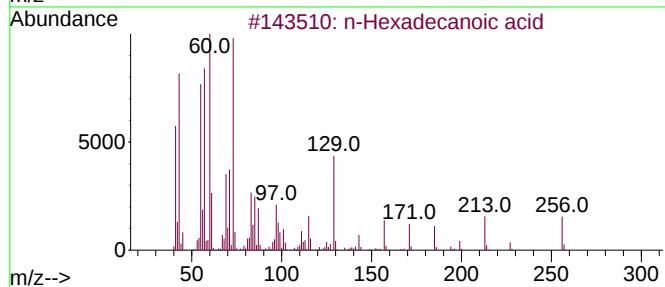
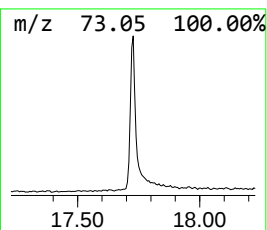
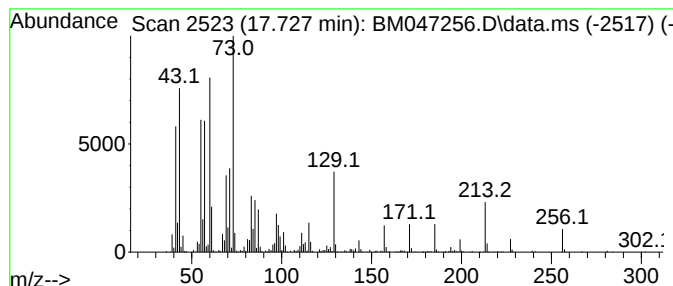
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.727	9.42 ng	1272280	Phenanthrene-d10	16.786

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	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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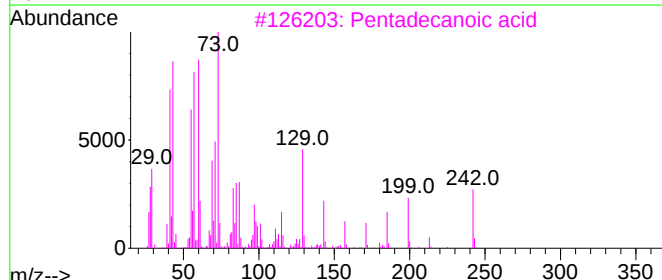
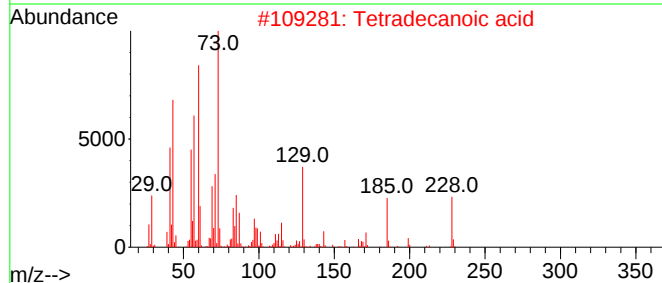
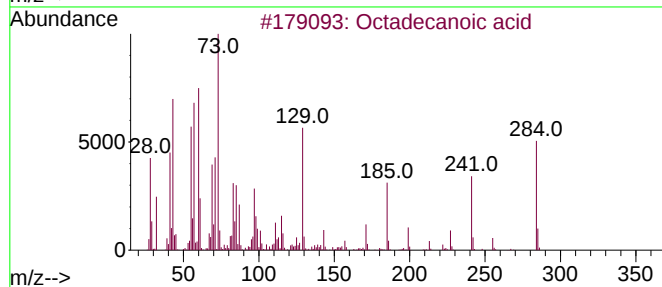
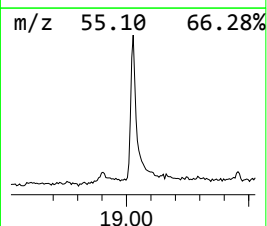
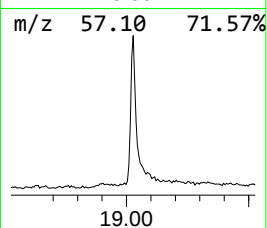
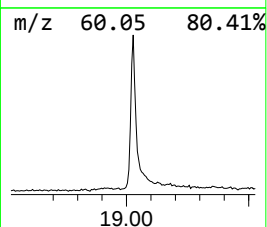
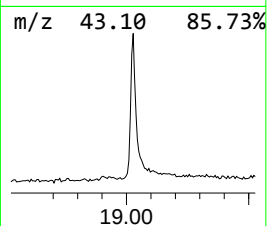
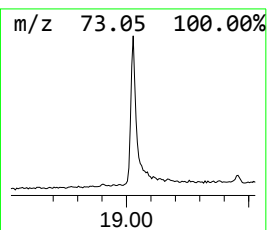
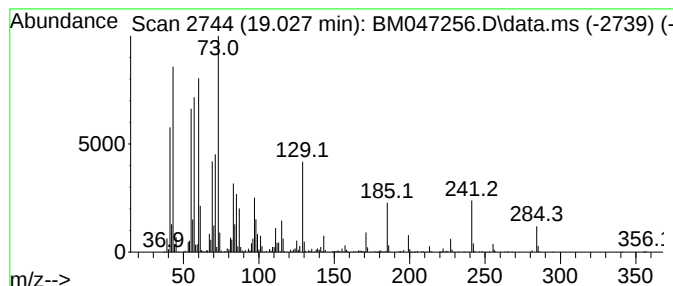
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Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.027	8.64 ng	1473120	Chrysene-d12	21.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
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
1-Phenoxypropan...	10.881	2.1	ng	156040	2	10.122	1480730	20.0
D-Allose	13.904	2.1	ng	217149	3	14.027	2092430	20.0
n-Hexadecanoic ...	17.727	9.4	ng	1272280	4	16.786	2702210	20.0
Octadecanoic acid	19.027	8.6	ng	1473120	5	21.027	3409350	20.0