

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111522\
 Data File : BG055634.D
 Acq On : 15 Nov 2022 23:13
 Operator : CG/JU
 Sample : N5431-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20221170-COMP-05-MODIFIED-ELUTRIATE

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_G\Methods\8270-BG110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055634.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.692	232	239	245	rBV3	13640	21753	1.13%	0.215%
2	5.309	338	344	351	rBV	41354	66932	3.49%	0.660%
3	5.779	418	424	432	rBV	211156	344510	17.94%	3.398%
4	7.389	690	698	707	rBV	179078	307132	16.00%	3.030%
5	8.258	839	846	852	rBV	140765	240939	12.55%	2.377%
6	9.427	1037	1045	1054	rVB	247708	439958	22.92%	4.340%
7	11.084	1319	1327	1335	rBV	201666	357637	18.63%	3.528%
8	13.505	1730	1739	1746	rBV	693505	1074565	55.97%	10.600%
9	14.880	1966	1973	1981	rVB	357952	557921	29.06%	5.504%
10	16.355	2218	2224	2236	rBV	651872	1021107	53.18%	10.073%
11	16.983	2322	2331	2339	rBV2	22287	38340	2.00%	0.378%
12	17.618	2432	2439	2445	rBV	524227	775454	40.39%	7.650%
13	18.258	2544	2548	2554	rVB	37077	46111	2.40%	0.455%
14	18.352	2560	2564	2573	rBV5	15032	25202	1.31%	0.249%
15	18.481	2578	2586	2597	rBV	263587	436076	22.71%	4.302%
16	19.416	2741	2745	2752	rVB4	22527	29351	1.53%	0.290%
17	19.621	2772	2780	2788	rBV8	24901	68315	3.56%	0.674%
18	19.739	2795	2800	2812	rBV	127308	211075	10.99%	2.082%
19	20.015	2843	2847	2856	rVB2	15745	27907	1.45%	0.275%
20	20.203	2873	2879	2886	rBV	1499343	1919920	100.00%	18.939%
21	21.537	3100	3106	3123	rBV3	67730	275839	14.37%	2.721%
22	21.778	3144	3147	3152	rVB2	20284	28618	1.49%	0.282%
23	21.913	3164	3170	3185	rVB2	494470	862348	44.92%	8.507%
24	23.681	3467	3471	3479	rVB4	33616	69041	3.60%	0.681%
25	25.326	3741	3751	3766	rVB2	290216	891256	46.42%	8.792%

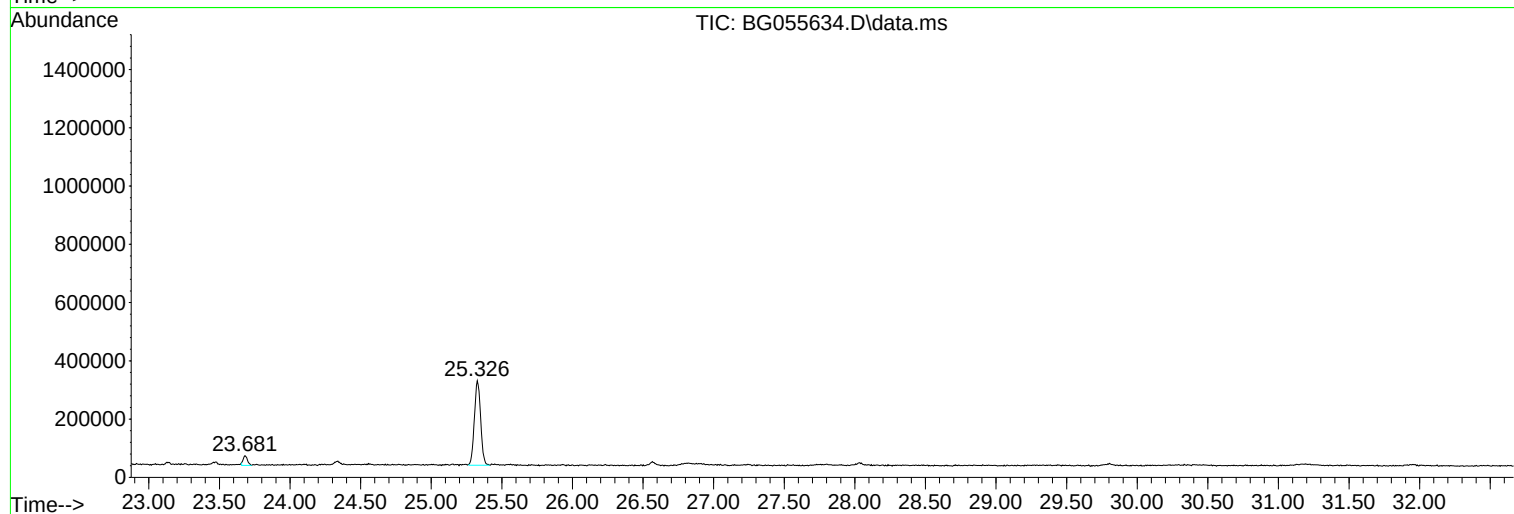
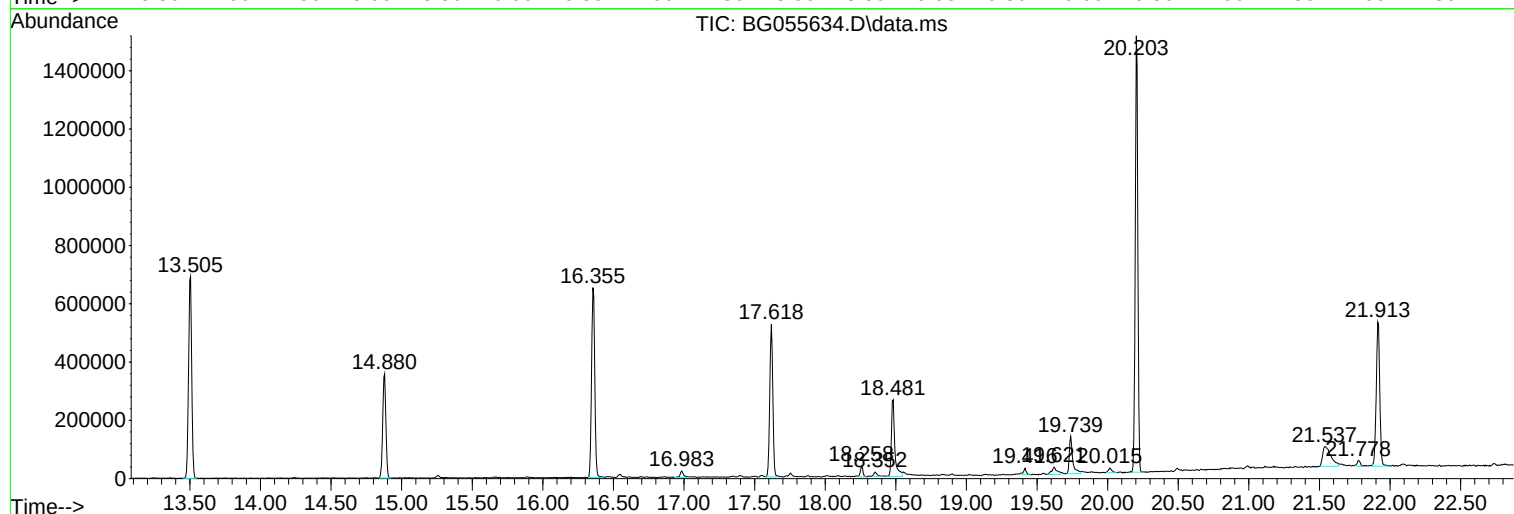
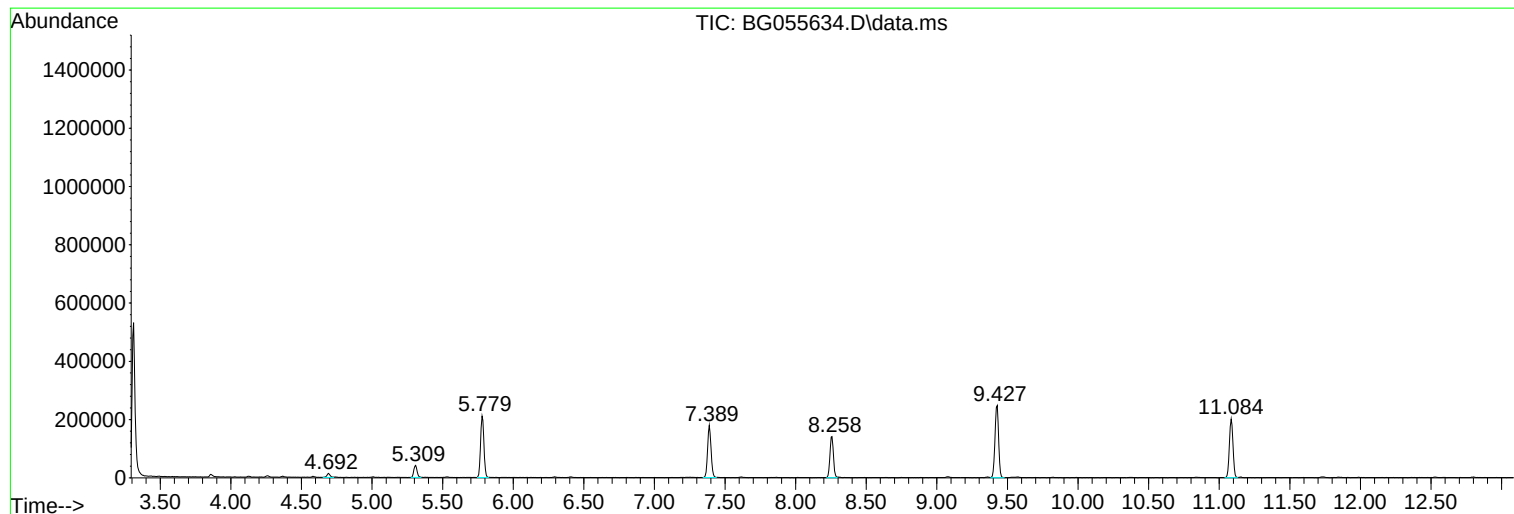
Sum of corrected areas: 10137307

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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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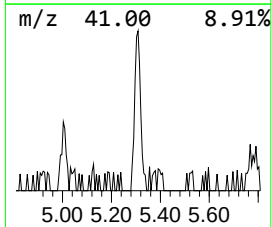
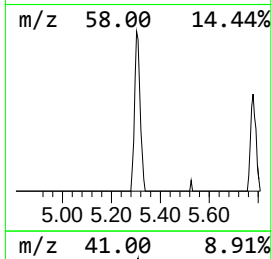
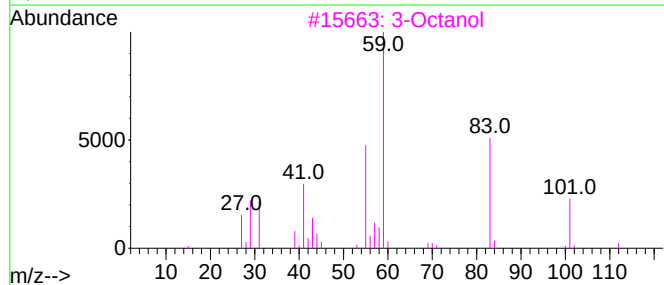
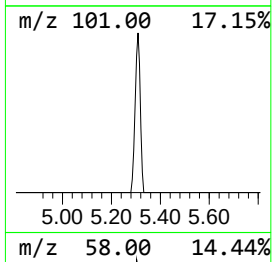
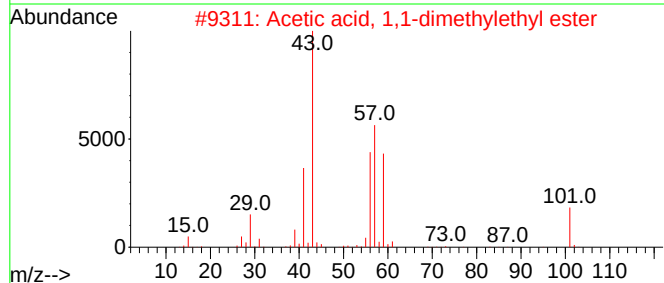
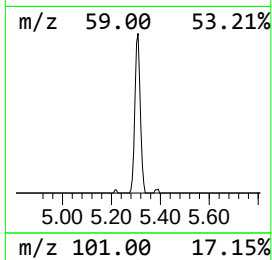
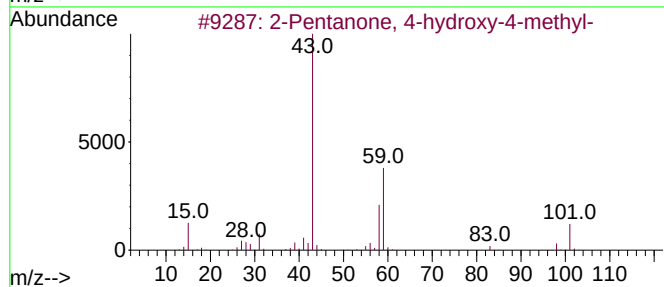
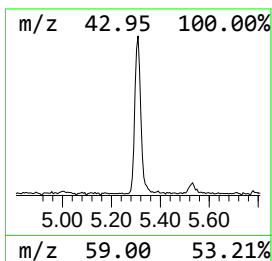
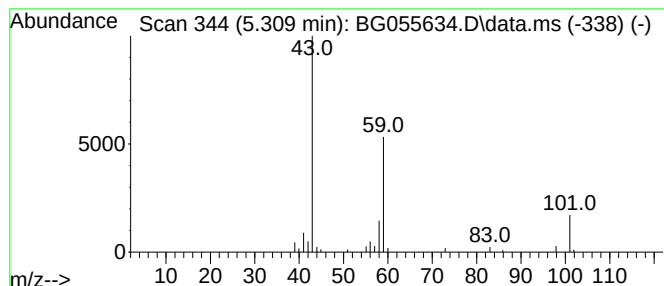
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.309	5.56 ng	66932	1,4-Dichlorobenzene-d4	8.258

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		3-Octanol	130	C8H18O	000589-98-0	36
4		3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	33
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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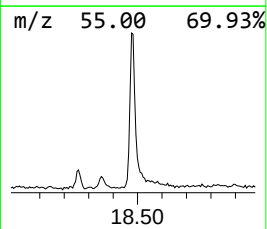
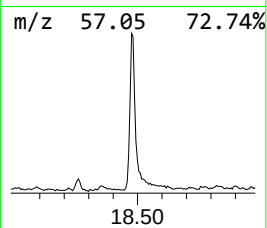
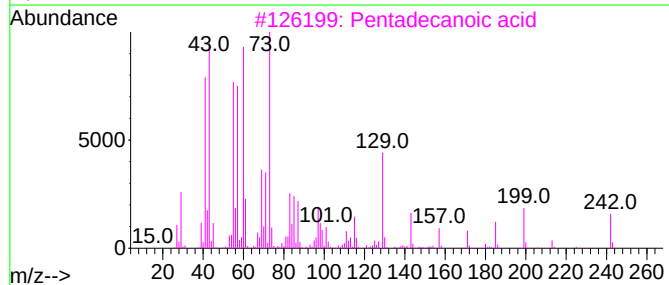
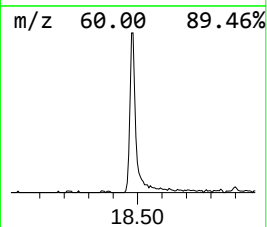
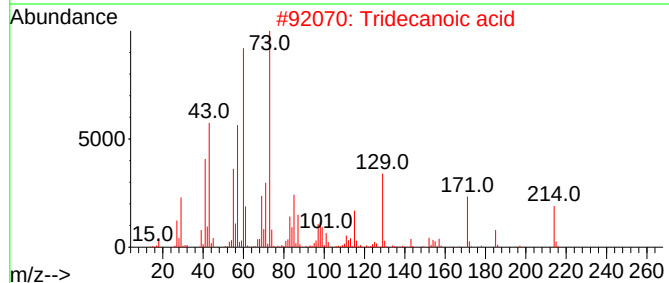
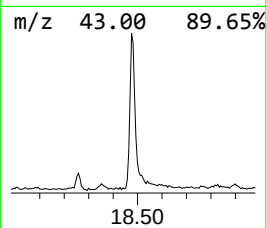
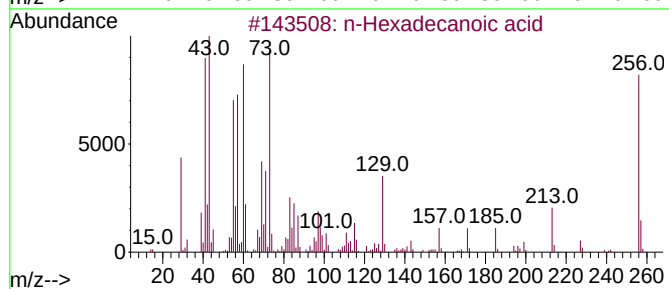
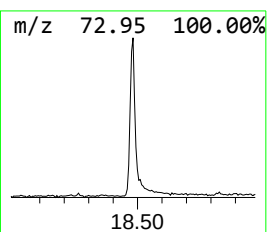
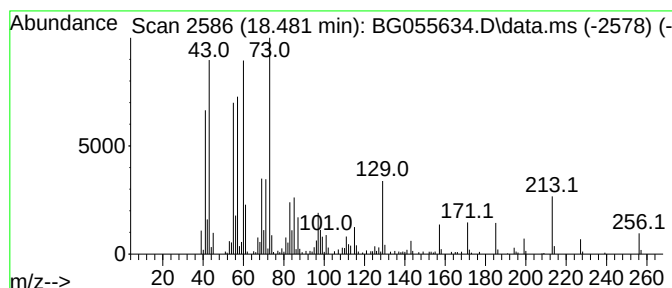
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.482	11.25 ng	436076	Phenanthrene-d10	17.618

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	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Octanoic acid	144	C8H16O2	000124-07-2	49



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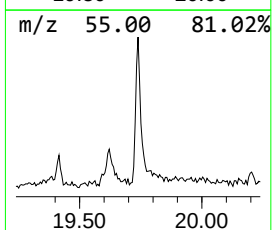
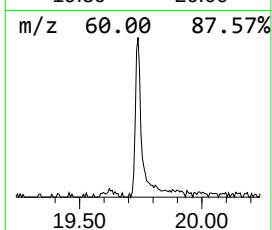
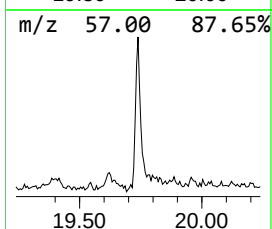
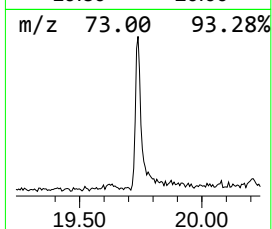
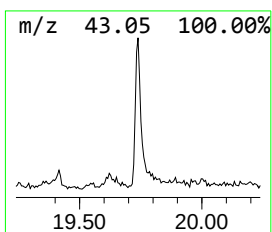
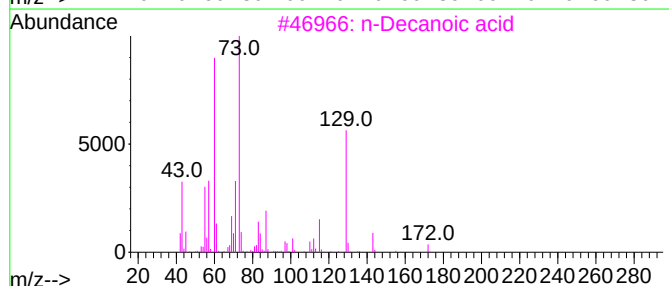
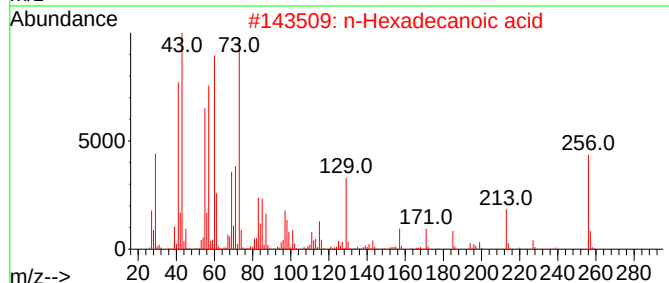
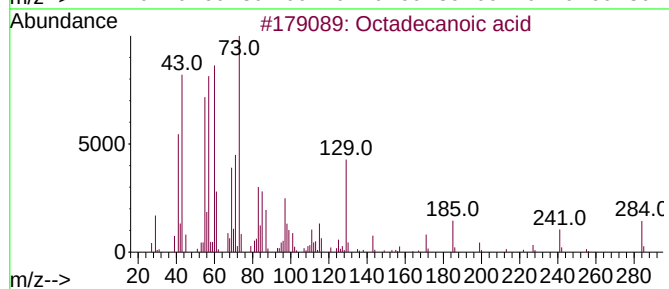
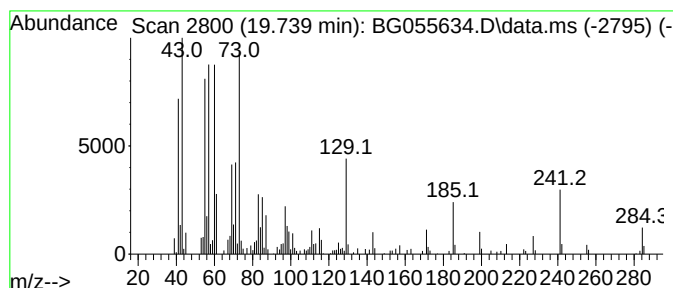
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Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.739	5.44 ng	211075	Phenanthrene-d10	17.618	
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	93
3	n-Decanoic acid	172	C10H20O2	000334-48-5	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	64



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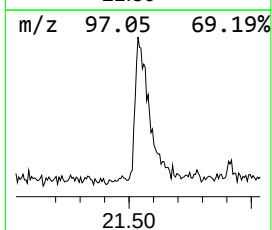
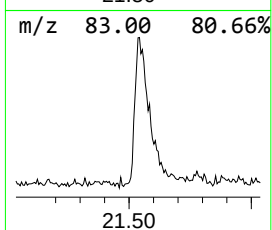
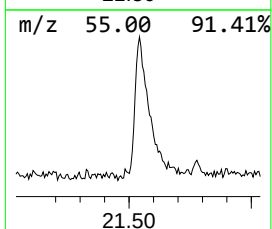
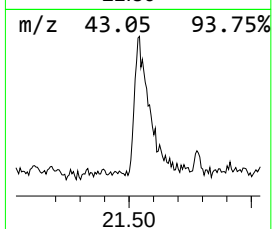
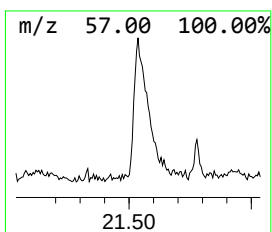
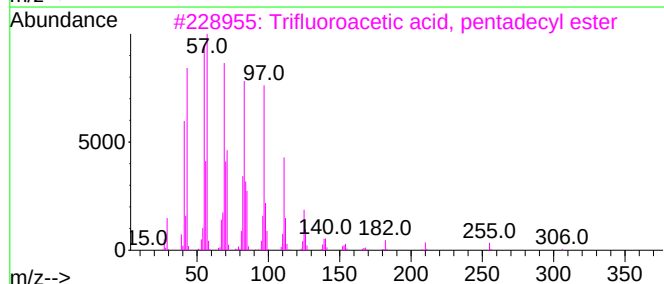
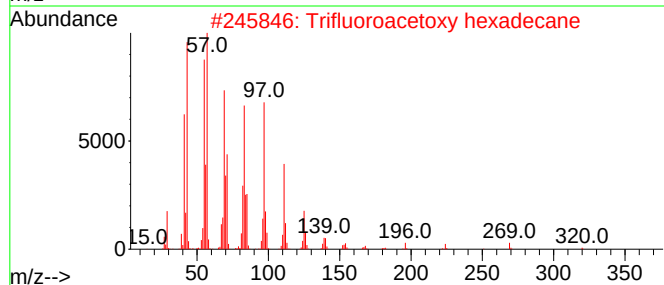
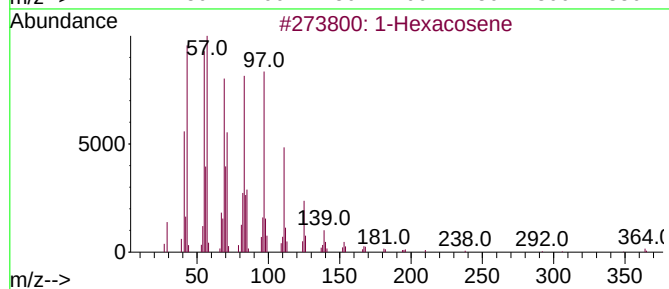
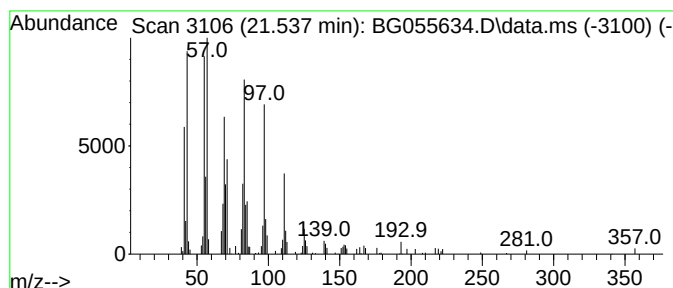
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Peak Number 4 1-Hexacosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.537	6.40 ng	275839	Chrysene-d12	21.913

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	94
2	Trifluoroacetoxy hexadecane			338	C18H33F3O2	006222-03-3	94
3	Trifluoroacetic acid, pentadecyl...			324	C17H31F3O2	959010-23-2	94
4	Behenic alcohol			326	C22H46O	000661-19-8	91
5	Cyclotetracosane			336	C24H48	000297-03-0	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.309	5.6	ng	66932	1	8.258	240939	20.0
n-Hexadecanoic ...	18.482	11.3	ng	436076	4	17.618	775454	20.0
Octadecanoic acid	19.739	5.4	ng	211075	4	17.618	775454	20.0
1-Hexacosene	21.537	6.4	ng	275839	5	21.913	862348	20.0