

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG083122\
 Data File : BG054804.D
 Acq On : 31 Aug 2022 13:13
 Operator : CG/JU
 Sample : N4423-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-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_G\Methods\8270-BG082522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054804.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.211	321	327	334	rVB	95234	146980	4.97%	0.945%
2	5.687	401	408	421	rBV	611811	979835	33.10%	6.299%
3	7.297	675	682	695	rVB	614761	1062635	35.90%	6.831%
4	8.149	819	827	834	rBV	133230	221797	7.49%	1.426%
5	9.324	1017	1027	1038	rBV	355787	655587	22.15%	4.215%
6	10.975	1300	1308	1316	rBV	174764	322118	10.88%	2.071%
7	13.408	1714	1722	1730	rBV	1066473	1660639	56.10%	10.676%
8	14.783	1949	1956	1964	rBV	295968	470764	15.90%	3.026%
9	16.269	2202	2209	2220	rBV	1003825	1540878	52.06%	9.906%
10	17.532	2417	2424	2430	rBV	397754	638398	21.57%	4.104%
11	18.173	2529	2533	2537	rVB	28326	35370	1.19%	0.227%
12	19.918	2810	2830	2845	rBV	235922	1072446	36.23%	6.894%
13	20.129	2860	2866	2879	rVB	2281157	2959899	100.00%	19.028%
14	21.434	3076	3088	3105	rVB2	334543	1128425	38.12%	7.254%
15	21.821	3147	3154	3160	rBV	403911	702638	23.74%	4.517%
16	22.632	3288	3292	3297	rVB2	18964	41015	1.39%	0.264%
17	23.108	3361	3373	3390	rVB2	154187	744987	25.17%	4.789%
18	23.355	3410	3415	3427	rVB4	36998	106547	3.60%	0.685%
19	25.194	3720	3728	3744	rVB2	312352	1064548	35.97%	6.844%

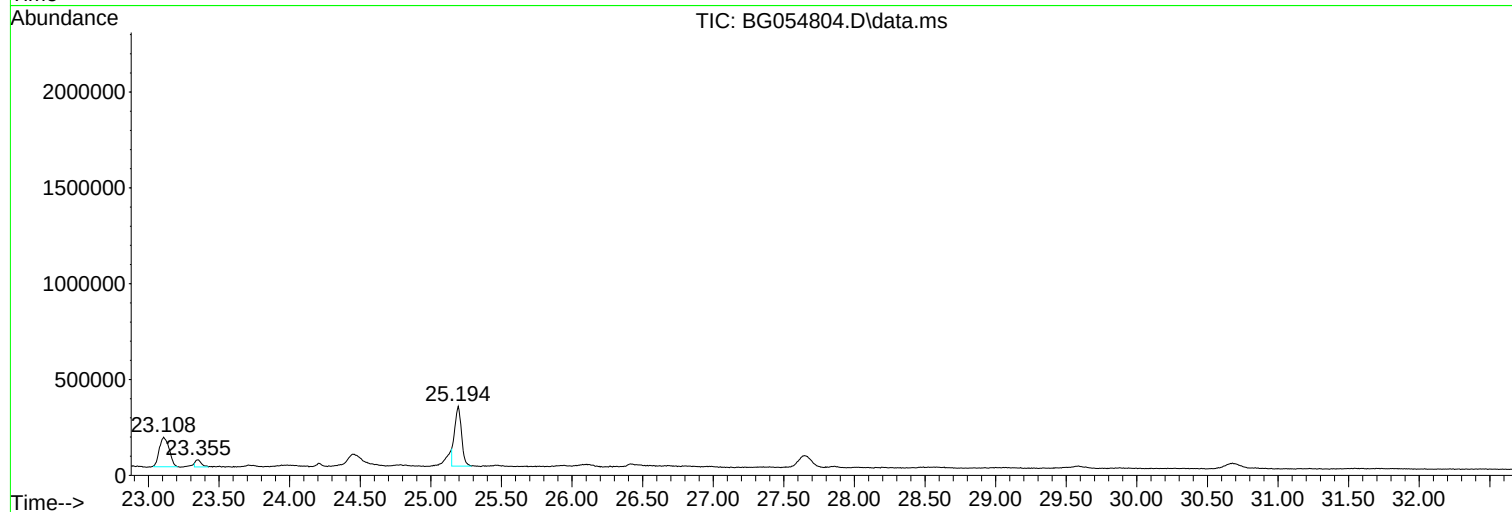
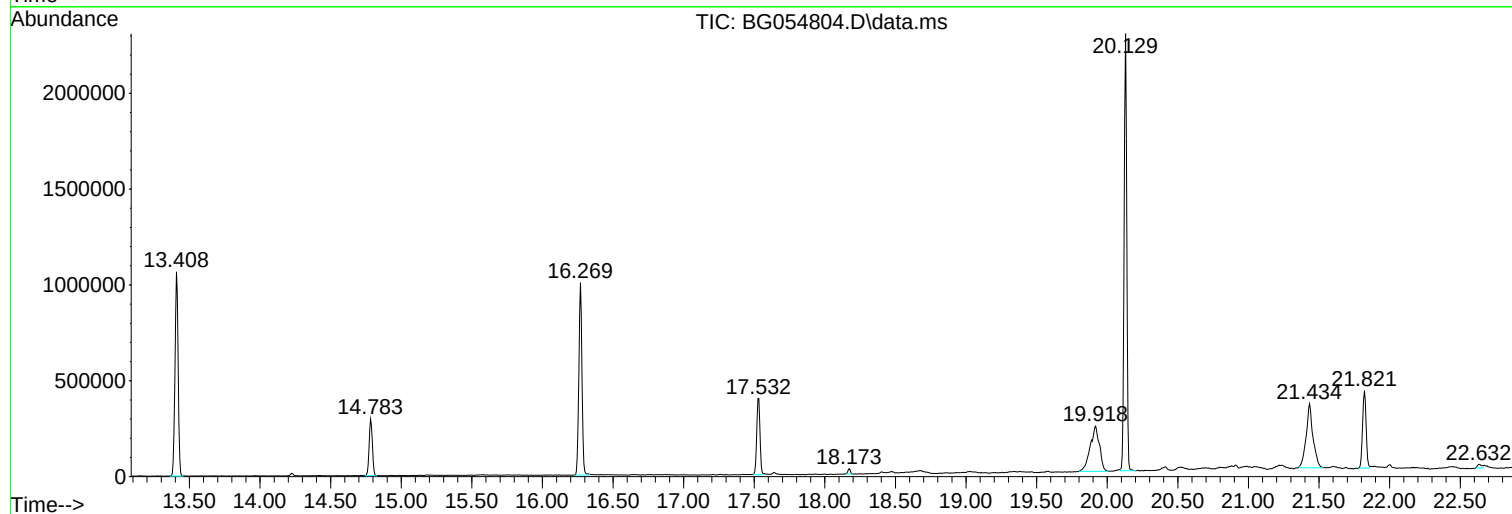
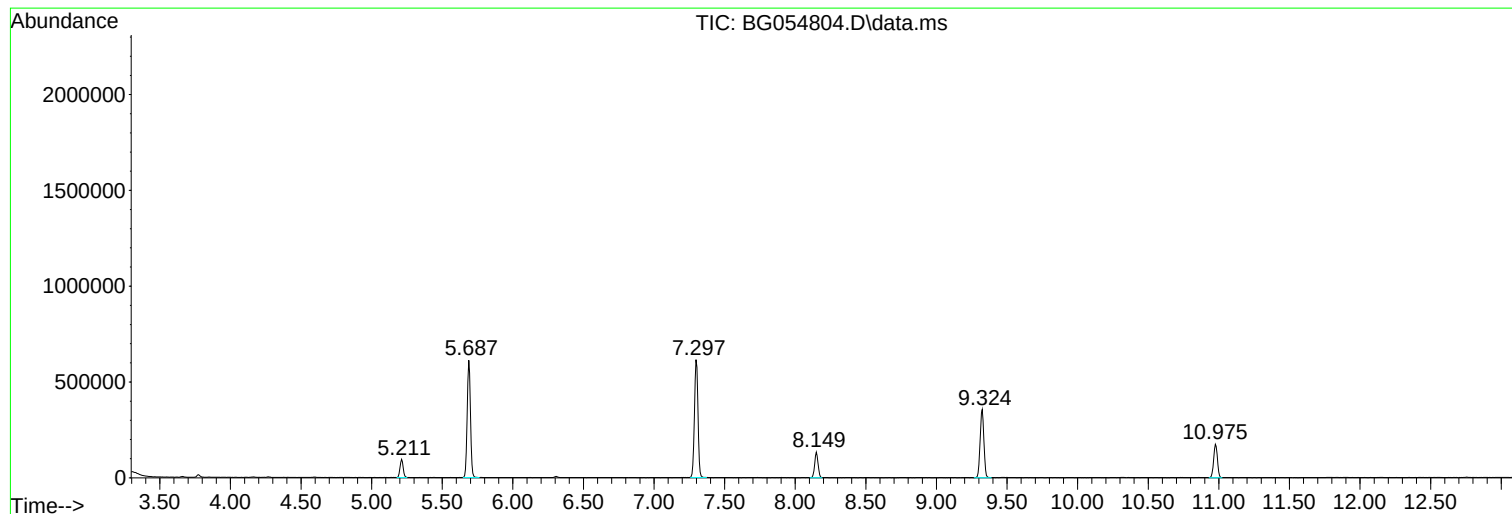
Sum of corrected areas: 15555506

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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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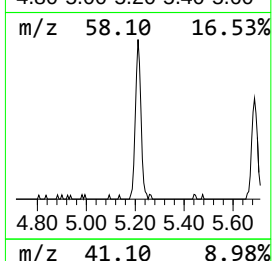
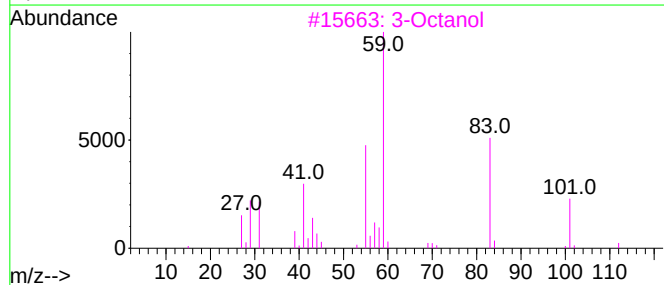
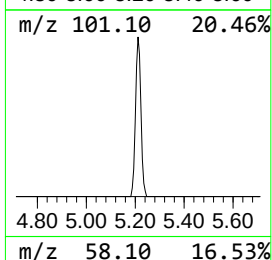
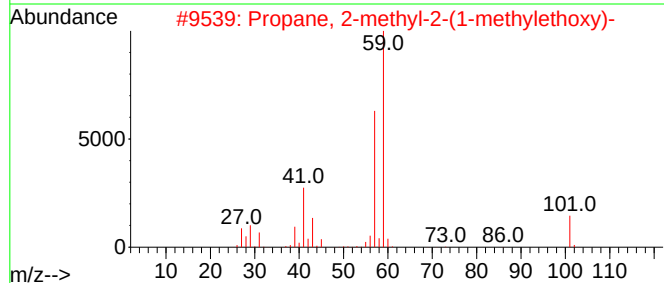
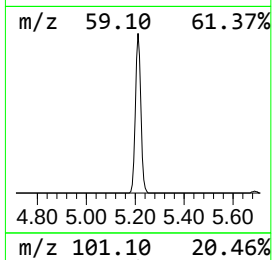
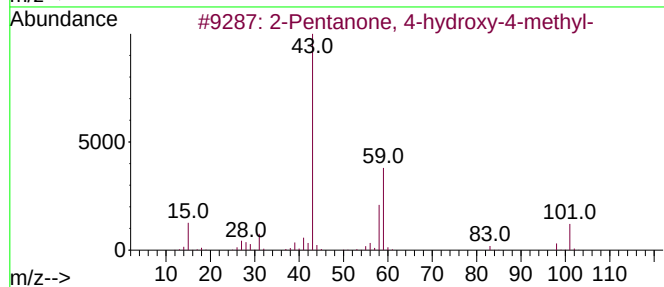
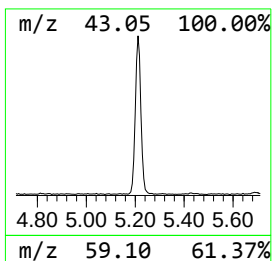
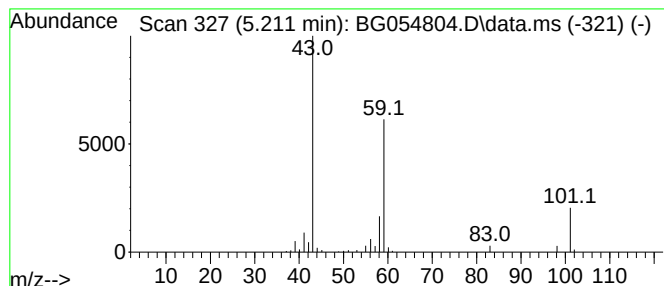
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.211	13.25 ng	146980	1,4-Dichlorobenzene-d4	8.149

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			3-Octanol	130	C8H18O	000589-98-0	36
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23



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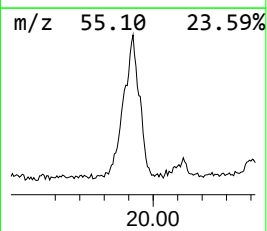
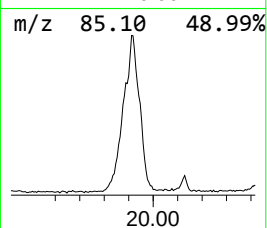
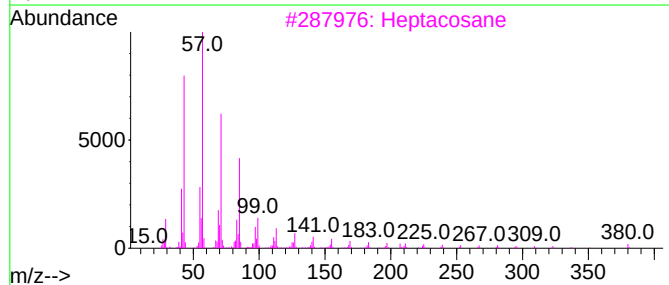
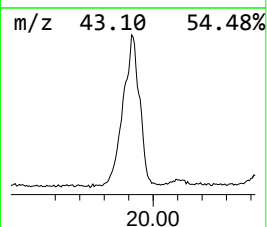
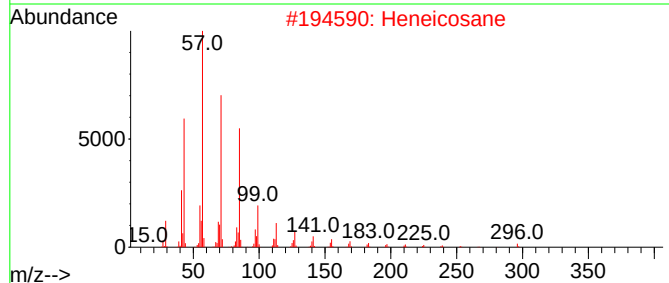
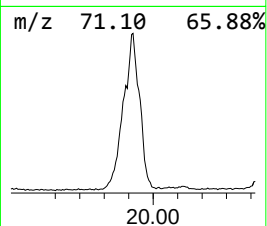
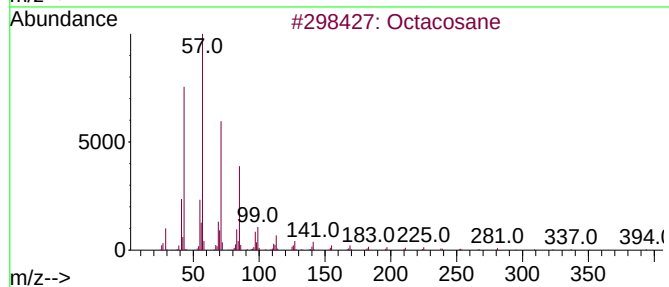
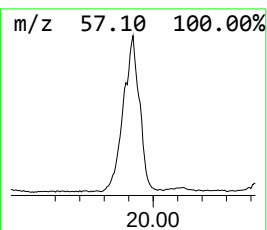
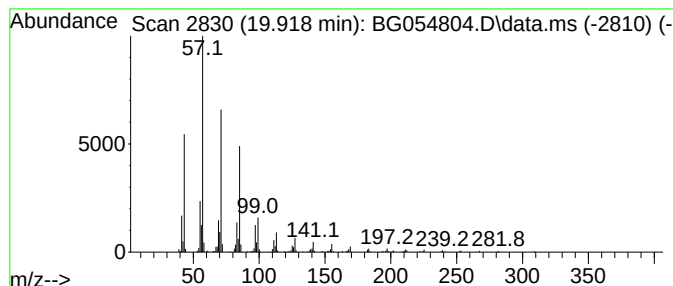
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.918	30.53 ng	1072450	Chrysene-d12	21.821

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Heptacosane	380	C27H56	000593-49-7	91
4			Triacontane	422	C30H62	000638-68-6	91
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



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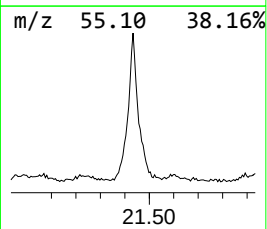
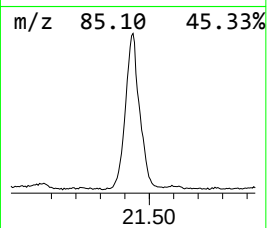
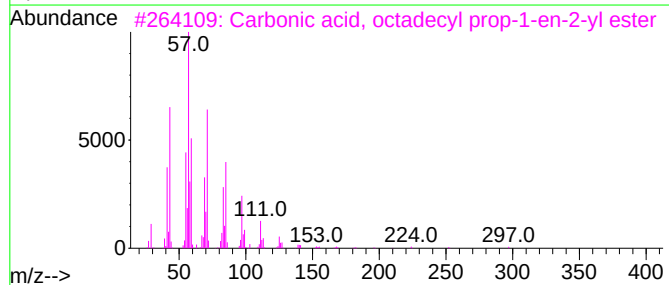
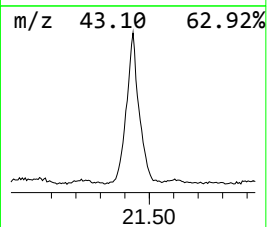
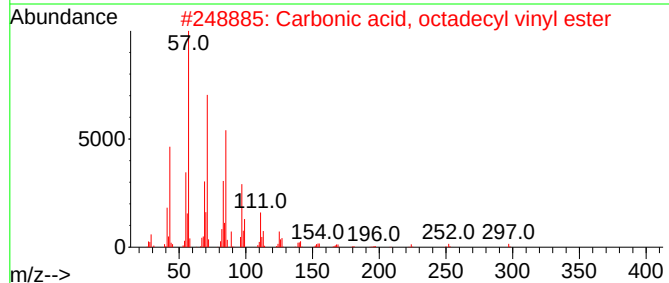
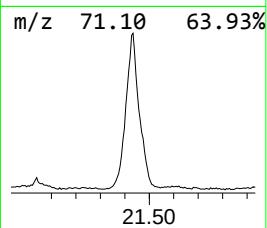
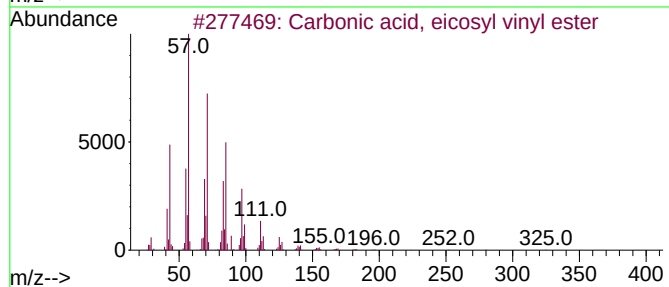
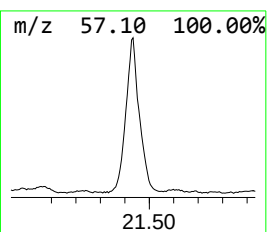
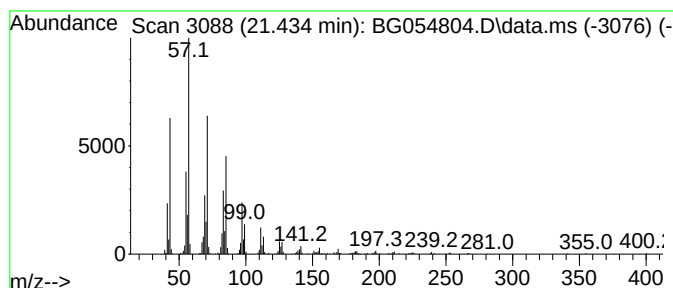
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Peak Number 3 Carbonic acid, eicosyl vinyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.434	32.12 ng	1128430	Chrysene-d12	21.821

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	94
2			Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	91
3			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
4			Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1010309-12-5	91
5			Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	91



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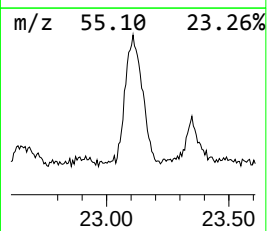
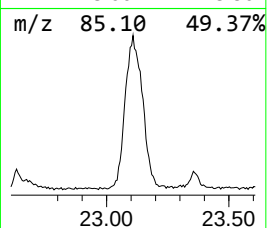
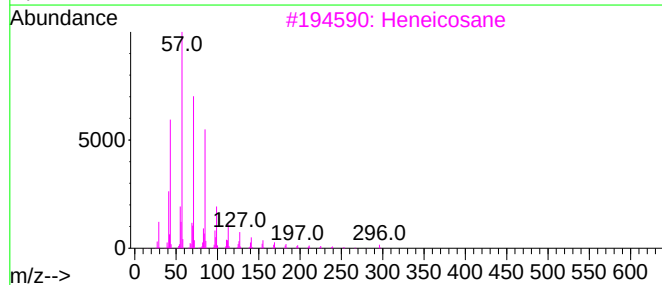
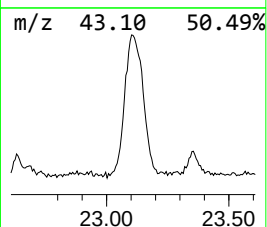
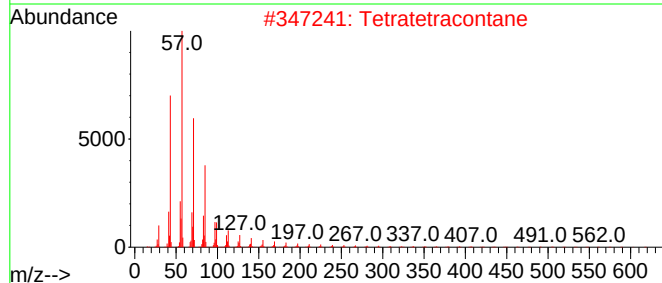
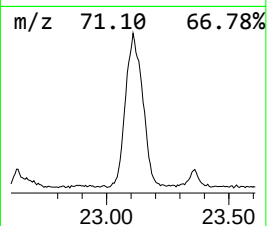
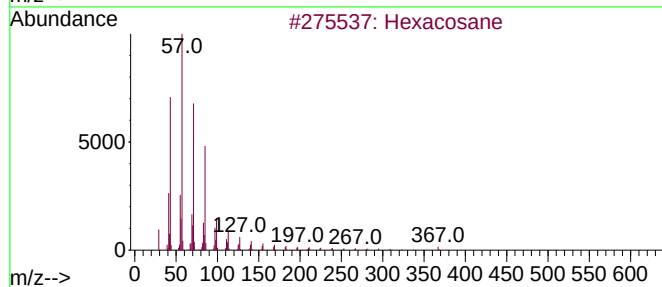
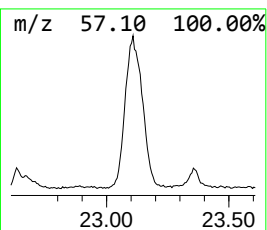
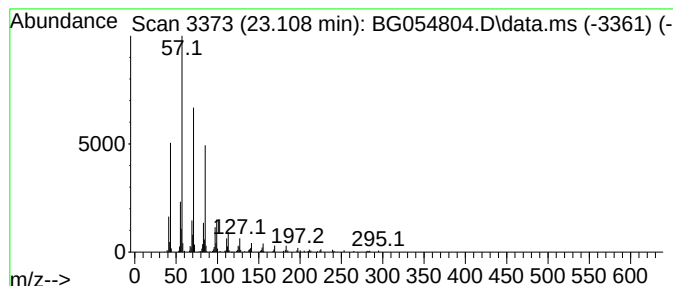
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Peak Number 4 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.108	21.21 ng	744987	Chrysene-d12	21.821

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	94
2			Tetratetracontane	619	C44H90	007098-22-8	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Triacontane	422	C30H62	000638-68-6	91
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91



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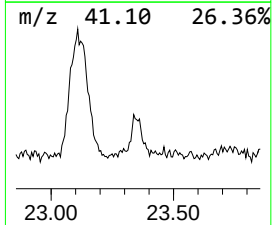
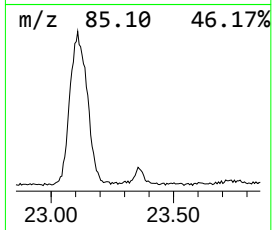
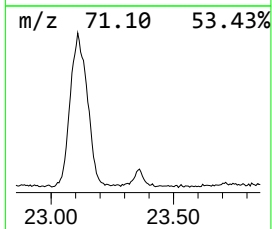
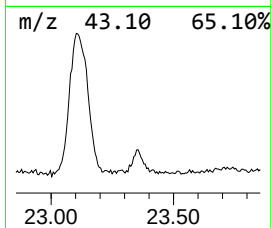
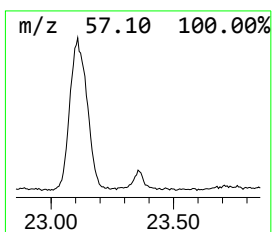
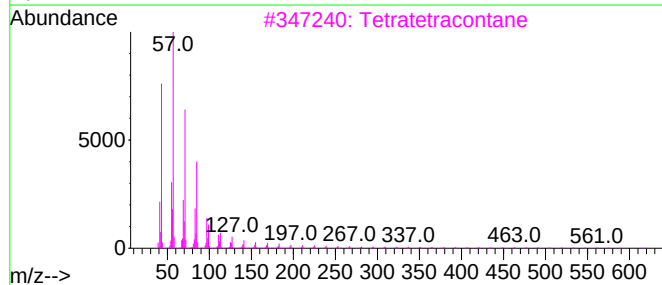
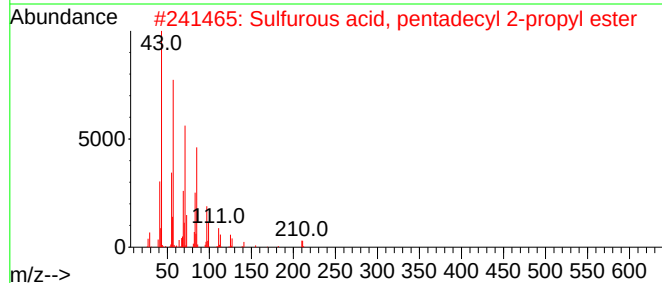
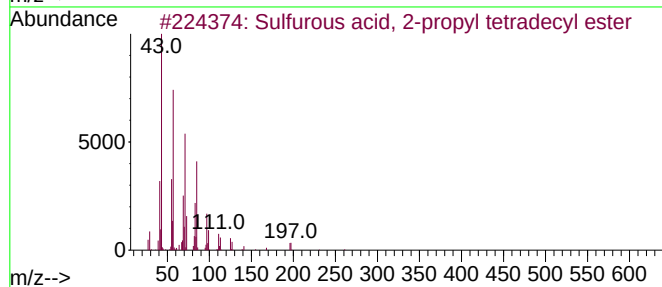
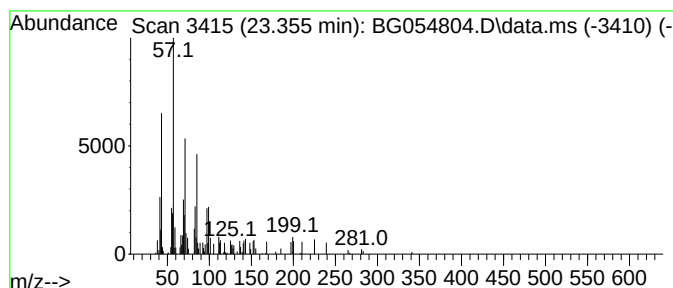
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Sulfurous acid, 2-propyl te... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.355	3.03 ng	106547	Chrysene-d12	21.821

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-propyl tetradecyl ester	320	C17H36O3S	1010309-12-5	74
2			Sulfurous acid, pentadecyl 2-propyl ester	334	C18H38O3S	1000309-12-6	72
3			Tetratetracontane	619	C44H90	007098-22-8	64
4			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	64
5			Sulfurous acid, dodecyl 2-propyl ester	292	C15H32O3S	1000309-12-3	64



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.211	13.3	ng	146980	1	8.149	221797	20.0
Octacosane	19.918	30.5	ng	1072450	5	21.821	702638	20.0
Carbonic acid, ...	21.434	32.1	ng	1128430	5	21.821	702638	20.0
Hexacosane	23.108	21.2	ng	744987	5	21.821	702638	20.0
Sulfurous acid,...	23.355	3.0	ng	106547	5	21.821	702638	20.0