

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071522\
 Data File : BM035834.D
 Acq On : 15 Jul 2022 17:36
 Operator : CG/JU
 Sample : N3726-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 HL-12-12.5

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-BM071322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035834.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.999	318	325	335	rVB2	75785	128905	1.16%	0.175%
2	5.463	397	404	422	rBV	5865700	8061543	72.78%	10.970%
3	7.069	669	677	687	rBV	5459392	8389399	75.74%	11.417%
4	7.904	812	819	827	rVB	1293095	1947885	17.59%	2.651%
5	9.069	1008	1017	1031	rBV	3188809	5208871	47.03%	7.088%
6	10.710	1288	1296	1305	rBV	1733540	2798328	25.26%	3.808%
7	13.169	1706	1714	1728	rBV	7614590	11076531	100.00%	15.073%
8	14.539	1936	1947	1958	rBV	2435958	3468774	31.32%	4.720%
9	16.021	2192	2199	2221	rBV	5289376	7591308	68.54%	10.331%
10	17.274	2406	2412	2422	rBV	2548760	3559333	32.13%	4.844%
11	17.398	2429	2433	2438	rVB	79779	111076	1.00%	0.151%
12	18.180	2561	2566	2576	rBV	1099071	1599725	14.44%	2.177%
13	18.492	2615	2619	2625	rBV2	86911	153606	1.39%	0.209%
14	19.457	2779	2783	2793	rBV	570894	859207	7.76%	1.169%
15	19.898	2853	2858	2868	rVB	9068325	10849417	97.95%	14.764%
16	21.180	3072	3076	3083	rBV	288836	386637	3.49%	0.526%
17	21.450	3117	3122	3131	rBV	2195604	2829056	25.54%	3.850%
18	22.568	3308	3312	3325	rVB2	933322	1457000	13.15%	1.983%
19	22.721	3334	3338	3347	rVB	325896	502818	4.54%	0.684%
20	23.827	3520	3526	3537	rVB2	1246208	2504423	22.61%	3.408%

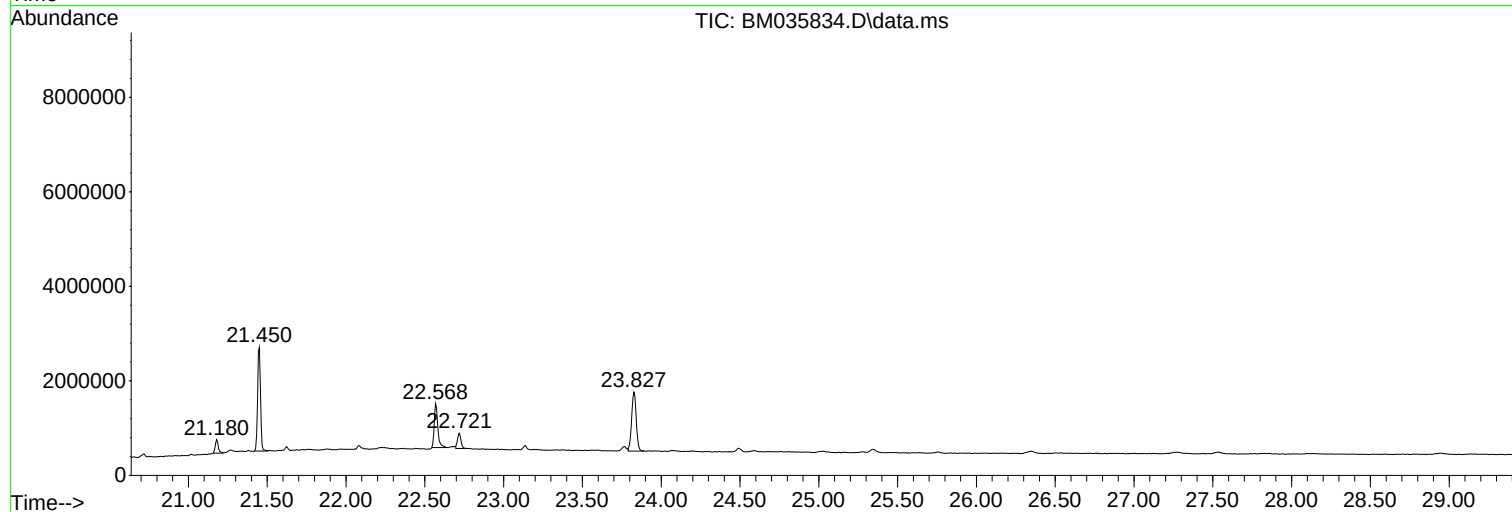
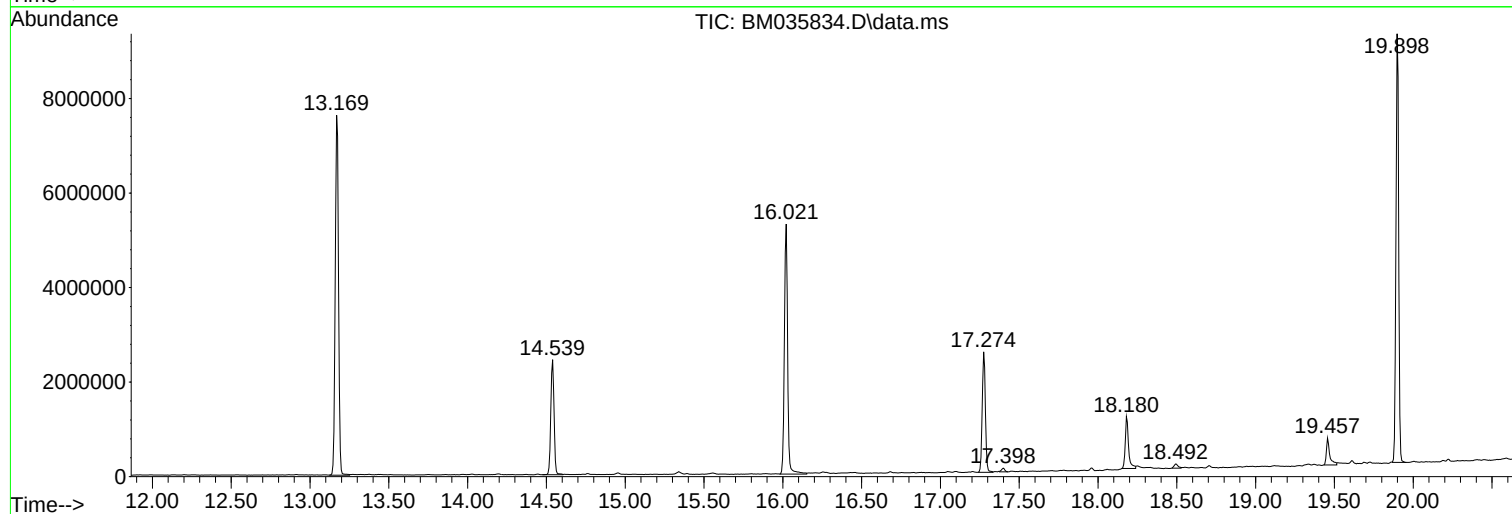
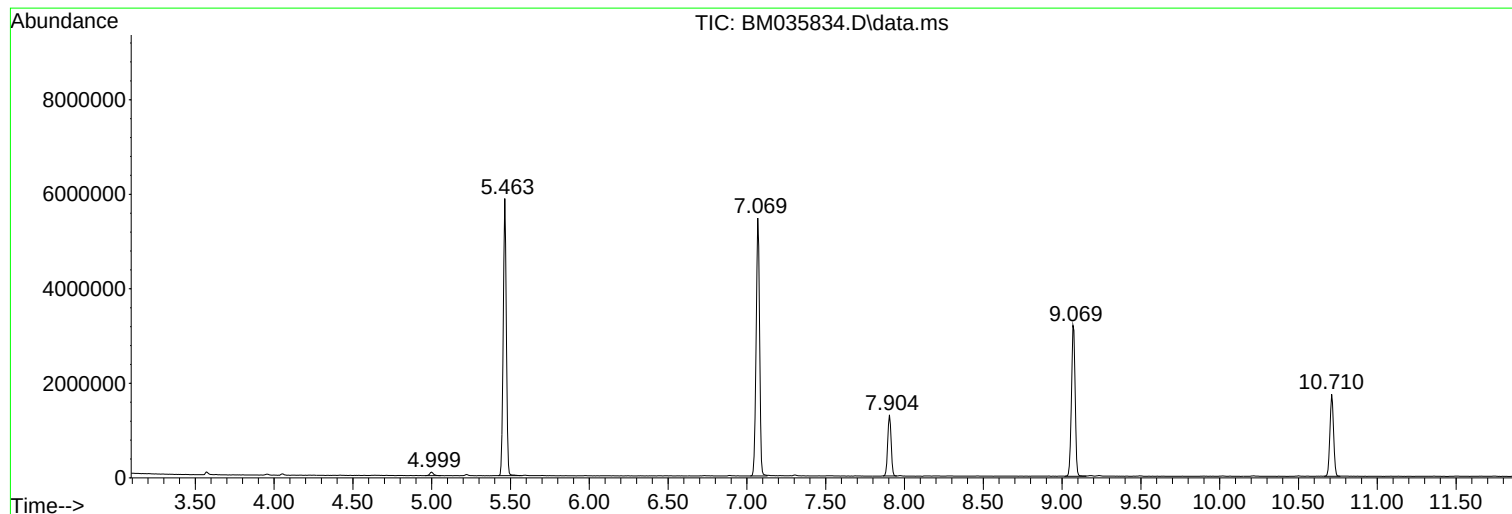
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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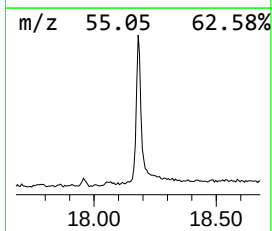
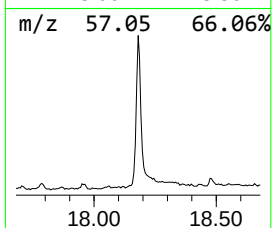
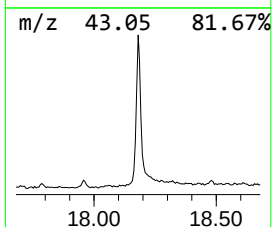
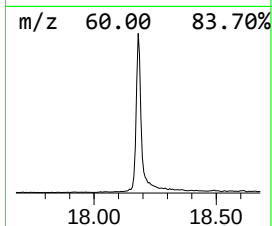
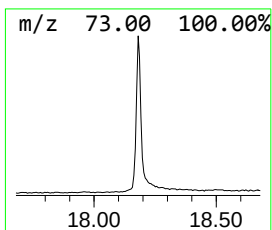
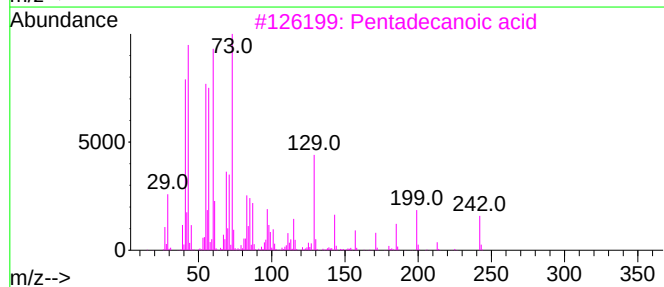
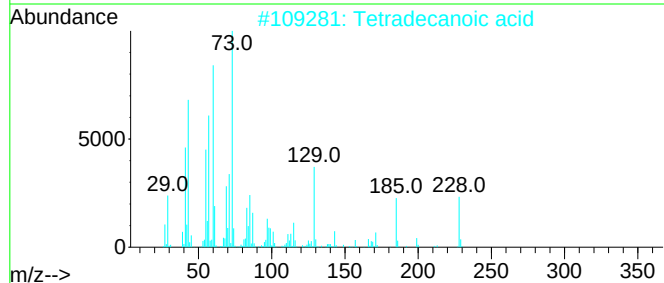
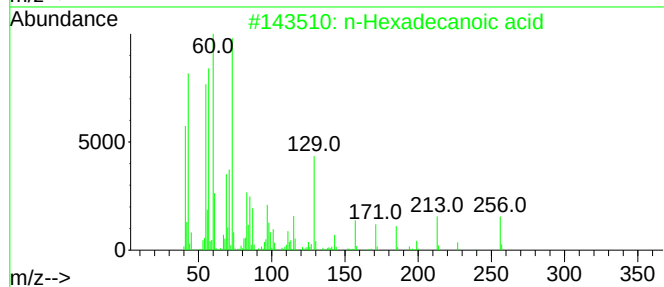
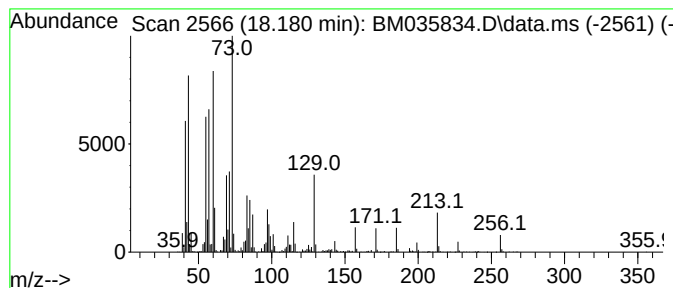
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.180	8.99 ng	1599730	Phenanthrene-d10	17.274

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			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	74
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



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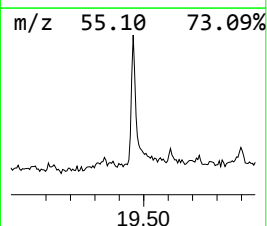
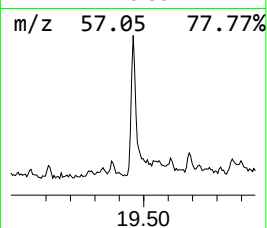
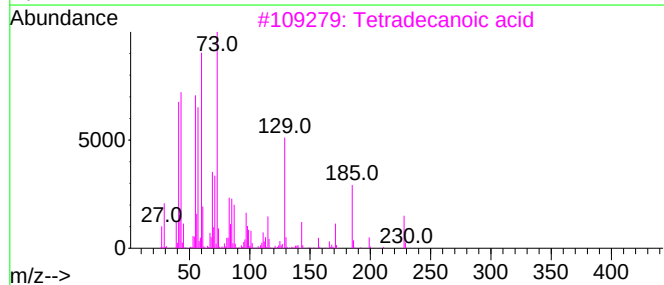
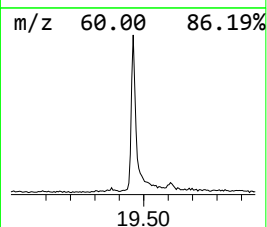
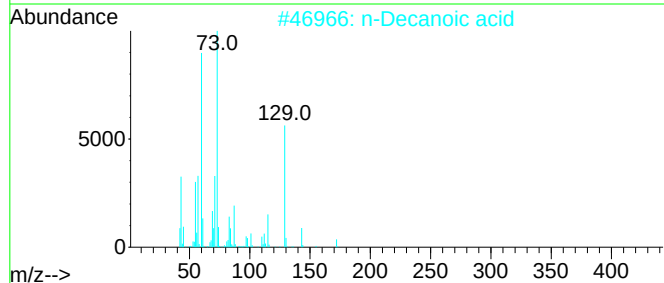
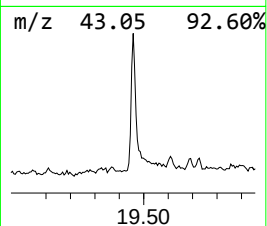
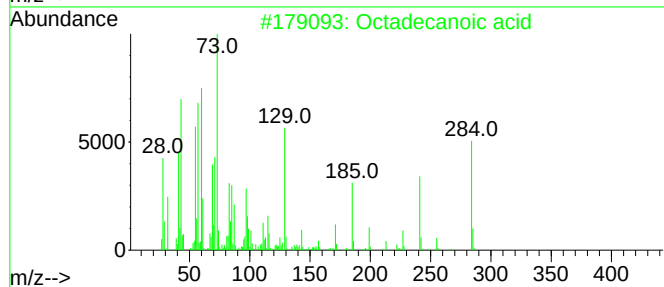
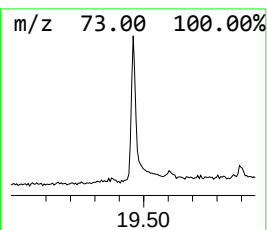
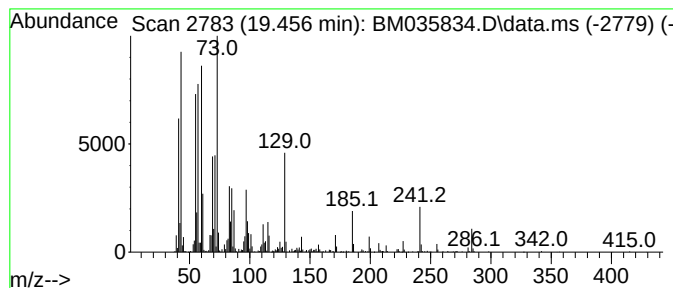
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.456	6.07 ng	859207	Chrysene-d12	21.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Decanoic acid	172	C10H20O2	000334-48-5	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83



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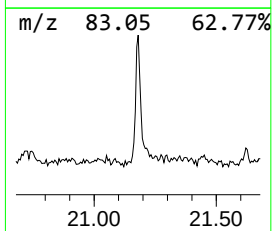
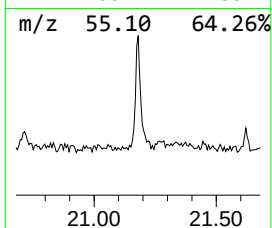
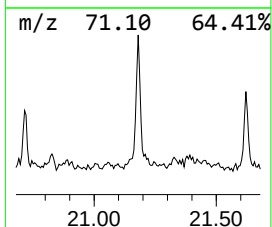
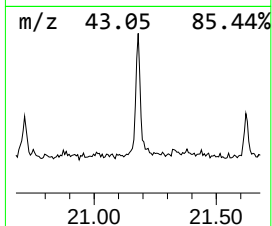
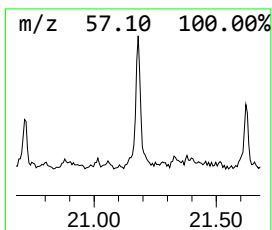
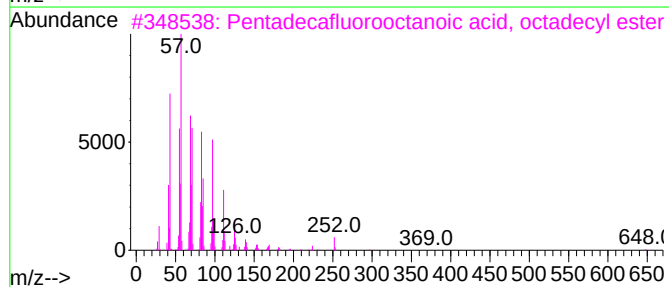
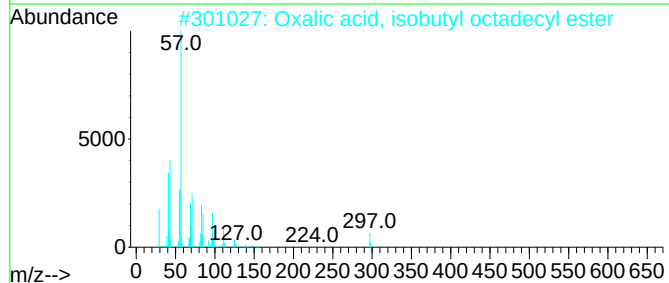
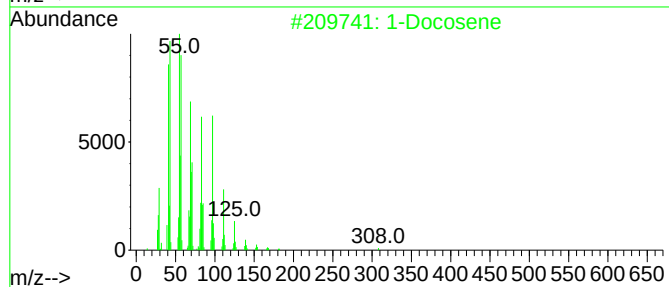
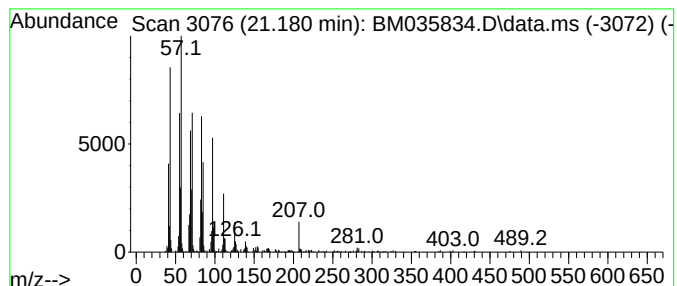
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	2.73 ng	386637	Chrysene-d12	21.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	91
2			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87
4			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
5			Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	87



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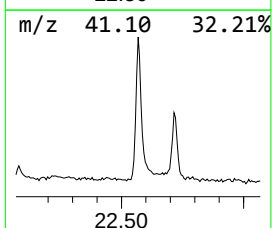
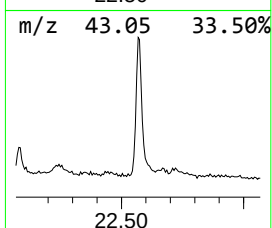
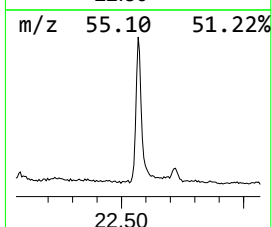
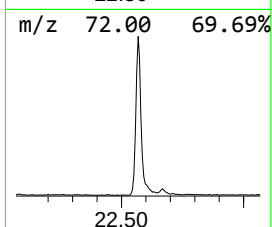
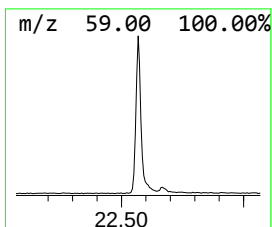
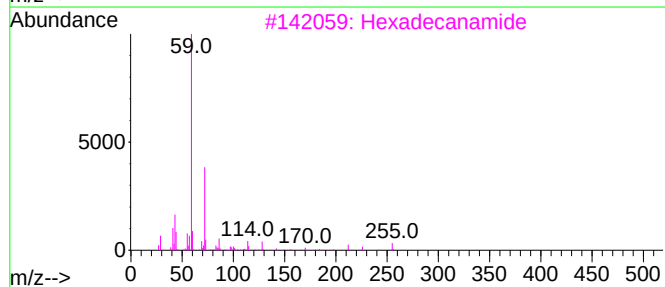
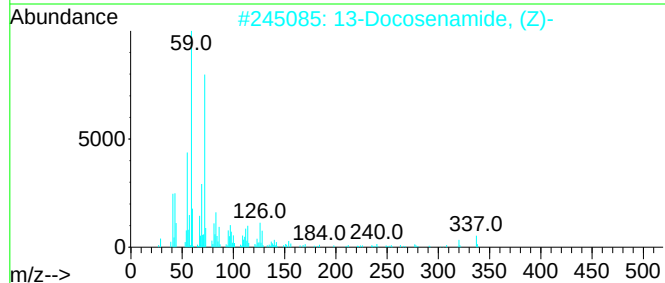
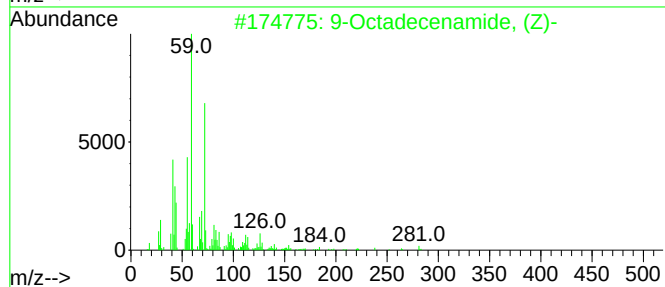
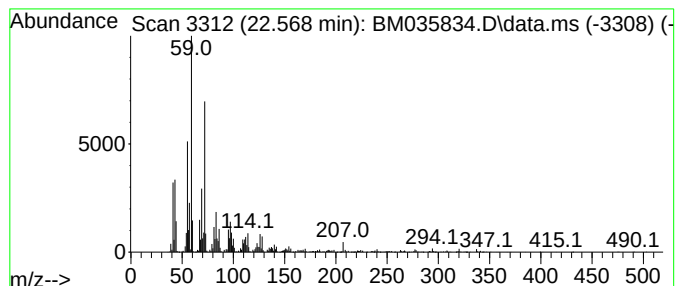
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.568	10.30 ng	1457000	Chrysene-d12	21.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
3			Hexadecanamide	255	C16H33NO	000629-54-9	64
4			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	53
5			Methyl 17-methoxy-10-methoxycarb...	386	C22H42O5	1000110-20-7	43



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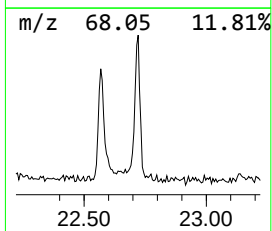
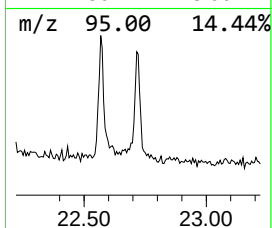
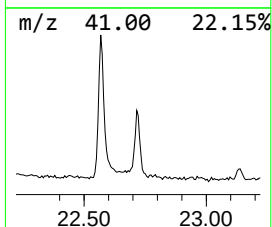
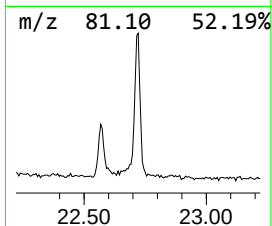
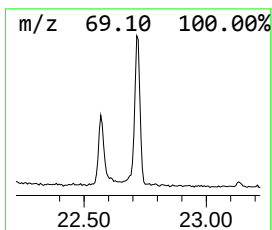
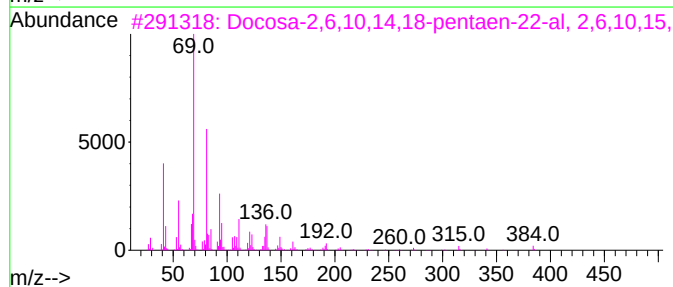
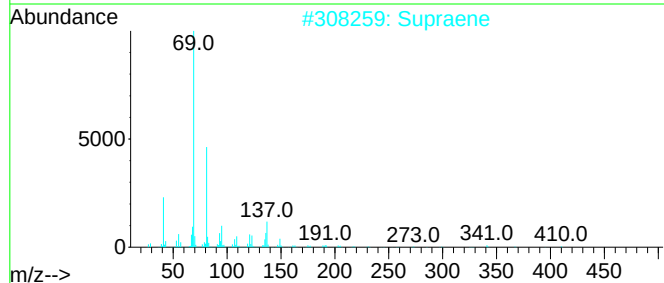
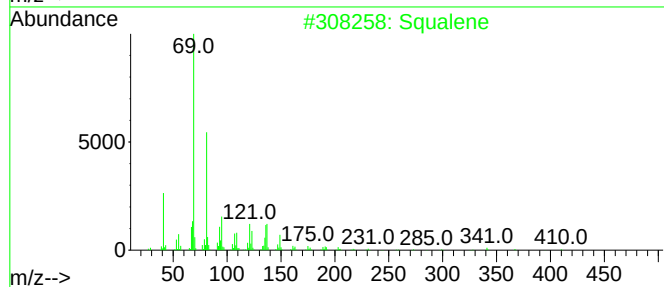
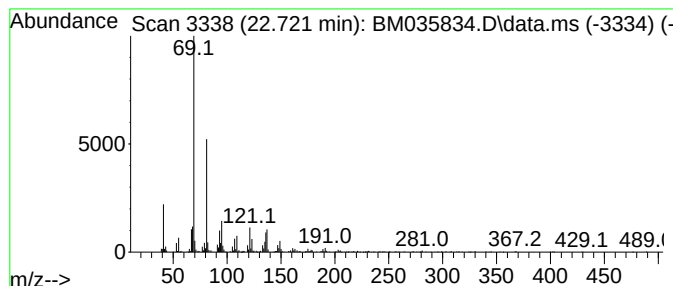
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.721	4.02 ng	502818	Perylene-d12	23.827

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	91
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4			2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	78
5			3,7,11-Tridecatrienoic acid, 4,8...	264	C17H28O2	036237-70-4	64



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.180	9.0	ng	1599730	4	17.274	3559330	20.0
Octadecanoic acid	19.456	6.1	ng	859207	5	21.451	2829060	20.0
1-Docosene	21.180	2.7	ng	386637	5	21.451	2829060	20.0
9-Octadecenamid...	22.568	10.3	ng	1457000	5	21.451	2829060	20.0
Squalene	22.721	4.0	ng	502818	6	23.827	2504420	20.0