

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020723\
 Data File : BG056572.D
 Acq On : 7 Feb 2023 18:02
 Operator : CG/JU
 Sample : 01462-15
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMP-3

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-BG012723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056572.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.302	336	343	351	rVB	96425	147972	6.91%	1.554%
2	5.790	419	426	441	rVB	392316	639015	29.86%	6.710%
3	7.417	695	703	713	rBV	399508	681573	31.85%	7.157%
4	8.269	841	848	855	rBB	99253	169534	7.92%	1.780%
5	9.444	1040	1048	1062	rBB	230276	413270	19.31%	4.339%
6	11.101	1322	1330	1337	rBV	136195	242856	11.35%	2.550%
7	13.510	1732	1740	1749	rBV	872149	1381585	64.56%	14.507%
8	14.891	1967	1975	1982	rBV	253567	402236	18.80%	4.224%
9	16.225	2198	2202	2210	rVB	17566	26728	1.25%	0.281%
10	16.371	2220	2227	2236	rBV	652071	1004039	46.92%	10.543%
11	17.629	2435	2441	2446	rBV	339322	525283	24.55%	5.516%
12	17.670	2446	2448	2453	rVB	30257	37425	1.75%	0.393%
13	18.469	2580	2584	2593	rBV3	44277	79450	3.71%	0.834%
14	18.692	2616	2622	2627	rBV4	10453	23099	1.08%	0.243%
15	19.662	2782	2787	2791	rBV	74412	102077	4.77%	1.072%
16	20.026	2844	2849	2856	rVB	66314	103841	4.85%	1.090%
17	20.202	2873	2879	2885	rVB	1673425	2139993	100.00%	22.471%
18	21.495	3095	3099	3108	rVB5	52007	101764	4.76%	1.069%
19	21.918	3163	3171	3177	rBV	329304	609952	28.50%	6.405%
20	23.628	3458	3462	3469	rVB	73376	135029	6.31%	1.418%
21	25.337	3744	3753	3765	rVB2	187328	556730	26.02%	5.846%

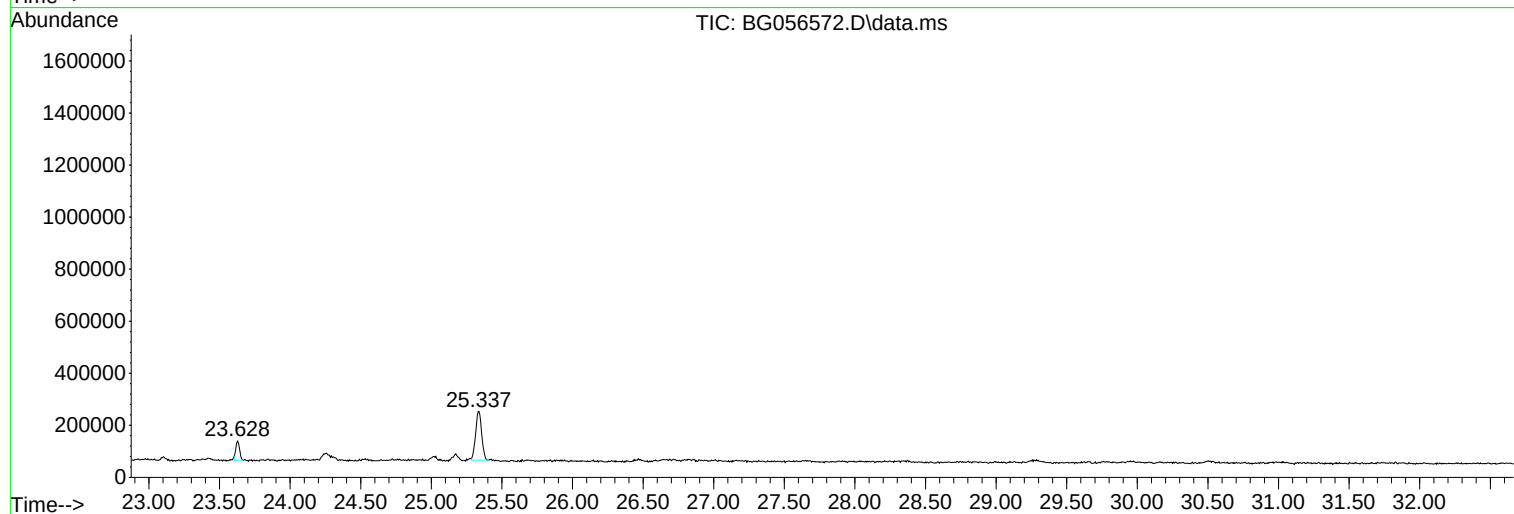
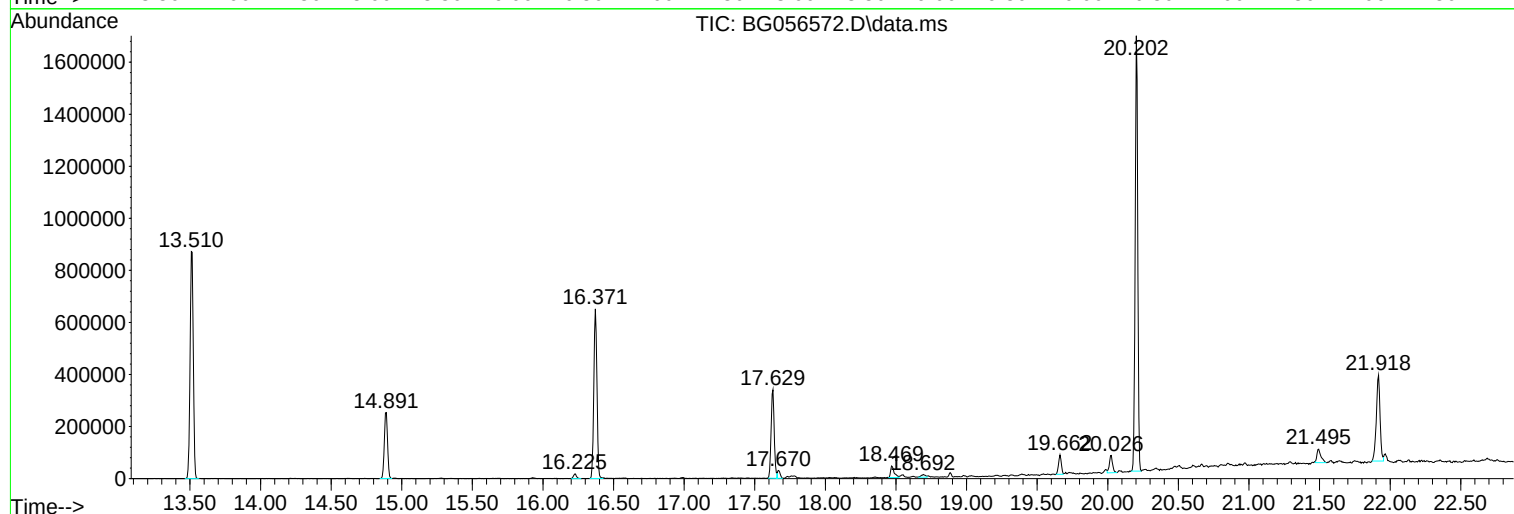
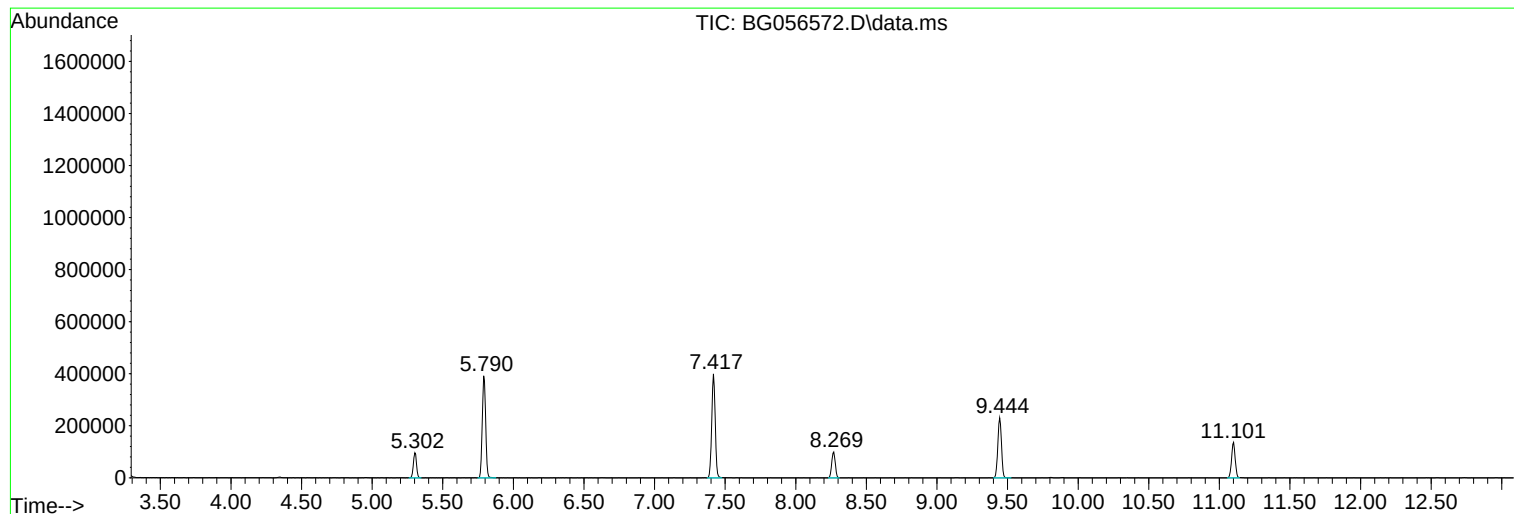
Sum of corrected areas: 9523451

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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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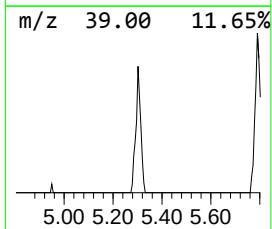
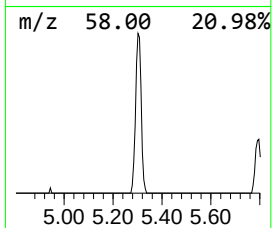
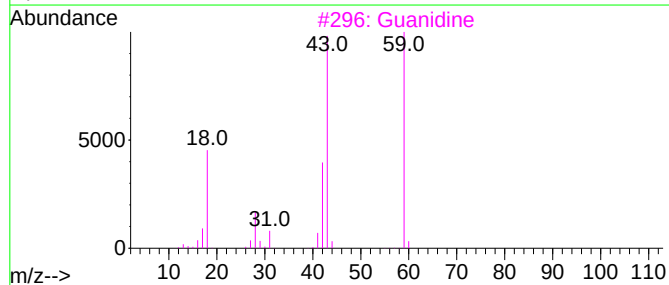
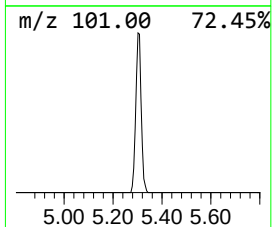
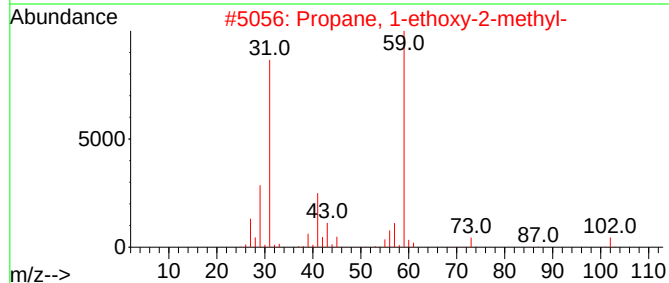
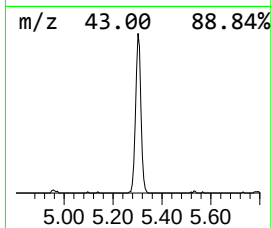
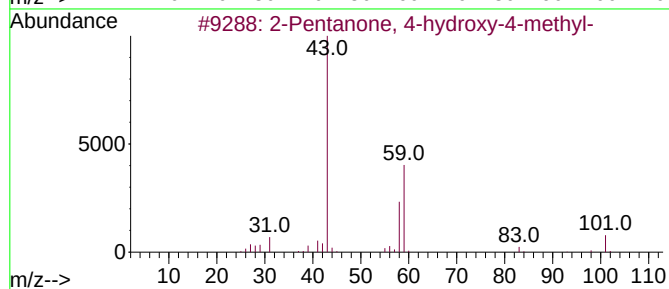
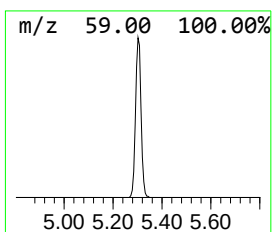
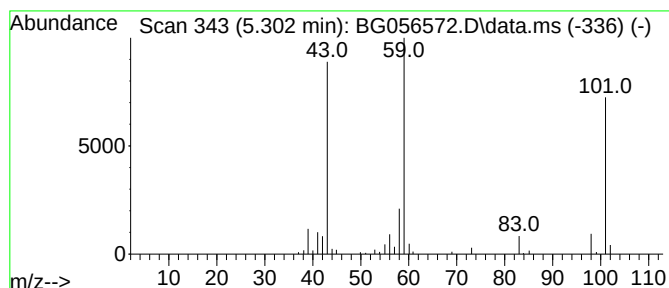
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.302	17.46 ng	147972	1,4-Dichlorobenzene-d4	8.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	32
3	Guanidine	59	CH5N3	000113-00-8	32
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17



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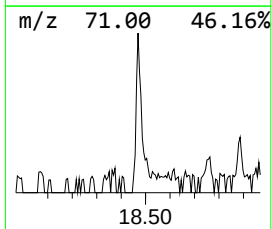
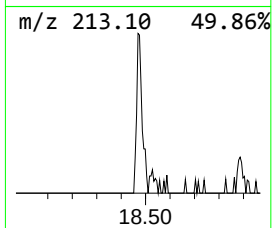
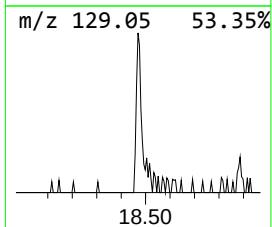
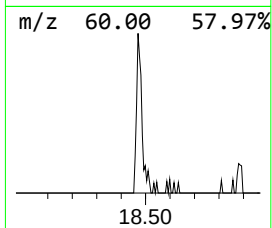
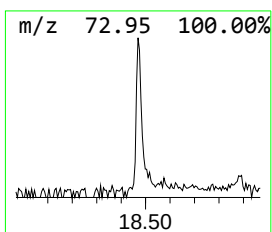
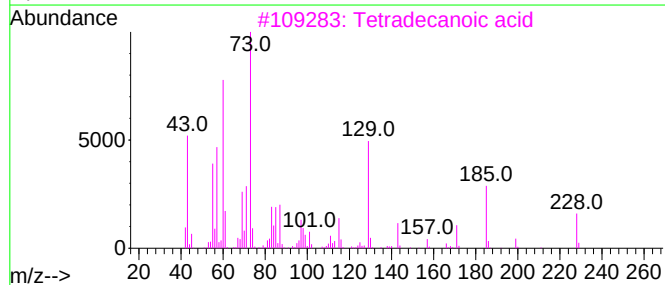
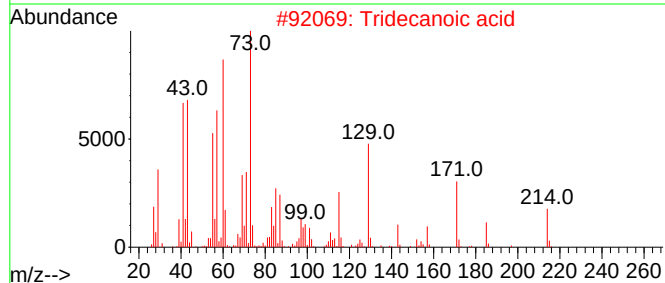
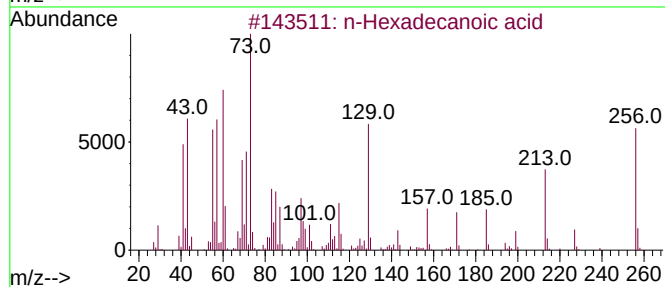
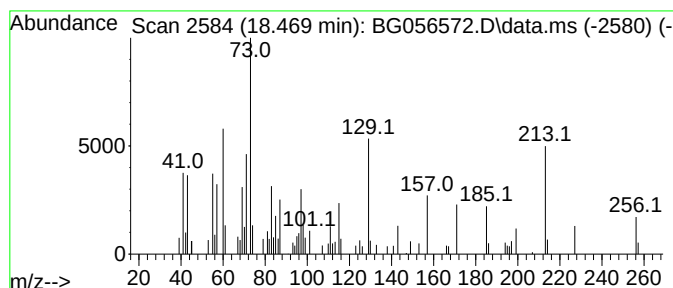
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.469	3.03 ng	79450	Phenanthrene-d10	17.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2			Tridecanoic acid	214	C13H26O2	000638-53-9	55
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4			Undecanoic acid	186	C11H22O2	000112-37-8	47
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	35



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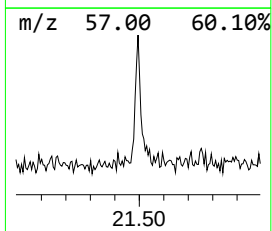
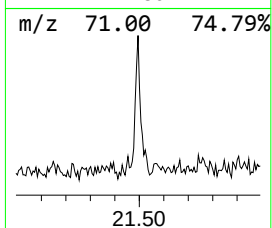
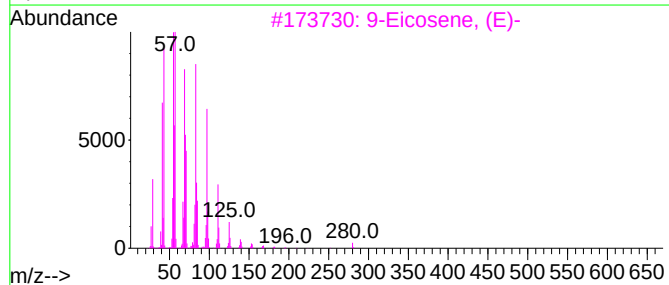
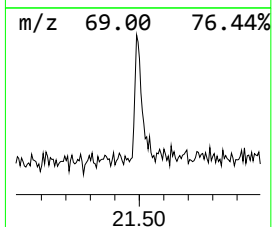
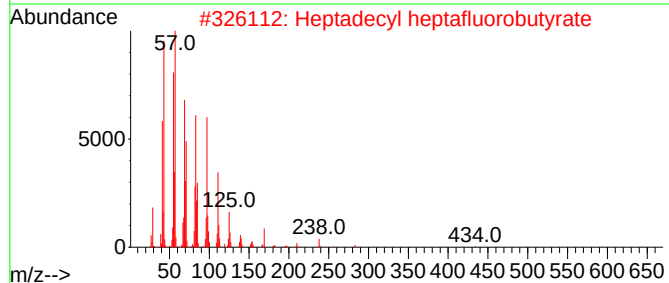
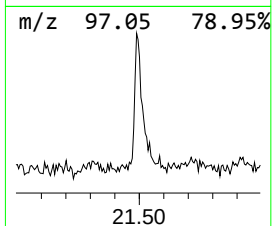
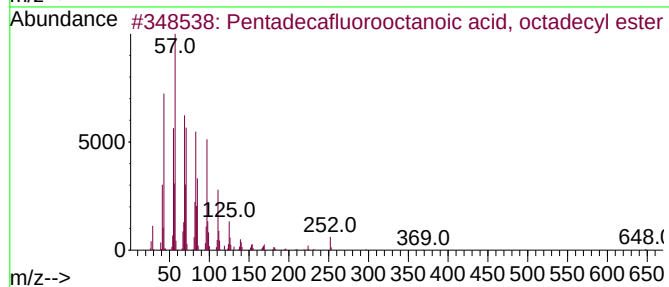
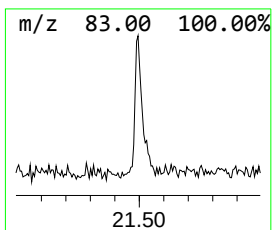
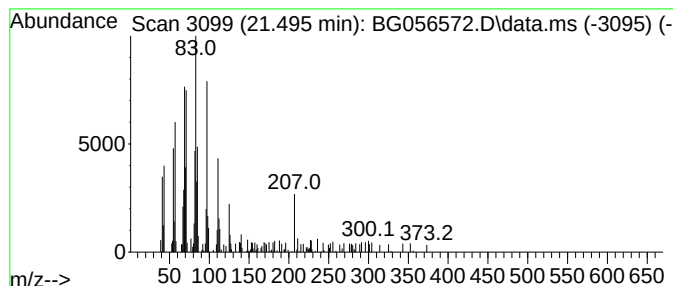
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Peak Number 3 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.495	3.34 ng	101764	Chrysene-d12	21.918	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	76
4	1-Tricosene	322	C23H46	018835-32-0	72
5	1-Hexacosene	364	C26H52	018835-33-1	72



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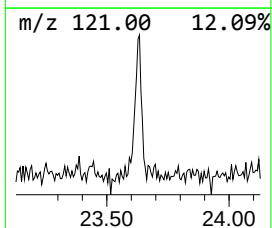
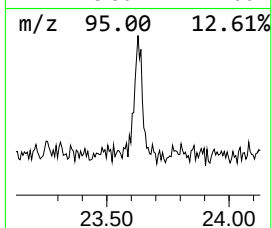
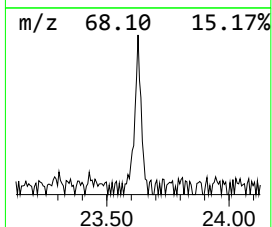
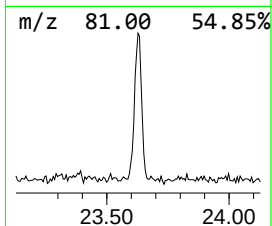
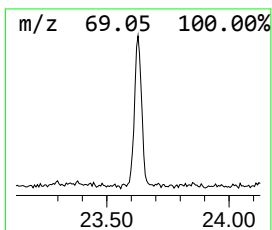
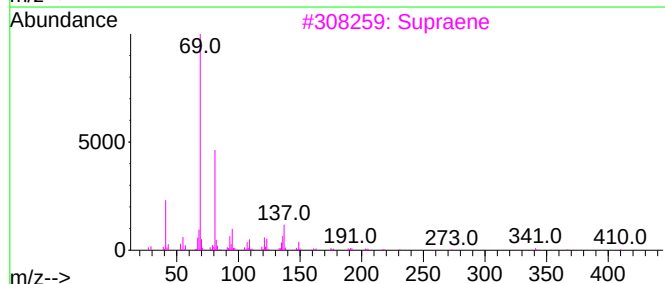
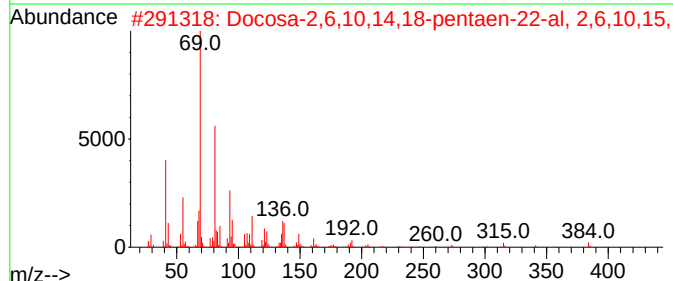
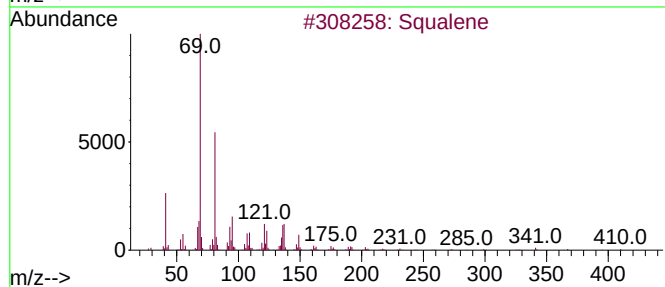
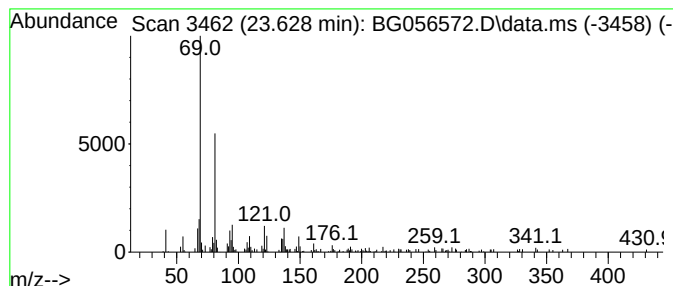
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Peak Number 4 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.628	4.85 ng	135029	Perylene-d12	25.332

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	83
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	80
3			Supraene	410	C30H50	007683-64-9	74
4			Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	72
5			1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.302	17.5	ng	147972	1	8.269	169534	20.0
n-Hexadecanoic ...	18.469	3.0	ng	79450	4	17.629	525283	20.0
Pentadecafluoro...	21.495	3.3	ng	101764	5	21.918	609952	20.0
Squalene	23.628	4.8	ng	135029	6	25.332	556730	20.0