

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
 Data File : BG055964.D
 Acq On : 14 Dec 2022 18:06
 Operator : CG/JU
 Sample : N6001-17
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-16

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-BG121322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055964.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.402	14	19	29	rBB	79311	111975	13.48%	4.192%
2	5.882	436	441	447	rBB	46296	71604	8.62%	2.681%
3	7.491	709	715	723	rBB2	30340	50431	6.07%	1.888%
4	8.373	859	865	870	rBB2	17182	26760	3.22%	1.002%
5	9.542	1057	1064	1070	rBB	62000	107580	12.95%	4.028%
6	11.205	1340	1347	1353	rBB	22619	39430	4.75%	1.476%
7	13.608	1749	1756	1763	rBB	246357	368592	44.37%	13.800%
8	14.977	1981	1989	1995	rBB	50455	76648	9.23%	2.870%
9	16.451	2234	2240	2248	rVB	331384	491438	59.16%	18.400%
10	17.715	2448	2455	2461	rBV	80816	119798	14.42%	4.485%
11	18.561	2596	2599	2606	rVB2	7881	11991	1.44%	0.449%
12	20.288	2887	2893	2899	rBV	658879	830655	100.00%	31.101%
13	21.604	3112	3117	3127	rVB3	11412	18783	2.26%	0.703%
14	22.016	3180	3187	3197	rVB2	88068	151490	18.24%	5.672%
15	23.843	3489	3498	3506	rVB2	14627	30116	3.63%	1.128%
16	25.511	3770	3782	3795	rBV	56683	163576	19.69%	6.124%

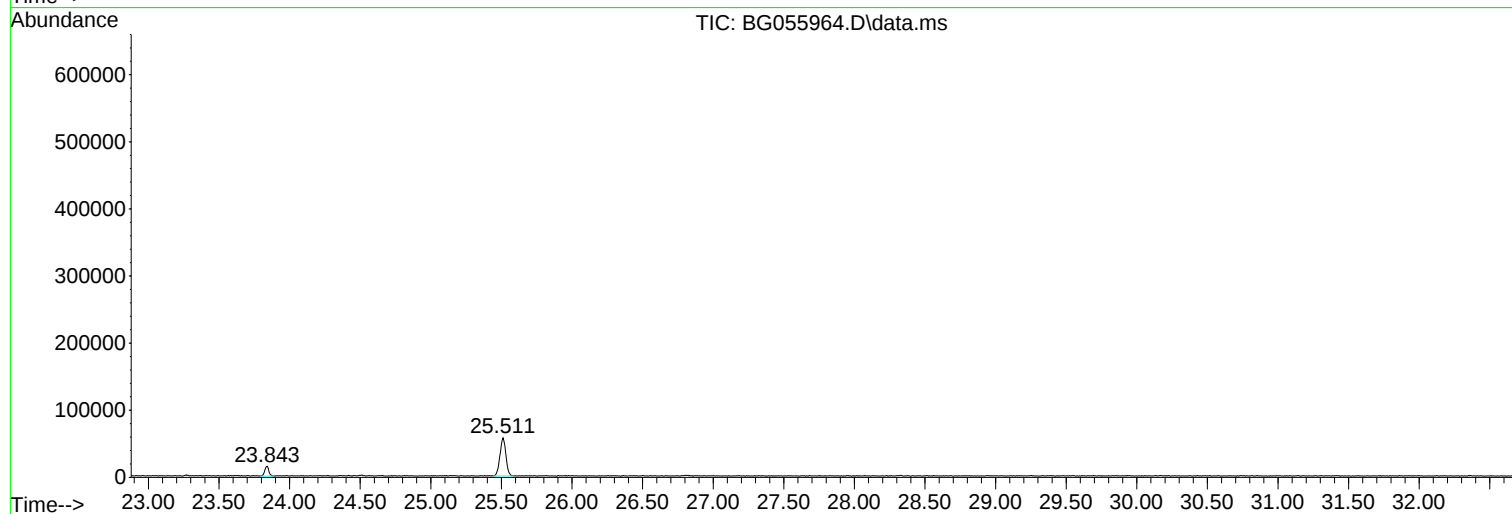
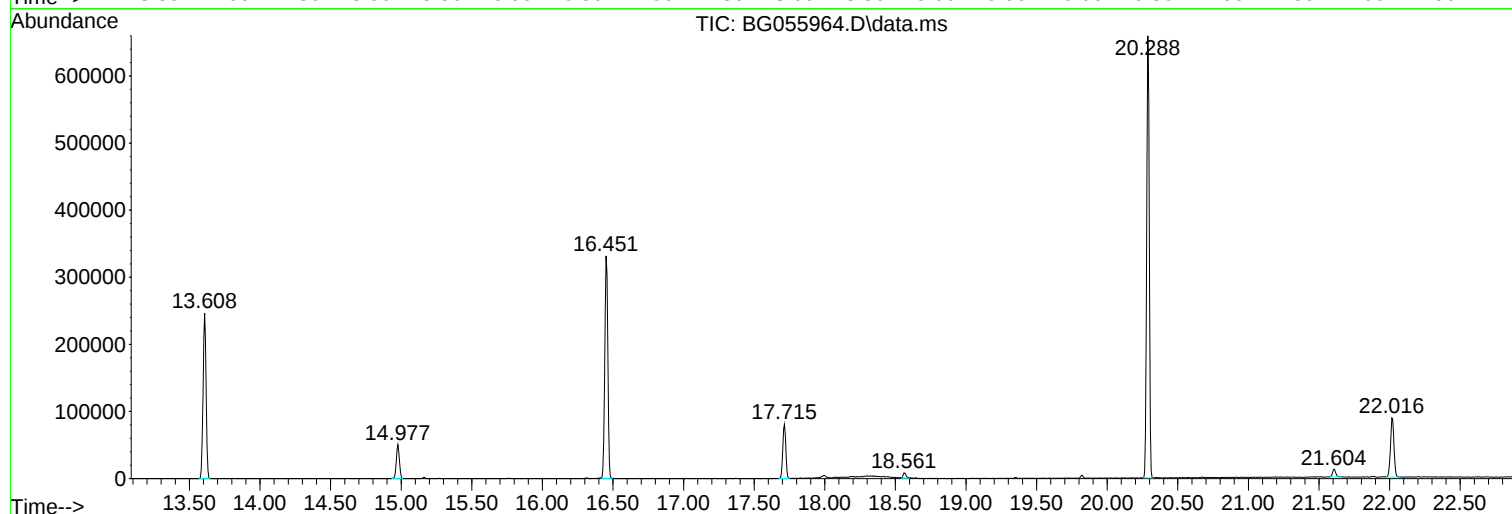
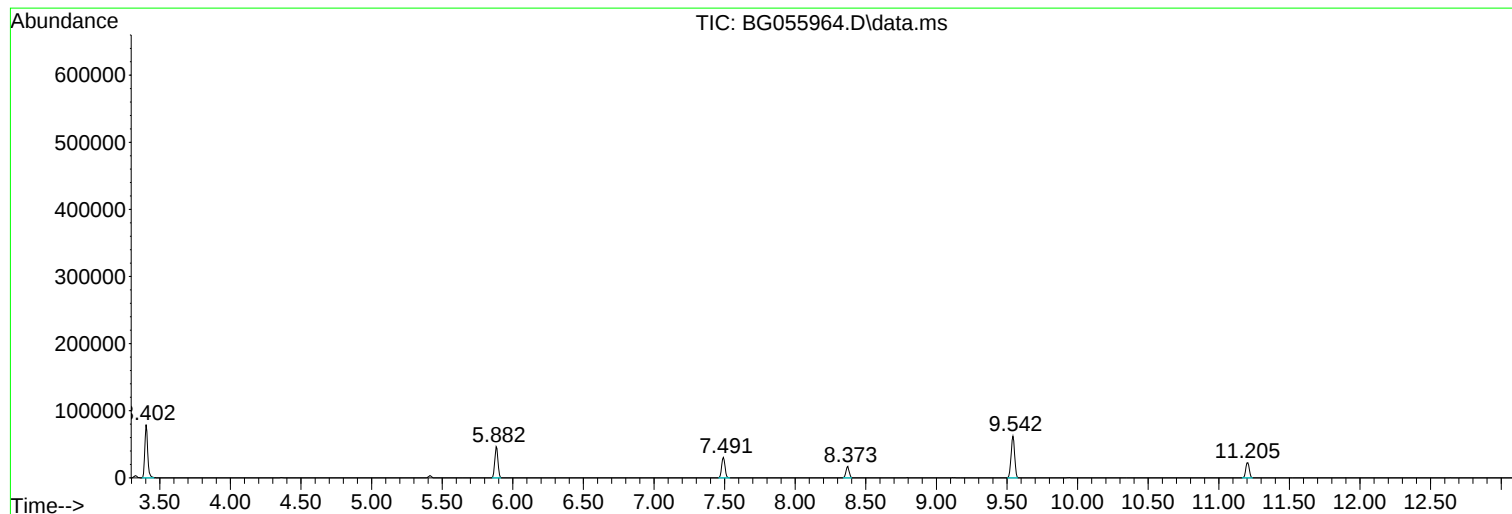
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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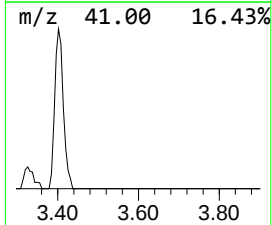
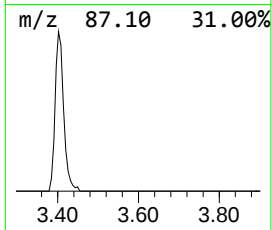
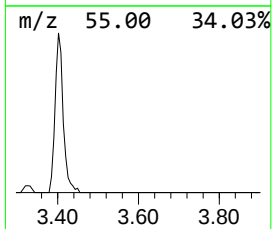
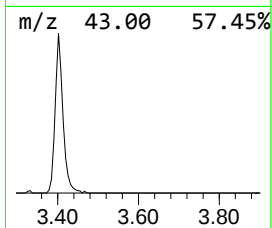
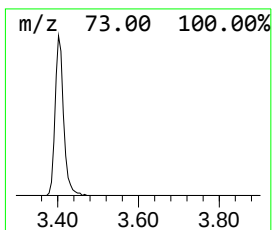
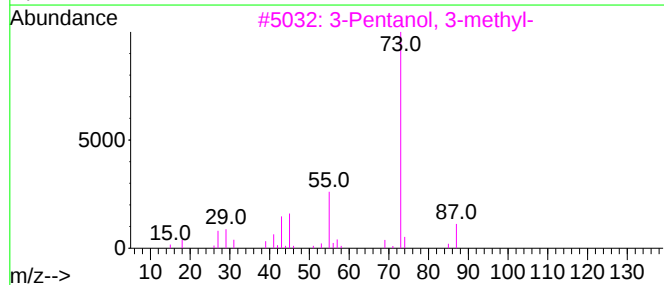
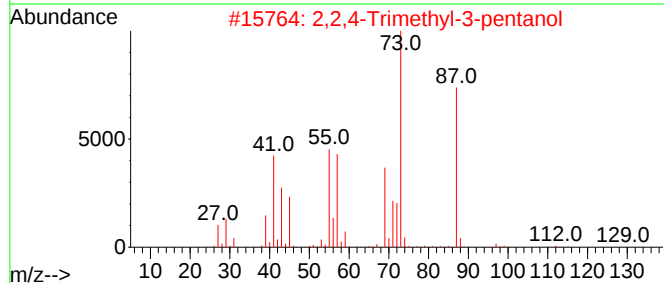
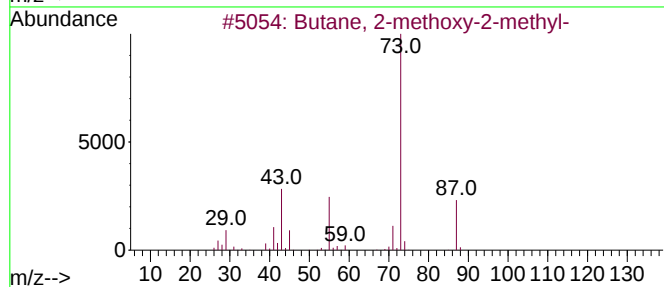
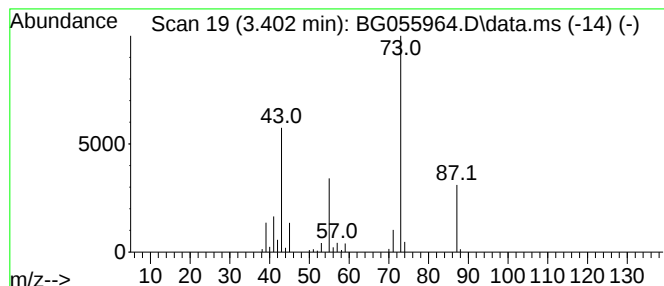
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.402	83.69 ng	111975	1,4-Dichlorobenzene-d4	8.373

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	33
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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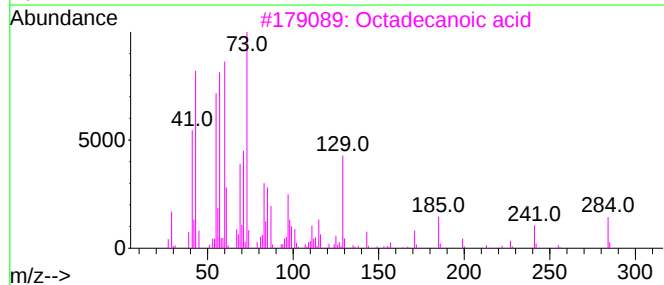
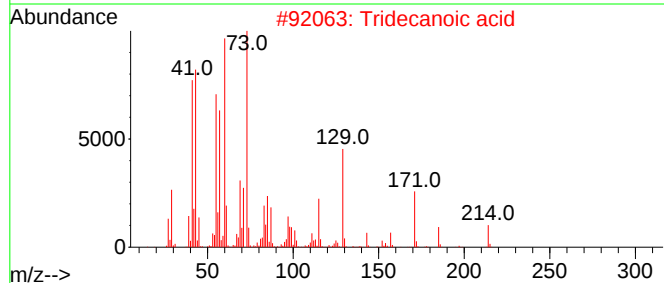
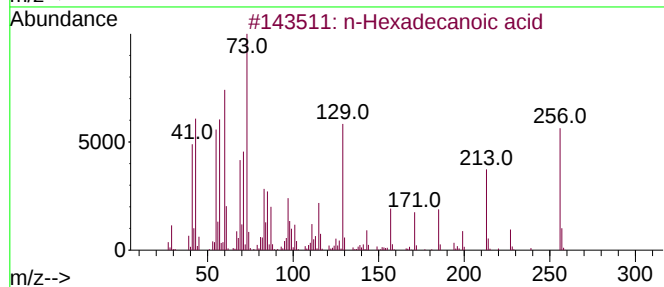
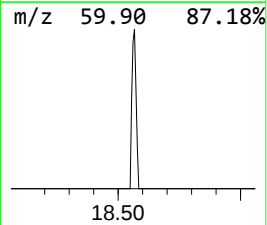
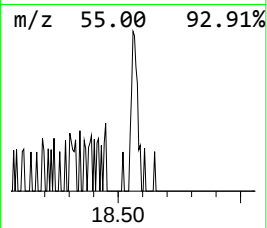
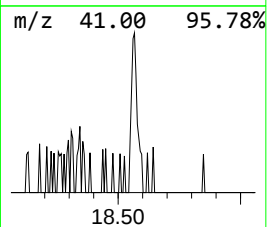
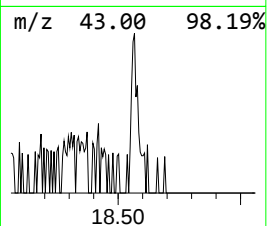
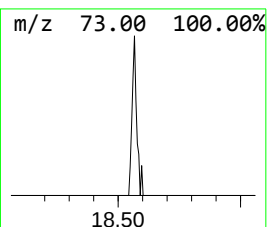
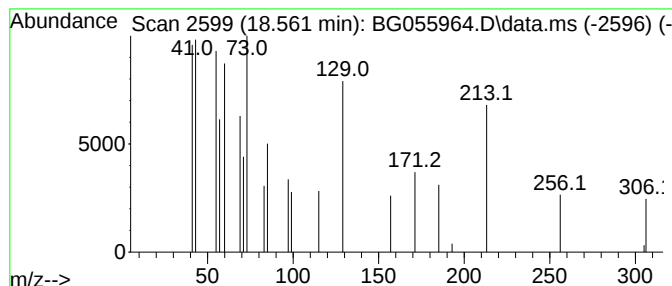
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.561	2.00 ng	11991	Phenanthrene-d10	17.715

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
2			Tridecanoic acid	214	C13H26O2	000638-53-9	47
3			Octadecanoic acid	284	C18H36O2	000057-11-4	43
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	43
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	42



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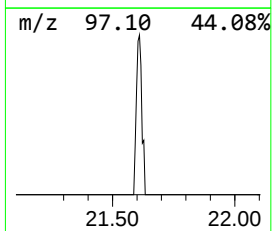
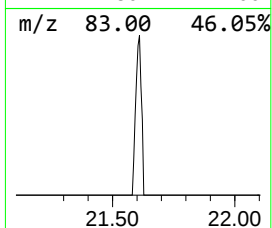
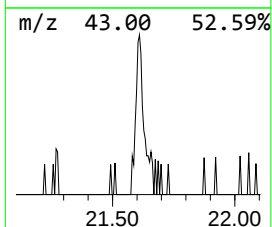
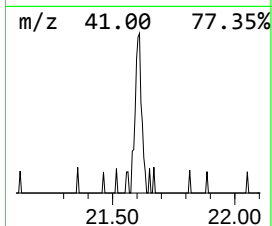
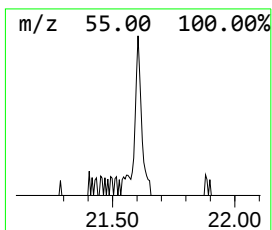
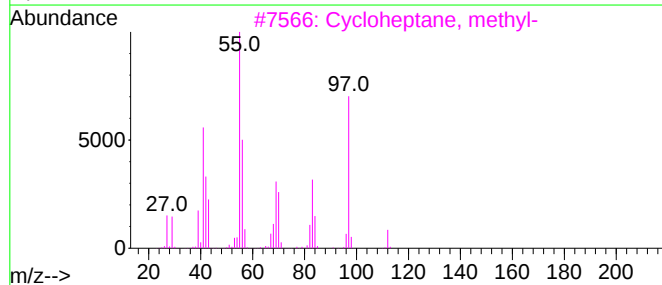
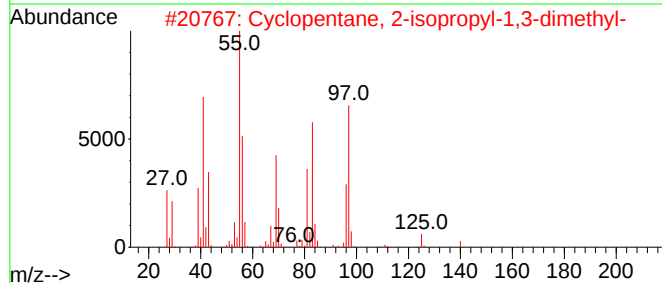
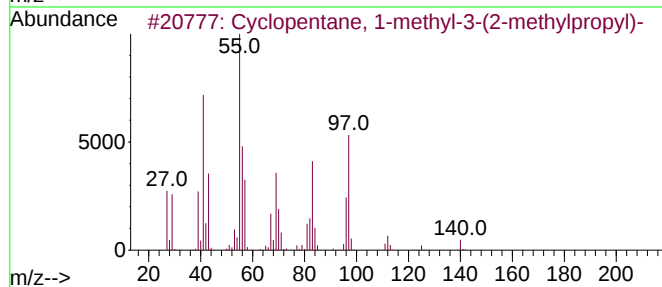
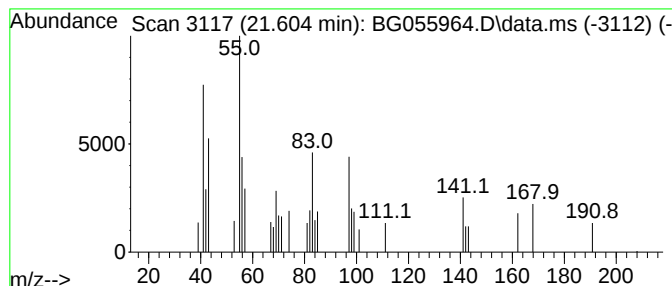
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Peak Number 3 unknown21.604 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.604	2.48 ng	18783	Chrysene-d12	22.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1-methyl-3-(2-meth...	140	C10H20	029053-04-1	43
2			Cyclopentane, 2-isopropyl-1,3-di...	140	C10H20	032281-85-9	43
3			Cycloheptane, methyl-	112	C8H16	004126-78-7	35
4			Cyclododecane	168	C12H24	000294-62-2	27
5			Cyclopentane, 1-ethyl-3-methyl-,...	112	C8H16	002613-65-2	22



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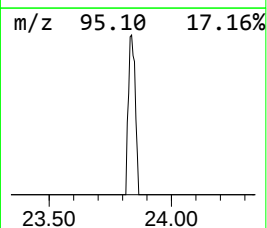
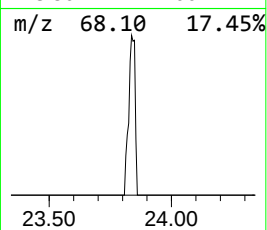
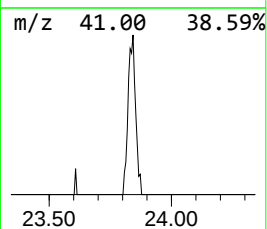
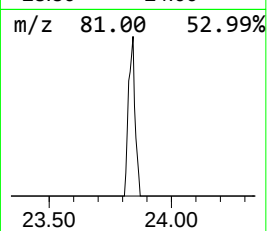
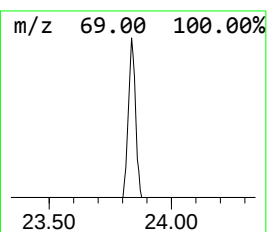
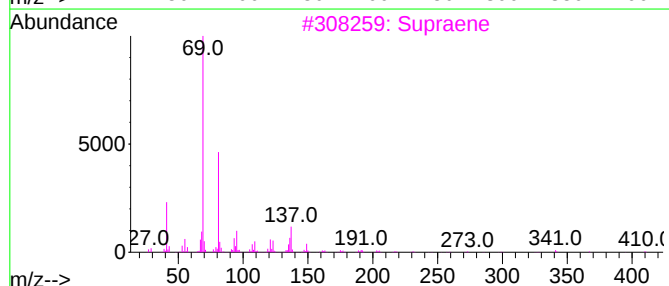
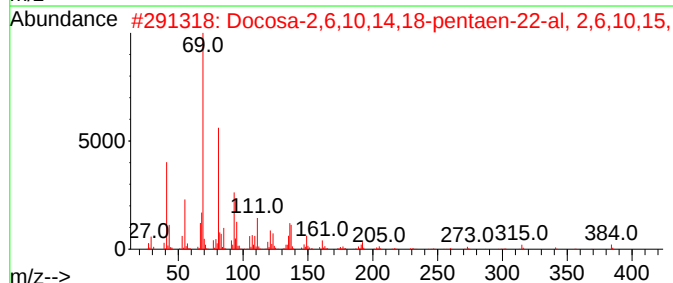
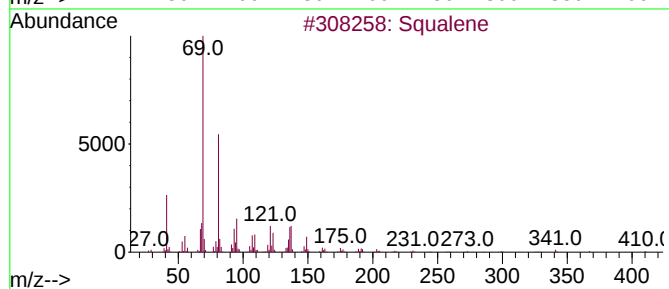
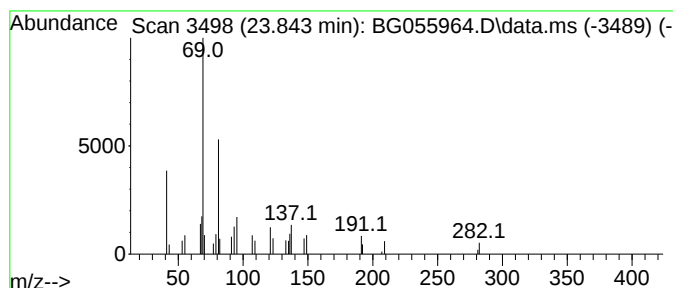
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Peak Number 4 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.843	3.68 ng	30116	Perylene-d12	25.512

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	80
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72
3			Supraene	410	C30H50	007683-64-9	72
4			3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	59
5			1-(3,5-Dinitrophenoxy)-3,7,11-tr...	388	C21H28N2O5	1000187-44-2	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.402	83.7	ng	111975	1	8.373	26760	20.0
n-Hexadecanoic ...	18.561	2.0	ng	11991	4	17.715	119798	20.0
unknown21.604	21.604	2.5	ng	18783	5	22.015	151490	20.0
Squalene	23.843	3.7	ng	30116	6	25.512	163576	20.0