

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
 Data File : BG060041.D
 Acq On : 15 Dec 2023 18:32
 Operator : MA/JU
 Sample : 05827-07
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RT-SB-09-13.75-14.75

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-BG121323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060041.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.144	4	9	20	rVB	202388	320068	5.27%	1.442%
2	5.523	408	414	426	rVB	765511	1211921	19.97%	5.460%
3	7.110	677	684	695	rVB	810931	1353423	22.30%	6.098%
4	7.956	820	828	835	rBV	248674	396277	6.53%	1.785%
5	9.113	1017	1025	1034	rBV	475503	843328	13.90%	3.799%
6	10.764	1298	1306	1313	rBV	307587	547286	9.02%	2.466%
7	13.214	1715	1723	1732	rBV	1612225	2492129	41.07%	11.228%
8	14.595	1952	1958	1966	rVB	552068	868490	14.31%	3.913%
9	16.081	2204	2211	2218	rBV	1200932	1787256	29.45%	8.052%
10	17.339	2418	2425	2436	rBV	937132	1446214	23.83%	6.516%
11	18.232	2571	2577	2590	rBV2	212996	333870	5.50%	1.504%
12	19.507	2790	2794	2798	rBV2	82670	116563	1.92%	0.525%
13	19.965	2866	2872	2878	rBV	4617233	6068573	100.00%	27.341%
14	21.264	3089	3093	3098	rBV2	144571	210746	3.47%	0.949%
15	21.610	3145	3152	3158	rBV	1196948	1938168	31.94%	8.732%
16	23.079	3397	3402	3412	rBV4	118674	271430	4.47%	1.223%
17	24.801	3686	3695	3706	rVB	728774	1990452	32.80%	8.968%

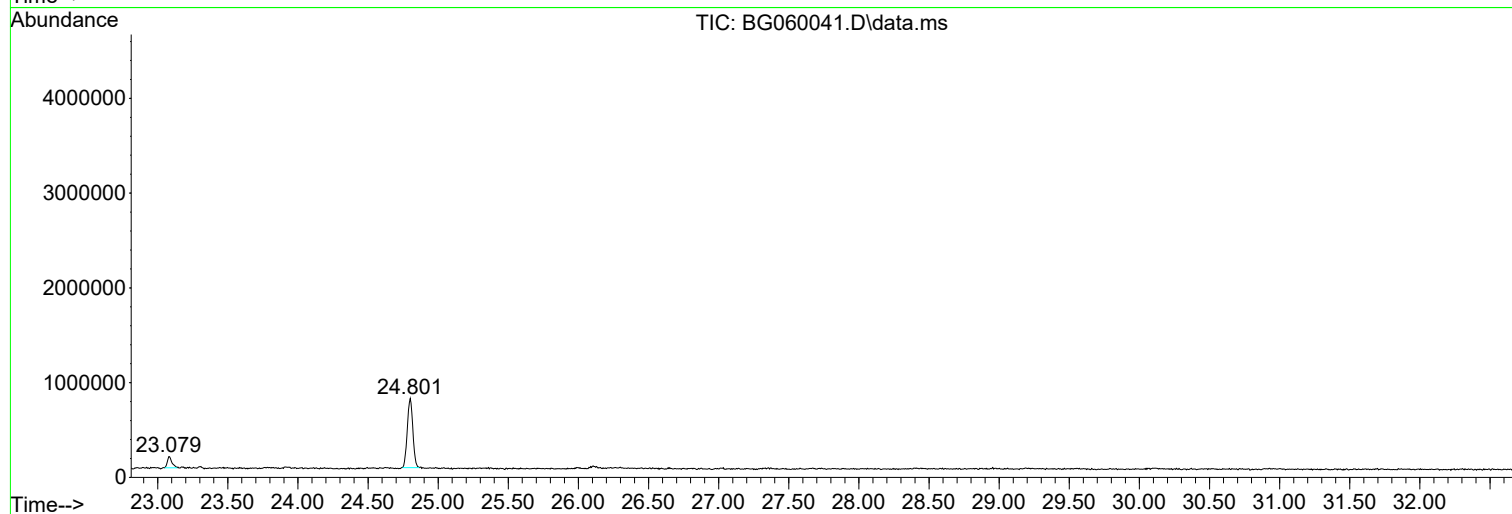
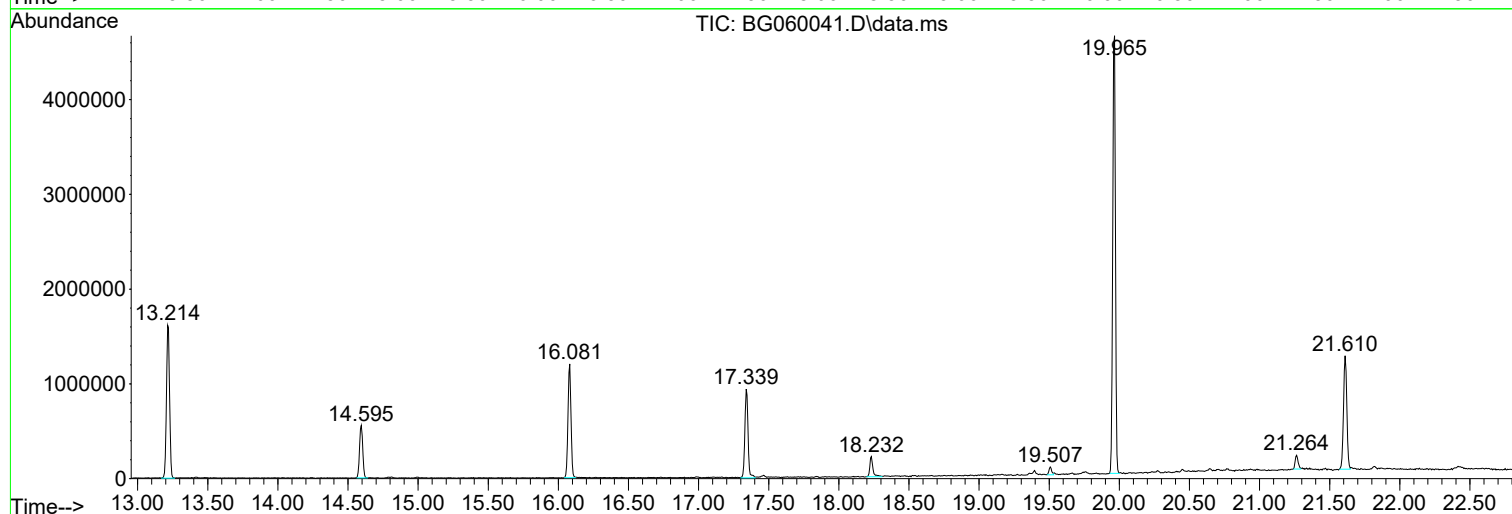
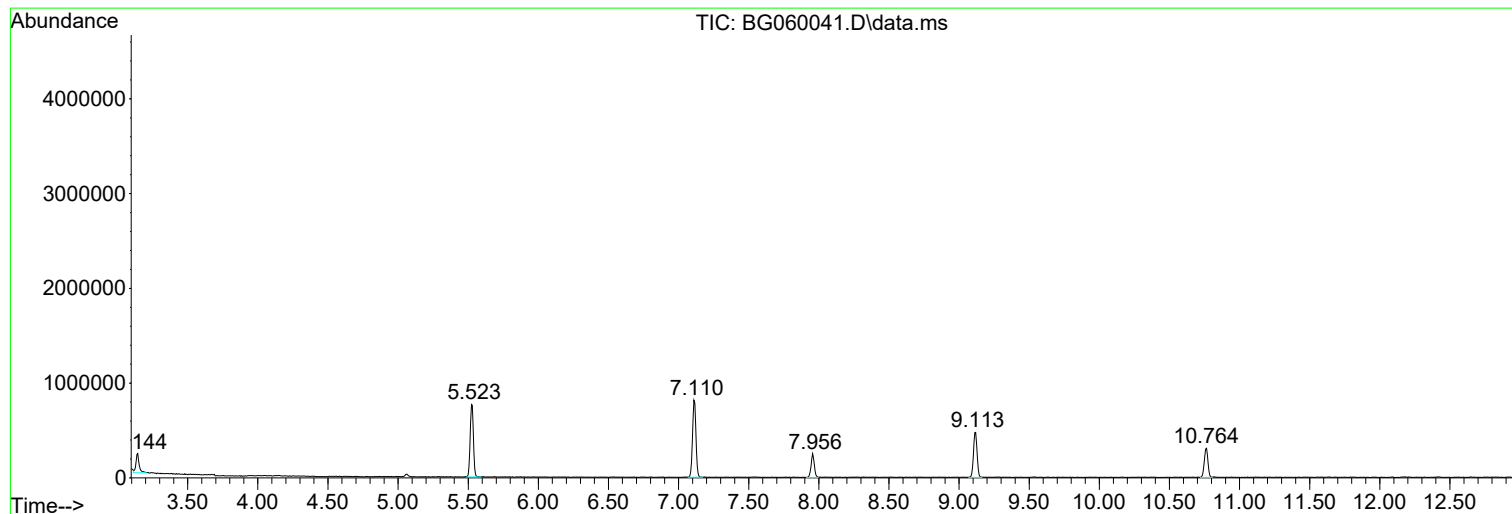
Sum of corrected areas: 22196194

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.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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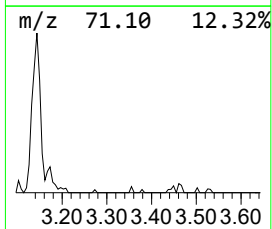
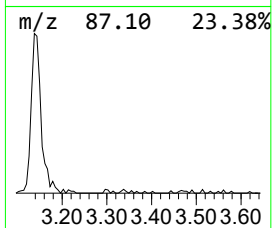
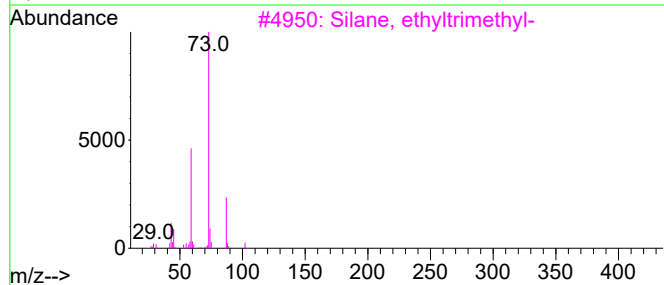
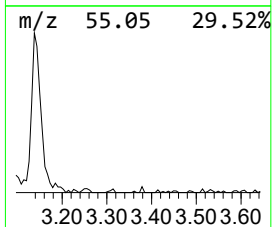
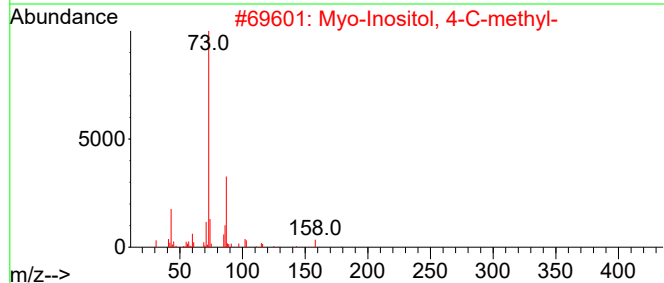
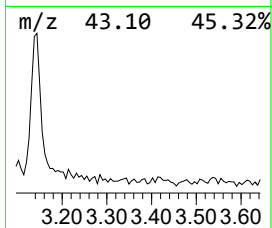
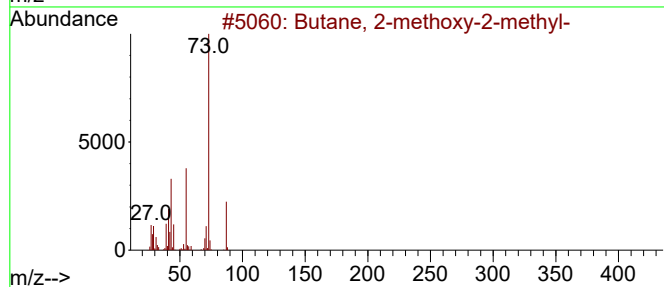
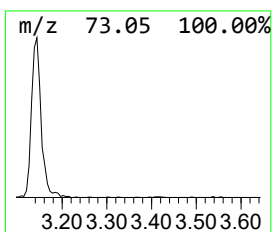
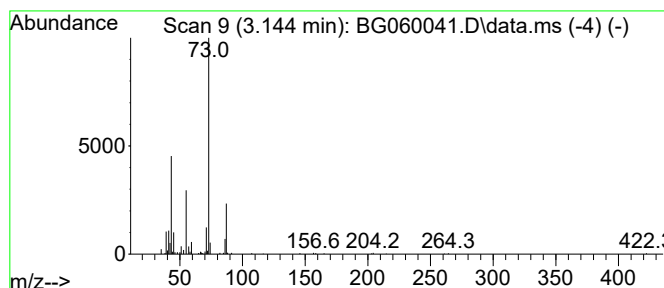
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.144	16.15 ng	320068	1,4-Dichlorobenzene-d4	7.956

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2			Myo-Inositol, 4-C-methyl-	194	C7H14O6	000472-95-7	33
3			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	28
4			2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	25
5			Silane, trimethyl(1-phenylethyl)-	178	C11H18Si	017961-78-3	16



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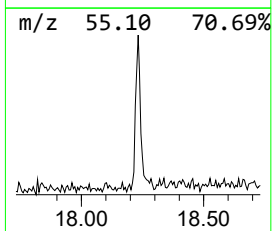
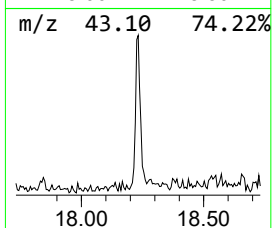
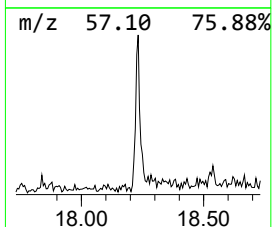
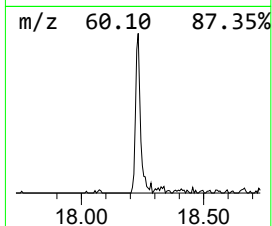
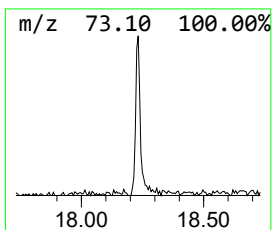
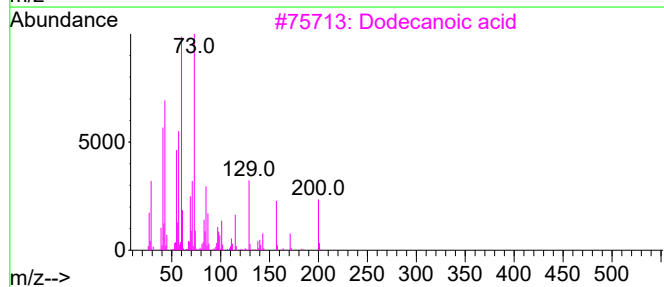
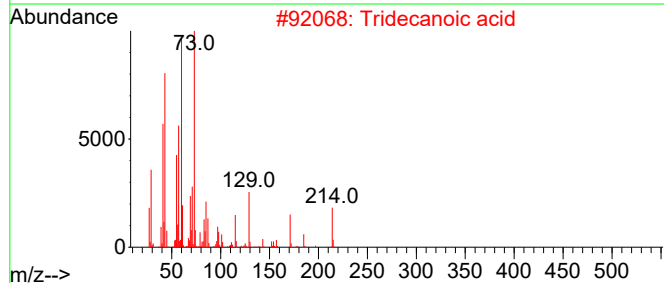
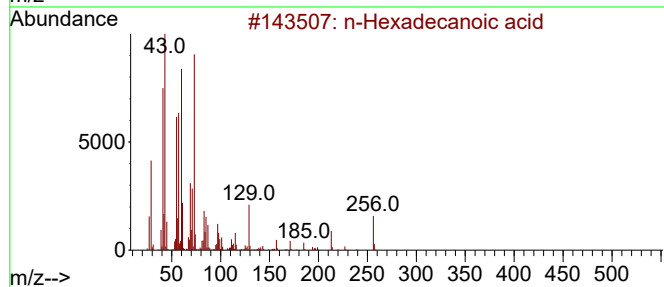
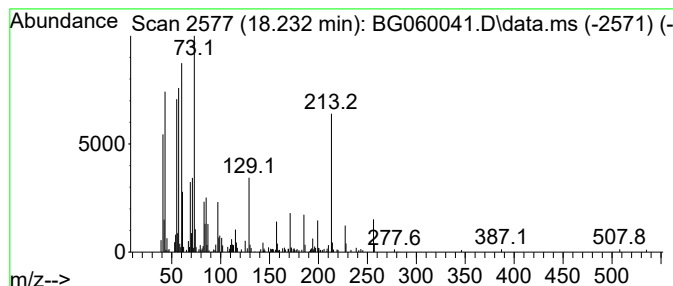
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.232	4.62 ng	333870	Phenanthrene-d10	17.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
2			Tridecanoic acid	214	C13H26O2	000638-53-9	52
3			Dodecanoic acid	200	C12H24O2	000143-07-7	50
4			Nonanoic acid	158	C9H18O2	000112-05-0	46
5			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	43



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Instrument :
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ClientSampleId :
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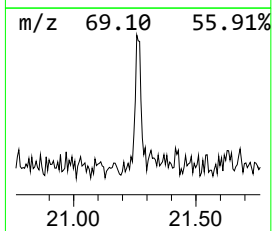
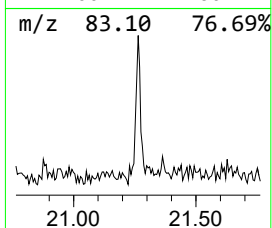
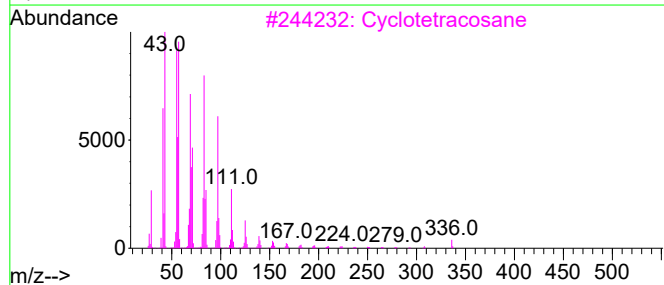
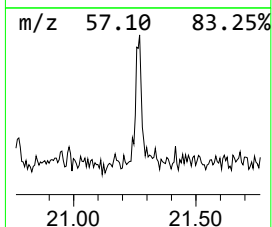
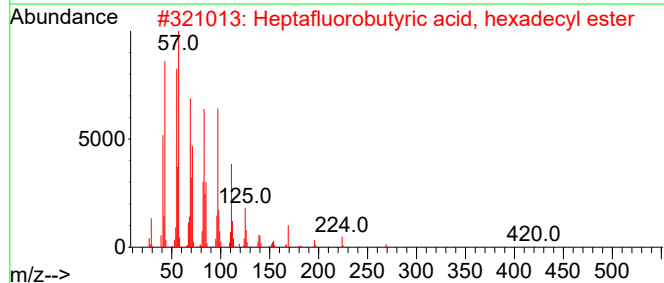
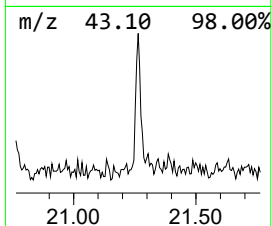
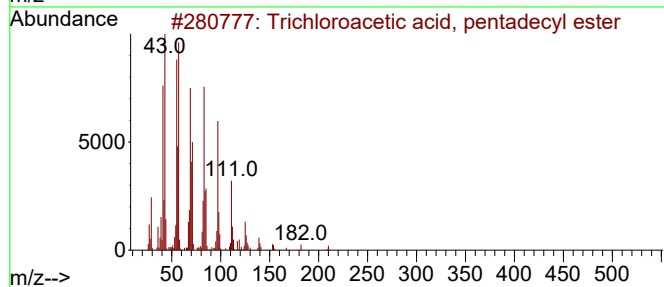
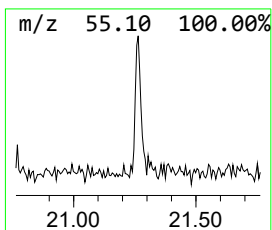
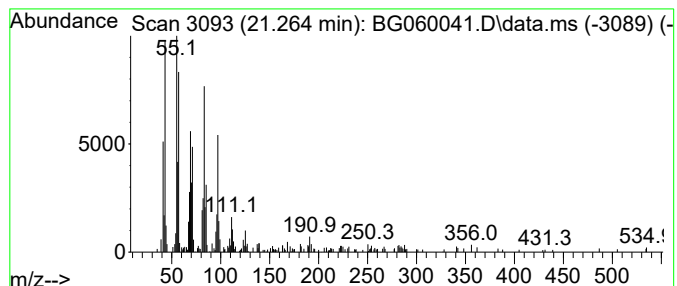
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Peak Number 3 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.264	2.17 ng	210746	Chrysene-d12	21.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
3			Cyclotetracosane	336	C24H48	000297-03-0	91
4			1-Heptadecene	238	C17H34	006765-39-5	90
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	83



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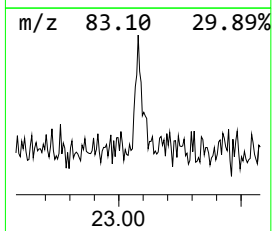
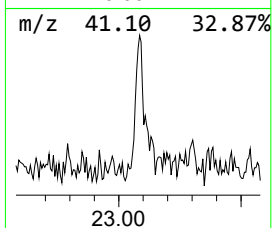
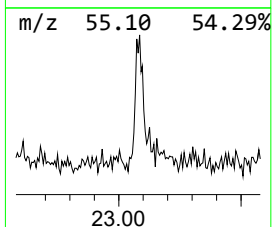
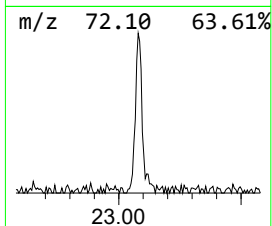
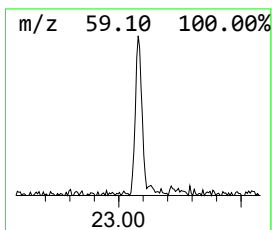
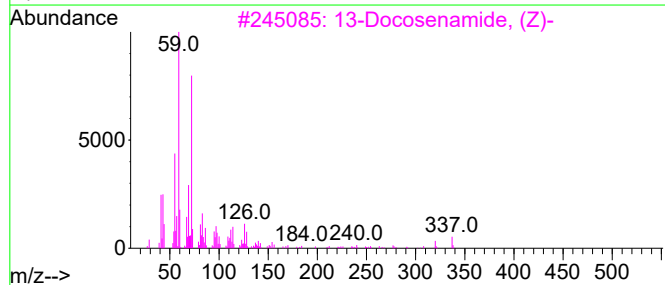
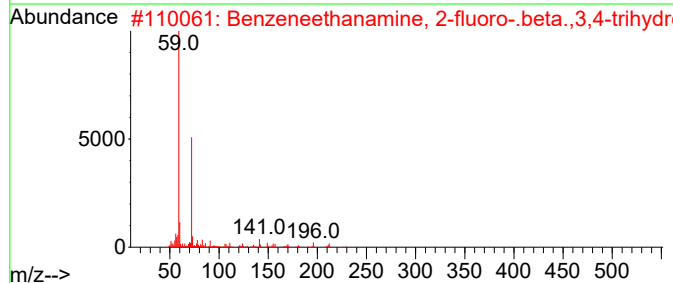
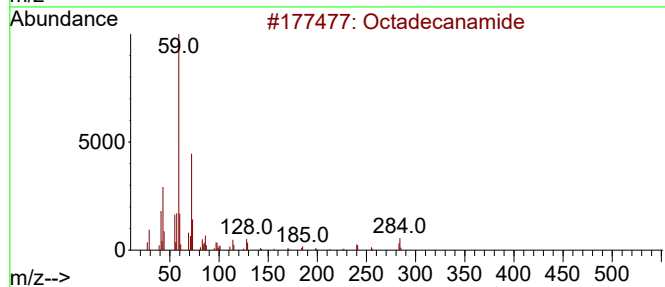
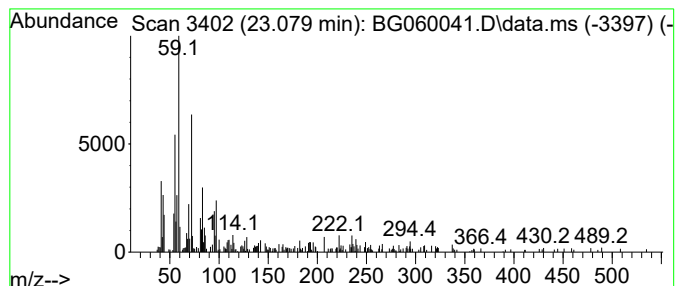
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Peak Number 4 Octadecanamide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.079	2.80 ng	271430	Chrysene-d12	21.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanamide	283	C18H37NO	000124-26-5	81
2			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	64
3			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	64
4			Hexadecanamide	255	C16H33NO	000629-54-9	50
5			3-Tridecanol	200	C13H28O	010289-68-6	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.144	16.1	ng	320068	1	7.956	396277	20.0
n-Hexadecanoic ...	18.232	4.6	ng	333870	4	17.339	1446210	20.0
Trichloroacetic...	21.264	2.2	ng	210746	5	21.610	1938170	20.0
Octadecanamide	23.079	2.8	ng	271430	5	21.610	1938170	20.0