

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102021\
 Data File : BG050647.D
 Acq On : 20 Oct 2021 16:04
 Operator : CG/JU
 Sample : M4286-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SW-RR-03-(SA)

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-BG100621.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050647.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.791	384	392	404	rVB	622366	1047532	29.54%	6.999%
2	7.389	655	664	674	rBV	464755	841199	23.72%	5.620%
3	8.247	804	810	817	rVB	153300	267027	7.53%	1.784%
4	9.422	1001	1010	1023	rBV	680409	1257857	35.47%	8.404%
5	10.820	1241	1248	1257	rBV	106819	188319	5.31%	1.258%
6	11.073	1284	1291	1298	rBV	201387	373394	10.53%	2.495%
7	13.494	1695	1703	1711	rVB	1596423	2536390	71.53%	16.947%
8	14.869	1930	1937	1944	rBV	309715	487377	13.74%	3.256%
9	16.355	2183	2190	2202	rBV	1250636	1946120	54.88%	13.003%
10	16.531	2214	2220	2228	rBV	29833	57097	1.61%	0.381%
11	17.613	2398	2404	2411	rBV	383915	596956	16.83%	3.989%
12	18.247	2507	2512	2517	rBV2	26673	36664	1.03%	0.245%
13	18.470	2542	2550	2558	rBV2	44419	77530	2.19%	0.518%
14	20.204	2839	2845	2852	rVB	2664191	3545976	100.00%	23.692%
15	20.979	2973	2977	2982	rVB2	26479	36951	1.04%	0.247%
16	21.508	3063	3067	3072	rBV2	88842	135184	3.81%	0.903%
17	21.608	3079	3084	3094	rVB	76624	119369	3.37%	0.798%
18	21.913	3129	3136	3147	rVB	379688	670833	18.92%	4.482%
19	23.658	3427	3433	3440	rVB2	41992	81979	2.31%	0.548%
20	25.321	3706	3716	3729	rVB3	215036	663000	18.70%	4.430%

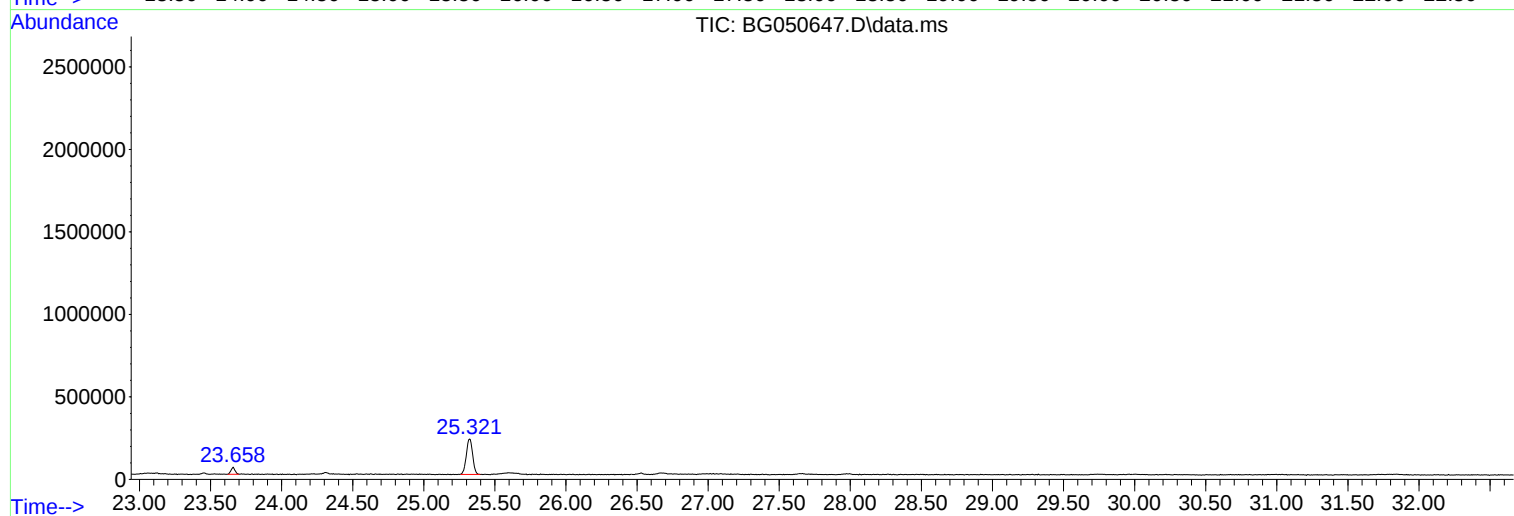
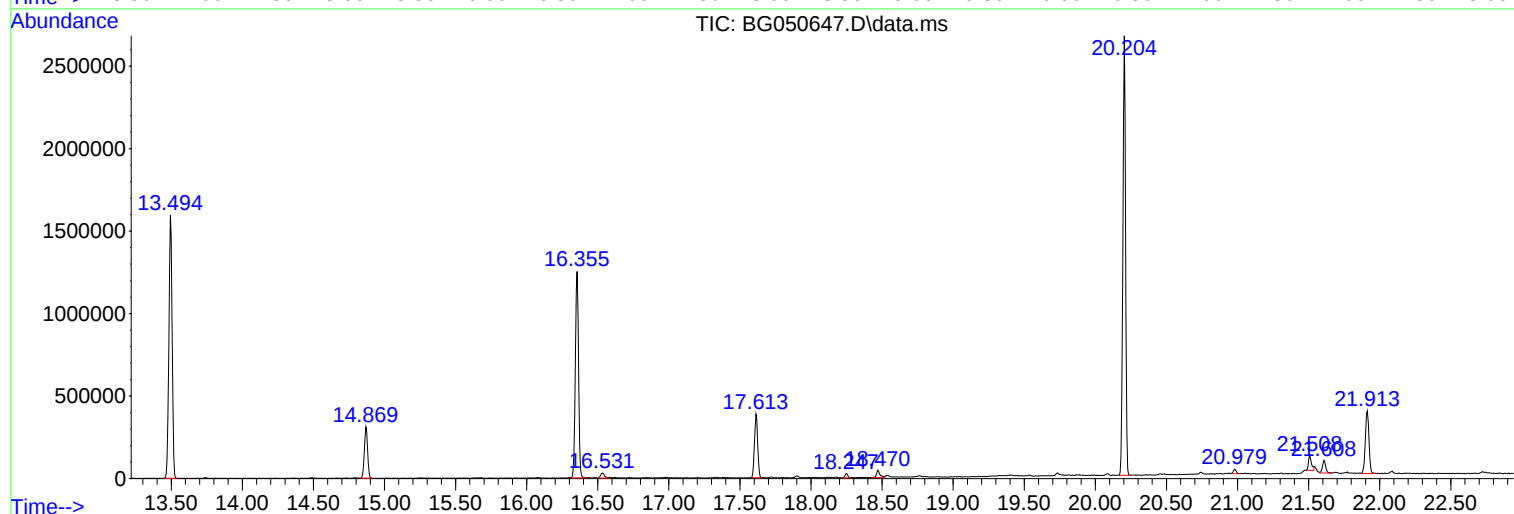
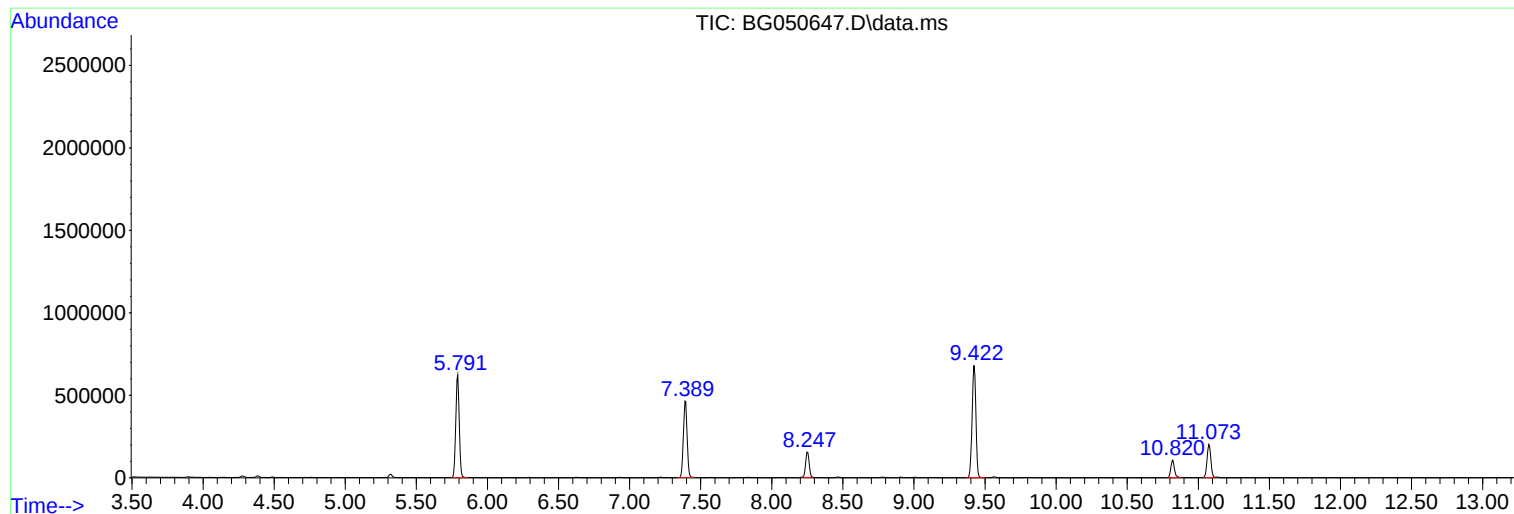
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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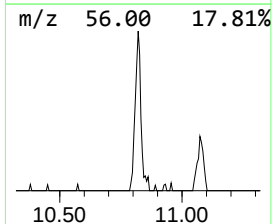
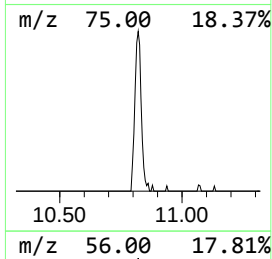
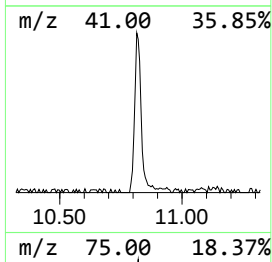
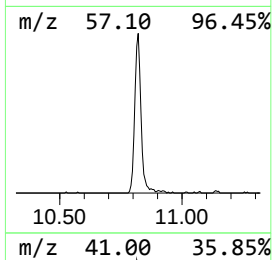
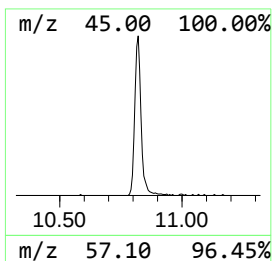
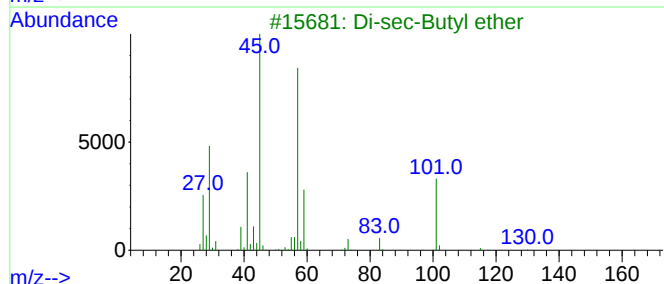
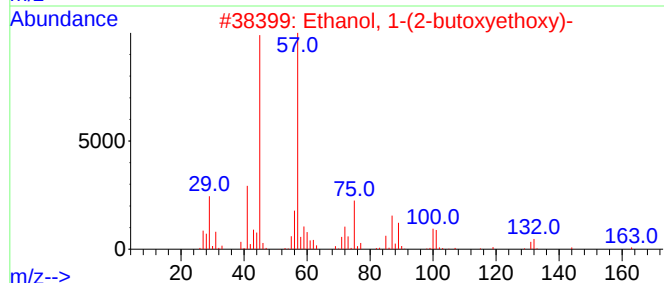
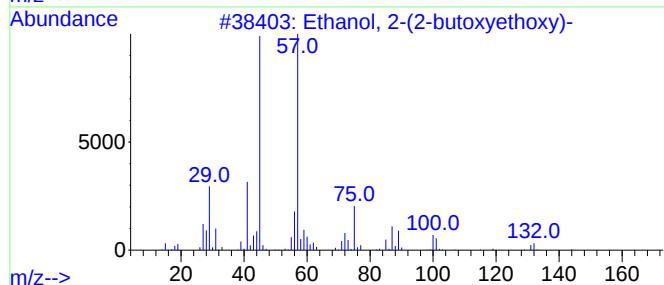
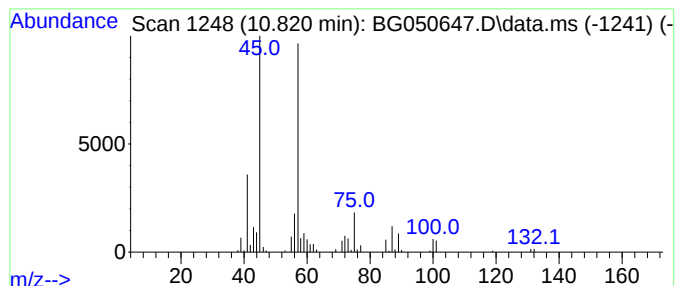
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.820	10.09 ng	188319	Naphthalene-d8	11.073

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	50



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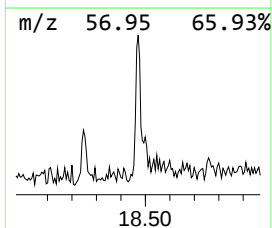
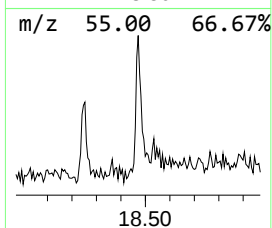
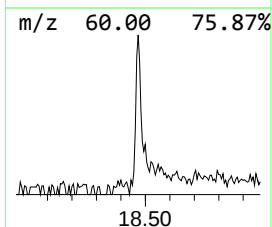
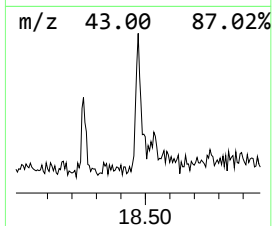
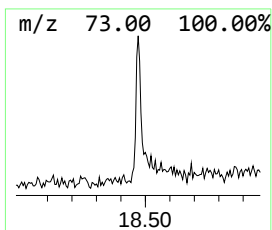
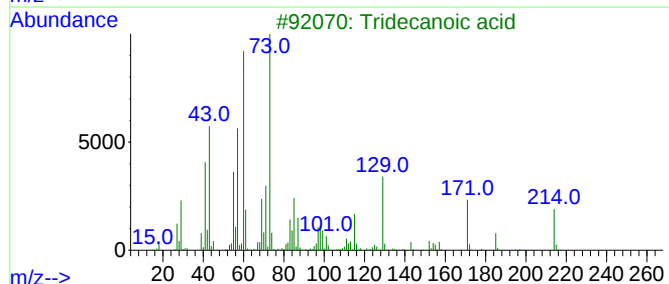
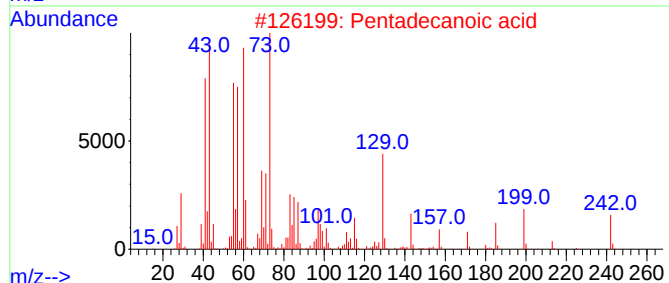
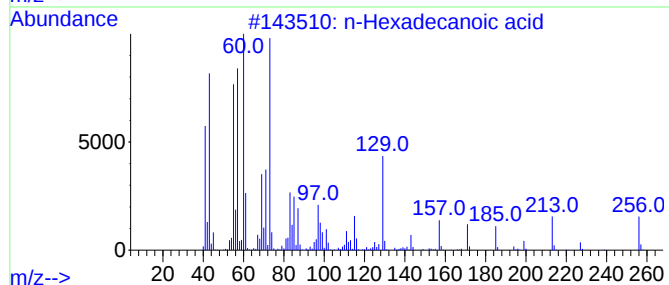
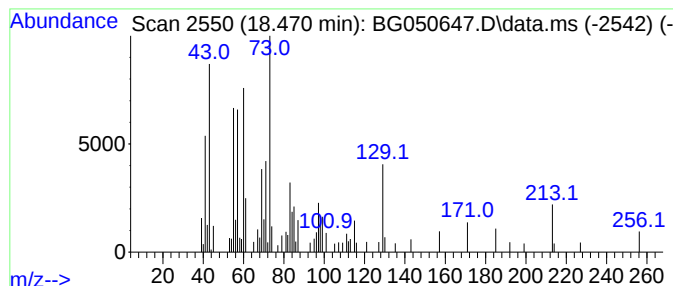
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.470	2.60 ng	77530	Phenanthrene-d10	17.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
3			Tridecanoic acid	214	C13H26O2	000638-53-9	53
4			n-Decanoic acid	172	C10H20O2	000334-48-5	47
5			Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25



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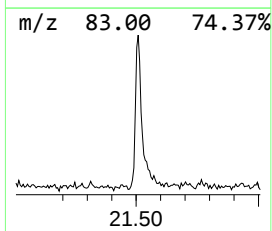
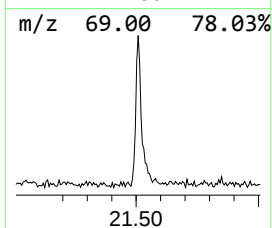
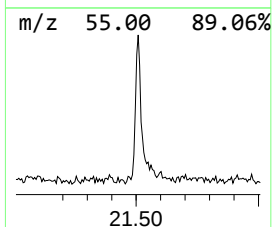
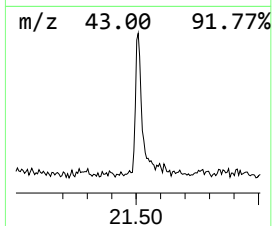
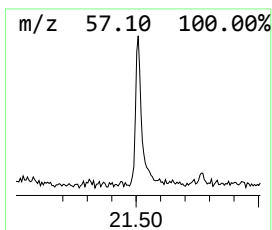
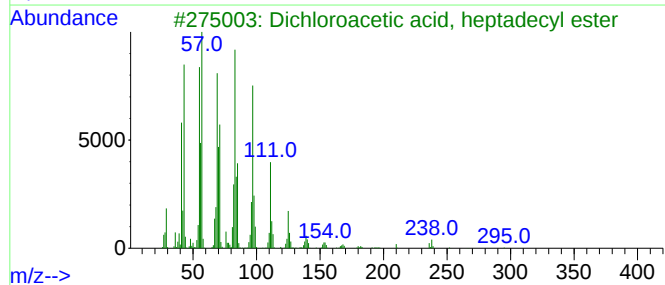
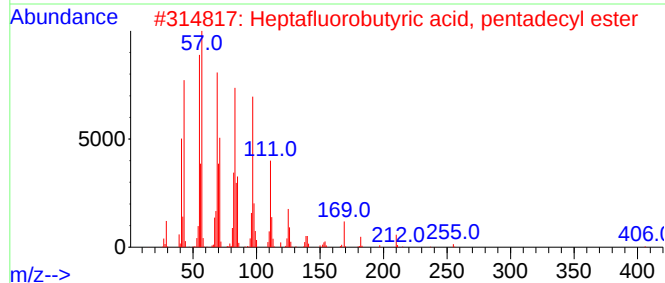
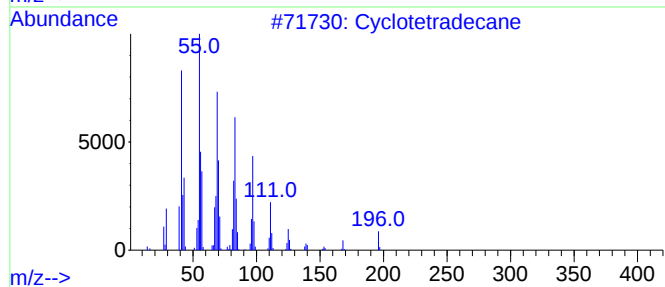
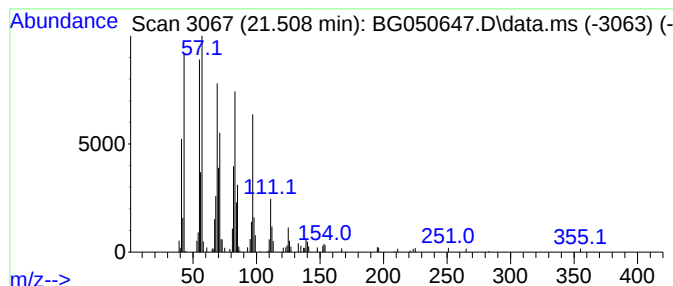
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Peak Number 3 Cyclotetradecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.508	4.03 ng	135184	Chrysene-d12	21.913

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	97
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4			Behenic alcohol	326	C22H46O	000661-19-8	91
5			1-Heptacosanol	396	C27H56O	002004-39-9	91



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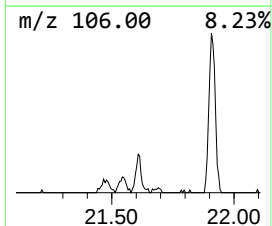
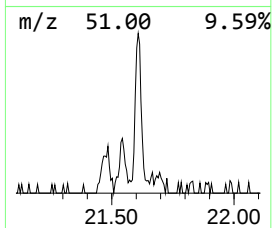
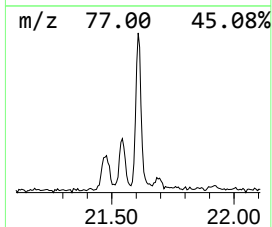
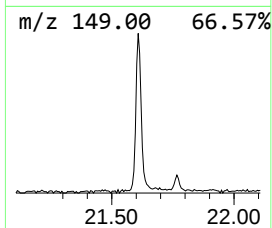
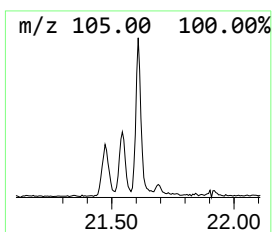
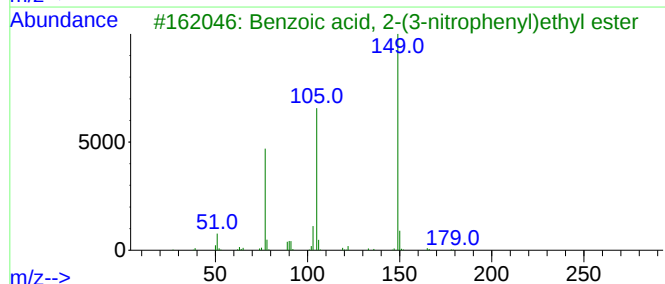
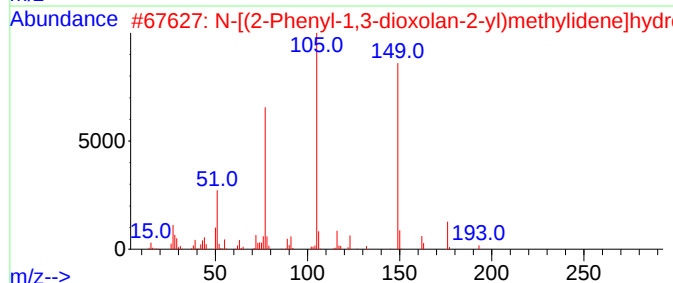
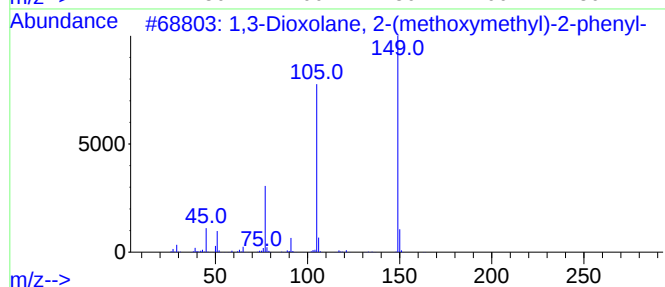
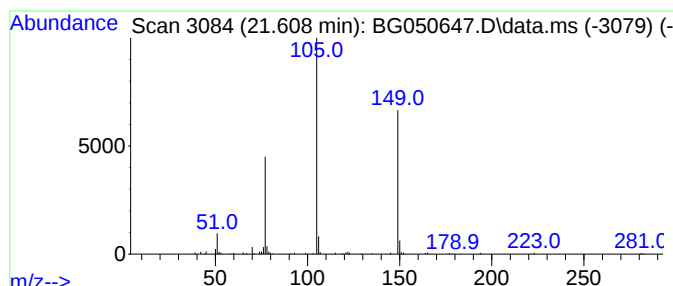
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Peak Number 4 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.608	3.56 ng	119369	Chrysene-d12	21.913

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83
2			N-[(2-Phenyl-1,3-dioxolan-2-yl)m...	193	C10H11NO3	1000411-48-9	64
3			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	64
4			N-(4-Cyanophenyl)benzamide	222	C14H10N2O	010278-46-3	47
5			Phenylglyoxylic acid, propyl ester	192	C11H12O3	1000453-46-7	47



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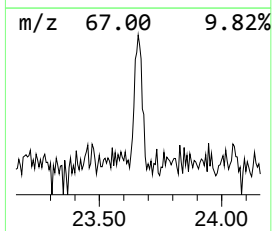
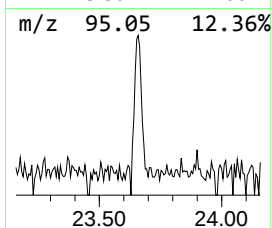
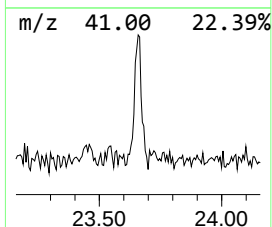
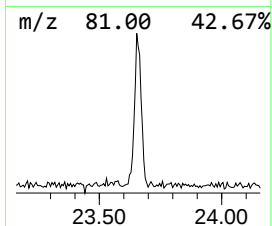
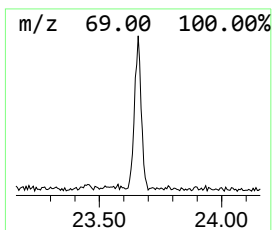
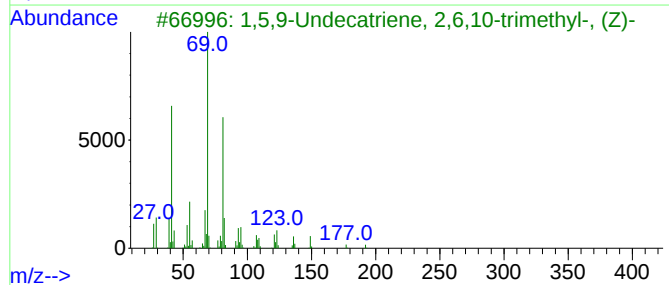
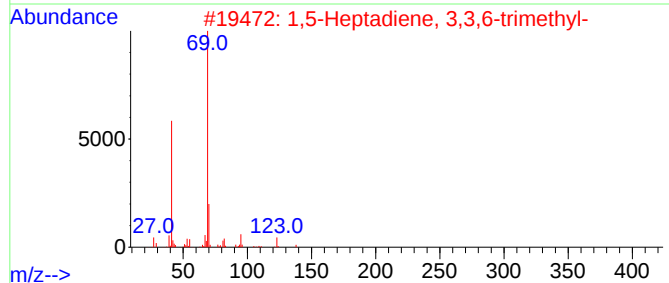
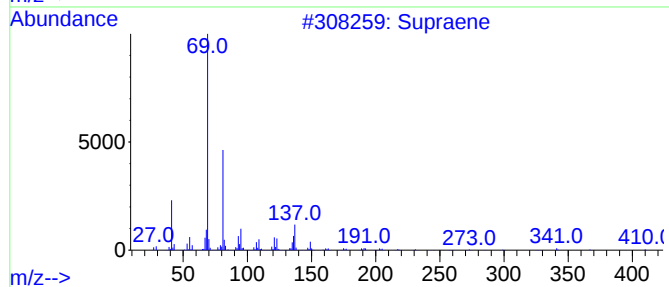
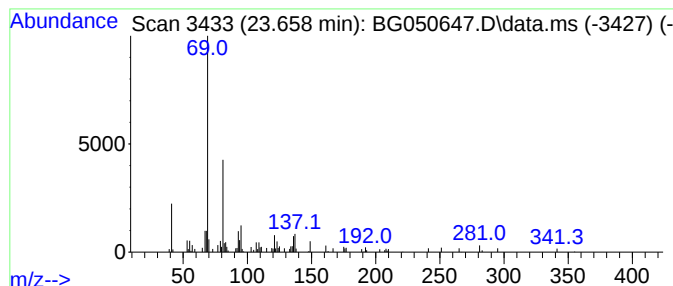
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Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.658	2.47 ng	81979	Perylene-d12	25.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	74
2			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	72
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
4			2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	64
5			4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	10.820	10.1	ng	188319	2	11.073	373394	20.0
n-Hexadecanoic ...	18.470	2.6	ng	77530	4	17.613	596956	20.0
Cyclotetradecane	21.508	4.0	ng	135184	5	21.913	670833	20.0
1,3-Dioxolane, ...	21.608	3.6	ng	119369	5	21.913	670833	20.0
Supraene	23.658	2.5	ng	81979	6	25.327	663000	20.0