

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040518\
 Data File : BG033600.D
 Acq On : 5 Apr 2018 19:49
 Operator : SJ/JU
 Sample : J2265-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PF-2

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:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.478	25	32	41	rBV	72665	135602	5.40%	0.944%
2	3.567	43	47	55	rVB	44387	66072	2.63%	0.460%
3	5.776	417	423	429	rBV	24822	45120	1.80%	0.314%
4	6.287	504	510	528	rBV	445484	909844	36.24%	6.333%
5	7.973	790	797	814	rBV	492986	1114187	44.38%	7.755%
6	8.373	858	865	889	rBV	470598	1053794	41.98%	7.335%
7	8.860	939	948	959	rBV	78966	188571	7.51%	1.313%
8	9.195	997	1005	1020	rBV	346363	725165	28.89%	5.047%
9	10.059	1145	1152	1168	rBV	270895	644115	25.66%	4.483%
10	11.739	1432	1438	1450	rBV	136674	298377	11.89%	2.077%
11	14.101	1832	1840	1857	rBV	916764	1600017	63.73%	11.137%
12	14.894	1965	1975	1985	rBV	72334	122416	4.88%	0.852%
13	15.300	2039	2044	2049	rBV2	24352	32581	1.30%	0.227%
14	15.476	2068	2074	2086	rBV2	309750	539066	21.47%	3.752%
15	16.240	2200	2204	2210	rVB	36805	50652	2.02%	0.353%
16	16.639	2264	2272	2277	rBV4	12365	25847	1.03%	0.180%
17	16.951	2318	2325	2341	rBV	883141	1526024	60.79%	10.622%
18	17.092	2344	2349	2360	rVB	35392	70618	2.81%	0.492%
19	18.208	2529	2539	2549	rBV	415988	720649	28.71%	5.016%
20	19.007	2671	2675	2685	rBV2	93166	142670	5.68%	0.993%
21	20.729	2962	2968	2977	rBV	1727462	2510484	100.00%	17.474%
22	22.068	3191	3196	3206	rBV	124605	221477	8.82%	1.542%
23	22.550	3271	3278	3287	rBV2	369150	758345	30.21%	5.278%
24	23.467	3428	3434	3443	rVB10	35627	75504	3.01%	0.526%
25	24.419	3592	3596	3602	rVB7	23867	46075	1.84%	0.321%
26	26.310	3907	3918	3936	rBV2	206737	744017	29.64%	5.179%

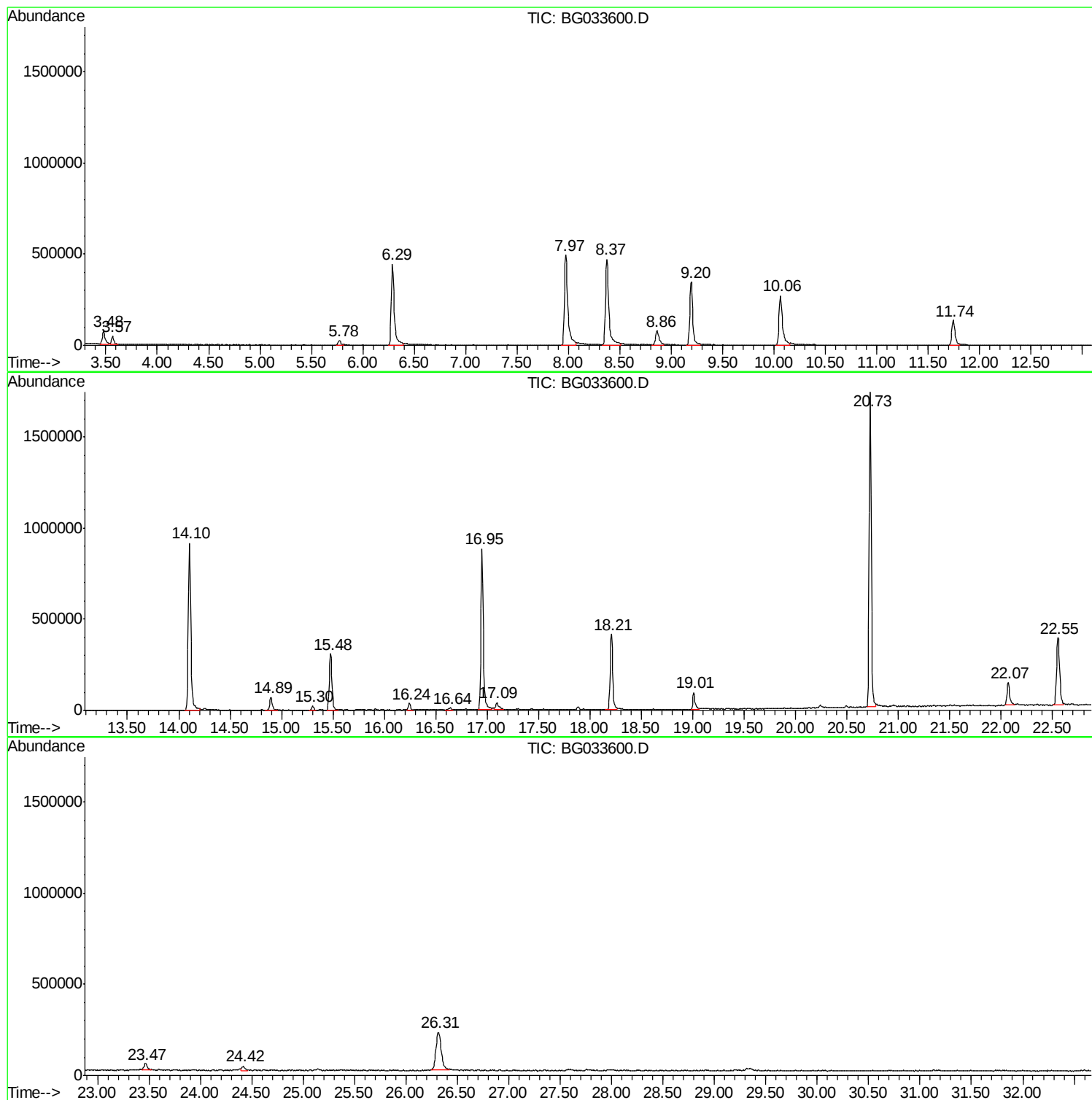
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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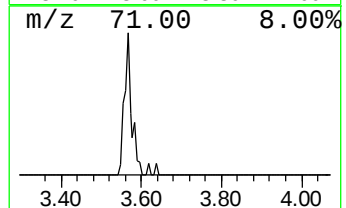
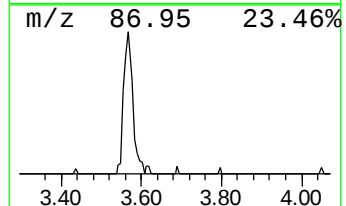
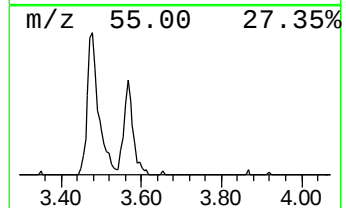
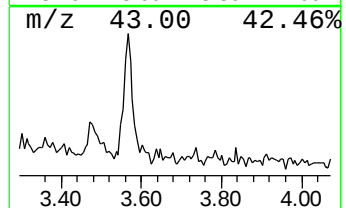
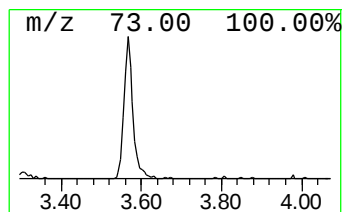
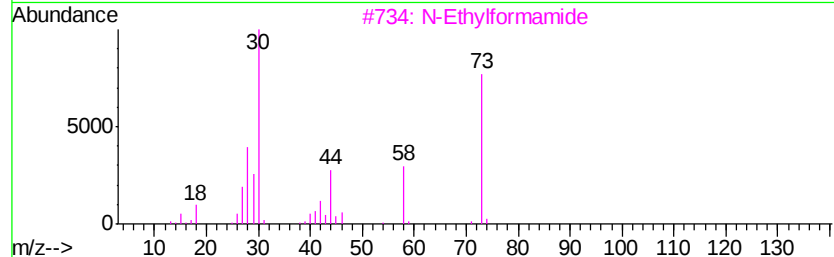
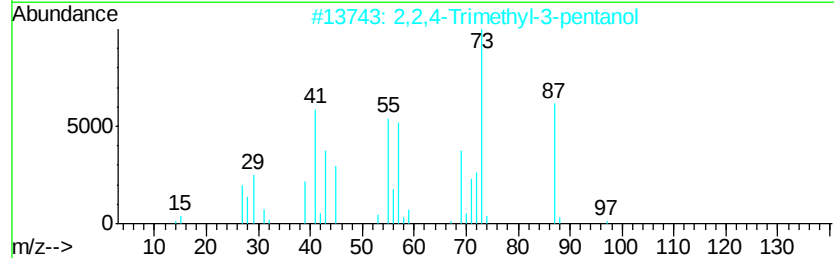
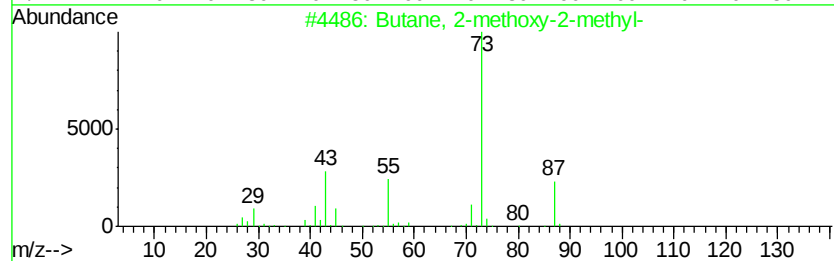
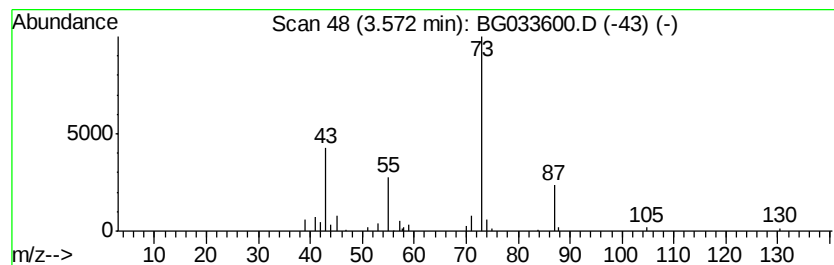
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.57	7.01 ng	66072	1,4-Dichlorobenzene-d4	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Myo-Inositol, 4-C-methyl-	194	C7H14O6	000472-95-7	9
5		Myo-Inositol, 2-C-methyl-	194	C7H14O6	000472-96-8	9



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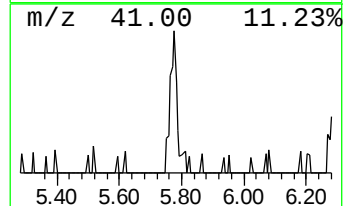
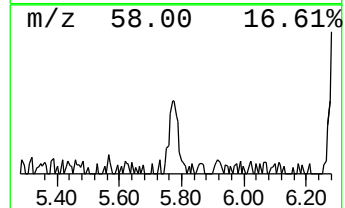
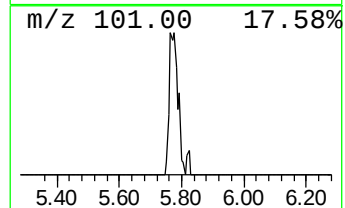
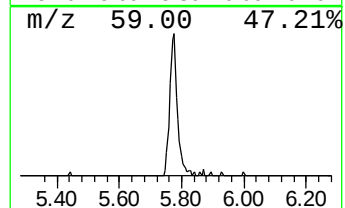
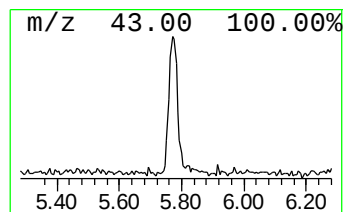
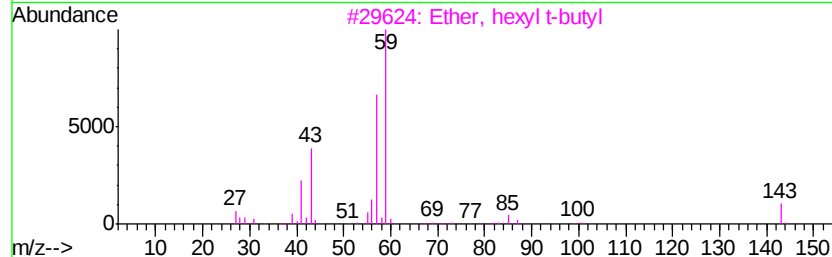
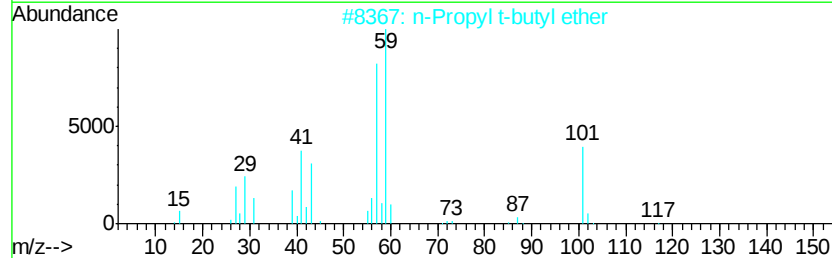
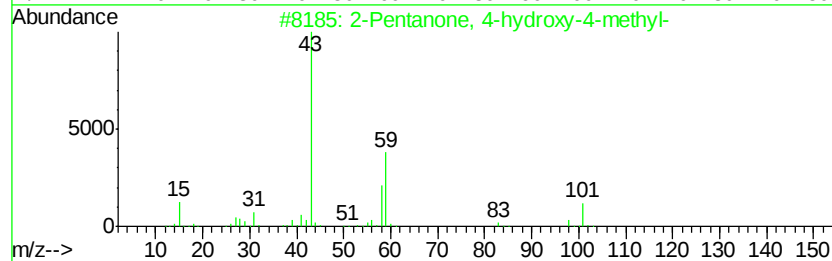
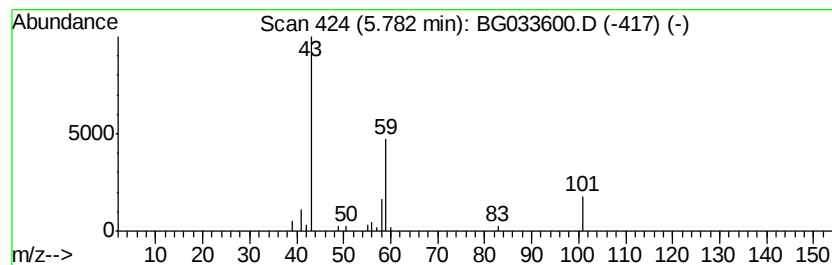
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.78	4.79 ng	45120	1,4-Dichlorobenzene-d4	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	25
2		n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	25
3		Ether, hexyl t-butyl	158	C10H22O	069775-79-7	23
4		2,11-Dodecanedione	198	C12H22O2	007029-09-6	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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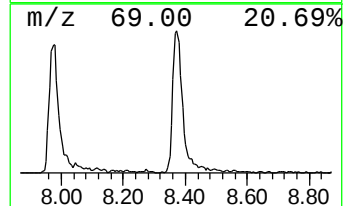
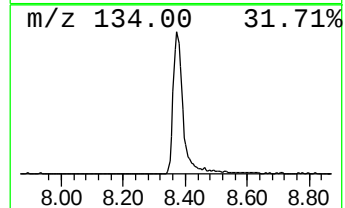
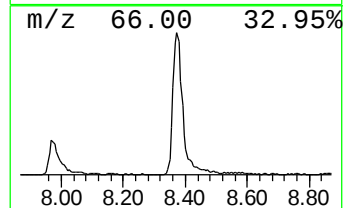
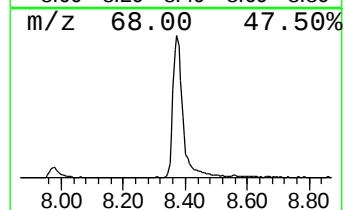
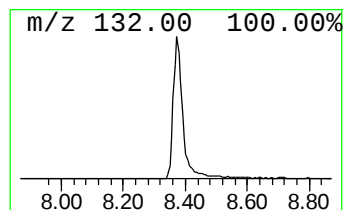
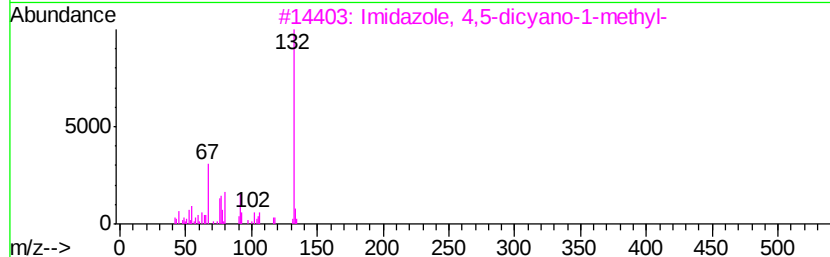
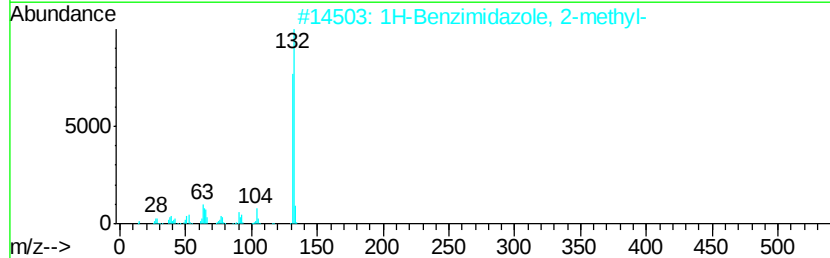
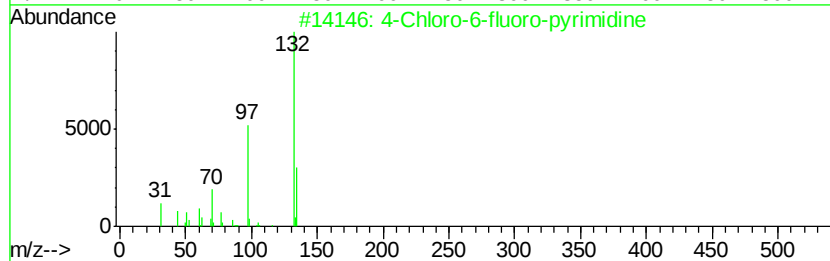
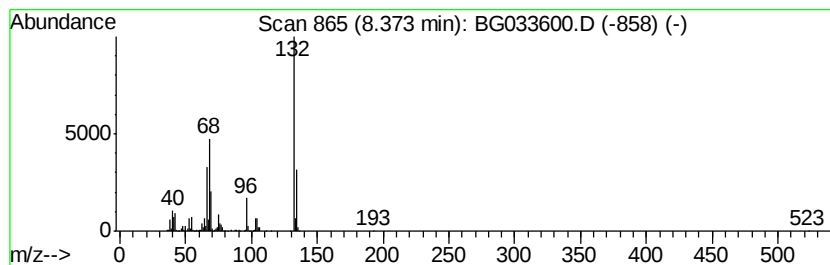
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Peak Number 4 unknown8.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.37	111.77 ng	1053790	1,4-Dichlorobenzene-d4	8.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		5-Aminoindole	132	C8H8N2	005192-03-0	10



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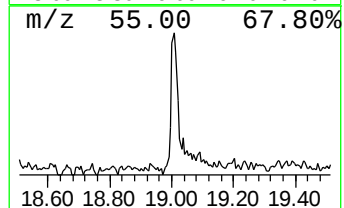
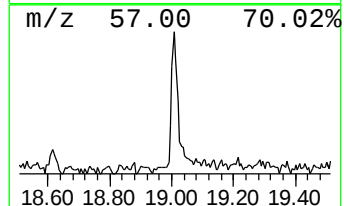
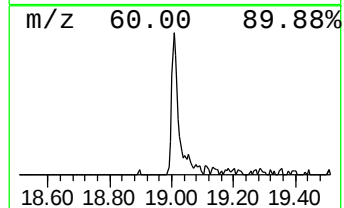
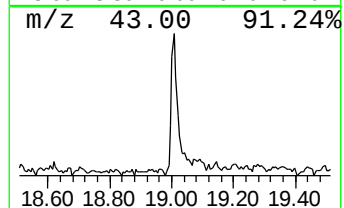
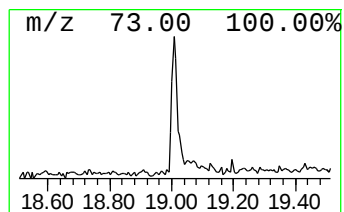
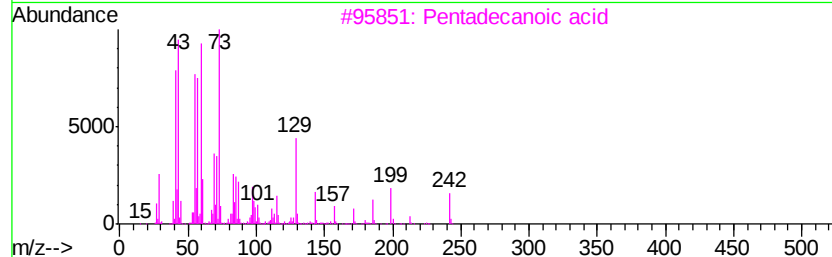
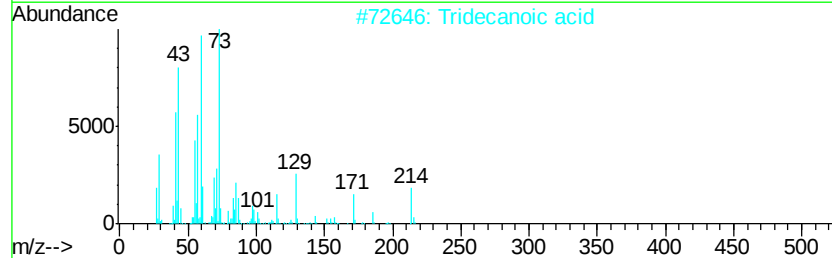
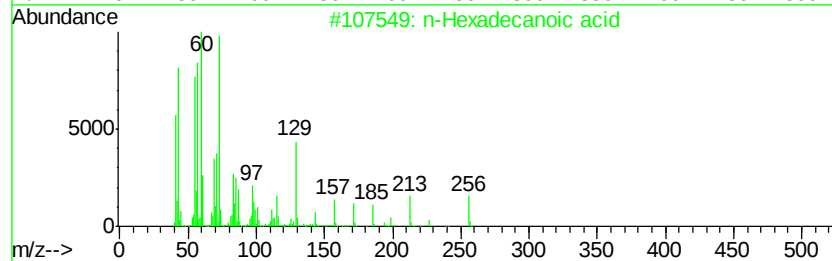
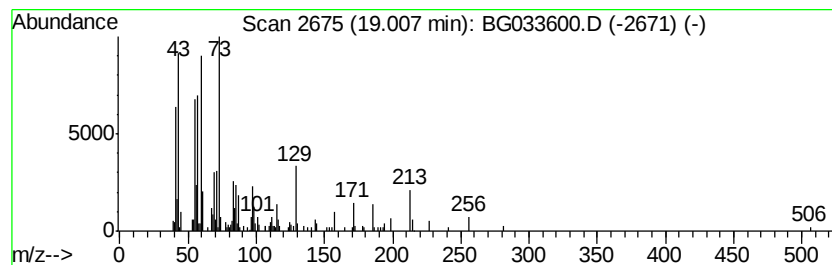
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.01	3.96 ng	142670	Phenanthrene-d10		18.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98	
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93	
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81	
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72	
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70	



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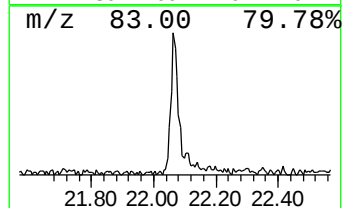
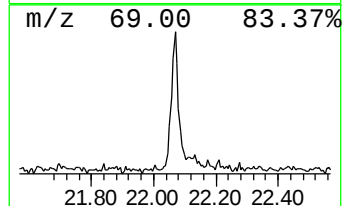
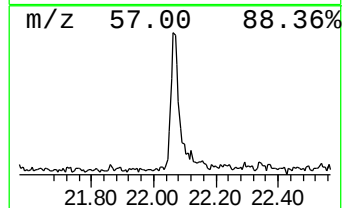
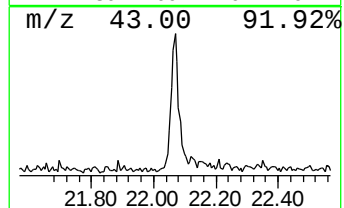
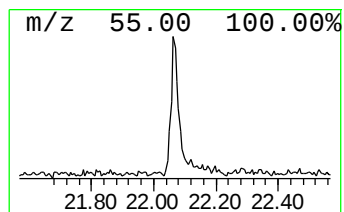
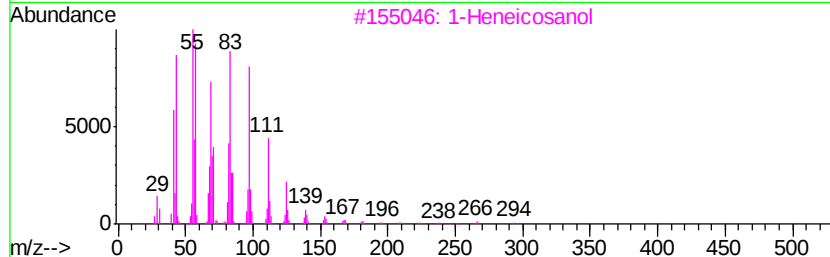
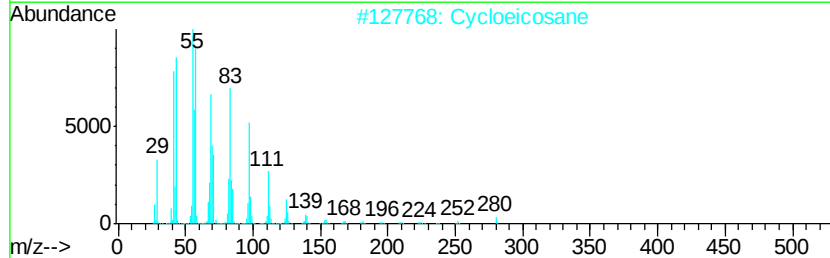
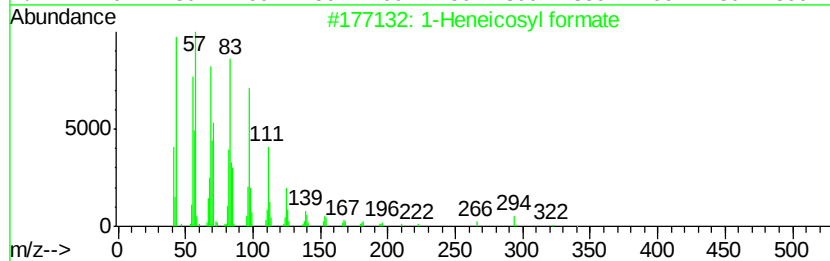
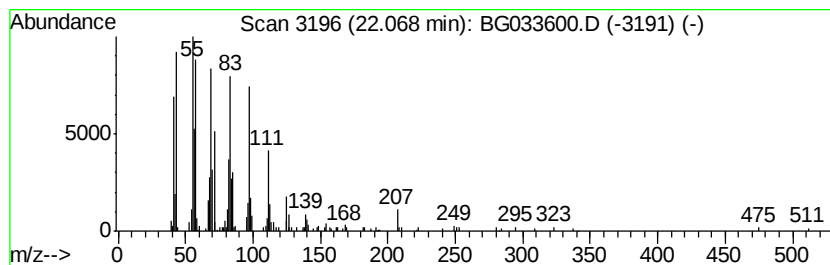
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Peak Number 7 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.07	5.84 ng	221477	Chrysene-d12	22.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl	formate	340	C22H44O2	077899-03-7	94
2	Cycloeicosane		280	C20H40	000296-56-0	93
3	1-Heneicosanol		312	C21H44O	015594-90-8	93
4	Heptadecyl	trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
5	Behenic	alcohol	326	C22H46O	000661-19-8	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.57	7.0	ng	66072	1	8.87	188571	20.0
2-Pentanone, 4-hy...	5.78	4.8	ng	45120	1	8.87	188571	20.0
unknown8.37	8.37	111.8	ng	1053790	1	8.87	188571	20.0
n-Hexadecanoic acid	19.01	4.0	ng	142670	4	18.21	720649	20.0
1-Heneicosyl formate	22.07	5.8	ng	221477	5	22.56	758345	20.0