

Data Path : Z:\HPCHEM1\BNA G\DATA\BG042415\
 Data File : BG016713.D
 Acq On : 25 Apr 2015 12:28
 Operator : TP/IZ
 Sample : G2006-04
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-4

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-BG042315.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	2.746	6	10	23	rVB	358524	452508	14.29%	3.129%
2	4.702	337	343	351	rVB	96939	133101	4.20%	0.920%
3	5.184	420	425	438	rVB	256390	356885	11.27%	2.468%
4	6.794	693	699	708	rBV	147169	233837	7.38%	1.617%
5	7.129	750	756	767	rBV	503270	761863	24.06%	5.269%
6	7.593	828	835	844	rBV	156133	243305	7.68%	1.683%
7	7.911	882	889	901	rVB	827823	1269268	40.08%	8.778%
8	8.751	1025	1032	1041	rBV	594311	959941	30.31%	6.639%
9	10.378	1302	1309	1321	rBV	215480	354796	11.20%	2.454%
10	12.864	1725	1732	1747	rBV	1697130	2386741	75.37%	16.506%
11	14.244	1960	1967	1978	rBV2	325282	484344	15.29%	3.350%
12	15.743	2216	2222	2235	rBV	609846	860681	27.18%	5.952%
13	16.988	2428	2434	2441	rBV2	439922	605437	19.12%	4.187%
14	17.899	2583	2589	2598	rBV	105382	180550	5.70%	1.249%
15	19.186	2803	2808	2827	rBV	180022	292468	9.24%	2.023%
16	19.626	2877	2883	2895	rBV	2619625	3166899	100.00%	21.901%
17	20.895	3095	3099	3105	rVB	36497	44642	1.41%	0.309%
18	21.177	3142	3147	3157	rBV	582373	735410	23.22%	5.086%
19	21.324	3169	3172	3176	rBV	36047	38792	1.22%	0.268%
20	21.753	3241	3245	3250	rBV	34358	44402	1.40%	0.307%
21	22.006	3284	3288	3296	rBV2	37209	55726	1.76%	0.385%
22	22.206	3318	3322	3326	rBV3	31643	38690	1.22%	0.268%
23	22.693	3403	3405	3413	rVB4	23562	35404	1.12%	0.245%
24	23.381	3515	3522	3531	rBV2	381311	724468	22.88%	5.010%

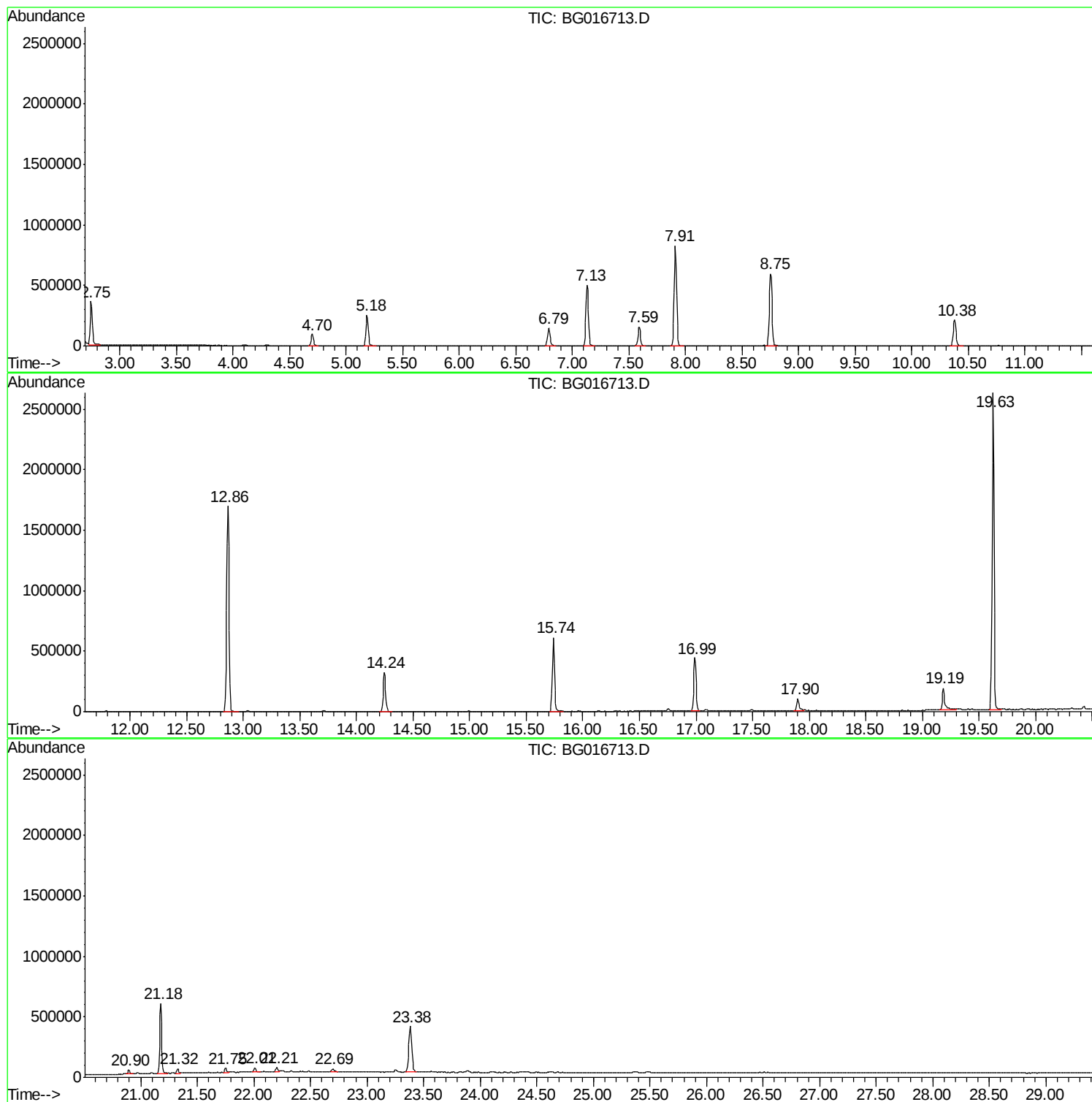
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG042315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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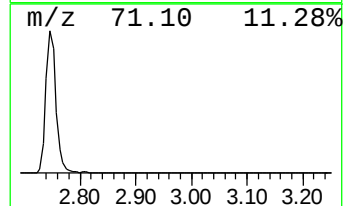
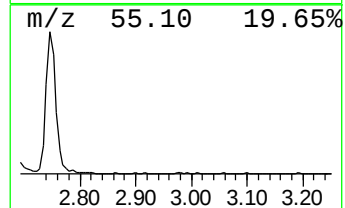
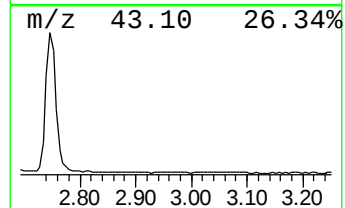
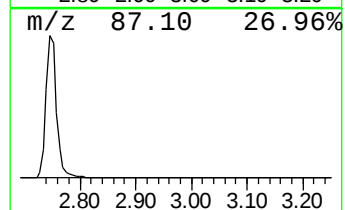
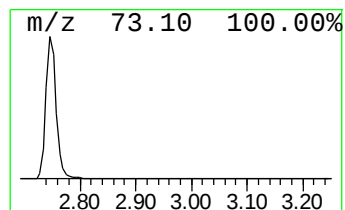
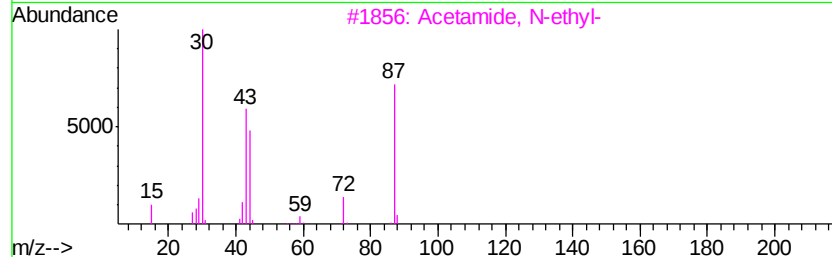
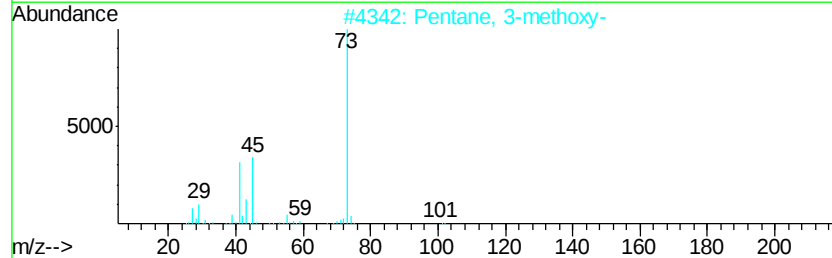
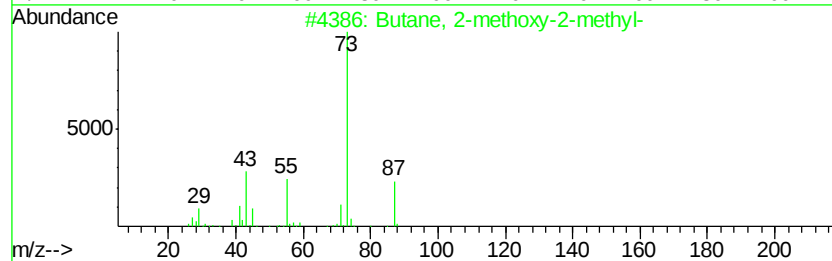
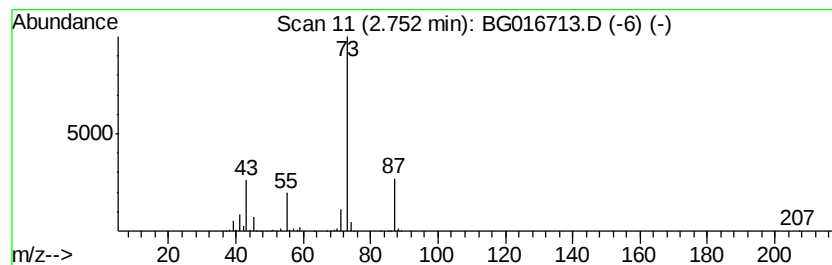
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG042315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.75	37.20 ng	452508	1,4-Dichlorobenzene-d4	7.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9



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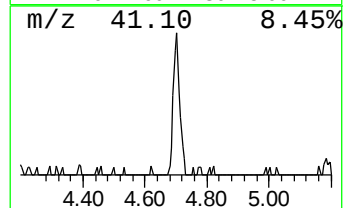
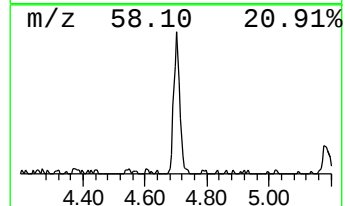
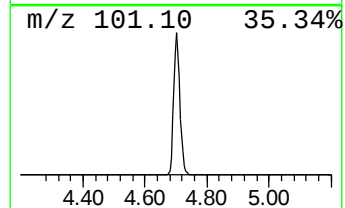
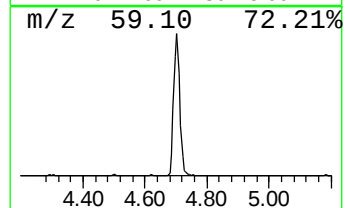
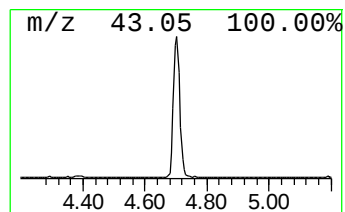
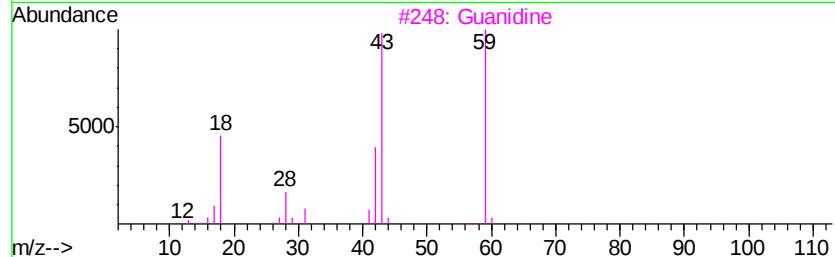
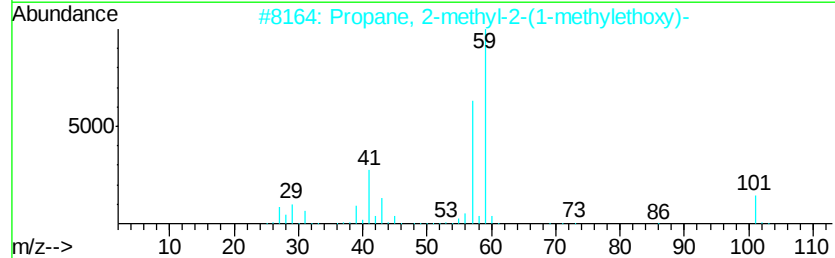
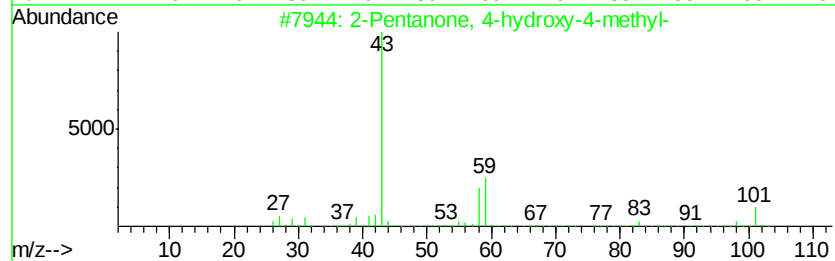
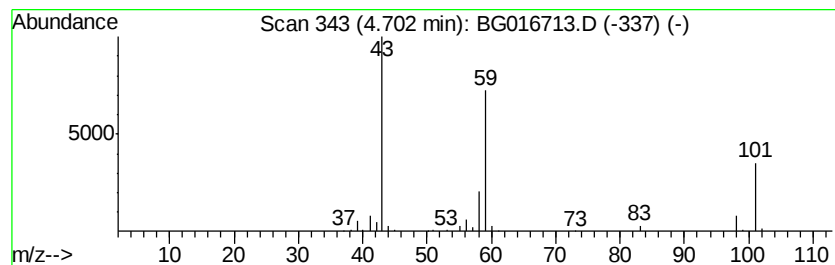
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	10.94 ng	133101	1,4-Dichlorobenzene-d4	7.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	47
3		Guanidine	59	CH5N3	000113-00-8	38
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		Acetone	58	C3H6O	000067-64-1	12



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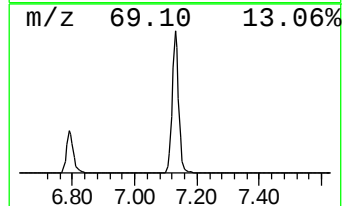
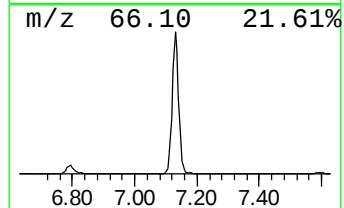
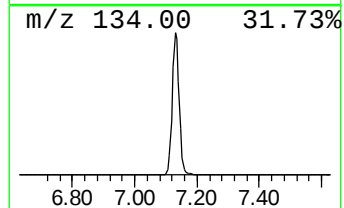
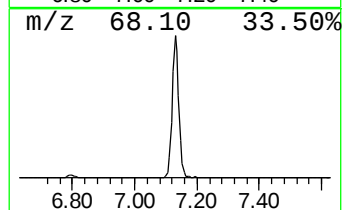
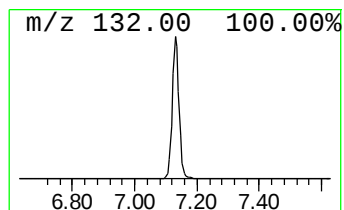
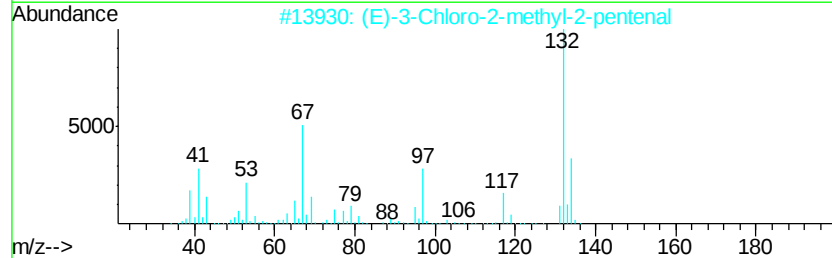
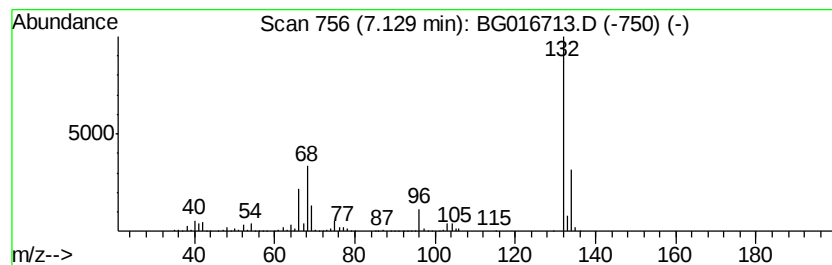
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.13 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.13	62.63 ng	761863	1,4-Dichlorobenzene-d4	7.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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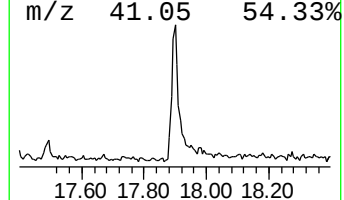
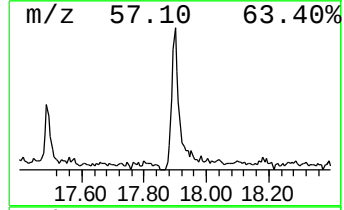
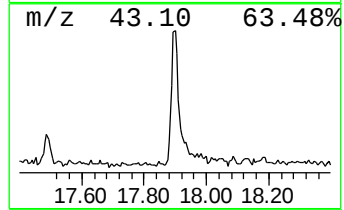
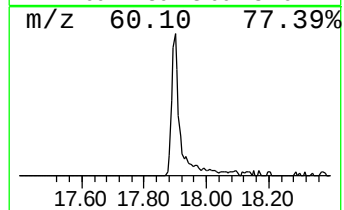
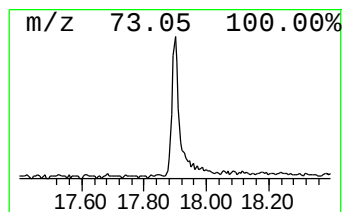
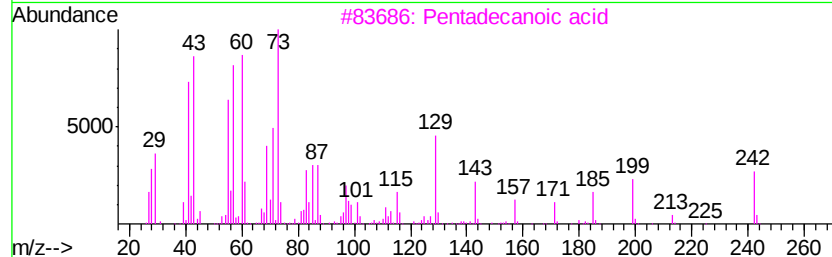
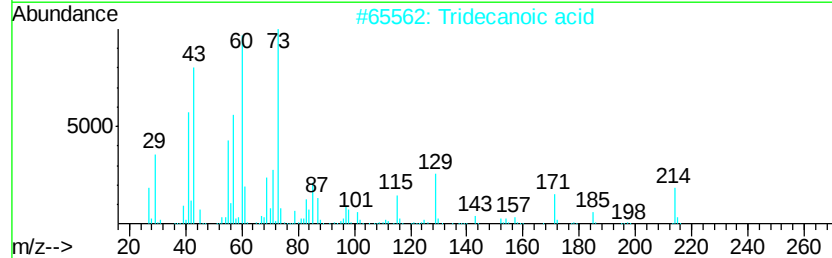
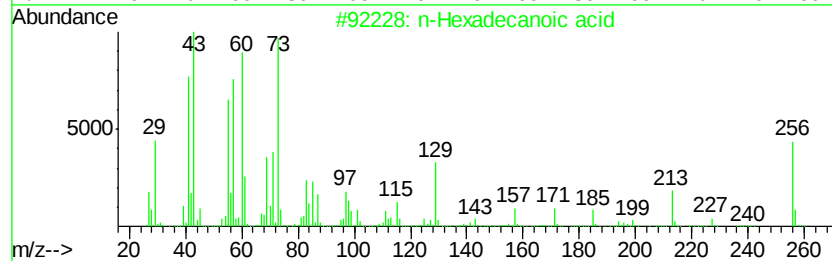
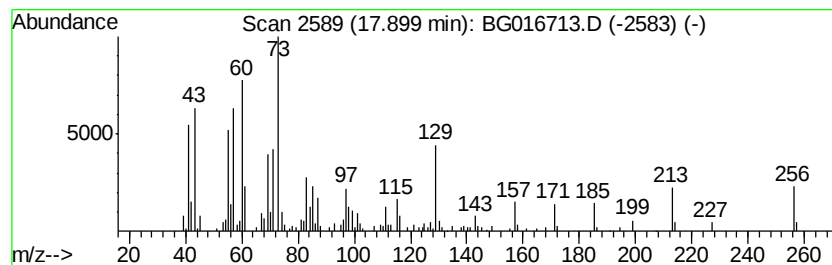
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.90	5.96 ng	180550	Phenanthrene-d10		16.99
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	58
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	43



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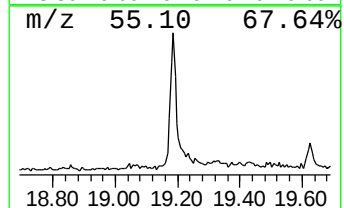
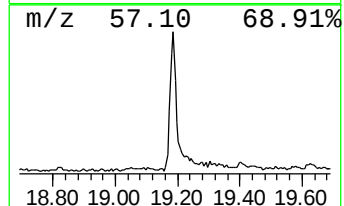
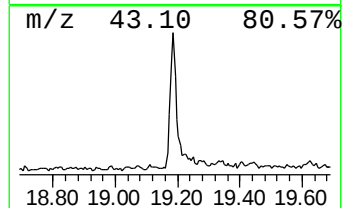
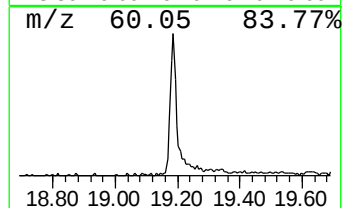
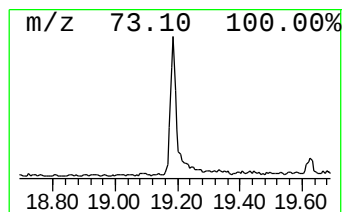
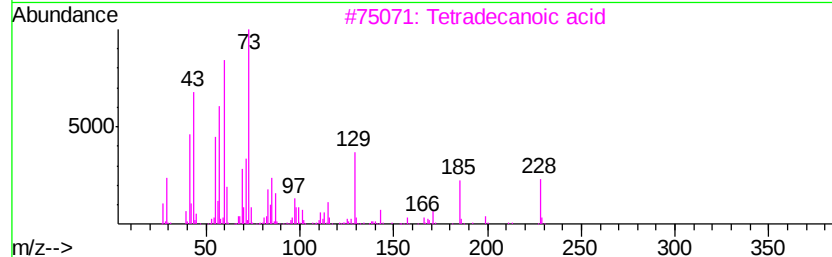
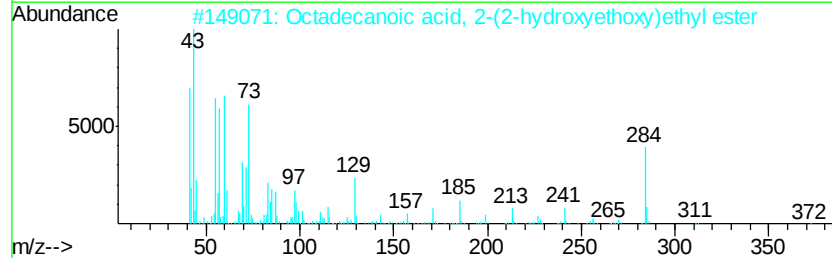
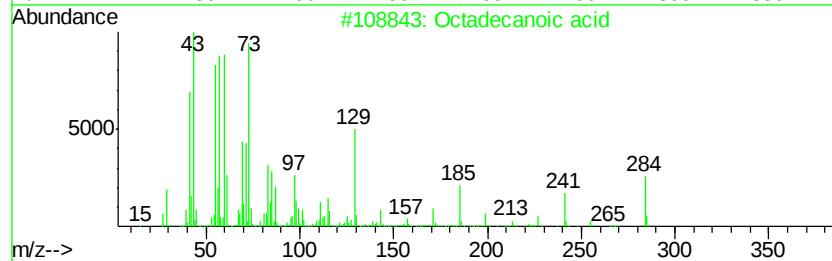
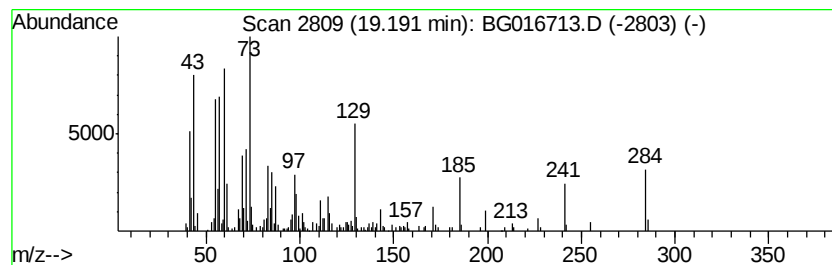
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.19	7.95 ng	292468	Chrysene-d12	21.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.75	37.2	ng	452508	1	7.59	243305	20.0
2-Pentanone, 4-hy...	4.70	10.9	ng	133101	1	7.59	243305	20.0
unknown7.13	7.13	62.6	ng	761863	1	7.59	243305	20.0
n-Hexadecanoic acid	17.90	6.0	ng	180550	4	16.99	605437	20.0
Octadecanoic acid	19.19	8.0	ng	292468	5	21.18	735410	20.0