

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041715\
 Data File : BG016496.D
 Acq On : 17 Apr 2015 19:52
 Operator : TP/IZ
 Sample : G1868-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P5-27(5-10)

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-BG040615.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	2.751	6	11	21	rVV	103425	186137	5.17%	0.856%
2	2.834	21	25	30	rVB	97142	129609	3.60%	0.596%
3	4.773	349	355	363	rVB	157531	212682	5.90%	0.978%
4	5.249	430	436	447	rBV	1252802	1770484	49.15%	8.144%
5	6.847	701	708	724	rBV	1224636	1925703	53.46%	8.858%
6	7.193	760	767	779	rBV	1249333	1968866	54.65%	9.057%
7	7.657	838	846	853	rBV	258145	389905	10.82%	1.794%
8	7.975	893	900	909	rBV	903414	1410010	39.14%	6.486%
9	8.815	1036	1043	1055	rBV	710907	1137381	31.57%	5.232%
10	10.442	1313	1320	1329	rBV	351972	569465	15.81%	2.619%
11	12.922	1735	1742	1751	rBV	1745356	2566745	71.25%	11.807%
12	13.762	1878	1885	1893	rBV	63244	91793	2.55%	0.422%
13	14.303	1970	1977	1986	rBV2	498120	749025	20.79%	3.445%
14	15.795	2223	2231	2243	rBV	1140314	1637782	45.46%	7.534%
15	16.012	2263	2268	2277	rBV2	22826	41940	1.16%	0.193%
16	17.041	2437	2443	2453	rBV2	651565	925509	25.69%	4.257%
17	17.945	2592	2597	2605	rBV2	66255	113377	3.15%	0.522%
18	19.232	2810	2816	2828	rBV4	20728	56283	1.56%	0.259%
19	19.673	2885	2891	2899	rBV	2750992	3602400	100.00%	16.571%
20	20.936	3102	3106	3116	rBV	128256	201072	5.58%	0.925%
21	21.224	3150	3155	3166	rBV	820885	1036889	28.78%	4.770%
22	23.457	3528	3535	3547	rBV2	540923	1016641	28.22%	4.676%

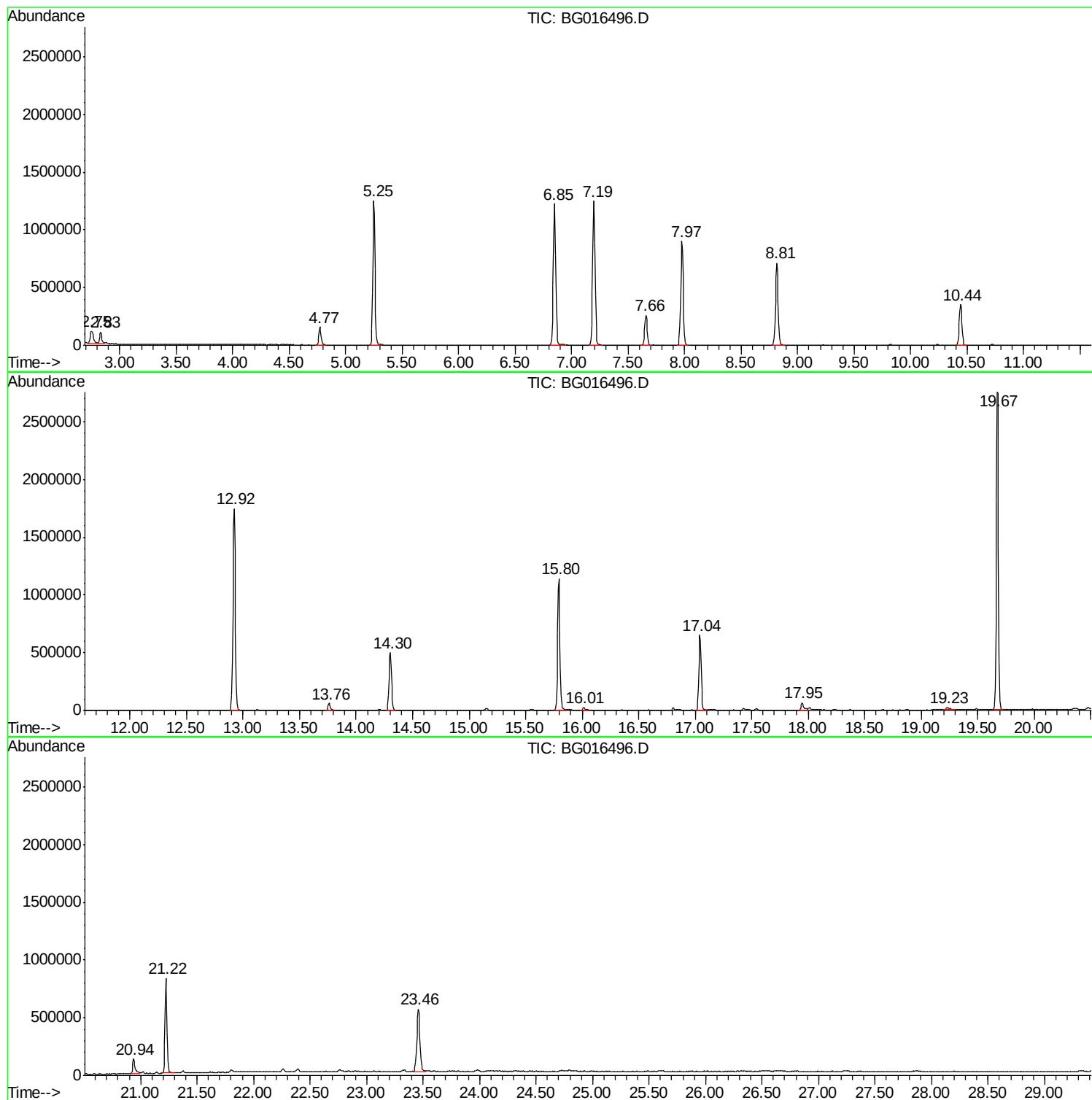
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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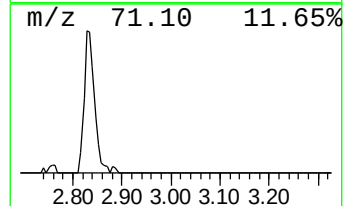
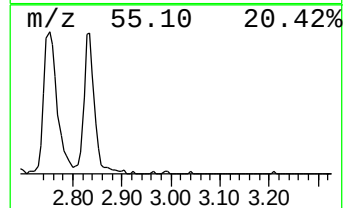
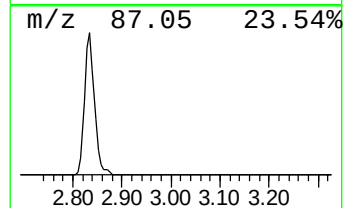
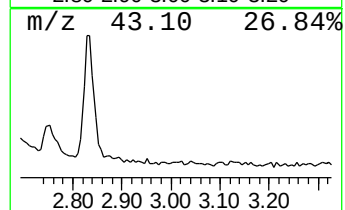
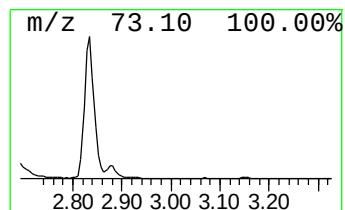
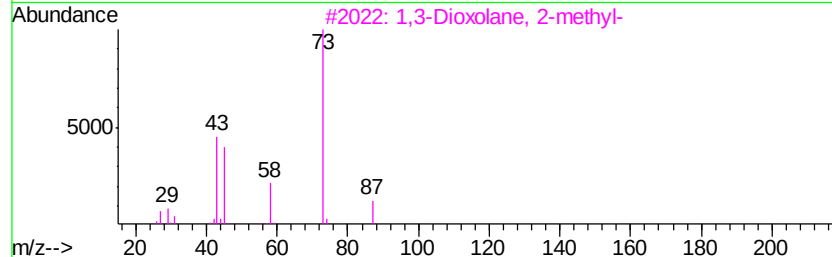
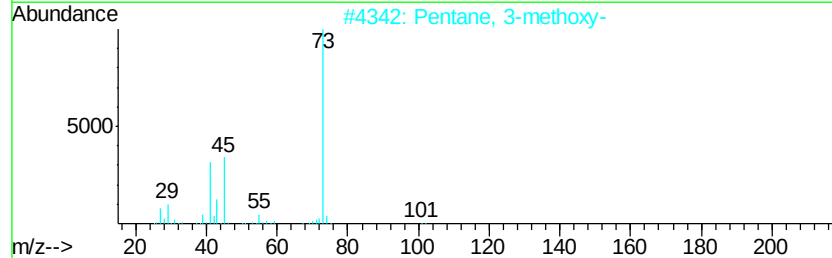
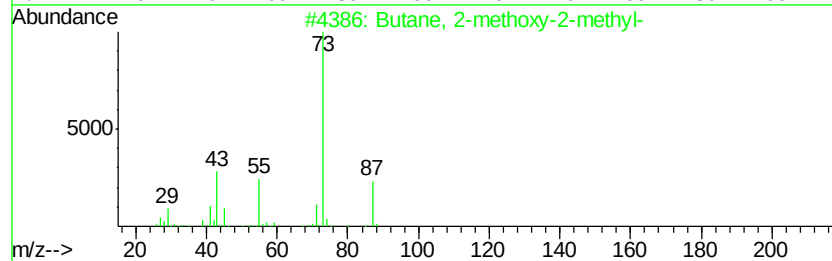
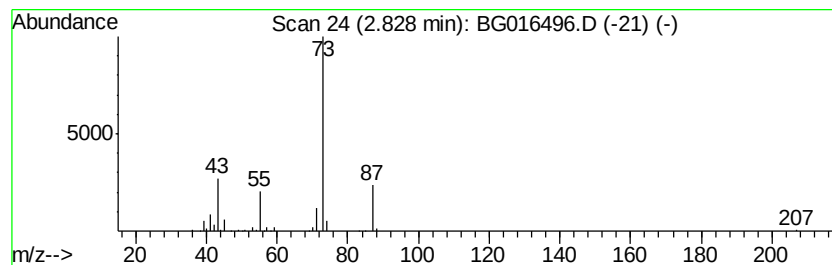
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.83	6.65 ng	129609	1,4-Dichlorobenzene-d4	7.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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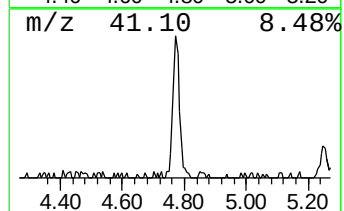
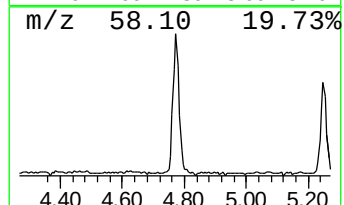
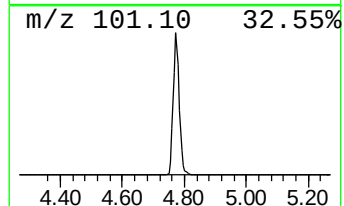
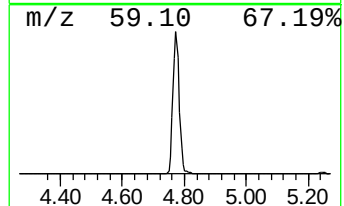
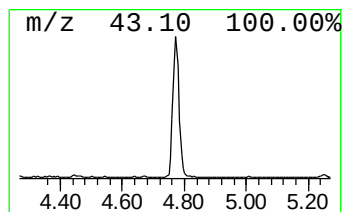
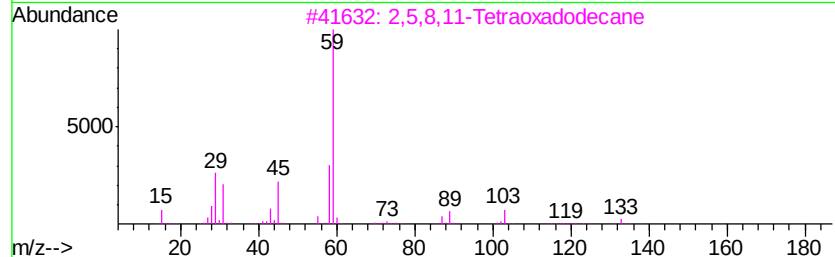
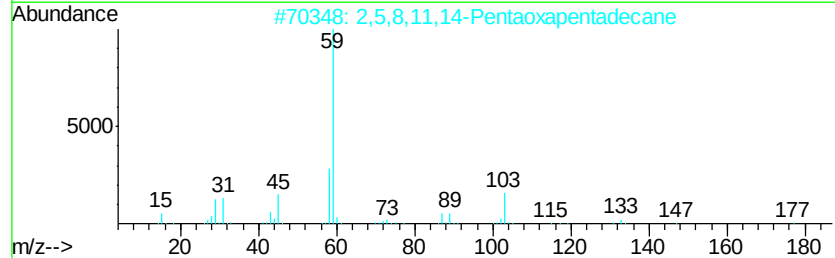
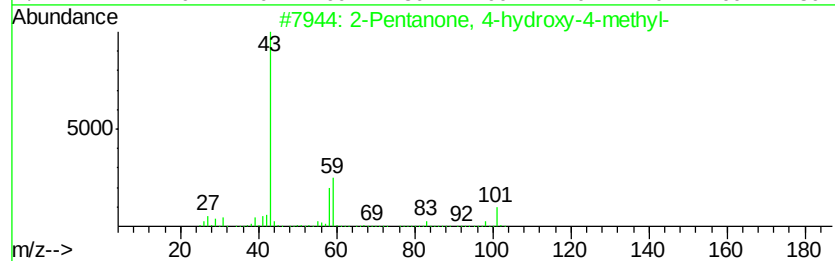
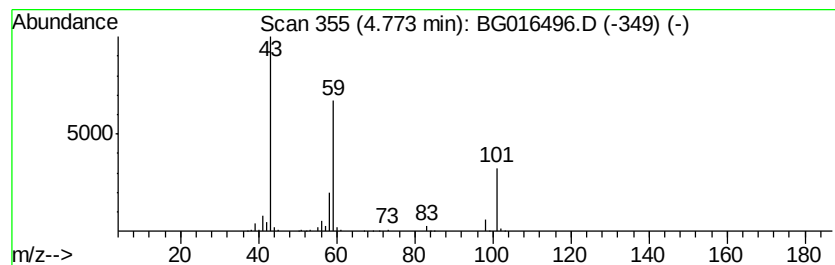
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.77	10.91 ng	212682	1,4-Dichlorobenzene-d4	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	25
3		2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	23
4		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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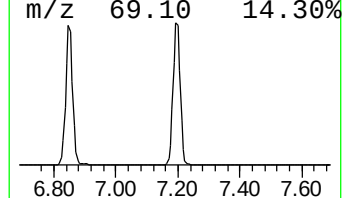
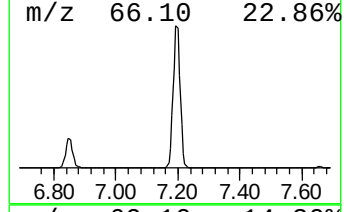
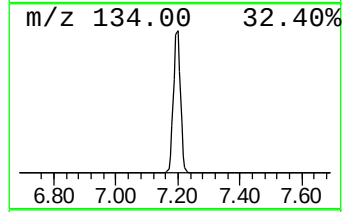
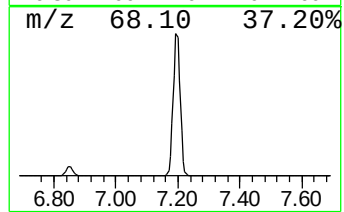
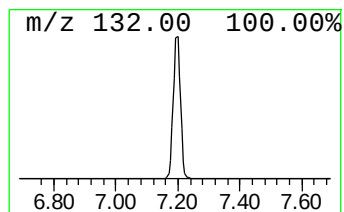
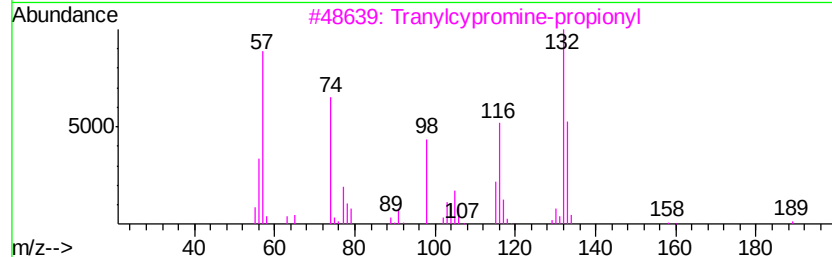
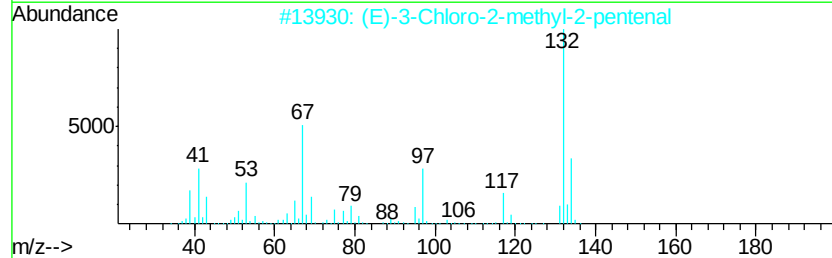
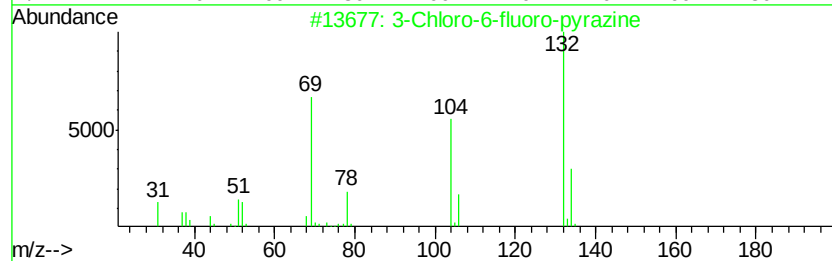
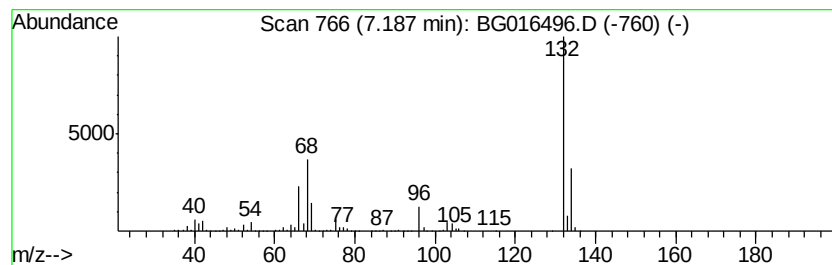
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Peak Number 4 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	100.99 ng	1968870	1,4-Dichlorobenzene-d4	7.66

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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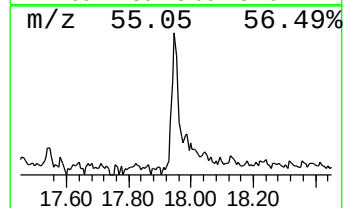
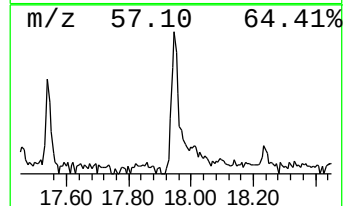
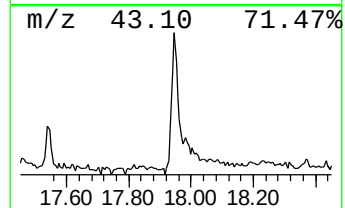
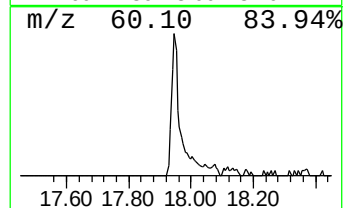
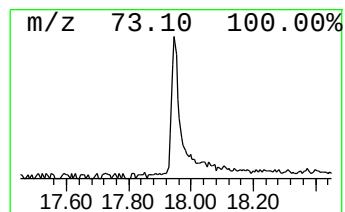
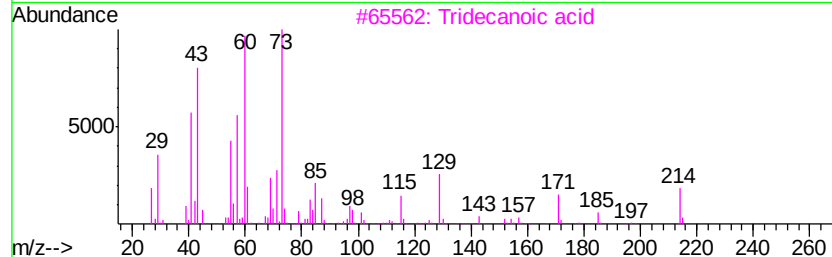
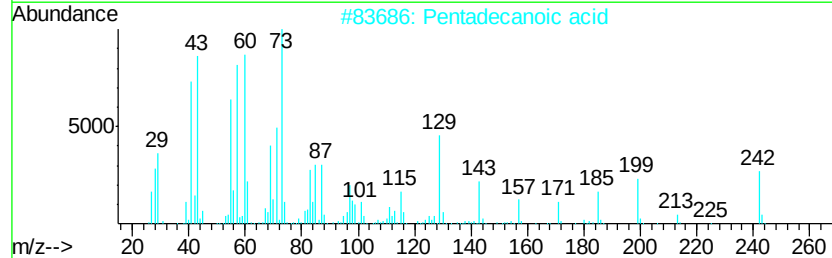
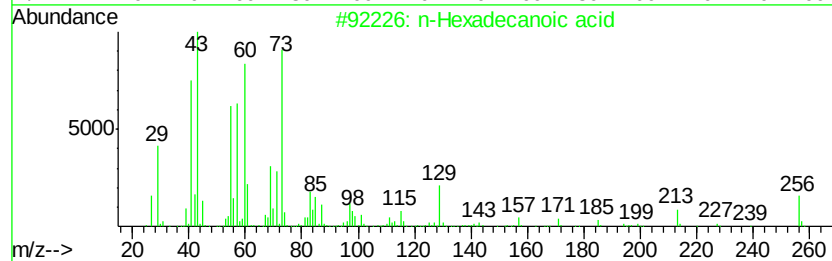
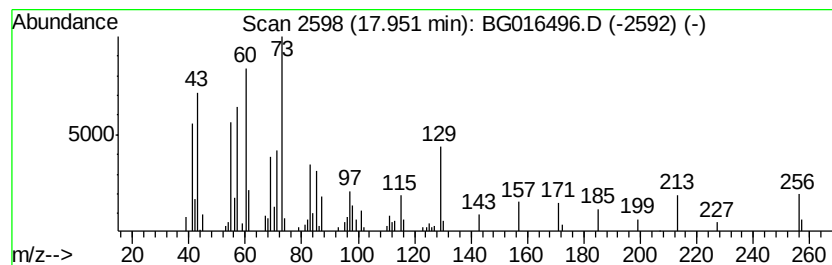
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.95	2.45 ng	113377	Phenanthrene-d10	17.04	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	74
4	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38
5	Nonanoic acid	158	C9H18O2	000112-05-0	38



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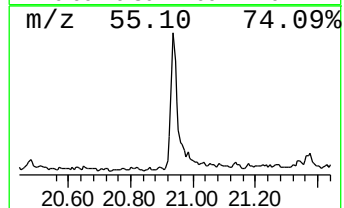
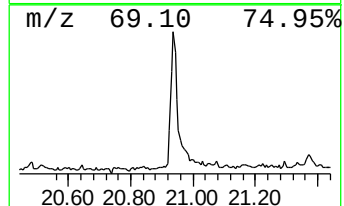
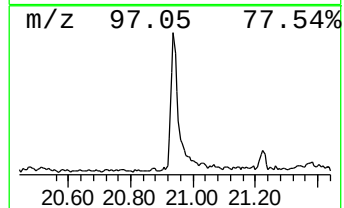
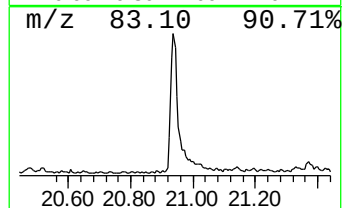
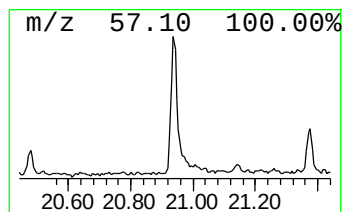
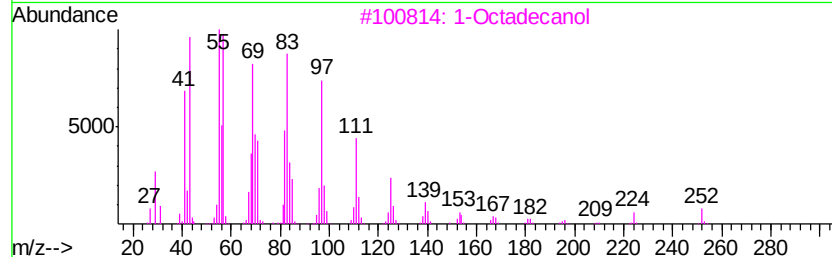
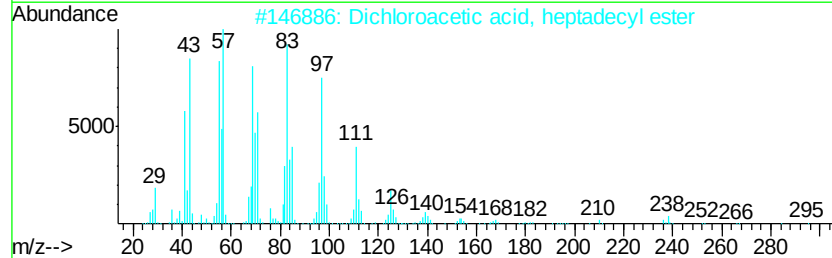
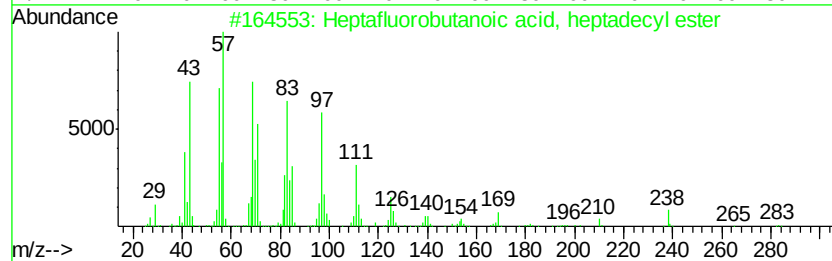
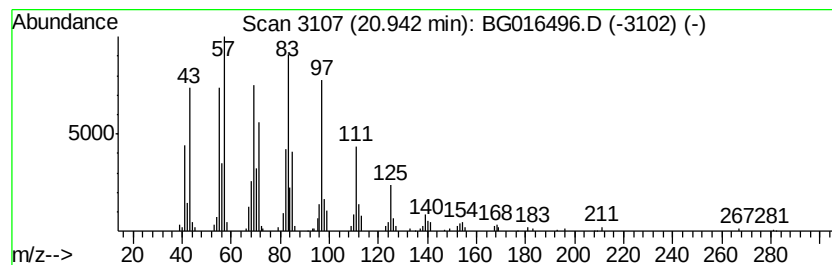
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 Heptafluorobutanoic acid, h... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.94	3.88 ng	201072	Chrysene-d12	21.22

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	93
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
3		1-Octadecanol	270	C18H38O	000112-92-5	93
4		1-Tetracosanol	354	C24H50O	000506-51-4	91
5		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.83	6.7	ng	129609	1	7.66	389905	20.0
2-Pentanone, 4-hy...	4.77	10.9	ng	212682	1	7.66	389905	20.0
unknown7.19	7.19	101.0	ng	1968870	1	7.66	389905	20.0
n-Hexadecanoic acid	17.95	2.5	ng	113377	4	17.04	925509	20.0
Heptafluorobutano...	20.94	3.9	ng	201072	5	21.22	1036890	20.0