

Data Path : Z:\HPCHEM1\BNA G\DATA\BG082316\
 Data File : BG023855.D
 Acq On : 23 Aug 2016 16:16
 Operator : UM/SJ
 Sample : H4528-15
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 VITALEFILL-MCMPH3-4

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.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	2.968	17	22	42	rVB	4794425	7899444	100.00%	20.018%
2	5.153	388	394	406	rVB	465810	716933	9.08%	1.817%
3	5.629	468	475	487	rBV	1262742	2147023	27.18%	5.441%
4	7.245	742	750	762	rBV	1307493	2394857	30.32%	6.069%
5	7.621	804	814	826	rBV	1325108	2316626	29.33%	5.870%
6	8.091	887	894	904	rBV	358717	617880	7.82%	1.566%
7	8.414	941	949	958	rBV	968278	1702744	21.56%	4.315%
8	9.271	1086	1095	1108	rBV	803290	1510483	19.12%	3.828%
9	10.928	1366	1377	1385	rBV	468208	869099	11.00%	2.202%
10	13.377	1784	1794	1803	rBV	2009146	3183826	40.30%	8.068%
11	14.206	1930	1935	1947	rVB	431085	678672	8.59%	1.720%
12	14.764	2023	2030	2039	rVB2	724643	1203117	15.23%	3.049%
13	16.262	2279	2285	2304	rBV	1772406	2857374	36.17%	7.241%
14	16.450	2312	2317	2326	rBV2	66037	117199	1.48%	0.297%
15	17.525	2494	2500	2511	rBV2	1005927	1648477	20.87%	4.177%
16	18.394	2643	2648	2656	rBV2	123134	197107	2.50%	0.499%
17	19.663	2861	2864	2870	rBV6	55576	87320	1.11%	0.221%
18	20.133	2938	2944	2952	rBV	4172075	5259975	66.59%	13.329%
19	21.443	3162	3167	3176	rBV8	70804	207376	2.63%	0.526%
20	21.837	3228	3234	3244	rBV2	1099694	1982146	25.09%	5.023%
21	25.220	3799	3810	3822	rVB2	624794	1864892	23.61%	4.726%

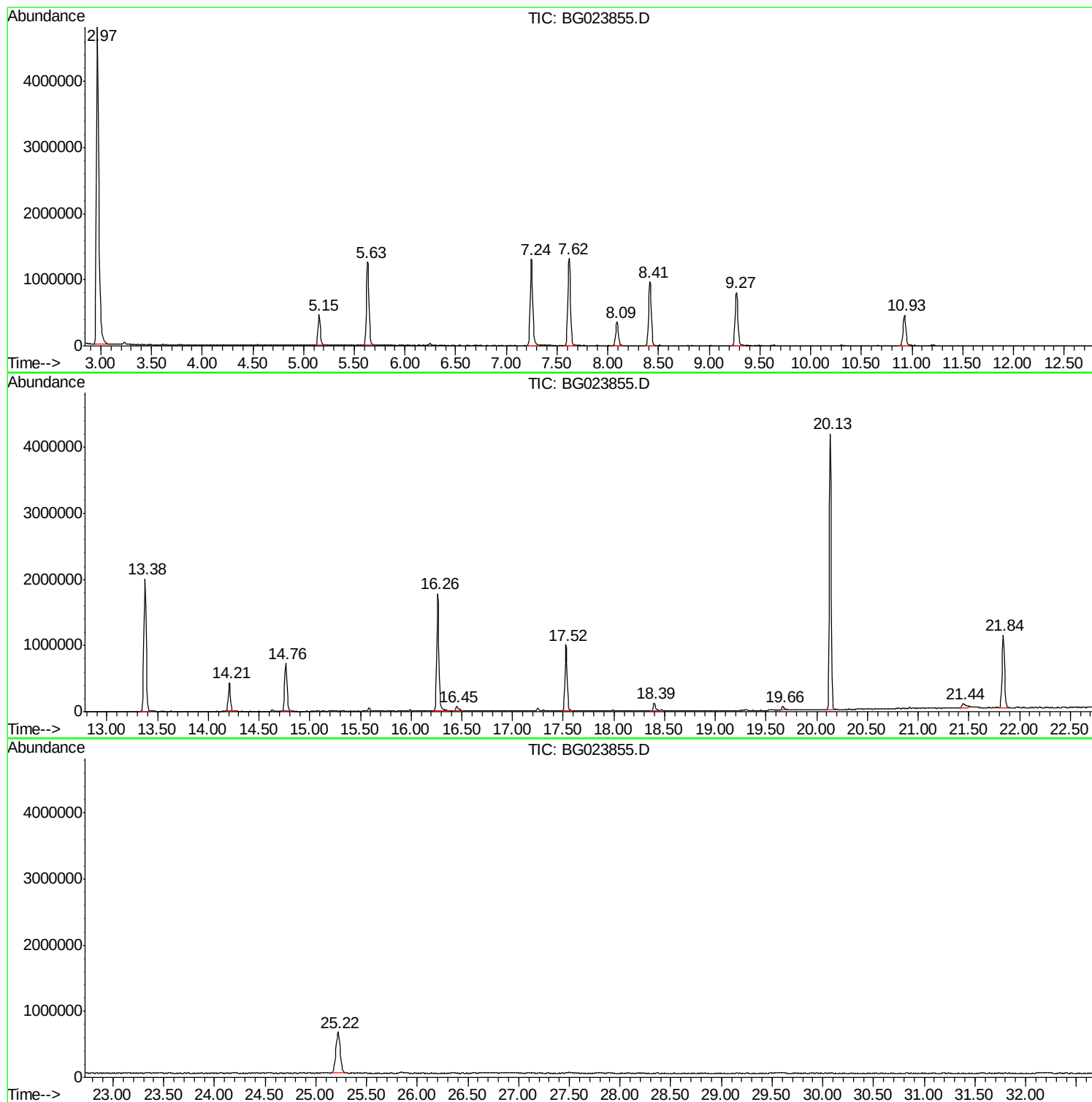
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Quant Method : Z:\HPCHEM1\BNA G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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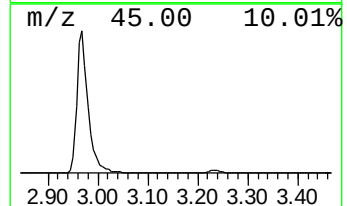
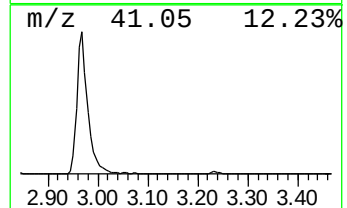
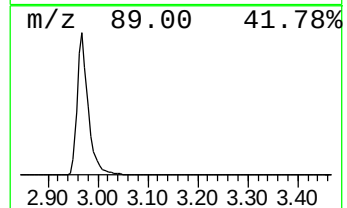
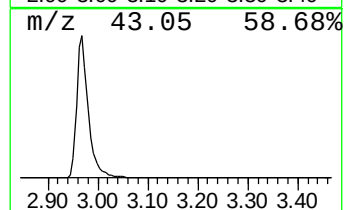
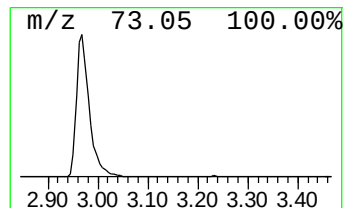
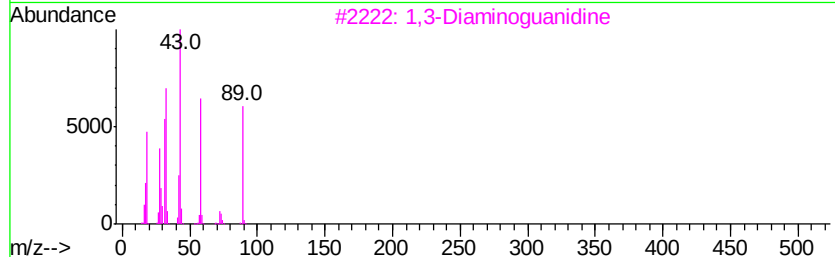
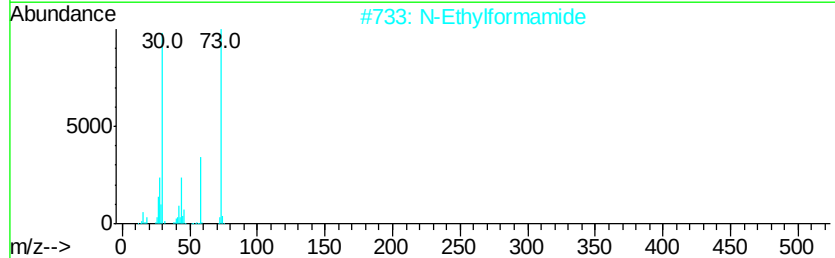
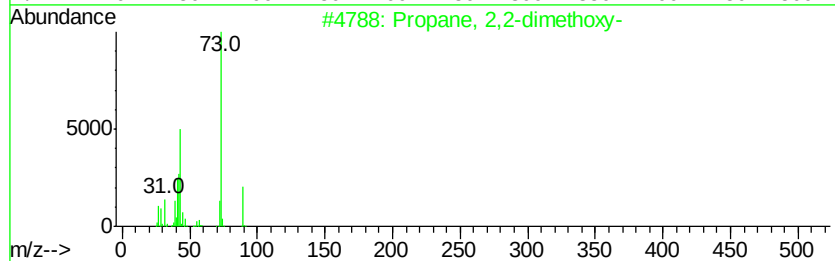
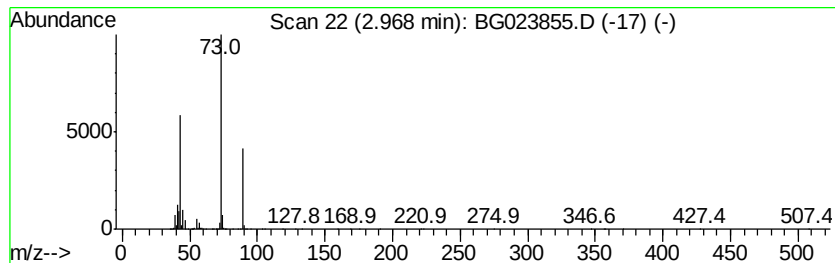
Quant Method : Z:\HPCHEM1\BNA G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.97	255.70 ng	7899440	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	78
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5		1-Propanol, 2-methyl-2-nitro-	119	C4H9NO3	000076-39-1	9



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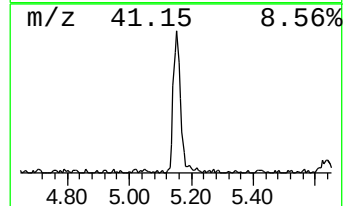
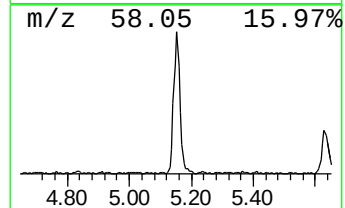
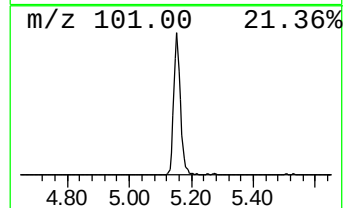
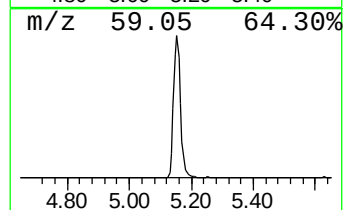
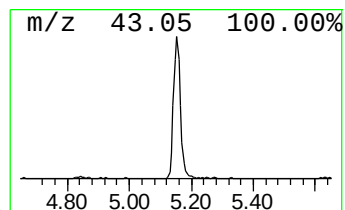
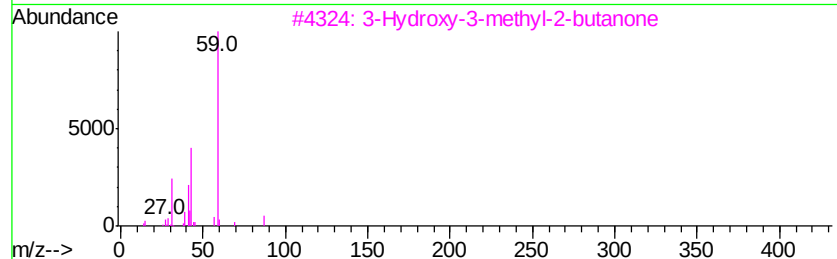
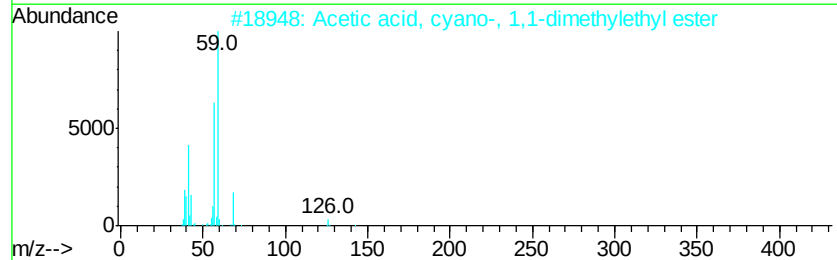
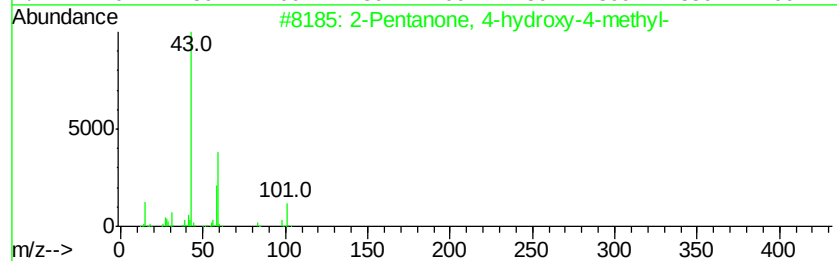
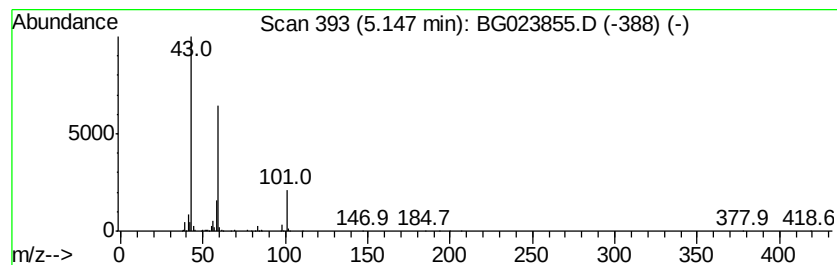
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	23.21 ng	716933	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Guanidine	59	CH5N3	000113-00-8	9



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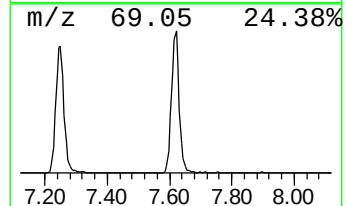
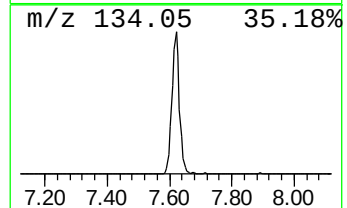
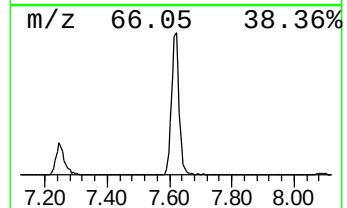
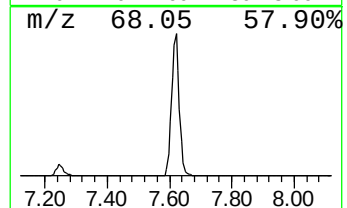
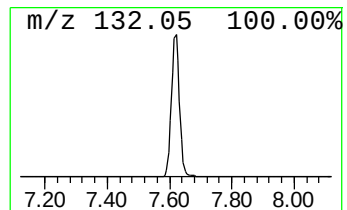
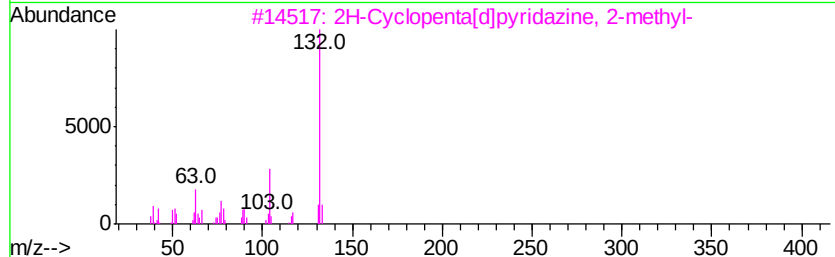
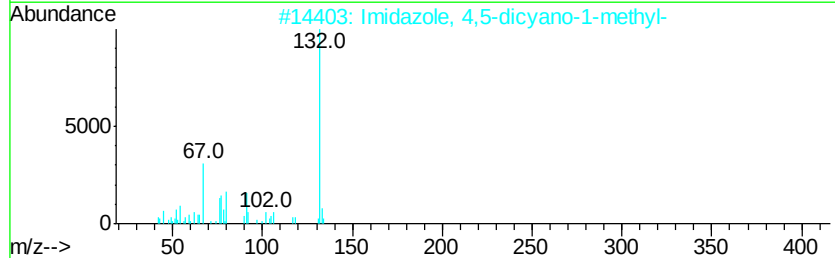
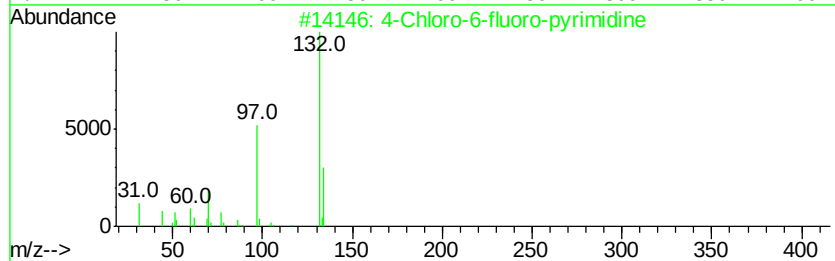
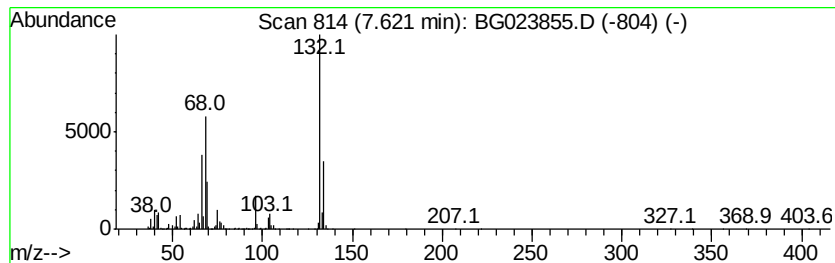
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Peak Number 3 unknown7.62 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	74.99 ng	2316630	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	10
3		2H-Cyclopentaf[d]pyridazine, 2-methyl-	132	C8H8N2	022291-85-6	10
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		Xenon	132	Xe	007440-63-3	9



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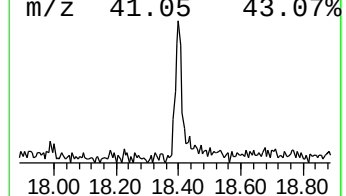
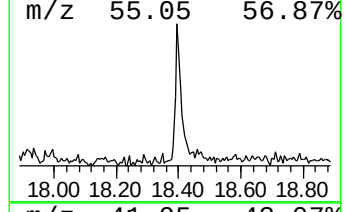
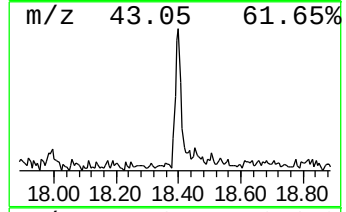
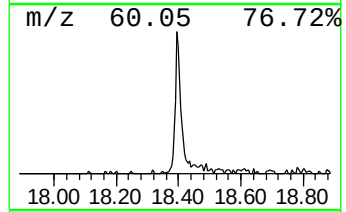
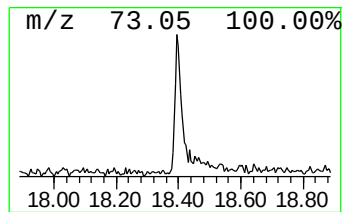
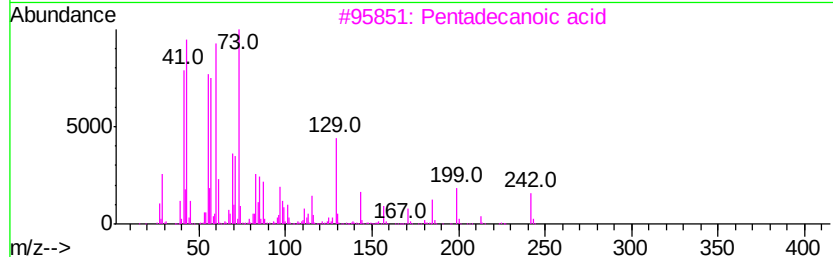
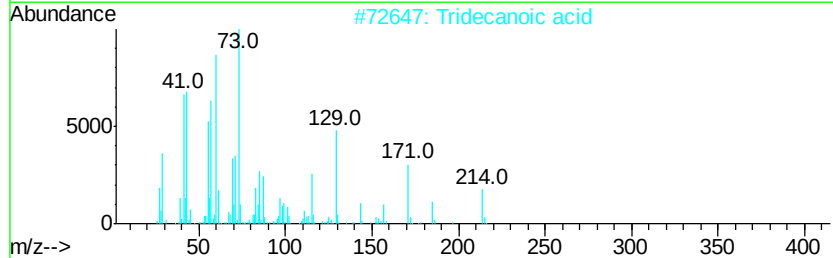
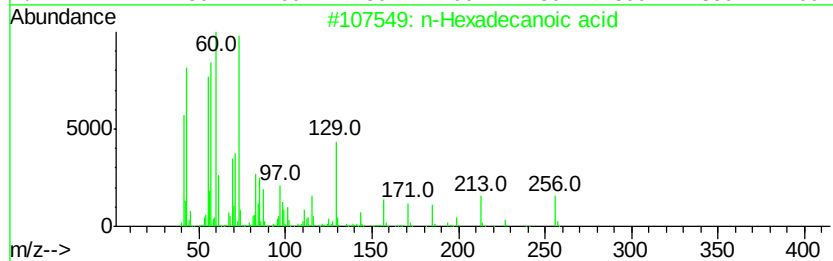
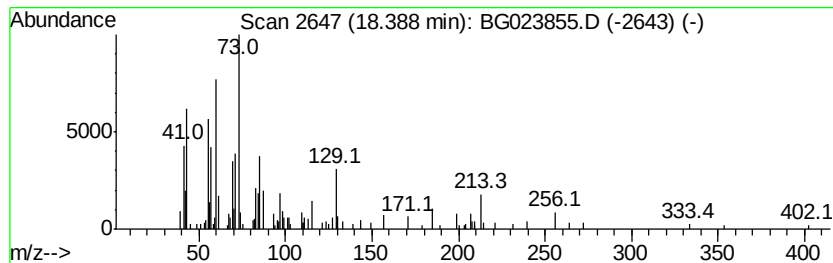
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	2.39 ng	197107	Phenanthrene-d10	17.52

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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Undecanoic acid	186	C11H22O2	000112-37-8	53



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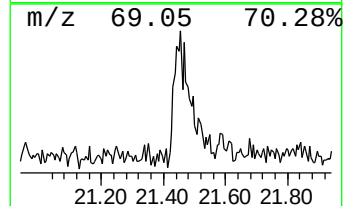
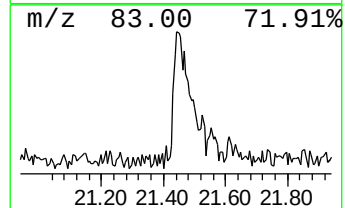
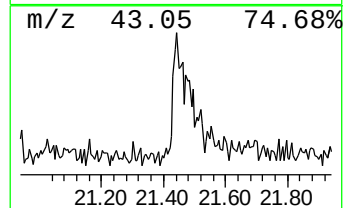
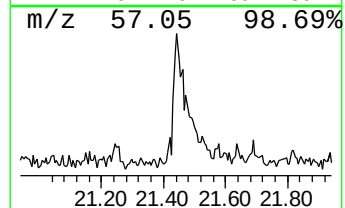
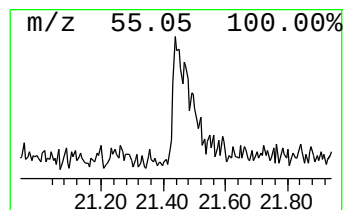
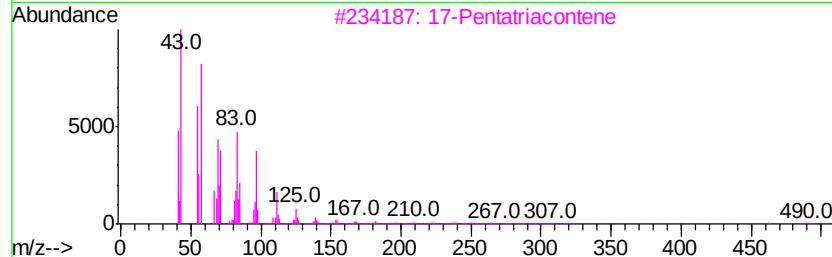
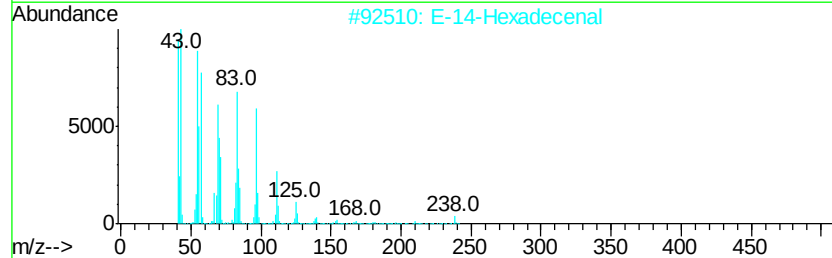
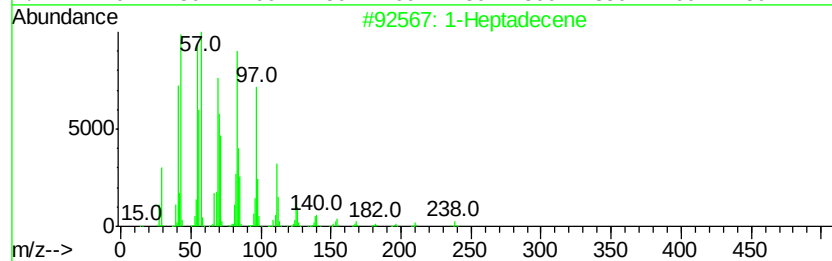
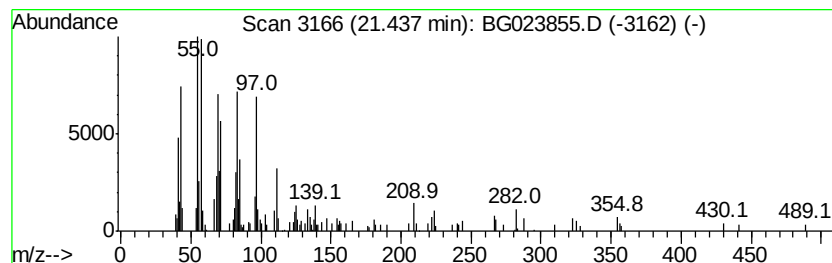
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 1-Heptadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.44	2.09 ng	207376	Chrysene-d12	21.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecene	238	C17H34	006765-39-5	87
2	E-14-Hexadecenal	238	C16H30O	330207-53-9	78
3	17-Pentatriacontene	491	C35H70	006971-40-0	72
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	68
5	Dodecane, 1-cyclopentyl-4-(3-cyc...	348	C25H48	007225-68-5	58



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	2.97	255.7	ng	7899440	1	8.09	617880	20.0
2-Pentanone, 4-hy...	5.15	23.2	ng	716933	1	8.09	617880	20.0
unknown7.62	7.62	75.0	ng	2316630	1	8.09	617880	20.0
n-Hexadecanoic acid	18.39	2.4	ng	197107	4	17.52	1648480	20.0
1-Heptadecene	21.44	2.1	ng	207376	5	21.84	1982150	20.0