

Data Path : Z:\HPCHEM1\BNA G\DATA\BG082316\
 Data File : BG023852.D
 Acq On : 23 Aug 2016 14:23
 Operator : UM/SJ
 Sample : H4528-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 VITALEFILL-MCMPH3-1

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-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	2.967	17	22	41	rVB	3986851	6425953	100.00%	15.122%
2	3.232	62	67	72	rBV2	42435	65685	1.02%	0.155%
3	5.152	388	394	404	rBV	569579	866084	13.48%	2.038%
4	5.634	469	476	487	rBV	1505911	2567451	39.95%	6.042%
5	7.244	744	750	761	rBV	1521534	2809552	43.72%	6.612%
6	7.620	806	814	825	rBV	1541006	2734452	42.55%	6.435%
7	8.090	884	894	902	rBV	369809	633692	9.86%	1.491%
8	8.413	941	949	959	rBV	1180683	2054315	31.97%	4.834%
9	9.270	1087	1095	1105	rBV	974123	1784421	27.77%	4.199%
10	10.927	1369	1377	1391	rBV	465993	896819	13.96%	2.110%
11	13.377	1784	1794	1806	rBV	2525943	3905972	60.78%	9.192%
12	14.205	1929	1935	1944	rBV	487757	744237	11.58%	1.751%
13	14.763	2024	2030	2039	rBV2	751647	1240966	19.31%	2.920%
14	15.585	2164	2170	2175	rVB	71109	95886	1.49%	0.226%
15	16.261	2278	2285	2301	rBV	2032785	3305098	51.43%	7.778%
16	16.449	2311	2317	2326	rBV	92215	145175	2.26%	0.342%
17	17.524	2493	2500	2514	rBV2	1012226	1674831	26.06%	3.941%
18	18.399	2645	2649	2654	rBV4	48880	80025	1.25%	0.188%
19	20.138	2938	2945	2950	rBV	4651139	6356253	98.92%	14.958%
20	21.442	3162	3167	3179	rBV6	86686	266224	4.14%	0.627%
21	21.842	3228	3235	3243	rBV2	1108843	1992239	31.00%	4.688%
22	25.219	3799	3810	3822	rVB2	624803	1847949	28.76%	4.349%

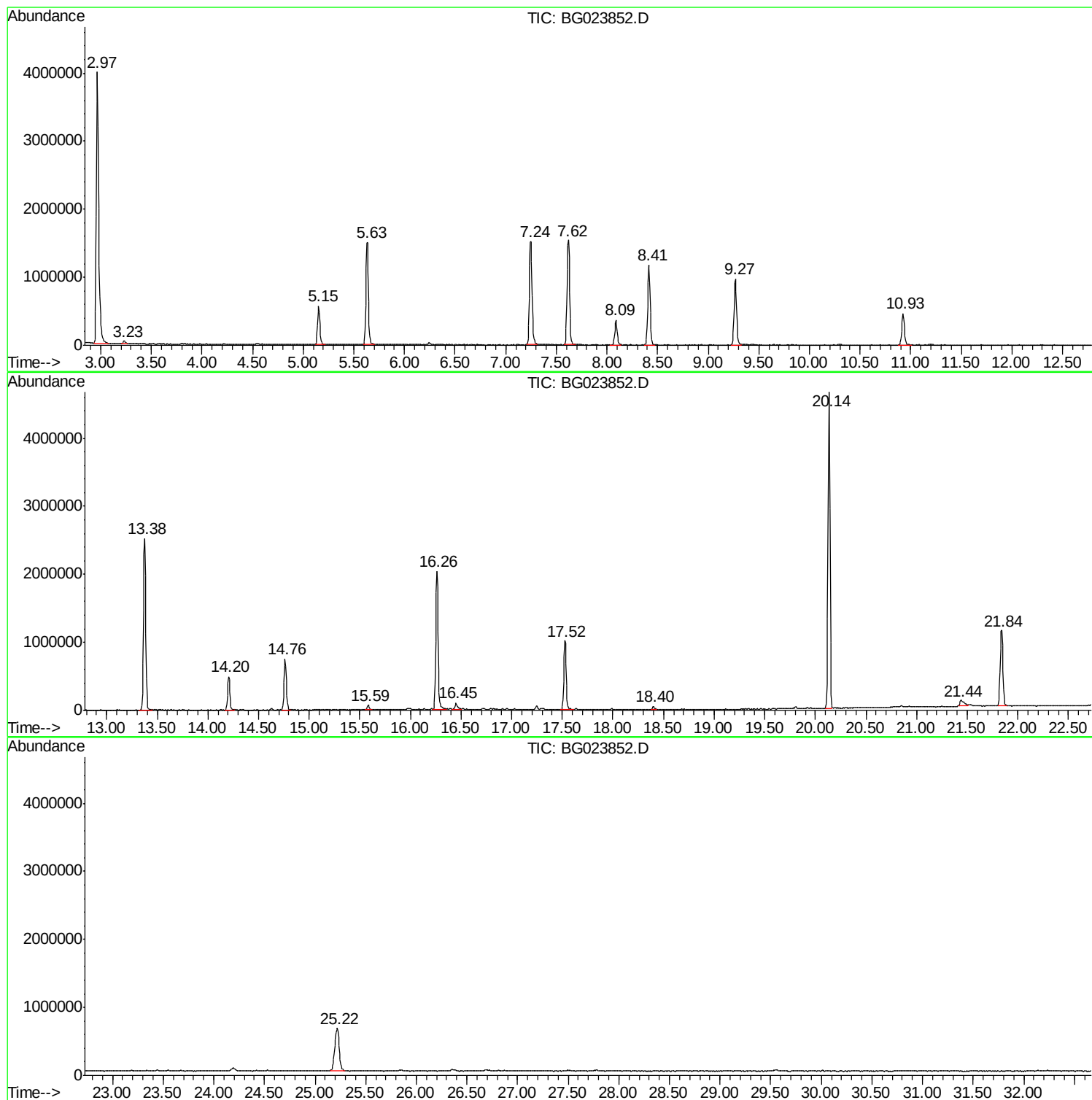
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Quant Method : Z:\HPCHEM1\BNA G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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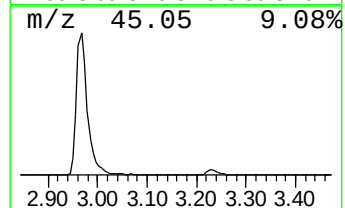
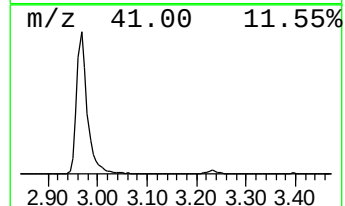
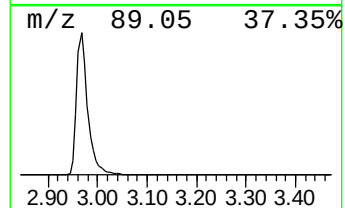
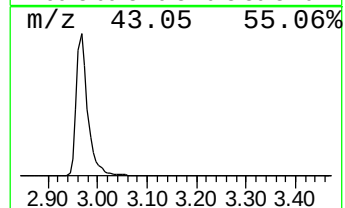
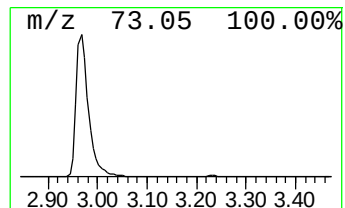
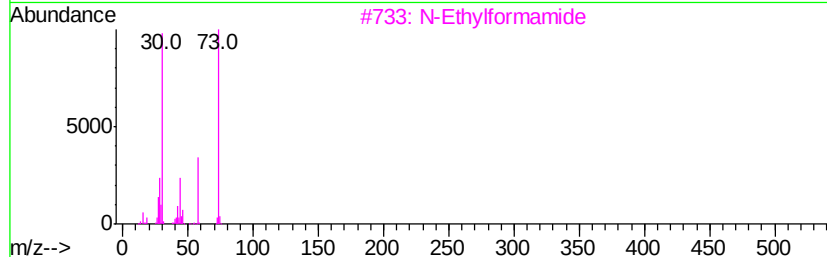
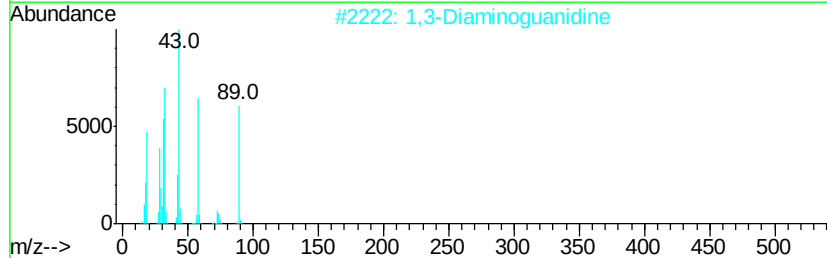
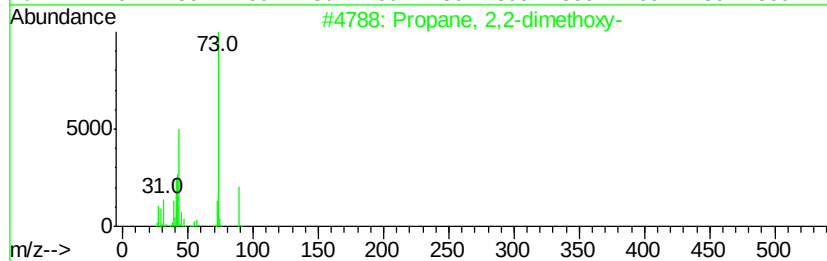
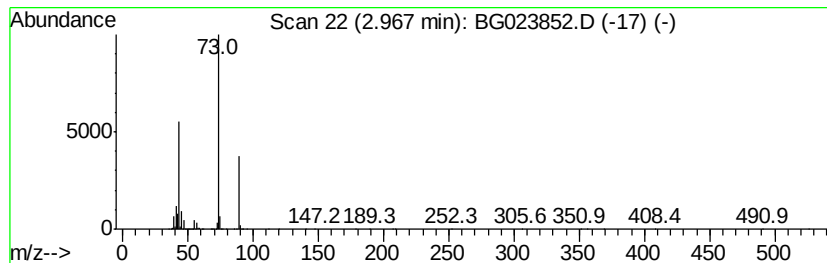
Quant Method : Z:\HPCHEM1\BNA G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.97 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.97	202.81 ng	6425950	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	40
2		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	25
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5		1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9



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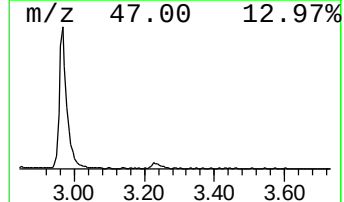
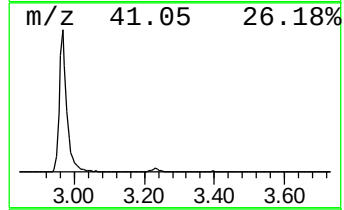
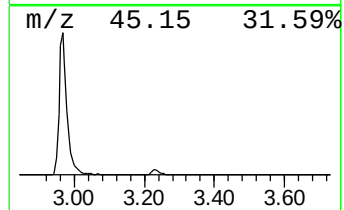
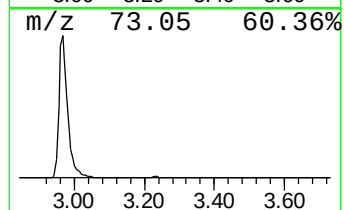
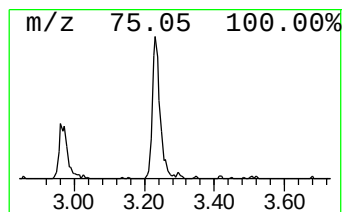
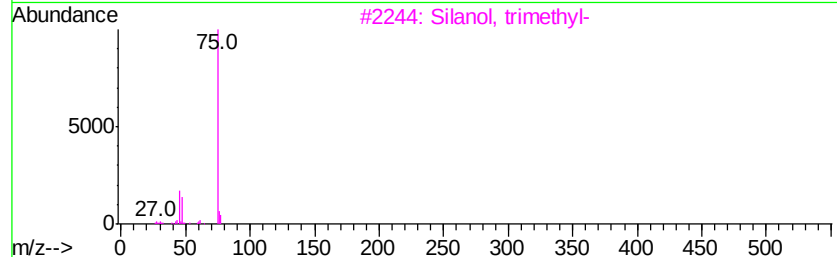
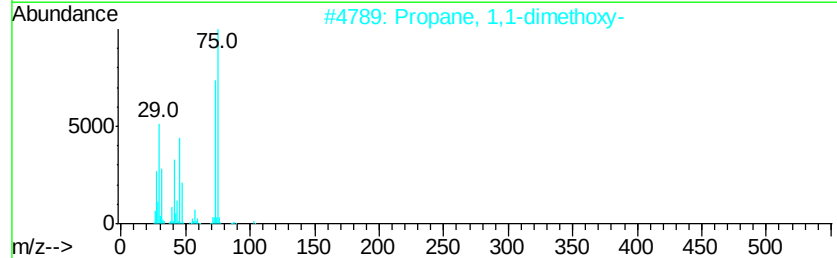
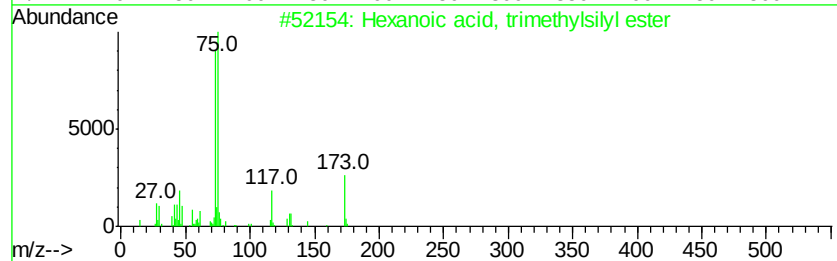
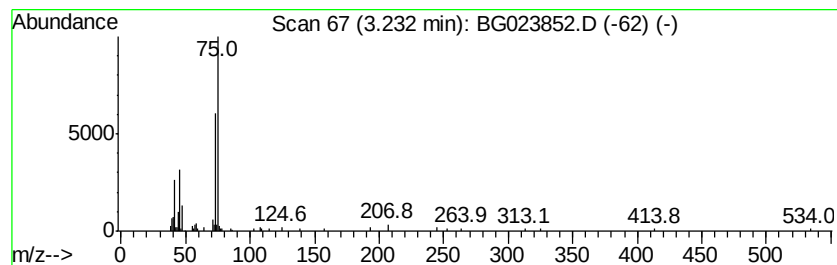
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Peak Number 2 unknown3.23 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	2.07 ng	65685	1,4-Dichlorobenzene-d4	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, trimethylsilyl ester	188	C9H20O2Si	014246-15-2	39
2		Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	38
3		Silanol, trimethyl-	90	C3H10OSi	001066-40-6	36
4		Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	36
5		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	14



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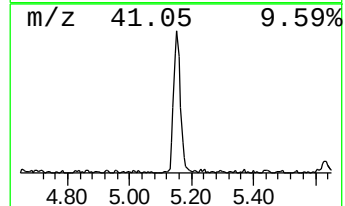
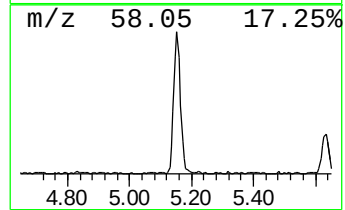
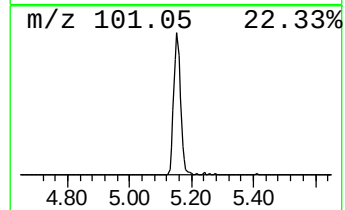
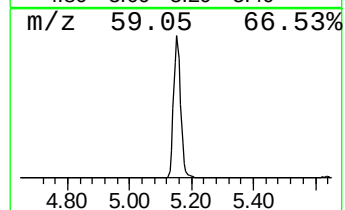
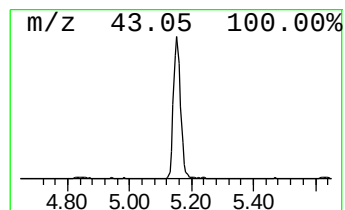
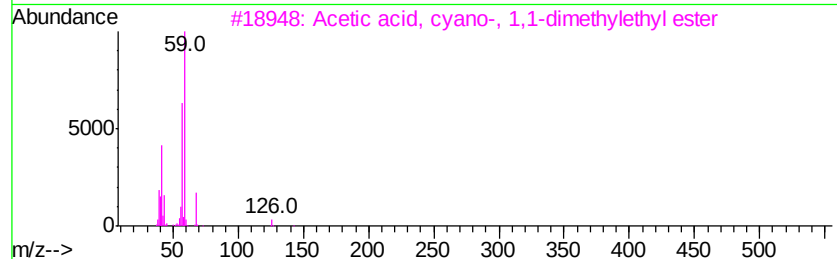
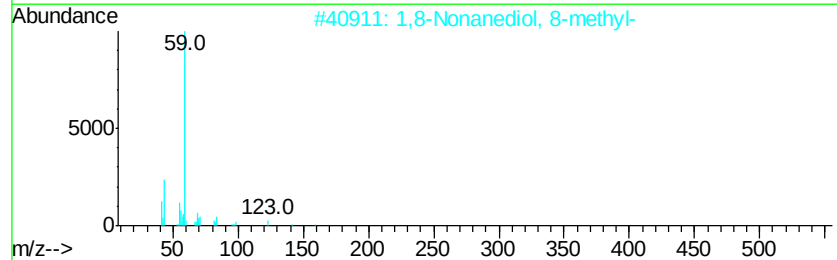
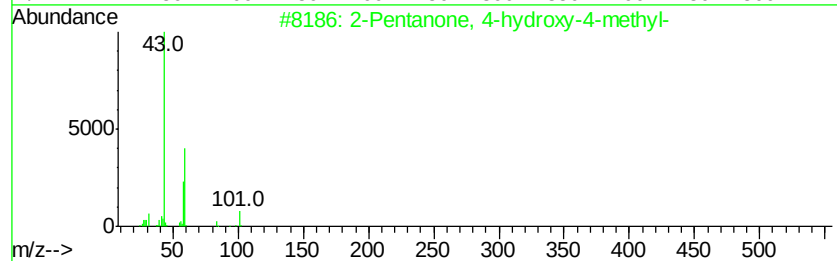
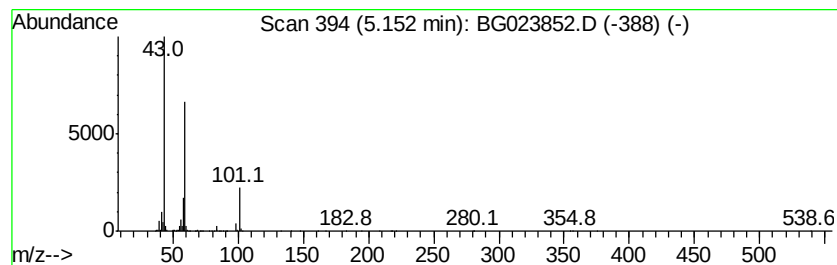
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	27.33 ng	866084	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	56
2		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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ClientSampleId :
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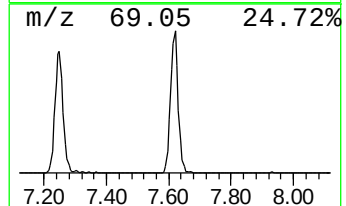
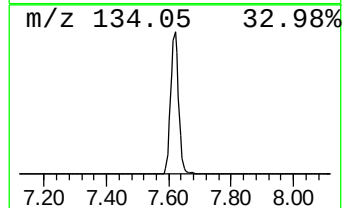
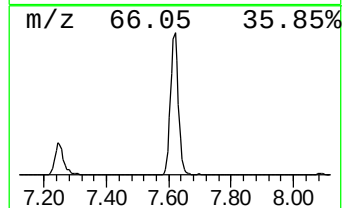
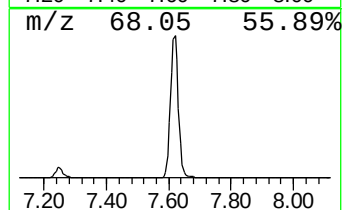
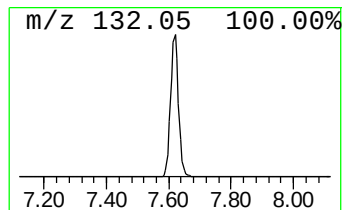
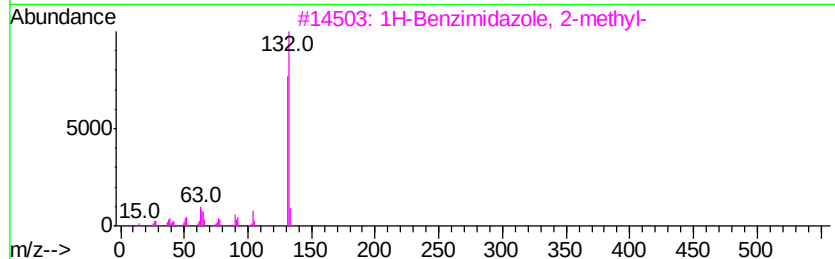
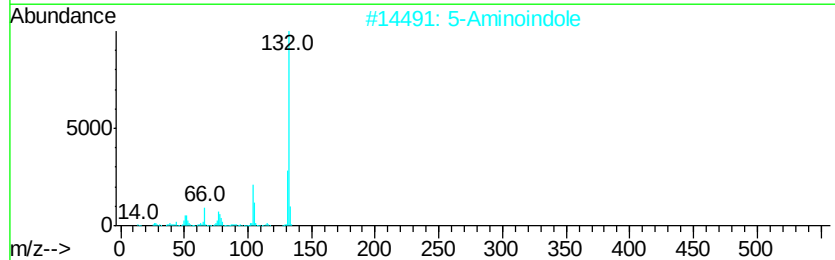
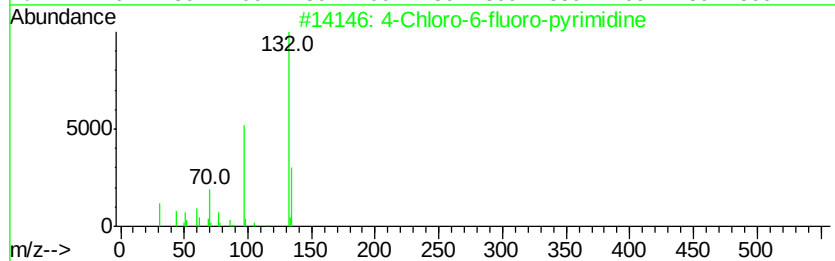
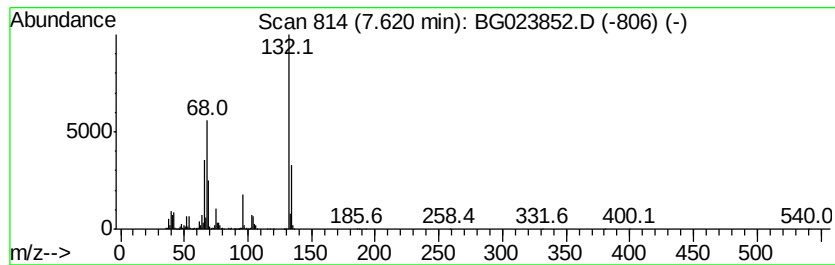
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Peak Number 4 unknown7.62 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	86.30 ng	2734450	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	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	22
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16



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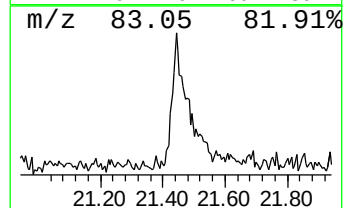
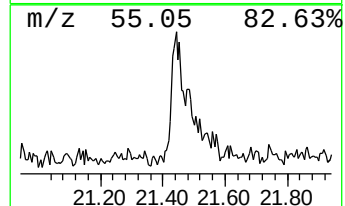
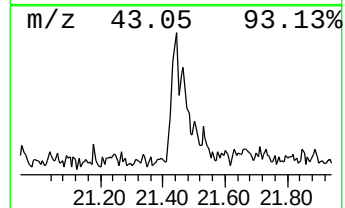
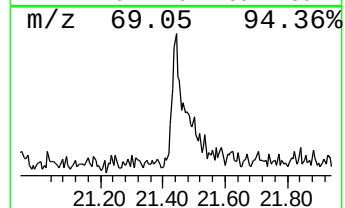
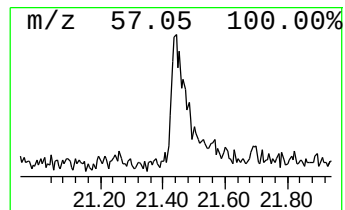
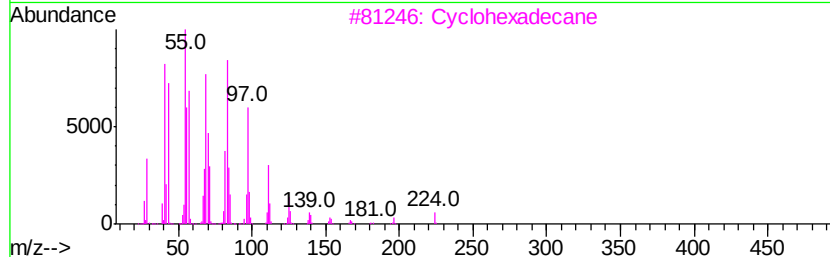
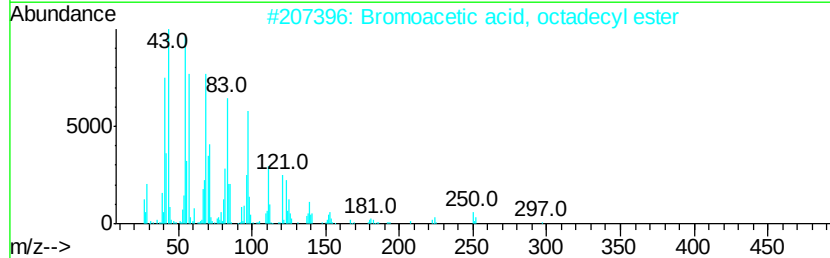
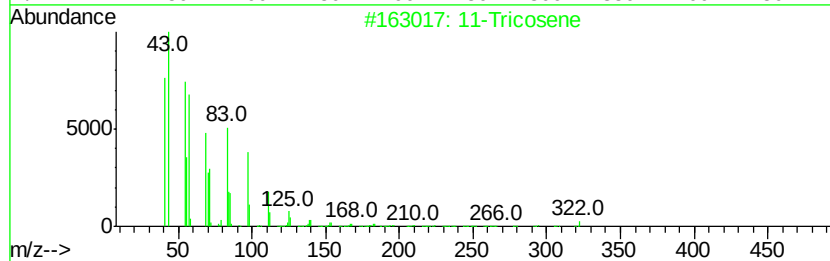
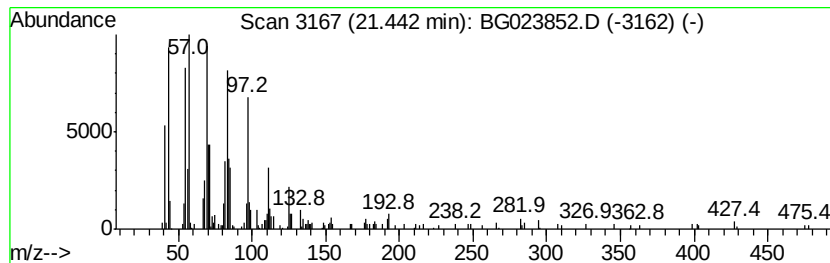
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Peak Number 6 11-Tricosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.44	2.67 ng	266224	Chrysene-d12	21.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Tricosene	322	C23H46	052078-56-5	91
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87
3	Cvclohexadecane	224	C16H32	000295-65-8	83
4	1-Nonadecene	266	C19H38	018435-45-5	70
5	10-Heneicosene (c,t)	294	C21H42	095008-11-0	70



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.97	2.97	202.8	ng	6425950	1	8.09	633692	20.0
unknown3.23	3.23	2.1	ng	65685	1	8.09	633692	20.0
2-Pentanone, 4-hy...	5.15	27.3	ng	866084	1	8.09	633692	20.0
unknown7.62	7.62	86.3	ng	2734450	1	8.09	633692	20.0
11-Tricosene	21.44	2.7	ng	266224	5	21.84	1992240	20.0