

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
 Data File : BG016985.D
 Acq On : 9 May 2015 9:57
 Operator : TP/IZ
 Sample : G2081-04
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MWHR3-8

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-BG050515.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	2.917	34	39	47	rBV	334910	529659	10.48%	2.269%
2	2.994	47	52	63	rVB	576999	730117	14.44%	3.128%
3	4.909	374	378	382	rBV	39514	54966	1.09%	0.235%
4	5.373	449	457	465	rBV	584245	825643	16.33%	3.537%
5	6.960	720	727	738	rBV	399298	620743	12.28%	2.659%
6	7.324	781	789	798	rBV	1068065	1668834	33.01%	7.149%
7	7.788	862	868	875	rBV	208453	338774	6.70%	1.451%
8	8.111	916	923	931	rVB	846912	1352673	26.75%	5.795%
9	8.945	1056	1065	1075	rBV	803520	1318200	26.07%	5.647%
10	10.579	1334	1343	1352	rBV	305852	519194	10.27%	2.224%
11	13.052	1757	1764	1770	rBV	1994779	2968035	58.70%	12.715%
12	14.427	1992	1998	2004	rBV2	500616	749769	14.83%	3.212%
13	15.168	2120	2124	2130	rBV	98969	131307	2.60%	0.563%
14	15.914	2244	2251	2264	rBV	2070171	2949599	58.34%	12.636%
15	17.171	2457	2465	2471	rBV	709271	1033335	20.44%	4.427%
16	18.064	2612	2617	2623	rBV2	59645	82095	1.62%	0.352%
17	19.797	2906	2912	2922	rBV	4046002	5056287	100.00%	21.661%
18	20.432	3016	3020	3025	rBV2	55383	70311	1.39%	0.301%
19	21.055	3122	3126	3132	rBV4	64132	89106	1.76%	0.382%
20	21.260	3157	3161	3166	rVB	119615	131204	2.59%	0.562%
21	21.343	3170	3175	3184	rVB	844411	1069048	21.14%	4.580%
22	23.640	3558	3566	3576	rVB	530889	1053590	20.84%	4.514%

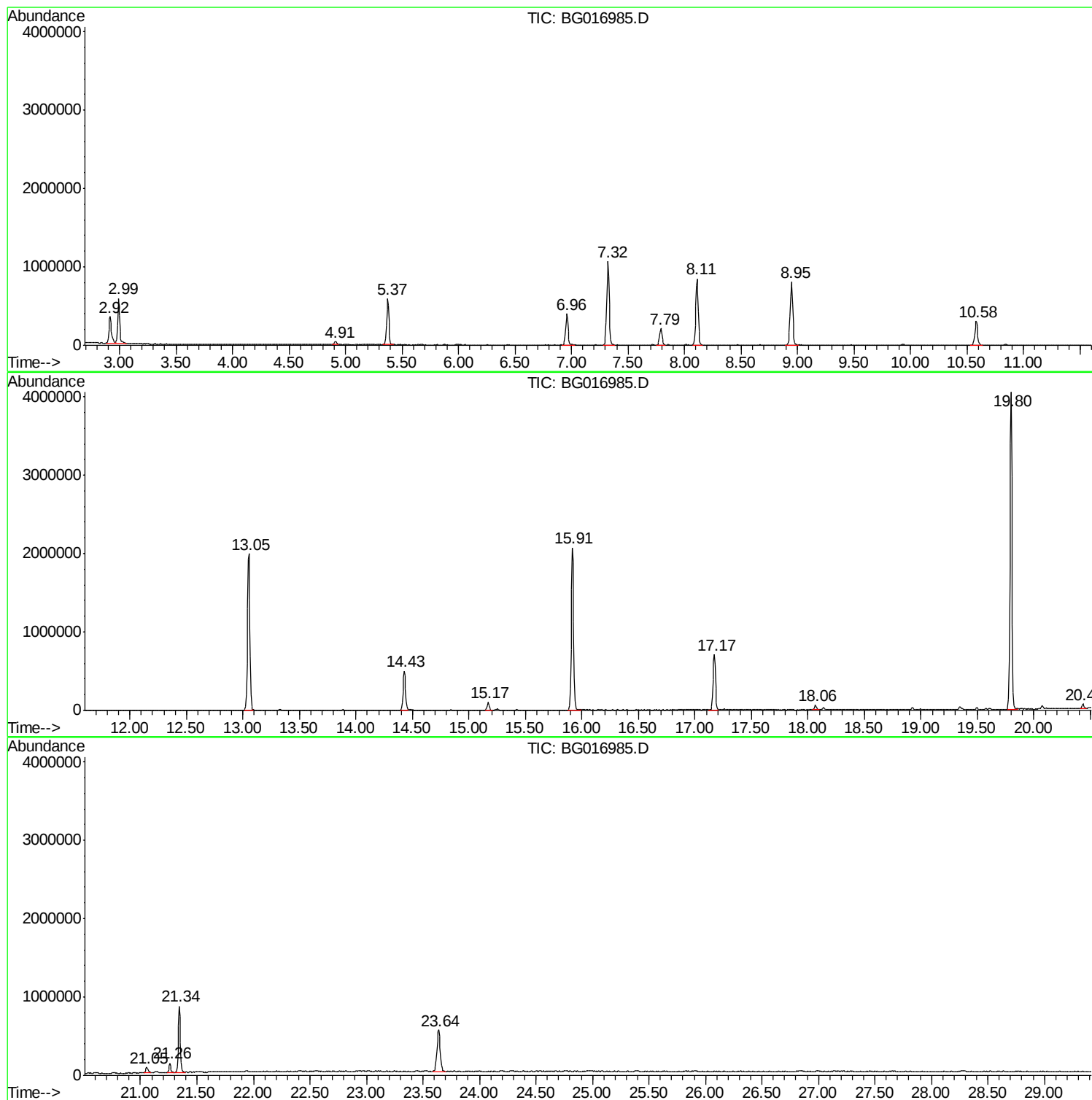
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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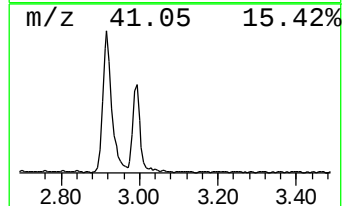
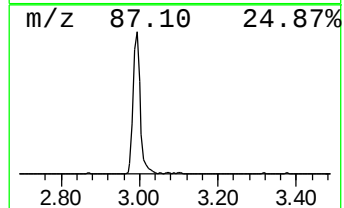
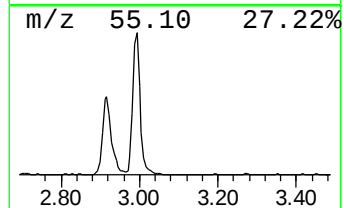
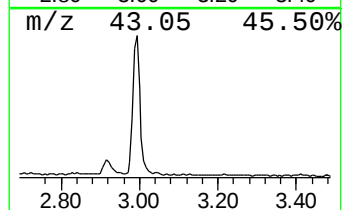
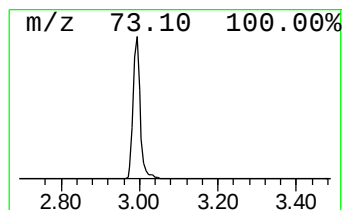
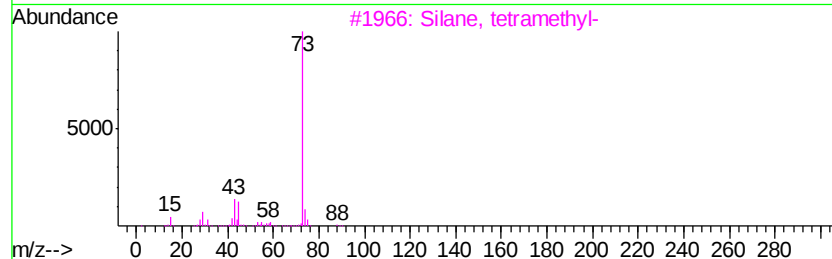
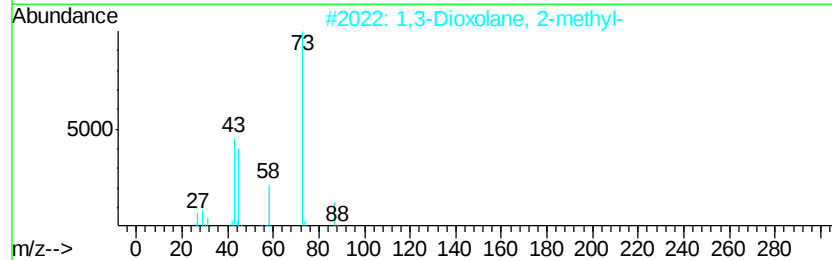
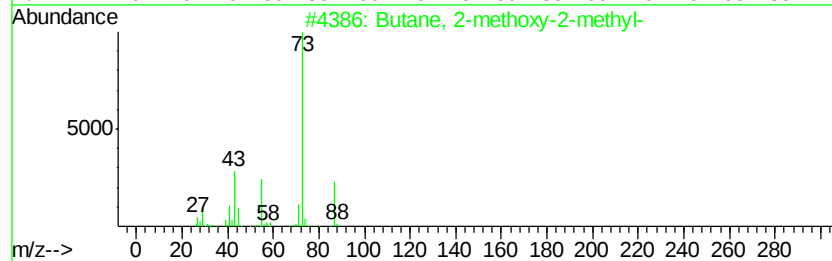
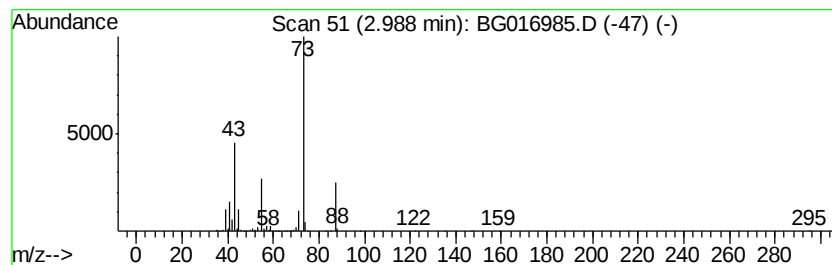
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	43.10 ng	730117	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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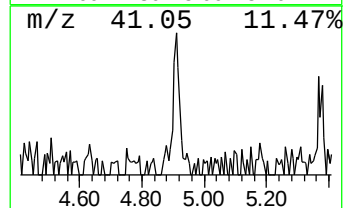
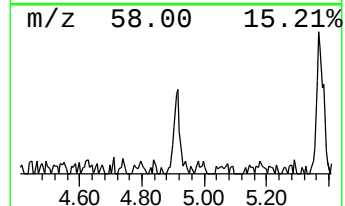
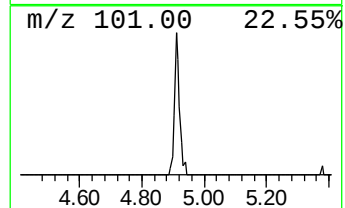
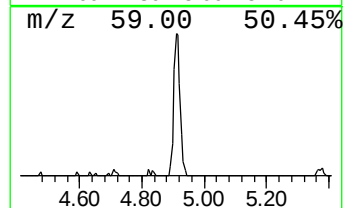
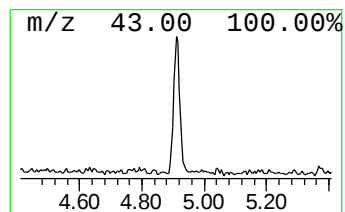
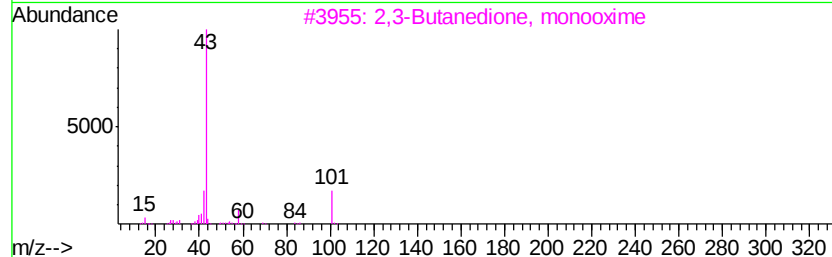
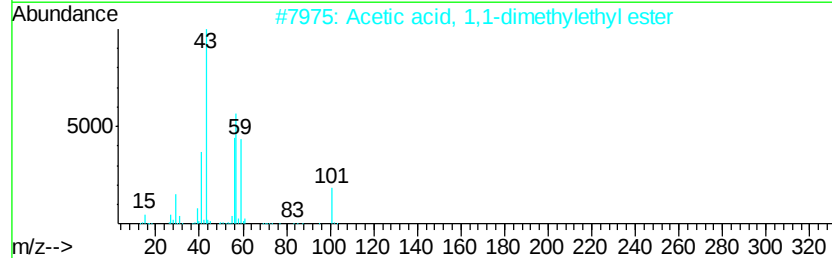
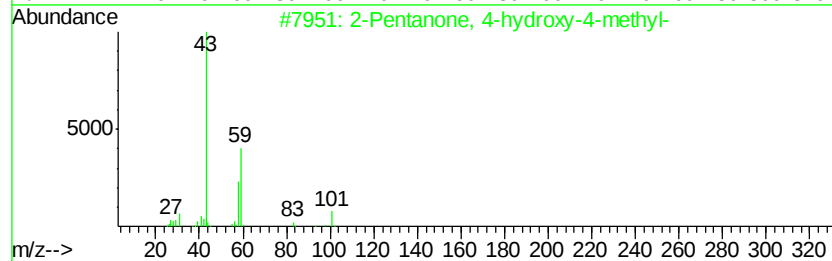
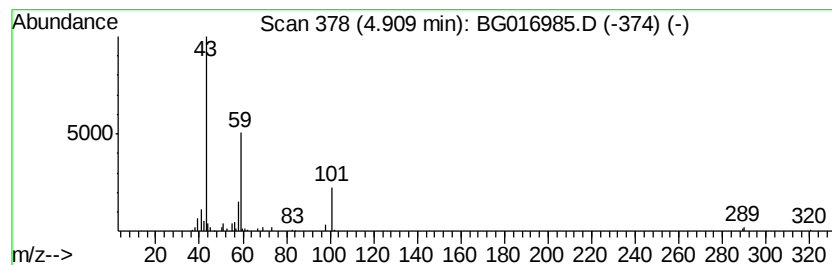
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	3.25 ng	54966	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4		1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	17
5		2-Nonanone	142	C9H18O	000821-55-6	10



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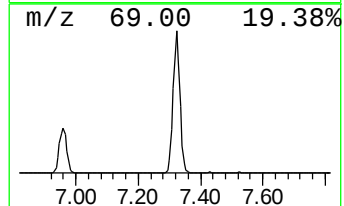
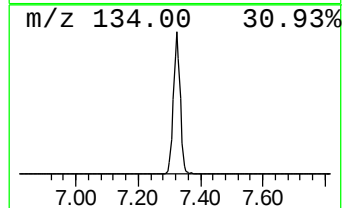
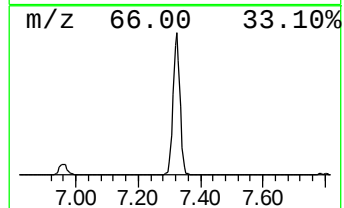
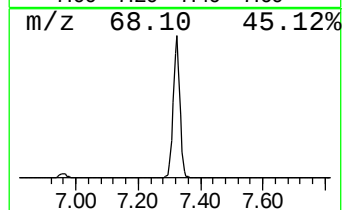
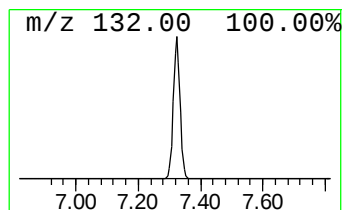
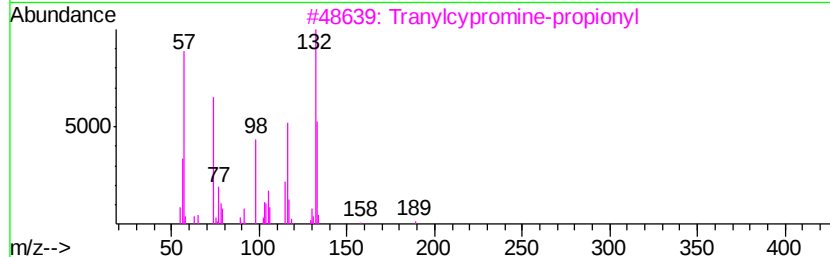
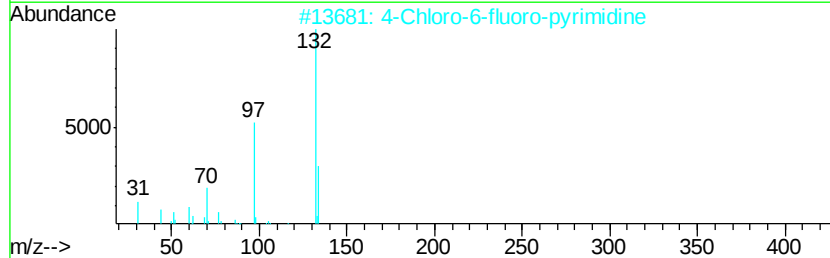
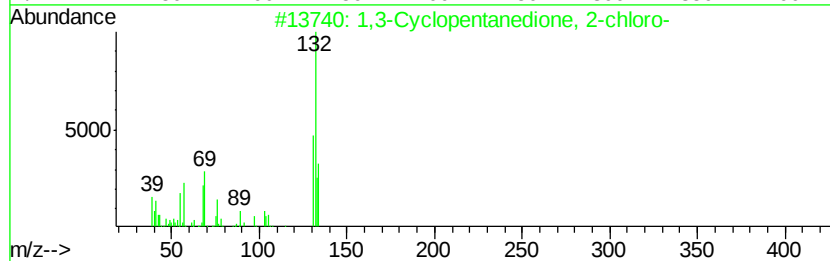
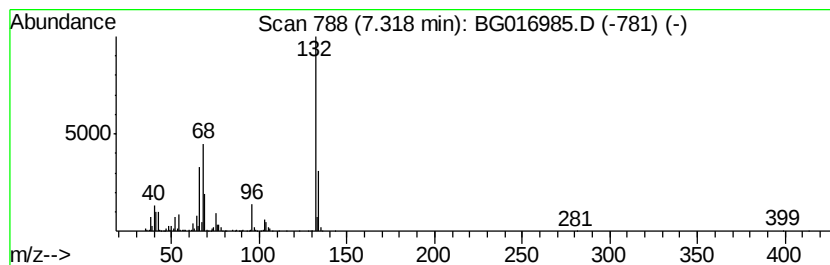
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Peak Number 4 unknown7.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	98.52 ng	1668830	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	35
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4		5-Aminoindole	132	C8H8N2	005192-03-0	22
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	18



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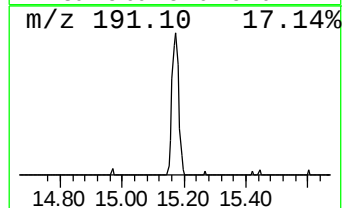
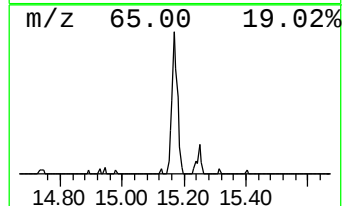
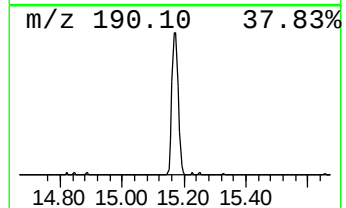
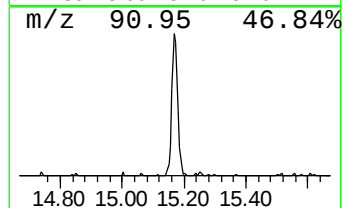
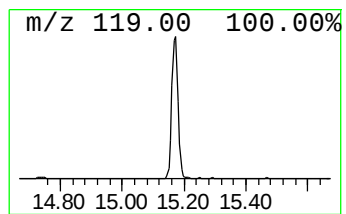
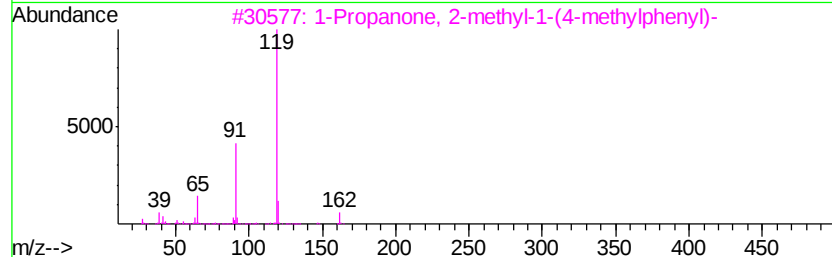
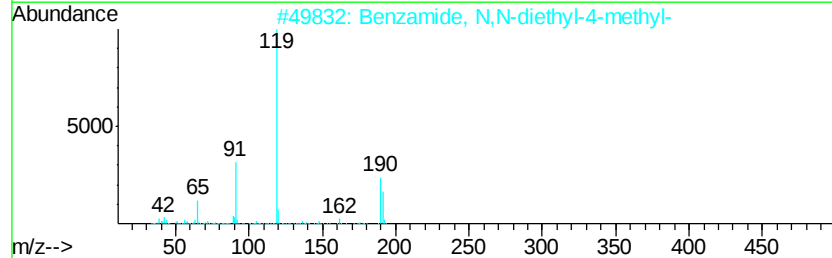
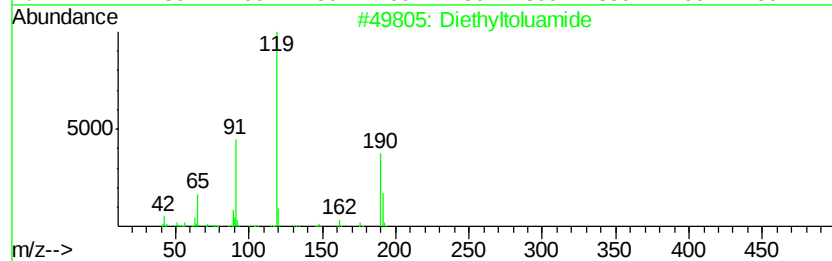
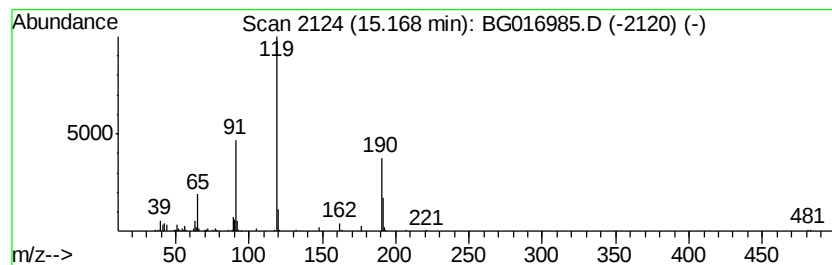
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Peak Number 6 Diethyltoluamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.17	3.50 ng	131307	Acenaphthene-d10	14.43	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	97
2	Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	90
3	1-Propanone, 2-methyl-1-(4-methylphenyl)-	162	C11H14O	050390-51-7	64
4	Benzamide, N-(1,1-dimethylethyl)-	191	C12H17NO	042498-32-8	59
5	Benzamide, 3-methyl-N-[5-(trifluoromethyl)phenyl]-	409	C18H14F7N02	339240-75-4	58



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.99	43.1	ng	730117	1	7.79	338774	20.0
2-Pentanone, 4-hy...	4.91	3.3	ng	54966	1	7.79	338774	20.0
unknown7.32	7.32	98.5	ng	1668830	1	7.79	338774	20.0
Diethyltoluamide	15.17	3.5	ng	131307	3	14.43	749769	20.0