

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040815\
 Data File : BG016279.D
 Acq On : 8 Apr 2015 17:26
 Operator : TP/IZ
 Sample : PB82625BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB82625BL

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	2.787	13	17	27	rVB	49802	83249	2.64%	0.423%
2	4.203	252	258	268	rBV	215973	282109	8.95%	1.433%
3	4.808	354	361	370	rBV	1914541	2600065	82.50%	13.204%
4	5.272	434	440	451	rVB	766812	1067101	33.86%	5.419%
5	5.878	538	543	549	rBV	90607	127025	4.03%	0.645%
6	6.865	704	711	721	rBV	795533	1164453	36.95%	5.913%
7	7.223	764	772	781	rBV	758470	1158566	36.76%	5.884%
8	7.687	845	851	861	rVB	243147	375159	11.90%	1.905%
9	8.010	899	906	913	rBV	698998	1097527	34.82%	5.574%
10	8.845	1040	1048	1061	rBV	544821	880835	27.95%	4.473%
11	10.478	1319	1326	1333	rBV	345966	572172	18.15%	2.906%
12	12.952	1740	1747	1754	rBV	1386003	2043298	64.83%	10.376%
13	14.332	1976	1982	1990	rBV2	522030	787963	25.00%	4.001%
14	15.825	2230	2236	2249	rBV	743323	1038766	32.96%	5.275%
15	17.076	2443	2449	2455	rBV2	776202	1018488	32.32%	5.172%
16	19.708	2891	2897	2906	rBV	2456206	3151740	100.00%	16.005%
17	21.254	3155	3160	3171	rBV	881637	1106806	35.12%	5.621%
18	23.381	3518	3522	3532	rVB7	16444	37137	1.18%	0.189%
19	23.498	3535	3542	3554	rVB2	556768	1060734	33.66%	5.387%
20	24.033	3626	3633	3641	rBV9	15421	38503	1.22%	0.196%

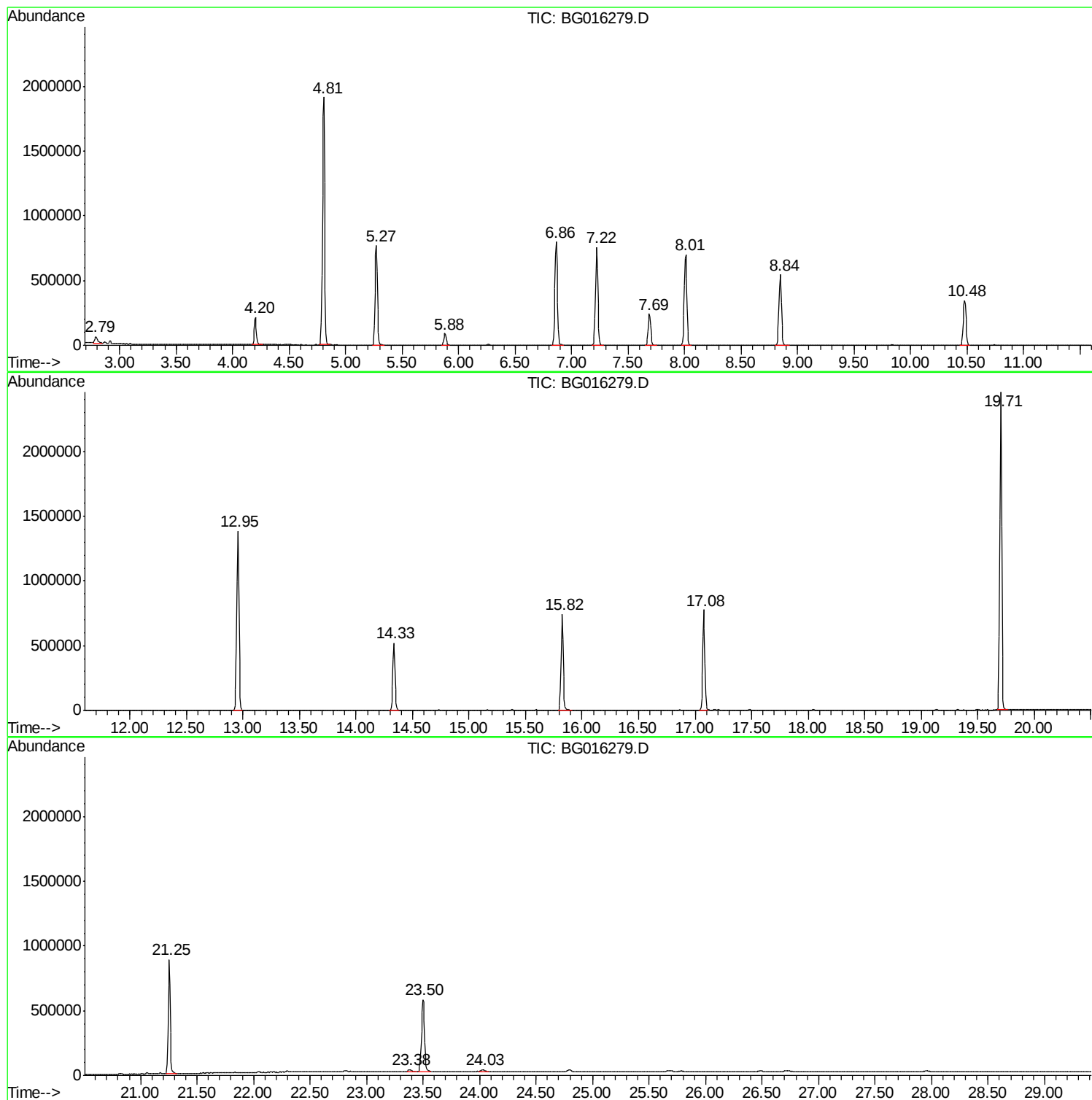
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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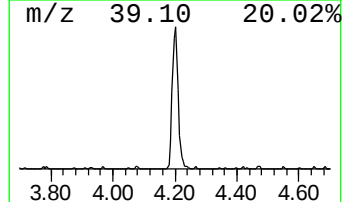
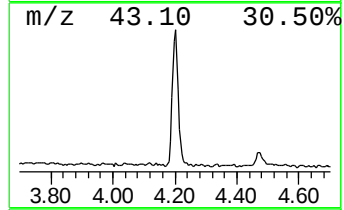
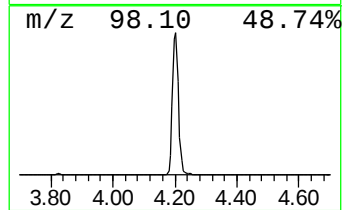
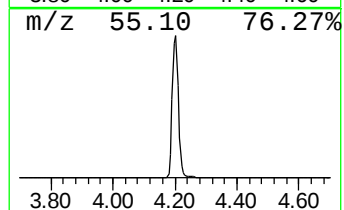
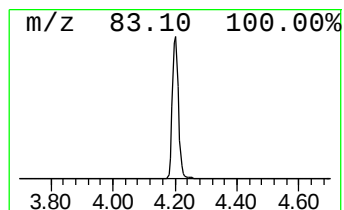
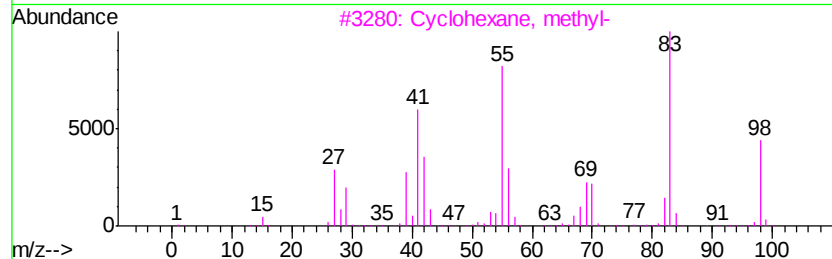
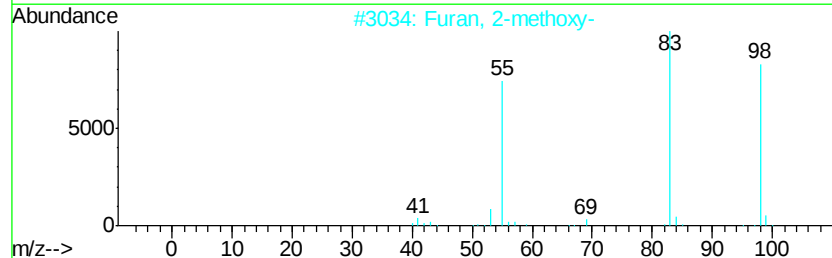
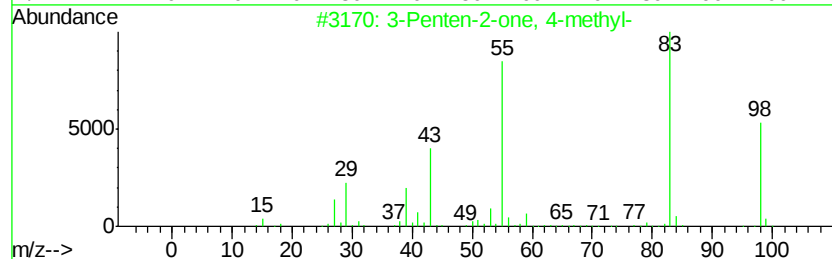
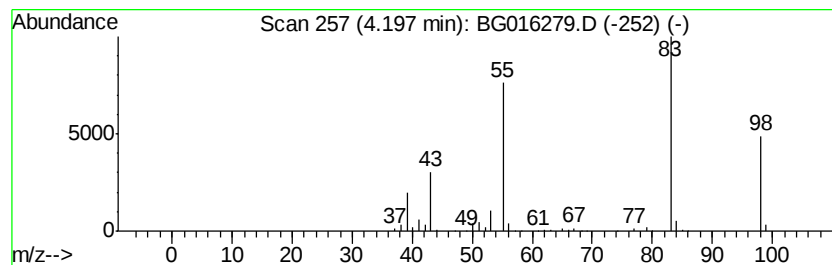
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.20	15.04 ng	282109	1,4-Dichlorobenzene-d4	7.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78
3		Cyclohexane, methyl-	98	C7H14	000108-87-2	72
4		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72
5		2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	72



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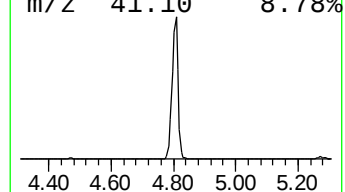
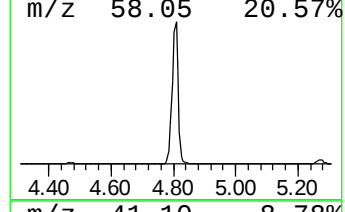
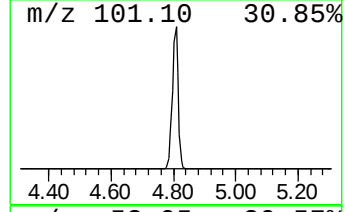
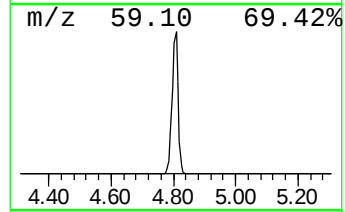
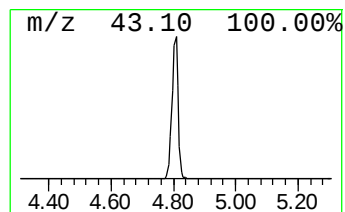
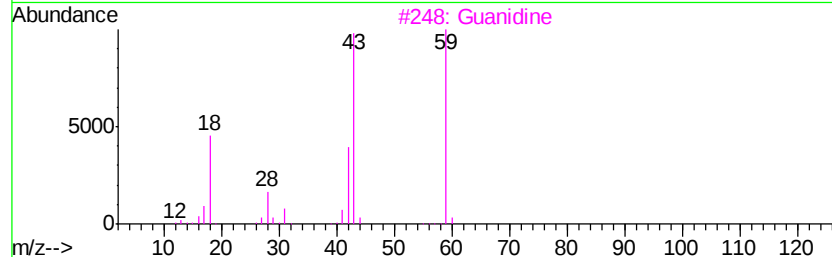
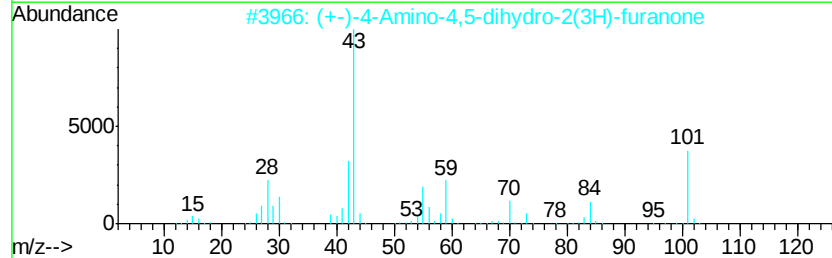
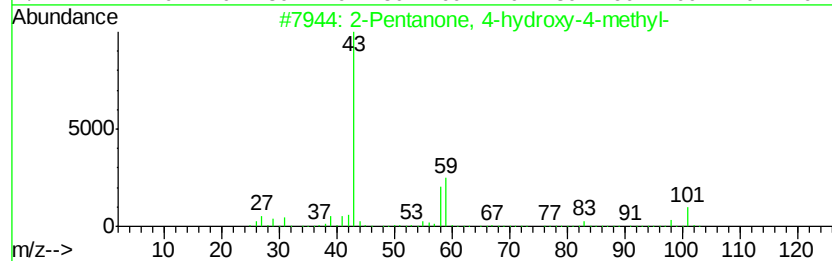
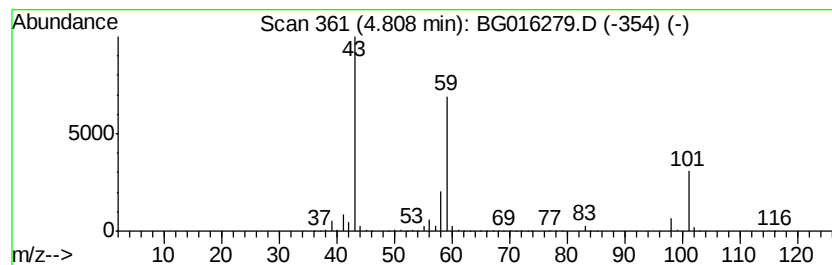
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	138.61 ng	2600070	1,4-Dichlorobenzene-d4	7.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	38
3		Guanidine	59	CH5N3	000113-00-8	38
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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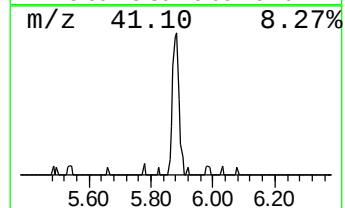
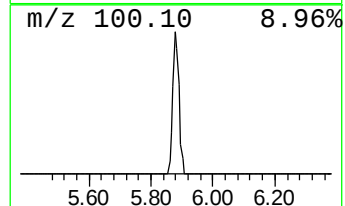
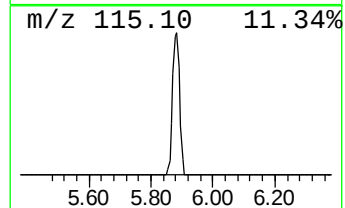
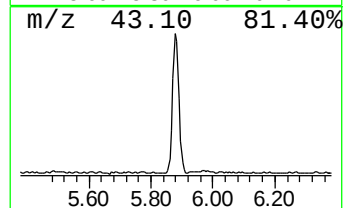
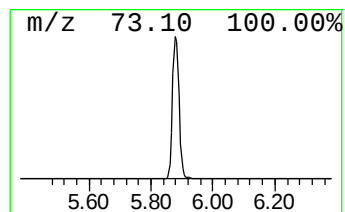
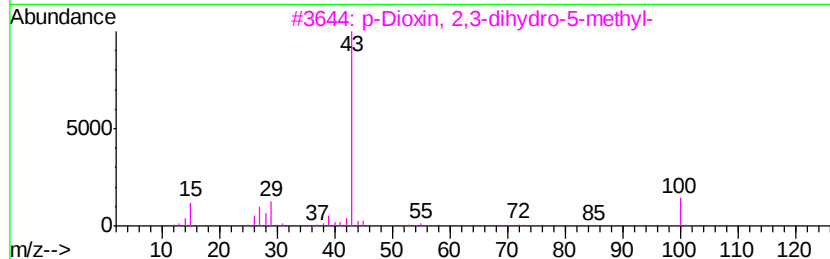
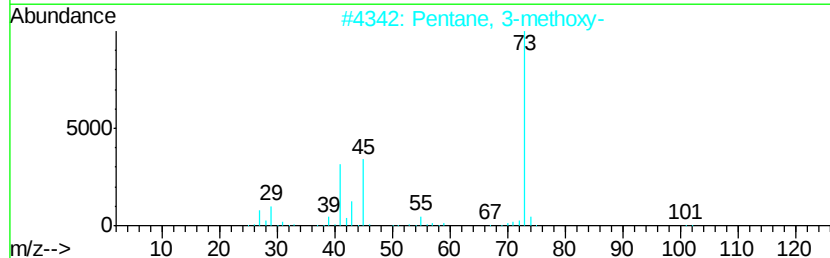
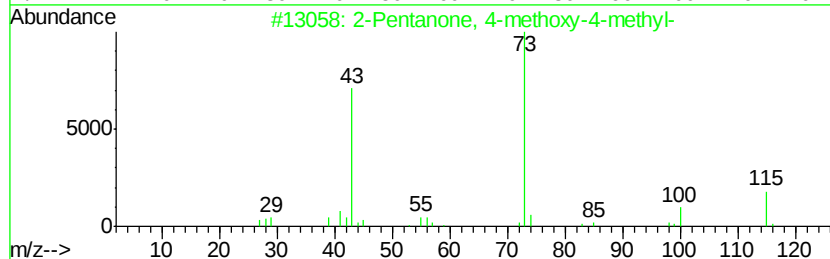
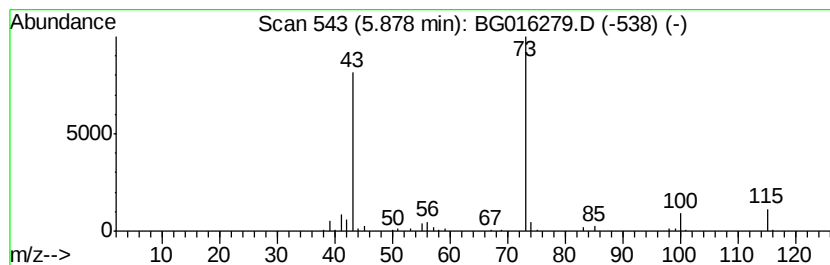
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.88	6.77 ng	127025	1,4-Dichlorobenzene-d4	7.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
3		p-Dioxin, 2,3-dihydro-5-methyl-	100	C5H8O2	003973-22-6	9
4		Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9
5		Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	9



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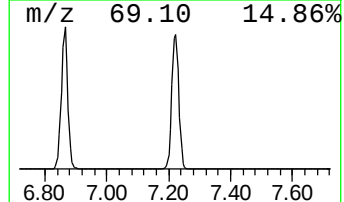
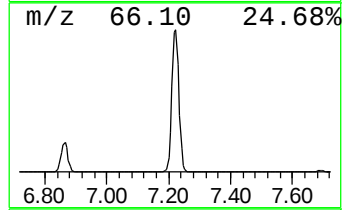
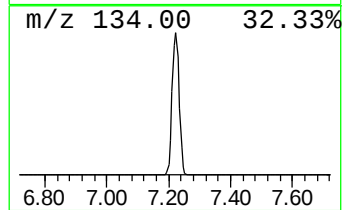
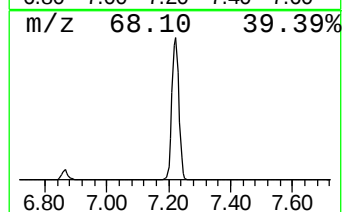
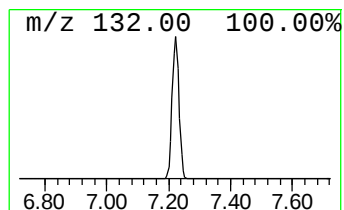
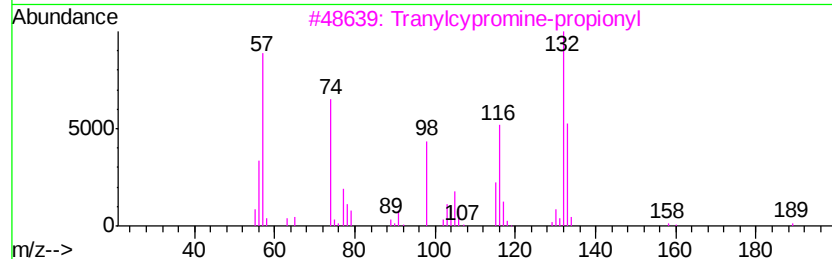
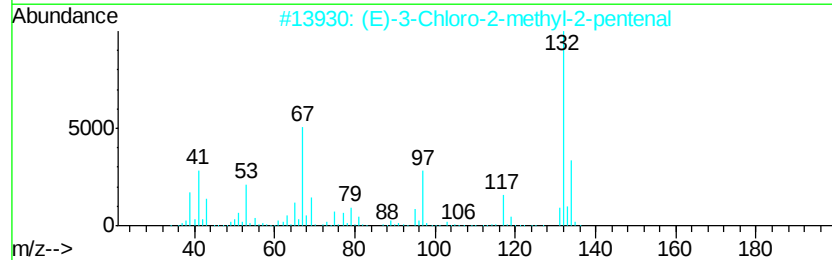
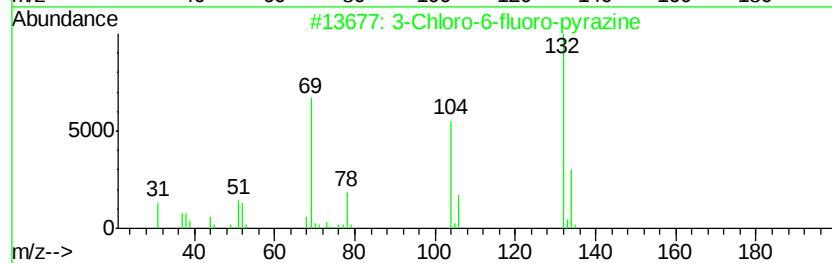
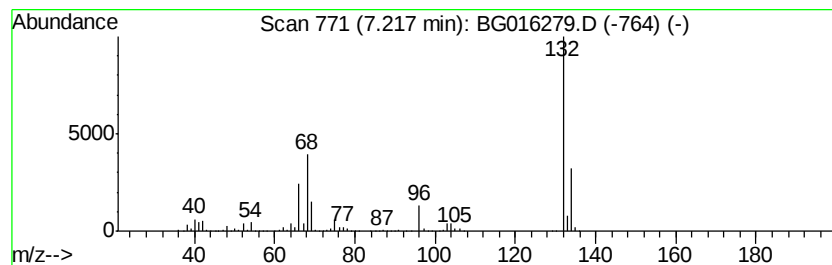
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Peak Number 5 unknown7.22 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	61.76 ng	1158570	1,4-Dichlorobenzene-d4	7.69

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	17
3		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.20	15.0	ng	282109	1	7.69	375159	20.0
2-Pentanone, 4-hy...	4.81	138.6	ng	2600070	1	7.69	375159	20.0
2-Pentanone, 4-me...	5.88	6.8	ng	127025	1	7.69	375159	20.0
unknown7.22	7.22	61.8	ng	1158570	1	7.69	375159	20.0