

Data Path : Z:\HPCHEM1\BNA G\DATA\BG032017\
 Data File : BG026353.D
 Acq On : 21 Mar 2017 8:37
 Operator : SJ/MA
 Sample : I2263-23
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-104I

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-BG032017.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	4.665	262	268	276	rBV	158125	268842	3.11%	0.728%
2	5.147	344	350	357	rBV	99982	160490	1.86%	0.435%
3	5.617	422	430	441	rBV	781947	1258704	14.57%	3.410%
4	7.204	693	700	711	rBV	445573	825648	9.56%	2.237%
5	7.580	755	764	777	rBV	1536708	2630298	30.44%	7.127%
6	8.044	835	843	855	rBV	344554	595481	6.89%	1.613%
7	8.367	890	898	909	rBV	1473159	2593198	30.01%	7.026%
8	9.201	1032	1040	1052	rBV	1122519	1993096	23.07%	5.400%
9	10.846	1311	1320	1329	rBV	502960	916300	10.61%	2.483%
10	13.279	1724	1734	1742	rBV	3500515	5515785	63.84%	14.945%
11	14.654	1959	1968	1977	rBV2	803059	1281087	14.83%	3.471%
12	16.134	2211	2220	2234	rBV	2632857	4051015	46.89%	10.976%
13	17.386	2426	2433	2446	rBV	1091249	1669683	19.32%	4.524%
14	18.255	2577	2581	2589	rBV2	67630	109110	1.26%	0.296%
15	19.525	2793	2797	2806	rBV2	73550	112875	1.31%	0.306%
16	19.983	2868	2875	2884	rBV	6599498	8640133	100.00%	23.410%
17	21.628	3149	3155	3163	rVB	1310972	2128130	24.63%	5.766%
18	24.812	3686	3697	3713	rBV2	750950	2157962	24.98%	5.847%

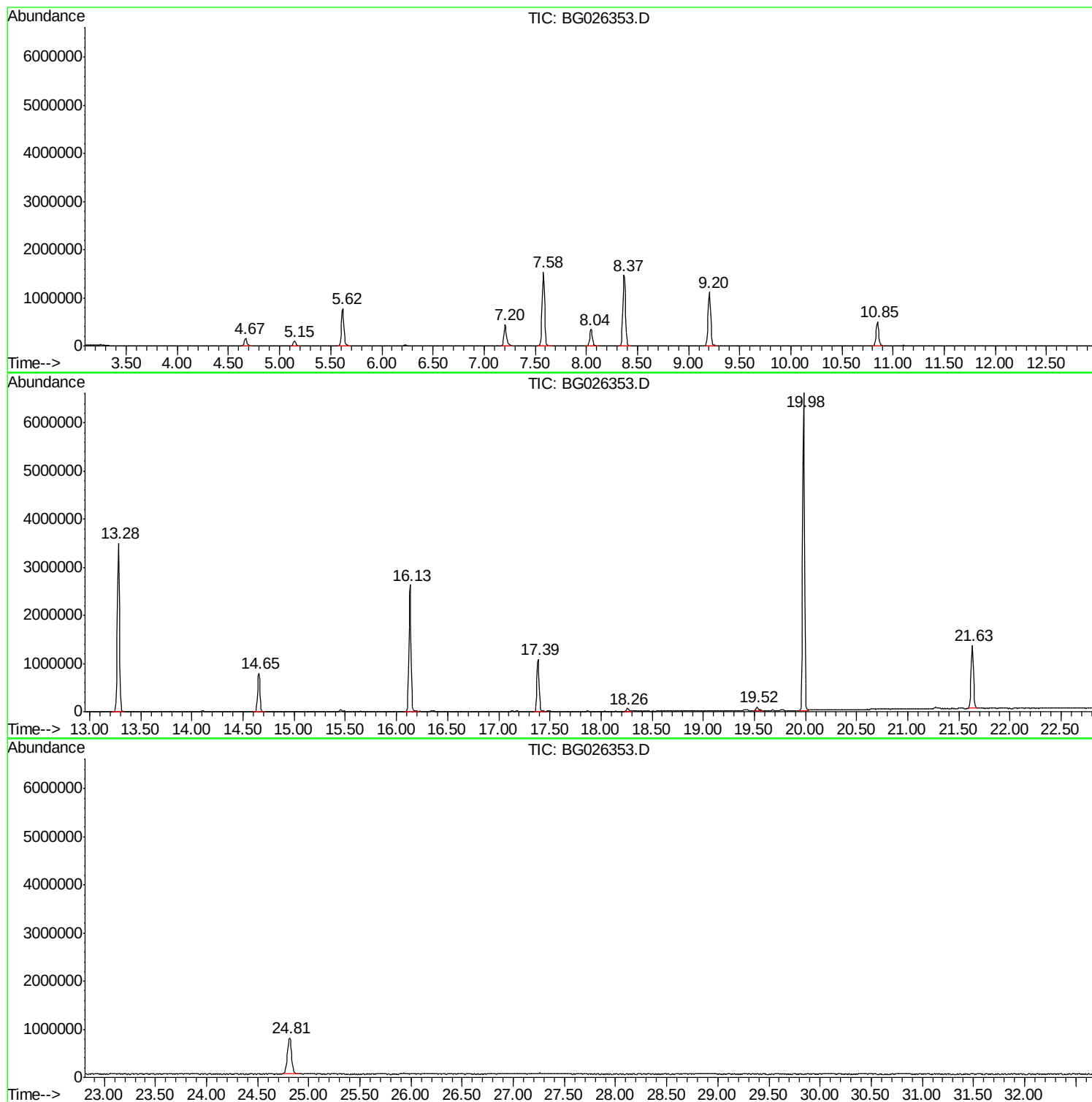
Sum of corrected areas: 36907837

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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG032017.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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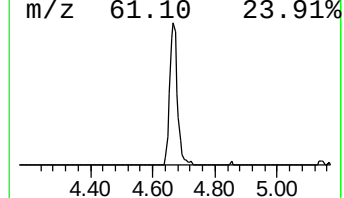
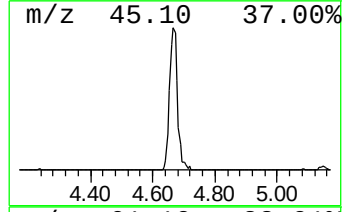
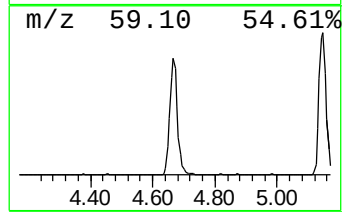
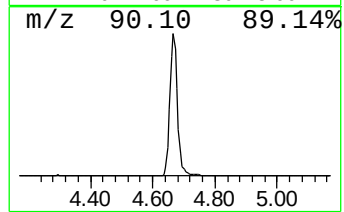
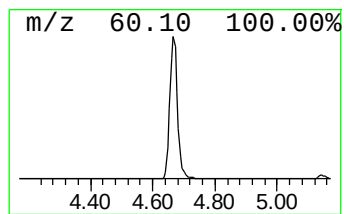
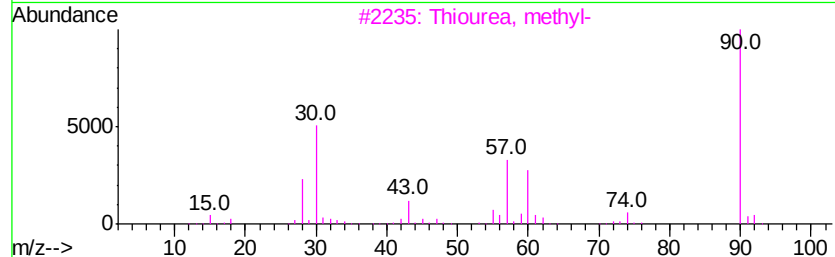
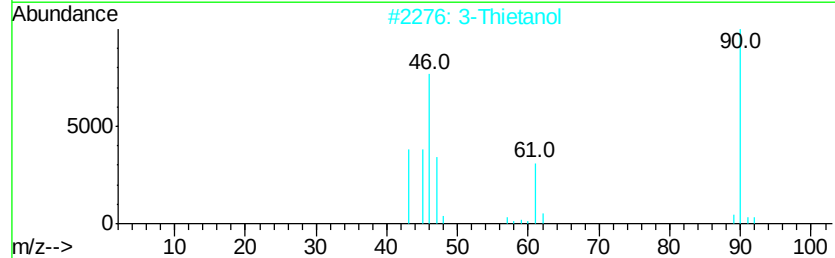
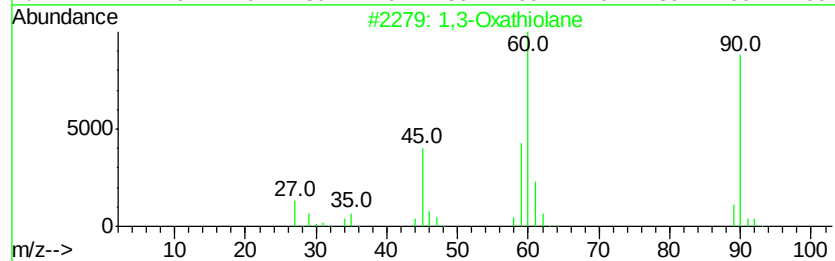
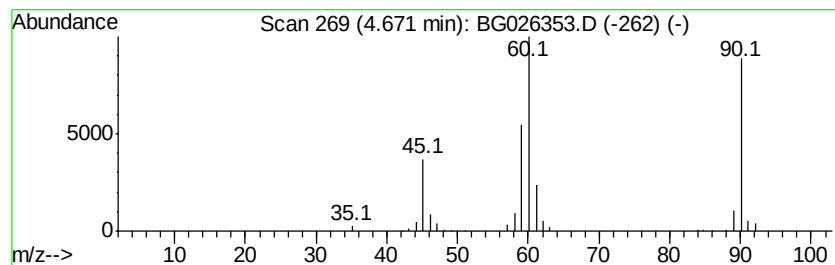
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3-Oxathiolane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.67	9.03 ng	268842	1,4-Dichlorobenzene-d4	8.04

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Oxathiolane	90	C3H6OS	002094-97-5	94
2			3-Thietanol	90	C3H6OS	010304-16-2	53
3			Thiourea, methyl-	90	C2H6N2S	000598-52-7	50
4			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	38
5			Thiirane	60	C2H4S	000420-12-2	18



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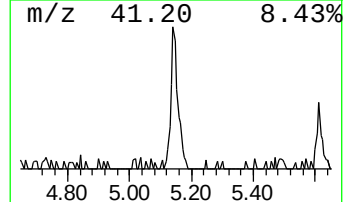
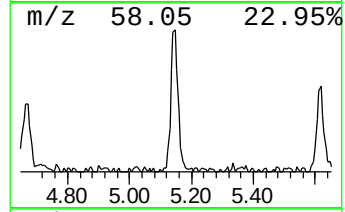
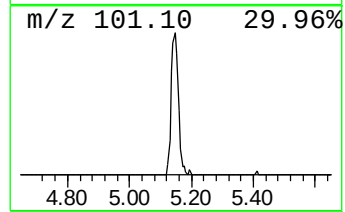
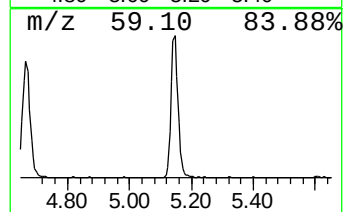
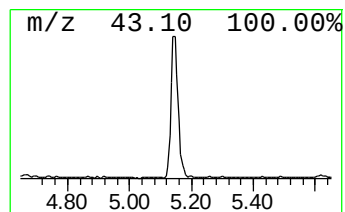
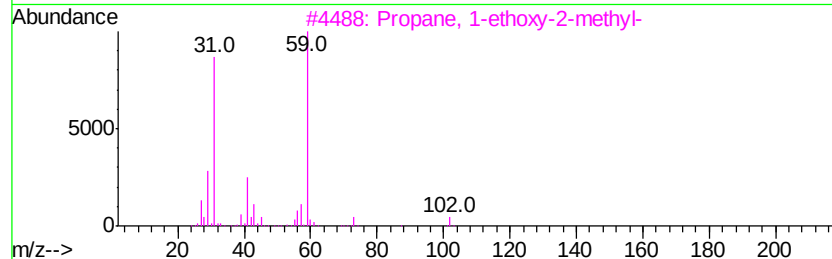
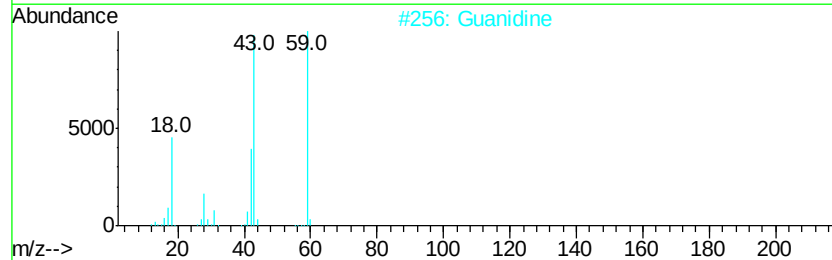
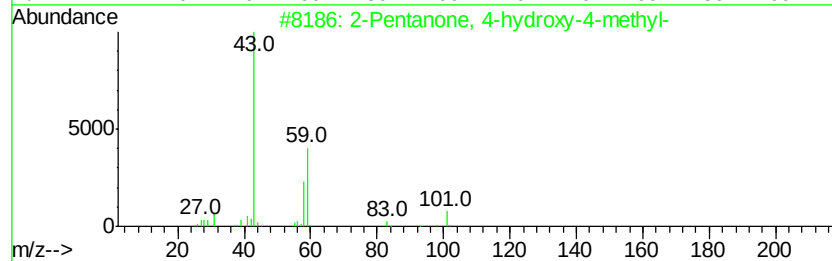
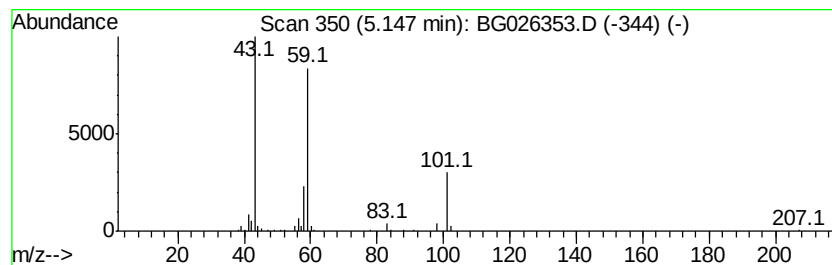
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	5.39 ng	160490	1,4-Dichlorobenzene-d4	8.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Guanidine	59	CH5N3	000113-00-8	47
3		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	43
4		Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	36
5		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	33



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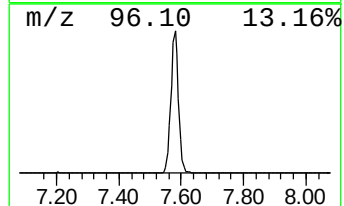
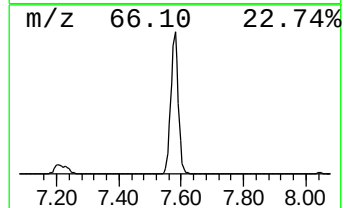
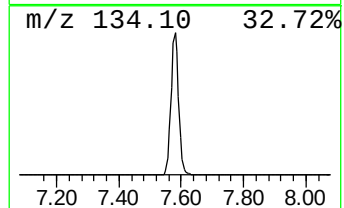
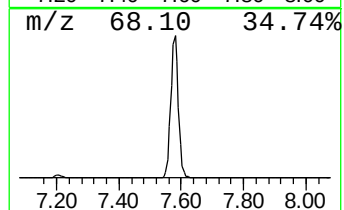
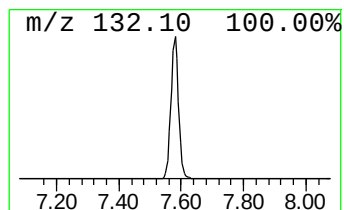
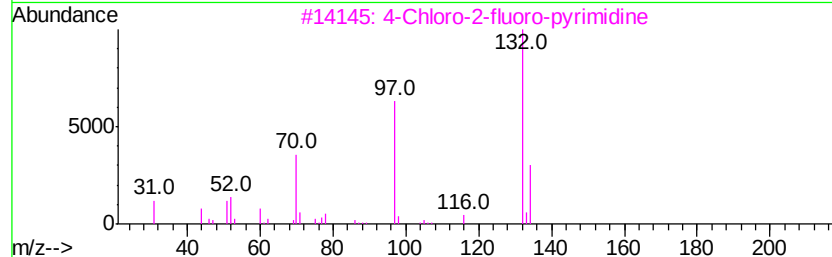
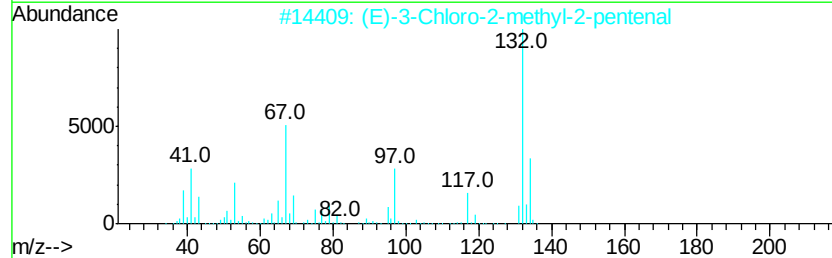
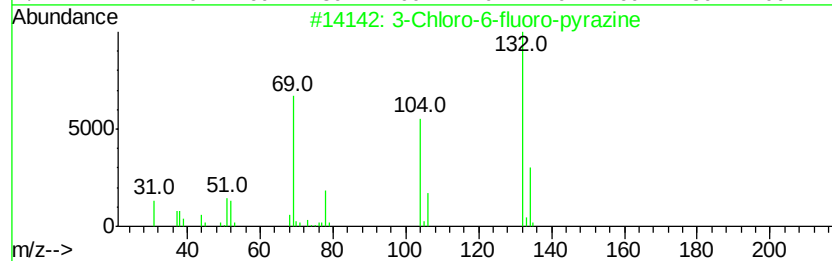
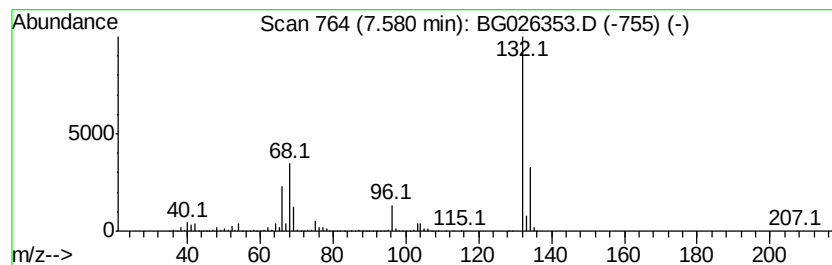
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Peak Number 3 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	88.34 ng	2630300	1,4-Dichlorobenzene-d4	8.04

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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
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
1,3-Oxathiolane	4.67	9.0	ng	268842	1	8.04	595481	20.0
2-Pentanone, 4-hy...	5.15	5.4	ng	160490	1	8.04	595481	20.0
unknown7.58	7.58	88.3	ng	2630300	1	8.04	595481	20.0