

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060917\
 Data File : BG027363.D
 Acq On : 10 Jun 2017 1:22
 Operator : SJ/MA
 Sample : I3575-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 HR-06-060817-A

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-BG060517.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	4.553	141	147	154	rBV	43171	71324	1.25%	0.295%
2	5.704	337	343	354	rVB	140536	248700	4.38%	1.030%
3	6.145	409	418	430	rBV	933585	1681779	29.59%	6.965%
4	7.690	667	681	693	rBV	907927	1706273	30.02%	7.067%
5	8.090	741	749	759	rBV	1022530	1883145	33.13%	7.799%
6	8.554	821	828	839	rVB	144052	263377	4.63%	1.091%
7	8.883	874	884	894	rBV	655025	1218029	21.43%	5.044%
8	9.717	1016	1026	1038	rBV	616733	1193965	21.01%	4.945%
9	11.374	1300	1308	1315	rBV	236233	455458	8.01%	1.886%
10	13.760	1706	1714	1724	rBV	1941126	3106106	54.65%	12.864%
11	15.135	1940	1948	1955	rBV2	421277	706273	12.43%	2.925%
12	16.621	2193	2201	2211	rBV	1951338	3160732	55.61%	13.090%
13	17.884	2409	2416	2428	rBV2	665492	1072323	18.87%	4.441%
14	20.464	2848	2855	2866	rBV	4025401	5683872	100.00%	23.540%
15	22.267	3154	3162	3172	rBV	527115	1001843	17.63%	4.149%
16	25.951	3778	3789	3809	rBV3	185913	692619	12.19%	2.868%

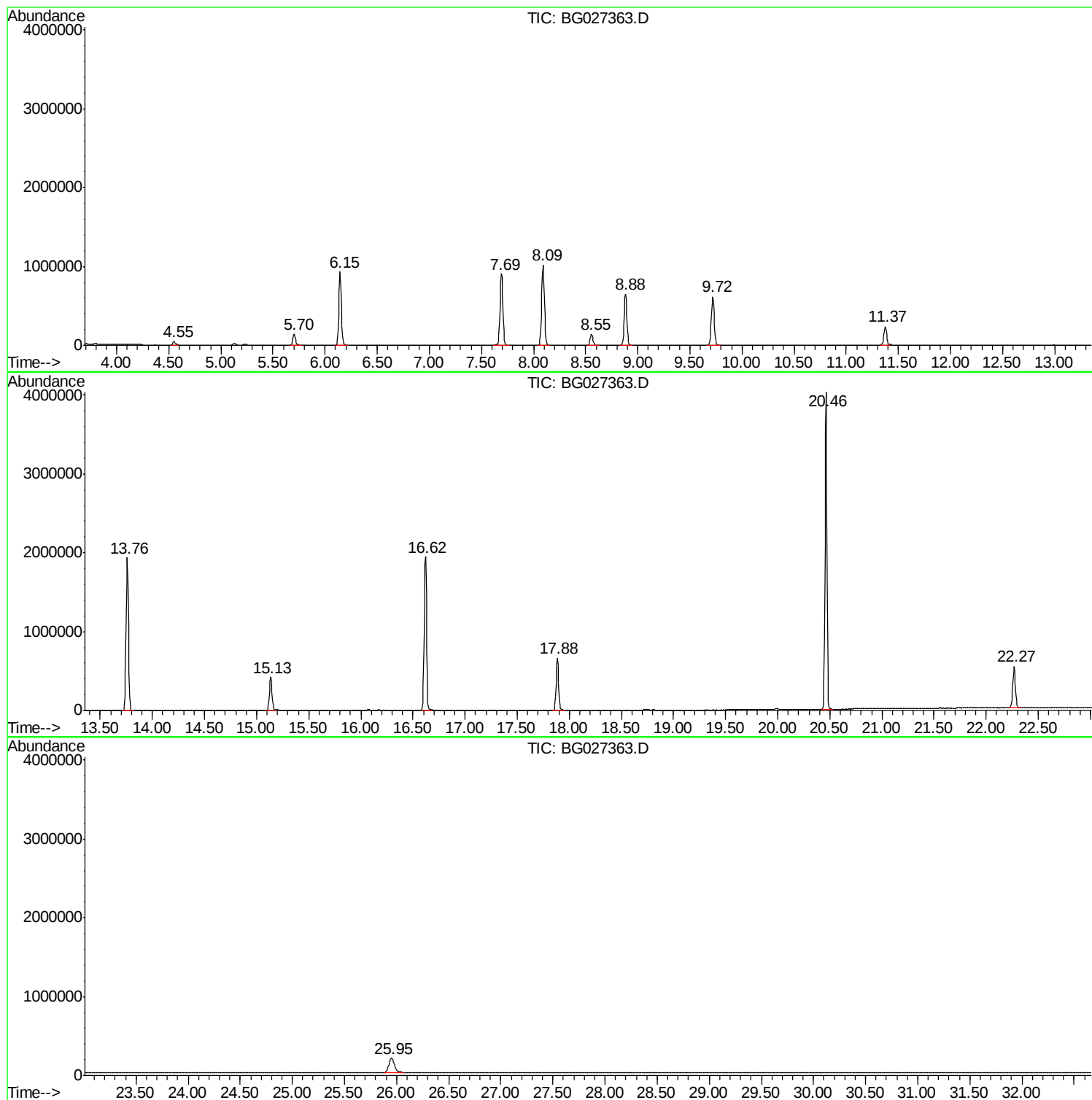
Sum of corrected areas: 24145818

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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.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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Instrument :
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ClientSampled :
HR-06-060817-A

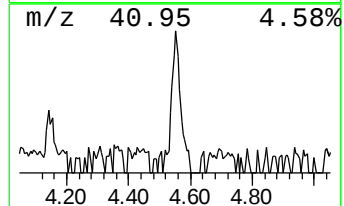
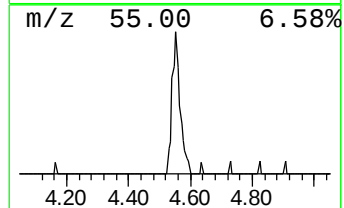
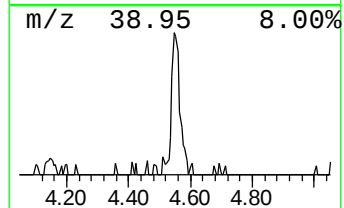
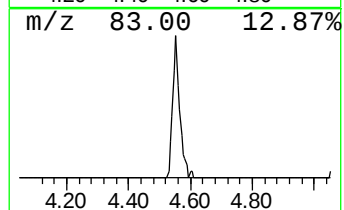
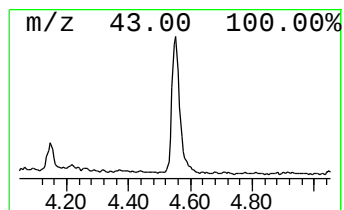
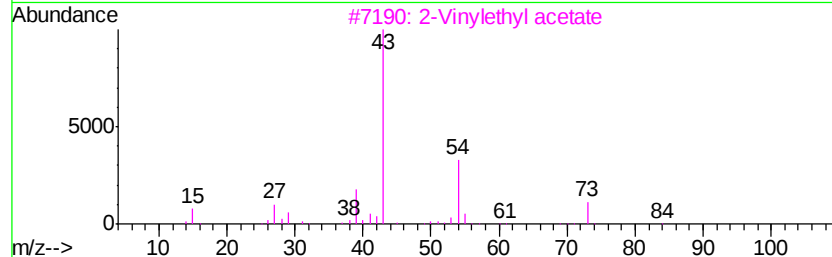
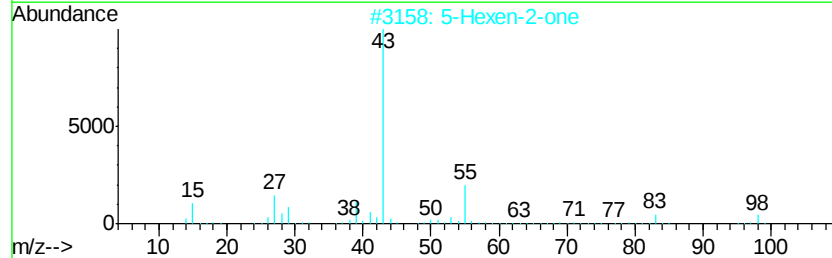
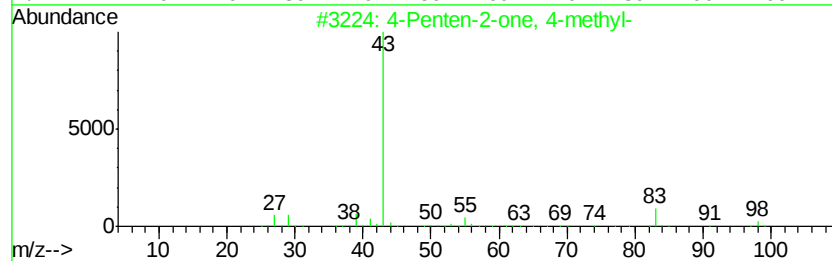
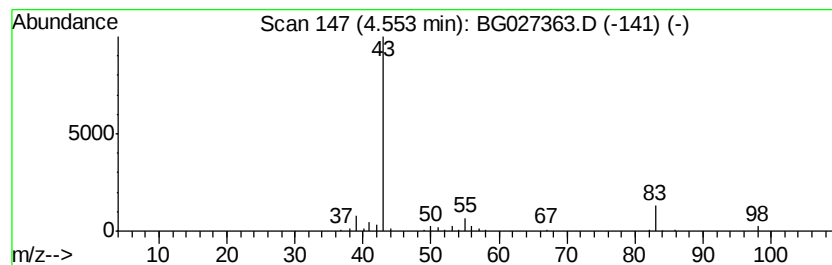
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	5.42 ng	71324	1,4-Dichlorobenzene-d4	8.55

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	64
2			5-Hexen-2-one	98	C6H10O	000109-49-9	43
3			2-Vinylethyl acetate	114	C6H10O2	001576-84-7	25
4			Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	10
5			2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	10



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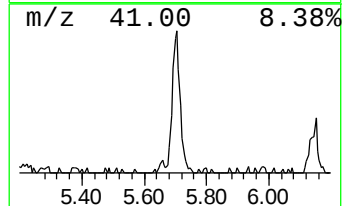
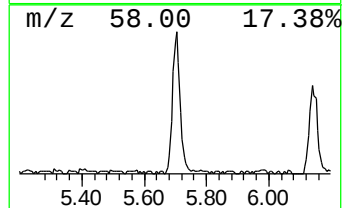
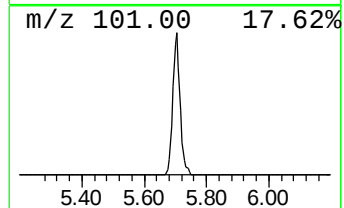
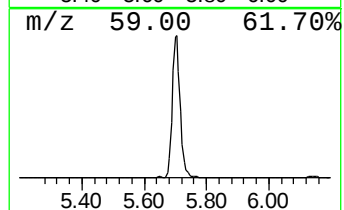
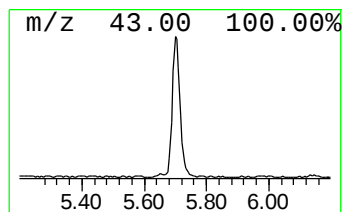
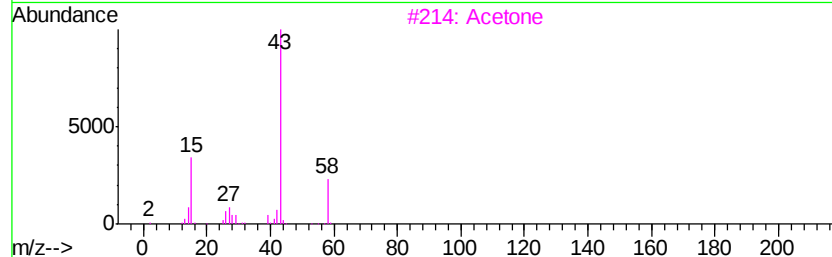
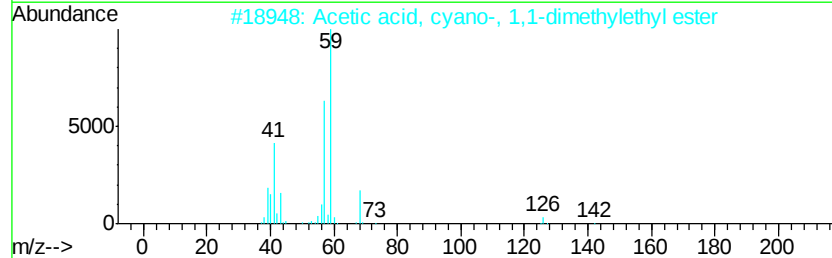
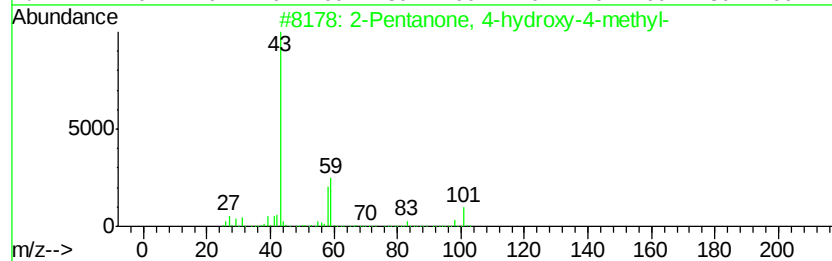
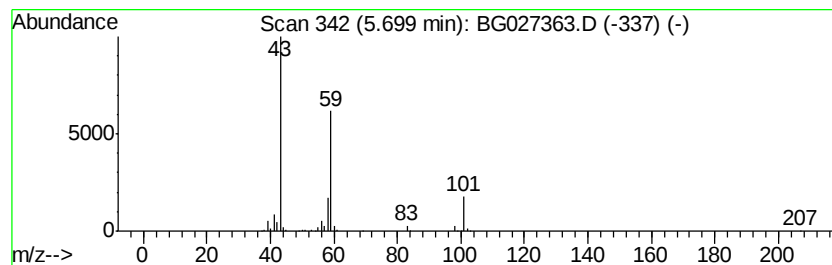
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.70	18.89 ng	248700	1,4-Dichlorobenzene-d4	8.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3		Acetone	58	C3H6O	000067-64-1	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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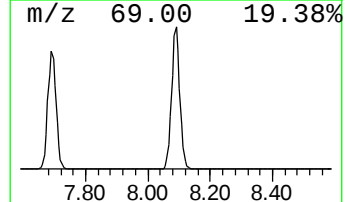
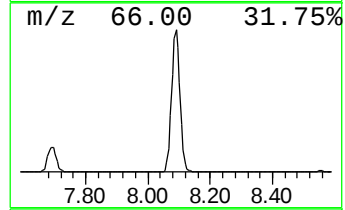
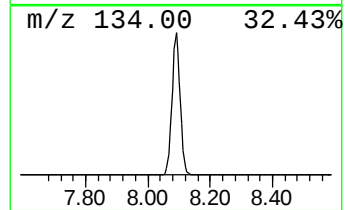
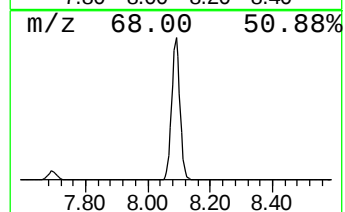
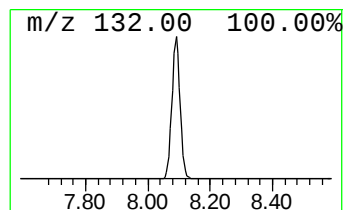
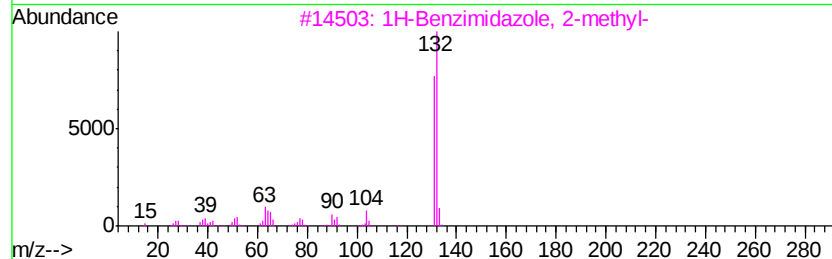
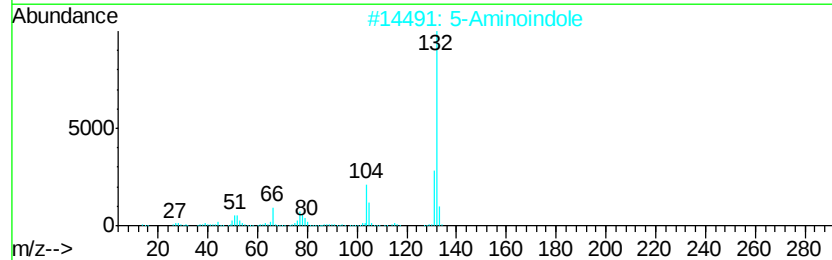
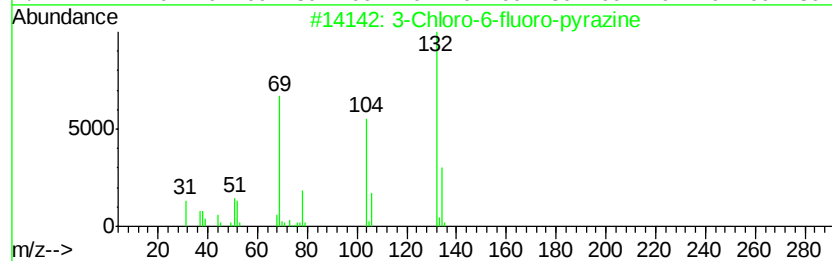
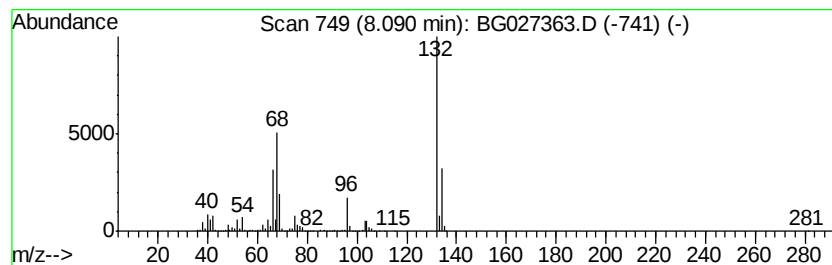
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Peak Number 3 unknown8.09 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.09	143.00 ng	1883150	1,4-Dichlorobenzene-d4	8.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	22
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one, 4...	4.55	5.4	ng	71324	1	8.55	263377	20.0
2-Pentanone, 4-hy...	5.70	18.9	ng	248700	1	8.55	263377	20.0
unknown8.09	8.09	143.0	ng	1883150	1	8.55	263377	20.0