

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG073116\
 Data File : BG023367.D
 Acq On : 31 Jul 2016 14:14
 Operator : UM/SJ
 Sample : PB92481BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB92481BL

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-BG072616.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	2.993	21	26	39	rVB	352564	532267	4.15%	0.840%
2	5.184	393	399	410	rVB	558533	865877	6.76%	1.367%
3	5.666	473	481	493	rBV	2517546	4123624	32.18%	6.509%
4	7.281	747	756	766	rBV	2600107	4595577	35.86%	7.254%
5	7.651	810	819	829	rBV	2530364	4396202	34.31%	6.939%
6	8.121	893	899	908	rVB	518421	911893	7.12%	1.439%
7	8.450	948	955	963	rBV	1729779	3047387	23.78%	4.810%
8	9.296	1092	1099	1111	rVB	1534220	2766011	21.59%	4.366%
9	10.953	1373	1381	1389	rBV	783283	1441043	11.25%	2.275%
10	13.402	1790	1798	1806	rBV	4457909	7271762	56.75%	11.478%
11	14.789	2024	2034	2042	rBV2	1437304	2457575	19.18%	3.879%
12	16.281	2280	2288	2304	rBV	4467715	7078298	55.24%	11.172%
13	17.544	2496	2503	2512	rBV2	2268911	3636111	28.38%	5.739%
14	20.158	2941	2948	2959	rBV	9107345	12814280	100.00%	20.226%
15	21.861	3231	3238	3246	rVB	2164973	3731304	29.12%	5.889%
16	25.245	3803	3814	3830	rVB3	1204461	3686996	28.77%	5.819%

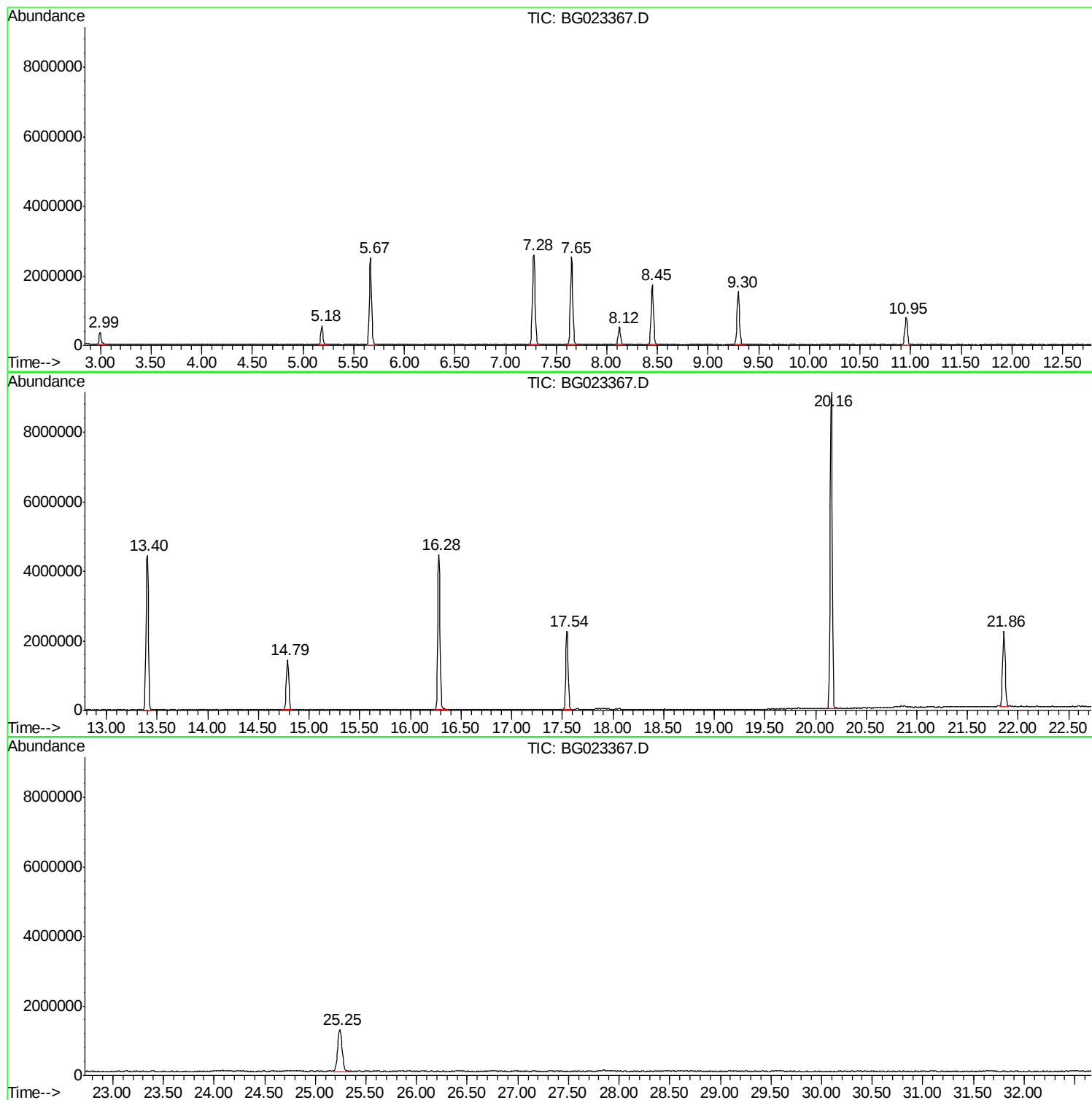
Sum of corrected areas: 63356207

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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.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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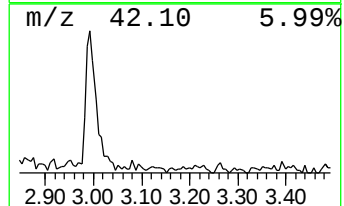
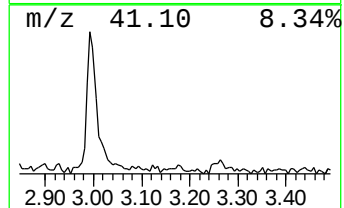
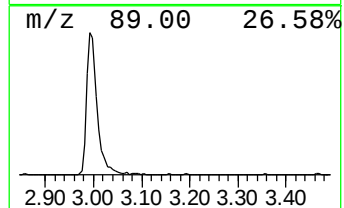
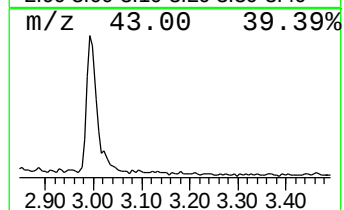
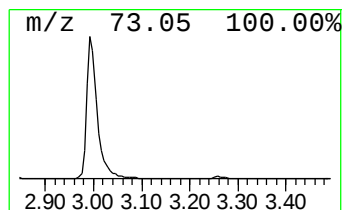
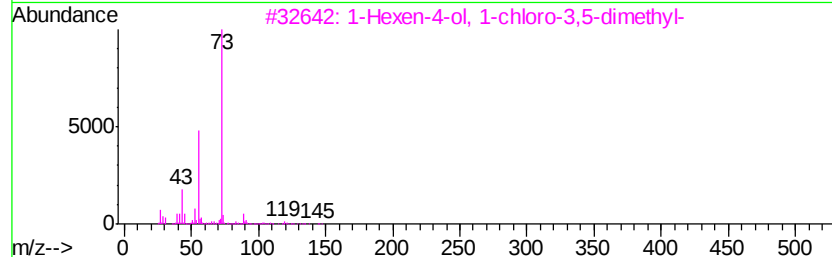
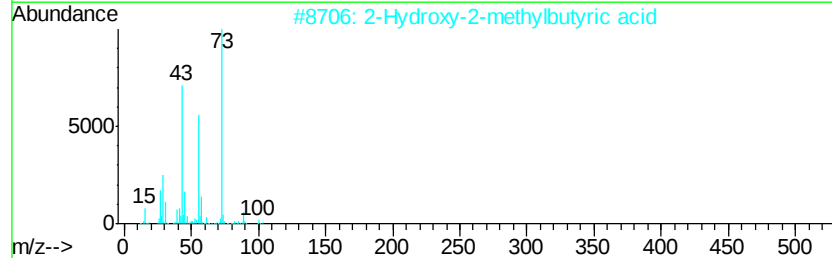
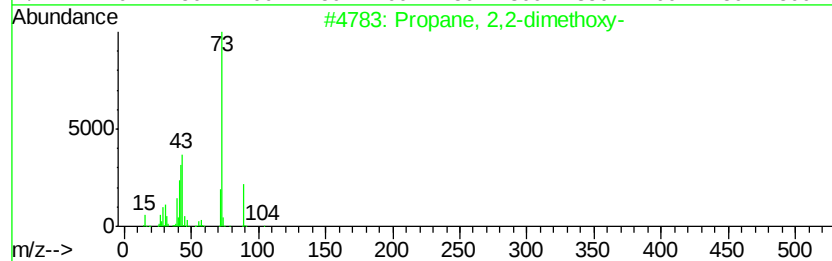
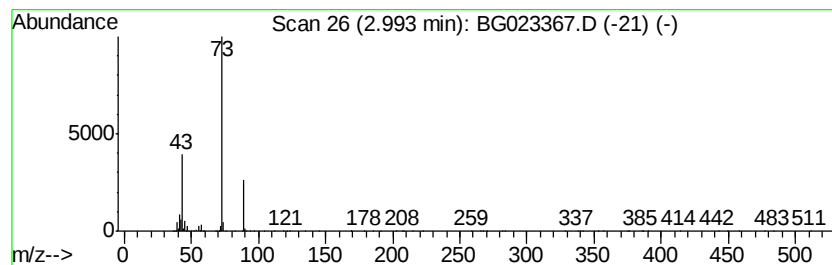
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	11.67 ng	532267	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	64
2		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
3		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
4		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5		1,3-Dioxolane, 2-(6-heptynyl)-	168	C10H16O2	025595-82-8	7



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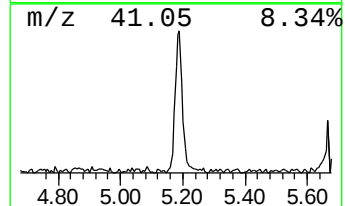
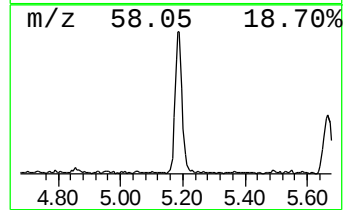
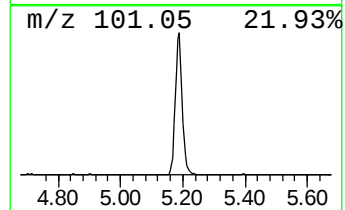
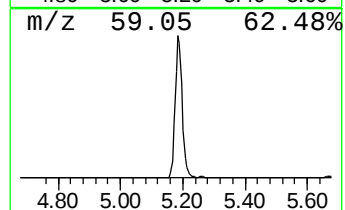
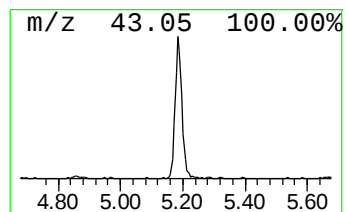
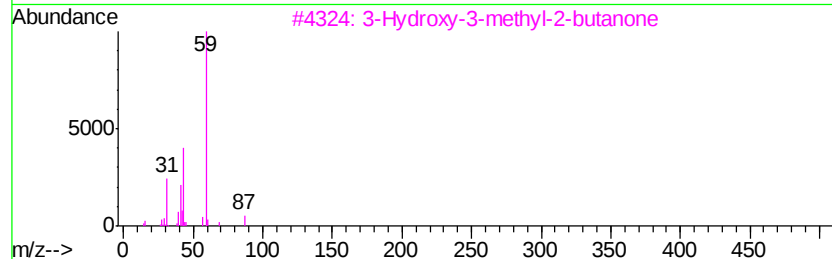
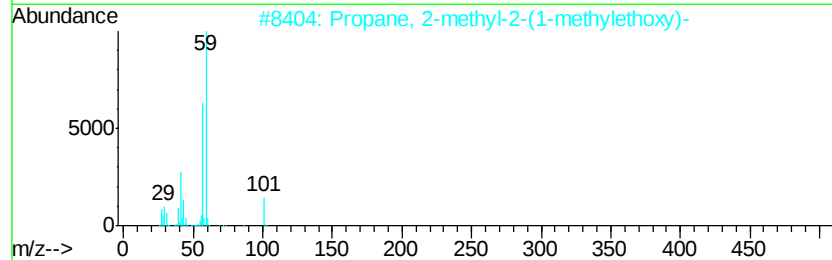
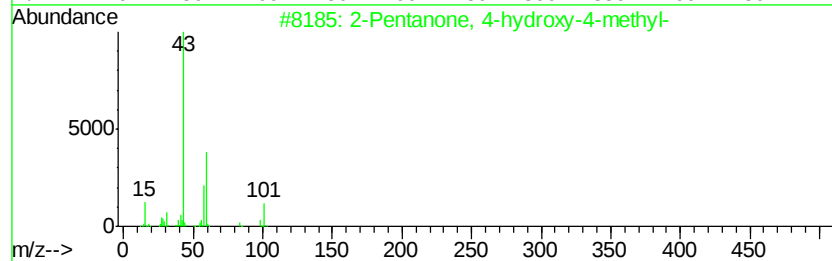
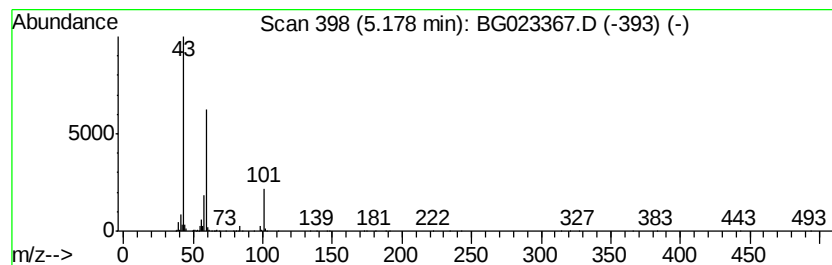
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	18.99 ng	865877	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
4		Guanidine	59	CH5N3	000113-00-8	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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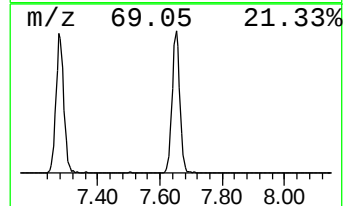
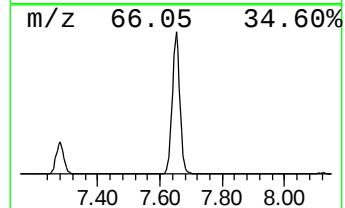
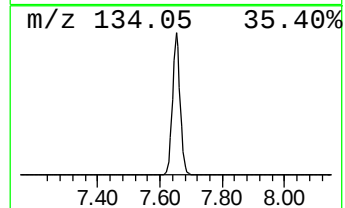
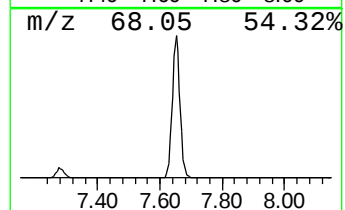
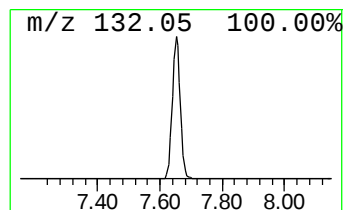
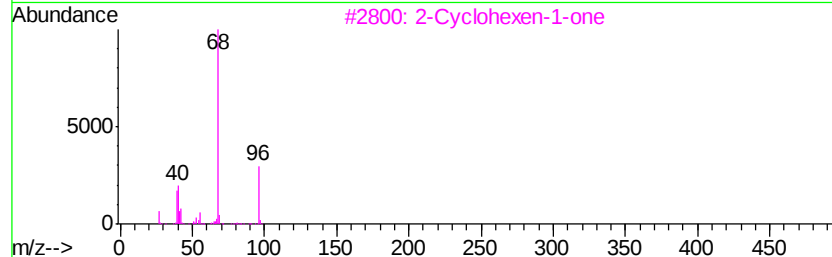
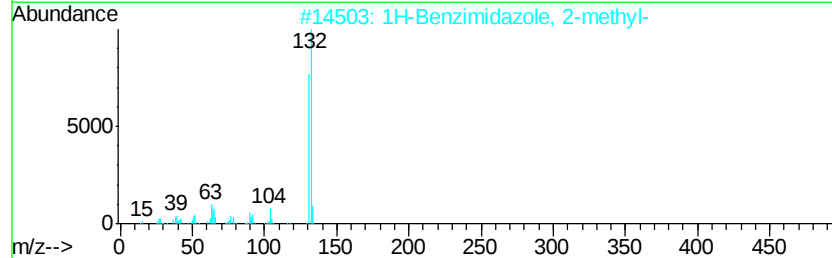
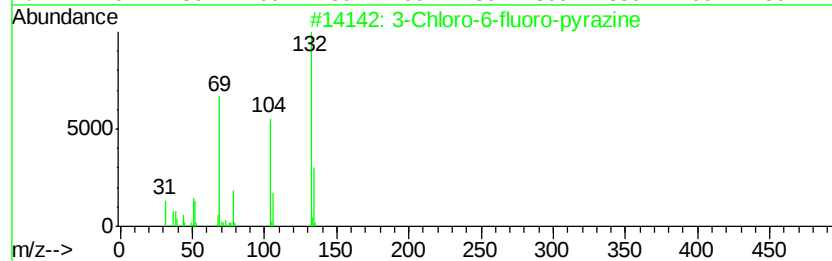
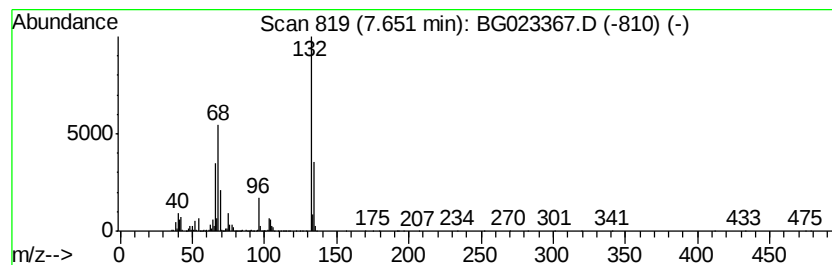
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Peak Number 3 unknown7.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	96.42 ng	4396200	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
4		5-Aminoindole	132	C8H8N2	005192-03-0	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	2.99	11.7	ng	532267	1	8.13	911893	20.0
2-Pentanone, 4-hy...	5.18	19.0	ng	865877	1	8.13	911893	20.0
unknown7.65	7.65	96.4	ng	4396200	1	8.13	911893	20.0