

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
 Data File : BF093629.D
 Acq On : 14 Mar 2017 1:35
 Operator : SJ/MA
 Sample : I2199-21
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D-87

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_F\METHODS\8270-BF030717.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	2.447	46	49	62	rVB	63105	210409	3.85%	0.444%
2	4.161	196	199	206	rVB	63069	101471	1.85%	0.214%
3	4.413	219	221	229	rBV	44064	110376	2.02%	0.233%
4	4.870	259	261	278	rBV	1243651	2438414	44.56%	5.142%
5	5.316	298	300	333	rBV	3582122	5343182	97.64%	11.267%
6	5.716	333	335	343	rVB	53983	97789	1.79%	0.206%
7	6.367	390	392	400	rBV	3280251	4987965	91.15%	10.518%
8	6.482	400	402	405	rVB	4728338	4817091	88.03%	10.158%
9	6.710	420	422	429	rVB	914583	1168210	21.35%	2.463%
10	6.859	433	435	438	rBV	3747542	3722037	68.02%	7.849%
11	7.282	470	472	487	rBV	3108045	3535155	64.60%	7.455%
12	8.002	532	535	543	rBV	1263571	1593040	29.11%	3.359%
13	9.076	627	629	632	rBV	3860214	5472171	100.00%	11.539%
14	9.762	686	689	691	rBV	1258699	1655403	30.25%	3.491%
15	10.551	756	758	761	rBV2	2243224	2945981	53.84%	6.212%
16	11.248	817	819	825	rBV	1788450	1732863	31.67%	3.654%
17	12.837	955	958	961	rBV	4521828	4898776	89.52%	10.330%
18	13.900	1049	1051	1059	rVB	1025121	1496796	27.35%	3.156%
19	15.305	1171	1174	1184	rBV	690680	1094927	20.01%	2.309%

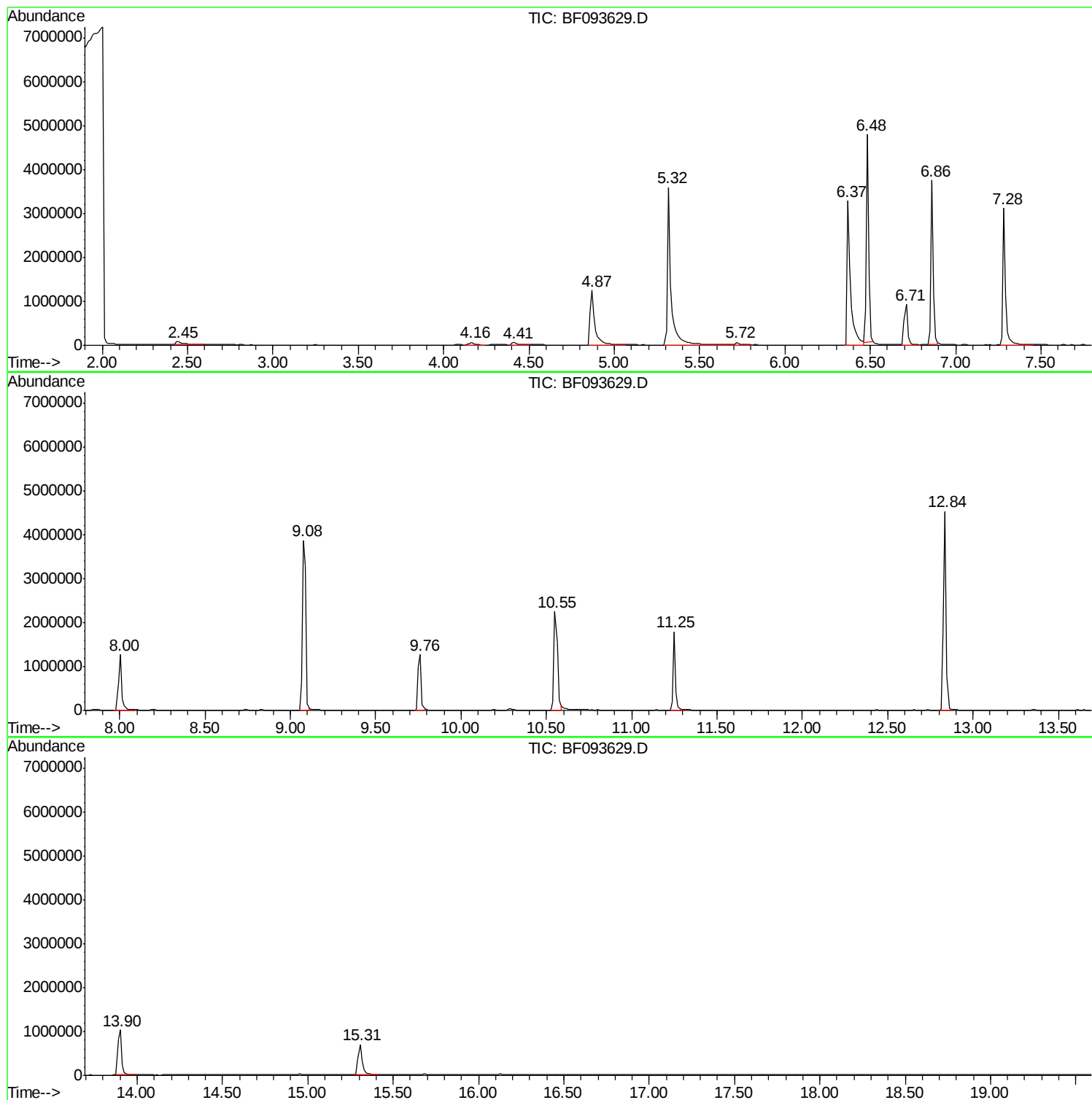
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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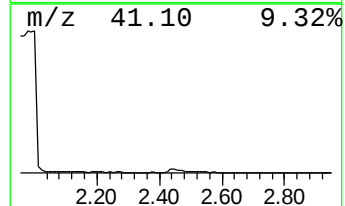
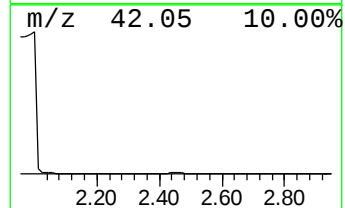
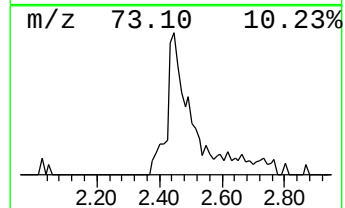
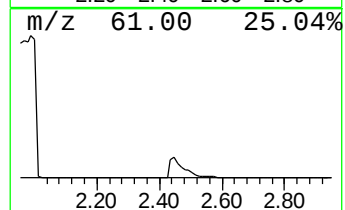
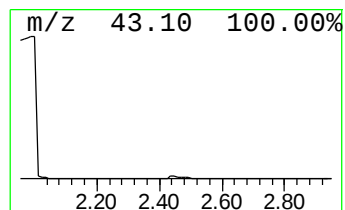
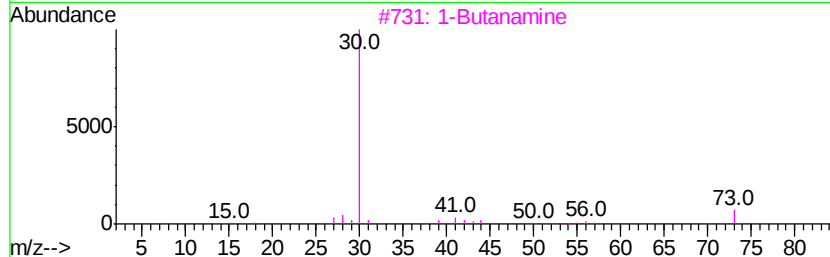
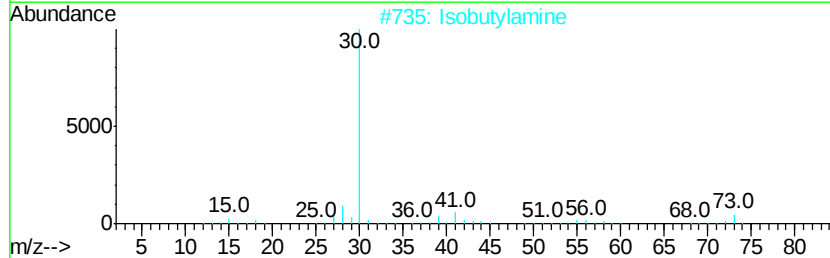
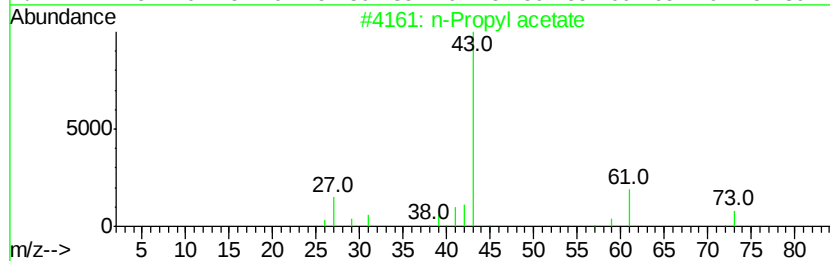
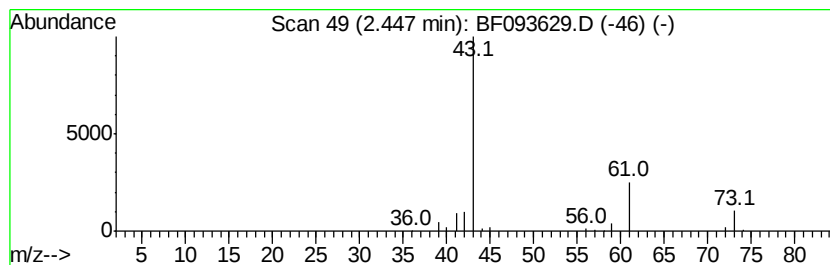
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	3.60 ng	210409	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	78
2			Isobutylamine	73	C4H11N	000078-81-9	7
3			1-Butanamine	73	C4H11N	000109-73-9	7
4			Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	5
5			Methylglyoxal	72	C3H4O2	000078-98-8	4



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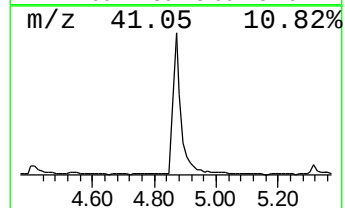
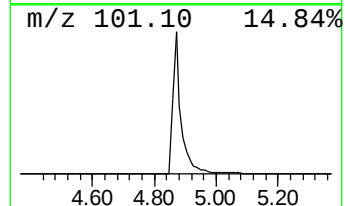
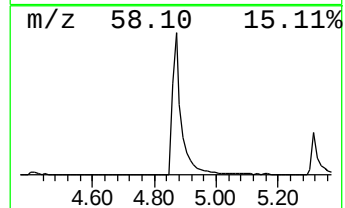
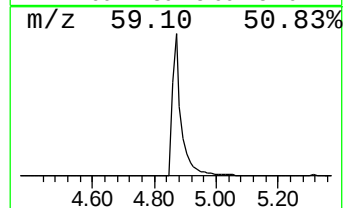
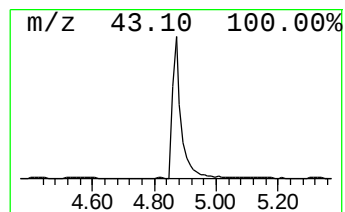
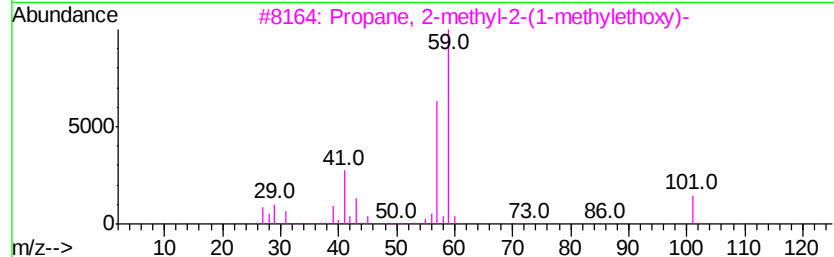
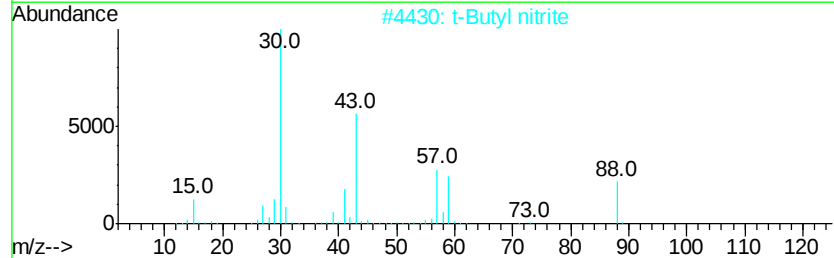
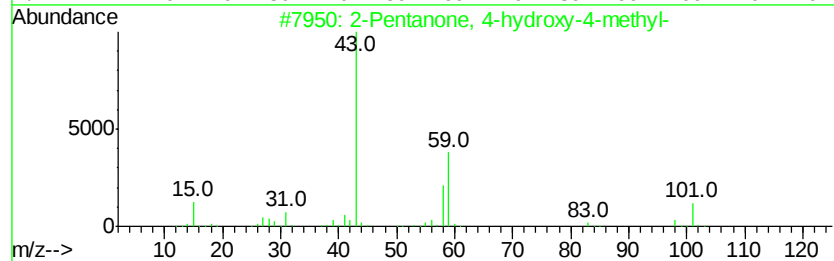
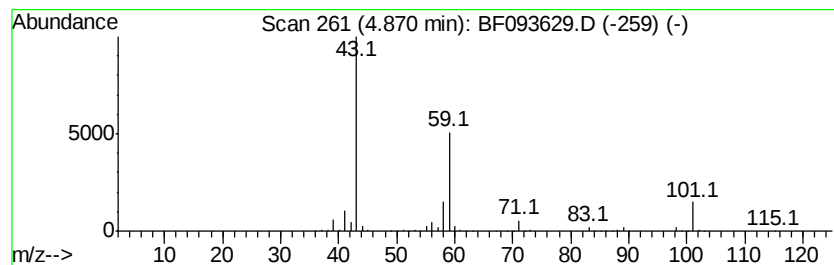
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	41.75 ng	2438410	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		t-Butyl nitrite	103	C4H9NO2	000540-80-7	39
3		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	33
4		1,2-Butanediol, (+/-)-	90	C4H10O2	026171-83-5	25
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25



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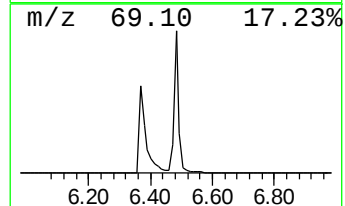
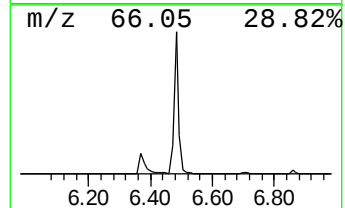
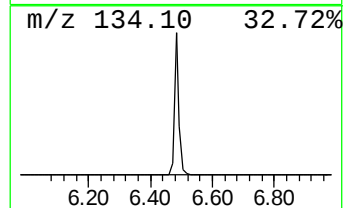
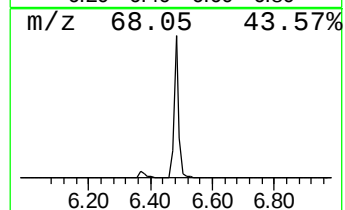
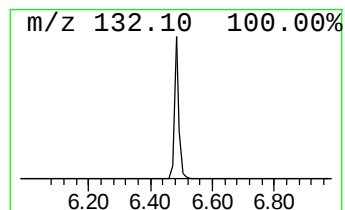
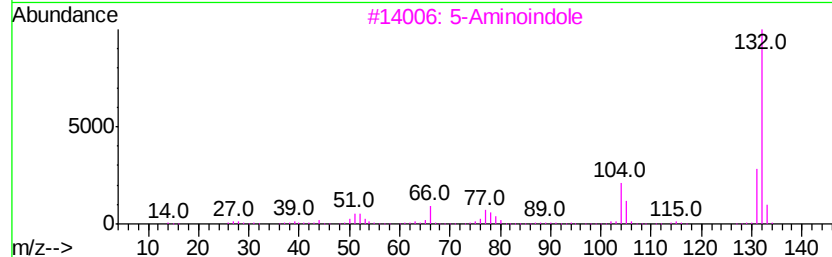
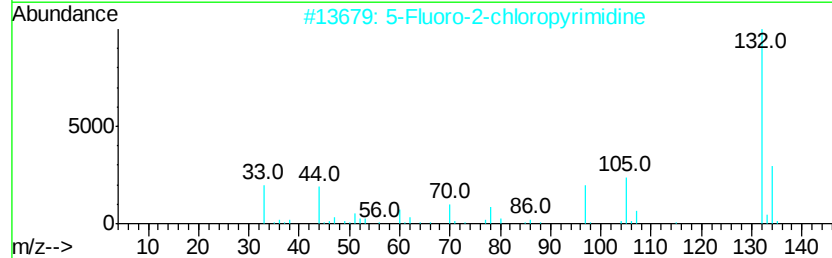
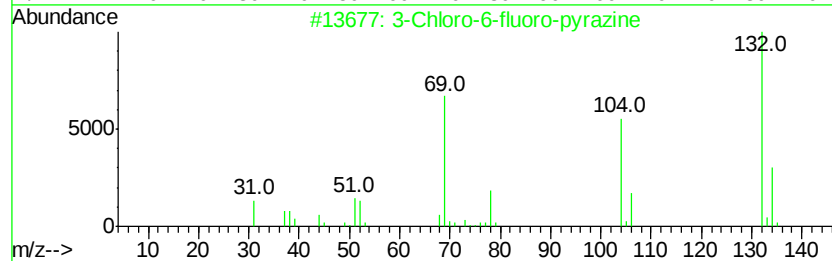
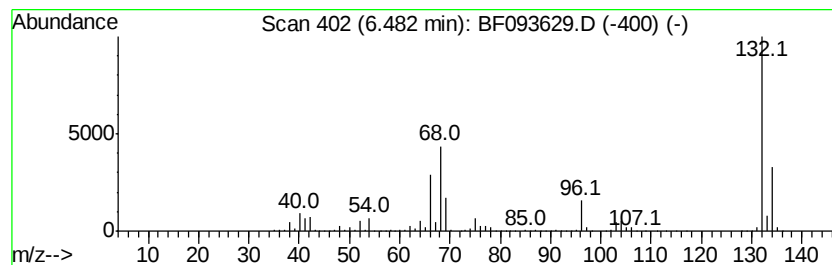
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Peak Number 3 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	82.47 ng	4817090	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.45	3.6	ng	210409	1	6.71	1168210	20.0
2-Pentanone, 4-hy...	4.87	41.8	ng	2438410	1	6.71	1168210	20.0
unknown6.48	6.48	82.5	ng	4817090	1	6.71	1168210	20.0