

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031117\
 Data File : BF093566.D
 Acq On : 11 Mar 2017 14:48
 Operator : SJ/MA
 Sample : PB97500BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB97500BL

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_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	1.944	3	5	22	rVB	109536	248191	4.86%	0.539%
2	4.881	259	262	276	rBV	587932	1241813	24.33%	2.699%
3	5.316	298	300	317	rBV	3070316	5104799	100.00%	11.093%
4	5.716	333	335	339	rVB	55246	60687	1.19%	0.132%
5	6.379	391	393	401	rBV	4275378	4498243	88.12%	9.775%
6	6.493	401	403	405	rBV	4479179	4665152	91.39%	10.138%
7	6.722	421	423	428	rBV	963296	1287551	25.22%	2.798%
8	6.870	434	436	439	rBV	3836427	3486519	68.30%	7.576%
9	7.293	471	473	475	rBV	3303094	3149709	61.70%	6.844%
10	8.002	533	535	538	rBV	1761790	1696615	33.24%	3.687%
11	8.162	544	549	556	rBV	27654	59612	1.17%	0.130%
12	8.425	569	572	582	rVB	38153	122297	2.40%	0.266%
13	9.076	627	629	632	rBV	3766043	4900542	96.00%	10.649%
14	9.728	675	686	687	rBV	433196	1244080	24.37%	2.703%
15	9.750	687	688	691	rVB	1825207	1852639	36.29%	4.026%
16	10.208	725	728	733	rBV	38245	81637	1.60%	0.177%
17	10.551	755	758	760	rBV	2429265	2809505	55.04%	6.105%
18	11.236	816	818	821	rBV	2057428	1862561	36.49%	4.047%
19	12.825	954	957	959	rBV	3923795	4707685	92.22%	10.230%
20	13.877	1047	1049	1056	rBV	1677940	1657353	32.47%	3.601%
21	15.271	1168	1171	1175	rBV	967070	1281276	25.10%	2.784%

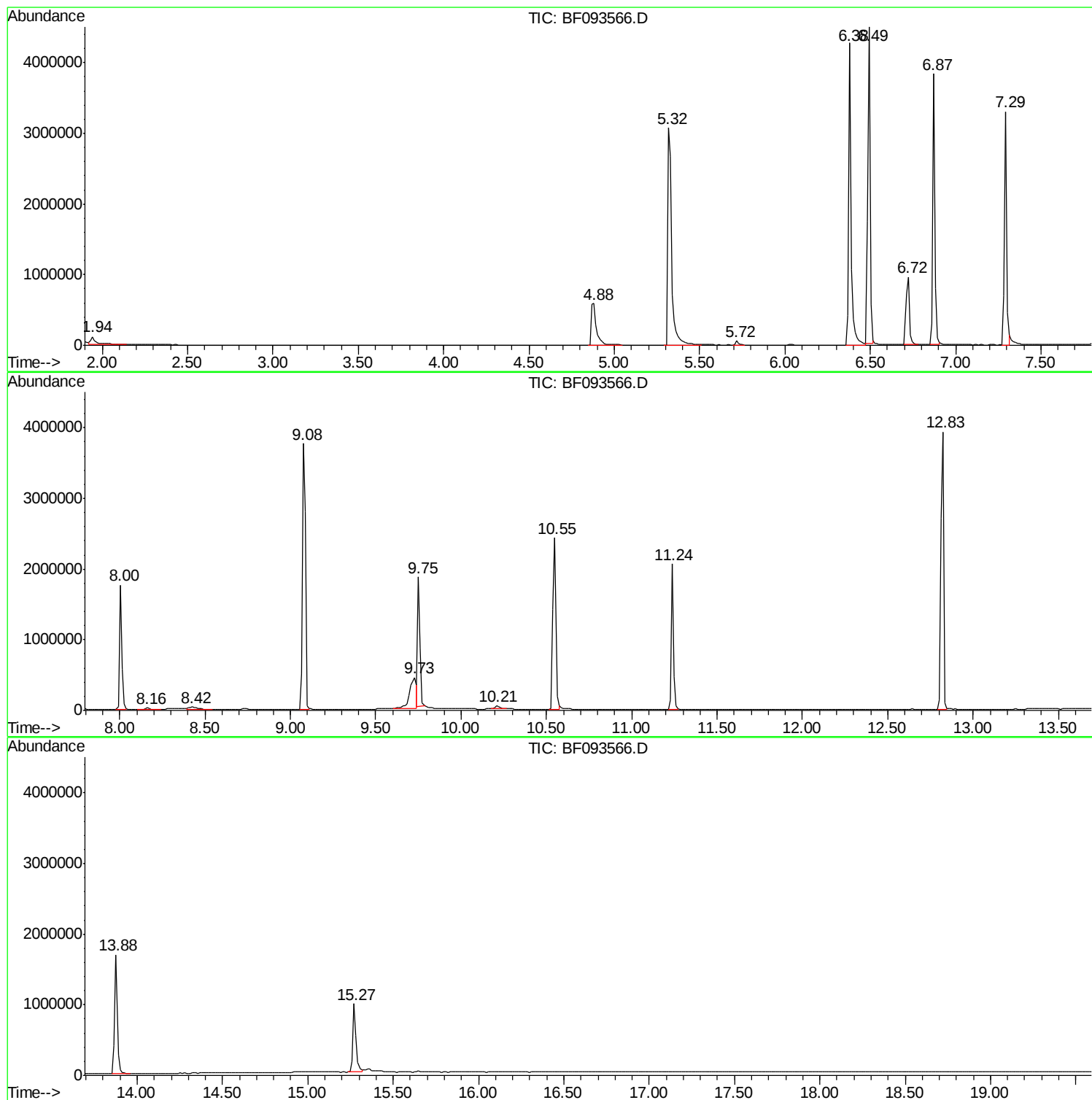
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PB97500BL

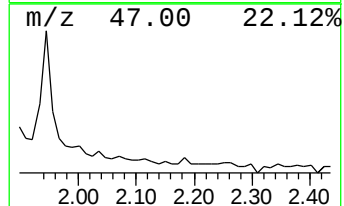
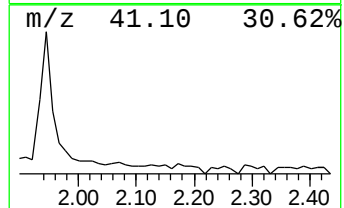
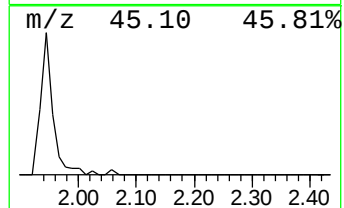
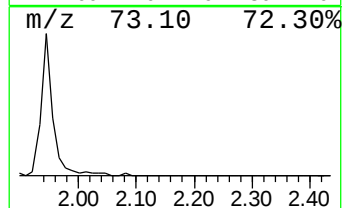
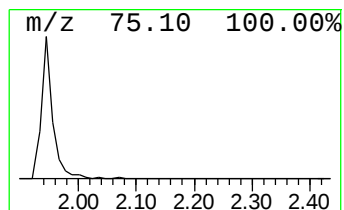
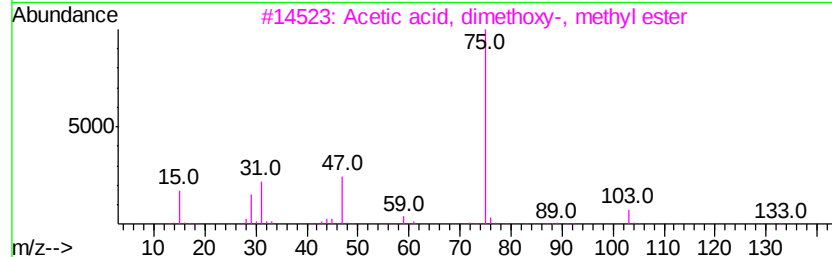
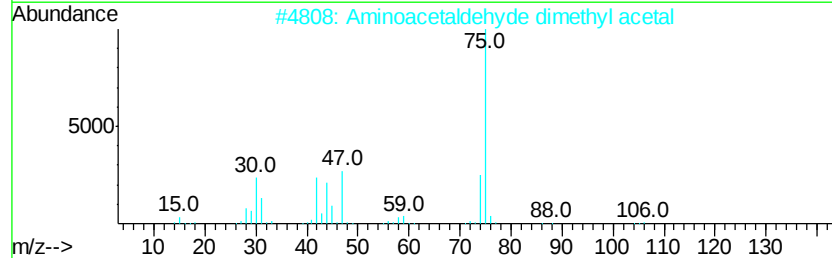
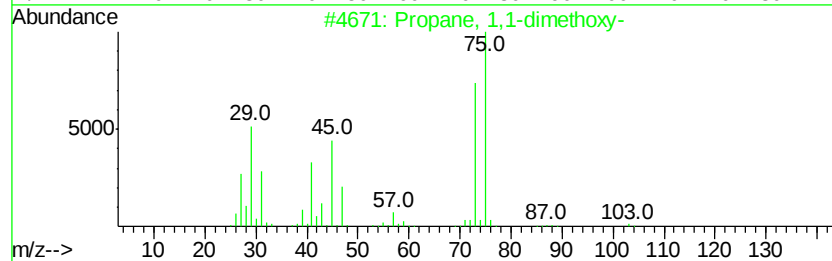
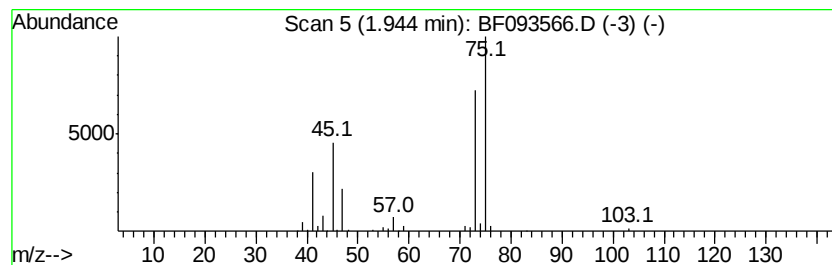
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.94	3.86 ng	248191	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	33
3		Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	33
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9



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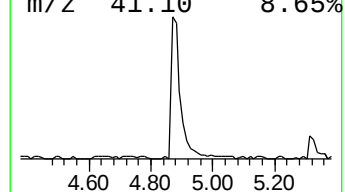
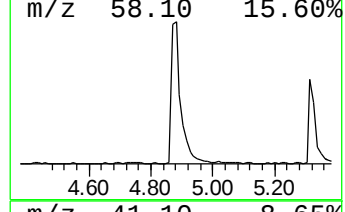
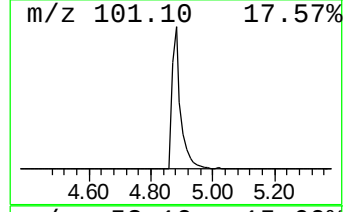
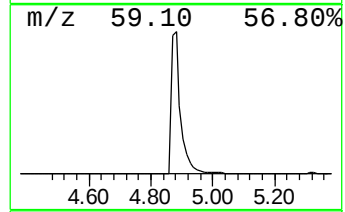
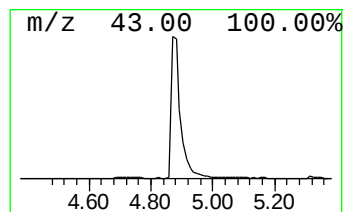
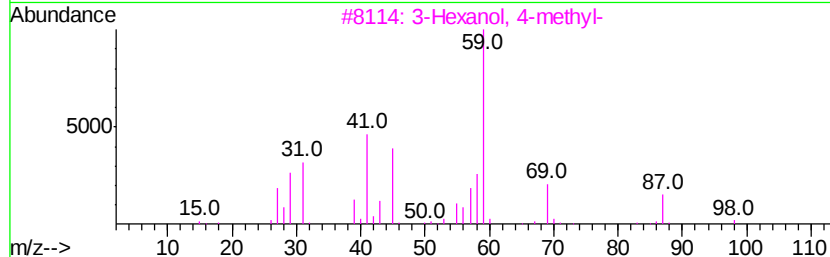
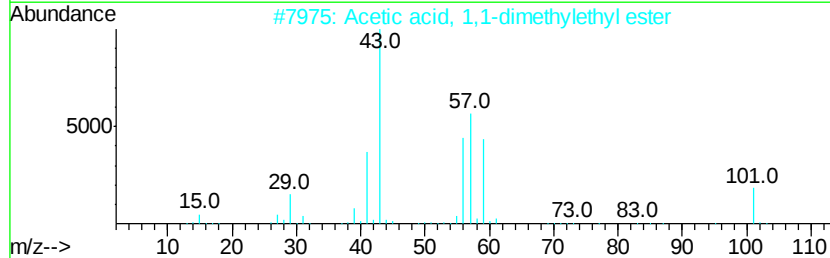
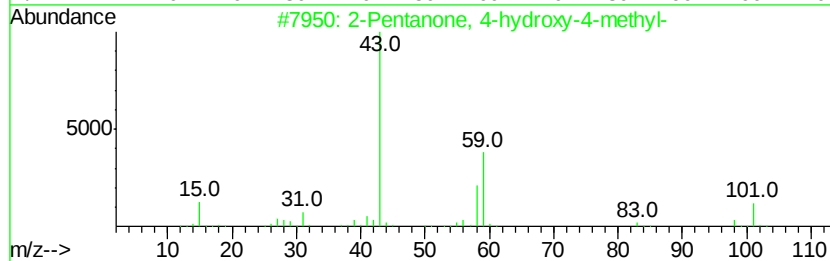
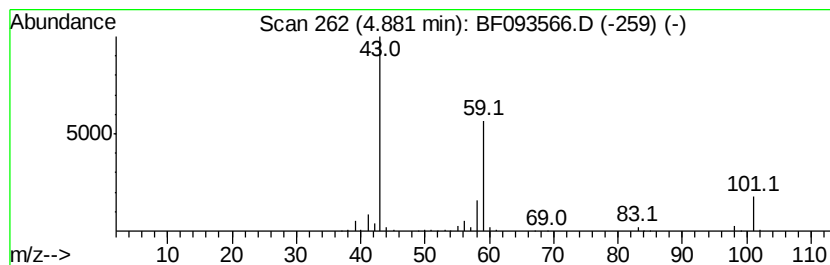
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	19.29 ng	1241810	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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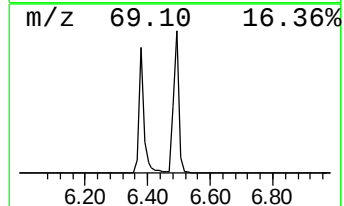
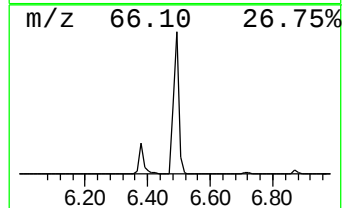
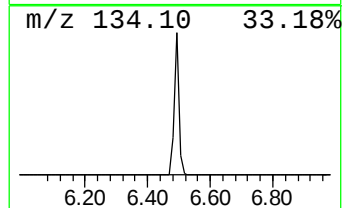
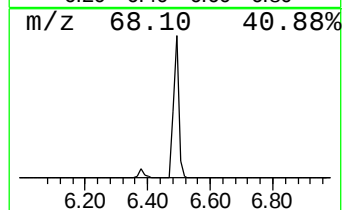
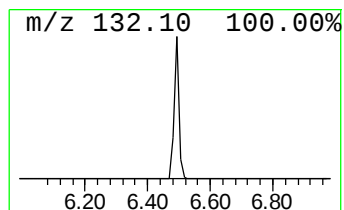
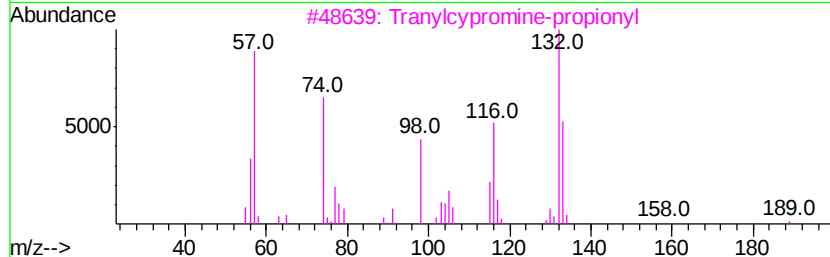
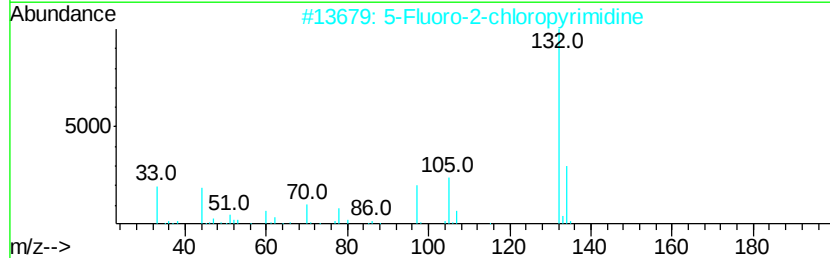
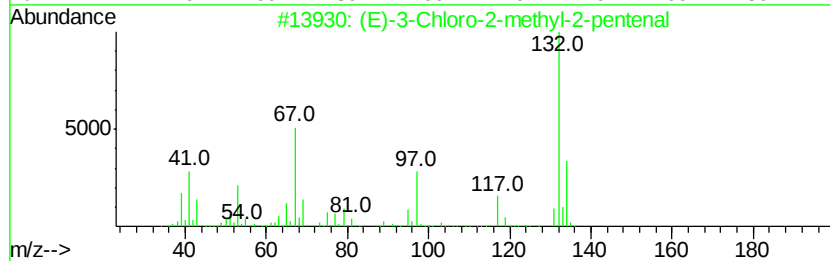
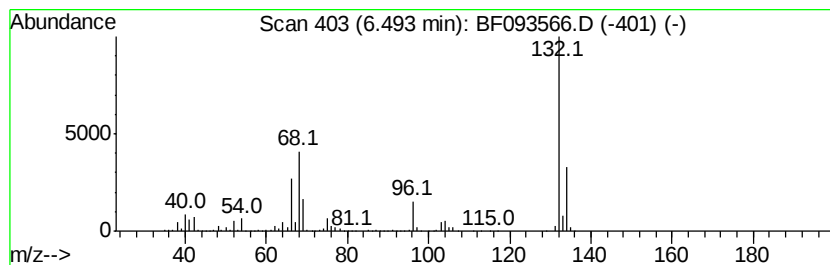
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Peak Number 3 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	72.47 ng	4665150	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
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
Propane, 1,1-dime...	1.94	3.9	ng	248191	1	6.72	1287550	20.0
2-Pentanone, 4-hy...	4.88	19.3	ng	1241810	1	6.72	1287550	20.0
unknown6.49	6.49	72.5	ng	4665150	1	6.72	1287550	20.0