

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122116\
 Data File : BF091851.D
 Acq On : 21 Dec 2016 23:24
 Operator : UM/SJ
 Sample : PB95527BL
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB95527BL

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-BF122116.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	4.270	189	191	198	rBV	191254	302832	3.82%	0.447%
2	4.933	245	249	262	rBV	2313738	4237684	53.47%	6.257%
3	5.367	283	287	289	rBV	6309086	7837802	98.89%	11.572%
4	6.396	374	377	379	rBV	5711149	6382349	80.53%	9.423%
5	6.522	385	388	390	rBV	5524021	7031363	88.72%	10.382%
6	6.739	405	407	410	rBV	1290855	1608106	20.29%	2.374%
7	6.899	418	421	424	rBV	4578487	5051488	63.74%	7.458%
8	7.310	454	457	460	rBV	3378430	4149232	52.35%	6.126%
9	8.030	517	520	523	rBV	2162276	2250334	28.39%	3.323%
10	9.116	610	615	617	rBV	4853535	7925744	100.00%	11.702%
11	9.779	670	673	676	rBV	2176542	2417719	30.50%	3.570%
12	10.568	738	742	745	rBV2	3422025	4529241	57.15%	6.687%
13	11.265	800	803	805	rBV	2495298	2503479	31.59%	3.696%
14	12.854	939	942	944	rBV	6379624	6736971	85.00%	9.947%
15	13.894	1030	1033	1035	rBV	2465389	2272658	28.67%	3.356%
16	15.288	1152	1155	1157	rBV	1461283	1928775	24.34%	2.848%
17	15.334	1157	1159	1165	rVB	80369	127449	1.61%	0.188%
18	15.723	1190	1193	1197	rBV	89012	127743	1.61%	0.189%
19	16.180	1230	1233	1238	rVB	78987	131434	1.66%	0.194%
20	16.717	1276	1280	1284	rBV	47225	94815	1.20%	0.140%
21	17.346	1330	1335	1343	rVB2	30581	81088	1.02%	0.120%

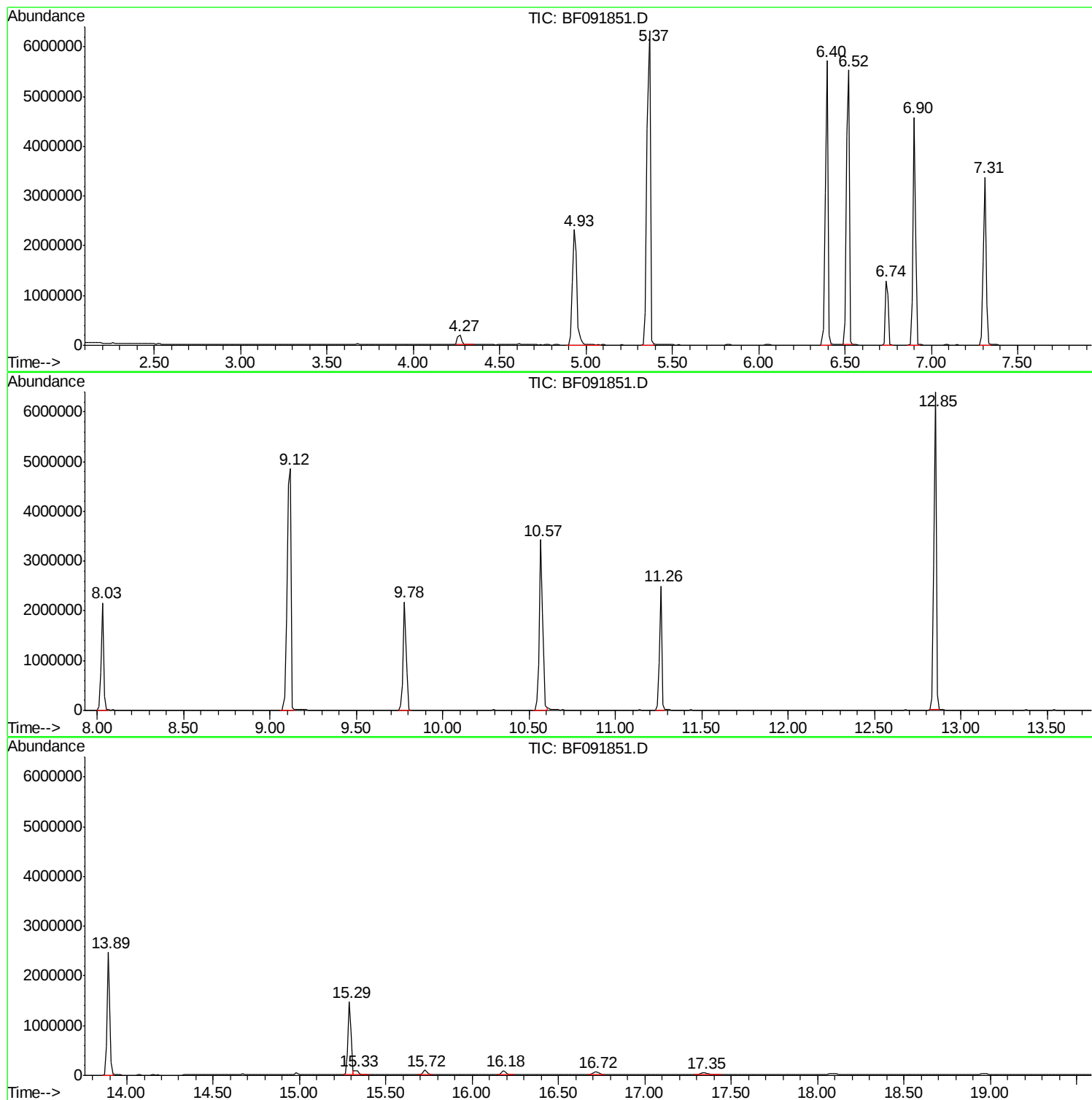
Sum of corrected areas: 67728306

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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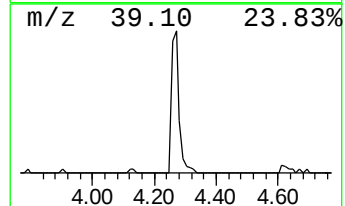
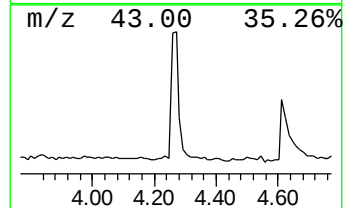
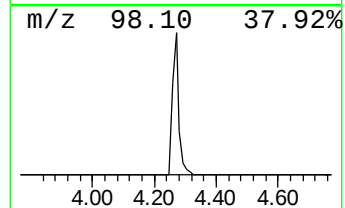
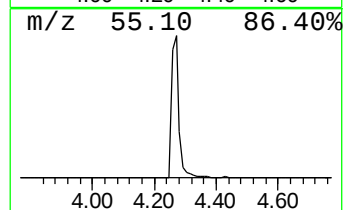
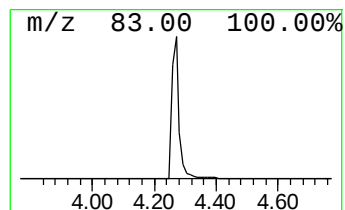
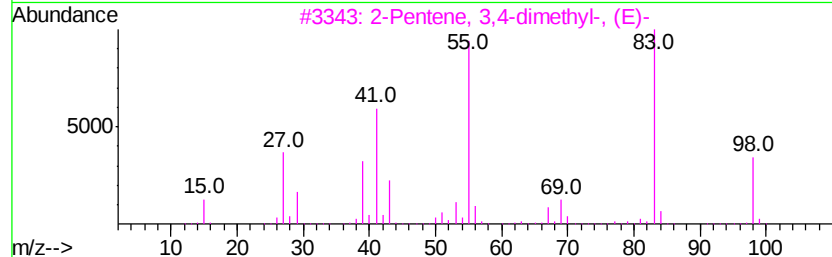
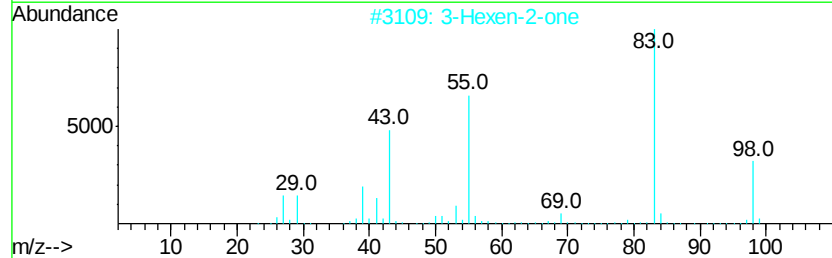
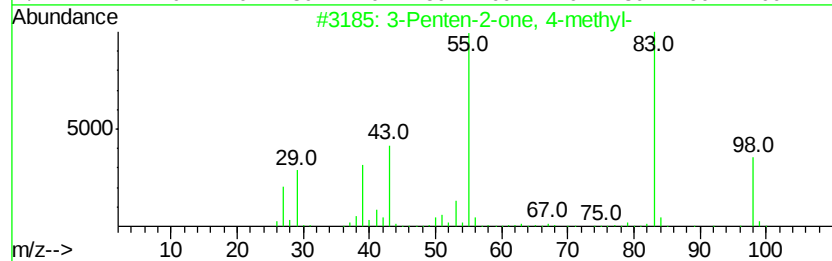
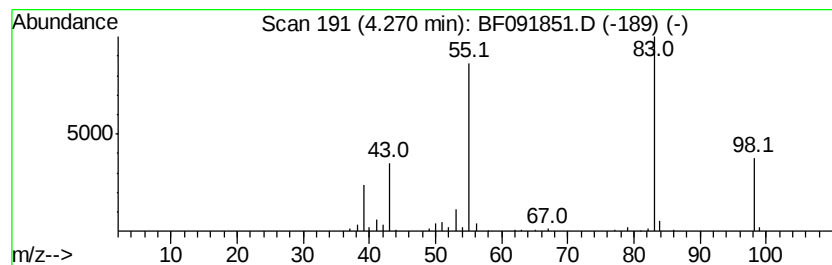
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.27	3.77 ng	302832	1,4-Dichlorobenzene-d4	6.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	90
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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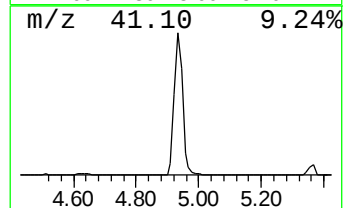
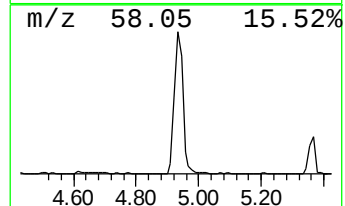
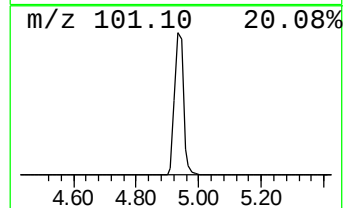
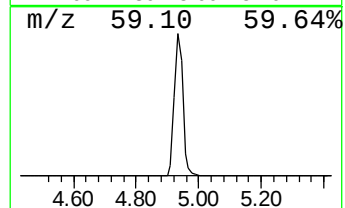
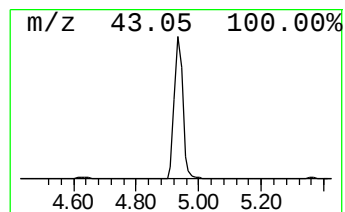
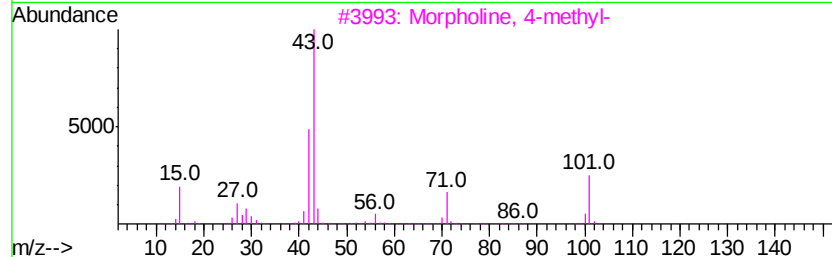
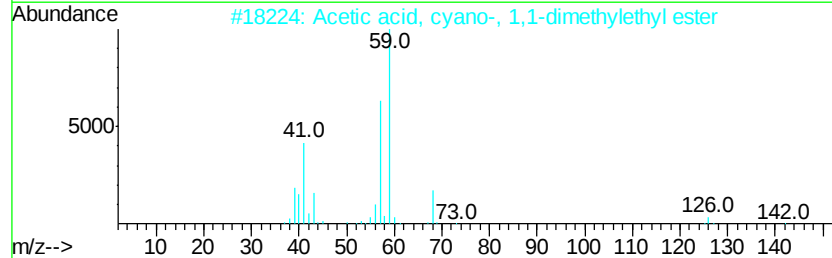
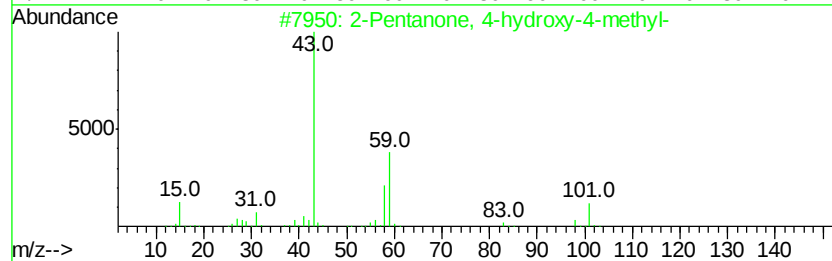
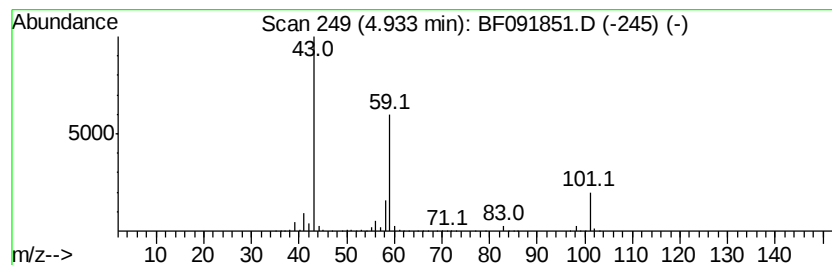
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	52.70 ng	4237680	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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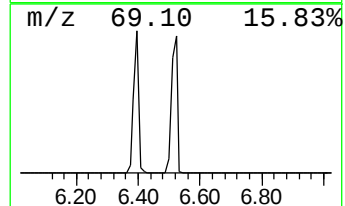
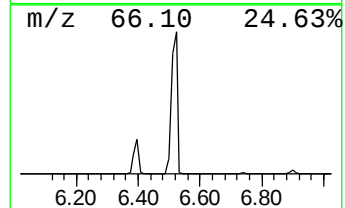
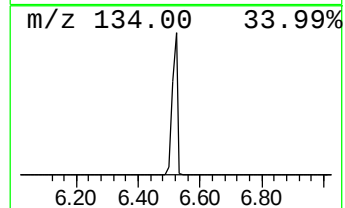
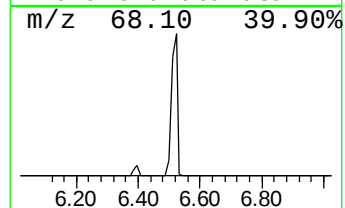
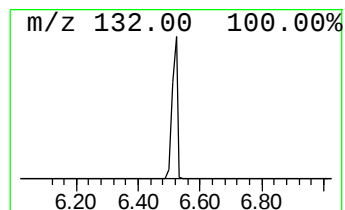
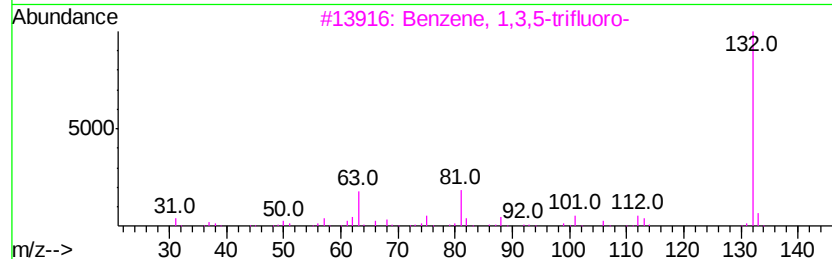
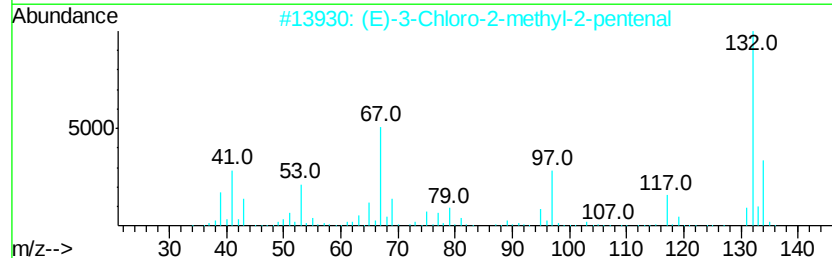
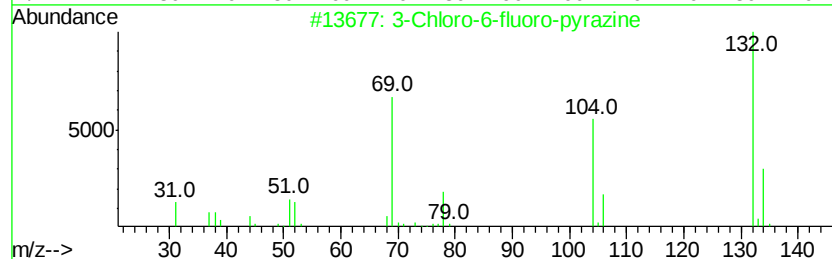
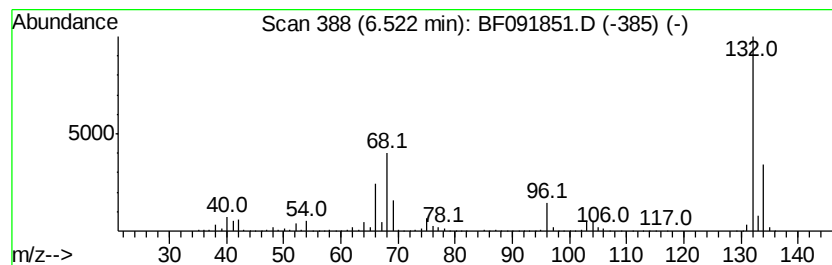
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Peak Number 3 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	87.45 ng	7031360	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.27	3.8	ng	302832	1	6.75	1608110	20.0
2-Pentanone, 4-hy...	4.93	52.7	ng	4237680	1	6.75	1608110	20.0
unknown6.52	6.52	87.5	ng	7031360	1	6.75	1608110	20.0