

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052716\
 Data File : BF087458.D
 Acq On : 27 May 2016 23:46
 Operator : UM/SJ
 Sample : H3291-02
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-12B

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-BF052316.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	1.633	3	4	36	rVB	2194004	4056394	89.75%	11.827%
2	4.707	271	273	296	rBV	187714	560170	12.39%	1.633%
3	5.381	330	332	354	rBV	792767	1731203	38.30%	5.047%
4	5.987	382	385	392	rBV	36563	94575	2.09%	0.276%
5	7.039	474	477	483	rBV	460782	1122207	24.83%	3.272%
6	7.130	483	485	500	rVB	1847306	3273691	72.43%	9.545%
7	7.485	514	516	528	rVB	550612	816529	18.07%	2.381%
8	7.713	534	536	553	rVB	1862705	2823325	62.47%	8.232%
9	8.399	594	596	610	rBV	1748471	2534343	56.08%	7.389%
10	9.519	692	694	705	rBV	671813	1038004	22.97%	3.026%
11	10.365	765	768	773	rVB	24857	46343	1.03%	0.135%
12	11.291	846	849	852	rBV	2959792	4341565	96.06%	12.658%
13	11.999	908	911	914	rBV	51479	92889	2.06%	0.271%
14	12.342	939	941	946	rBV	909713	1200130	26.55%	3.499%
15	13.177	1011	1014	1017	rBV	41263	58252	1.29%	0.170%
16	13.634	1051	1054	1069	rBV	1998247	2915953	64.52%	8.502%
17	13.954	1079	1082	1087	rBV	45908	81913	1.81%	0.239%
18	14.742	1148	1151	1163	rVB	866398	1185250	26.23%	3.456%
19	15.737	1235	1238	1244	rBV	25736	45244	1.00%	0.132%
20	17.097	1354	1357	1360	rBV	3215158	4519533	100.00%	13.177%
21	18.446	1473	1475	1485	rBV	768241	1067275	23.61%	3.112%
22	20.114	1619	1621	1627	rBV	354640	694222	15.36%	2.024%

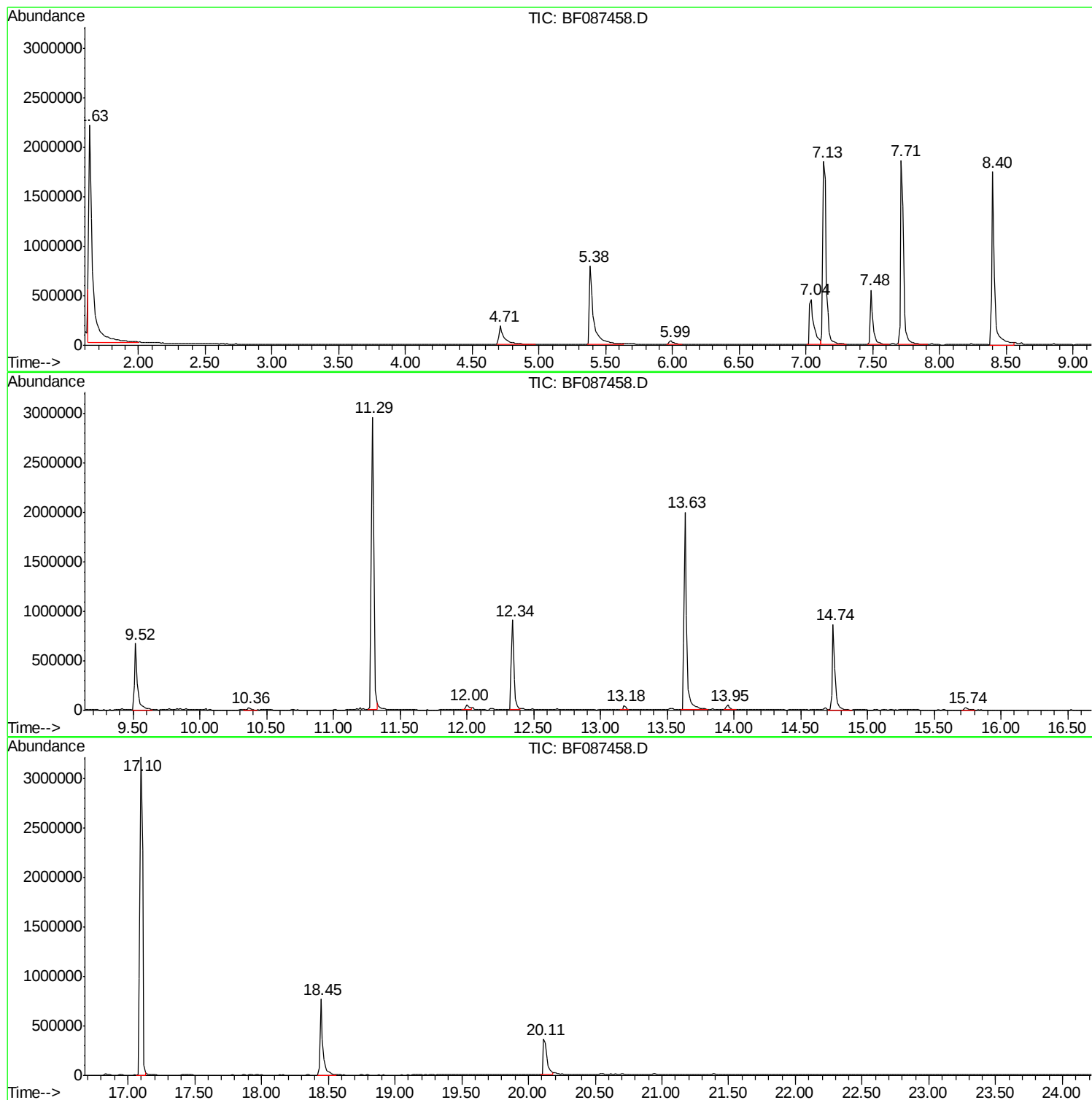
Sum of corrected areas: 34299010

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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF052316.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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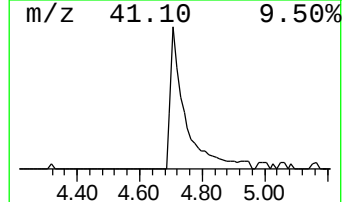
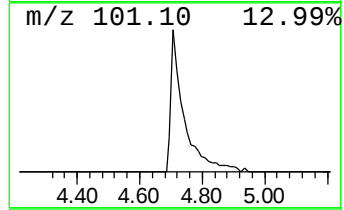
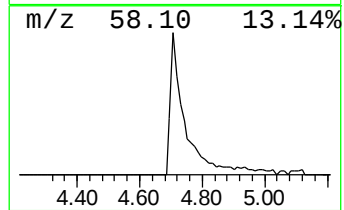
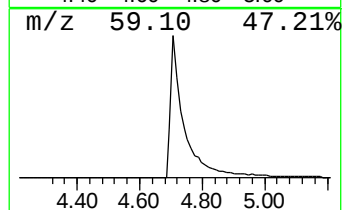
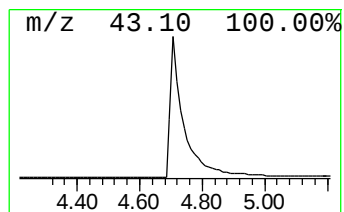
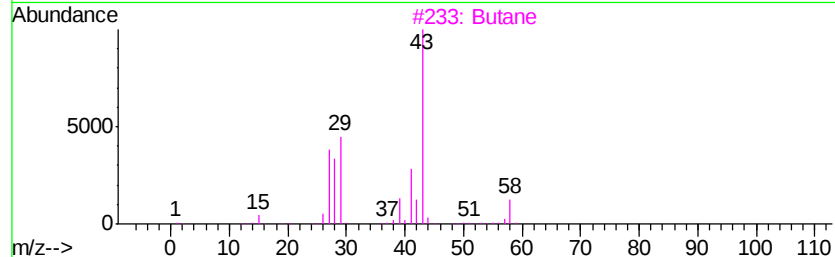
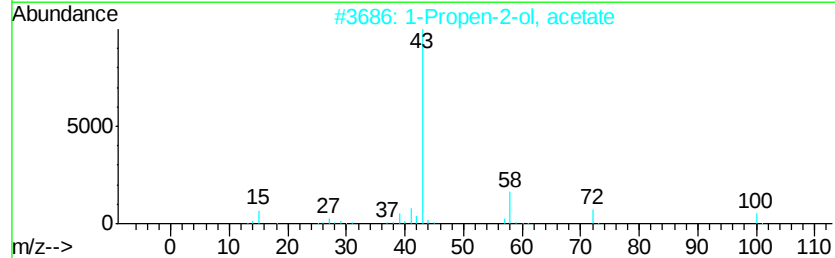
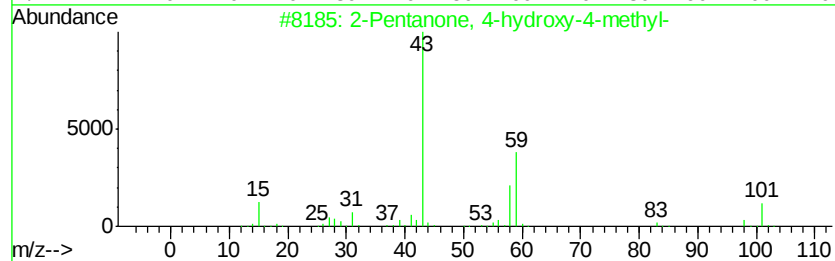
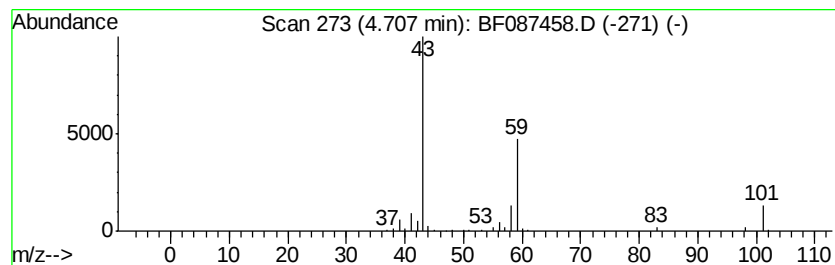
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	13.72 ng	560170	1,4-Dichlorobenzene-d4	7.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		Butane	58	C4H10	000106-97-8	9
4		Diacetamide	101	C4H7NO2	000625-77-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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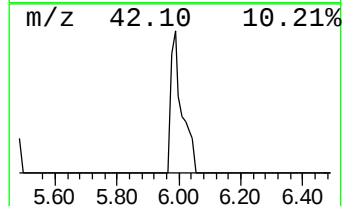
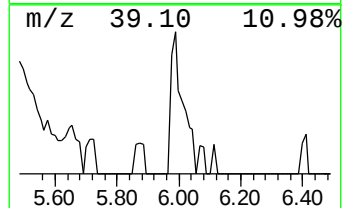
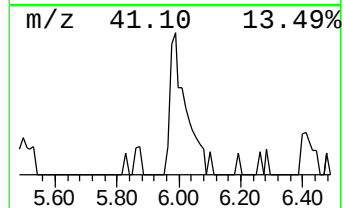
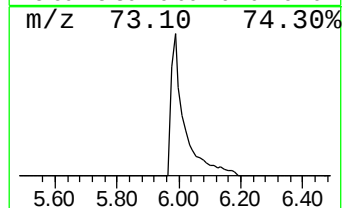
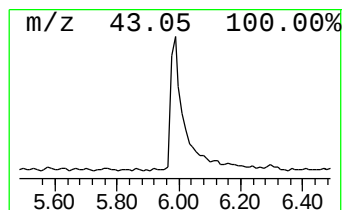
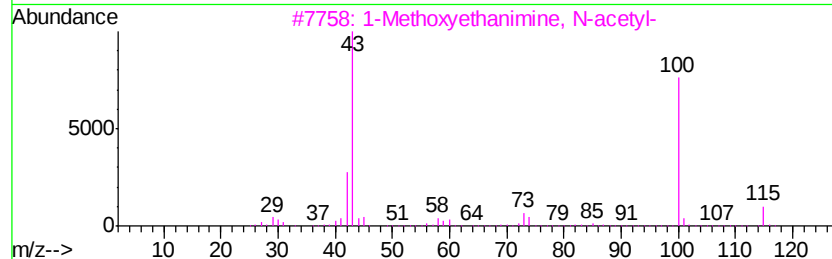
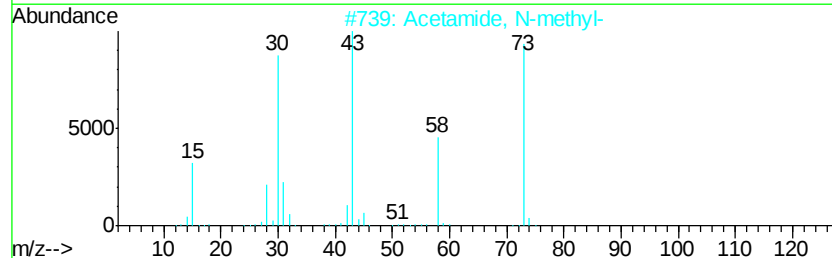
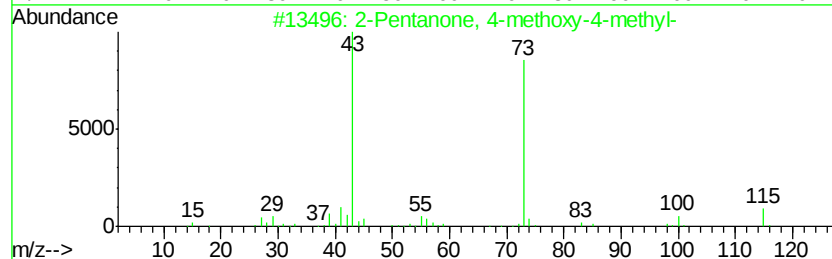
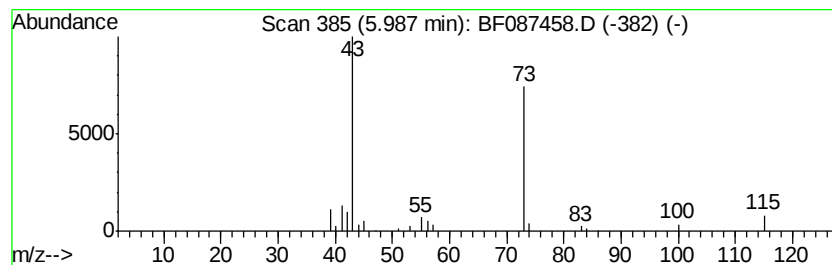
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.99	2.32 ng	94575	1,4-Dichlorobenzene-d4	7.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	58
3		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9
4		Guanidine, methyl-	73	C2H7N3	000471-29-4	9
5		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9



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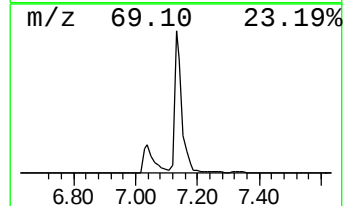
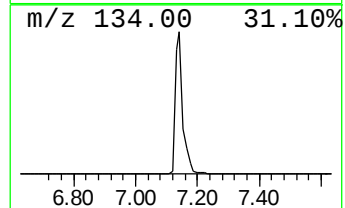
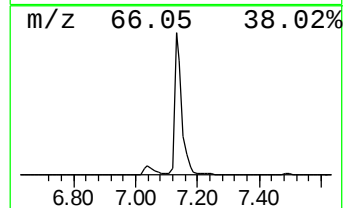
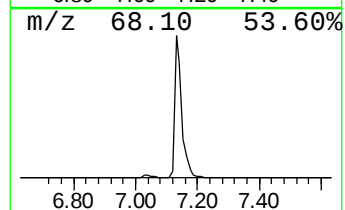
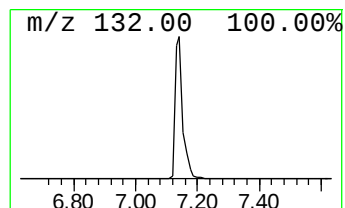
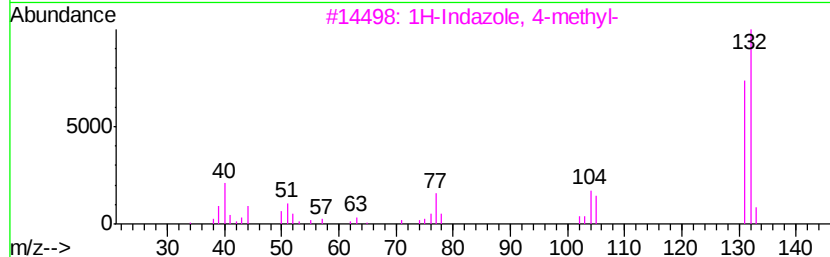
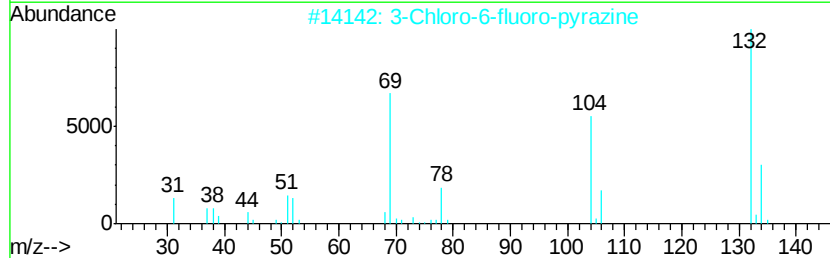
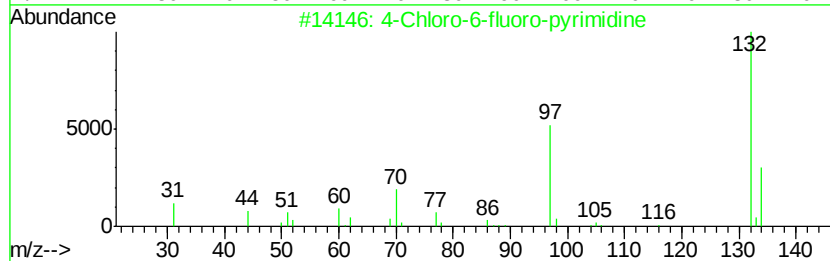
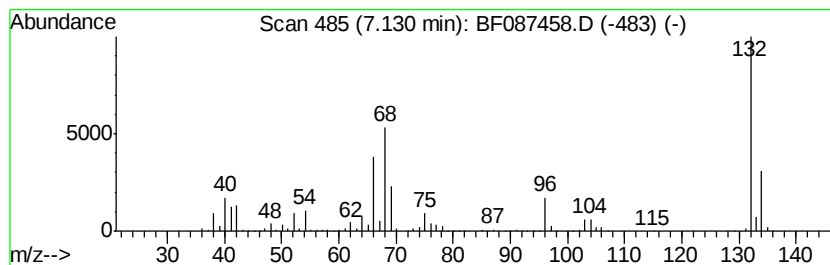
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Peak Number 4 unknown7.13 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.13	80.19 ng	3273690	1,4-Dichlorobenzene-d4	7.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Indazole, 4-methyl-	132	C8H8N2	1000316-00-9	25
4		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.71	13.7	ng	560170	1	7.48	816529	20.0
2-Pentanone, 4-me...	5.99	2.3	ng	94575	1	7.48	816529	20.0
unknown7.13	7.13	80.2	ng	3273690	1	7.48	816529	20.0