

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111414\
 Data File : BF075507.D
 Acq On : 14 Nov 2014 21:30
 Operator : TP / JJ
 Sample : PB80238BL
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB80238BL

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-BF111214.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	1.624	44	47	50	rBV	2122151	2474182	100.00%	15.393%
2	1.761	56	59	64	rVB	22742	49780	2.01%	0.310%
3	1.830	64	65	71	rVB	24542	35961	1.45%	0.224%
4	1.967	75	77	84	rBV	92153	138229	5.59%	0.860%
5	5.339	370	372	382	rBV	544027	711019	28.74%	4.424%
6	5.841	413	416	418	rBV	1377541	1407283	56.88%	8.756%
7	6.344	458	460	462	rVB	28339	26355	1.07%	0.164%
8	7.087	523	525	528	rBV	1043204	1317096	53.23%	8.194%
9	7.259	537	540	542	rBV	1527628	1391979	56.26%	8.660%
10	7.545	563	565	568	rBV	215296	275284	11.13%	1.713%
11	7.739	579	582	584	rBV	1148275	1049552	42.42%	6.530%
12	8.242	623	626	628	rVB	885531	838475	33.89%	5.217%
13	9.133	701	704	706	rVB	374500	381318	15.41%	2.372%
14	10.471	819	821	824	rBV	1203724	1495822	60.46%	9.306%
15	11.305	892	894	897	rBV	290130	399978	16.17%	2.489%
16	12.288	978	980	983	rBV	875089	922952	37.30%	5.742%
17	13.157	1054	1056	1059	rVB	420589	410719	16.60%	2.555%
18	15.157	1228	1231	1233	rBV	1611630	1746492	70.59%	10.866%
19	16.460	1342	1345	1347	rBV	384673	477534	19.30%	2.971%
20	18.220	1496	1499	1502	rBV	416610	522961	21.14%	3.254%

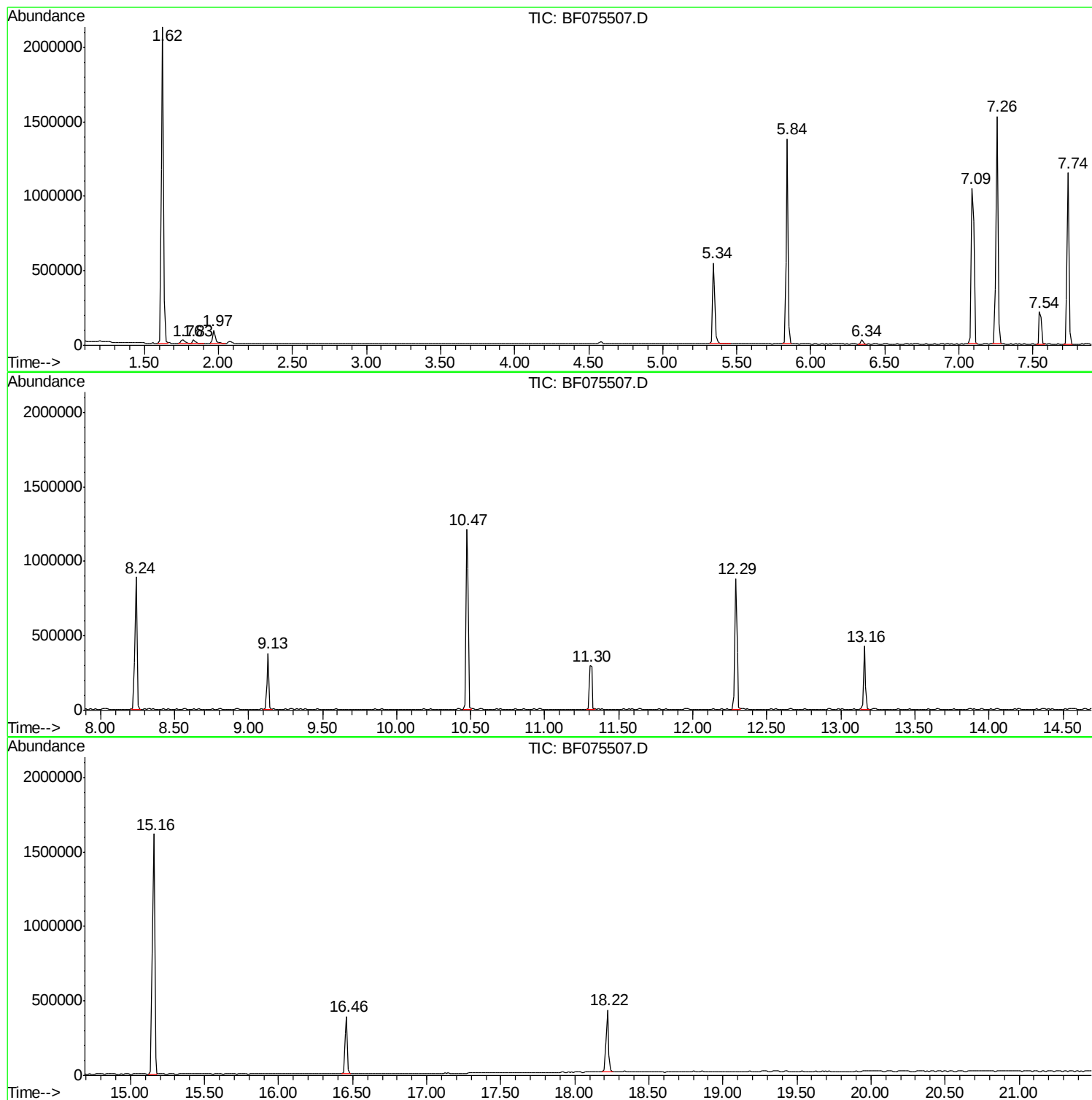
Sum of corrected areas: 16072971

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.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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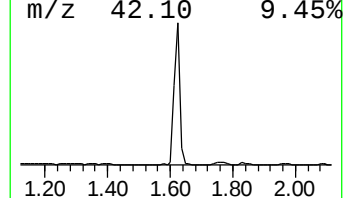
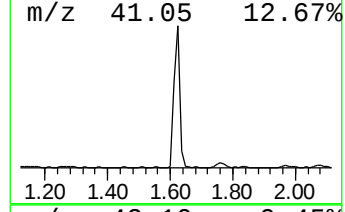
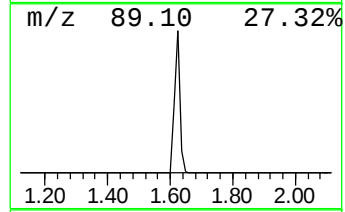
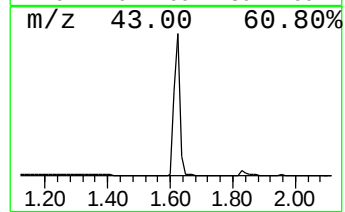
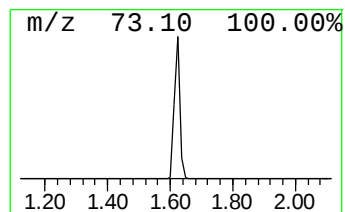
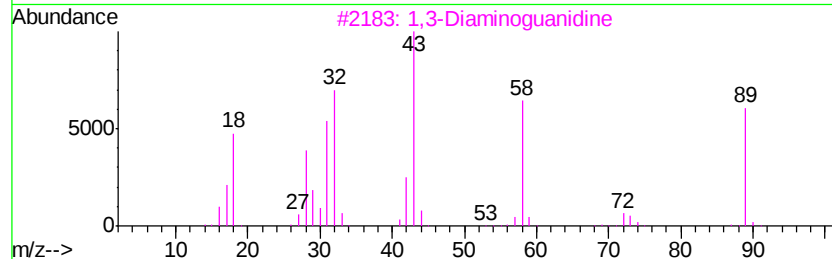
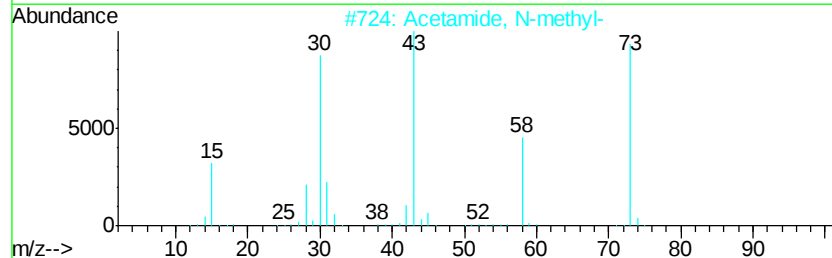
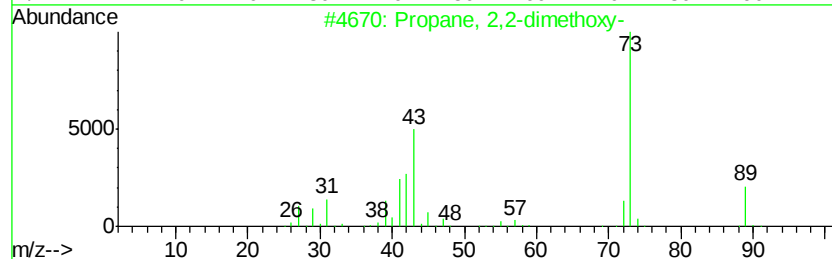
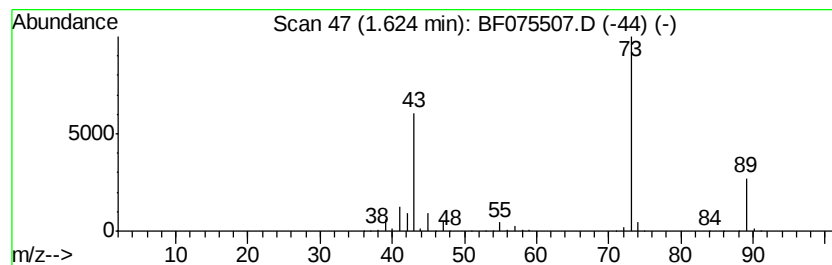
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.62	179.76 ng	2474180	1,4-Dichlorobenzene-d4	7.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	64	
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9	
3	1,3-Diaminoquanidine	89	CH7N5	004364-78-7	9	
4	Propanoic acid, 2-methyl-, pentv...	158	C9H18O2	002445-72-9	9	
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9	



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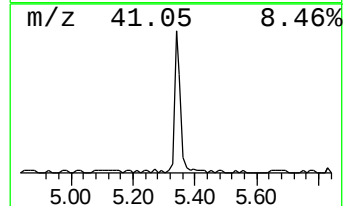
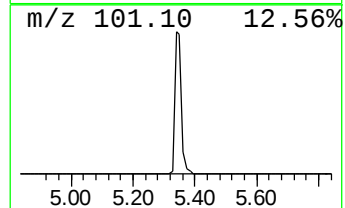
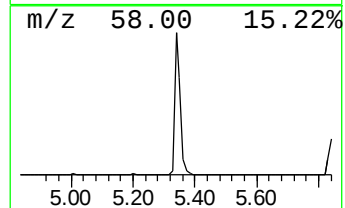
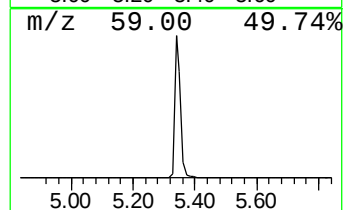
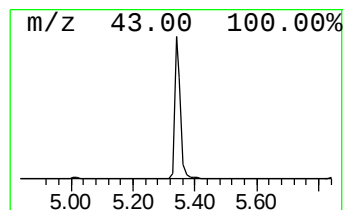
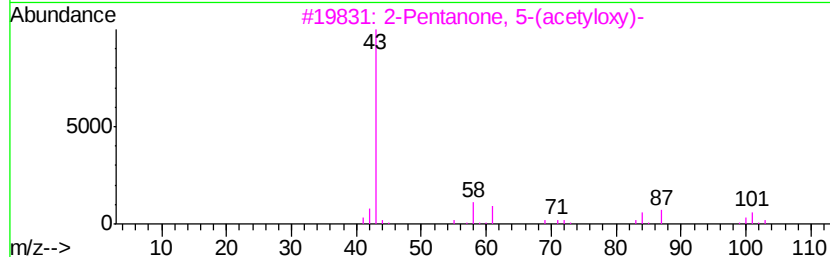
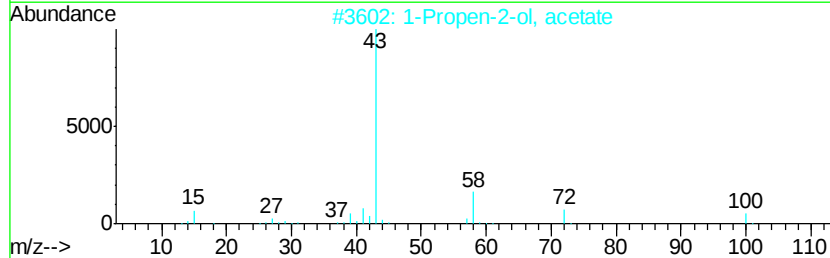
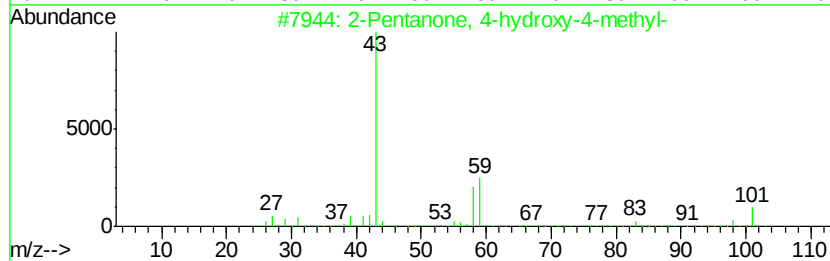
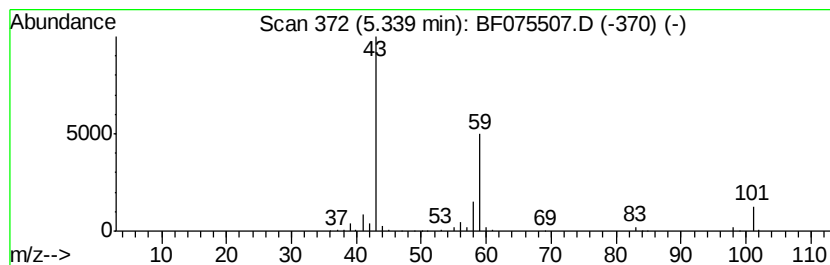
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.34	51.66 ng	711019	1,4-Dichlorobenzene-d4	7.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2-Pentanone, 5-(acetyloxy)-	144	C7H12O3	005185-97-7	9
4		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7
5		Acetone	58	C3H6O	000067-64-1	7



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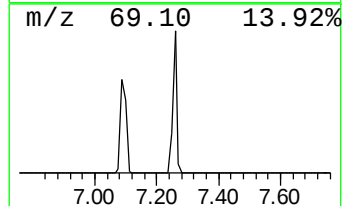
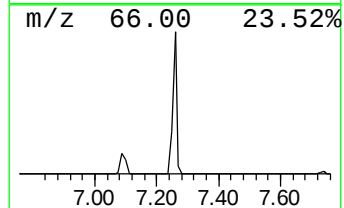
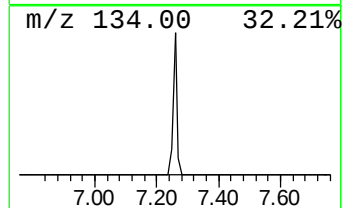
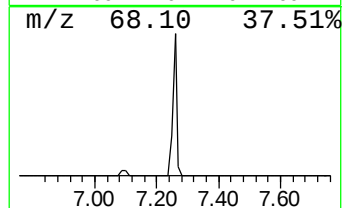
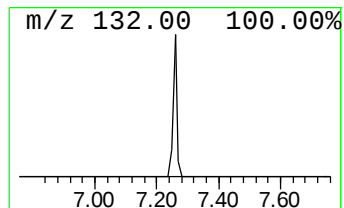
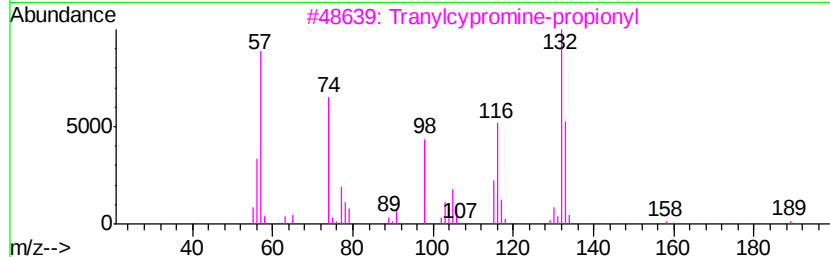
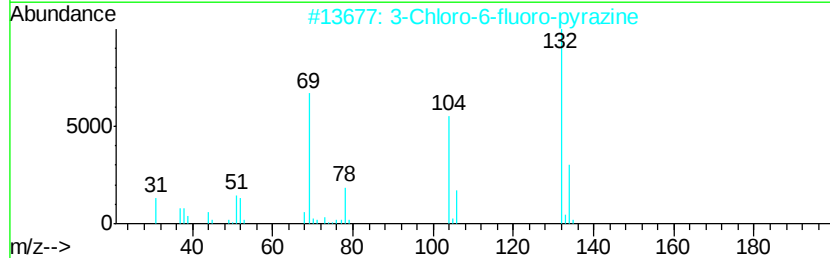
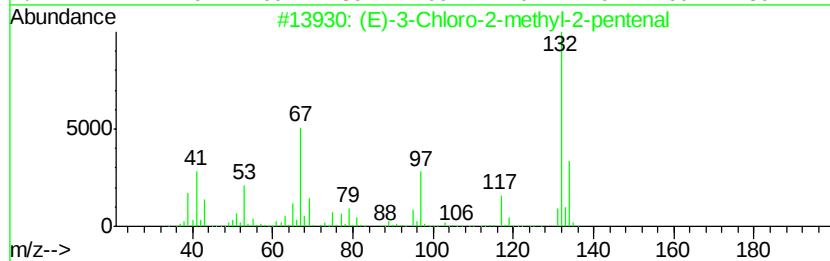
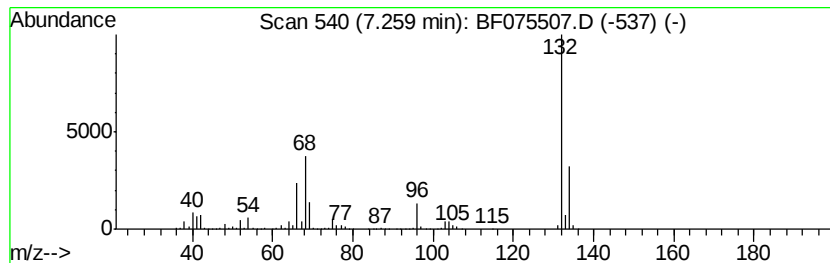
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Peak Number 6 unknown7.26 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.26	101.13 ng	1391980	1,4-Dichlorobenzene-d4	7.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35	
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35	
3	Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12	
4	5-Aminoindole	132	C8H8N2	005192-03-0	10	
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.62	179.8	ng	2474180	1	7.56	275284	20.0
2-Pentanone, 4-hy...	5.34	51.7	ng	711019	1	7.56	275284	20.0
unknown7.26	7.26	101.1	ng	1391980	1	7.56	275284	20.0