

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111516\
 Data File : BF091175.D
 Acq On : 15 Nov 2016 13:02
 Operator : UM/SJ
 Sample : H5636-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CPS073041

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-BF110316.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	1.744	3	5	60	rVB	2858512	8609833	100.00%	17.048%
2	4.761	267	269	282	rBV	373045	566203	6.58%	1.121%
3	5.219	307	309	331	rBV	2134445	2512795	29.19%	4.976%
4	6.282	400	402	410	rBV	1316843	1642575	19.08%	3.252%
5	6.407	410	413	415	rBV	3672635	4460226	51.80%	8.832%
6	6.636	431	433	444	rVB	853960	961724	11.17%	1.904%
7	6.784	444	446	449	rBV	3140301	4149962	48.20%	8.217%
8	7.207	480	483	485	rBV	3139609	3244743	37.69%	6.425%
9	7.916	543	545	548	rBV	1054012	1292746	15.01%	2.560%
10	8.339	579	582	589	rBV	202905	324209	3.77%	0.642%
11	9.002	637	640	642	rBV	5835932	5780507	67.14%	11.446%
12	9.402	673	675	677	rBV	243661	219573	2.55%	0.435%
13	9.665	696	698	701	rBV	1509363	1581301	18.37%	3.131%
14	10.465	765	768	770	rBV	3314709	4075500	47.34%	8.070%
15	11.151	826	828	830	rBV	1695159	1693660	19.67%	3.354%
16	12.739	964	967	969	rBV	5691474	6376650	74.06%	12.626%
17	13.779	1055	1058	1060	rBV	1338926	1530126	17.77%	3.030%
18	14.237	1096	1098	1103	rBV	92658	117219	1.36%	0.232%
19	15.140	1175	1177	1180	rBV	926007	1226068	14.24%	2.428%
20	16.614	1297	1306	1316	rVB4	21120	136941	1.59%	0.271%

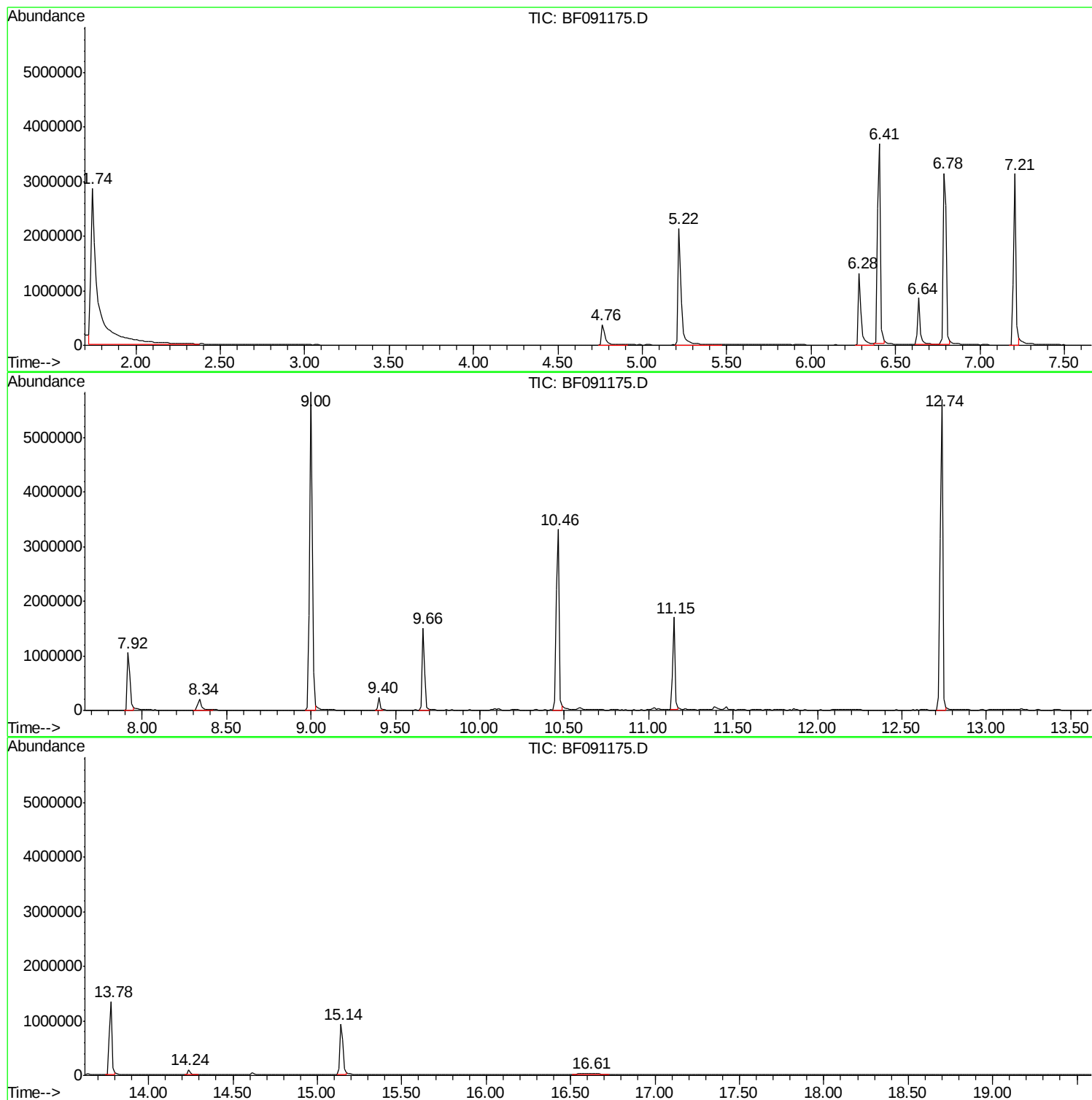
Sum of corrected areas: 50502561

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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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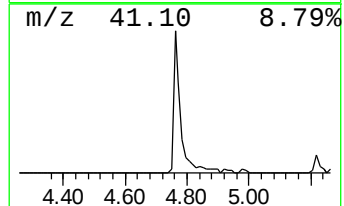
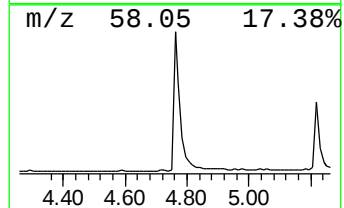
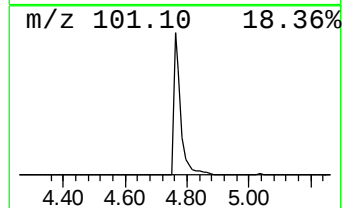
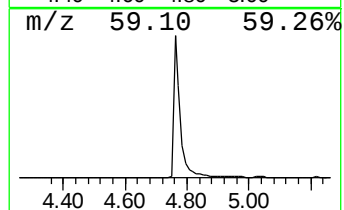
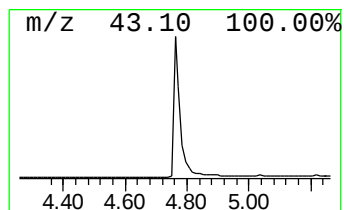
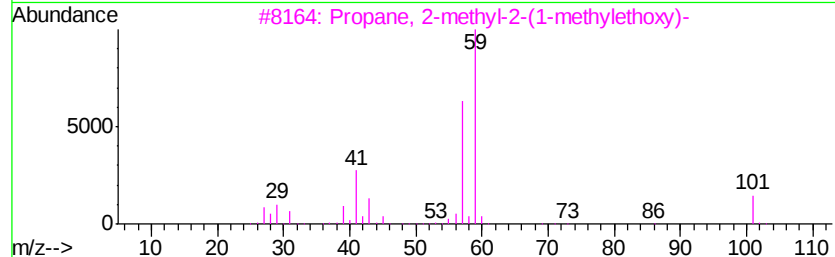
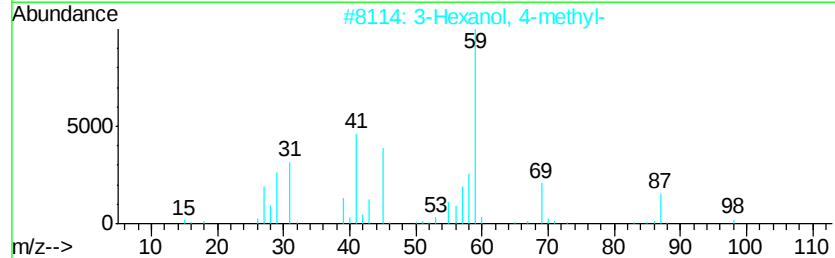
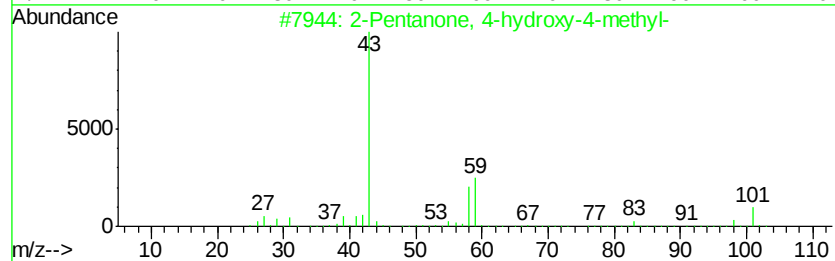
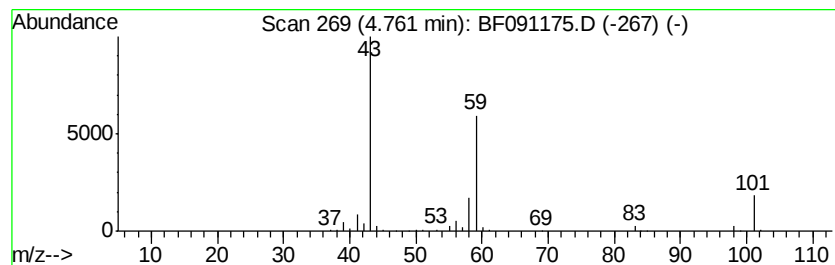
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	11.77 ng	566203	1,4-Dichlorobenzene-d4	6.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	33
4			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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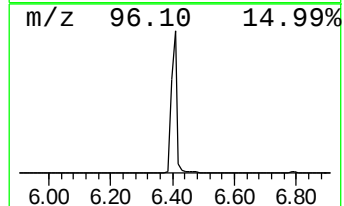
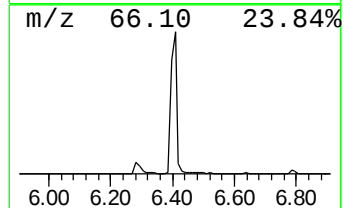
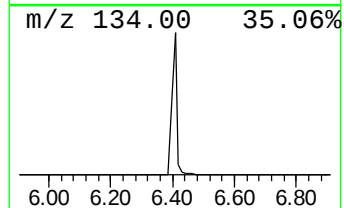
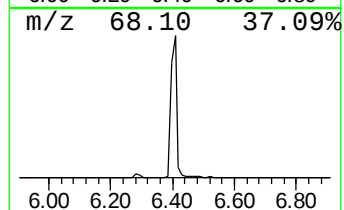
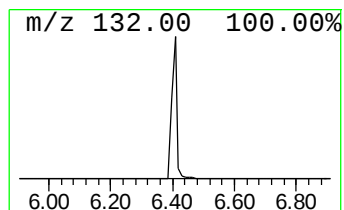
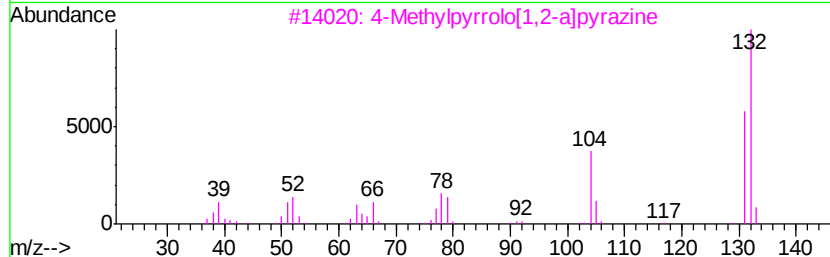
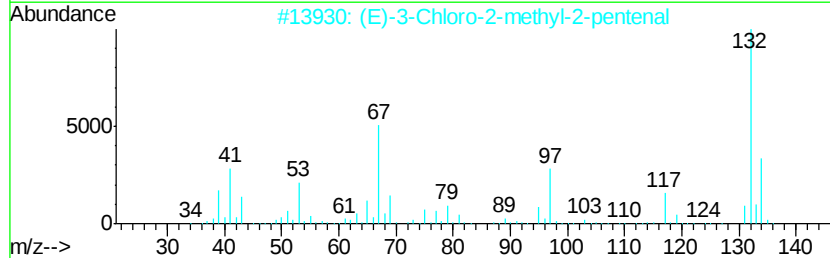
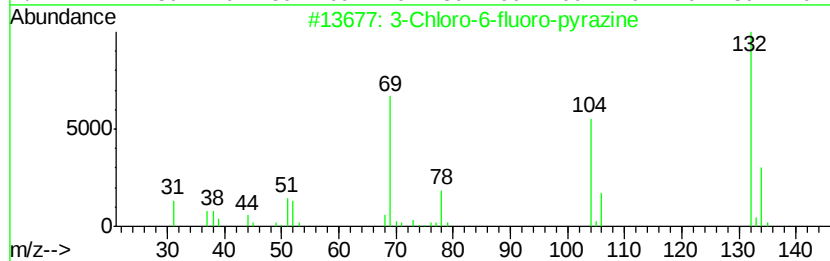
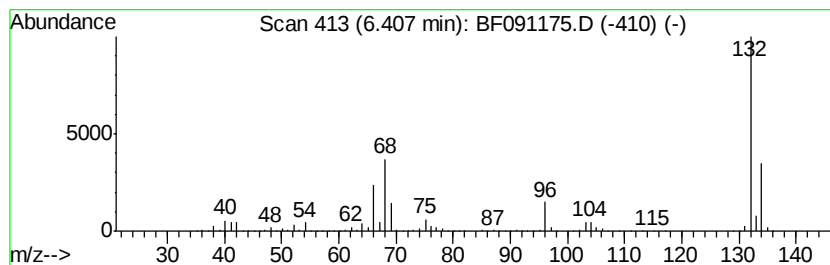
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Peak Number 3 unknown6.41 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	92.75 ng	4460230	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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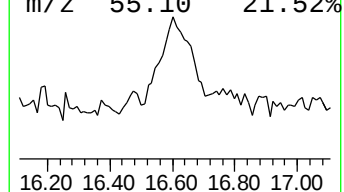
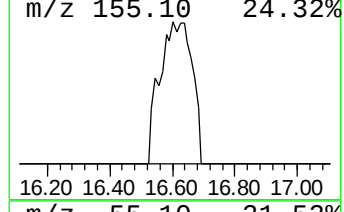
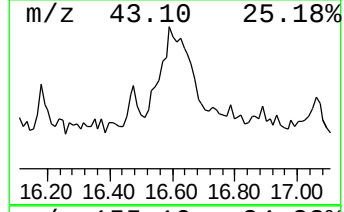
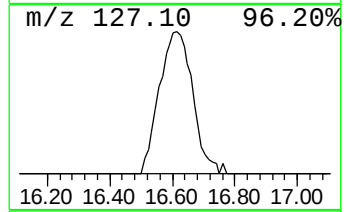
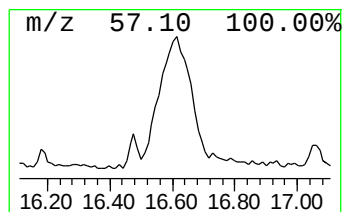
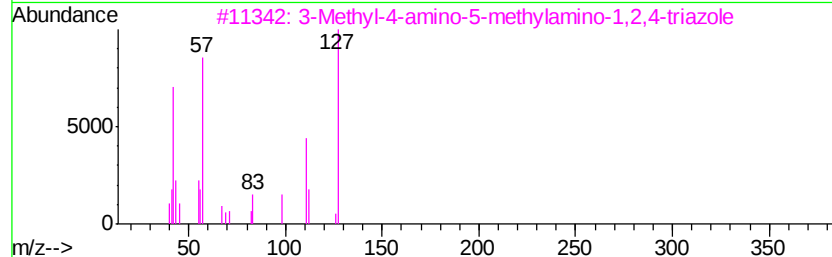
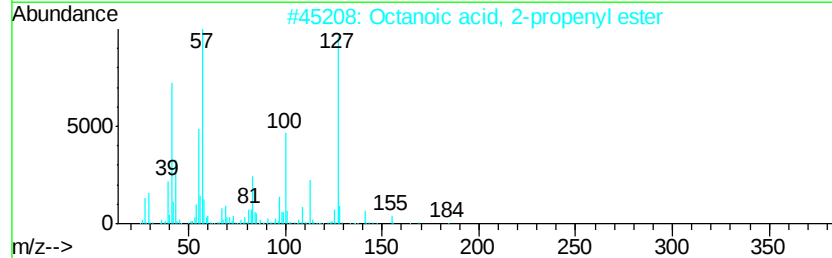
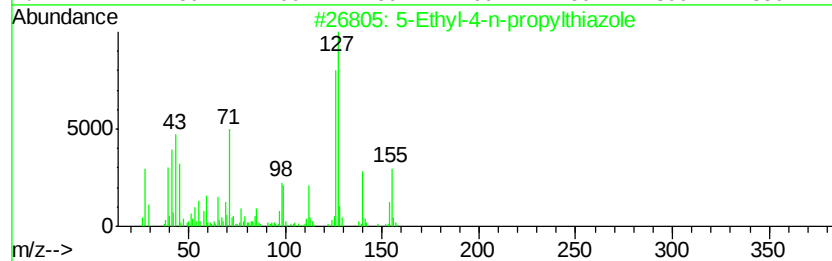
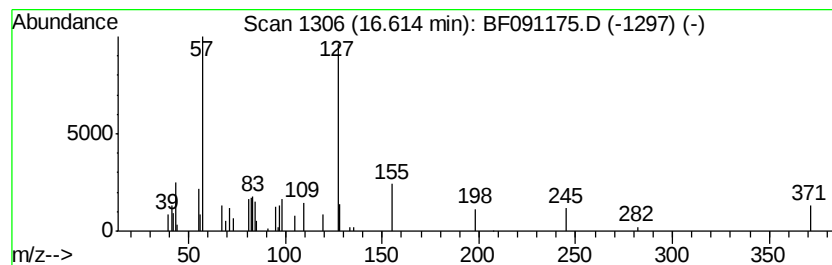
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Peak Number 5 5-Ethyl-4-n-propylthiazole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.61	2.23 ng	136941	Perylene-d12	15.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Ethyl-4-n-propylthiazole	155	C8H13NS	035508-67-9	50	
2	Octanoic acid, 2-propenyl ester	184	C11H20O2	004230-97-1	47	
3	3-Methyl-4-amino-5-methylamino-1...	127	C4H9N5	065901-89-5	43	
4	2-Cyclohexyl-3-isopropyl-pent-4-...	210	C14H26O	1000194-91-7	38	
5	2,3-Dimethyl-1,4-dioxo-spiro[4.7...	198	C12H22O2	062406-91-1	38	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.76	11.8	ng	566203	1	6.64	961724	20.0
unknown6.41	6.41	92.8	ng	4460230	1	6.64	961724	20.0
5-Ethyl-4-n-propy...	16.61	2.2	ng	136941	6	15.14	1226070	20.0