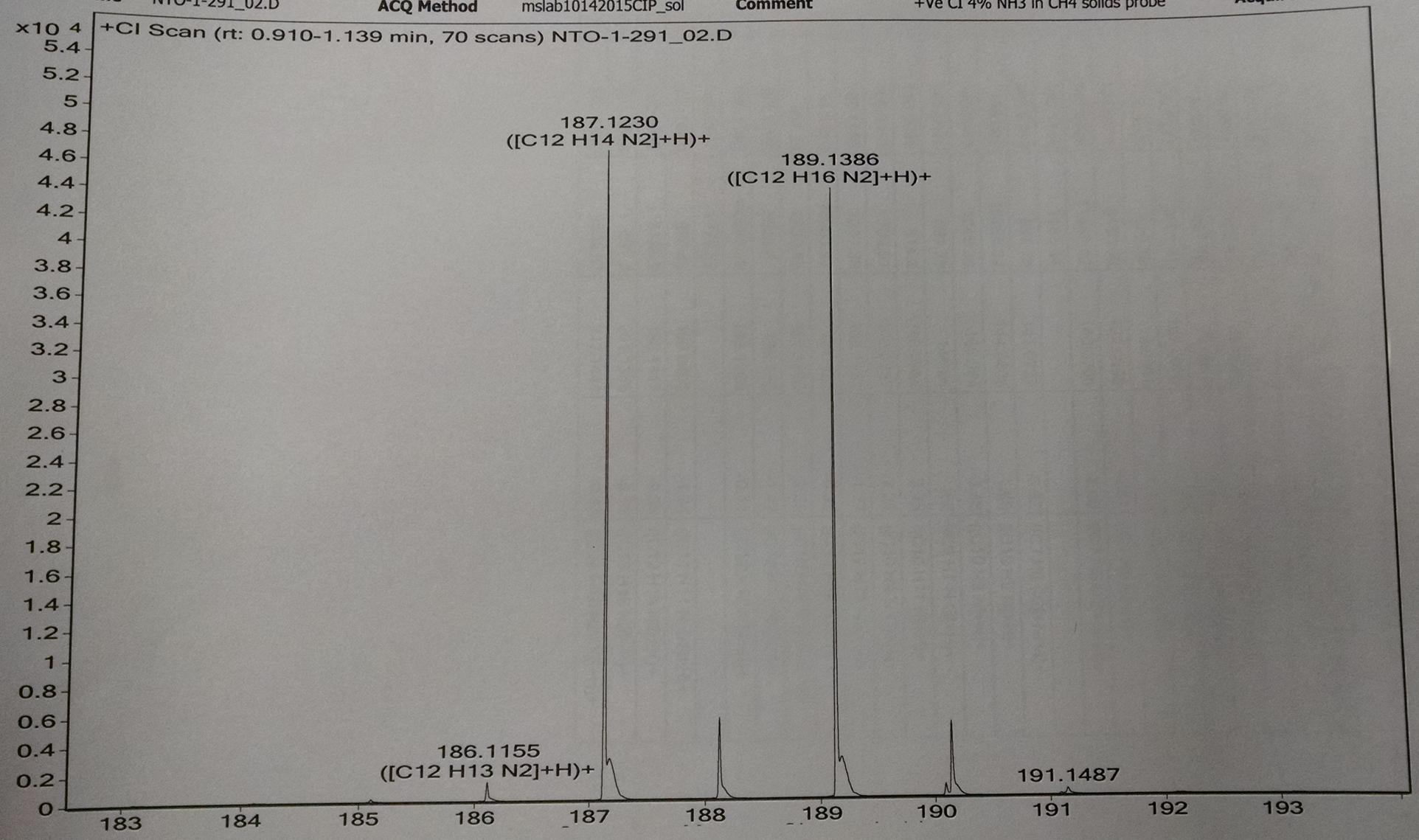
Sample Name	Dimethyltryptophan	**Position**	2	**Instrument Name**	Agilent QTOF	**User Name**	
Inj Vol	-1.79769313486232E+3	**InjPosition**		**SampleType**		**IRM Calibration Status**	
Data Filename	NTO-1-291_02.D	**ACQ Method**	mslab10142015CIP_sol	**Comment**	+Ve CI 4% NH3 in CH4 solids probe	**Acquired Time**	



MS Peaks One: + Scan (rt: 0.910-1.139 min) (NTO-1-291_02.D)

m/z	Abund	m/z (Calc)	Diff (ppm)	Formula & Ion Species
60.0809	12541.69	60.0808	-2.7	([C3 H9 N]+H)+
60.1076	1032.39			
75.0554	618.63	75.0553	-1.35	([C2 H6 N2 O]+H)+
75.0917	1997.92	75.0917	0.06	([C3 H10 N2]+H)+
105.0337	2691.31	105.0335	-1.78	([C7 H4 O]+H)+
118.0653	629.38	118.0651	-1.11	([C8 H7 N]+H)+
132.0811	2483.68	132.0808	-2.31	([C9 H9 N]+H)+
140.0709	11466.42	140.0706	-2.08	([C7 H6 O2]+NH4)+
140.1114	1183.34			
141.0743	887.75	141.0737	-3.82	([C7 H6 O2]+NH4)+
144.081	15868.32	144.0808	-1.86	([C10 H9 N]+H)+
145.0845	1649.36	145.084	-3.48	([C10 H9 N]+H)+
146.0605	691.75	146.06	-3.2	([C9 H7 N O]+H)+
146.0959	814.2	146.0964	3.75	([C10 H11 N]+H)+
160.0761	1702.51	160.0757	-2.28	([C10 H9 N O]+H)+
186.1155	1287.38	186.1151	-1.77	([C12 H13 N2]+H)+
187.123	48093.97	187.123	-0.39	([C12 H14 N2]+H)+
187.18	2830.85	187.1805	2.39	([C10 H19 N O]+NH4)+
188.1263	5558.41	188.126	-1.47	([C12 H14 N2]+H)+
189.1386	**44997.92**	**189.1386**	**-0.11**	**([C12 H16 N2]+H)+**
189.1947	2772.89			
190.0865	836.48	190.0863	-1.34	([C11 H11 N O2]+H)+
190.1419	5188.2	190.1417	-0.96	([C12 H16 N2]+H)+
201.1388	697.2	201.1386	-0.75	([C13 H16 N2]+H)+
247.1441	2035.83	247.1441	-0.13	([C14 H18 N2 O2]+H)+