

CWC Labs Analysis of Tide Laundry Pods via LC-MS-TOF (CWCLabs.com)

Analysis conducted on January 29, 2018
Analysis by Mike Adams, lab science director
and author of Food Forensics



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Published on Science.news

Instrument conditions and method:

C18 column, 5% to 95% MeOH gradient, 25 min. run time for LC

MS-TOF conditions: Positive mode, 350C gas temp, 10 L/min. drying gas

Vcap 4000V, Fragmentor 100V

Mass tune and calibration on 1/29/2018 using multi-mass tune solution for TOF

Reference masses: 121.0509, 922.0098

Sample injection volume: 0.5uL

Blank subtraction used to exclude non-sample mass list

Explanation of results

The chemical formulas shown here are software-derived "best fit" formulas based on accurate molecular mass.

The score (MFE) field indicates confidence of the Molecular Feature Extraction, which includes peak shape and isotopic spread.

Vol = Area response of chemical peak using automated software integration.

m/z = mass-to-charge ratio of the molecule; Z=2 indicates doubly charged.

RT = Retention Time

Formula (MFG)	Score	Score (MFE)	Mass	Avg Mass	Base Peak	Height	Vol	m/z	Z	Count	Ions	Polarity	RT	Start	End	Width	File	Mining Algorithm
C6 H14 O3	99.07	99.5	134.0947	134.1722	152.1285	1771675	33018458	152.1285	1	8	Positive	5.456	5.334	5.904	0.23	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C17 H31 N O3 S	98.62	100	329.2029	329.4608	330.2101	1007016	27751906	330.2101	1	3	Positive	17.226	16.802	17.503	0.337	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C18 H33 N O3 S	98.23	100	343.2187	343.4896	344.2259	933706	24788514	344.2259	1	3	Positive	18.031	17.631	18.255	0.332	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C22 H43 N O	99.06	100	337.335	337.5712	338.3422	805521	24451532	338.3422	1	11	Positive	23.336	22.997	23.721	0.217	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C32 H63 N5 O5	99.12	100	597.4828	597.861	598.49	856236	16672282	598.49	1	5	Positive	21.469	21.278	21.709	0.202	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C31 H61 N5 O5	99.35	100	583.467	583.8405	584.4742	849137	16352751	584.4742	1	5	Positive	20.783	20.604	21.046	0.209	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C34 H67 N5 O6	99.31	100	641.5091	641.9108	642.5162	800906	15949622	642.5162	1	5	Positive	21.444	21.261	21.797	0.213	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C30 H59 N5 O4	99.2	100	553.4565	553.8058	554.4636	858561	15920932	554.4636	1	4	Positive	21.495	21.306	21.737	0.197	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C29 H57 N5 O4	98.99	100	539.4408	539.7643	540.448	801979	14961347	540.448	1	3	Positive	20.803	20.615	21.151	0.212	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C33 H65 N5 O6	99.42	100	627.4933	627.8905	628.5005	816686	14232766	628.5005	1	5	Positive	20.76	20.593	20.996	0.168	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C36 H71 N5 O7	99.37	100	685.5354	685.963	686.5426	709682	13535223	686.5426	1	5	Positive	21.416	21.25	21.676	0.199	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C28 H55 N5 O3	98.32	100	509.4302	509.7474	510.4374	772841	13433137	510.4374	1	4	Positive	21.528	21.322	21.825	0.206	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C35 H69 N5 O7	99.49	100	671.5197	671.9368	672.5269	741923	13314796	672.5269	1	5	Positive	20.743	20.587	20.957	0.176	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C16 H29 N O3 S	97.43	100	315.1875	315.4286	316.1948	602322	12526922	316.1948	1	3	Positive	16.507	16.199	16.691	0.25	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C27 H53 N5 O3	98.35	100	495.4146	495.728	496.4219	637240	11164989	496.4219	1	4	Positive	20.824	20.626	21.173	0.211	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C28 H55 N5 O3	98.53	100	509.43	509.7574	510.4372	997317	11141967	510.4372	1	5	Positive	20.288	20.14	20.466	0.127	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C37 H73 N5 O8	99.4	100	715.546	715.9856	716.5533	625328	10975622	716.5533	1	5	Positive	20.725	20.571	20.957	0.176	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C26 H51 N5 O2	97.86	100	465.4037	465.6984	466.4109	985351	10885438	466.4109	1	4	Positive	20.219	20.068	20.488	0.132	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C38 H75 N5 O8	99.26	100	729.5617	730.0147	730.5691	603509	10818261	730.5691	1	5	Positive	21.388	21.223	21.676	0.185	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C6 H14 O3	98.19	100	134.0948	134.1136	152.1285	1127992	10708815	152.1285	1	5	Positive	5.239	5.169	5.329	0.102	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C25 H52 O6	99	96.6	448.3765	448.67	466.4112	654483	10003822	466.4112	1	10	Positive	21.546	21.339	21.875	0.169	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C30 H59 N5 O4	98.54	100	553.4564	553.803	554.4636	858331	10003416	554.4636	1	4	Positive	20.344	20.2	20.759	0.145	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C25 H46 N4 O2	97.23	100	434.3619	434.6238	452.3958	442783	8959911	452.3958	1	7	Positive	20.841	20.631	21.471	0.257	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C40 H79 N5 O9	98.89	100	773.5881	774.0679	774.5956	508072	8812567	774.5956	2	6	Positive	21.363	21.206	21.626	0.189	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C39 H77 N5 O9	98.9	100	759.5725	760.0371	760.5799	502880	8708336	760.5799	1	5	Positive	20.705	20.56	21.234	0.179	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C32 H63 N5 O5	99.12	100	597.4828	597.8577	598.49	715588	8532394	598.49	1	4	Positive	20.393	20.256	20.698	0.146	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C29 H57 N5 O4	98.21	100	539.4407	539.7725	540.448	649047	7980724	540.448	1	4	Positive	19.698	19.51	20.012	0.164	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C31 H61 N5 O5	99.09	100	583.4671	583.8287	584.4743	628299	7957653	584.4743	1	4	Positive	19.741	19.493	20.057	0.155	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C21 H44 O4	97.57	100	360.3248	360.5592	378.3587	597718	7890873	378.3587	1	9	Positive	20.003	19.841	20.278	0.135	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C27 H53 N5 O3	97.96	100	495.4143	495.7222	496.4215	759024	7747106	496.4215	1	4	Positive	19.644	19.526	19.847	0.125	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C18 H33 N O3 S	96.86	87	343.2189	343.4763	344.2263	545175	7599982	344.2263	1	3	Positive	18.363	18.261	18.614	0.171	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C33 H65 N5 O6	99.08	100	627.4932	627.8854	628.5004	557928	7548938	628.5004	1	4	Positive	19.785	19.565	20.057	0.153	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C31 H61 N5 O6	98.2	100	599.4624	599.8272	600.4699	489252	7409242	600.4699	1	4	Positive	19.487	19.338	19.769	0.172	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C33 H65 N5 O7	98.34	100	643.4888	643.8781	644.4963	469473	7401952	644.4963	1	4	Positive	19.492	19.344	19.979	0.188	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C42 H83 N5 O10	98.62	100	817.6143	818.1175	818.6218	386614	7322766	818.6218	2	11	Positive	21.34	21.184	21.676	0.178	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C34 H67 N5 O6	98.57	100	641.5093	641.905	642.5166	567413	7158905	642.5166	1	5	Positive	20.438	20.289	20.736	0.142	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C29 H57 N5 O5	97.94	100	555.436	555.7729	556.4434	462356	7095705	556.4434	1	4	Positive	19.48	19.333	19.825	0.186	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	
C18 H38 O3	97.16	100	302.2824	302.4652	320.3165	294648	7056239	320.3165	1	8	Positive	19.074	18.813	19.421	0.206	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature	

C35 H62 N20 O	71.29	100	778.5423	778.8581	779.5495	4996	47398	779.5495	1	2	Positive	20.544	20.46	20.637	0.099	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C60 H89 N3 O8	88.73	100	979.6649	980.2977	980.6716	4086	47206	980.6716	1	3	Positive	19.057	18.979	19.167	0.109	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C32 H67 N11 O4	73.83	98.9	669.5377	669.8309	670.5449	3560	47151	670.5449	1	2	Positive	21.814	21.681	21.958	0.147	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C16 H23 N8	81.94	96.6	327.2039	327.3902	328.2111	4880	46774	328.2111	1	2	Positive	14.054	13.944	14.221	0.155	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C29 H53 N25 O2	73.56	96.2	783.4819	783.7271	784.4887	3997	45516	784.4887	2	3	Positive	7.717	7.639	7.838	0.111	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C24 H51 N11 O3	79.27	100	541.4183	541.6667	542.4252	4790	45439	542.4252	1	2	Positive	17.479	17.371	17.586	0.117	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C28 H36 N13 O3	75.67	100	602.3073	602.5625	603.3144	5445	44732	603.3144	1	2	Positive	19.656	19.576	19.758	0.098	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C18 H29 N11 O	82.61	100	415.2564	415.4508	416.2634	5445	44316	416.2634	1	2	Positive	16.241	16.161	16.348	0.104	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C23 H48 N20 O9	74.88	100	748.39	748.6575	375.2022	5223	44114	375.2022	1	2	Positive	6.041	5.975	6.147	0.098	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C34 H62 N29 O	70.52	100	892.5688	892.8833	447.2916	4082	44070	447.2916	1	2	Positive	9.066	8.971	9.175	0.118	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C25 H14 N9 O13	75.58	100	648.0711	648.2787	649.0784	5138	43825	649.0784	1	2	Positive	9.52	9.402	9.645	0.133	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C34 H43 N22 O4	70.99	100	823.3838	823.6744	824.3908	4365	42199	824.3908	1	2	Positive	14.396	14.32	14.503	0.106	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C31 H57 O4	75.1	71.2	493.4253	493.6696	494.432	3598	41536	494.432	1	2	Positive	21.621	21.488	21.814	0.185	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C24 H45 N5 O2	79.86	85.5	435.3573	435.5981	436.3648	5843	41530	436.3648	1	2	Positive	20.615	20.537	20.731	0.096	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C25 H55 N25 O	72.06	100	721.5027	721.7193	722.5098	4275	41004	722.5098	1	2	Positive	19.891	19.808	19.979	0.093	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C19 H41 N25	77.08	100	619.3969	619.6533	620.4038	5467	39088	620.4038	1	2	Positive	19.699	19.626	19.802	0.105	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C36 H70 N13 O3	70.41	100	732.5729	732.9031	367.2936	3309	38485	367.2936	1	2	Positive	20.715	20.62	20.88	0.152	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C35 H44 N17 O2	71.16	100	734.3862	734.66	735.3931	3636	38392	735.3931	1	2	Positive	19.825	19.714	19.935	0.129	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C20 H43 N25	77.74	100	633.4129	633.6755	634.4198	4749	37724	634.4198	1	2	Positive	20.342	20.261	20.444	0.1	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C13 H27 N8 O3	86.18	100	343.2206	343.3789	344.2278	6627	37471	344.2278	1	2	Positive	4.887	4.826	4.986	0.089	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C18 H28 N3 O	72.48	100	802.2238	802.4465	303.2312	3730	36980	303.2312	1	2	Positive	16.558	16.459	16.702	0.148	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C18 H23 N15 O	81.07	93.8	465.2205	465.4509	466.2275	4206	36253	466.2275	1	2	Positive	9.626	9.545	9.75	0.125	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C17 H35 N8 O5	81.81	100	431.2725	431.4515	432.2795	5904	35527	432.2795	1	2	Positive	5.911	5.848	6.009	0.09	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C18 H37 N O	77.94	99.9	283.2872	283.4973	284.2945	4358	34824	284.2945	1	2	Positive	21.297	21.217	21.416	0.119	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C20 H28 O2	81.95	100	300.2083	300.4011	301.2158	4571	34493	301.2158	1	2	Positive	17.751	17.675	17.863	0.114	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C25 H32 N22 O3	75.1	94.3	688.3031	688.588	689.31	3488	34246	689.31	1	2	Positive	17.124	17.006	17.211	0.122	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C26 H55 N11 O4	78.95	100	585.4444	585.6828	586.4515	3896	33544	586.4515	1	2	Positive	17.543	17.459	17.653	0.111	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C25 H53 N25 O3	71.74	100	751.4758	751.7595	752.4825	3569	33078	752.4825	1	2	Positive	19.838	19.753	19.935	0.106	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C20 H27 N18 O2	79.26	80	551.2568	551.4996	552.2639	4019	32646	552.2639	1	2	Positive	10.751	10.678	10.861	0.112	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C18 H33 N15 O	84.06	100	475.2989	475.4997	476.3061	4831	32165	476.3061	1	2	Positive	6.078	6.014	6.174	0.092	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C42 H86 N3 O8 S3	85.15	100	856.5579	857.1519	429.2865	3758	32087	429.2865	1	3	Positive	19.896	19.825	19.99	0.091	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C15 H31 N8 O4	83.13	100	387.2465	387.4341	388.2536	5324	32075	388.2536	1	2	Positive	5.723	5.66	5.815	0.087	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C23 H47 N22 O2	77.12	100	663.4247	663.7117	664.4318	3453	31624	664.4318	1	2	Positive	19.742	19.659	19.847	0.105	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C33 H65 N18	70.61	100	713.5645	713.8757	714.5717	2724	31390	714.5717	1	2	Positive	21.836	21.709	21.969	0.153	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C31 H57 N25 O3	72.48	100	827.5078	827.7828	828.5147	3312	31035	828.5147	1	2	Positive	7.892	7.816	8.004	0.109	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C36 H64 N20 O2	70.35	99.3	808.552	808.8902	809.5591	3367	29919	809.5591	1	2	Positive	19.928	19.858	20.012	0.089	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C25 H55 N28 O3	73.16	100	795.5012	795.7962	796.5082	3633	29214	796.5082	1	2	Positive	19.877	19.802	19.968	0.095	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C34 H50 N13 O2	73.68	100	672.4217	672.7113	673.4289	3069	27792	673.4289	1	2	Positive	17.427	17.343	17.515	0.102	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C38 H53 N13 O	70.85	100	707.4492	707.7339	708.4561	3314	27553	708.4561	1	2	Positive	19.783	19.703	19.885	0.106	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C22 H39 N12 O3	72.13	100	519.3275	519.5447	520.3322	4034	26652	520.3322	1	2	Positive	6.234	6.169	6.324	0.092	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C24 H48 N16 O4	78.03	100	624.4055	624.6498	313.2099	3681	26269	313.2099	1	2	Positive	6.516	6.451	6.605	0.094	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C24 H33 N18 O4	74.11	100	637.2926	637.5624	638.2994	3298	26005	638.2994	1	2	Positive	11.757	11.679	11.85	0.103	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C37 H48 N17 O3	70.65	94.7	778.4124	778.7235	779.4195	3420	25887	779.4195	1	2	Positive	19.88	19.802	19.946	0.083	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C39 H53 N10 O	71.85	100	677.4403	677.7463	678.4476	3102	24184	678.4476	1	2	Positive	20.393	20.322	20.482	0.096	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C35 H60 N20 O3	71.38	100	808.516	808.7952	405.2653	3109	24021	405.2653	1	2	Positive	6.535	6.462	6.628	0.1	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C29 H53 N26	74.6	100	765.495	765.7905	766.5025	2585	21573	766.5025	1	2	Positive	20.484	20.399	20.576	0.111	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C27 H44 N6 O2	73.78	100	688.5459	688.8567	345.28	2951	21558	345.28	1	2	Positive	19.837	19.758	19.913	0.096	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C37 H67 N12 O4	70.47	100	743.5408	743.8534	744.5478	2429	20002	744.5478	1	2	Positive	20.098	20.029	20.189	0.101	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C35 H68 N13 O2	72.44	96.7	702.5627	702.8469	352.2885	2800	18936	352.2885	1	2	Positive	20.484	20.41	20.56	0.092	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C27 H44 N6 O2	80.73	83	484.3525	484.5993	243.1836	3786	17819	243.1836	1	2	Positive	4.706	4.666	4.776	0.07	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature
C29 H55 N29	72.64	94.1	809.52	809.8183	810.5276	2564	17166	810.5276	1	2	Positive	20.511	20.444	20.576	0.086	Tide-Laundry-Pods-0-5ul.d	Find by Molecular Feature