

AAA and AAB Triacylglycerols by Name

Abbrev.	ECN	Mass		Mass		[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
		Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺					
LaLaLa	36	638.55	639.56	639	656.58	660.53	645.56		439.38	
LaLaM	38	666.58	667.59	667	684.61	688.56	673.60	439.38	467.41	
LaLaP	40	694.61	695.62	695	712.65	716.59	701.63	439.38	495.44	
LaLaPo	38	692.60	693.60	693	710.63	714.58	699.61	439.38	493.43	
LaLaS	42	722.64	723.65	723	740.68	744.62	729.66	439.38	523.47	
LaLaO	40	720.63	721.63	721	738.66	742.61	727.64	439.38	521.46	
LaLaL	38	718.61	719.62	719	736.65	740.59	725.63	439.38	519.44	
LaLaLn	36	716.60	717.60	717	734.63	738.58	723.61	439.38	517.43	
LaLaA	44	750.67	751.68	751	768.71	772.66	757.69	439.38	551.50	
LaLaG	42	748.66	749.67	749	766.69	770.64	755.67	439.38	549.49	
LaLaB	46	778.71	779.71	779	796.74	800.69	785.72	439.38	579.54	
LaLaE	44	776.69	777.70	777	794.72	798.67	783.71	439.38	577.52	
LaLaLg	48	806.74	807.74	807	824.77	828.72	813.75	439.38	607.57	
LaLaN	46	804.72	805.73	805	822.76	826.70	811.74	439.38	605.55	
LaLaCe	50	834.77	835.78	835	852.80	856.75	841.78	439.38	635.60	
LaLaXi	48	832.75	833.76	833	850.79	854.73	839.77	439.38	633.58	
LaLaMo	52	862.80	863.81	863	880.83	884.78	869.81	439.38	663.63	
LaLa28:1	50	860.78	861.79	861	878.82	882.77	867.80	439.38	661.61	
LaLa30	54	890.83	891.84	891	908.86	912.81	897.85	439.38	691.66	
LaLa30:1	52	888.81	889.82	889	906.85	910.80	895.83	439.38	689.64	
MMM	42	722.64	723.65	723	740.68	744.62	729.66		495.44	
MMLa	40	694.61	695.62	695	712.65	716.59	701.63	495.44	467.41	
MMP	44	750.67	751.68	751	768.71	772.66	757.69	495.44	523.47	
MMPo	42	748.66	749.67	749	766.69	770.64	755.67	495.44	521.46	
MMS	46	778.71	779.71	779	796.74	800.69	785.72	495.44	551.50	
MMO	44	776.69	777.70	777	794.72	798.67	783.71	495.44	549.49	
MML	42	774.67	775.68	775	792.71	796.66	781.69	495.44	547.47	
MMLn	40	772.66	773.67	773	790.69	794.64	779.67	495.44	545.46	
MMA	48	806.74	807.74	807	824.77	828.72	813.75	495.44	579.54	
MMG	46	804.72	805.73	805	822.76	826.70	811.74	495.44	577.52	
MMB	50	834.77	835.78	835	852.80	856.75	841.78	495.44	607.57	
MME	48	832.75	833.76	833	850.79	854.73	839.77	495.44	605.55	
MMLg	52	862.80	863.81	863	880.83	884.78	869.81	495.44	635.60	
MMN	50	860.78	861.79	861	878.82	882.77	867.80	495.44	633.58	
MMCe	54	890.83	891.84	891	908.86	912.81	897.85	495.44	663.63	
MMXi	52	888.81	889.82	889	906.85	910.80	895.83	495.44	661.61	
MMMo	56	918.86	919.87	919	936.90	940.84	925.88	495.44	691.66	
MM28:1	54	916.85	917.85	917	934.88	938.83	923.86	495.44	689.64	
MM30	58	946.89	947.90	947	964.93	968.87	953.91	495.44	719.69	
MM30:1	56	944.88	945.89	945	962.91	966.86	951.89	495.44	717.68	
PPP	48	806.74	807.74	807	824.77	828.72	813.75		551.50	
PPLa	44	750.67	751.68	751	768.71	772.66	757.69	551.50	495.44	
PPM	46	778.71	779.71	779	796.74	800.69	785.72	551.50	523.47	
PPPo	46	804.72	805.73	805	822.76	826.70	811.74	551.50	549.49	
PPS	50	834.77	835.78	835	852.80	856.75	841.78	551.50	579.54	
PPO	48	832.75	833.76	833	850.79	854.73	839.77	551.50	577.52	
PPL	46	830.74	831.74	831	848.77	852.72	837.75	551.50	575.50	
PPLn	44	828.72	829.73	829	846.76	850.70	835.74	551.50	573.49	
PPA	52	862.80	863.81	863	880.83	884.78	869.81	551.50	607.57	
PPG	50	860.78	861.79	861	878.82	882.77	867.80	551.50	605.55	
PPB	54	890.83	891.84	891	908.86	912.81	897.85	551.50	635.60	

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
PPE	52	888.81	889.82	889	906.85	910.80	895.83	551.50	633.58	
PPLg	56	918.86	919.87	919	936.90	940.84	925.88	551.50	663.63	
PPN	54	916.85	917.85	917	934.88	938.83	923.86	551.50	661.61	
PPCe	58	946.89	947.90	947	964.93	968.87	953.91	551.50	691.66	
PPXi	56	944.88	945.89	945	962.91	966.86	951.89	551.50	689.64	
PPMo	60	974.92	975.93	975	992.96	996.91	981.94	551.50	719.69	
PP28:1	58	972.91	973.92	973	990.94	994.89	979.92	551.50	717.68	
PP30	62	1002.96	1003.96	1003	1020.99	1024.94	1009.97	551.50	747.72	
PP30:1	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	551.50	745.71	
PoPoPo	42	800.69	801.70	801	818.72	822.67	807.71		547.47	
PoPoLa	40	746.64	747.65	747	764.68	768.62	753.66	547.47	493.43	
PoPoM	42	774.67	775.68	775	792.71	796.66	781.69	547.47	521.46	
PoPoP	44	802.71	803.71	803	820.74	824.69	809.72	547.47	549.49	
PoPoS	46	830.74	831.74	831	848.77	852.72	837.75	547.47	577.52	
PoPoO	44	828.72	829.73	829	846.76	850.70	835.74	547.47	575.50	
PoPoL	42	826.71	827.71	827	844.74	848.69	833.72	547.47	573.49	
PoPoLn	40	824.69	825.70	825	842.72	846.67	831.71	547.47	571.47	
PoPoA	48	858.77	859.78	859	876.80	880.75	865.78	547.47	605.55	
PoPoG	46	856.75	857.76	857	874.79	878.73	863.77	547.47	603.54	
PoPoB	50	886.80	887.81	887	904.83	908.78	893.81	547.47	633.58	
PoPoE	48	884.78	885.79	885	902.82	906.77	891.80	547.47	631.57	
PoPoLg	52	914.83	915.84	915	932.86	936.81	921.85	547.47	661.61	
PoPoN	50	912.81	913.82	913	930.85	934.80	919.83	547.47	659.60	
PoPoCe	54	942.86	943.87	943	960.90	964.84	949.88	547.47	689.64	
PoPoXi	52	940.85	941.85	941	958.88	962.83	947.86	547.47	687.63	
PoPoMo	56	970.89	971.90	971	988.93	992.87	977.91	547.47	717.68	
PoPo28:1	54	968.88	969.89	969	986.91	990.86	975.89	547.47	715.66	
PoPo30	58	998.92	999.93	999	1016.96	1020.91	1005.94	547.47	745.71	
PoPo30:1	56	996.91	997.92	997	1014.94	1018.89	1003.92	547.47	743.69	
SSS	54	890.83	891.84	891	908.86	912.81	897.85		607.57	
SSLa	48	806.74	807.74	807	824.77	828.72	813.75	607.57	523.47	
SSM	50	834.77	835.78	835	852.80	856.75	841.78	607.57	551.50	
SSP	52	862.80	863.81	863	880.83	884.78	869.81	607.57	579.54	
SSPo	50	860.78	861.79	861	878.82	882.77	867.80	607.57	577.52	
SSO	52	888.81	889.82	889	906.85	910.80	895.83	607.57	605.55	
SSL	50	886.80	887.81	887	904.83	908.78	893.81	607.57	603.54	
SSLn	48	884.78	885.79	885	902.82	906.77	891.80	607.57	601.52	
SSA	56	918.86	919.87	919	936.90	940.84	925.88	607.57	635.60	
SSG	54	916.85	917.85	917	934.88	938.83	923.86	607.57	633.58	
SSB	58	946.89	947.90	947	964.93	968.87	953.91	607.57	663.63	
SSE	56	944.88	945.89	945	962.91	966.86	951.89	607.57	661.61	
SSLg	60	974.92	975.93	975	992.96	996.91	981.94	607.57	691.66	
SSN	58	972.91	973.92	973	990.94	994.89	979.92	607.57	689.64	
SSCe	62	1002.96	1003.96	1003	1020.99	1024.94	1009.97	607.57	719.69	
SSXi	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	607.57	717.68	
SSMo	64	1030.99	1031.99	1031	1049.02	1052.97	1038.00	607.57	747.72	
SS28:1	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	607.57	745.71	
SS30	66	1059.02	1060.03	1059	1077.05	1081.00	1066.03	607.57	775.75	
SS30:1	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	607.57	773.74	
OOO	48	884.78	885.79	885	902.82	906.77	891.80		603.54	
OOLa	44	802.71	803.71	803	820.74	824.69	809.72	603.54	521.46	
OOM	46	830.74	831.74	831	848.77	852.72	837.75	603.54	549.49	
OOP	48	858.77	859.78	859	876.80	880.75	865.78	603.54	577.52	
OOPo	46	856.75	857.76	857	874.79	878.73	863.77	603.54	575.50	
OOS	50	886.80	887.81	887	904.83	908.78	893.81	603.54	605.55	

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
OOL	46	882.77	883.78	883	900.80	904.75	889.78	603.54	601.52	
OOLn	44	880.75	881.76	881	898.79	902.73	887.77	603.54	599.50	
OOA	52	914.83	915.84	915	932.86	936.81	921.85	603.54	633.58	
OOG	50	912.81	913.82	913	930.85	934.80	919.83	603.54	631.57	
OOB	54	942.86	943.87	943	960.90	964.84	949.88	603.54	661.61	
OOE	52	940.85	941.85	941	958.88	962.83	947.86	603.54	659.60	
OOLg	56	970.89	971.90	971	988.93	992.87	977.91	603.54	689.64	
OON	54	968.88	969.89	969	986.91	990.86	975.89	603.54	687.63	
OOCe	58	998.92	999.93	999	1016.96	1020.91	1005.94	603.54	717.68	
OOXi	56	996.91	997.92	997	1014.94	1018.89	1003.92	603.54	715.66	
OOMo	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	603.54	745.71	
OO28:1	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	603.54	743.69	
OO30	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	603.54	773.74	
OO30:1	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	603.54	771.72	
LLL	42	878.74	879.74	879	896.77	900.72	885.75		599.50	
LLLa	40	798.67	799.68	799	816.71	820.66	805.69	599.50	519.44	
LLM	42	826.71	827.71	827	844.74	848.69	833.72	599.50	547.47	
LLP	44	854.74	855.74	855	872.77	876.72	861.75	599.50	575.50	
LLPo	42	852.72	853.73	853	870.76	874.70	859.74	599.50	573.49	
LLS	46	882.77	883.78	883	900.80	904.75	889.78	599.50	603.54	
LLO	44	880.75	881.76	881	898.79	902.73	887.77	599.50	601.52	
LLLn	40	876.72	877.73	877	894.76	898.70	883.74	599.50	597.49	
LLA	48	910.80	911.81	911	928.83	932.78	917.81	599.50	631.57	
LLG	46	908.78	909.79	909	926.82	930.77	915.80	599.50	629.55	
LLB	50	938.83	939.84	939	956.86	960.81	945.85	599.50	659.60	
LLE	48	936.81	937.82	937	954.85	958.80	943.83	599.50	657.58	
LLLg	52	966.86	967.87	967	984.90	988.84	973.88	599.50	687.63	
LLN	50	964.85	965.85	965	982.88	986.83	971.86	599.50	685.61	
LLCe	54	994.89	995.90	995	1012.93	1016.87	1001.91	599.50	715.66	
LLXi	52	992.88	993.89	993	1010.91	1014.86	999.89	599.50	713.64	
LLMo	56	1022.92	1023.93	1023	1040.96	1044.91	1029.94	599.50	743.69	
LL28:1	54	1020.91	1021.92	1021	1038.94	1042.89	1027.92	599.50	741.68	
LL30	58	1050.96	1051.96	1051	1068.99	1072.94	1057.97	599.50	771.72	
LL30:1	56	1048.94	1049.95	1049	1066.97	1070.92	1055.96	599.50	769.71	
LnLnLn	36	872.69	873.70	873	890.72	894.67	879.71		595.47	
LnLnLa	36	794.64	795.65	795	812.68	816.62	801.66	595.47	517.43	
LnLnM	38	822.67	823.68	823	840.71	844.66	829.69	595.47	545.46	
LnLnP	40	850.71	851.71	851	868.74	872.69	857.72	595.47	573.49	
LnLnPo	38	848.69	849.70	849	866.72	870.67	855.71	595.47	571.47	
LnLnS	42	878.74	879.74	879	896.77	900.72	885.75	595.47	601.52	
LnLnO	40	876.72	877.73	877	894.76	898.70	883.74	595.47	599.50	
LnLnL	38	874.71	875.71	875	892.74	896.69	881.72	595.47	597.49	
LnLnA	44	906.77	907.78	907	924.80	928.75	913.78	595.47	629.55	
LnLnG	42	904.75	905.76	905	922.79	926.73	911.77	595.47	627.54	
LnLnB	46	934.80	935.81	935	952.83	956.78	941.81	595.47	657.58	
LnLnE	44	932.78	933.79	933	950.82	954.77	939.80	595.47	655.57	
LnLnLg	48	962.83	963.84	963	980.86	984.81	969.85	595.47	685.61	
LnLnN	46	960.81	961.82	961	978.85	982.80	967.83	595.47	683.60	
LnLnCe	50	990.86	991.87	991	1008.90	1012.84	997.88	595.47	713.64	
LnLnXi	48	988.85	989.85	989	1006.88	1010.83	995.86	595.47	711.63	
LnLnMo	52	1018.89	1019.90	1019	1036.93	1040.87	1025.91	595.47	741.68	
LnLn28:1	50	1016.88	1017.89	1017	1034.91	1038.86	1023.89	595.47	739.66	
LnLn30	54	1046.92	1047.93	1047	1064.96	1068.91	1053.94	595.47	769.71	
LnLn30:1	52	1044.91	1045.92	1045	1062.94	1066.89	1051.92	595.47	767.69	
AAA	60	974.92	975.93	975	992.96	996.91	981.94		663.63	
AALa	52	862.80	863.81	863	880.83	884.78	869.81	663.63	551.50	

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
AAM	54	890.83	891.84	891	908.86	912.81	897.85	663.63	579.54	
AAP	56	918.86	919.87	919	936.90	940.84	925.88	663.63	607.57	
AAPo	54	916.85	917.85	917	934.88	938.83	923.86	663.63	605.55	
AAS	58	946.89	947.90	947	964.93	968.87	953.91	663.63	635.60	
AAO	56	944.88	945.89	945	962.91	966.86	951.89	663.63	633.58	
AAL	54	942.86	943.87	943	960.90	964.84	949.88	663.63	631.57	
AALn	52	940.85	941.85	941	958.88	962.83	947.86	663.63	629.55	
AAG	58	972.91	973.92	973	990.94	994.89	979.92	663.63	661.61	
AAB	62	1002.96	1003.96	1003	1020.99	1024.94	1009.97	663.63	691.66	
AAE	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	663.63	689.64	
AALg	64	1030.99	1031.99	1031	1049.02	1052.97	1038.00	663.63	719.69	
AAN	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	663.63	717.68	
AACe	66	1059.02	1060.03	1059	1077.05	1081.00	1066.03	663.63	747.72	
AAXi	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	663.63	745.71	
AAMo	68	1087.05	1088.06	1088	1105.08	1109.03	1094.07	663.63	775.75	
AA28:1	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	663.63	773.74	
AA30	70	1115.08	1116.09	1116	1133.12	1137.06	1122.10	663.63	803.79	
AA30:1	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	663.63	801.77	
GGG	54	968.88	969.89	969	986.91	990.86	975.89		659.60	
GGLa	48	858.77	859.78	859	876.80	880.75	865.78	659.60	549.49	
GGM	50	886.80	887.81	887	904.83	908.78	893.81	659.60	577.52	
GGP	52	914.83	915.84	915	932.86	936.81	921.85	659.60	605.55	
GGPo	50	912.81	913.82	913	930.85	934.80	919.83	659.60	603.54	
GGS	54	942.86	943.87	943	960.90	964.84	949.88	659.60	633.58	
GGO	52	940.85	941.85	941	958.88	962.83	947.86	659.60	631.57	
GGL	50	938.83	939.84	939	956.86	960.81	945.85	659.60	629.55	
GGLn	48	936.81	937.82	937	954.85	958.80	943.83	659.60	627.54	
GGA	56	970.89	971.90	971	988.93	992.87	977.91	659.60	661.61	
GGB	58	998.92	999.93	999	1016.96	1020.91	1005.94	659.60	689.64	
GGE	56	996.91	997.92	997	1014.94	1018.89	1003.92	659.60	687.63	
GGLg	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	659.60	717.68	
GGN	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	659.60	715.66	
GGCe	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	659.60	745.71	
GGXi	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	659.60	743.69	
GGMo	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	659.60	773.74	
GG28:1	62	1081.00	1082.01	1081	1099.04	1102.98	1088.02	659.60	771.72	
GG30	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	659.60	801.77	
GG30:1	64	1109.03	1110.04	1109	1127.07	1131.02	1116.05	659.60	799.75	
BBB	66	1059.02	1060.03	1059	1077.05	1081.00	1066.03		719.69	
BBLa	56	918.86	919.87	919	936.90	940.84	925.88	719.69	579.54	
BBM	58	946.89	947.90	947	964.93	968.87	953.91	719.69	607.57	
BBP	60	974.92	975.93	975	992.96	996.91	981.94	719.69	635.60	
BBPo	58	972.91	973.92	973	990.94	994.89	979.92	719.69	633.58	
BBS	62	1002.96	1003.96	1003	1020.99	1024.94	1009.97	719.69	663.63	
BBO	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	719.69	661.61	
BBL	58	998.92	999.93	999	1016.96	1020.91	1005.94	719.69	659.60	
BBLn	56	996.91	997.92	997	1014.94	1018.89	1003.92	719.69	657.58	
BBA	64	1030.99	1031.99	1031	1049.02	1052.97	1038.00	719.69	691.66	
BBG	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	719.69	689.64	
BBE	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	719.69	717.68	
BBLg	68	1087.05	1088.06	1088	1105.08	1109.03	1094.07	719.69	747.72	
BBN	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	719.69	745.71	
BBCe	70	1115.08	1116.09	1116	1133.12	1137.06	1122.10	719.69	775.75	
BBXi	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	719.69	773.74	
BBMo	72	1143.11	1144.12	1144	1161.15	1165.09	1150.13	719.69	803.79	

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
BB28:1	70	1141.10	1142.10	1142	1159.13	1163.08	1148.11	719.69	801.77	
BB30	74	1171.14	1172.15	1172	1189.18	1193.13	1178.16	719.69	831.82	
BB30:1	72	1169.13	1170.14	1170	1187.16	1191.11	1176.14	719.69	829.80	
EEE	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99		715.66	
EELa	52	914.83	915.84	915	932.86	936.81	921.85	715.66	577.52	
EEM	54	942.86	943.87	943	960.90	964.84	949.88	715.66	605.55	
EEP	56	970.89	971.90	971	988.93	992.87	977.91	715.66	633.58	
EEPo	54	968.88	969.89	969	986.91	990.86	975.89	715.66	631.57	
EES	58	998.92	999.93	999	1016.96	1020.91	1005.94	715.66	661.61	
EEO	56	996.91	997.92	997	1014.94	1018.89	1003.92	715.66	659.60	
EEL	54	994.89	995.90	995	1012.93	1016.87	1001.91	715.66	657.58	
EELn	52	992.88	993.89	993	1010.91	1014.86	999.89	715.66	655.57	
EEA	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	715.66	689.64	
EEG	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	715.66	687.63	
EEB	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	715.66	717.68	
EELg	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	715.66	745.71	
EEN	62	1081.00	1082.01	1081	1099.04	1102.98	1088.02	715.66	743.69	
EECe	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	715.66	773.74	
EEXi	64	1109.03	1110.04	1109	1127.07	1131.02	1116.05	715.66	771.72	
EEMo	68	1139.08	1140.09	1140	1157.12	1161.06	1146.10	715.66	801.77	
EE28:1	66	1137.06	1138.07	1138	1155.10	1159.05	1144.08	715.66	799.75	
EE30	70	1167.11	1168.12	1168	1185.15	1189.09	1174.13	715.66	829.80	
EE30:1	68	1165.10	1166.10	1166	1183.13	1187.08	1172.11	715.66	827.79	
LgLgLg	72	1143.11	1144.12	1144	1161.15	1165.09	1150.13		775.75	
LgLgLa	60	974.92	975.93	975	992.96	996.91	981.94	775.75	607.57	
LgLgM	62	1002.96	1003.96	1003	1020.99	1024.94	1009.97	775.75	635.60	
LgLgP	64	1030.99	1031.99	1031	1049.02	1052.97	1038.00	775.75	663.63	
LgLgPo	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	775.75	661.61	
LgLgS	66	1059.02	1060.03	1059	1077.05	1081.00	1066.03	775.75	691.66	
LgLgO	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	775.75	689.64	
LgLgL	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	775.75	687.63	
LgLgLn	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	775.75	685.61	
LgLgA	68	1087.05	1088.06	1088	1105.08	1109.03	1094.07	775.75	719.69	
LgLgG	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	775.75	717.68	
LgLgB	70	1115.08	1116.09	1116	1133.12	1137.06	1122.10	775.75	747.72	
LgLgE	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	775.75	745.71	
LgLgN	70	1141.10	1142.10	1142	1159.13	1163.08	1148.11	775.75	773.74	
LgLgCe	74	1171.14	1172.15	1172	1189.18	1193.13	1178.16	775.75	803.79	
LgLgXi	72	1169.13	1170.14	1170	1187.16	1191.11	1176.14	775.75	801.77	
LgLgMo	76	1199.17	1200.18	1200	1217.21	1221.16	1206.19	775.75	831.82	
LgLg28:1	74	1197.16	1198.17	1198	1215.19	1219.14	1204.17	775.75	829.80	
LgLg30	78	1227.21	1228.21	1228	1245.24	1249.19	1234.22	775.75	859.85	
LgLg30:1	76	1225.19	1226.20	1226	1243.22	1247.17	1232.21	775.75	857.83	
NNN	66	1137.06	1138.07	1138	1155.10	1159.05	1144.08		771.72	
NNLa	56	970.89	971.90	971	988.93	992.87	977.91	771.72	607.57	
NNM	58	998.92	999.93	999	1016.96	1020.91	1005.94	771.72	635.60	
NNP	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	771.72	663.63	
NNPo	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	771.72	661.61	
NNS	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	771.72	691.66	
NNO	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	771.72	689.64	
NNL	58	1050.96	1051.96	1051	1068.99	1072.94	1057.97	771.72	687.63	
NNLn	56	1048.94	1049.95	1049	1066.97	1070.92	1055.96	771.72	685.61	
NNA	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	771.72	719.69	
NNG	62	1081.00	1082.01	1081	1099.04	1102.98	1088.02	771.72	717.68	
NNB	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	771.72	747.72	
NNE	64	1109.03	1110.04	1109	1127.07	1131.02	1116.05	771.72	745.71	

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
NNLg	68	1139.08	1140.09	1140	1157.12	1161.06	1146.10	771.72	775.75	
NNCe	70	1167.11	1168.12	1168	1185.15	1189.09	1174.13	771.72	801.77	
NNXi	68	1165.10	1166.10	1166	1183.13	1187.08	1172.11	771.72	799.75	
NNMo	72	1195.14	1196.15	1196	1213.18	1217.13	1202.16	771.72	829.80	
NN28:1	70	1193.13	1194.14	1194	1211.16	1215.11	1200.14	771.72	827.79	
NN30	74	1223.17	1224.18	1224	1241.21	1245.16	1230.19	771.72	857.83	
NN30:1	72	1221.16	1222.17	1222	1239.19	1243.14	1228.17	771.72	855.82	
CeCeCe	78	1227.21	1228.21	1228	1245.24	1249.19	1234.22		831.82	
XiXiXi	72	1221.16	1222.17	1222	1239.19	1243.14	1228.17		827.79	
MoMoMo	84	1311.30	1312.31	1312	1329.33	1333.28	1318.32		887.88	
28:1,28:1,28:1	78	1305.25	1306.26	1306	1323.29	1327.23	1312.27		883.85	
30,30,30	90	1395.39	1396.40	1396	1413.43	1417.38	1402.41		943.94	
30:1,30:1,30:1	84	1389.35	1390.35	1390	1407.38	1411.33	1396.36		939.91	
32,32,32	96	1479.49	1480.50	1480	1497.52	1501.47	1486.50		1000.00	
32:1,32:1,32:1	90	1473.44	1474.45	1474	1491.47	1495.42	1480.46		995.97	
34,34,34	102	1563.58	1564.59	1564	1581.62	1585.56	1570.60		1056.07	
34:1,34:1,34:1	96	1557.53	1558.54	1558	1575.57	1579.52	1564.55		1052.04	
36,36,36	108	1647.68	1648.68	1648	1665.71	1669.66	1654.69		1112.13	
36:1,36:1,36:1	102	1641.63	1642.64	1642	1659.66	1663.61	1648.64		1108.10	