

ABC Triacylglycerols by Name (C₁₂ to C₃₀)

Abbrev.	ECN	Mass		Mass		[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3	
		Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺					
LaMP	42	722.64	723.65	723	740.68	744.62	729.66	467.41	523.47	495.44
LaMPo	40	720.63	721.63	721	738.66	742.61	727.64	467.41	521.46	493.43
LaMS	44	750.67	751.68	751	768.71	772.66	757.69	467.41	551.50	523.47
LaMO	42	748.66	749.67	749	766.69	770.64	755.67	467.41	549.49	521.46
LaML	40	746.64	747.65	747	764.68	768.62	753.66	467.41	547.47	519.44
LaMLn	38	744.63	745.63	745	762.66	766.61	751.64	467.41	545.46	517.43
LaMA	46	778.71	779.71	779	796.74	800.69	785.72	467.41	579.54	551.50
LaMG	44	776.69	777.70	777	794.72	798.67	783.71	467.41	577.52	549.49
LaMB	48	806.74	807.74	807	824.77	828.72	813.75	467.41	607.57	579.54
LaME	46	804.72	805.73	805	822.76	826.70	811.74	467.41	605.55	577.52
LaMLg	50	834.77	835.78	835	852.80	856.75	841.78	467.41	635.60	607.57
LaMN	48	832.75	833.76	833	850.79	854.73	839.77	467.41	633.58	605.55
LaMCe	52	862.80	863.81	863	880.83	884.78	869.81	467.41	663.63	635.60
LaMXi	50	860.78	861.79	861	878.82	882.77	867.80	467.41	661.61	633.58
LaMMo	54	890.83	891.84	891	908.86	912.81	897.85	467.41	691.66	663.63
LaM28:1	52	888.81	889.82	889	906.85	910.80	895.83	467.41	689.64	661.61
LaM30	56	918.86	919.87	919	936.90	940.84	925.88	467.41	719.69	691.66
LaM30:1	54	916.85	917.85	917	934.88	938.83	923.86	467.41	717.68	689.64
LaPPo	42	748.66	749.67	749	766.69	770.64	755.67	495.44	549.49	493.43
LaPS	46	778.71	779.71	779	796.74	800.69	785.72	495.44	579.54	523.47
LaPO	44	776.69	777.70	777	794.72	798.67	783.71	495.44	577.52	521.46
LaPL	42	774.67	775.68	775	792.71	796.66	781.69	495.44	575.50	519.44
LaPLn	40	772.66	773.67	773	790.69	794.64	779.67	495.44	573.49	517.43
LaPA	48	806.74	807.74	807	824.77	828.72	813.75	495.44	607.57	551.50
LaPG	46	804.72	805.73	805	822.76	826.70	811.74	495.44	605.55	549.49
LaPB	50	834.77	835.78	835	852.80	856.75	841.78	495.44	635.60	579.54
LaPE	48	832.75	833.76	833	850.79	854.73	839.77	495.44	633.58	577.52
LaPLg	52	862.80	863.81	863	880.83	884.78	869.81	495.44	663.63	607.57
LaPN	50	860.78	861.79	861	878.82	882.77	867.80	495.44	661.61	605.55
LaPCe	54	890.83	891.84	891	908.86	912.81	897.85	495.44	691.66	635.60
LaPXi	52	888.81	889.82	889	906.85	910.80	895.83	495.44	689.64	633.58
LaPMo	56	918.86	919.87	919	936.90	940.84	925.88	495.44	719.69	663.63
LaP28:1	54	916.85	917.85	917	934.88	938.83	923.86	495.44	717.68	661.61
LaP30	58	946.89	947.90	947	964.93	968.87	953.91	495.44	747.72	691.66
LaP30:1	56	944.88	945.89	945	962.91	966.86	951.89	495.44	745.71	689.64
LaPoS	44	776.69	777.70	777	794.72	798.67	783.71	493.43	577.52	523.47
LaPoO	42	774.67	775.68	775	792.71	796.66	781.69	493.43	575.50	521.46
LaPoL	40	772.66	773.67	773	790.69	794.64	779.67	493.43	573.49	519.44
LaPoLn	38	770.64	771.65	771	788.68	792.62	777.66	493.43	571.47	517.43
LaPoA	46	804.72	805.73	805	822.76	826.70	811.74	493.43	605.55	551.50
LaPoG	44	802.71	803.71	803	820.74	824.69	809.72	493.43	603.54	549.49
LaPoB	48	832.75	833.76	833	850.79	854.73	839.77	493.43	633.58	579.54
LaPoE	46	830.74	831.74	831	848.77	852.72	837.75	493.43	631.57	577.52
LaPoLg	50	860.78	861.79	861	878.82	882.77	867.80	493.43	661.61	607.57
LaPoN	48	858.77	859.78	859	876.80	880.75	865.78	493.43	659.60	605.55
LaPoCe	52	888.81	889.82	889	906.85	910.80	895.83	493.43	689.64	635.60
LaPoXi	50	886.80	887.81	887	904.83	908.78	893.81	493.43	687.63	633.58
LaPoMo	54	916.85	917.85	917	934.88	938.83	923.86	493.43	717.68	663.63
LaPo28:1	52	914.83	915.84	915	932.86	936.81	921.85	493.43	715.66	661.61
LaPo30	56	944.88	945.89	945	962.91	966.86	951.89	493.43	745.71	691.66
LaPo30:1	54	942.86	943.87	943	960.90	964.84	949.88	493.43	743.69	689.64
LaSO	46	804.72	805.73	805	822.76	826.70	811.74	523.47	605.55	521.46
LaSL	44	802.71	803.71	803	820.74	824.69	809.72	523.47	603.54	519.44
LaSLn	42	800.69	801.70	801	818.72	822.67	807.71	523.47	601.52	517.43
LaSA	50	834.77	835.78	835	852.80	856.75	841.78	523.47	635.60	551.50

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
LaSG	48	832.75	833.76	833	850.79	854.73	839.77	523.47	633.58	549.49
LaSB	52	862.80	863.81	863	880.83	884.78	869.81	523.47	663.63	579.54
LaSE	50	860.78	861.79	861	878.82	882.77	867.80	523.47	661.61	577.52
LaSLg	54	890.83	891.84	891	908.86	912.81	897.85	523.47	691.66	607.57
LaSN	52	888.81	889.82	889	906.85	910.80	895.83	523.47	689.64	605.55
LaSCe	56	918.86	919.87	919	936.90	940.84	925.88	523.47	719.69	635.60
LaSXi	54	916.85	917.85	917	934.88	938.83	923.86	523.47	717.68	633.58
LaSMo	58	946.89	947.90	947	964.93	968.87	953.91	523.47	747.72	663.63
LaS28:1	56	944.88	945.89	945	962.91	966.86	951.89	523.47	745.71	661.61
LaS30	60	974.92	975.93	975	992.96	996.91	981.94	523.47	775.75	691.66
LaS30:1	58	972.91	973.92	973	990.94	994.89	979.92	523.47	773.74	689.64
LaOL	42	800.69	801.70	801	818.72	822.67	807.71	521.46	601.52	519.44
LaOLn	40	798.67	799.68	799	816.71	820.66	805.69	521.46	599.50	517.43
LaOA	48	832.75	833.76	833	850.79	854.73	839.77	521.46	633.58	551.50
LaOG	46	830.74	831.74	831	848.77	852.72	837.75	521.46	631.57	549.49
LaOB	50	860.78	861.79	861	878.82	882.77	867.80	521.46	661.61	579.54
LaOE	48	858.77	859.78	859	876.80	880.75	865.78	521.46	659.60	577.52
LaOLg	52	888.81	889.82	889	906.85	910.80	895.83	521.46	689.64	607.57
LaON	50	886.80	887.81	887	904.83	908.78	893.81	521.46	687.63	605.55
LaOCe	54	916.85	917.85	917	934.88	938.83	923.86	521.46	717.68	635.60
LaOXi	52	914.83	915.84	915	932.86	936.81	921.85	521.46	715.66	633.58
LaOMo	56	944.88	945.89	945	962.91	966.86	951.89	521.46	745.71	663.63
LaO28:1	54	942.86	943.87	943	960.90	964.84	949.88	521.46	743.69	661.61
LaO30	58	972.91	973.92	973	990.94	994.89	979.92	521.46	773.74	691.66
LaO30:1	56	970.89	971.90	971	988.93	992.87	977.91	521.46	771.72	689.64
LaLLn	38	796.66	797.67	797	814.69	818.64	803.67	519.44	597.49	517.43
LaLA	46	830.74	831.74	831	848.77	852.72	837.75	519.44	631.57	551.50
LaLG	44	828.72	829.73	829	846.76	850.70	835.74	519.44	629.55	549.49
LaLB	48	858.77	859.78	859	876.80	880.75	865.78	519.44	659.60	579.54
LaLE	46	856.75	857.76	857	874.79	878.73	863.77	519.44	657.58	577.52
LaLLg	50	886.80	887.81	887	904.83	908.78	893.81	519.44	687.63	607.57
LaLN	48	884.78	885.79	885	902.82	906.77	891.80	519.44	685.61	605.55
LaLCe	52	914.83	915.84	915	932.86	936.81	921.85	519.44	715.66	635.60
LaLXi	50	912.81	913.82	913	930.85	934.80	919.83	519.44	713.64	633.58
LaLMo	54	942.86	943.87	943	960.90	964.84	949.88	519.44	743.69	663.63
LaL28:1	52	940.85	941.85	941	958.88	962.83	947.86	519.44	741.68	661.61
LaL30	56	970.89	971.90	971	988.93	992.87	977.91	519.44	771.72	691.66
LaL30:1	54	968.88	969.89	969	986.91	990.86	975.89	519.44	769.71	689.64
LaLnA	44	828.72	829.73	829	846.76	850.70	835.74	517.43	629.55	551.50
LaLnG	42	826.71	827.71	827	844.74	848.69	833.72	517.43	627.54	549.49
LaLnB	46	856.75	857.76	857	874.79	878.73	863.77	517.43	657.58	579.54
LaLnE	44	854.74	855.74	855	872.77	876.72	861.75	517.43	655.57	577.52
LaLnLg	48	884.78	885.79	885	902.82	906.77	891.80	517.43	685.61	607.57
LaLnN	46	882.77	883.78	883	900.80	904.75	889.78	517.43	683.60	605.55
LaLnCe	50	912.81	913.82	913	930.85	934.80	919.83	517.43	713.64	635.60
LaLnXi	48	910.80	911.81	911	928.83	932.78	917.81	517.43	711.63	633.58
LaLnMo	52	940.85	941.85	941	958.88	962.83	947.86	517.43	741.68	663.63
LaLn28:1	50	938.83	939.84	939	956.86	960.81	945.85	517.43	739.66	661.61
LaLn30	54	968.88	969.89	969	986.91	990.86	975.89	517.43	769.71	691.66
LaLn30:1	52	966.86	967.87	967	984.90	988.84	973.88	517.43	767.69	689.64
LaAG	50	860.78	861.79	861	878.82	882.77	867.80	551.50	661.61	549.49
LaAB	54	890.83	891.84	891	908.86	912.81	897.85	551.50	691.66	579.54
LaAE	52	888.81	889.82	889	906.85	910.80	895.83	551.50	689.64	577.52
LaALg	56	918.86	919.87	919	936.90	940.84	925.88	551.50	719.69	607.57
LaAN	54	916.85	917.85	917	934.88	938.83	923.86	551.50	717.68	605.55
LaACe	58	946.89	947.90	947	964.93	968.87	953.91	551.50	747.72	635.60
LaAXi	56	944.88	945.89	945	962.91	966.86	951.89	551.50	745.71	633.58
LaAMo	60	974.92	975.93	975	992.96	996.91	981.94	551.50	775.75	663.63
LaA28:1	58	972.91	973.92	973	990.94	994.89	979.92	551.50	773.74	661.61

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
LaA30	62	1002.96	1003.96	1003	1020.99	1024.94	1009.97	551.50	803.79	691.66
LaA30:1	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	551.50	801.77	689.64
LaGB	52	888.81	889.82	889	906.85	910.80	895.83	549.49	689.64	579.54
LaGE	50	886.80	887.81	887	904.83	908.78	893.81	549.49	687.63	577.52
LaGLg	54	916.85	917.85	917	934.88	938.83	923.86	549.49	717.68	607.57
LaGN	52	914.83	915.84	915	932.86	936.81	921.85	549.49	715.66	605.55
LaGCe	56	944.88	945.89	945	962.91	966.86	951.89	549.49	745.71	635.60
LaGXi	54	942.86	943.87	943	960.90	964.84	949.88	549.49	743.69	633.58
LaGMo	58	972.91	973.92	973	990.94	994.89	979.92	549.49	773.74	663.63
LaG28:1	56	970.89	971.90	971	988.93	992.87	977.91	549.49	771.72	661.61
LaG30	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	549.49	801.77	691.66
LaG30:1	58	998.92	999.93	999	1016.96	1020.91	1005.94	549.49	799.75	689.64
LaBE	54	916.85	917.85	917	934.88	938.83	923.86	579.54	717.68	577.52
LaBLg	58	946.89	947.90	947	964.93	968.87	953.91	579.54	747.72	607.57
LaBN	56	944.88	945.89	945	962.91	966.86	951.89	579.54	745.71	605.55
LaBCe	60	974.92	975.93	975	992.96	996.91	981.94	579.54	775.75	635.60
LaBXi	58	972.91	973.92	973	990.94	994.89	979.92	579.54	773.74	633.58
LaBMo	62	1002.96	1003.96	1003	1020.99	1024.94	1009.97	579.54	803.79	663.63
LaB28:1	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	579.54	801.77	661.61
LaB30	64	1030.99	1031.99	1031	1049.02	1052.97	1038.00	579.54	831.82	691.66
LaB30:1	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	579.54	829.80	689.64
LaELg	56	944.88	945.89	945	962.91	966.86	951.89	577.52	745.71	607.57
LaEN	54	942.86	943.87	943	960.90	964.84	949.88	577.52	743.69	605.55
LaLgN	58	972.91	973.92	973	990.94	994.89	979.92	607.57	773.74	605.55
LaPoCe	52	888.81	889.82	889	906.85	910.80	895.83	493.43	689.64	635.60
LaPoXi	50	886.80	887.81	887	904.83	908.78	893.81	493.43	687.63	633.58
LaPoMo	54	916.85	917.85	917	934.88	938.83	923.86	493.43	717.68	663.63
LaPo28:1	52	914.83	915.84	915	932.86	936.81	921.85	493.43	715.66	661.61
LaPo30	56	944.88	945.89	945	962.91	966.86	951.89	493.43	745.71	691.66
LaPo30:1	54	942.86	943.87	943	960.90	964.84	949.88	493.43	743.69	689.64
MPPo	44	776.69	777.70	777	794.72	798.67	783.71	523.47	549.49	521.46
MPS	48	806.74	807.74	807	824.77	828.72	813.75	523.47	579.54	551.50
MPO	46	804.72	805.73	805	822.76	826.70	811.74	523.47	577.52	549.49
MPL	44	802.71	803.71	803	820.74	824.69	809.72	523.47	575.50	547.47
MPLn	42	800.69	801.70	801	818.72	822.67	807.71	523.47	573.49	545.46
MPA	50	834.77	835.78	835	852.80	856.75	841.78	523.47	607.57	579.54
MPG	48	832.75	833.76	833	850.79	854.73	839.77	523.47	605.55	577.52
MPB	52	862.80	863.81	863	880.83	884.78	869.81	523.47	635.60	607.57
MPE	50	860.78	861.79	861	878.82	882.77	867.80	523.47	633.58	605.55
MPLg	54	890.83	891.84	891	908.86	912.81	897.85	523.47	663.63	635.60
MPN	52	888.81	889.82	889	906.85	910.80	895.83	523.47	661.61	633.58
MPCe	56	918.86	919.87	919	936.90	940.84	925.88	523.47	691.66	663.63
MPXi	54	916.85	917.85	917	934.88	938.83	923.86	523.47	689.64	661.61
MPMo	58	946.89	947.90	947	964.93	968.87	953.91	523.47	719.69	691.66
MP28:1	56	944.88	945.89	945	962.91	966.86	951.89	523.47	717.68	689.64
MP30	60	974.92	975.93	975	992.96	996.91	981.94	523.47	747.72	719.69
MP30:1	58	972.91	973.92	973	990.94	994.89	979.92	523.47	745.71	717.68
MPoS	46	804.72	805.73	805	822.76	826.70	811.74	521.46	577.52	551.50
MPoO	44	802.71	803.71	803	820.74	824.69	809.72	521.46	575.50	549.49
MPoL	42	800.69	801.70	801	818.72	822.67	807.71	521.46	573.49	547.47
MPoLn	40	798.67	799.68	799	816.71	820.66	805.69	521.46	571.47	545.46
MPoA	48	832.75	833.76	833	850.79	854.73	839.77	521.46	605.55	579.54
MPoG	46	830.74	831.74	831	848.77	852.72	837.75	521.46	603.54	577.52
MPoB	50	860.78	861.79	861	878.82	882.77	867.80	521.46	633.58	607.57
MPoE	48	858.77	859.78	859	876.80	880.75	865.78	521.46	631.57	605.55
MPoLg	52	888.81	889.82	889	906.85	910.80	895.83	521.46	661.61	635.60
MPoN	50	886.80	887.81	887	904.83	908.78	893.81	521.46	659.60	633.58
MPoCe	54	916.85	917.85	917	934.88	938.83	923.86	521.46	689.64	663.63
MPoXi	52	914.83	915.84	915	932.86	936.81	921.85	521.46	687.63	661.61

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
MPoMo	56	944.88	945.89	945	962.91	966.86	951.89	521.46	717.68	691.66
MPo28:1	54	942.86	943.87	943	960.90	964.84	949.88	521.46	715.66	689.64
MPo30	58	972.91	973.92	973	990.94	994.89	979.92	521.46	745.71	719.69
MPo30:1	56	970.89	971.90	971	988.93	992.87	977.91	521.46	743.69	717.68
MSO	48	832.75	833.76	833	850.79	854.73	839.77	551.50	605.55	549.49
MSL	46	830.74	831.74	831	848.77	852.72	837.75	551.50	603.54	547.47
MSLn	44	828.72	829.73	829	846.76	850.70	835.74	551.50	601.52	545.46
MSA	52	862.80	863.81	863	880.83	884.78	869.81	551.50	635.60	579.54
MSG	50	860.78	861.79	861	878.82	882.77	867.80	551.50	633.58	577.52
MSB	54	890.83	891.84	891	908.86	912.81	897.85	551.50	663.63	607.57
MSE	52	888.81	889.82	889	906.85	910.80	895.83	551.50	661.61	605.55
MSLg	56	918.86	919.87	919	936.90	940.84	925.88	551.50	691.66	635.60
MSN	54	916.85	917.85	917	934.88	938.83	923.86	551.50	689.64	633.58
MSCe	58	946.89	947.90	947	964.93	968.87	953.91	551.50	719.69	663.63
MSXi	56	944.88	945.89	945	962.91	966.86	951.89	551.50	717.68	661.61
MSMo	60	974.92	975.93	975	992.96	996.91	981.94	551.50	747.72	691.66
MS28:1	58	972.91	973.92	973	990.94	994.89	979.92	551.50	745.71	689.64
MS30	62	1002.96	1003.96	1003	1020.99	1024.94	1009.97	551.50	775.75	719.69
MS30:1	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	551.50	773.74	717.68
MOL	44	828.72	829.73	829	846.76	850.70	835.74	549.49	601.52	547.47
MOLn	42	826.71	827.71	827	844.74	848.69	833.72	549.49	599.50	545.46
MOA	50	860.78	861.79	861	878.82	882.77	867.80	549.49	633.58	579.54
MOG	48	858.77	859.78	859	876.80	880.75	865.78	549.49	631.57	577.52
MOB	52	888.81	889.82	889	906.85	910.80	895.83	549.49	661.61	607.57
MOE	50	886.80	887.81	887	904.83	908.78	893.81	549.49	659.60	605.55
MOLg	54	916.85	917.85	917	934.88	938.83	923.86	549.49	689.64	635.60
MON	52	914.83	915.84	915	932.86	936.81	921.85	549.49	687.63	633.58
MOCe	56	944.88	945.89	945	962.91	966.86	951.89	549.49	717.68	663.63
MOXi	54	942.86	943.87	943	960.90	964.84	949.88	549.49	715.66	661.61
MOMo	58	972.91	973.92	973	990.94	994.89	979.92	549.49	745.71	691.66
MO28:1	56	970.89	971.90	971	988.93	992.87	977.91	549.49	743.69	689.64
MO30	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	549.49	773.74	719.69
MO30:1	58	998.92	999.93	999	1016.96	1020.91	1005.94	549.49	771.72	717.68
MLLn	40	824.69	825.70	825	842.72	846.67	831.71	547.47	597.49	545.46
MLA	48	858.77	859.78	859	876.80	880.75	865.78	547.47	631.57	579.54
MLG	46	856.75	857.76	857	874.79	878.73	863.77	547.47	629.55	577.52
MLB	50	886.80	887.81	887	904.83	908.78	893.81	547.47	659.60	607.57
MLE	48	884.78	885.79	885	902.82	906.77	891.80	547.47	657.58	605.55
MLLg	52	914.83	915.84	915	932.86	936.81	921.85	547.47	687.63	635.60
MLN	50	912.81	913.82	913	930.85	934.80	919.83	547.47	685.61	633.58
MLCe	54	942.86	943.87	943	960.90	964.84	949.88	547.47	715.66	663.63
MLXi	52	940.85	941.85	941	958.88	962.83	947.86	547.47	713.64	661.61
MLMo	56	970.89	971.90	971	988.93	992.87	977.91	547.47	743.69	691.66
ML28:1	54	968.88	969.89	969	986.91	990.86	975.89	547.47	741.68	689.64
ML30	58	998.92	999.93	999	1016.96	1020.91	1005.94	547.47	771.72	719.69
ML30:1	56	996.91	997.92	997	1014.94	1018.89	1003.92	547.47	769.71	717.68
MLnA	46	856.75	857.76	857	874.79	878.73	863.77	545.46	629.55	579.54
MLnG	44	854.74	855.74	855	872.77	876.72	861.75	545.46	627.54	577.52
MLnB	48	884.78	885.79	885	902.82	906.77	891.80	545.46	657.58	607.57
MLnE	46	882.77	883.78	883	900.80	904.75	889.78	545.46	655.57	605.55
MLnLg	50	912.81	913.82	913	930.85	934.80	919.83	545.46	685.61	635.60
MLnN	48	910.80	911.81	911	928.83	932.78	917.81	545.46	683.60	633.58
MLnCe	52	940.85	941.85	941	958.88	962.83	947.86	545.46	713.64	663.63
MLnXi	50	938.83	939.84	939	956.86	960.81	945.85	545.46	711.63	661.61
MLnMo	54	968.88	969.89	969	986.91	990.86	975.89	545.46	741.68	691.66
MLn28:1	52	966.86	967.87	967	984.90	988.84	973.88	545.46	739.66	689.64
MLn30	56	996.91	997.92	997	1014.94	1018.89	1003.92	545.46	769.71	719.69
MLn30:1	54	994.89	995.90	995	1012.93	1016.87	1001.91	545.46	767.69	717.68
MAG	52	888.81	889.82	889	906.85	910.80	895.83	579.54	661.61	577.52

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
MAB	56	918.86	919.87	919	936.90	940.84	925.88	579.54	691.66	607.57
MAE	54	916.85	917.85	917	934.88	938.83	923.86	579.54	689.64	605.55
MALg	58	946.89	947.90	947	964.93	968.87	953.91	579.54	719.69	635.60
MAN	56	944.88	945.89	945	962.91	966.86	951.89	579.54	717.68	633.58
MACe	60	974.92	975.93	975	992.96	996.91	981.94	579.54	747.72	663.63
MAXi	58	972.91	973.92	973	990.94	994.89	979.92	579.54	745.71	661.61
MAMo	62	1002.96	1003.96	1003	1020.99	1024.94	1009.97	579.54	775.75	691.66
MA28:1	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	579.54	773.74	689.64
MA30	64	1030.99	1031.99	1031	1049.02	1052.97	1038.00	579.54	803.79	719.69
MA30:1	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	579.54	801.77	717.68
MGB	54	916.85	917.85	917	934.88	938.83	923.86	577.52	689.64	607.57
MGE	52	914.83	915.84	915	932.86	936.81	921.85	577.52	687.63	605.55
MGLg	56	944.88	945.89	945	962.91	966.86	951.89	577.52	717.68	635.60
MGN	54	942.86	943.87	943	960.90	964.84	949.88	577.52	715.66	633.58
MGCe	58	972.91	973.92	973	990.94	994.89	979.92	577.52	745.71	663.63
MGXi	56	970.89	971.90	971	988.93	992.87	977.91	577.52	743.69	661.61
MGMo	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	577.52	773.74	691.66
MG28:1	58	998.92	999.93	999	1016.96	1020.91	1005.94	577.52	771.72	689.64
MG30	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	577.52	801.77	719.69
MG30:1	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	577.52	799.75	717.68
MBE	56	944.88	945.89	945	962.91	966.86	951.89	607.57	717.68	605.55
MBLg	60	974.92	975.93	975	992.96	996.91	981.94	607.57	747.72	635.60
MBN	58	972.91	973.92	973	990.94	994.89	979.92	607.57	745.71	633.58
MBCe	62	1002.96	1003.96	1003	1020.99	1024.94	1009.97	607.57	775.75	663.63
MBXi	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	607.57	773.74	661.61
MBMo	64	1030.99	1031.99	1031	1049.02	1052.97	1038.00	607.57	803.79	691.66
MB28:1	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	607.57	801.77	689.64
MB30	66	1059.02	1060.03	1059	1077.05	1081.00	1066.03	607.57	831.82	719.69
MB30:1	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	607.57	829.80	717.68
MELg	58	972.91	973.92	973	990.94	994.89	979.92	605.55	745.71	635.60
MEN	56	970.89	971.90	971	988.93	992.87	977.91	605.55	743.69	633.58
MECe	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	605.55	773.74	663.63
MEXi	58	998.92	999.93	999	1016.96	1020.91	1005.94	605.55	771.72	661.61
MEMo	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	605.55	801.77	691.66
ME28:1	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	605.55	799.75	689.64
ME30	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	605.55	829.80	719.69
ME30:1	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	605.55	827.79	717.68
MLgN	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	635.60	773.74	633.58
MLgCe	64	1030.99	1031.99	1031	1049.02	1052.97	1038.00	635.60	803.79	663.63
MLgXi	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	635.60	801.77	661.61
MLgMo	66	1059.02	1060.03	1059	1077.05	1081.00	1066.03	635.60	831.82	691.66
MLg28:1	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	635.60	829.80	689.64
MLg30	68	1087.05	1088.06	1088	1105.08	1109.03	1094.07	635.60	859.85	719.69
MLg30:1	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	635.60	857.83	717.68
PPoS	48	832.75	833.76	833	850.79	854.73	839.77	549.49	577.52	579.54
PPoO	46	830.74	831.74	831	848.77	852.72	837.75	549.49	575.50	577.52
PPoL	44	828.72	829.73	829	846.76	850.70	835.74	549.49	573.49	575.50
PPoLn	42	826.71	827.71	827	844.74	848.69	833.72	549.49	571.47	573.49
PPoA	50	860.78	861.79	861	878.82	882.77	867.80	549.49	605.55	607.57
PPoG	48	858.77	859.78	859	876.80	880.75	865.78	549.49	603.54	605.55
PPoB	52	888.81	889.82	889	906.85	910.80	895.83	549.49	633.58	635.60
PPoE	50	886.80	887.81	887	904.83	908.78	893.81	549.49	631.57	633.58
PPoLg	54	916.85	917.85	917	934.88	938.83	923.86	549.49	661.61	663.63
PPoN	52	914.83	915.84	915	932.86	936.81	921.85	549.49	659.60	661.61
PPoCe	56	944.88	945.89	945	962.91	966.86	951.89	549.49	689.64	691.66
PPoXi	54	942.86	943.87	943	960.90	964.84	949.88	549.49	687.63	689.64
PPoMo	58	972.91	973.92	973	990.94	994.89	979.92	549.49	717.68	719.69
PPo28:1	56	970.89	971.90	971	988.93	992.87	977.91	549.49	715.66	717.68
PPo30	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	549.49	745.71	747.72

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
PPo30:1	58	998.92	999.93	999	1016.96	1020.91	1005.94	549.49	743.69	745.71
PSO	50	860.78	861.79	861	878.82	882.77	867.80	579.54	605.55	577.52
PSL	48	858.77	859.78	859	876.80	880.75	865.78	579.54	603.54	575.50
PSLn	46	856.75	857.76	857	874.79	878.73	863.77	579.54	601.52	573.49
PSA	54	890.83	891.84	891	908.86	912.81	897.85	579.54	635.60	607.57
PSG	52	888.81	889.82	889	906.85	910.80	895.83	579.54	633.58	605.55
PSB	56	918.86	919.87	919	936.90	940.84	925.88	579.54	663.63	635.60
PSE	54	916.85	917.85	917	934.88	938.83	923.86	579.54	661.61	633.58
PSLg	58	946.89	947.90	947	964.93	968.87	953.91	579.54	691.66	663.63
PSN	56	944.88	945.89	945	962.91	966.86	951.89	579.54	689.64	661.61
PSCe	60	974.92	975.93	975	992.96	996.91	981.94	579.54	719.69	691.66
PSXi	58	972.91	973.92	973	990.94	994.89	979.92	579.54	717.68	689.64
PSMo	62	1002.96	1003.96	1003	1020.99	1024.94	1009.97	579.54	747.72	719.69
PS28:1	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	579.54	745.71	717.68
PS30	64	1030.99	1031.99	1031	1049.02	1052.97	1038.00	579.54	775.75	747.72
PS30:1	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	579.54	773.74	745.71
POL	46	856.75	857.76	857	874.79	878.73	863.77	577.52	601.52	575.50
POLn	44	854.74	855.74	855	872.77	876.72	861.75	577.52	599.50	573.49
POA	52	888.81	889.82	889	906.85	910.80	895.83	577.52	633.58	607.57
POG	50	886.80	887.81	887	904.83	908.78	893.81	577.52	631.57	605.55
POB	54	916.85	917.85	917	934.88	938.83	923.86	577.52	661.61	635.60
POE	52	914.83	915.84	915	932.86	936.81	921.85	577.52	659.60	633.58
POLg	56	944.88	945.89	945	962.91	966.86	951.89	577.52	689.64	663.63
PON	54	942.86	943.87	943	960.90	964.84	949.88	577.52	687.63	661.61
POCe	58	972.91	973.92	973	990.94	994.89	979.92	577.52	717.68	691.66
POXi	56	970.89	971.90	971	988.93	992.87	977.91	577.52	715.66	689.64
POMo	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	577.52	745.71	719.69
PO28:1	58	998.92	999.93	999	1016.96	1020.91	1005.94	577.52	743.69	717.68
PO30	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	577.52	773.74	747.72
PO30:1	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	577.52	771.72	745.71
PLLn	42	852.72	853.73	853	870.76	874.70	859.74	575.50	597.49	573.49
PLA	50	886.80	887.81	887	904.83	908.78	893.81	575.50	631.57	607.57
PLG	48	884.78	885.79	885	902.82	906.77	891.80	575.50	629.55	605.55
PLB	52	914.83	915.84	915	932.86	936.81	921.85	575.50	659.60	635.60
PLE	50	912.81	913.82	913	930.85	934.80	919.83	575.50	657.58	633.58
PLLg	54	942.86	943.87	943	960.90	964.84	949.88	575.50	687.63	663.63
PLN	52	940.85	941.85	941	958.88	962.83	947.86	575.50	685.61	661.61
PLCe	56	970.89	971.90	971	988.93	992.87	977.91	575.50	715.66	691.66
PLXi	54	968.88	969.89	969	986.91	990.86	975.89	575.50	713.64	689.64
PLMo	58	998.92	999.93	999	1016.96	1020.91	1005.94	575.50	743.69	719.69
PL28:1	56	996.91	997.92	997	1014.94	1018.89	1003.92	575.50	741.68	717.68
PL30	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	575.50	771.72	747.72
PL30:1	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	575.50	769.71	745.71
PLnA	48	884.78	885.79	885	902.82	906.77	891.80	573.49	629.55	607.57
PLnG	46	882.77	883.78	883	900.80	904.75	889.78	573.49	627.54	605.55
PLnB	50	912.81	913.82	913	930.85	934.80	919.83	573.49	657.58	635.60
PLnE	48	910.80	911.81	911	928.83	932.78	917.81	573.49	655.57	633.58
PLnLg	52	940.85	941.85	941	958.88	962.83	947.86	573.49	685.61	663.63
PLnN	50	938.83	939.84	939	956.86	960.81	945.85	573.49	683.60	661.61
PLnCe	54	968.88	969.89	969	986.91	990.86	975.89	573.49	713.64	691.66
PLnXi	52	966.86	967.87	967	984.90	988.84	973.88	573.49	711.63	689.64
PLnMo	56	996.91	997.92	997	1014.94	1018.89	1003.92	573.49	741.68	719.69
PLn28:1	54	994.89	995.90	995	1012.93	1016.87	1001.91	573.49	739.66	717.68
PLn30	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	573.49	769.71	747.72
PLn30:1	56	1022.92	1023.93	1023	1040.96	1044.91	1029.94	573.49	767.69	745.71
PAG	54	916.85	917.85	917	934.88	938.83	923.86	607.57	661.61	605.55
PAB	58	946.89	947.90	947	964.93	968.87	953.91	607.57	691.66	635.60
PAE	56	944.88	945.89	945	962.91	966.86	951.89	607.57	689.64	633.58
PALg	60	974.92	975.93	975	992.96	996.91	981.94	607.57	719.69	663.63

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
PAN	58	972.91	973.92	973	990.94	994.89	979.92	607.57	717.68	661.61
PACe	62	1002.96	1003.96	1003	1020.99	1024.94	1009.97	607.57	747.72	691.66
PAXi	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	607.57	745.71	689.64
PAMo	64	1030.99	1031.99	1031	1049.02	1052.97	1038.00	607.57	775.75	719.69
PA28:1	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	607.57	773.74	717.68
PA30	66	1059.02	1060.03	1059	1077.05	1081.00	1066.03	607.57	803.79	747.72
PA30:1	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	607.57	801.77	745.71
PGB	56	944.88	945.89	945	962.91	966.86	951.89	605.55	689.64	635.60
PGE	54	942.86	943.87	943	960.90	964.84	949.88	605.55	687.63	633.58
PGLg	58	972.91	973.92	973	990.94	994.89	979.92	605.55	717.68	663.63
PGN	56	970.89	971.90	971	988.93	992.87	977.91	605.55	715.66	661.61
PGCe	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	605.55	745.71	691.66
PGXi	58	998.92	999.93	999	1016.96	1020.91	1005.94	605.55	743.69	689.64
PGMo	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	605.55	773.74	719.69
PG28:1	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	605.55	771.72	717.68
PG30	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	605.55	801.77	747.72
PG30:1	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	605.55	799.75	745.71
PBE	58	972.91	973.92	973	990.94	994.89	979.92	635.60	717.68	633.58
PBLg	62	1002.96	1003.96	1003	1020.99	1024.94	1009.97	635.60	747.72	663.63
PBN	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	635.60	745.71	661.61
PBCe	64	1030.99	1031.99	1031	1049.02	1052.97	1038.00	635.60	775.75	691.66
PBXi	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	635.60	773.74	689.64
PBMo	66	1059.02	1060.03	1059	1077.05	1081.00	1066.03	635.60	803.79	719.69
PB28:1	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	635.60	801.77	717.68
PB30	68	1087.05	1088.06	1088	1105.08	1109.03	1094.07	635.60	831.82	747.72
PB30:1	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	635.60	829.80	745.71
PELg	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	633.58	745.71	663.63
PEN	58	998.92	999.93	999	1016.96	1020.91	1005.94	633.58	743.69	661.61
PECe	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	633.58	773.74	691.66
PEXi	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	633.58	771.72	689.64
PEMo	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	633.58	801.77	719.69
PE28:1	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	633.58	799.75	717.68
PE30	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	633.58	829.80	747.72
PE30:1	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	633.58	827.79	745.71
PLgN	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	663.63	773.74	661.61
PLgCe	66	1059.02	1060.03	1059	1077.05	1081.00	1066.03	663.63	803.79	691.66
PLgXi	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	663.63	801.77	689.64
PLgMo	68	1087.05	1088.06	1088	1105.08	1109.03	1094.07	663.63	831.82	719.69
PLg28:1	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	663.63	829.80	717.68
PLg30	70	1115.08	1116.09	1116	1133.12	1137.06	1122.10	663.63	859.85	747.72
PLg30:1	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	663.63	857.83	745.71
PoSO	48	858.77	859.78	859	876.80	880.75	865.78	577.52	605.55	575.50
PoSL	46	856.75	857.76	857	874.79	878.73	863.77	577.52	603.54	573.49
PoSLn	44	854.74	855.74	855	872.77	876.72	861.75	577.52	601.52	571.47
PoSA	52	888.81	889.82	889	906.85	910.80	895.83	577.52	635.60	605.55
PoSG	50	886.80	887.81	887	904.83	908.78	893.81	577.52	633.58	603.54
PoSB	54	916.85	917.85	917	934.88	938.83	923.86	577.52	663.63	633.58
PoSE	52	914.83	915.84	915	932.86	936.81	921.85	577.52	661.61	631.57
PoSLg	56	944.88	945.89	945	962.91	966.86	951.89	577.52	691.66	661.61
PoSN	54	942.86	943.87	943	960.90	964.84	949.88	577.52	689.64	659.60
PoSce	58	972.91	973.92	973	990.94	994.89	979.92	577.52	719.69	689.64
PoSXi	56	970.89	971.90	971	988.93	992.87	977.91	577.52	717.68	687.63
PoSMo	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	577.52	747.72	717.68
PoS28:1	58	998.92	999.93	999	1016.96	1020.91	1005.94	577.52	745.71	715.66
PoS30	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	577.52	775.75	745.71
PoS30:1	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	577.52	773.74	743.69
PoOL	44	854.74	855.74	855	872.77	876.72	861.75	575.50	601.52	573.49
PoOLn	42	852.72	853.73	853	870.76	874.70	859.74	575.50	599.50	571.47
PoOA	50	886.80	887.81	887	904.83	908.78	893.81	575.50	633.58	605.55

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
PoOG	48	884.78	885.79	885	902.82	906.77	891.80	575.50	631.57	603.54
PoOB	52	914.83	915.84	915	932.86	936.81	921.85	575.50	661.61	633.58
PoOE	50	912.81	913.82	913	930.85	934.80	919.83	575.50	659.60	631.57
PoOLg	54	942.86	943.87	943	960.90	964.84	949.88	575.50	689.64	661.61
PoON	52	940.85	941.85	941	958.88	962.83	947.86	575.50	687.63	659.60
PoOCe	56	970.89	971.90	971	988.93	992.87	977.91	575.50	717.68	689.64
PoOXi	54	968.88	969.89	969	986.91	990.86	975.89	575.50	715.66	687.63
PoOMo	58	998.92	999.93	999	1016.96	1020.91	1005.94	575.50	745.71	717.68
PoO28:1	56	996.91	997.92	997	1014.94	1018.89	1003.92	575.50	743.69	715.66
PoO30	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	575.50	773.74	745.71
PoO30:1	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	575.50	771.72	743.69
PoLLn	40	850.71	851.71	851	868.74	872.69	857.72	573.49	597.49	571.47
PoLA	48	884.78	885.79	885	902.82	906.77	891.80	573.49	631.57	605.55
PoLG	46	882.77	883.78	883	900.80	904.75	889.78	573.49	629.55	603.54
PoLB	50	912.81	913.82	913	930.85	934.80	919.83	573.49	659.60	633.58
PoLE	48	910.80	911.81	911	928.83	932.78	917.81	573.49	657.58	631.57
PoLLg	52	940.85	941.85	941	958.88	962.83	947.86	573.49	687.63	661.61
PoLN	50	938.83	939.84	939	956.86	960.81	945.85	573.49	685.61	659.60
PoLnA	46	882.77	883.78	883	900.80	904.75	889.78	571.47	629.55	605.55
PoLnCe	52	966.86	967.87	967	984.90	988.84	973.88	571.47	713.64	689.64
PoLnXi	50	964.85	965.85	965	982.88	986.83	971.86	571.47	711.63	687.63
PoLnMo	54	994.89	995.90	995	1012.93	1016.87	1001.91	571.47	741.68	717.68
PoLn28:1	52	992.88	993.89	993	1010.91	1014.86	999.89	571.47	739.66	715.66
PoLn30	56	1022.92	1023.93	1023	1040.96	1044.91	1029.94	571.47	769.71	745.71
PoLn30:1	54	1020.91	1021.92	1021	1038.94	1042.89	1027.92	571.47	767.69	743.69
PoAG	52	914.83	915.84	915	932.86	936.81	921.85	605.55	661.61	603.54
PoAB	56	944.88	945.89	945	962.91	966.86	951.89	605.55	691.66	633.58
PoAE	54	942.86	943.87	943	960.90	964.84	949.88	605.55	689.64	631.57
PoALg	58	972.91	973.92	973	990.94	994.89	979.92	605.55	719.69	661.61
PoAN	56	970.89	971.90	971	988.93	992.87	977.91	605.55	717.68	659.60
PoACe	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	605.55	747.72	689.64
PoAXi	58	998.92	999.93	999	1016.96	1020.91	1005.94	605.55	745.71	687.63
PoAMo	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	605.55	775.75	717.68
PoA28:1	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	605.55	773.74	715.66
PoA30	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	605.55	803.79	745.71
PoA30:1	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	605.55	801.77	743.69
PoGB	54	942.86	943.87	943	960.90	964.84	949.88	603.54	689.64	633.58
PoGE	52	940.85	941.85	941	958.88	962.83	947.86	603.54	687.63	631.57
PoGLg	56	970.89	971.90	971	988.93	992.87	977.91	603.54	717.68	661.61
PoGN	54	968.88	969.89	969	986.91	990.86	975.89	603.54	715.66	659.60
PoGCe	58	998.92	999.93	999	1016.96	1020.91	1005.94	603.54	745.71	689.64
PoGXi	56	996.91	997.92	997	1014.94	1018.89	1003.92	603.54	743.69	687.63
PoGMo	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	603.54	773.74	717.68
PoG28:1	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	603.54	771.72	715.66
PoG30	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	603.54	801.77	745.71
PoG30:1	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	603.54	799.75	743.69
PoBE	56	970.89	971.90	971	988.93	992.87	977.91	633.58	717.68	631.57
PoBLg	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	633.58	747.72	661.61
PoBN	58	998.92	999.93	999	1016.96	1020.91	1005.94	633.58	745.71	659.60
PoBCe	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	633.58	775.75	689.64
PoBXi	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	633.58	773.74	687.63
PoBMo	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	633.58	803.79	717.68
PoB28:1	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	633.58	801.77	715.66
PoB30	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	633.58	831.82	745.71
PoB30:1	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	633.58	829.80	743.69
PoELg	58	998.92	999.93	999	1016.96	1020.91	1005.94	631.57	745.71	661.61
PoEN	56	996.91	997.92	997	1014.94	1018.89	1003.92	631.57	743.69	659.60
PoECe	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	631.57	773.74	689.64
PoEXi	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	631.57	771.72	687.63

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
PoEMo	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	631.57	801.77	717.68
PoE28:1	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	631.57	799.75	715.66
PoE30	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	631.57	829.80	745.71
PoE30:1	62	1081.00	1082.01	1081	1099.04	1102.98	1088.02	631.57	827.79	743.69
PoLgN	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	661.61	773.74	659.60
PoLgCe	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	661.61	803.79	689.64
PoLgXi	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	661.61	801.77	687.63
PoLgMo	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	661.61	831.82	717.68
PoLg28:1	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	661.61	829.80	715.66
PoLg30	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	661.61	859.85	745.71
PoLg30:1	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	661.61	857.83	743.69
SOL	48	884.78	885.79	885	902.82	906.77	891.80	605.55	601.52	603.54
SOLn	46	882.77	883.78	883	900.80	904.75	889.78	605.55	599.50	601.52
SOA	54	916.85	917.85	917	934.88	938.83	923.86	605.55	633.58	635.60
SOG	52	914.83	915.84	915	932.86	936.81	921.85	605.55	631.57	633.58
SOB	56	944.88	945.89	945	962.91	966.86	951.89	605.55	661.61	663.63
SOE	54	942.86	943.87	943	960.90	964.84	949.88	605.55	659.60	661.61
SOLg	58	972.91	973.92	973	990.94	994.89	979.92	605.55	689.64	691.66
SON	56	970.89	971.90	971	988.93	992.87	977.91	605.55	687.63	689.64
SOCe	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	605.55	717.68	719.69
SOXi	58	998.92	999.93	999	1016.96	1020.91	1005.94	605.55	715.66	717.68
SOMo	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	605.55	745.71	747.72
SO28:1	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	605.55	743.69	745.71
SO30	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	605.55	773.74	775.75
SO30:1	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	605.55	771.72	773.74
SLLn	44	880.75	881.76	881	898.79	902.73	887.77	603.54	597.49	601.52
SLA	52	914.83	915.84	915	932.86	936.81	921.85	603.54	631.57	635.60
SLG	50	912.81	913.82	913	930.85	934.80	919.83	603.54	629.55	633.58
SLB	54	942.86	943.87	943	960.90	964.84	949.88	603.54	659.60	663.63
SLE	52	940.85	941.85	941	958.88	962.83	947.86	603.54	657.58	661.61
SLLg	56	970.89	971.90	971	988.93	992.87	977.91	603.54	687.63	691.66
SLN	54	968.88	969.89	969	986.91	990.86	975.89	603.54	685.61	689.64
SLCe	58	998.92	999.93	999	1016.96	1020.91	1005.94	603.54	715.66	719.69
SLXi	56	996.91	997.92	997	1014.94	1018.89	1003.92	603.54	713.64	717.68
SLML	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	603.54	743.69	747.72
SL28:1	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	603.54	741.68	745.71
SL30	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	603.54	771.72	775.75
SL30:1	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	603.54	769.71	773.74
SLnA	50	912.81	913.82	913	930.85	934.80	919.83	601.52	629.55	635.60
SLnG	48	910.80	911.81	911	928.83	932.78	917.81	601.52	627.54	633.58
SLnB	52	940.85	941.85	941	958.88	962.83	947.86	601.52	657.58	663.63
SLnE	50	938.83	939.84	939	956.86	960.81	945.85	601.52	655.57	661.61
SLnLg	54	968.88	969.89	969	986.91	990.86	975.89	601.52	685.61	691.66
SLnN	52	966.86	967.87	967	984.90	988.84	973.88	601.52	683.60	689.64
SLnCe	56	996.91	997.92	997	1014.94	1018.89	1003.92	601.52	713.64	719.69
SLnXi	54	994.89	995.90	995	1012.93	1016.87	1001.91	601.52	711.63	717.68
SLnMo	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	601.52	741.68	747.72
SLn28:1	56	1022.92	1023.93	1023	1040.96	1044.91	1029.94	601.52	739.66	745.71
SLn30	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	601.52	769.71	775.75
SLn30:1	58	1050.96	1051.96	1051	1068.99	1072.94	1057.97	601.52	767.69	773.74
SAG	56	944.88	945.89	945	962.91	966.86	951.89	635.60	661.61	633.58
SAB	60	974.92	975.93	975	992.96	996.91	981.94	635.60	691.66	663.63
SAE	58	972.91	973.92	973	990.94	994.89	979.92	635.60	689.64	661.61
SALg	62	1002.96	1003.96	1003	1020.99	1024.94	1009.97	635.60	719.69	691.66
SAN	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	635.60	717.68	689.64
SACe	64	1030.99	1031.99	1031	1049.02	1052.97	1038.00	635.60	747.72	719.69
SAXi	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	635.60	745.71	717.68
SAMo	66	1059.02	1060.03	1059	1077.05	1081.00	1066.03	635.60	775.75	747.72
SA28:1	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	635.60	773.74	745.71

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
SA30	68	1087.05	1088.06	1088	1105.08	1109.03	1094.07	635.60	803.79	775.75
SA30:1	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	635.60	801.77	773.74
SGB	58	972.91	973.92	973	990.94	994.89	979.92	633.58	689.64	663.63
SGE	56	970.89	971.90	971	988.93	992.87	977.91	633.58	687.63	661.61
SGLg	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	633.58	717.68	691.66
SGN	58	998.92	999.93	999	1016.96	1020.91	1005.94	633.58	715.66	689.64
SGCe	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	633.58	745.71	719.69
SGXi	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	633.58	743.69	717.68
SGMo	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	633.58	773.74	747.72
SG28:1	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	633.58	771.72	745.71
SG30	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	633.58	801.77	775.75
SG30:1	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	633.58	799.75	773.74
SBE	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	663.63	717.68	661.61
SBLg	64	1030.99	1031.99	1031	1049.02	1052.97	1038.00	663.63	747.72	691.66
SBN	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	663.63	745.71	689.64
SBCe	66	1059.02	1060.03	1059	1077.05	1081.00	1066.03	663.63	775.75	719.69
SBXi	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	663.63	773.74	717.68
SBMo	68	1087.05	1088.06	1088	1105.08	1109.03	1094.07	663.63	803.79	747.72
SB28:1	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	663.63	801.77	745.71
SB30	70	1115.08	1116.09	1116	1133.12	1137.06	1122.10	663.63	831.82	775.75
SB30:1	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	663.63	829.80	773.74
SELg	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	661.61	745.71	691.66
SEN	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	661.61	743.69	689.64
SECe	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	661.61	773.74	719.69
SEXi	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	661.61	771.72	717.68
SEMo	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	661.61	801.77	747.72
SE28:1	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	661.61	799.75	745.71
SE30	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	661.61	829.80	775.75
SE30:1	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	661.61	827.79	773.74
SLgN	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	691.66	773.74	689.64
SLgCe	68	1087.05	1088.06	1088	1105.08	1109.03	1094.07	691.66	803.79	719.69
SLgXi	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	691.66	801.77	717.68
SLgMo	70	1115.08	1116.09	1116	1133.12	1137.06	1122.10	691.66	831.82	747.72
SLg28:1	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	691.66	829.80	745.71
SLg30	72	1143.11	1144.12	1144	1161.15	1165.09	1150.13	691.66	859.85	775.75
SLg30:1	70	1141.10	1142.10	1142	1159.13	1163.08	1148.11	691.66	857.83	773.74
OLLn	42	878.74	879.74	879	896.77	900.72	885.75	601.52	597.49	599.50
OLA	50	912.81	913.82	913	930.85	934.80	919.83	601.52	631.57	633.58
OLG	48	910.80	911.81	911	928.83	932.78	917.81	601.52	629.55	631.57
OLB	52	940.85	941.85	941	958.88	962.83	947.86	601.52	659.60	661.61
OLE	50	938.83	939.84	939	956.86	960.81	945.85	601.52	657.58	659.60
OLLg	54	968.88	969.89	969	986.91	990.86	975.89	601.52	687.63	689.64
OLN	52	966.86	967.87	967	984.90	988.84	973.88	601.52	685.61	687.63
OLCe	56	996.91	997.92	997	1014.94	1018.89	1003.92	601.52	715.66	717.68
OLXi	54	994.89	995.90	995	1012.93	1016.87	1001.91	601.52	713.64	715.66
OLMo	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	601.52	743.69	745.71
OL28:1	56	1022.92	1023.93	1023	1040.96	1044.91	1029.94	601.52	741.68	743.69
OL30	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	601.52	771.72	773.74
OL30:1	58	1050.96	1051.96	1051	1068.99	1072.94	1057.97	601.52	769.71	771.72
OLnA	48	910.80	911.81	911	928.83	932.78	917.81	599.50	629.55	633.58
OLnG	46	908.78	909.79	909	926.82	930.77	915.80	599.50	627.54	631.57
OLnB	50	938.83	939.84	939	956.86	960.81	945.85	599.50	657.58	661.61
OLnE	48	936.81	937.82	937	954.85	958.80	943.83	599.50	655.57	659.60
OLnLg	52	966.86	967.87	967	984.90	988.84	973.88	599.50	685.61	689.64
OLnN	50	964.85	965.85	965	982.88	986.83	971.86	599.50	683.60	687.63
OLnCe	54	994.89	995.90	995	1012.93	1016.87	1001.91	599.50	713.64	717.68
OLnXi	52	992.88	993.89	993	1010.91	1014.86	999.89	599.50	711.63	715.66
OLnMo	56	1022.92	1023.93	1023	1040.96	1044.91	1029.94	599.50	741.68	745.71
OLn28:1	54	1020.91	1021.92	1021	1038.94	1042.89	1027.92	599.50	739.66	743.69

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
OLn30	58	1050.96	1051.96	1051	1068.99	1072.94	1057.97	599.50	769.71	773.74
OLn30:1	56	1048.94	1049.95	1049	1066.97	1070.92	1055.96	599.50	767.69	771.72
OAG	54	942.86	943.87	943	960.90	964.84	949.88	633.58	661.61	631.57
OAB	58	972.91	973.92	973	990.94	994.89	979.92	633.58	691.66	661.61
OAE	56	970.89	971.90	971	988.93	992.87	977.91	633.58	689.64	659.60
OALg	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	633.58	719.69	689.64
OAN	58	998.92	999.93	999	1016.96	1020.91	1005.94	633.58	717.68	687.63
OACe	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	633.58	747.72	717.68
OAXi	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	633.58	745.71	715.66
OAMo	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	633.58	775.75	745.71
OA28:1	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	633.58	773.74	743.69
OA30	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	633.58	803.79	773.74
OA30:1	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	633.58	801.77	771.72
OGB	56	970.89	971.90	971	988.93	992.87	977.91	631.57	689.64	661.61
OGE	54	968.88	969.89	969	986.91	990.86	975.89	631.57	687.63	659.60
OGLg	58	998.92	999.93	999	1016.96	1020.91	1005.94	631.57	717.68	689.64
OGN	56	996.91	997.92	997	1014.94	1018.89	1003.92	631.57	715.66	687.63
OGCe	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	631.57	745.71	717.68
OGXi	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	631.57	743.69	715.66
OGMo	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	631.57	773.74	745.71
OG28:1	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	631.57	771.72	743.69
OG30	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	631.57	801.77	773.74
OG30:1	62	1081.00	1082.01	1081	1099.04	1102.98	1088.02	631.57	799.75	771.72
OBE	58	998.92	999.93	999	1016.96	1020.91	1005.94	661.61	717.68	659.60
OBLg	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	661.61	747.72	689.64
OBN	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	661.61	745.71	687.63
OBCe	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	661.61	775.75	717.68
OBXi	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	661.61	773.74	715.66
OBMo	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	661.61	803.79	745.71
OB28:1	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	661.61	801.77	743.69
OB30	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	661.61	831.82	773.74
OB30:1	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	661.61	829.80	771.72
OELg	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	659.60	745.71	689.64
OEN	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	659.60	743.69	687.63
OECe	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	659.60	773.74	717.68
OEXi	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	659.60	771.72	715.66
OEMo	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	659.60	801.77	745.71
OE28:1	62	1081.00	1082.01	1081	1099.04	1102.98	1088.02	659.60	799.75	743.69
OE30	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	659.60	829.80	773.74
OE30:1	64	1109.03	1110.04	1109	1127.07	1131.02	1116.05	659.60	827.79	771.72
OLgN	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	689.64	773.74	687.63
OLgCe	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	689.64	803.79	717.68
OLgXi	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	689.64	801.77	715.66
OLgMo	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	689.64	831.82	745.71
OLg28:1	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	689.64	829.80	743.69
OLg30	70	1141.10	1142.10	1142	1159.13	1163.08	1148.11	689.64	859.85	773.74
OLg30:1	68	1139.08	1140.09	1140	1157.12	1161.06	1146.10	689.64	857.83	771.72
LLnA	46	908.78	909.79	909	926.82	930.77	915.80	597.49	629.55	631.57
LLnG	44	906.77	907.78	907	924.80	928.75	913.78	597.49	627.54	629.55
LLnB	48	936.81	937.82	937	954.85	958.80	943.83	597.49	657.58	659.60
LLnE	46	934.80	935.81	935	952.83	956.78	941.81	597.49	655.57	657.58
LLnLg	50	964.85	965.85	965	982.88	986.83	971.86	597.49	685.61	687.63
LLnN	48	962.83	963.84	963	980.86	984.81	969.85	597.49	683.60	685.61
LLnCe	52	992.88	993.89	993	1010.91	1014.86	999.89	597.49	713.64	715.66
LLnXi	50	990.86	991.87	991	1008.90	1012.84	997.88	597.49	711.63	713.64
LLnMo	54	1020.91	1021.92	1021	1038.94	1042.89	1027.92	597.49	741.68	743.69
LLn28:1	52	1018.89	1019.90	1019	1036.93	1040.87	1025.91	597.49	739.66	741.68
LLn30	56	1048.94	1049.95	1049	1066.97	1070.92	1055.96	597.49	769.71	771.72
LLn30:1	54	1046.92	1047.93	1047	1064.96	1068.91	1053.94	597.49	767.69	769.71

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
LAG	52	940.85	941.85	941	958.88	962.83	947.86	631.57	661.61	629.55
LAB	56	970.89	971.90	971	988.93	992.87	977.91	631.57	691.66	659.60
LAE	54	968.88	969.89	969	986.91	990.86	975.89	631.57	689.64	657.58
LALg	58	998.92	999.93	999	1016.96	1020.91	1005.94	631.57	719.69	687.63
LAN	56	996.91	997.92	997	1014.94	1018.89	1003.92	631.57	717.68	685.61
LACe	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	631.57	747.72	715.66
LAXi	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	631.57	745.71	713.64
LAMo	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	631.57	775.75	743.69
LA28:1	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	631.57	773.74	741.68
LA30	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	631.57	803.79	771.72
LA30:1	62	1081.00	1082.01	1081	1099.04	1102.98	1088.02	631.57	801.77	769.71
LGB	54	968.88	969.89	969	986.91	990.86	975.89	629.55	689.64	659.60
LGE	52	966.86	967.87	967	984.90	988.84	973.88	629.55	687.63	657.58
LGLg	56	996.91	997.92	997	1014.94	1018.89	1003.92	629.55	717.68	687.63
LGN	54	994.89	995.90	995	1012.93	1016.87	1001.91	629.55	715.66	685.61
LGCe	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	629.55	745.71	715.66
LGXi	56	1022.92	1023.93	1023	1040.96	1044.91	1029.94	629.55	743.69	713.64
LGMo	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	629.55	773.74	743.69
LG28:1	58	1050.96	1051.96	1051	1068.99	1072.94	1057.97	629.55	771.72	741.68
LG30	62	1081.00	1082.01	1081	1099.04	1102.98	1088.02	629.55	801.77	771.72
LG30:1	60	1078.99	1079.99	1079	1097.02	1100.97	1086.00	629.55	799.75	769.71
LBE	56	996.91	997.92	997	1014.94	1018.89	1003.92	659.60	717.68	657.58
LBLg	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	659.60	747.72	687.63
LBN	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	659.60	745.71	685.61
LBCe	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	659.60	775.75	715.66
LBXi	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	659.60	773.74	713.64
LBMo	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	659.60	803.79	743.69
LB28:1	62	1081.00	1082.01	1081	1099.04	1102.98	1088.02	659.60	801.77	741.68
LB30	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	659.60	831.82	771.72
LB30:1	64	1109.03	1110.04	1109	1127.07	1131.02	1116.05	659.60	829.80	769.71
LELg	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	657.58	745.71	687.63
LEN	56	1022.92	1023.93	1023	1040.96	1044.91	1029.94	657.58	743.69	685.61
LECe	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	657.58	773.74	715.66
LEXi	58	1050.96	1051.96	1051	1068.99	1072.94	1057.97	657.58	771.72	713.64
LEMo	62	1081.00	1082.01	1081	1099.04	1102.98	1088.02	657.58	801.77	743.69
LE28:1	60	1078.99	1079.99	1079	1097.02	1100.97	1086.00	657.58	799.75	741.68
LE30	64	1109.03	1110.04	1109	1127.07	1131.02	1116.05	657.58	829.80	771.72
LE30:1	62	1107.02	1108.03	1107	1125.05	1129.00	1114.03	657.58	827.79	769.71
LLgN	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	687.63	773.74	685.61
LLgCe	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	687.63	803.79	715.66
LLgXi	62	1081.00	1082.01	1081	1099.04	1102.98	1088.02	687.63	801.77	713.64
LLgMo	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	687.63	831.82	743.69
LLg28:1	64	1109.03	1110.04	1109	1127.07	1131.02	1116.05	687.63	829.80	741.68
LLg30	68	1139.08	1140.09	1140	1157.12	1161.06	1146.10	687.63	859.85	771.72
LLg30:1	66	1137.06	1138.07	1138	1155.10	1159.05	1144.08	687.63	857.83	769.71
LnAG	50	938.83	939.84	939	956.86	960.81	945.85	629.55	661.61	627.54
LnAB	54	968.88	969.89	969	986.91	990.86	975.89	629.55	691.66	657.58
LnAE	52	966.86	967.87	967	984.90	988.84	973.88	629.55	689.64	655.57
LnALg	56	996.91	997.92	997	1014.94	1018.89	1003.92	629.55	719.69	685.61
LnAN	54	994.89	995.90	995	1012.93	1016.87	1001.91	629.55	717.68	683.60
LnACe	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	629.55	747.72	713.64
LnAXi	56	1022.92	1023.93	1023	1040.96	1044.91	1029.94	629.55	745.71	711.63
LnAMo	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	629.55	775.75	741.68
LnA28:1	58	1050.96	1051.96	1051	1068.99	1072.94	1057.97	629.55	773.74	739.66
LnA30	62	1081.00	1082.01	1081	1099.04	1102.98	1088.02	629.55	803.79	769.71
LnA30:1	60	1078.99	1079.99	1079	1097.02	1100.97	1086.00	629.55	801.77	767.69
LnGB	52	966.86	967.87	967	984.90	988.84	973.88	627.54	689.64	657.58
LnGE	50	964.85	965.85	965	982.88	986.83	971.86	627.54	687.63	655.57
LnGLg	54	994.89	995.90	995	1012.93	1016.87	1001.91	627.54	717.68	685.61

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
LnGN	52	992.88	993.89	993	1010.91	1014.86	999.89	627.54	715.66	683.60
LnGCe	56	1022.92	1023.93	1023	1040.96	1044.91	1029.94	627.54	745.71	713.64
LnGXi	54	1020.91	1021.92	1021	1038.94	1042.89	1027.92	627.54	743.69	711.63
LnGMo	58	1050.96	1051.96	1051	1068.99	1072.94	1057.97	627.54	773.74	741.68
LnG28:1	56	1048.94	1049.95	1049	1066.97	1070.92	1055.96	627.54	771.72	739.66
LnG30	60	1078.99	1079.99	1079	1097.02	1100.97	1086.00	627.54	801.77	769.71
LnG30:1	58	1076.97	1077.98	1077	1095.01	1098.95	1083.99	627.54	799.75	767.69
LnBE	54	994.89	995.90	995	1012.93	1016.87	1001.91	657.58	717.68	655.57
LnBLg	58	1024.94	1025.95	1025	1042.97	1046.92	1031.96	657.58	747.72	685.61
LnBN	56	1022.92	1023.93	1023	1040.96	1044.91	1029.94	657.58	745.71	683.60
LnBCe	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	657.58	775.75	713.64
LnBXi	58	1050.96	1051.96	1051	1068.99	1072.94	1057.97	657.58	773.74	711.63
LnBMo	62	1081.00	1082.01	1081	1099.04	1102.98	1088.02	657.58	803.79	741.68
LnB28:1	60	1078.99	1079.99	1079	1097.02	1100.97	1086.00	657.58	801.77	739.66
LnB30	64	1109.03	1110.04	1109	1127.07	1131.02	1116.05	657.58	831.82	769.71
LnB30:1	62	1107.02	1108.03	1107	1125.05	1129.00	1114.03	657.58	829.80	767.69
LnELg	56	1022.92	1023.93	1023	1040.96	1044.91	1029.94	655.57	745.71	685.61
LnEN	54	1020.91	1021.92	1021	1038.94	1042.89	1027.92	655.57	743.69	683.60
LnECe	58	1050.96	1051.96	1051	1068.99	1072.94	1057.97	655.57	773.74	713.64
LnEXi	56	1048.94	1049.95	1049	1066.97	1070.92	1055.96	655.57	771.72	711.63
LnEMo	60	1078.99	1079.99	1079	1097.02	1100.97	1086.00	655.57	801.77	741.68
LnE28:1	58	1076.97	1077.98	1077	1095.01	1098.95	1083.99	655.57	799.75	739.66
LnE30	62	1107.02	1108.03	1107	1125.05	1129.00	1114.03	655.57	829.80	769.71
LnE30:1	60	1105.00	1106.01	1105	1123.04	1126.98	1112.02	655.57	827.79	767.69
LnLgN	58	1050.96	1051.96	1051	1068.99	1072.94	1057.97	685.61	773.74	683.60
LnLgCe	62	1081.00	1082.01	1081	1099.04	1102.98	1088.02	685.61	803.79	713.64
LnLgXi	60	1078.99	1079.99	1079	1097.02	1100.97	1086.00	685.61	801.77	711.63
LnLgMo	64	1109.03	1110.04	1109	1127.07	1131.02	1116.05	685.61	831.82	741.68
LnLg28:1	62	1107.02	1108.03	1107	1125.05	1129.00	1114.03	685.61	829.80	739.66
LnLg30	66	1137.06	1138.07	1138	1155.10	1159.05	1144.08	685.61	859.85	769.71
LnLg30:1	64	1135.05	1136.06	1135	1153.08	1157.03	1142.07	685.61	857.83	767.69
AGB	60	1000.94	1001.95	1001	1018.97	1022.92	1007.96	661.61	689.64	691.66
AGE	58	998.92	999.93	999	1016.96	1020.91	1005.94	661.61	687.63	689.64
AGLg	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	661.61	717.68	719.69
AGN	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	661.61	715.66	717.68
AGCe	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	661.61	745.71	747.72
AGXi	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	661.61	743.69	745.71
AGMo	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	661.61	773.74	775.75
AG28:1	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	661.61	771.72	773.74
AG30	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	661.61	801.77	803.79
AG30:1	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	661.61	799.75	801.77
ABE	62	1028.97	1029.98	1029	1047.01	1050.95	1035.99	691.66	717.68	689.64
ABLg	66	1059.02	1060.03	1059	1077.05	1081.00	1066.03	691.66	747.72	719.69
ABN	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	691.66	745.71	717.68
ABCe	68	1087.05	1088.06	1088	1105.08	1109.03	1094.07	691.66	775.75	747.72
ABXi	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	691.66	773.74	745.71
ABMo	70	1115.08	1116.09	1116	1133.12	1137.06	1122.10	691.66	803.79	775.75
AB28:1	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	691.66	801.77	773.74
AB30	72	1143.11	1144.12	1144	1161.15	1165.09	1150.13	691.66	831.82	803.79
AB30:1	70	1141.10	1142.10	1142	1159.13	1163.08	1148.11	691.66	829.80	801.77
AELg	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	689.64	745.71	719.69
AEN	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	689.64	743.69	717.68
AECe	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	689.64	773.74	747.72
AEXi	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	689.64	771.72	745.71
AEMo	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	689.64	801.77	775.75
AE28:1	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	689.64	799.75	773.74
AE30	70	1141.10	1142.10	1142	1159.13	1163.08	1148.11	689.64	829.80	803.79
AE30:1	68	1139.08	1140.09	1140	1157.12	1161.06	1146.10	689.64	827.79	801.77
ALgN	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	719.69	773.74	717.68

Abbrev.	ECN	Accurate	[M+H] ⁺	Nominal	[M+NH ₄] ⁺	[M+Na] ⁺	[M+Li] ⁺	DAG 1,2	DAG 2,3	DAG 1,3
ALgCe	70	1115.08	1116.09	1116	1133.12	1137.06	1122.10	719.69	803.79	747.72
ALgXi	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	719.69	801.77	745.71
ALgMo	72	1143.11	1144.12	1144	1161.15	1165.09	1150.13	719.69	831.82	775.75
ALg28:1	70	1141.10	1142.10	1142	1159.13	1163.08	1148.11	719.69	829.80	773.74
ALg30	74	1171.14	1172.15	1172	1189.18	1193.13	1178.16	719.69	859.85	803.79
ALg30:1	72	1169.13	1170.14	1170	1187.16	1191.11	1176.14	719.69	857.83	801.77
GBE	60	1026.96	1027.96	1027	1044.99	1048.94	1033.97	689.64	717.68	687.63
GBLg	64	1057.00	1058.01	1057	1075.04	1078.98	1064.02	689.64	747.72	717.68
GBN	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	689.64	745.71	715.66
GBCe	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	689.64	775.75	745.71
GBXi	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	689.64	773.74	743.69
GBMo	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	689.64	803.79	773.74
GB28:1	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	689.64	801.77	771.72
GB30	70	1141.10	1142.10	1142	1159.13	1163.08	1148.11	689.64	831.82	801.77
GB30:1	68	1139.08	1140.09	1140	1157.12	1161.06	1146.10	689.64	829.80	799.75
GELg	62	1054.99	1055.99	1055	1073.02	1076.97	1062.00	687.63	745.71	717.68
GEN	60	1052.97	1053.98	1053	1071.01	1074.95	1059.99	687.63	743.69	715.66
GECe	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	687.63	773.74	745.71
GEXi	62	1081.00	1082.01	1081	1099.04	1102.98	1088.02	687.63	771.72	743.69
GEMo	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	687.63	801.77	773.74
GE28:1	64	1109.03	1110.04	1109	1127.07	1131.02	1116.05	687.63	799.75	771.72
GE30	68	1139.08	1140.09	1140	1157.12	1161.06	1146.10	687.63	829.80	801.77
GE30:1	66	1137.06	1138.07	1138	1155.10	1159.05	1144.08	687.63	827.79	799.75
GLgN	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	717.68	773.74	715.66
GLgCe	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	717.68	803.79	745.71
GLgXi	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	717.68	801.77	743.69
GLgMo	70	1141.10	1142.10	1142	1159.13	1163.08	1148.11	717.68	831.82	773.74
GLg28:1	68	1139.08	1140.09	1140	1157.12	1161.06	1146.10	717.68	829.80	771.72
GLg30	72	1169.13	1170.14	1170	1187.16	1191.11	1176.14	717.68	859.85	801.77
GLg30:1	70	1167.11	1168.12	1168	1185.15	1189.09	1174.13	717.68	857.83	799.75
BELg	66	1085.03	1086.04	1085	1103.07	1107.02	1092.05	717.68	745.71	747.72
BEN	64	1083.02	1084.03	1083	1101.05	1105.00	1090.03	717.68	743.69	745.71
BECe	68	1113.06	1114.07	1114	1131.10	1135.05	1120.08	717.68	773.74	775.75
BEXi	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	717.68	771.72	773.74
BEMo	70	1141.10	1142.10	1142	1159.13	1163.08	1148.11	717.68	801.77	803.79
BE28:1	68	1139.08	1140.09	1140	1157.12	1161.06	1146.10	717.68	799.75	801.77
BE30	72	1169.13	1170.14	1170	1187.16	1191.11	1176.14	717.68	829.80	831.82
BE30:1	70	1167.11	1168.12	1168	1185.15	1189.09	1174.13	717.68	827.79	829.80
ELgN	66	1111.05	1112.06	1112	1129.08	1133.03	1118.07	745.71	773.74	743.69
ELgCe	70	1141.10	1142.10	1142	1159.13	1163.08	1148.11	745.71	803.79	773.74
ELgXi	68	1139.08	1140.09	1140	1157.12	1161.06	1146.10	745.71	801.77	771.72
ELgMo	72	1169.13	1170.14	1170	1187.16	1191.11	1176.14	745.71	831.82	801.77
ELg28:1	70	1167.11	1168.12	1168	1185.15	1189.09	1174.13	745.71	829.80	799.75
ELg30	74	1197.16	1198.17	1198	1215.19	1219.14	1204.17	745.71	859.85	829.80
ELg30:1	72	1195.14	1196.15	1196	1213.18	1217.13	1202.16	745.71	857.83	827.79