

SUPPLEMENTAL MATERIALS

Native Top-Down Mass Spectrometry and Ion Mobility MS for Characterizing the Cobalt and Manganese Metal Binding of α -Synuclein Protein

Piriya Wongkongkathep^{1,#}, Jong Yoon Han², Tae Su Choi², Sheng Yin¹, Hugh I. Kim², and
Joseph A. Loo^{1,3*}

¹Department of Chemistry and Biochemistry, University of California-Los Angeles, Los Angeles,
CA, 90095-1569, USA

²Department of Chemistry, Korea University, Seoul, Republic of Korea

³Department of Biological Chemistry, David Geffen School of Medicine at UCLA, UCLA
Molecular Biology Institute, and UCLA/DOE Institute for Genomics and Proteomics, University
of California-Los Angeles, Los Angeles, CA, 90095-1569, USA

Journal of the American Society for Mass Spectrometry

[#]*Current address:* Faculty of Medicine, Chulalongkorn University, Bangkok, Thailand

^{*}*Correspondence to:* Joseph A. Loo; *e-mail:* JLoo@chem.ucla.edu

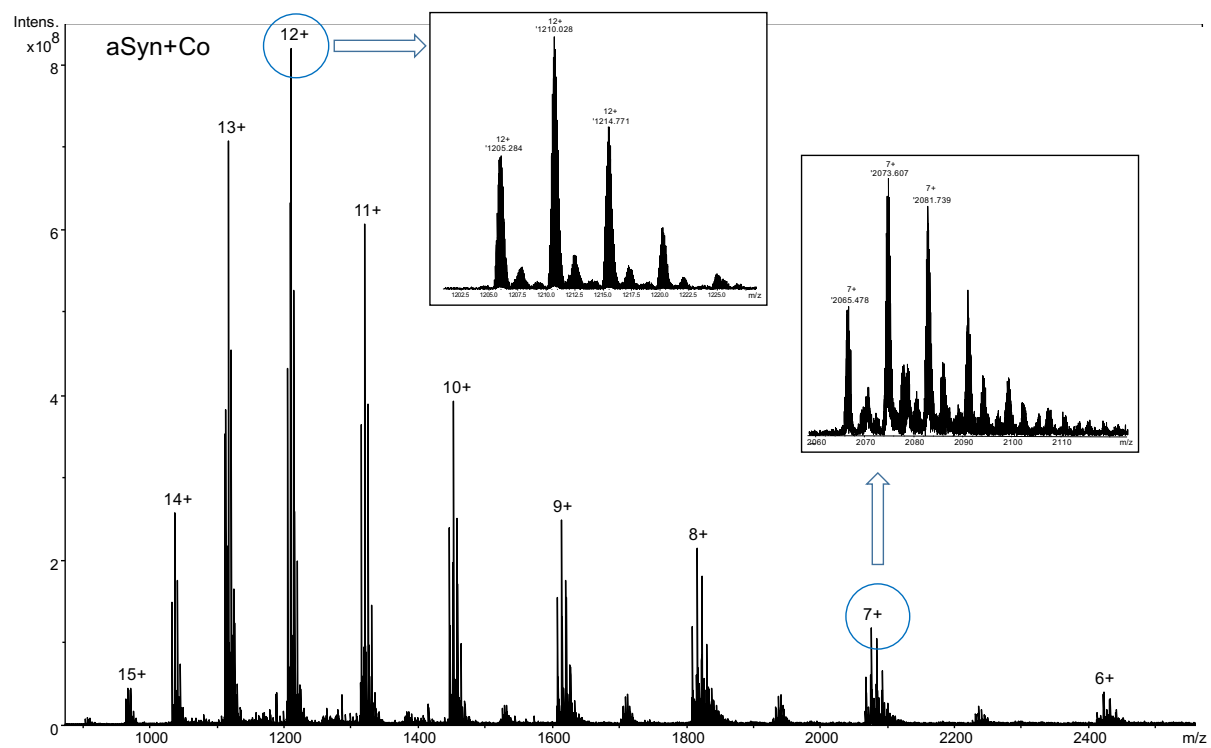
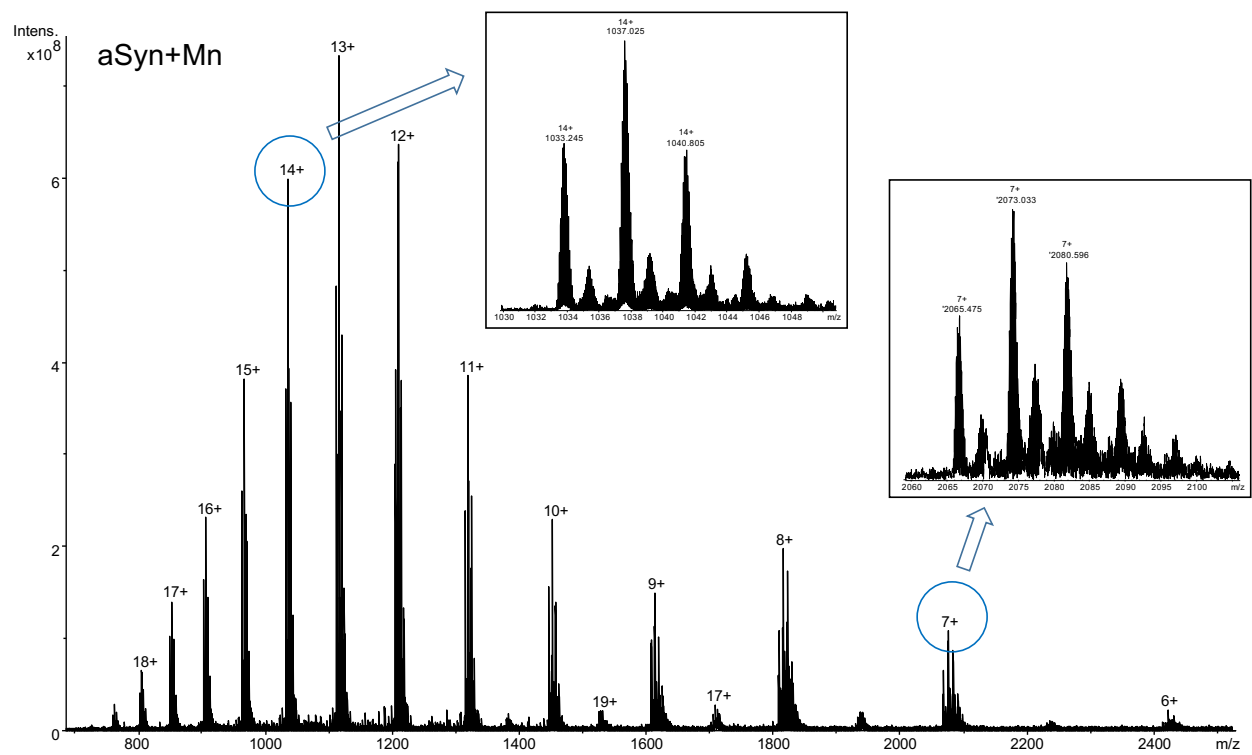


Figure S1. Native ESI-MS of α Syn with (top) Mn- and (bottom) Co-binding. The ratio of metal-bound and apo-proteins are consistent throughout the charge state envelopes.

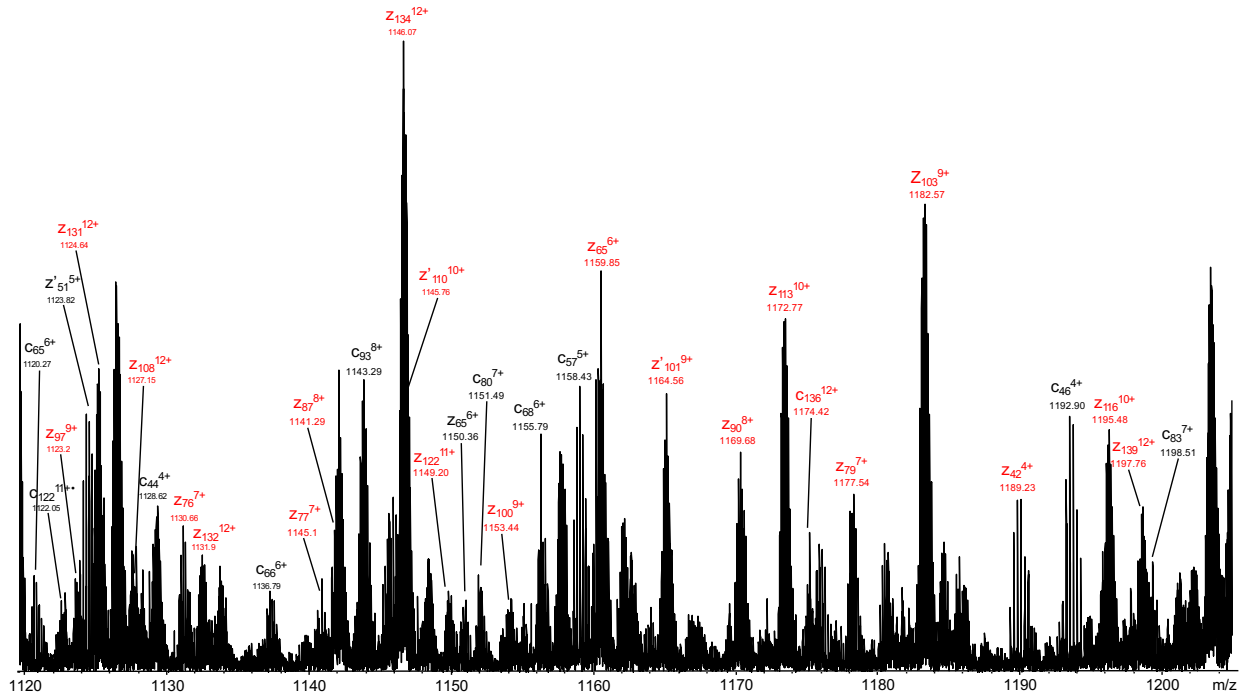


Figure S2. Magnified view of ECD spectrum of 14+-charged cobalt-bound α Syn. Cobalt-bound product ions are labeled in red.

Table S1. Measured masses of α Syn and α Syn-Co complex

Cobalt						
Charge state	Observed αSyn m/z	Calculated $[M+H]^+$	ppm	Observed αSyn+Co m/z	Calculated $[M+Co-H]^+$	ppm
15+	964.4293	14452.3370	7.66	968.2233	14509.2477	7.08
14+	1033.2447	14452.3309	7.24	1037.3103	14509.2494	7.20
13+	1112.6474	14452.3288	7.10	1117.0256	14509.2457	6.94
12+	1205.2842	14452.3301	7.18	1210.0278	14509.2529	7.44
11+	1314.7639	14452.3297	7.15	1319.9381	14509.2462	6.98
10+	1446.1388	14452.3221	6.63	1451.8307	14509.2414	6.65
9+	1606.7086	14452.3190	6.41	1613.0328	14509.2370	6.35
8+	1807.4187	14452.2983	4.98	1814.5339	14509.2205	5.21
7+	2065.4776	14452.2999	5.09	2073.6074	14509.2083	4.36

Table S2. Measured masses of α Syn and α Syn-Mn complex

Manganese						
Charge state	Observed αSyn m/z	Calculated $[M+H]^+$	ppm	Observed αSyn+Mn m/z	Calculated $[M+Mn-H]^+$	ppm
15+	964.4292	14452.3359	7.59	967.9575	14505.2606	7.64
14+	1033.2448	14452.3320	7.31	1037.0250	14505.2558	7.31
13+	1112.6476	14452.3320	7.31	1116.7184	14505.2517	7.03
12+	1205.2837	14452.3241	6.77	1209.6947	14505.2560	7.32
11+	1314.7640	14452.3308	7.23	1319.5744	14505.2458	6.62
10+	1446.1381	14452.3157	6.18	1451.4309	14505.2435	6.46
9+	1606.7064	14452.2990	5.03	1612.5868	14505.2230	5.05
8+	1807.4173	14452.2874	4.22	1814.0337	14505.2190	4.77
7+	2065.4750	14452.2813	3.81	2073.0332	14505.1885	2.67