CHEMISTRY
A EUROPEAN JOURNAL

Supporting Information

A Simple and Effective Catalytic System for Epoxidation of Aliphatic Terminal Alkenes with Manganese(II) as the Catalyst

Kam-Piu Ho, Wing-Leung Wong, Kin-Ming Lam, Cheuk-Piu Lai, Tak-Hang Chan, and Kwok-Yin Wong*

Department Applied Biology and Chemical Technology
The Hong Kong Polytechnic University
Hung Hom, Kwoloon
Hong Kong, SAR China
E-mail: bckywong@polyu.edu.hk
Fax: (+ 852) 23649932

List of Contents:

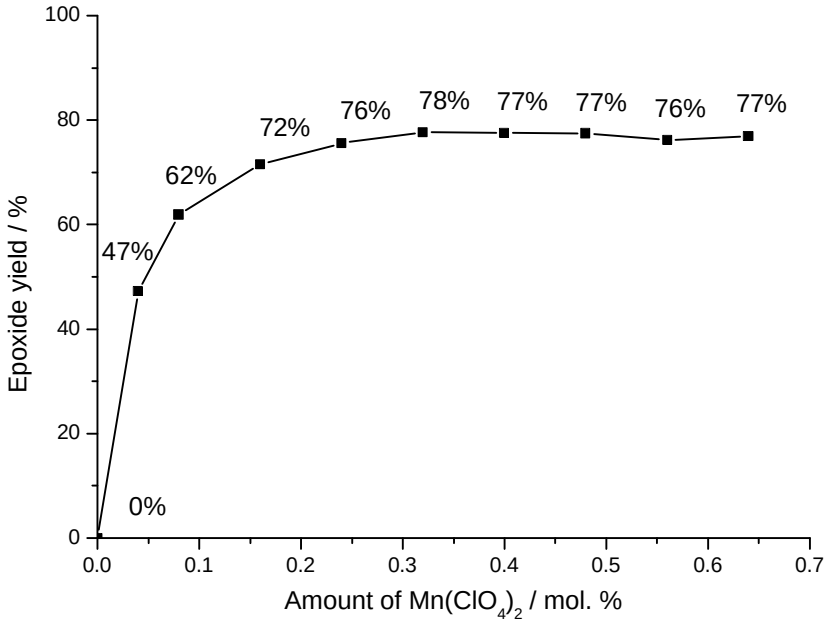


Figure S1. Effect of $Mn(ClO_4)_2$ loading on the catalytic epoxidation of 1-decene at room temperature; epoxide yields determined by GC after reaction of 15 min with tetradecane as the internal standard.

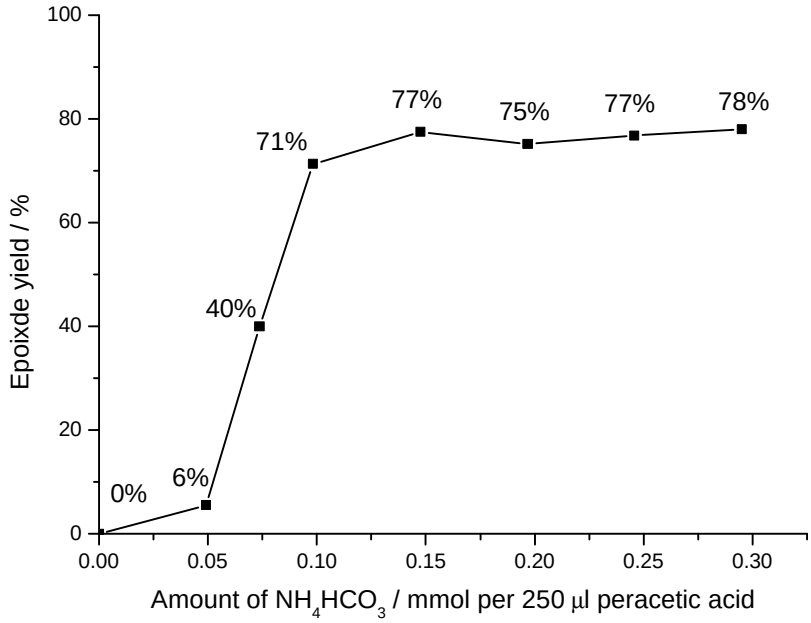


Figure S2. Effect of NH_4HCO_3 loading on the catalytic epoxidation of 1-decene at room temperature; epoxide yields determined by GC after reaction of 15 min with tetradecane as the internal standard.

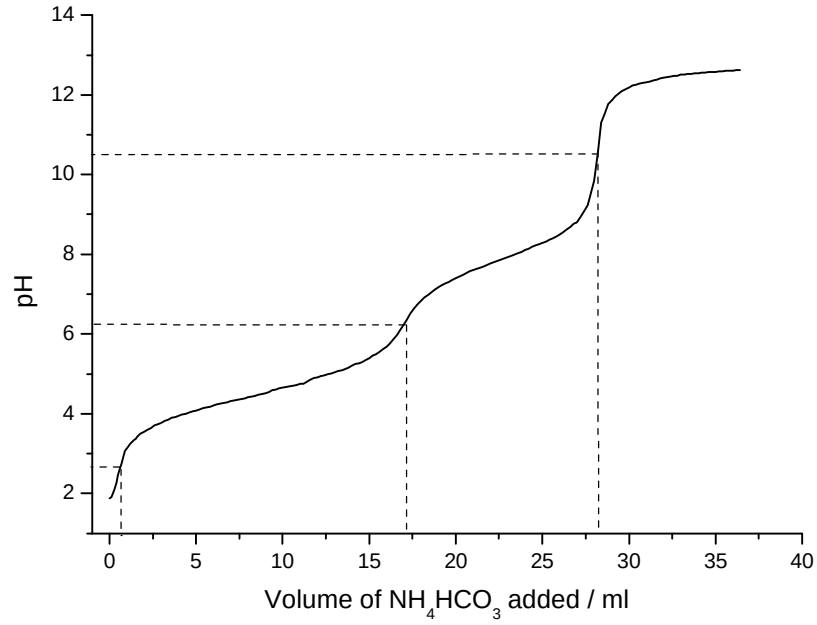


Figure S3. Titration of 0.5 M $NH_4HCO_{3(aq)}$ against 32 wt. % of peracetic acid (500 µl).

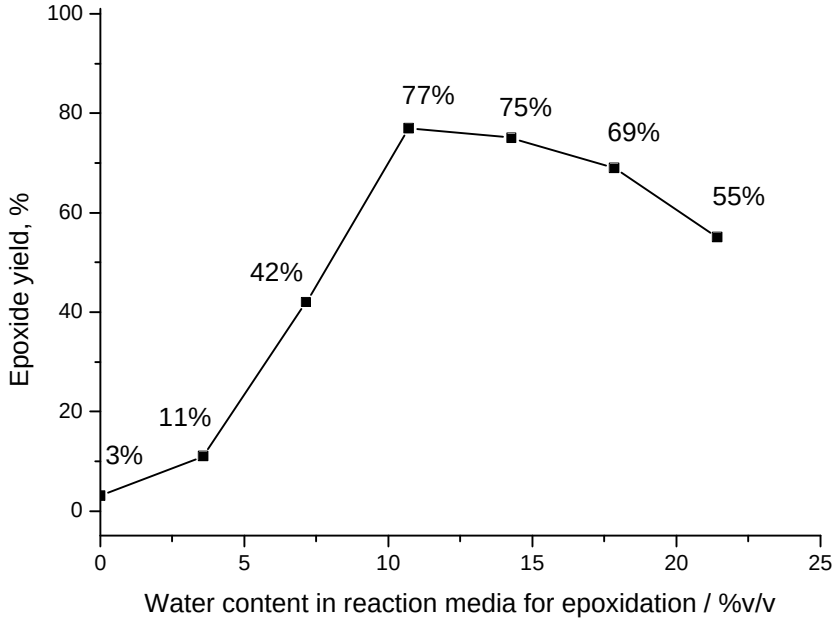


Figure S4. Effect of water content in the acetonitrile on the catalytic epoxidation of 1-decene at room temperature; epoxide yields determined by GC after reaction of 15 min with tetradecane as the internal standard.

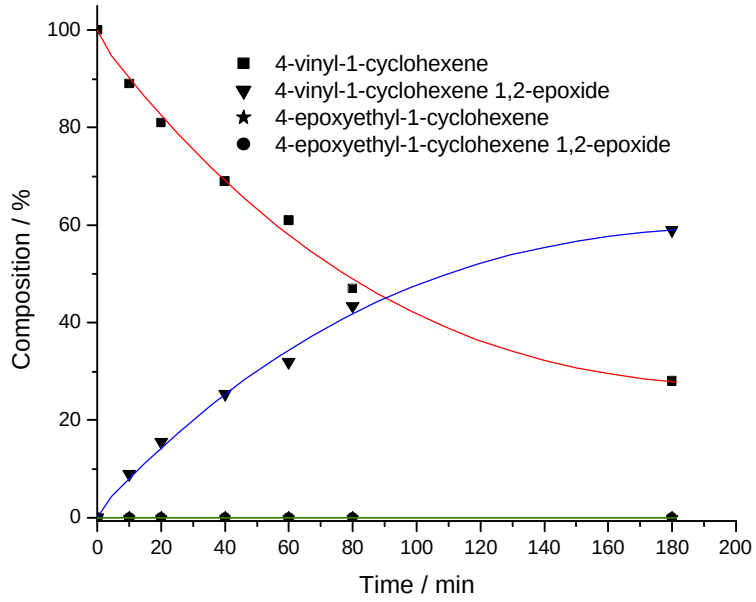


Figure S5. Control experiment in the regioselectivity study with 4-vinyl-1-cyclohexene as the substrate without adding the Mn-catalyst at 25°C.

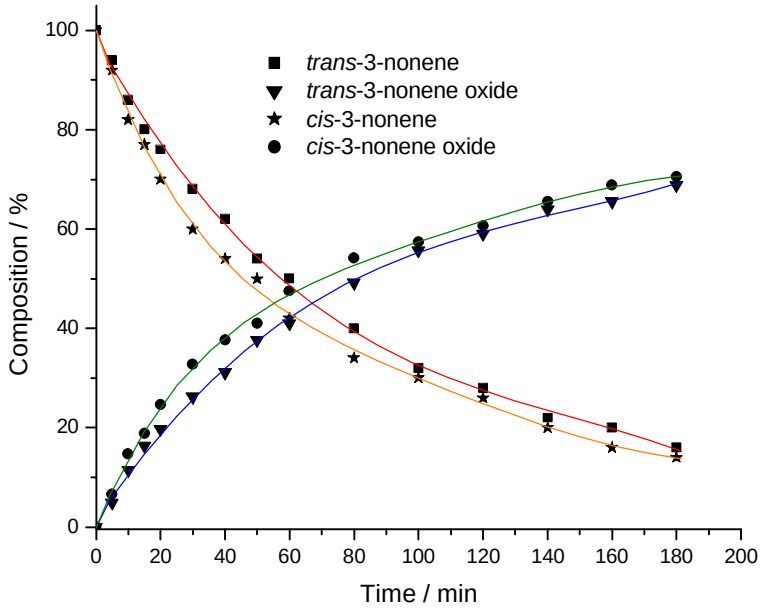


Figure S6. Control experiment for the *trans*-3-nonene/*cis*-3-nonene inter-molecular competition reaction studies without adding the Mn-catalyst at 25°C.

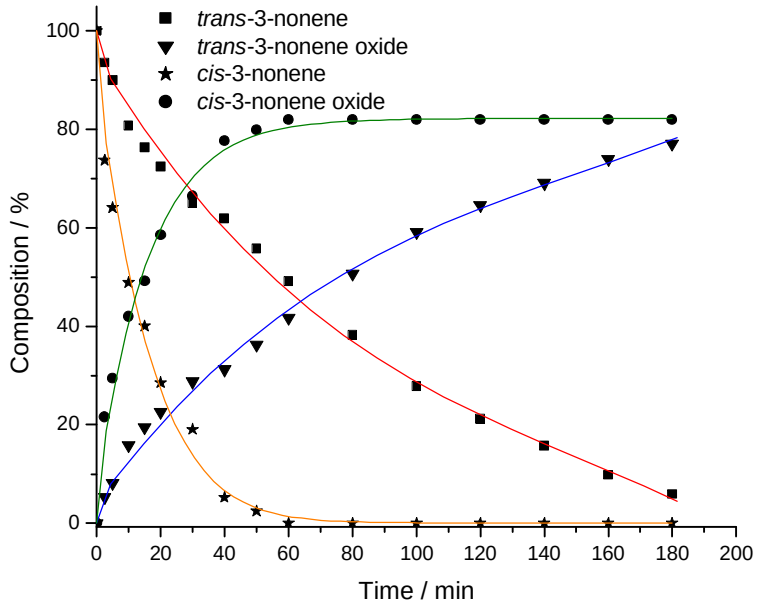


Figure S7. The *trans*-3-nonene/*cis*-3-nonene inter-molecular competition reaction studies with the Mn-catalyst at 25^{o}C.

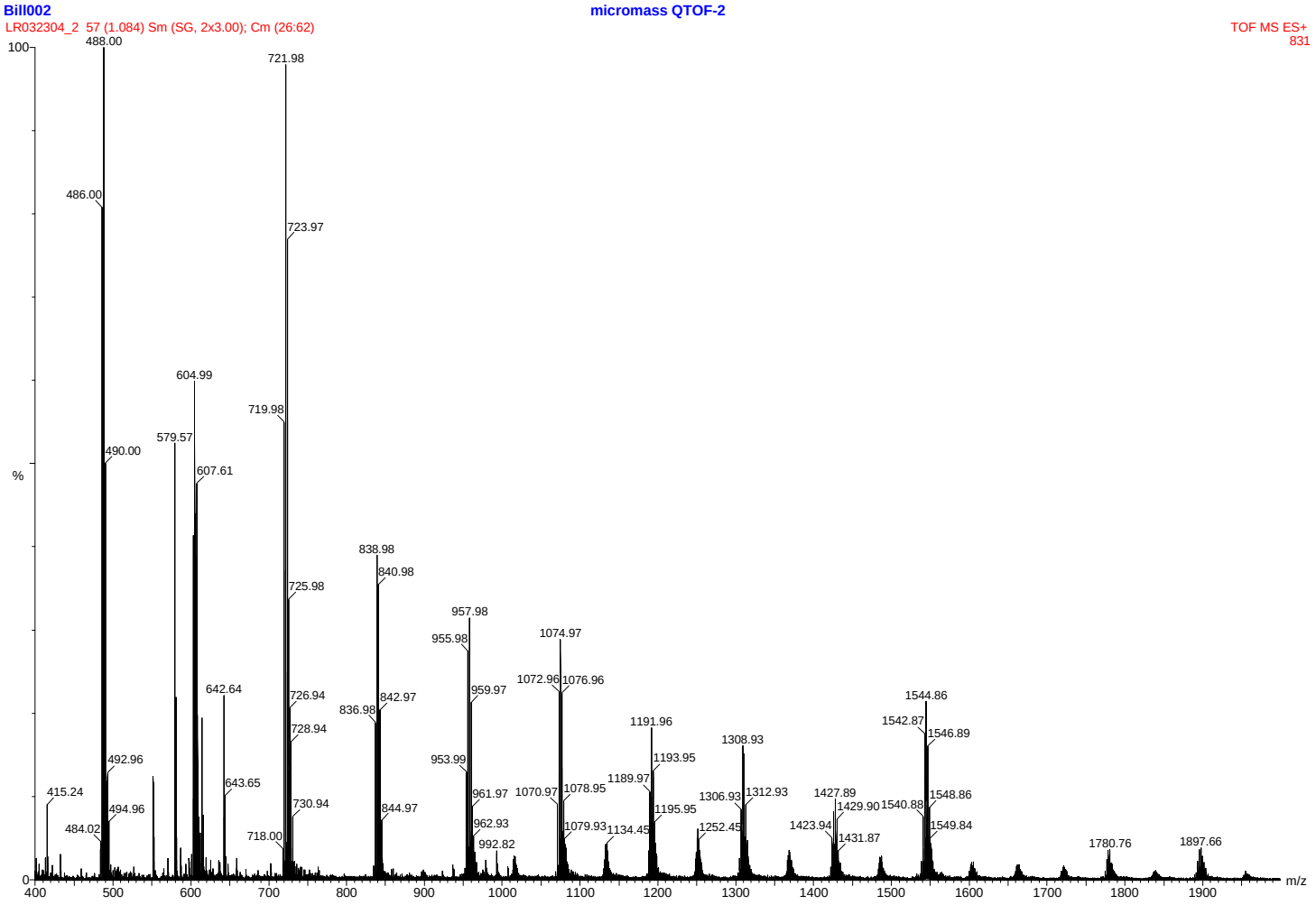


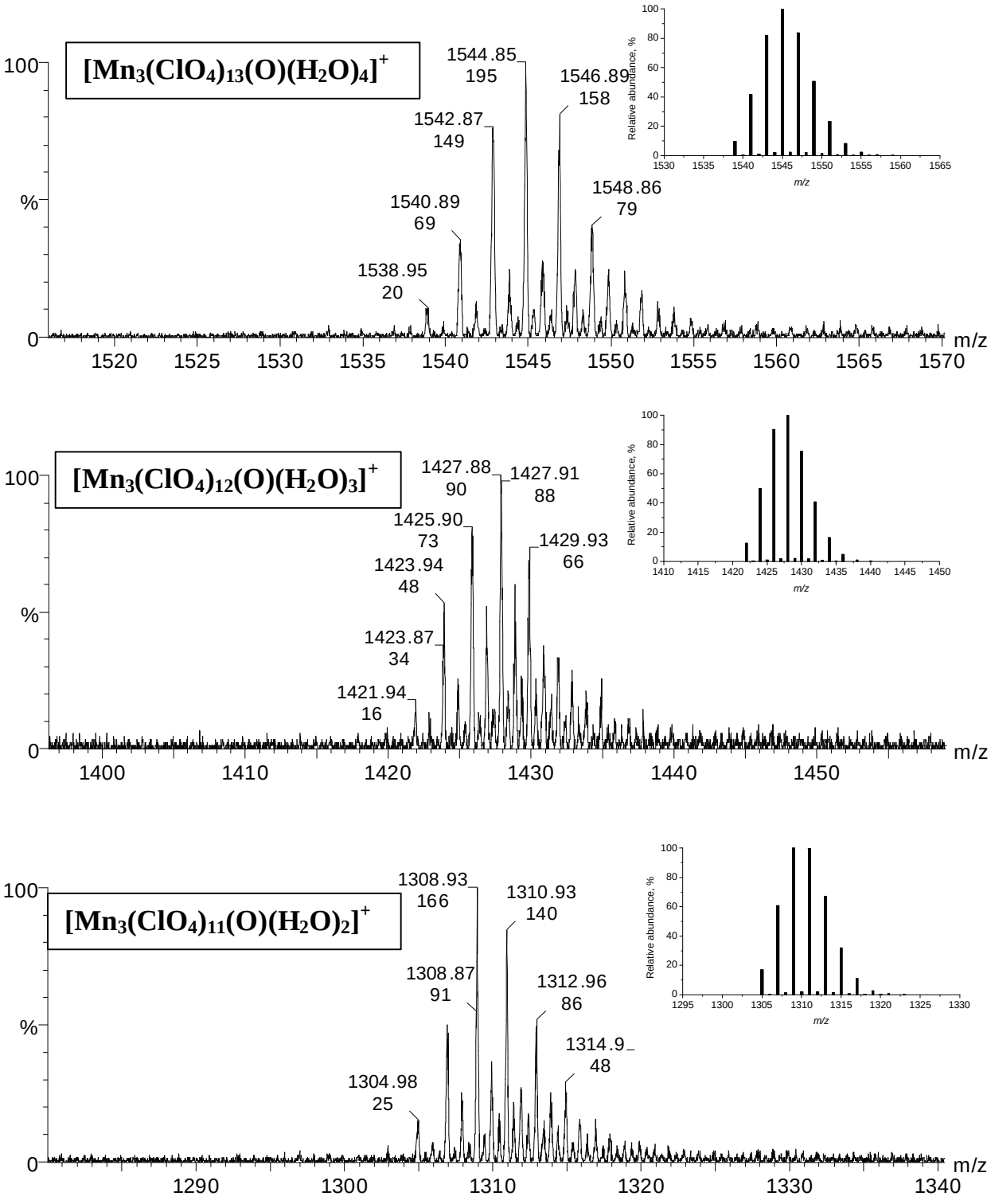
Figure S8. The full MS spectrum of the polymetallic Mn-oxo clusters.

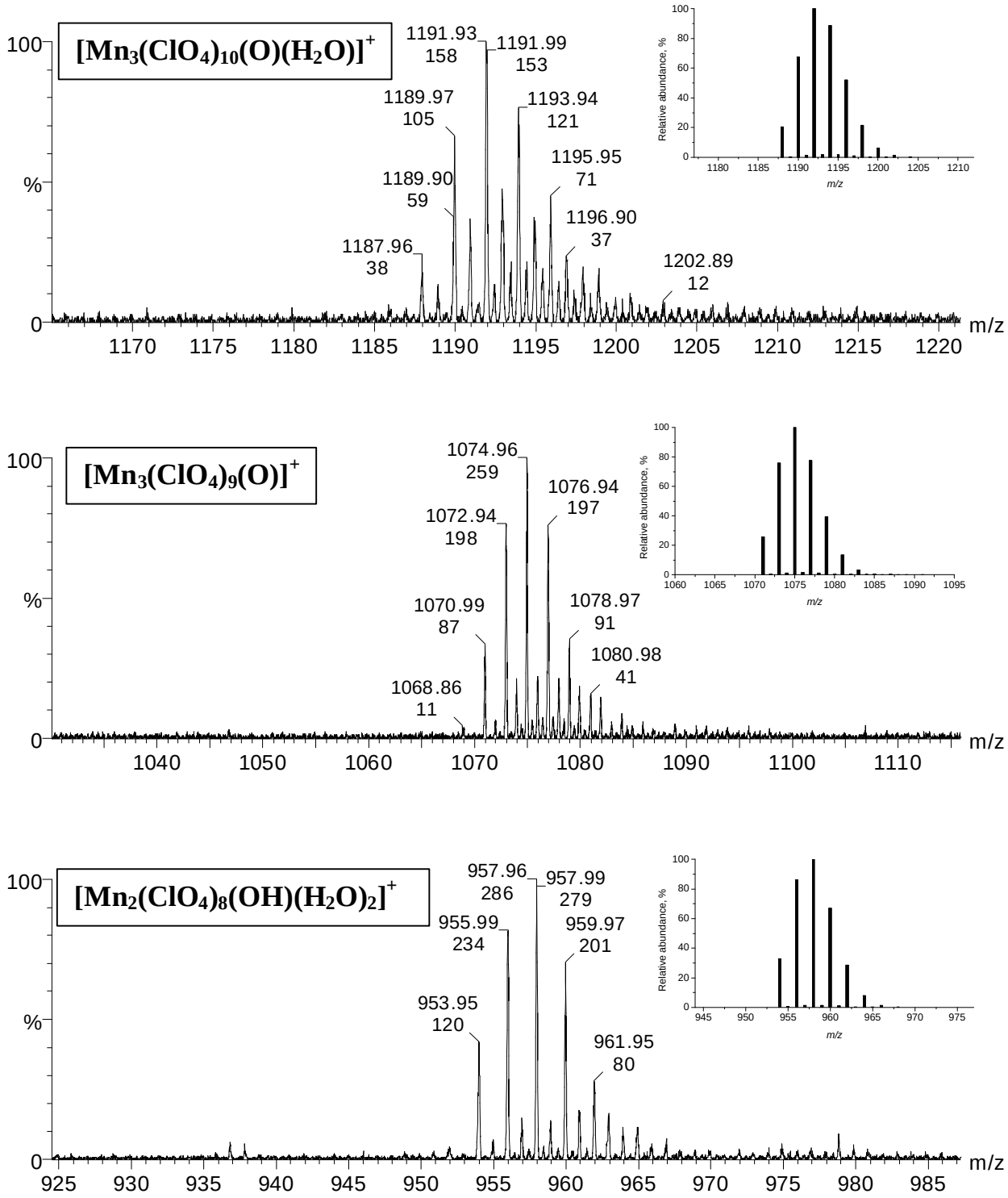
Table S1. Assignment of the fragment/molecule ions produced from ESI-MS in the reaction mixture of the Mn-catalyzed epoxidation and their relatively isotopic abundances (%) in the ion series.[a]

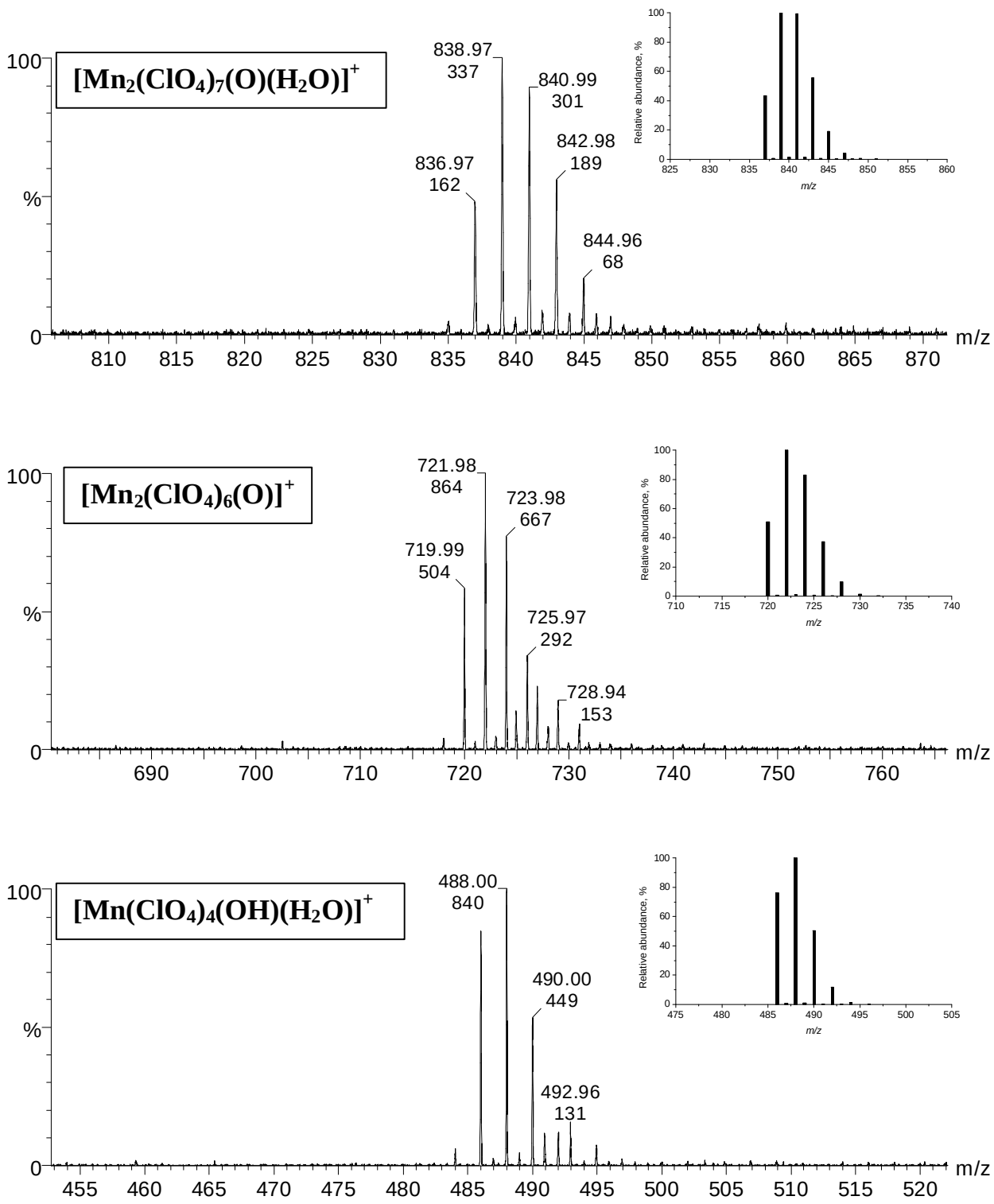
	m/z	486	488	490	492	494		
$[Mn(ClO_4)_4(OH)(H_2O)]^+$	Calc.(%)	76	100	50	12	1.2		
	Obs.(%)	83	100	52	11	--		
	m/z	720	722	724	726	728	730	732
$[Mn_2(ClO_4)_6(O)]^+$	Calc.(%)	51	100	83	37	9.8	1.5	0.1
	Obs.(%)	58	100	76	43	8.0	1.0	--
	m/z	837	839	841	843	845	847	849
$[Mn_2(ClO_4)_7(O)(H_2O)]^+$	Calc.(%)	44	100	99	56	19	4.1	0.5
	Obs.(%)	48	100	88	56	19	5.0	--
	m/z	954	956	958	960	962	964	966
$[Mn_2(ClO_4)_8(OH)(H_2O)_2]^+$	Calc.(%)	33	86	100	67	29	8.0	1.5
	Obs.(%)	40	80	100	69	28	10	3.0
	m/z	1071	1073	1075	1077	1079	1081	1083	1085
$[Mn_3(ClO_4)_9(O)]^+$	Calc.(%)	26	77	100	78	39	14	3.2	0.5
	Obs.(%)	31	77	100	76	32	13	3.0	--
	m/z	1188	1190	1192	1194	1196	1198	1200	202
$[Mn_3(ClO_4)_{10}(O)(H_2O)]^+$	Calc.(%)	21	67	100	89	52	21	6.3	1.3
	Obs.(%)	22	64	100	74	44	18	7.0	2.0
	m/z	1305	1307	1309	1311	1313	1315	1317	1319
$[Mn_3(ClO_4)_{11}(O)(H_2O)_2]^+$	Calc(%)	17	61	100	99	67	32	11	2.8
	Obs(%)	14	46	100	82	51	29	15	3.0
	m/z	1422	1424	1426	1428	1430	1432	1434	1436	1438
$[Mn_3(ClO_4)_{12}(O)(H_2O)_3]^+$	Calc(%)	13	50	90	100	75	41	16	4.9	1.1
	Obs(%)	18	51	80	100	70	31	17	6.0	--
	m/z	1539	1541	1543	1545	1547	1549	1551	1553	1555
$[Mn_3(ClO_4)_{13}(O)(H_2O)_4]^+$	Calc(%)	10	42	82	100	84	51	23	8.1	2.2
	Obs(%)	9	31	74	100	80	37	21	10	4.0

[a] The assignment of chemical formulas to the fragment ions is based on the relatively isotopic abundances and confirmed by comparing with the theoretical calculations.

List S1. A series of ESI-MS fragment/molecule ions for the polymetallic Mn-oxo clusters.




[Mn3(ClO4)10(O)(H2O)]+
1191.93 158
1191.99 153
1189.97 105
1193.94 121
1195.95 71
1189.90 59
1196.90 37
1187.96 38
1202.89 12
100
%
0
1170 1175 1180 1185 1190 1195 1200 1205 1210 1215 1220
m/z
Relative abundance, %
1180 1185 1190 1195 1200 1205 1210
[Mn3(ClO4)9(O)]+
1074.96 259
1076.94 197
1072.94 198
1070.99 87
1078.97 91
1080.98 41
1068.86 11
1040 1050 1060 1070 1080 1090 1100 1110
[Mn2(ClO4)8(OH)(H2O)2]+
957.96 286
957.99 279
955.99 234
959.97 201
953.95 120
961.95 80
925 930 935 940 945 950 955 960 965 970 975 980 985


[Mn2(ClO4)7(O)(H2O)]+
838.97
337
840.99
301
842.98
189
836.97
162
844.96
68
Relative abundance, %
m/z
[Mn2(ClO4)6(O)]+
721.98
864
723.98
667
719.99
504
725.97
292
728.94
153
[Mn(ClO4)4(OH)(H2O)]+
488.00
840
490.00
449
492.96
131
100
%
0
m/z