Supplementary Information

Magnetostructural Coupling, Kondo-like Behavior, and Magnetocaloric Performance in Fe-doped $Nd_{0.5}(Sr_{0.4}Ba_{0.1})CoO_3$ Perovskites

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Table S1: Structural parameters of the $Nd_{0.5}Sr_{0.4}Ba_{0.1}Co_{1-x}Fe_xO_3$ (x = 0–0.2) samples at room temperature obtained through SXRD data Rietveld refinements.

	$Nd_{0.5}Sr_{0.4}Ba_{0.1}Co_{1-x}Fe_xO_3$			
x	**0.0**	**0.04**	**0.12**	**0.2**
	Atoms positions			
(Nd/Sr/Ba) x	0.50193(1)	0.50027(4)	0.50073(4)	0.50419(4)
y	0.25	0.25	0.25	0.25
z	0.50118(5)	0.49754(3)	0.49807(4)	0.50326(5)
(Co/Fe) x	0.5	0.5	0.5	0.5
y	0.0	0.0	0.0	0.0
z	0.0	0.0	0.0	0.0
(O1) x	0.03872(7)	0.03808(1)	0.03272(2)	0.02668(5)
y	0.25	0.25	0.25	0.25
z	0.45818(2)	0.50887(4)	0.49685(5)	0.53159(6)
O2 x	0.24686(5)	0.25416(3)	0.24795(4)	0.26537(2)
y	0.00911(3)	0.02713(6)	0.02448(7)	-0.01051(2)
z	0.73411(3)	0.76462(2)	0.75156(3)	0.72905(4)
	B_{iso}			
Nd/Sr/Ba	0.767(9)	0.726(7)	0.687(7)	0.686(1)
Co/Fe	0.430(1)	0.428(1)	0.372(9)	0.413(1)
O1	0.940(2)	0.552(9)	1.118(1)	1.793(2)
O2	0.940(2)	0.552(9)	1.118(1)	1.793(2)
	Lattice parameters			
a (Å)	5.4144(1)	5.4302(8)	5.4300(2)	5.4232(4)
b (Å)	7.6502(3)	7.6220(3)	7.6334(1)	7.6524(0)
c (Å)	5.3985(2)	5.3929(8)	5.3996(2)	5.4098(6)
V (Å^3)	223.61(4)	223.21(4)	223.81(2)	224.51(4)
	Average bonds (Å) and angles (°)			
$\langle Nd/Sr/Ba - O1\rangle$	2.63(4)	2.64(3)	2.65(2)	2.65(3)
$\langle Nd/Sr/Ba - O2\rangle$	2.70(6)	2.65(1)	2.70(7)	2.70(9)
$\langle Nd/Sr/Ba - O\rangle$	2.67(0)	2.64(7)	2.67(9)	2.68(1)
$\langle Co/Fe - O1\rangle$	1.931(3)	1.917(3)	1.916(7)	1.926(4)
$\langle Co/Fe - O2\rangle$	1.91(8)	1.925(1)	1.92(2)	1.922(2)
$\langle Co/Fe - O\rangle$	1.924(7)	1.921(2)	1.919(4)	1.924(3)
$\langle Co/Fe - O1 - Co/Fe\rangle$	164.1(9)	167.3(6)	169.3(7)	166.5(2)
$\langle Co/Fe - O2 - Co/Fe\rangle$	174.5(1)	167.4(4)	168.8(4)	170.4(1)
$\langle Co/Fe - O - Co/Fe\rangle$	169.3(5)	167.4(0)	169.1(1)	168.4(7)
	Reliability factors			
R_p (%)	13.0	7.68	12.3	11.9
R_{wp} (%)	17.3	9.84	16.8	17.1
R_{exp} (%)	2.99	5.25	2.84	3.73
R_{Bragg} (%)	5.73	5.07	6.86	7.73
χ^2	33.7	3.51	37.8	21.0

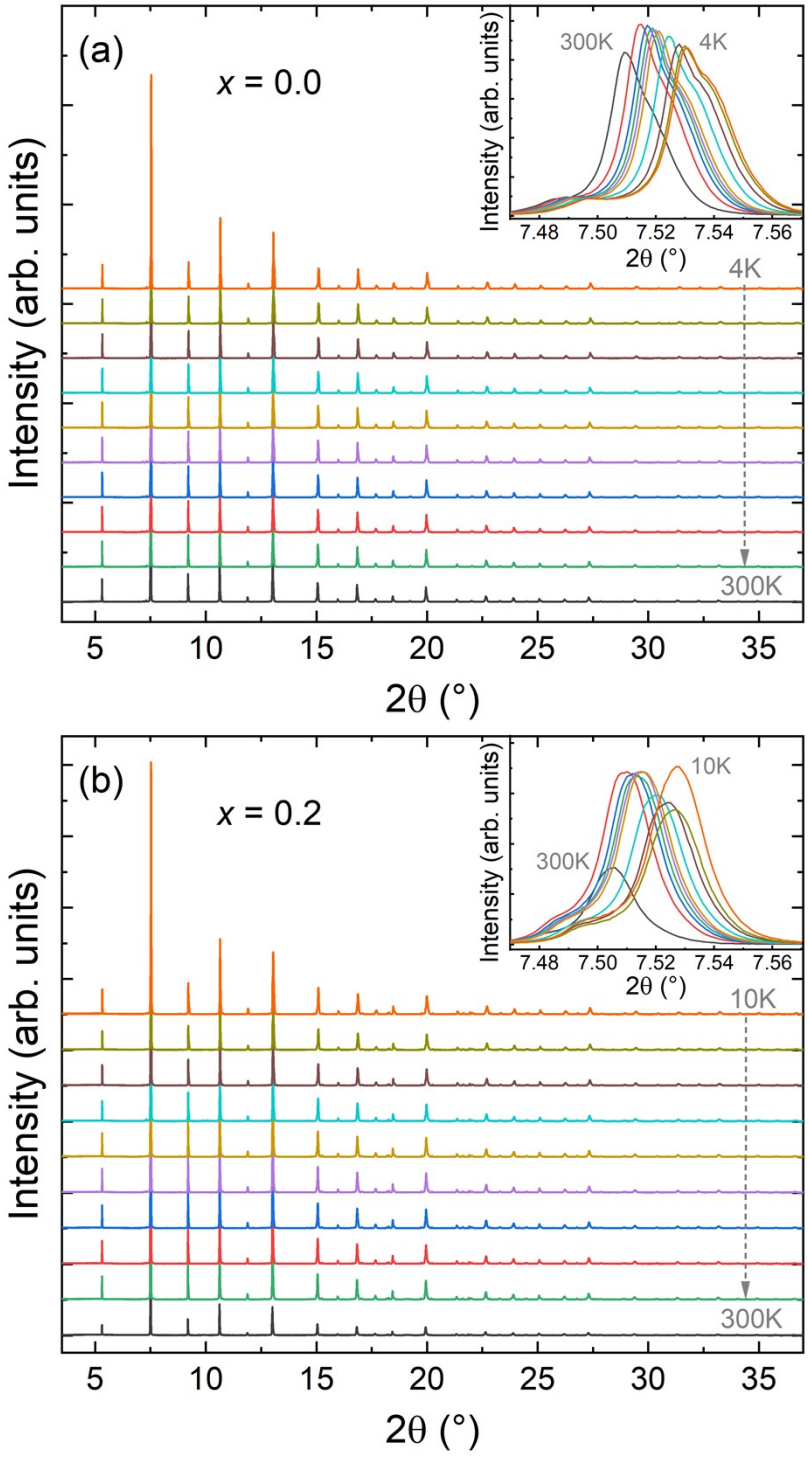

Fig. S1: SXRD temperature-dependent in the 4-300K range for the x = 0.0 (a) and x = 0.2 (b) samples.

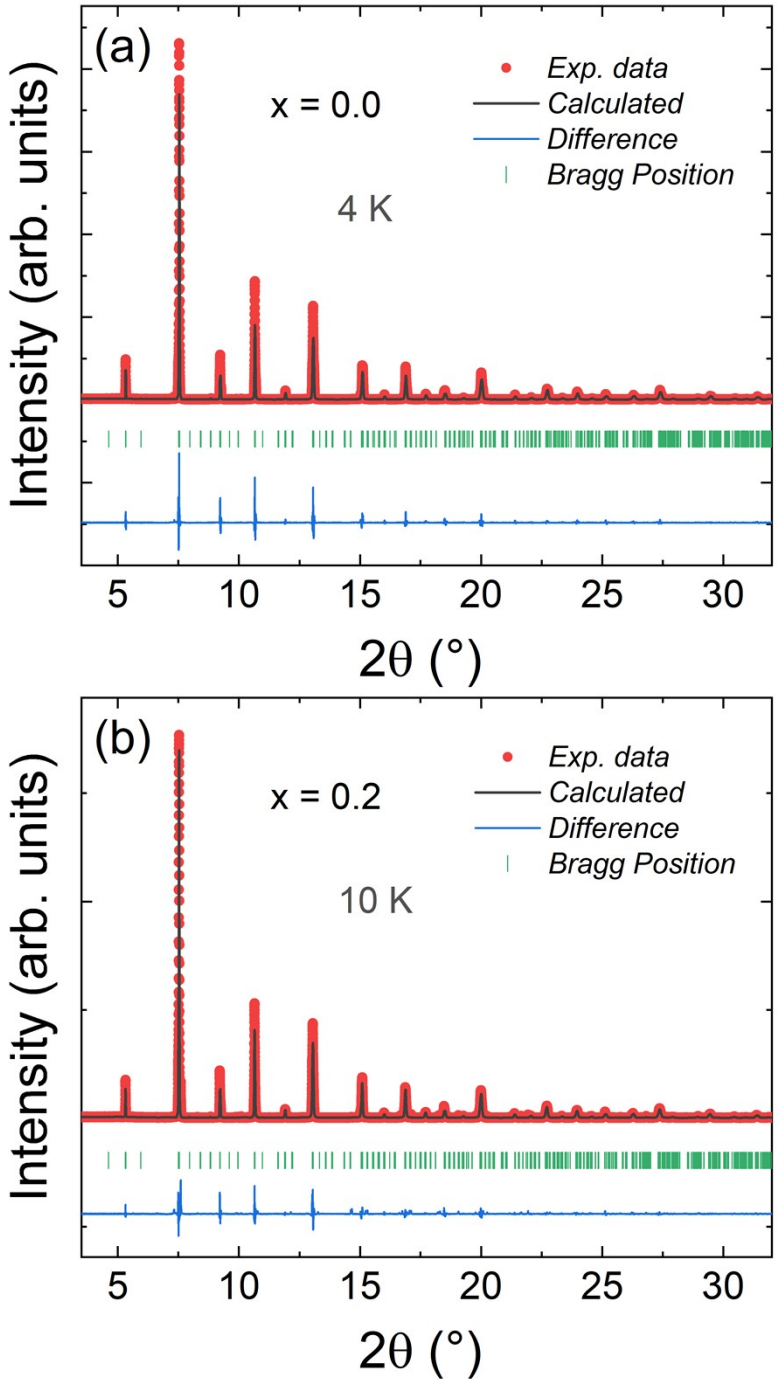

Fig. S2: Rietveld refinement of the SXRD data for (a) x = 0.0 at 4 K, and (b) x = 0.2 at 10 K.

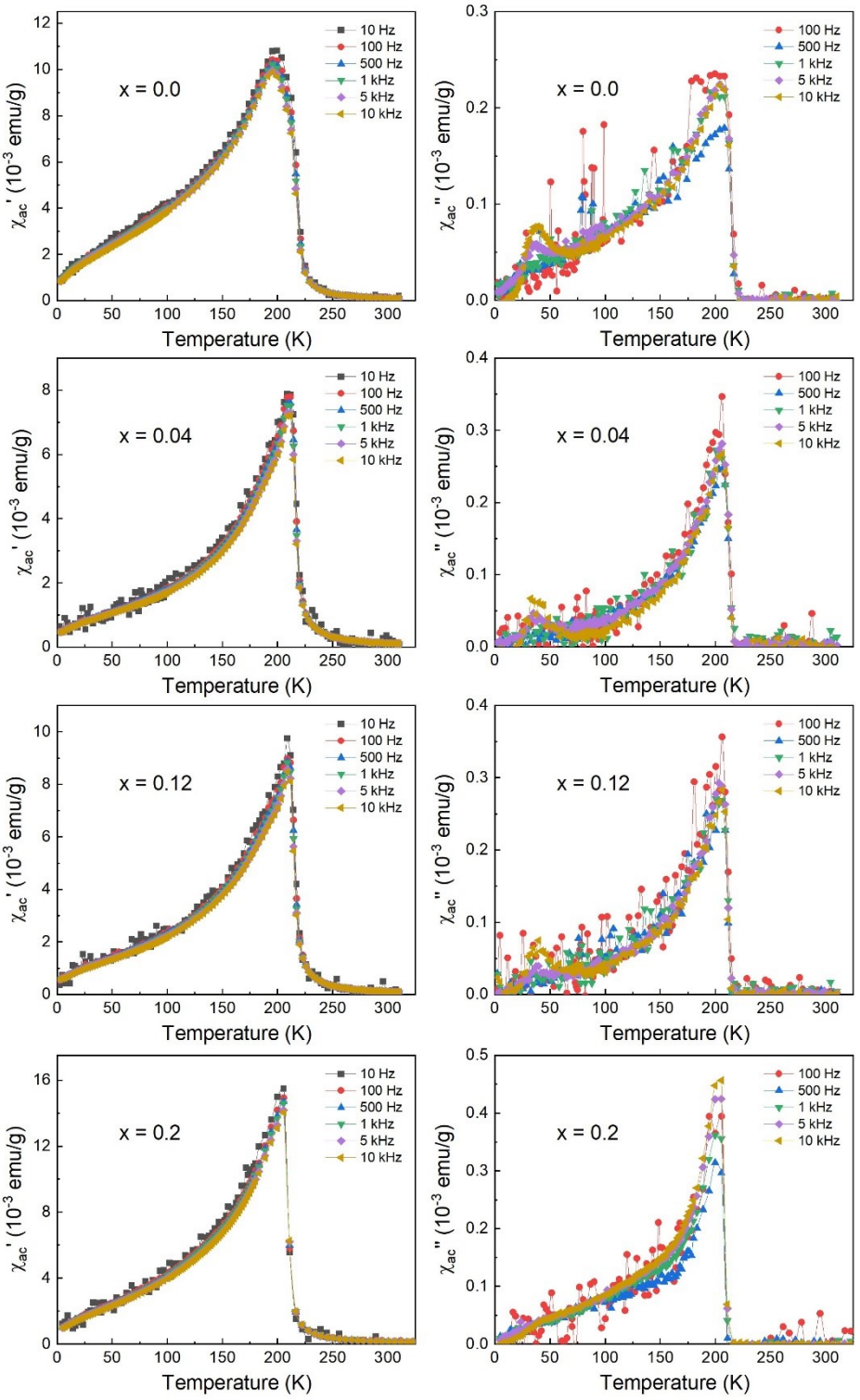

Fig. S3: *ac* magnetic susceptibility (χ_{ac}) data taken at frequencies (f) between 0.1–10 kHz as a function of Fe-content.

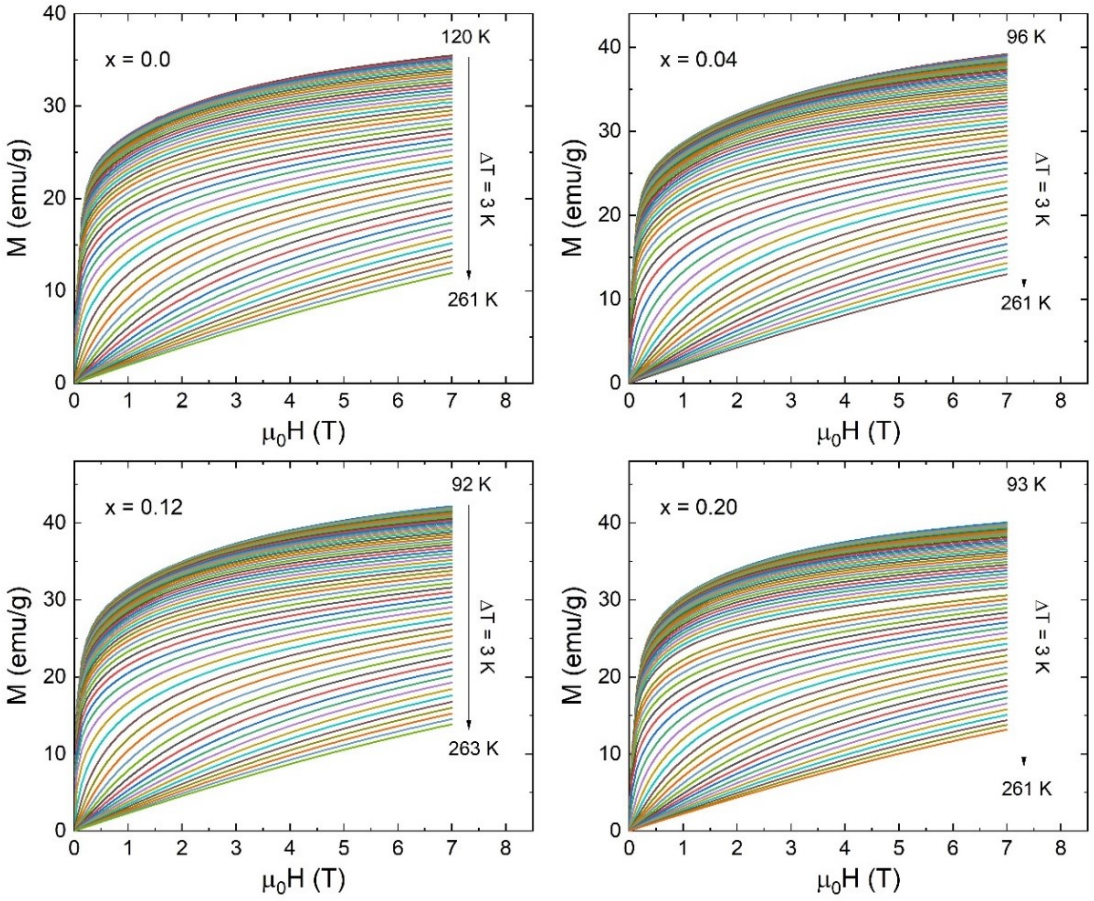

Fig. S4: *M*(*H*) isotherms temperature-dependent for the $Nd_{0.5}Sr_{0.4}Ba_{0.1}Co_{1-x}Fe_xO_3$ (x = 0–0.2) samples.

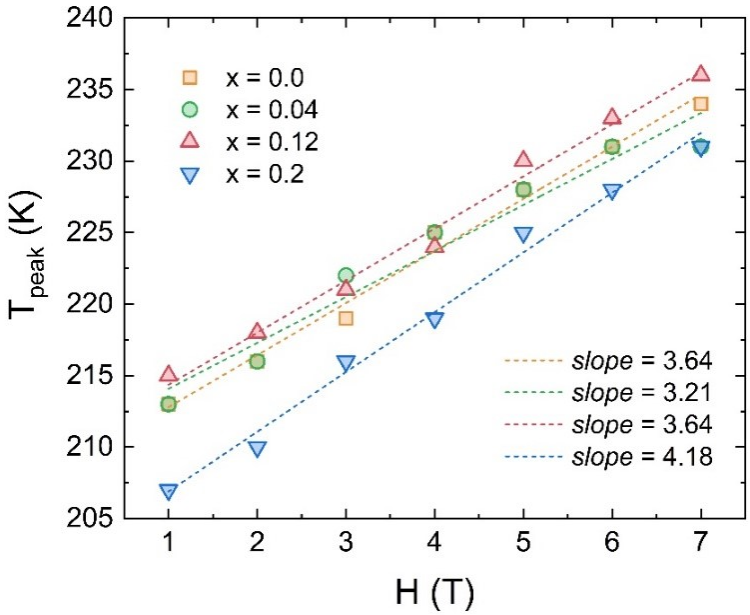

Fig. S5: Linear fitting of T_{peak} data for the $Nd_{0.5}Sr_{0.4}Ba_{0.1}Co_{1-x}Fe_xO_3$ (x = 0–0.2) samples.

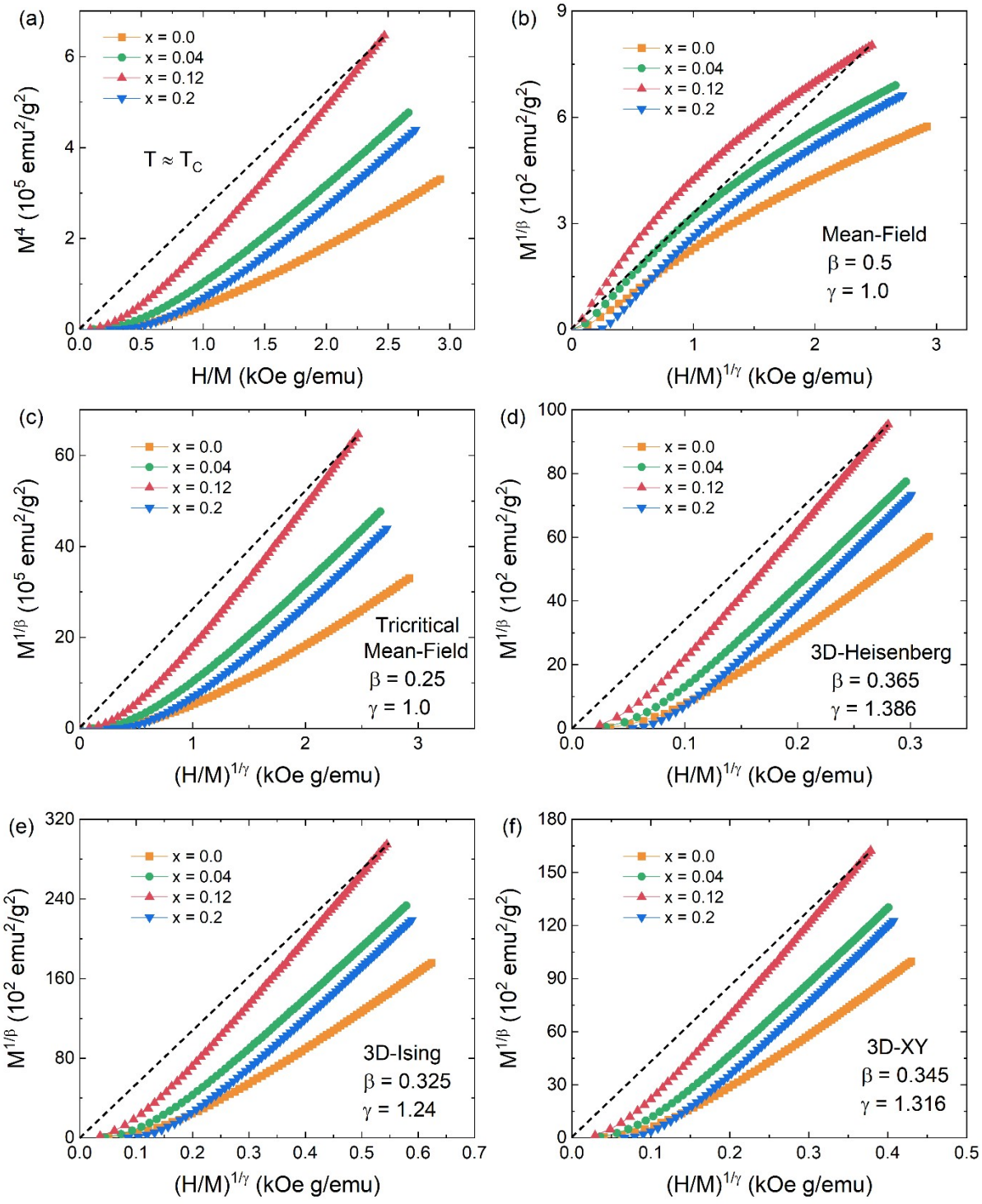

Fig. S6: (a) M^4 versus H/M plots for the $Nd_{0.5}Sr_{0.4}Ba_{0.1}Co_{1-x}Fe_xO_3$ ($x = 0$–0.2) samples. Modified Arrott-plots $M^{1/\beta}$ vs $(H/M)^{1/\gamma}$ for curves at $T = T_C$ with the models: (b) mean-field, (c) tricritical mean-field, (d) 3D-Heisenberg, (e) 3D-Ising, and (f) 3D XY.

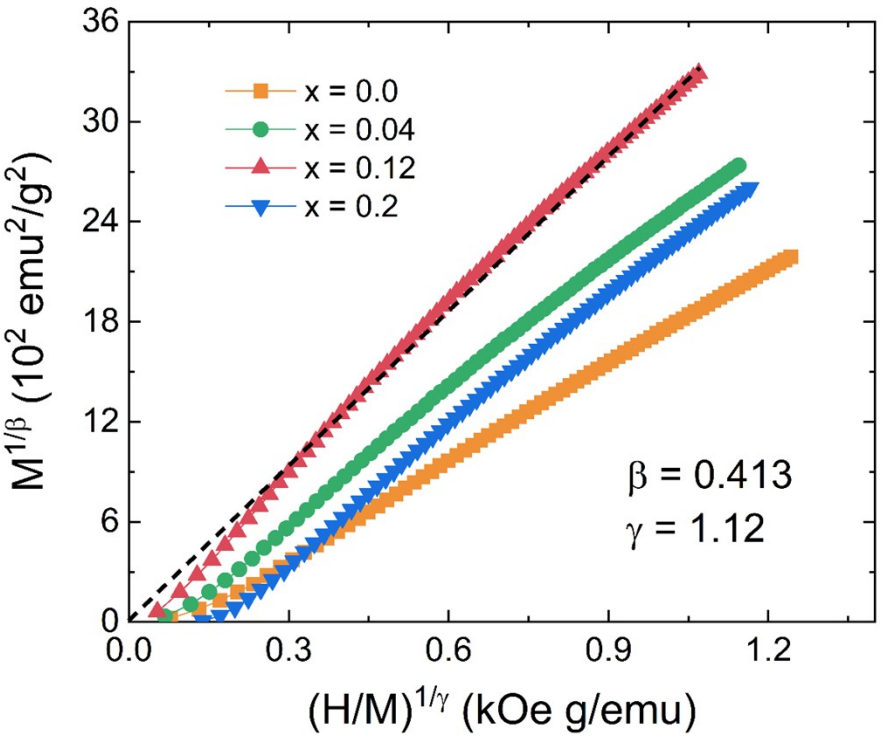

Fig. S7: Modified Arrott-plots [$M^{1/\beta}$ vs $(H/M)^{1/\gamma}$] constructed with the critical exponents β = 0.413 and γ = 1.12.

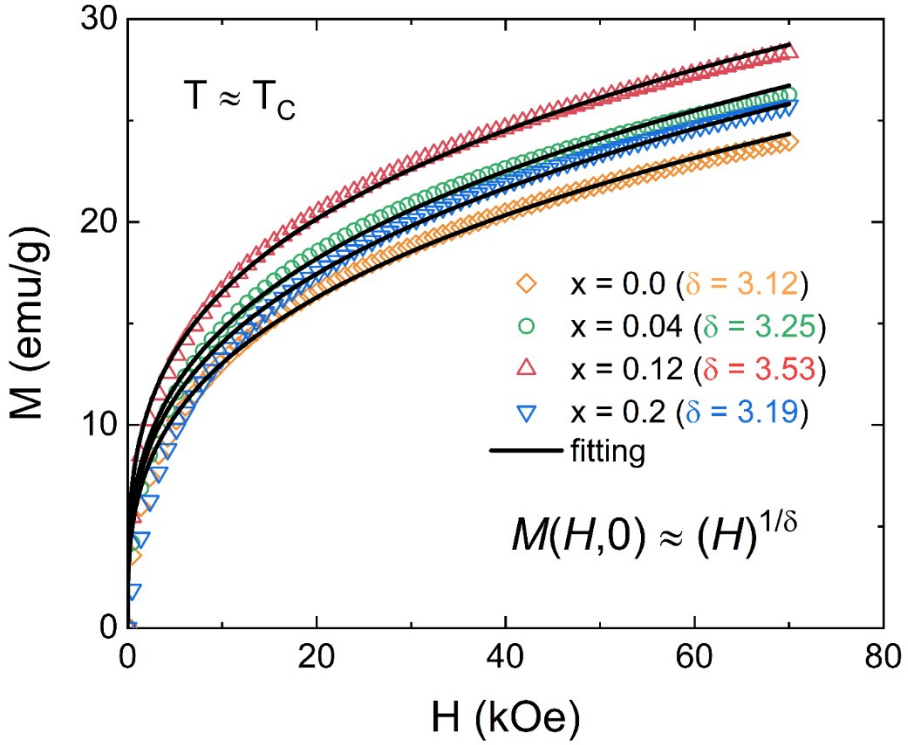

Fig. S8: Fitting of the isotherms at $T = T_C$ by $M(H,0) \approx (H)^{1/\delta}$ relation for the $Nd_{0.5}Sr_{0.4}Ba_{0.1}Co_{1-x}Fe_xO_3$ (x = 0–0.2) samples.

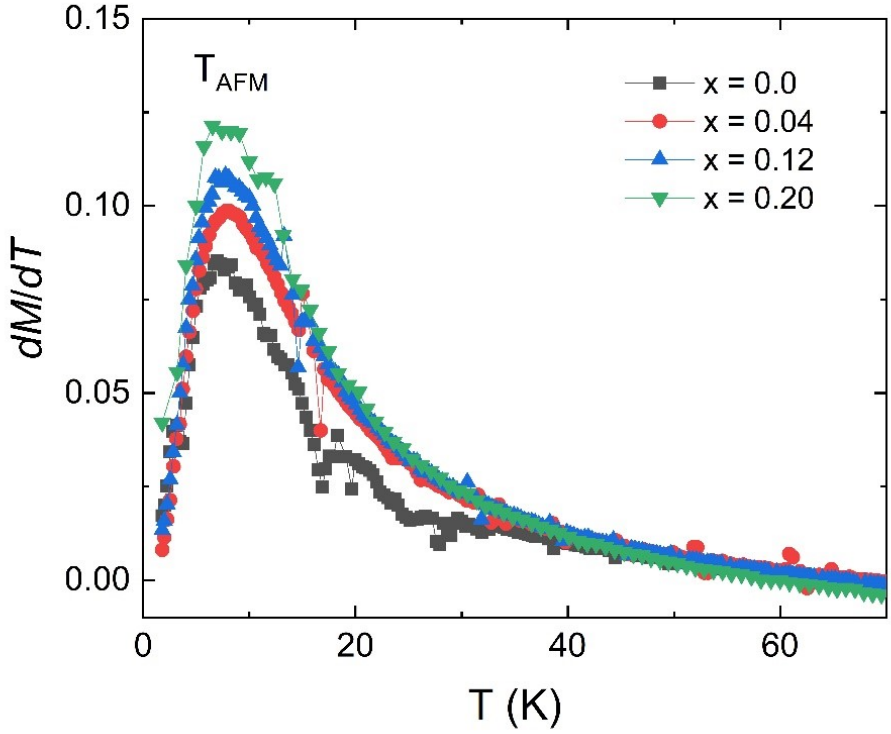

Fig. S9: *dM*/*dT*(*T*) curves at lower temperature for the $Nd_{0.5}Sr_{0.4}Ba_{0.1}Co_{1-x}Fe_xO_3$ (x = 0–0.2) samples.