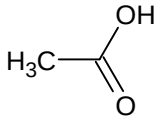
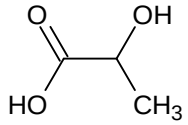
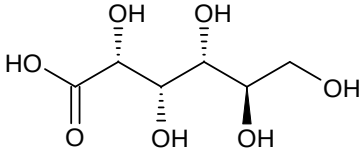
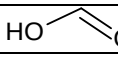
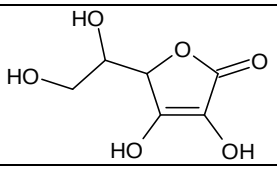
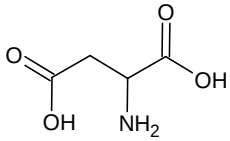
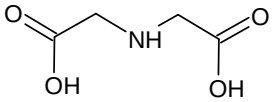
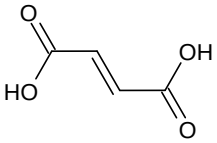
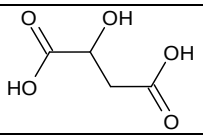
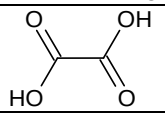
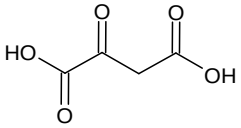
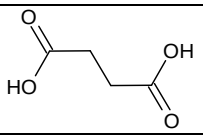
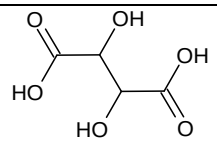
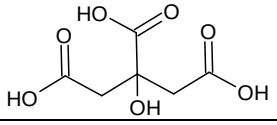
Table S1. Leading groups of organic acids, formula, dissociation reactions, and corresponding pKa [2,132,133].

Type of organic acid	Organic acid	Formula	Dissociation reaction	Chemical structure
Monocarboxylic	Acetic	$C_2H_4O_2$	$HC_2H_3O_2 \rightarrow C_2H_3O_2^- + H^+ \ (pKa1 = 4.76)$	
	Lactic	$C_3H_6O_3$	$HC_3H_5O_3 \rightarrow C_3H_5O_3^- + H^+ \ (pKa1 = 3.86)$	
	Gluconic	$C_6H_{12}O_7$	$HC_6H_{11}O_7^- \rightarrow C_6H_{11}O_7^- + H^+ \ (pKa1 = 3.86)$	
Dicarboxylic acid	Formic	CH_2O_2	$HC_2HO_2 \rightarrow C_2HO_2^- + H^+ \ (pKa1 = 3.75)$	
	Ascorbic	$C_6H_8O_6$	$H_2C_6H_6O_6 \rightarrow HC_6H_6O_6^- + H^+ \ (pKa1 = 4.17)$ $HC_6H_6O_6^- \rightarrow C_6H_6O_6^{2-} + H^+ \ (pKa2 = 11.57)$	
	Aspartic	$C_4H_7NO_4$	$H_2C_4H_5NO_4 \rightarrow HC_4H_5NO_4^- + H^+ \ (pKa1 = 2.10)$ $HC_4H_5NO_4^- \rightarrow C_4H_5NO_4^{2-} + H^+ \ (pKa2 = 3.86)$	
	Iminodiacetic	$C_4H_7NO_4$	$H_2C_4H_5NO_4 \rightarrow HC_4H_5NO_4^- + H^+ \ (pKa1 = 2.54)$ $HC_4H_6NO_4^- \rightarrow C_4H_5NO_4^{2-} + H^+ \ (pKa2 = 9.12)$	
	Maleic	$C_4H_4O_4$	$H_2C_4H_2O_4 \rightarrow HC_4H_2O_4^- + H^+ \ (pKa1 = 1.83)$ $HC_4H_2O_4^- \rightarrow C_4H_2O_4^{2-} + H^+ \ (pKa2 = 6.07)$	
	Malic	$C_4H_6O_5$	$H_2C_4H_2O_5 \rightarrow HC_4H_2O_5^- + H^+ \ (pKa1 = 3.40)$ $HC_4H_4O_5^- \rightarrow C_4H_4O_5^{2-} + H^+ \ (pKa2 = 5.11)$	
	Oxalic	$C_2H_2O_4$	$H_2C_2O_4 \rightarrow HC_2O_4^- + H^+ \ (pKa1 = 1.23)$ $HC_2O_4^- \rightarrow C_2O_4^{2-} + H^+ \ (pKa2 = 4.19)$	
	Oxaloacetic	$C_4H_4O_5$	$H_2C_4H_2O_5 \rightarrow HC_4H_2O_5^- + H^+ \ (pKa1 = 2.22)$ $HC_4H_2O_5^- \rightarrow C_4H_2O_5^{2-} + H^+ \ (pKa2 = 3.89)$	
	Succinic	$C_4H_6O_4$	$H_2C_4H_4O_4 \rightarrow HC_4H_4O_4^- + H^+ \ (pKa1 = 4.22)$ $HC_4H_4O_4^- \rightarrow C_4H_4O_4^{2-} + H^+ \ (pKa2 = 5.70)$	
	Tartaric	$C_4H_6O_6$	$H_2C_4H_4O_6 \rightarrow HC_4H_4O_6^- + H^+ \ (pKa1 = 3.03)$	

Type of organic acid	Organic acid	Formula	Dissociation reaction	Chemical structure
			$HC_4H_4O_6^- \rightarrow C_4H_4O_6^{2-} + H^+ \ (pKa2 = 4.37)$	
Tricarboxylic acid	Citric	$C_6H_8O_7$	$H_3C_6H_5O_7 \rightarrow H_2C_6H_5O_7^- + H^+ \ (pKa1 = 2.79)$ $H_2C_6H_5O_7^- \rightarrow HC_6H_5O_7^{2-} + H^+ \ (pKa2 = 4.30)$ $HC_6H_5O_7^{2-} \rightarrow C_6H_5O_7^{3-} + H^+ \ (pKa3 = 5.65)$	
	Isocitric	$C_6H_8O_7$	$H_3C_6H_5O_7 \rightarrow H_2C_6H_5O_7^- + H^+ \ (pKa1 = 3.28)$ $H_2C_6H_5O_7^- \rightarrow HC_6H_5O_7^{2-} + H^+ \ (pKa2 = 4.71)$ $HC_6H_5O_7^{2-} \rightarrow C_6H_5O_7^{3-} + H^+ \ (pKa3 = 6.39)$	