

Equilibria in Aqueous Cobalt(II) – Reduced Schiff Base *N*-(2-hydroxybenzyl)alanine System: Chemical Characterization, Kinetic Analysis, Antimicrobial and Cytotoxic Properties

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- Page 3. **Figure S1.** Species distribution curves as a function of pH for AlaSal; $C_{\text{AlaSal}} = 2.0 \times 10^{-2}$ M.
- Page 4. **Figure S2.** Tandem mass spectrum of $[\text{LH}_3]^+$ – $m/z = 196.0$, $C_{\text{AlaSal}} = 1.0 \times 10^{-2}$ M.
- Page 5. **Figure S3.** ESI-MS spectra for ligand in positive ion-mode at various pH, $C_{\text{AlaSal}} = 1.0 \times 10^{-2}$ M. Explanation of the adduct signal described in the text:
 $m/z = 111.0$ [fragment ion $m/z = 79 + \text{CH}_3\text{OH}]^+$
 $m/z = 174.0$ [deprotonated fragment ion $m/z = 152 + \text{Na}]^+$
 $m/z = 211.0$ [fragment ion $m/z = 152 + \text{NaOH} + \text{H}_2\text{O}]^+$.
- Page 6. **Figure S4.** ESI-MS spectra for ligand in negative ion-mode at various pH, $C_{\text{AlaSal}} = 1.0 \times 10^{-2}$ M.
- Page 7. **Figure S5.** Negative-ion ESI-MS spectra for the complexes formed in the $\text{Co}(\text{NO}_3)_2/\text{AlaSal}$ system at ligand-to-metal molar ratio 2:1, at various pH, $C_{\text{AlaSal}} = 2 \times 10^{-2}$ M. Explanation of the signal described in the text:
 $m/z = 615.0$ [$\text{CoL}_2\text{H} + \text{deprotonated fragment ion } m/z = 107 + \text{HNO}_3]^-$.
- Page 8. **Figure S6.** Positive-ion ESI-MS spectra for the complexes formed in the $\text{Co}(\text{NO}_3)_2/\text{AlaSal}$ system at ligand-to-metal molar ratio 2:1, at various pH, $C_{\text{AlaSal}} = 2 \times 10^{-2}$ M. Explanation of the signal described in the text:
 $m/z = 218.0$ [$\text{Co}(\text{II}) + \text{fragment ion } m/z = 79 + 2\text{OH} + \text{NO}_2]^+$
 $m/z = 576.0$ [$\text{CoL}_2\text{H} + \text{fragment ion } m/z = 107 + \text{Na}]^+$
 $m/z = 618.0$ [$\text{CoL}_2\text{H} + \text{fragment ion } m/z = 108 + \text{H} + \text{HNO}_3]^+$
 $m/z = 662.0$ [$\text{CoL}_2\text{H} + \text{fragment ion } m/z = 152 + \text{H} + \text{HNO}_3]^+$.

Page 9. **Figure S7. (a)** UV spectra of AlaSal during titration within the pH range 1.90–11.30, $C_{\text{AlaSal}} = 2 \times 10^{-4}$ M; **(b)** Molar absorption coefficients (ϵ) of various ligand ionic forms.

Page 10. **Figure S8. (a)** UV/Vis spectra during titration of the Co(II) – AlaSal system at ligand-to-metal molar ratio 2:1, pH range 1.80–11.43; $C_{\text{AlaSal}} = 2 \times 10^{-3}$ M. **(b)** Molar absorption coefficients (ϵ) of the two complexes accepted by HypSpec deconvolution.

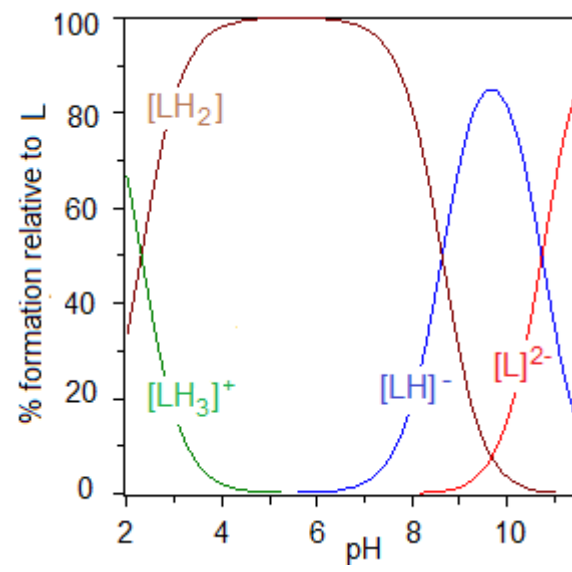


Figure S1. Species distribution curves as a function of pH for AlaSal; $C_{\text{AlaSal}} = 2.0 \times 10^{-2}$ M.

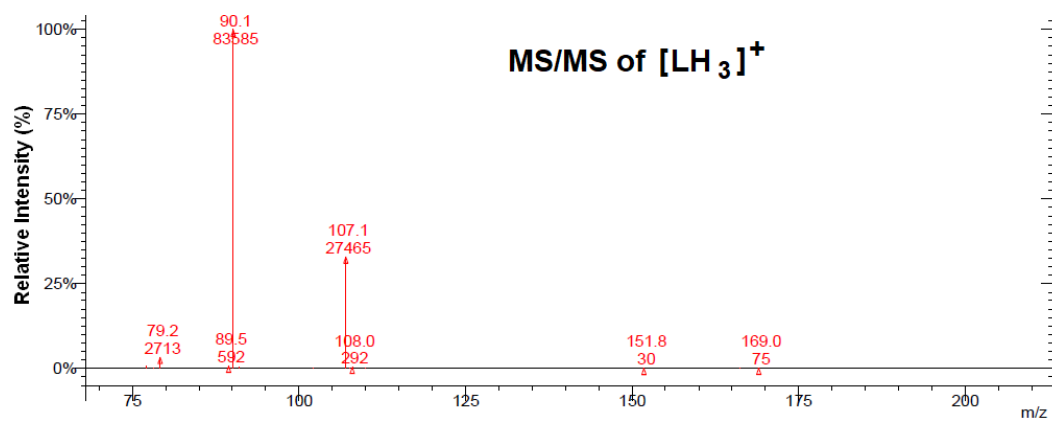


Figure S2. Tandem mass spectrum of $[LH_3]^+$ – $m/z = 196.0$, $C_{AlaSal} = 1.0 \times 10^{-2}$ M.

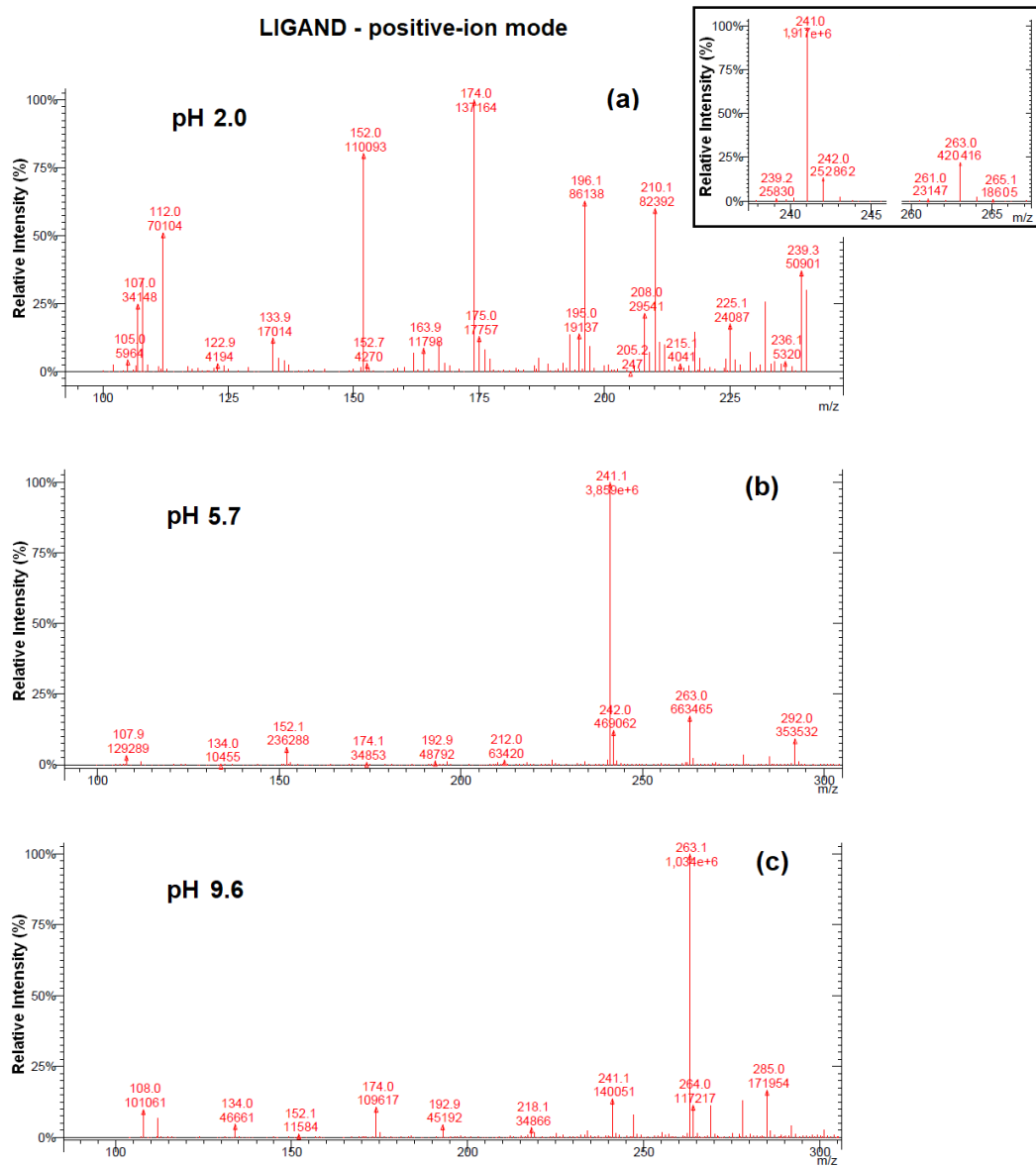


Figure S3. ESI-MS spectra for ligand in positive ion-mode at various pH, $C_{AlaSal} = 1.0 \times 10^{-2}$ M.

Explanation of the adduct signal described in the text:

$m/z = 111.0$ [fragment ion $m/z = 79 + CH_3OH$]⁺

$m/z = 174.0$ [deprotonated fragment ion $m/z = 152 + Na$]⁺

$m/z = 211.0$ [fragment ion $m/z = 152 + NaOH + H_2O$]⁺.

LIGAND - negative-ion mode

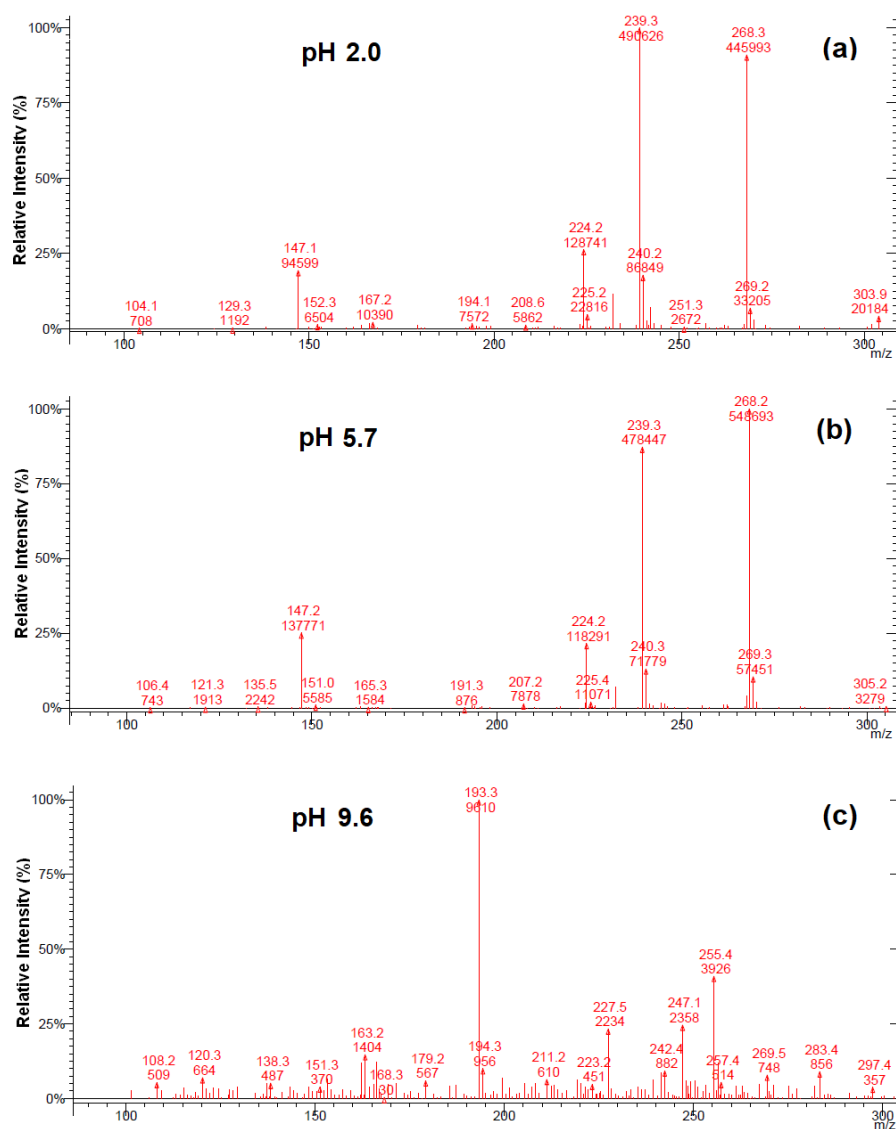


Figure S4. ESI-MS spectra for ligand in negative ion-mode at various pH, $C_{AlaSal} = 1.0 \times 10^{-2}$ M.

ligand-to-metal molar ratio 2:1
(negative-ion mode)

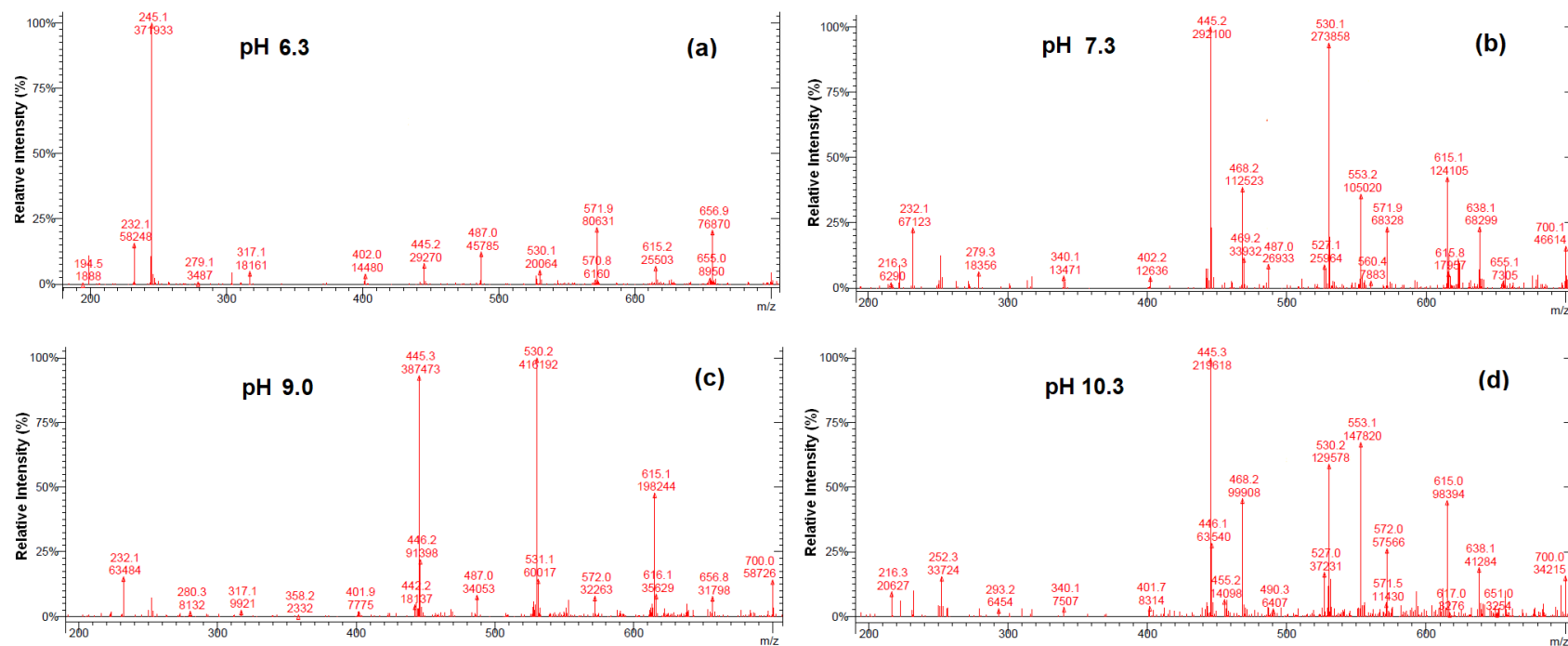


Figure S5. Negative-ion ESI-MS spectra for the complexes formed in the $\text{Co}(\text{NO}_3)_2/\text{AlaSal}$ system at ligand-to-metal molar ratio 2:1, at various pH, $C_{\text{AlaSal}} = 2 \times 10^{-2}$ M. Explanation of the signal described in the text: $m/z = 615.0$ [$\text{CoL}_2\text{H} + \text{deprotonated fragment ion } m/z = 107 + \text{HNO}_3$].

ligand-to-metal molar ratio 2:1
(positive-ion mode)

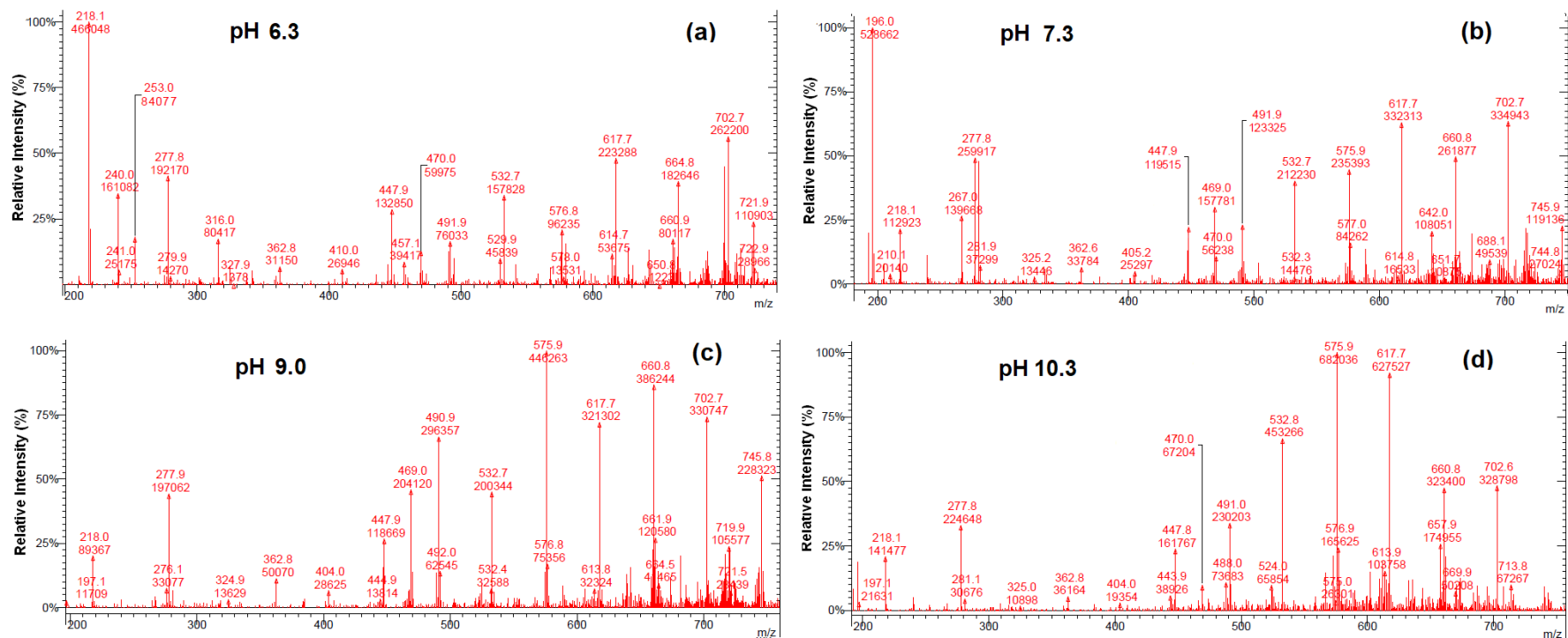


Figure S6. Positive-ion ESI-MS spectra for the complexes formed in the $\text{Co}(\text{NO}_3)_2/\text{AlaSal}$ system at ligand-to-metal molar ratio 2:1, at various pH, $C_{\text{AlaSal}} = 2 \times 10^{-2}$ M. Explanation of the signal described in the text:
 $m/z = 218.0$ [$\text{Co}(\text{II}) + \text{fragment ion } m/z = 79 + 2\text{OH} + \text{NO}_2$]⁺
 $m/z = 576.0$ [$\text{CoL}_2\text{H} + \text{fragment ion } m/z = 107 + \text{Na}$]⁺
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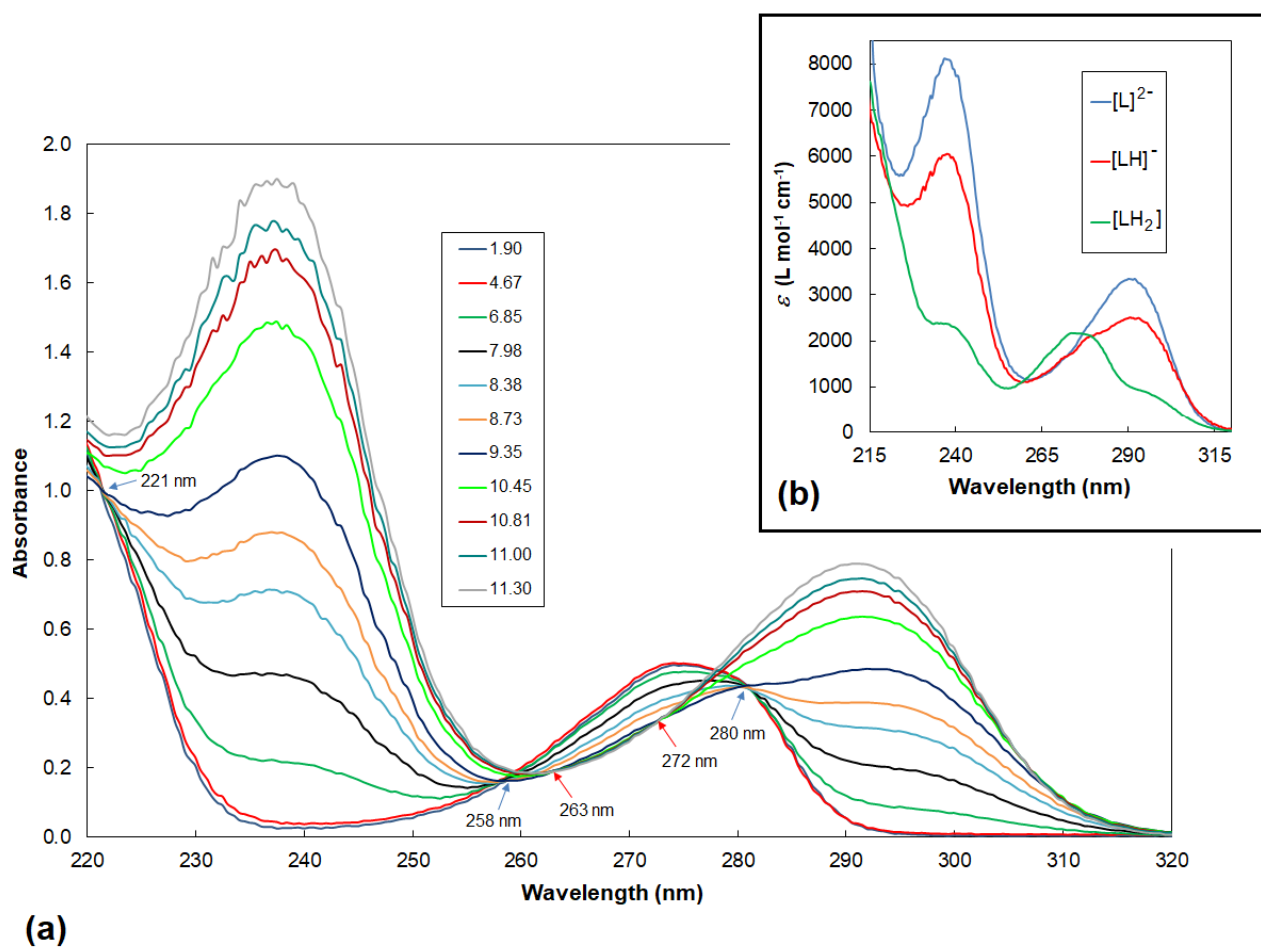


Figure S7. (a) UV spectra of AlaSal during titration within the pH range 1.90–11.30, $C_{\text{AlaSal}} = 2 \times 10^{-4}$ M; (b) Molar absorption coefficients (ϵ) of various ligand ionic forms.

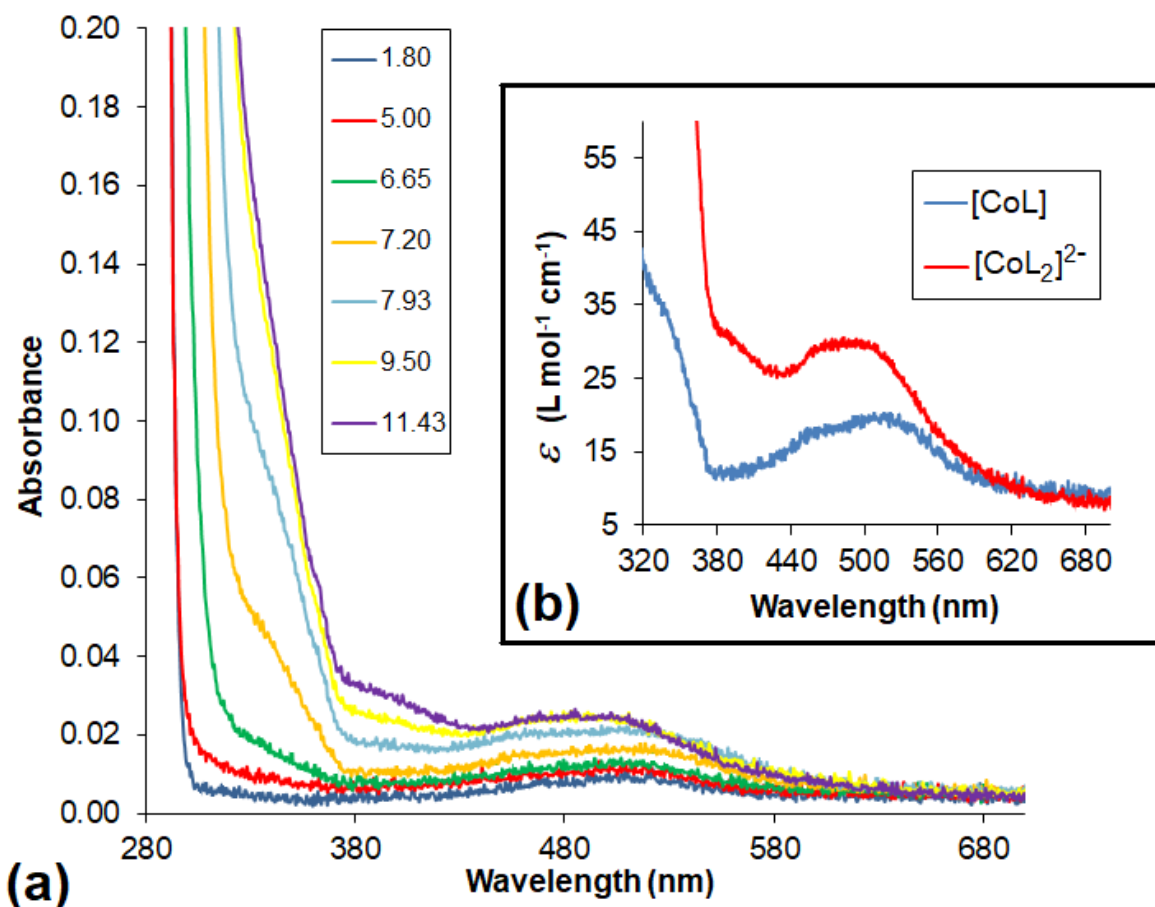


Figure S8. (a) UV/Vis spectra during titration of the Co(II) – AlaSal system at ligand-to-metal molar ratio 2:1, pH range 1.80–11.43; $C_{\text{AlaSal}} = 2 \times 10^{-3}$ M. (b) Molar absorption coefficients (ϵ) of the two complexes accepted by HypSpec deconvolution.