Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Synthesis and properties of differently charged chemiluminescent acridinium ester labels

(Supplementary Material)

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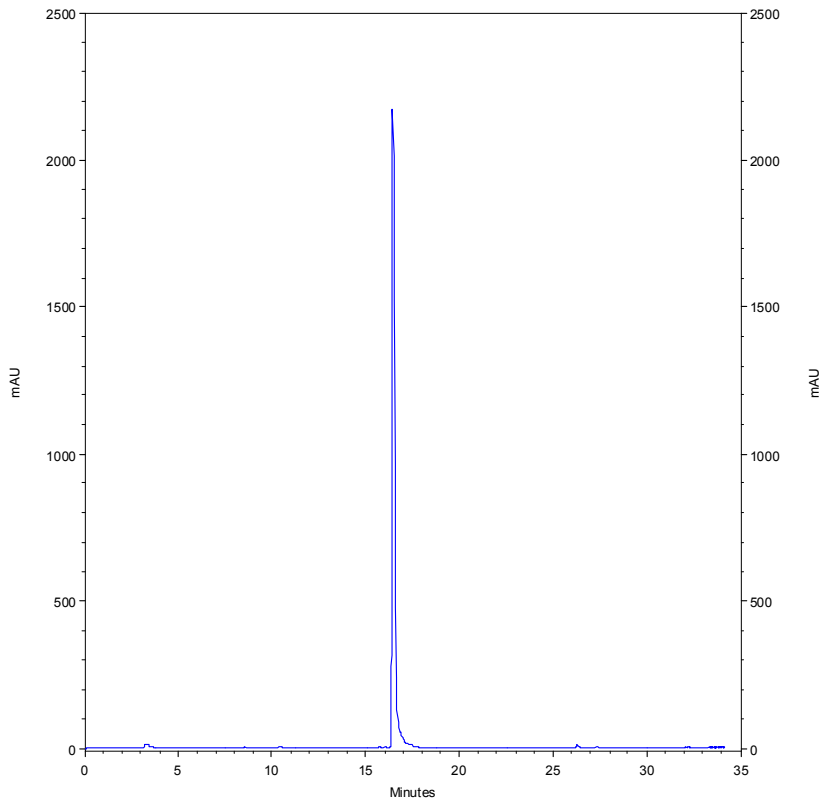
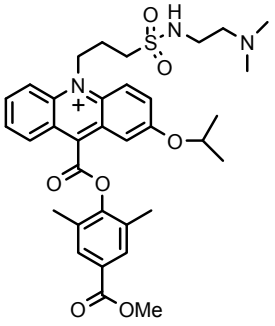


Figure S1. HPLC trace of compound **2**. HPLC conditions: Phenomenex C_{18}, 10 micron, 3.9 x 300 mm column, 30 minute gradient of 10 → 100% MeCN/water (each with 0.05% TFA), 1 mL/minute, UV detection at 260 nm.



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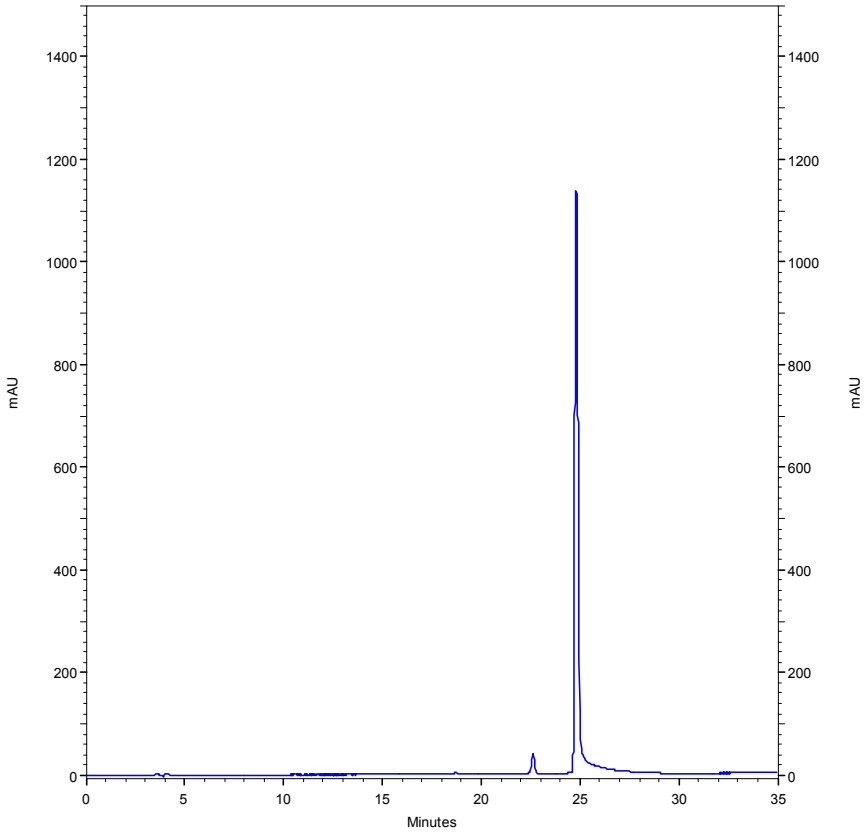
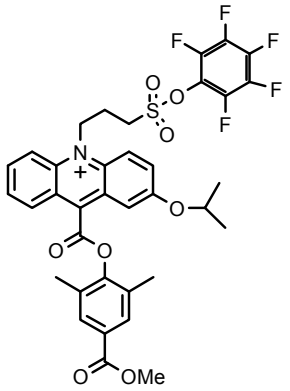


Figure S2. HPLC trace of compound **3a**. HPLC conditions: Phenomenex C_{18}, 10 micron, 3.9 x 300 mm column, 30 minute gradient of 10 → 100% MeCN/water (each with 0.05% TFA), 1 mL/minute, UV detection at 260 nm.



3a

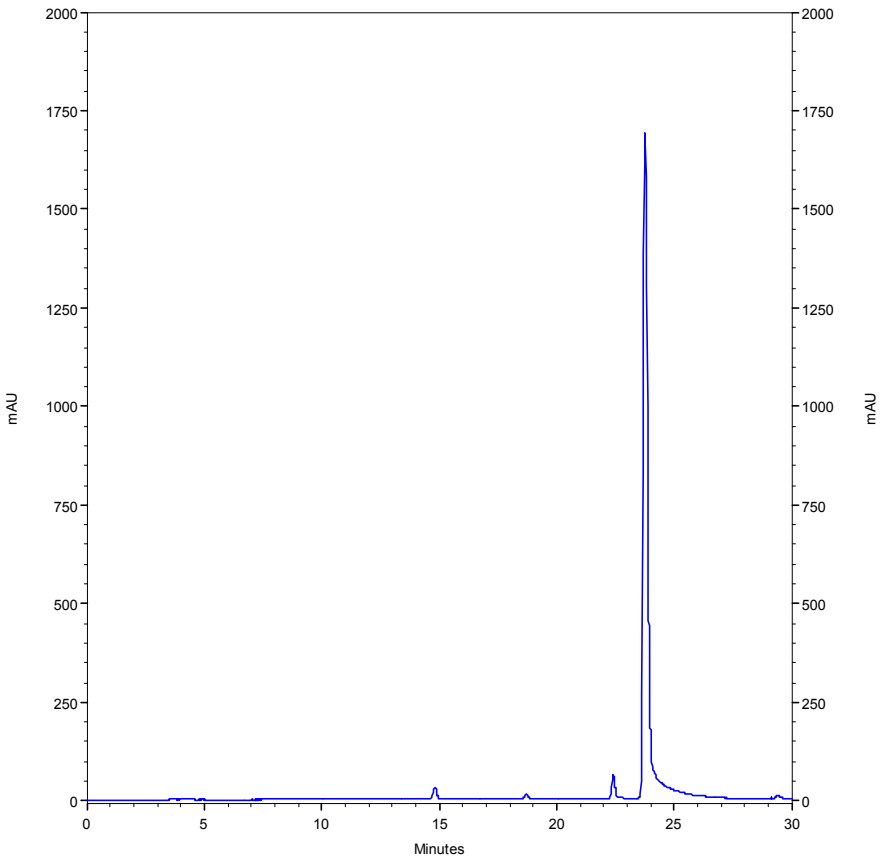
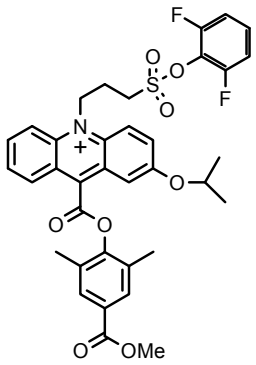


Figure S3. HPLC trace of compound **3b**. HPLC conditions: Phenomenex C_{18}, 10 micron, 3.9 x 300 mm column, 30 minute gradient of 10 → 100% MeCN/water (each with 0.05% TFA), 1 mL/minute, UV detection at 260 nm.



3b

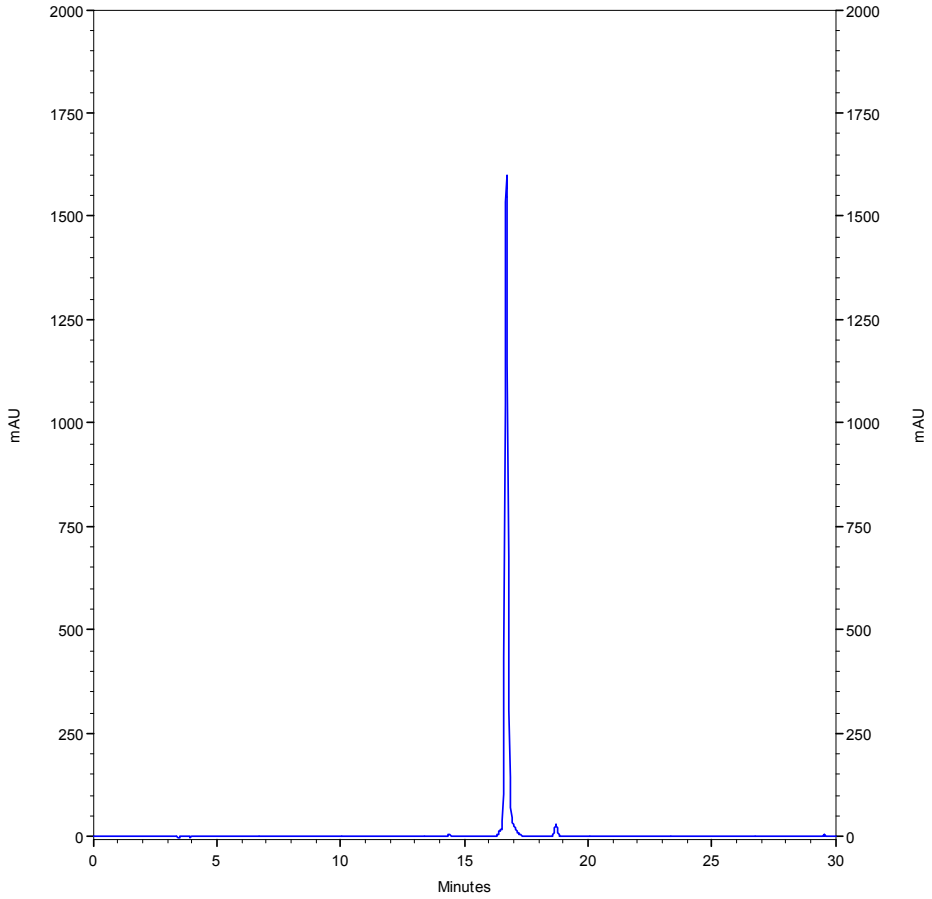
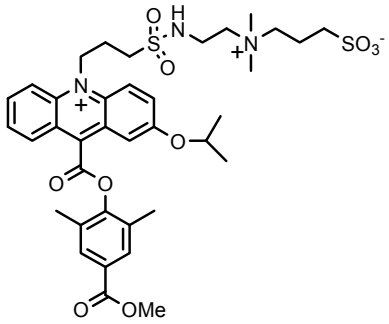


Figure S4. HPLC trace of compound **5**. HPLC conditions: Phenomenex C_{18}, 10 micron, 3.9 x 300 mm column, 30 minute gradient of 10 → 100% MeCN/water (each with 0.05% TFA), 1 mL/minute, UV detection at 260 nm.



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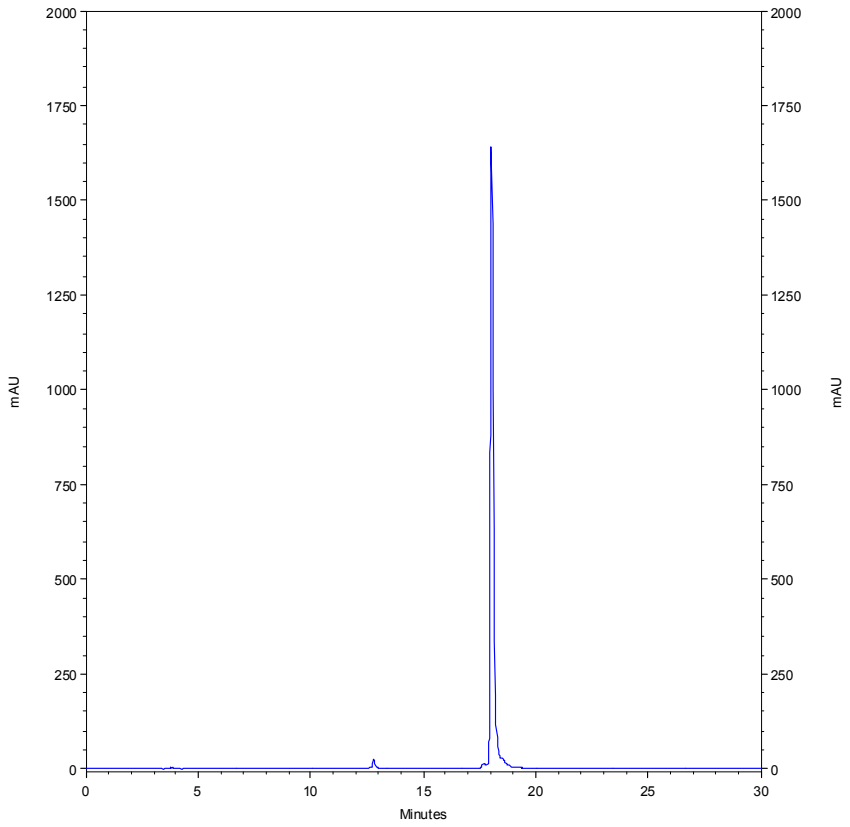
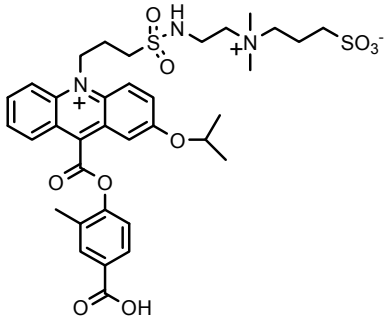


Figure S5. HPLC trace of compound **6**. Phenomenex C_{18}, 10 micron, 3.9 x 300 mm column, 30 minute gradient of 10 → 70% MeCN/water (each with 0.05% TFA), 1 mL/minute, UV detection at 260 nm.



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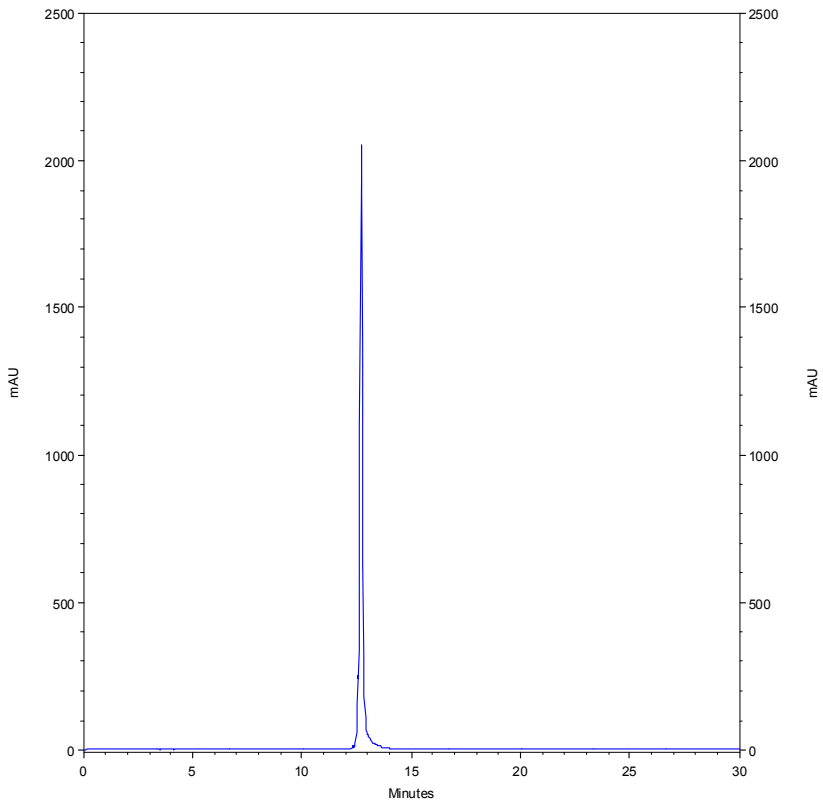
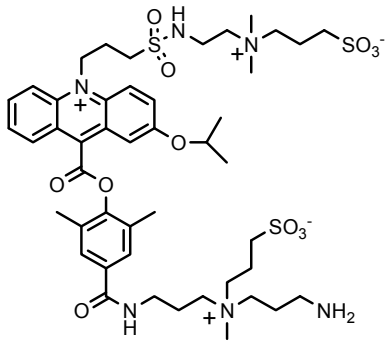


Figure S6. HPLC trace of compound **8**. HPLC conditions: Phenomenex C_{18}, 10 micron, 3.9 x 300 mm column, 30 minute gradient of 10 → 70% MeCN/water (each with 0.05% TFA), 1 mL/minute, UV detection at 260 nm.



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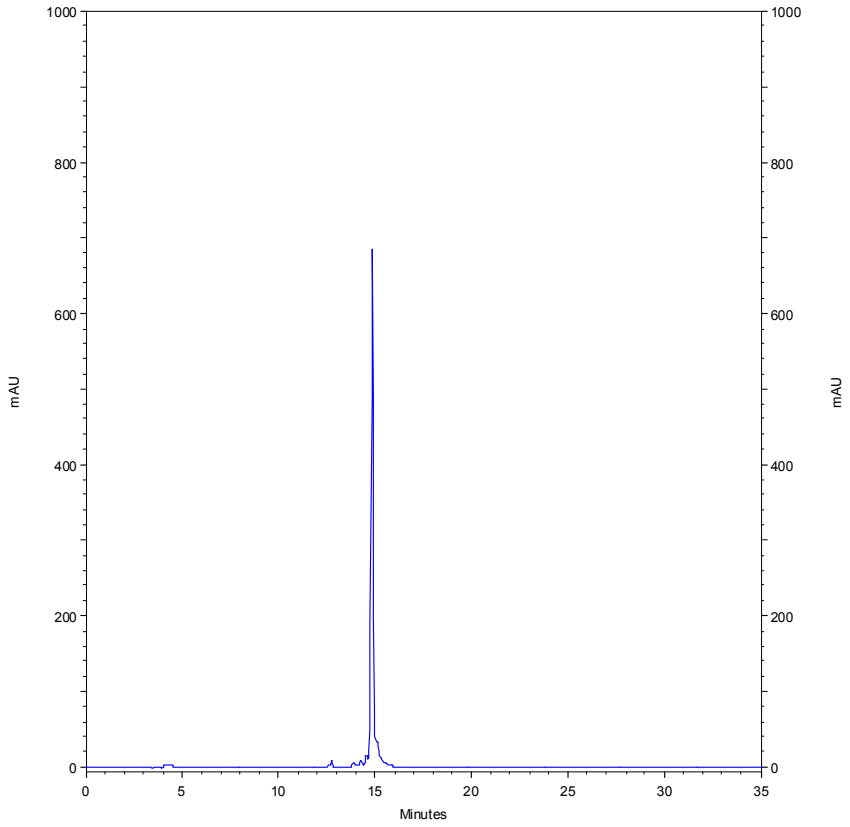
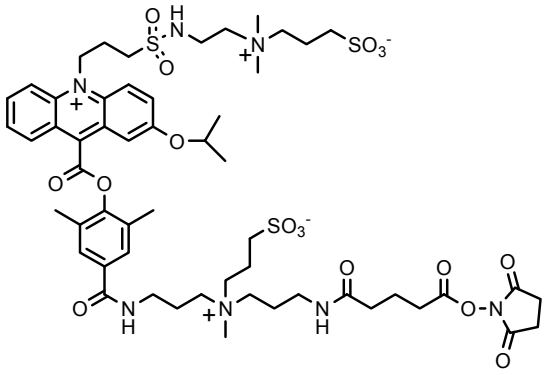


Figure S7. HPLC trace of compound **9**. HPLC conditions: Phenomenex C_{18}, 10 micron, 3.9 x 300 mm column, 30 minute gradient of 10 → 70% MeCN/water (each with 0.05% TFA), 1 mL/minute, UV detection at 260 nm.



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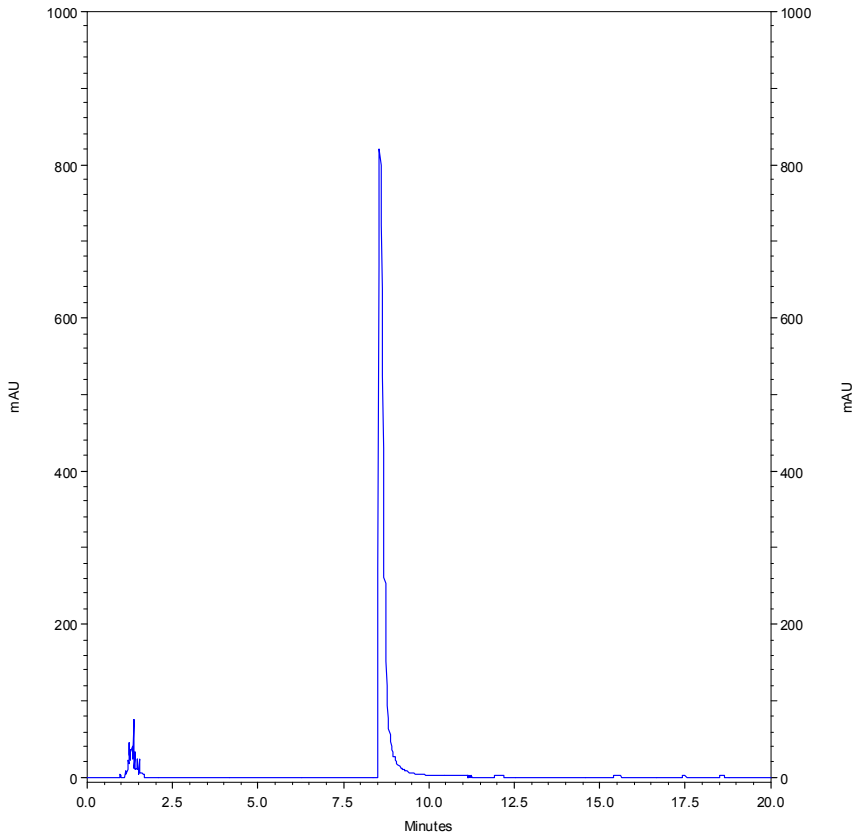
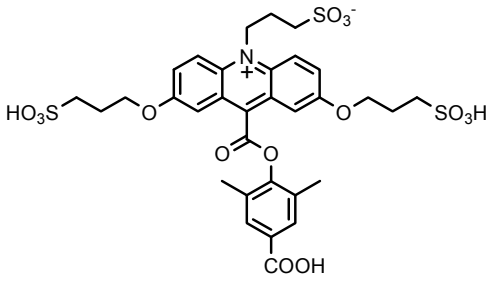


Figure S8. HPLC trace of compound **12**. HPLC conditions: Phenomenex C_8, 5 micron, 4.6 x 100 mm column, 40 minute gradient of 10 → 60% MeCN/water (each with 0.05% TFA), 1 mL/minute, UV detection at 260 nm.



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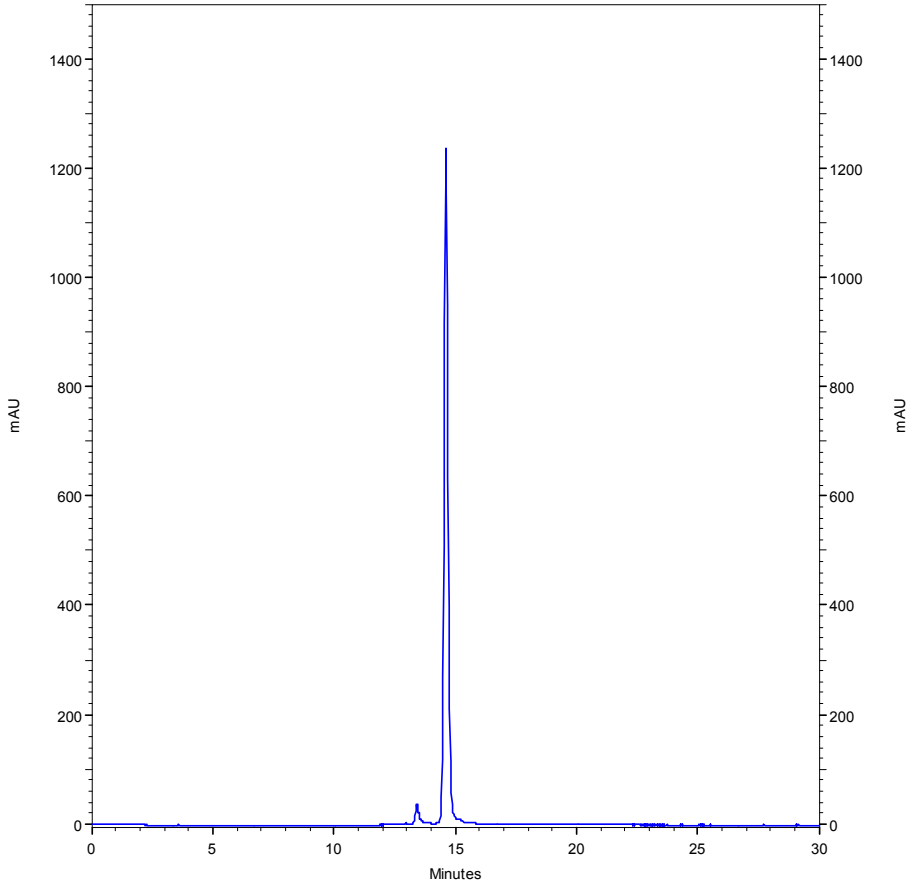
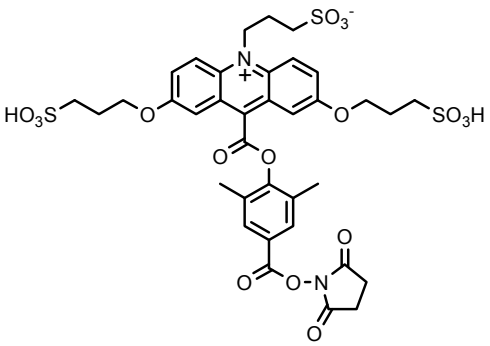


Figure S9. HPLC trace of compound **13**. HPLC conditions: Phenomenex C_{18}, 10 micron, 3.9 x 300 mm column, 30 minute gradient of 10 → 70% MeCN/water (each with 0.05% TFA), 1 mL/minute, UV detection at 260 nm.



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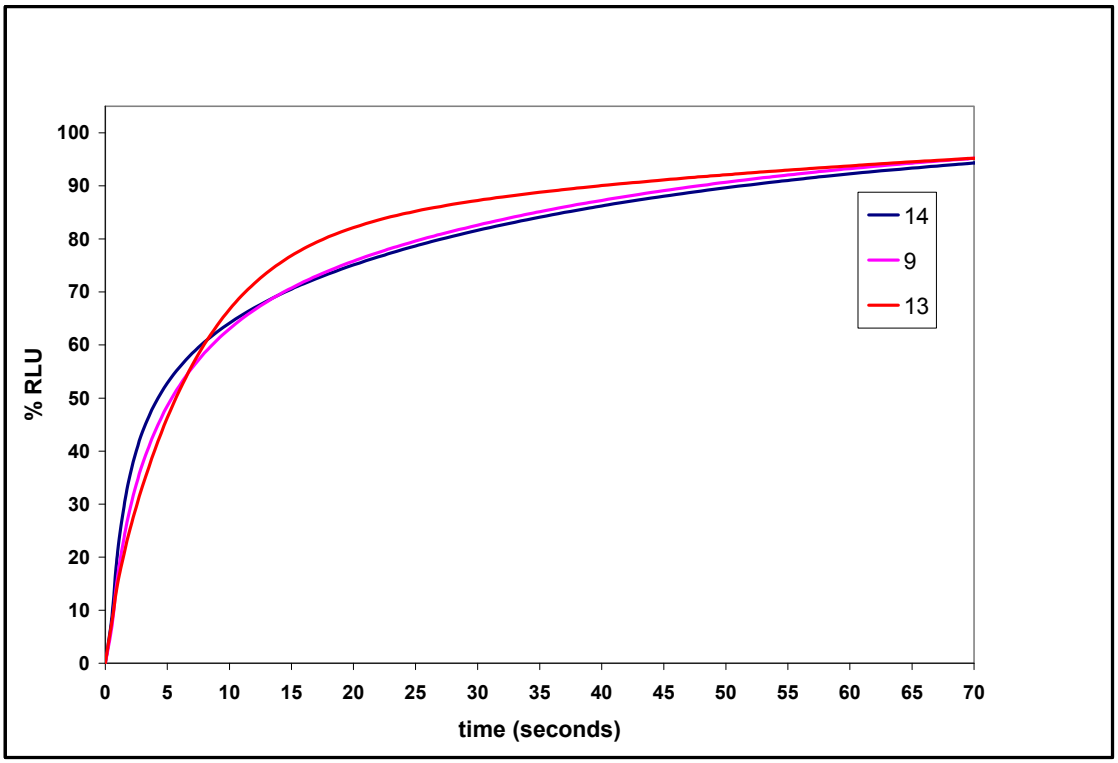

Figure S10. Chemiluminescence emission profiles of acridinium esters **9**, **13** and **14** in the absence of CTAC. Light emission was observed to be slow for all three acridinium esters in the absence of surfactant requiring more than 60 seconds for > 95% emission.

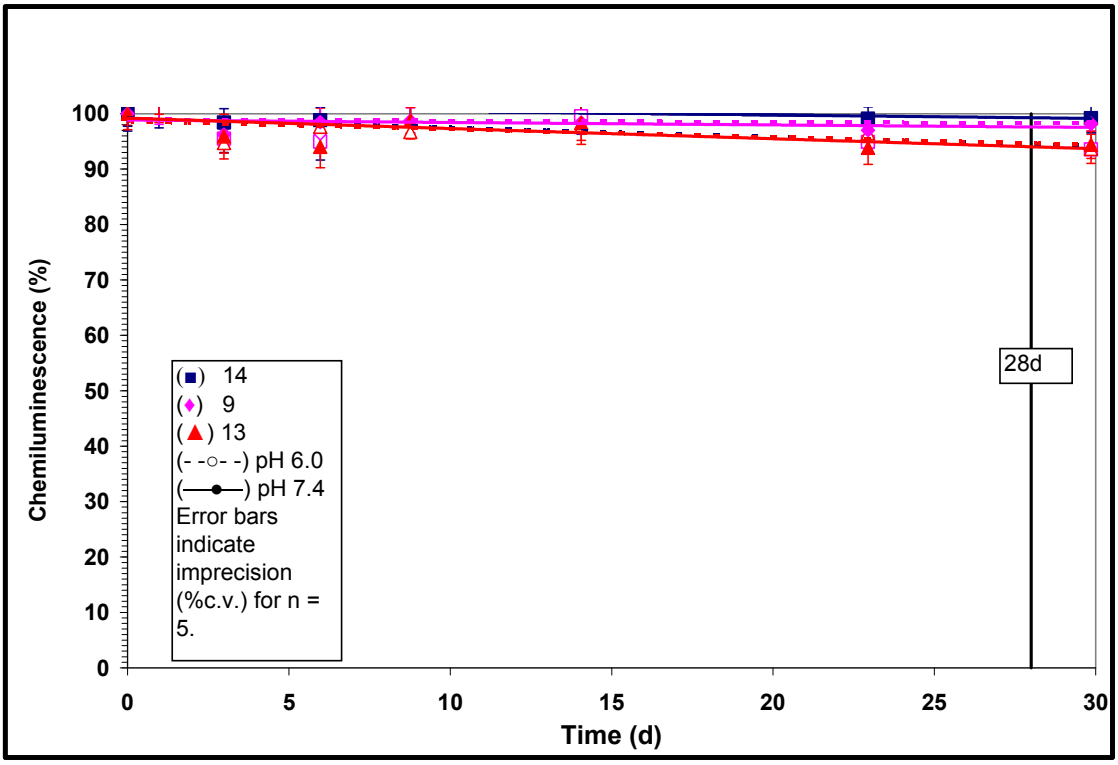

Figure S11. Apparent chemiluminescence stability of anti-HBsAg antibody conjugates of acridinium ester labels **9**, **13** and **14** at pH = 6.0 and 7.4 at 4^{o}C. There was no discernible loss of chemiluminescence even after 30 days for all three labels.