

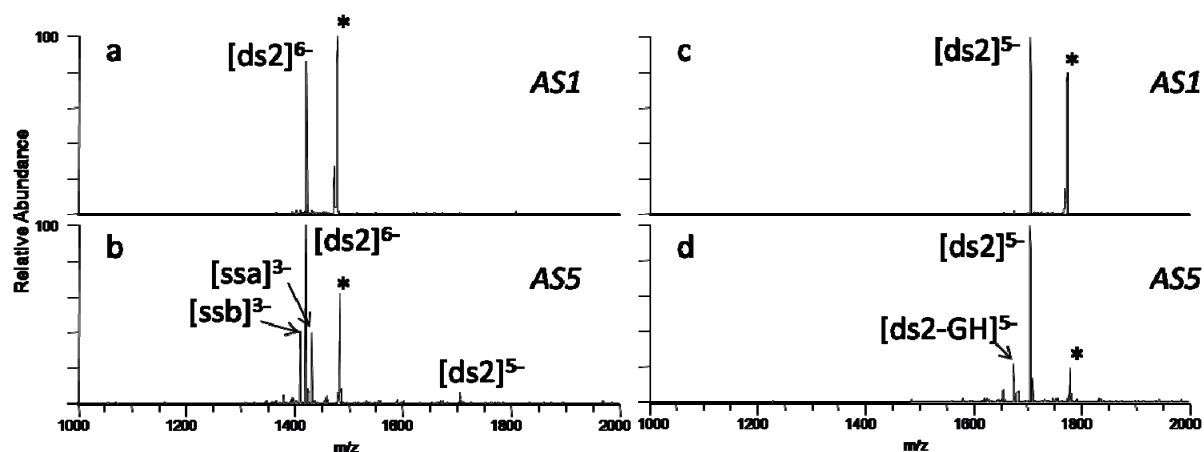
## Interactions of Sulfur-Containing Acridine Ligands with DNA by ESI-MS

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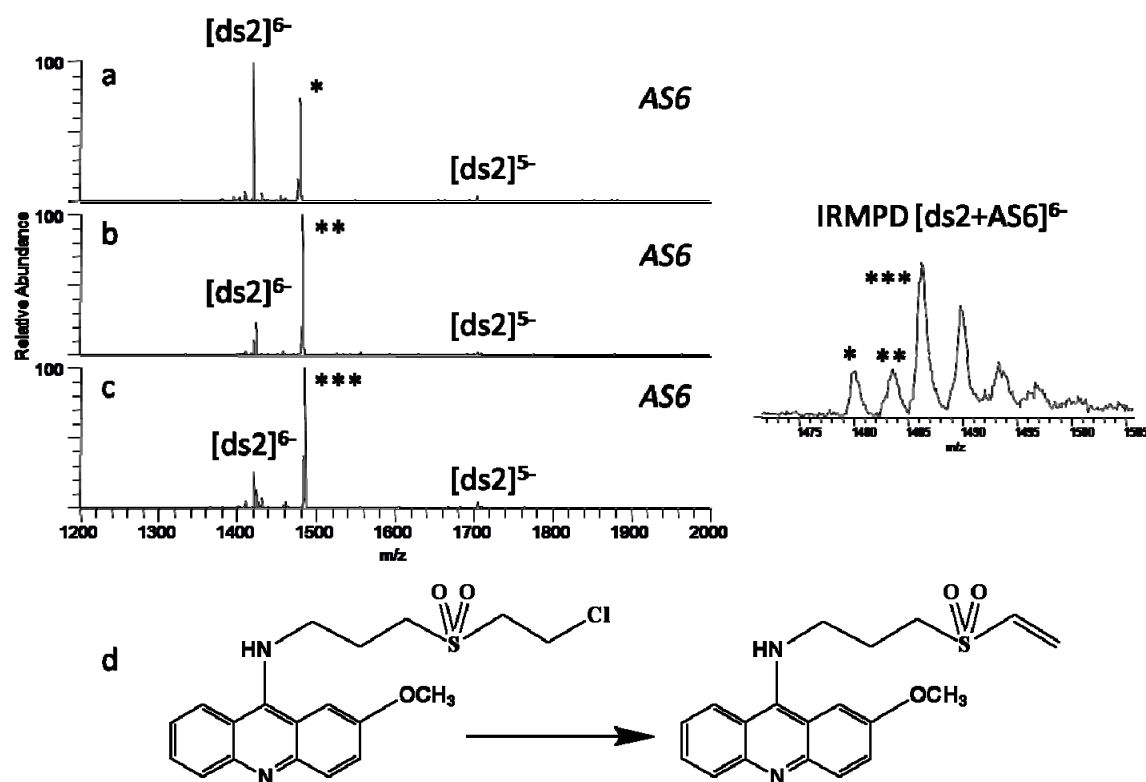
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**Supplemental Figure 1.** IRMPD mass spectra of (a) [ds2 + AS1]<sup>6-</sup> with an irradiation time of 0.75 ms, (b) [ds2 + AS5]<sup>6-</sup> with an irradiation time of 1.0 ms, (c) [ds2 + AS1]<sup>5-</sup> with an irradiation time of 0.75 ms, and (d) [ds2 + AS5]<sup>5-</sup> with an irradiation time of 1.0 ms. The parent ion is denoted with an asterisk.



**Supplemental Figure 2.** (a-c) IRMPD mass spectra of  $[\text{ds}2 + \text{AS}6]^{6-}$  with an irradiation time of 0.75 ms. Each precursor ion, shown on the right with one, two, or three asterisks, was isolated and subjected to IRMPD. (d) Proposed pathway for formation of the lowest mass adduct.

**Supplemental Table 1.** Change in melting temperature of duplex 3 upon addition of acridine ligands

Ligand	$\Delta T_m$ (°C)
AS1	6.2
AS2	6.0
AS3	6.6
AS4	7.0
AS5	7.9
AS6	7.2
AN1	6.4