Supporting information

Ion Mobility Mass Spectrometry of $Au_{25}(SCH_2CH_2Ph)_{18}$ Nanoclusters

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Figure S1. Mass spectra of Au25 (a) positive scan (b) negative scan

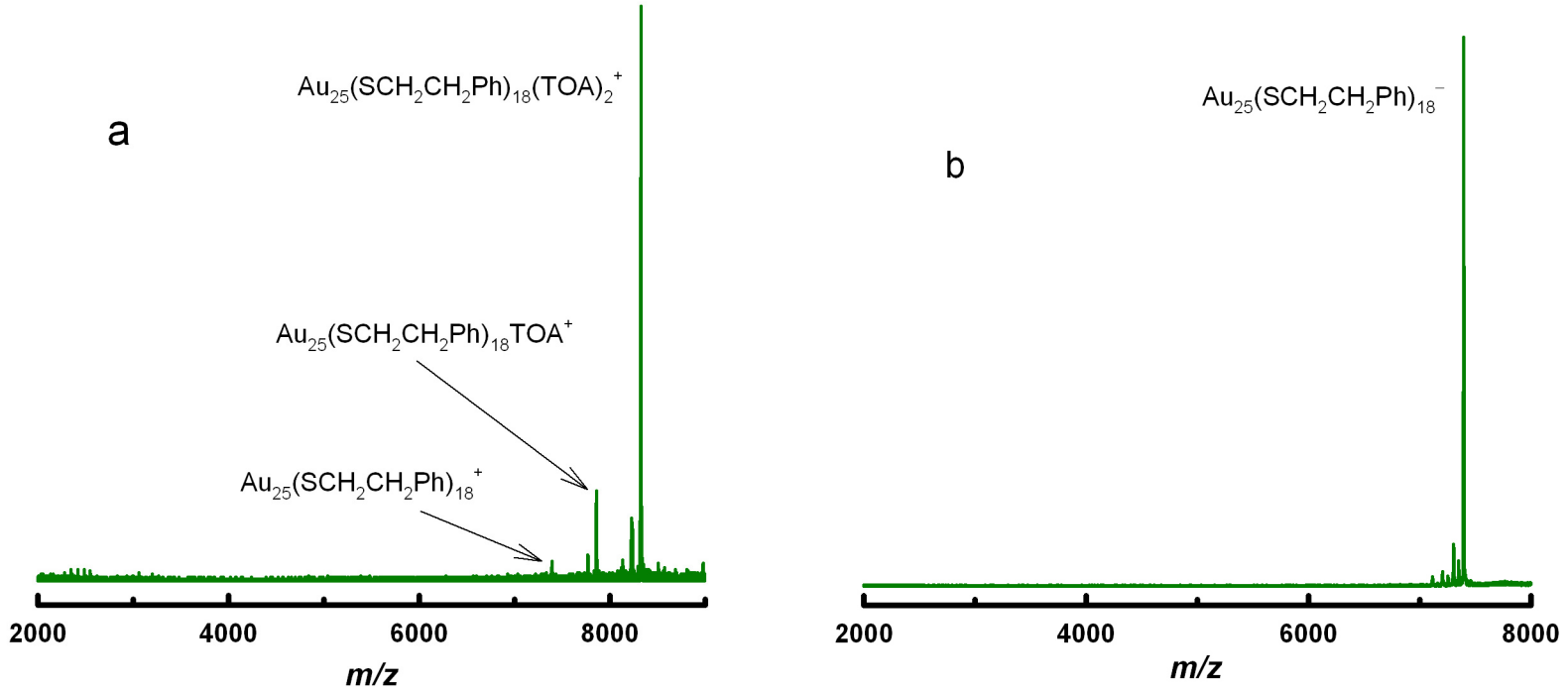


Figure S2: Expanded version of Figure 1. IM-MS/MS of $Au_{25}(SCH_2CH_2Ph)_{18}^-$ taken by resolving the $Au_{25}(SCH_2CH_2Ph)_{18}^-$ parent ion and applying 100 V lab kinetic energy to the trap T-wave cell.

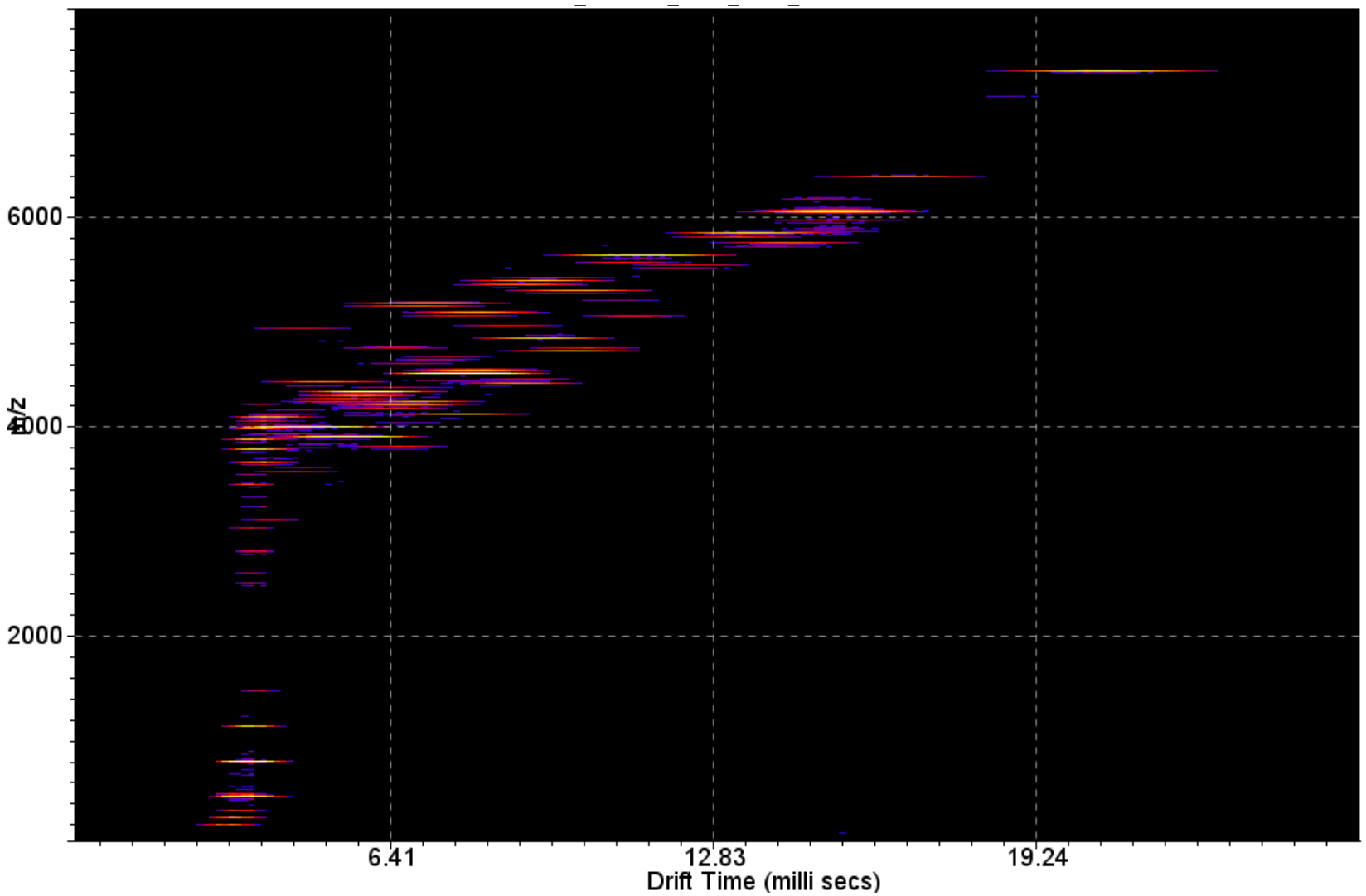


Figure S3: Expanded and full mass range version of Figure 2. IM-MS/MS of $Au_{25}(SCH_2CH_2Ph)_{18}^-$ taken without resolving the $Au_{25}(SCH_2CH_2Ph)_{18}^-$ parent ion and applying 200 V lab kinetic energy to the trap T-wave cell.

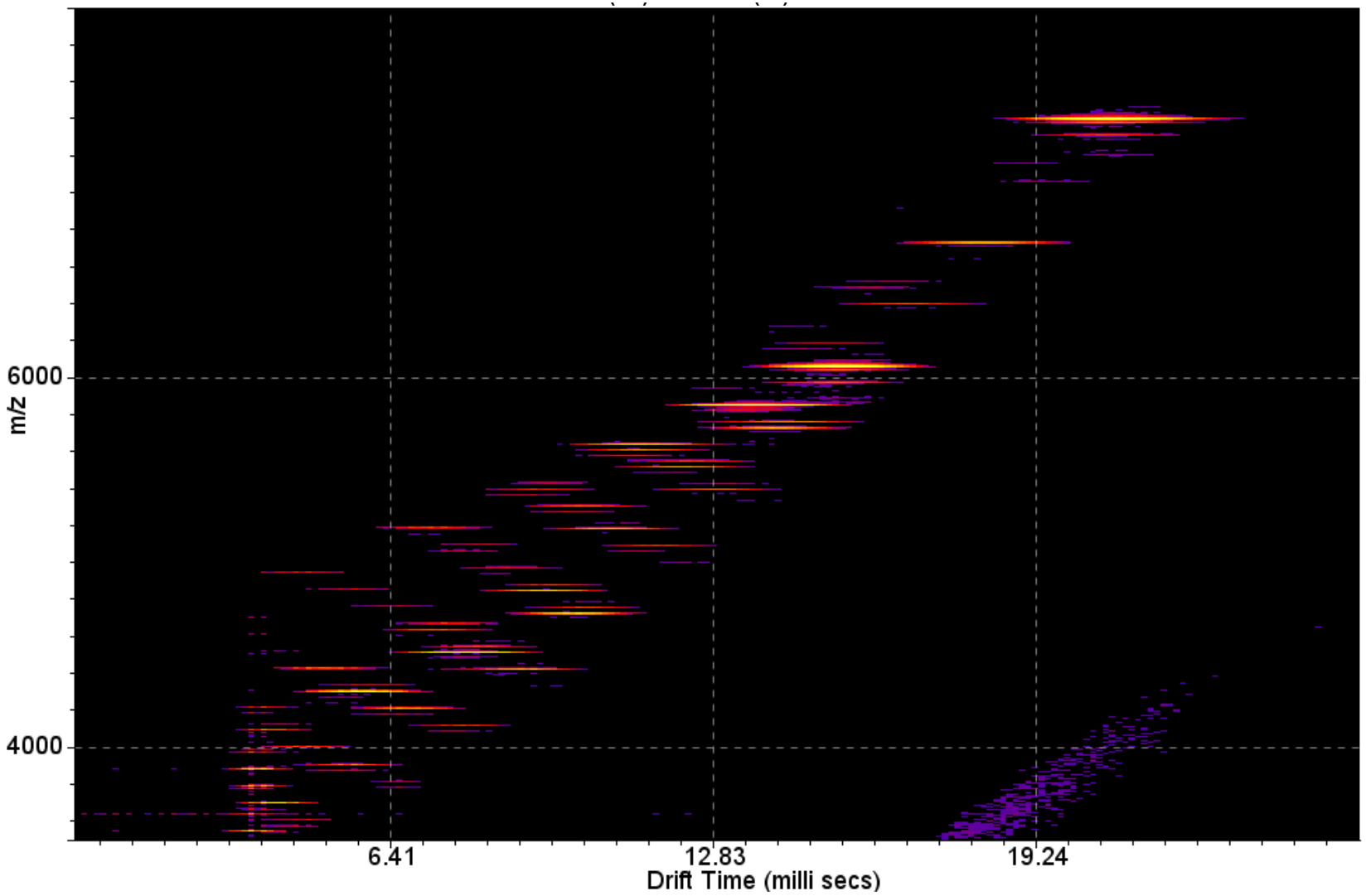
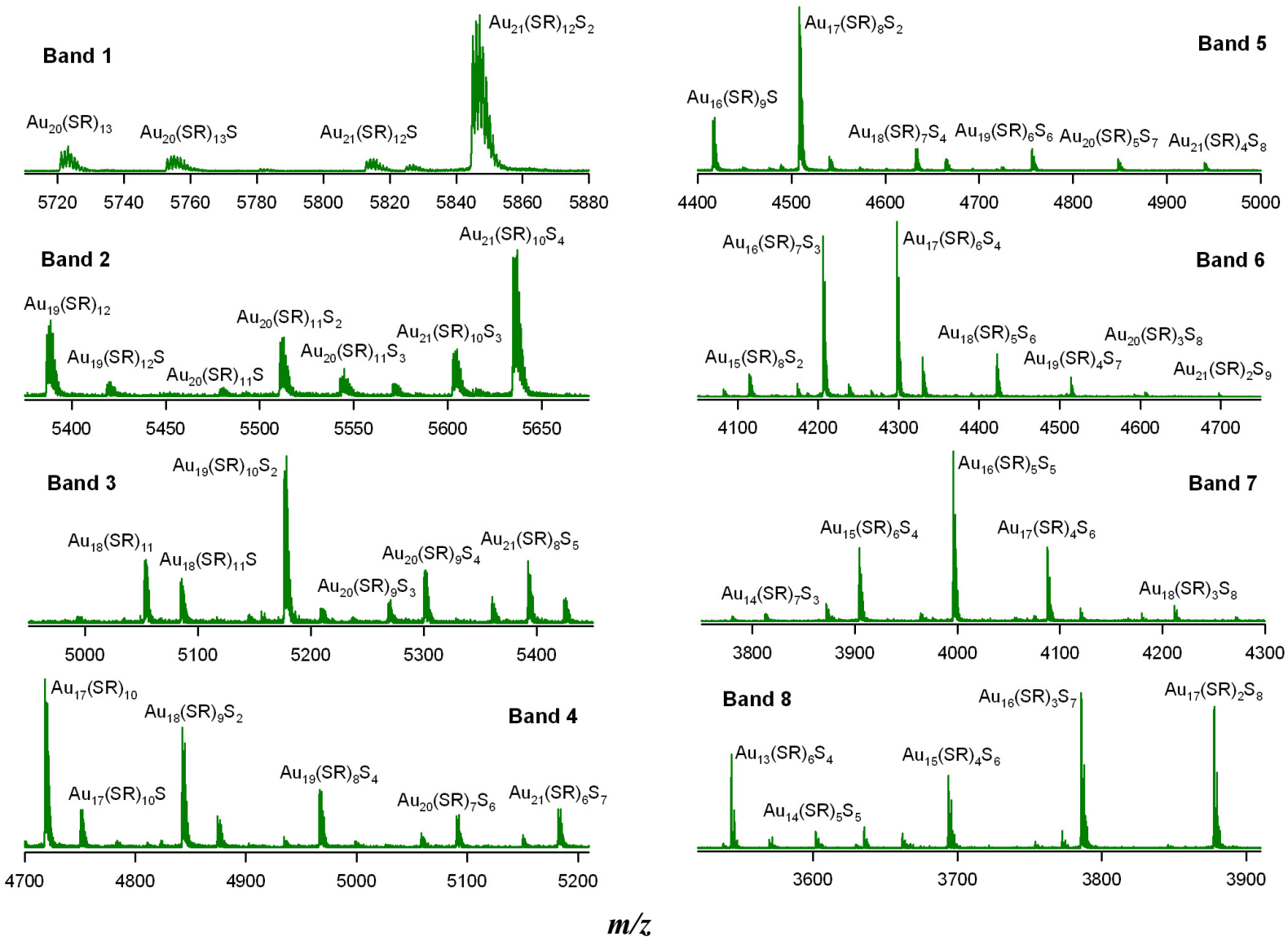


Figure S4: Expanded version of Figure 3



Band	High mass species	Low mass species	Δ –Au, –S, +R	Δ mass across band, amu
1	$Au_{21}(SR)_{12}S_2^-$	$Au_{20}(SR)_{13}^-$	Δ –1Au, –1S, +1R	Δ –124
2	$Au_{21}(SR)_{10}S_4^-$	$Au_{19}(SR)_{12}^-$	Δ –2Au, –2S, +2R	Δ –248
3	$Au_{21}(SR)_8S_6^-$	$Au_{18}(SR)_{11}^-$	Δ –3Au, –3S, +3R	Δ –372
4	$Au_{21}(SR)_6S_7^-$	$Au_{17}(SR)_{10}^-$	Δ –4Au, –3S, +4R	Δ –464
5	$Au_{21}(SR)_4S_8^-$	$Au_{16}(SR)_9S^-$	Δ –5Au, –2S, +5R	Δ –524
6	$Au_{21}(SR)_2S_9^-$	$Au_{15}(SR)_8S^-$	Δ –6Au, –2S, +6R	Δ –616
7	$Au_{18}(SR)_3S_8^-$	$Au_{14}(SR)_7S^-$	Δ –4Au, –3S, +4R	Δ –464
8	$Au_{17}(SR)_2S_8^-$	$Au_{13}(SR)_6S_4^-$	Δ –4Au, –0S, +4R	Δ –368

Table S1. Assignments of the high and low mass species contained in the individual bands 1 to 8 and the changes in mass that accompanies them, where R = CH_2CH_2Ph.

Consecutive bands display an increased incremental loss of Au atoms and increased incremental gain of -CH_2CH_2Ph. For example in band 2, the high and low mass species are $Au_{21}(SR)_{10}S_4^-$ and $Au_{19}(SR)_{12}^-$, respectively, showing a loss of 2 Au atoms and gain of 2 -CH_2CH_2Ph ligands. The Δ*m* across band 2 is two times greater than that of band 1; Δ*m* = –2Au (396) –2S (64) +2R (210) = –250 amu. Band 3 has high and low mass species of $Au_{21}(SR)_8S_7^-$ and $Au_{18}(SR)_{11}^-$ giving Δ*m* that is three times greater than that of band 1 Δ*m* = –3Au (591) –3S (96) +3R (315) = –372 amu. Band 4 has high and low mass species of $Au_{21}(SR)_6S_7^-$ and $Au_{17}(SR)_{10}^-$ exhibiting Δ*m* = –4Au (788) –3S (96) +4R (420) = –464 amu. Band 5 has high and low mass species of $Au_{21}(SR)_4S_8^-$ and $Au_{16}(SR)_9S^-$ exhibiting Δ*m* = –5Au (985) –2S (64) +5R (525) = –524 amu. Band 6 contains high and low mass species of $Au_{21}(SR)_2S_9^-$ and $Au_{15}(SR)_8S^-$ exhibiting Δ*m* = –6Au (1182) –2S (64) +6R (630) = –616 amu. Bands 7 and 8 do not contain a $Au_{21}(SR)_nS_m^-$ species, but band 7 contains a low mass species $Au_{14}(SR)_mS_n^-$, representing the loss of 7 Au, and band 8 contains the low mass species $Au_{13}(SR)_nS_m^-$, representing the loss of 8 Au. The $Au_{13}(SR)_mS_n^-$ species has now lost all the Au atoms from the outer protecting "staple" shell and contains only Au atoms that are in the Au_{13} core with a combination of stabilizing S and SR units.

Figure S5: Schematic of the Synapt HDMS design accessible at www.waters.com