

# The Retention Behavior of CAPCELL CORE ADME S2.7, a Novel Adamantyl Stationary Phase in the Reversed-Phase Chromatography of Polar Compounds

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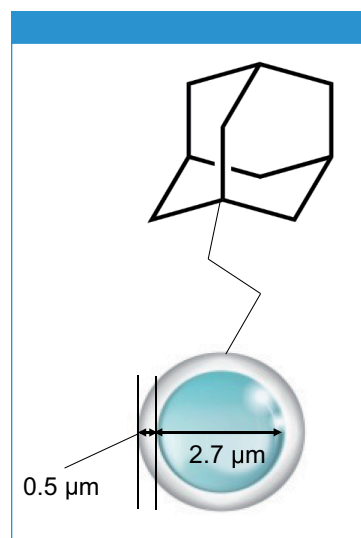
*CAPCELL CORE ADME S2.7 (ADME) is a column packed with a novel stationary phase of superficially porous silica (core-shell particle) modified by adamantyl functional groups. ADME has separation characteristics with a balance between moderate hydrophobicity and extra-high surface polarity which is completely different from the conventional C<sub>18</sub>. Therefore, The ADME is found to exhibit retention behavior different from the conventional C<sub>18</sub> phase, because ADME has a higher surface polarity and a tendency to maintain a hydrophobicity. In addition, it is suggested simply use as a significant alternative to the C<sub>18</sub> phase for the improved separation of highly polar substances such as metabolites, and biological samples.*

The C<sub>18</sub> column is the most popular one used in reversed-phase chromatography, but this phase has difficulty in retaining the highly polar compounds. Therefore, in order to increase the retention, separation modes such as HILIC (1) and ion exchange are some of the choices. However, these are in separation mechanism different from the reversed phase mode, the column selection and the mobile phase condition becomes complicated.

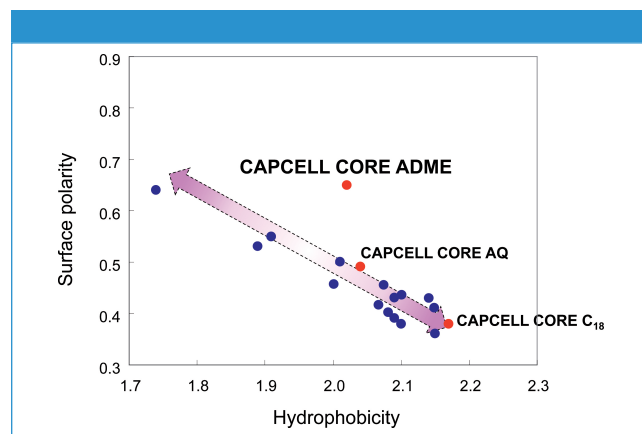
In general, in order to increase the retention of highly polar compounds in the reversed phase mode, packing material with enhanced surface polarity by decreasing the density of alkyl groups or embedding polar functional group is conventionally used, but has slight effect on changing the retention of them.

Shiseido succeeded in development of CAPCELL CORE ADME S2.7, a novel stationary phase with an adamantyl group having a cage structure. This is characterized as alkyl group; therefore, the packed column is still easy to use just as a reversed-phase column.

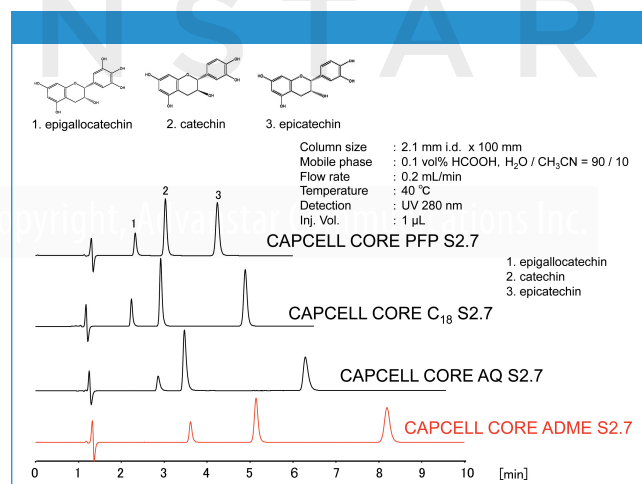
In this study, the characteristics of CAPCELL CORE ADME S2.7 and the retention behavior of highly polar compounds on the same mobile phase were evaluated.



**Figure 1:** Superficially porous silica (core-shell particle) modified by adamantyl functional groups.



**Figure 2:** Parameter map of separation.



**Figure 3:** Chromatograms of catechines.

## Experimental

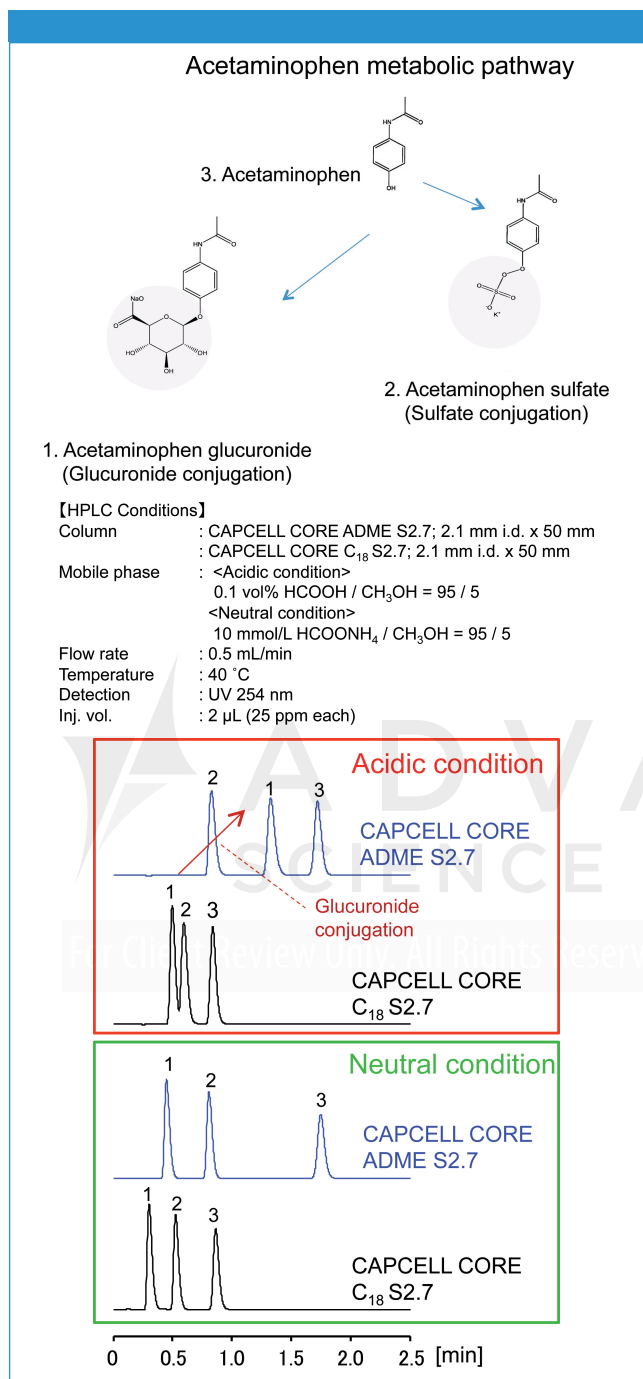
### 1. Basic Feature of CAPCELL CORE ADME S2.7

#### (1) Determination of Separation Parameters

CAPCELL CORE ADME S2.7 (ADME) is a column packed with a novel particle with 1.7- $\mu\text{m}$  solid core and 0.5- $\mu\text{m}$  porous layer modified with adamantyl functional group (Figure 1). The parameter of Hydrophobicity and Surface polarity was determined with ADME by the resolution factor of toluene with benzoate, and toluene with methyl benzoate (2).

#### (2) Comparison of Separation Characteristics

The effect of separation parameters on retention and separation were determined by comparison of the analysis of catechines with CAPCELL CORE C<sub>18</sub> S2.7 and CAPCELL CORE AQ S2.7, and CAPCELL CORE PFP S2.7, respectively.



**Figure 4:** Chromatograms of acetaminophen and its metabolites.

## 2. Application of CAPCELL CORE ADME S2.7

Acetaminophen and its conjugated metabolites were analyzed under acidic and neutral conditions with CAPCELL CORE ADME S2.7 and CAPCELL CORE C<sub>18</sub> S2.7, respectively.

## Results and Discussion

### 1. Basic Feature of CAPCELL CORE ADME S2.7

(1) Determination of Separation Parameters

In Figure 2, the parameters of hydrophobicity and surface polarity of CAPCELL CORE ADME S2.7 (ADME) derived from the resolution factors of toluene with benzoate, and toluene with methyl benzoate, were plotted on the parameter graph including CAPCELL CORE C<sub>18</sub> S2.7, CAPCELL CORE AQ S2.7, CAPCELL CORE PFP S2.7, and other reverse-phase columns. In the parameter map, ADME is positioned with moderate hydrophobicity and extra-high surface polarity.

(2) Comparison of Separation Characteristics

As shown in the chromatograms in Figure 3, CAPCELL CORE ADME S2.7 (ADME) showed a large retention and a highly resolution of catechines compared with more hydrophobic CAPCELL CORE C<sub>18</sub> S2.7, similarly hydrophilic CAPCELL CORE AQ S2.7 and CAPCELL CORE PFP S2.7. Therefore, it is suggested that not only the hydrophobicity but also the high surface polarity of ADME provided effect on the separation of catechines.

## 2. Application of CAPCELL CORE ADME S2.7

Acetaminophen and its conjugated metabolites containing glycoside were analyzed under acidic and neutral conditions with CAPCELL CORE ADME S2.7 and CAPCELL CORE C<sub>18</sub> S2.7, respectively (Figure 4). It is clear that the metabolites of acetaminophen, conjugate of sulfuric acid, and glucuronic acid were certainly separated under acidic and neutral conditions. In particular, a good separation and large retention was obtained with CAPCELL CORE ADME S2.7 under acidic conditions.

## Conclusion

CAPCELL CORE ADME S2.7 is a novel core-shell type column with adamantly-functional group modified stationary phase and provides improved separation to highly polar metabolites which was previously unavailable by the conventional C<sub>18</sub> and PFP columns. It is suggested particularly useful in retaining and separation of highly polar compounds. It is also an easy-to-use reverse-phase column and is expected to work as an alternative to the C<sub>18</sub> column in the improved separation of highly polar compounds and matrix components in biological samples.

## References

- (1) A.J. Alpert, *J. Chromatogr. A* **499**, 177–196 (1990).
- (2) S. Kobayashi, I. Tanaka, O. Shirota, T. Kanda, and Y. Ohtsu. *J. Chromatogr. A* **828**, 75–81 (1998).

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