

Solvent switched weak interaction of a 4-quinazolinone inhibitor with a cavitand derivative

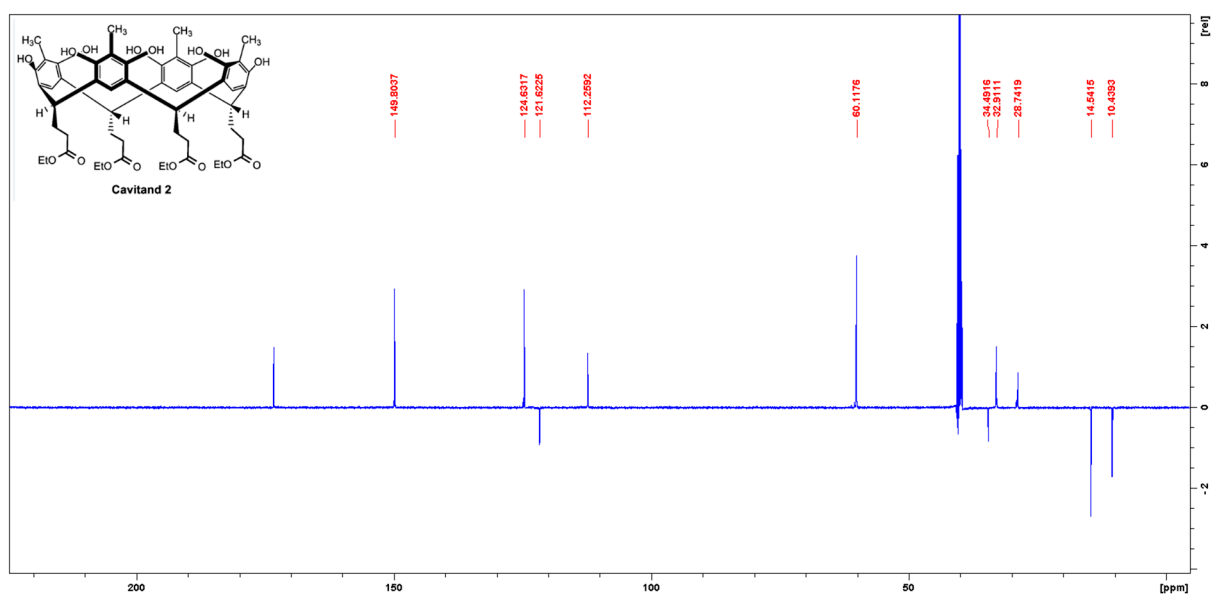
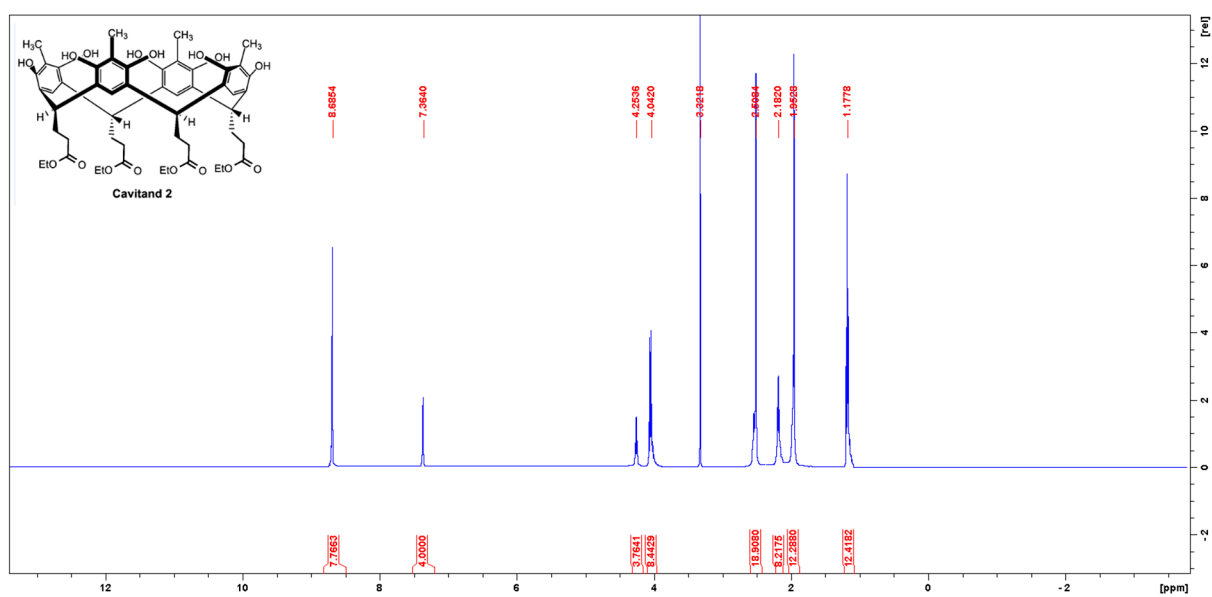
Zoltán Nagymihály, Beáta Lemli, László Kollár and Sándor Kunsági-Máté

Supplementary Material

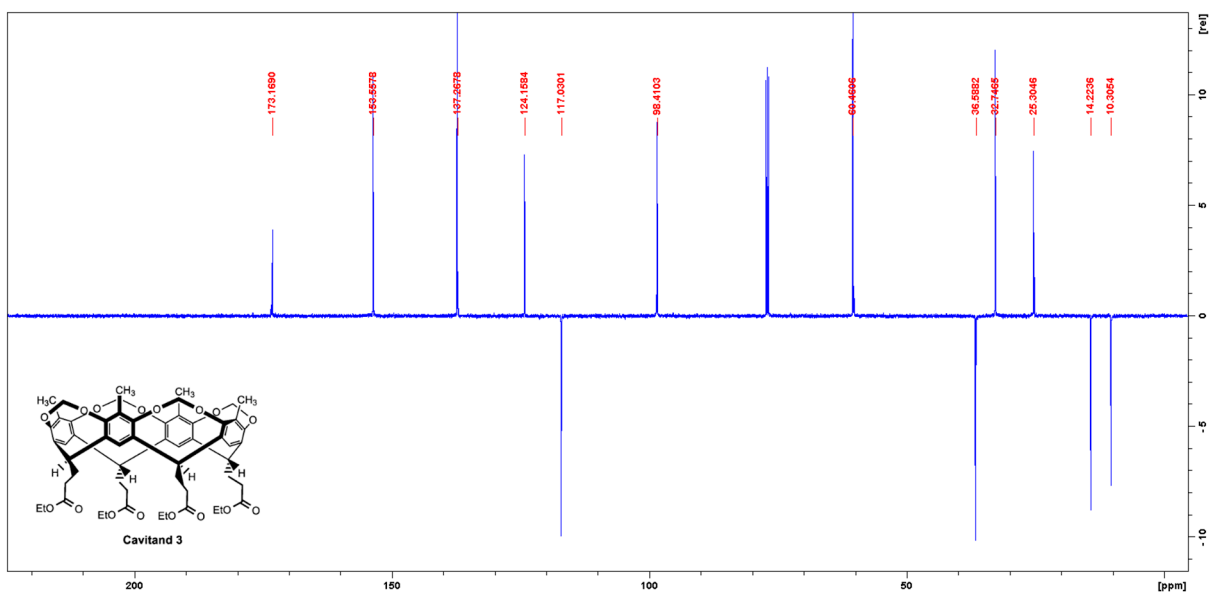
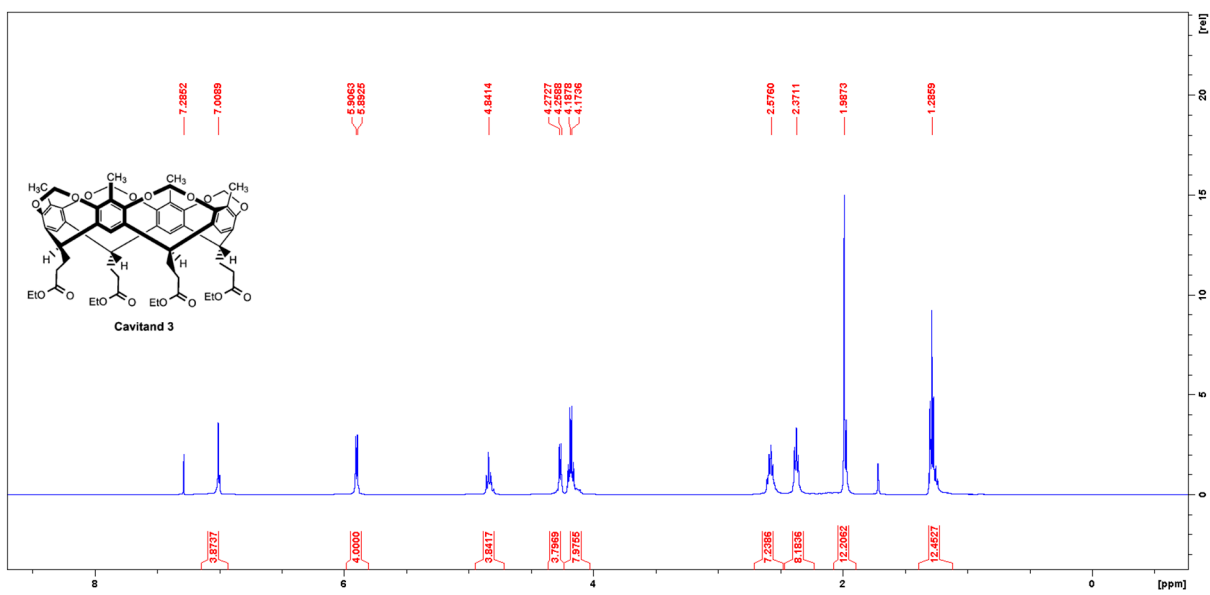
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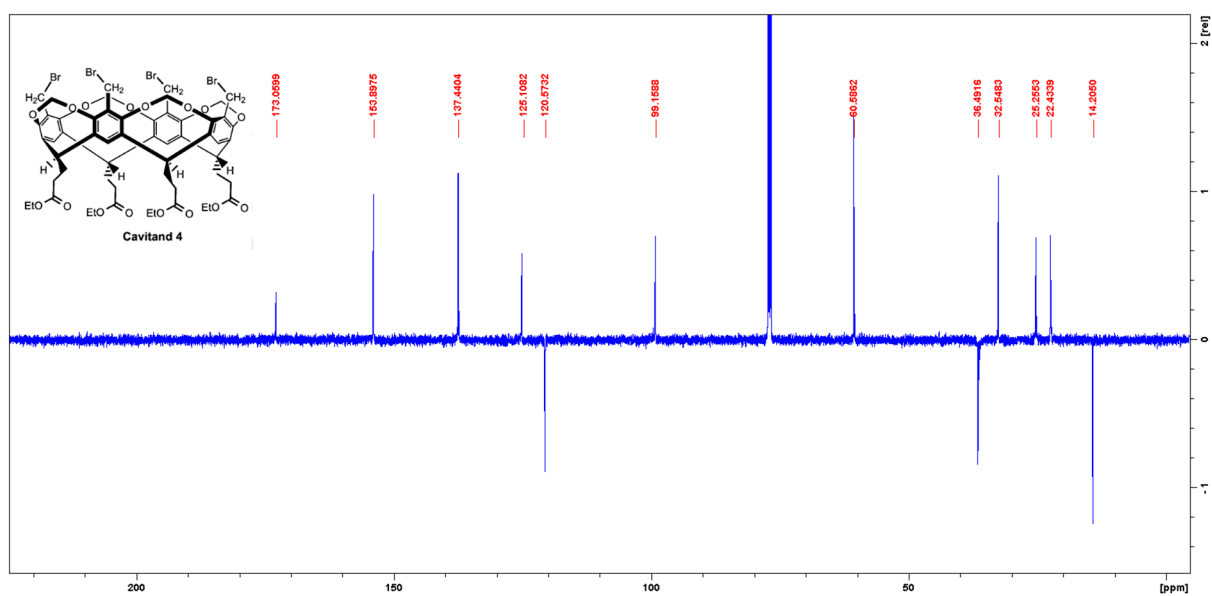
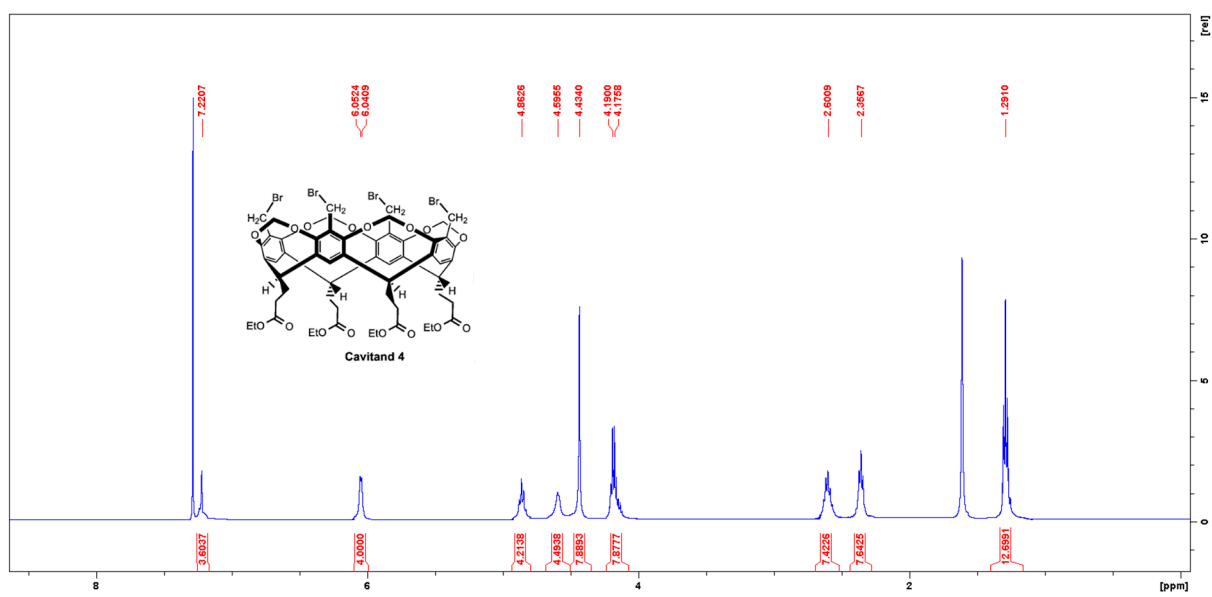
¹H and ³¹P NMR spectra of Cavitant 2



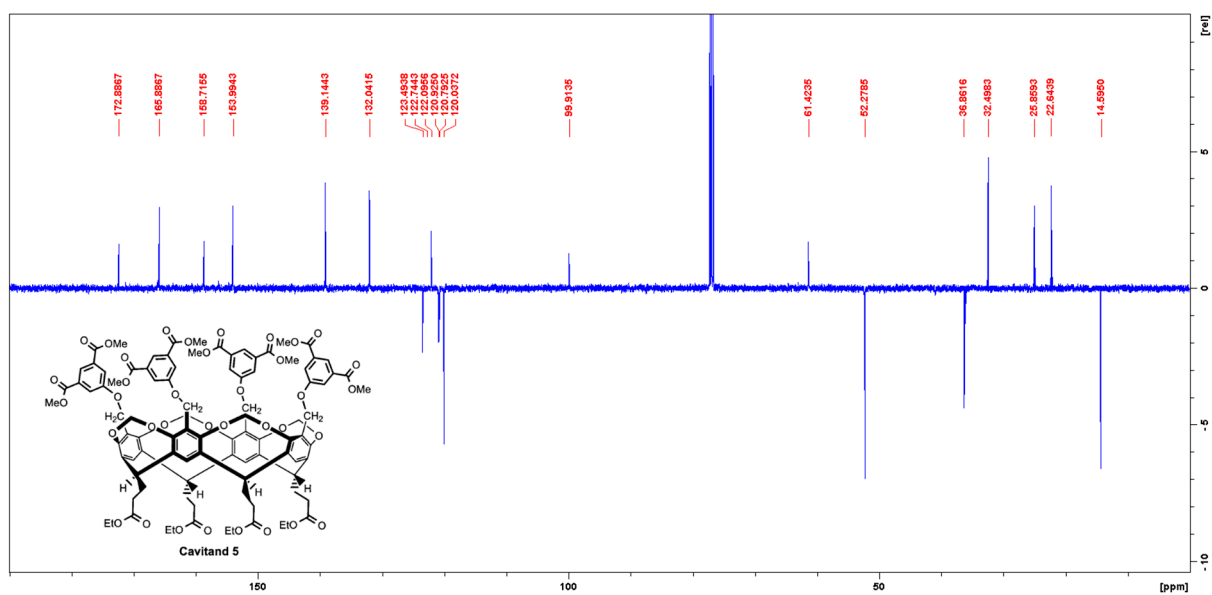
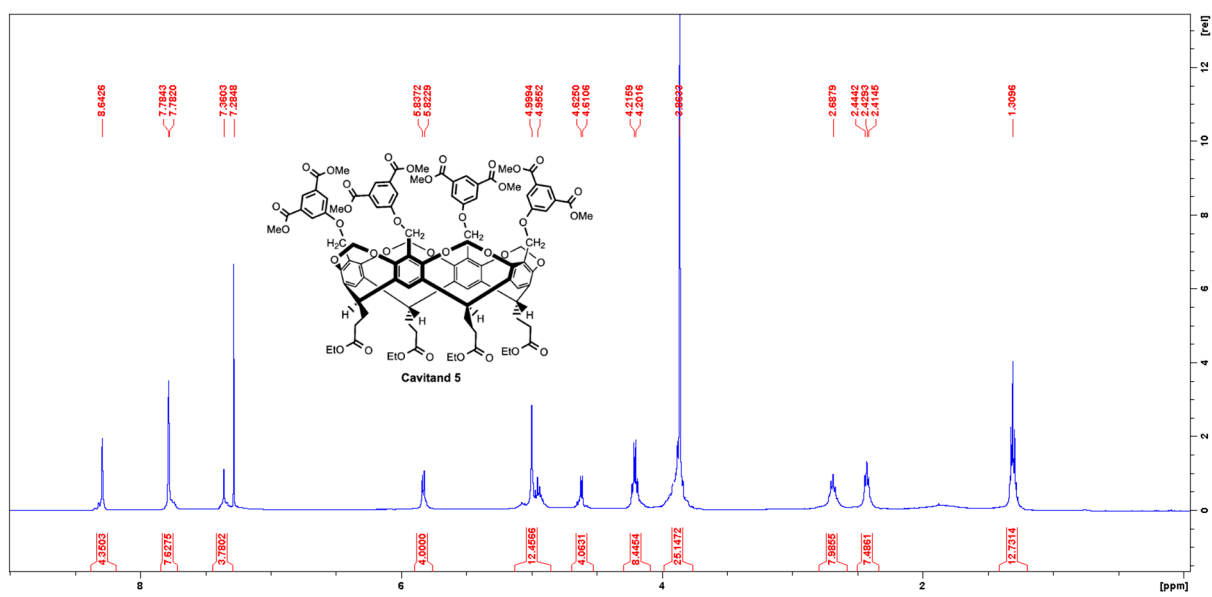
¹H and ³¹P NMR spectra of Cavitant 3



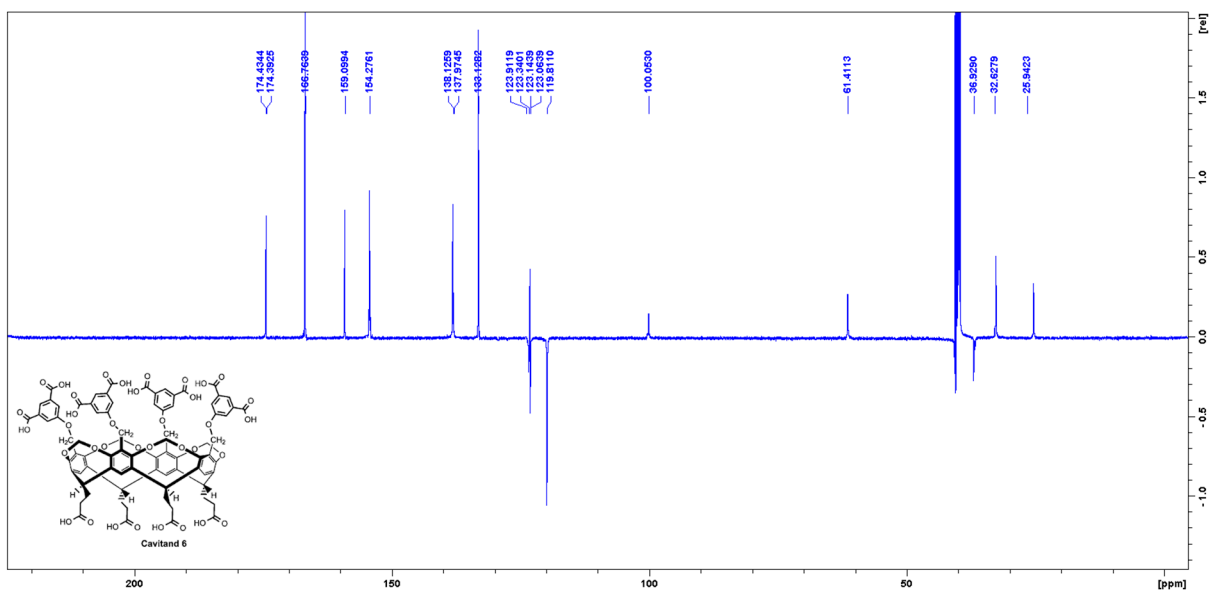
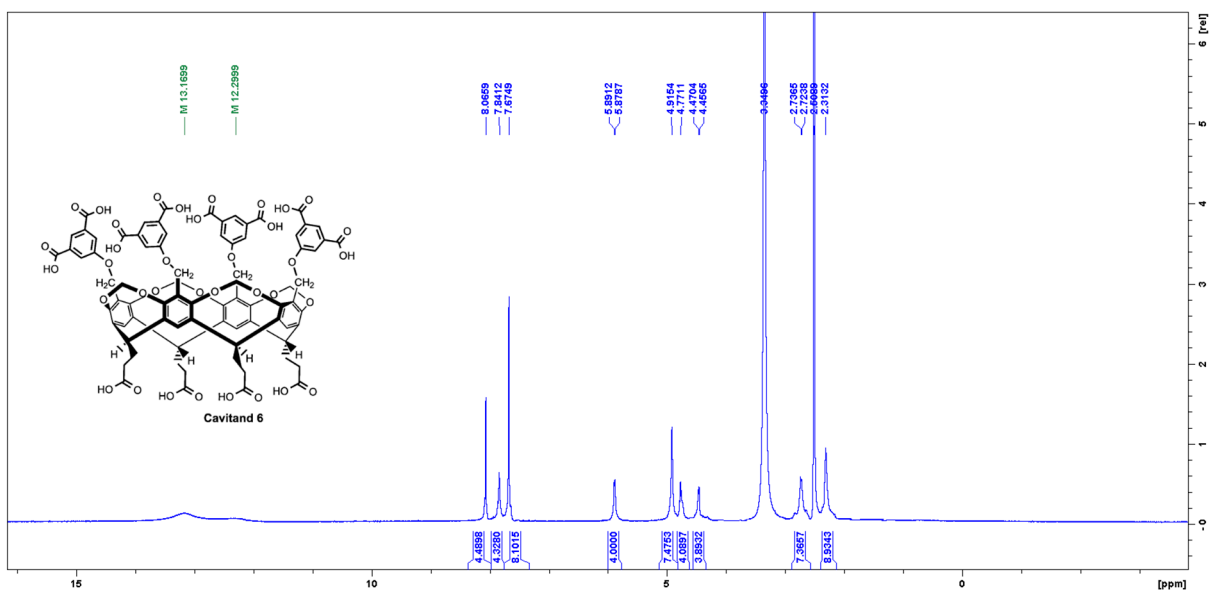
¹H and ³¹P NMR spectra of Cavitand 4



¹H and ³¹P NMR spectra of Cavitant 5



¹H and ³¹P NMR spectra of Cavitant 6



Complex stability constants (log K values) associated to the complex formation of **1** with **6** in methanol or DMF solvent determined in the different temperatures.

Table S1: results derived by the Benesi-Hildebrand method

solvent	Temperature (K)								
	289.16	291.16	293.16	295.16	297.16	299.16	301.16	303.16	305.16
methanol	5.34	5.31	5.27	5.22	5.17	5.15	5.13	5.1	5.09
DMF	6.07	6.01	5.98	5.93	5.87	5.83	5.8	5.79	5.77

Table S2: results derived by the Hyperquad code

solvent	Temperature (K)								
	289.16	291.16	293.16	295.16	297.16	299.16	301.16	303.16	305.16
methanol	5.32	5.30	5.25	5.22	5.16	5.15	5.13	5.11	5.09
DMF	6.06	6.03	5.99	5.94	5.86	5.83	5.82	5.80	5.78