Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Quick temperature-swept pure-shift NMR: case of solvent effects in atorvastatin

Supporting Information

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Results for D_2O and H_2O

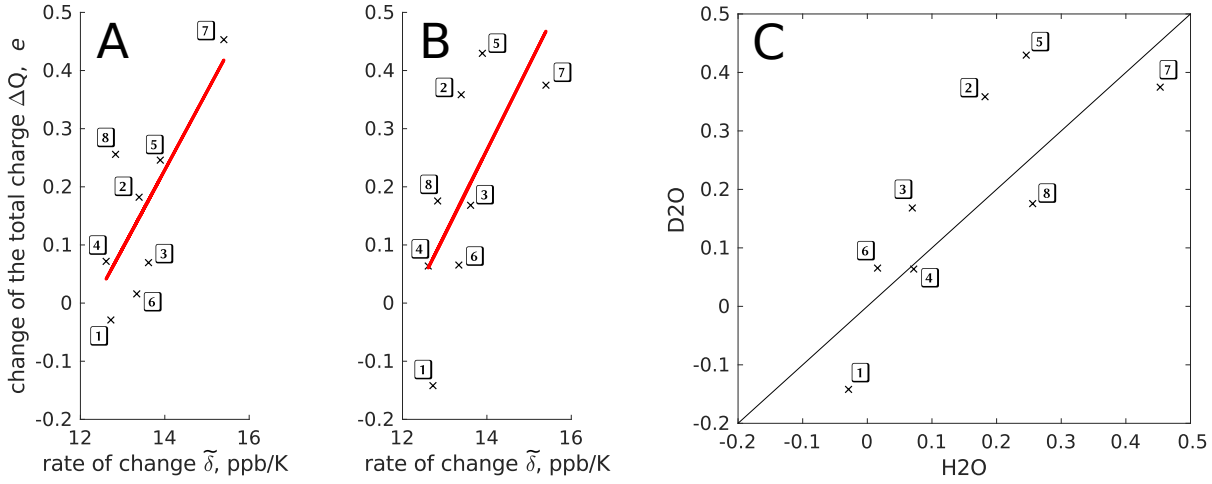

Figure 1: Comparison between experimental temperature coefficients of atorvastatin (in D_2O) aromatic peaks and temperature-driven change of solvent charge enclosed in spherical volume centred around each hydrogen nucleus (Eq. 4 in the main text).
A – simulation in H_2O vs experiment in D_2O, linear fit: $y = 0.13(5)x - 1.7(6)$, Pearson's correlation coefficient, $r = 0.77$,
B – simulation in D_2O vs experiment in D_2O, linear fit: $y = 0.15(5)x - 1.8(9)$, $r = 0.68$,
C – direct comparison between simulation results for H_2O and D_2O.

List of simulations

Table 1: Summary of simulation length (in μs) for considered systems at lower and higher temperature.

	298 K	350 K
H_2O	3.5	2.5
D_2O	1.0	1.0
CH_3OH	3.0	2.0

Structure and partial charges of atorvastatin

A listing of atorvastatin atomic coordinates (starting structure), types, and partial charges in mol2 file format is given below.

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@<TRIPOS>MOLECULE
MOL
   76    79     1     0     0
SMALL

@<TRIPOS>ATOM
      1 F1           4.2320    4.8490   -0.2410 f          1 MOL      -0.137900
      2 O1           3.3900   -2.4370    3.0600 oh         1 MOL      -0.605800
      3 O2           5.8230   -0.9360   -0.1690 oh         1 MOL      -0.608800
      4 O3          -4.0480   -0.0240    1.5870 o          1 MOL      -0.602100
      5 O4           5.9510   -3.8220   -3.4780 oh         1 MOL      -0.600100
      6 O5           5.7340   -1.5960   -3.0710 o          1 MOL      -0.564000
      7 N1           0.3210    0.0760    1.5170 na         1 MOL      -0.047100
      8 N2          -3.4510   -1.1570   -0.3630 n          1 MOL      -0.464100
      9 C1          -0.8540   -0.6250    1.6000 cc         1 MOL      -0.014600
     10 C2           1.5800   -0.3340    2.1280 c3         1 MOL       0.026300
     11 C3           0.1280    1.2100    0.7720 cc         1 MOL      -0.064300
     12 C4          -0.9530   -1.9000    2.3430 c3         1 MOL      -0.008400
     13 C5           2.4470   -1.2160    1.2190 c3         1 MOL      -0.097400
     14 C6          -1.8120    0.0730    0.8980 cd         1 MOL      -0.217600
     15 C7          -1.1910    1.2340    0.3740 cd         1 MOL      -0.071000
     16 C8           3.7420   -1.7120    1.8780 c3         1 MOL       0.143100
     17 C9           4.5790   -2.6490    0.9880 c3         1 MOL      -0.110400
     18 C10          1.1950    2.1550    0.5090 ca         1 MOL      -0.035000
     19 C11         -1.3240   -3.1000    1.4400 c3         1 MOL      -0.095600
     20 C12         -1.9350   -1.8320    3.5350 c3         1 MOL      -0.095600
     21 C13         -1.7590    2.2830   -0.4270 ca         1 MOL      -0.021000
     22 C14          5.0320   -2.1040   -0.3740 c3         1 MOL       0.154100
     23 C15         -3.1790   -0.3430    0.7530 c          1 MOL       0.718700
     24 C16          5.8130   -3.1250   -1.2010 c3         1 MOL      -0.171400
     25 C17          1.9990    2.0030   -0.6210 ca         1 MOL      -0.088000
     26 C18          1.4170    3.2180    1.3850 ca         1 MOL      -0.088000
     27 C19         -2.3260    3.4000    0.1870 ca         1 MOL      -0.120000
     28 C20         -1.7440    2.1850   -1.8180 ca         1 MOL      -0.120000
     29 C21          3.0250    2.9130   -0.8740 ca         1 MOL      -0.169000
     30 C22          2.4430    4.1280    1.1310 ca         1 MOL      -0.169000
     31 C23         -2.8780    4.4190   -0.5900 ca         1 MOL      -0.130500
     32 C24         -2.2960    3.2030   -2.5950 ca         1 MOL      -0.130500
     33 C25          3.2470    3.9760    0.0020 ca         1 MOL       0.132900
     34 C26         -4.6780   -1.7490   -0.7540 ca         1 MOL       0.075600
     35 C27          5.8310   -2.7460   -2.6620 c          1 MOL       0.638100
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36 C28        -2.8630     4.3200    -1.9810 ca        1 MOL      -0.124000
37 C29        -5.8250    -1.5490     0.0140 ca        1 MOL      -0.172000
38 C30        -4.7390    -2.5310    -1.9080 ca        1 MOL      -0.172000
39 C31        -7.0330    -2.1310    -0.3720 ca        1 MOL      -0.105500
40 C32        -5.9470    -3.1130    -2.2930 ca        1 MOL      -0.105500
41 C33        -7.0940    -2.9130    -1.5250 ca        1 MOL      -0.163000
42 H1          2.1380     0.5730     2.3850 h1        1 MOL       0.076700
43 H2          1.3710    -0.8000     3.0950 h1        1 MOL       0.076700
44 H3          0.0080    -2.1840     2.7780 hc        1 MOL       0.058700
45 H4          1.8520    -2.0870     0.9140 hc        1 MOL       0.062200
46 H5          2.6840    -0.6640     0.3050 hc        1 MOL       0.062200
47 H6          4.3430    -0.8510     2.1900 h1        1 MOL       0.057700
48 H7          5.4690    -2.9410     1.5620 hc        1 MOL       0.061700
49 H8          4.0140    -3.5780     0.8350 hc        1 MOL       0.061700
50 H9         -0.6940    -3.1290     0.5450 hc        1 MOL       0.046533
51 H10        -1.1780    -4.0400     1.9850 hc        1 MOL       0.046533
52 H11        -2.3700    -3.0710     1.1260 hc        1 MOL       0.046533
53 H12        -1.8630    -2.7440     4.1390 hc        1 MOL       0.046533
54 H13        -1.7020    -0.9800     4.1830 hc        1 MOL       0.046533
55 H14        -2.9740    -1.7380     3.2090 hc        1 MOL       0.046533
56 H15         4.1470    -1.8000    -0.9460 h1        1 MOL       0.047700
57 H16         6.8510    -3.2030    -0.8610 hc        1 MOL       0.095200
58 H17         5.3310    -4.1060    -1.1200 hc        1 MOL       0.095200
59 H18         1.8370     1.1820    -1.3150 ha        1 MOL       0.144500
60 H19         0.7990     3.3500     2.2700 ha        1 MOL       0.144500
61 H20         4.2170    -2.6970     3.5010 ho        1 MOL       0.409000
62 H21        -2.3460     3.4930     1.2710 ha        1 MOL       0.137000
63 H22        -1.3070     1.3200    -2.3120 ha        1 MOL       0.137000
64 H23        -2.6660    -1.3610    -0.9790 hn        1 MOL       0.323500
65 H24         3.6510     2.7950    -1.7540 ha        1 MOL       0.151500
66 H25         2.6160     4.9550     1.8130 ha        1 MOL       0.151500
67 H26         5.2440    -0.2440     0.1900 ho        1 MOL       0.431000
68 H27        -3.3190     5.2880    -0.1120 ha        1 MOL       0.133000
69 H28        -2.2840     3.1270    -3.6790 ha        1 MOL       0.133000
70 H29        -3.2920     5.1130    -2.5870 ha        1 MOL       0.133000
71 H30        -5.8620    -0.9590     0.9180 ha        1 MOL       0.149000
72 H31        -3.8530    -2.6950    -2.5150 ha        1 MOL       0.149000
73 H32         5.9550    -3.5650    -4.4250 ho        1 MOL       0.450000
74 H33        -7.9270    -1.9760     0.2260 ha        1 MOL       0.129500
75 H34        -5.9950    -3.7220    -3.1910 ha        1 MOL       0.129500
76 H35        -8.0340    -3.3660    -1.8250 ha        1 MOL       0.130000
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