Supporting Information

A Collective Coordinate to Obtain Free Energy Profiles for Complex Reactions in Condensed Phases

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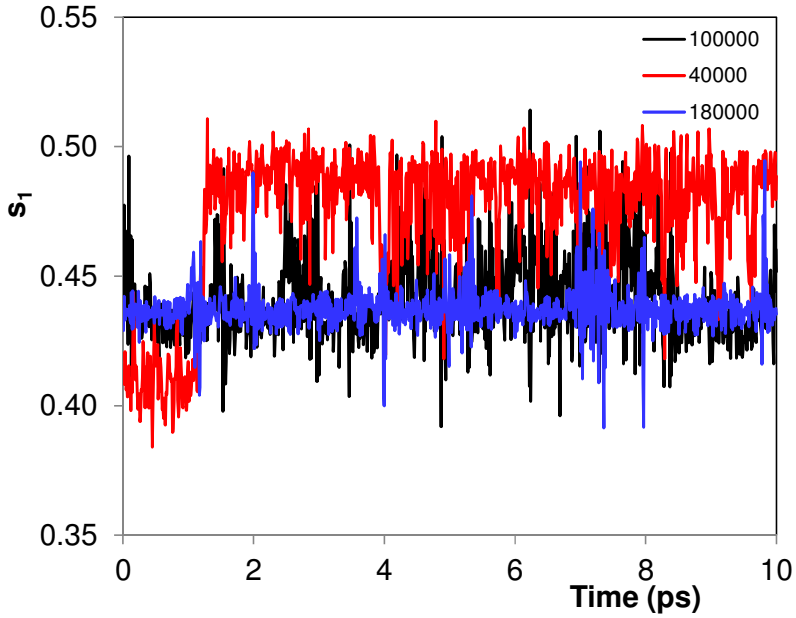

Figure S1. Oscillations of the $s_1(\mathbf{q})$ coordinate with different values of the force constant (in kJ·mol^{-1}). Results correspond to the simulation of the enzymatic TS and λ=500 Å^{-2}.

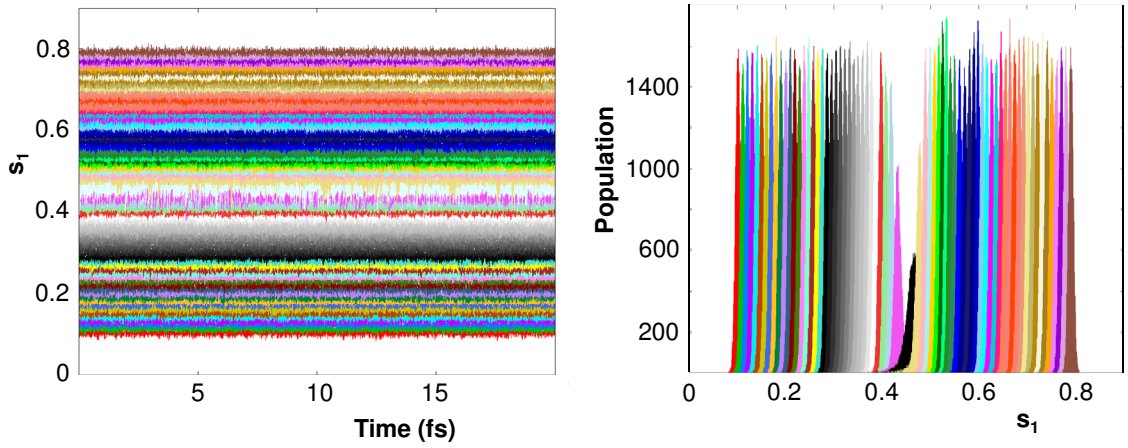

Figure S1. $s_1(\mathbf{q})$ values obtained in the simulation windows used to trace the enzymatic PMF with λ=500 Å^{-2}. Left, values of the coordinate versus simulation time coloured by window. Right, histogram of $s_1(\mathbf{q})$ for each simulation window.

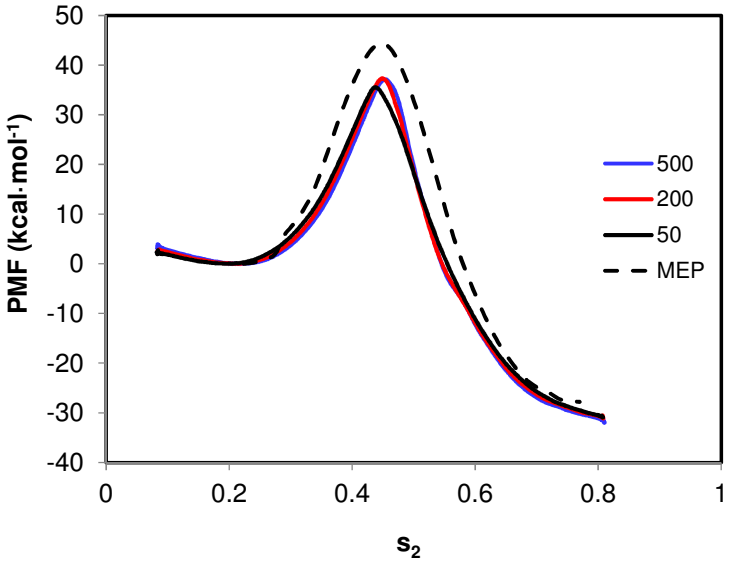

Figure S3. PMF and MEP for the isochorismate transformation into pyruvate and salycilate as a function of the $s_2(\mathbf{q})$ coordinate and different values of λ (in $Å^{-2}$).

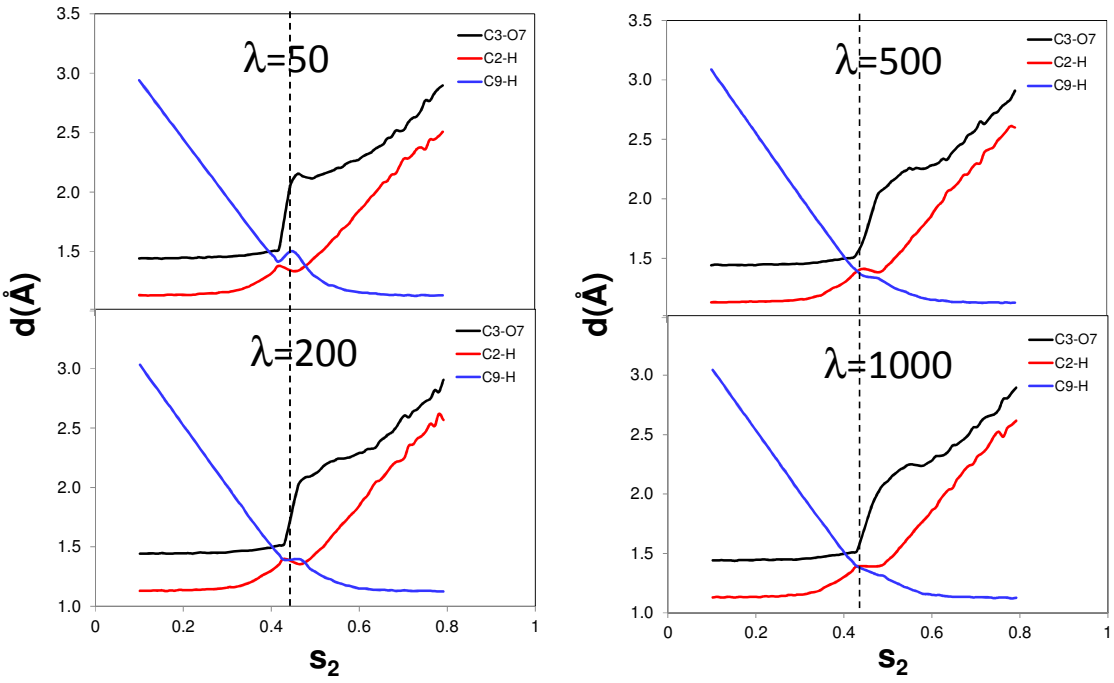

Figure S4. Averaged values of distances corresponding to bonds broken or formed during the reaction as a function of the $s_2(\mathbf{q})$ reaction coordinate. Each plot corresponds to a different values of λ (in $Å^{-2}$). Position of the TS is shown with a vertical dashed line.

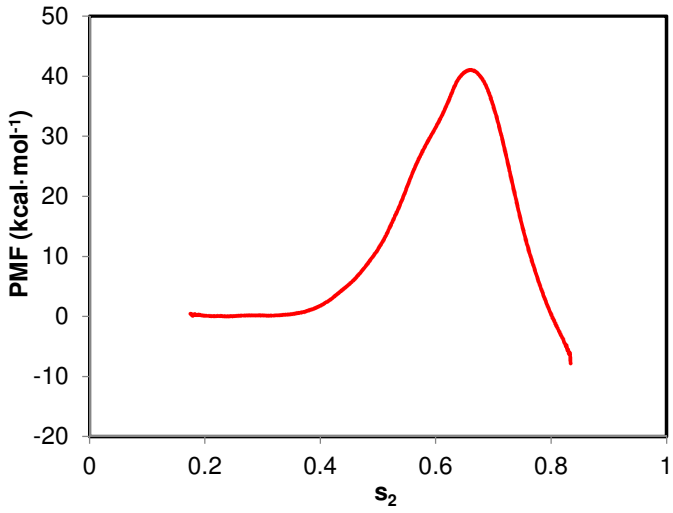

Figure S5. PMF and the isochorismate transformation into pyruvate and salycilate in aqueous solution as a function of the $s_2(\mathbf{q})$ coordinate with λ=500 Å^{-2}.

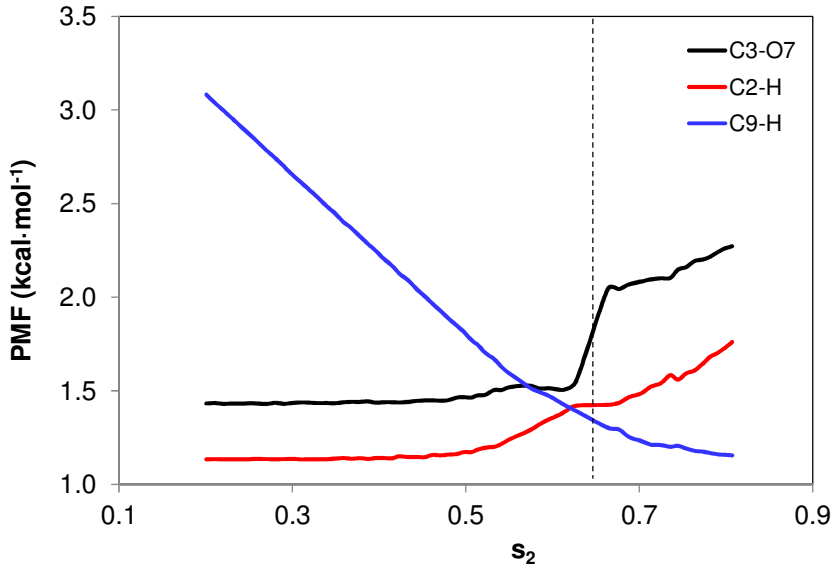

Figure S6. Evolution of averaged values of distances corresponding to bonds broken or formed during the reaction in aqueous solution as a function of the $s_2(\mathbf{q})$ reaction coordinate with λ=500 Å^{-2}. Position of the TS is indicated by a vertical dashed line.

Implementation of the s coordinate in fDynamo

The method was implemented as a separate module (cvsd.F90) that can be obtained from the authors upon request.

In addition, small changes must be made in other modules of the fDynamo library. The definition of the new module must be included in module dynamo.F90. Module energy.F90 must be also changed in subroutines energy, gradient, energy_initialize and print_initialize to add and print the energy terms coming from the new module

dynamo.F90 : Definition of the new module

USE CVSZD

energy.F90 : Definition of the subroutine cvszd_calc, and the corresponding energy term

USE CVSZD, ONLY : CVSZD_CALC

REAL (KIND = DP) :: ECVSZD = 0.0_DP

Subroutine CVSZD_CALC must be called in the subroutine ENERGY:

CALL CVSZD_CALC(ECVSZD)

ETOTAL = ETOTAL + ECVSZD

The same in subroutine GRADIENT:

CALL CVSZD_CALC(ECVSZD, ATMDER)

ETOTAL = ETOTAL + ECVSZD

In the initialization procedure (subroutine ENERGY_INITIALIZE):

ECVSZD = 0.0_DP

And in the subroutine ENERGY_PRINT:

WRITE (PRINT_LINE, "(F16.4)") ECVSZD ; CALL PRINT_SUMMARY_ELEMENT ("Colective var. SZD")