# Experimental and Theoretical Insights into the Structure and Molecular Dynamics of 2,3,3',4'-Tetramethoxy-trans-stilbene – a Chemopreventive Agent

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## Supporting Information

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## 1. The synthesis of the 2,3,3',4'-tetramethoxy-trans-stilbene

Synthesis of TeTS was performed according to the Horner–Wadsworth–Emmons reaction. The synthesis (Fig S1) were carried out in N,N-dimethylformamide as a solvent and strong base – sodium methanolate, diethyl 3,4-dimethoxybenzyl)phosphonate and 2,3-dimethyl benzaldehyde. The reaction mixture was kept in temperature range 0 to 25 °C by 30 minutes and next 1h in temperature 100 °C. Cooled reaction mixture was poured into distilled water and precipitated raw product was recrystalized from ethanol. The applied procedure allowed to obtain product with a yield of 52%.

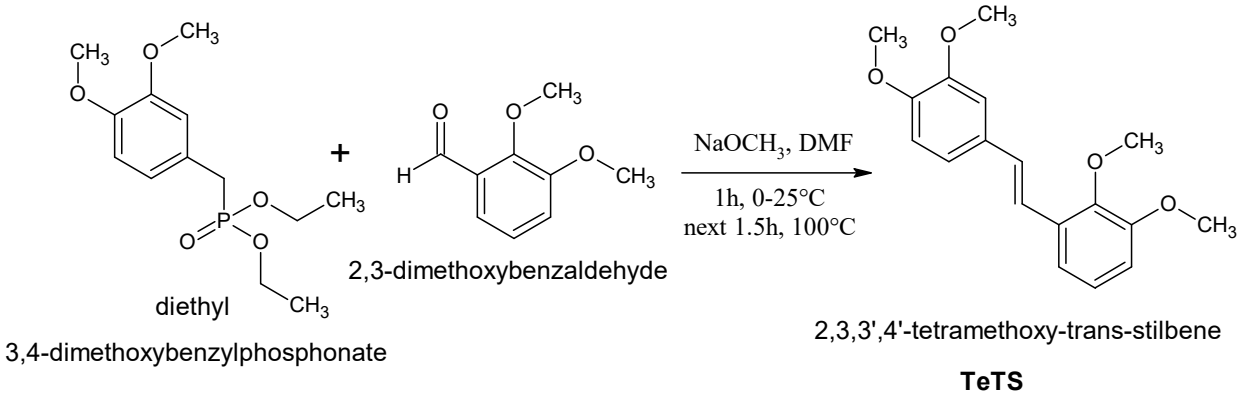



*Fig. S1. Scheme describing procedure of synthesis of 2,3,3',4'-tetramethoxy-trans-stilbene*

## 2. Mass spectrometry

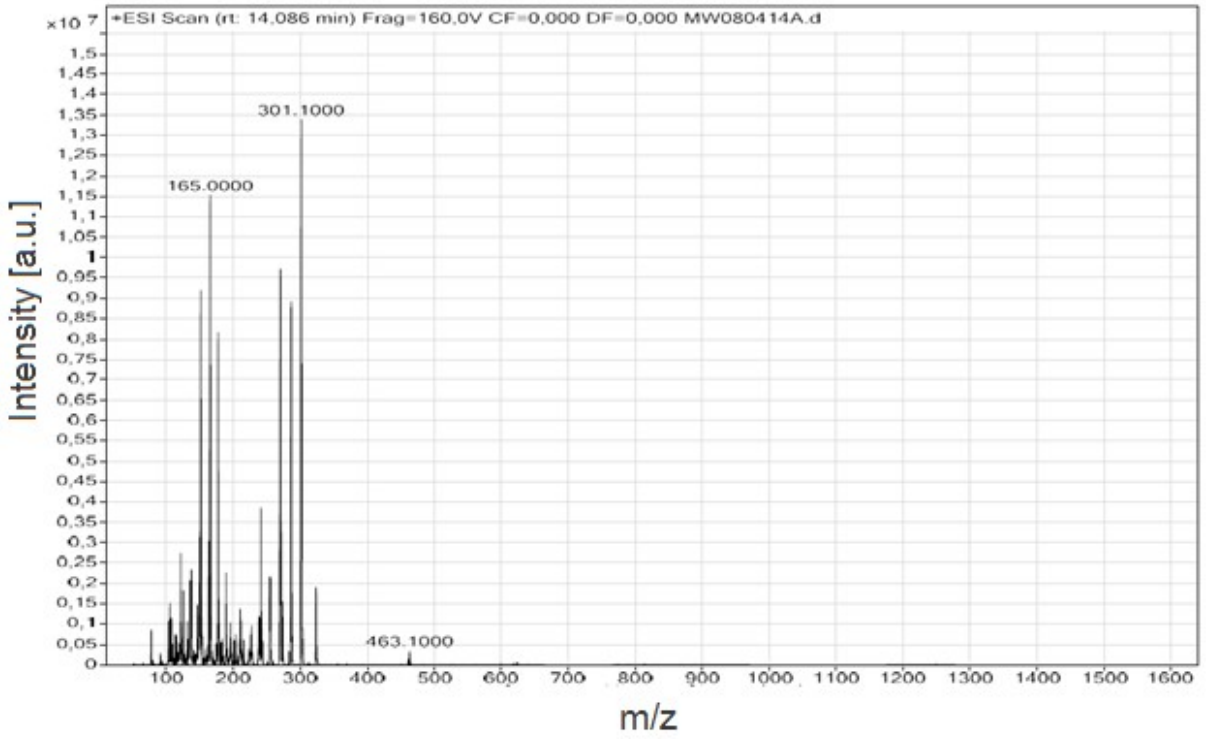



*Fig. S2. Mass spectra of 2,3,3',4'-tetramethoxy-trans-stilbene*

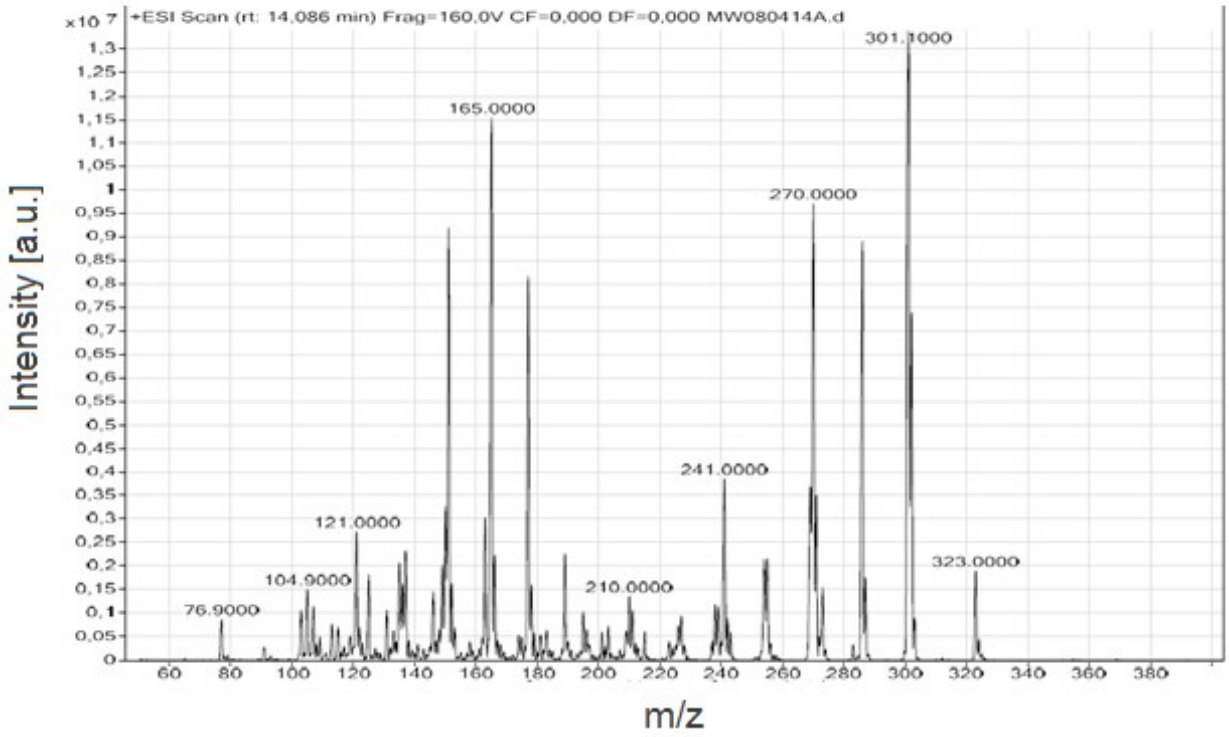



*Fig. S3. Mass spectra of 2,3,3',4'-tetramethoxy-trans-stilbene.*

## 3. $^{1}$H and $^{13}$C liquid-state NMR

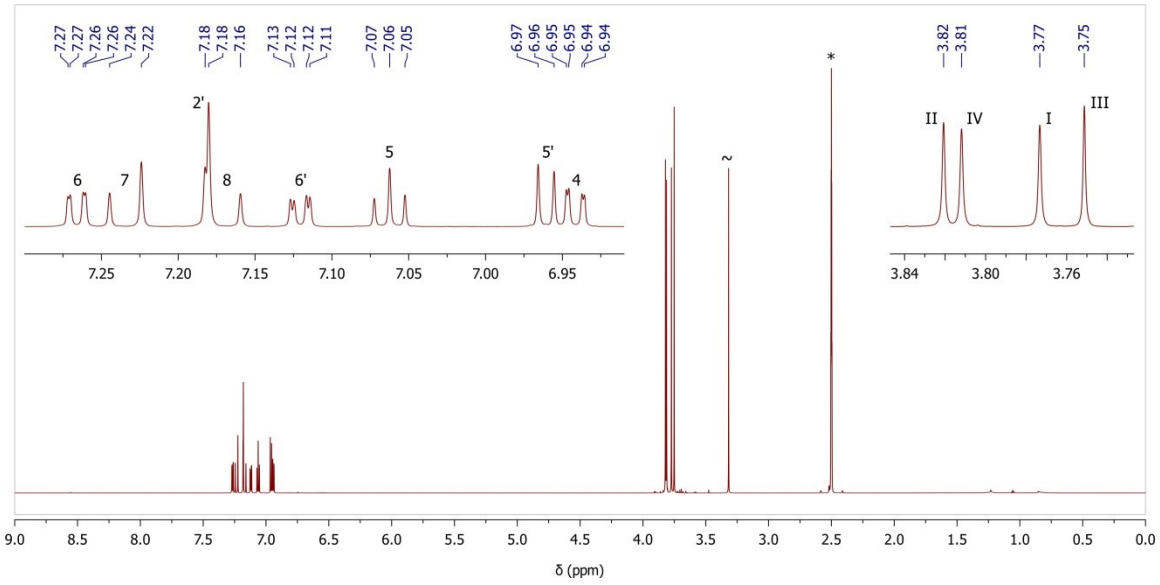



*Fig. S4. $^{1}$H NMR spectrum of 2,3,3',4'-tetramethoxy-trans-stilbene (DMSO-$d_6$, 298 K). The symbols * and ~ indicate DMSO-$d_6$ and water residual peaks, respectively.*

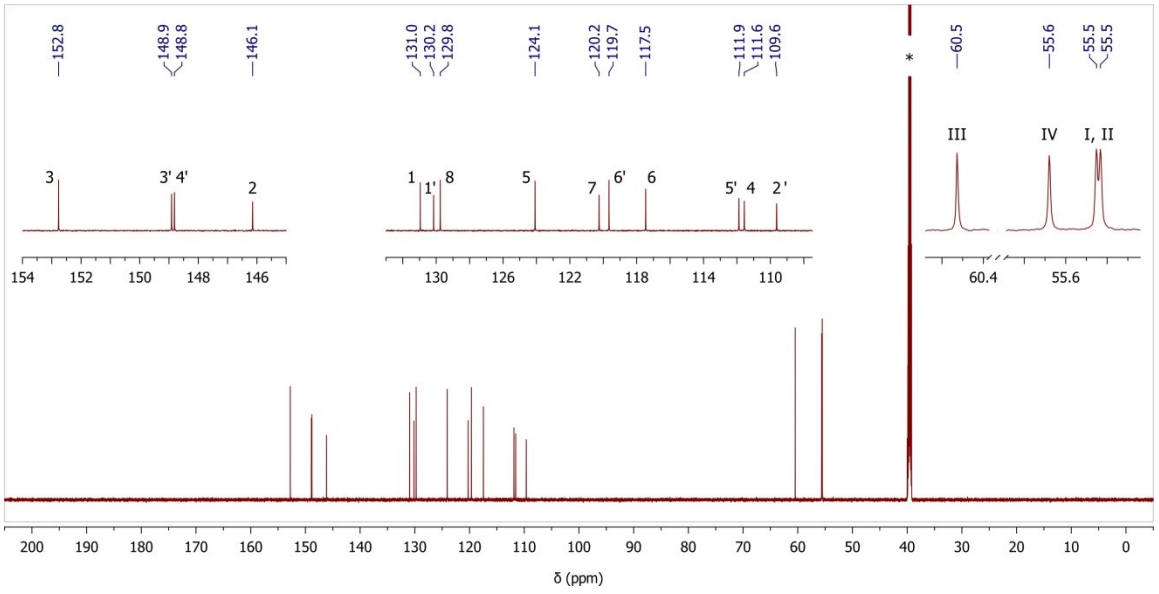



*Fig. S5. $^{13}$C NMR spectrum of 2,3,3',4'-tetramethoxy-trans-stilbene (DMSO-$d_6$, 298 K). The symbol * indicates DMSO-$d_6$ peak.*

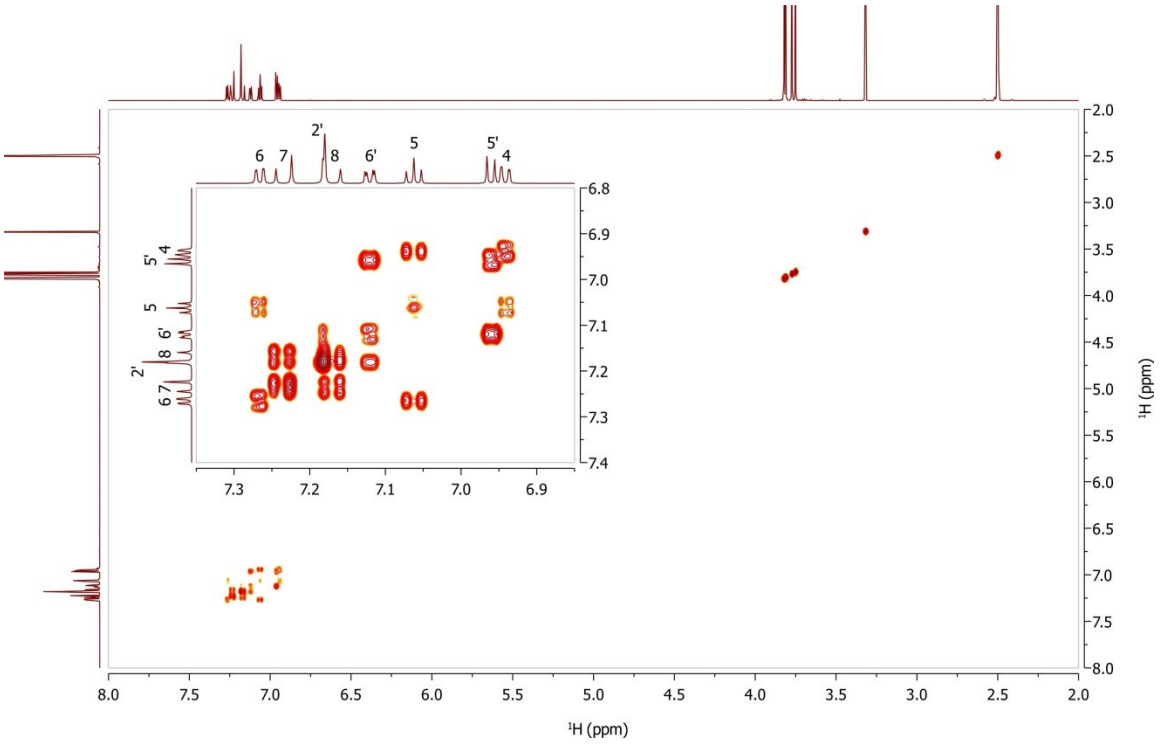



*Fig. S6. $^{1}H$-$^{1}H$ COSY spectrum of 2,3,3',4'-tetramethoxy-trans-stilbene (DMSO-$d_6$, 298 K). Expansion reveal correlations via $^{3}J_{HH}$ within the vinylene and aromatic group.*

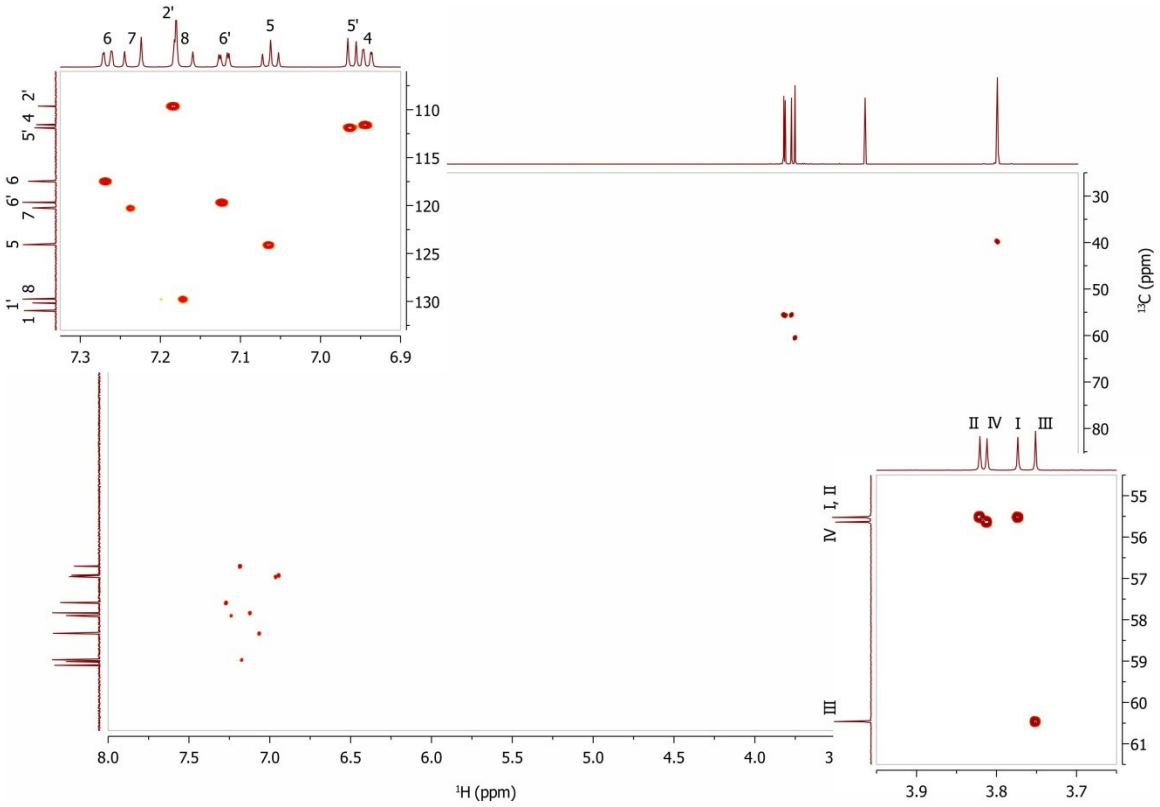



*Fig. S7. $^{1}H$-$^{13}C$ HSQC spectrum of 2,3,3',4'-tetramethoxy-trans-stilbene (DMSO-$d_6$, 298 K). Expanded regions show the one-bond $^{1}H$-$^{13}C$ correlations within the vinylene and aromatic groups (top left) and the methyl groups (bottom right).*

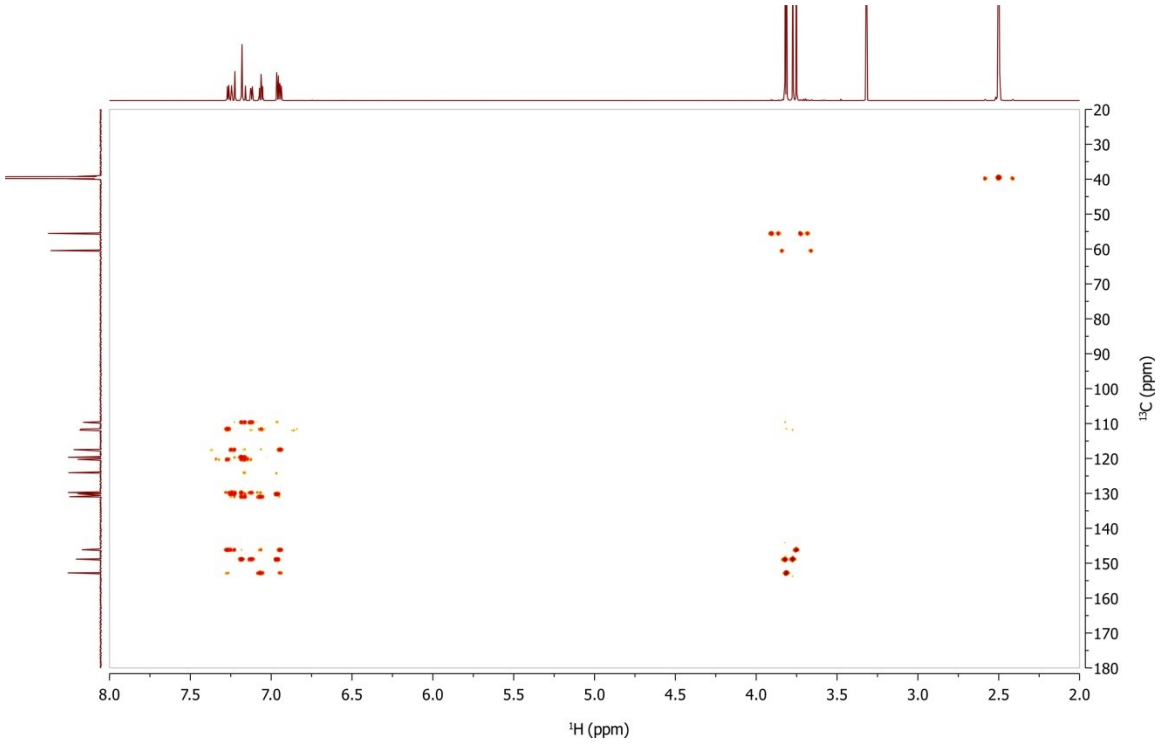



*Fig. S8. $^{1}H$-$^{13}C$ HMBC spectrum of 2,3,3',4'-tetramethoxy-trans-stilbene (DMSO-$d_6$, 298 K).*

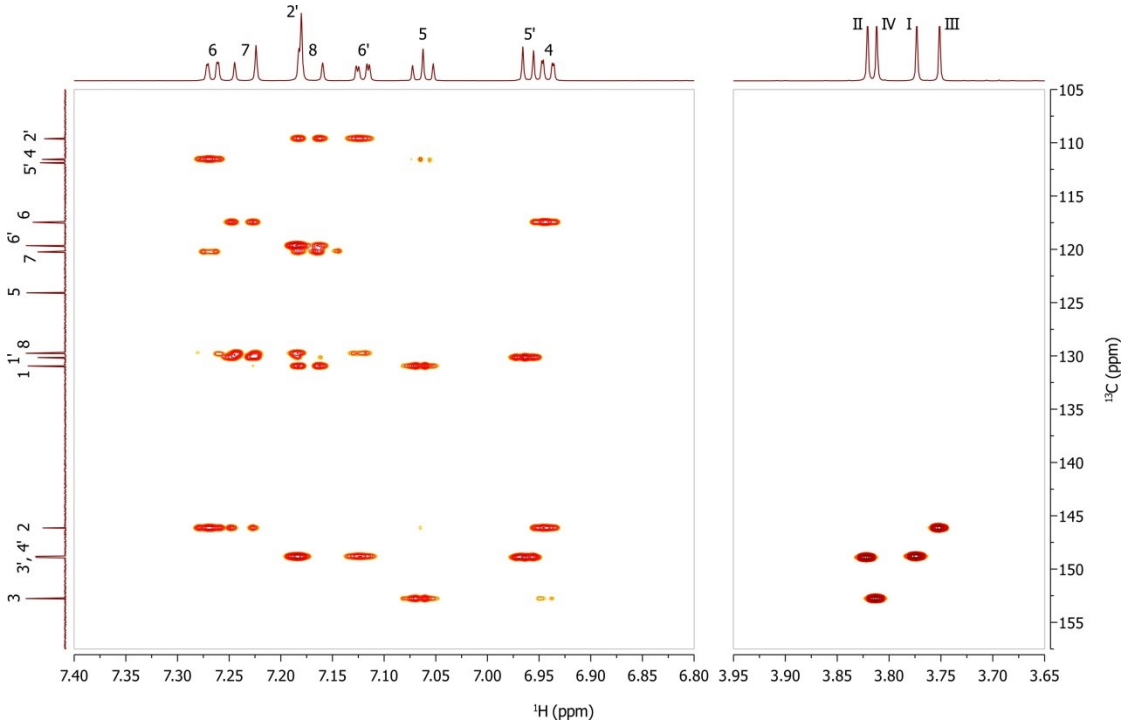



*Fig. S9. Selected region of $^{1}H$-$^{13}C$ HMBC spectrum of 2,3,3',4'-tetramethoxy-trans-stilbene (DMSO-$d_6$, 298 K) presenting two- and three-bond correlations within vinylene and aromatic groups (left) and three-bond correlations between methyl protons and ring carbons (right).*

## 4. Crystallographic data

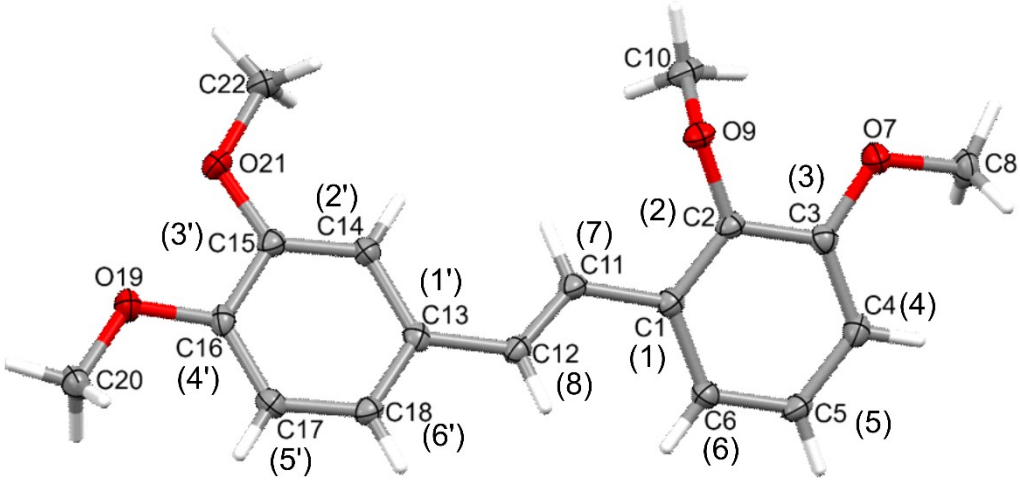



*Fig. S10. View of 2,3,3',4'-tetramethoxy-trans-stilbene, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. The figure shows both ways of numbering crystallographic and IUPAC (in brackets).*

Table S1 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 2,3,3',4'-tetramethoxy-trans-stilbene. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalised $U_{IJ}$ tensor.

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| O19 | -211(2) | 4450.5(4) | 3428.1(4) | 23.2(3) |
| O9 | 10197(2) | 1822.5(4) | 4529.3(4) | 19.5(3) |
| O7 | 13430(2) | 935.2(4) | 4433.4(4) | 23.2(3) |
| O21 | 3442(2) | 4301.8(4) | 4106.6(4) | 24.3(3) |
| C1 | 8928(3) | 1737.3(6) | 3615.4(6) | 17.0(3) |
| C2 | 10450(3) | 1555.1(6) | 4039.9(5) | 16.7(3) |
| C3 | 12072(3) | 1079.6(6) | 3986.2(6) | 18.4(3) |
| C13 | 3813(3) | 2911.6(6) | 3402.4(6) | 17.0(3) |
| C11 | 7342(3) | 2250.1(6) | 3674.8(5) | 17.8(3) |
| C6 | 9059(3) | 1436.3(6) | 3131.3(6) | 18.8(3) |
| C18 | 1799(3) | 2996.2(6) | 3049.5(6) | 18.6(3) |
| C14 | 4381(3) | 3351.3(6) | 3769.6(6) | 18.1(3) |
| C17 | 399(3) | 3503.1(6) | 3045.5(6) | 18.7(3) |
| C4 | 12171(3) | 786.7(6) | 3504.9(6) | 20.1(3) |
| C16 | 994(3) | 3932.6(6) | 3401.6(6) | 18.0(3) |
| C15 | 2997(3) | 3851.0(6) | 3773.7(5) | 18.0(3) |
| C5 | 10656(3) | 969.7(6) | 3081.1(6) | 19.8(3) |
| C12 | 5298(3) | 2382.5(6) | 3377.0(6) | 18.0(3) |
| C22 | 5421(3) | 4234.0(7) | 4496.2(6) | 23.5(4) |
| C20 | -2203(3) | 4554.4(7) | 3049.6(6) | 23.9(4) |
| C10 | 12423(3) | 2131.8(7) | 4705.0(6) | 24.4(4) |
| C8 | 15340(3) | 502.4(6) | 4375.5(7) | 23.8(4) |

Table S2 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 2,3,3',4'-tetramethoxy-trans-stilbene. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| O19 | 26.1(6) | 17.7(5) | 25.7(6) | -1.7(4) | -5.5(5) | 6.6(5) |
| O9 | 22.8(6) | 20.9(5) | 14.7(5) | -3.4(4) | 0.7(4) | 1.2(4) |
| O7 | 27.7(6) | 22.0(5) | 19.8(5) | 0.1(4) | -2.4(5) | 8.0(5) |
| O21 | 31.8(7) | 17.1(5) | 24.0(6) | -5.5(4) | -6.7(5) | 3.5(5) |
| C1 | 19.1(8) | 14.9(6) | 17.0(7) | 1.0(5) | 2.3(6) | -2.0(6) |
| C2 | 20.7(8) | 15.2(6) | 14.2(7) | -1.0(5) | 3.0(6) | -1.4(6) |
| C3 | 19.9(8) | 17.6(7) | 17.8(7) | 2.0(6) | 0.1(6) | -0.6(6) |
| C13 | 19.0(8) | 15.8(6) | 16.1(7) | 2.7(5) | 3.4(6) | -0.6(6) |
| C11 | 24.0(8) | 15.7(6) | 13.9(6) | -1.2(5) | 1.5(6) | -0.2(6) |
| C6 | 23.5(8) | 17.0(7) | 16.0(7) | 0.8(6) | -1.2(6) | -0.5(6) |
| C18 | 22.9(8) | 17.1(7) | 15.7(7) | -0.9(5) | 1.6(6) | -2.5(6) |
| C14 | 20.5(8) | 17.0(7) | 16.7(7) | 1.7(6) | -1.8(6) | 0.9(6) |
| C17 | 18.8(8) | 20.2(7) | 17.0(7) | 2.8(6) | -0.9(6) | -0.1(6) |

Table S2 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 2,3,3',4'-tetramethoxy-trans-stilbene. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| C4 | 22.7(8) | 15.3(7) | 22.4(7) | -0.4(6) | 4.3(6) | 1.8(6) |
| C16 | 20.2(8) | 14.9(6) | 18.9(7) | 3.2(6) | 3.4(6) | 2.6(6) |
| C15 | 22.6(8) | 16.2(7) | 15.3(7) | -0.6(5) | 1.6(6) | -0.7(6) |
| C5 | 26.1(9) | 17.2(7) | 16.1(7) | -3.7(6) | 2.7(6) | -2.4(6) |
| C12 | 23.2(8) | 14.8(7) | 16.0(7) | -0.8(5) | 2.7(6) | -1.7(6) |
| C22 | 27.9(9) | 21.8(7) | 20.7(7) | -5.4(6) | -4.4(7) | -0.1(7) |
| C20 | 23.9(9) | 23.1(7) | 24.6(8) | 3.9(6) | -2.3(7) | 5.1(7) |
| C10 | 29.6(9) | 24.1(7) | 19.6(7) | -5.5(6) | 1.3(7) | -4.1(7) |
| C8 | 21.4(8) | 20.3(7) | 29.8(8) | 1.1(6) | -3.2(7) | 5.9(6) |

Table S3 Bond Lengths for 2,3,3',4'-tetramethoxy-trans-stilbene.

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| O19 | C16 | 1.3687(17) | C3 | C4 | 1.387(2) |
| O19 | C20 | 1.4264(19) | C13 | C18 | 1.386(2) |
| O9 | C2 | 1.3818(16) | C13 | C14 | 1.412(2) |
| O9 | C10 | 1.4373(19) | C13 | C12 | 1.463(2) |
| O7 | C3 | 1.3665(18) | C11 | C12 | 1.337(2) |
| O7 | C8 | 1.4289(18) | C6 | C5 | 1.380(2) |
| O21 | C15 | 1.3654(17) | C18 | C17 | 1.395(2) |
| O21 | C22 | 1.4278(19) | C14 | C15 | 1.376(2) |
| C1 | C2 | 1.393(2) | C17 | C16 | 1.380(2) |
| C1 | C11 | 1.467(2) | C4 | C5 | 1.390(2) |
| C1 | C6 | 1.403(2) | C16 | C15 | 1.412(2) |
| C2 | C3 | 1.406(2) | | | |

Table S4 Bond Angles for 2,3,3',4'-tetramethoxy-trans-stilbene.

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| C16 | O19 | C20 | 116.97(12) | C14 | C13 | C12 | 122.41(14) |
| C2 | O9 | C10 | 115.00(12) | C12 | C11 | C1 | 125.70(13) |
| C3 | O7 | C8 | 116.99(12) | C5 | C6 | C1 | 120.43(14) |
| C15 | O21 | C22 | 116.94(12) | C13 | C18 | C17 | 121.55(14) |
| C2 | C1 | C11 | 119.69(13) | C15 | C14 | C13 | 121.08(14) |
| C2 | C1 | C6 | 118.43(13) | C16 | C17 | C18 | 119.94(14) |
| C6 | C1 | C11 | 121.80(13) | C3 | C4 | C5 | 119.22(14) |
| O9 | C2 | C1 | 118.82(13) | O19 | C16 | C17 | 125.10(14) |
| O9 | C2 | C3 | 120.12(13) | O19 | C16 | C15 | 115.33(13) |
| C1 | C2 | C3 | 120.87(13) | C17 | C16 | C15 | 119.57(14) |
| O7 | C3 | C2 | 115.46(13) | O21 | C15 | C14 | 125.03(14) |

Table S4 Bond Angles for 2,3,3',4'-tetramethoxy-trans-stilbene.

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| O7 | C3 | C4 | 124.67(14) | O21 | C15 | C16 | 115.04(13) |
| C4 | C3 | C2 | 119.86(14) | C14 | C15 | C16 | 119.90(13) |
| C18 | C13 | C14 | 117.95(13) | C6 | C5 | C4 | 121.19(13) |
| C18 | C13 | C12 | 119.63(13) | C11 | C12 | C13 | 126.46(14) |

Table S5Torsion Angles for 2,3,3',4'-tetramethoxy-trans-stilbene.

| A | B | C | D | Angle/° | A | B | C | D | Angle/° |
|---|---|---|---|---|---|---|---|---|---|
| O19 | C16 | C15 | O21 | -0.04(19) | C6 | C1 | C2 | C3 | -0.3(2) |
| O19 | C16 | C15 | C14 | -178.08(13) | C6 | C1 | C11 | C12 | 23.6(2) |
| O9 | C2 | C3 | O7 | -3.7(2) | C18 | C13 | C14 | C15 | -0.7(2) |
| O9 | C2 | C3 | C4 | 175.11(14) | C18 | C13 | C12 | C11 | 177.23(14) |
| O7 | C3 | C4 | C5 | 178.73(14) | C18 | C17 | C16 | O19 | 178.75(14) |
| C1 | C2 | C3 | O7 | -178.69(13) | C18 | C17 | C16 | C15 | -1.0(2) |
| C1 | C2 | C3 | C4 | 0.1(2) | C14 | C13 | C18 | C17 | 1.4(2) |
| C1 | C11 | C12 | C13 | -174.91(14) | C14 | C13 | C12 | C11 | -1.5(2) |
| C1 | C6 | C5 | C4 | -0.1(2) | C17 | C16 | C15 | O21 | 179.74(13) |
| C2 | C1 | C11 | C12 | -159.62(15) | C17 | C16 | C15 | C14 | 1.7(2) |
| C2 | C1 | C6 | C5 | 0.3(2) | C12 | C13 | C18 | C17 | -177.42(13) |
| C2 | C3 | C4 | C5 | 0.0(2) | C12 | C13 | C14 | C15 | 178.10(14) |
| C3 | C4 | C5 | C6 | 0.0(2) | C22 | O21 | C15 | C14 | -3.2(2) |
| C13 | C18 | C17 | C16 | -0.6(2) | C22 | O21 | C15 | C16 | 178.88(13) |
| C13 | C14 | C15 | O21 | -178.68(14) | C20 | O19 | C16 | C17 | -1.3(2) |
| C13 | C14 | C15 | C16 | -0.9(2) | C20 | O19 | C16 | C15 | 178.48(13) |
| C11 | C1 | C2 | O9 | 7.7(2) | C10 | O9 | C2 | C1 | -114.96(15) |
| C11 | C1 | C2 | C3 | -177.22(14) | C10 | O9 | C2 | C3 | 69.94(17) |
| C11 | C1 | C6 | C5 | 177.16(14) | C8 | O7 | C3 | C2 | -172.10(13) |
| C6 | C1 | C2 | O9 | -175.35(13) | C8 | O7 | C3 | C4 | 9.2(2) |

Table S6 Hydrogen Atom Coordinates (Å×$10^4$) and Isotropic Displacement Parameters (Å$^2$×$10^3$) for 2,3,3',4'-tetramethoxy-trans-stilbene.

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H11 | 7797 | 2505 | 3943 | 21 |
| H6 | 8065 | 1552 | 2842 | 23 |
| H18 | 1372 | 2708 | 2810 | 22 |
| H14 | 5713 | 3302 | 4013 | 22 |
| H17 | -936 | 3552 | 2803 | 22 |
| H4 | 13238 | 471 | 3466 | 24 |
| H5 | 10719 | 774 | 2758 | 24 |
| H12 | 4767 | 2112 | 3129 | 22 |
| H22A | 7029 | 4170 | 4319 | 35 |

Table S6 Hydrogen Atom Coordinates (Å×$10^4$) and Isotropic Displacement Parameters (Å$^2$×$10^3$) for 2,3,3',4'-tetramethoxy-trans-stilbene.

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H22B | 5030 | 3914 | 4721 | 35 |
| H22C | 5534 | 4573 | 4710 | 35 |
| H20A | -1506 | 4543 | 2695 | 36 |
| H20B | -2940 | 4923 | 3114 | 36 |
| H20C | -3505 | 4267 | 3085 | 36 |
| H10A | 12644 | 2465 | 4487 | 37 |
| H10B | 13910 | 1893 | 4675 | 37 |
| H10C | 12202 | 2244 | 5071 | 37 |
| H8A | 16537 | 613 | 4103 | 36 |
| H8B | 14535 | 150 | 4276 | 36 |
| H8C | 16231 | 454 | 4708 | 36 |

# 5. Computational data

Table S7. Atomic coordinates of local minimum 1 of 2,3,3',4'-tetramethoxy-trans-stilbene

| type | x [Å] | y [Å] | z [Å] |
|---|---|---|---|
| C | -0.320768924 | 0.706834953 | -0.095076281 |
| H | -0.253658134 | 1.785709489 | 0.034897106 |
| C | 0.818834989 | -0.008840559 | -0.204983984 |
| H | 0.764719112 | -1.089040852 | -0.298027968 |
| C | 2.18213876O | 0.530278589 | -0.196902283 |
| C | 2.469051412 | 1.910835725 | -0.284882650 |
| C | 3.266342119 | -0.36574232H | -0.114277866 |
| C | 3.778178510 | 2.366578010 | -0.267790962 |
| C | 4.599575670 | 0.101604935 | -0.108520270 |
| C | 4.853187274 | 1.473075365 | -0.178839974 |
| H | 1.65701667O | 2.623892580 | -0.377137293 |
| H | 3.98048322H | 3.431331595 | -0.334649151 |
| H | 5.86840593H | 1.849828902 | -0.175102050 |
| C | -1.691031705 | 0.187498084 | -0.113286631 |
| C | -2.75304469H | 1.093382497 | 0.112183982 |
| C | -2.014058717 | -1.15673538C | -0.342402813 |
| C | -4.080018863 | 0.677940780 | 0.116855393 |
| C | -3.342340894 | -1.587031029 | -0.339622159 |
| C | -4.38581716H | -0.688205490 | -0.111459829 |

| | | | |
|---|---|---|---|
| H | -2.516213392 | 2.136387410 | 0.287954499 |
| H | -1.233347413 | -1.885651884 | -0.531480789 |
| H | -3.558440219 | -2.632918630 | -0.520862385 |
| O | 3.029654952 | -1.724799002 | -0.090235826 |
| C | 3.184727932 | -2.34208316O | 1.196618856 |
| H | 4.209149574 | -2.233310097 | 1.564194332 |
| H | 2.484940303 | -1.911218447 | 1.922220550 |
| H | 2.956838014 | -3.40076712C | 1.059201425 |
| O | 5.561962297 | -0.863869275 | -0.036635867 |
| C | 6.92631406O | -0.44940315C | -0.022454435 |
| H | 7.19007654H | 0.090764224 | -0.938889125 |
| H | 7.145054194 | 0.182906400 | 0.845658661 |
| H | 7.51553245C | -1.364587594 | 0.039414716 |
| O | -5.709416267 | -1.011688912 | -0.089980292 |
| C | -6.06774472C | -2.37317422C | -0.314056134 |
| H | -5.74997251O | -2.713813220 | -1.306330370 |
| H | -5.637479595 | -3.032214530 | 0.448901241 |
| H | -7.155593235 | -2.40976317C | -0.251095026 |
| O | -5.154136260 | 1.49304582C | 0.328803961 |
| C | -4.90671668H | 2.87645554C | 0.562459630 |
| H | -4.300736503 | 3.03029400O | 1.463084557 |
| H | -4.40644208O | 3.345733619 | -0.292809194 |
| H | -5.885700873 | 3.335313404 | 0.703870925 |

Table S8. Atomic coordinates of global minimum 2 of 2,3,3',4’-tetramethoxy-trans-stilbene

| type | x [Å] | y [Å] | z [Å] |
|---|---|---|---|
| C | 0.335125870 | -1.221608100 | 0.003360400 |
| H | 0.133100197 | -2.28218353H | 0.145582891 |
| C | -0.705851154 | -0.376331510 | -0.146705405 |
| H | -0.52448711O | 0.690366862 | -0.232891537 |
| C | -2.121637742 | -0.751881283 | -0.184568401 |
| C | -2.562212310 | -2.079479233 | -0.374368320 |
| C | -3.09594887H | 0.25565667O | -0.048591315 |
| C | -3.913589602 | -2.383204807 | -0.400543828 |
| C | -4.472145740 | -0.055911363 | -0.088789614 |

| | | | |
|---|---|---|---|
| C | -4.87971568H | -1.38005776O | -0.257374118 |
| H | -1.832278389 | -2.868488502 | -0.519473100 |
| H | -4.234675603 | -3.41013133C | -0.547928692 |
| H | -5.931570274 | -1.63629715C | -0.290614026 |
| C | 1.756726610 | -0.876137805 | 0.023968813 |
| C | 2.235597470 | 0.425783010 | -0.253741319 |
| C | 2.695472889 | -1.866709995 | 0.328241313 |
| C | 3.590470767 | 0.721063560 | -0.215838755 |
| C | 4.064323117 | -1.583949990 | 0.369728967 |
| C | 4.528260960 | -0.298894702 | 0.103058504 |
| H | 1.529363843 | 1.204271822 | -0.511758256 |
| H | 2.357205609 | -2.876584723 | 0.542247916 |
| H | 4.762892490 | -2.375989560 | 0.611238760 |
| O | -2.699951410 | 1.569714667 | 0.071217211 |
| C | -2.849474285 | 2.134167607 | 1.376894849 |
| H | -3.899383230 | 2.149251857 | 1.684548405 |
| H | -2.256885480 | 1.578749130 | 2.114866358 |
| H | -2.476073075 | 3.158461420 | 1.311765126 |
| O | -5.321479919 | 1.007560450 | 0.045841052 |
| C | -6.716060729 | 0.758460860 | -0.024446021 |
| H | -6.999874627 | 0.320552044 | -0.989738582 |
| H | -7.052586343 | 0.094221872 | 0.782164795 |
| H | -7.200602353 | 1.729768183 | 0.085111202 |
| O | 5.834546419 | 0.085258934 | 0.113475682 |
| C | 6.811222673 | -0.895944412 | 0.418194313 |
| H | 6.670158942 | -1.310015439 | 1.425102008 |
| H | 6.802056100 | -1.717434892 | -0.309997158 |
| H | 7.774102324 | -0.385309800 | 0.371545972 |
| O | 4.131878107 | 1.945864060 | -0.472194136 |
| C | 3.250739020 | 3.005289145 | -0.804771750 |
| H | 2.687260714 | 2.792454560 | -1.722501791 |
| H | 2.542471130 | 3.214908424 | 0.007408212 |
| H | 3.882040277 | 3.880384444 | -0.965646862 |

Table S9. Atomic coordinates of local minimum 3 of 2,3,3',4’-tetramethoxy-trans-stilbene

| type | x [Å] | y [Å] | z [Å] |
|---|---|---|---|
| C | -0.097992505 | -0.347495959 | -0.203914775 |
| H | 0.38356672C | -1.310721017 | -0.328812110 |
| C | 0.681756582 | 0.752917930 | -0.124145101 |
| H | 0.193360139 | 1.723560463 | -0.048299194 |
| C | 2.143710715 | 0.858936147 | -0.168875512 |
| C | 2.694894673 | 2.15038501C | -0.332568934 |
| C | 3.04023674H | -0.22288507H | -0.054442517 |
| C | 4.064019650 | 2.35417565H | -0.391542017 |
| C | 4.434992412 | -0.01283824H | -0.122835721 |
| C | 4.947384630 | 1.275618214 | -0.290230399 |
| H | 2.018406189 | 2.99589746C | -0.417813455 |
| H | 4.459485159 | 3.357209012 | -0.520613111 |
| H | 6.01582333C | 1.444566703 | -0.343917223 |
| C | -1.56121032O | -0.381957042 | -0.167336233 |
| C | -2.361097840 | 0.751698224 | 0.109826948 |
| C | -2.212812839 | -1.594571403 | -0.414287506 |
| C | -3.746156883 | 0.674138863 | 0.125722127 |
| C | -3.607880947 | -1.688102894 | -0.402283039 |
| C | -4.388431905 | -0.56658939O | -0.136365668 |
| H | -1.882252952 | 1.698318602 | 0.324980517 |
| H | -1.62405248C | -2.48196051C | -0.627638439 |
| H | -4.077666464 | -2.643676470 | -0.602094858 |
| O | 2.57088602O | -1.510652294 | 0.079192782 |
| C | 2.710226864 | -2.073049889 | 1.388572235 |
| H | 3.763341677 | -2.15110649H | 1.673954774 |
| H | 2.167191617 | -1.475923042 | 2.131073698 |
| H | 2.272636274 | -3.072380517 | 1.339743987 |
| O | 5.202149475 | -1.140249805 | -0.014089902 |
| C | 6.610113252 | -1.00125164O | -0.112474925 |
| H | 6.90778228H | -0.577739252 | -1.080030821 |
| H | 7.015546952 | -0.374150247 | 0.692189904 |
| H | 7.018108647 | -2.00900641O | -0.021723999 |

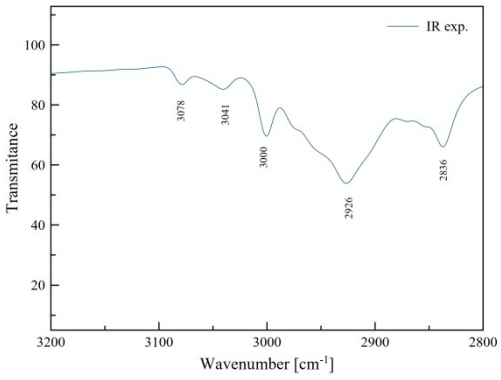
| | | | |
|---|---|---|---|
| O | -5.749513615 | -0.544685984 | -0.097069983 |
| C | -6.438716075 | -1.757607717 | -0.348614031 |
| H | -6.227697492 | -2.143172917 | -1.354579053 |
| H | -6.184834400 | -2.529354657 | 0.389751478 |
| H | -7.500768199 | -1.52098522C | -0.270115342 |
| O | -4.586111094 | 1.717087525 | 0.385789727 |
| C | -4.009822877 | 2.983197445 | 0.654419110 |
| H | -3.374911145 | 2.959570702 | 1.549908927 |
| H | -3.41573691H | 3.347833124 | -0.193876934 |
| H | -4.845894937 | 3.662915810 | 0.825585995 |

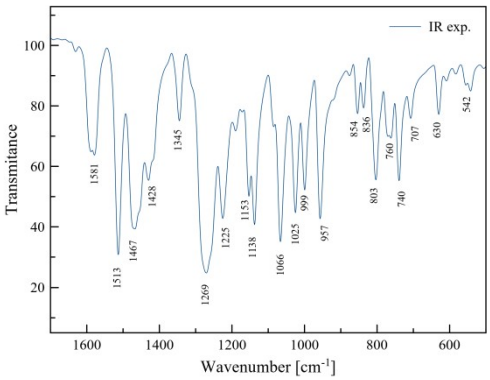
Table S10. Atomic coordinates of local minimum 4 of 2,3,3',4'-tetramethoxy-trans-stilbene

| type | x [Å] | y [Å] | z [Å] |
|---|---|---|---|
| C | 0.11249447H | -0.147584105 | -0.080122552 |
| H | -0.248635407 | 0.871027482 | -0.168374419 |
| C | -0.792581734 | -1.150294812 | -0.080928447 |
| H | -0.420558153 | -2.17354795C | -0.052150107 |
| C | -2.25494228C | -1.07892005C | -0.163951582 |
| C | -2.948813634 | -2.283741524 | -0.419164513 |
| C | -3.02079981H | 0.093441890 | -0.002592675 |
| C | -4.330156324 | -2.318948750 | -0.520553344 |
| C | -4.427953603 | 0.055582787 | -0.113784354 |
| C | -5.08305534H | -1.15063162O | -0.371929554 |
| H | -2.374047300 | -3.19718845O | -0.541283988 |
| H | -4.837010622 | -3.258334762 | -0.719929550 |
| H | -6.16195161H | -1.18768185H | -0.459176491 |
| C | 1.56830208C | -0.29934863H | -0.004069713 |
| C | 2.371426983 | 0.83352660C | -0.267649625 |
| C | 2.216613099 | -1.496281687 | 0.322253648 |
| C | 3.75930907C | 0.774385127 | -0.226954956 |
| C | 3.610142550 | -1.56996022H | 0.368503716 |
| C | 4.396152977 | -0.450389957 | 0.095359103 |
| H | 1.879229630 | 1.766462524 | -0.517152367 |
| H | 1.64036176C | -2.38382600O | 0.561159933 |
| H | 4.08061469C | -2.510801967 | 0.628395332 |

| | | | |
|---|---|---|---|
| O | -2.407295564 | 1.306179184 | 0.221307459 |
| C | -2.515377313 | 1.799870807 | 1.561018787 |
| H | -3.559648584 | 1.982930585 | 1.830459940 |
| H | -2.06476831O | 1.099097045 | 2.274150795 |
| H | -1.964379504 | 2.74245044C | 1.584699712 |
| O | -5.060113867 | 1.257910959 | 0.048485850 |
| C | -6.471541945 | 1.29295107C | -0.086038344 |
| H | -6.790723035 | 0.966240323 | -1.083796880 |
| H | -6.969051799 | 0.671393619 | 0.669769373 |
| H | -6.760997773 | 2.334742210 | 0.059424370 |
| O | 5.75834145C | -0.42174517O | 0.117016559 |
| C | 6.442361260 | -1.622170922 | 0.432817705 |
| H | 6.19430386O | -1.97838595O | 1.441279856 |
| H | 6.222038735 | -2.417986352 | -0.290674217 |
| H | 7.50563864H | -1.38187061O | 0.389076207 |
| O | 4.59655729H | 1.82238696C | -0.475968038 |
| C | 4.015226089 | 3.071172554 | -0.808776320 |
| H | 3.41698825H | 3.009684962 | -1.727251538 |
| H | 3.38301415H | 3.455098125 | 0.002637256 |
| H | 4.848827960 | 3.75668978H | -0.968619716 |

# 6. FT-IR Spectroscopy



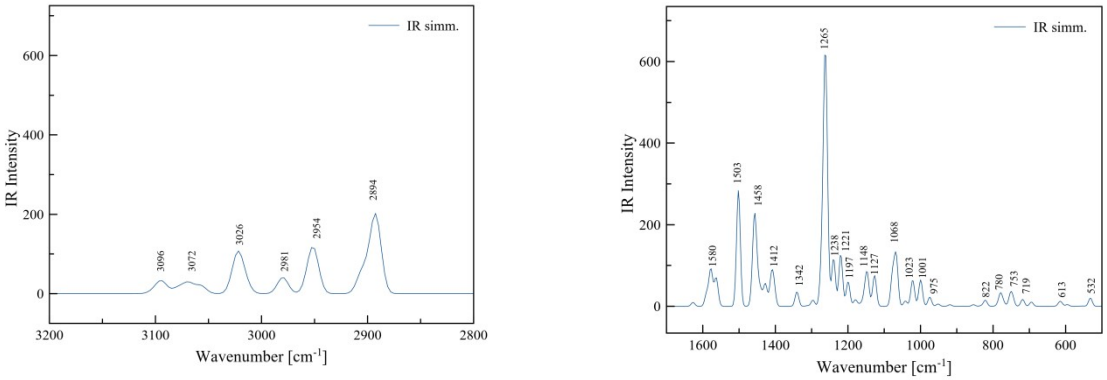



*Fig S11. The experimental FT-IR spectra of 2,3,3',4'-tetramethoxy-trans-stilbene (top) along with simulated spectrum by computational method B3LYP/6-31G(d,p) model (bottom). Theoretical spectra were plotted with a value of FWHM = 12. The wavenumber axis values were scaled by 0.961 factor according to CCCBDB.*

Table S11. Observed and theoretical FT-IR vibrational assignments of 2,3,3',4'-tetramethoxy-trans-stilbene for selected bands Scaling factor is 0.961 according to the reference [S1].

| Band number | Observed band maxima [$cm^{-1}$] | Main calculated normal modes [$cm^{-1}$] | | Assignment |
|---|---|---|---|---|
| | | unscaled | scaled | |
| 1 | 3078 | 3223 | 3096 | Ring C-H stretching |
| 2 | 3041 | 3197 | 3072 | Vinylene C-H and ring C-H stretching |
| 3 | 3000 | 3149 | 3026 | Asymmetrical $CH_3$ C-H stretching |
| 4 | 2926 | 3074 | 2954 | Asymmetrical $CH_3$ C-H stretching |
| 5 | 2836 | 3012 | 2894 | Symmetrical $CH_3$ C-H stretching |
| 6 | 1581 | 1644 | 1580 | Ring -C=C- stretching |
| 7 | 1513 | 1565 | 1503 | Ring C-H rocking |
| 8 | 1467 | 1518 | 1458 | Ring C-H rocking and $CH_3$ C-H bending |
| 9 | 1428 | 1470 | 1412 | Ring C-H rocking and $CH_3$ C-H bending |
| 10 | 1345 | 1463 | 1343 | Vinylene C-H rocking |
| 11 | 1269 | 1316 | 1265 | Vinylene C-H rocking and ring C-H rocking |
| 12 | 1225 | 1271 | 1221 | Vinylene C-H rocking and ring C-H rocking |
| 13 | 1153 | 1195 | 1148 | Ring C-H rocking and $CH_3$ C-H wagging |
| 14 | 1138 | 1173 | 1127 | Ring C-H rocking |
| 15 | 1066 | 1111 | 1068 | Ring C-H rocking and $H_3C$-O stretching |
| 16 | 1025 | 1064 | 1023 | Ring -C=C- rocking and $H_3C$-O stretching |
| 17 | 999 | 1041 | 1001 | Ring -C=C- breathing and $H_3C$-O stretching |
| 18 | 957 | 1015 | 975 | Vinylene C-H out of plane |
| 19 | 854 | 889 | 856 | Vinylene C-H out of plane and ring C-H out of plane |
| 20 | 803 | 855 | 822 | Ring C-H out of plane |
| 21 | 760 | 812 | 780 | Ring C-H out of plane |
| 22 | 740 | 783 | 753 | Ring -C=C- breathing and ring C-H out of plane |
| 23 | 707 | 748 | 719 | Ring C-H out of plane |
| 24 | 630 | 638 | 613 | Ring C=C bending and $CH_3$ C-H wagging |
| 25 | 542 | 554 | 532 | Ring -C=C- bending and $CH_3$ C-H wagging |

## 6. $^{13}$C CP MAS solid-state NMR data

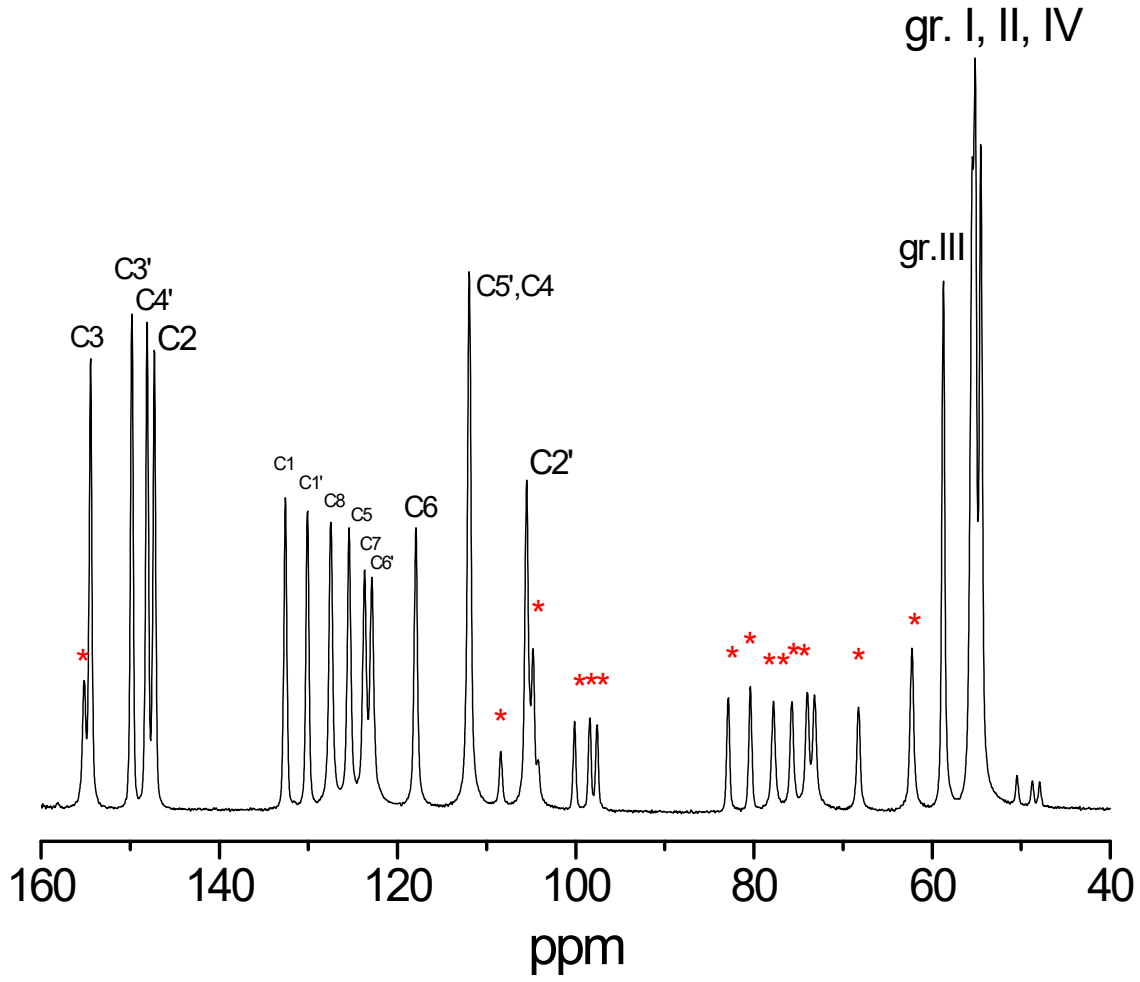



*Fig. S12. $^{13}$C CP MAS solid-state NMR spectrum along with assignments of methyl groups and other carbons based on liquid-state NMR (section III.1 of the paper). The asterix denote satellite peaks.*

*Table S12*
*The chemical shift for carbons in TeTS derived from liquid and solid NMR experiments*

| Carbon nucleus | $^{13}$C NMR liquid [ppm] | $^{13}$C CP/MAS NMR [ppm] |
|---|---|---|
| C_methyl_I or C_methyl_II | 55.5 | 54.5 |
| C_methyl_I or C_methyl_II | 55.5 | 55.3 |
| C_methyl_IV | 55.7 | 55.5 |
| C_methyl_III | 60.5 | 58.9 |
| C2’ | 109.6 | 105.6 |
| C4 | 111.6 | 111.8 |
| C5’ | 111.9 | 111.8 |
| C6 | 117.5 | 118.1 |
| C6’ | 119.7 | 122.9 |
| C7 | 120.3 | 123.7 |

| | | |
|---|---|---|
| C5 | 124.1 | 125.5 |
| C8 | 129.8 | 127.5 |
| C1’ | 130.2 | 130.2 |
| C1 | 131.0 | 132.7 |
| C2 | 146.2 | 147.3 |
| C4’ | 148.7 | 148.2 |
| C3’ | 148.9 | 149.9 |
| C3 | 152.8 | 154.5 |

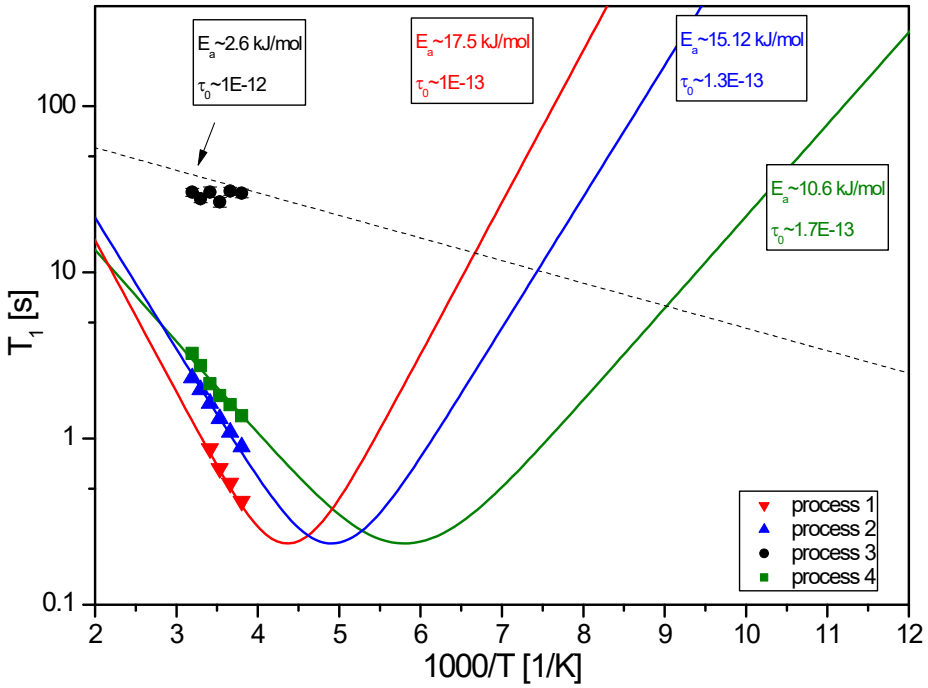



*Fig. S13. $^{13}C$ $T_1$ relaxation data along with simulated BPP curves representing four different methyl groups.*

Fig. S13 illustrates four different BPP curves simulated for each individual methyl group relying on both a) $^{13}C$ $T_1$ experimental data points and b) activation parameters estimated via QENS and $^{1}H$ NMR relaxation data. Unfortunately, an experimentally available temperature window does not allow determining the actual position of $T_1$ minima and hence the relaxation amplitudes remain unknown. However, one can simulate hypothetical curves taking into account a) equal relaxation amplitudes for all individual methyl group reorientations and b) estimated energy barriers corresponding to four inequivalent methyl group positions. It is worth pointing out that the slopes of the BPP curves shoulders fit nicely to the experimental data points. Moreover, simulated BPP formula (dashed line) with the activation energy $E_a$=*2.6 kJ/mol* determined via QENS, explains clearly relatively long relaxation times observed in the case of the methyl group number III.

## REFERENCES

S1. NIST Computational Chemistry Comparison and Benchmark Database, NIST Standard Reference Database Number 101 Release 18, October 2016, Editor: Russell D. Johnson III http://cccbdb.nist.gov/