Electronic Supplementary Information for

Decoloration Rates of a Photomerocyanine Dye as a Visual Probe Into Hydrogen Bonding Interactions

Simone Ciampi, Paul K. Eggers, Naomi L. Haworth, Nadim Darwish, Pawel Wagner, Michelle L. Coote, Gordon G. Wallace and Colin L. Raston

S1. Experimental Methods 2
S1.1 Materials 2
S1.1.1 Chemicals 2
S1.1.2 Purification and Analysis of Synthesized Compounds 3
S1.2 Calculation Methods 9
S2. Spectroscopic characterization of compounds **SP-1** to **SP-5** 11
S3. Additional Experimental and Computational results 26
S3.1 Theoretical hydrogen bond strengths 26
S3.2 Experimental and theoretical hydroxyl (8-OH) infrared (IR) stretching frequencies and scaling factors 27
S3.3 Computed energies (**SP-1** to **SP-5**) 28
S3.4 Experimental fading rates for S**P-1**/**-2**/**-3**-/-4 solutions (MC→SP) 31
S3.5 Hydroxyl groups absorption region in the IR spectrum of SP-1 and SP-3 solutions 36
S3.6 Computed hydroxyls (8-OH) infrared stretching frequencies for the SP and *trans*-MC isomers of **SP-2** and **SP-3** 37
S3.7 "Closed-ring control"; spectroscopic data for **SP-3** (5′-NO_2-6-NO_2-8-OH BIPS) 38
S3.8 MC→SP (**SP-2**) thermal fading; computed reaction profiles 40
S3.9 Representative UV/V spectra of **SP-2** samples showing the photochemical opening and thermal fading of photocolored solutions 42
S3.10 Thermal decoloration of **SP-4** solutions; k_{obs} vs solvent polarity ($E_T(30)$ scale) 43
S3.11 **SP-2** and **SP-4**; computed Gibb's Free Energy reaction profiles 44
S3.12 "Open-ring control"; spectroscopic data for **SP-5** (8-COOH BIPS) 46
S3.13 Thermal decoloration of **SP-2** solutions; k_{obs} vs solvent polarity ($E_T(30)$ scale) 48
S3.14 Shear stress effects on the thermal decoloration of **SP-2** solutions; high rpms 48
S4. M06-2X/6-31G(2df,p) optimized geometries 49
S5. References 74

S1. Experimental Methods

S1.1 Materials

S1.1.1 Chemicals

All chemicals, unless noted otherwise, were of analytical grade and used as received. Dichloromethane, chloroform, chlorobenzene, 1,2-dichloroethane, hexane, *n*-propanol, ethanol, methanol, ethyl acetate, diethyl ether, tetrahydrofuran, 1,4-dioxane, benzene, toluene, acetonitrile and *N*,*N*-dimethylformamide, for chemical reactions, purification procedures and UV-visible absorption measurements were redistilled prior to use. Anhydrous solvents used in chemical reactions were purified under nitrogen by a solvent drying system from LC Technology Solutions Inc. Anhydrous chloroform was distilled from phosphorus pentoxide. Although we are aware of the limitations of using a single physical quantity in defining solvent polarity, we tentatively used the $E_T(30)$ scale by Dimroth as empirical measure of solvent polarity.[1] $E_T(30)$ parameters relevant to this study are taken from ref. 2 and ref. 3.[2] $E_T(30)$ values expressed in kcal mol^{-1} are as follow: 2,2,2-trifluoroethanol, 59.8; methanol, 55.4; 2-chloroethanol, 55.1; ethanol, 51.9; nitromethane, 46.3; propylene carbonate, 46.0; acetonitrile, 45.6; dimethyl sulfoxide, 45.1; *N*,*N*-dimethylformamide, 43.2; acetone, 42.2; 1,2-dichloroethane, 41.3; dichloromethane 40.7; acetophenone, 40.6; pyridine, 40.5; *i*-butyl methyl ketone, 39.4; chloroform, 39.1; *n*-butyl acetate, 38.5; 1,2-dimethoxyethane (*monoglyme*, 38.2; ethyl acetate, 38.1; 1,2-dichlorobenzene, 38.0; tetrahydrofuran, 37.4; fluorobenzene, 37.0; chlorobenzene, 36.8; 1-bromobutane, 36.6; 1,4-dioxane, 36.0; trichloroethene, 35.9; diethyl ether, 34.5; benzene, 34.3; toluene, 33.9. Electric dipole moments for solvents used in this study are expressed in non SI units of debye (1 debye = 3.336×10^{-30} Coulomb meter) and are taken from ref. 4:[3] propylene carbonate, 4.90; dimethyl sulfoxide, 3.96; acetonitrile, 3.93; *N*,*N*-dimethylformamide, 3.82; nitromethane, 3.46; acetophenone, 3.05; acetone, 2.88; *i*-butyl methyl ketone, 2.69; 2,2,2-trifluoroethanol, 2.52; 1,2-dichlorobenzene, 2.50; pyridine, 2.22; 1-bromobutane, 2.08; butyl acetate, 1.87; 1,2-dichloroethane, 1.83; ethyl acetate, 1.78; 2-chloroethanol, 1.77; tetrahydrofuran, 1.75; 1,2-dimethoxyethane (*monoglyme*), 1.71; methanol, 1.70; chlorobenzene, 1.69; ethanol, 1.69; fluorobenzene, 1.66; dichloromethane, 1.60; diethyl ether, 1.15; chloroform, 1.04; trichloroethene, 0.80; toluene, 0.36; benzene, 0.0; 1,4-dioxane, 0.0. Taft and Kamlet α and β empirical solvent parameters for hydrogen-bond acceptor (β, HBA) basicities and hydrogen-bond donor (α, HBD) acidities are taken from either ref. 5,[4] or from the web-based database at http://www.stenutz.eu/chem/solv26.php and are as follow (α, β): dimethyl sulfoxide, (0.00,

0.76); *N*,*N*-dimethylformamide, (0.00,0.69); pyridine, (0.00, 0.64); tetrahydrofuran, (0.00, 0.55); diethyl ether, (0.00, 0.47); butyl acetate, (0.00, 0.46); *i*-butyl methyl ketone, (0.02, 0.48); acetophenone, (0.04, 0.49); ethyl acetate, (0.00, 0.45); propylene carbonate, (0.00, 0.40); acetone, (0.08, 0.48); 1,4-dioxane, (0.00, 0.37); 1,2-dimethoxyethane, (0.00, 0.31); acetonitrile, (0.19, 0.40); 1-bromobutane, (0.00, 0.13); toluene, (0.00, 0.11); benzene, (0.00, 0.10); chlorobenzene, (0.00, 0.07); fluorobenzene, (0.00, 0.07); trichloroethene, (0.00, 0.05); 1,2-dichlorobenzene, (0.00, 0.03); 1,2-dichloroethane, (0.00, 0.00); dichloromethane, (0.13, 0.10); chloroform, (0.20, 0.10); ethanol, (0.86, 0.75); nitromethane, (0.22, 0.06); methanol, (0.98, 0.66); 2-chloroethanol, (1.28, 0.53); 2,2,2-trifluoroethanol, (1.55, 0.00).

S1.1.2 Purification and Analysis of Synthesized Compounds

Thin-layer chromatography (TLC) was performed either on silica gel or neutral aluminium oxide Merck aluminium sheets (60 F_{254}). Merck 60 Å silica gel (220−400 mesh particle size) and Sigma-Aldrich activated aluminum oxide, neutral, 58 Å (150 mesh particle size) was used for column chromatography. Unless otherwise specified NMR spectra were recorded on a Bruker Avance 400 spectrometer in deuteriochloroform ($CDCl_3$ from Aldrich, passed through basic aluminum oxide) using the residual solvent signal as internal reference. Unless otherwise specified, NMR samples were equilibrated in dark (3 h) prior to analysis. Gas chromatography-mass spectrometry (GC-MS) analyses were performed by means of an Agilent Technologies 7890A GC system equipped with a HP-5 capillary column (5% phenyl methyl siloxan, 30 m × 250 μm × 0.25 μm) and interfaced with an Agilent 5975N MSD scheme. The flow rate of the helium carrier gas was 14 mL/min and unless otherwise specified a temperature program from 100 °C to 280 °C at a ramping rate of 15 °C/min was used. The column was held at the initial temperature for 5 min and the final temperature was then held for an additional 5 min. When noted, the total ion current chromatograms of the GC/MS station were used to monitor extent of conversions and to assay the purity of synthesized compounds and commercial precursors.[5] Electrospray ionization mass spectra (ESI-MS) were obtained using a single-quadrupole liquid chromatograph mass spectrometer (LC-MS) 2020 system from Shimadzu. The MS heat-block and desolvation line (DL) temperatures were set at 200 °C and 250 °C, respectively. The DL (equivalent to the cone voltage), interface and detector voltages were set to 0 V, 4.5 kV and −1.1 kV, respectively. Nitrogen gas was used as both nebulizers (1.5 L min^{-1}) as well as drying gas (15 L min^{-1}). UV-visible absorption spectra were obtained at a room temperature of *ca*. 23 °C using a Shimadzu UV-1800 spectrophotometer and all solutions were prepared at the concentration

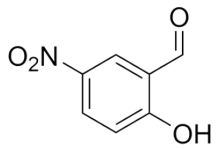
of 2.0 × 10^{-5} mol L^{-1}. The apparent rate constant for the first-order merocyanine-to-spiropyran dark relaxation kinetics (k_{obs}, MC→SP) was estimated from absorbance data and by considering only data for thermal fading times up to *ca*. 4 half-life times ($t_{1/2}$= ln 2/k_{obs}).[6] The decay in MC absorbance do translate into a k_{obs} value by the following equation[7]:

$$A_t = A_\infty + A_0 e^{-k_{obs}t}$$

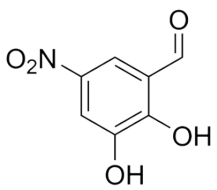
where A_∞ ,A_t and A_0 are the MC absorbances (λ_{max}) values at infinity, at a specified time after the removal of the UV stimulus, and at the time of removing the UV stimulus, respectively. A mounted high-power LED from Thorlabs (model M365L2) with a 365 nm nominal wavelength and a nominal typical output of 360 mW was used for the coloration of **SP-1** (6-NO_2 BIPS), **SP-2** (6-NO_2-8-OH BIPS), and **SP-4** (6-NO_2-8-OMe BIPS), samples. Samples of **SP-3** (5′-NO_2-6-NO_2-8-OH BIPS were colored by exposure to the UV radiation from a DYMAX® curing spot light source (model 38920) with typical nominal output intensities of *ca*. 3 W cm^{-2} (320−390 nm), *ca.* 3.5 W cm^{-2} (390−450 nm) and *ca.* 1 W cm^{-2} (280−320 nm). For each solute (**SP-1**, **SP-2**, **SP-3** and **SP-4**)/solvent system the number of repeated relaxation measures was between three and eight. The 95% confidence limit of the mean is given for each k_{obs} value and is calculated as $t_{n-1}\, s/n^{1/2}$ where t_{n-1} was between 4.30 and 2.45,[8] s is the standard deviation, and n is the number of repeated measurements. Solutions of **SP-2** and **SP-4** for visible relaxation experiments under shearing in vortex fluidic films of were prepared in dimethylsulfoxide, tetrahydrofuran and dichloromethane at the concentration of 4.0 × 10^{-4} mol L^{-1}. Samples were prepared in triplicate. The schematic of the vortex fluidic device (VFD) is detailed elsewhere.[9] In brief, a 10 mm (ID) glass NMR tube, 160 mm long, was inclined at 45º and operated in confined mode at 4000, 6000 and 9000 rpm. The liquid sample was photocolorated by exposure to 365 nm radiation (360 mW) and the MC absorbance was monitored over time through a modular fiber optic-coupled spectrometer from Ocean Optics (USB4000-VIS-NIR model). The spectrometer accepts light transmitted from the tungsten halogen light source (DT-MINI-2-GS model from Ocean Optics; deuterium UV source is kept off during measurements) through the vortexed sample via a 1000 μm optical fiber. FTIR spectra of solid samples were recorded by attenuated total reflectance (Ge ATR, PIKE MIRacle™) on a Shimadzu IR-Prestige-21 spectrometer by accumulating a minimum of 1000 scans and selecting a resolution of 2 cm^{-1}. FTIR spectra of anhydrous chloroform solutions of **SP-2** (2 mM) and **SP-3** (2 mM) were recorded in

transmission mode using a long optical path (25 mm) liquid cell from International Crystal Laboratories (Garfield, NJ, Fig. S2) by accumulating a minimum of 64 scans and selecting a resolution of 2 cm^{-1}.

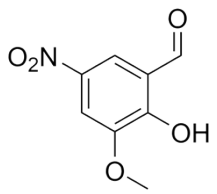
5-Nitrosalicylaldehyde **a** and 3-methoxy-5-nitrosalicylaldehyde **c** and were obtained by nitration of salicylaldehyde and *o*-vanillin, respectively, according to literature procedures[10] with minor modifications. 3-Hydroxy-5-nitrosalicylaldehyde **b** was prepare by demethylation of the methyl phenyl ether of aldehyde **c** according literature procedures[10a] with minor modifications. 6-Nitro indoline spiropyrans **SP-1, SP-2**, and **SP-4** were prepared via condensation of the Fischer`s base 1,3,3-trimethyl-2-methyleneindoline (Aldrich, 98% pure by GC-MS analysis) with aldehydes **a**, **b**, and **c**, respectively, through conventional methods[11] with minor modifications. 5',6-Dinitro-8-hydroxy indoline spiropyran **SP-3** was prepared via condensation of the methylene base 1,3,3-trimethyl-2-methylene-5-nitroindoline **d** with aldehyde **b** and follows modification of conventional literature procedures[12] for some of the synthetic steps. The "reverse photochromic"[13] control molecule **SP-5**, with a 8-carboxylic acid substitution, was prepared via condensation of the Fischer`s base 1,3,3-trimethyl-2-methyleneindoline with 3-formylsalicylic acid.



*5-Nitrosalicylaldehyde (**a**)*. Aldehyde **a** was prepared from salicylaldehyde following previously published procedures.[14] Aldehyde **b** was 96% pure by GC-MS analysis and no effort was made to remove *ca*. 4% of 3-nitrosalicylaldehyde side-product. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.59 (1H, s), 10.00 (1H, s), 8.56 (1H, d, J = 3 Hz), 8.41 (1H, dd, J = 3 Hz, J = 9 Hz), 7.12 (1H, d, J = 9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.4, 166.1, 137.1, 131.7, 129.7, 119.4, 119.0; MS (EI, 70 eV), *m*/*z* (rel intensity) 167 (100) $[M]^+$, 166 (23) $[M-1]^+$, 137 (19) $[M-NO]^+$, 120 (14), 65 (29).

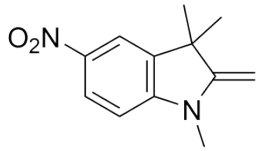


*3-Hydroxy-5-nitrosalicylaldehyde (**b**)*. Aldehyde **b** was prepared from aldehyde **c** following previously published procedures.[10a] ^{1}H NMR (400 MHz, CD_3CN) δ 11.41 (1H, s), 10.01 (1H, s), 8.22 (1H, d, J = 3 Hz), 7.90 (1H, d, J = 3 Hz), 7.58 (1H, s); ^{13}C NMR (100 MHz, CD_3CN) δ 197.1, 155.3, 146.6, 141.2, 120.7, 120.3, 115.9; MS (ESI, negative-ion mode), *m*/*z* 182 $[M-1]^-$.



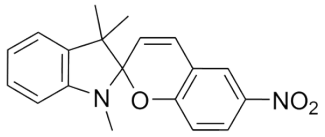
*3-Methoxy-5-nitrosalicylaldehyde (**c**)*. Aldehyde **c** was prepared from *o*-vanillin following literature procedures.[14] ^{1}H NMR (400 MHz, $CDCl_3$) δ

11.69 (1H, s), 10.00 (1H, s), 8.23 (1H, d, *J* = 3 Hz), 7.94 (1H, d, *J* = 3 Hz), 4.03 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.4, 156.9, 149.1, 140.5, 120.4, 118.8, 111.4, 56.8; MS (EI, 70 eV), *m*/*z* (rel intensity) 197 (100) $[M]^+$, 167 (10) $[M\text{-}NO]^+$, 151 (43), 136 (30), 108 (30), 80 (17).



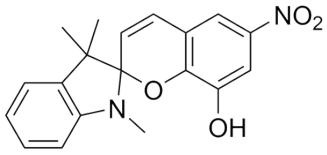
*1,3,3-Trimethyl-2-methylene-5-nitroindoline (**d**)*. The methylene base **d** was prepared according to previously published procedures.[14] ^{1}H NMR (400 MHz, C_6D_6) δ 8.05 (1H, dd, *J* = 2 Hz, *J* = 9 Hz), 7.93 (1H, d, *J* = 2 Hz), 5.73 (1H, d, *J* = 9 Hz), 3.87 (1H, d, *J* = 2 Hz), 3.81 (1H, d, *J* = 2 Hz), 2.26 (3H, s), 1.00 (6H, s); ^{13}C NMR (100 MHz, C_6D_6) δ 161.8, 151.4, 141.4, 138.4, 126.4, 118.5, 104.3, 78.6, 43.8, 29.7, 28.6; MS (EI, 70 eV), *m*/*z* (rel intensity) 218 (45) $[M]^+$, 203 (100) $[M\text{-}Me]^+$, 157 (61); TLC [SiO_2, dichloromethane/hexane (7:3, v/v)], Rf = 0.4 (UV).

6-Nitro-1',3',3'-trimethylspiro-[2H-1-benzopyran-2,2'-indoline] (SP-1)



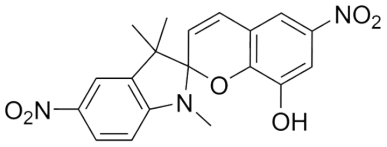
1,3,3-Trimethyl-2-methyleneindoline (1.180 g, 6.81 mmol) in ethanol (*ca*. 10 mL) was added in small portions over 5 min to a stirred solution of 5-nitrosalicylaldehyde (**a**, 1.252 g, 7.50 mmol) in ethanol (*ca*. 25 mL). The obtained solution was refluxed under an argon atmosphere for 2 h. The crude reaction mixture was concentrated *in vacuo* (bath temperature not exceeding 45 °C) to leave a dark red slurry which was then suspended in *ca*. 5 mL of ice-cold ethanol. The solid that separated was recovered by centrifugation and further washed with ice-cold ethanol (5 × 10 mL) to give the pure title compound **SP-1** as a yellow powder (421 mg, 19%). ^{1}H NMR (400 MHz, CD_3CN) δ 8.08 (1H, d, *J* = 3 Hz), 8.00 (1H, dd, *J* = 3 Hz, *J* = 9 Hz), 7.15 (1H, dt, *J* = 1 Hz, *J* = 8 Hz), 7.12 (1H, dd, *J* = 1 Hz, *J* = 7 Hz), 7.06 (1H, d, *J* = 10 Hz), 6.83 (1H, dt, *J* = 1 Hz, *J* = 7 Hz), 6.74 (1H, d, *J* = 9 Hz), 6.60 (1H, d, *J* = 8 Hz), 5.95 (1H, d, *J* = 10 Hz), 2.72 (3H, s), 1.27 (3H, s), 1.16 (3H, s); ^{13}C NMR (100 MHz, CD_3CN) δ 160.7, 148.9, 142.2, 137.3, 129.2, 128.8, 126.6, 123.7, 122.64, 122.62, 120.7, 120.2, 116.2, 108.1, 107.7, 53.1, 29.2, 26.2, 20.1; MS (EI, 70 eV), *m*/*z* (rel intensity) 323 (18), 322 (88) $[M]^+$, 307 (42), 207 (15), 159 (100), 158 (58), 144 (26); UV-vis (MeCN), λ_{max}/nm (ε_{SP}, [10^2 $M^{-1}cm^{-1}$]) 266 (231), 297 (108), 342 (125).

6-Nitro-8-hydroxy-1',3',3'-trimethylspiro-[2H-1-benzopyran-2,2'-indoline] (**SP-2**)



A solution of 1,3,3-trimethyl-2-methyleneindoline (450 mg, 2.60 mmol) in *n*-propanol (*ca*. 10 mL) was added at room temperature in one portion to an off-green stirred suspension of 3-hydroxy-5-nitrosalicylaldehyde (**b**, 551 mg, 3.01 mmol) in *n*-propanol (*ca*. 20 mL). Upon addition of the methylene base the suspension acquired a deep-blue coloration. The reaction mixture was refluxed under an argon atmosphere for a 30 min period, cooled to room temperature and concentrated *in vacuo* to leave a dark blue solid. The crude solid was suspended in 10 mL of ice-cold ethanol and the solid that separated was recovered by centrifugation and further washed with ice-cold ethanol (2 × 10 mL) to give the pure title compound **SP-2** as a fine blue powder (670 mg, 76%). ^{1}H NMR (400 MHz, (THF-d_8) δ 8.54 (1H, s), 7.61 (1H, d, J = 3 Hz), 7.51 (1H, d, J = 3 Hz), 7.10-7.04 (2H, m), 7.01 (1H, d, J = 10 Hz), 6.76 (1H, dt, J = 1 Hz, J = 7 Hz), 6.54 (1H, d, J = 8 Hz), 5.89 (1H, d, J = 10 Hz), 2.76 (3H, s), 1.30 (3H, s), 1.16 (3H, s); ^{13}C NMR (100 MHz, $(CD_3)_2SO$) δ 148.0, 147.5, 144.6, 139.7, 135.9, 128.3, 127.5, 121.5, 121.4, 119.1, 118.9, 113.6, 110.7, 10 6.8, 105.5, 51.7, 28.3, 25.8, 19.5; UV-vis (THF), λ_{max}/nm (ε_{SP}, [10^2 $M^{-1}cm^{-1}$]) 288 (94), 354 (101). MS (ESI, positive-ion mode), m/z 339 $[M+1]^+$. *Note*: integration values of NMR low ppm-absorptions peaks that are associated with an equilibrium amount of merocyanine form (MC) of **SP-2** were used to estimate dark equilibrium constants (K_{eq} = $[MC]_{eq}/[SP]_{eq}$, dark equilibration time was 3 h). NMR samples were prepared at the concentration of 2.0 × 10^{-3} M. Measured K_{eq} values are: (a) 0.00, tetrahydrofuran-d_8; (b) 0.13, acetone-d_6; (c) 0.55, dichloromethane-d_2; (d) 0.21, dimethylsulfoxide-d_6; (e) 0.28, methanol-d_4.

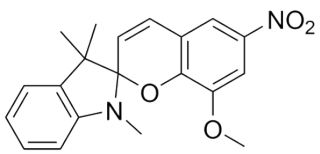
5',6-Dinitro-8-hydroxy-1',3',3'-trimethylspiro-[2H-1-benzopyran-2,2'-indoline] (SP-3).



1,3,3-Trimethyl-2-methylene-5-nitroindoline **d** (108 mg, 0.49 mmol) was added at room temperature in small portions over 10 min to a stirred suspension of 3-hydroxy-5-nitrosalicylaldehyde (**b**, 110 mg, 0.60 mmol) in *n*-propanol (*ca*. 20 mL). The orange solution was refluxed under an argon atmosphere for 12 h. The crude reaction mixture was concentrated *in vacuo* to leave an orange slurry which was then suspended in 10 mL of ice-cold ethanol. The solid that separated was recovered by centrifugation and further washed with ice-cold ethanol (2 × 10 mL) to give the pure title compound **SP-3** as an orange powder (155 mg, 82%). ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 8.79 (1H, s), 8.17 (1H, dd, J = 2 Hz, J = 9 Hz), 7.98 (1H, d, J = 2 Hz), 7.75 (1H, d, J = 2 Hz), 7.61

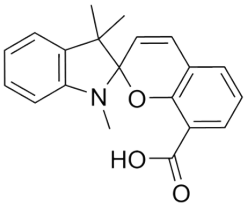
(1H, d, J = 2 Hz), 7.25 (1H, d, J = 10 Hz), 6.77 (1H, d, J = 9 Hz), 6.08 (1H, d, J = 10 Hz), 2.96 (3H, s), 1.44 (3H, s), 1.28 (3H, s); ^{1}H NMR (400 MHz, ($CDCl_3$) δ 8.20 (1H, dd, J = 2 Hz, J = 9 Hz), 7.97 (1H, d, J = 2 Hz), 7.73 (1H, d, J = 2 Hz), 7.68 (1H, d, J = 2 Hz), 7.00 (1H, d, J = 10 Hz), 6.57 (1H, d, J = 9 Hz), 5.86 (1H, d, J = 10 Hz), 5.43 (1H, s), 2.90 (3H, s), 1.36 (3H, s), 1.24 (3H, s); ^{1}H NMR (400 MHz, (CD_3CN) δ 8.18 (1H, dd, J = 2 Hz, J = 9 Hz), 8.00 (1H, d, J = 2 Hz), 7.70 (1H, d, J = 2 Hz), 7.58 (1H, d, J = 2 Hz), 7.15 (1H, s), 7.08 (1H, d, J = 10 Hz), 6.68 (1H, d, J = 9 Hz), 5.95 (1H, d, J = 10 Hz), 2.88 (3H, s), 1.33 (3H, s), 1.21 (3H, s); ^{13}C NMR (100 MHz, $(CD_3)_2CO$) 153. 2, 146.8, 144.6, 141.3, 140.7, 137.3, 129.1, 125.7, 120.3 , 118.8, 117.9, 113.8, 111.4, 10 6.1, 105.8, 51.6, 28.0, 25.1, 18.6; MS (ESI, positive-ion mode), m/z 384 $[M+1]^+$. *Note*: NMR data (*vide supra*) in either acetone-d_6, chloroform-*d* or acetonitrile-d_3 showed only absorptions peaks that are associated with the ring-closed SP form of **SP-4**. IR (ATR, cm^{-1}) 1602 (w), 1486 (s, $\nu_{as}NO_2$), 1457 (s), 1363 (m, ν_sNO_2), 1252 (s, N−Me/N−Ph), 1229 (s, N^+−O^- stretching in NO_2), 1183 (s), 1112 (m), 1022 (s), 972 (s), 923 (s, N−C_{spiro}−O); UV-vis (MeCN), λ_{max}/nm (ε_{SP}, [10^2 $M^{-1}cm^{-1}$) 250 (257), 372 (253).

6-Nitro-8-methoxy-1',3',3'-trimethylspiro-[2H-1-benzopyran-2,2'-indoline] (SP-4)



1,3,3-Trimethyl-2-methyleneindoline (780 mg, 4.50 mmol) in *n*-propanol (*ca*. 10 mL) was added in small portions over 5 min to a stirred suspension of 3-methoxy-5-nitrosalicylaldehyde (**c**, 960 mg, 4.87 mmol) in *n*-propanol (*ca*. 25 mL). The obtained deep blue solution was refluxed for 4 h. The crude reaction mixture was cooled to room temperature and concentrated *in vacuo* to leave a green residue which was then suspended in *ca*. 10 mL of ice-cold ethanol. The solid that separated was recovered by centrifugation and further washed with ice-cold ethanol (3 × 10 mL) to give the pure title compound **SP-4** as an orange powder (1018 mg, 64%). ^{1}H NMR (400 MHz, CD_3CN) δ 7.77 (1H, d, J = 3 Hz), 7.67 (1H, d, J = 3 Hz), 7.18 (1H, dt, J = 1 Hz, J = 8 Hz), 7.11 (1H, dd, J = 1 Hz, J = 7 Hz), 7.02 (1H, d, J = 10 Hz), 6.85 (1H, dt, J = 1 Hz, J = 7 Hz), 6.59 (1H, d, J = 8 Hz), 5.93 (1H, d, J = 10 Hz), 3.77 (3H, s), 2.73 (3H, s), 1.25 (3H, s), 1.14 (3H, s); ^{13}C NMR (100 MHz, CD_3CN) δ 150.2, 148.8, 148.2, 141.6, 137.3, 129.3, 128.9, 122.7, 122.6, 120.6, 120.0, 116.3, 108.5, 108.0, 107.8, 57.1, 53.1, 29.1, 26.3, 20.0; MS (EI, 70 eV), *m*/*z* (rel intensity) 352 (62) $[M]^+$, 337 (23) $[M-Me]^+$, 159 (100), 158 (143), 144 (18); UV-vis (THF), λ_{max}/nm (ε_{SP}, [10^2 $M^{-1}cm^{-1}$]) 287 (105), 297 (91), 356 (109).

1',3',3'-Trimethylspiro-[2H-1-benzopyran-2,2'-indoline]-8-carboxylic acid (SP-5)



1,3,3-Trimethyl-2-methyleneindoline (376 mg, 2.17 mmol) in ethanol (*ca*. 20 mL) was added in one portion at room temperature to a stirred solution of 3-formylsalycilic acid (400 mg, 2.41 mmol) in ethanol (*ca*. 20 mL). The obtained solution was refluxed for 4 h. The crude reaction mixture was concentrated *in vacuo* to leave a deep-red slurry which was then suspended in *ca*. 20 mL of dichloromethane. The solid that separated was recovered by centrifugation and further washed with dichloromethane aliquots (3 × 10 mL) to give the pure title compound **SP-5** as a brown powder (474 mg, 68%). ^{1}H NMR (400 MHz, CD_3OD) δ 8.65 (1H, d, J = 16 Hz, MC form, trans-coupled vinylic proton), 8.11 (1H, dd, J = 2 Hz, J = 8 Hz), 7.96 (1H, dd, J = 2 Hz, J = 8 Hz), 7.88 (1H, d, J = 16 Hz), 7.78-7.74 (1H, m), 7.65-7.58 (1H, m), 6.91 (1H, t, J = 8 Hz), 4.10 (3H, s), 1.85 (6H, s); ^{13}C NMR (100 MHz, $(CD_3)_2SO$) δ 181.6, 172.7, 169.5, 152.0, 142.8, 141.9, 136.9, 128.7, 128.1, 123.0, 122.6, 120.0, 114.1, 11 3.7, 109.1, 51.1, 33.3, 26.4; MS (ESI, positive-ion mode), m/z 322 $[M+1]^+$. *Note*: NMR data (dark equilibration time of 3 h) in methanol-d_4, dimethylsulfoxide-d_6 or acetonitrile-d_3 showed only absorptions peaks that are associated with the open-ring MC form of **SP-5**. UV-vis (MeCN), λ_{max}/nm (ε_{SP}, [10^2 $M^{-1}cm^{-1}$]) 296 (42), 368 (166), 523 (283).

S1.2 Calculation Methods

Experimental data were corroborated by theoretical calculations that were performed to give insights into hydroxyls infrared (IR) frequencies, hydrogen-bond (HB) strengths and HB effects on the pathway and barriers for the MC/SP thermal relaxation. Molecular geometries of the SP (closed-ring) structures (**SP-1**, **SP-2, SP-3, SP-4** and **SP-5**), MC isomers, transition states and intermediates (MC→SP) were determined using the M06-2X density functional[15] coupled with 6-31G(2*df*,*p*) basis sets[16]. Harmonic vibrational frequencies, calculated using the same model chemistry, were checked to ensure that each optimized geometry was a stationary point of the appropriate order. Earlier studies have identified two potential reaction pathways for the decolouration reaction.[17] Both pathways were investigated here. Starting geometries for intermediates and transition states were modelled on those reported in published literature.[17] Optimized geometries for all structures investigated in this study are reported in Table S10.

Accurate gas-phase energies for the species of interest were determined using the high-level composite G3MP2(CC) level of theory.[18] Free energies of solvation were estimated for a selection of solvents at the M05-2X[19]/6-31G(*d*)[16] level of theory using the SMD continuum

solvent model[20] and the gas-phase optimized geometries. For the calculation of zero-point energies and partition functions, the M06-2X harmonic vibrational frequencies were scaled using the scaling factors recommended for M05-2X/6-31G(2*df*,*p*).[21] Partition functions and hence entropies and thermal corrections to the energies were calculated using standard textbook formulae for the statistical thermodynamics of an ideal gas under the harmonic oscillator rigid rotor approximation. Gas-phase Gibbs free energies could therefore be calculated and combined with free energies of solvation to give Gibbs free energies in solution; appropriate phase change corrections were included.[22] Kinetic parameters could then be determined using the Eyring equation.[23] When solvent effects were considered, the rates of both possible reaction pathways were found to be comparable. In addition, decoloration of the planar merocyanine can produce either the R or S isomer of the spiropyran. This means that there are four possible reaction pathways which can contribute to the decoloration process. Calculated rates for all four of these pathways were summed to give final overall reaction rates.[24]

The strength of intramolecular 8-O–H···9-O (phenolate) hydrogen-bonds was estimated via the difference in Gibbs free energy between structures with the 8-O-H hydrogen pointing towards and away from 9-O (Fig. S3). For **SP-5** the "non-hydrogen-bonded" conformation is likely to experience some stabilization due to interaction between the O-H and the carbonyl, hence the predicted hydrogen bond energies are likely to be an underestimation. We note that the published scaling factors for harmonic vibrational frequencies[21] are designed to be applicable to vibrations over the whole energy range. For the very high-energy hydroxyl stretching vibrations, use of these averaged scaling factors can give large errors. Instead, hydroxyl IR frequencies were scaled by a factor of 0.9374. This factor was determined by comparison of the calculated OH stretching frequencies with experimental values for a variety of phenols taken from the NIST Webbook (Table S3). To evaluate the effect solvation in chloroform on the IR frequencies, structures were re-optimized using M06-2X/6-31G(2*df*,*p*) coupled with the SMD solvent model and harmonic vibrational frequencies were calculated using the same model chemistry. Frequencies were again scaled by 0.9374.

S2. Spectroscopic characterization of compounds SP-1 to SP-5

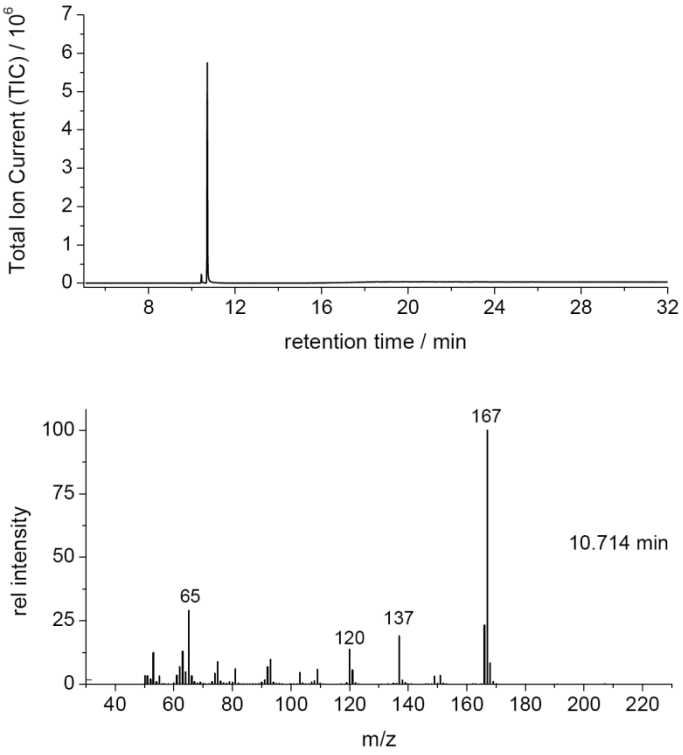


Fig. 1 Plot of the total GC-MS ion current chromatogram and normalized mass profile at the specified peak elution time for aldehyde **a**. Aldehyde **a** was 97% pure by GC-MS analysis and no effort was made to remove *ca*. 3% of 3-nitrosalicylaldehyde side-product.

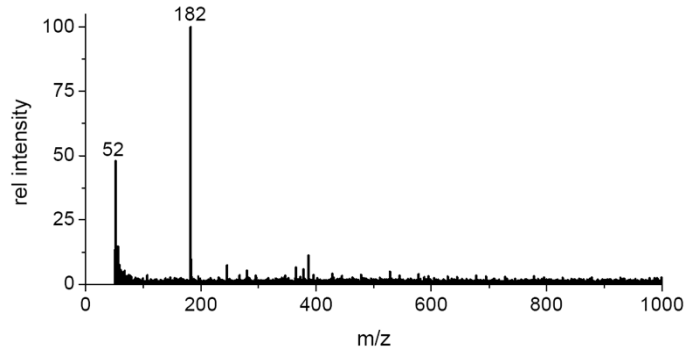


Fig. 2a Plot of the normalized mass profile (ESI, negative-ion mode) for aldehyde **b**.

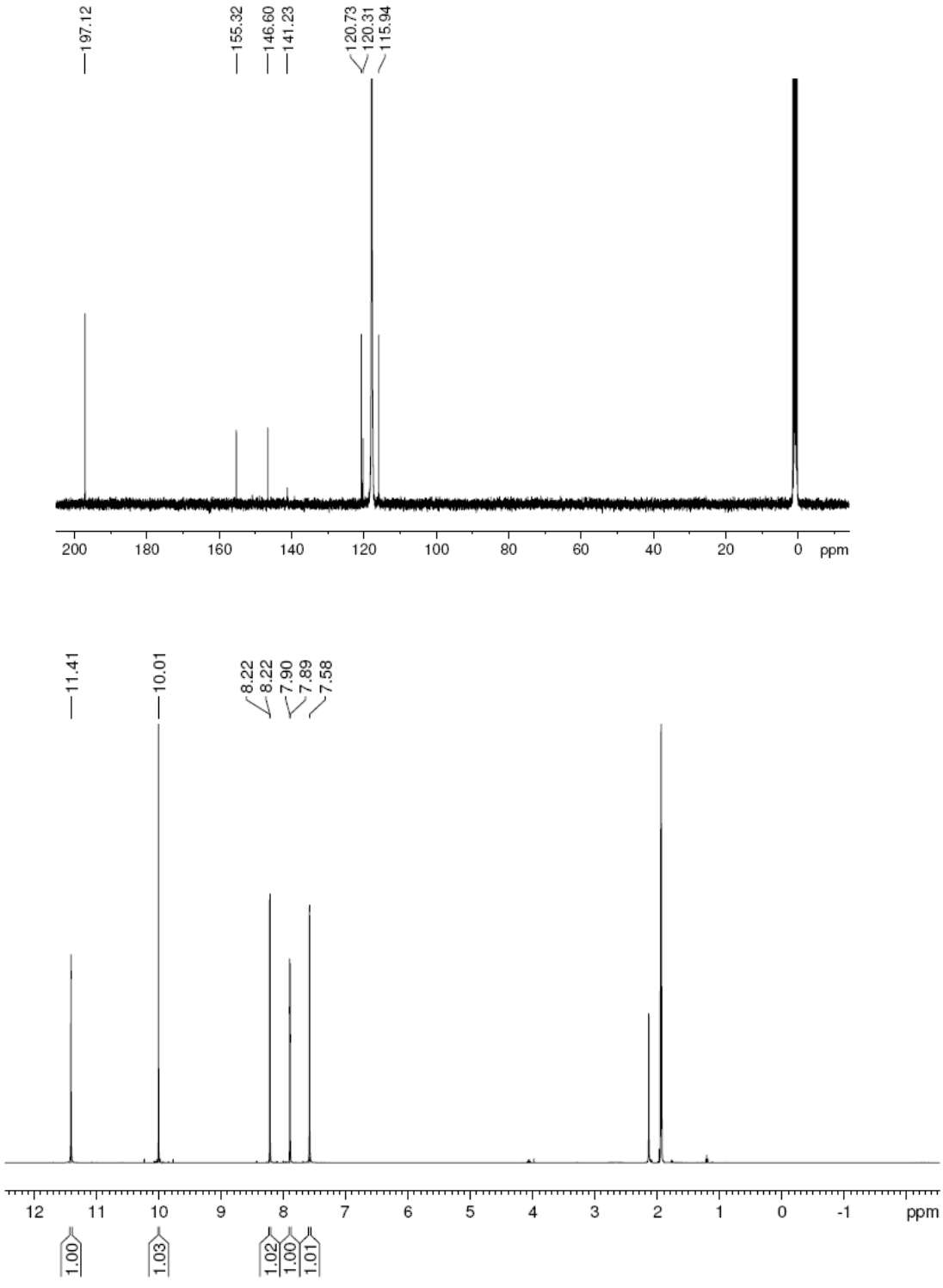


Fig. 2b ^{1}H NMR spectrum (400 MHz, CD_3CN) of compound **b**.

Fig. 2c ^{13}C NMR spectrum (100 MHz, CD_3CN) of compound **b**.

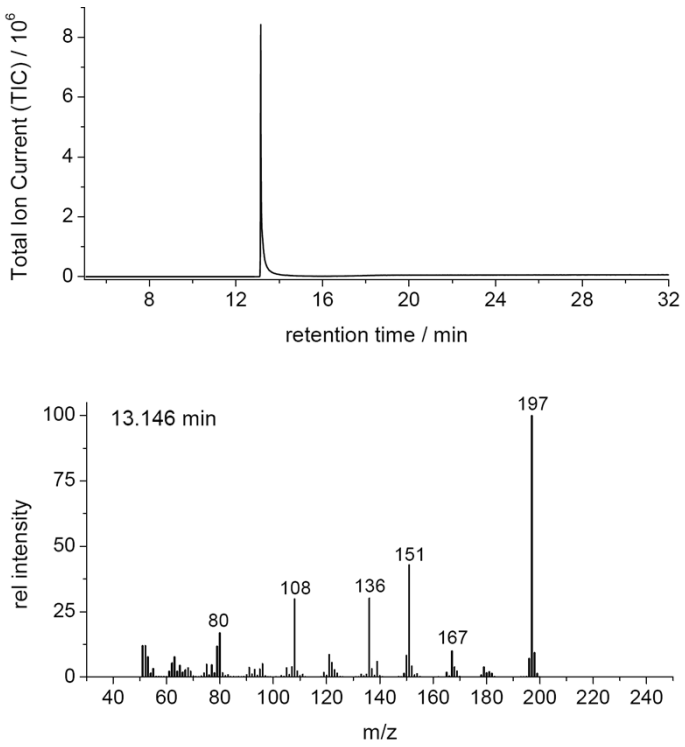


Fig. 3a Plot of the total GC-MS ion current chromatogram and normalized mass profile at the specified peak elution time for aldehyde **c**.

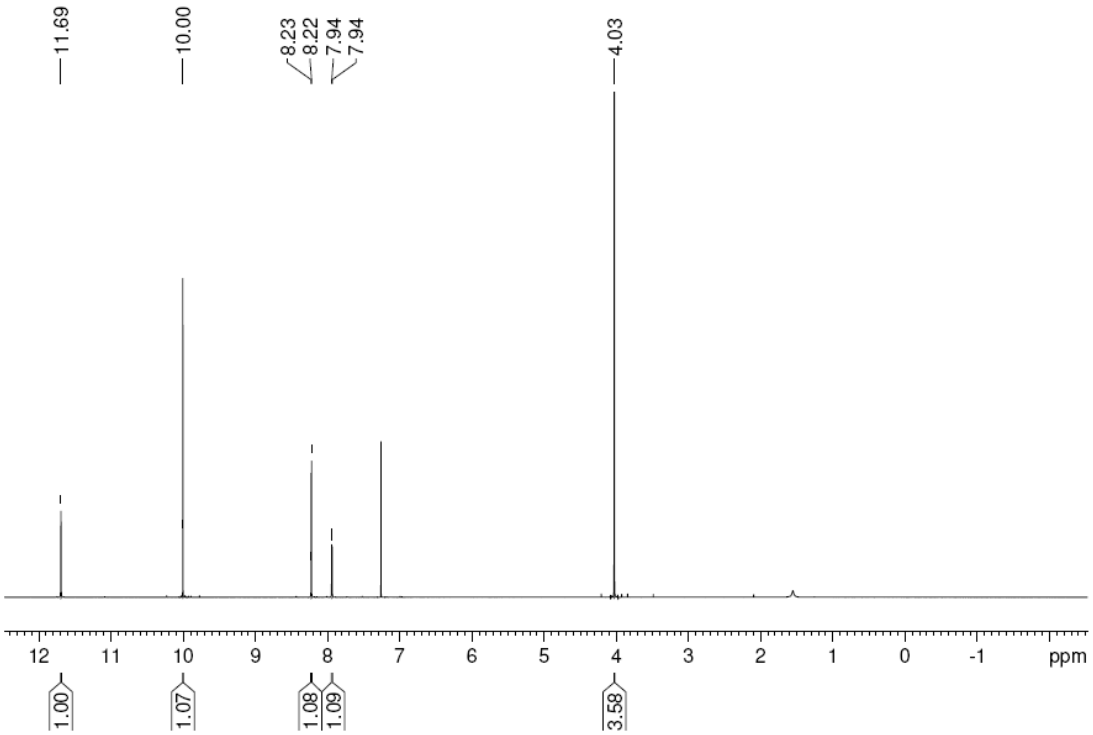


Fig. 3b ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **c**.

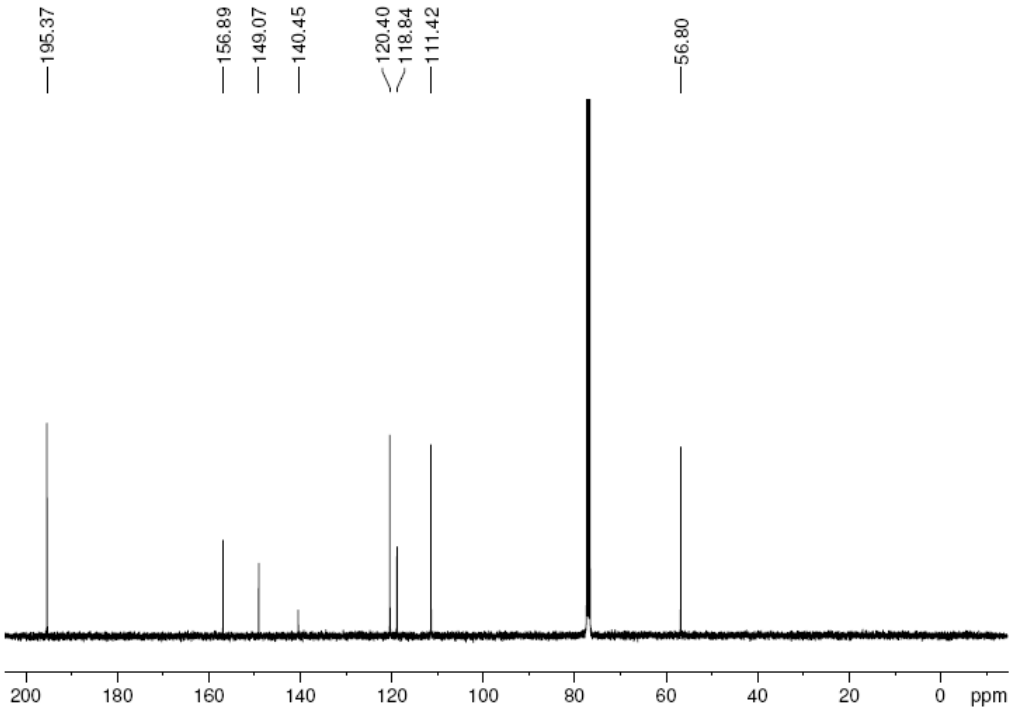


Fig. 3c ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of compound **c**.

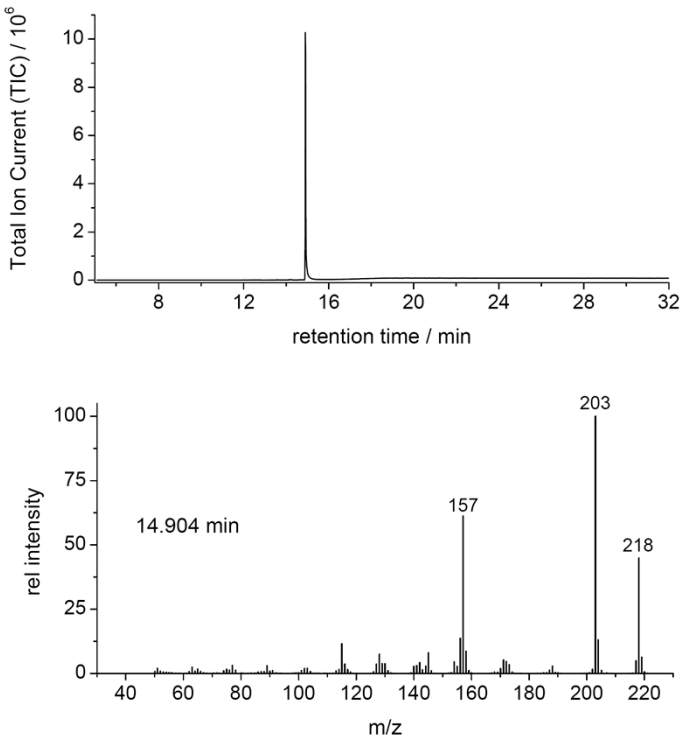


Fig. 4a Plot of the total GC-MS ion current chromatogram and normalized mass profile at the specified peak elution time for the methylene base **d** (Fischer base).

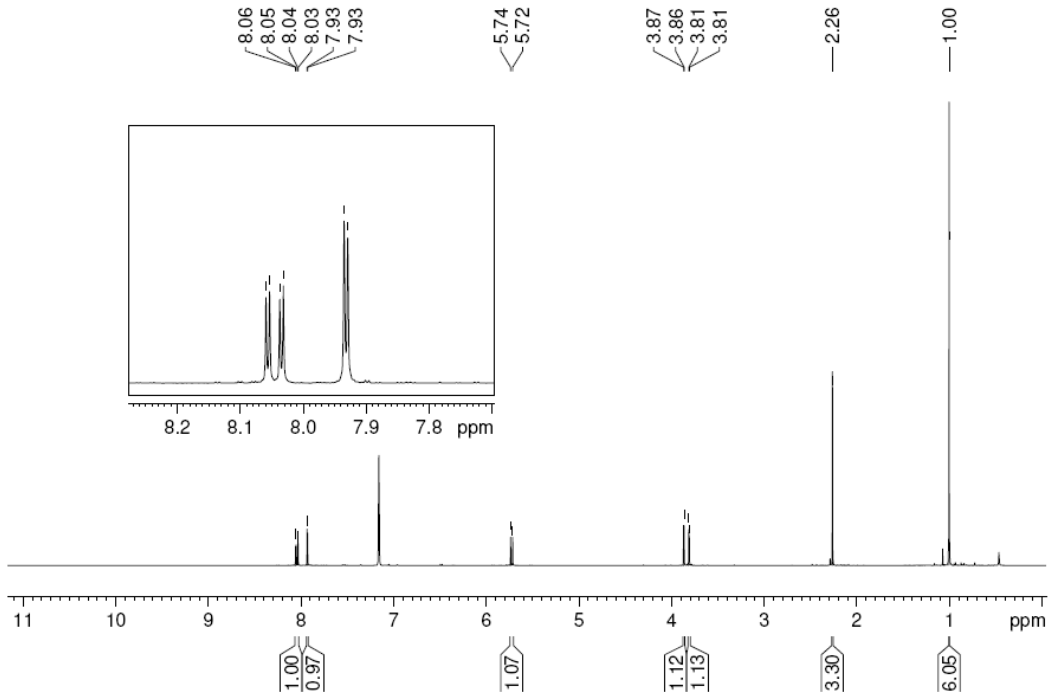


Fig. 4b ^{1}H NMR spectrum (400 MHz, C_6D_6) of compound **d**.

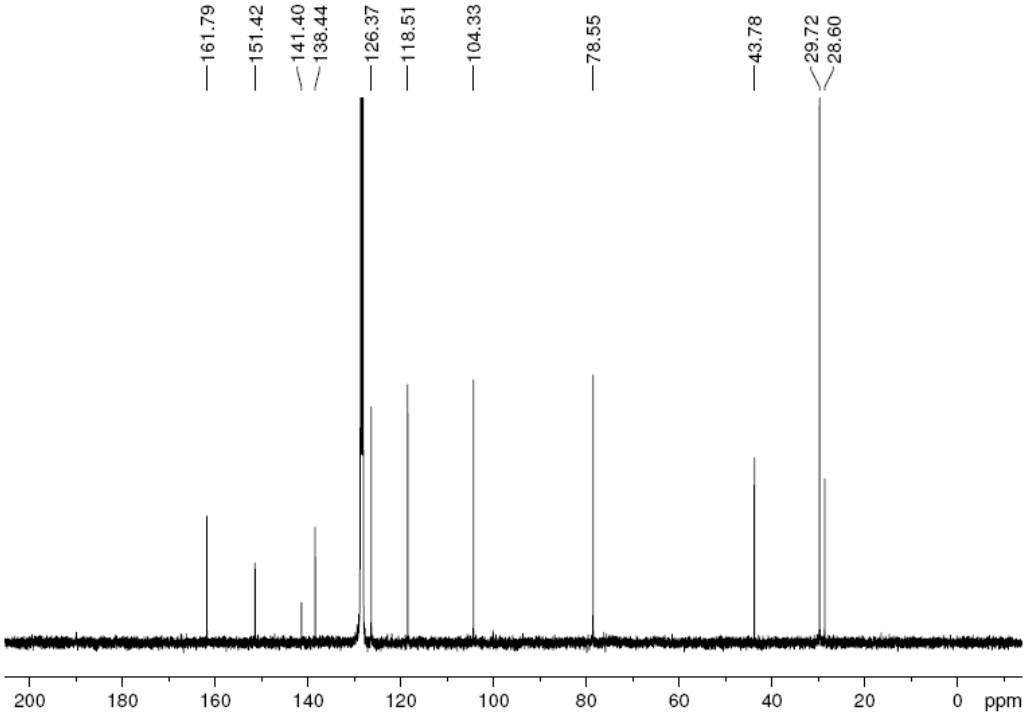


Fig. 4c ^{1}H NMR spectrum (400 MHz, C_6D_6) of compound **d**.

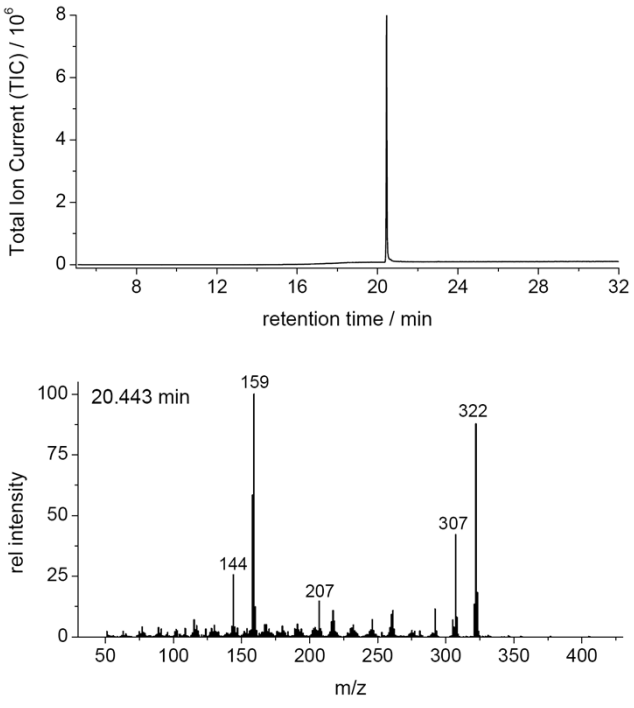


Fig. 5a Plot of the total GC-MS ion current chromatogram and normalized mass profile at the specified peak elution time for the indoline spiropyran **SP-1** (6-NO_2 BIPS).

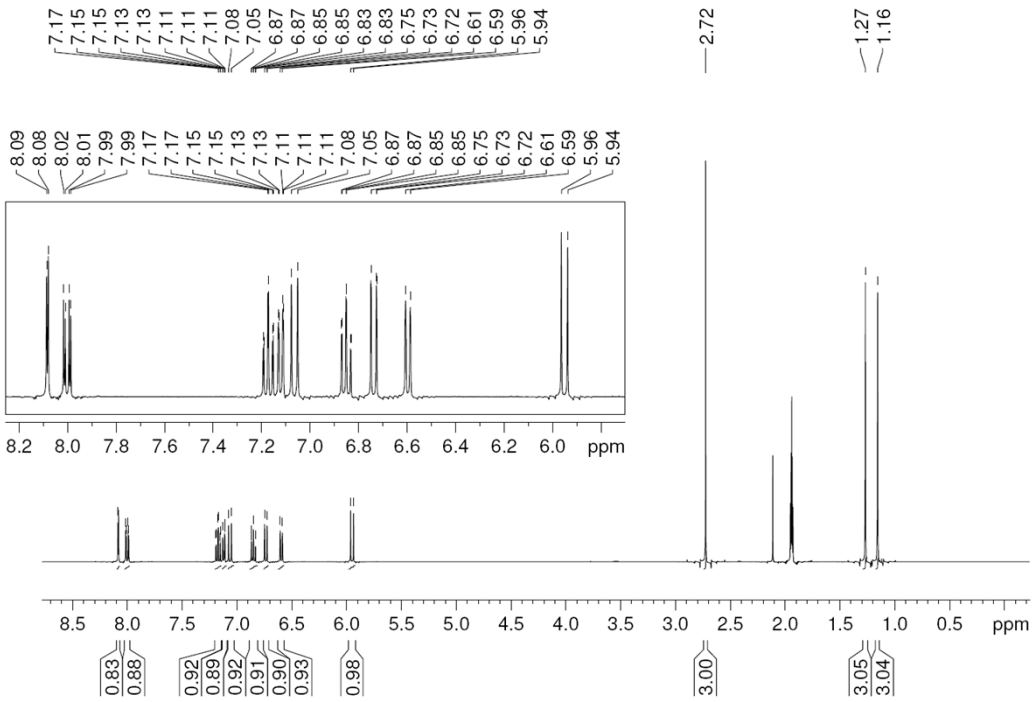


Fig. 5b ^{1}H NMR spectrum (400 MHz, CD_3CN) of compound **SP-1**.

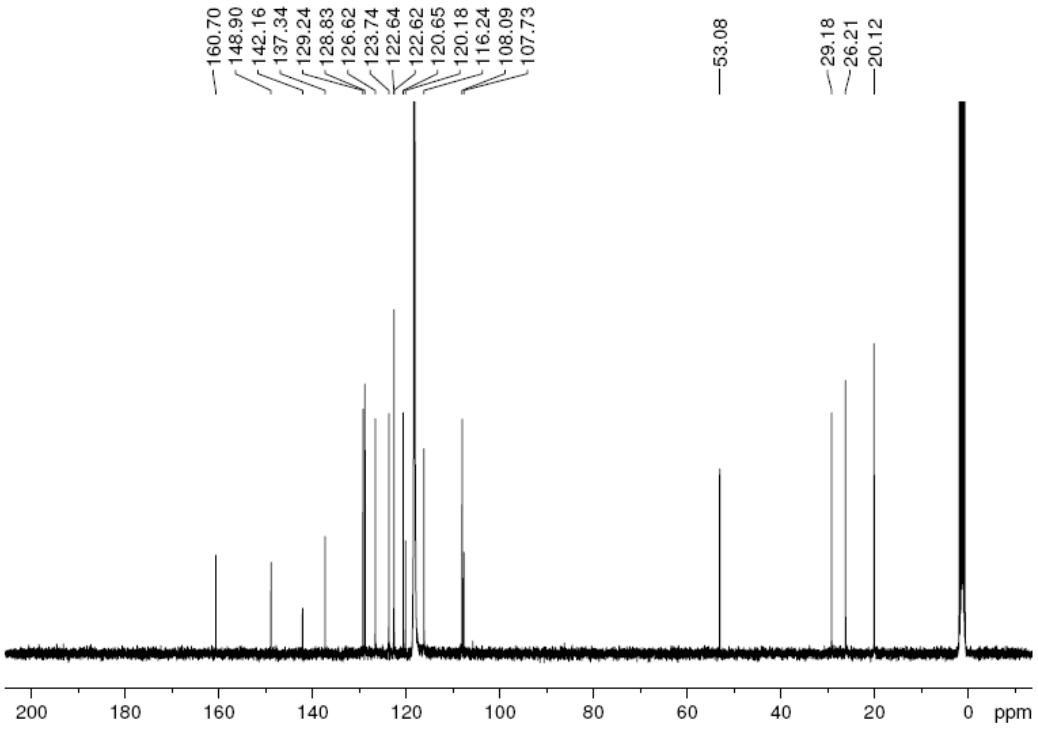


Fig. 5c ^{13}C NMR spectrum (100 MHz, CD_3CN) of compound **SP-1**.

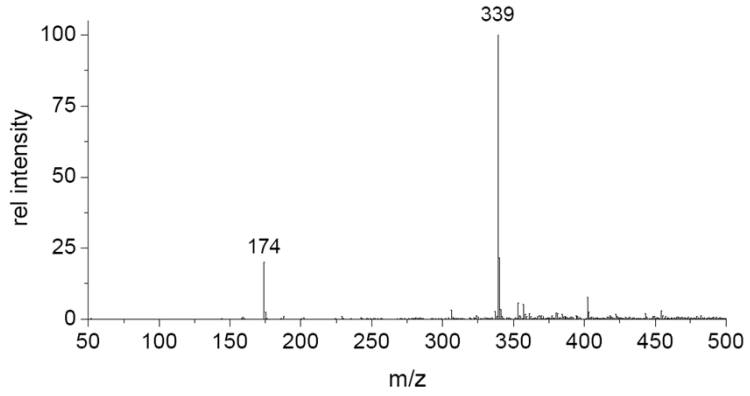


Fig. 6a Plot of the normalized mass profile (ESI, positive-ion mode) for 6-NO_2-8-OH BIPS **SP-2**.

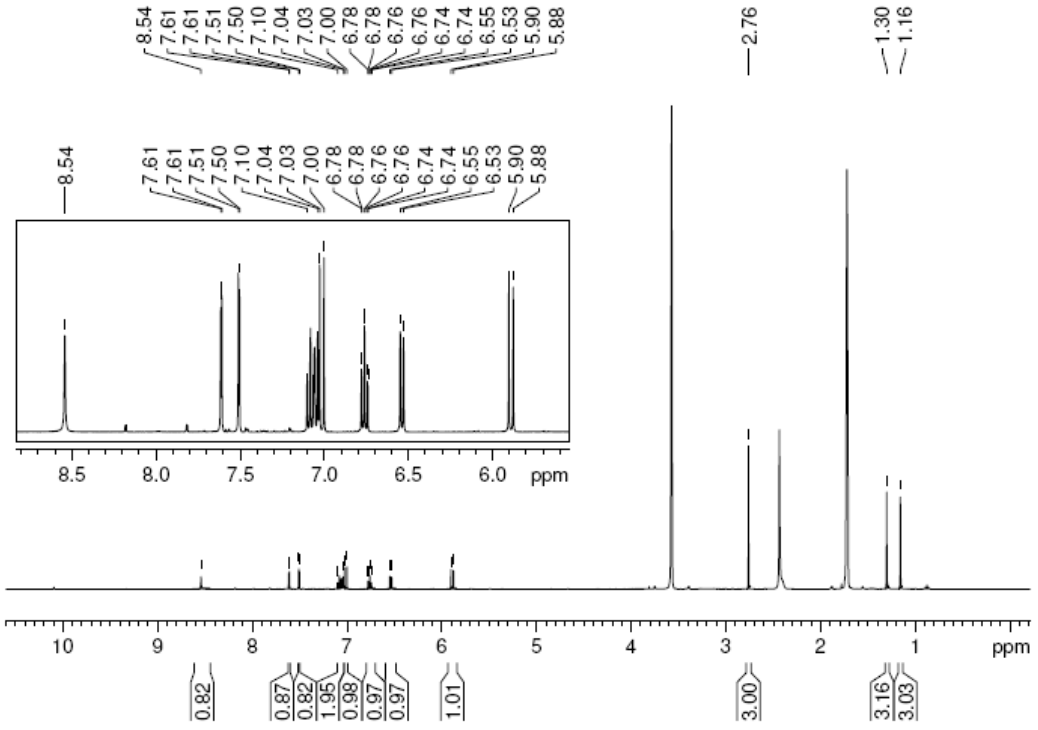


Fig. 6b ^{1}H NMR spectrum (400 MHz, THF-d_8) of compound **SP-2**.

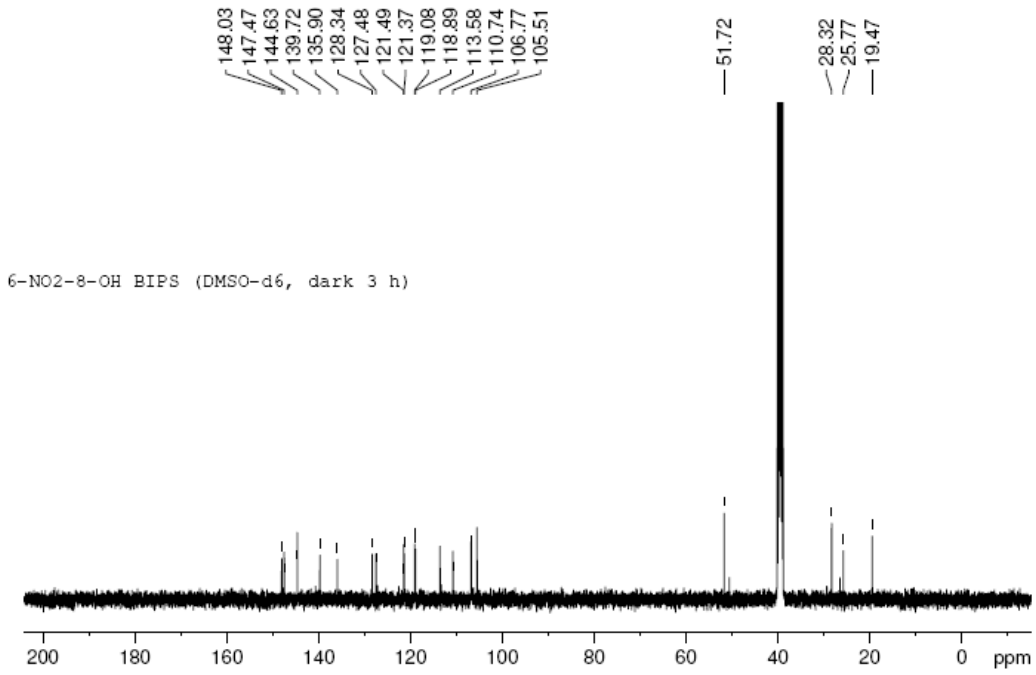


Fig. 6c ^{13}C NMR spectrum (100 MHz, DMSO-d_6) of compound **SP-2**.

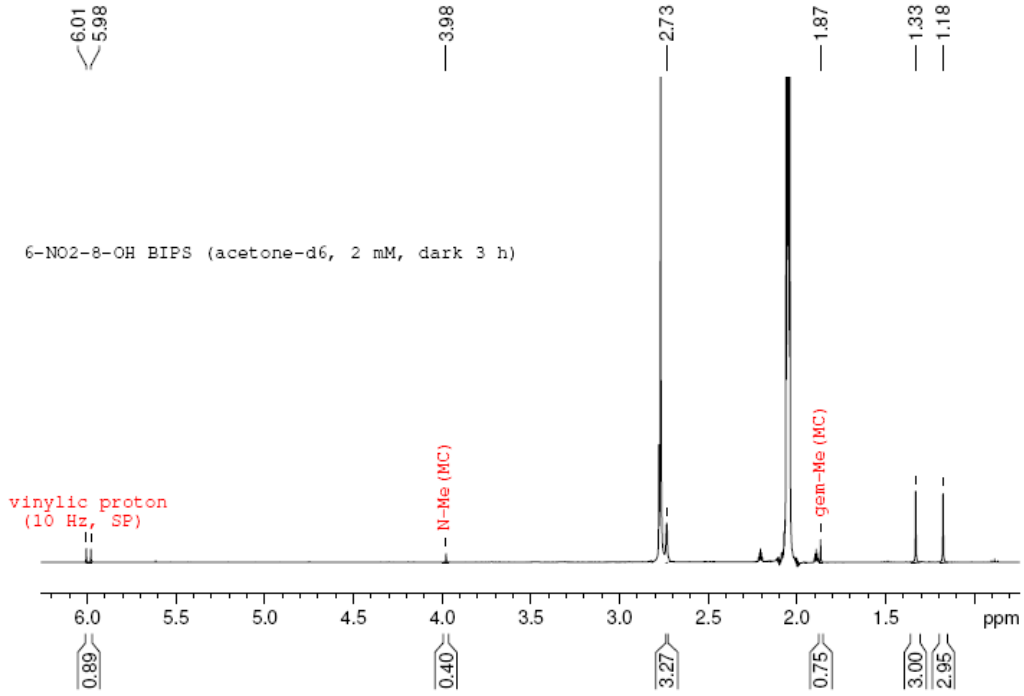


Fig. 6d ^{1}H NMR spectra (400 MHz, acetone-d_6) of compound **SP-2**. NMR absorptions peaks associated with an equilibrium amount of open-ring merocyanine form (MC) of **SP-2** are indicated with text labels in the low ppm region (dark equilibrium constant, $K_{eq} = [MC]_{eq}/[SP]_{eq}$, was *ca*. 0.13).

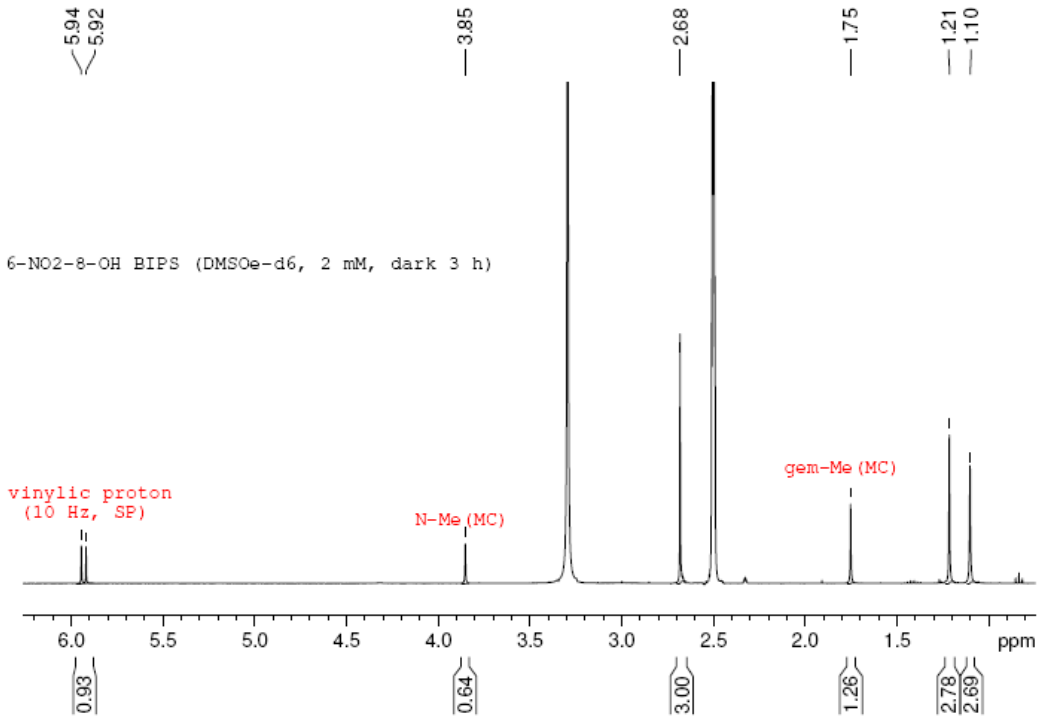


Fig. 6e ^{1}H NMR spectra (400 MHz, DMSO-d_6) of compound **SP-2**. NMR absorptions peaks associated with an equilibrium amount of merocyanine form (MC) of **SP-2** are indicated with text labels in the low ppm region (dark equilibrium constant, $K_{eq} = [MC]_{eq}/[SP]_{eq}$, was *ca*. 0.21).

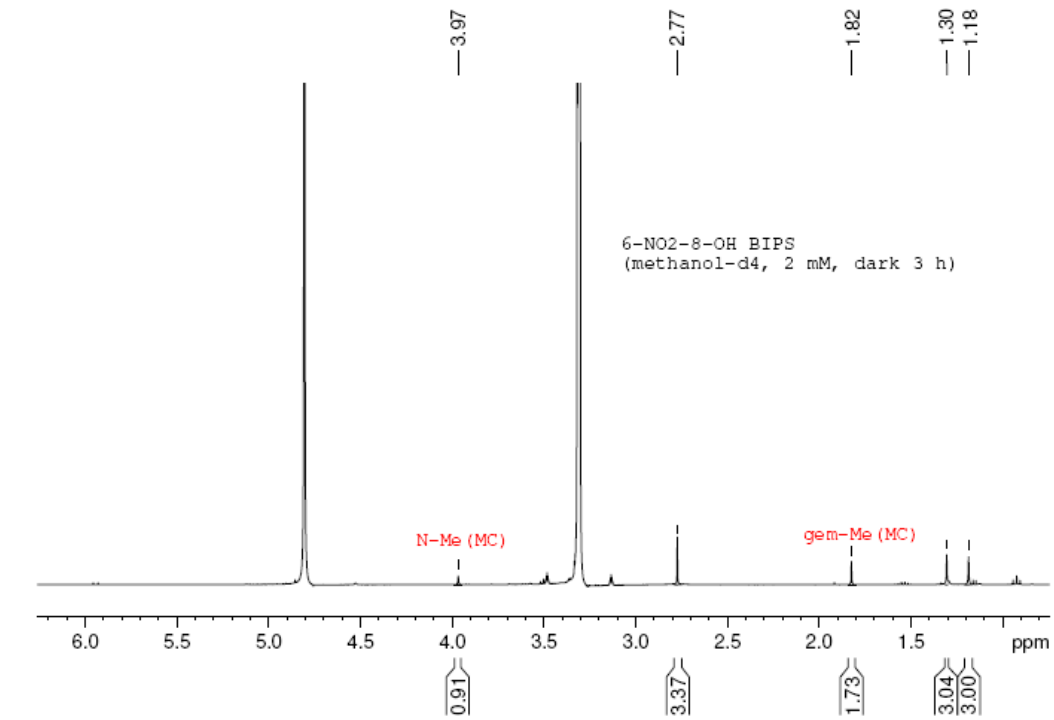


Fig. 6f ^{1}H NMR spectra (400 MHz, methanol-d_4) of compound **SP-2**. NMR absorptions peaks associated with an equilibrium amount of merocyanine form (MC) of **SP-2** are indicated with text labels in the low ppm region (dark equilibrium constant, $K_{eq} = [MC]_{eq}/[SP]_{eq}$, was *ca*. 0.28).

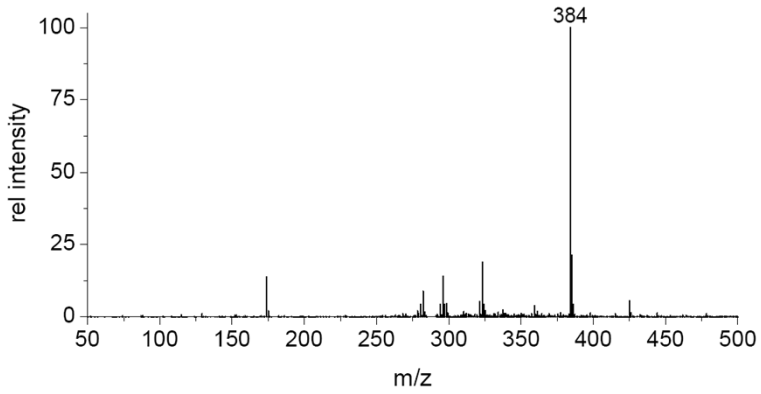


Fig. 7a Plot of the normalized mass profile (ESI, positive-ion mode) for 5`-NO_2-6-NO_2-8-OH BIPS **SP-3**.

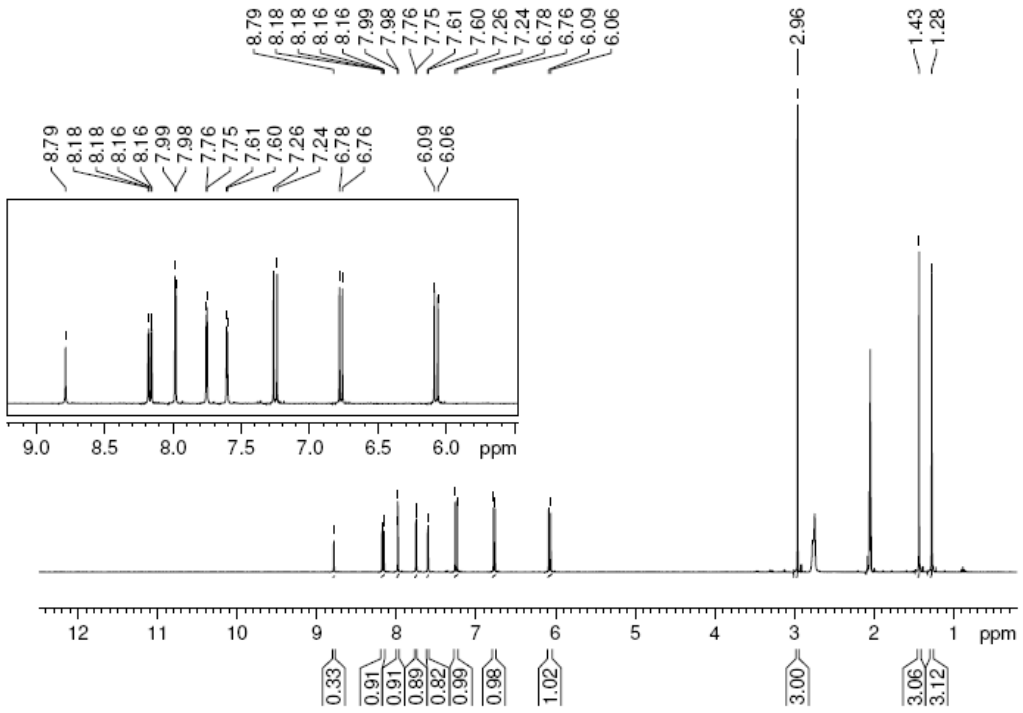


Fig. 7b ^{1}H NMR spectrum (400 MHz, acetone-d_6) of compound **SP-3**.

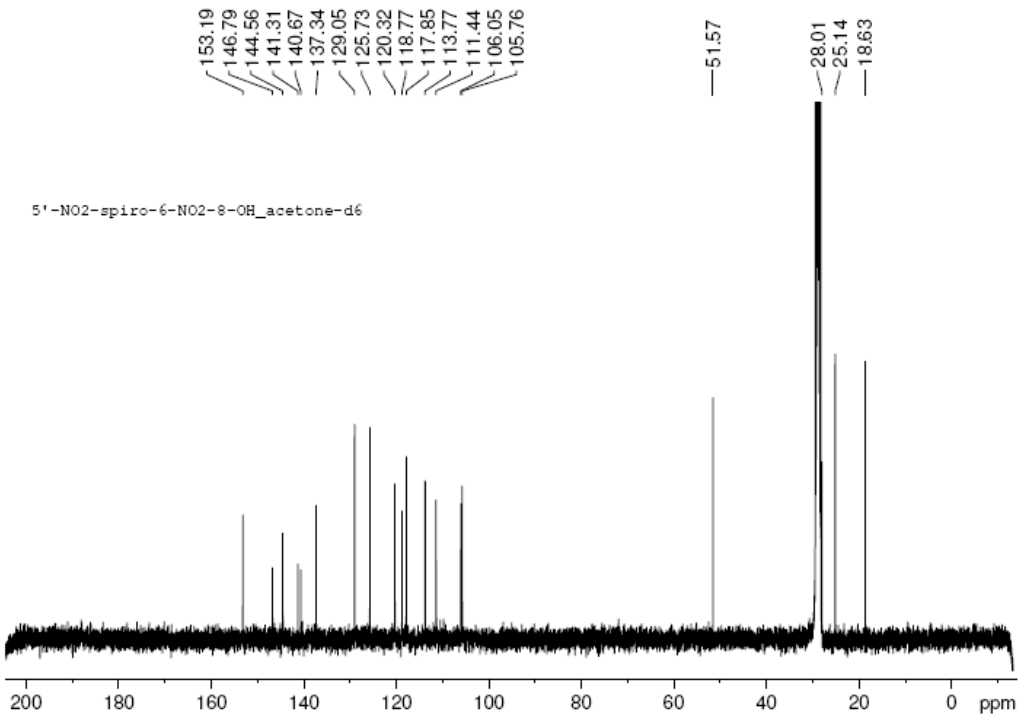


Fig. 7c ^{13}C NMR spectrum (100 MHz, acetone-d_6) of compound **SP-3**.

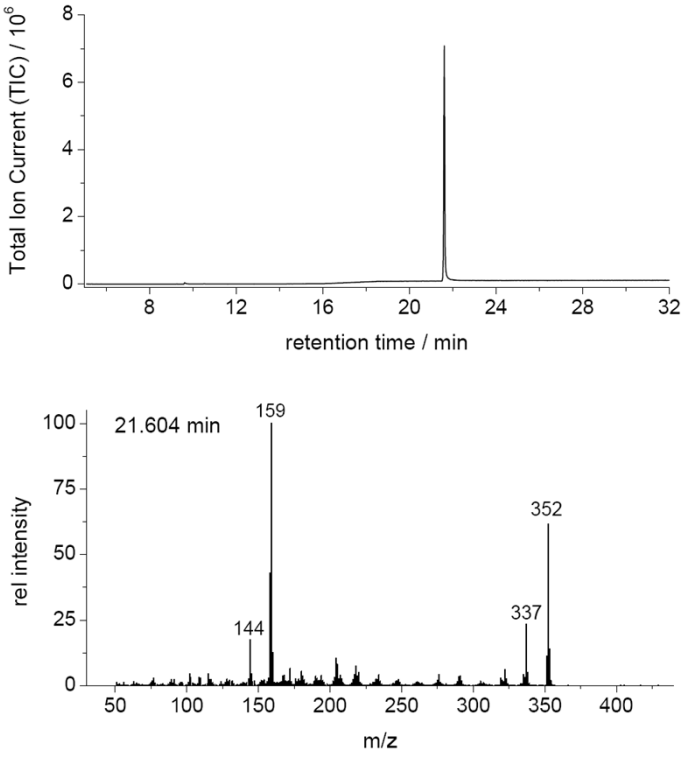


Fig. 8a Plot of the total GC-MS ion current chromatogram and normalized mass profile averaged around the specified peak elution time for the 6-NO_2-8-OMe BIPS **SP-4**.

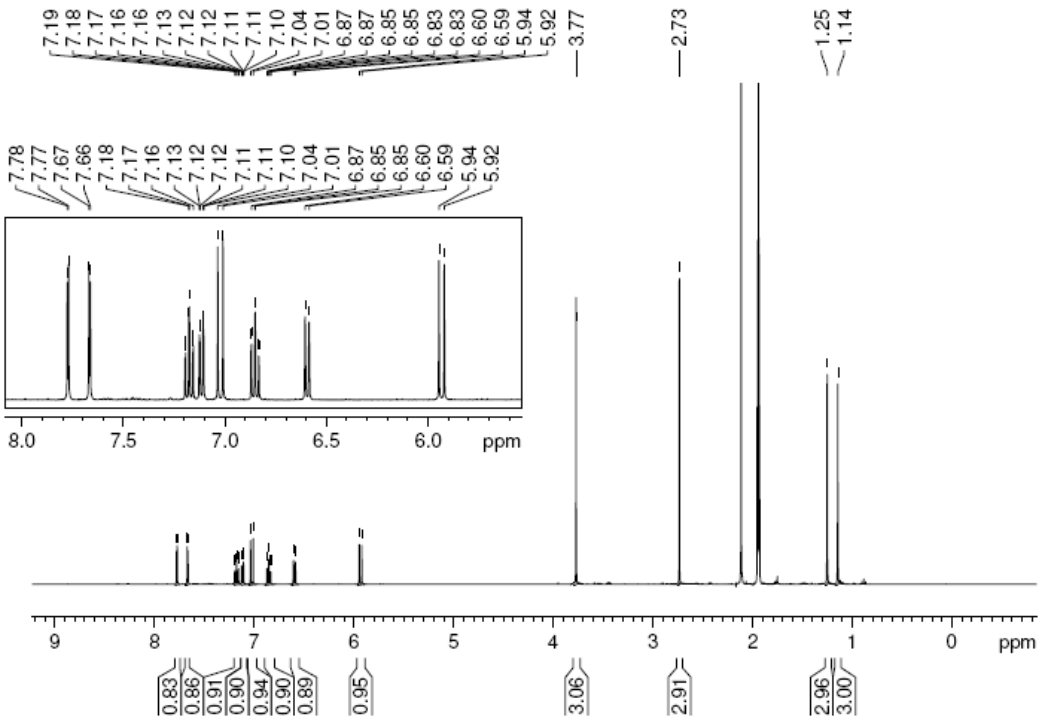


Fig. 8b ^{1}H NMR spectra (400 MHz, CD_3CN) of compound **SP-4**.

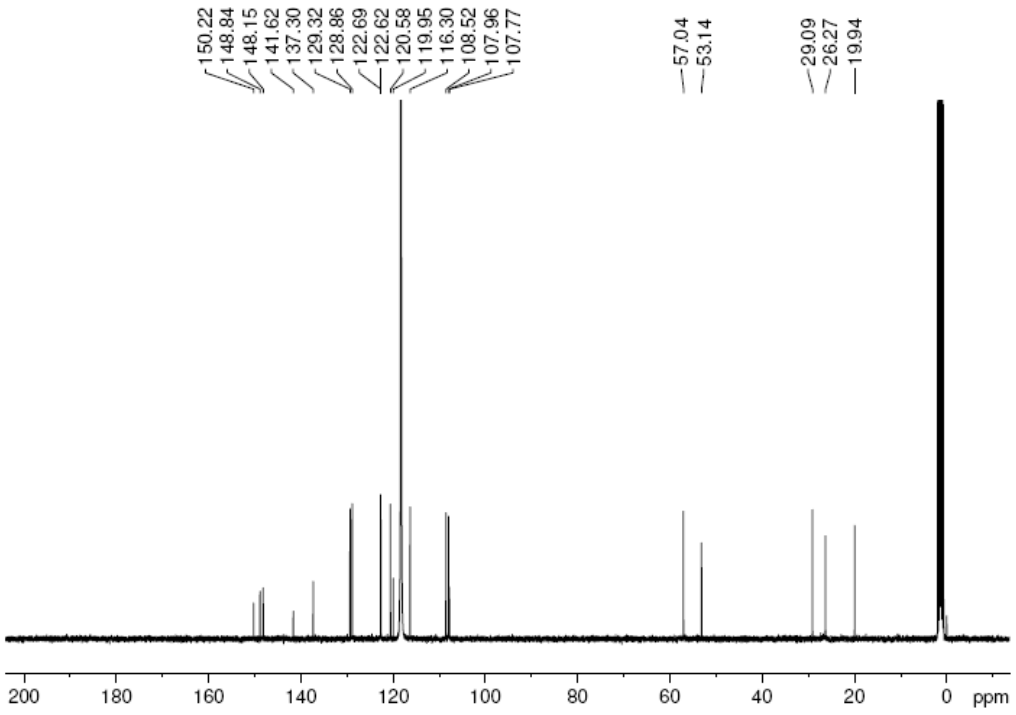


Fig. 8c ^{13}C NMR spectrum (400 MHz, CD_3CN) of compound **SP-4**.

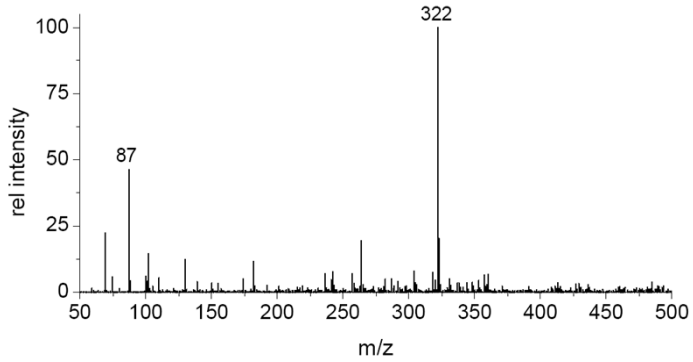


Fig. 9a Plot of the normalized mass profile (ESI,positive-ion mode) for 8-COOH BIPS **SP-5**.

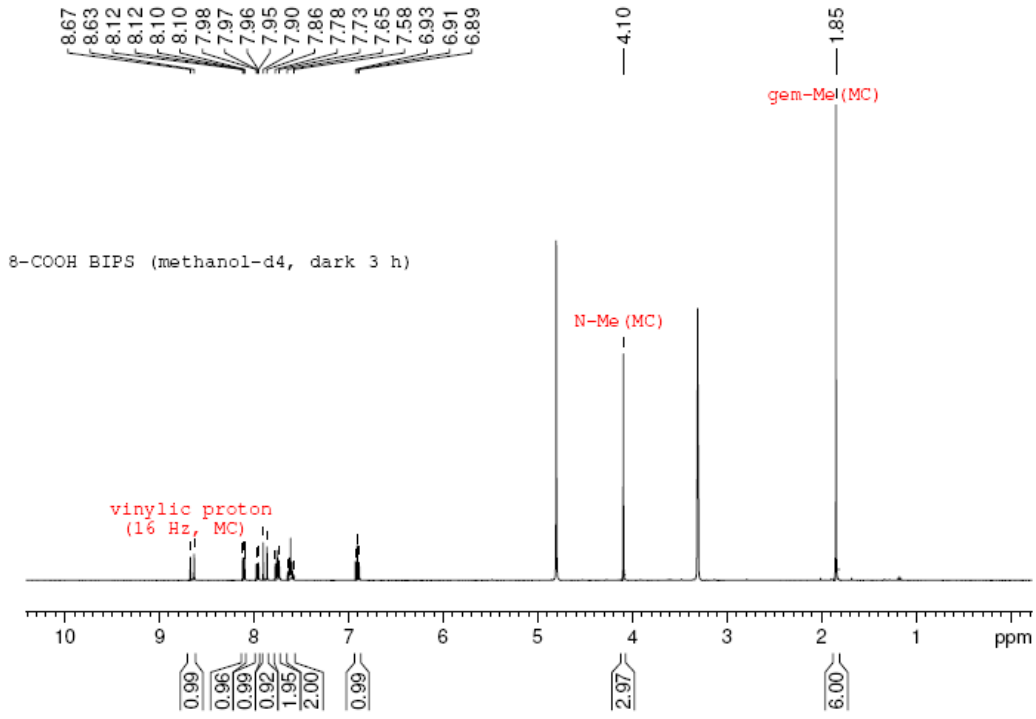


Fig. 9b ^{1}H NMR spectrum (400 MHz, methanol-d_4) of compound **SP-5**. NMR absorptions peaks associated with characteristic signals from the open-ring merocyanine form (MC) of **SP-5** are indicated with labels.

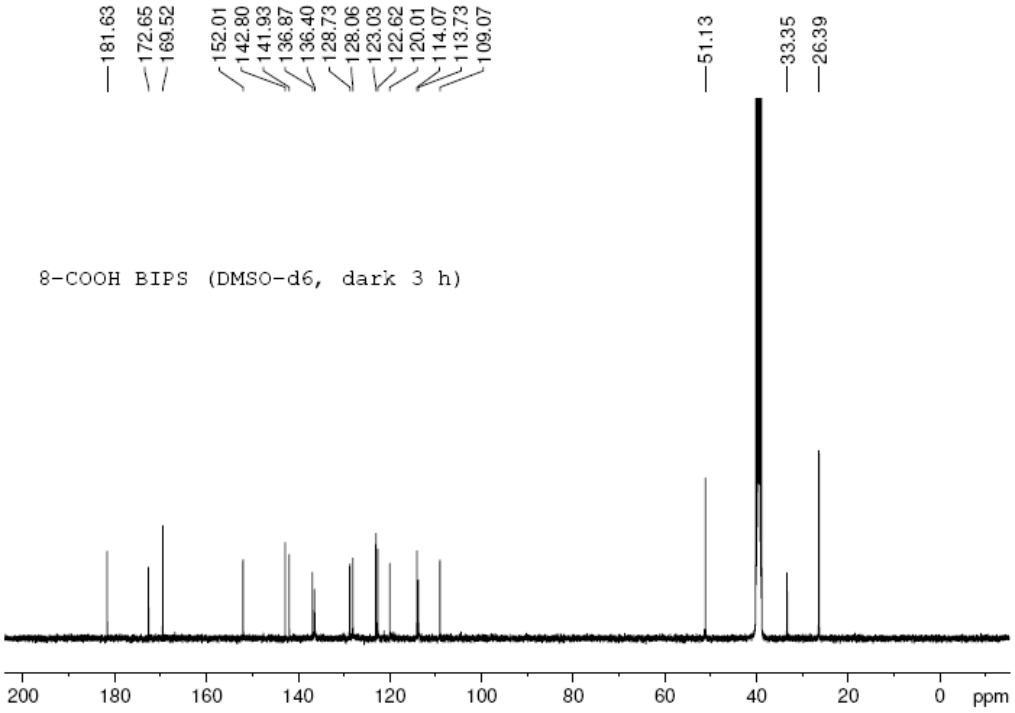


Fig. 9c ^{13}C NMR spectrum (100 MHz, DMSO-d_6) of compound **SP-5**.

S3. Additional Experimental and Computational results

S3.1 Theoretical hydrogen bond strengths

Table S1. Theoretical hydrogen bond strengths (kJ mol^{-1}) of closed- ring (SP) and open-ring (MC-TTC) isomers of **SP-2**, **SP-3** and **SP-5** and putative transition states (pathway 1 and pathway 2) of **SP-2**. HB strengths calculated as the difference in Gibbs free energy between hydrogen bonded and non-hydrogen bonded conformations, as shown for **SP-2** and **SP-3** in Fig. S3.

SP / isomer / *pathway*	Gas phase	diethyl ether	chloroform	THF	DCM	1,2-DCE	ethanol	methanol	water
SP-2 / SP / –	16	11	9	10	8	7	2	1	1
SP-2 / CCC / *2*	33	29	25	27	24	24	15	13	13
SP-2 / CTC / *2*	32	27	24	26	23	23	14	13	13
SP-2 / MC / –	32	28	24	26	23	23	15	13	13
SP-2 / TS2 / *1*	27	21	17	19	16	16	8	7	7
SP-2 / TS3 / *2*	29	26	22	24	21	21	12	11	10
SP-2 / TS4 / *2*	28	21	18	20	17	16	9	8	8
SP-2 / TS5 / *2*	37	32	27	30	27	27	17	15	15
SP-3 / SP / –	14	10	8	9	7	7	2	2	2
SP-3 / MC / –	31	26	22	25	22	22	13	12	12
SP-5 / SP / –	8	13	9	13	10	11	7	6	9
SP-5 / MC / –	33	41	37	42	39	39	31	29	30

S3.2 Experimental and theoretical hydroxyl (8-OH) infrared (IR) stretching frequencies and scaling factors

Table S2. Experimental and theoretical hydroxyl (8-OH) infrared (IR) stretching frequencies and calculated hydrogen bond strengths for closed-ring (SP) and open-ring (MC *trans*-isomer, MC-TTC) isomers of **SP-2** and **SP-3**.

SP / isomer / solvent	Experimental OH stretching frequencies[a] / cm^{-1}		Computed OH stretching frequencies[b] / cm^{-1}		Hydrogen bond strength[c] / kJ mol^{-1}
	red-shifted band	blue-shifted band	with HB	without HB	
SP-2 / MC / gas phase			3467	3638	32
SP-2 / SP / gas phase			3585	3646	16
SP-2 / MC / chloroform		3608	3432	3604	24
SP-2 / SP / chloroform	3541		3559	3605	9
SP-3 / MC / gas phase			3477	3637	31
SP-3 / SP / gas phase			3595	3646	14
SP-3 / MC / chloroform	–		3444	3601	22
SP-3 / SP / chloroform		3548	3564	3601	8

[a]The experimental absorption band centered at *ca*. 3600 cm^{-1} was assigned to free hydroxyls groups while the red-shifted band at *ca*. 3500 cm^{-1} was ascribed to hydroxyls groups involved in intramolecular hydrogen bonding. [b]Harmonic vibrational frequencies calculated at the M06-2X/6-31G(2*df*,*p*) level of theory scaled by 0.9374. Scaling factor determined by comparison of OH stretching frequencies of selected phenols with experimental values from the NIST webbook (see §S1.2 and Table S3). See Fig. S3 for "with HB" and "without HB" structures. [c]Calculated at the M06-2X/6-31G(2*df*,*p*) level of theory as the difference in Gibbs free energy between the conformers with and without the intramolecular hydrogen bond (see Fig. S3).

Table S3. Determination of IR scaling factor for OH stretching frequencies by comparison of M06-2X/6-31G(2*df*,*p*) theoretical values with experimental results[a]

	Experimental OH stretching frequencies[a] / cm^{-1}	Computed OH stretching frequencies / cm^{-1}	Scaling factor
phenol	3650	3891	0.9381
catechol (1)	3658	3909	0.9358
catechol (2)	3602	3856	0.9341
resorcinol (1)	3658	3894	0.9394
resorcinol (2)	3650	3893	0.9376
hydroquinone (1)	3654	3901	0.9367
hydroquinone (2)	3654	3890	0.9393
3-nitrophenol	3650	3890	0.9383
			0.9374 (average)

[a]Experimental values from the NIST webbook (see §1.2).

S3.3 Computed energies (SP-1 to SP-5)

Table S4. Total electronic energies (E) at G3(MP2,CC) and component levels of theory and corresponding zero-point vibrational energies (ZPVE), thermal corrections (T
entropies (S), gas-phase enthalpies (H_{gas}) and gas-phase Gibbs free energies (G_{gas}) at 298.15 K (Hartrees or Hartrees / K)[a].

SP	Isomer	E(MP2/ 6-31G*)	E(MP2/ GTMP2Large)	E(CCSD(T)/ 6-31G*)	HLC	E(G3(MP2, CC))	ZPVE	TC	S x 10^3 [a]	H_{gas}	
SP-1	SP	-1066.64803	-1067.79626	-1066.89083	-0.57419	-1068.03906	0.32756	0.02196	0.23924	-1068.26374	-
	MC	-1066.61565	-1067.76439	-1066.86246	-0.57419	-1068.01121	0.32604	0.02346	0.25626	-1068.23591	-
	CCC	-1066.61454	-1067.76568	-1066.85874	-0.57419	-1068.00987	0.32635	0.02277	0.24616	-1068.23494	-
	CTC	-1066.61203	-1067.76038	-1066.85887	-0.57419	-1068.00722	0.32634	0.02318	0.25392	-1068.23190	-
	TS2	-1066.58307	-1067.73065	-1066.83571	-0.57419	-1067.98329	0.32388	0.02316	0.25481	-1068.21045	-
	TS3	-1066.61432	-1067.76469	-1066.85907	-0.57419	-1068.00945	0.32593	0.02204	0.23952	-1068.23566	-
	TS4	-1066.58076	-1067.72808	-1066.83375	-0.57419	-1067.98108	0.32360	0.02331	0.25770	-1068.20836	-
	TS5	-1066.58329	-1067.73306	-1066.82920	-0.57419	-1067.97897	0.32445	0.02277	0.24996	-1068.20595	-
SP-2	SP	-1141.68516	-1142.92247	-1141.93041	-0.60243	-1143.16773	0.33236	0.02308	0.24630	-1143.41472	-
with HB	MC	-1141.65977	-1142.89763	-1141.90888	-0.60243	-1143.14673	0.33106	0.02445	0.26310	-1143.39366	-
	CCC	-1141.65982	-1142.89979	-1141.90591	-0.60243	-1143.14588	0.33130	0.02378	0.25352	-1143.39323	-
	CTC	-1141.65630	-1142.89373	-1141.90540	-0.60243	-1143.14283	0.33134	0.02416	0.26094	-1143.38975	-
	TS2	-1141.62653	-1142.86319	-1141.88142	-0.60243	-1143.11808	0.32885	0.02416	0.26164	-1143.36750	-
	TS3	-1141.65792	-1142.89716	-1141.90430	-0.60243	-1143.14354	0.33059	0.02319	0.24792	-1143.39219	-
	TS4	-1141.62434	-1142.86059	-1141.87957	-0.60243	-1143.11581	0.32861	0.02430	0.26497	-1143.36532	-
	TS5	-1141.62860	-1142.86718	-1141.87672	-0.60243	-1143.11529	0.32951	0.02381	0.25743	-1143.36440	-
SP-2	SP	-1141.67744	-1142.91551	-1141.92271	-0.60243	-1143.16078	0.33191	0.02325	0.24777	-1143.40806	-
no HB	MC	-1141.64636	-1142.88424	-1141.89592	-0.60243	-1143.13380	0.33063	0.02465	0.26439	-1143.38095	-
	CCC	-1141.64563	-1142.88602	-1141.89216	-0.60243	-1143.13255	0.33070	0.02405	0.25557	-1143.38023	-
	CTC	-1141.64271	-1142.88020	-1141.89230	-0.60243	-1143.12979	0.33082	0.02440	0.26257	-1143.37700	-
	TS2	-1141.61479	-1142.85150	-1141.86992	-0.60243	-1143.10664	0.32832	0.02439	0.26410	-1143.35635	-
	TS3	-1141.64497	-1142.88483	-1141.89183	-0.60243	-1143.13168	0.33010	0.02338	0.24912	-1143.38064	-
	TS4	-1141.61251	-1142.84894	-1141.86799	-0.60243	-1143.10442	0.32817	0.02449	0.26639	-1143.35420	-
	TS5	-1141.61286	-1142.85206	-1141.86131	-0.60243	-1143.10051	0.32887	0.02406	0.25904	-1143.35001	-
SP-3	SP	-1345.69460	-1347.13654	-1345.94950	-0.67774	-1347.39145	0.33550	0.02575	0.26956	-1347.70793	-
with HB	MC	-1345.66558	-1347.10788	-1345.92496	-0.67774	-1347.36726	0.33415	0.02709	0.28589	-1347.68375	-
SP-3	SP	-1345.68837	-1347.13092	-1345.94327	-0.67774	-1347.38582	0.33521	0.02586	0.27051	-1347.70249	-
no HB	MC	-1345.65298	-1347.09518	-1345.91281	-0.67774	-1347.35502	0.33371	0.02729	0.28718	-1347.67174	-
SP-4	SP	-1180.83351	-1182.11784	-1181.09547	-0.63067	-1182.37980	0.35961	0.02465	0.25895	-1182.62621	-
	MC	-1180.80271	-1182.08711	-1181.06899	-0.63067	-1182.35339	0.35820	0.02608	0.27584	-1182.59978	-
	CCC	-1180.80168	-1182.08845	-1181.06494	-0.63067	-1182.35171	0.35836	0.02544	0.26657	-1182.59858	-
	CTC	-1180.79910	-1182.08318	-1181.06543	-0.63067	-1182.34950	0.35854	0.02579	0.27341	-1182.59585	-
	TS2	-1180.77191	-1182.05534	-1181.04358	-0.63067	-1182.32702	0.35594	0.02582	0.27557	-1182.57593	-
	TS3	-1180.80074	-1182.08700	-1181.06435	-0.63067	-1182.35060	0.35767	0.02479	0.26034	-1182.59881	-
	TS4	-1180.76965	-1182.05271	-1181.04168	-0.63067	-1182.32474	0.35587	0.02589	0.27690	-1182.57366	-
	TS5	-1180.76835	-1182.05388	-1181.03355	-0.63067	-1182.31908	0.35644	0.02546	0.27011	-1182.56785	-
SP-5	SP	-1050.73429	-1051.87762	-1050.98355	-0.57419	-1052.12687	0.33979	0.02212	0.23766	-1052.33916	-
with HB	MC	-1050.70687	-1051.85125	-1050.95969	-0.57419	-1052.10407	0.33818	0.02347	0.25536	-1052.31661	-
SP-5	SP	-1050.73060	-1051.87363	-1050.98011	-0.57419	-1052.12315	0.33955	0.02228	0.24019	-1052.33551	-
no HB	MC	-1050.69311	-1051.83556	-1050.94723	-0.57419	-1052.08968	0.33796	0.02388	0.26232	-1052.30204	-

Table S5. Gibbs free energies of solvation (ΔG_{solv}, kJ mol^{-1}) in various solvents calculated using the SMD implicit solvent model. Gibbs free energies in solution should be calculated as: $G_{soln} = G_{gas} + \Delta G_{solv} + RTln(R'T)$ where R and R' are the gas constant in units of J mol^{-1} K^{-1} and L atm mol^{-1} K^{-1}, respectively (R = 8.31446 J mol^{-1} K^{-1}, R' = 0.0820575 L atm mol^{-1} K^{-1}) and T is the temperature.

SP	Isomer	Solvent and its Dielectric Constant						
		Diethylether	$CHCl_3$	DCM	DCE	Ethanol	Methanol	Water
		4.2	4.7	8.9	10.1	24.9	32.6	78.3
SP-1	SP	-60.2	-62.3	-68.9	-63.9	-54.9	-52.3	-26.0
	MC	-81.0	-82.9	-93.4	-88.8	-85.5	-84.5	-59.5
	CCC	-74.9	-77.8	-87.4	-82.9	-82.3	-82.4	-55.5
	CTC	-82.6	-84.6	-95.3	-90.6	-87.9	-86.9	-61.6
	TS2	-67.1	-67.9	-76.4	-71.5	-66.4	-64.9	-39.0
	TS3	-74.4	-77.7	-87.2	-82.6	-81.4	-81.1	-54.6
	TS4	-67.5	-68.6	-77.1	-72.2	-67.9	-66.4	-40.3
	TS5	-115.1	-119.9	-135.1	-131.1	-137.1	-138.2	-113.0
SP-2 with HB	SP	-62.4	-63.5	-70.2	-65.3	-60.2	-57.8	-34.0
	MC	-83.3	-82.7	-93.8	-89.3	-86.7	-85.3	-62.9
	CCC	-77.4	-77.8	-88.1	-83.6	-83.4	-82.9	-58.7
	CTC	-84.4	-84.0	-95.3	-90.8	-88.7	-87.2	-64.4
	TS2	-68.2	-67.1	-75.6	-70.9	-66.9	-64.9	-41.3
	TS3	-77.3	-78.3	-88.2	-83.8	-83.3	-82.6	-58.3
	TS4	-68.2	-67.3	-75.9	-71.1	-68.0	-65.9	-42.1
	TS5	-117.6	-119.6	-135.5	-131.6	-138.0	-138.6	-116.2
SP-2 no HB	SP	-67.2	-70.9	-79.0	-74.4	-74.5	-72.8	-49.0
	MC	-87.9	-91.2	-103.1	-98.8	-104.4	-104.2	-81.8
	CCC	-81.3	-85.6	-96.5	-92.3	-101.1	-102.3	-78.1
	CTC	-89.2	-92.6	-104.7	-100.4	-106.5	-106.4	-83.7
	TS2	-74.9	-77.3	-87.1	-82.6	-85.8	-84.9	-61.5
	TS3	-81.1	-85.8	-96.4	-92.3	-100.6	-101.3	-77.5
	TS4	-75.0	-77.6	-87.5	-83.0	-87.1	-86.1	-62.3
	TS5	-122.4	-128.7	-145.2	-141.6	-157.9	-160.0	-137.8
SP-3 with HB	SP	-72.1	-70.2	-79.6	-74.5	-67.4	-64.2	-43.9
	MC	-90.5	-86.4	-100.0	-95.2	-88.8	-86.1	-67.3
SP-3 no HB	SP	-75.6	-76.1	-86.1	-81.3	-78.8	-76.1	-55.6
	MC	-95.0	-94.7	-108.7	-104.1	-105.9	-104.3	-85.6
SP-4	SP	-62.8	-64.0	-71.8	-66.5	-60.5	-58.4	-31.9
	MC	-83.4	-84.5	-95.9	-91.0	-90.6	-89.9	-64.9
	CCC	-77.0	-79.3	-89.8	-85.0	-88.1	-88.5	-61.3
	CTC	-84.4	-85.6	-97.2	-92.3	-92.5	-91.8	-66.4
	TS2	-70.4	-70.3	-79.7	-74.6	-71.5	-69.9	-43.7
	TS3	-76.5	-79.3	-89.7	-84.8	-87.6	-87.9	-61.3
	TS4	-70.4	-70.5	-80.0	-74.9	-72.4	-71.0	-44.9
	TS5	-118.2	-122.7	-138.9	-134.7	-145.3	-146.9	-121.7
SP-5 with HB	SP	-67.4	-68.2	-75.7	-71.3	-72.0	-70.9	-47.4
	MC	-91.5	-91.7	-103.8	-99.7	-101.3	-101.0	-77.3
SP-5 no HB	SP	-62.3	-66.5	-72.8	-68.3	-72.1	-72.3	-45.9
	MC	-83.5	-87.3	-97.4	-93.2	-103.3	-105.2	-79.7

Table S6. Theoretical prediction of the effects of HB on the **SP-2** Gibbs free energy reaction profile (G3(MP2,CC), gas-phase[a])

SP / **isomer** / *pathway*	Free Energy Relative to MC / kJ mol^{-1}		Difference
	with HB	without HB	
SP-2 / **MC-TCC**	0.0	0.0	0.0
SP-2 / **TS5** / *pathway 2*	81.2	85.4	4.2
SP-2 / **CTC** / *pathway 2*	11.9	11.8	-0.1
SP-2 / **TS4** / *pathway 2*	72.9	68.7	-4.2
SP-2 / **CCC** / *pathway 2*	8.6	8.8	0.2
SP-2 / **TS3** / *pathway 2*	15.7	12.8	-3.0
SP-2 / **TS2** / *pathway 1*	69.8	64.8	-5.0
SP-2/ **SP**	-42.1	-58.2	-16.0

[a]Reaction profile as in Fig. S9.

Table S7. Calculated $\Delta G^{\ddagger}$ and ΔG_r (in kJ mol^{-1}) for **SP-1**, **SP-2** and **SP-4** in various solvents.[a]

Solvent		Gas Phase	Diethyether	$CHCl_3$	DCM	DCE	Ethanol	Methanol	Water
Dielectric Constant		1.0	4.2	4.7	8.9	10.1	24.9	32.6	78.3
SP-1	E_a Pathway 1	68	82	83	85	85	87	88	88
	E_a Pathway 2	84	85	86	88	88	89	89	90
	ΔG_r	-60	-39	-39	-35	-35	-29	-27	-26
SP-2	E_a Pathway 1	70	85	85	88	88	90	90	91
with HB	E_a Pathway 2	81	88	88	91	91	92	92	94
	ΔG_r	-42	-21	-23	-19	-18	-16	-15	-13
SP-2	E_a Pathway 1	65	79	78	81	81	83	84	85
no HB	E_a Pathway 2	85	82	82	84	84	86	87	88
	ΔG_r	-58	-38	-37	-34	-34	-28	-27	-25
SP-4	E_a Pathway 1	63	76	77	79	79	82	83	84
	E_a Pathway 2	88	81	82	84	84	86	87	88
	ΔG_r	-56	-36	-36	-32	-32	-26	-25	-23

[a]Derived from gas phase Gibbs free energies calculated with G3(MP2,CC) and Gibbs free energies of solvation calculated using the SMD implicit solvation model, as described in §S1.2.

Table S8. Calculated decoloration reaction rate constants (in s^{-1}) for **SP-1**, **SP-2** and **SP-4** in various solvents.[a]

Solvent		Gas Phase	Diethyether	$CHCl_3$	DCM	DCE	Ethanol	Methanol	Water
Dielectric Constant		1.0	4.2	4.7	8.9	10.1	24.9	32.6	78.3
SP-1	Pathway 1	1.5E+01	5.6E-02	3.6E-02	1.6E-02	1.4E-02	7.0E-03	5.4E-03	3.9E-03
	Pathway 2	2.8E-02	1.8E-02	1.3E-02	5.6E-03	5.2E-03	3.4E-03	2.7E-03	1.8E-03
	Overall	1.5E+01	7.4E-02	4.9E-02	2.1E-02	1.9E-02	1.0E-02	8.2E-03	5.6E-03
SP-2	Pathway 1	7.3E+00	1.7E-02	1.4E-02	4.7E-03	4.2E-03	2.5E-03	2.0E-03	1.2E-03
with HB	Pathway 2	7.2E-02	4.8E-03	4.2E-03	1.5E-03	1.3E-03	1.1E-03	8.4E-04	4.7E-04
	Overall	7.3E+00	2.1E-02	1.8E-02	6.2E-03	5.6E-03	3.6E-03	2.8E-03	1.7E-03
SP-2	Pathway 1	5.5E+01	2.9E-01	2.0E-01	8.8E-02	8.1E-02	3.0E-02	2.3E-02	1.5E-02
no HB	Pathway 2	1.4E-02	6.1E-02	4.8E-02	2.2E-02	2.0E-02	1.1E-02	7.7E-03	4.4E-03
	Overall	5.5E+01	3.5E-01	2.5E-01	1.1E-01	1.0E-01	4.1E-02	3.1E-02	1.9E-02
SP-4	Pathway 1	1.2E+02	6.4E-01	4.0E-01	1.7E-01	1.6E-01	5.4E-02	3.7E-02	2.4E-02
	Pathway 2	4.2E-03	8.9E-02	6.0E-02	2.7E-02	2.5E-02	1.1E-02	8.0E-03	5.2E-03
	Overall	1.2E+02	7.3E-01	4.6E-01	2.0E-01	1.9E-01	6.5E-02	4.5E-02	2.9E-02

[a] Derived from gas phase Gibbs free energies calculated with G3(MP2,CC) and Gibbs free energies of solvation calculated using the SMD implicit solvation model, as described in §S1.2.

S3.4 Experimental fading rates for SP-1/-2/-3-/-4 solutions (MC→SP)

Table S9. SP-2 (6-NO_2-8-OH BIPS). Experimental data on thermal fading of photo-colored solutions of **SP-2** (MC→SP)

entry / solvent	$E_T(30)^a$ / (kcal mol^{-1})	μ^b / debye	$\beta - \alpha^c$	experimental k_{obs} / ($\times 10^{-3}$ s^{-1})^d	number of repeated measurements	$\lambda_{MC}{}^e$/ nm
1 / 2,2,2-trifluoroethanol	59.8	2.52	-1.51	0	3	506
2 / methanol	55.4	1.7	-0.32	3.1 ± 0.5	6	549
3 / 2-chloroethanol	55.1	1.77	-0.75	0	3	380
4 / ethanol	51.9	1.69	-0.11	4.2 ± 0.3	4	554
5 / nitromethane	46.3	3.46	-0.16	2.7 ± 0.6	4	560
6 / propylene carbonate	46.0	4.9	0.40	2.2 ± 0.3	4	560
7 / acetonitrile	45.6	3.93	0.21	2.7 ± 0.2	7	559
8 / dimethylsulfoxide	45.1	3.96	0.76	3.1 ± 0.2	7	567
8[f] (VFD) / dimethylsulfoxide	45.1	3.96		2.1 ± 0.4	8	
9 / *N*,*N*-dimethylformamide	43.2	3.82	0.69	3.8 ± 0.4	4	569
10 / acetone	42.2	2.88	0.40	5.5 ± 0.8	4	582
11 / 1,2-dichloroethane	41.3	1.83	0.00	7.6 ± 2.2	2	581
12 / dichloromethane	40.7	1.6	-0.03	10.7 ± 1.6	4	582
12[f] (VFD) / dichloromethane	40.7	1.6		9.7 ± 3.1	4	582
13 / acetophenone	40.6	3.05	0.45	7.1 ± 1.2	4	573
14 / pyridine	40.5	2.22	0.64	47.0 ± 0.8	4	600
15 / *i*-butyl methyl ketone	39.4	2.69	0.46	8.1 ± 0.9	3	576
16 / chloroform	39.1	1.04	-0.10	12.0 ± 1.8	5	586
17 / butyl acetate	38.5	1.87	0.46	21.1 ± 1.9	4	584
18 / 1,2-dimethoxyethane	38.2	1.71	0.31	19.4 ± 2.8	3	579
19 / ethyl acetate	38.1	1.78	0.45	17.1 ± 1.7	4	578
20 / 1,2-dichlorobenzene	38.0	2.5	0.03	9.2 ± 2.1	7	606
21 / tetrahydrofuran	37.4	31.75	0.55	32.4 ± 3.5	5	588
21[f] (VFD) / tetrahydrofuran	37.4	1.75		22.7 ± 4.1	4	
22 / fluorobenzene	37.0	1.66	0.07	18.6 ± 2.2	7	589
23 / chlorobenzene	36.8	1.69	0.07	15.3 ± 1.2	4	597
24 / 1-bromobutane	36.6	2.08	0.13	15.6 ± 1.6	5	591
25 / 1,4-dioxane	36.0	0.0	0.37	38.8 ± 1.3	4	598
26 / trichloroethene	35.9	0.8	0.05	27.7 ± 1.9	4	595
27 / diethyl ether	34.5	1.15	0.47	19.9 ± 2.6	4	597
28 / benzene	34.3	0.0	0.10	32.1 ± 0.7	4	600
29 / toluene	33.9	0.36	0.11	28.1 ± 3.0	3	603

[a]Dimroth as empirical measure of solvent polarity. [b]Electric dipole moments for solvents used in this study are expressed in non SI units of debye (1 debye = 3.336×10^{-30} Coulomb meter). [c]Algebraic difference between the Kamlet and Taft empirical β and α values (HBA and HBD, respectively). Individual α and β values are listed in §S1.1.1. [d]The 95% confidence limit of the mean for each k_{obs} value and is calculated as $t_{n-1}\ s/n^{1/2}$ where t_{n-1} was between 4.30 and 2.45 (see §S1.1.2). [e]Position of the absorbance λ_{max} for the open-ring merocyanine form. [f]Decoloration rate measured in a VFD device inclined at 45º and operated in confined mode at 4000 rpm (see §S1.1.2).

Table S10. SP-3 (5′-NO_2-6-NO_2-8-OH BIPS). Experimental data on thermal fading of photo-colored solutions of **SP-3** (MC→SP)

entry / solvent	$E_T(30)^a$ / (kcal mol^{-1})	μ^b / debye	$\beta - \alpha^c$	experimental k_{obs} / ($\times 10^{-2}$ s^{-1})^d	number of repeated measurements	$\lambda_{MC}{}^e$/ nm
7 / acetonitrile	45.6	3.93	0.21	10.7 ± 0.8	4	602
9 / *N*,*N*-dimethylformamide	43.2	3.82	0.69	4.5 ± 0.7	4	477
10 / acetone	42.2	2.88	0.40	6.0 ± 0.6	4	601
11 / 1,2-dichloroethane	41.3	1.83	0.00	4.6 ± 0.5	4	614
12 / dichloromethane	40.7	1.6	-0.03	5.5 ± 0.3	5	615
19 / ethyl acetate	38.1	1.78	0.45	6.6 ± 0.6	5	617
21 / tetrahydrofuran	37.4	1.75	0.55	12.1 ± 1.0	5	623
29 / toluene	33.9	0.36	0.11	23.0 ± 7.7	6	632

[a]Dimroth as empirical measure of solvent polarity. [b]Electric dipole moments for solvents used in this study are expressed in non SI units of debye (1 debye = 3.336×10^{-30} Coulomb meter). [c]Algebraic difference between the Kamlet and Taft empirical β and α values (HBA and HBD, respectively). Individual α and β values are listed in §S1.1.1. [d]The 95% confidence limit of the mean for each k_{obs} value and is calculated as $t_{n-1}\ s/n^{1/2}$ where t_{n-1} was between 4.30 and 2.57 (see §S1.1.2). [e]Position of the absorbance λ_{max} for the open-ring merocyanine form.

Table S11. SP-4 (6-NO_2-8-OMe BIPS). Experimental data on thermal fading of photocolored solutions of **SP-4** (MC→SP)

entry / solvent	$E_T(30)^a$ / (kcal mol^{-1})	μ^b / debye	$\beta - \alpha^c$	experimental k_{obs} / ($\times 10^{-3}$ s^{-1})^d	number of trials	$\lambda_{MC}{}^e$/ nm
2 / methanol	55.4	1.7	-0.32	1.7 ± 0.1	5	552
4 / ethanol	51.9	1.69	-0.11	6.3 ± 2.0	3	565
5 / nitromethane	46.3	3.46	-0.16	16.4 ± 1.3	4	580
7 / acetonitrile	45.6	3.93	0.21	18.1 ± 0.4	6	578
8 / dimethylsulfoxide	45.1	3.96	0.76	4.9 ± 0.4	4	581
8^f (VFD) / dimethylsulfoxide	45.1	3.96		4.7 ± 0.5	3	
10 / acetone	42.2	2.88	0.40	36.7 ± 2.6	4	589
11 / 1,2-dichloroethane	41.3	1.83	0.00	51.2 ± 2.3	4	603
12 / dichloromethane	40.7	1.6	-0.03	62.0 ± 2.8	5	603
15 / *i*-butyl methyl ketone	39.4	2.69	0.46	63.4 ± 5.7	4	599
16 / chloroform	39.1	1.04	-0.10	63.1 ± 5.0	5	606
17 / butyl acetate	38.5	1.87	0.46	39.2 ± 6.2	3	603
18 / 1,2-dimethoxyethane	38.2	1.71	0.31	77.7 ± 4.3	7	596
19 / ethyl acetate	38.1	1.78	0.45	43.8 ± 1.4	4	601
20 / 1,2-dichlorobenzene	38.0	2.5	0.03	37.1 ± 1.7	3	617
21 / tetrahydrofuran	37.4	1.75	0.55	42.5 ± 3.9	5	604
23 / chlorobenzene	36.8	1.69	0.07	33.8 ± 2.1	4	616
25 / 1,4-dioxane	36.0	0.0	0.37	22.8 ± 1.0	4	606
26 / trichloroethene	35.9	0.8	0.05	24.6 ± 0.4	3	614
27 / diethyl ether	34.5	1.15	0.47	14.6 ± 2.2	4	609
28 / benzene	34.3	0.0	0.10	21.7 ± 3.4	3	

[a]Dimroth as empirical measure of solvent polarity. [b]Electric dipole moments for solvents used in this study are expressed in non SI units of debye (1 debye = 3.336×10^{-30} Coulomb meter). [c]Algebraic difference between the Kamlet and Taft empirical β and α values (HBA and HBD, respectively). Individual α and β values are listed in §S1.1.1. [d]The 95% confidence limit of the mean for each k_{obs} value and is calculated as $t_{n-1}\ s/n^{1/2}$ where t_{n-1} was between 4.30 and 2.45 (see §S1.1.2). [e]Position of the absorbance λ_{max} for the open-ring merocyanine form. . [f]Decoloration rate measured in a VFD device inclined at 45º and operated in confined mode at 4000 rpm (see §S1.1.2).

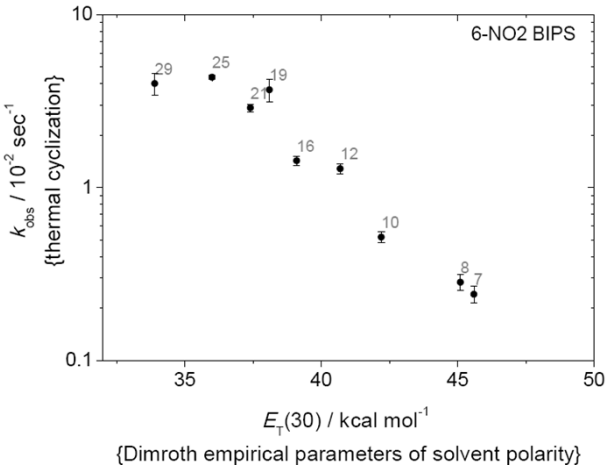


Fig. S1 Thermal decolorization kinetic data for solutions of 6-NO_2 BIPS (**SP-1**). Experimental rate constants (k_{obs}) for the thermal fade of **SP-1** are obtained upon UV irradiation (365 nm nominal wavelength and a nominal typical output of 360 mW, §S1.1.2) at 23 ºC of 2.0 ×10^{-5} mol L^{-1} solutions in acetonitrile (7), dimethylsulfoxide (8), acetone (10), dichloromethane (12), chloroform (16), ethyl acetate (19), tetrahydrofuran (21), 1,4-dioxane (25) and toluene (29). Experimental values of k_{obs} are plotted against the solvent polarity expressed in the Dimroth $E_T(30)$ scale.

S3.5 Hydroxyl groups absorption region in the IR spectrum of SP-1 and SP-3 solutions

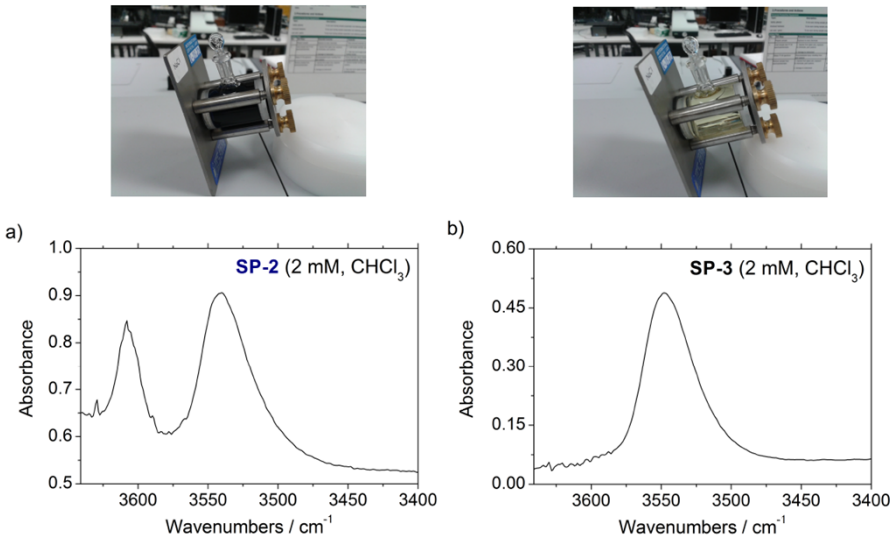
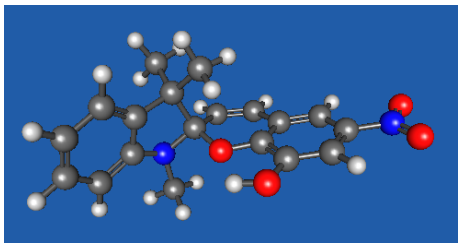


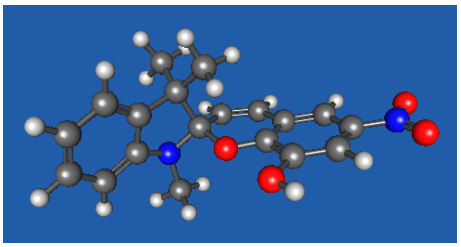
Fig. S2 Hydroxyl groups absorption region in the IR spectrum of **SP-1** (a) and **SP-3** (b) in 2.0×10^{-3} mol L^{-1} solutions in chloroform. (a) **SP-2**; based both on literature data,[25] and on simulation results (Fig. S3 and Table S2) the high energy absorption band was assigned to free hydroxyls groups while the red-shifted band was ascribed to hydroxyls groups involved in intramolecular hydrogen bonding.

S3.6 Computed hydroxyls (8-OH) infrared stretching frequencies for the SP and *trans*-MC isomers of SP-2 and SP-3

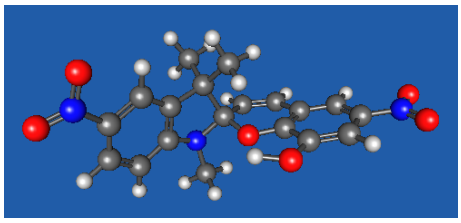
SP-2/HB 3584 cm^{-1}



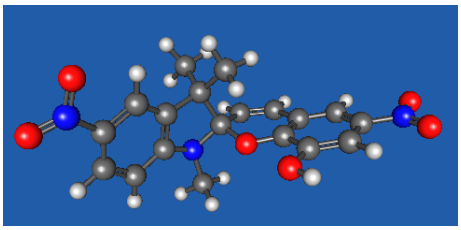
SP-2/non-HB 3647 cm^{-1}



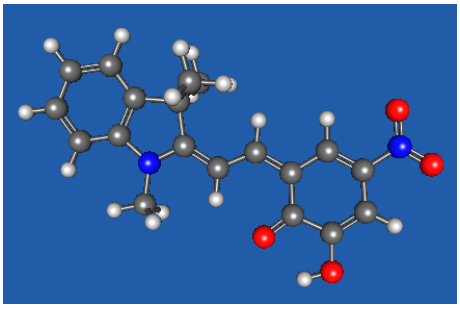
SP-3/HB 3595 cm^{-1}



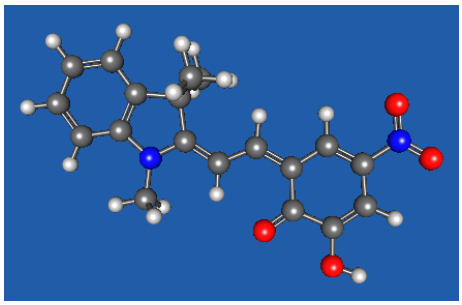
SP-3/non-HB 3645 cm^{-1}



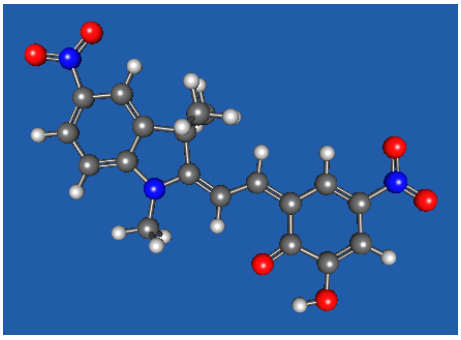
MC-2/HB 3468 cm^{-1}



MC-2/non-HB 3638 cm^{-1}



MC-3/HB 3477 cm^{-1}



MC-3/non-HB 3637 cm^{-1}

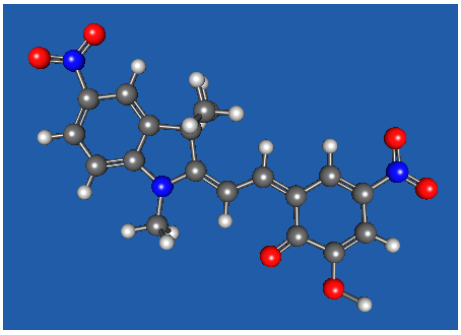


Fig. S3 Computed gas-phase hydroxyls (8-OH) IR stretching frequencies for SP and *trans*-MC isomers of **SP-2** and **SP-3**. IR frequencies calculated at the M06-2X/6-31G(2*df,p*) level of theory are indicated in figure next to the corresponding molecular graphics.

S3.7 "Closed-ring control"; spectroscopic data for SP-3 (5′-NO_2-6-NO_2-8-OH BIPS)

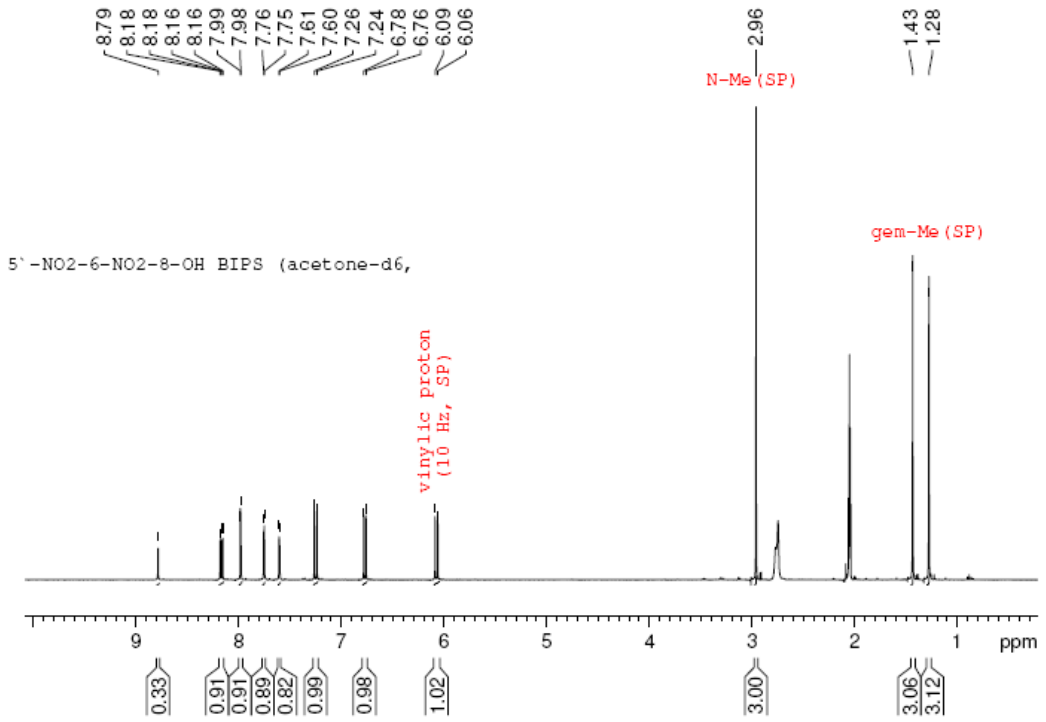


Fig. S4 ^{1}H NMR spectrum (400 MHz, acetone-d_6) of compound **SP-3**. A pair of distinct *gem*-Me signals (1.76 ppm), the upfield position of the *N*-Me absorption (3.97 ppm), and *cis*-coupled vinylic protons (J = 10 Hz) are in agreement with the presence of only the closed-ring SP isomer.

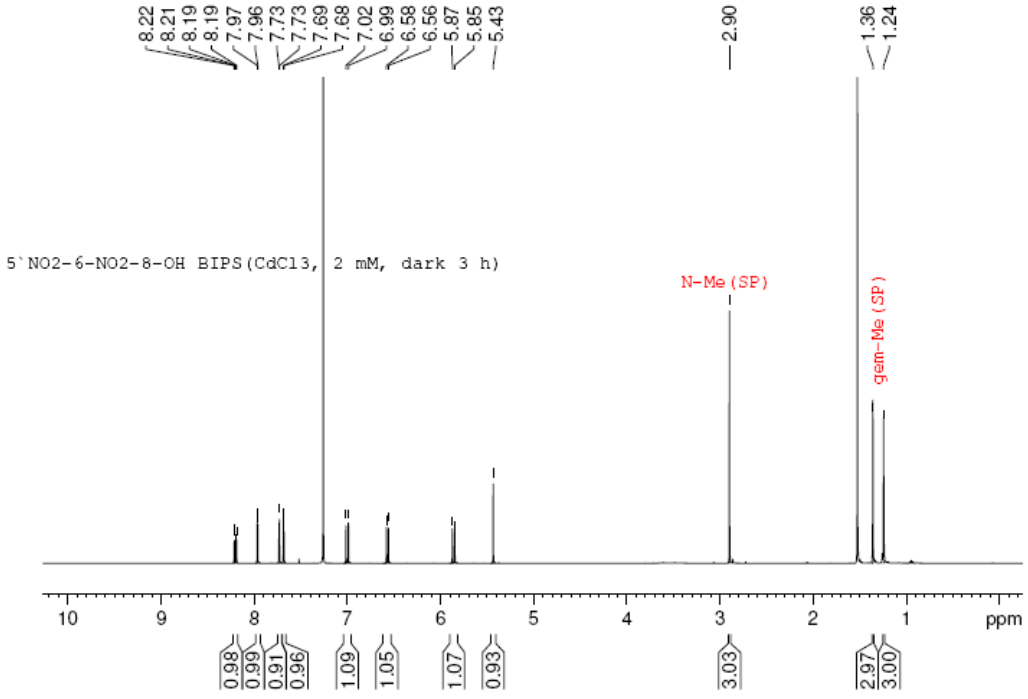


Fig. S5 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **SP-3**.

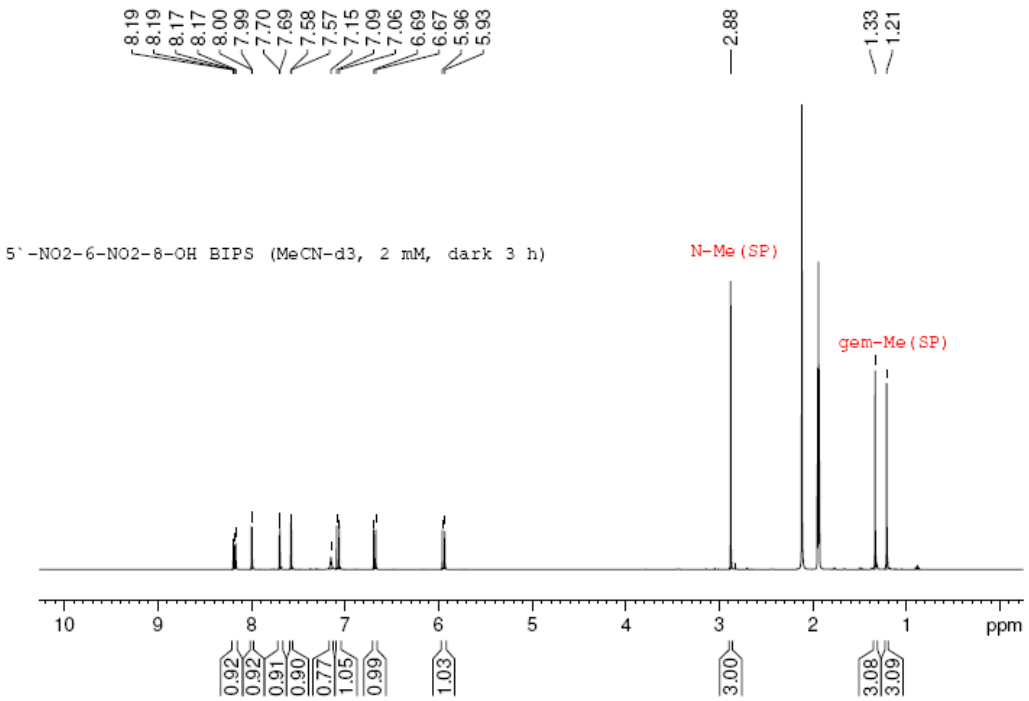


Fig. S6 ^{1}H NMR spectrum (400 MHz, CD_3CN) of compound **SP-3**.

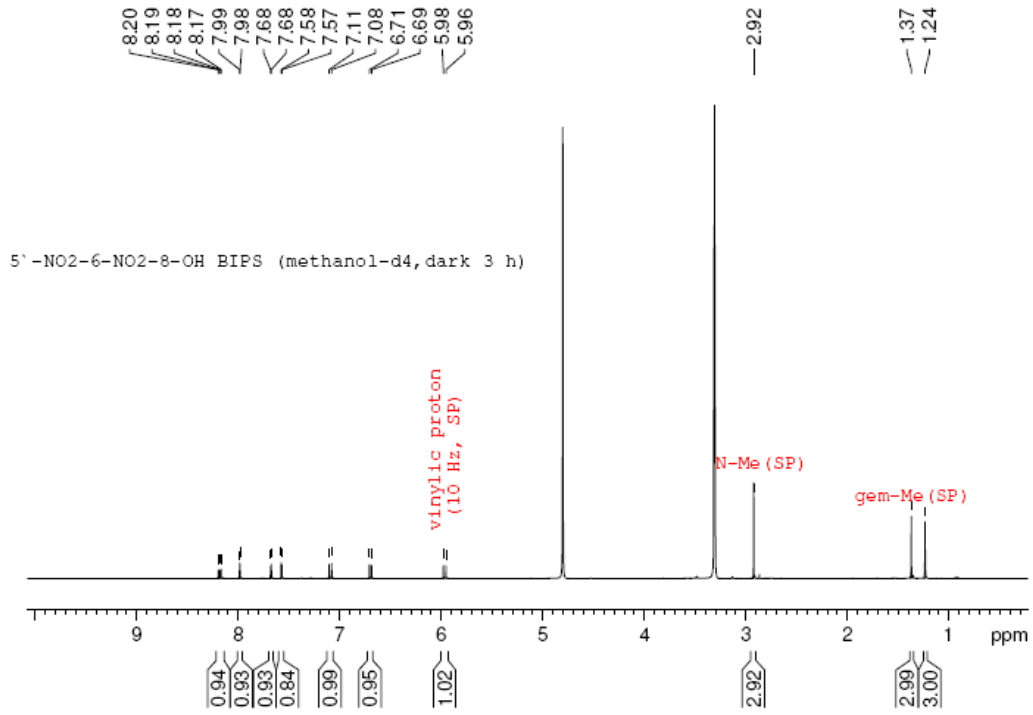


Fig. S7 ^{1}H NMR spectrum (400 MHz, methanol-d_4) of compound **SP-3**.

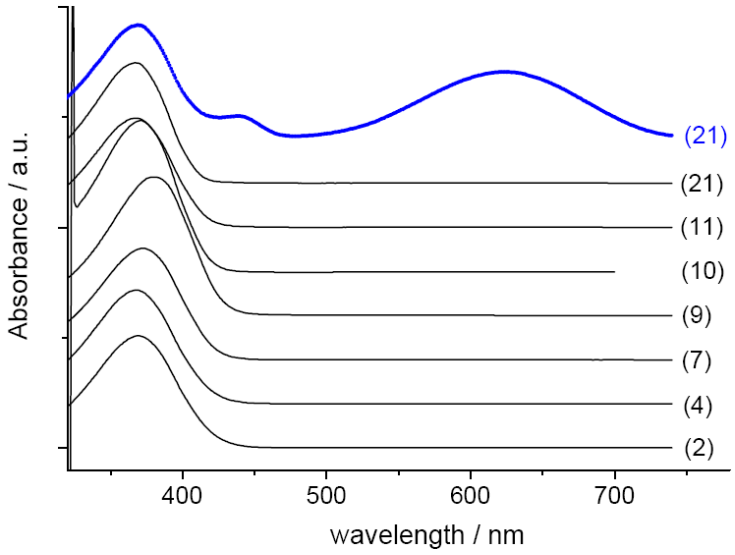


Fig. S8 Representative Steady-state (dark) absorption spectra of **SP-3** in in methanol (2), ethanol (4), acetonitrile (7), *N*,*N*-dimethylformamide (9), acetone (10), 1,2-dichloroethane (11) and tetrahydrofuran (21) solutions. All solutions were prepared at 23 ºC at a 2.0×10^{-5} mol L^{-1} concentration. Absent from the red portion of the spectra are absorptions associated to equilibrium amounts of the open-ring MC isomer. Blue trace shows the MC contribution to the spectra after irradiation at 365 nm of **SP-3** solutions in THF. All spectra are vertically offset for clarity.

S3.8 MC→SP (SP-2) thermal fading; computed reaction profiles

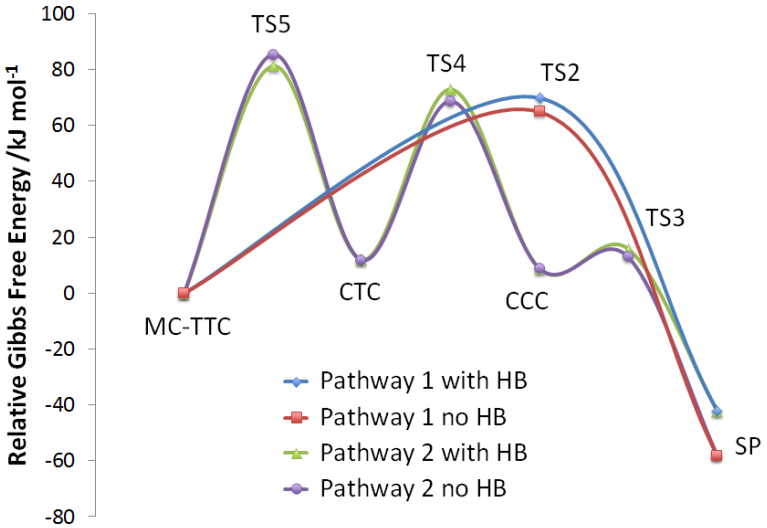


Fig. S9 Effects of hydrogen bonding on MC→SP (**SP-2**) thermal fading; computed gas-phase Gibbs free energy reaction profiles for pathway 1 and 2. All free energies calculated relative to that of the relevant MC form as in Table S6. Geometries of each point on the reaction profiles optimized with M06-2X/6-31G(2*df*,*p*) (see Fig. S10). Free energies calculated with G3(MP2,CC).

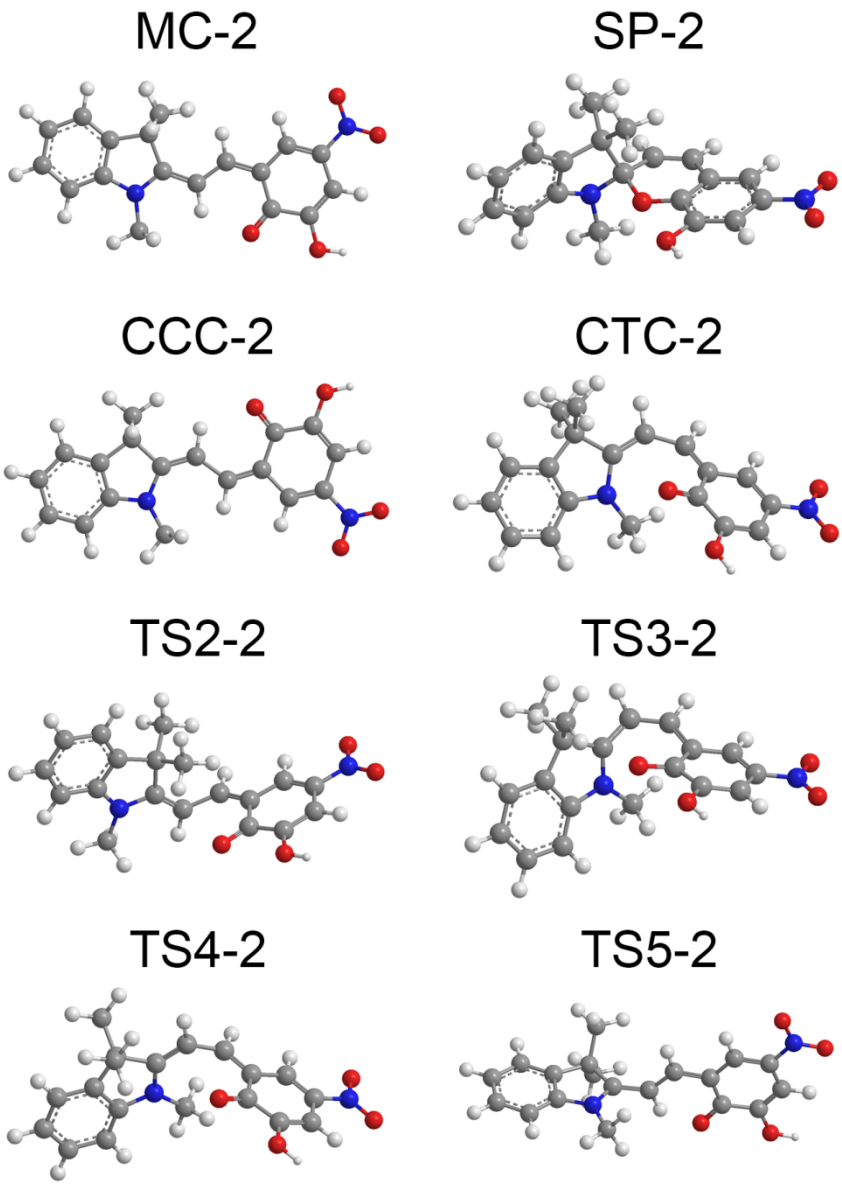


Fig. S10 SP-2 species along the MC→SP thermal fading reaction profile. Geometries optimised using M06-2X/6-31G(2*df*,*p*).

S3.9 Representative UV/V spectra of SP-2 samples showing the photochemical opening and thermal fading of photocolored solutions

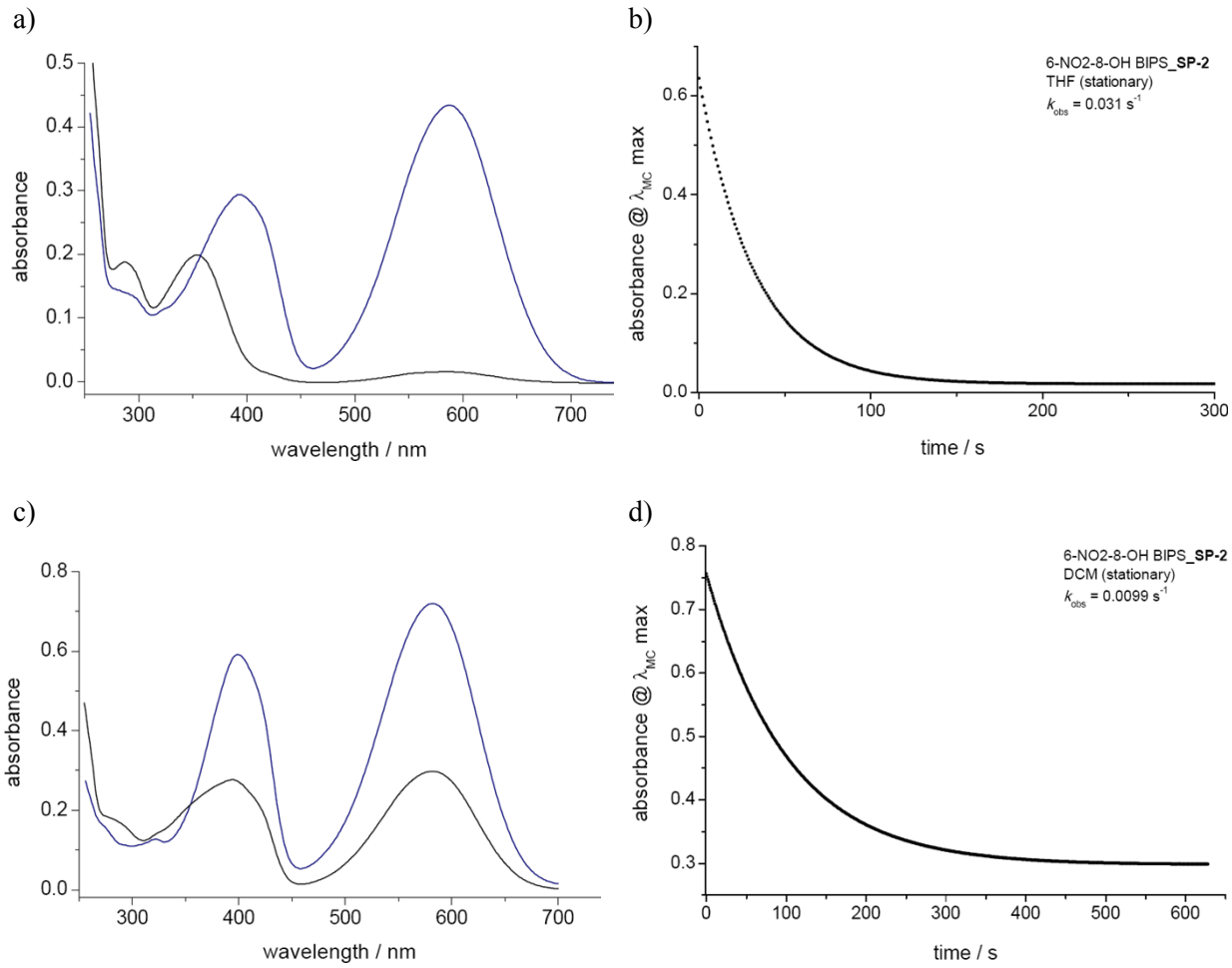


Fig. S11 Representative UV/V spectra of **SP-2** samples showing the photochemical opening and thermal decoloration kinetic (thermal fading times up to *ca*. 10 half-life times, $t_{1/2} = \ln 2/k_{obs}$). All solutions were prepared at the concentration of 2.0×10^{-5} mol L^{-1} in either THF (a-b) and DCM (c-d).

S3.10 Thermal decoloration of SP-4 solutions; k_{obs} vs solvent polarity ($E_T(30)$ scale)

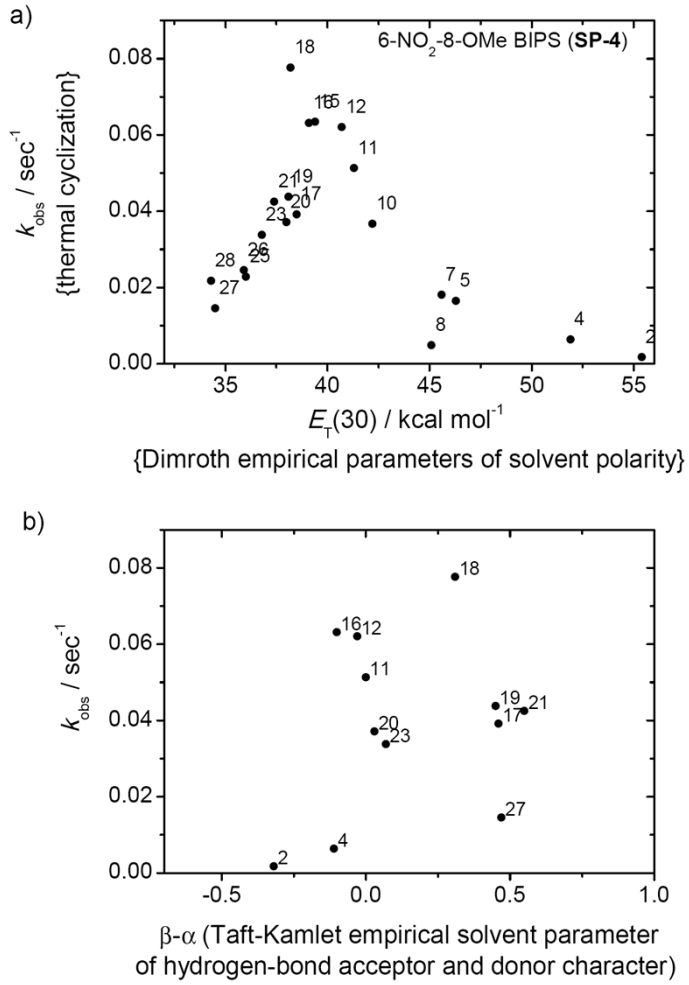


Fig. S12 Solvent effects on the thermal decolouration of **SP-4** (MC/SP relaxation). Plots of experimental k_{obs} *vs.* (a) $E_T(30)$ values from the Dimroth polarity scale, and (b) algebraic difference between the Kamlet and Taft empirical β and α values (HBA and HBD, respectively). Panel (b) includes only solvents systems of intermediate μ values (*ca*. 2.5-1.0 D). Solvents are numbered in order of increasing $E_T(30)$ value (§S1.1.1): methanol, (2); 55.4; ethanol, (4); nitromethane, (5); acetonitrile, (7); dimethyl sulfoxide, (8); acetone, (10); 1,2-dichloroethane, (11); dichloromethane, (12); *i*-butyl methyl ketone, (15); chloroform, (16); *n*-butyl acetate, (17); 1,2-dimethoxyethane (*monoglyme*), (18); ethyl acetate, (19); 1,2-dichlorobenzene, (20); tetrahydrofuran, (21); chlorobenzene, (23); 1,4-dioxane, (25); trichloroethene, (26); diethyl ether, (27); benzene, (28). Data in plot are tabled in Table S11. Despite the thermal fading vs polarity data for **SP-1** (Fig. S1) and **SP-2** (Fig. S18) being in line with a general trends found in literature for 6-NO2 BIPS derivatives, the increase in k_{obs} with decreasing polarity is in fact not shared by the methyl ether **SP-4** (Fig. S12a). Data in our hand for control **SP-4** in 21 different solvents do challenge the general notion of more polar solvents lowering the rate of thermal fading, and points out at a need to clarify further the reaction pathway for this rather common SP molecule.

S3.11 SP-2 and SP-4; computed Gibb's Free Energy reaction profiles

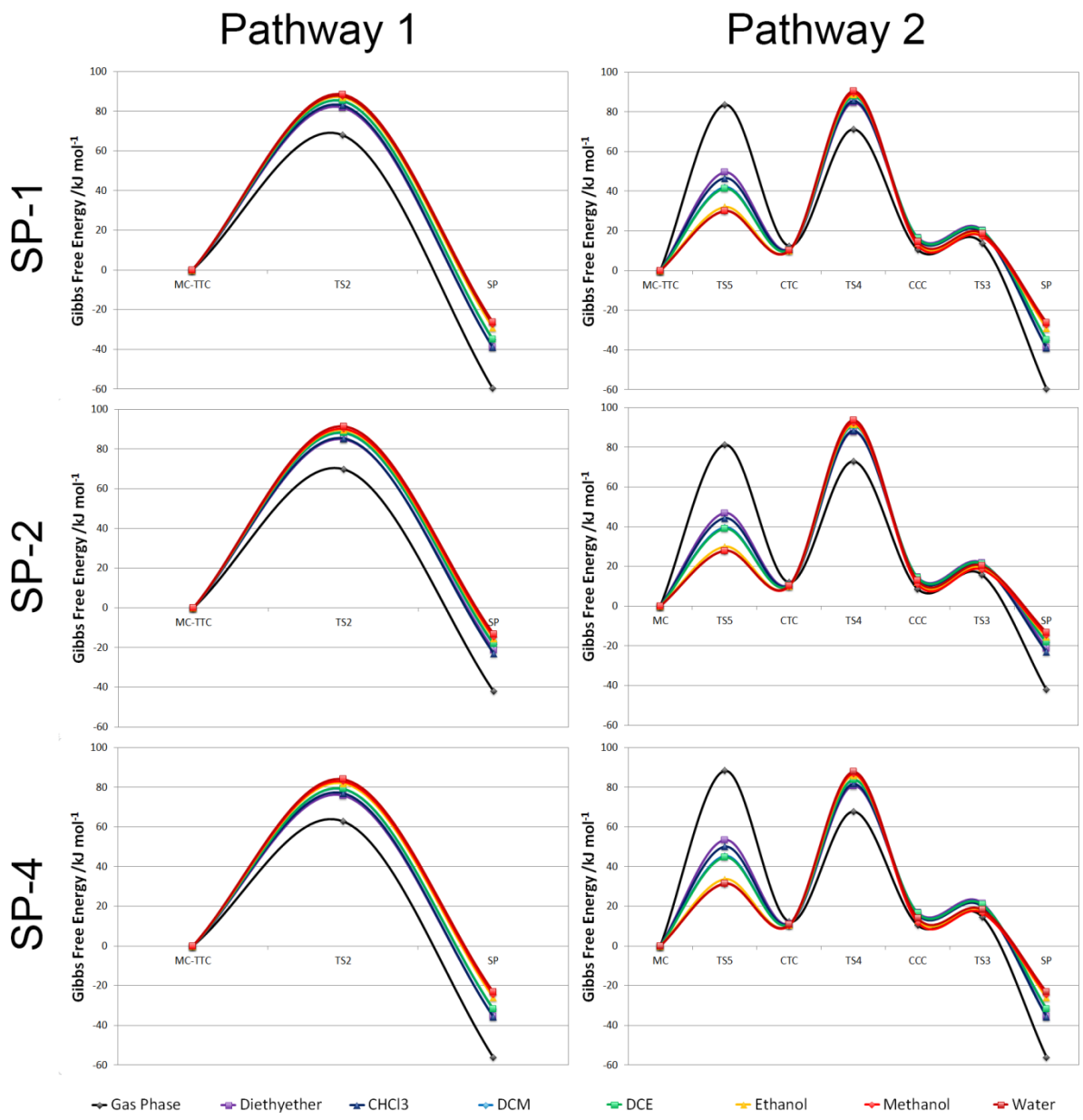


Fig. S13 SP-1, **SP-2** and **SP-4** computed Gibbs Free Energy reaction profiles for MC→SP. Reaction pathways as shown in Fig.s S9 and S10. Profiles for different implicit solvents systems are coloured according to a rainbow with polarity, *i.e.* water (ε=78) is red through to diethyl ether (ε=4.2) being purple. The black line represents the reaction in the gas phase (vacuum). Free energies are calculated with respect to the MC form in the relevant solvent. Note that although pathway 1 is favoured for the gas phase reaction, solvent effects lower the activation barrier for pathway 2 so that passage over TS4 rather than TS5 becomes the rate limiting step. As a result both pathways are competitive for all three spiropyrans.

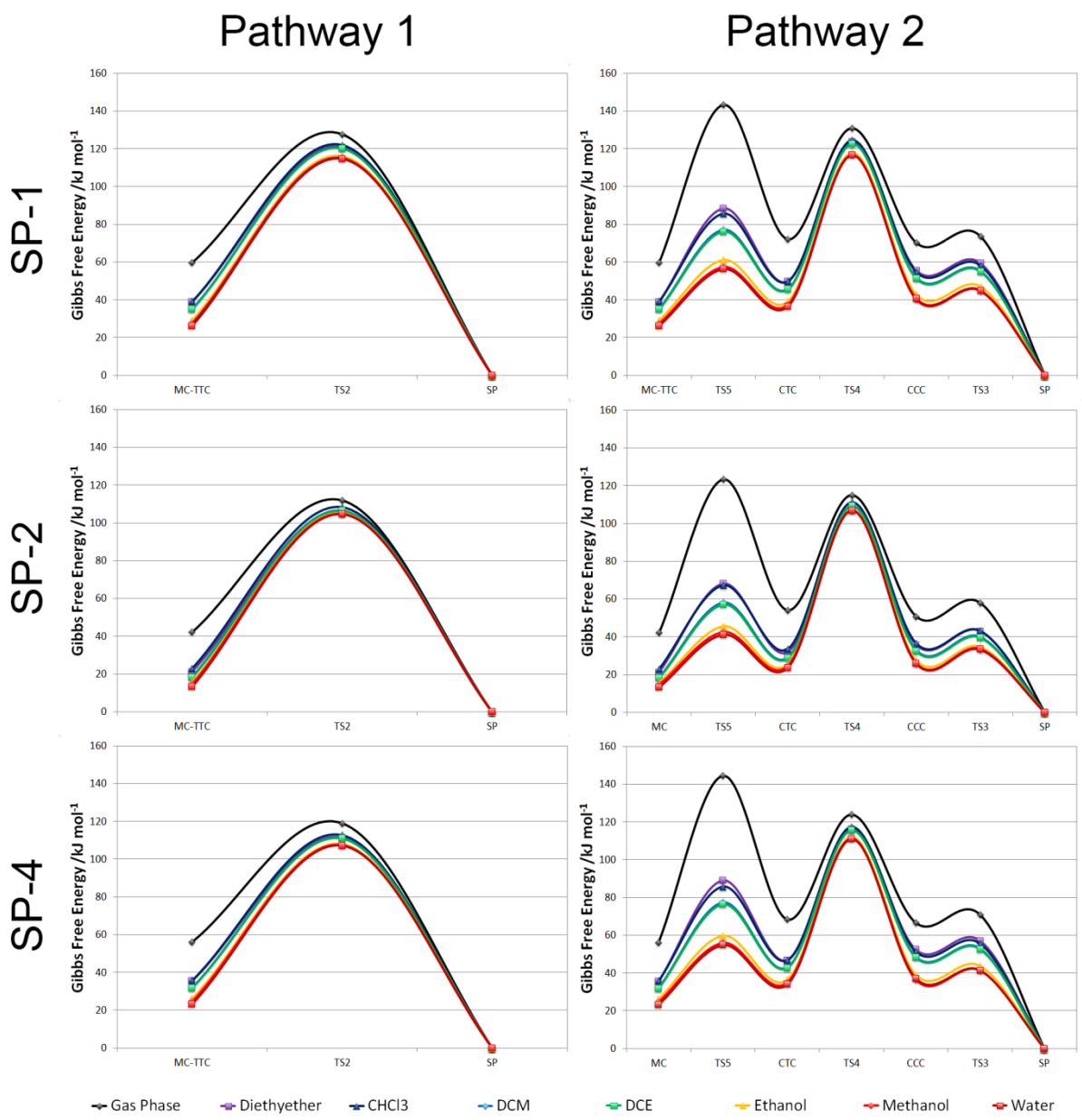


Fig. S14. **SP-1**, **SP-2** and **SP-4** computed Gibbs Free Energy reaction profiles for MC→SP. Reaction pathways as shown in Fig.s S9 and S10. Profiles for different implicit solvents systems are coloured according to a rainbow with polarity, *i.e.* water (ε=78) is red through to diethyl ether (ε=4.2) being purple. The black line represents the reaction in the gas phase (vacuum). Free energies are calculated with respect to the SP form in the relevant solvent. This allows the effects of solvation on each of the steps along the reaction pathway to be clearly seen. Open-ring isomers are preferentially stabilized by more polar solvents in comparison to the closed-ring SP form. This is consistent with the expectation that these isomers may have some zwitterionic character.

S3.12 “Open-ring control”; spectroscopic data for SP-5 (8-COOH BIPS)

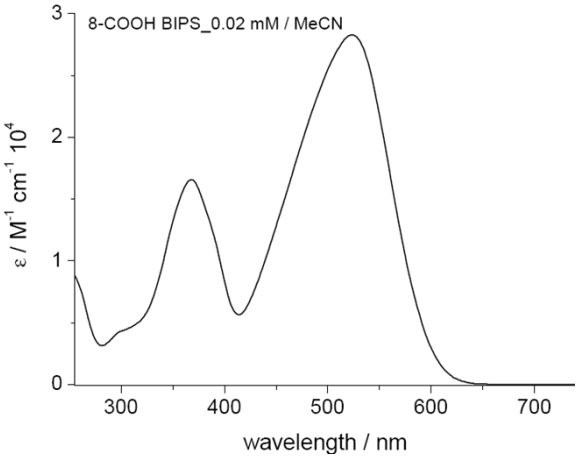


Fig. S15 Representative dark equilibrated (30 min) absorption spectra of **SP-5** solutions in acetonitrile (2.0 $\times 10^{-5}$ mol L^{-1}).

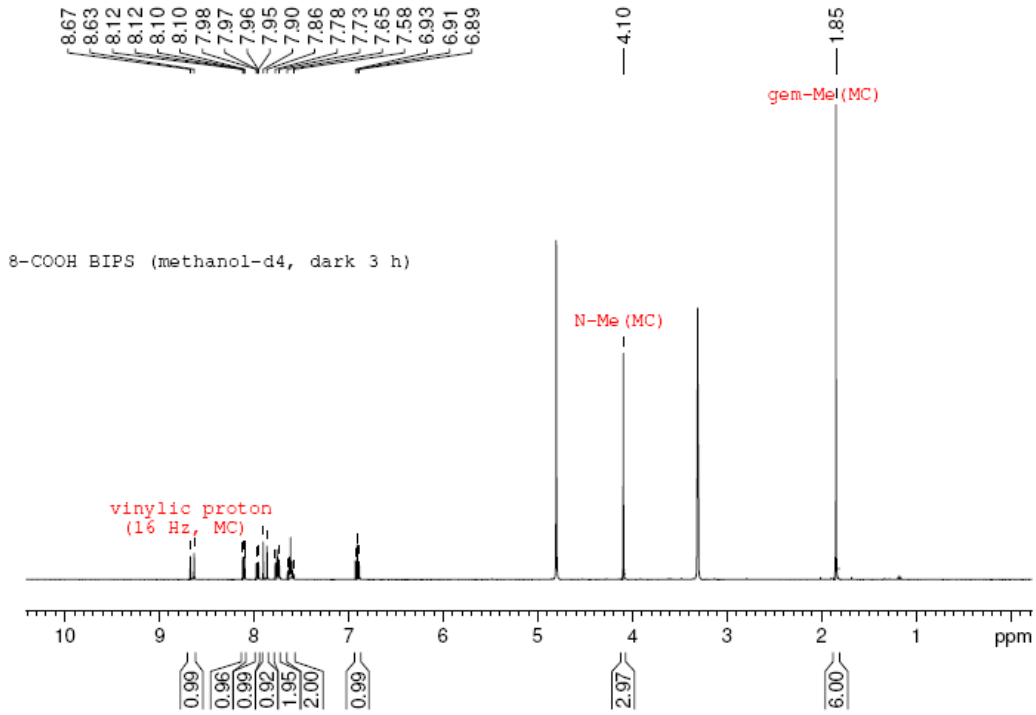


Fig. S16 ^{1}H NMR spectrum (400 MHz, methanol-d_4) of compound **SP-5**. NMR absorptions peaks associated with characteristic signals from the open-ring merocyanine form (MC) of **SP-5** are indicated with labels. Absent from the spectra are signals from the closed-ring isomer (SP).

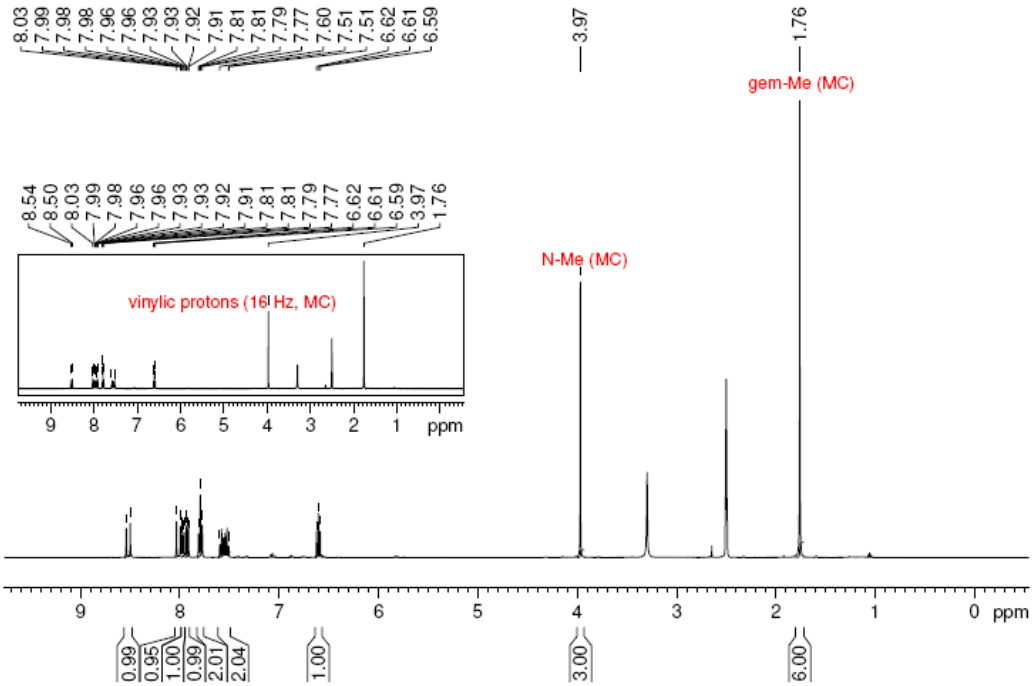


Fig. S17 ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **SP-5**. A single downfield *gem*-Me signal (1.76 ppm), the downfield shift for the *N*-Me absorption (3.97 ppm), and *trans*-coupled vinylic protons (J = 16 Hz) are in agreement with the presence of only merocyanine isomers.

S3.13 Thermal decoloration of SP-2 solutions; k_{obs} vs solvent polarity ($E_T(30)$ scale)

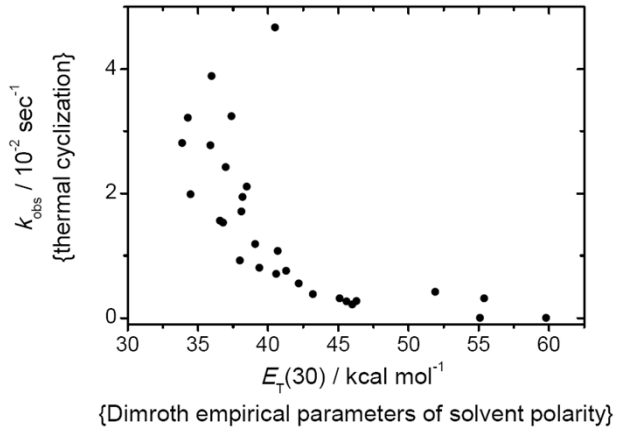


Fig. S18 Solvent effects on the thermal decolouration of **SP-2** (MC/SP relaxation). Plots of experimental k_{obs} *vs*. $E_T(30)$ values from the Dimroth polarity scale. Data in plot are in Table S9.

S3.14 Shear stress effects on the thermal decoloration of SP-2 solutions; high rpms

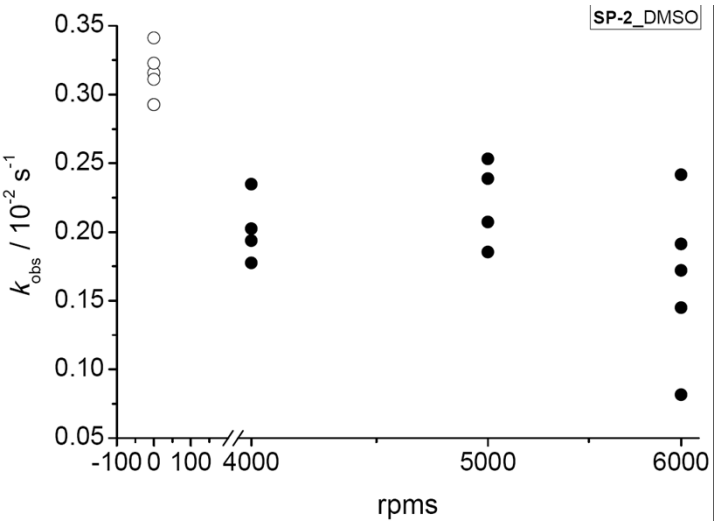


Fig. S19 SP-2 (6-NO_2-8-OH BIPS); shear stress effect on the thermal fading rate of a dynamic thin film. Thermal decoloration data obtained above 4000 rpms may indicate a progressive drop in the HBA character of the solvent as shearing is increased by means of increasing the rotational speed of the VFD tube (●). However, noise in the absorbance with the shortening of the optical path at high rpms will require further modifications of the current optical system coupled to the VFD device (S1.1.2). All data are for **SP-2** solutions in DMSO. Thermal fading data for the stationary system are shown for comparison and are indicated as hollow symbols (○).

S4. M06-2X/6-31G(2df,p) optimized geometries

Molecular geometries (in Gaussian archive format) for all calculations discussed in this work. Unless otherwise stated, optimization was performed in the gas phase.

```
SP-1

MC-1
 1\1\GINC-R2217\FOpt\RM062X\6-31G(2df,p)\C19H18N2O3\ROOT\07-Nov-2014\0\
 \# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) ma
 xdisk=3221225472\\MC0-TTC.M062X\\0,1\C,-1.1952743301,0.9825572608,-0.9
 961683157\N,-0.2343193369,1.9499047437,-0.5105112225\C,1.0469855259,1.
 6346495565,-0.2050113872\C,1.5196218858,0.3471504657,-0.3424118397\C,2
 .8273504579,-0.0521471747,-0.0465592864\C,3.364468741,-1.327300629,-0.
 1623645159\C,2.5793012866,-2.4916138267,-0.6397719397\O,1.3996982578,-
 2.4226986668,-0.968799681\C,4.729525826,-1.5072970912,0.1970294327\C,5
 .3188605969,-2.7247878238,0.108824824\C,4.6012848192,-3.8765759332,-0.
 3462139506\C,3.3054334796,-3.7627990147,-0.6995559439\N,6.7160118062,-
 2.867702464,0.4854871461\O,7.3111781254,-1.8794873818,0.8699315106\O,7
 .2104477156,-3.974289512,0.3932855878\C,1.7622328785,2.8985556777,0.27
 28416536\C,0.6560130413,3.9258090437,0.169713521\C,-0.5023216141,3.311
 4264818,-0.2985290808\C,2.9232914075,3.2820781467,-0.6595553408\C,2.22
 62929541,2.771728346,1.7333583838\C,0.6573949055,5.2742990593,0.457535
 5063\C,-0.5177779901,6.0038619897,0.2707627318\C,-1.6653519334,5.37654
 87743,-0.19722603\C,-1.6789272751,4.0140893456,-0.4915649341\H,-0.8482
 180916,0.5407127073,-1.9339079273\H,-1.3297165058,0.1814727414,-0.2646
 199121\H,0.8525423927,-0.4226843383,-0.7014294698\H,3.5206528547,0.702
 7131659,0.3168029989\H,5.3157793873,-0.6651460821,0.5476969204\H,5.130
 6683905,-4.8194760225,-0.3932584794\H,2.5784944393,3.3605123308,-1.693
 0104283\H,3.7331085803,2.5520152853,-0.6213438877\H,3.3225261371,4.253
 9195492,-0.3568614042\H,1.3920048702,2.4917653705,2.3803917249\H,2.614
 7795334,3.735697004,2.0729617028\H,3.014478726,2.0258209931,1.84581314
 13\H,1.5554127863,5.762139732,0.8230280844\H,-0.5354258778,7.063972911
 2,0.4915554802\H,-2.5717606063,5.9533985174,-0.3383609458\H,-2.5821384
 585,3.5413923098,-0.8555903852\H,-2.1494271453,1.4766783413,-1.1649295
 881\H,2.7330173563,-4.6139938899,-1.0481044543\\Version=ES64L-G09RevD.
 01\State=1-A\HF=-1069.5609154\RMSD=9.657e-09\RMSF=5.495e-06\Dipole=-2.
 8601689,3.2595125,-0.1370959\Quadrupole=-6.8319752,3.3699128,3.4620624
 ,7.4383059,-1.4014169,2.155935\PG=C01 [X(C19H18N2O3)]\\@

SP-1
 1\1\GINC-R2363\FOpt\RM062X\6-31G(2df,p)\C19H18N2O3\ROOT\07-Nov-2014\0\
 \# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) ma
 xdisk=3221225472\\SP0.M062X\\0,1\C,0.0586688131,-1.7436051094,-1.44521
 8285\N,-1.3233025602,-1.9321118757,-1.0618266928\C,-2.1275640092,-0.76
 71430581,-0.7888200046\C,-2.3256890271,0.0873467782,-2.005596914\C,-2.
 2529961866,1.4153917655,-1.9641471486\C,-1.9015996024,2.0974767313,-0.
 7262937216\C,-1.4925972389,1.2987794059,0.3536019718\O,-1.446152221,-0
 .0386694147,0.2654104922\C,-1.9056814203,3.4771199642,-0.5813126458\C,
 -1.5076386645,4.0333538552,0.6221900702\C,-1.0891261692,3.2530880734,1
 .6909377502\C,-1.0785259277,1.8773261145,1.5522630203\N,-1.5210663065,
 5.4903887575,0.7680006262\O,-1.8916519622,6.1461557913,-0.1828892905\O
 ,-1.1608901412,5.9514203384,1.8300932246\C,-3.4462392911,-1.3724459915
 ,-0.193886725\C,-2.8976341557,-2.6239938706,0.4553436528\C,-1.65315215
 73,-2.9073382501,-0.1133052782\C,-4.1401216793,-0.4102534799,0.7638146
 201\C,-4.4069116156,-1.77599414,-1.3232265374\C,-3.4387570416,-3.46117
 53921,1.4048277523\C,-2.7208215852,-4.5958813077,1.7961550327\C,-1.483
 9762986,-4.8651663999,1.229712488\C,-0.9261108651,-4.0218115902,0.2660
 815225\H,0.4278983968,-2.6434341208,-1.9428449348\H,0.1218977384,-0.91
 33232496,-2.152006936\H,-2.5644527747,-0.4465246025,-2.9176050825\H,-2
 .4330585704,2.0163315753,-2.8494688634\H,-2.2094254677,4.1251439866,-1
 .3939005925\H,-0.7843658177,3.7352466908,2.6097259669\H,-3.521443786,-
 0.1988886201,1.6372177128\H,-5.0830218796,-0.8454257111,1.1063592026\H
 ,-4.3748100634,0.5334344441,0.2591179559\H,-5.243464235,-2.3361598702,
 -0.8984868731\H,-3.9057283298,-2.4159666657,-2.0543480529\H,-4.8061200
 314,-0.8951820199,-1.8348854736\H,-4.4043533872,-3.240942677,1.8496594
 997\H,-3.1287914099,-5.2614184771,2.5470777651\H,-0.9305869417,-5.7427
 211552,1.544624753\H,0.047796968,-4.2335461007,-0.1587285241\H,0.70234
 911,-1.5229783496,-0.5840290248\H,-0.7605222051,1.2285472268,2.3586825
 212\\Version=ES64L-G09RevD.01\State=1-A\HF=-1069.5903297\RMSD=6.351e-0
 9\RMSF=3.767e-06\Dipole=-0.1051093,-1.8076217,-0.6716712\Quadrupole=9.
 9543148,-20.5909786,10.6366638,-3.1733071,-1.192554,-4.5903323\PG=C01
 [X(C19H18N2O3)]\\@
```

CCC-1
1\1\GINC-R2034\FOpt\RM062X\6-31G(2df,p)\C19H18N2O3\ROOT\07-Nov-2014\0\
\# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) ma
xdisk=3221225472\\CCC0.M062X\\0,1\C,-0.675830669,0.9251533435,-2.68371
55222\C,-0.6636243665,0.801595073,-1.2770066953\C,0.6058015385,0.94645
81374,-0.5505580464\C,1.7855620367,1.1545373739,-1.37880218\C,1.733590
5491,1.2075898995,-2.7312193842\C,0.4800677422,1.0965414533,-3.3878411
224\C,-1.9171195222,0.7055150649,-0.6246025349\C,-2.2394382995,0.42447
87748,0.6829814084\C,-1.4494442093,-0.1842096317,1.6765642314\N,-0.613
1135739,-1.197575554,1.5081790653\C,0.0419514487,-1.5258933774,2.71559
75035\C,-0.4703491683,-0.7292325074,3.7326631558\C,-1.4959414402,0.205
4757917,3.1449113716\C,-0.0130663579,-0.8889636086,5.0245314094\C,0.97
07919702,-1.8473210469,5.2709930627\C,1.4786438384,-2.6257990961,4.237
188458\C,1.0186372605,-2.4789035531,2.9297551697\O,0.6968739302,0.9078
143825,0.6844095781\N,0.4262110651,1.1824418767,-4.8354687863\O,-0.660
0853906,1.0957332659,-5.3766570426\O,1.4762861139,1.3357421624,-5.4299
577469\H,1.4267737654,-3.0751264273,2.1234265638\H,2.2491298819,-3.358
0589777,4.4469643625\H,1.3487256574,-1.9818971154,6.2772675536\H,-0.40
25470182,-0.2778286231,5.8320216182\C,-2.8900307504,-0.031300835,3.745
0995225\C,-1.0769656477,1.6779736179,3.2868072946\H,-3.2156032315,0.75
31778276,1.0285292426\H,-2.7646686378,0.9933766129,-1.2467983462\H,2.6
203887873,1.3473399437,-3.3359148076\H,-1.611389745,0.8655125505,-3.22
8575311\C,-0.3739876833,-1.9202242543,0.2804010201\H,-3.6301220195,0.6
254308015,3.2810573931\H,-2.8642634297,0.1934720858,4.8144758367\H,-3.
2065786126,-1.0693488941,3.6190955953\H,-1.8229637848,2.3234735406,2.8
156209079\H,-0.116418644,1.8444251204,2.7974626309\H,-1.0067709267,1.9
360872601,4.3470695297\H,-1.2432044718,-1.8100611862,-0.3665154083\H,-
0.2267362513,-2.9736332893,0.5243660625\H,0.5072539504,-1.5278690403,-
0.234127232\H,2.7230743159,1.2529710577,-0.8443293818\\Version=ES64L-G
09RevD.01\State=1-A\HF=-1069.5582889\RMSD=7.905e-09\RMSF=1.834e-05\Dip
ole=-1.0745186,-1.5810644,3.6570013\Quadrupole=9.7544502,8.0255582,-17
.7800084,-5.3609937,1.835359,4.907221\PG=C01 [X(C19H18N2O3)]\\@

CTC-1
1\1\GINC-R2036\FOpt\RM062X\6-31G(2df,p)\C19H18N2O3\ROOT\07-Nov-2014\0\
\# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) ma
xdisk=3221225472\\CTC0.M062X\\0,1\C,-2.3680461152,-3.6048927724,-0.157
241108\C,-3.1318835531,-2.4474662934,-0.0393901175\C,-2.9879883061,-4.
8271886686,-0.3095694928\C,-4.3827040842,-4.8738457277,-0.3517922271\C
,-5.1293270034,-3.7076740447,-0.2436787786\C,-4.5141699277,-2.46587133
39,-0.0868346588\H,-2.4033265148,-5.737167998,-0.3974703975\H,-4.88628
14278,-5.8248197779,-0.4749242477\H,-6.2109107225,-3.7575079736,-0.286
5732373\H,-5.1056989431,-1.5612171713,-0.0218580211\N,-2.2733989409,-1
.3412268592,0.1224083157\C,-2.7696999924,-0.0272422318,0.4659100594\C,
-0.9082087666,-3.2369255288,-0.0772906707\C,-0.145977139,-3.6382669518
,-1.3471926508\C,-0.9747361119,-1.7169874519,0.0577838252\C,0.16907356
47,-0.9496741303,0.1135362644\C,0.2778621608,0.4395050298,-0.025247266
\H,-0.6203853058,1.0074416556,-0.2541963235\H,1.0996230912,-1.49269606
26,0.2077012064\C,1.4385934937,1.2012013774,0.0275721672\C,1.322929871
7,2.5999094062,-0.2054386857\H,0.3536756096,3.0391391071,-0.4140625745
\C,2.7731823599,0.6203001343,0.3121355196\O,2.9583084337,-0.5723323454
,0.5283211215\C,3.8881167567,1.5713582553,0.3221033344\H,4.5494562273,
3.5859043891,0.1078244669\C,2.4126375149,3.4055547967,-0.1706824197\C,
3.7208562534,2.889612496,0.0960894434\N,2.2512090012,4.830244247,-0.41
05885147\O,1.1327614848,5.2520206128,-0.6349584387\O,3.2502795244,5.52
14853766,-0.3722123225\C,-0.2436510879,-3.8500006065,1.1665576346\H,-3
.7434510845,-0.1360461194,0.9447157133\H,-2.8762028701,0.6146921828,-0
.413543014\H,-2.0827384077,0.4400797696,1.1738095927\H,-0.6051626674,-
3.197798619,-2.2350280695\H,-0.1591800559,-4.7263238172,-1.4546082627\
H,0.8934915283,-3.3068092473,-1.2902240807\H,-0.263050779,-4.940457431
1,1.0883867117\H,-0.7737575858,-3.5597672342,2.0765584917\H,0.79643171
34,-3.5250514469,1.2470788014\H,4.8640488029,1.1476590087,0.5267629106
\\Version=ES64L-G09RevD.01\State=1-A\HF=-1069.5573348\RMSD=8.949e-09\R
MSF=7.273e-06\Dipole=-3.0171488,-2.9807529,0.1146599\Quadrupole=9.9983
023,-13.7030667,3.7047645,-5.1537039,-0.9244864,4.2123527\PG=C01 [X(C1
9H18N2O3)]\\@

TS2-1
1\1\GINC-R2363\FTS\RM062X\6-31G(2df,p)\C19H18N2O3\ROOT\07-Nov-2014\0\\
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noei
gentest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS02.M062X\\0,1\C,
0.0422764626,-0.0732240086,-0.1030147949\C,0.004233462,-0.0618678219,1
.427214333\N,1.3071011046,-0.1535387065,1.8933241933\C,2.2218980675,-0
.0674481525,0.8496143399\C,1.5336530197,-0.0034383945,-0.364847467\C,2
.2245069455,0.0791538011,-1.5528009881\C,3.622064879,0.1053848844,-1.5
287457541\C,4.2937829503,0.0455875411,-0.3165968947\C,3.6063290286,-0.

0401148092,0.894926773\H,4.1484377067,-0.0737718763,1.831886768\H,5.37
76115451,0.0697149059,-0.3030694464\H,4.1790361464,0.1742978313,-2.454
9073697\H,1.6911668182,0.1242733998,-2.4977197735\C,-0.6959524224,1.12
37294358,-0.7080679615\C,-0.5258420637,-1.3915480694,-0.6540568637\C,1
.6283468572,-0.2718195602,3.2872245926\C,-1.0619151534,0.0180399568,2.
2312531688\H,-0.9167752069,0.0308947607,3.3087938915\C,-2.4650360815,0
.0836571051,1.8079564357\H,-2.9055306411,1.0803741024,1.7117216053\C,-
3.3134262337,-0.9482562146,1.5893542387\C,-2.9044727835,-2.3894737138,
1.7425036536\O,-1.7992872061,-2.7290223263,2.1069014738\C,-4.676427236
8,-0.6510623768,1.1987597866\H,-4.9974549621,0.3796849213,1.1007567893
\C,-3.9435479317,-3.3885568563,1.4264186286\C,-5.1836341066,-3.0413228
823,1.0528396453\H,-5.9460786358,-3.7745183569,0.8243637314\C,-5.54148
0819,-1.6443424249,0.9474835937\N,-6.9120573153,-1.3089804564,0.545635
0077\O,-7.6624174139,-2.2353857065,0.3234616492\O,-7.2081297505,-0.137
108391,0.4608273671\H,-0.5612571186,1.1341254214,-1.793628394\H,-0.315
7509529,2.0647626836,-0.3043754143\H,-1.7699045337,1.0626526184,-0.508
4580347\H,-0.3078025308,-1.4645219091,-1.7236683126\H,-1.6095449421,-1
.4307563654,-0.5205287009\H,-0.0837401297,-2.2502612401,-0.1447402332\
H,2.6791646833,-0.5382057966,3.3981900675\H,1.0215770503,-1.0641194435
,3.7380465012\H,1.4415937195,0.6633611543,3.8301191581\H,-3.6405942748
,-4.4242586637,1.5204490108\\Version=ES64L-G09RevD.01\State=1-A\HF=-10
69.5303191\RMSD=8.092e-09\RMSF=5.379e-06\Dipole=1.4026444,0.414178,0.4
488136\Quadrupole=-13.2694267,3.5735555,9.6958712,2.2419029,-0.6986948
,1.8967803\PG=C01 [X(C19H18N2O3)]\\@

TS3-1
1\1\GINC-R2428\FTS\RM062X\6-31G(2df,p)\C19H18N2O3\ROOT\07-Nov-2014\0\\
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noei
gentest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS03.M062X\\0,1\C,
-2.822813943,0.9059733182,0.0964182428\C,-1.5477016674,0.676987533,-0.
4301792994\C,-0.9140339821,-0.6183172143,-0.2652729116\C,-1.6775298657
,-1.615149639,0.4401266263\C,-2.8991070055,-1.346248672,0.9813259348\C
,-3.4731539788,-0.0718679512,0.8091853256\C,-0.9529053336,1.6706897177
,-1.2773810505\C,0.3241982199,1.7265482344,-1.7181033871\C,1.42290013,
0.9327521579,-1.2268149466\N,1.8696732098,0.9496999752,0.0195028382\C,
3.0218478698,0.1399648716,0.1495366641\C,3.4166679972,-0.279805219,-1.
1157536163\C,2.4726626848,0.3090127146,-2.132936964\C,4.5360772804,-1.
0730747938,-1.2558304059\C,5.2390938346,-1.4439498147,-0.1082912528\C,
4.8241914902,-1.0185515483,1.1479515252\C,3.6980745112,-0.2104149298,1
.3007164253\O,0.2322791821,-0.88248233,-0.7116067088\N,-4.7796491175,0
.2050586775,1.3719781806\O,-5.2540396464,1.3133478559,1.2028326221\O,-
5.3326646195,-0.687647211,1.9863560773\H,3.3670443232,0.1067313506,2.2
816763277\H,5.3792418806,-1.3230914883,2.0271685691\H,6.1146800179,-2.
0757155731,-0.1965739698\H,4.8593786149,-1.4110928042,-2.234723083\C,3
.1836060106,1.4430115741,-2.9047396587\C,1.8825077045,-0.7067776737,-3
.1114356117\H,0.5737280403,2.3909109457,-2.5396639168\H,-1.6382466434,
2.4129064469,-1.6829899247\H,-3.4531797692,-2.0914065323,1.5375837848\
H,-3.3129404374,1.8628838677,-0.0430141142\C,1.1650381486,1.4774869305
,1.1663344067\H,2.5076695003,1.9007979254,-3.6312341586\H,4.0315576845
,1.0206342892,-3.4487970138\H,3.5594901257,2.214463701,-2.2278404921\H
,1.1301007243,-0.2230806831,-3.7403207343\H,1.4089925104,-1.5240332633
,-2.571139271\H,2.6775775998,-1.0907252649,-3.7568985464\H,0.505063420
1,2.2793632668,0.8397201352\H,1.8925736455,1.8642282968,1.8815546436\H
,0.5675221555,0.6854320042,1.6287972313\H,-1.2161325068,-2.5893430488,
0.5476054772\\Version=ES64L-G09RevD.01\State=1-A\HF=-1069.5561295\RMSD
=7.531e-09\RMSF=7.751e-06\Dipole=4.0800826,0.8079249,-0.9480758\Quadru
pole=-17.4047265,7.4707912,9.9339353,-0.6204737,10.4376845,-1.9611707\
PG=C01 [X(C19H18N2O3)]\\@

TS4-1
1\1\GINC-R2434\FTS\RM062X\6-31G(2df,p)\C19H18N2O3\ROOT\07-Nov-2014\0\\
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noei
gentest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS04.M062X\\0,1\C,
1.0711869669,-2.9614962112,3.1094528544\C,0.104054387,-2.0340482484,2.
7564898962\C,-0.6759025846,-1.3954600408,3.7235057794\C,-0.5115400498,
-1.6923559555,5.057998786\C,0.44984453,-2.6348828308,5.4335928027\C,1.
2273996708,-3.2527155577,4.4654178947\C,-1.6100813062,-0.4176637229,3.
0464067466\C,-1.2559369858,-0.622574073,1.570179909\N,-0.2631286926,-1
.586510575,1.4882360888\C,-1.8201751411,0.0754283428,0.5796215826\C,-1
.5038186672,0.0834306402,-0.8536371687\C,-0.6293463615,0.8985398003,-1
.4887201789\C,-0.4793307002,0.7694957625,-2.9233534172\C,0.415001708,1
.5211975441,-3.5817684005\C,1.2621812401,2.4897207899,-2.9223665177\C,
1.1648974786,2.6720755105,-1.5974901026\C,0.2069590247,1.9191077267,-0
.7640292671\O,0.1103846659,2.131763153,0.4254592544\N,0.5493450837,1.3
579383532,-5.0335334788\O,1.3692229249,2.0553630168,-5.5919949309\O,-0
.1604761267,0.542730387,-5.5812294109\H,1.6991400229,-3.4447387537,2.3

713064989\H,1.9780206529,-3.9764636485,4.7623221604\H,0.5920284006,-2.
8773926884,6.4794263475\H,-1.1183412184,-1.1968168792,5.8098393134\C,-
3.078649344,-0.7557394778,3.3218647974\C,-1.2949638196,1.0236856017,3.
4677975149\H,-2.5692017509,0.8076888703,0.8743383538\H,-2.0676420929,-
0.5948591808,-1.5002426664\H,1.9588997312,3.0478242051,-3.5341341472\H
,-1.0867278047,0.0557434186,-3.4680602744\C,0.3373762859,-2.0450245011
,0.2644154555\H,-3.7385036297,-0.0757381863,2.7753917077\H,-3.29321382
99,-0.6558023904,4.3899444453\H,-3.3071421878,-1.7800315941,3.01846297
75\H,-1.9435476243,1.728608665,2.9404282232\H,-0.260681907,1.279286782
9,3.2295043176\H,-1.4523204311,1.1413776711,4.5440771069\H,-0.43304719
05,-2.2146486338,-0.4921051603\H,0.8365727555,-2.9978662535,0.44407309
84\H,1.0675714113,-1.3310290194,-0.1332967049\H,1.7784425056,3.3922621
804,-1.0700620865\\Version=ES64L-G09RevD.01\State=1-A\HF=-1069.527904\
RMSD=9.751e-09\RMSF=6.864e-06\Dipole=-0.3347581,-0.6335874,0.9786077\Q
uadrupole=8.4727738,6.402358,-14.8751318,-2.4975107,1.5352367,2.285967
5\PG=C01 [X(C19H18N2O3)]\\@

TS5-1
1\1\GINC-R2503\FTS\RM062X\6-31G(2df,p)\C19H18N2O3\ROOT\07-Nov-2014\0\\
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noei
gentest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS05.M062X\\0,1\C,
-5.3246508624,-0.3900831378,1.3733741931\C,-6.4044937068,-0.7914200474
,0.58730065\C,-6.2785023469,-0.9323095826,-0.7917438671\C,-5.068144437
8,-0.6764369802,-1.4324692554\C,-4.0199265101,-0.2800798126,-0.6269910
239\C,-4.1186455712,-0.131551351,0.7508089124\H,-5.4325588914,-0.28352
05331,2.4472237982\H,-7.3587574003,-0.9975277564,1.0569305587\H,-7.133
2980081,-1.2456105963,-1.378507724\H,-4.9634386435,-0.7843990803,-2.50
5080801064\C,-2.779978165,0.3068408157,1.2811944631\C,-2.1505100298,-0.7
249911125,2.2331659764\C,-2.8155314996,1.6960640479,1.9407667287\N,-2.
6876617401,0.0421932546,-1.013413667\C,-2.2452704426,-0.0022863086,-2.
3992169106\C,-1.9525952295,0.3810921006,0.0143489116\C,-0.5804352531,0
.8174320912,-0.0654897709\C,0.473110845,-0.0243386493,0.0592794948\C,1
.8549275862,0.3388307019,0.0027321861\H,0.2733679907,-1.0876173017,0.2
104842422\H,-0.3762219324,1.8806910973,-0.2080749086\O,1.4313970019,2.
653626676,-0.347416184\C,2.2520193808,1.730267642,-0.2100693706\C,2.81
46726187,-0.6624890396,0.1471681477\H,2.5188395898,-1.6944598293,0.303
5320036\C,4.1570914842,-0.3649704182,0.0947255057\N,5.1243593331,-1.42
07917628,0.2462968831\O,4.7186462089,-2.5596542819,0.4192617546\O,6.30
66230905,-1.1271667502,0.1941103787\C,4.5930811664,0.9650947514,-0.107
9831413\C,3.6833193743,1.964073433,-0.2536740254\H,5.6586380289,1.1539
167666,-0.1425498333\H,-2.1103501018,-1.7166221806,1.7756565754\H,-2.7
563549022,-0.7878527714,3.1401232467\H,-1.1384372205,-0.4145576059,2.5
008203272\H,-3.2575797121,2.4405697519,1.2747139474\H,-1.8008569933,2.
0082255949,2.197564864\H,-2.8493483747,0.691353681,-2.9872283843\H,-2.
377466776,-1.0160086969,-2.7820882004\H,-1.1950236552,0.2823345496,-2.
4301835771\H,-3.4160205135,1.6448112104,2.8519881564\H,3.9945052204,2.
9903274207,-0.4103519553\\Version=ES64L-G09RevD.01\State=1-A\HF=-1069.
5272563\RMSD=5.572e-09\RMSF=3.747e-06\Dipole=-7.600981,-0.3751951,-0.3
865026\Quadrupole=-10.8574848,-7.0128543,17.8703392,12.4162754,1.04214
75,3.3232648\PG=C01 [X(C19H18N2O3)]\\@

SP-2

MC-2 with HB
1\1\GINC-R96\FOpt\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\03-Oct-2014\0\\#
 M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxd
isk=3221225472\\MC-OH-TTC.M062X\\0,1\C,-1.200507197,0.9853502519,-0.99
67163012\N,-0.2381450255,1.9511449637,-0.5111173432\C,1.0424205596,1.6
35595904,-0.2058821973\C,1.5171372966,0.3480403165,-0.3427761415\C,2.8
258772264,-0.045454548,-0.045464142\C,3.3724487553,-1.3167263987,-0.15
78013148\C,2.5994081504,-2.4651784331,-0.6283097447\O,1.4126656532,-2.
4483563773,-0.9704974749\C,4.7432870936,-1.5074978767,0.2008881693\C,5
.3104811107,-2.7312518848,0.1047801956\C,4.6032394375,-3.8892031047,-0
.3485965063\C,3.3055736985,-3.7576706364,-0.6985926011\N,6.7131303568,
-2.8840201959,0.4808383488\O,7.3144134902,-1.9003356572,0.8661380997\O
,7.19960894,-3.9924698978,0.3858646594\C,1.758785896,2.8988596825,0.27
21364417\C,0.6531764981,3.926610863,0.1690073659\C,-0.5056276377,3.313
5747036,-0.2990551408\C,2.9197800731,3.2825861806,-0.6604623973\C,2.22
2211786,2.7724149883,1.7330276982\C,0.6558878134,5.2751486982,0.457005
8256\C,-0.5186741179,6.005573864,0.2703780195\C,-1.6669246911,5.379347
843,-0.19757719\C,-1.6817459107,4.0168543421,-0.4920594164\H,-0.855099
2629,0.5443345306,-1.9355189731\H,-1.3359763541,0.1843158709,-0.265227
3396\H,0.8482735081,-0.4201371151,-0.7020739292\H,3.5150680854,0.71281
223,0.3174415847\H,5.337368067,-0.6730225642,0.5522124829\H,5.11130499
69,-4.8414359878,-0.4039388777\O,2.5522439523,-4.7760963368,-1.1355861

064\H,2.5749103497,3.3611304378,-1.6938894745\H,3.7305117133,2.5535786
323,-0.6224220415\H,3.3181464168,4.2546777755,-0.3576198226\H,1.387651
5719,2.4927277575,2.3798368961\H,2.6099296695,3.7368215441,2.072094827
2\H,3.0109131332,2.0273192887,1.8468886765\H,1.5543408977,5.7622147009
,0.8224585245\H,-0.5354182891,7.0656793522,0.4912586461\H,-2.572780795
2,5.9570886867,-0.3385502511\H,-2.5854403268,3.5450177112,-0.856095159
7\H,-2.1541830529,1.4806852835,-1.1643428434\H,1.6812964637,-4.3775593
891,-1.3042337317\\Version=ES64L-G09RevD.01\State=1-A\HF=-1144.7754741
\RMSD=8.088e-09\RMSF=1.816e-05\Dipole=-3.2875188,3.802697,-0.1453617\Q
uadrupole=-4.3150312,-0.5445188,4.85955,9.4690967,-0.6051138,1.63851\P
G=C01 [X(C19H18N2O4)]\\@

SP-2 with HB
1\1\GINC-R110\FOpt\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\10-Oct-2014\0\\
# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) max
disk=3221225472\\SP-OH.M062X.M062X\\0,1\C,0.0508773255,-1.8120346933,-
1.4968510911\N,-1.3271584081,-1.9648877758,-1.0841618647\C,-2.10651009
81,-0.7833100718,-0.8197595158\C,-2.2858867281,0.0704780072,-2.0432642
336\C,-2.2003311358,1.3989316706,-2.0118070889\C,-1.8792265291,2.09117
31963,-0.7688494478\C,-1.4988041972,1.2920283278,0.305059257\O,-1.3966
541259,-0.051890133,0.2169959787\C,-1.9191802523,3.4728594117,-0.60643
46399\C,-1.5847284852,3.9991722709,0.6265793088\C,-1.2113881,3.2161796
224,1.711710166\C,-1.167645345,1.843430935,1.5484589557\N,-1.629376310
1,5.4563043024,0.8039810156\O,-1.9621081606,6.1266500436,-0.1502216676
\O,-1.3310588586,5.8984591204,1.8921132635\C,-3.4298116996,-1.35359777
22,-0.2040084329\C,-2.8947908411,-2.6027705955,0.4623667783\C,-1.66147
85405,-2.9177798726,-0.1145547375\C,-4.101349824,-0.3694588666,0.74824
49503\C,-4.4053981832,-1.7565361764,-1.3203781354\C,-3.4371547795,-3.4
114243454,1.435810992\C,-2.7320982992,-4.5490408602,1.8419648828\C,-1.
5067125898,-4.8499081782,1.2664368267\C,-0.947095623,-4.0355740598,0.2
790576757\H,0.3908341395,-2.7273935482,-1.9868095721\H,0.1185454444,-0
.9937205997,-2.2167191038\H,-2.5191063125,-0.4671181871,-2.9547435796\
H,-2.3629836042,1.9926063187,-2.9050993468\H,-2.2039651623,4.131637097
4,-1.4155965224\H,-0.9699181617,3.6697353547,2.6626366982\O,-0.8275386
295,1.0375266503,2.5742583734\H,-3.4679592081,-0.1449353496,1.60879907
98\H,-5.0381630233,-0.7957875175,1.1173862117\H,-4.3426786711,0.566071
9167,0.2326892759\H,-5.2506444549,-2.2928419335,-0.8824228582\H,-3.920
9381353,-2.4173961902,-2.0440427018\H,-4.789135497,-0.875747954,-1.843
6070105\H,-4.3935706964,-3.1671486474,1.8876941406\H,-3.1410044623,-5.
1921594177,2.6115771541\H,-0.9635442106,-5.7295214754,1.5929861751\H,0
.0177644732,-4.2718351425,-0.1533931317\H,0.7168074546,-1.5926585254,-
0.6522929899\H,-0.8611314946,0.1268636429,2.2545305119\\Version=ES64L-
G09RevD.01\State=1-A\HF=-1144.7975173\RMSD=8.071e-09\RMSF=8.086e-06\Di
pole=-0.1896779,-2.228498,-1.0447373\Quadrupole=10.0927664,-18.5868578
,8.4940914,-3.4504103,-2.4478294,-6.1014062\PG=C01 [X(C19H18N2O4)]\\@

CCC-2 with HB
1\1\GINC-R185\FOpt\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\10-Oct-2014\0\\
# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) max
disk=3221225472\\CCC-OH-2.M062X\\0,1\C,-0.6548666609,0.9258910073,-2.6
948658733\C,-0.6533378696,0.8080778414,-1.2772041765\C,0.5999099477,0.
9468300069,-0.5642096782\C,1.8027824752,1.1642713742,-1.3748064457\C,1
.7690365824,1.2174661538,-2.7281698166\C,0.508483562,1.0983821291,-3.3
747095086\C,-1.9028026483,0.7260886553,-0.6205950876\C,-2.2226170451,0
.4549679216,0.6924977282\C,-1.4433998722,-0.1682926666,1.6806584413\N,
-0.5992440653,-1.1760730683,1.502832499\C,0.0547371109,-1.5128385776,2
.7085231417\C,-0.4633729766,-0.7289659822,3.7326384035\C,-1.4952409235
,0.2048131982,3.1536887556\C,-0.0064202445,-0.8983299712,5.0234113636\
C,0.9834011107,-1.8526200904,5.2618732467\C,1.4968620763,-2.6183140974
,4.2212498677\C,1.0369198217,-2.4621128526,2.914872333\O,0.7521660303,
0.9156508716,0.6744422195\N,0.4651823455,1.1809284109,-4.8301572982\O,
-0.6154179866,1.0843667852,-5.3791577421\O,1.5183339694,1.3412274941,-
5.414013389\H,1.4491763613,-3.0487525895,2.1035395688\H,2.2715888719,-
3.3478512121,4.4247034148\H,1.3614075652,-1.9942339115,6.2671124491\H,
-0.4008841295,-0.2978793359,5.8365086348\C,-2.8883282955,-0.0507157912
,3.7487842762\C,-1.0889545784,1.6784140349,3.3142041832\H,-3.189337015
6,0.8070309334,1.0416048478\H,-2.7491576095,1.0171314841,-1.2427630072
\O,2.9358012265,1.2857312439,-0.6648580998\H,2.666441195,1.3641852658,
-3.3122079572\H,-1.5835332189,0.8620283155,-3.2480631333\C,-0.37484626
69,-1.9037094439,0.2755574677\H,-3.6337807836,0.603056368,3.2890976643
\H,-2.867455124,0.1636248546,4.8204057187\H,-3.1942278307,-1.090422329
3,3.6113972284\H,-1.8401724253,2.3248528256,2.8528161108\H,-0.13012662
62,1.8604106241,2.8266800627\H,-1.0174921675,1.9248226134,4.3770585654
\H,2.6394517002,1.2286381315,0.2602478573\H,-1.2543924347,-1.802220133
3,-0.3589100886\H,-0.2186137492,-2.9547358719,0.5237673124\H,0.4959805
962,-1.5130856195,-0.2580490602\\Version=ES64L-G09RevD.01\State=1-A\HF

=-1144.7726478\RMSD=6.660e-09\RMSF=7.559e-06\Dipole=-1.5275422,-1.6386
637,4.0079556\Quadrupole=6.6656226,8.969932,-15.6355546,-6.1408504,3.4
650811,5.0317154\PG=C01 [X(C19H18N2O4)]\\@

CTC-2 with HB
1\1\GINC-R480\FOpt\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\10-Oct-2014\0\\
# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) max
disk=3221225472\\CTC-OH-2.M062X\\0,1\C,-2.3671678713,-3.6085089012,-0.
1562514621\C,-3.1326608993,-2.4525804768,-0.0366093402\C,-2.9850960755
,-4.8319369727,-0.307908011\C,-4.3797520107,-4.88080101,-0.3471551607\
C,-5.1281446928,-3.7159145525,-0.2370525878\C,-4.5149353602,-2.4730719
219,-0.0811638705\H,-2.3991101082,-5.7408803629,-0.3974637549\H,-4.882
0506033,-5.8325160173,-0.4695901014\H,-6.2097154317,-3.7676400815,-0.2
774298552\H,-5.1080346318,-1.5695919783,-0.0146484579\N,-2.2751896113,
-1.3447468452,0.1239203551\C,-2.7736684608,-0.0309724184,0.4664231155\
C,-0.9078409101,-3.2382897549,-0.0790714219\C,-0.1482653831,-3.6375257
098,-1.3512624727\C,-0.9769063492,-1.7185442074,0.0570763914\C,0.16591
72826,-0.9483389135,0.1109776542\C,0.2703304167,0.4405602616,-0.029727
3741\H,-0.6291409557,1.0055966196,-0.2595426047\H,1.0951664533,-1.4937
952977,0.2034366807\C,1.4270441712,1.2080209458,0.0232602371\C,1.32642
47754,2.6144418283,-0.2123047962\H,0.3657483386,3.0653926693,-0.427808
2515\C,2.7401536165,0.6333160036,0.3110191567\O,2.9754008163,-0.557886
1455,0.5351092355\C,3.8831553357,1.5653124226,0.3348642117\O,5.0617687
23,0.986764073,0.6012962825\H,4.5824941323,3.5630680062,0.1281936068\C
,2.4294115703,3.3956994256,-0.1680791504\C,3.7384702854,2.888507029,0.
1070059042\N,2.2820158718,4.8276424468,-0.4118542388\O,1.1692219359,5.
2590326375,-0.6436132029\O,3.2864973672,5.5082925481,-0.3680833468\C,-
0.2402869414,-3.8518062563,1.1629499019\H,-3.7466025805,-0.1413235124,
0.9463723612\H,-2.8823234912,0.6092917753,-0.4139203512\H,-2.087140861
3,0.4387439436,1.1731441652\H,-0.6098373273,-3.1965288318,-2.237551203
6\H,-0.1609286504,-4.725433713,-1.4597813019\H,0.8912185579,-3.3056309
674,-1.2969673612\H,-0.2588318993,-4.9421387262,1.0836549355\H,-0.7688
094881,-3.5630643383,2.0743052919\H,0.7998425792,-3.5266176483,1.24207
84493\H,4.8477683652,0.0451819252,0.7185037431\\Version=ES64L-G09RevD.
01\State=1-A\HF=-1144.7720117\RMSD=7.621e-09\RMSF=3.476e-06\Dipole=-3.
4743797,-3.501779,0.1308771\Quadrupole=7.4216176,-12.3952689,4.9736514
,-8.5210006,-1.0420153,3.7338083\PG=C01 [X(C19H18N2O4)]\\@

TS2-2 with HB
1\1\GINC-R675\FTS\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\10-Oct-2014\0\\#
 M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeig
entest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS2-OH-2.M062X\\0,1
\C,-1.8119002587,-0.8953882359,-0.1805078843\C,-1.6393588209,0.1773970
833,0.8977835068\N,-2.8371871935,0.8637667494,1.0212686746\C,-3.838333
9211,0.2694750389,0.2591881061\C,-3.2961058696,-0.7918803717,-0.469748
3046\C,-4.091640162,-1.5361189673,-1.3117404055\C,-5.4491412139,-1.221
4053114,-1.4220463511\C,-5.9766340152,-0.1681091828,-0.6895956754\C,-5
.1813869802,0.5958359039,0.1656862422\H,-5.6141956827,1.4072290203,0.7
37686359\H,-7.0308421395,0.0696163153,-0.7761165568\H,-6.0883001854,-1
.8007253603,-2.0766826218\H,-3.6712442511,-2.3587641667,-1.8825303452\
C,-1.4273908756,-2.2888572915,0.323780687\C,-1.0063608023,-0.537941082
8,-1.4404820736\C,-3.0013810841,1.9911609829,1.8944051182\C,-0.5520224
392,0.4544205733,1.6273975132\H,-0.5979822029,1.2440381065,2.373562171
4\C,0.7488532606,-0.2180381733,1.5344600832\H,0.9231495896,-1.05596025
64,2.2154369275\C,1.8030455064,0.1184629032,0.7546958347\C,1.761114185
3,1.2741539914,-0.1842590968\O,0.8111248813,2.0191857867,-0.3442233579
\C,3.0279051432,-0.6550443584,0.8333772541\H,3.0944385036,-1.496685725
7,1.5108341915\C,2.9864593663,1.5360977052,-0.985194848\O,2.8917948548
,2.5790982054,-1.8124853409\C,4.0872897126,0.7713145269,-0.8708389724\
H,4.9757229974,0.9628373008,-1.4552571181\C,4.0740023103,-0.3283655893
,0.0608703218\N,5.2978143445,-1.1403853668,0.1647467872\O,6.2300006489
,-0.8242208554,-0.5418351231\O,5.2984738773,-2.0682118153,0.9441447566
\H,-1.6635020642,-3.0377619298,-0.4377224478\H,-1.9726671702,-2.541009
139,1.2359759343\H,-0.3538961746,-2.3501423404,0.5256525172\H,-1.28893
98042,-1.2082881953,-2.2574397591\H,0.0651535729,-0.6506035269,-1.2587
214157\H,-1.200868725,0.4915809285,-1.7481427116\H,-3.9546049129,2.476
9441873,1.6882325109\H,-2.1993537195,2.7153240923,1.7169118865\H,-2.97
64459611,1.6951501086,2.9507536372\H,1.9971198748,2.9342877324,-1.6785
176119\\Version=ES64L-G09RevD.01\State=1-A\HF=-1144.7450959\RMSD=5.858
e-09\RMSF=1.969e-06\Dipole=-2.1229963,0.4097354,0.6844091\Quadrupole=-
13.8553183,5.6267492,8.2285691,3.0352295,-0.0221308,5.0912355\PG=C01 [
X(C19H18N2O4)]\\@

TS3-2 with HB
1\1\GINC-R159\FTS\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\10-Oct-2014\0\\#
 M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeig

```
 entest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS3-OH-2.M062X\\0,1
 \C,-2.8278929517,0.9065353724,0.1017284057\C,-1.5490447245,0.704028994
 4,-0.446248354\C,-0.9026462598,-0.5569399096,-0.2953104418\C,-1.614215
 789,-1.5910969229,0.4155550648\C,-2.8373780943,-1.3653051521,0.9753035
 309\C,-3.433043604,-0.0991327037,0.8066969448\C,-0.9594934759,1.700848
 9254,-1.2988902683\C,0.3184143415,1.7417113167,-1.7279287776\C,1.39720
 52191,0.9141854485,-1.2263416692\N,1.8666297898,0.9741156788,0.0134156
 583\C,3.0049670987,0.1463879018,0.152732255\C,3.3810321079,-0.31176162
 93,-1.1054703507\C,2.4485475136,0.2849792633,-2.1294461\C,4.4797435696
 ,-1.1351064431,-1.2344042146\C,5.181075618,-1.497352624,-0.0826569918\
 C,4.7859972327,-1.0326178066,1.165827827\C,3.6809692387,-0.1933843099,
 1.3070464187\O,0.2509664089,-0.8507214645,-0.755014062\N,-4.744575564,
 0.139772273,1.3914526895\O,-5.249453143,1.2355962587,1.2362221121\O,-5
 .2635911115,-0.7714850781,2.0053865545\H,3.3646504477,0.1544847017,2.2
 825000757\H,5.3393355799,-1.3307551754,2.0482896323\H,6.03973922,-2.15
 30481111,-0.1619392059\H,4.7883962871,-1.5027206544,-2.2073157651\C,3.
 1776653746,1.428793667,-2.8727504506\C,1.8732599174,-0.7074716042,-3.1
 370770929\H,0.5960809091,2.4168203541,-2.5310092168\H,-1.6414266192,2.
 4459766869,-1.7033893817\O,-0.9853702625,-2.7790913415,0.5189066066\H,
 -3.3495974297,-2.1380395125,1.5314179843\H,-3.3422967003,1.8513366586,
 -0.0208816314\C,1.1801559901,1.5350831113,1.1563192395\H,2.5186032495,
 1.8951783801,-3.6092235558\H,4.0372276504,1.011031962,-3.4016411783\H,
 3.5389557597,2.1921238453,-2.1789348554\H,1.1220375723,-0.2134487097,-
 3.7593072828\H,1.4012368987,-1.5437208484,-2.626247144\H,2.6747592247,
 -1.0692636972,-3.7872610787\H,0.5077814694,2.3212891541,0.8176474348\H
 ,1.9184959028,1.9503338164,1.8441766686\H,0.5982381852,0.7555405868,1.
 658488998\H,-0.1484790475,-2.6550506593,0.0449779683\\Version=ES64L-G0
 9RevD.01\State=1-A\HF=-1144.7675814\RMSD=7.652e-09\RMSF=2.068e-06\Dipo
 le=4.3510367,1.1873749,-1.2182229\Quadrupole=-15.5989377,5.5971151,10.
 0018227,-2.5103113,10.6085516,-0.1396119\PG=C01 [X(C19H18N2O4)]\\@

TS4-2 with HB
 1\1\GINC-R195\FTS\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\10-Oct-2014\0\\#
  M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeig
 entest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS4-OH-2.M062X\\0,1
 \C,1.0662584609,-2.9652134414,3.1042961052\C,0.0991938394,-2.036195122
 7,2.7558620306\C,-0.6693090077,-1.3889466439,3.7257954494\C,-0.4933068
 581,-1.6783504067,5.0605802156\C,0.4686359151,-2.6218694048,5.43219935
 77\C,1.2345554033,-3.2487143494,4.460404572\C,-1.608368126,-0.41440389
 57,3.0506834466\C,-1.2592738045,-0.6207849156,1.573086634\N,-0.2768881
 595,-1.593996043,1.4877735512\C,-1.8213397471,0.0813774618,0.583246735
 5\C,-1.5075218442,0.0780552965,-0.850826435\C,-0.6331493086,0.88746803
 1,-1.4935714777\C,-0.4643472989,0.7659928308,-2.9289321361\C,0.4329323
 899,1.5350289568,-3.5627272864\C,1.2677901692,2.5154918466,-2.91558427
 97\C,1.1512559174,2.6882596972,-1.5864908552\C,0.1888517614,1.89815543
 32,-0.7722376048\O,0.133209395,2.1333130612,0.4213908516\N,0.583623500
 8,1.3740178272,-5.0185492371\O,1.399204422,2.0807415756,-5.5693605413\
 O,-0.1111293684,0.5503219731,-5.5729605938\H,1.6854357866,-3.454221446
 8,2.3625357539\H,1.9855972068,-3.9730543113,4.7546598122\H,0.620396450
 8,-2.8583406397,6.4780613077\H,-1.0913536397,-1.1768284792,5.815441182
 \C,-3.0749063261,-0.7605889412,3.3290003883\C,-1.3008825078,1.02785728
 82,3.4728461388\H,-2.5653457508,0.8185972554,0.8780444806\H,-2.0692649
 564,-0.6051145374,-1.493640874\O,1.8692215633,3.5703982099,-0.88861490
 42\H,1.9645001954,3.0939018045,-3.5051353394\H,-1.0551173476,0.0497696
 44,-3.4854620739\C,0.3005964978,-2.0777520335,0.2619611973\H,-3.739727
 2288,-0.0842815411,2.7839732183\H,-3.2872501931,-0.6627389326,4.397664
 8744\H,-3.2979723784,-1.7860641618,3.0255864538\H,-1.9526270294,1.7305
 962041,2.9463765951\H,-0.266711477,1.2873639661,3.2380493037\H,-1.4600
 980811,1.1443159258,4.5489274077\H,1.5662403932,3.4804289247,0.0305251
 877\H,-0.4804239033,-2.2275154143,-0.4873834112\H,0.769944738,-3.04533
 9837,0.4440370718\H,1.0506673357,-1.3907447144,-0.1460822728\\Version=
 ES64L-G09RevD.01\State=1-A\HF=-1144.742783\RMSD=7.073e-09\RMSF=1.303e-
 06\Dipole=-0.6857501,-0.9005621,1.5836836\Quadrupole=7.9067948,6.19064
 64,-14.0974412,-5.1755838,3.5873035,5.3434547\PG=C01 [X(C19H18N2O4)]\\
 @

TS5-2 with HB
 1\1\GINC-R165\FTS\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\10-Oct-2014\0\\#
  M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeig
 entest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS5-OH-2.M062X\\0,1
 \C,-5.3155543462,-0.4123534692,1.374823515\C,-6.3899635244,-0.82816210
 95,0.5889566476\C,-6.26378631,-0.9637341712,-0.7907247986\C,-5.0584857
 641,-0.6878337803,-1.4324326792\C,-4.0155704196,-0.2776291681,-0.62693
 91258\C,-4.1144423149,-0.1338360095,0.7511913055\H,-5.4236778868,-0.31
 0568765,2.4490830812\H,-7.3403035203,-1.0502731205,1.0592500518\H,-7.1
 144265803,-1.2890152096,-1.3769974821\H,-4.9535292966,-0.791879783,-2.
```

5053850374\C,-2.7815351302,0.3222608635,1.2807899107\C,-2.1380359003,-
0.7014605359,2.2322791231\C,-2.8357329106,1.7105818623,1.9414374056\N,
-2.6880126134,0.0648641831,-1.014016048\C,-2.2468734533,0.0267745242,-
2.4007169605\C,-1.9568978251,0.4104962635,0.0132279924\C,-0.5844208887
,0.8550788841,-0.0674257524\C,0.4618465242,0.0029938495,0.0583242475\C
,1.8478933541,0.3430329098,0.00322075\H,0.2473346346,-1.0573251004,0.2
093285208\H,-0.3920314795,1.9175951195,-0.210445327\O,1.4920219355,2.6
863616518,-0.352678947\C,2.2579836075,1.7043509602,-0.206771501\C,2.81
15136037,-0.6712362938,0.1484990538\H,2.5140571889,-1.701116045,0.3060
494447\C,4.144442002,-0.3684323649,0.092716969\N,5.1113681386,-1.43389
77733,0.2451423019\O,4.7013495817,-2.5701006445,0.4186053176\O,6.29262
39133,-1.1432787092,0.1921017866\C,4.6086842743,0.9569264009,-0.111304
455\C,3.6944413014,1.9506664971,-0.2553524801\O,4.0298520552,3.2396327
762,-0.4546170239\H,5.6703147159,1.1569563735,-0.1498070973\H,-2.08477
82387,-1.6922932357,1.774441299\H,-2.7434701009,-0.7726802919,3.138880
1653\H,-1.130344363,-0.3779490985,2.5007402653\H,-3.2887591386,2.44955
21568,1.2765595207\H,-1.8254157029,2.0361508144,2.1987679242\H,-2.8606
353104,0.7130273314,-2.9872560477\H,-2.3676044972,-0.9884514212,-2.783
3041496\H,-1.2001026039,0.3234880078,-2.4332778987\H,-3.4349203877,1.6
501537082,2.8528998624\H,3.1662546768,3.6858569627,-0.5149806504\\Vers
ion=ES64L-G09RevD.01\State=1-A\HF=-1144.7417794\RMSD=4.266e-09\RMSF=3.
610e-06\Dipole=-8.2412654,-0.4903584,-0.3652365\Quadrupole=-11.6909296
,-6.5636622,18.2545918,10.017111,1.6619779,3.4286271\PG=C01 [X(C19H18N
2O4)]\\@

MC-2 no HB
1\1\GINC-R93\FOpt\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\03-Oct-2014\0\\#
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxd
isk=3221225472\\MC-OH-TTC2.M062X\\0,1\C,-1.208136341,0.9973962006,-0.9
947505697\N,-0.2431257728,1.9600452716,-0.5092729453\C,1.0389559268,1.
638583333,-0.2062025668\C,1.5070163471,0.3511133484,-0.3461163261\C,2.
8166040678,-0.0501934162,-0.0512569553\C,3.362521159,-1.3198166821,-0.
1645132251\C,2.5746292745,-2.4749751944,-0.6410071946\O,1.3997654723,-
2.4214041957,-0.9715669796\C,4.7326672896,-1.4952632646,0.1963635481\C
,5.3120591533,-2.7124264373,0.1040638059\C,4.6036783034,-3.8708146449,
-0.3501839858\C,3.3053620988,-3.7640033472,-0.7048515486\N,6.710371671
7,-2.8636134279,0.4783035465\O,7.3125958947,-1.8808206601,0.8640515309
\O,7.1983649283,-3.9734963133,0.3824203101\C,1.7594790455,2.8994989148
,0.2727009529\C,0.6566647852,3.9308843999,0.1730031827\C,-0.5049129698
,3.3216476235,-0.2945091368\C,2.9201159989,3.2816882803,-0.660712185\C
,2.2250677407,2.7697783368,1.7324422679\C,0.6642032732,5.2787156159,0.
4632786124\C,-0.5080352207,6.0140435924,0.2799715266\C,-1.6588020779,5
.3922499053,-0.1872395583\C,-1.6786497625,4.0302689989,-0.4841083121\H
,-0.8652090819,0.5561729925,-1.9344466853\H,-1.3442002474,0.1949758512
,-0.2647897206\H,0.8356059517,-0.4143396347,-0.7055329154\H,3.50725690
24,0.7067741731,0.311895044\H,5.3184871226,-0.6541615527,0.5469205948\
H,5.1362204707,-4.8131027593,-0.3972720341\O,2.5432423537,-4.785261275
7,-1.1453850776\H,2.5735452199,3.3633129148,-1.693331981\H,3.728149305
,2.549475311,-0.6258024321\H,3.3226149637,4.2518433842,-0.3568060559\H
,1.3904831108,2.4920756288,2.3800765428\H,2.6171077134,3.7321438775,2.
0726218775\H,3.0108637443,2.0211567705,1.8436884351\H,1.5650703772,5.7
618692449,0.8281546556\H,-0.5207022377,7.0738038943,0.502783355\H,-2.5
630928501,5.9731116545,-0.3258507107\H,-2.5845043587,3.562120504,-0.84
75501379\H,-2.1610767989,1.4950383049,-1.1602992957\H,3.075558053,-5.5
859255218,-1.1622212529\\Version=ES64L-G09RevD.01\State=1-A\HF=-1144.7
63001\RMSD=7.916e-09\RMSF=1.166e-05\Dipole=-2.5610243,2.7909737,-0.146
1459\Quadrupole=-10.4200185,10.409456,0.0105625,2.5036503,-2.5382651,2
.9281111\PG=C01 [X(C19H18N2O4)]\\@

SP-2 no HB
1\1\GINC-R107\FOpt\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\10-Oct-2014\0\\
# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) max
disk=3221225472\\SP-OH-2.M062X.M062X\\0,1\C,0.0695662425,-1.761590622,
-1.4444258292\N,-1.3135353764,-1.9402171025,-1.0600414224\C,-2.1084460
175,-0.7695177927,-0.7852386289\C,-2.3025752437,0.0780410355,-2.009645
6056\C,-2.214500706,1.405339261,-1.9810109361\C,-1.8749202545,2.098205
5484,-0.7441029444\C,-1.4876512624,1.2995016739,0.3331789591\O,-1.4125
96237,-0.0365382804,0.2538810207\C,-1.896826884,3.483820608,-0.6115784
28\C,-1.5358047844,4.0345690999,0.5997546581\C,-1.1500597331,3.2599751
014,1.6878140356\C,-1.1230249943,1.8838962531,1.5582307622\N,-1.558166
9674,5.4910161991,0.7558977956\O,-1.9004544085,6.1530613358,-0.2001967
084\O,-1.2323601961,5.9449334828,1.8330299838\C,-3.4270778718,-1.36065
45734,-0.1738916903\C,-2.890753644,-2.6277356997,0.455249535\C,-1.6515
364282,-2.9194057959,-0.1194138857\C,-4.0822425799,-0.4003405442,0.813
66964\C,-4.415559469,-1.7331851862,-1.2889619297\C,-3.4398473622,-3.46

97093849,1.3958494083\C,-2.7353934643,-4.6177267261,1.772008226\C,-1.5
027675611,-4.8948427756,1.2000613079\C,-0.9369830511,-4.0469312974,0.2
454454749\H,0.4305658517,-2.6626716787,-1.9459304576\H,0.1387123671,-0
.9291990547,-2.1481970606\H,-2.5434724193,-0.4612671457,-2.9180099933\
H,-2.3837457783,2.0000079804,-2.8724940965\H,-2.1871518782,4.125735089
2,-1.4325910101\H,-0.8866783524,3.7475501765,2.618388564\O,-0.77723920
16,1.0388319471,2.5547945229\H,-3.4286235514,-0.2035450838,1.665450145
6\H,-5.0153117617,-0.8333827524,1.1848953174\H,-4.3287370866,0.5484947
942,0.3245471197\H,-5.2576617099,-2.2777416647,-0.8548482374\H,-3.9415
826685,-2.3788885758,-2.0332459878\H,-4.8025357148,-0.8395577259,-1.78
76829781\H,-4.4015181684,-3.2430164188,1.8459323495\H,-3.1500274063,-5
.2872071089,2.5157476782\H,-0.9591517339,-5.7825232286,1.503499981\H,0
.0336053751,-4.2648856961,-0.1837696927\H,0.7148913624,-1.5487411543,-
0.5827501367\H,-0.5531192708,1.5481834828,3.3384611742\\Version=ES64L-
G09RevD.01\State=1-A\HF=-1144.790668\RMSD=5.733e-09\RMSF=6.299e-06\Dip
ole=0.0172921,-1.4342664,-0.2968219\Quadrupole=8.4572462,-21.5392171,1
3.0819709,-1.6700464,0.2091218,-1.1577077\PG=C01 [X(C19H18N2O4)]\\@

CCC-2 no HB
1\1\GINC-R452\FOpt\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\09-Oct-2014\0\\
# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) max
disk=3221225472\\CCC-OH.M062X\\0,1\C,-0.6849961372,0.9180444845,-2.706
7599907\C,-0.6592680338,0.7870170434,-1.293541125\C,0.6035013571,0.934
726371,-0.5692513602\C,1.7945024456,1.1602206109,-1.4077958034\C,1.728
4497352,1.2220505735,-2.75933618\C,0.4652157184,1.1062352288,-3.403484
7211\C,-1.9018202524,0.6919289948,-0.6289887507\C,-2.2172810955,0.4286
298605,0.6884427153\C,-1.4394073974,-0.1832568827,1.6830878934\N,-0.59
34679536,-1.1930626262,1.5185101012\C,0.0471311046,-1.5263409622,2.731
1813733\C,-0.4791510468,-0.7373334806,3.7472764125\C,-1.496571352,0.20
24196281,3.1530406728\C,-0.0380978471,-0.9046911534,5.0436320869\C,0.9
441025946,-1.8630524143,5.297010983\C,1.4665165218,-2.6335324551,4.264
5625663\C,1.0230920345,-2.4787197727,2.9523802272\O,0.7167733858,0.896
8474871,0.6584788308\N,0.413371091,1.2069875463,-4.8515506297\O,-0.668
751212,1.1103786486,-5.3978667121\O,1.4639234284,1.3825226853,-5.44035
35463\H,1.4434675007,-3.0680288492,2.1472406141\H,2.2358785621,-3.3656
32236,4.479134818\H,1.3093991992,-2.0035391635,6.3071203392\H,-0.43908
64285,-0.2993205658,5.8498983391\C,-2.8954572538,-0.0232598838,3.74446
78457\C,-1.0653835127,1.6712639956,3.2988467162\H,-3.1862554206,0.7785
140807,1.0337520878\H,-2.755024942,0.9680893013,-1.2487483619\O,2.9395
993665,1.2721610701,-0.6973484785\H,2.6101987326,1.3735118674,-3.37060
88887\H,-1.6220040922,0.853521087,-3.2464390378\C,-0.3572916376,-1.923
2214189,0.295390178\H,-3.6276241205,0.6394289335,3.2762079158\H,-2.875
4582189,0.2004172236,4.8142676651\H,-3.2194028756,-1.0585900868,3.6152
034874\H,-1.8014494687,2.3239029741,2.821921549\H,-0.0990639926,1.8298
660989,2.8177081554\H,-0.999582284,1.9290971958,4.3594815881\H,3.66487
40034,1.4337373006,-1.3073555347\H,-1.2292825203,-1.8192387594,-0.3490
034937\H,-0.2081865105,-2.9748448491,0.5462267672\H,0.5217188249,-1.53
6024732,-0.2266393145\\Version=ES64L-G09RevD.01\State=1-A\HF=-1144.759
8702\RMSD=9.327e-09\RMSF=5.458e-06\Dipole=-0.7294869,-1.455229,3.25567
59\Quadrupole=11.7923561,6.500858,-18.2932141,-3.5226651,-2.9634678,3.
5437414\PG=C01 [X(C19H18N2O4)]\\@

CTC-2 no HB
1\1\GINC-R1822\FOpt\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\09-Oct-2014\0\
\# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) ma
xdisk=3221225472\\CTC-OH.M062X\\0,1\C,-2.3695243411,-3.6063260539,-0.1
578134932\C,-3.1303875385,-2.4467840175,-0.0392375048\C,-2.9922823758,
-4.827361287,-0.307553933\C,-4.3873197978,-4.8716497838,-0.3461161597\
C,-5.1310286357,-3.7038640627,-0.2370769546\C,-4.5129111078,-2.4630653
978,-0.0831739246\H,-2.4094684269,-5.7385087899,-0.3959518805\H,-4.893
051767,-5.8217598278,-0.4670073161\H,-6.2128746751,-3.7513880104,-0.27
67760157\H,-5.1025976649,-1.5572243634,-0.0177135648\N,-2.270020047,-1
.3425405407,0.1194679076\C,-2.7631462153,-0.0286261011,0.4668712486\C,
-0.9084500749,-3.2421950339,-0.0809378942\C,-0.1503549612,-3.647996218
6,-1.3517730249\C,-0.9705197654,-1.7214495886,0.052157315\C,0.17388354
26,-0.9575947919,0.1040582027\C,0.2833931078,0.4339668688,-0.032827237
2\H,-0.6160428881,0.998305632,-0.264958124\H,1.1018785125,-1.505036351
6,0.1944140177\C,1.4366007887,1.2031923289,0.0237023902\C,1.3179933231
,2.6058948606,-0.2129203494\H,0.3517397917,3.0452728228,-0.4294275083\
C,2.760447281,0.6178366463,0.3184145678\O,2.9581882757,-0.5671195218,0
.5376067492\C,3.8928738254,1.5760735378,0.3385323576\O,5.0774859883,0.
9919758475,0.6080466752\H,4.5480694402,3.59421527,0.1254207521\C,2.409
9433893,3.4006989567,-0.1689166686\C,3.7205578949,2.8952286069,0.10832
49405\N,2.2589118894,4.8275900917,-0.4112221086\O,1.1460085215,5.25726
28042,-0.6449891683\O,3.2627923786,5.5124909603,-0.3649657152\C,-0.243
9846406,-3.8565466255,1.1621935293\H,-3.7349281943,-0.1369738645,0.950

0387859\H,-2.8731781486,0.6153765041,-0.4107390786\H,-2.0728507354,0.4
372726555,1.1725492574\H,-0.609760443,-3.2067963757,-2.239134552\H,-0.
1676188969,-4.7361405287,-1.4580635731\H,0.8904756621,-3.320320559,-1.
2976231284\H,-0.2665176566,-4.9470460061,1.0850404432\H,-0.7720338371,
-3.5640208366,2.0726575614\H,0.797146172,-3.5345575251,1.2413834546\H,
5.7640030503,1.6652976692,0.6073687217\\Version=ES64L-G09RevD.01\State
=1-A\HF=-1144.7593837\RMSD=5.030e-09\RMSF=9.458e-06\Dipole=-2.5994065,
-2.5960214,0.1187089\Quadrupole=14.9243435,-15.1457911,0.2214475,1.319
3959,-0.6456657,4.9464728\PG=C01 [X(C19H18N2O4)]\\@

TS2-2 no HB
1\1\GINC-R96\FTS\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\09-Oct-2014\0\\#
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeige
ntest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS2-OH.M062X\\0,1\C,
0.0469927821,-0.0738061565,-0.1053413298\C,0.006771972,-0.0655871737,1
.4249069201\N,1.3095707717,-0.1558856309,1.8924101038\C,2.2253631259,-
0.0673135167,0.8500878097\C,1.5386595963,-0.0026348088,-0.3652414458\C
,2.231183902,0.0822766591,-1.5520570913\C,3.6286869927,0.1103847275,-1
.5260415303\C,4.2988289949,0.049864287,-0.3130556276\C,3.6097785523,-0
.0382799628,0.8972804198\H,4.1505229521,-0.0725138967,1.8350109622\H,5
.3826107903,0.0754467767,-0.2979479104\H,4.1867906804,0.18152224,-2.45
13526237\H,1.6992771645,0.1280849336,-2.4977678467\C,-0.6907141059,1.1
247204112,-0.7081699086\C,-0.5203412937,-1.3902695923,-0.6615074551\C,
1.6298619486,-0.2746145338,3.2864645015\C,-1.0600029168,0.0138940342,2
.2283367037\H,-0.9136696562,0.0319063945,3.3056799804\C,-2.4631086721,
0.0823722038,1.8042254298\H,-2.9012350466,1.0802474346,1.7118215215\C,
-3.3174651872,-0.943366771,1.5809749435\C,-2.8991833864,-2.3770638219,
1.7387496207\O,-1.7980008374,-2.7260669961,2.0905279863\C,-4.682190498
9,-0.6472054089,1.1924045431\H,-5.0067071201,0.3805850039,1.088178167\
C,-3.9496473909,-3.3970400138,1.4371115641\O,-3.5070209109,-4.65535140
27,1.5802206435\C,-5.1940960711,-3.0452539001,1.0656435365\H,-5.960123
0262,-3.7787207155,0.8468747414\C,-5.5384757375,-1.6494691038,0.954127
2534\N,-6.9140328315,-1.3234934445,0.5546990398\O,-7.6628854772,-2.255
1622255,0.3466252937\O,-7.2162647384,-0.1544751977,0.4574772846\H,-0.5
53684243,1.1384554773,-1.793403033\H,-0.3116058325,2.0646616037,-0.300
8788369\H,-1.7648818192,1.0623165116,-0.5104148589\H,-0.30286238,-1.45
83042568,-1.731554888\H,-1.6040113883,-1.4298257757,-0.5276756283\H,-0
.0774100642,-2.2511872797,-0.1566749794\H,2.6807145703,-0.5406298705,3
.3979450211\H,1.0231526059,-1.0673418177,3.7365499419\H,1.4423555114,0
.6601847125,3.8297958282\H,-4.2186222811,-5.2698301368,1.3754652327\\V
ersion=ES64L-G09RevD.01\State=1-A\HF=-1144.7337323\RMSD=8.357e-09\RMSF
=1.620e-06\Dipole=1.1216213,0.0883398,0.38747\Quadrupole=-13.0674596,5
.7567359,7.3107237,7.3836685,-0.7555696,2.5141738\PG=C01 [X(C19H18N2O4
)]\\@

TS3-2 no HB
1\1\GINC-R3264\FTS\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\09-Oct-2014\0\\
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noei
gentest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS3-OH.M062X\\0,1\
C,-2.8335175686,0.9185982628,0.1062280472\C,-1.5474063032,0.6929292627
,-0.4121698249\C,-0.9075988628,-0.5896108088,-0.2649821429\C,-1.678147
316,-1.6149625918,0.4184712746\C,-2.904006259,-1.3535015897,0.95212129
77\C,-3.4788622895,-0.0741822634,0.7898860806\C,-0.9474326791,1.686458
0925,-1.2554869196\C,0.3279269009,1.7319795271,-1.7024457745\C,1.42185
70825,0.9273418453,-1.2152478523\N,1.8847448846,0.9587358711,0.0265948
932\C,3.0355479728,0.1470489953,0.1524781382\C,3.4173466459,-0.2850949
725,-1.1126202119\C,2.4647666592,0.2968718099,-2.1262031376\C,4.533101
2942,-1.0827318511,-1.2560842114\C,5.246207456,-1.4452490243,-0.111981
0416\C,4.8443495121,-1.007472187,1.1440999781\C,3.7218616671,-0.194943
1312,1.3001177585\O,0.2405061828,-0.8587120696,-0.6990327142\N,-4.7927
193756,0.1775733635,1.3477965138\O,-5.2787965387,1.2830086602,1.198406
9986\O,-5.3405324907,-0.7349599936,1.9391099149\H,3.4005146171,0.13108
2942,2.2813805741\H,5.4065859653,-1.3061041343,2.0207989278\H,6.118958
1546,-2.0805460281,-0.2029922179\H,4.845771028,-1.430698223,-2.2349380
563\C,3.1696646706,1.4266827425,-2.909599522\C,1.8693255892,-0.7250066
182,-3.0948291453\H,0.5805525846,2.3972197892,-2.5222216175\H,-1.62911
29379,2.4351013981,-1.6549982219\O,-1.0560690402,-2.8162874922,0.50771
34351\H,-3.4614111061,-2.1088749061,1.4938115489\H,-3.3237780271,1.875
7445071,-0.0231801716\C,1.1913583658,1.496826995,1.1750980326\H,2.4894
5077,1.8775196024,-3.636525924\H,4.0162118469,1.0020985896,-3.45409904
\H,3.5468128419,2.2041421827,-2.2402358639\H,1.1064700999,-0.247523232
1,-3.7159267277\H,1.4077064788,-1.5445223643,-2.547506667\H,2.65919692
89,-1.1053998017,-3.7488281162\H,0.5303562924,2.2977526541,0.848245321
1\H,1.9255573831,1.8876370373,1.8812903529\H,0.596317215,0.709906229,1
.6493191276\H,-1.6430662957,-3.431907076,0.9549669067\\Version=ES64L-G
09RevD.01\State=1-A\HF=-1144.7566314\RMSD=4.586e-09\RMSF=4.767e-06\Dip

ole=3.7128021,0.5668392,-0.7311494\Quadrupole=-17.3865509,8.5234201,8.
8631308,3.606925,8.7768255,-3.8751565\PG=C01 [X(C19H18N2O4)]\\@

TS4-2 no HB
1\1\GINC-R2217\FTS\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\09-Oct-2014\0\\
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noei
gentest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS4-OH.M062X\\0,1\
C,1.0765838429,-2.9512875471,3.0944979363\C,0.1039122623,-2.0272134602
,2.7477516283\C,-0.6697122704,-1.3883148234,3.7196269161\C,-0.49322298
63,-1.6817000389,5.0533354014\C,0.474108629,-2.6206648799,5.4229673189
\C,1.2451013409,-3.2388491098,4.449752056\C,-1.6130447419,-0.415871273
4,3.0474791411\C,-1.2668872541,-0.6196775427,1.5690236015\N,-0.2740403
368,-1.5838226231,1.4815786651\C,-1.8361308973,0.0783686341,0.58125814
09\C,-1.5190413358,0.086512962,-0.8523471342\C,-0.6424905618,0.8972467
896,-1.4896944609\C,-0.4783673718,0.7666179816,-2.9234989529\C,0.42941
36035,1.5185664997,-3.5602716912\C,1.2761657088,2.4843396954,-2.905083
0729\C,1.1667309399,2.6741269673,-1.5774426575\C,0.1787171793,1.913938
7579,-0.751215751\O,0.0731628831,2.1421513595,0.4298257237\N,0.5859575
468,1.3577721623,-5.0120729118\O,1.4181466034,2.0522977253,-5.55706711
95\O,-0.118336428,0.5477876701,-5.5737520306\H,1.6999417797,-3.4334753
564,2.3517408003\H,2.0004909597,-3.9594876391,4.7421636257\H,0.6261589
261,-2.8598940123,6.4681900421\H,-1.0950669175,-1.1861935362,5.8091814
901\C,-3.0778796609,-0.763721608,3.3313511936\C,-1.3052847557,1.027330
662,3.4674982607\H,-2.5857766443,0.8084507416,0.8794982774\H,-2.081035
0126,-0.5924680714,-1.4993402328\O,1.8896769029,3.5414890014,-0.853393
7475\H,1.9818414757,3.0386409954,-3.511209155\H,-1.0790496685,0.055998
4116,-3.4773033045\C,0.3069176281,-2.0593982928,0.2547262735\H,-3.7453
556936,-0.0887781934,2.7878797287\H,-3.2869417416,-0.6644415054,4.4006
043171\H,-3.3010009318,-1.789855544,3.030049549\H,-1.9625956929,1.7281
065931,2.9454501375\H,-0.2745003273,1.2908990563,3.2227943967\H,-1.456
3841665,1.1431907138,4.5449164356\H,2.4994371014,4.0107455996,-1.43126
09234\H,-0.4734512662,-2.2148976146,-0.4942481823\H,0.7864643647,-3.02
24752923,0.4345991374\H,1.0491369856,-1.3636510154,-0.1529988666\\Vers
ion=ES64L-G09RevD.01\State=1-A\HF=-1144.7313546\RMSD=7.923e-09\RMSF=1.
260e-06\Dipole=-0.058072,-0.3800677,0.7645595\Quadrupole=9.0085303,7.6
589899,-16.6675202,0.7736254,-0.8601265,-0.9810925\PG=C01 [X(C19H18N2O
4)]\\@

TS5-2 no HB
1\1\GINC-R1715\FTS\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\09-Oct-2014\0\\
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noei
gentest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS5-OH.M062X\\0,1\
C,-5.3169651618,-0.4108969702,1.3751158269\C,-6.3925883546,-0.82451925
77,0.5896128844\C,-6.2665460842,-0.9611167193,-0.7898587414\C,-5.06037
43656,-0.6885391874,-1.4315469515\C,-4.0161891803,-0.2805439796,-0.626
5894875\C,-4.1150649325,-0.1358824035,0.7516101333\H,-5.4247701559,-0.
3080161718,2.449325541\H,-7.343499946,-1.0439456907,1.060037482\H,-7.1
179252307,-1.2845279017,-1.3761385966\H,-4.955528642,-0.79329346,-2.50
44501158\C,-2.7811021381,0.3174651983,1.2809928151\C,-2.1395109352,-0.
706509129,2.2331486609\C,-2.8320130058,1.7065957709,1.9399626803\N,-2.
6882008809,0.0579339283,-1.0138219767\C,-2.2466880166,0.0202464063,-2.
4001167468\C,-1.9551689592,0.4024454031,0.0135822918\C,-0.5853073839,0
.847858617,-0.0671394982\C,0.4676258671,0.0025496936,0.0564262094\C,1.
8520316109,0.3476689973,0.0014575016\H,0.2594309245,-1.0592661327,0.20
638343\H,-0.3905124655,1.9113557744,-0.2086714794\O,1.4508465496,2.667
179346,-0.3494621492\C,2.2486987183,1.7301424204,-0.2105025372\C,2.803
5703261,-0.6710060389,0.1475003242\H,2.4982361001,-1.6992873181,0.3037
45582\C,4.1398334733,-0.379176585,0.0948632274\N,5.1061514486,-1.43497
48762,0.2458291042\O,4.7027311234,-2.5743982699,0.4185159851\O,6.28908
91817,-1.1394387681,0.19324562\C,4.5935328524,0.9501253172,-0.10813265
53\C,3.6963081201,1.958935554,-0.2548648085\O,4.0449783055,3.255621938
7,-0.4536628916\H,5.6620767141,1.130192509,-0.1422575816\H,-2.08965827
,-1.6981658461,1.776645118\H,-2.7433049236,-0.7747324409,3.1411102188\
H,-1.1303013784,-0.3851822824,2.4986394694\H,-3.2840193578,2.445453701
1,1.2742843652\H,-1.820553648,2.0306559471,2.194689972\H,-2.8602958721
,0.7064444096,-2.9869559007\H,-2.3661552052,-0.9948494433,-2.783566504
4\H,-1.2001675706,0.3183694551,-2.4312711803\H,-3.4303218271,1.6487597
739,2.8522275076\H,5.0042125759,3.3106587112,-0.4657521477\\Version=ES
64L-G09RevD.01\State=1-A\HF=-1144.7277216\RMSD=4.616e-09\RMSF=2.577e-0
6\Dipole=-7.1593733,-0.4057053,-0.3807495\Quadrupole=-1.1228293,-12.64
52173,13.7680467,17.0006628,0.4251492,3.6453073\PG=C01 [X(C19H18N2O4)]
\\@

MC-2 with HB optimized in implicit CHCl3
1\1\GINC-R96\FOpt\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\03-Oct-2014\0\\#

M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxd
isk=3221225472\\MC-OH-TTC.M062X\\0,1\C,-1.200507197,0.9853502519,-0.99
67163012\N,-0.2381450255,1.9511449637,-0.5111173432\C,1.0424205596,1.6
35595904,-0.2058821973\C,1.5171372966,0.3480403165,-0.3427761415\C,2.8
258772264,-0.045454548,-0.045464142\C,3.3724487553,-1.3167263987,-0.15
78013148\C,2.5994081504,-2.4651784331,-0.6283097447\O,1.4126656532,-2.
4483563773,-0.9704974749\C,4.7432870936,-1.5074978767,0.2008881693\C,5
.3104811107,-2.7312518848,0.1047801956\C,4.6032394375,-3.8892031047,-0
.3485965063\C,3.3055736985,-3.7576706364,-0.6985926011\N,6.7131303568,
-2.8840201959,0.4808383488\O,7.3144134902,-1.9003356572,0.8661380997\O
,7.19960894,-3.9924698978,0.3858646594\C,1.758785896,2.8988596825,0.27
21364417\C,0.6531764981,3.926610863,0.1690073659\C,-0.5056276377,3.313
5747036,-0.2990551408\C,2.9197800731,3.2825861806,-0.6604623973\C,2.22
2211786,2.7724149883,1.7330276982\C,0.6558878134,5.2751486982,0.457005
8256\C,-0.5186741179,6.005573864,0.2703780195\C,-1.6669246911,5.379347
843,-0.19757719\C,-1.6817459107,4.0168543421,-0.4920594164\H,-0.855099
2629,0.5443345306,-1.9355189731\H,-1.3359763541,0.1843158709,-0.265227
3396\H,0.8482735081,-0.4201371151,-0.7020739292\H,3.5150680854,0.71281
223,0.3174415847\H,5.337368067,-0.6730225642,0.5522124829\H,5.11130499
69,-4.8414359878,-0.4039388777\O,2.5522439523,-4.7760963368,-1.1355861
064\H,2.5749103497,3.3611304378,-1.6938894745\H,3.7305117133,2.5535786
323,-0.6224220415\H,3.3181464168,4.2546777755,-0.3576198226\H,1.387651
5719,2.4927277575,2.3798368961\H,2.6099296695,3.7368215441,2.072094827
2\H,3.0109131332,2.0273192887,1.8468886765\H,1.5543408977,5.7622147009
,0.8224585245\H,-0.5354182891,7.0656793522,0.4912586461\H,-2.572780795
2,5.9570886867,-0.3385502511\H,-2.5854403268,3.5450177112,-0.856095159
7\H,-2.1541830529,1.4806852835,-1.1643428434\H,1.6812964637,-4.3775593
891,-1.3042337317\\Version=ES64L-G09RevD.01\State=1-A\HF=-1144.7754741
\RMSD=8.088e-09\RMSF=1.816e-05\Dipole=-3.2875188,3.802697,-0.1453617\Q
uadrupole=-4.3150312,-0.5445188,4.85955,9.4690967,-0.6051138,1.63851\P
G=C01 [X(C19H18N2O4)]\\@

SP-2 with HB optimized in implicit CHCl3
1\1\GINC-R110\FOpt\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\10-Oct-2014\0\\
# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) max
disk=3221225472\\SP-OH.M062X.M062X\\0,1\C,0.0508773255,-1.8120346933,-
1.4968510911\N,-1.3271584081,-1.9648877758,-1.0841618647\C,-2.10651009
81,-0.7833100718,-0.8197595158\C,-2.2858867281,0.0704780072,-2.0432642
336\C,-2.2003311358,1.3989316706,-2.0118070889\C,-1.8792265291,2.09117
31963,-0.7688494478\C,-1.4988041972,1.2920283278,0.305059257\O,-1.3966
541259,-0.051890133,0.2169959787\C,-1.9191802523,3.4728594117,-0.60643
46399\C,-1.5847284852,3.9991722709,0.6265793088\C,-1.2113881,3.2161796
224,1.711710166\C,-1.167645345,1.843430935,1.5484589557\N,-1.629376310
1,5.4563043024,0.8039810156\O,-1.9621081606,6.1266500436,-0.1502216676
\O,-1.3310588586,5.8984591204,1.8921132635\C,-3.4298116996,-1.35359777
22,-0.2040084329\C,-2.8947908411,-2.6027705955,0.4623667783\C,-1.66147
85405,-2.9177798726,-0.1145547375\C,-4.101349824,-0.3694588666,0.74824
49503\C,-4.4053981832,-1.7565361764,-1.3203781354\C,-3.4371547795,-3.4
114243454,1.435810992\C,-2.7320982992,-4.5490408602,1.8419648828\C,-1.
5067125898,-4.8499081782,1.2664368267\C,-0.947095623,-4.0355740598,0.2
790576757\H,0.3908341395,-2.7273935482,-1.9868095721\H,0.1185454444,-0
.9937205997,-2.2167191038\H,-2.5191063125,-0.4671181871,-2.9547435796\
H,-2.3629836042,1.9926063187,-2.9050993468\H,-2.2039651623,4.131637097
4,-1.4155965224\H,-0.9699181617,3.6697353547,2.6626366982\O,-0.8275386
295,1.0375266503,2.5742583734\H,-3.4679592081,-0.1449353496,1.60879907
98\H,-5.0381630233,-0.7957875175,1.1173862117\H,-4.3426786711,0.566071
9167,0.2326892759\H,-5.2506444549,-2.2928419335,-0.8824228582\H,-3.920
9381353,-2.4173961902,-2.0440427018\H,-4.789135497,-0.875747954,-1.843
6070105\H,-4.3935706964,-3.1671486474,1.8876941406\H,-3.1410044623,-5.
1921594177,2.6115771541\H,-0.9635442106,-5.7295214754,1.5929861751\H,0
.0177644732,-4.2718351425,-0.1533931317\H,0.7168074546,-1.5926585254,-
0.6522929899\H,-0.8611314946,0.1268636429,2.2545305119\\Version=ES64L-
G09RevD.01\State=1-A\HF=-1144.7975173\RMSD=8.071e-09\RMSF=8.086e-06\Di
pole=-0.1896779,-2.228498,-1.0447373\Quadrupole=10.0927664,-18.5868578
,8.4940914,-3.4504103,-2.4478294,-6.1014062\PG=C01 [X(C19H18N2O4)]\\@

CCC-2 with HB optimized in implicit CHCl3
1\1\GINC-R185\FOpt\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\10-Oct-2014\0\\
# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) max
disk=3221225472\\CCC-OH-2.M062X\\0,1\C,-0.6548666609,0.9258910073,-2.6
948658733\C,-0.6533378696,0.8080778414,-1.2772041765\C,0.5999099477,0.
9468300069,-0.5642096782\C,1.8027824752,1.1642713742,-1.3748064457\C,1
.7690365824,1.2174661538,-2.7281698166\C,0.508483562,1.0983821291,-3.3
747095086\C,-1.9028026483,0.7260886553,-0.6205950876\C,-2.2226170451,0
.4549679216,0.6924977282\C,-1.4433998722,-0.1682926666,1.6806584413\N,
-0.5992440653,-1.1760730683,1.502832499\C,0.0547371109,-1.5128385776,2

.7085231417\C,-0.4633729766,-0.7289659822,3.7326384035\C,-1.4952409235
,0.2048131982,3.1536887556\C,-0.0064202445,-0.8983299712,5.0234113636\
C,0.9834011107,-1.8526200904,5.2618732467\C,1.4968620763,-2.6183140974
,4.2212498677\C,1.0369198217,-2.4621128526,2.914872333\O,0.7521660303,
0.9156508716,0.6744422195\N,0.4651823455,1.1809284109,-4.8301572982\O,
-0.6154179866,1.0843667852,-5.3791577421\O,1.5183339694,1.3412274941,-
5.414013389\H,1.4491763613,-3.0487525895,2.1035395688\H,2.2715888719,-
3.3478512121,4.4247034148\H,1.3614075652,-1.9942339115,6.2671124491\H,
-0.4008841295,-0.2978793359,5.8365086348\C,-2.8883282955,-0.0507157912
,3.7487842762\C,-1.0889545784,1.6784140349,3.3142041832\H,-3.189337015
6,0.8070309334,1.0416048478\H,-2.7491576095,1.0171314841,-1.2427630072
\O,2.9358012265,1.2857312439,-0.6648580998\H,2.666441195,1.3641852658,
-3.3122079572\H,-1.5835332189,0.8620283155,-3.2480631333\C,-0.37484626
69,-1.9037094439,0.2755574677\H,-3.6337807836,0.603056368,3.2890976643
\H,-2.867455124,0.1636248546,4.8204057187\H,-3.1942278307,-1.090422329
3,3.6113972284\H,-1.8401724253,2.3248528256,2.8528161108\H,-0.13012662
62,1.8604106241,2.8266800627\H,-1.0174921675,1.9248226134,4.3770585654
\H,2.6394517002,1.2286381315,0.2602478573\H,-1.2543924347,-1.802220133
3,-0.3589100886\H,-0.2186137492,-2.9547358719,0.5237673124\H,0.4959805
962,-1.5130856195,-0.2580490602\\Version=ES64L-G09RevD.01\State=1-A\HF
=-1144.7726478\RMSD=6.660e-09\RMSF=7.559e-06\Dipole=-1.5275422,-1.6386
637,4.0079556\Quadrupole=6.6656226,8.969932,-15.6355546,-6.1408504,3.4
650811,5.0317154\PG=C01 [X(C19H18N2O4)]\\@

CTC-2 with HB optimized in implicit CHCl3
1\1\GINC-R480\FOpt\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\10-Oct-2014\0\\
# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) max
disk=3221225472\\CTC-OH-2.M062X\\0,1\C,-2.3671678713,-3.6085089012,-0.
1562514621\C,-3.1326608993,-2.4525804768,-0.0366093402\C,-2.9850960755
,-4.8319369727,-0.307908011\C,-4.3797520107,-4.88080101,-0.3471551607\
C,-5.1281446928,-3.7159145525,-0.2370525878\C,-4.5149353602,-2.4730719
219,-0.0811638705\H,-2.3991101082,-5.7408803629,-0.3974637549\H,-4.882
0506033,-5.8325160173,-0.4695901014\H,-6.2097154317,-3.7676400815,-0.2
774298552\H,-5.1080346318,-1.5695919783,-0.0146484579\N,-2.2751896113,
-1.3447468452,0.1239203551\C,-2.7736684608,-0.0309724184,0.4664231155\
C,-0.9078409101,-3.2382897549,-0.0790714219\C,-0.1482653831,-3.6375257
098,-1.3512624727\C,-0.9769063492,-1.7185442074,0.0570763914\C,0.16591
72826,-0.9483389135,0.1109776542\C,0.2703304167,0.4405602616,-0.029727
3741\H,-0.6291409557,1.0055966196,-0.2595426047\H,1.0951664533,-1.4937
952977,0.2034366807\C,1.4270441712,1.2080209458,0.0232602371\C,1.32642
47754,2.6144418283,-0.2123047962\H,0.3657483386,3.0653926693,-0.427808
2515\C,2.7401536165,0.6333160036,0.3110191567\O,2.9754008163,-0.557886
1455,0.5351092355\C,3.8831553357,1.5653124226,0.3348642117\O,5.0617687
23,0.986764073,0.6012962825\H,4.5824941323,3.5630680062,0.1281936068\C
,2.4294115703,3.3956994256,-0.1680791504\C,3.7384702854,2.888507029,0.
1070059042\N,2.2820158718,4.8276424468,-0.4118542388\O,1.1692219359,5.
2590326375,-0.6436132029\O,3.2864973672,5.5082925481,-0.3680833468\C,-
0.2402869414,-3.8518062563,1.1629499019\H,-3.7466025805,-0.1413235124,
0.9463723612\H,-2.8823234912,0.6092917753,-0.4139203512\H,-2.087140861
3,0.4387439436,1.1731441652\H,-0.6098373273,-3.1965288318,-2.237551203
6\H,-0.1609286504,-4.725433713,-1.4597813019\H,0.8912185579,-3.3056309
674,-1.2969673612\H,-0.2588318993,-4.9421387262,1.0836549355\H,-0.7688
094881,-3.5630643383,2.0743052919\H,0.7998425792,-3.5266176483,1.24207
84493\H,4.8477683652,0.0451819252,0.7185037431\\Version=ES64L-G09RevD.
01\State=1-A\HF=-1144.7720117\RMSD=7.621e-09\RMSF=3.476e-06\Dipole=-3.
4743797,-3.501779,0.1308771\Quadrupole=7.4216176,-12.3952689,4.9736514
,-8.5210006,-1.0420153,3.7338083\PG=C01 [X(C19H18N2O4)]\\@

TS2-2 with HB optimized in implicit CHCl3
1\1\GINC-R675\FTS\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\10-Oct-2014\0\\#
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeig
entest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS2-OH-2.M062X\\0,1
\C,-1.8119002587,-0.8953882359,-0.1805078843\C,-1.6393588209,0.1773970
833,0.8977835068\N,-2.8371871935,0.8637667494,1.0212686746\C,-3.838333
9211,0.2694750389,0.2591881061\C,-3.2961058696,-0.7918803717,-0.469748
3046\C,-4.091640162,-1.5361189673,-1.3117404055\C,-5.4491412139,-1.221
4053114,-1.4220463511\C,-5.9766340152,-0.1681091828,-0.6895956754\C,-5
.1813869802,0.5958359039,0.1656862422\H,-5.6141956827,1.4072290203,0.7
37686359\H,-7.0308421395,0.0696163153,-0.7761165568\H,-6.0883001854,-1
.8007253603,-2.0766826218\H,-3.6712442511,-2.3587641667,-1.8825303452\
C,-1.4273908756,-2.2888572915,0.323780687\C,-1.0063608023,-0.537941082
8,-1.4404820736\C,-3.0013810841,1.9911609829,1.8944051182\C,-0.5520224
392,0.4544205733,1.6273975132\H,-0.5979822029,1.2440381065,2.373562171
4\C,0.7488532606,-0.2180381733,1.5344600832\H,0.9231495896,-1.05596025
64,2.2154369275\C,1.8030455064,0.1184629032,0.7546958347\C,1.761114185
3,1.2741539914,-0.1842590968\O,0.8111248813,2.0191857867,-0.3442233579

\C,3.0279051432,-0.6550443584,0.8333772541\H,3.0944385036,-1.496685725
7,1.5108341915\C,2.9864593663,1.5360977052,-0.985194848\O,2.8917948548
,2.5790982054,-1.8124853409\C,4.0872897126,0.7713145269,-0.8708389724\
H,4.9757229974,0.9628373008,-1.4552571181\C,4.0740023103,-0.3283655893
,0.0608703218\N,5.2978143445,-1.1403853668,0.1647467872\O,6.2300006489
,-0.8242208554,-0.5418351231\O,5.2984738773,-2.0682118153,0.9441447566
\H,-1.6635020642,-3.0377619298,-0.4377224478\H,-1.9726671702,-2.541009
139,1.2359759343\H,-0.3538961746,-2.3501423404,0.5256525172\H,-1.28893
98042,-1.2082881953,-2.2574397591\H,0.0651535729,-0.6506035269,-1.2587
214157\H,-1.200868725,0.4915809285,-1.7481427116\H,-3.9546049129,2.476
9441873,1.6882325109\H,-2.1993537195,2.7153240923,1.7169118865\H,-2.97
64459611,1.6951501086,2.9507536372\H,1.9971198748,2.9342877324,-1.6785
176119\\Version=ES64L-G09RevD.01\State=1-A\HF=-1144.7450959\RMSD=5.858
e-09\RMSF=1.969e-06\Dipole=-2.1229963,0.4097354,0.6844091\Quadrupole=-
13.8553183,5.6267492,8.2285691,3.0352295,-0.0221308,5.0912355\PG=C01 [
X(C19H18N2O4)]\\@

TS3-2 with HB optimized in implicit CHCl3
1\1\GINC-R159\FTS\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\10-Oct-2014\0\\#
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeig
entest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS3-OH-2.M062X\\0,1
\C,-2.8278929517,0.9065353724,0.1017284057\C,-1.5490447245,0.704028994
4,-0.446248354\C,-0.9026462598,-0.5569399096,-0.2953104418\C,-1.614215
789,-1.5910969229,0.4155550648\C,-2.8373780943,-1.3653051521,0.9753035
309\C,-3.433043604,-0.0991327037,0.8066969448\C,-0.9594934759,1.700848
9254,-1.2988902683\C,0.3184143415,1.7417113167,-1.7279287776\C,1.39720
52191,0.9141854485,-1.2263416692\N,1.8666297898,0.9741156788,0.0134156
583\C,3.0049670987,0.1463879018,0.152732255\C,3.3810321079,-0.31176162
93,-1.1054703507\C,2.4485475136,0.2849792633,-2.1294461\C,4.4797435696
,-1.1351064431,-1.2344042146\C,5.181075618,-1.497352624,-0.0826569918\
C,4.7859972327,-1.0326178066,1.165827827\C,3.6809692387,-0.1933843099,
1.3070464187\O,0.2509664089,-0.8507214645,-0.755014062\N,-4.744575564,
0.139772273,1.3914526895\O,-5.249453143,1.2355962587,1.2362221121\O,-5
.2635911115,-0.7714850781,2.0053865545\H,3.3646504477,0.1544847017,2.2
825000757\H,5.3393355799,-1.3307551754,2.0482896323\H,6.03973922,-2.15
30481111,-0.1619392059\H,4.7883962871,-1.5027206544,-2.2073157651\C,3.
1776653746,1.428793667,-2.8727504506\C,1.8732599174,-0.7074716042,-3.1
370770929\H,0.5960809091,2.4168203541,-2.5310092168\H,-1.6414266192,2.
4459766869,-1.7033893817\O,-0.9853702625,-2.7790913415,0.5189066066\H,
-3.3495974297,-2.1380395125,1.5314179843\H,-3.3422967003,1.8513366586,
-0.0208816314\C,1.1801559901,1.5350831113,1.1563192395\H,2.5186032495,
1.8951783801,-3.6092235558\H,4.0372276504,1.011031962,-3.4016411783\H,
3.5389557597,2.1921238453,-2.1789348554\H,1.1220375723,-0.2134487097,-
3.7593072828\H,1.4012368987,-1.5437208484,-2.626247144\H,2.6747592247,
-1.0692636972,-3.7872610787\H,0.5077814694,2.3212891541,0.8176474348\H
,1.9184959028,1.9503338164,1.8441766686\H,0.5982381852,0.7555405868,1.
658488998\H,-0.1484790475,-2.6550506593,0.0449779683\\Version=ES64L-G0
9RevD.01\State=1-A\HF=-1144.7675814\RMSD=7.652e-09\RMSF=2.068e-06\Dipo
le=4.3510367,1.1873749,-1.2182229\Quadrupole=-15.5989377,5.5971151,10.
0018227,-2.5103113,10.6085516,-0.1396119\PG=C01 [X(C19H18N2O4)]\\@

TS4-2 with HB optimized in implicit CHCl3
1\1\GINC-R195\FTS\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\10-Oct-2014\0\\#
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeig
entest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS4-OH-2.M062X\\0,1
\C,1.0662584609,-2.9652134414,3.1042961052\C,0.0991938394,-2.036195122
7,2.7558620306\C,-0.6693090077,-1.3889466439,3.7257954494\C,-0.4933068
581,-1.6783504067,5.0605802156\C,0.4686359151,-2.6218694048,5.43219935
77\C,1.2345554033,-3.2487143494,4.460404572\C,-1.608368126,-0.41440389
57,3.0506834466\C,-1.2592738045,-0.6207849156,1.573086634\N,-0.2768881
595,-1.593996043,1.4877735512\C,-1.8213397471,0.0813774618,0.583246735
5\C,-1.5075218442,0.0780552965,-0.850826435\C,-0.6331493086,0.88746803
1,-1.4935714777\C,-0.4643472989,0.7659928308,-2.9289321361\C,0.4329323
899,1.5350289568,-3.5627272864\C,1.2677901692,2.5154918466,-2.91558427
97\C,1.1512559174,2.6882596972,-1.5864908552\C,0.1888517614,1.89815543
32,-0.7722376048\O,0.133209395,2.1333130612,0.4213908516\N,0.583623500
8,1.3740178272,-5.0185492371\O,1.399204422,2.0807415756,-5.5693605413\
O,-0.1111293684,0.5503219731,-5.5729605938\H,1.6854357866,-3.454221446
8,2.3625357539\H,1.9855972068,-3.9730543113,4.7546598122\H,0.620396450
8,-2.8583406397,6.4780613077\H,-1.0913536397,-1.1768284792,5.815441182
\C,-3.0749063261,-0.7605889412,3.3290003883\C,-1.3008825078,1.02785728
82,3.4728461388\H,-2.5653457508,0.8185972554,0.8780444806\H,-2.0692649
564,-0.6051145374,-1.493640874\O,1.8692215633,3.5703982099,-0.88861490
42\H,1.9645001954,3.0939018045,-3.5051353394\H,-1.0551173476,0.0497696
44,-3.4854620739\C,0.3005964978,-2.0777520335,0.2619611973\H,-3.739727
2288,-0.0842815411,2.7839732183\H,-3.2872501931,-0.6627389326,4.397664

8744\H,-3.2979723784,-1.7860641618,3.0255864538\H,-1.9526270294,1.7305
962041,2.9463765951\H,-0.266711477,1.2873639661,3.2380493037\H,-1.4600
980811,1.1443159258,4.5489274077\H,1.5662403932,3.4804289247,0.0305251
877\H,-0.4804239033,-2.2275154143,-0.4873834112\H,0.769944738,-3.04533
9837,0.4440370718\H,1.0506673357,-1.3907447144,-0.1460822728\\Version=
ES64L-G09RevD.01\State=1-A\HF=-1144.742783\RMSD=7.073e-09\RMSF=1.303e-
06\Dipole=-0.6857501,-0.9005621,1.5836836\Quadrupole=7.9067948,6.19064
64,-14.0974412,-5.1755838,3.5873035,5.3434547\PG=C01 [X(C19H18N2O4)]\\
@

TS5-2 with HB optimized in implicit CHCl3
1\1\GINC-R165\FTS\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\10-Oct-2014\0\\#
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeig
entest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS5-OH-2.M062X\\0,1
\C,-5.3155543462,-0.4123534692,1.374823515\C,-6.3899635244,-0.82816210
95,0.5889566476\C,-6.26378631,-0.9637341712,-0.7907247986\C,-5.0584857
641,-0.6878337803,-1.4324326792\C,-4.0155704196,-0.2776291681,-0.62693
91258\C,-4.1144423149,-0.1338360095,0.7511913055\H,-5.4236778868,-0.31
0568765,2.4490830812\H,-7.3403035203,-1.0502731205,1.0592500518\H,-7.1
144265803,-1.2890152096,-1.3769974821\H,-4.9535292966,-0.791879783,-2.
5053850374\C,-2.7815351302,0.3222608635,1.2807899107\C,-2.1380359003,-
0.7014605359,2.2322791231\C,-2.8357329106,1.7105818623,1.9414374056\N,
-2.6880126134,0.0648641831,-1.014016048\C,-2.2468734533,0.0267745242,-
2.4007169605\C,-1.9568978251,0.4104962635,0.0132279924\C,-0.5844208887
,0.8550788841,-0.0674257524\C,0.4618465242,0.0029938495,0.0583242475\C
,1.8478933541,0.3430329098,0.00322075\H,0.2473346346,-1.0573251004,0.2
093285208\H,-0.3920314795,1.9175951195,-0.210445327\O,1.4920219355,2.6
863616518,-0.352678947\C,2.2579836075,1.7043509602,-0.206771501\C,2.81
15136037,-0.6712362938,0.1484990538\H,2.5140571889,-1.701116045,0.3060
494447\C,4.144442002,-0.3684323649,0.092716969\N,5.1113681386,-1.43389
77733,0.2451423019\O,4.7013495817,-2.5701006445,0.4186053176\O,6.29262
39133,-1.1432787092,0.1921017866\C,4.6086842743,0.9569264009,-0.111304
455\C,3.6944413014,1.9506664971,-0.2553524801\O,4.0298520552,3.2396327
762,-0.4546170239\H,5.6703147159,1.1569563735,-0.1498070973\H,-2.08477
82387,-1.6922932357,1.774441299\H,-2.7434701009,-0.7726802919,3.138880
1653\H,-1.130344363,-0.3779490985,2.5007402653\H,-3.2887591386,2.44955
21568,1.2765595207\H,-1.8254157029,2.0361508144,2.1987679242\H,-2.8606
353104,0.7130273314,-2.9872560477\H,-2.3676044972,-0.9884514212,-2.783
3041496\H,-1.2001026039,0.3234880078,-2.4332778987\H,-3.4349203877,1.6
501537082,2.8528998624\H,3.1662546768,3.6858569627,-0.5149806504\\Vers
ion=ES64L-G09RevD.01\State=1-A\HF=-1144.7417794\RMSD=4.266e-09\RMSF=3.
610e-06\Dipole=-8.2412654,-0.4903584,-0.3652365\Quadrupole=-11.6909296
,-6.5636622,18.2545918,10.017111,1.6619779,3.4286271\PG=C01 [X(C19H18N
2O4)]\\@

MC-2 no HB optimized in implicit CHCl3
1\1\GINC-R93\FOpt\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\03-Oct-2014\0\\#
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxd
isk=3221225472\\MC-OH-TTC2.M062X\\0,1\C,-1.208136341,0.9973962006,-0.9
947505697\N,-0.2431257728,1.9600452716,-0.5092729453\C,1.0389559268,1.
638583333,-0.2062025668\C,1.5070163471,0.3511133484,-0.3461163261\C,2.
8166040678,-0.0501934162,-0.0512569553\C,3.362521159,-1.3198166821,-0.
1645132251\C,2.5746292745,-2.4749751944,-0.6410071946\O,1.3997654723,-
2.4214041957,-0.9715669796\C,4.7326672896,-1.4952632646,0.1963635481\C
,5.3120591533,-2.7124264373,0.1040638059\C,4.6036783034,-3.8708146449,
-0.3501839858\C,3.3053620988,-3.7640033472,-0.7048515486\N,6.710371671
7,-2.8636134279,0.4783035465\O,7.3125958947,-1.8808206601,0.8640515309
\O,7.1983649283,-3.9734963133,0.3824203101\C,1.7594790455,2.8994989148
,0.2727009529\C,0.6566647852,3.9308843999,0.1730031827\C,-0.5049129698
,3.3216476235,-0.2945091368\C,2.9201159989,3.2816882803,-0.660712185\C
,2.2250677407,2.7697783368,1.7324422679\C,0.6642032732,5.2787156159,0.
4632786124\C,-0.5080352207,6.0140435924,0.2799715266\C,-1.6588020779,5
.3922499053,-0.1872395583\C,-1.6786497625,4.0302689989,-0.4841083121\H
,-0.8652090819,0.5561729925,-1.9344466853\H,-1.3442002474,0.1949758512
,-0.2647897206\H,0.8356059517,-0.4143396347,-0.7055329154\H,3.50725690
24,0.7067741731,0.311895044\H,5.3184871226,-0.6541615527,0.5469205948\
H,5.1362204707,-4.8131027593,-0.3972720341\O,2.5432423537,-4.785261275
7,-1.1453850776\H,2.5735452199,3.3633129148,-1.693331981\H,3.728149305
,2.549475311,-0.6258024321\H,3.3226149637,4.2518433842,-0.3568060559\H
,1.3904831108,2.4920756288,2.3800765428\H,2.6171077134,3.7321438775,2.
0726218775\H,3.0108637443,2.0211567705,1.8436884351\H,1.5650703772,5.7
618692449,0.8281546556\H,-0.5207022377,7.0738038943,0.502783355\H,-2.5
630928501,5.9731116545,-0.3258507107\H,-2.5845043587,3.562120504,-0.84
75501379\H,-2.1610767989,1.4950383049,-1.1602992957\H,3.075558053,-5.5
859255218,-1.1622212529\\Version=ES64L-G09RevD.01\State=1-A\HF=-1144.7

63001\RMSD=7.916e-09\RMSF=1.166e-05\Dipole=-2.5610243,2.7909737,-0.146
1459\Quadrupole=-10.4200185,10.409456,0.0105625,2.5036503,-2.5382651,2
.9281111\PG=C01 [X(C19H18N2O4)]\\@

SP-2 no HB optimized in implicit CHCl3
1\1\GINC-R107\FOpt\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\10-Oct-2014\0\\
# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) max
disk=3221225472\\SP-OH-2.M062X.M062X\\0,1\C,0.0695662425,-1.761590622,
-1.4444258292\N,-1.3135353764,-1.9402171025,-1.0600414224\C,-2.1084460
175,-0.7695177927,-0.7852386289\C,-2.3025752437,0.0780410355,-2.009645
6056\C,-2.214500706,1.405339261,-1.9810109361\C,-1.8749202545,2.098205
5484,-0.7441029444\C,-1.4876512624,1.2995016739,0.3331789591\O,-1.4125
96237,-0.0365382804,0.2538810207\C,-1.896826884,3.483820608,-0.6115784
28\C,-1.5358047844,4.0345690999,0.5997546581\C,-1.1500597331,3.2599751
014,1.6878140356\C,-1.1230249943,1.8838962531,1.5582307622\N,-1.558166
9674,5.4910161991,0.7558977956\O,-1.9004544085,6.1530613358,-0.2001967
084\O,-1.2323601961,5.9449334828,1.8330299838\C,-3.4270778718,-1.36065
45734,-0.1738916903\C,-2.890753644,-2.6277356997,0.455249535\C,-1.6515
364282,-2.9194057959,-0.1194138857\C,-4.0822425799,-0.4003405442,0.813
66964\C,-4.415559469,-1.7331851862,-1.2889619297\C,-3.4398473622,-3.46
97093849,1.3958494083\C,-2.7353934643,-4.6177267261,1.772008226\C,-1.5
027675611,-4.8948427756,1.2000613079\C,-0.9369830511,-4.0469312974,0.2
454454749\H,0.4305658517,-2.6626716787,-1.9459304576\H,0.1387123671,-0
.9291990547,-2.1481970606\H,-2.5434724193,-0.4612671457,-2.9180099933\
H,-2.3837457783,2.0000079804,-2.8724940965\H,-2.1871518782,4.125735089
2,-1.4325910101\H,-0.8866783524,3.7475501765,2.618388564\O,-0.77723920
16,1.0388319471,2.5547945229\H,-3.4286235514,-0.2035450838,1.665450145
6\H,-5.0153117617,-0.8333827524,1.1848953174\H,-4.3287370866,0.5484947
942,0.3245471197\H,-5.2576617099,-2.2777416647,-0.8548482374\H,-3.9415
826685,-2.3788885758,-2.0332459878\H,-4.8025357148,-0.8395577259,-1.78
76829781\H,-4.4015181684,-3.2430164188,1.8459323495\H,-3.1500274063,-5
.2872071089,2.5157476782\H,-0.9591517339,-5.7825232286,1.503499981\H,0
.0336053751,-4.2648856961,-0.1837696927\H,0.7148913624,-1.5487411543,-
0.5827501367\H,-0.5531192708,1.5481834828,3.3384611742\\Version=ES64L-
G09RevD.01\State=1-A\HF=-1144.790668\RMSD=5.733e-09\RMSF=6.299e-06\Dip
ole=0.0172921,-1.4342664,-0.2968219\Quadrupole=8.4572462,-21.5392171,1
3.0819709,-1.6700464,0.2091218,-1.1577077\PG=C01 [X(C19H18N2O4)]\\@

CCC-2 no HB optimized in implicit CHCl3
1\1\GINC-R452\FOpt\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\09-Oct-2014\0\\
# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) max
disk=3221225472\\CCC-OH.M062X\\0,1\C,-0.6849961372,0.9180444845,-2.706
7599907\C,-0.6592680338,0.7870170434,-1.293541125\C,0.6035013571,0.934
726371,-0.5692513602\C,1.7945024456,1.1602206109,-1.4077958034\C,1.728
4497352,1.2220505735,-2.75933618\C,0.4652157184,1.1062352288,-3.4034847211\C,-1.9018202524,0.6919289948,-0.6289887507\C,-2.2172810955,0.4286
298605,0.6884427153\C,-1.4394073974,-0.1832568827,1.6830878934\N,-0.59
34679536,-1.1930626262,1.5185101012\C,0.0471311046,-1.5263409622,2.731
1813733\C,-0.4791510468,-0.7373334806,3.7472764125\C,-1.496571352,0.20
24196281,3.1530406728\C,-0.0380978471,-0.9046911534,5.0436320869\C,0.9
441025946,-1.8630524143,5.297010983\C,1.4665165218,-2.6335324551,4.264
5625663\C,1.0230920345,-2.4787197727,2.9523802272\O,0.7167733858,0.896
8474871,0.6584788308\N,0.413371091,1.2069875463,-4.8515506297\O,-0.668
751212,1.1103786486,-5.3978667121\O,1.4639234284,1.3825226853,-5.44035
35463\H,1.4434675007,-3.0680288492,2.1472406141\H,2.2358785621,-3.3656
32236,4.479134818\H,1.3093991992,-2.0035391635,6.3071203392\H,-0.43908
64285,-0.2993205658,5.8498983391\C,-2.8954572538,-0.0232598838,3.74446
78457\C,-1.0653835127,1.6712639956,3.2988467162\H,-3.1862554206,0.7785
140807,1.0337520878\H,-2.755024942,0.9680893013,-1.2487483619\O,2.9395
993665,1.2721610701,-0.6973484785\H,2.6101987326,1.3735118674,-3.37060
88887\H,-1.6220040922,0.853521087,-3.2464390378\C,-0.3572916376,-1.923
2214189,0.295390178\H,-3.6276241205,0.6394289335,3.2762079158\H,-2.875
4582189,0.2004172236,4.8142676651\H,-3.2194028756,-1.0585900868,3.6152
034874\H,-1.8014494687,2.3239029741,2.821921549\H,-0.0990639926,1.8298
660989,2.8177081554\H,-0.999582284,1.9290971958,4.3594815881\H,3.66487
40034,1.4337373006,-1.3073555347\H,-1.2292825203,-1.8192387594,-0.3490
034937\H,-0.2081865105,-2.9748448491,0.5462267672\H,0.5217188249,-1.53
6024732,-0.2266393145\\Version=ES64L-G09RevD.01\State=1-A\HF=-1144.759
8702\RMSD=9.327e-09\RMSF=5.458e-06\Dipole=-0.7294869,-1.455229,3.25567
59\Quadrupole=11.7923561,6.500858,-18.2932141,-3.5226651,-2.9634678,3.
5437414\PG=C01 [X(C19H18N2O4)]\\@

CTC-2 no HB optimized in implicit CHCl3
1\1\GINC-R1822\FOpt\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\09-Oct-2014\0\
\# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) ma
xdisk=3221225472\\CTC-OH.M062X\\0,1\C,-2.3695243411,-3.6063260539,-0.1

578134932\C,-3.1303875385,-2.4467840175,-0.0392375048\C,-2.9922823758,
-4.827361287,-0.307553933\C,-4.3873197978,-4.8716497838,-0.3461161597\
C,-5.1310286357,-3.7038640627,-0.2370769546\C,-4.5129111078,-2.4630653
978,-0.0831739246\H,-2.4094684269,-5.7385087899,-0.3959518805\H,-4.893
051767,-5.8217598278,-0.4670073161\H,-6.2128746751,-3.7513880104,-0.27
67760157\H,-5.1025976649,-1.5572243634,-0.0177135648\N,-2.270020047,-1
.3425405407,0.1194679076\C,-2.7631462153,-0.0286261011,0.4668712486\C,
-0.9084500749,-3.2421950339,-0.0809378942\C,-0.1503549612,-3.647996218
6,-1.3517730249\C,-0.9705197654,-1.7214495886,0.052157315\C,0.17388354
26,-0.9575947919,0.1040582027\C,0.2833931078,0.4339668688,-0.032827237
2\H,-0.6160428881,0.998305632,-0.264958124\H,1.1018785125,-1.505036351
6,0.1944140177\C,1.4366007887,1.2031923289,0.0237023902\C,1.3179933231
,2.6058948606,-0.2129203494\H,0.3517397917,3.0452728228,-0.4294275083\
C,2.760447281,0.6178366463,0.3184145678\O,2.9581882757,-0.5671195218,0
.5376067492\C,3.8928738254,1.5760735378,0.3385323576\O,5.0774859883,0.
9919758475,0.6080466752\H,4.5480694402,3.59421527,0.1254207521\C,2.409
9433893,3.4006989567,-0.1689166686\C,3.7205578949,2.8952286069,0.10832
49405\N,2.2589118894,4.8275900917,-0.4112221086\O,1.1460085215,5.25726
28042,-0.6449891683\O,3.2627923786,5.5124909603,-0.3649657152\C,-0.243
9846406,-3.8565466255,1.1621935293\H,-3.7349281943,-0.1369738645,0.950
0387859\H,-2.8731781486,0.6153765041,-0.4107390786\H,-2.0728507354,0.4
372726555,1.1725492574\H,-0.609760443,-3.2067963757,-2.239134552\H,-0.
1676188969,-4.7361405287,-1.4580635731\H,0.8904756621,-3.320320559,-1.
2976231284\H,-0.2665176566,-4.9470460061,1.0850404432\H,-0.7720338371,
-3.5640208366,2.0726575614\H,0.797146172,-3.5345575251,1.2413834546\H,
5.7640030503,1.6652976692,0.6073687217\\Version=ES64L-G09RevD.01\State
=1-A\HF=-1144.7593837\RMSD=5.030e-09\RMSF=9.458e-06\Dipole=-2.5994065,
-2.5960214,0.1187089\Quadrupole=14.9243435,-15.1457911,0.2214475,1.319
3959,-0.6456657,4.9464728\PG=C01 [X(C19H18N2O4)]\\@

TS2-2 no HB optimized in implicit CHCl3
1\1\GINC-R96\FTS\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\09-Oct-2014\0\\#
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeige
ntest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS2-OH.M062X\\0,1\C,
0.0469927821,-0.0738061565,-0.1053413298\C,0.006771972,-0.0655871737,1
.4249069201\N,1.3095707717,-0.1558856309,1.8924101038\C,2.2253631259,-
0.0673135167,0.8500878097\C,1.5386595963,-0.0026348088,-0.3652414458\C
,2.231183902,0.0822766591,-1.5520570913\C,3.6286869927,0.1103847275,-1
.5260415303\C,4.2988289949,0.049864287,-0.3130556276\C,3.6097785523,-0
.0382799628,0.8972804198\H,4.1505229521,-0.0725138967,1.8350109622\H,5
.3826107903,0.0754467767,-0.2979479104\H,4.1867906804,0.18152224,-2.45
13526237\H,1.6992771645,0.1280849336,-2.4977678467\C,-0.6907141059,1.1
247204112,-0.7081699086\C,-0.5203412937,-1.3902695923,-0.6615074551\C,
1.6298619486,-0.2746145338,3.2864645015\C,-1.0600029168,0.0138940342,2
.2283367037\H,-0.9136696562,0.0319063945,3.3056799804\C,-2.4631086721,
0.0823722038,1.8042254298\H,-2.9012350466,1.0802474346,1.7118215215\C,
-3.3174651872,-0.943366771,1.5809749435\C,-2.8991833864,-2.3770638219,
1.7387496207\O,-1.7980008374,-2.7260669961,2.0905279863\C,-4.682190498
9,-0.6472054089,1.1924045431\H,-5.0067071201,0.3805850039,1.088178167\
C,-3.9496473909,-3.3970400138,1.4371115641\O,-3.5070209109,-4.65535140
27,1.5802206435\C,-5.1940960711,-3.0452539001,1.0656435365\H,-5.960123
0262,-3.7787207155,0.8468747414\C,-5.5384757375,-1.6494691038,0.954127
2534\N,-6.9140328315,-1.3234934445,0.5546990398\O,-7.6628854772,-2.255
1622255,0.3466252937\O,-7.2162647384,-0.1544751977,0.4574772846\H,-0.5
53684243,1.1384554773,-1.793403033\H,-0.3116058325,2.0646616037,-0.300
8788369\H,-1.7648818192,1.0623165116,-0.5104148589\H,-0.30286238,-1.45
83042568,-1.731554888\H,-1.6040113883,-1.4298257757,-0.5276756283\H,-0
.0774100642,-2.2511872797,-0.1566749794\H,2.6807145703,-0.5406298705,3
.3979450211\H,1.0231526059,-1.0673418177,3.7365499419\H,1.4423555114,0
.6601847125,3.8297958282\H,-4.2186222811,-5.2698301368,1.3754652327\\V
ersion=ES64L-G09RevD.01\State=1-A\HF=-1144.7337323\RMSD=8.357e-09\RMSF
=1.620e-06\Dipole=1.1216213,0.0883398,0.38747\Quadrupole=-13.0674596,5
.7567359,7.3107237,7.3836685,-0.7555696,2.5141738\PG=C01 [X(C19H18N2O4
)]\\@

TS3-2 no HB optimized in implicit CHCl3
1\1\GINC-R3264\FTS\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\09-Oct-2014\0\\
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noei
gentest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS3-OH.M062X\\0,1\
C,-2.8335175686,0.9185982628,0.1062280472\C,-1.5474063032,0.6929292627
,-0.4121698249\C,-0.9075988628,-0.5896108088,-0.2649821429\C,-1.678147
316,-1.6149625918,0.4184712746\C,-2.904006259,-1.3535015897,0.95212129
77\C,-3.4788622895,-0.0741822634,0.7898860806\C,-0.9474326791,1.686458
0925,-1.2554869196\C,0.3279269009,1.7319795271,-1.7024457745\C,1.42185
70825,0.9273418453,-1.2152478523\N,1.8847448846,0.9587358711,0.0265948
932\C,3.0355479728,0.1470489953,0.1524781382\C,3.4173466459,-0.2850949

725,-1.1126202119\C,2.4647666592,0.2968718099,-2.1262031376\C,4.533101
2942,-1.0827318511,-1.2560842114\C,5.246207456,-1.4452490243,-0.111981
0416\C,4.8443495121,-1.007472187,1.1440999781\C,3.7218616671,-0.194943
1312,1.3001177585\O,0.2405061828,-0.8587120696,-0.6990327142\N,-4.7927
193756,0.1775733635,1.3477965138\O,-5.2787965387,1.2830086602,1.198406
9986\O,-5.3405324907,-0.7349599936,1.9391099149\H,3.4005146171,0.13108
2942,2.2813805741\H,5.4065859653,-1.3061041343,2.0207989278\H,6.118958
1546,-2.0805460281,-0.2029922179\H,4.845771028,-1.430698223,-2.2349380
563\C,3.1696646706,1.4266827425,-2.909599522\C,1.8693255892,-0.7250066
182,-3.0948291453\H,0.5805525846,2.3972197892,-2.5222216175\H,-1.62911
29379,2.4351013981,-1.6549982219\O,-1.0560690402,-2.8162874922,0.50771
34351\H,-3.4614111061,-2.1088749061,1.4938115489\H,-3.3237780271,1.875
7445071,-0.0231801716\C,1.1913583658,1.496826995,1.1750980326\H,2.4894
5077,1.8775196024,-3.636525924\H,4.0162118469,1.0020985896,-3.45409904
\H,3.5468128419,2.2041421827,-2.2402358639\H,1.1064700999,-0.247523232
1,-3.7159267277\H,1.4077064788,-1.5445223643,-2.547506667\H,2.65919692
89,-1.1053998017,-3.7488281162\H,0.5303562924,2.2977526541,0.848245321
1\H,1.9255573831,1.8876370373,1.8812903529\H,0.596317215,0.709906229,1
.6493191276\H,-1.6430662957,-3.431907076,0.9549669067\\Version=ES64L-G
09RevD.01\State=1-A\HF=-1144.7566314\RMSD=4.586e-09\RMSF=4.767e-06\Dip
ole=3.7128021,0.5668392,-0.7311494\Quadrupole=-17.3865509,8.5234201,8.
8631308,3.606925,8.7768255,-3.8751565\PG=C01 [X(C19H18N2O4)]\\@

TS4-2 no HB optimized in implicit CHCl3
1\1\GINC-R2217\FTS\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\09-Oct-2014\0\\
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noei
gentest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS4-OH.M062X\\0,1\
C,1.0765838429,-2.9512875471,3.0944979363\C,0.1039122623,-2.0272134602
,2.7477516283\C,-0.6697122704,-1.3883148234,3.7196269161\C,-0.49322298
63,-1.6817000389,5.0533354014\C,0.474108629,-2.6206648799,5.4229673189
\C,1.2451013409,-3.2388491098,4.449752056\C,-1.6130447419,-0.415871273
4,3.0474791411\C,-1.2668872541,-0.6196775427,1.5690236015\N,-0.2740403
368,-1.5838226231,1.4815786651\C,-1.8361308973,0.0783686341,0.58125814
09\C,-1.5190413358,0.086512962,-0.8523471342\C,-0.6424905618,0.8972467
896,-1.4896944609\C,-0.4783673718,0.7666179816,-2.9234989529\C,0.42941
36035,1.5185664997,-3.5602716912\C,1.2761657088,2.4843396954,-2.905083
0729\C,1.1667309399,2.6741269673,-1.5774426575\C,0.1787171793,1.913938
7579,-0.751215751\O,0.0731628831,2.1421513595,0.4298257237\N,0.5859575
468,1.3577721623,-5.0120729118\O,1.4181466034,2.0522977253,-5.55706711
95\O,-0.118336428,0.5477876701,-5.5737520306\H,1.6999417797,-3.4334753
564,2.3517408003\H,2.0004909597,-3.9594876391,4.7421636257\H,0.6261589
261,-2.8598940123,6.4681900421\H,-1.0950669175,-1.1861935362,5.8091814
901\C,-3.0778796609,-0.763721608,3.3313511936\C,-1.3052847557,1.027330
662,3.4674982607\H,-2.5857766443,0.8084507416,0.8794982774\H,-2.081035
0126,-0.5924680714,-1.4993402328\O,1.8896769029,3.5414890014,-0.853393
7475\H,1.9818414757,3.0386409954,-3.511209155\H,-1.0790496685,0.055998
4116,-3.4773033045\C,0.3069176281,-2.0593982928,0.2547262735\H,-3.7453
556936,-0.0887781934,2.7878797287\H,-3.2869417416,-0.6644415054,4.4006
043171\H,-3.3010009318,-1.789855544,3.030049549\H,-1.9625956929,1.7281
065931,2.9454501375\H,-0.2745003273,1.2908990563,3.2227943967\H,-1.456
3841665,1.1431907138,4.5449164356\H,2.4994371014,4.0107455996,-1.43126
09234\H,-0.4734512662,-2.2148976146,-0.4942481823\H,0.7864643647,-3.02
24752923,0.4345991374\H,1.0491369856,-1.3636510154,-0.1529988666\\Vers
ion=ES64L-G09RevD.01\State=1-A\HF=-1144.7313546\RMSD=7.923e-09\RMSF=1.
260e-06\Dipole=-0.058072,-0.3800677,0.7645595\Quadrupole=9.0085303,7.6
589899,-16.6675202,0.7736254,-0.8601265,-0.9810925\PG=C01 [X(C19H18N2O
4)]\\@

TS5-2 no HB optimized in implicit CHCl3
1\1\GINC-R1715\FTS\RM062X\6-31G(2df,p)\C19H18N2O4\ROOT\09-Oct-2014\0\\
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noei
gentest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS5-OH.M062X\\0,1\
C,-5.3169651618,-0.4108969702,1.3751158269\C,-6.3925883546,-0.82451925
77,0.5896128844\C,-6.2665460842,-0.9611167193,-0.7898587414\C,-5.06037
43656,-0.6885391874,-1.4315469515\C,-4.0161891803,-0.2805439796,-0.626
5894875\C,-4.1150649325,-0.1358824035,0.7516101333\H,-5.4247701559,-0.
3080161718,2.449325541\H,-7.343499946,-1.0439456907,1.060037482\H,-7.1
179252307,-1.2845279017,-1.3761385966\H,-4.955528642,-0.79329346,-2.50
44501158\C,-2.7811021381,0.3174651983,1.2809928151\C,-2.1395109352,-0.
706509129,2.2331486609\C,-2.8320130058,1.7065957709,1.9399626803\N,-2.
6882008809,0.0579339283,-1.0138219767\C,-2.2466880166,0.0202464063,-2.
4001167468\C,-1.9551689592,0.4024454031,0.0135822918\C,-0.5853073839,0
.847858617,-0.0671394982\C,0.4676258671,0.0025496936,0.0564262094\C,1.
8520316109,0.3476689973,0.0014575016\H,0.2594309245,-1.0592661327,0.20
638343\H,-0.3905124655,1.9113557744,-0.2086714794\O,1.4508465496,2.667
179346,-0.3494621492\C,2.2486987183,1.7301424204,-0.2105025372\C,2.803

5703261,-0.6710060389,0.1475003242\H,2.4982361001,-1.6992873181,0.3037
45582\C,4.1398334733,-0.379176585,0.0948632274\N,5.1061514486,-1.43497
48762,0.2458291042\O,4.7027311234,-2.5743982699,0.4185159851\O,6.28908
91817,-1.1394387681,0.19324562\C,4.5935328524,0.9501253172,-0.10813265
53\C,3.6963081201,1.958935554,-0.2548648085\O,4.0449783055,3.255621938
7,-0.4536628916\H,5.6620767141,1.130192509,-0.1422575816\H,-2.08965827
,-1.6981658461,1.776645118\H,-2.7433049236,-0.7747324409,3.1411102188\
H,-1.1303013784,-0.3851822824,2.4986394694\H,-3.2840193578,2.445453701
1,1.2742843652\H,-1.820553648,2.0306559471,2.194689972\H,-2.8602958721
,0.7064444096,-2.9869559007\H,-2.3661552052,-0.9948494433,-2.783566504
4\H,-1.2001675706,0.3183694551,-2.4312711803\H,-3.4303218271,1.6487597
739,2.8522275076\H,5.0042125759,3.3106587112,-0.4657521477\\Version=ES
64L-G09RevD.01\State=1-A\HF=-1144.7277216\RMSD=4.616e-09\RMSF=2.577e-0
6\Dipole=-7.1593733,-0.4057053,-0.3807495\Quadrupole=-1.1228293,-12.64
52173,13.7680467,17.0006628,0.4251492,3.6453073\PG=C01 [X(C19H18N2O4)]
\\@

SP-3

MC-3 with HB
1\1\GINC-R2758\FOpt\RM062X\6-31G(2df,p)\C19H17N3O6\ROOT\18-Oct-2014\0\
\# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) ma
xdisk=3489660928\\MC4-OH-TTC.M062X\\0,1\C,-1.1695717098,1.0185972836,-
0.9857905987\N,-0.1990814905,1.9786485135,-0.5032340442\C,1.0884572048
,1.6470725844,-0.1986785137\C,1.5434045437,0.3602854514,-0.3361155228\
C,2.8538884092,-0.0542209696,-0.0416569383\C,3.3770904823,-1.328802948
9,-0.1565460462\C,2.5826583143,-2.4685037004,-0.6265205337\O,1.3974678
289,-2.430413507,-0.9634259697\C,4.7490471663,-1.5446883881,0.19745483
6\C,5.2908797631,-2.7769654449,0.0969202446\C,4.5636860795,-3.92484761
12,-0.3552081197\C,3.2678446573,-3.774062637,-0.7006924007\N,6.6949117
253,-2.9556657408,0.4680520676\O,7.312969791,-1.9830660479,0.851670871
1\O,7.1587265217,-4.0724640623,0.3690283313\C,1.8179095456,2.903713273
2,0.2764074347\C,0.7198394723,3.9391765882,0.1737922502\C,-0.449173073
1,3.332942164,-0.2928387763\C,2.979704003,3.279363225,-0.6588291269\C,
2.2829103601,2.7778658993,1.7370669753\C,0.7403469157,5.2829622701,0.4
607806923\C,-0.4405213423,5.9956054092,0.26650886\C,-1.6053124693,5.40
5669209,-0.1955452229\C,-1.6237044967,4.0467624418,-0.4851215556\H,-0.
8274207409,0.5736304824,-1.923797705\H,-1.309478447,0.2209194244,-0.25
16143602\H,0.8641933307,-0.3996448686,-0.6931397237\H,3.5542391669,0.6
94585494,0.3191614184\H,5.3591614957,-0.7214492838,0.5474914115\H,5.05
75597855,-4.8843728724,-0.4125448624\O,2.4988767656,-4.7800407713,-1.1
352372512\H,2.6346439696,3.3601613622,-1.6919783974\H,3.7833784437,2.5
427037536,-0.6211739783\H,3.3880488269,4.2473339601,-0.3563222265\H,1.
4482675362,2.5064478348,2.3872203865\H,2.6816568912,3.7388014332,2.072
9642875\H,3.0648980296,2.0255589574,1.8489372991\H,1.6211839679,5.7973
981823,0.8244459894\H,-2.4858314883,6.0204801084,-0.3229795678\H,-2.53
17324051,3.5828490517,-0.8463385538\H,-2.1205301711,1.518626496,-1.154
3393404\H,1.63167659,-4.3740492486,-1.3025131085\N,-0.4491940432,7.432
4853503,0.5645054984\O,0.5837665831,7.9227887177,0.9672069099\O,-1.485
4022893,8.0353931814,0.3894666809\\Version=ES64L-G09RevD.01\State=1-A\
HF=-1349.2208648\RMSD=3.891e-09\RMSF=5.197e-06\Dipole=-2.7250813,1.347
311,-0.5094363\Quadrupole=8.3620054,-30.1843589,21.8223535,25.1805379,
1.2327727,-3.6467672\PG=C01 [X(C19H17N3O6)]\\@

SP-3 with HB
1\1\GINC-R1580\FOpt\RM062X\6-31G(2df,p)\C19H17N3O6\ROOT\18-Oct-2014\0\
\# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) ma
xdisk=3489660928\\SP4-OH.M062X\\0,1\C,0.049371795,-1.8372821573,-1.478
9456686\N,-1.3232811343,-1.9630391726,-1.0379518262\C,-2.1015217047,-0
.7720454858,-0.7886326538\C,-2.2614526358,0.0734010654,-2.02041472\C,-
2.1650738273,1.4011086676,-1.9931908578\C,-1.8508736363,2.0957616647,-
0.750138075\C,-1.4865311689,1.2993898151,0.3310152387\O,-1.3931874549,
-0.0488720617,0.2471176454\C,-1.883134192,3.4784486875,-0.5952980345\C
,-1.5563482171,4.007467392,0.6384257324\C,-1.1978277701,3.2274442309,1
.7298270961\C,-1.1616909764,1.852909513,1.5740932443\N,-1.5920796015,5
.4668457931,0.8085946899\O,-1.9138722974,6.1331543885,-0.1516268463\O,
-1.2976461414,5.910978873,1.896358239\C,-3.4368296521,-1.3343980634,-0
.1887720788\C,-2.9262481131,-2.6015608406,0.4606032458\C,-1.6846314979
,-2.923920549,-0.1079813096\C,-4.0995917775,-0.3568070963,0.7763000183
\C,-4.4127058855,-1.7102922664,-1.3144779598\C,-3.4957189728,-3.417435
6396,1.40468933\C,-2.7911767066,-4.5660369075,1.7715591977\C,-1.564198
1647,-4.8954243939,1.222186418\C,-0.9878062248,-4.0650652318,0.2664408
386\H,0.3589833059,-2.754200558,-1.9854200897\H,0.1179415143,-1.012518
9093,-2.19060163\H,-2.4918520387,-0.4664979428,-2.9312362872\H,-2.3146
371067,1.9920373157,-2.8905167373\H,-2.156170714,4.1353697542,-1.41003

79131\H,-0.9608469037,3.6838703758,2.6806641446\O,-0.834097618,1.05339
11895,2.6083816603\H,-3.4636830112,-0.1454155618,1.6381443205\H,-5.039
0527556,-0.780237543,1.1415139331\H,-4.3337572535,0.5852180773,0.27001
67652\H,-5.2701161301,-2.2350762572,-0.8866853822\H,-3.9381487579,-2.3
721683334,-2.0440023667\H,-4.7765080622,-0.8168114703,-1.8294290766\H,
-4.4497065251,-3.204624638,1.8706325468\H,-1.0692485553,-5.7965158414,
1.5581496609\H,-0.0214977146,-4.3049034865,-0.1586168591\H,0.734420218
9,-1.6398431734,-0.6453330591\H,-0.8640734331,0.1401892096,2.297390646
6\N,-3.3714622144,-5.4518228403,2.7822594931\O,-2.7461549542,-6.444404
1047,3.0902310531\O,-4.4461353329,-5.1377654869,3.2503242731\\Version=
ES64L-G09RevD.01\State=1-A\HF=-1349.2467541\RMSD=3.786e-09\RMSF=9.194e
-06\Dipole=0.5710681,-0.6877057,-2.4200476\Quadrupole=18.5092927,-32.1
833844,13.6740916,-11.974605,2.071009,9.0744752\PG=C01 [X(C19H17N3O6)]
\\@

MC-3 no HB
1\1\GINC-R2522\FOpt\RM062X\6-31G(2df,p)\C19H17N3O6\ROOT\18-Oct-2014\0\
\# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) ma
xdisk=3489660928\\MC4-OH-TTC2.M062X\\0,1\C,-1.1776578172,1.0108866299,
-0.9727521769\N,-0.204606575,1.9710979717,-0.4965950259\C,1.0853484801
,1.6361506588,-0.1946765864\C,1.5347104826,0.349315114,-0.3297150518\C
,2.8470437518,-0.070313581,-0.0386391594\C,3.3697804218,-1.3436380242,
-0.1497804851\C,2.5604985932,-2.492309818,-0.6181120392\O,1.3864107969
,-2.4218423651,-0.9411603679\C,4.7426560403,-1.5425711068,0.2039725041
\C,5.2963936017,-2.7688085743,0.1113849024\C,4.567836461,-3.9199002045
,-0.3343561285\C,3.2700463272,-3.7950913109,-0.6817288028\N,6.69762661
14,-2.9435773319,0.4782239448\O,7.3170333798,-1.9698938121,0.856111816
4\O,7.1629528228,-4.0620224409,0.3823495154\C,1.8185840349,2.893289832
6,0.2738649543\C,0.722287786,3.9309026397,0.1711273549\C,-0.4498741857
,3.3249640889,-0.2899409021\C,2.9783041934,3.2634165133,-0.6658632986\
C,2.2881124158,2.7718281671,1.7332585008\C,0.7468514909,5.2752731179,0
.453455299\C,-0.4328195557,5.9909637977,0.2607458865\C,-1.6003775673,5
.4019133037,-0.1956093942\C,-1.6231495332,4.0422321454,-0.4804777461\H
,-0.8386369755,0.5609901213,-1.9096000713\H,-1.3166358466,0.2156859296
,-0.2356397829\H,0.8531154232,-0.4104920328,-0.6817755951\H,3.54921170
75,0.6793806582,0.317082162\H,5.3455751791,-0.711023413,0.5479494491\H
,5.0867215629,-4.8696767776,-0.3802289137\O,2.4872466249,-4.8018137281
,-1.1134772235\H,2.6298521473,3.3421838002,-1.698035645\H,3.7795758346
,2.5240235075,-0.6290438821\H,3.3908168571,4.231033757,-0.3676233489\H
,1.454694767,2.5050638058,2.3869060346\H,2.6909541886,3.732666919,2.06
47791086\H,3.0678775008,2.0171461025,1.8450902934\H,1.6303345759,5.788
4041665,0.8125258251\H,-2.4798836007,6.0183394826,-0.3223038193\H,-2.5
334667371,3.5793304169,-0.8371839423\H,-2.1283967071,1.5116595798,-1.1
408358088\H,3.0020642734,-5.61399504,-1.1319449578\N,-0.4368054549,7.4
279868391,0.5538212532\O,0.5986639731,7.91768793,0.9515794834\O,-1.471
9817512,8.0337125644,0.3804318677\\Version=ES64L-G09RevD.01\State=1-A\
HF=-1349.20906\RMSD=3.943e-09\RMSF=6.253e-06\Dipole=-2.0035928,0.28926
03,-0.5151623\Quadrupole=1.7224288,-17.4614921,15.7390632,16.7201803,-
0.7939582,-2.1334681\PG=C01 [X(C19H17N3O6)]\\@

SP-3 no HB
1\1\GINC-R2524\FOpt\RM062X\6-31G(2df,p)\C19H17N3O6\ROOT\18-Oct-2014\0\
\# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) ma
xdisk=3489660928\\SP4-OH-2.M062X\\0,1\C,0.0620547342,-1.7978796229,-1.
433509894\N,-1.3164432023,-1.9452235242,-1.0180891819\C,-2.1084706366,
-0.7610924851,-0.7685715146\C,-2.2784770999,0.0729266097,-2.0057172854
\C,-2.1807322723,1.3998108501,-1.9850371166\C,-1.8556796114,2.09931775
14,-0.7478804182\C,-1.4876741253,1.307057421,0.3395450462\O,-1.4136614
604,-0.0328778735,0.2658566789\C,-1.87571342,3.4859100681,-0.623053113
2\C,-1.532088579,4.0401246929,0.5915275922\C,-1.1665264521,3.270787777
1,1.6896490447\C,-1.1418405077,1.8934152404,1.5677733333\N,-1.55197347
22,5.4988803042,0.7399742185\O,-1.8779404823,6.1554653648,-0.224948161
1\O,-1.2405230264,5.9560067149,1.8193069632\C,-3.4404266901,-1.3378048
28,-0.1704346078\C,-2.9269574908,-2.612996807,0.4593454369\C,-1.678898
8437,-2.9186215358,-0.1029175616\C,-4.0912245534,-0.3744919768,0.81705
75596\C,-4.42484524,-1.6978990702,-1.2932940297\C,-3.4993757525,-3.446
0691444,1.3858208822\C,-2.791374697,-4.5959142648,1.7423552918\C,-1.55
70068489,-4.9087851754,1.1994102989\C,-0.9782438641,-4.061042556,0.261
2975148\H,0.3934571954,-2.7074094451,-1.939706422\H,0.1313024298,-0.96
8649009,-2.1401967369\H,-2.5126111395,-0.4717519427,-2.9126662987\H,-2
.333973307,1.9887480461,-2.883101851\H,-2.1516984335,4.1252652045,-1.4
509546387\H,-0.9166643995,3.763010264,2.6215404244\O,-0.816494207,1.05
0825929,2.5723917583\H,-3.4383634726,-0.1816993307,1.6702721136\H,-5.
0277534041,-0.8017354723,1.1857527538\H,-4.3299464453,0.5753044065,0.3
267632544\H,-5.2799007106,-2.2270235229,-0.8658951511\H,-3.9570847954,

-2.3520003272,-2.0343631954\H,-4.7915435126,-0.7980661789,-1.795259689
1\H,-4.4581401618,-3.245031229,1.8470003467\H,-1.0587599314,-5.8111724
358,1.526837002\H,-0.0058658568,-4.2873678994,-0.1571339874\H,0.727047
5404,-1.594616903,-0.5855247427\H,-0.6088669385,1.5600490998,3.3609619
668\N,-3.3744202214,-5.4992761401,2.7340339214\O,-2.7465870547,-6.4934
470063,3.0333959399\O,-4.4552295796,-5.1994367019,3.1985162547\\Versio
n=ES64L-G09RevD.01\State=1-A\HF=-1349.2412593\RMSD=9.784e-09\RMSF=7.68
6e-06\Dipole=0.7932179,0.1640965,-1.6654766\Quadrupole=16.6645035,-34.
2310172,17.5665137,-9.9668594,4.8092076,14.7101666\PG=C01 [X(C19H17N3O
6)]\\@

SP-4

MC-4
1\1\GINC-R3229\FOpt\RM062X\6-31G(2df,p)\C20H20N2O4\ROOT\17-Oct-2014\0\
\# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) ma
xdisk=3221225472\\MC3-OH-TTC.M062X\\0,1\C,-1.1878397337,0.979867465,-0
.9914214003\N,-0.2325370474,1.9523133593,-0.5070805733\C,1.0524705053,
1.6427533279,-0.2006350823\C,1.5319697225,0.3598010931,-0.3361250767\C
,2.8451517686,-0.0302421712,-0.0384916836\C,3.4022195148,-1.2944404749
,-0.1473836541\C,2.6272312844,-2.4593304303,-0.6214880793\O,1.45296051
66,-2.4155701624,-0.9528721811\C,4.7733981519,-1.4579090441,0.21552429
02\C,5.3621436335,-2.6701303804,0.1269213363\C,4.6709052373,-3.8414931
293,-0.3243411959\C,3.3697693735,-3.7465406803,-0.6814799939\N,6.76260
46532,-2.8041873736,0.5045543118\O,7.3526930705,-1.8129394611,0.887842
612\O,7.2644897798,-3.9081190949,0.413934496\C,1.7605720054,2.91174958
37,0.2759420635\C,0.648673677,3.9329654291,0.1709185447\C,-0.506604505
5,3.3118325207,-0.296865761\C,2.919689273,3.3014743237,-0.6561944269\C
,2.2244107111,2.7907095273,1.7369630654\C,0.6437003656,5.2816270753,0.
4570807896\C,-0.5345926847,6.0060887307,0.2694613889\C,-1.6788879812,5
.3726502857,-0.1979067922\C,-1.6861240912,4.0096552212,-0.4906488074\H
,-0.8391170153,0.538363867,-1.9289086168\H,-1.318745851,0.1785259802,-
0.259250821\H,0.8676481068,-0.4121453424,-0.6943939185\H,3.528764929,0
.7337647314,0.3234168915\H,5.3518233115,-0.6110608743,0.5645825153\H,5
.2244107868,-4.7679822738,-0.3621631379\O,2.6014682041,-4.7563313625,-
1.120560597\H,2.5742023516,3.3779073268,-1.6895717853\H,3.7335510988,2
.5758858196,-0.6182756466\H,3.313640763,4.2755827574,-0.3537329078\H,1
.390785702,2.5083559152,2.3838163058\H,2.6079394425,3.7573610365,2.074
6906069\H,3.0159503187,2.0487778831,1.8521868709\H,1.5396038733,5.7737
878147,0.8221380599\H,-0.5569562371,7.0663433998,0.4890496056\H,-2.588
047543,5.9450328048,-0.3399178879\H,-2.5872176786,3.5325107899,-0.8542
711318\H,-2.1447754436,1.4684920526,-1.1608659888\C,3.2116703049,-6.01
99453465,-1.2126545956\H,2.4491733282,-6.7056184053,-1.5796888256\H,3.
5707380271,-6.3588361146,-0.2333181934\H,4.0571120198,-6.0016679997,-1
.9110749926\\Version=ES64L-G09RevD.01\State=1-A\HF=-1184.0481943\RMSD=
9.742e-09\RMSF=8.271e-06\Dipole=-2.6693563,2.5963001,-0.2183331\Quadru
pole=-12.184002,13.5708241,-1.3868221,2.0913944,-2.6763046,3.8050948\P
G=C01 [X(C20H20N2O4)]\\@

SP-4
1\1\GINC-R217\FOpt\RM062X\6-31G(2df,p)\C20H20N2O4\ROOT\29-Oct-2014\0\\
# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) max
disk=3221225472\\SP3-OH.M062X\\0,1\C,0.0649304875,-1.7540379154,-1.402
789113\N,-1.3240650141,-1.9266426629,-1.0374499088\C,-2.1216494789,-0.
751201217,-0.7896115929\C,-2.2956456204,0.0812150257,-2.0272045964\C,-
2.2038401708,1.4084207068,-2.0118549871\C,-1.8805587838,2.114272027,-0
.777920299\C,-1.5129005035,1.3298169217,0.3139154246\O,-1.4409799154,-
0.0068864548,0.2509819311\C,-1.8978301849,3.5025776034,-0.6616499122\C
,-1.5518462348,4.0639079034,0.5471212982\C,-1.1852785176,3.3047813763,
1.65556513\C,-1.1638937471,1.9257018449,1.5432666915\N,-1.568565116,5.
5231293756,0.6825583788\O,-1.8934494815,6.1737869278,-0.2877134201\O,-
1.2559529095,5.9919976505,1.7572114789\C,-3.4498149471,-1.3332411856,-
0.1901652898\C,-2.9245915259,-2.5930313108,0.4626487678\C,-1.677166605
6,-2.8931101111,-0.0895848501\C,-4.1171942528,-0.3600557149,0.77633661
71\C,-4.4227261444,-1.7180451119,-1.3146239719\C,-3.4886758115,-3.4225
061787,1.405527376\C,-2.7912782513,-4.5663503881,1.8068923616\C,-1.550
4454229,-4.8518417756,1.2572268702\C,-0.9694274602,-4.0165800341,0.300
5307918\H,0.432835596,-2.6617916861,-1.8869647983\H,0.1455643771,-0.93
07789229,-2.1159739986\H,-2.5243362877,-0.4680765608,-2.9326919925\H,-
2.3577427087,1.9936676571,-2.9123744779\H,-2.1728895278,4.1359714185,-
1.4944511776\H,-0.9361729739,3.8158209464,2.5736000962\O,-0.8455055657
,1.0700703751,2.5337158999\H,-3.4741856464,-0.1531606772,1.6338192112\
H,-5.055511522,-0.7876097106,1.1406502756\H,-4.3558151297,0.5828930639
,0.2722313732\H,-5.2722709503,-2.2555123066,-0.88618666\H,-3.939365036
7,-2.3738280364,-2.0439215224\H,-4.8003425057,-0.8299499472,-1.8300503

897\H,-4.4569256558,-3.1894372307,1.8379339014\H,-1.0126365545,-5.7362
802058,1.5799234081\H,0.0072071902,-4.2409052572,-0.1113419906\H,0.697
1243987,-1.5305042701,-0.5341044461\C,-0.4981611642,1.6324965873,3.778
5542373\H,-0.2775507347,0.7955722911,4.4392775714\H,-1.3255943823,2.21
89225541,4.1944570614\H,0.3866925775,2.2734448674,3.6915989395\H,-3.21
81721809,-5.2260622516,2.5524943022\\Version=ES64L-G09RevD.01\State=1-
A\HF=-1184.0751191\RMSD=5.685e-09\RMSF=1.029e-05\Dipole=0.0650183,-1.5
599884,-0.1417842\Quadrupole=8.4233142,-22.5389942,14.11568,-1.8680009
,0.6426522,-0.823604\PG=C01 [X(C20H20N2O4)]\\@

CCC-4
1\1\GINC-R2940\FOpt\RM062X\6-31G(2df,p)\C20H20N2O4\ROOT\17-Oct-2014\0\
\# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) ma
xdisk=3221225472\\CCC3-OH.M062X\\0,1\C,-0.7177520297,0.9122890747,-2.7
181153504\C,-0.6815711663,0.7842662399,-1.3041301473\C,0.5887647828,0.
9343000355,-0.5930290832\C,1.7791233325,1.1509290312,-1.4435428177\C,1
.7014223419,1.2093895313,-2.7967826775\C,0.426890602,1.0951550947,-3.4
228947005\C,-1.9172352509,0.6903803848,-0.6307008951\C,-2.2235143787,0
.4333997856,0.6919966184\C,-1.4428428987,-0.1784600214,1.6815349164\N,
-0.5919416746,-1.1851649032,1.5122977306\C,0.0519033848,-1.5192594928,
2.722580811\C,-0.4748413944,-0.7345215629,3.7420007577\C,-1.4962566533
,0.2039691708,3.1528205292\C,-0.0313128636,-0.9035220698,5.0371738257\
C,0.9541607574,-1.8594853696,5.2871142388\C,1.4769835844,-2.6258537684
,4.2519177572\C,1.0311648725,-2.4692150221,2.9406656006\O,0.7094213682
,0.9049796682,0.6328757549\N,0.3594064482,1.1923891188,-4.8720030774\O
,-0.7296259455,1.1008205705,-5.4055318032\O,1.4034679295,1.3599254136,
-5.4741754187\H,1.4519730413,-3.0557100502,2.1336908764\H,2.2485867455
,-3.3565451605,4.4634095923\H,1.3211696198,-2.0013885904,6.296399328\H
,-0.433213417,-0.3012791278,5.8453593273\C,-2.8922054386,-0.02459515,3
.7494730857\C,-1.0661560824,1.6730438375,3.2994566646\H,-3.187983632,0
.7903678825,1.0426584258\H,-2.775640054,0.9605927778,-1.2459934911\O,2
.9120875814,1.2566817987,-0.7230963046\H,2.5645435681,1.3557762044,-3.
4291891387\H,-1.65926204,0.8486918983,-3.2500295515\C,-0.3637027727,-1
.9167421139,0.2887340354\H,-3.6272383924,0.6377365214,3.2852773827\H,-
2.8685444234,0.1971538831,4.8196528627\H,-3.2151952843,-1.0601131783,3
.6194944386\H,-1.8056127244,2.3259136123,2.8281722607\H,-0.1027889824,
1.8340559781,2.8130839538\H,-0.9941677755,1.9290122483,4.3601601861\C,
4.0996922662,1.4715929706,-1.4432975656\H,-1.2439077985,-1.8209823356,
-0.3459673364\H,-0.2044181642,-2.966621221,0.5406141788\H,0.5059692065
,-1.5253628625,-0.2459103525\H,4.8995313597,1.5435196648,-0.7071418878
\H,4.0500657982,2.4009235323,-2.0236203421\H,4.3060826464,0.6403260713
,-2.1288831981\\Version=ES64L-G09RevD.01\State=1-A\HF=-1184.0447786\RM
SD=5.219e-09\RMSF=1.629e-05\Dipole=-0.5768302,-1.4136401,3.3170397\Qua
drupole=12.6396791,6.1411841,-18.7808632,-2.6554071,-3.8976491,3.21632
02\PG=C01 [X(C20H20N2O4)]\\@

CTC-4
1\1\GINC-R3227\FOpt\RM062X\6-31G(2df,p)\C20H20N2O4\ROOT\17-Oct-2014\0\
\# M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) ma
xdisk=3221225472\\CTC3-OH.M062X\\0,1\C,-2.3654892646,-3.6072423053,-0.
1573526964\C,-3.1300586507,-2.4500046547,-0.0387844957\C,-2.9843399698
,-4.8301679553,-0.3076892074\C,-4.3792642815,-4.8790846578,-0.34694563
41\C,-5.1267033551,-3.7137437458,-0.2377521688\C,-4.5125955941,-2.4710
185553,-0.0831938268\H,-2.3984832708,-5.7393875869,-0.396208428\H,-4.8
81811338,-5.8307993071,-0.4685589137\H,-6.2083853395,-3.7647355701,-0.
2780260422\H,-5.1051846597,-1.567076917,-0.0176014898\N,-2.273927465,-
1.343006063,0.1199783417\C,-2.7717435108,-0.0315899353,0.4696735358\C,
-0.9054700949,-3.2384076946,-0.0793763639\C,-0.1442923843,-3.644631443
2,-1.3480687806\C,-0.9723023223,-1.7174523641,0.0516865351\C,0.1684327
546,-0.9493581973,0.1010000937\C,0.2712113882,0.4436124939,-0.03611579
47\H,-0.6320169457,1.0025607817,-0.2664655672\H,1.099082242,-1.4925069
408,0.1891953674\C,1.4187868218,1.2197407754,0.0175668349\C,1.29118575
55,2.6220372808,-0.2184829375\H,0.3215638531,3.0555529682,-0.431517209
8\C,2.7483698904,0.6453360802,0.3076811259\O,2.9524564258,-0.537904131
,0.5262448578\C,3.8790243287,1.6118758905,0.3234641328\O,5.0523856718,
1.0162764362,0.5888569688\H,4.5069572667,3.6472186323,0.1030274462\C,2
.3784092879,3.4222773869,-0.1782698181\C,3.6975903064,2.9323762669,0.0
931658562\N,2.2136313563,4.8490412546,-0.4207992398\O,1.0954585539,5.2
689205763,-0.6479285231\O,3.211072705,5.5434068831,-0.3815884391\C,-0.
2412340779,-3.848462354,1.1659759967\H,-3.7422721616,-0.1444378794,0.9
544264608\H,-2.8860808099,0.6133356434,-0.4067824345\H,-2.0822907818,0
.4365088839,1.1747289042\H,-0.6030523635,-3.2057758552,-2.2369112545\H
,-0.1588141709,-4.7329946788,-1.4527435641\H,0.8956921656,-3.314451525
8,-1.2926819851\H,-0.2597865066,-4.9392157646,1.0911012845\H,-0.771817
1673,-3.5559325981,2.0749741764\H,0.7985642729,-3.5224130471,1.2462275
878\C,6.1873805253,1.8457640006,0.6279043019\H,7.0349607955,1.19959881

03,0.852378588\H,6.0917153722,2.6114041756,1.4073680917\H,6.3483047466
,2.3423465068,-0.3366816735\\Version=ES64L-G09RevD.01\State=1-A\HF=-11
84.0446139\RMSD=6.765e-09\RMSF=7.369e-06\Dipole=-2.3913311,-2.6635394,
0.1627689\Quadrupole=18.1061795,-16.7895125,-1.316667,2.4750371,-0.144
9369,5.0440379\PG=C01 [X(C20H20N2O4)]\\@

TS2-4
1\1\GINC-R90\FTS\RM062X\6-31G(2df,p)\C20H20N2O4\ROOT\18-Oct-2014\0\\#
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeige
ntest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS23-OH.M062X\\0,1\C
,0.0392206937,-0.0735876276,-0.1013201645\C,0.0013396593,-0.0576368394
,1.4289569115\N,1.304806575,-0.151816815,1.8949723494\C,2.2192691426,-
0.0763039068,0.8507033369\C,1.5309191348,-0.0149791191,-0.3639537873\C
,2.2218612452,0.0565060269,-1.5525502848\C,3.6195874739,0.0741784891,-
1.5293501321\C,4.2914072657,0.0173888173,-0.317142968\C,3.6039865199,-
0.0569757055,0.8950531928\H,4.1463592975,-0.0886711043,1.8319236957\H,
5.3753757114,0.0348691092,-0.3042039274\H,4.1766129919,0.134070554,-2.
4561156244\H,1.6883297997,0.0995254265,-2.4974758329\C,-0.6900735948,1
.1280395226,-0.708545676\C,-0.5393791926,-1.3879429222,-0.6507165103\C
,1.6262963633,-0.2629275989,3.2892903253\C,-1.0636785257,0.0296728567,
2.2336679579\H,-0.9154110043,0.0503049712,3.3106658646\C,-2.4672948768
,0.1048002338,1.8115099616\H,-2.8992148129,1.1052174455,1.7173996073\C
,-3.3281556026,-0.9156330268,1.5911403409\C,-2.9196096231,-2.352149788
7,1.74899404\O,-1.8217580058,-2.7040885368,2.1069029535\C,-4.691139544
2,-0.6128435267,1.2027316875\H,-5.0109859581,0.4165656349,1.1007771681
\C,-3.9742197711,-3.3701995633,1.4391593332\O,-3.5214092372,-4.6182933
709,1.5822159362\C,-5.2192050659,-3.0114124393,1.0658216813\H,-5.99562
40552,-3.7269505104,0.840402218\C,-5.5505591518,-1.6111951481,0.961176
539\N,-6.9247177714,-1.2740177145,0.5613590536\O,-7.6804932517,-2.1986
787853,0.3478291064\O,-7.2190509905,-0.1023644366,0.4692126059\H,-0.55
59509724,1.1350583946,-1.7942336614\H,-0.3017801003,2.0667323337,-0.30
70737415\H,-1.7641374765,1.0759151828,-0.5071852653\H,-0.3229576818,-1
.4631817128,-1.7205273525\H,-1.6232109568,-1.417372217,-0.5161075081\H
,-0.1037971144,-2.2501205451,-0.1415631959\H,2.6768840532,-0.529599301
7,3.4015087847\H,1.0188830875,-1.0518756248,3.7451347265\H,1.440428372
3,0.6754203606,3.8270871822\C,-4.4333052795,-5.6598713499,1.3159237376
\H,-3.8936110375,-6.5905765774,1.4819362322\H,-4.7864288072,-5.6162855
699,0.2791050997\H,-5.2963779249,-5.6068339745,1.9896140028\\Version=E
S64L-G09RevD.01\State=1-A\HF=-1184.0194583\RMSD=7.722e-09\RMSF=8.417e-
07\Dipole=1.1700713,-0.1221948,0.4108735\Quadrupole=-14.185886,7.54521
21,6.6406739,8.1159366,-0.7585068,2.3179923\PG=C01 [X(C20H20N2O4)]\\@

TS3-4
1\1\GINC-R204\FTS\RM062X\6-31G(2df,p)\C20H20N2O4\ROOT\18-Oct-2014\0\\#
 M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noeig
entest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS33-OH.M062X\\0,1\
C,-2.8369488939,0.9458856285,0.1103938609\C,-1.5506458698,0.7152570835
,-0.4059751818\C,-0.9174545948,-0.5685979488,-0.2520967796\C,-1.692360
5233,-1.594678291,0.434177436\C,-2.9209524443,-1.3281208365,0.96443928
91\C,-3.4847772168,-0.0429308329,0.7952483271\C,-0.9478637285,1.701277
3032,-1.2550061624\C,0.3269095325,1.7372998289,-1.7052810673\C,1.41595
34028,0.9289660921,-1.2138552392\N,1.8830698309,0.9698676758,0.0270103
174\C,3.0288690499,0.1522318899,0.1573284604\C,3.4049350469,-0.2935960
259,-1.1049200477\C,2.4545363551,0.2864521448,-2.1215859262\C,4.515196
2413,-1.0994655378,-1.2443549408\C,5.229323999,-1.4565461791,-0.099141
6895\C,4.8337125739,-1.0049398344,1.1539815504\C,3.7165476233,-0.18418
69538,1.3059035384\O,0.2300748237,-0.8414528209,-0.6838994943\N,-4.799
4838394,0.2176629394,1.3496180458\O,-5.2787158861,1.325827492,1.196584
5969\O,-5.3551007888,-0.6894980351,1.9416816038\H,3.4003044784,0.15270
01285,2.2851653235\H,5.3966989428,-1.2988698338,2.0318157717\H,6.09803
2542,-2.09782957,-0.1869211206\H,4.8229524395,-1.457859686,-2.22102731
25\C,3.1654536988,1.4070724748,-2.912670839\C,1.8528816133,-0.73822582
03,-3.083121148\H,0.5815394745,2.3946196983,-2.5307280445\H,-1.6267911
148,2.4510945744,-1.6571420602\O,-1.0538566148,-2.7827745701,0.5106826
946\H,-3.4945235628,-2.0661027329,1.5059480751\H,-3.3243680899,1.90401
56486,-0.0223516886\C,1.1933776325,1.5209649286,1.1714248994\H,2.48690
16741,1.8587642086,-3.6406001163\H,4.0079963076,0.9738305897,-3.456588
557\H,3.5492171855,2.1854171285,-2.2481189653\H,1.0945381572,-0.259786
8084,-3.7090167543\H,1.3843657148,-1.5499523719,-2.5300824418\H,2.6406
553482,-1.1297400917,-3.7330904938\H,0.5424686885,2.3279872004,0.83908
41501\H,1.9301940365,1.9068981395,1.8775073865\H,0.5875787489,0.743626
268,1.6479611363\C,-1.7381772773,-3.8251142445,1.1572355239\H,-1.09042
62397,-4.6997874192,1.1051807926\H,-2.6915556624,-4.0458750226,0.66146
28506\H,-1.9381028149,-3.5816875987,2.2083204404\\Version=ES64L-G09Rev
D.01\State=1-A\HF=-1184.0412366\RMSD=4.213e-09\RMSF=3.279e-06\Dipole=3
.7854744,0.4268555,-0.7447156\Quadrupole=-17.683327,9.323356,8.3599711

,4.6301295,8.5658478,-4.1486963\PG=C01 [X(C20H20N2O4)]\\@

TS4-4
1\1\GINC-R1499\FTS\RM062X\6-31G(2df,p)\C20H20N2O4\ROOT\18-Oct-2014\0\\
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noei
gentest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS43-OH.M062X\\0,1
\C,1.0743775599,-2.9544549651,3.0992088445\C,0.1041279348,-2.028489749
1,2.7504240898\C,-0.6692468964,-1.3876507572,3.7215111413\C,-0.4951505
87,-1.6810559472,5.0555742519\C,0.4694744085,-2.6220258373,5.426885903
\C,1.240452124,-3.2419906664,4.4547654189\C,-1.6098717573,-0.413437660
6,3.0480566213\C,-1.263433226,-0.6191956458,1.5698680001\N,-0.27195971
02,-1.5852798478,1.4838236882\C,-1.8325340741,0.0778654787,0.581495374
3\C,-1.5264915163,0.076135234,-0.8547151151\C,-0.6550703716,0.88018623
95,-1.5066274282\C,-0.506030501,0.7404278128,-2.9409367493\C,0.3960999
693,1.4873760442,-3.5908708469\C,1.2551483376,2.4578040142,-2.95725336
84\C,1.1597052496,2.6563068528,-1.6268943924\C,0.1770247589,1.90007908
15,-0.7849819742\O,0.0834402482,2.132406292,0.3959147919\N,0.534053699
1,1.3148934604,-5.0444848042\O,1.3598952699,2.003067709,-5.6066703722\
O,-0.1788330972,0.5016654529,-5.5909008827\H,1.6973421571,-3.439153333
3,2.3578103435\H,1.9936976978,-3.9644488593,4.7482275432\H,0.619239429
5,-2.8615132526,6.472388886\H,-1.0969698443,-1.183938919,5.8104300364\
C,-3.0757022228,-0.7575839912,3.3310395619\C,-1.2990826796,1.029259406
4,3.4673569272\H,-2.5807439345,0.809442007,0.8796696043\H,-2.096012949
7,-0.6064984386,-1.4912185173\O,1.8796142863,3.5169496224,-0.903236693
1\H,1.9480799283,2.997662612,-3.5850032059\H,-1.1138226324,0.027667405
5,-3.484092175\C,0.3191803767,-2.0504673578,0.2577926563\H,-3.74107504
8,-0.081311544,2.7865989226\H,-3.2857705168,-0.6574627294,4.4000436386
\H,-3.3010283548,-1.7832445759,3.0297801986\H,-1.9520888069,1.73141518
16,2.9417157092\H,-0.2663533377,1.2885689176,3.2263511644\H,-1.4537225
446,1.1472711629,4.5440528094\C,2.8303629329,4.2925532134,-1.597651983
4\H,-0.4561872426,-2.2175635237,-0.4938982752\H,0.8141319208,-3.005536
3437,0.437752554\H,1.0508657004,-1.3418338396,-0.1467592908\H,3.312797
3463,4.9248239329,-0.8543610731\H,2.3466215361,4.9170028365,-2.3576678
021\H,3.57803898,3.6543678145,-2.0827637316\\Version=ES64L-G09RevD.01\
State=1-A\HF=-1184.017111\RMSD=4.538e-09\RMSF=5.331e-06\Dipole=0.06594
96,-0.219399,0.8614022\Quadrupole=9.1923339,8.8675588,-18.0598927,1.93
49551,-1.0605827,-1.011574\PG=C01 [X(C20H20N2O4)]\\@

TS5-4
1\1\GINC-R2412\FTS\RM062X\6-31G(2df,p)\C20H20N2O4\ROOT\18-Oct-2014\0\\
M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT=(TS,calcfc,noei
gentest,maxcyc=200) IOP(2/17=4) maxdisk=3221225472\\TS53-OH.M062X\\0,1
\C,-5.3246983047,-0.3875922972,1.3715544615\C,-6.4028431221,-0.7912036
617,0.5843790248\C,-6.2751464461,-0.9316352801,-0.7945553307\C,-5.0647
034309,-0.6729340594,-1.4339734533\C,-4.0180546271,-0.2746579361,-0.62
74087742\C,-4.118504483,-0.1265357496,0.7503203452\H,-5.4338028397,-0.
2815609846,2.4453294139\H,-7.3571243592,-0.9997369377,1.0529709076\H,-
7.1285697342,-1.2471696022,-1.3821200669\H,-4.9585908717,-0.7805032447
,-2.5064770188\C,-2.7808990465,0.3133815239,1.281833557\C,-2.151289665
,-0.7176402563,2.2345166098\C,-2.818313854,1.702490199,1.9414065208\N,
-2.6859551055,0.0496287642,-1.0123448595\C,-2.2420168864,0.0053753702,
-2.3976372901\C,-1.9515956185,0.389178124,0.0159489644\C,-0.578271248,
0.823296252,-0.0630393738\C,0.46920875,-0.0290678041,0.0621737777\C,1.
8555449339,0.3058784855,0.0081636615\H,0.2536261954,-1.0893496373,0.21
27227471\H,-0.3762330038,1.8853242192,-0.2050781129\O,1.4720751216,2.6
250727601,-0.3449287723\C,2.2638998373,1.6840811674,-0.2048495053\C,2.
8012319531,-0.7179652,0.1555957973\H,2.4898806337,-1.7443437744,0.3128
326472\C,4.1383767055,-0.4337093777,0.1030178234\N,5.095720998,-1.4986
729778,0.2559943534\O,4.6816250794,-2.6343545843,0.4297278892\O,6.2815
217087,-1.215304086,0.2041281268\C,4.6094486445,0.8909038567,-0.101193
7902\C,3.7167675082,1.9064776412,-0.2495017941\O,4.0424142254,3.204141
2712,-0.4499738202\H,5.6783935609,1.0442301296,-0.1321558444\H,-2.1123
608457,-1.7098573096,1.7781613601\H,-2.7561860449,-0.7789677892,3.1422
343744\H,-1.1386464712,-0.4075191633,2.5002911639\H,-3.2603317236,2.44
67065014,1.2749887503\H,-1.8039719179,2.0151955798,2.1988136889\H,-2.8
440745527,0.7004487092,-2.9860260574\H,-2.3755763464,-1.0078981964,-2.
7812571635\H,-1.1912038698,0.2882949983,-2.4262369226\H,-3.4195088609,
1.6508503194,2.8521546598\C,5.410227572,3.5061765562,-0.503691249\H,5.
4861526004,4.581332973,-0.6668672391\H,5.9069014834,2.9764045691,-1.32
69567725\H,5.917115768,3.2428799391,0.4337225849\\Version=ES64L-G09Rev
D.01\State=1-A\HF=-1184.0123813\RMSD=3.208e-09\RMSF=2.999e-06\Dipole=-
7.181676,-0.2137778,-0.4089392\Quadrupole=2.184512,-13.5645043,11.3799
924,19.94677,0.1249174,3.5338913\PG=C01 [X(C20H20N2O4)]\\@

SP-5

MC-5 with HB

```
 1\1\GINC-R279\FOpt\RM062X\6-31G(2df,p)\C20H19N1O3\ROOT\12-Nov-2014\0\\
 # M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) max
 disk=3221225472\\MC5-COOH1-TTC.M062X\\0,1\C,-1.2255917671,1.0350618648
 ,-0.9757911923\N,-0.2508034621,1.9916468818,-0.4962493081\C,1.02890999
 78,1.6630781994,-0.1981628349\C,1.4878588055,0.3705016821,-0.337425233
 \C,2.7949387005,-0.0375428959,-0.0477789986\C,3.3456400915,-1.30797564
 98,-0.1559440372\C,2.5765443915,-2.4692220604,-0.6199443162\O,1.375578
 2331,-2.3842261719,-0.9468039757\C,4.7203143185,-1.477028083,0.2031659
 363\C,5.3444719632,-2.6798126353,0.1303075154\C,4.6063484401,-3.809264
 6516,-0.3181386191\C,3.2949477961,-3.7344734247,-0.6788209679\C,1.7599
 382984,2.9202008742,0.2747300862\C,0.6637692439,3.9587016073,0.1775206
 23\C,-0.50351509,3.3561298205,-0.2834134844\C,2.9186691663,3.292343081
 9,-0.6651387954\C,2.2304713843,2.7904270513,1.7329099171\C,0.681068624
 4,5.3072538963,0.4646035005\C,-0.4874517588,6.0490130751,0.2844939099\
 C,-1.6442560804,5.4333837544,-0.1762551849\C,-1.6738501818,4.070950901
 5,-0.4697616279\H,-0.8893195447,0.5890182355,-1.9154725583\H,-1.365942
 456,0.2364741549,-0.2426078043\H,0.8074453803,-0.3884630513,-0.6919179
 525\H,3.4871036942,0.7211382028,0.3099130205\H,5.2614924099,-0.5975476
 435,0.5427314115\H,5.0779011839,-4.7848201869,-0.3871812039\C,2.623675
 4768,-5.0016295689,-1.1369208197\H,2.5679391544,3.3733891612,-1.696366
 4903\H,3.7218890803,2.554755381,-0.6321281275\H,3.3284670411,4.2608090
 999,-0.3656979955\H,1.3968206382,2.5192301278,2.3844391653\H,2.6295915
 939,3.7511516342,2.0694170419\H,3.0117450495,2.0368424384,1.8424963975
 \H,1.5862842735,5.7859675942,0.824465433\H,-0.4927259108,7.1093547976,
 0.5047931201\H,-2.5454389081,6.0195690599,-0.3122674268\H,-2.584162548
 9,3.607563869,-0.828056542\H,-2.1748505031,1.540010863,-1.1397350318\O
 ,3.2113407321,-6.049908899,-1.1879140595\O,1.3472775002,-4.885636378,-
 1.4788996235\H,1.0876252183,-3.9375297683,-1.3547667814\H,6.38522033,-
 2.7891062415,0.4060939144\\Version=ES64L-G09RevD.01\State=1-A\HF=-1053
 .6482005\RMSD=5.226e-09\RMSF=3.813e-06\Dipole=-0.8024271,5.1780777,0.8
 548424\Quadrupole=21.6481215,-26.6639282,5.0158067,-0.1373459,4.729553
 8,-6.6875143\PG=C01 [X(C20H19N1O3)]\\@
```

SP-5 with HB

```
 1\1\GINC-R578\FOpt\RM062X\6-31G(2df,p)\C20H19N1O3\ROOT\12-Nov-2014\0\\
 # M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) max
 disk=3221225472\\SP5-COOH1.M062X\\0,1\C,0.0360455307,-1.8205275181,-1.
 5225878444\N,-1.3408054993,-1.9704183205,-1.1026910265\C,-2.1109753998
 ,-0.7864809685,-0.8237326199\C,-2.287058789,0.0846026192,-2.0304677882
 \C,-2.1672938862,1.4087038254,-1.9700574657\C,-1.8277358278,2.07919812
 26,-0.7213608047\C,-1.4627833172,1.2755900415,0.3652612914\O,-1.381367
 3449,-0.0724798639,0.2158504954\C,-1.8380886586,3.4600739546,-0.567818
 524\C,-1.4977104066,4.0422177203,0.646579266\C,-1.1513926029,3.2319927
 075,1.7140106005\C,-1.1316597138,1.8405234221,1.5978192218\C,-3.430191
 456,-1.3515001759,-0.1972170166\C,-2.8911728262,-2.601265533,0.4654042
 941\C,-1.6660106026,-2.9213557059,-0.1260464618\C,-4.090545643,-0.3670
 909259,0.7628068592\C,-4.4143079978,-1.7490645868,-1.3076913124\C,-3.4
 212309846,-3.40327702,1.451894204\C,-2.7130860596,-4.5400612672,1.8526
 821136\C,-1.4959146655,-4.8462009732,1.2623026276\C,-0.9475770932,-4.0
 379499412,0.264226881\H,0.3696445599,-2.7357289929,-2.0170689604\H,0.1
 023542025,-0.9999800992,-2.2399004123\H,-2.5404762076,-0.4312360601,-2
 .9489097225\H,-2.3227334398,2.0222461788,-2.8518339471\H,-2.1168329355
 ,4.0770635734,-1.4164251263\H,-0.892022417,3.6455748704,2.6810868868\C
 ,-0.7871279065,1.0695821907,2.8467903704\H,-3.4630963655,-0.170254888,
 1.6346364988\H,-5.0393950046,-0.7798173102,1.1163258673\H,-4.306702313
 9,0.5810615643,0.2591427716\H,-5.2569707722,-2.2861342135,-0.865800197
 2\H,-3.9358546398,-2.4067985451,-2.0381641018\H,-4.8004661985,-0.86503
 99448,-1.823776975\H,-4.36865617,-3.1524990857,1.9185839747\H,-0.94872
 09866,-5.7234781129,1.5882091155\H,0.0125708475,-4.2761520462,-0.17740
 2972\H,0.7066271874,-1.6067576486,-0.6801836575\O,-0.4737512968,1.6318
 416174,3.857952713\O,-0.8743610803,-0.2621185566,2.8042773262\H,-3.110
 5998236,-5.1763570047,2.6337313189\H,-1.0850390085,-0.5644452223,1.907
 3065243\H,-1.5079069865,5.1189981228,0.758845714\\Version=ES64L-G09Rev
 D.01\State=1-A\HF=-1053.6714834\RMSD=5.040e-09\RMSF=6.633e-06\Dipole=-
 0.7056884,-0.0271616,-2.3050696\Quadrupole=1.1323707,7.188422,-8.32079
 27,-3.7553252,-6.4464596,-7.8572141\PG=C01 [X(C20H19N1O3)]\\@
```

MC-5 no HB

```
 1\1\GINC-R516\FOpt\RM062X\6-31G(2df,p)\C20H19N1O3\ROOT\12-Nov-2014\0\\
 # M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) max
 disk=3221225472\\MC5-COOH2-TTC.M062X\\0,1\C,-1.2336395473,1.050241641,
 -0.9749920886\N,-0.2596396814,2.0051462582,-0.4960017099\C,1.025218227
 5,1.669149367,-0.198023102\C,1.4779933686,0.380988167,-0.3381347457\C,
```

```
 2.7894049415,-0.0386401612,-0.0496419152\C,3.3271867816,-1.3072366703,
 -0.161098616\C,2.5298347907,-2.4725620339,-0.6340729172\O,1.3529389908
 ,-2.3670548633,-0.9497868707\C,4.7017231443,-1.4802189258,0.1971967908
 \C,5.3228633974,-2.6824253239,0.123639791\C,4.5813305003,-3.8115482598
 ,-0.325713916\C,3.2700779467,-3.7479359609,-0.6887425523\C,1.758434253
 7,2.9257167505,0.2754037816\C,0.6641367527,3.9671667371,0.1794148802\C
 ,-0.5056719245,3.366893855,-0.2817766708\C,2.9177848812,3.2965694977,-
 0.6635904287\C,2.2301597215,2.7949128027,1.7327050891\C,0.685841974,5.
 3149402952,0.4676561457\C,-0.4798043034,6.0626146109,0.2896573629\C,-1
 .6383326271,5.4508873414,-0.1707824556\C,-1.6728359851,4.0886410627,-0
 .4657203976\H,-0.8979592377,0.6022056762,-1.9143619266\H,-1.3741773225
 ,0.2500177694,-0.2430851624\H,0.7981047007,-0.3788194331,-0.692641094\
 H,3.4861455823,0.7160122251,0.3085344966\H,5.245910138,-0.6022366711,0
 .5373132575\H,5.0636162034,-4.7818258438,-0.3905318913\C,2.6680208955,
 -5.035184492,-1.1311729919\H,2.5661602711,3.3808034727,-1.6942830057\H
 ,3.7174648673,2.5548762679,-0.633209067\H,3.3323797732,4.2628533966,-0
 .3629341115\H,1.3957118694,2.5269150445,2.3845777477\H,2.634260907,3.7
 53536344,2.0699453153\H,3.0075041056,2.0369193187,1.840897186\H,1.5935
 429072,5.7893965927,0.8273467144\H,-0.4807964475,7.1227206814,0.511181
 8979\H,-2.5379609565,6.0399870212,-0.3057002881\H,-2.5851938986,3.6289
 742739,-0.8238313522\H,-2.1832885858,1.5550018044,-1.1391252005\O,3.27
 96406851,-6.0755548142,-1.1735505\O,1.3791316001,-4.969274831,-1.48725
 6141\H,1.1470813244,-5.8721717908,-1.7429699093\H,6.3632580149,-2.7971
 442002,0.398225571\\Version=ES64L-G09RevD.01\State=1-A\HF=-1053.634516
 2\RMSD=4.587e-09\RMSF=2.729e-06\Dipole=-0.8184427,3.1784632,0.4313188\
 Quadrupole=11.498617,-9.7898908,-1.7087262,3.8132014,4.9776938,-0.3148
 554\PG=C01 [X(C20H19N1O3)]\\@

SP-5 no HB
 1\1\GINC-R640\FOpt\RM062X\6-31G(2df,p)\C20H19N1O3\ROOT\12-Nov-2014\0\\
 # M062X/6-31G(2df,p) SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) max
 disk=3221225472\\SP5-COOH2.M062X\\0,1\C,0.0519214709,-1.787531686,-1.4
 788387744\N,-1.3297942415,-1.9595293152,-1.0863790391\C,-2.1129034556,
 -0.7790515249,-0.8027390475\C,-2.3042696193,0.0805807076,-2.0166041844
 \C,-2.1955327186,1.405727692,-1.9606901185\C,-1.8463747506,2.076938186
 1,-0.7154853698\C,-1.4745253858,1.2652469803,0.3691854475\O,-1.4007669
 488,-0.0678441407,0.2324600486\C,-1.8352817317,3.458105033,-0.57436665
 56\C,-1.4577842447,4.0520732076,0.6238519875\C,-1.0957305693,3.2464605
 868,1.6881020304\C,-1.1116067982,1.8530186985,1.5865284357\C,-3.430653
 7453,-1.3639107265,-0.1858326523\C,-2.8892218809,-2.6206106067,0.45925
 57177\C,-1.6570965246,-2.9231324635,-0.1262342545\C,-4.0897095185,-0.3
 939447586,0.7888571893\C,-4.4150065223,-1.7527105525,-1.2990310609\C,-
 3.4244992577,-3.4429409993,1.4244442652\C,-2.7146012618,-4.5836133501,
 1.814202184\C,-1.4902292841,-4.872450972,1.2307339441\C,-0.9377045711,
 -4.043358612,0.2516969404\H,0.4078075806,-2.6927824881,-1.9766806949\H
 ,0.1198995074,-0.9590909065,-2.1872328989\H,-2.5568333063,-0.440412412
 6,-2.932420844\H,-2.359390269,2.0180755878,-2.8419584407\H,-2.12126903
 45,4.0696995151,-1.4247902517\H,-0.7979822905,3.6690127142,2.640276774
 9\C,-0.7497483508,1.1055647477,2.8238267719\H,-3.4455170527,-0.2032647
 583,1.6489151819\H,-5.0333952539,-0.8157426974,1.1468037379\H,-4.31841
 22662,0.5558339025,0.2928354394\H,-5.2555320111,-2.2978464242,-0.86238
 14409\H,-3.9356816241,-2.4010586908,-2.0375888404\H,-4.8052593166,-0.8
 648519982,-1.8055829042\H,-4.3795876899,-3.2061649716,1.8833507093\H,-
 0.9423561221,-5.7542651922,1.5438737698\H,0.0273255812,-4.2696945724,-
 0.1857440499\H,0.7022500936,-1.5718110932,-0.6214830989\O,-0.216598477
 2,1.6175698176,3.7730046259\O,-1.111327025,-0.1860253536,2.8199289689\
 H,-3.1191275329,-5.2382634087,2.5766485327\H,-0.8455729104,-0.53796357
 82,3.6801791788\H,-1.4482236701,5.1298968773,0.7236247398\\Version=ES6
 4L-G09RevD.01\State=1-A\HF=-1053.6682893\RMSD=4.442e-09\RMSF=1.571e-05
 \Dipole=-0.3948103,0.0314329,-1.0171993\Quadrupole=-1.5917258,1.918226
 9,-0.326501,-4.6408173,-3.6957304,-8.2281134\PG=C01 [X(C20H19N1O3)]\\@
```


S5. References

1 M. S. Tunuli, M. A. Rauf and Farhataziz, *J. Photochem.*, 1984, **24**, 411-413.

2 (a) C. Reichardt, in *Solvents and Solvent Effects in Organic Chemistry*, Wiley-VCH Verlag GmbH & Co. KGaA, 2004, pp. 389-469; (b) J. P. Cerón-Carrasco, D. Jacquemin, C. Laurence, A. Planchat, C. Reichardt and K. Sraïdi, *J. Phys. Org. Chem.*, 2014, **27**, 512-518.

3 D. R. Lide, ed., *CRC Handbook of Chemistry and Physics , Internet Version 2005, <**Error! Hyperlink reference not valid.***, Boca Raton, FL, 2005.

4 M. J. Kamlet, J. L. M. Abboud, M. H. Abraham and R. W. Taft, *J. Org. Chem.*, 1983, **48**, 2877-2887.

5 The ion current is a function of the compound characteristics and is not a true quantification.

6 S. Delbaere, J.-C. Micheau and G. Vermeersch, *J. Org. Chem.*, 2003, **68**, 8968-8973.
7 N. T. Lu, V. N. Nguyen, S. Kumar and A. McCurdy, *J. Org. Chem.*, 2005, **70**, 9067-9070.
8 J. N. Miller and J. C. Miller, *Statistics and Chemometrics for Analytical Chemistry*, 5th edn., Prentice Hall, 2005.
9 L. Yasmin, X. Chen, K. A. Stubbs and C. L. Raston, *Sci. Rep.*, 2013, **3**.
10 (a) D. A. Davis, A. Hamilton, J. Yang, L. D. Cremar, D. Van Gough, S. L. Potisek, M. T. Ong, P. V. Braun, T. J. Martinez, S. R. White, J. S. Moore and N. R. Sottos, *Nature*, 2009, **459**, 68-72; (b) M. Bieniek, A. Michrowska, Ł. Gułajski and K. Grela, *Organometallics*, 2007, **26**, 1096-1099.
11 (a) Y. Hirshberg and E. Fischer, *Journal of the Chemical Society*, 1954, 297-303; (b) Y. J. Cho, S. H. Lee, J. W. Bae, H.-J. Pyun and C. M. Yoon, *Tetrahedron Lett.*, 2000, **41**, 3915-3917.
12 C. J. Roxburgh, P. G. Sammes and A. Abdullah, *Dyes Pigments*, 2009, **82**, 226-237.
13 (a) E. Inoue, H. Kokado, I. Shimizu, H. Kobayashi and Y. Takahashi, *B. Chem. Soc. Jpn.*, 1972, **45**, 1951-1956; (b) I. Shimizu, H. Kokado and E. Inoue, *B. Chem. Soc. Jpn.*, 1969, **42**, 1730-1734.
14 N. A. Darwish, A. C. Aragones, T. A. Darwish, S. Ciampi and I. Díez-Pérez, *Nano Lett.*, 10.1021/nl5034599.
15 Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **119**, 525.
16 (a) W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257-2261; (b) M. J. Frisch, J. A. Pople and J. S. Binkley, *J. Chem. Phys.*, 1984, **80**, 3265-3269.
17 Y. Sheng, J. Leszczynski, A. A. Garcia, R. Rosario, D. Gust and J. Springer, *J. Phys. Chem. B*, 2004, **108**, 16233-16243.
18 L. A. Curtiss, K. Raghavachari, P. C. Redfern, A. G. Baboul and J. A. Pople, *Chem. Phys. Lett.*, 1999, **314**, 101-107.
19 Y. Zhao, N. E. Schultz and D. G. Truhlar, *J. Chem. Theory Comput.*, 2006, **2**, 364-382.
20 A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. A*, 2009, **113**, 6378-6396.
21 J. P. Merrick, D. Moran and L. Radom, *J. Phys. Chem. A*, 2007, **111**, 11683-11700.
22 J. Ho and M. Coote, *Theor. Chem. Acc.*, 2010, **125**, 3-21.
23 (a) H. Eyring, *J. Chem. Phys.*, 1935, **3**, 107-115; (b) M. G. Evans and M. Polanyi, *Trans. Faraday Soc.*, 1935, **31**, 875-894.
24 A. J. Karas, R. G. Gilbert and M. A. Collins, *Chem. Phys. Lett.*, 1992, **193**, 181-184.
25 D. C. Solha, T. M. Barbosa, R. V. Viesser, R. Rittner and C. F. Tormena, *J. Phys. Chem. A*, 2014, **118**, 2794-2800.