Supporting Information for

Rigidochromism by imide functionalisation of an aminomaleimide fluorophore

Jonathan T. Husband,[a] Yujie Xie,[a] Thomas R. Wilks,[a] Louise Male,[a] Miquel Torrent-Sucarrat,[b,c] Vasilios G. Stavros[d] and Rachel K. O'Reilly[a]

a. School of Chemistry, University of Birmingham, Edgbaston, Birmingham, B15 2TT, United Kingdom.
b. Department of Organic Chemistry I, Universidad del País Vasco (UPV/EHU), and Donostia International Physics Center (DIPC), Manuel Lardizabal Ibilbidea 3, Donostia 20018, Spain.
c. Ikerbasque, Basque Foundation for Science, Plaza Euskadi 5, 48009 Bilbao, Euskadi, Spain.
d. Department of Chemistry, University of Warwick, Coventry, CV4 8AL, United Kingdom.

1 Contents

2 Experimental

2.1 Materials

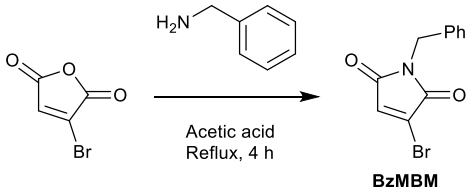
All non-synthesized chemicals were obtained from either Sigma Aldrich, Fisher Chemicals, Acros Chemicals, Alfa Aesar or Fluorochem and used as received.

2.2 Instrumentation

NMR spectra were recorded with a Bruker Avance III HD 300, Bruker Avance III HD 400 or a Bruker Avance III HD 500 spectrometer at 298 K and 300, 400 and 500 MHz, respectively. Shifts are quoted in parts per million and relative to the internal standard trimethylsilane. High-resolution mass spectra (HR-MS) were recorded using a Bruker UHR-Q-ToF MaXis spectrometer or a Waters Xevo G2-XS QTof instrument with electrospray ionization. FTIR spectroscopy was carried out using an Agilent Technologies Cary 630 FTIR spectrometer. 16 scans from 600 to 4000 cm^{-1} were taken at a resolution of 4 cm^{-1}, and the spectra were corrected for background absorbance. UV–visible spectroscopy was carried out with a Perkin Elmer Lambda 35 UV–visible spectrometer or an Agilent Cary 60 UV–visible spectrometer at room temperature. Fluorescence emission and excitation spectrum were obtained with an Edinburgh Instruments FS5 Spectrofluorometer in quartz 3.5 mL cuvettes for liquid samples (Starna Cell, Type: 3/Q/10), and analyzed in Fluoracle (Edinburgh Instruments) and Origin 2019 (Origin Labs). For solid state samples the SC-30 integrating sphere module of the FS5 was used on 1-10 mg of dye.

2.3 Synthetic Methods

3-bromo-1-trityl-1H-pyrrole-2,5-dione (BzMBM)



Scheme S1. *Synthesis of* ***BzMBM****.*

In this case, bromomaleic anhydride (1 g, 5.6 mmol) was dissolved in acetic acid (25 mL) in a round bottom flask containing a stirrer bar. To this benzylamine (642 mg, 6.4 mmol) was slowly added. This was refluxed for 4 hours and then left to cool. The solvent is removed *in vacuo* and then purified by silica column chromatography and eluted with 20% DCM in hexane. The product was obtained as a yellow powder (984 mg, 66%). ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.38-7.28 (m, 5H, Ar*H*), 6.87 (s, 1H, C*H*), 4.71 (s, 2H, CH_2) ppm. ^{13}C NMR ($CDCl_3$, 101 MHz) δ = 168.2 (*C*O), 165.0 (*C*O), 135.6 (*C*H), 131.9 (*C*Br), 131.5 (Ar*C*), 128.8 (Ar*C*), 128.6 (Ar*C*), 128.1 (Ar*C*), 42.4 (CH_2) ppm. HR-MS (MaXis): [M+Na^+] – calculated m/z 265.9813, observed m/z 265.9817. FTIR: *v* = 3093 (υAr-C-H), 2933 (υC-H), 1705 (υC=O) cm^{-1}.

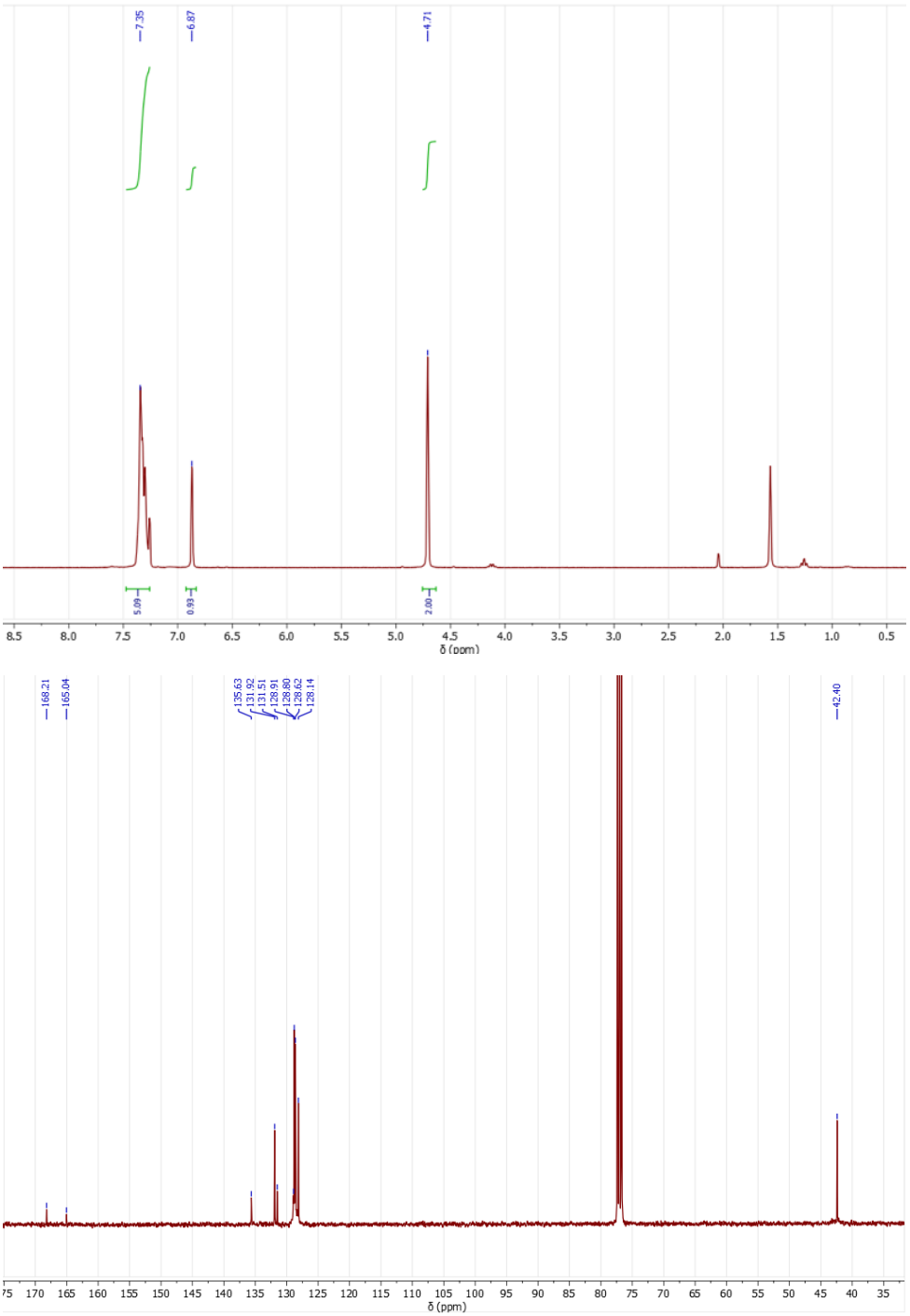
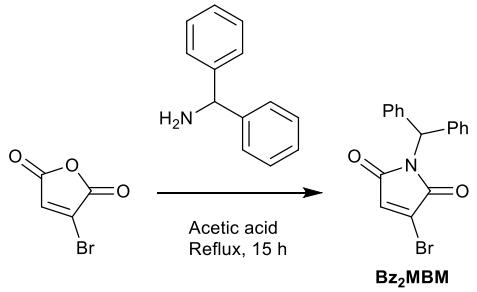


Figure S1. *^{1}H (top) and ^{13}C (lower) NMR spectra for* ***BzMBM****. Solvent: $CDCl_3$.*

1-benzhydryl-3-bromo-1H-pyrrole-2,5-dione (Bz_2MBM)



Scheme S2. *Synthesis of* ***Bz_2MBM****.*

In this case, bromomaleic anhydride (1 g, 5.6 mmol) was dissolved in acetic acid (25 mL) in a round bottom flask containing a stirrer bar. To this diphenylmethylamine (1.03 g, 5.6 mmol) was slowly added. This was refluxed for 15 hours and then left to cool. The solvent is removed *in vacuo* and then the orange solid was purified by silica column chromatography and eluted with 10% diethyl ether in hexane (R_f = 0.1). The product was obtained as a yellow powder (415 mg, 22%). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.48 – 7.17 (m, 10H, Ar*H*), 6.89 (s, 1H, C*H*), 6.54 (s, 1H, ArC*H*) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ = 168.1 (*C*O), 164.9 (*C*O), 137.6 (Ar*C*), 131.8(*C*H), 131.5(*C*Br), 128.6 (Ar*C*), 128.5 (Ar*C*), 128.0 (Ar*C*), 58.5 (*C*H) ppm. HR-MS (MaXis): [M+Na^+] – calculated m/z 363.9944 observed m/z 363.9942. FTIR: *v* = 3096 (υAr-C-H), 2910 (υC-H), 1705 (υC=O), 1656 (υC=O) cm^{-1}.

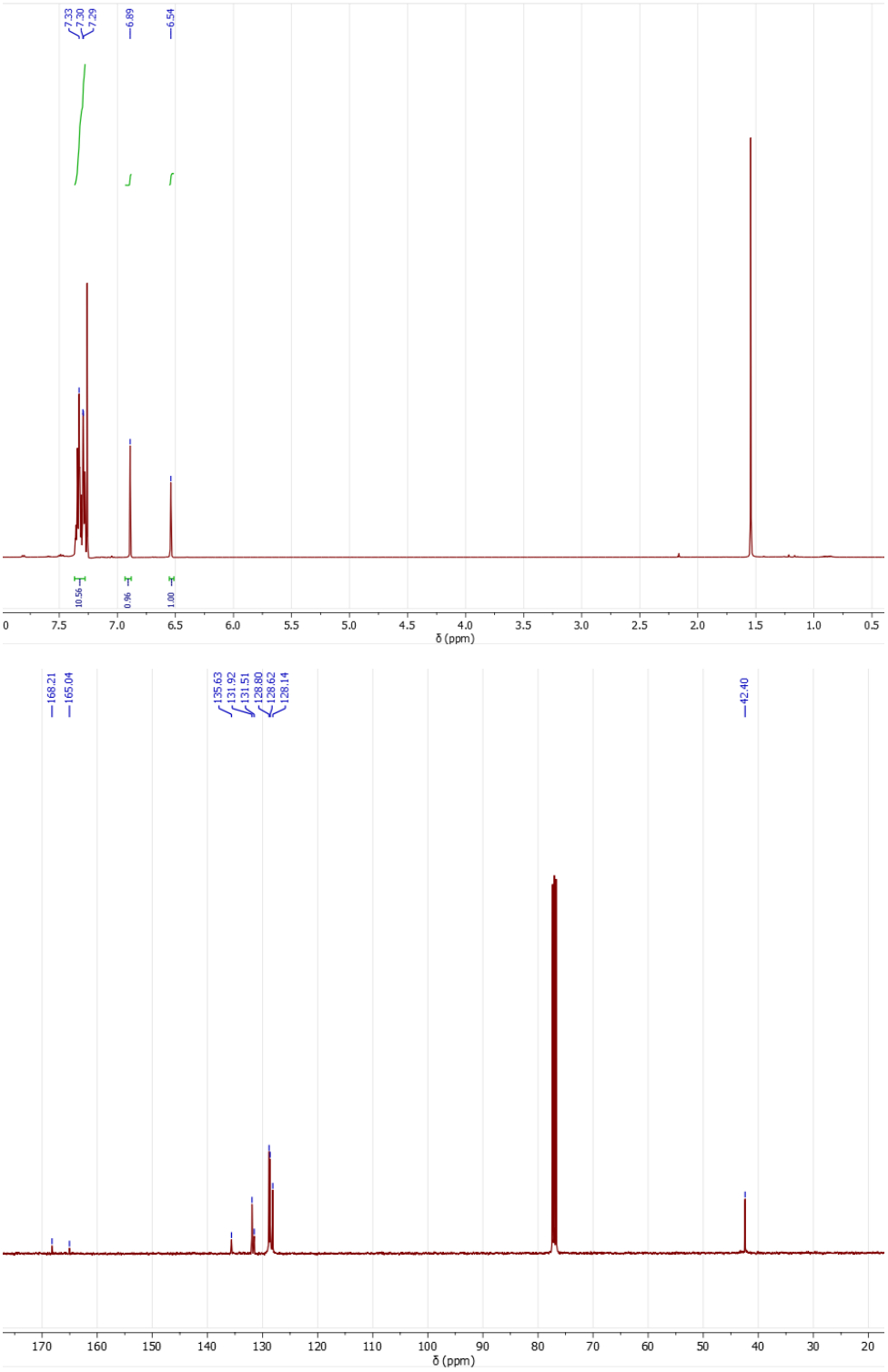
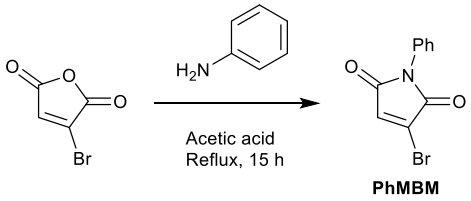


Figure S2. *^{1}H (top) and ^{13}C (lower) NMR spectra for* ***BzMBM****. Solvent: $CDCl_3$.*

3-bromo-1-phenyl-1H-pyrrole-2,5-dione (PhMBM)



Scheme S3. *Synthesis of* ***PhMBM****.*

Bromomaleic anhydride (1 g, 5.6 mmol) was dissolved in acetic acid (25 mL) in a round bottom flask containing a stirrer bar. To this aniline (0.82 g, 8.9 mmol) was slowly added. This was refluxed for 15 hours and then left to cool. This was poured onto ice and the precipitate filtered, and washed with cold water. This solid was purified by silica column chromatography on a 12 g RediSep Rf silica flash column and eluted with an ethyl acetate and hexane gradient eluent on a CombiFlash Rf+ Lumen by Teledyne. The product was obtained as a yellow powder (358 mg, 17%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.46 – 7.37 (m, 2H, Ar*H*), 7.37-7.23 (m, 3H, Ar*H*), 6.96 (s, 1H, C*H*) ppm. ^{13}C NMR ($CDCl_3$, 101 MHz) δ = 167.4 (*C*O), 164.2 (*C*O), 131.9 (C*H*), 131.9 (*C*Br) 131.0 (ArC), 129.3 (Ar*C*), 128.4 (Ar*C*), 126.1 (Ar*C*) ppm. HR-MS (Xevo): [M+H^{+}] – calculated m/z 265.9817 observed m/z 265.9813. FTIR: *v* = 3093 (υAr-C-H), 1705 (υC=O), 1690 (υC=O) cm^{-1}.

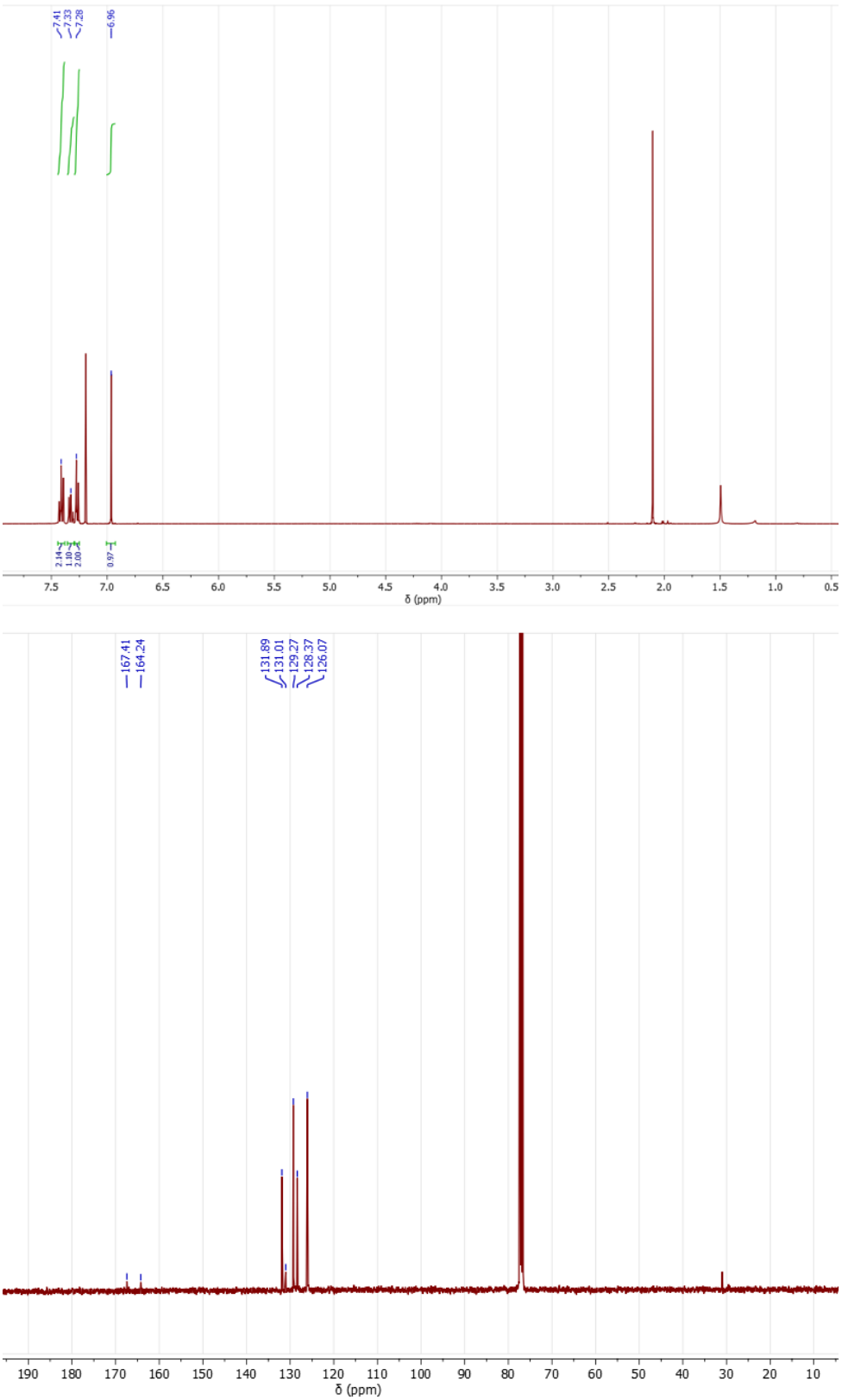
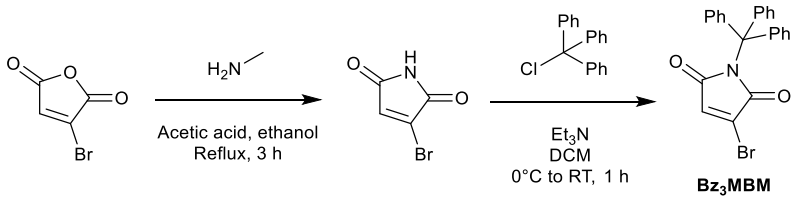


Figure S3. *^{1}H (top) and ^{13}C (lower) NMR spectra for* ***PhMBM****. Solvent: $CDCl_3$.*

2.3.1 3-bromo-1-trityl-1H-pyrrole-2,5-dione (Bz_3MBM)



Scheme S4. *Synthesis of* ***Bz_3MBM****.*

Step 1: Monobromomaleimide was synthesized based on a previously reported literature procedure.[1] To a solution of bromomaleic anhydride (1 g, 5.65 mmol) in acetic acid (20 ml) was added methyl amine in ethanol (695 µl, 5.65 mmol.) The solution was refluxed for 3 hours after which the solvent was removed *in vacuo*. The resultant solid was purified by silica column chromatography and eluted with 10% ethyl acetate in petroleum ether 40-60 °C to give a cream coloured solid (15%.) R_f : 0.2. Characterisation data matched those from the literature. ^{1}H NMR ($CDCl_3$, 300 MHz) δ =7.52 (br, 1H, N*H*), 6.90 (s, 1H, C*H*CBr) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ = 168.6, 165.5, 132.2, 131.4 ppm. MS (ESI): $[M+H]^+$ – calculated: 189.9; observed: 190.0.

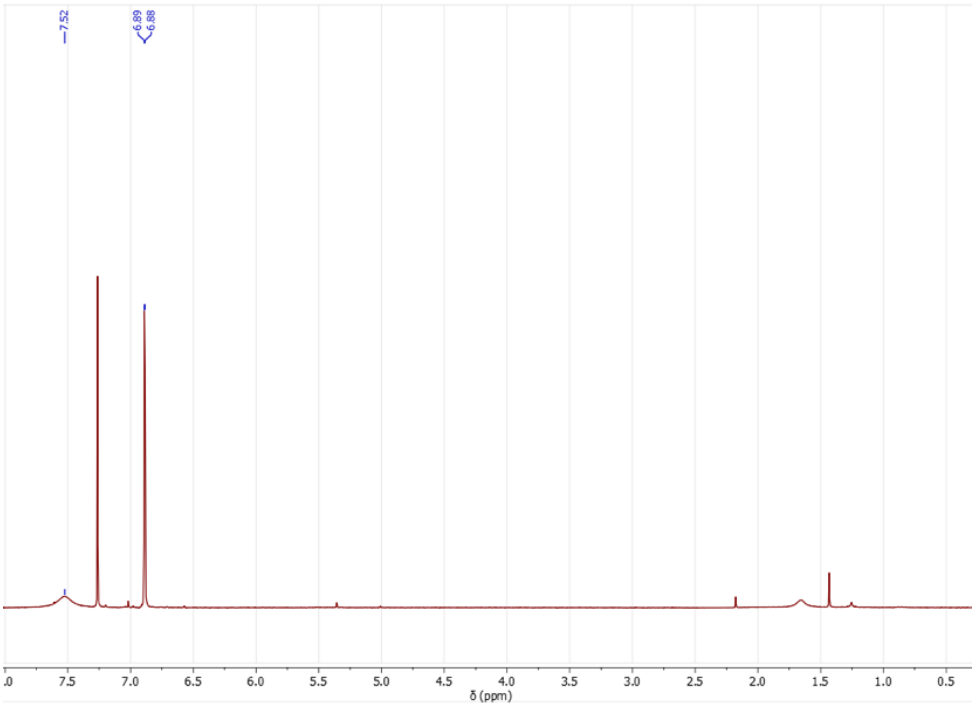


Figure S4. *^{1}H NMR spectrum of monobromomaleimide. Solvent: $CDCl_3$.*

Step 2: To a solution of dry DCM (25 mL) under nitrogen, was added monobromomaleimide from step 1 (0.25 g, 1.4 mmol) and trityl chloride (0.42 g, 1.5 mmol). This was put onto ice to cool, and triethylamine (160 mg, 1.65 mmol) was slowly added. The ice bath was removed and the reaction was left for 1 hour at room temperature. The solution was dried under vacuum and purified by silica column chromatography (2% ethyl acetate in petroleum ether as the eluent, R_f = 0.1) to give a white solid (238 mg, 47%). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.36 (d, $^3J_{HH}$ = 7.5 Hz, 6H), 7.32 – 7.14 (m, 9H), 6.76 (s, 1H) ppm. ^{13}C NMR ($CDCl_3$, 126MHz) δ = 168.4 (*C*O), 165.1 (*C*O), 141.9 (*C*H), 132.6 (*C*Ar), 131.6 (*C*Br), 128.6 (*C*Ar), 127.7 (*C*Ar), 126.9 (*C*Ar), 74.3 (*C*) ppm. HR-MS (MaXis): $[M+Na^+]$ – calculated m/z 440.0257 observed m/z 440.0256. FTIR: *v* = 3096 (υC-H), 1707 (υC=O), 1686 (υC=O) cm^{-1}.

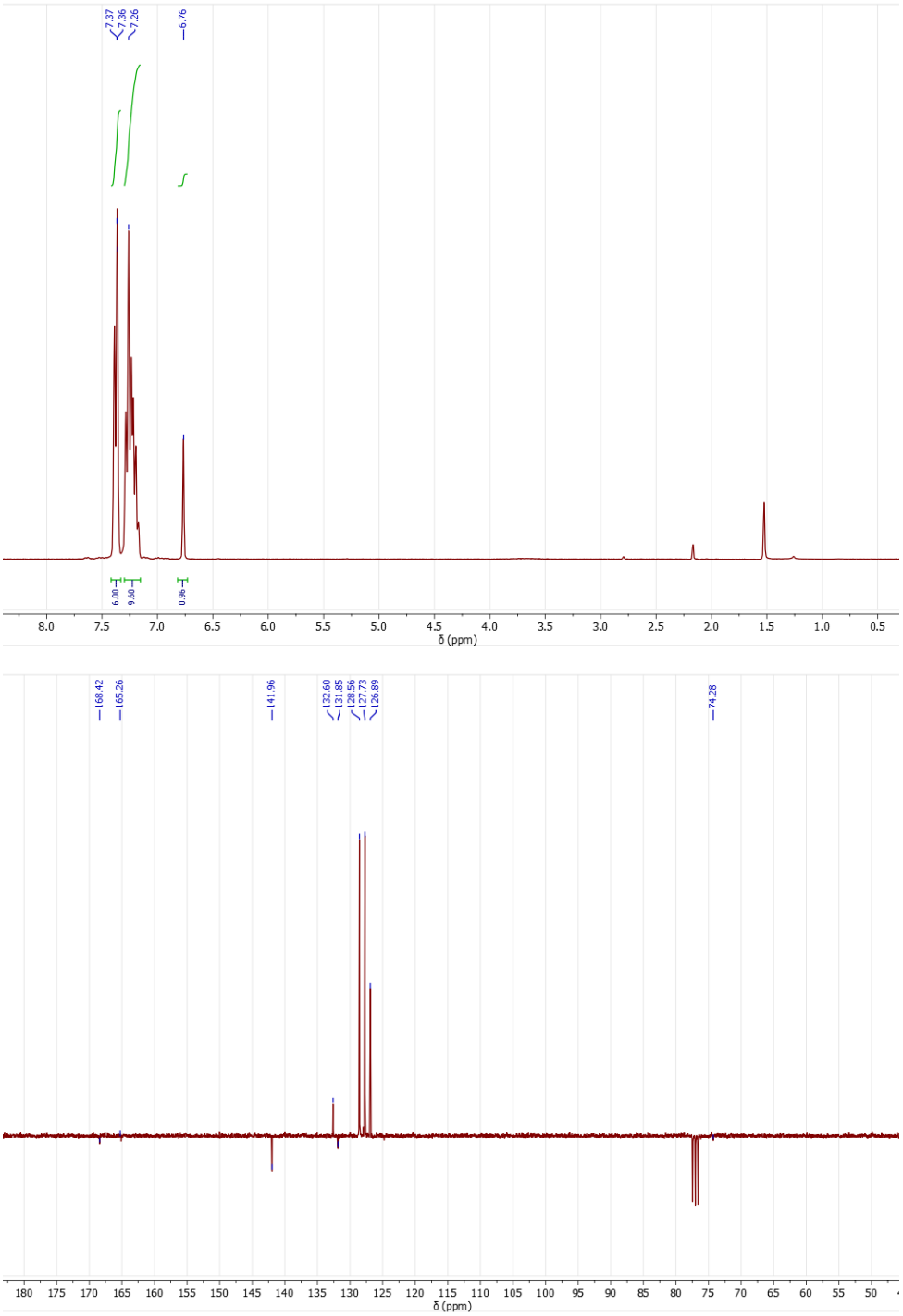
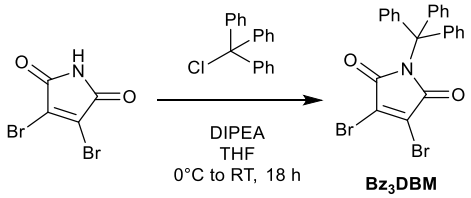


Figure S5. *^{1}H (top) and ^{13}C (lower) NMR spectra for* ***Bz_3MBM****. Solvent: $CDCl_3$.*

3,4-dibromo-1-trityl-1H-pyrrole-2,5-dione (Bz_3DBM)



Scheme S5. *Synthesis of* ***Bz_3DBM****.*

To a solution of Dry THF (50 mL) under nitrogen, was added dibromomaleimide (0. 5 g, 1.9 mmol) and trityl chloride (0.58 g, 2.1 mmol). This was put onto ice to cool, to which diisopropylethylamine (DIPEA) (390 mg, 2.46 mmol) was slowly added. The ice bath was removed and the reaction was left for 18 hours at room temperature. The solution was dried under vacuum and purified by silica column chromatography (2-5% ethyl acetate in petroleum ether as the eluent) to give a white solid (240 mg, 26%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ = 7.31 – 7.29 (d), 7.22 – 7.09 (m) ppm. ^{13}C NMR ($CDCl_3$, 101 MHz) δ = 163.7 (*C*O), 141.7 (*C*Br), 130.2 (*C*Ar), 128.5 (*C*Ar), 127.8 (*C*Ar), (*C*Ar), 127.0 (*C*Ar), 75.2 (*C*N) ppm. HR-MS (Xevo): [M+Na^++MeOH] – calculated m/z 549.9624 observed m/z 549.9611. FTIR: *v* = 3056 (υC-H), 1716 (υC=O) cm^{-1}.

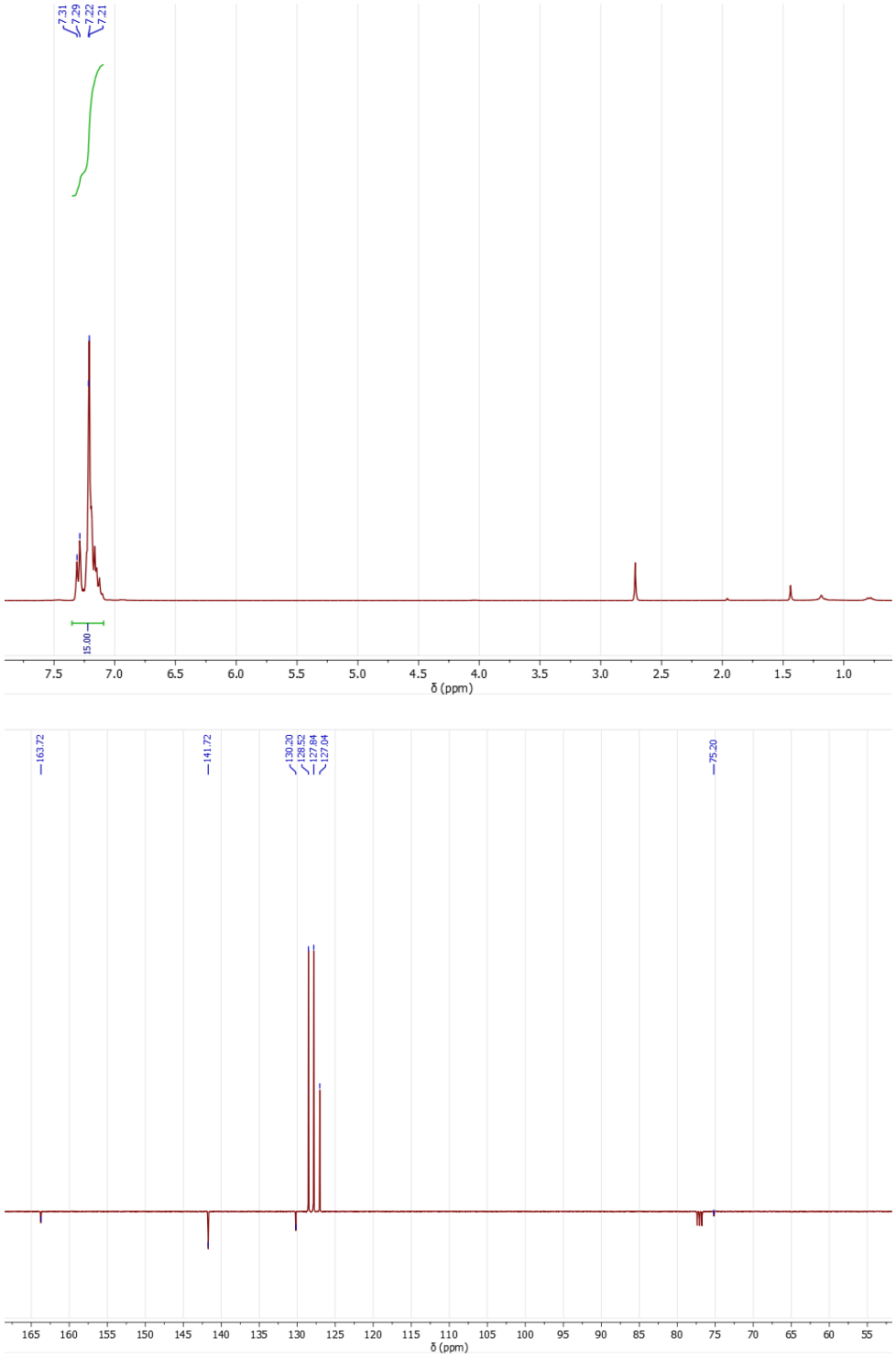
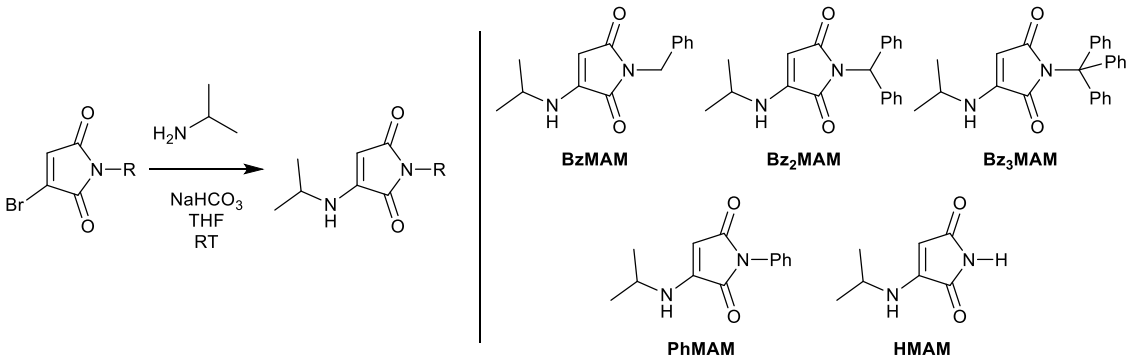


Figure S6. *^{1}H (top) and ^{13}C (lower) NMR spectra for* ***Bz_3DBM****. Solvent: $CDCl_3$.*

General synthesis of aminomaleimides



Scheme S6. *General synthetic procedure for monoaminomaleimides.*

The synthesis was developed from a previously reported protocol.[2] Initially, the bromomaleimide (1 equiv.) was added to a round bottom flask, which contained THF and a magnetic stirrer bar. To this $NaHCO_3$ (1.5 equiv.) was added. A solution of isopropylamine (1.05 equiv.) in 10-20 mL of THF was added to a dropping funnel. Over 10 minutes this was added dropwise to the stirred solution of base and bromomaleimide. This was left for another 60-90 minutes, after which it was filtered to remove the base and dried *in vacuo.* The crude solid was purified by silica column chromatography with conditions listed for each individual product. The fractions containing product were combined and dried *in vacuo.*

3-(isopropylamino)-pyrrole-2,5-dione (HMAM)

An eluent of 75% ethyl acetate in petroleum ether was used to isolate a yellow solid (160 mg, 75%). ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.17 (s, 1H), 5.26 (s, 1H), 4.80 (s, 1H), 3.51 (dq, $^3J_{HH}$ = 13.1, 6.5 Hz, 1H), 1.64 (s, 1H), 1.27 (d, $^3J_{HH}$ = 6.5 Hz, 1H) ppm. ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 172.3 (*C*O), 167.9 (*C*O), 148.6 (*CN*H), 85.2 (*C*H), 46.4 (*C*H), 21.8 (*C*H_3) ppm. HR-MS (MaXis): [M+Na^+] – calculated m/z 177.0634 observed m/z 177.0635. FTIR: *v* = 3178 (υN-H), 2983 (υC-H), 1697 (υC=O), 1618 (υC=O) cm^{-1}.

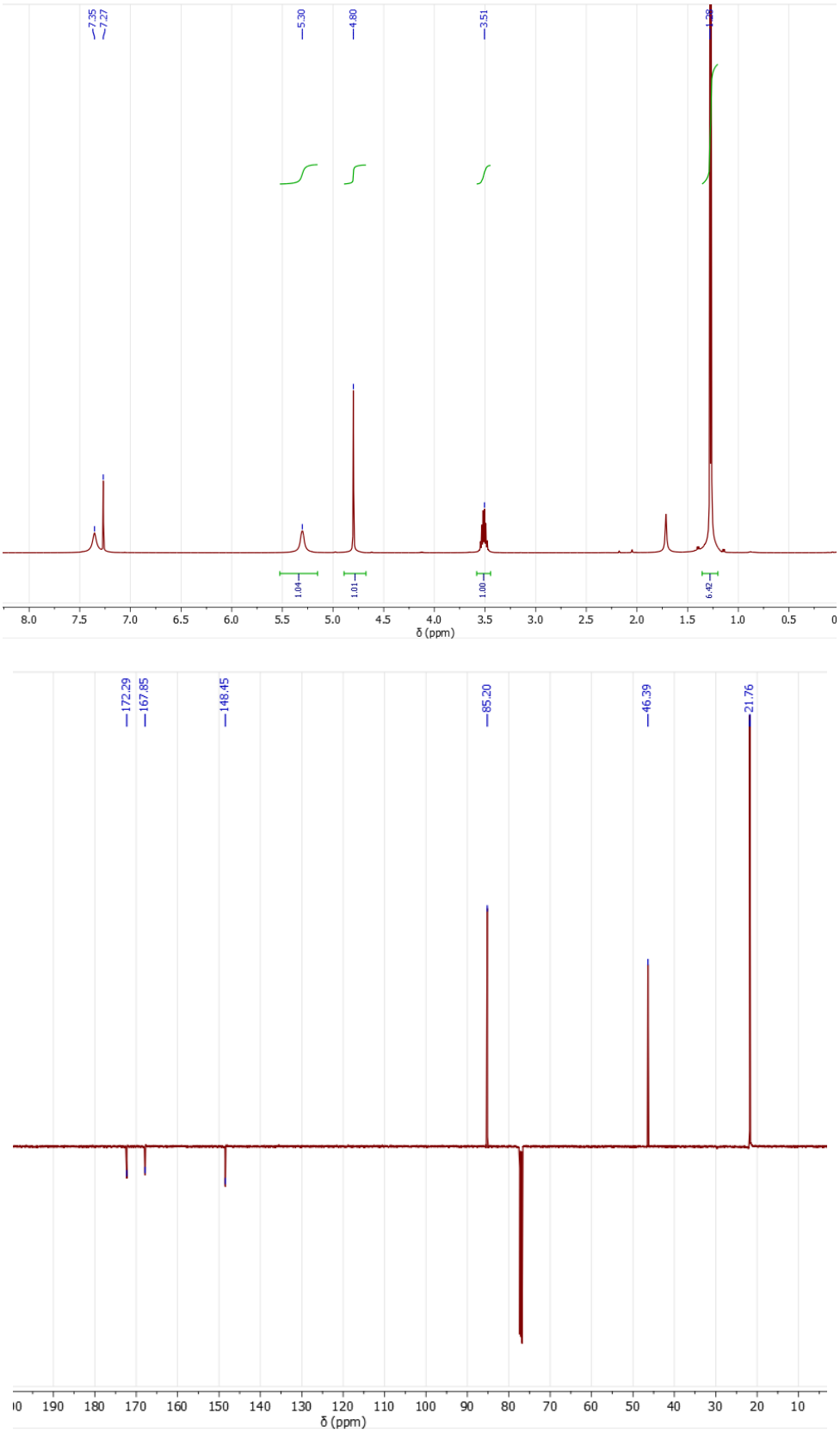


Figure S7. *^{1}H (top) and ^{13}C (lower) NMR spectra for* ***HMAM****. Solvent: $CDCl_3$.*

1-benzyl-3-(isopropylamino)-pyrrole-2,5-dione (BzMAM)

An eluent of 75% ethyl acetate in petroleum ether was used to isolate a yellow solid (160 mg, 75%). ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.37-7.28 (m, 5H), 5.30 (br, 1H), 4.82 (br d, $^{3}J_{HH}$ = 13.1 Hz, 1H), 4.65 (s, 2H), 3.51 (dq, $^{3}J_{HH}$ = 13.1, 6.5 Hz, 1H), 1.27 (d, *J* = 6.5 Hz, 9H) ppm. ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 172.9 (*C*O), 167.5 (*C*O), 148.5 (*C*NH), 136.5 (Ar*C*), 128.7-127.4 (m, Ar*C*), 84.4 (*C*H), 46.1 (*C*H), 41.0 (CH_2), 21.8 (CH_3) ppm. HR-MS (MaXis): [M+Na^+] – calculated m/z 267.1104 observed m/z 267.1104. FTIR: *v* = 3103 (υAr-C-H), 2971 (υC-H), 1698 (υC=O), 1621 (υC=O) cm^{-1}.

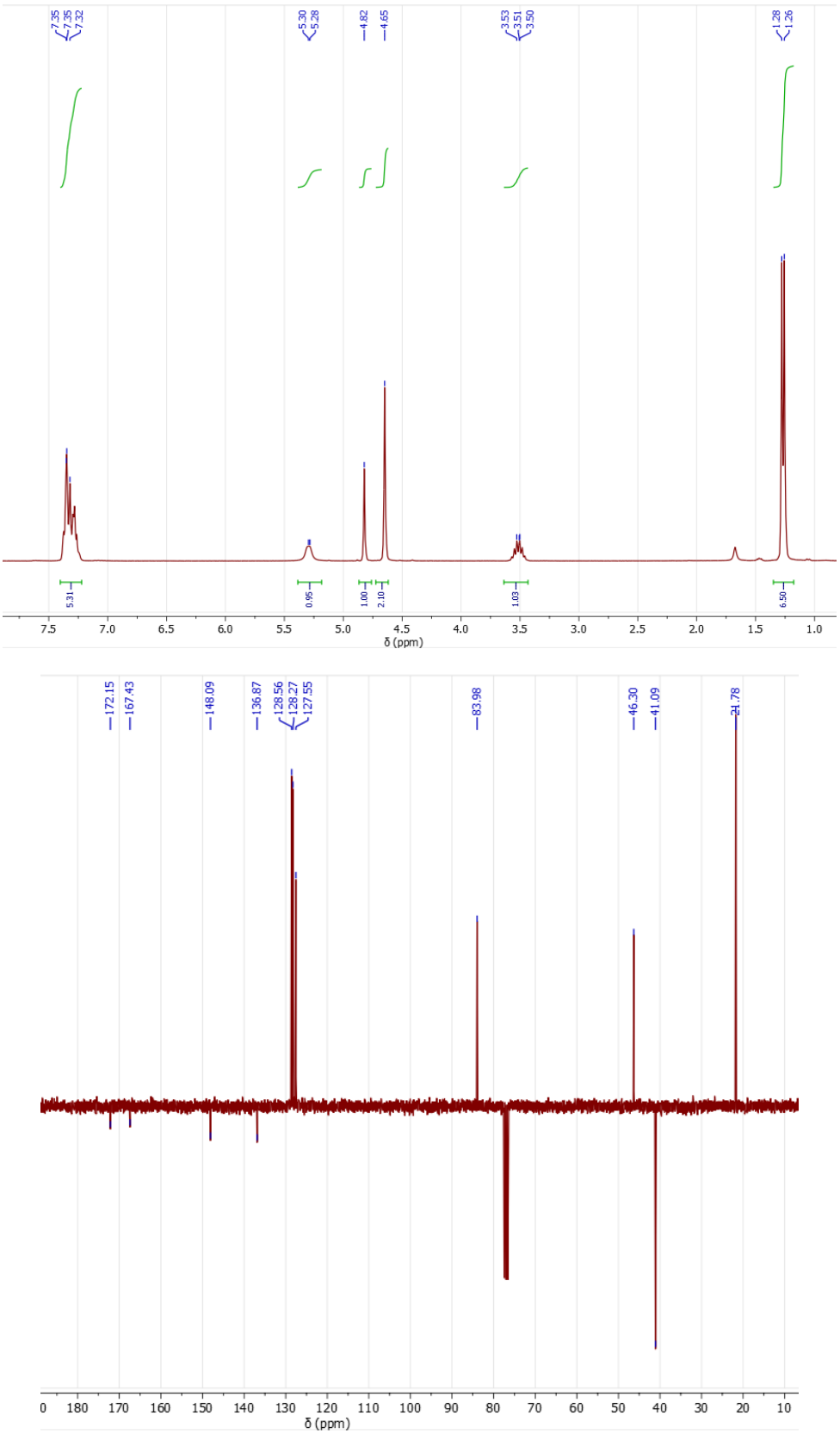


Figure S8. *^{1}H (top) and ^{13}C (lower) NMR spectra for* ***BzMAM****. Solvent: $CDCl_3$.*

1-benzhydryl-3-(isopropylamino)-pyrrole-2,5-dione (Bz_2MAM)

An eluent of 10 % ethyl acetate in petroleum ether was used to isolate a light yellow solid (198 mg, 62 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.28 (m, 10H, Ar*H*), 6.49 (s, 1H, ArC*H*), 5.19 (s, 1H, N*H*), 4.84 (s, 1H, C*H*), 3.51 (dq, $^{3}J_{HH}$ = 6.5 Hz, 1H, C*H*), 1.25 (d, $^{3}J_{HH}$ = 6.5 Hz, 6H, CH_3) ppm. ^{13}C NMR (126MHz, $CDCl_3$) δ = 171.9 (*C*O), 167.2 (*C*O), 147.8 (*C*N), 138.7 (*C*Ar), 128.6 (*C*Ar), 128.2 (*C*Ar), 127.5 (*C*Ar), 84.0 (*C*H), 56.9 (*C*H), 46.3 (*C*H), 21.8 (*C*H_3) ppm. HR-MS (MaXis): [M+Na$^+$] - calculated m/z 343.1417 observed m/z 343.1422. FTIR: *v* = 2973 (υC-H), 1704 (υC=O), 1634 (υC=O) cm^{-1}.

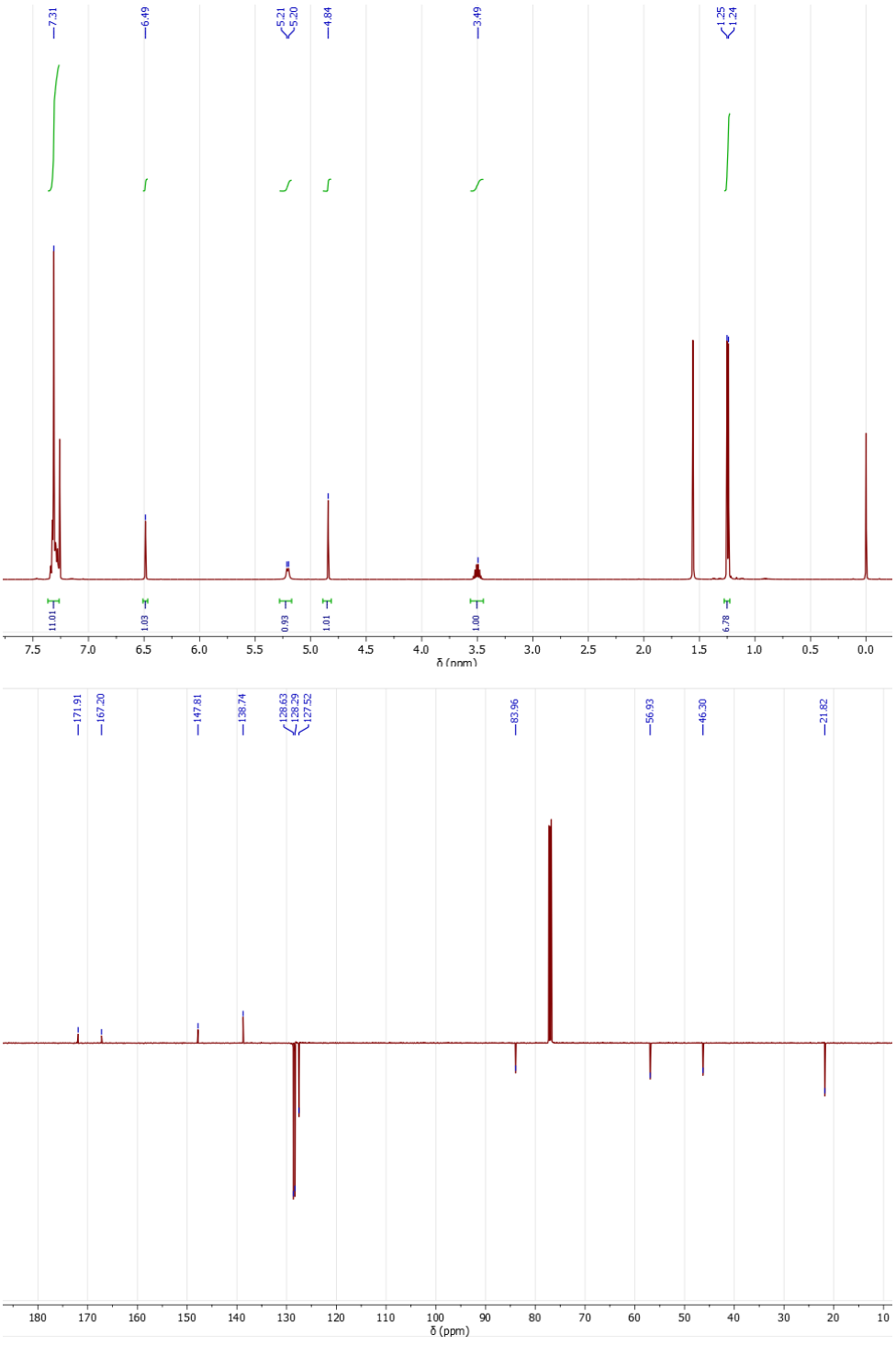


Figure S9. *^{1}H (top) and ^{13}C (lower) NMR spectra for* ***Bz_2MAM****. Solvent: $CDCl_3$.*

3-(isopropylamino)-1-trityl-pyrrole-2,5-dione (Bz_3MAM)

An eluent of 5% ethyl acetate in petroleum ether was used to isolate a light yellow solid (36 mg, 37%). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.33 (s, 6H, ArH), 7.11-7.20 (m, under solvent peak, ArH), 5.02 (d, 1H, N*H*), 4.68 (s, 1H, C*H*), 3.37 (dq, $^3J_{HH}$ = 13.2, 6.6 Hz, 1H, C*H*), 1.13 (d, $^3J_{HH}$ = 6.5 Hz, 6H, CH_3) ppm. ^{13}C NMR ($CDCl_3$, 126 MHz) δ = 172.1 (*C*O), 168.0 (*C*O), 147.5 (*C*N), 142.9 (Ar*C*), 128.8 (Ar*C*), 127.4 (Ar*C*), 126.5 (Ar*C*), 85.7 (*C*Ph$_3$), 46.1 (*C*H), 21.8 (*C*H$_3$) ppm. HR-MS (MaXis): [M+Na$^+$] – calculated m/z 419.1703 observed m/z 419.1730. FTIR: *v* = 3018 (υC-H), 2983 (υC-H), 1700 (υC=O), 1624 (υC=O) cm^{-1}.

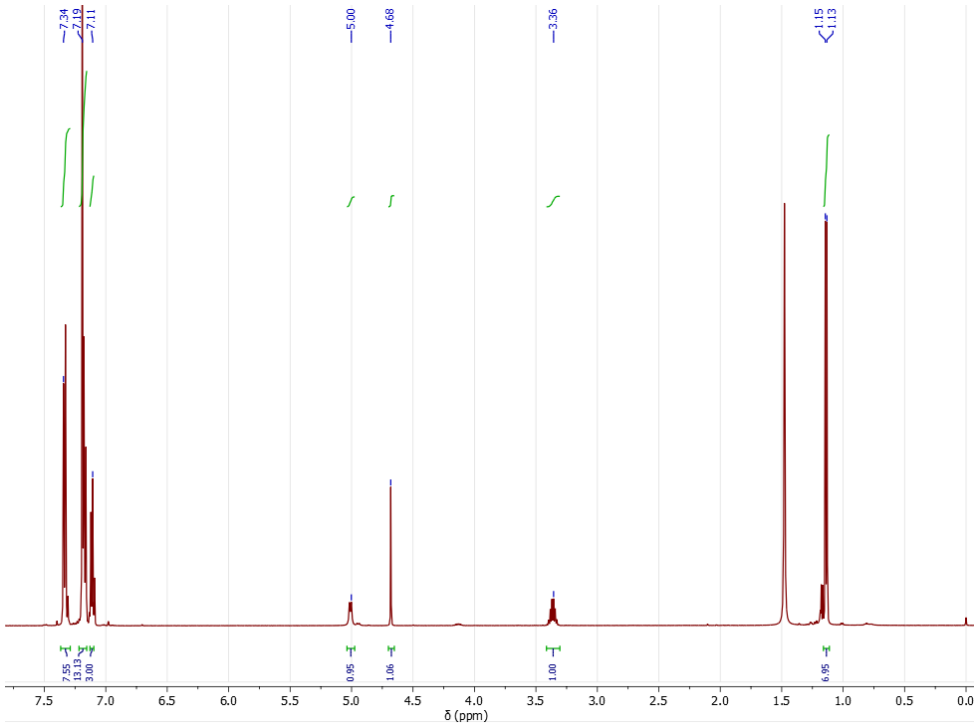


Figure S10. *^{1}H NMR spectrum for **Bz_3MAM**. Solvent: $CDCl_3$.*

3-bromo-4-(isopropylamino)-1-trityl-pyrrole-2,5-dione (Bz_3ABM)

An eluent of 10 % ethyl acetate in petroleum ether was used to isolate a light yellow solid (16 mg, 9 %). ^{1}H NMR (300 MHz, DMSO-d_6) δ = 7.38 – 7.00 (m, 15H, Ar*H*), 5.06 (d, J = 8.9 Hz, 1H, N*H*), 4.33 – 4.08 (m, 1H, C*H*), 1.17 (d, $^3J_{HH}$ = 6.6 Hz, 6H, CH_3) ppm. ^{13}C NMR (126 MHz, DMSO-d_6) δ = 171.1 (*C*O), 162.4 (*C*O), 146.9 (*C*N), 142.4 (*C*Br), 128.7 (*C*Ar), 128.0 (*C*Ar), 127.3 (*C*Ar), 126.7 (*C*Ar), 44.7 (*C*H), 21.8 (*C*H$_3$) ppm. HR-MS (MaXis): [M+Na$^+$] - calculated m/z 497.0838 observed m/ 497.0841. FTIR: *v* = 2966 (υC-H), 1704 (υC-H), 1620 (υC-H) cm^{-1}.

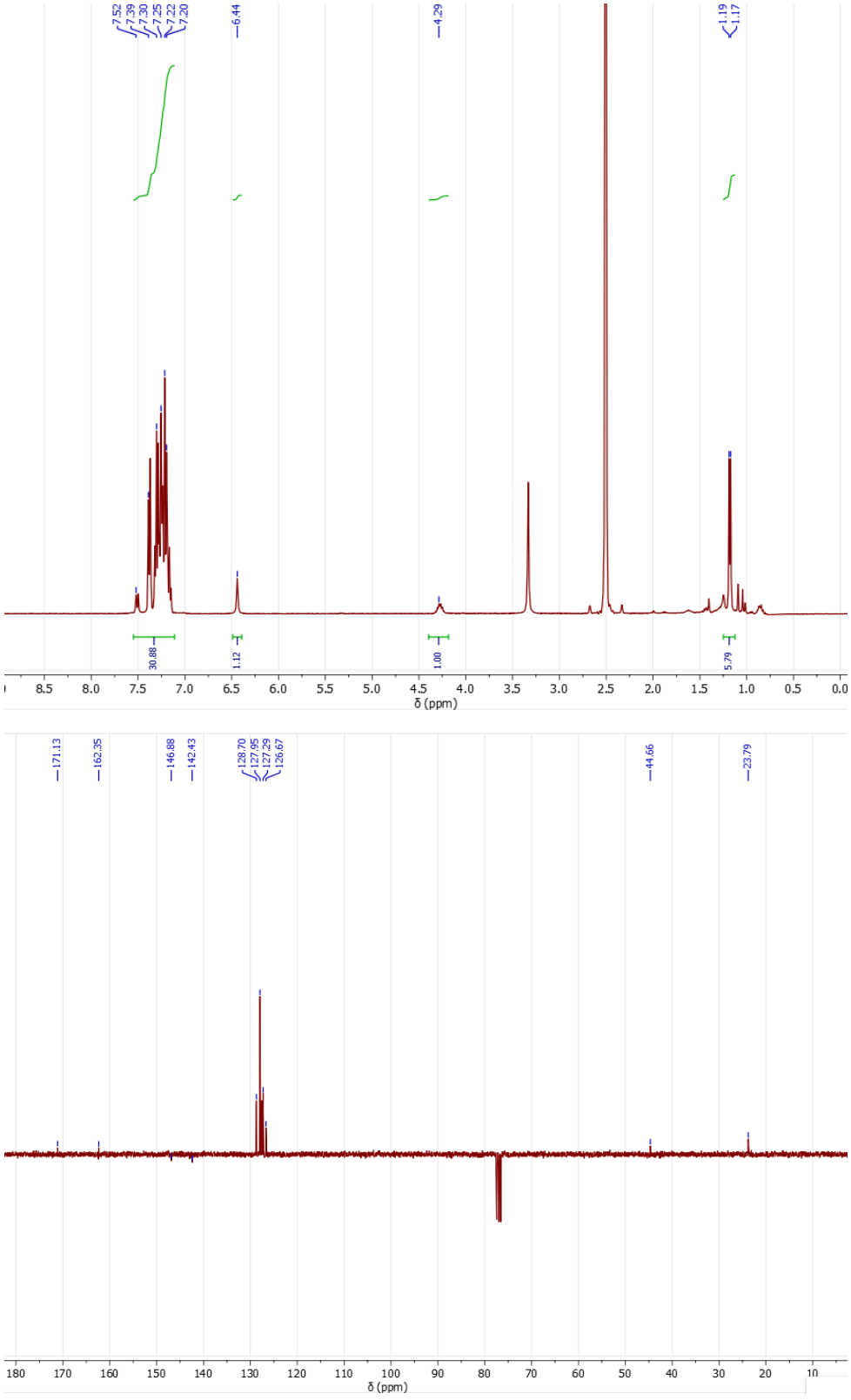


Figure S11. *^{1}H (top) and ^{13}C (lower) NMR spectra for* ***Bz$_3$MBM****. Solvent: DMSO-d$_6$.*

3-(isopropylamino)-1-phenyl-1H-pyrrole-2,5-dione (PhMAM)

This was purified by silica column chromatography on a 4 g RediSep Rf silica flash column and eluted with an ethyl acetate and hexane gradient eluent on a CombiFlash Rf+ Lumen by Teledyne, to isolate

a yellow solid (39 mg, 49%). ^{1}H NMR (300 MHz, DMSO-d_6) δ = 7.88 (br d, 1H, N*H*), 7.52 – 7.29 (m, 5H, Ar*H*), 5.06 (s, 1H, C*H*), 3.58 (dq, $^{3}J_{HH}$ = 7.8, 6.4 Hz, 1H, C*H*), 1.22 (d, $^{3}J_{HH}$ = 6.5 Hz, 6H, CH_3) ppm. ^{13}C NMR (DMSO-d_6, 101 MHz) δ = 171.2 (*C*O), 166.5 (*C*O), 147.8 (*C*N), 131.9 (*C*Ar), 129.0 (*C*Ar), 127.3 (*C*Ar), 125.9 (*C*Ar), 84.2 (*C*H), 46.5 (*C*H), 21.9 (*C*H_3) ppm. HR-MS (Xevo): [M+H$^+$] – calculated m/z 230.1055 observed m/z 230.1057. FTIR: *v* = 3091 (υC-H), 2974 (υC-H), 1705 (υC=O), 1656 (υC=O) cm^{-1}.

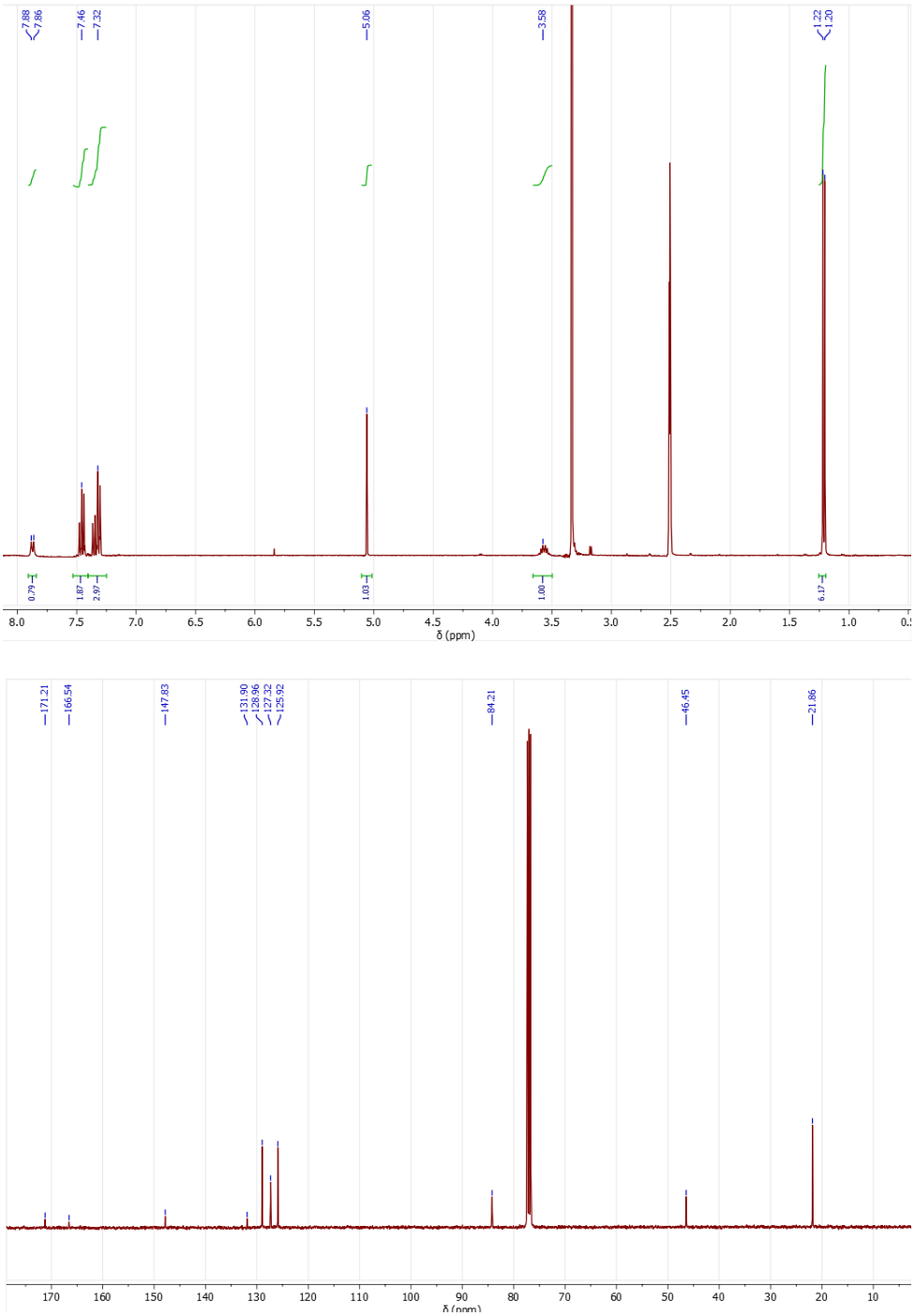


Figure S12. *^{1}H (top) and ^{13}C (lower) NMR spectra for* ***PhMAM****. Solvent: DMSO-d_6.*

2.4 Quantum yield fluorescence analysis

Solution state quantum yield analysis was based on a previously reported literature procedure.[3] A solution of quinine sulfate dihydrate (15 µmol) in 0.105 mol L^{-1} perchloric acid was used a standard ($\Phi_{quinine}$ = 59%), from which a UV–visible spectrum was recorded. The sample was diluted until the absorbance was between 0.05 and 0.1 and then the emission spectrum at λ_{max} was measured.

For solid-state fluorescence, absolute fluorescence quantum yields were recorded with an integrating sphere set up. Powers of each dye were crushed, and approximately 10 mg of the dye was placed onto a circular solid-state holder for analysis. All dyes were recorded with 375 nm excitation; with a 7-8 nm excitation slit and 0.1-0.2 nm emission slit width. Dyes were measured in triplicate and the mean and standard deviation (σ) recorded. For polymer films, 10 mg of **Bz_3MAM** was added to 1 mL of a 0.5 g mL^{-1} solution of the polymer in chloroform. The polymer and **Bz_3MAM** were fully dissolved and then drop cast onto glass slides to evaporate the solvent. The films were dried and then their fluorescence properties measured as for the solid samples.

3 Fluorescence Data

3.1 Solution state fluorescence

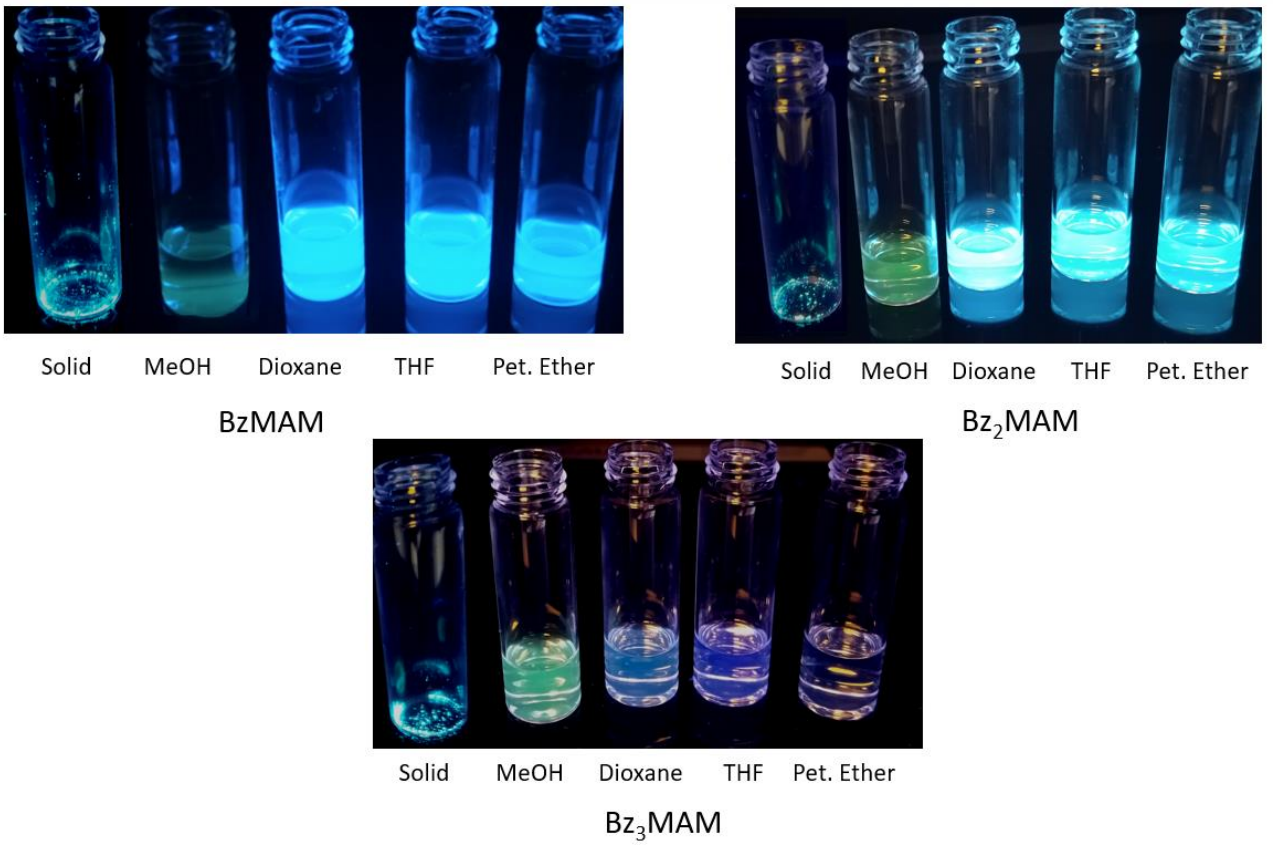


Figure S13. *Digital photographs of* ***BzMAM, Bz_2MAM*** *and* ***Bz_3MAM*** *under UV illumination.*

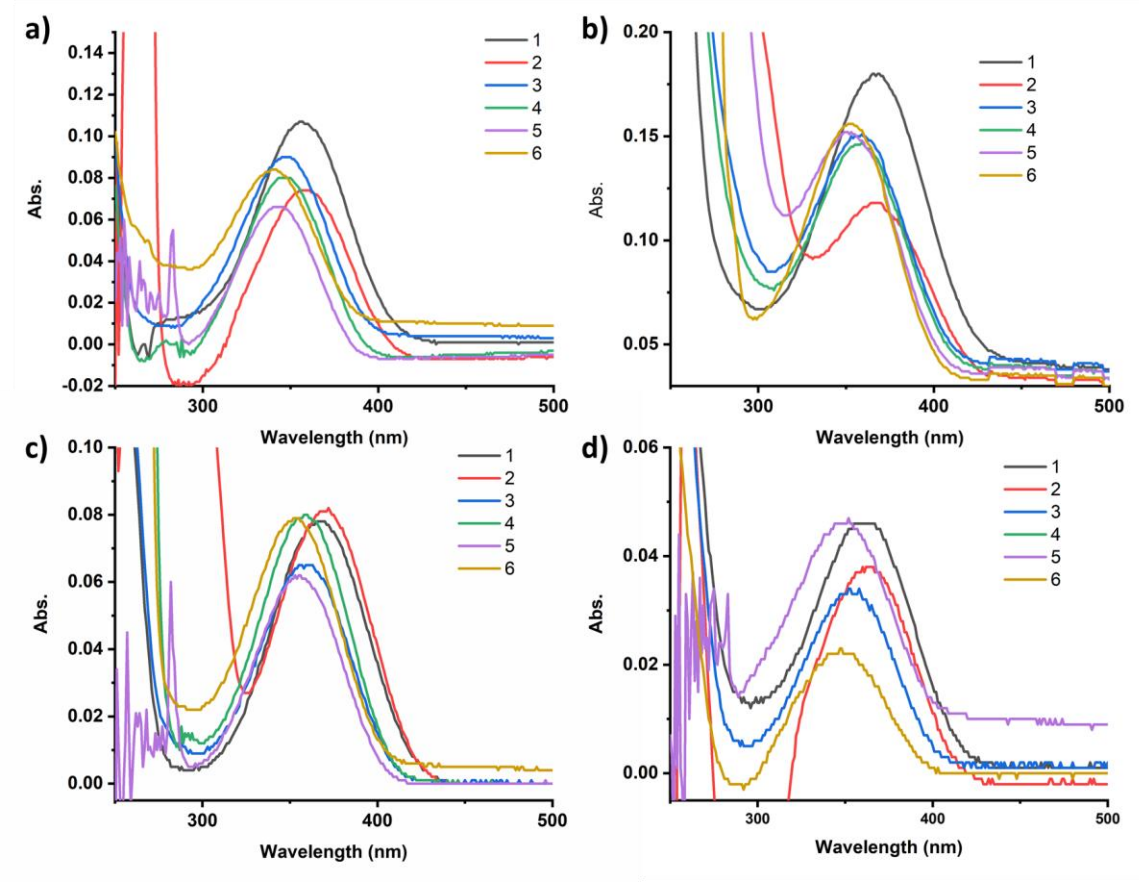


Figure S14. *UV-vis absorption spectra of HMAM (a), BzMAM (b), Bz_2MAM (c) and Bz_3MAM (d) in six different solvents. 1-6: Methanol, DMSO, dioxane, THF, toluene, diethyl ether.*

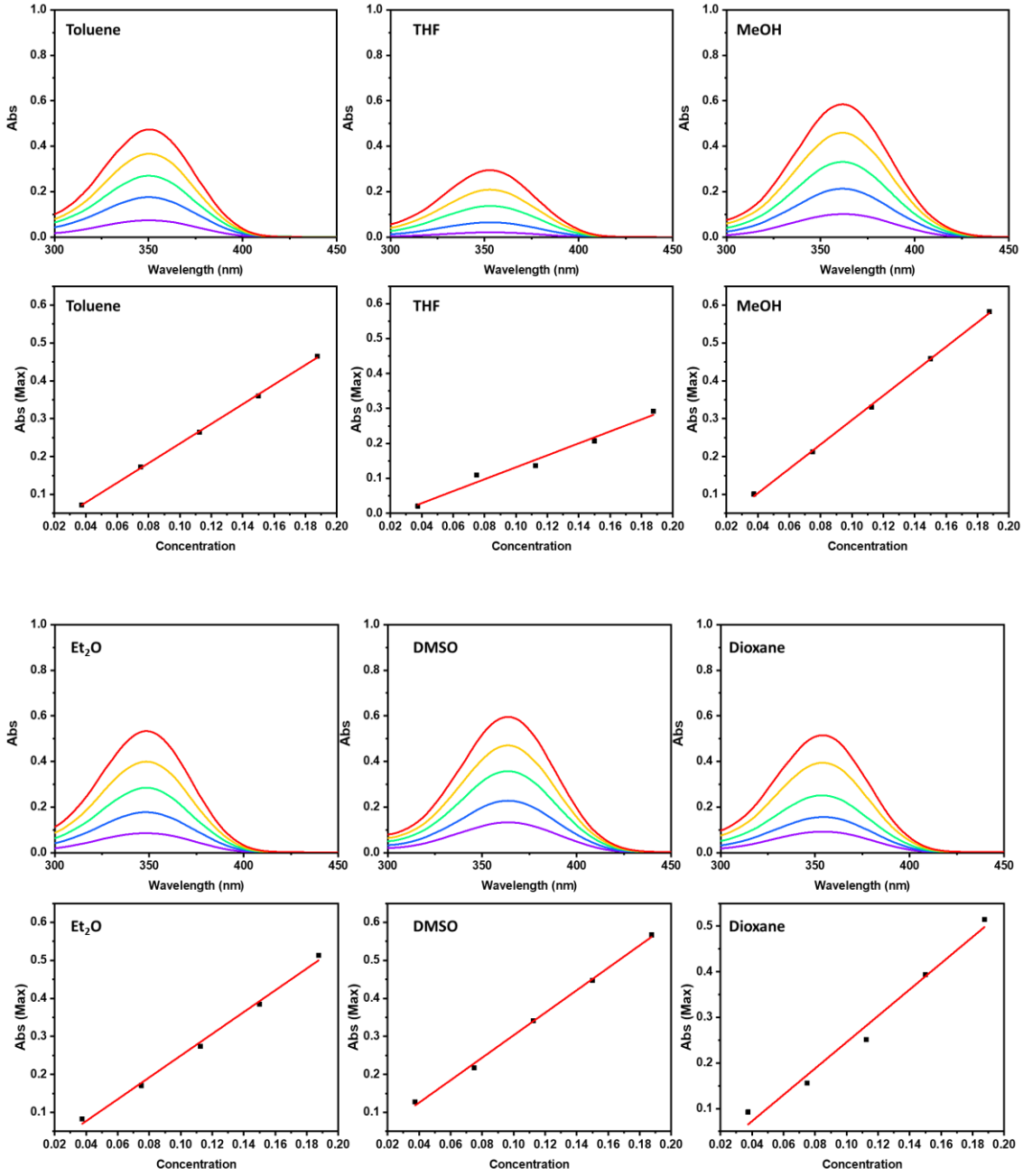


Figure S15. *UV-vis data for* ***Bz$_3$MAM*** *in a range of solvents used for the calculation of molar extinction coefficients.*

Table S1. *Molar extinction coefficients calculated from the data in Figure S15 for* ***Bz$_3$MAM*** *in a range of solvents.*

Solvent	ε_{max} / $M^{-1}cm^{-1}$	R^2
Toluene	**2596**	**0.999**
THF	**1711**	**0.989**

Solvent	ε_{max} / $M^{-1}cm^{-1}$	R^2
DMSO	2957	0.998
Dioxane	2886	0.991
Et2O	2868	0.995
MeOH	3225	0.999

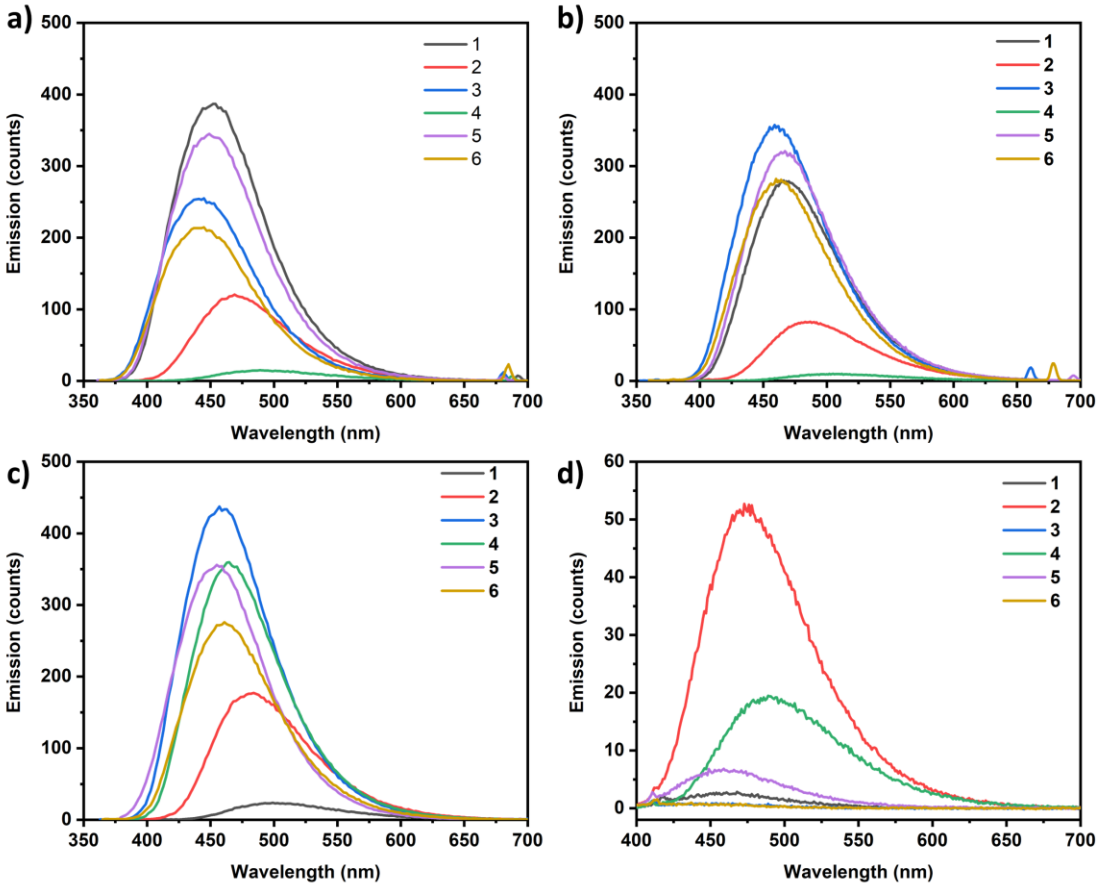


Figure S16. *Fluorescence emission spectra of HMAM (a), BzMAM (b), Bz_2MAM (c) and Bz_3MAM (d) in six different solvents. 1-6: dioxane, DMSA, diethyl ether, methanol, THF, toluene.*

Table S2. *Solution state fluorescence quantum yields for the dye series calculated using a reference method.*

Dye	Solution State Quantum Yield

	MeOH	DMSO	Dioxane	THF	Toluene	Ether
HMAM	2.4	20.2	47.2	54.5	66.7	47.1
PhMAM	0.0	1.3	0.1	0.1	0.3	0.2
BzMAM	1.7	27.9	49.3	52.6	61.7	57.4
Bz_2MAM	3.1	26.4	59.3	58.4	48.6	46.5
Bz_3MAM	3.8	11.3	1.4	1.39	0.8	0.1
Bz_3ABM	3.0	27.8	34.0	22.5	9.5	15.3

3.2 Solid state fluorescence

Table S3. *Solid (aggregate) state fluorescence quantum yields with standard deviation over 3 runs (σ), recorded at 375 nm excitation.*

Dye	$\Phi_{f(\%)}$	σ
HMAM	25.3	1.63
PhMAM	7.8	1.28
BzMAM	24.7	5.27
Bz_2MAM	27.7	3.50
Bz_3MAM	73.5	10.16
Bz_3ABM	5.7	0.35

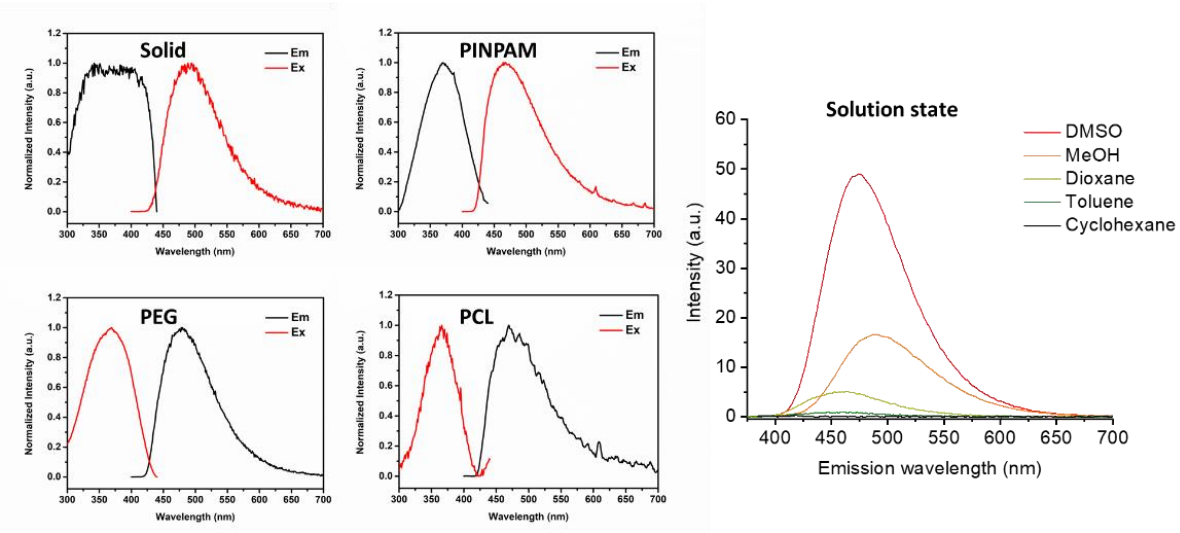


Figure S17. *Comparison of fluorescence emission profiles of* ***Bz$_3$MAM*** *in the solid state, dispersed in different polymer matrices, and in solution.*

3.3 Aggregation-induced emission

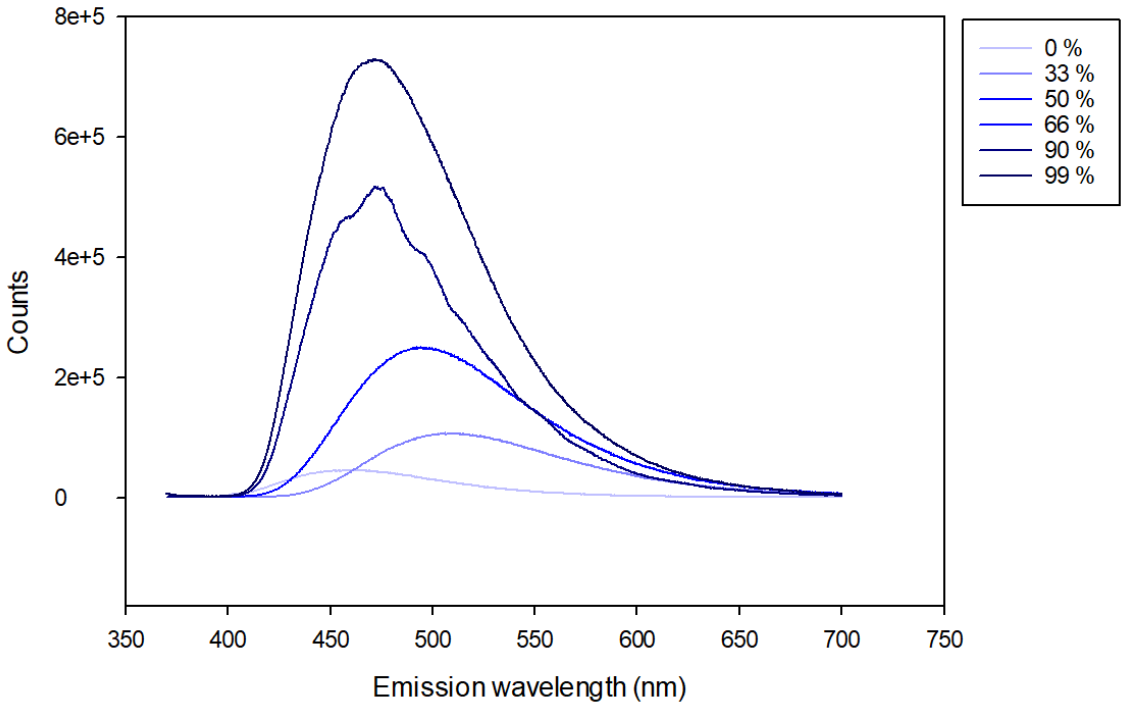


Figure S18. *Fluorescence of* ***Bz$_3$MAM*** *in water/dioxane mixtures. Emission at 470 nm (375 nm excitation) plotted against water content.*

3.4 Temperature-Dependent Emission

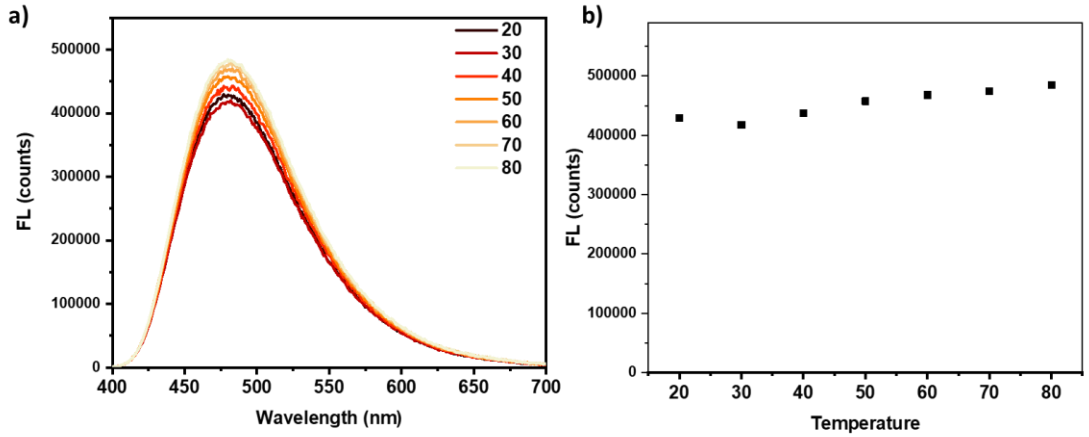


Figure S19. *a) Fluorescence emission spectra of* ***Bz$_3$MAM*** *in DMSO (Slit widths:1 nm, 1 nm) at different temperatures from 20-80 °C. b) Fluorescence intensity at 480 nm plotted against temperature.*

3.5 Viscosity-Dependent Emission

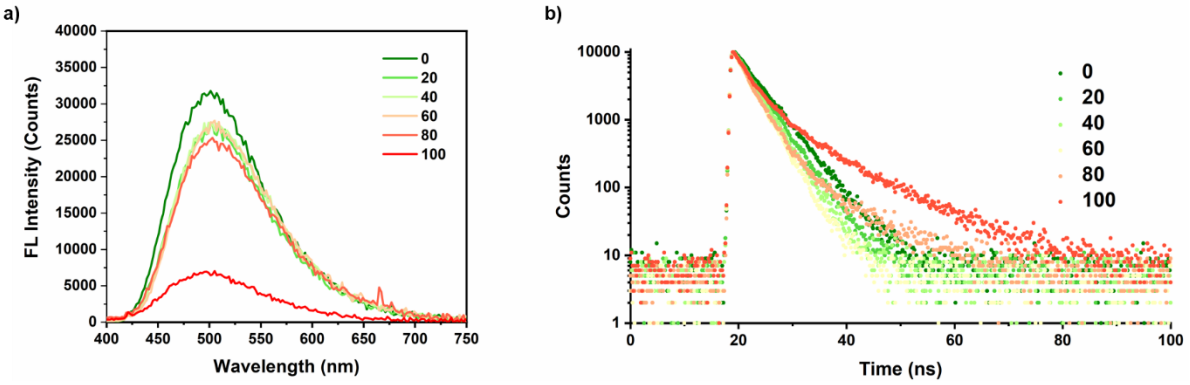


Figure S20. *a) Fluorescence emission spectra of* ***Bz$_3$MAM*** *in MeOH/glycerol mixtures. b) Fluorescence decay spectra of* ***Bz$_3$MAM*** *in MeOH/glycerol mixtures. Numbers in legends refer to the vol% of glycerol present in the mixture.*

4 Crystallography

4.1 Crystal growth

Crystals were grown by dissolving several milligrams of the dye in around 5 mL of DCM/hexane, in a small vial with a lid. This was placed in a sealed jar quarter filled with hexane. A needle was placed into the vial to allow solvent exchange with the jar reservoir. This was left on a windowsill for 2-4 weeks until crystals were observed.

4.2 Crystal structure determination

The datasets for **HMAM**, **BzMAM**, **Bz_2MAM** and **Bz_3MAM** were collected on an Agilent SuperNova diffractometer using an Atlas detector. The data were processed using CrysAlisPro.[19] The structures were solved using ShelXT [20] and were refined by a full-matrix least-squares procedure on F^2 in ShelXL.[21] Figures and reports were produced using OLEX2.[22] All non-hydrogen atoms in all structures were refined with anisotropic displacement parameters. Unless otherwise stated, in all structures, the hydrogen atoms were fixed as riding models and the U_{iso} of all hydrogen atoms were based on the U_{eq} of the parent atoms.

4.3 Crystallographic data

HMAM Crystal Data

For $C_7H_{10}N_2O_2$ (*M* =154.17 g/mol): orthorhombic, space group Ccc2 (no. 37), *a* = 10.9082(7) Å, *b* = 19.5765(18) Å, *c* = 7.2562(5) Å, *V* = 1549.5(2) Å^3, *Z* = 8, *T* = 100.00(10) K, μ(CuKα) = 0.821 mm^{-1}, *Dcalc* = 1.322 g/cm^3, 2842 reflections measured (9.034° ≤ 2Θ ≤ 148.636°), 1044 unique (R_{int} = 0.0275, R_{sigma} = 0.0244) which were used in all calculations. The final R_1 was 0.0309 (I > 2σ(I)) and wR_2 was 0.0842 (all data). The structure occupies a chiral space group. It was not possible to determine the absolute structure due to the large error in the Flack parameter and low Friedel pair coverage. The hydrogen atoms bonded to N(1) and N(2) were located in the electron density and the positions and thermal parameters refined.

BzMAM Crystal Data

For $C_{14}H_{16}N_2O_2$ (*M* =244.29 g/mol): monoclinic, space group $P2_1/n$ (no. 14), *a* = 5.8960(2) Å, *b* = 21.5637(8) Å, *c* = 9.9291(4) Å, *β* = 94.217(3)°, *V* = 1258.96(8) Å^3, *Z* = 4, *T* = 100.01(10) K, μ(CuKα) = 0.706 mm^{-1}, *Dcalc* = 1.289 g/cm^3, 4605 reflections measured (8.2° ≤ 2Θ ≤ 147.512°), 2461 unique (R_{int} = 0.0243, R_{sigma} = 0.0319) which were used in all calculations. The final R_1 was 0.0363 (I > 2σ(I)) and wR_2 was 0.0948 (all data). The hydrogen atom bonded to N(2) was located in the electron density and the position and thermal parameters refined.

Bz_2MAM Crystal Data

For $C_{20}H_{20}N_2O_2$ (*M* =320.38 g/mol): triclinic, space group P-1 (no. 2), *a* = 10.4304(12) Å, *b* = 12.5881(13) Å, *c* = 13.5096(14) Å, *α* = 87.170(9)°, *β* = 83.950(9)°, *γ* = 79.063(9)°, *V* = 1731.1(3) Å^3, *Z* = 4, *T* = 100.00(10) K, μ(CuKα) = 0.639 mm^{-1}, *Dcalc* = 1.229 g/cm^3, 10696 reflections measured (8.676° ≤ 2Θ ≤ 151.596°), 10696 unique (R_{int} = ?, R_{sigma} = 0.0338) which were used in all calculations. The final R_1 was 0.0803 (I > 2σ(I)) and wR_2 was 0.2665 (all data). The crystal was a non-merohedral twin with the two domains related by −180° about the direct direction [0 0 1]. The structure contains two crystallographically independent molecules. The hydrogen atoms bonded to N(2) and N(102) were located in the electron density and the positions and thermal parameters refined.

Bz_3MAM Crystal Data

For $C_{26}H_{24}N_2O_2$ (*M* =396.47 g/mol): tetragonal, space group $P4_32_12$ (no. 96), *a* = 9.27140(10) Å, *c* = 48.3513(8) Å, *V* = 4156.22(11) $Å^3$, *Z* = 8, *T* = 100.01(10) K, μ(CuKα) = 0.637 mm^{-1}, *Dcalc* = 1.267 g/cm^3, 77228 reflections measured (7.314° ≤ 2Θ ≤ 143.684°), 4081 unique (R_{int} = 0.0614, R_{sigma} = 0.0191) which were used in all calculations. The final R_1 was 0.0662 (I > 2σ(I)) and wR_2 was 0.1493 (all data). The structure occupies a chiral space group. It was not possible to determine the absolute structure due to the slightly large error in the Flack parameter. The hydrogen atom bonded to N(2) was located in the electron density and the position refined while the isotropic thermal parameters (U_{iso}) was based on the U_{eq} of the parent atom.

Hydrogen bond lengths

Table S4. *Hydrogen bonding parameters measured from solvent crystal structures.*

Dye	Bonds	Length (dH-A) / Å	Angle / °	Form
HMAM	N2−H2···O1^{i}	2.11 (±0.02)	167 (±2)	Dimer
	N1-H1···O2^{i}	2.03 (±0.03)	170 (±3)	Imide H-Bond
BzMAM	N2−H2···O2^{i}	2.19 (±0.02)	151.7 (±1.7)	Dimer
	H4···O1^{i}	2.47 (±0.10)	174.2 (±0.8)	Dimer
Bz$_2$MAM	N2−H2···O1^{i}	2.07 (±0.04)	156 (±3)	Dimer
	N102−H102···O101^{i}	2.11 (±0.04)	157 (±3)	Dimer
Bz$_3$MAM	H3···O1^{i}	2.92 (±0.04)	n.d.*	Chain
	N2−H2···O2^{i}	2.14 (±0.06)	162 (±4)	Chain

n.d. = not determined.* ***HMAM* *i= 1-X, +Y, -1/2+Z.* ***BzMAM*** *i= 1-X, 1-Y, 1-Z.* ***Bz$_2$MAM*** *i= 1-X, 1-Y, -Z.* ***Bz$_3$MAM*** *i= +Y, +X, 1-Z*

Ring stacking data

Table S5. *Maleimide ring separation parameters measured from solvent crystal structures.*

Dye	Solid state $\Phi_{f(\%)}$	Ring plane angle†	Ring centroid distance / Å†	Inter-plane distance / Å‡	Ring shift / Å§	Ring to plane twist angle*	Ring to plane fold angle*
HMAM	25.3	9.8° (±0.1)	3.649 (±0.001)	3.520 (±0.001)	0.648 (±0.005)	23.1° (±0.04)	8.4° (±0.1)
BzMAM	24.7	0.0° (±0.1)	4.053 (±0.001)	3.519 (±0.002)	2.070 (±0.003)	0.0° (±0.1)	0.0° (±0.1)
Bz_2MAM	27.6	0.0° (±0.1)	5.042 (±0.003)	2.764 (±0.009)	4.216 (±0.006)	0.0° (±0.2)	0.0° (±0.5)
Bz_3MAM	73.5	13.0° (±0.3)	6.464 (±0.004)	5.885 (±0.007)	2.674 (±0.013)	150.1° (±0.7)	166.6° (±0.3)

*† Measured distance and angle between ring centroid of N1C1C2C3C4 and $N1^iC1^iC2^iC3^iC4^i$. * Angles between mean plane created from atom selection N1C1C2C3C4 and $N1^iC1^iC2^iC3^iC4^i$.*

‡ Distance between ring centroid of N1C1C2C3C4 and plane of $N1^iC1^iC2^iC3^iC4^i$.

§ Distance in horizontal shift between ring centroids of N1C1C2C3C4 and $N1^iC1^iC2^iC3^iC4^i$.

HMAM *i= 1-X, +Y, -1/2+Z.* ***BzMAM*** *i= 1-X, 1-Y, 1-Z.* ***Bz_2MAM*** *i= 1-X, 1-Y, -Z.* ***Bz_3MAM*** *i= +Y, +X, 1-Z*

Detailed crystallographic data and refinement parameters

Table S6. *Crystallographic data from solvent crystal structures*

Dye	HMAM	BzMAM	Bz_2MAM	Bz_3MAM
Empirical formula	$C_7H_{10}N_2O_2$	$C_{14}H_{16}N_2O_2$	$C_{20}H_{20}N_2O_2$	$C_{26}H_{24}N_2O_2$
Formula weight / Da	154.17	244.29	320.38	396.47
Temperature / K	100.00(10)	100.01(10)	100.00(10)	100.01(10)

Dye	HMAM	BzMAM	Bz_2MAM	Bz_3MAM
Crystal system	orthorhombic	monoclinic	triclinic	tetragonal
Space group	Ccc2	$P2_1/n$	P-1	$P4_32_12$
a / Å	10.9082(7)	5.8960(2)	10.4304(12)	9.27140(10)
b / Å	19.5765(18)	21.5637(8)	12.5881(13)	9.27140(10)
c / Å	7.2562(5)	9.9291(4)	13.5096(14)	48.3513(8)
α / °	90	90	87.170(9)	90
β / °	90	94.217(3)	83.950(9)	90
γ / °	90	90	79.063(9)	90
Volume / $Å^3$	1549.5(2)	1258.96(8)	1731.1(3)	4156.22(11)
Z	8	4	4	8
ρ_{calc} / g cm^{-3}	1.322	1.289	1.229	1.267
μ / mm^{-1}	0.821	0.706	0.639	0.637
F(000)	656.0	520.0	680.0	1680.0
Crystal size / mm^3	0.119 × 0.08 × 0.036	0.212 × 0.096 × 0.077	0.154 × 0.106 × 0.067	0.234 × 0.115 × 0.093
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection / °	9.034 to 148.636	8.2 to 147.512	8.676 to 151.596	7.314 to 143.684

Dye	HMAM	BzMAM	Bz_2MAM	Bz_3MAM
Index ranges	-12 ≤ h ≤ 13, -24 ≤ k ≤ 23, -5 ≤ l ≤ 8	-4 ≤ h ≤ 7, -26 ≤ k ≤ 24, -11 ≤ l ≤ 12	-13 ≤ h ≤ 13, -15 ≤ k ≤ 15, -12 ≤ l ≤ 16	-11 ≤ h ≤ 11, -11 ≤ k ≤ 11, -59 ≤ l ≤ 59
Reflections collected	2842	4605	10696	77228
Independent reflections	1044 [R_{int} = 0.0275, R_{sigma} = 0.0244]	2461 [R_{int} = 0.0243, R_{sigma} = 0.0319]	10696 [R_{int} = ?, R_{sigma} = 0.0338]	4081 [R_{int} = 0.0614, R_{sigma} = 0.0191]
Data/restraints/ parameters	1044/1/110	2461/0/169	10696/0/445	4081/0/276
Goodness-of-fit on F^2	1.058	1.052	1.041	1.110
Final R indexes [I>=2σ (I)]	R_1 = 0.0309, wR_2 = 0.0826	R_1 = 0.0363, wR_2 = 0.0898	R_1 = 0.0803, wR_2 = 0.2269	R1 = 0.0662, wR_2 = 0.1484
Final R indexes [all data]	R_1 = 0.0331, wR_2 = 0.0842	R_1 = 0.0421, wR_2 = 0.0948	R_1 = 0.1026, wR_2 = 0.2665	R1 = 0.0681, wR2 = 0.1493
Largest diff. peak/hole / e $Å^{-3}$	0.23/-0.17	0.23/-0.20	0.53/-0.51	0.36/-0.30
Flack parameter	0.2(3)	n/a	n/a	-0.05(7)

4.4 Crystallographic data availability

CCDC 1955637-CCDC 1955640 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

5 Computational Studies

5.1 Computational methods

The geometries for all studied systems in the ground state were fully optimized with the CAM-B3LYP[1] functional and the 6-311G(d,p) basis set.[2,3] The dispersion effects and the solvent were included in the optimization process. The D3-Grimme's dispersion[4] with Becke-Johnson damping factor[5,6] was used to evaluate the dispersion effects. The solvent was considered using the polarization continuum model (PCM).[7,8] The calculations were performed using the same solvents as in the experiments; *i.e.* toluene (ε = 2.3741), diethyl ether (ε = 4.24), tetrahydrofuran (ε = 7.4257), methanol (ε = 32.613), and dimethyl sulfoxide (ε = 46.826).

The time-dependent density functional theory (TD-DFT)[9,10] was applied to compute the absorption and emission (fluorescence) spectra. In the TD-DFT calculations, the first 40 excited states have been considered, although only the results of the first excitation have been displayed, wich correspond to HOMO → LUMO transitions ($\pi \rightarrow \pi^*$). The charge distribution was obtained following the natural bond orbital (NBO) partition scheme by Weinhold and co-workers.[11] All geometry optimizations, frequencies, and TD-DFT calculations were calculated using the Gaussian 09 program package.[12]

To quantify the electron redistribution of the different substituents in the aminomaleimide ring, four indices have been defined. The first two are based on the sum of the natural population charges (see Figure S21 for atom numbering system)

$$Q_{NBO1} = q_{NBO,C1} + q_{NBO,C2} + q_{NBO,C3} + q_{NBO,C4} + q_{NBO,O1} + q_{NBO,O2} \quad (1)$$

and

$$Q_{NBO2} = Q_{NBO1} + q_{NBO,N1} + q_{NBO,N2} \quad (2)$$

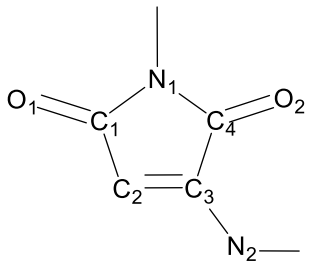


Figure S21. *Atom numbering scheme used in this work.*

The other two indices are obtained by integrating the HOMO density along the aminomaleimide ring

$$Q_{HOMO1} = \int_{\Omega_{i=C1,C2,C3,C4,O1,O2}} \rho_{HOMO}(\vec{r}) w_i(\vec{r}) d\vec{r} \quad (3)$$

and

$$Q_{HOMO2} = Q_{HOMO1} + \int_{\Omega_{i=N1,N2}} \rho_{HOMO}(\vec{r}) w_i(\vec{r}) d\vec{r} \quad (4)$$

The integrals of Equations (3) and (4) have been evaluated using Becke's multicentre integration scheme.[13] The atomic regions have been defined using the fuzzy Voronoi polyhedral, where $w_i(\vec{r})$ is the weight function for the atomic integration proposed by Becke,[13] tuned by the Bragg–Slater set of atomic radii.[14] The Q_{HOMO1} and Q_{HOMO2} values have been obtained using a program developed from our laboratory.[15,16]

The non-covalent interactions (NCI) descriptor is a well-established methodology that allows the visualization of both attractive (van der Waals and hydrogen bonding) and repulsive (steric) interactions.[17,18] The NCI index is based on the electron density, $\rho(\vec{r})$, and the reduced density gradient, $s(\vec{r})$, which is defined as

$$s(\vec{r}) = \frac{|\nabla \rho(\vec{r})|}{2(3\pi^2)^{1/3}\rho(\vec{r})^{4/3}} \quad (5)$$

The 3D representation of the $s(\vec{r})$ isosurface is colourized according to a Red-Blue-Green scheme over the range of the second eigenvalue of the electron-density Hessian, λ_2, showing van der Waals interactions, hydrogen bonds, steric repulsions, and covalent bonds. Negative values of λ_2 are characteristic of hydrogen bonds (strong attractions are indicated in the NCI plots by the blue colour). On the other hand, nonbonding interactions (steric repulsions) are represented by positive values (and red colour in the NCI plots). Finally, weak interactions (π stacking) show small λ_2 values (and represented in the NCI plots (section S5.4) by the green colour). Taking into account all these aspects, for some specific crystal structures, the NCI analysis has been performed using the NCIPLOT program.[17] The wave functions have been obtained at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in the gas phase.

5.2 Computational results and discussion

Table S7 contains the photophysical parameters of the absorption and emission spectra of aminomaleimide compounds studied in this work computed at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM methodology with diethyl ether. All excitation energies correspond to HOMO → LUMO transitions (and emission energies to LUMO → HOMO). Figures S22-28 display the HOMO and LUMO Kohn-Sham orbital isosurfaces, which mainly represent π bonding and π^* antibonding, respectively, interactions of the aminomaleimide ring. A good agreement between the theoretical and experimental values of the absorption and emission wavelengths has been obtained; although the TD-DFT results predict lower λ_{ex} and λ_{em} values than the experimental ones (these variations are more relevant in the polar solvents). Nevertheless, it is pertinent to note that the inclusion of explicit solvent molecules mitigates these differences (*vide infra*).

Table S7. *TD-DFT excitation and emission energies and their corresponding oscillator strengths of the aminomaleimide derivatives studied in this work.[a,b]*

Dye	λ_{exc} [c]	f_{exc} [d]	λ_{em} [e]	f_{em} [d]	$\Delta\lambda$ [f]
HMAM	312.2	0.139	406.7	0.111	94.5

Dye	λ_{exc} [c]	f_{exc} [d]	λ_{em} [e]	f_{em} [d]	$\Delta\lambda$ [f]
PhMAM	328.3	0.066	478.2	0.015	149.8
BzMAM	323.2	0.100	436.8	0.067	113.6
Bz_2MAM	321.0	0.106	432.4	0.070	111.3
Bz_3MAM	317.7	0.105	428.1	0.069	110.4
Bz_3ABM	334.0	0.097	450.9	0.078	116.8

[a] All excitation and emission energies correspond to the first excited state ($\pi \rightarrow \pi^*$ and $\pi^* \rightarrow \pi$ transitions, respectively). [b] All values computed at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM with diethyl ether (ε = 4.24). [c] Excitation wavelength, in nm. [d] Oscillator strength. [e] Emission wavelength, in nm. [f] Stokes shift (λ_{em} - λ_{ex}).

The imide functionalization provokes an important electron redistribution in the aminomaleimide ring (Table S8). The increase of the electron withdrawing character of the substituent results in an important reduction of Q_{HOMO1} and Q_{HOMO2} (and corresponding growth of Q_{NBO1} and Q_{NBO2}) values. For instance, the imide functionalization with the trityl group and the replacement of the maleic proton by a bromine atom generate Q_{HOMO1} values smaller by 4.34 a.u. and positive Q_{NBO1} values. Moreover, as can be seen in Figure S22, a good correlation between $\Phi_{f(\%)}$ and Q_{HOMO1} is obtained.

Table S8. *Charge descriptors of the electron withdrawing effect of the imide functionalization in the aminomaleimide ring.[a]*

Dye	Q_{NBO1}	Q_{NBO2}	Q_{HOMO1}	Q_{HOMO2}
HMAM	-0.074	-1.333	0.570	0.899
PhMAM	-0.019	-1.124	0.435	0.722
BzMAM	-0.057	-1.148	0.545	0.872
Bz_2MAM	-0.036	-1.138	0.541	0.865
Bz_3MAM	0.006	-1.127	0.369	0.586
Bz_3ABM	0.126	-0.993	0.399	0.664

[a] All values are in atomic units and computed at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM with diethyl ether (ε = 4.24).

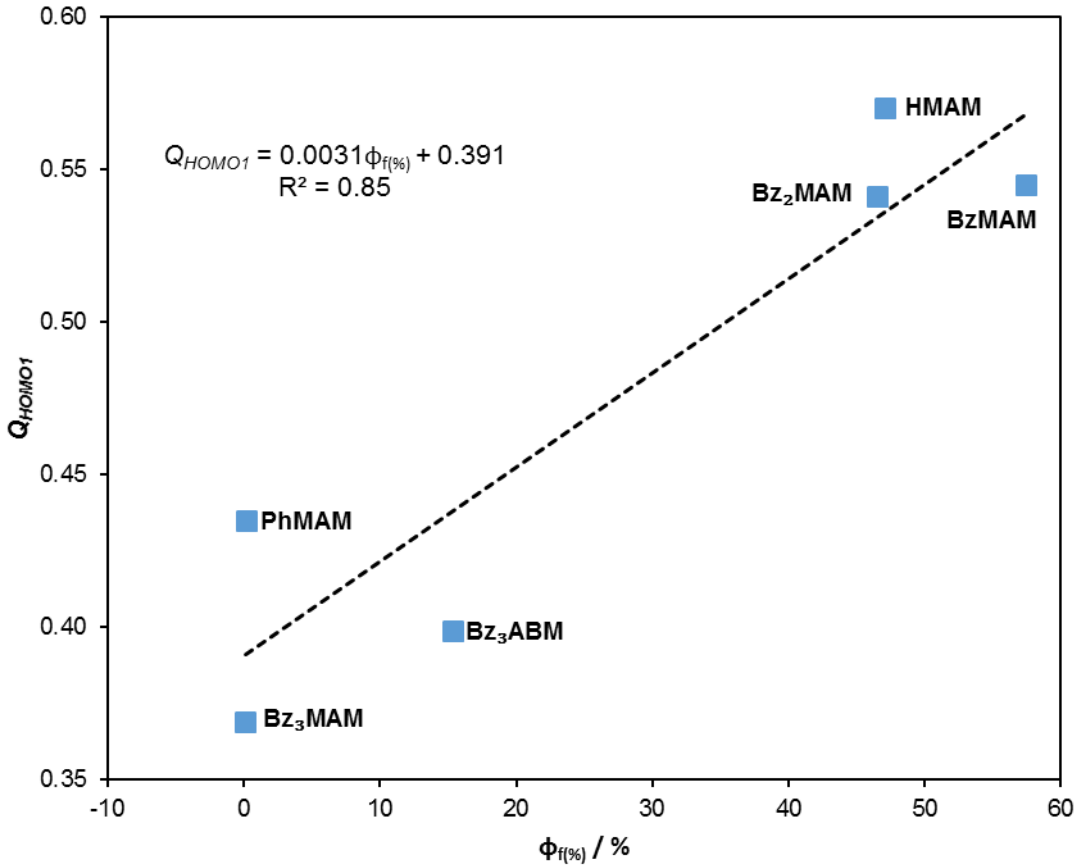
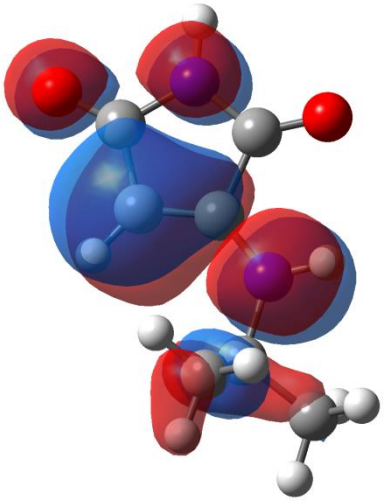
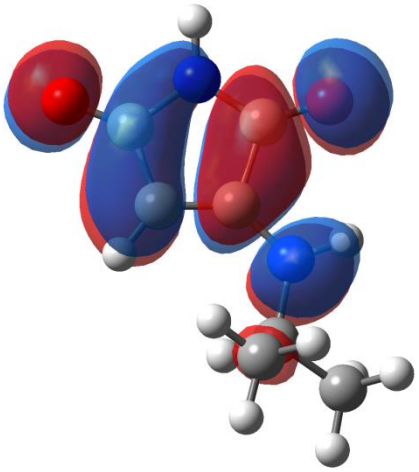


Figure S22. *Correlation between quantum yield, $\Phi_{f(\%)}$, (in diethyl ether solution) and the atomic integration of HOMO along the π conjugated structure of the aminomaleimide ring, Q_{HOMO1}*

5.3 Orbital visualisations

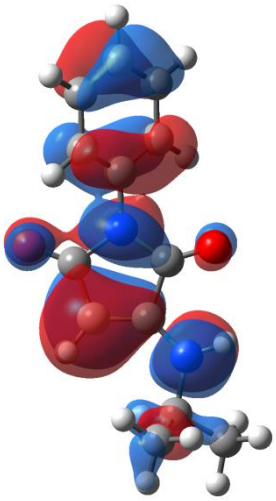


HMAM HOMO (-6.29)

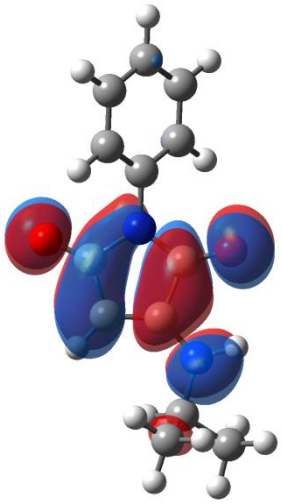


HMAM LUMO (-1.97)

Figure S23. *Representation of the HOMO and LUMO Kohn-Sham orbital isosurfaces of* ***HMAM*** *evaluated at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM with ε = 4.24. The values in parenthesis are the orbital energies (eV).*

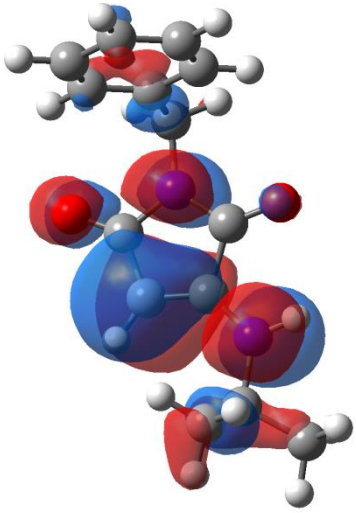


PhMAM HOMO (-7.64)

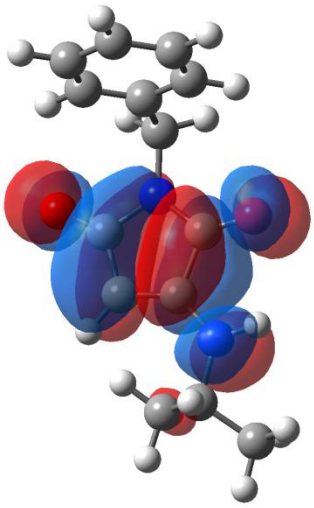


PhMAM LUMO (-0.79)

Figure S24. *Representation of the HOMO and LUMO Kohn-Sham orbital isosurfaces of* ***PhMAM*** *evaluated at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM with ε = 4.24. The values in parenthesis are the orbital energies (eV).*

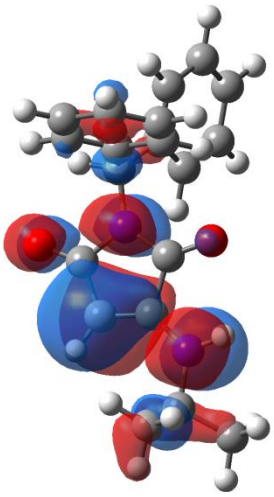


BzMAM HOMO (-6.22)

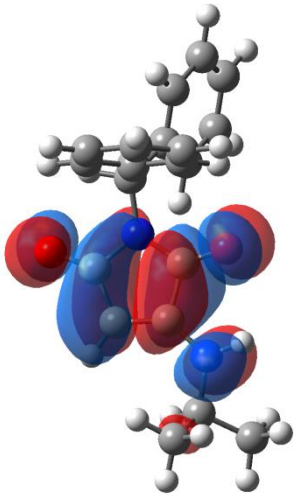


BzMAM LUMO (-1.97)

Figure S25. *Representation of the HOMO and LUMO Kohn-Sham orbital isosurfaces of* ***BzMAM*** *evaluated at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM with ε = 4.24. The values in parenthesis are the orbital energies (eV).*

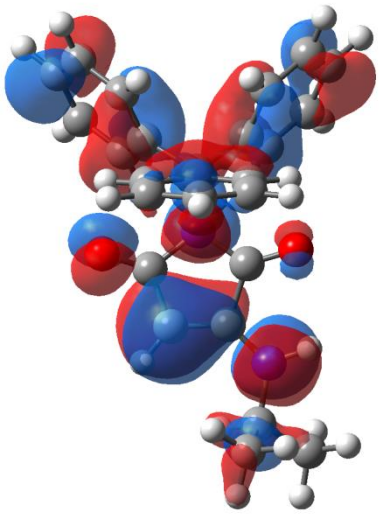


Bz$_2$MAM HOMO (-6.27)

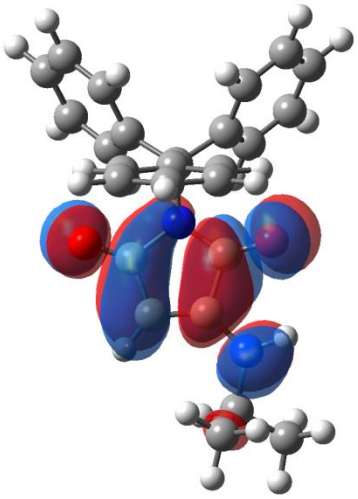


Bz$_2$MAM LUMO (-2.00)

Figure S26. *Representation of the HOMO and LUMO Kohn-Sham orbital isosurfaces of* ***Bz$_2$MAM*** *evaluated at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM with ε = 4.24. The values in parenthesis are the orbital energies (eV).*

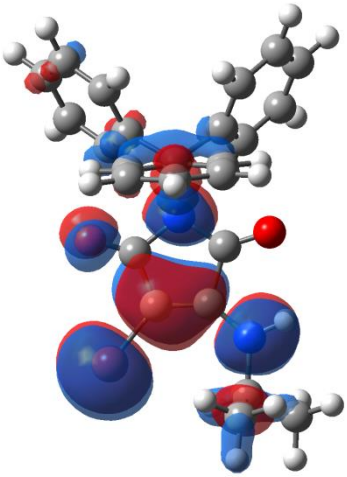


Bz$_3$MAM HOMO (-6.23)

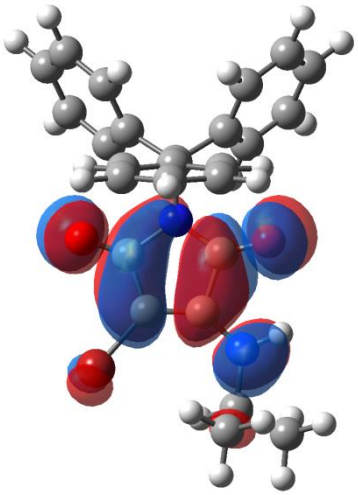


Bz$_3$MAM LUMO (-1.97)

Figure S27. *Representation of the HOMO and LUMO Kohn-Sham orbital isosurfaces of* ***Bz$_3$MAM*** *evaluated at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM with ε = 4.24. The values in parenthesis are the orbital energies (eV).*



Bz$_3$ABM HOMO (-6.17)



Bz$_3$ABM LUMO (-2.16)

Figure S28. *Representation of the HOMO and LUMO Kohn-Sham orbital isosurfaces of* ***Bz$_3$ABM*** *evaluated at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM with ε = 4.24. The values in parenthesis are the orbital energies (eV).*

5.4 Visualisations of non-covalent interactions

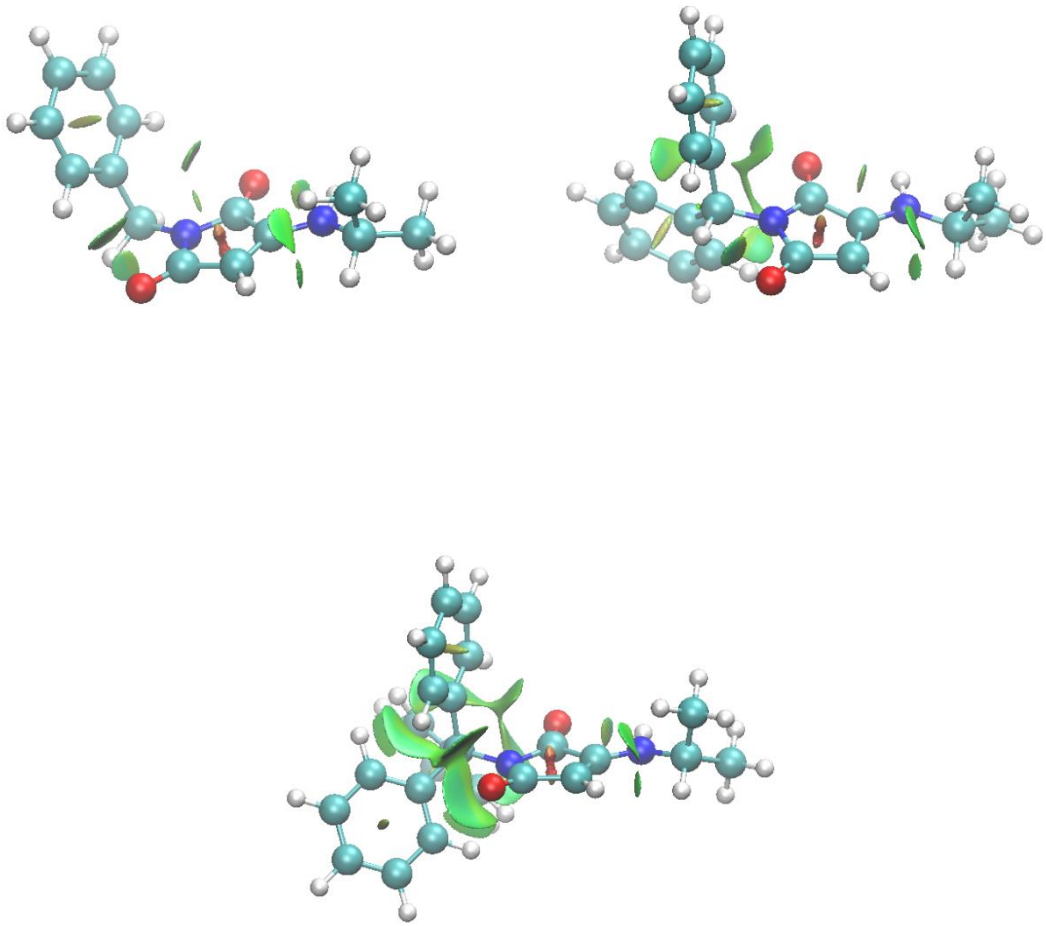


Figure S29. *CAM-B3LYP-D3BJ/6-311G(d,p) gradient isosurfaces with s=0.5 for* ***BzMAM****,* ***Bz$_2$MAM****, and* ***Bz$_3$MAM*** *with a blue-green-red colour scale from -0.05 < ρ sign(λ2) < 0.05 au.*

5.5 Natural population charge distributions

To rationalize the electron density reduction in the π-conjugated maleimide ring along the **BzMAM**, **Bz$_2$MAM**, and **Bz$_3$MAM** series, we have analyzed the natural population charge distribution of these maleimides. Figure S30 shows that the electron densities of the carbonyl oxygens reduce as the number of phenyls increases. Two factors can explain this electronic redistribution. The electron-withdrawing character of the N-substituent increases with the number of phenyls (the trityl group is a well-known electron-withdrawing substituent). Additionally, **Bz$_3$MAM** presents the shortest hydrogen bonds between the carbonyl oxygens of the maleimide and the hydrogens of the phenyl groups, see Figure S31. These hydrogen bonds may also favour electron transfer from the maleimide ring to the N-substituent.

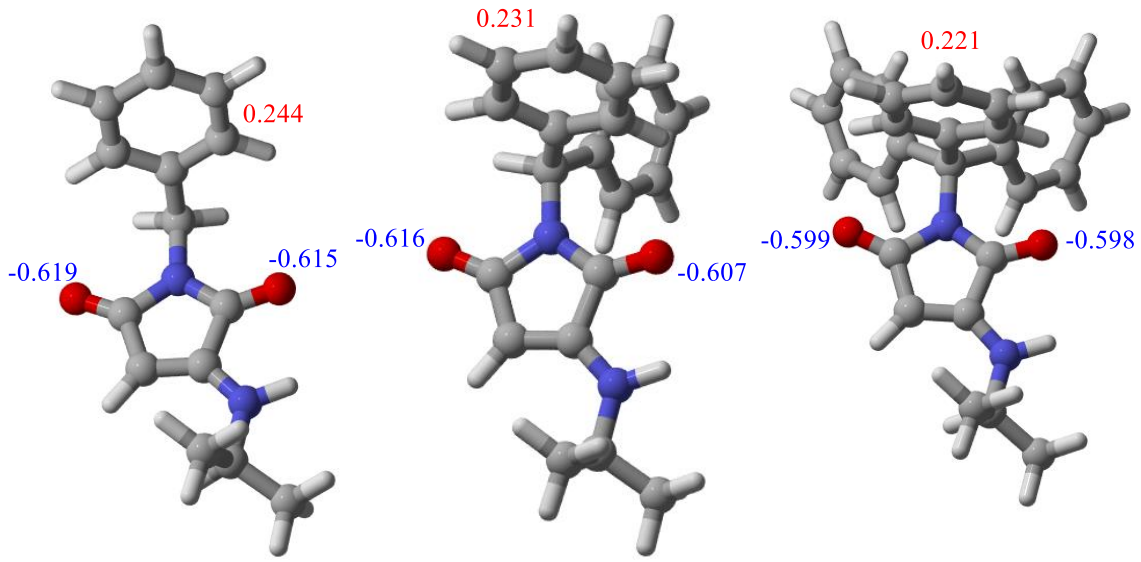


Figure S30. *CAM-B3LYP-D3BJ/6-311G(d,p)-optimized geometries of* ***BzMAM****,* ***Bz$_2$MAM****, and* ***Bz$_3$MAM*** *aminomaleimides indicating the natural population charges of the carbonyl oxygens (numbers in blue) and the N-substituents (numbers in red). All values are in atomic units.*

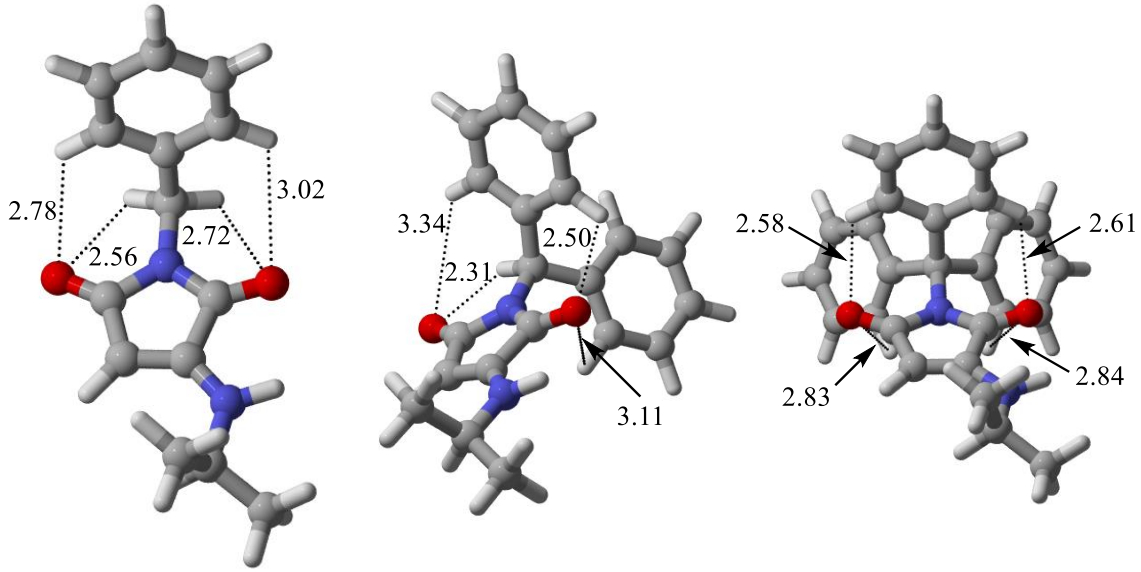


Figure S31. *CAM-B3LYP-D3BJ/6-311G(d,p)-optimized geometries of* ***BzMAM****,* ***Bz$_2$MAM****, and* ***Bz$_3$MAM*** *aminomaleimides indicating the most relevant hydrogen between the carbonyl oxygens of the maleimide ring and the hydrogens of the N-substituents. Bond distances are given in Å.*

5.6 Solvent effects

To rationalize the effect of solvent, the photophysical parameters of the absorption and emission spectra of seven aminomaleimides (**HMAM**, **PhMAM**, **BzMAM**, **Bz$_2$MAM**, **Bz$_3$MAM**, and **Bz$_3$ABM**) in six different media (1,4-dioxane, toluene, diethyl ether, tetrahydrofuran, methanol, and dimethyl sulfoxide) and were obtained using the PCM methodology (Tables Table **S9**-Table **S14**). A small

bathochromic shift (less than 20 nm) of the λ_{ex} and λ_{em} values was observed with increasing solvent polarity for all the studied systems (with the exception of **PhMAM** emission).

Table S9. *TD-DFT excitation and emission energies and their corresponding oscillator strengths of **HMAM** using six different solvents (PCM model).[a,b] Charge descriptors along the π-conjugated structure of the aminomaleimide ring.*

Solvent	λ_{exc}[c]	f_{exc}[d]	λ_{em}[e]	f_{em}[d]	$\Delta\lambda$[f]	Q_{NBO1}	Q_{HOMO1}
1,4-Dioxane	309.0	0.142	397.0	0.095	87.9	-0.057	0.570
Toluene	310.0	0.146	398.2	0.097	88.2	-0.059	0.570
Diethyl Ether	312.2	0.139	406.7	0.111	94.5	-0.074	0.570
Tetrahydrofuran	314.5	0.143	412.5	0.122	98.0	-0.083	0.571
Methanol	316.0	0.139	418.9	0.135	102.9	-0.094	0.571
Dimethyl Sulfoxide	316.9	0.145	419.5	0.136	102.6	-0.095	0.571

[a] All excitation and emission energies correspond to the first excited state ($\pi \rightarrow \pi^*$ and $\pi^* \rightarrow \pi$ transitions, respectively). [b] All values computed at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM model. [c] Excitation wavelength, in nm. [d] Oscillator strength. [e] Emission wavelength, in nm. [f] Stokes shift (λ_{em} - λ_{exc}).

Table S10. *TD-DFT excitation and emission energies and their corresponding oscillator strengths of **PhMAM** using six different solvents (PCM model).[a,b] Charge descriptors along the π-conjugated structure of the aminomaleimide ring.*

Solvent	λ_{exc}[c]	f_{exc}[d]	λ_{em}[e]	f_{em}[d]	$\Delta\lambda$[f]	Q_{NBO1}	Q_{HOMO1}
1,4-Dioxane	327.3	0.058	491.9	0.006	164.6	-0.057	0.399
Toluene	327.8	0.061	489.9	0.007	162.0	-0.007	0.404
Diethyl Ether	328.3	0.066	478.2	0.015	149.8	-0.019	0.435
Tetrahydrofuran	329.3	0.074	473.3	0.024	144.0	-0.026	0.454
Methanol	329.9	0.078	470.0	0.036	140.1	-0.036	0.474

Solvent	λ_{exc}[c]	f_{exc}[d]	λ_{em}[e]	f_{em}[d]	$\Delta\lambda$[f]	Q_{NBO1}	Q_{HOMO1}
Dimethyl Sulfoxide	330.5	0.082	469.8	0.037	139.3	-0.037	0.475

[a] All excitation and emission energies correspond to the first excited state ($\pi \rightarrow \pi^*$ and $\pi^* \rightarrow \pi$ transitions, respectively). [b] All values computed at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM model. [c] Excitation wavelength, in nm. [d] Oscillator strength. [e] Emission wavelength, in nm. [f] Stokes shift (λ_{em} - λ_{exc}).

Table S11. *TD-DFT excitation and emission energies and their corresponding oscillator strengths of **BzMAM** using six different solvents (PCM model).[a,b] Charge descriptors along the π-conjugated structure of the aminomaleimide ring.*

Solvent	λ_{exc}[c]	f_{exc}[d]	λ_{em}[e]	f_{em}[d]	$\Delta\lambda$[f]	Q_{NBO1}	Q_{HOMO1}
1,4-Dioxane	320.3	0.099	429.2	0.053	108.9	-0.043	0.541
Toluene	321.2	0.103	430.2	0.055	109.0	-0.045	0.541
Diethyl Ether	323.2	0.100	436.8	0.067	113.6	-0.057	0.545
Tetrahydrofuran	325.3	0.105	441.5	0.076	116.2	-0.065	0.547
Methanol	326.9	0.105	446.6	0.087	119.8	-0.074	0.549
Dimethyl Sulfoxide	327.7	0.109	447.1	0.089	119.5	-0.075	0.550

[a] All excitation and emission energies correspond to the first excited state ($\pi \rightarrow \pi^*$ and $\pi^* \rightarrow \pi$ transitions, respectively). [b] All values computed at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM model. [c] Excitation wavelength, in nm. [d] Oscillator strength. [e] Emission wavelength, in nm. [f] Stokes shift (λ_{em} - λ_{exc}).

Table S12. *TD-DFT excitation and emission energies and their corresponding oscillator strengths of **Bz$_2$MAM** using six different solvents (PCM model).[a,b] Charge descriptors along the π-conjugated structure of the aminomaleimide ring.*

Solvent	λ_{exc}[c]	f_{exc}[d]	λ_{em}[e]	f_{em}[d]	$\Delta\lambda$[f]	Q_{NBO1}	Q_{HOMO1}
1,4-Dioxane	315.0	0.103	421.7	0.054	106.8	0.019	0.536
Toluene	315.7	0.107	422.5	0.056	106.8	0.018	0.536

Solvent	λ_{exc}[c]	f_{exc}[d]	λ_{em}[e]	f_{em}[d]	$\Delta\lambda$[f]	Q_{NBO1}	Q_{HOMO1}
Diethyl Ether	321.0	0.106	432.4	0.070	111.3	-0.036	0.541
Tetrahydrofuran	319.8	0.110	432.1	0.079	112.3	-0.002	0.543
Methanol	321.6	0.110	437.5	0.094	115.9	-0.011	0.546
Dimethyl Sulfoxide	322.4	0.114	438.0	0.095	115.7	-0.012	0.547

[a] All excitation and emission energies correspond to the first excited state ($\pi \rightarrow \pi^*$ and $\pi^* \rightarrow \pi$ transitions, respectively). [b] All values computed at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM model. [c] Excitation wavelength, in nm. [d] Oscillator strength. [e] Emission wavelength, in nm. [f] Stokes shift (λ_{em} - λ_{exc}).

Table S13. *TD-DFT excitation and emission energies and their corresponding oscillator strengths of* ***Bz$_3$MAM*** *using six different solvents (PCM model).[a,b] Charge descriptors along the π-conjugated structure of the aminomaleimide ring.*

Solvent	λ_{exc}[c]	f_{exc}[d]	λ_{em}[e]	f_{em}[d]	$\Delta\lambda$[f]	Q_{NBO1}	Q_{HOMO1}
1,4-Dioxane	315.0	0.103	421.7	0.054	106.8	0.019	0.179
Toluene	315.7	0.107	422.5	0.056	106.8	0.018	0.200
Diethyl Ether	317.7	0.105	428.1	0.069	110.4	0.006	0.369
Tetrahydrofuran	319.8	0.110	432.1	0.079	112.3	-0.002	0.443
Methanol	321.6	0.110	437.5	0.094	115.9	-0.011	0.489
Dimethyl Sulfoxide	322.4	0.114	438.0	0.095	115.7	-0.012	0.492

[a] All excitation and emission energies correspond to the first excited state ($\pi \rightarrow \pi^*$ and $\pi^* \rightarrow \pi$ transitions, respectively). [b] All values computed at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM model. [c] Excitation wavelength, in nm. [d] Oscillator strength. [e] Emission wavelength, in nm. [f] Stokes shift (λ_{em} - λ_{exc}).

***Table S14**. TD-DFT excitation and emission energies and their corresponding oscillator strengths of **Bz_3ABM** using six different solvents (PCM model).[a,b] Charge descriptors along the π-conjugated structure of the aminomaleimide ring.*

Solvent	λ_{exc}[c]	f_{exc}[d]	λ_{em}[e]	f_{em}[d]	$\Delta\lambda$[f]	Q_{NBO1}	Q_{HOMO1}
1,4-Dioxane	332.1	0.098	443.9	0.063	111.9	0.136	0.389
Toluene	332.7	0.101	444.8	0.064	112.1	0.135	0.390
Diethyl Ether	334.0	0.097	450.9	0.078	116.8	0.126	0.399
Tetrahydrofuran	335.7	0.101	455.2	0.088	119.4	0.120	0.405
Methanol	337.1	0.099	460.7	0.102	123.7	0.113	0.410
Dimethyl Sulfoxide	337.8	0.104	461.3	0.103	123.6	0.112	0.410

[a] All excitation and emission energies correspond to the first excited state ($\pi \rightarrow \pi^*$ and $\pi^* \rightarrow \pi$ transitions, respectively). [b] All values computed at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM model. [c] Excitation wavelength, in nm. [d] Oscillator strength. [e] Emission wavelength, in nm. [f] Stokes shift (λ_{em} - λ_{exc}).

For **HMAM**, we then performed the calculations again, but with the addition of one or two explicit solvent molecules, see Table S15 and Figures Figure **S32**-Figure **S34**. It is worth noting that three and four explicit solvent molecules were also studied, but the high endergonic values obtained indicate that these complexes are quite unprovable to exist in solution. In the case of one solvent molecule, two different conformers were studied (1a and 1b). Additionally, with two solvent molecules, also several conformations were calculated, but only the most stable conformation found is displayed for clarity purposes. The results shown in Table S15 present larger bathochromic shift of the λ_{exc} and λ_{em} values than the ones considering the PCM methodology, (c.f. Table S9). Additionally, when two solvent molecules are included, an important reduction of the error between theoretical and experimental λ_{ex} and λ_{em} values is found. This improvement becomes especially significant for the polar solvents.

***Table S15.** TD-DFT excitation and emission energies and their corresponding oscillator strengths of **HMAM** using six different solvents and considering n explicit solvent molecules.[a,b] For one solvent molecule two different conformers were modelled (1a and 1b). Charge descriptors along the π-conjugated structure of the aminomaleimide ring.*

Solvent	n	λ_{exc}[c]	f_{exc}[d]	λ_{em}[e]	f_{em}[d]	$\Delta\lambda$[f]	Q_{NBO1}	Q_{HOMO1}
Dioxane	1a	319.4	0.150	417.2	0.101	97.8	-0.087	0.568

Solvent	n	λ_{exc}[c]	f_{exc}[d]	λ_{em}[e]	f_{em}[d]	$\Delta\lambda$[f]	Q_{NBO1}	Q_{HOMO1}
	1b	311.4	0.141	403.2	0.091	91.8	-0.088	0.568
	2	321.6	0.147	422.4	0.096	100.8	-0.117	0.567
	1a	317.2	0.103	442.9	0.053	125.7	-0.051	0.524
Toluene	1b	310.8	0.137	402.6	0.088	91.8	-0.066	0.565
	2	321.5	0.097	443.7	0.052	122.3	-0.061	0.410
	1a	320.5	0.152	424.3	0.122	103.8	-0.100	0.570
Diethyl Ether	1b	314.7	0.130	413.5	0.100	98.7	-0.095	0.567
	2	322.6	0.142	430.4	0.111	107.8	-0.120	0.567
	1a	323.1	0.150	428.6	0.128	105.5	-0.111	0.571
THF	1b	316.5	0.131	418.7	0.107	102.3	-0.110	0.568
	2	321.8	0.136	435.1	0.114	113.3	-0.121	0.564
	1a	328.9	0.139	451.6	0.127	122.7	-0.112	0.571
Methanol	1b	322.4	0.144	430.9	0.131	108.5	-0.104	0.572
	2	334.9	0.143	463.8	0.123	128.9	-0.125	0.575
	1a	330.6	0.152	450.3	0.141	119.7	-0.138	0.574
Dimethyl Sulfoxide	1b	322.0	0.142	430.6	0.122	108.6	-0.136	0.568
	2	335.8	0.150	460.4	0.129	124.6	-0.180	0.573

[a] All excitation and emission energies correspond to the first excited state ($\pi \rightarrow \pi^*$ and $\pi^* \rightarrow \pi$ transitions, respectively). [b] All values computed at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM model. [c] Excitation wavelength, in nm. [d] Oscillator strength. [e] Emission wavelength, in nm. [f] Stokes shift (λ_{em} - λ_{exc}).

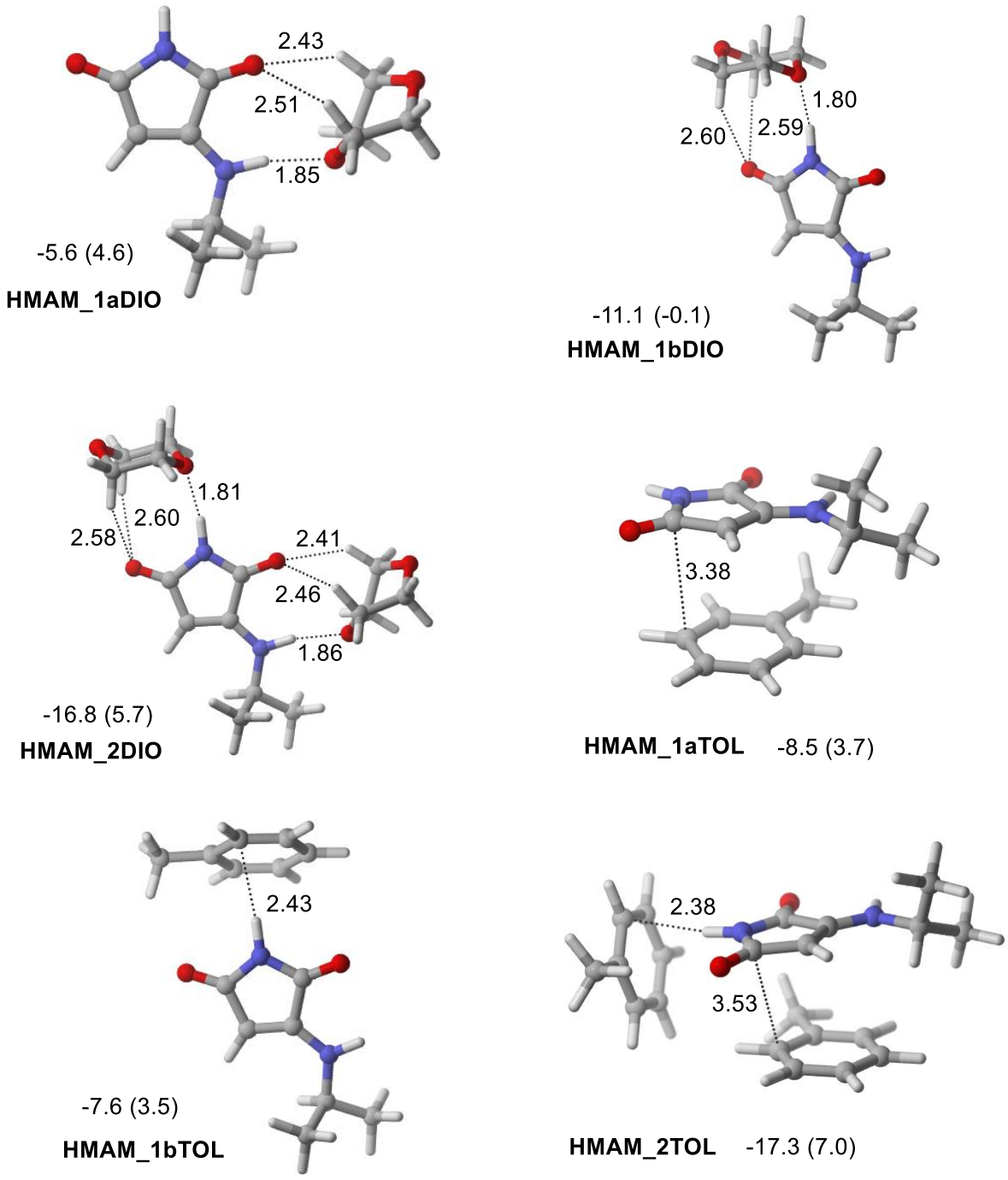


Figure S32. *CAM-B3LYP-D3BJ/6-311G(d,p)-optimized geometries for complexes formed between **HMAM** and one or two solvent molecules of 1,4-dioxane (DIO) and toluene (TOL). In the case of one solvent molecule, two different conformers were modelled (1a and 1b). Bond distances are given in Å. The adjacent values to the name of the complexes correspond to their relative stability with respect to their isolated solvent molecules (the parentheses values are the relative Gibbs energies at 298 K) and they are given in kcal/mol.*

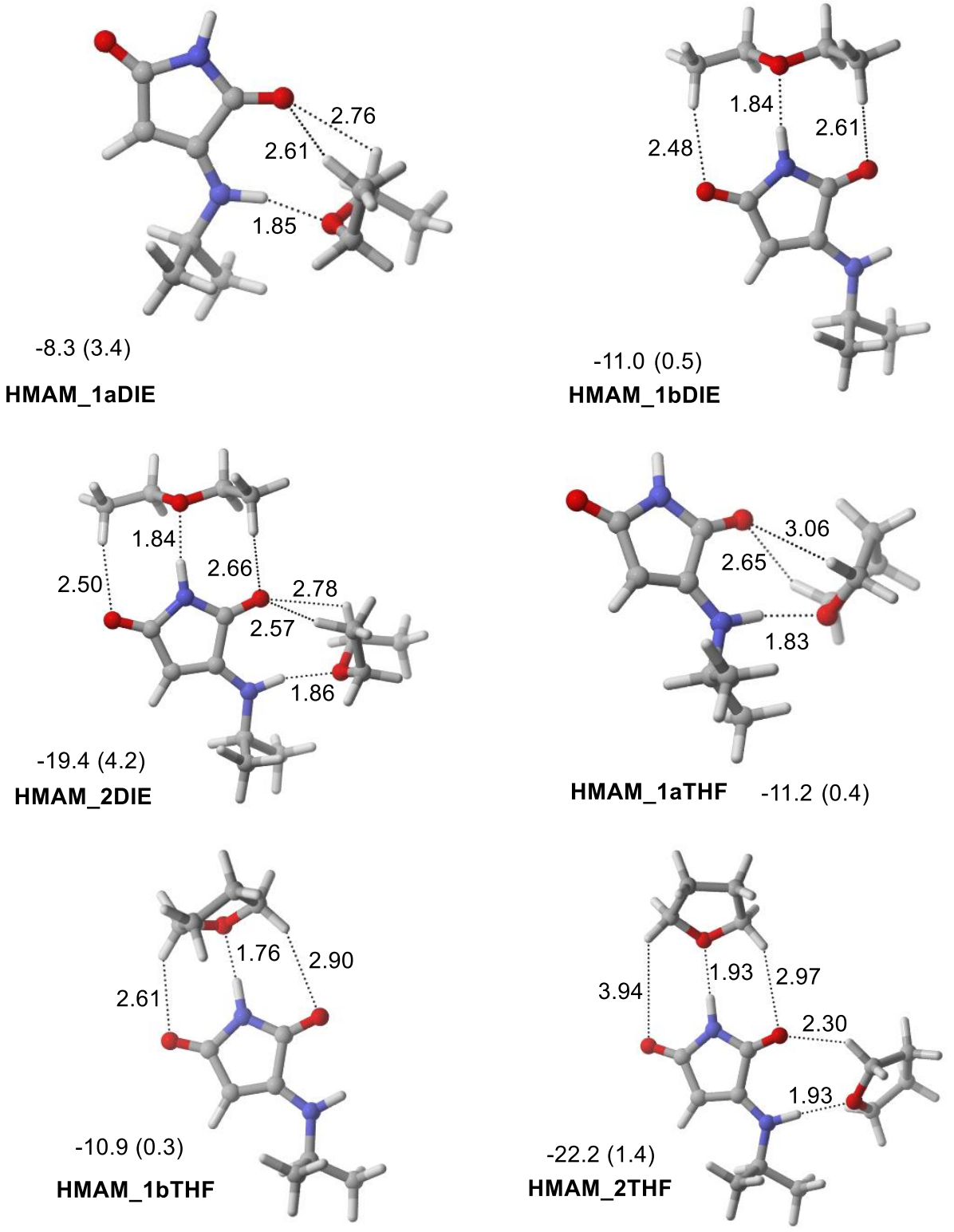


Figure S33. *CAM-B3LYP-D3BJ/6-311G(d,p)-optimized geometries for complexes formed between* ***HMAM*** *and one or two solvent molecules of diethyl ether (DIE) and tetrahydrofuran (THF). In the case of one solvent molecule, two different conformers were modelled (1a and 1b). Bond distances are given in Å. The adjacent values to the name of the complexes correspond to their relative stability with respect to their isolated solvent molecules (the parentheses values are the relative Gibbs energies at 298 K) and they are given in kcal/mol.*

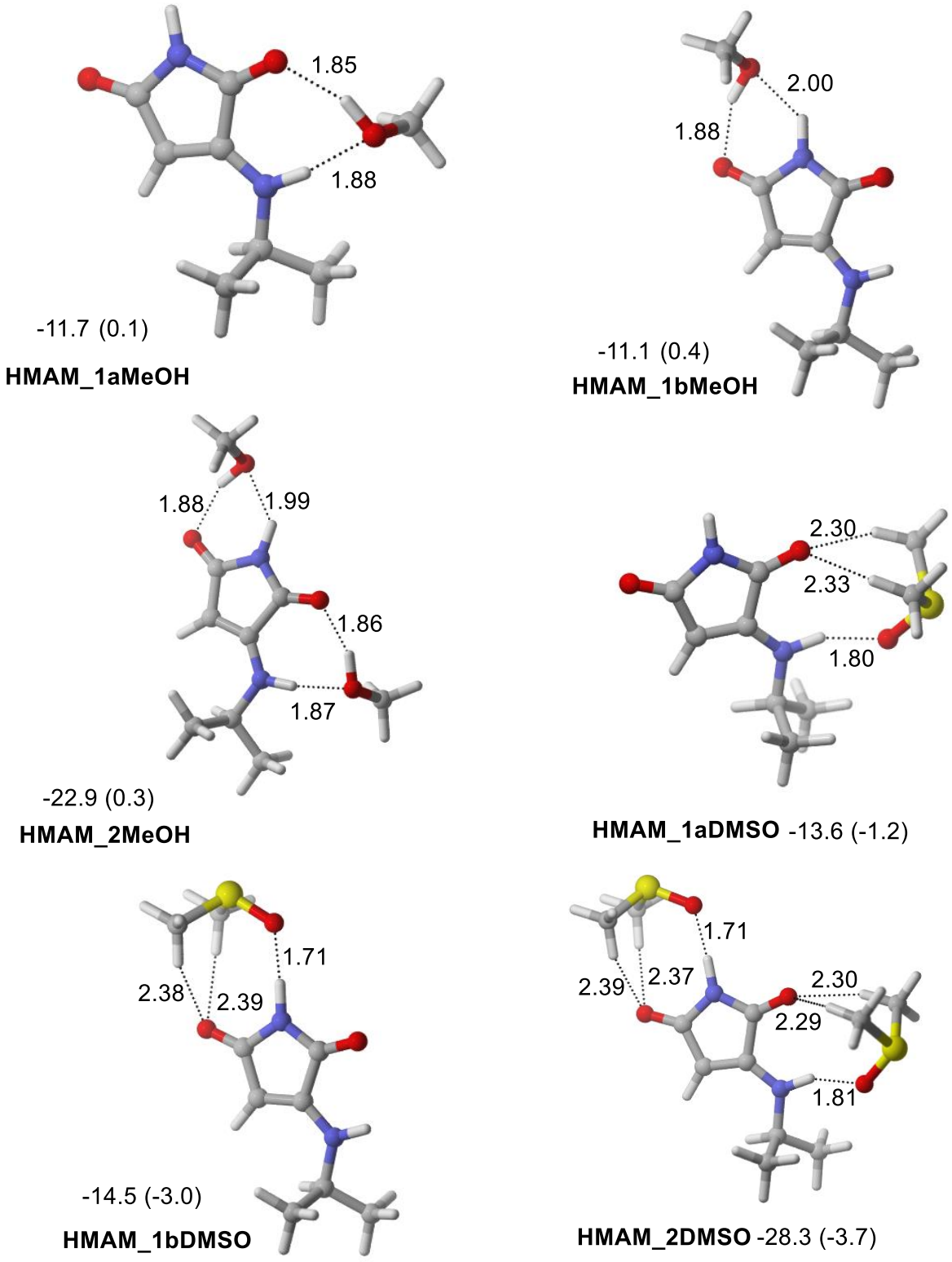


Figure S34. *CAM-B3LYP-D3BJ/6-311G(d,p)-optimized geometries for complexes formed between* ***HMAM*** *and one or two solvent molecules of methanol (MeOH) and dimethyl sulfoxide (DMSO). In the case of one solvent molecule, two different conformers were modelled (1a and 1b). Bond distances are given in Å. The adjacent values to the name of the complexes correspond to their relative stability with respect to their isolated solvent molecules (the parentheses values are the relative Gibbs energies at 298 K) and they are given in kcal/mol.*

These results motivated us to study the effect of the explicit solvent for five additional aminomaleimides (**BzMAM**, **Bz$_2$MAM**, **Bz$_3$MAM**, and **Bz$_3$ABM**) but only for the polar solvents (methanol and dimethyl sulfoxide), see Table S16 and Figures Figure **S35**-Figure **S38**. When two solvent molecules are considered, the errors between theoretical and experimental λ_{em} (λ_{exc}) values become smaller than 10 nm (are reduced by 50%).

Table S16. *TD-DFT excitation and emission energies and their corresponding oscillator strengths of **BzMAM**, **Bz$_2$MAM**, **Bz$_3$MAM**, and **Bz$_3$ABM** using two different solvents and considering one or two explicit solvent molecules of methanol and dimethylsulfoxide.[a,b] For one solvent molecule two different conformers were modelled (1a and 1b). Charge descriptors along the π-conjugated structure of the aminomaleimide ring.*

Dye	Solvent	n	λ_{exc}[c]	f_{exc}[d]	λ_{em}[e]	f_{em}[d]	$\Delta\lambda$[f]	Q_{NBO1}	Q_{HOMO1}
BzMAM	MeOH	1a	339.3	0.104	476.1	0.086	136.8	-0.094	0.556
		1b	336.1	0.112	462.0	0.091	126.0	-0.071	0.542
		2	348.5	0.110	495.0	0.088	146.5	-0.095	0.551
	DMSO	1a	339.4	0.115	473.2	0.102	133.7	-0.116	0.559
		1b	331.5	0.121	456.9	0.091	125.4	-0.080	0.530
		2	343.6	0.132	480.8	0.105	137.1	-0.123	0.555
Bz$_2$MAM	MeOH	1a	337.2	0.108	475.2	0.090	138.0	-0.073	0.553
		1b	334.4	0.116	457.6	0.095	123.2	-0.053	0.531
		2	346.7	0.115	491.0	0.092	144.4	-0.077	0.544
	DMSO	1a	337.3	0.120	469.0	0.101	131.7	-0.093	0.555
		1b	328.4	0.126	453.8	0.092	125.4	-0.062	0.542
		2	340.2	0.132	471.5	0.114	131.3	-0.103	0.554
Bz$_3$MAM	MeOH	1a	333.4	0.109	467.8	0.091	134.3	-0.033	0.507

Dye	Solvent	n	λ_{exc}[c]	f_{exc}[d]	λ_{em}[e]	f_{em}[d]	$\Delta\lambda$[f]	Q_{NBO1}	Q_{HOMO1}
Bz_3ABM		1b	328.9	0.120	449.6	0.098	120.7	-0.020	0.484
		2	340.5	0.119	481.4	0.093	140.9	-0.043	0.509
	DMSO	1a	333.0	0.125	462.6	0.112	129.6	-0.049	0.529
		1b	326.2	0.125	445.0	0.096	118.7	-0.017	0.478
		2	336.5	0.136	468.7	0.112	132.3	-0.053	0.523
	MeOH	1a	348.8	0.102	495.7	0.099	146.8	0.090	0.418
		1b	345.0	0.106	474.7	0.102	129.7	0.104	0.407
		2	356.5	0.109	511.1	0.098	154.6	0.079	0.415
	DMSO	1a	347.5	0.118	483.5	0.115	136.0	0.077	0.426
		1b	342.0	0.112	468.9	0.104	126.9	0.107	0.405
		2	350.5	0.129	490.2	0.114	139.7	0.074	0.422

[a] All excitation and emission energies correspond to the first excited state ($\pi \rightarrow \pi^*$ and $\pi^* \rightarrow \pi$ transitions, respectively). [b] All values computed at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM model. [c] Excitation wavelength, in nm. [d] Oscillator strength. [e] Emission wavelength, in nm. [f] Stokes shift (λ_{em} - λ_{exc}).

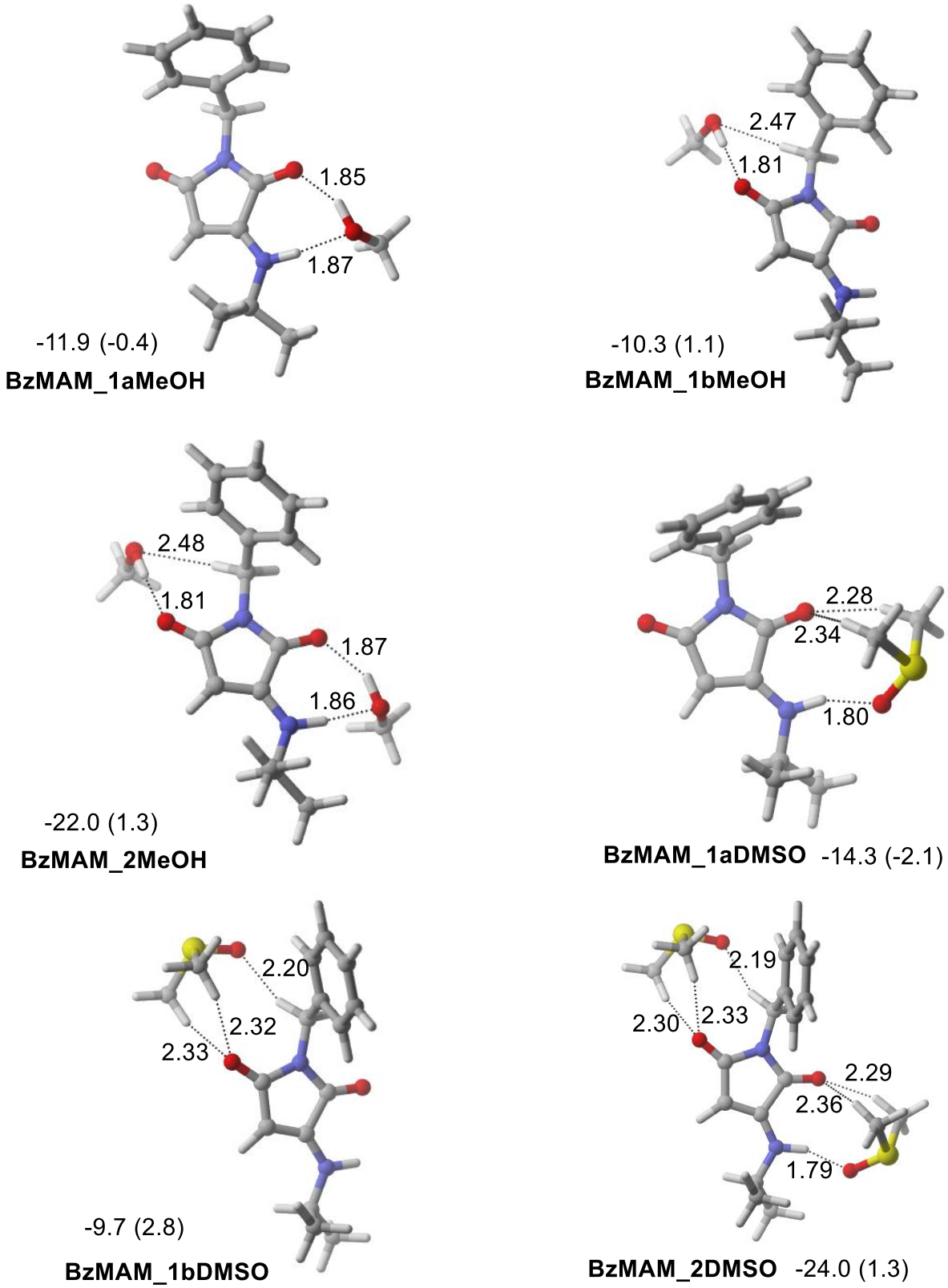


Figure S35. *CAM-B3LYP-D3BJ/6-311G(d,p)-optimized geometries for complexes formed between* ***BzMAM*** *and one and two solvent molecules of methanol (MeOH) and dimethyl sulfoxide (DMSO) . In the case of one solvent molecule, two different conformers were modelled (1a and 1b). Bond distances are given in Å. The adjacent values to the name of the complexes correspond to their relative stability with respect to their isolated solvent molecules (the parentheses values are the relative Gibbs energies at 298 K) and they are given in kcal/mol.*

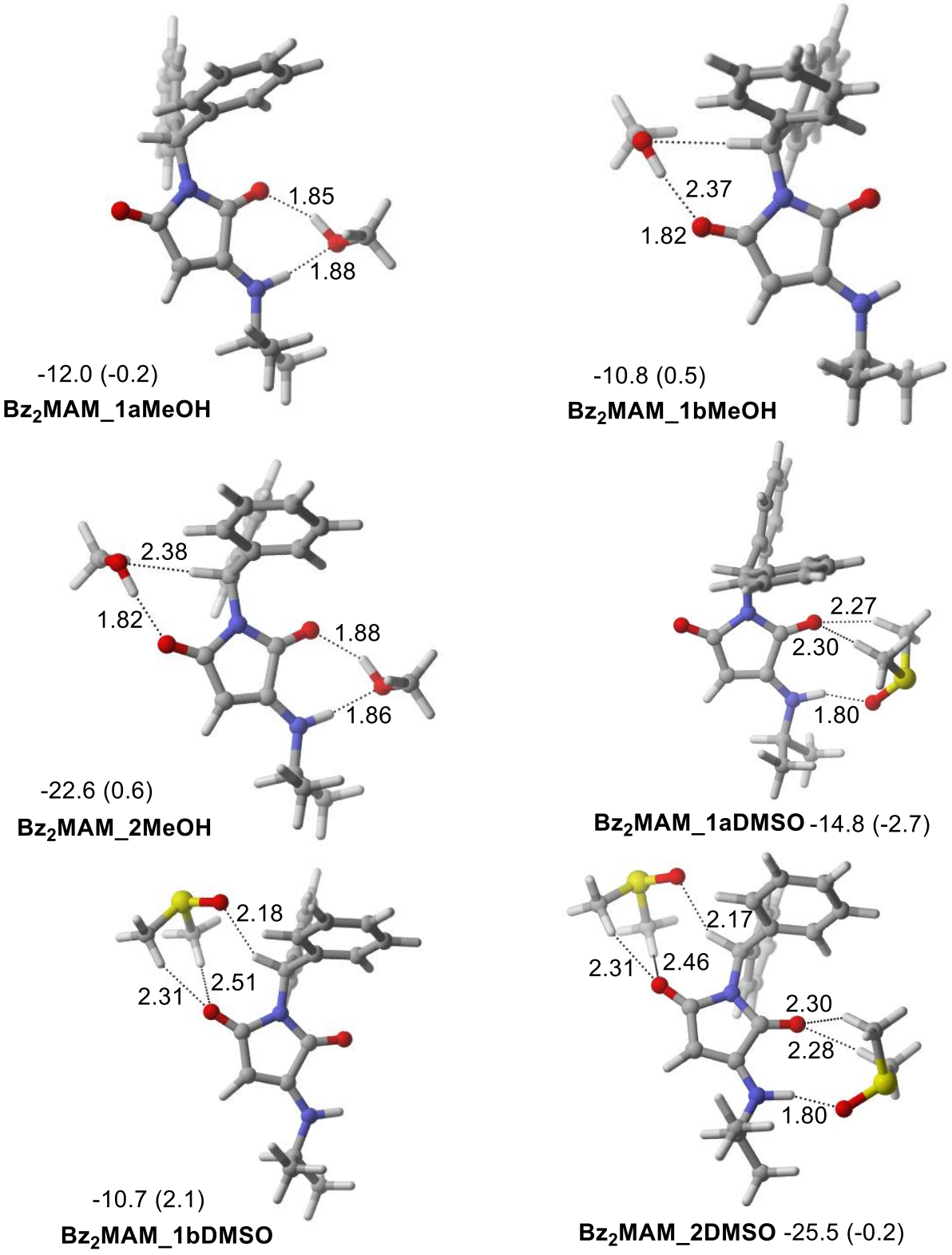


Figure S36. *CAM-B3LYP-D3BJ/6-311G(d,p)-optimized geometries for complexes formed between* ***Bz$_2$MAM*** *and one and two solvent molecules of methanol (MeOH) and dimethyl sulfoxide (DMSO) . In the case of one solvent molecule, two different conformers were modelled (1a and 1b). Bond distances are given in Å. The adjacent values to the name of the complexes correspond to their relative stability with respect to their isolated solvent molecules (the parentheses values are the relative Gibbs energies at 298 K) and they are given in kcal/mol.*

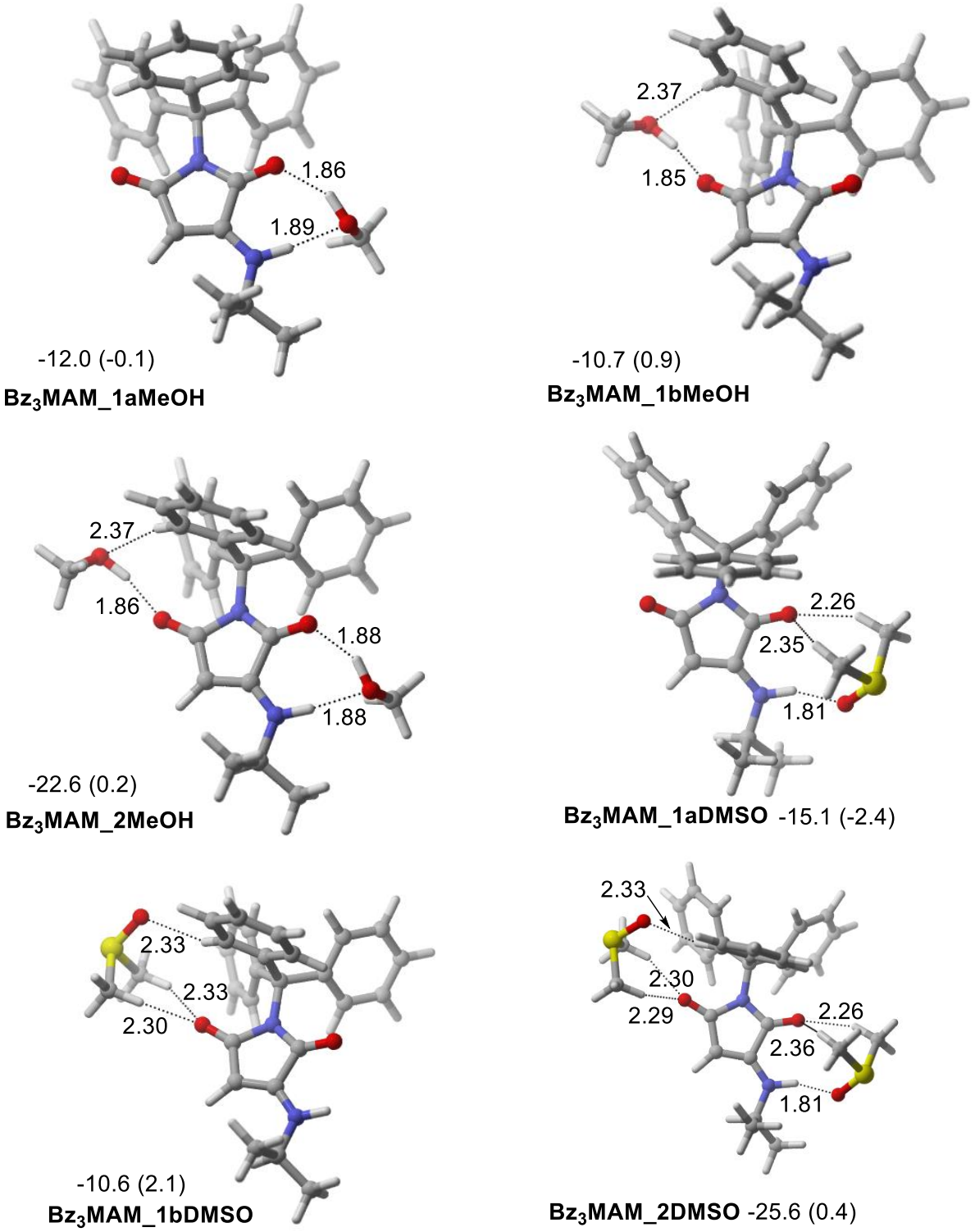


Figure S37. *CAM-B3LYP-D3BJ/6-311G(d,p)-optimized geometries for complexes formed between* ***Bz₃MAM*** *and one and two solvent molecules of methanol (MeOH) and dimethyl sulfoxide (DMSO) . In the case of one solvent molecule, two different conformers were modelled (1a and 1b). Bond distances are given in Å. The adjacent values to the name of the complexes correspond to their relative stability with respect to their isolated solvent molecules (the parentheses values are the relative Gibbs energies at 298 K) and they are given in kcal/mol.*

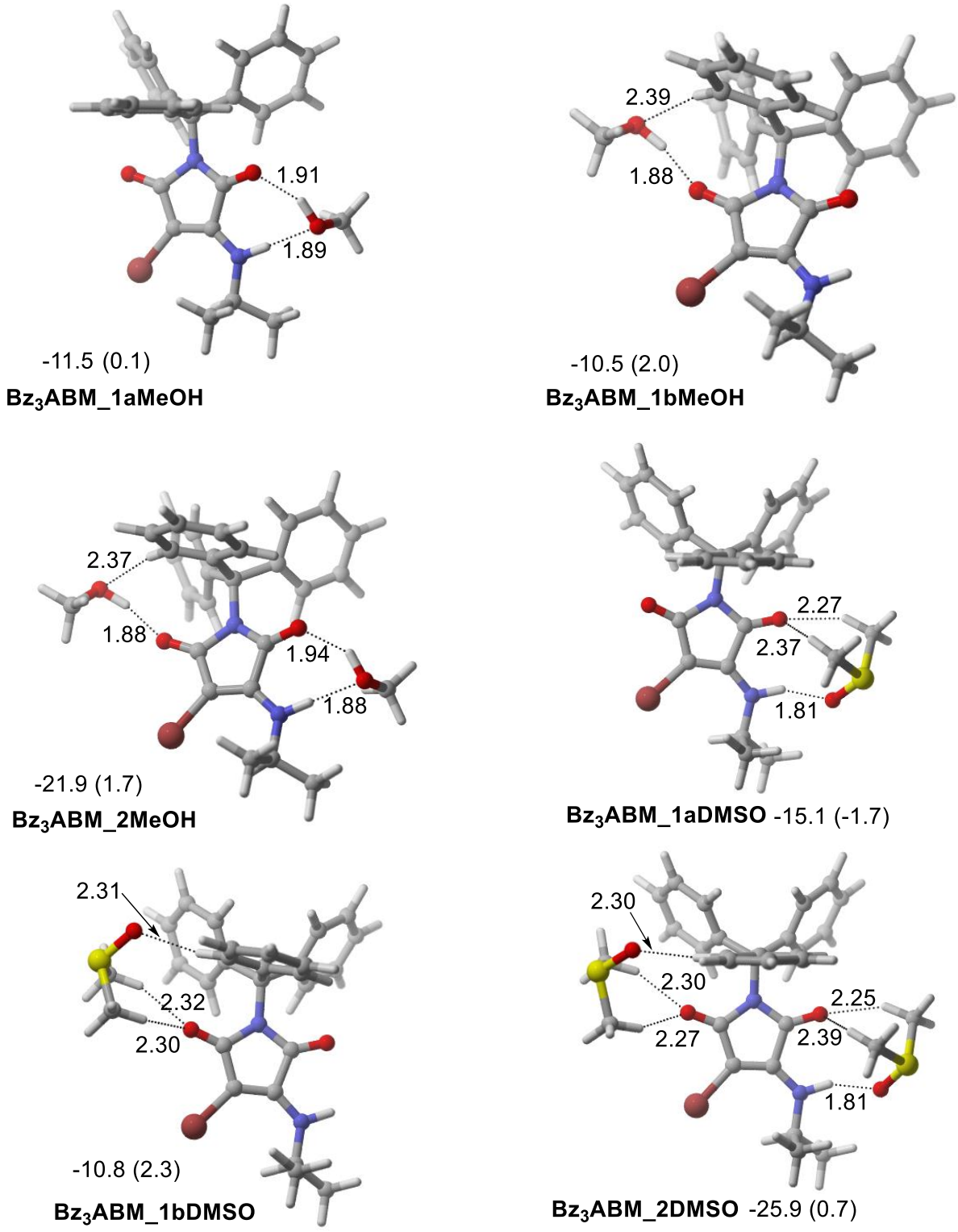


Figure S38. *CAM-B3LYP-D3BJ/6-311G(d,p)-optimized geometries for complexes formed between* ***Bz$_3$ABM*** *and one and two solvent molecules of methanol (MeOH) and dimethyl sulfoxide (DMSO) . In the case of one solvent molecule, two different conformers were modelled (1a and 1b). Bond distances are given in Å. The adjacent values to the name of the complexes correspond to their relative stability with respect to their isolated solvent molecules (the parentheses values are the relative Gibbs energies at 298 K) and they are given in kcal/mol.*

In conclusion, these results support the conclusion that solvent polarity and the interactions between the solvent molecules and the aminomaleimide play a critical role in determining the photophysical parameters of these dyes. Furthermore, they also reinforce the conclusion that the fluorescence quenching observed in polar solvents can be attributed to electron-driven proton transfer (Q_{NBO1} values become more negative when increasing the polarity of the solvent, and with the addition of explicit polar solvent molecules).

5.7 Rotational barriers

To rationalize the unusual quantum yield behaviour of **Bz$_3$MAM** in the solid state and in polar solvents, the rotational barriers of **BzMAM**, **Bz$_2$MAM**, **Bz$_3$MAM**, **Bz$_3$ABM**, and **TPE** were evaluated in two different solvent conditions: a) only the PCM methodology with ε = 4.240 (diethyl ether); and b) two explicit molecules of methanol or dimethyl sulfoxide in addition to the PCM methodology with ε = 32.613 or 46.826, respectively (see Table S17). In the **BzMAM** and **Bz$_2$MAM** fluorophores, the two solvent conditions present similar energetic barriers, even a small reduction of them is observed with the inclusion of the explicit polar molecules. On the other hand, for **Bz$_3$MAM**, an increase of *ca.* 2 kcal/mol is observed, indicating that the hydrogen bonds formed between the solvent and the carbonyl oxygen and the hydrogen of the phenyl groups can reduce the rotation of the trityl substituent. Additionally, the computational rotational barriers obtained from **Bz$_3$ABM** display again that a tiny decrease is observed when the inclusion of the explicit polar molecules is considered. The electron withdrawing nature of the bromine atom reduces the effect of the trityl substituent, increasing its ability to rotate. For the sake of comparison, the rotational barrier of the archetypical aggregation-induced emission dye, tetraphenylethylene (**TPE**), has been evaluated and was calculated to be 3 kcal mol^{-1} lower than **Bz$_3$MAM**, illustrating the relevance of the trityl steric hindrance. This difference helps to understand that in flexible polymers a larger quenching effect is observed with **TPE** than **Bz$_3$MAM.**

Table S17. *Relative energies, energies plus ZPE, enthalpies, and free energies (in kcal/mol at 298K) calculated for the rotational barriers of **BzMAM**, **Bz$_2$MAM**, **Bz$_3$MAM**, **Bz$_3$ABM**, and **TPE** both isolated and with the presence of two explicit solvent molecules of methanol or dimethylsulfoxide (for **TPE** only the isolated molecule was studied).*[a]

Dye	Solvent[b]	ΔE	$\Delta E(E+ZPE)$	ΔH	ΔG
BzMAM	Et_2O	5.4	5.2	4.7	6.5
	MeOH	5.9	5.5	5.0	6.6
	DMSO	4.6	4.1	3.2	5.7
Bz$_2$MAM	Et_2O	7.1	6.7	6.2	8.4
	MeOH	7.3	6.8	6.3	8.1
	DMSO	4.9	5.0	4.2	8.0

Dye	Solvent[b]	ΔE	$\Delta E(E+ZPE)$	ΔH	ΔG
	Et_2O	8.2	8.2	7.7	8.9
Bz_3MAM	MeOH	10.4	10.2	9.7	11.0
	DMSO	10.5	10.5	10.0	10.5
	Et_2O	8.2	8.1	7.7	9.9
Bz_3ABM	MeOH	10.1	9.8	9.4	9.8
	DMSO	10.2	10.0	9.7	9.5
TPE	Et_2O	5.7	5.3	5.0	5.6

[a] All values are in atomic units and computed at CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution. [b] For Et_2O, calculations were made using the PCM with ε = 4.240; for MeOH and DMSO calculations were made using the PCM with ε = 32.613 and 46.826, respectively, and two explicit molecules of solvent.

5.8 Cartesian coordinates

Table S18. *Cartesian coordinates (in Å) of the stationary points in the ground state optimized at the CAM-B3LYP-D3BJ/6-311G(d,p) level of theory in solution using the PCM model (the solvent used is indicated in parenthesis).*

HMAM (diethyl ether)

C	-2.506011	-1.164675	-0.084737
C	-1.072170	-1.007527	-0.297634
C	-0.772396	0.310290	-0.196386
C	-2.047036	1.077003	0.106111
N	-3.028374	0.135779	0.152723
O	-3.191582	-2.156601	-0.087966
O	-2.126282	2.270048	0.264822
N	0.345453	1.017333	-0.318190
H	0.263600	2.010886	-0.146529
C	1.662105	0.437833	-0.559731
H	-4.001588	0.324046	0.336419
H	-0.419871	-1.841843	-0.493526
C	2.249638	-0.144611	0.723006
H	1.576683	-0.881420	1.164006
H	3.203294	-0.633916	0.516187
H	2.419510	0.647685	1.455614
C	2.561203	1.496888	-1.177691
H	2.697850	2.334372	-0.487700
H	3.544479	1.078629	-1.394447
H	2.134893	1.878796	-2.106464
H	1.518478	-0.370379	-1.283536

HABM (diethyl ether)

C	-2.587019	-1.162381	-0.106159
C	-1.145688	-1.055993	-0.355475
C	-0.762212	0.238549	-0.231115
C	-2.006096	1.042138	0.123977

N	-3.031771	0.149338	0.173961
O	-3.302037	-2.127512	-0.119514
O	-2.023426	2.230342	0.316581
N	0.358913	0.938858	-0.346513
H	0.257742	1.922345	-0.124267
C	1.711919	0.420871	-0.553250
H	-3.989717	0.380652	0.389000
C	2.307415	-0.081513	0.758271
H	1.682148	-0.859383	1.198152
H	3.300812	-0.500033	0.585833
H	2.397625	0.738058	1.475185
C	2.552539	1.517201	-1.188767
H	2.622415	2.383714	-0.524942
H	3.564336	1.155667	-1.373792
H	2.121018	1.840549	-2.136943
H	1.632072	-0.412647	-1.251160
Br	-0.152777	-2.591206	-0.778296

BzMAM (diethyl ether)

C	-2.267908	-0.740400	-0.792392
C	-0.829709	-0.967977	-0.772198
C	-0.249338	0.090290	-0.155493
C	-1.337510	1.059690	0.264662
N	-2.507265	0.515276	-0.163189
O	-3.161814	-1.422724	-1.232755
O	-1.165593	2.098658	0.857689
N	1.004435	0.428276	0.121260
H	1.127272	1.284619	0.645667
C	2.164212	-0.410376	-0.160889
H	-0.375204	-1.850475	-1.189645
C	2.300072	-1.525866	0.872257
H	1.388941	-2.123427	0.926790
H	3.127639	-2.187594	0.609752
H	2.494711	-1.105128	1.861442
C	3.402813	0.468915	-0.228553
H	3.579796	0.957094	0.734038
H	4.281140	-0.132193	-0.465057
H	3.294309	1.239334	-0.993308
H	1.993212	-0.856768	-1.145360
C	-3.827779	1.065867	0.089923
H	-4.474704	0.707347	-0.709687
H	-3.752657	2.150516	0.015107
C	-4.373178	0.661082	1.438077
C	-4.224251	1.495395	2.540858
C	-5.002501	-0.570708	1.597080
C	-4.700644	1.106879	3.785656
H	-3.724162	2.449692	2.423225
C	-5.478348	-0.960277	2.840298
H	-5.107750	-1.225849	0.740115
C	-5.329106	-0.121232	3.937290
H	-4.581074	1.764870	4.638031
H	-5.968706	-1.919726	2.953318
H	-5.702608	-0.424353	4.908003

Bz_2MAM (diethyl ether)

C	0.355764	-1.799496	-0.500977
C	1.681979	-1.455331	-0.017110
C	1.863224	-0.126611	-0.212426
C	0.608236	0.449184	-0.839620
N	-0.243109	-0.601881	-1.006994
O	-0.219666	-2.860312	-0.515442
O	0.447856	1.612116	-1.121882
N	2.865295	0.714124	0.009884
H	2.683091	1.685525	-0.207245
C	4.120347	0.347697	0.657360
H	2.349210	-2.181622	0.415005
C	3.949489	0.254751	2.171309
H	3.155701	-0.445939	2.434276
H	4.875346	-0.086967	2.637736
H	3.694970	1.233282	2.584970
C	5.192303	1.348656	0.256296
H	4.928773	2.352449	0.601346
H	6.147986	1.080214	0.707259
H	5.316154	1.376012	-0.827251
H	4.394544	-0.638086	0.269108
C	-1.618365	-0.565572	-1.491692
C	-2.523456	0.146562	-0.501964
C	-2.589966	1.536677	-0.436508

C	-3.281028	-0.609525	0.385291
C	-3.399812	2.153694	0.504221
H	-1.996615	2.130068	-1.118673
C	-4.094718	0.007674	1.326366
H	-3.230548	-1.691619	0.340667
C	-4.155123	1.391781	1.387409
H	-3.443083	3.235403	0.547733
H	-4.681829	-0.594494	2.009186
H	-4.789585	1.877231	2.119194
C	-1.720728	-0.080197	-2.929878
C	-2.947960	0.345294	-3.431912
C	-0.630143	-0.132805	-3.790892
C	-3.078119	0.718911	-4.761282
H	-3.809736	0.388526	-2.778152
C	-0.757674	0.244121	-5.120268
H	0.330020	-0.473867	-3.426104
C	-1.981828	0.673734	-5.610969
H	-4.040790	1.049346	-5.132533
H	0.105475	0.201273	-5.773616
H	-2.081299	0.970645	-6.647920
H	-1.903577	-1.620294	-1.486178

Bz_3MAM (diethyl ether)

C	0.930033	-0.704901	-1.579032
C	2.365965	-0.487266	-1.626535
C	2.709724	0.273688	-0.563895
C	1.463055	0.567355	0.236844
N	0.398174	0.101242	-0.500828
O	0.254251	-1.427348	-2.264380
O	1.471411	1.084206	1.326278
N	3.853135	0.771203	-0.106376
H	3.800216	1.238526	0.789797
C	5.161419	0.481493	-0.683525
H	2.987231	-0.930709	-2.386219
C	5.653046	-0.901760	-0.265105
H	4.929936	-1.673142	-0.534019
H	6.599459	-1.133915	-0.757061
H	5.807911	-0.937922	0.815686
C	6.130302	1.584167	-0.286895
H	6.255008	1.612716	0.799295
H	7.109861	1.405332	-0.731084
H	5.770787	2.558765	-0.619988
H	5.031411	0.499332	-1.769760
C	-0.966797	-0.081305	0.055113
C	-0.891224	-1.364396	0.895714
C	-0.445976	-1.314171	2.216052
C	-1.104496	-2.611557	0.312102
C	-0.251746	-2.479342	2.943286
H	-0.236076	-0.357881	2.673701
C	-0.911618	-3.776489	1.040511
H	-1.403572	-2.672296	-0.724265
C	-0.490993	-3.715598	2.360933
H	0.090716	-2.417458	3.969249
H	-1.086917	-4.735661	0.568397
H	-0.342578	-4.625568	2.929806
C	-2.010294	-0.117672	-1.075559
C	-1.829647	0.626981	-2.236840
C	-3.230573	-0.752986	-0.878091
C	-2.828589	0.704634	-3.192405
H	-0.898643	1.152216	-2.401660
C	-4.233836	-0.677488	-1.834911
H	-3.409629	-1.312222	0.030297
C	-4.036409	0.047125	-2.999448
H	-2.661568	1.282091	-4.093688
H	-5.174191	-1.187083	-1.662409
H	-4.817274	0.105433	-3.747829
C	-1.395492	1.168294	0.847529
C	-0.985947	2.437939	0.451963
C	-2.337511	1.062833	1.864316
C	-1.476043	3.570233	1.080487
H	-0.277444	2.548979	-0.357764
C	-2.831397	2.196354	2.495659
H	-2.697153	0.090077	2.171093
C	-2.399072	3.455647	2.111348
H	-1.135199	4.547855	0.761500
H	-3.560237	2.088893	3.289952
H	-2.781831	4.340791	2.604514

Bz_3ABM (diethyl ether)

C	0.736005	-1.145024	-0.179751
C	2.126209	-0.720202	-0.342916
C	2.177601	0.629830	-0.387136
C	0.753227	1.128438	-0.239876
N	-0.079697	0.033333	-0.287208
O	0.315483	-2.248932	0.027295
O	0.476900	2.289094	-0.080463
N	3.105816	1.570945	-0.506200
H	2.746835	2.513441	-0.403142
C	4.557436	1.388500	-0.466289
C	5.045749	1.224944	0.969784
H	4.558808	0.377413	1.453637
H	6.123628	1.052497	0.984522
H	4.832570	2.125343	1.551026
C	5.208267	2.570161	-1.168348
H	4.974769	3.504284	-0.649390
H	6.292292	2.453576	-1.174507
H	4.861941	2.650991	-2.199501
H	4.780141	0.479173	-1.024640
C	-1.510214	0.072412	0.123086
C	-1.484534	0.095679	1.658072
C	-1.357172	1.302736	2.343800
C	-1.420400	-1.092608	2.383289
C	-1.204819	1.321320	3.722552
H	-1.364280	2.234094	1.795668
C	-1.268473	-1.073105	3.762014
H	-1.470745	-2.039023	1.864497
C	-1.167175	0.133735	4.438489
H	-1.112594	2.270540	4.236415
H	-1.224555	-2.008446	4.306668
H	-1.051314	0.148356	5.515484
C	-2.276269	-1.114464	-0.487246
C	-1.932938	-1.615711	-1.739064
C	-3.432052	-1.586325	0.123255
C	-2.705184	-2.589519	-2.348832
H	-1.052413	-1.246031	-2.247109
C	-4.208437	-2.562801	-0.486341
H	-3.738215	-1.191632	1.082558
C	-3.846154	-3.073368	-1.722535
H	-2.412641	-2.973252	-3.318717
H	-5.101432	-2.921158	0.011331
H	-4.449111	-3.837246	-2.198018
C	-2.217183	1.280180	-0.519442
C	-1.853657	1.731858	-1.784374
C	-3.345795	1.826630	0.080816
C	-2.577374	2.728531	-2.417261
H	-0.998811	1.301613	-2.288687
C	-4.073521	2.825117	-0.551821
H	-3.669191	1.472328	1.050082
C	-3.689803	3.285610	-1.801385
H	-2.270412	3.070104	-3.398396
H	-4.946358	3.239696	-0.062132
H	-4.255683	4.065956	-2.295304
Br	3.492138	-2.003691	-0.411096

PhMAM (diethyl ether)

C	-2.220718	-0.707794	-0.526769
C	-0.787768	-0.943237	-0.566690
C	-0.162327	0.161802	-0.096643
C	-1.207183	1.185977	0.287768
N	-2.421721	0.612394	0.015523
O	-3.130463	-1.421787	-0.861197
O	-0.970841	2.278187	0.741545
N	1.108887	0.503841	0.069934
H	1.273639	1.411075	0.486296
C	2.239699	-0.377308	-0.202621
H	-0.366442	-1.867237	-0.924851
C	2.432278	-1.387515	0.925137
H	1.521610	-1.963336	1.096410
H	3.235363	-2.084036	0.677284
H	2.694307	-0.874115	1.853049
C	3.479749	0.471091	-0.435826
H	3.724682	1.046056	0.461633
H	4.334053	-0.164764	-0.669294
H	3.329120	1.166092	-1.263158
H	2.000201	-0.915202	-1.125155
C	-3.684603	1.228679	0.212549
C	-4.729730	0.501849	0.771388

C	-3.869922	2.557902	-0.150435
C	-5.962328	1.108450	0.957323
H	-4.577688	-0.532173	1.044594
C	-5.101736	3.159700	0.056128
H	-3.050597	3.116866	-0.580100
C	-6.152082	2.437722	0.605494
H	-6.776663	0.538112	1.386958
H	-5.240983	4.197192	-0.221802
H	-7.114911	2.909173	0.758890

PhABM (diethyl ether)

C	-0.521847	-1.076611	-0.117623
C	0.882234	-0.669227	-0.130851
C	0.960846	0.680876	-0.052720
C	-0.460857	1.209280	0.022175
N	-1.294526	0.122828	-0.016861
O	-0.997754	-2.176402	-0.176372
O	-0.747068	2.375855	0.104012
N	1.915106	1.601419	-0.034107
H	1.573850	2.548679	0.081819
C	3.360080	1.379392	0.042202
C	3.786380	1.066551	1.473046
H	3.262586	0.189241	1.854274
H	4.858747	0.866021	1.510892
H	3.569847	1.912788	2.129336
C	4.063345	2.607033	-0.515229
H	3.831638	3.490864	0.086073
H	5.143793	2.462812	-0.494341
H	3.759372	2.798173	-1.545242
H	3.586210	0.523118	-0.593393
C	-2.714732	0.172481	0.021697
C	-3.412844	-0.697581	0.849802
C	-3.393035	1.093540	-0.766870
C	-4.797927	-0.646866	0.879254
H	-2.874126	-1.412901	1.454580
C	-4.777421	1.147658	-0.716116
H	-2.839160	1.767242	-1.405705
C	-5.483339	0.276478	0.101877
H	-5.342272	-1.329623	1.519739
H	-5.305289	1.870238	-1.325977
H	-6.565047	0.316837	0.133291
Br	2.228831	-1.969339	-0.257530

HMAM_1aDIO (1,4-dioxane)

C	-1.741720	1.706098	0.158846
C	-0.473098	2.418675	0.178554
C	0.533995	1.507172	0.156141
C	-0.079396	0.117410	0.104943
N	-1.423605	0.317619	0.117125
O	-2.874496	2.115912	0.169144
O	0.524699	-0.927897	0.060879
N	1.856974	1.605915	0.187325
H	2.412864	0.752858	0.081227
C	2.560106	2.883036	0.172552
H	-2.115336	-0.414650	0.086206
H	-0.415496	3.493762	0.202009
C	2.669698	3.428079	-1.249912
H	1.685201	3.515766	-1.712253
H	3.136264	4.415276	-1.248315
H	3.279588	2.760354	-1.863066
C	3.923104	2.706120	0.826594
H	4.505935	1.952987	0.292223
H	4.475047	3.646871	0.814126
H	3.816461	2.381717	1.863177
H	1.966776	3.579208	0.773245
O	3.717162	-0.548888	-0.069546
C	3.547507	-1.371340	-1.226939
H	2.482983	-1.575983	-1.371584
H	3.916462	-0.796347	-2.076814
C	3.816492	-1.287749	1.154117
H	4.871192	-1.361708	1.438218
H	3.288741	-0.718167	1.921541
C	3.214352	-2.668698	1.018931
H	3.325772	-3.210980	1.958768
H	2.148746	-2.581814	0.789025
C	4.326158	-2.659805	-1.088022
H	4.203277	-3.266911	-1.987275
H	5.392782	-2.429561	-0.974328

O	3.881220	-3.432334	0.019945

HMAM_1bDIO (1,4-dioxane)

C	-1.746498	1.689628	0.136851
C	-0.490388	2.433634	0.181748
C	0.522417	1.536206	0.146166
C	-0.072124	0.140346	0.063869
N	-1.419977	0.315166	0.067472
O	-2.883718	2.101518	0.149666
O	0.568154	-0.881256	0.006794
N	1.848733	1.626817	0.182125
H	2.350836	0.752501	0.098807
C	2.587671	2.882414	0.206136
H	-2.124447	-0.427651	0.017202
H	-0.453466	3.508946	0.230863
C	2.640154	3.517983	-1.181018
H	1.636743	3.661179	-1.584502
H	3.132978	4.491215	-1.137129
H	3.198355	2.879352	-1.869556
C	3.974051	2.627889	0.776779
H	4.529259	1.934355	0.138867
H	4.540264	3.558197	0.830003
H	3.912336	2.202039	1.779303
H	2.044962	3.551214	0.881931
O	-3.567649	-1.507223	-0.072977
C	-4.399915	-1.539188	1.085822
H	-4.995410	-2.459958	1.071251
H	-3.734135	-1.559076	1.949062
C	-4.339576	-1.408764	-1.269067
H	-4.932392	-2.323764	-1.387039
H	-3.630550	-1.334853	-2.094135
C	-5.310124	-0.327497	1.113962
H	-6.002678	-0.387165	1.954096
H	-4.710226	0.586190	1.197946
C	-5.250535	-0.198795	-1.209493
H	-5.898929	-0.162863	-2.085440
H	-4.649406	0.716679	-1.161140
O	-6.092850	-0.280551	-0.069654

HMAM_2DIO (1,4-dioxane)

C	1.430885	-2.507069	-0.020782
C	0.029317	-2.815595	0.221383
C	-0.674845	-1.655717	0.158636
C	0.298718	-0.527673	-0.150787
N	1.521992	-1.109279	-0.233937
O	2.391575	-3.242704	-0.054922
O	0.007008	0.637859	-0.290069
N	-1.956182	-1.351872	0.323237
H	-2.254382	-0.389121	0.145215
C	-2.988406	-2.354208	0.557158
H	2.401359	-0.628044	-0.446735
H	-0.320591	-3.817257	0.405720
C	-3.422600	-3.005831	-0.754061
H	-2.567136	-3.433816	-1.279092
H	-4.143933	-3.803842	-0.566436
H	-3.891204	-2.265014	-1.406341
C	-4.154294	-1.704990	1.289349
H	-4.560627	-0.880004	0.700566
H	-4.947405	-2.433779	1.461624
H	-3.834209	-1.308636	2.254571
H	-2.547126	-3.119893	1.202770
O	4.069392	-0.050866	-0.830779
O	-3.142430	1.234329	-0.025601
C	5.023483	-0.153641	0.225294
H	5.857819	0.527614	0.019426
H	4.517684	0.167178	1.136406
C	4.606233	-0.515427	-2.068743
H	5.421751	0.150366	-2.375745
H	3.801172	-0.453824	-2.801611
C	5.527550	-1.578375	0.341897
H	6.314144	-1.647273	1.093931
H	4.700471	-2.244181	0.614823
C	5.116555	-1.935142	-1.921633
H	5.599864	-2.266561	-2.841196
H	4.283767	-2.606612	-1.682480
O	6.092397	-1.995341	-0.892119
C	-2.866658	1.896484	-1.263120
H	-1.814868	1.749741	-1.523231

H	-3.489751	1.418250	-2.019486
C	-2.863538	2.034524	1.129767
H	-3.803308	2.450323	1.507599
H	-2.445433	1.372800	1.891012
C	-1.891062	3.148434	0.811404
H	-1.715350	3.748990	1.704813
H	-0.939903	2.720150	0.483310
C	-3.195691	3.369137	-1.168875
H	-2.998624	3.855269	-2.126691
H	-4.261198	3.490014	-0.937168
O	-2.413112	4.026578	-0.179711

HMAM_1aTOL (toluene)

C	-0.009524	1.544427	-1.568370
C	-1.403681	1.447940	-1.151661
C	-1.430237	1.139408	0.164779
C	-0.005788	1.039955	0.670348
N	0.778141	1.324424	-0.404119
O	0.469624	1.761123	-2.652053
O	0.320841	0.754859	1.797563
N	-2.403795	0.902554	1.040950
H	-2.111453	0.703359	1.987509
C	-3.821317	0.915329	0.707806
H	1.784961	1.287924	-0.409240
H	-2.222016	1.573683	-1.839660
C	-4.349024	2.342852	0.589991
H	-3.767807	2.918049	-0.131961
H	-5.390890	2.338408	0.263394
H	-4.291820	2.849514	1.556168
C	-4.580100	0.107820	1.748648
H	-4.469407	0.557719	2.739397
H	-5.643682	0.084337	1.509787
H	-4.213768	-0.918730	1.792643
H	-3.916400	0.418380	-0.263207
C	-1.186112	-2.243975	0.102995
C	0.000474	-2.032950	-0.597767
C	-2.380810	-2.238038	-0.610190
C	-0.007217	-1.815010	-1.966699
H	0.941435	-2.032229	-0.057918
C	-2.394696	-2.017984	-1.981093
H	-3.314202	-2.407203	-0.084621
C	-1.207489	-1.801936	-2.664234
H	0.924703	-1.640622	-2.490917
H	-3.337337	-2.013577	-2.515887
H	-1.214629	-1.617967	-3.731378
C	-1.162014	-2.459850	1.591514
H	-0.683212	-1.617495	2.095951
H	-2.170013	-2.572977	1.992313
H	-0.596960	-3.358697	1.849552

HMAM_1bTOL (toluene)

C	0.400497	1.727945	-0.993086
C	-1.044823	1.519041	-0.950355
C	-1.388565	1.236127	0.328117
C	-0.134858	1.260030	1.183701
N	0.875353	1.589163	0.334951
O	1.116705	1.976483	-1.931862
O	-0.095315	1.026910	2.366726
N	-2.532629	0.943094	0.939849
H	-2.474256	0.802926	1.939803
C	-3.832518	0.916790	0.281739
H	1.856761	1.575077	0.579757
H	-1.667799	1.598910	-1.825247
C	-4.370838	2.329189	0.067361
H	-3.659680	2.939761	-0.490856
H	-5.308031	2.299141	-0.491847
H	-4.557822	2.813552	1.028590
C	-4.782747	0.055659	1.098713
H	-4.931798	0.486113	2.093122
H	-5.756397	-0.002720	0.611437
H	-4.392362	-0.956521	1.214302
H	-3.678856	0.444591	-0.694110
C	4.024273	0.601121	-0.504675
C	3.336615	-0.605358	-0.630001
C	4.232061	1.109210	0.776485
C	2.863849	-1.278125	0.486334
H	3.160039	-1.012788	-1.619055
C	3.757783	0.438800	1.899186

H	4.768821	2.043935	0.896443
C	3.068442	-0.756609	1.757445
H	2.325311	-2.210392	0.364052
H	3.922227	0.856583	2.885070
H	2.687588	-1.273009	2.629378
C	4.473038	1.355187	-1.724428
H	5.224695	2.105088	-1.475018
H	4.895077	0.682086	-2.472915
H	3.615248	1.861053	-2.174190

HMAM_2TOL (toluene)

C	0.262740	1.503864	-1.101221
C	-1.190573	1.539682	-0.985198
C	-1.518788	1.167446	0.273069
C	-0.242933	0.907726	1.048674
N	0.768448	1.141065	0.171690
O	0.968775	1.721018	-2.056679
O	-0.185293	0.556970	2.203319
N	-2.669116	0.976413	0.912627
H	-2.595016	0.662069	1.870219
C	-3.978598	1.092327	0.286651
H	1.751690	1.027023	0.377559
H	-1.831853	1.778992	-1.816125
C	-4.408569	2.552645	0.175736
H	-3.660382	3.141606	-0.356696
H	-5.354091	2.632420	-0.364529
H	-4.540250	2.985944	1.169851
C	-4.976225	0.255748	1.071590
H	-5.062268	0.623318	2.098132
H	-5.963915	0.312084	0.612941
H	-4.668255	-0.790405	1.102384
H	-3.881659	0.671280	-0.719408
C	4.117933	0.642158	-0.468919
C	3.834451	-0.721258	-0.539462
C	4.089320	1.254527	0.783570
C	3.522182	-1.446758	0.600983
H	3.853436	-1.216535	-1.503928
C	3.769212	0.532919	1.927972
H	4.310678	2.313271	0.861345
C	3.479577	-0.821215	1.839911
H	3.305401	-2.505428	0.522230
H	3.738434	1.032844	2.888351
H	3.221161	-1.383320	2.728356
C	4.387608	1.436474	-1.715726
H	4.958634	2.339414	-1.495715
H	4.943687	0.847952	-2.447238
H	3.439505	1.733761	-2.171400
C	-0.724120	-2.395069	0.163412
C	0.041335	-2.017936	-0.939831
C	-2.108261	-2.424410	0.022553
C	-0.555900	-1.684205	-2.144733
H	1.119997	-1.976938	-0.847887
C	-2.712725	-2.092177	-1.183144
H	-2.720902	-2.717708	0.868269
C	-1.938323	-1.721581	-2.271878
H	0.059270	-1.380354	-2.983064
H	-3.792507	-2.129031	-1.271500
H	-2.406766	-1.460843	-3.213195
C	-0.066617	-2.743392	1.471386
H	0.285712	-1.843205	1.980002
H	-0.763532	-3.252816	2.138196
H	0.794249	-3.396744	1.317161

HMAM_1aDIE (diethyl ether)

C	-1.817412	-2.200604	0.239762
C	-0.437633	-2.634908	0.104834
C	0.348188	-1.535055	-0.047344
C	-0.542812	-0.302912	-0.006415
N	-1.805890	-0.780731	0.164044
O	-2.831145	-2.838443	0.392914
O	-0.182197	0.844864	-0.104356
N	1.649077	-1.364131	-0.233402
H	2.026121	-0.411310	-0.232362
C	2.599936	-2.470123	-0.257386
H	-2.633281	-0.208730	0.229638
H	-0.151674	-3.672567	0.139178
C	3.029658	-2.849823	1.157925
H	2.163730	-3.083206	1.779667

H	3.683344	-3.724130	1.138472
H	3.574896	-2.024595	1.622196
C	3.782960	-2.091878	-1.137490
H	4.266863	-1.190408	-0.756981
H	4.514022	-2.901308	-1.157184
H	3.456009	-1.895098	-2.159911
H	2.082611	-3.321594	-0.708896
O	3.141051	1.065835	-0.183468
C	2.757056	2.045081	-1.146385
H	2.484046	1.465303	-2.028877
C	3.465143	1.540288	1.120503
H	3.741483	0.642618	1.675608
H	4.353842	2.177889	1.072418
C	2.324507	2.257130	1.820073
H	2.596466	2.439772	2.861737
H	2.103332	3.222430	1.361818
H	1.417349	1.652941	1.791182
H	1.855983	2.563457	-0.809732
C	3.866329	3.023014	-1.483807
H	4.772157	2.489542	-1.778788
H	3.553672	3.656498	-2.316398
H	4.108216	3.677623	-0.644602

HMAM_1bDIE (diethyl ether)

C	-1.818503	-2.183062	0.205070
C	-0.443360	-2.651602	0.062123
C	0.353054	-1.565142	-0.079197
C	-0.517433	-0.322615	-0.017468
N	-1.788326	-0.768528	0.149173
O	-2.837405	-2.818565	0.343663
O	-0.113437	0.814388	-0.102483
N	1.656845	-1.387672	-0.266806
H	1.973933	-0.427335	-0.291718
C	2.637637	-2.466670	-0.287928
H	-2.610069	-0.161944	0.243496
H	-0.180262	-3.695878	0.077948
C	2.972086	-2.933707	1.126403
H	2.071084	-3.234726	1.662936
H	3.652113	-3.787104	1.094608
H	3.453584	-2.129157	1.687077
C	3.868937	-2.000256	-1.048385
H	4.333121	-1.149599	-0.541535
H	4.607088	-2.800960	-1.101873
H	3.610084	-1.698954	-2.064446
H	2.177289	-3.294908	-0.835562
O	-3.966335	1.069424	0.107258
C	-3.374461	2.340148	-0.143581
H	-4.162826	3.045605	-0.430919
C	-4.784823	0.608124	-0.962349
H	-5.497867	1.396944	-1.229047
H	-2.670576	2.259984	-0.981534
H	-4.160245	0.412301	-1.844145
C	-5.505795	-0.642804	-0.515579
H	-6.129302	-0.427330	0.353876
H	-6.147894	-1.010717	-1.318321
H	-4.799218	-1.430595	-0.249678
C	-2.667330	2.802833	1.108468
H	-2.264293	3.806389	0.959484
H	-3.362770	2.828364	1.948881
H	-1.836125	2.140184	1.349487

HMAM_2DIE (diethyl ether)

C	-1.813255	-2.190736	0.256096
C	-0.435928	-2.636240	0.110560
C	0.351312	-1.538663	-0.044299
C	-0.542496	-0.308894	0.006207
N	-1.804189	-0.775938	0.187059
O	-2.826266	-2.836058	0.406385
O	-0.176663	0.840242	-0.095994
N	1.651183	-1.366421	-0.241901
H	2.026366	-0.413510	-0.232029
C	2.603284	-2.470728	-0.270710
H	-2.631956	-0.178799	0.276264
H	-0.155713	-3.675738	0.138624
C	3.033571	-2.857155	1.142711
H	2.167351	-3.091467	1.763644
H	3.685793	-3.732517	1.119268
H	3.580408	-2.034766	1.610353
C	3.786202	-2.086521	-1.148555

H	4.267518	-1.185765	-0.763216
H	4.519257	-2.894090	-1.171236
H	3.459537	-1.885786	-2.170325
H	2.086947	-3.320670	-0.726404
O	-3.976684	1.073000	0.106915
O	3.146871	1.069279	-0.169808
C	-3.364962	2.341697	-0.101816
H	-4.133340	3.056097	-0.420113
C	-4.736842	0.624416	-1.009523
H	-5.449736	1.407957	-1.292373
C	2.772797	2.039150	-1.145341
H	2.500183	1.451020	-2.022515
C	3.448149	1.555768	1.135286
H	3.729717	0.665105	1.698956
H	4.328477	2.205442	1.094366
C	2.288677	2.260777	1.815869
H	2.545362	2.454820	2.859396
H	2.058960	3.219308	1.347680
H	1.391053	1.643216	1.779331
H	-2.620016	2.264112	-0.903397
H	-4.068775	0.457912	-1.865074
H	1.873248	2.567015	-0.819421
C	-5.456621	-0.647834	-0.624804
H	-6.120863	-0.463156	0.221252
H	-6.056926	-1.006035	-1.463428
H	-4.750219	-1.431463	-0.345713
C	-2.716494	2.786694	1.187802
H	-2.290071	3.784259	1.065959
H	-3.452811	2.818580	1.992521
H	-1.909702	2.108841	1.466685
C	3.889665	3.006491	-1.488785
H	4.793287	2.463769	-1.773407
H	3.585182	3.632767	-2.329922
H	4.132110	3.669025	-0.656002

HMAM_1aTHF (tetrahydrofuran)

C	-1.468192	-2.322887	-0.398234
C	-0.070304	-2.650359	-0.184804
C	0.656419	-1.501317	-0.250833
C	-0.299386	-0.348041	-0.515142
N	-1.533378	-0.915125	-0.589135
O	-2.447574	-3.030316	-0.422107
O	-0.000547	0.816436	-0.630669
N	1.949495	-1.235345	-0.151125
H	2.254820	-0.255775	-0.153363
C	2.950308	-2.253572	0.149863
H	-2.389366	-0.410672	-0.760274
H	0.268317	-3.655588	0.001604
C	3.014338	-2.526344	1.651065
H	2.035045	-2.811313	2.039192
H	3.714936	-3.336585	1.862384
H	3.349968	-1.633207	2.183496
C	4.292927	-1.807241	-0.410919
H	4.589731	-0.854369	0.031925
H	5.060666	-2.549734	-0.189688
H	4.236996	-1.677731	-1.493085
H	2.637660	-3.168102	-0.362981
C	2.539032	2.029578	1.213435
O	3.096781	1.346994	0.076864
C	1.833140	3.258537	0.658537
H	3.354907	2.301722	1.889659
C	3.004469	2.179469	-1.092970
C	2.674467	3.572780	-0.578797
H	1.799903	4.076872	1.377713
H	0.815740	2.999548	0.364758
H	3.953181	2.122925	-1.627370
H	2.204223	1.794118	-1.730112
H	3.587617	4.102235	-0.296004
H	2.144576	4.171980	-1.319099
H	1.866846	1.342902	1.730561

HMAM_1bTHF (tetrahydrofuran)

C	-1.491342	-2.310046	-0.369590
C	-0.096332	-2.664739	-0.133756
C	0.648213	-1.542794	-0.291992
C	-0.284764	-0.394194	-0.636443
N	-1.529202	-0.931307	-0.681794
O	-2.485112	-2.999316	-0.314651

O	0.056094	0.752978	-0.812581
N	1.946801	-1.274826	-0.218318
H	2.208138	-0.305534	-0.343331
C	2.965973	-2.247010	0.161500
H	-2.393440	-0.411730	-0.887621
H	0.217257	-3.660716	0.130358
C	2.997812	-2.445907	1.674627
H	2.017444	-2.741126	2.051657
H	3.714858	-3.224895	1.940466
H	3.293738	-1.519361	2.172047
C	4.309223	-1.796711	-0.390574
H	4.600058	-0.836031	0.043559
H	5.082723	-2.524086	-0.142663
H	4.269486	-1.689081	-1.475456
H	2.687067	-3.191739	-0.315028
C	-3.644410	1.790689	-0.362159
O	-3.914293	0.477800	-0.895554
C	-4.302596	1.840453	1.018178
H	-4.042587	2.539302	-1.048917
C	-4.735472	-0.258980	0.026343
C	-4.444342	0.361409	1.381517
H	-5.288003	2.306465	0.954819
H	-3.707215	2.403752	1.736070
H	-5.788021	-0.141053	-0.251019
H	-4.455966	-1.309664	-0.054282
H	-5.232200	0.170456	2.109827
H	-3.504491	-0.031199	1.777029
H	-2.558776	1.909250	-0.308833

HMAM_2THF (tetrahydrofuran)

C	0.732316	-3.755349	0.150982
C	-0.682371	-3.654806	0.476017
C	-1.098864	-2.390977	0.200162
C	0.079670	-1.629777	-0.399012
N	1.130159	-2.490022	-0.345076
O	1.486659	-4.695771	0.244587
O	0.065634	-0.514579	-0.863237
N	-2.273425	-1.791000	0.351671
H	-2.365879	-0.794051	0.168943
C	-3.471916	-2.503076	0.788645
H	2.064403	-2.273771	-0.691185
H	-1.247729	-4.477667	0.880316
C	-4.074527	-3.302227	-0.364070
H	-3.342657	-3.991191	-0.788891
H	-4.930422	-3.884788	-0.017069
H	-4.411872	-2.627576	-1.154365
C	-4.457552	-1.498366	1.366017
H	-4.726212	-0.752722	0.613454
H	-5.368123	-2.003535	1.690104
H	-4.026925	-0.978986	2.222848
H	-3.171099	-3.196593	1.581133
C	3.900382	-0.477404	-1.698419
O	3.835910	-1.863716	-1.347475
C	4.594053	-0.375183	-3.064021
H	4.454678	0.065649	-0.922652
C	4.674879	-2.668681	-2.178280
C	5.052950	-1.814259	-3.402135
H	5.441209	0.314998	-3.015612
H	3.905349	0.004078	-3.827599
H	5.557343	-2.990047	-1.598455
H	4.109504	-3.565096	-2.468663
H	6.128419	-1.856375	-3.585516
H	4.547240	-2.181888	-4.303171
H	2.876955	-0.095197	-1.722990
C	-1.856241	2.039618	-0.610469
O	-2.536595	1.126677	0.259678
C	-1.583076	3.322494	0.179970
H	-2.492816	2.222901	-1.478160
C	-2.666396	1.634513	1.585504
C	-2.088543	3.054000	1.611389
H	-2.103546	4.172377	-0.265340
H	-0.516392	3.554632	0.178724
H	-3.726498	1.621426	1.860658
H	-2.128772	0.967538	2.269710
H	-2.852666	3.777686	1.901725
H	-1.275881	3.128114	2.336590
H	-0.943063	1.551311	-0.940647

HMAM_1aMET (methanol)

C	-1.831409	-0.998407	-0.513432
C	-0.474382	-1.504482	-0.450421
C	0.356100	-0.478151	-0.119190
C	-0.491908	0.775669	0.054345
N	-1.764288	0.388044	-0.194522
O	-2.871102	-1.556584	-0.770591
O	-0.106546	1.887035	0.352209
N	1.668849	-0.403497	0.043824
H	2.080174	0.487223	0.332812
C	2.554848	-1.556917	-0.087728
H	-2.566518	0.998717	-0.161098
H	-0.228829	-2.536065	-0.637711
C	2.531325	-2.411059	1.177177
H	1.515797	-2.727876	1.419398
H	3.144564	-3.303960	1.042149
H	2.926937	-1.844238	2.023055
C	3.954179	-1.062646	-0.421862
H	4.338515	-0.427980	0.380788
H	4.633156	-1.907479	-0.540437
H	3.954322	-0.485599	-1.347875
H	2.180329	-2.152529	-0.925824
O	2.612859	2.262991	0.630098
H	1.650368	2.386299	0.663564
C	3.074602	2.782406	-0.610979
H	2.589629	2.291501	-1.461120
H	2.903736	3.860211	-0.681004
H	4.146413	2.596188	-0.667972

HMAM_1bMET (methanol)

C	-1.845724	-0.986071	-0.531701
C	-0.505335	-1.532649	-0.486498
C	0.338981	-0.521941	-0.148877
C	-0.479222	0.746033	0.046050
N	-1.765705	0.383947	-0.203803
O	-2.903443	-1.533176	-0.792392
O	-0.037536	1.823823	0.358494
N	1.648941	-0.434214	0.016886
H	2.002749	0.466593	0.313266
C	2.570366	-1.563420	-0.082783
H	-2.595741	0.972203	-0.169156
H	-0.284888	-2.567099	-0.688484
C	2.552499	-2.395236	1.196502
H	1.542781	-2.736999	1.429013
H	3.192657	-3.272128	1.084982
H	2.919544	-1.803498	2.038109
C	3.958677	-1.039485	-0.413428
H	4.325772	-0.393002	0.388388
H	4.657110	-1.869490	-0.522392
H	3.950284	-0.469294	-1.343456
H	2.216753	-2.179814	-0.914342
O	-4.563059	0.646353	-0.345025
H	-4.237094	-0.224111	-0.633554
C	-5.170256	0.478453	0.928458
H	-4.462900	0.090176	1.669305
H	-5.517705	1.455943	1.261659
H	-6.030545	-0.195765	0.878604

HMAM_2MET (methanol)

C	-2.064239	-0.947906	-1.061390
C	-0.640609	-1.040099	-0.848871
C	-0.226343	0.116301	-0.255803
C	-1.449482	1.010664	-0.065632
N	-2.490503	0.308388	-0.567824
O	-2.840954	-1.743994	-1.559372
O	-1.477676	2.116668	0.430974
N	0.962268	0.547793	0.129199
H	1.030721	1.460342	0.588564
C	2.182947	-0.244503	-0.004019
H	-3.466835	0.595515	-0.612384
H	-0.060004	-1.903852	-1.124028
C	2.291312	-1.270461	1.120890
H	1.412932	-1.916893	1.150576
H	3.172344	-1.898063	0.975391
H	2.381251	-0.765711	2.085429
C	3.375294	0.699317	-0.039662
H	3.440496	1.270184	0.890136
H	4.299533	0.132548	-0.155149

H	3.293552	1.401411	-0.870808
H	2.118370	-0.770575	-0.961216
O	-5.169115	-0.282498	-1.157358
H	-4.545795	-0.955431	-1.482284
C	-5.845602	-0.827284	-0.032642
H	-5.150831	-1.092779	0.771499
H	-6.532521	-0.068271	0.340397
H	-6.424752	-1.715263	-0.302899
O	0.933655	3.222710	1.193913
H	-0.017488	3.059526	1.089142
C	1.348526	4.076934	0.134643
H	1.124637	3.644347	-0.845939
H	0.872385	5.058768	0.204651
H	2.426772	4.206701	0.219232

HMAM_1aDMSO (dimethyl sulfoxide)

C	1.709397	1.518700	0.037933
C	0.427402	2.189750	0.027811
C	-0.549792	1.255492	-0.157577
C	0.117590	-0.108015	-0.261140
N	1.447992	0.131198	-0.147923
O	2.829755	1.955022	0.173651
O	-0.440888	-1.171575	-0.407392
N	-1.863421	1.327509	-0.273782
H	-2.421729	0.462649	-0.311017
C	-2.602646	2.578448	-0.126880
H	2.163949	-0.578790	-0.166367
H	0.327816	3.253976	0.158472
C	-2.990746	2.797841	1.333259
H	-2.107519	2.801128	1.974550
H	-3.506432	3.752542	1.453730
H	-3.657464	1.999167	1.665642
C	-3.814009	2.559823	-1.048742
H	-4.467171	1.723938	-0.793520
H	-4.375238	3.490398	-0.950987
H	-3.504850	2.449576	-2.089654
H	-1.932302	3.381766	-0.442185
O	-3.889732	-0.577761	-0.218158
S	-4.020409	-2.072548	0.079510
C	-3.108740	-2.922503	-1.220364
H	-3.088441	-3.988361	-0.994071
H	-3.648832	-2.754813	-2.150144
H	-2.104727	-2.505792	-1.271798
C	-2.897328	-2.413915	1.445566
H	-2.904133	-3.485434	1.643386
H	-1.901189	-2.065834	1.178409
H	-3.278072	-1.877953	2.312822

HMAM_1bDMSO (dimethyl sulfoxide)

C	1.697935	1.578527	0.015008
C	0.413232	2.260638	-0.010652
C	-0.545144	1.318864	-0.201264
C	0.134007	-0.039319	-0.296346
N	1.462317	0.200675	-0.162253
O	2.812703	2.043626	0.160616
O	-0.439038	-1.091797	-0.457898
N	-1.864269	1.353308	-0.327604
H	-2.326022	0.457725	-0.421334
C	-2.673028	2.562645	-0.209322
H	2.215836	-0.511804	-0.173028
H	0.310351	3.325774	0.111908
C	-2.884158	2.938320	1.254831
H	-1.929969	3.059075	1.769976
H	-3.433937	3.878362	1.329031
H	-3.456704	2.161060	1.766116
C	-3.985653	2.351874	-0.947036
H	-4.552181	1.533599	-0.494080
H	-4.596558	3.253390	-0.894186
H	-3.809874	2.112915	-1.996893
H	-2.112722	3.361422	-0.704211
O	3.529942	-1.600947	-0.172334
S	4.990844	-1.169479	-0.020885
C	5.257592	0.131993	-1.237786
H	4.528275	0.924583	-1.074375
H	6.276089	0.504488	-1.131315
H	5.133572	-0.319605	-2.220094
C	5.059548	-0.144633	1.459447
H	6.075774	0.231249	1.575777

H	4.345679	0.671886	1.357240
H	4.806565	-0.784730	2.302433

HMAM_2DMSO (dimethyl sulfoxide)

C	1.615534	-1.263149	0.424177
C	0.243252	-1.634852	0.159070
C	-0.519656	-0.505582	0.233154
C	0.408948	0.659018	0.558472
N	1.650218	0.130979	0.655043
O	2.617464	-1.955498	0.459063
O	0.073839	1.816482	0.697207
N	-1.812390	-0.269723	0.107081
H	-2.152655	0.702178	0.090625
C	-2.779188	-1.302639	-0.253893
H	2.516783	0.654094	0.878760
H	-0.057919	-2.644265	-0.064590
C	-2.957690	-1.355336	-1.769043
H	-2.004681	-1.545134	-2.266223
H	-3.654204	-2.149034	-2.046358
H	-3.353556	-0.403751	-2.130417
C	-4.091415	-1.039955	0.472495
H	-4.486139	-0.062377	0.191254
H	-4.825028	-1.805437	0.214500
H	-3.942758	-1.053102	1.553694
H	-2.369491	-2.255008	0.090817
O	3.998426	1.418091	1.258713
O	-3.304219	2.051387	-0.247983
S	-3.090442	3.564065	-0.163890
S	5.321777	0.663522	1.408878
C	-2.379933	3.875690	1.461243
H	-2.123689	4.932132	1.536044
H	-3.145742	3.631256	2.194913
H	-1.503432	3.242120	1.584788
C	-1.631103	3.920618	-1.157351
H	-1.399639	4.981969	-1.070575
H	-0.806952	3.302576	-0.805709
H	-1.884363	3.683944	-2.189002
C	4.993107	-0.709753	2.528126
H	4.174559	-1.306102	2.126363
H	5.901960	-1.302884	2.626722
H	4.729925	-0.279600	3.492459
C	5.527423	-0.293768	-0.103316
H	6.434783	-0.890953	-0.015440
H	4.650499	-0.925047	-0.243703
H	5.634713	0.417685	-0.919835

BzMAM_1aMET (methanol)

C	-0.412997	-1.919763	-1.010268
C	0.919311	-1.998354	-0.451142
C	1.367175	-0.731354	-0.231768
C	0.268174	0.232637	-0.656287
N	-0.744469	-0.533510	-1.121000
O	-1.181937	-2.789552	-1.349222
O	0.287450	1.446859	-0.595859
N	2.508994	-0.251608	0.236070
H	2.608059	0.760457	0.349217
C	3.607588	-1.102342	0.686438
H	1.416627	-2.933830	-0.259481
C	3.348996	-1.625432	2.096926
H	2.398874	-2.159060	2.150557
H	4.143166	-2.311183	2.397707
H	3.319641	-0.796428	2.807712
C	4.905283	-0.314163	0.593569
H	4.867852	0.564366	1.242897
H	5.745119	-0.933527	0.909700
H	5.087153	0.020193	-0.428970
H	3.657785	-1.949742	-0.003915
C	-2.027192	-0.028860	-1.581882
H	-2.431365	-0.783379	-2.255429
H	-1.842645	0.880805	-2.152326
C	-2.982859	0.239760	-0.444476
C	-3.202862	1.536705	0.005287
C	-3.634487	-0.818302	0.185257
C	-4.064057	1.776424	1.068528
H	-2.692006	2.362131	-0.476638
C	-4.492883	-0.581061	1.248271
H	-3.459409	-1.830365	-0.161283
C	-4.710029	0.718110	1.691857

H	-4.229415	2.791114	1.410166
H	-4.996523	-1.410385	1.730226
H	-5.382088	0.903835	2.520930
O	2.623146	2.632189	0.253188
H	1.696649	2.476556	0.006910
C	3.330035	2.992586	-0.927313
H	4.379145	3.113199	-0.659867
H	3.253061	2.218190	-1.697587
H	2.964200	3.937370	-1.338850

BzMAM_1bMET (methanol)

C	0.183230	1.176760	-0.532515
C	1.597196	1.044172	-0.813525
C	2.130938	0.224430	0.129178
C	1.017367	-0.220793	1.058137
N	-0.113259	0.397615	0.612897
O	-0.660968	1.824425	-1.122562
O	1.134970	-0.978142	1.991117
N	3.351706	-0.218756	0.382165
H	3.440510	-0.870534	1.151462
C	4.520926	0.066622	-0.446714
H	2.077747	1.540891	-1.639031
C	4.552264	-0.841173	-1.672832
H	3.633806	-0.747292	-2.254194
H	5.392923	-0.576245	-2.316418
H	4.664200	-1.884397	-1.369017
C	5.773774	-0.064564	0.404618
H	5.883692	-1.088514	0.772250
H	6.656677	0.175483	-0.188269
H	5.737264	0.610379	1.260857
H	4.422057	1.105653	-0.773486
C	-1.441785	0.209004	1.177058
H	-1.970587	1.157896	1.122271
H	-1.298941	-0.043604	2.227994
C	-2.232435	-0.867407	0.470723
C	-1.814297	-2.195924	0.522384
C	-3.382704	-0.543120	-0.239665
C	-2.533592	-3.183613	-0.132516
H	-0.922040	-2.454612	1.081325
C	-4.106206	-1.534264	-0.892542
H	-3.705599	0.490837	-0.281264
C	-3.682920	-2.854294	-0.842349
H	-2.200897	-4.213621	-0.085844
H	-5.001123	-1.271676	-1.444025
H	-4.245854	-3.626493	-1.352714
O	-3.137137	2.786665	-0.330669
H	-2.309076	2.420839	-0.682899
C	-2.813617	3.945709	0.416081
H	-3.744104	4.374109	0.788997
H	-2.174924	3.715948	1.277209
H	-2.308624	4.700098	-0.196832

BzMAM_2MET (methanol)

C	-0.44375700	-1.43056400	0.51442000
C	0.91389100	-1.50365000	0.99281100
C	1.64534900	-0.55623800	0.34083300
C	0.70629400	0.19120600	-0.59577500
N	-0.51144800	-0.38890600	-0.45128600
O	-1.41304600	-2.09876000	0.81985400
O	0.98048600	1.12424500	-1.32266100
N	2.92379500	-0.22509700	0.38156700
H	3.24894200	0.55871900	-0.19203800
C	3.88897800	-0.87134200	1.26881500
H	1.23361000	-2.21430200	1.73537500
C	3.78709300	-0.30754300	2.68344900
H	2.77444500	-0.41043900	3.07621400
H	4.46802300	-0.83833200	3.35113400
H	4.05322400	0.75180800	2.68798500
C	5.28121600	-0.70301700	0.67976000
H	5.54235400	0.35600000	0.60940200
H	6.01944500	-1.19273900	1.31530600
H	5.33918400	-1.14021000	-0.31821500
H	3.63875600	-1.93611400	1.29022500
C	-1.72725600	0.04942700	-1.12225100
H	-2.31585700	-0.83289000	-1.36299900
H	-1.41416000	0.51858000	-2.05504100
C	-2.54514900	1.00669800	-0.28708100
C	-2.03981700	2.26299200	0.04271900

C	-3.80925500	0.64200500	0.16224400
C	-2.78676700	3.13824900	0.81591400
H	-1.05768600	2.55496100	-0.31143000
C	-4.55988200	1.52158600	0.93344200
H	-4.19989100	-0.33662600	-0.09213300
C	-4.05033900	2.76882900	1.26332000
H	-2.38560100	4.11285100	1.06685900
H	-5.54384500	1.22820900	1.27934500
H	-4.63437000	3.45368300	1.86625400
O	3.64475100	1.85483400	-1.46885300
H	2.67956900	1.86797900	-1.56656400
C	4.19034700	1.19794100	-2.60716200
H	5.26956400	1.14441900	-2.46981500
H	3.80056600	0.18029100	-2.71283800
H	3.98236600	1.75363800	-3.52545500
O	-3.78818400	-2.62912100	-0.50677800
H	-3.00741700	-2.43035500	0.03555700
C	-3.41461400	-3.61106800	-1.45656800
H	-4.29620700	-3.85560700	-2.04932100
H	-2.63527000	-3.24951300	-2.13791000
H	-3.05621900	-4.52863100	-0.97768000

BzMAM_1aDMSO (dimethyl sulfoxide)

C	-1.183838	-2.640261	-0.494585
C	0.177328	-2.794752	-0.033747
C	0.845820	-1.629577	-0.274307
C	-0.124956	-0.661335	-0.927983
N	-1.298433	-1.328637	-1.051538
O	-2.124970	-3.402155	-0.457419
O	0.108476	0.480484	-1.260888
N	2.087902	-1.232317	-0.069143
H	2.327989	-0.239385	-0.205060
C	3.077524	-2.051765	0.625205
H	0.535010	-3.696680	0.433085
C	2.993278	-1.822576	2.132214
H	1.990997	-2.042823	2.504013
H	3.703485	-2.463816	2.657764
H	3.227869	-0.781262	2.362909
C	4.461284	-1.741434	0.072136
H	4.698048	-0.687173	0.225525
H	5.213790	-2.348513	0.577693
H	4.506534	-1.953522	-0.997478
H	2.835099	-3.094999	0.407581
C	-2.539447	-0.737967	-1.520302
H	-3.186367	-1.566944	-1.804200
H	-2.321022	-0.149279	-2.411022
C	-3.195745	0.117826	-0.463338
C	-3.876309	-0.480131	0.594946
C	-3.097145	1.503992	-0.509175
C	-4.448344	0.297017	1.591031
H	-3.949843	-1.561070	0.635328
C	-3.670320	2.284358	0.486967
H	-2.562146	1.973575	-1.326140
C	-4.346121	1.682176	1.539005
H	-4.977324	-0.177690	2.408688
H	-3.587627	3.363586	0.440873
H	-4.793513	2.289452	2.316550
O	3.222925	1.302144	0.035476
S	2.703526	2.739844	0.094965
C	2.044239	3.102974	-1.541204
H	1.571635	4.084601	-1.517028
H	2.887901	3.118773	-2.228533
H	1.334628	2.323566	-1.811469
C	1.141763	2.678886	0.990864
H	0.707195	3.678158	1.001487
H	0.480351	1.965808	0.502824
H	1.369089	2.366425	2.008225

BzMAM_1bDMSO (dimethyl sulfoxide)

C	-0.639030	-0.844195	-0.508310
C	-2.055866	-1.029138	-0.763786
C	-2.741193	-0.324503	0.172525
C	-1.739754	0.364815	1.079921
N	-0.508916	0.013815	0.615618
O	0.321818	-1.300164	-1.090946
O	-2.010118	1.078674	2.016467
N	-4.027428	-0.146353	0.434501
H	-4.246083	0.483856	1.195388

C	-5.114851	-0.696204	-0.370995
H	-2.430467	-1.630245	-1.574946
C	-5.322906	0.125636	-1.640033
H	-4.403205	0.187183	-2.223777
H	-6.092812	-0.331814	-2.263907
H	-5.639664	1.139806	-1.386474
C	-6.370705	-0.770919	0.482271
H	-6.678928	0.229335	0.798774
H	-7.188564	-1.209194	-0.090087
H	-6.203853	-1.381042	1.371127
H	-4.813628	-1.710639	-0.648719
C	0.753725	0.441920	1.181908
H	1.447429	-0.400491	1.195169
H	0.547878	0.723095	2.216913
C	1.390615	1.602917	0.451538
C	0.640657	2.537327	-0.253468
C	2.773306	1.756148	0.517632
C	1.260940	3.610212	-0.881018
H	-0.435366	2.431031	-0.320916
C	3.393275	2.830150	-0.104633
H	3.356802	1.006855	1.040107
C	2.638590	3.761813	-0.806659
H	0.664253	4.329528	-1.429270
H	4.470504	2.935074	-0.049667
H	3.122122	4.598009	-1.297140
O	3.392099	-1.424574	1.317340
S	3.934974	-2.204483	0.125335
C	3.648413	-1.189110	-1.336612
H	4.272962	-0.303279	-1.242904
H	3.946700	-1.759263	-2.216421
H	2.594263	-0.918583	-1.378048
C	2.717397	-3.484893	-0.236642
H	1.749582	-3.014566	-0.405166
H	3.042568	-4.040067	-1.116470
H	2.686261	-4.148443	0.625517

BzMAM_2DMSO (dimethyl sulfoxide)

C	-0.76859900	-1.58847000	0.39666100
C	0.49174900	-2.21459100	0.71796700
C	1.49028200	-1.48227400	0.14324700
C	0.84876900	-0.31473300	-0.58748800
N	-0.49012400	-0.43896200	-0.39834800
O	-1.90231500	-1.90021000	0.69957100
O	1.42542000	0.55433000	-1.20367700
N	2.80268800	-1.60979100	0.10151800
H	3.37402200	-0.84888700	-0.29516600
C	3.51845100	-2.65730100	0.82551400
H	0.56459900	-3.09972800	1.32666100
C	3.81976600	-2.20651700	2.25267000
H	2.90182900	-1.93643300	2.77779400
H	4.31206000	-3.00548000	2.81039900
H	4.47943100	-1.33628100	2.23742400
C	4.78046800	-3.02363400	0.05750600
H	5.42544300	-2.14912100	-0.04222700
H	5.32691000	-3.80743600	0.58414200
H	4.53307600	-3.38568300	-0.94192000
H	2.85854300	-3.52803000	0.85768400
C	-1.49060700	0.46872400	-0.91532600
H	-2.37424100	-0.10092200	-1.20930700
H	-1.06962000	0.91961400	-1.81643800
C	-1.89898100	1.55613300	0.05326000
C	-1.12176800	1.91572100	1.14727600
C	-3.09253300	2.23612700	-0.18014900
C	-1.52657700	2.94149500	1.99354900
H	-0.19604200	1.39223200	1.35289100
C	-3.49501600	3.26284100	0.66019200
H	-3.71610000	1.92768300	-1.01113900
C	-2.71182300	3.62025800	1.75171400
H	-0.91130300	3.20860000	2.84451700
H	-4.42804500	3.77999600	0.46945100
H	-3.02758000	4.41890600	2.41199800
O	4.81702500	0.18335200	-0.55619100
O	-4.46927900	-0.37994500	-1.76839000
S	4.90896500	1.70677900	-0.66200500
C	4.10641100	2.15113900	-2.21164100
H	4.06192900	3.23765500	-2.28312800
H	4.72533200	1.75566800	-3.01462100
H	3.11291900	1.70773800	-2.23071200

C	3.67138500	2.36934700	0.46719500
H	3.66635100	3.45541500	0.37931400
H	2.69931000	1.94890600	0.21712300
H	3.97201300	2.08394400	1.47350800
S	-5.40494700	-1.12796400	-0.82585100
C	-4.98528300	-0.60763600	0.84896200
H	-5.22979600	0.44931500	0.92930600
H	-5.59026100	-1.18169400	1.55073700
H	-3.92164200	-0.77256000	1.01494800
C	-4.76934200	-2.81210200	-0.71589300
H	-3.72879700	-2.77574000	-0.39596500
H	-5.37965100	-3.37307300	-0.00813200
H	-4.86024900	-3.25174500	-1.70744600

Bz_2MAM_1aMET (methanol)

C	0.392540	0.237806	-2.338265
C	1.814397	0.335614	-2.105193
C	2.024586	0.388003	-0.761221
C	0.671805	0.314471	-0.068889
N	-0.254835	0.246665	-1.055888
O	-0.236989	0.155009	-3.366494
O	0.469038	0.324145	1.128471
N	3.120510	0.498293	-0.027864
H	3.035801	0.459150	0.991029
C	4.464751	0.530536	-0.598966
H	2.536189	0.350559	-2.903871
C	4.936480	-0.876010	-0.958373
H	4.239017	-1.362349	-1.642031
H	5.914932	-0.835621	-1.440392
H	5.019662	-1.488107	-0.057294
C	5.397005	1.215663	0.388429
H	5.442252	0.654533	1.325422
H	6.405416	1.271679	-0.022448
H	5.055332	2.227989	0.609176
H	4.409322	1.132429	-1.510806
C	-1.694274	0.056088	-0.907416
C	-1.998660	-1.324261	-0.350310
C	-1.943244	-1.597663	1.014752
C	-2.305155	-2.353708	-1.233680
C	-2.186144	-2.880350	1.481972
H	-1.702617	-0.803466	1.707731
C	-2.550587	-3.638581	-0.767019
H	-2.350109	-2.148119	-2.297233
C	-2.490566	-3.904357	0.593109
H	-2.139658	-3.081830	2.545450
H	-2.791501	-4.429385	-1.466997
H	-2.682852	-4.904831	0.961368
C	-2.370195	1.213332	-0.188150
C	-3.658798	1.053936	0.316152
C	-1.766414	2.462519	-0.093711
C	-4.322806	2.116157	0.911970
H	-4.148067	0.090699	0.245892
C	-2.428134	3.525723	0.505559
H	-0.772019	2.615726	-0.492524
C	-3.707961	3.356720	1.013440
H	-5.323830	1.971678	1.300189
H	-1.938202	4.489468	0.574650
H	-4.223353	4.185326	1.483517
H	-2.046144	0.069517	-1.941448
O	2.649241	0.144676	2.801734
H	1.746589	0.281510	2.472345
C	2.816810	-1.248796	3.034299
H	2.644886	-1.835071	2.125638
H	3.843810	-1.407278	3.361093
H	2.142479	-1.606599	3.817189

Bz_2MAM_1bMET (methanol)

C	-0.887650	-0.421298	1.640983
C	-2.323677	-0.375539	1.488347
C	-2.591139	0.012593	0.214363
C	-1.275533	0.213728	-0.513131
N	-0.294934	-0.053756	0.400078
O	-0.228904	-0.706611	2.622352
O	-1.165019	0.545543	-1.667807
N	-3.702255	0.243707	-0.463995
H	-3.587654	0.495551	-1.437811
C	-5.049170	0.053157	0.070143
H	-3.003361	-0.617853	2.287375
C	-5.441292	-1.421247	0.042609

H	-4.719552	-2.030299	0.588968
H	-6.421448	-1.558756	0.502518
H	-5.488340	-1.781858	-0.987335
C	-6.017451	0.925689	-0.712066
H	-6.043270	0.624326	-1.762770
H	-7.024892	0.822690	-0.308395
H	-5.728452	1.976244	-0.658374
H	-5.022234	0.396146	1.108410
C	1.151820	-0.013793	0.183988
C	1.650325	-1.233384	-0.565946
C	1.273385	-1.498035	-1.881899
C	2.509951	-2.111982	0.084755
C	1.745802	-2.629423	-2.528872
H	0.611818	-0.813466	-2.396170
C	2.986732	-3.243215	-0.566733
H	2.803284	-1.903521	1.108031
C	2.604382	-3.504991	-1.873781
H	1.446219	-2.827642	-3.551022
H	3.655996	-3.920069	-0.049356
H	2.973425	-4.386986	-2.383232
C	1.597851	1.332018	-0.371354
C	2.650118	1.432647	-1.273465
C	1.001293	2.501641	0.096528
C	3.089857	2.676746	-1.710114
H	3.132732	0.537313	-1.641612
C	1.437473	3.742509	-0.339480
H	0.185353	2.443517	0.807009
C	2.484462	3.835057	-1.248449
H	3.909123	2.735760	-2.416497
H	0.958467	4.640428	0.031829
H	2.824903	4.804257	-1.591896
H	1.563750	-0.089071	1.189261
O	2.480454	-0.782590	3.266931
C	2.763289	0.535160	3.706258
H	2.500005	1.284620	2.950669
H	2.236178	0.778659	4.634679
H	3.835256	0.602085	3.891384
H	1.525807	-0.840705	3.103833

Bz_2MAM_2MET (methanol)

C	0.24477400	-2.06044400	0.05058600
C	1.67957400	-2.14580600	-0.01506900
C	2.17139700	-0.88743500	-0.19392000
C	0.99314500	0.07495800	-0.22882000
N	-0.12376400	-0.68708100	-0.08829800
O	-0.57918500	-2.94300300	0.19113900
O	1.04729900	1.27947800	-0.35901800
N	3.39625100	-0.41572200	-0.33940600
H	3.52858100	0.59734400	-0.41365700
C	4.59057100	-1.25569200	-0.27101100
H	2.21297700	-3.07683300	0.07078500
C	4.96766600	-1.54101500	1.18021200
H	4.13923000	-2.00403300	1.71845000
H	5.82314100	-2.21747400	1.22235600
H	5.23503100	-0.61268700	1.69018700
C	5.71295300	-0.56958900	-1.03443500
H	5.95163700	0.39530900	-0.57997100
H	6.61224100	-1.18573900	-1.01472200
H	5.43087500	-0.40049300	-2.07465300
H	4.34620600	-2.19818600	-0.76922400
C	-1.51028500	-0.21989700	-0.02507100
C	-1.84618900	0.36953200	1.33133800
C	-1.25661900	1.54490800	1.79525500
C	-2.76801200	-0.29160300	2.13596300
C	-1.58015600	2.04046500	3.04885200
H	-0.54721500	2.06975100	1.16967300
C	-3.09525800	0.20910600	3.39036700
H	-3.23031400	-1.20264200	1.77176100
C	-2.50030400	1.37423500	3.85026900
H	-1.11524500	2.95342100	3.40126100
H	-3.81524900	-0.31477700	4.00749800
H	-2.75245000	1.76539000	4.82857000
C	-1.87067500	0.63816100	-1.22968400
C	-2.76466500	1.69660700	-1.12147100
C	-1.37022100	0.30866800	-2.48800000
C	-3.14121900	2.42112300	-2.24610700
H	-3.17195700	1.96212000	-0.15519300
C	-1.74307500	1.03181400	-3.60976300

H	-0.67954000	-0.51929600	-2.59398200
C	-2.63030600	2.09475700	-3.49266300
H	-3.83607000	3.24574100	-2.14203700
H	-1.33951400	0.76426700	-4.57884100
H	-2.92071600	2.66221100	-4.36836100
H	-2.09238400	-1.13648700	-0.10832600
O	3.54598500	2.45897900	-0.34296200
H	2.59120700	2.33839000	-0.46251700
C	3.76830200	2.84474800	1.00875000
H	3.36894300	2.10653000	1.71178400
H	4.84491900	2.91948700	1.15633700
H	3.31783200	3.81737800	1.22424100
O	-3.35901800	-3.11778200	0.25831100
C	-3.73468700	-3.25077400	-1.10214900
H	-3.35291400	-2.42622700	-1.71555900
H	-3.38415400	-4.19458400	-1.53268400
H	-4.82335100	-3.23363000	-1.15053800
H	-2.39007300	-3.13697000	0.30096700

Bz_2MAM_1aDMSO (dimethyl sulfoxide)

C	-0.41117600	-2.55010400	1.19726100
C	1.01759100	-2.68672500	1.04734800
C	1.47466700	-1.62633100	0.32047600
C	0.28426800	-0.75902400	-0.04498500
N	-0.80816900	-1.36565500	0.49000900
O	-1.21441100	-3.23284900	1.79240300
O	0.32190600	0.26434500	-0.69013400
N	2.66897000	-1.25545000	-0.10070100
H	2.78565500	-0.31641400	-0.51015500
C	3.89207000	-1.96923800	0.25703300
H	1.57362700	-3.49660300	1.48811600
C	4.42200100	-1.47818400	1.60214800
H	3.67221500	-1.60154100	2.38565600
H	5.31382800	-2.03838200	1.88946400
H	4.68264200	-0.41972700	1.53584500
C	4.91182200	-1.80035900	-0.86022000
H	5.13537500	-0.74209000	-1.00622500
H	5.83516400	-2.32476100	-0.60988300
H	4.52742100	-2.20397500	-1.79854000
H	3.62940300	-3.02696800	0.34079500
C	-2.15795500	-0.82026900	0.56231600
C	-2.15602800	0.47099000	1.36661100
C	-1.94392200	1.71233200	0.77331500
C	-2.31222700	0.39998900	2.74719200
C	-1.88375900	2.85983400	1.55034300
H	-1.81672700	1.77690800	-0.29835900
C	-2.25370600	1.54728000	3.52676300
H	-2.47658500	-0.56409400	3.21566000
C	-2.03747900	2.78088000	2.92888300
H	-1.71457100	3.81976100	1.07733900
H	-2.37991000	1.47669900	4.60031100
H	-1.99165100	3.67846300	3.53366500
C	-2.84149900	-0.73571600	-0.79239100
C	-4.06450400	-0.07512100	-0.89538400
C	-2.32101500	-1.35646500	-1.92121000
C	-4.74383700	-0.02584600	-2.10268900
H	-4.48709600	0.40910700	-0.02339600
C	-2.99864500	-1.30537000	-3.13306200
H	-1.38193500	-1.89017800	-1.86109300
C	-4.21018400	-0.63807800	-3.22988100
H	-5.69240700	0.49391100	-2.16355100
H	-2.57396800	-1.79079400	-4.00351500
H	-4.73718300	-0.59612600	-4.17526000
H	-2.69423700	-1.56904300	1.14985700
O	3.61363800	1.21873400	-0.94749700
S	3.07074100	2.63651800	-1.13807900
C	1.94774100	2.94426700	0.23697500
H	2.54795100	2.94645400	1.14489100
H	1.48923600	3.92313700	0.09792100
H	1.19668800	2.15791000	0.26781600
C	1.84551400	2.53107600	-2.45382200
H	1.35584900	3.49932300	-2.55401200
H	2.38264300	2.29486400	-3.37034900
H	1.13361400	1.74686300	-2.20518500

Bz_2MAM_1bDMSO (dimethyl sulfoxide)

C	-0.96092000	-1.28805800	-0.85449300
C	-2.39134900	-1.51124200	-0.81176200

C	-2.94065100	-0.52664400	-0.05600700
C	-1.83148300	0.39493300	0.41685400
N	-0.67629700	-0.10441400	-0.10753400
O	-0.08922000	-1.93714000	-1.38999100
O	-1.99024300	1.35551100	1.13153900
N	-4.17184400	-0.24706500	0.34165000
H	-4.28177000	0.59399600	0.89400600
C	-5.35730100	-1.00647900	-0.04705000
H	-2.86905100	-2.33774100	-1.31000100
C	-5.82653900	-0.60712000	-1.44309100
H	-5.02864000	-0.73384200	-2.17639000
H	-6.67256300	-1.22551400	-1.74826500
H	-6.14120200	0.43891000	-1.45209400
C	-6.43663600	-0.80920600	1.00535200
H	-6.73069800	0.24247500	1.06086700
H	-7.32168700	-1.39235300	0.74981900
H	-6.08586500	-1.12441600	1.98908500
H	-5.06132500	-2.05952200	-0.05811400
C	0.67230800	0.43946200	0.02116200
C	0.77593900	1.83145200	-0.57765500
C	0.39026800	2.97429600	0.11836300
C	1.27275100	1.96138100	-1.87081500
C	0.48309200	4.22284600	-0.47855900
H	0.00636400	2.88053900	1.12472100
C	1.36560500	3.21107300	-2.46967300
H	1.61677500	1.07557900	-2.39073900
C	0.96732000	4.34469800	-1.77552800
H	0.17749400	5.10541200	0.07082700
H	1.75767100	3.29909000	-3.47594500
H	1.04068200	5.32132700	-2.23897800
C	1.23268400	0.30372000	1.42525500
C	2.45181500	0.90974500	1.72419900
C	0.63256800	-0.49653400	2.38944500
C	3.05338100	0.72130200	2.95829300
H	2.93748400	1.52407600	0.97699400
C	1.23187800	-0.68436400	3.62928100
H	-0.30517100	-0.99301000	2.17684500
C	2.44414500	-0.07734700	3.91899900
H	4.00270400	1.19829300	3.17088600
H	0.74690200	-1.31100500	4.36813600
H	2.91256300	-0.22428400	4.88456100
H	1.28543700	-0.20573700	-0.61346700
O	3.27077700	-0.59099500	-1.43150300
S	3.74726600	-2.01553900	-1.17750000
C	2.89225600	-3.05189100	-2.38002900
H	1.82405900	-2.85106200	-2.31319100
H	3.27635700	-2.78480500	-3.36275600
H	3.11574500	-4.09780800	-2.17003600
C	2.88731400	-2.60652300	0.29467400
H	3.19050500	-3.63687700	0.47929000
H	3.19397100	-1.97368200	1.12524600
H	1.81284200	-2.53506500	0.13623200

Bz_2MAM_2DMSO (dimethyl sulfoxide)

C	-0.53751400	2.07653700	-0.38970500
C	0.73852000	2.74468400	-0.32097500
C	1.68029600	1.82512800	0.03922000
C	0.98053800	0.49283600	0.24029500
N	-0.33033400	0.69994700	-0.05521100
O	-1.63708400	2.50931300	-0.66503800
O	1.50728200	-0.53252500	0.60893500
N	2.98083500	1.88469800	0.25029300
H	3.50756500	1.00755700	0.37909900
C	3.76519700	3.09658000	0.02734000
H	0.86196600	3.78967600	-0.54932400
C	4.18596100	3.19779100	-1.43684400
H	3.31533900	3.18593900	-2.09494100
H	4.73694400	4.12360100	-1.61303700
H	4.82955000	2.35530100	-1.69905300
C	4.95922000	3.09799900	0.97124600
H	5.58501400	2.22347900	0.78541100
H	5.55679500	3.99809600	0.82024200
H	4.62974500	3.07092900	2.01135800
H	3.11806700	3.94278200	0.27258100
C	-1.38703900	-0.30506000	-0.11416700
C	-1.05942800	-1.38059000	-1.13677200
C	-0.26448400	-2.48354700	-0.83554900
C	-1.55952300	-1.24019500	-2.42765700

C	0.04268000	-3.41570600	-1.81589300
H	0.12249400	-2.60409700	0.16654400
C	-1.25333600	-2.17266300	-3.41008400
H	-2.21612900	-0.40703100	-2.64734200
C	-0.44657800	-3.26057900	-3.10722100
H	0.66696200	-4.26688200	-1.57102200
H	-1.65187400	-2.05272400	-4.41046800
H	-0.20614900	-3.99023700	-3.87122200
C	-1.79216000	-0.81986600	1.25414200
C	-2.69849300	-1.87586400	1.33431600
C	-1.37620600	-0.20778300	2.42966900
C	-3.17339900	-2.31063400	2.56140500
H	-3.04122500	-2.35200400	0.42457500
C	-1.84861200	-0.64369600	3.66200900
H	-0.68690900	0.62553300	2.39259700
C	-2.74842700	-1.69595100	3.73351600
H	-3.87946000	-3.13139800	2.60351500
H	-1.51091000	-0.15426400	4.56769600
H	-3.11765400	-2.03569700	4.69351600
H	-2.25420200	0.23047000	-0.50897700
O	4.89987900	-0.12599800	0.32832600
O	-4.31642500	0.10210900	-1.18487200
S	4.96597700	-1.64977200	0.20792700
S	-5.21253000	1.12676500	-0.50088800
C	3.80893200	-2.11286300	-1.09305100
H	4.18573000	-1.68584300	-2.02052800
H	3.79146900	-3.19980000	-1.17064000
H	2.82368400	-1.71825300	-0.85431800
C	4.05026000	-2.30322100	1.61429800
H	3.98094400	-3.38611900	1.51495100
H	4.61854000	-2.05257500	2.50798200
H	3.06626700	-1.83952400	1.63447400
C	-4.89549500	2.69693900	-1.32852900
H	-3.82147700	2.87684100	-1.32783600
H	-5.27326600	2.60391000	-2.34507500
H	-5.43302600	3.48916100	-0.80766600
C	-4.44300100	1.53306600	1.08002500
H	-5.05459000	2.28649900	1.57617700
H	-4.42291600	0.62068000	1.67299600
H	-3.43263800	1.89833700	0.90454000

Bz_3MAM_1aMET (methanol)

C	0.34485800	-1.63254000	-1.24161200
C	1.78046000	-1.72288600	-1.37815600
C	2.34537800	-0.71418900	-0.66655600
C	1.22900900	0.05579400	0.00806600
N	0.05159800	-0.41456100	-0.50736300
O	-0.50762600	-2.39647800	-1.61848200
O	1.37519500	0.89673700	0.86883300
N	3.59992000	-0.33730200	-0.47349700
C	4.74383900	-1.05107200	-1.03515700
H	2.25519400	-2.50588500	-1.94448200
C	5.07713600	-2.28643100	-0.20313700
H	4.21383700	-2.94812300	-0.11773900
H	5.89177400	-2.84594500	-0.66647400
H	5.38680400	-1.99223000	0.80224400
C	5.91768000	-0.08850300	-1.13294600
H	6.19374500	0.28011400	-0.14164600
H	6.78418100	-0.59363200	-1.56054600
H	5.66976000	0.76765300	-1.76230900
H	4.45928700	-1.36705500	-2.04342800
C	-1.27944200	-0.09222800	0.06682200
C	-1.39624000	-0.95879800	1.32974000
C	-0.90505100	-0.50453500	2.55247200
C	-1.84655300	-2.27519000	1.24214100
C	-0.89560100	-1.33344800	3.66544200
H	-0.51574200	0.49986400	2.63450800
C	-1.83841400	-3.10331800	2.35490300
H	-2.18939200	-2.66025700	0.29265300
C	-1.36882300	-2.63412400	3.57358800
H	-0.51343600	-0.95806400	4.60703400
H	-2.19798100	-4.12127500	2.26535600
H	-1.36471400	-3.28007300	4.44318100
C	-2.38697800	-0.32913000	-0.97592200
C	-2.15479000	-0.07791400	-2.32552100
C	-3.68316800	-0.62061200	-0.56813400
C	-3.18472800	-0.15115100	-3.24797400
H	-1.15982300	0.17800300	-2.66441100

C	-4.71840800	-0.69494200	-1.49170600
H	-3.89807200	-0.78960500	0.47822000
C	-4.47403000	-0.46597000	-2.83641300
H	-2.97891500	0.03923600	-4.29441100
H	-5.71961300	-0.93049200	-1.15160100
H	-5.27974600	-0.52504900	-3.55785400
C	-1.40102600	1.42311600	0.32096100
C	-0.75861500	2.34202800	-0.50425900
C	-2.29315300	1.90007400	1.27491100
C	-0.97115800	3.70263200	-0.35306400
H	-0.08540900	1.99878200	-1.27821500
C	-2.50891700	3.26329900	1.42799100
H	-2.83278500	1.20788800	1.90690100
C	-1.84407500	4.17229200	0.61968300
H	-0.45203200	4.39861400	-1.00087400
H	-3.20362700	3.61100800	2.18294500
H	-2.00918000	5.23594800	0.73977200
O	3.85485600	2.05886800	1.14315100
H	2.94012400	1.79319200	1.32586900
C	3.81007800	3.13847800	0.21763400
H	4.83750500	3.41461000	-0.01609100
H	3.30483600	2.85476000	-0.71151200
H	3.30215500	4.00827700	0.64319300
H	3.78562600	0.45539100	0.14494700

Bz_3MAM_1bMET (methanol)

C	0.88656500	-1.24086000	-0.82668700
C	2.32009100	-1.31624600	-0.98658100
C	2.84928200	-0.15118100	-0.54129300
C	1.72159400	0.72052300	-0.03598500
N	0.54679500	0.08234500	-0.37675900
O	0.06748600	-2.11395300	-1.01044400
O	1.88720100	1.74478700	0.57608600
N	4.07780200	0.33264100	-0.45524900
C	5.28167800	-0.41564000	-0.80990300
H	2.81250100	-2.19344700	-1.37039400
C	5.67912100	-1.37078900	0.31184300
H	4.86057200	-2.04868600	0.55869700
H	6.53969400	-1.97034800	0.00986100
H	5.94632800	-0.80985200	1.21026100
C	6.38940000	0.56618200	-1.15622800
H	6.63921000	1.18508800	-0.29008500
H	7.28903700	0.02729400	-1.45441400
H	6.08927200	1.22066200	-1.97573100
H	5.03219500	-0.99677500	-1.70212900
C	-0.79569900	0.44035000	0.15241700
C	-0.90048600	-0.25967900	1.51624100
C	-0.20377400	0.26933700	2.60456500
C	-1.55236700	-1.47836600	1.67380500
C	-0.18304200	-0.38948800	3.82350700
H	0.33184900	1.20253800	2.49474100
C	-1.53353600	-2.13709200	2.89730700
H	-2.06787500	-1.93473700	0.84116900
C	-0.85490500	-1.59520200	3.97751100
H	0.36045800	0.04186300	4.65540400
H	-2.05188500	-3.08305400	2.99873400
H	-0.84294000	-2.10970100	4.93071900
C	-1.89434100	0.05874900	-0.85576300
C	-1.62983300	-0.05143400	-2.21677000
C	-3.21841800	-0.00207900	-0.43041900
C	-2.65794200	-0.25444400	-3.12543400
H	-0.61542300	0.02667400	-2.58223700
C	-4.24772400	-0.20796000	-1.33649200
H	-3.45544300	0.11932400	0.61818500
C	-3.97225900	-0.34077700	-2.68981800
H	-2.42662600	-0.34429300	-4.17991000
H	-5.26931000	-0.26041700	-0.98020000
H	-4.77481100	-0.50229200	-3.39893700
C	-0.94846300	1.97289700	0.22588200
C	-0.47986500	2.76959400	-0.81678300
C	-1.69592500	2.56890600	1.23302600
C	-0.71982200	4.13206900	-0.83144900
H	0.07844700	2.32231400	-1.62900300
C	-1.94326600	3.93704900	1.21758500
H	-2.09593800	1.97123800	2.04025200
C	-1.45186100	4.72567100	0.19068400
H	-0.33667100	4.73381100	-1.64668400
H	-2.52523700	4.38141000	2.01595100

H	-1.64131700	5.79202100	0.17959600
H	-1.62928700	-2.85895500	-1.07021200
O	-2.33745000	-3.50048400	-0.91716100
C	-1.73744600	-4.64792000	-0.34452700
H	-1.26895500	-4.42676900	0.62109400
H	-2.52136200	-5.38883600	-0.18361100
H	-0.97895600	-5.08566900	-1.00257400
H	4.17184700	1.22885600	0.00622600

Bz_3MAM_2MET (methanol)

C	0.17970900	-1.60815600	-0.79519400
C	1.54325600	-2.04868000	-0.93389000
C	2.35883300	-1.06073300	-0.47974300
C	1.47917000	0.06195100	0.03340100
N	0.19269300	-0.23939200	-0.33668600
O	-0.83839000	-2.23111500	-0.99820600
O	1.86232800	1.00849700	0.68304300
N	3.67235400	-0.93745100	-0.40487700
C	4.59938800	-1.98905500	-0.81798700
H	1.79772300	-3.01913000	-1.32415200
C	4.73045500	-3.05339100	0.26789700
H	3.75784400	-3.47573500	0.52503500
H	5.37514800	-3.86468900	-0.07471100
H	5.16816000	-2.62050200	1.17016900
C	5.93573700	-1.35064500	-1.16430100
H	6.35578800	-0.84469000	-0.29127200
H	6.64415200	-2.11352300	-1.48823200
H	5.82331400	-0.61907700	-1.96596800
H	4.18060700	-2.44787600	-1.71856200
C	-1.01217200	0.47974600	0.15724000
C	-1.32181200	-0.13254300	1.53210500
C	-0.56362300	0.24934400	2.64007800
C	-2.24142600	-1.16689800	1.68066500
C	-0.73894900	-0.36896800	3.86835500
H	0.17546900	1.03175600	2.53883900
C	-2.41781200	-1.78435400	2.91243300
H	-2.82049300	-1.51006400	0.83539600
C	-1.67257900	-1.38648100	4.01171200
H	-0.14235300	-0.05313700	4.71559700
H	-3.14229500	-2.58444400	3.00632100
H	-1.81305500	-1.86822900	4.97173800
C	-2.15958300	0.37851500	-0.86301200
C	-1.91619200	0.19300100	-2.21993700
C	-3.46058700	0.65559500	-0.45396900
C	-2.95295800	0.24323900	-3.13961400
H	-0.91083900	0.01058000	-2.57345300
C	-4.49923900	0.70439600	-1.37136200
H	-3.67109400	0.84075700	0.59087500
C	-4.25184400	0.49201200	-2.71946700
H	-2.74082700	0.08710000	-4.19037200
H	-5.50514500	0.91224600	-1.02750500
H	-5.06194100	0.52761400	-3.43744800
C	-0.74597200	1.99866300	0.18794100
C	-0.03785200	2.60365800	-0.84849200
C	-1.34062800	2.80836900	1.14661300
C	0.10696300	3.97874600	-0.90130900
H	0.40743100	1.99619300	-1.62578200
C	-1.20175100	4.19066600	1.09235200
H	-1.92078400	2.36928800	1.94631100
C	-0.47215000	4.78200800	0.07431700
H	0.67169800	4.42598600	-1.71035300
H	-1.67022600	4.80242900	1.85378000
H	-0.36023300	5.85852100	0.03391000
O	4.55513600	1.61104700	0.64267100
H	3.62444600	1.62023300	0.91269100
C	4.68933500	2.49009900	-0.46850700
H	5.72453500	2.44046400	-0.80347400
H	4.03848000	2.19636700	-1.29836600
H	4.46075200	3.52224300	-0.18943800
H	-2.67761500	-2.48330500	-1.08749700
O	-3.52699700	-2.92039500	-0.93391500
C	-3.24230200	-4.18609400	-0.36646600
H	-2.73498200	-4.09685100	0.60084100
H	-4.19044200	-4.70173300	-0.20989200
H	-2.61985700	-4.80064500	-1.02574200
H	4.06419300	-0.08856600	0.01176200

Bz_3MAM_1aDMSO (dimethyl sulfoxide)

C	-0.55184100	-2.32956700	-0.24001100
C	0.79766600	-2.76655400	-0.50467300
C	1.57853800	-1.66876400	-0.69212700
C	0.70131800	-0.44809100	-0.53936700
N	-0.59447400	-0.88971500	-0.42638500
O	-1.50894200	-2.97918100	0.10515100
O	1.10948800	0.68780400	-0.48329900
N	2.86219500	-1.48925100	-0.94597300
C	3.81998900	-2.59129900	-0.98588900
H	1.07670900	-3.80636700	-0.48392500
C	4.34180500	-2.89335800	0.41685000
H	3.51995300	-3.12467800	1.09688200
H	5.02187400	-3.74715900	0.39695900
H	4.88172300	-2.02813400	0.80744300
C	4.94075000	-2.24397600	-1.95525500
H	5.44551900	-1.33220000	-1.63141400
H	5.66930800	-3.05508000	-1.99523500
H	4.54629700	-2.08245200	-2.95994100
H	3.28323600	-3.46534100	-1.36347900
C	-1.68588400	-0.01823200	0.07886800
C	-1.42066200	0.11864500	1.58614500
C	-0.60317900	1.13294800	2.08150100
C	-1.85313300	-0.87380700	2.46526900
C	-0.24810800	1.16821100	3.42299800
H	-0.22852600	1.89483800	1.41387800
C	-1.50104100	-0.83713600	3.80634500
H	-2.45426500	-1.69111700	2.09297100
C	-0.69989500	0.18669100	4.29265300
H	0.38777400	1.96711700	3.78509500
H	-1.85184600	-1.61664000	4.47183800
H	-0.42486200	0.21525200	5.34000900
C	-3.06227500	-0.60690000	-0.27637800
C	-3.25513300	-1.26362300	-1.48905800
C	-4.17032800	-0.33716400	0.51722900
C	-4.51859600	-1.67051700	-1.88155600
H	-2.40990200	-1.46114800	-2.13461200
C	-5.44015000	-0.74419000	0.12525300
H	-4.05329300	0.19776500	1.44988400
C	-5.62011300	-1.41703900	-1.07247400
H	-4.64447100	-2.18832600	-2.82480700
H	-6.28908900	-0.52888600	0.76289200
H	-6.60881200	-1.73650200	-1.37851000
C	-1.70221000	1.31859100	-0.68710200
C	-1.29368400	1.39125000	-2.01546000
C	-2.28749900	2.44102600	-0.11094400
C	-1.43144200	2.56635700	-2.73702600
H	-0.86374600	0.52406000	-2.49815100
C	-2.42591800	3.61983500	-0.83107700
H	-2.64601500	2.40183200	0.90886900
C	-1.99263800	3.69084400	-2.14636200
H	-1.09783700	2.60176400	-3.76709200
H	-2.87819900	4.48330300	-0.35841200
H	-2.09787100	4.61019500	-2.70923300
O	4.50396600	0.74146900	-0.62687900
S	4.43827300	1.96235700	0.29236800
C	3.26603400	3.10260900	-0.46351600
H	2.33832700	2.57087300	-0.66306100
H	3.10939200	3.94135000	0.21451700
H	3.71857900	3.45737000	-1.38753100
C	3.44547000	1.47920600	1.71637500
H	3.32440200	2.34625700	2.36543600
H	2.48278400	1.10764200	1.37256000
H	3.99709300	0.70183700	2.24168600
H	3.25621500	-0.53909500	-0.88393200

Bz_3MAM_1bDMSO (dimethyl sulfoxide)

C	0.64532200	-1.23480700	-0.76180400
C	1.89172700	-1.94729000	-0.94257400
C	2.90081800	-1.11683800	-0.58773000
C	2.30046900	0.19060000	-0.12224700
N	0.95199600	0.12622600	-0.39687900
O	-0.48461000	-1.65180600	-0.86161400
O	2.93278800	1.06476300	0.41574500
N	4.22051500	-1.22506600	-0.55573000
C	4.95087100	-2.45239400	-0.86208800
H	1.92914100	-2.97033300	-1.27688400
C	4.92627300	-3.41164000	0.32466000
H	3.90201600	-3.63443500	0.62763700

H	5.41685900	-4.35054900	0.06212500
H	5.45107000	-2.97358600	1.17684000
C	6.36542600	-2.09250000	-1.28742900
H	6.89711400	-1.59540400	-0.47139800
H	6.91993200	-2.99396800	-1.54947200
H	6.35589400	-1.42694000	-2.15167300
H	4.43483700	-2.91654400	-1.70723300
C	-0.06904300	1.05106300	0.16091600
C	-0.36063000	0.52816000	1.57549400
C	0.54608600	0.79798400	2.60288700
C	-1.42070700	-0.33437100	1.83415700
C	0.38144600	0.23931900	3.86079500
H	1.39313700	1.44329900	2.41386100
C	-1.58592000	-0.89195900	3.09577000
H	-2.13509800	-0.60117900	1.06984000
C	-0.69124900	-0.60601900	4.11513500
H	1.09514900	0.46585800	4.64383500
H	-2.42598300	-1.55501900	3.26204800
H	-0.82257200	-1.04046900	5.09902900
C	-1.29120500	1.12400600	-0.77171200
C	-1.16540200	0.91402900	-2.14158700
C	-2.50742200	1.58864700	-0.28191300
C	-2.23457300	1.13650300	-2.99536300
H	-0.22388200	0.57772800	-2.55394800
C	-3.58068800	1.80826000	-1.13383800
H	-2.62353700	1.79065600	0.77423800
C	-3.45077800	1.58157200	-2.49562000
H	-2.11438200	0.95989100	-4.05746500
H	-4.52025100	2.16171700	-0.72670200
H	-4.28718000	1.75289800	-3.16217500
C	0.44466000	2.50424000	0.12719500
C	1.18020500	2.96584200	-0.96193000
C	0.04049800	3.41928600	1.09124000
C	1.53265100	4.30027200	-1.06578500
H	1.48134400	2.27767200	-1.74067200
C	0.38959200	4.76063800	0.98736000
H	-0.55440700	3.09307000	1.93308300
C	1.14180600	5.20664400	-0.08717500
H	2.11368800	4.63510200	-1.91661200
H	0.06728000	5.45561600	1.75332400
H	1.41706100	6.25111700	-0.16778200
O	-4.12306600	-1.80979100	0.97491600
S	-4.20555900	-2.81421900	-0.16622300
C	-2.76907000	-3.89350300	-0.00996000
H	-2.78196800	-4.61224900	-0.82958900
H	-1.86026900	-3.29421400	-0.03384200
H	-2.86927500	-4.41892900	0.93805900
C	-3.69126500	-1.94095100	-1.65587800
H	-2.71897000	-1.48158100	-1.48647200
H	-3.65314000	-2.65082500	-2.48241000
H	-4.44269700	-1.18084100	-1.85714100
H	4.72018600	-0.44226000	-0.15285100

Bz_3MAM_2DMSO (dimethyl sulfoxide)

C	-0.52294700	-1.33043700	-1.04525800
C	0.58333400	-2.18664500	-1.38935900
C	1.73739200	-1.49048800	-1.20163600
C	1.36820700	-0.11293200	-0.69901100
N	-0.00094700	-0.00903400	-0.77056400
O	-1.69772200	-1.60496400	-0.95309800
O	2.16079800	0.69403300	-0.27586600
N	3.01658600	-1.78013200	-1.34849900
C	3.48765900	-3.11511100	-1.70930000
H	0.44570200	-3.21165700	-1.68922700
C	3.64041800	-3.98029800	-0.46061200
H	2.69922200	-4.04204700	0.08873700
H	3.94640000	-4.99261600	-0.73138700
H	4.39893400	-3.55227900	0.19819900
C	4.78934500	-2.99104800	-2.48799000
H	5.54332400	-2.49070600	-1.87784600
H	5.15899100	-3.97965300	-2.76435700
H	4.64015400	-2.40954900	-3.39937200
H	2.72683000	-3.55539000	-2.35878700
C	-0.77567900	1.04050600	-0.05690800
C	-0.80438300	0.58875400	1.41120400
C	0.28179600	0.85688100	2.24643800
C	-1.82386300	-0.22956600	1.88950700
C	0.33822100	0.33251000	3.52932100

H	1.09453900	1.47287400	1.88920700
C	-1.76907900	-0.74919700	3.17577900
H	-2.67729200	-0.48488100	1.27922400
C	-0.69064200	-0.47147200	4.00225700
H	1.19123700	0.55496200	4.15939500
H	-2.58588400	-1.37445100	3.51462300
H	-0.64862400	-0.87819300	5.00567400
C	-2.15933700	1.22613600	-0.70415500
C	-2.34029900	1.03104900	-2.07049100
C	-3.20360900	1.77579500	0.03095400
C	-3.54197100	1.35273000	-2.68043800
H	-1.53587700	0.62631400	-2.66963000
C	-4.40911200	2.09865400	-0.57771700
H	-3.08140800	1.96245500	1.08906800
C	-4.58571300	1.88703800	-1.93610800
H	-3.66216100	1.18535300	-3.74405300
H	-5.21053000	2.51900000	0.01773500
H	-5.52570200	2.13761900	-2.41242200
C	-0.13080200	2.42263300	-0.27729500
C	0.46352800	2.74334100	-1.49490600
C	-0.27700700	3.42520400	0.67410000
C	0.93455900	4.02235600	-1.73973000
H	0.56242000	1.98816200	-2.26326600
C	0.19266800	4.70982100	0.43045800
H	-0.76213800	3.21185200	1.61681000
C	0.80703000	5.01344500	-0.77418900
H	1.40310600	4.24605500	-2.69053800
H	0.07357100	5.47345200	1.18960800
H	1.17692500	6.01356400	-0.96417700
O	5.29848500	-0.60709600	-0.26238900
O	-4.72693700	-1.51261700	1.66833700
S	5.53095100	0.16637400	1.03684900
C	5.02027800	1.86299600	0.71142000
H	4.01298800	1.85393000	0.30094600
H	5.06827400	2.42703000	1.64257700
H	5.72856500	2.27591400	-0.00433000
C	4.19385100	-0.29608500	2.15259300
H	4.28850300	0.28551600	3.06908900
H	3.24003600	-0.10859300	1.66495400
H	4.31424000	-1.35453200	2.37545700
S	-5.20367200	-2.46212800	0.57765500
C	-3.90003300	-3.68917500	0.35782700
H	-4.19821700	-4.37855100	-0.43233200
H	-2.96867600	-3.18562200	0.10285500
H	-3.81167100	-4.22883400	1.29898800
C	-4.98919400	-1.59643200	-0.98765300
H	-3.96485800	-1.23514600	-1.06120100
H	-5.22549700	-2.28228400	-1.80150100
H	-5.68936900	-0.76423400	-0.99259000
H	3.72329800	-1.12923500	-0.97523300

Bz_3ABM_1aMET (methanol)

C	0.39978900	-1.47949100	-0.32316800
C	1.83441400	-1.24018700	-0.35755500
C	2.08414100	0.07505500	-0.12325500
C	0.73093600	0.72205900	0.12774100
N	-0.23656500	-0.19633700	-0.18624100
O	-0.18938000	-2.52536000	-0.37589700
O	0.57392300	1.83785200	0.56430300
N	3.15132100	0.85241100	-0.05461000
C	4.55045300	0.42795600	-0.14853100
C	5.05056700	-0.07173700	1.20318400
H	4.44152600	-0.90225300	1.56251900
H	6.08294900	-0.41637600	1.11849200
H	5.01322500	0.73109100	1.94327100
C	5.36780600	1.60184500	-0.66786800
H	5.29196400	2.45356000	0.01260600
H	6.41810500	1.32021500	-0.74747400
H	5.01709200	1.91562200	-1.65219000
H	4.59984200	-0.38514200	-0.87190100
C	-1.67670400	-0.01964900	0.14385500
C	-1.78714700	-0.32818000	1.64405100
C	-1.55922400	0.66833500	2.59164500
C	-1.95303700	-1.64011600	2.08452600
C	-1.53077600	0.36593200	3.94553300
H	-1.39052100	1.68597400	2.27046500
C	-1.92533500	-1.94217000	3.43814900
H	-2.08711200	-2.43360100	1.36362000

C	-1.72051800	-0.93944700	4.37513500
H	-1.35666300	1.15648100	4.66535000
H	-2.06089600	-2.96790200	3.75897400
H	-1.70129900	-1.17504300	5.43226300
C	-2.54711700	-0.91168200	-0.75885100
C	-2.17110000	-1.18153000	-2.07164100
C	-3.80909300	-1.31028100	-0.33375000
C	-3.02085700	-1.86395100	-2.92630600
H	-1.20582500	-0.85776900	-2.43744500
C	-4.66324200	-1.99408300	-1.18917700
H	-4.13973100	-1.08576800	0.67128900
C	-4.27178500	-2.27927900	-2.48783300
H	-2.70337300	-2.07118200	-3.94106700
H	-5.63973500	-2.30026300	-0.83396600
H	-4.93604900	-2.81390600	-3.15563600
C	-2.14200900	1.39407000	-0.25570700
C	-1.60363100	2.03489400	-1.36838900
C	-3.22625700	1.98028000	0.38713100
C	-2.10876200	3.24958900	-1.80184900
H	-0.78227400	1.58581600	-1.91066100
C	-3.73631100	3.19693600	-0.04717300
H	-3.68646700	1.48879200	1.23347800
C	-3.17600100	3.84150800	-1.13893000
H	-1.66650900	3.73395500	-2.66395900
H	-4.57781400	3.63754600	0.47352700
H	-3.57087400	4.79192500	-1.47623300
O	2.63306500	3.67756600	0.42103100
H	1.77965300	3.31590200	0.69902200
C	2.45501900	4.26020000	-0.86539600
H	3.43093600	4.60062700	-1.20871200
H	2.06276500	3.53624300	-1.58675500
H	1.77905500	5.11848500	-0.82356800
H	2.99628600	1.83595600	0.18304300
Br	2.99949300	-2.67752000	-0.67775200

Bz_3ABM _1bMET (methanol)

C	0.75318300	-0.80688400	-0.40985600
C	2.16671800	-0.47203400	-0.46897800
C	2.31524900	0.85942400	-0.26426200
C	0.92456800	1.42325700	-0.03541800
N	0.01891000	0.41228900	-0.28599300
O	0.25578200	-1.90555600	-0.44311400
O	0.72580200	2.54937200	0.33592000
N	3.30857200	1.72909500	-0.19972400
C	4.74445300	1.43707900	-0.22034100
C	5.22441700	1.00210900	1.16039600
H	4.67929700	0.12232500	1.50475300
H	6.28701400	0.75494400	1.12717900
H	5.07868400	1.80653200	1.88499300
C	5.47795200	2.66821500	-0.72839500
H	5.32194600	3.51564200	-0.05502700
H	6.54907600	2.47097600	-0.77691400
H	5.13072500	2.94666200	-1.72417300
H	4.89235800	0.62024200	-0.92625900
C	-1.41863400	0.45804000	0.10768000
C	-1.44192400	0.07841200	1.59590800
C	-1.07786900	1.02914900	2.55098700
C	-1.67073700	-1.22987400	2.01258100
C	-0.97082000	0.68583900	3.88960700
H	-0.86917100	2.04469900	2.24389800
C	-1.56554300	-1.57204000	3.35478600
H	-1.92085800	-1.99744100	1.29422900
C	-1.22036400	-0.61729900	4.29876500
H	-0.69110100	1.44077100	4.61430700
H	-1.75213600	-2.59523000	3.65804700
H	-1.14057100	-0.88616700	5.34505700
C	-2.25841100	-0.45471100	-0.80208900
C	-1.86118900	-0.75782100	-2.10012600
C	-3.52868000	-0.84401300	-0.38800400
C	-2.69718400	-1.46692800	-2.94973800
H	-0.89407300	-0.43866200	-2.46360300
C	-4.36540000	-1.55441200	-1.23512500
H	-3.87661100	-0.58858100	0.60395400
C	-3.95158900	-1.87508900	-2.51964300
H	-2.36292100	-1.69956600	-3.95349800
H	-5.34601800	-1.85507000	-0.88700100
H	-4.60295500	-2.43163800	-3.18215300
C	-2.00658600	1.84889200	-0.19883100

C	-1.66395300	2.50854700	-1.37696000
C	-3.00996800	2.38638700	0.59706900
C	-2.28224500	3.69506800	-1.73048200
H	-0.90722900	2.09238900	-2.02929900
C	-3.63585200	3.57530600	0.24122100
H	-3.31665400	1.88069700	1.50209100
C	-3.27148800	4.23833000	-0.91911300
H	-1.99291000	4.19636600	-2.64610800
H	-4.41310500	3.97884900	0.87874200
H	-3.75682500	5.16627300	-1.19552400
H	-1.18457100	-3.12017700	-0.41921000
O	-1.66857500	-3.90270100	-0.12314000
C	-0.77265100	-4.67050000	0.66066600
H	-0.43021500	-4.12254700	1.54554400
H	-1.30401000	-5.56274600	0.99340300
H	0.10667800	-4.98508100	0.08854300
H	3.02333200	2.66717900	0.05916500
Br	3.43667600	-1.82214100	-0.75932200

Bz_3ABM_2MET (methanol)

C	0.28687100	-1.22244900	-0.38996700
C	1.73504400	-1.27534500	-0.40514700
C	2.23580400	-0.04038900	-0.12988200
C	1.03181400	0.85249200	0.13440900
N	-0.09605400	0.14439900	-0.20442500
O	-0.48988500	-2.13915300	-0.49969900
O	1.09461000	1.96370100	0.60038000
N	3.43214300	0.50746500	-0.02976500
C	4.72130300	-0.18379400	-0.12663100
C	5.08901100	-0.81568000	1.21200900
H	4.32167300	-1.52022500	1.53537200
H	6.03406800	-1.35517400	1.12589800
H	5.19826300	-0.04554300	1.97899900
C	5.76323300	0.81986200	-0.59804000
H	5.84982200	1.64632300	0.11151700
H	6.73694100	0.33633400	-0.68039400
H	5.49611100	1.22955600	-1.57326400
H	4.61927600	-0.96690800	-0.87703500
C	-1.48506300	0.57270900	0.12750200
C	-1.69666300	0.16809600	1.59410800
C	-1.17365000	0.96683300	2.61203600
C	-2.26939900	-1.05432300	1.93532300
C	-1.24303200	0.56443600	3.93688400
H	-0.70141700	1.90749100	2.36616000
C	-2.33960000	-1.45547600	3.26310400
H	-2.65840100	-1.71006200	1.16961200
C	-1.83177800	-0.64799800	4.26926800
H	-0.83409300	1.20228100	4.71103400
H	-2.79336800	-2.40867100	3.50645200
H	-1.88924800	-0.96202300	5.30438900
C	-2.48890400	-0.04425400	-0.86198700
C	-2.11957500	-0.37229900	-2.16266500
C	-3.83502100	-0.11081500	-0.51685900
C	-3.06667600	-0.79316300	-3.08367600
H	-1.08597500	-0.29819000	-2.47191000
C	-4.78379500	-0.53388600	-1.43587900
H	-4.15395400	0.17317200	0.47695600
C	-4.40393500	-0.88237700	-2.72334500
H	-2.75461000	-1.05171100	-4.08821600
H	-5.82467000	-0.58705500	-1.14104700
H	-5.14328200	-1.21430100	-3.44176800
C	-1.64938500	2.08098000	-0.14443800
C	-1.04431600	2.66472300	-1.25522100
C	-2.53239800	2.84383500	0.60893700
C	-1.28341700	3.98893900	-1.57908700
H	-0.37835000	2.08240900	-1.87864100
C	-2.77847700	4.17212500	0.28213500
H	-3.03987100	2.40847100	1.45866000
C	-2.15043000	4.75325800	-0.80734700
H	-0.79259300	4.42509600	-2.44063400
H	-3.46700900	4.74983600	0.88674900
H	-2.33849500	5.78950900	-1.05993600
O	3.49790700	3.34974600	0.53324000
H	2.58319200	3.18904200	0.80260300
C	3.46808700	4.01118800	-0.72731400
H	4.49816100	4.11880800	-1.06399400
H	2.91319300	3.43396500	-1.47361100
H	3.02044400	5.00499300	-0.64400800

H	-2.18455200	-2.94513700	-0.54027200
O	-2.86909600	-3.57523900	-0.27861800
C	-2.23522900	-4.57195500	0.50351200
H	-1.78759600	-4.15532700	1.41270600
H	-2.99515200	-5.29724300	0.79599100
H	-1.45364800	-5.09674200	-0.05614500
H	3.47200500	1.49699100	0.23404300
Br	2.59399100	-2.90477400	-0.76685200

Bz_3ABM_1aDMSO (dimethyl sulfoxide)

C	-0.37889000	-1.90597900	-0.02361800
C	1.03736300	-2.12237400	-0.25961800
C	1.64404100	-0.93559200	-0.53951200
C	0.55115000	0.11613400	-0.48605500
N	-0.65364500	-0.52706800	-0.33370900
O	-1.19942500	-2.68770900	0.38093400
O	0.75733800	1.30261500	-0.53247900
N	2.86171800	-0.50935800	-0.80994300
C	4.07835000	-1.32500000	-0.81505300
C	4.71888000	-1.32079300	0.56956400
H	4.02820700	-1.71328700	1.31798600
H	5.61834200	-1.93959500	0.57410700
H	4.99433700	-0.30206200	0.84952500
C	5.01909400	-0.79532000	-1.88856200
H	5.28261700	0.24251600	-1.67912400
H	5.93156300	-1.39308000	-1.91320000
H	4.54797900	-0.84343600	-2.87182600
H	3.78735000	-2.34184300	-1.07212300
C	-1.88774300	0.19300000	0.08353100
C	-1.66236100	0.54250600	1.56257000
C	-1.08622600	1.75360000	1.93906800
C	-1.87685100	-0.42479900	2.54468100
C	-0.75876500	2.00254900	3.26512400
H	-0.87876100	2.50626500	1.19279100
C	-1.55075000	-0.17612500	3.86919200
H	-2.28776300	-1.38536100	2.26738800
C	-0.99430500	1.04150400	4.23659200
H	-0.31324500	2.95258300	3.53438900
H	-1.72989700	-0.94037500	4.61568000
H	-0.74036200	1.23627800	5.27142700
C	-3.13349900	-0.66818700	-0.18775700
C	-3.20909100	-1.44491400	-1.34156900
C	-4.26425300	-0.54924700	0.60972700
C	-4.37477900	-2.11455500	-1.66950000
H	-2.34860100	-1.53075400	-1.99201900
C	-5.43708900	-1.21948800	0.28120000
H	-4.24288000	0.07101900	1.49525100
C	-5.49674400	-2.00895000	-0.85542300
H	-4.40853300	-2.72143500	-2.56622900
H	-6.30552100	-1.11740300	0.92066900
H	-6.40933900	-2.53320500	-1.11129400
C	-2.12932800	1.40972200	-0.82891500
C	-1.68923000	1.42640700	-2.14843100
C	-2.94555300	2.44675000	-0.38818800
C	-2.02406100	2.47240100	-2.99455900
H	-1.08046300	0.61771400	-2.52912000
C	-3.28088300	3.49568400	-1.23255900
H	-3.33157400	2.43973400	0.62239400
C	-2.81634800	3.51726900	-2.53927300
H	-1.66248700	2.46819500	-4.01568200
H	-3.91164400	4.29569900	-0.86443100
H	-3.07552200	4.33577100	-3.19951200
O	3.98625400	2.03018300	-0.64460700
S	3.69675100	3.26042700	0.21701100
C	2.33457100	4.12879100	-0.58078500
H	1.51784700	3.42979600	-0.74579100
H	2.02984800	4.95923100	0.05557900
H	2.71371000	4.51202400	-1.52621800
C	2.81266100	2.66999500	1.67176100
H	2.53872700	3.52822900	2.28479600
H	1.93200200	2.11520700	1.35686100
H	3.49774900	2.02903200	2.22347800
H	3.01817200	0.51092000	-0.81903200
Br	1.74668900	-3.85116800	-0.05416900

Bz_3ABM_1bDMSO (dimethyl sulfoxide)

C	0.71148800	-0.64729000	-0.44654700
C	2.15354000	-0.84223500	-0.48898400

C	2.76814800	0.33907700	-0.24023800
C	1.67076700	1.36039000	0.00363600
N	0.46812000	0.75432800	-0.28682100
O	-0.15462300	-1.48132800	-0.51042800
O	1.88858300	2.47026000	0.41418700
N	4.00769000	0.79084800	-0.14485300
C	5.24164200	0.00200300	-0.17339500
C	5.51196500	-0.62532200	1.19030700
H	4.68021500	-1.25918100	1.50054700
H	6.41317700	-1.23977500	1.14879300
H	5.65697600	0.15108400	1.94504700
C	6.37698500	0.90295300	-0.63309500
H	6.52325800	1.72754100	0.06997100
H	7.30688800	0.33613500	-0.68412800
H	6.16961700	1.31981800	-1.61945600
H	5.09697000	-0.78838000	-0.90960000
C	-0.86843000	1.28446300	0.10543200
C	-1.04977100	0.86835600	1.57265000
C	-0.38383000	1.58314400	2.57079000
C	-1.73125700	-0.29166700	1.92623600
C	-0.41971900	1.16107500	3.89049600
H	0.17413400	2.47273800	2.31215800
C	-1.76842200	-0.71182200	3.24988600
H	-2.24060400	-0.89786700	1.19178400
C	-1.11828500	0.01145000	4.23749700
H	0.10079400	1.73317700	4.64908200
H	-2.31318000	-1.61626200	3.49142600
H	-1.14950200	-0.31758700	5.26933900
C	-1.94883900	0.76478300	-0.85922900
C	-1.64373600	0.43918700	-2.17721100
C	-3.28521500	0.78826300	-0.47415000
C	-2.64576600	0.11458800	-3.07836500
H	-0.61565000	0.43966700	-2.51294300
C	-4.28974100	0.45947500	-1.37324900
H	-3.55270300	1.06976300	0.53524700
C	-3.97532700	0.11820800	-2.67993500
H	-2.38323100	-0.14322900	-4.09727000
H	-5.32239100	0.47441900	-1.04660200
H	-4.75830600	-0.13890400	-3.38276800
C	-0.92960000	2.80594400	-0.12774400
C	-0.34586500	3.36747100	-1.26111700
C	-1.70783200	3.61571400	0.68969800
C	-0.50549500	4.71179100	-1.54882100
H	0.24020100	2.75083900	-1.93000300
C	-1.87357700	4.96505300	0.40010900
H	-2.19543600	3.20003400	1.56062200
C	-1.26885800	5.52089300	-0.71545900
H	-0.03360800	5.12950300	-2.42991400
H	-2.48117200	5.57893400	1.05391700
H	-1.39479400	6.57292100	-0.94012600
O	-3.64705800	-2.73347900	1.15149900
S	-3.21788200	-3.86843800	0.23209300
C	-1.51238100	-4.26742200	0.66309500
H	-1.15968700	-5.05554400	-0.00232700
H	-0.89593100	-3.37515400	0.56829200
H	-1.52095100	-4.63172500	1.68875000
C	-2.89422700	-3.12846400	-1.37829200
H	-2.19437600	-2.30303500	-1.26135100
H	-2.49300600	-3.89439100	-2.04215500
H	-3.84632100	-2.76895900	-1.76216900
H	4.07503400	1.75979800	0.14638200
Br	2.85610400	-2.55061700	-0.82023900

Bz_3ABM_2DMSO (dimethyl sulfoxide)

C	-0.60658300	-1.05083800	-0.67658700
C	0.49405800	-1.98162200	-0.82808400
C	1.67556800	-1.30529700	-0.77023000
C	1.31244200	0.15377500	-0.55727200
N	-0.05418800	0.27394500	-0.66215400
O	-1.78071300	-1.29570000	-0.55582700
O	2.11683500	1.01247700	-0.29981300
N	2.95960500	-1.59293800	-0.83162600
C	3.53639600	-2.93613900	-0.92909000
C	3.79173200	-3.49910500	0.46559800
H	2.86573500	-3.54555700	1.04146700
H	4.20518900	-4.50731600	0.39809400
H	4.50272900	-2.86540600	0.99941300
C	4.80612400	-2.86539200	-1.76589300

H	5.52840000	-2.19464300	-1.29827700
H	5.25090100	-3.85788200	-1.85277900
H	4.58655800	-2.49606000	-2.76908200
H	2.81120600	-3.56514900	-1.44217100
C	-0.79490600	1.46687500	-0.16098200
C	-0.75901900	1.34104600	1.36956400
C	0.31409500	1.85397100	2.09845100
C	-1.70917300	0.56919000	2.03563900
C	0.42522000	1.61606400	3.46110500
H	1.07513800	2.43505000	1.59822000
C	-1.59806700	0.33565200	3.39903300
H	-2.54989000	0.13299600	1.51531500
C	-0.53333200	0.85786500	4.11900400
H	1.26699000	2.02522200	4.00691700
H	-2.35916100	-0.26118600	3.88634700
H	-0.44822600	0.67445900	5.18344800
C	-2.20619000	1.52308100	-0.77123200
C	-2.42530600	1.11071100	-2.08296600
C	-3.23951300	2.15807800	-0.09313000
C	-3.65497000	1.30125900	-2.69031500
H	-1.62920500	0.63522600	-2.64049400
C	-4.47288900	2.35395200	-0.70187000
H	-3.08976000	2.50994000	0.91821300
C	-4.68835700	1.92388100	-2.00106200
H	-3.80577800	0.96348300	-3.70854100
H	-5.26571700	2.84585100	-0.15145400
H	-5.65043900	2.07347400	-2.47564200
C	-0.15427700	2.75682800	-0.70620300
C	0.46806300	2.78387300	-1.95052500
C	-0.33725800	3.95778200	-0.02915200
C	0.92999000	3.97530500	-2.48685800
H	0.59732500	1.86921700	-2.51315600
C	0.12386100	5.15276700	-0.56443600
H	-0.84682100	3.96927700	0.92497000
C	0.76593800	5.16709300	-1.79341300
H	1.42027800	3.97048700	-3.45282000
H	-0.02399100	6.07486700	-0.01550700
H	1.12874500	6.09806100	-2.21142800
O	5.19424700	-0.14915500	-0.01074700
O	-4.52657800	-0.88717200	2.11537700
S	5.43176100	0.86513900	1.10936300
C	4.88821000	2.46144700	0.47481200
H	3.87604400	2.36246800	0.08996800
H	4.94118700	3.19300700	1.28083500
H	5.57945100	2.73970400	-0.31837700
C	4.12172500	0.60630500	2.31901600
H	4.22194500	1.35362700	3.10571800
H	3.15537800	0.68235400	1.82591400
H	4.26491700	-0.38814900	2.73737800
S	-5.12740500	-1.96931100	1.22853700
C	-3.87129300	-3.25172600	1.05625400
H	-4.25201600	-4.02742400	0.39170300
H	-2.95838900	-2.81093200	0.65891900
H	-3.70615500	-3.66914500	2.04795600
C	-5.06896800	-1.34121900	-0.45926600
H	-4.05685700	-1.00848300	-0.68215400
H	-5.38556800	-2.13303200	-1.13849100
H	-5.76490900	-0.50730800	-0.51579400
H	3.62882300	-0.84321500	-0.59415600
Br	0.12708800	-3.81841500	-0.98433700

TS_BzMAM (diethyl ether)

C	0.271288	-1.803551	-0.242336
C	1.654507	-1.501870	0.090607
C	1.855563	-0.187120	-0.159496
C	0.559963	0.422931	-0.671117
N	-0.343490	-0.599775	-0.699173
O	-0.339622	-2.843552	-0.176751
O	0.434973	1.585327	-0.969595
N	2.900709	0.625888	-0.065689
H	2.725994	1.595156	-0.298330
C	4.205711	0.232431	0.452885
H	2.338356	-2.242493	0.469294
C	4.192073	0.160350	1.977667
H	3.412125	-0.515165	2.332175
H	5.152336	-0.201778	2.349774
H	4.008219	1.150129	2.401894
C	5.256480	1.199362	-0.069297

H	5.058986	2.212504	0.292149
H	6.246796	0.906678	0.280532
H	5.265180	1.215769	-1.160101
H	4.413099	-0.764848	0.052238
C	-1.752025	-0.609244	-1.095939
H	-2.331772	-0.964337	-0.242302
H	-1.865093	-1.350922	-1.888197
C	-2.273998	0.724073	-1.557091
C	-2.216243	1.076399	-2.900223
C	-2.837339	1.611690	-0.648015
C	-2.699429	2.304005	-3.327673
H	-1.784333	0.385500	-3.615671
C	-3.323898	2.839197	-1.071142
H	-2.890879	1.340178	0.400351
C	-3.252399	3.189420	-2.412698
H	-2.647111	2.569196	-4.376770
H	-3.760113	3.523655	-0.353594
H	-3.632191	4.147941	-2.745252

TS_Bz$_2$MAM (diethyl ether)

C	-1.007422	-0.205072	1.938550
C	-2.409702	-0.107212	1.557752
C	-2.469482	0.108751	0.225087
C	-1.058823	0.141726	-0.317178
N	-0.219691	0.093702	0.768918
O	-0.534022	-0.502990	3.003835
O	-0.782176	0.170607	-1.490617
N	-3.457352	0.277202	-0.647865
H	-3.179387	0.338104	-1.618946
C	-4.873022	0.162045	-0.315959
H	-3.206796	-0.237199	2.270245
C	-5.294942	-1.300485	-0.201037
H	-4.678282	-1.831101	0.525922
H	-6.336553	-1.371893	0.117692
H	-5.195046	-1.800661	-1.167197
C	-5.686591	0.917184	-1.355201
H	-5.551000	0.472778	-2.345331
H	-6.748310	0.871954	-1.110985
H	-5.385547	1.964717	-1.401658
H	-5.004352	0.647337	0.655961
C	1.233639	-0.077752	0.659852
C	1.823610	0.781144	-0.449164
C	1.453341	2.109954	-0.628084
C	2.818904	0.244768	-1.254219
C	2.068506	2.885561	-1.596779
H	0.667392	2.539829	-0.019488
C	3.440498	1.021065	-2.223146
H	3.110242	-0.791569	-1.125807
C	3.067004	2.344722	-2.397470
H	1.765157	3.916985	-1.730592
H	4.213780	0.586788	-2.845325
H	3.546751	2.952030	-3.155296
C	1.964027	0.237752	1.956132
C	2.885365	-0.673384	2.450427
C	1.796541	1.453221	2.612216
C	3.629490	-0.381931	3.587049
H	3.019153	-1.624876	1.948621
C	2.530469	1.743806	3.748592
H	1.076884	2.172490	2.242455
C	3.453073	0.826955	4.240296
H	4.342957	-1.105452	3.962827
H	2.383404	2.689852	4.255675
H	4.027943	1.056285	5.129296
H	1.435168	-1.123440	0.413751

TS_Bz$_3$MAM (diethyl ether)

C	-0.992649	-1.721068	-0.320129
C	-2.440200	-1.670919	-0.399127
C	-2.823991	-0.410640	-0.112996
C	-1.587984	0.416740	0.154553
N	-0.493079	-0.367381	-0.175010
O	-0.303852	-2.709067	-0.304734
O	-1.653301	1.522581	0.628072
N	-3.995273	0.195831	0.035808
H	-3.955886	1.171107	0.301067
C	-5.287549	-0.458514	-0.133994
H	-3.031022	-2.552870	-0.580153
C	-5.635924	-0.606606	-1.612570

H	-4.852783	-1.144538	-2.148934
H	-6.570420	-1.158637	-1.729314
H	-5.754560	0.376728	-2.073295
C	-6.340934	0.327672	0.630325
H	-6.429650	1.340729	0.227963
H	-7.313948	-0.155573	0.538844
H	-6.087110	0.395870	1.689276
H	-5.198086	-1.455003	0.310963
C	0.958463	0.005773	-0.017583
C	1.036515	1.534437	0.167574
C	1.684785	2.113147	1.245853
C	0.498093	2.373785	-0.810865
C	1.790477	3.497944	1.353044
H	2.115166	1.494038	2.019331
C	0.598670	3.746181	-0.708513
H	-0.005466	1.940705	-1.666676
C	1.248991	4.318155	0.381235
H	2.300242	3.927144	2.207173
H	0.168284	4.375142	-1.478326
H	1.329885	5.395193	0.465221
C	1.802198	-0.373886	-1.278770
C	1.960960	-1.705811	-1.673090
C	2.537793	0.581469	-1.982340
C	2.757037	-2.053517	-2.752507
H	1.464432	-2.482838	-1.119957
C	3.342535	0.234583	-3.061147
H	2.514538	1.618544	-1.692432
C	3.448757	-1.084344	-3.463722
H	2.844084	-3.097966	-3.027786
H	3.892859	1.011354	-3.578533
H	4.073752	-1.356693	-4.305762
C	1.513079	-0.706561	1.224435
C	0.696214	-0.936191	2.327479
C	2.858614	-1.047576	1.314232
C	1.205074	-1.504782	3.484669
H	-0.350609	-0.664770	2.295580
C	3.371879	-1.614500	2.472771
H	3.517168	-0.868356	0.475583
C	2.547179	-1.849157	3.562237
H	0.548311	-1.679105	4.328339
H	4.422317	-1.875414	2.518761
H	2.945709	-2.296932	4.464440

TS_Bz_3ABM (diethyl ether)

C	-0.814306	-1.147326	-0.013023
C	-2.214762	-0.736174	-0.054592
C	-2.280699	0.606557	0.051972
C	-0.852978	1.109156	0.164386
N	-0.003754	0.039905	-0.079755
O	-0.403730	-2.267387	0.119419
O	-0.615370	2.246964	0.472684
N	-3.223313	1.535512	0.135497
H	-2.867208	2.479794	0.224207
C	-4.667038	1.346904	-0.010269
C	-5.052777	1.228688	-1.481349
H	-4.526228	0.400804	-1.957743
H	-6.125407	1.049575	-1.577141
H	-4.806521	2.149564	-2.015171
C	-5.373066	2.502250	0.681876
H	-5.110462	3.453394	0.210013
H	-6.453967	2.380097	0.609005
H	-5.100647	2.551515	1.737050
H	-4.924841	0.418862	0.500818
C	1.505826	0.059930	-0.012520
C	1.949757	1.534250	-0.069062
C	2.757530	2.097914	0.903703
C	1.578235	2.319603	-1.163078
C	3.183105	3.419683	0.794571
H	3.064027	1.517249	1.761634
C	1.996356	3.629638	-1.274765
H	0.953356	1.893110	-1.938647
C	2.805369	4.189183	-0.289755
H	3.812560	3.840707	1.569200
H	1.691461	4.219978	-2.130283
H	3.135551	5.217510	-0.373623
C	2.162453	-0.691581	-1.216163
C	1.962412	-2.059885	-1.421397
C	3.086999	-0.059482	-2.049900

C	2.598098	-2.740260	-2.447589
H	1.312954	-2.606160	-0.761568
C	3.732333	-0.741617	-3.074211
H	3.339655	0.977669	-1.906339
C	3.482787	-2.084817	-3.290635
H	2.405750	-3.798910	-2.575237
H	4.440509	-0.208513	-3.697155
H	3.982468	-2.618045	-4.090444
C	1.941007	-0.581327	1.312540
C	1.156432	-0.446769	2.454075
C	3.168513	-1.226238	1.424058
C	1.578554	-0.955773	3.672336
H	0.205111	0.066301	2.405808
C	3.595595	-1.733344	2.643498
H	3.801613	-1.334570	0.554303
C	2.801245	-1.604304	3.772427
H	0.947438	-0.844579	4.545632
H	4.553606	-2.235104	2.706221
H	3.130939	-2.005881	4.722813
Br	-3.566895	-2.035372	-0.105519

TPE (diethyl ether)

C	-2.262464	0.358027	0.000113
C	-0.914805	0.356641	0.000280
C	-3.062355	1.610007	-0.097941
C	-4.099581	1.852363	0.802790
C	-2.818499	2.545435	-1.102600
C	-4.848545	3.016287	0.724369
H	-4.313360	1.123046	1.575112
C	-3.574189	3.704361	-1.189549
H	-2.026325	2.361258	-1.817089
C	-4.587185	3.947712	-0.271945
H	-5.641234	3.195251	1.440946
H	-3.371300	4.419705	-1.977505
H	-5.175223	4.855175	-0.337183
C	-3.064803	-0.892431	0.097816
C	-4.102073	-1.132560	-0.803461
C	-2.823354	-1.828496	1.102468
C	-4.853518	-2.294914	-0.725529
H	-4.313926	-0.402689	-1.575796
C	-3.581505	-2.985855	1.188910
H	-2.031128	-1.646123	1.817357
C	-4.594585	-3.226986	0.270811
H	-5.646227	-2.472147	-1.442514
H	-3.380464	-3.701723	1.976864
H	-5.184539	-4.133232	0.335668
C	-0.112175	1.606884	0.098078
C	-0.354543	2.543609	1.101912
C	0.926219	1.846243	-0.802118
C	0.403761	3.700842	1.188553
H	-1.147627	2.361824	1.815998
C	1.677817	3.008490	-0.724010
H	1.138864	1.115890	-1.573770
C	1.417946	3.941213	0.271470
H	0.201983	4.417206	1.975866
H	2.471401	3.185108	-1.440178
H	2.008034	4.847361	0.336472
C	-0.115204	-0.895574	-0.097496
C	-0.358203	-1.830423	-1.102879
C	0.920848	-1.138686	0.804364
C	0.397254	-2.989535	-1.189518
H	-1.149567	-1.645702	-1.818132
C	1.669553	-2.302795	0.726256
H	1.133904	-0.409785	1.577286
C	1.409094	-3.233637	-0.270844
H	0.195053	-3.704453	-1.978036
H	2.461326	-2.482372	1.443692
H	1.996926	-4.141251	-0.335829

TS_TPE (diethyl ether)

C	-2.254262	0.356443	0.046975
C	-0.921064	0.356037	-0.053871
C	-3.041413	1.625741	0.044355
C	-3.658200	2.104061	1.198010
C	-3.178308	2.349669	-1.137519
C	-4.387407	3.283850	1.172192
H	-3.551917	1.562549	2.129767
C	-3.909248	3.528248	-1.165718

H	-2.700047	1.985972	-2.038769
C	-4.516116	3.999559	-0.010174
H	-4.852711	3.647430	2.080572
H	-4.002315	4.080877	-2.092958
H	-5.084958	4.921188	-0.029983
C	-3.040237	-0.912878	0.083836
C	-3.129737	-1.706035	-1.057685
C	-3.704134	-1.323747	1.237418
C	-3.856584	-2.887352	-1.044898
H	-2.617549	-1.394549	-1.959626
C	-4.428298	-2.506751	1.253178
H	-3.642512	-0.724636	2.137154
C	-4.507095	-3.292807	0.111815
H	-3.912083	-3.493740	-1.941024
H	-4.929776	-2.817026	2.162085
H	-5.072157	-4.216888	0.124511
C	-0.135077	1.625348	-0.090738
C	-0.045644	2.418563	1.050749
C	0.528917	2.036142	-1.244291
C	0.681227	3.599865	1.037954
H	-0.557900	2.107133	1.952670
C	1.253105	3.219131	-1.260060
H	0.467352	1.436986	-2.144001
C	1.331834	4.005245	-0.118731
H	0.736674	4.206297	1.934052
H	1.754659	3.529347	-2.168945
H	1.896917	4.929314	-0.131434
C	-0.133923	-0.913269	-0.051230
C	0.482835	-1.391639	-1.204879
C	0.002990	-1.637152	1.130669
C	1.212032	-2.571434	-1.179030
H	0.376537	-0.850165	-2.136656
C	0.733920	-2.815737	1.158899
H	-0.475248	-1.273415	2.031915
C	1.340761	-3.287098	0.003361
H	1.677315	-2.935054	-2.087405
H	0.827001	-3.368330	2.086159
H	1.909595	-4.208731	0.023194

TS_BzMAM_2MET (methanol)

C	0.06385000	2.15404400	-0.69850700
C	1.47604200	1.89852300	-0.59952100
C	1.63888800	0.57577100	-0.32111200
C	0.25767700	-0.07093000	-0.25559800
N	-0.63407900	0.92866600	-0.49220100
O	-0.53021100	3.19606100	-0.90962200
O	0.03919700	-1.24157100	-0.03152600
N	2.70671600	-0.16897200	-0.09772000
H	2.58281300	-1.17104800	0.07063200
C	4.07186900	0.35018800	-0.15325900
H	2.22081400	2.66606000	-0.72155300
C	4.55756300	0.44590700	-1.59694200
H	3.88799700	1.06378800	-2.19714000
H	5.55424500	0.88944100	-1.63138000
H	4.60526800	-0.54858000	-2.04619600
C	4.96553900	-0.53852500	0.69840700
H	4.97063100	-1.56043600	0.31080100
H	5.98974600	-0.16500900	0.68474300
H	4.61978800	-0.56372200	1.73292800
H	4.04906900	1.35324600	0.28281100
C	-2.09880600	0.88627800	-0.59914800
H	-2.35683900	1.30955500	-1.57130200
H	-2.50875100	1.55225700	0.16003800
C	-2.69423500	-0.48771500	-0.46424400
C	-3.14915500	-0.93578800	0.77026200
C	-2.81913000	-1.31482300	-1.57507300
C	-3.70099000	-2.20231200	0.89944500
H	-3.06328600	-0.29066300	1.63731400
C	-3.36940900	-2.58156600	-1.45015900
H	-2.47574300	-0.96607900	-2.54261300
C	-3.80808700	-3.02955100	-0.21051400
H	-4.05005500	-2.54314200	1.86669900
H	-3.45955700	-3.21951000	-2.32105300
H	-4.23931100	-4.01840400	-0.11178300
O	2.13452900	-2.92396200	0.56538100
H	1.25578000	-2.59957200	0.31189100
C	2.17636000	-2.98988600	1.98585900
H	3.18027900	-3.30098500	2.27214300

H	1.96873500	-2.01642600	2.44215500
H	1.46084200	-3.72081100	2.37242900
O	-2.53707300	3.81240300	0.93780400
H	-1.94969400	3.70478700	0.17430200
C	-1.73558700	3.69116400	2.09982200
H	-2.37929100	3.84290500	2.96647800
H	-1.28092700	2.69638800	2.18401100
H	-0.93689500	4.43998800	2.12849000

TS_BzMAM_2DMSO (dimethyl sulfoxide)

C	-1.42312100	-1.52786000	1.66194000
C	-0.35305500	-2.42094600	1.29014200
C	0.62141700	-1.67619300	0.69315800
C	0.16879400	-0.22244500	0.68027200
N	-1.06085600	-0.20477600	1.26129900
O	-2.48762800	-1.75433000	2.20044600
O	0.81867400	0.68978900	0.22303200
N	1.78472100	-1.96313000	0.14356500
H	2.39193200	-1.19473100	-0.18037800
C	2.34590100	-3.31118200	0.12911200
H	-0.37671700	-3.47833500	1.49174500
C	3.17639800	-3.55625800	1.38617600
H	2.57602300	-3.40497500	2.28500200
H	3.56034800	-4.57817700	1.39762300
H	4.02398100	-2.86786400	1.41653700
C	3.15522800	-3.50560000	-1.14530800
H	3.96617900	-2.77693100	-1.19224700
H	3.58003800	-4.51017000	-1.17092000
H	2.52495800	-3.37324700	-2.02648400
H	1.50168200	-4.00542400	0.11999900
C	-1.97633000	0.91684200	1.50339500
H	-2.13695000	0.98486000	2.58075300
H	-2.92002800	0.66219500	1.02051800
C	-1.47466400	2.23001000	0.96586700
C	-1.80021500	2.61549800	-0.33046500
C	-0.68775700	3.06666100	1.74933000
C	-1.31708000	3.81060200	-0.84576900
H	-2.43864100	1.96751000	-0.92075000
C	-0.20428600	4.26139700	1.23637700
H	-0.44075100	2.77337600	2.76378700
C	-0.51240600	4.63240700	-0.06671900
H	-1.57137200	4.10401000	-1.85757500
H	0.41273200	4.90439500	1.85270100
H	-0.13472300	5.56463800	-0.46961300
O	3.87308700	-0.34233400	-0.74620900
O	-4.04344000	0.30444800	-0.93997800
S	4.18424400	1.14055200	-0.95701300
C	2.86840400	1.79580200	-1.99843600
H	3.01368500	2.87062600	-2.10485700
H	2.96374100	1.31523500	-2.97028600
H	1.90856900	1.56633500	-1.54065100
C	3.74306400	1.97787500	0.57576200
H	3.87068000	3.05096100	0.43495400
H	2.71434100	1.72956500	0.82789500
H	4.43097200	1.62388800	1.34125900
S	-4.12784200	-1.01744100	-1.69175700
C	-4.60573900	-2.25950000	-0.47556200
H	-5.63893800	-2.05470500	-0.20119500
H	-4.53612900	-3.24726400	-0.93033400
H	-3.95902800	-2.17766500	0.39788600
C	-2.43041100	-1.56570500	-1.95426500
H	-1.91207300	-1.63043900	-1.00003300
H	-2.44238700	-2.53418700	-2.45306000
H	-1.95199100	-0.82693300	-2.59438900

TS_Bz$_2$MAM_2MET (methanol)

C	0.06195900	1.50994100	-0.45833300
C	1.45920300	1.68785000	-0.15205300
C	2.01668100	0.45838500	0.00684400
C	0.93040400	-0.57569900	-0.22887600
N	-0.24634600	0.11463200	-0.35911500
O	-0.75974100	2.34590800	-0.77827100
O	1.09288800	-1.77155000	-0.32011200
N	3.24292600	0.05889700	0.29772300
H	3.44677700	-0.94415200	0.30373100
C	4.35948600	0.98559000	0.47184200
H	1.91493000	2.66292000	-0.11920100
C	4.91024200	1.43042600	-0.88038200

H	4.12795800	1.87873600	-1.49472400
H	5.70147500	2.16940000	-0.74214600
H	5.32534800	0.57550700	-1.41908100
C	5.41847100	0.31738600	1.33480000
H	5.80137400	-0.58153100	0.84486200
H	6.25503000	0.99752500	1.49724200
H	5.00856800	0.03321600	2.30509200
H	3.96766600	1.85860900	1.00183700
C	-1.52308500	-0.50043200	-0.74955800
C	-1.73380300	-1.85151100	-0.08206100
C	-1.50352600	-2.04591900	1.27665400
C	-2.25116600	-2.89613200	-0.83574400
C	-1.78384700	-3.26700700	1.86750500
H	-1.08738000	-1.24677600	1.87734900
C	-2.53866700	-4.11981300	-0.24417500
H	-2.42952800	-2.75542000	-1.89570400
C	-2.30539900	-4.30910200	1.10946400
H	-1.59258200	-3.40767800	2.92446700
H	-2.94048800	-4.92618900	-0.84567400
H	-2.52441200	-5.26320800	1.57299900
C	-2.71771200	0.38506500	-0.43009200
C	-3.67990300	0.59513700	-1.40724100
C	-2.91277800	0.92069500	0.83978400
C	-4.82349400	1.33332100	-1.12600300
H	-3.53416100	0.18509000	-2.39998600
C	-4.04741900	1.66244200	1.12062600
H	-2.16779100	0.77335900	1.61148500
C	-5.00955600	1.87067500	0.13793100
H	-5.56489200	1.49136200	-1.89990800
H	-4.18331500	2.08169800	2.11027200
H	-5.89729300	2.45042700	0.35944600
H	-1.50405700	-0.65895800	-1.82990400
O	3.64775300	-2.78175400	0.00596200
H	2.68203300	-2.73252700	-0.06829000
C	4.17539700	-2.92635800	-1.30764500
H	3.87236400	-2.09961600	-1.95852900
H	5.26176000	-2.92586800	-1.22757700
H	3.85911600	-3.86877900	-1.76278700
O	0.46388600	4.77935300	-0.23303200
C	0.10442900	4.92310800	1.12878400
H	-0.97609800	5.05112600	1.25879100
H	0.42417800	4.06390200	1.73078500
H	0.60218800	5.81278400	1.51616300
H	-0.01860700	4.00639600	-0.57008200

TS_Bz$_2$MAM_2DMSO (dimethyl sulfoxide)

C	0.71076000	-1.52923100	1.28817300
C	-0.61885900	-1.69384000	1.83084700
C	-1.35287300	-0.60242900	1.48779200
C	-0.44637200	0.34273400	0.73057800
N	0.81809100	-0.19256700	0.77864000
O	1.59782300	-2.35069400	1.20719000
O	-0.80498400	1.36130200	0.19229400
N	-2.61226000	-0.25020400	1.67867800
H	-2.99033700	0.55030300	1.15132000
C	-3.58020400	-1.12137800	2.33846100
H	-0.93058600	-2.59816700	2.32594100
C	-4.17577600	-2.12084600	1.34973000
H	-3.39222000	-2.71135400	0.87302700
H	-4.85632200	-2.80458600	1.86072500
H	-4.73374300	-1.59310700	0.57345100
C	-4.64862500	-0.26462400	3.00203900
H	-5.15851500	0.34312000	2.25236300
H	-5.38386100	-0.89711700	3.50174000
H	-4.20399800	0.40209500	3.74284700
H	-3.03535800	-1.67014400	3.11161300
C	1.88318200	0.29141900	-0.10493800
C	1.99516900	1.80823500	-0.06626100
C	1.93482300	2.52182500	1.12643700
C	2.23908300	2.49264000	-1.24981400
C	2.11138100	3.89647600	1.13226000
H	1.72833900	2.00375100	2.05475900
C	2.42038400	3.86977900	-1.24677600
H	2.28052500	1.94477800	-2.18446100
C	2.35663900	4.57676200	-0.05483100
H	2.05346400	4.44100200	2.06720500
H	2.60540900	4.38996900	-2.17901200
H	2.49259600	5.65139800	-0.04932800

C	3.24693900	-0.29137000	0.22307100
C	4.03039500	-0.78680700	-0.80972100
C	3.77323200	-0.25505700	1.51155100
C	5.31776700	-1.25078900	-0.56422700
H	3.63188400	-0.81340800	-1.81716400
C	5.05265200	-0.72089800	1.76087400
H	3.17346400	0.12528500	2.32892800
C	5.83183400	-1.22159200	0.72246300
H	5.91491000	-1.63762300	-1.38130400
H	5.44669100	-0.69525700	2.76986600
H	6.83314600	-1.58506800	0.91918600
H	1.61149300	-0.00686700	-1.11871000
O	-4.19340600	1.53401300	0.23530000
O	-0.35535600	-1.06716900	-1.83180800
S	-4.19004300	1.74082000	-1.28090200
S	-0.36926100	-2.46245000	-2.44329000
C	-3.36794100	0.30974900	-2.00135200
H	-3.98550800	-0.55783600	-1.77487400
H	-3.32855000	0.45190500	-3.08151400
H	-2.36499100	0.18286900	-1.59589200
C	-2.91723700	2.96764500	-1.62643500
H	-2.81787300	3.06778900	-2.70707900
H	-3.25872600	3.90950000	-1.20105100
H	-1.98575200	2.64761300	-1.16472600
C	-1.34613100	-3.48525400	-1.32647600
H	-0.96835000	-3.36543200	-0.31248700
H	-2.37306300	-3.13082700	-1.38891700
H	-1.29277800	-4.52363100	-1.65147600
C	1.24457100	-3.18840100	-2.09390500
H	1.22916600	-4.23771300	-2.38761100
H	1.97322600	-2.65155300	-2.69814100
H	1.47287900	-3.07429700	-1.03441800

TS_Bz$_3$MAM_2MET (methanol)

C	0.22117000	1.60200600	0.65639400
C	1.58780200	2.03312100	0.54875400
C	2.33001400	0.96849700	0.15410700
C	1.39177900	-0.21316700	-0.00347400
N	0.10263300	0.27434800	0.09895100
O	-0.69714200	2.18971000	1.18797600
O	1.76941100	-1.35576300	-0.11388500
N	3.62686300	0.79187700	-0.02841500
H	3.96381600	-0.12756500	-0.32465600
C	4.60613900	1.86478700	0.13585900
C	4.63292000	2.76800200	-1.09403000
H	3.64317400	3.17619200	-1.30430300
H	5.31929100	3.60168500	-0.93543900
H	4.96726700	2.20552900	-1.96865400
C	5.96506500	1.24688000	0.42690000
H	6.28571700	0.61535500	-0.40553100
H	6.71092500	2.02987200	0.56567000
H	5.93221200	0.63686300	1.33080700
H	4.29205600	2.45342100	1.00316200
C	-1.18037500	-0.51530800	-0.00753000
C	-0.84286600	-1.88277800	-0.63439900
C	-1.19048700	-3.07688600	-0.02434200
C	-0.21845700	-1.93252000	-1.88351900
C	-0.91447900	-4.29641300	-0.63878100
H	-1.67715200	-3.07612300	0.94001900
C	0.05865100	-3.13832900	-2.49561100
H	0.05464400	-1.01050600	-2.38238000
C	-0.28872700	-4.33321400	-1.87121500
H	-1.19323700	-5.21718700	-0.14088900
H	0.54771900	-3.14995800	-3.46197800
H	-0.07254300	-5.28138700	-2.34829800
C	-2.22424000	0.19971500	-0.92832300
C	-2.76970500	1.43900700	-0.58242500
C	-2.74671600	-0.41844500	-2.06606100
C	-3.72610500	2.06099500	-1.36840600
H	-2.45204800	1.92751400	0.31865100
C	-3.71561200	0.19628500	-2.85089800
H	-2.42227000	-1.40309200	-2.35787600
C	-4.20298000	1.44775900	-2.51728600
H	-4.09881300	3.03174400	-1.06442800
H	-4.08910300	-0.32117100	-3.72633900
H	-4.95342300	1.93042300	-3.13164500
C	-1.75287200	-0.70423500	1.40336900
C	-0.90179800	-0.83680600	2.49660400

C	-3.12165000	-0.84700400	1.60638800
C	-1.40474400	-1.09019900	3.76350500
H	0.16890600	-0.74971600	2.36739500
C	-3.62813300	-1.10376500	2.87342900
H	-3.80304500	-0.76265000	0.77105300
C	-2.77271700	-1.22281200	3.95840500
H	-0.72351700	-1.18434800	4.60039200
H	-4.69769200	-1.20869000	3.00923200
H	-3.16760800	-1.41813100	4.94785600
O	4.42970900	-1.93868300	-0.59413200
H	3.46559000	-2.03151600	-0.57113600
C	4.93599300	-2.43749400	0.63849600
H	6.01174100	-2.26675900	0.64595600
H	4.49331300	-1.92003100	1.49579100
H	4.75173900	-3.51051300	0.73975900
O	-1.93355800	4.59370400	0.54003800
H	-1.46891500	3.84331500	0.93600500
C	-1.28862200	4.87277900	-0.68917200
H	-1.35590300	4.03120700	-1.38772100
H	-1.78812700	5.73055700	-1.14103500
H	-0.23103500	5.12650300	-0.55171300
H	1.90301100	3.02110700	0.83812000

TS_Bz$_3$MAM_2DMSO (dimethyl sulfoxide)

C	-0.84225000	1.26740200	0.51011700
C	0.04993400	2.39495700	0.53326000
C	1.32245800	1.92436100	0.47241700
C	1.25254100	0.41419700	0.39180700
N	-0.07740200	0.07156500	0.21430000
O	-2.02865900	1.26333400	0.75378700
O	2.22390900	-0.28665000	0.53157000
N	2.51369100	2.48629000	0.53699800
H	3.35626900	1.90244800	0.42916200
C	2.71039900	3.93146200	0.60918800
C	2.83550000	4.52104700	-0.79332000
H	1.95418800	4.28733200	-1.39335500
H	2.94005100	5.60663400	-0.74436200
H	3.71462100	4.11070500	-1.29504400
C	3.92926000	4.22922600	1.47147200
H	4.81594400	3.75809500	1.04397400
H	4.09478200	5.30605600	1.53004300
H	3.78971200	3.84456800	2.48324100
H	1.82483400	4.35051800	1.09334300
C	-0.64202600	-1.32380300	0.12862100
C	0.53287900	-2.28462400	-0.14649100
C	0.82464000	-3.35380700	0.68406200
C	1.30946400	-2.10543400	-1.29437300
C	1.87357100	-4.22152400	0.38553300
H	0.24385800	-3.52331300	1.57904800
C	2.34698700	-2.96372200	-1.59630600
H	1.09558100	-1.27617000	-1.95789300
C	2.63745500	-4.03117800	-0.75113700
H	2.08551500	-5.04817000	1.05282400
H	2.93489200	-2.80269500	-2.49155100
H	3.45275000	-4.70545300	-0.98364200
C	-1.67888000	-1.47238100	-1.03431300
C	-2.87840000	-0.75437600	-1.03835200
C	-1.51743400	-2.42506300	-2.04321400
C	-3.82977000	-0.92393500	-2.03231200
H	-3.09221500	-0.05500700	-0.25117900
C	-2.47147100	-2.60429700	-3.03850700
H	-0.65085700	-3.06426900	-2.06711700
C	-3.62897200	-1.84563400	-3.04929100
H	-4.73004000	-0.32453600	-1.97266200
H	-2.29952900	-3.35339700	-3.80235300
H	-4.37137300	-1.98372500	-3.82656800
C	-1.30607100	-1.66658700	1.46975500
C	-0.81365900	-1.13898200	2.65977800
C	-2.35003900	-2.58423800	1.53376500
C	-1.35823900	-1.50628300	3.88112300
H	0.00825900	-0.43556400	2.64604400
C	-2.89524000	-2.95673200	2.75494900
H	-2.74255000	-3.01752500	0.62410700
C	-2.40461200	-2.41665500	3.93451200
H	-0.96186600	-1.07765300	4.79360600
H	-3.70946200	-3.67082900	2.78033400
H	-2.83312000	-2.70222300	4.88740500
O	5.07969900	1.46842900	0.13472100

S	5.64352500	0.32264900	-0.70712300
C	5.30349300	-1.19690900	0.19896700
H	4.24326500	-1.24006300	0.43723900
H	5.60732100	-2.04233700	-0.41774600
H	5.90704300	-1.16726600	1.10414700
C	4.48184600	0.07897700	-2.06121300
H	4.81203700	-0.77057000	-2.65799500
H	3.48991400	-0.09371300	-1.65021900
H	4.50068600	0.98375200	-2.66552100
O	-5.61677700	1.30845800	-0.53784800
S	-5.34176400	2.80093600	-0.64564200
C	-4.62696300	3.30576800	0.93193000
H	-3.75725300	2.68409600	1.14075600
H	-4.35405300	4.35944400	0.87176500
H	-5.39797800	3.16993700	1.68821200
C	-3.84941200	2.98089000	-1.64295800
H	-3.56850800	4.03351900	-1.66954800
H	-3.05868200	2.37348300	-1.20679200
H	-4.08840600	2.63743100	-2.64754900
H	-0.30515200	3.40278600	0.66635600

TS_Bz$_3$MAM_2MET (methanol)

C	-0.36154100	-1.15928400	0.40099700
C	-1.79933700	-1.09432400	0.24728800
C	-2.15744300	0.18734000	-0.02193200
C	-0.86543900	0.99417100	-0.02872400
N	0.19310800	0.10431000	0.01624300
O	0.27879500	-2.08435700	0.84242300
O	-0.85117000	2.19871500	-0.00619200
N	-3.28553300	0.84654500	-0.20875900
H	-3.21437200	1.84874000	-0.40695700
C	-4.62656000	0.25984100	-0.29893200
C	-4.85890300	-0.33053500	-1.68615100
H	-4.10798400	-1.08593700	-1.92144200
H	-5.84259200	-0.80126400	-1.73368500
H	-4.81249800	0.45307300	-2.44587500
C	-5.64297400	1.33750800	0.04668500
H	-5.57109100	2.17324400	-0.65355100
H	-6.65229800	0.92948500	-0.01109300
H	-5.48111100	1.71783500	1.05625900
H	-4.68863900	-0.53510600	0.44346000
C	1.67106600	0.43525200	0.00921900
C	1.82019000	1.90795400	-0.41951400
C	2.49980400	2.83237100	0.35688900
C	1.30716000	2.32340700	-1.65112600
C	2.65858800	4.14624300	-0.07819500
H	2.91232700	2.54449400	1.31276500
C	1.46087800	3.62443900	-2.08581000
H	0.77875100	1.61514200	-2.27779800
C	2.14017000	4.54769000	-1.29551600
H	3.19140800	4.85214100	0.54721900
H	1.05010900	3.92274300	-3.04256200
H	2.26272200	5.56955500	-1.63331000
C	2.45504400	-0.45730800	-1.00792900
C	2.54357100	-1.84240600	-0.84348800
C	3.20266600	0.09906100	-2.04769400
C	3.27524200	-2.63514000	-1.71274500
H	2.04585000	-2.31788700	-0.02020000
C	3.94752900	-0.69159000	-2.91499000
H	3.23612400	1.16544900	-2.19488800
C	3.97867800	-2.06676200	-2.76409300
H	3.29449700	-3.70592300	-1.54936300
H	4.50984100	-0.21510000	-3.70894200
H	4.55445800	-2.68427000	-3.44280300
C	2.21710200	0.23455900	1.42869700
C	1.41592200	0.49191300	2.53727300
C	3.54827800	-0.11152600	1.63684500
C	1.92612700	0.39071700	3.82245400
H	0.38132200	0.78169700	2.40890600
C	4.06288700	-0.20978600	2.92250800
H	4.19491500	-0.30275500	0.79157500
C	3.25348800	0.03672500	4.02120300
H	1.28235600	0.59005700	4.67039900
H	5.10178600	-0.48291700	3.06178400
H	3.65293000	-0.04513000	5.02458700
Br	-2.83301800	-2.62931800	0.56347000
O	-3.09576000	3.73844200	-0.55395100
H	-2.15080100	3.53637400	-0.52186300

C	-3.45577500	4.28966000	0.70825400
H	-4.53233700	4.45368400	0.69943100
H	-3.21100400	3.60860300	1.52948400
H	-2.95724300	5.24719200	0.88068500
O	0.74150000	-4.68830800	-0.05690400
H	0.46121000	-3.88215700	0.39664000
C	0.14313300	-4.67768100	-1.34071000
H	0.46021800	-3.81224800	-1.93325600
H	0.46044200	-5.58125600	-1.86245400
H	-0.95091100	-4.67838500	-1.28458600

TS_Bz$_3$MAM_2DMSO (dimethyl sulfoxide)

C	-0.88835900	0.79085500	0.37220900
C	-0.10421300	2.00364400	0.28629900
C	1.21513300	1.68038400	0.21278900
C	1.27625800	0.16038200	0.25191900
N	-0.01375600	-0.32714100	0.13469500
O	-2.05895500	0.70171600	0.65250300
O	2.31334000	-0.42639000	0.41835000
N	2.37131000	2.30564300	0.16730300
H	3.23035500	1.73263400	0.16767100
C	2.59980200	3.75117700	0.12023100
C	3.27130300	4.10974400	-1.20112900
H	2.64111200	3.82284200	-2.04477800
H	3.45143800	5.18507800	-1.25398500
H	4.22698700	3.58943900	-1.28590900
C	3.43764700	4.16628000	1.32385000
H	4.39682400	3.64528200	1.30813600
H	3.62315800	5.24167700	1.30212800
H	2.92330000	3.92255600	2.25497400
H	1.63050900	4.24074900	0.17223400
C	-0.43350900	-1.77891300	0.15431000
C	0.82976500	-2.62781600	-0.09227200
C	1.24547800	-3.60651600	0.79491900
C	1.55989600	-2.44466500	-1.26976800
C	2.37124900	-4.38143100	0.52233100
H	0.70327300	-3.77580600	1.71382900
C	2.67359300	-3.21164000	-1.54524900
H	1.24951100	-1.68632100	-1.97862700
C	3.08811300	-4.18836300	-0.64398300
H	2.68016500	-5.13807900	1.23330100
H	3.22401100	-3.04943500	-2.46378300
H	3.96315500	-4.79063400	-0.85593900
C	-1.47051900	-2.10600500	-0.96928600
C	-2.72991300	-1.50063700	-1.00248100
C	-1.23652100	-3.11579600	-1.90569300
C	-3.67488400	-1.82957800	-1.96204200
H	-2.99714400	-0.76765400	-0.26390900
C	-2.18404000	-3.45682100	-2.86389000
H	-0.31503400	-3.67338200	-1.89793800
C	-3.40498800	-2.80632300	-2.90923100
H	-4.62314900	-1.30678600	-1.93209800
H	-1.95572700	-4.24508000	-3.57140300
H	-4.14200500	-3.06924000	-3.65886400
C	-1.02972700	-2.09341000	1.53296100
C	-0.55662000	-1.44968700	2.67285400
C	-1.98609000	-3.09247000	1.68405500
C	-1.03662100	-1.78398000	3.93006000
H	0.20045300	-0.68084800	2.59255100
C	-2.46579900	-3.43203300	2.94185300
H	-2.36105500	-3.61553400	0.81516700
C	-1.99645400	-2.77678700	4.07041200
H	-0.65757400	-1.26520500	4.80212800
H	-3.21226900	-4.21140100	3.03566700
H	-2.37448000	-3.03698000	5.05148600
Br	-0.96281000	3.66904200	0.44085400
O	5.01128300	1.42444900	0.10902800
S	5.71391500	0.29366300	-0.64511900
C	5.42190800	-1.21456400	0.29656800
H	4.35387000	-1.33483400	0.45993500
H	5.83580500	-2.05464400	-0.26054200
H	5.95146200	-1.10429900	1.24101400
C	4.66695800	-0.07960900	-2.06226500
H	5.08752700	-0.92987900	-2.59784200
H	3.66093000	-0.29786300	-1.71100900
H	4.67238300	0.79952500	-2.70370100
O	-5.67363400	0.37598300	-0.73812800
S	-5.50388400	1.87956600	-0.90041800

C	-4.87210000	2.49548200	0.67256300
H	-3.96599300	1.95010600	0.93179000
H	-4.67096600	3.56237800	0.57676200
H	-5.65406500	2.33422600	1.41250800

C	-4.00426100	2.12672900	-1.87092500
H	-3.79019100	3.19362900	-1.92617800
H	-3.18537300	1.58891800	-1.39803000
H	-4.19740500	1.73535300	-2.86783600

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