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Supplementary Material

Crystal Structures of the Amide and Iminol Tautomers O-(3,5-dinitrobenzoyloxy)benzohydroxamate. A case of a disappearing solvate?

Abigail L. Albright,[A] *Lucy Collins*,[A] *John Li*,[A] *Benjamin Harris*,[A] and *Jonathan M. White*[A,B]

[A]School of Chemistry, Bio21 Institute, The University of Melbourne, Parkville 3010, Australia.
[B]Corresponding author. Email: whitejm@unimelb.edu.au

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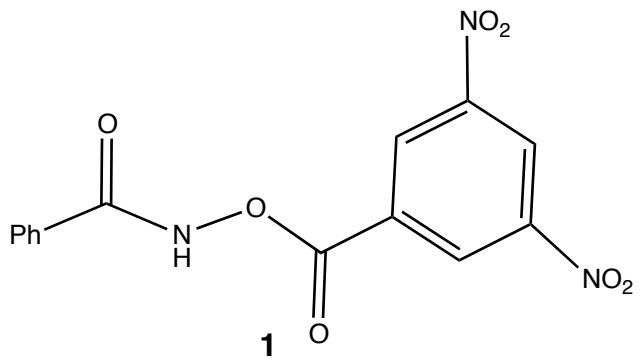
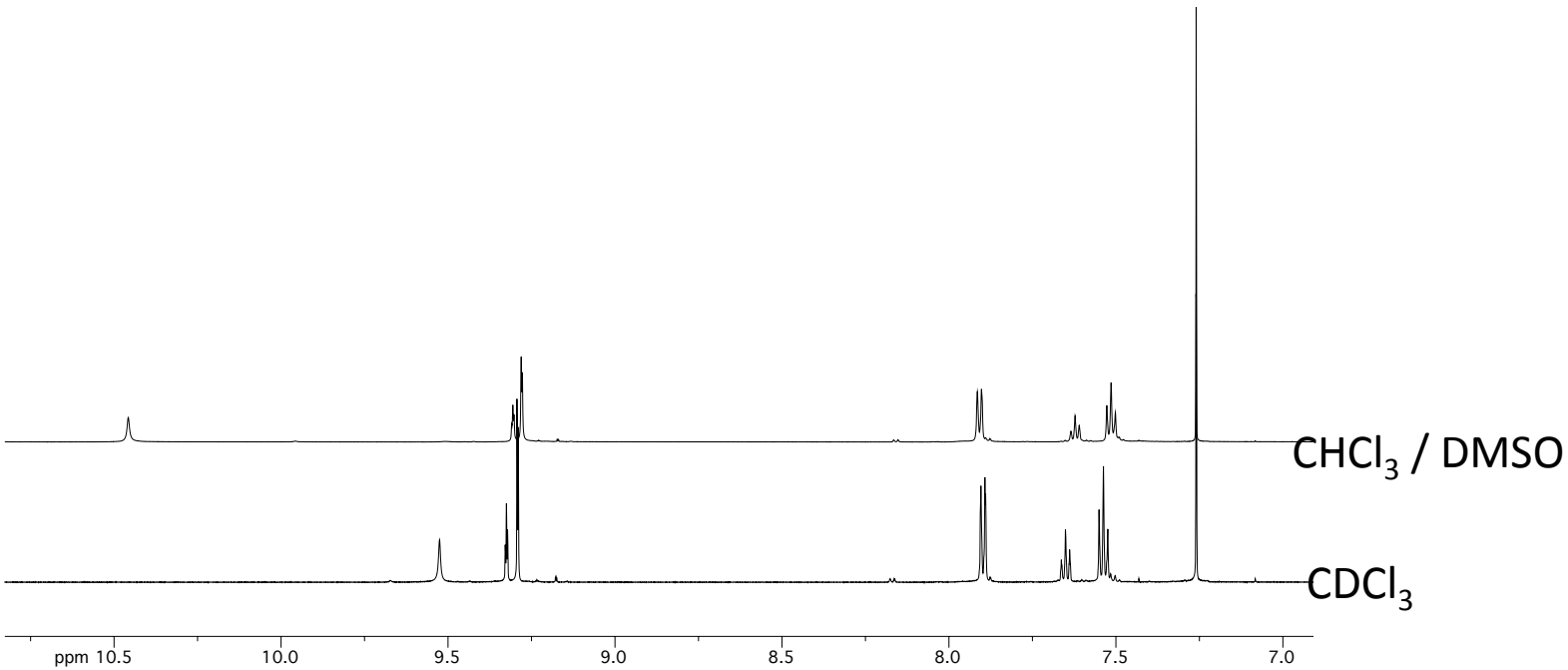
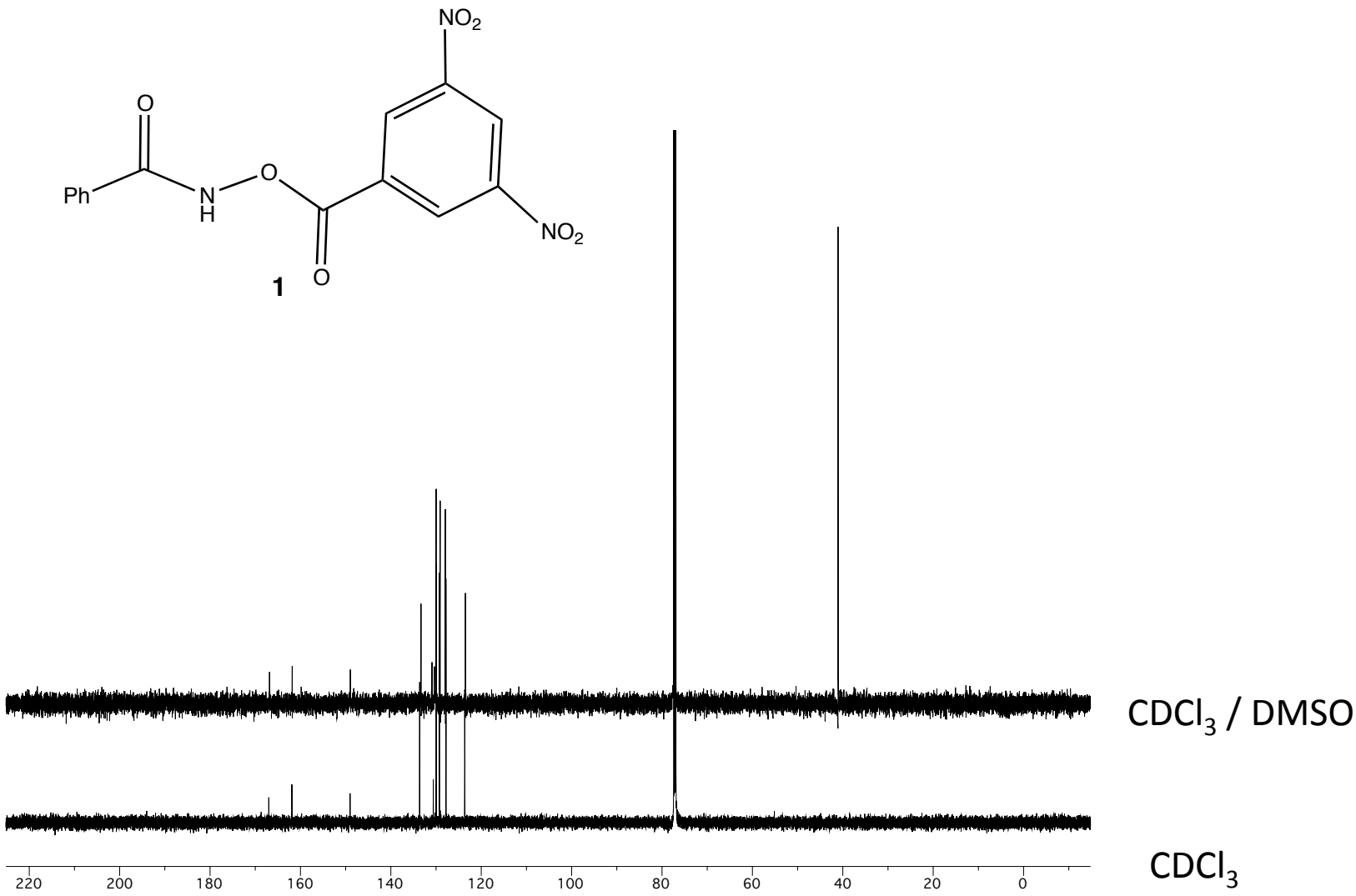
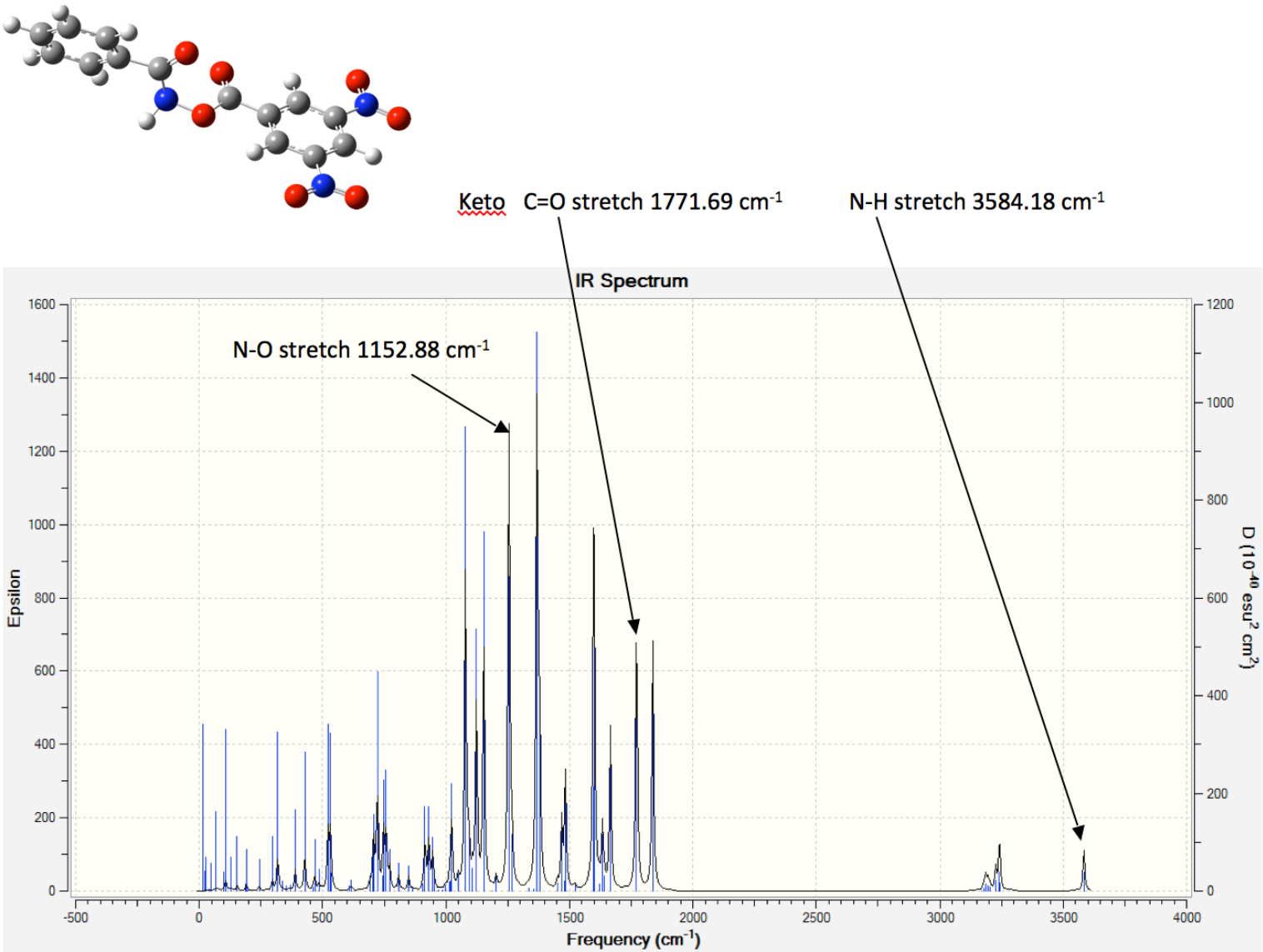




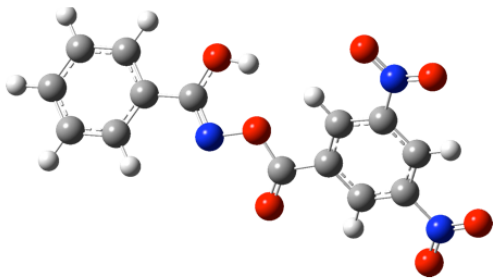
SUPP_Figure 1. ^{1}H NMR spectrum of **1** in $CDCl_3$ with added DMSO (~ 2.5 eq.)

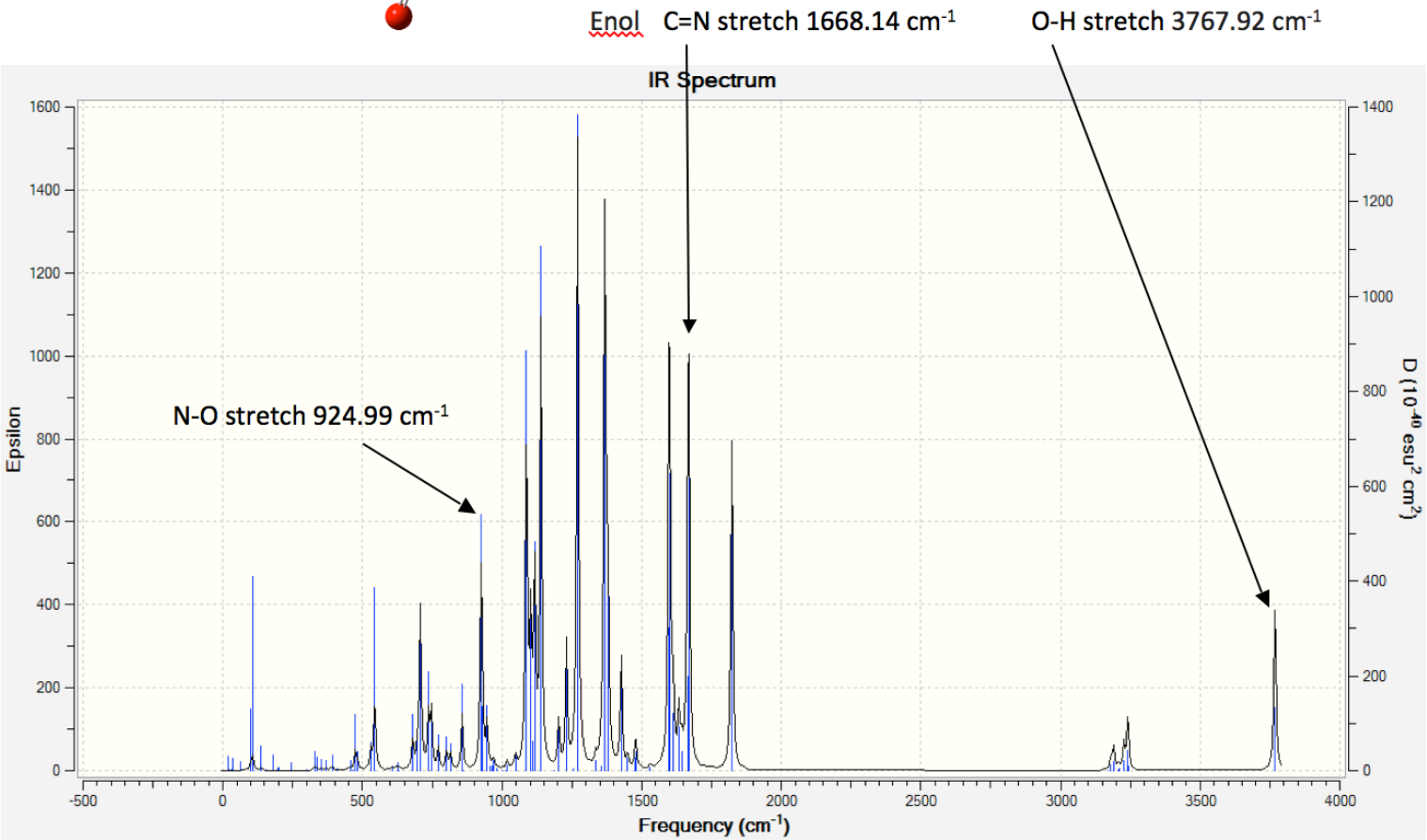


SUPP_Figure 2. ^{13}C NMR spectrum of **1** in $CDCl_3$ with added DMSO (~ 2.5 eq.)



SUPP_Figure 3. Computed IR spectrum of the amide tautomer of 1

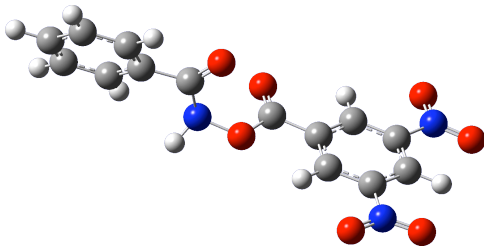




SUPP_Figure 4. Computed IR spectrum of the iminol tautomer of 1

ZPE -1229.623606 a.u. 9.88 kJ/mol more stable than the enol

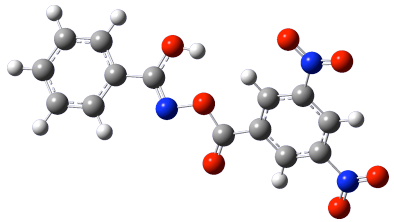
Symbol	X	Y	Z
O	2.3342720	0.1660780	1.4273780
O	0.8273510	0.2844650	-0.7444140
O	0.4189140	-1.9286200	-0.3753880
O	-4.2979100	-3.2136000	0.3003880
O	-5.8431380	-1.6966110	0.4676840
O	-4.6967570	2.9729650	0.0634950
O	-2.6405980	3.5562490	-0.3205250
N	2.1926520	-0.0327930	-0.8469720
N	-4.6865010	-2.0559230	0.3071410
N	-3.5149670	2.7260970	-0.1214160
C	4.3841480	0.0115100	0.1942360
C	4.9976910	-0.6038120	-0.9045730
C	6.3868130	-0.6312480	-1.0002380
C	7.1676080	-0.0458680	-0.0049790
C	6.5590030	0.5580740	1.0959430
C	5.1728620	0.5816200	1.2003070
C	2.9007080	0.0735480	0.3623020
C	0.0336800	-0.8005490	-0.4573090
C	-1.3845790	-0.3612750	-0.2725480
C	-2.3403260	-1.3606450	-0.0744300
C	-3.6668420	-0.9940700	0.1011380
C	-4.0822300	0.3307080	0.0918000
C	-3.1065190	1.2973490	-0.1054160
C	-1.7655740	0.9824230	-0.2860860
H	4.3979470	-1.0958980	-1.6612730
H	6.8585460	-1.1198180	-1.8448930
H	8.2487430	-0.0685750	-0.0819090
H	7.1659140	1.0062200	1.8741020
H	4.6840750	1.0347330	2.0539850
H	-2.0480300	-2.4018180	-0.0566780
H	-5.1196740	0.5969360	0.2333370
H	-1.0428020	1.7723480	-0.4270880
H	2.5612460	0.4602150	-1.6506680



SUPP Table 1. B3LYP 631-G** Minimised geometry of amide tautomer of 1

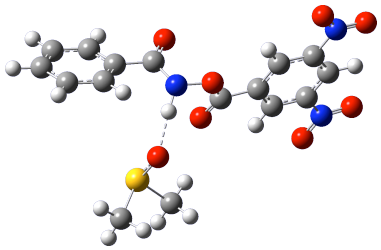
ZPE -1229.619843 a.u. 9.88 kJ/mol less stable than the keto

Symbol	X	Y	Z
O	2.6678840	1.3641710	0.9520850
O	0.8578050	-0.0978950	-0.0598440
O	0.1599560	-2.2533030	-0.2965770
O	-2.3425310	3.4941830	-0.4054790
O	-4.4757580	3.1083050	-0.2778490
O	-6.0686930	-1.4114460	0.3207870
O	-4.6576480	-3.0615160	0.3774110
N	2.1974650	-0.5553320	-0.2975460
N	-3.3081450	2.7521360	-0.2959770
N	-4.9401660	-1.8776220	0.2813320
C	4.4717450	0.0600830	0.0964580
C	4.9540160	-1.0426510	-0.6236810
C	6.3226070	-1.2407750	-0.7521140
C	7.2214860	-0.3458620	-0.1681800
C	6.7449810	0.7500920	0.5472300
C	5.3743350	0.9561860	0.6815430
C	3.0198400	0.2788590	0.2430560
C	-0.0773250	-1.0873350	-0.1744890
C	-1.4610020	-0.5115260	-0.1099760
C	-1.7200480	0.8554790	-0.2262950
C	-3.0365020	1.2966620	-0.1720580
C	-4.1084800	0.4316770	-0.0074830
C	-3.8154960	-0.9212200	0.1022060
C	-2.5185480	-1.4111780	0.0507210
H	1.7018340	1.4005810	0.9985750
H	4.2516190	-1.7333760	-1.0720660
H	6.6906680	-2.0950970	-1.3082700
H	8.2889740	-0.5045950	-0.2711670
H	7.4391510	1.4470380	1.0022630
H	5.0024880	1.8068240	1.2372040
H	-0.9250630	1.5720410	-0.3695940
H	-5.1256190	0.7938640	0.0321440
H	-2.3258940	-2.4724860	0.1303480



SUPP Table 2. B3LYP 631-G** Minimised geometry of iminol tautomer of 1

ZPE	-1782.831968 a.u.	0.71 kJ/mol more stable than the enol	
Keto	N-H	1.03578 Å	
DMSO	O-H	1.75527 Å	
	N-H-O	177.35174°	
Symbol	X	Y	Z
O	1.1694860	-2.1071380	1.2532270
O	0.1020190	-0.8152440	-0.7681980
O	0.1201620	0.9527940	0.6630810
O	-4.2880890	2.8152910	1.8825010
O	-6.1124060	1.7508010	1.3790020
O	-5.8963580	-2.3073360	-1.2205070
O	-3.9761450	-3.0699920	-1.8886830
N	1.5001700	-0.9171720	-0.6717600
N	-4.8987480	1.8899020	1.3679900
N	-4.6772600	-2.2654650	-1.2950940
C	3.4265310	-1.6873050	0.5783210
C	4.2954500	-1.4838440	-0.5007440
C	5.6711950	-1.6044120	-0.3180860
C	6.1869780	-1.9235180	0.9371790
C	5.3231290	-2.1304130	2.0132500
C	3.9487100	-2.0183220	1.8340070
C	1.9353930	-1.5968910	0.4575980
C	-0.4752100	0.1160500	0.0371140
C	-1.9653110	-0.0171460	0.0057290
C	-2.7157570	0.9551020	0.6690080
C	-4.0995320	0.8509690	0.6696210
C	-4.7684020	-0.1898130	0.0398320
C	-3.9914650	-1.1397640	-0.6081070
C	-2.6039960	-1.0793200	-0.6396210
H	3.9032700	-1.2478220	-1.4817350
H	6.3395900	-1.4594170	-1.1593670
H	7.2583680	-2.0189690	1.0750410
H	5.7213950	-2.3838660	2.9891580
H	3.2611380	-2.1883910	2.6532720
H	-2.2255110	1.7735210	1.1775770
H	-5.8464290	-0.2583220	0.0541320
H	-2.0391240	-1.8461660	-1.1494810
H	1.9723660	-0.0525260	-0.9915280
O	2.6999720	1.4425270	-1.5539940
S	3.2123160	2.5240790	-0.5957360
C	1.8438560	3.7131320	-0.3909540
H	1.0649340	3.1839270	0.1561040
H	2.1995300	4.5682010	0.1868990
H	1.4849610	4.0182620	-1.3748300
C	4.3084460	3.5709580	-1.6124380
H	4.6202610	4.4385070	-1.0282890
H	5.1745950	2.9622080	-1.8688030
H	3.7752480	3.8683420	-2.5160000



SUPP Table 3. B3LYP 631-G** Minimised geometry of amide tautomer of 1.DMSO

ZPE	-1782.831696 a.u.	0.71 kJ/mol less stable than the keto	
Enol	O-H	0.99481 Å	
DMSO	O-H	1.68509 Å	
	O-H-O	158.12193°	
Symbol	X	Y	Z
S	0.5256690	3.5754770	0.6053120
O	0.4891580	2.0396860	0.6057930
O	2.6748770	0.6600530	0.0962580
O	0.6277960	-0.9641570	0.0155830
O	-0.2147530	-3.0517550	0.3627480
O	-2.4097370	2.7529170	-0.7924930
O	-4.5193200	2.5323770	-0.3422050
O	-6.3832070	-1.9080860	0.0299580
O	-5.0686020	-3.6094520	0.3316340
N	1.9206200	-1.5663330	-0.0397760
N	-3.3896470	2.0880450	-0.4752600
N	-5.2788880	-2.4209880	0.1443770
C	4.2448440	-1.1118760	-0.1114430
C	4.5505320	-2.4754520	-0.2309430
C	5.8744830	-2.8873700	-0.3202190
C	6.9085120	-1.9495480	-0.2939190
C	6.6095690	-0.5944380	-0.1765560
C	5.2841070	-0.1751800	-0.0846330
C	2.8352450	-0.6566240	-0.0101230
C	-0.3652190	-1.8766940	0.1752560
C	-1.7161690	-1.2250870	0.0674350
C	-1.8907460	0.1468770	-0.1332250
C	-3.1877860	0.6383840	-0.2449150
C	-4.3132220	-0.1689160	-0.1530040
C	-4.0987490	-1.5248630	0.0489770
C	-2.8263770	-2.0687020	0.1583680
C	2.2135090	4.0333140	1.1361770
C	0.6631640	4.0802850	-1.1429200
H	1.7429630	0.9699740	0.2547800
H	3.7447220	-3.1976010	-0.2500340
H	6.1016970	-3.9434750	-0.4106140
H	7.9402610	-2.2754110	-0.3642230
H	7.4077890	0.1389580	-0.1552890
H	5.0493140	0.8764990	0.0091640
H	-1.0452900	0.8239870	-0.1624490
H	-5.3108610	0.2368480	-0.2347320
H	-2.6894950	-3.1304660	0.3119190
H	2.3059530	3.7348610	2.1798330
H	2.3283280	5.1148290	1.0456740
H	2.9430090	3.5007290	0.5256570
H	1.4931570	3.5459190	-1.6064410
H	0.8115980	5.1606950	-1.1858540
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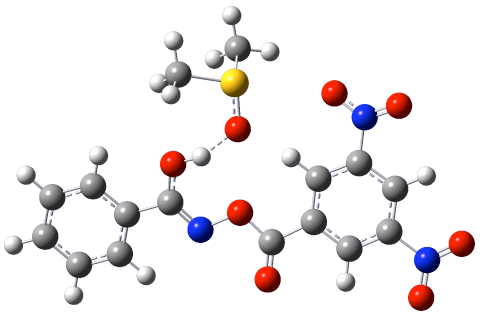

SUPP Table 4. B3LYP 631-G** Minimised geometry of iminol tautomer of **1.**DMSO