Supplementary Information

Experimental Results and Computational Insight into Sequential Reactions of β-(2-aminophenyl)-α,β-Ynones with Aryl Isocyanates/Benzoyl Isothiocyanate

Antonio Arcadi,*[a] Massimiliano Aschi,*[a] Marco Chiarini, [b] Fabio Marinelli, [a] Vincenzo Marsicano,[a] and Gustavo Portalone. [c]

[a] *Dipartimento di Scienze Fisiche e Chimiche Università degli Studi di L'Aquila; Via Vetoio, 67100 Coppito (AQ), Italy*

e-mail: antonio.arcadi@univaq.it; massimiliano.aschi@univaq.it

[b] *Facoltà di Bioscienze e Tecnologie Agro-alimentari e Ambientali, Università di Teramo, Via Balzarini 1, 64100 Teramo (TE), Italy*

[c] *Dipartimento di Chimica, Sapienza Università di Roma, P.le A. Moro 5, 00185 Roma, Italy*

Contents:

Kinetic calculations.

In order to assess whether the proposed mechanism is consistent with the experimental findings we have estimated the kinetics of the two reactions. The Kinetic Master Equation has been constructed using the reported free energy diagrams and adopting the Eyring equation

$$\boldsymbol{k = \frac{k_B T}{h} e^{-\frac{\Delta G^{\#}}{RT}}}$$

for the estimation of the reactions coefficients.

Scheme 1. Master equation based on the kinetic Scheme in Figure S01.

$$\frac{d[R_1]}{dt} = -k_1[R_1][R_2] + k_{-1}[2A]$$

$$\frac{d[R_2]}{dt} = -k_1[R_1][R_2] + k_{-1}[2A]$$

$$\frac{d[2A]}{dt} = k_1[R_1][R_2] - k_{-1}[2A] - k_2[2A][NEt_3]$$

$$\frac{d[3A]}{dt} = k_{-1}[2A] + k_{-N}[N_1^-] + k_{-O}[O_1^-] - (k_N + k_O)[3A]$$

$$\frac{d[N_1^-]}{dt} = k_N[3A] - (k_{-N} + k_d[NEt_3H^+])[N_1^-]$$

$$\frac{d[O_1^-]}{dt} = k_O[3A] - (k_O + k_d[NEt_3H^+])[O_1^-]$$

$$\frac{d[N_1]}{dt} = k_d[NEt_3H^+][N_1^-]$$

$$\frac{d[O_1]}{dt} = k_d[NEt_3H^+][O_1^-] - k_5[O_1][NEt_3]$$

$$\frac{d[O_2^-]}{dt} = k_5([NEt_3][O_1] - [NEt_3H^+][O_2^-])$$

$$\frac{d[O_2]}{dt} = k_5[NEt_3H^+][O_2^-]$$

$$\frac{d[NEt_3]}{dt} = -k_2[2A][NEt_3] + k_d[N_1^-][NEt_3H^+] + k_d[O_1^-][NEt_3H^+]$$

$$\frac{d[NEt_3H^+]}{dt} = k_2[2A] - k_d[NEt_3H^+][N_1^-] - k_d[NEt_3H^+][O_1^-]$$

Scheme 2. Master equation based on the kinetic Scheme in Figure S02.

$$\frac{d[R_1]}{dt} = -k_1[R_1][R_2] + k_{-1}[1B] - k_5[CO_3^-][R_1]$$

$$\frac{d[R_2]}{dt} = -k_1[R_1][R_2] + k_{-1}[1B] - k_6[R_1^-]$$

$$\frac{d[1B]}{dt} = k_1[R_1][R_2] + k_{-3}[3B] - k_{-1}[1B] - k_2[1B] - k_3[1B] - k_d[CO_3^{2-}][1B]$$

$$\frac{d[2B]}{dt} = k_2[1B] - k[2B] - k_d[2B][CO_3^{2-}]$$

$$\frac{d[3B]}{dt} = k_3[1B] - k_{-3}[3B] - k_d[3B][CO_3^{2-}]$$

$$\frac{d[1B^-]}{dt} = k_6[R_1^-][R_2] - k_4[1B^-] + k_{-4}[3B^-] + k[CO_3^-][1B] - k_7[1B^-] + k_{-7}[3B^-]$$

$$\frac{d[3B^-]}{dt} = k_d[CO_3^{2-}][3B] + k_4[1B^-] + k_{-4}[3B^-] - k_d[HCO_3^-][3B^-]$$

$$\frac{d[R_1^-]}{dt} = k_5[R_1][CO_3^{2-}] - k_6[R_1^-][R_2]$$

The Kinetic Schemes and the time course of the relevant species obtained by the integration of the above equations, are reported in the Figure S01 and S02. It is important to note that, as previously commented, in our model we have not addressed the explicit calculation of the free energy barriers related to the bimolecular proton transfer channels involving CO_3^{2-} and NEt_3. This is a very difficult task since, for a fully quantitative estimation of these processes, quantum effects may play a relevant role and – moreover – the presence of the solvent might severely influence the bimolecular rate coefficients for the formation of the primary encounter complexes. In this study, in which we are not explicitly reporting a kinetic assessment of the reaction under study, we have then assumed that all the proton transfer steps are diffusion-controlled and, for this reason, all these steps are kinetically treated using the diffusion rate constant (k_d). This may cause an underestimation of the overall reaction time. It follows that the results presented in this section do not have any quantitative value and their sole purpose is to assess whether the global reaction time predicted by our calculations can be considered as compatible with the times observed in the experiments (order of minutes).

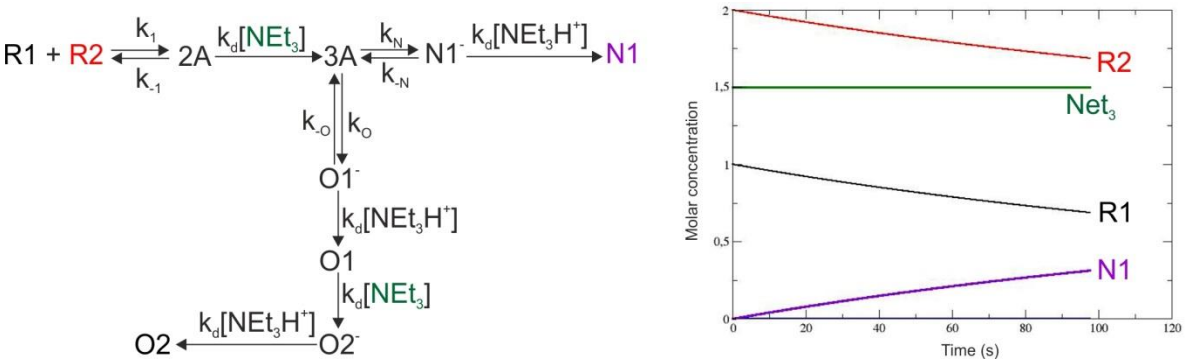

Figure S01. Kinetic model (left side, see Figure 1 of the main text for additional details) and time-course of the relevant species for the Reaction A.

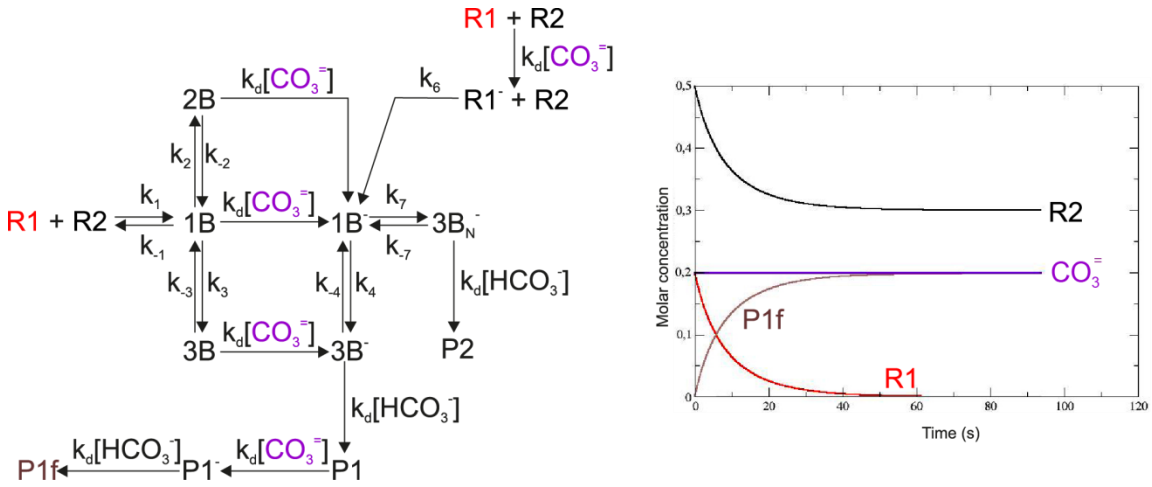

Figure S02. Kinetic model (left side, see Figure 4 for additional details) and time-course of the relevant species for the Reaction B.

The formation of the most stable product (P_{1f}) has been assumed to occur through a sequence of bimolecular proton-transfer steps involving the carbonate-bicarbonate couple. The results reported in the Figures clearly, although qualitatively, demonstrate that the kinetics emerged by our free-energy are in both the reactions are not incompatible with the times necessary for completing the two reactions. As a matter of fact, in both the cases the reaction is completed or reaches rather high values of progress within the minutes time-scale.

Copies of ^{1}H and ^{13}C NMR Spectra:

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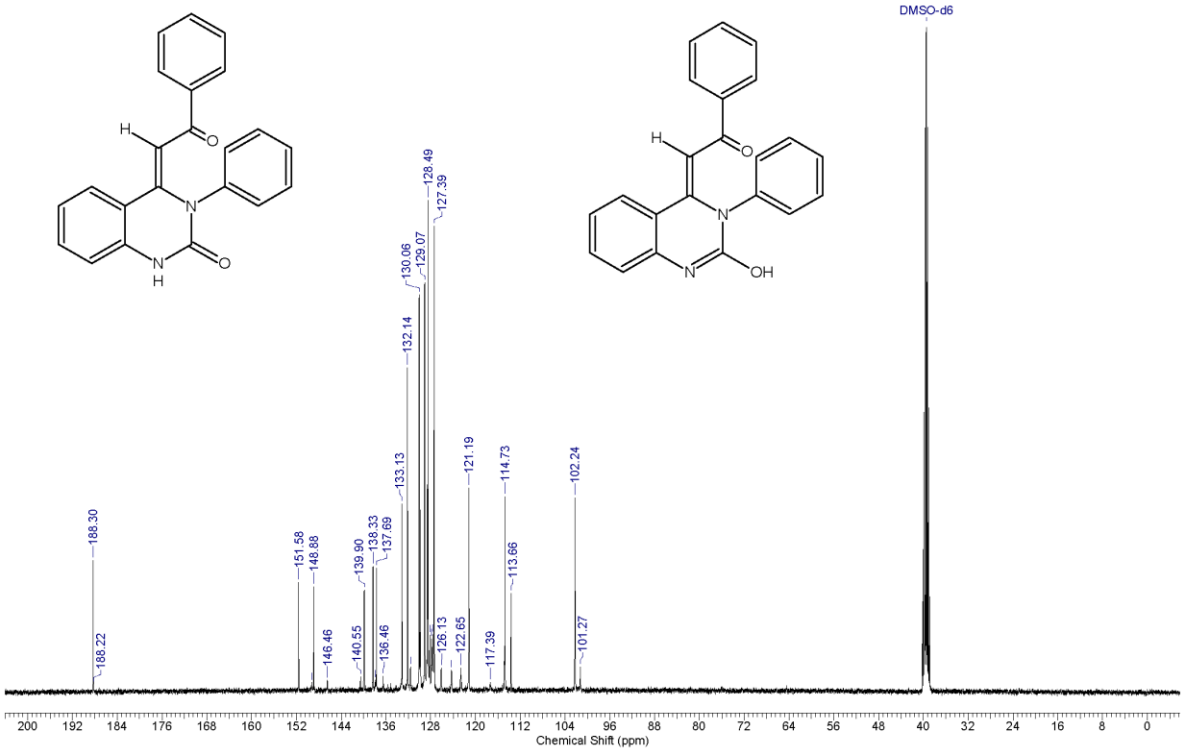

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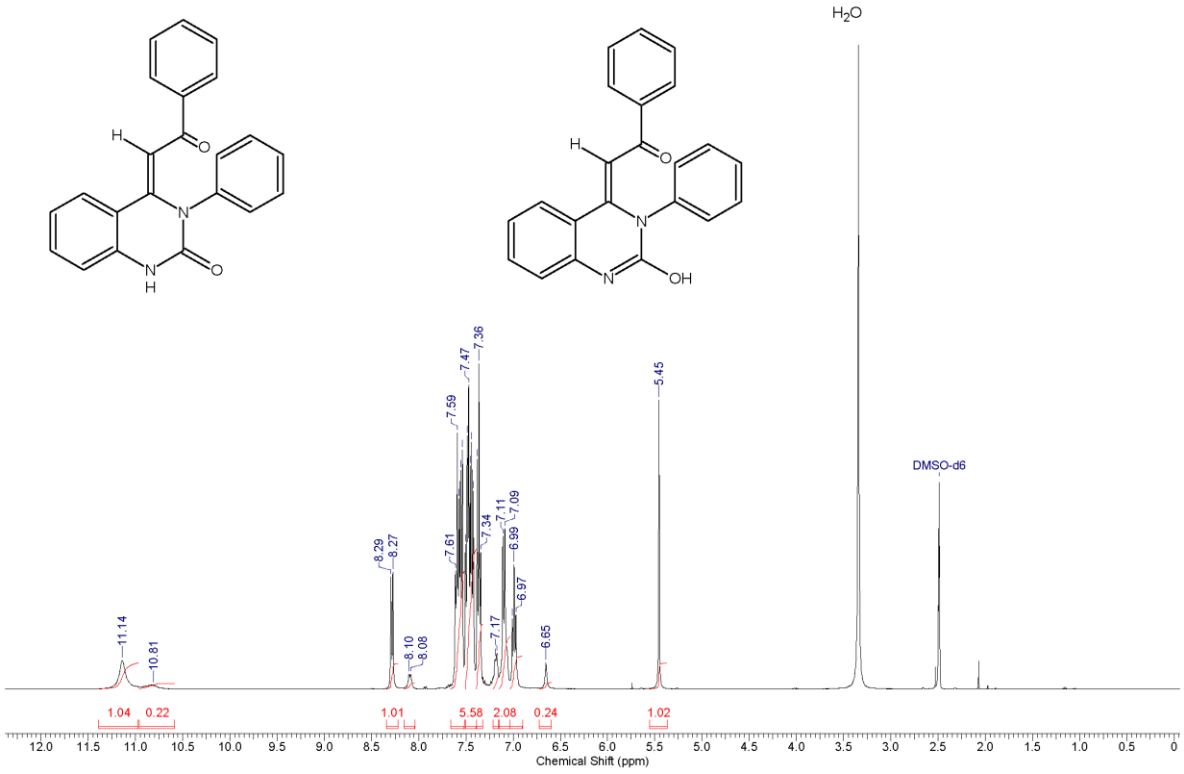

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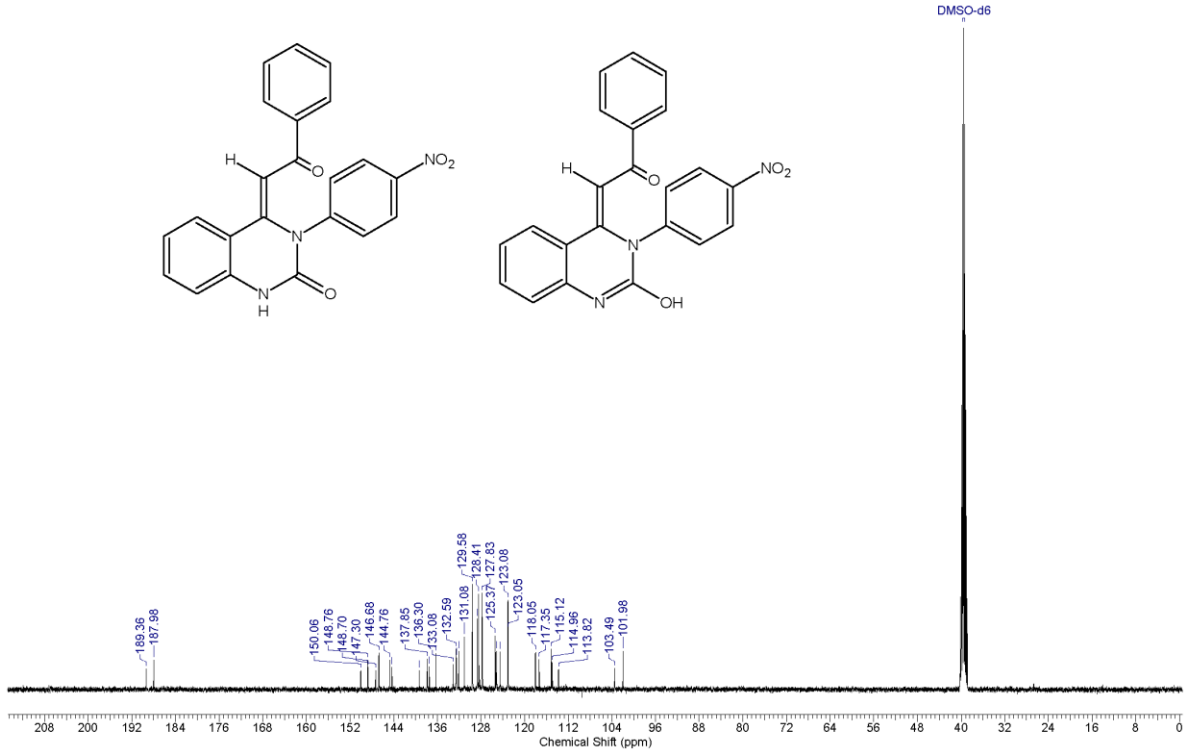
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129.58
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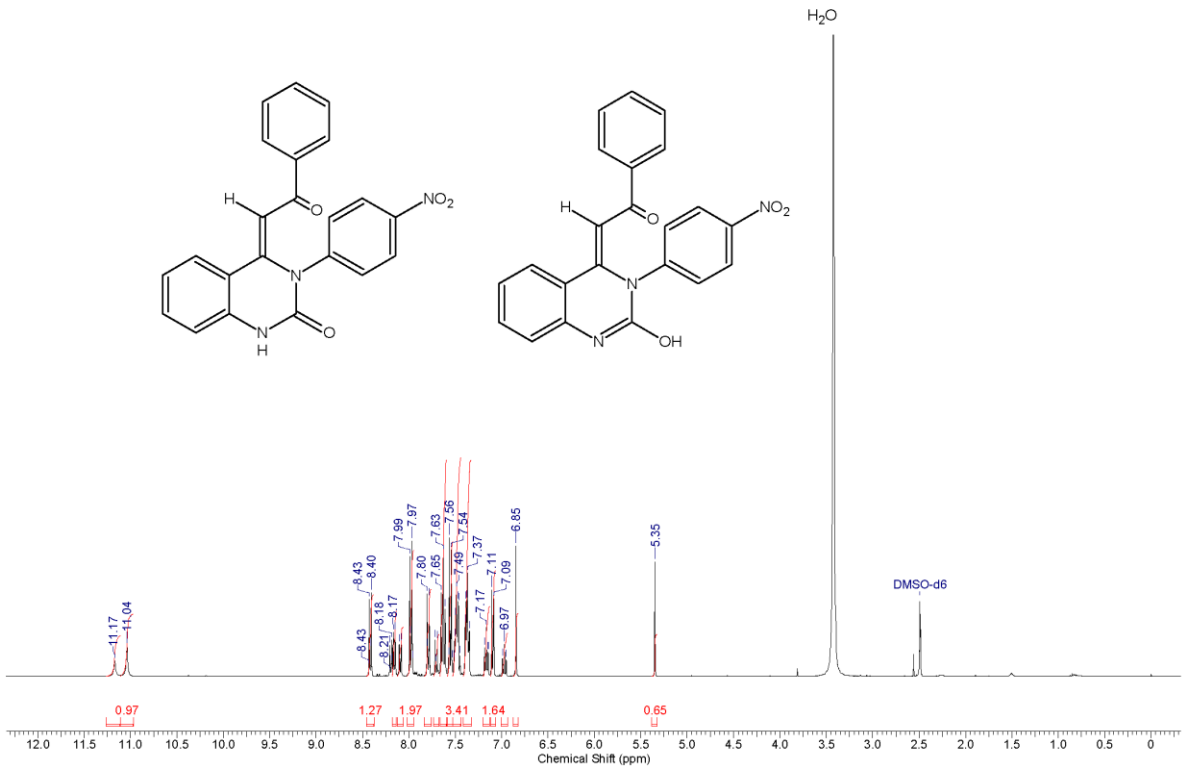
Chemical Shift (ppm)

5ab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7.63
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7.17
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Chemical Shift (ppm)

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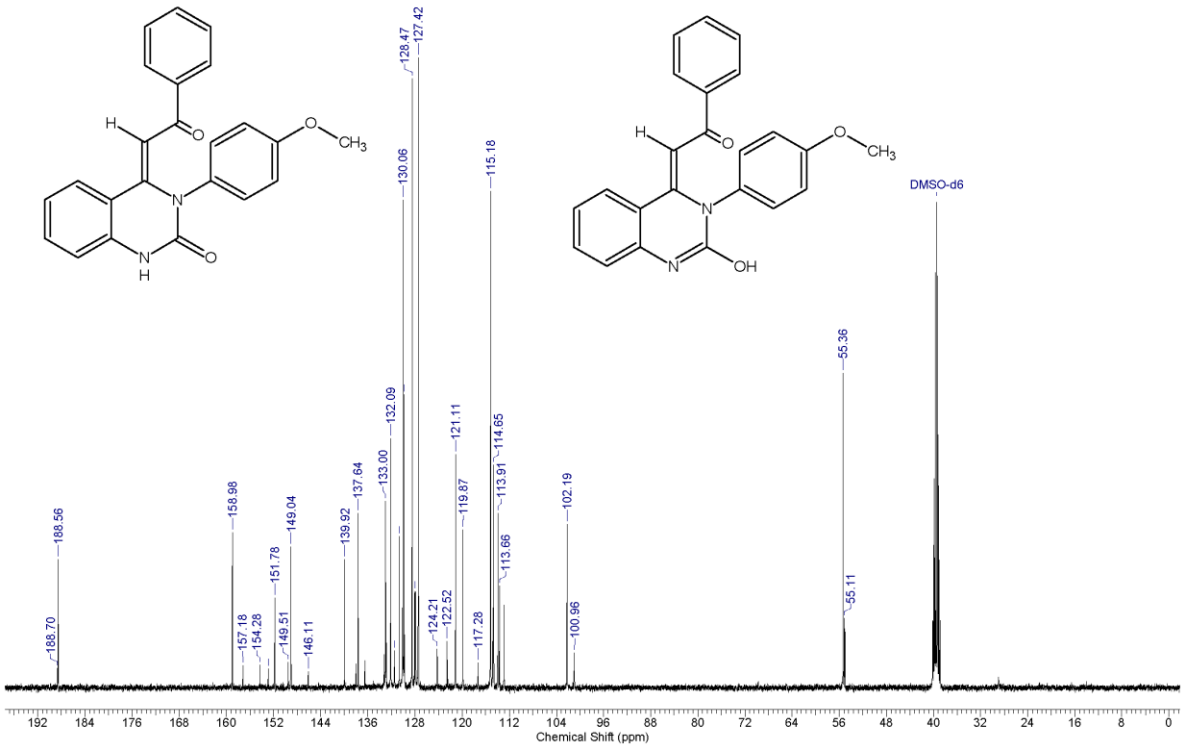
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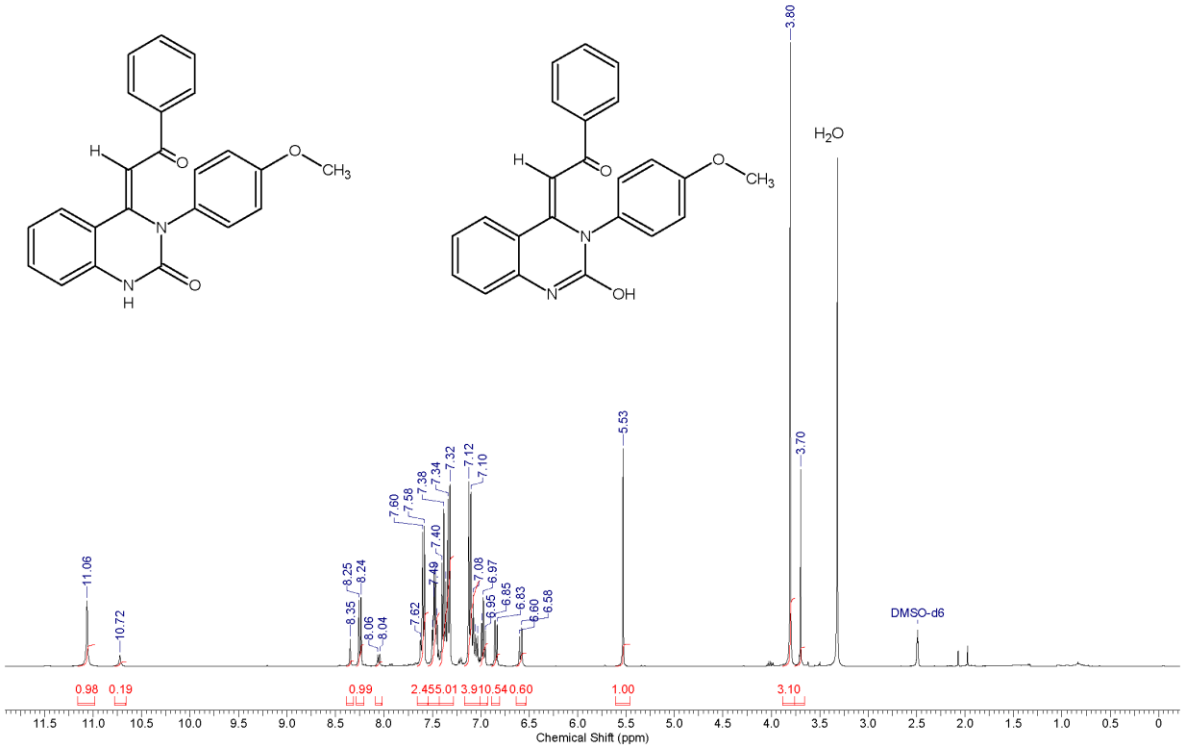
55.11
DMSO-d6
Chemical Shift (ppm)

5ac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7.10
7.08
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6.83
6.60
6.58
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3.70
DMSO-d6
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Chemical Shift (ppm)

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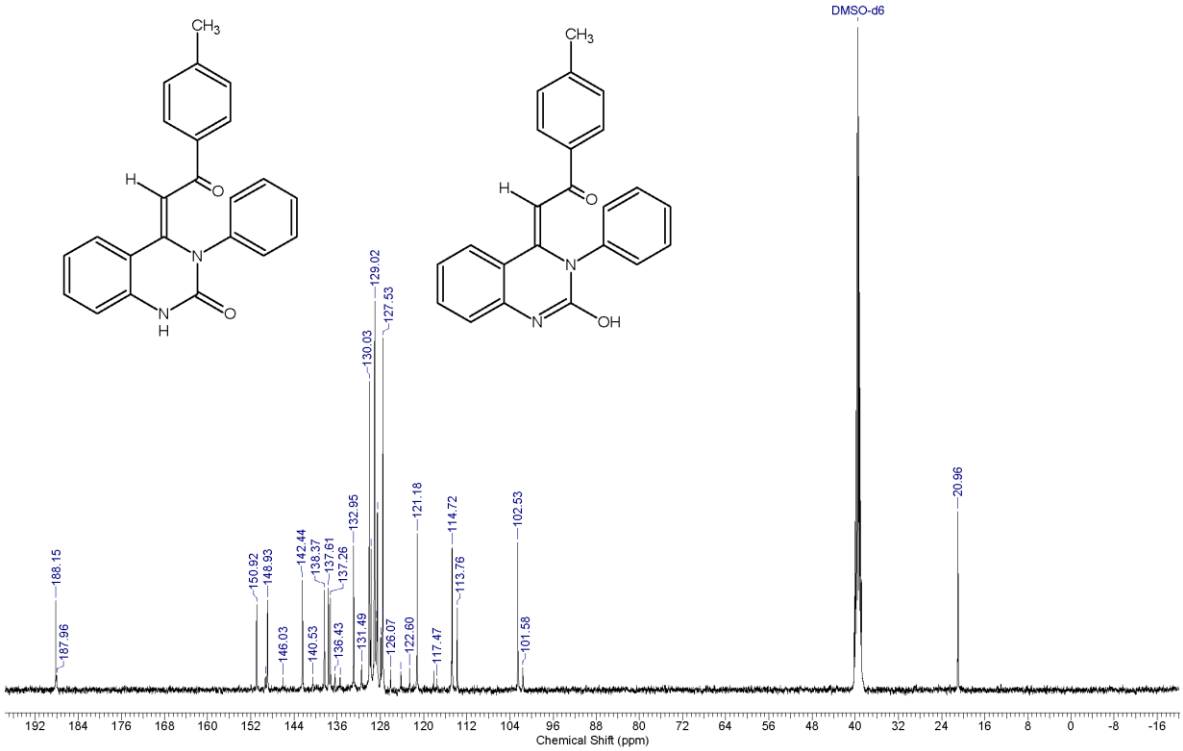
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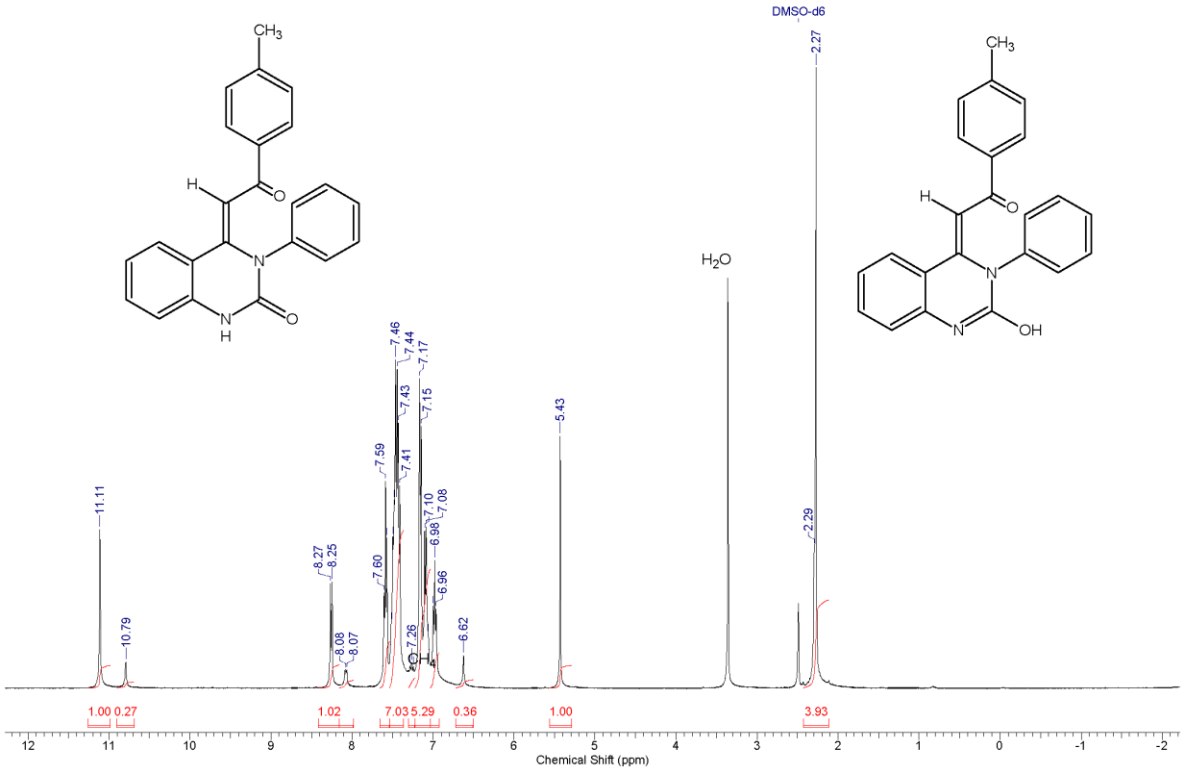
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7.10
7.08
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6.62
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Chemical Shift (ppm)

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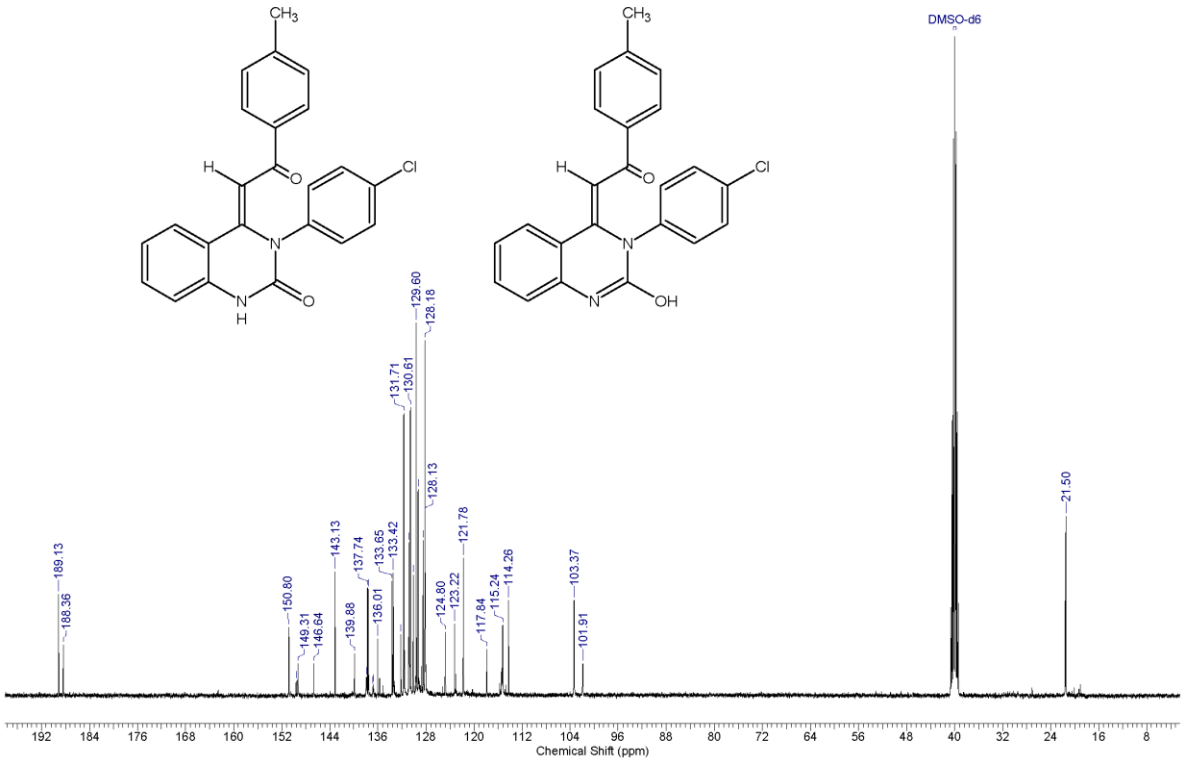
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Cl
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Chemical Shift (ppm)

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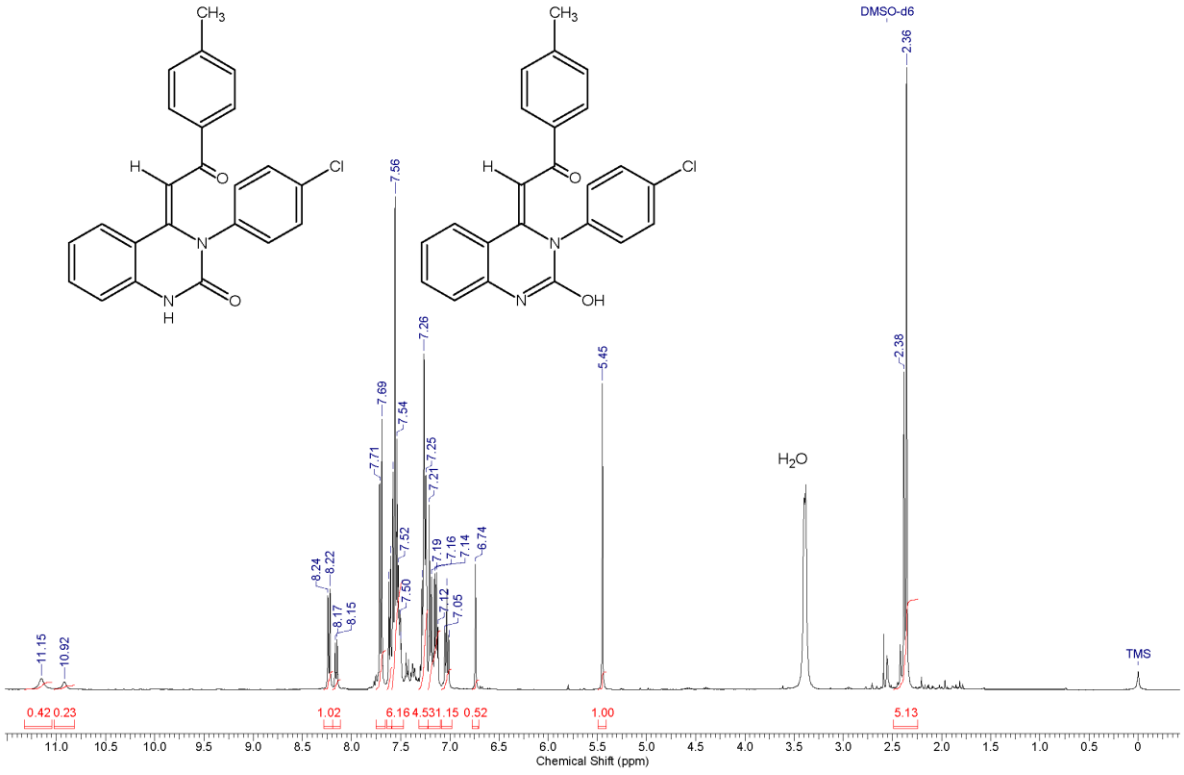
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OH
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5.45
7.69
7.54
7.71
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7.21
7.52
7.19
7.16
7.14
6.74
8.24
8.22
7.50
8.17
8.15
7.12
7.05
H2O
11.15
10.92
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Chemical Shift (ppm)

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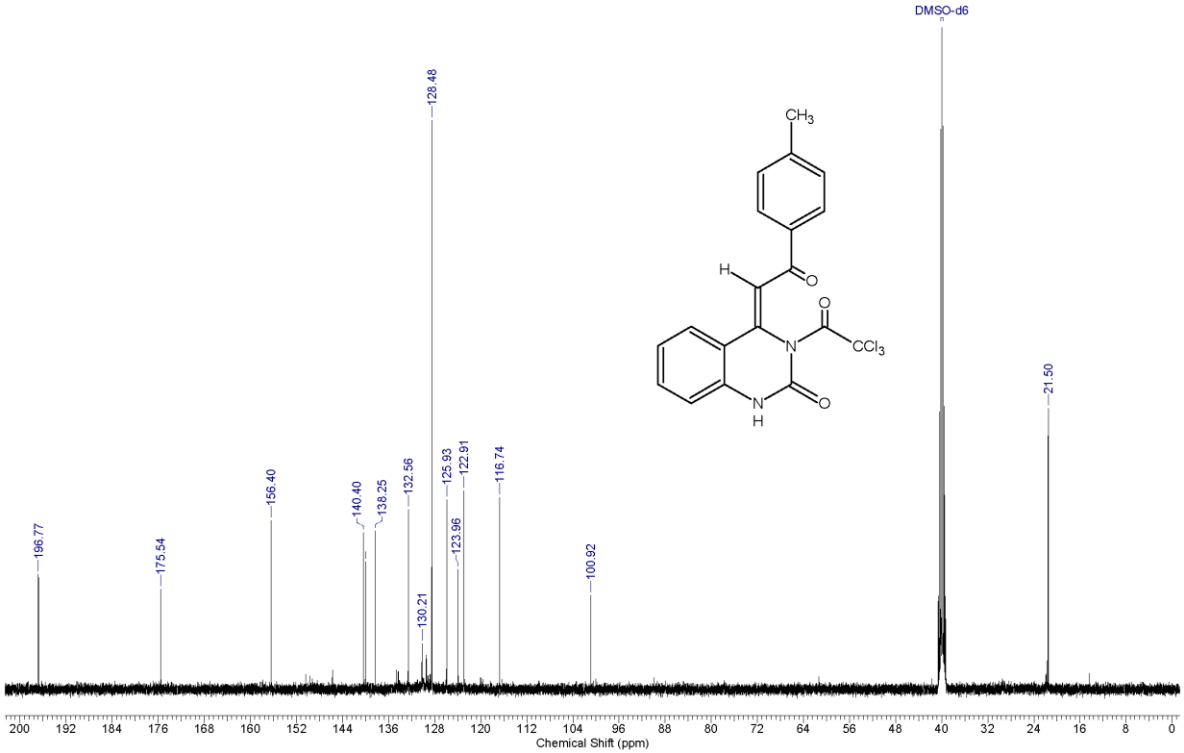
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Chemical Shift (ppm)

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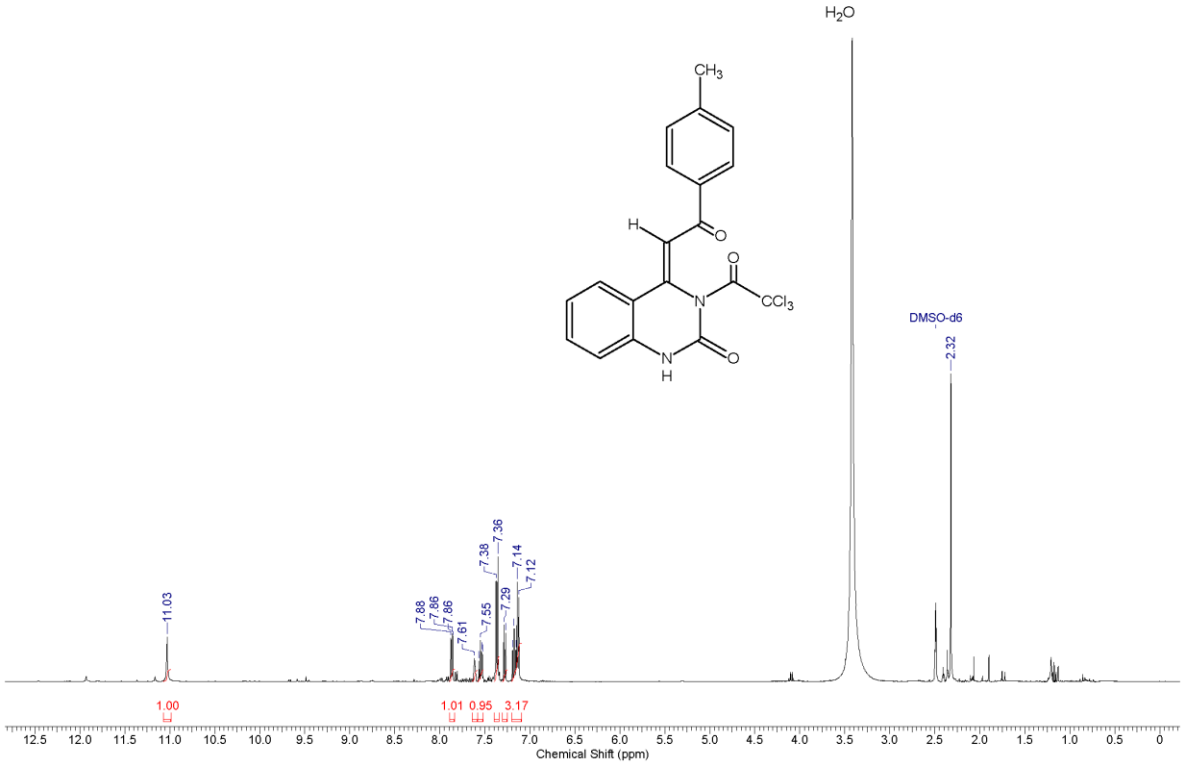
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Chemical Shift (ppm)

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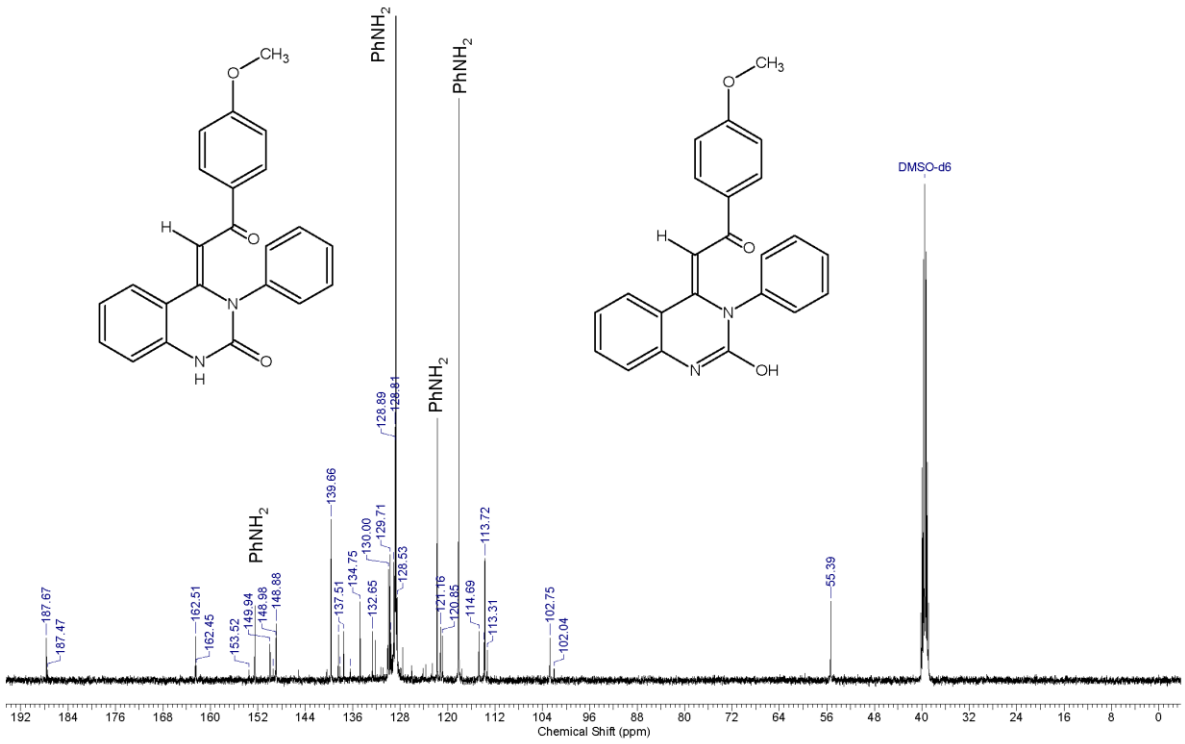
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Chemical Shift (ppm)

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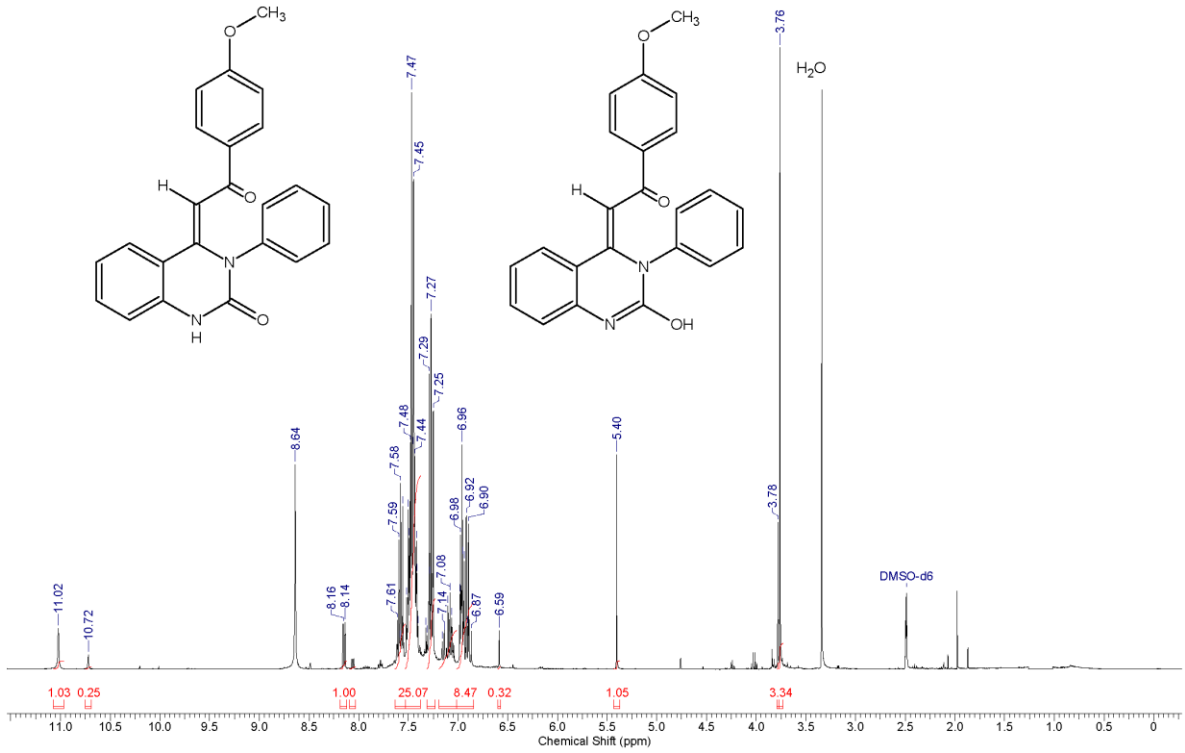
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Chemical Shift (ppm)

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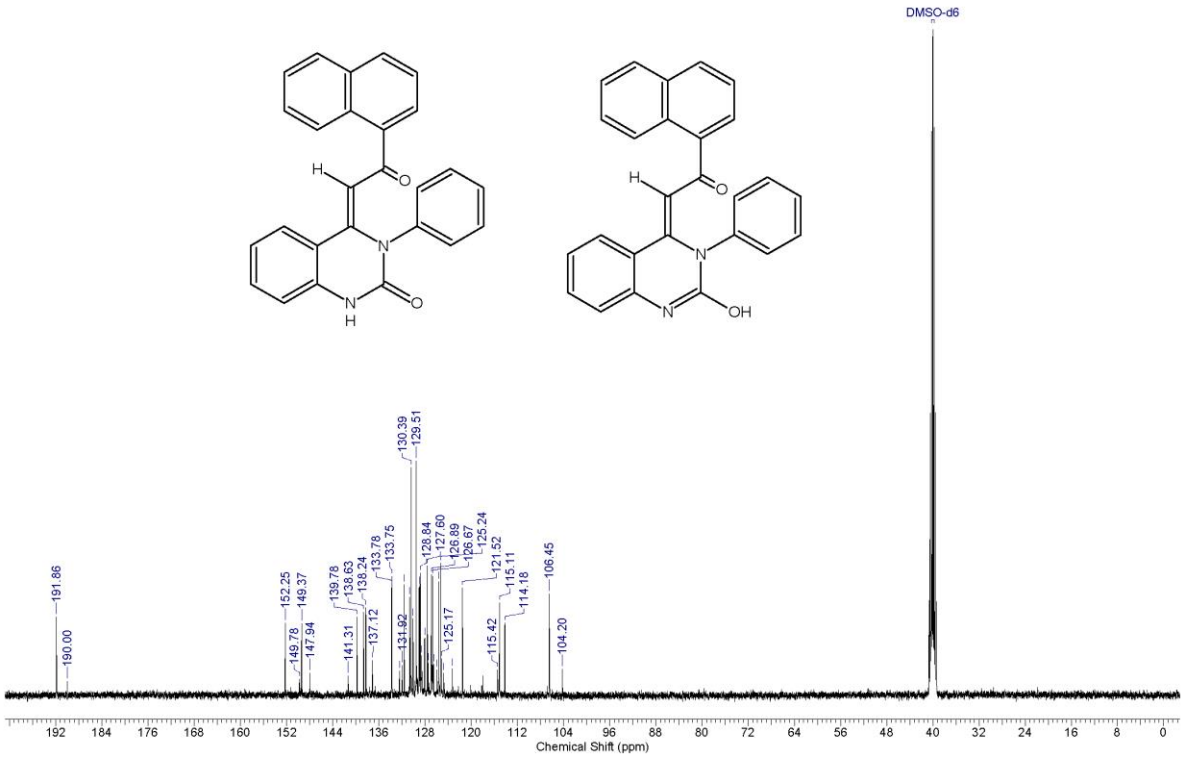
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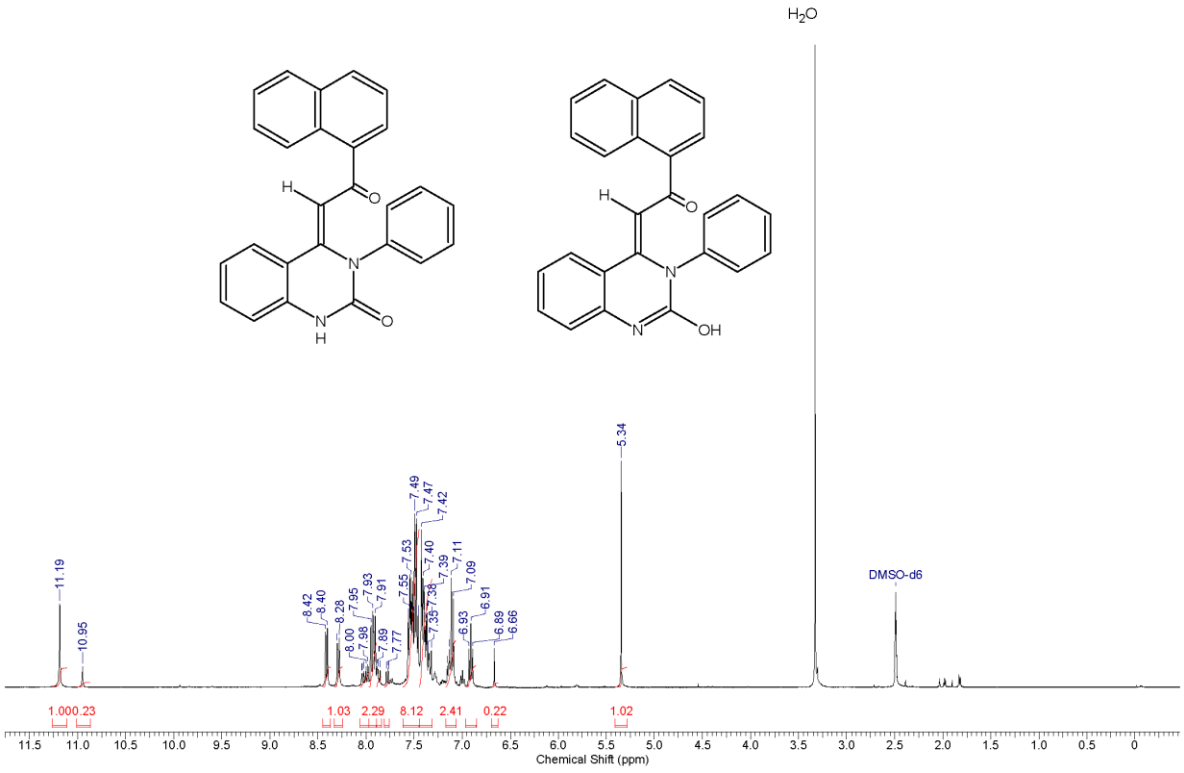
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Chemical Shift (ppm)

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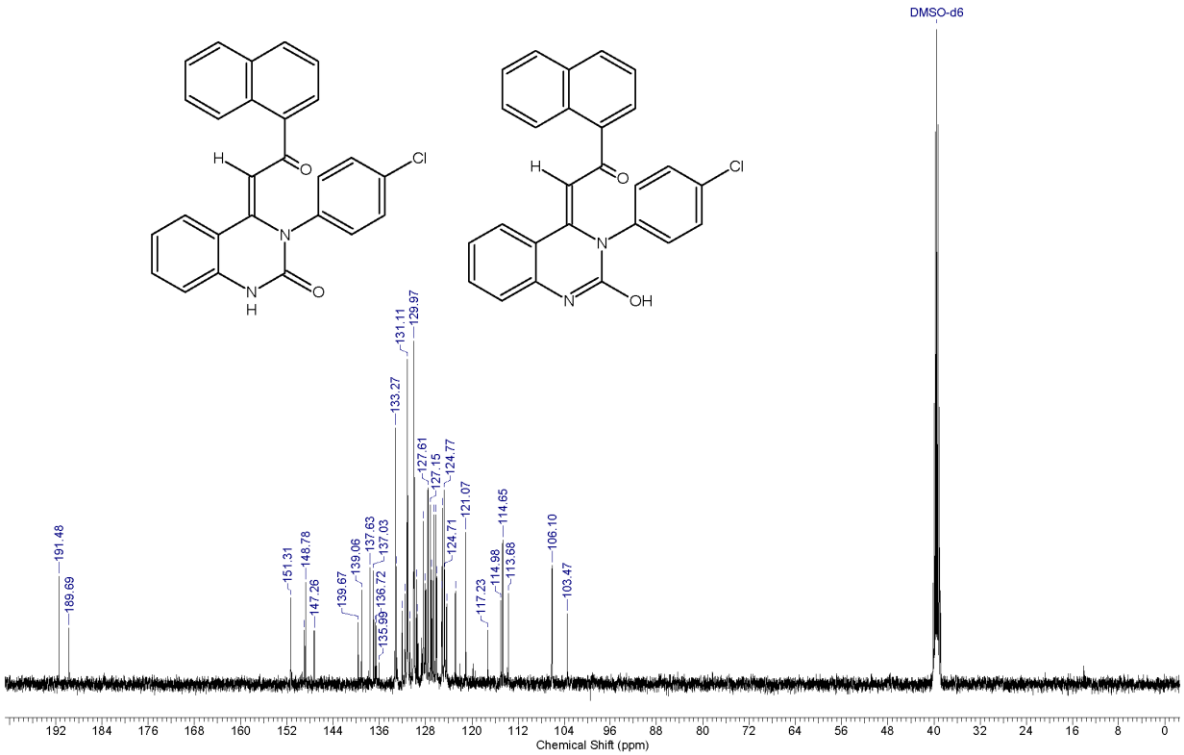
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Chemical Shift (ppm)

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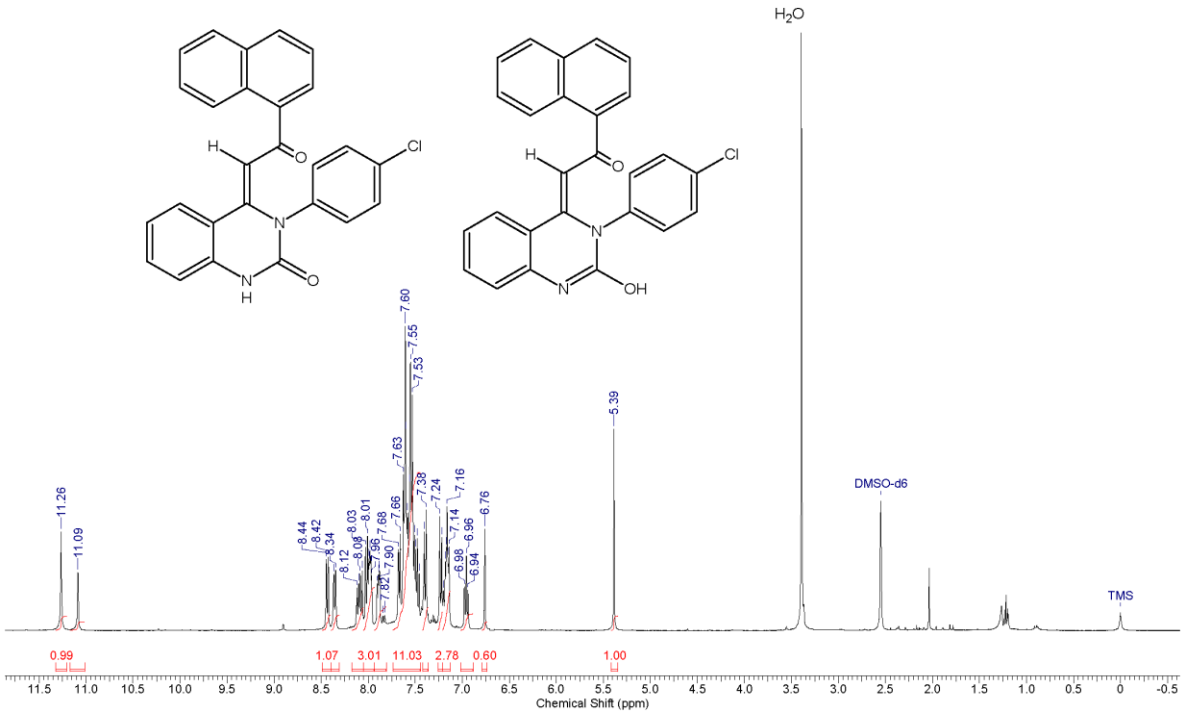
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Chemical Shift (ppm)

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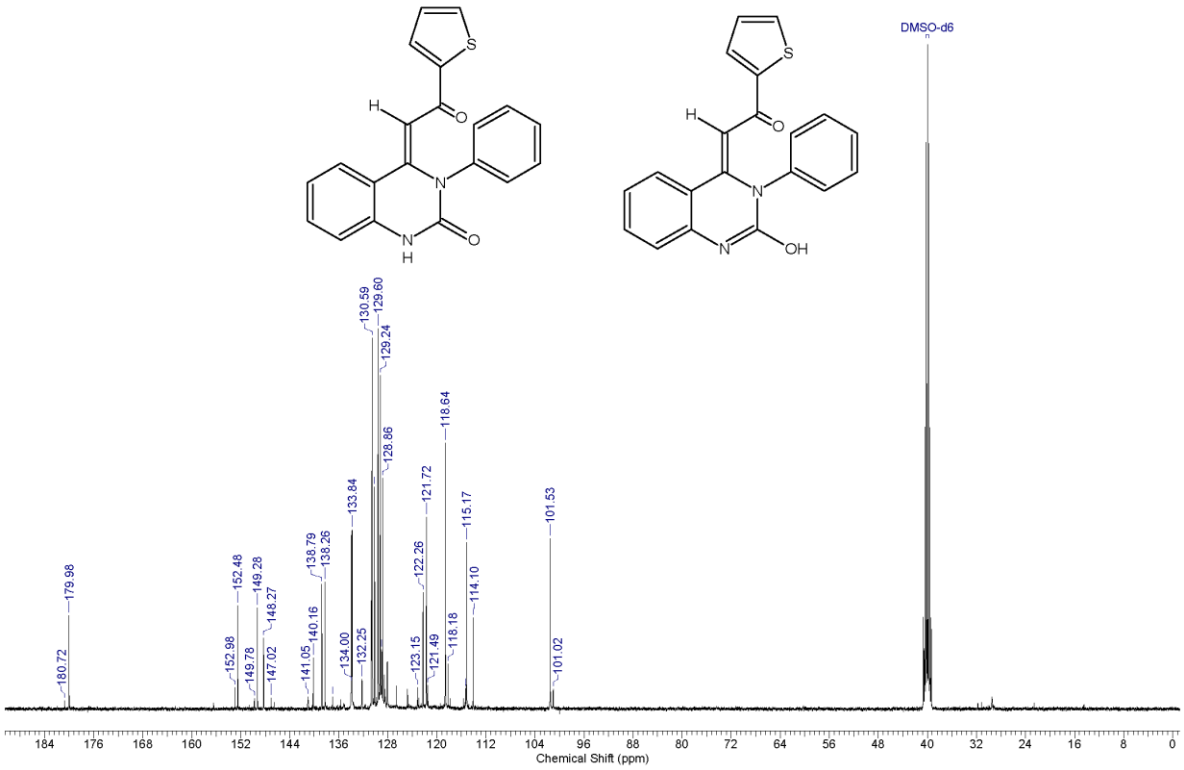
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Chemical Shift (ppm)

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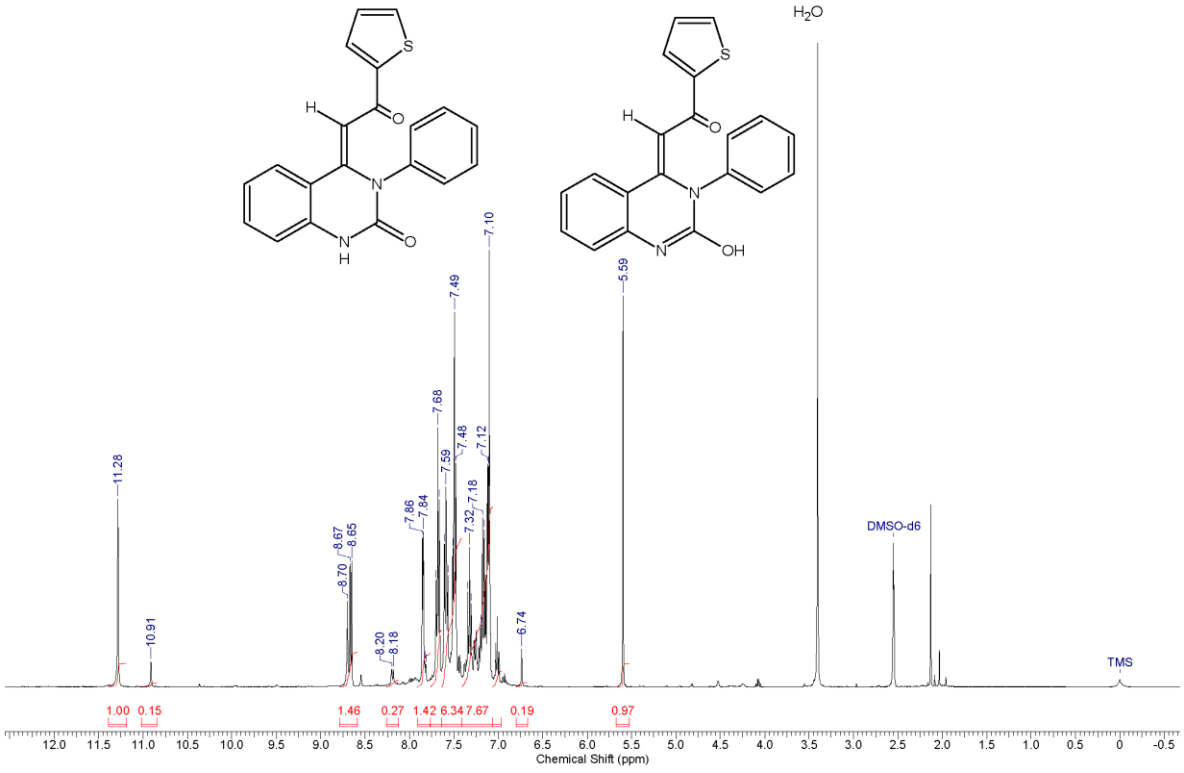
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Chemical Shift (ppm)

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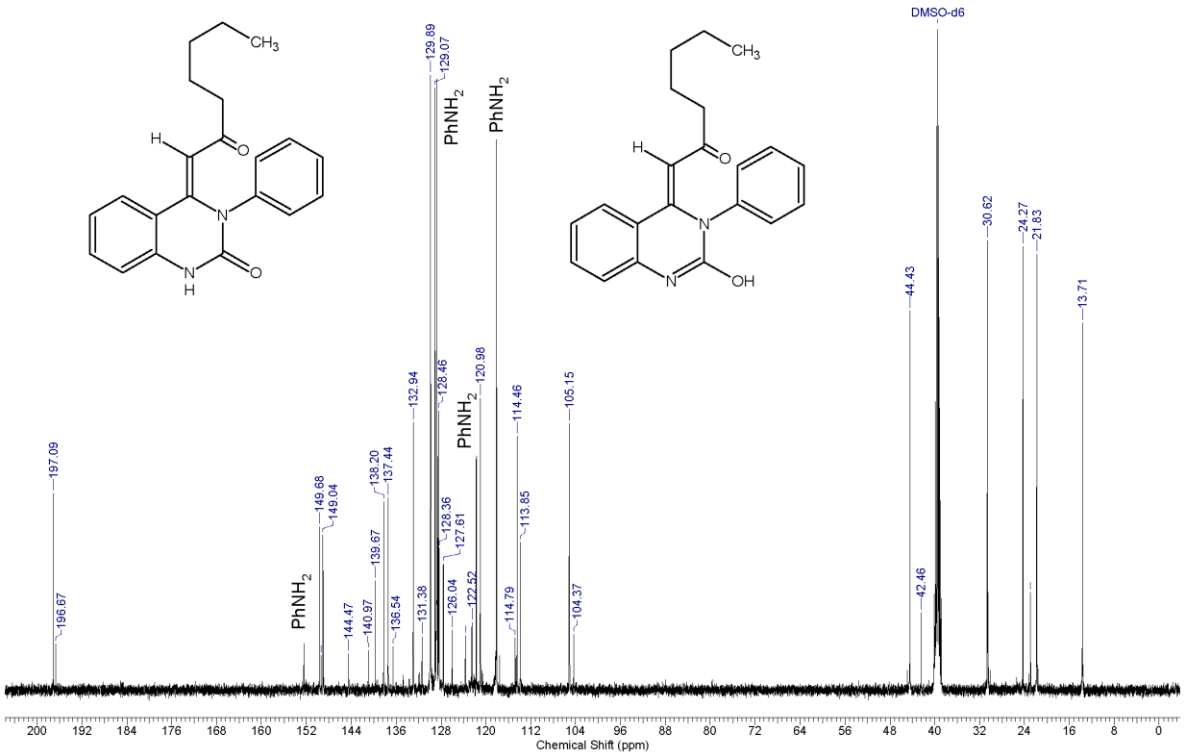
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Chemical Shift (ppm)

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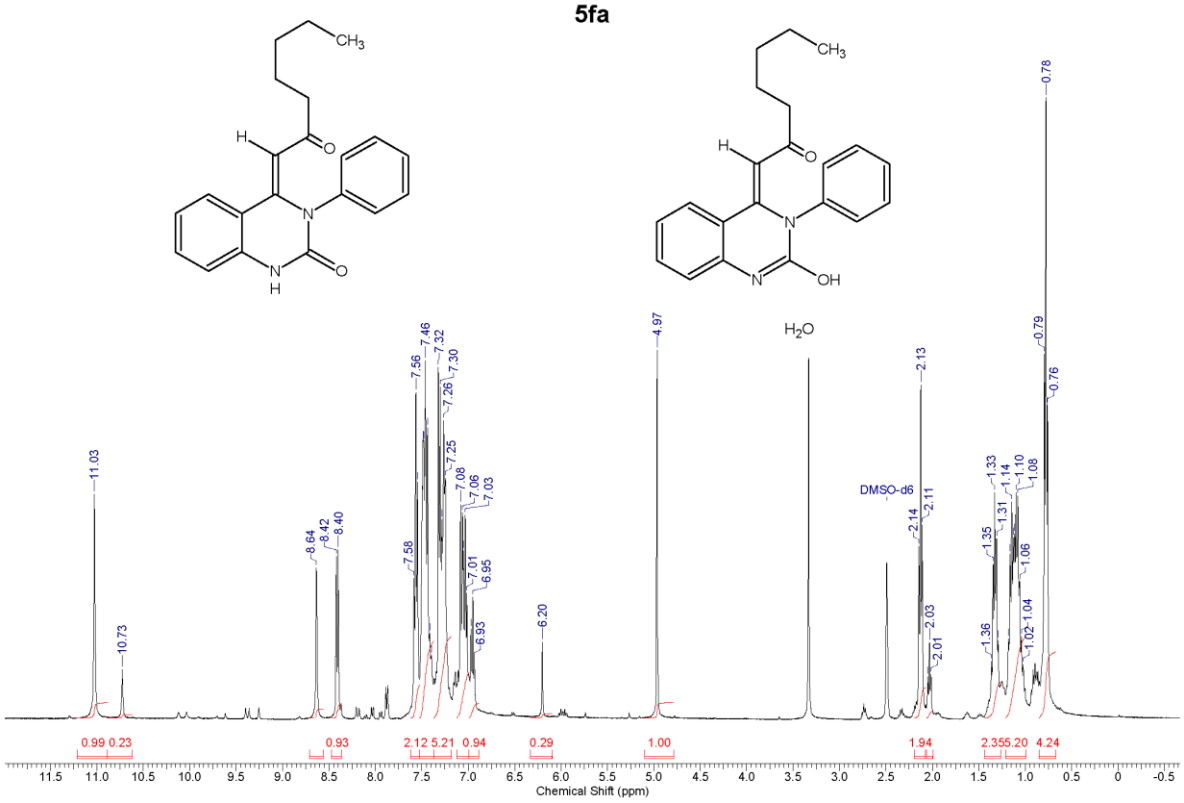
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Chemical Shift (ppm)

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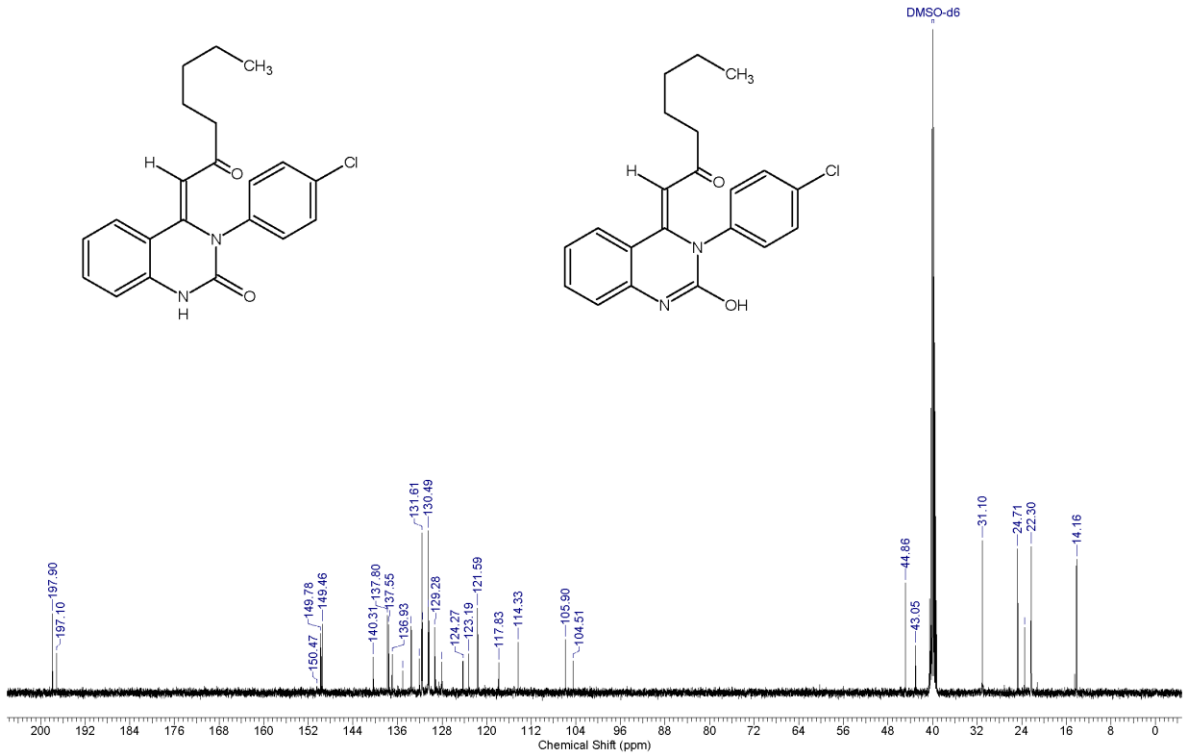
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124.27
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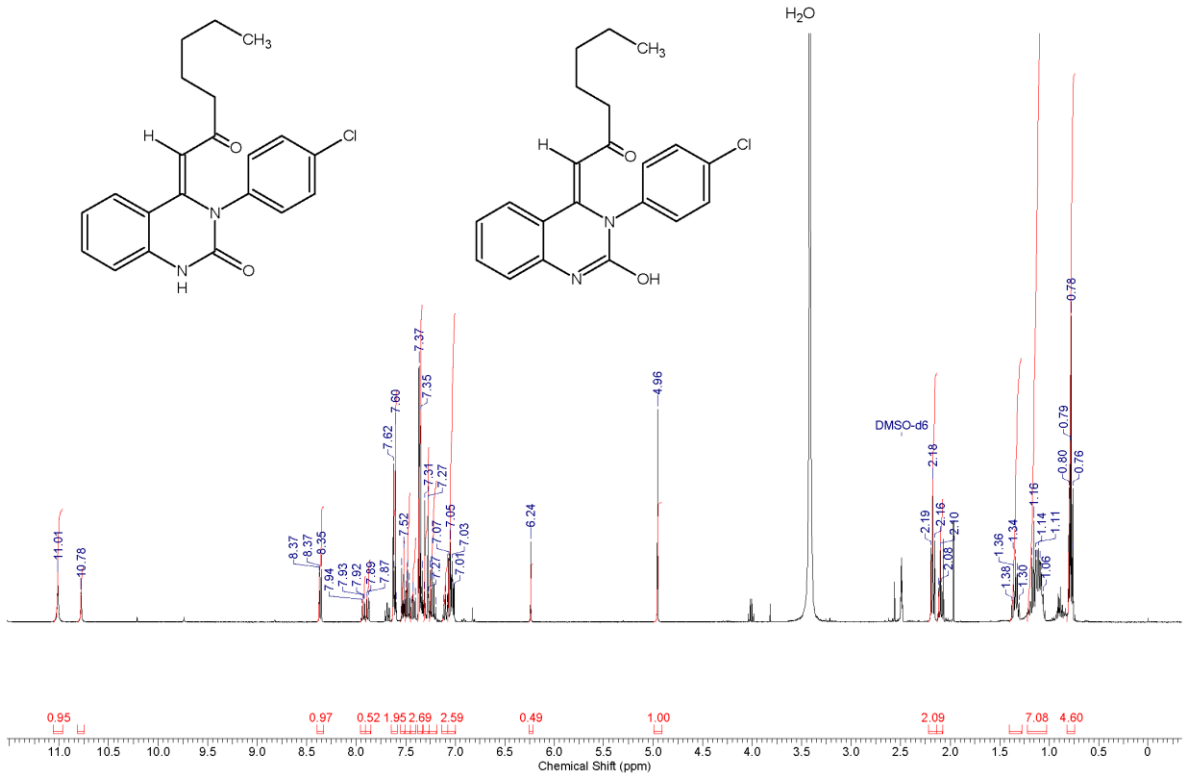
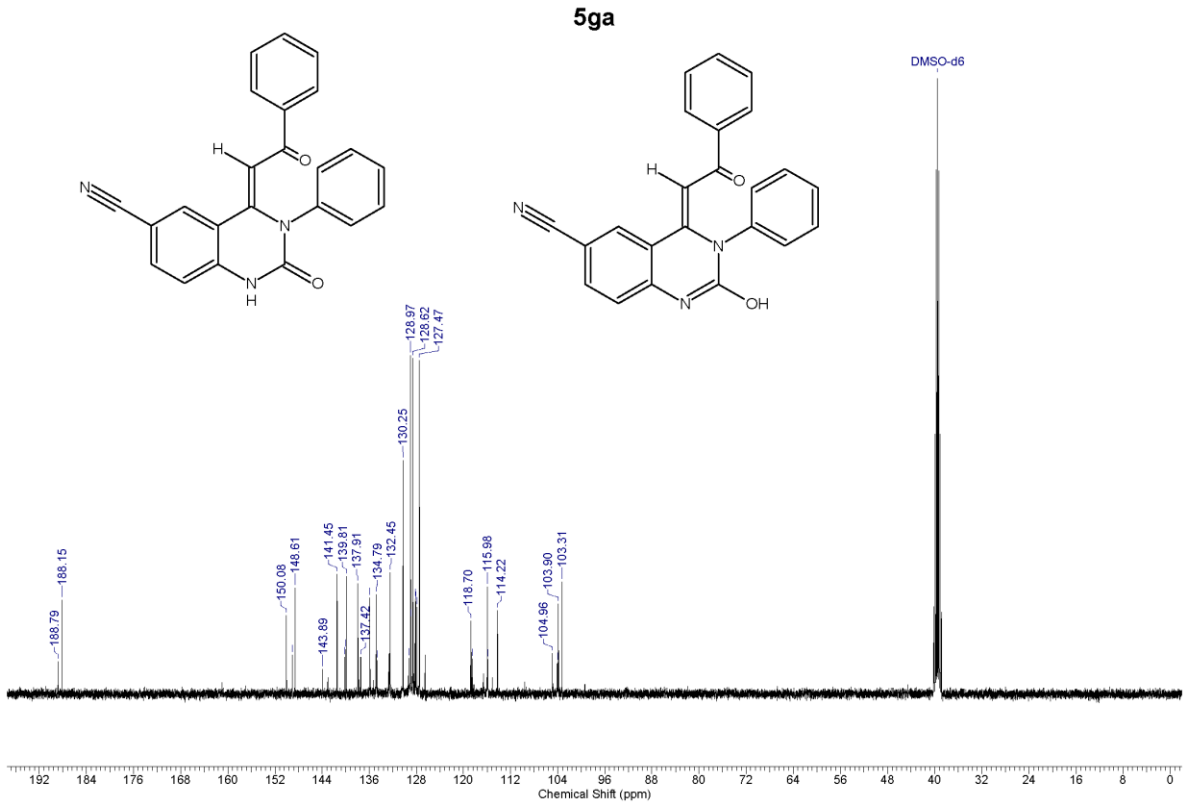
121.59
117.83
114.33
105.90
104.51
44.86
43.05
31.10
24.71
22.30
14.16
Chemical Shift (ppm)

5fd


H2O
DMSO-d6
11.01
10.78
8.37
8.37
8.35
7.94
7.93
7.92
7.89
7.87
7.62
7.60
7.52
7.37
7.35
7.31
7.27
7.27
7.07
7.05
7.03
7.01
6.24
4.96
2.18
2.19
2.16
2.10
2.08
1.38
1.36
1.34
1.30
1.16
1.14
1.11
1.06
0.80
0.79
0.78
0.76
0.95
0.97
0.52
1.95
2.69
2.59
0.49
1.00
2.09
7.08
4.60
Chemical Shift (ppm)


5ga
DMSO-d6
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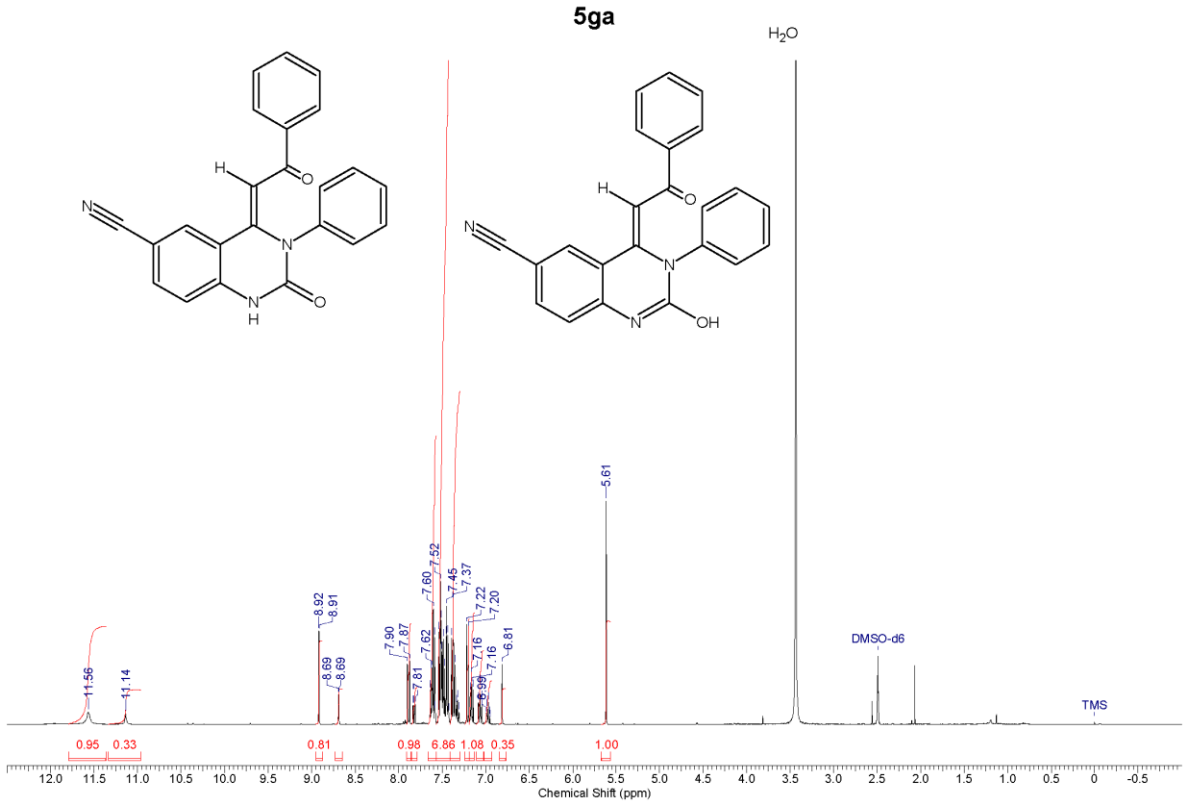
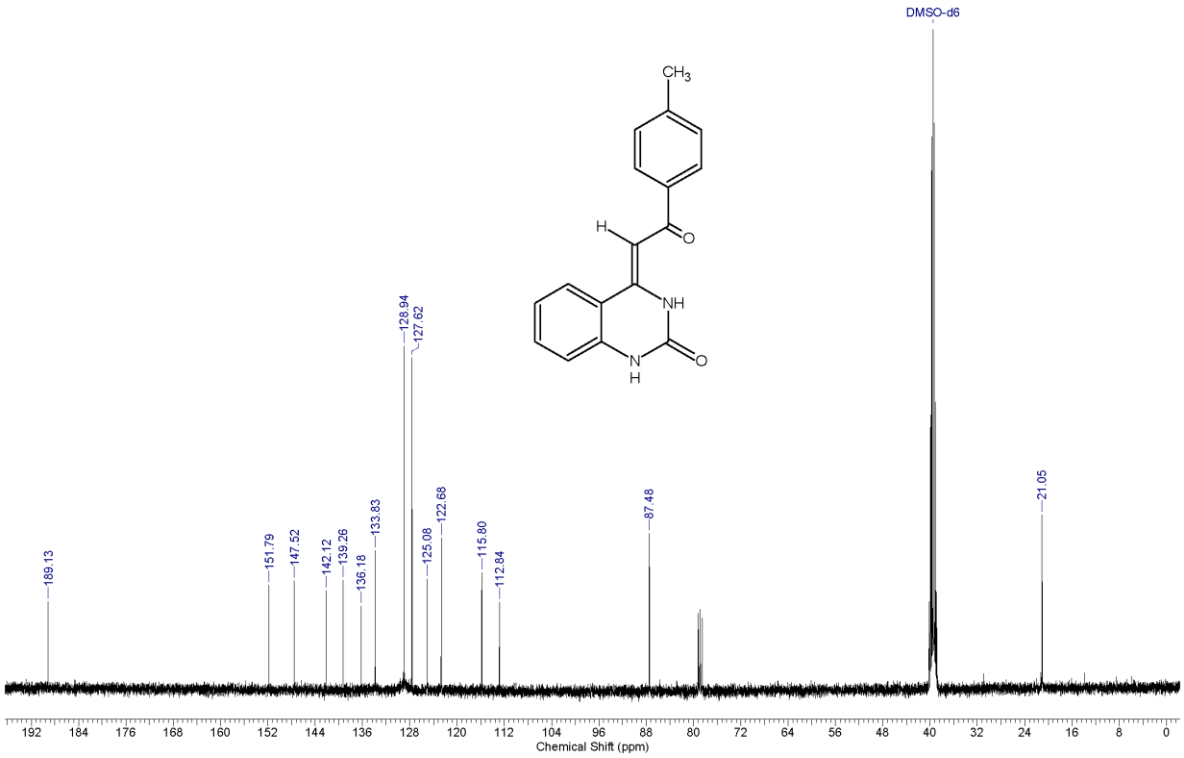
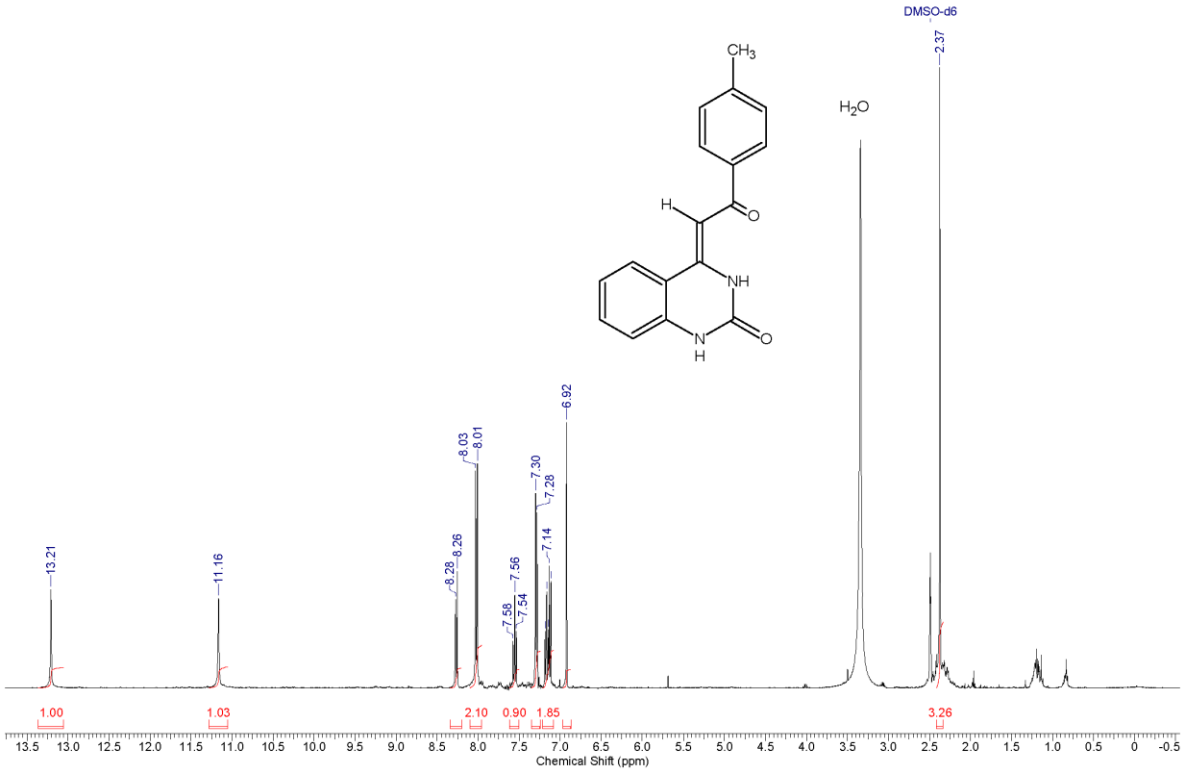
188.79
150.08
148.61
143.89
141.45
139.81
137.91
137.42
134.79
132.45
130.25
128.97
128.62
127.47
118.70
115.98
114.22
104.96
103.90
103.31
Chemical Shift (ppm)


5ga
H2O
DMSO-d6
TMS
11.56
11.14
8.92
8.91
8.69
8.69
7.90
7.87
7.81
7.62
7.60
7.52
7.45
7.37
7.22
7.20
7.16
7.16
6.99
6.81
5.61
0.95
0.33
0.81
0.98
6.86
1.08
0.35
1.00
Chemical Shift (ppm)

6b


DMSO-d6
189.13
151.79
147.52
142.12
139.26
136.18
133.83
128.94
127.62
125.08
122.68
115.80
112.84
87.48
21.05
Chemical Shift (ppm)

6b


DMSO-d6
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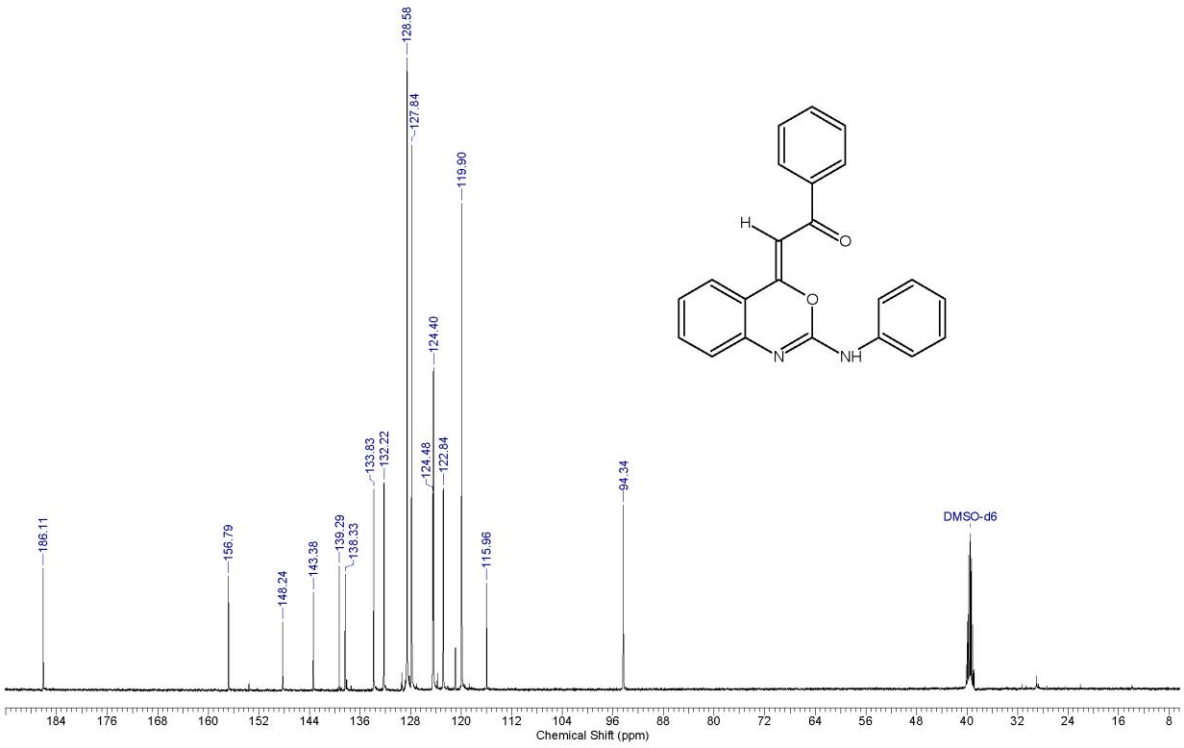
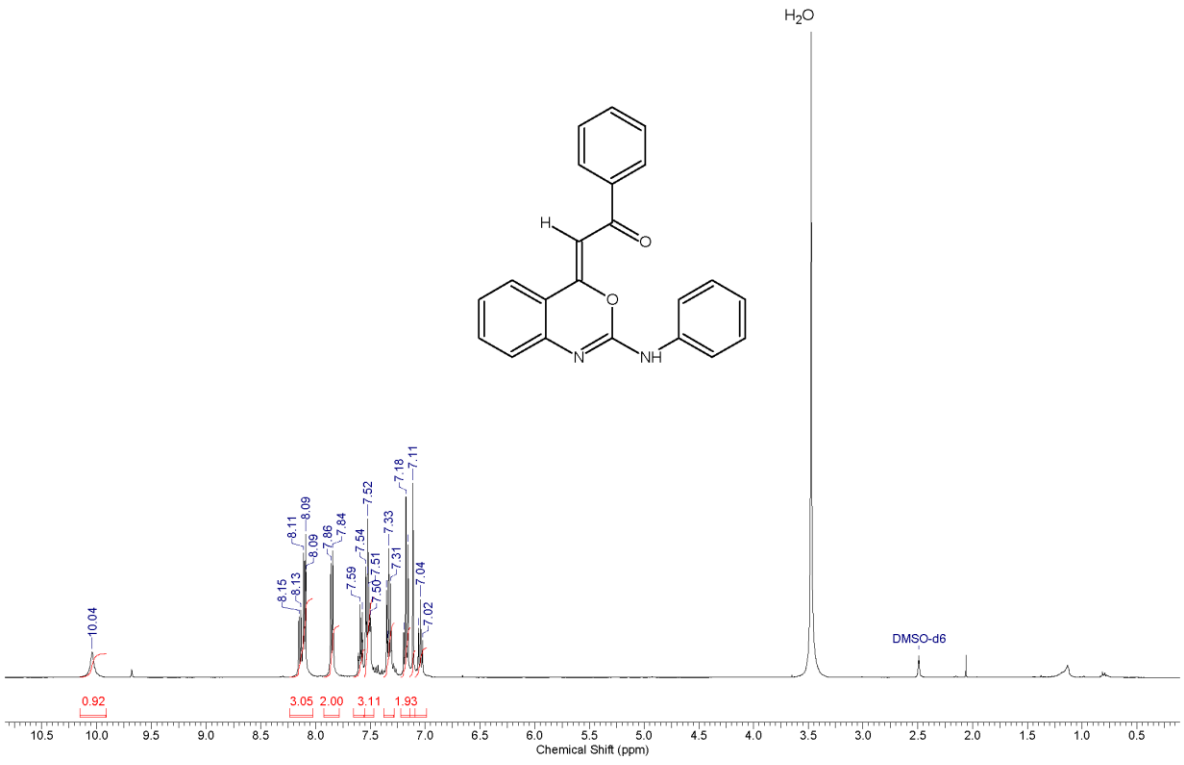
H2O
13.21
11.16
8.28
8.26
8.03
8.01
7.58
7.56
7.54
7.30
7.28
7.14
6.92
1.00
1.03
2.10
0.90
1.85
3.26
Chemical Shift (ppm)

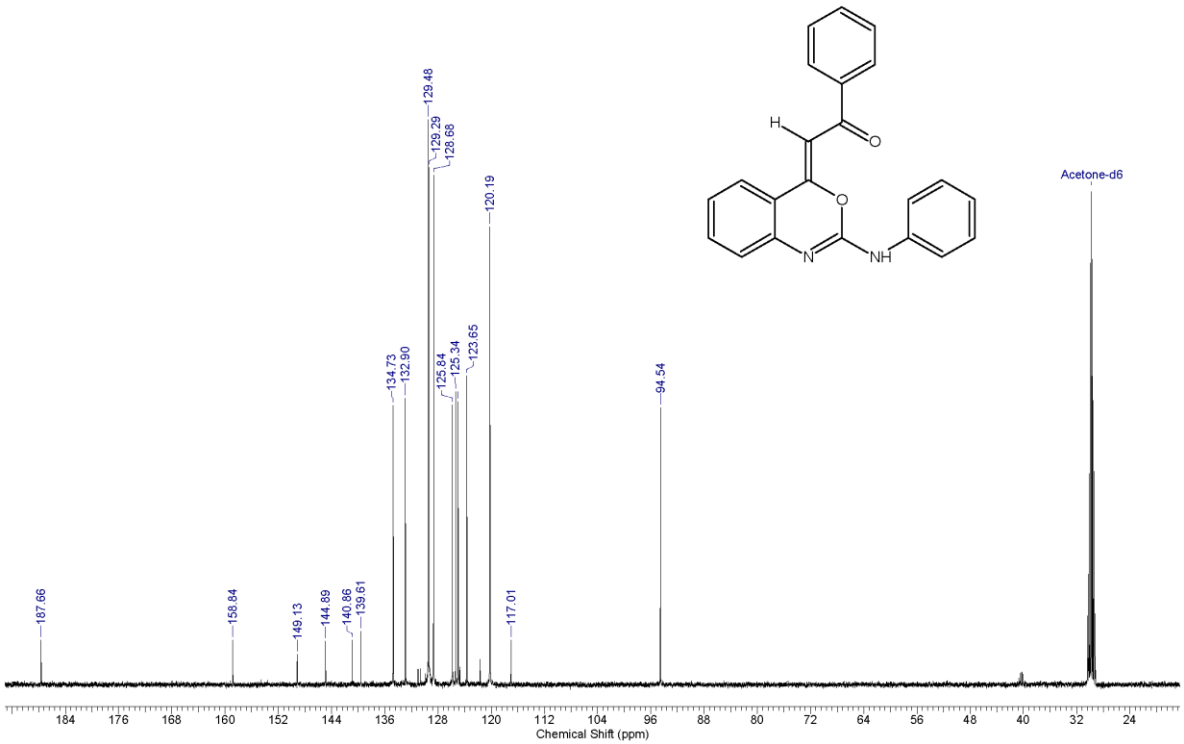
7aa - DMSO



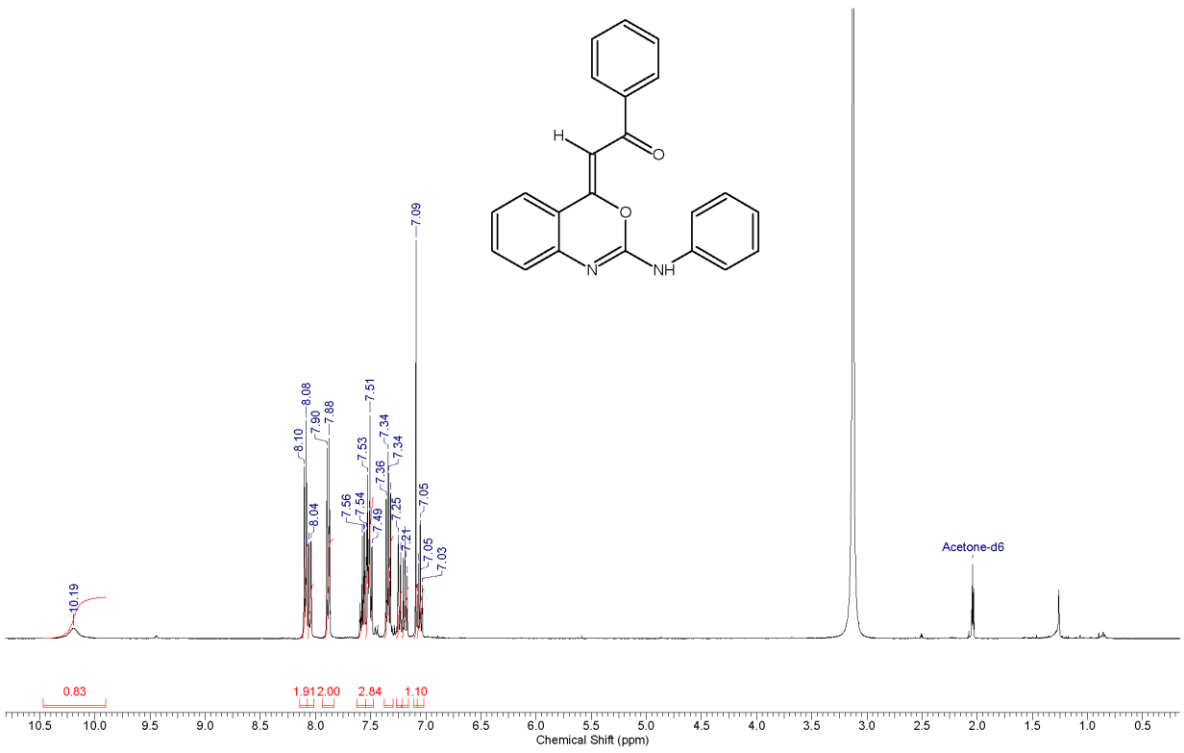
7aa - DMSO



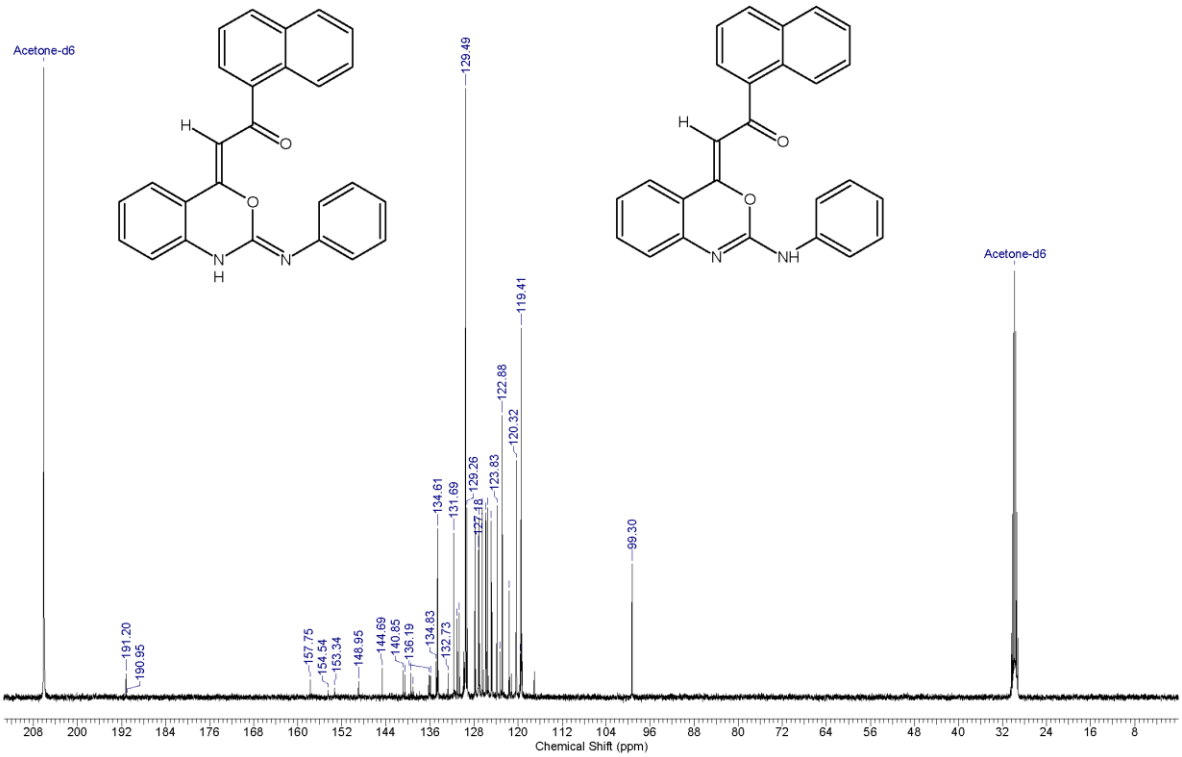
7aa - Acetone-d6



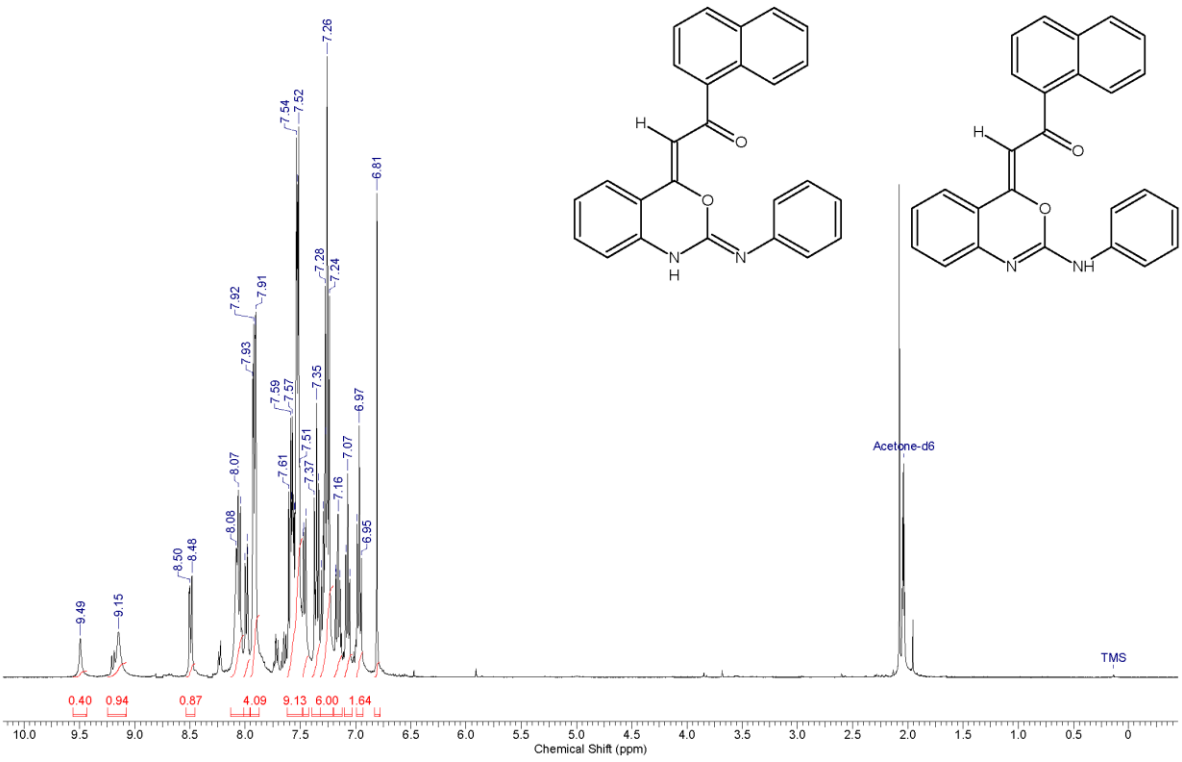
7aa - Acetone-d6



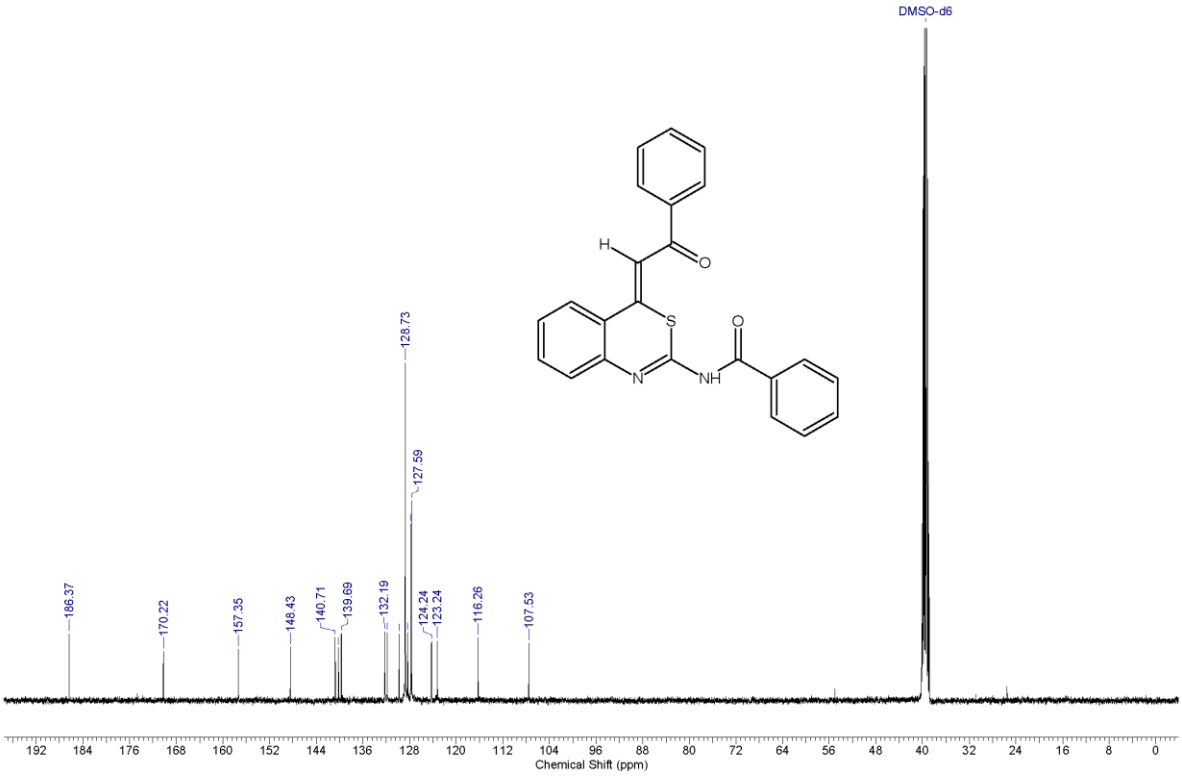
7da


Acetone-d6
129.49
119.41
122.88
120.32
134.61
131.69
129.26
123.83
127.18
99.30
Acetone-d6
191.20
190.95
157.75
154.54
153.34
148.95
144.69
140.85
136.19
134.83
132.73
Chemical Shift (ppm)

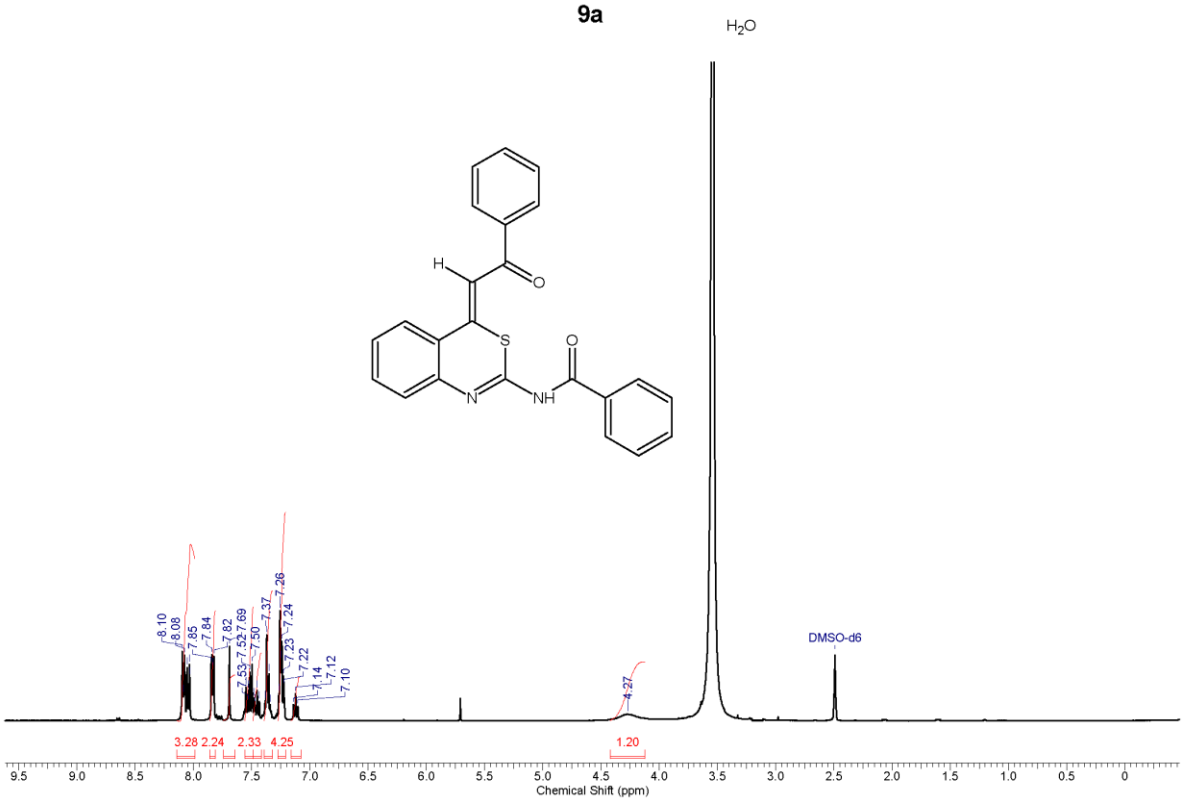
7da


7.26
7.54
7.52
6.81
7.28
7.24
7.92
7.91
7.93
7.59
7.57
7.35
6.97
7.51
8.07
7.61
7.37
7.16
7.07
8.08
6.95
8.50
8.48
9.49
9.15
Acetone-d6
TMS
0.40
0.94
0.87
4.09
9.13
6.00
1.64
Chemical Shift (ppm)

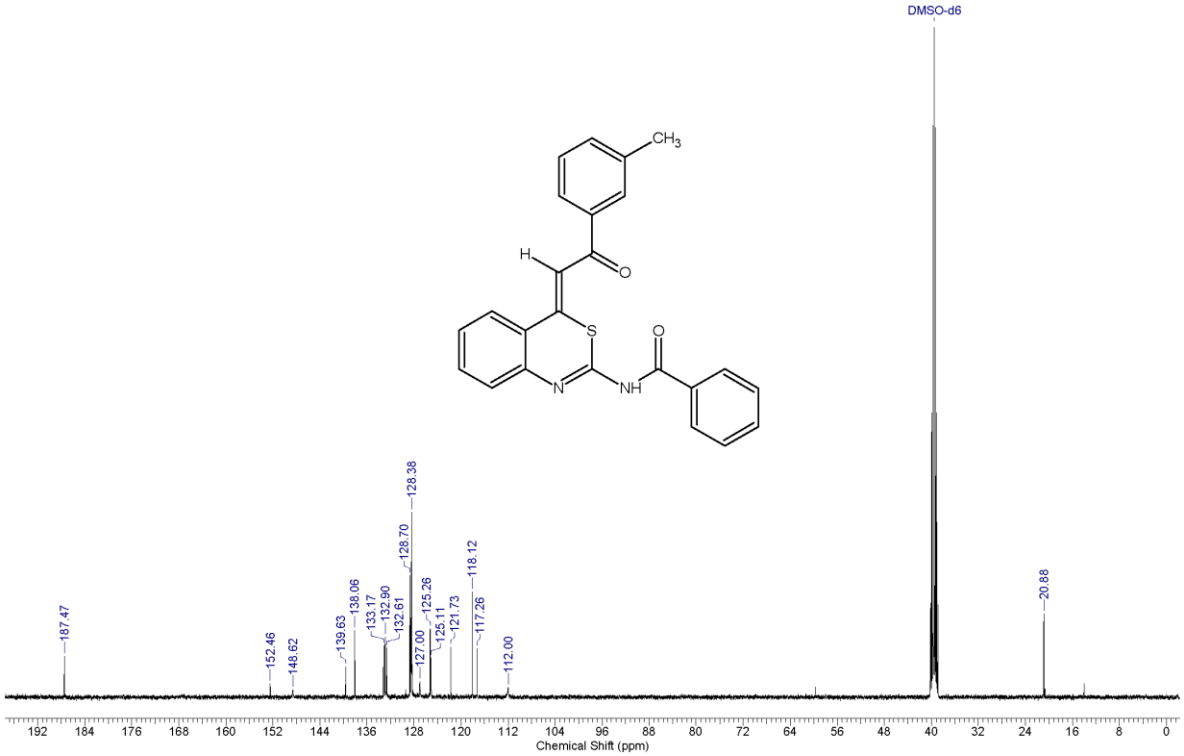
9a


DMSO-d6
H
O
S
N
NH
O
128.73
127.59
186.37
170.22
157.35
148.43
140.71
139.69
132.19
124.24
123.24
116.26
107.53
192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0
Chemical Shift (ppm)

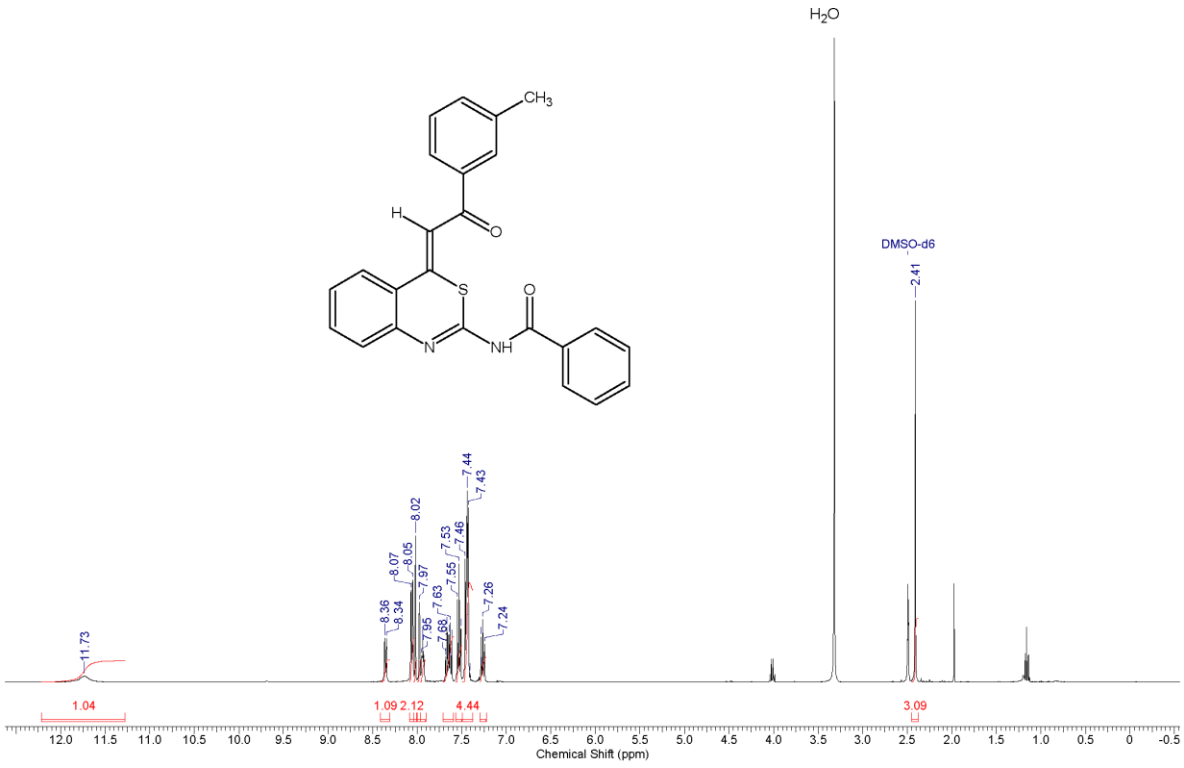
9a


H2O
H
O
S
N
NH
O
DMSO-d6
8.10
8.08
7.85
7.84
7.82
7.69
7.53
7.50
7.37
7.26
7.24
7.23
7.22
7.14
7.12
7.10
4.27
3.28 2.24 2.33 4.25
1.20
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
Chemical Shift (ppm)

9h


DMSO-d6
CH3
H
O
S
N
NH
O
187.47
152.46
148.62
139.63
138.06
133.17
132.90
132.61
128.38
128.70
127.00
125.26
125.11
121.73
118.12
117.26
112.00
20.88
Chemical Shift (ppm)

9h


H2O
DMSO-d6
2.41
CH3
H
O
S
N
NH
O
11.73
8.36
8.34
8.07
8.05
8.02
7.97
7.95
7.68
7.63
7.55
7.53
7.46
7.44
7.43
7.26
7.24
1.04
1.09
2.12
4.44
3.09
Chemical Shift (ppm)

NMR - Structural characterization in solution:

In order to better understand the structure of **5aa**, **5ba**, **6b**, **7aa** and **9a**, as model compounds, they were analysed by NMR spectroscopy (^{1}H, ^{13}C, H–H Cosy, H–H Noesy, H–C HSQC and H–C HMBC).

(Z)-4-(2-oxo-2-phenylethylidene)-3-phenyl-3,4-dihydroquinazolin-2(1H)-one (5aa)

Key NOE interactions to establish the absolute stereochemistry for **5aa** are those of the proton H(7) with proton of the NH(1) (for structure numbering see Figure S06) of the dihydroquinazolin-2(1H)-one and those of the H(18a) of the ethylidene. Analysis of Noesy spectrum showed proximity between the ethylidene proton H(18a) and the proton H(10) of the dihydroquinazolin-2(1H)-one (Figure S07A), the proximity of the proton H(7) with the proton NH(1) of the dihydroquinazolin-2(1H)-one (Figure S07B) and also the proximity of the ethylidene proton H(18a) with the protons H(22,26) of the 2-phenil (Figure S07A).

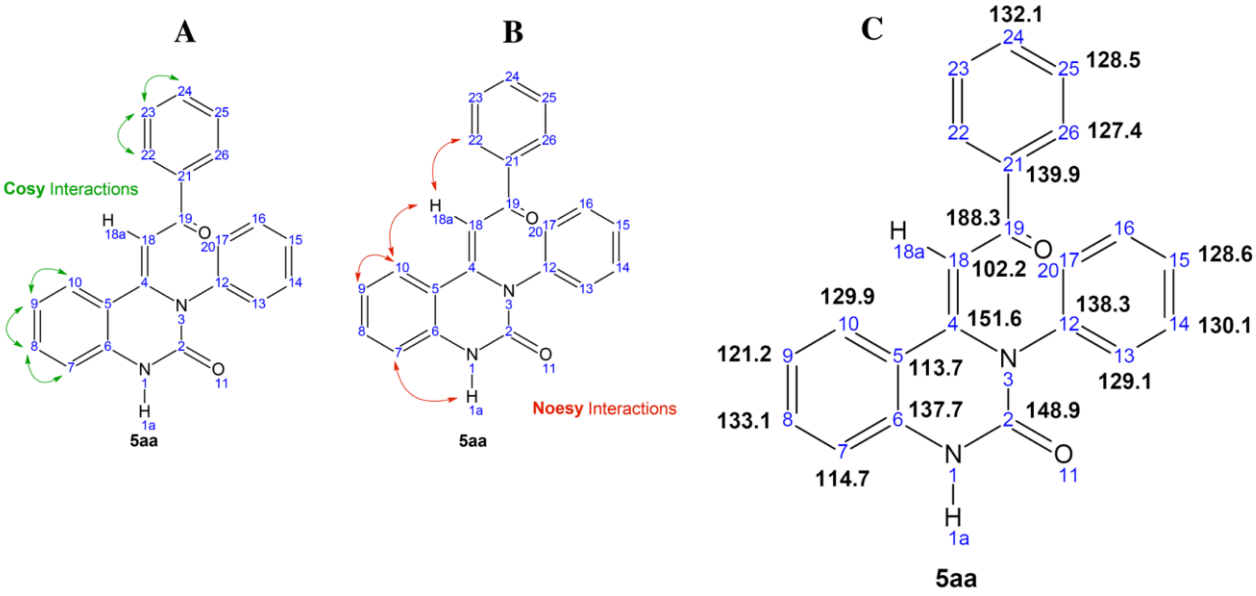


Figure S06. A) Relevant Cosy interactions; B) Relevant Noesy interactions C) ^{13}C assignment

Analysis of Cosy spectrum allowed to establish the correct proton assignment for proton resonances of H(8) and H(9) and H(22,26), H(23,25) and H(24) as shown in Figure S08.

Analysis of HSQC spectrum provides correlations between carbons and the attached proton for all protonated carbons as shown in Figure S09.

In order to completely assign the ^{13}C-NMR resonances, HMBC spectra, optimized for 5 and 8Hz long rang coupling constant, were acquired (Figure S10).

Resonances for C(12) and C(21) were respectively 138.3 and 139.9 and were assigned considering that proton H(18a) correlated with 139.9 and 137.7 ppm for HMBC spectrum acquired for 5Hz long range coupling constant and that the aromatic protons C(14,16) correlate with the quaternary carbon at 138.3 ppm. Finally phenyl protons H(22,26) correlated with C(24) and C(19) confirming the assignment.

As shown in the Figure S10 the proton H(10) correlated with C(8) and with the quaternary carbons at 151.6 and 133.7 ppm, the proton H(9) correlated with C(7) and the quaternary carbon at 113.7 ppm, and the proton H(7) correlated with C(9) and the quaternary carbon at 113.7 ppm; the correlations just indicated were for $^{3}J_{CH}$ couplings, so we assigned at C(5) 113.7 ppm as resonance. In order to assign the other two resonances, we considered that proton H(18a) correlated with the quaternary carbon at 113.7 and 151.6 ppm, so we assigned at C(4), and C(6) the resonances 151.6, and 133.7 ppm respectively.

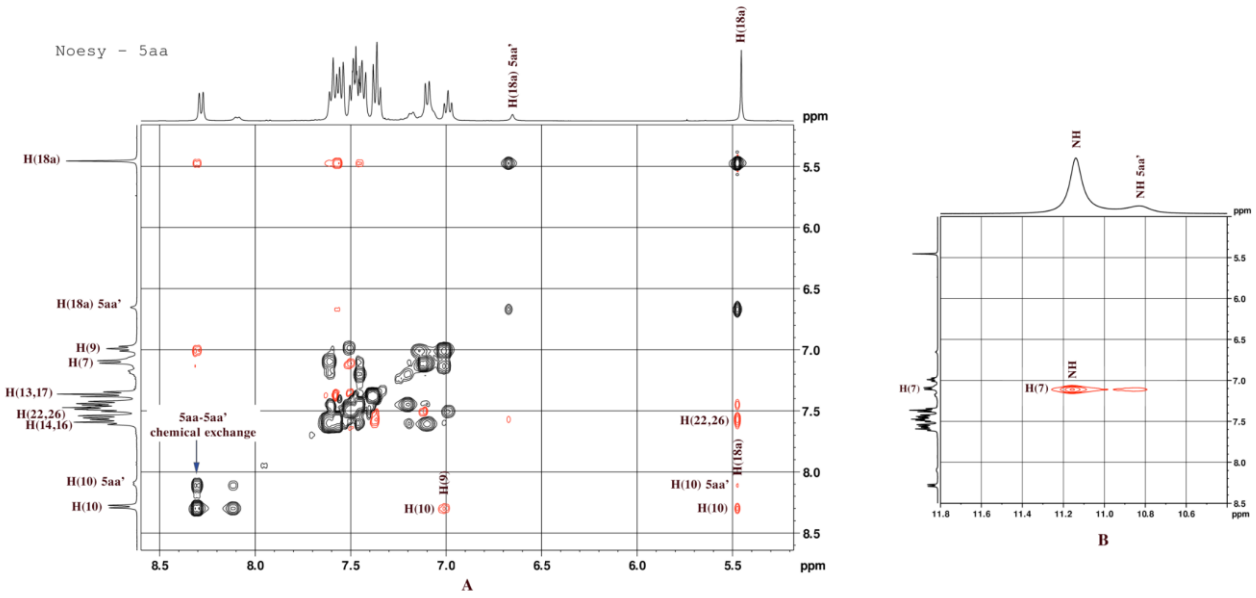


Figure S07. Key NOESY correlations for **5aa**.

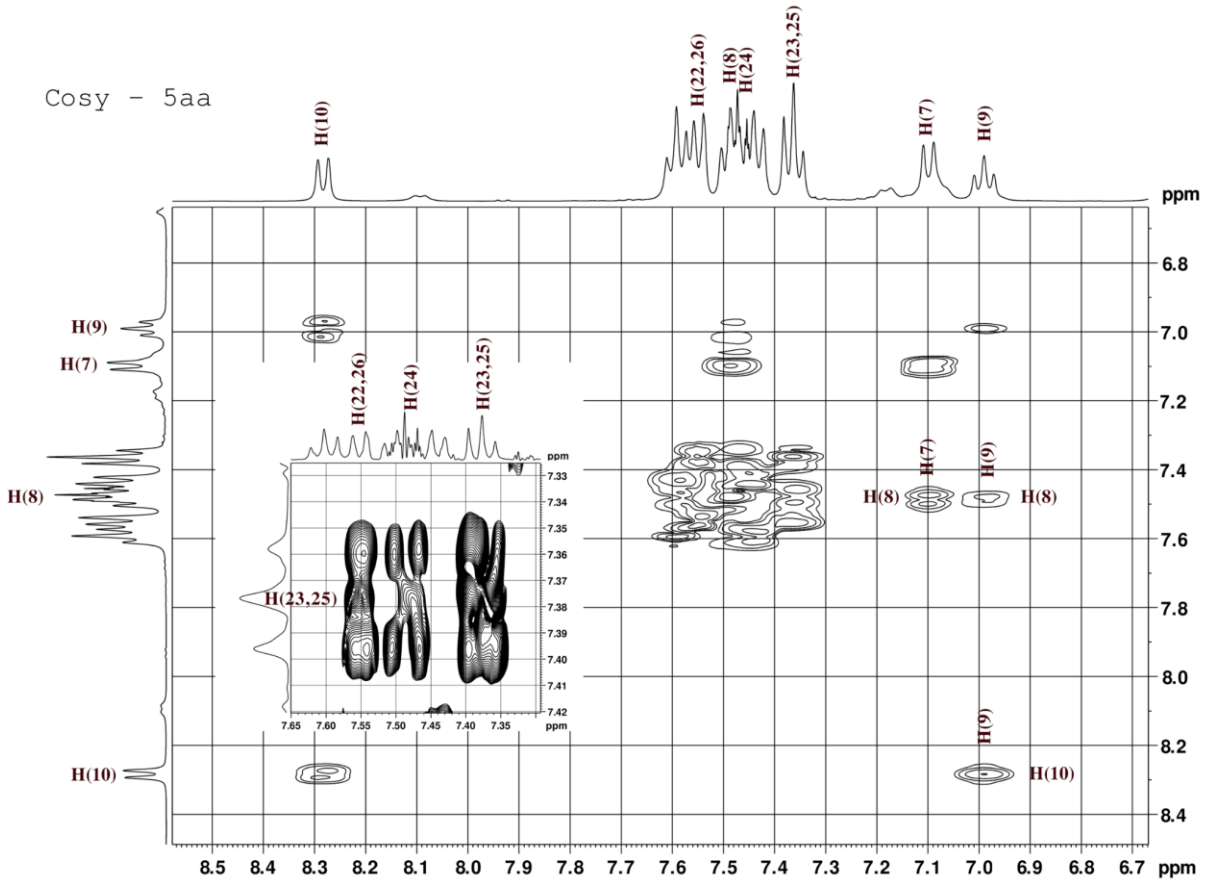


Figure S08. COSY correlations. Relevant coupling interactions for **5aa**.

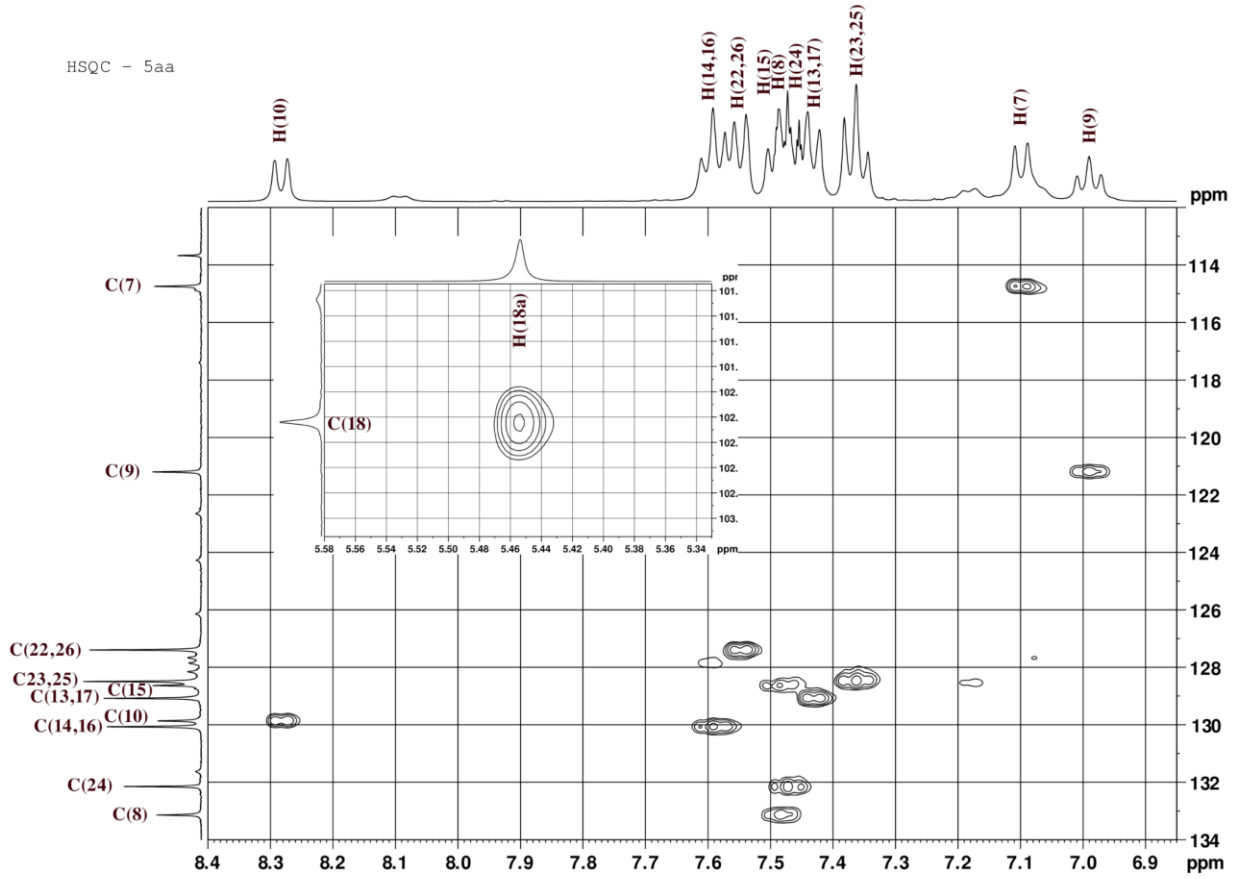


Figure S09. HSQC. Correlations between protons and directly attached (one bond) carbon for **5aa**.

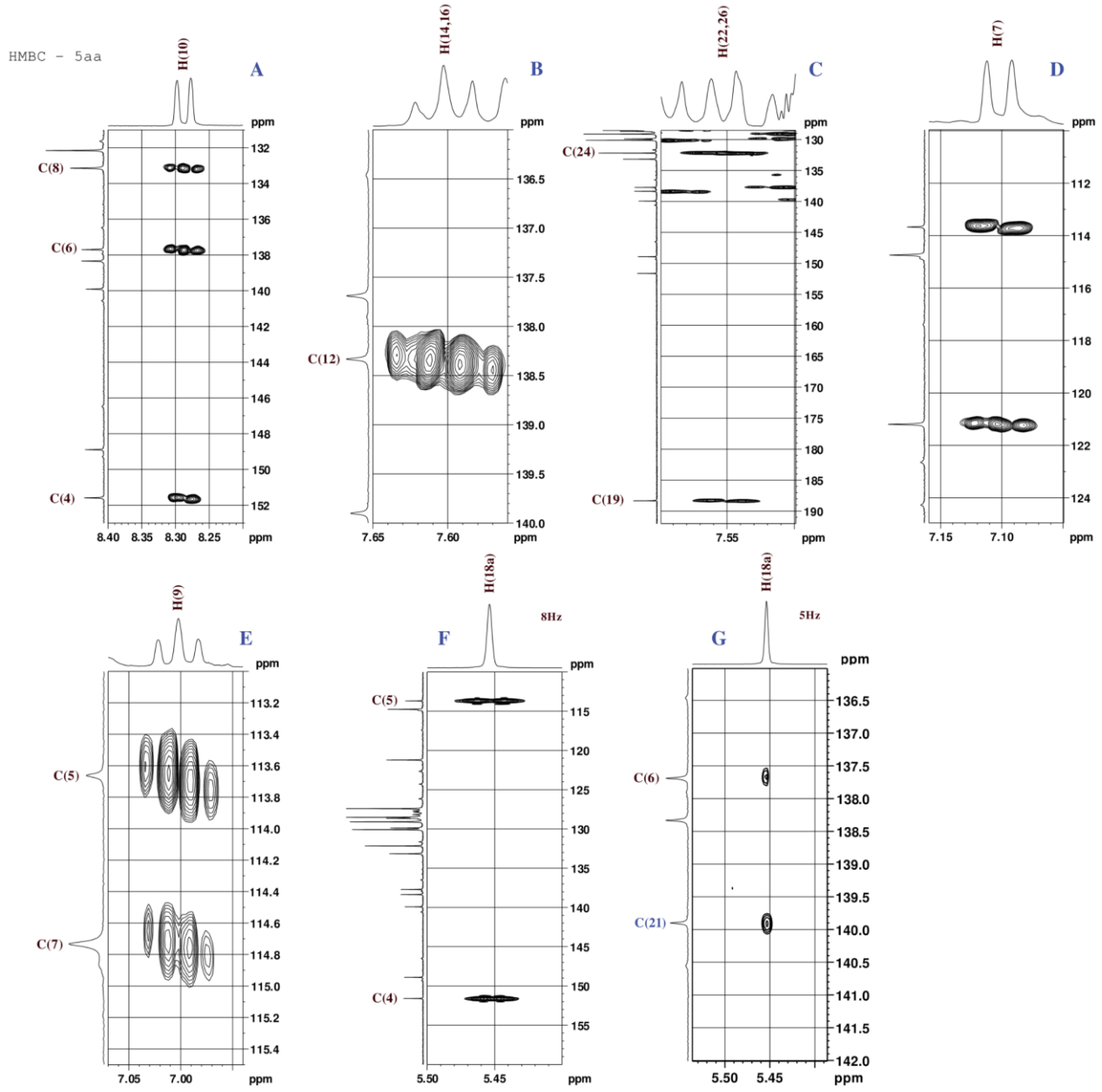


Figure S10. HMBC. Correlations between protons and carbons through long range coupling constant for **5aa**.

(Z)-4-[2-(4-methylphenyl)-2-oxoethylidene]-3-phenyl-3,4-dihydroquinazolin-2(1H)-one (5ba)

The **5ba** sample used for all the NMR spectra was the one deriving from the X-ray crystallographic analysis.

Key NOE interactions to establish the absolute stereochemistry for **5ba** are those of the proton H(7) with the proton of the NH(1) (for structure numbering see Figure S11) of the dihydroquinazolin-2(1H)-one and those of the proton H(18a) of the ethylidene. In fact, from the noesy interaction of the proton H(7) with the proton NH(1) (Figure S12B), we assigned the correct resonance at the proton H(7). The Noesy spectrum showed proximity between the ethylidene proton H(18a) and the proton H(10) of the dihydroquinazolin-2(1H)-one (Figure S12A), and the noesy interactions between the proton H(18a) and the protons H(22,26). Moreover, from Noesy interactions between the Me(27) and the protons H(23,25) we distinguished resonances for 4-methylphenyl from that for the phenyl (Figure S12C). Noesy spectrum also showed a weak interaction between the Me(27) and

the protons H(22,26), Figure S11C, and noe interactions between the protons H(9) and H10, the protons H(7) and H(8) and the protons H(23,25) and H(22,26).

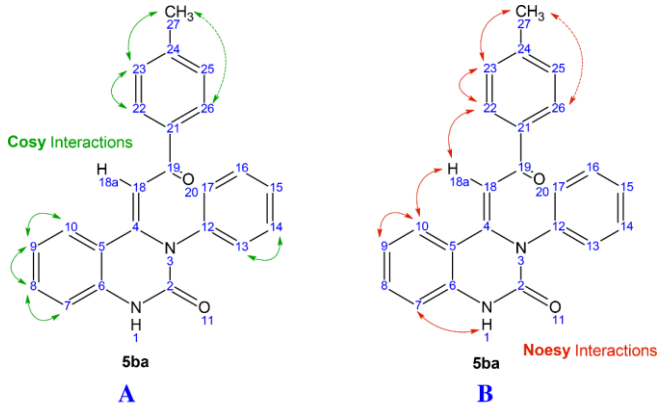


Figure S11. A) Relevant Cosy interactions; B) Relevant Noesy interactions.

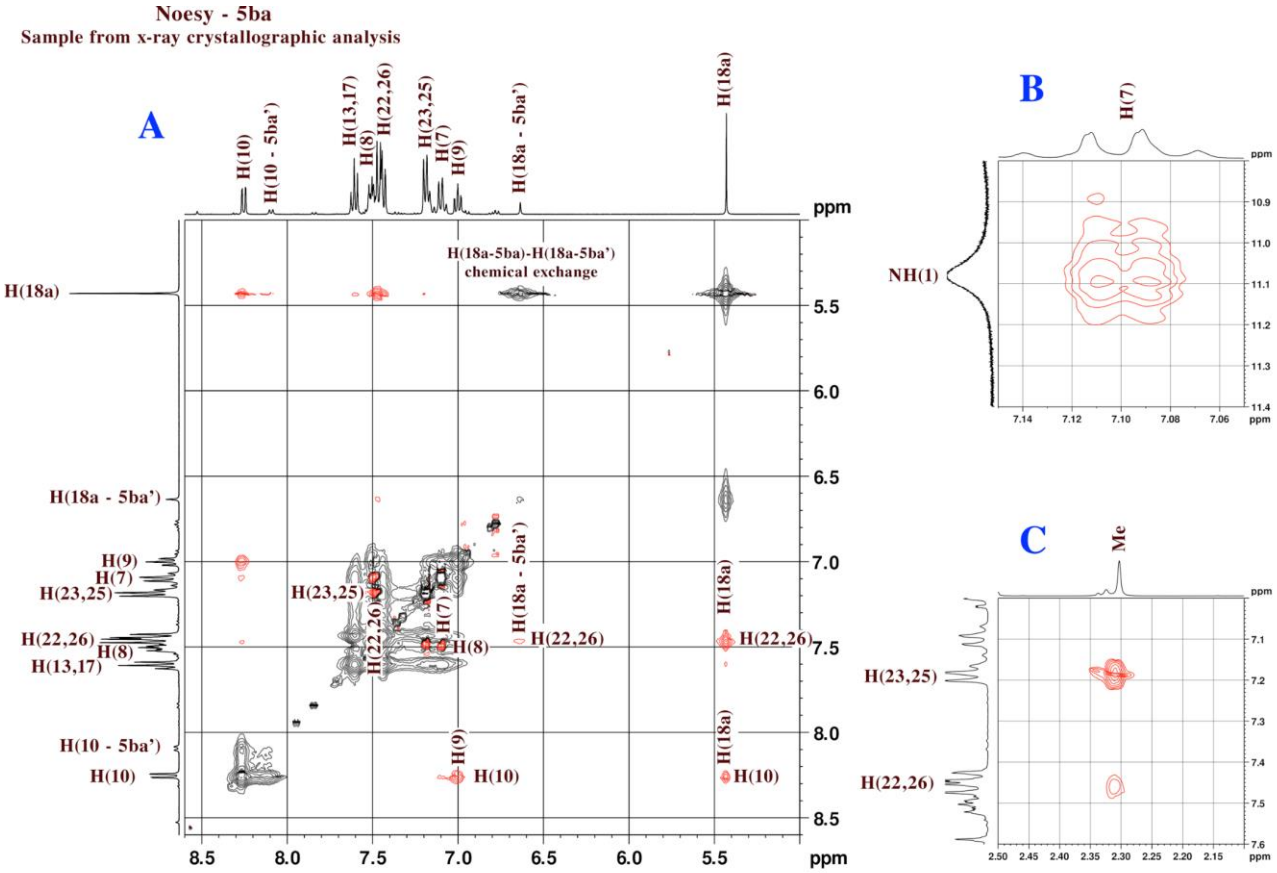


Figure S12. Key NOESY correlations for **5ba**.

Analysis of Cosy spectrum allowed to confirm, among the others, the correct proton assignment for the resonances of H(10), H(22,26) and H(23,25), as shown in Figure S13, confirming that in solution we have the ***Z*** isomer.

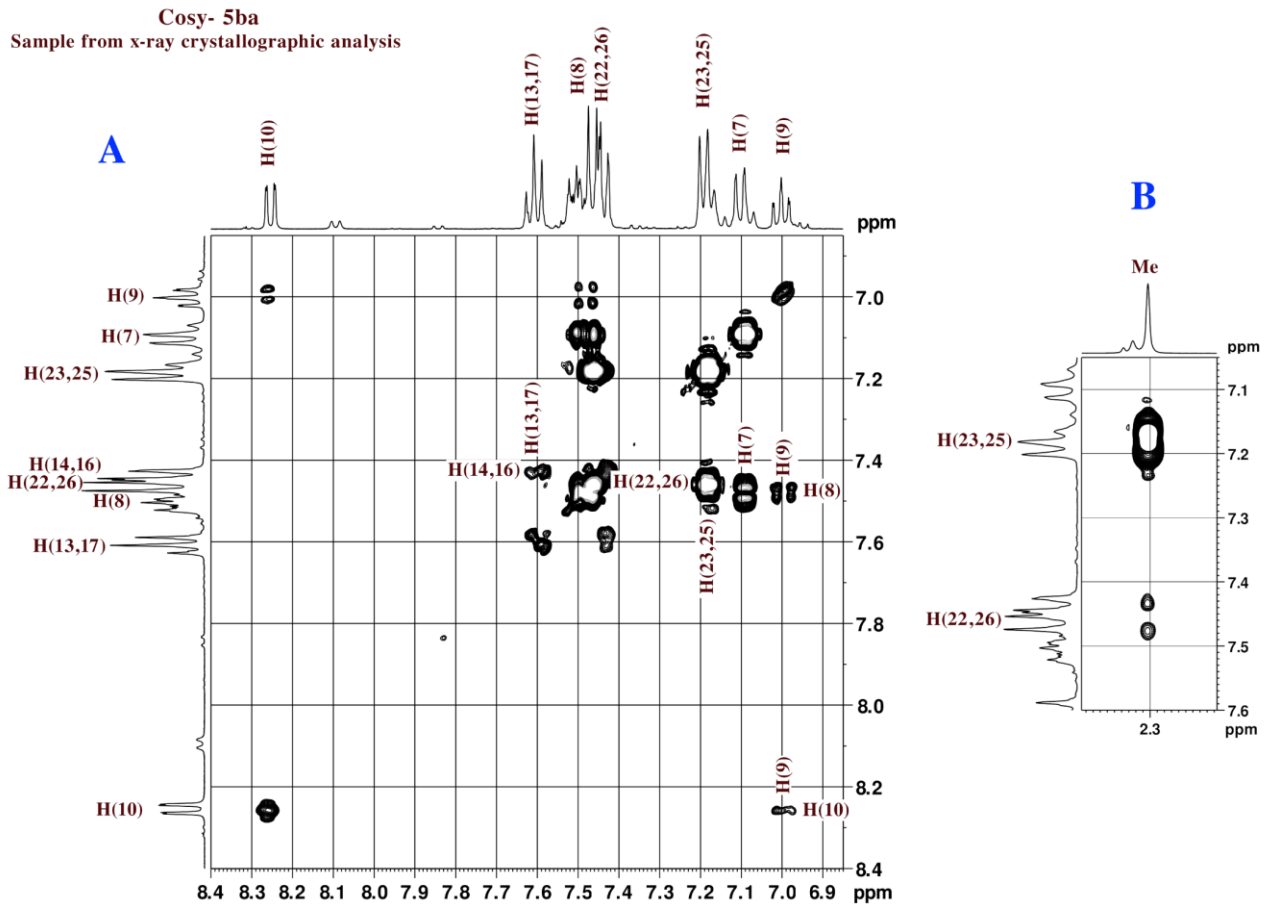


Figure S13. COSY correlations. A) Relevant coupling interactions for **5ba**. B) Cosy interactions for the methyl group.

(4Z)-4-[2-(4-methylphenyl)-2-oxoethylidene]-3,4-dihydroquinazolin-2(1H)-one (6b).

In order to assign the correct stereochemistry to the derivative **6b** it is necessary to assign the correct resonance to the two NH and to the proton H(10) of the 3,4-dihydroquinazolin-2(1H)-one (for structure numbering see Figure S14). In fact, key NOE interactions are those of the proton H(12a) of the 2-oxoethylidene. The Noesy analysis showed the resonance position of the protons H(1a) (see Figure S15), in fact, there was noe interaction between NH(1a) and H(7), while no interaction of NH(3a) with H(7), was seen, nor chemical exchange between NH(1a) and NH(3a), Figure S15. From the analysis of the Noesy spectrum, it was evident that the proton H(12a) interacted with the proton H(10), indicating that the geometry of the double bond was ***Z***, Figure S16A. Moreover, the resonance of NH(3a) was confirmed by the noesy interaction with the protons H(10) and H(16,20) (see Figure S16B). The Noesy spectrum showed also some small interactions between NH(3a) and the protons H(12a) and H(16,20), Figure S16B, and between the methyl group and H(16,20), Figure S16B.

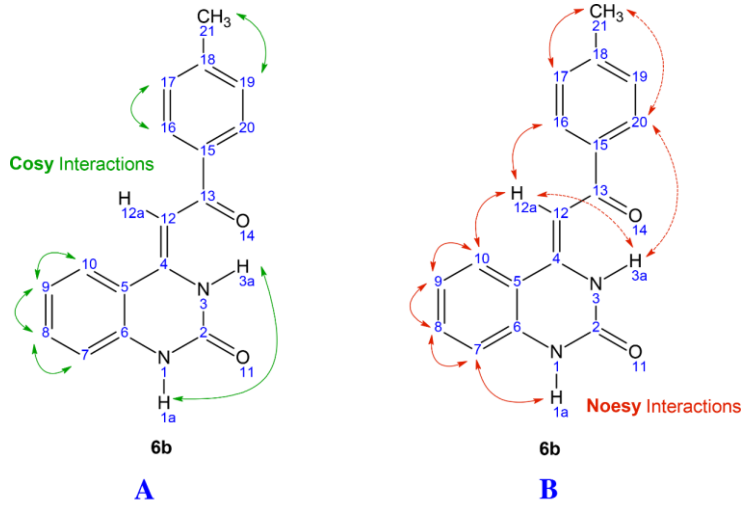


Figure S14. A) Relevant Cosy interactions; B) Relevant Noesy interactions for **6b**.

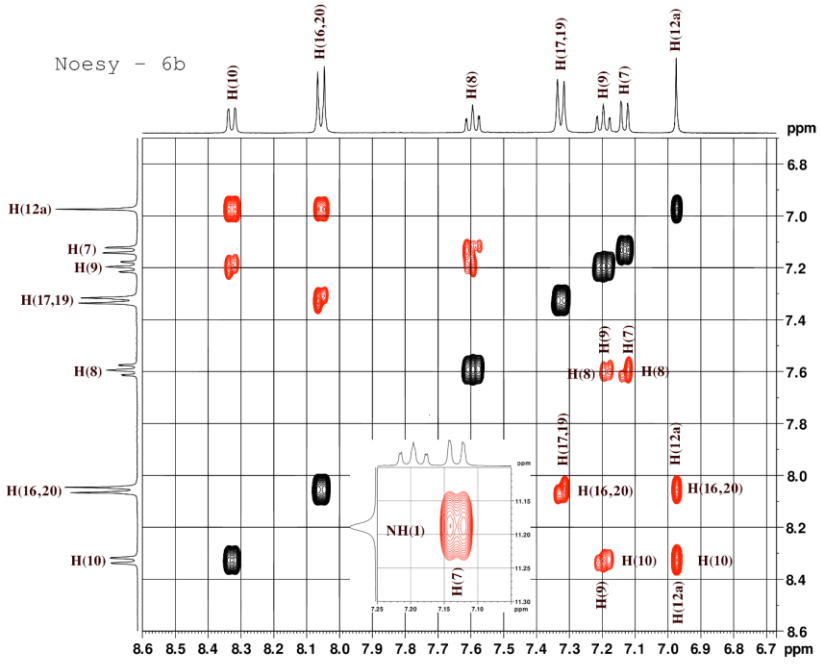


Figure S15. NOESY correlations for **6b**.

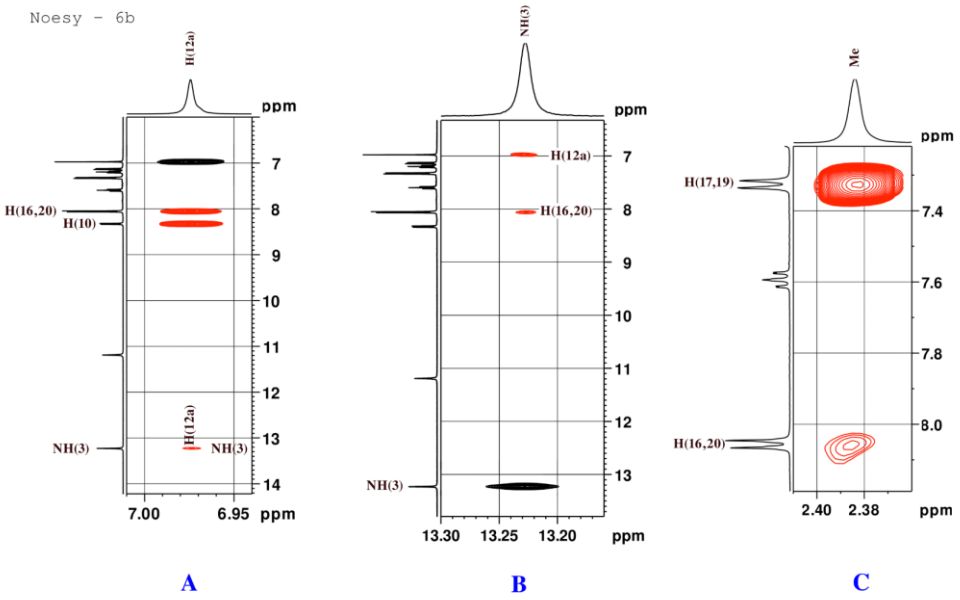


Figure S16. Key NOESY correlations for **6b** A) Noesy for H(12a); B) Noesy for NH(3a); C) Noesy for Me

Analysis of Cosy spectrum allowed to confirm the correct proton assignment (Figure S17).

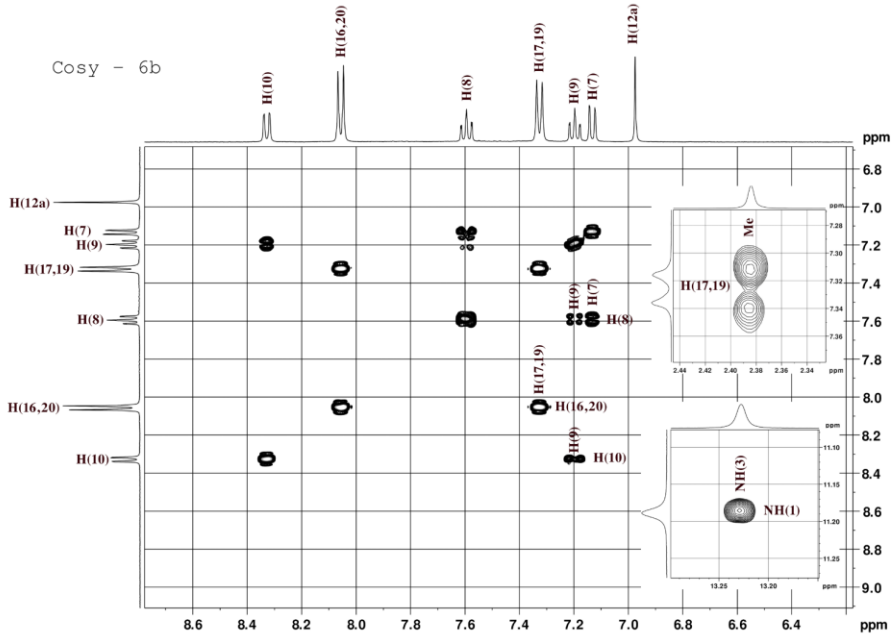


Figure S17. COSY correlations for **6b**.

(2Z)-2-(2-anilino-4H-3,1-benzoxazin-4-ylidene)-1-phenylethanone (7aa).

Spectra for **7aa** acquired in DMSO-d6 at 303 K (Figure S18) showed some overlaps for ^{13}C-NMR, so we decided to acquire the spectra also using acetone-d6 as a solvent at 313 K. Changing from DMSO to Acetone, relative shifts were small, but sufficient to resolve some overlaps on 4H-3,1-benzoxazin-4-ylidene (Figure S18).

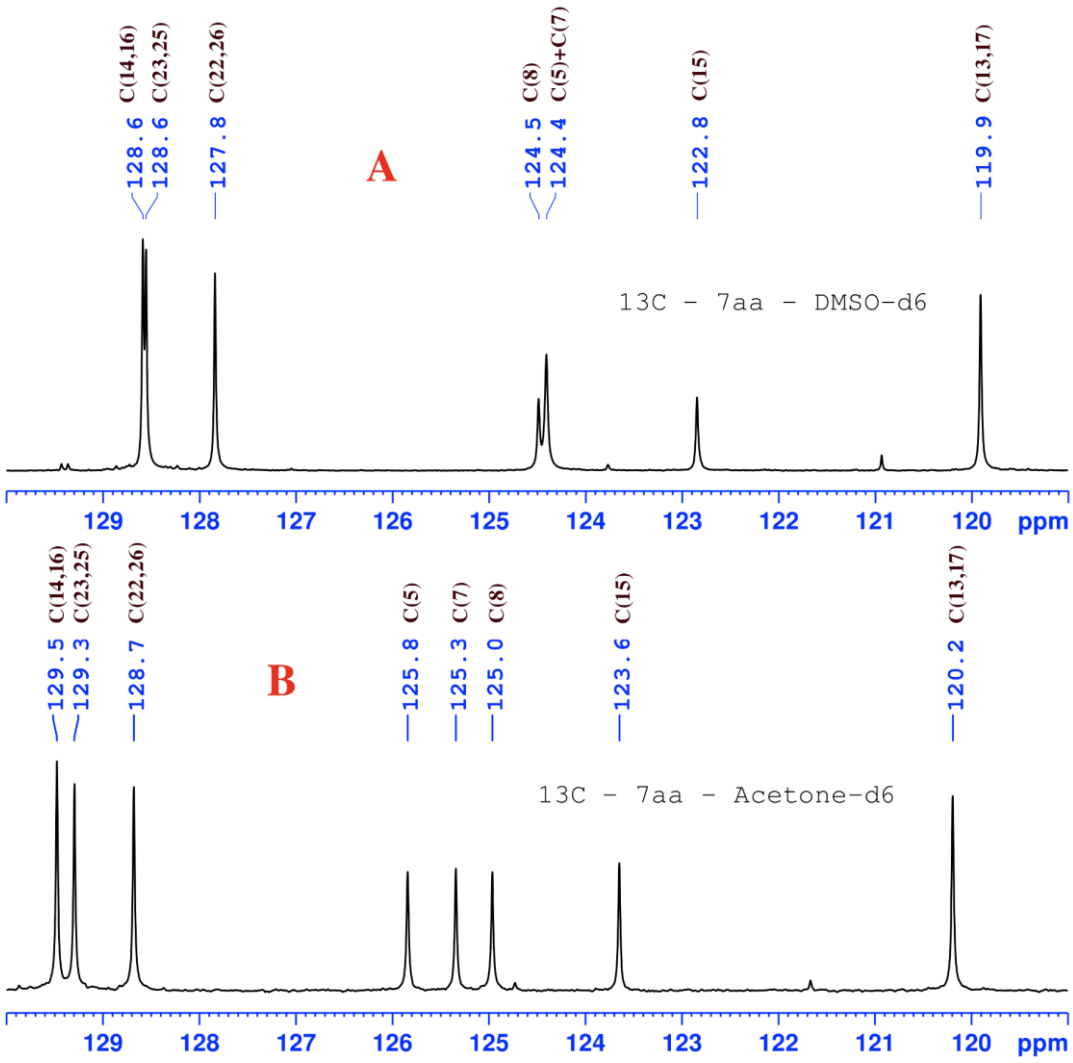


Figure S18. ^{13}C NMR. A) Expansion of ^{13}C NMR for **7aa** in DMSO-d6 at 303 K B) Expansion of ^{13}C NMR for **7aa** in acetone-d6 at 313 K.

Key NOE interactions to establish the absolute stereochemistry for **7aa**, are those of the protons H(13,17) with and NH(11) (for structure numbering see Figure S19) of the anilino, in fact those allow to distinguish the resonances of the anilino from that of the phenylethanone, and those of H(18a). The Noesy analysis showed the resonance position of the protons H(13,17) (see Figure S20A) and consequently the proximity between the proton H(18a) and the proton H(8) of 4H-3,1-benzoxazin-4-ylidene, as well as with the protons (22,26) of phenylethanone (Figure S20B), showing that in solution we have the ***Z*** isomer. The Noesy has also shown the interactions between all protons of the anilino, all protons of the 4H-3,1-benzoxazin-4-ylidene and noesy interaction between the protons H(22,26) and H(23,25) of the phenylethanone (Figure 19A).

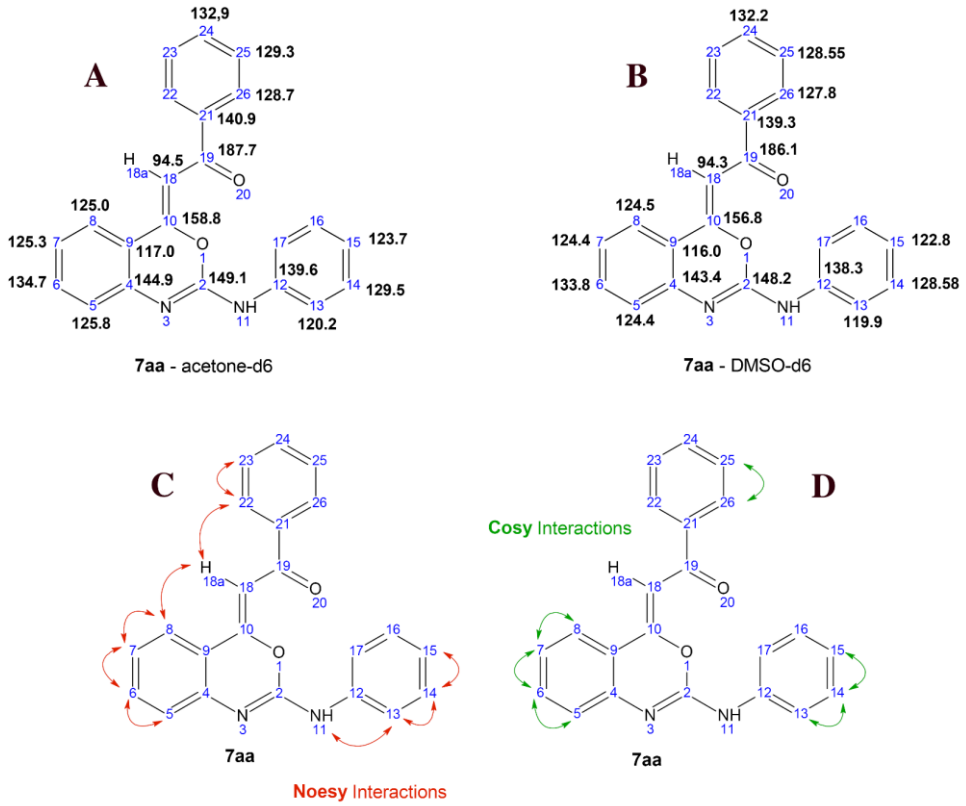


Figure S19. A) ^{13}C assignment in acetone-d6; B) ^{13}C assignment in DMSO-d6; C) Relevant Noesy interactions both in Acetone-d6 and DMSO-d6; D) Relevant Cosy interactions both in Acetone-d6 and DMSO-d6.

The analysis of the Cosy spectrum allowed to confirm the correct assignment of the protons made with the Noesy analysis, as shown in Figure S21.
Analysis of HSQC spectrum provides correlations between carbons and the attached proton for all protonated carbons as shown in Figure S22.
In order to completely assign the ^{13}C-NMR resonances, the HMBC spectra, optimized for 8Hz long rang coupling constant, was acquired (Figure S23).
As shown in the Figure S23A the proton H(15) correlated with the quaternary carbon at 139.6 ppm, so we assigned that resonance at C(12). The quaternary carbon at 149.1 ppm correlated only with the proton H(18a) so we assigned that resonance at C(2), Figure S23B. The quaternary carbon at 140.9 ppm correlated with the protons H(24) and H(23,25) so we assigned that resonance at C(21) Figure S23C. Because the quaternary carbons at 117.0 ppm and 144.9 ppm correlated both with the proton H(6) but only the quaternary carbon at 117.0 ppm correlated with the proton H(18a) we assigned at C(4) the resonance 144.9 ppm and at C(9) the resonance 117.0 ppm Figure S23D. Finally, at the carbon C(10) has been assigned the resonance of 158.8 ppm because it correlated with both the protons H(18a) and H(8), Figure S23E.

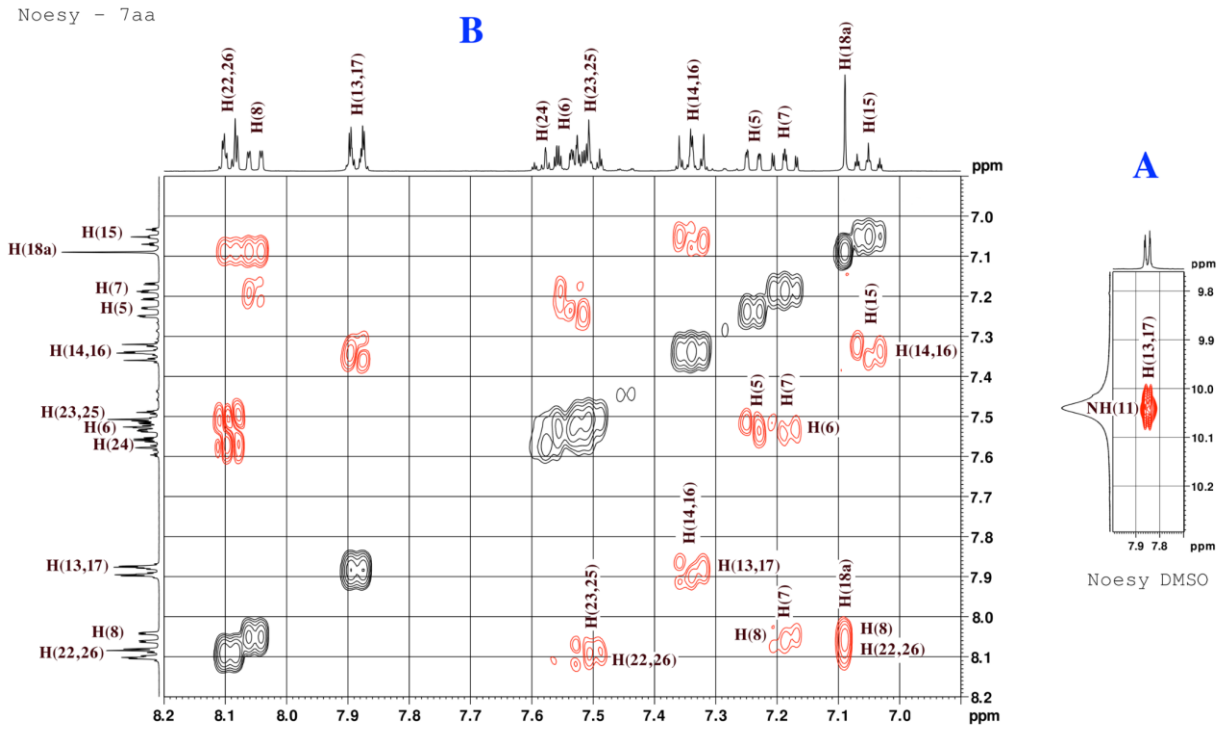


Figure S20. Key NOESY correlations for **7aa**. A) Relevant Noesy interactions for **7aa** in acetone-d6. B) Noesy interaction of the protons H(13,17) with and NH(11) in DMSO-d6 for **7aa**.

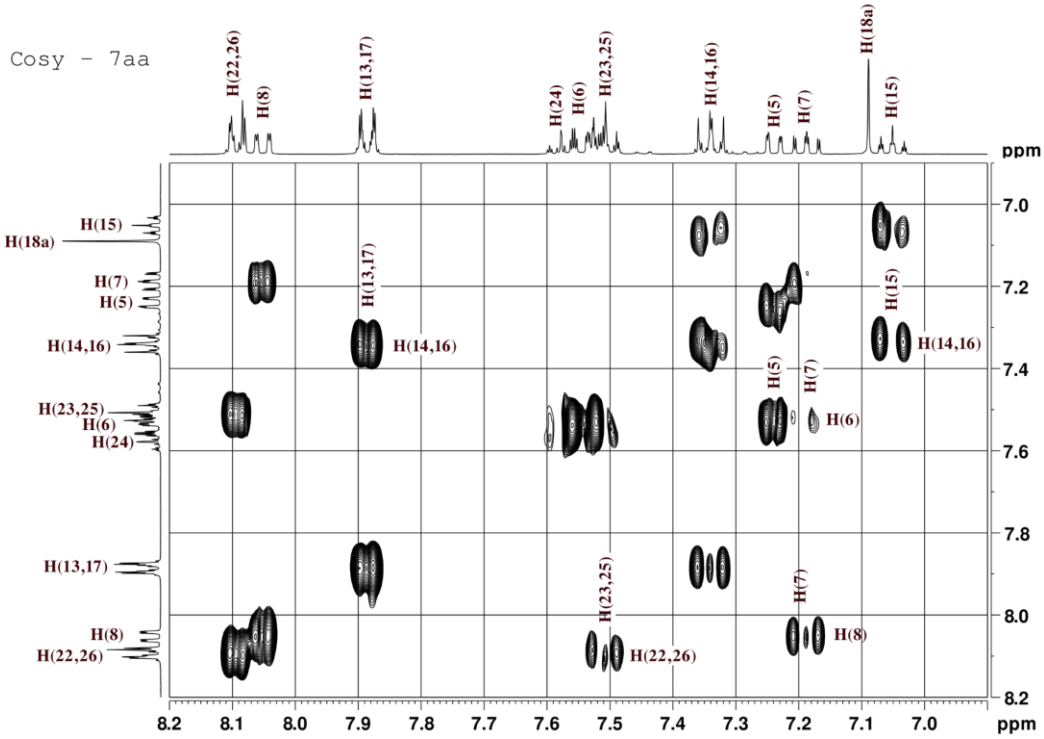


Figure S21. COSY correlations. Relevant coupling interactions for **7aa**.

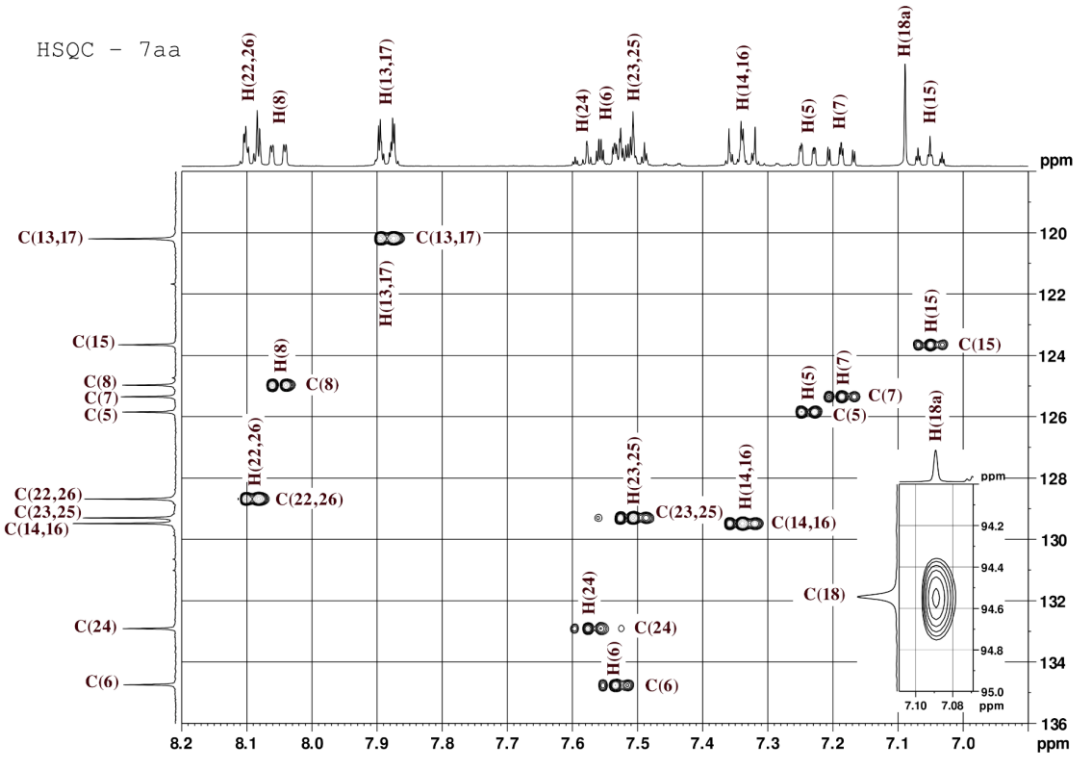


Figure S22. HSQC. Correlations between protons and directly attached (one bond) carbon for **7aa**.

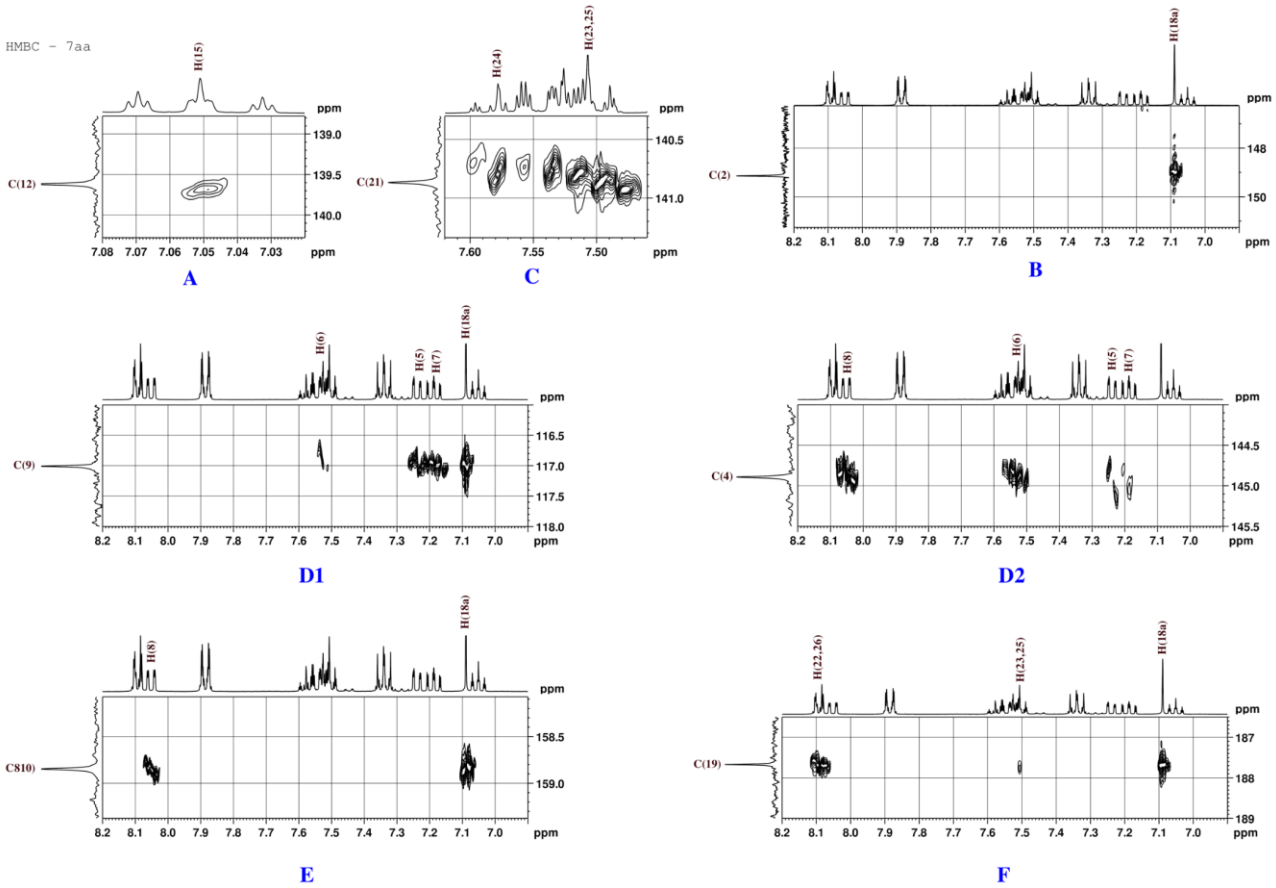


Figure S23. Correlations between protons and carbons through long range coupling constant for **7aa**.

Complete NMR spectra assignment has been made also for **7aa** acquired in DMSO at 303, with similar considerations already

The complete NMR spectra assignment for **7aa**, acquired in DMSO-d6 at 303 K, was made with similar considerations already exploited for the same compound acquired in acetone-d6 at 313 K. No significant changes were recorded, and the Z geometry is also confirmed in DMSO-d6.

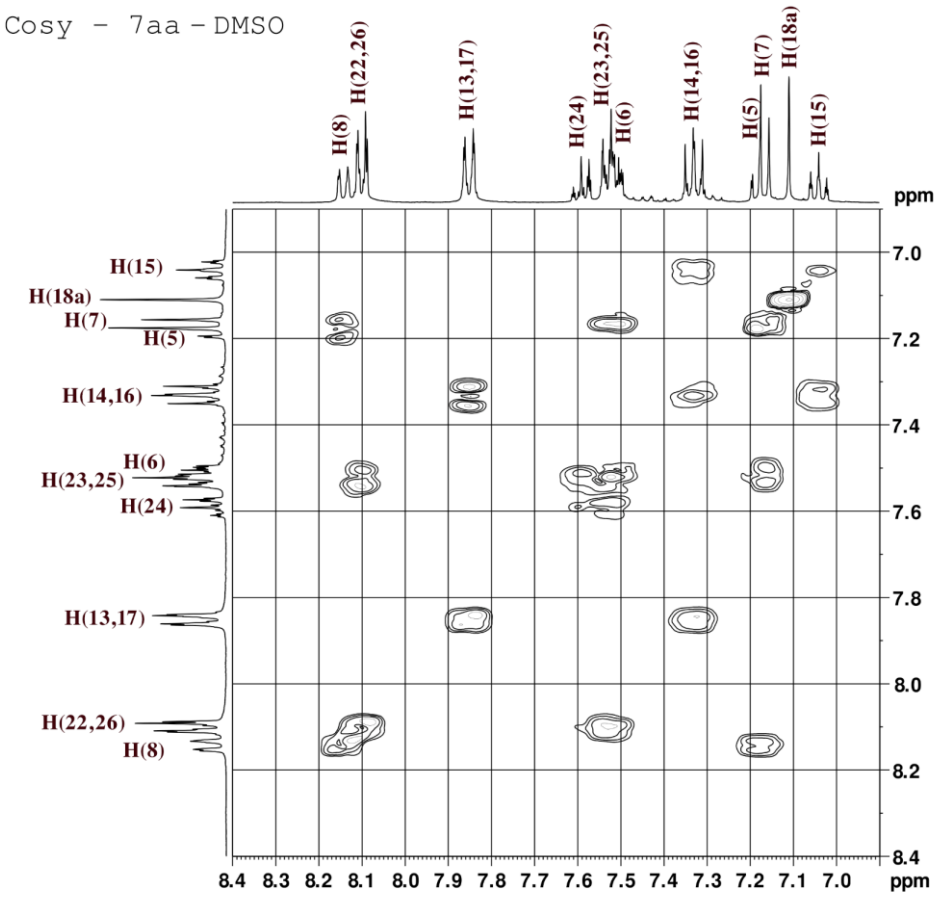


Figure S24. COSY correlations. Relevant coupling interactions for **7aa**.

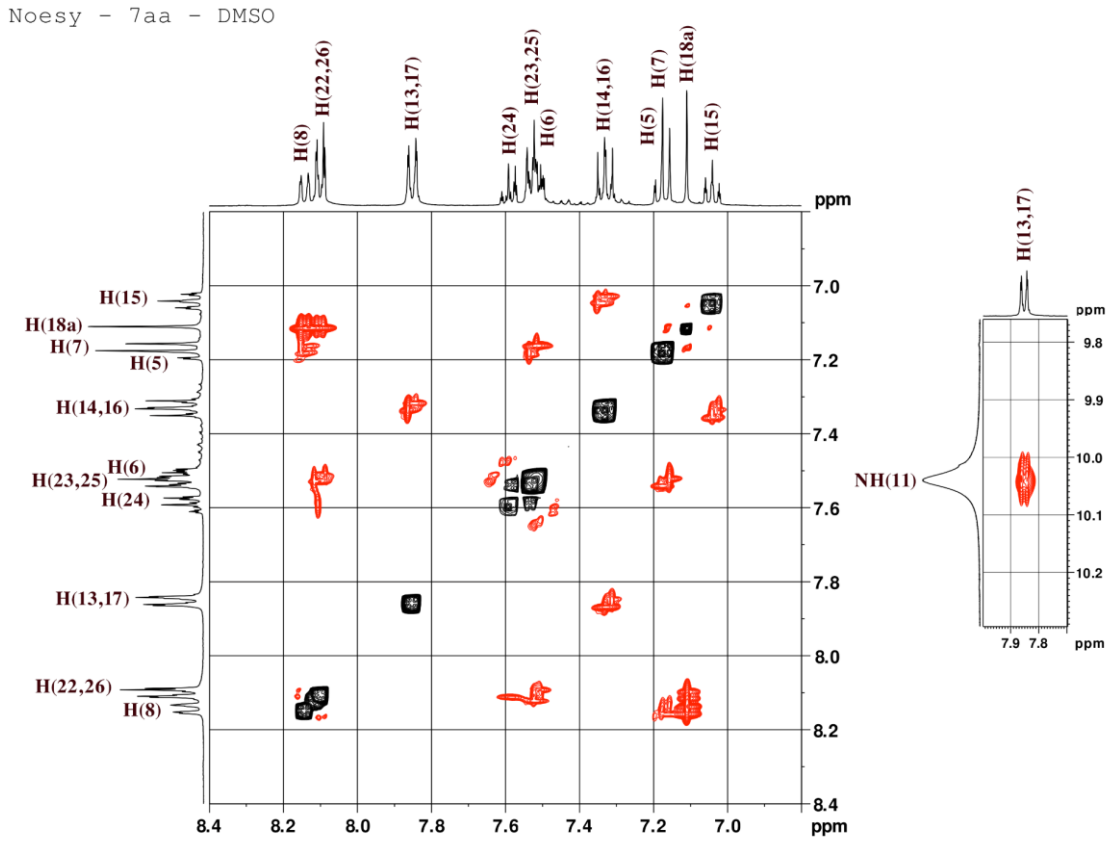


Figure S25. Key NOESY correlations for **7aa** in DMSO-d6

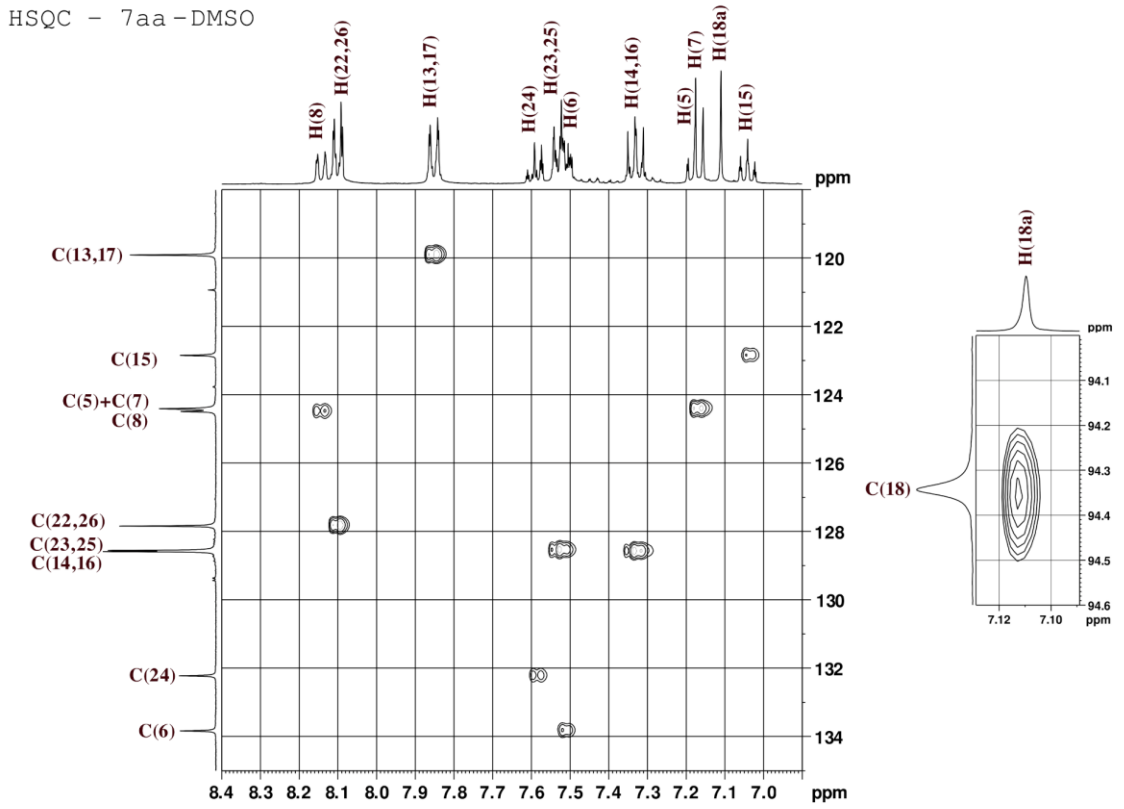


Figure S26. HSQC. Correlations between protons and directly attached (one bond) carbon for **7aa**.

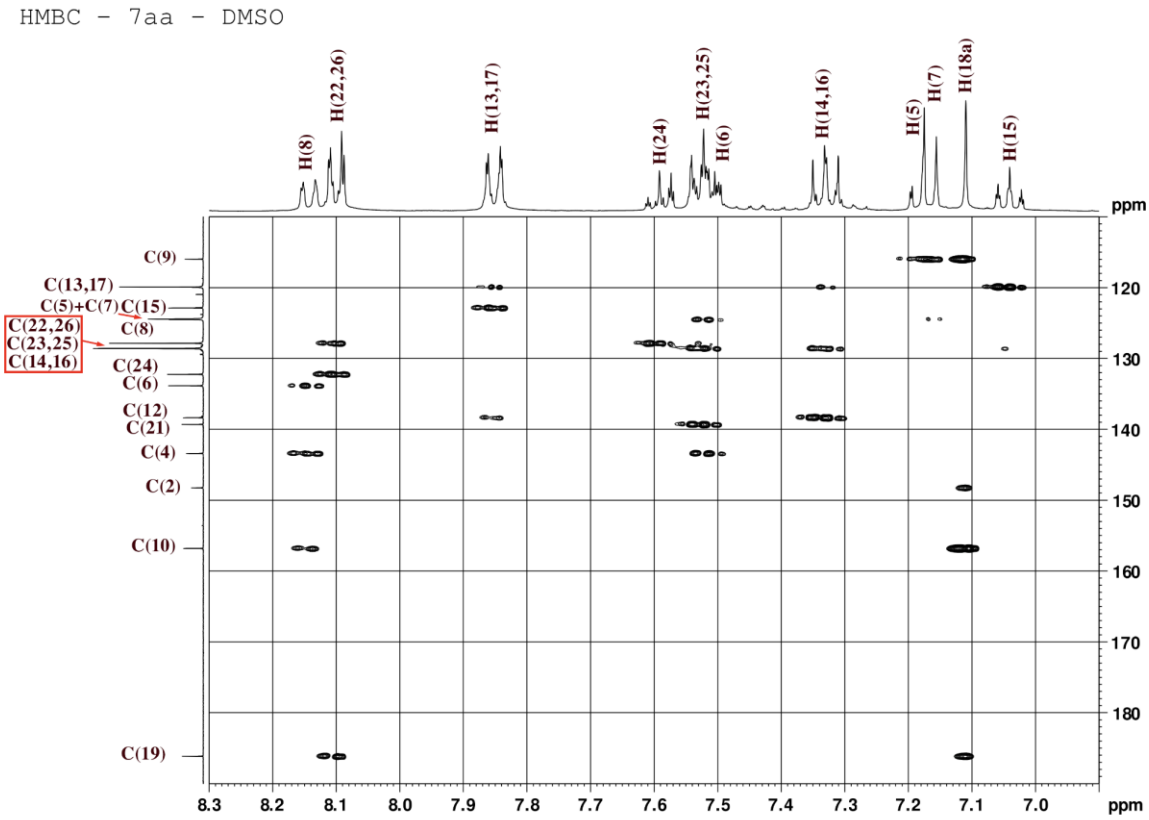


Figure S27. Correlations between protons and carbons through long range coupling constant for **7aa** in DMSO-d6 at 303K.

N-[(4Z)-4-(2-oxo-2-phenylethylidene)-4H-3,1-benzothiazin-2-yl]benzamide (9a)

The Noesy interactions shown in the spectrum for **9a** (Figure S28) indicated that in solution the isomeric structure of **9a** was the same obtained by the X-ray crystallographic analysis of **9h**.

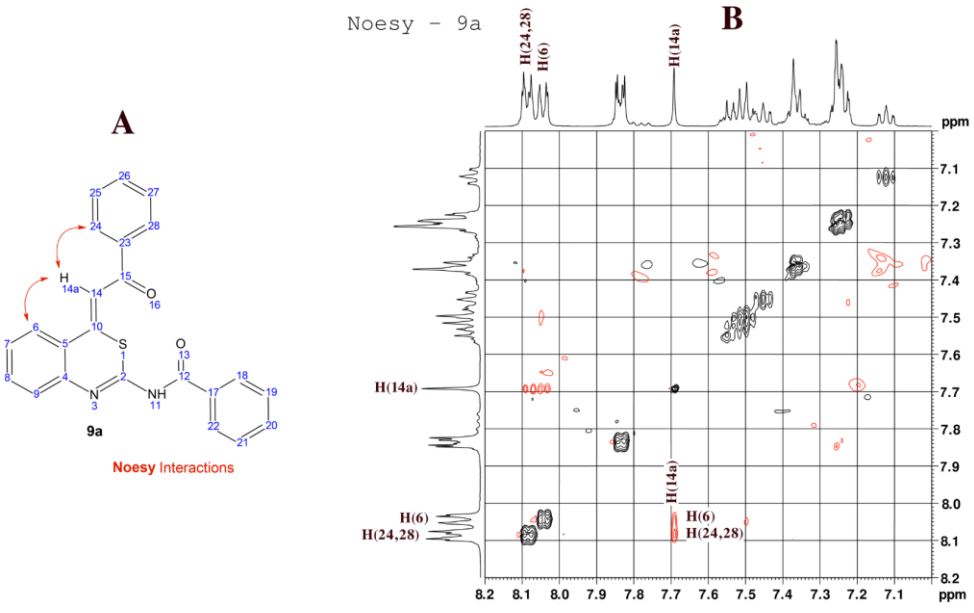


Figure S28. NOESY correlations for **9a**. A) Structure numbering and interactions B) NOESY spectrum for **9a**.

Crystal packing

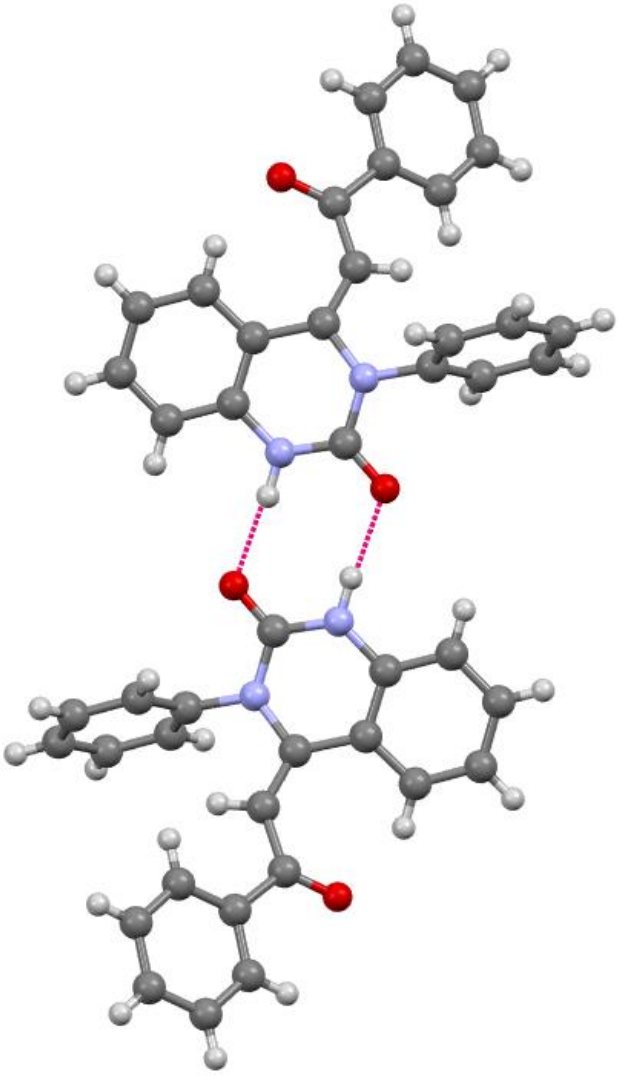


Figure S03. Part of the crystal structure of **5aa''**, showing the formation of a hydrogen bonding network.

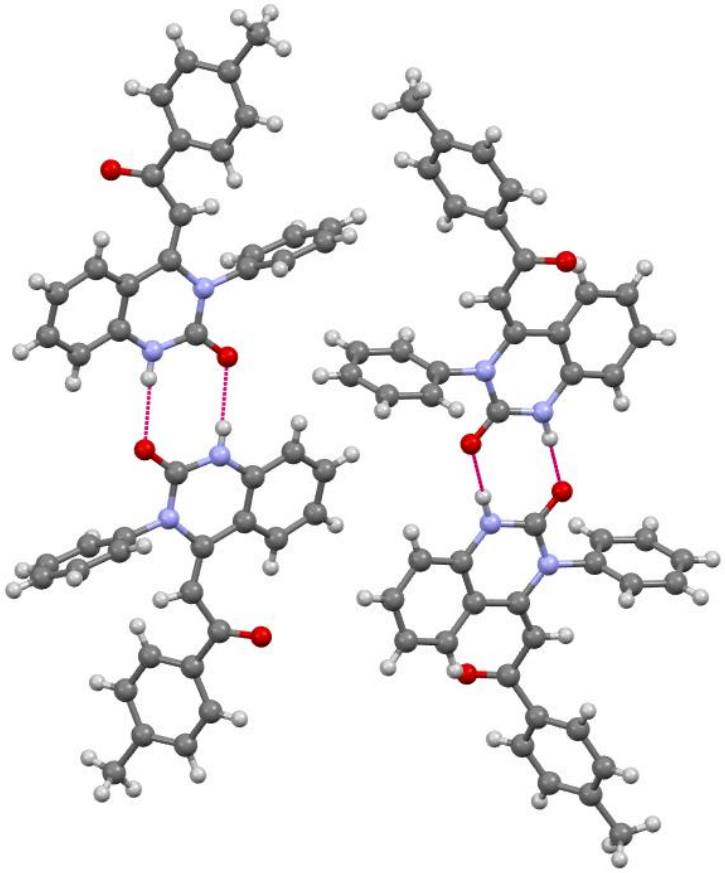


Figure S04. Part of the crystal structure of **5ba''**, showing the formation of a hydrogen bonding network.

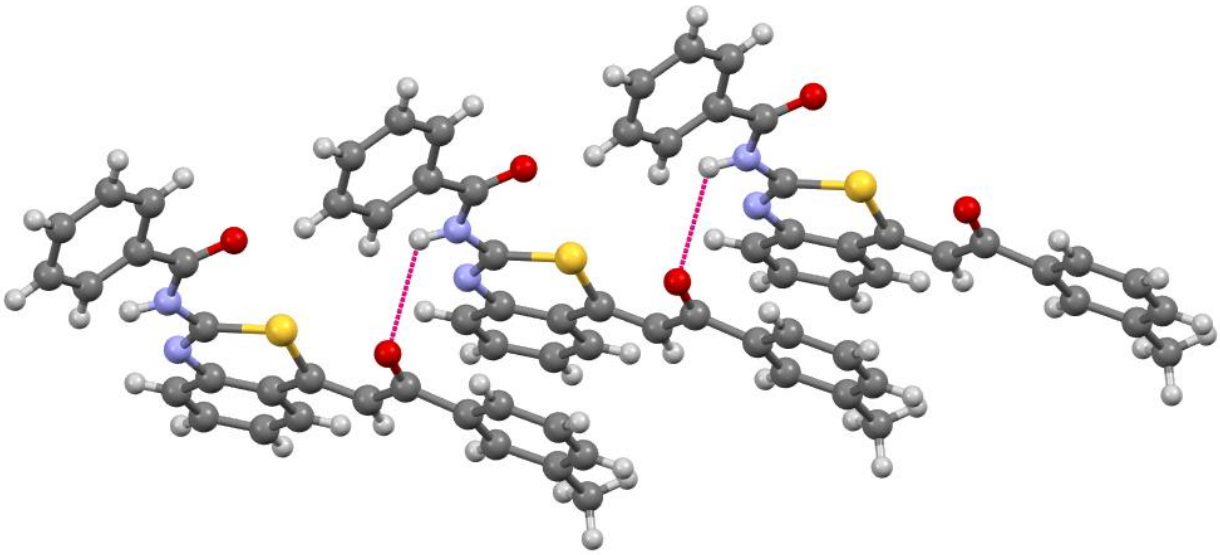


Figure S05. Part of the crystal structure of **9h**, showing the formation of a hydrogen bonding network.

Quantum-Chemical calculations: optimized geometries (see Figures 1 and 4 of the main text), energies and harmonic frequencies

Reaction B

R2

C	0.145989	-0.000000	-0.122484
C	0.002989	-0.000000	1.267912
C	1.129062	-0.000000	2.078939
C	2.400394	-0.000000	1.505858
C	2.544928	-0.000000	0.120971
C	1.419316	-0.000000	-0.694899
H	-0.995422	0.000000	1.692079
H	1.018434	-0.000000	3.158894
H	3.280871	-0.000000	2.141729
H	3.535053	-0.000000	-0.324171
H	1.522470	-0.000000	-1.774730
C	-1.081424	0.000000	-0.950943
O	-2.206141	0.000000	-0.506618
N	-0.846420	0.000000	-2.344402
C	-1.491954	0.000000	-3.363482
S	-2.221053	0.000000	-4.745152

Frequencies

41.3395	55.9696	88.3037
170.6648	200.3670	321.2937
423.9269	442.0005	448.5596
494.2619	500.1749	636.1237
670.9365	701.6034	726.4135
744.8172	829.0753	884.0821
891.4022	984.2260	1023.7880
1030.6812	1042.0588	1065.5807
1121.3455	1151.8298	1198.4139
1214.3860	1313.1085	1358.0928
1370.2444	1512.4728	1555.6107
1672.6239	1691.1092	1800.2142
2082.6417	3215.0148	3226.0515
3235.0305	3245.1460	3249.3637

Energy -835.808185223 a.u.
PCM=-835.9339254

R1

C	-1.499473	-1.517807	0.040718
C	-0.824704	-0.287139	-0.001909
C	-1.562589	0.920878	-0.028596
C	-2.964114	0.845327	-0.002237
C	-3.606732	-0.379248	0.044174
C	-2.880822	-1.574533	0.064095

C	0.595389	-0.231195	-0.007880
C	1.801884	-0.105830	-0.003503
C	3.240101	0.056075	-0.000378
C	4.058514	-1.209670	-0.051643
N	-0.924732	2.133345	-0.120216
O	3.745271	1.164548	0.041846
H	-3.542804	1.764807	-0.027038
H	-4.692471	-0.406065	0.063289
H	-3.391932	-2.530603	0.098663
H	-0.908902	-2.428397	0.059194
H	3.820808	-1.774431	-0.959441
H	5.119800	-0.955948	-0.038349
H	3.816211	-1.850395	0.802891
H	-1.438552	2.965300	0.127469
H	0.070103	2.168704	0.056326

Frequencies

40.3680	50.5083	69.3488
103.6357	158.8604	168.4109
244.5928	286.1247	347.0302
395.0330	413.4945	437.3448
495.7149	520.6409	525.6487
585.4522	592.9918	623.0694
629.6842	690.7516	772.1227
776.6990	836.8022	883.9522
896.9963	980.0864	1001.4637
1012.5805	1060.0420	1062.1510
1091.0511	1172.2467	1197.7883
1207.2148	1301.1683	1337.7466
1360.8806	1375.5693	1425.2759
1492.9820	1499.8956	1520.7703
1555.1551	1648.5272	1682.4006
1703.6500	1781.6411	2324.6017
3081.7847	3147.3059	3190.8094
3205.0236	3220.8101	3227.7080
3243.8192	3609.0332	3720.0649

Energy: -516.145936015
PCM: -516.2671146

TS1B

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C	4.016035	-2.264559	-0.164799
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C	2.421127	-4.029097	-0.540820
N	0.668198	-0.781769	-0.855497
C	-0.513517	-0.677484	0.488285

S	0.195519	-0.685879	1.949398
C	3.311359	0.091514	-0.350935
C	3.492429	1.287935	-0.366332
C	3.664684	2.732739	-0.383193
O	2.826942	3.438386	-0.911675
N	-1.602103	-0.572237	-0.149626
C	-2.854692	-0.692326	0.470463
O	-3.107112	-1.559578	1.283052
C	-3.886665	0.278470	-0.003220
C	-5.171527	0.192517	0.538435
C	-6.158582	1.083708	0.138570
C	-5.868651	2.068308	-0.804762
C	-4.589260	2.158872	-1.346108
C	-3.600130	1.265893	-0.946947
C	4.903042	3.272800	0.279486
H	0.401299	-3.407049	-0.959796
H	2.183471	-5.086632	-0.592011
H	4.497211	-4.351162	-0.065309
H	5.021278	-1.931053	0.068892
H	5.797882	2.837722	-0.178289
H	4.922771	4.359146	0.180779
H	4.910465	2.993980	1.338769
H	0.053242	-0.980147	-1.645357
H	-2.601409	1.328552	-1.363975
H	-4.360796	2.926651	-2.079361
H	-6.640729	2.765967	-1.116561
H	-7.155679	1.013325	0.563008
H	-5.374135	-0.578992	1.273556
H	1.035520	0.168680	-0.949407

Frequencies:

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22.4597	35.2534	36.5108
50.9686	54.3148	67.7591
86.0469	111.7524	118.5290
147.8083	165.8979	183.0304
205.3558	233.8379	275.6157
289.8481	374.9113	387.3368
403.3099	425.5419	443.9561
478.0376	486.0835	494.2969
504.7003	528.2774	568.7710
585.5832	607.6234	615.8552
627.9813	637.2943	688.4592
694.5716	712.1604	732.3665
765.3268	774.5793	788.2774
802.7017	829.5375	849.0994
883.9867	884.3291	904.8315
916.2098	980.4575	991.6492
1003.9981	1021.7257	1029.9720
1031.1000	1037.2895	1062.8144
1064.0091	1080.0884	1102.5288

1119.3710	1131.8262	1182.5719
1195.2707	1197.4985	1204.5409
1210.4846	1215.6186	1261.3338
1313.3241	1333.4118	1336.8380
1355.0452	1365.2620	1373.4523
1427.0946	1491.6839	1497.8646
1509.8536	1520.1469	1554.3196
1562.6088	1658.4761	1671.5823
1678.4262	1691.4053	1695.3812
1700.7555	1790.8167	1795.0873
2349.1283	3082.4202	3147.7905
3195.1421	3208.9164	3220.8595
3222.7624	3230.8188	3231.1695
3241.8069	3248.2976	3249.9812
3250.1311	3467.5681	3558.1484

Energy: -1351.9247889
PCM: -1352.179599

1B

C	0.546984	-0.276471	-0.220144
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C	1.398774	-0.632953	2.011210
C	2.667423	-0.861691	1.488962
C	2.876395	-0.796175	0.114006
C	1.814501	-0.502906	-0.740186
C	-1.040568	-0.073164	1.675787
O	-1.991641	0.092078	0.933069
N	-1.183399	-0.116735	3.063247
C	-1.710601	0.821336	3.727216
S	-2.148050	2.418102	3.595289
N	-2.047234	0.281504	5.241685
C	-1.829120	-1.114398	5.560810
C	-2.746232	-2.060494	5.085591
C	-2.533770	-3.406126	5.402202
C	-1.428714	-3.787468	6.152440
C	-0.522311	-2.832008	6.602908
C	-0.724073	-1.487811	6.306090
C	-3.846462	-1.643684	4.277412
C	-4.732684	-1.237988	3.562664
C	-5.740389	-0.768550	2.607450
C	-5.367334	0.453352	1.821008
O	-6.787567	-1.372436	2.485259
H	-0.019496	-0.736592	6.652680
H	0.342115	-3.129405	7.187370
H	-1.273674	-4.835848	6.385463
H	-3.241253	-4.144953	5.042050
H	-5.223947	1.304911	2.496412
H	-4.406487	0.302679	1.314902

H	-6.157583	0.675801	1.102080
H	1.223664	-0.688447	3.079967
H	3.493822	-1.092339	2.154802
H	3.867615	-0.973784	-0.293308
H	1.977135	-0.450645	-1.812541
H	-0.293365	-0.045958	-0.866104
H	-3.031986	0.544960	5.346893
H	-1.522497	0.904038	5.859765

Frequencies

13.0308	25.7534	29.6648
37.4452	51.1016	57.6677
65.4937	74.5012	86.2817
129.8992	149.8330	157.7681
166.1191	169.0135	219.5412
226.6889	239.7527	295.8498
349.3055	370.0681	389.6191
420.8918	424.0720	444.5177
475.8224	486.0710	501.3629
529.1951	551.9235	556.1242
584.5095	612.6699	615.4545
635.3216	637.4239	688.7326
692.2088	713.0569	740.8500
761.4017	777.9349	788.3650
832.0454	845.3630	868.9279
882.7531	899.0025	906.9673
915.8545	979.4394	989.2707
1011.9271	1019.8633	1031.0619
1031.2939	1037.0991	1063.4075
1064.7460	1081.7700	1113.2266
1135.6264	1138.4904	1195.6387
1201.5232	1209.2164	1209.6215
1219.2529	1244.0131	1291.5621
1320.1759	1321.8524	1332.3695
1356.3707	1365.7077	1374.4681
1438.1711	1487.8242	1498.2298
1510.3099	1518.4264	1554.9557
1562.5388	1648.3031	1665.8864
1671.6892	1692.1280	1703.9758
1713.0512	1781.0685	1801.5765
2362.0484	3074.1054	3137.7281
3191.2506	3209.1056	3214.1166
3220.3707	3230.1493	3231.3477
3243.1134	3245.2522	3249.3930
3251.7364	3457.0488	3535.2124

Energy: -1351.92818625
PCM: -1352.1846862

2B

C	-0.000342	-0.481263	-0.012785
C	0.175125	-0.055696	1.320343
C	1.411662	-0.216423	1.941393
C	2.477049	-0.791604	1.257302
C	2.318698	-1.192508	-0.066567
C	1.091491	-1.034683	-0.695435
N	-0.901479	0.490482	2.069605
H	1.528379	0.118266	2.967751
H	3.433269	-0.915026	1.755979
H	3.149853	-1.632594	-0.608116
H	0.951771	-1.354420	-1.722648
C	-1.269659	-0.382792	-0.660092
C	-2.338407	-0.303645	-1.218923
C	-3.633106	-0.186442	-1.883969
O	-3.747037	-0.499831	-3.054071
C	-4.761992	0.339767	-1.044800
H	-4.894795	-0.285027	-0.154815
H	-4.518719	1.347206	-0.689620
H	-5.677770	0.352464	-1.638201
H	-1.217699	-0.018386	2.886062
C	-1.689677	1.563816	1.756401
S	-3.095256	1.861624	2.567129
N	-1.129063	2.381602	0.788141
H	-0.139241	2.254533	0.613888
C	-1.792899	3.216204	-0.115702
O	-2.988462	3.179634	-0.303437
C	-0.888111	4.134059	-0.875703
C	0.321184	4.604155	-0.357770
C	1.107749	5.476098	-1.103743
C	0.693855	5.876246	-2.370884
C	-0.515803	5.415539	-2.886793
C	-1.307889	4.553985	-2.139399
H	0.636526	4.327317	0.644207
H	2.039592	5.849822	-0.690578
H	1.310324	6.554040	-2.953821
H	-0.843087	5.730983	-3.872669
H	-2.258623	4.195780	-2.519614

Frequencies

14.2124	27.2031	29.6013
42.2582	59.1585	65.5757
73.9690	83.6335	98.3610
128.6225	148.0517	162.5417
170.6325	183.0495	222.1298
250.6395	261.8966	302.7478
350.7236	383.8880	402.8160
417.1910	422.0599	458.0974

477.0257	506.7175	514.4733
537.3996	563.1784	569.3832
580.4677	613.9076	618.8957
632.4620	636.9637	650.5298
691.7670	699.6777	711.1898
731.1779	762.0764	791.2514
811.0313	847.5630	856.8388
880.6556	901.8879	922.0259
928.6875	970.3907	998.2123
1010.3580	1015.4233	1029.9633
1031.2525	1037.7351	1066.1368
1068.0083	1081.4745	1120.5930
1138.4671	1148.2175	1198.5910
1199.2559	1210.3154	1220.0306
1236.7582	1268.9158	1280.6918
1301.3729	1325.1619	1341.6265
1351.0270	1372.6609	1375.6859
1433.1519	1490.4757	1497.9504
1499.4179	1508.8064	1531.7990
1553.1895	1556.8396	1584.5142
1653.3430	1671.6448	1686.1467
1693.0184	1793.2410	1830.3056
2361.0760	3080.4473	3147.9852
3191.4351	3211.4148	3219.1425
3220.5018	3229.1322	3229.6085
3238.1965	3238.9852	3247.7224
3249.2343	3606.4909	3622.2695

Energy: -1351.97248823
PCM:-1352.22283588

TS2B

C	5.783156	-1.151447	-1.798305
H	6.571277	-1.451794	-2.482666
C	4.457172	-1.146894	-2.221930
H	4.208001	-1.443309	-3.236483
C	6.096968	-0.770596	-0.495240
H	7.130015	-0.773641	-0.160716
C	3.447049	-0.762309	-1.346481
H	2.417334	-0.763356	-1.683884
C	3.755631	-0.378781	-0.039552
C	5.088501	-0.386659	0.378987
H	5.311447	-0.087887	1.397577
C	2.722879	0.044855	0.958827
O	3.020716	0.369764	2.092911
N	1.410867	0.043993	0.487414
C	0.319771	0.337648	1.214630
S	-0.096565	0.739351	2.730305
N	-0.681084	0.147493	0.073287

C	-1.497490	1.251481	-0.336739
C	-2.851086	1.038819	-0.640434
C	-0.933439	2.513315	-0.472215
H	0.110887	2.666980	-0.220585
C	-1.715264	3.572452	-0.915283
H	-1.270900	4.557620	-1.014065
C	-3.059050	3.376439	-1.229327
H	-3.665982	4.206498	-1.575471
C	-3.623031	2.117666	-1.094076
H	-4.668228	1.948328	-1.329334
C	-3.436847	-0.254104	-0.485028
C	-3.936010	-1.348983	-0.351107
C	-4.586494	-2.642120	-0.184289
O	-5.705656	-2.826862	-0.619064
C	-3.801109	-3.698994	0.547493
H	-2.866868	-3.911941	0.016123
H	-3.535429	-3.346553	1.550026
H	-4.398828	-4.608827	0.619969
H	0.441401	-0.094261	-0.461055
H	-1.255878	-0.681821	0.240412

Frequencies

i1743.2821	12.2561	17.0876
21.0100	28.0885	36.4734
45.9768	68.1036	81.6908
97.8512	109.9374	132.9252
149.1044	166.7864	196.0722
208.8745	241.1927	259.0949
293.6848	327.3608	392.6900
421.6289	423.7579	452.4773
471.5494	482.5561	504.1868
513.0912	549.7315	569.4203
573.6910	602.1069	629.4134
637.5862	663.6433	691.0342
708.8717	714.2784	735.6573
757.4423	785.5480	805.2616
839.9408	848.7982	880.5789
882.8296	910.9078	933.1478
974.3822	986.9066	997.6926
1002.4321	1008.9110	1019.1790
1031.1072	1031.4133	1038.9465
1061.6556	1068.7112	1084.5241
1120.6363	1136.2223	1194.6446
1196.8639	1203.6613	1207.2063
1215.9272	1256.2968	1295.0946
1331.7578	1334.5603	1340.0010
1360.8971	1366.8469	1374.1829
1426.0837	1454.3215	1476.0075
1492.3743	1499.5268	1509.2849
1519.6430	1556.1015	1562.6295
1666.5826	1670.6002	1692.1134

1698.0777	1781.2798	1800.5740
2073.4096	2344.2697	3080.2253
3144.9628	3194.1962	3210.8641
3221.6559	3226.0283	3232.9524
3235.7638	3243.7212	3249.4876
3250.6370	3251.6922	3492.4932

Energy: -1351.89761375
PCM: -1352.147759

TS3B

C	-3.706498	-0.265955	-0.155260
C	-4.089582	0.597289	0.873736
H	-3.328385	1.105103	1.453576
C	-5.437639	0.799092	1.149467
H	-5.730939	1.470008	1.951344
C	-6.408642	0.140883	0.399790
H	-7.461156	0.298881	0.616536
C	-6.030712	-0.721771	-0.627985
H	-6.787067	-1.236537	-1.212623
C	-4.685676	-0.925008	-0.904290
H	-4.370807	-1.593436	-1.698401
C	-2.278616	-0.522564	-0.492268
O	-1.947820	-1.279401	-1.386402
N	-1.350603	0.185462	0.300163
C	-0.097281	-0.002743	0.120940
S	0.886415	-0.954643	-0.868578
N	0.699130	0.876006	1.085319
H	-0.002240	1.392746	1.625143
H	1.208747	0.233978	1.713761
C	1.674517	1.759847	0.436003
C	1.524598	3.135248	0.452679
H	0.670878	3.603585	0.934920
C	2.509041	3.901542	-0.162910
H	2.425053	4.983053	-0.167712
C	3.600240	3.276557	-0.766417
H	4.369311	3.880462	-1.237910
C	3.715791	1.890670	-0.778968
H	4.562670	1.402835	-1.248902
C	2.736123	1.099777	-0.177159
C	2.754661	-0.360984	-0.110708
C	3.563394	-1.232620	0.372346
C	3.536845	-2.623136	0.675227
O	2.969954	-3.049284	1.685480
C	4.307123	-3.557647	-0.235911
H	5.285918	-3.764552	0.210787
H	3.763788	-4.502729	-0.314162
H	4.468700	-3.130772	-1.229995

Frequencies

i190.8529	9.4528	25.7219
30.8936	49.8775	61.0463
70.9176	74.8840	81.9476
109.8698	136.5886	148.8072
175.4197	199.5089	215.1010
248.8289	281.8418	325.3871
360.5315	373.1216	423.8741
432.6829	452.0263	460.7972
484.7036	501.8964	508.7446
541.3945	563.7760	577.4895
611.2993	637.2646	648.9104
663.6089	693.3469	708.6777
724.0308	740.2396	743.4543
766.9732	781.2600	832.9792
845.2854	848.8480	883.5762
886.5762	905.6846	951.5240
982.0338	983.3325	1010.6665
1022.0053	1024.8586	1030.0122
1032.7243	1039.2353	1056.1215
1066.5273	1070.8154	1107.5466
1123.1465	1149.0282	1195.5881
1196.6878	1199.3611	1210.2640
1221.1070	1260.3986	1314.7320
1328.9699	1333.2935	1355.8112
1366.9392	1378.5624	1381.4568
1415.4257	1500.4393	1503.5292
1510.3273	1518.2088	1548.9253
1554.3422	1621.5719	1629.7321
1664.5393	1670.1737	1691.3423
1695.1012	1705.7529	1778.9622
1864.2997	3079.0598	3148.6070
3172.8393	3211.9088	3214.8946
3223.2848	3226.8952	3233.9058
3243.9432	3249.7156	3251.8276
3258.1025	3358.0216	3494.5649

Energy: -1351.89002930
PCM: -1352.14880222

3B

C	0.150932	-0.846389	0.243198
C	0.083543	-0.208435	1.485437
C	1.170713	0.543302	1.937610
C	2.314443	0.653867	1.154514
C	2.377240	0.015679	-0.081288
C	1.293617	-0.734327	-0.536478
C	-1.161180	-0.361344	2.282791

O	-2.113711	-1.014326	1.894459
N	-1.156764	0.304453	3.527691
C	-2.177197	0.186094	4.286059
N	-2.011962	0.956251	5.568543
C	-2.099515	0.109534	6.775229
C	-3.351226	-0.472416	6.951621
C	-4.347399	-0.150952	5.912502
S	-3.667499	-0.645279	4.207391
C	-3.539229	-1.235744	8.102704
C	-2.490740	-1.408867	9.001537
C	-1.241873	-0.828928	8.774423
C	-1.033105	-0.047193	7.641729
C	-5.422924	0.595546	6.051138
C	-6.138340	1.283728	5.031964
C	-7.536927	0.827182	4.674687
O	-5.654782	2.303625	4.515939
H	-4.511614	-1.681206	8.282701
H	-2.646131	-2.007624	9.893728
H	-0.432322	-0.979039	9.480746
H	-0.072500	0.424834	7.454820
H	1.113419	1.037837	2.899830
H	3.157531	1.239406	1.508542
H	3.271215	0.102970	-0.691879
H	1.341636	-1.230715	-1.500827
H	-0.703469	-1.423753	-0.093358
H	-7.736444	-0.195798	5.007805
H	-8.263954	1.491539	5.154206
H	-7.671111	0.904926	3.592364
H	-1.115208	1.446838	5.493045
H	-2.787368	1.645242	5.603753

Frequencies

14.2610	24.8293	33.1786
51.7726	67.5785	71.4411
80.4286	92.1309	124.7199
135.1662	146.1349	179.1084
183.4799	219.2338	247.7234
291.2519	336.6400	354.3124
372.9808	383.0226	423.4095
444.7246	454.6042	469.2620
487.5903	505.5583	532.3785
561.2727	582.2879	598.7619
631.0317	637.0327	646.6296
666.6359	698.1662	708.3118
723.1300	742.9916	759.0313
774.9491	805.1605	832.5730
846.7565	863.6993	881.7363
883.5912	905.3305	964.1225
981.3539	983.6007	1010.5696
1022.3727	1029.1091	1030.7403
1039.6907	1056.5810	1060.8609

1067.2083	1076.6221	1108.3873
1123.7134	1148.6164	1190.5873
1196.0114	1197.2097	1211.5188
1221.1062	1272.0824	1315.1415
1328.3496	1335.1958	1357.0538
1367.8980	1381.5554	1395.5530
1414.8208	1500.8291	1503.0052
1510.8515	1516.1529	1544.0379
1554.6908	1616.9141	1637.1934
1661.8304	1665.3883	1669.7973
1691.2394	1703.2323	1728.4512
1779.2830	3077.8370	3147.7798
3167.4704	3213.0723	3215.7771
3224.5228	3225.8403	3234.7643
3242.9354	3249.5726	3250.1742
3258.1036	3291.0402	3493.4368

Energy: -1351.89118531
PCM: -1352.14848778

1B-

C	0.641833	0.288088	-0.142806
C	0.279382	-0.262679	1.091483
C	1.262033	-0.955357	1.834278
C	2.543951	-1.121950	1.292763
C	2.881124	-0.584429	0.058800
C	1.925295	0.139697	-0.651377
N	-1.010568	-0.052891	1.580133
C	-1.926998	-1.038440	1.979267
S	-3.468142	-0.453248	2.420331
C	1.005768	-1.402981	3.164213
C	0.839570	-1.735630	4.315468
C	0.510338	-2.122334	5.673462
O	1.337648	-2.647711	6.404972
N	-1.499419	-2.271917	1.843261
C	-1.968634	-3.360620	2.488173
O	-2.341219	-3.426520	3.662960
C	-1.915552	-4.635657	1.673211
C	-2.351314	-5.826273	2.255868
C	-2.335250	-7.014861	1.533478
C	-1.880822	-7.025203	0.215805
C	-1.444319	-5.839709	-0.371695
C	-1.461920	-4.651652	0.353676
C	-0.903033	-1.834726	6.092983
H	-0.114960	0.819386	-0.713534
H	2.173305	0.573793	-1.616422
H	3.881949	-0.719686	-0.340396
H	3.279978	-1.666371	1.876088
H	-1.115472	-0.764956	5.986009
H	-1.594485	-2.354806	5.416834
H	-1.047690	-2.150007	7.128790

H	-1.122446	-3.719974	-0.085440
H	-1.087349	-5.840625	-1.398713
H	-1.866786	-7.953471	-0.350416
H	-2.677991	-7.936246	1.997998
H	-2.700975	-5.791493	3.282426
H	-1.458906	0.822466	1.346733

Frequencies

16.8176	25.6897	30.9785
41.8192	57.8558	68.1673
76.6859	91.7843	111.9861
134.7518	159.4524	171.5887
176.1207	194.0923	230.3029
250.7703	260.4961	294.8666
359.0542	388.3542	405.2303
428.2251	454.3557	466.2490
482.3185	494.2886	512.3252
547.6299	560.1059	585.5580
616.6502	619.5716	632.0094
638.3457	642.6809	695.4677
698.8718	713.8334	726.9520
757.3885	774.6747	800.9009
837.2638	849.5394	880.3075
888.8132	908.8331	929.3803
970.5052	975.9008	1002.9684
1014.5457	1020.3750	1023.6526
1030.4774	1063.0273	1068.4080
1082.5695	1104.7270	1124.6188
1151.5595	1171.7195	1186.5687
1193.0177	1204.3964	1210.4332
1286.1891	1289.8563	1330.7585
1341.2130	1352.4868	1357.6360
1368.6604	1438.4143	1468.3415
1490.7103	1503.6850	1506.4136
1511.4499	1549.1658	1557.4332
1589.8331	1652.6527	1662.6029
1684.3763	1688.2787	1712.7084
1766.9526	2350.7473	3057.7662
3129.0481	3173.9825	3186.6647
3198.3088	3199.8790	3212.7523
3213.5150	3221.4008	3233.9331
3242.1373	3246.6355	3636.9220

Energy: -1351.45361416
PCM: -1351.76385044

TS3B-

C	2.953739	0.942390	0.097761

C	4.271529	1.421790	0.116650
H	5.069510	0.705505	-0.052786
C	4.558606	2.759419	0.346565
H	5.589653	3.103095	0.346898
C	3.510118	3.650723	0.579507
H	3.713707	4.702146	0.768206
C	2.202475	3.192238	0.570385
H	1.372362	3.866611	0.758985
C	1.889219	1.846025	0.317841
C	2.759395	-0.486337	-0.065836
C	3.238913	-1.610081	0.201792
C	3.246073	-3.023679	0.219867
O	3.959260	-3.728630	-0.502878
C	2.300718	-3.666801	1.224358
H	1.268392	-3.523933	0.884564
H	2.517402	-4.736095	1.292212
H	2.390366	-3.199630	2.210177
N	0.541304	1.513862	0.357977
C	0.039226	0.549124	-0.352990
N	-1.354027	0.428409	-0.107741
H	-1.635901	1.079627	0.614617
C	-2.340300	-0.267585	-0.747718
O	-2.220796	-0.887931	-1.790247
C	-3.683780	-0.202048	-0.054886
C	-3.832885	-0.030527	1.322520
H	-2.958524	0.054672	1.961154
C	-5.101799	-0.006847	1.895958
H	-5.204467	0.116070	2.970503
C	-6.232263	-0.149424	1.097220
H	-7.222236	-0.127686	1.544779
C	-6.088492	-0.330143	-0.277318
H	-6.966977	-0.448906	-0.905623
C	-4.821511	-0.364639	-0.846716
H	-4.685653	-0.525480	-1.911131
S	0.852738	-0.515818	-1.417883

Frequencies

i209.3872	16.5582	21.3248
39.0530	48.3312	56.7563
62.8441	73.7521	82.8514
98.5027	106.9394	154.0981
165.6822	201.2684	232.0376
256.1075	266.3678	304.5615
322.8184	390.6317	413.7179
421.4398	424.8763	482.8177
493.1371	517.0072	522.6015
563.4133	580.2769	596.6450
611.3797	637.9383	639.8059
665.7916	690.3248	702.6398
708.4595	714.9978	728.8022
736.5965	766.2517	781.7112

818.0987	844.7321	879.9030
891.1012	902.0644	945.5476
965.0508	974.3616	995.1346
996.0687	1012.2544	1026.3444
1029.9423	1054.2795	1067.9861
1079.4426	1117.4108	1127.8539
1152.2562	1184.2256	1192.5345
1199.0474	1217.0822	1232.9349
1267.1743	1296.6672	1300.6051
1319.3483	1348.4385	1351.6341
1369.3231	1407.6279	1488.5350
1498.2152	1502.1915	1505.3429
1531.6241	1546.7220	1561.1292
1592.1050	1640.2329	1670.1079
1679.4803	1692.9991	1695.4413
1795.4190	2062.7057	3071.2010
3140.1877	3164.3160	3188.5476
3199.4807	3206.6326	3210.6070
3220.0024	3222.0651	3229.0355
3229.8672	3243.9933	3617.0752

Energy: -1351.4313989
PCM: -1351.75916441

TS3B$_N$-

C	-2.404437	0.426637	-0.065697
C	-3.447652	1.362274	-0.039986
H	-3.180815	2.400523	0.128280
C	-4.771515	1.000069	-0.237622
H	-5.552627	1.754171	-0.211778
C	-5.081068	-0.338788	-0.474524
H	-6.110178	-0.648470	-0.635556
C	-4.069040	-1.283850	-0.497981
H	-4.304813	-2.330548	-0.676548
C	-2.729003	-0.923123	-0.292071
C	-1.045617	0.930490	0.064440
C	-0.359616	1.967976	0.002515
C	0.393568	3.145301	-0.073978
O	0.918621	3.575173	-1.110887
C	0.568016	3.904413	1.235980
H	1.269320	3.364812	1.881701
H	0.969455	4.897397	1.018036
H	-0.378097	3.991062	1.780223
N	-1.773195	-1.929871	-0.348046
H	-2.107973	-2.872234	-0.489500
C	-0.497619	-1.878733	0.188510
N	-0.121223	-0.690859	0.590411
C	1.137824	-0.469604	1.169923

O	1.249995	-0.239382	2.359107
C	2.318885	-0.401690	0.255749
C	2.169566	-0.189197	-1.113657
H	1.175584	-0.072548	-1.530040
C	3.291572	-0.093118	-1.930383
H	3.168161	0.089915	-2.993820
C	4.565367	-0.222046	-1.385507
H	5.440872	-0.152102	-2.026201
C	4.718136	-0.433827	-0.015428
H	5.711892	-0.534553	0.413242
C	3.598822	-0.512901	0.802234
H	3.693682	-0.669070	1.871719
S	0.373776	-3.343830	0.264552

Frequencies

i284.1196	-55.2147	-2.0250
22.2586	27.7541	40.9741
52.0100	72.4130	78.0298
97.8369	113.2871	144.1661
164.6986	199.8299	228.0988
251.4407	265.4586	303.0043
349.4621	392.2508	400.5802
421.9079	430.2925	466.7393
497.2212	530.2066	539.7488
569.6638	581.0017	585.8088
591.9117	623.1446	637.0076
641.1387	652.9586	663.6318
707.2317	708.9062	728.5222
757.8949	763.8150	770.5058
848.2911	854.6425	871.1365
877.1850	905.4177	937.5895
966.2057	967.6234	995.2325
1002.0646	1008.7986	1020.7285
1031.4774	1053.8310	1065.7183
1087.1867	1111.7070	1126.9009
1157.7881	1190.1681	1192.6161
1201.4225	1211.7772	1222.8178
1283.6141	1298.0364	1320.4252
1342.0411	1352.4697	1366.8944
1371.0334	1410.8527	1476.0143
1497.5969	1503.4992	1508.4204
1526.3190	1554.8004	1563.7984
1602.4571	1667.5919	1672.6530
1682.7961	1688.8717	1692.6671
1781.1716	2095.5803	3073.5496
3141.6528	3164.9871	3190.0379
3193.0171	3205.7891	3209.0725
3220.4800	3222.2813	3236.5320
3241.3039	3255.6504	3650.6408

Energy: -1351.43029024

PCM: -1351.75633465

$3B_N$-

C	-0.050083	0.015583	-0.176372
C	-0.214344	1.217129	0.513687
C	0.893045	2.026287	0.762931
C	2.154106	1.635520	0.328241
C	2.315825	0.433701	-0.355908
C	1.210360	-0.376811	-0.607460
C	-1.594502	1.609847	0.917713
O	-2.579191	1.016499	0.561821
N	-1.700454	2.800972	1.744297
C	-2.218375	3.930226	1.238639
N	-2.368996	4.958349	2.134083
C	-1.753737	5.011317	3.390785
C	-1.213356	3.830492	3.914482
C	-1.363725	2.569419	3.161786
C	-1.686308	6.212362	4.094064
C	-1.060861	6.249733	5.335972
C	-0.494055	5.090164	5.860419
C	-0.564723	3.895480	5.149543
S	-2.633502	4.192975	-0.376289
C	-1.202433	1.323311	3.569159
C	-0.872165	0.713188	4.785067
O	0.283315	0.470022	5.200330
C	-2.052064	0.189505	5.605804
H	-0.108215	2.991956	5.540667
H	0.011477	5.114778	6.821631
H	-1.009975	7.185929	5.885332
H	-2.124442	7.111863	3.667027
H	-1.897526	0.460628	6.655802
H	-2.074208	-0.904662	5.544466
H	-3.013105	0.578196	5.255528
H	0.765509	2.955633	1.306267
H	3.013657	2.267474	0.532297
H	3.303695	0.126207	-0.689079
H	1.333039	-1.317476	-1.137430
H	-0.924588	-0.599071	-0.360515
H	-2.672492	5.820990	1.704768

Frequencies

15.8921	28.7824	36.6673
51.6239	68.3279	77.9827
89.6173	100.0252	123.4091
149.4409	159.8093	166.5346
206.5204	239.1107	269.2158
275.0229	284.9642	377.2023
391.2699	416.8740	422.3717

436.4132	440.1965	504.5277
525.4579	531.2177	549.2137
574.9371	589.9738	606.2774
635.7806	636.2939	638.0169
653.2069	676.5630	699.1877
708.8015	719.0422	771.2331
776.1853	784.7386	812.2187
870.4552	870.8757	886.1311
905.2328	949.2702	967.1560
967.6508	996.4156	1009.4466
1017.9337	1021.4156	1024.6097
1032.0819	1055.5420	1067.4640
1084.6860	1119.7349	1131.6267
1174.6243	1190.4115	1191.0283
1212.3505	1216.7054	1265.6964
1283.9379	1294.2533	1320.9787
1334.2786	1352.7809	1354.3176
1367.2674	1398.1625	1470.3924
1498.2886	1502.8545	1505.2636
1510.7561	1556.5074	1557.9240
1566.6743	1614.3648	1674.5502
1674.8248	1688.4411	1693.4588
1798.9726	1842.6704	3063.5190
3130.6679	3148.6241	3188.4650
3196.7824	3204.4232	3211.5240
3220.6849	3222.7058	3241.1290
3246.0607	3251.4760	3649.3995

Energy: -1351.45056525
PCM: -1351.77943999

3B-

C	-5.002441	-1.142705	-0.650441
C	-4.027724	-0.386634	0.011518
C	-4.458886	0.641366	0.859476
C	-5.816960	0.922240	1.016752
C	-6.766894	0.173905	0.333104
C	-6.356354	-0.866069	-0.499677
C	-2.587779	-0.619896	-0.211929
S	-1.527004	-0.313346	1.252687
C	-2.263264	1.104288	1.939614
N	-3.524991	1.435916	1.546556
N	-1.734444	1.941691	2.809602
C	-0.517439	1.697843	3.376263
O	0.108879	0.640010	3.325489
C	-1.999984	-1.101990	-1.289303
C	-2.389487	-1.542171	-2.555551
O	-2.738125	-2.707880	-2.857423

C	0.051288	2.860666	4.150462
C	1.286791	2.700049	4.779886
C	1.853390	3.746025	5.499624
C	1.188154	4.966864	5.597506
C	-0.044725	5.133500	4.971129
C	-0.610470	4.085344	4.250859
C	-2.253473	-0.518132	-3.683104
H	-4.667432	-1.946481	-1.299324
H	-7.091174	-1.464225	-1.031310
H	-7.822667	0.397873	0.459342
H	-6.124558	1.730681	1.677135
H	-3.877825	2.248082	2.037836
H	-1.568794	4.198893	3.757698
H	-0.567351	6.083848	5.042952
H	1.629974	5.785847	6.159441
H	2.816515	3.610476	5.984697
H	1.785911	1.741084	4.687803
H	-3.178555	-0.522972	-4.269983
H	-1.435692	-0.819422	-4.347825
H	-2.052540	0.492032	-3.312963

Frequencies

15.4975	28.9448	51.0077
57.2284	66.4543	74.6827
87.8116	110.6326	123.6061
134.9928	154.2691	165.3007
202.7371	229.5859	264.3370
278.3824	313.3245	360.0050
368.3925	426.1079	427.7538
446.7878	464.8896	487.1320
504.4915	508.1448	543.4744
571.5082	575.8240	601.4081
638.2381	645.8900	674.4515
680.1310	691.9875	703.3057
713.8253	732.8799	740.0189
768.4255	776.8555	832.0746
839.1123	858.8483	882.9451
888.2904	920.1603	941.8163
968.4011	975.9397	999.9804
1021.8125	1022.0860	1028.6965
1031.0525	1051.9511	1063.7380
1085.0407	1108.4402	1134.6159
1156.6005	1189.0073	1191.8742
1203.7104	1215.3329	1259.3573
1290.3020	1312.1229	1330.3517
1350.9049	1357.8751	1359.7119
1378.4685	1398.2038	1466.7243
1498.2980	1503.3724	1505.2046
1515.6975	1550.7993	1554.6141
1578.7543	1601.8619	1665.5358
1669.3970	1685.1865	1690.3108

1727.9179	1789.3951	3062.2096
3129.7523	3146.2106	3183.9796
3193.2288	3202.9529	3205.9303
3218.9194	3219.5043	3233.8433
3243.9537	3254.4377	3615.8534

Energy: -1351.41854681
PCM: -1351.77430662

P1

C	-0.664231	4.069605	4.335557
C	0.005116	2.870505	4.082478
C	1.298584	2.683812	4.576357
C	1.916205	3.685232	5.314180
C	1.245274	4.881172	5.564204
C	-0.044271	5.071560	5.074573
C	-0.616791	1.771861	3.288412
O	-0.017234	0.721274	3.073256
N	-1.901413	2.016585	2.841352
C	-2.435901	1.233805	1.956923
S	-1.621774	-0.124255	1.169594
C	-2.717346	-0.378386	-0.234362
C	-4.159212	-0.323675	0.043889
C	-4.618755	0.642366	0.951168
N	-3.723435	1.497426	1.605629
C	-5.981449	0.778573	1.216360
C	-6.891071	-0.079950	0.618926
C	-6.444605	-1.086836	-0.234513
C	-5.092651	-1.201670	-0.519118
C	-2.062508	-0.643264	-1.385481
C	-2.588314	-0.871218	-2.754514
C	-1.528738	-0.891553	-3.835402
O	-3.767093	-1.009931	-3.031649
H	-4.747781	-1.966388	-1.199730
H	-7.150216	-1.774655	-0.688363
H	-7.949639	0.026478	0.835101
H	-6.319574	1.544426	1.909125
H	-4.118930	2.260834	2.142958
H	-1.668438	4.204972	3.951537
H	-0.568504	6.002552	5.269274
H	1.728080	5.664395	6.141726
H	2.921729	3.534927	5.695831
H	1.802992	1.745821	4.370405
H	-1.999797	-1.053292	-4.805555
H	-0.801561	-1.688684	-3.641672
H	-0.974359	0.053759	-3.848449
H	-0.976758	-0.598477	-1.338753

Frequencies

17.4098	25.4565	32.1219
55.0377	60.2022	80.9035
98.4715	122.8626	135.1099
161.8263	180.8280	193.4125
205.6677	224.4426	261.1591
269.6434	302.6055	339.7087
383.1873	399.5945	425.3488
459.7758	466.6105	490.3943
517.7579	537.0383	550.5270
570.1495	586.7871	623.1651
637.3257	638.4732	681.9269
690.3276	697.1916	712.1705
736.0338	743.3876	747.1914
771.7241	782.0810	844.5887
856.2029	873.7332	884.3958
887.1623	896.2080	941.7988
974.4923	982.6191	982.8000
1017.0229	1019.3574	1022.5063
1031.1278	1036.8744	1061.8762
1065.2220	1090.6679	1115.2372
1136.9970	1159.5266	1195.1348
1201.3088	1209.5114	1220.7898
1232.0498	1266.6725	1306.7124
1335.6235	1349.9614	1356.2812
1363.3649	1390.3053	1421.2919
1446.2705	1479.0137	1496.8306
1504.2766	1510.1971	1542.0530
1552.8065	1556.7234	1610.1983
1657.9570	1668.4341	1682.6800
1692.0540	1698.4591	1738.2247
1807.2518	3075.4312	3136.1742
3193.3249	3195.2785	3208.5059
3209.0651	3220.4863	3226.8338
3231.0349	3241.2653	3247.3669
3257.3970	3292.8066	3607.0423

Energy: -1352.02021844
PCM: -1352.27877541

P2

C	-0.072494	0.092280	-0.255749
C	-0.222659	1.217616	0.566606
H	0.634848	1.851345	0.741594
C	-1.438916	1.505166	1.168498
H	-1.525080	2.380917	1.803130
C	-2.538181	0.673657	0.964377
H	-3.488789	0.891788	1.441417

C	-2.425303	-0.430066	0.134945
H	-3.278917	-1.075773	-0.051554
C	-1.205948	-0.706575	-0.481577
N	-1.109925	-1.788626	-1.349723
C	-0.095159	-1.967336	-2.230695
N	1.000990	-1.175594	-2.016644
C	1.193183	-0.316296	-0.894211
C	2.481333	-0.024027	-0.564811
H	3.231368	-0.572096	-1.119474
C	3.093805	0.810546	0.483304
C	4.545915	0.471181	0.756122
H	4.919687	1.101624	1.563690
H	5.149951	0.635959	-0.143595
H	4.654401	-0.584527	1.027648
O	2.557470	1.721405	1.098572
C	2.091926	-1.337896	-2.997083
O	2.980581	-2.115890	-2.772071
C	2.042670	-0.431129	-4.165958
C	1.068813	0.559751	-4.305737
H	0.298862	0.677750	-3.551297
C	1.084518	1.396374	-5.414864
H	0.327231	2.166801	-5.520243
C	2.067202	1.242586	-6.388989
H	2.075257	1.894931	-7.257212
C	3.039244	0.252398	-6.253928
H	3.803050	0.130721	-7.015617
C	3.029714	-0.580875	-5.144919
H	3.775355	-1.358882	-5.022247
S	-0.205831	-3.056089	-3.484941
H	-1.927367	-2.358917	-1.524009

Frequencies

13.0242	28.5201	37.1073
42.5039	50.7787	78.9481
113.3868	124.7419	154.1371
159.8420	162.3900	191.4049
219.9122	246.6974	259.2105
267.2455	286.0992	351.9063
388.9974	397.0461	421.0618
437.9807	443.8012	514.1110
528.2811	551.2263	560.0618
592.6500	611.2956	615.5328
635.7661	641.6458	651.2673
676.0947	689.9382	708.3135
721.3170	734.8325	777.2464
782.7356	793.8485	827.0041
875.0428	878.7783	895.2060
898.5314	928.6376	978.2474
991.3639	996.4943	1005.5402
1019.9728	1030.8492	1040.0173

1040.1358	1062.2087	1067.1647
1083.9987	1093.3339	1127.9646
1140.3064	1181.6998	1198.6257
1201.7794	1216.0708	1224.7867
1248.9681	1280.0404	1295.4758
1309.9719	1348.2601	1356.0012
1371.8278	1372.6802	1422.0606
1423.2246	1489.7551	1498.0604
1505.7714	1510.0335	1513.3430
1555.6088	1559.8004	1584.4480
1638.4032	1672.2566	1680.6667
1690.5082	1702.4106	1791.4951
1841.7110	3077.6831	3139.3847
3193.7304	3211.4116	3216.1915
3226.9731	3227.6872	3236.3222
3241.2498	3247.9150	3251.4173
3257.0277	3284.2249	3636.6144

Energy: -1352.02330437
PCM: -1352.28291720

$3B_2$-

C	-4.842561	-0.581525	-1.110083
C	-3.986422	-0.059497	-0.138778
C	-4.525662	0.468570	1.035100
C	-5.898586	0.452970	1.247376
C	-6.749076	-0.077669	0.279223
C	-6.219077	-0.588555	-0.901766
C	-2.490046	0.002594	-0.302322
O	-1.829749	0.845175	0.283280
N	-1.965048	-0.952562	-1.126621
C	-0.631744	-1.146886	-1.548690
S	0.517653	0.161498	-1.380613
C	1.672892	-0.327472	-2.722892
C	1.881027	-1.787925	-2.811900
C	0.841683	-2.691582	-2.517211
N	-0.428513	-2.299729	-2.071568
C	1.042452	-4.066010	-2.695256
C	2.262362	-4.557584	-3.135969
C	3.301023	-3.667446	-3.415765
C	3.106773	-2.301634	-3.256493
C	2.243681	0.629432	-3.422202
C	3.189741	0.758176	-4.438110
C	2.625420	0.873318	-5.856014
O	4.429012	0.883754	-4.289279
H	3.904995	-1.598707	-3.476182
H	4.263746	-4.038136	-3.758505
H	2.404423	-5.628101	-3.262152
H	0.211596	-4.731900	-2.479326

H	-4.443822	-0.955428	-2.048554
H	-6.877492	-0.986683	-1.668480
H	-7.823295	-0.085684	0.441948
H	-6.307723	0.859230	2.168079
H	-3.846681	0.893668	1.766852
H	3.170108	0.176899	-6.503202
H	2.802073	1.886847	-6.234650
H	1.552878	0.660050	-5.901332
H	-2.539577	-1.749888	-1.370763

Frequencies

17.6500	28.9043	46.1460
56.8120	63.6795	78.1979
86.1390	108.7699	111.9519
127.4851	148.0933	160.0119
197.0144	245.8296	265.1559
285.2600	316.5437	357.3275
368.7245	415.8060	424.2394
436.8403	453.9828	493.2184
513.5147	525.0146	545.3147
572.4650	591.2079	605.7547
637.2567	646.0386	668.4021
671.5041	682.9771	691.1323
710.5428	724.8660	729.1801
773.7441	789.6205	818.5621
828.9395	854.9617	880.4577
903.7715	915.9598	947.6377
966.6780	979.2364	1000.0904
1013.3404	1017.5794	1028.5148
1030.7003	1051.1971	1068.1247
1080.5149	1118.2764	1129.4852
1153.0554	1184.7932	1193.7963
1211.7072	1218.3436	1248.7362
1266.5707	1297.1303	1307.5250
1319.6833	1345.3509	1349.6688
1370.9974	1396.6048	1497.9905
1498.4251	1502.8509	1506.4468
1533.1701	1546.8071	1566.7707
1598.6681	1641.1234	1654.1160
1670.5406	1689.3938	1694.0345
1790.2942	1802.2041	3060.3676
3126.9302	3144.8265	3189.1502
3202.8639	3206.3143	3213.2306
3219.1732	3222.1972	3230.8927
3231.1759	3245.3369	3621.4826

Energy: -1351.43997747
PCM: -1351.75160231

TS-P1-P2

C	-5.070551	-1.038416	-0.501386
C	-4.038155	-0.238823	0.007921
C	-4.375012	0.756666	0.953563
C	-5.711494	0.994116	1.284139
C	-6.713394	0.211663	0.735849
C	-6.390776	-0.824199	-0.140931
N	-3.396789	1.493118	1.604704
C	-2.132994	1.134747	1.706321
S	-1.351695	-0.118660	0.825238
C	-2.637352	-0.419176	-0.405966
N	-1.635996	1.943363	2.661742
C	-0.333434	1.925459	3.094294
O	0.462722	1.084057	2.685726
C	-2.117790	-0.817364	-1.590735
C	-2.763679	-1.069146	-2.901438
O	-3.962630	-1.012856	-3.114098
C	0.051752	2.966229	4.090369
C	-0.830990	3.959242	4.519569
C	-0.416891	4.907450	5.448444
C	0.879977	4.868404	5.953893
C	1.763944	3.879280	5.527597
C	1.351764	2.932232	4.598945
C	-1.792339	-1.367803	-4.024637
H	-4.829661	-1.826246	-1.199529
H	-7.169410	-1.456120	-0.555108
H	-7.748767	0.396873	1.005732
H	-5.937659	1.782110	1.994959
H	-2.943025	2.305295	2.579237
H	-1.840433	3.993331	4.125886
H	-1.107217	5.678278	5.777586
H	1.202067	5.609332	6.679848
H	2.775788	3.847097	5.920284
H	2.023278	2.154211	4.252238
H	-2.346494	-1.551271	-4.945750
H	-1.180249	-2.243867	-3.780992
H	-1.106514	-0.525668	-4.172459
H	-1.032084	-0.871150	-1.638937

Frequencies

i1974.6740	19.1448	25.3896
28.5114	48.3357	60.5996
75.6812	97.7812	116.7980
132.1251	153.8675	163.8872
195.9133	199.2135	225.2378
263.4857	285.8579	295.3608
332.1701	385.7778	410.7165
422.7406	455.5144	456.9557
487.7082	523.1611	531.0379
556.4711	576.1367	585.4463
626.8972	637.4685	642.6862
694.7892	709.5495	715.1997

730.5552	742.6695	764.3517
777.3942	785.0957	833.3561
854.2471	880.0639	881.3105
884.0079	897.4616	974.5772
976.0407	986.0107	995.4894
1016.6623	1018.9692	1019.5340
1031.9698	1037.8851	1060.5599
1066.3882	1069.2627	1088.8526
1120.2329	1141.6247	1183.4541
1195.6950	1196.8767	1214.7494
1218.1350	1232.6885	1309.0568
1325.1835	1336.9180	1351.0812
1368.0854	1369.9435	1420.5500
1439.5116	1467.9017	1496.8501
1504.2374	1504.6920	1510.5589
1545.4309	1557.2474	1598.0264
1641.9399	1656.9236	1668.9486
1693.4117	1694.3260	1737.2891
1805.4720	2075.9250	3074.9399
3135.7296	3184.5418	3194.8441
3211.2400	3218.8000	3222.6135
3233.0008	3234.0479	3241.9142
3249.2654	3250.6973	3296.2433

Energy: -1351.95504641
PCM: -1352.19077085

P1f

C	0.015586	-0.182927	1.332799
C	1.365756	-0.349917	1.689226
H	1.628842	-0.494340	2.730285
C	2.371418	-0.366486	0.740763
H	3.402649	-0.504476	1.050207
C	2.051994	-0.215749	-0.611603
H	2.834900	-0.222001	-1.363920
C	0.730976	-0.078613	-0.988576
H	0.446819	0.020575	-2.030773
C	-0.298901	-0.078623	-0.034816
N	-1.586403	0.016979	-0.541008
C	-2.621598	-0.168690	0.187376
S	-2.723391	-0.428833	1.934356
C	-1.029151	-0.113753	2.368537
N	-3.831759	-0.103898	-0.503323
H	-3.685528	0.076255	-1.488979
C	-5.107167	-0.382672	-0.056071
O	-5.321796	-0.815781	1.061744
C	-6.204401	-0.135853	-1.042642
C	-7.401521	-0.827457	-0.847682

H	-7.479366	-1.503164	-0.002682
C	-8.465182	-0.643432	-1.721416
H	-9.390363	-1.190485	-1.568277
C	-8.346122	0.243861	-2.788879
H	-9.179289	0.390764	-3.469694
C	-7.161540	0.949732	-2.977367
H	-7.071042	1.655820	-3.797033
C	-6.091966	0.760185	-2.108521
H	-5.187995	1.345127	-2.252022
C	-0.732243	0.151108	3.667443
H	0.293033	0.390816	3.923630
C	-1.698139	0.179709	4.763581
O	-2.859411	-0.182462	4.613556
C	-1.200922	0.679142	6.101834
H	-2.013084	0.643588	6.829121
H	-0.831086	1.707174	6.015384
H	-0.367148	0.062101	6.456013

Frequencies

19.0690	29.9968	47.4503
50.7289	68.1395	78.3830
88.0477	113.8284	114.9194
133.8294	163.1008	183.8158
214.9881	227.1476	264.5010
297.6617	319.1234	325.7034
391.1071	411.3595	421.8222
432.3630	459.3781	495.0398
524.7864	538.5390	555.6379
590.2666	603.4928	622.2200
637.0285	650.9363	675.2824
677.0990	682.2962	708.1510
714.8123	725.9623	729.9013
771.4443	788.6356	821.5738
848.7309	854.6588	879.4098
902.4681	908.6944	954.5083
969.3345	987.4087	996.0989
1015.6266	1021.6586	1024.1278
1030.0668	1038.1037	1062.4559
1068.8768	1088.5627	1119.3073
1138.0284	1158.3826	1197.9960
1198.6086	1222.9752	1226.6065
1267.0715	1278.2170	1294.1275
1305.2762	1333.4535	1352.7457
1354.1456	1374.9852	1383.6151
1424.4929	1496.3580	1503.3665
1505.4940	1510.7147	1536.0532
1551.8803	1569.9850	1603.7411
1646.4329	1671.4563	1679.5933
1693.7819	1701.6867	1775.9189
1801.2283	3074.9345	3135.4186
3191.1344	3211.2589	3216.8152

3218.6678	3228.9952	3229.0577
3235.9672	3238.3289	3243.7350
3249.6022	3253.8453	3626.7173

Energy: -1352.02820062
PCM: -1352.26845759

R1-

C	-3.624091	-0.457459	-0.026528
C	-2.801230	-1.539947	0.028341
C	-1.379139	-1.402899	0.039891
C	-0.851426	-0.138861	-0.006415
C	-1.665163	1.025533	-0.064708
C	-3.129953	0.911802	-0.077467
C	-1.056876	2.276178	-0.109741
C	-0.534317	3.388168	-0.147130
C	0.149924	4.623724	-0.190406
O	-0.395575	5.729102	-0.260872
N	-3.994896	1.888560	-0.128627
C	1.669371	4.541936	-0.108615
H	-4.704883	-0.570821	-0.034799
H	-3.236575	-2.538151	0.064608
H	-0.737747	-2.278438	0.084335
H	0.227719	0.002806	0.001024
H	2.055041	3.620026	-0.552416
H	2.102375	5.414626	-0.605086
H	1.970332	4.560818	0.945911
H	-3.504827	2.785124	-0.160478

Frequencies

30.8801	58.0817	60.4530
62.4964	127.1481	160.4888
218.2641	291.6554	412.3034
424.3176	492.4363	514.2727
540.8598	575.7484	588.7498
605.3636	630.0484	674.5001
726.7215	737.3962	818.7892
825.9816	855.7333	907.0381
957.5260	996.3857	1000.1761
1030.9221	1051.6427	1100.6905
1167.6601	1187.3179	1212.8957
1300.6163	1363.0950	1387.3220
1410.9495	1458.1605	1499.5895
1504.7233	1515.8947	1564.8589
1592.3189	1692.6196	1709.4795
2217.3484	3069.7392	3138.5478
3164.8587	3166.9484	3181.2571
3207.8716	3214.2327	3470.7089

Energy: -515.578028232
PCM: -515.767349723

TSHB-

C	-2.561638	0.335383	0.063561
C	-2.698968	-1.041271	-0.106535
C	-3.690108	-1.542789	-0.954546
C	-4.544730	-0.671968	-1.617283
C	-4.405064	0.705882	-1.444451
C	-3.411081	1.207881	-0.609647
C	-1.800284	-2.011975	0.579822
O	-1.790262	-3.199281	0.315330
N	-1.047291	-1.501445	1.631901
C	0.121177	-1.233445	1.846549
S	1.407992	-0.821698	2.687309
N	0.824310	-1.425750	-0.409600
C	2.044959	-1.036796	-0.741229
C	3.077229	-1.935832	-1.197599
C	4.339422	-1.513471	-1.520352
C	4.709289	-0.151962	-1.415119
C	3.759730	0.746377	-0.982829
C	2.444120	0.351327	-0.649267
C	1.530386	1.350904	-0.272949
C	0.784058	2.270965	0.025765
C	-0.017146	3.389878	0.378945
C	0.712059	4.720061	0.461467
O	-1.224236	3.328325	0.614338
H	2.819054	-2.990165	-1.276814
H	5.073912	-2.243162	-1.857624
H	5.713901	0.173605	-1.667770
H	4.007756	1.801415	-0.893625
H	1.225350	4.934749	-0.481715
H	-0.005387	5.512633	0.686325
H	1.475560	4.678836	1.245913
H	0.740281	-2.434925	-0.543279
H	-1.780529	0.739255	0.696051
H	-3.268952	2.275307	-0.476381
H	-5.070112	1.387860	-1.968836
H	-5.317769	-1.064697	-2.272804
H	-3.770829	-2.617326	-1.082009

Frequencies

i213.8730	20.8117	30.5428
33.3743	43.9836	53.9509
58.5704	62.6770	72.6240
78.4009	81.0398	83.6999
138.0237	156.6146	167.0580
208.0735	215.8766	256.2355

283.6351	312.9478	384.7787
414.1562	419.9736	423.8558
437.8572	478.9953	493.4029
506.4739	528.7880	547.0183
581.7140	596.9737	612.6235
631.9499	634.8032	644.1484
685.8330	699.4068	712.6682
734.7671	735.5394	757.1971
792.8665	822.1536	835.2578
863.2253	883.2845	886.7464
909.9250	962.5593	975.9085
987.3899	993.6806	1014.7527
1029.6097	1044.0482	1056.0413
1057.3641	1060.4577	1115.9820
1117.7399	1145.0530	1180.0420
1188.4006	1190.3460	1206.8826
1220.0748	1307.8497	1314.9844
1351.2056	1358.0753	1363.9263
1392.8274	1413.8778	1433.2795
1496.7076	1503.1233	1506.6095
1523.3408	1540.6474	1551.1914
1588.9981	1670.8267	1679.4762
1689.8518	1722.5741	1769.4529
2000.2484	2257.3371	3075.3816
3141.9257	3170.5111	3172.3958
3190.9680	3193.2195	3195.5000
3211.3995	3219.2641	3239.3923
3243.1761	3272.0503	3480.8024

Energy: -1351.3928098
PCM: -1351.70844910

TS-3B-3B_2-

C	-5.236168	-1.027156	-0.302667
C	-4.147096	-0.243579	0.081144
C	-4.375496	0.947667	0.771408
C	-5.673754	1.349684	1.070928
C	-6.756360	0.565229	0.681357
C	-6.533756	-0.625694	-0.006778
C	-2.768246	-0.740296	-0.270470
O	-2.620691	-1.836854	-0.807544
N	-1.754287	0.104482	0.036907
C	-0.410248	-0.096650	-0.149634
N	0.096520	1.064110	0.221873
C	1.429652	1.450453	0.084713
C	2.441596	0.512721	-0.211590
C	2.189616	-0.949898	-0.305489
S	0.453296	-1.449947	-0.723507

C	1.735661	2.803892	0.248847
C	3.040418	3.256945	0.112782
C	4.050461	2.347275	-0.192850
C	3.744682	1.000691	-0.348993
C	3.031241	-1.948447	-0.177367
C	4.376630	-2.239787	0.031137
C	5.198071	-2.483446	-1.240122
O	4.939787	-2.422119	1.134010
H	4.533460	0.287630	-0.562108
H	5.078358	2.682222	-0.301724
H	3.266046	4.311843	0.244475
H	0.926891	3.489378	0.486673
H	-1.218331	1.276448	0.389798
H	-3.534197	1.557518	1.080051
H	-5.839469	2.277585	1.611543
H	-7.769972	0.880102	0.915060
H	-7.374007	-1.243512	-0.311959
H	-5.036113	-1.952235	-0.832903
H	6.138764	-1.926851	-1.160130
H	4.668184	-2.190217	-2.152578
H	5.449132	-3.548152	-1.306460

i1929.8092	14.3419	21.1987
40.2983	48.9197	62.6672
69.3036	83.9588	114.0629
120.3067	138.1132	146.6285
156.6622	193.9184	237.4980
267.4574	290.3004	303.5761
353.7611	378.1668	419.3959
424.9583	443.7190	457.7881
469.8900	488.4516	514.6618
544.7655	566.3868	586.9638
599.9751	638.3439	647.4629
670.7297	697.2312	709.2208
726.5207	730.4432	743.2044
769.9903	774.5233	811.6274
828.3699	865.2121	880.7327
889.7831	910.5218	967.1129
970.1929	996.1355	996.9903
998.1004	1015.6101	1030.4217
1031.5268	1047.8275	1051.4748
1067.0573	1084.6791	1114.4479
1131.5510	1177.2173	1184.9615
1191.0162	1201.8002	1210.7042
1276.0231	1295.4995	1313.2270
1319.0561	1343.7522	1353.7313
1363.2051	1396.8311	1449.4298
1495.8329	1498.5542	1504.3907
1506.8689	1537.6387	1554.2531
1590.0226	1610.1465	1650.7384
1666.9224	1682.3530	1692.4049

1735.9195	1814.3930	2106.1462
3059.0335	3127.6956	3138.9824
3195.0409	3197.5571	3209.3133
3210.1004	3221.3450	3222.4013
3244.9420	3245.9749	3249.9110

Energy: -1351.3818048
PCM: -1351.70699985

Reaction A

R2

C	4.668496	-3.876809	3.652956
C	5.066457	-4.115309	2.336030
C	6.418172	-4.252691	2.025531
C	7.369752	-4.151170	3.033659
C	6.980638	-3.913463	4.349253
C	5.628488	-3.777111	4.653129
N	4.134019	-4.222431	1.300658
C	2.955116	-4.182936	1.074878
O	1.829782	-4.164951	0.737975
H	6.707095	-4.437618	0.996488
H	8.421797	-4.258784	2.787730
H	7.726668	-3.834811	5.133788
H	5.315067	-3.591575	5.676043
H	3.613522	-3.770825	3.887500

Frequencies

61.0171	78.5529	248.5325
389.2560	426.9172	470.0986
515.3930	584.5372	631.6037
642.2337	708.5368	780.3632
782.0118	862.9337	943.2647
1002.6343	1025.7233	1029.9608
1065.2261	1119.0175	1168.8002
1195.5791	1214.6930	1335.1448
1370.2796	1511.6929	1516.5946
1597.8062	1671.5780	1693.8495
2404.8222	3213.8123	3220.9506
3229.5180	3238.3505	3245.7237

Energy: -399.540944199
PCM: -399.638637519

TS1

C	-2.238161	1.321692	0.074370

C	-2.699242	2.508782	0.660789
H	-3.689987	2.522658	1.102244
C	-1.904427	3.643898	0.670321
H	-2.272349	4.557975	1.124634
C	-0.632774	3.606337	0.099345
H	-0.004121	4.490976	0.111536
C	-0.154613	2.436691	-0.476922
H	0.845187	2.386927	-0.897081
C	-0.955962	1.301180	-0.495104
N	-0.426605	0.087491	-1.043669
H	-1.138870	-0.644257	-1.089413
H	0.012540	0.222873	-1.953124
C	-3.057721	0.154278	0.029008
C	-3.712413	-0.859529	-0.062016
C	-4.472920	-2.093123	-0.186145
O	-4.123413	-2.949257	-0.976029
C	-5.699437	-2.221543	0.677817
H	-6.493577	-1.589601	0.261271
H	-5.507040	-1.875926	1.697320
H	-6.035266	-3.259573	0.677729
C	0.934206	-0.550654	-0.049689
O	0.483940	-1.090247	0.924542
N	1.950251	-0.189622	-0.721856
C	3.251089	-0.474738	-0.250882
C	4.310731	-0.052482	-1.061891
C	5.627776	-0.277817	-0.684134
C	5.913058	-0.930636	0.513607
C	4.863360	-1.354425	1.322894
C	3.540098	-1.132550	0.951585
H	4.076381	0.453382	-1.993505
H	6.435916	0.057153	-1.328530
H	6.942224	-1.108274	0.811172
H	5.071841	-1.866344	2.258374
H	2.731490	-1.469179	1.590221

Frequencies

i131.8069	15.1961	16.6898
28.0170	37.6348	45.4045
62.9836	74.5269	95.7235
108.1196	122.4818	168.4488
188.8019	252.2906	266.3024
289.8994	303.5762	364.7108
398.8317	408.1957	430.8276
494.2824	501.5709	510.0251
524.9445	551.0329	578.5578
589.8459	610.1613	629.6288
636.4117	680.4078	697.2831
716.0578	732.2560	773.6734
789.2275	792.0371	803.2661
834.8172	867.7860	872.4065
894.1136	914.6627	944.0102

995.7370	1002.5609	1007.9255
1019.6064	1026.7066	1031.2319
1061.7195	1067.5564	1079.8997
1119.1188	1121.1318	1138.0118
1169.7859	1191.6446	1199.7365
1203.5261	1212.6988	1217.9866
1261.4049	1332.4759	1334.6341
1335.7762	1370.7058	1373.3561
1388.3515	1426.0483	1493.1940
1498.9103	1511.5712	1518.7051
1557.6760	1563.1904	1657.4949
1663.5423	1677.1265	1688.2396
1698.2040	1794.2648	1982.0231
2347.9181	3079.1210	3149.1606
3196.4677	3203.2848	3211.5940
3224.3951	3225.2234	3233.0053
3233.5772	3241.2418	3248.6935
3250.8029	3480.6568	3579.5370

Energy: -915.6641747
PCM: -915.897940566

2A

C	-0.207228	2.483904	-0.431591
C	-0.965065	1.323484	-0.439029
C	-2.276621	1.305319	0.051425
C	-2.818072	2.495229	0.555526
C	-2.067845	3.661544	0.558671
C	-0.764915	3.656372	0.064398
N	-0.356019	0.097752	-0.925771
C	0.882998	-0.383755	-0.035271
O	0.526761	-0.812184	1.050562
C	-3.038990	0.098994	0.011600
C	-3.637652	-0.948719	-0.075977
C	-4.325940	-2.227041	-0.197128
O	-3.896474	-3.076932	-0.952372
N	1.930167	-0.154526	-0.751932
C	3.216685	-0.448399	-0.263690
C	3.503185	-0.980528	1.002355
C	4.823036	-1.223243	1.374385
C	5.875259	-0.946009	0.507208
C	5.595333	-0.418358	-0.752338
C	4.282729	-0.173337	-1.131384
C	-5.555135	-2.413878	0.649969
H	-3.832179	2.487491	0.939974
H	-2.497889	4.577318	0.950885
H	-0.174573	4.566793	0.073299
H	0.816002	2.454169	-0.793138
H	-1.047347	-0.660089	-0.931473

H	0.034547	0.212298	-1.864526
H	-6.288713	-1.630559	0.431092
H	-5.293405	-2.328576	1.710226
H	-5.986141	-3.396244	0.451382
H	4.053336	0.235023	-2.111112
H	6.404381	-0.197871	-1.443535
H	6.901015	-1.139806	0.807020
H	5.026824	-1.636586	2.358664
H	2.692243	-1.202491	1.684874

Frequencies

10.2300	14.8483	27.6345
37.2681	44.1433	64.3074
77.8749	108.2159	113.2796
124.5552	151.1106	175.4128
243.9604	263.3600	278.2813
306.8697	366.7072	384.8453
404.0222	431.1772	457.7961
492.5630	510.5789	528.9905
561.9177	568.0298	584.6631
603.4761	609.3969	629.6947
636.7571	688.1658	716.7548
723.5742	772.4015	786.9185
792.5342	796.3758	834.1072
867.6354	870.1204	890.6550
919.7554	946.6293	955.2290
1001.4274	1003.5448	1003.9895
1019.9669	1025.7118	1035.4589
1063.0239	1067.7706	1080.4215
1118.6356	1127.5942	1174.4253
1190.6905	1202.2802	1208.2735
1216.1611	1222.1551	1250.3368
1280.5791	1328.0361	1334.0022
1335.9032	1370.0241	1380.2182
1401.2593	1427.0111	1491.1732
1497.6943	1510.4559	1518.5755
1557.1475	1563.7670	1654.0925
1660.2324	1672.2767	1687.5374
1700.9721	1798.8508	1872.4569
2351.8457	3082.2301	3147.6120
3195.3500	3199.9153	3208.1562
3222.1423	3226.8503	3230.3432
3235.2626	3243.6110	3250.4658
3263.3206	3436.2104	3518.4823

Energy: -915.662839364
PCM: -915.901439364

3A

C	0.581400	-0.407711	-0.038496
C	0.410460	-0.049815	1.310469
H	1.237126	-0.222260	1.995222
C	-0.779698	0.478770	1.783651
H	-0.870767	0.731224	2.837268
C	-1.861384	0.662458	0.921692
H	-2.802817	1.061772	1.286869
C	-1.708059	0.339423	-0.417476
H	-2.522124	0.500456	-1.117703
C	-0.503325	-0.175080	-0.920535
C	-0.388060	-0.348909	-2.329877
C	-0.355692	-0.394200	-3.540061
C	-0.196619	-0.640878	-4.952107
O	-1.013065	-0.262839	-5.781789
C	1.042186	-1.414335	-5.329028
H	1.935476	-0.914344	-4.940525
H	1.015275	-2.404833	-4.861666
H	1.098192	-1.508334	-6.415740
N	1.810808	-0.880618	-0.457098
H	2.587641	-0.660811	0.152398
C	2.108753	-2.095827	-1.186397
O	3.332413	-2.325970	-1.281826
N	1.037838	-2.751594	-1.587542
C	1.130958	-3.889813	-2.360144
C	-0.092374	-4.512498	-2.703018
C	-0.143777	-5.650312	-3.493934
C	1.028898	-6.227758	-3.986722
C	2.245233	-5.631326	-3.660311
C	2.310126	-4.489842	-2.865252
H	-1.003416	-4.058539	-2.323144
H	-1.109821	-6.091531	-3.732855
H	0.993006	-7.118937	-4.608546
H	3.173288	-6.063806	-4.031389
H	3.262584	-4.042108	-2.614249

Frequencies

22.8901	30.3715	36.2488
47.4333	54.7425	73.1339
81.6036	118.4366	126.2983
141.3637	164.3917	188.6300
241.8649	262.3923	279.7383
341.6611	374.0407	403.0266
414.8524	435.9534	477.0970
492.7077	534.5828	540.6269
560.2520	573.4616	587.5260
611.7019	623.4874	634.1685
659.8106	704.2214	714.1049
717.8162	762.9178	770.9502
776.8399	793.2621	856.0487
862.1561	875.2193	887.0058

919.9101	928.3308	971.0326
990.8900	996.0711	1005.1604
1006.3776	1008.7433	1022.7107
1060.1810	1063.2695	1086.9087
1110.4115	1145.3736	1180.8017
1192.7934	1198.6070	1203.3427
1257.0899	1279.0108	1299.0043
1323.3162	1338.7136	1362.1765
1368.6023	1420.7451	1427.3684
1451.5172	1491.1690	1495.2738
1502.9761	1517.4093	1549.1050
1560.5215	1634.2494	1648.3208
1661.5198	1683.3872	1716.7317
1762.5360	2337.8372	3079.6697
3148.4269	3170.0156	3178.7636
3178.8113	3191.4125	3203.3720
3206.7275	3216.3235	3217.6814
3230.9791	3270.8622	3626.7797

Energy: -915.167382714
PCM: -915.4447123

TSo

C	5.456559	-4.905431	0.458006
H	4.775266	-5.422525	-0.223314
H	5.986064	-5.627427	1.086908
H	4.873783	-4.253824	1.119320
C	6.419008	-4.040988	-0.348641
O	6.127441	-3.715495	-1.503689
C	7.616043	-3.684583	0.315716
C	8.190012	-2.940419	1.150599
C	9.446558	-2.739937	1.847097
C	10.363287	-3.796051	1.901973
H	10.067701	-4.737495	1.450257
C	11.614627	-3.652692	2.487127
H	12.306074	-4.490169	2.507325
C	11.969618	-2.423970	3.041905
H	12.944109	-2.288255	3.503854
C	11.071484	-1.367437	3.014455
H	11.340923	-0.409414	3.453498
C	9.807700	-1.507428	2.424437
N	8.950314	-0.422735	2.394454
H	9.252180	0.441697	2.820606
C	7.560464	-0.513444	2.262390
O	7.097706	-1.646524	1.876116
N	6.927559	0.581598	2.583447
C	5.553952	0.735039	2.452428
C	4.998350	1.874099	3.068944
H	5.674196	2.527409	3.613640

C	3.643355	2.162311	2.988488
H	3.254249	3.050770	3.481982
C	2.784032	1.324549	2.277080
H	1.722195	1.546767	2.207829
C	3.317567	0.198519	1.654199
H	2.667637	-0.465433	1.088206
C	4.673838	-0.102766	1.736337
H	5.065823	-0.985164	1.248720

Frequency:

i256.9845	18.6714	29.1094
29.9020	43.0498	56.9309
68.0936	87.3101	101.9752
119.4436	153.5096	225.5705
241.6432	261.2049	296.5426
342.5091	371.8197	405.6309
432.4255	441.7993	484.0857
504.9002	521.9612	541.5531
566.7784	577.3969	586.6200
609.5289	635.2729	649.7990
663.8187	714.2795	722.5488
752.4757	760.0301	765.7205
782.4841	815.9374	834.1052
861.5871	872.7844	875.7964
926.6321	931.4957	963.7590
990.3160	991.5277	997.8359
1007.8344	1017.8338	1042.3827
1054.4589	1066.3502	1087.1702
1115.7659	1146.2198	1183.2564
1190.2401	1200.4403	1208.5082
1264.7549	1294.1813	1304.5923
1325.3697	1331.1328	1363.5893
1367.1296	1405.7503	1428.6935
1461.1769	1497.9657	1502.6354
1505.1937	1532.2449	1559.0203
1569.2771	1638.9084	1645.4861
1667.5204	1685.1907	1694.7617
1709.9207	2028.2084	3071.3788
3141.3720	3161.7832	3178.2800
3187.5671	3189.7041	3202.5475
3208.5306	3217.5503	3218.1009
3235.7039	3276.7124	3654.4493

Energy: -915.1532732
PCM: -915.427097569

TSN

C	2.511483	-1.662330	-0.435932
C	1.542491	-0.996901	0.340933

C	2.000413	-0.214371	1.417350
C	3.352908	-0.104737	1.712640
C	4.302120	-0.770883	0.938720
C	3.863603	-1.546924	-0.133410
N	0.178167	-1.009569	0.105255
C	-0.417215	-1.980201	-0.583898
O	0.021127	-3.055145	-1.026408
N	-1.800746	-1.741502	-0.797105
C	-2.573448	-0.762367	-0.200103
C	-2.050238	0.508214	0.116138
C	-2.892161	1.457342	0.705596
C	-4.230994	1.191179	0.965557
C	-4.749925	-0.056942	0.627416
C	-3.927798	-1.019299	0.059243
C	-0.702345	0.901276	-0.231631
C	0.085551	1.781955	-0.597202
C	1.168063	2.609723	-0.973364
C	1.959793	3.248858	0.157643
O	1.485471	2.839881	-2.143134
H	-2.469871	2.429638	0.940037
H	-4.860796	1.950018	1.420928
H	-5.794991	-0.288531	0.817201
H	-4.328430	-1.999531	-0.189461
H	2.880332	2.673263	0.301025
H	1.409132	3.252667	1.102291
H	2.230526	4.269410	-0.129040
H	-2.274704	-2.578447	-1.106791
H	1.259324	0.303819	2.018518
H	3.668801	0.506342	2.555932
H	5.361853	-0.686738	1.166107
H	4.588610	-2.073443	-0.750834
H	2.181679	-2.280403	-1.260811

Frequencies

i204.9054	26.6801	31.0458
51.8947	68.1408	74.4104
85.1723	88.7241	91.5824
137.2732	157.5684	211.9805
249.7220	256.0879	286.4512
341.6910	372.7124	400.2493
423.9568	430.8948	467.9504
508.0306	530.8283	537.9179
549.1539	569.8529	584.3968
598.0296	635.0011	644.5331
666.7921	705.4582	711.4653
729.6209	759.1212	767.0736
768.1746	787.9895	855.8846
858.5553	873.4290	883.9244
925.5961	932.1474	961.8473
988.0497	990.7665	1001.7693
1013.3433	1019.8794	1041.0279

1056.0179	1067.2047	1088.1851
1115.3600	1144.3305	1183.4874
1190.7582	1199.2692	1206.4869
1270.2227	1284.8248	1308.7473
1332.2004	1339.0935	1364.2169
1368.7523	1411.2614	1431.9014
1451.1072	1499.5879	1502.4919
1505.3508	1525.4995	1555.7655
1565.1589	1647.9752	1663.2060
1671.7771	1683.6725	1699.1209
1728.9854	2153.4080	3076.3117
3150.5120	3161.7137	3177.3287
3186.5885	3186.7144	3201.6483
3208.1397	3215.1530	3223.2107
3230.5217	3268.5431	3646.5062

Energy: -915.1582631
PCM: -915.434810803

O1-

C	0.110049	-0.292197	0.671006
C	1.403738	-0.246222	1.225699
C	1.510084	-0.044479	2.614405
C	0.388841	0.114978	3.416018
C	-0.887401	0.072503	2.855228
C	-1.009471	-0.132888	1.483894
N	2.616317	-0.402619	0.553666
C	2.755536	-0.449910	-0.726519
N	4.042990	-0.577554	-1.209934
C	4.333562	-0.935314	-2.526485
C	3.327290	-0.777659	-3.489317
C	2.018449	-0.246703	-3.096863
O	1.787780	-0.390788	-1.619806
C	5.599476	-1.401230	-2.880116
C	5.879077	-1.712415	-4.206747
C	4.888186	-1.564357	-5.176128
C	3.626375	-1.105384	-4.812260
C	1.059610	0.241978	-3.838312
C	-0.218607	0.754417	-3.540715
C	-0.297982	2.263002	-3.300410
O	-1.281261	0.105726	-3.543674
H	2.838331	-0.975744	-5.547163
H	5.096686	-1.809335	-6.214024
H	6.867594	-2.073355	-4.478282
H	6.364051	-1.511363	-2.113861
H	-0.929554	2.719800	-4.070824
H	-0.779696	2.431325	-2.331084
H	0.684695	2.743597	-3.308645

H	2.508215	-0.016576	3.041727
H	0.511352	0.272320	4.485447
H	-1.770299	0.196715	3.476887
H	-1.994184	-0.170071	1.024701
H	-0.020090	-0.447557	-0.391088
H	4.733189	-0.721669	-0.487440

Frequencies

24.7827	30.0354	41.4817
49.8082	68.7232	84.1773
97.1337	106.9924	118.4737
161.6152	209.6253	247.7198
272.7314	287.6823	300.7679
399.7095	422.4372	432.3441
457.1907	496.4560	520.8063
522.7673	535.3533	544.7169
557.0306	587.2108	625.3446
635.8308	649.2933	662.3543
676.2131	715.5365	734.8763
763.7635	764.9834	784.7189
803.4268	833.8208	848.1749
867.5143	875.9561	901.1980
934.3684	938.6259	957.5666
994.8503	999.0329	1002.5878
1019.9318	1020.4955	1039.0330
1055.1526	1068.1890	1077.5634
1120.5374	1140.9085	1185.2142
1185.5444	1207.9990	1215.7072
1265.9919	1287.6684	1312.0295
1322.1239	1326.6612	1358.7930
1369.0136	1397.5445	1423.0071
1468.3252	1498.1266	1505.3182
1506.3966	1536.6307	1557.4779
1566.2833	1647.6916	1649.7483
1669.3643	1676.0501	1690.0907
1716.9356	1815.0990	3064.9689
3132.9323	3150.8758	3184.1256
3184.8007	3199.1715	3200.0812
3214.3772	3216.8684	3222.3482
3237.0325	3285.3927	3662.3575

Energy: -915.159237243
PCM: -915.434827261

O1

C	0.269673	0.218380	0.877416
C	1.440839	-0.367326	1.372300
H	1.493891	-0.665463	2.413260

C	2.542805	-0.558668	0.556108
H	3.443365	-1.011272	0.956966
C	2.488115	-0.158981	-0.781814
H	3.346834	-0.307145	-1.429328
C	1.348305	0.440095	-1.289250
H	1.305443	0.762720	-2.325658
C	0.241691	0.638160	-0.458142
C	-0.948146	0.401973	1.676161
C	-1.168826	-0.185363	2.872164
H	-0.391682	-0.847522	3.233317
C	-2.347338	-0.054855	3.741098
O	-3.310888	0.652848	3.493162
C	-2.301152	-0.878775	5.012333
H	-1.439782	-0.590059	5.625821
H	-3.219507	-0.723561	5.579882
H	-2.191139	-1.943681	4.777317
N	-0.908039	1.237648	-0.933144
N	-2.760672	2.523245	-0.585110
C	-1.915191	1.715293	-0.116033
O	-1.911605	1.227400	1.162945
C	-3.886556	3.093598	0.032556
C	-4.548796	4.065196	-0.729767
C	-5.681436	4.703147	-0.243521
C	-6.179313	4.374986	1.015908
C	-5.528863	3.406623	1.774337
C	-4.388327	2.764962	1.298533
H	-4.151782	4.304214	-1.711319
H	-6.178359	5.455198	-0.849965
H	-7.067055	4.868683	1.400628
H	-5.907107	3.138329	2.756766
H	-3.906131	2.017351	1.914109
H	-0.925076	1.629651	-1.864653

Frequencies:

19.9299	25.5237	56.4393
73.5664	83.3637	101.6093
102.3535	122.6298	130.0101
172.0064	223.4296	256.6803
268.8849	296.2248	303.3371
332.9227	432.0345	432.4824
454.3524	499.2304	530.6943
535.7301	537.6349	560.2195
569.2108	594.3259	633.6035
652.5909	673.6998	675.7908
700.4289	719.5887	737.3938
755.4892	779.9480	795.1699
799.5506	834.8523	846.4053
881.5501	882.9395	912.9217
931.8087	966.5269	977.5079
986.2330	1012.5498	1014.8577
1028.2340	1032.7164	1044.9681

1061.2776	1070.1856	1085.2230
1120.2968	1130.7800	1172.6135
1191.6153	1199.3781	1221.5247
1228.2218	1257.3089	1286.2310
1301.7502	1320.7149	1334.9801
1363.5203	1372.2263	1383.9783
1412.1525	1424.0450	1479.5385
1496.6462	1505.8160	1511.0514
1552.6526	1560.7788	1577.4628
1663.7456	1671.6135	1677.1043
1691.0123	1703.7477	1803.4200
1821.5858	3073.6864	3134.3854
3192.0638	3204.0698	3213.2210
3214.7926	3226.8551	3227.1669
3234.9042	3235.9645	3245.5931
3255.2112	3283.1794	3652.1892

Energy: -915.738965818
PCM: -915.954905702

O2

C	0.257870	0.190387	0.833085
C	1.295121	-0.670503	1.225458
H	1.246518	-1.184986	2.178302
C	2.389814	-0.875636	0.408016
H	3.183932	-1.544013	0.724592
C	2.469313	-0.218739	-0.827383
H	3.329117	-0.378816	-1.471155
C	1.459047	0.631432	-1.230061
H	1.497050	1.151424	-2.181385
C	0.342841	0.846631	-0.407309
C	-0.922774	0.445870	1.655513
C	-1.163304	-0.099614	2.871150
H	-0.406739	-0.777324	3.244816
C	-2.312722	0.103741	3.753096
O	-3.262848	0.832596	3.500669
C	-2.267689	-0.669290	5.056539
H	-1.376309	-0.398982	5.634145
H	-3.161269	-0.447888	5.641511
H	-2.215756	-1.746844	4.862776
N	-0.645004	1.704409	-0.848210
N	-2.646292	2.723364	-0.484886
C	-1.660121	1.887647	-0.078528
O	-1.851414	1.314956	1.131367
C	-3.871204	3.160666	0.065976
H	-2.421078	3.105471	-1.394350
C	-4.604345	4.057526	-0.720295
C	-5.822171	4.550161	-0.274167

C	-6.326475	4.155486	0.962580
C	-5.592306	3.264577	1.737511
C	-4.368215	2.760330	1.305051
H	-4.216848	4.370246	-1.687396
H	-6.376711	5.245012	-0.897914
H	-7.278976	4.538674	1.315216
H	-5.967107	2.943919	2.704994
H	-3.825981	2.069485	1.935552

Frequencies

22.3595	27.9967	48.9939
68.6185	91.4916	91.5749
94.7733	134.3522	152.0132
177.7106	217.8075	239.9692
264.5830	291.7842	294.3097
331.6936	428.9377	443.5764
470.4547	507.2334	525.0701
538.0678	538.8634	570.9273
595.3369	626.8338	636.1188
659.1006	681.4571	683.6751
719.8573	731.9501	747.0624
766.4121	785.4494	786.6322
811.2207	836.0280	842.1768
871.7686	896.7281	927.3509
938.5054	955.0867	982.5350
994.5575	1006.9031	1022.4071
1026.5972	1047.1429	1055.8978
1061.1821	1074.7089	1081.9752
1116.6172	1141.3427	1165.8302
1196.2379	1197.1015	1223.6412
1237.7073	1257.3864	1287.4978
1312.6856	1340.5170	1358.4107
1370.0765	1396.5022	1397.4438
1423.2578	1465.6717	1488.2069
1497.1069	1506.2871	1529.1910
1543.2434	1557.5063	1585.7339
1641.1126	1657.6851	1681.7314
1691.7416	1697.9542	1739.3200
1793.2500	3074.2699	3135.1305
3190.7724	3193.3208	3214.4542
3217.5274	3224.6547	3230.1058
3237.2216	3241.1718	3245.6019
3260.6073	3287.5045	3633.0494

Energy: -915.7488937
PCM: -915.961976099

N1

C	0.134447	0.425414	0.814969
C	1.332522	0.055121	1.433507
C	1.373753	0.005113	2.830417
H	2.282688	-0.314721	3.328437
C	0.263371	0.341313	3.589729
H	0.312141	0.290797	4.672415
C	-0.914445	0.739389	2.955381
H	-1.786473	1.008544	3.543278
C	-0.983965	0.778075	1.571929
H	-1.901978	1.072824	1.071135
N	0.100389	0.445868	-0.574222
C	0.979557	-0.258196	-1.371174
N	2.162039	-0.649670	-0.742874
C	2.491389	-0.216447	0.558354
C	3.759968	-0.055777	1.003201
H	3.875396	0.167239	2.058314
C	5.010228	-0.011407	0.226477
O	5.040671	0.192925	-0.976594
C	6.287560	-0.163275	1.024887
H	7.148007	-0.034356	0.366819
H	6.331204	0.574546	1.834044
H	6.327210	-1.156316	1.487708
O	0.720020	-0.501036	-2.533908
C	2.943693	-1.664615	-1.405115
C	3.143141	-2.874200	-0.747184
C	3.869452	-3.887160	-1.364971
C	4.378894	-3.694837	-2.645753
C	4.164960	-2.484823	-3.300218
C	3.455006	-1.463207	-2.680921
H	2.726944	-3.022973	0.244819
H	4.021735	-4.830852	-0.849610
H	4.939998	-4.486551	-3.133357
H	4.564058	-2.327042	-4.297442
H	3.304738	-0.512622	-3.174858

Frequencies

31.0314	53.3890	60.3196
71.1185	86.8513	94.8024
104.1963	133.6747	159.9498
188.2506	238.5540	262.6189
276.5236	281.2495	326.0543
374.8235	407.7790	427.0311
453.5516	474.8109	522.9092
541.6829	552.5878	566.3852
576.9591	591.8349	629.6270
637.1698	667.0385	685.4560
710.8098	723.0903	729.5974
761.5782	769.8006	780.5896
791.8916	841.7750	858.1064
863.2343	889.4423	922.8130

947.9370	958.9137	979.8654
995.8846	999.7618	1014.7635
1022.2297	1033.2511	1047.3159
1065.6951	1074.7758	1090.9888
1121.2637	1154.4439	1180.5844
1194.7174	1199.4688	1216.5576
1230.8965	1269.0014	1293.4583
1311.6319	1325.0227	1347.0998
1361.4534	1370.7144	1388.4025
1422.3576	1449.1453	1468.0775
1495.5368	1505.4507	1514.6959
1555.4273	1561.4063	1562.8075
1664.9462	1680.0848	1686.0418
1690.6611	1703.4371	1797.3178
1819.5089	3073.6478	3134.1203
3189.4695	3208.5892	3211.4779
3218.2747	3222.9818	3227.4289
3228.2345	3235.8682	3236.5563
3246.2702	3277.3123	3645.3139

Energy: -915.766208
PCM: -915.986495040

N1-

C	0.235596	-0.314019	0.776227
C	1.341902	0.088216	1.516600
C	1.172339	0.585336	2.806477
C	-0.101622	0.693016	3.352859
C	-1.211982	0.287545	2.614924
C	-1.037764	-0.220412	1.330803
N	2.658210	-0.015416	0.969620
C	3.263853	1.152489	0.613498
N	4.550455	1.034965	0.110697
C	5.339709	-0.110463	0.230017
C	4.703046	-1.318721	0.535917
C	3.232575	-1.369197	0.717732
C	5.495418	-2.463826	0.627980
C	6.869299	-2.418778	0.417043
C	7.485059	-1.206327	0.110269
C	6.717445	-0.050491	0.019149
O	2.754091	2.269839	0.710139
C	2.533167	-2.481455	0.696240
C	1.315275	-3.127427	0.780243
C	0.932331	-3.670763	2.158448
O	0.537246	-3.376702	-0.178812
H	4.988691	-3.396674	0.854778
H	7.458596	-3.328804	0.492209
H	8.557903	-1.156807	-0.057052
H	7.181357	0.903497	-0.223898
H	-0.040193	-3.247940	2.435747

H	0.819162	-4.759664	2.100522
H	1.667738	-3.424734	2.931490
H	2.046827	0.896162	3.369422
H	-0.226716	1.089034	4.357466
H	-2.208461	0.359661	3.043674
H	-1.893169	-0.561268	0.754688
H	0.373838	-0.739278	-0.211363
H	4.993938	1.929121	-0.041444

Frequencies

18.0192	34.6033	63.5219
80.8380	88.3601	95.9813
101.0989	126.4272	141.3840
162.1225	224.8909	242.8527
272.0217	291.0276	364.3255
385.1621	429.6033	432.2048
440.7444	461.0854	500.1489
503.7899	531.0793	534.8602
566.7615	592.2031	601.0851
637.5733	652.0644	671.7826
679.6241	714.2517	728.8186
759.8700	765.6499	769.4899
783.2698	850.3222	861.7526
870.6069	877.0867	923.5887
945.3152	957.9123	993.9720
1001.9284	1003.4406	1011.7374
1026.8030	1034.7745	1053.5512
1069.4069	1080.2327	1114.1203
1136.7352	1142.1985	1184.4509
1187.7801	1211.7919	1223.6882
1277.0047	1294.0709	1312.2956
1319.4352	1340.1416	1357.0155
1368.1900	1396.8909	1449.9164
1455.8370	1497.5842	1501.9825
1509.2192	1536.0364	1556.4862
1563.7259	1588.7977	1673.6933
1675.7907	1686.9669	1691.2674
1753.1387	1861.0073	3056.9381
3124.3564	3137.8961	3181.5502
3190.4044	3197.2313	3206.5770
3214.4123	3221.0876	3230.1417
3231.5544	3253.9769	3661.9281

Energy: -915.1822528
PCM: -915.463951044

TS-5-cycle

C	-1.695226	-3.334292	-4.460609
C	-2.343411	-2.217306	-3.906013
C	-3.620244	-1.882482	-4.381573
C	-4.240375	-2.645879	-5.361411
C	-3.594145	-3.752678	-5.900136
C	-2.318918	-4.082579	-5.448007
N	-1.807405	-1.436380	-2.885100
C	-0.504651	-1.382527	-2.558396
O	0.521493	-1.780790	-3.091480
C	-0.578331	-0.708792	-1.207213
C	-1.859276	-0.696534	-0.890585
C	-3.314678	-0.765534	-0.662542
C	-3.979485	-2.094521	-0.891073
C	0.472313	-0.209912	-0.340853
C	-0.005413	0.388002	0.828202
C	0.871922	0.891725	1.773365
C	2.240917	0.798129	1.526879
C	2.718202	0.216709	0.354097
C	1.837403	-0.292322	-0.593454
N	-1.432668	0.375516	0.906417
O	-3.915857	0.217356	-0.274872
H	0.501477	1.353713	2.683342
H	2.941233	1.188760	2.258125
H	3.787642	0.156861	0.180895
H	2.176037	-0.761530	-1.510789
H	-1.811414	0.058203	1.794687
H	-4.104653	-0.996999	-3.980615
H	-5.229281	-2.366523	-5.713332
H	-4.073535	-4.347111	-6.671615
H	-1.800253	-4.938106	-5.871461
H	-0.695759	-3.581535	-4.126017
H	-3.289346	-2.924725	-0.727412
H	-4.840835	-2.166581	-0.223973
H	-4.326829	-2.162339	-1.926189
H	-1.896897	1.243906	0.646795

Energy (PCM)=-915.852862

-522.2564	32.4091	44.7121
47.2968	58.8314	94.2364
109.0321	115.0136	138.6244
160.9563	183.7244	194.0908
214.8582	241.4551	293.4140
315.8867	338.6256	381.8721
400.8102	429.5346	447.3251
457.5692	496.4281	528.7283
540.6902	552.9955	582.5612
582.8895	605.1262	636.2165
639.6010	682.1977	722.1417

740.5202	764.5256	788.3445
799.0685	804.3731	849.7124
860.2454	872.8372	888.9703
915.8439	919.7484	946.4436
993.4679	994.7539	1013.6642
1021.1900	1026.2722	1038.3366
1050.5788	1064.3777	1069.4971
1072.5721	1123.3888	1144.2694
1161.8394	1194.1368	1197.7644
1206.1227	1215.8217	1237.3766
1279.9082	1327.3117	1335.3969
1350.7895	1372.8946	1375.2521
1428.7423	1434.8686	1497.9936
1505.1614	1517.2081	1527.9759
1557.9037	1562.5885	1654.6118
1664.3289	1684.3741	1690.9282
1706.4052	1787.4170	1797.6675
1812.1926	3096.8197	3172.2938
3195.1621	3205.1959	3212.4269
3220.4617	3223.2542	3231.0911
3234.5789	3242.7356	3255.6232
3267.3317	3525.8522	3611.1407

Part 2. Quantum-Chemical calculations: optimized geometries for structures involving silver cation.

TS-N-attack

C	-4.316053	0.934202	-0.646526
C	-2.974947	0.655501	-0.404788
C	-2.595574	-0.623983	0.034185
C	-3.568920	-1.607099	0.208022
C	-4.910165	-1.325764	-0.033853
C	-5.280225	-0.051715	-0.454169
N	-2.001189	1.657319	-0.538763
C	-0.654586	1.406368	-0.720343
O	0.148686	2.341283	-0.409834
C	-1.208727	-0.877910	0.368034
C	-0.368743	-1.337148	1.170168
C	0.885330	-1.583769	1.731016
O	1.618408	-0.666438	2.198390
N	-0.366795	0.174643	-1.150960
C	0.931833	-0.218891	-1.482764
C	2.021304	0.647566	-1.715615
C	3.271054	0.134744	-2.071863
C	3.476631	-1.232046	-2.201469
C	2.398690	-2.095127	-1.998079
C	1.152364	-1.599400	-1.648670
C	1.367222	-3.004954	1.854086
H	-3.261614	-2.591013	0.547525

H	-5.659911	-2.098237	0.103466
H	-6.323900	0.177036	-0.647494
H	-4.600082	1.924387	-0.991213
H	2.436646	-3.046567	1.634540
H	0.817576	-3.678683	1.193346
H	1.219114	-3.336571	2.888218
H	-2.211053	2.587469	-0.203298
H	0.313041	-2.273437	-1.516946
H	2.529281	-3.166475	-2.124449
H	4.451753	-1.621484	-2.477207
H	4.085825	0.827727	-2.264022
H	1.872031	1.719000	-1.688841
Ag	1.468330	1.255976	1.088123

TS-O-attack

C	9.452081	-2.743356	1.962976
C	10.413218	-3.739640	1.730108
H	10.120179	-4.590014	1.123903
C	11.695988	-3.649119	2.243576
H	12.420429	-4.431320	2.042118
C	12.037222	-2.547372	3.028507
H	13.035344	-2.459016	3.446818
C	11.099656	-1.562035	3.288464
H	11.363356	-0.709744	3.909274
C	9.803148	-1.640365	2.763214
N	8.920252	-0.607964	3.047855
H	9.277748	0.230827	3.482499
C	7.595929	-0.548170	2.668308
O	7.095618	-1.624225	2.137019
C	8.152960	-2.921714	1.349842
C	7.478456	-3.635657	0.563320
C	6.238297	-3.926840	-0.010533
C	5.670615	-5.312123	0.166347
H	4.579867	-5.264279	0.207020
H	5.953541	-5.918981	-0.701652
H	6.068931	-5.797119	1.060705
O	5.586043	-3.106698	-0.718639
Ag	5.571051	-1.106479	0.240323
N	6.966655	0.565898	2.871875
C	5.664478	0.692531	2.410717
C	4.556033	0.497400	3.248265
C	3.263163	0.694734	2.778284
C	3.023146	1.078701	1.457841
C	4.104066	1.288173	0.608148
C	5.420724	1.098350	1.071726
H	4.733387	0.199185	4.276335
H	2.425244	0.542632	3.452893
H	2.008910	1.230614	1.103586
H	3.943983	1.643808	-0.405949
H	6.266688	1.427787	0.470040