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Characterization and Density Functional Theory Investigations of 3-Monoacylaminoquinazolinone Derivatives

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1- Synthesis of MAQs

2.2 Synthesis of N-N-monoacylaminoquinazolinone (MAQ)

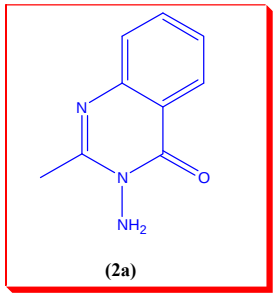
Synthesis of 3-aminoquinazolinones **(2)** was carried out under microwave irradiation. The availability of these 3-aminoquinazolinones having a ring of alkyl group size in the Q-2 substituent would enable the important of this alkyl group on the chemoselectivity process to be assessed 3-aminoquinazolinones **(2)** was synthesized from the corresponding acid chloride. The synthesis can be accomplished in tow steps **(Scheme 1)**; acid chloride was accomplished with freshly distilled thionyl chloride, the acid chloride was reacted with an ether solution of methyl anthranilate and the *N*-acylanthranilate (**1)** obtained was reacted with hydrazine (5 mol equiv.) to give 3-aminoquinazolinone (**2)** in good yield.

Synthesis of 3-monoacylaminoquinazolinones (MAQs); in general monoacylation of the 3-aminoquinazolinones **(2)** with acid chloride and pyridine proceeded in high yields and most of the products **(MAQs) (Scheme 1)**, were crystalline; with short reaction times and absence of excess acid chloride, formation of diacylation products was not competitive. The overall yield was with no need for chromatography at any stage.

General Procedure (I) for 3-Aminoquinazolin-4 (3H) -one Q (NH_2) (2)

Carboxylic acid (0.014 mol) was added to freshly distilled thionyl chloride (6 ml) and one drop of DMF added as catalyst. The solution was heated at 40°C for 4h (with exclusion of moisture), cooled to room temperature and excess thionyl chloride was removed under reduced pressure. The acid chloride was diluted with dry ether (5 ml) then added briskly to an efficiently stirred solution of methyl anthranilate hydrochloride was filtered off, the other solution washed with hydrochloric acid (2M, 20 ml) (twice), then water, dried and the solvent evaporated under reduced pressure. N-(acyl) anthranilate (48) (0.009 mol) was dissolved in ethanol (60 ml) and hydrazine monohydrate (1.24 ml, 0.005 mol) added. The reaction mixture was heated under reflux for 2h then cooled to room temperature and excess ethanol removed under reduced pressure.

Preparation of 3-amino-2-methyl- quinazolin -4 (3H) -one (2a)



(2a)

Acetic acid (3g, 0.05 mol) was added to freshly distilled thionyl chloride (6 ml) and one drop of DMF added as catalyst. The solution was heated at 40 ˚C for 4h (with exclusion of moisture), cooled to room temperature and excess thionyl chloride was removed under reduced pressure. The acid chloride was diluted with dry ether (5 ml) then added briskly to an efficiently stirred solution of methyl anthranilate hydrochloride was filtered off, the other solution washed with hydrochloric acid (2M, 20 ml) (twice), then water, dried and the solvent evaporated under reduced pressure. Methyl – N (methylethanoyl) anthranilate (3.1g 0.016 mol) was dissolved in ethanol (60 ml) and hydrazine monohydrate (1.24 ml, 0.005 mol) added. The reaction mixture was heated under reflux for 2h then cooled to room temperature and excess ethanol removed under reduced pressure. The foregoing 2- (methylethanoyl) aminobenzoic acid hydrazide (2.7g, 0.014 mol) was dissolved in ethanol (10 ml) and heated in a sealed tube at 185˚C for 2 days on cooling to room temperature and standing overnight, the product crystallizedout. Recrystallisation from ethanol gave colourless crystals of the title compound **(49a)** (2.7g 90%) m.p 121-123˚C. δ H ($CDCl_3$, 125 MHz) 1.25 (3H, s, CH_3), 4.94 (2H, s, br, NH_2), and 7.40-8.61 [4H, m, 4 × C<u>H</u> (Q)]; δ C ($CDCl_3$, 500 MHz) 22.19 (<u>C</u>H_3),119.91 [<u>C</u>CO (Q)], 126.17, 126.30, 126.80, 130.69 and 134.57 [4 × <u>C</u>H (Q)], 146.85 [CN=<u>C</u> (Q)], 155.42 [<u>C</u>N (Q)] and 168.6 [<u>C</u>O (Q)].

5.5.2 Preparation of 3-amino -2-ethyl- quinazolin -4 (3H) -one (2b)

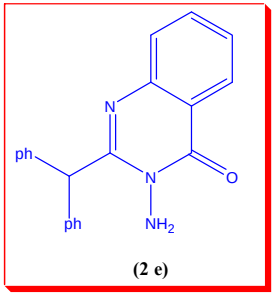
Propionic acid (3g, 0.04mol) was added to freshly distilled thionyl chloride (6 ml) and one drop of DMF added as catalyst. The solution was heated at 40°C for 4h (with exclusion of moisture), cooled to room temperature and excess thionyl chloride was removed under reduced pressure. The acid chloride was diluted with dry ether (5 ml) then added briskly to an efficiently stirred solution of methyl anthranilate hydrochloride was filtered off, the other solution washed with hydrochloric acid (2M, 20 ml) (twice), then water, dried and the solvent evaporated under reduced pressure. Methyl – N (ethylethanoyl) anthranilate (3.1g 0.015 mol) was dissolved in ethanol (60 ml) and hydrazine monohydrate (1.24 ml, 0.005 mol) added. The reaction mixture was heated under reflux for 2h then cooled to room temperature and excess ethanol removed under reduced pressure. The foregoing 2- (ethylethanoyl) aminobenzoic acid hydrazide (2.7g, 0.0.13 mol) was dissolved in ethanol (10 ml) and heated in a sealed tube at 185°C for 2 days on cooling to room temperature and standing overnight, the product crystallizedout. Recrystallisation from ethanol gave colourless crystals of the title compound **(2b)** (2.8g 94%) m.p 113-115°C. δH ($CDCl_3$, 500 MHz) 1.03 (3H, t, *J* 7.5, C<u>H</u>$_3$), 3.04 (2H, q, *J* 7.5, C<u>H</u>$_2$), 4.90 (2H, s, br, NH_2) and 7.40-8.20 [4H, m, 4 × C<u>H</u> (Q)]; δ C ($CDCl_3$, 125 MHz) 11.02, 11.17 (<u>C</u>H_3), 27.90, 28.03 (<u>C</u>H_2), 119.96 [<u>C</u>CO (Q)], 126.19, 126.37, 126.88, 127.15, 127.35, 134.16 and 134.36 [4 × <u>C</u>H (Q)], 147.05 [CN=<u>C</u> (Q)], 159.02 [<u>C</u>N (Q)] and 161.82 [<u>C</u>O (Q)].

Preparation of 3-amino -2-isopropyl-quinazolin -4 (3H) -one (2c)

Isobutyric acid (3g, 0.034 mol) was added to freshly distilled thionyl chloride (6 ml) and one drop of DMF added as catalyst. The solution was heated at 40°C for 4h (with exclusion of moisture), cooled to room temperature and excess thionyl chloride was removed under reduced pressure. The acid chloride was diluted with dry ether (5 ml) then added briskly to an efficiently stirred solution of methyl anthranilate hydrochloride was filtered off, the other solution washed with hydrochloric acid (2M, 20 ml) (twice), then water, dried and the solvent evaporated under reduced pressure. Methyl – N (isobutylethanoyl) anthranilate (3.1g 0.014 mol) was dissolved in ethanol (60 ml) and hydrazine monohydrate (1.24 ml, 0.005 mol) added. The reaction mixture was heated under reflux for

2h then cooled to room temperature and excess ethanol removed under reduced pressure. The foregoing 2- (isobutylethanoyl) aminobenzoic acid hydrazide (2.7g, 0.012 mol) was dissolved in ethanol (10 ml) and heated in a sealed tube at 185°C for 2 days on cooling to room temperature and standing overnight, the product crystallizedout. Recrystallisation from ethanol gave colourless crystals of the title compound **(2c)** (2.6g 88%) m.p 207-210. δ H ($CDCl_3$, 500 MHz) 1.32, 1.34, 1.40, 1.42 (6H, q, *J* 10, 2 × C<u>H</u>$_3$), 3.74, 3.75, 3.77, 3.78, 3.79 (1H, h, *J* 7, C<u>H</u>), 4.88 (2H, s, br, NH_2), 7.4-8.22 [4H, m, 4 × C<u>H</u> (Q)]; δ C ($CDCl_3$, 125 MHz) 20.34, 20.49, 20.61, 20.80 (2 × C<u>H</u>$_3$), 31.04 (<u>C</u>H), 119.93 [<u>C</u>CO(Q)], 126.13, 126.24, 125.34, 127.13, 127.41, 127.65, 134.06 [4 × CH (Q)], 147.11 [CN=<u>C</u>(Q)], 161.96 [<u>C</u>N(Q)] and 162.15 [<u>C</u>O(Q)].

Preparation of 3-amino -2-(di phenyl methyl) quinazolin -4 (3H)-one (2e)



(2 e)

Diphenylacetic acid (3g, 0.014 mol) was added to freshly distilled thionyl chloride (6 ml) and one drop of DMF added as catalyst. The solution was heated at 40°C for 4h (with exclusion of moisture), cooled to room temperature and excess thionyl chloride was removed under reduced pressure. The acid chloride was diluted with dry ether (5 ml) then added briskly to an efficiently stirred solution of methyl anthranilate hydrochloride was filtered off, the other solution washed with hydrochloric acid (2M, 20 ml) (twice), then water, dried and the solvent evaporated under reduced pressure. Methyl – N (diphenylethanoyl) anthranilate (3.1g 0.009 mol) was dissolved in ethanol (60 ml) and hydrazine monohydrate (1.24 ml, 0.005 mol) added. The reaction mixture was heated under reflux for 2h then cooled to room temperature and excess ethanol removed under reduced pressure. The foregoing 2- (Diphenylethanoyl)

aminobenzoic acid hydrazide (2.7g, 0.008 mol) was dissolved in ethanol (10 ml) and heated in a sealed tube at 185°C for 2 days on cooling to room temperature and standing overnight, the product crystallizedout. Recrystallisation from ethanol gave colourless crystals of the title compound **(2e)** (2.4g 85%) m.p 211-213. δ H ($CDCl_3$, 500 MHz) 4.73 (2H, s, br, $N\underline{H}_2$), 6.24 [1H, s, $(ph)_2C\underline{H}$], 7.4-8.2 [14H, m, 10H (Ar) and 4H (Q)]; δ C ($CDCl_3$, 500 MHz) 53.85 [$(ph)_2\underline{C}H$], 119.96 [$\underline{C}CO(Q)$], 126.36, 126.69, 127.13, 128.15, 129.21 and 134.05 [7 × CH (Ar)], 139.90 [2 × C (ph)], 146.56 [$\underline{C}N{=}C$ (Q)], 157.03 [$\underline{C}N$ (Q)] and 161.65 [$\underline{C}O$ (Q)].

General Procedure (II) for Mono- Acylation of N-Aminoquinazolin-4 (3H)-ones MAQ (3)

To the given carboxylic acid (1 mol equiv.) an excess of freshly distilled thinoyl chloride and one drop of DMF were added and the mixture was then heated at 40°C until the reaction was complete, (1- 2h, as shown by the appearance of bands at 1835 and 1780 cm^{-1} in the IR spectrum). Excess thionyl chloride was then removed under reduced pressure, the residual acid chloride diluted with dichloromethane (~1 ml/1g) and added dropwise with stirring over 2 min to the 3- aminoquinzolinone (0.9 mol equiv.) in dichloromethane (~2 ml/1g) containing pyridine (1 mol equiv.). The resulting mixture was then stirred at room temperature for approximately 5h. Further dichloromethane (40 ml) was added and the solution washed with sodium hydrogen carbonate solution, then water, dried and the solvent evaporated.

3-Acetylamino-2-methylquinazolin -4 (3H) –one MAQ (3a)

The general procedure **(II)** for monoacylation was followed using 3-aminoquinazolinone (QNH_2) **(2a)** (2g, 11.42 mmol), followed by addition acetyl chloride (1.08g, 13.70 mmol) and stirring continued for tow days at room temperature. The pale brown solid obtained after work-up was triturated with ethyl acetate-light petroleum and the solid obtained crystallized to give **MAQ (3a)** (1.6g 64.5%). (from light petroleum) δ H 1.25 (3H, s, $C\underline{H}_3$), 2.15 (3H, s, $C\underline{H}_3CO$), 7.63 [1H, ddd, *J* 10.0, 5.0, 2.0, 6-H (Q)], 7.81[2H, m, 7and 8-H (Q)], and 8.2 [1H, dd, J10, 5, 5-H (Q)] 8.4 (1H,s, $N\underline{H}$); δC ($CDCl_3$,125MHz) 20 ($\underline{C}H_3$), 25 ($\underline{C}H_3CO$), 120.4 [$\underline{C}CO$ (Q)]

126.5, 126.7, 127.6 127.7, 127.8, 127.9, 128.4, 128.6, and 134.9 [4×CH (Q)], 147.3 [C-N=C (Q)], 161.6 [C=N(Q)], 162.0 [CO (Q)] and 167.1[CH_3CON].

3-Acetylamino-2-ethylquinazolin -4 (3H)-one MAQ (2b)

The general procedure **(II)** for monoacylation was followed using 3-aminoquinazolinone (QNH_2) **(2b)** (2g, 10.57 mmol), followed by addition acetyl chloride (0.996g, 12.68 mmol) and stirring continued for tow days at room temperature. The pale brown solid obtained after work-up was triturated with ethyl acetate-light petroleum and the solid obtained crystallized to give **MAQ (3b)** (1.5g 61.4%). (from light petroleum) δ H 1.03 (3H, t, *J* 7.5, CH_3CH_2), 3.04 (2H, q, *J* 7.5, CH_3CH_2) 2.15 (3H, s, CH_3CO), 7.63 [1H, ddd, *J* 10.0, 5.0, 2.0, 6-H (Q)], 7.81 [2H, m, 7and 8-H (Q)], and 8.2 [1H, dd, *J*10, 5, 5-H (Q)] 8.4 (1H, s, NH); δ C ($CDCl_3$,125 MHz) 10 (CH_3CH_2), 21 (CH_3CH_2), 25 (CH_3CO), 120.4 [CCO (Q)] 126.5, 126.7, 127.6 127.7, 127.8, 127.9, 128.4, 128.6, and 134.9 [4×CH (Q)], 147.3 [C-N=C (Q)], 161.6 [C=N (Q)], 162.0 [CO (Q)] and 167.1 [CH_3CON].

3-Acetylamino-2- Isopropylquinazolin -4 (3H) –one MAQ (3c)

The general procedure II for monoacylation was followed using 3-aminoquinazolinone (QNH_2) **(2c)** (2g, 9.84 mmol), followed by addition acetyl chloride (0.927g, 11.81 mmol) and stirring continued for tow days at room temperature. The pale brown solid obtained after work-up was triturated with ethyl acetate-light petroleum and the solid obtained crystallized to give **MAQ (3c)** (1.7g 70.4%). (from light petroleum) δ H 1.25 and 1.27 (6H, 2×d, *J* 5.0, CH_3CHCH_3), 3.15 (1H, h, *J* 5, CH_3CHCH_3), 2.15 (3H, s, CH_3CO), 7.63 [1H, ddd, *J* 10, 5, 2, 6-H (Q)], 7.81 [2H, m, 7 and 8-H (Q)], and 8.2 [1H, dd, *J* 10, 5, 5-H (Q)] 8.4 (1H, s, NH); δ C ($CDCl_3$, 125 MHz) 20, 21.4 (CH_3CHCH_3), 31.3 (CH_3CHCH_3), 25 (CH_3CO), 120.4 [CCO (Q)]126.7, 127.8, 128.4, 128.6, and 134.9 [4×CH (Q)], 147.3 [C-N=C (Q)], 161.6 [C=N (Q)], 162.0 [CO (Q)] and 167.1 [CH_3CON].

3-Acetylamino-2-phenyl quinazolin -4 (3H) –one MAQ (3d)

The general procedure **(II)** for monoacylation was followed using 3-aminoquinazolinone (QNH_2) **(2d)** (2g, 8.43 mmol), followed by addition acetyl chloride (0.794g, 10.12 mmol) and stirring continued for tow days at room temperature. The pale brown solid obtained after work-up was triturated with ethyl acetate-light petroleum and the solid obtained crystallized to give **MAQ (3d)** (1.7g 75%) m.p 124-126 ˚C. (from light petroleum) δ H 2.15 (3H, s, CH_3CO), 7.17-7.20 [2H, m, CH (ph)], 7.30-7.39 [2H, m, CH (ph)], 7.58 [1H, m, CH (ph)], 7.63 [1H, ddd, *J* 10, 5, 2, 6-H (Q)], 7.81 [2H, m, 7and 8-H (Q)], and 8.2 [1H, dd, *J* 10, 5, 5-H (Q)] 8.4 (1H,s, NH); δ C ($CDCl_3$, 125 MHz) 25 (CH_3CO), 120.4 [CCO (Q)] 126.7, 127.8, 128.4, 128.6, and 134.9 [(4×CH (Q)) and (5×CH (ph))], 130.4 [2×C (ph)], 147.3 [C-N=C (Q)], 161.6 [C=N (Q)], 162.0 [CO (Q)] and 167.1 [CH_3CON].

3-Benzoylamino-2-methylquinazolin -4 (3H) –one MAQ (3e)

The general procedure **(II)** for monoacylation was followed using 3-aminoquinazolinone (QNH_2) **(2e)** (2g, 11.42 mmol), followed by addition benzoyl chloride (1.93g, 13.7 mmol) and stirring continued for tow days at room temperature. The pale brown solid obtained after work-up was triturated with ethyl acetate-light petroleum and the solid obtained crystallized to give **MAQ (3e)** (2.3g 72%). (from light petroleum) δ H 1.3 (3H, s, CH_3), 7.17-7.20 [2H, m, CH (ph)], 7.30-7.39 [2H, m, CH (ph)], 7.58 [1H, m, CH (ph)], 7.63 [1H, ddd, *J* 10, 5, 2, 6-H (Q)], 7.81 [2H, m, 7 and 8-H (Q)], and 8.2 [1H, dd, *J* 10, 5, 5-H (Q)] 8.4 (1H, s, NH); δ C ($CDCl_3$, 125 MHz) 19.9 (CH_3 Q), 120.4 [CCO (Q)] 126.5, 126.7, 127.6 127.7, 127.8, 127.9, 128.4, 128.6, and 134.9 [(4×CH (Q)) and (5×CH(ph))], 130.4 [C(ph)], 147.3 [C-N=C (Q)], 161.6 [C=N(Q)], 162.0 [CO(Q)] and 167.1 [phCON].

3-Benzoylamino-2-isopropylquinazolin -4 (3H) –one MAQ (3 f)

The general procedure **(II)** for monoacylation was followed using 3-aminoquinazolinone (QNH_2) **(2c)** (2g, 9.84 mol), followed by addition benzoyl chloride (1.65g, 11.81 mmol) and stirring continued for tow days at room temperature. The pale brown solid

obtained after work-up was triturated with ethyl acetate-light petroleum and the solid obtained crystallized to give **MAQ (3f)** (2g 66%) m.p 174-176 ˚C. (from light petroleum) δH 1.25 and 1.27 (6H, 2× d, *J* 6.6, C$\underline{H}_3$CHC$\underline{H}_3$), 3.15 (1H, h, J6.6, $CH_3C\underline{H}CH_3$), 7.17-7.20 [2H, m, CH(ph)], 7.30-7.39 [2H, m, CH(ph)], 7.58 [1H, m, CH(ph)], 7.63 [1H, ddd, *J* 10, 5, 2, 6-H (Q)], 7.81 [2H, m, 7 and 8-H (Q)], and 8.2 [1H, dd, *J* 10, 5, 5-H (Q)] and 11.6 (1H, s, br, NH); δ C ($CDCl_3$, 125 MHz) 20, 21.4 ($\underline{C}H_3CH\underline{C}H_3$), 31.3 ($CH_3\underline{C}HCH_3$), 120.4 [$\underline{C}$CO (Q)] 126.7, 127.8, 127.9, 128.6, and 134.9 [(4×$\underline{C}$H (Q)) and (5×$\underline{C}$H (ph))], 130.4 [$\underline{C}$ (ph)], 147.3 [$\underline{C}$-N=C (Q)], 161.6 [$\underline{C}$=N (Q)], 162.0 [$\underline{C}$O (Q)] and 167.1 [ph$\underline{C}$ON]; IR ν/cm^{-1} :3262 (N-H), 1671 (C=O), 1536 (C=N).

5.6.7 3-Benzoylamino-2-ethylquinazolin -4 (3H) –one MAQ (3 g)

The general procedure **(II)** for monoacylation was followed using 3-aminoquinazolinone (QNH_2) (**2b)** (2g, 10.57 mmol), followed by addition benzoyl chloride (1.78g, 12.68 mmol) and stirring continued for two days at room temperature. The pale yellow solid obtained after work-up was triturated with ethyl acetate-light petroleum and the solid obtained crystallized to give **MAQ (3g)** (2.2 g 70%) m.p 106-109 ˚C. (from light petroleum) δ H 1.33 (3H, t, *J* 5, $CH_2C\underline{H}_3$), 2.85 (2H, q, *J* 5, $CH_3C\underline{H}_2$), 7.17-7.20 [2H, m, C$\underline{H}$(ph)], 7.30-7.39 [2H, m, C$\underline{H}$(ph)], 7.58 [1H, m, C$\underline{H}$(ph)], 7.63 [1H, ddd, *J* 10, 5, 2, 6-H (Q)], 7.81 [2H, m, 7 and 8-H (Q)], and 8.2 [1H, dd, *J* 10, 5, 5-H (Q)], 10.23 (1H, s, br, NH); δ C ($CDCl_3$, 125 MHz) 27.12, 27.9 ($\underline{C}H_2CH_3$), 10.82, 11.27 ($CH_2\underline{C}H_3$), 120.4 [$\underline{C}$CO (Q)] 126.5, 126.7, 127.6 127.7, 127.8, 127.9, 128.4, 128.6, and 134.9 [(4×$\underline{C}$H (Q)) and (5×$\underline{C}$H(ph))], 130.4 [$\underline{C}$(ph)], 147.3 [$\underline{C}$-N=C (Q)], 161.6 [$\underline{C}$=N (Q)], 162.0 [$\underline{C}$O (Q)] and 167.1 [ph$\underline{C}$ON].

3-Acetylamino -2-diphenylmethylquinazolin -4 (3H) –one MAQ (3h)

The general procedure **(**II) for monoacylation was followed using 3-aminoquinazolinone (QNH_2) (**3h)** (2 g, 6.11 mmol), followed by addition acetyl chloride (0.575 g, 7.33 mmol) and stirring continued for tow days at room temperature. The pale white

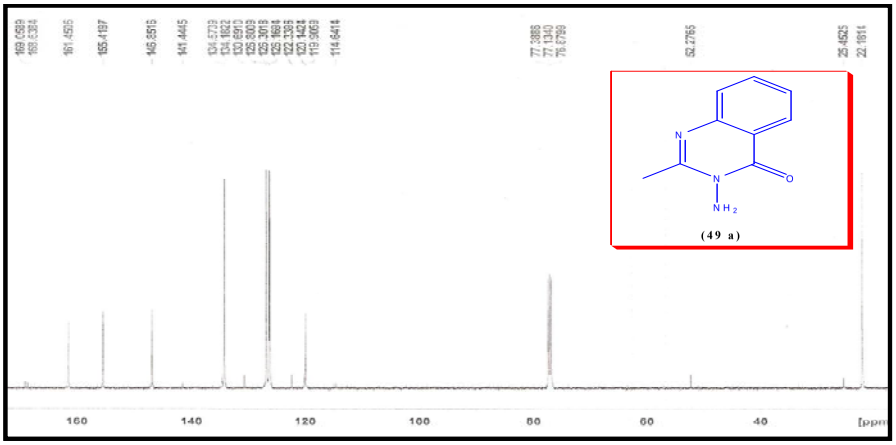
solid obtained after work-up was triturated with ethanol and the solid obtained crystallized to give **MAQ (3h)** (1.4 g 62%) m.p 201-203 °C. (from ethanol) δ H 2.61 (3H, s, C<u>H</u>$_3$CO), 4.91 [1H, s, C<u>H</u>(ph)$_2$] 7.25-7.41 [10H, m, C<u>H</u>(Ar)], 7.45 [2H, ddd, *J* 10, 5, 2, 7 and 8-H (Q)], 7.63[1H, ddd, *J* 10.5.2. 6-H (Q)], and 8.23 [1H, d, *J* 10, 5-H (Q)] and 11.0 (1H, s, N<u>H</u>); δ C ($CDCl_3$, 125 MHz) 22.2 (<u>C</u>H$_3$CO), 52.3 [<u>C</u>H (ph)$_2$], 120.0 [<u>C</u>CO (Q)] 120.2, 122.4, 126.3 126.4, 126.9, 134.3 [7 × <u>C</u>H (Ar)], 140.0 [2 × <u>C</u>(ph)], 146.9 [<u>C</u>-N=C (Q)], 155.4 [<u>C</u>=N (Q)], 161.5 [2 × <u>C</u>O]; MS m/z(%): 370 (M^{+2}, 8.18), 368 (M^+, 46.20), 326 (68.19), 309(35), 235(54.14), 167 (94.65), 1.66 (28.81), 165 (81.43), 152 (35.70), 102 (20.04), 77 (27.57), 76 (22.20), 63 (22.54), 51 (28.47), 50 (25.80), 43 (100).

3-Benzoylamino -2-diphenylmethylquinazolin -4 (3H) –one MAQ (3i)

The general procedure **(II)** for monoacylation was follwed using 3-aminoquinazolinone (QNH$_2$) **(2c)** (2 g, 6.11 mmol), followed by addition benzoyl chloride (1.03 g, 7.33 mmol) and stirring continued for tow days at room temperature. The pale white solid obtained after work-up was triturated with ethanol and the solid obtained crystallized to give MAQ **(3i)** (1.4 g 55%) m.p 165-172 °C. (from ethanol) δ H (DMSO), 5.90 [1H, s, C<u>H</u>(ph)$_2$], 7.2- 7.37 [10H, m, C<u>H</u>(Ar)], 7.4 [3H, m, C<u>H</u>(ph)], 7.57-7.61 [2H, m, C<u>H</u>(ph)], 7.63 [2H, ddd, *J* 10, 5, 2, 6, 7-H (Q)], 7.81 [1H, d, *J* 10, 8-H (Q)], 8.19 [1H, d, *J* 10, 5-H(Q)] and 11.51 (1H, s, N<u>H</u>); δ C (DMSO, 125 MHz) 52.0 [<u>C</u>H(ph)$_2$], 120.5 [<u>C</u>CO (Q)], 123.4, 126.4, 126.7, 127.1, 127.3, 127.5, 127.8, 128.1, 128.5, 128.6, 128.7, 129.0, 129.2, 129.3, 131.3, 132.4, 132.7, 135.1 and 135.2 [19×<u>C</u>H(Ar)], 139.4, 139.5 and 139.7 [3×<u>C</u>H(ph)], 146.0 [<u>C</u>-N=C (Q)], 158.8 [<u>C</u>=N (Q)], 162.6 [<u>C</u>O (Q)] and 166.4 (<u>C</u>O).

2. IR, NMR and mass spectra

Fig.(S2): ^{13}C NMR Spectrum for **Q(NH_2) (2a)**



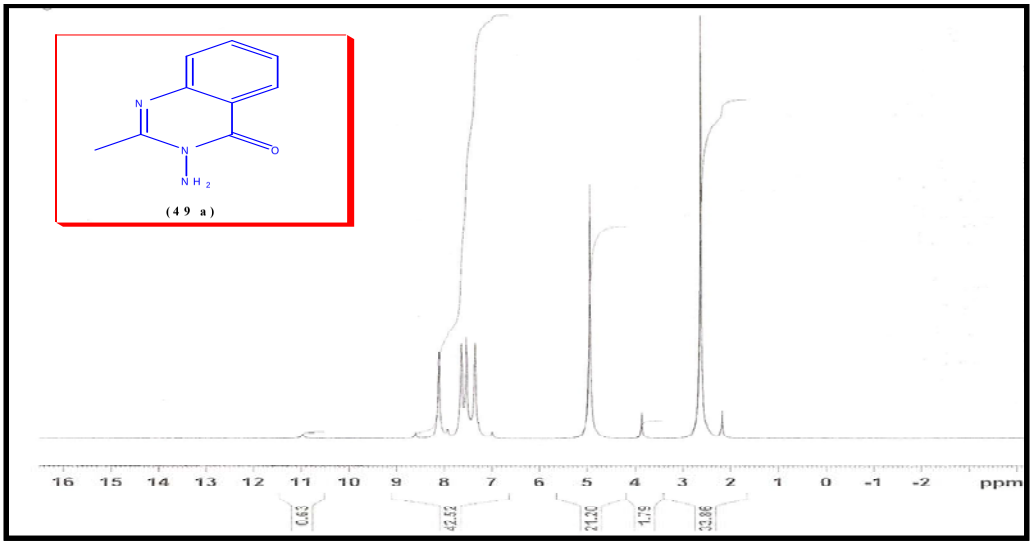


Fig.(S1): ^{1}H NMR Spectrum for **Q(NH_2) (2a)**

Fig.(S3): ^{1}H NMR Spectrum for **Q(NH_2) (2b)**

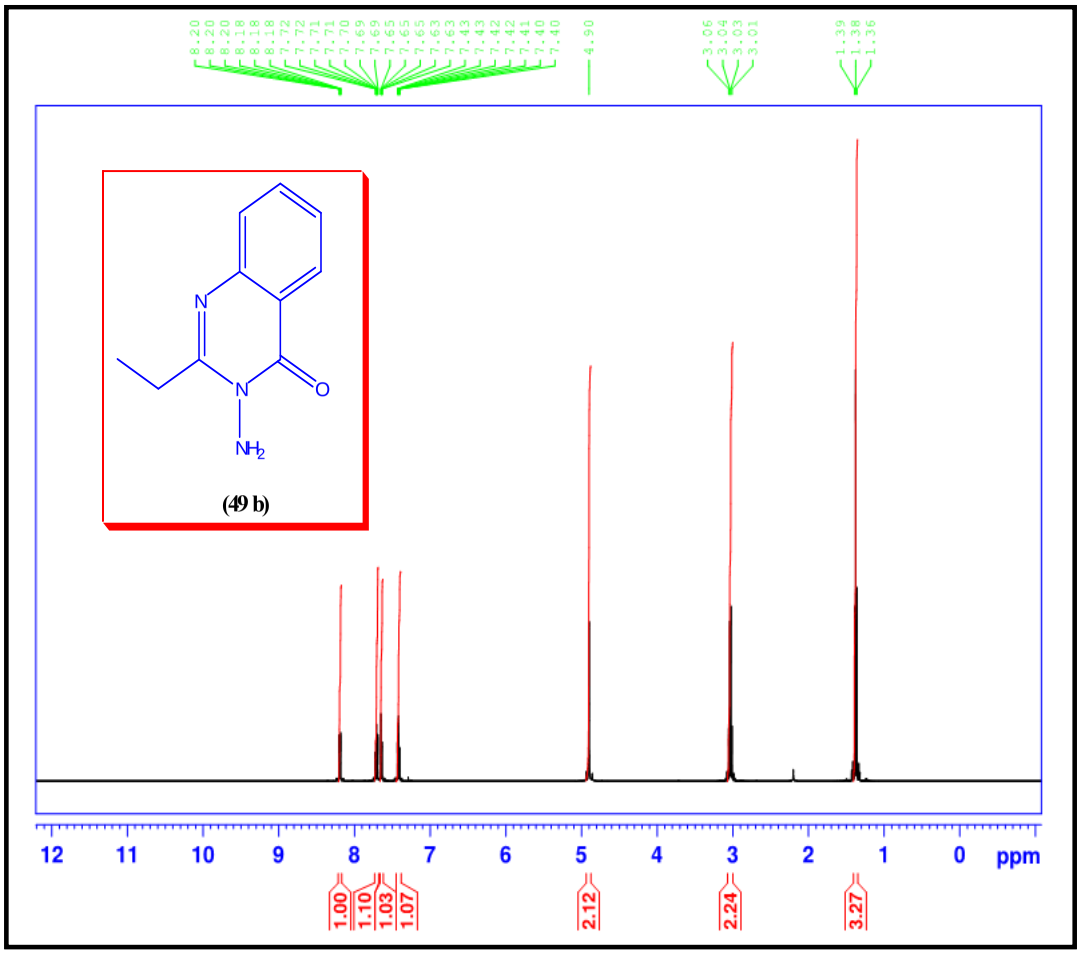


Fig.(S4): ^{1}H NMR Spectrum for **Q(NH_2) (2b)**

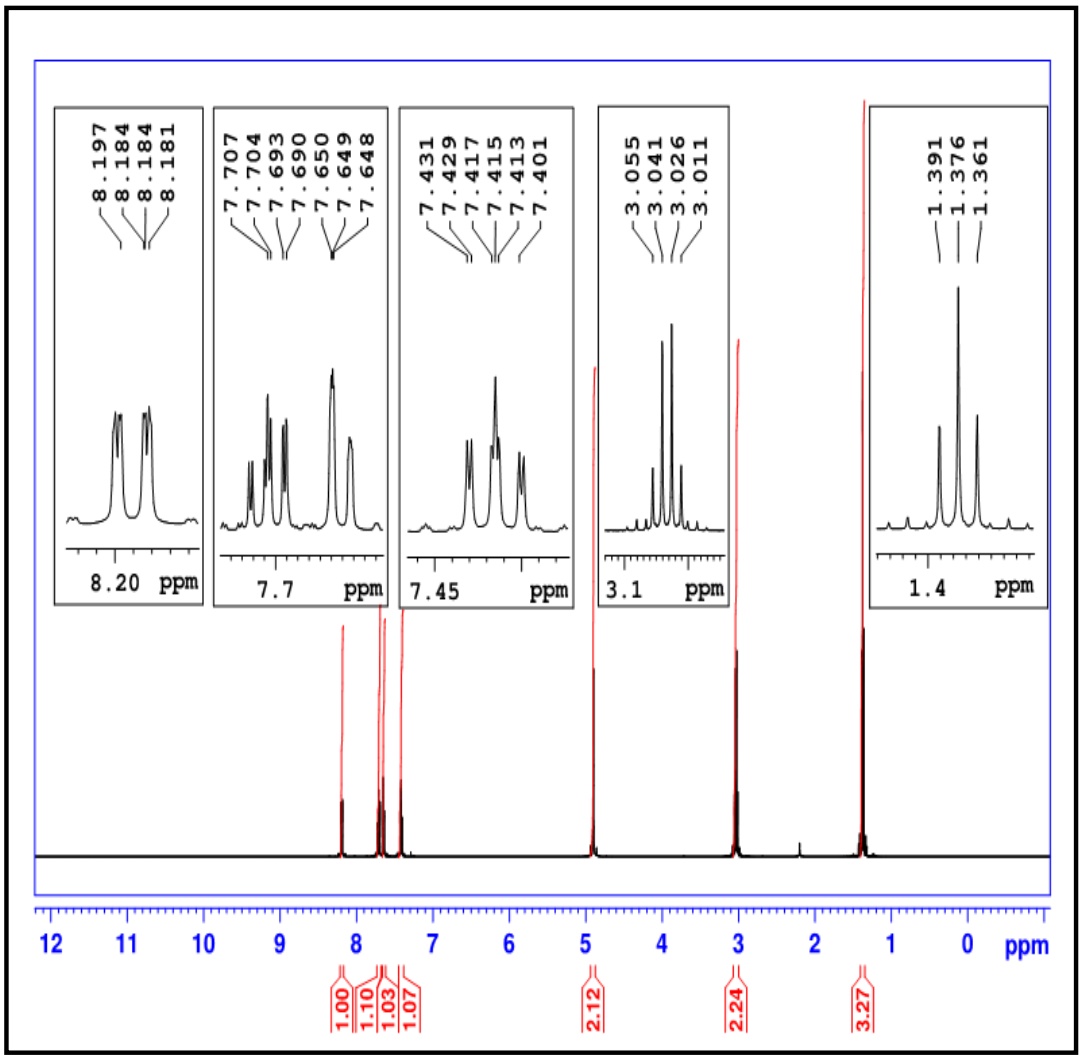


Fig.(S5): ^{13}C NMR Spectrum for **Q(NH_2) (2b)**

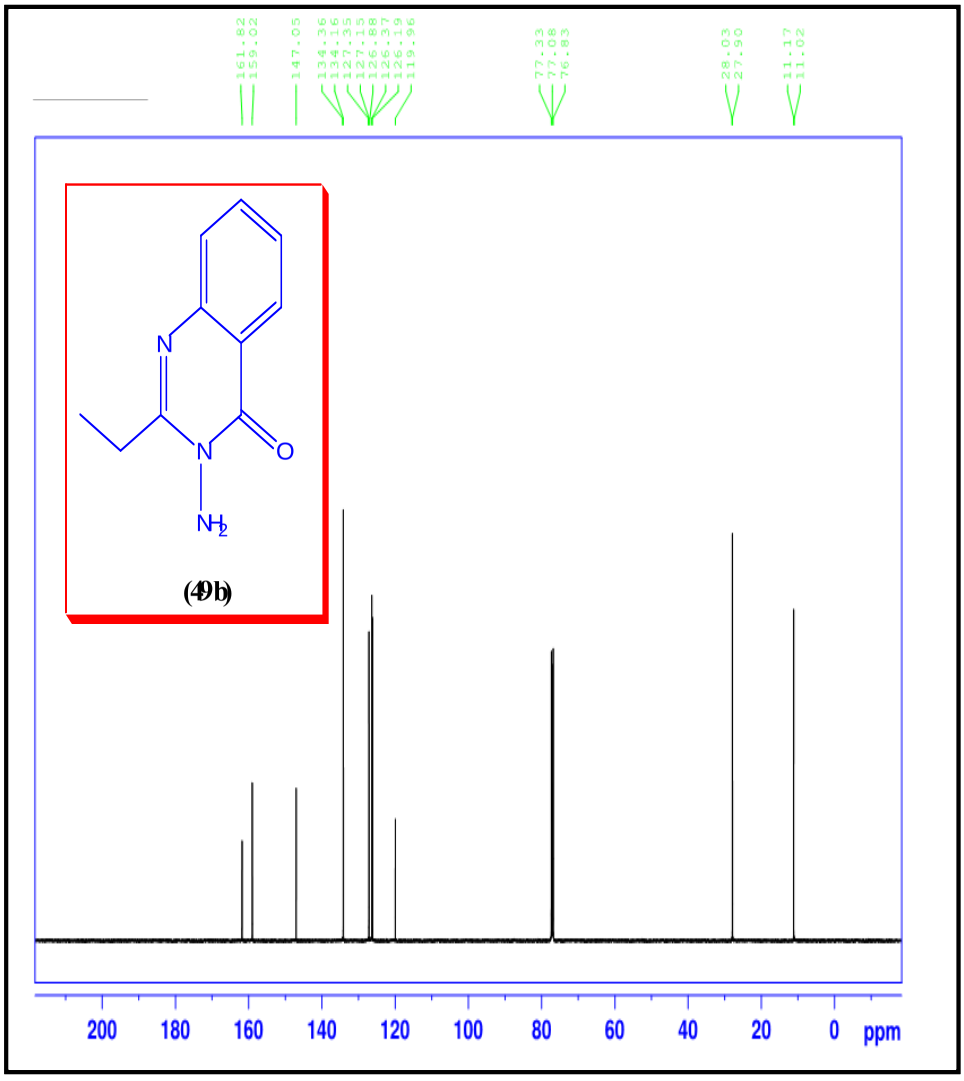


Fig.(S6): ^{1}H NMR Spectrum for **Q(NH_2) (2c)**

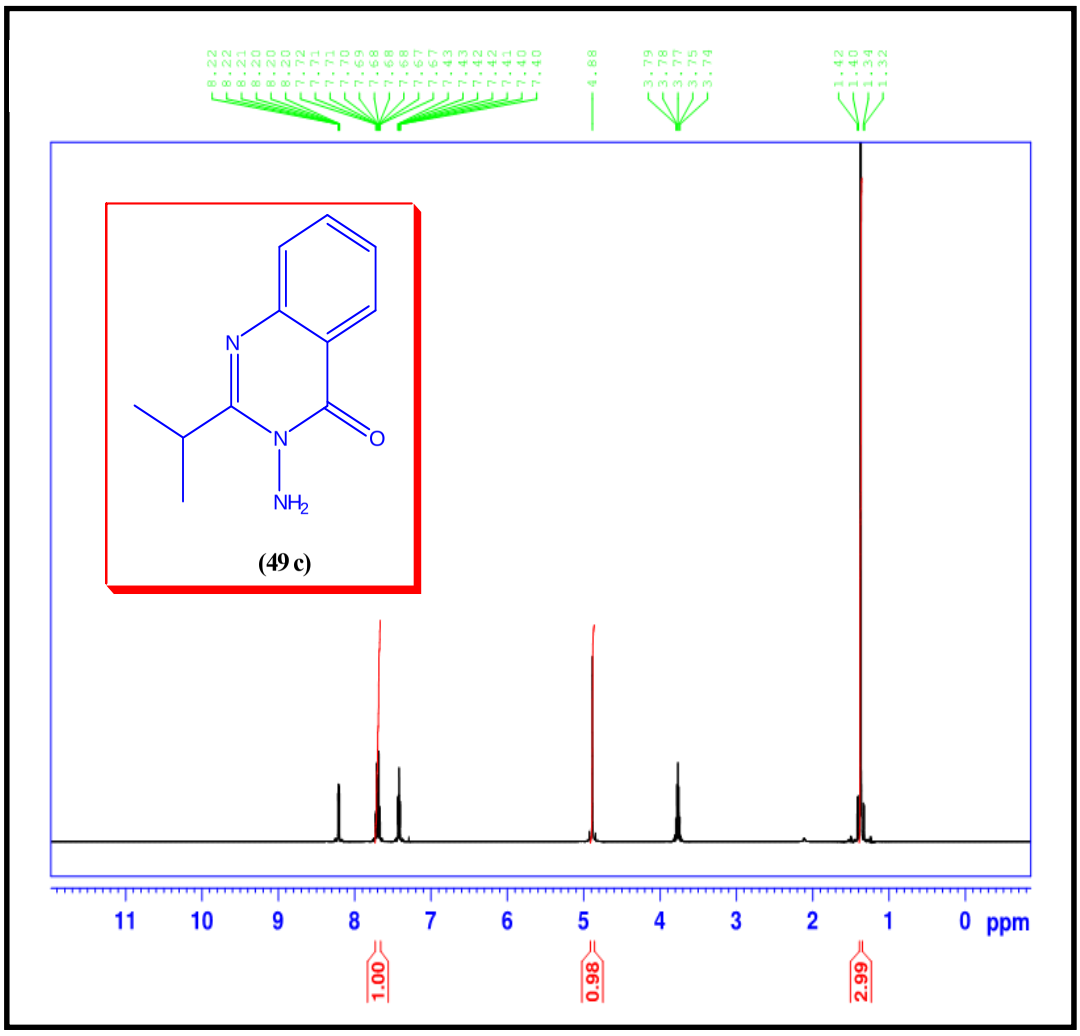


Fig.(S7): ^{13}C NMR Spectrum for **Q(NH_2) (2c)**

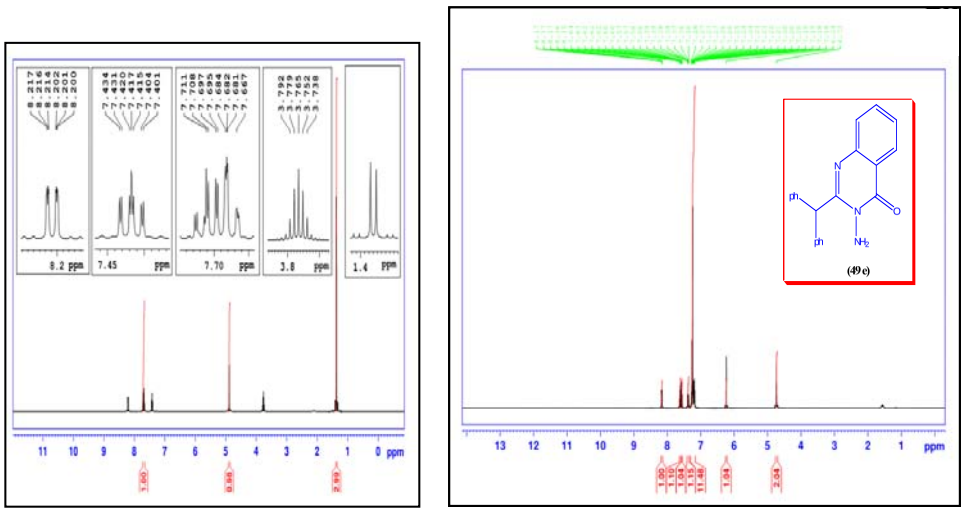


Fig.(S8): ^{1}H NMR Spectrum for **Q(NH_2) (2e)**

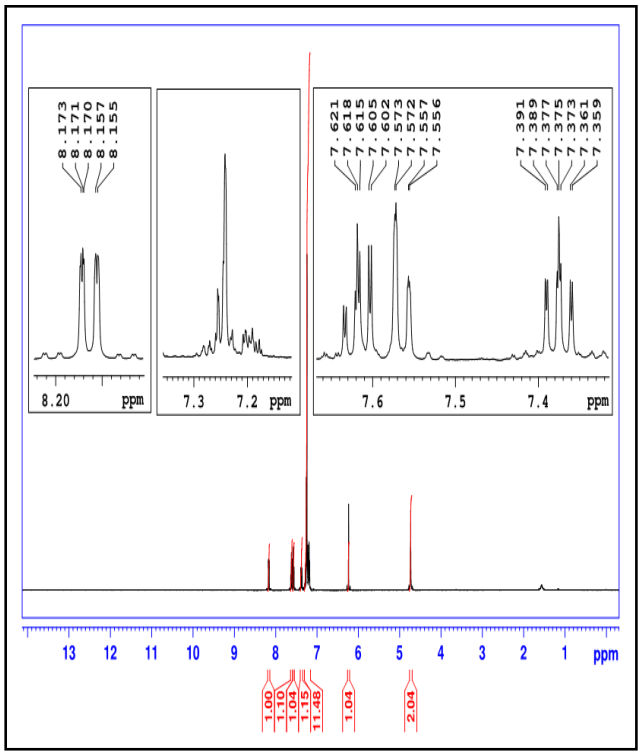


Fig.(S9): ^{1}H NMR Spectrum for **Q(NH_2) (2e)**

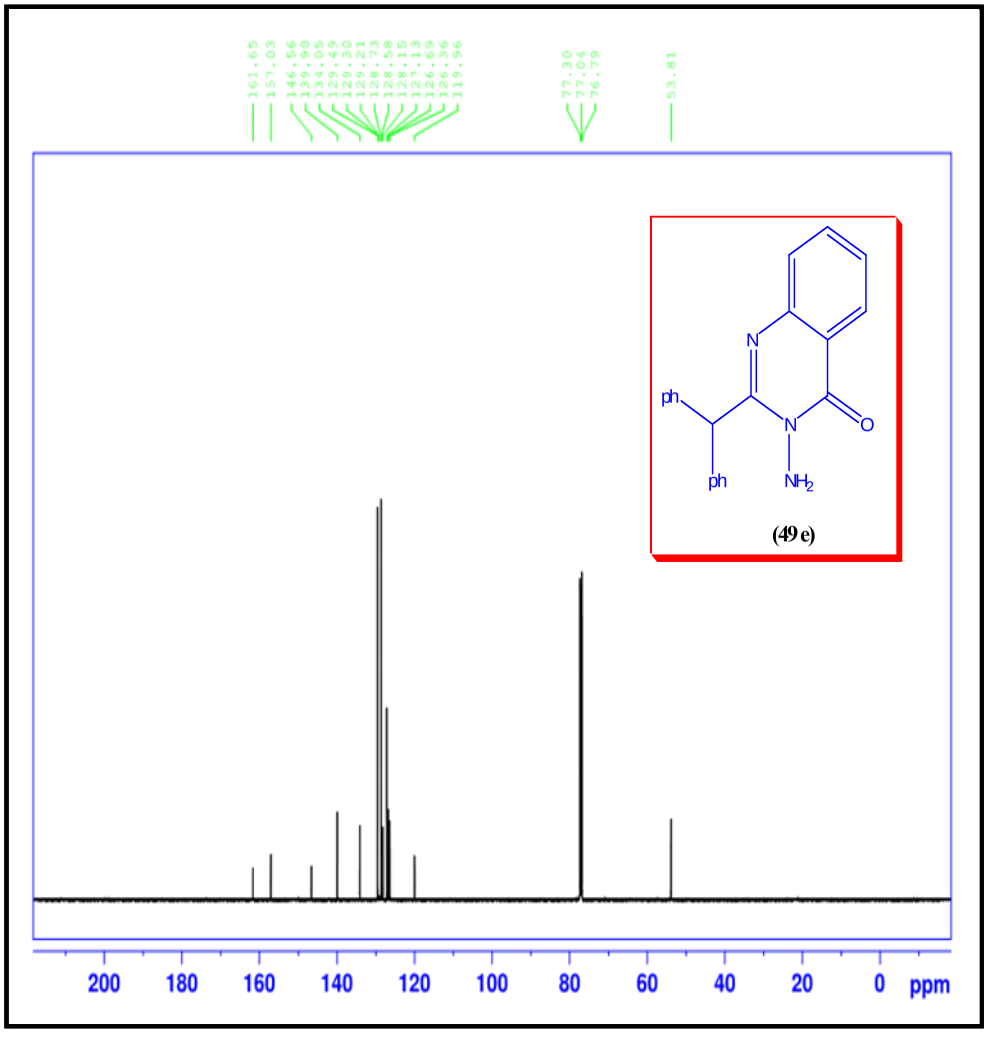


Fig.(S10): ^{1}H NMR Spectrum for **MAQ (3f)**

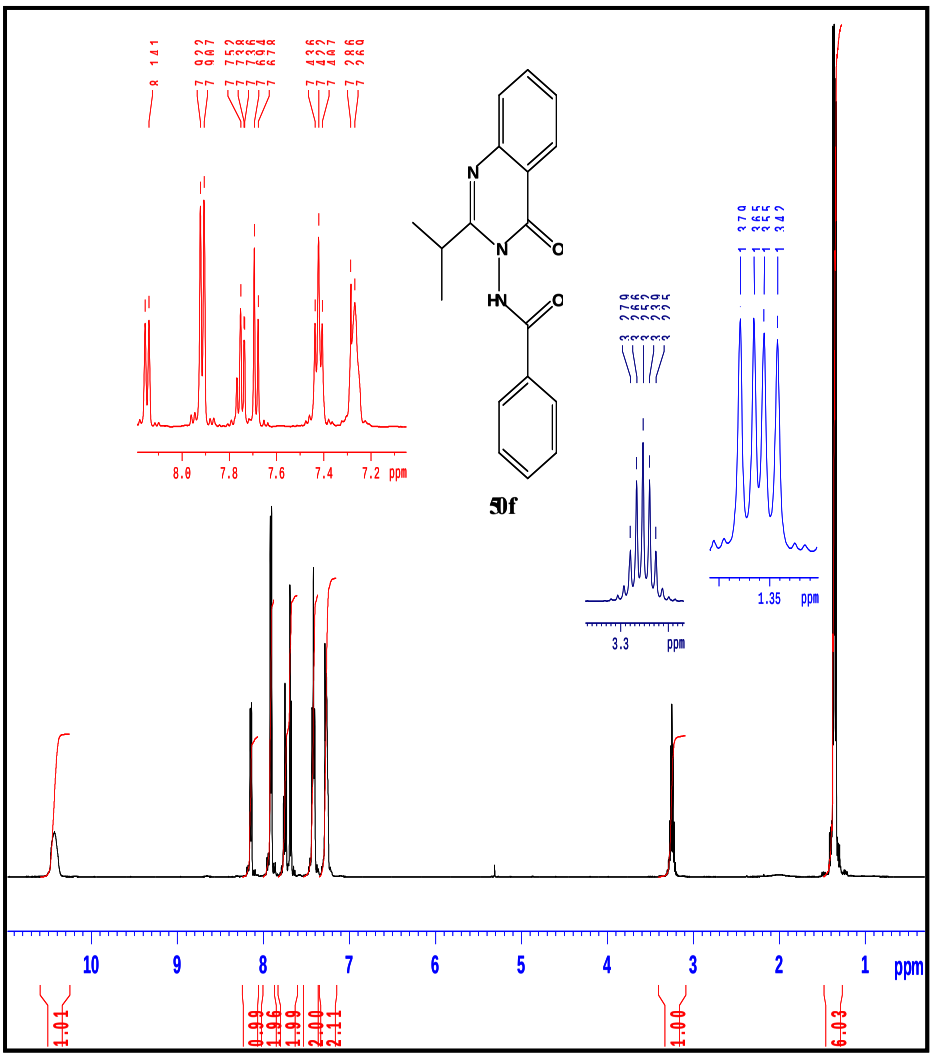


Fig.(S11): ^{1}H NMR Spectrum for **MAQ (3f)**

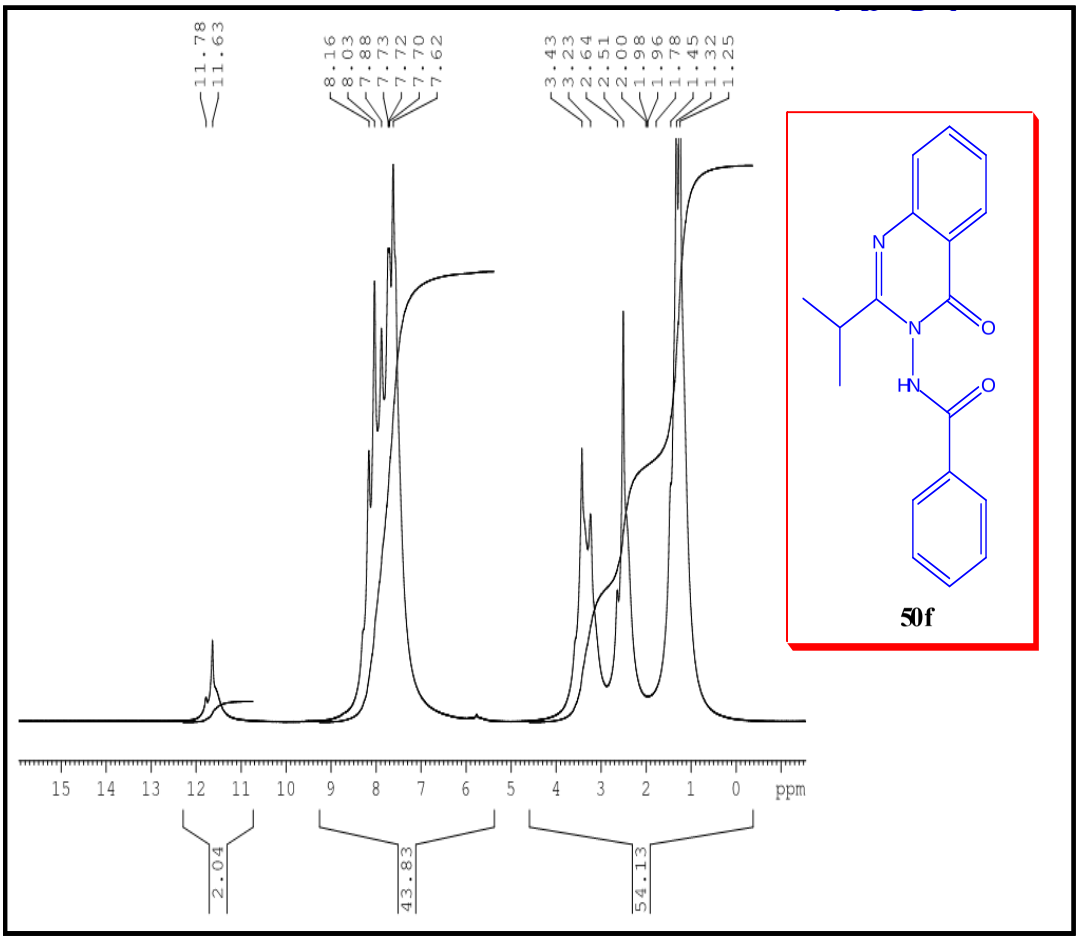


Fig.(S12): ^{13}C NMR Spectrum for **MAQ (3f)**

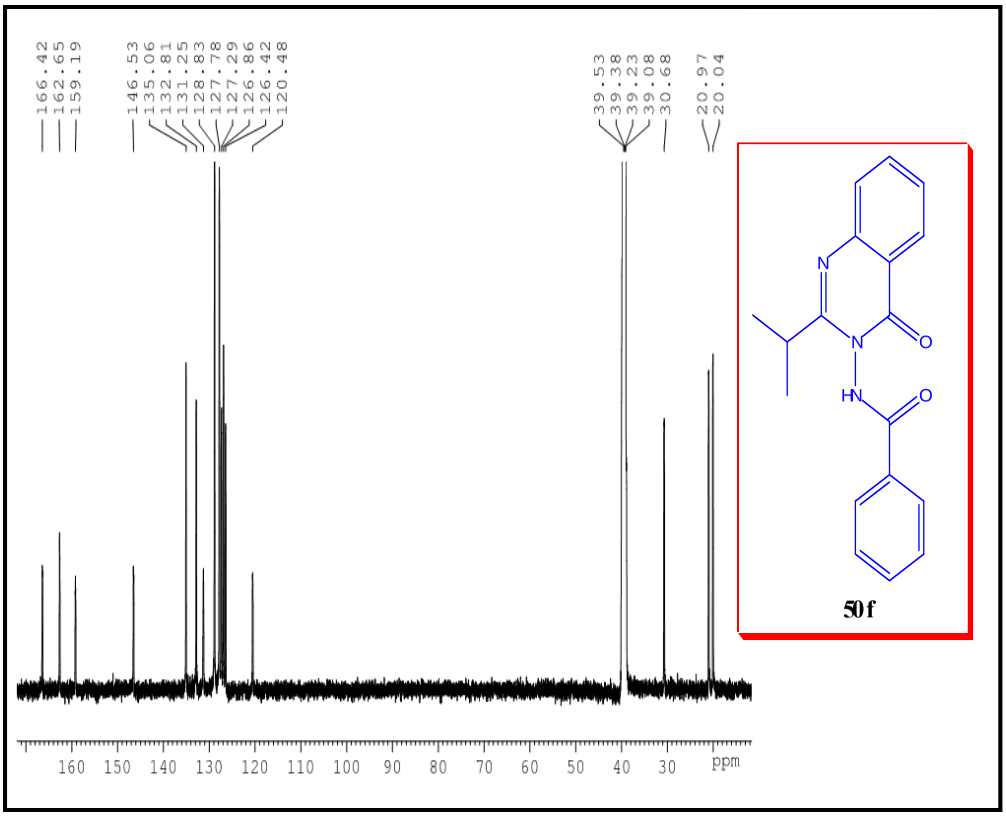


Fig. (S13): ^{1}H NMR Spectrum for **MAQ (3g)**

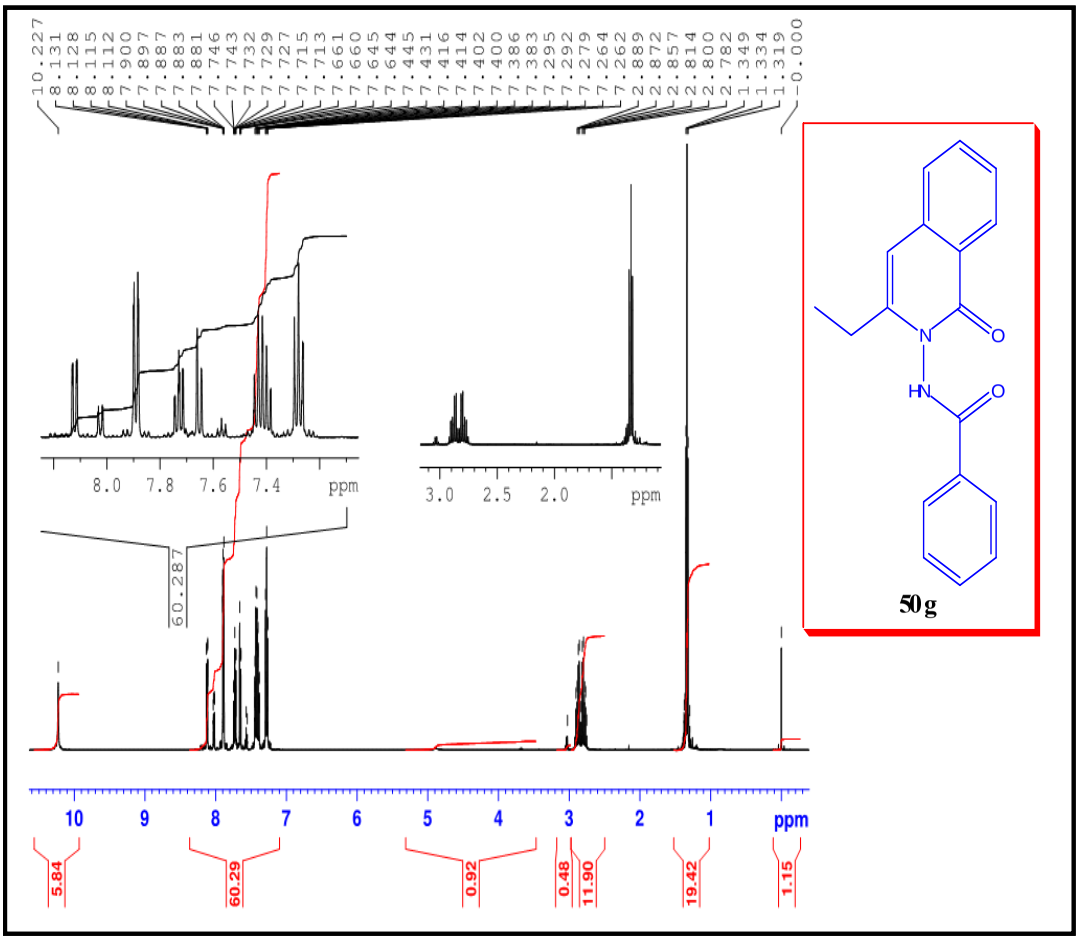


Fig.(S14): ^{13}C NMR Spectrum for **MAQ (3g)**

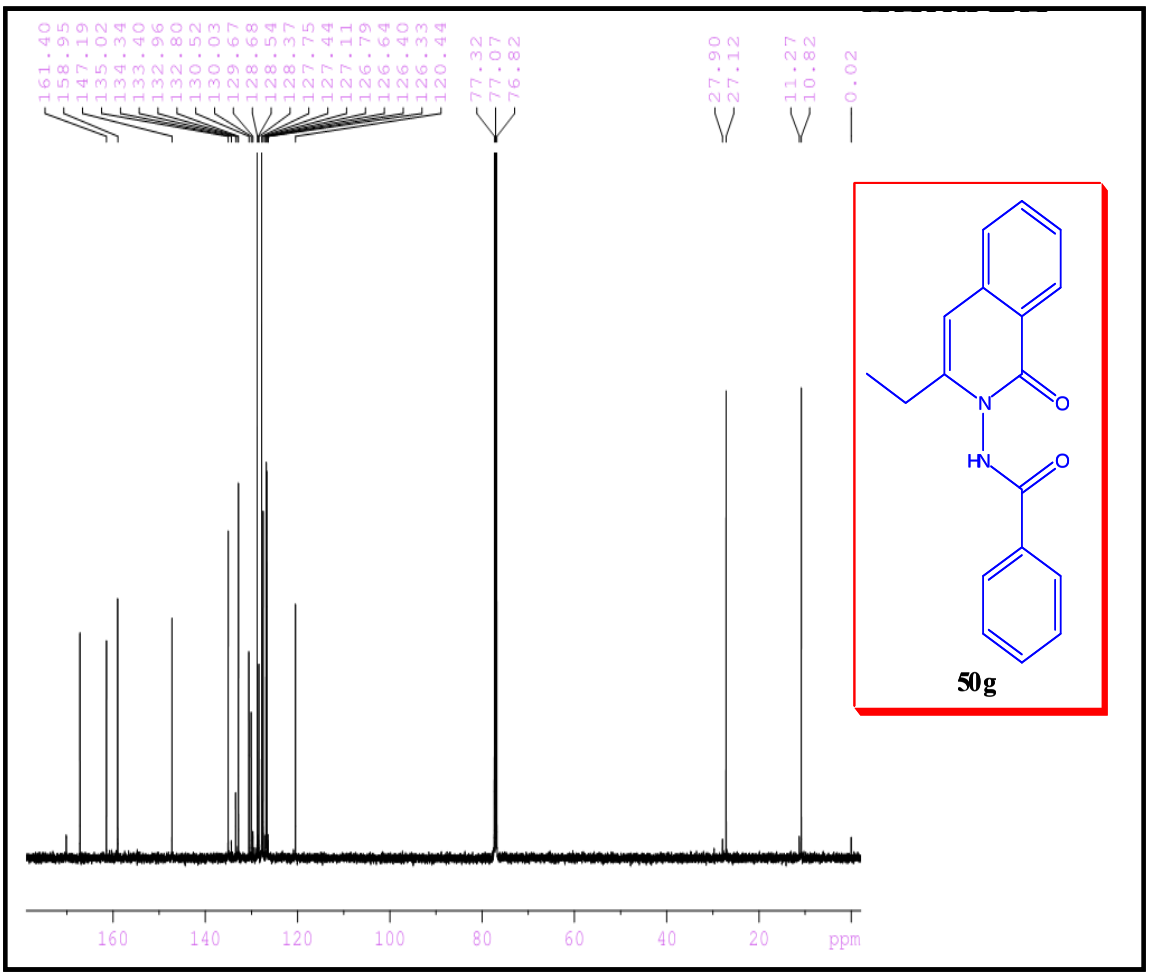


Fig.(S15): ^{1}H NMR Spectrum for **MAQ (3h)**

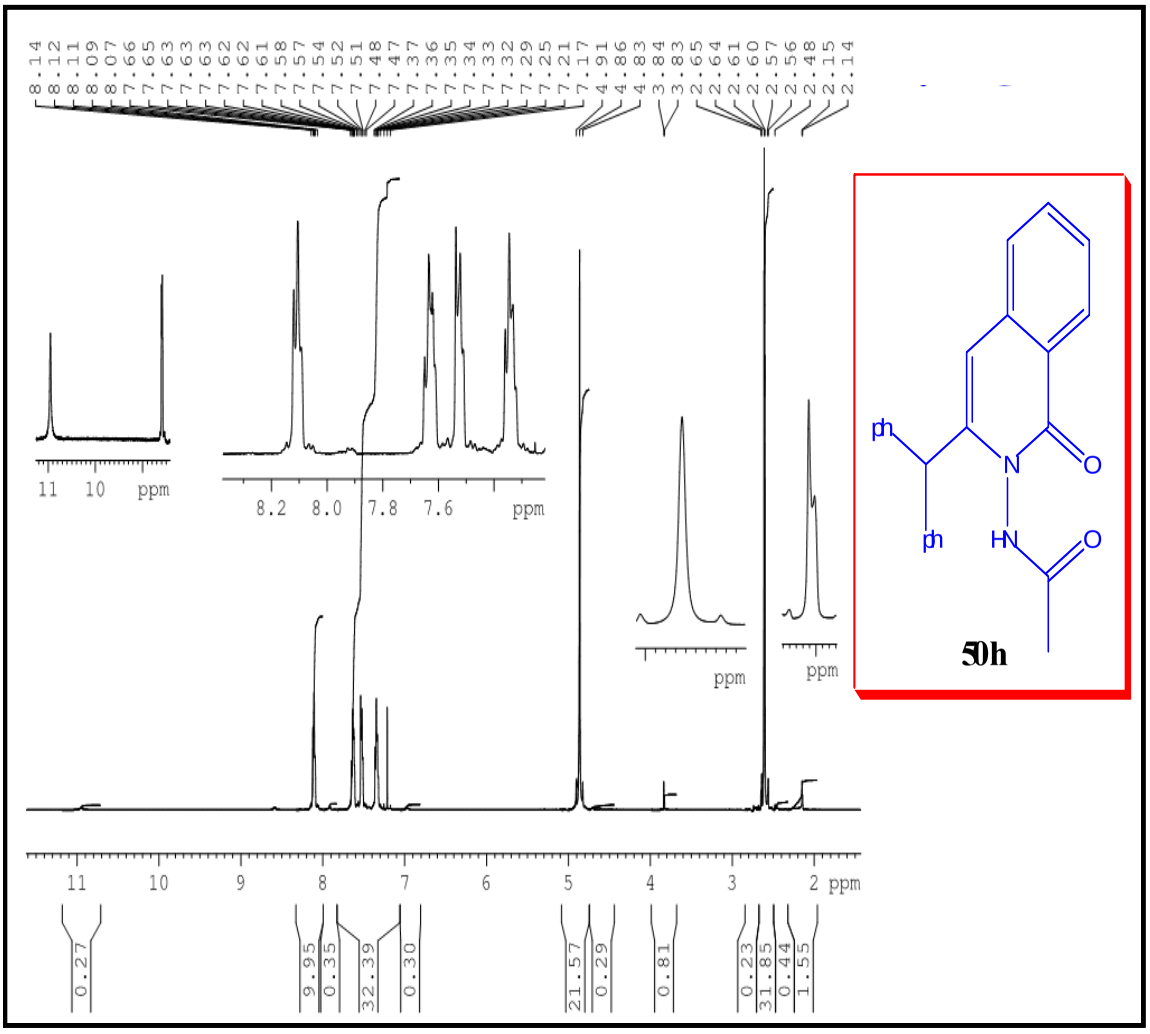


Fig.(S16): ^{13}C NMR Spectrum for **MAQ (3h)**

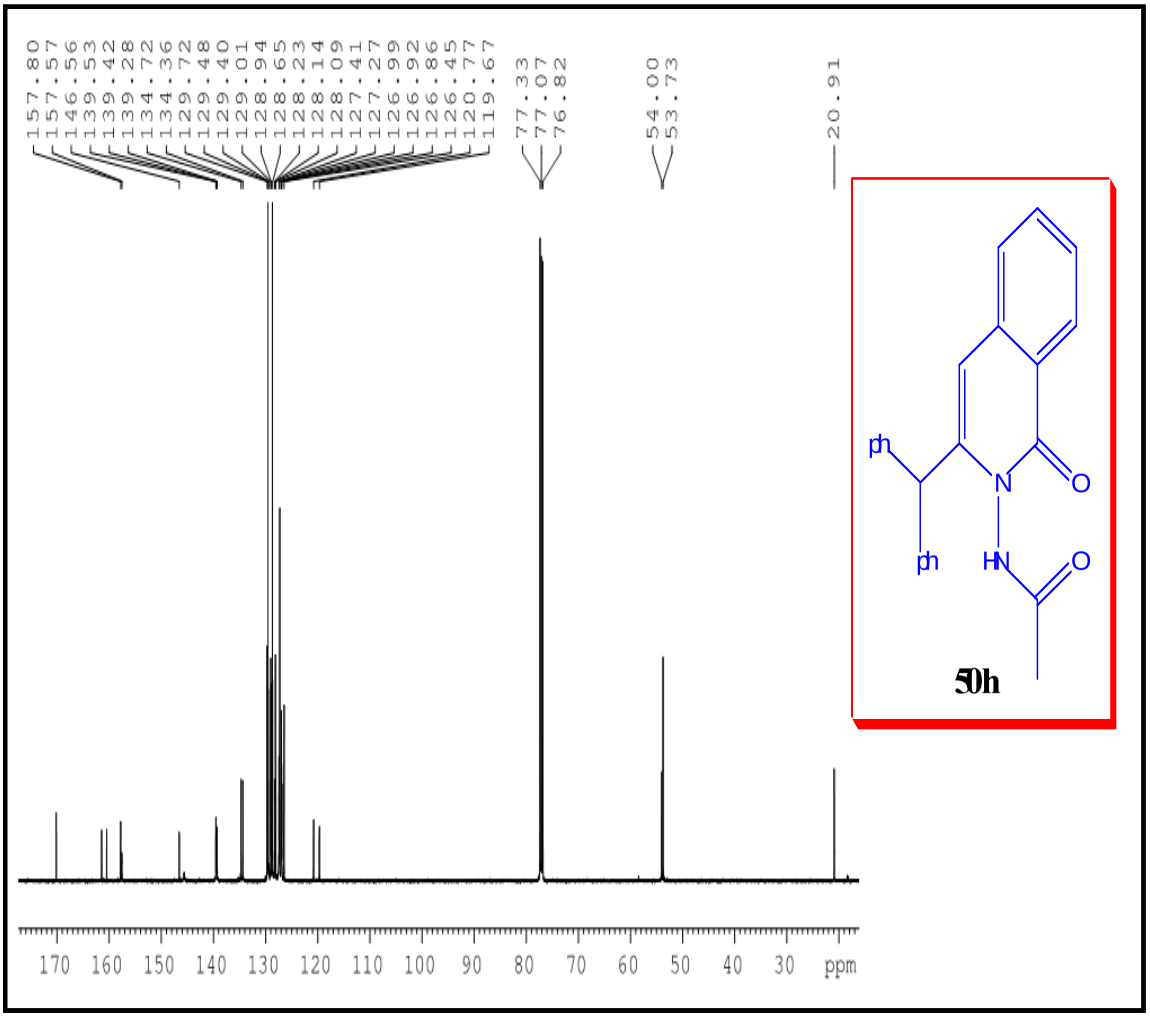


Fig.(S17): ^{1}H NMR Spectrum for **MAQ (3i)**

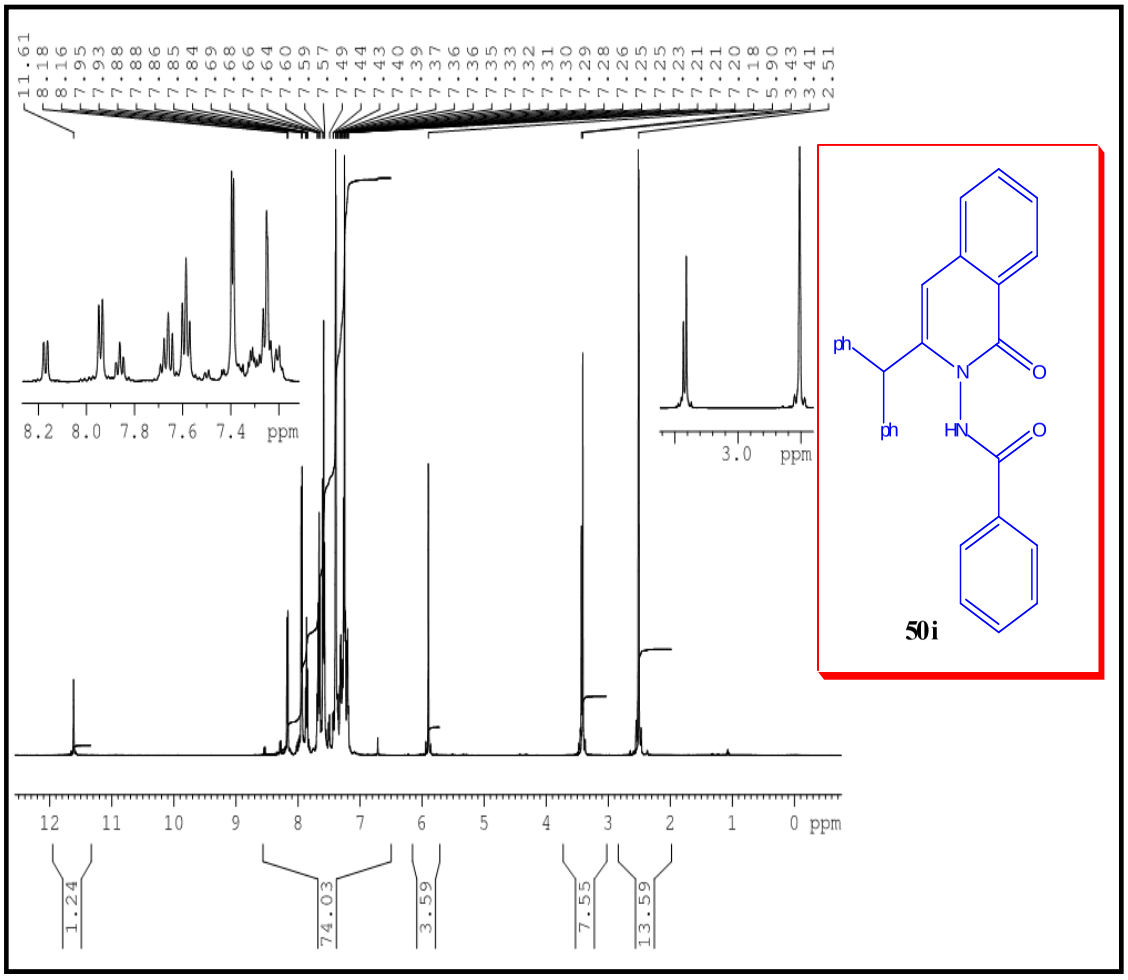
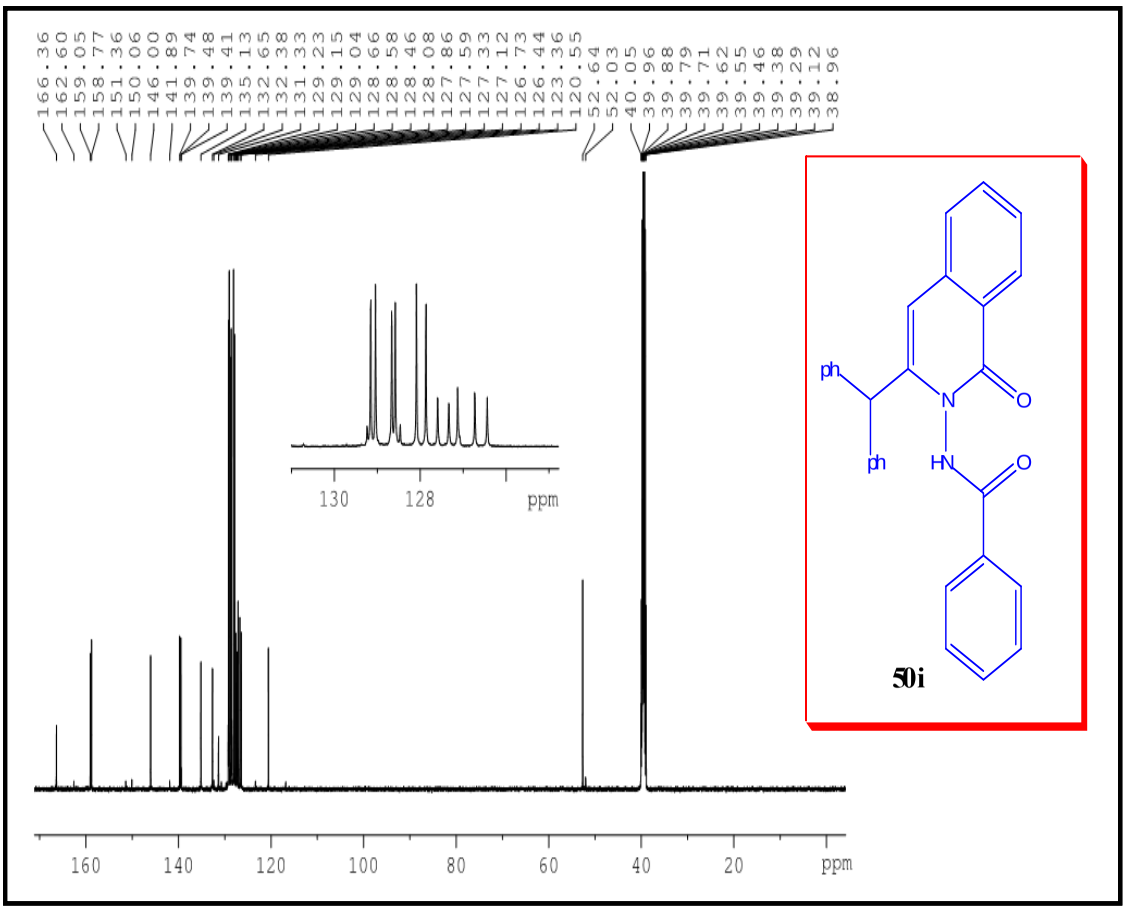


Fig.(S18): ^{13}C NMR Spectrum for **MAQ (3i)**



Mass Spectral of Selected Compounds

Fig.(S19): Mass Spectrum for **Q**(NH_2) **(2 e)**

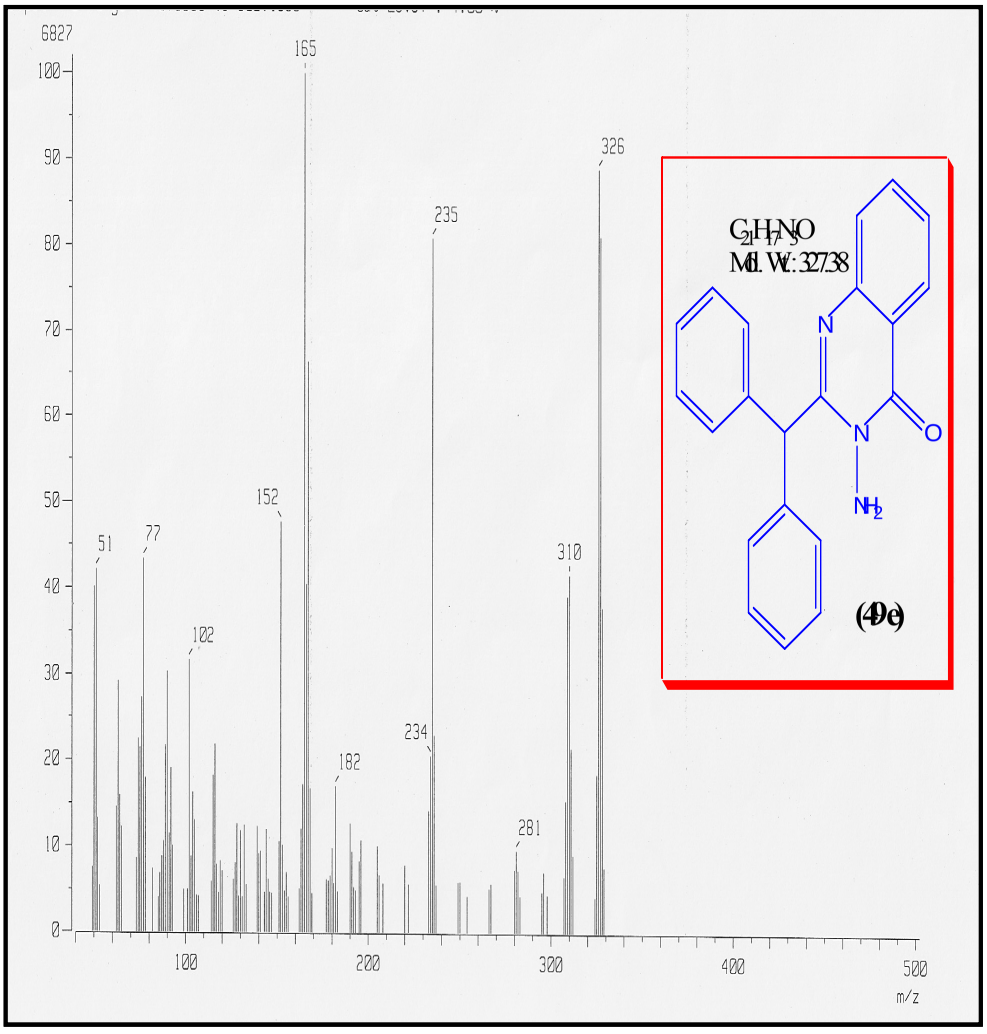
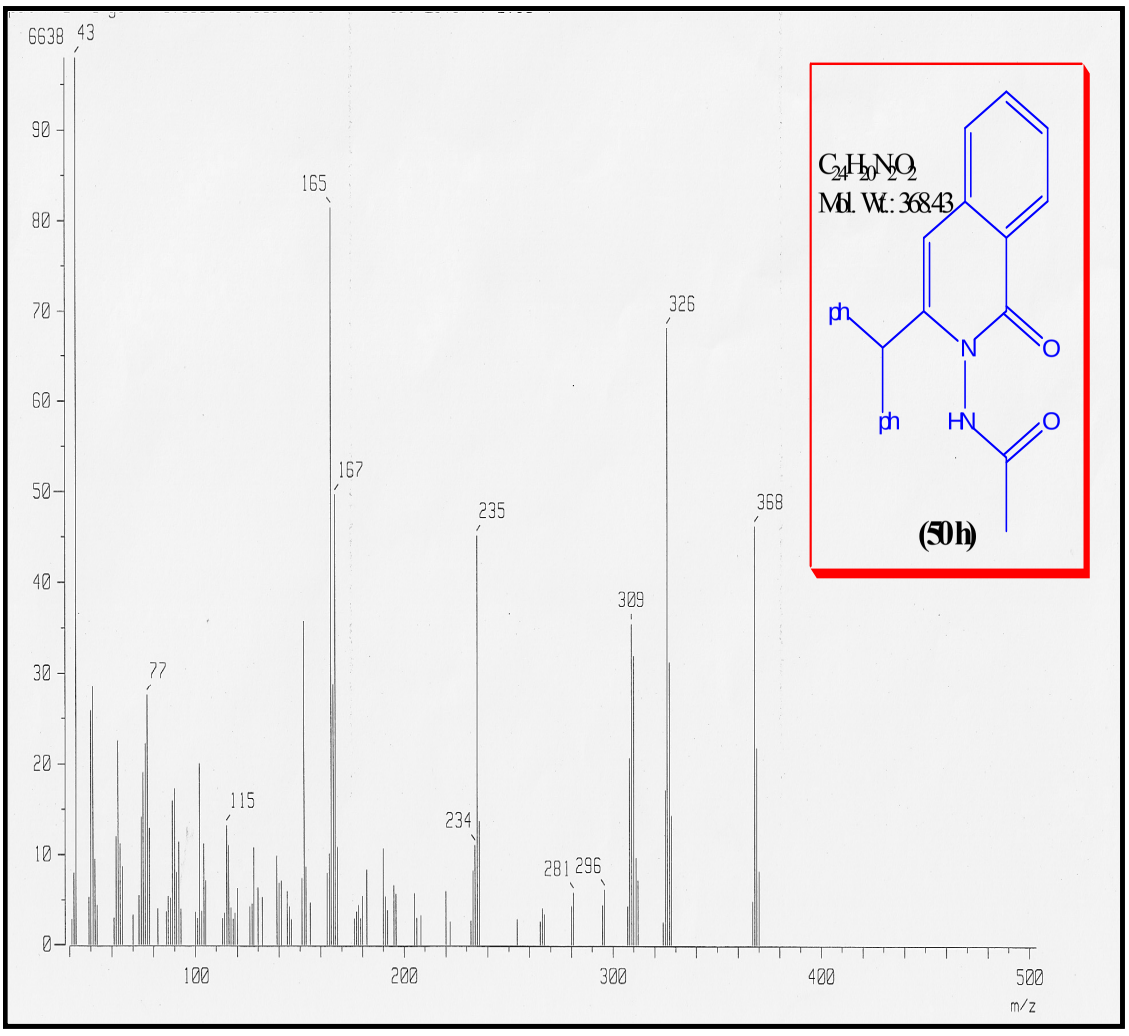
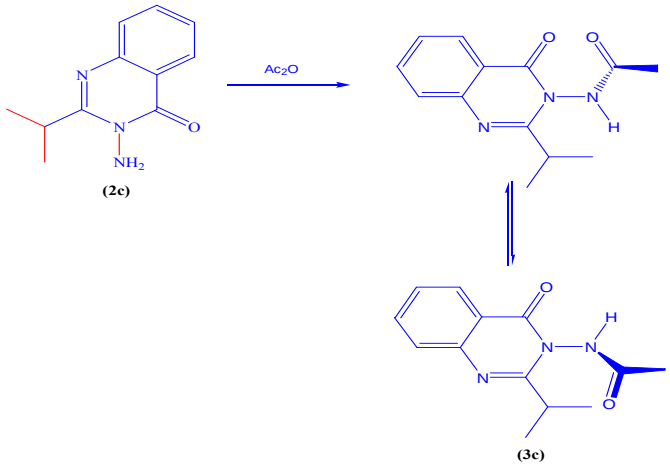


Fig.(S20): Mass Spectrum for **MAQ (3 h)**



3- Scheme S1.



In general the NMR chemical shifts of some **MAQ** protons were shown to be concentration dependent, possibly resulting from reversible dimer formation as in **(3)**A or **(3)**B, a factor which was not helpful in NMR analysis of reaction mixtures containing **MAQs**.

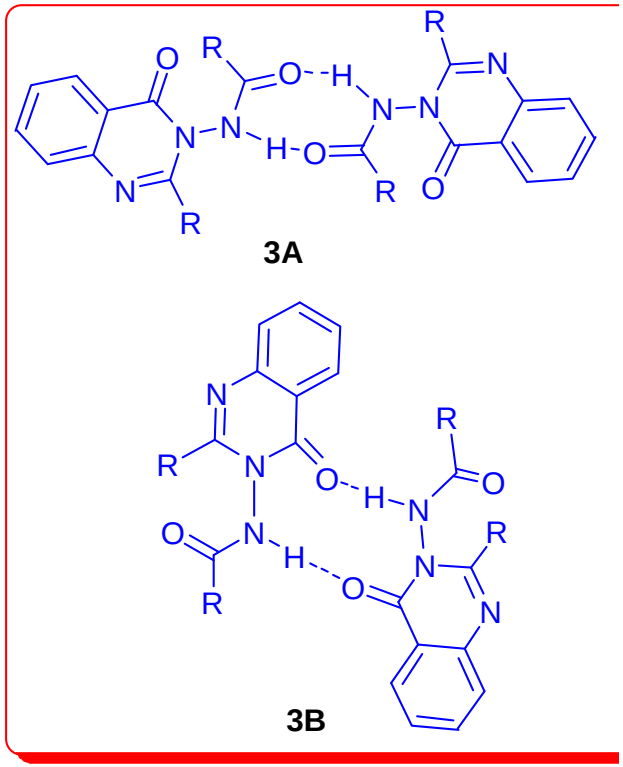


Fig. S21_dimer. The dimer formation of **MAQ**.

4.1. Properties of the *N-N* Bond

Over the past decade, enantiopure 1,1-binphthyl derives have been extensively used as chiral auxiliaries in stereoselective synthesis. By contrast, little use has been made of other molecules capable of sustaining a chiral axis. Hydrazine systems have been shown to possess a chiral axis when appropriately substituted. This type of chirality arise form the restricted rotation around the *N-N* bond. For example bond rotational barriers which are strongly influenced by type of substitute present on both sides of nitrogen atoms. The type

of chirality can also be present in substituted hydrazine systems. In this case, it is the restricted rotation around the *N-N* bond which gives rise to the chiral axis.

4-Potential energy surfaces of dihedral angle S23-S26

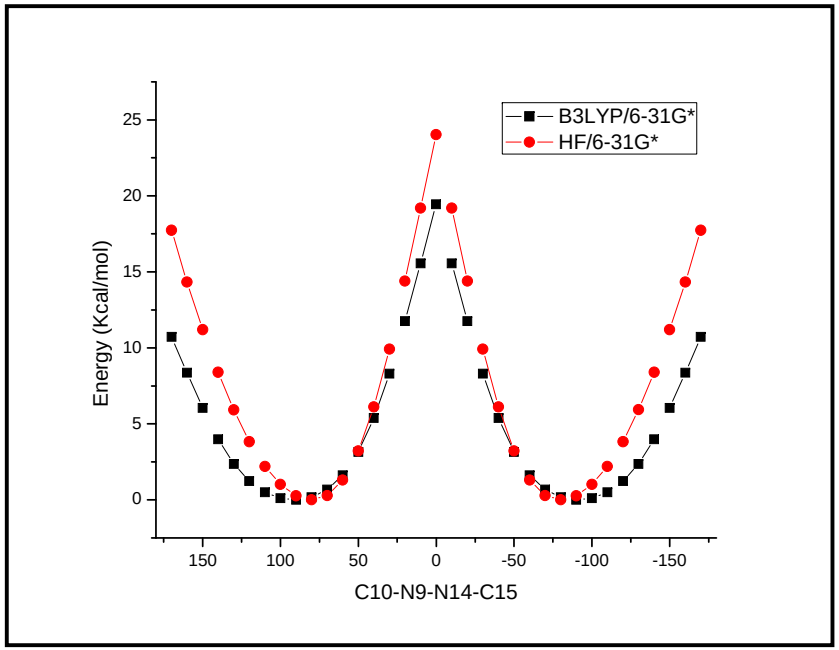


Fig. S22. Potential energy scan (Kcal/mol) versus torsion angles a (C10-N9-N14-C15) for **MAQ** compound **(3a)**.

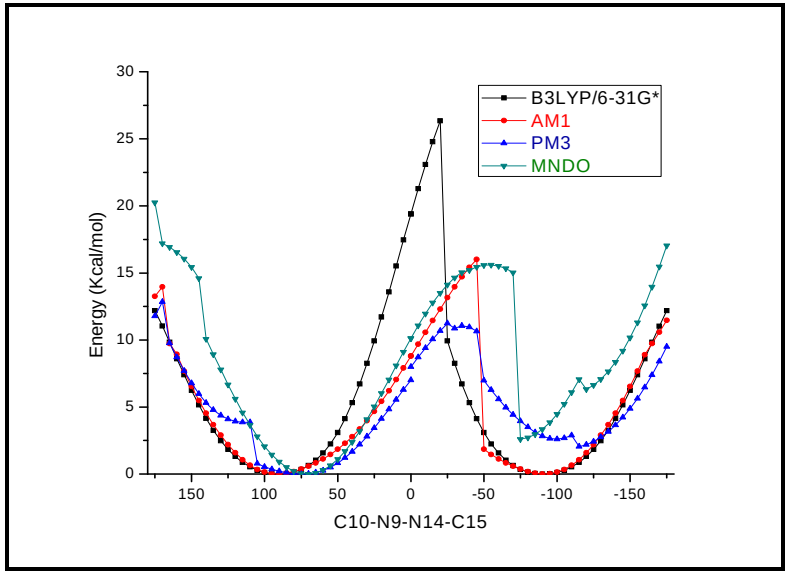


Fig. S23. Potential energy scan (Kcal/mol) versus torsion angles a (C10-N9-N14-C15) for **MAQ** compound **(3b)**.

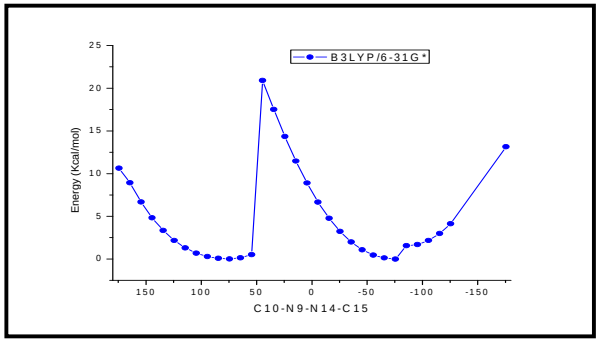


Fig. S24. Potential energy scan (Kcal/mol) versus torsion angles a (C10-N9-N14-C15) for **MAQ** compound **(3c)**.

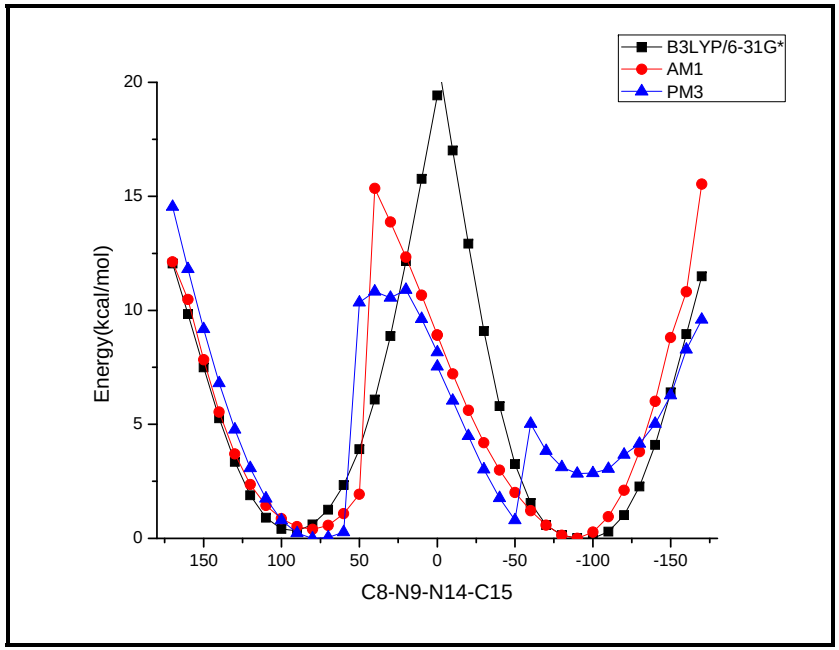


Fig. S25. Potential energy scan (Kcal/mol) versus torsion angles a (C8-N9-N14-C15) for MAQ compound **(3f)**.

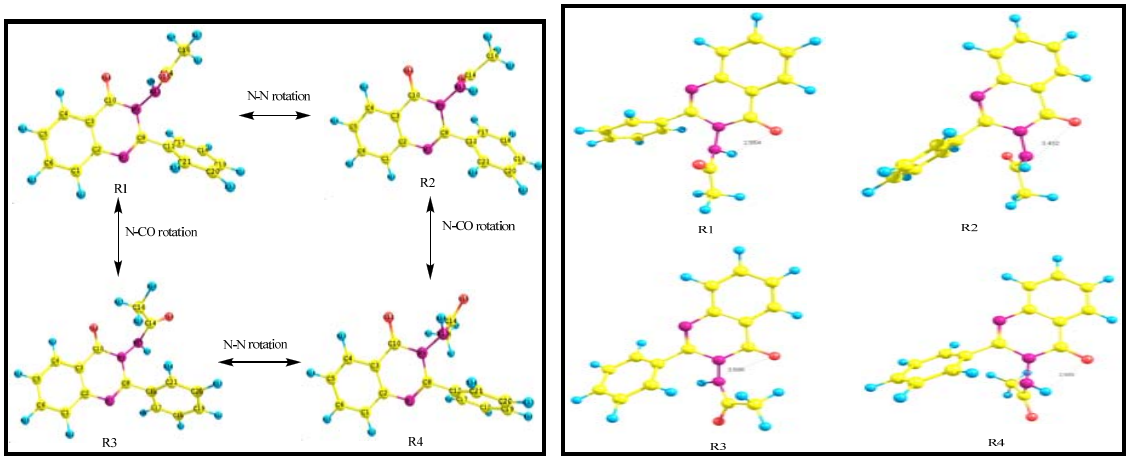
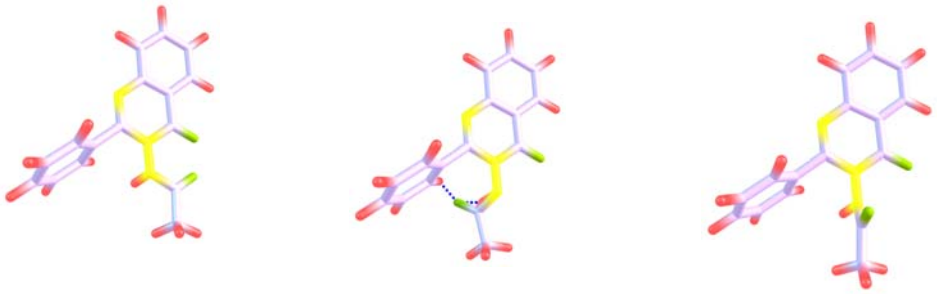


Fig. S26. Isomaric presentation of the passable conformers of **3d** that result from the rotation around the *N-N* and *N-CO* bonds (left) and conformers showing H-bonding (right).



(A) (B) (C)

Fig. S27. Molecular structures of most stable conformer and two transitions states of **MAQ (3d)** optimized at the B3LYP/6-31G(d) level of theory (A) R1, (B) TS1 for N-N rotation and (C) TS2 for N-N rotation.

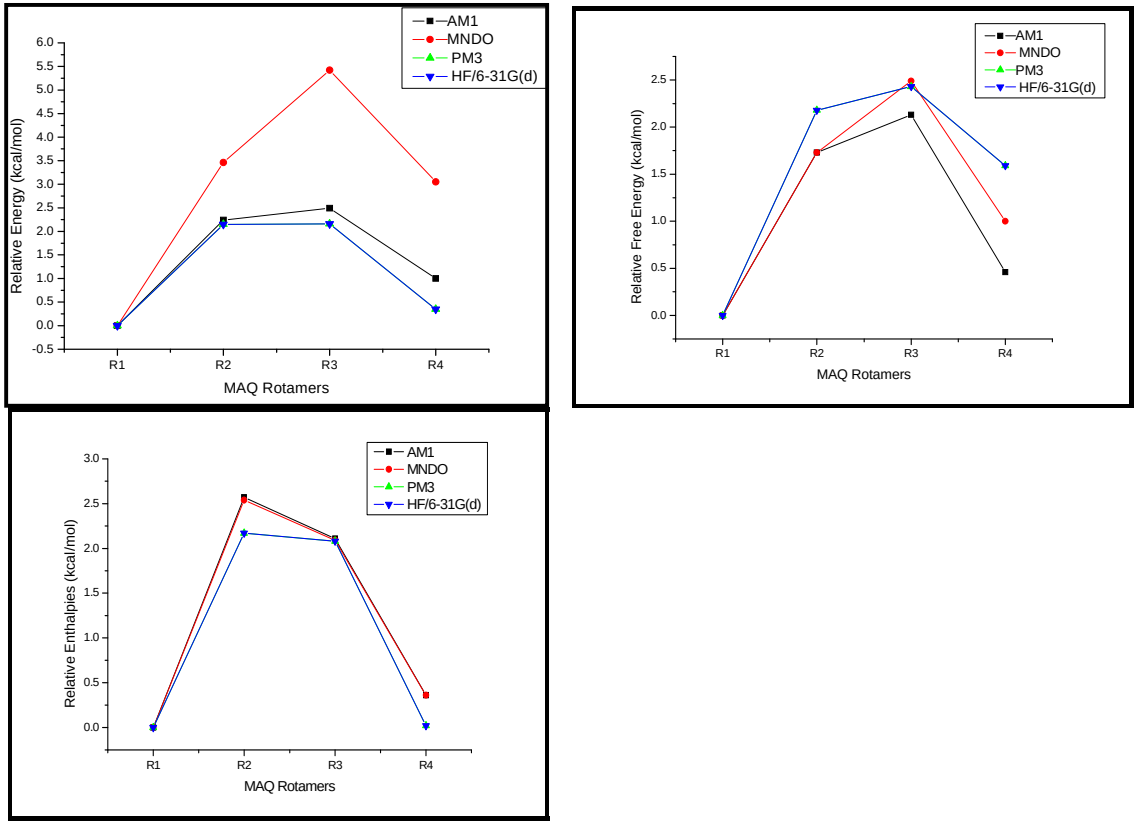
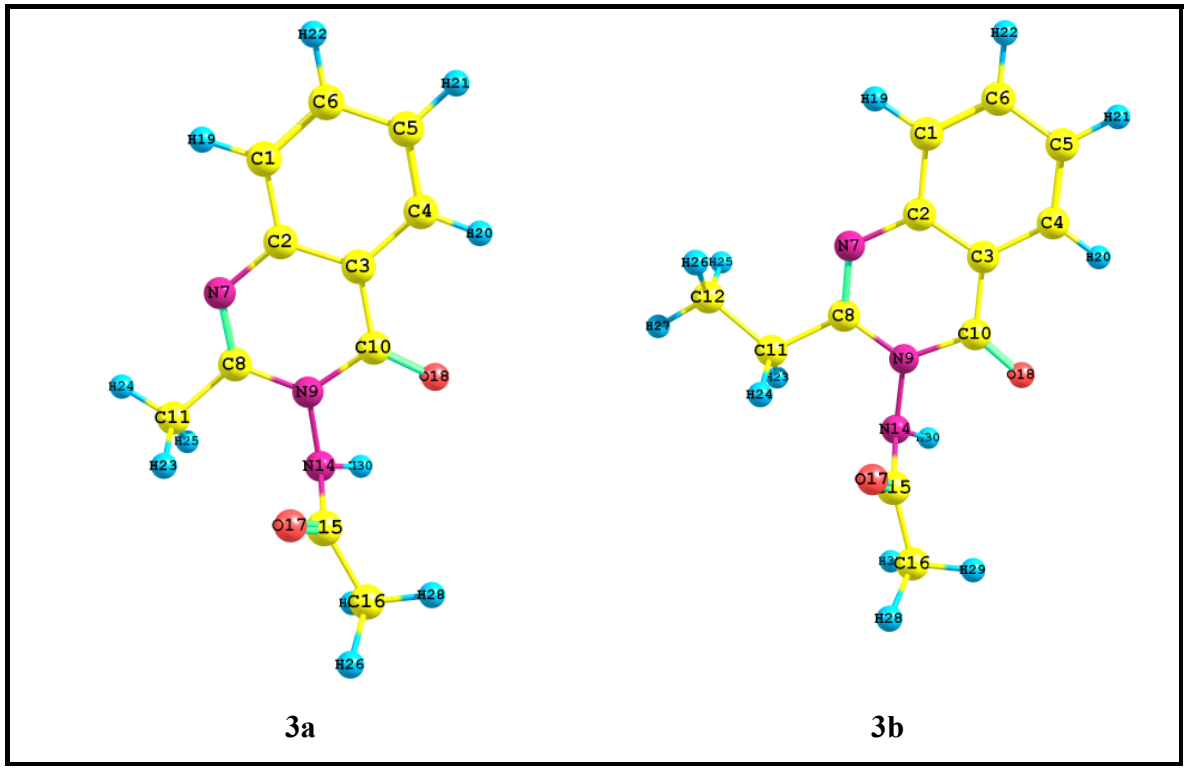
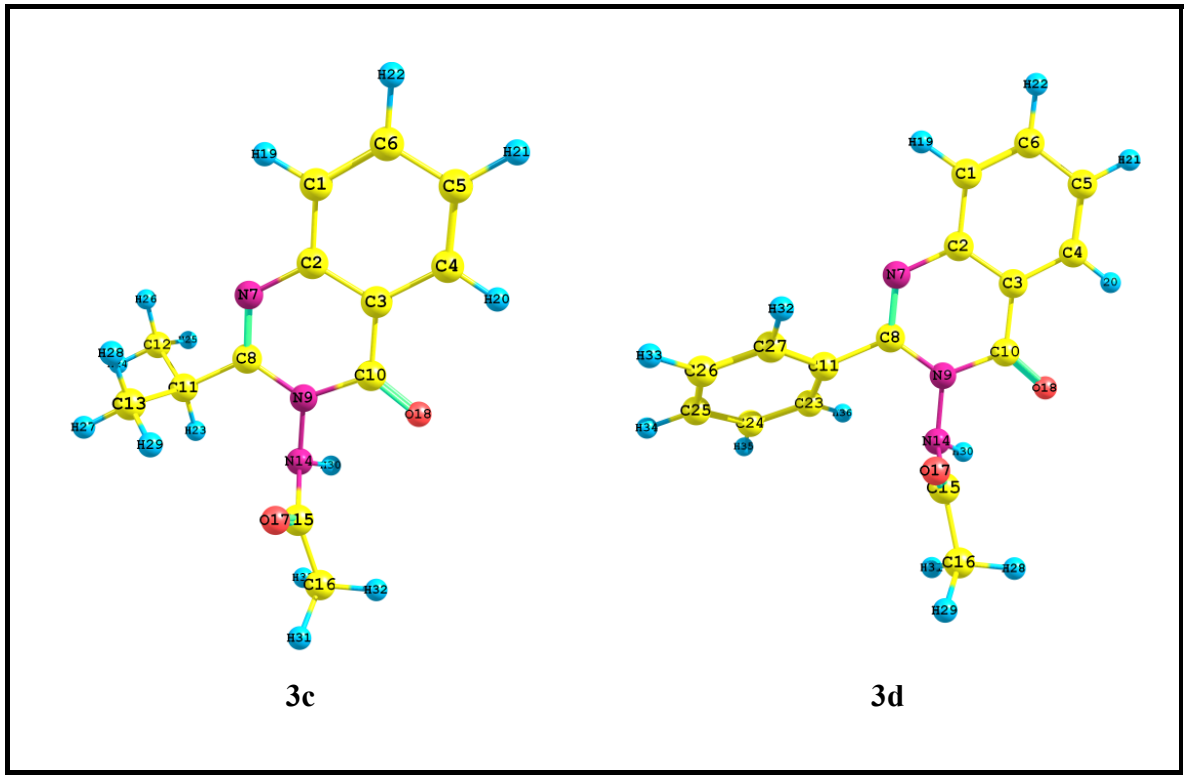


Fig. S28A Relative energy, Relative free energy and Relative Enthlpies (kcal/mol) of **3d** rotamers at different levels.


H22
C6
H21
H19
C1
C5
C4
H20
C2
C3
N7
C10
C8
O18
H24
N9
C11
H25
H23
N14
H30
O17
15
C16
H28
H26
3a
H22
H19
C6
C1
H21
C5
C2
C4
N7
H20
C3
H26
H25
C12
C8
C10
H27
C11
N9
O18
H24
N14
H30
O17
15
C16
H29
H28
3b


H22
C6
H19
C1
C5
H21
C2
C4
N7
C3
H20
H26
C12
H28
C8
C10
C11
N9
O18
C13
H27
H23
H29
N14
O17
C15
C16
H32
H31
H22
C6
H19
C1
C5
H21
C2
C4
N7
C3
H32
C27
H33
C26
C11
C8
C10
N9
O18
C25
C23
C24
N14
O17
C15
C16
H29

3c **3d**

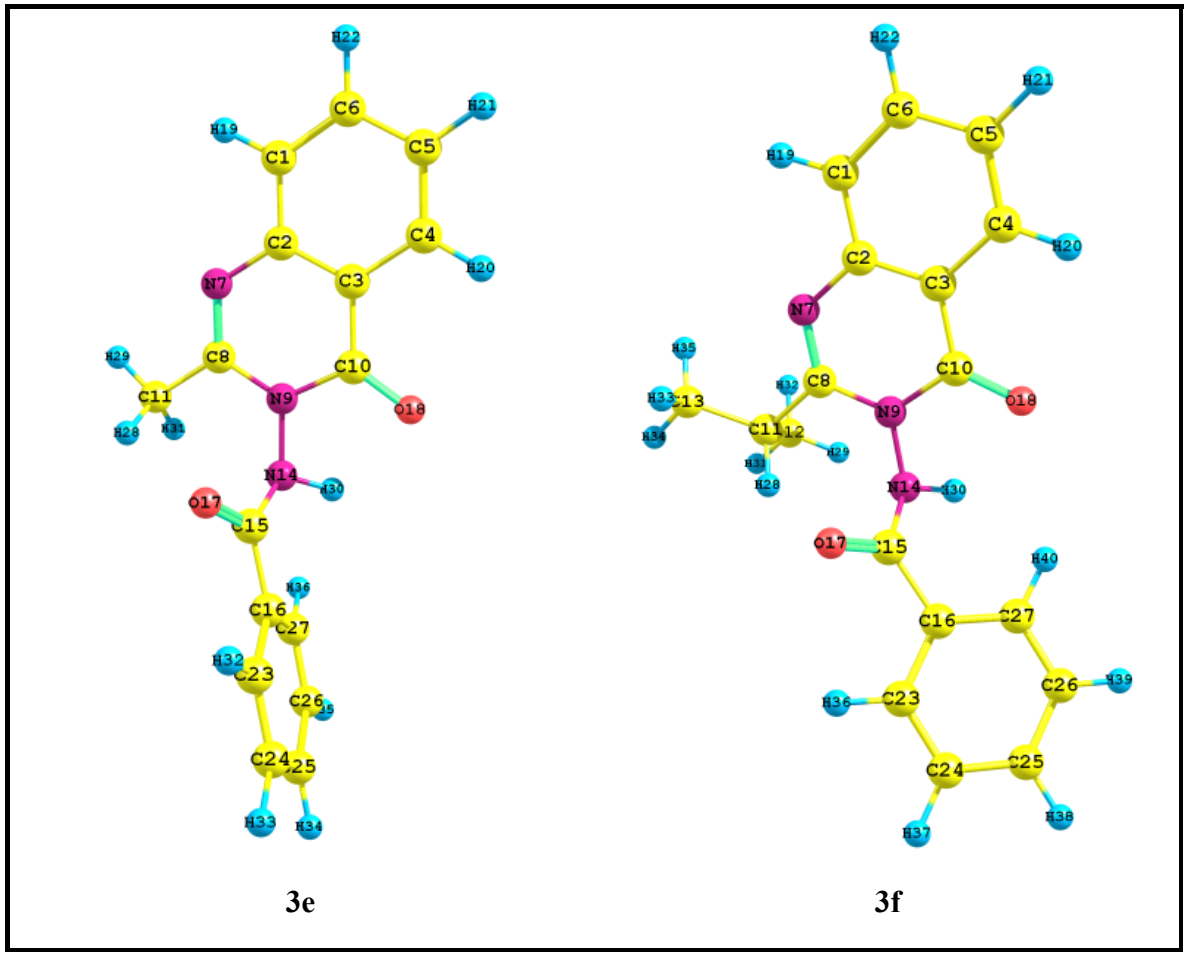


Fig. S29. Optimized structures for the more stable rotamers of **MAQs (3a-f)** calculated using Density Function Theory method at B3LYP/6-31G(d,p).

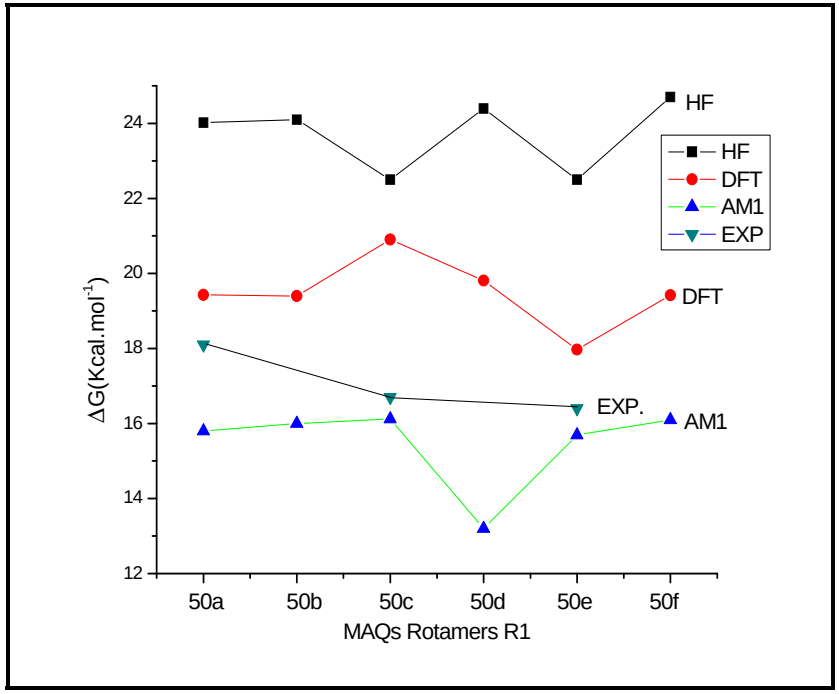


Fig. S30. Free energy (kcal/mol) of **MAQs** rotamers (R1) at different levels.

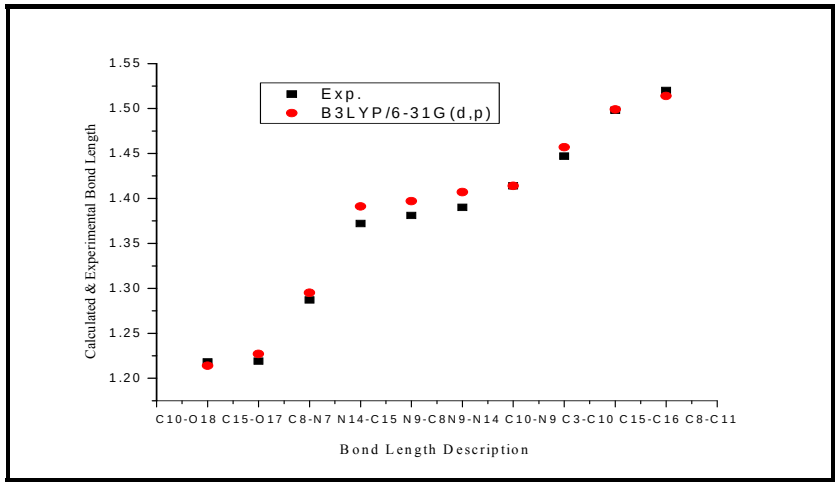


Fig. S31. Calculated vs experimental bond length for **MAQ (3a)** (Me-Me-R1 rotamer) at *B3LYP/6-31G(d,p)* level.

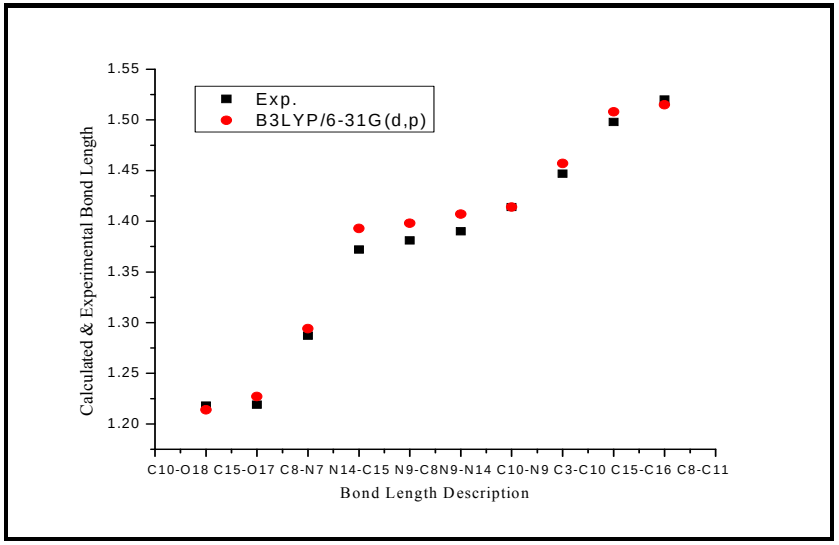


Fig. S32. Calculated vs experimental bond length for **MAQ (3b)** (Et-Me-R1 rotamer) at *B3LYP/6-31G(d,p)* level.

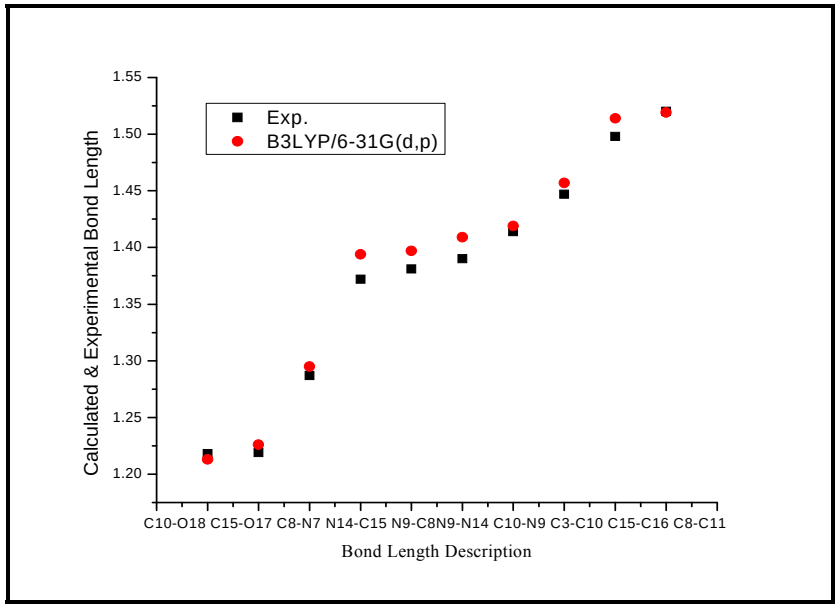


Fig. S33. Calculated vs experimental bond length for **MAQ (3c)** (Pr^i-Me-R1 rotamer) at *B3LYP/6-31G(d,p)* level.

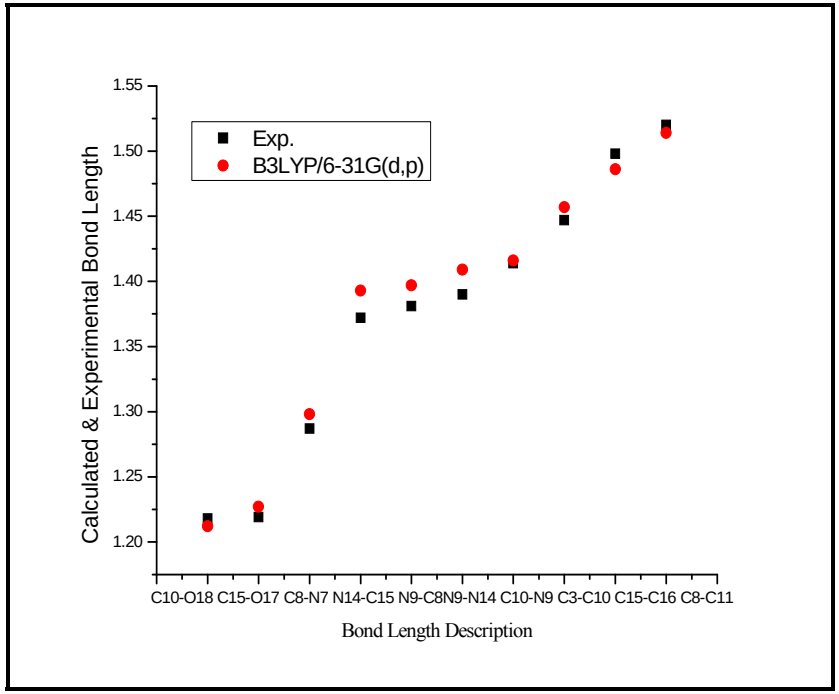


Fig. S34. Calculated vs experimental bond length for **MAQ (3d)** (Ph-Me-R1 rotamer) at *B3LYP/6-31G(d,p)* level.

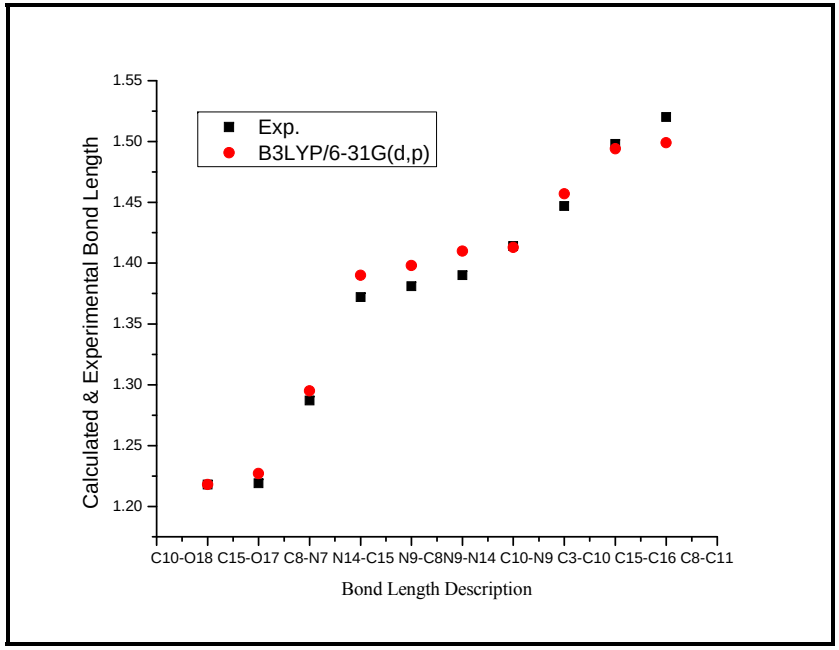


Fig. S35. Calculated vs experimental bond length for **MAQ (3e)** (Me-Ph-R1 rotamer) at *B3LYP/6-31G(d,p)* level.

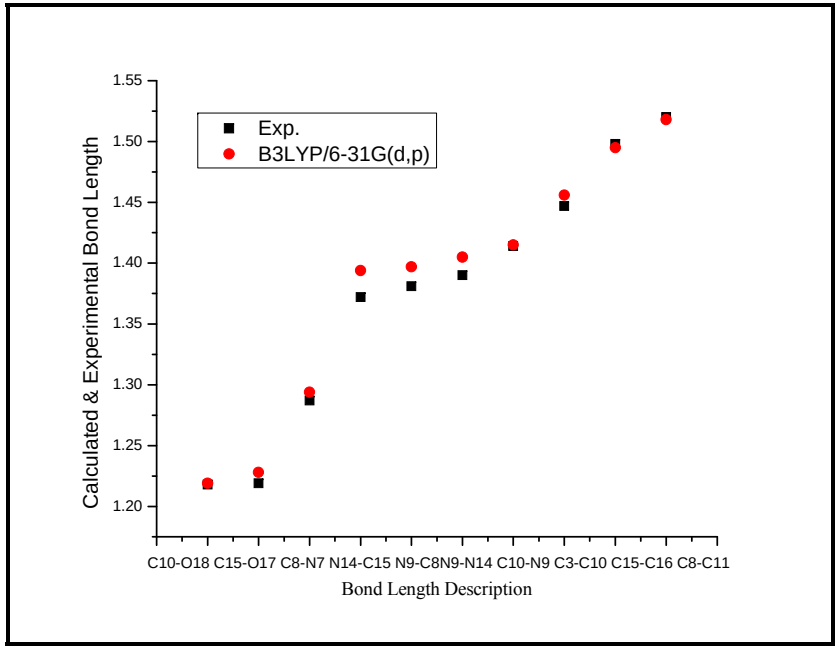


Fig. S36. Calculated vs experimental bond length for **MAQ (3f)** (Pr^{i}-Ph-R1 rotamer) at *B3LYP/6-31G(d,p)* level.

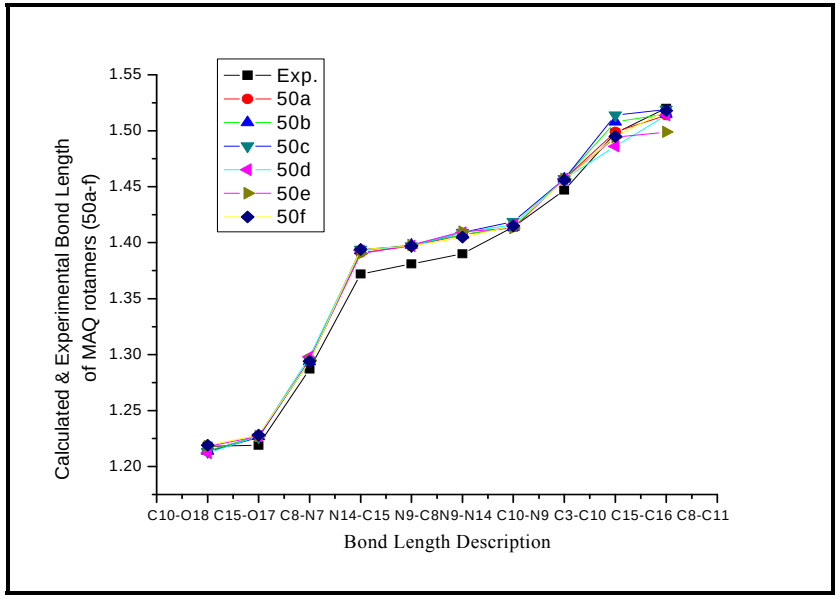


Fig. S37. Calculated vs experimental bond length for **MAQs** rotamers **(3a-f)** at *B3LYP/6-31G(d,p)* level.

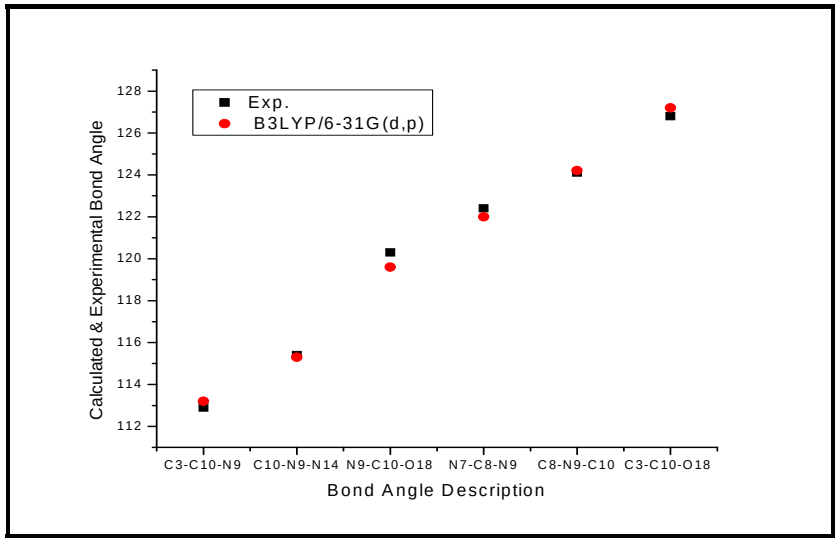


Fig. S38. Calculated vs experimental bond angles for **MAQ (3a)** (Me-Me-R1 rotamer) at *B3LYP/6-31G(d,p)* level.

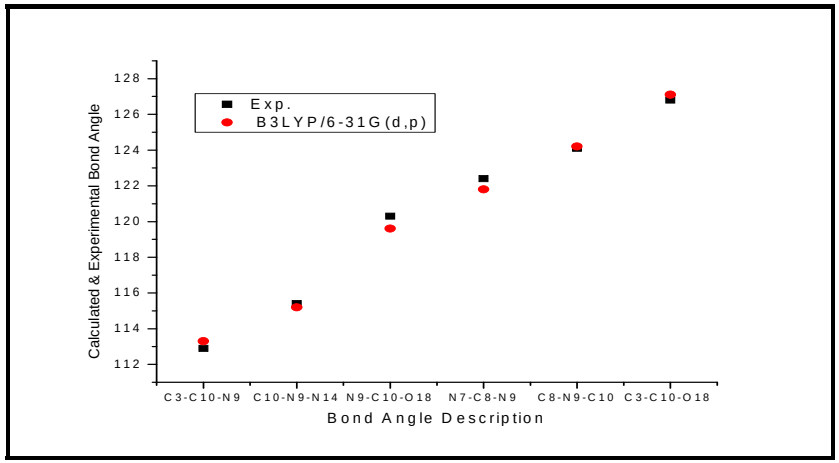


Fig. S39. Calculated vs experimental bond angles for **MAQ (3b)** (Et-Me-R1 rotamer) at *B3LYP/6-31G(d,p)* level.

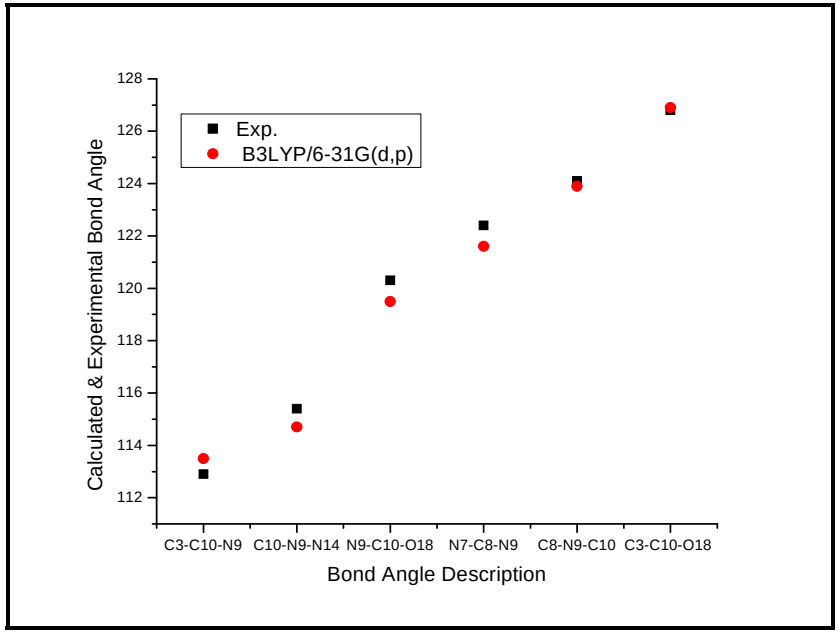


Fig. S40. Calculated vs experimental bond angles for **MAQ (3c)** (Pr^i-Me-R1 rotamer) at *B3LYP/6-31G(d,p)* level.

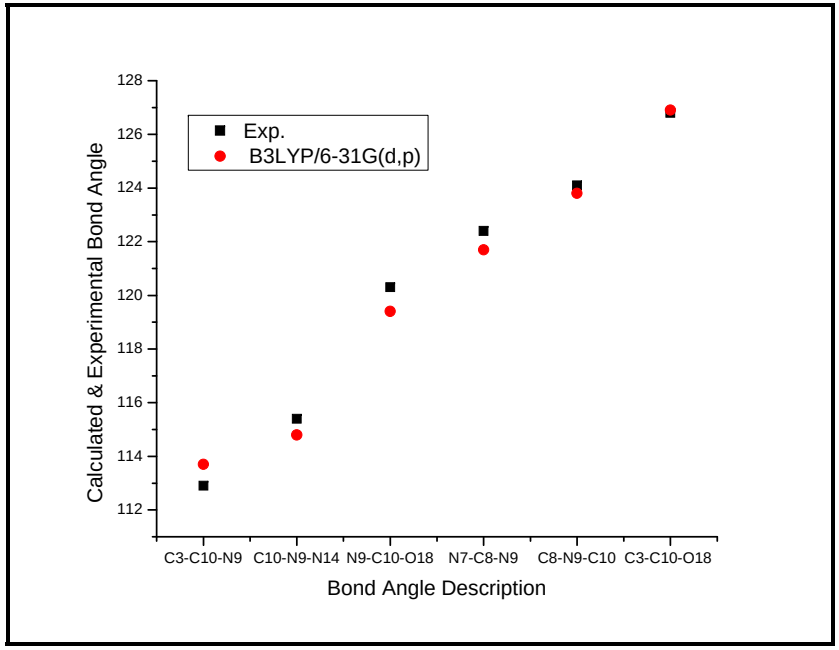


Fig. S41. Calculated vs experimental bond angles for **MAQ (3d)** (Ph-Me -R1 rotamer) at *B3LYP/6-31G(d,p)* level.

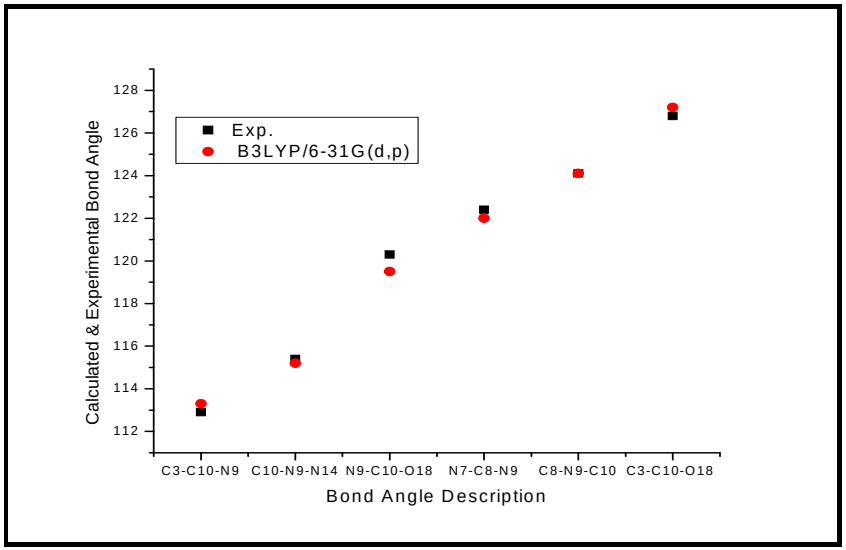


Fig. S42. Calculated vs experimental bond angles for **MAQ (3e)** (Me-Ph- R1 rotamer) at *B3LYP/6-31G(d,p)* level.

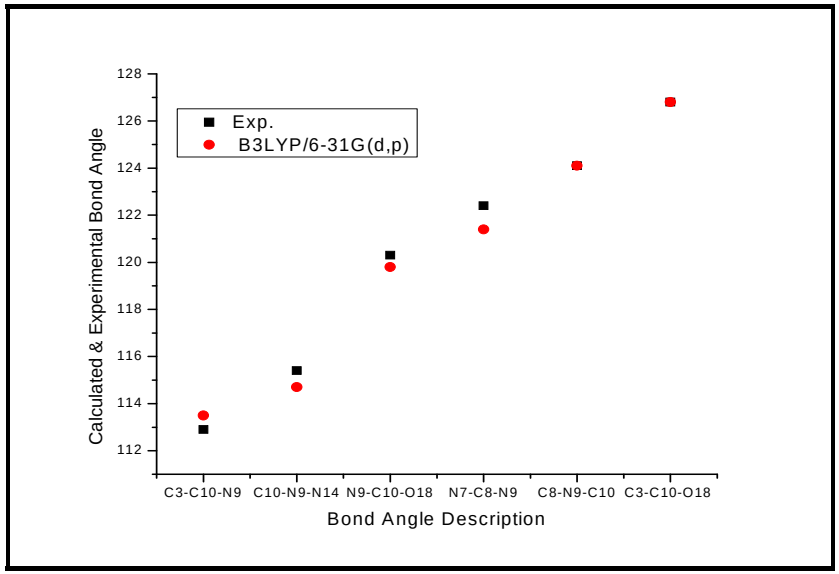


Fig. S43. Calculated vs experimental bond angles for **MAQ (3f)** (Pr^{i}-Ph-R1 rotamer) at *B3LYP/6-31G(d,p)* level.

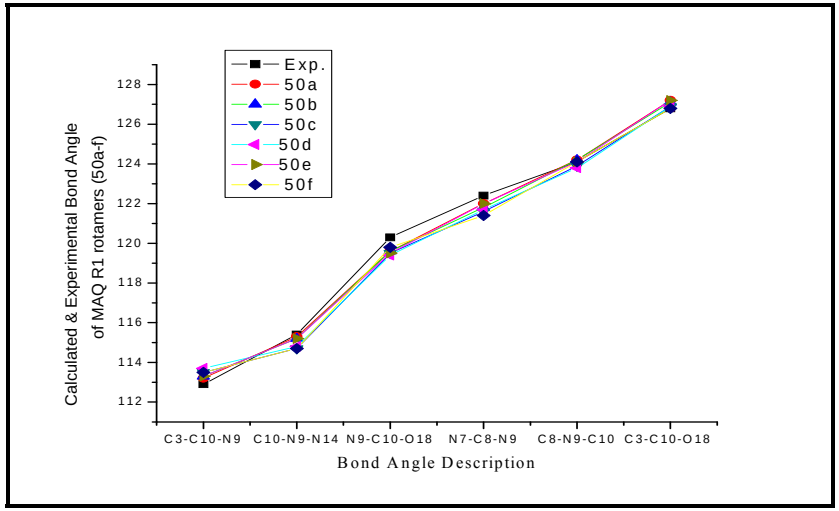


Fig. S44. Calculated vs experimental bond angle of **MAQs** rotamers **(3a-f)** at *B3LYP/6-31G(d,p)* level.

Table S1 Thermodynamic parameters (kcal/mol) for **MAQ (3d)** rotamers at different levels

Species	***AM1***			***MNDO***			***PM3***			***HF/6-31G(d)***		
	ΔE_0	ΔH_{298}	ΔG_{298}	ΔE_0	ΔH_{298}	ΔG_{298}	ΔE_0	ΔH_{298}	ΔG_{298}	ΔE_0	ΔH_{298}	ΔG_{298}
R1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
R2	2.24	2.57	1.73	3.46	2.54	1.73	2.15	2.17	2.18	2.15	2.17	2.18
R3	2.49	2.11	2.13	5.42	2.09	2.49	2.16	2.08	2.43	2.16	2.08	2.43
R4	1.00	0.36	0.46	3.05	0.36	1.00	0.35	0.02	1.59	0.35	0.02	1.59

Table S2 H bond in **MAQ (3d)** (A°) and Thermodynamic parameters.

parameters		***R1***	***R2***	***R3***	***R4***
	NH..O	2.554	3.432	3.586	2.609
AM1	ΔE_0	0.00	2.24	2.49	1.00
	ΔH_{298}	0.00	2.57	2.11	0.36
	ΔG_{298}	0.00	1.73	2.13	0.46
	NH..O	2.695	3.336	3.265	2.758
MNDO	ΔE_0	0.00	3.46	2.42	3.05
	ΔH_{298}	0.00	2.54	2.09	0.36
	ΔG_{298}	0.00	1.73	2.49	1.00
	NH..O	2.645	3.526	3.529	2.657
PM3	ΔE_0	0.00	2.15	2.16	0.35
	ΔH_{298}	0.00	2.17	2.08	0.02
	ΔG_{298}	0.00	2.18	2.43	1.59
	NH..O	2.512	2.602	2.834	2.659
HF	ΔE_0	0.00	2.15	2.16	0.35
	ΔH_{298}	0.00	2.17	2.08	0.02
	ΔG_{298}	0.00	2.18	2.43	1.59

Table (S3) Optimized ***geometrical*** parameters (bond lengths (Å) and bond angles (degrees) for **MAQ (50a)** R1-R4

For numbering of the atoms, see Figure 22 (Chapter 2).

parameters	***HF/6-31G(d,p)***				***b3lyp/6-31G(d,p)***				***cbs***				***x-ray***
	R1	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	
	bond lengths												
C1-C2	1.400	1.400	1.400	1.400	1.409	1.409	1.408	1.409	1.409	1.409	1.400	1.409	1.394
C1-C6	1.373	1.373	1.373	1.373	1.385	1.385	1.386	1.385	1.385	1.385	1.373	1.385	1.368
C1-H19	1.074	1.074	1.074	1.074	1.085	1.085	1.085	1.085	1.085	1.085	1.074	1.085	
C2-C3	1.392	1.392	1.391	1.391	1.414	1.414	1.413	1.414	1.414	1.414	1.391	1.414	1.399
C2-N7	1.385	1.385	1.386	1.386	1.386	1.386	1.388	1.386	1.386	1.386	1.386	1.386	1.396
C3-C4	1.398	1.398	1.398	1.398	1.405	1.405	1.405	1.405	1.405	1.405	1.398	1.405	1.394
C3-C10	1.459	1.459	1.461	1.461	1.457	1.457	1.462	1.457	1.457	1.457	1.461	1.457	1.447
C4-C5	1.371	1.371	1.372	1.372	1.385	1.385	1.386	1.385	1.385	1.385	1.372	1.385	1.381
C4-H20	1.074	1.074	1.074	1.074	1.085	1.085	1.085	1.085	1.085	1.085	1.074	1.085	
C5-C6	1.400	1.401	1.400	1.400	1.408	1.408	1.407	1.408	1.408	1.408	1.400	1.408	1.385
C5-H21	1.075	1.075	1.075	1.075	1.085	1.085	1.085	1.085	1.085	1.085	1.075	1.085	
C6-H22	1.076	1.076	1.076	1.076	1.086	1.086	1.086	1.086	1.086	1.086	1.076	1.086	
N7-C8	1.268	1.268	1.267	1.267	1.295	1.295	1.293	1.295	1.295	1.295	1.267	1.295	1.287
C8-N9	1.383	1.383	1.389	1.389	1.391	1.391	1.398	1.391	1.391	1.391	1.389	1.391	1.381
C8-C11	1.499	1.499	1.501	1.501	1.499	1.499	1.501	1.499	1.499	1.499	1.501	1.499	1.520
N9-C10	1.391	1.391	1.396	1.396	1.414	1.414	1.422	1.414	1.414	1.414	1.396	1.414	1.414
N9-N14	1.376	1.376	1.376	1.376	1.397	1.397	1.394	1.397	1.397	1.397	1.376	1.397	1.390
C10-O18	1.200	1.200	1.200	1.197	1.227	1.227	1.222	1.227	1.227	1.227	1.197	1.227	1.218
C11-H23	1.083	1.083	1.083	1.083	1.094	1.094	1.094	1.094	1.094	1.094	1.083	1.094	
C11-H24	1.079	1.079	1.079	1.079	1.089	1.089	1.089	1.089	1.089	1.089	1.079	1.089	
C11-H25	1.083	1.083	1.083	1.083	1.094	1.094	1.094	1.094	1.094	1.094	1.083	1.094	

N14-C15	1.391	1.391	1.392	1.392	1.407	1.407	1.407	1.407	1.407	1.407	1.392	1.407	1.372
N14-H30	0.997	0.997	0.999	0.999	1.016	1.016	1.016	1.016	1.016	1.016	0.999	1.016	
C15-O17	1.189	1.189	1.190	1.190	1.214	1.214	1.214	1.214	1.214	1.214	1.190	1.214	1.219
C15-C16	1.507	1.507	1.508	1.508	1.514	1.515	1.512	1.515	1.515	1.515	1.507	1.515	1.498
C16-H26	1.080	1.080	1.080	1.080	1.100	1.100	1.094	1.096	1.096	1.096	1.080	1.096	
C16-H27	1.084	1.084	1.083	1.083	1.090	1.090	1.090	1.090	1.090	1.090	1.083	1.090	
C16-H28	1.086	1.086	1.084	1.083	1.094	1.094	1.093	1.094	1.094	1.094	1.084	1.094	
O18…..H30	2.515	2.515	2.767	2.767	2.312	2.312	2.809	2.312	2.312	2.312	2.767	2.312	

parameters	***HF/6-31G(d,p)***				***b3lyp/6-31G(d,p)***				***cbs***				***x-ray***
	R1	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	
	bond angles												
C1-C2-C3	118.9	118.9	119.0	119.0	118.6	118.6	118.7	118.6	118.6	118.6	119.0	118.6	119.1
C1-C2-N7	118.7	118.7	118.7	118.7	118.6	118.6	118.6	118.6	118.6	118.6	118.7	118.6	118.5
C1-C6-C5	121.1	121.1	121.1	121.1	120.8	120.8	120.8	120.8	120.8	120.8	121.1	120.8	121.7
C1-C6-H22	119.5	119.5	119.5	119.5	119.6	119.6	119.6	119.6	119.6	119.6	119.5	119.6	
C2-C1-C6	119.9	119.9	119.8	119.8	120.2	120.2	120.1	120.2	120.2	120.2	119.8	120.2	120
C2-C1-H19	118.5	118.5	118.5	118.5	118.0	118.0	118.1	118.5	118.5	118.5	118.5	118.0	
C2-C3-C4	120.9	120.9	120.9	120.9	120.8	120.8	120.7	120.8	120.8	120.8	120.9	120.8	119.8
C2-C3-C10	118.7	118.7	118.9	118.9	119.0	119.0	119.3	119.0	119.0	119.0	118.9	119.0	119.7
C2-N7-C8	119.0	119.0	119.1	119.1	118.8	118.8	118.8	118.8	118.8	118.8	119.1	118.8	118.4
C3-C2-N7	122.5	122.5	122.3	122.3	122.8	122.8	122.7	122.8	122.8	122.8	122.3	122.8	122.4
C3-C4-C5	119.7	119.7	119.7	119.7	119.8	119.8	119.8	119.8	119.8	119.8	119.7	119.8	120.6
C3-C4-H20	118.7	118.7	118.8	118.8	118.4	118.4	118.4	118.4	118.4	118.4	118.8	118.4	
C3-C10-N9	113.6	113.6	113.7	113.7	113.2	113.2	113.2	113.2	113.2	113.2	113.7	113.2	112.9
C3-C10-O18	126.3	126.3	126.0	126.0	127.2	127.1	126.6	127.2	127.2	127.1	126.0	127.1	126.8
C4-C3-C10	120.4	120.4	120.3	120.3	120.3	120.3	120.0	120.3	120.3	120.3	120.3	120.3	120.5
C4-C5-C6	119.6	119.6	119.6	119.6	119.9	119.9	119.9	119.9	119.9	119.9	119.6	119.9	118.8
C4-C5-H21	120.4	120.4	120.4	120.4	120.2	120.2	120.2	120.2	120.2	120.2	120.4	120.2	119.1
C5-C4-H20	121.6	121.6	121.6	121.6	121.8	121.8	121.8	121.8	121.8	121.8	121.6	121.8	118.5

C5-C6-H22	119.4	119.4	119.4	119.4	119.6	119.6	119.6	119.6	119.6	119.6	119.4	119.6	
C6-C1-H19	121.7	121.7	121.7	121.7	121.8	121.8	121.7	121.8	121.8	121.8	121.7	121.8	
C6-C5-H21	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	
N7-C8-N9	122.5	122.5	122.8	122.8	122.0	122.0	122.6	122.0	122.0	122.0	122.8	122.0	122.4
N7-C8-C11	120.0	120.0	119.7	119.7	120.3	120.3	119.9	120.3	120.3	120.3	119.7	120.3	120.8
C8-N9-C10	123.7	123.7	123.1	123.1	124.2	142.2	123.4	124.2	124.2	124.2	123.1	124.2	124.1
C8-N9-N14	119.8	119.8	118.8	118.8	120.5	120.5	119.0	120.5	120.5	120.5	118.8	120.5	120.5
C8-C11-H23	110.2	110.2	110.9	110.9	110.2	110.2	111.3	110.2	110.2	110.2	110.9	110.2	
C8-C11-H24	107.8	107.8	107.7	107.7	108.0	108.0	107.8	108.0	108.0	108.0	107.7	108.0	
C8-C11-H25	111.1	111.1	111.4	111.4	111.2	111.2	111.6	111.2	111.2	111.2	111.4	111.2	
N9-C8-C11	117.5	117.5	117.5	117.5	117.7	117.7	117.6	117.7	117.7	117.7	117.5	117.7	116.7
N9-C10-O18	120.1	120.1	120.3	120.3	119.6	119.6	120.2	119.6	119.6	119.6	120.3	119.6	120.3
N9-N14-C15	116.6	116.6	120.9	120.9	116.8	116.8	121.2	116.8	116.8	116.8	120.9	116.8	116.2
N9-N14-H30	111.5	111.5	113.8	113.8	109.2	109.2	113.6	109.2	109.2	109.2	113.8	109.2	
C10-N9-N14	116.4	116.4	117.8	117.8	115.3	115.3	117.5	115.3	115.3	115.3	117.8	115.3	115.4
N14-C15-C16	113.9	113.9	117.8	117.8	113.3	113.3	117.1	113.3	113.3	113.3	117.8	113.3	116.1
N14-C15-O17	121.7	121.7	118.6	118.6	122.0	122.0	118.6	122.0	122.0	122.0	118.6	122.0	120.7
C15-N14-H30	115.5	115.5	112.1	112.1	114.5	114.5	111.7	114.5	114.5	114.5	112.1	114.5	
C15-C16-H26	109.0	109.0	109.4	109.4	109.0	109.0	109.1	109.0	109.0	109.0	109.4	109.4	
C15-C16-H27	111.6	111.6	112.2	112.2	112.0	112.0	112.6	112.0	112.0	112.0	112.2	112.0	
C15-C16-H28	108.7	108.7	107.7	107.7	108.9	108.9	108	108.9	108.9	108.9	107.7	108.9	
C16-C15-O17	124.4	124.4	123.6	123.6	124.6	124.6	124.3	124.6	124.6	124.6	123.6	124.6	123.2

parameters	***HF/6-31G(d,p)***				***b3lyp/6-31G(d,p)***				***cbs***			
	R1	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**
	Dihedral angles											
C1-C2-C3-C4	0.165	-0.161	-0.124	0.125	0.037	-0.038	-0.132	-0.037	0.037	-0.038	-0.124	-0.038
C1-C2-C3-C10	180.0	-180.0	179.8	-179.8	179.7	-179.7	179.8	-179.7	179.7	-179.7	179.8	-179.7

C1-C2-N7-C8	180.0	-179.9	-179.7	179.7	-179.7	179.7	-179.9	179.7	-179.7	179.7	-179.7	179.7
C1-C6-C5-C4	0.025	-0.021	-0.043	0.043	0.000	0.000	-0.048	0.000	0.000	0.000	-0.043	0.000
C1-C6-C5-H21	-179.9	179.9	180.0	-180.0	-180.0	-180.0	180.0	-180.0	180.0	-180.0	180.0	-180.0
C2-C1-C6-C5	-0.003	0.006	0.066	-0.065	0.069	-0.069	0.043	-0.069	0.069	-0.069	0.066	-0.069
C2-C1-C6-H22	-179.9	179.9	-180.0	180.0	-179.9	179.9	180.0	179.9	-179.9	179.9	-180.0	179.9
C2-C3-C4-C5	-0.144	0.148	0.148	-0.148	0.030	-0.030	0.129	-0.030	0.030	-0.030	0.148	-0.030
C2-C3-C4-H20	179.8	-179.8	-179.9	179.9	180.0	-180.0	-179.9	-180.0	180.0	-180.0	-179.9	-180.0
C2-C3-C10-N9	0.960	-0.974	-1.109	1.108	-0.139	0.146	-0.459	0.142	-0.139	0.146	-1.109	0.146
C2-C3-C10-O18	179.5	-179.5	179.6	-179.6	178.5	-178.5	-179.8	-178.5	178.5	-178.5	179.6	-178.5
C2-N7-C8-N9	-0.799	0.797	0.995	-0.995	0.146	-0.148	0.830	-0.146	0.146	-0.148	0.995	-0.148
C2-N7-C8-C11	179.1	-179.1	-179.0	179.0	179.8	-179.8	-179.2	-179.8	179.8	-179.8	-179.0	-179.8
C3-C2-C1-C6	-0.090	0.084	0.017	-0.019	-0.086	0.086	0.046	0.087	-0.086	0.086	0.017	0.087
C3-C2-C1-H19	-179.9	179.9	179.9	-179.9	180.0	-180.0	180.0	-180.0	180.0	-180.0	179.9	-180.0
C3-C2-N7-C8	-0.153	0.172	0.665	-0.664	0.634	-0.635	0.356	-0.638	0.634	-0.635	0.665	-0.635
C3-C4-C5-C6	0.048	-0.055	-0.063	0.063	-0.049	0.049	-0.038	0.049	-0.049	0.049	-0.063	0.049
C3-C4-C5-H21	180.0	-180.0	179.9	-179.9	180.0	-180.0	179.9	-180.0	180.0	-180.0	179.9	-180.0
C3-C10-N9-C8	-1.940	1.972	2.759	-2.757	0.913	-0.924	1.629	-0.919	0.913	-0.924	2.759	-0.923
C3-C10-N9-N14	-178.4	178.4	177.0	-177.0	-179.0	179.0	177.8	179.0	-179.0	179.0	177.0	179.0
C4-C3-C2-N7	-179.8	179.8	179.5	-179.5	179.7	-179.7	179.6	-179.7	179.7	-179.7	179.5	-179.7
C4-C3-C10-N9	-179.2	179.2	178.8	-178.9	179.5	-179.5	179.4	-179.5	179.5	-179.5	178.8	-179.5
C4-C3-C10-O18	-0.741	0.730	-0.411	0.410	-1.826	1.831	0.045	1.829	-1.826	1.831	-0.411	1.830
C4-C5-C6-H22	180.0	-179.9	-180.0	180.0	180.0	-180.0	180.0	-180.0	180.0	-180.0	-180.0	-180.0
C5-C4-C3-C10	-179.9	179.9	-179.8	179.8	-179.6	179.6	-179.8	179.6	-179.6	179.6	-179.8	179.6
C5-C6-C1-H19	179.8	-179.8	-179.9	179.9	180.0	-180.0	-179.9	-180.0	180.0	-180.0	-179.9	-180.0
C6-C1-C2-N7	179.9	-179.8	-179.6	179.6	-179.8	179.8	-179.7	179.8	-179.8	179.8	-179.6	179.8
C6-C5-C4-H20	-179.9	179.9	180.0	-180.0	-180.0	180.0	-180.0	180.0	-180.0	180.0	180.0	180.0
N7-C2-C1-H19	-0.001	0.010	0.301	-0.300	0.293	-0.294	0.238	-0.294	0.293	-0.294	0.301	-0.294
N7-C2-C3-C10	0.027	-0.037	-0.543	0.542	-0.619	0.617	-0.507	0.621	-0.619	0.617	-0.543	0.617
N7-C8-N9-C10	1.979	-2.005	-2.882	2.880	-0.974	0.983	-1.932	0.979	-0.974	0.983	-2.882	0.983
N7-C8-N9-N14	178.3	-178.3	-177.1	177.1	179.0	-179.0	-178.0	-179.0	179.0	-179.0	-177.1	-179.0

N7-C8-C11-H23	-117.0	117.0	119.6	-119.6	-114.3	114.3	-120.2	114.3	-114.3	114.3	119.6	-126.2
N7-C8-C11-H24	2.710	-2.695	-0.586	0.586	5.432	-5.404	0.189	-5.412	5.432	-5.404	-0.586	-5.404
N7-C8-C11-H25	123.2	-123.2	-121.0	121.0	126.2	-126.2	120.5	-126.2	126.2	-126.2	-121.0	114.3
C8-N9-C10-O18	179.5	-179.4	-177.9	177.9	-177.8	177.8	-178.9	177.8	-177.8	177.8	-177.9	177.8
C8-N9-N14-C15	-96.26	96.23	-114.6	114.6	-87.11	87.11	-114.5	87.11	-87.11	87.11	-114.6	87.11
C8-N9-N14-H30	128.1	-128.1	107.4	-107.4	141.0	-140.9	108.2	-140.9	141.0	-140.9	107.4	-140.9
N9-C8-C11-H23	62.95	-62.94	-60.38	60.38	65.41	-65.37	59.76	-65.38	65.41	-65.37	-60.38	54.18
N9-C8-C11-H24	-177.4	177.4	179.4	-179.4	-174.9	174.9	-179.8	174.9	-174.9	174.9	179.4	174.9
N9-C8-C11-H25	-56.85	56.87	59.05	-59.05	-54.15	54.18	-59.45	54.17	-54.15	54.18	59.05	-65.37
N9-N14-C15-C16	-158.9	158.9	21.36	-21.36	-159.0	159.0	21.95	159.0	-159.0	159.0	21.36	159.0
N9-N14-C15-O17	23.12	-23.13	-161.3	161.3	23.56	-23.56	-160.7	-23.56	23.56	-23.56	-161.3	-23.56
C10-C3-C4-H20	0.018	-0.018	0.147	-0.147	0.296	-0.294	0.164	-0.298	0.296	-0.294	0.147	-0.294
C10-N9-C8-C11	-177.9	177.9	177.1	-177.1	179.4	-179.4	178.1	-179.4	179.4	-179.4	177.1	-179.4
C10-N9-N14-C15	80.34	-80.34	70.88	-70.89	92.85	-92.86	69.20	-92.85	92.85	-92.86	70.88	-92.86
C10-N9-N14-H30	-55.29	55.29	-67.13	67.13	-39.08	39.08	-68.14	39.10	-39.08	39.08	-67.13	39.08
C11-C8-N9-N14	-1.618	1.624	2.865	-2.867	-0.672	0.664	1.953	0.679	-0.672	0.664	2.865	0.665
N14-N9-C10-O18	3.013	-3.011	-3.648	3.648	2.200	-2.200	-2.775	-2.206	2.200	-2.200	-3.648	-2.195
N14-C15-C16-H26	-162.4	162.4	163.6	-163.6	-158.2	158.4	162.5	158.3	-158.2	158.4	163.6	158.4
N14-C15-C16-H27	-40.81	40.82	42.40	-42.40	-36.45	36.65	40.89	36.52	-36.45	36.65	42.40	36.64
N14-C15-C16-H28	78.71	-78.71	-78.00	78.00	83.23	-83.03	-79.18	-83.16	83.23	-83.03	-78.00	-83.04
C16-C15-N14-H30	-25.11	25.10	160.0	-160.0	-29.51	29.49	160.0	29.49	-29.51	29.49	160.00	29.49
O17-C15-N14-H30	156.9	-157.0	-22.62	22.62	153.0	-153.0	-22.56	-153.0	153.0	-153.0	-22.62	-153.0
O17-C15-C16-H26	-103.4	103.4	104.8	-104.8	-99.36	99.57	103.6	99.43	-99.38	99.57	104.8	99.56
O17-C15-C16-H27	137.1	-137.1	-134.8	134.8	141.0	-140.8	-136.3	-140.9	141.0	-140.8	-134.8	-140.8
O17-C15-C16-H28	15.47	-15.46	-13.65	13.65	19.20	-18.98	-14.69	-19.11	19.18	-19.00	-13.65	-18.99
H19-C1-C6-H22	-0.081	0.083	0.085	-0.084	0.005	-0.004	0.065	-0.004	0.005	-0.004	0.085	-0.004
H20-C4-C5-H21	0.035	-0.033	-0.011	0.011	0.046	-0.046	0.020	-0.047	0.046	-0.046	-0.011	-0.046
H21-C5-C6-H22	0.004	-0.006	0.013	-0.014	-0.030	0.030	0.015	0.030	-0.030	0.030	0.013	0.030

Table (S4) Optimized geometrical parameters (bond lengths (Å) and bond angles (degrees)) for **MAQ (50b)** R1-R4. For numbering of the atoms, see Figure 22 (Chapter 2).

parameters	***HF/6-31G(d,p)***				***b3lyp/6-31G(d,p)***				***cbs***				***mpwpw91/6-31+G(d,p)***				***x-ray***
	R1	R2	R3	R4	R1	R2	R3	R4	R1	R2	R3	R4	R1	R2	R3	R4	
	bond lengths																
C1-C2	1.400	1.400	1.399	1.399	1.409	1.409	1.408	1.408	1.400	1.407	1.400	1.399	1.417	1.417	1.416	1.416	1.394
C1-C6	1.373	1.373	1.373	1.373	1.385	1.385	1.386	1.386	1.373	1.383	1.373	1.373	1.393	1.393	1.394	1.394	1.368
C1-H19	1.074	1.074	1.074	1.074	1.085	1.085	1.085	1.085	1.074	1.083	1.074	1.074	1.092	1.092	1.092	1.092	
C2-C3	1.391	1.391	1.390	1.390	1.414	1.414	1.413	1.413	1.391	1.410	1.390	1.390	1.424	1.424	1.423	1.423	1.399
C2-N7	1.385	1.385	1.386	1.386	1.385	1.385	1.388	1.388	1.385	1.384	1.386	1.386	1.387	1.387	1.390	1.390	1.396
C3-C4	1.398	1.398	1.398	1.398	1.405	1.405	1.405	1.405	1.398	1.403	1.398	1.398	1.412	1.412	1.412	1.412	1.394
C3-C10	1.459	1.459	1.461	1.461	1.457	1.457	1.462	1.462	1.459	1.457	1.461	1.461	1.459	1.459	1.464	1.464	1.447
C4-C5	1.371	1.371	1.372	1.372	1.385	1.385	1.386	1.386	1.371	1.382	1.372	1.372	1.393	1.393	1.394	1.394	1.381
C4-H20	1.074	1.074	1.074	1.074	1.085	1.085	1.085	1.085	1.074	1.083	1.074	1.074	1.092	1.092	1.092	1.092	
C5-C6	1.400	1.400	1.400	1.400	1.408	1.408	1.407	1.407	1.400	1.405	1.400	1.400	1.415	1.415	1.414	1.414	1.385
C5-H21	1.075	1.075	1.075	1.075	1.085	1.085	1.085	1.085	1.075	1.084	1.075	1.075	1.092	1.092	1.092	1.092	
C6-H22	1.076	1.076	1.076	1.076	1.086	1.086	1.086	1.086	1.076	1.084	1.076	1.076	1.093	1.093	1.093	1.093	
N7-C8	1.267	1.267	1.266	1.266	1.294	1.294	1.292	1.292	1.267	1.289	1.266	1.266	1.306	1.306	1.304	1.304	1.287
C8-N9	1.385	1.385	1.391	1.391	1.393	1.393	1.400	1.400	1.385	1.393	1.391	1.391	1.399	1.399	1.405	1.406	1.381
C8-C11	1.507	1.507	1.510	1.510	1.508	1.508	1.511	1.511	1.507	1.507	1.510	1.510	1.509	1.509	1.512	1.512	1.520
N9-C10	1.391	1.391	1.395	1.395	1.414	1.414	1.422	1.422	1.391	1.415	1.395	1.395	1.424	1.424	1.433	1.433	1.414
N9-N14	1.377	1.377	1.377	1.377	1.398	1.398	1.394	1.394	1.377	1.395	1.377	1.377	1.401	1.401	1.398	1.398	1.390
C10-O18	1.200	1.200	1.197	1.197	1.227	1.227	1.222	1.222	1.200	1.220	1.197	1.197	1.240	1.240	1.233	1.233	1.218
C11-C12	1.524	1.524	1.524	1.524	1.528	1.528	1.528	1.528	1.524	1.527	1.524	1.524	1.531	1.531	1.531	1.531	
C11-H23	1.086	1.086	1.085	1.085	1.097	1.097	1.097	1.097	1.086	1.095	1.085	1.085	1.104	1.104	1.104	1.104	
C11-H24	1.085	1.085	1.085	1.085	1.097	1.097	1.097	1.097	1.085	1.095	1.085	1.085	1.104	1.104	1.104	1.104	
C12-H25	1.083	1.083	1.083	1.083	1.093	1.093	1.092	1.092	1.083	1.090	1.083	1.083	1.100	1.100	1.100	1.100	
C12-H26	1.082	1.082	1.082	1.082	1.092	1.092	1.092	1.092	1.082	1.091	1.082	1.082	1.099	1.099	1.099	1.099	
C12-H27	1.085	1.085	1.085	1.085	1.094	1.094	1.094	1.094	1.085	1.093	1.085	1.085	1.200	1.100	1.099	1.099	
N14-C15	1.391	1.391	1.391	1.391	1.407	1.407	1.406	1.406	1.391	1.406	1.391	1.391	1.411	1.411	1.408	1.408	1.372
N14-H30	0.997	0.997	0.999	0.999	1.016	1.016	1.016	1.016	0.997	1.014	0.999	0.999	1.025	1.025	1.023	1.023	
C15-C16	1.507	1.507	1.507	1.507	1.515	1.515	1.512	1.512	1.507	1.513	1.507	1.507	1.517	1.517	1.514	1.514	1.219
C15-O17	1.189	1.189	1.190	1.190	1.214	1.214	1.214	1.214	1.189	1.207	1.190	1.190	1.226	1.226	1.228	1.228	1.498
C16-H28	1.080	1.080	1.080	1.080	1.090	1.090	1.090	1.090	1.080	1.088	1.080	1.080	1.098	1.098	1.096	1.096	
C16-H29	1.086	1.086	1.083	1.083	1.096	1.096	1.094	1.094	1.086	1.092	1.083	1.083	1.099	1.099	1.100	1.102	
C16-H31	1.084	1.084	1.084	1.084	1.094	1.094	1.093	1.093	1.084	1.094	1.084	1.084	1.101	1.101	1.102	1.100	
O18…..H30	2.514	2.514	2.590	2.762	2.313	2.313	2.807	2.806	2.514	2.357	2.762	2.762	2.246	2.246	2.821	2.821	

parameters	***HF/6-31G(d,p)***	***b3lyp/6-31G(d,p)***	***cbs***	***mpwpw91/6-31+G(d,p)***	***x-ray***

	R1	R2	R3	R4	R1	R2	R3	R4	R1	R2	R3	R4	R1	R2	R3	R4	
	bond angles																
C1-C2-C3	118.9	118.9	119.0	119.0	118.6	118.6	118.8	118.8	118.9	118.6	119.0	119.0	118.6	118.6	118.7	118.7	119.1
C1-C2-N7	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.5	118.5	118.4	118.4	118.5
C1-C6-C5	121.1	121.1	121.1	121.1	120.8	120.8	120.8	120.8	121.1	120.8	121.1	121.1	120.8	120.8	120.7	120.7	121.7
C1-C6-H22	119.5	119.5	119.5	119.5	119.6	119.6	119.6	119.6	119.5	119.6	119.5	119.5	119.6	119.6	119.6	119.6	
C2-C1-C6	119.9	119.9	119.8	119.8	120.2	120.2	120.1	120.1	119.9	120.2	119.8	119.8	120.3	120.3	120.2	120.2	120
C2-C1-H19	118.5	118.5	118.6	118.6	118.1	118.1	118.1	118.1	118.5	118.0	118.6	118.6	118.1	118.1	118.1	118.1	
C2-C3-C4	120.9	120.9	120.9	120.9	120.8	120.8	120.7	120.7	120.9	120.7	120.9	120.9	120.7	120.7	120.6	120.6	119.8
C2-C3-C10	118.6	118.6	118.8	118.8	118.9	118.9	119.2	119.2	118.6	119.0	118.8	118.8	118.9	118.9	119.3	119.3	119.7
C2-N7-C8	119.3	119.3	119.5	119.5	119.1	119.1	119.1	119.1	119.3	119.3	119.5	119.5	119.0	119.0	118.9	118.9	118.4
C3-C2-N7	122.4	122.4	122.3	122.3	122.7	122.7	122.6	122.6	122.4	122.7	122.3	122.3	122.9	122.9	122.8	122.8	122.4
C3-C4-C5	119.7	119.7	119.7	119.7	119.7	119.7	119.8	119.8	119.7	119.8	119.7	119.7	119.8	119.8	119.8	119.8	120.6
C3-C4-H20	118.7	118.7	118.8	118.8	118.4	118.4	118.4	118.4	118.7	118.5	118.8	118.8	118.5	118.5	118.5	118.5	
C3-C10-N9	113.7	113.7	113.8	113.8	113.3	113.3	113.3	113.3	113.7	113.2	113.8	113.8	113.3	113.3	113.1	113.1	112.9
C3-C10-O18	126.2	126.2	125.9	125.9	127.1	127.1	126.5	126.5	126.2	127.0	125.9	125.9	127.3	127.3	126.8	126.8	126.8
C4-C3-C10	120.5	120.5	120.3	120.3	120.3	120.3	120.1	120.1	120.5	120.3	120.3	120.3	120.4	120.4	120.1	120.1	120.5
C4-C5-C6	119.6	119.6	119.6	119.6	119.9	119.9	119.9	119.9	119.6	119.9	119.6	119.6	120.0	120.0	120.0	120.0	118.8
C4-C5-H21	120.4	120.4	120.4	120.4	120.2	120.2	120.1	120.1	120.4	120.2	120.3	120.4	120.1	120.1	120.0	120.0	119.1
C5-C4-H20	121.6	121.6	121.6	121.6	121.8	121.8	121.8	121.8	121.6	121.8	121.6	121.6	121.7	121.7	121.7	121.7	118.5
C5-C6-H22	119.4	119.4	119.4	119.5	119.6	119.6	119.6	119.6	119.4	119.6	119.4	119.5	119.6	119.6	119.7	119.7	
C6-C1-H19	121.7	121.7	121.7	121.7	121.7	121.7	121.7	121.7	121.7	121.8	121.7	121.7	121.7	121.7	121.7	121.7	
C6-C5-H21	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	
N7-C8-N9	122.2	122.2	122.5	122.5	121.8	121.8	122.3	122.3	122.2	121.8	122.5	122.5	121.5	121.5	122.2	122.2	122.4
N7-C8-C11	120.8	120.8	120.5	120.5	120.9	120.9	120.5	120.5	120.8	120.9	120.5	120.5	120.9	120.9	120.7	120.7	120.8
C8-N9-C10	123.7	123.7	123.1	123.1	124.2	124.2	123.5	123.5	123.7	124.0	123.1	123.1	124.2	124.2	123.6	123.6	124.1
C8-N9-N14	120.1	120.1	119.1	119.1	120.6	120.6	119.1	119.1	120.1	120.5	119.1	119.1	120.9	120.9	119.0	119.0	120.5
C8-C11-C12	113.4	113.4	113.4	113.4	113.5	113.5	113.4	113.4	113.4	113.6	113.4	113.4	113.7	113.7	113.6	113.6	
C8-C11-H23	108.3	108.3	108.7	108.6	108.3	108.3	108.7	108.7	108.3	108.3	108.7	108.6	108.1	108.1	108.7	108.3	
C8-C11-H24	107.7	107.7	108.2	108.2	107.5	107.5	108.4	108.4	107.7	107.4	108.2	108.2	107.7	107.7	108.3	108.7	
N9-C8-C11	116.9	116.9	117.0	117.0	117.4	117.4	117.2	117.2	116.9	117.3	117.0	117.0	117.5	117.5	117.2	117.2	116.7
N9-C10-O18	120.1	120.1	120.3	120.3	119.6	119.6	120.2	120.2	120.1	119.7	120.3	120.3	119.4	119.4	120.1	120.1	120.3
N9-N14-C15	116.6	116.6	120.9	120.9	116.8	116.8	121.2	121.2	116.6	117.3	120.9	120.9	118.1	118.1	121.8	121.8	116.2
N9-N14-H30	111.4	111.4	113.8	113.8	109.2	109.2	113.7	113.7	111.4	110.0	113.8	113.8	109.0	109.0	114.3	114.3	
C10-N9-N14	116.1	116.1	117.6	117.6	115.2	115.2	117.3	117.3	116.1	115.4	117.6	117.6	114.8	114.8	117.3	117.3	115.4
C11-C12-H25	111.4	111.4	111.4	111.4	111.4	111.3	111.2	111.2	111.4	111.4	111.4	111.4	111.4	109.6	109.6	109.6	
C11-C12-H26	111.2	111.2	111.3	111.3	111.1	111.1	111.2	111.2	111.2	111.1	111.3	111.3	111.2	111.2	111.3	111.3	
C11-C12-H27	109.3	109.3	109.2	109.2	109.7	109.7	109.7	109.7	109.3	109.7	109.2	109.2	109.6	111.4	111.3	111.3	
C12-C11-H23	110.6	110.6	110.5	110.5	110.9	110.9	110.7	110.7	110.6	110.9	110.5	110.5	110.9	110.9	110.5	110.7	

C12-C11-H24	110.4	110.4	110.4	110.4	110.6	110.6	110.6	110.6	110.4	110.4	110.4	110.4	110.4	110.4	110.7	110.5	
N14-C15-C16	113.9	113.9	117.8	117.8	113.3	113.3	117.1	117.1	113.9	113.3	117.8	117.8	113.5	113.5	117.1	117.1	116.1
N14-C15-O17	121.7	121.7	118.6	118.6	122.0	122.0	118.6	118.6	121.7	122.1	118.6	118.6	122.3	122.3	118.5	118.5	120.7
C15-N14-H30	115.5	115.5	112.1	112.1	114.4	114.4	111.7	111.7	115.5	114.8	112.1	112.1	115.1	115.1	113.0	113.0	
C15-C16-H28	109.0	109.0	109.3	109.3	109.1	109.1	109.1	109.1	109.0	108.8	109.3	109.3	108.9	108.9	108.2	108.2	
C15-C16-H29	108.7	108.7	107.7	107.7	108.9	108.9	108.0	108.0	108.7	108.8	107.7	107.7	108.3	113.5	112.9	109.1	
C15-C16-H31	111.6	111.6	112.3	112.3	112.0	112.0	112.6	112.6	111.6	112.1	112.3	112.3	113.5	108.3	109.1	113.0	
C16-C15-O17	124.4	124.4	123.5	123.5	124.6	124.6	124.3	124.3	124.4	124.6	123.5	123.5	124.1	124.1	124.3	124.3	123.2

parameters	***HF/6-31G (d,p)***				***b3lyp/6-31G (d,p)***				***cbs***				***mpwpw91/6-31+G(d,p)***			
	R1	R2	R3	R4	R1	R2	R3	R4	R1	R2	R3	R4	R1	R2	R3	R4
	Dihedral angles															
C1-C2-C3-C4	0.153	-0.153	-0.125	0.130	0.019	-0.019	-0.144	0.144	0.153	0.002	-0.125	0.130	-0.169	0.170	-0.193	0.192
C1-C2-C3-C10	180.0	-180.0	179.8	-179.8	179.7	-179.7	179.7	-179.7	180.0	-179.6	179.8	-179.8	179.6	-179.6	179.6	-179.6
C1-C2-N7-C8	179.9	-179.9	-179.7	179.7	-179.7	179.7	-179.9	179.9	179.9	179.6	-179.7	179.7	-178.9	178.9	-179.6	179.6
C1-C6-C5-C4	0.021	-0.021	-0.043	0.046	-0.020	0.020	-0.068	0.069	0.021	0.020	-0.043	0.046	-0.067	0.067	-0.119	0.118
C1-C6-C5-H21	-179.9	179.9	180.0	-179.9	180.0	-180.0	180.0	-180.0	-179.9	-180.0	180.0	-179.9	179.9	-179.9	179.9	-179.9
C2-C1-C6-C5	-0.001	0.001	0.069	-0.069	0.082	-0.082	0.056	-0.056	-0.001	-0.085	0.069	-0.069	0.219	-0.219	0.143	-0.143
C2-C1-C6-H22	-179.9	179.9	-180.0	180.0	-179.9	179.9	-180.0	180.0	-179.9	179.9	-180.0	180.0	-179.9	179.9	-180.0	180.0
C2-C3-C4-C5	-0.134	0.134	0.152	-0.154	0.041	-0.041	0.133	-0.133	-0.134	-0.065	0.152	-0.154	0.321	-0.321	0.217	-0.218
C2-C3-C4-H20	179.8	-179.8	-179.9	179.9	180.0	-180.0	-179.9	179.9	179.8	-179.9	-179.9	179.9	-179.9	179.9	-179.9	179.9
C2-C3-C10-N9	0.859	-0.865	-1.162	1.160	-0.163	0.163	-0.439	0.436	0.859	0.197	-1.162	1.160	-1.953	1.951	-0.861	0.874
C2-C3-C10-O18	179.4	-179.4	179.6	-179.6	178.5	-178.5	-179.8	179.8	179.4	-178.6	179.6	-179.6	177.2	-177.2	179.6	-179.6
C2-N7-C8-N9	-0.760	0.759	1.016	-1.017	0.210	-0.210	0.838	-0.840	-0.760	-0.217	1.016	-1.017	0.856	-0.857	0.929	-0.930
C2-N7-C8-C11	179.2	-179.2	-179.0	179.0	179.8	-179.8	-179.2	179.2	179.2	-179.8	-179.9	179.0	-179.0	179.0	-179.0	179.0
C3-C2-C1-C6	-0.086	0.085	0.014	-0.019	-0.080	0.080	0.049	-0.049	-0.086	0.073	0.014	-0.019	-0.100	0.099	0.013	-0.012
C3-C2-C1-H19	-179.9	179.9	179.9	-179.9	180.0	-180.0	180.0	-180.0	-179.9	-180.0	179.9	-179.9	179.9	-179.9	179.9	-179.9
C3-C2-N7-C8	-0.107	0.110	0.707	-179.9	0.676	-0.676	0.404	-0.406	-0.107	-0.684	0.707	-0.711	2.028	-2.029	0.924	-0.930
C3-C4-C5-C6	0.045	-0.045	-0.067	0.065	-0.041	0.041	-0.027	0.026	0.045	0.055	-0.067	0.065	-0.202	0.202	-0.061	0.063
C3-C4-C5-H21	180.0	-180.0	179.9	-179.9	180.0	-180.0	179.9	-179.9	180.0	-179.9	179.9	-179.9	179.8	-179.8	179.9	-179.9
C3-C10-N9-C8	-1.755	1.764	2.884	-2.885	1.045	-1.045	1.667	-1.669	-1.755	-1.092	2.884	-2.885	4.914	-4.914	2.707	-2.727
C3-C10-N9-N14	-178.4	178.4	177.1	-177.1	-179.1	179.1	177.9	-177.9	-178.4	179.0	177.1	-177.1	-178.8	178.8	179.4	-179.4
C4-C3-C2-N7	-179.8	179.8	179.5	-179.5	179.7	-179.7	179.6	-179.6	-179.8	-179.7	179.5	-179.5	178.9	-178.9	179.3	-179.3
C4-C3-C10-N9	-179.3	179.3	178.8	-178.8	179.5	-179.5	179.4	-179.4	-179.3	-179.4	178.8	-178.8	177.8	-177.8	178.9	-178.9
C4-C3-C10-O18	-0.818	0.810	-0.448	0.453	-1.859	1.859	0.049	-0.049	-0.818	1.782	-0.448	0.453	-3.097	3.096	-0.603	0.607
C4-C5-C6-H22	180.0	-180.0	-180.0	180.0	180.0	-180.0	180.0	-180.0	180.0	-180.0	-180.0	180.0	-180.0	180.0	-180.0	180.0

C5-C4-C3-C10	-179.9	179.9	-179.8	179.8	-179.6	179.6	-179.7	179.7	-179.9	179.6	-179.8	179.8	-179.4	179.4	-179.6	179.6
C5-C6-C1-H19	179.9	-179.9	-179.9	179.8	-180.0	180.0	-179.9	179.9	179.9	180.0	-179.9	179.8	-179.8	179.8	-179.8	179.8
C6-C1-C2-N7	179.9	-179.9	-179.6	179.6	-179.8	179.8	-179.7	179.7	179.9	179.8	-179.6	179.6	-179.2	179.2	-179.5	179.5
C6-C5-C4-H20	-179.9	179.9	180.0	-180.0	-180.0	180.0	-179.9	179.9	-179.9	179.9	180.0	-180.0	-180.0	180.0	-180.0	180.0
N7-C2-C1-H19	0.004	-0.003	0.317	-0.314	0.297	-0.297	0.253	-0.254	0.004	-0.282	0.317	-0.314	0.782	-0.782	0.402	-0.402
N7-C2-C3-C10	0.019	-0.018	-0.568	0.573	-0.678	0.678	-0.571	0.575	0.019	0.670	-0.568	0.573	-1.354	1.357	-0.896	0.895
N7-C8-N9-C10	1.811	-1.816	-2.990	2.994	-1.133	1.133	-1.984	1.988	1.811	1.170	-2.990	2.994	-4.617	4.619	-2.914	2.929
N7-C8-N9-N14	178.4	-178.4	-177.1	177.1	179.0	-179.0	-178.1	178.1	178.4	-178.9	-177.1	177.1	179.3	-179.3	-179.5	179.5
N7-C8-C11-C12	2.557	-2.551	-0.649	0.619	6.219	-6.219	0.453	-0.494	2.557	-6.393	-0.649	0.619	7.777	-7.789	1.388	-1.423
N7-C8-C11-H23	125.7	-125.7	-123.8	123.8	129.9	-129.9	123.8	-123.9	125.7	-130.1	-123.8	123.8	131.4	-131.4	-122.2	-124.9
N7-C8-C11-H24	-119.9	119.9	122.3	-122.3	-116.3	116.3	-123.0	123.0	-119.9	116.1	122.3	-122.3	-114.9	114.9	124.9	122.1
C8-N9-C10-O18	179.6	-179.6	-177.8	177.8	-177.7	177.7	-178.9	178.9	179.6	177.8	-177.8	177.8	-174.3	174.3	-177.7	177.7
C8-N9-N14-C15	-97.04	97.04	-114.7	114.7	-87.98	87.98	-114.4	114.4	-97.04	88.43	-144.7	114.7	-83.13	83.12	-110.1	110.1
C8-N9-N14-H30	127.5	-127.5	107.2	-107.2	140.3	-140.3	108.0	-108.0	127.5	-137.9	107.2	-107.2	143.1	-143.2	108.3	-108.3
C8-C11-C12-H25	60.16	-60.16	-60.19	60.19	60.21	-60.21	59.89	-59.89	60.16	59.41	-60.19	60.19	-60.24	-179.7	-180.0	180.0
C8-C11-C12-H26	-60.08	60.08	60.04	-60.04	-59.45	59.45	-59.69	59.69	-60.08	-60.31	60.04	-60.04	59.60	60.24	59.88	59.81
C8-C11-C12-H27	-179.9	179.9	179.9	-179.9	-179.6	179.6	-179.9	179.9	-179.9	179.5	179.9	-179.9	179.7	-59.61	-59.80	-59.88
N9-C8-C11-C12	-177.5	177.5	179.4	-179.4	-174.1	174.1	-179.6	179.6	-177.5	174.0	179.4	-179.4	-172.1	172.0	-178.5	178.5
N9-C8-C11-H23	-54.31	54.32	56.23	-56.26	-50.50	50.50	-56.20	56.16	-54.31	50.28	56.23	57.63	-48.44	48.42	57.93	55.01
N9-C8-C11-H24	60.10	-60.09	-57.66	57.63	63.30	-63.30	57.00	-57.00	60.10	-63.55	-57.66	-56.26	65.29	-65.30	-55.05	-57.96
N9-N14-C15-C16	-158.8	158.8	21.30	-21.30	-158.9	158.9	21.85	-21.84	-158.8	159.3	21.30	-21.30	-162.8	162.8	18.18	-18.16
N9-N14-C15-O17	23.25	-23.26	-161.3	161.3	23.66	-23.66	-160.7	160.7	23.25	-22.90	-161.3	161.3	20.25	-20.25	-164.1	164.1
C10-C3-C4-H20	0.011	-0.012	0.153	-0.160	0.322	-0.322	0.196	-0.199	0.011	-0.311	0.153	-0.160	0.344	-0.345	0.331	-0.33
C10-N9-C8-C11	-178.2	178.2	177.0	-177.0	179.2	-179.2	178.1	-178.1	-178.2	-179.2	177.0	-177.0	175.2	-175.2	177.0	-177.0
C10-N9-N14-C15	79.76	-79.75	70.85	-70.84	92.14	-92.14	69.21	-69.24	79.76	-91.67	70.85	-70.84	100.4	-100.5	73.05	-73.05
C10-N9-N14-H30	-55.74	55.74	-67.25	67.27	-39.60	39.60	-68.34	68.32	-55.74	41.96	-67.25	67.27	-33.28	33.27	-68.51	68.50
C11-C8-N9-N14	-1.622	1.625	2.847	-2.840	-0.644	0.644	1.943	-1.937	-1.622	0.692	2.847	-2.840	-0.861	0.863	0.386	-0.386
N14-N9-C10-O18	2.971	-2.967	-3.619	3.606	2.154	-2.155	-2.731	2.726	2.971	-2.117	-3.619	3.606	2.007	-2.008	-1.039	1.033
N14-C15-C16-H28	-162.5	162.4	163.4	-163.4	-158.8	158.8	162.2	-162.3	-162.5	157.4	163.4	-163.4	-134.2	134.2	160.8	-160.7
N14-C15-C16-H29	78.67	-78.71	-78.24	78.22	82.62	-82.62	-79.58	79.49	78.67	-84.14	-78.24	78.22	108.9	12.01	38.77	81.20
N14-C15-C16-H31	-40.85	40.81	42.16	-42.18	-37.06	37.06	40.48	-40.57	-40.85	35.60	42.16	-42.18	-11.99	-108.9	-81.15	-38.73
C16-C15-N14-H30	-25.07	25.07	160.1	-160.1	-29.53	29.53	160.2	-160.1	-25.07	27.87	160.1	-160.1	-31.78	31.78	160.2	-160.2
O17-C15-N14-H30	157.0	-157.0	-22.55	22.54	153.0	-153.0	-22.37	22.39	157.0	-154.4	-22.55	22.54	151.3	-151.3	-22.06	22.07
O17-C15-C16-H28	15.44	-15.48	-13.90	13.87	18.61	-18.61	-15.13	15.05	15.44	-20.24	-13.90	13.87	42.70	-42.68	-16.85	16.90
O17-C15-C16-H29	-103.4	103.4	104.5	-104.5	-99.97	99.97	103.1	103.2	-103.4	98.18	104.5	-104.5	-74.19	-164.9	-138.8	-101.2
O17-C15-C16-H31	137.0	-137.1	-135.1	135.1	140.4	-140.4	-136.8	136.7	137.0	-142.1	-135.1	135.1	164.9	74.21	101.2	138.9
H19-C1-C6-H22	-0.074	0.074	0.086	-0.087	0.019	-0.019	0.078	-0.078	-0.074	-0.030	0.086	-0.087	0.127	-0.127	0.122	-0.122
H20-C4-C5-H21	0.032	-0.033	-0.011	0.010	0.055	-0.056	0.026	-0.027	0.032	-0.056	-0.011	0.010	0.046	-0.047	-0.007	0.007
H21-C5-C6-H22	0.010	-0.010	0.014	-0.014	-0.023	0.023	0.013	-0.013	0.010	0.015	0.014	-0.014	0.029	-0.029	0.033	-0.033

Table (S5) Optimized geometrical parameters (bond lengths (Å) and bond angles (degrees) for **MAQ (50c)** R1-R4 . For numbering of the atoms, see Figure 22 (Chapter 2).

parameters	*HF/6-31G(d,p)*				*b3lyp/6-31G(d)*				*b3lyp/6-31G(d,p)*				*x-ray*
	R1	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	
	bond lengths												
C1-C2	1.400	1.400	1.399	1.399	1.411	1.411	1.410	1.410	1.410	1.410	1.409	1.408	1.394
C1-C6	1.372	1.372	1.373	1.373	1.387	1.387	1.388	1.388	1.385	1.385	1.386	1.386	1.368
C1-H19	1.074	1.074	1.074	1.074	1.086	1.086	1.086	1.086	1.085	1.085	1.085	1.085	
C2-C3	1.39	1.39	1.389	1.389	1.414	1.414	1.413	1.413	1.413	1.413	1.412	1.412	1.399
C2-N7	1.383	1.383	1.384	1.384	1.383	1.383	1.387	1.387	1.383	1.385	1.386	1.386	1.396
C3-C4	1.399	1.399	1.398	1.398	1.407	1.407	1.407	1.407	1.405	1.405	1.405	1.405	1.394
C3-C10	1.458	1.458	1.459	1.459	1.457	1.457	1.46	1.46	1.457	1.457	1.461	1.461	1.447
C4-C5	1.371	1.371	1.371	1.371	1.386	1.386	1.387	1.387	1.385	1.385	1.385	1.385	1.381
C4-H20	1.074	1.074	1.074	1.074	1.086	1.086	1.086	1.086	1.085	1.085	1.085	1.085	
C5-C6	1.401	1.401	1.401	1.401	1.401	1.41	1.409	1.409	1.408	1.408	1.407	1.407	1.385
C5-H21	1.075	1.075	1.075	1.075	1.086	1.086	1.086	1.086	1.085	1.085	1.085	1.085	
C6-H22	1.076	1.076	1.077	1.076	1.087	1.087	1.087	1.087	1.086	1.086	1.086	1.086	
N7-C8	1.268	1.268	1.27	1.27	1.295	1.295	1.27	1.297	1.295	1.294	1.293	1.293	1.287
C8-N9	1.387	1.387	1.391	1.391	1.396	1.396	1.401	1.401	1.394	1.393	1.402	1.401	1.381
C8-C11	1.518	1.518	1.523	1.523	1.519	1.519	1.524	1.524	1.519	1.518	1.521	1.519	1.520
N9-C10	1.394	1.394	1.398	1.398	1.418	1.418	1.425	1.425	1.419	1.415	1.424	1.423	1.414
N9-N14	1.377	1.377	1.377	1.377	1.396	1.396	1.395	1.395	1.397	1.398	1.395	1.395	1.390
C10-O18	1.2	1.2	1.198	1.198	1.228	1.228	1.224	1.224	1.226	1.227	1.222	1.222	1.218
C11-C12	1.537	1.537	1.536	1.536	1.542	1.542	1.542	1.542	1.543	1.544	1.543	1.533	
C11-C13	1.531	1.531	1.534	1.534	1.541	1.541	1.541	1.541	1.537	1.533	1.535	1.544	
C11-H23	1.081	1.081	1.082	1.082	1.092	1.092	1.095	1.095	1.092	1.093	1.093	1.094	
C12-H24	1.086	1.086	1.085	1.085	1.097	1.096	1.096	1.096	1.095	1.095	1.094	1.094	
C12-H25	1.083	1.083	1.086	1.086	1.095	1.097	1.096	1.096	1.095	1.093	1.094	1.094	

C12-H26	1.085	1.085	1.081	1.082	1.095	1.094	1.093	1.094	1.092	1.092	1.092	1.092	
C13-H27	1.086	1.086	1.085	1.085	1.096	1.097	1.096	1.096	1.095	1.095	1.094	1.094	
C13-H28	1.082	1.082	1.082	1.081	1.094	1.095	1.094	1.093	1.094	1.094	1.095	1.095	
C13-H29	1.085	1.085	1.086	1.086	1.097	1.095	1.096	1.096	1.093	1.093	1.093	1.094	
N14-C15	1.391	1.391	1.394	1.394	1.405	1.405	1.405	1.405	1.409	1.409	1.408	1.407	1.372
N14-H30	0.997	0.997	0.999	0.999	1.017	1.017	1.018	1.018	1.016	1.016	1.017	1.016	
C15-O17	1.189	1.189	1.19	1.19	1.216	1.216	1.218	1.218	1.213	1.213	1.214	1.213	1.219
C15-C16	1.507	1.507	1.506	1.506	1.514	1.514	1.511	1.511	1.514	1.514	1.511	1.512	1.498
C16-H31	1.08	1.08	1.08	1.08	1.091	1.097	1.092	1.092	1.09	1.09	1.09	1.09	
C16-H32	1.084	1.084	1.082	1.082	1.095	1.092	1.093	1.093	1.094	1.094	1.092	1.094	
C16-H33	1.086	1.087	1.084	1.084	1.097	1.095	1.096	1.096	1.096	1.096	1.094	1.093	
O18…..H30	2.549	2.549	2.752	2.752	2.418	2.419	2.802	2.801	2.4	3.115	2.852	2.78	

parameters	***HF/6-31G(d,p)***				***b3lyp/6-31G(d)***				***b3lyp/6-31G(d,p)***				***x-ray***
	R1	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	
	bond angles												
C1-C2-C3	118.9	118.9	119	119	118.7	118.7	118.9	118.9	118.6	118.6	118.7	118.7	119.1
C1-C2-N7	118.8	118.8	118.8	118.8	118.8	118.8	118.6	118.6	118.8	118.7	118.8	118.7	118.5
C1-C6-C5	121.1	121.1	121.1	121.1	120.8	120.8	120.8	120.8	120.8	120.8	120.8	120.8	121.7
C1-C6-H22	119.5	119.5	119.5	119.5	119.6	119.6	119.6	119.6	119.6	119.6	119.6	119.6	
C2-C1-C6	119.8	119.8	119.8	119.8	120.2	120.2	120.1	120.1	120.2	120.2	120.1	120.1	120
C2-C1-H19	118.5	118.5	118.6	118.6	118.2	118.2	118.3	118.3	118.1	118.1	118.1	118.1	
C2-C3-C4	121	121	121	121	120.7	120.7	120.7	120.7	120.8	120.8	120.7	120.7	119.8
C2-C3-C10	118.5	118.5	118.6	118.6	118.8	118.8	118.9	118.9	118.9	118.8	119.2	119.2	119.7
C2-N7-C8	119.8	119.8	119.9	119.9	119.7	119.7	119.8	119.8	119.5	119.4	119.5	119.4	118.4
C3-C2-N7	122.3	122.3	122.2	122.2	122.5	122.5	122.5	122.5	122.6	122.7	122.5	122.5	122.4
C3-C4-C5	119.7	119.7	119.6	119.6	119.8	119.8	119.7	119.7	119.7	119.7	119.7	119.7	120.6
C3-C4-H20	118.7	118.7	118.8	118.8	118.6	118.6	118.7	118.7	118.4	118.4	118.4	118.4	

C3-C10-N9	113.9	113.9	114.1	114.1	113.7	113.7	113.8	113.8	113.5	113.4	113.5	113.5	112.9
C3-C10-O18	126.1	126.1	125.7	125.7	126.7	126.8	126.3	126.3	126.9	126.9	126.4	126.5	126.8
C4-C3-C10	120.5	120.5	120.5	120.5	120.5	120.5	120.4	120.4	120.3	120.4	120.1	120.1	120.5
C4-C5-C6	119.6	119.6	119.6	199.6	119.9	119.9	119.9	119.9	119.9	119.9	119.9	119.9	118.8
C4-C5-H21	120.4	120.4	120.4	120.4	120.1	120.1	120.1	120.1	120.2	120.2	120.2	120.2	119.1
C5-C4-H20	121.6	121.6	121.6	121.6	121.6	121.6	121.6	121.6	121.8	121.8	121.8	121.8	118.5
C5-C6-H22	119.4	119.4	119.4	119.4	119.6	119.6	119.6	119.6	119.6	119.6	119.6	119.6	
C6-C1-H19	121.7	121.7	121.7	121.7	121.6	121.6	121.6	121.6	121.8	121.8	121.7	121.7	
C6-C5-H21	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	119.9	120.0	120.0	
N7-C8-N9	121.9	121.9	121.9	121.9	121.5	121.5	121.5	121.5	121.6	121.5	122.0	122.0	122.4
N7-C8-C11	119.1	119.1	116.8	116.8	119	199	117.2	117.2	119	120.2	119.4	119.8	120.8
C8-N9-C10	123.5	123.5	123.1	123.1	123.8	123.8	123.4	123.4	123.9	124.2	123.2	123.4	124.1
C8-N9-N14	121.0	121.0	119.8	119.8	121.2	121.2	119.9	119.9	121.4	121	119.6	119.8	120.5
C8-C11-C12	109.4	109.4	113.2	113.2	110.0	110.0	113.3	113.3	110.3	111.2	110.9	111.3	
C8-C11-C13	110.8	110.8	114.9	114.9	110.1	110.1	114.9	114.9	109.5	109.8	110.3	109.6	
C8-C11-H23	108.4	108.4	101.2	101.2	108.4	108.4	101.5	101.5	108.2	107.7	107.9	108.0	
N9-C8-C11	118.9	118.9	121.3	121.3	119.5	119.5	121.3	121.3	119.4	118.2	118.6	118.2	116.7
N9-C10-O18	119.9	119.9	120.1	120.1	119.6	119.6	119.9	119.9	119.5	119.6	120.2	120.1	120.3
N9-N14-C15	116.6	116.6	120.8	120.8	117.2	117.2	121.5	121.5	116.4	116.4	121.6	121.1	116.2
N9-N14-H30	111.5	111.5	113.5	113.5	110.6	110.6	113.5	113.5	109.8	109.1	113.8	113.5	
C10-N9-N14	115.5	115.5	116.9	116.9	115	115	116.6	116.6	114.7	114.9	116.9	116.7	115.4
C11-C12-H24	109.7	109.7	108.8	109.0	109.7	109.7	108.9	109.1	109.8	109.5	109.5	109.6	
C11-C12-H25	111.7	111.7	111.3	111.2	111.1	111.6	111.4	111.4	111.6	111.1	111.4	111.4	
C11-C12-H26	110.2	110.2	112.6	112.4	110.4	110.6	112.3	112.2	110.5	111.1	111,0	111.1	
C11-C13-H27	109.4	109.4	109.0	108.8	109.7	109.7	109.1	108.9	109.9	109.9	109.9	109.9	
C11-C13-H28	111.1	111.1	112.4	112.6	110.7	110.4	112.2	112.3	110.1	110.5	110.5	110.4	
C11-C13-H29	111.4	111.4	111.2	111.3	111.6	111.1	111.4	111.4	111.1	111.8	112	111.9	
C12-C11-C13	111.3	111.3	112.2	112.2	111.4	111.4	111.9	111.9	111.4	111.3	111	111.2	
C12-C11-H23	108.4	108.4	107.1	107.1	108.5	108.4	107.1	107.2	108.9	108.3	109	109	
C13-C11-H23	108.5	108.5	107.1	107.1	108.4	108.5	107.2	107.1	108.6	108.5	107.7	107.6	

N14-C15-C16	113.7	113.7	118.4	118.4	113.8	113.8	118	118	113.3	113.4	117.9	117.0	116.1
N14-C15-O17	122.1	122.1	118.2	118.2	121.8	121.8	118.2	118.2	122.1	121.8	118.2	118.6	120.7
C15-N14-H30	114.9	114.9	111.3	111.3	115.2	115.2	112	112	114.1	114.1	111.2	111.5	
C15-C16-H31	108.9	108.9	107.7	107.7	109.0	108.6	108.2	108.2	108.9	108.9	108.0	107.9	
C15-C16-H32	111.7	111.7	112.7	112.7	112.6	112.6	113.0	113.0	112.1	112	113.3	109.3	
C15-C16-H33	108.6	108.6	108.8	108.8	108.6	109.0	108.8	108.8	108.8	109	108.2	112.5	
C16-C15-O17	124.2	124.2	123.3	123.3	124.	124.4	123.7	123.7	124.6	124.0	123.0	124.3	123.2

parameters	***HF/6-31G(d,p)***				***b3lyp/6-31G(d)***				***b3lyp/6-31G(d,p)***			
	R1	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**
	Dihedral angles											
C1-C2-C3-C4	-0.054	-0.054	-0.220	0.220	-0.068	0.064	-0.376	0.378	0.055	-0.085	-0.278	0.102
C1-C2-C3-C10	-179.9	-179.9	179.5	-179.5	-179.7	179.8	179.7	-179.7	179.8	-179.7	179.6	-179.9
C1-C2-N7-C8	179.3	179.3	-179.0	179.0	179.6	-179.6	-179.2	179.2	-179.7	180	-179.2	-179.8
C1-C6-C5-C4	0.018	0.017	-0.096	0.096	-0.028	0.027	-0.140	0.143	0.016	-0.038	-0.114	0.023
C1-C6-C5-H21	180.0	180.0	179.9	-179.9	180.0	-180.0	179.9	-179.8	-180.0	180.0	179.9	180.0
C2-C1-C6-C5	-0.090	-0.092	0.152	-0.151	-0.060	0.062	0.161	-0.160	0.055	0.002	0.161	0.008
C2-C1-C6-H22	180.0	179.9	-180.0	180.0	180.0	-179.9	180.0	-180.0	-180.0	179.9	-180.0	-180.0
C2-C3-C4-C5	-0.02	-0.019	0.277	-0.277	-0.020	0.024	0.400	-0.398	0.014	0.050	0.327	-0.073
C2-C3-C4-H20	-179.9	-179.9	-179.8	179.8	-179.9	179.9	-179.7	179.7	179.9	-177.9	-179.8	180.0
C2-C3-C10-N9	0.461	0.461	-2.025	2.025	0.021	-0.032	-1.803	1.782	-0.064	-0.444	-1.799	0.177
C2-C3-C10-O18	-178.4	-178.4	179.2	179.2	-178.7	178.7	179.0	-179.0	178.7	-179.1	179.4	179.7
C2-N7-C8-N9	0.567	0.567	1.199	-1.199	0.156	-0.173	1.116	-1.114	0.050	-0.007	1.101	-0.842
C2-N7-C8-C11	-178.6	-178.6	-177.4	177.4	179.9	-179.9	177.3	177.3	179.1	177.7	-179.7	177.2
C3-C2-C1-C6	0.108	0.108	0.006	-0.007	0.108	-0.106	0.095	-0.099	-0.089	0.058	0.034	-0.069
C3-C2-C1-H19	-180.0	-180.0	179.9	-179.9	-180.0	-180.0	179.9	-179.9	180.0	180.0	179.9	180.0
C3-C2-N7-C8	-0.987	-0.987	1.893	-1.893	-0.651	0.628	1.684	-1.676	0.544	-0.263	1.643	-0.053
C3-C4-C5-C6	0.038	0.038	-0.117	0.117	0.068	-0.069	-0.140	0.316	-0.050	0.012	-0.130	0.010
C3-C4-C5-H21	-180.0	-179.9	179.9	-179.9	-180.0	179.9	179.9	-179.9	180.0	-180.0	179.9	-180.0
C3-C10-N9-C8	-0.894	-0.894	5.129	-5.129	-0.505	0.478	4.628	-4.597	0.650	0.206	4.548	-1.057

C3-C10-N9-N14	177.7	177.7	179.0	-179.0	178.0	-178.0	179.8	-179.8	-178.5	178.6	179.4	-177.6
C4-C3-C2-N7	-179.7	-179.7	178.9	-178.9	-179.8	179.8	178.7	-178.7	179.8	-179.9	178.9	-179.7
C4-C3-C10-N9	-179.4	-179.4	177.7	-177.7	-179.7	179.7	178.3	-178.3	179.6	180.0	178.1	-179.8
C4-C3-C10-O18	1.795	1.795	-1.102	1.101	1.579	-1.569	-0.927	0.913	-1.600	1.288	-0.745	-0.287
C4-C5-C6-H22	-180.0	-180.0	-180.0	180.0	-180.0	180.0	-180.0	180.0	-180.0	-180.0	-180.0	-180.0
C5-C4-C3-C10	179.8	179.8	-179.4	179.4	179.6	-179.7	-179.7	179.7	-179.7	179.6	-179.6	179.9
C5-C6-C1-H19	-180.0	180.0	-179.7	179.7	-180.0	180.0	-179.6	179.6	180.0	-179.9	-179.7	179.9
C6-C1-C2-N7	179.8	179.8	-179.2	179.2	179.8	-179.8	-179.0	179.0	-179.8	179.9	-179.2	179.7
C6-C5-C4-H20	180.0	179.9	-180.0	180.0	180.0	-179.9	179.9	-179.9	-179.9	180.0	-180.0	180.0
N7-C2-C1-H19	-0.287	-0.288	0.683	-0.683	-0.272	0.262	0.771	-0.771	0.243	-0.183	0.638	-0.220
N7-C2-C3-C10	0.434	0.434	-1.352	1.352	0.548	-0.511	-1.221	1.225	-0.523	0.502	-1.177	0.372
N7-C8-N9-C10	0.407	0.407	-4.989	4.988	0.443	-0.400	-4.519	4.497	-0.681	0.023	-4.455	1.470
N7-C8-N9-N14	-178.1	-178.1	178.7	178.7	-178.0	178.0	-179.5	179.5	178.5	-178.3	-179.2	177.9
N7-C8-C11-C12	82.27	82.27	-115.5	115.5	64.51	-64.55	-115.5	115.5	-74.24	24.11	32.91	28.42
N7-C8-C11-C13	-40.75	-40.75	113.7	113.7-	-58.59	58.59	114.1	114.1	48.70	-99.49	-90.39	-95.00
N7-C8-C11-H23	-159.7	-159.7	-0.600	0.600	-177.0	176.9	-0.398	0.399	167.7	142.6	152.2	148.1
C8-N9-C10-O18	178.0	178.0	-176.0	176	178.4	-178.4	-176.1	176.2	-178.2	179.0	-176.5	179.4
C8-N9-N14-C15	104.0	104.0	-118.8	118.8	91.90	-92.00	-117.1	117.1	-95.64	89.63	-120.7	114.1
C8-N9-N14-H30	-121.2	-121.2	105.1	-105.1	-133.3	133.3	104.8	-104.9	132.8	-139.4	102.1	-109.2
C8-C11-C12-H24	177.0	117.0	165.8	164.7	179.2	179.2	166.8	166.6	-179.3	178.3	178.5	178.7
C8-C11-C12-H25	56.68	56.68	47.70	46.31	59.40	59.49	48.48	47.95	60.89	58.58	58.75	58.93
C8-C11-C12-H26	-63.78	-63.78	-75.00	-76.03	-61.21	-61.04	-74.07	-74.36	-59.30	-61.44	-61.26	-61.00
C8-C11-C13-H27	-178.0	-178.0	-164.6	-165.8	-179.2	-179.3	-166.6	166.8	-178.2	-178.5	178.8	-179.2
C8-C11-C13-H28	61.91	61.91	76.04	75.00	61.04	61.19	74.37	74.06	62.45	02.29	59.45	61.46
C8-C11-C13-H29	-58.64	-58.64	-46.31	-47.7	-59.49	-59.42	-47.95	-48.49	-57.88	-58.68	-61.65	059.4
N9-C8-C11-C12	-96.93	-96.93	65.84	64.87	-115.8	115.8	66.05	-66.05	-132.2	-158.1	-147.8	-153.5
N9-C8-C11-C13	140.1	140.1	-64.87	-65.84	121.1	-121.2	-64.29	64.29	104.8	78.34	88.86	83.15
N9-C8-C11-H23	21.14	21.14	-179.2	179.2	2.75	-2.786	-178.8	178.8	-13.26	-39.59	-28.56	-33.8
N9-N14-C15-C16	158.6	158.6	21.15	-21.15	159.8	-159.8	19.99	-20.04	-158.0	157.8	21.15	-22.96
N9-N14-C15-O17	-23.10	-23.10	-161.3	161.3	-22.50	22.45	-162.5	162.5	24.10	-24.85	-160.8	160.0

C10-C3-C4-H20	-0.678	-0.068	0.447	-0.447	-0.218	0.200	0.259	-0.264	0.211	-0.314	0.286	-0.085
C10-N9-C8-C11	179.6	179.6	173.6	-173.6	-179.3	179.3	173.8	-173.9	-179.7	-177.8	176.3	-176.6
C10-N9-N14-C15	-74.58	-74.58	67.14	-67.14	-86.64	86.57	67.63	-67.59	83.58	-88.85	64.25	-69.26
C10-N9-N14-H30	60.18	60.18	-68.92	68.92	48.11	-48.19	-70.47	70.45	-47.94	42.09	-72.99	67.49
C11-C8-N9-N14	1.081	1.081	-0.115	0.115	2.266	-2.281	-1.148	1.164	-0.605	3.900	1.590	-0.188
C12-C11-C13-H27	60.02	60.02	63.31	63.01	58.57	58.43	-57.50	-56.97	59.51	57.91	55.54	57.40
C12-C11-C13-H28	-60.04	-60.04	-56.00	-56.20	-61.23	-61.11	61.56	62.15	-59.84	-61.27	-63.78	-61.99
C12-C11-C13-H29	179.4	179.4	-178.3	-178.9	78.2	178.3	-179.8	-179.5	179.8	177.8	175.1	177.1
C13-C11-C12-H24	-60.26	-60.26	-63.01	-63.31	-58.45	-58.56	-62.16	-61.55	-57.52	-58.9	-58.60	-58.79
C13-C11-C12-H25	179.4	179.4	178.9	178.3	-178.3	-178.2	179.5	179.8	-177.3	-178.7	-178.4	-178.6
C13-C11-C12-H26	58.94	58.94	56.21	56.00	61.09	61.23	56.96	57.50	62.49	61.33	61.63	61.47
N14-N9-C10-O18	-3.409	-3.409	-2.158	2.158	-3.100	3.119	-0.994	0.990	2.608	-2.583	-1.674	2.900
N14-C15-C16-H31	161.6	161.6	158.3	-158.3	151.1	90.93	155.9	-155.7	-158.0	159.4	154.0	-163.2
N14-C15-C16-H32	39.93	39.93	36.64	-36.64	29.10	-29.03	33.92	-33.71	-36.20	37.65	31.55	78.43
N14-C15-C16-H33	-79.67	-79.67	-83.87	83.87	-90.87	-151	-86.31	86.53	83.49	-81.96	-88.46	-41.72
C16-C15-N14-H30	25.31	25.31	158.1	-158.1	27.13	-27.12	158.7	-158.7	-28.44	29.25	159.4	-160.5
O17-C15-N14-H30	-156.3	-156.3	-24.36	24.36	-155.2	155.2	-23.84	23.86	153.6	-153.4	-22.58	22.48
O17-C15-C16-H31	-16.69	-16.69	-19.18	19.18	-26.54	-91.43	-21.41	21.6	19.84	-17.87	-23.90	13.63
O17-C15-C16-H32	-138.4	-138.4	-140.8	140.8	-148.6	148.6	-143.4	143.6	141.7	-139.6	-146.4	-104.7
O17-C15-C16-H33	102.0	102.0	98.70	-98.70	91.49	26.6	96.34	-96.13	-98.63	100.8	93.60	135.1
H19-C1-C6-H22	-0.006	-0.006	0.173	-0.173	0.005	-0.011	0.191	-0.19	0.009	0.023	0.193	-0.055
H20-C4-C5-H21	-0.032	-0.032	0.007	-0.007	-0.051	0.05	-0.048	0.046	0.047	-0.046	0.009	0.003
H21-C5-C6-H22	-0.034	-0.035	0.027	-0.027	-0.009	0.007	0.021	-0.019	0.008	0.020	0.034	-0.011
H23-C11-C12-H24	59.01	59.01	54.26	53.91	60.77	60.73	54.98	55.53	62.15	60.24	59.85	59.68
H23-C11-C12-H25	-61.33	-61.33	-63.82	-64.44	-59.08	-58.94	-63.36	-63.11	57.66	-59.52	-59.9	-60.12
H23-C11-C12-H26	178.21	178.2	173.5	173.2	-179.7	-179.5	174.1	174.6	-177.8	-179.5	-179.9	179.9
H23-C11-C13-H27	-59.20	-59.2	-53.91	-54.26	-60.73	-60.79	-55.52	-55.00	-60.34	-61.12	-63.67	-61.94
H23-C11-C13-H28	-179.3	-179.3	-173.2	-173.5	179.48	179.7	-174.6	-174.1	-179.7	179.7	177.0	178.7
H23-C11-C13-H29	60.19	60.19	64.44	63.82	58.95	59.05	63.11	63.35	59.98	58.74	55.92	57.79

Table (S6) Optimized ***geometrical*** parameters (bond lengths (Å) and bond angles (degrees) for **MAQ (50d)** R1-R4

For numbering of the atoms, see Figure 22 (Chapter 2).

parameters	***HF/6-31g(d)***				***B3LYP/6-31G(d,p)***				***RAM1***				***MNDO***				***PM3***			
	R1	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**
	bond lengths																			
C1-C2	1.400	1.400	1.399	1.399	1.410	1.410	1.409	1.409	1.418	1.417	1.417	1.417	1.425	1.423	1.422	1.423	1.405	1.404	1.403	1.404
C1-C6	1.373	1.373	1.373	1.373	1.385	1.385	1.386	1.386	1.385	1.386	1.386	1.386	1.397	1.398	1.399	1.398	1.385	1.386	1.386	1.385
C1-H19	1.074	1.074	1.073	1.074	1.085	1.085	1.085	1.085	1.101	1.101	1.101	1.101	1.091	1.091	1.091	1.091	1.097	1.096	1.097	1.097
C2-C3	1.391	1.390	1.389	1.390	1.414	1.414	1.412	1.412	1.418	1.416	1.416	1.417	1.424	1.424	1.424	1.424	1.405	1.405	1.405	1.405
C2-N7	1.384	1.384	1.384	1.384	1.382	1.382	1.383	1.383	1.397	1.399	1.398	1.397	1.399	1.400	1.401	1.400	1.416	1.417	1.417	1.416
C3-C4	1.398	1.398	1.398	1.398	1.405	1.405	1.405	1.405	1.403	1.402	1.403	1.403	1.421	1.420	1.420	1.421	1.401	1.399	1.399	1.400
C3-C10	1.459	1.459	1.460	1.460	1.457	1.457	1.460	1.460	1.470	1.477	1.476	1.471	1.479	1.485	1.485	1.480	1.470	1.477	1.477	1.471
C4-C5	1.372	1.372	1.372	1.372	1.385	1.385	1.386	1.386	1.387	1.388	1.387	1.387	1.398	1.399	1.400	1.398	1.385	1.386	1.386	1.385
C4-H20	1.073	1.073	1.073	1.073	1.085	1.085	1.085	1.085	1.102	1.103	1.103	1.103	1.091	1.091	1.091	1.091	1.097	1.097	1.097	1.097
C5-C6	1.401	1.401	1.401	1.401	1.408	1.408	1.407	1.407	1.402	1.401	1.401	1.402	1.414	1.413	1.413	1.414	1.398	1.397	1.397	1.398
C5-H21	1.075	1.075	1.074	1.074	1.085	1.085	1.085	1.085	1.100	1.100	1.100	1.100	1.090	1.090	1.091	1.090	1.095	1.095	1.095	1.095
C6-H22	1.075	1.075	1.075	1.075	1.086	1.086	1.086	1.086	1.101	1.101	1.101	1.102	1.091	1.091	1.091	1.091	1.096	1.095	1.096	1.096
C8-N7	1.268	1.268	1.268	1.269	1.298	1.298	1.297	1.297	1.317	1.315	1.316	1.317	1.310	1.309	1.308	1.309	1.311	1.309	1.308	1.311
C8-N9	1.386	1.387	1.394	1.392	1.393	1.393	1.404	1.404	1.430	1.431	1.432	1.430	1.421	1.422	1.427	1.425	1.432	1.436	1.439	1.435
C8-C11	1.491	1.493	1.495	1.493	1.486	1.486	1.490	1.490	1.490	1.492	1.491	1.491	1.492	1.492	1.492	1.492	1.481	1.481	1.481	1.481
N9-C10	1.394	1.395	1.399	1.398	1.416	1.416	1.428	1.428	1.434	1.440	1.437	1.434	1.450	1.455	1.457	1.453	1.446	1.454	1.456	1.449
N9-N14	1.376	1.375	1.376	1.377	1.397	1.397	1.394	1.394	1.369	1.359	1.361	1.365	1.372	1.367	1.368	1.372	1.449	1.446	1.454	1.451
C10-O18	1.199	1.199	1.197	1.197	1.227	1.227	1.221	1.221	1.245	1.239	1.241	1.243	1.226	1.222	1.222	1.225	1.223	1.217	1.217	1.221
C11-C23	1.390	1.390	1.390	1.390	1.402	1.402	1.405	1.405	1.398	1.398	1.399	1.399	1.415	1.415	1.416	1.414	1.396	1.395	1.396	1.396
C11-C27	1.388	1.388	1.390	1.390	1.403	1.403	1.404	1.404	1.399	1.398	1.399	1.398	1.415	1.416	1.415	1.415	1.395	1.397	1.395	1.396
N14- C15	1.390	1.389	1.389	1.389	1.409	1.409	1.403	1.403	1.440	1.418	1.421	1.435	1.453	1.441	1.447	1.455	1.453	1.448	1.448	1.452
N14-H30	0.997	0.998	1.000	1.000	1.016	1.016	1.016	1.016	1.013	1.004	1.009	1.014	1.021	1.016	1.020	1.024	0.998	0.998	1.002	1.000
C15-C16	1.507	1.507	1.508	1.508	1.514	1.514	1.512	1.512	1.506	1.508	1.499	1.499	1.524	1.524	1.521	1.521	1.504	1.505	1.499	1.501
C15- O17	1.189	1.190	1.191	1.191	1.212	1.212	1.215	1.215	1.238	1.240	1.242	1.240	1.223	1.224	1.227	1.226	1.216	1.217	1.219	1.217
C16-H28	1.086	1.084	1.080	1.080	1.096	1.096	1.093	1.093	1.117	1.116	1.120	1.118	1.109	1.109	1.109	1.110	1.099	1.098	1.099	1.098
C16-H29	1.084	1.085	1.082	1.082	1.094	1.094	1.094	1.094	1.117	1.118	1.117	1.118	1.109	1.109	1.110	1.108	1.098	1.099	1.098	1.098
C16-H31	1.080	1.080	1.083	1.083	1.090	1.090	1.090	1.090	1.118	1.118	1.117	1.119	1.109	1.109	1.108	1.107	1.098	1.098	1.098	1.105
C23-C24	1.383	1.384	1.384	1.384	1.392	1.392	1.392	1.392	1.394	1.395	1.395	1.394	1.406	1.407	1.405	1.406	1.391	1.391	1.391	1.390
C23-H36	1.074	1.073	1.073	1.073	1.084	1.084	1.084	1.084	1.100	1.103	1.101	1.100	1.091	1.091	1.091	1.091	1.095	1.096	1.096	1.101

C24-C25	1.387	1.386	1.384	1.384	1.396	1.396	1.396	1.396	1.395	1.395	1.395	1.395	1.406	1.405	1.406	1.405	1.391	1.391	1.391	1.391
C24-H35	1.075	1.075	1.075	1.075	1.086	1.086	1.086	1.086	1.100	1.100	1.100	1.100	1.090	1.091	1.091	1.091	1.095	1.095	1.095	1.095
C25-C26	1.384	1.385	1.386	1.386	1.396	1.396	1.395	1.395	1.395	1.395	1.396	1.395	1.405	1.406	1.406	1.406	1.391	1.392	1.391	1.391
C25-H34	1.075	1.075	1.075	1.075	1.086	1.086	1.086	1.086	1.100	1.100	1.100	1.100	1.090	1.090	1.090	1.090	1.100	1.095	1.095	1.095
C26-C27	1.385	1.385	1.383	1.383	1.394	1.394	1.394	1.394	1.395	1.395	1.394	1.395	1.406	1.405	1.406	1.406	1.395	1.390	1.391	1.391
C26-H33	1.075	1.075	1.075	1.075	1.086	1.086	1.086	1.086	1.100	1.100	1.100	1.100	1.091	1.091	1.091	1.091	1.095	1.095	1.095	1.095
C27-H32	1.073	1.074	1.072	1.072	1.084	1.084	1.082	1.082	1.101	1.100	1.101	1.100	1.091	1.091	1.091	1.091	1.096	1.096	1.096	1.095

parameters	***HF/6-31g(d)***				***B3LYP/6-31G(d,p)***				***RAM1***				***MNDO***				***PM3***			
	R1	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**
	bond angles																			
C1-C2-C3	118.9	119.0	119.1	119.1	118.6	118.6	118.8	118.8	118.5	118.7	118.7	118.5	120.3	120.5	120.6	120.4	120.2	120.4	120.4	120.3
C1-C2-N7	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.7	120.1	120.0	120.1	120.1	118.0	117.9	118.0	118.1	118.6	118.5	118.6	118.6
C1-C6-C5	121.1	121.1	121.0	121.0	120.8	120.8	120.8	120.8	121.1	121.0	121.0	121.1	120.5	120.4	120.4	120.5	120.7	120.6	120.6	120.7
C1-C6-H22	119.5	119.5	119.5	119.5	119.6	119.6	119.6	119.6	119.5	119.5	119.6	119.5	120.0	120.0	120.0	120.0	119.8	119.8	119.8	119.8
C2-C1-C6	119.8	119.8	119.7	119.7	120.1	120.1	120.1	120.1	119.9	119.8	119.8	119.8	119.5	119.4	119.4	119.4	119.2	119.2	119.2	119.2
C2-C1-H19	118.5	118.5	118.6	118.6	118.1	118.1	118.1	118.1	119.6	119.7	119.7	119.6	120.4	120.4	120.5	120.4	120.1	120.2	120.2	120.1
C2-C3-C4	120.9	120.9	120.9	120.9	120.8	120.8	120.7	120.7	120.8	120.6	120.6	120.7	118.9	118.8	118.8	118.9	119.7	119.5	119.5	119.7
C2-C3-C10	118.6	118.6	118.7	118.7	118.8	118.8	119.1	119.1	119.4	120.2	120.1	119.5	118.8	119.1	119.0	118.7	119.1	119.7	119.6	119.1
C2-N7-C8	119.4	119.5	119.8	119.8	119.3	119.3	119.7	119.7	119.6	119.1	119.2	119.6	121.3	121.2	121.3	121.4	121.3	121.0	121.1	121.4
C3-C2-N7	122.4	122.4	122.2	122.2	122.7	122.7	122.5	122.5	121.4	121.3	121.2	121.3	121.6	121.6	121.4	121.5	121.2	121.1	121.0	121.1
C3-C4-C5	119.7	119.7	119.6	119.6	119.7	119.7	119.7	119.7	119.7	119.8	119.8	119.7	120.3	120.4	120.3	120.3	119.7	119.8	119.8	119.7
C3-C4-H20	118.8	118.8	118.9	118.9	118.4	118.4	118.5	118.5	119.0	119.0	119.0	119.0	120.5	120.6	120.6	120.6	119.6	119.7	119.7	119.7
C3-C10-N9	114.0	113.9	114.2	114.2	113.7	113.7	113.9	113.9	116.5	115.6	115.8	116.4	114.9	114.4	114.3	114.8	116.2	115.6	115.9	116.2
C3-C10-O18	126.1	126.0	125.6	125.6	126.9	126.9	126.1	126.1	124.2	123.0	122.9	124.0	127.7	126.9	126.6	127.4	126.8	125.8	125.5	126.6
C4-C3-C10	120.5	120.5	120.4	120.4	120.4	120.4	120.2	120.2	119.8	119.3	119.3	119.7	122.3	122.1	122.2	122.4	121.2	120.8	120.9	121.2
C4-C5-C6	119.6	119.6	119.6	119.6	119.9	119.9	119.9	119.9	120.0	120.1	120.1	120.1	120.4	120.5	120.5	120.5	120.5	120.5	120.5	120.5
C4-C5-H21	120.4	120.4	120.4	120.4	120.2	120.2	120.1	120.1	120.1	120.1	120.1	120.1	120.0	119.9	119.9	119.9	119.9	119.8	119.8	119.8
C5-C4-H20	121.5	121.5	121.5	121.5	121.8	121.8	121.8	121.8	121.3	121.2	121.2	121.2	119.2	119.0	119.0	119.2	120.7	120.5	120.5	120.6
C5-C6-H22	119.4	119.4	119.4	119.4	119.6	119.6	119.6	119.6	119.4	119.4	119.4	119.4	119.5	119.6	119.6	119.5	119.5	119.6	119.6	119.5
C6-C1-H19	121.7	121.7	121.7	121.7	121.8	121.8	121.8	121.8	120.5	120.5	120.5	120.5	120.2	120.1	120.1	120.1	120.7	120.6	120.6	120.7
C6-C5-H21	120.0	120.0	120.0	120.0	119.9	119.9	119.9	119.9	119.8	119.9	119.8	119.8	119.6	119.6	119.6	119.6	119.7	119.7	119.7	119.7
N7-C8-N9	122.4	122.3	122.3	122.3	121.7	121.7	121.9	121.9	124.0	124.8	124.6	124.0	121.3	121.7	121.5	121.3	121.4	122.1	122.2	121.4
N7-C8-C11	118.5	118.3	117.6	117.6	118.3	118.3	117.4	117.4	118.0	117.8	117.9	117.9	117.8	117.2	117.1	117.6	118.8	118.7	118.7	118.4
C8-N9-C10	123.2	123.3	122.6	122.6	123.8	123.8	122.9	122.9	119.1	119.0	119.0	119.1	121.9	121.9	121.0	121.0	120.6	120.2	119.5	120.0
C8-N9-N14	120.0	120.9	119.6	119.6	120.8	120.8	119.9	119.9	119.4	121.5	120.9	119.4	116.3	122.5	121.8	115.7	118.0	119.8	118.6	117.2

C8-C11-C23	121.9	122.0	117.2	117.7	117.9	117.9	116.9	116.9	120.1	119.8	119.3	119.2	120.4	120.6	120.3	120.7	119.8	119.8	119.8	120.2
C8-C11-C27	118.4	118.2	123.5	122.8	122.7	122.7	124.2	124.2	119.4	119.5	120.3	120.3	120.5	120.4	120.7	120.3	119.8	119.9	119.8	119.5
N9-C8-C11	119.1	119.3	120.0	119.8	120.0	120.0	120.7	120.7	118.0	117.3	117.5	118.0	120.8	121.1	121.3	121.1	119.8	119.1	119.1	120.1
N9-C10-O18	119.9	120.0	120.2	120.1	119.4	119.4	120.0	120.0	119.3	121.3	121.2	119.6	117.4	118.7	119.0	117.7	116.9	118.6	118.6	117.2
N9-N14-C15	116.3	117.1	121.4	120.7	115.9	115.9	122.0	122.0	120.4	123.7	122.5	120.5	118.7	120.6	120.0	119.3	119.0	120.0	118.2	117.8
N9-N14-H30	111.8	111.7	113.9	113.2	109.3	109.3	114.1	114.1	108.9	112.4	113.0	110.6	110.4	112.5	112.6	111.0	108.5	109.1	110.3	110.0
C10-N9-N14	115.8	115.7	117.0	116.8	114.8	114.9	116.4	116.4	121.1	119.1	119.7	121.4	121.8	115.6	115.4	121.7	120.4	118.0	117.4	120.3
C11-C23-C24	120.2	119.9	120.5	120.4	120.4	120.2	120.7	120.7	119.5	119.5	119.6	119.6	120.4	120.3	120.4	120.4	119.6	119.6	119.6	119.7
C11-C23-H36	120.2	120.1	119.3	119.4	118.8	120.1	118.7	118.7	120.3	120.1	120.2	120.2	120.6	120.6	120.6	120.6	119.6	120.2	120.4	120.2
C11-C27-C26	120.2	120.2	120.3	120.2	120.2	120.4	120.3	120.3	119.5	119.5	119.7	119.5	120.3	120.4	120.4	120.4	119.5	119.7	119.6	119.6
C11-C27-H32	119.4	119.5	120.6	120.4	120.1	118.8	120.5	120.5	120.2	120.2	120.3	120.4	120.6	120.6	120.6	120.6	120.3	120.4	120.3	120.4
N14-C15-C16	113.7	113.7	118.4	117.4	113.2	113.2	117.6	117.6	114.6	114.7	120.0	120.0	115.2	114.8	119.8	120.5	115.5	115.3	120.7	120.6
N14-C15-O17	121.7	122.0	118.5	118.7	121.9	121.9	118.5	118.5	122.8	122.7	116.3	116.6	119.7	120.0	115.7	115.3	119.4	119.8	114.2	114.4
C15-N14-H30	116.1	115.3	112.3	112.0	114.9	114.9	112.2	112.2	111.2	116.5	115.1	112.2	111.6	114.3	113.7	111.8	113.2	114.4	115.2	114.7
C15-C16-H28	109.0	111.6	107.8	107.8	109.2	109.2	113.2	113.2	110.1	111.2	110.2	109.0	110.5	111.0	110.8	110.4	110.9	111.7	111.1	111.2
C15-C16-H29	111.5	108.7	113.3	110.2	111.9	111.9	108.0	108.0	110.8	110.0	108.9	109.7	111.3	110.9	110.5	111.1	111.4	110.7	111.2	111.0
C15-C16-H31	108.9	109.0	108.5	111.5	108.8	108.8	108.4	108.4	108.6	108.4	110.2	110.8	110.8	110.7	111.8	111.7	111.4	111.4	111.3	111.5
C16-C15-O17	124.5	124.2	123.0	123.8	124.8	124.8	123.9	123.9	122.4	122.4	123.5	123.2	124.9	124.9	124.2	123.9	124.9	124.8	124.9	124.8
C23-C11-C27	119.5	119.7	119.1	119.3	119.2	119.2	118.8	118.8	120.5	120.6	120.4	120.5	119.0	118.9	118.9	118.9	120.4	120.3	120.4	120.2
C23-C24-C25	120.1	120.3	120.0	120.0	120.1	120.1	120.1	120.1	120.2	120.2	120.2	120.2	120.2	120.3	120.2	120.3	120.2	120.2	120.2	120.1
C23-C24-H35	119.8	119.6	119.7	119.7	119.7	119.7	119.7	119.7	119.8	119.7	119.7	119.8	119.8	119.7	119.8	119.7	119.8	119.7	119.8	119.8
C24-C23-H36	119.6	120.0	120.2	120.3	120.9	120.9	120.6	120.6	120.2	120.5	120.3	120.2	119.0	119.0	119.0	119.0	120.0	120.2	120.0	120.0
C24-C25-C26	119.9	119.9	119.8	119.9	119.8	119.8	119.7	119.7	120.1	120.1	120.1	120.1	119.8	119.7	119.7	119.7	120.1	120.1	120.1	120.0
C24-C25-H34	120.0	120.0	120.2	120.1	120.2	120.2	120.2	120.2	119.9	120.0	120.0	120.0	120.1	120.2	120.1	120.1	120.1	120.0	119.9	120.0
C25-C24-H35	120.2	120.1	120.3	120.2	120.2	120.2	120.2	120.2	120.1	120.1	120.1	120.1	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0
C25-C26-C27	120.1	120.0	120.2	120.2	120.3	120.3	120.4	120.4	120.2	120.1	120.1	120.2	120.3	120.2	120.2	120.3	120.2	120.2	120.2	120.2
C25-C26-H33	120.2	120.2	120.2	120.2	120.1	120.1	120.2	120.2	120.1	120.1	120.1	120.1	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0
C26-C25-H34	120.1	120.1	120.0	120.0	120.1	120.1	120.1	120.1	120.0	119.9	119.9	120.0	120.1	120.1	120.1	120.1	120.0	119.9	120.0	120.0
C26-C27-H32	120.5	120.3	119.0	119.4	119.8	119.8	119.2	119.2	120.3	120.3	120.0	120.1	119.1	119.0	119.0	119.0	120.1	119.9	120.1	120.0
C27-C26-H33	119.7	119.8	119.6	119.6	119.6	119.6	119.4	119.4	119.7	119.8	119.8	119.7	119.7	119.8	119.7	119.7	119.7	119.8	119.8	119.8
H28-C16-H29	108.5	108.5	110.0	109.0	108.2	108.2	108.1	108.1	109.2	109.2	109.3	109.0	108.6	108.6	107.6	107.4	107.9	107.9	107.6	107.4
H28-C16-H31	109.1	109.9	108.8	109.7	108.7	108.7	108.8	108.8	109.0	109.1	109.1	109.2	107.8	107.7	108.7	107.3	107.5	107.6	108.0	107.6
H29-C16-H31	109.9	109.1	108.3	108.5	109.9	109.9	110.2	110.2	109.0	108.9	109.2	109.1	107.7	107.8	107.3	108.7	107.6	107.8	107.5	108.0

parameters	*HF/6-31g(d)*				*B3LYP/6-31G(d,p)*				*RAM1*				*MNDO*				*PM3*			
	R1	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**
	Dihedral angles																			
C1-C2-C3-C4	0.248	0.037	-0.311	-0.012	-0.001	0.002	-0.253	0.253	0.118	-0.201	-0.331	0.068	0.167	-0.125	-0.175	0.304	0.231	-0.247	-0.477	0.408
C1-C2-C3-C10	178.5	178.9	-179.5	-178.9	177.7	-177.7	-178.8	178.8	179.2	-179.6	179.9	-179.9	179.9	-179.9	-179.6	180.0	179.5	-179.5	-180.0	-180.0
C1-C2-N7-C8	180.0	179.2	-178.9	-180.0	-179.6	179.6	-179.4	179.4	-179.1	178.9	179.3	179.9	-178.2	177.3	-177.1	177.6	-179.4	179.2	-179.5	178.8
C1-C6-C5-C4	-0.084	-0.075	-0.032	0.080	-0.169	0.169	0.030	-0.030	-0.045	0.008	-0.100	0.012	0.019	-0.010	-0.002	0.057	0.013	-0.011	-0.123	0.116
C1-C6-C5-H21	-180.0	179.9	179.9	-179.9	179.9	-179.9	-180.0	180.0	180.0	179.9	179.9	-179.9	-179.9	179.9	-180.0	-180.0	-179.9	180.0	179.9	-179.9
C2-C1-C6-C5	0.035	-0.069	0.121	-0.072	0.075	-0.075	0.076	-0.076	-0.020	0.035	0.010	-0.021	0.027	-0.041	0.091	-0.084	-0.043	0.055	0.131	-0.124
C2-C1-C6-H22	-180.0	179.9	-179.9	-180.0	180.0	-180.0	-179.9	179.9	-180.0	179.9	180.0	-180.0	-179.9	179.9	-179.9	180.0	-180.0	180.0	-179.9	180.0
C2-C3-C4-C5	-0.298	-0.181	0.401	0.020	-0.091	-0.181	0.359	-0.359	-0.184	0.246	0.245	-0.078	-0.122	0.074	0.264	-0.331	-0.260	0.290	0.484	-0.415
C2-C3-C4-H20	179.6	179.9	-179.6	-179.9	179.6	-179.6	-179.6	179.6	179.8	-179.7	-179.8	179.9	179.8	-179.8	-179.9	179.8	179.7	-179.7	-179.6	179.7
C2-C3-C10-N9	2.880	2.344	-3.475	-0.558	2.550	-2.548	-3.161	3.161	1.142	-1.549	1.230	0.912	-2.309	3.583	-8.360	7.054	2.242	-2.824	-4.919	5.232
C2-C3-C10-O18	-177.6	-175.7	177.1	178.3	-177.5	177.5	177.0	-177.0	179.3	-179.8	-177.0	-178.9	176.7	-175.8	173.3	-174.5	179.9	179.6	178.3	-176.6
C2-N7-C8-N9	0.048	1.344	0.429	-1.683	1.132	-1.132	-0.026	0.026	-1.356	3.077	0.436	-1.020	-0.828	1.147	2.875	-2.943	-2.685	3.496	4.217	-3.261
C2-N7-C8-C11	-178.9	-179.9	-177.8	179.7	-177.5	177.5	-178.5	178.5	-179.8	-179.3	-178.9	179.5	-179.9	179.3	-178.3	177.7	179.7	179.9	-178.3	178.5
C3-C2-C1-C6	-0.116	0.087	0.050	0.037	0.009	-0.010	0.036	-0.036	-0.016	0.061	0.203	-0.018	-0.120	0.109	0.000	-0.098	-0.079	0.075	0.170	-0.139
C3-C2-C1-H19	179.8	179.8	-179.9	-179.7	179.8	-179.8	-179.9	179.9	-180.0	179.9	-179.8	-179.9	180.0	-180.0	180.0	179.9	-179.9	180.0	-180.0	179.9
C3-C2-N7-C8	0.755	-0.530	1.362	-0.768	1.552	-1.550	0.503	-0.503	1.094	-0.909	-0.650	-0.332	2.061	-3.110	3.668	-3.345	0.447	-0.649	1.300	-1.886
C3-C4-C5-C6	0.212	0.198	-0.226	-0.053	0.175	-0.175	-0.245	0.245	0.146	-0.147	-0.027	0.038	0.030	-0.007	-0.178	0.155	0.140	-0.164	-0.188	0.156
C3-C4-C5-H21	-179.9	-179.8	179.8	180.0	-179.9	179.9	179.8	-179.8	-179.9	179.9	179.9	180.0	180.0	-180.0	179.8	-179.8	-179.9	179.9	179.8	-179.8
C3-C10-N9-C8	-2.252	-1.679	5.346	-1.777	-0.065	0.065	3.755	-3.755	-1.345	3.425	-1.43	-2.135	3.572	-5.581	14.80	-13.25	-4.406	5.504	10.06	-10.16
C3-C10-N9-N14	-171.3	-177.2	174.5	178.6	-171.5	171.5	173.7	-173.7	-174.5	176.5	171.8	-178.8	-176.0	173.6	179.8	-178.7	-172.7	169.6	165.8	-171.6
C4-C3-C2-N7	179.5	179.7	179.5	-179.2	178.8	-178.8	179.8	-179.8	179.9	179.6	179.6	-179.7	179.9	-179.7	179.0	-178.7	-179.6	179.6	178.8	-178.9
C4-C3-C10-N9	-178.9	-178.8	177.4	-179.5	-179.7	179.7	178.2	-178.2	-179.8	179.0	-178.6	-179.1	177.4	-176.2	172.2	-173.3	-178.5	178.0	175.6	-175.2
C4-C3-C10-O18	0.615	3.170	-2.095	-0.581	0.181	-0.181	-1.559	1.559	-1.630	0.762	3.183	1.135	-3.613	4.446	-6.154	5.152	-0.790	0.347	-1.163	3.039
C4-C5-C6-H22	179.9	180.0	-180.0	180.0	179.9	-179.9	-180.0	180.0	179.9	-179.9	179.9	180.0	180.0	-180.0	-180.0	-180.0	179.9	-179.9	179.9	-180.0
C5-C4-C3-C10	-178.5	-179.0	179.5	178.9	-177.8	177.8	178.9	-178.9	-179.3	179.7	-180.0	179.9	-179.8	179.8	179.7	-180.0	-179.6	179.5	180.0	180.0
C5-C6-C1-H19	-179.9	-179.8	-179.9	179.7	-179.7	179.7	-180.0	180.0	179.9	-179.8	-179.9	179.9	179.9	-179.9	-179.9	179.9	179.8	-179.8	-179.7	179.8
C6-C1-C2-N7	-179.4	-179.6	-179.7	179.3	-178.9	178.9	180.0	-180.0	-179.8	-179.8	-179.7	179.7	-179.9	179.7	-179.2	179.0	179.8	-179.8	-179.1	179.2
C6-C5-C4-H20	-179.6	-179.9	179.8	179.8	-179.5	179.5	179.8	-179.8	-179.8	179.8	-180.0	-179.9	-179.9	179.9	180.0	180.0	-179.9	179.8	179.9	-180.0

N7-C2-C1-H19	0.581	0.115	0.298	-0.526	0.924	-0.922	0.037	-0.037	0.253	0.021	0.246	-0.176	0.216	-0.390	0.788	-0.987	-0.119	0.088	0.786	-0.731
N7-C2-C3-C10	-2.295	-1.394	0.313	1.872	-3.457	3.454	1.229	-1.229	-1.017	0.246	-0.212	0.341	-0.352	0.520	-0.477	0.921	-0.282	0.408	-0.732	0.692
N7-C8-N9-C10	0.836	-0.169	-4.062	3.067	-1.886	1.886	-2.292	2.292	1.530	-4.469	0.66	2.319	-2.125	3.436	-12.71	11.73	4.794	-6.105	-10.17	9.538
N7-C8-N9-N14	169.4	175.2	-172.9	-177.3	169.1	-169.1	-171.9	171.9	174.8	-177.4	-172.5	179.1	177.5	-175.7	-176.8	178.0	173.4	-169.9	-165.6	171.5
N7-C8-C11-C23	127.2	122.7	45.19	45.37	-39.91	39.92	37.43	-37.43	116.4	105.7	60.44	61.75	93.9	81.6	92.70	81.29	93.0	73.3	92.57	102.9
N7-C8-C11-C27	-48.65	-53.18	-130.8	-130.3	135.4	-135.4	-138.6	138.6	-61.87	-71.63	-117.2	-116.5	-83.88	-94.55	-83.60	-96.16	-85.12	-104.5	-85.44	-75.09
C8-N9-C10-O18	178.2	176.5	-175.2	179.3	-180.0	180.0	-176.4	176.4	-179.6	-178.3	176.9	177.7	-175.5	173.8	-166.7	168.1	177.7	-176.7	-172.9	171.5
C8-N9-N14-C15	-91.06	110.2	-124.0	106.6	-81.44	81.45	-125.0	125.0	-92.41	82.86	-101.6	97.46	-108.7	81.36	-84.31	121.8	-96.19	78.22	-104.2	112.4
C8-N9-N14-H30	132.4	-113.7	96.59	-116.6	146.7	-146.7	94.91	-94.91	137.49	-65.93	43.10	-129.0	120.64	-58.35	53.66	-106.0	132.51	-56.55	31.36	-113.5
C8-C11-C23-C24	-175.9	-176.3	-177.4	-177.2	176.6	-176.6	-177.5	177.5	-178.4	-177.8	-178.5	-178.7	-178.3	-177.5	-177.6	-178.4	-178.6	-178.5	-178.7	-178.7
C8-C11-C23-H36	3.203	2.388	2.334	2.403	-3.362	3.362	2.211	-2.211	1.514	2.068	1.029	0.639	1.341	2.037	1.974	1.191	0.970	1.158	0.667	0.639
C8-C11-C27-C26	176.9	177.4	176.2	176.0	-175.7	175.7	176.4	-176.4	178.6	178.1	178.2	178.5	178.4	177.5	177.6	178.3	178.6	178.4	178.7	178.2
C8-C11-C27-H32	-3.176	-2.295	-2.902	-3.239	3.418	-3.417	-2.526	2.526	-1.385	-1.089	-1.688	-1.595	-1.397	-1.899	-1.976	-1.359	-1.388	-0.589	-0.912	-1.428
N9-C8-C11-C23	-51.72	-58.54	-133.0	-133.3	141.4	-141.4	-141.1	141.1	-62.17	-76.46	-119.0	-117.8	-85.17	-100.2	-88.44	-98.05	-84.62	-110.2	-89.87	-75.35
N9-C8-C11-C27	132.4	125.6	50.93	51.05	-43.25	43.26	42.94	-42.94	119.6	106.2	63.38	64.00	97.09	83.66	95.27	84.51	97.22	72.06	92.12	106.7
N9-N14-C15-C16	-162.2	157.6	21.23	-23.10	-162.0	162.0	21.98	-21.98	-166.7	-178.7	-24.39	-26.76	-165.0	-175.0	-39.67	-34.06	-162.6	-173.2	-29.80	-26.68
N9-N14-C15-O17	19.67	-24.39	-161.1	160.1	20.38	-20.38	-160.7	160.7	18.217	5.140	160.7	158.5	20.289	10.160	147.0	152.1	21.274	10.361	154.6	157.9
C10-N9-C8-C11	179.8	-178.9	174.1	-178.3	176.8	-176.8	176.1	-176.1	180.0	177.9	-180.0	-178.2	176.9	-174.7	168.5	-169.0	-177.6	177.5	172.4	-172.3
C10-N9-N14-C15	78.34	-74.10	66.47	-73.74	90.30	-90.30	64.75	-64.75	80.73	-90.01	85.35	-85.88	70.96	-97.80	110.8	-72.05	72.43	-85.93	99.83	-85.66
C10-N9-N14-H30	-58.16	61.94	-72.90	63.05	-41.51	41.52	-75.33	75.33	-49.36	121.19	-130.0	47.71	-59.72	122.50	-111.2	60.22	-58.88	139.30	-124.6	48.44
C11-C8-N9-N14	-11.66	-3.576	5.206	1.293	-12.27	12.27	6.555	-6.555	-6.735	4.997	6.862	-1.450	-3.495	6.204	4.404	-2.668	-9.008	13.700	16.95	-10.34
C11-C23-C24-C25	-0.785	-0.563	1.168	1.258	-0.915	0.915	0.987	-0.987	-0.095	0.591	0.457	0.249	0.190	0.591	0.462	0.361	0.167	0.367	0.226	-0.169
C11-C23-C24-H35	179.2	179.2	-179.2	-179.2	179.2	-179.2	-179.2	179.2	179.8	179.6	-179.8	-180.0	-180.0	-179.8	-179.7	-179.8	179.9	-180.0	-179.8	179.9
C11-C27-C26-C25	-1.038	-1.156	0.790	0.781	-0.527	0.527	0.609	-0.609	-0.340	-0.544	-0.083	-0.017	-0.270	-0.479	-0.501	-0.267	-0.198	-0.174	-0.249	-0.317
C11-C27-C26-H33	179.3	179.4	-179.4	-179.4	179.2	-179.2	-179.4	179.4	179.8	-180.0	179.8	179.9	179.9	179.9	179.6	179.8	180.0	-179.7	179.8	179.9
N14-N9-C10-O18	9.201	0.932	-6.003	-0.377	8.556	-8.554	-6.499	6.499	7.253	-5.208	-9.917	0.988	4.866	-6.993	-1.692	2.677	9.369	-12.62	-17.23	10.05
N14-C15-C16-H28	77.68	40.92	153.3	-168.2	82.85	-82.73	-86.97	86.97	68.02	58.66	-50.77	-166.6	71.81	65.35	-56.83	-165.6	68.33	58.10	-53.70	-167.1
N14-C15-C16-H29	-42.02	-78.75	31.30	72.88	-37.01	37.13	32.97	-32.97	-52.93	-62.38	-170.6	74.10	-49.01	-55.50	-176.0	75.39	-51.88	-62.09	-173.5	73.40
N14-C15-C16-H31	-163.4	162.4	-89.10	-47.73	-158.6	158.7	155.2	-155.2	-172.7	178.6	69.63	-46.46	-168.8	-175.2	64.62	-46.17	-172.0	178.4	66.65	-47.01
C16-C15-N14-H30	-27.55	23.16	161.2	-160.4	-32.81	32.81	162.8	-162.8	-37.68	-31.11	-168.4	-159.7	-34.91	-35.95	-177.2	-166.0	-33.42	-40.65	-163.3	-158.7
O17-C15-N14-H30	154.3	-158.9	-21.15	22.83	149.5	-149.5	-19.88	19.88	147.3	152.8	16.73	25.62	150.4	149.2	9.438	20.232	150.5	142.9	21.04	25.90
O17-C15-C16-H28	-104.2	-137.0	-24.27	8.414	-99.56	99.69	95.82	-95.83	-116.9	-125.2	123.7	7.705	-113.8	-120.1	115.9	7.682	-115.8	-125.7	121.4	7.778

O17-C15-C16-H29	136.1	103.3	-146.3	-110.5	140.6	-140.5	-144.2	144.2	122.1	113.7	3.908	-111.6	125.4	119.1	-3.226	-111.4	124.0	114.1	1.651	-111.7
O17-C15-C16-H31	14.69	-15.49	93.35	128.9	18.97	-18.85	-21.97	21.97	2.404	-5.272	-115.9	127.9	5.569	-0.583	-122.6	127.1	3.860	-5.359	-118.2	127.8
C23-C11-C27-C26	0.957	1.417	0.255	0.377	-0.409	0.409	0.489	-0.489	0.400	0.781	0.610	0.340	0.605	1.245	1.238	0.830	0.478	0.677	0.694	0.209
C23-C11-C27-H32	-179.2	-178.2	-178.9	-178.8	178.7	-178.7	-178.4	178.4	-179.6	-178.4	-179.3	-179.8	-179.2	-178.1	-178.3	-178.9	-179.5	-178.3	-178.9	-179.4
C23-C24-C25-C26	0.707	0.827	-0.113	-0.091	-0.028	0.028	0.125	-0.125	0.155	0.202	0.065	0.070	0.153	0.195	0.294	0.215	0.110	0.132	0.216	0.063
C23-C24-C25-H34	-179.5	-179.6	179.7	179.6	-179.8	179.8	179.9	-179.9	-180.0	179.8	180.0	180.0	180.0	179.9	-179.9	-179.9	179.9	179.8	-179.8	-179.9
C24-C23-C11-C27	-0.047	-0.557	-1.233	-1.396	1.129	-1.129	-1.287	1.287	-0.183	-0.526	-0.796	-0.456	-0.565	-1.299	-1.219	-0.877	-0.463	-0.773	-0.683	0.033
C25-C24-C23-H36	-179.9	-179.3	-178.6	-178.3	179.1	-179.1	-178.7	178.7	180.0	-179.9	-179.0	-179.1	-179.5	-179.0	-179.1	-179.2	-179.4	-179.3	-179.1	179.0
C25-C26-C27-H32	179.1	178.5	179.9	180.0	-179.6	179.6	179.5	-179.5	179.7	178.7	179.9	-179.9	179.5	178.9	179.1	179.4	179.8	178.8	179.4	179.3
C26-C25-C24-H35	-179.3	-179.0	-179.7	-179.6	179.9	-179.9	-179.7	179.7	-179.7	-179.4	-179.7	-179.7	-179.7	-179.4	-179.5	-179.6	-179.7	-179.5	-179.7	180.0
C27-C26-C25-H34	-179.6	-179.5	179.4	179.3	-179.5	179.5	179.3	-179.3	-179.8	-179.6	179.8	179.9	-179.9	-179.9	179.9	179.9	-179.9	-179.9	179.9	-179.8
H19-C1-C6-H22	0.088	0.121	0.029	-0.194	0.200	-0.200	-0.011	0.011	-0.034	0.135	0.020	-0.073	-0.025	0.022	0.072	-0.086	-0.103	0.090	0.198	-0.116
H20-C4-C5-H21	0.247	0.140	-0.153	-0.14	0.392	-0.393	-0.242	0.242	0.136	-0.103	-0.021	0.042	0.062	-0.062	-0.019	0.008	0.100	-0.120	-0.081	0.072
H21-C5-C6-H22	0.035	-0.022	0.007	-0.031	-0.017	0.017	0.039	-0.039	-0.059	0.038	-0.025	0.000	0.020	-0.020	0.048	0.000	-0.022	0.027	-0.033	0.009
H32-C27-C26-H33	-0.612	-0.957	-0.313	-0.218	0.127	-0.127	-0.487	0.487	-0.187	-0.785	-0.312	0.078	-0.327	-0.719	-0.791	-0.475	-0.014	-0.750	-0.571	-0.557
H33-C26-C25-H34	0.113	-0.042	-0.420	-0.457	0.717	-0.717	-0.619	0.619	0.051	-0.124	0.001	-0.057	-0.112	-0.285	-0.235	-0.203	-0.062	-0.296	-0.213	-0.007
H34-C25-C24-H35	0.526	0.575	0.067	0.125	0.111	-0.111	0.046	-0.046	0.180	0.243	0.224	0.227	0.150	0.224	0.270	0.211	0.150	0.119	0.216	0.013
H35-C24-C23-H36	0.085	0.485	1.005	1.18	-0.792	0.791	1.100	-1.100	-0.158	-0.304	0.726	0.689	0.341	0.656	0.745	0.643	0.344	0.361	0.812	-0.897

Table (S7) Optimized geometrical parameters (bond lengths (Å) and bond angles (degrees) for MAQ (50e) R1-R4. For numbering of the atoms, see Figure22 (Chapter 2)

parameters	*RHF/6-31G(d,p)*				*b3lyp/6-31G(d,p)*				*x-ray*
	R1	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	
	bond lengths								
C1-C2	1.400	1.400	1.399	1.398	1.410	1.409	1.408	1.408	1.394
C1-C6	1.373	1.372	1.373	1.374	1.385	1.385	1.386	1.386	1.368
C1-H19	1.074	1.074	1.074	1.074	1.085	1.085	1.085	1.085	
C2-C3	1.391	1.392	1.391	1.391	1.414	1.414	1.413	1.413	1.399
C2-N7	1.385	1.385	1.385	1.387	1.385	1.385	1.387	1.388	1.396
C3-C4	1.398	1.398	1.398	1.398	1.405	1.405	1.405	1.404	1.394
C3-C10	1.460	1.459	1.461	1.462	1.457	1.457	1.461	1.462	1.447
C4-C5	1.371	1.371	1.372	1.372	1.385	1.385	1.385	1.386	
C4-H20	1.074	1.074	1.074	1.074	1.085	1.085	1.085	1.085	1.385
C5-C6	1.400	1.401	1.400	1.400	1.408	1.408	1.407	1.407	
C5-H21	1.075	1.075	1.075	1.075	1.085	1.085	1.085	1.085	
C6-H22	1.076	1.076	1.076	1.076	1.086	1.086	1.086	1.086	
N7-C8	1.268	1.268	1.267	1.267	1.295	1.295	1.293	1.293	1.287
C8-N9	1.383	1.384	1.391	1.388	1.390	1.392	1.400	1.396	1.381
C8-C11	1.499	1.499	1.500	1.502	1.499	1.498	1.500	1.502	1.520
N9-C10	1.391	1.391	1.394	1.396	1.413	1.414	1.420	1.423	
N9-N14	1.377	1.375	1.372	1.379	1.398	1.396	1.389	1.398	
C10-O18	1.199	1.200	1.198	1.196	1.227	1.228	1.223	1.221	1.218
C11-H28	1.083	1.083	1.083	1.084	1.094	1.094	1.094	1.095	
C11-H29	1.079	1.079	1.079	1.079	1.089	1.089	1.089	1.089	
C11-H31	1.084	1.084	1.083	1.082	1.094	1.094	1.094	1.093	
N14-C15	1.392	1.386	1.384	1.397	1.410	1.404	1.397	1.413	1.372
N14-H30	0.997	0.994	0.998	1.000	1.018	1.014	1.014	1.018	
C15-C16	1.494	1.494	1.501	1.496	1.494	1.495	1.499	1.494	1.498

C15-O17	1.192	1.193	1.193	1.192	1.218	1.219	1.219	1.218	1.219
C16-C23	1.390	1.390	1.388	1.388	1.402	1.401	1.401	1.401	
C16-C27	1.390	1.390	1.390	1.391	1.403	1.403	1.402	1.403	
C23-C24	1.382	1.382	1.385	1.385	1.392	1.392	1.395	1.395	
C23-H32	1.074	1.074	1.073	1.073	1.084	1.085	1.084	1.083	
C24-C25	1.387	1.387	1.385	1.384	1.397	1.398	1.396	1.395	
C24-H33	1.075	1.075	1.075	1.075	1.086	1.086	1.086	1.086	
C25-C26	1.385	1.385	1.386	1.386	1.396	1.396	1.397	1.397	
C25-H34	1.076	1.076	1.076	1.076	1.086	1.086	1.086	1.086	
C26-C27	1.384	1.385	1.383	1.382	1.394	1.395	1.393	1.391	
C26-H35	1.075	1.075	1.075	1.075	1.086	1.086	1.086	1.086	
C27-H36	1.075	1.076	1.075	1.073	1.085	1.087	1.085	1.084	

parameters	***RHF/6-31G(d,p)***				***b3lyp/6-31G(d,p)***				
	R1	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**	
	bond angles								
C1-C2-C3	118.9	118.8	119.0	119.0	118.6	118.6	118.7	118.8	119.1
C1-C2-N7	118.7	118.7	118.7	118.7	118.7	118.6	118.6	118.6	
C1-C6-C5	121.1	121.1	121.1	121.0	120.8	120.8	120.8	120.8	121.7
C1-C6-H22	119.5	119.5	119.5	119.5	119.6	119.6	119.6	119.6	
C2-C1-C6	119.9	119.9	119.8	119.8	120.2	120.2	120.1	120.1	
C2-C1-H19	118.5	118.5	118.5	118.6	118.0	118.0	118.1	118.1	
C2-C3-C4	120.9	120.9	120.9	120.9	120.8	120.8	120.7	120.7	119.8
C2-C3-C10	118.7	118.7	118.9	118.9	118.9	118.9	119.3	119.3	119.7
C2-N7-C8	119.0	119.1	119.2	119.1	118.8	118.8	118.9	118.7	126.8
C3-C2-N7	122.5	122.5	122.3	122.3	122.8	122.8	122.6	122.6	
C3-C4-C5	119.7	119.7	119.7	119.7	119.7	119.8	119.8	119.8	
C3-C4-H20	118.7	118.7	118.8	118.7	118.4	118.4	118.4	118.4	
C3-C10-N9	113.5	113.6	113.8	113.6	113.3	113.2	113.3	113.1	
C3-C10-O18	126.3	126.2	125.8	126.0	127.2	127.0	126.5	126.6	

C4-C3-C10	120.4	120.4	120.3	120.3	120.3	120.3	120.0	120.0	
C4-C5-C6	119.6	119.6	119.6	119.6	119.9	119.9	119.9	119.9	118.8
C4-C5-H21	120.4	120.4	120.4	120.4	120.2	120.2	120.2	120.1	
C5-C4-H20	121.6	121.6	121.6	121.6	121.8	121.8	121.8	121.8	
C5-C6-H22	119.4	119.4	119.4	119.5	119.6	119.6	119.6	119.6	
C6-C5-H21	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	
N7-C8-N9	122.6	122.5	122.8	122.8	122.0	122.0	122.5	122.6	122.4
N7-C8-C11	119.9	120.1	119.7	119.5	120.1	120.3	119.9	119.7	120.8
C8-N9-C10	123.7	123.7	123.0	123.1	124.1	124.2	123.4	123.4	124.1
C8-N9-N14	119.7	120.0	119.1	118.8	120.7	120.7	119.3	118.8	120.5
C8-C11-H28	111.1	110.2	110.9	110.4	111.2	110.1	111.2	111.0	116.7
C8-C11-H29	107.8	107.8	107.6	107.6	107.9	108.0	107.8	107.8	
C8-C11-H31	110.4	111.0	111.1	112.1	110.3	111.1	111.4	112.1	
N9-C8-C11	117.5	117.5	117.6	117.7	117.9	117.7	117.6	117.7	
N9-C10-O18	120.2	120.2	120.4	120.4	119.5	119.8	120.1	120.3	120.3
N9-N14-C15	116.0	117.5	124.9	121.0	116.4	117.9	126.1	121.3	116.2
N9-N14-H30	111.0	112.5	114.7	112.9	108.1	110.0	114.9	112.6	
C10-N9-N14	116.5	116.3	117.5	117.9	115.2	115.2	117.0	117.6	
N14-C15-C16	115.2	115.2	119.7	120.3	114.6	114.6	119.4	119.9	
N14-C15-O17	121.5	121.3	118.0	117.7	121.8	121.6	117.9	117.5	
C15-N14-H30	115.0	117.5	113.2	109.2	114.0	116.0	113.6	108.5	
C15-C16-C23	117.4	118.1	123.2	123.9	117.1	118.0	123.0	124.3	
C15-C16-C27	122.9	122.0	116.9	116.5	123.3	122.1	117.1	116.3	
C16-C23-C24	120.1	120.0	119.8	120.2	120.2	120.1	119.9	120.2	
C16-C23-H32	119.0	119.2	120.3	120.8	118.4	118.8	120.1	120.6	
C16-C27-C26	120.1	119.9	120.2	120.2	120.1	119.9	120.2	120.4	
C16-C27-H36	120.6	120.4	119.5	119.0	120.5	120.2	119.1	118.5	
C23-C24-C25	120.0	120.0	120.3	120.0	120.1	120.0	120.3	120.2	
C23-C24-H33	119.9	119.9	119.6	119.7	119.9	119.9	119.6	119.7	
C24-C23-H32	120.9	120.8	119.8	119.0	121.4	121.2	120.0	119.2	

C24-C25-C26	120.1	120.2	120.0	120.0	120.0	120.1	119.9	119.9	
C24-C25-H34	120.0	119.9	120.0	119.9	120.0	120.0	120.0	120.0	
C25-C24-H33	120.1	120.1	120.1	120.2	120.1	120.1	120.1	120.2	
C25-C26-C27	120.0	120.0	119.9	120.0	120.1	120.1	120.0	120.0	
C25-C26-H35	120.2	120.2	120.2	120.2	120.1	120.2	120.2	120.1	
C26-C25-H34	119.9	119.9	120.0	120.0	119.9	119.9	120.0	120.1	
C26-C27-H36	119.3	119.6	120.4	120.8	119.5	119.8	120.7	121.2	
C27-C26-H35	119.8	119.8	119.9	119.8	119.8	119.7	119.8	119.8	
H28-C11-H29	110.0	109.8	109.6	109.5	110.0	109.9	109.3	109.3	
H28-C11-H31	108.1	108.2	107.8	107.1	107.9	107.8	107.3	106.6	
H29-C11-H31	109.6	109.9	109.9	110.1	109.5	110.0	109.9	110.0	

parameters	***RHF/6-31G(d,p)***				***b3lyp/6-31G(d,p)***			
	R1	**R2**	**R3**	**R4**	**R1**	**R2**	**R3**	**R4**
	Dihedral angles							
C1-C2-C3-C4	0.142	-0.124	0.160	-0.179	0.009	0.002	0.069	-0.315
C1-C2-C3-C10	180.0	-180.0	-179.8	179.8	179.8	-179.8	-179.7	179.9
C1-C2-N7-C8	-180.0	179.7	179.6	-178.6	-179.3	179.3	-179.9	-179.0
C1-C6-C5-C4	0.018	-0.017	0.056	-0.068	0.014	-0.001	0.033	-0.101
C1-C6-C5-H21	-179.9	179.9	-179.9	179.9	180.0	-180.0	-179.9	179.9
C2-C1-C6-C5	0.020	-0.039	-0.111	0.182	0.143	-0.143	-0.075	0.165
C2-C1-C6-H22	-179.9	179.9	180.0	-180.0	-179.9	179.9	180.0	-180.0
C2-C3-C4-C5	-0.106	0.069	-0.215	0.294	0.145	-0.144	-0.111	0.381
C2-C3-C4-H20	179.9	-179.9	179.8	-179.9	-180.0	180.0	179.9	-179.8
C2-C3-C10-N9	0.705	-0.187	1.384	-2.906	-1.234	1.275	0.678	-2.142
C2-C3-C10-O18	179.0	-178.8	-179.2	177.9	177.4	-177.5	-179.9	178.6
C2-N7-C8-N9	-0.782	0.614	-1.228	0.928	0.381	-0.442	-1.487	0.758
C2-N7-C8-C11	179.2	-179.5	179.1	-177.4	-179.8	179.7	179.3	-178.1

C3-C2-C1-C6	-0.098	0.108	0.003	-0.058	-0.152	0.141	0.024	0.042
C3-C2-C1-H19	-180.0	180.0	-179.9	179.8	179.9	-179.9	-179.9	179.9
C3-C2-N7-C8	0.058	-0.376	-0.946	2.318	1.312	-1.313	-0.396	1.661
C3-C4-C5-C6	0.024	0.002	0.106	-0.168	-0.157	0.143	0.06	-0.172
C3-C4-C5-H21	180.0	-180.0	-179.9	179.8	179.9	-179.9	-180.0	179.8
C3-C10-N9-C8	-1.448	0.430	-3.541	6.177	2.970	-3.075	-2.533	4.584
C3-C10-N9-N14	-178.0	178.2	-175.9	179.7	-179.2	178.8	-175.9	179.2
C4-C3-C2-N7	-179.9	180.0	-179.3	178.9	179.4	-179.4	-179.5	179.0
C4-C3-C10-N9	-179.5	180.0	-178.6	177.0	178.5	-178.5	-179.1	178.0
C4-C3-C10-O18	-1.222	1.327	0.831	-2.199	-2.820	2.709	0.329	-1.246
C4-C5-C6-H22	180.0	-180.0	180.0	-179.9	-180.0	180.0	180.0	-180.0
C5-C4-C3-C10	-179.9	179.9	179.7	-179.7	-179.6	179.6	179.7	-179.8
C5-C6-C1-H19	179.9	-179.9	179.8	-179.7	-179.9	179.9	179.9	-179.7
C6-C1-C2-N7	179.9	180.0	179.5	-179.2	-179.6	179.6	179.6	-179.3
C6-C5-C4-H20	-179.9	179.9	-179.9	-180.0	180.0	-180.0	180.0	-180.0
N7-C2-C1-H19	0.053	-0.135	-0.469	0.699	0.484	-0.476	-0.376	0.587
N7-C2-C3-C10	-0.052	0.166	0.786	-1.160	-0.807	0.815	0.751	-0.835
N7-C8-N9-C10	1.582	-0.683	3.692	-5.541	-2.699	2.822	3.124	-4.153
N7-C8-N9-N14	178.1	-178.4	175.9	-179.0	179.6	-179.2	176.3	-178.7
N7-C8-C11-H28	123.7	117.1	118.3	115.9	127.8	114.9	176.3	116.3
N7-C8-C11-H29	3.183	-2.696	-1.561	-3.592	7.010	-5.088	-3.357	-3.475
N7-C8-C11-H31	-116.4	-123.1	-121.9	-124.8	-112.6	-125.8	-124.0	-124.6
C8-N9-C10-O18	-179.8	179.2	177.0	-174.5	-175.8	175.8	178.0	-176.1
C8-N9-N14-C15	-94.14	93.74	101.4	-127.1	-83.24	86.37	95.14	-128.8
C8-N9-N14-H30	132.1	-125.1	-110.6	100.9	147.0	-137.6	-112.6	100.3
N9-C8-C11-H28	-56.32	-63.00	-61.38	-62.54	-52.34	-65.01	-62.85	-62.65
N9-C8-C11-H29	-176.8	177.2	178.8	178.0	-173.1	175.0	177.4	177.6
N9-C8-C11-H31	63.58	56.80	58.43	56.79	67.30	54.36	56.71	56.49
C10-C3-C4-H20	0.032	-0.026	-0.254	0.165	0.242	-0.251	-0.257	-0.003
C10-N9-C8-C11	-178.4	179.4	-176.7	172.8	177.4	-177.3	-177.6	174.7

C10-N9-N14-C15	82.59	-84.14	-85.98	59.14	98.83	-95.48	-91.22	56.32
C10-N9-N14-H30	-51.20	57.00	62.07	-72.94	-30.91	40.56	61.09	-74.53
C11-C8-N9-N14	-1.910	1.723	-4.427	-0.614	-0.286	0.684	-4.4	0.164
N14-N9-C10-O18	3.593	-3.034	4.681	-1.026	2.058	-2.258	4.623	-1.459
N14-C15-C16-C23	159.4	140.5	63.57	34.27	164.7	143.6	56.62	28.31
N14-C15-C16-C27	-21.55	-41.81	-120.8	-149.1	-15.98	-39.28	-128.4	-155.1
C15-C16-C23-C24	-179.9	179.5	176.8	176.9	-179.6	179.0	176.3	177.1
C15-C16-C23-H32	-0.095	-0.455	-0.758	-1.764	0.268	-0.966	-0.683	-1.453
C15-C16-C27-C26	-179.5	-178.6	-178.1	-178.0	180.0	-178.3	-177.7	-178.1
C15-C16-C27-H36	-1.253	-1.768	1.473	2.228	-1.956	-2.035	1.991	2.007
C16-C23-C24-C25	-0.728	-1.158	0.463	0.646	-0.561	-1.052	0.483	0.479
C16-C23-C24-H33	179.4	179.3	-179.3	-179.4	179.5	179.2	-179.2	-179.4
C16-C27-C26-C25	-0.254	-0.363	1.559	1.079	-0.014	-0.203	1.619	1.003
C16-C27-C26-H35	179.5	179.1	-179.2	-179.2	179.6	179.1	-179.1	-179.2
C23-C16-C15-O17	-23.12	-35.03	-122.76	-142.8	-18.33	-31.83	-128.6	-147.6
C23-C16-C27-C26	-0.538	-0.996	-2.264	-1.191	-0.730	-1.241	-2.483	-1.312
C23-C16-C27-H36	177.7	175.9	177.3	179.0	177.3	175.0	177.2	178.8
C23-C24-C25-C26	-0.068	-0.205	-1.174	-0.763	-0.189	-0.398	-1.356	-0.797
C23-C24-C25-H34	-179.8	-179.6	179.5	179.5	-179.8	-179.7	179.4	179.5
C24-C23-C16-C27	1.029	1.758	1.250	0.327	1.018	1.87	1.429	0.570
C24-C25-C26-C27	0.559	0.967	0.160	-0.099	0.476	1.026	0.303	0.056
C24-C25-C26-H35	-179.2	-178.5	-179.1	-179.8	-179.1	-178.3	-179.0	-179.7
C25-C24-C23-H32	179.4	178.8	178.0	179.3	179.5	178.9	177.5	179.0
C25-C26-C27-H36	-178.5	-177.3	-178.0	-179.1	-178.1	-176.5	-178.0	-179.1
C26-C25-C24-H33	179.8	179.4	178.6	179.2	179.7	179.3	178.3	179.1
C27-C16-C15-O17	155.9	142.7	52.91	33.85	161.0	145.3	46.40	29.01
C27-C16-C23-H32	-179.1	-178.2	-176.3	-178.3	-179.1	-178.1	-175.6	-178.0
C27-C26-C25-H34	-179.7	-179.7	179.5	179.6	-179.9	-179.7	179.5	179.7
H19-C1-C6-H22	-0.068	0.048	-0.090	0.189	0.051	-0.048	-0.077	0.167
H20-C4-C5-H21	0.029	-0.032	0.032	0.017	0.024	-0.037	-0.029	0.015

H21-C5-C6-H22	0.005	-0.017	0.009	0.070	-0.011	0.014	0.000	0.053
H32-C23-C24-H33	-0.422	-0.789	-1.720	-0.701	-0.379	-0.755	-2.19	-0.829
H33-C24-C25-H34	0.101	0.010	-0.720	-0.497	0.083	0.021	-0.891	-0.604
H34-C25-C26-H35	0.542	0.871	0.247	-0.039	0.555	0.989	0.243	-0.013
H35-C26-C27-H36	1.165	2.201	1.219	0.546	1.459	2.852	1.238	0.637

Table (S8) Optimized geometrical parameters, bond lengths (Å) and bond angles (degrees) for **MAQ (3f)** R1. For numbering of the atoms see Figure 22 (Chapter 2).

Parameters	**R1**		***x-ray***
	HF/6-31G(d,p)	***b3lyp/6-31G(d,p)***	
	bond lengths		
C1-C2	1.400	1.410	1.394
C1-C6	1.372	1.385	1.368
C1-H19	1.074	1.085	
C2-C3	1.390	1.413	1.399
C2-N7	1.383	1.384	1.396
C3-C4	1.399	1.405	1.394
C3-C10	1.458	1.456	1.447
C4-C5	1.371	1.385	1.381
C4-H20	1.074	1.085	
C5-C6	1.401	1.408	1.385
C5-H21	1.075	1.085	
C6-H22	1.076	1.086	
N7-C8	1.268	1.294	1.287
C8-N9	1.387	1.394	1.381
C8-C11	1.517	1.518	1.520
N9-C10	1.392	1.415	1.414
N9-N14	1.376	1.397	1.390
C10-O18	1.201	1.228	1.218
C11-C12	1.537	1.544	
C11-C13	1.529	1.533	
C11-H28	1.081	1.092	
C12-H29	1.084	1.094	
C12-H31	1.085	1.095	
C12-H32	1.085	1.094	
C13-H33	1.082	1.092	
C13-H34	1.083	1.093	
C13-H35	1.086	1.095	
N14-C15	1.386	1.405	1.372
N14-H30	0.994	1.014	
C15-O17	1.192	1.219	1.219
C15-C16	1.494	1.495	1.498
C16-C23	1.390	1.401	1.387
C16-C27	1.390	1.403	1.398
O18…..H30	2.521	2.330	
C23-C24	1.382	1.392	1.386
C23-H36	1.074	1.085	
C24-C25	1.387	1.398	1.362
C24-H37	1.075	1.086	
C25-C26	1.385	1.396	1.384
C25-H38	1.076	1.086	
C26-C27	1.385	1.395	1.390
C26-H39	1.075	1.086	

C27-H40	1.076	1.087	

parameters	R1		x-ray
	HF/6-31G(d,p)	*b3lyp/6-31G(d,p)*	
	bond angles		
C1-C2-C3	118.9	118.6	119.1
C1-C2-N7	118.8	118.7	118.5
C1-C6-C5	121.1	120.8	121.7
C1-C6-H22	119.5	119.6	
C2-C1-C6	119.8	120.2	120.0
C2-C1-H19	118.5	118.1	
C2-C3-C4	121.0	120.8	119.8
C2-C3-C10	118.5	118.8	119.7
C2-N7-C8	119.7	119.4	118.4
C3-C2-N7	122.4	122.7	122.4
C3-C4-C5	119.7	119.7	120.6
C3-C4-H20	118.7	118.4	
C3-C10-N9	113.8	113.5	112.9
C3-C10-O18	126.0	126.8	126.8
C4-C3-C10	120.5	120.4	120.5
C4-C5-C6	119.6	119.9	118.8
C4-C5-H21	120.4	120.2	
C5-C4-H20	121.6	121.8	
C5-C6-H22	119.4	119.6	
C6-C1-H19	121.7	121.8	
C6-C5-H21	120.0	119.9	
N7-C8-N9	121.9	121.4	122.4
N7-C8-C11	120.1	120.3	120.8
C8-N9-C10	123.7	124.1	124.1
C8-N9-N14	120.6	121.2	120.5
C8-C11-C12	109.5	109.6	
C8-C11-C13	111.3	111.2	
C8-C11-H28	107.9	107.6	
N9-C8-C11	118.0	118.2	116.7
N9-C10-O18	120.1	119.8	120.3
N9-N14-C15	117.2	117.5	116.2
N9-N14-H30	112.3	109.8	
C10-N9-N14	115.6	114.7	115.4
C11-C12-H29	112.0	111.8	
C11-C12-H31	110.5	110.6	
C11-C12-H32	109.9	109.9	
C11-C13-H33	111.5	111.2	
C11-C13-H34	111.1	111.1	
C11-C13-H35	109.2	109.5	
C12-C11-C13	111.2	111.3	
C12-C11-H28	108.7	108.7	
C13-C11-H28	108.2	108.3	

N14-C15-C16	115.3	114.7	116.1
N14-C15-O17	121.2	121.4	120.7
C15-N14-H30	117.2	115.8	
C15-C16-C23	118.0	118.1	117.1
C15-C16-C27	122.0	122.1	123.3
C16-C15-O17	123.4	123.8	123.2
C16-C23-C24	120.0	120.1	119.7
C16-C23-H36	119.2	118.8	
C16-C27-C26	119.9	119.9	119.6
C16-C27-H40	120.4	120.2	
C23-C16-C27	120.0	119.8	119.6
C23-C24-C25	120.0	120.0	120.7
C23-C24-H37	119.9	119.9	
C24-C23-H36	120.8	121.2	
C24-C25-C26	120.2	120.1	120.4
C24-C25-H38	119.9	120.0	
C25-C24-H37	120.1	120.1	
C25-C26-C27	120.0	120.1	119.8
C25-C26-H39	120.2	120.1	
C26-C25-H38	119.9	119.9	
C26-C27-H40	119.6	119.8	
C27-C26-H39	119.8	119.7	
H29-C12-H31	108.4	108.5	
H29-C12-H32	107.8	107.9	
H31-C12-H32	108.1	108.1	
H33-C13-H34	108.0	107.8	
H33-C13-H35	108.7	108.8	
H34-C13-H35	108.3	108.4	

Parameters	**R1**	
	HF/6-31G(d,p)	***b3lyp/6-31G(d,p)***
	Dihedral angles	
C1-C2-C3-C4	0.130	-0.024
C1-C2-C3-C10	179.8	179.6
C1-C2-N7-C8	-179.8	-179.4
C1-C6-C5-C4	0.014	-0.003
C1-C6-C5-H21	-179.9	180.0
C2-C1-C6-C5	0.015	0.074
C2-C1-C6-H22	-180.0	-180.0
C2-C3-C4-C5	-0.102	0.095
C2-C3-C4-H20	179.9	180.0
C2-C3-C10-N9	0.052	-0.679
C2-C3-C10-O18	179.3	178.2
C2-N7-C8-N9	-0.045	0.048
C2-C3-C10-O18	179.3	178.2
C2-N7-C8-C11	-177.9	-176.9
C3-C2-C1-C6	-0.086	-0.060
C3-C2-C1-H19	-180.0	180.0

C3-C2-N7-C8	0.332	1.125
C3-C4-C5-C6	0.028	-0.081
C3-C4-C5-H21	180.0	180.0
C3-C10-N9-N14	-177.6	-178.2
C3-C10-N9-C8	-0.663	2.300
C4-C3-C2-N7	180.0	179.4
C4-C3-C10-N9	-179.8	178.9
C4-C3-C10-O18	-1.041	-2.183
C4-C5-C6-H22	180.0	-180.0
C5-C4-C3-C10	-179.8	-179.5
C5-C6-C1-H19	179.9	-179.9
C6-C1-C2-N7	-179.9	-179.5
C6-C5-C4-H20	-179.9	-179.9
N7-C2-C1-H19	0.185	0.466
N7-C2-C3-C10	-0.379	-0.97
N7-C8-N9-C10	0.662	-2.325
N7-C8-N9-N14	177.5	178.2
N7-C8-C11-C12	97.80	98.80
N7-C8-C11-C13	-25.47	-24.50
N7-C8-C11-H28	-144.0	-143.1
C8-N9-C10-O18	-179.5	-176.7
C8-N9-N14-C15	-93.80	-87.00
C8-N9-N14-H30	126.2	137.9
C8-C11-C12-H29	58.74	58.8
C8-C11-C12-H31	-62.27	-62.27
C8-C11-C12-H32	178.5	178.5
C8-C11-C13-H33	62.90	61.10
C8-C11-C13-H34	-57.60	-59.04
C8-C11-C13-H35	-177.0	-178.7
N9-C8-C11-C12	-79.70	-78.60
N9-C8-C11-C13	157.0	157.9
N9-C8-C11-H28	38.40	39.40
N9-N14-C15-C16	-156.1	-153.1
N9-N14-C15-O17	28.50	31.70
C10-C3-C4-H20	0.156	0.342
C10-N9-C8-C11	178.2	175.1
C10-N9-N14-C15	83.30	93.50
C10-N9-N14-H30	-56.80	-41.60
C11-C8-N9-N14	-5.001	-4.403
C12-C11-C13-H33	-59.50	-61.50
C12-C11-C13-H34	180.0	178.4
C12-C11-C13-H35	60.60	58.70
C13-C11-C12-H29	-177.9	-177.7
C13-C11-C12-H31	61.10	61.20
C13-C11-C12-H32	-58.20	-58.00
N14-N9-C10-O18	3.500	2.800
N14-C15-C16-C23	-140.4	-143.1
N14-C15-C16-C27	41.90	39.80
C15-C16-C23-H36	0.421	0.892
C15-C16-C23-C24	-179.5	-179.1
C15-C16-C27-C26	178.7	178.4
C15-C16-C27-H40	1.825	2.148
C16-C15-N14-H30	-18.10	-20.50

C16-C23-C24-C25	1.153	1.080
C16-C23-C24-H37	-179.3	-179.2
C16-C27-C26-C25	0.358	0.207
C16-C27-C26-H39	-179.1	-179.1
O17-C15-N14-H30	166.5	164.2
O17-C15-C16-C23	34.90	32.04
O17-C15-C16-C27	-142.8	-145.1
C23-C16-C27-C26	0.999	1.266
C23-C16-C27-H40	-175.9	-175.0
C23-C24-C25-C26	0.208	0.401
C23-C24-C25-H38	179.6	179.7
C24-C23-C16-C27	-1.757	-1.911
C24-C25-C26-C27	-0.966	-1.045
C24-C25-C26-H39	178.5	178.3
C25-C24-C23-H36	-178.8	-178.9
C25-C26-C27-H40	177.2	176.4
C26-C25-C24-H37	-179.4	179.3
C27-C16-C23-H36	178.2	178.1
C27-C26-C25-H38	179.7	179.7
H19-C1-C6-H22	-0.046	0.061
H20-C4-C5-H21	0.059	0.080
H21-C5-C6-H22	0.023	0.011
H28-C11-C12-H29	-58.90	-58.90
H28-C11-C12-H31	-180.0	-179.7
H28-C11-C12-H32	60.80	61.10
H28-C11-C13-H33	111.5	111.2
H28-C11-C13-H34	60.80	59.03
H28-C11-C13-H35	-58.60	-60.60
H36-C23-C24-H37	0.788	0.753
H37-C24-C25-H38	-0.013	-0.024
H38-C25-C26-H39	-0.873	-0.992
H39-C26-C27-H40	-2.219	-2.883