SUPPORTING INFORMATION FOR

Optimization on the 2-Arylquinazoline-4(*3H*)one Scaffold for an Selective and Potent Antitrypanosomal Agent: Mechanism of Action Modulated through Chemical Functionalization

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1. General Chemistry Information

The 2-arylquinazolin-4-hydrazines **2a-g** used herein were previously prepared.[1] The rest of reagents were purchased from commercial sources and used without further purification. Solvents were anhydrous HPLC grade. ^{1}H NMR and ^{13}C NMR spectra were recorded on a 400 MHz NMR-spectrometer (Bruker-400). Multiplicity is indicated as follows: s (singlet), d (doublet), t (triplet), m (multiplet), dd (doublet of doublets), brs (broad singlet); chemical shifts were measured in parts per million (δ) and coupling constant (J) are given in Hz. Proton chemical shifts were given in relative to tetramethylsilane (δ 0.00 ppm) in DMSO-d_6 solvents. Carbon chemical shifts are internally referenced to the deuterated solvent signals in CDCl$_3$ (δ 77.00 ppm) or DMSO-d_6 (δ 40.02 ppm). Elemental analyses of the synthesized compounds were performed using a Perkin Elmer 2400 CHN analyser: results fell in the range of 0.4% of the required theoretical values. TLC was performed using commercially available 100-400 mesh silica gel plates (GF254), visualized under UV light (at 254 nm). Absorption spectra data were obtained from a Thermo Scientific Varioskans Flash Multimode instrument for air-equilibrated solutions at 25 ℃.

2. Synthetic Procedures and Characterization Data

2.1. General procedure for the synthesis of (*E/Z*)-4-(2-((5-nitrofuran-2-yl)methylene)hydrazineyl)-2-phenylquinazoline 3a-h. The corresponding starting material **2a-g** (0.5 mmol, 1.0 eq.) was initially dissolved in aqueous acidic solution (1 mL, 1M in HCl) and the corresponding furfuraldehyde (furfural or 5-nitro-2-furfurylcarbaldehyde) (0.6 mmol, 1.2 eq.) was added following reported protocol with a few modifications.[2,3] The reaction mixture was stirred for 10-20 minutes at 60 ℃. The mixture was cooled at room-temperature and neutralized with addition of sodium carbonate solution until to reach pH of 7. The formed precipitate was filtered by vacuum and, the resulting solid was washed several times with aqueous solution to obtain an orange or red solid **3a-h**, which was recrystallized in methanol/DMF mixture. The product were characterized by NMR spectroscopy and they were reported as a *E/Z* mixture from ^{1}H-NMR spectroscopic analysis. A general nomenclature, for example, **3a_E** was assigned for the *E*-isomer of compound **3a**, whereas **3a_Z** was assigned for the *Z*-isomer of the compound **3a**.

2.2. Characterization data for the synthesized compounds 3a-h

2.2.1.(*E/Z*)-4-(2-((5-nitrofuran-2yl)methylene)hydrazinyl)-2-(phenyl)quinazoline 3a

3a_Z   or   **3a_E**
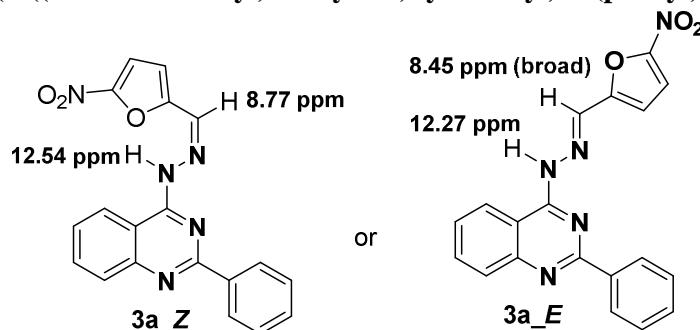
^{1}H-NMR (400 MHz, DMSO-d_6): Mixture *E/Z* isomers. *E (69%):* δ 12.27 (br, 1H), 8.77 (m, 1H), 8.55 (d, *J*= 5.6 Hz, 2H), 8.45 (s broad, 1H), 7.92 (m, 2H), 7.85 (d, *J*=3.6 Hz, 1H), 7.55 (m, 4H), 7.34 (d, *J*=3.6 Hz, 1H); *Z (31%):* δ 12.54 (br, 1H), 8.77 (s, 1H), 8.20 (d, *J* =6.4 Hz, 1H), 8.17 (d, *J*=8.8 Hz, 2H), 7.82 (d, *J*=3.6 Hz, 1H), 7.75 (d, J= 8.0 Hz, 1H), 7.61 (m, 1H), 7.55 (m, 4H), 7.46 (d, *J*=3.6 Hz, 1H). **^{13}C-NMR** (400 MHz, DMSO-d_6): ~ 34 different signals (see spectrum at end of S.I.). **Anal. Calc. for C$_{19}$H$_{13}$N$_5$O$_3$:** C, 63.51; H, 3.65; N, 19.49. Found: C, 63.46; H, 3.58; N, 19.40.

2.2.2.   (*E/Z*)-4-(2-((5-nitrofuran-2yl)methylene)hydrazinyl)-2-(4-fluorophenyl)quinazoline 3b

3b_Z   or   **3b_E**

minor isomer (11 %)   *majoritary isomer (89 %)*
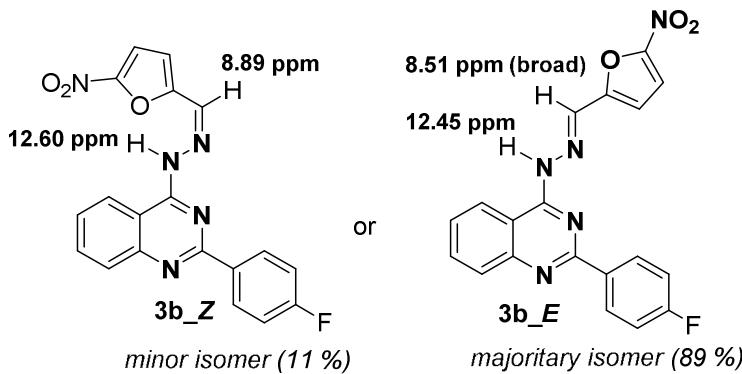
^{1}H-NMR (400 MHz, DMSO-d_6): *E* (89 %) δ 12.45 (br, 1H), 8.81 (s broad, 1H), 8.58 (m, 2H), 8.56 (s, 1H), 7.91 (m, 2H), 7.85 (d, *J*=3.6 Hz, 1H), 7.63 (m, 1H), 7.44 (d, *J*=8.4 Hz, 2H), 7.35 (d, *J*=3.6 Hz, 1H); *Z* (~11 %). **^{13}C-NMR** (400 MHz, DMSO-d_6): δ 165.48 (d, *J*$_{C-F}$=984.4 Hz), 158.73, 157.46, 152.91, 152.33, 134.80, 134.18, 133.78, 130.85 (d, *J*$_{C-C-C-F}$=34.8 Hz), 128.45, 126.74, 124.99, 115.70 (d, *J*$_{C-C-F}$=86.4 Hz), 115.50, 114.73, 113.14. **HSQC** (400 MHz, DMSO-d_6): δ 152.91, 152.27, 134.01, 130.85, 128.40,

126.93, 115.88, 115.66, 115.29. ^{19}**F-NMR** (400 MHz, DMSO-d$_6$): -111.11. **Anal. Calc. for C$_{19}$H$_{12}$FN$_5$O$_3$:** C, 60.48; H, 3.21; F, 5.03; N, 18.56. Found: C, 60.42; H, 3.17; N, 18.40.

2.2.3. **(E/Z)-4-(2-((5-nitrofuran-2yl)methylene)hydrazinyl)-2-(4-chlorophenyl)quinazoline 3c**
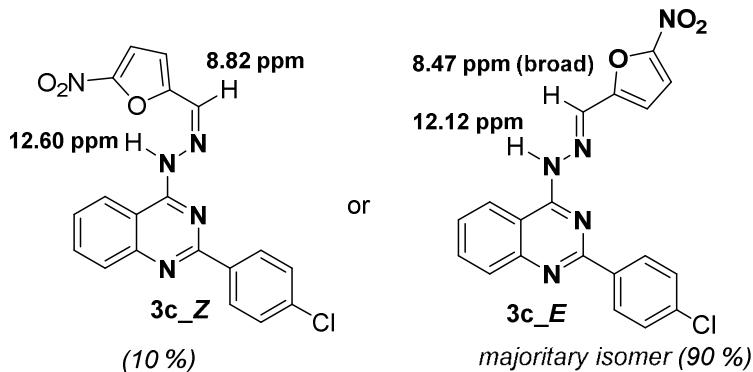
^{1}**H-NMR** (400 MHz, DMSO-d$_6$): **E** (90 %) δ 12.12 (br, 1H), 8.81 (d, J= 7.4 Hz, 1H), 8.52 (d, J=8.0 Hz, 2H), 8.47 (s broad, 1H), 7.90 (m, 2H), 7.75 (d, J=3.6 Hz, 1H), 7.60 (m, 3H), 7.27 (sa, 1H); **Z** (10 %). ^{13}**C-NMR** (400 MHz, DMSO-d$_6$): δ 161.70, 157.07, 156.74, 150.83, 150.47, 135.30, 133.94, 132.38, 131.84, 130.29, 128.32, 127.13, 126.70, 125.10, 113.63, 113.03, 111.12. **Anal. Calc. for C$_{19}$H$_{12}$ClN$_5$O$_3$**: C, 57.95; H, 3.07; N, 17.78. Found: C, 57.83; H, 3.04; N, 17.63.

2.2.4. **(E/Z)-4-(2-((5-nitrofuran-2yl)methylene)hydrazinyl)-2-(4-bromorophenyl)quinazoline 3d**
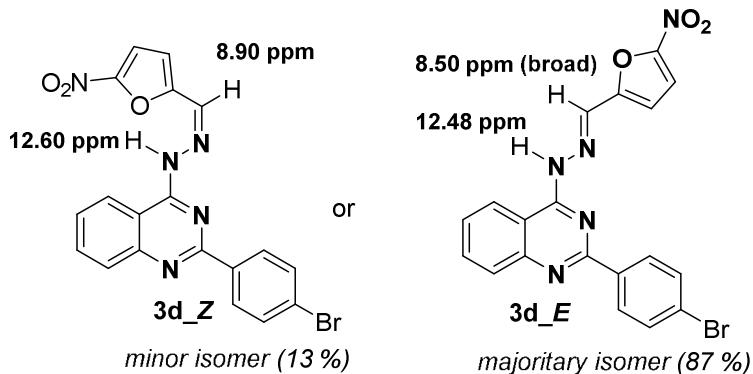
^{1}**H-NMR** (400 MHz, DMSO-d$_6$): **E** (87 %) δ 12.38 (br, 1H), 8.78 (s, 1H), 8.48 (s broad, 1H), 8.48-8.45 (m, 2H), 7.92 (m, 2H), 7.85 (s, 1H), 7.77-7.75 (m, 2H), 7.60 (m, 1H), 7.35 (s, 1H); **Z** (13 %). ^{13}**C-NMR** (400 MHz, DMSO-d$_6$): δ 162.82, 159.86, 157.44,

152.75, 152.30, 134.31, 132.58, 131.97, 130.47, 130.29, 128.48, 127.05, 124.88, 121.45, 115.52, 114.94, 113.27. **HSQC** (400 MHz, DMSO-d_6): 134.11, 133.57, 130.45, 130.40, 128.53, 126.75, 115.24, 114.76. **Anal. Calc. for C$_{19}$H$_{12}$BrN$_5$O$_3$:** C, 52.07; H, 2.76; N, 15.98. Found: C, 52.02; H, 2.78; N, 15.91.

2.2.5. (*E/Z*)-4-(2-((5-nitrofuran-2yl)methylene)hydrazinyl)-2-(4-methylphenyl)quinazoline 3e

E/Z (68/32)
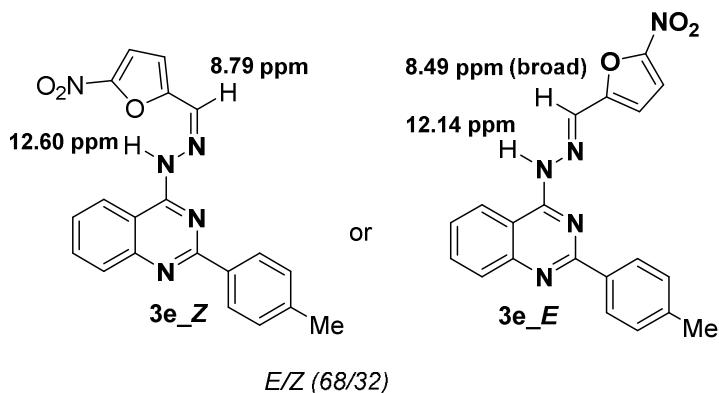
^{1}H-NMR (400 MHz, DMSO-d_6)a and **^{13}C-NMR** (400 MHz, DMSO-d_6) can be found at end of S.I. **Anal. Calc. for C$_{20}$H$_{15}$N$_5$O$_3$**: C, 64.34; H, 4.05; N, 18.76. Found: C, 64.12; H, 3.98; N, 18.71.

2.2.6. (*E/Z*)-4-(2-((5-nitrofuran-2yl)methylene)hydrazinyl)-2-(3-chlorophenyl)quinazoline 3f

minor isomer (4 %)   majoritary isomer (96 %)
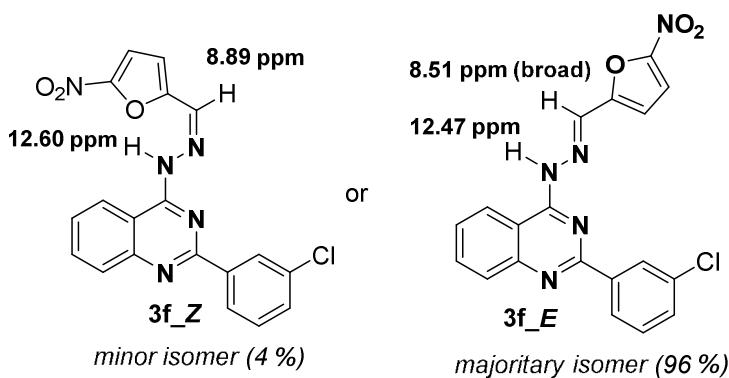
^{1}H-NMR (400 MHz, DMSO-d_6): **E** (96%) δ 12.47 (br, 1H), 8.82 (d, *J*= 7.4 Hz, 1H), 8.51 (s, 1H), 8.51-8.47 (m, 2H), 7.93 (m, 2H), 7.85 (d, *J*=4.0 Hz, 1H), 7.64-7.59 (m, 4H), 7.32 (d, *J*=3.6 Hz, 1H); **Z** (4 %). **^{13}C-NMR** (400 MHz, DMSO-d_6): δ 158.07, 157.48, 152.66, 152.24, 151.36, 140.21, 134.28, 133.84, 130.88, 130.75, 128.40,

128.13, 127.13, 126.94, 125.15, 115.43, 115.02, 113.36. **Anal. Calc. for C19H12ClN5O3:** C, 57.95; H, 3.07; N, 17.78. Found: C, 57.89; H, 3.05; N, 17.70.

2.2.7. (*E*)-4-(2-((5-nitrofuran-2-yl)methylene)hydrazinyl)-2-(3-bromophenyl)quinazoline 3g

E-3g
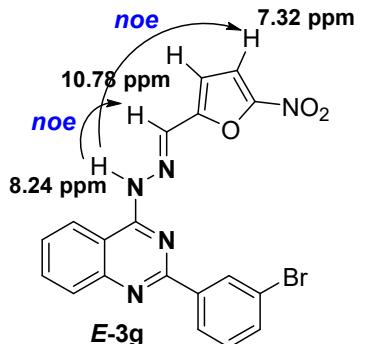
majoritary isomer (96-97 %)

1H-NMR (400 MHz, DMSO-*d6*): ***E*** (≥ 97%) δ 10.78 (br, 1H), 8.65 (m, 2H), 8.24 (s, 1H), 8.19 (m, 2H), 7.94 (m, 3H), 7.72 (m, 1H), 7.29 (m, 1H), 7.32 (m, 1H). **13C-NMR** (400 MHz, DMSO-*d6*): δ 161.57, 161.44, 157.84, 155.58, 150.52, 141.72, 140.67, 134.13, 133.30, 130.95, 128.68, 128.63, 127.10, 126.84, 123.21, 122.16, 113.84, 113.43, 112.26. **HSQC** (400 MHz, DMSO-*d6*): 133.92, 133.38, 130.80, 130.75 (2C), 128.24, 126.89, 126.77, 123.19. **Anal. Calc. for C19H12BrN5O3:** C, 52.07; H, 2.76; N, 15.98. Found: C, 52.02; H, 2.78; N, 15.91.

2.2.8. (*E*)-4-(2-(furan-2-yl-methylene)hydrazinyl)-2-(4-fluorophenyl)quinazoline 3h

E-3h

majority isomer
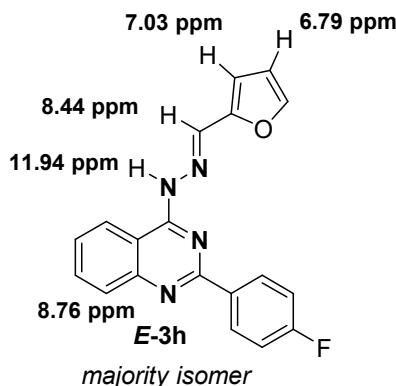
1H-NMR (400 MHz, DMSO-*d6*): ***E*** (98 %) δ 11.91 (br, 1H), 8.76 (m, 1H), 8.56 (m, 1H), 8.44 (s, 1H), 7.94 (d, *J*= 0.8 Hz, 1H), 7.87 (m, 2H), 7.60 (m, 1H), 7.38 (dd, *J*$_{H-F}$= 8.6 Hz, *J*$_{HH}$= 8.4 Hz, 2H), 7.03 (d, *J*= 2.4 Hz, 1H), 6.79 (dd, *J*= 2.0, 1.6 Hz, 1H); ***Z*** (2 %) δ 12.57 (br, 1H). **13C-NMR** (400 MHz, DMSO-*d6*): δ 165.52 (d, *J*$_{C-F}$= 984.4 Hz),

163.78, 158.64, 157.42, 150.03, 145.74, 144.19, 136.55, 134.66, 133.94, 130.76 (d, $J_{C\text{-}C\text{-}F}$= 33.2 Hz), 127.92, 126.43, 115.90 (d, $J_{C\text{-}C\text{-}F}$= 85.6 Hz), 114.10, 113.09, 112.81. **^{19}F-NMR** (400 MHz, DMSO-d_6): -110.81. **HSQC** (400 MHz, DMSO-d_6): δ 133.92, 133.38, 130.80, 130.75 (2C), 128.24, 126.89, 126.77, 123.19. **Anal. Calc. for $C_{19}H_{13}FN_4O$:** C, 68.67; H, 3.94; N, 16.86. Found: C, 68.62; H, 3.86; N, 16.78.

3. Biological Experimental Information

Parasite and cultures. Tests were carried out on promastigotes of *Leishmania (V) infantum* (MHOM MA67I7MAP263) and epimastigote of *T. cruzi* CL Brener clone. Promastigote of *L. infantum* were provided by Dr. M. Comini (Lab. Redox Biology of Trypanosomes, Institut Pasteur, Mataojo 2020, Montevideo, Uruguay). Both parasites were maintained in brain-heart infusion medium (BHI, Oxoid) supplemented with 10 % heat inactivated fetal bovine serum (FBS, Capricorn), penicillin (100 units per mL) and streptomycin (100 mg per mL) at 28 °C and harvested during the exponential phase of growth. For differentiation and maintenance of promastigote culture was used medium LIT (tryptose 15 g/L, yeast extract 5 g/L, liver extract 2 g/L, hemin-NaOH 0.02 g/L, glucose 4 g/L, NaCl 9 g/L, KCl 0.4 g/L, Na_2HPO_4 7.5 g/L, pH 7.4) supplemented with 10 % fetal bovine serum and maintained at 29 °C. Macrophages J774.1A and peritoneal were grown in DMEN medium. Macrophages were grown in a humidified incubator with 5 % CO_2 and 95 % air at 37 °C until they reach the exponential growth phase. For treatments, exponentially growing cells were collected, counted, re-suspended in fresh culture medium and incubated in 96-sterile-well plates.

4. Biological Procedures

4.1. *In vitro* anti-*T.cruzi* evaluation on epimastigote form. The effect of the compounds **1a-g**, **2a-g** and (*E/Z*)-4-(2-((5-nitrofuran/furan-2-yl)methylene)hydrazineyl)-2-phenylquinazolines **3a-h** on the epimastigotes viability of *T. cruzi* (CL Brener clone) was determined through turbidimetric technique.[4] Stock solutions (at 3000 μM) of the tested compounds in DMSO were prepared. Fresh solutions were diluted in the culture medium to obtain the different concentrations from 0.5 to 25 μM. All controls and tested well contains no more than 1 % of DMSO. The screening was performed in 24-well microliter plates maintained at 25 °C. Briefly, 2×10^6 parasites/mL were exposed to increasing concentrations from 0.5 to 25.0 μM

(0.5, 1.0, 2.5, 5.0, 10.0, 25 μM) of each compound for 120 h at 25 ºC. Controls contain 1 % of DMSO and medium. Biological effect of these compounds was evaluated through absorbance measurements at 595 nm using a spectrometer El301 microwell at 5 days. Untreated control parasites were used to calculate the relative proliferation. Nifurtimox was used as reference drug. The IC_{50} value (50 % growth inhibitory concentration) was determined as follows: % parasite growth = (A_p A_{0p})/(A_c A_{0c}) -100, where:

 A_p = A_{595} of the culture containing the compound at day 5;

 A_{0p} = A_{595} of the culture containing the compound at day 0;

 A_c = A_{595} of the culture in the absence of any drug (control) at day 5;

 A_{0c} = A_{595} in the absence of any drug at day 0.

4.2. *In vitro* anti-*Leishmania* evaluation on promastigote. The cell viability of the compounds **1a-g, 2a-g** and **3a-h** on *Leishmania infantum* (MHOM MA67I7MAP263) strain was assessed using the 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assays with a few modifications.[2] Stock solutions (at 3000 μM) of the tested compounds in DMSO were prepared. Fresh solutions were diluted in the culture medium to obtain the different concentrations from 0.5 to 25 μM. All controls and tested well contains no more than 1 % of DMSO. The screening was performed in 96-well microliter plates maintained at 25 ºC. Briefly, 2×10^6 parasites/mL were exposed to increasing concentrations from 0.5 to 25.0 μM (0.5, 1.0, 2.5, 5.0, 10.0 and 25.0 μM) of each compound for 72 h at 25 ºC. Controls contain 1 % of DMSO and medium. After incubation, cells were treated with 100 μL 0.4 mg/mL MTT for 4h at 37 ºC. Subsequently, the medium was removed and 100 μL DMSO was added to the resulting mixture to dissolved formazan salt. The solubilized formazan product was quantified through absorbance measurements at 570 nm using a Thermo Scientific Varioskan Flash Multimode instrument at 72 h. Miltefosine and glucantime were used as reference drugs. Untreated control parasites were used to calculate the relative proliferation. The percentage of parasite inhibition with regard to controls was calculated as= 100 - [(parasite counts in treated cells/parasite counts in untreated cells)-100].

4.3. *In vitro* antiamastigote activity of *L. infantum*. Axenic amastigote forms of *L. infantum* were cultured as described in literature.[5] The promastigotes were transformed into amastigotes by culturing for three days in BHI medium supplemented with 10%

heat-inactivated fetal calf serum, 1 g/L β-alanine, 100 mg/L L-asparagine, 200 mg/L sucrose, 50 mg/L sodium pyruvate, 320 mg/L malic acid, 40 mg/L fumaric acid, 70 mg/L succinic acid, 200 mg/L α-ketoglutaric acid, 300 mg/L citric acid, 1.1 g/L sodium bicarbonate, 5 g/L 2-[morpholino]ethanesulfonic acid, 0.4 mg/L hemin and 10 mg/L gentamicin at a *pH* of 5.4 at 37 °C. The screening was performed in 96-well microtiter plates maintained at 37 °C. Briefly, 2×10^6 parasites/mL were exposed to increasing concentrations (0.5, 1.0, 2.5, 5.0, 10.0 and 25.0 μM) of each compound **3a-h**. Controls contained 1% of DMSO. Miltefosine and glucantime were used as reference drug. The effect of the derivatives **3a-h** against amastigote forms was tested at 48 h using conventional counting parasite in Neubauer chamber (optical microscopy, 1000x magnification) using tripan blue. Untreated control parasites were used to calculate the relative proliferation. The antileishmanial effects were expressed as IC_{50}.

4.4. Cytotoxicity. Peritoneal and J774.1A macrophages were grown in DMEM medium supplemented with 10 % heat inactivated fetal bovine serum, 1 % of L-glutamine, 1 % streptomicyn, 100 units/mL penicillin. Cell viability was assessed using MTT protocol.[2,4] Stock solutions (at 25000 μM) of the tested compounds in DMSO were prepared. Cells were grown in 96-well plates (5×10^4 cells/well) for 24 h. Cultures were carried out at 37 °C in a humidified atmosphere with 5 % CO_2 and incubated with the (*E/Z*)-4-(2-((5-nitrofuran/furan-2-yl)methylene)hydrazineyl)-2-phenylquinazolines **3a, 3b, 3f** and **3h** at 0, 10.0, 25.0, 50.0, 75, 100 μM concentrations for 48 h. After incubation, the medium was removed and, the cells were treated with 100 μL 0.4 mg/mL MTT for 4 h at 37 °C. Subsequently, 100 μL DMSO was added to the mixture. The solubilized formazan product was quantified through absorbance measurements at 570 nm. The absorbance values were transformed to the percentage of cytotoxicity compared to the negative controls.

4.5. Mutagenicity Ames test.[6] *In vitro* genetic toxicity *Salmonella typhimurium* TA 98 strain was incubated in agar minimum glucose milieu solution (Difco BactoR agar) and aqueous glucose solution (40 %). The direct toxicity of the derivatives **3b** and **3f** against *S. typhimurium* TA 98 strain was studied. From these data, the mutagenic assay was performed incubating **3b** or **3f** in phosphate buffer (0.1 M, pH 7.4) and DMSO (10 % v/v) at six doses. Control positive consisted of NPD (20.0 mg/plate) and negative controls consisted of phosphate buffer and DMSO (10 % v/v) solutions. The revertant

numbers were counted and the studied system was considered mutagenic if the colonies number was at least doubled the natural revertants (negative control) for two or more consecutive doses.

4.6. Statistical analysis. All biological experiments were performed at least three times. The results are expressed as mean ± SD. Anova test were performed. Only post hoc Dunnet test p< 0.01 was considered to be statistically significant. The dose-response curves were plotted using GraphPad prism v.5.02 software.[7]

4.7. Drulikeness properties predictions. Firstly, we proceeded to explore the analysis the existence of false positive agents, PAINS, through the filter named False Positive Remover.[8] ADME properties were analysed from the Swiss-ADME platform.[9] Drug-likeness maps can be found in Figure S7.

5. Mechanistic Assays

5.1. Effect of Divalent Metal. Similar to point 4.1, 2×10^6 parasites/mL (epimastigote of *T. cruzi* or promastigote of *L. infantum*) were exposed to three concentrations from 6.25 to 25.0 μM (6.25, 12.5 and 25.0 μM) of each compound for 120 h at 25 ºC.[1] This experiment of parasite treated with the (*E/Z*)-4-(2-((5-nitrofuran/furan-2-yl)methylene)hydrazineyl)-2-phenylquinazolines **3a, 3b** and **3f** was repeated in presence of copper (II), iron (III) and zinc (II) at a final concentration of 1 μM in separated experiments. Three controls containing copper(II), iron (III) and zinc(II) salts were performed. All treated and untreated wells contain 1 % of DMSO. Antiepimastigote effect of these compounds was evaluated through absorbance measurements at 595 nm using a spectrometer EL301 microwell at 5 days, whereas antipromastigote effect was determined using MTT protocol. Untreated control parasites were used to calculate the relative proliferation. Assays were performed by triplicate for all cases. The IC_{50} values (50 % growth inhibitory concentration) for the antiepimastigote and antipromastigote activities were determined as described in points 4.1 and 4.2, respectively.

5.2. Antifolate activity. Similar to point 4.1, 2×10^6 parasites/mL (epimastigote of *T.cruzi* or promastigote of *L.infantum*) were exposed to three concentrations from 6.25 to 25.0 μM (6.25, 12.5 and 25.0 μM) of each compound for 120 h at 25 ºC. This experiment of parasite treated with the (*E/Z*)-4-(2-((5-nitrofuran/furan-2-

yl)methylene)hydrazineyl)-2-phenylquinazolines **3a, 3b, 3f** and **3h** was repeated in presence of increasing concentration of *d,l*-folic acid (10 nM, 100 nM and 1000 nM) in separated experiments.[10a] Three controls containing folic acid at the three mentioned concentrations were performed. All treated and untreated wells contain 1 % of DMSO. Antiepimastigote effect of these compounds was evaluated through absorbance measurements at 595 nm using a spectrometer EL301 microwell at 5 days, whereas antipromastigote effect was determined using MTT protocol. Untreated control parasites were used to calculate the relative proliferation. Assays were performed by triplicate for all cases. The IC_{50} values (50 % growth inhibitory concentration) for the antiepimastigote and antipromastigote activities were determined as described in points 4.1 and 4.2, respectively. Further assays were performed for key 2-arylquinazolin-4(*3H*)ones **1b** and **1c** and, 2-arylquinazolin-4-hydrazines **2c** and **2d**.

5.3. Determination of nitrite concentration. Nitrite (NO_2^-) accumulation was determined in supernatants of promastigote or epimastigote culture, which were incubated (6×10^6) for 5 days in the presence of the (*E/Z*)-4-(2-((5-nitrofuran-2-yl)methylene)hydrazineyl)-2-(3-chlorophenyl)quinazolines **3f** at increasing concentrations (25, 50 and 100 μM). Three wells with untreated parasites were incubated as negative control. The assay was performed by the Griess reaction (detection limit: 1.56 μM) with sodium nitrite as a standard as previously described.[2] In brief, 100 μL of Griess reagent 1% sulphanilamide in 50% of acetic acid was added to 400 μL of each sample. Blank reference and standard curve were determined. After 15 min, 100 μL of a solution of *N*-[naphthyl]ethylenediamine dihydrochloride (1 %) in acetic acid in 50% was added. The absorbance was measured at 540 nm for that resulting final solution. Nitrite content was quantified by the extrapolation from sodium nitrite standard curve in each experiment. All the assays were performed by triplicate. The results were expressed amount of nitrite ion (in μM). Further assays were performed for key 2-arylquinazolin-4(*3H*)ones **1c** and 2-arylquinazolin-4-hydrazines **2c**.

5.4. Measurement of reactive oxygen species (ROS). To estimate the level of ROS, the cell-permeant probe H2DCFDA (2',7'-dichlorodihydrofluorescein diacetate) was used and analyzed by flow cytometry as described previously.[11] H2DCFDA is a non-fluorescent dye that is converted into fluorescent DCF (2',7'-dichlorofluorescein) in the presence of proper oxidants inside the cells. Promastigotes were treated with the $2 \times IC_{50}$

concentration of studied compounds, and the induction of ROS was estimated at 48 h at room temperature for 20 min in the dark. The induction of ROS in promastigotes was compared with the positive inducer H_2O_2.

6. Theoretical Calculations

6.1. Optimization structures. All theoretical calculations, in gas phase, were performed by using the B3LYP functional[12a] in conjunction with the 6-31G(d,p) basis set[12b] at Gaussian09 quantum chemistry software.[13] The B3LYP/6-31G(d,p) approach allowed us to obtain a consistent prediction for analogue structures such as the (*E*)-4-(2-((aryl-2-yl)methylene)hydrazineyl)-phthalazines[14] and 2-arylquinazolin-4-hydrazines[1]. Geometry of the free compounds **3a**, as E-form, and, their cation-compound complexes for copper(II), iron(III) and zinc (II) cations were optimized. HOMO-LUMO orbital frontiers orbital maps were obtained for free compounds and metal-ligand complexes. HOMO and LUMO frontier orbital maps can be found in Figure S4-S5.

6.2. Molecular Docking. Docking calculations and analysis were carried out using the X-ray crystallographic PTR1-*Leishmania major* (PDB code: 1E7W) [15] and DHFT-TS of *T. cruzi* (PDB code: 3INV) [16]. Their structure was minimized using the CHARMm on Swiss-PdbViewer v4.0.1 software [17]. Binding site definition was determined by comparison with reported interactions for the respective co-crystalized ligand. The prepared protein was exported to ArgusLab v.4.0.1 program package [18] and save as Agl document. Then, molecular docking for the most stable extended geometry of the 5 tested derivates were performed using AMBER method on the selected protein implemented in the ArgusLab (v4.0.1) package program under Windows 10.0 environment. The docking experiment on the tested enzyme was carried out between the energy-minimized ligand into the binding site through their respective grid map dimensions and with a grid point spacing of 0.375 Aº. Rigid ligand models were used in the docking and subsequent optimization scheme. As a test of docking accuracy and for docking energy comparison, co-crystallized ligands were re-docked into the protein structures. Different orientations of the ligands were searched and ranked based on their energy scores. Reproducibility of the calculated affinity energy and the minimum energy pose were evaluated through 10 replicates for each ligand [19]. Affinity energy is reported as mean of the 10 replicates. The lowest energy (strongest-docking) poses for each ligand in binding site of the protein are summarized in Table 3.

7. Experimental Evidences

7.1. Analysis of *E/Z*-isomers in compounds 3a-h

The compounds **3a-h** were found as a *E/Z* isomeric mixture in turn to the imine (-HC=N-) bond in solution. From nuclear Overhauser effect (NOESY) experiments for compounds **3f**, **3g** and **3h**, it should be noted that hydrazinyl proton (NH) (~ 11 ppm) showed spatial correlations with adjacente ylidenic proton (H-C=N-) (~ 8.57-8.44 ppm) for all these cases (Figures S1-S3). Extra correlations between the hydrazynil proton with furyl protons can be noted in Fiigure S2 and S3, which suggested that the furylic oxygen is oriented in "*cisoide*" configuration concerning to the adjacent imine nitrogen (H-C=N-). Theoretical calculations on the compounds **3b** and **3f** revealed that they prefer a cisoide configuration between the furylic oxygen and the imine nitrogen (Figure S4), which implies a specific disposition of the furyl ring into the quinazolin-hydrazone structure as depicted in Figure S4. With a ylidenic proton at 8.57-8.44 ppm, all synthesized compounds **3a-h** showed a dominant *E*-isomer and the *Z*-isomer is identified by having higher chemical shifts for hydrazynil (~12.60 ppm) and ylidenic (~8.90 ppm) protons (see details in section 2 and NMR spectra at end of S.I.). From ¹H-NMR spectra, a clear *E/Z*-isomeric ratio was estimated for all compounds **3a-h** (see details in section 2).
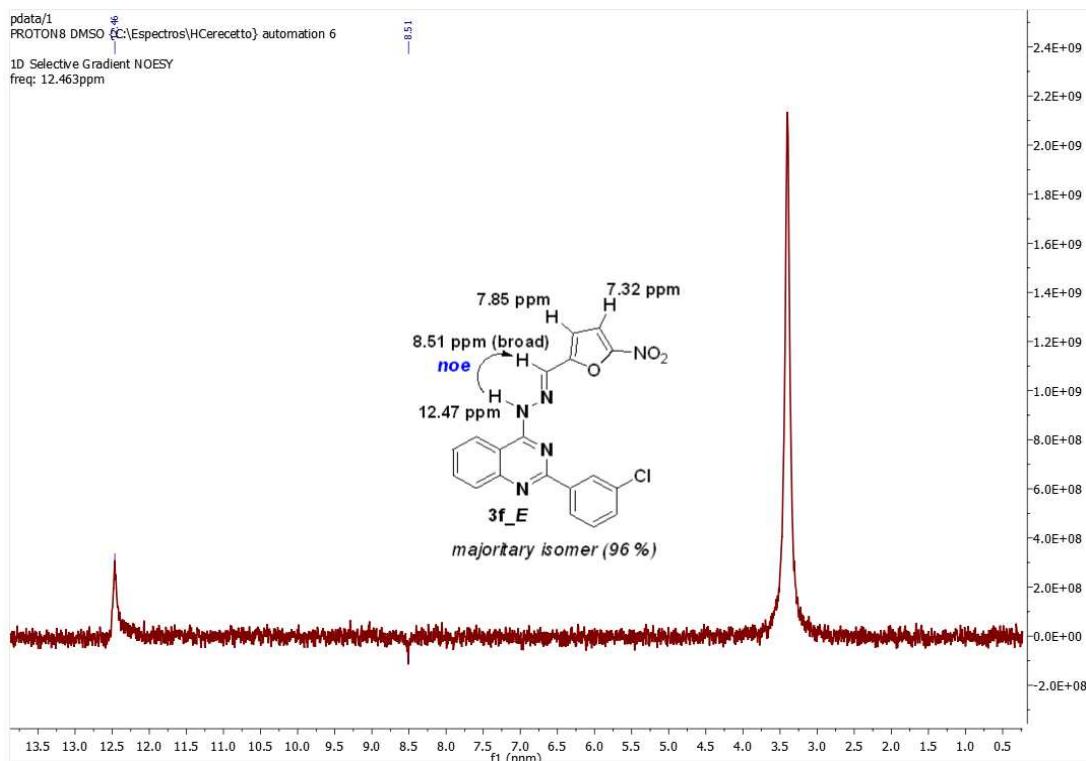
Figure S1. NOE experiments for compound **3f** with selective gradient at 12.463 ppm.
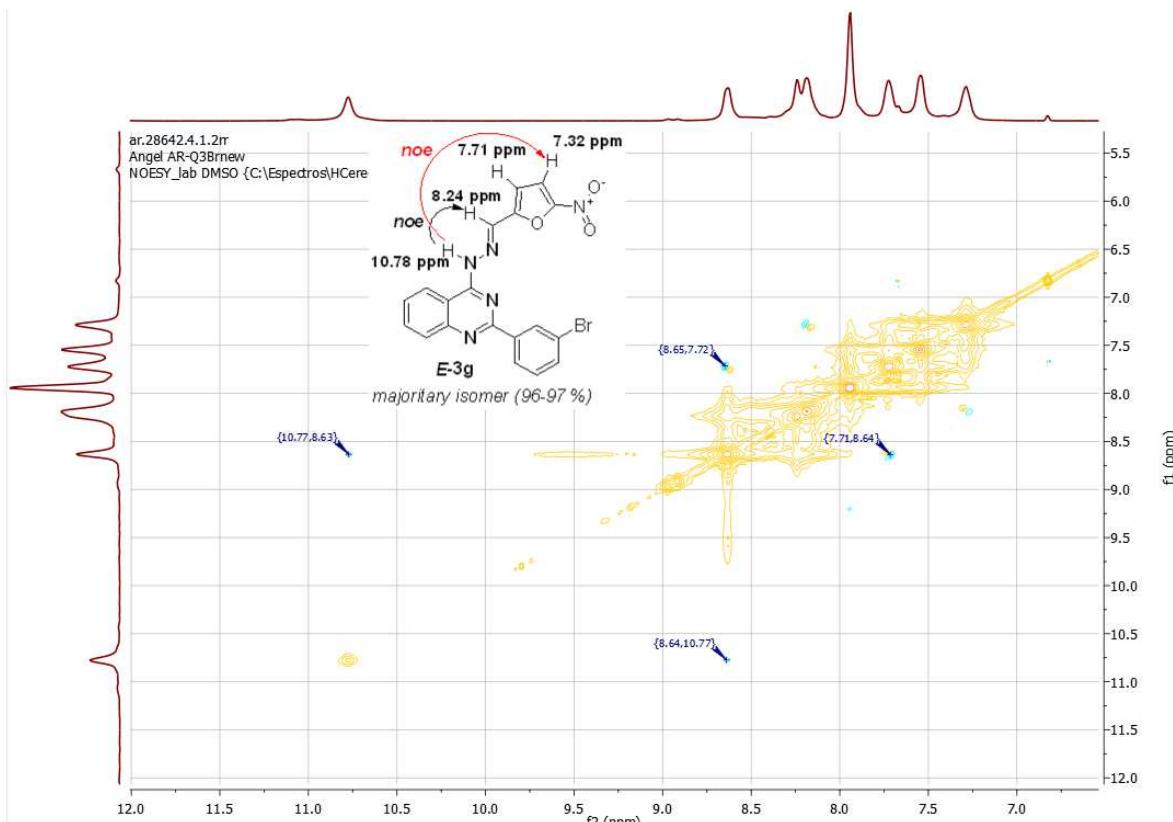
Figure S2. NOESY experiment for compound **3g**.
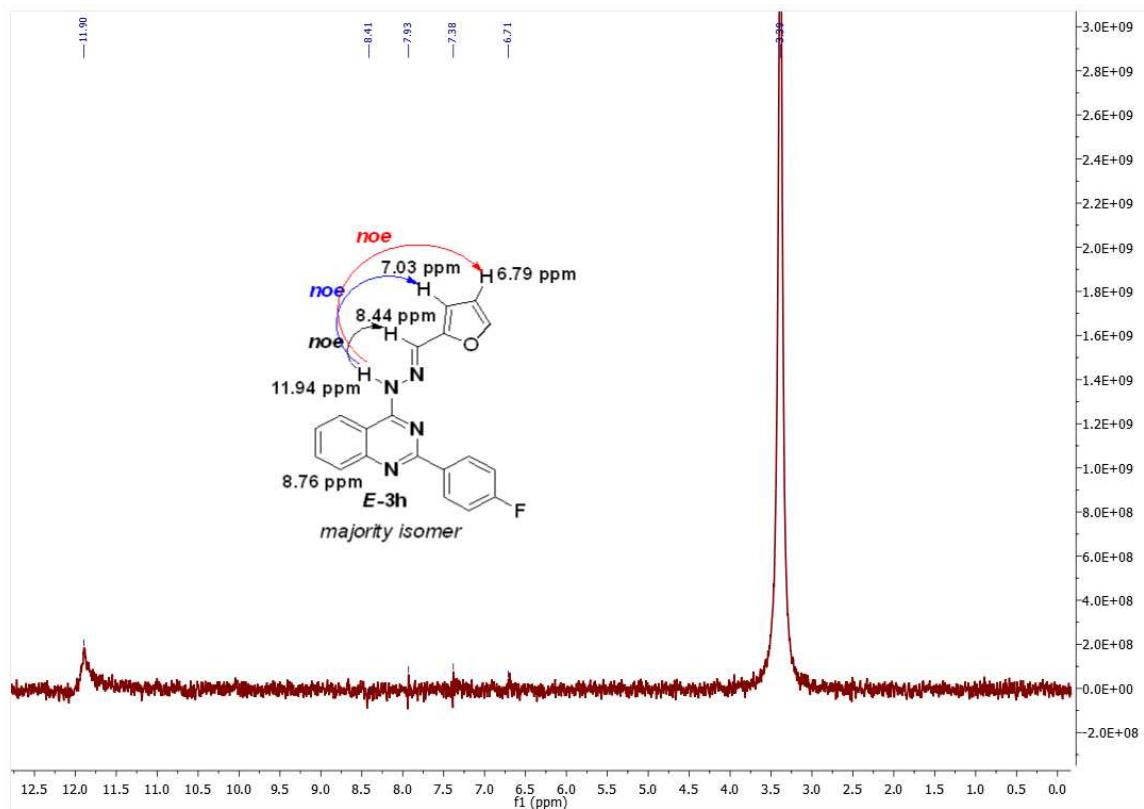
Figure S3. NOE spectra for compound **3h** with selective gradient at 11.90 ppm.

S14
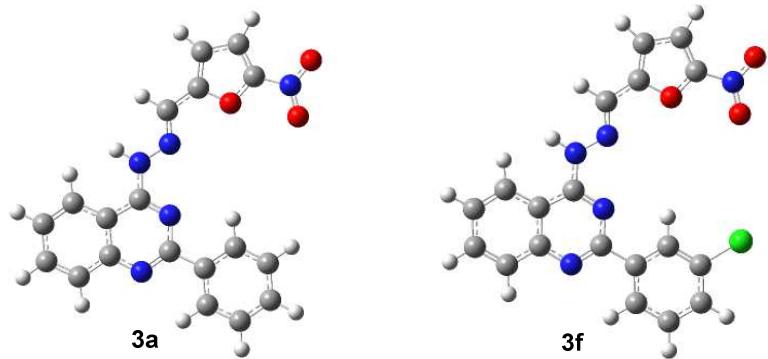
Figure S4. Theoretical structures of the compounds **3a** and **3f** from B3LYP/6-31G(d,p) calculations. Details in section 9 of S.I.

7.2. Molecular docking results
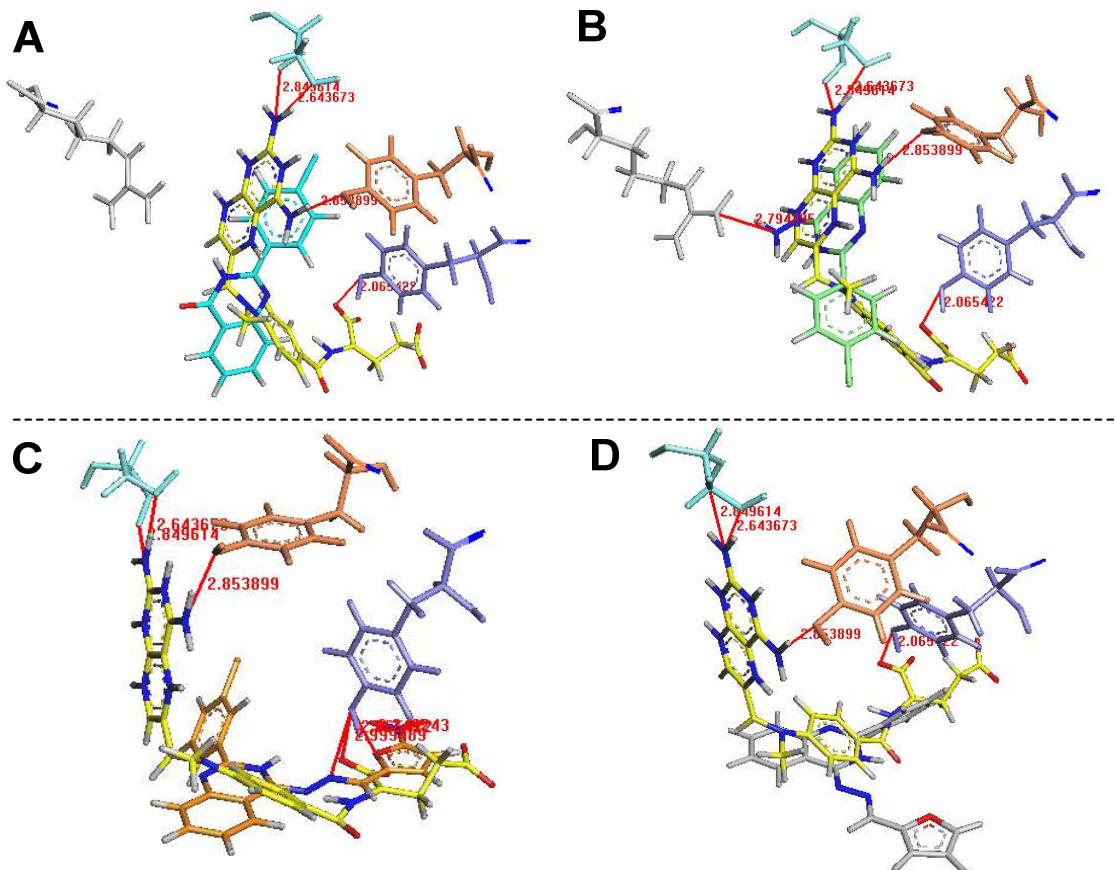
Figure S5. H-Interaction in the binding site of the PTR1-*Leishmania* protein for the compounds **1c** (cyan color, **A), 2c** (green color, **B), 3f** (orange color, **C), 3h** (gray color, **D)** and methotrexate (yellow color)**.** Residues color: Arg-300 (gray), Tyr-452 (purple), Tyr-455 (orange), Ser-385 (cyan).
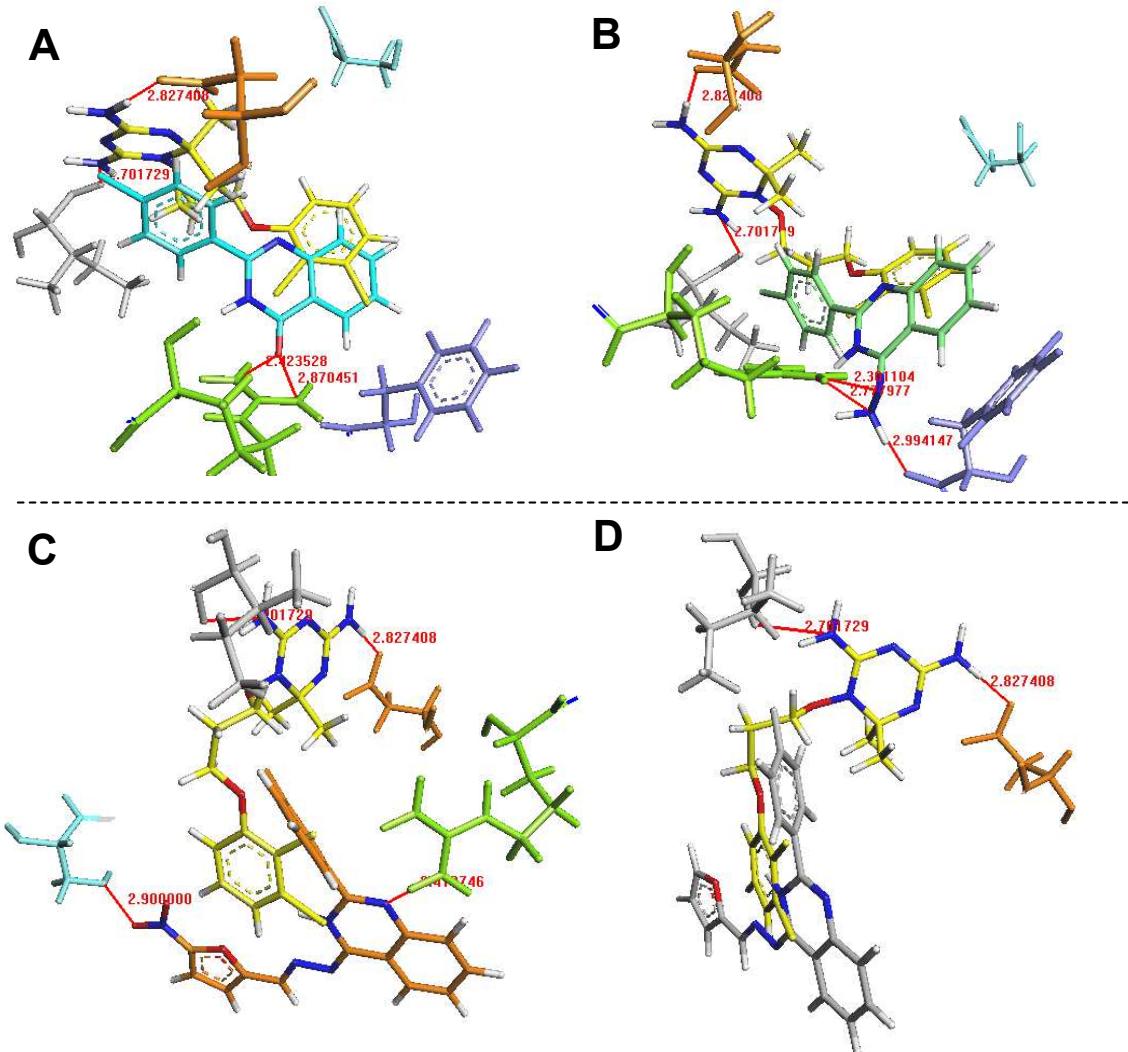
Figure S6. H-Interaction in the binding site of the DHFR-TS/*T. cruzi* protein for the compounds **1c** (cyan color, **A**), **2c** (green color, **B**), **3f** (orange color, **C**), **3h** (gray color, **D**) and C50 (yellow color). Residues color: Arg-300 (gray), Tyr-452 (purple), Tyr-455 (orange), Ser-385 (cyan).
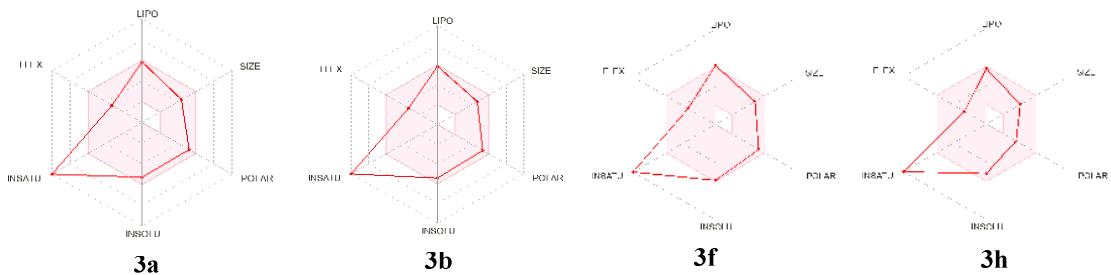
Figure S7. Druglikeness map for the most active (*E/Z*)-4-(2-((5-nitrofuran/furan-2-yl)methylene)hydrazineyl)-2-phenylquinazolines **3a, 3b, 3f** and **3h.**

Table S1. *In vitro* cytotoxicity using macrophage J774.1A of the compounds **3a, 3b and 3f** in absence and presence of Cu^{2+} and Fe^{3+} cations.

3a-h
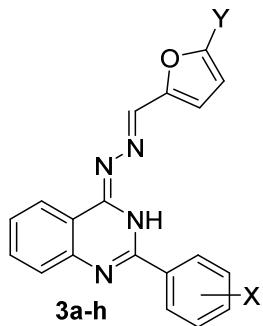
Entries	Compds	CC_{50} ($\pm$S.D.), macrophages J774.1A		
	(X, Y)	**No metal**	Fe^{3+}	Cu^{2+}
1	**2a** (H, NO$_2$)	**15.06 $\pm$ 0.11**	14.87 $\pm$ 0.89	14.78 $\pm$ 0.15
2	**2b** (4-F, NO$_2$)	**69.06 $\pm$ 3.99**	65.56 $\pm$ 2.79	64.45 $\pm$ 3.88
6	**2f** (3-Cl, NO$_2$)	**41.55 $\pm$ 1.87**	43.01 $\pm$ 1.99	40.01 $\pm$ 1.82
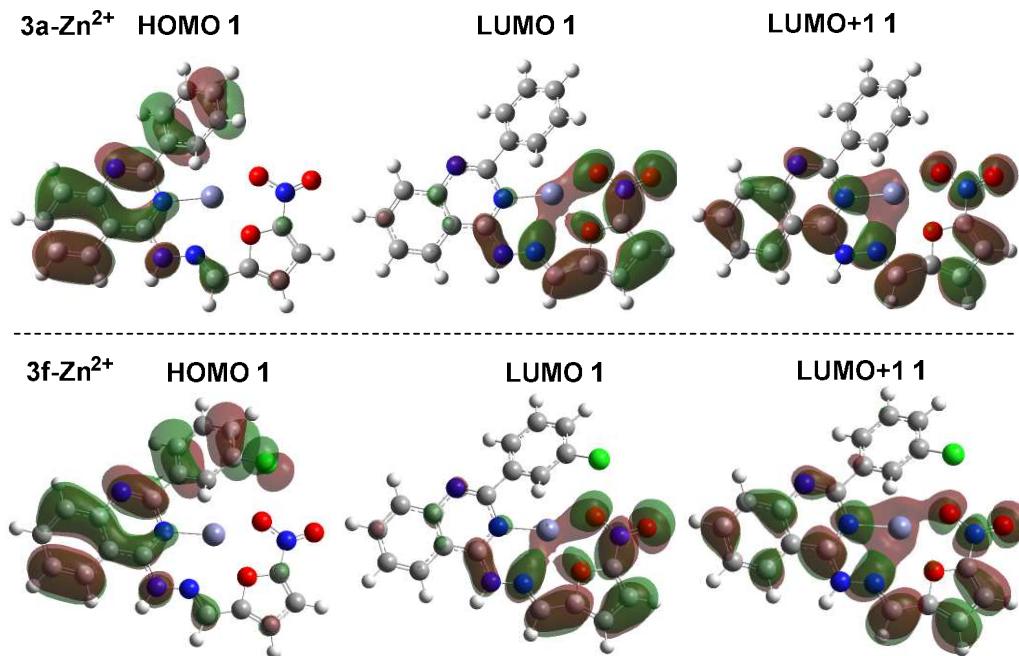
Figure S8. HOMO, LUMO and LUMO+1 orbital maps for (*E/Z*)-4-(2-((5-nitrofuran/furan-2-yl)methylene)hydrazineyl)-2-phenylquinazolines **3a** and **3f** in complexation with Zn (II) cation.
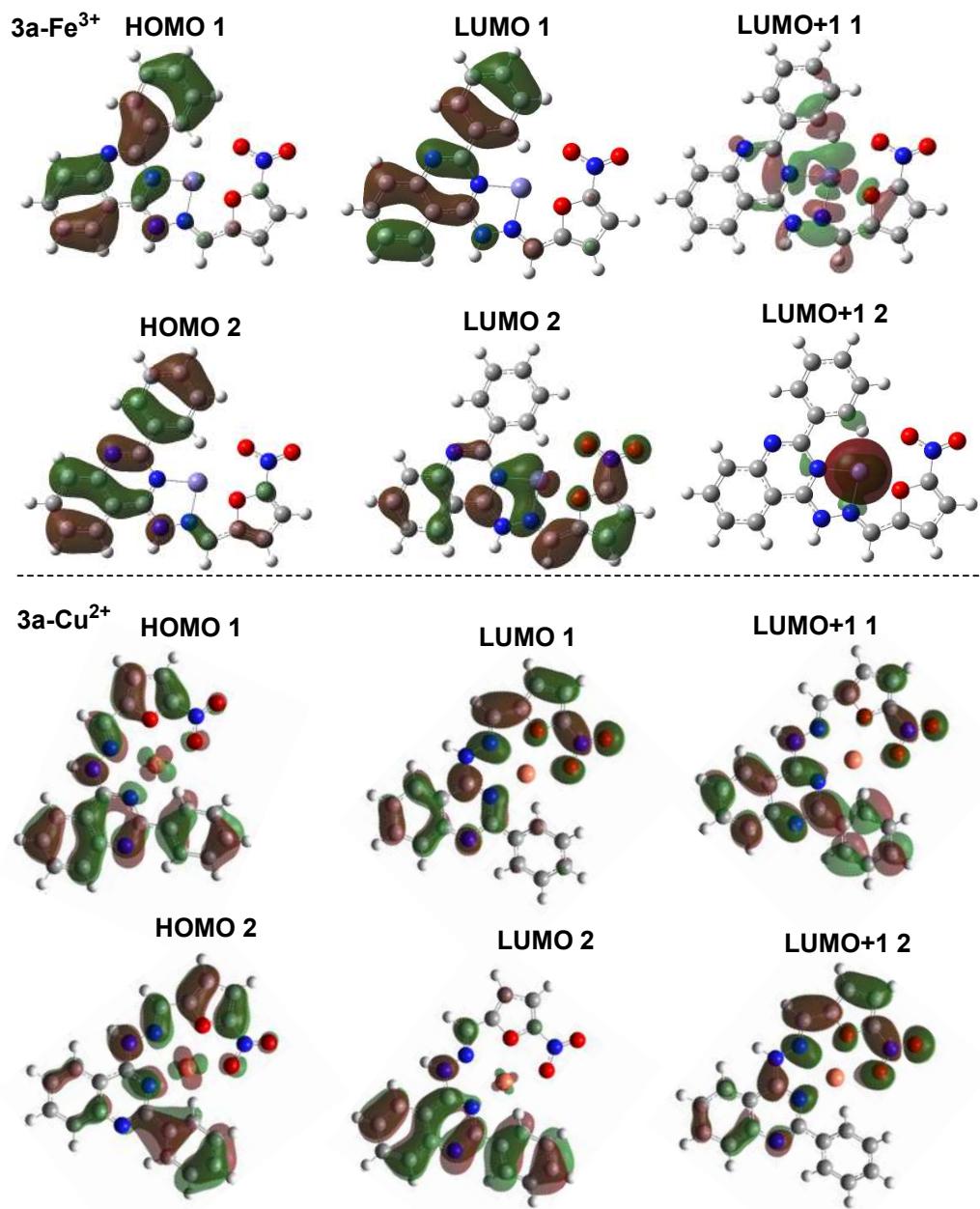
Figure S9. HOMO1, HOMO2, LUMO1, LUMO2, LUMO+1 1 and LUMO+1 2 orbital maps for (*E/Z*)-4-(2-((5-nitrofuran)methylene)hydrazineyl)-2-phenylquinazoline **3a** in complexation with Fe (III) and Cu (II) cations.

8. References

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9. Theoretical Output of the tested compounds

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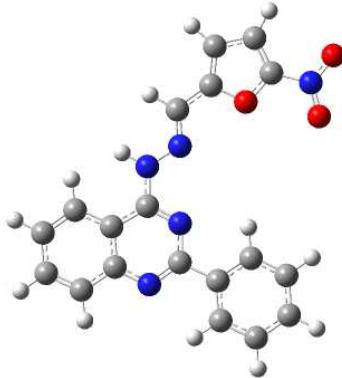
Optimized geometry:

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IRaf=   1 NMat= 1 IRICut=   1 DoRegI=T DoRafI=F ISym2E= 0.
FoFCou: FMM=F IPFlag=   0 FMFlag=   100000 FMFlg1=   0
NFxFlg=   0 DoJE=T BraDBF=F KetDBF=F FulRan=T
           wScrn= 0.000000 ICntrl=   500 IOpCl= 0 I1Cent=   0 NGrid=   0
           NMat0=   1 NMatS0=   1 NMatT0=   0 NMatD0=   1 NMtDS0=   0
      NMtDT0=   0
 Symmetry not used in FoFCou.
E= -1230.55631681931
DIIS: error= 2.45D-08 at cycle   1 NSaved=   1.
NSaved= 1 IEnMin= 1 EnMin= -1230.55631681931   IErMin= 1 ErrMin= 2.45D-08
ErrMax= 2.45D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.05D-13 BMatP= 2.05D-13
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: 0.100D+01
Coeff: 0.100D+01
Gap=   0.211 Goal= None   Shift=   0.000
RMSDP=2.49D-09 MaxDP=1.76D-07   OVMax= 3.53D-07

       SCF Done: E(RCAM-B3LYP) = -1230.55631682   A.U. after   1 cycles
           NFock= 1 Conv=0.25D-08   -V/T= 2.0087
 KE= 1.219914373228D+03 PE=-7.221
902069917D+03 EE= 2.592503998689D+03

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
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2	6	0	-2.954563	-3.208537	0.000052

3	6	0	-2.686385	-1.821562	-0.000014
4	6	0	-3.762476	-0.903235	0.000157
5	6	0	-5.087064	-1.401627	0.000363
6	6	0	-5.321820	-2.750722	0.000405
7	1	0	-4.446578	-4.731311	0.000293
8	1	0	-2.148096	-3.935518	-0.000059
9	6	0	-1.387872	-1.209100	-0.000234
10	1	0	-5.892852	-0.676872	0.000488
11	1	0	-6.340629	-3.124084	0.000566
12	6	0	-2.330169	0.870475	-0.000062
13	7	0	-3.570994	0.442532	0.000132
14	7	0	-1.222549	0.083180	-0.000251
15	7	0	-0.265759	-2.015098	-0.000416
16	7	0	0.969444	-1.496484	-0.000351
17	6	0	-2.084951	2.332841	-0.000082
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22	6	0	-2.930664	4.592630	-0.000019
23	1	0	-4.166683	2.825340	0.000101
24	6	0	-1.628076	5.083035	-0.000135
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30	1	0	1.828615	-3.400594	-0.000396
31	6	0	3.317430	-1.836498	-0.000221
32	6	0	4.504165	-2.522873	-0.000199
33	8	0	3.546671	-0.502928	-0.000057
34	6	0	5.533294	-1.547981	0.000010
35	1	0	4.618982	-3.596411	-0.000301
36	6	0	4.882191	-0.355819	0.000091
37	1	0	6.602288	-1.686636	0.000113
38	7	0	5.400556	0.974223	0.000341
39	8	0	4.608070	1.900720	0.000431
40	8	0	6.623022	1.066436	0.000448

Rotational constants (GHZ):   0.2387349   0.1058125   0.0733169
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2	O	-19.255362	29.033123
3	O	-19.252746	29.033049
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5	O	-14.495797	21.957540

6	O	-14.477339	21.963441
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10	O	-10.365160	15.882509
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21	O	-10.272431	15.878989
22	O	-10.255354	15.878273
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31	O	-1.139674	2.801317
32	O	-1.070953	1.829727
33	O	-0.991429	1.982037
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35	O	-0.936453	1.883855
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37	O	-0.926002	1.516875
38	O	-0.906575	1.966091
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41	O	-0.816748	1.767973
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75	O	-0.444451	0.986779
76	O	-0.432428	1.441849
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85	O	-0.361647	2.574561
86	O	-0.358156	1.998009
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88	O	-0.334427	1.177239
89	O	-0.311927	1.259548
90	O	-0.308095	1.961370
91	O	-0.292219	1.126889
92	O	-0.284047	1.451741
93	O	-0.264157	1.454084
94	V	-0.053086	2.099493
95	V	-0.017720	1.694727
96	V	0.001524	1.537037
97	V	0.017447	1.769876
98	V	0.058150	1.429273
99	V	0.066534	1.402748
100	V	0.092107	1.162844
101	V	0.092887	1.733979
102	V	0.107329	2.062734
103	V	0.129620	1.302956
104	V	0.130706	1.675283
105	V	0.148788	1.043257

106	V	0.154488	1.739024
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112	V	0.213953	0.992584
113	V	0.221608	1.304031
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115	V	0.234825	1.825129
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117	V	0.243577	1.499702
118	V	0.245597	1.880270
119	V	0.255569	1.321327
120	V	0.265275	1.663528
121	V	0.276529	2.001277
122	V	0.281462	1.832154
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125	V	0.317293	2.496474
126	V	0.319921	2.106588
127	V	0.328544	2.481173
128	V	0.339673	2.199009
129	V	0.353697	1.770153
130	V	0.361683	1.897543
131	V	0.369460	1.683645
132	V	0.376382	1.676387
133	V	0.389358	1.747554
134	V	0.400363	2.261689
135	V	0.406964	2.095531
136	V	0.410589	2.293334
137	V	0.422754	2.068847
138	V	0.435125	2.424773
139	V	0.446083	1.921894
140	V	0.455437	2.096622
141	V	0.475879	2.150113
142	V	0.487717	2.379440
143	V	0.499766	2.291772
144	V	0.527295	1.916007
145	V	0.536348	2.011109
146	V	0.544980	2.015283
147	V	0.549615	1.999376
148	V	0.560242	2.265120
149	V	0.569511	2.220763
150	V	0.577169	2.405859
151	V	0.577675	2.087241
152	V	0.584046	2.016016
153	V	0.593624	2.229647
154	V	0.598370	2.022356
155	V	0.605979	2.297783

156	V	0.609792	2.224202
157	V	0.616395	2.497419
158	V	0.619448	2.507731
159	V	0.623923	2.103889
160	V	0.624644	2.312509
161	V	0.638429	2.324492
162	V	0.638754	2.142609
163	V	0.640283	2.238112
164	V	0.642252	2.120406
165	V	0.646464	2.466125
166	V	0.655172	2.078376
167	V	0.657728	2.057375
168	V	0.660140	2.235149
169	V	0.663575	2.163947
170	V	0.666584	2.067811
171	V	0.666633	2.346748
172	V	0.669988	2.574207
173	V	0.671649	2.162151
174	V	0.677360	2.431237
175	V	0.686168	2.190194
176	V	0.690655	2.116317
177	V	0.691505	2.355032
178	V	0.696843	2.179643
179	V	0.706551	2.366096
180	V	0.708604	2.726565
181	V	0.711565	2.344903
182	V	0.726994	2.263825
183	V	0.737369	2.744100
184	V	0.737663	2.235686
185	V	0.741503	2.298633
186	V	0.755882	3.151033
187	V	0.768771	2.734082
188	V	0.800511	2.300391
189	V	0.806819	2.531126
190	V	0.814222	2.531299
191	V	0.826828	2.614755
192	V	0.827123	2.431380
193	V	0.833942	2.680873
194	V	0.839116	2.712874
195	V	0.846247	2.673759
196	V	0.850527	2.363022
197	V	0.852368	2.480438
198	V	0.868635	2.640231
199	V	0.872812	2.605910
200	V	0.875386	2.556870
201	V	0.877892	2.549191
202	V	0.880525	2.714491
203	V	0.890966	2.628719
204	V	0.898920	2.733250
205	V	0.900009	2.633047

206	V	0.903654	2.422021
207	V	0.917108	2.376339
208	V	0.926218	2.715227
209	V	0.930202	2.675454
210	V	0.938071	2.401485
211	V	0.952938	2.398159
212	V	0.960428	2.753105
213	V	0.966755	2.595909
214	V	0.980986	2.579293
215	V	0.983120	2.664179
216	V	0.986148	2.542085
217	V	0.986407	3.402680
218	V	1.000332	2.574362
219	V	1.017635	2.545882
220	V	1.025213	2.643838
221	V	1.025438	2.647638
222	V	1.028647	2.609779
223	V	1.037043	2.543466
224	V	1.043299	2.588435
225	V	1.053092	3.379903
226	V	1.060289	2.465242
227	V	1.077395	2.617526
228	V	1.085683	3.261972
229	V	1.092135	2.573530
230	V	1.099681	2.593077
231	V	1.106134	2.261148
232	V	1.132954	2.408776
233	V	1.137181	2.479309
234	V	1.147362	2.380910
235	V	1.153552	2.463513
236	V	1.168181	2.318273
237	V	1.172749	2.464352
238	V	1.199122	2.805460
239	V	1.218486	2.504759
240	V	1.229253	2.596471
241	V	1.245782	2.468516
242	V	1.262492	2.590680
243	V	1.271556	2.585333
244	V	1.272897	2.400977
245	V	1.281152	2.653276
246	V	1.284739	2.390131
247	V	1.291452	2.397148
248	V	1.311589	2.651529
249	V	1.320978	2.634880
250	V	1.335003	2.614010
251	V	1.341776	2.418074
252	V	1.346665	2.478151
253	V	1.347909	2.668855
254	V	1.361050	2.478371
255	V	1.366045	2.440721

256	V	1.368824	2.567196
257	V	1.368964	2.506885
258	V	1.385820	2.497366
259	V	1.392192	2.506755
260	V	1.401886	2.830772
261	V	1.403088	2.452365
262	V	1.434394	2.462476
263	V	1.441490	2.728140
264	V	1.450329	2.531560
265	V	1.458266	2.534226
266	V	1.464364	2.594638
267	V	1.469309	2.561340
268	V	1.471168	2.730676
269	V	1.471910	2.682819
270	V	1.480485	2.587199
271	V	1.490012	2.497098
272	V	1.505176	2.543725
273	V	1.509752	2.564000
274	V	1.520999	2.713287
275	V	1.529482	2.623032
276	V	1.530389	2.662662
277	V	1.545658	2.752739
278	V	1.566608	2.726907
279	V	1.578003	2.687769
280	V	1.582015	2.694930
281	V	1.601294	2.701020
282	V	1.604183	3.014709
283	V	1.652533	2.967392
284	V	1.662998	2.985434
285	V	1.679546	3.166665
286	V	1.685988	2.738987
287	V	1.709596	3.055133
288	V	1.720354	3.025443
289	V	1.780743	2.840692
290	V	1.797913	3.010374
291	V	1.808946	3.174274
292	V	1.828465	2.912205
293	V	1.830416	3.076220
294	V	1.846093	3.171569
295	V	1.859081	3.152298
296	V	1.873254	3.201091
297	V	1.874373	3.324163
298	V	1.876512	2.864943
299	V	1.878864	3.158232
300	V	1.880546	2.927790
301	V	1.892690	3.209320
302	V	1.895270	2.971777
303	V	1.911126	3.164800
304	V	1.912792	3.197970
305	V	1.939442	3.235603

306	V	1.948428	3.248962
307	V	1.957503	3.194681
308	V	1.964624	3.413394
309	V	1.965343	3.273422
310	V	1.976792	3.251857
311	V	1.977402	3.180336
312	V	1.977880	3.041843
313	V	1.983504	3.094635
314	V	1.993830	3.300405
315	V	2.004248	3.497718
316	V	2.021614	3.433455
317	V	2.021914	3.093576
318	V	2.025985	3.356012
319	V	2.034567	3.152300
320	V	2.049236	3.463463
321	V	2.056390	2.994483
322	V	2.061664	3.324144
323	V	2.063197	3.026678
324	V	2.065842	3.507822
325	V	2.088008	3.017403
326	V	2.089048	3.502572
327	V	2.111247	3.364867
328	V	2.124090	3.457253
329	V	2.135253	3.216723
330	V	2.141421	3.497282
331	V	2.150619	3.419796
332	V	2.151253	3.183256
333	V	2.158288	3.421475
334	V	2.163477	3.794898
335	V	2.190936	3.661396
336	V	2.213232	3.810470
337	V	2.217672	3.365791
338	V	2.232734	3.591633
339	V	2.236411	3.356972
340	V	2.247621	3.373697
341	V	2.269915	3.693200
342	V	2.279517	3.757159
343	V	2.304292	3.478873
344	V	2.313254	3.798165
345	V	2.324228	3.426642
346	V	2.332534	3.501681
347	V	2.334612	3.919275
348	V	2.347148	3.513842
349	V	2.380356	3.907688
350	V	2.383400	3.504772
351	V	2.388339	3.550370
352	V	2.396614	3.520518
353	V	2.405325	3.528737
354	V	2.410619	3.838565
355	V	2.418267	3.760519

356	V	2.426090	3.888281
357	V	2.434309	3.779604
358	V	2.436818	3.384645
359	V	2.446819	3.363965
360	V	2.455308	3.630472
361	V	2.456792	3.355903
362	V	2.463850	3.586057
363	V	2.481597	3.455175
364	V	2.484509	3.757801
365	V	2.496476	3.432081
366	V	2.505178	3.493979
367	V	2.512521	3.928539
368	V	2.517155	3.602828
369	V	2.524388	3.891879
370	V	2.531726	3.832741
371	V	2.534529	3.543540
372	V	2.535175	3.732731
373	V	2.555748	3.910917
374	V	2.582152	3.918699
375	V	2.587863	3.765258
376	V	2.590438	4.019457
377	V	2.606736	4.007792
378	V	2.615041	3.707744
379	V	2.619822	4.171649
380	V	2.629704	3.962986
381	V	2.641336	4.138348
382	V	2.644172	3.641385
383	V	2.649582	4.030950
384	V	2.661641	3.649919
385	V	2.684138	4.009273
386	V	2.688667	3.880254
387	V	2.690277	3.710765
388	V	2.703192	3.749335
389	V	2.723966	4.018082
390	V	2.740080	4.534533
391	V	2.747905	4.211382
392	V	2.749800	3.949999
393	V	2.764539	4.273624
394	V	2.768275	3.914204
395	V	2.777612	3.913308
396	V	2.784921	3.892050
397	V	2.793623	4.298772
398	V	2.801949	4.452530
399	V	2.803417	3.988729
400	V	2.807060	4.321753
401	V	2.845123	4.390442
402	V	2.850468	3.842045
403	V	2.860759	4.426630
404	V	2.873395	4.070742
405	V	2.874678	4.487622

406	V	2.888190	4.410671
407	V	2.890381	4.466917
408	V	2.912901	4.599377
409	V	2.940138	4.694522
410	V	2.952939	4.893560
411	V	2.967014	5.087709
412	V	2.968645	4.707443
413	V	2.978864	4.657702
414	V	2.997752	4.684201
415	V	3.009750	4.585472
416	V	3.056215	4.644355
417	V	3.094806	4.866710
418	V	3.143427	4.842014
419	V	3.146174	4.752384
420	V	3.161433	4.454877
421	V	3.177986	5.011225
422	V	3.223055	4.964650
423	V	3.253123	4.890087
424	V	3.274948	5.012196
425	V	3.293087	4.950015
426	V	3.303558	4.949161
427	V	3.326610	4.868040
428	V	3.330407	4.868692
429	V	3.331507	5.026529
430	V	3.351525	4.878779
431	V	3.364616	5.199192
432	V	3.411950	5.114060
433	V	3.430196	5.328903
434	V	3.505772	5.226091
435	V	3.526206	5.280920
436	V	3.543233	5.354146
437	V	3.581179	5.506904
438	V	3.603979	5.692776
439	V	3.622232	5.449428
440	V	3.685213	5.976144
441	V	3.764619	8.618362
442	V	3.786518	7.693065
443	V	3.933282	8.779196
444	V	3.935529	7.423514
445	V	3.973838	9.989864
446	V	4.008732	6.039206
447	V	4.082369	10.396891
448	V	4.129006	10.209396
449	V	4.161222	10.146942
450	V	4.190426	10.090022
451	V	4.197749	10.113033
452	V	4.209641	10.125430
453	V	4.219236	10.105138
454	V	4.226328	10.142707
455	V	4.246625	10.157609

456	V	4.272289	10.187873
457	V	4.373992	10.084415
458	V	4.381707	10.118418
459	V	4.395858	9.994798
460	V	4.437588	10.600591
461	V	4.504305	10.429617
462	V	4.522439	10.075595
463	V	4.523967	10.256895
464	V	4.574131	10.511127
465	V	4.589307	10.878250
466	V	4.642807	10.025514
467	V	4.775660	11.103655
468	V	4.827527	10.299130
469	V	4.911218	10.206319
470	V	4.970058	10.227859

Total kinetic energy from orbitals= 1.219914374160D+03

9.2. (*E/Z*)-4-(2-((5-nitrofuran-2-yl)methylene)hydrazineyl)-2-phenylquinazolines **3a** in complex with Fe(III)
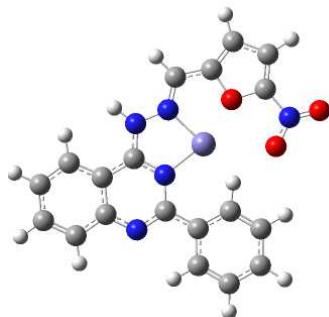
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-5.242032	-2.486374	0.000111
2	6	0	-3.843083	-2.553370	-0.000795
3	6	0	-3.093082	-1.380376	-0.000209
4	6	0	-3.768421	-0.111198	0.001259
5	6	0	-5.190757	-0.075003	0.002258
6	6	0	-5.910773	-1.254054	0.001669
7	1	0	-5.814804	-3.408544	-0.000413
8	1	0	-3.382171	-3.536253	-0.002044
9	6	0	-1.666019	-1.298680	-0.000888
10	1	0	-5.676044	0.895240	0.003403
11	1	0	-6.995681	-1.230682	0.002372
12	6	0	-1.780133	1.062131	0.000483
13	7	0	-3.106857	1.049127	0.001613
14	7	0	-1.029863	-0.110250	-0.000616

15	7	0	-0.861492	-2.388335	-0.001726
16	7	0	0.481046	-2.134084	-0.001698
17	6	0	-1.109710	2.328481	0.000195
18	6	0	0.300295	2.460902	-0.001775
19	6	0	-1.896980	3.520305	0.001843
20	6	0	0.903999	3.688180	-0.002024
21	1	0	1.002312	1.617810	-0.003169
22	6	0	-1.294535	4.762322	0.001604
23	1	0	-2.975725	3.425378	0.003330
24	6	0	0.096773	4.856717	-0.000318
25	1	0	1.985311	3.769327	-0.003490
26	1	0	-1.901303	5.661108	0.002910
27	1	0	0.577731	5.830641	-0.000526
28	1	0	-1.204420	-3.343514	-0.001422
29	6	0	1.420658	-3.025665	0.000162
30	1	0	1.239756	-4.099887	0.001184
31	6	0	2.751413	-2.490729	0.001054
32	6	0	4.040701	-2.928569	0.002413
33	8	0	2.744056	-1.093229	0.000713
34	6	0	4.886823	-1.766792	0.002854
35	1	0	4.374623	-3.959473	0.003037
36	6	0	4.055413	-0.704596	0.001690
37	1	0	5.969665	-1.740455	0.003801
38	7	0	4.223388	0.723081	0.000737
39	8	0	3.163524	1.365750	-0.001620
40	8	0	5.341212	1.155881	0.002176
41	26	0	0.880906	-0.265633	-0.002953

 Rotational constants (GHZ):   0.2560772   0.1300303   0.0862397

 Cycle   8 Pass 1 IDiag 1:
 RMSU= 1.92D-08   CP: 1.00D+00 1.04D+00 8.33D-01 1.04D+00 7.44D-01
 E= -1230.50034853501   Delta-E=   -0.000000000166 Rises=F Damp=F
 DIIS: error= 9.90D-08 at cycle   6 NSaved=   6.
 NSaved= 6 IEnMin= 6 EnMin= -1230.50034853501   IErMin= 6 ErrMin= 9.90D-08
 ErrMax= 9.90D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.29D-11 BMatP= 5.56D-
10
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com: 0.727D-03-0.276D-01-0.948D-02 0.128D+00 0.293D+00 0.615D+00
 Coeff: 0.727D-03-0.276D-01-0.948D-02 0.128D+00 0.293D+00 0.615D+00
 Gap=   0.197 Goal= None   Shift=   0.000
 Gap=   0.197 Goal= None   Shift=   0.000
 RMSDP=7.77D-09 MaxDP=4.12D-07 DE=-1.66D-10 OVMax= 8.61D-07

 SCF Done: E(UCAM-B3LYP) = -1230.50034854   A.U. after   8 cycles
        NFock= 8 Conv=0.78D-08   -V/T= 2.0066
 <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.0000 <S**2>= 0.0000 S= 0.0000
 <L.S>= 0.000000000000E+00
 KE= 1.222477580584D+03 PE=-7.379816511258D+03 EE= 2.670955262334D+03
 Annihilation of the first spin contaminant:

S**2 before annihilation   0.0000,   after   0.0000

Leave Link   502 at Wed Nov 2 12:11:04 2022, MaxMem= 2147483648 cpu: 1626.2

(Enter /opt/gaussian/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

Leave Link 701 at Wed Nov 2 12:11:04 2022, MaxMem= 2147483648 cpu: 4.7

(Enter /opt/gaussian/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Wed Nov 2 12:11:04 2022, MaxMem= 2147483648 cpu: 0.9

(Enter /opt/gaussian/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT=   0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl=   2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl=   2127 DoSepK=T KAlg= 0 I1Cent=   0 FoldK=F

IRaf=   1 NMat= 1 IRICut=   1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag=   0 FMFlag=   100000 FMFlg1=   800

      NFxFlg=   0 DoJE=F BraDBF=F KetDBF=F FulRan=T

      wScrn= 0.000000 ICntrl=   2527 IOpCl= 0 I1Cent=   0 NGrid=   0

      NMat0=   1 NMatS0=   1 NMatT0=   0 NMatD0=   1 NMtDS0=   0

NMtDT0=   0

Symmetry not used in FoFCou.

Leave Link   703 at Wed Nov 2 12:12:46 2022, MaxMem= 2147483648 cpu: 809.6

(Enter /opt/gaussian/g09/l716.exe)

Dipole   =-1.29672797D-01-3.25664643D+00 1.35986156D-03

***** Axes restored to original set *****

Cartesian Forces: Max   0.067369325 RMS   0.016207602

Leave Link 716 at Wed Nov 2 12:12:46 2022, MaxMem= 2147483648 cpu: 0.7

(Enter /opt/gaussian/g09/l122.exe)

CPIOFr: IOpCl= 1 IRwI=-1 IRwCP= 731 ICalc= 4 LCPTot=   338287 Len1MO= 1090774 IndFrg=   5792157

Restoring MOs from calculation   1 to rwf.

CPIOFr: IOpCl= 1 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot=   338287 Len1MO= 1090774 IndFrg=   1429061

Counterpoise corrected energy =   -1352.996105014944

        BSSE energy =   -0.133081306096

      sum of monomers = -1351.538250634977

    complexation energy =   -831.31 kcal/mole (raw)

    complexation energy =   -914.82 kcal/mole (corrected)

Leave Link 122 at Wed Nov 2 12:12:46 2022, MaxMem= 2147483648 cpu: 0.5

(Enter /opt/gaussian/g09/l716.exe)

Rotating derivatives to standard orientation.

Dipole   =-1.69536516D+00-3.17169454D+00 6.32188506D-04

Orbital energies and kinetic energies (alpha):

		1	2
1	O	-19.725999	29.117625
2	O	-19.615450	29.122444

3	O	-19.607622	29.122516
4	O	-15.013875	22.048548
5	O	-14.908169	22.049812
6	O	-14.898917	22.046686
7	O	-14.846432	22.050308
8	O	-14.792328	22.051931
9	O	-10.778748	15.952939
10	O	-10.748922	15.951033
11	O	-10.746688	15.952331
12	O	-10.738365	15.952842
13	O	-10.729926	15.951556
14	O	-10.685495	15.953429
15	O	-10.668665	15.953898
16	O	-10.663897	15.953852
17	O	-10.659195	15.953016
18	O	-10.656132	15.956154
19	O	-10.649595	15.954179
20	O	-10.648595	15.953350
21	O	-10.631688	15.955890
22	O	-10.626759	15.955572
23	O	-10.625289	15.956814
24	O	-10.625222	15.955156
25	O	-10.621238	15.954127
26	O	-10.618608	15.953086
27	O	-10.600252	15.952865
28	O	-4.055218	2.062319
29	O	-2.857638	3.846621
30	O	-2.854500	3.839228
31	O	-2.794204	3.831054
32	O	-1.680834	2.483759
33	O	-1.624474	2.512326
34	O	-1.554724	1.970040
35	O	-1.500407	2.793228
36	O	-1.471322	1.851732
37	O	-1.399296	1.950125
38	O	-1.359368	1.970460
39	O	-1.318314	1.608539
40	O	-1.298422	1.596475
41	O	-1.296847	1.793869
42	O	-1.278169	1.934486
43	O	-1.236776	1.671735
44	O	-1.221066	1.636960
45	O	-1.192783	1.610137
46	O	-1.187467	1.860525
47	O	-1.171675	1.721987
48	O	-1.142448	1.655797
49	O	-1.127957	1.921664
50	O	-1.097303	1.765186
51	O	-1.092181	1.677197
52	O	-1.073626	1.678586

53	O	-1.052777	1.729220
54	O	-1.043373	1.575129
55	O	-1.036129	1.620676
56	O	-1.033617	1.779564
57	O	-1.006209	1.745057
58	O	-0.994218	2.173078
59	O	-0.986464	1.674808
60	O	-0.984822	1.546503
61	O	-0.969786	1.557704
62	O	-0.959529	1.729386
63	O	-0.956818	1.466531
64	O	-0.950551	1.769797
65	O	-0.936513	1.959690
66	O	-0.928662	2.485749
67	O	-0.911167	1.946757
68	O	-0.903898	1.787401
69	O	-0.896521	1.484573
70	O	-0.890759	1.610668
71	O	-0.885839	1.726579
72	O	-0.872683	1.671983
73	O	-0.869858	1.590609
74	O	-0.867225	1.649324
75	O	-0.864196	1.660061
76	O	-0.861063	1.524651
77	O	-0.849866	1.819898
78	O	-0.845948	1.734609
79	O	-0.841456	5.480043
80	O	-0.838473	1.566887
81	O	-0.815953	1.548538
82	O	-0.802711	5.266880
83	O	-0.801551	6.099777
84	O	-0.800500	1.823689
85	O	-0.786051	5.477361
86	O	-0.780320	1.668169
87	O	-0.778322	1.530444
88	O	-0.765951	1.588466
89	O	-0.762543	1.743048
90	O	-0.759227	1.475649
91	O	-0.744128	1.883216
92	O	-0.731350	1.548754
93	O	-0.730559	2.558892
94	O	-0.721512	2.388202
95	O	-0.717191	2.648495
96	O	-0.703598	2.101061
97	O	-0.691131	1.377670
98	O	-0.667273	1.483807
99	O	-0.664198	1.212606
100	O	-0.644860	1.262359
101	V	-0.505954	1.317669
102	V	-0.445949	6.062714

103	V	-0.441435	1.703432
104	V	-0.381065	1.989403
105	V	-0.379405	1.486830
106	V	-0.357456	2.049308
107	V	-0.329752	1.466935
108	V	-0.308217	0.907192
109	V	-0.290288	1.362699
110	V	-0.281858	1.296995
111	V	-0.275509	0.806855
112	V	-0.273710	1.693378
113	V	-0.266556	1.888517
114	V	-0.262297	0.574262
115	V	-0.235606	1.688878
116	V	-0.231008	1.599579
117	V	-0.230396	1.134229
118	V	-0.215883	1.686833
119	V	-0.197458	1.554918
120	V	-0.194651	0.668903
121	V	-0.179745	1.492663
122	V	-0.171204	1.645297
123	V	-0.164811	1.935887
124	V	-0.162067	1.341651
125	V	-0.151144	1.304282
126	V	-0.143469	1.426323
127	V	-0.126786	1.506638
128	V	-0.122467	1.758065
129	V	-0.117413	2.133386
130	V	-0.106973	1.298734
131	V	-0.104631	1.738354
132	V	-0.101216	1.508951
133	V	-0.097872	1.974980
134	V	-0.091395	1.595478
135	V	-0.085679	2.057295
136	V	-0.079091	1.425026
137	V	-0.070286	1.707479
138	V	-0.060950	2.021287
139	V	-0.052250	1.460069
140	V	-0.046083	1.773813
141	V	-0.041700	1.804650
142	V	-0.033386	1.950559
143	V	-0.026935	1.416222
144	V	-0.022573	2.281758
145	V	-0.012226	2.060543
146	V	0.000403	1.936787
147	V	0.005943	1.935640
148	V	0.016804	2.053504
149	V	0.029565	2.061204
150	V	0.032925	1.796022
151	V	0.045991	2.126938
152	V	0.051167	1.837459

153	V	0.058428	2.386335
154	V	0.062618	2.334044
155	V	0.078057	2.214539
156	V	0.092128	1.926837
157	V	0.097638	2.335867
158	V	0.109178	2.232222
159	V	0.121625	2.626771
160	V	0.145862	2.497562
161	V	0.154913	2.370867
162	V	0.167001	2.458201
163	V	0.172298	2.088389
164	V	0.178518	2.316317
165	V	0.201347	2.602924
166	V	0.209055	2.229521
167	V	0.212637	2.495803
168	V	0.220723	2.304288
169	V	0.223971	2.148015
170	V	0.232865	2.129639
171	V	0.238378	2.291467
172	V	0.247483	2.461494
173	V	0.247994	2.186031
174	V	0.254246	2.061179
175	V	0.260718	2.115331
176	V	0.261864	2.299058
177	V	0.266722	2.439096
178	V	0.270701	2.214174
179	V	0.272232	2.136924
180	V	0.276984	2.337271
181	V	0.288420	2.529953
182	V	0.291651	2.767264
183	V	0.297822	2.137891
184	V	0.299175	2.574636
185	V	0.311901	2.308002
186	V	0.315740	2.065213
187	V	0.317179	2.239170
188	V	0.323253	2.236005
189	V	0.328550	2.131084
190	V	0.334095	2.470813
191	V	0.340947	2.187358
192	V	0.341754	2.093181
193	V	0.345258	2.321355
194	V	0.348357	2.419861
195	V	0.353472	2.180410
196	V	0.357281	2.404671
197	V	0.358838	2.161010
198	V	0.372787	2.388776
199	V	0.376786	2.209393
200	V	0.379384	2.259132
201	V	0.389857	2.217511
202	V	0.411015	2.378869

203	V	0.414472	2.722229
204	V	0.420786	2.349409
205	V	0.439884	2.854138
206	V	0.443437	2.306738
207	V	0.455045	2.542250
208	V	0.457369	2.403893
209	V	0.466210	2.495815
210	V	0.478795	2.678058
211	V	0.487520	2.384113
212	V	0.496949	2.561522
213	V	0.503545	2.484618
214	V	0.508324	2.637562
215	V	0.517225	2.763717
216	V	0.522411	2.545279
217	V	0.531950	2.813647
218	V	0.538336	2.373160
219	V	0.544955	2.586596
220	V	0.548185	2.619375
221	V	0.549476	2.752552
222	V	0.556809	2.760444
223	V	0.560228	2.635170
224	V	0.567221	2.617151
225	V	0.573679	2.713667
226	V	0.578153	2.696091
227	V	0.579135	2.743564
228	V	0.581108	2.609284
229	V	0.595247	2.598546
230	V	0.609580	2.523471
231	V	0.618429	2.499082
232	V	0.622221	2.503344
233	V	0.633828	2.589292
234	V	0.640055	2.577333
235	V	0.648010	2.582601
236	V	0.650873	2.641091
237	V	0.657619	3.259232
238	V	0.658248	2.595538
239	V	0.672113	2.715689
240	V	0.680270	3.069574
241	V	0.682318	2.756897
242	V	0.699346	2.879818
243	V	0.714060	2.736442
244	V	0.715559	2.614503
245	V	0.726160	2.571686
246	V	0.728033	3.212311
247	V	0.740597	2.584058
248	V	0.751834	3.190808
249	V	0.752404	2.641515
250	V	0.759423	2.534729
251	V	0.778948	2.481005
252	V	0.788085	2.403526

253	V	0.789357	2.579464
254	V	0.799588	2.349394
255	V	0.835709	2.513785
256	V	0.837552	2.772580
257	V	0.860948	2.537130
258	V	0.863310	2.761494
259	V	0.872374	2.625637
260	V	0.883436	2.401193
261	V	0.904773	2.535514
262	V	0.915287	2.406066
263	V	0.927648	2.564547
264	V	0.931591	2.435626
265	V	0.942760	2.797818
266	V	0.943037	2.744833
267	V	0.945881	2.490111
268	V	0.961862	2.765359
269	V	0.962043	2.437895
270	V	0.976237	2.765423
271	V	0.977268	2.457878
272	V	0.988883	2.752419
273	V	0.990784	2.499906
274	V	0.992548	2.472946
275	V	1.000313	2.798979
276	V	1.008881	2.527979
277	V	1.016900	2.810098
278	V	1.033487	2.524018
279	V	1.056877	2.446619
280	V	1.065994	3.011883
281	V	1.067843	2.454819
282	V	1.074438	2.765494
283	V	1.087801	3.009835
284	V	1.092773	2.551947
285	V	1.116280	3.027231
286	V	1.117105	2.518992
287	V	1.119689	2.568451
288	V	1.124652	2.658239
289	V	1.130903	2.597791
290	V	1.136914	2.937049
291	V	1.137949	2.555793
292	V	1.144469	2.550672
293	V	1.163907	2.675457
294	V	1.168211	2.861560
295	V	1.177962	2.663756
296	V	1.178846	2.732983
297	V	1.190090	2.979929
298	V	1.222027	3.133586
299	V	1.228398	3.084803
300	V	1.252127	2.814961
301	V	1.268445	2.795720
302	V	1.286746	3.071777

303	V	1.300708	2.887396
304	V	1.319279	2.891339
305	V	1.336180	3.081818
306	V	1.355090	3.008549
307	V	1.385509	3.334332
308	V	1.409647	3.198423
309	V	1.417458	2.838041
310	V	1.442364	2.895337
311	V	1.444936	3.447114
312	V	1.452202	3.306048
313	V	1.465560	3.409503
314	V	1.485320	3.372181
315	V	1.485789	3.279491
316	V	1.488535	2.924178
317	V	1.489238	3.343213
318	V	1.502995	3.350389
319	V	1.507310	2.941332
320	V	1.513304	3.300804
321	V	1.528096	2.862281
322	V	1.538355	3.302720
323	V	1.545985	3.332780
324	V	1.560982	3.273397
325	V	1.566390	3.363770
326	V	1.585481	3.347289
327	V	1.588270	3.488968
328	V	1.600136	3.054866
329	V	1.602001	3.304722
330	V	1.612083	3.436147
331	V	1.617593	3.360663
332	V	1.621226	3.257210
333	V	1.629509	3.088313
334	V	1.630240	3.242724
335	V	1.644606	3.437003
336	V	1.647906	3.470286
337	V	1.648951	3.070041
338	V	1.654673	3.431936
339	V	1.656813	3.280901
340	V	1.685512	3.503711
341	V	1.694549	3.040722
342	V	1.699213	3.393601
343	V	1.705053	3.464476
344	V	1.713858	3.494784
345	V	1.718861	3.062339
346	V	1.724262	3.049269
347	V	1.726894	3.368891
348	V	1.748958	3.615536
349	V	1.751326	3.088192
350	V	1.764163	3.219317
351	V	1.766715	3.431010
352	V	1.769516	3.513136

353	V	1.785495	3.595908
354	V	1.797465	3.321447
355	V	1.804227	3.524803
356	V	1.829563	3.823998
357	V	1.836211	3.669922
358	V	1.851972	3.348676
359	V	1.858817	3.671675
360	V	1.873618	3.791491
361	V	1.878783	3.805872
362	V	1.886166	3.373228
363	V	1.902343	3.437323
364	V	1.907205	3.770224
365	V	1.931401	3.886624
366	V	1.933876	3.481648
367	V	1.946303	3.496302
368	V	1.959847	3.870180
369	V	1.967392	3.481123
370	V	1.992652	3.898077
371	V	1.993979	3.498727
372	V	2.004823	3.532115
373	V	2.009055	3.889564
374	V	2.026351	3.529427
375	V	2.048448	3.604485
376	V	2.056792	3.479889
377	V	2.062561	3.773978
378	V	2.073937	3.594493
379	V	2.079362	3.565978
380	V	2.098230	3.504181
381	V	2.103883	3.923988
382	V	2.113407	3.737679
383	V	2.120343	3.910998
384	V	2.126566	3.310859
385	V	2.135071	3.558331
386	V	2.140689	3.874503
387	V	2.143340	3.331411
388	V	2.149080	3.740855
389	V	2.151199	3.437617
390	V	2.165870	3.795501
391	V	2.169940	3.590385
392	V	2.183695	3.831593
393	V	2.195384	3.821878
394	V	2.198049	3.605653
395	V	2.205263	3.962665
396	V	2.212581	3.889933
397	V	2.236581	4.041802
398	V	2.239010	3.713227
399	V	2.252568	4.075363
400	V	2.261248	4.112319
401	V	2.282174	3.991137
402	V	2.282565	3.645519

403	V	2.291822	3.972493
404	V	2.298036	3.816409
405	V	2.298947	4.064520
406	V	2.305321	3.638270
407	V	2.324266	3.835158
408	V	2.325761	4.027363
409	V	2.331546	3.601514
410	V	2.354983	4.078677
411	V	2.367915	4.208733
412	V	2.367951	3.931468
413	V	2.377003	4.240779
414	V	2.391888	3.924674
415	V	2.406940	4.230897
416	V	2.412177	3.899045
417	V	2.417164	3.917994
418	V	2.418031	4.235290
419	V	2.437494	4.452158
420	V	2.448452	4.290225
421	V	2.461671	4.009787
422	V	2.469501	4.490858
423	V	2.482105	3.828875
424	V	2.485314	4.341950
425	V	2.491320	3.940307
426	V	2.499585	4.355874
427	V	2.517645	4.395769
428	V	2.535329	4.301360
429	V	2.571211	4.550041
430	V	2.583796	4.546724
431	V	2.589804	4.607555
432	V	2.608231	4.536599
433	V	2.621306	4.619231
434	V	2.646819	4.649423
435	V	2.672994	4.922281
436	V	2.684960	4.590537
437	V	2.722440	4.759097
438	V	2.726505	4.797914
439	V	2.764493	4.745304
440	V	2.768495	4.621065
441	V	2.810351	4.766895
442	V	2.834845	4.806688
443	V	2.858769	4.877247
444	V	2.879041	5.068993
445	V	2.902830	4.891145
446	V	2.932950	4.937791
447	V	2.960222	4.786317
448	V	2.965702	4.896956
449	V	2.989036	4.847695
450	V	2.999648	4.843563
451	V	3.014519	5.023087
452	V	3.020850	5.051630

453	V	3.070756	5.024542
454	V	3.074954	5.144190
455	V	3.138916	5.100621
456	V	3.173660	5.201703
457	V	3.198624	5.210353
458	V	3.227155	5.259857
459	V	3.259817	5.352553
460	V	3.265638	5.275790
461	V	3.322583	5.550470
462	V	3.471395	5.539669
463	V	3.601946	5.634618
464	V	3.649144	5.649988
465	V	7.504365	3.566019

Orbital energies and kinetic energies (beta):

		1	2
1	O	-19.725731	29.117844
2	O	-19.615554	29.122358
3	O	-19.607654	29.122495
4	O	-15.013825	22.048584
5	O	-14.908934	22.049414
6	O	-14.899300	22.046373
7	O	-14.846738	22.050196
8	O	-14.796679	22.048265
9	O	-10.778880	15.952811
10	O	-10.749252	15.950764
11	O	-10.747032	15.952039
12	O	-10.737612	15.953408
13	O	-10.729738	15.951712
14	O	-10.684813	15.953920
15	O	-10.668907	15.953692
16	O	-10.664669	15.953181
17	O	-10.658942	15.953231
18	O	-10.658450	15.954131
19	O	-10.650209	15.953601
20	O	-10.648506	15.953382
21	O	-10.634547	15.953398
22	O	-10.630219	15.952571
23	O	-10.628610	15.953821
24	O	-10.627121	15.953524
25	O	-10.622007	15.953455
26	O	-10.616791	15.954613
27	O	-10.599098	15.953808
28	O	-3.950766	2.056192
29	O	-2.744683	3.823895
30	O	-2.733049	3.823474
31	O	-2.693078	3.843371
32	O	-1.680867	2.484005
33	O	-1.623938	2.510382
34	O	-1.555584	1.972458
35	O	-1.500524	2.793377

36	O	-1.473643	1.851329
37	O	-1.402655	1.965296
38	O	-1.361609	1.974955
39	O	-1.321995	1.602216
40	O	-1.303182	1.549971
41	O	-1.296993	1.839171
42	O	-1.279139	1.935965
43	O	-1.239454	1.671939
44	O	-1.224321	1.639435
45	O	-1.193977	1.601154
46	O	-1.189752	1.821809
47	O	-1.180024	1.770144
48	O	-1.145238	1.651461
49	O	-1.128222	1.924312
50	O	-1.100258	1.759860
51	O	-1.092352	1.657777
52	O	-1.075171	1.685870
53	O	-1.052557	1.683179
54	O	-1.045993	1.576350
55	O	-1.038417	1.628055
56	O	-1.033687	1.756299
57	O	-1.008268	1.739496
58	O	-0.994791	2.192501
59	O	-0.986126	1.546638
60	O	-0.985611	1.650095
61	O	-0.971404	1.534435
62	O	-0.960310	1.656247
63	O	-0.956681	1.428987
64	O	-0.950535	1.719227
65	O	-0.932850	1.752509
66	O	-0.928811	2.500414
67	O	-0.909568	1.604769
68	O	-0.901633	1.829931
69	O	-0.897240	1.467029
70	O	-0.893485	1.396793
71	O	-0.885671	1.494714
72	O	-0.872787	1.579490
73	O	-0.870914	1.503196
74	O	-0.866667	1.556528
75	O	-0.865363	1.515328
76	O	-0.860542	1.438522
77	O	-0.848918	1.713343
78	O	-0.844771	1.452138
79	O	-0.837891	1.622437
80	O	-0.824754	1.230481
81	O	-0.814655	1.257647
82	O	-0.785182	1.288914
83	O	-0.782858	1.509124
84	O	-0.780141	1.531614
85	O	-0.769927	2.083879

86	O	-0.761429	1.764754
87	O	-0.755882	4.275838
88	O	-0.755785	1.794711
89	O	-0.748411	4.389782
90	O	-0.735778	2.538060
91	O	-0.727581	2.992931
92	O	-0.721073	2.667124
93	O	-0.716276	2.728025
94	O	-0.706478	2.547381
95	O	-0.700774	1.311914
96	O	-0.682538	1.293798
97	O	-0.670400	1.610041
98	O	-0.665276	1.274741
99	O	-0.638811	1.379851
100	V	-0.444135	2.204535
101	V	-0.436687	4.540982
102	V	-0.434063	4.671849
103	V	-0.398453	1.565815
104	V	-0.389358	5.992485
105	V	-0.373551	2.820749
106	V	-0.359561	2.121469
107	V	-0.314042	1.262480
108	V	-0.308260	2.511400
109	V	-0.307098	1.350401
110	V	-0.286492	1.236385
111	V	-0.283407	1.382689
112	V	-0.275424	0.832114
113	V	-0.267731	1.998847
114	V	-0.261515	0.603388
115	V	-0.235700	1.734486
116	V	-0.231592	1.613038
117	V	-0.228720	1.167125
118	V	-0.223526	1.846381
119	V	-0.196324	1.654171
120	V	-0.191640	0.615246
121	V	-0.178366	1.518282
122	V	-0.170703	1.635118
123	V	-0.165159	1.961562
124	V	-0.162505	1.345656
125	V	-0.151499	1.276488
126	V	-0.143308	1.462195
127	V	-0.132005	1.766635
128	V	-0.127424	1.521906
129	V	-0.117991	2.125850
130	V	-0.107675	2.002999
131	V	-0.106938	1.309269
132	V	-0.104997	1.783442
133	V	-0.101391	1.490831
134	V	-0.092418	1.593345
135	V	-0.086224	2.044445

136	V	-0.079401	1.409390
137	V	-0.070341	1.730196
138	V	-0.061927	2.052607
139	V	-0.051341	1.436793
140	V	-0.046900	1.884711
141	V	-0.042429	1.776495
142	V	-0.034649	1.943239
143	V	-0.027582	1.380204
144	V	-0.021883	2.424550
145	V	-0.013182	2.046784
146	V	-0.000499	1.988052
147	V	0.006006	1.894064
148	V	0.015579	2.065009
149	V	0.028627	2.067653
150	V	0.032819	1.799067
151	V	0.045648	2.145166
152	V	0.049993	1.823516
153	V	0.058158	2.391626
154	V	0.062546	2.344763
155	V	0.079394	2.203673
156	V	0.091829	1.935403
157	V	0.098758	2.376577
158	V	0.110491	2.386204
159	V	0.127125	2.743996
160	V	0.153567	2.557009
161	V	0.155517	2.361311
162	V	0.171712	2.102001
163	V	0.175169	2.327558
164	V	0.178333	2.338284
165	V	0.199916	2.612313
166	V	0.211581	2.490634
167	V	0.214744	2.244754
168	V	0.219713	2.311593
169	V	0.223797	2.153025
170	V	0.237088	2.156235
171	V	0.238864	2.298531
172	V	0.246389	2.472086
173	V	0.247532	2.324748
174	V	0.253210	2.071771
175	V	0.261286	2.299237
176	V	0.261497	2.319025
177	V	0.265809	2.424518
178	V	0.270223	2.234394
179	V	0.271157	2.297180
180	V	0.275788	2.339082
181	V	0.286013	2.504561
182	V	0.290036	2.765927
183	V	0.296915	2.164031
184	V	0.297791	2.600639
185	V	0.308396	2.049690

186	V	0.308942	2.295507
187	V	0.316073	2.200246
188	V	0.321362	2.204928
189	V	0.326647	2.154262
190	V	0.331739	2.469637
191	V	0.341962	2.127433
192	V	0.343131	2.219886
193	V	0.343364	2.250168
194	V	0.346874	2.532685
195	V	0.347179	2.207688
196	V	0.355785	2.384937
197	V	0.361719	2.204435
198	V	0.373363	2.399101
199	V	0.375405	2.211725
200	V	0.377616	2.241108
201	V	0.385172	2.266512
202	V	0.409051	2.401098
203	V	0.416304	2.727699
204	V	0.419337	2.391468
205	V	0.439903	2.862572
206	V	0.440375	2.290549
207	V	0.455178	2.534603
208	V	0.455385	2.413878
209	V	0.467170	2.506661
210	V	0.478412	2.681005
211	V	0.483871	2.369335
212	V	0.496689	2.577313
213	V	0.503038	2.497039
214	V	0.508264	2.628555
215	V	0.516730	2.656921
216	V	0.523936	2.559024
217	V	0.532991	2.828344
218	V	0.535215	2.381921
219	V	0.544452	2.598203
220	V	0.548346	2.565021
221	V	0.552285	2.723095
222	V	0.552801	2.810142
223	V	0.561297	2.702096
224	V	0.567596	2.645278
225	V	0.573733	2.710660
226	V	0.577618	2.709237
227	V	0.580353	2.606128
228	V	0.583636	2.828161
229	V	0.595415	2.669471
230	V	0.609302	2.527085
231	V	0.618493	2.501981
232	V	0.621936	2.500822
233	V	0.634718	2.596386
234	V	0.638919	2.604549
235	V	0.647749	2.613428

236	V	0.648977	2.638883
237	V	0.656994	3.212524
238	V	0.657540	2.605175
239	V	0.671872	2.728368
240	V	0.679026	3.110761
241	V	0.682224	2.757284
242	V	0.700396	2.883648
243	V	0.714144	2.717049
244	V	0.714305	2.634711
245	V	0.725881	2.585926
246	V	0.728621	3.224917
247	V	0.740239	2.549409
248	V	0.751314	2.629356
249	V	0.752647	3.212910
250	V	0.760408	2.585924
251	V	0.777264	2.469586
252	V	0.786643	2.387965
253	V	0.789829	2.621016
254	V	0.797905	2.347865
255	V	0.834331	2.537489
256	V	0.837514	2.762490
257	V	0.860588	2.552329
258	V	0.864534	2.788030
259	V	0.871864	2.631713
260	V	0.881636	2.401200
261	V	0.903489	2.532655
262	V	0.912862	2.401647
263	V	0.926071	2.569173
264	V	0.930341	2.439243
265	V	0.942435	2.823912
266	V	0.943421	2.705496
267	V	0.944286	2.494195
268	V	0.956310	2.420079
269	V	0.961858	2.814114
270	V	0.973452	2.468157
271	V	0.974980	2.763183
272	V	0.987583	2.470473
273	V	0.988549	2.762730
274	V	0.990838	2.505882
275	V	0.999961	2.802137
276	V	1.008663	2.528474
277	V	1.016764	2.815735
278	V	1.033124	2.525464
279	V	1.050623	2.449869
280	V	1.063191	2.454312
281	V	1.065408	3.011868
282	V	1.073325	2.756499
283	V	1.087993	3.024738
284	V	1.088521	2.548287
285	V	1.114389	2.522326

286	V	1.116148	3.033882
287	V	1.117678	2.546861
288	V	1.121234	2.611510
289	V	1.127797	2.656309
290	V	1.132347	2.566805
291	V	1.135873	2.957132
292	V	1.138248	2.553927
293	V	1.162614	2.665205
294	V	1.167644	2.873501
295	V	1.175373	2.664680
296	V	1.177584	2.717811
297	V	1.189183	2.996271
298	V	1.221619	3.134741
299	V	1.228887	3.103094
300	V	1.250819	2.824075
301	V	1.267313	2.796673
302	V	1.285335	3.068406
303	V	1.302607	2.907936
304	V	1.318233	2.895756
305	V	1.334387	3.077220
306	V	1.354780	3.013179
307	V	1.384033	3.328130
308	V	1.408605	3.206365
309	V	1.417252	2.838171
310	V	1.439789	2.894128
311	V	1.443651	3.410440
312	V	1.450933	3.321314
313	V	1.464480	3.420855
314	V	1.483801	3.347318
315	V	1.484348	2.942604
316	V	1.484728	3.268098
317	V	1.488430	3.371331
318	V	1.500860	3.344499
319	V	1.506324	2.941733
320	V	1.511531	3.293799
321	V	1.527915	2.861771
322	V	1.535404	3.318010
323	V	1.545819	3.334555
324	V	1.558768	3.244788
325	V	1.565730	3.387682
326	V	1.584306	3.356304
327	V	1.587681	3.469361
328	V	1.594639	3.054360
329	V	1.600541	3.314609
330	V	1.611257	3.416485
331	V	1.615075	3.357515
332	V	1.620155	3.263547
333	V	1.628418	3.259886
334	V	1.629492	3.087188
335	V	1.641256	3.422638

336	V	1.645984	3.076521
337	V	1.646323	3.476280
338	V	1.652563	3.441415
339	V	1.654495	3.282781
340	V	1.684874	3.504978
341	V	1.690528	3.039254
342	V	1.699026	3.399122
343	V	1.703171	3.446630
344	V	1.712997	3.503356
345	V	1.714481	3.085445
346	V	1.720850	3.031885
347	V	1.726385	3.369717
348	V	1.746623	3.602479
349	V	1.748321	3.076768
350	V	1.760624	3.428541
351	V	1.762250	3.229505
352	V	1.768394	3.527535
353	V	1.785220	3.598020
354	V	1.796797	3.318591
355	V	1.802163	3.526996
356	V	1.829078	3.815104
357	V	1.834571	3.674862
358	V	1.851404	3.348745
359	V	1.858375	3.669857
360	V	1.872440	3.755990
361	V	1.877654	3.842438
362	V	1.885980	3.374071
363	V	1.899142	3.435772
364	V	1.907276	3.774288
365	V	1.929825	3.895520
366	V	1.932846	3.478518
367	V	1.944127	3.501501
368	V	1.959054	3.869737
369	V	1.963059	3.486125
370	V	1.987555	3.498506
371	V	1.990799	3.897007
372	V	2.001097	3.532452
373	V	2.008033	3.884933
374	V	2.023331	3.529848
375	V	2.046516	3.603851
376	V	2.055835	3.478892
377	V	2.059205	3.781052
378	V	2.072949	3.594830
379	V	2.075587	3.567076
380	V	2.097000	3.506950
381	V	2.103873	3.916199
382	V	2.112123	3.738056
383	V	2.119889	3.915416
384	V	2.125070	3.308814
385	V	2.134861	3.558381

386	V	2.139624	3.870996
387	V	2.141319	3.333785
388	V	2.148261	3.745265
389	V	2.149848	3.426544
390	V	2.165785	3.797225
391	V	2.168903	3.586244
392	V	2.182548	3.836377
393	V	2.193845	3.823913
394	V	2.195851	3.610354
395	V	2.204520	3.960740
396	V	2.211450	3.890605
397	V	2.235219	4.040740
398	V	2.237752	3.712802
399	V	2.249570	4.074399
400	V	2.260705	4.121660
401	V	2.278352	3.643613
402	V	2.280675	3.997298
403	V	2.290672	3.973885
404	V	2.296623	3.824456
405	V	2.298063	4.062025
406	V	2.300466	3.626800
407	V	2.323144	3.836255
408	V	2.324573	4.029598
409	V	2.329893	3.601325
410	V	2.353841	4.078473
411	V	2.363286	3.915319
412	V	2.367352	4.227506
413	V	2.376468	4.243804
414	V	2.388957	3.931328
415	V	2.405352	4.227063
416	V	2.409535	3.895009
417	V	2.416590	3.913806
418	V	2.416951	4.236401
419	V	2.437301	4.448044
420	V	2.446158	4.288233
421	V	2.461504	4.009117
422	V	2.468927	4.493573
423	V	2.478933	3.826680
424	V	2.483892	4.345222
425	V	2.488133	3.939432
426	V	2.497902	4.356936
427	V	2.516691	4.393880
428	V	2.532119	4.303417
429	V	2.570712	4.548313
430	V	2.582746	4.548540
431	V	2.588307	4.605174
432	V	2.607721	4.535335
433	V	2.619841	4.619023
434	V	2.646229	4.647994
435	V	2.672784	4.922550

436	V	2.683817	4.591785
437	V	2.721855	4.759796
438	V	2.726216	4.797587
439	V	2.763859	4.743906
440	V	2.767585	4.619623
441	V	2.809802	4.769055
442	V	2.834225	4.806629
443	V	2.858290	4.876805
444	V	2.878829	5.069417
445	V	2.900607	4.891596
446	V	2.930872	4.940150
447	V	2.959460	4.786566
448	V	2.964330	4.895296
449	V	2.988735	4.847357
450	V	2.999135	4.842444
451	V	3.014369	5.019748
452	V	3.020663	5.054422
453	V	3.070085	5.023541
454	V	3.074902	5.144288
455	V	3.137957	5.099554
456	V	3.172772	5.201305
457	V	3.197607	5.209710
458	V	3.226209	5.259392
459	V	3.259210	5.354966
460	V	3.265188	5.273641
461	V	3.322002	5.550537
462	V	3.471353	5.539655
463	V	3.600906	5.634455
464	V	3.647962	5.649983
465	V	7.480087	3.567334

Total kinetic energy from orbitals= 1.292665684137D+03

9.3. (*E/Z*)-4-(2-((5-nitrofuran-2-yl)methylene)hydrazineyl)-2-phenylquinazoline **3a** in complex with Cu(II)
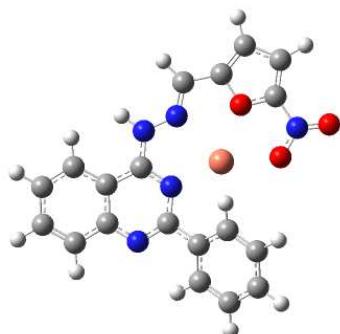
Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	-4.959877	-2.883396	-0.096146
2	6	0	-3.569798	-2.795027	-0.200751
3	6	0	-2.939913	-1.561811	-0.078952
4	6	0	-3.736828	-0.392361	0.137010
5	6	0	-5.149646	-0.512949	0.266427
6	6	0	-5.746329	-1.746821	0.145566
7	1	0	-5.435902	-3.852876	-0.197946
8	1	0	-3.016876	-3.710477	-0.384183
9	6	0	-1.512975	-1.331016	-0.102103
10	1	0	-5.720425	0.392611	0.438070
11	1	0	-6.822710	-1.845648	0.230356
12	6	0	-1.873326	0.950411	0.012973
13	7	0	-3.193972	0.823571	0.204833
14	7	0	-1.003172	-0.099534	-0.063898
15	7	0	-0.665310	-2.391447	-0.145111
16	7	0	0.652773	-2.142220	-0.115364
17	6	0	-1.380660	2.301026	-0.110162
18	6	0	-0.161007	2.599443	-0.768699
19	6	0	-2.148737	3.362086	0.439097
20	6	0	0.296727	3.894595	-0.824044
21	1	0	0.373421	1.823948	-1.310981
22	6	0	-1.676330	4.656807	0.387669
23	1	0	-3.088769	3.130091	0.922924
24	6	0	-0.454309	4.926739	-0.233016
25	1	0	1.220322	4.127352	-1.341433
26	1	0	-2.250555	5.462994	0.829509
27	1	0	-0.086487	5.946842	-0.277950
28	1	0	-1.022987	-3.340737	-0.125867
29	6	0	1.567945	-3.038772	-0.134098
30	1	0	1.410764	-4.116014	-0.193830
31	6	0	2.908794	-2.474746	-0.056626
32	6	0	4.223618	-2.856862	-0.036008
33	8	0	2.845927	-1.124414	0.033045
34	6	0	5.003877	-1.659348	0.074073
35	1	0	4.609126	-3.865246	-0.091542
36	6	0	4.091113	-0.652316	0.110570
37	1	0	6.079850	-1.571968	0.119136
38	7	0	4.083763	0.774055	0.210308
39	8	0	2.955969	1.315634	0.212587
40	8	0	5.134810	1.355092	0.281511
41	29	0	1.049826	0.192537	0.101191

Rotational constants (GHZ):   0.2429866   0.1310050   0.0860669

Cycle   9 Pass 1 IDiag 1:
RMSU= 7.83D-09   CP: 1.00D+00 1.04D+00 9.27D-01 1.06D+00 8.00D-01
          CP: 1.11D+00
E= -1230.50015307063   Delta-E=   -0.000000000042 Rises=F Damp=F
DIIS: error= 4.32D-08 at cycle   7 NSaved=   7.
NSaved= 7 IEnMin= 7 EnMin= -1230.50015307063   IErMin= 7 ErrMin= 4.32D-08

ErrMax= 4.32D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.98D-12 BMatP= 2.50D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.773D-05 0.140D-02-0.501D-02-0.973D-01-0.633D-01 0.314D+00

Coeff-Com: 0.850D+00

Coeff: 0.773D-05 0.140D-02-0.501D-02-0.973D-01-0.633D-01 0.314D+00

Coeff: 0.850D+00

Gap=   0.204 Goal= None   Shift=   0.000

Gap=   0.204 Goal= None   Shift=   0.000

RMSDP=7.32D-09 MaxDP=4.70D-07 DE=-4.18D-11 OVMax= 1.11D-06

SCF Done: E(UCAM-B3LYP) = -1230.50015307   A.U. after   9 cycles

        NFock= 9 Conv=0.73D-08   -V/T= 2.0064

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 0.0000 <S**2>= 0.0000 S= 0.0000

<L.S>= 0.000000000000E+00

KE= 1.222727256475D+03 PE=-7.370827779908D+03 EE= 2.666256415164D+03

Annihilation of the first spin contaminant:

S**2 before annihilation   0.0000,   after   0.0000

Leave Link   502 at Thu Sep 22 03:54:39 2022, MaxMem=   2147483648 cpu: 1906.5

(Enter /opt/gaussian/g09/l701.exe)

Compute integral first derivatives.

... and contract with generalized density number 0.

Leave Link 701 at Thu Sep 22 03:54:39 2022, MaxMem= 2147483648 cpu: 4.5

(Enter /opt/gaussian/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Thu Sep 22 03:54:39 2022, MaxMem= 2147483648 cpu: 0.5

(Enter /opt/gaussian/g09/l703.exe)

Compute integral first derivatives, UseDBF=F ICtDFT=   0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl=   2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl=   2127 DoSepK=T KAlg= 0 I1Cent=   0 FoldK=F

IRaf=   1 NMat= 1 IRICut=   1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag=   0 FMFlag=   100000 FMFlg1=   800

     NFxFlg=   0 DoJE=F BraDBF=F KetDBF=F FulRan=T

     wScrn= 0.000000 ICntrl=   2527 IOpCl= 0 I1Cent=   0 NGrid=   0

     NMat0=   1 NMatS0=   1 NMatT0=   0 NMatD0=   1 NMtDS0=   0

NMtDT0=   0

Symmetry not used in FoFCou.

Leave Link 703 at Thu Sep 22 03:56:25 2022, MaxMem= 2147483648 cpu: 847.0

(Enter /opt/gaussian/g09/l716.exe)

Dipole   =-2.20606259D-01-3.20457782D+00-2.62306603D-01

***** Axes restored to original set *****

Cartesian Forces: Max   0.048232877 RMS   0.011696893

Leave Link 716 at Thu Sep 22 03:56:26 2022, MaxMem= 2147483648 cpu: 1.0

(Enter /opt/gaussian/g09/l1122.exe)

CPIOFr: IOpCl= 1 IRwI=-1 IRwCP= 731 ICalc= 4 LCPTot=   338287 Len1MO= 1090774 IndFrg=   5792157

Restoring MOs from calculation   1 to rwf.

CPIOFr: IOpCl= 1 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot=   338287 Len1MO= 1090774 IndFrg=   1429061
 Counterpoise corrected energy =   -1426.063306408361
              BSSE energy =   0.011530177425
           sum of monomers = -1425.493130401567
         complexation energy =   -365.03 kcal/mole (raw)
         complexation energy =   -357.79 kcal/mole (corrected)
 Leave Link 122 at Thu Sep 22 03:56:26 2022, MaxMem= 2147483648 cpu: 0.5
 (Enter /opt/gaussian/g09/l716.exe)
 Rotating derivatives to standard orientation.
 Dipole   =-2.04827069D+00-2.73171297D+00-1.95395818D-01

Orbital energies and kinetic energies (alpha):

		1	2
1	O	-19.558362	29.116819
2	O	-19.497706	29.122489
3	O	-19.493996	29.121956
4	O	-14.893671	22.048957
5	O	-14.759193	22.045778
6	O	-14.722929	22.049514
7	O	-14.693036	22.050236
8	O	-14.677966	22.048057
9	O	-10.638678	15.952994
10	O	-10.609812	15.953424
11	O	-10.605723	15.949837
12	O	-10.583905	15.953681
13	O	-10.583462	15.950153
14	O	-10.565770	15.953740
15	O	-10.547575	15.953106
16	O	-10.534299	15.953736
17	O	-10.527647	15.953999
18	O	-10.527053	15.953050
19	O	-10.525567	15.953599
20	O	-10.520580	15.953268
21	O	-10.519457	15.952416
22	O	-10.509213	15.953163
23	O	-10.508588	15.954357
24	O	-10.506056	15.953536
25	O	-10.503819	15.953384
26	O	-10.493223	15.953478
27	O	-10.484590	15.953688
28	O	-4.581928	2.684574
29	O	-3.096573	5.088141
30	O	-3.090851	5.075689
31	O	-3.089812	5.079120
32	O	-1.558782	2.483329
33	O	-1.484048	2.495621
34	O	-1.403868	1.969347
35	O	-1.376610	2.795062
36	O	-1.341208	1.835449

37	O	-1.260382	2.005025
38	O	-1.226512	1.794707
39	O	-1.194584	1.725833
40	O	-1.180853	1.519466
41	O	-1.151883	1.993819
42	O	-1.145437	1.800052
43	O	-1.116373	1.700011
44	O	-1.103128	1.629931
45	O	-1.068160	1.624841
46	O	-1.064496	1.677863
47	O	-1.049423	1.917044
48	O	-1.008009	1.693411
49	O	-0.994281	1.853260
50	O	-0.968164	1.739864
51	O	-0.956664	1.511534
52	O	-0.941507	1.810644
53	O	-0.923508	1.595048
54	O	-0.913783	1.509365
55	O	-0.900884	1.762402
56	O	-0.892573	1.800403
57	O	-0.877080	1.970107
58	O	-0.871374	1.699290
59	O	-0.859009	1.686414
60	O	-0.856797	1.639730
61	O	-0.844306	1.527153
62	O	-0.828771	1.354331
63	O	-0.815820	2.376890
64	O	-0.809790	1.332217
65	O	-0.800468	1.757854
66	O	-0.792769	1.659387
67	O	-0.787359	1.552416
68	O	-0.778587	1.409924
69	O	-0.764743	1.461628
70	O	-0.757886	1.387691
71	O	-0.753152	1.369993
72	O	-0.744747	1.480305
73	O	-0.740048	1.920613
74	O	-0.735558	1.484232
75	O	-0.730942	1.399316
76	O	-0.726882	1.629333
77	O	-0.722442	1.246935
78	O	-0.704827	1.615884
79	O	-0.695386	1.243561
80	O	-0.678878	1.385933
81	O	-0.675180	1.474424
82	O	-0.667843	1.750778
83	O	-0.662489	1.198579
84	O	-0.649355	2.199920
85	O	-0.645636	2.142742
86	O	-0.638151	1.455016

87	O	-0.626246	2.727715
88	O	-0.618217	2.662669
89	O	-0.609760	1.815272
90	O	-0.605941	2.787793
91	O	-0.598257	1.918953
92	O	-0.593434	2.326511
93	O	-0.581246	1.557107
94	O	-0.568475	4.129396
95	O	-0.564761	8.462917
96	O	-0.563658	8.573294
97	O	-0.555433	5.247079
98	O	-0.549268	4.527298
99	O	-0.542644	6.307067
100	O	-0.533975	2.128390
101	O	-0.523836	5.787960
102	O	-0.516617	2.377482
103	V	-0.299542	1.829929
104	V	-0.275848	1.699993
105	V	-0.256205	1.834881
106	V	-0.224050	1.875226
107	V	-0.195786	1.474895
108	V	-0.192598	1.546846
109	V	-0.172834	1.384539
110	V	-0.168520	1.631441
111	V	-0.165671	0.560364
112	V	-0.148670	0.745865
113	V	-0.141237	0.370019
114	V	-0.126020	2.007885
115	V	-0.117380	0.885057
116	V	-0.109456	1.674417
117	V	-0.093225	1.703982
118	V	-0.079126	1.560597
119	V	-0.072503	0.681037
120	V	-0.060736	1.276383
121	V	-0.051948	1.938938
122	V	-0.043883	1.224135
123	V	-0.042686	1.265498
124	V	-0.028776	1.375419
125	V	-0.021464	1.611656
126	V	-0.008207	1.785117
127	V	-0.006336	1.684308
128	V	-0.000751	1.468621
129	V	0.007228	1.536336
130	V	0.010381	1.255641
131	V	0.014538	1.591077
132	V	0.018283	1.468177
133	V	0.021202	1.835400
134	V	0.031308	1.670448
135	V	0.033922	1.510470
136	V	0.044568	2.276782

137	V	0.054653	1.917886
138	V	0.055357	1.534711
139	V	0.065302	1.528400
140	V	0.069860	1.905713
141	V	0.076695	2.083864
142	V	0.086452	2.026008
143	V	0.097816	2.181545
144	V	0.105242	1.883073
145	V	0.115211	1.958335
146	V	0.128155	2.720722
147	V	0.137197	1.488821
148	V	0.140947	2.166943
149	V	0.147275	1.708026
150	V	0.159536	1.865239
151	V	0.166582	1.899630
152	V	0.173313	2.173602
153	V	0.183662	2.219715
154	V	0.188478	2.274296
155	V	0.204268	1.761499
156	V	0.212044	2.386365
157	V	0.231322	2.302668
158	V	0.235544	2.394484
159	V	0.255859	2.301768
160	V	0.285352	1.998559
161	V	0.298122	2.054375
162	V	0.308975	2.016394
163	V	0.327735	2.723681
164	V	0.331113	2.129122
165	V	0.336088	2.150194
166	V	0.337348	2.173153
167	V	0.347147	2.085663
168	V	0.353703	2.126192
169	V	0.357355	2.178093
170	V	0.360360	2.212194
171	V	0.364564	2.123016
172	V	0.367216	2.158498
173	V	0.375754	2.221358
174	V	0.379726	2.462859
175	V	0.384722	2.091374
176	V	0.390644	2.448789
177	V	0.398073	2.476416
178	V	0.402611	2.290804
179	V	0.409689	2.492143
180	V	0.413353	2.424983
181	V	0.418774	2.214189
182	V	0.421120	2.278618
183	V	0.424546	2.208071
184	V	0.427854	2.401293
185	V	0.429394	2.512322
186	V	0.436457	2.185001

187	V	0.437754	2.182949
188	V	0.443168	2.099165
189	V	0.445152	2.335985
190	V	0.453396	2.303911
191	V	0.456973	2.311575
192	V	0.459160	2.167435
193	V	0.460357	2.208974
194	V	0.470509	2.385442
195	V	0.474388	2.470501
196	V	0.480965	2.404841
197	V	0.482263	2.495641
198	V	0.493644	2.562844
199	V	0.508873	2.302782
200	V	0.513288	2.462416
201	V	0.525186	2.224954
202	V	0.535148	2.598412
203	V	0.552263	2.487231
204	V	0.557049	2.626564
205	V	0.566844	2.721527
206	V	0.577606	2.522166
207	V	0.585376	2.927734
208	V	0.589202	2.738175
209	V	0.602808	2.693289
210	V	0.607291	2.537227
211	V	0.617689	2.587770
212	V	0.619374	2.492958
213	V	0.631425	2.583353
214	V	0.641863	2.538666
215	V	0.646305	2.619573
216	V	0.650738	2.678820
217	V	0.652357	2.560191
218	V	0.659332	2.556326
219	V	0.665347	2.682151
220	V	0.666636	2.745746
221	V	0.672690	2.847478
222	V	0.679677	2.756599
223	V	0.682032	2.762258
224	V	0.689155	2.744080
225	V	0.696846	2.642558
226	V	0.700336	2.646234
227	V	0.717841	2.631779
228	V	0.722740	2.670364
229	V	0.729769	2.656592
230	V	0.734302	2.525378
231	V	0.743875	2.956600
232	V	0.751268	2.757378
233	V	0.762658	2.788515
234	V	0.768673	2.654329
235	V	0.772610	2.709661
236	V	0.775964	2.714330

237	V	0.791106	2.851731
238	V	0.796065	2.780647
239	V	0.798499	3.157855
240	V	0.809554	2.949970
241	V	0.822070	2.831884
242	V	0.827799	2.714234
243	V	0.832309	2.946835
244	V	0.838412	2.962903
245	V	0.848935	2.821650
246	V	0.856629	2.446577
247	V	0.861902	2.593586
248	V	0.868866	2.609901
249	V	0.881327	3.142021
250	V	0.899225	2.733977
251	V	0.903207	2.468872
252	V	0.907560	2.653577
253	V	0.912995	3.051759
254	V	0.922178	2.793905
255	V	0.930093	3.134190
256	V	0.946667	2.799761
257	V	0.952548	2.517143
258	V	0.968556	2.611268
259	V	0.985510	2.543442
260	V	0.987369	2.684193
261	V	1.004667	2.659392
262	V	1.016038	2.599105
263	V	1.030619	2.523900
264	V	1.040793	2.480743
265	V	1.049448	2.689278
266	V	1.058533	2.624699
267	V	1.063979	2.555479
268	V	1.076437	2.695534
269	V	1.078721	2.700906
270	V	1.089335	2.646745
271	V	1.094517	2.684841
272	V	1.114383	2.726379
273	V	1.118336	2.547427
274	V	1.128900	2.623599
275	V	1.129927	2.621459
276	V	1.140823	2.594761
277	V	1.155929	2.658281
278	V	1.161822	2.587108
279	V	1.165333	2.616530
280	V	1.171077	2.566025
281	V	1.175954	2.601942
282	V	1.182652	2.572450
283	V	1.184236	2.631530
284	V	1.215913	2.613555
285	V	1.224105	2.609069
286	V	1.227606	2.682290

287	V	1.234886	2.590020
288	V	1.244847	2.635254
289	V	1.249214	2.733151
290	V	1.257069	2.658597
291	V	1.263694	2.776237
292	V	1.275126	2.933698
293	V	1.278022	2.776553
294	V	1.288418	2.732235
295	V	1.292137	2.732991
296	V	1.308894	2.792629
297	V	1.331870	2.738746
298	V	1.337157	2.776783
299	V	1.349607	2.835916
300	V	1.377710	2.930253
301	V	1.392991	2.980273
302	V	1.402000	2.936462
303	V	1.440136	2.995528
304	V	1.459123	2.938692
305	V	1.468371	3.054519
306	V	1.489387	3.243280
307	V	1.512421	3.275323
308	V	1.545419	2.877629
309	V	1.555674	3.519114
310	V	1.562987	3.164092
311	V	1.567507	3.151636
312	V	1.570413	3.245351
313	V	1.582089	3.183085
314	V	1.597224	3.131763
315	V	1.609322	3.269231
316	V	1.616979	3.238155
317	V	1.629848	3.561289
318	V	1.642782	3.142609
319	V	1.645826	3.097954
320	V	1.647744	3.255708
321	V	1.653035	3.349434
322	V	1.660654	3.433661
323	V	1.663681	2.965689
324	V	1.673823	3.115189
325	V	1.689341	3.241950
326	V	1.703681	3.267210
327	V	1.716606	3.195832
328	V	1.722274	3.174983
329	V	1.730208	3.306468
330	V	1.733699	3.201123
331	V	1.737971	3.263949
332	V	1.743159	3.442186
333	V	1.750125	3.336952
334	V	1.751822	3.176283
335	V	1.758118	3.515248
336	V	1.767858	3.273955

337	V	1.774983	3.405170
338	V	1.778831	3.375580
339	V	1.785576	3.357704
340	V	1.788924	3.567063
341	V	1.794703	3.367295
342	V	1.821752	3.341255
343	V	1.823942	3.045685
344	V	1.830700	3.269515
345	V	1.838320	3.396266
346	V	1.838878	3.493029
347	V	1.841836	3.097014
348	V	1.869538	3.454565
349	V	1.879551	3.455450
350	V	1.886565	3.428343
351	V	1.898529	3.307935
352	V	1.907133	3.239829
353	V	1.908041	3.597359
354	V	1.921438	3.485892
355	V	1.922363	3.676680
356	V	1.958368	3.687691
357	V	1.959576	3.389038
358	V	1.964471	3.650355
359	V	1.992306	3.633804
360	V	1.999912	3.942438
361	V	2.011726	3.395769
362	V	2.016012	3.381273
363	V	2.029414	3.561899
364	V	2.044899	3.651123
365	V	2.068554	3.789550
366	V	2.076692	3.733945
367	V	2.083877	3.532156
368	V	2.096575	3.537926
369	V	2.100679	3.682526
370	V	2.114460	3.559408
371	V	2.122007	3.878622
372	V	2.130634	3.598212
373	V	2.140982	3.684270
374	V	2.146622	3.731092
375	V	2.157024	3.554561
376	V	2.176323	3.700375
377	V	2.183968	3.709858
378	V	2.188200	3.540896
379	V	2.206612	3.493379
380	V	2.217259	3.886308
381	V	2.222171	3.631896
382	V	2.228857	3.406860
383	V	2.232997	3.554985
384	V	2.241656	3.582409
385	V	2.248227	3.493621
386	V	2.261451	3.623856

387	V	2.265332	3.578499
388	V	2.271513	3.955524
389	V	2.274618	3.454677
390	V	2.288304	3.833393
391	V	2.293372	3.670600
392	V	2.298058	3.684312
393	V	2.300837	3.744912
394	V	2.315158	3.838248
395	V	2.331721	3.903023
396	V	2.335880	3.878765
397	V	2.346762	3.891232
398	V	2.355650	4.026828
399	V	2.376029	3.828002
400	V	2.378295	3.972810
401	V	2.381086	4.129356
402	V	2.391075	3.939156
403	V	2.398283	3.654813
404	V	2.413308	3.726250
405	V	2.417761	3.882699
406	V	2.433024	4.017614
407	V	2.440086	3.853355
408	V	2.457019	3.909552
409	V	2.457872	3.718983
410	V	2.472393	3.856465
411	V	2.482083	4.199173
412	V	2.493900	3.968000
413	V	2.506597	4.187193
414	V	2.510237	4.054480
415	V	2.528360	4.257609
416	V	2.531588	3.960533
417	V	2.542054	3.910185
418	V	2.542909	4.330781
419	V	2.550782	4.309456
420	V	2.561212	4.182201
421	V	2.576657	4.371824
422	V	2.589898	3.980518
423	V	2.596744	4.006453
424	V	2.613480	4.020793
425	V	2.617524	4.370168
426	V	2.626292	4.304739
427	V	2.631738	4.234443
428	V	2.666821	4.352910
429	V	2.678126	4.560544
430	V	2.701892	4.583788
431	V	2.720964	4.533189
432	V	2.738037	4.531982
433	V	2.740284	4.594983
434	V	2.752984	4.687800
435	V	2.758989	4.649304
436	V	2.804543	4.845905

		1	2
437	V	2.811735	4.584025
438	V	2.840783	4.583232
439	V	2.878841	4.748810
440	V	2.895978	4.701641
441	V	2.910625	4.495807
442	V	2.919615	4.784803
443	V	2.970421	4.839321
444	V	2.992029	4.945835
445	V	3.008367	4.890455
446	V	3.019703	4.909222
447	V	3.040302	4.941240
448	V	3.070426	4.793515
449	V	3.076787	4.943210
450	V	3.092779	4.847021
451	V	3.107782	4.846842
452	V	3.119007	4.870057
453	V	3.163819	5.206434
454	V	3.179490	5.037662
455	V	3.225585	5.214199
456	V	3.259351	5.103321
457	V	3.265214	5.114400
458	V	3.312002	5.200527
459	V	3.333223	5.299795
460	V	3.389522	5.229983
461	V	3.409836	5.444970
462	V	3.487838	5.526783
463	V	3.612637	5.554127
464	V	3.713829	5.643662
465	V	3.777205	5.661245

Orbital energies and kinetic energies (beta):

		1	2
1	O	-19.558342	29.116836
2	O	-19.497574	29.122597
3	O	-19.493967	29.121978
4	O	-14.893719	22.048922
5	O	-14.758079	22.046673
6	O	-14.723368	22.049156
7	O	-14.693260	22.050054
8	O	-14.672352	22.052711
9	O	-10.638729	15.952988
10	O	-10.610208	15.953157
11	O	-10.605464	15.950051
12	O	-10.583721	15.953767
13	O	-10.583324	15.950350
14	O	-10.566731	15.953016
15	O	-10.545954	15.954494
16	O	-10.534658	15.953469
17	O	-10.525882	15.955548
18	O	-10.525706	15.953477

19	O	-10.523777	15.955906
20	O	-10.520307	15.953509
21	O	-10.516135	15.955303
22	O	-10.510429	15.952808
23	O	-10.508639	15.953691
24	O	-10.503221	15.956027
25	O	-10.502324	15.954700
26	O	-10.493427	15.953336
27	O	-10.485522	15.952925
28	O	-4.581250	2.684528
29	O	-3.096323	5.088194
30	O	-3.089893	5.075616
31	O	-3.088841	5.078924
32	O	-1.558702	2.483247
33	O	-1.483976	2.495646
34	O	-1.402898	1.968957
35	O	-1.376470	2.794786
36	O	-1.337143	1.831008
37	O	-1.256052	1.985869
38	O	-1.224814	1.804468
39	O	-1.190718	1.714531
40	O	-1.176197	1.524873
41	O	-1.151368	1.988384
42	O	-1.145042	1.807603
43	O	-1.113637	1.697831
44	O	-1.099883	1.624762
45	O	-1.066125	1.601951
46	O	-1.058157	1.744840
47	O	-1.047523	1.875861
48	O	-1.004903	1.701915
49	O	-0.993562	1.837279
50	O	-0.966373	1.737137
51	O	-0.954955	1.518769
52	O	-0.940657	1.809807
53	O	-0.921047	1.581491
54	O	-0.911868	1.510275
55	O	-0.899773	1.771158
56	O	-0.892152	1.815538
57	O	-0.876248	1.949655
58	O	-0.870490	1.695161
59	O	-0.858697	1.687815
60	O	-0.855790	1.629317
61	O	-0.842051	1.515436
62	O	-0.827380	1.378712
63	O	-0.815568	2.366174
64	O	-0.806980	1.382621
65	O	-0.800023	1.763203
66	O	-0.790922	1.634998
67	O	-0.785737	1.543720
68	O	-0.777538	1.407061

69	O	-0.762509	1.457222
70	O	-0.754175	1.350205
71	O	-0.749905	1.417442
72	O	-0.740516	1.741333
73	O	-0.739219	1.622086
74	O	-0.735346	1.480129
75	O	-0.729825	1.407023
76	O	-0.726454	1.618452
77	O	-0.721623	1.253981
78	O	-0.702273	1.746151
79	O	-0.685258	1.126006
80	O	-0.674234	1.470831
81	O	-0.670980	1.332474
82	O	-0.666140	1.755990
83	O	-0.649016	2.066140
84	O	-0.648228	2.048143
85	O	-0.638673	1.445026
86	O	-0.636573	1.462858
87	O	-0.625698	2.708516
88	O	-0.616529	2.692563
89	O	-0.605642	2.769080
90	O	-0.602524	1.962085
91	O	-0.595796	1.845624
92	O	-0.585500	2.318340
93	O	-0.573856	2.074987
94	O	-0.564095	8.493694
95	O	-0.563485	8.723778
96	O	-0.559329	7.172185
97	O	-0.548381	4.943163
98	O	-0.542050	6.132481
99	O	-0.537600	1.365971
100	O	-0.521626	5.982292
101	O	-0.516346	2.520242
102	V	-0.389379	1.452316
103	V	-0.295774	1.926029
104	V	-0.258962	1.712196
105	V	-0.251853	1.747864
106	V	-0.219727	1.858629
107	V	-0.190399	1.515518
108	V	-0.175983	1.515395
109	V	-0.168749	1.238526
110	V	-0.165136	0.656341
111	V	-0.157010	1.598324
112	V	-0.148281	0.766074
113	V	-0.140920	0.381868
114	V	-0.124671	2.027400
115	V	-0.116808	0.845958
116	V	-0.101723	1.631474
117	V	-0.091851	1.709362
118	V	-0.078696	1.560337

119	V	-0.071844	0.719050
120	V	-0.059768	1.298053
121	V	-0.051341	1.928243
122	V	-0.042925	1.272951
123	V	-0.042142	1.182435
124	V	-0.027630	1.376556
125	V	-0.016329	1.613734
126	V	-0.006694	1.734353
127	V	-0.003575	1.656778
128	V	0.001213	1.368435
129	V	0.009732	1.456106
130	V	0.011283	1.509856
131	V	0.016228	1.600790
132	V	0.019755	1.446519
133	V	0.023165	1.783189
134	V	0.032484	1.647356
135	V	0.036120	1.556640
136	V	0.045200	2.280995
137	V	0.055639	1.891159
138	V	0.056522	1.556622
139	V	0.066362	1.524324
140	V	0.070833	1.911710
141	V	0.078333	2.049887
142	V	0.088728	2.073289
143	V	0.099070	2.199205
144	V	0.106965	1.865398
145	V	0.116965	1.957630
146	V	0.128409	2.723940
147	V	0.137931	1.486283
148	V	0.142130	2.152005
149	V	0.148195	1.702977
150	V	0.160212	1.868278
151	V	0.167454	1.894083
152	V	0.174992	2.182563
153	V	0.184541	2.258643
154	V	0.189171	2.230367
155	V	0.205269	1.760856
156	V	0.213050	2.385072
157	V	0.232107	2.271174
158	V	0.236872	2.424322
159	V	0.256329	2.299155
160	V	0.285983	1.998880
161	V	0.299313	2.053410
162	V	0.310110	2.018805
163	V	0.330533	2.714526
164	V	0.332186	2.167125
165	V	0.337609	2.196684
166	V	0.339028	2.120992
167	V	0.349186	2.096133
168	V	0.354689	2.120921

169	V	0.358608	2.199041
170	V	0.363601	2.258764
171	V	0.367482	2.075196
172	V	0.369854	2.151948
173	V	0.377440	2.215110
174	V	0.380671	2.481873
175	V	0.387069	2.114752
176	V	0.391963	2.449274
177	V	0.399612	2.454507
178	V	0.404173	2.330228
179	V	0.412021	2.489399
180	V	0.416038	2.533182
181	V	0.421795	2.247679
182	V	0.425473	2.227722
183	V	0.426413	2.238929
184	V	0.428687	2.613600
185	V	0.431519	2.274943
186	V	0.437320	2.135569
187	V	0.439849	2.230431
188	V	0.444496	2.007831
189	V	0.447221	2.387949
190	V	0.455328	2.291544
191	V	0.459319	2.270975
192	V	0.459921	2.183267
193	V	0.464016	2.244217
194	V	0.471863	2.402958
195	V	0.476330	2.470826
196	V	0.481984	2.493930
197	V	0.485009	2.401611
198	V	0.496029	2.619912
199	V	0.510676	2.349775
200	V	0.516296	2.469049
201	V	0.527848	2.234152
202	V	0.537705	2.581971
203	V	0.553428	2.535892
204	V	0.559320	2.631977
205	V	0.569242	2.668191
206	V	0.579914	2.530932
207	V	0.585748	2.952284
208	V	0.589883	2.738449
209	V	0.603324	2.698178
210	V	0.608507	2.526417
211	V	0.619276	2.591843
212	V	0.622320	2.512631
213	V	0.632043	2.572155
214	V	0.643179	2.539033
215	V	0.646981	2.633800
216	V	0.652032	2.693088
217	V	0.653759	2.544386
218	V	0.660061	2.540436

219	V	0.666661	2.631803
220	V	0.668281	2.798407
221	V	0.673366	2.847118
222	V	0.682359	2.749000
223	V	0.684930	2.773863
224	V	0.690161	2.789755
225	V	0.698266	2.687331
226	V	0.701514	2.605277
227	V	0.718904	2.636241
228	V	0.723127	2.663433
229	V	0.731029	2.708624
230	V	0.735488	2.495755
231	V	0.744754	2.951637
232	V	0.752072	2.764872
233	V	0.763935	2.779462
234	V	0.769175	2.663686
235	V	0.773115	2.712063
236	V	0.777936	2.699055
237	V	0.791988	2.889425
238	V	0.796452	2.788025
239	V	0.799560	3.133309
240	V	0.810805	2.962691
241	V	0.822477	2.811543
242	V	0.828630	2.688959
243	V	0.833385	2.955356
244	V	0.839053	2.971602
245	V	0.850117	2.834411
246	V	0.858116	2.460297
247	V	0.862930	2.598581
248	V	0.869964	2.615802
249	V	0.882137	3.125596
250	V	0.900678	2.756822
251	V	0.904585	2.477253
252	V	0.908464	2.626675
253	V	0.913806	3.048923
254	V	0.922669	2.784719
255	V	0.931318	3.137095
256	V	0.948132	2.809783
257	V	0.953606	2.498555
258	V	0.970293	2.612723
259	V	0.986558	2.625682
260	V	0.989126	2.588970
261	V	1.005468	2.663034
262	V	1.017727	2.602743
263	V	1.032286	2.526432
264	V	1.043641	2.498571
265	V	1.051151	2.690975
266	V	1.061053	2.603728
267	V	1.065279	2.561914
268	V	1.077499	2.699871

269	V	1.080088	2.701139
270	V	1.091369	2.680428
271	V	1.096212	2.641792
272	V	1.115529	2.724595
273	V	1.121896	2.539681
274	V	1.129840	2.648430
275	V	1.130440	2.595350
276	V	1.143563	2.605849
277	V	1.158869	2.707609
278	V	1.163231	2.555771
279	V	1.166907	2.598116
280	V	1.171847	2.571305
281	V	1.177765	2.613342
282	V	1.184805	2.682211
283	V	1.186691	2.500260
284	V	1.219799	2.664645
285	V	1.228007	2.579480
286	V	1.230113	2.678759
287	V	1.238666	2.587945
288	V	1.248714	2.647314
289	V	1.249684	2.729764
290	V	1.258741	2.669372
291	V	1.265758	2.760458
292	V	1.277335	2.957220
293	V	1.279971	2.732644
294	V	1.289680	2.727332
295	V	1.294568	2.732880
296	V	1.310208	2.788239
297	V	1.333259	2.744500
298	V	1.339281	2.774209
299	V	1.350778	2.828452
300	V	1.379572	2.931294
301	V	1.393543	2.980190
302	V	1.402628	2.933912
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304	V	1.461650	2.959465
305	V	1.469449	3.027651
306	V	1.489865	3.242920
307	V	1.513139	3.273767
308	V	1.545765	2.875325
309	V	1.556692	3.547061
310	V	1.564850	3.199630
311	V	1.569764	3.125940
312	V	1.572114	3.241197
313	V	1.584753	3.164954
314	V	1.599886	3.137047
315	V	1.610760	3.274180
316	V	1.619636	3.233451
317	V	1.630681	3.553728
318	V	1.643999	3.124735

319	V	1.647107	3.148755
320	V	1.649625	3.251754
321	V	1.654258	3.327742
322	V	1.662027	3.421414
323	V	1.664295	2.970718
324	V	1.676071	3.120629
325	V	1.691657	3.239697
326	V	1.705919	3.260273
327	V	1.718424	3.252290
328	V	1.726601	3.152747
329	V	1.731419	3.311262
330	V	1.736626	3.183187
331	V	1.740421	3.251451
332	V	1.743867	3.441897
333	V	1.751533	3.159312
334	V	1.753101	3.366564
335	V	1.760145	3.502226
336	V	1.769056	3.280585
337	V	1.776157	3.400844
338	V	1.779720	3.410422
339	V	1.787020	3.320278
340	V	1.790773	3.557952
341	V	1.794971	3.371341
342	V	1.823139	3.362241
343	V	1.826636	3.029631
344	V	1.832830	3.305413
345	V	1.838934	3.520466
346	V	1.840619	3.341016
347	V	1.844946	3.081513
348	V	1.870241	3.450346
349	V	1.882788	3.459323
350	V	1.892268	3.432809
351	V	1.901041	3.346616
352	V	1.907932	3.296357
353	V	1.909434	3.499769
354	V	1.922088	3.522003
355	V	1.923134	3.644293
356	V	1.958504	3.686854
357	V	1.960846	3.379478
358	V	1.966817	3.659049
359	V	1.995643	3.645559
360	V	2.000461	3.929243
361	V	2.012255	3.397433
362	V	2.016210	3.376052
363	V	2.031616	3.578991
364	V	2.046894	3.632822
365	V	2.070626	3.817567
366	V	2.078073	3.717215
367	V	2.087897	3.525160
368	V	2.097513	3.522152

369	V	2.102507	3.698386
370	V	2.118984	3.637851
371	V	2.124473	3.794278
372	V	2.134149	3.603244
373	V	2.142380	3.729314
374	V	2.148458	3.684741
375	V	2.159728	3.547461
376	V	2.179456	3.664604
377	V	2.185967	3.747150
378	V	2.191994	3.523921
379	V	2.207744	3.500963
380	V	2.217674	3.886661
381	V	2.223334	3.635469
382	V	2.230241	3.424902
383	V	2.233931	3.538102
384	V	2.242498	3.602966
385	V	2.249560	3.489818
386	V	2.262484	3.619661
387	V	2.266130	3.575769
388	V	2.272181	3.949747
389	V	2.275477	3.464182
390	V	2.289401	3.819978
391	V	2.294654	3.694345
392	V	2.298901	3.675142
393	V	2.301445	3.729822
394	V	2.316899	3.849188
395	V	2.333717	3.889949
396	V	2.338635	3.883077
397	V	2.348898	3.898347
398	V	2.357025	4.027872
399	V	2.377084	3.861704
400	V	2.379359	3.953729
401	V	2.382040	4.112699
402	V	2.392001	3.936023
403	V	2.401883	3.654448
404	V	2.415862	3.806384
405	V	2.419874	3.804832
406	V	2.433993	4.014394
407	V	2.441834	3.855658
408	V	2.458786	3.748281
409	V	2.459079	3.871422
410	V	2.473972	3.860497
411	V	2.483560	4.206466
412	V	2.497361	3.968944
413	V	2.507318	4.204021
414	V	2.513704	4.036434
415	V	2.529156	4.246161
416	V	2.531844	3.970495
417	V	2.543393	3.972688
418	V	2.543821	4.264905

419	V	2.553140	4.315526
420	V	2.563071	4.183385
421	V	2.578647	4.372499
422	V	2.591023	3.979570
423	V	2.598442	4.016390
424	V	2.615949	4.023726
425	V	2.619039	4.359767
426	V	2.628133	4.306506
427	V	2.633858	4.227561
428	V	2.669510	4.338289
429	V	2.678593	4.570175
430	V	2.702155	4.584164
431	V	2.721709	4.535013
432	V	2.738945	4.528767
433	V	2.740953	4.603133
434	V	2.753581	4.703421
435	V	2.759331	4.637364
436	V	2.804658	4.848157
437	V	2.812667	4.581155
438	V	2.841129	4.582716
439	V	2.879440	4.750694
440	V	2.896815	4.701339
441	V	2.911151	4.496142
442	V	2.919748	4.783652
443	V	2.971113	4.841718
444	V	2.992213	4.944758
445	V	3.009119	4.889872
446	V	3.021653	4.908845
447	V	3.042170	4.939911
448	V	3.071102	4.794224
449	V	3.077892	4.943138
450	V	3.093132	4.847096
451	V	3.108158	4.847475
452	V	3.119068	4.870303
453	V	3.163910	5.206741
454	V	3.180208	5.038397
455	V	3.225649	5.214189
456	V	3.260252	5.104558
457	V	3.266040	5.114959
458	V	3.312802	5.201036
459	V	3.334186	5.299962
460	V	3.389818	5.230039
461	V	3.410194	5.444840
462	V	3.488135	5.527047
463	V	3.612711	5.554150
464	V	3.714828	5.643817
465	V	3.778102	5.661262

Total kinetic energy from orbitals= 1.350375837688D+03

9.4. (*E/Z*)-4-(2-((5-nitrofuran-2-yl)methylene)hydrazineyl)-2-phenylquinazoline **3a** in complex with Zn(II)
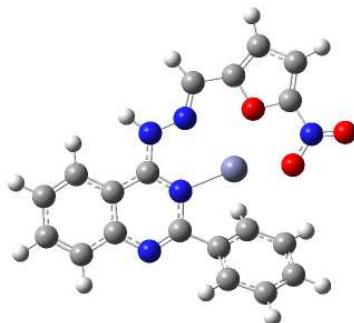
Standard orientation:

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
| Number | Number | Type | X | Y | Z |

1	6	0	5.422971	-2.106802	0.113708
2	6	0	4.066266	-2.260855	-0.004418
3	6	0	3.230951	-1.118960	-0.013498
4	6	0	3.806724	0.181299	0.092877
5	6	0	5.202570	0.306351	0.215402
6	6	0	5.991297	-0.818046	0.226869
7	1	0	6.068216	-2.977938	0.119078
8	1	0	3.658316	-3.262815	-0.092794
9	6	0	1.817702	-1.148228	-0.088892
10	1	0	5.620787	1.303014	0.291546
11	1	0	7.067661	-0.720381	0.319129
12	6	0	1.767120	1.183332	-0.050480
13	7	0	3.046021	1.319251	0.058606
14	7	0	1.105838	-0.027331	-0.082604
15	7	0	1.100577	-2.326820	-0.158421
16	7	0	-0.227181	-2.218015	-0.155724
17	6	0	0.849025	2.340498	-0.146708
18	6	0	-0.271690	2.253790	-1.010599
19	6	0	1.031967	3.476374	0.631733
20	6	0	-1.197687	3.303191	-1.060054
21	1	0	-0.247220	1.546410	-1.848139
22	6	0	0.096951	4.507387	0.575310
23	1	0	1.897235	3.543509	1.281588
24	6	0	-1.022641	4.416823	-0.249619
25	1	0	-2.026664	3.262522	-1.758254
26	1	0	0.242213	5.391231	1.187555
27	1	0	-1.738532	5.230328	-0.283179
28	1	0	1.563118	-3.228726	-0.152911
29	6	0	-1.057122	-3.195546	-0.183617
30	1	0	-0.802613	-4.252880	-0.232840
31	6	0	-2.439745	-2.752264	-0.094349
32	6	0	-3.705255	-3.258634	-0.006070
33	8	0	-2.504024	-1.390074	0.001334

S75

34	6	0	-4.596386	-2.150595	0.171154
35	1	0	-3.987634	-4.301536	-0.046497
36	6	0	-3.799841	-1.050286	0.172138
37	1	0	-5.670703	-2.179783	0.292645
38	7	0	-3.928732	0.343602	0.359147
39	8	0	-2.838992	0.997147	0.346651
40	8	0	-5.006305	0.839795	0.518178
41	30	0	-0.922811	0.159477	-0.063286

 Rotational constants (GHZ):   0.2650736   0.1355138   0.0915378

 Cycle 10 Pass 1 IDiag 1:
 RMSU= 6.25D-09   CP: 1.00D+00 1.04D+00 6.19D-01 1.10D+00 8.05D-01
              CP: 1.23D+00 1.15D+00
 E= -1230.48999739917   Delta-E=   0.000000000005 Rises=F Damp=F
 DIIS: error= 6.62D-08 at cycle   8 NSaved= 8.
 NSaved= 8 IEnMin= 7 EnMin= -1230.48999739917   IErMin= 8 ErrMin= 6.62D-08
 ErrMax= 6.62D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.14D-12 BMatP= 3.81D-
12
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com: -0.166D-03 0.684D-02 0.325D-02-0.699D-01-0.881D-01-0.379D-01
 Coeff-Com: 0.410D+00 0.776D+00
 Coeff: -0.166D-03 0.684D-02 0.325D-02-0.699D-01-0.881D-01-0.379D-01
 Coeff: 0.410D+00 0.776D+00
 Gap=   0.217 Goal=   None   Shift=   0.000
 RMSDP=6.56D-09 MaxDP=5.18D-07 DE= 4.55D-12 OVMax= 1.74D-06

 SCF Done: E(RCAM-B3LYP) = -1230.48999740   A.U. after   10 cycles
          NFock= 10 Conv=0.66D-08   -V/T= 2.0063
 KE= 1.222744431539D+03 PE=-7.432092622106D+03 EE= 2.697104146851D+03
 Leave Link   502 at Thu Sep 15 17:05:16 2022, MaxMem=   2147483648 cpu:
1564.9
 (Enter /opt/gaussian/g09/l701.exe)
 Compute integral first derivatives.
 ... and contract with generalized density number 0.
 Leave Link 701 at Thu Sep 15 17:05:17 2022, MaxMem= 2147483648 cpu: 5.7
 (Enter /opt/gaussian/g09/l702.exe)
 L702 exits ... SP integral derivatives will be done elsewhere.
 Leave Link 702 at Thu Sep 15 17:05:17 2022, MaxMem= 2147483648 cpu: 0.8
 (Enter /opt/gaussian/g09/l703.exe)
 Compute integral first derivatives, UseDBF=F ICtDFT=   0.
 Integral derivatives from FoFJK, PRISM(SPDF).
 Calling FoFJK, ICntrl=   2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1
 NMatS=1 NMatT=0.
 FoFJK: IHMeth= 1 ICntrl=   2127 DoSepK=T KAlg= 0 I1Cent=   0 FoldK=F
 IRaf=   1 NMat= 1 IRICut=   1 DoRegI=T DoRafI=F ISym2E= 0.
 FoFCou: FMM=F IPFlag=   0 FMFlag=   100000 FMFlg1=   800
      NFxFlg=   0 DoJE=F BraDBF=F KetDBF=F FulRan=T
      wScrn= 0.000000 ICntrl=   2527 IOpCl= 0 I1Cent=   0 NGrid=   0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0
NMtDT0= 0
Symmetry not used in FoFCou.
Leave Link 703 at Thu Sep 15 17:07:03 2022, MaxMem= 2147483648 cpu: 849.0
(Enter /opt/gaussian/g09/l716.exe)
Dipole = 7.86255013D-01-3.21191683D+00-2.55910265D-01
***** Axes restored to original set *****
Cartesian Forces: Max 0.076524475 RMS 0.012357602
Leave Link 716 at Thu Sep 15 17:07:04 2022, MaxMem= 2147483648 cpu: 0.8
(Enter /opt/gaussian/g09/l1122.exe)
CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 4 LCPTot= 332729 Len1MO=
859619 IndFrg= 4630824
Restoring MOs from calculation 1 to rwf.
CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot= 332729 Len1MO=
859619 IndFrg= 1192348
Counterpoise corrected energy = -1295.567377170607
           BSSE energy = 0.012400118580
        sum of monomers = -1295.069316729376
      complexation energy = -320.32 kcal/mole (raw)
      complexation energy = -312.54 kcal/mole (corrected)
Leave Link 122 at Thu Sep 15 17:07:04 2022, MaxMem= 2147483648 cpu: 0.4
(Enter /opt/gaussian/g09/l716.exe)
Rotating derivatives to standard orientation.
Dipole =-1.02340469D+00-3.22105232D+00-4.20267598D-02

Orbital energies and kinetic energies (alpha):

		1	2
1	O	-19.602883	29.117244
2	O	-19.543404	29.122550
3	O	-19.536732	29.122124
4	O	-14.935730	22.048939
5	O	-14.753451	22.046288
6	O	-14.750140	22.049361
7	O	-14.690581	22.049144
8	O	-14.635367	22.049810
9	O	-10.641608	15.949527
10	O	-10.623179	15.952528
11	O	-10.620247	15.952262
12	O	-10.596816	15.951643
13	O	-10.579534	15.952914
14	O	-10.564986	15.953690
15	O	-10.548986	15.953244
16	O	-10.534406	15.954284
17	O	-10.515822	15.953610
18	O	-10.514876	15.954573
19	O	-10.507867	15.953407
20	O	-10.497037	15.953914
21	O	-10.495373	15.953485
22	O	-10.486451	15.954544
23	O	-10.485620	15.952885

24	O	-10.480548	15.954716
25	O	-10.480004	15.953461
26	O	-10.479726	15.953217
27	O	-10.471619	15.952977
28	O	-1.600874	2.484780
29	O	-1.520408	2.497606
30	O	-1.417159	2.750974
31	O	-1.410806	2.020585
32	O	-1.327611	1.848590
33	O	-1.250789	1.923370
34	O	-1.215774	1.989445
35	O	-1.192890	1.919399
36	O	-1.184106	1.738981
37	O	-1.175473	1.692849
38	O	-1.158964	1.679505
39	O	-1.102518	1.724463
40	O	-1.083436	1.794069
41	O	-1.063167	1.847071
42	O	-1.061568	1.731886
43	O	-1.044331	1.735298
44	O	-1.010114	7.687710
45	O	-1.007905	6.494897
46	O	-1.002592	3.862603
47	O	-1.000128	10.096717
48	O	-0.997576	11.070563
49	O	-0.995423	11.082978
50	O	-0.986393	6.350547
51	O	-0.975355	2.229146
52	O	-0.952744	2.068015
53	O	-0.937096	2.657672
54	O	-0.930280	1.816143
55	O	-0.923127	2.571373
56	O	-0.912855	1.637194
57	O	-0.899755	1.734145
58	O	-0.898459	1.691852
59	O	-0.889818	1.771380
60	O	-0.867451	1.676907
61	O	-0.856922	2.565053
62	O	-0.842928	1.489824
63	O	-0.834373	1.769731
64	O	-0.829675	1.516568
65	O	-0.816000	1.516731
66	O	-0.811129	1.548647
67	O	-0.801278	1.408409
68	O	-0.779963	1.922182
69	O	-0.767783	1.483616
70	O	-0.765818	1.477928
71	O	-0.760954	1.506409
72	O	-0.756575	1.392399
73	O	-0.751759	1.510266

74	O	-0.742148	1.377104
75	O	-0.736045	1.435139
76	O	-0.721144	1.451886
77	O	-0.717105	1.371246
78	O	-0.715387	1.239859
79	O	-0.704151	1.479973
80	O	-0.678205	1.321326
81	O	-0.669758	2.449201
82	O	-0.663375	1.303069
83	O	-0.658389	2.234357
84	O	-0.654158	1.783929
85	O	-0.650967	1.472894
86	O	-0.645333	2.301629
87	O	-0.643566	1.556150
88	O	-0.635187	1.601890
89	O	-0.632772	1.540027
90	O	-0.632349	1.499196
91	O	-0.628960	1.617951
92	O	-0.605710	1.458573
93	O	-0.562967	1.507146
94	O	-0.559739	1.798181
95	O	-0.545771	1.311917
96	O	-0.540547	1.299502
97	O	-0.532075	1.259348
98	O	-0.501145	1.352349
99	V	-0.333143	2.069237
100	V	-0.273718	1.842187
101	V	-0.262531	1.350665
102	V	-0.232968	1.625128
103	V	-0.226637	1.568080
104	V	-0.206187	0.761220
105	V	-0.189273	1.254462
106	V	-0.167124	1.410741
107	V	-0.161148	2.011279
108	V	-0.145385	0.841436
109	V	-0.142248	1.088867
110	V	-0.137706	0.979530
111	V	-0.123058	1.665100
112	V	-0.119300	1.033667
113	V	-0.096336	1.710005
114	V	-0.088949	1.371932
115	V	-0.082130	2.138537
116	V	-0.065469	1.047049
117	V	-0.060420	1.263153
118	V	-0.053706	1.094779
119	V	-0.035041	1.179903
120	V	-0.027907	1.587080
121	V	-0.022463	2.007121
122	V	-0.018489	1.475821
123	V	-0.015531	1.699624

124	V	-0.004171	1.662164
125	V	-0.000829	1.646523
126	V	0.005158	1.407243
127	V	0.018501	1.445553
128	V	0.023760	1.698523
129	V	0.030213	1.847507
130	V	0.033936	1.775610
131	V	0.038992	1.771677
132	V	0.046138	1.510403
133	V	0.050923	1.386717
134	V	0.058950	1.652727
135	V	0.066066	1.635121
136	V	0.073865	2.191405
137	V	0.084126	1.882122
138	V	0.090382	2.071875
139	V	0.099281	2.301288
140	V	0.110818	2.109374
141	V	0.122859	1.786346
142	V	0.129751	1.926193
143	V	0.141889	1.956722
144	V	0.143252	1.672263
145	V	0.147664	2.235498
146	V	0.158368	1.979385
147	V	0.164283	2.208905
148	V	0.180631	1.890256
149	V	0.188203	2.204064
150	V	0.190664	1.955133
151	V	0.205626	1.926177
152	V	0.216865	2.264081
153	V	0.232537	2.097477
154	V	0.245728	2.155111
155	V	0.262452	2.066823
156	V	0.282329	1.927552
157	V	0.306926	2.006113
158	V	0.318813	2.079723
159	V	0.324009	2.049175
160	V	0.325733	2.081710
161	V	0.340577	2.248419
162	V	0.343180	2.640199
163	V	0.352572	2.323407
164	V	0.356685	2.426567
165	V	0.360896	2.294519
166	V	0.369131	2.301604
167	V	0.371873	2.359824
168	V	0.375332	2.268851
169	V	0.379708	2.233645
170	V	0.385175	2.244005
171	V	0.386369	2.168333
172	V	0.395241	2.513755
173	V	0.399038	2.128654

174	V	0.403954	2.153534
175	V	0.406900	2.232304
176	V	0.414610	2.180684
177	V	0.416623	2.378294
178	V	0.422481	2.266960
179	V	0.427416	2.353719
180	V	0.436727	2.377322
181	V	0.439963	2.326032
182	V	0.447510	2.153764
183	V	0.455593	2.238398
184	V	0.457596	2.428696
185	V	0.463606	2.337715
186	V	0.463904	2.251615
187	V	0.469368	2.324889
188	V	0.476605	2.074099
189	V	0.478815	2.166332
190	V	0.479929	2.240815
191	V	0.486594	2.224964
192	V	0.488729	2.484924
193	V	0.497938	2.392182
194	V	0.506659	2.602338
195	V	0.519904	2.426604
196	V	0.527341	2.367710
197	V	0.538855	2.767513
198	V	0.549258	2.670920
199	V	0.555316	2.317642
200	V	0.562150	2.641258
201	V	0.571253	2.732412
202	V	0.577743	2.628847
203	V	0.591100	2.699603
204	V	0.595002	2.715357
205	V	0.604276	2.533379
206	V	0.606039	2.414282
207	V	0.611337	2.648897
208	V	0.619049	2.672807
209	V	0.626402	2.546403
210	V	0.635073	2.743487
211	V	0.647507	2.843859
212	V	0.649795	2.777570
213	V	0.658086	2.863516
214	V	0.665724	2.563843
215	V	0.673807	2.502350
216	V	0.679212	2.757759
217	V	0.683699	2.655450
218	V	0.689945	2.649637
219	V	0.694973	2.647636
220	V	0.695591	2.625115
221	V	0.700994	2.676191
222	V	0.703485	2.619107
223	V	0.719943	2.583807

224	V	0.730495	2.682238
225	V	0.736202	3.016625
226	V	0.741252	2.523193
227	V	0.745338	2.609316
228	V	0.753954	2.573233
229	V	0.760423	2.670152
230	V	0.766914	2.816729
231	V	0.780359	2.951205
232	V	0.785275	2.955234
233	V	0.799249	2.830439
234	V	0.804544	2.735481
235	V	0.814700	2.952125
236	V	0.819269	2.732738
237	V	0.822017	2.691318
238	V	0.830604	2.781916
239	V	0.841648	2.724031
240	V	0.843992	2.962504
241	V	0.851403	2.631723
242	V	0.869819	2.845872
243	V	0.873111	2.828139
244	V	0.882525	2.601108
245	V	0.895839	2.474187
246	V	0.902108	2.942841
247	V	0.912322	2.466939
248	V	0.924721	2.669224
249	V	0.933258	2.439884
250	V	0.967787	2.549539
251	V	0.978525	2.939222
252	V	0.986323	2.646738
253	V	1.005640	2.666036
254	V	1.011469	2.862683
255	V	1.016487	2.560236
256	V	1.031896	2.734216
257	V	1.039627	2.916075
258	V	1.053218	2.694188
259	V	1.058341	2.556025
260	V	1.060697	2.653698
261	V	1.075245	2.638312
262	V	1.081529	2.714700
263	V	1.085924	2.849732
264	V	1.090450	2.680594
265	V	1.099626	2.639750
266	V	1.103695	2.599743
267	V	1.118374	2.620142
268	V	1.127632	2.837122
269	V	1.130612	2.695921
270	V	1.138074	2.699676
271	V	1.141397	2.764839
272	V	1.161987	3.037602
273	V	1.171550	2.785320

274	V	1.186493	2.885367
275	V	1.194657	2.730174
276	V	1.204808	2.547956
277	V	1.209690	2.762364
278	V	1.220860	2.873431
279	V	1.223390	2.936943
280	V	1.233083	2.900548
281	V	1.249496	2.934204
282	V	1.253449	2.953451
283	V	1.262652	2.557980
284	V	1.266941	2.575012
285	V	1.269496	2.685942
286	V	1.277147	2.978745
287	V	1.284564	3.057945
288	V	1.294505	2.852220
289	V	1.308712	3.548562
290	V	1.318554	2.812854
291	V	1.338473	2.878506
292	V	1.343050	3.055483
293	V	1.344042	2.855855
294	V	1.359872	3.491044
295	V	1.394127	3.614065
296	V	1.417810	3.906765
297	V	1.424077	3.086982
298	V	1.440056	2.985576
299	V	1.453689	3.042225
300	V	1.479103	3.653187
301	V	1.483312	3.516150
302	V	1.493574	3.725050
303	V	1.509969	2.992488
304	V	1.540483	3.808440
305	V	1.569623	3.634400
306	V	1.582968	3.394729
307	V	1.589721	3.005836
308	V	1.596502	3.464798
309	V	1.598211	3.211658
310	V	1.608837	3.278967
311	V	1.611722	3.371437
312	V	1.614608	3.142429
313	V	1.628000	3.181936
314	V	1.630710	3.152342
315	V	1.638921	3.300541
316	V	1.648497	3.490055
317	V	1.664287	3.368240
318	V	1.670587	3.557828
319	V	1.676497	3.543008
320	V	1.683947	3.335861
321	V	1.698067	3.249693
322	V	1.705934	3.194162
323	V	1.710617	3.460710

324	V	1.719389	3.651091
325	V	1.729166	3.782321
326	V	1.737950	3.354826
327	V	1.740833	3.286802
328	V	1.748697	3.271952
329	V	1.753372	3.470975
330	V	1.759440	3.251536
331	V	1.766093	3.594261
332	V	1.768757	3.400092
333	V	1.780918	3.381437
334	V	1.789149	3.570950
335	V	1.796327	3.164801
336	V	1.807082	3.529796
337	V	1.816972	3.407922
338	V	1.833137	3.607672
339	V	1.843347	3.727448
340	V	1.852509	3.165336
341	V	1.855630	3.464378
342	V	1.859855	3.003945
343	V	1.863887	3.182961
344	V	1.872247	3.707402
345	V	1.880646	3.216806
346	V	1.901224	4.126253
347	V	1.909289	3.603416
348	V	1.917067	3.671636
349	V	1.918369	3.729920
350	V	1.928197	3.589754
351	V	1.940603	3.484807
352	V	1.947611	3.446476
353	V	1.954245	3.947410
354	V	1.969108	3.634891
355	V	1.978444	3.410921
356	V	1.993967	3.689975
357	V	1.997389	3.411173
358	V	2.007694	3.686984
359	V	2.017220	3.716897
360	V	2.053192	3.499362
361	V	2.067665	3.886612
362	V	2.077995	3.542037
363	V	2.084156	3.498818
364	V	2.094633	3.784413
365	V	2.105526	3.799707
366	V	2.115156	3.558877
367	V	2.130192	3.747616
368	V	2.136694	3.742103
369	V	2.138407	3.663253
370	V	2.147764	3.667789
371	V	2.163692	3.742342
372	V	2.176463	3.491816
373	V	2.193592	3.703876

374	V	2.200809	3.660952
375	V	2.208049	4.052527
376	V	2.222580	3.585836
377	V	2.227279	3.593725
378	V	2.231951	3.657371
379	V	2.243029	3.745181
380	V	2.245583	3.464920
381	V	2.250942	3.720637
382	V	2.251848	3.785387
383	V	2.258358	3.362011
384	V	2.263229	3.769762
385	V	2.276799	3.470643
386	V	2.280459	3.806655
387	V	2.296306	3.685691
388	V	2.310928	3.733068
389	V	2.313090	3.864256
390	V	2.327369	3.917169
391	V	2.328264	3.985808
392	V	2.332992	3.857154
393	V	2.341235	3.869950
394	V	2.351408	3.838773
395	V	2.370487	3.787960
396	V	2.374668	3.907773
397	V	2.387875	4.044538
398	V	2.402423	4.055540
399	V	2.410583	3.734870
400	V	2.415405	3.925677
401	V	2.424766	3.867465
402	V	2.446554	3.893269
403	V	2.448591	3.643245
404	V	2.451822	3.691944
405	V	2.464311	4.051756
406	V	2.473682	3.898794
407	V	2.477607	4.208391
408	V	2.481418	4.122320
409	V	2.490094	4.068879
410	V	2.496673	4.449220
411	V	2.529688	4.081431
412	V	2.537346	4.000531
413	V	2.542955	4.093652
414	V	2.554628	4.059206
415	V	2.566105	4.329205
416	V	2.573401	4.096396
417	V	2.585653	4.145563
418	V	2.594663	4.041089
419	V	2.611853	4.141111
420	V	2.629105	4.413806
421	V	2.631966	4.139840
422	V	2.644470	4.271710
423	V	2.647812	4.382391

424	V	2.661339	4.505088
425	V	2.676341	4.597184
426	V	2.707229	4.512740
427	V	2.722115	4.803136
428	V	2.735816	4.632419
429	V	2.752243	4.656363
430	V	2.758857	4.558306
431	V	2.776937	4.779245
432	V	2.790063	4.733272
433	V	2.829021	4.616206
434	V	2.845417	4.818856
435	V	2.881897	4.715660
436	V	2.897589	4.481720
437	V	2.927437	4.753151
438	V	2.941499	4.964548
439	V	2.972756	4.819892
440	V	2.991565	4.903084
441	V	3.038604	4.924780
442	V	3.054421	4.977078
443	V	3.099918	4.922627
444	V	3.101883	4.812625
445	V	3.111835	4.868212
446	V	3.117916	4.878238
447	V	3.124393	4.853682
448	V	3.133897	5.194475
449	V	3.186387	5.205287
450	V	3.206101	5.020245
451	V	3.237344	5.069652
452	V	3.268201	5.085721
453	V	3.344716	5.256726
454	V	3.356868	5.285075
455	V	3.372032	5.226635
456	V	3.402420	5.411689
457	V	3.487781	5.563759
458	V	3.579923	5.554575
459	V	3.755066	5.647573
460	V	3.768529	5.640077
461	V	7.063015	2.534052

Total kinetic energy from orbitals= 1.337453319717D+03

9.5. (*E/Z*)-4-(2-((5-nitrofuran-2-yl)methylene)hydrazineyl)-2-(3-chlorophenyl)quinazolines **3f**
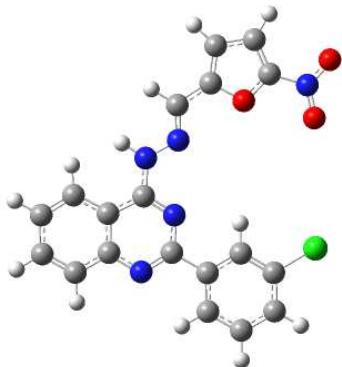
Standard orientation:

```
---------------------------------------------------------------------
Center   Atomic    Atomic        Coordinates (Angstroms)
Number   Number     Type       X        Y        Z
---------------------------------------------------------------------
```

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	4.545455	3.790549	-0.000293
2	6	0	3.230278	3.401486	-0.000075
3	6	0	2.890809	2.030312	-0.000067
4	6	0	3.918578	1.058804	-0.000256
5	6	0	5.266947	1.486966	-0.000489
6	6	0	5.571091	2.822281	-0.000502
7	1	0	4.799017	4.844941	-0.000307
8	1	0	2.462933	4.169487	0.000069
9	6	0	1.560796	1.487349	0.000161
10	1	0	6.034233	0.721613	-0.000644
11	1	0	6.607713	3.142714	-0.000672
12	6	0	2.395883	-0.635473	0.000048
13	7	0	3.656904	-0.275889	-0.000223
14	7	0	1.329137	0.203706	0.000280
15	7	0	0.486135	2.351139	0.000458
16	7	0	-0.779234	1.904339	0.000323
17	6	0	2.079936	-2.086255	0.000165
18	6	0	0.749985	-2.508256	-0.000010
19	6	0	3.108812	-3.029303	0.000410
20	6	0	0.472302	-3.866149	0.000047
21	1	0	-0.046035	-1.774558	-0.000180
22	6	0	2.809066	-4.383085	0.000496
23	1	0	4.133922	-2.680618	0.000516
24	6	0	1.487094	-4.814039	0.000309
25	1	0	3.609478	-5.115488	0.000714
26	1	0	1.241850	-5.869641	0.000351
27	1	0	0.657695	3.349098	0.000716
28	6	0	-1.707444	2.781930	0.000429
29	1	0	-1.509813	3.859694	0.000670
30	6	0	-3.102360	2.405339	0.000273
31	6	0	-4.233798	3.179023	0.000296

32	8	0	-3.430864	1.092638	0.000074
33	6	0	-5.333377	2.284168	0.000103
34	1	0	-4.267461	4.258198	0.000417
35	6	0	-4.773435	1.046829	0.000005
36	1	0	-6.389010	2.502153	0.000076
37	7	0	-5.392343	-0.240843	-0.000353
38	8	0	-4.673084	-1.224159	-0.000698
39	8	0	-6.618348	-0.237347	-0.000270
40	17	0	-1.192944	-4.398158	-0.000252

Rotational constants (GHZ): 0.1781282 0.1039344 0.0656367

Cycle 9 Pass 1 IDiag 1:
RMSU= 6.60D-09 CP: 1.00D+00 1.24D+00 1.31D+00 7.98D-01 1.34D+00
          CP: 1.22D+00 9.91D-01 9.61D-01
E= -1690.15325925696   Delta-E=   0.000000000003 Rises=F Damp=F
DIIS: error= 6.32D-08 at cycle 9 NSaved= 9.
NSaved= 9 IEnMin= 8 EnMin= -1690.15325925696   IErMin= 9 ErrMin= 6.32D-08
ErrMax= 6.32D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.13D-12 BMatP= 8.48D-
12
IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
Coeff-Com: -0.471D-04-0.449D-04 0.545D-02 0.117D-02-0.338D-01-0.569D-01
Coeff-Com: -0.308D-02 0.277D+00 0.810D+00
Coeff: -0.471D-04-0.449D-04 0.545D-02 0.117D-02-0.338D-01-0.569D-01
Coeff: -0.308D-02 0.277D+00 0.810D+00
Gap=   0.215 Goal= None   Shift=   0.000
RMSDP=5.18D-09 MaxDP=3.67D-07 DE= 2.73D-12 OVMax= 1.47D-06

SCF Done: E(RCAM-B3LYP) = -1690.15325926   A.U. after   9 cycles
      NFock= 9 Conv=0.52D-08   -V/T= 2.0072
KE= 1.678102729444D+03 PE=-8.887476039495D+03 EE= 3.053661797712D+03
Leave Link 502 at Fri Sep 9 15:46:30 2022, MaxMem= 2147483648 cpu: 1909.8
(Enter /opt/gaussian/g09/l701.exe)
Compute integral first derivatives.
... and contract with generalized density number 0.
Leave Link 701 at Fri Sep 9 15:46:31 2022, MaxMem= 2147483648 cpu: 7.1
(Enter /opt/gaussian/g09/l702.exe)
L702 exits ... SP integral derivatives will be done elsewhere.
Leave Link 702 at Fri Sep 9 15:46:31 2022, MaxMem= 2147483648 cpu: 0.8
(Enter /opt/gaussian/g09/l703.exe)
Compute integral first derivatives, UseDBF=F ICtDFT=   0.
Integral derivatives from FoFJK, PRISM(SPDF).
Calling FoFJK, ICntrl=   2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1
NMatS=1 NMatT=0.
FoFJK: IHMeth= 1 ICntrl=   2127 DoSepK=T KAlg= 0 I1Cent=   0 FoldK=F
IRaf=   1 NMat= 1 IRICut=   1 DoRegI=T DoRafI=F ISym2E= 0.
FoFCou: FMM=F IPFlag=   0 FMFlag=   100000 FMFlg1=   800
      NFxFlg=   0 DoJE=F BraDBF=F KetDBF=F FulRan=T
      wScrn= 0.000000 ICntrl=   2527 IOpCl= 0 I1Cent=   0 NGrid=   0

NMat0=   1 NMatS0=   1 NMatT0=   0 NMatD0=   1 NMtDS0=   0
NMtDT0=   0
Symmetry not used in FoFCou.
Leave Link 703 at Fri Sep 9 15:48:19 2022, MaxMem= 2147483648 cpu: 862.2
(Enter /opt/gaussian/g09/l716.exe)
Dipole   = 1.49170142D+00 3.71086493D+00 8.55175443D-04

Orbital energies and kinetic energies (alpha):

		1	2
1	O	-101.602777	136.916771
2	O	-19.328100	29.025821
3	O	-19.254595	29.033119
4	O	-19.251739	29.033048
5	O	-14.658935	21.965603
6	O	-14.498658	21.957511
7	O	-14.479119	21.963488
8	O	-14.404701	21.960007
9	O	-14.399692	21.960624
10	O	-10.377404	15.880718
11	O	-10.369871	15.882560
12	O	-10.360085	15.881430
13	O	-10.339279	15.881954
14	O	-10.335627	15.877533
15	O	-10.315749	15.881245
16	O	-10.312815	15.882019
17	O	-10.305639	15.878327
18	O	-10.298728	15.878922
19	O	-10.295537	15.874468
20	O	-10.294933	15.882813
21	O	-10.286125	15.874414
22	O	-10.285537	15.884251
23	O	-10.276563	15.878996
24	O	-10.268836	15.878511
25	O	-10.267099	15.878069
26	O	-10.263347	15.879512
27	O	-10.260768	15.879081
28	O	-10.258005	15.879917
29	O	-9.519790	21.535382
30	O	-7.284848	20.526569
31	O	-7.274988	20.553887
32	O	-7.274692	20.548548
33	O	-1.320027	2.494469
34	O	-1.242483	2.495416
35	O	-1.146503	1.989739
36	O	-1.139097	2.804901
37	O	-1.076260	1.831102
38	O	-0.995860	1.986692
39	O	-0.970745	1.695496
40	O	-0.961234	1.888585
41	O	-0.939129	1.888561

42	O	-0.929505	1.874497
43	O	-0.910457	2.072107
44	O	-0.906828	2.035452
45	O	-0.866614	1.743495
46	O	-0.854058	1.658498
47	O	-0.826954	1.687454
48	O	-0.814126	1.915272
49	O	-0.801023	2.009617
50	O	-0.753161	1.724864
51	O	-0.747909	1.748841
52	O	-0.722114	1.655991
53	O	-0.714617	1.794409
54	O	-0.702038	1.649639
55	O	-0.680153	1.586950
56	O	-0.669641	1.604467
57	O	-0.664014	1.640065
58	O	-0.650698	1.654233
59	O	-0.629104	2.198037
60	O	-0.623279	1.671550
61	O	-0.623062	1.713983
62	O	-0.604983	1.690418
63	O	-0.597237	1.530706
64	O	-0.580037	1.380287
65	O	-0.576995	2.459523
66	O	-0.561132	1.619303
67	O	-0.560284	1.543730
68	O	-0.543881	1.466393
69	O	-0.542569	1.308420
70	O	-0.540162	1.494314
71	O	-0.519924	1.532610
72	O	-0.518455	1.482151
73	O	-0.517502	1.506984
74	O	-0.511737	1.511219
75	O	-0.506239	1.596252
76	O	-0.498890	1.261597
77	O	-0.489210	1.442998
78	O	-0.482050	1.640350
79	O	-0.479776	2.217922
80	O	-0.459710	1.044161
81	O	-0.455076	1.528008
82	O	-0.437016	1.176005
83	O	-0.436996	1.440914
84	O	-0.417912	1.600302
85	O	-0.416313	1.378040
86	O	-0.409139	1.587286
87	O	-0.386134	1.901098
88	O	-0.382342	1.692325
89	O	-0.380502	1.609582
90	O	-0.376626	2.422750
91	O	-0.367916	2.352817

92	O	-0.365418	2.054261
93	O	-0.360585	2.584726
94	O	-0.357132	2.297171
95	O	-0.355705	1.408219
96	O	-0.338279	1.206724
97	O	-0.315965	1.269288
98	O	-0.314150	1.961877
99	O	-0.294423	1.355361
100	O	-0.286806	1.560806
101	O	-0.268779	1.524943
102	V	-0.053602	2.062023
103	V	-0.021455	1.684945
104	V	-0.004301	1.548758
105	V	0.015266	1.800670
106	V	0.048552	1.429914
107	V	0.056159	1.465215
108	V	0.086610	1.725952
109	V	0.089323	1.162632
110	V	0.104953	2.050588
111	V	0.106287	2.109314
112	V	0.127741	1.298752
113	V	0.129548	1.674987
114	V	0.146371	1.047699
115	V	0.148132	1.754115
116	V	0.167072	1.304291
117	V	0.176698	1.545540
118	V	0.180074	1.236259
119	V	0.189320	1.197527
120	V	0.201288	1.487543
121	V	0.217219	1.195523
122	V	0.223525	1.758481
123	V	0.229368	1.740078
124	V	0.231523	1.566163
125	V	0.234458	1.772354
126	V	0.241464	1.502745
127	V	0.247241	1.826772
128	V	0.256285	1.623536
129	V	0.268146	2.034151
130	V	0.276455	1.812620
131	V	0.281237	2.451315
132	V	0.301341	1.971849
133	V	0.314129	2.284386
134	V	0.317189	2.218168
135	V	0.325576	2.081622
136	V	0.330312	2.265332
137	V	0.340789	1.941160
138	V	0.345308	1.760370
139	V	0.356673	1.929137
140	V	0.361110	1.817597
141	V	0.381989	1.823396

142	V	0.394635	2.082522
143	V	0.405066	2.175180
144	V	0.407875	2.217107
145	V	0.410946	2.345358
146	V	0.431701	2.484860
147	V	0.435508	2.005445
148	V	0.442797	1.932130
149	V	0.468990	2.038527
150	V	0.476440	2.247252
151	V	0.483799	2.511905
152	V	0.487622	2.349588
153	V	0.498049	2.289486
154	V	0.511119	2.496503
155	V	0.517035	2.597145
156	V	0.531804	1.994786
157	V	0.542497	2.017664
158	V	0.543146	2.118433
159	V	0.547168	2.001170
160	V	0.558108	2.368992
161	V	0.567627	2.197127
162	V	0.576792	2.085678
163	V	0.578036	2.437672
164	V	0.580039	2.040790
165	V	0.593033	1.981532
166	V	0.594258	2.044870
167	V	0.601684	2.298172
168	V	0.604379	2.369854
169	V	0.617887	2.506387
170	V	0.619543	2.102033
171	V	0.621210	2.638432
172	V	0.623153	2.549543
173	V	0.632794	2.099614
174	V	0.638175	2.144767
175	V	0.638363	2.107494
176	V	0.640177	2.460724
177	V	0.646069	2.517523
178	V	0.648549	2.065959
179	V	0.653123	2.034206
180	V	0.655756	2.301820
181	V	0.661492	2.177150
182	V	0.661866	2.189008
183	V	0.667377	2.674507
184	V	0.668027	2.116457
185	V	0.673326	2.441010
186	V	0.674365	2.221247
187	V	0.680248	2.178428
188	V	0.681701	2.192105
189	V	0.692329	2.172758
190	V	0.697556	2.576324
191	V	0.706842	2.882337

192	V	0.710690	2.344140
193	V	0.716560	2.284383
194	V	0.726314	2.251033
195	V	0.734899	2.892076
196	V	0.737771	2.311713
197	V	0.752129	3.113084
198	V	0.769622	2.728639
199	V	0.790073	2.308559
200	V	0.802375	2.475429
201	V	0.812103	2.562373
202	V	0.823287	2.430900
203	V	0.823593	2.624341
204	V	0.833844	2.577066
205	V	0.835902	2.714001
206	V	0.837548	2.629269
207	V	0.842500	2.388076
208	V	0.845972	2.690378
209	V	0.851483	2.484477
210	V	0.865098	2.627238
211	V	0.869333	2.613327
212	V	0.869892	2.508054
213	V	0.872088	2.569476
214	V	0.880917	2.736562
215	V	0.886679	2.810845
216	V	0.889539	2.587051
217	V	0.898458	2.433624
218	V	0.905889	2.458170
219	V	0.918548	2.702001
220	V	0.919835	2.457862
221	V	0.928753	2.560247
222	V	0.942064	2.496679
223	V	0.950830	2.595588
224	V	0.953473	2.419334
225	V	0.958897	2.586064
226	V	0.964364	2.622135
227	V	0.968740	2.603234
228	V	0.979964	2.670578
229	V	0.984925	2.592076
230	V	0.987316	3.402379
231	V	0.996665	2.565571
232	V	1.002181	2.509355
233	V	1.011214	2.604332
234	V	1.022550	2.629384
235	V	1.024176	2.581147
236	V	1.028650	2.731907
237	V	1.037099	2.573028
238	V	1.041464	2.535741
239	V	1.053619	3.385518
240	V	1.058342	2.474262
241	V	1.068781	2.345941

242	V	1.074578	2.633978
243	V	1.086442	3.257098
244	V	1.092720	2.560269
245	V	1.099709	2.597942
246	V	1.121241	2.359391
247	V	1.134655	2.564676
248	V	1.139891	2.463018
249	V	1.148292	2.436845
250	V	1.153370	2.503829
251	V	1.172192	2.478288
252	V	1.181881	2.859395
253	V	1.199628	2.875109
254	V	1.210784	2.502374
255	V	1.227830	2.681705
256	V	1.239339	2.471177
257	V	1.266627	2.685960
258	V	1.271032	2.398659
259	V	1.273062	2.596113
260	V	1.279178	2.578884
261	V	1.280308	2.391833
262	V	1.288442	2.399382
263	V	1.305918	2.624537
264	V	1.324264	2.697319
265	V	1.325849	2.412613
266	V	1.335867	2.673569
267	V	1.344158	2.483559
268	V	1.346924	2.734598
269	V	1.358126	2.488737
270	V	1.365829	2.458041
271	V	1.368037	2.594421
272	V	1.368374	2.509328
273	V	1.384416	2.499829
274	V	1.390247	2.500991
275	V	1.398292	2.828189
276	V	1.399355	2.454920
277	V	1.414312	2.800793
278	V	1.441740	2.495497
279	V	1.442691	2.672532
280	V	1.447533	2.514441
281	V	1.454130	2.544527
282	V	1.463722	2.654830
283	V	1.465515	2.546920
284	V	1.471607	2.669239
285	V	1.477088	2.614331
286	V	1.484279	2.552324
287	V	1.486965	2.748145
288	V	1.487829	2.538868
289	V	1.517515	2.713605
290	V	1.528679	2.729052
291	V	1.528836	2.624386

292	V	1.551848	2.826626
293	V	1.567744	2.794620
294	V	1.570640	2.686246
295	V	1.587451	2.817391
296	V	1.598033	2.699686
297	V	1.601328	3.031654
298	V	1.623212	2.770704
299	V	1.652190	2.969993
300	V	1.661303	2.965631
301	V	1.678351	3.185484
302	V	1.682745	2.731881
303	V	1.710381	3.077425
304	V	1.720219	3.034184
305	V	1.781148	2.841718
306	V	1.796581	3.015187
307	V	1.802670	3.167932
308	V	1.824260	2.911658
309	V	1.828145	3.093904
310	V	1.842601	3.163632
311	V	1.856620	3.147982
312	V	1.869289	3.204525
313	V	1.871954	2.937867
314	V	1.873391	3.357701
315	V	1.876008	3.165452
316	V	1.877785	2.862033
317	V	1.889352	3.272655
318	V	1.889830	3.171190
319	V	1.893876	2.968331
320	V	1.910912	3.194229
321	V	1.934873	3.231622
322	V	1.942785	3.271881
323	V	1.951787	3.192620
324	V	1.958325	3.166343
325	V	1.963082	3.437927
326	V	1.971747	3.313471
327	V	1.973706	3.042034
328	V	1.975557	3.278514
329	V	1.984360	3.093631
330	V	1.986391	3.379272
331	V	2.002401	3.509433
332	V	2.018640	3.095110
333	V	2.018978	3.471549
334	V	2.035609	3.148625
335	V	2.039035	3.403762
336	V	2.050522	3.459013
337	V	2.052841	2.994282
338	V	2.058905	3.024195
339	V	2.065559	3.508252
340	V	2.074597	3.421433
341	V	2.089568	3.522390

342	V	2.109418	3.370867
343	V	2.121288	3.450060
344	V	2.122765	3.193827
345	V	2.134585	3.216961
346	V	2.141486	3.502721
347	V	2.144808	3.417284
348	V	2.162271	3.160034
349	V	2.164021	3.803515
350	V	2.171712	3.498011
351	V	2.188584	3.665835
352	V	2.213861	3.804877
353	V	2.215160	3.362093
354	V	2.229319	3.596310
355	V	2.235991	3.350790
356	V	2.245768	3.382288
357	V	2.272133	3.705878
358	V	2.278705	3.763000
359	V	2.299592	3.481122
360	V	2.310081	3.800884
361	V	2.319212	3.427945
362	V	2.331787	3.921386
363	V	2.332215	3.501490
364	V	2.341342	3.513341
365	V	2.371892	3.543600
366	V	2.378679	3.530738
367	V	2.378852	3.913383
368	V	2.386986	3.531528
369	V	2.406107	3.528846
370	V	2.409768	3.812922
371	V	2.416100	3.816413
372	V	2.424410	3.821458
373	V	2.433587	3.862201
374	V	2.433665	3.379214
375	V	2.444809	3.376013
376	V	2.451299	3.676611
377	V	2.457134	3.425124
378	V	2.473723	3.706283
379	V	2.479161	3.769552
380	V	2.479525	3.382868
381	V	2.498243	3.576565
382	V	2.509822	3.950816
383	V	2.514843	3.632610
384	V	2.523927	3.882575
385	V	2.529715	3.542426
386	V	2.530066	3.862537
387	V	2.555705	3.951982
388	V	2.576173	3.879097
389	V	2.585956	3.766595
390	V	2.596585	4.052747
391	V	2.607235	3.597909

392	V	2.613201	4.002217
393	V	2.618239	4.177173
394	V	2.618285	3.658739
395	V	2.633903	4.082745
396	V	2.639361	4.023374
397	V	2.641616	3.634281
398	V	2.660138	3.647325
399	V	2.672984	4.003358
400	V	2.687909	3.891696
401	V	2.688807	4.086050
402	V	2.693433	3.839288
403	V	2.711010	4.033872
404	V	2.737666	3.947552
405	V	2.739709	4.412580
406	V	2.745136	4.315583
407	V	2.760331	4.302399
408	V	2.764101	3.919286
409	V	2.773449	4.414079
410	V	2.776103	3.856283
411	V	2.779020	3.918791
412	V	2.797566	4.348446
413	V	2.801605	4.349507
414	V	2.802860	3.984895
415	V	2.807841	3.846994
416	V	2.839988	4.386617
417	V	2.843596	4.397052
418	V	2.858910	4.455457
419	V	2.868176	4.069114
420	V	2.887563	4.453862
421	V	2.890191	4.574633
422	V	2.909650	4.569981
423	V	2.937065	4.648879
424	V	2.953260	4.915138
425	V	2.958787	4.475619
426	V	2.968464	5.092973
427	V	2.973486	4.892788
428	V	2.989622	4.654729
429	V	3.000888	4.686941
430	V	3.051010	4.637612
431	V	3.064012	4.451559
432	V	3.093669	4.866637
433	V	3.142385	4.770533
434	V	3.143251	4.828580
435	V	3.176948	5.012661
436	V	3.218345	4.869423
437	V	3.234409	4.920076
438	V	3.266043	5.030604
439	V	3.286648	4.996523
440	V	3.297476	4.927552
441	V	3.309162	4.984564

442	V	3.321217	4.873802
443	V	3.329451	4.892476
444	V	3.362635	5.214880
445	V	3.405017	5.092327
446	V	3.429192	5.330060
447	V	3.481136	5.186519
448	V	3.485736	5.262529
449	V	3.534812	5.421496
450	V	3.541321	5.351049
451	V	3.582122	5.491304
452	V	3.600104	5.693946
453	V	3.681917	5.963215
454	V	3.765339	8.468520
455	V	3.786931	7.846000
456	V	3.908860	6.181351
457	V	3.931456	6.328976
458	V	3.936088	9.909790
459	V	3.973326	9.990463
460	V	4.081783	10.395491
461	V	4.129339	10.210384
462	V	4.157021	10.170606
463	V	4.174269	10.405650
464	V	4.183294	10.070858
465	V	4.193280	10.125157
466	V	4.206611	10.139694
467	V	4.215647	10.100304
468	V	4.224822	10.175360
469	V	4.268317	10.190985
470	V	4.363832	11.016767
471	V	4.369031	11.689773
472	V	4.380460	10.665410
473	V	4.393712	10.018088
474	V	4.432714	10.628193
475	V	4.496394	10.904119
476	V	4.503932	10.460502
477	V	4.516726	10.299393
478	V	4.566087	10.414325
479	V	4.586425	11.130217
480	V	4.632824	10.060846
481	V	4.776534	11.087344
482	V	4.827175	10.330951
483	V	4.879368	10.281641
484	V	4.955005	10.270800

Total kinetic energy from orbitals= 1.678102681267D+03

9.6. (*E*)-4-(2-((5-nitrofuran-2-yl)methylene)hydrazineyl)-2-(3-chlorophenyl)quinazoline **3f** in complex with Zn(II)
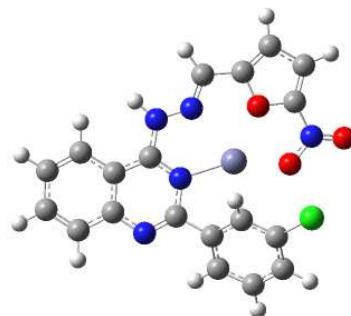
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.873915	-1.518125	-0.142860
2	6	0	-4.547035	-1.852928	-0.222560
3	6	0	-3.562851	-0.844341	-0.100751
4	6	0	-3.958530	0.511825	0.097213
5	6	0	-5.327814	0.823181	0.176432
6	6	0	-6.263934	-0.175467	0.059747
7	1	0	-6.632558	-2.286833	-0.236767
8	1	0	-4.277217	-2.892514	-0.379142
9	6	0	-2.164926	-1.067513	-0.126944
10	1	0	-5.608097	1.859564	0.322692
11	1	0	-7.319767	0.066032	0.118890
12	6	0	-1.796261	1.222679	0.119713
13	7	0	-3.047325	1.530603	0.188371
14	7	0	-1.307961	-0.062919	0.012569
15	7	0	-1.611264	-2.322848	-0.287933
16	7	0	-0.280827	-2.399549	-0.237989
17	6	0	-0.722395	2.243166	0.145768
18	6	0	0.419907	2.029399	-0.666854
19	6	0	-0.781382	3.347840	0.981743
20	6	0	1.487816	2.935388	-0.606345
21	1	0	0.339425	1.402743	-1.560708
22	6	0	0.298940	4.228772	1.026864
23	1	0	-1.659652	3.509687	1.595869
24	6	0	1.439321	4.023246	0.255912
25	1	0	0.256357	5.090917	1.684200
26	1	0	2.271104	4.716650	0.300070
27	1	0	-2.190082	-3.146559	-0.405165
28	6	0	0.414219	-3.470603	-0.363980
29	1	0	0.024423	-4.470206	-0.548323
30	6	0	1.839311	-3.233411	-0.185262
31	6	0	3.023976	-3.909488	-0.118635
32	8	0	2.075043	-1.912945	0.079464
33	6	0	4.040347	-2.958003	0.226083
34	1	0	3.173254	-4.968603	-0.277073

35	6	0	3.392605	-1.769889	0.338096
36	1	0	5.094004	-3.145570	0.382262
37	7	0	3.679719	-0.438947	0.723333
38	8	0	2.675955	0.336678	0.780738
39	8	0	4.800150	-0.108384	0.980649
40	17	0	2.844888	2.706545	-1.647541
41	30	0	0.719525	-0.193604	0.137862

Rotational constants (GHZ):   0.2187655   0.1235568   0.0836900

Cycle 8 Pass 1 IDiag 1:
 RMSU= 2.14D-08   CP: 1.00D+00 1.04D+00 7.04D-01 1.08D+00 7.27D-01
 E= -1690.08311289256   Delta-E=   -0.000000000226 Rises=F Damp=F
 DIIS: error= 8.55D-08 at cycle   6 NSaved=   6.
 NSaved= 6 IEnMin= 6 EnMin= -1690.08311289256   IErMin= 6 ErrMin= 8.55D-08
 ErrMax= 8.55D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.67D-12 BMatP= 1.60D-10
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com: 0.555D-03-0.191D-01-0.557D-02 0.849D-01 0.136D+00 0.803D+00
 Coeff: 0.555D-03-0.191D-01-0.557D-02 0.849D-01 0.136D+00 0.803D+00
 Gap=   0.222 Goal= None   Shift=   0.000
 RMSDP=8.22D-09 MaxDP=4.20D-07 DE=-2.26D-10 OVMax= 1.48D-06

 SCF Done: E(RCAM-B3LYP) = -1690.08311289   A.U. after   8 cycles
        NFock= 8 Conv=0.82D-08   -V/T= 2.0051
 KE= 1.681516923743D+03 PE=-9.160933961420D+03 EE= 3.189679730761D+03
 Leave Link 502 at Fri Oct 14 11:38:21 2022, MaxMem= 2147483648 cpu: 1277.6
 (Enter /opt/gaussian/g09/l701.exe)
 Compute integral first derivatives.
 ... and contract with generalized density number 0.
 Leave Link 701 at Fri Oct 14 11:38:22 2022, MaxMem= 2147483648 cpu: 5.0
 (Enter /opt/gaussian/g09/l702.exe)
 L702 exits ... SP integral derivatives will be done elsewhere.
 Leave Link 702 at Fri Oct 14 11:38:22 2022, MaxMem= 2147483648 cpu: 0.8
 (Enter /opt/gaussian/g09/l703.exe)
 Compute integral first derivatives, UseDBF=F ICtDFT=   0.
 Integral derivatives from FoFJK, PRISM(SPDF).
 Calling FoFJK, ICntrl=   2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1
 NMatS=1 NMatT=0.
 FoFJK: IHMeth= 1 ICntrl=   2127 DoSepK=T KAlg= 0 I1Cent=   0 FoldK=F
 IRaf=   1 NMat= 1 IRICut=   1 DoRegI=T DoRafI=F ISym2E= 0.
 FoFCou: FMM=F IPFlag=   0 FMFlag=   100000 FMFlg1=   800
      NFxFlg=   0 DoJE=F BraDBF=F KetDBF=F FulRan=T
      wScrn= 0.000000 ICntrl=   2527 IOpCl= 0 I1Cent=   0 NGrid=   0
      NMat0=   1 NMatS0=   1 NMatT0=   0 NMatD0=   1 NMtDS0=   0
 NMtDT0=   0
 Symmetry not used in FoFCou.
 Leave Link 703 at Fri Oct 14 11:40:08 2022, MaxMem= 2147483648 cpu: 843.6
 (Enter /opt/gaussian/g09/l716.exe)

Dipole   =-1.77793373D+00-3.04933610D+00-2.33034480D-01
***** Axes restored to original set *****
 Cartesian Forces: Max   0.075219074 RMS   0.012454398
 Leave Link 716 at Fri Oct 14 11:40:08 2022, MaxMem= 2147483648 cpu: 0.8
 (Enter /opt/gaussian/g09/l122.exe)
 CPIOFr: IOpCl= 0 IRwI=-1 IRwCP= 731 ICalc= 4 LCPTot=   350968 Len1MO=
 908432 IndFrg=   4893128
 Restoring MOs from calculation   1 to rwf.
 CPIOFr: IOpCl= 0 IRwI=-2 IRwCP= 731 ICalc= 0 LCPTot=   350968 Len1MO=
 908432 IndFrg=   1259400
 Counterpoise corrected energy =   -1755.156462399315
          BSSE energy =   0.012354005752
       sum of monomers =   -1754.662432222770
      complexation energy =   -317.76 kcal/mole (raw)
      complexation energy =   -310.01 kcal/mole (corrected)
 Leave Link 122 at Fri Oct 14 11:40:08 2022, MaxMem= 2147483648 cpu: 0.4
 (Enter /opt/gaussian/g09/l716.exe)

Orbital energies and kinetic energies (alpha):

		1	2
1	O	-101.812887	137.071065
2	O	-19.603997	29.117157
3	O	-19.543568	29.122529
4	O	-19.536769	29.122024
5	O	-14.935955	22.048972
6	O	-14.755311	22.046333
7	O	-14.752193	22.049342
8	O	-14.692480	22.049082
9	O	-14.638673	22.049839
10	O	-10.642509	15.949617
11	O	-10.625519	15.952561
12	O	-10.621034	15.952266
13	O	-10.599284	15.951736
14	O	-10.582951	15.952938
15	O	-10.565321	15.953704
16	O	-10.555047	15.958512
17	O	-10.550197	15.953292
18	O	-10.536653	15.954301
19	O	-10.522649	15.954662
20	O	-10.518066	15.953630
21	O	-10.514410	15.953115
22	O	-10.497219	15.953481
23	O	-10.495718	15.954230
24	O	-10.490687	15.953212
25	O	-10.490023	15.953206
26	O	-10.482407	15.954725
27	O	-10.481597	15.953211
28	O	-10.473689	15.952980
29	O	-9.745017	21.703139
30	O	-7.509661	20.522876

31	O	-7.499341	20.549741
32	O	-7.498889	20.545554
33	O	-1.601160	2.486054
34	O	-1.521732	2.499071
35	O	-1.417778	2.740973
36	O	-1.412255	2.029353
37	O	-1.330217	1.848801
38	O	-1.253064	1.924891
39	O	-1.218106	1.968707
40	O	-1.205623	1.808241
41	O	-1.191792	2.004610
42	O	-1.183191	1.791344
43	O	-1.164821	1.843439
44	O	-1.146108	2.068596
45	O	-1.103616	1.747029
46	O	-1.085130	1.820434
47	O	-1.064747	1.904810
48	O	-1.057445	1.838220
49	O	-1.037566	2.003157
50	O	-1.011650	6.242669
51	O	-1.009193	7.415358
52	O	-1.004202	3.815976
53	O	-1.001016	9.973498
54	O	-0.997933	11.007738
55	O	-0.996003	10.937204
56	O	-0.988819	6.921206
57	O	-0.976377	2.342189
58	O	-0.956647	2.028668
59	O	-0.939697	2.562982
60	O	-0.933323	2.030697
61	O	-0.923714	2.604952
62	O	-0.913877	1.690690
63	O	-0.900769	1.756778
64	O	-0.899449	1.761761
65	O	-0.892775	1.805730
66	O	-0.865823	1.820185
67	O	-0.856573	2.550661
68	O	-0.845717	1.490854
69	O	-0.835539	1.776785
70	O	-0.829327	1.621523
71	O	-0.817630	1.501434
72	O	-0.814370	1.537280
73	O	-0.803320	1.411634
74	O	-0.781294	1.915821
75	O	-0.774227	1.519157
76	O	-0.768070	1.482456
77	O	-0.766226	1.484767
78	O	-0.762563	1.532581
79	O	-0.753595	1.544131
80	O	-0.745329	1.383168

81	O	-0.743548	1.452991
82	O	-0.724373	1.498480
83	O	-0.721425	1.317189
84	O	-0.719092	1.682563
85	O	-0.709903	1.424914
86	O	-0.692603	1.457233
87	O	-0.670834	2.394125
88	O	-0.666832	1.378758
89	O	-0.661224	1.677655
90	O	-0.657170	1.657113
91	O	-0.656265	2.000411
92	O	-0.653512	1.556602
93	O	-0.647068	2.110150
94	O	-0.644586	2.027957
95	O	-0.637381	1.530113
96	O	-0.635677	1.620426
97	O	-0.633447	1.770671
98	O	-0.613713	1.750582
99	O	-0.606152	1.503400
100	O	-0.585368	2.376664
101	O	-0.565149	1.602637
102	O	-0.562287	1.682675
103	O	-0.552733	1.398774
104	O	-0.535429	1.366023
105	O	-0.526665	1.563282
106	O	-0.502476	1.399955
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108	V	-0.275452	1.833556
109	V	-0.264911	1.398739
110	V	-0.235941	1.585564
111	V	-0.229164	1.623932
112	V	-0.207872	0.911147
113	V	-0.192640	1.198975
114	V	-0.171484	1.443377
115	V	-0.162473	1.997052
116	V	-0.147806	0.915505
117	V	-0.142912	1.243508
118	V	-0.138228	0.894608
119	V	-0.124305	1.681640
120	V	-0.118622	1.010277
121	V	-0.113016	2.008316
122	V	-0.097557	1.719128
123	V	-0.089449	1.492081
124	V	-0.083342	2.133885
125	V	-0.067229	0.995885
126	V	-0.061707	1.277345
127	V	-0.043457	1.415485
128	V	-0.036777	1.182339
129	V	-0.027141	1.576391
130	V	-0.023333	2.374896

131	V	-0.018767	1.070441
132	V	-0.016111	1.558728
133	V	-0.003382	1.866687
134	V	0.000763	1.762736
135	V	0.013101	1.445618
136	V	0.019913	1.447154
137	V	0.024156	1.786462
138	V	0.028907	1.910225
139	V	0.035921	1.837438
140	V	0.037420	1.781571
141	V	0.046592	1.322365
142	V	0.057675	1.558453
143	V	0.063254	1.807956
144	V	0.072120	2.195624
145	V	0.077187	1.878478
146	V	0.085235	2.118622
147	V	0.095523	2.266139
148	V	0.107323	2.073993
149	V	0.110541	1.805483
150	V	0.127491	1.971612
151	V	0.129566	1.570556
152	V	0.138500	2.081246
153	V	0.146200	2.191748
154	V	0.152663	2.082183
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156	V	0.167187	2.012138
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158	V	0.188844	2.289674
159	V	0.197232	1.931469
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161	V	0.230340	2.167304
162	V	0.240123	2.112706
163	V	0.247428	1.973620
164	V	0.258679	2.183495
165	V	0.271097	2.390130
166	V	0.286819	2.709933
167	V	0.297014	2.401446
168	V	0.307029	2.127136
169	V	0.309596	2.027912
170	V	0.320489	2.220911
171	V	0.326763	2.112643
172	V	0.335123	2.157091
173	V	0.340841	2.468270
174	V	0.342962	2.528509
175	V	0.354584	2.321286
176	V	0.362593	2.356995
177	V	0.364662	2.189204
178	V	0.366043	2.462052
179	V	0.369787	2.322086
180	V	0.373942	2.282151

181	V	0.377386	2.302409
182	V	0.386168	2.153123
183	V	0.386975	2.220476
184	V	0.396270	2.522982
185	V	0.401187	2.300562
186	V	0.403948	2.235486
187	V	0.409453	2.311223
188	V	0.415862	2.227584
189	V	0.420098	2.431140
190	V	0.426063	2.378512
191	V	0.427983	2.181004
192	V	0.440052	2.236812
193	V	0.446055	2.165416
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195	V	0.454737	2.372383
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197	V	0.465380	2.238506
198	V	0.469633	2.522040
199	V	0.471115	2.139279
200	V	0.476792	2.258197
201	V	0.477551	2.183484
202	V	0.483262	2.289767
203	V	0.486971	2.541706
204	V	0.490282	2.369893
205	V	0.500112	2.578437
206	V	0.515421	2.624116
207	V	0.525661	2.443743
208	V	0.537146	2.633907
209	V	0.541579	2.854129
210	V	0.551474	2.298153
211	V	0.558488	2.560411
212	V	0.566055	2.743107
213	V	0.574958	2.628722
214	V	0.584309	2.623414
215	V	0.592085	2.648077
216	V	0.594870	2.776982
217	V	0.601567	2.365785
218	V	0.607397	2.634939
219	V	0.617988	2.721783
220	V	0.624269	2.608837
221	V	0.633021	2.533405
222	V	0.635252	2.766866
223	V	0.642041	2.775805
224	V	0.649340	2.667602
225	V	0.656072	2.796248
226	V	0.666142	2.579732
227	V	0.670111	2.518709
228	V	0.674371	2.825391
229	V	0.680955	2.593678
230	V	0.682936	2.687303

231	V	0.692662	2.572265
232	V	0.695002	2.618679
233	V	0.696997	2.710350
234	V	0.701879	2.621394
235	V	0.712213	2.863076
236	V	0.722182	2.602894
237	V	0.728911	2.643773
238	V	0.737080	2.695294
239	V	0.740415	2.604529
240	V	0.743631	2.579073
241	V	0.747824	2.550371
242	V	0.763072	2.792173
243	V	0.766922	2.862307
244	V	0.777774	2.866948
245	V	0.785097	2.916476
246	V	0.791048	2.964171
247	V	0.801348	2.917633
248	V	0.810073	2.601171
249	V	0.818970	2.852415
250	V	0.820592	2.831923
251	V	0.823122	2.759986
252	V	0.835388	2.670080
253	V	0.841447	2.728043
254	V	0.850840	3.044331
255	V	0.855997	2.752553
256	V	0.868173	2.621490
257	V	0.870860	2.948809
258	V	0.884210	2.654142
259	V	0.892816	2.691230
260	V	0.893948	2.468116
261	V	0.896499	2.614507
262	V	0.927434	2.511799
263	V	0.936301	2.666997
264	V	0.957364	2.986827
265	V	0.974784	3.086632
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268	V	1.004862	2.701153
269	V	1.010831	2.965050
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271	V	1.028064	2.720398
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273	V	1.051916	2.824500
274	V	1.056870	2.731179
275	V	1.059435	2.585111
276	V	1.069037	2.696701
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278	V	1.081915	2.795936
279	V	1.086538	2.642279
280	V	1.096770	2.713193

281	V	1.104641	2.694004
282	V	1.113190	2.592263
283	V	1.119759	2.809119
284	V	1.130034	2.654312
285	V	1.135694	2.696567
286	V	1.139553	2.856499
287	V	1.153701	2.969673
288	V	1.170631	2.788974
289	V	1.175325	2.681663
290	V	1.194041	2.602917
291	V	1.196315	2.974362
292	V	1.208161	2.606634
293	V	1.213633	2.825059
294	V	1.219695	2.989602
295	V	1.235315	2.840522
296	V	1.237848	3.043160
297	V	1.251394	2.923356
298	V	1.256903	2.589650
299	V	1.260879	2.888806
300	V	1.266100	2.651628
301	V	1.273238	2.970631
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303	V	1.297227	2.875206
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310	V	1.376511	3.064928
311	V	1.405578	3.371501
312	V	1.420553	3.888563
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320	V	1.550351	3.731315
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322	V	1.579410	3.471642
323	V	1.587498	2.976738
324	V	1.596233	3.323061
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326	V	1.609079	3.373168
327	V	1.611367	3.335575
328	V	1.614223	3.099269
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330	V	1.630612	3.280466

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333	V	1.661916	3.417813
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335	V	1.676666	3.543686
336	V	1.680139	3.400025
337	V	1.698534	3.257532
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340	V	1.716392	3.655510
341	V	1.730219	3.719034
342	V	1.739109	3.282272
343	V	1.746424	3.346149
344	V	1.748387	3.315963
345	V	1.755459	3.475969
346	V	1.760594	3.475195
347	V	1.762090	3.365130
348	V	1.770139	3.657910
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350	V	1.792437	3.559990
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354	V	1.837913	3.556027
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356	V	1.854906	3.474556
357	V	1.857654	3.085171
358	V	1.859661	3.447262
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374	V	2.013228	3.597672
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376	V	2.052196	3.508335
377	V	2.066816	3.857416
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379	V	2.088811	3.609106
380	V	2.093921	3.800005

381	V	2.105623	3.751586
382	V	2.107260	3.607695
383	V	2.125220	3.679906
384	V	2.133841	3.821150
385	V	2.135517	3.654177
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387	V	2.156469	3.791708
388	V	2.174923	3.497922
389	V	2.196854	3.722133
390	V	2.202355	3.726902
391	V	2.208249	3.971880
392	V	2.221718	3.646993
393	V	2.227642	3.676777
394	V	2.232172	3.675668
395	V	2.244922	3.808765
396	V	2.248114	3.787827
397	V	2.250506	3.730908
398	V	2.256465	3.353940
399	V	2.261063	3.663288
400	V	2.265396	3.590788
401	V	2.276389	3.824978
402	V	2.296233	3.687159
403	V	2.314430	3.896397
404	V	2.322205	3.950402
405	V	2.327213	3.889321
406	V	2.329048	3.932861
407	V	2.342947	3.776048
408	V	2.362152	3.792329
409	V	2.363710	3.733377
410	V	2.370911	3.889893
411	V	2.387317	3.807620
412	V	2.393870	3.901963
413	V	2.406282	4.022329
414	V	2.415423	3.908777
415	V	2.422794	3.862092
416	V	2.434533	3.852118
417	V	2.447906	3.736328
418	V	2.452793	3.928173
419	V	2.462311	4.053878
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421	V	2.477164	4.201222
422	V	2.481418	4.175023
423	V	2.490121	4.077907
424	V	2.495960	4.416357
425	V	2.522034	4.259099
426	V	2.526842	4.033475
427	V	2.539407	3.960703
428	V	2.550464	4.045365
429	V	2.556396	4.193283
430	V	2.562788	3.978011

431	V	2.572108	4.354376
432	V	2.574558	3.974750
433	V	2.604739	4.288470
434	V	2.616771	4.336548
435	V	2.626917	4.385877
436	V	2.635669	4.063276
437	V	2.650875	4.430044
438	V	2.660223	4.512721
439	V	2.675758	4.579819
440	V	2.702029	4.508134
441	V	2.721522	4.782115
442	V	2.733651	4.625414
443	V	2.748969	4.623290
444	V	2.752925	4.708079
445	V	2.772360	4.748776
446	V	2.779455	4.701897
447	V	2.790958	4.487892
448	V	2.828861	4.603701
449	V	2.844699	4.828782
450	V	2.879482	4.714436
451	V	2.919410	4.756085
452	V	2.939802	4.962720
453	V	2.967130	4.802565
454	V	2.983374	4.901792
455	V	3.029727	4.929285
456	V	3.046874	4.960943
457	V	3.093532	4.942244
458	V	3.099732	4.787914
459	V	3.109972	4.870866
460	V	3.122446	4.855344
461	V	3.132204	5.205680
462	V	3.178212	5.025656
463	V	3.185373	5.199238
464	V	3.212946	5.078789
465	V	3.261921	5.084330
466	V	3.264681	5.100249
467	V	3.342534	5.261268
468	V	3.356687	5.299122
469	V	3.399810	5.410935
470	V	3.484224	5.563998
471	V	3.577600	5.551741
472	V	3.682330	5.563280
473	V	3.754262	5.651007
474	V	7.174543	2.544914

Total kinetic energy from orbitals= 1.796225271171D+03

3a

ar.28298.1.1.1r
PROTON8 DMSO {C:\Espectros\HCerecetto} automation 5
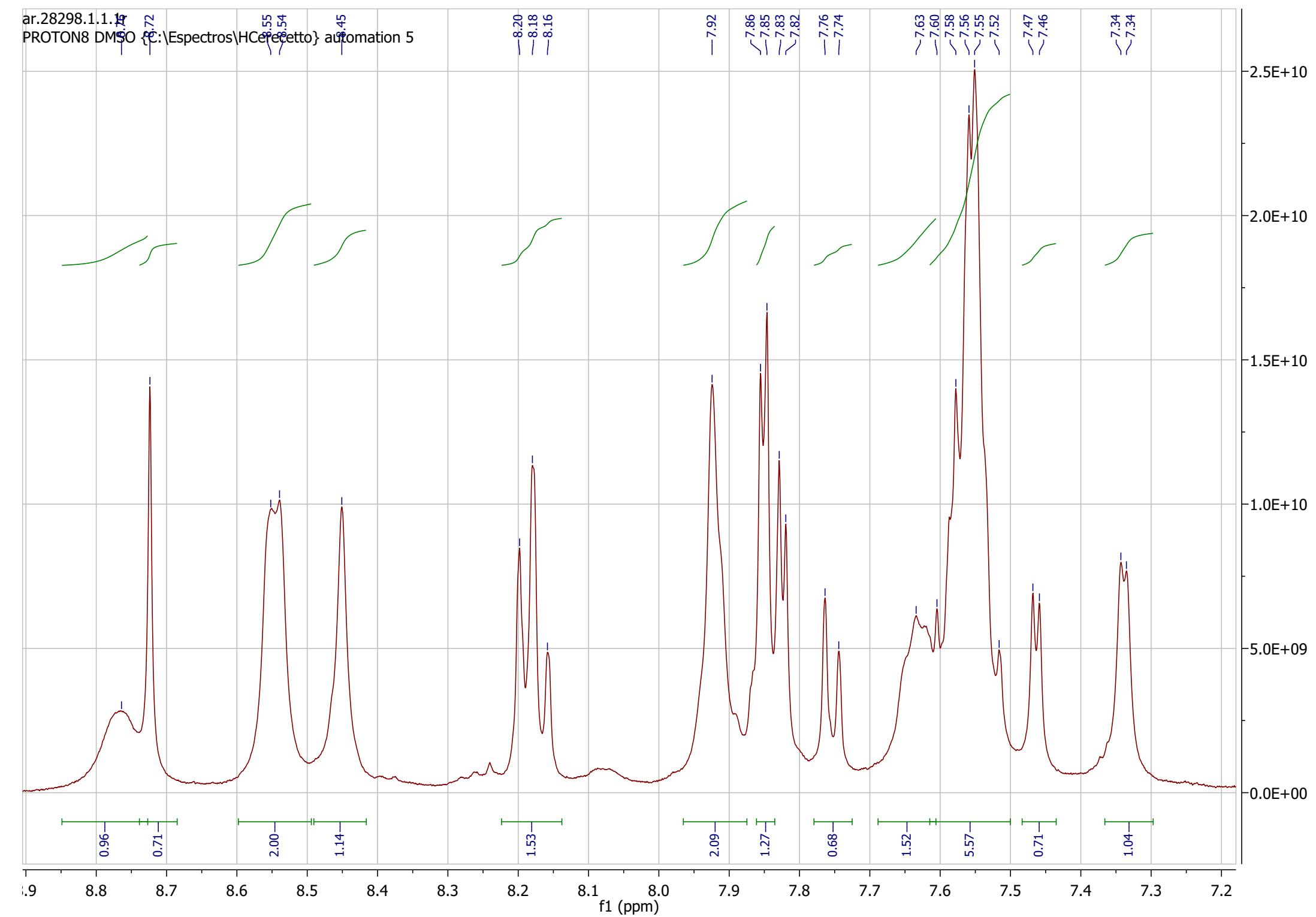
3a
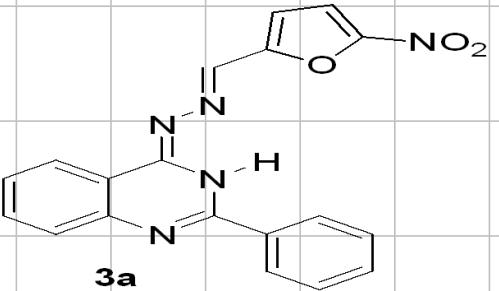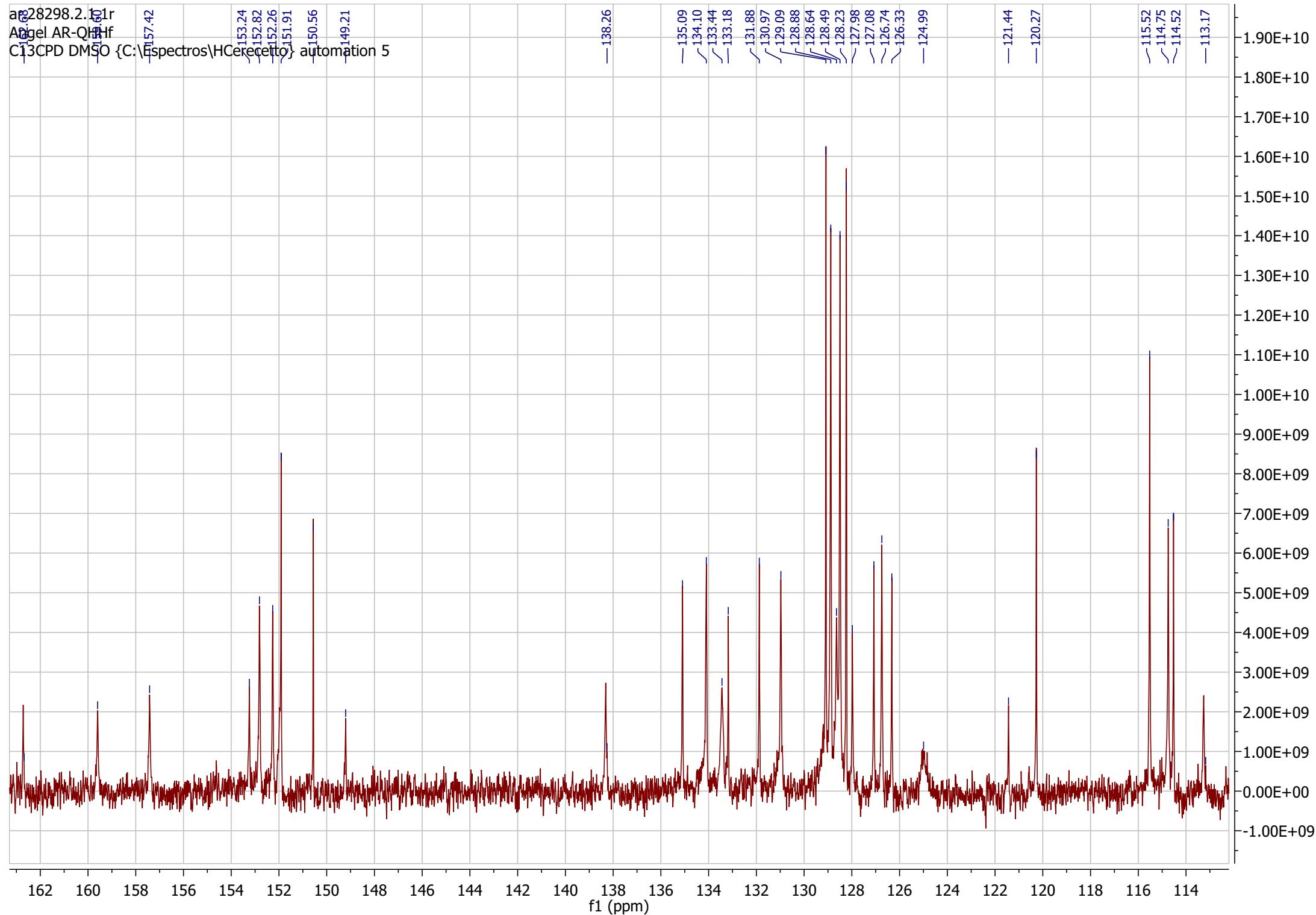
ar.28176.1.1.1r
Angel AR-Q4F 27oC
PROTON8 DMSO {C:\Espectros\HCerecetto} automation 3
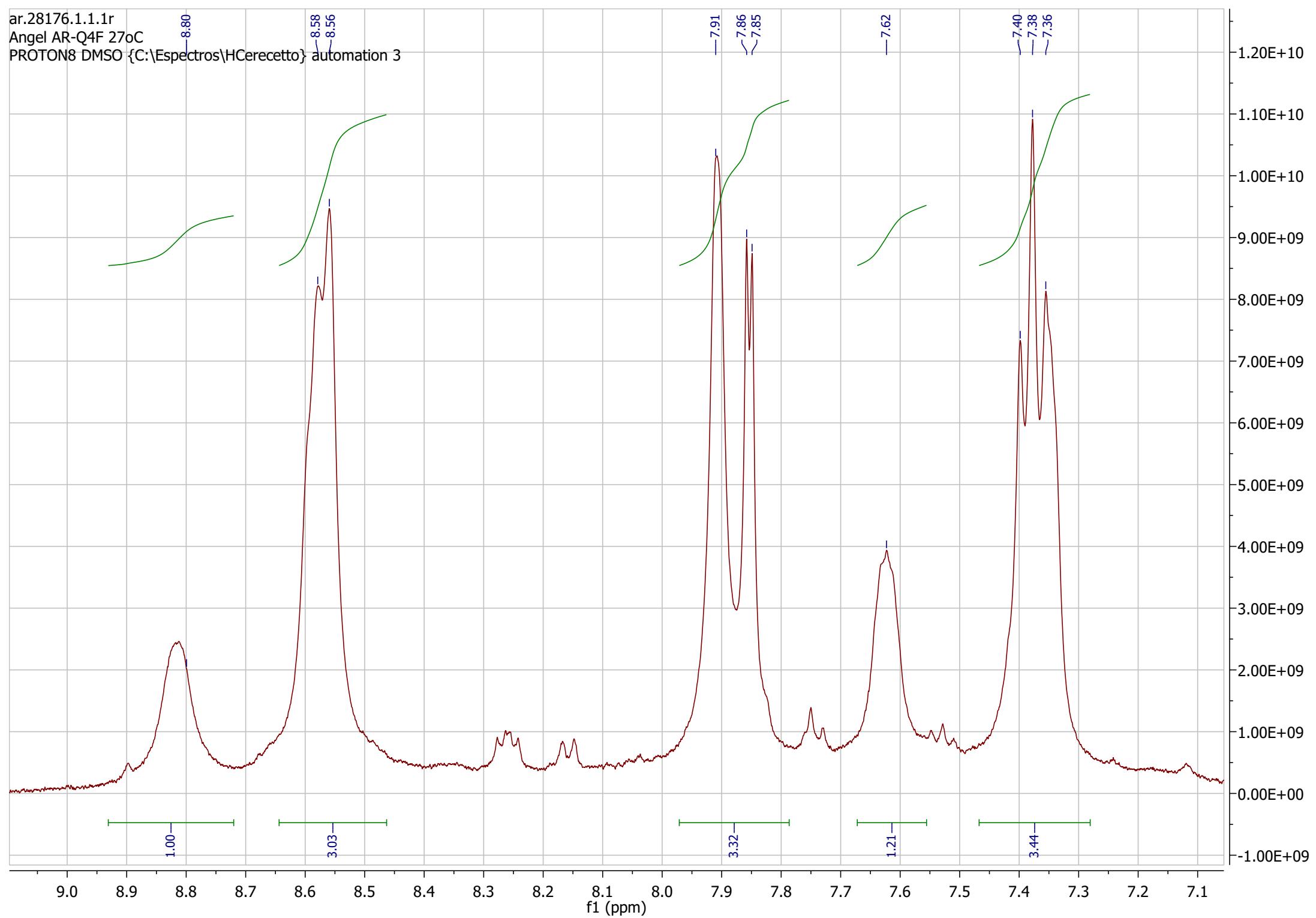
ar28176.31.1r
Angel AR-Q4F 27oC
C13CPD DMSO {C:\Espectros\HCerecetto} automation 13
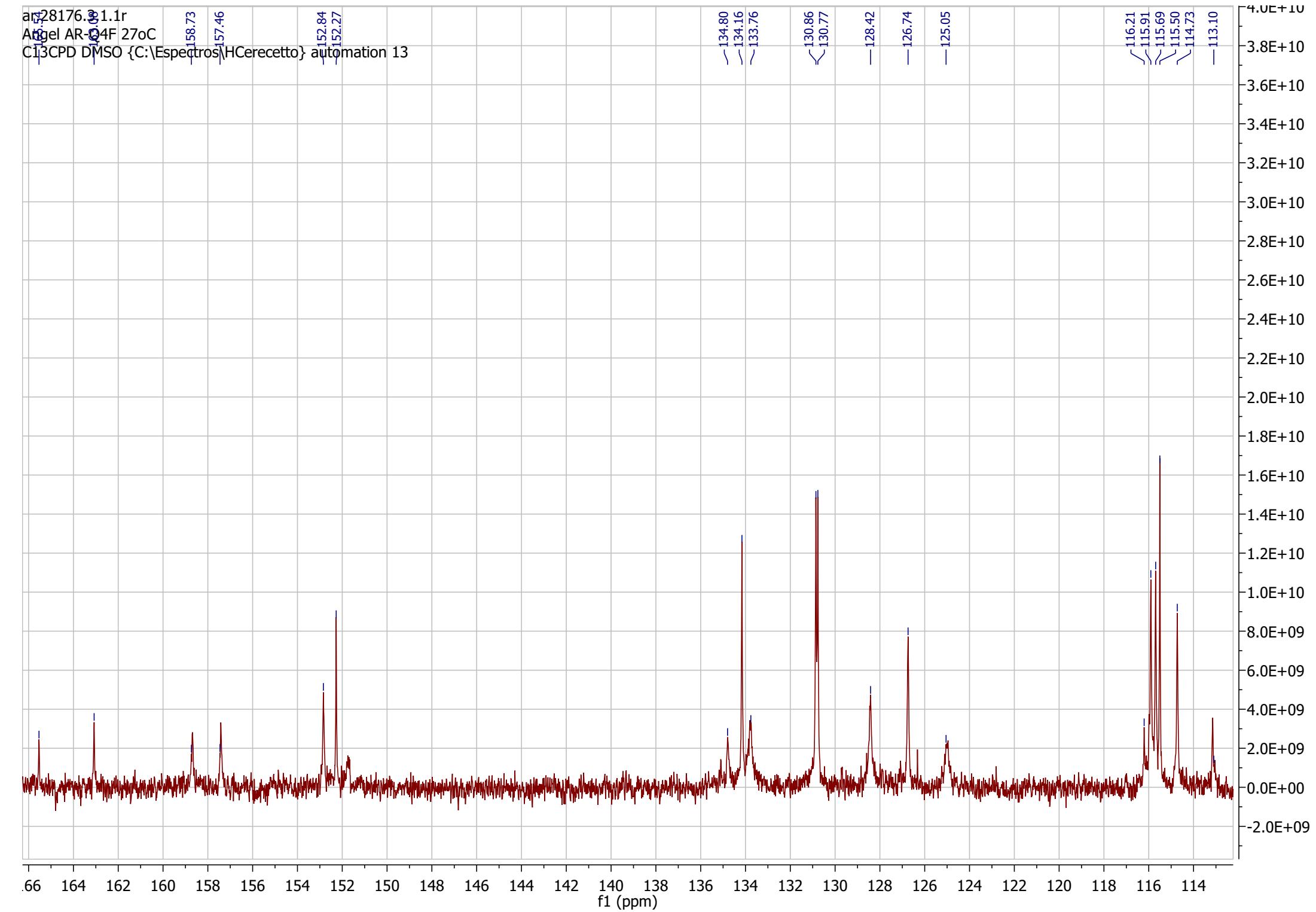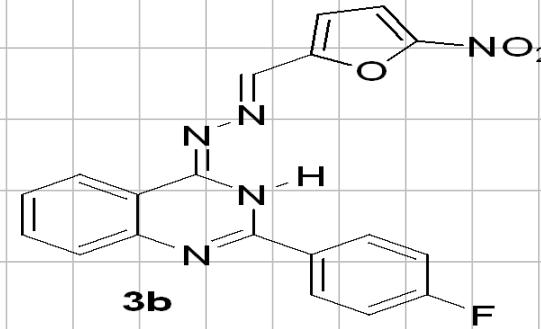
3b

ar.28176.6.1.2rr
Angel AR-Q4F 25oC (1/07)
COSY DMSO {C:\Espectros\HCerecetto} automation 1

{8.58,7.37}

{7.38,8.57}

3b

ar.28176.7.1.2rr
Angel AR-Q4F 25oC (1/07)
HSQC DMSO {C:\Espectros\HCerecetto} automation 1

{7.86,115.60}
{7.39,115.57}
{7.64,126.86}
{7.92,128.45}
{8.57,130.91}
{8.55,133.71}
{7.91,133.94}

3c
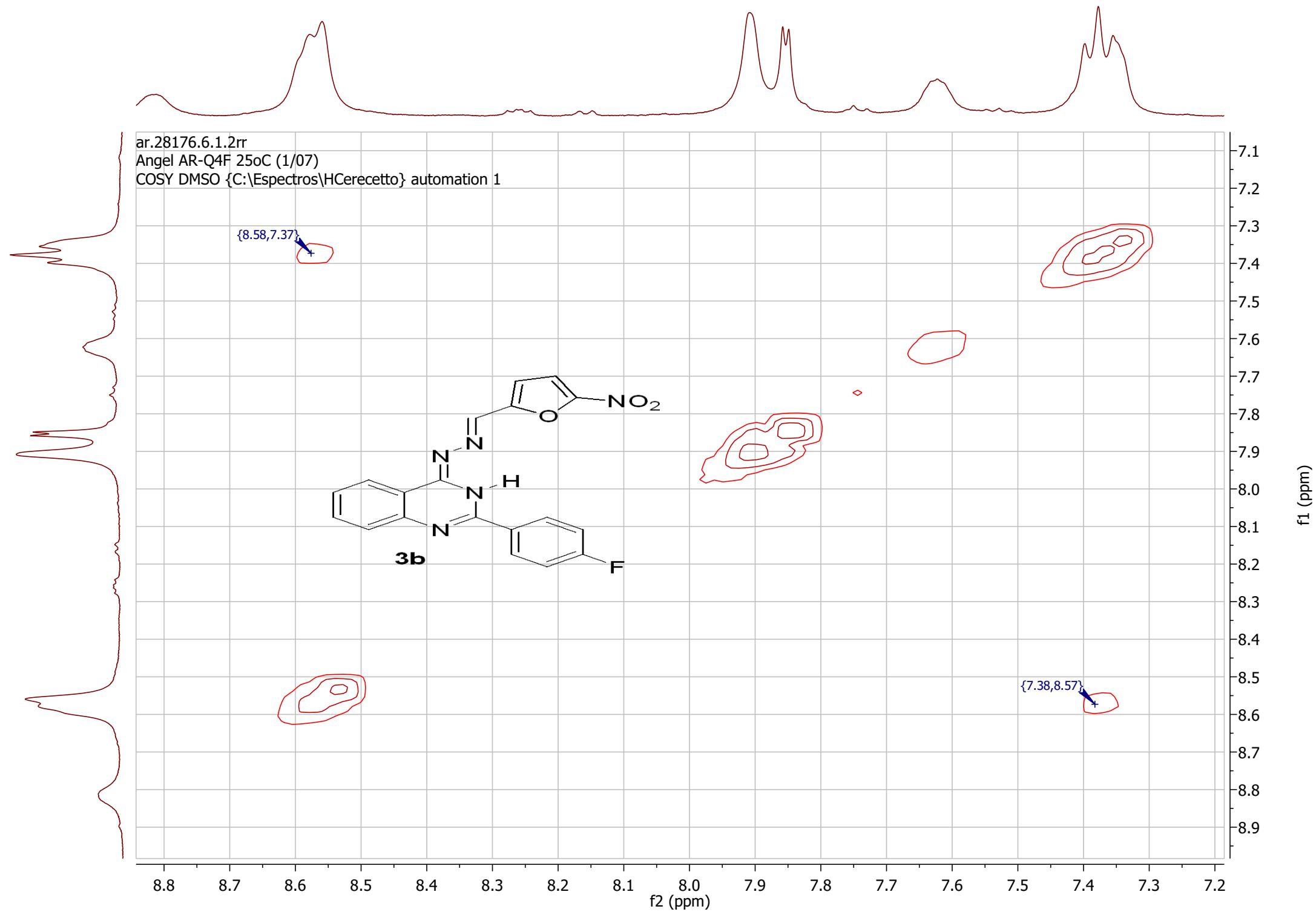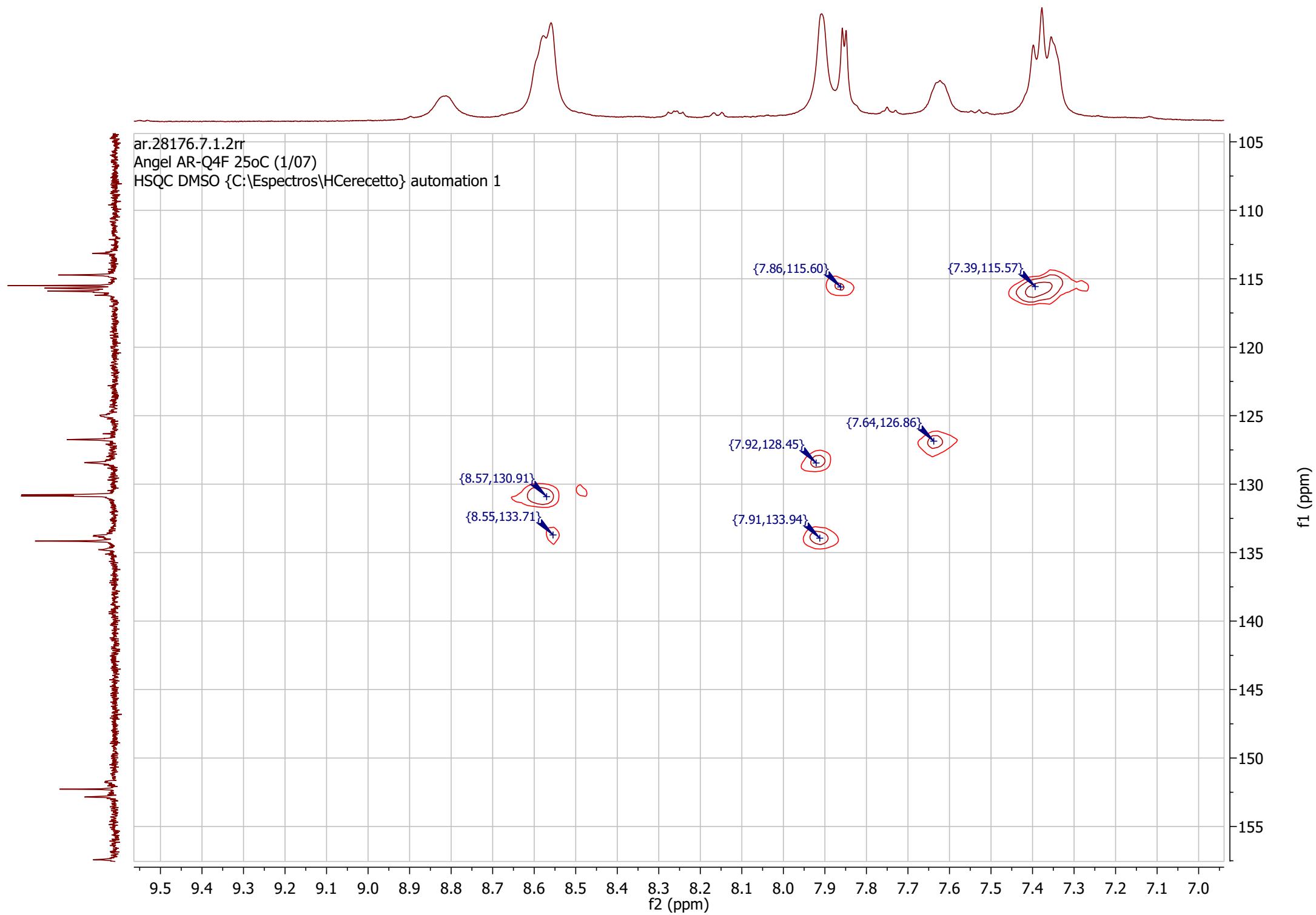
ar.28177.1.1.1r
Angel AR-Q4ClF 27oC
PROTON8 DMSO {C:\Espectros\HCerecetto} automation 4
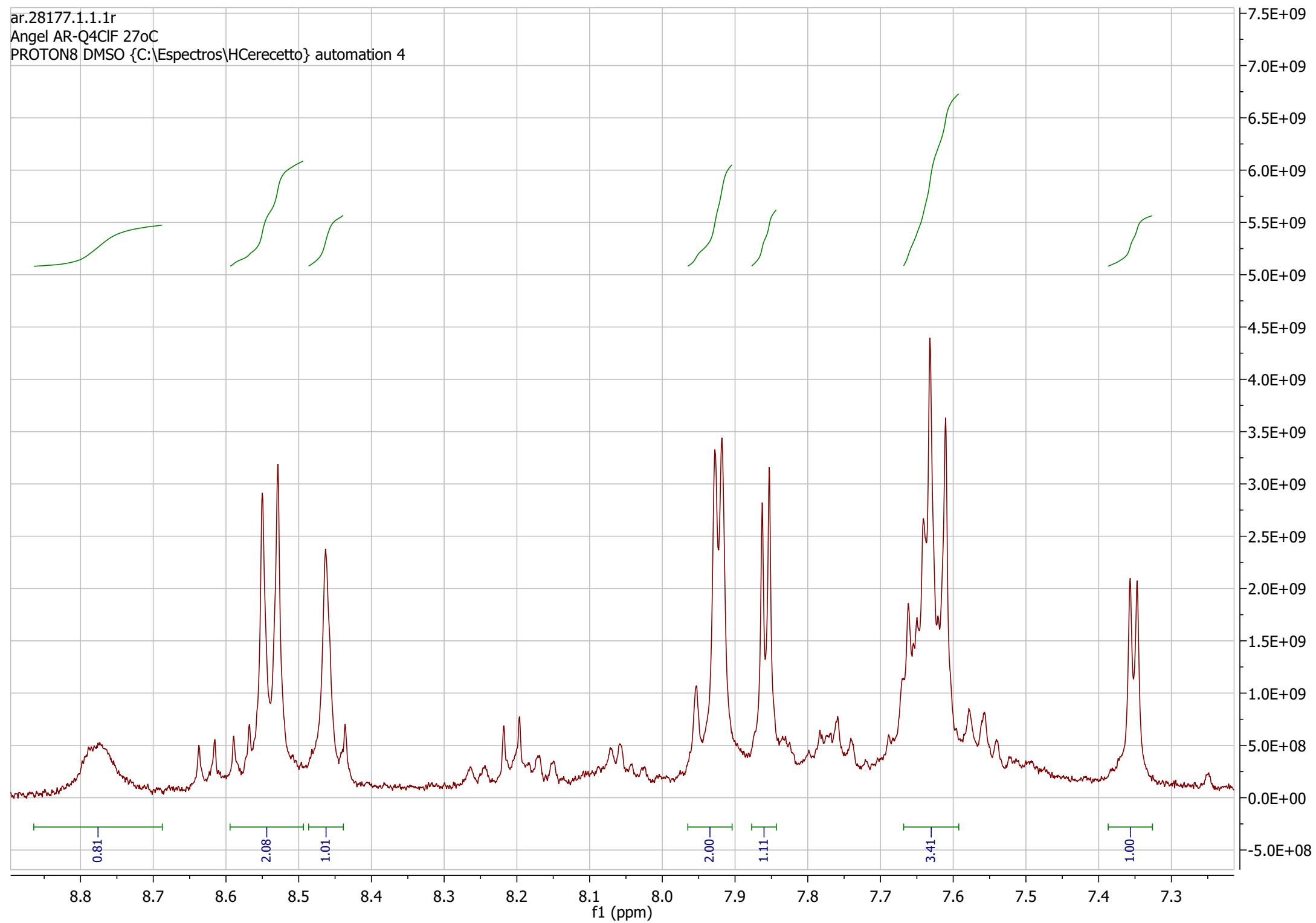
156.74
155.57
152.65
150.83
150.41
135.29
133.94
132.38
131.84
128.31
127.13
126.75
125.10
113.63
113.00
111.47
29.28
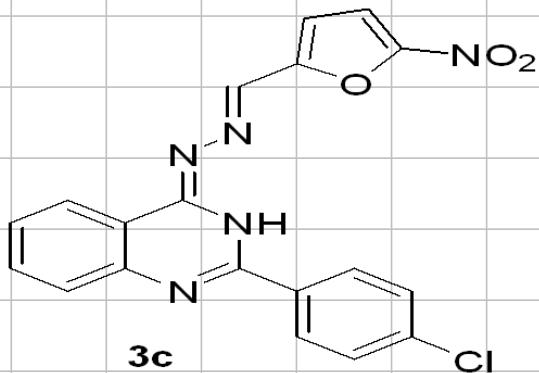
3c

f1 (ppm)
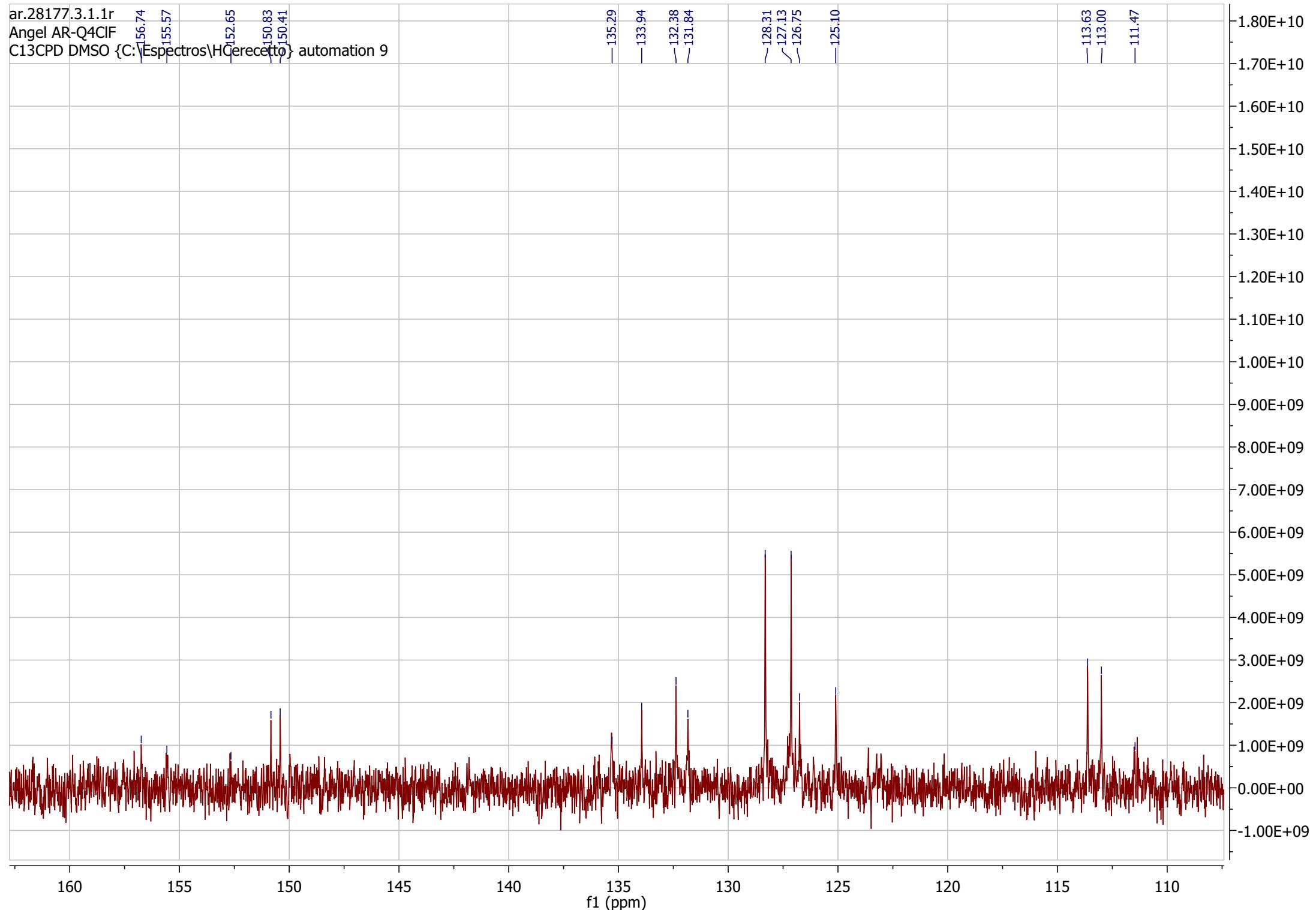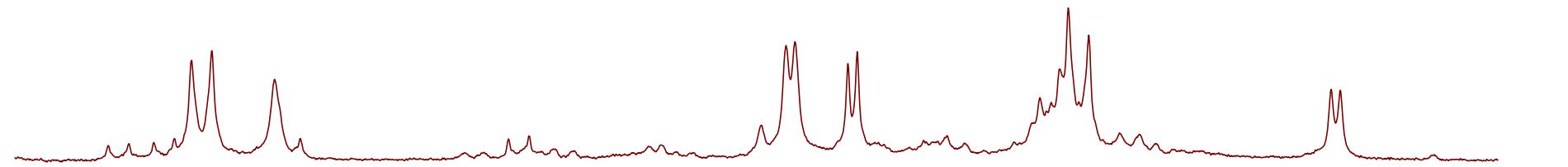
ar.28177.5.1.2rr
AR Q4Cl final
COSY DMSO {C:\Espectros\HCerecetto} automation 5

{7.86,7.35}
{8.55,7.63}
{8.45,7.60}
{7.92,7.63}
{7.91,7.67}
{7.35,7.86}
{7.63,7.93}
{7.67,7.91}
{7.58,8.45}
{7.63,8.59}

3c

f1 (ppm)
f2 (ppm)

ar.28296.1.1.1r
Angel AR-Q4Brf
PROTON8 DMSO {C:\Espectros\HCerecetto} automation 3

ar.28296.1.1.1r
Angel ARQ4Brf
PROTON8 DMSO {C:\Espectros\HCerecetto} automation 3

162.58
159.86
152.75
152.30
140.17
134.31
132.24
132.11
131.97
130.48
130.29
128.43
127.05
124.88
115.51
114.94

3d
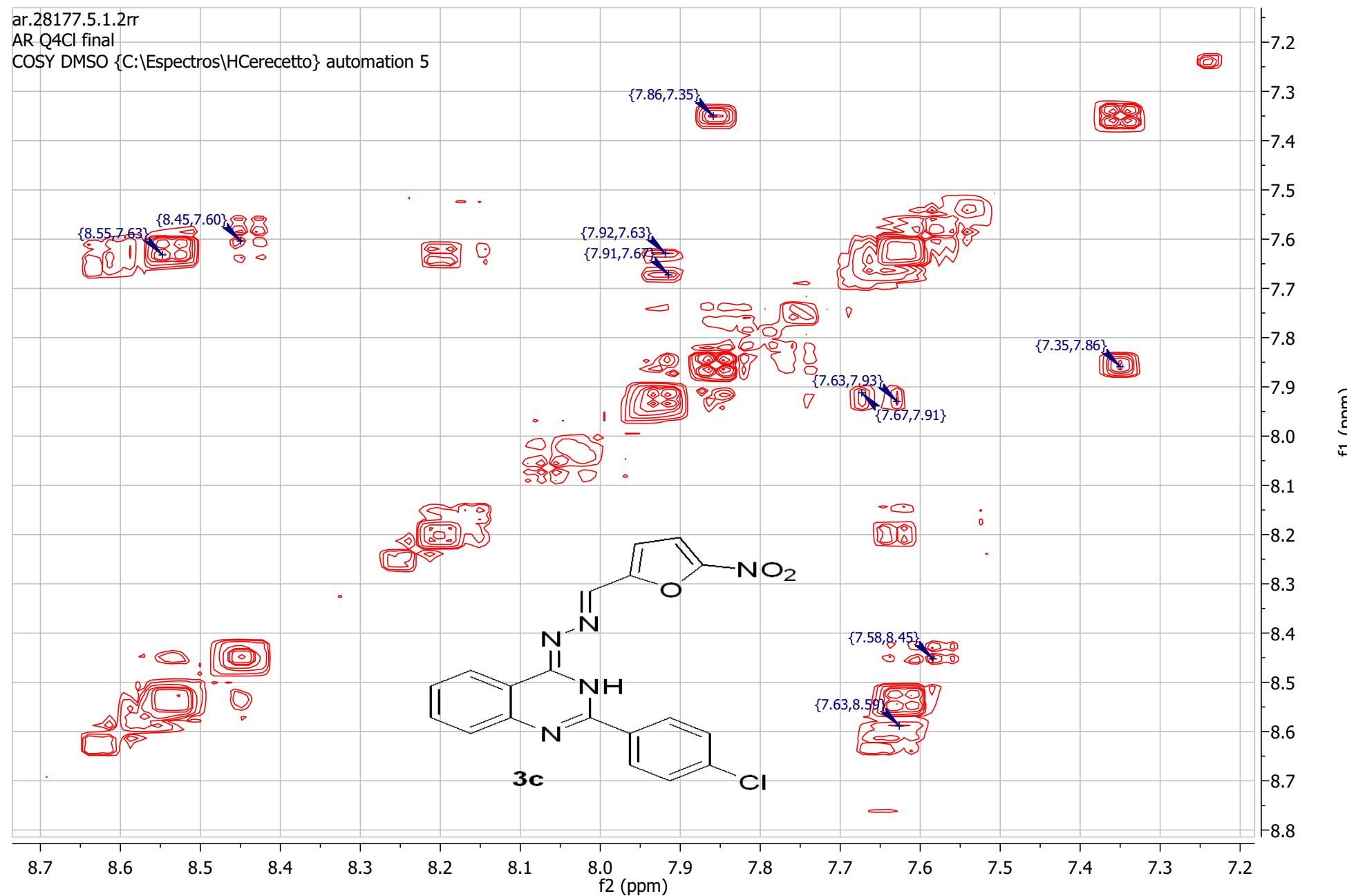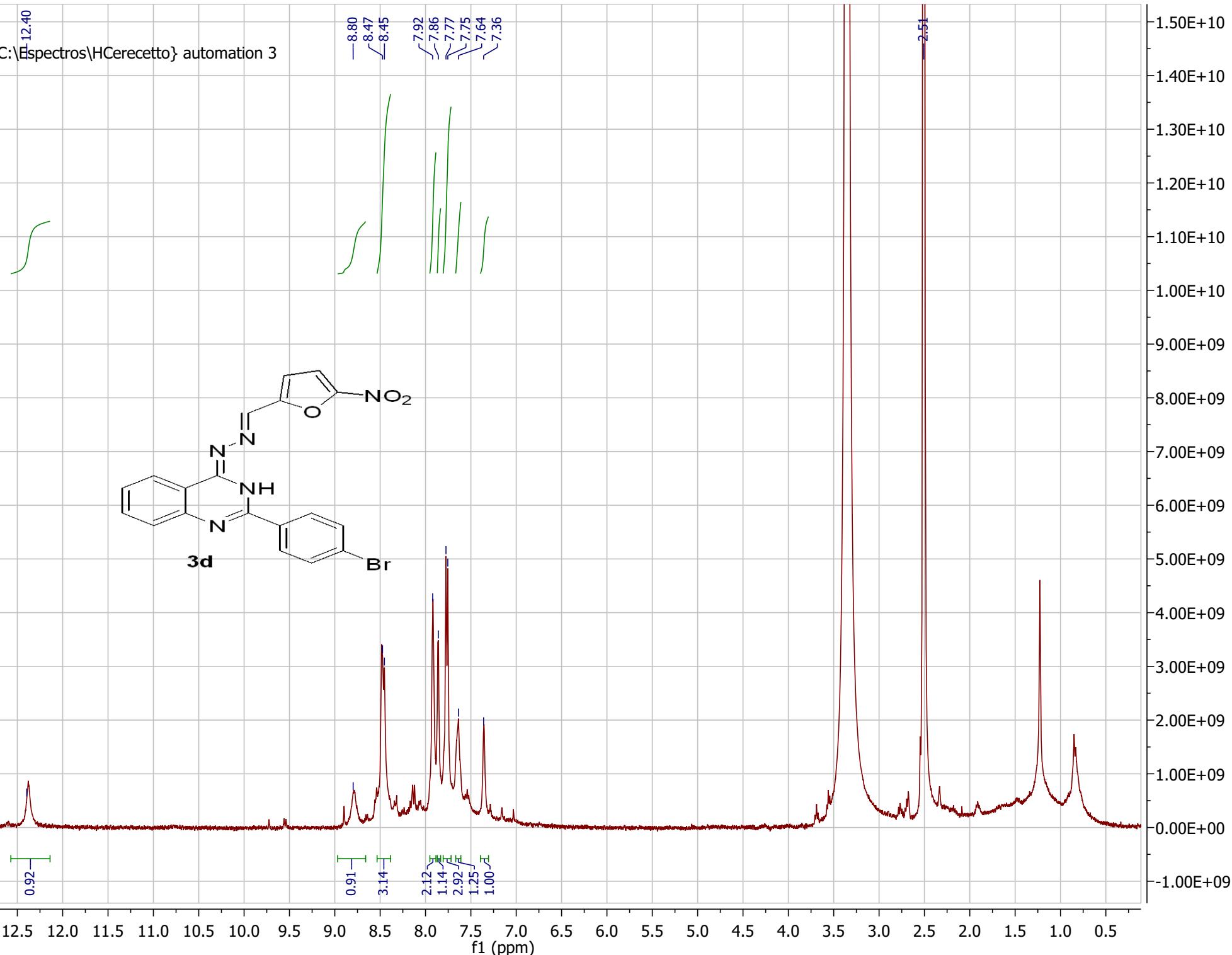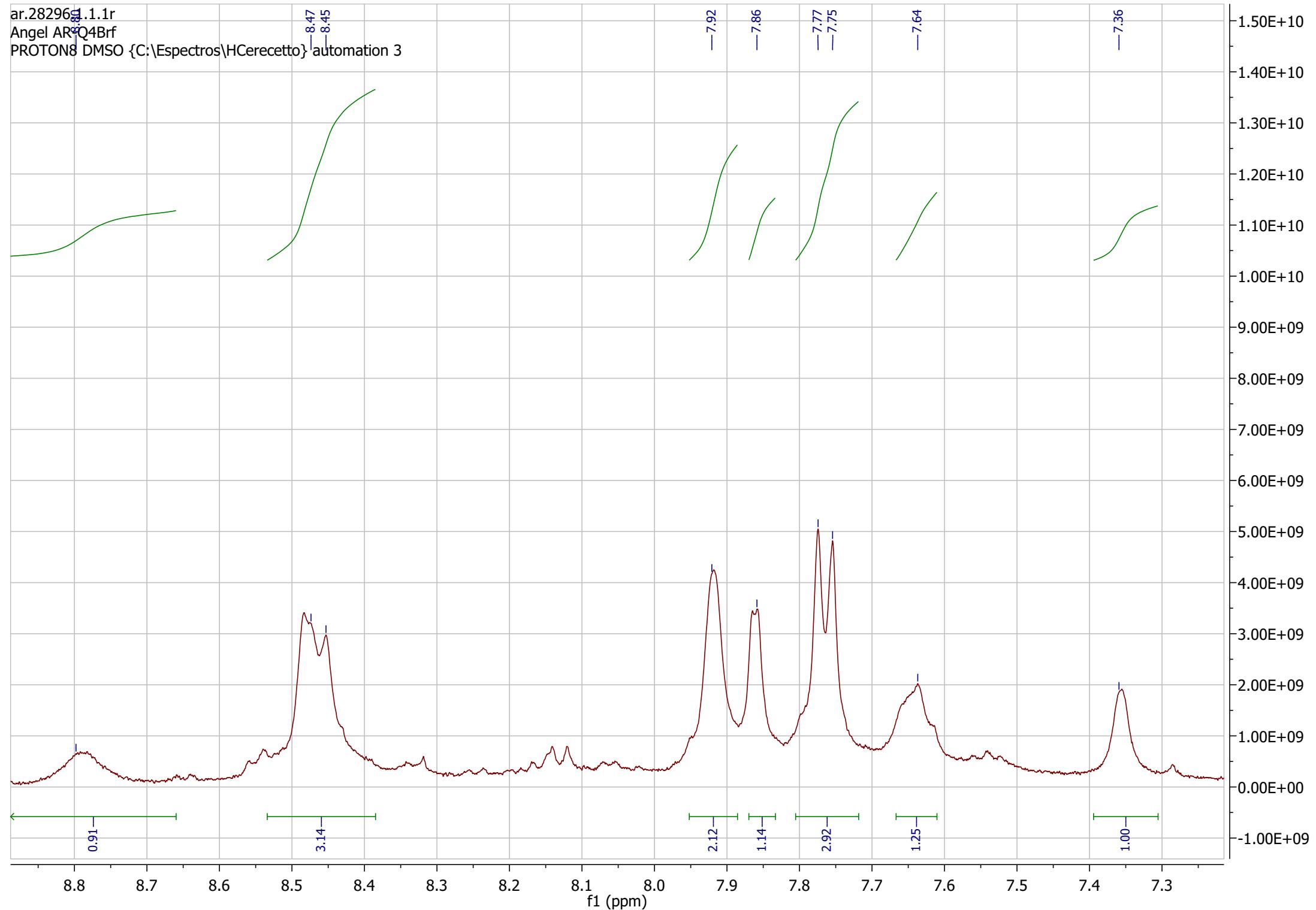
ar.28296.8.1.1r
AR-4BrQf
C13CPD DMSO {C:\Espectros\HCerecetto} automation 15
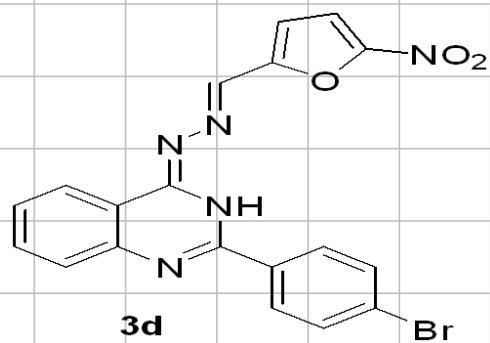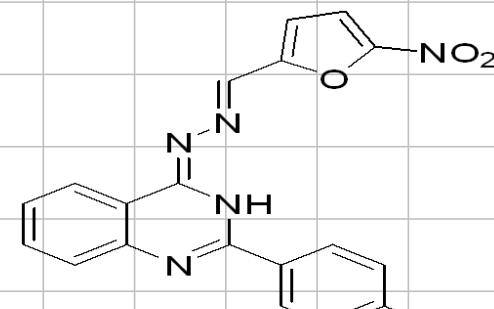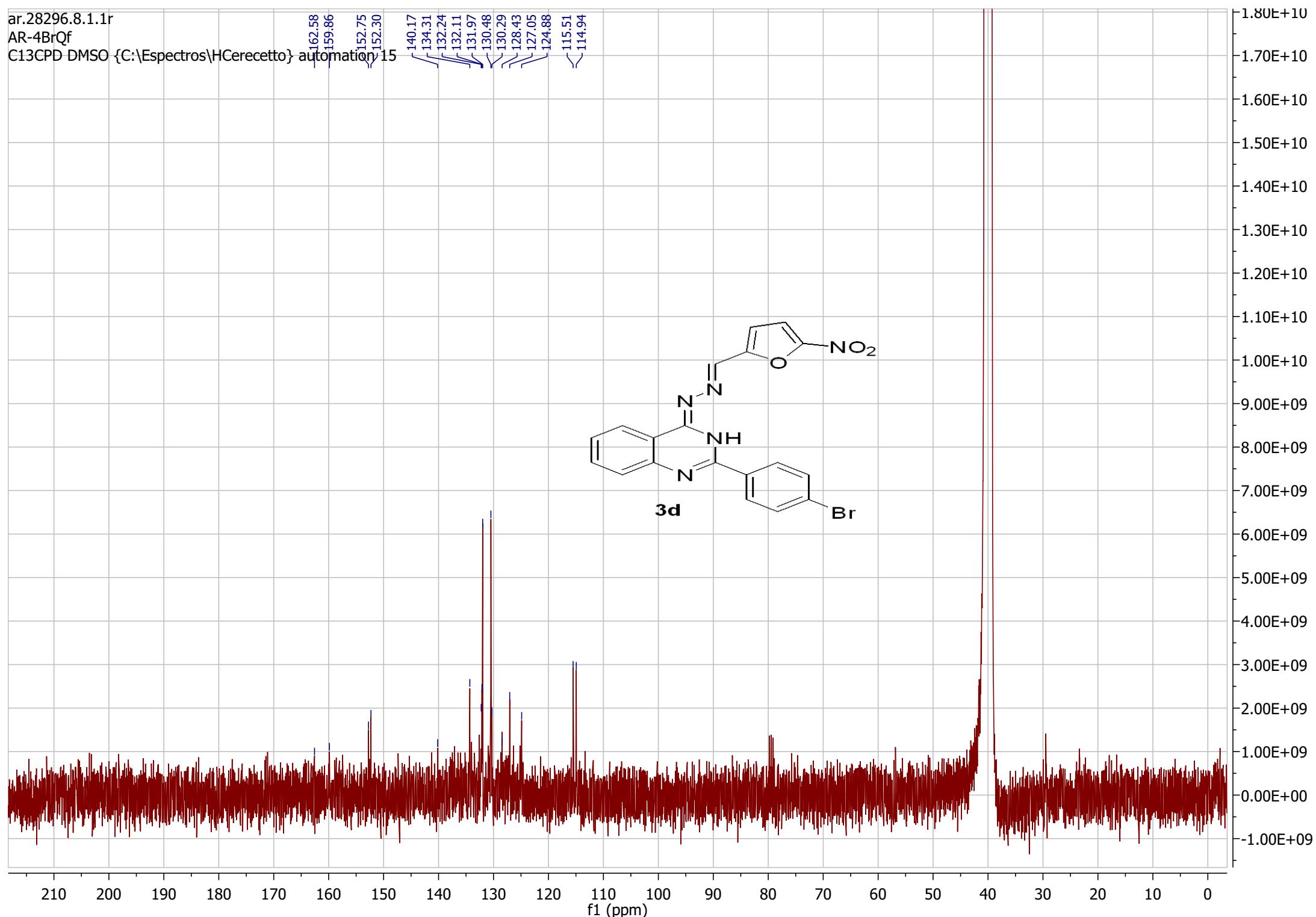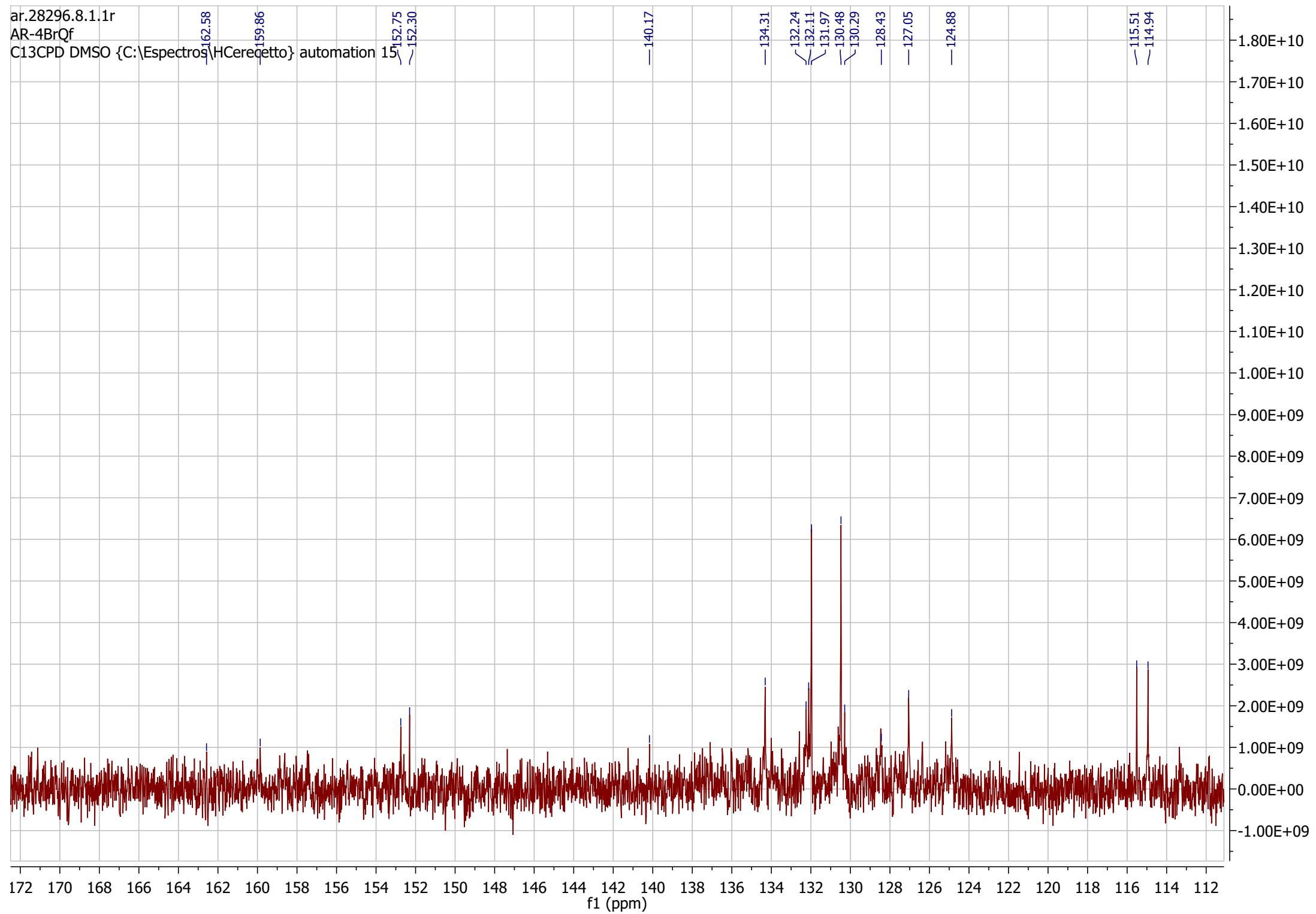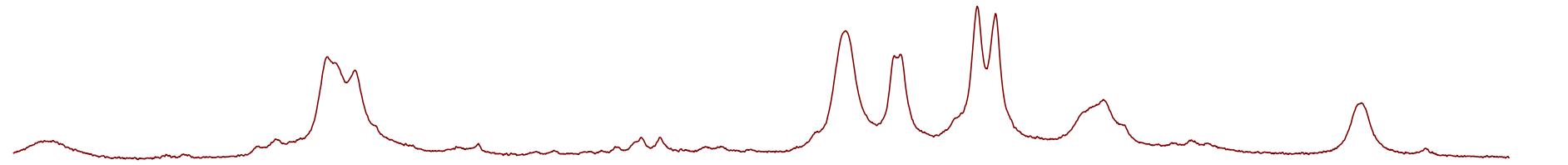
ar.28296.5.1.2rr
AR-4BrQf
COSY DMSO {C:\Espectros\HCerecetto} automation 15

{7.86,7.35}
{8.45,7.76}
{7.91,7.86}
{8.45,7.95}
{7.83,7.94}
{7.35,7.86}
{7.92,8.45}
{7.77,8.45}

3d

3e
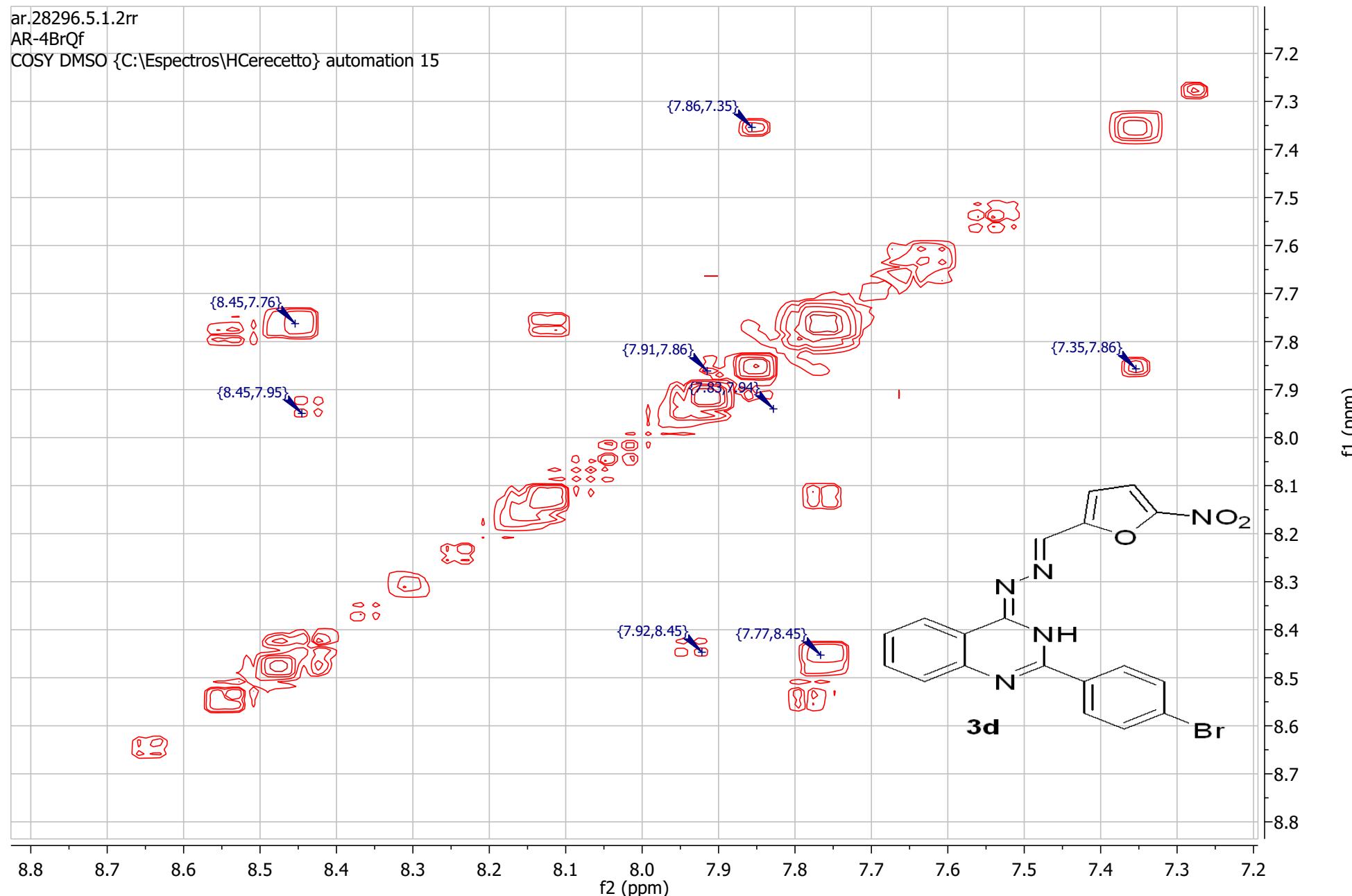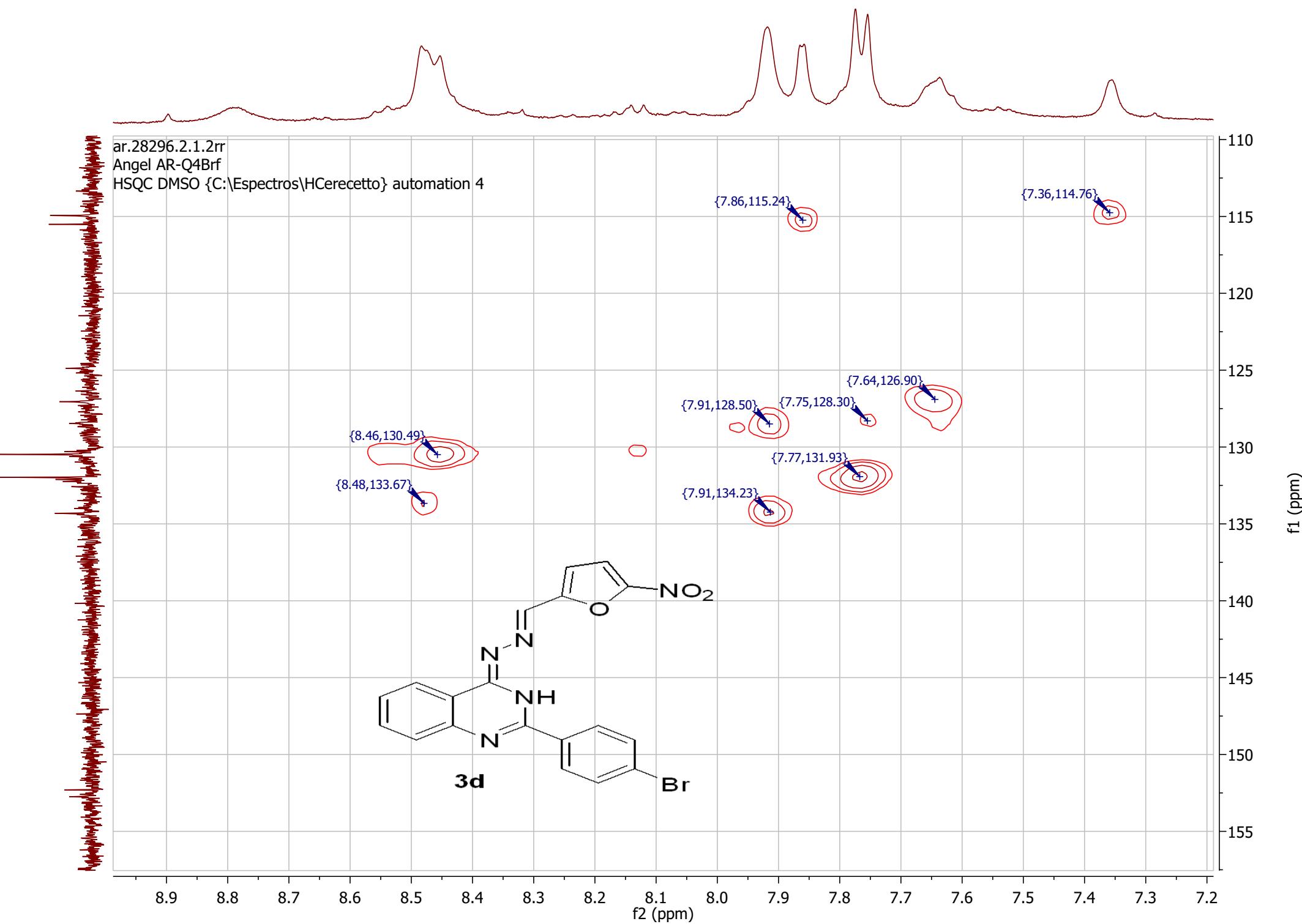
Peak labels: 8.79, 8.49, 8.41, 8.15, 8.13, 8.11, 8.09, 7.86, 7.75, 7.74, 7.55, 7.35, 7.33, 7.26, 12.14

Integrations: 0.84, 0.77, 0.96, 2.17, 0.34, 2.04, 1.01, 0.99, 2.23, 1.00
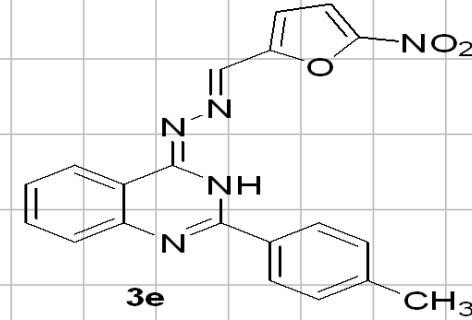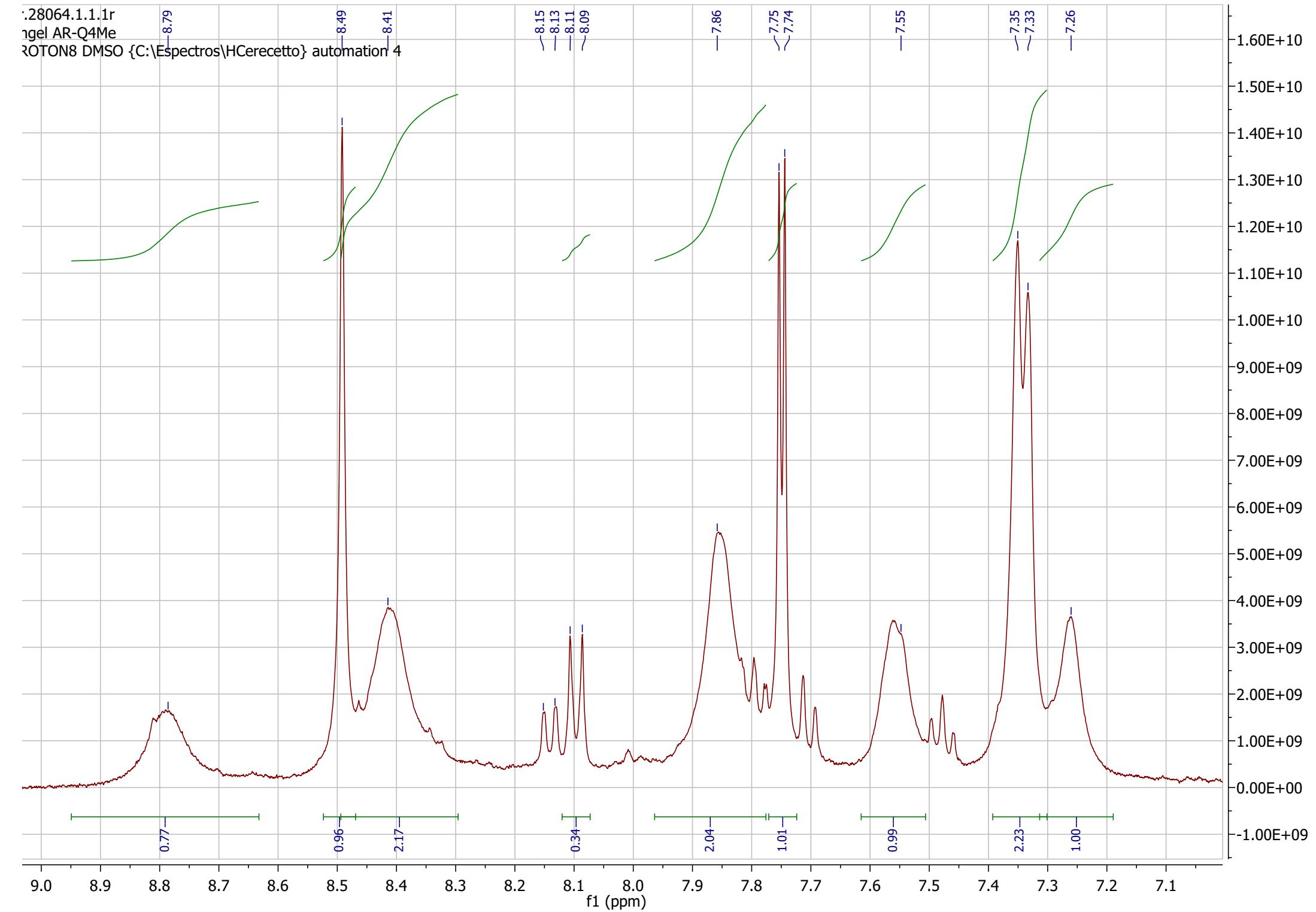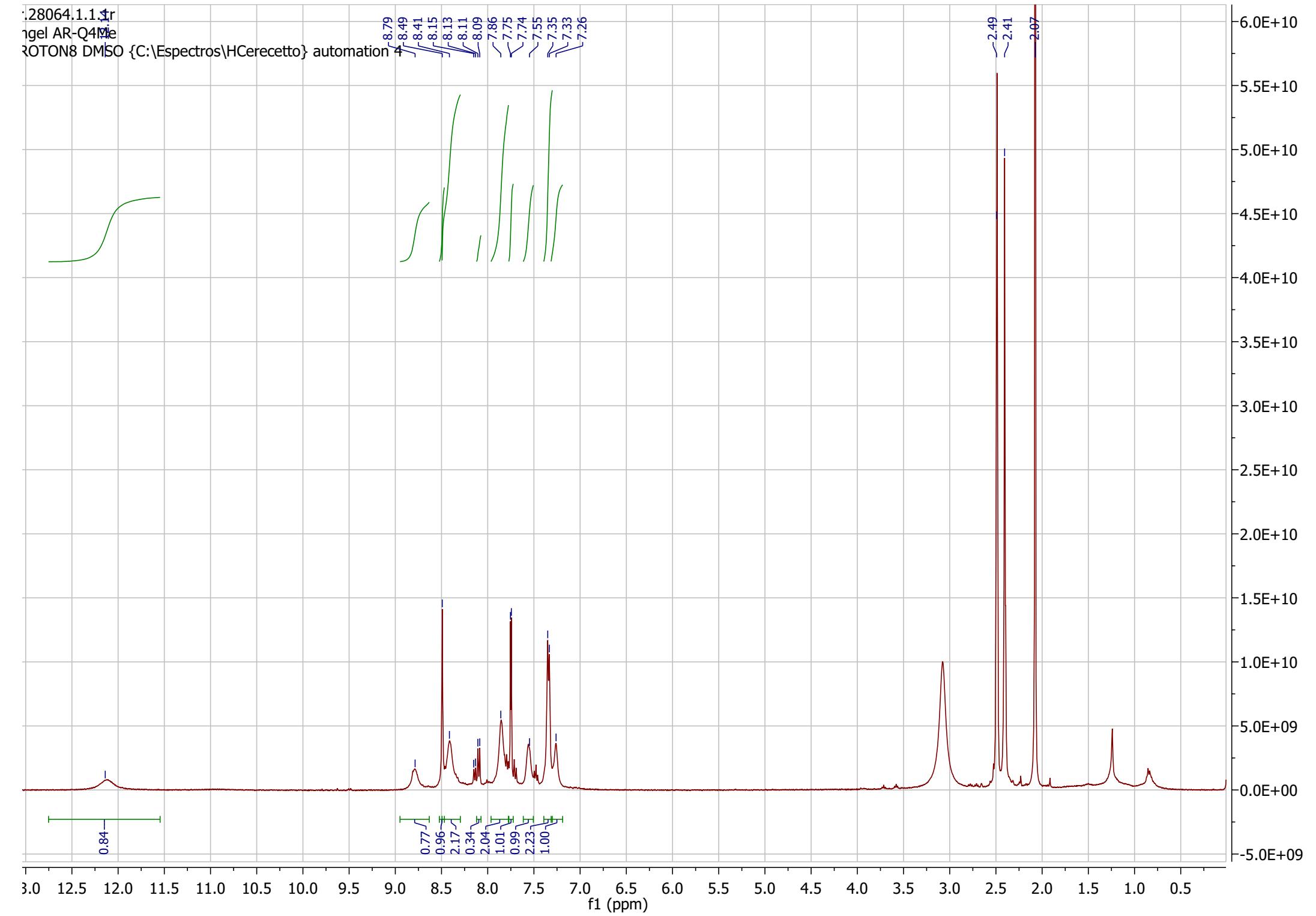
Peaks (ppm): 159.61, 157.38, 152.85, 152.27, 141.95, 140.75, 135.06, 134.06, 130.35, 129.68, 129.53, 128.51, 128.15, 126.89, 126.55, 126.32, 115.53, 114.76, 31.16, 21.52

3e

ar.28064.2.1.2rr
Angel AR-Q4Me
HSQC DMSO {C:\Espectros\HCerecetto} automation 5

{7.83,115.32}
{7.32,114.63}
{8.77,125.08}
{8.42,128.37}
{7.88,128.40}
{7.49,126.77}
{7.59,126.44}
{7.35,129.55}
{8.47,133.46}
{7.88,133.99}

3e

3f

168.04
157.52
152.66
142.30
151.57
134.28
133.85
130.88
128.13
126.95
125.43
115.02
113.32
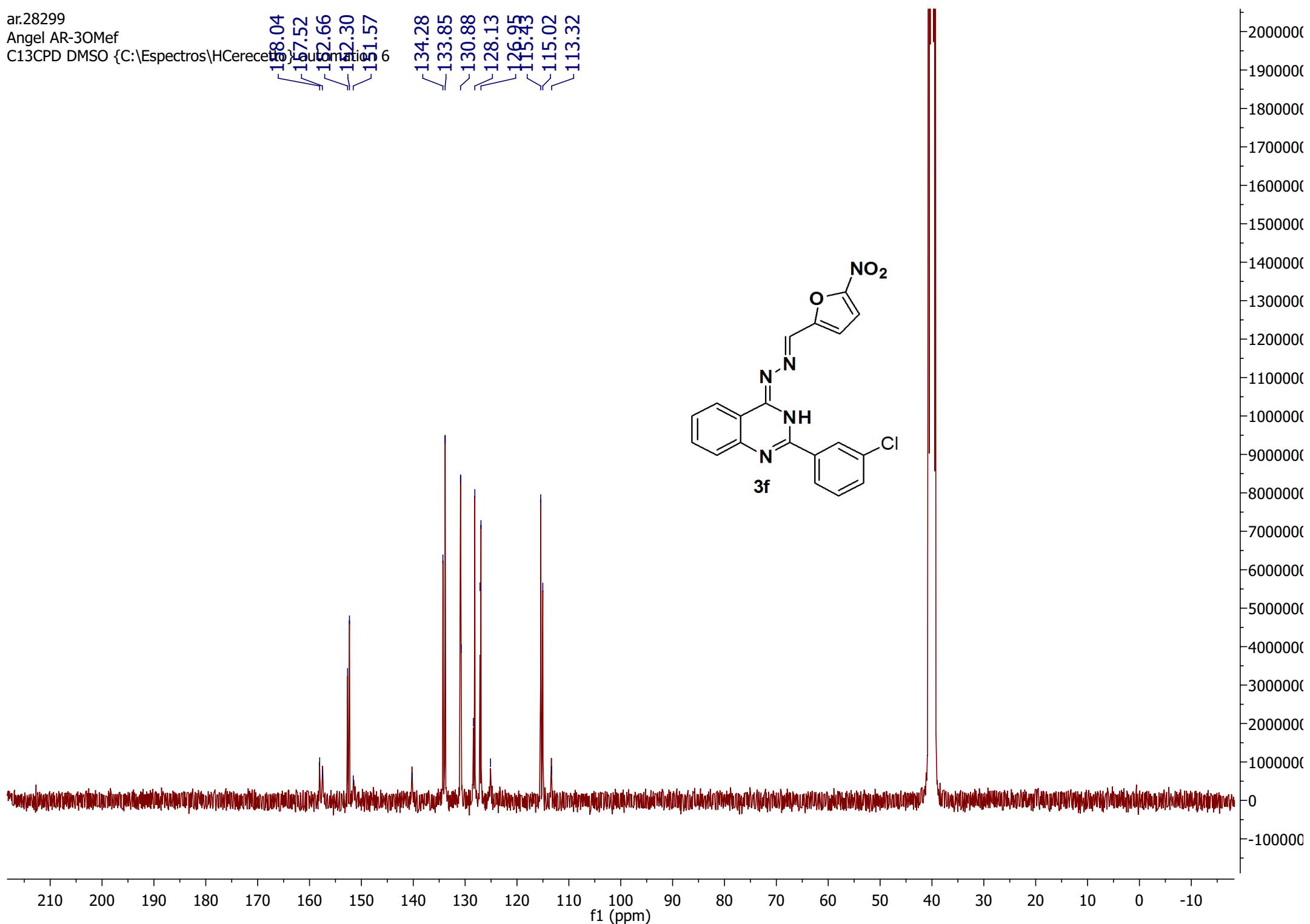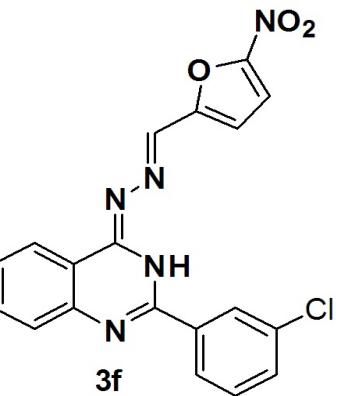
3f

158.04
152

152.66
152.30
151.57

140.21

134.28
133.85

130.88
130.75

128.40
128.13
127.13
126.95
125.10

115.43
115.02
113.32
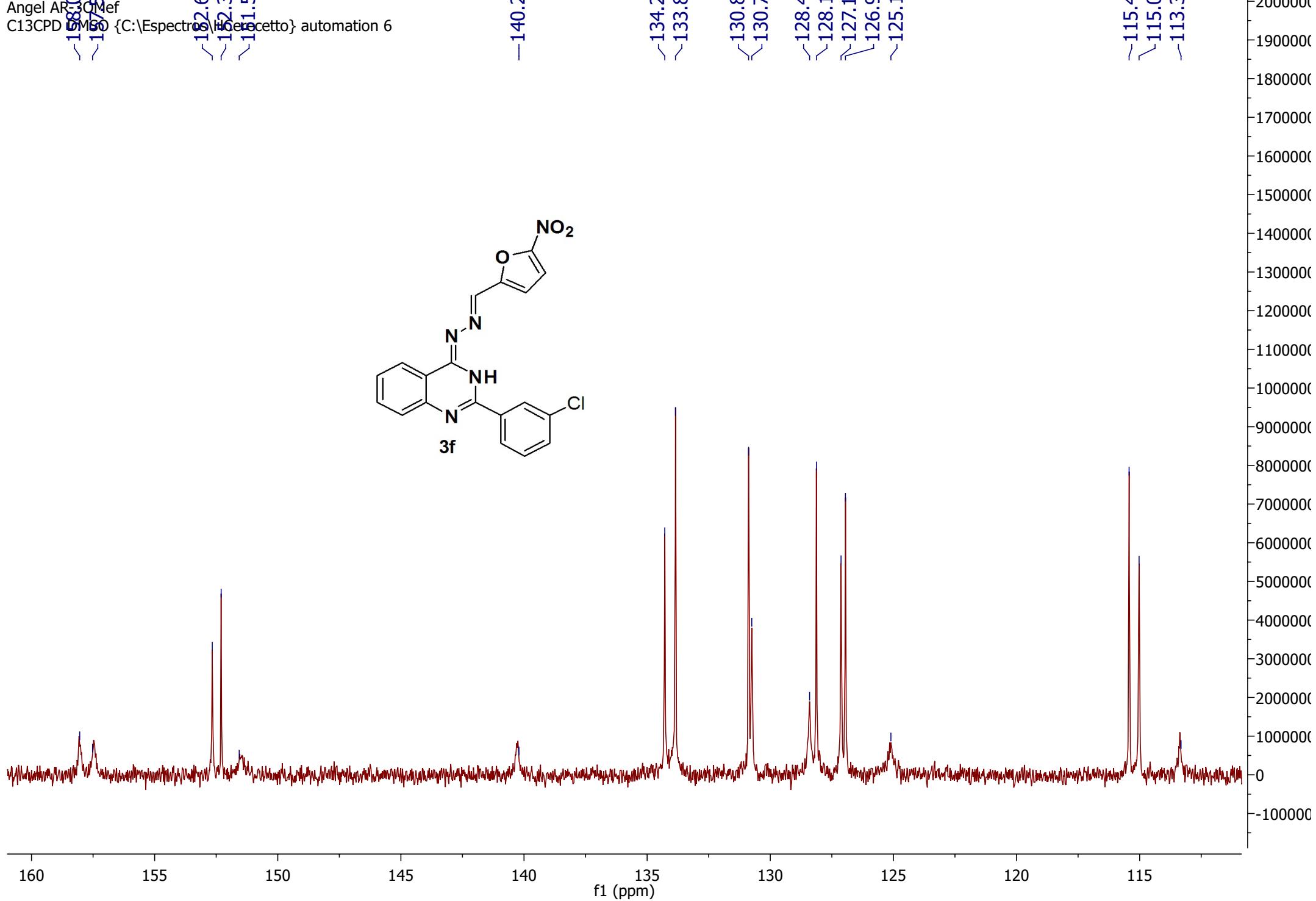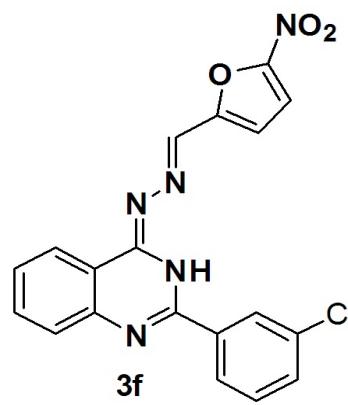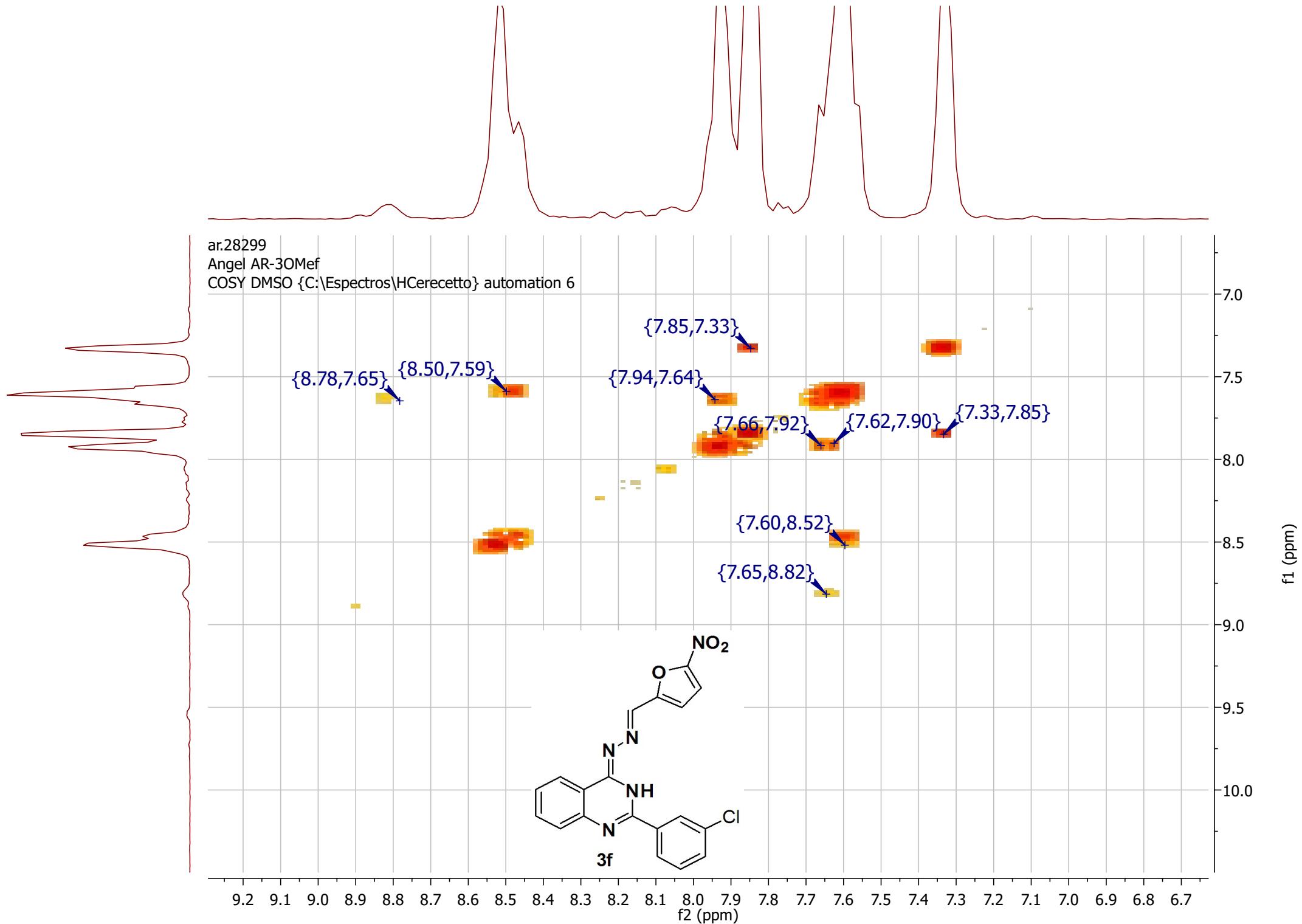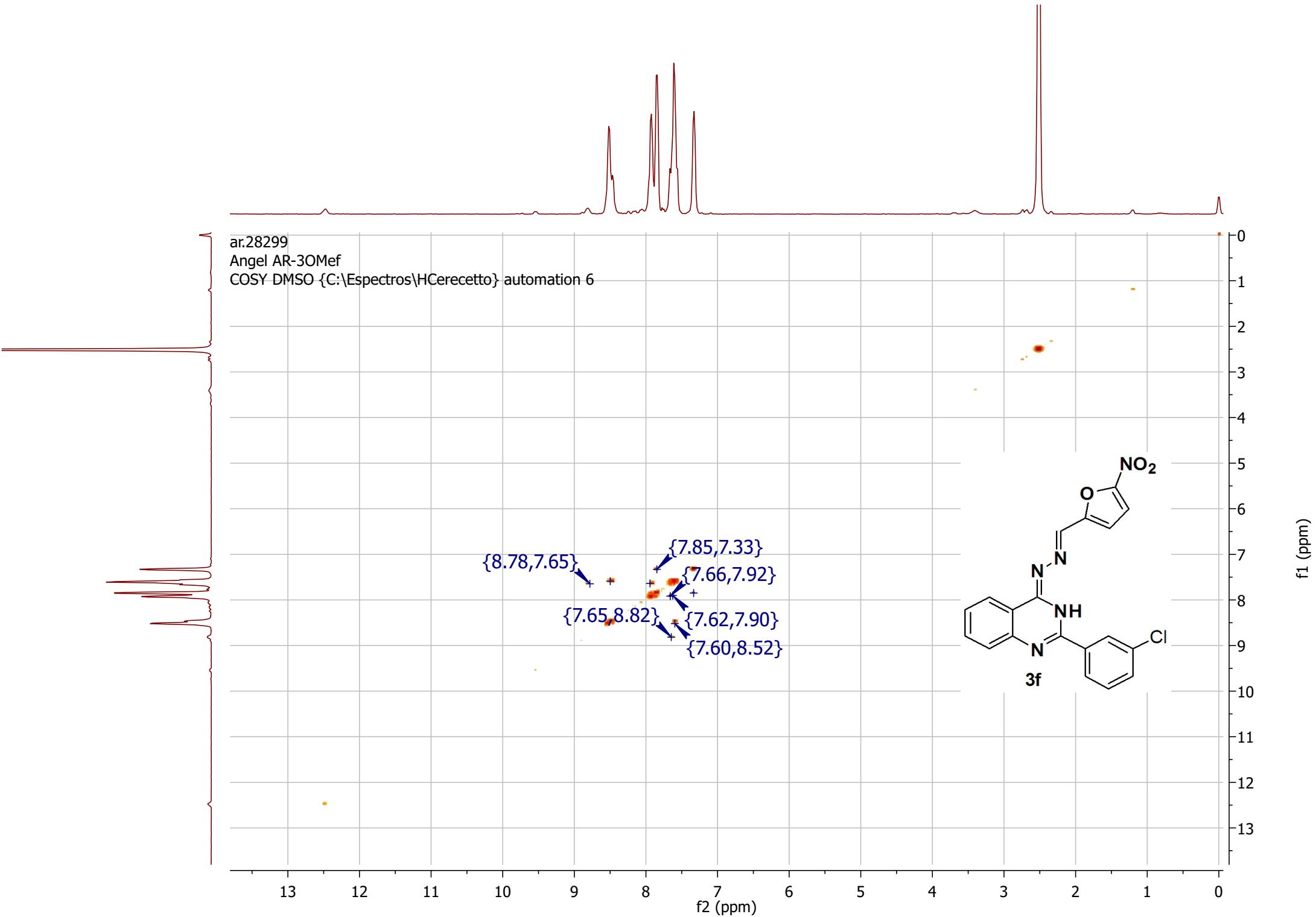
3f

ar.28299
Angel AR-3OMef
COSY DMSO {C:\Espectros\HCerecetto} automation 6

{7.85,7.33}
{8.78,7.65}
{8.50,7.59}
{7.94,7.64}
{7.66,7.92}
{7.62,7.90}
{7.33,7.85}
{7.60,8.52}
{7.65,8.82}

3f

ar.28299
Angel AR-3OMef
COSY DMSO {C:\Espectros\HCerecetto} automation 6

{8.78,7.65}
{7.85,7.33}
{7.66,7.92}
{7.65,8.82}
{7.62,7.90}
{7.60,8.52}

3f

12.46

8.51

3f

3g
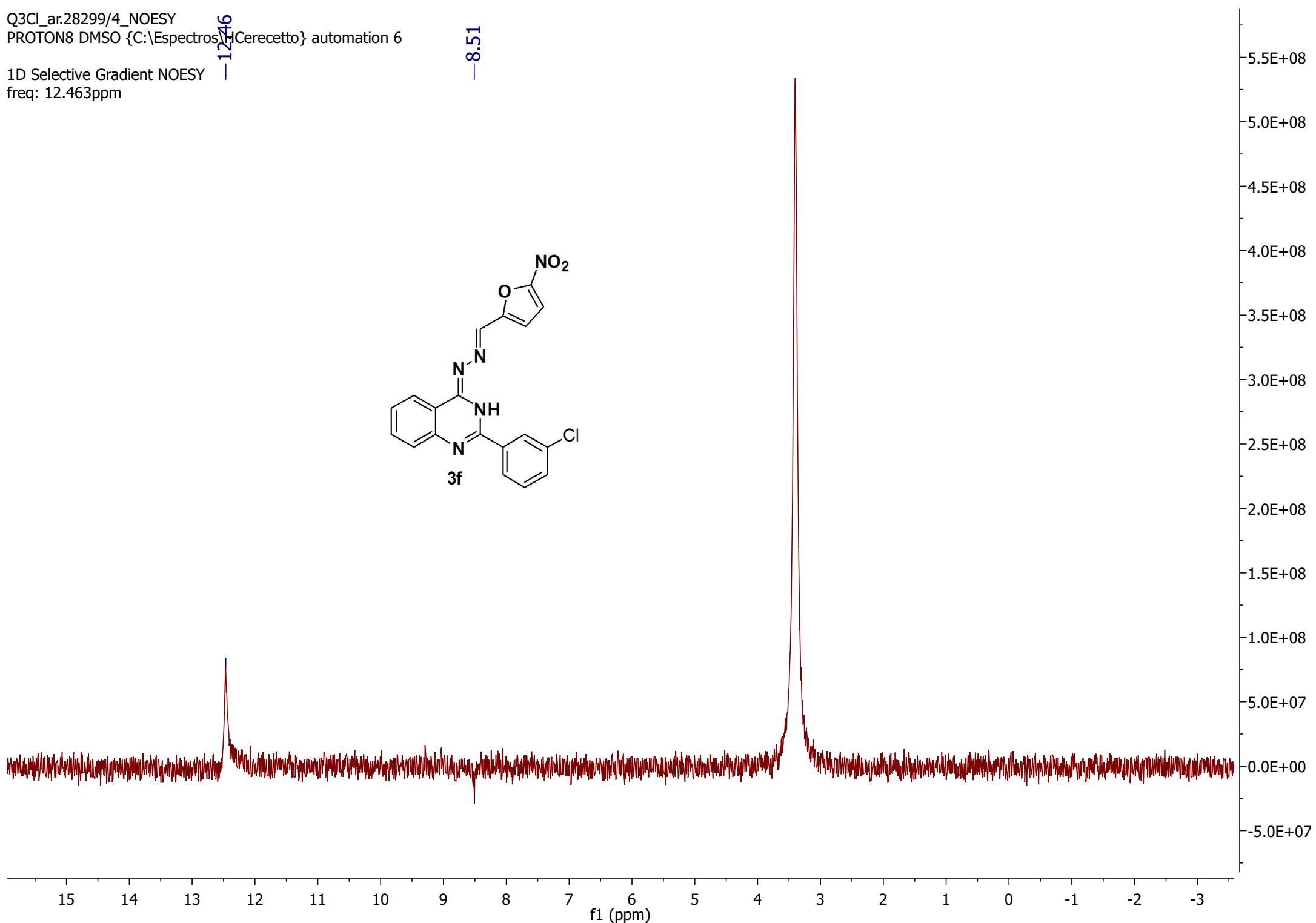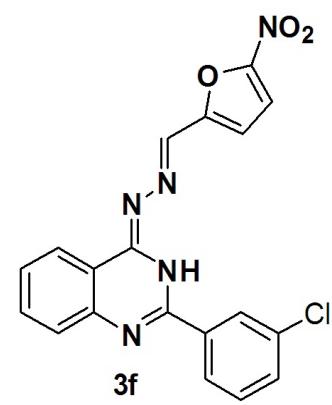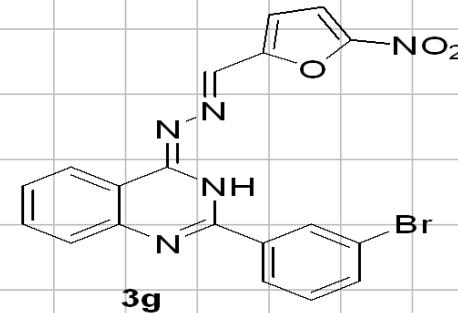
ar.28642.5.1.1r
Angel AR-Q3Brnew
C13CPD DMSO {C:\Espectros\HCerecetto} automation 1

ar.28642.2.1.2rr
Angel AR-Q3Brnew
COSY DMSO {C:\Espectros\HCerecetto} automation 1

{8.20,7.30}
{7.55,7.30}
{7.26,7.54}
{8.64,7.73}
{7.94,7.70}
{7.70,7.94}
{7.30,8.20}
{7.73,8.64}

3g

1.91

8.80
8.56
8.44
7.94
7.87
7.61
7.60
7.59
7.41
7.39
7.36
7.03
7.03
6.71
6.71
6.70
6.70

0.88

3h

3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00

0.97

0.97
2.02
1.06
1.06
2.04
1.04
2.13
0.97
1.00

14   13   12   11   10   9   8   7   6   5   4   3   2   1
f1 (ppm)
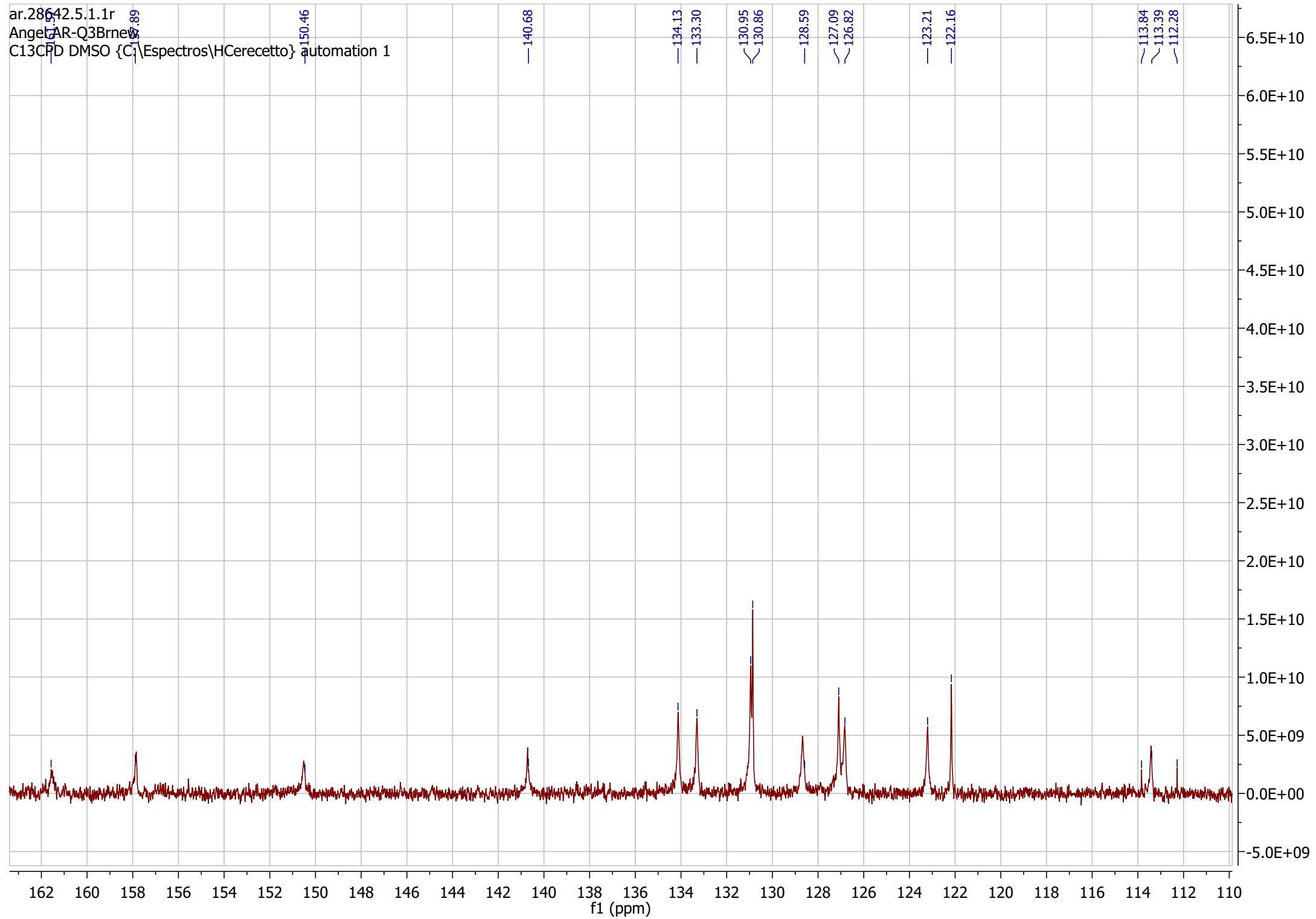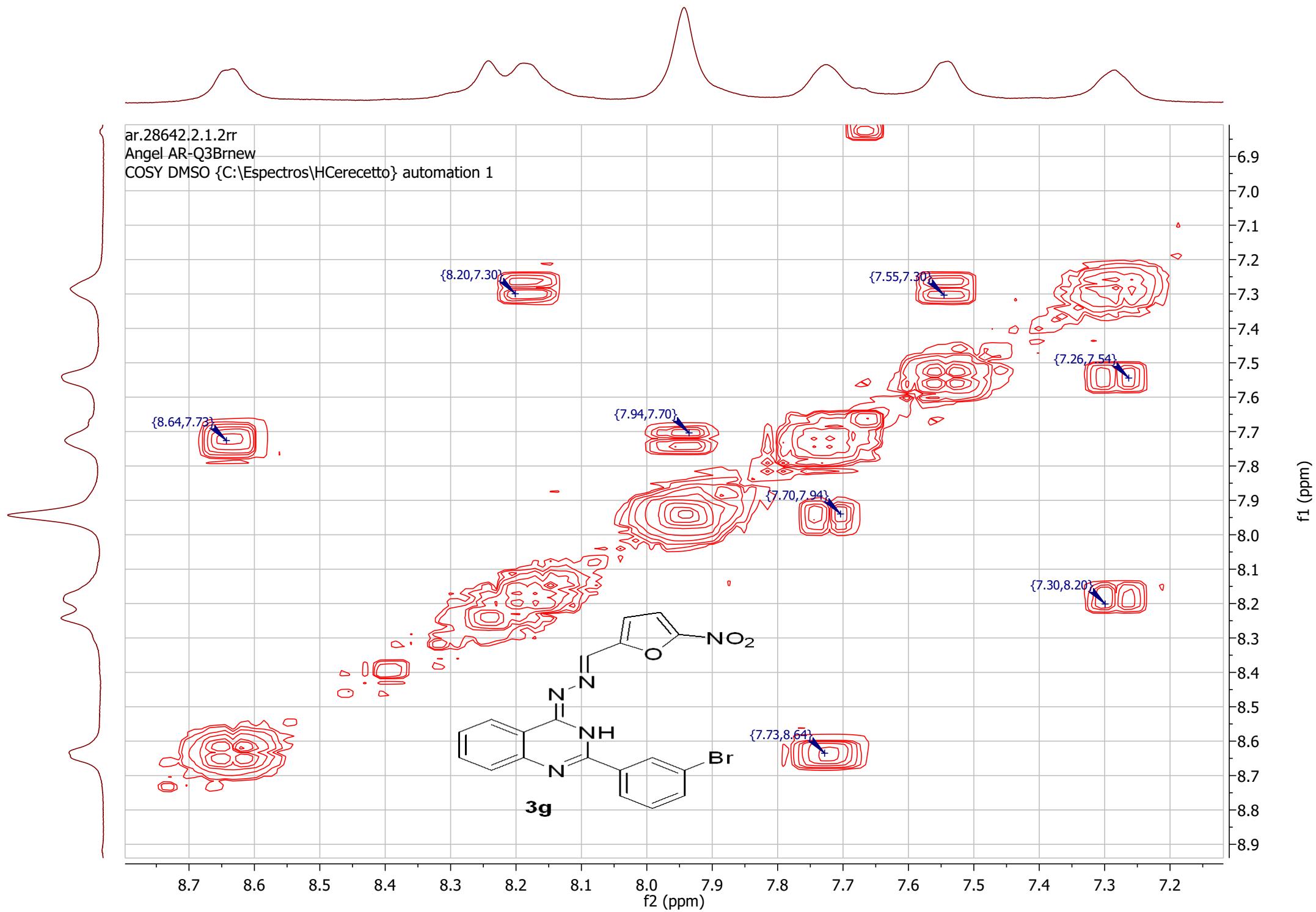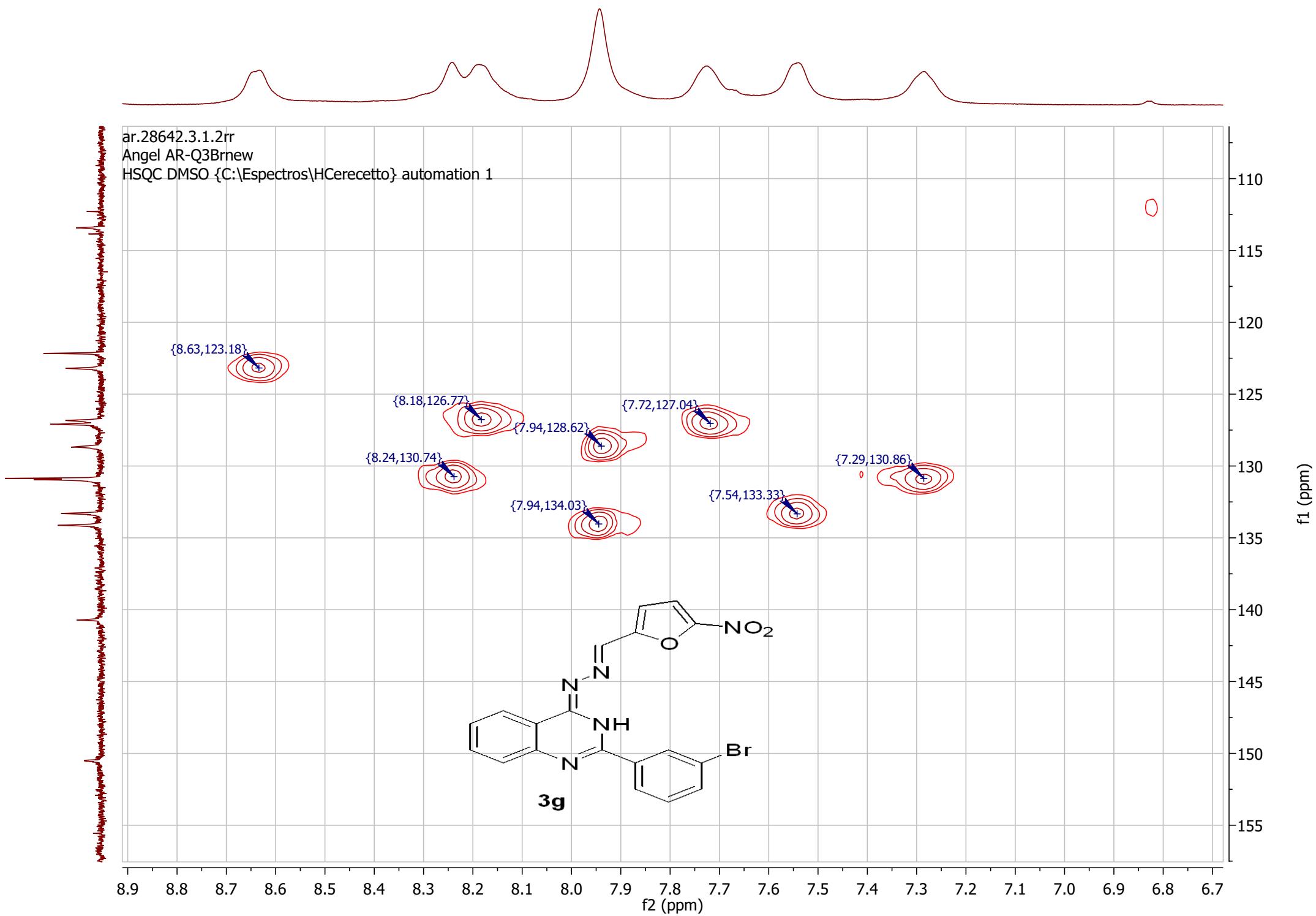
ar.28297
Angel AR-Q4FFurf
PROTON8 DMSO {C:\Espectros\HCerecetto} automation 4

8.80
8.56
8.44
7.94
7.87
7.61
7.60
7.59
7.41
7.39
7.36
7.03
7.03
6.71
6.71
6.70
6.70

3h

0.97
2.02
1.06
1.06
2.04
1.04
2.13
0.97
1.00

f1 (ppm)
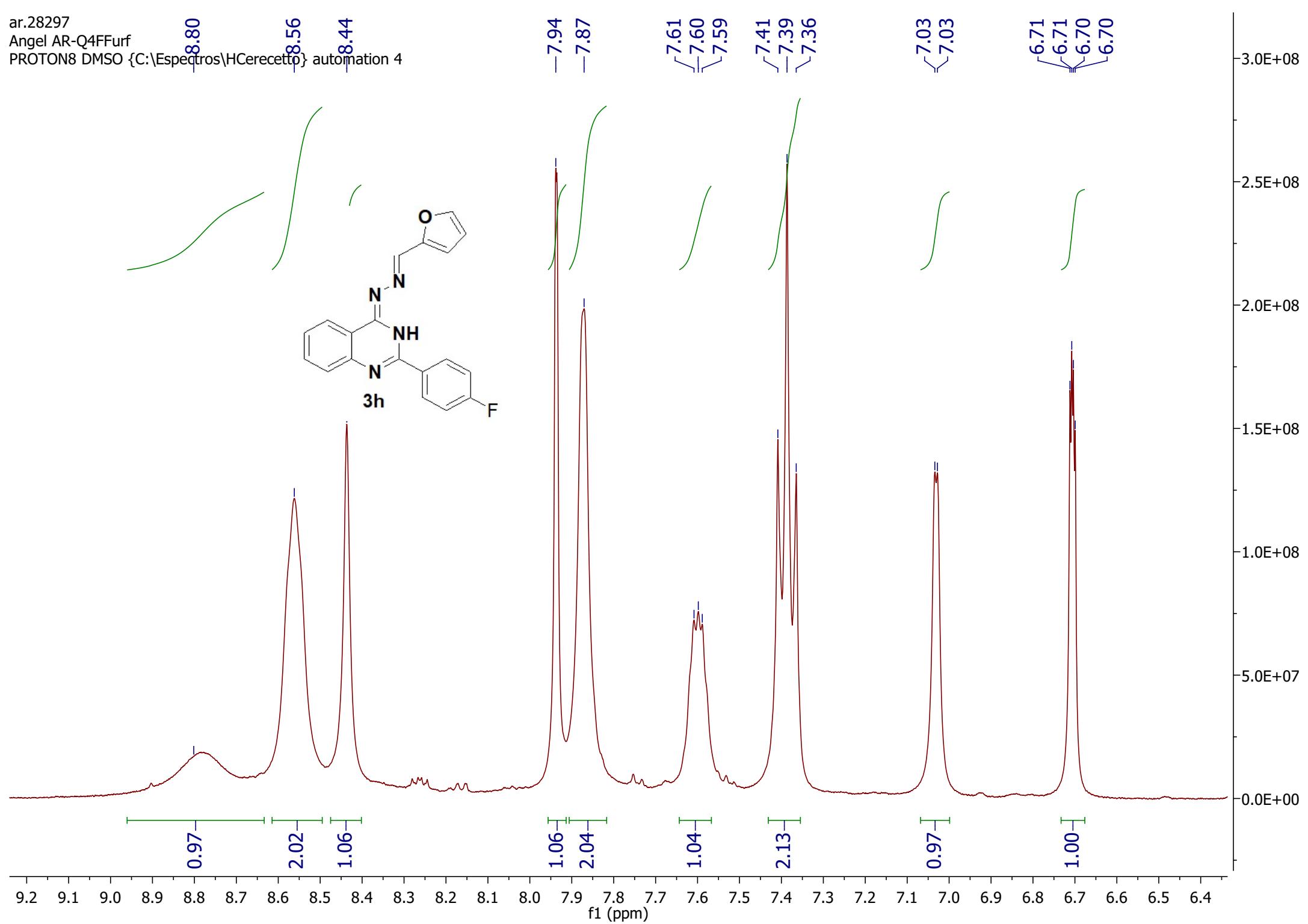
ar.28297
Angel AR-Q4FFurf
C13CPD DMSO {C:\Espectros\Cerecetto automation}

165.52
163.06
158.55
157.54
150.03
145.93
144.19
136.71
134.61
133.95
130.85
130.76
127.82
126.43
115.90
115.68
114.10
113.09
112.81

3h

3h

-109.03
-110.91

3h

ar.28297
Angel AR-Q4FFurf
COSY DMSO {C:\Espectros\HCerecetto} automation 4

{7.95,6.71}
{6.99,6.77}
{6.71,7.04}
{8.28,7.42}
{8.54,7.36}
{7.87,7.60}
{7.58,7.87}
{6.69,7.95}
{7.40,8.29}
{7.36,8.55}
{7.41,8.55}