## Supporting Information

*Org. Commun.* 12:4 (2019) 217-221

# Oxidation of some benzyl substituted fused quinazoline derivatives

**Dmytro Kravtsov**

*Department of Organic and Bioorganic Chemistry, Zaporizhzhia State Medical University, Mayakovsky ave., 26, 69035, Zaporizhzhia, Ukraine*

**Table of Contents** **Page**

**General Procedure**

A mixture of the phenylacetic acid (4.4 mmol), CDI (4.8 mmol) and dioxane (20 mL) was stirred at 80 °C for 1 h. Then, the appropriate amine **1a-d** (4.4 mmol) was added and the mixture was refluxed for 3 h., after which $H_2O$ (75 mL) was added. The precipitate was filtered,[a] washed thoroughly with $H_2O$ and dried at 60 °C. The crude product was dissolved in AcOH (50 mL) and refluxed for 8 h. After that, the solvent was removed *in vacuo* and MeOH (10 mL) was added. The resulting precipitate was filtered and washed with cold MeOH and dried at 60 °C.[b] A solution of $CrO_3$ (4.2 mmol (~ three-fold excess)) in AcOH (40 mL) was added to a stirred solution of the crude product in AcOH (20 mL) over 30 min at 60-63 °C. The mixture was stirred for 3.5 h. at 60-63 °C, then, poured into a solution of $Na_2SO_3$ (2.8 mmol) in ice-water (100 mL). The residue was filtered,[c] washed thoroughly with $H_2O$ and dried at 60 °C. The resulting material was purified to obtain the products (silica gel column chromatography EtOAc-$CHCl_3$-PE (6:2:2) **4a**[d] and **4b**. Crystallization from DMF-$H_2O$ afforded **4c** and **4d**).

[a]In the case of amines **1c-d**, the crude product was extracted with EtOAc (3×100 mL), washed with brine, dried over $Na_2SO_4$, and concentrated under reduced pressure.
[b]After crystallization from DMF-$H_2O$, 97.1% pure **3a**, according to LC-MS analysis, was obtained.
[c]Benzoic acid **6** was isolated from the filtrate by acid-base extraction with ether and crystallized from water.
[d]The resulting material was triturated in acetone to provide quinazolinone **5a**. The filtrate contained ketone **4a** and a small impurity of quinazolinone **5a**. This solution was used for chromatography.

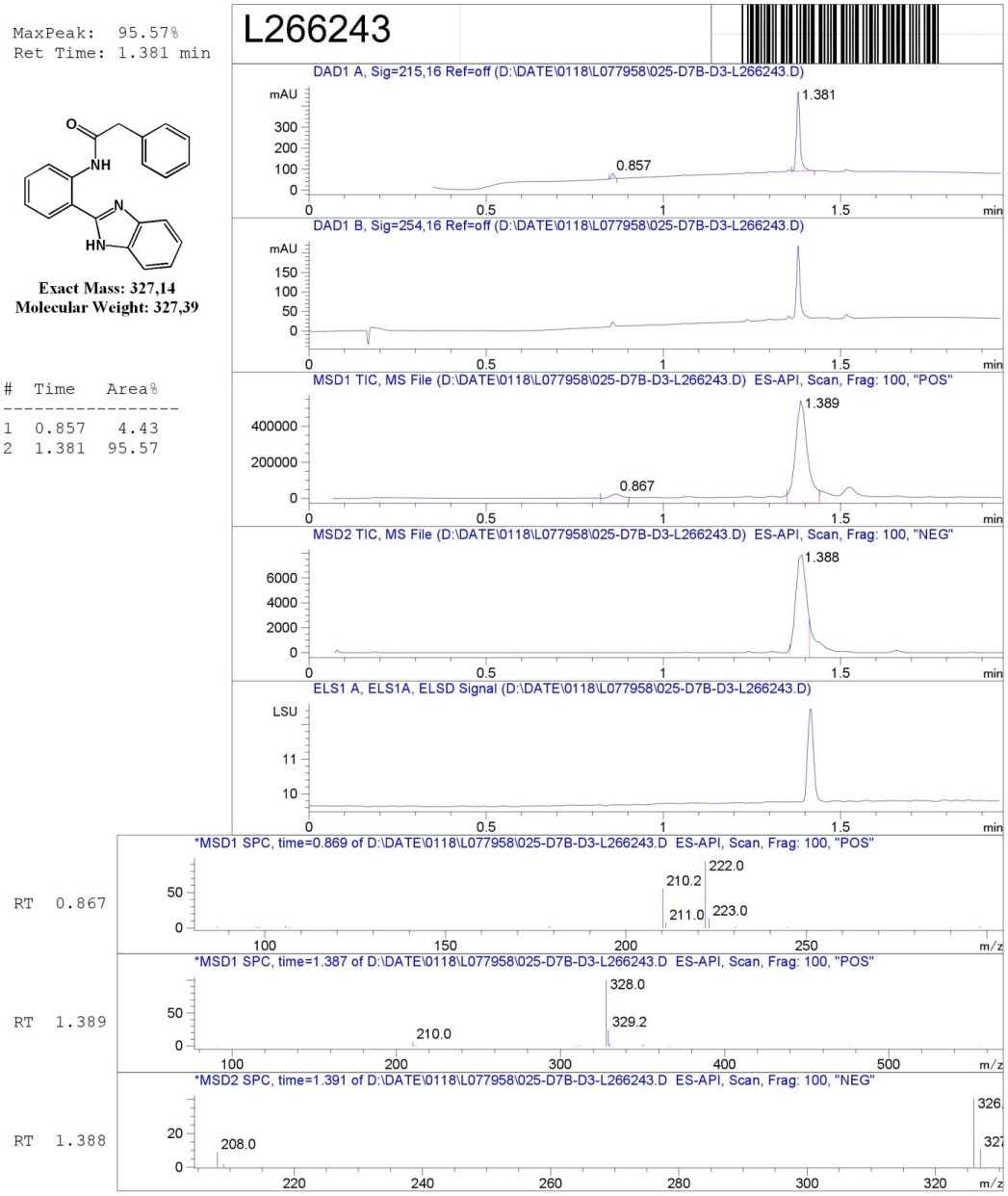


**Figure S1:** LC-MS spectrum of compound **2a** (N-(2-(1*H*-Benzo[*d*]imidazol-2-yl)phenyl)-2-phenylacetamide)

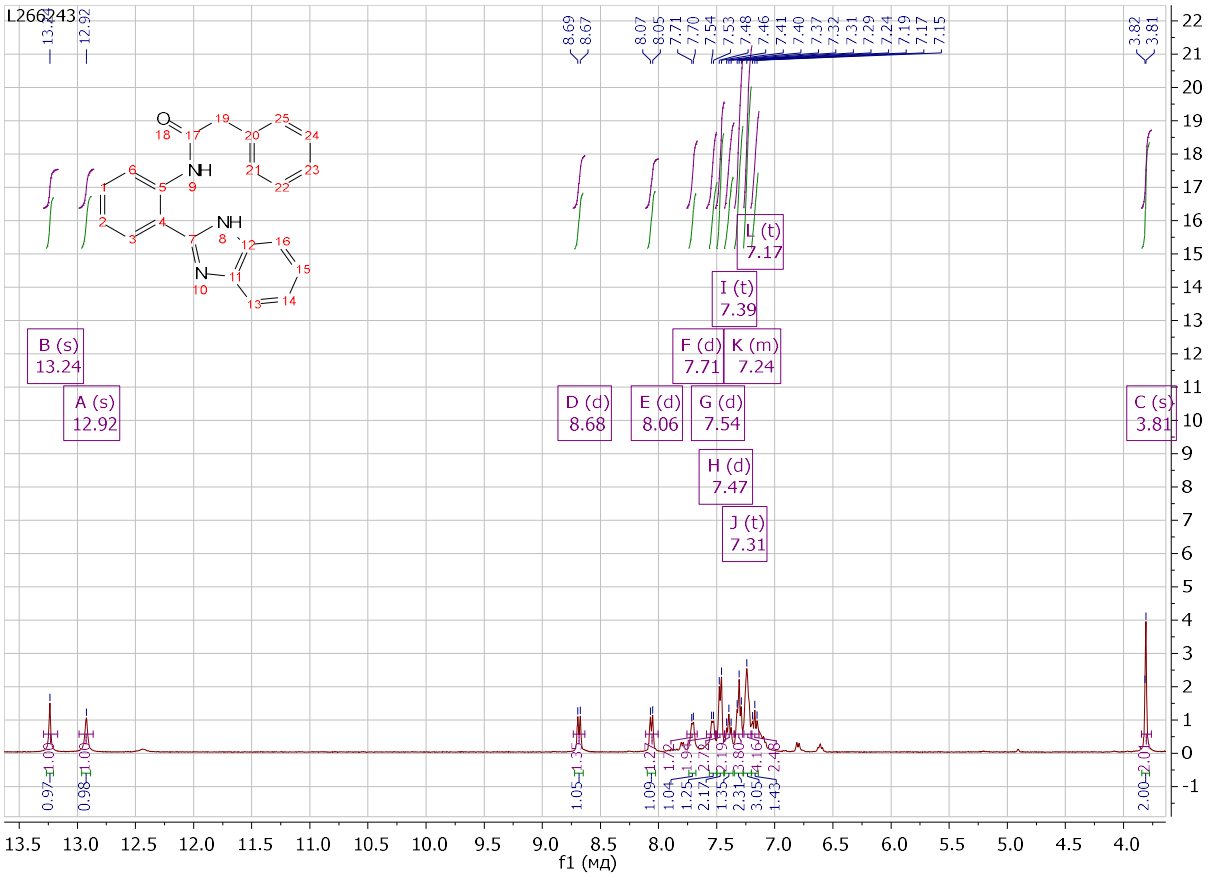


**Figure S2 :** $^{1}$H NMR spectrum of compound **2a**

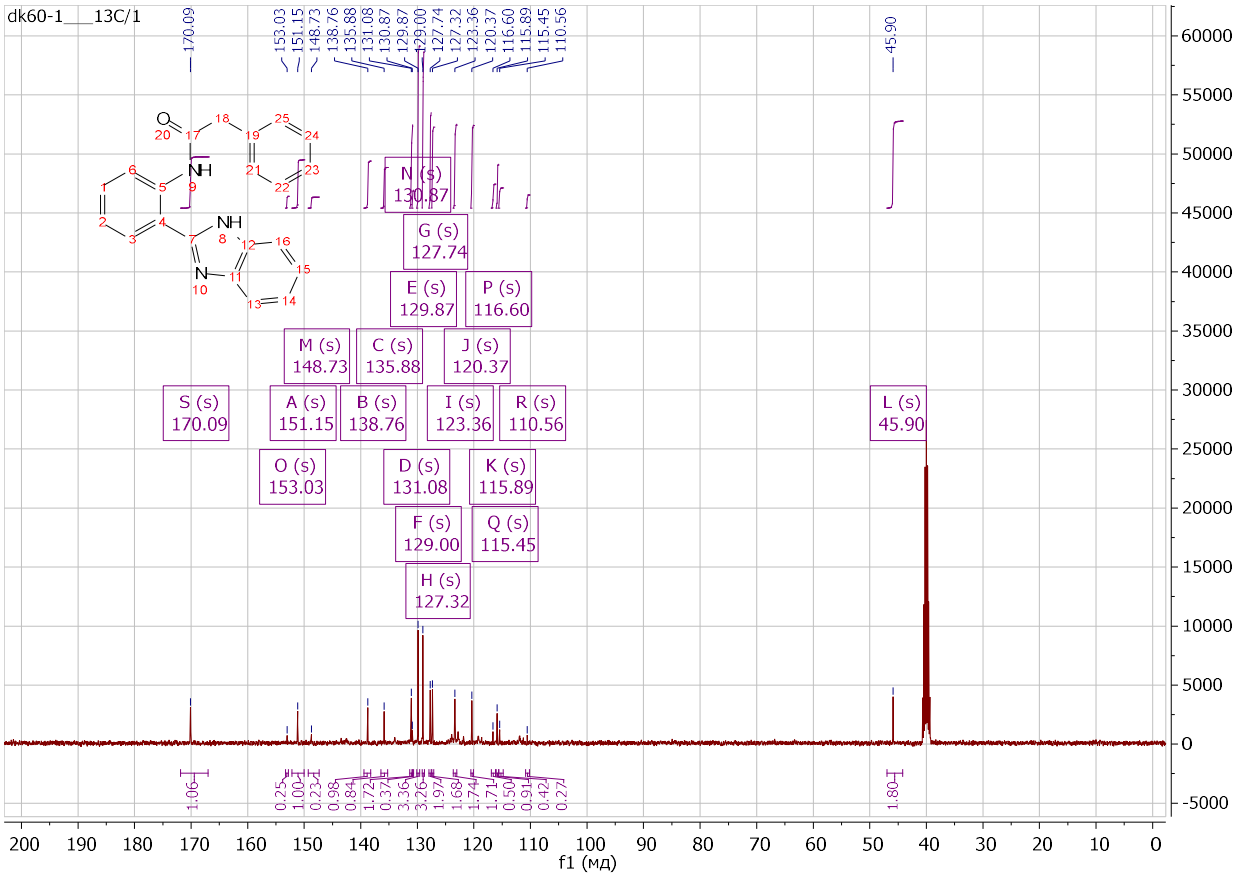


**Figure S3:** $^{13}$C NMR spectrum of compound **2a**

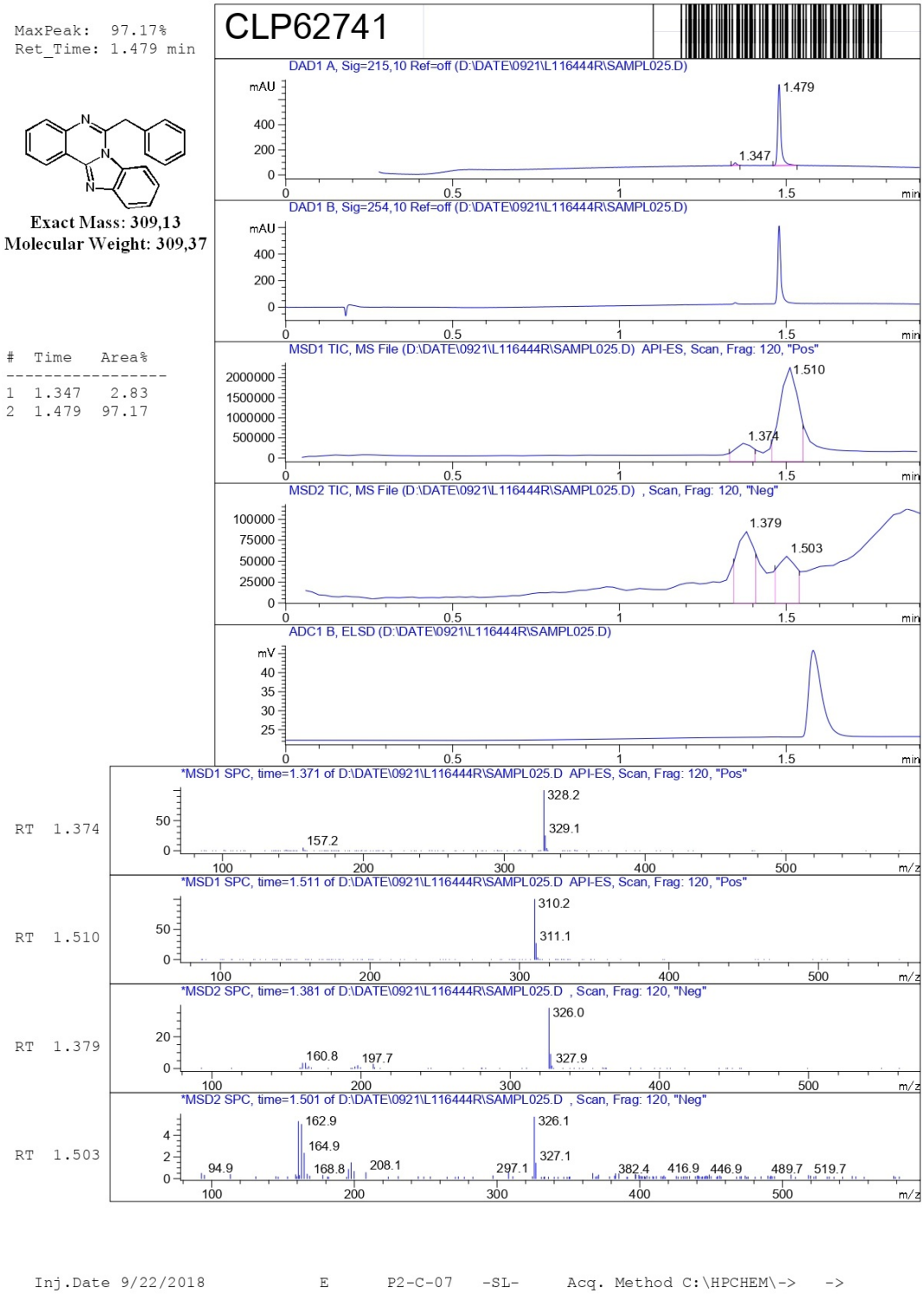


**Figure S4:** LC-MS spectrum of compound **3a** (6-Benzylbenzo[4,5]imidazo[1,2-*c*]quinazoline )

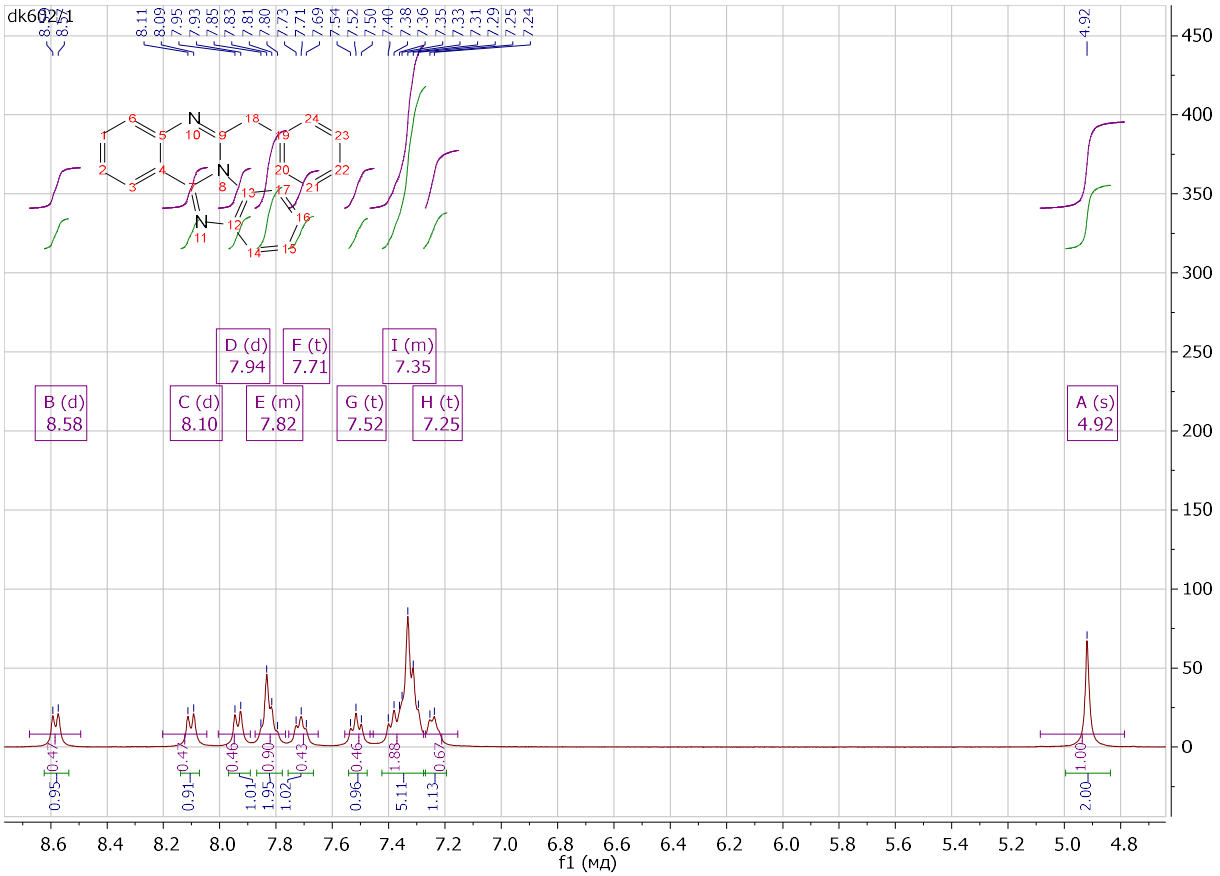


**Figure S5 :** $^{1}$H NMR spectrum of compound **3a**

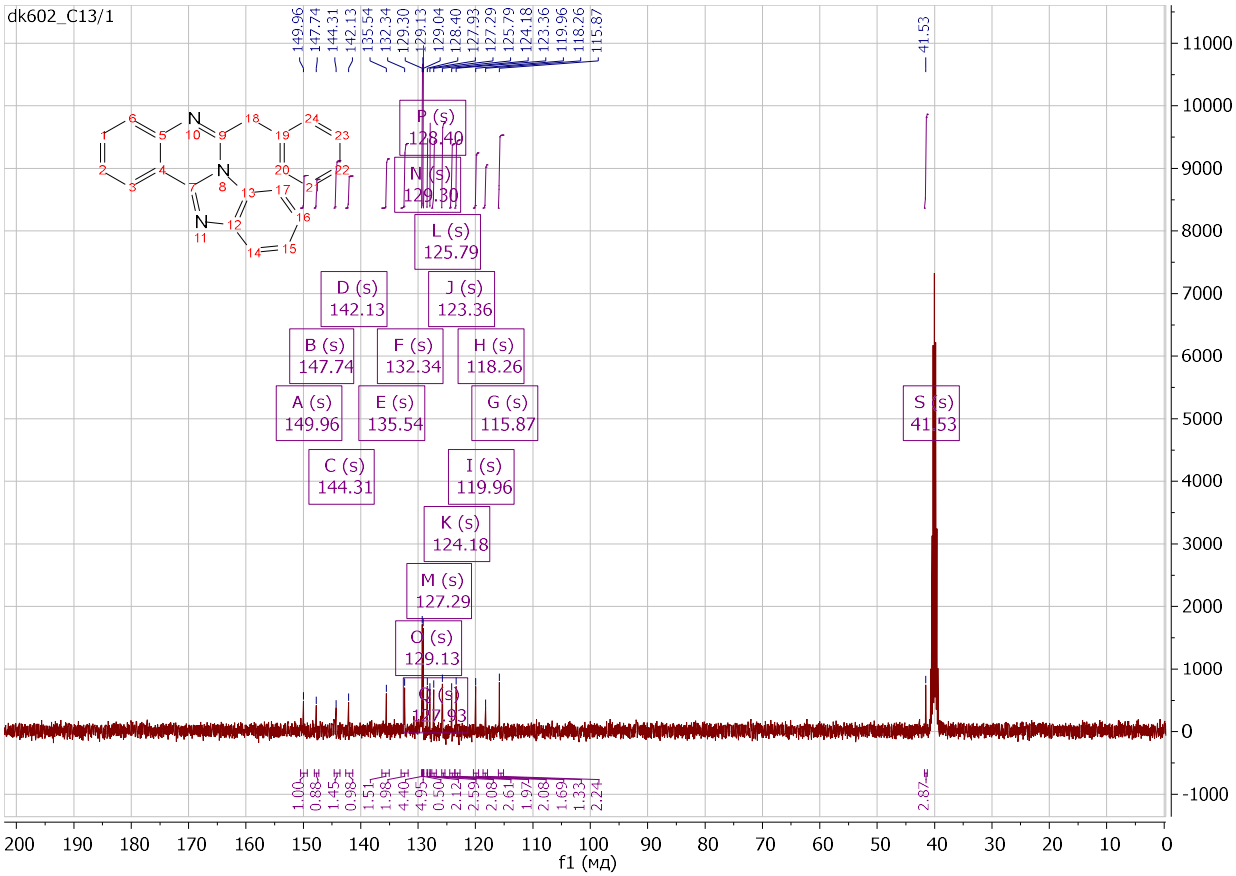


**Figure S6 :** $^{13}$C NMR spectrum of compound **3a**

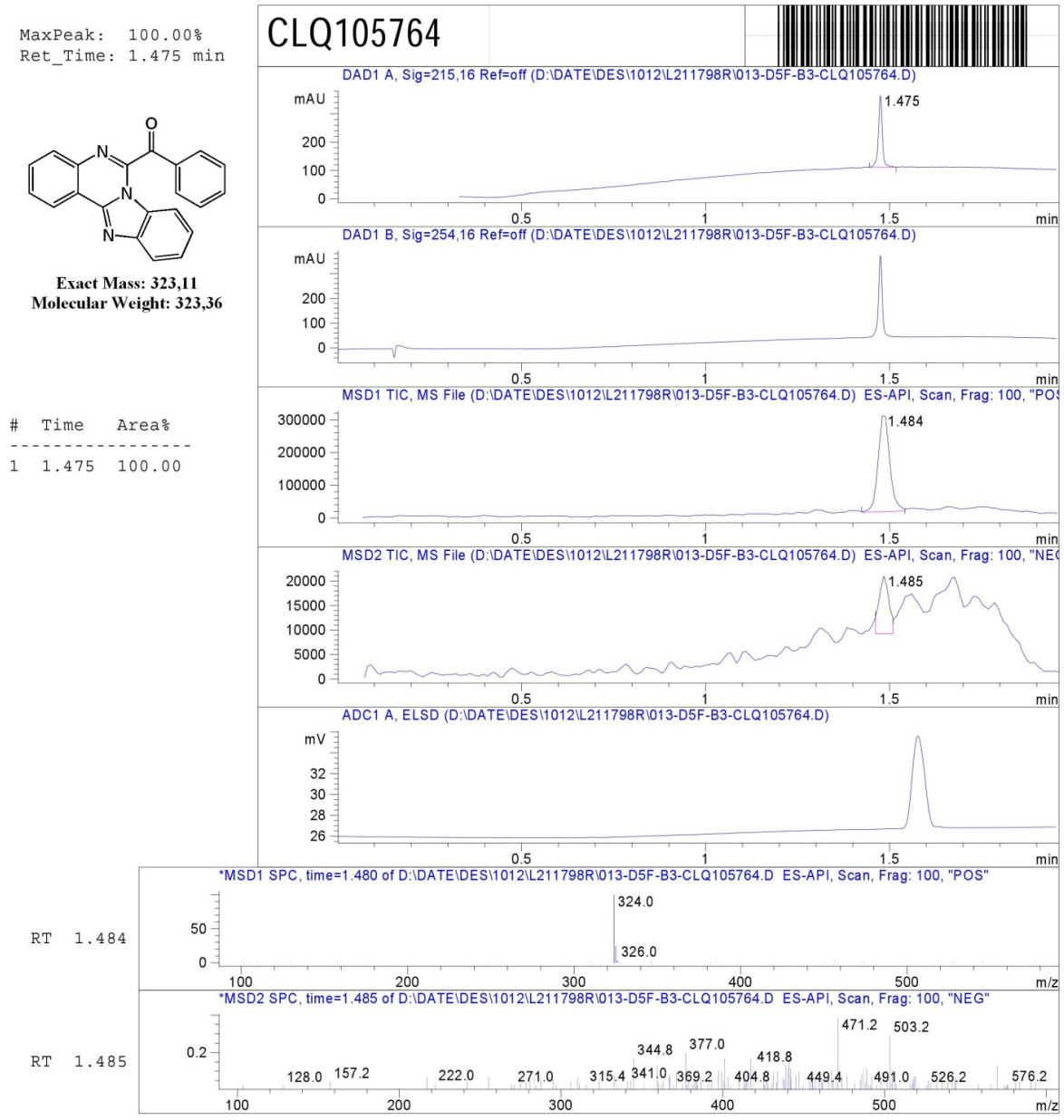


**Figure S7:** LC-MS spectrum of compound **4a** (Benzo[4,5]imidazo[1,2-*c*]quinazolin-6-yl(phenyl)methanone)

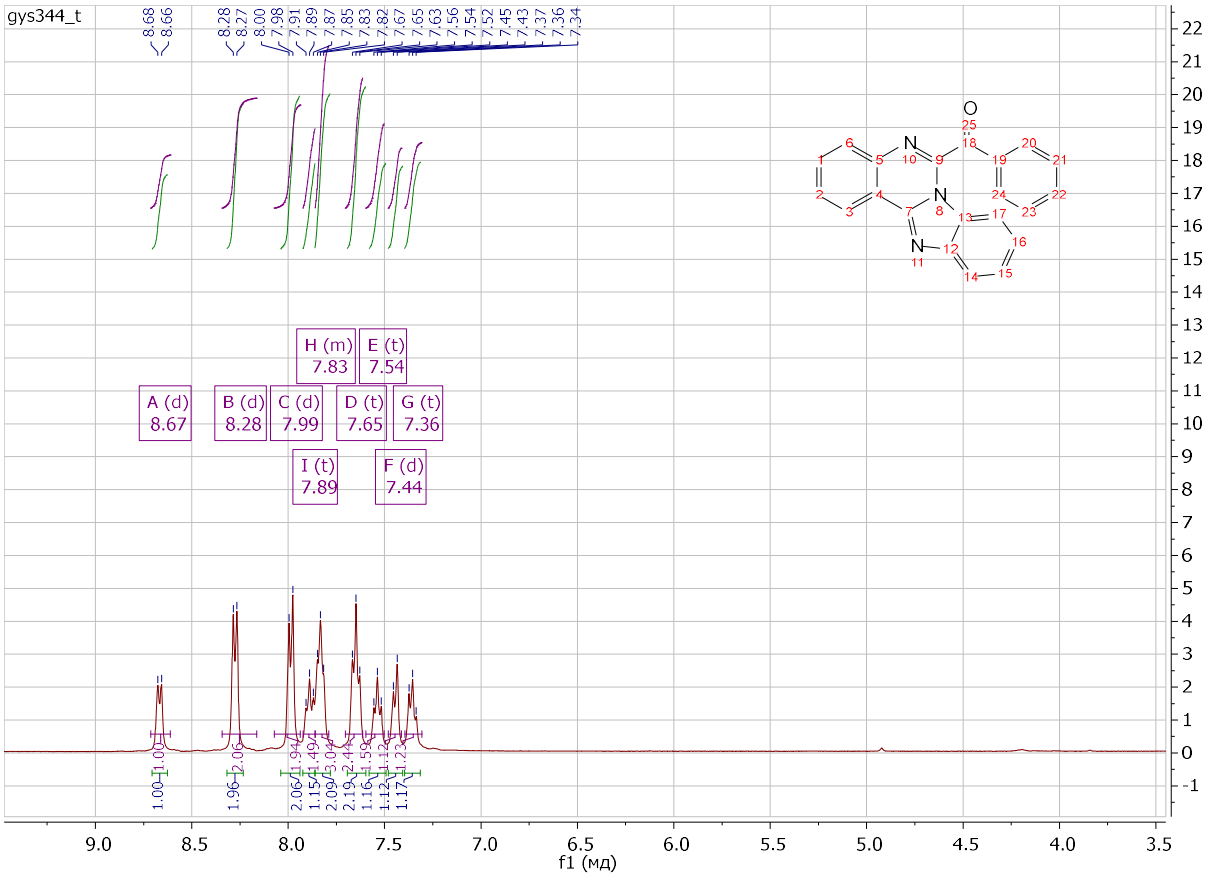


**Figure S8 :** $^{1}$H NMR spectrum of compound **4a**

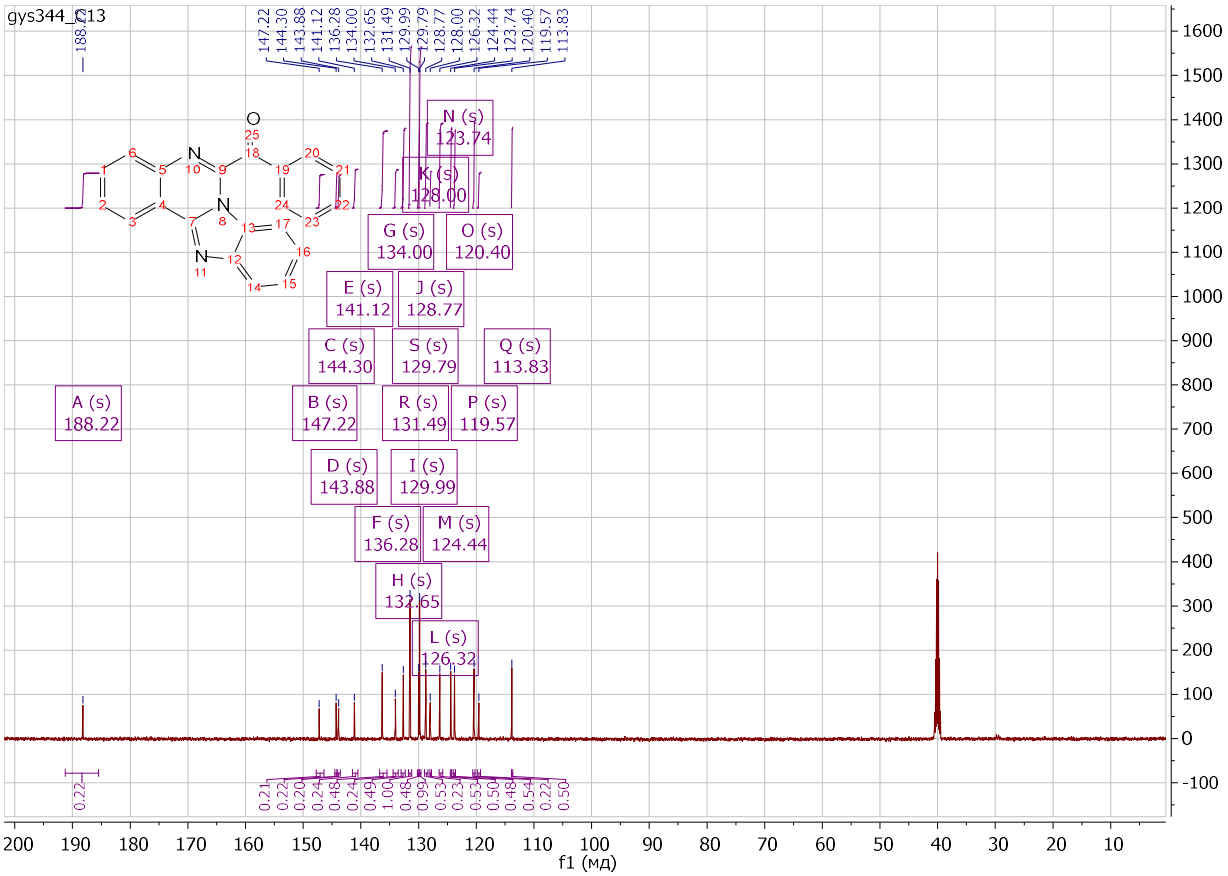


**Figure S9 :** $^{13}$C NMR spectrum of compound **4a**

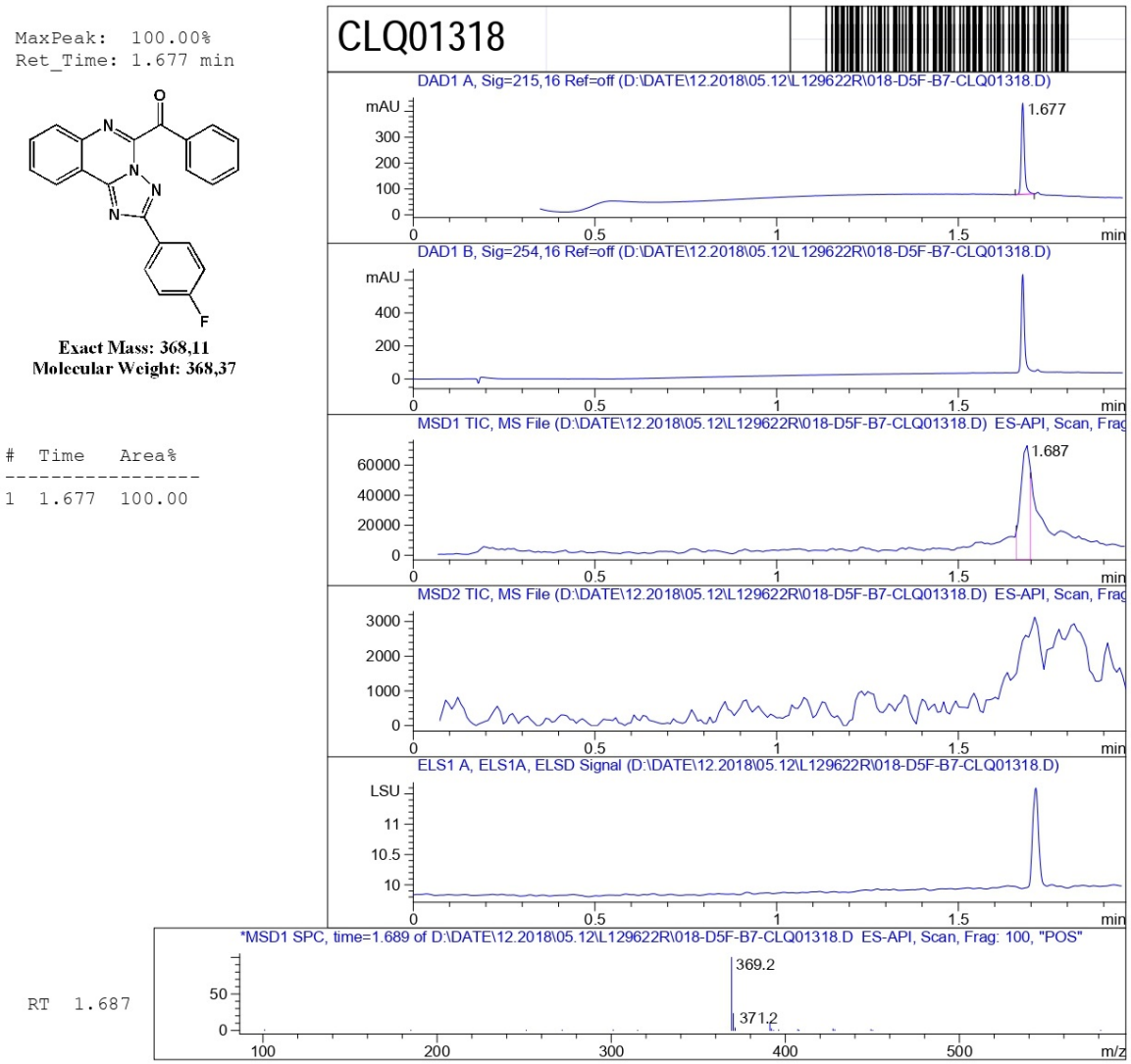


**Figure S10:** LC-MS spectrum of compound **4b** ((2-(4-Fluorophenyl)-[1,2,4]triazolo[1,5-*c*]quinazolin-5-yl)(phenyl)methanone)

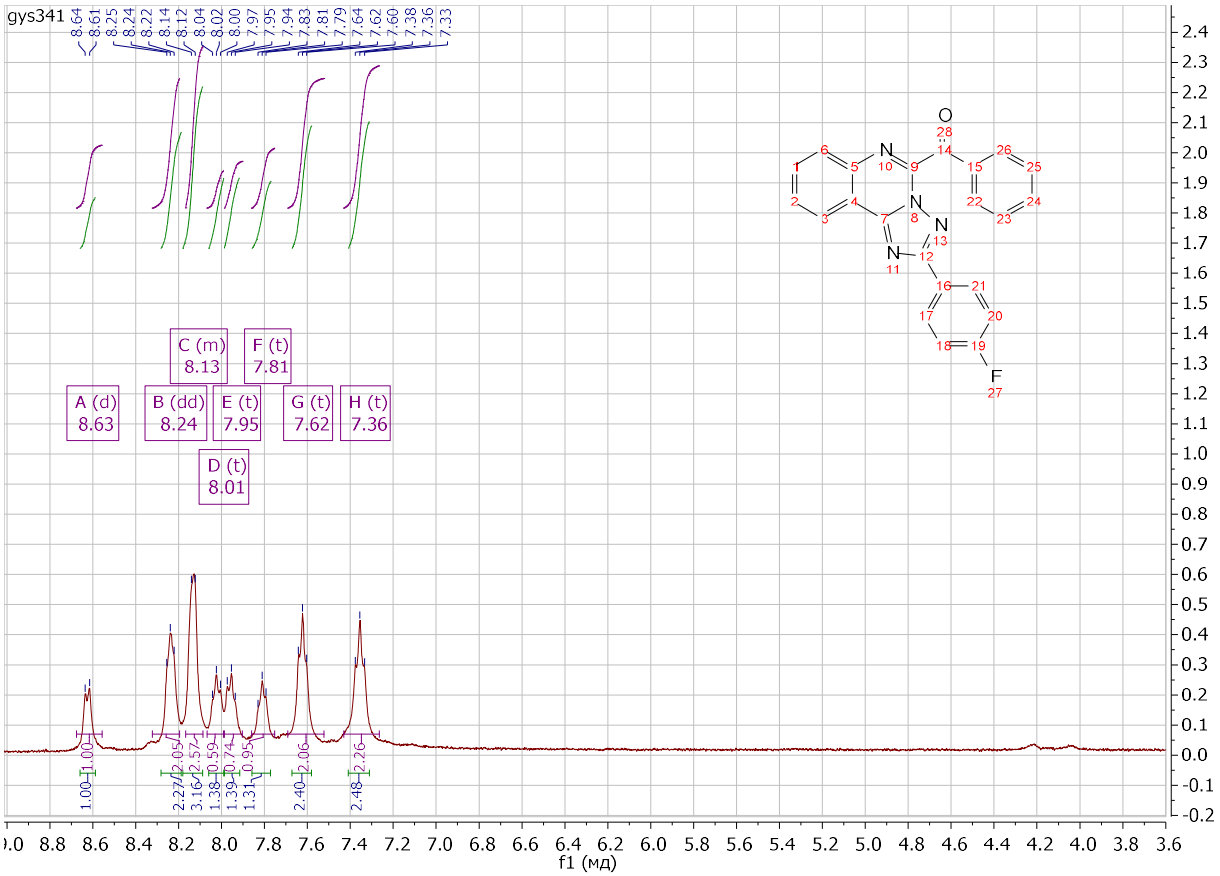


**Figure S11 :** $^{1}$H NMR spectrum of compound **4b**

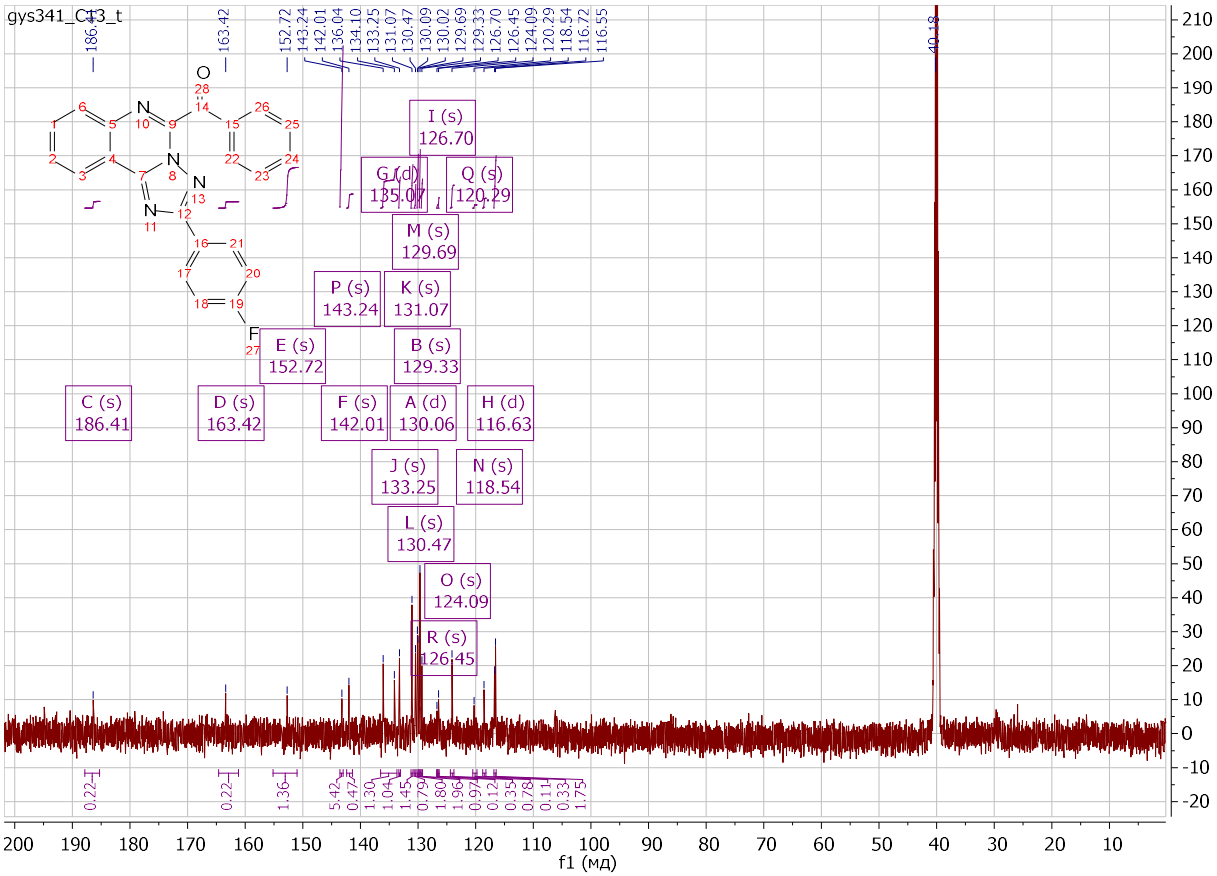


**Figure S12 :** $^{13}$C NMR spectrum of compound **4b**

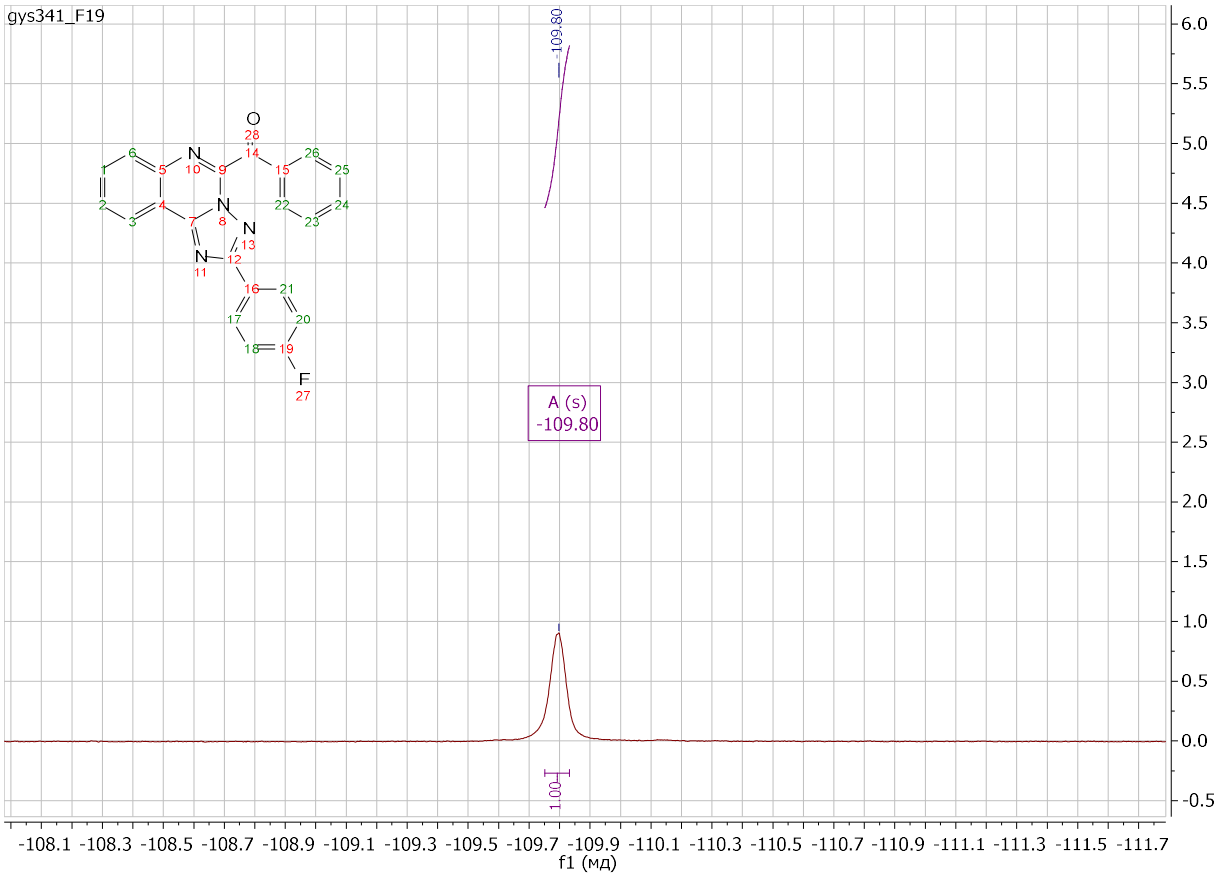


**Figure S13 :** $^{19}$F NMR spectrum of compound **4b**

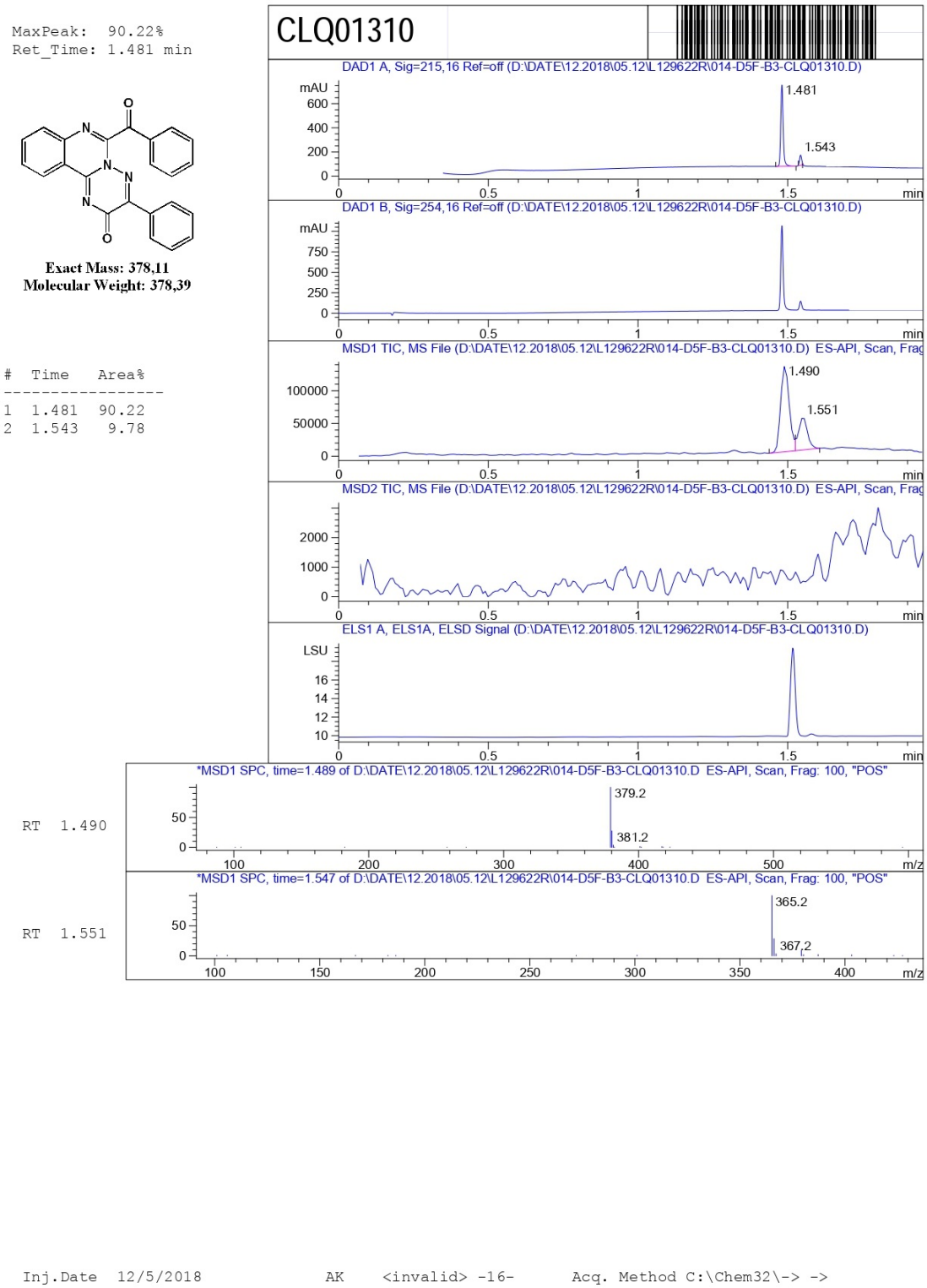


**Figure S14:** LC-MS spectrum of compound **4c** (6-Benzoyl-3-phenyl-2*H*-[1,2,4]triazino[2,3-*c*]quinazolin-2-one)

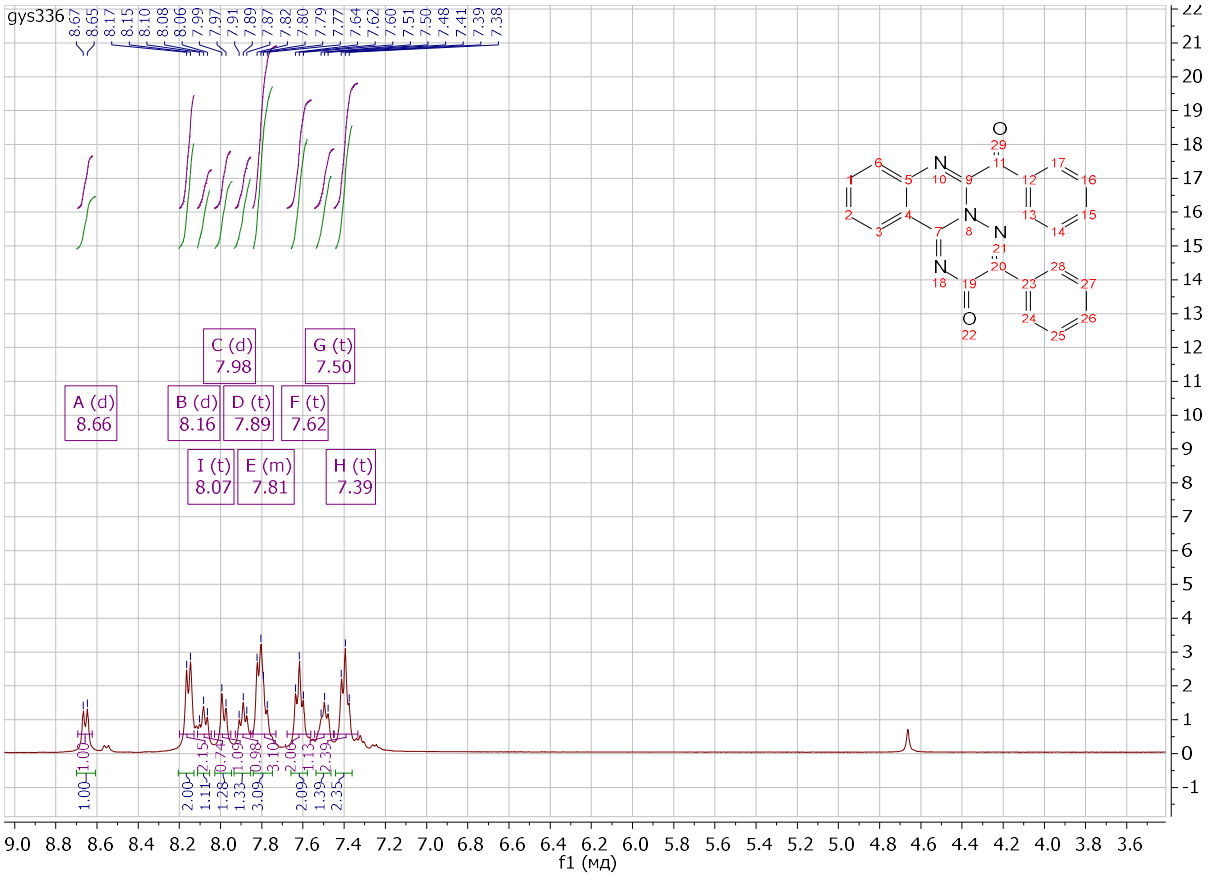


**Figure S15 :** $^{1}$H NMR spectrum of compound **4c**

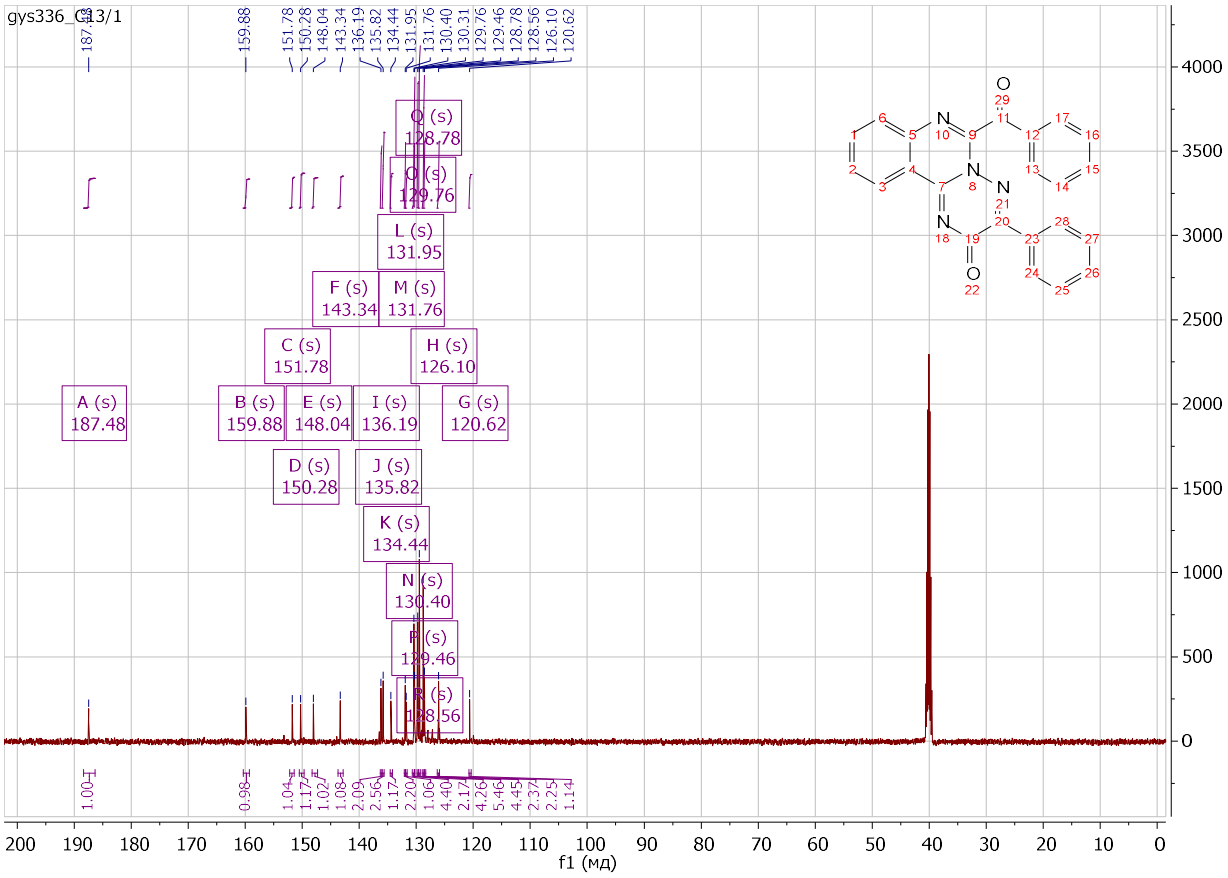


**Figure S16:** $^{13}$C NMR spectrum of compound **4c**

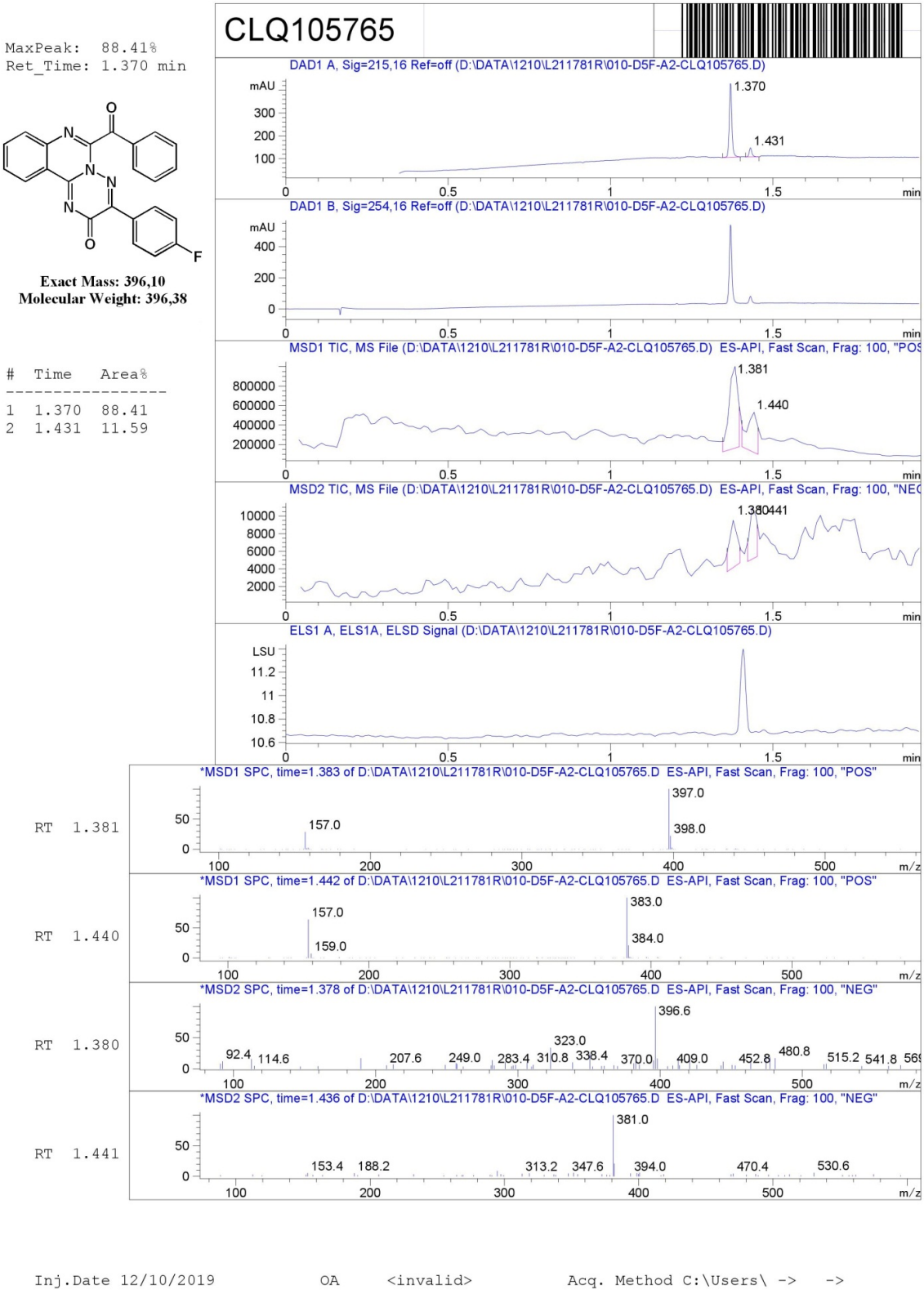


**Figure S17:** LC-MS spectrum of compound **4d** (6-Benzoyl-3-(4-fluorophenyl)-2*H*-[1,2,4]triazino[2,3-*c*]quinazolin-2-one)

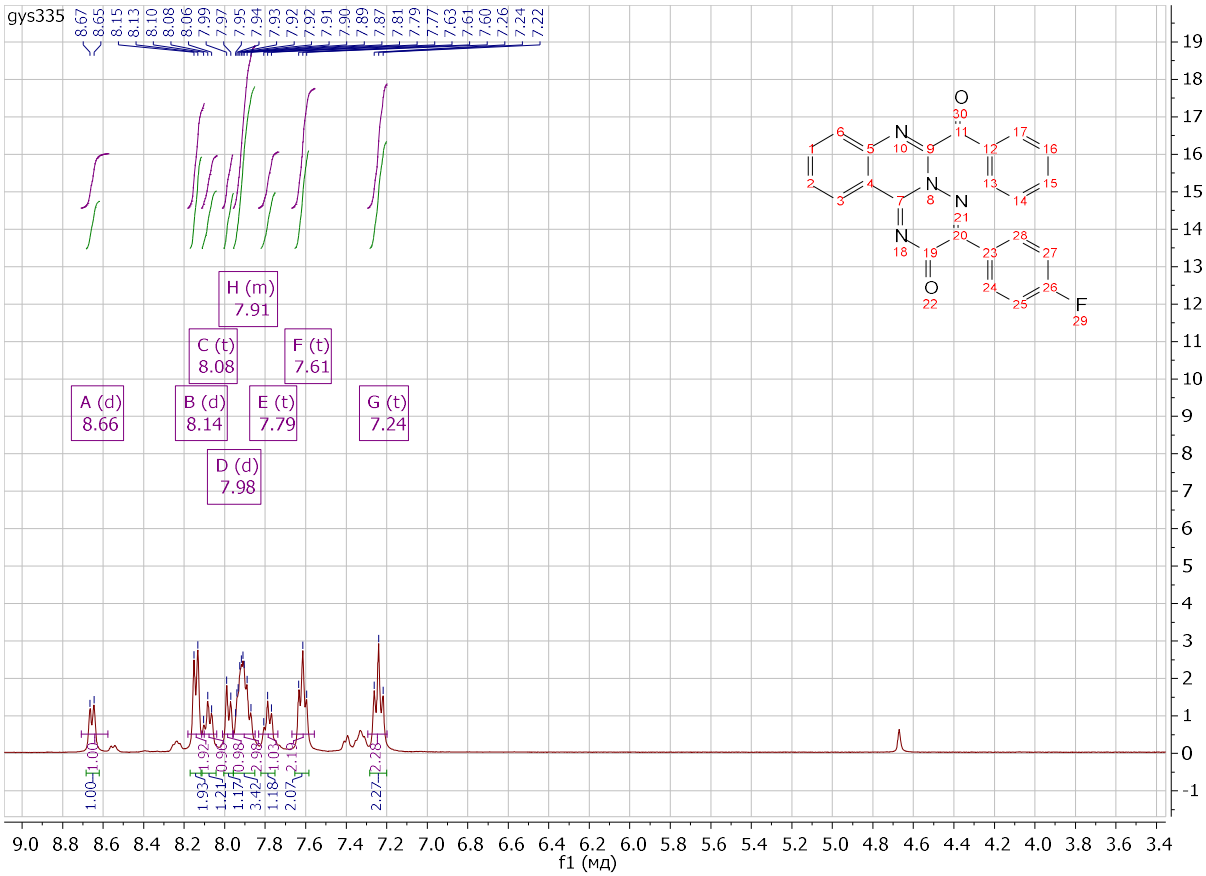


**Figure S18 :** $^{1}$H NMR spectrum of compound **4d**

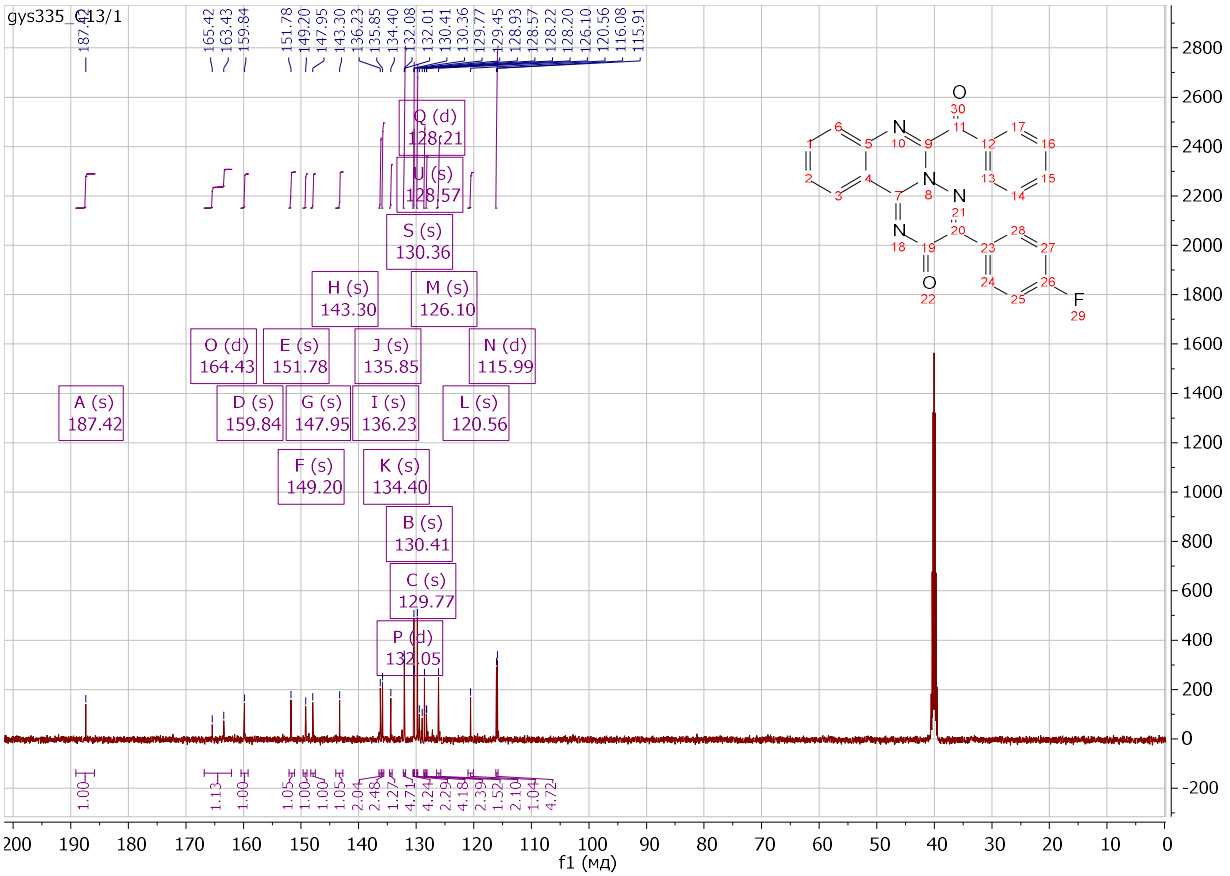


**Figure S19 :** $^{13}$C NMR spectrum of compound **4d**

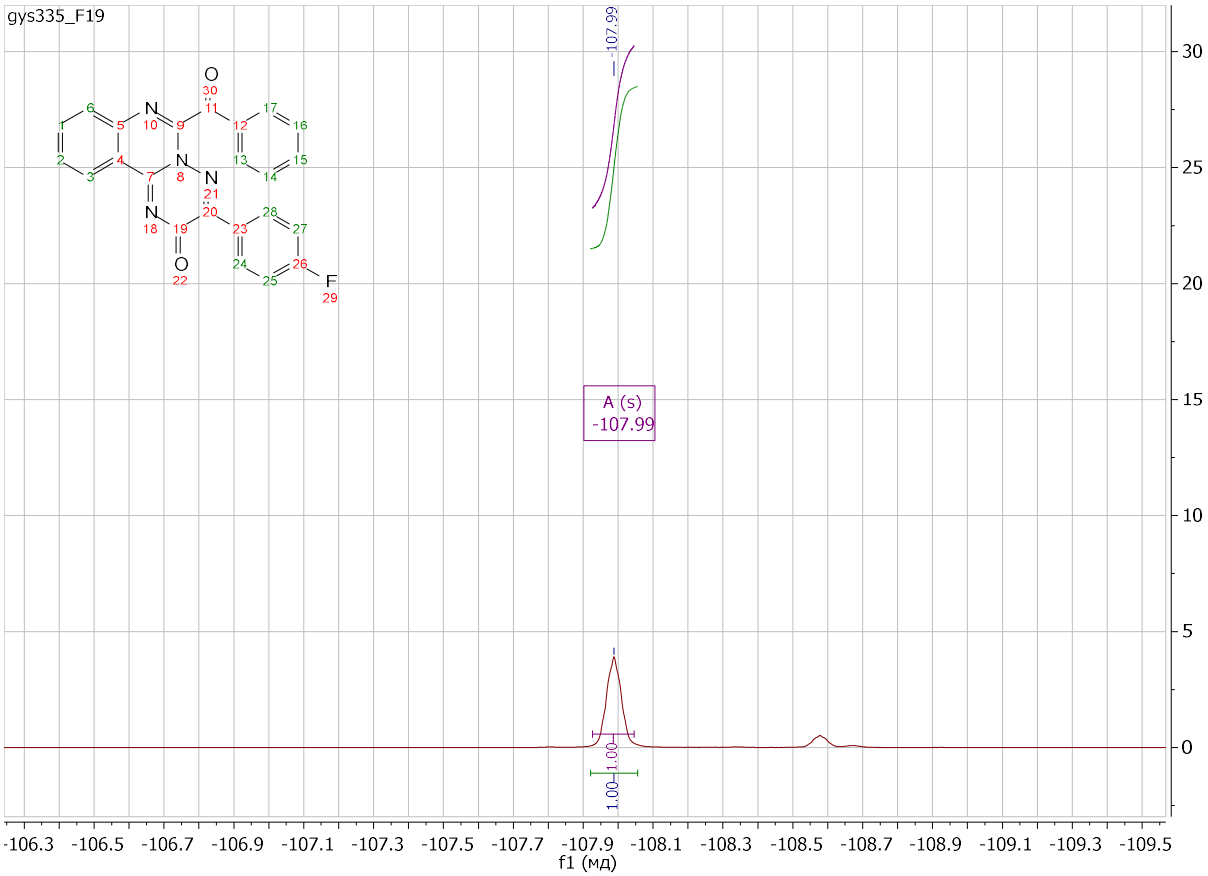


**Figure S20 :** $^{19}$F NMR spectrum of compound **4d**

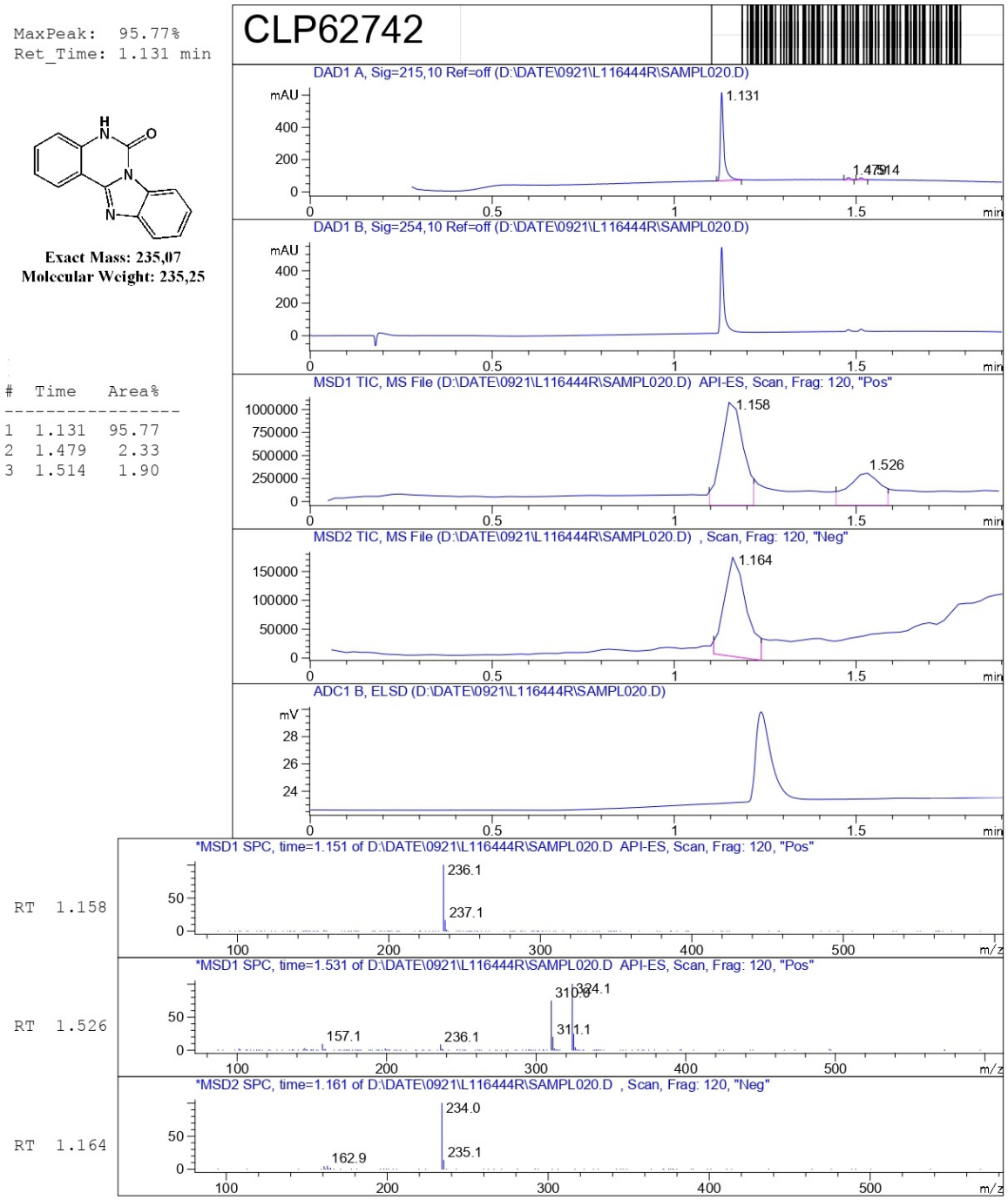


**Figure S21:** LC-MS spectrum of compound **5a** (Benzo[4,5]imidazo[1,2-*c*]quinazolin-6(5*H*)-one)

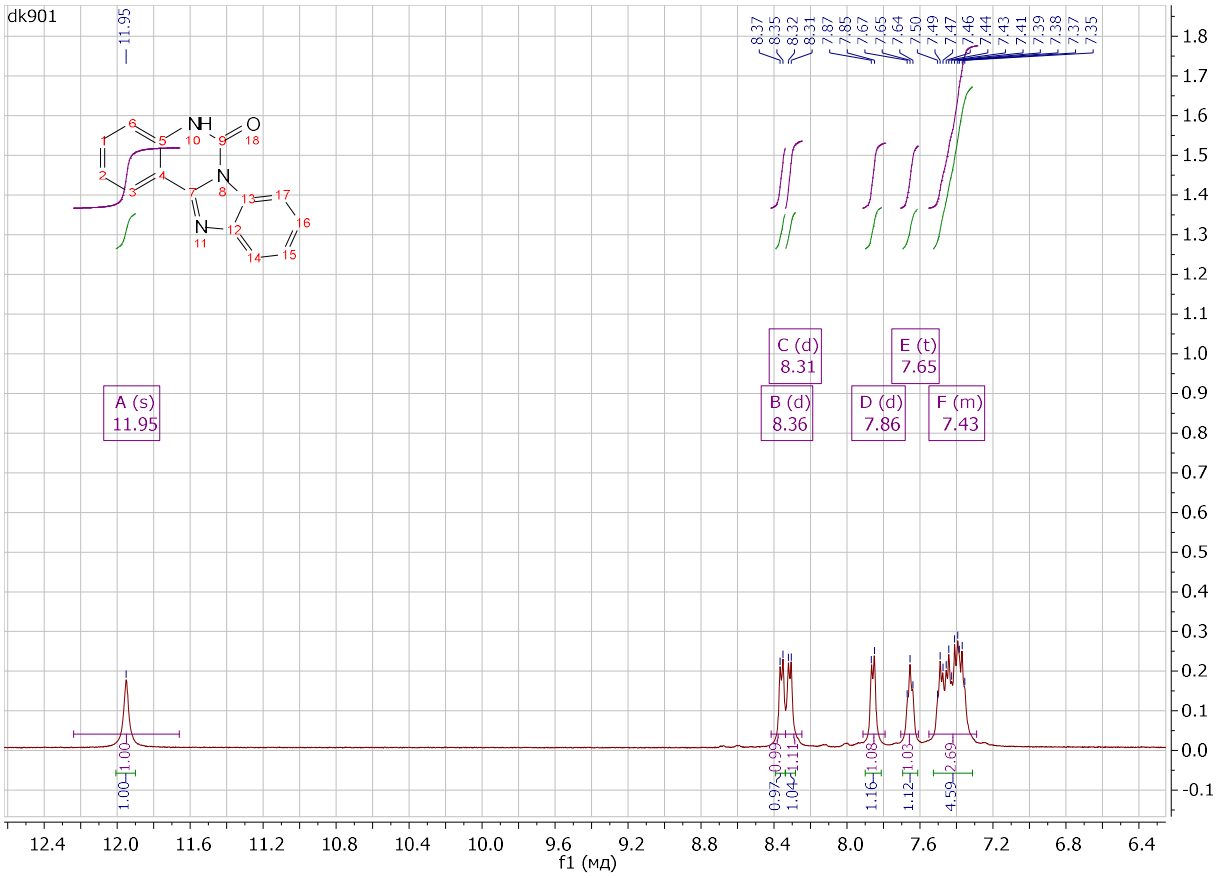


**Figure S22:** $^{1}$H NMR spectrum of compound **5a**

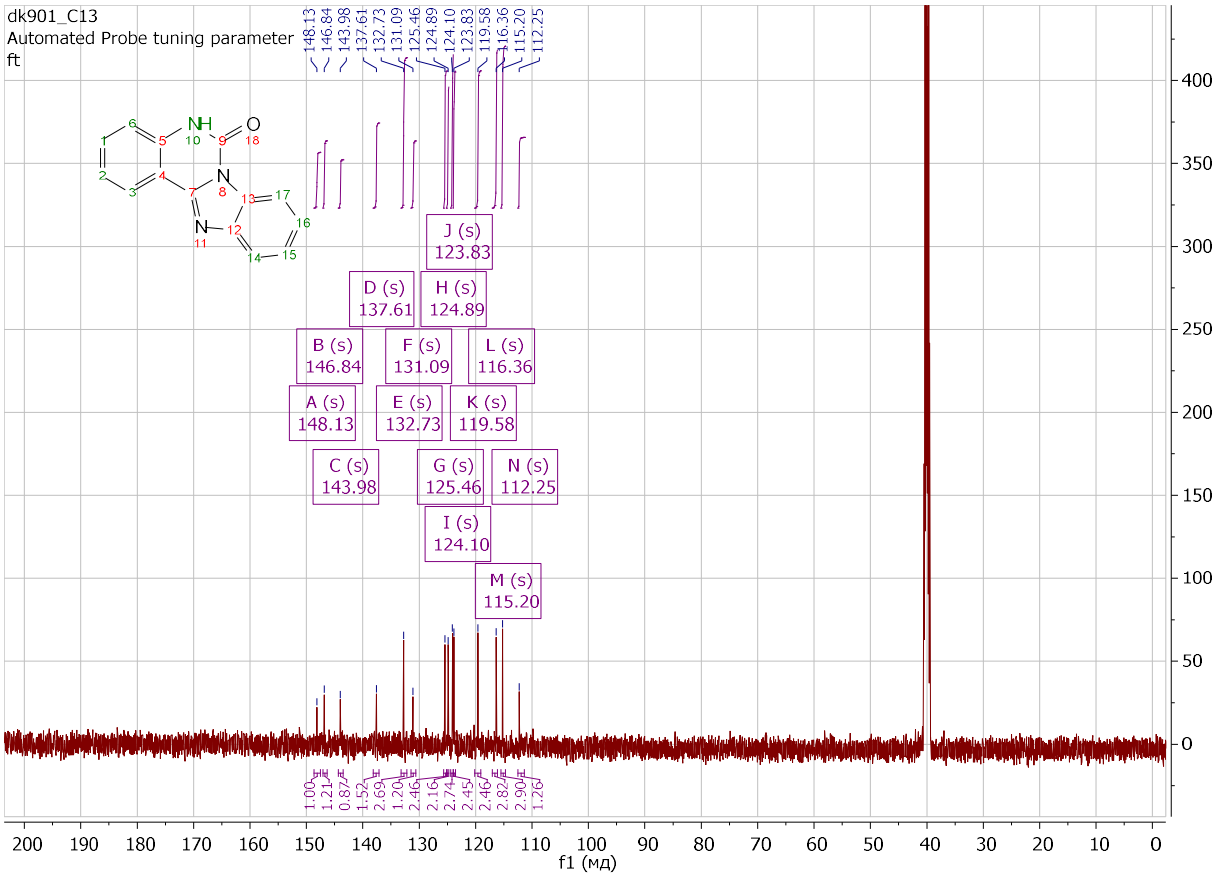


**Figure S23:** $^{13}$C NMR spectrum of compound **5a**

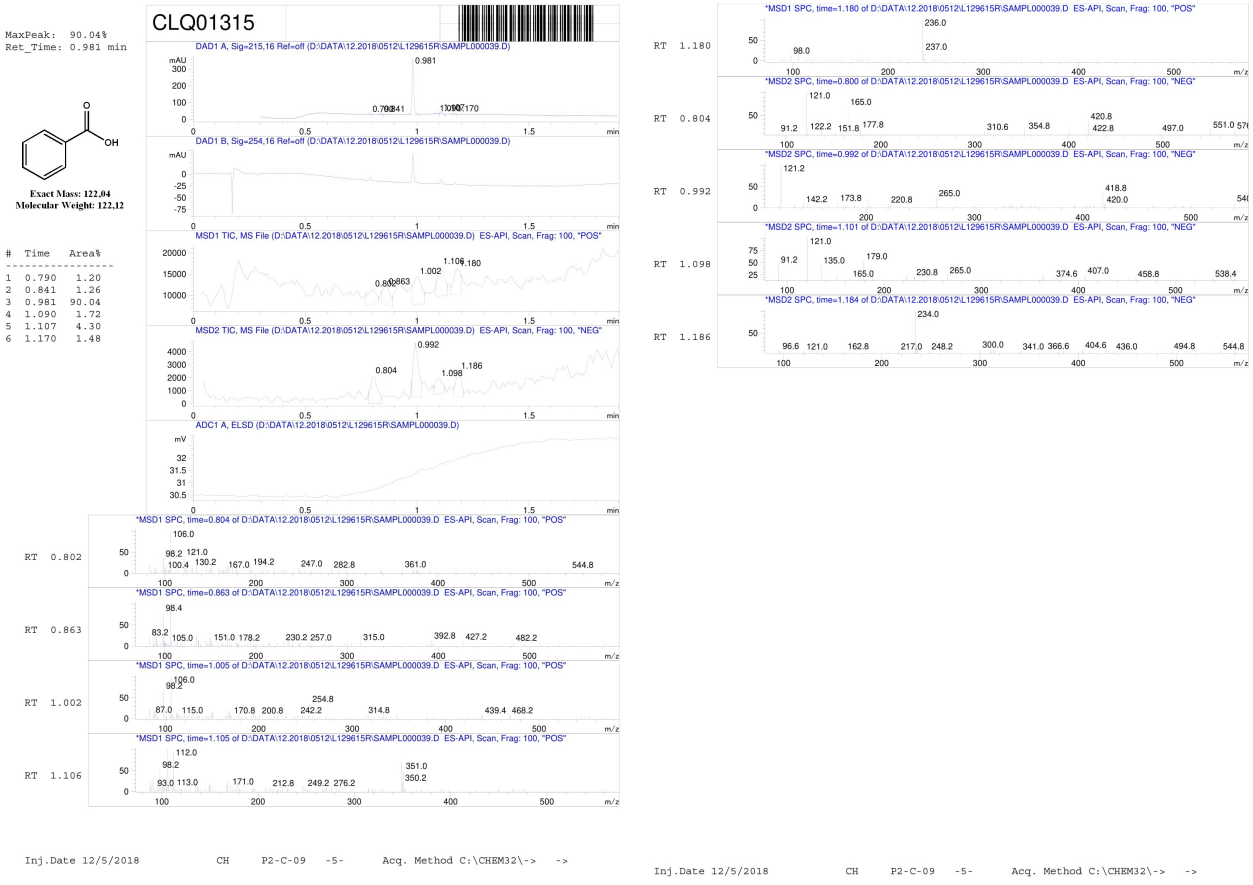


**Figure S24:** LC-MS spectrum of compound **6** (Benzoic acid)

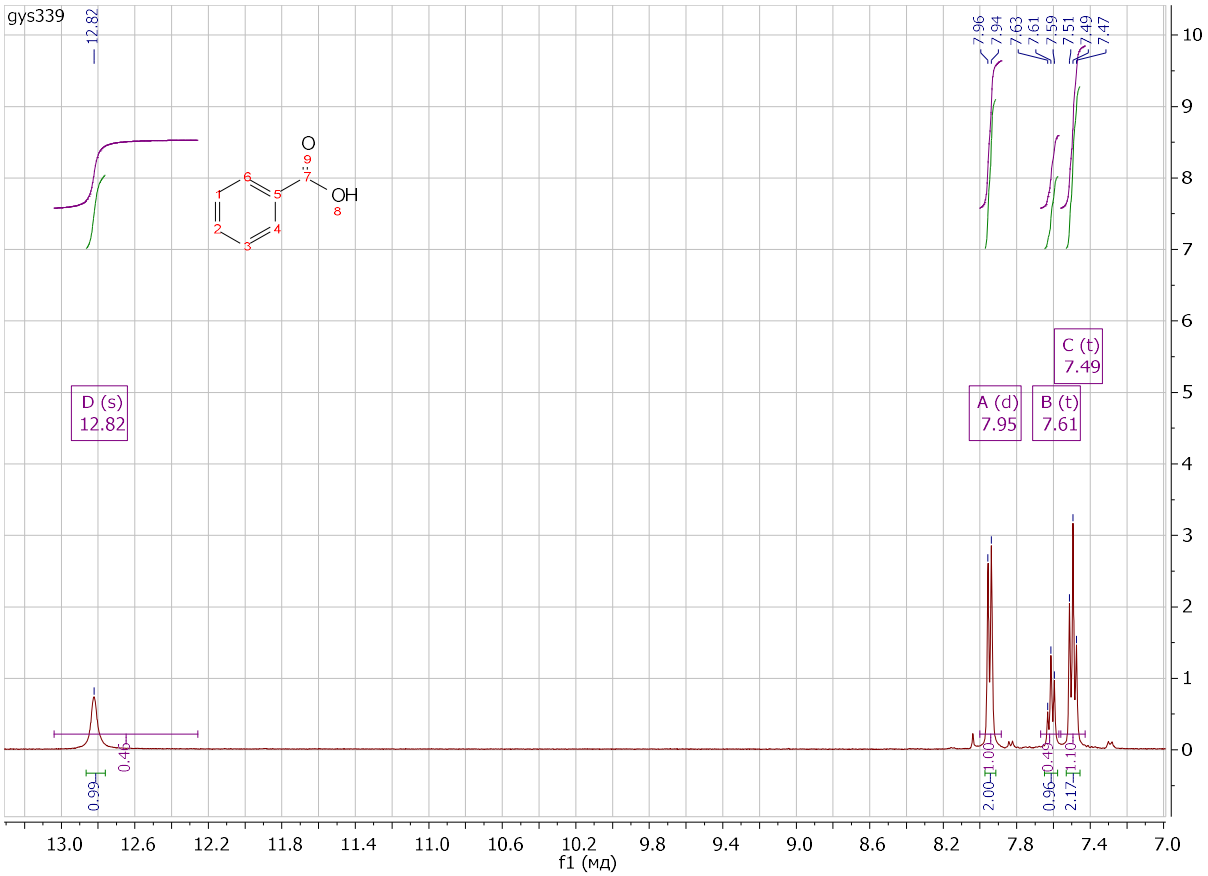


**Figure S25 :** $^{1}$H NMR spectrum of compound **6**

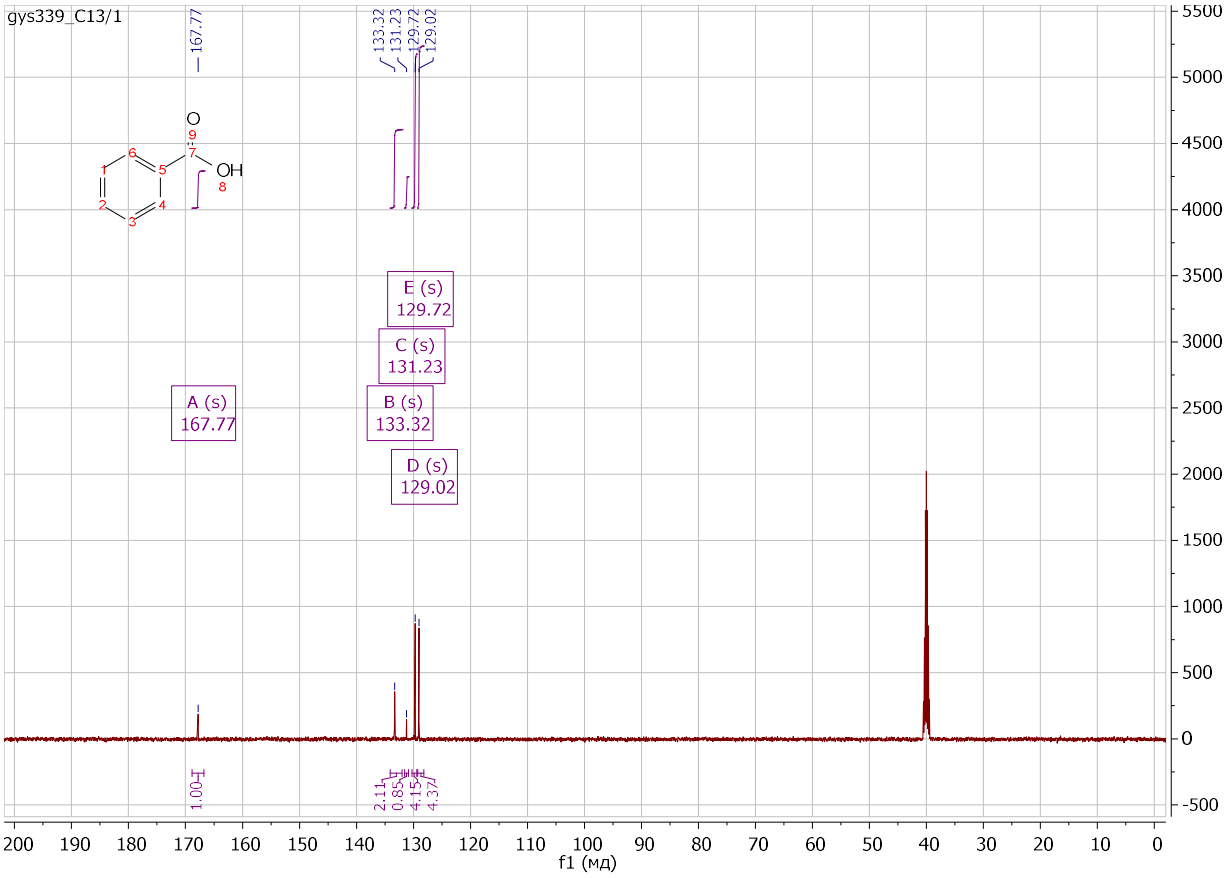


**Figure S26 :** $^{13}$C NMR spectrum of compound **6**