

Supporting Information

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Oxidation of some benzyl substituted fused quinazoline derivatives

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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 H₂O (75 mL) was added. The precipitate was filtered,^a washed thoroughly with H₂O 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 CrO₃ (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 Na₂SO₃ (2.8 mmol) in ice-water (100 mL). The residue was filtered,^c washed thoroughly with H₂O and dried at 60 °C. The resulting material was purified to obtain the products (silica gel column chromatography EtOAc-CHCl₃-PE (6:2:2) **4a**^d and **4b**. Crystallization from DMF-H₂O afforded **4c** and **4d**).

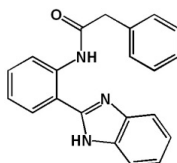
^aIn the case of amines **1c-d**, the crude product was extracted with EtOAc (3×100 mL), washed with brine, dried over Na₂SO₄, and concentrated under reduced pressure.

^bAfter crystallization from DMF-H₂O, 97.1% pure **3a**, according to LC-MS analysis, was obtained.

^cBenzoic acid **6** was isolated from the filtrate by acid-base extraction with ether and crystallized from water.

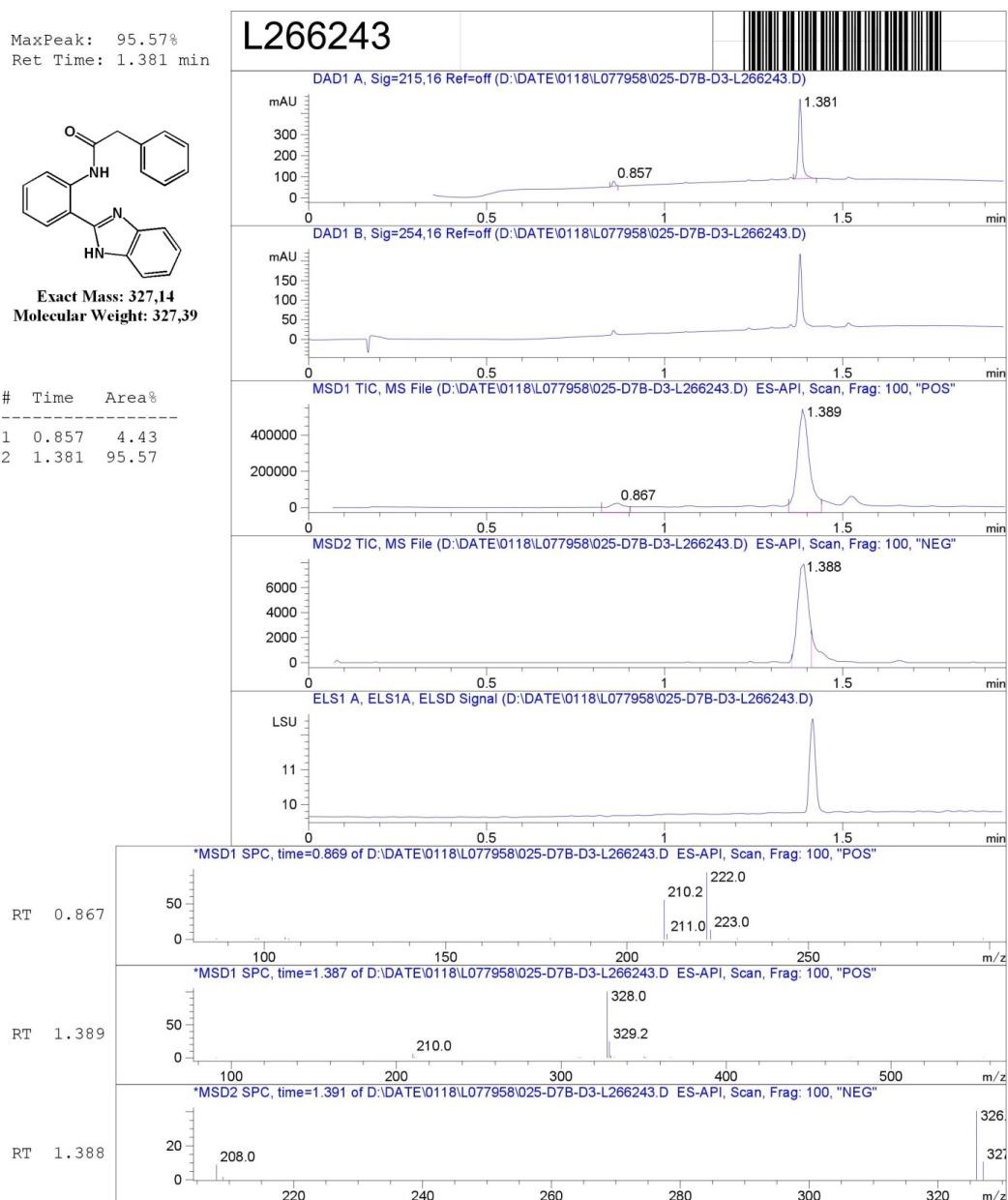
^dThe resulting material was triturated in acetone to provide quinazolinone **5a**. The filtrate contained ketone **4a** and a small impurity of quinazolinone **5a**. This solution was used for chromatography.

MaxPeak: 95.57%
Ret Time: 1.381 min



Exact Mass: 327.14
Molecular Weight: 327.39

#	Time	Area%
1	0.857	4.43
2	1.381	95.57



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

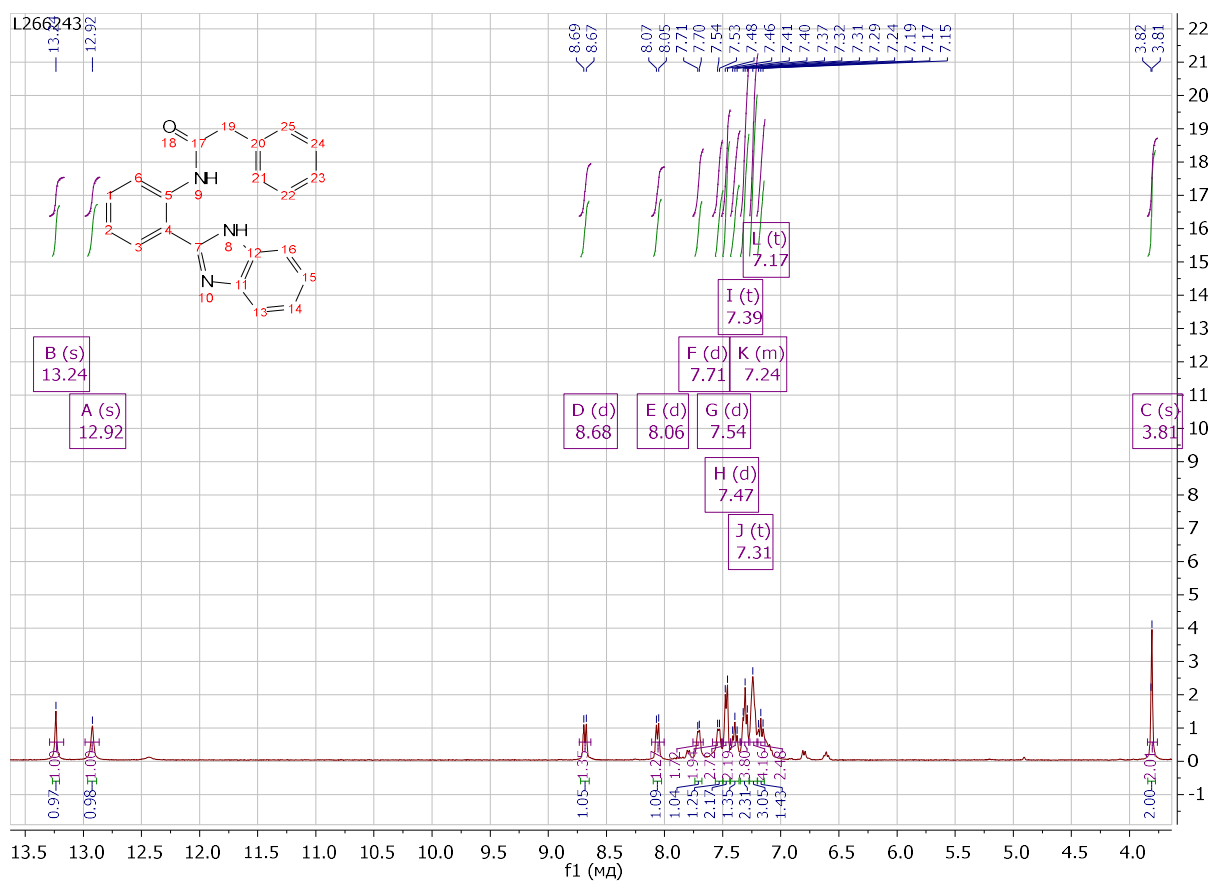


Figure S2 : ¹H NMR spectrum of compound 2a

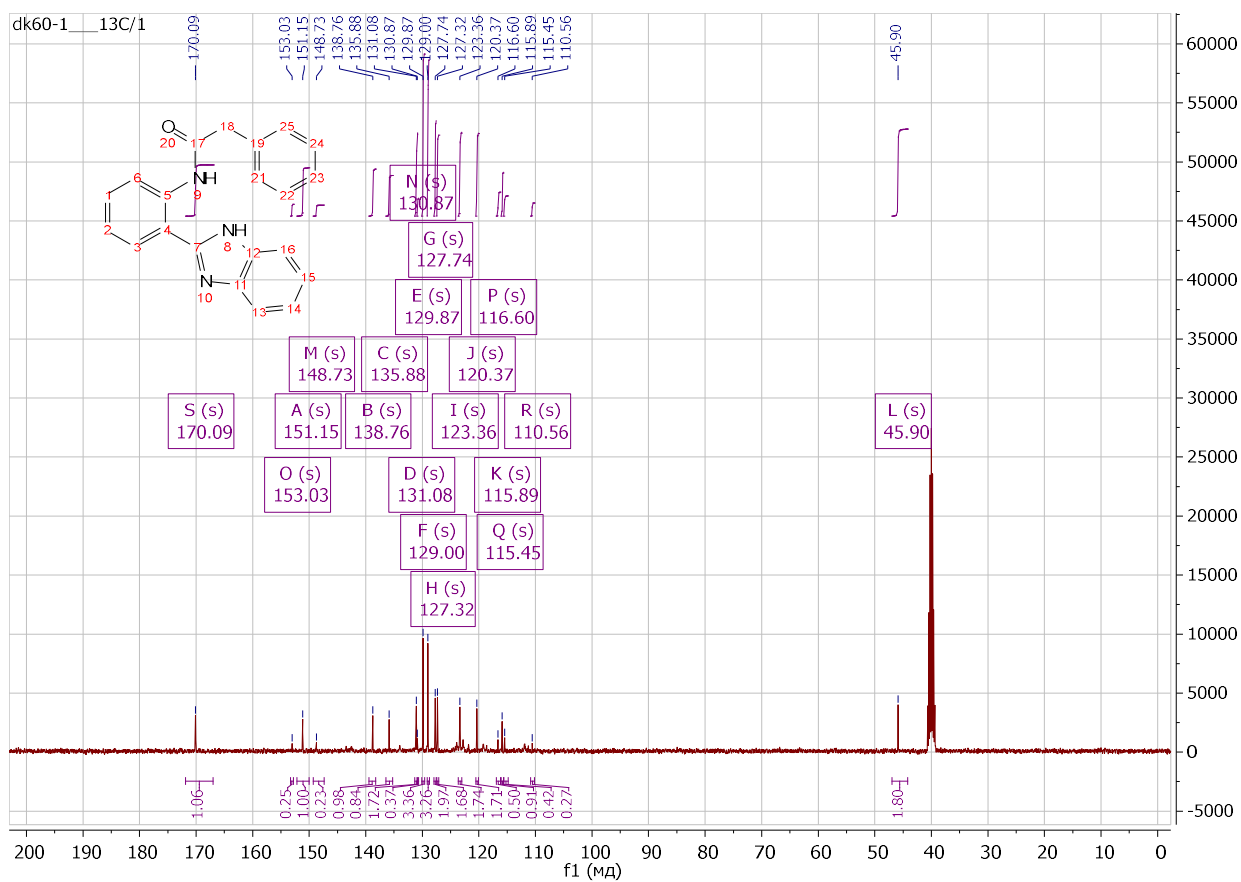
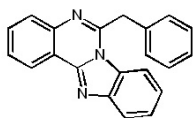


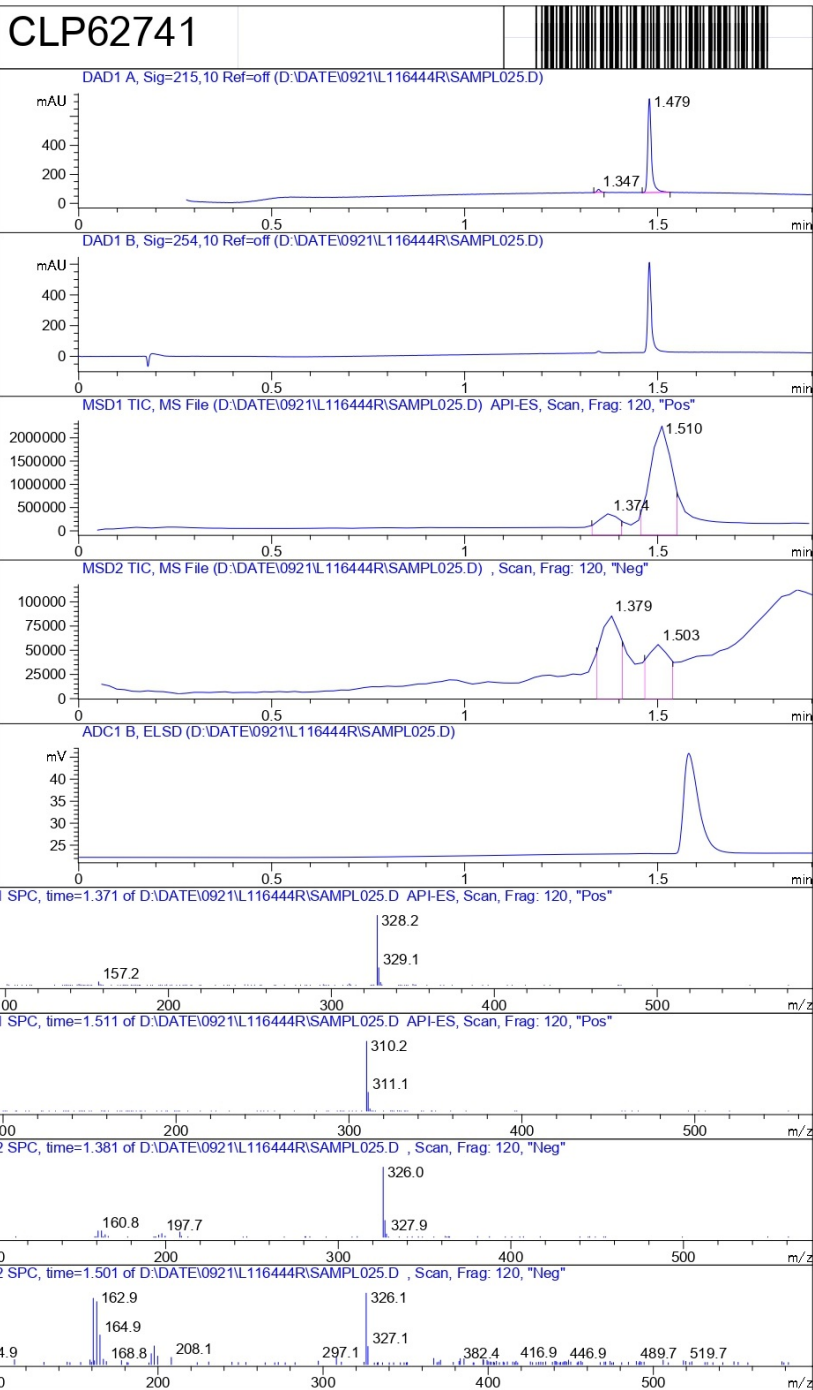
Figure S3: ^{13}C NMR spectrum of compound 2a

MaxPeak: 97.17%
Ret_Time: 1.479 min



Exact Mass: 309,13
Molecular Weight: 309,37

#	Time	Area%
1	1.347	2.83
2	1.479	97.17



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

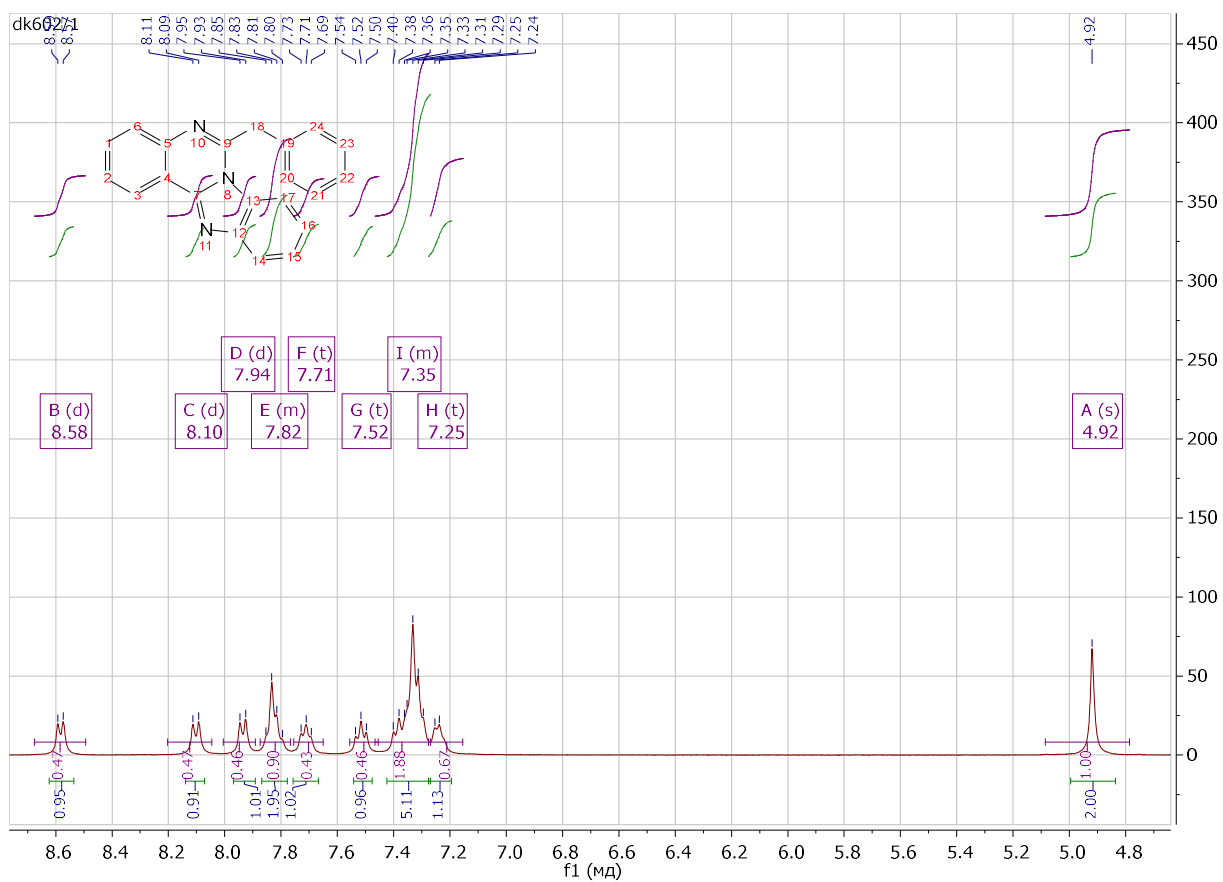


Figure S5 : ^1H NMR spectrum of compound **3a**

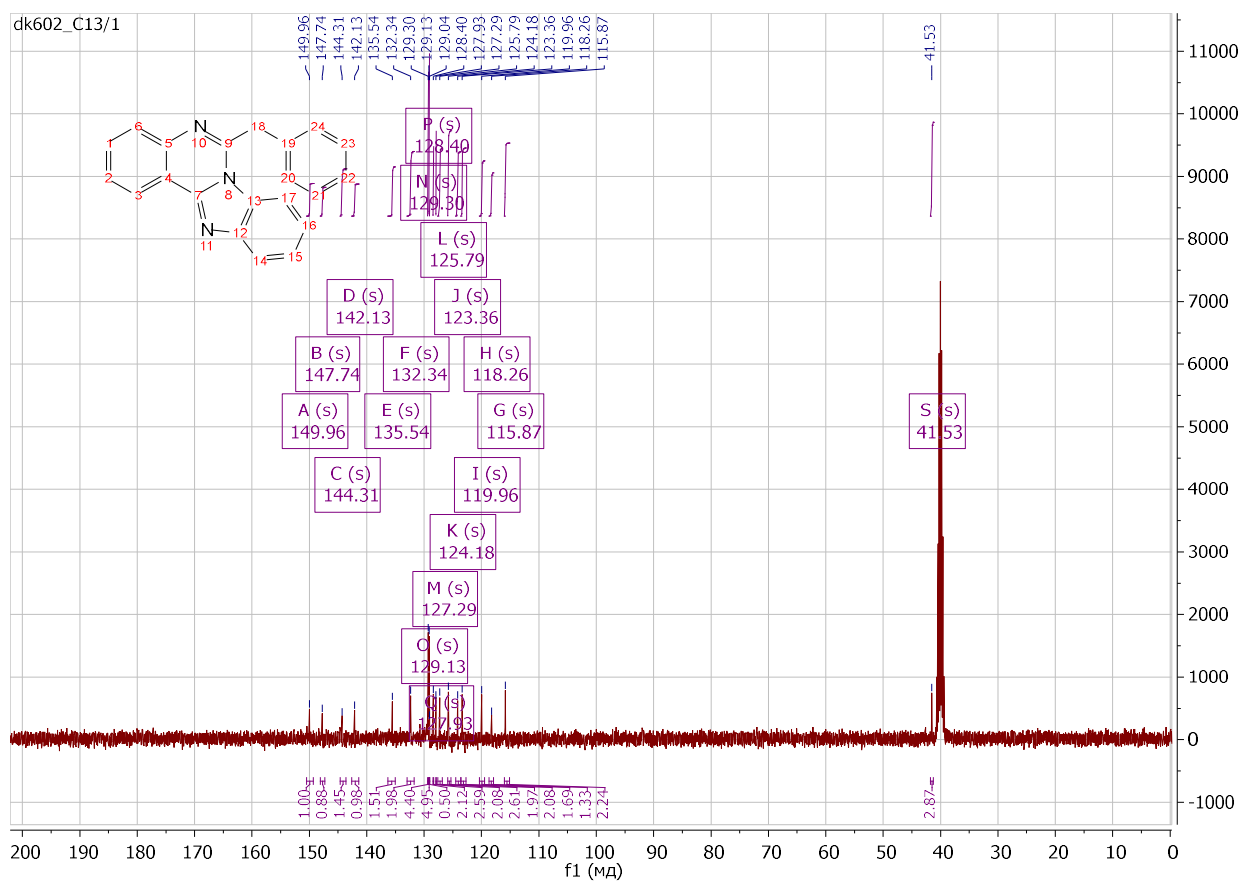
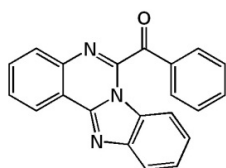


Figure S6 : ^{13}C NMR spectrum of compound 3a

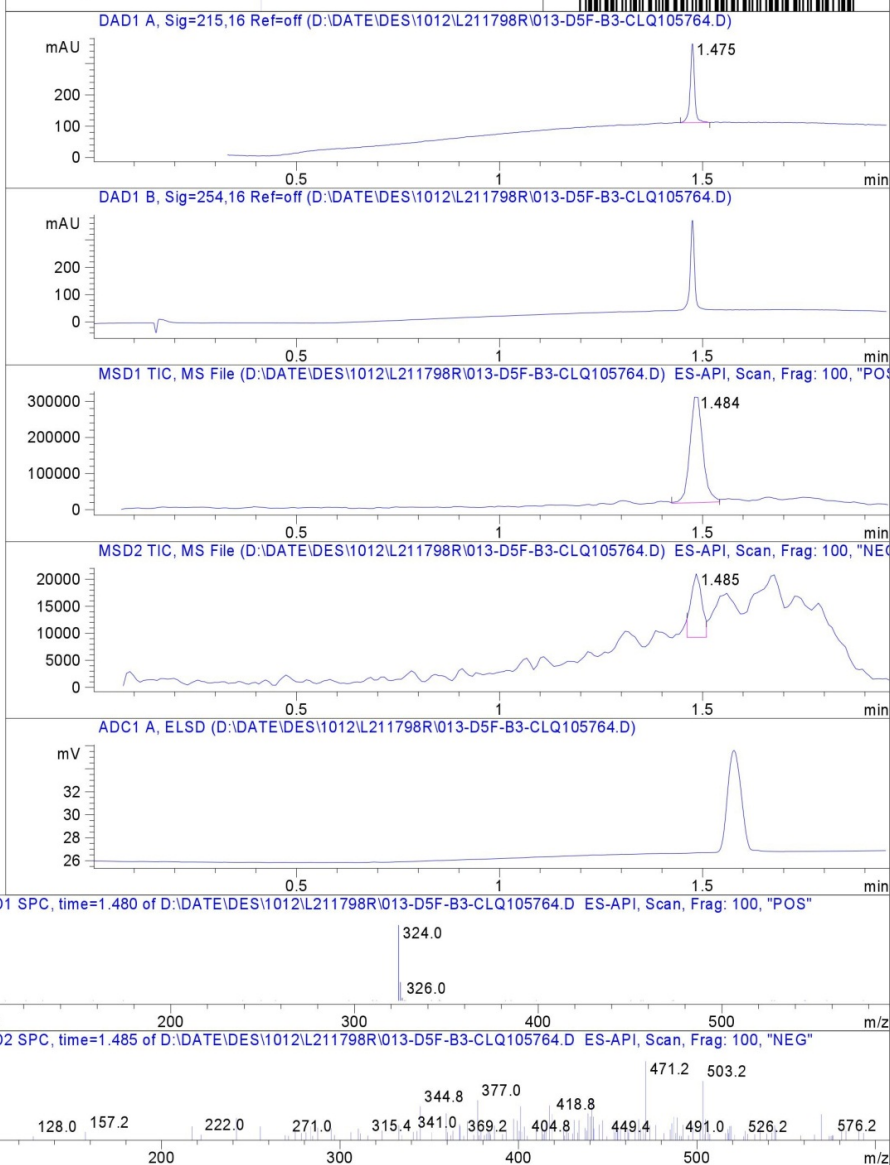
MaxPeak: 100.00%
Ret_Time: 1.475 min



Exact Mass: 323,11
Molecular Weight: 323,36

#	Time	Area%
1	1.475	100.00

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

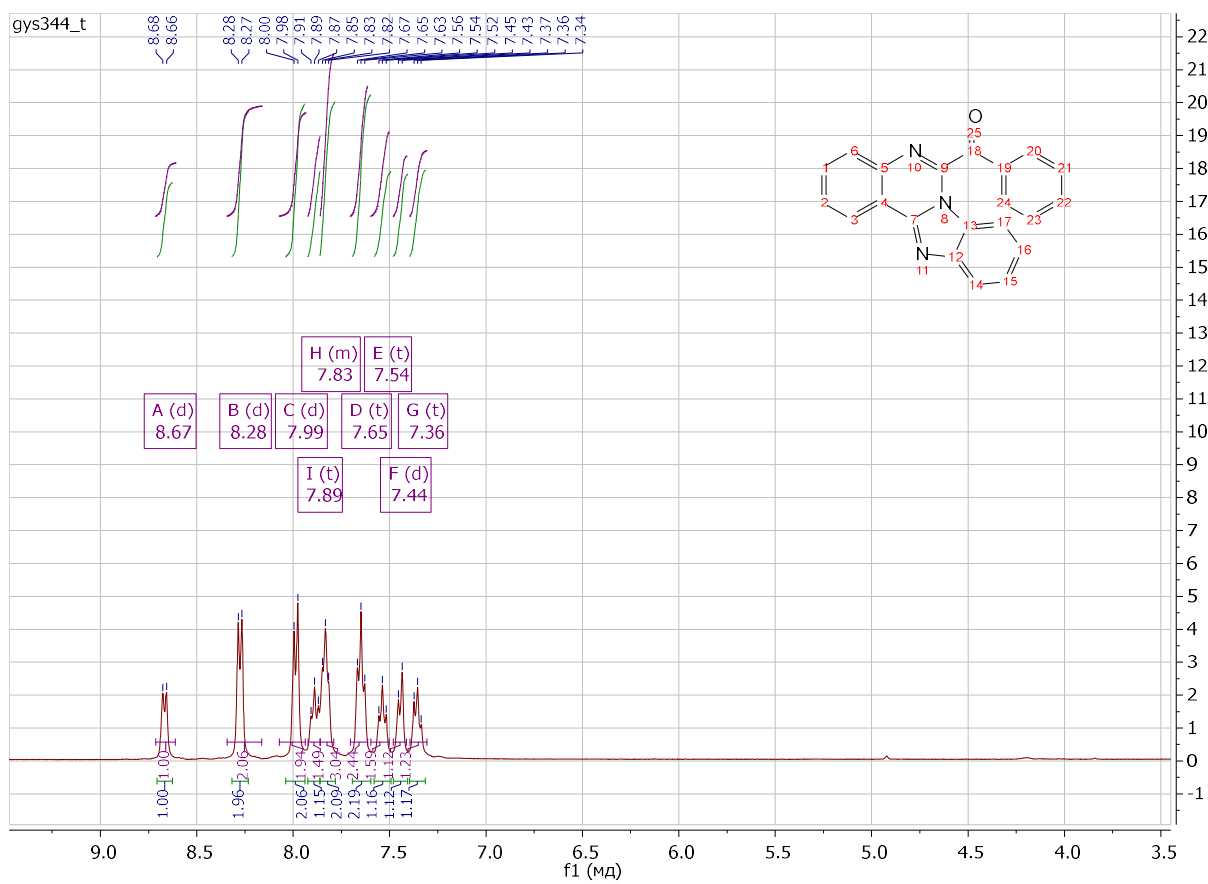


Figure S8 : ^1H NMR spectrum of compound 4a

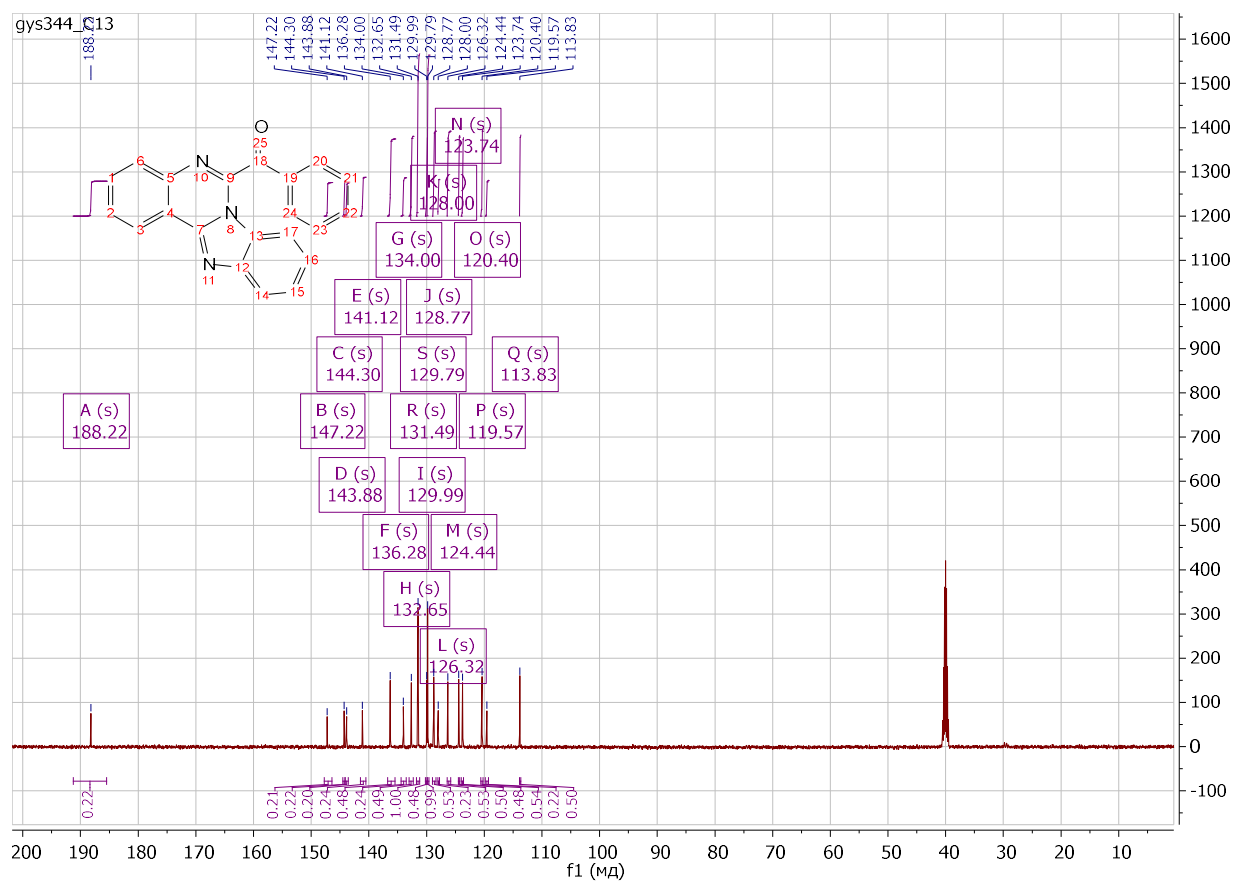
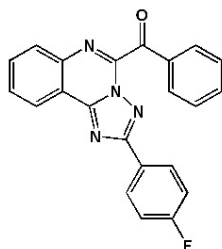


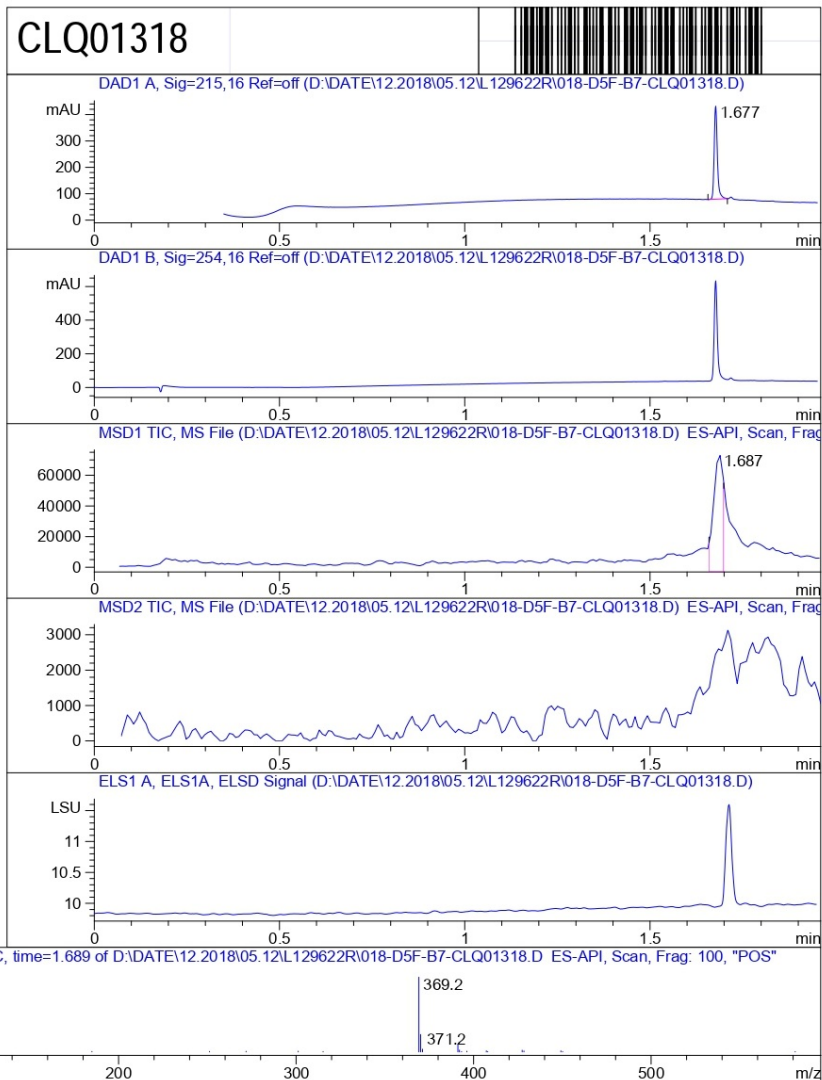
Figure S9 : ^{13}C NMR spectrum of compound 4a

MaxPeak: 100.00%
Ret_Time: 1.677 min



Exact Mass: 368,11
Molecular Weight: 368,37

#	Time	Area%
1	1.677	100.00



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

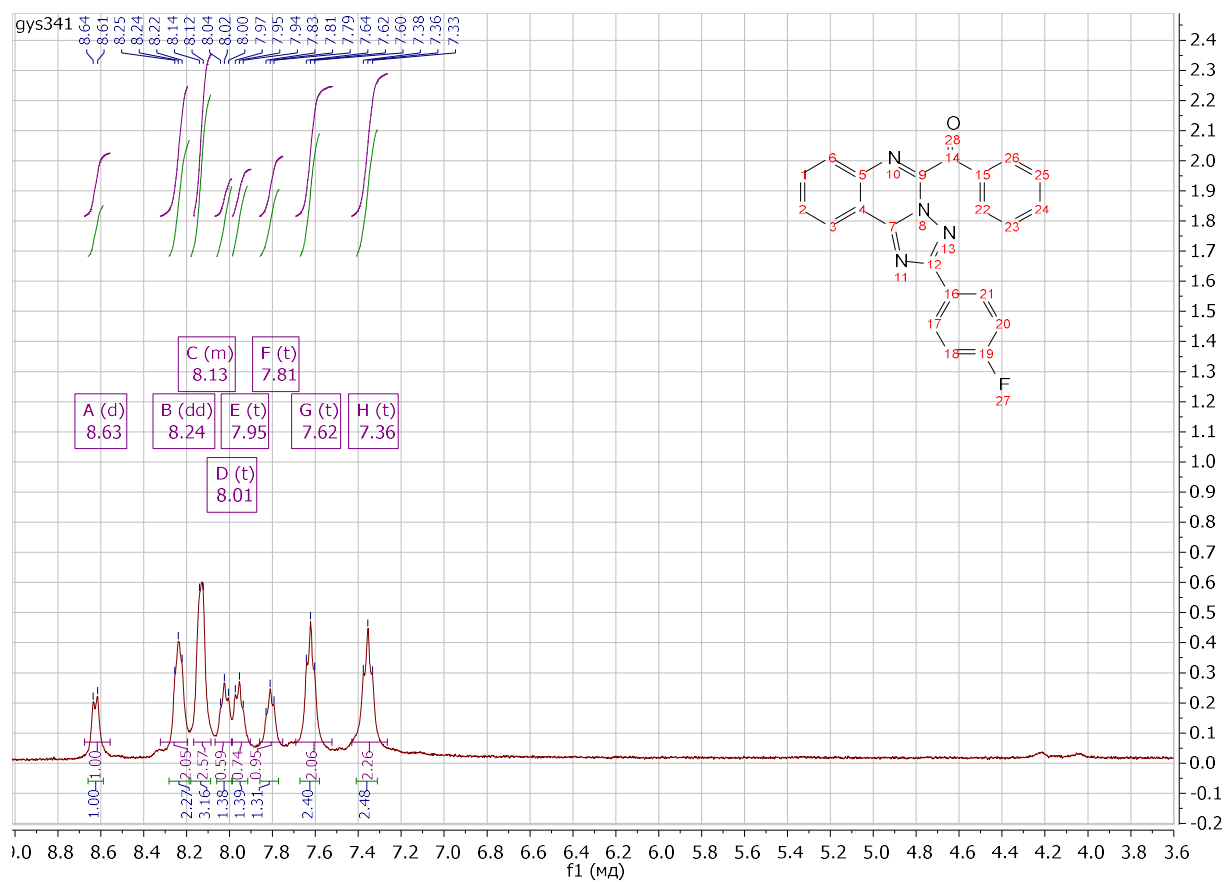


Figure S11 : ^1H NMR spectrum of compound 4b

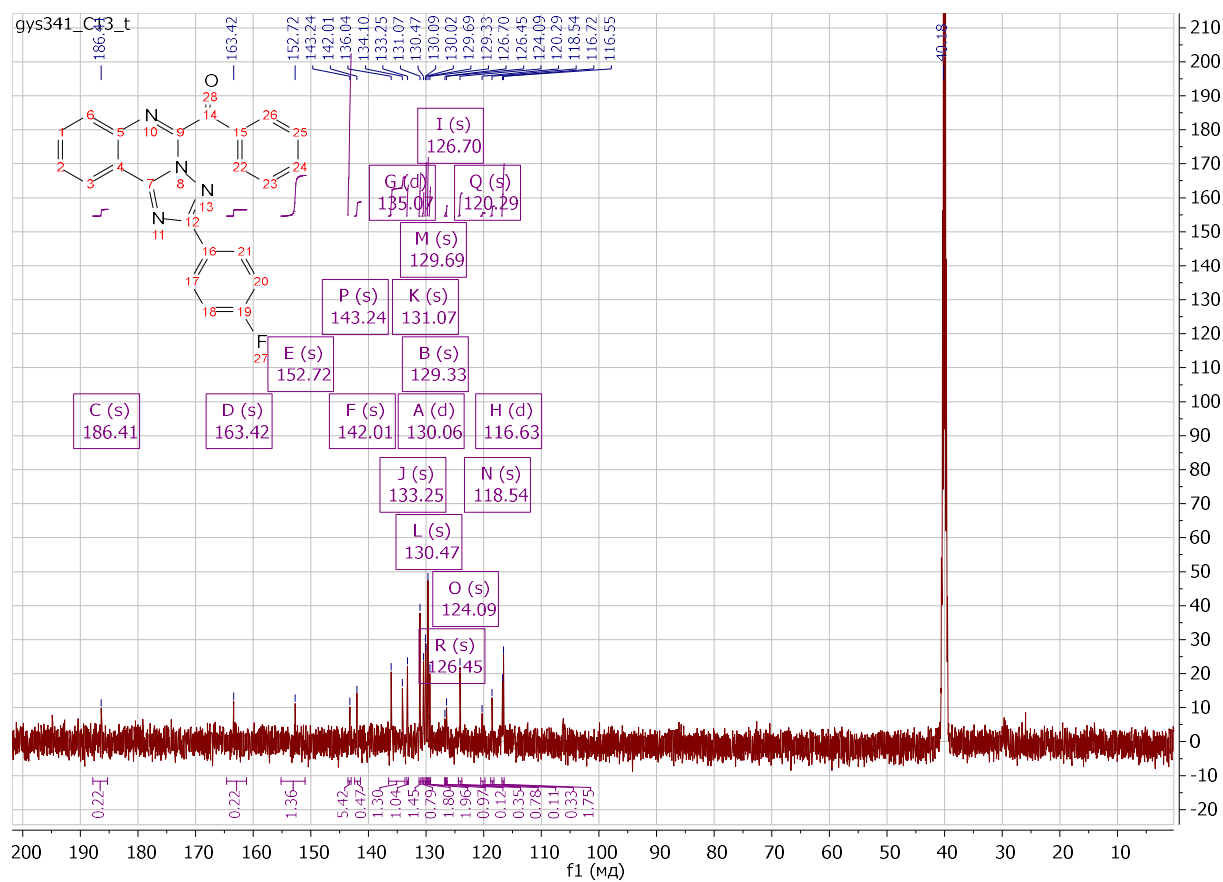
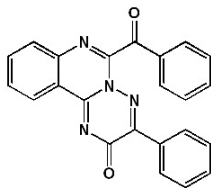


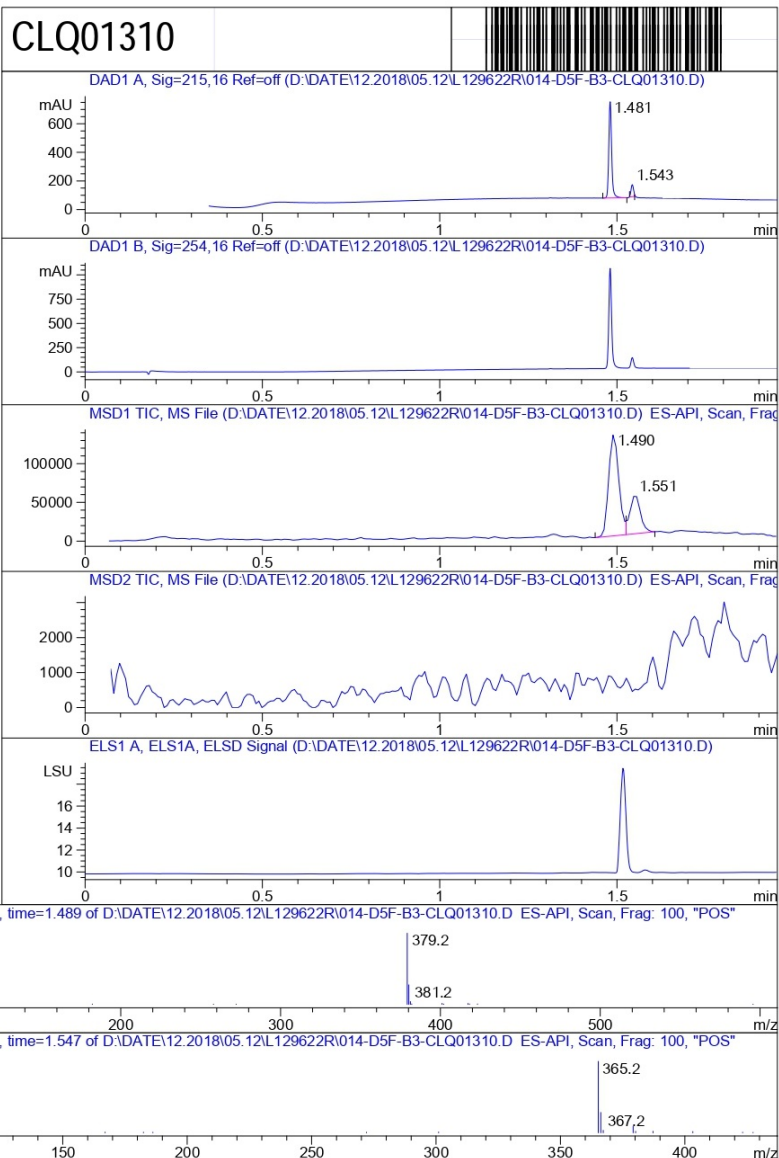
Figure S12 : ^{13}C NMR spectrum of compound 4b

MaxPeak: 90.22%
Ret_Time: 1.481 min



Exact Mass: 378.11
Molecular Weight: 378.39

#	Time	Area%
1	1.481	90.22
2	1.543	9.78



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

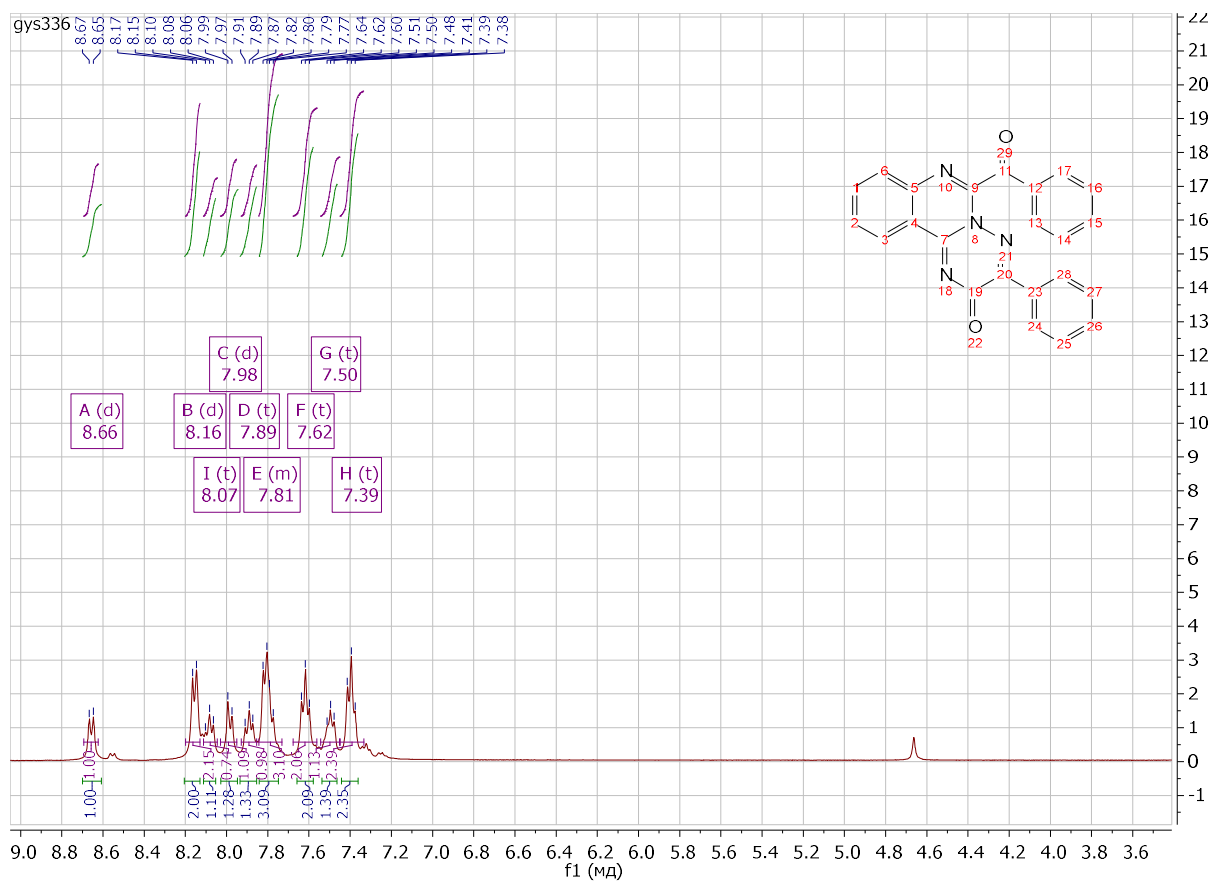


Figure S15 : ^1H NMR spectrum of compound 4c

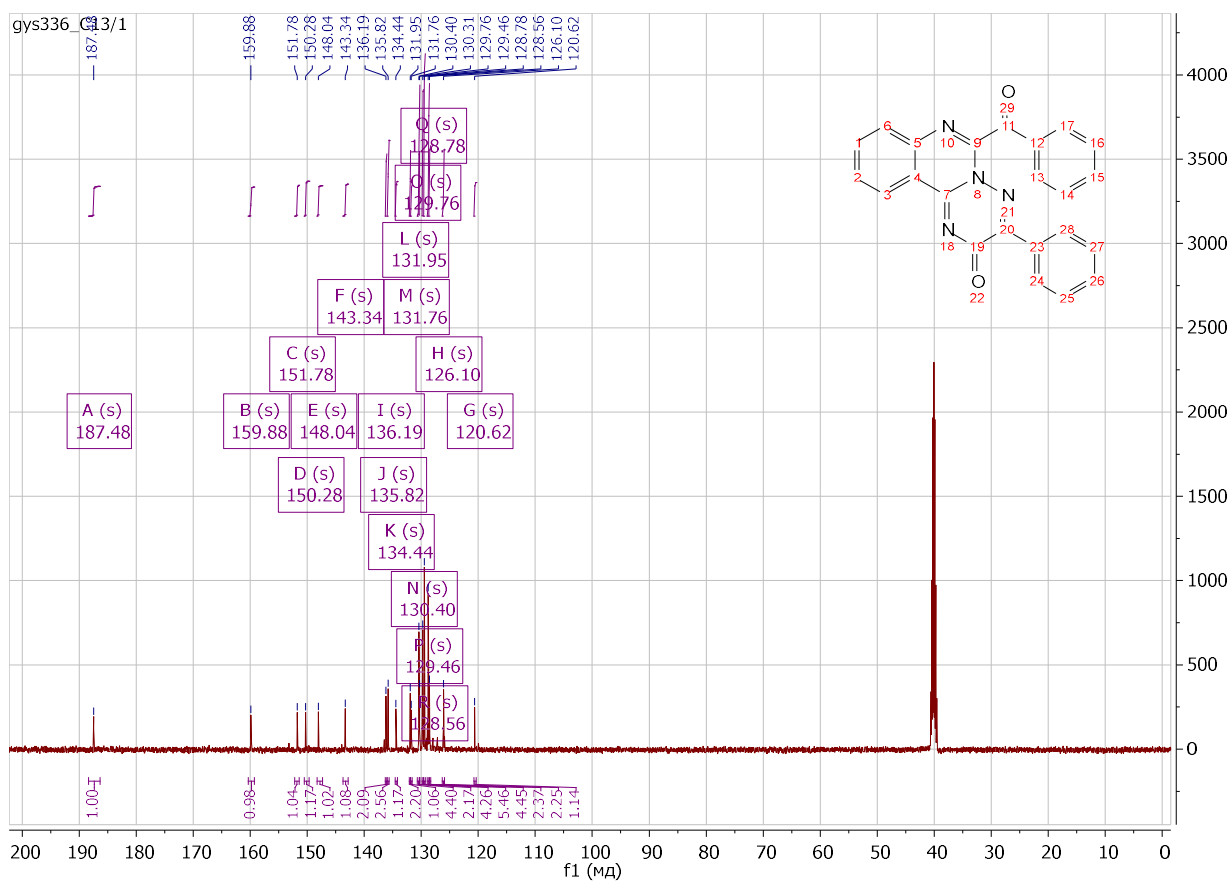
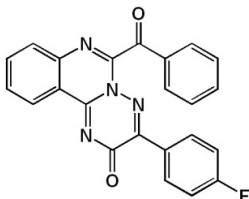


Figure S16: ^{13}C NMR spectrum of compound 4c

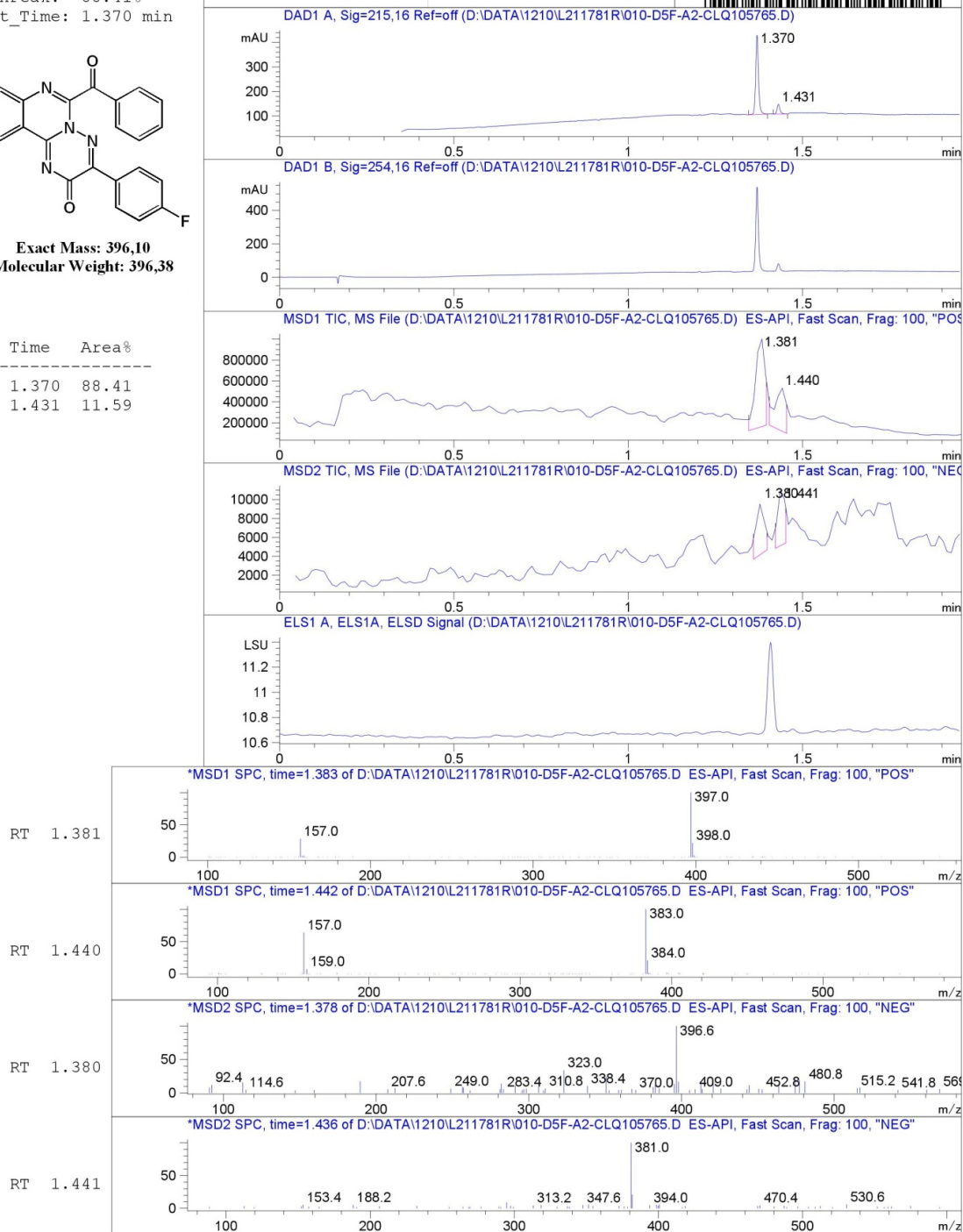
MaxPeak: 88.41%
Ret_Time: 1.370 min



Exact Mass: 396,10
Molecular Weight: 396,38

#	Time	Area%
1	1.370	88.41
2	1.431	11.59

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

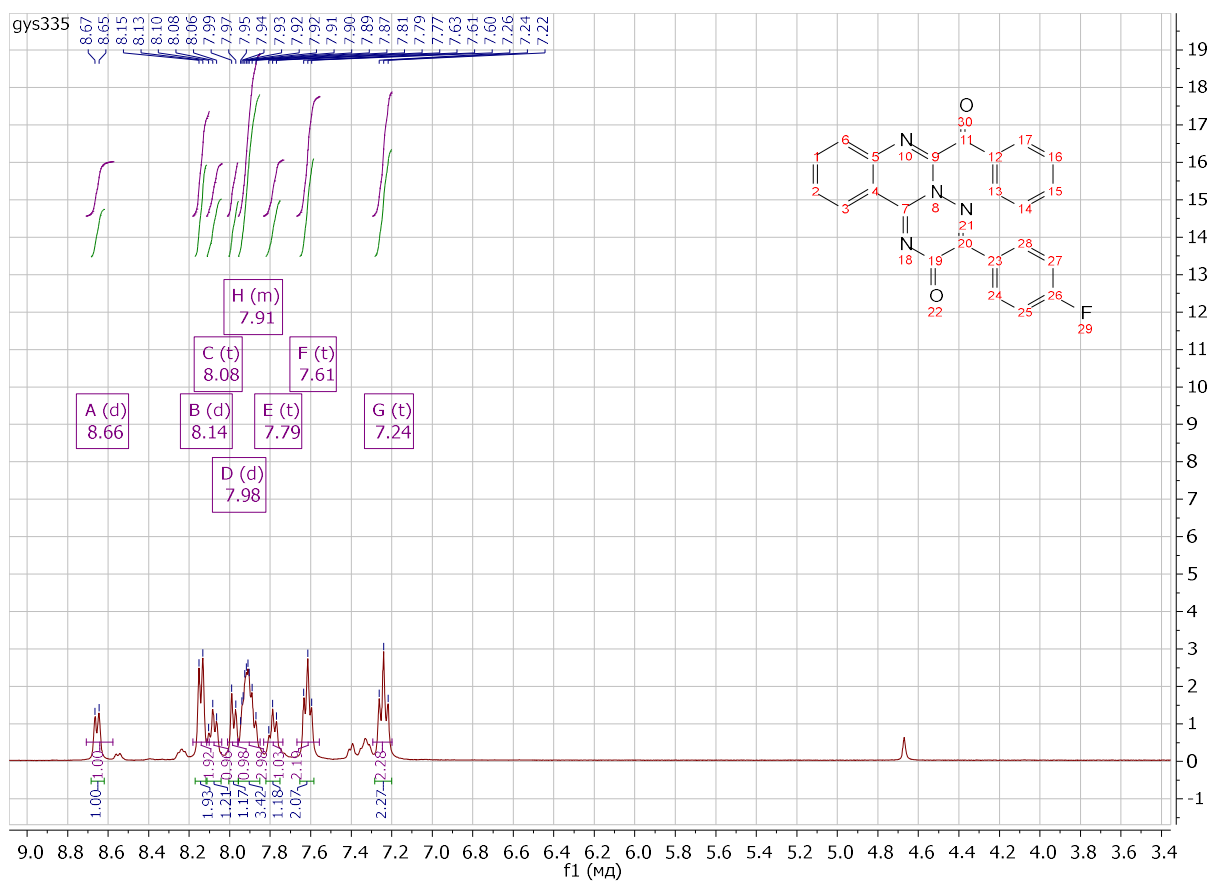


Figure S18 : ^1H NMR spectrum of compound **4d**

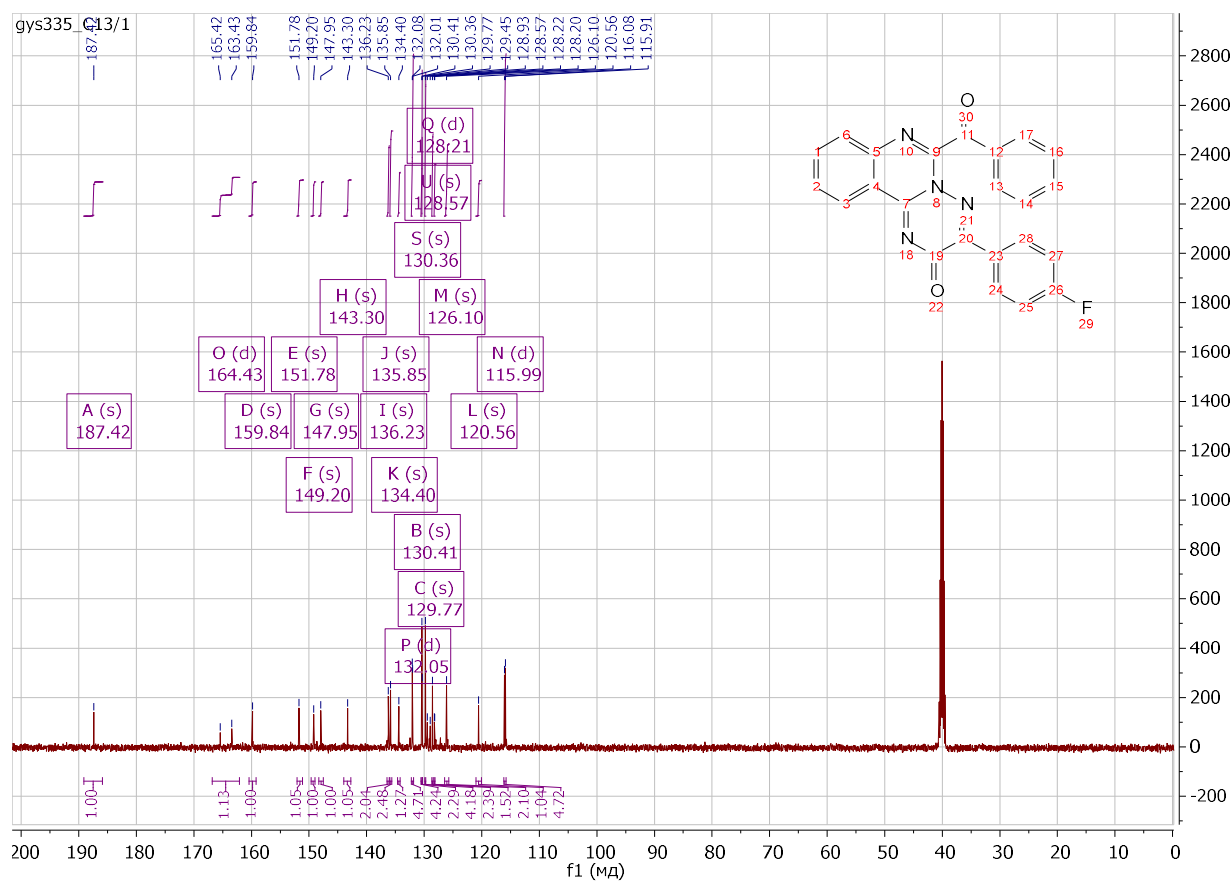


Figure S19 : ^{13}C NMR spectrum of compound 4d

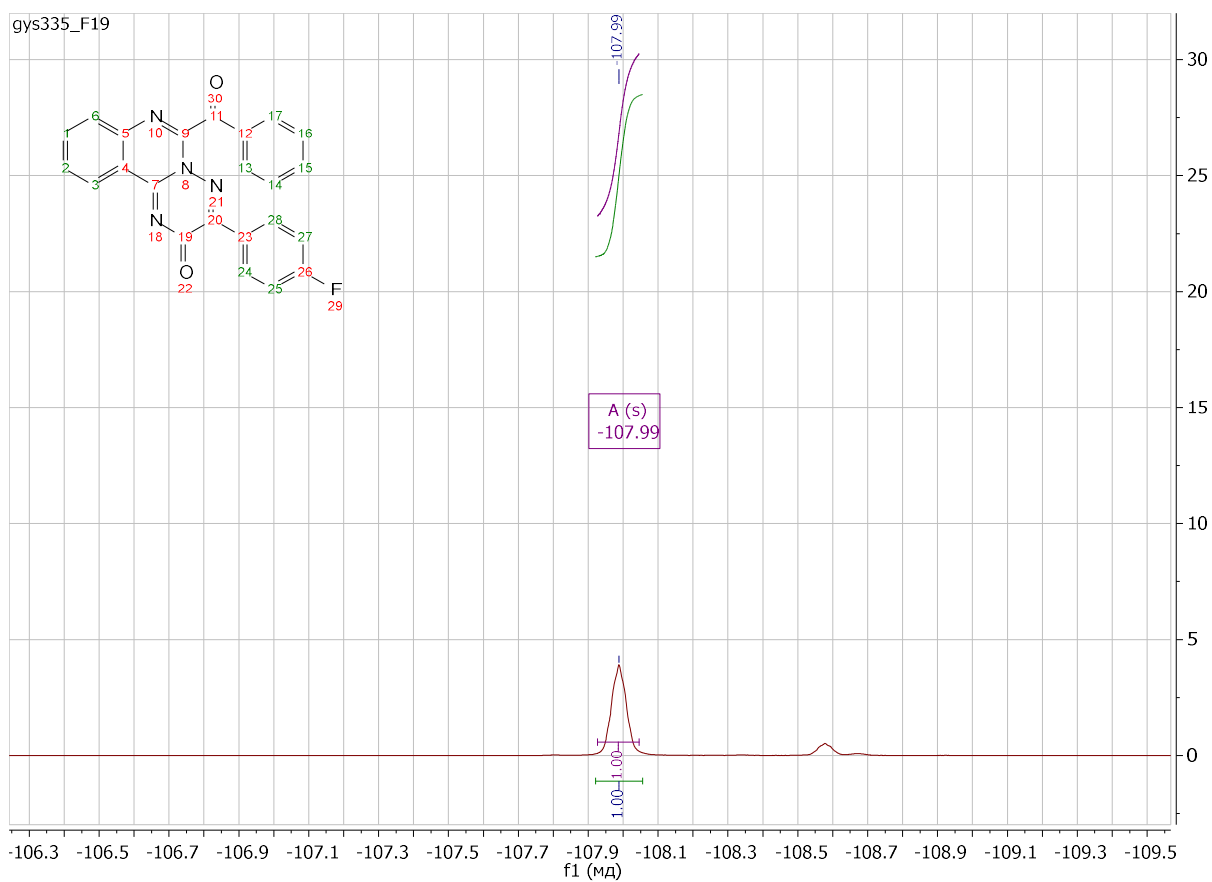
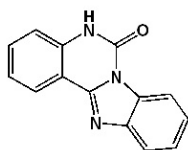


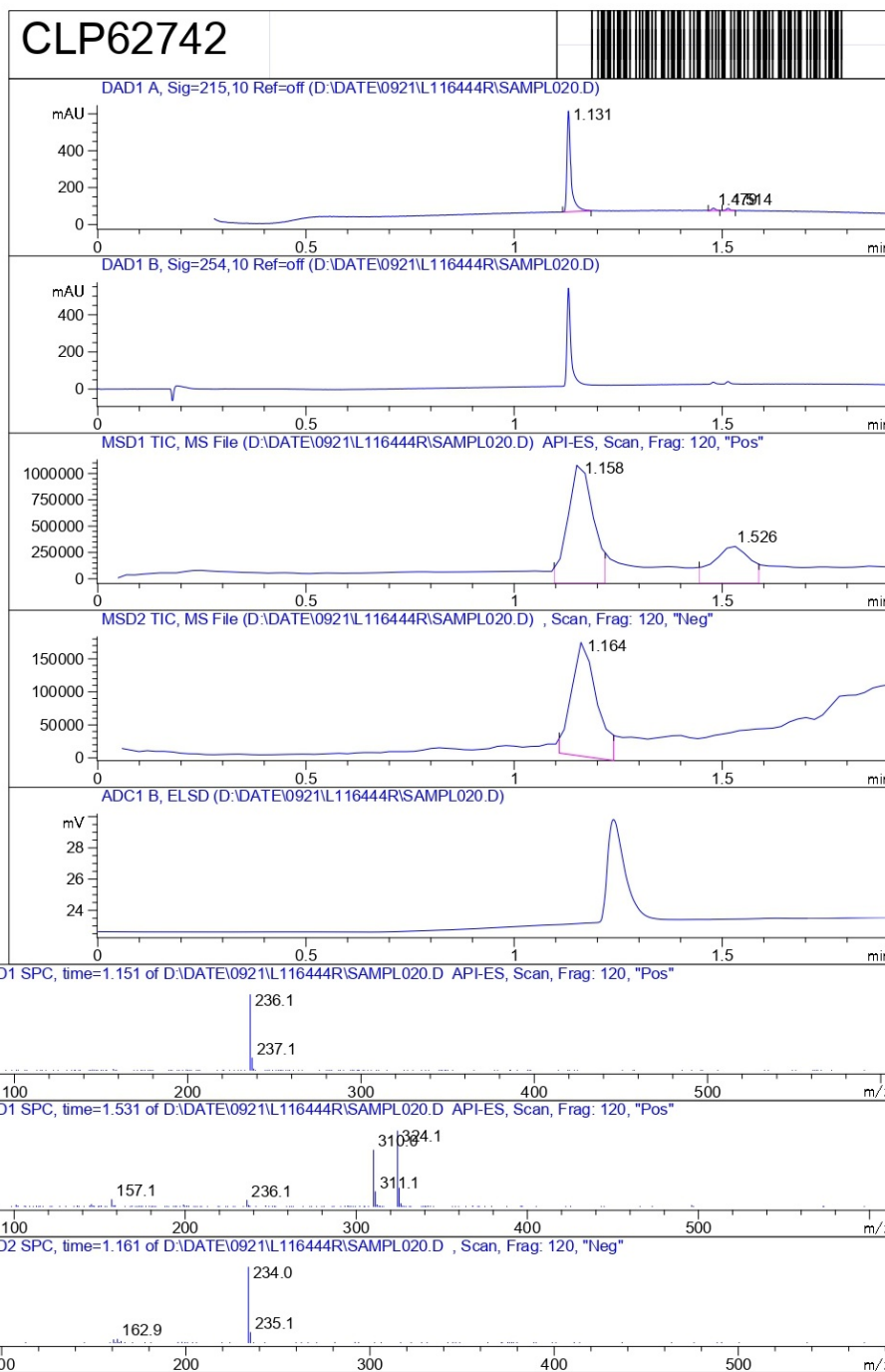
Figure S20 : ^{19}F NMR spectrum of compound **4d**

MaxPeak: 95.77%
Ret_Time: 1.131 min



Exact Mass: 235,07
Molecular Weight: 235,25

#	Time	Area%
1	1.131	95.77
2	1.479	2.33
3	1.514	1.90



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

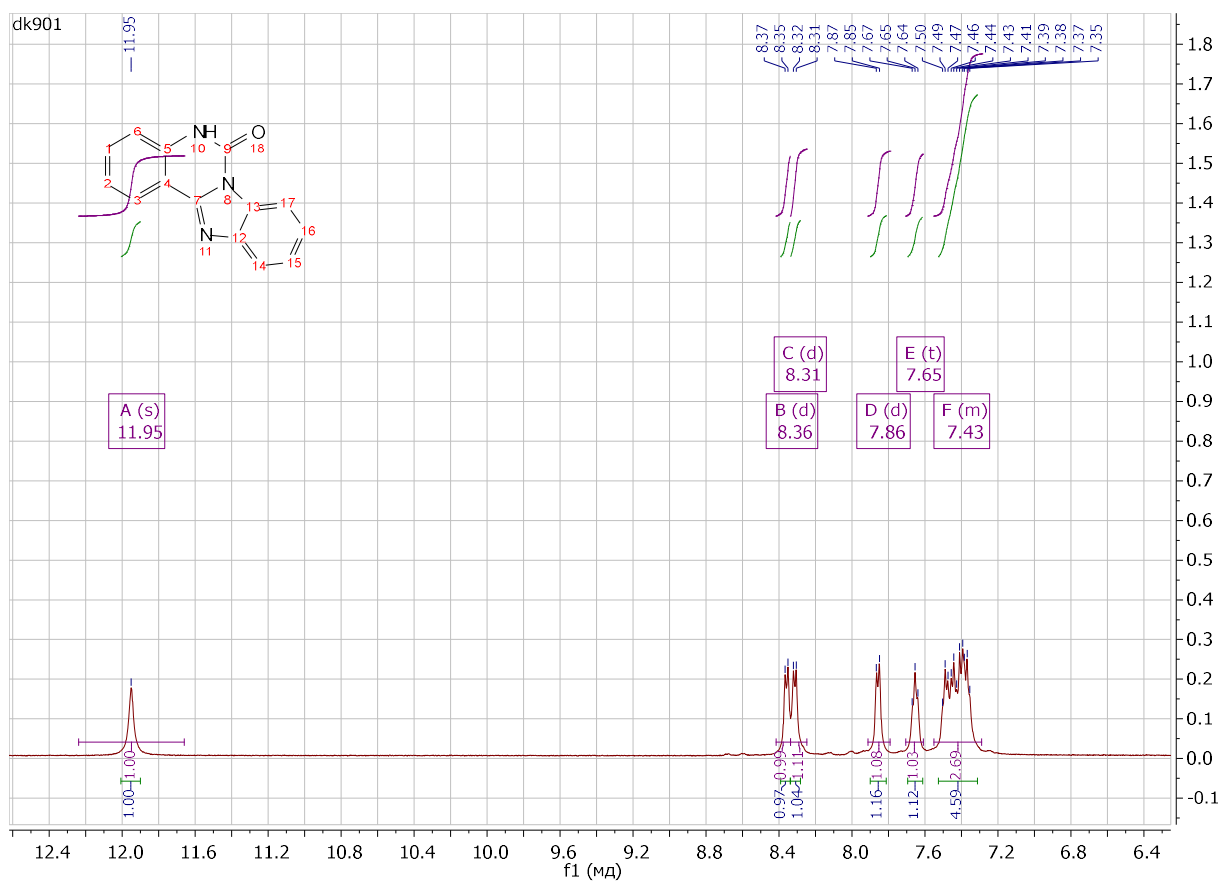


Figure S22: ^1H NMR spectrum of compound 5a

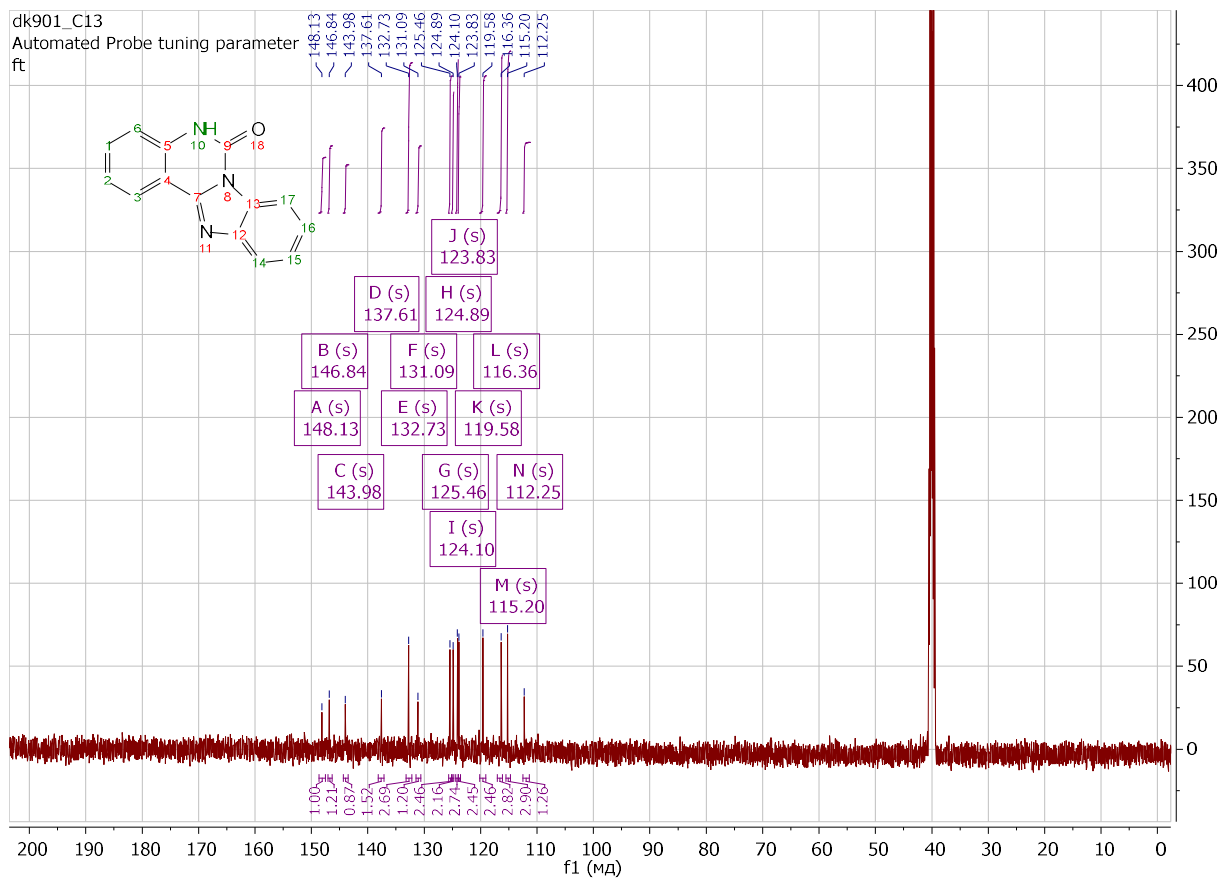
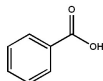


Figure S23: ^{13}C NMR spectrum of compound 5a

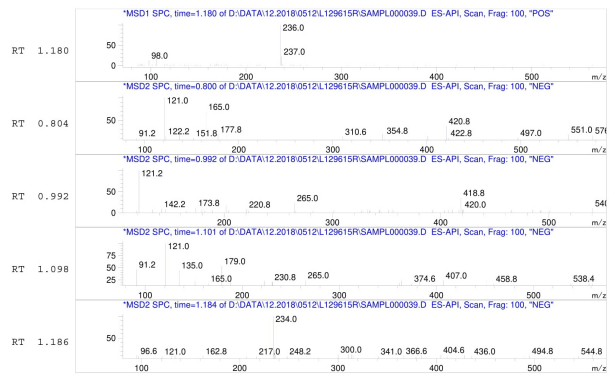
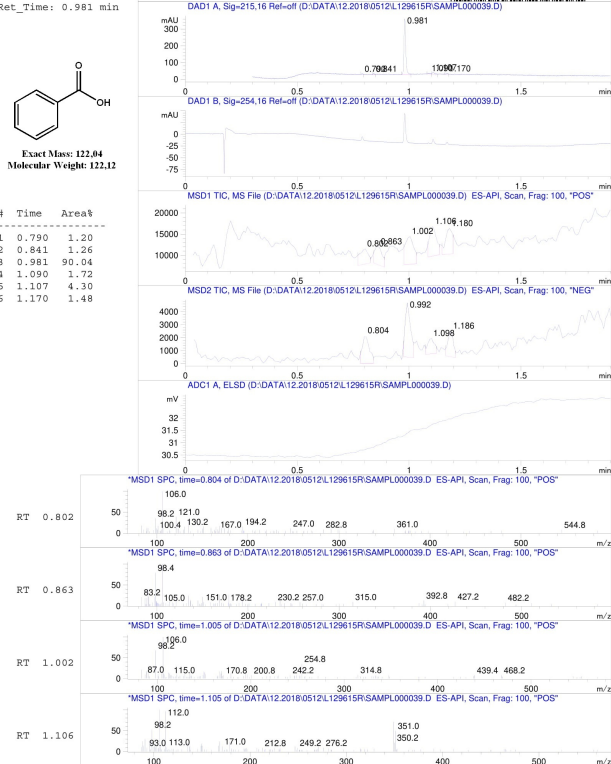
MaxPeak: 90.04%
Ret_Time: 0.981 min



Exact Mass: 122.04
Molecular Weight: 122.12

#	Time	Area%
1	0.790	1.20
2	0.841	1.26
3	0.981	90.04
4	1.090	1.72
5	1.107	4.30
6	1.170	1.48

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

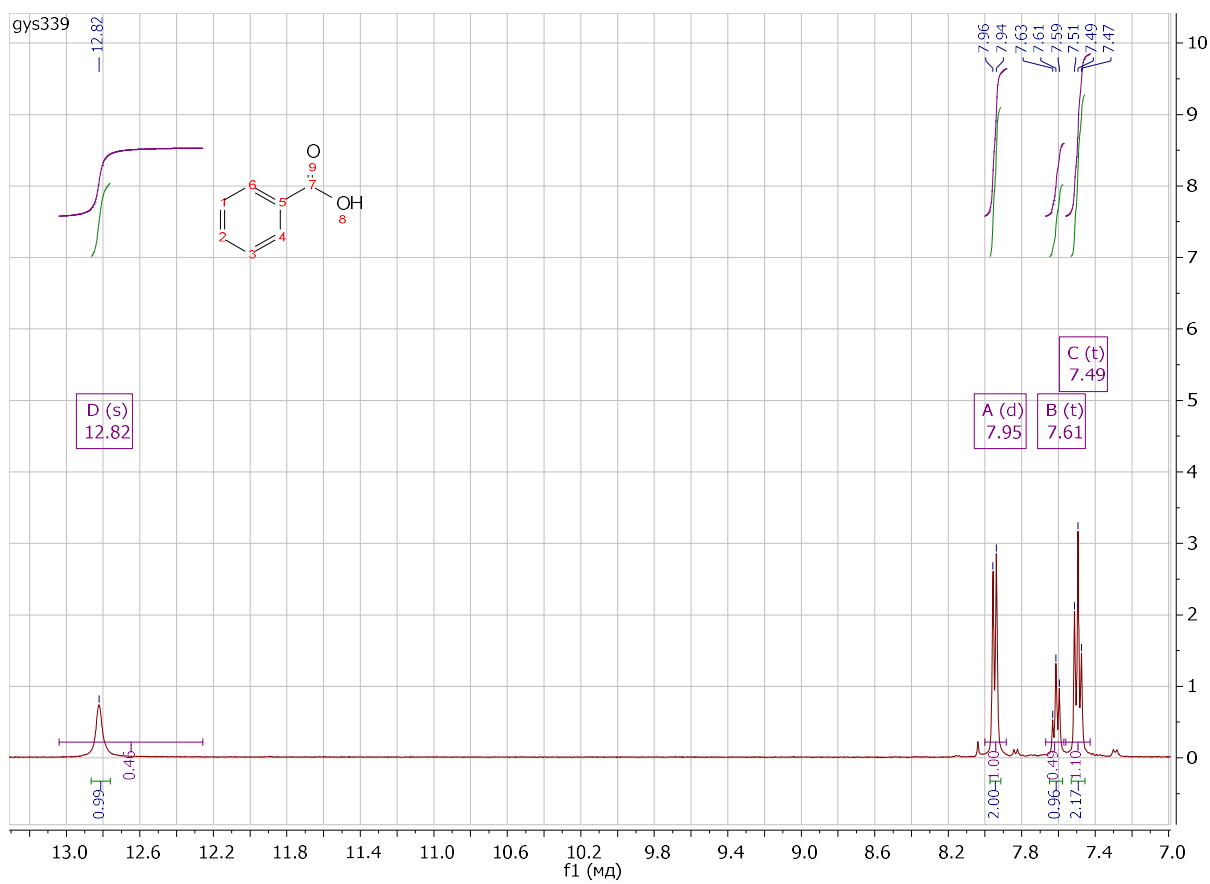


Figure S25 : ^1H NMR spectrum of compound 6

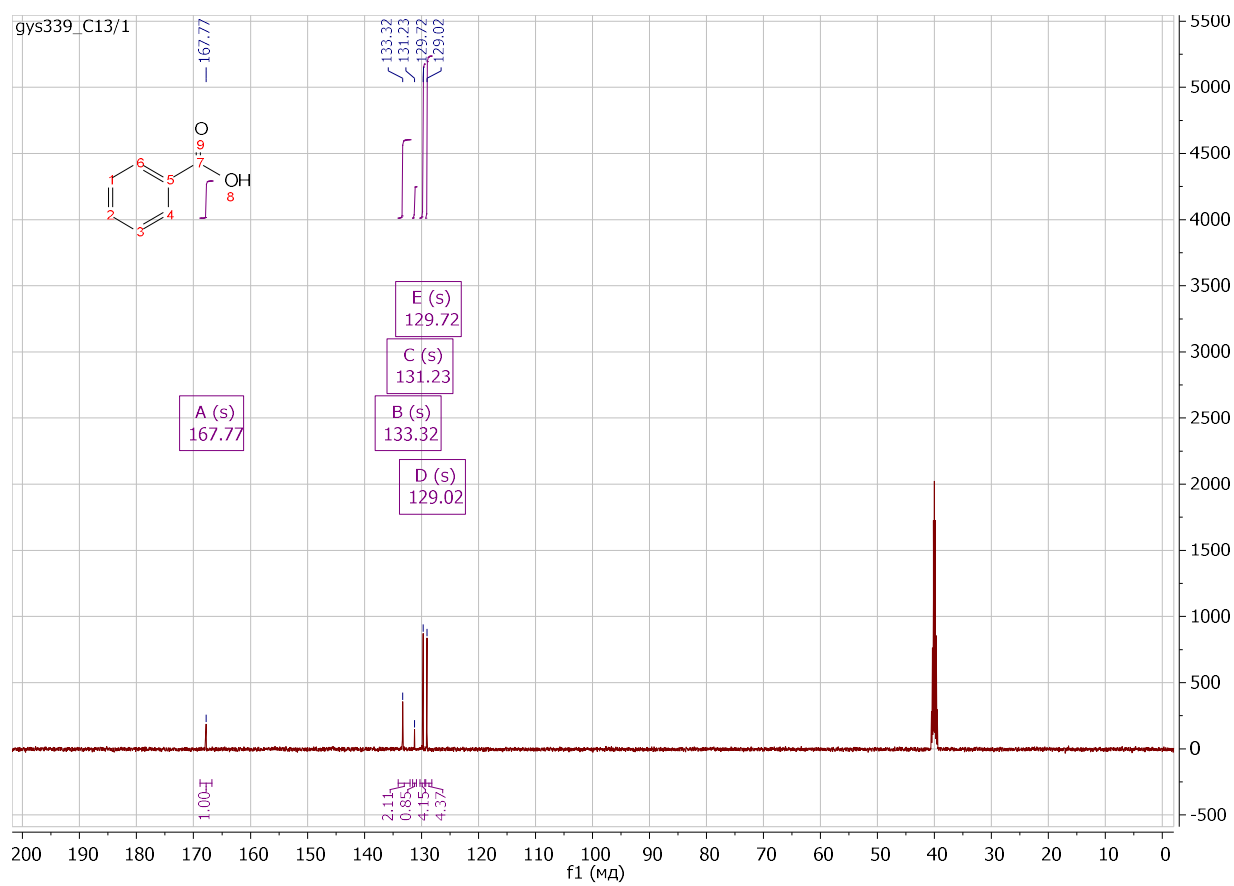


Figure S26 : ^{13}C NMR spectrum of compound 6