Chimica Techno Acta

Supplementary materials

Synthesis and cytotoxic activity of (2-arylquinazolin-4-yl)hydrazones of 2-hydroxybenzaldehydes

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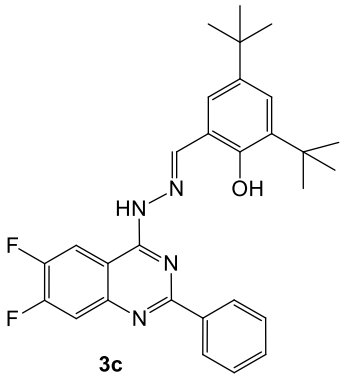


3c

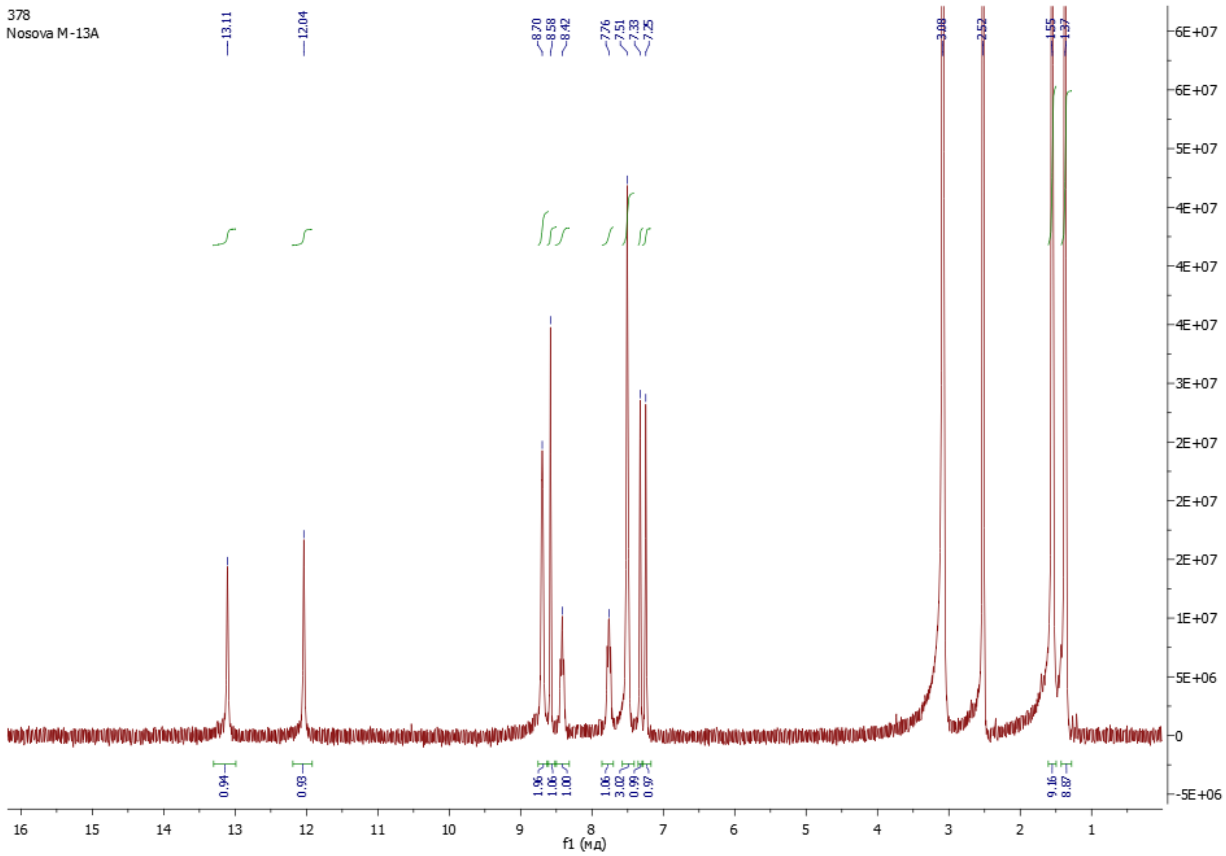


Figure S1 NMR ^{1}H spectra of salicylidenehydrazonoquinazoline **3c** in DMSO-d_6.

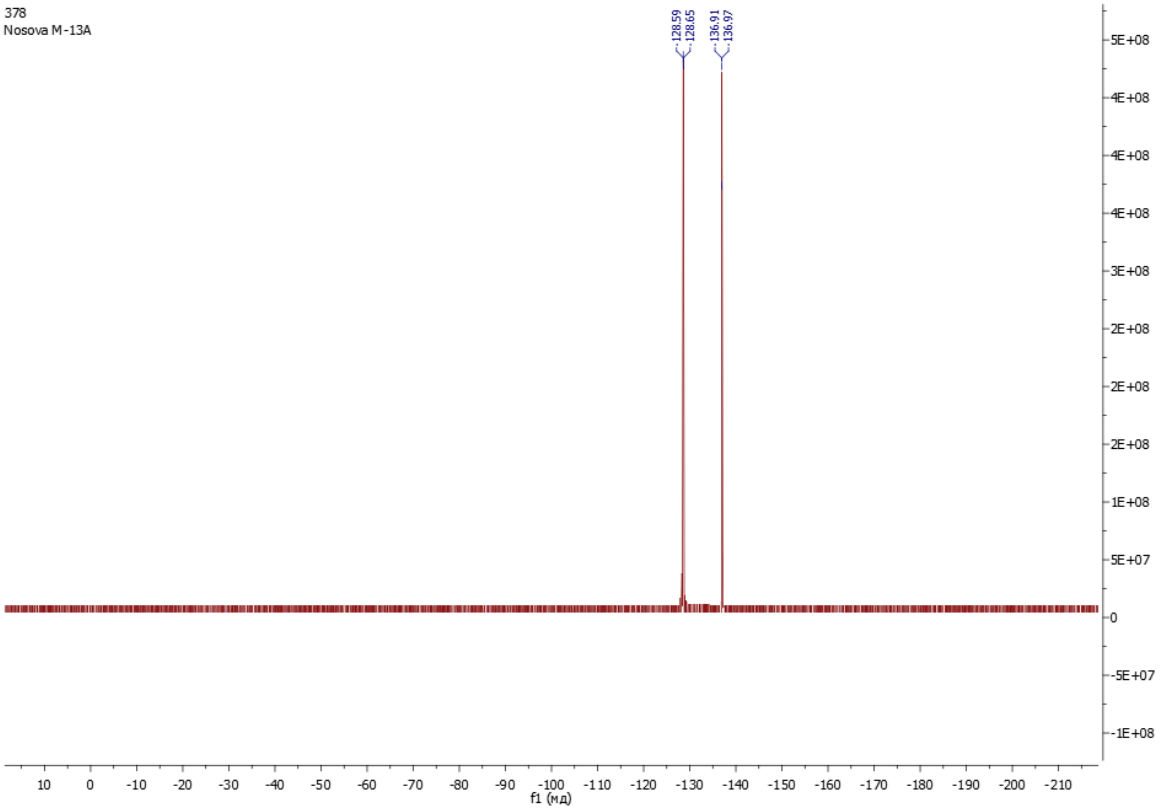


Figure S2 NMR ^{19}F spectra of salicylidenehydrazonoquinazoline **3c** in DMSO-d$_6$.

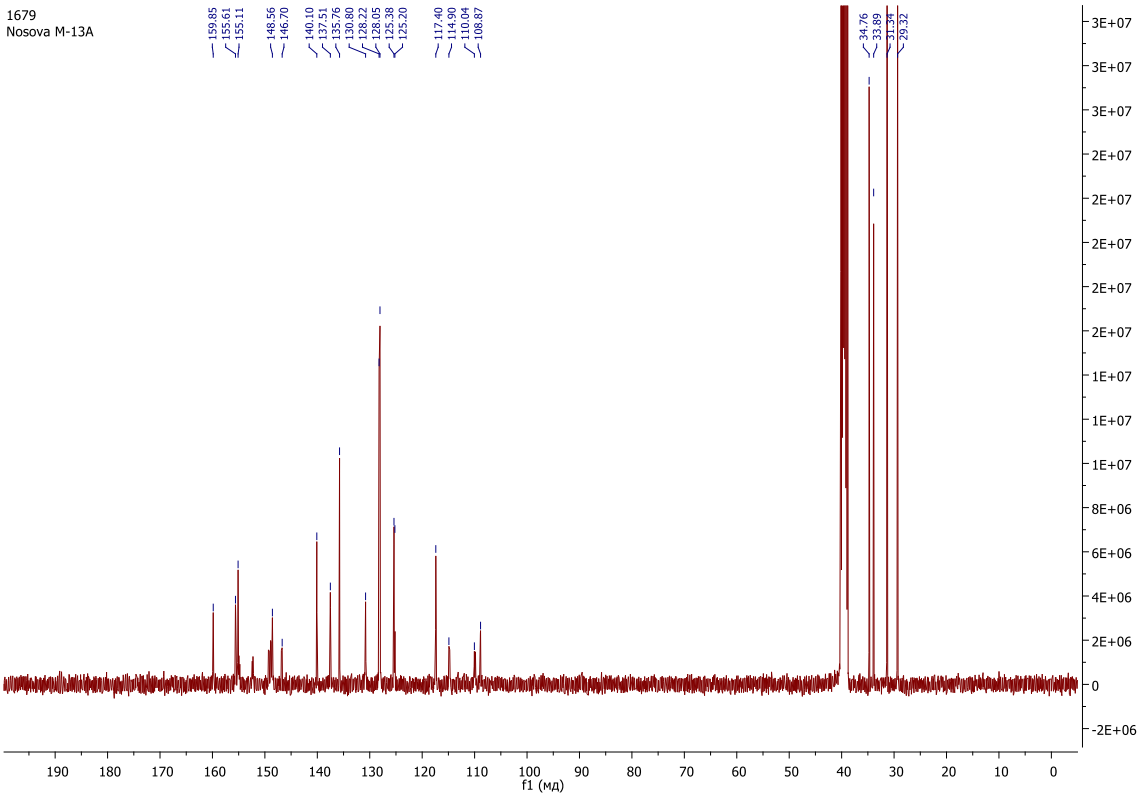


Figure S3 NMR ^{13}C spectra of salicylidenehydrazonoquinazoline **3c** in DMSO-d$_6$.

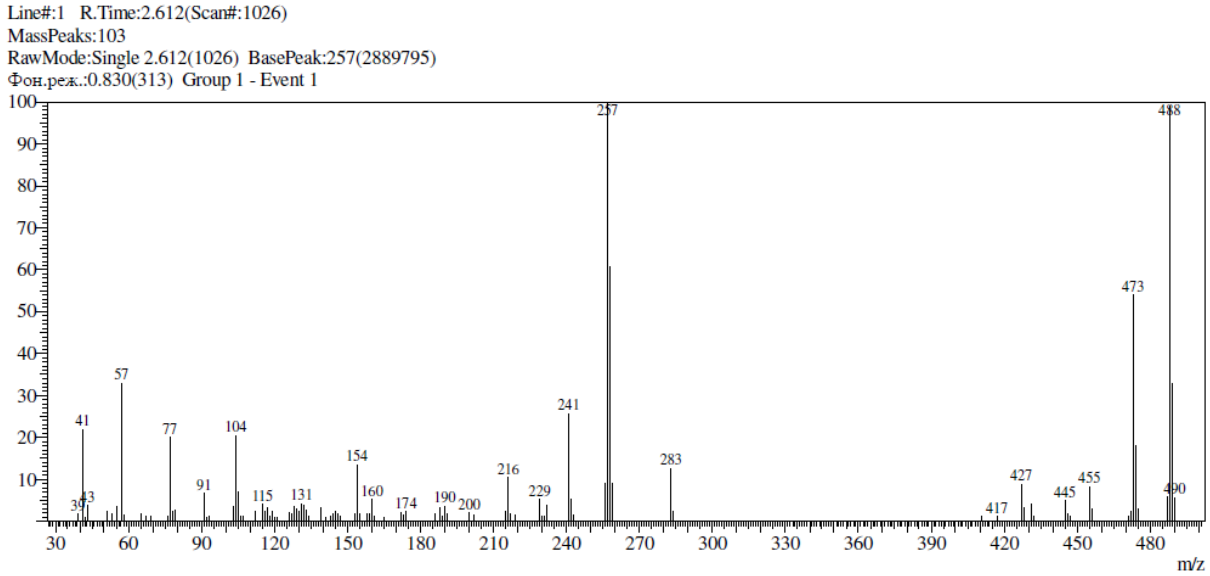


Figure S4 Mass spectra (EI) of salicylidenehydrazonoquinazoline **3c.**

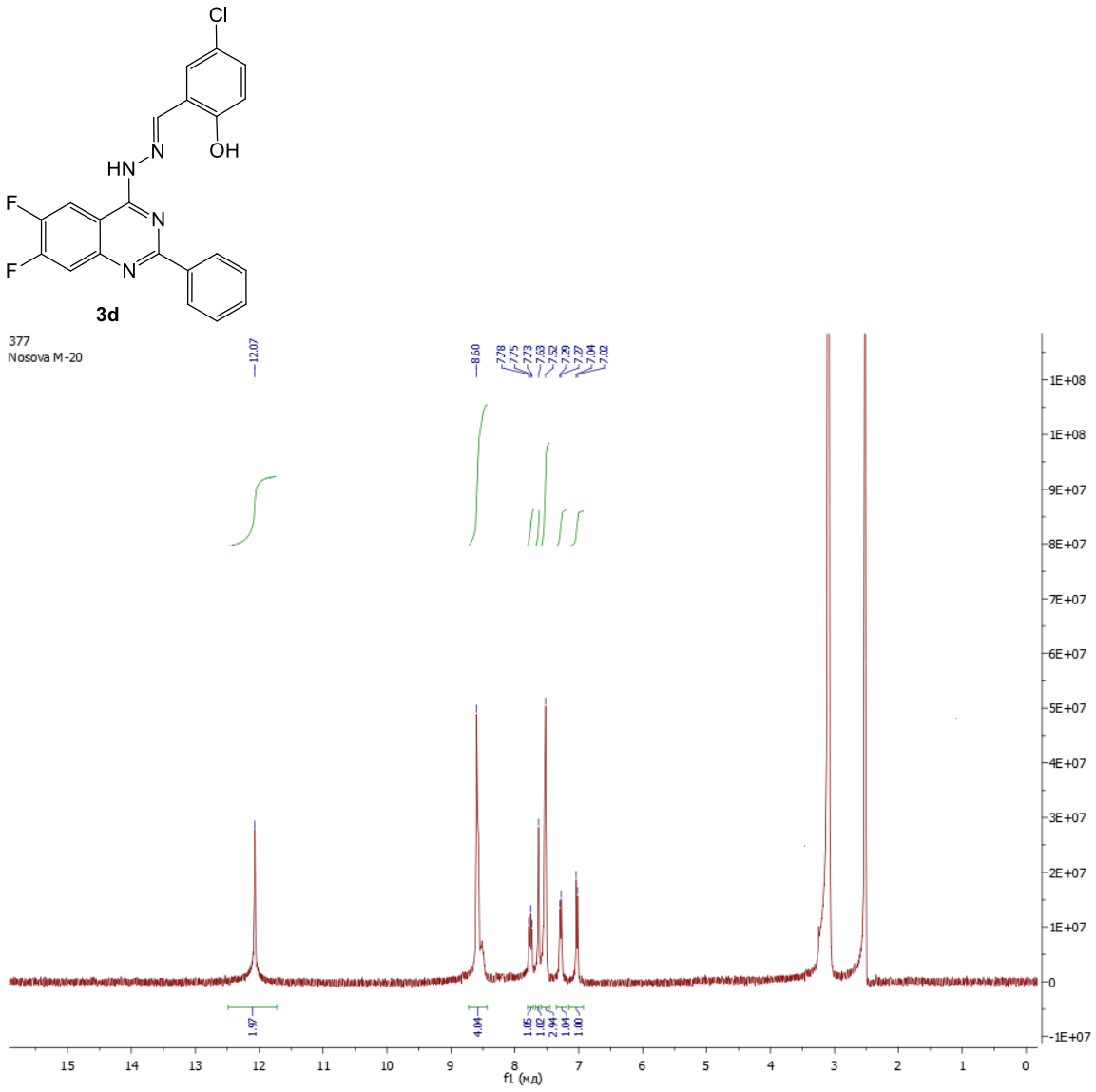


Figure S5 NMR ^{1}H spectra of salicylidenehydrazonoquinazoline **3d** in DMSO-d_6.

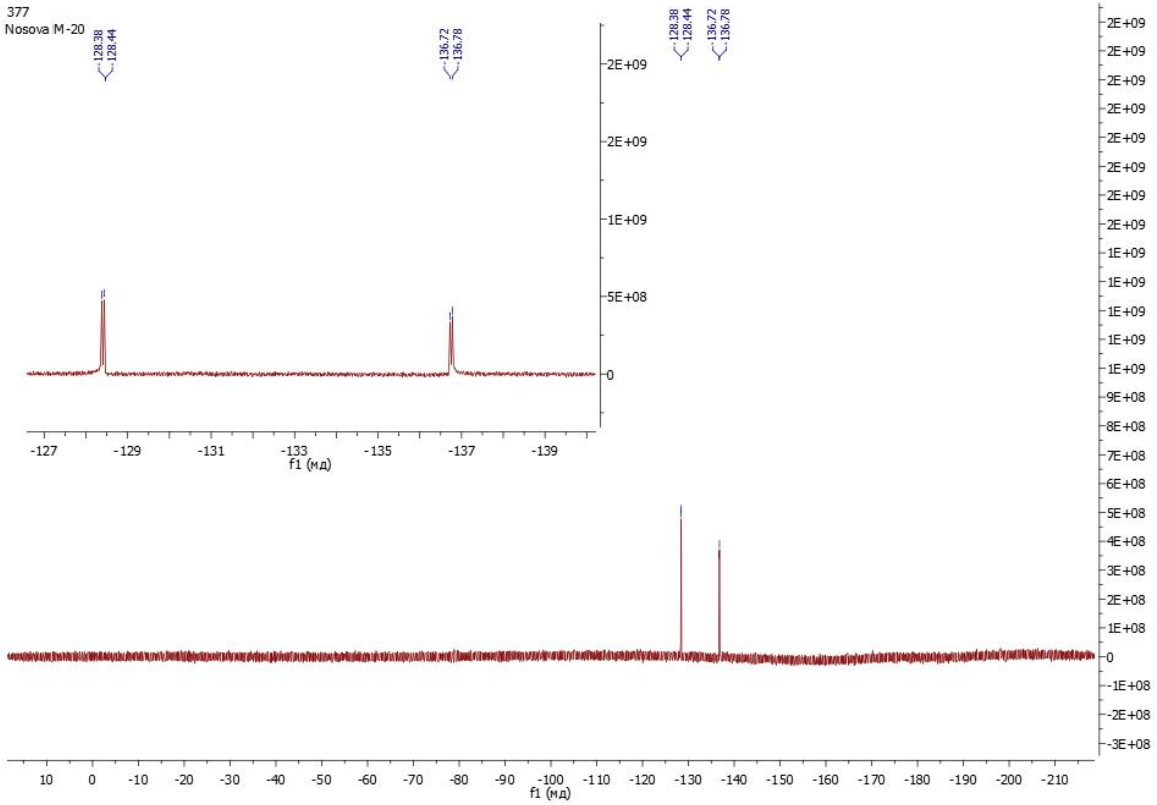


Figure S6 NMR ^{19}F spectra of salicylidenehydrazonoquinazoline **3d** in DMSO-d_6.

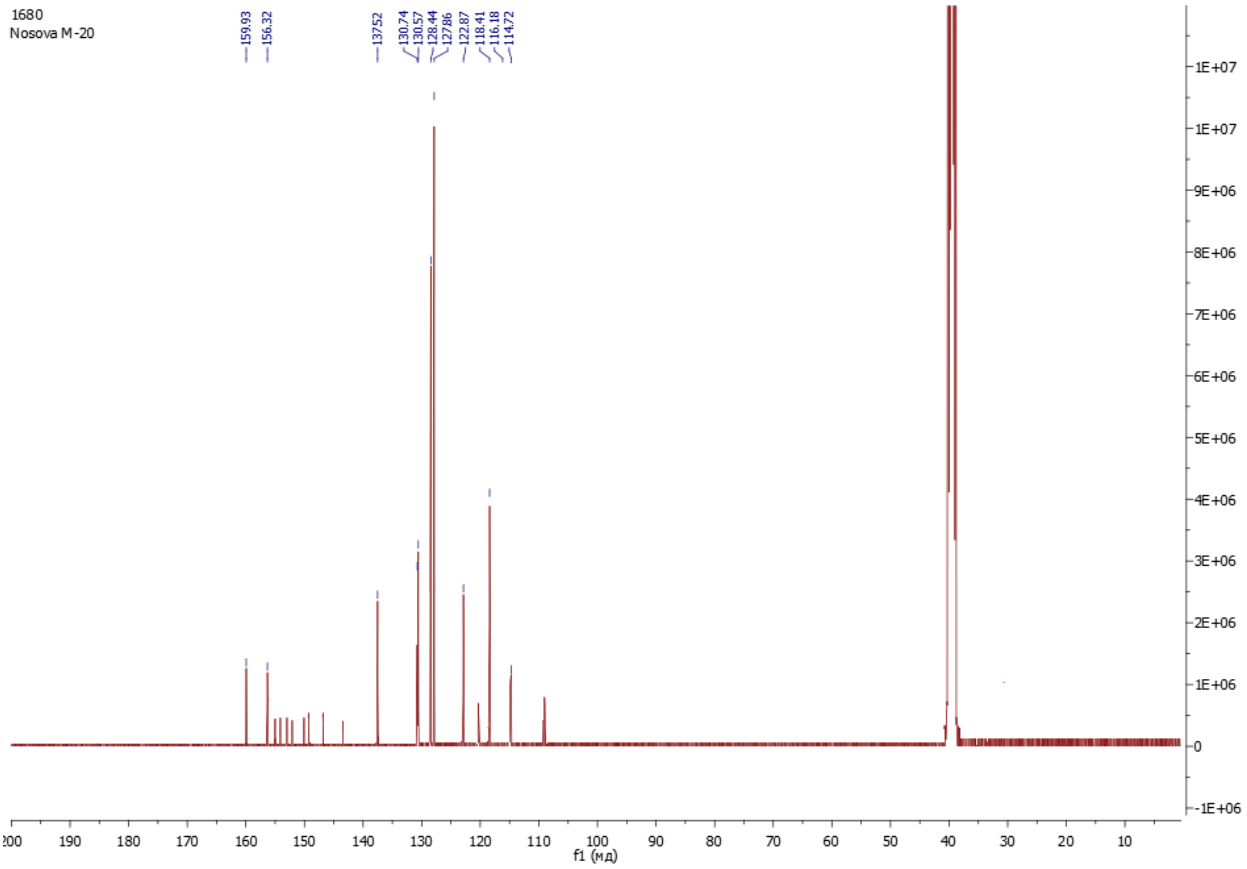


Figure S7 NMR ^{13}C spectra of salicylidenehydrazonoquinazoline **3d** in DMSO-d_6.

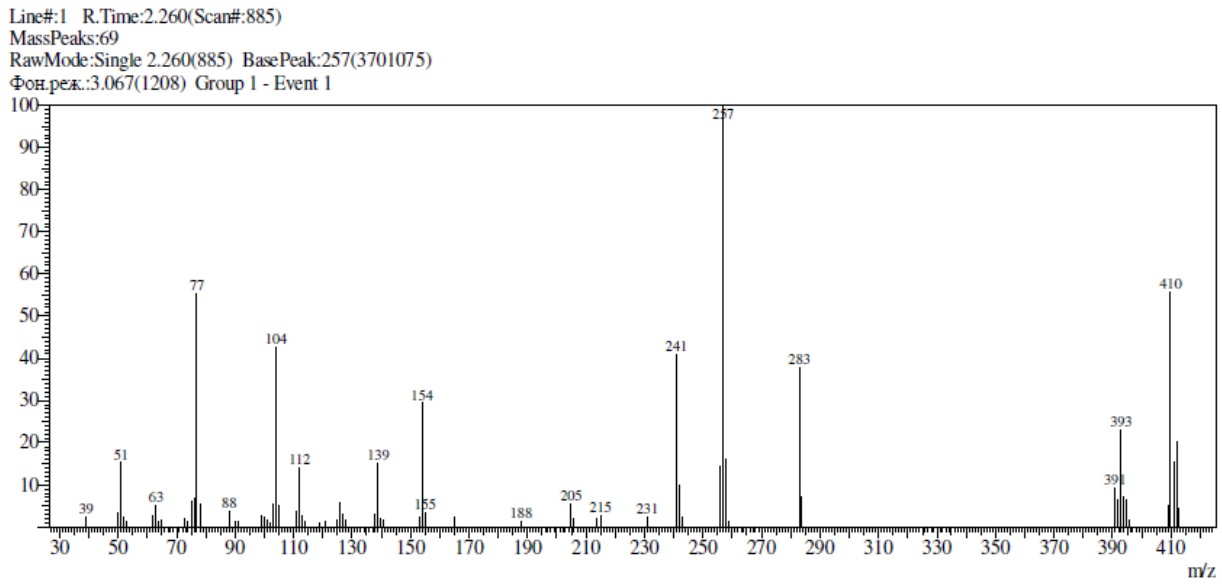
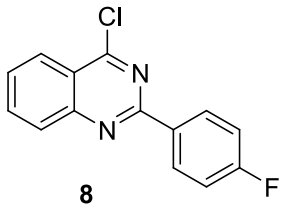


Figure S8 Mass spectra (EI) of salicylidenehydrazonoquinazoline **3d.**



8

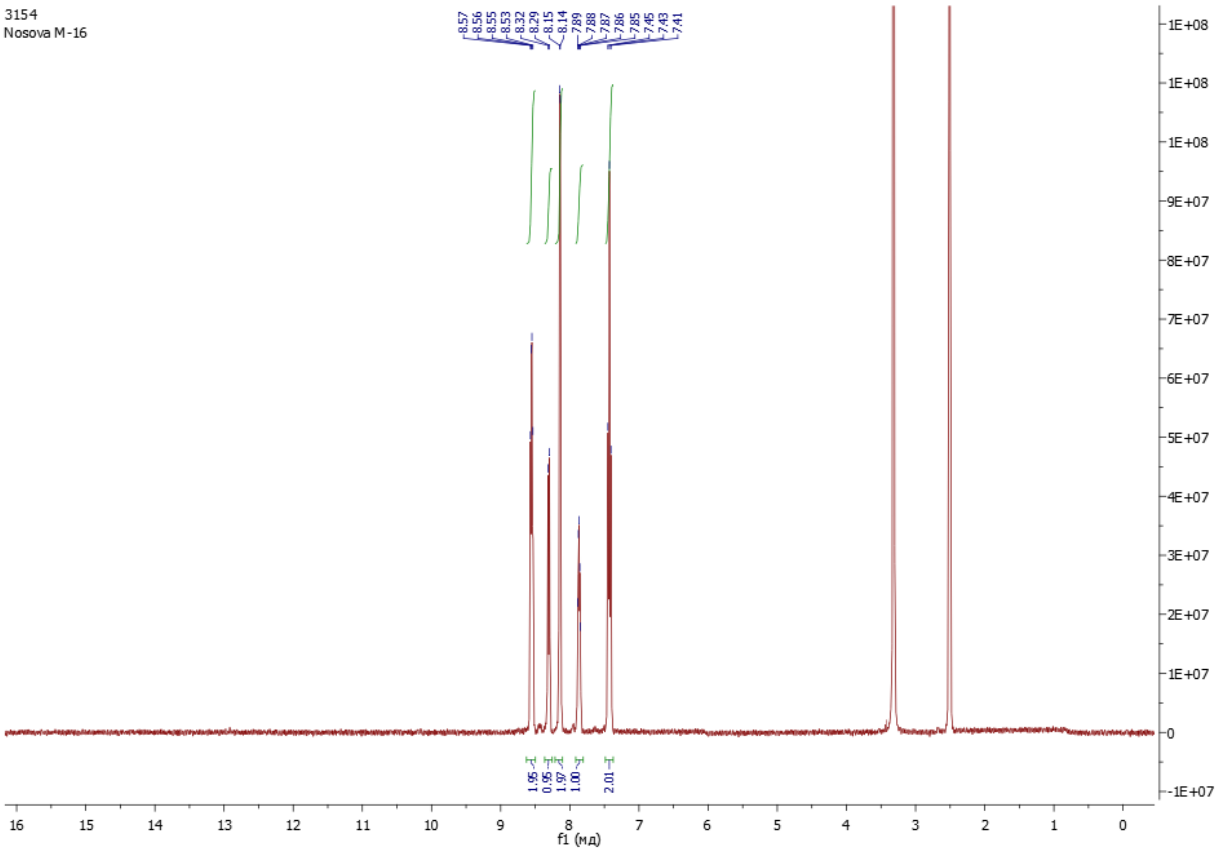


Figure S9 NMR ^{1}H spectra of chloroquinazoline **8** in DMSO-d_6.

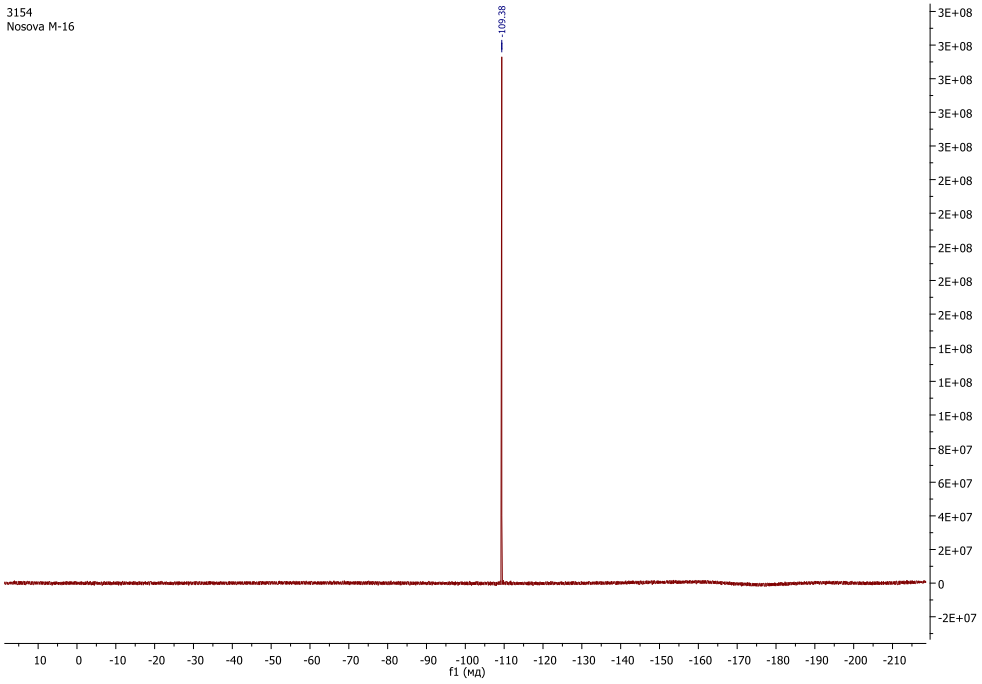
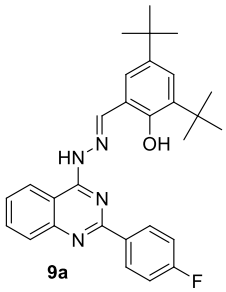


Figure S10 NMR ^{19}F spectra of chloroquinazoline **8** in DMSO-d_6.



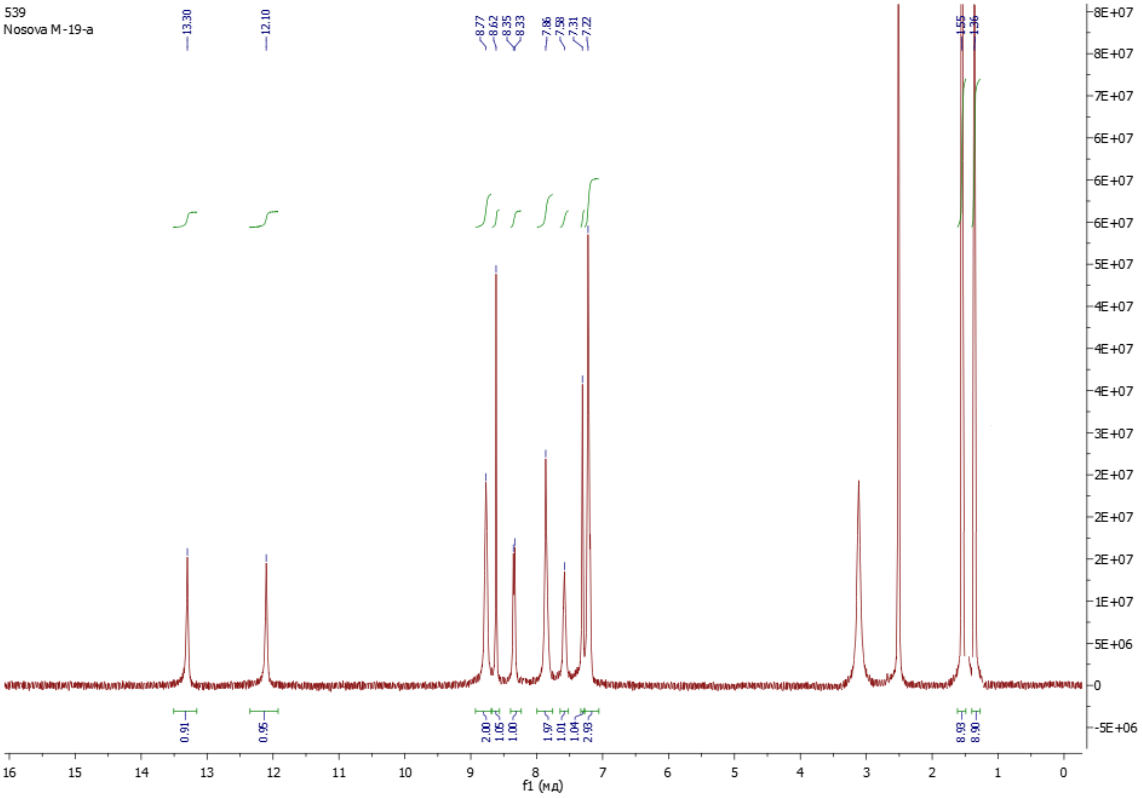


Figure S11 NMR ^{1}H spectra of salicylidenehydrazonoquinazoline **9a** in DMSO-d_6.

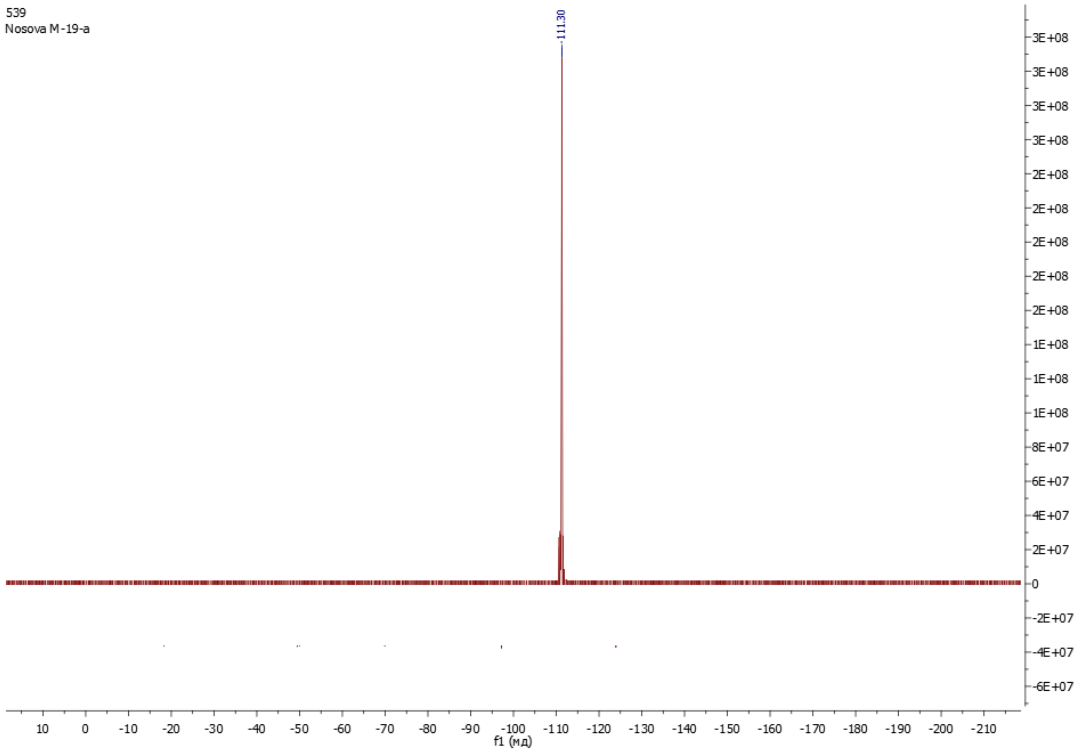


Figure S12 NMR ^{19}F spectra of salicylidenehydrazonoquinazoline **9a** in DMSO-d_6.

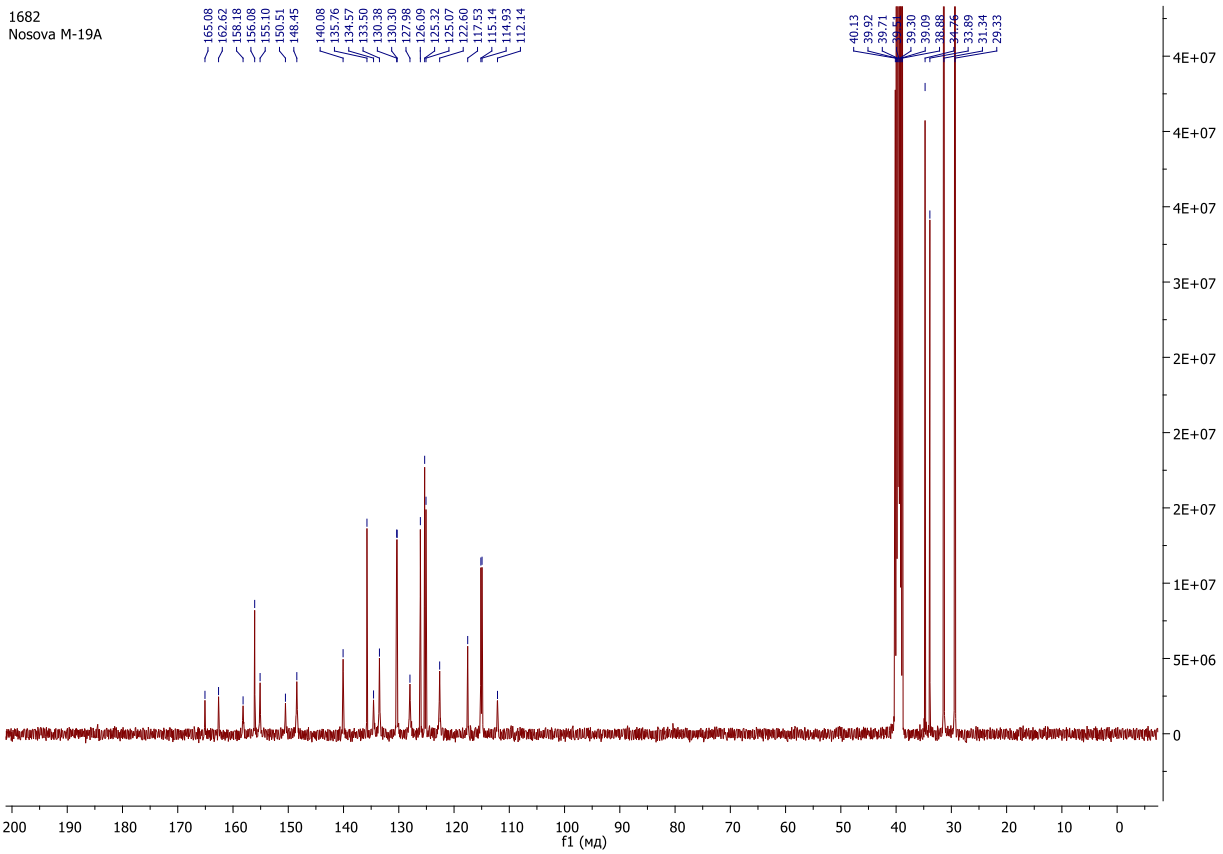


Figure 13 NMR ^{13}C spectra of salicylidenehydrazonoquinazoline **9a** in DMSO-d_6.

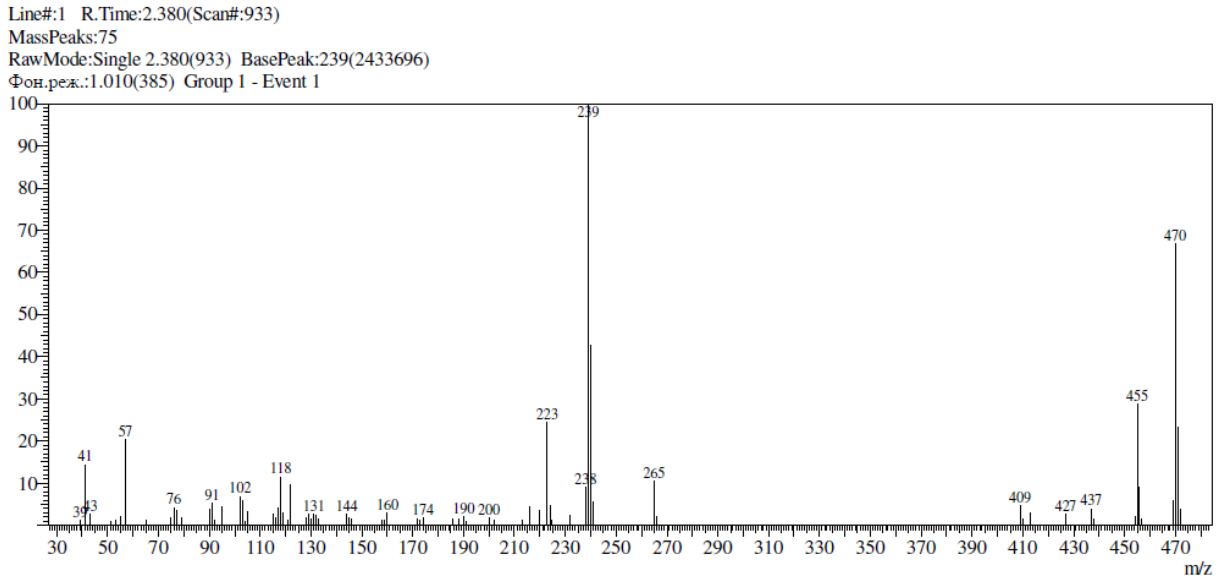
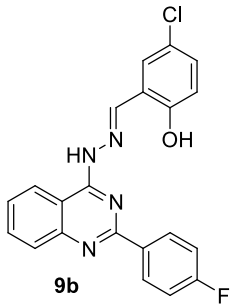


Figure S14 Mass spectra (EI) of salicylidenehydrazonoquinazoline **9a.**



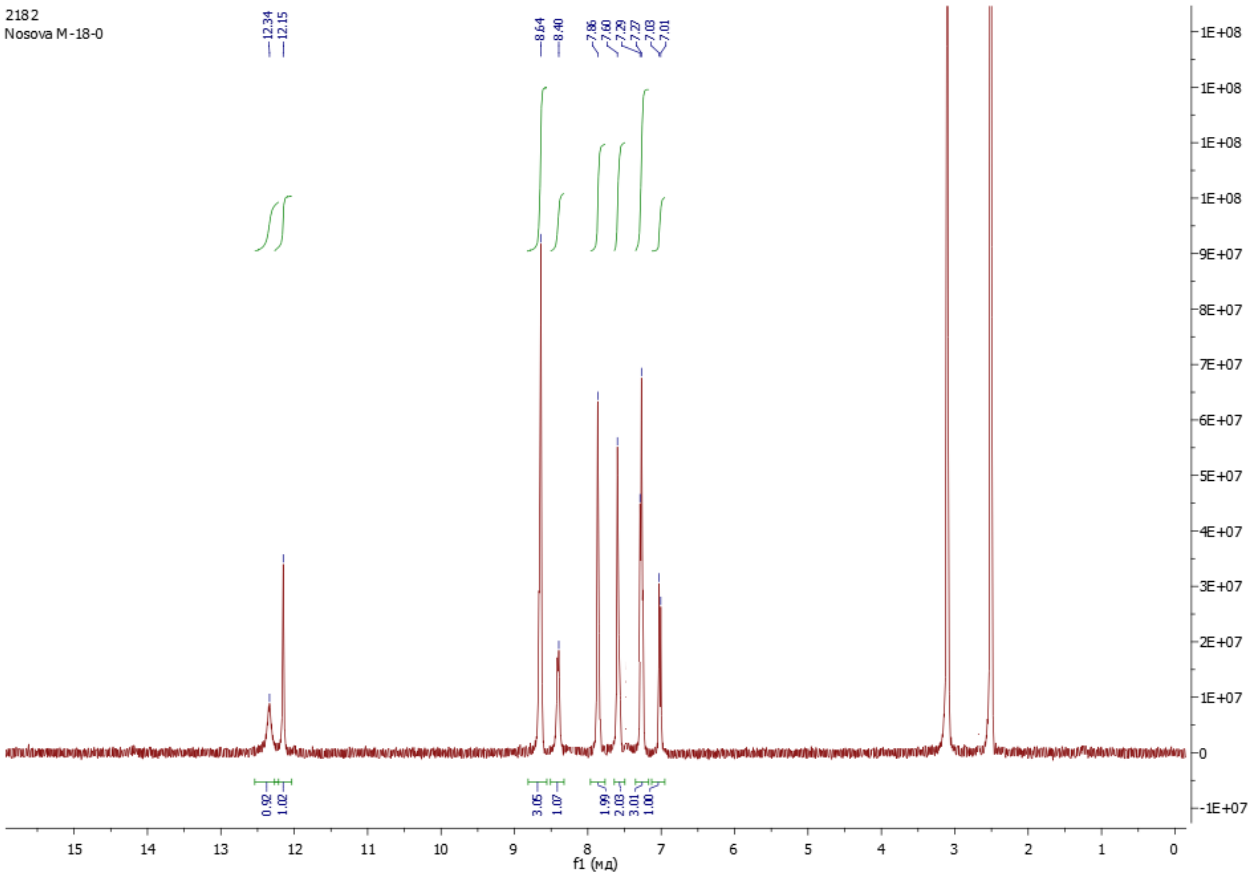


Figure S15 NMR ^{1}H spectra of salicylidenehydrazonoquinazoline **9b** in DMSO-d_6.

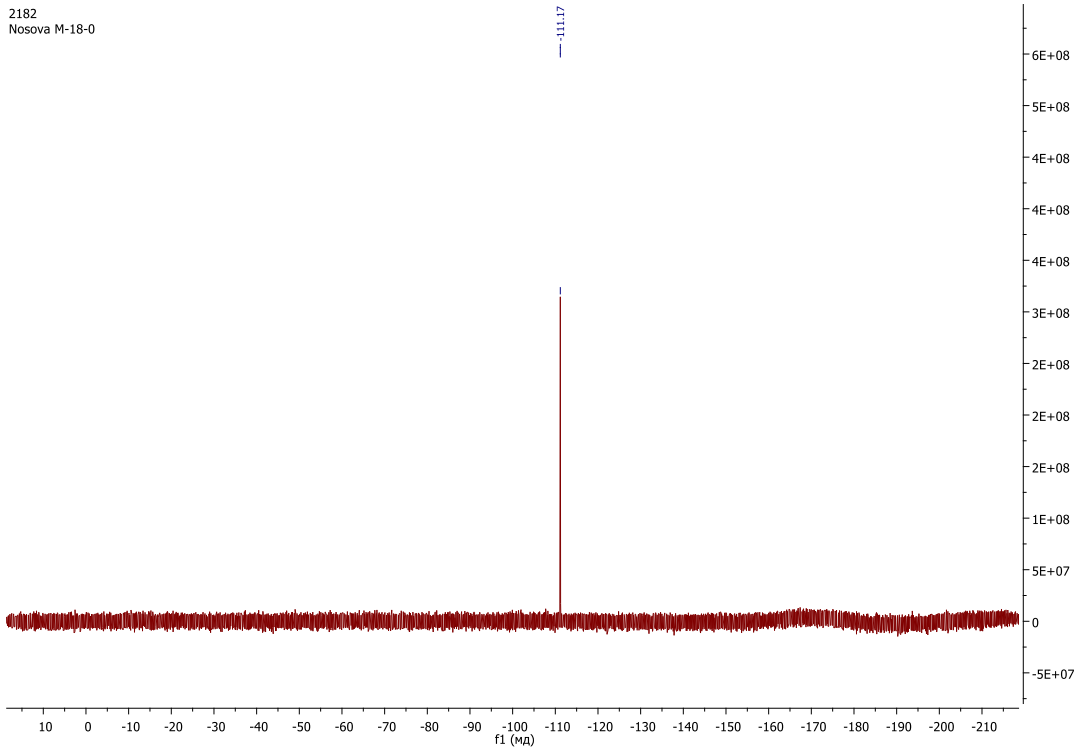


Figure S16 NMR ^{19}F spectra of salicylidenehydrazonoquinazoline **9b** in DMSO-d_6.

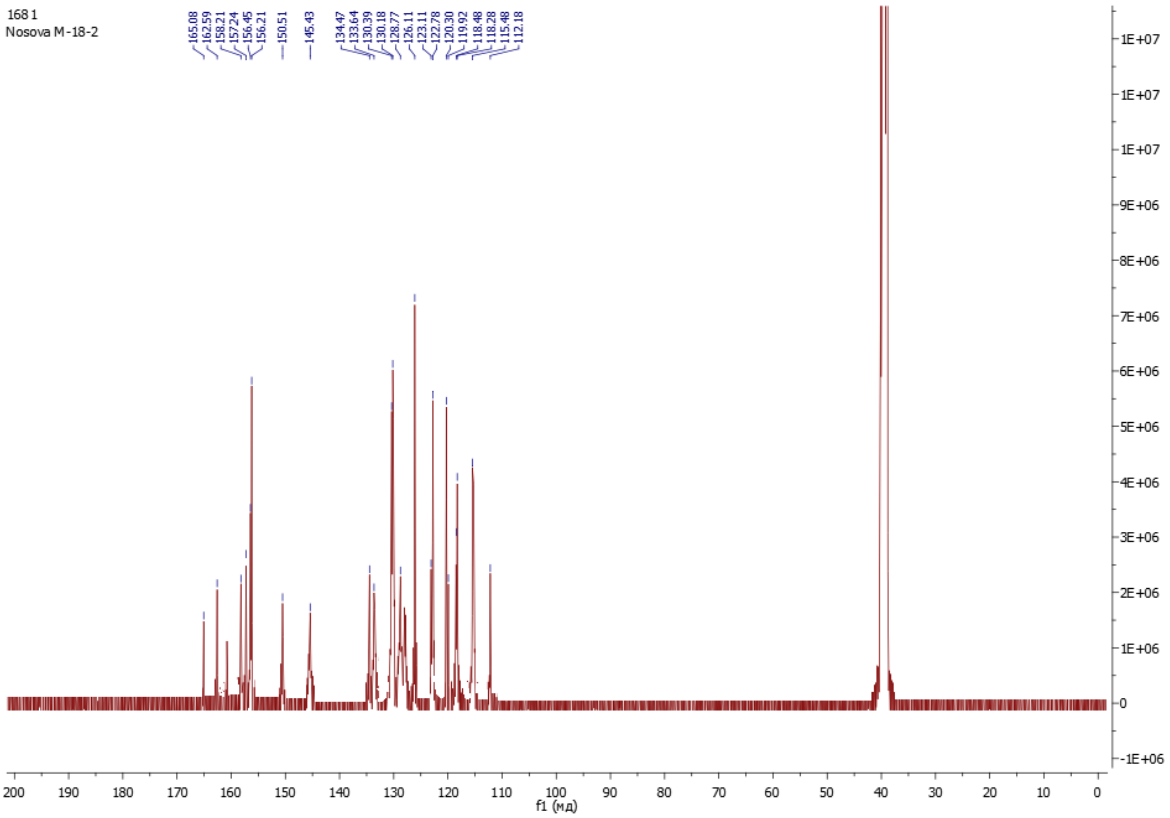


Figure S17 NMR ^{13}C spectra of salicylidenehydrazonoquinazoline **9b** in DMSO-d_6.

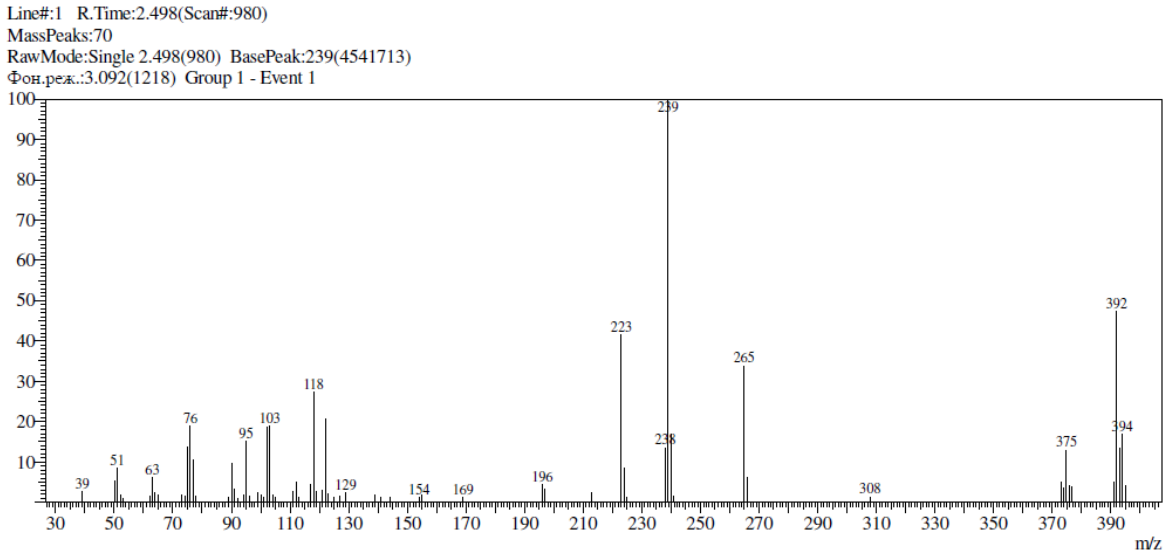


Figure S18 Mass spectra (EI) of salicylidenhydrazonoquinazoline **9b.**

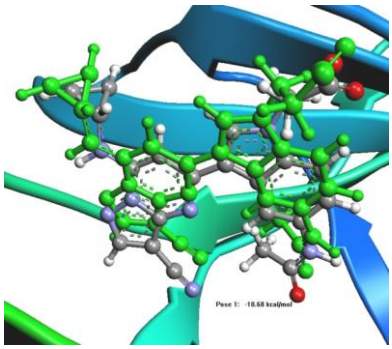
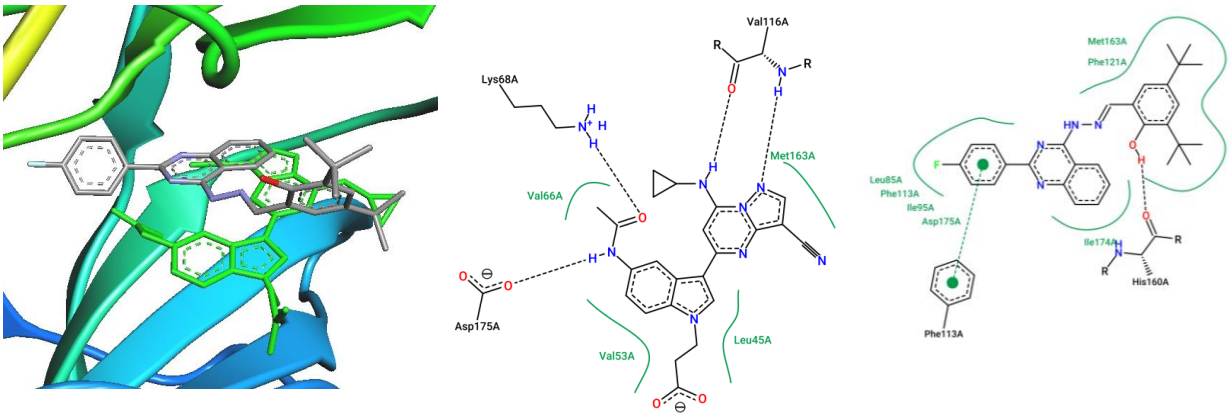


Figure S19 Redocking results of azolopyrimidine derivative, CK2 inhibitor (CHEMBL2062585): real position of ligand is shown in green; calculated positions are colored; RMSD(CHEMBL2062585) = 0.89Å, $\Delta G_{CHEMBL2062585}$ = −10.67 kcal/mol.



A | B (CHEMBL2062585, –10.67 kcal/mol) | C (**9a**, -13.86 kcal/mol)

Figure S20 Docking results for ligand **9a**: A – The positions of native ligand CHEMBL2062585 (green) and docked ligand **9a** (colored atoms) in active center of CK2; B –Non-covalent interactions of the native ligand CHEMBL2062585; C – Non-covalent interactions of the docked ligand **9a**.

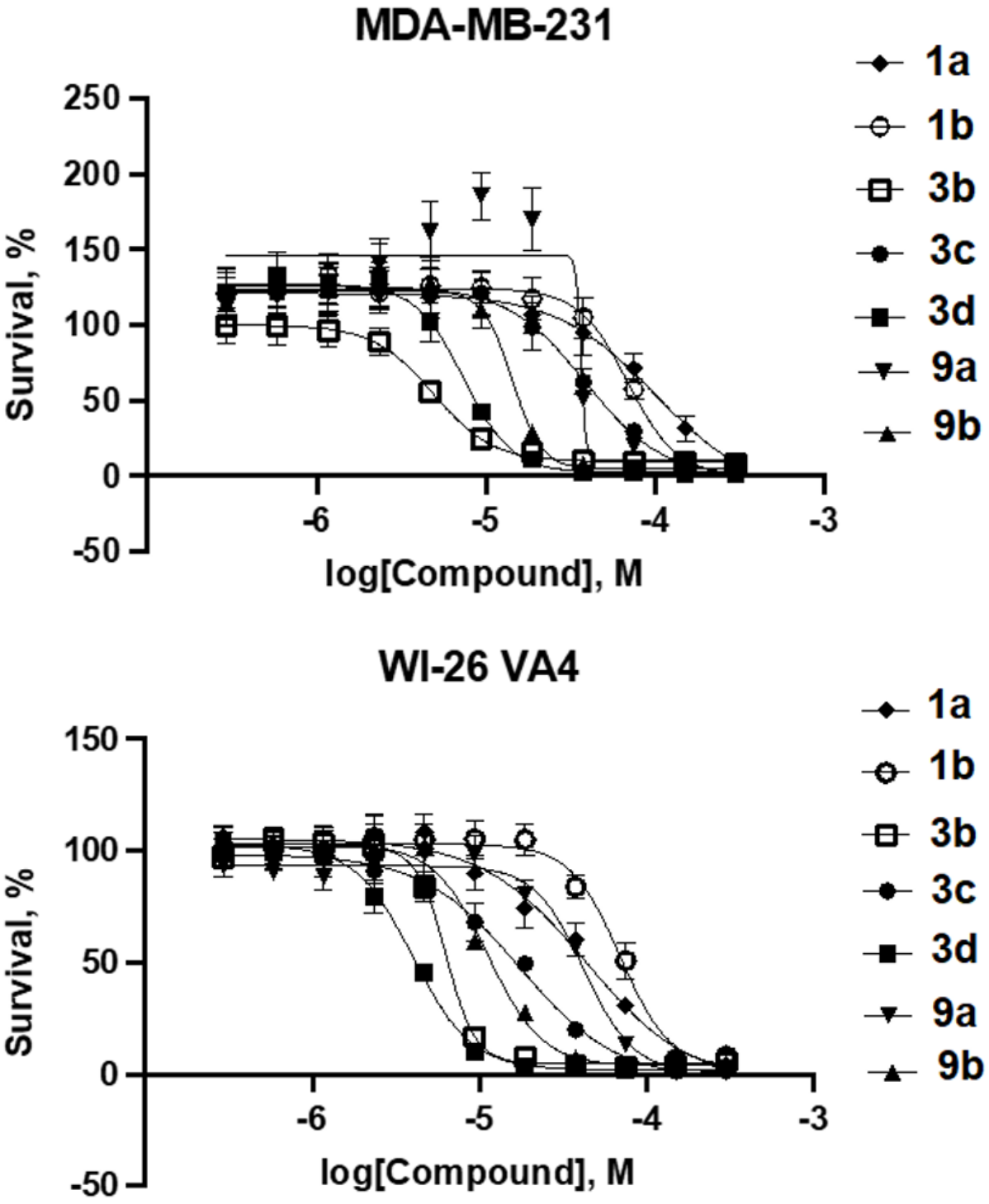


Figure S21 Cell growth inhibition curves for salicylidenehydrazones **1, 3, 9.**