



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

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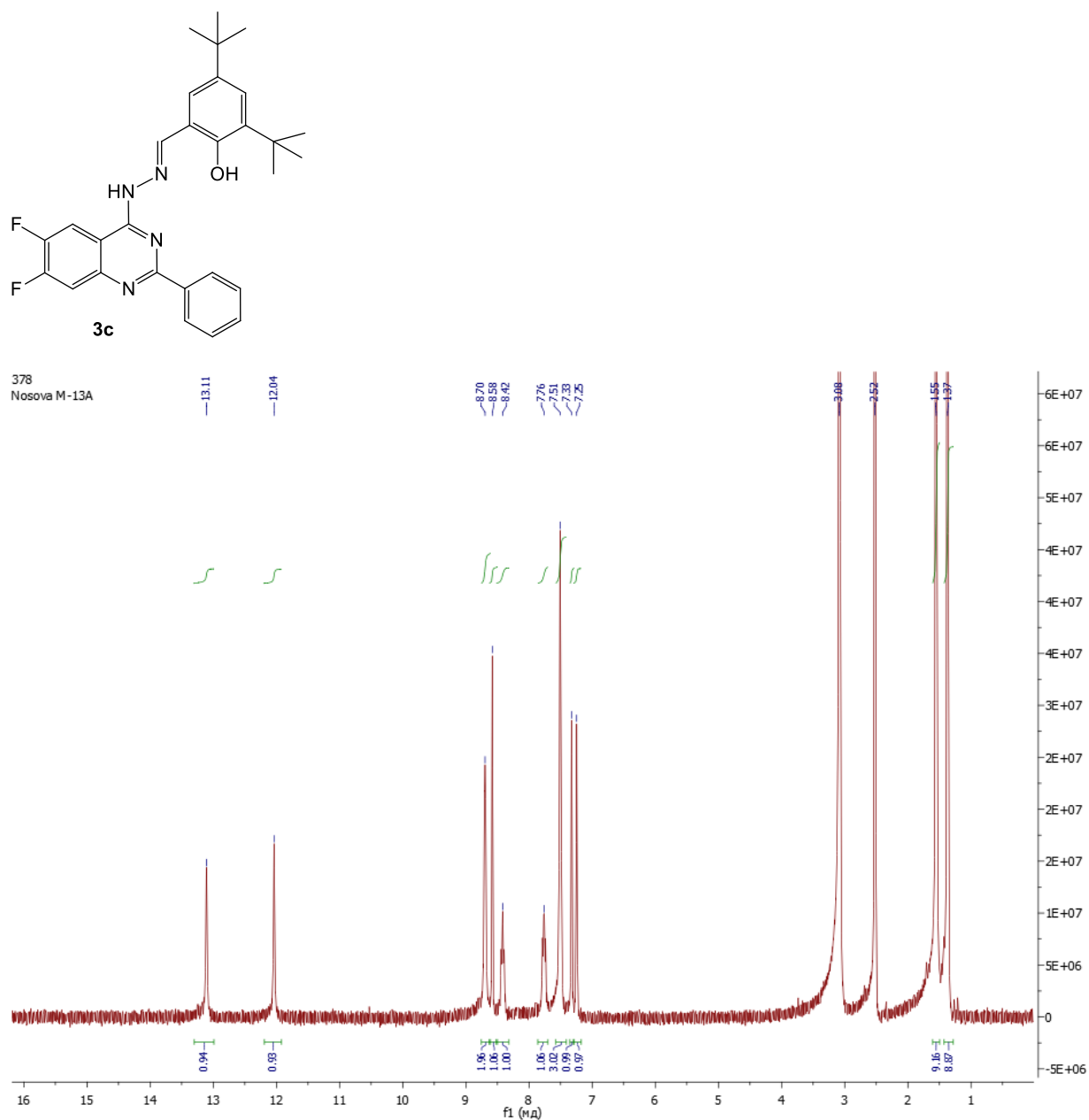


Figure S1 NMR ^1H spectra of salicylidenehydrazonequinazoline **3c** in DMSO-d_6 .

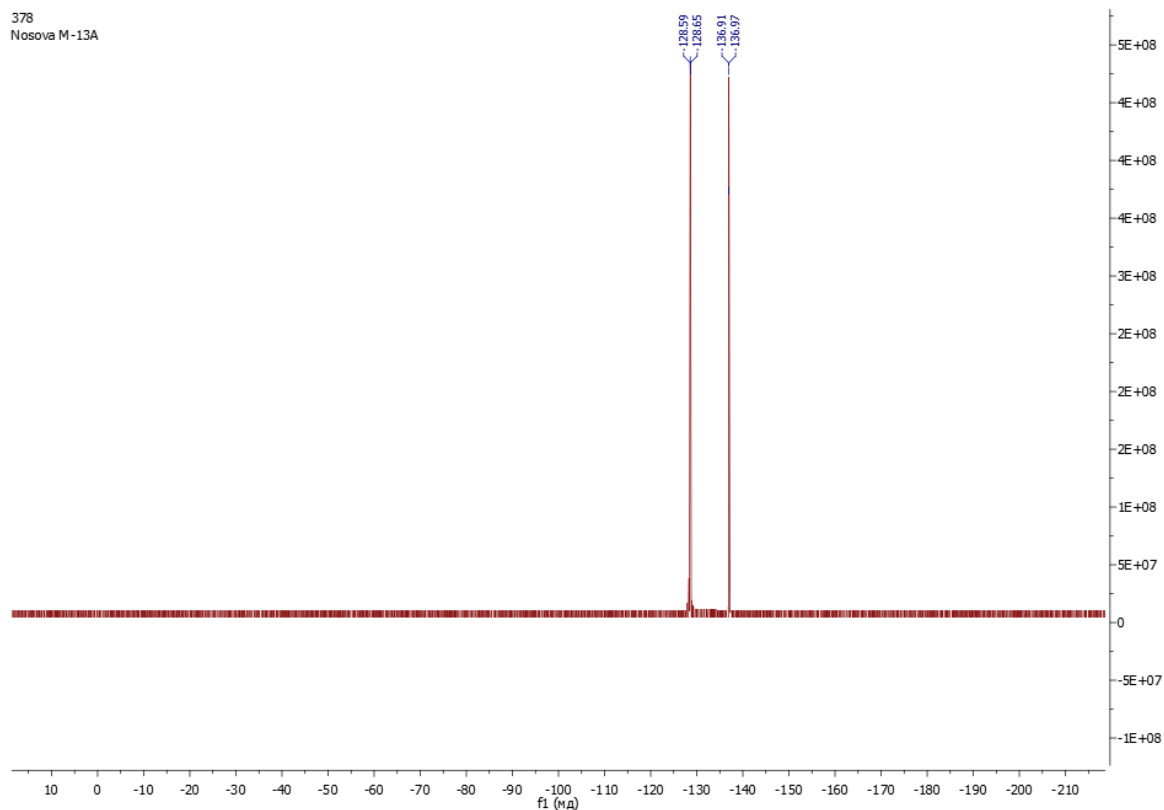


Figure S2 NMR ^{19}F spectra of salicylidenehydrazonequinazoline **3c** in DMSO- d_6 .

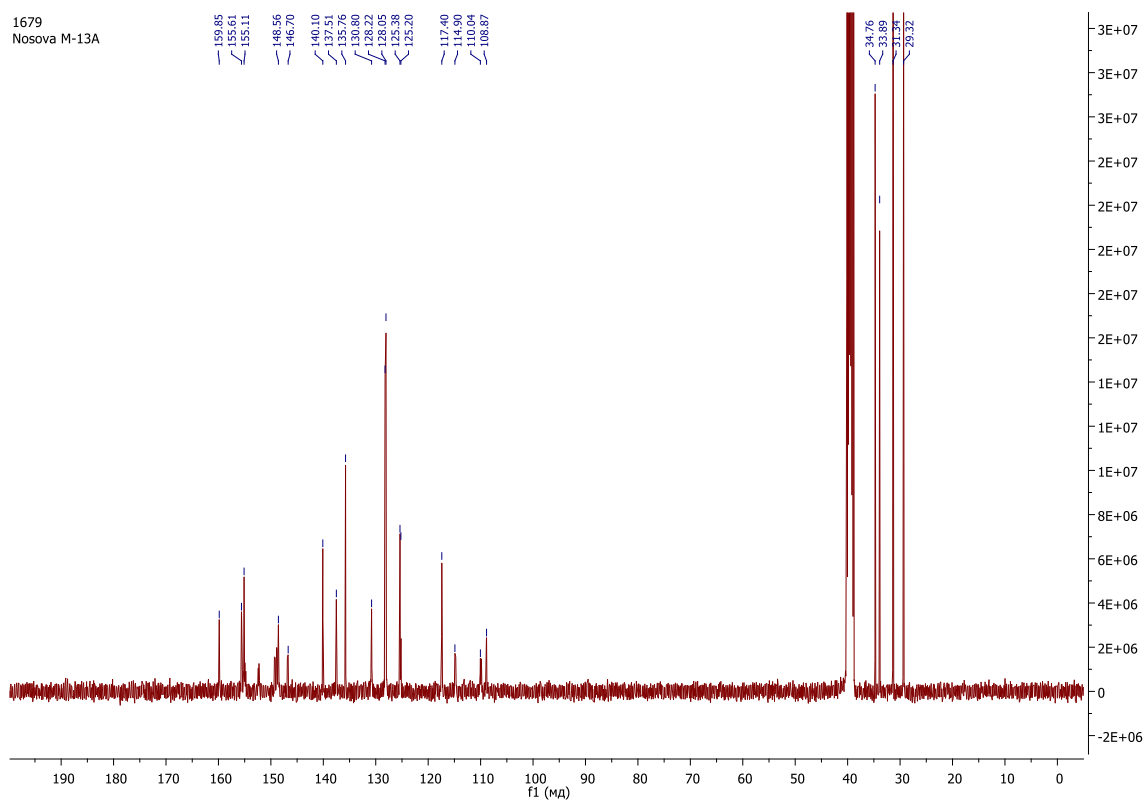


Figure S3 NMR ^{13}C spectra of salicylidenehydrazonequinazoline **3c** in DMSO- d_6 .



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Фон.реш.:0.830(313) Group 1 - Event 1

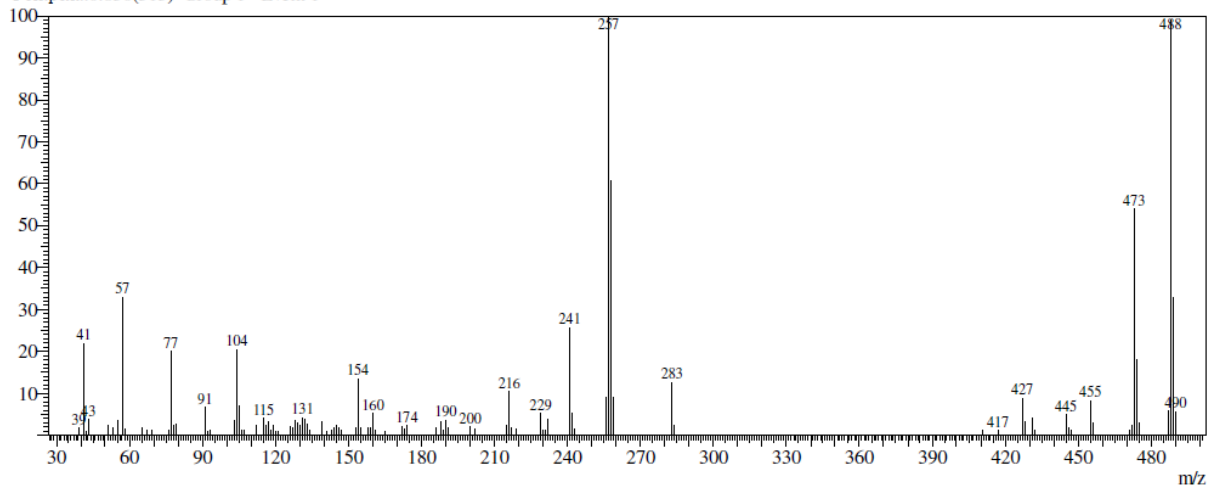


Figure S4 Mass spectra (EI) of salicylidenehydrazonequinazoline **3c**.

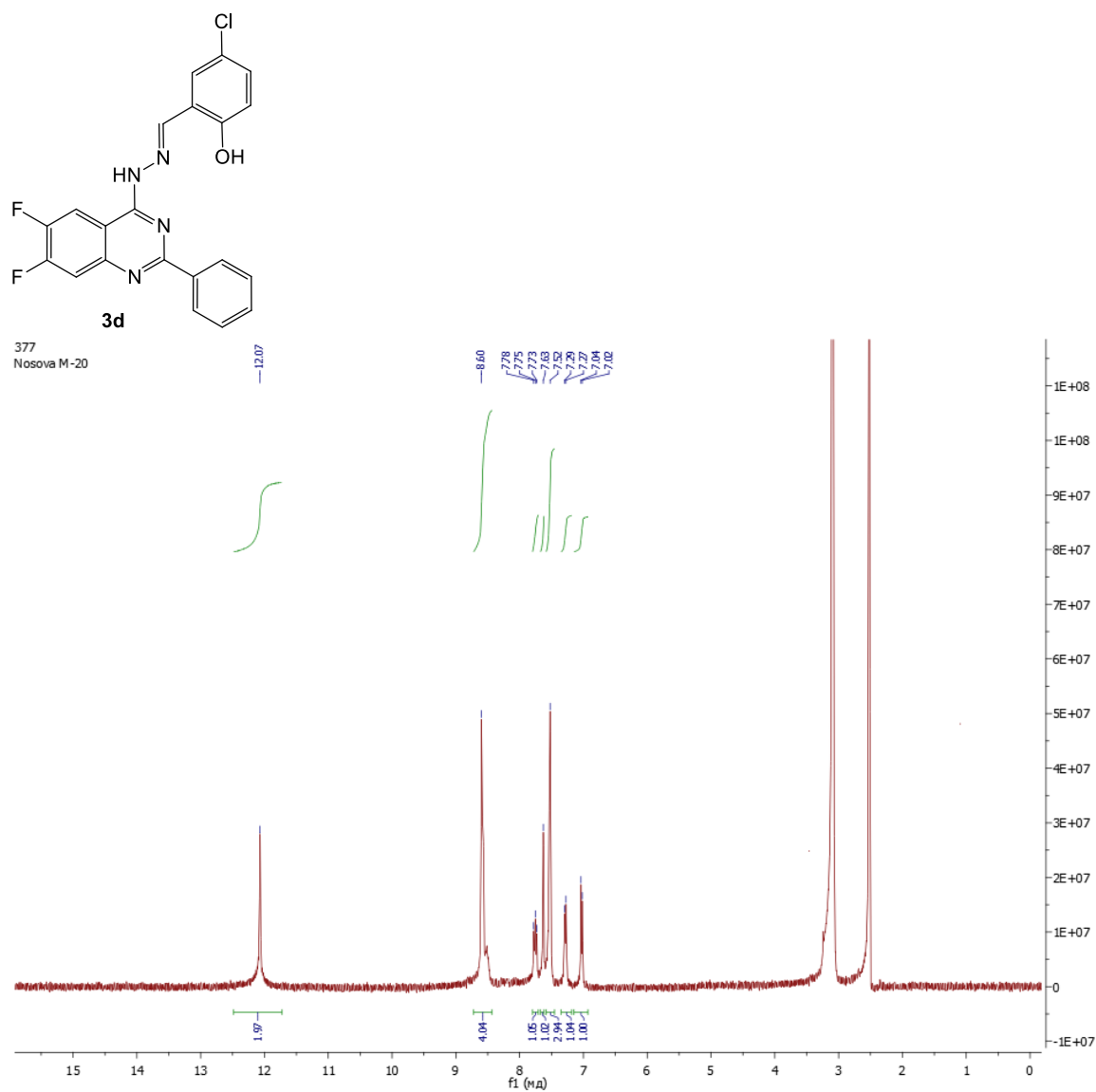


Figure S5 NMR ¹H spectra of salicylidenehydrazonequinazoline **3d** in DMSO-d₆.

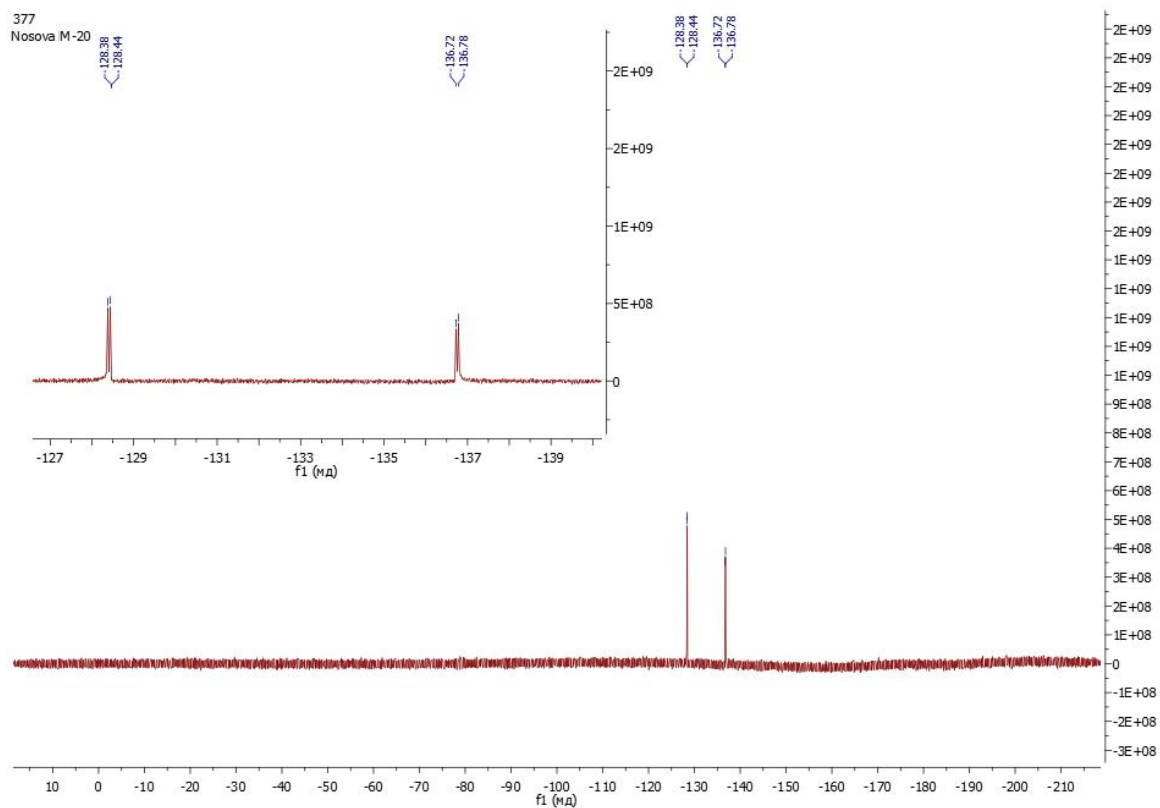


Figure S6 NMR ^{19}F spectra of salicylidenehydrazonoquinazoline **3d** in DMSO-d_6 .

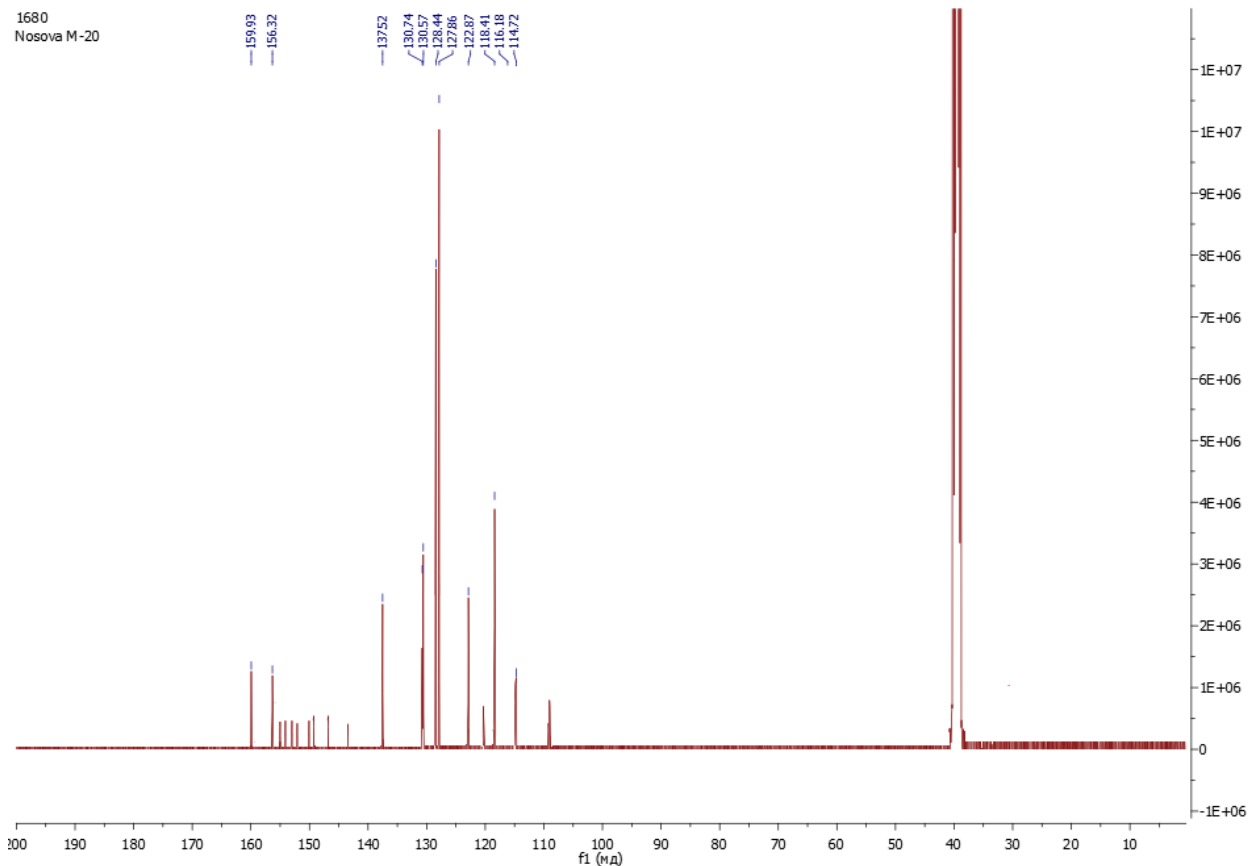


Figure S7 NMR ^{13}C spectra of salicylidenehydrazonequinazoline **3d** in DMSO- d_6 .

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Фон.р.ж.:3.067(1208) Group 1 - Event 1

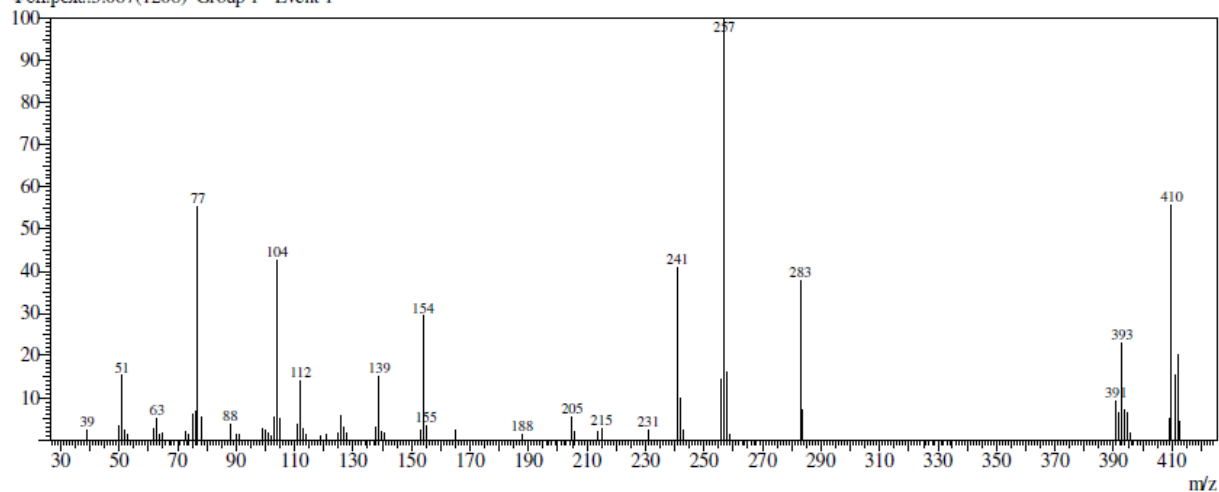
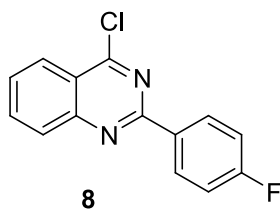


Figure S8 Mass spectra (EI) of salicylidenehydrazonequinazoline **3d**.



3154
Nosova M-16

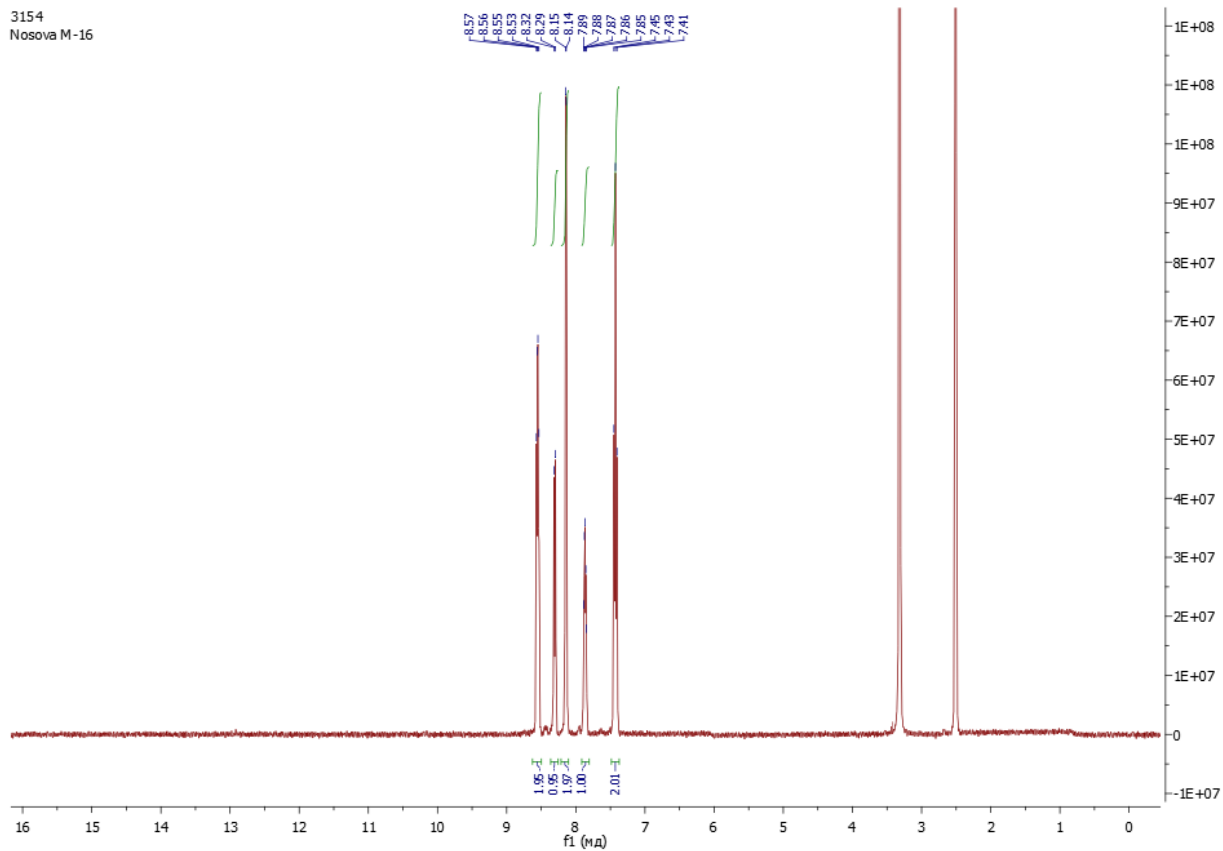


Figure S9 NMR ^1H spectra of chloroquinazoline **8** in DMSO-d_6 .

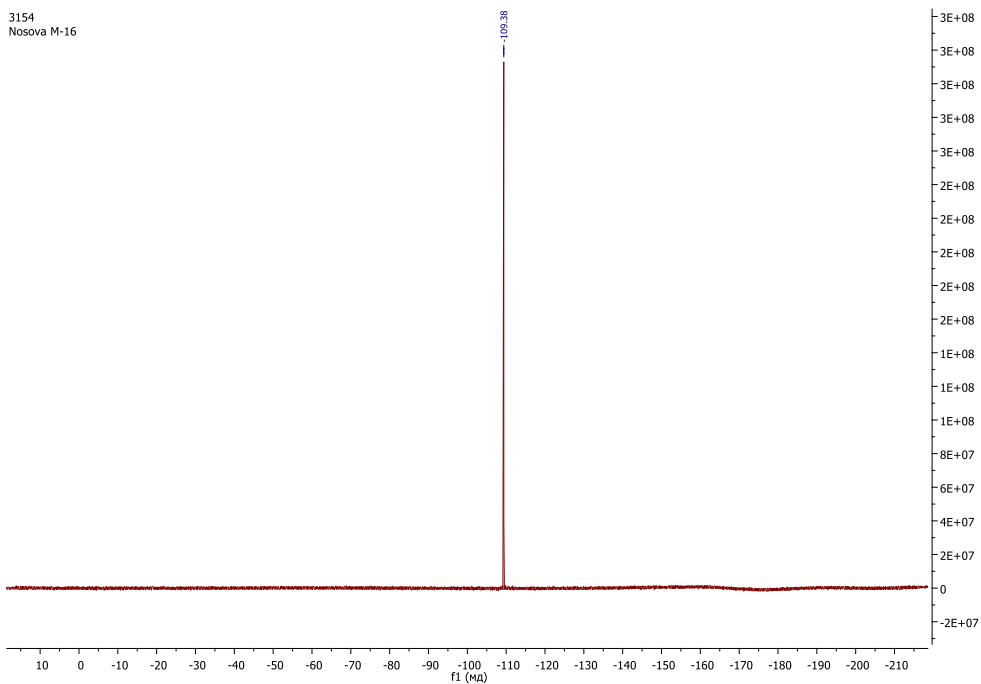


Figure S10 NMR ^{19}F spectra of chloroquinazoline **8** in DMSO-d_6 .

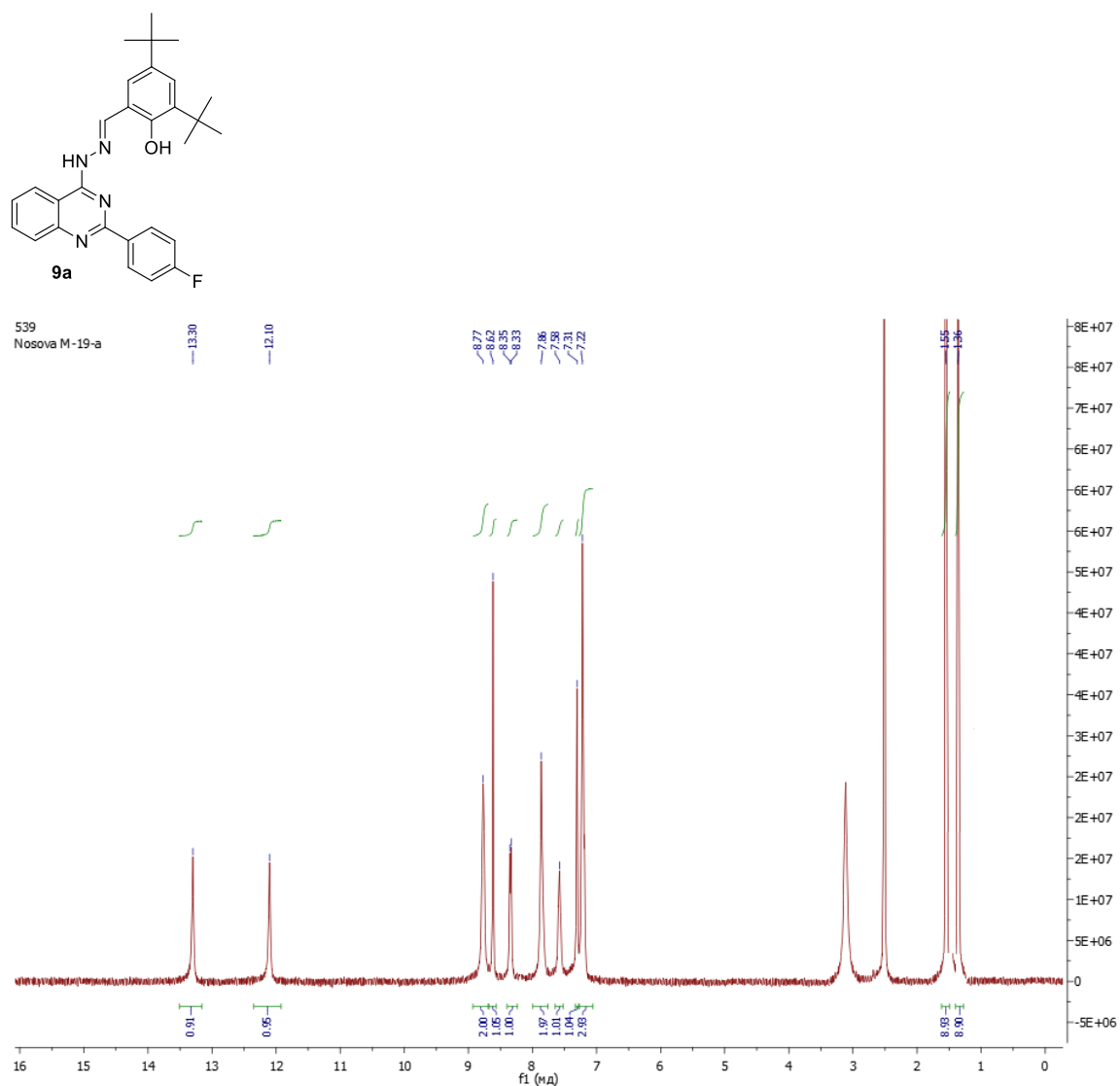


Figure S11 NMR ^1H spectra of salicylidenehydrazonoquinazoline **9a** in DMSO-d_6 .

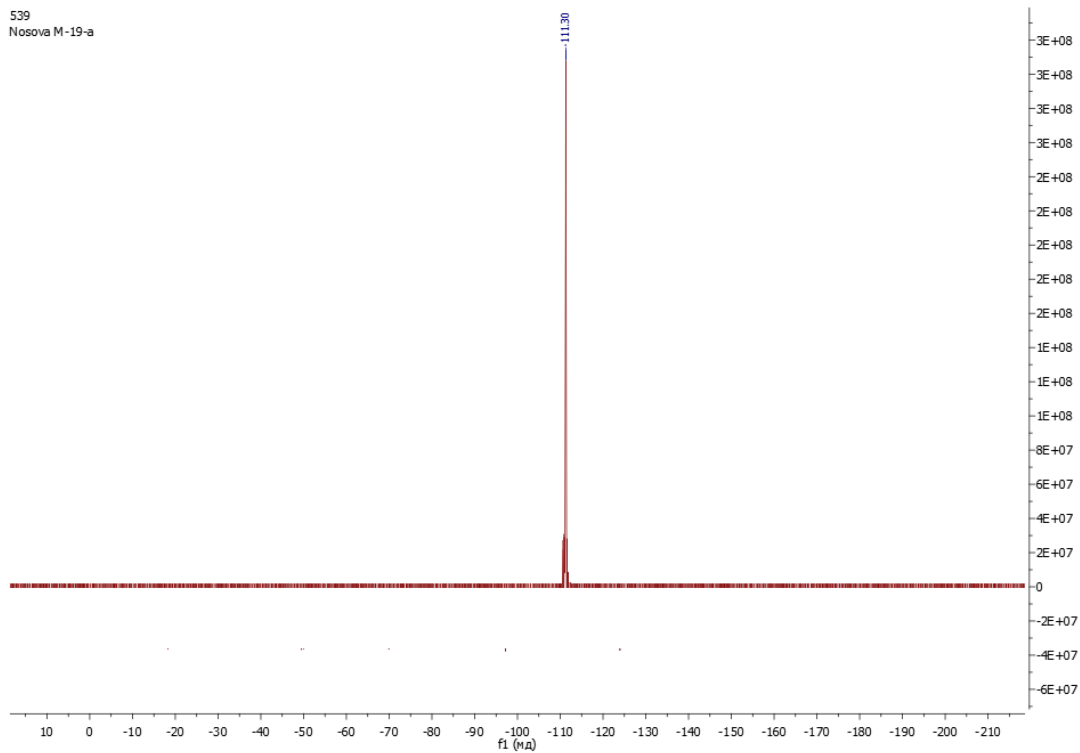


Figure S12 NMR ^{19}F spectra of salicylidenehydrazonoquinazoline **9a** in DMSO- d_6 .

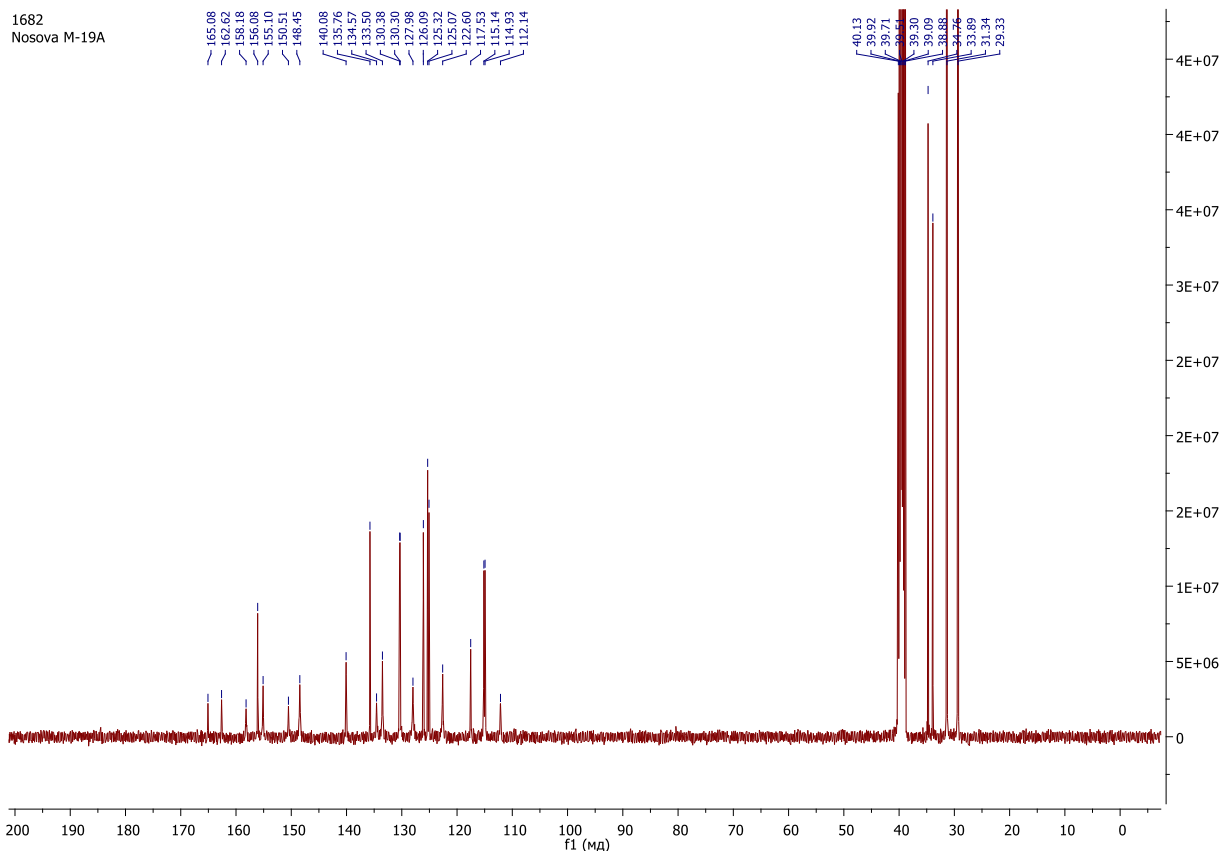


Figure 13 NMR ^{13}C spectra of salicylidenehydrazonequinazoline **9a** in DMSO- d_6 .

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Фон.реж.:1.010(385) Group 1 - Event 1

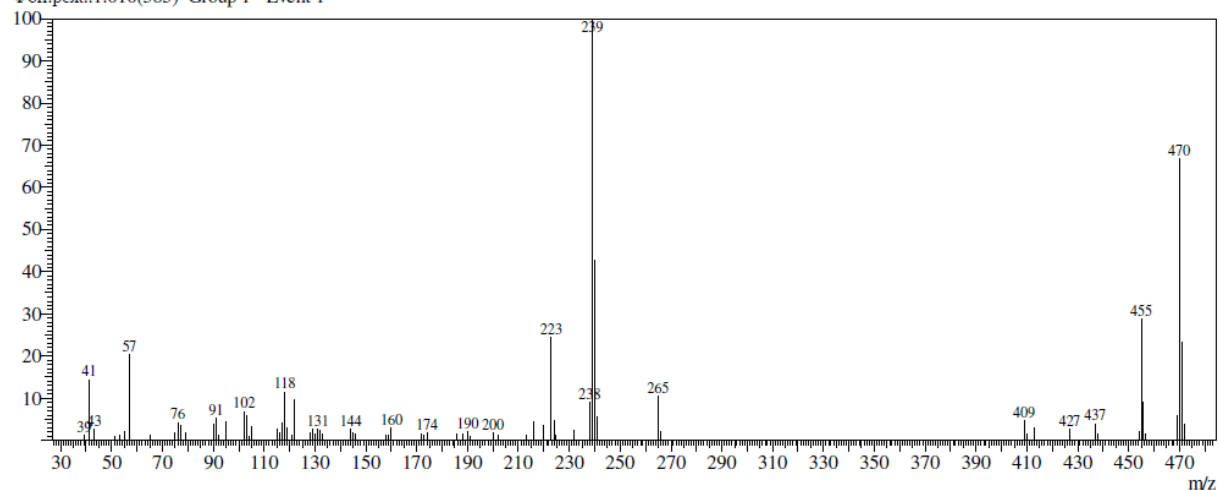
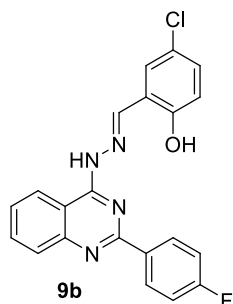


Figure S14 Mass spectra (EI) of salicylidenehydrazonequinazoline **9a**.



2182
Nosova M-18-0

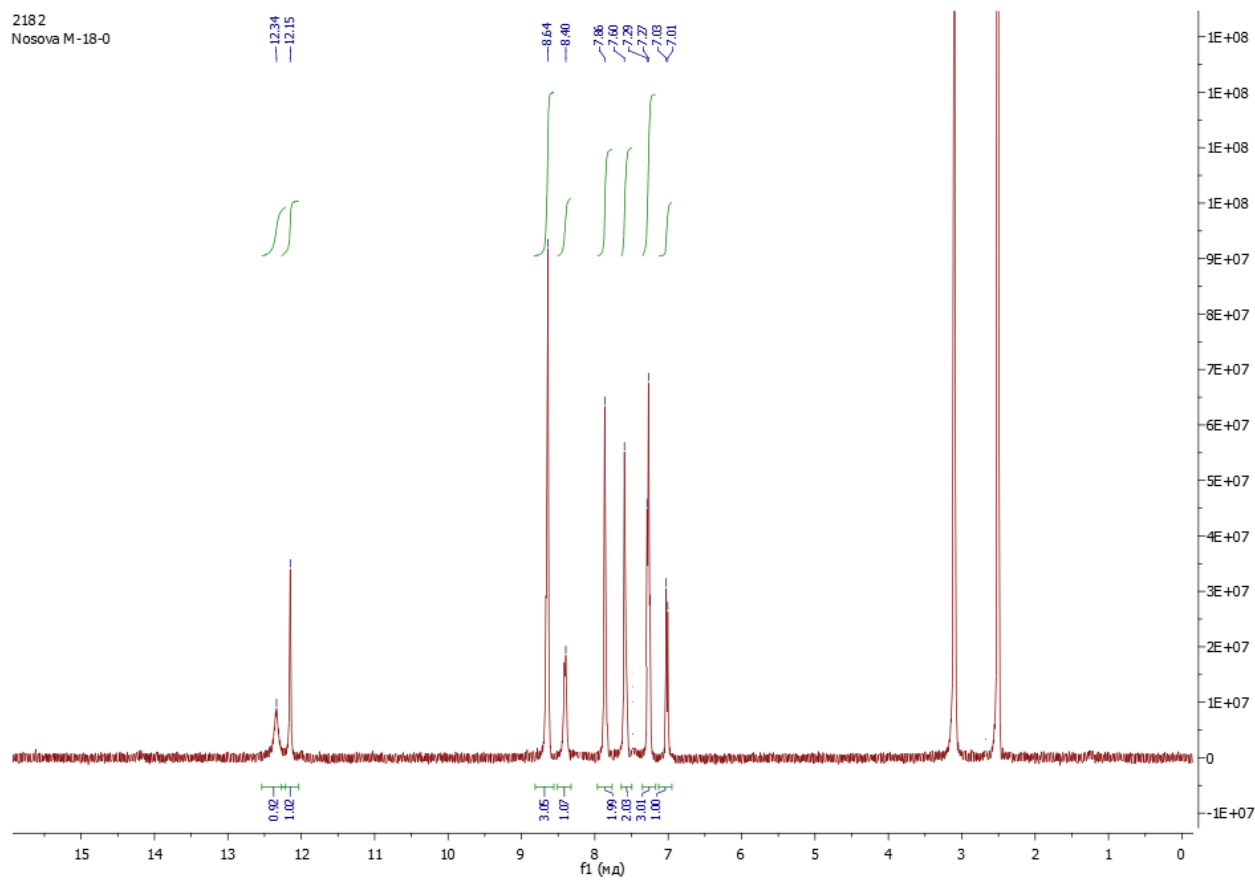


Figure S15 NMR ^1H spectra of salicylidenehydrazonequinazoline **9b** in DMSO- d_6 .



2182
Nosova M-18-0

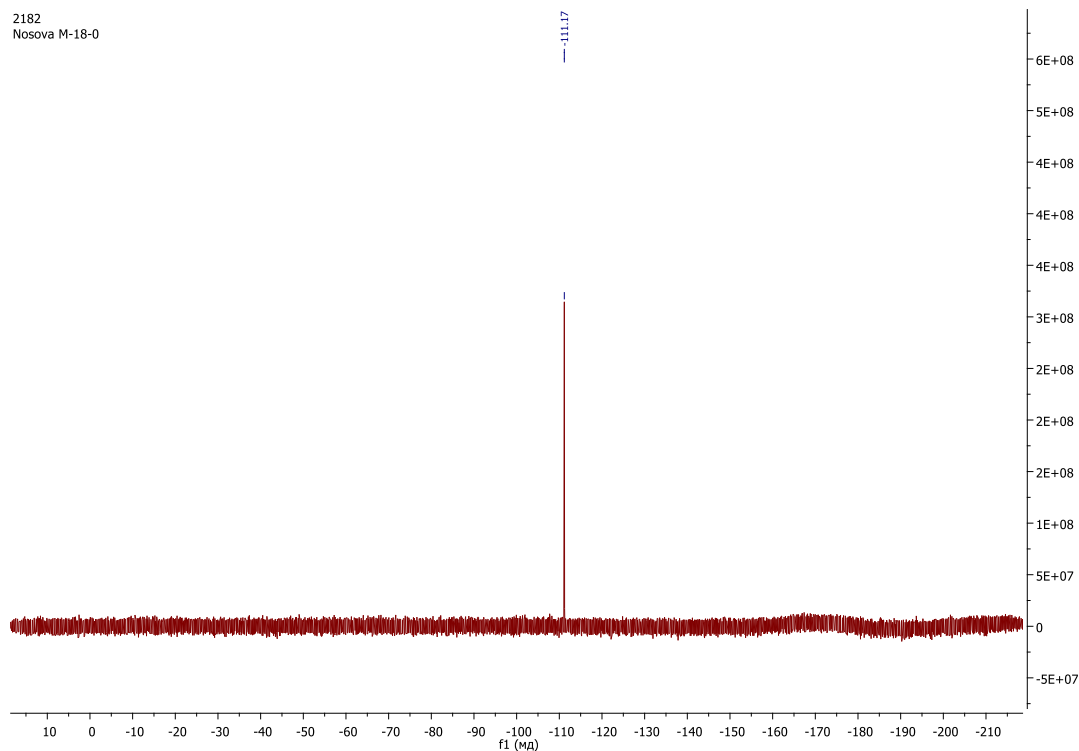


Figure S16 NMR ^{19}F spectra of salicylidenehydrazonequinazoline **9b** in DMSO- d_6 .

1681
Nosova M-18-2

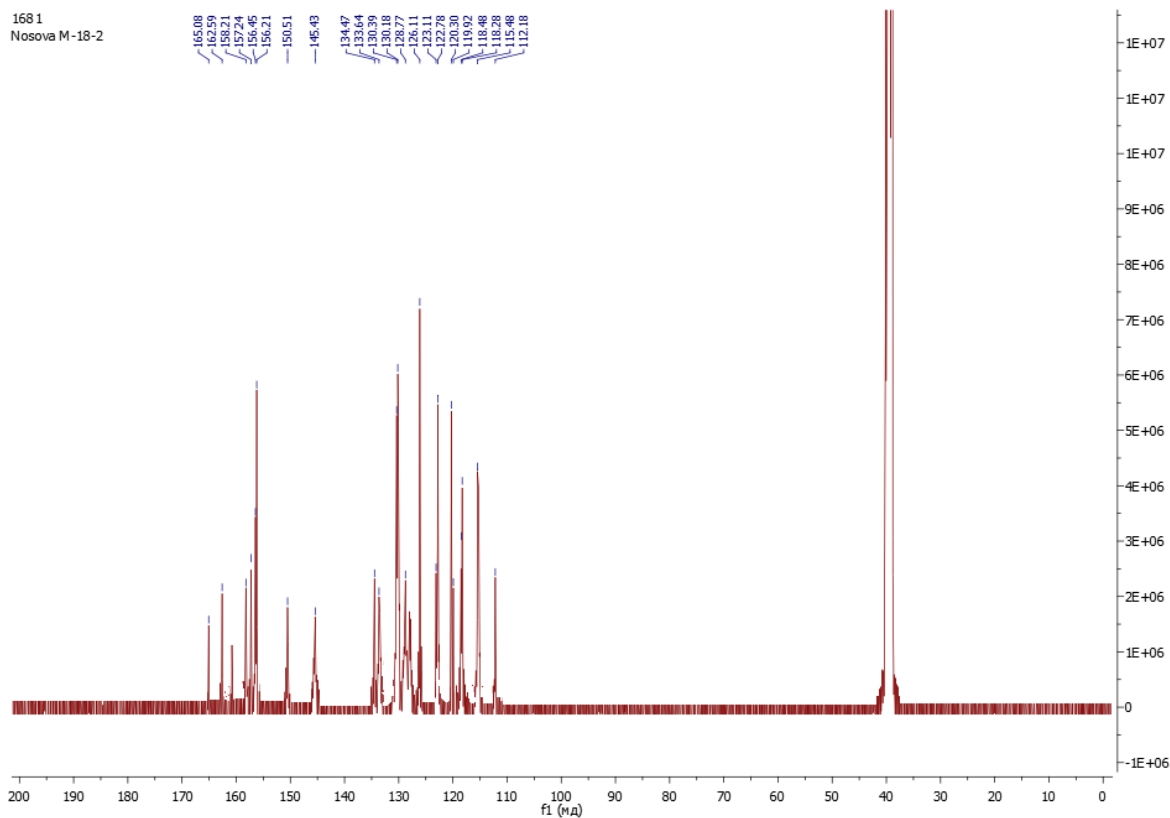


Figure S17 NMR ^{13}C spectra of salicylidenehydrazonequinazoline **9b** in DMSO- d_6 .



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Фон.реж.:3.092(1218) Group 1 - Event 1

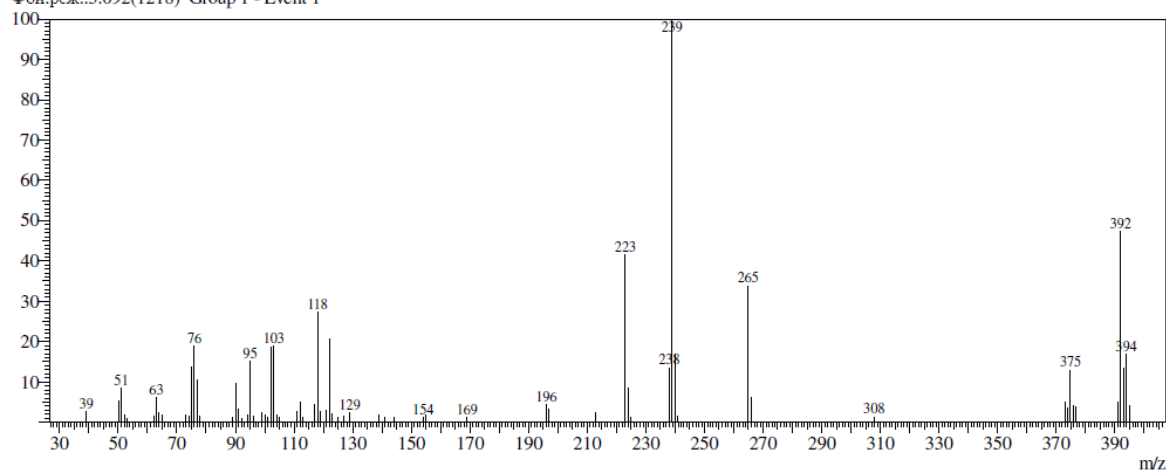


Figure S18 Mass spectra (EI) of salicylidenhydrazonoquinazoline **9b**.

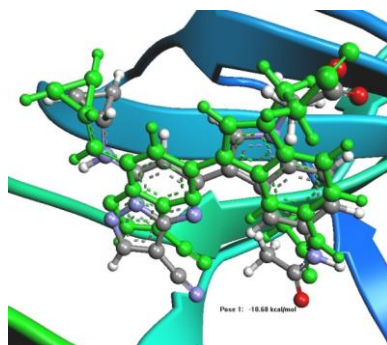


Figure S19 Redocking results of azolopyrimidine derivative, CK2 inhibitor (CHEMBL2062585): real position of ligand is shown in green; calculated positions are colored; $\text{RMSD}(\text{CHEMBL2062585}) = 0.89\text{\AA}$, $\Delta G_{\text{CHEMBL2062585}} = -10.67 \text{ kcal/mol}$.

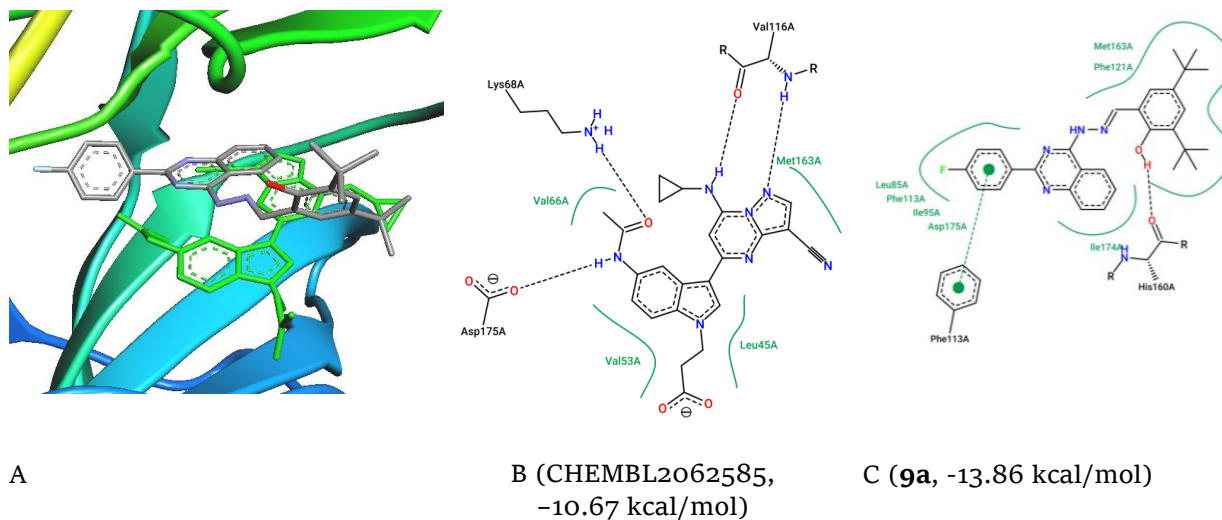


Figure S20 Docking results for ligand **9a**: A - The positions of native ligand CHEMBL2062585 (green) and docked ligand **9a** (colored atoms) in active center of CK2; B - Non-covalent interactions of the native ligand CHEMBL2062585; C - Non-covalent interactions of the docked ligand **9a**.

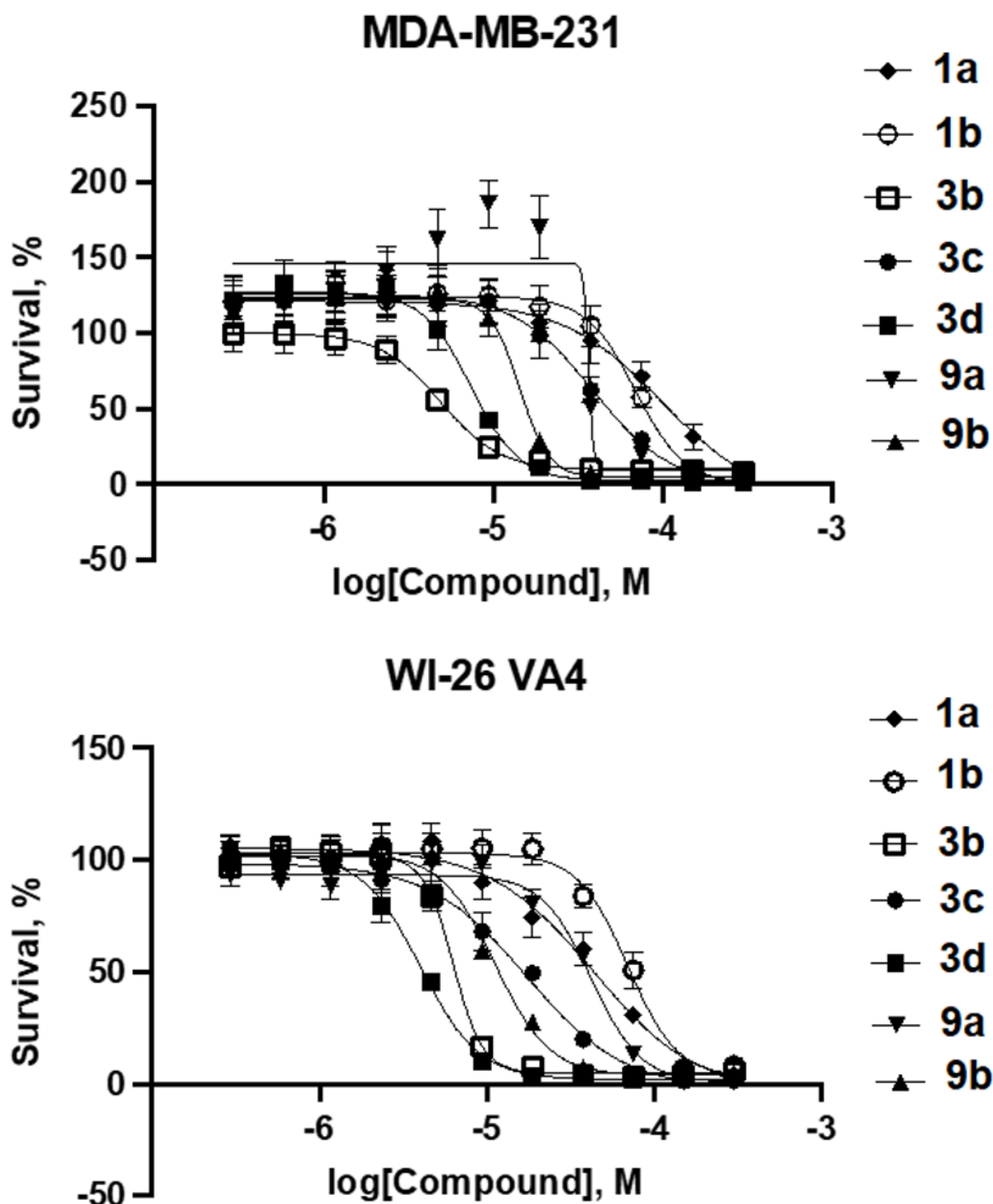


Figure S21 Cell growth inhibition curves for salicylidenehydrazones 1, 3, 9.