Supplementary Information

2-Acetyl quinoline analogues: Synthesis, ADME analysis and molecular docking studies

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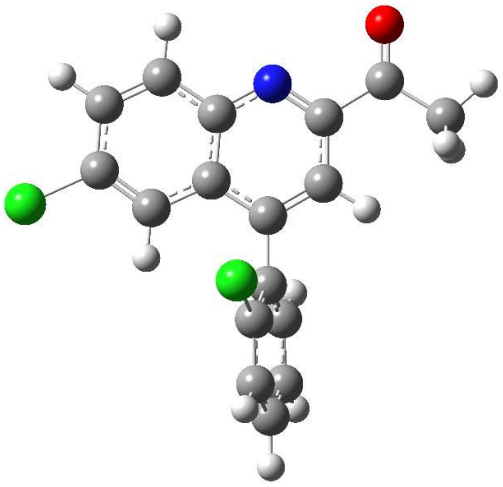
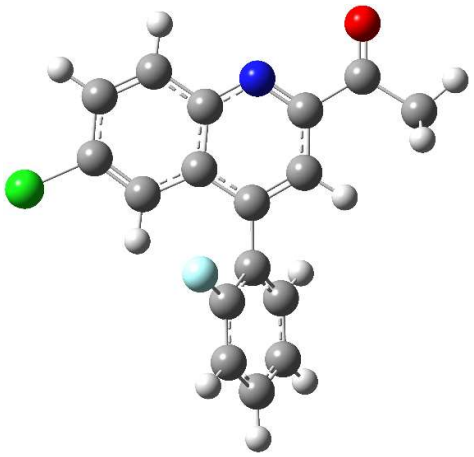


Supp. Fig. S1. Optimized structure of 3c.



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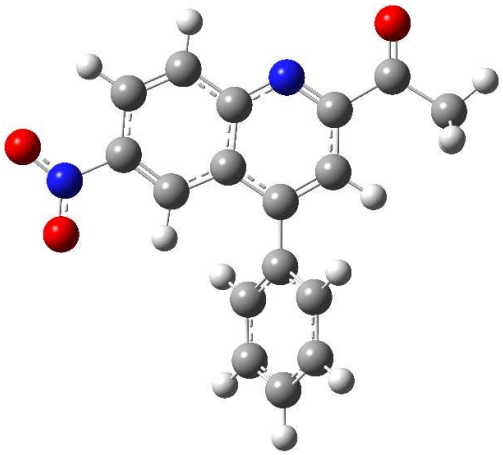
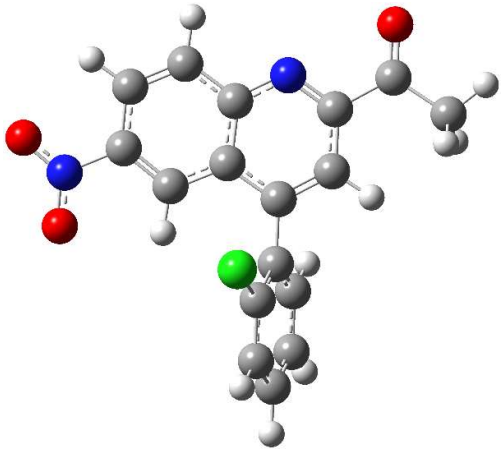


Supp. Fig. S3. Optimized structure of 3e.



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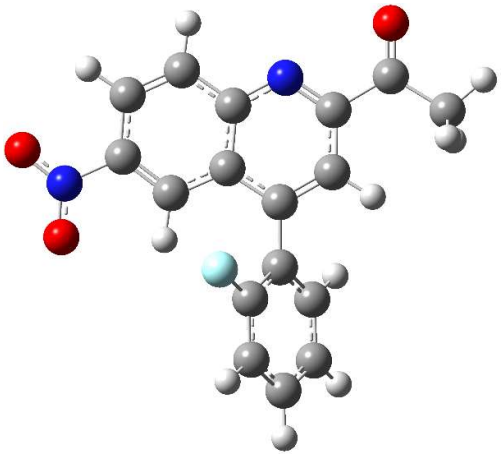

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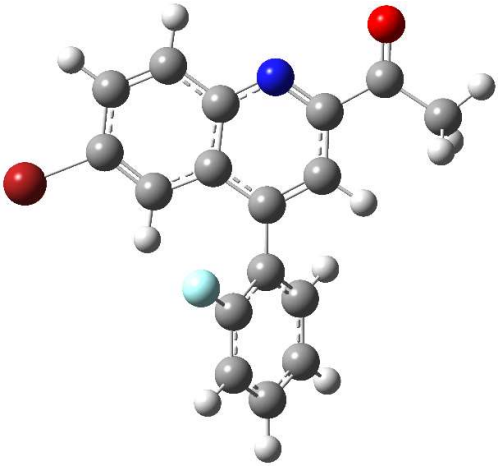

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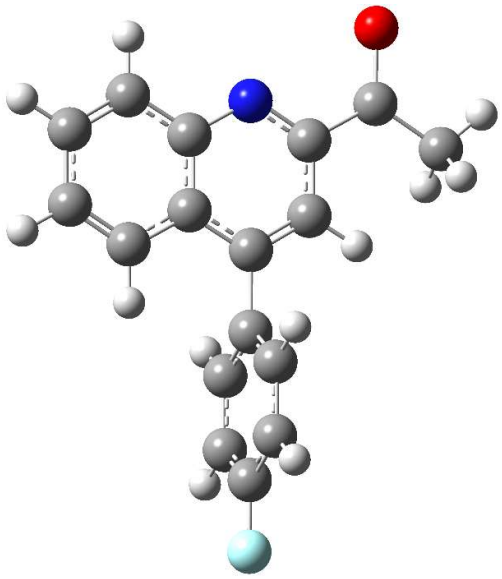
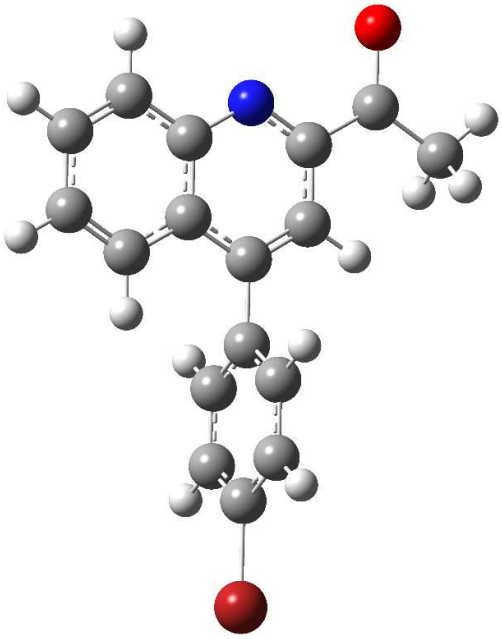
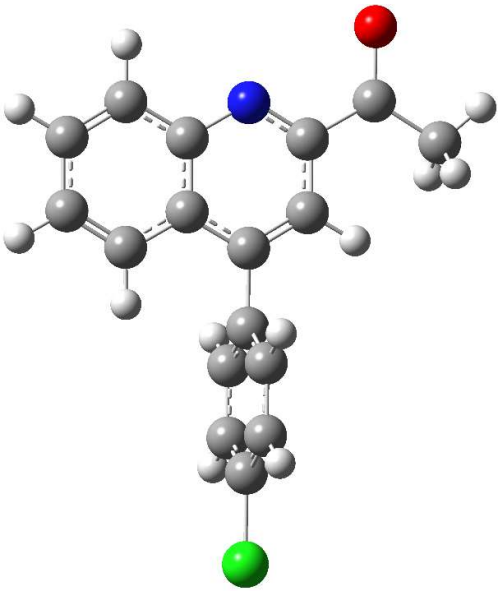


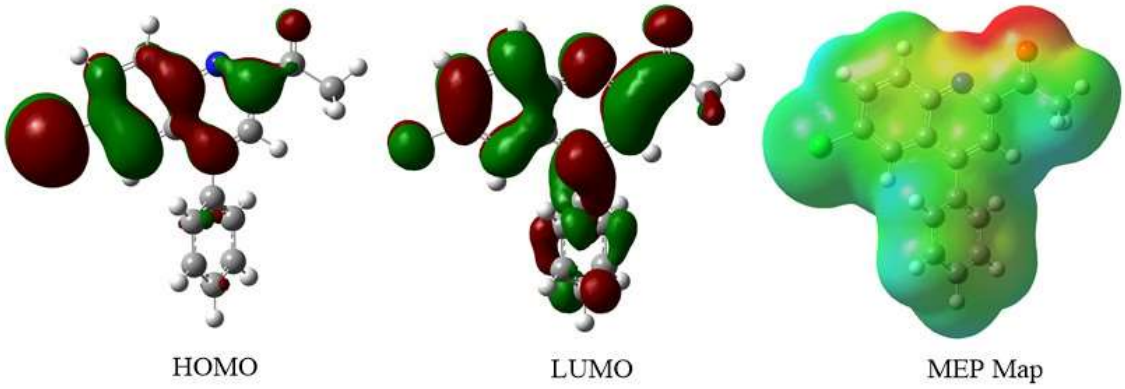
Supp. Fig. S7. Optimized structure of 3i.



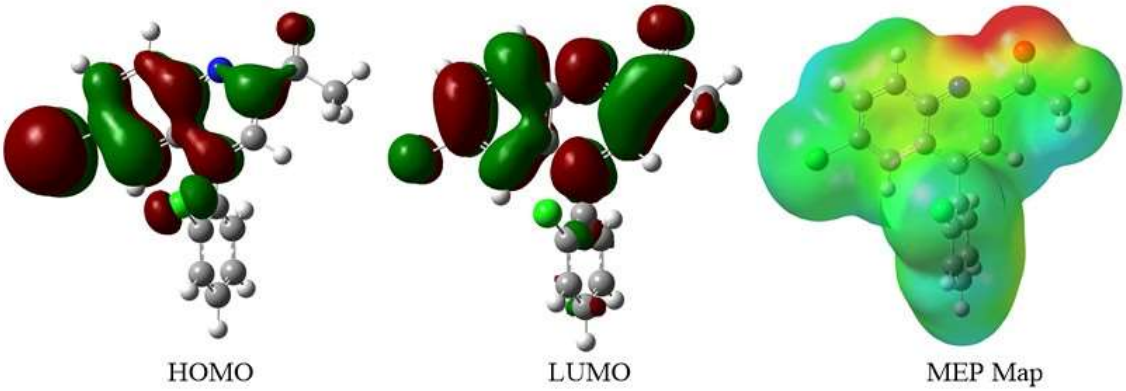
Supp. Fig. S8. Optimized structure of 3j.



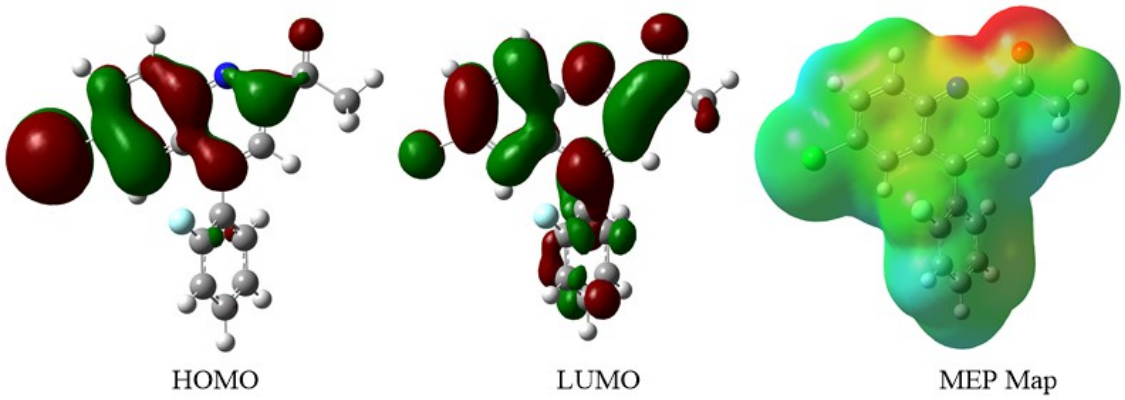
Supp. Fig. S9. Optimized structure of 3k.



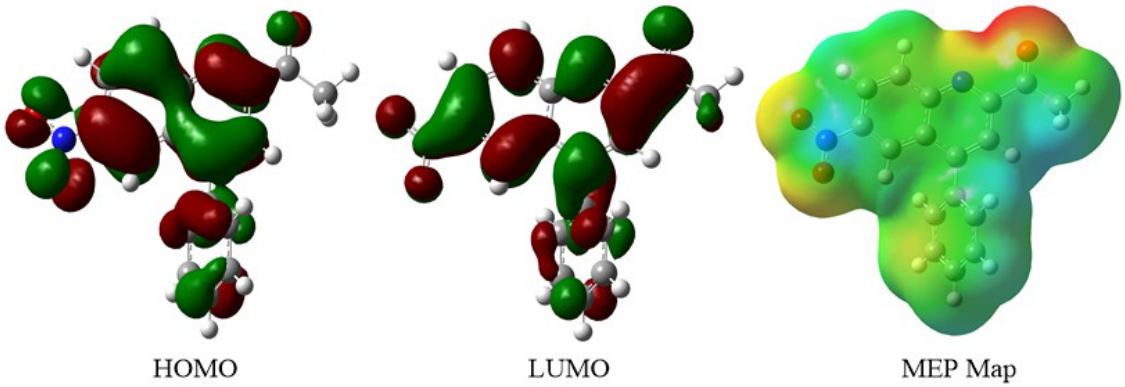
Supp. Fig. S10. Contour plot of HOMO, LUMO, and MEP map of compound **3b**.



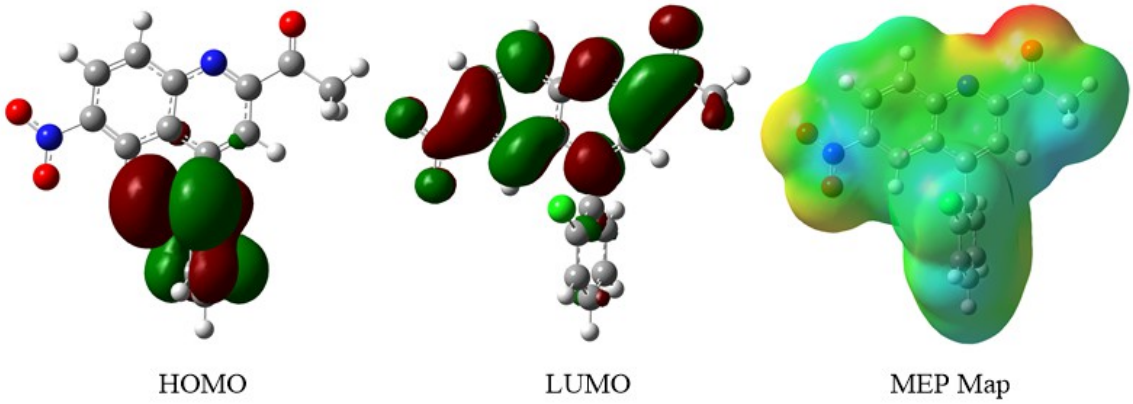
Supp. Fig. S11. Contour plot of HOMO, LUMO, and MEP map of compound **3c**.



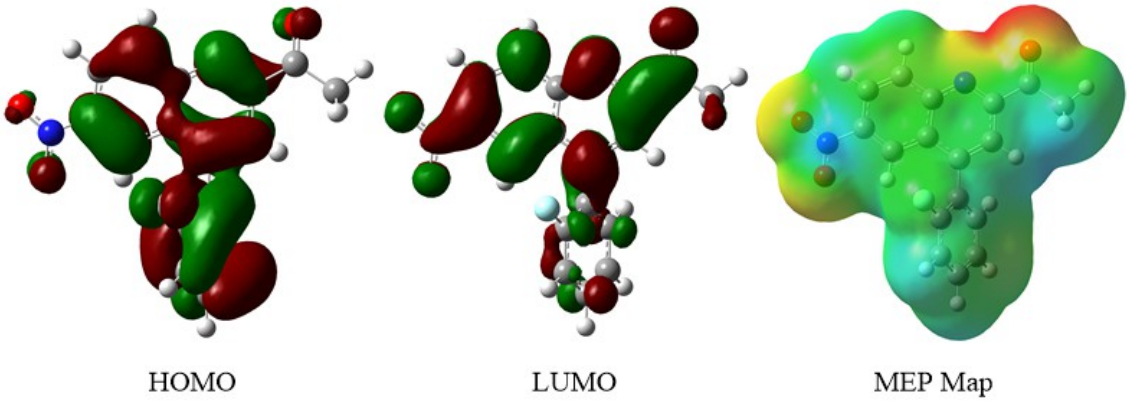
Supp. Fig. S12. Contour plot of HOMO, LUMO, and MEP map of compound **3d**.



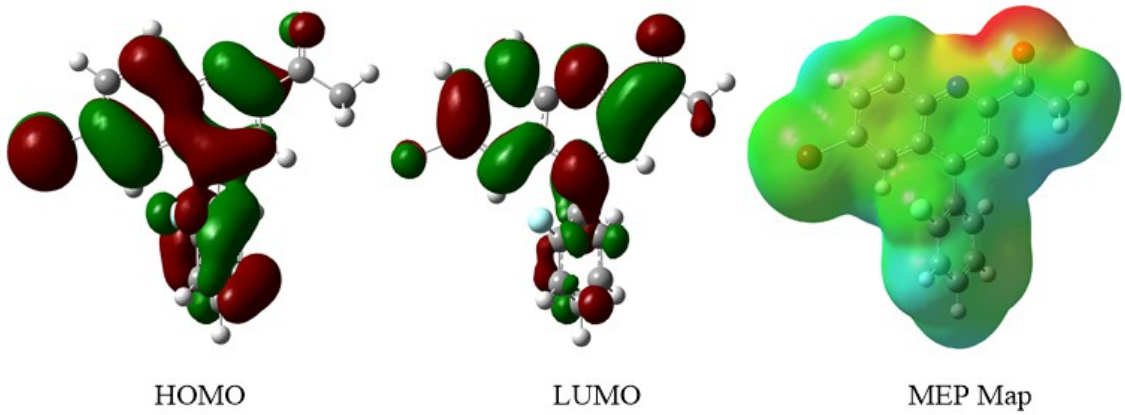
Supp. Fig. S13. Contour plot of HOMO, LUMO, and MEP map of compound **3e**.



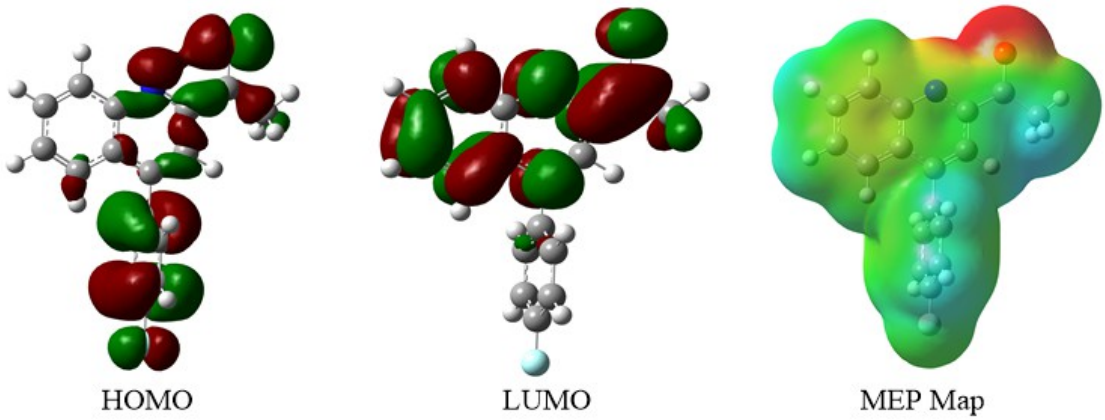
Supp. Fig. S14. Contour plot of HOMO, LUMO, and MEP map of compound **3f**.



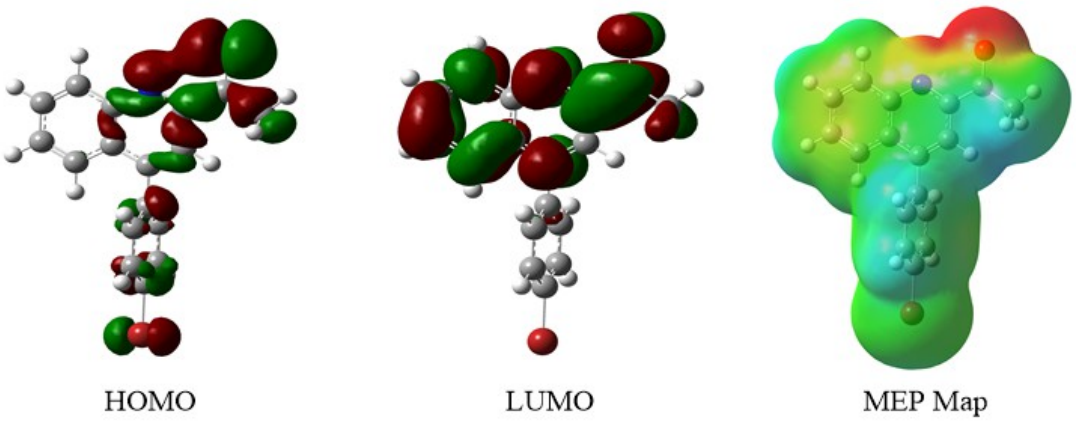
Supp. Fig. S15. Contour plot of HOMO, LUMO, and MEP map of compound **3g**.



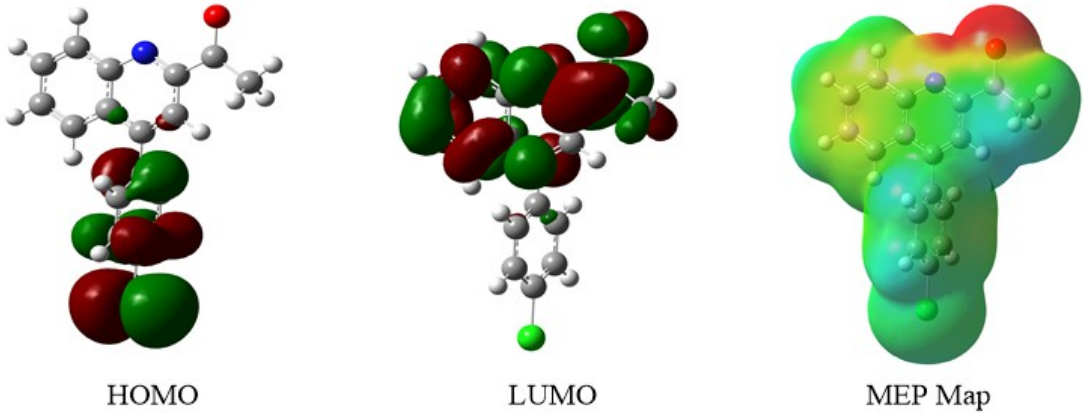
Supp. Fig. S16. Contour plot of HOMO, LUMO, and MEP map of compound **3h**.



Supp. Fig. S17. Contour plot of HOMO, LUMO, and MEP map of compound **3i**.



Supp. Fig. S18. Contour plot of HOMO, LUMO, and MEP map of compound **3j**.



Supp. Fig. S19. Contour plot of HOMO, LUMO, and MEP map of compound **3k**.

Supp. Table S1. Calculated QikProp parameters of studied compounds for ADME analyses

Parameters[a]	3h	3i	3j	3k	RV[b]
Stars	1.0	0.0	0.0	0.0	0-5
Amine	0.0	0.0	0.0	0.0	0-1
rtvFG	0.0	0.0	0.0	0.0	0-2
SASA	549.3	531.4	550.8	545.8	300.0-1000.0
FOSA	84.0	100.6	100.6	100.6	0.0-750.0
FISA	59.1	53.7	53.7	53.7	7.0-330.0
PISA	293.5	330.3	319.3	320.0	0.0-450.0
WPSA	112.7	46.8	77.3	71.5	0.0-175.0
donorHB	0.0	1.0	1.0	1.0	0.0-6.0
AccptHB	3.0	2.7	2.7	2.7	2.0-20.0
QPpolrz	32.6	31.0	32.3	32.0	13.0-70.0
QPPCaco	2724.6	3068.1	3068.4	3067.9	<25 poor >500 great
QPlogBB	0.2	0.0	0.1	0.1	-3.0- 1.2
QPPMDCK	6054.8	2999.9	4404.5	4095.7	<25 poor

QPlogKp					>500 great -8.0-
	-1.4	-1.1	-1.1	-1.1	-1.0
metab	0.0	1.0	1.0	1.0	1-8
QPlogKhsa	0.4	0.4	0.5	0.5	-1.5- 1.5
Percent Human-Oral Absorption	100.0	100.0	100.0	100.0	>80% is high <25% is poor
PSA	38.6	32.7	32.7	32.7	7.0- 200.0
RuleOfFive	0.0	0.0	0.0	0.0	Max is 4
RuleOfThree	0.0	0.0	0.0	0.0	Max is 3

[a] **Stars**: Number of property or descriptor values that fall outside the 95% range of similar values for known drugs; **Amine**: Number of non-conjugated amine groups; **rtvFG**: Number of reactive functional groups; **SASA**: Total solvent accessible surface area; FOSA: Hydrophobic component of the SASA; **FISA**: Hydrophilic component of the SASA; **PISA**: π (carbon and attached hydrogen) component of the SASA; **WPSA**: Weakly polar component of the SASA; **donorHB**: Estimated number of hydrogen bonds that would be donated; **AccptHB**: Estimated number of hydrogen bonds that would be accepted; **QPpolrz**: Predicted polarizability in cubic angstroms; **QPPCaco**: Predicted apparent Caco-2 cell permeability in nm/sec; **QPlogBB**: Predicted brain/blood partition coefficient; **QPPMDCK**: Predicted apparent MDCK cell permeability in nm/sec; **QPlogKp**: Predicted skin permeability; **metab**: Number of likely metabolic reactions; **QPlogKhsa**: Prediction of binding to human serum albumin; **PercentHuman-OralAbsorption**: Predicted human oral absorption on 0 to 100% scale; **PSA**: Van der Waals surface area of polar nitrogen and oxygen atoms; **RuleOfFive**: Number of violations of Lipinski's rule of five; **RuleOfThree**: Number of violations of Jorgensen's rule of three.

[b] RV: Recommended Value

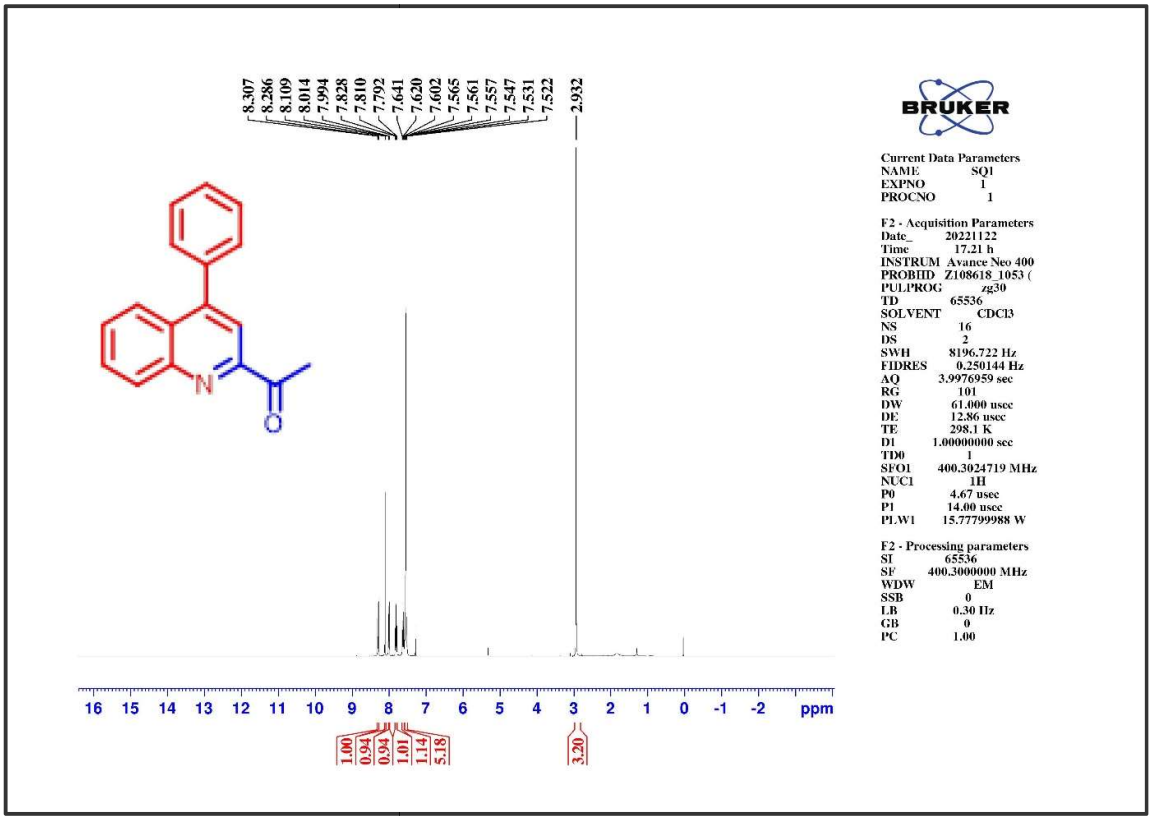


Fig. S20 The [1]H-NMR of the molecule 3a

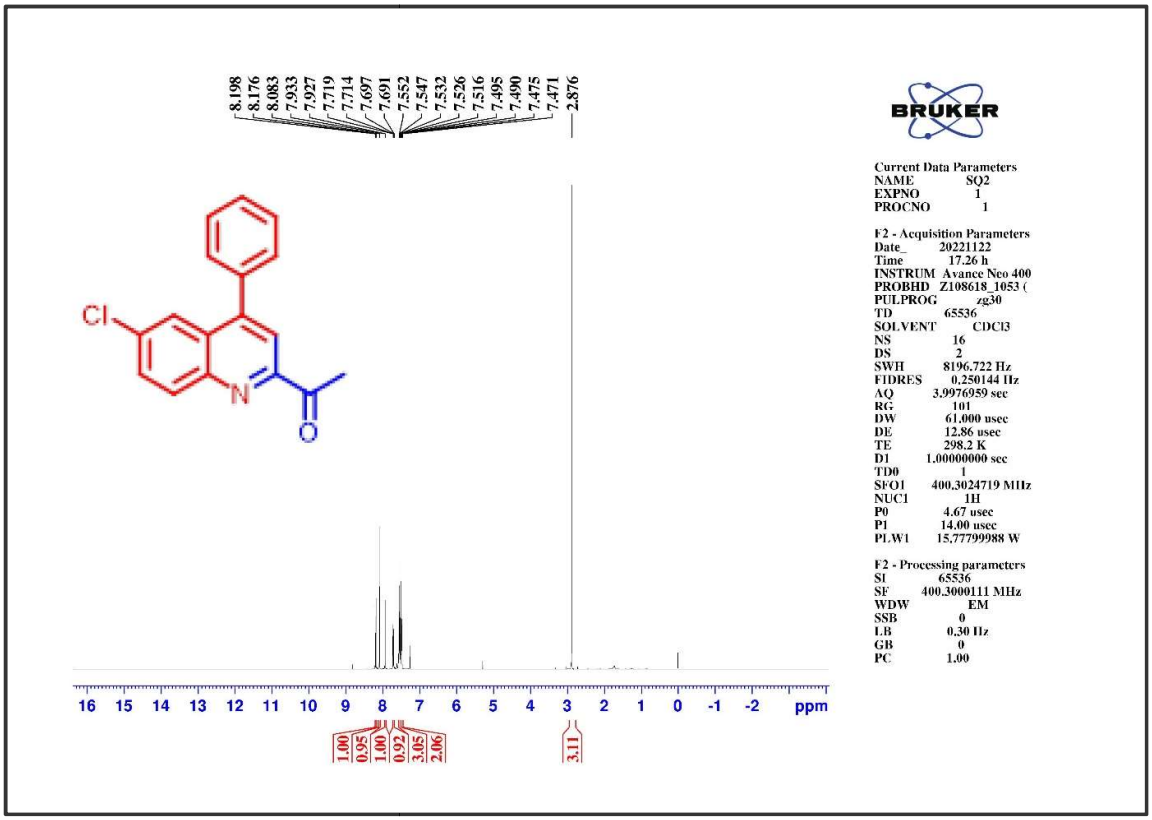


Fig. S21 The ^{1}H-NMR of the molecule 3b

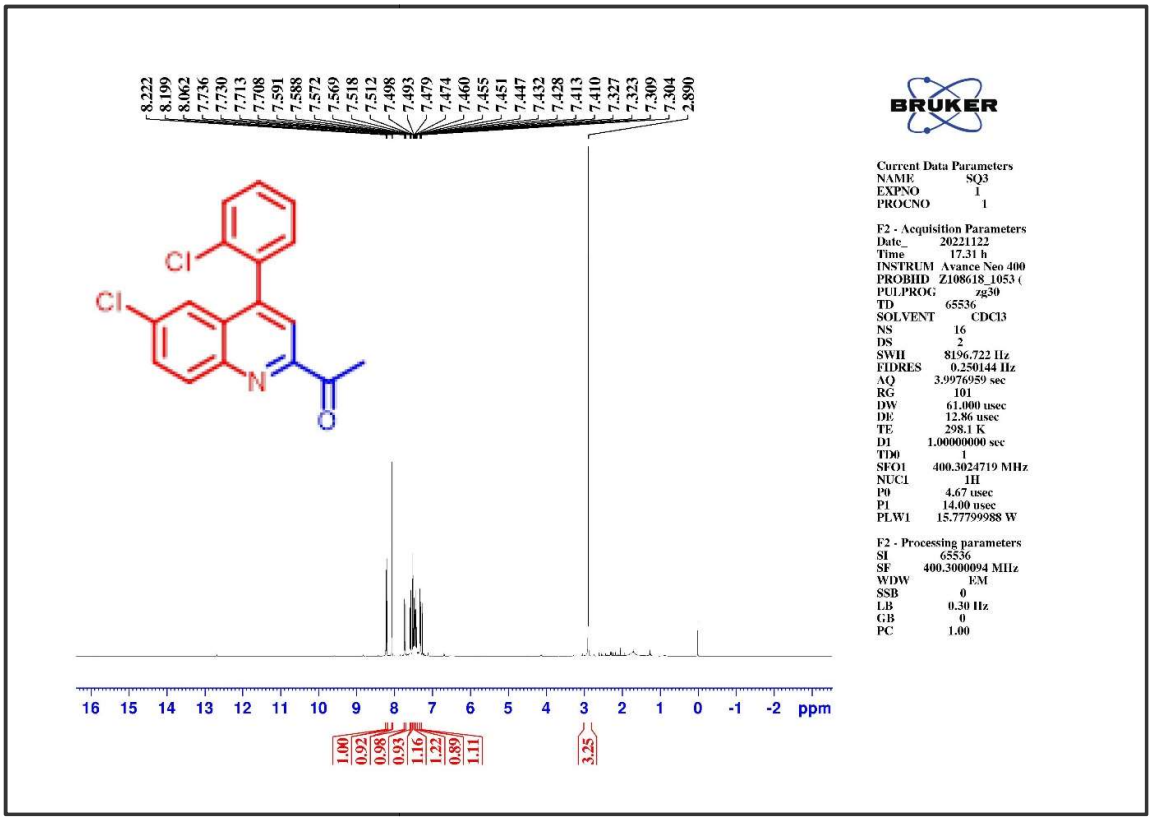


Fig. S22 The ^{1}H-NMR of the molecule 3c

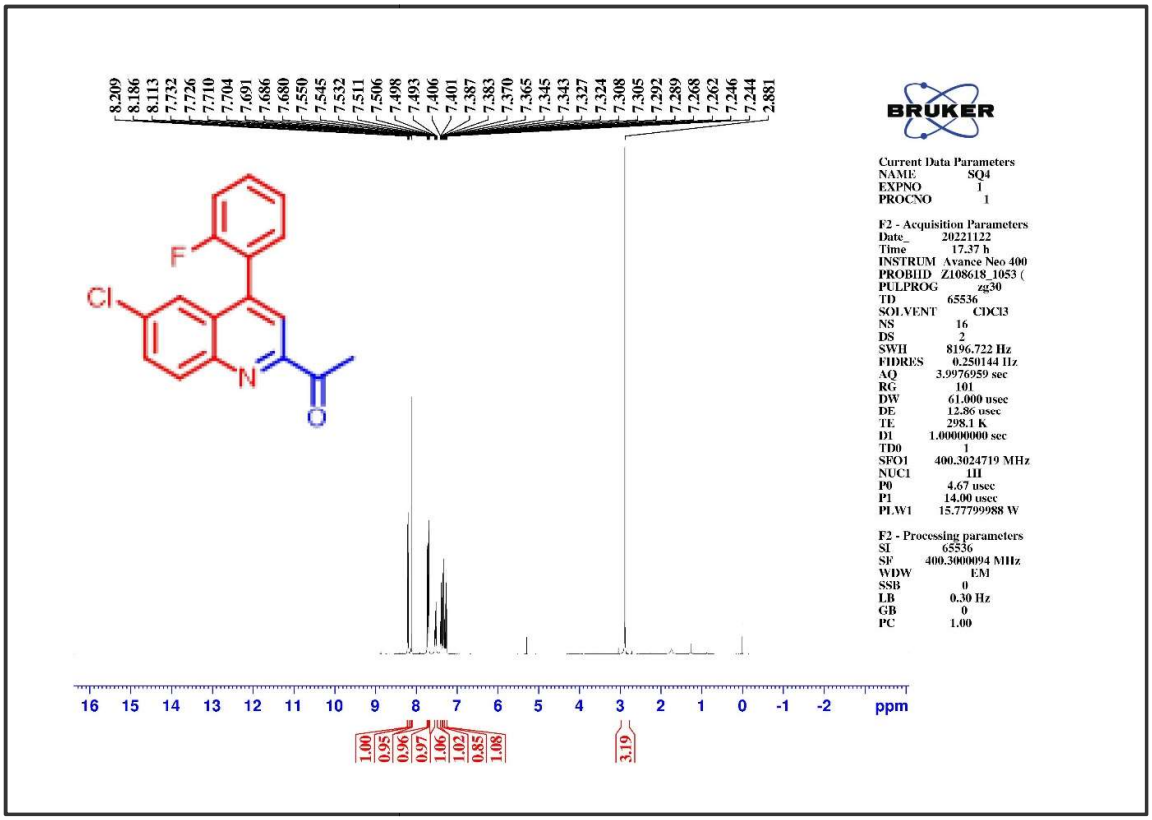


Fig. S23 The ^{1}H-NMR of the molecule 3d

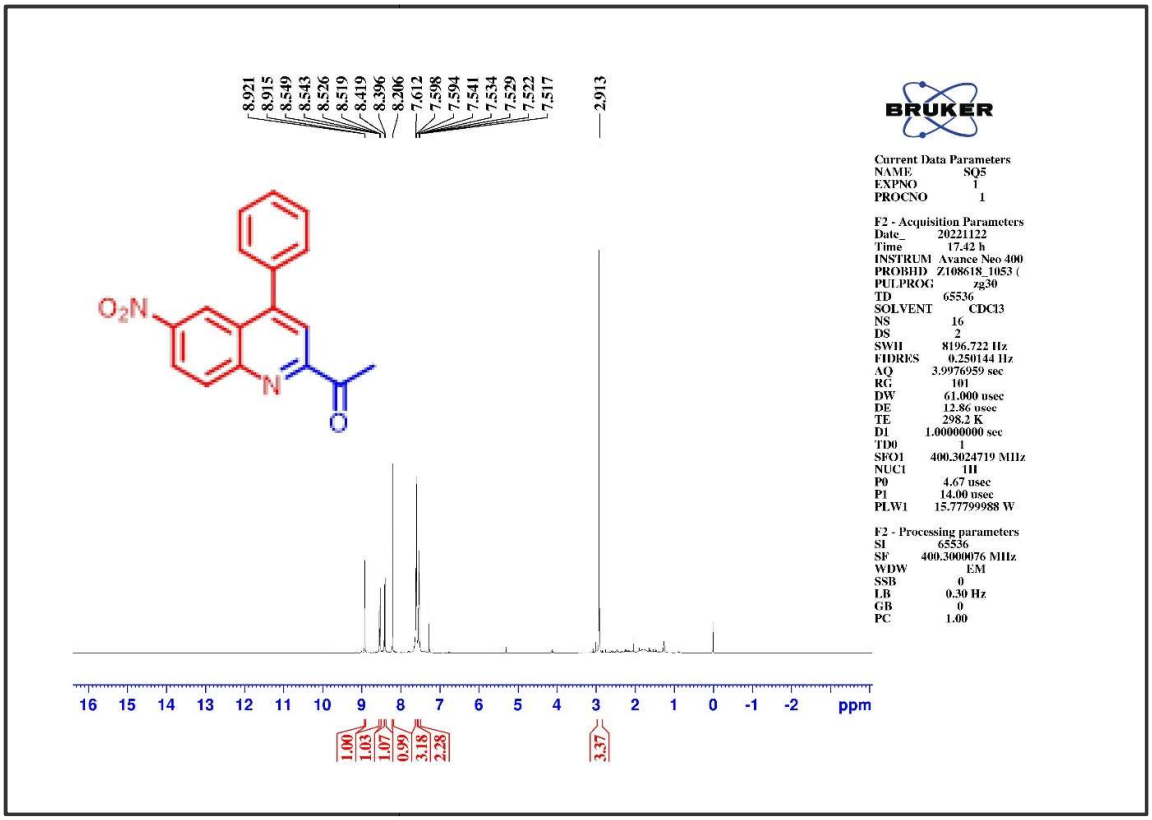


Fig. S24 The ^{1}H-NMR of the molecule 3e

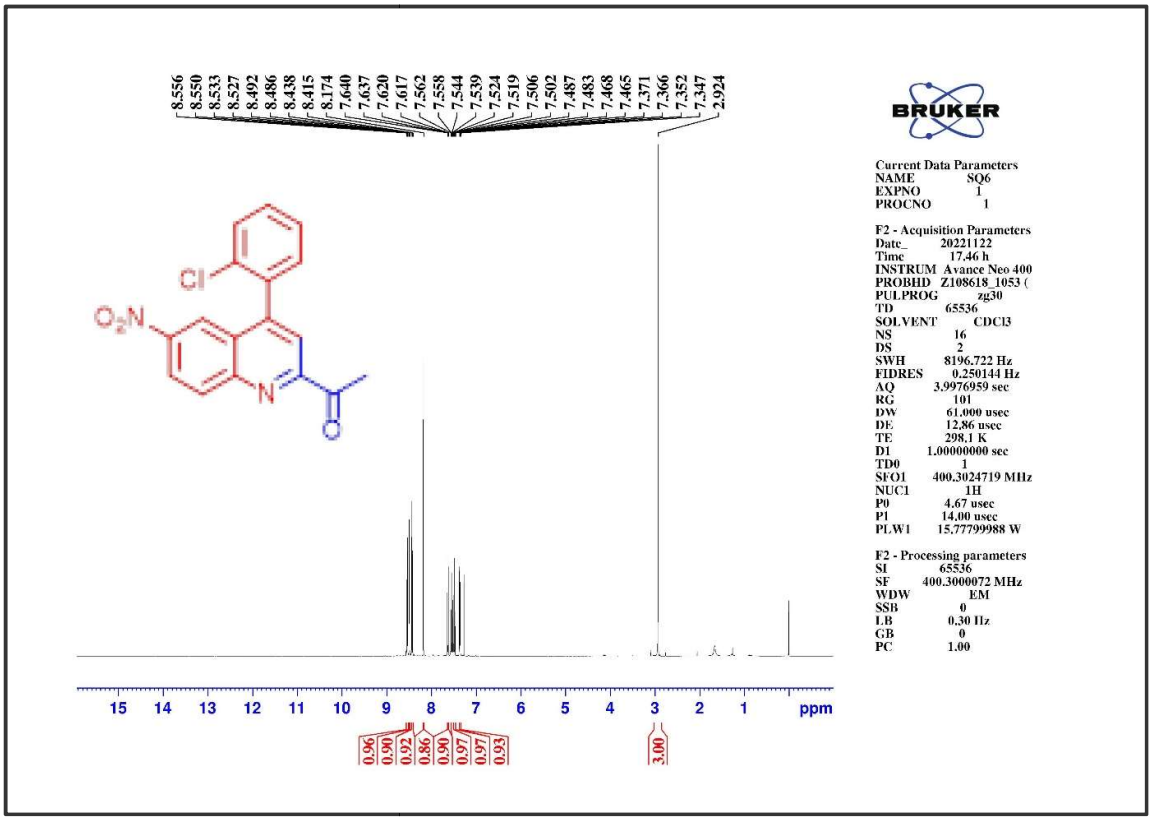


Fig. S25 The ^{1}H-NMR of the molecule 3f

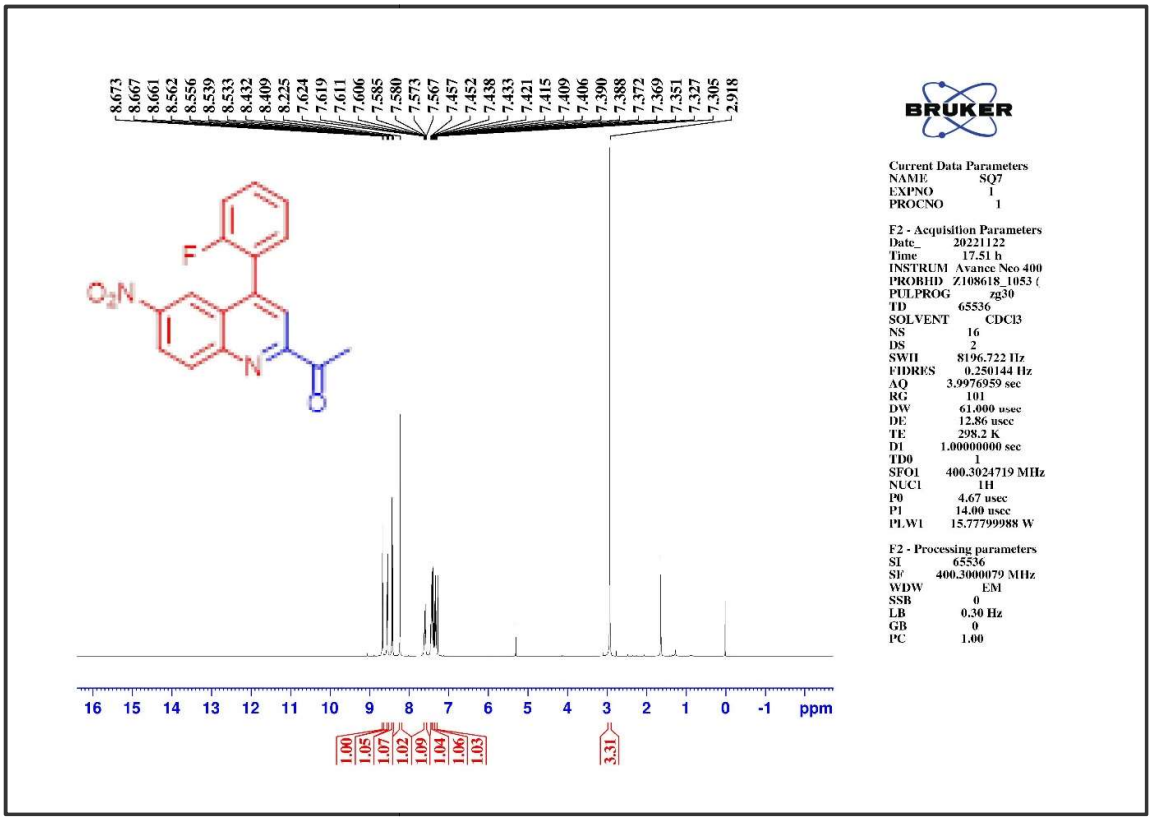


Fig. S26 The ^{1}H-NMR of the molecule 3g

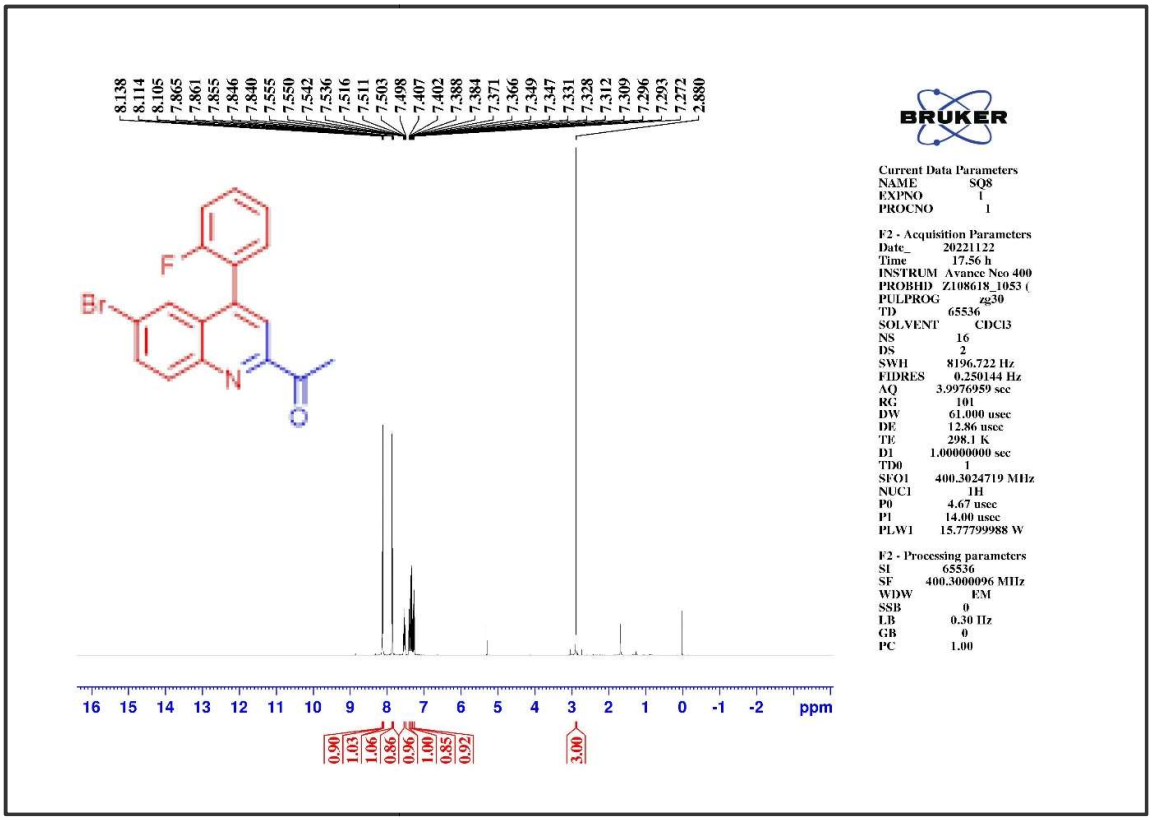


Fig. S27 The ^{1}H-NMR of the molecule 3h

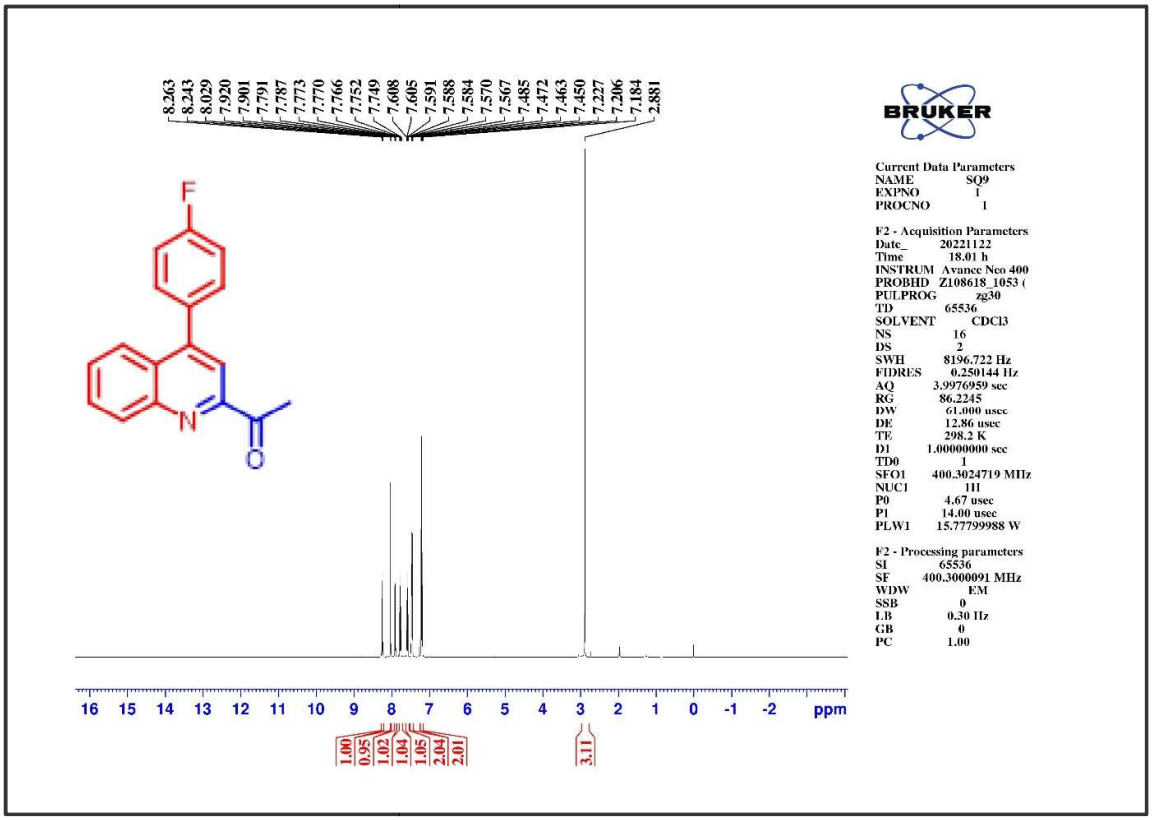


Fig. S28 The ^{1}H-NMR of the molecule 3i

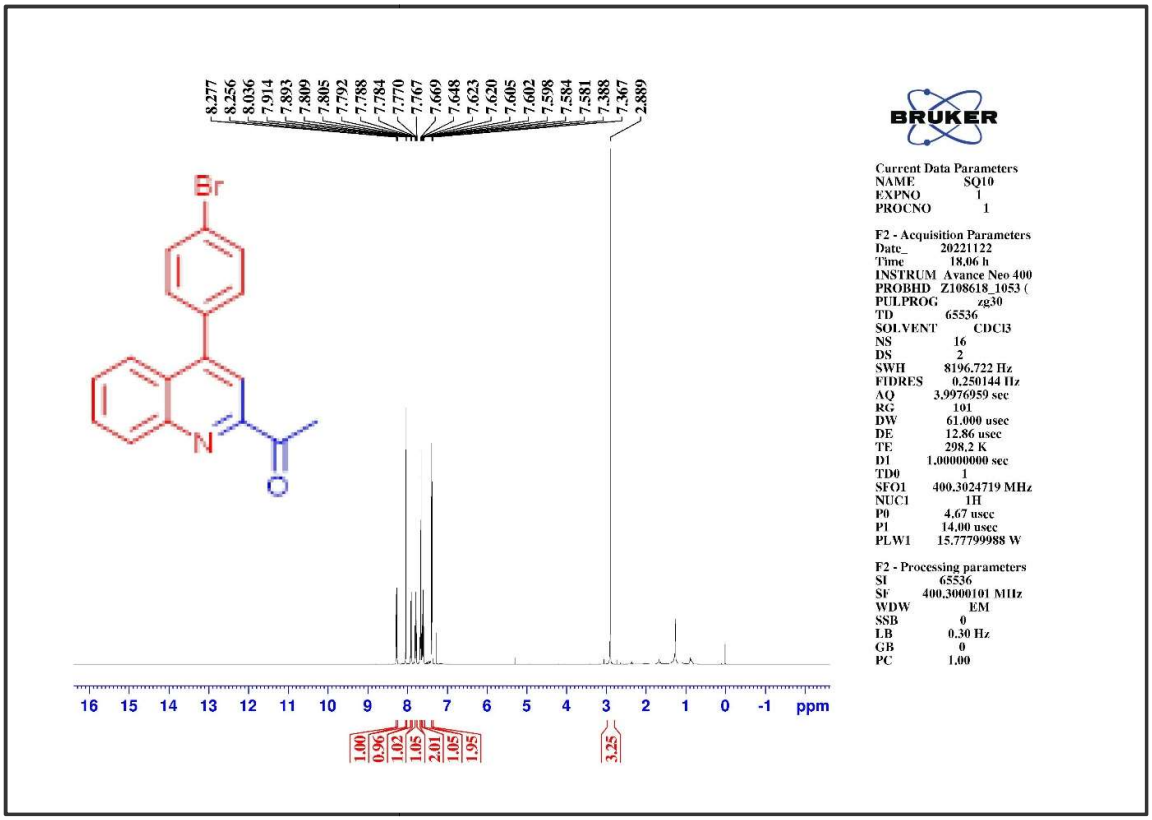


Fig. S29 The ^{1}H-NMR of the molecule 3j

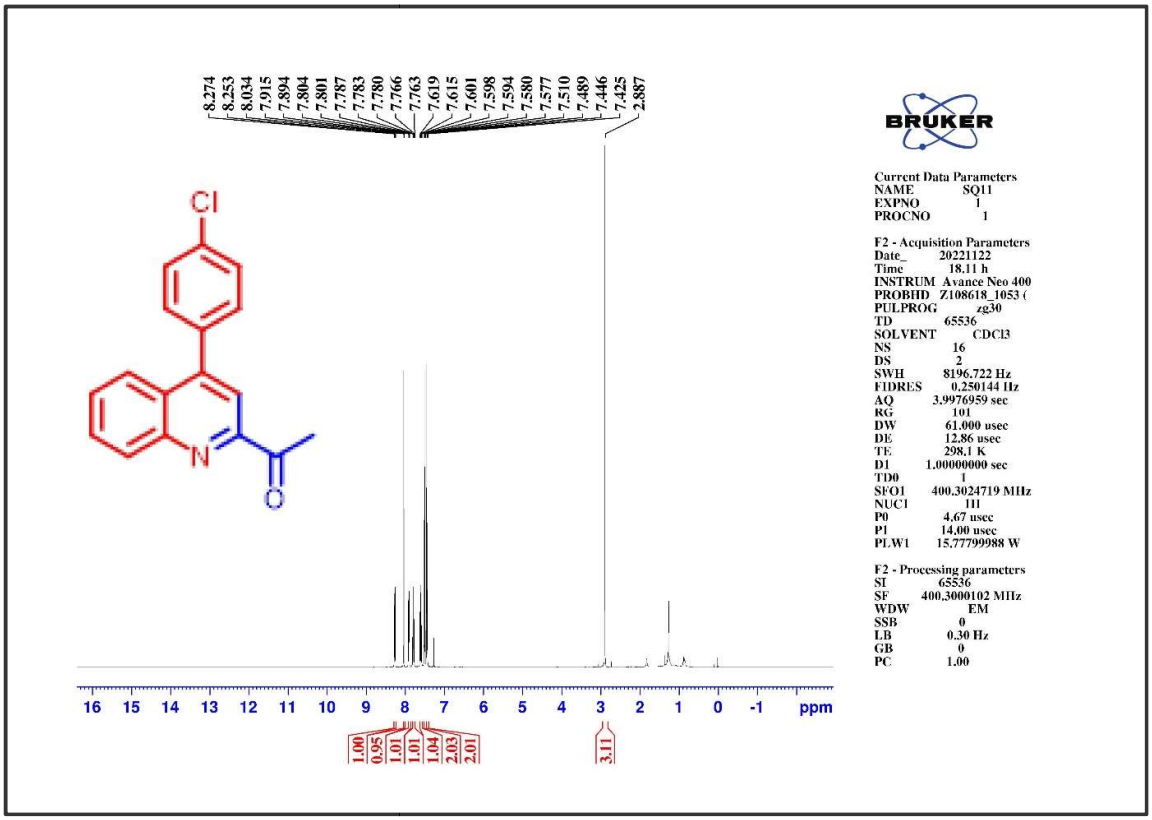


Fig. S30 The ^{1}H-NMR of the molecule 3k