Crystal Structure, Hirshfeld Surface Analysis, and Computational Study of Quinolin-8-yl 4-Chlorobenzoate: Insights from Spectroscopic, Thermal, and Antitumor Properties

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SUPPORTING INFORMATION

1. Copy of the EI-MS spectrum for compound 3

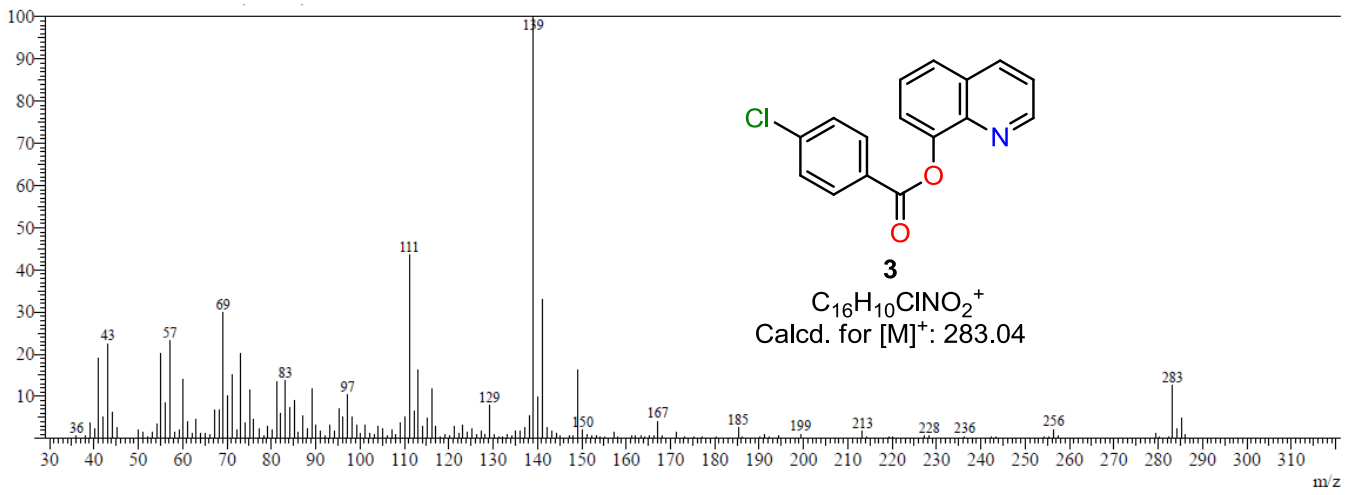


Figure S1: EI-MS spectrum for compound **3**.

2. Copies of FT-IR spectra for compound 3

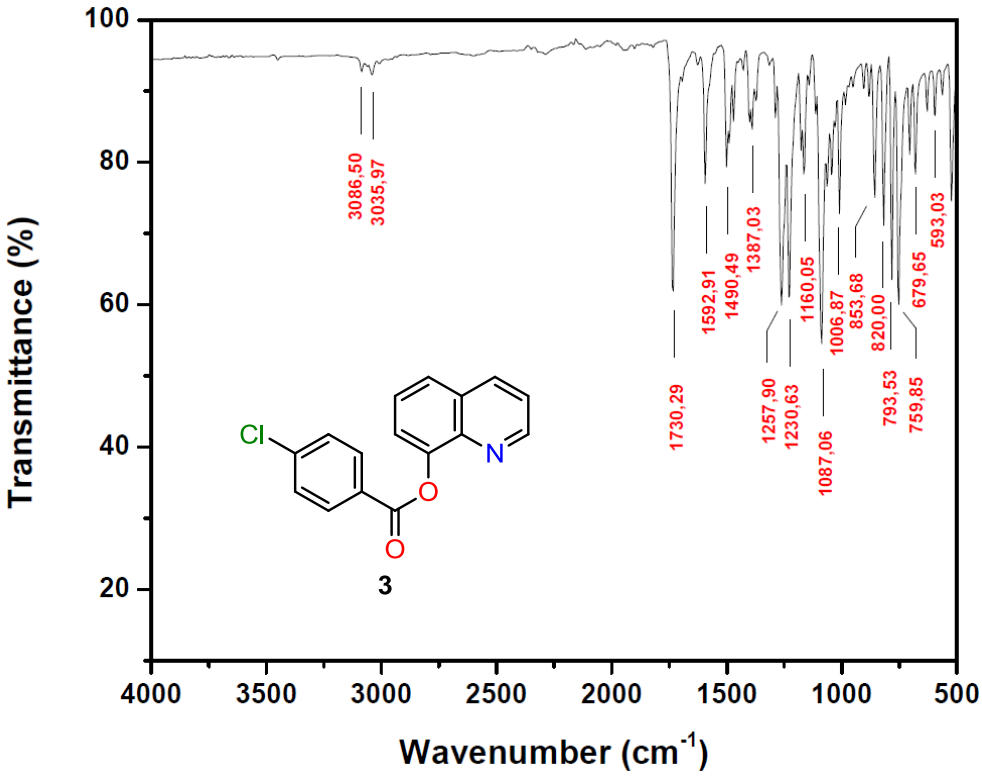


Figure S2: FT-IR spectrum for compound **3**.

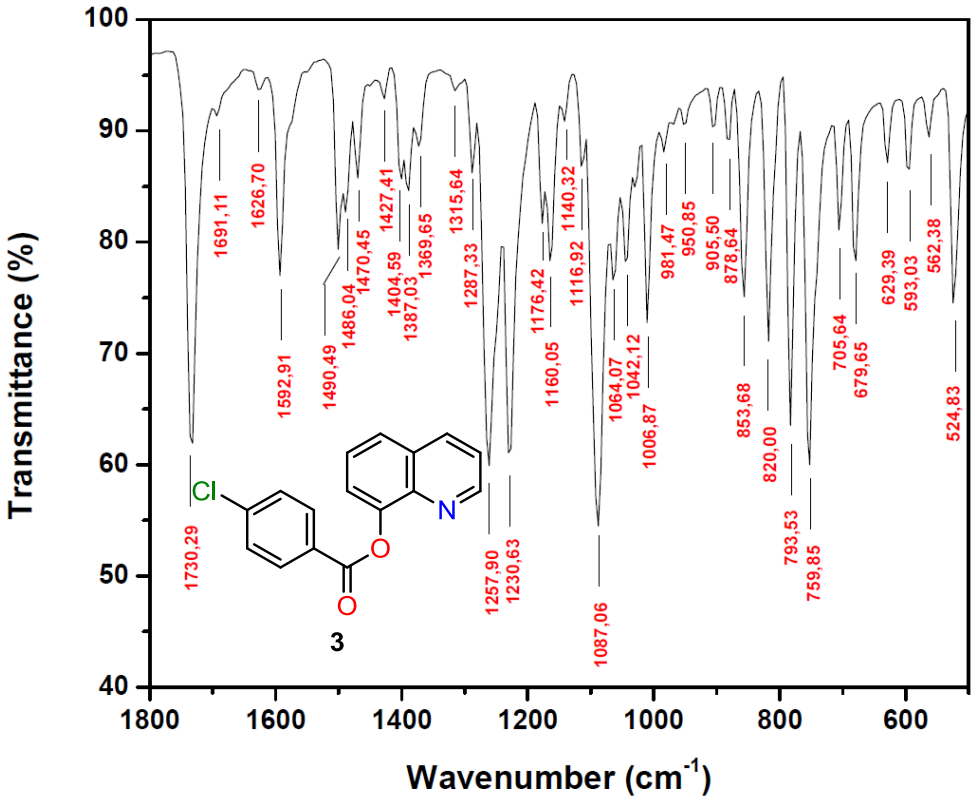


Figure S3: Expansion of the IR spectrum for compound **3**.

3. Copies of UV-Vis spectra for compounds 1 and 3

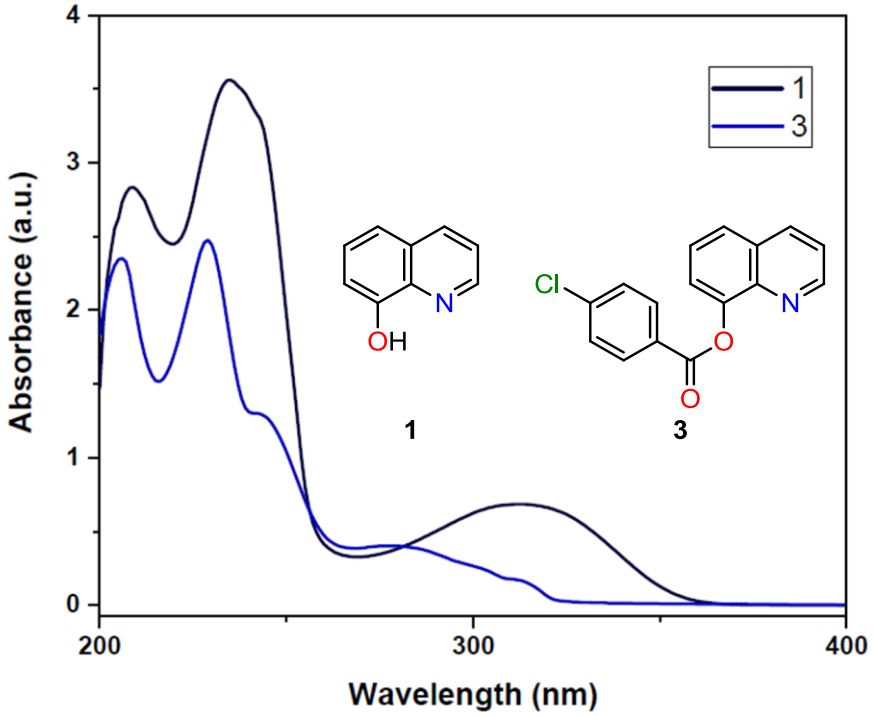


Figure S4: UV-Vis spectra for compounds **1** and **3**.

4. Copies of ^{1}H, ^{13}C and DEPT-135 spectra for compound 3

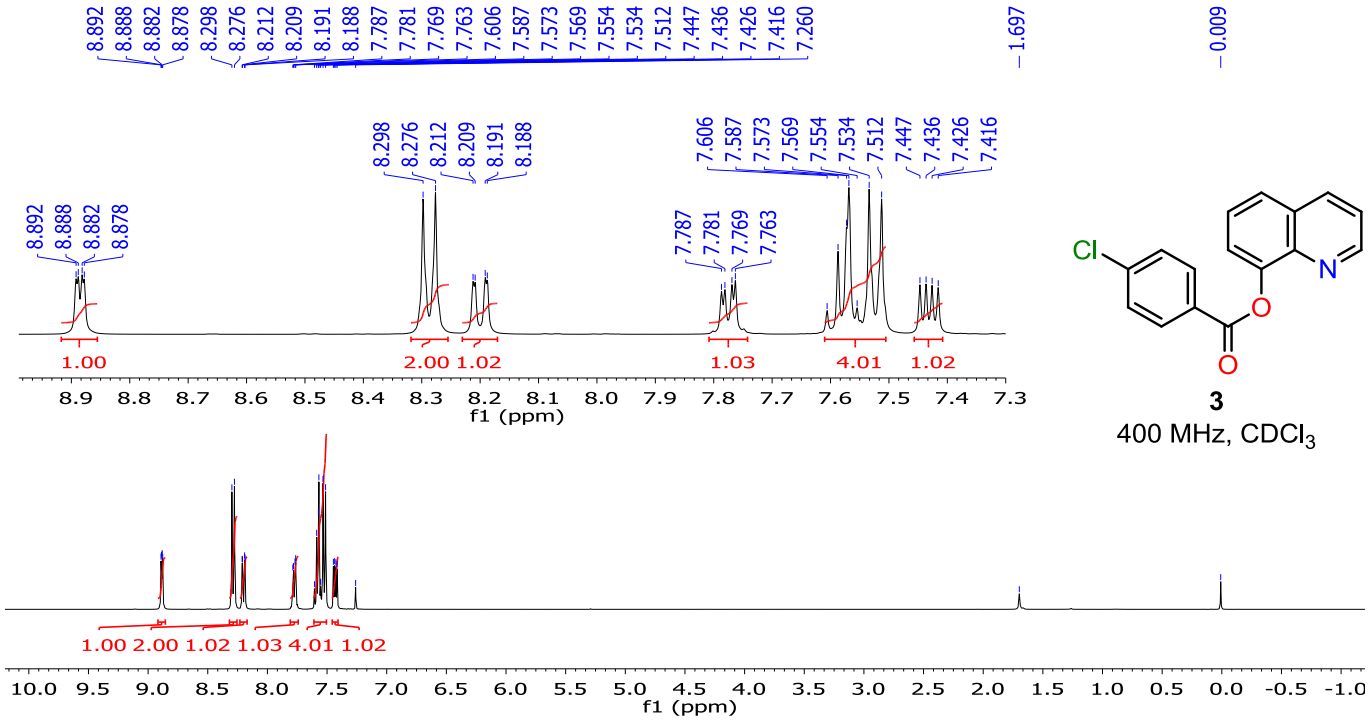


Figure S5: ^{1}H NMR spectrum for compound **3**.

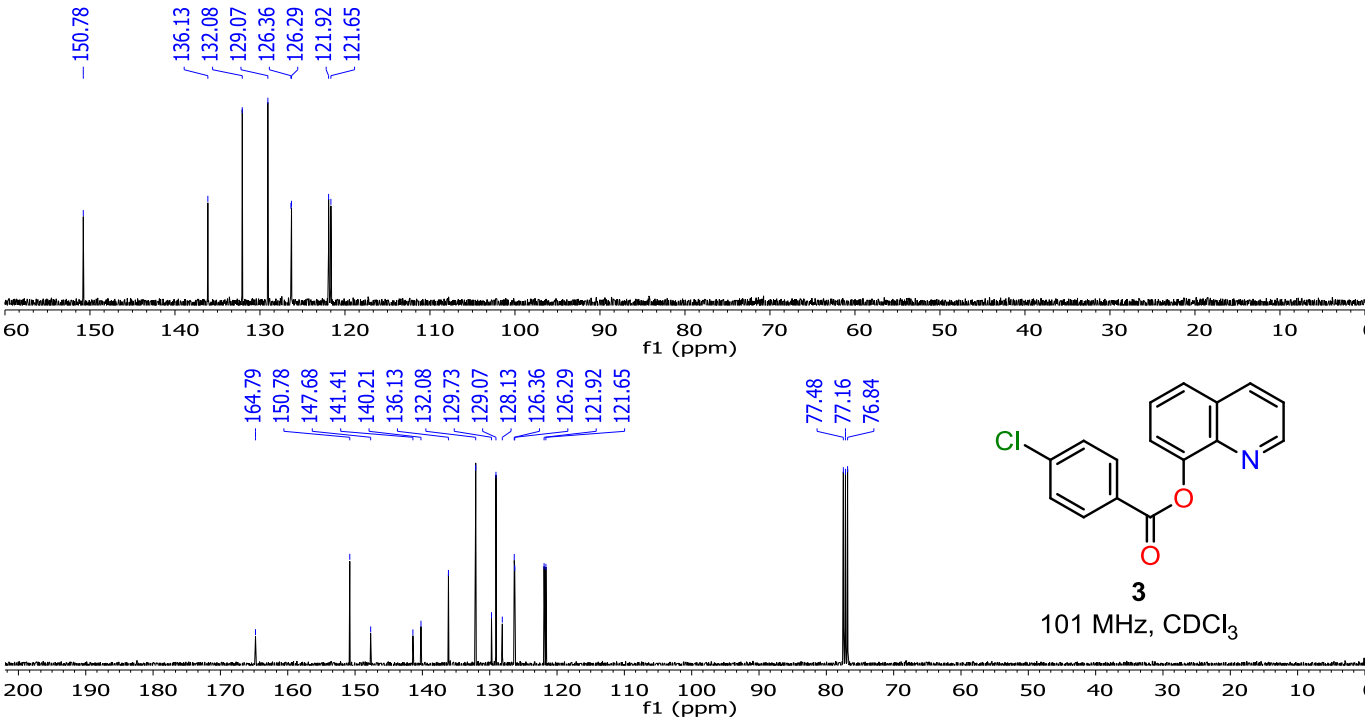


Figure S6: $^{13}C\{^{1}H\}$ NMR and DEPT-135 spectra for compound **3**.

5. Copies of HSQC, HMBC, and COSY spectra for compound 3

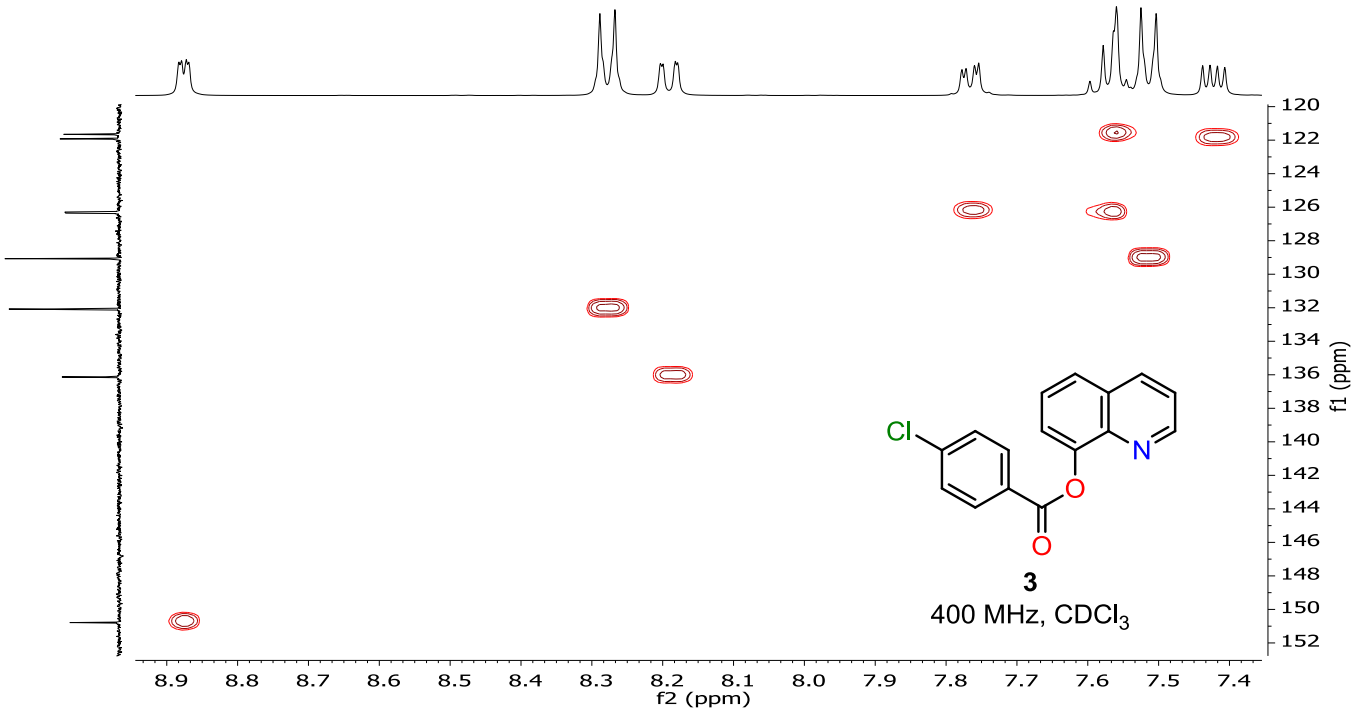


Figure S7: HSQC 2D C–H correlation spectrum for compound **3**.

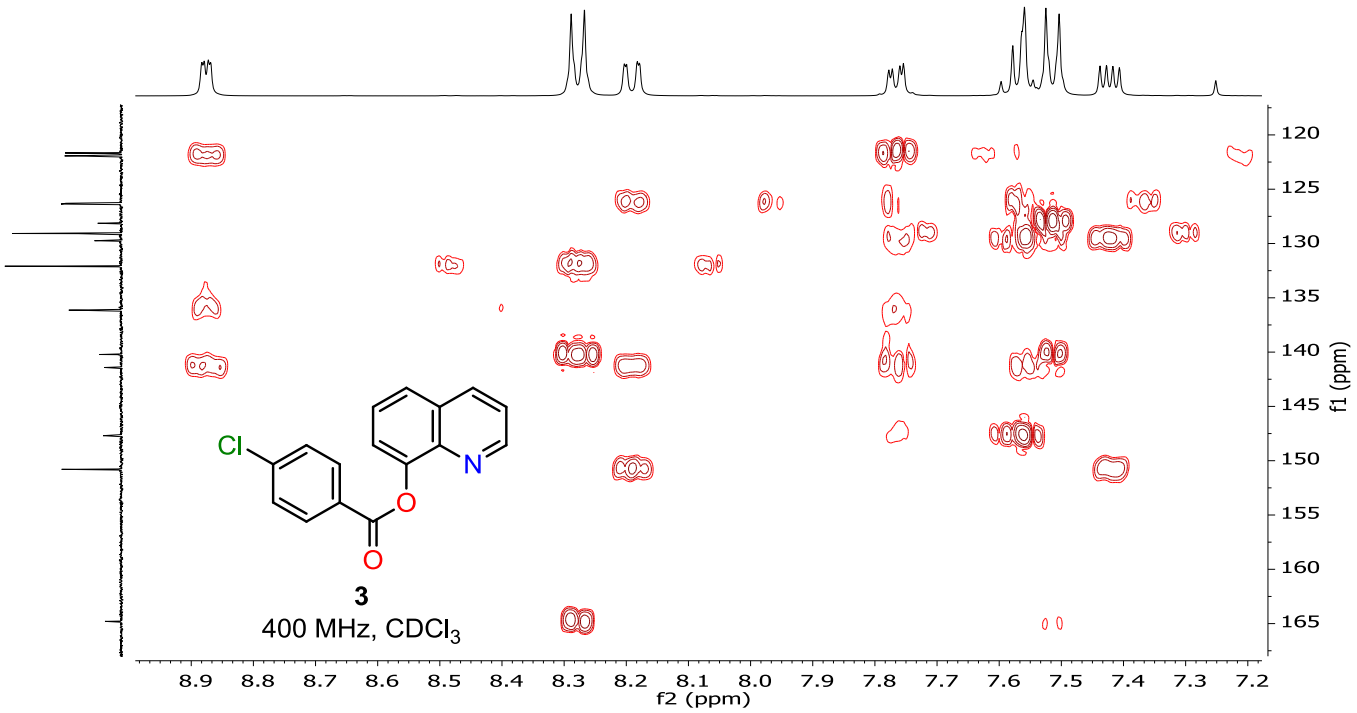


Figure S8: HMBC 2D C–H correlation spectrum for compound **3**.

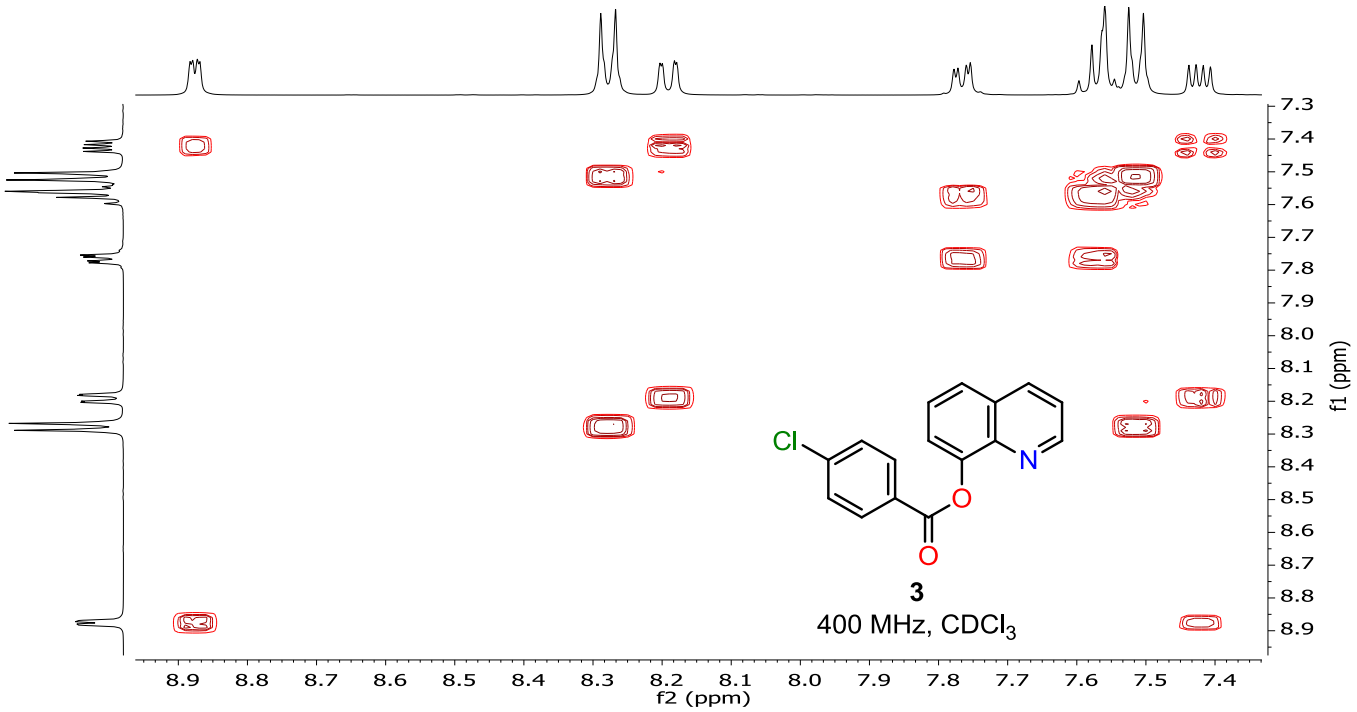


Figure S9: COSY 2D C–H correlation spectrum for compound **3**.

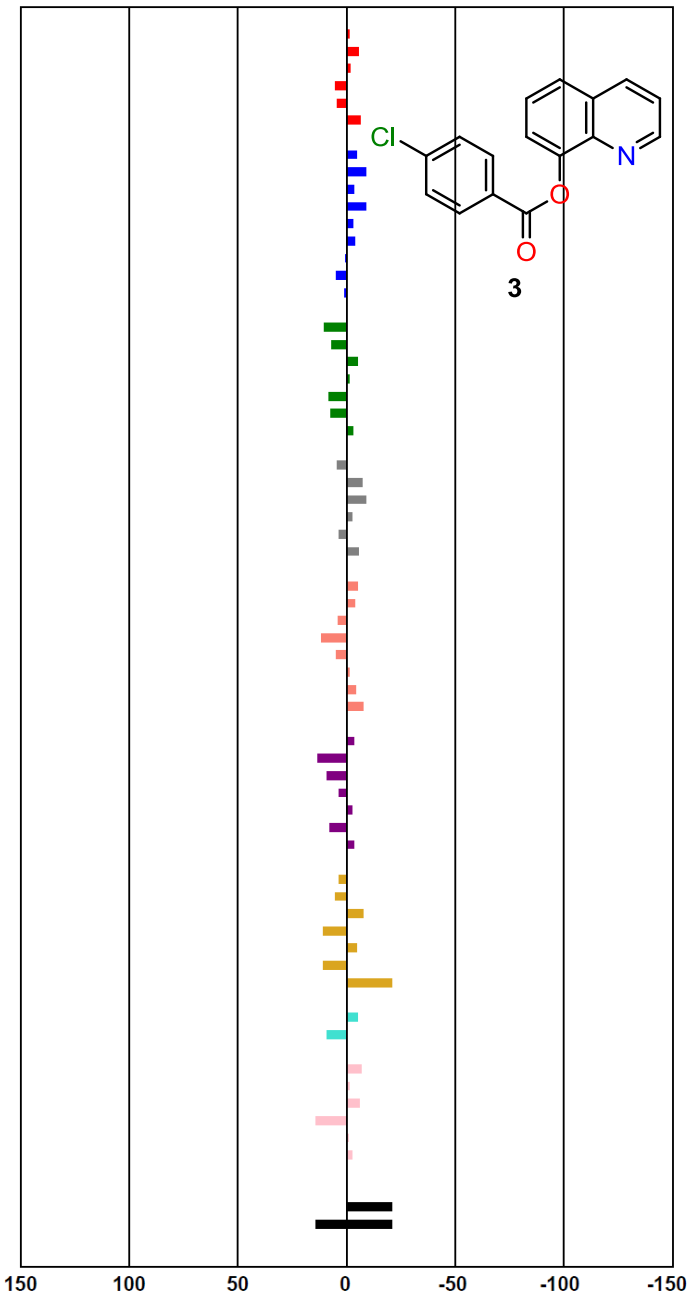
6. Mean growth, %GI, and lethality values for compound 3

Table S1: Mean growth, %GI, and lethality values displayed by the tested compound **3** against 60 NCI human cancer cell lines at 10 μM.

Developmental Therapeutics Program
One Dose Mean Graph

NSC: D-832410 / 1	Conc: 1.00E-5 Molar	Test Date: Aug 30, 2021
Experiment ID: 2108OS84		Report Date: Oct 11, 2021

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	101.46
HL-60(TB)	97.21
K-562	100.83
MOLT-4	107.22
RPMI-8226	106.38
SR	96.13
Non-Small Cell Lung Cancer	
A549/ATCC	98.23
EKVX	93.58
HOP-62	99.21
HOP-92	93.77
NCI-H226	99.68
NCI-H23	98.83
NCI-H322M	102.70
NCI-H460	106.80
NCI-H522	103.27
Colon Cancer	
COLO 205	112.57
HCC-2998	108.91
HCT-116	97.57
HCT-15	101.40
HT29	110.49
KM12	109.42
SW-620	99.82
CNS Cancer	
SF-268	106.44
SF-295	95.36
SF-539	93.83
SNB-19	100.36
SNB-75	105.74
U251	97.04
Melanoma	
MALME-3M	97.68
M14	99.03
MDA-MB-435	106.19
SK-MEL-2	113.92
SK-MEL-28	107.04
SK-MEL-5	101.65
UACC-257	98.33
UACC-62	94.99
Ovarian Cancer	
IGROV1	99.14
OVCAR-3	115.49
OVCAR-4	111.13
OVCAR-5	105.81
OVCAR-8	99.99
NCI/ADR-RES	109.92
SK-OV-3	99.38
Renal Cancer	
786-0	105.79
ACHN	107.53
CAKI-1	95.09
RXF 393	112.99
SN12C	97.96
TK-10	112.78
UO-31	81.85
Prostate Cancer	
PC-3	97.61
DU-145	111.29
Breast Cancer	
MCF7	95.97
MDA-MB-231/ATCC	101.60
HS 578T	96.70
BT-549	116.48
T-47D	101.89
MDA-MB-468	99.98
Mean	102.40
Delta	20.55
Range	34.63



7. X-Ray crystallography for compound 3

Table S2: Experimental bond lengths (Å) and bond/valence angles (°) obtained from single crystal X-ray measurements for compound **3**.

1. Bond Lengths (Angstrom). - (Bonds are ordered on the first label, left to right and top to bottom) - su in last digit in ().
2. ==========
3. Cl(1) - C(2) 1.729(2) O(7) - C(6) 1.357(2) O(7) - C(8) 1.395(2) O(18) - C(6) 1.195(2)
4. N(10) - C(9) 1.362(2) N(10) - C(11) 1.325(3) C(2) - C(3) 1.383(3) C(2) - C(20) 1.371(3)
5. C(3) - C(4) 1.376(3) C(4) - C(5) 1.384(3) C(5) > C(6) 1.475(2) C(5) - C(19) 1.387(3)
6. C(8) - C(9) 1.418(2) C(8) - C(17) 1.360(3) C(9) - C(14) 1.413(2) C(11) - C(12) 1.396(3)
7. C(12) - C(13) 1.355(3) C(13) - C(14) 1.414(2) C(14) - C(15) 1.416(3) C(15) - C(16) 1.354(3)
8. C(16) - C(17) 1.396(3) C(19) - C(20) 1.375(3)
9.
10. C(3) - H(3) 0.93 C(4) - H(4) 0.93 C(11) - H(11) 0.93 C(12) - H(12) 0.93
11. C(13) - H(13) 0.93 C(15) - H(15) 0.93 C(16) - H(16) 0.93 C(17) - H(17) 0.93
12. C(19) - H(19) 0.93 C(20) - H(20) 0.93
13.
14. Bond/Valence Angles (Degrees) - (Angles are ordered on the middle label, left to right and top to bottom) - su in last digit in ().
15. ==========
16. C(6) - O(7) - C(8) 117.53(14) C(9) - N(10) - C(11) 116.71(16) Cl(1) - C(2) - C(3) 119.01(15)
17. Cl(1) - C(2) - C(20) 119.50(17) C(3) - C(2) - C(20) 121.49(18) C(2) - C(3) - C(4) 119.07(18)
18. C(3) - C(4) - C(5) 120.38(18) C(4) - C(5) - C(6) 121.82(16) C(4) - C(5) - C(19) 119.37(17)
19. C(6) - C(5) - C(19) 118.81(17) O(7) - C(6) - O(18) 122.68(17) O(7) - C(6) - C(5) 111.94(15)
20. O(18) - C(6) - C(5) 125.38(18) O(7) - C(8) - C(9) 118.09(15) O(7) - C(8) - C(17) 119.64(15)
21. C(9) - C(8) - C(17) 122.09(16) N(10) - C(9) - C(8) 119.34(15) N(10) - C(9) - C(14) 123.17(16)
22. C(8) - C(9) - C(14) 117.49(15) N(10) - C(11) - C(12) 124.4(2) C(11) - C(12) - C(13) 119.1(2)
23. C(12) - C(13) - C(14) 119.53(19) C(9) - C(14) - C(13) 117.10(17) C(9) - C(14) - C(15) 119.17(17)
24. C(13) - C(14) - C(15) 123.73(18) C(14) - C(15) - C(16) 121.05(19) C(15) - C(16) - C(17) 120.57(19)
25. C(8) - C(17) - C(16) 119.63(17) C(5) - C(19) - C(20) 120.69(19) C(2) - C(20) - C(19) 119.0(2)
26.
27. C(2) - C(3) - H(3) 120 C(4) - C(3) - H(3) 120 C(3) - C(4) - H(4) 120
28. C(5) - C(4) - H(4) 120 N(10) - C(11) - H(11) 118 C(12) - C(11) - H(11) 118
29. C(11) - C(12) - H(12) 120 C(13) - C(12) - H(12) 120 C(12) - C(13) - H(13) 120
30. C(14) - C(13) - H(13) 120 C(14) - C(15) - H(15) 119 C(16) - C(15) - H(15) 119
31. C(15) - C(16) - H(16) 120 C(17) - C(16) - H(16) 120 C(8) - C(17) - H(17) 120
32. C(16) - C(17) - H(17) 120 C(5) - C(19) - H(19) 120 C(20) - C(19) - H(19) 120
33. C(2) - C(20) - H(20) 120 C(19) - C(20) - H(20) 120
34.
35. Torsion/Dihedral Angles (Deg.) - Klyne & Prelog Convention (Dunitz, p241) - (Excl. Minor Disorder & Embedded Bond Angl. > 160. Deg.)
36. ==========
37. Cl(1) C(2) C(3) C(4) 179.34(14) C(20) C(2) C(3) C(4) -0.5(3) Cl(1) C(2) C(20) C(19) -179.35(17)
38. C(3) C(2) C(20) C(19) 0.5(3) C(2) C(3) C(4) C(5) 0.1(3) C(3) C(4) C(5) C(6) -178.40(16)
39. C(3) C(4) C(5) C(19) 0.3(3) C(4) C(5) C(6) O(7) -7.8(2) C(4) C(5) C(6) O(18) 172.90(18)
40. C(19) C(5) C(6) O(7) 173.47(17) C(19) C(5) C(6) O(18) -5.8(3) C(4) C(5) C(19) C(20) -0.3(3)

C(6)	C(5)	C(19)	C(20)	178.4(2)	O(18)	C(6)	O(7)	C(8)	-8.9(3)	C(5)	C(6)	O(7)	C(8)	171.81(14)
C(9)	C(8)	O(7)	C(6)	-80.2(2)	C(17)	C(8)	O(7)	C(6)	104.5(2)	O(7)	C(8)	C(9)	N(10)	5.3(2)
O(7)	C(8)	C(9)	C(14)	-174.63(15)	C(17)	C(8)	C(9)	N(10)	-179.58(17)	C(17)	C(8)	C(9)	C(14)	0.5(3)
O(7)	C(8)	C(17)	C(16)	175.44(17)	C(9)	C(8)	C(17)	C(16)	0.4(3)	C(8)	C(9)	N(10)	C(11)	-178.33(17)
C(14)	C(9)	N(10)	C(11)	1.6(3)	N(10)	C(9)	C(14)	C(13)	-1.4(3)	N(10)	C(9)	C(14)	C(15)	179.27(17)
C(8)	C(9)	C(14)	C(13)	178.45(17)	C(8)	C(9)	C(14)	C(15)	-0.8(2)	C(12)	C(11)	N(10)	C(9)	-0.6(3)
N(10)	C(11)	C(12)	C(13)	-0.4(3)	C(11)	C(12)	C(13)	C(14)	0.5(3)	C(12)	C(13)	C(14)	C(9)	0.3(3)
C(12)	C(13)	C(14)	C(15)	179.6(2)	C(9)	C(14)	C(15)	C(16)	0.3(3)	C(13)	C(14)	C(15)	C(16)	-178.95(19)
C(14)	C(15)	C(16)	C(17)	0.6(3)	C(15)	C(16)	C(17)	C(8)	-0.9(3)	C(5)	C(19)	C(20)	C(2)	-0.1(3)

Cl(1)	C(2)	C(3)	H(3)	-1	C(20)	C(2)	C(3)	H(3)	180	Cl(1)	C(2)	C(20)	H(20)	1
C(3)	C(2)	C(20)	H(20)	-179	C(2)	C(3)	C(4)	H(4)	-180	H(3)	C(3)	C(4)	C(5)	-180
H(3)	C(3)	C(4)	H(4)	0	H(4)	C(4)	C(5)	C(6)	2	H(4)	C(4)	C(5)	C(19)	-180
C(4)	C(5)	C(19)	H(19)	180	C(6)	C(5)	C(19)	H(19)	-2	O(7)	C(8)	C(17)	H(17)	-5
C(9)	C(8)	C(17)	H(17)	-180	H(11)	C(11)	N(10)	C(9)	179	N(10)	C(11)	C(12)	H(12)	180
H(11)	C(11)	C(12)	C(13)	180	H(11)	C(11)	C(12)	H(12)	0	C(11)	C(12)	C(13)	H(13)	-179
H(12)	C(12)	C(13)	C(14)	-179	H(12)	C(12)	C(13)	H(13)	1	H(13)	C(13)	C(14)	C(9)	-180
H(13)	C(13)	C(14)	C(15)	0	C(9)	C(14)	C(15)	H(15)	-180	C(13)	C(14)	C(15)	H(15)	1
C(14)	C(15)	C(16)	H(16)	-179	H(15)	C(15)	C(16)	C(17)	-179	H(15)	C(15)	C(16)	H(16)	1
C(15)	C(16)	C(17)	H(17)	179	H(16)	C(16)	C(17)	C(8)	179	H(16)	C(16)	C(17)	H(17)	-1
C(5)	C(19)	C(20)	H(20)	180	H(19)	C(19)	C(20)	C(2)	180	H(19)	C(19)	C(20)	H(20)	0