Electronic Supporting Information

for

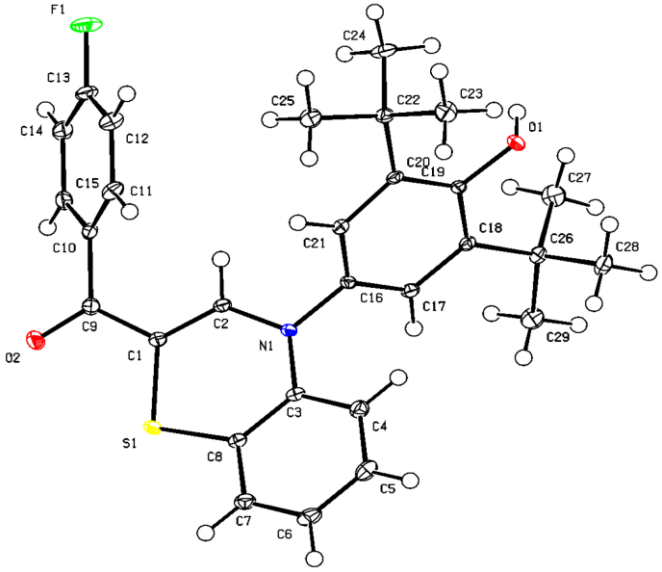
Cyclization of *ortho*-(*S*-phenacyl)-substituted *N*-phenylquinone imine, occurring with the introduction of an additional carbon unit

E. S. Khodykina,[a] A. V. Skorova,[a] V. I. Malay,[a] O. P. Demidov,[b] A. A. Kolodina,[a]★ V. M. Chernyshev[c]

[a]Institute of Physical and Organic Chemistry, Southern Federal University,
194/2 Stachki St., Rostov on Don, 344090, Russian Federation.
E-mail: akolodina@sfedu.ru
[b]Department of Organic Chemistry, North Caucasus Federal University,
Pushkin st. 1, Stavropol, 355017, Russian Federation
[c]Platov South-Russian State Polytechnic University (NPI),
132 ul. Prosveschenya, Novocherkassk, 346428, Russian Federation

Corresponding Author:
Alexandra Kolodina − orcid.org/ 0000-0003-0485-7223; Email: akolodina@sfedu.ru

Table S1. Crystal data and structure refinement for **12a.**



CCDC Number	2482017
Empirical formula	$C_{29}H_{30}FNO_2S$
Formula weight	475.60
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.46370(10)
b/Å	21.9076(2)
c/Å	12.11560(10)
α/°	90
β/°	103.2410(10)
γ/°	90
Volume/Å^3	2445.11(4)
Z	4
ρ_{calc}g/cm^3	1.292
μ/mm^{-1}	1.452
F(000)	1008.0
Crystal size/mm^3	0.264 × 0.188 × 0.089
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.072 to 153.124
Index ranges	$-11 \le h \le 9$, $-27 \le k \le 27$, $-14 \le l \le 15$
Reflections collected	25786
Independent reflections	5096 [R_{int} = 0.0306, R_{sigma} = 0.0207]
Data/restraints/parameters	5096/0/317
Goodness-of-fit on F^2	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0311, wR_2 = 0.0784
Final R indexes [all data]	R_1 = 0.0326, wR_2 = 0.0797
Largest diff. peak/hole / e Å^{-3}	0.27/-0.32

Table S2. Bond Lengths for **12a.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	C8	1.7760(11)	C1	C9	1.4406(14)
S1	C1	1.7658(11)	C10	C15	1.3992(15)
F1	C13	1.3574(13)	C10	C9	1.5021(14)
O1	C19	1.3734(12)	C10	C11	1.3955(16)
O2	C9	1.2430(14)	C20	C22	1.5419(14)
N1	C16	1.4448(13)	C15	C14	1.3919(16)
N1	C3	1.4298(13)	C4	C5	1.3936(15)
N1	C2	1.3554(13)	C22	C23	1.5378(15)
C16	C21	1.3853(15)	C22	C25	1.5396(15)
C16	C17	1.3845(15)	C22	C24	1.5378(15)
C18	C19	1.4173(14)	C7	C6	1.3927(16)
C18	C17	1.3984(15)	C12	C11	1.3903(16)
C18	C26	1.5400(14)	C12	C13	1.3799(16)
C19	C20	1.4141(14)	C26	C28	1.5401(15)
C21	C20	1.3953(15)	C26	C27	1.5424(15)
C3	C8	1.4027(15)	C26	C29	1.5373(15)
C3	C4	1.3937(15)	C13	C14	1.3802(17)
C2	C1	1.3561(15)	C6	C5	1.3847(17)
C8	C7	1.3938(14)			

Table S3. Bond Angles for **12a.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	S1	C8	99.02(5)	C21	C20	C19	117.18(9)
C3	N1	C16	120.47(9)	C21	C20	C22	120.23(9)
C2	N1	C16	115.76(8)	C14	C15	C10	120.42(10)
C2	N1	C3	121.33(9)	O2	C9	C1	120.08(10)
C21	C16	N1	118.35(9)	O2	C9	C10	120.90(10)
C17	C16	N1	120.41(9)	C1	C9	C10	119.02(9)
C17	C16	C21	121.21(10)	C5	C4	C3	120.51(10)
C19	C18	C26	122.03(9)	C23	C22	C20	110.84(9)
C17	C18	C19	117.60(9)	C23	C22	C25	107.43(9)
C17	C18	C26	120.34(9)	C25	C22	C20	111.48(9)
O1	C19	C18	118.72(9)	C24	C22	C20	109.99(9)
O1	C19	C20	118.68(9)	C24	C22	C23	110.22(9)
C20	C19	C18	122.41(10)	C24	C22	C25	106.78(9)
C16	C21	C20	121.10(10)	C6	C7	C8	120.73(11)
C8	C3	N1	120.91(9)	C13	C12	C11	117.91(11)
C4	C3	N1	119.54(10)	C12	C11	C10	120.87(10)
C4	C3	C8	119.49(10)	C18	C26	C27	111.88(9)
N1	C2	C1	127.07(10)	C28	C26	C18	109.24(9)
C16	C17	C18	120.47(10)	C28	C26	C27	110.05(10)
C3	C8	S1	124.18(8)	C29	C26	C18	111.40(9)

Table S3. Bond Angles for **12a.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C7	C8	S1	116.38(8)	C29	C26	C28	107.46(9)
C7	C8	C3	119.44(10)	C29	C26	C27	106.70(9)
C2	C1	S1	122.15(8)	F1	C13	C12	117.76(10)
C2	C1	C9	121.12(10)	F1	C13	C14	119.00(10)
C9	C1	S1	116.24(8)	C12	C13	C14	123.24(10)
C15	C10	C9	119.68(10)	C13	C14	C15	118.19(10)
C11	C10	C15	119.36(10)	C5	C6	C7	119.73(10)
C11	C10	C9	120.95(9)	C6	C5	C4	120.07(10)
C19	C20	C22	122.59(9)				

Table S4. Torsion Angles for **12a.**

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	C8	C7	C6	179.43(9)	C2	N1	C16	C17	-120.75(11)
S1	C1	C9	O2	-4.81(14)	C2	N1	C3	C8	17.00(15)
S1	C1	C9	C10	175.97(8)	C2	N1	C3	C4	-160.38(10)
F1	C13	C14	C15	179.43(10)	C2	C1	C9	O2	167.36(10)
O1	C19	C20	C21	-173.56(9)	C2	C1	C9	C10	-11.87(15)
O1	C19	C20	C22	5.98(14)	C17	C16	C21	C20	0.41(15)
N1	C16	C21	C20	-177.61(9)	C17	C18	C19	O1	175.14(9)
N1	C16	C17	C18	179.25(9)	C17	C18	C19	C20	0.27(15)
N1	C3	C8	S1	1.92(14)	C17	C18	C26	C28	-114.68(11)
N1	C3	C8	C7	-178.17(10)	C17	C18	C26	C27	123.22(11)
N1	C3	C4	C5	178.74(10)	C17	C18	C26	C29	3.88(14)
N1	C2	C1	S1	-7.65(16)	C8	S1	C1	C2	20.57(10)
N1	C2	C1	C9	-179.34(10)	C8	S1	C1	C9	-167.35(8)
C16	N1	C3	C8	178.49(9)	C8	C3	C4	C5	1.32(16)
C16	N1	C3	C4	1.11(15)	C8	C7	C6	C5	1.24(17)
C16	N1	C2	C1	-176.70(10)	C1	S1	C8	C3	-17.81(10)
C16	C21	C20	C19	-1.65(14)	C1	S1	C8	C7	162.28(9)
C16	C21	C20	C22	178.80(9)	C10	C15	C14	C13	-0.47(17)
C18	C19	C20	C21	1.31(14)	C15	C10	C9	O2	-50.08(15)
C18	C19	C20	C22	-179.15(9)	C15	C10	C9	C1	129.14(11)
C19	C18	C17	C16	-1.56(15)	C15	C10	C11	C12	-0.88(17)
C19	C18	C26	C28	63.29(12)	C9	C10	C15	C14	179.93(10)
C19	C18	C26	C27	-58.81(13)	C9	C10	C11	C12	-179.58(10)
C19	C18	C26	C29	-178.15(9)	C4	C3	C8	S1	179.30(8)

Table S4. Torsion Angles for **12a.**

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
C19	C20	C22	C23	-60.11(13)	C4	C3	C8	C7	-0.79(15)
C19	C20	C22	C25	-179.73(9)	C7	C6	C5	C4	-0.70(17)
C19	C20	C22	C24	62.02(13)	C12	C13	C14	C15	-0.64(18)
C21	C16	C17	C18	1.27(15)	C11	C10	C15	C14	1.21(16)
C21	C20	C22	C23	119.41(10)	C11	C10	C9	O2	128.62(12)
C21	C20	C22	C25	-0.21(13)	C11	C10	C9	C1	-52.16(14)
C21	C20	C22	C24	-118.45(11)	C11	C12	C13	F1	-179.11(10)
C3	N1	C16	C21	-105.18(11)	C11	C12	C13	C14	0.96(18)
C3	N1	C16	C17	76.77(13)	C26	C18	C19	O1	-2.89(14)
C3	N1	C2	C1	-14.39(16)	C26	C18	C19	C20	-177.75(9)
C3	C8	C7	C6	-0.49(16)	C26	C18	C17	C16	176.49(9)
C3	C4	C5	C6	-0.58(17)	C13	C12	C11	C10	-0.18(17)
C2	N1	C16	C21	57.29(13)					