SUPPORTING INFORMATION for

Synthesis and characterization of (E)-3-(2-(4-methylthiazol-2-yl)hydrazineylidene)chromane-2,4-dione

Fatlinda Rahmani [1], Aurélien Crochet[1], Fabio Zobi [1,*]

[1] Department of Chemistry, University of Fribourg, Chemin du Musée 10, 1700 Fribourg, Switzerland.

*To whom all the correspondence should be addressed

Phone (+41) 26 300 87 85, Fax (+41) 26 300 97 37, E-mail : fabio.zobi@unifr.ch

Table of contents

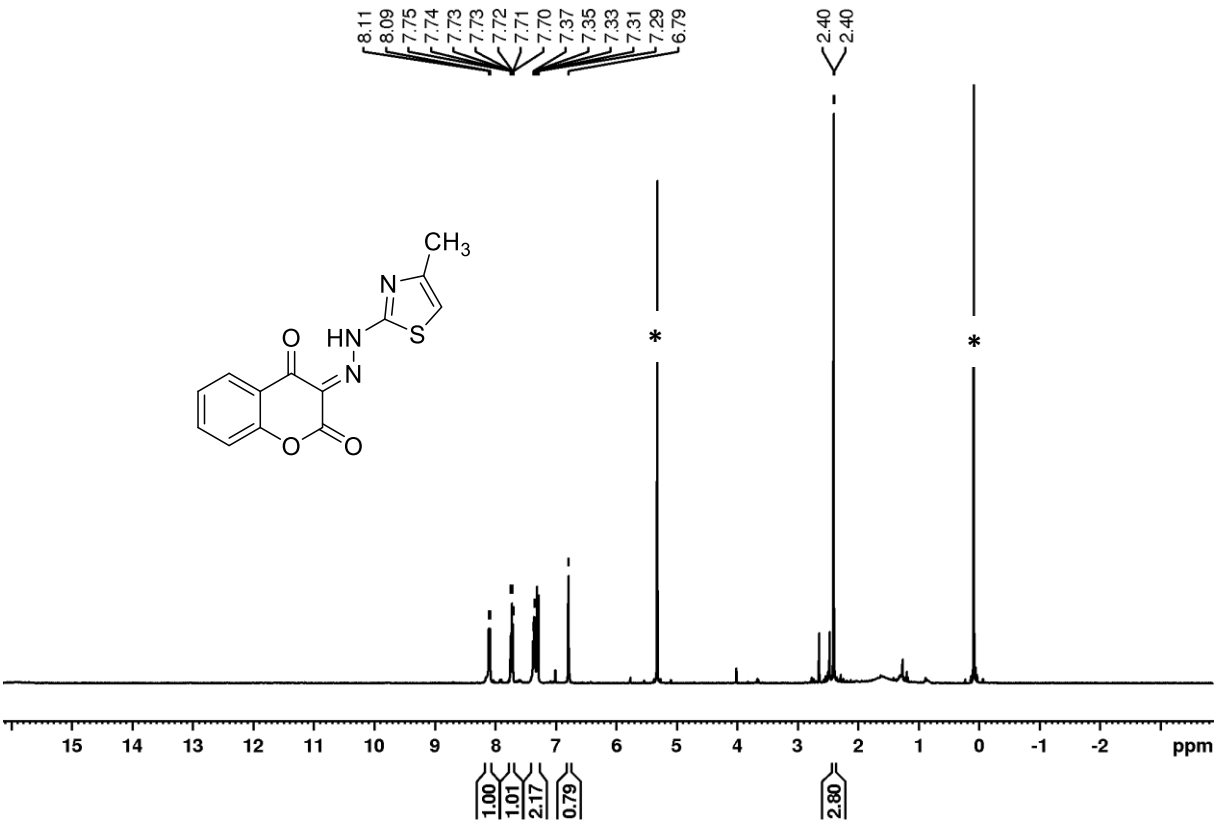


Fig.S1. ^{1}H spectra of (*E*)-3-(2-(4-methylthiazol-2 yl)hydrazineylidene)chromane-2,4-dione dione (in CD_2Cl_2, * = solvent residual peak)

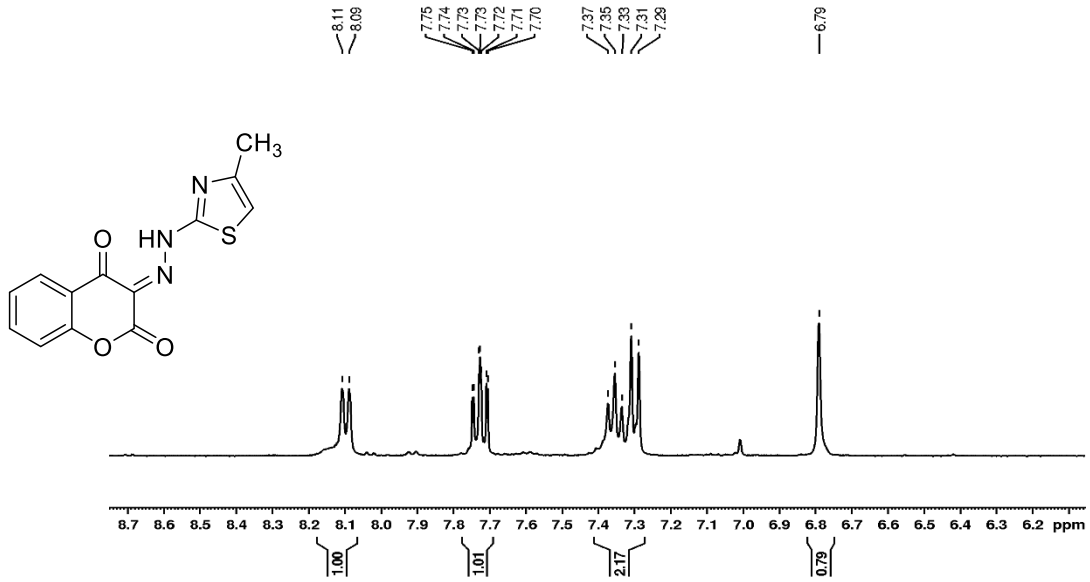


Fig.S2 ^{1}H spectra of (*E*)-3-(2-(4-methylthiazol-2 yl)hydrazineylidene)chromane-2,4-dione dione (in CD_2Cl_2, * = solvent residual peak)

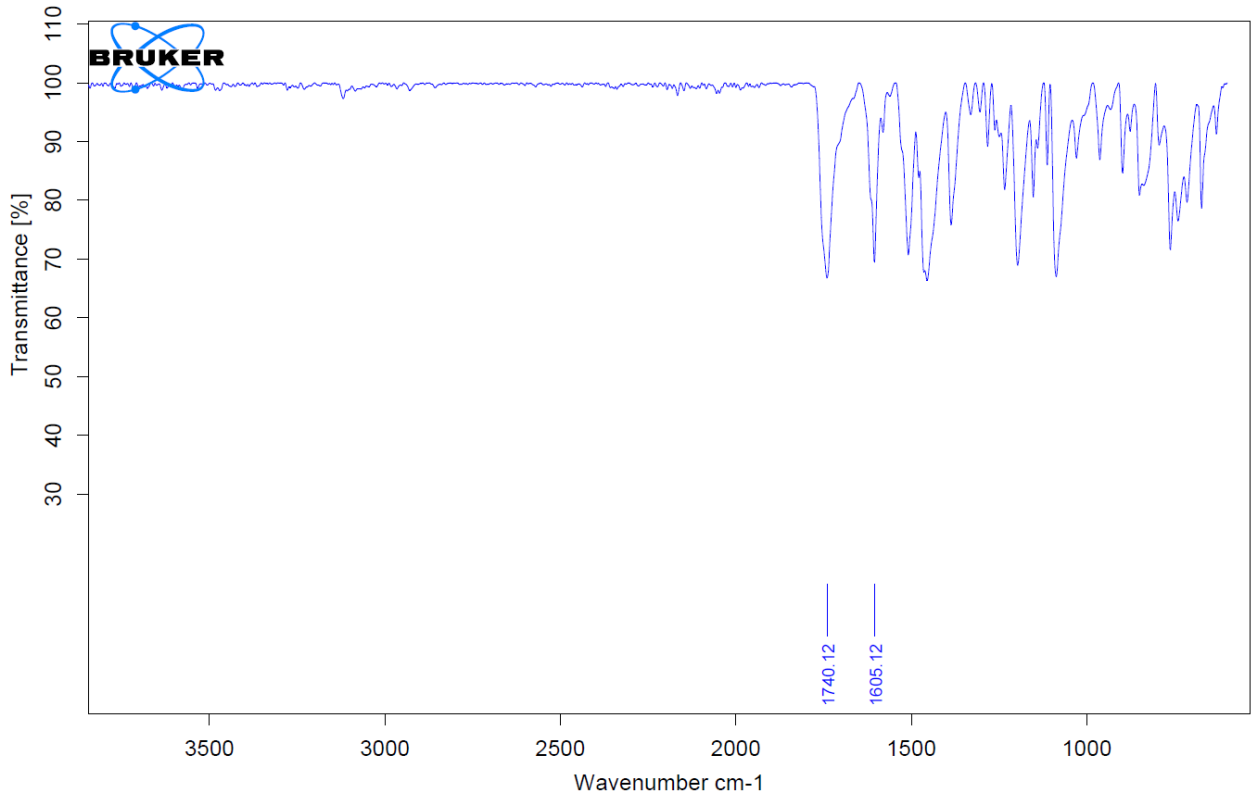


Fig.S3 IR spectra of (*E*)-3-(2-(4-methylthiazol-2 yl)hydrazineylidene)chromane-2,4-dione

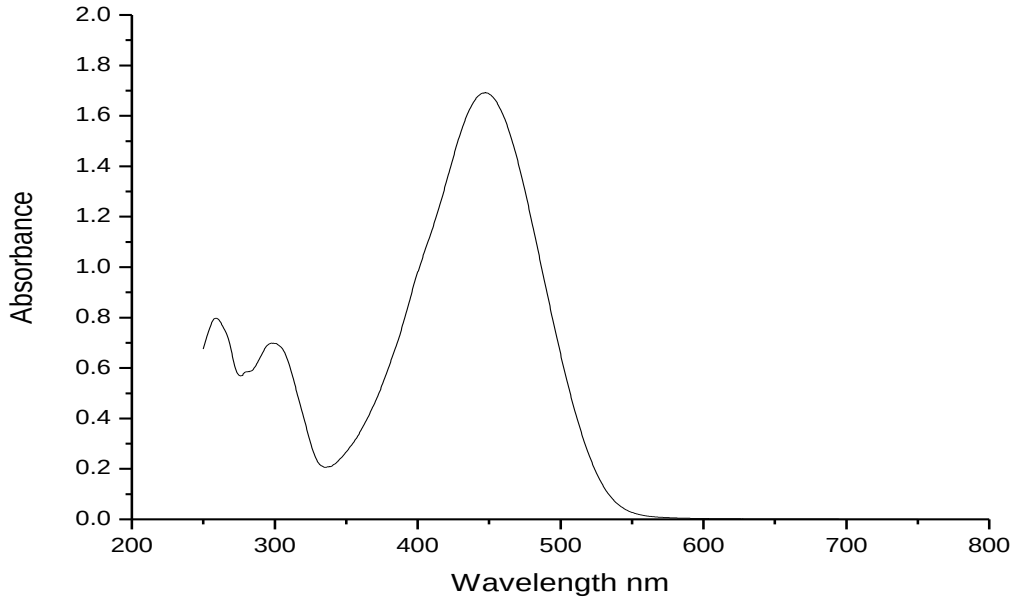


Fig.S4 UV-Vis spectra of (*E*)-3-(2-(4-methylthiazol-2 yl)hydrazineylidene)chromane-2,4-dione (DCMλ_{max}/nm) = 260, 350 and 450

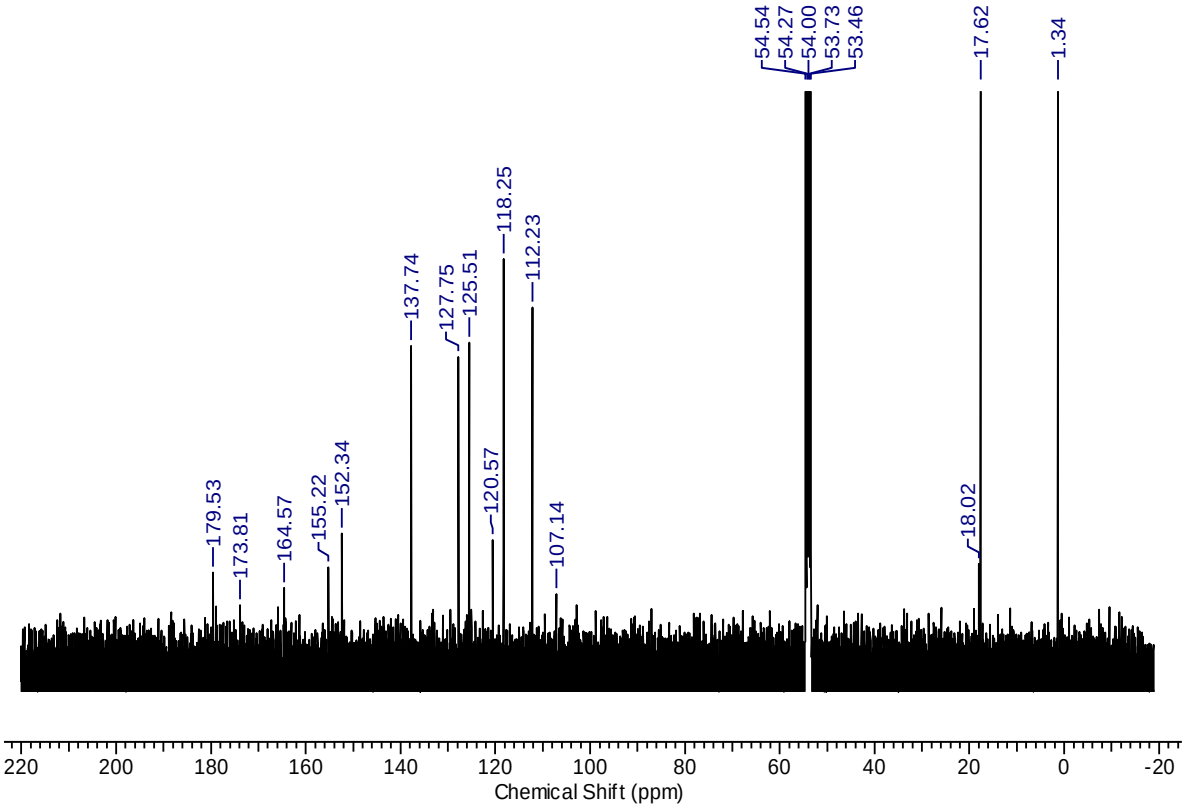
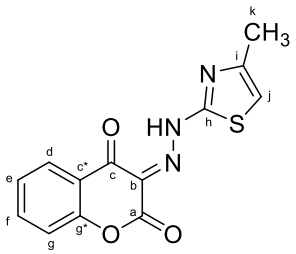


Fig.S5 ^{13}C NMR spectra of (*E*)-3-(2-(4-methylthiazol-2 yl)hydrazineylidene)chromane-2,4-dione dione (in CD_2Cl_2, * = solvent residual peak)

Table S1 – ^{13}C NMR shift (ppm) of compound 3



C	Chemical Shift (ppm)
a	155.22
b	127.75
c	179.53
c*	125.51
d	118.25
e	120.57
f	137.74
g	112.23
g*	164.57
h	173.81
j	107.14
i	152.34
k	18.02
solvent residual signal	1.34

Table S2 – Crystallographic Details

Compound Id	***3***
Empirical formula	$C_{13}H_9N_3O_3S$
Formula weight	287.29
Temperature/K	250(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	7.7866(2)
b/Å	18.6704(4)
c/Å	8.9217(2)
α/°	90
β/°	105.695(2)
γ/°	90
Volume/Å³	1248.67(5)
Z	4
$\rho_{calc}g/cm^3$	1.528
Final R indexes [I>=2σ (I)]	R_1 = 0.0282, wR_2 = 0.0734
Final R indexes [all data]	R_1 = 0.0359, wR_2 = 0.0756
Largest diff. peak/hole / e Å⁻³	0.12/-0.22

Table S3. Bond Lengths for compound 3

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	C10	1.7121(14)	C1	C9	1.473(2)
S1	C11	1.7181(16)	C2	C3	1.387(2)
O1	C1	1.191(2)	C2	C7	1.3889(19)
O2	C1	1.372(2)	C3	C4	1.372(2)
O2	C2	1.3805(19)	C4	C5	1.392(3)
O3	C8	1.2434(17)	C5	C6	1.376(2)
N1	N2	1.3051(17)	C6	C7	1.394(2)
N1	C9	1.3241(19)	C7	C8	1.456(2)
N2	C10	1.3885(19)	C8	C9	1.453(2)
N3	C10	1.2997(19)	C11	C12	1.353(2)
N3	C12	1.3808(19)	C12	C13	1.490(2)

Table S4. Bond Angles for compound 3

10	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C10	S1	C11	87.53(7)	C2	C7	C8	119.58(14)
C1	O2	C2	122.62(11)	C6	C7	C8	121.58(13)
N2	N1	C9	118.28(12)	O3	C8	C7	122.38(13)
N1	N2	C10	119.36(12)	O3	C8	C9	121.29(13)
C10	N3	C12	109.30(13)	C9	C8	C7	116.32(12)
O1	C1	O2	117.31(14)	N1	C9	C1	113.34(13)
O1	C1	C9	125.75(16)	N1	C9	C8	124.95(13)
O2	C1	C9	116.93(13)	C8	C9	C1	121.70(13)
O2	C2	C3	116.14(13)	N2	C10	S1	122.56(11)
O2	C2	C7	122.80(13)	N3	C10	S1	117.13(11)
C3	C2	C7	121.05(15)	N3	C10	N2	120.26(13)
C4	C3	C2	118.93(15)	C12	C11	S1	111.47(12)
C3	C4	C5	121.25(15)	N3	C12	C13	119.87(14)
C6	C5	C4	119.28(17)	C11	C12	N3	114.57(14)
C5	C6	C7	120.64(15)	C11	C12	C13	125.56(15)
C2	C7	C6	118.84(14)				

Table S5. Hydrogen Bonds for compound 3

D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**
N2	H2	O3	0.93(2)	1.79(2)

Table S6. Torsion Angles for compound 3

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	C11	C12	N3	-0.74(18)	C2	C7	C8	C9	1.2(2)
S1	C11	C12	C13	178.22(14)	C3	C2	C7	C6	-0.7(2)
O1	C1	C9	N1	-0.9(2)	C3	C2	C7	C8	-179.93(13)
O1	C1	C9	C8	179.96(16)	C3	C4	C5	C6	-0.2(3)
O2	C1	C9	N1	178.52(13)	C4	C5	C6	C7	0.7(2)
O2	C1	C9	C8	-0.6(2)	C5	C6	C7	C2	-0.3(2)
O2	C2	C3	C4	-178.75(14)	C5	C6	C7	C8	178.97(14)
O2	C2	C7	C6	179.27(13)	C6	C7	C8	O3	2.4(2)
O2	C2	C7	C8	0.0(2)	C6	C7	C8	C9	-178.02(13)
O3	C8	C9	N1	-0.3(2)	C7	C2	C3	C4	1.2(2)
O3	C8	C9	C1	178.65(14)	C7	C8	C9	N1	-179.94(13)
N1	N2	C10	S1	-4.20(19)	C7	C8	C9	C1	-0.9(2)
N1	N2	C10	N3	178.56(13)	C9	N1	N2	C10	177.73(12)
N2	N1	C9	C1	-179.83(12)	C10	S1	C11	C12	0.73(13)
N2	N1	C9	C8	-0.8(2)	C10	N3	C12	C11	0.28(19)
C1	O2	C2	C3	178.24(14)	C10	N3	C12	C13	-178.74(15)
C1	O2	C2	C7	-1.7(2)	C11	S1	C10	N2	-177.94(13)
C2	O2	C1	O1	-178.57(14)	C11	S1	C10	N3	-0.62(12)
C2	O2	C1	C9	1.9(2)	C12	N3	C10	S1	0.32(16)
C2	C3	C4	C5	-0.8(2)	C12	N3	C10	N2	177.71(13)
C2	C7	C8	O3	-178.36(14)					

Table S7. Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for compound 3

Atom	x	y	z	U(eq)
H3	11108.99	2668.45	6736.6	64
H4	12795.79	2949.84	9220.67	69
H5	12592.95	4075.43	10283.49	65
H6	10682.39	4925.1	8830.18	55
H11	1932.57	6779.02	-268.68	59
H13A	2227.06	7847.34	2971.14	93
H13B	1826.42	7938.08	1143.68	93
H13C	3751.01	8112.65	2233.5	93
H2	6640(30)	5790(10)	4840(30)	75