Supporting Information

for

9a-phenyl-2,3,3a,3b,9a,9b-hexahydro-4H furo[3',2':3,4]-cyclobuta- [1,2-b]chromen-4-one: a flavone-based 2+2-photocycloadduct

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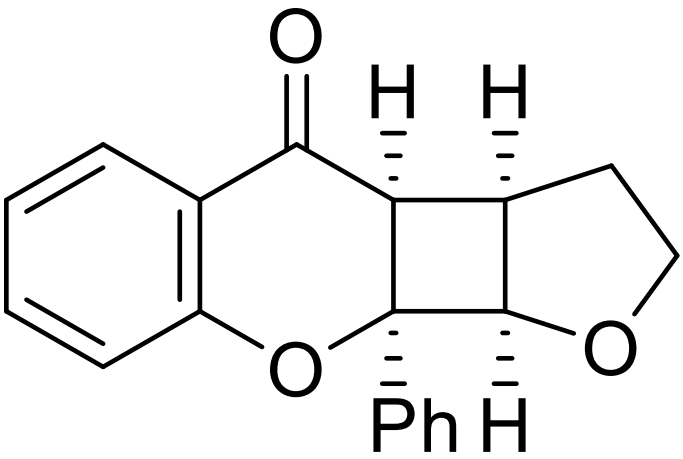

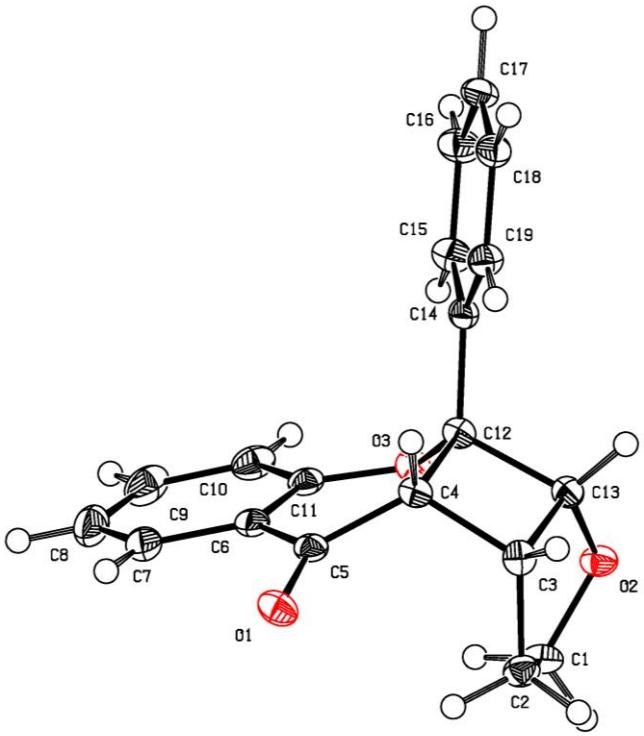

Figure S1. Cyclobutane **6**: X-ray ellipsoid picture.

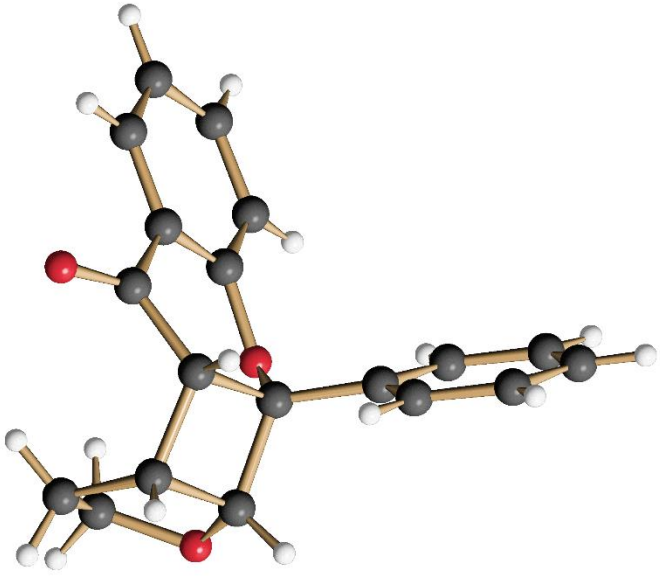

Figure S2. Cyclobutane **6**: ball/stick picture.

Compound name and **CCDC-number**	9a-phenyl-2,3,3a,3b,9a,9b-hexahydro-4H-furo[3',2':3,4]cyclobuta- [1,2-b]chromen-4-one; CCDC 2089434
Moiety formula	$C_{19}H_{16}O_3$
Formula weight	292.32 g/mol
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a= 13.5434(9) Å α= 90° b= 5.6782(4) Å β= 96.264(2)° c= 18.4927(12) Å γ= 90°
Volume	1413.64(16) $Å^3$
Z	4
Density (calculated)	1.373 Mg/m^3
Absorption coefficient	0.744 mm^{-1}
F(000)	616
Crystal size	0.200 x 0.100 x 0.030 mm^3
θ-range for data collection	3.283 to 71.993°
Index ranges	-16<=h<=16, -6<=k<=6, -22<=l<=22
Collected / Independent reflections	29141
Data / restraints / parameters	2763 [R(int) = 0.0493]
max. and min. transmission	0.7536 and 0.4978
Data / restraints / parameters	2763 / 0 / 199
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0345, wR2 = 0.0871
R indices (all data)	R1 = 0.0365, wR2 = 0.0879
Largest diff. peak and hole	0.259 and -0.210 $eÅ^{-3}$

Table S1. Cyclobutane **6**: data for X-ray structure analysis

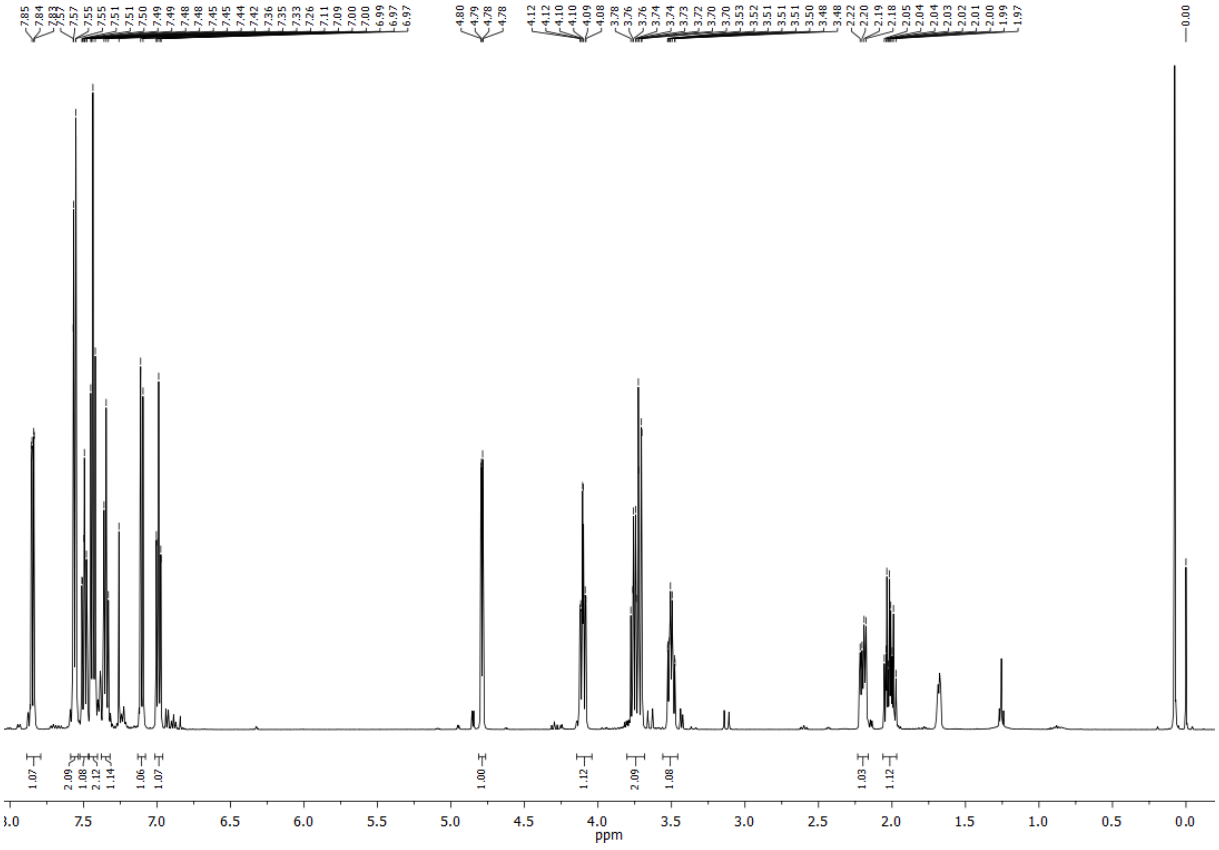

Figure S3. Cyclobutane **6**: ^{1}H-NMR spectrum (500 MHz, $CDCl_3$).

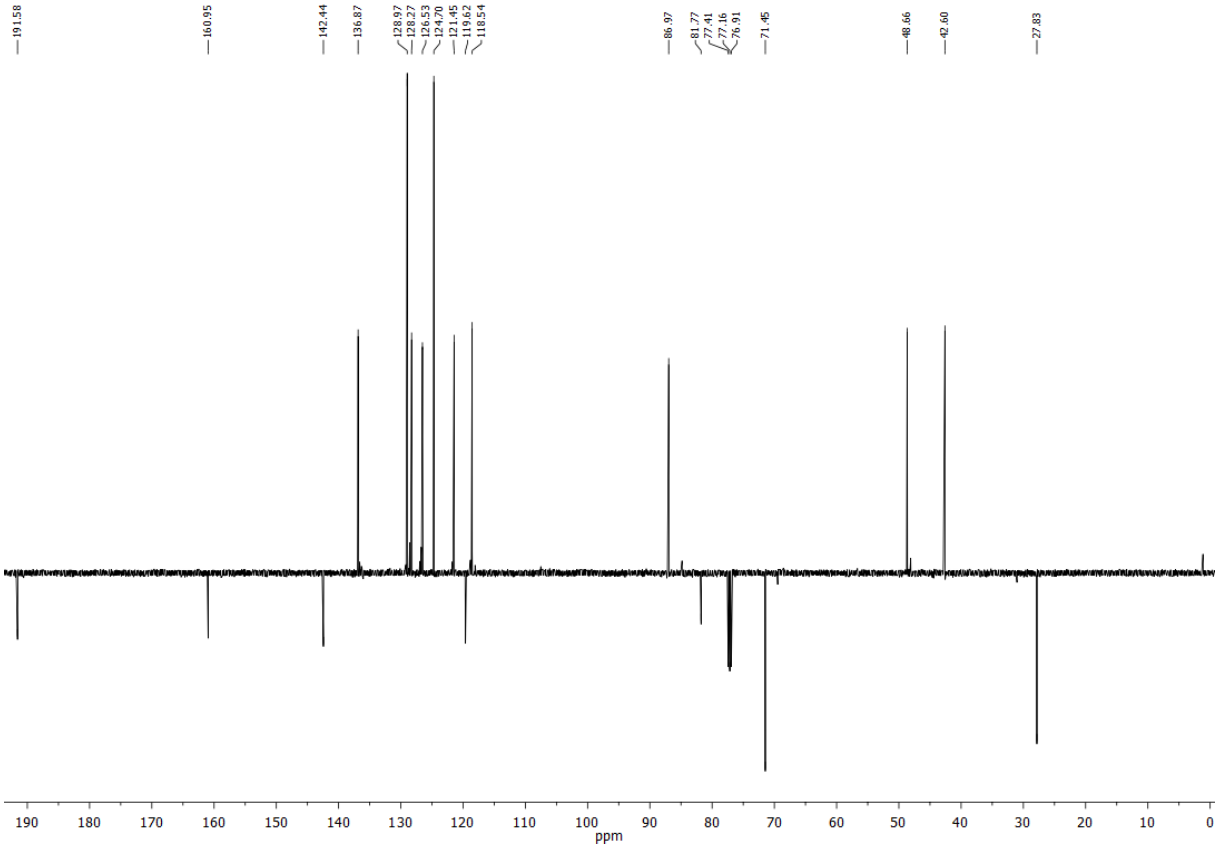

Figure S4. Cyclobutane **6**: ^{13}C-NMR spectrum (125 MHz, $CDCl_3$).

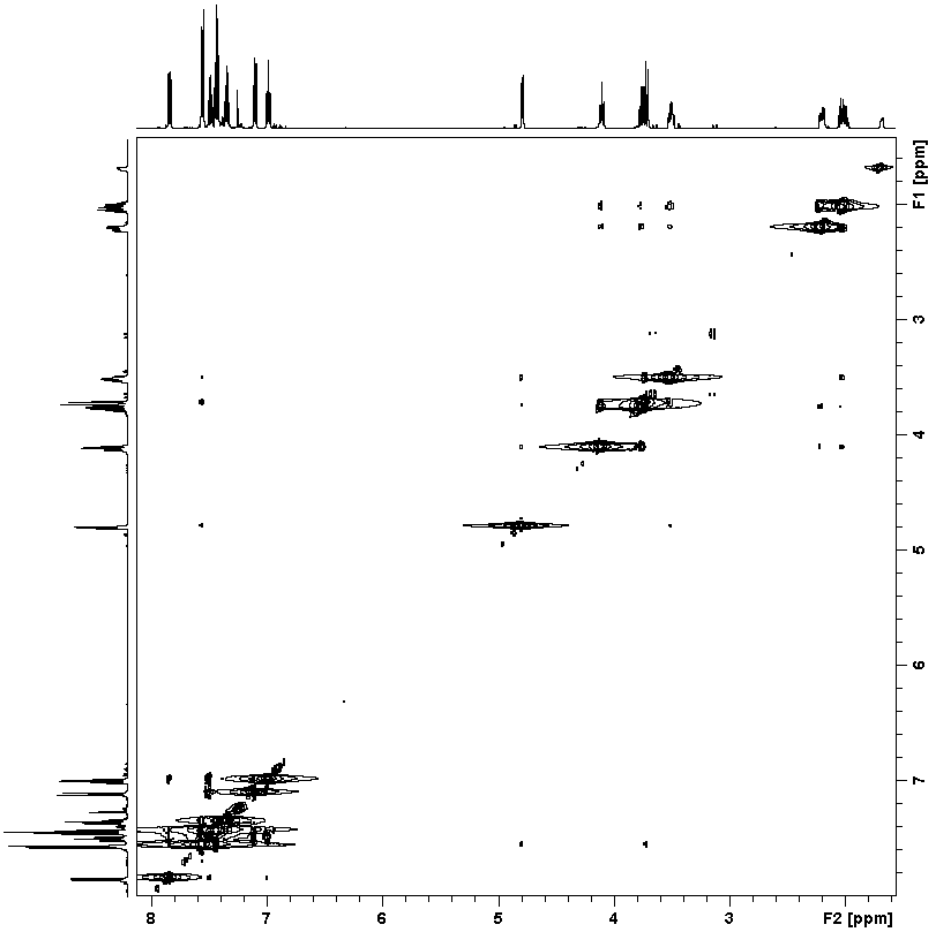

Figure S5. Cyclobutane **6**: NOESY-NMR spectrum (500 MHz, $CDCl_3$).

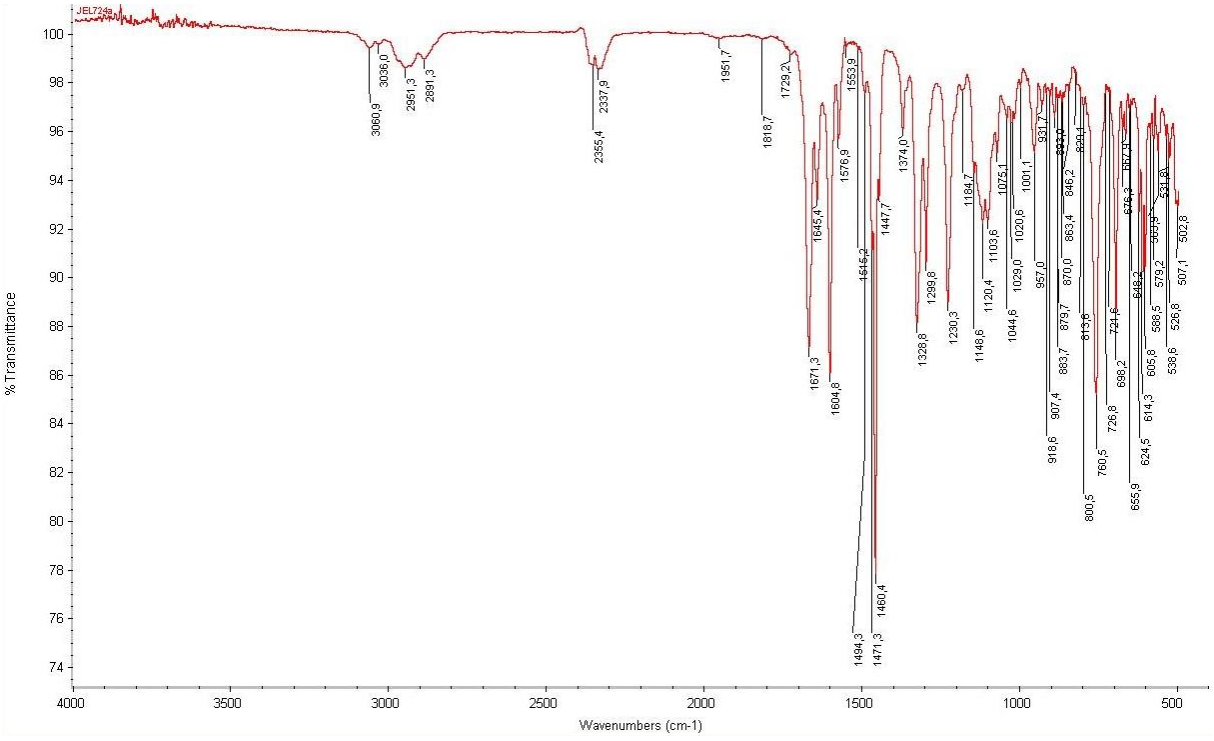

Figure S6. Cyclobutane **6**: IR spectrum.

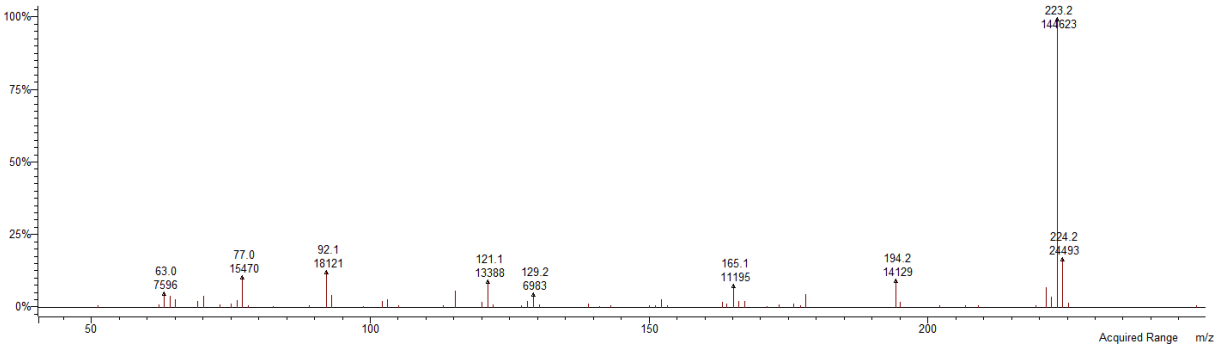

Figure S7. Cyclobutane **6**: mass spectrometric analysis (EI, 70 eV).

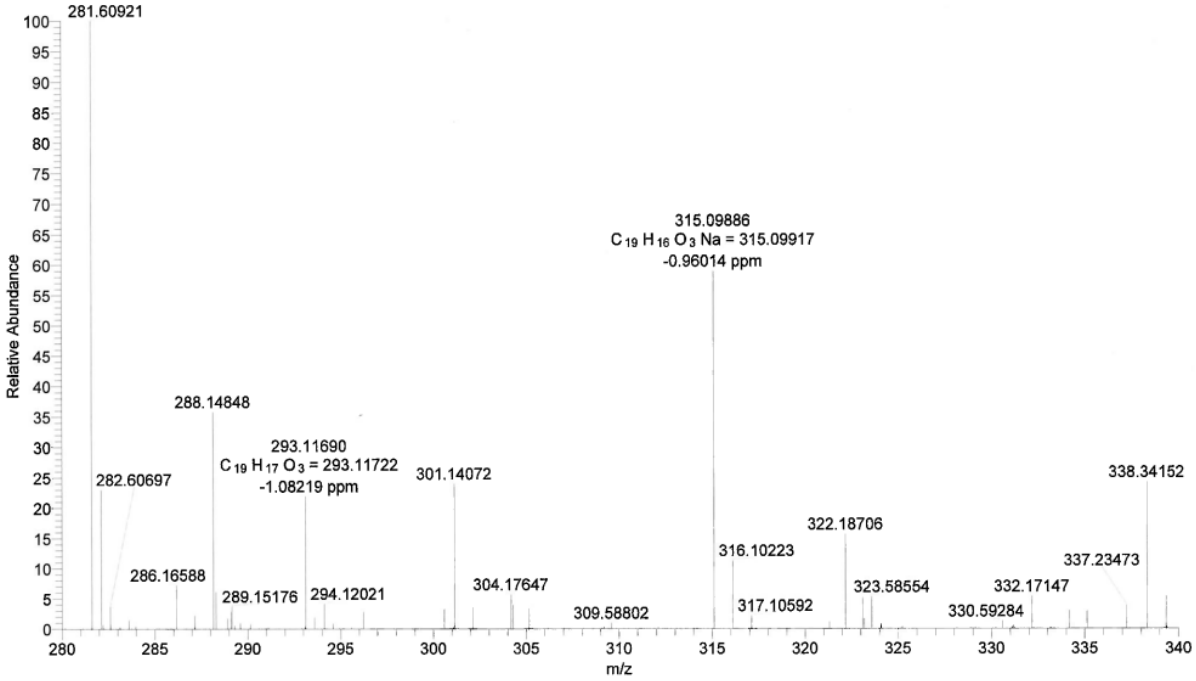

Figure S8. Cyclobutane **6**: mass spectrometric analysis (ESI HR-MS).