Supplementary Material: (*E*)-1-(2-Aminophenyl)-3-(benzo[*d*][1,3]dioxol-5-yl)prop-2-en-1-one

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Content

- Copies of ^{1}H, ^{13}C, DEPT-135 NMR and IR spectra and HMBC, HSQC and COSY experiments and mass spectrum for chalcone **3**.
- Copy of the checkCIF file for compound **3**.
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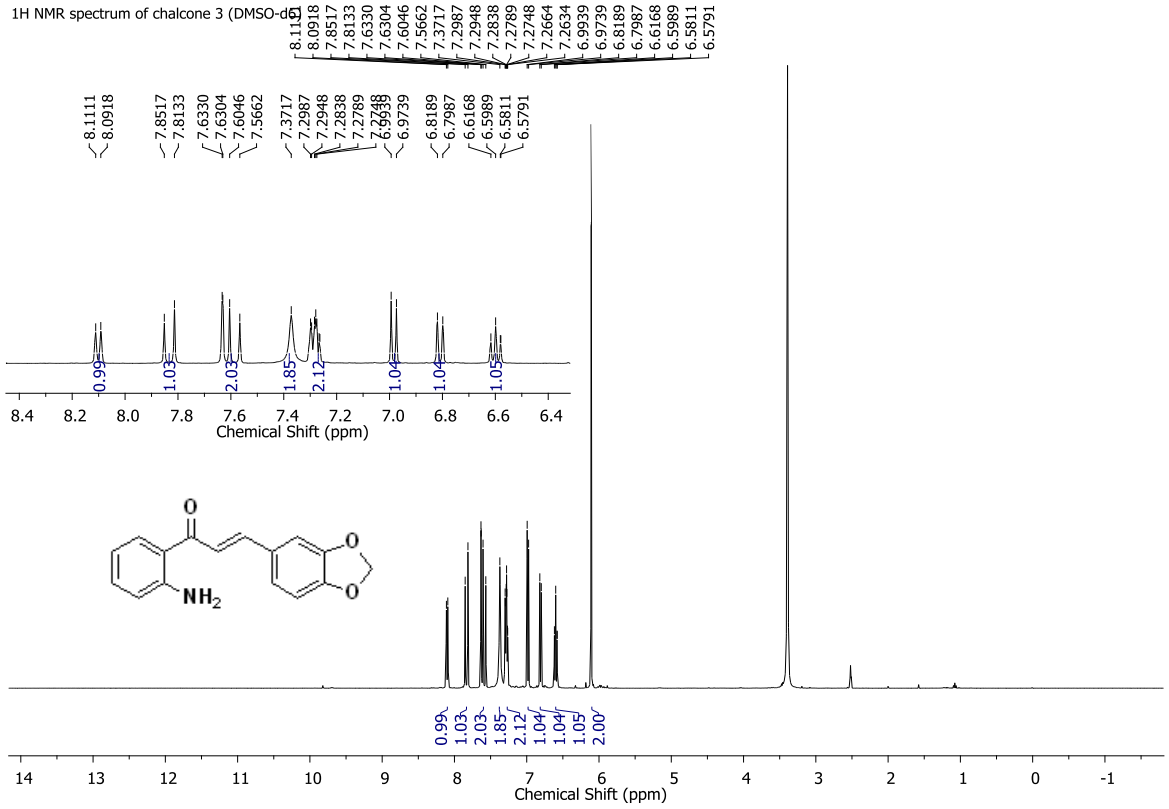

Figure S1. ^{1}H-NMR spectrum of chalcone **3**.

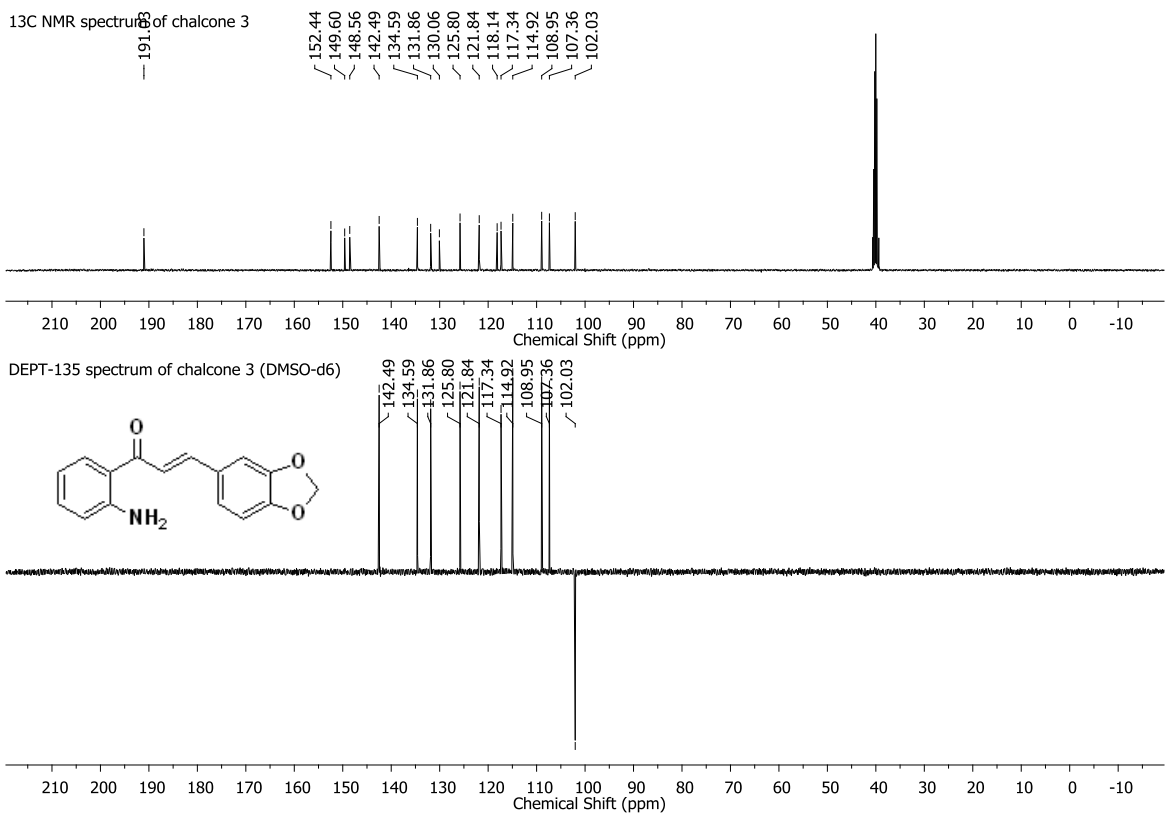

Figure S2. ^{13}C-NMR and DEPT-135 spectra of chalcone **3**.

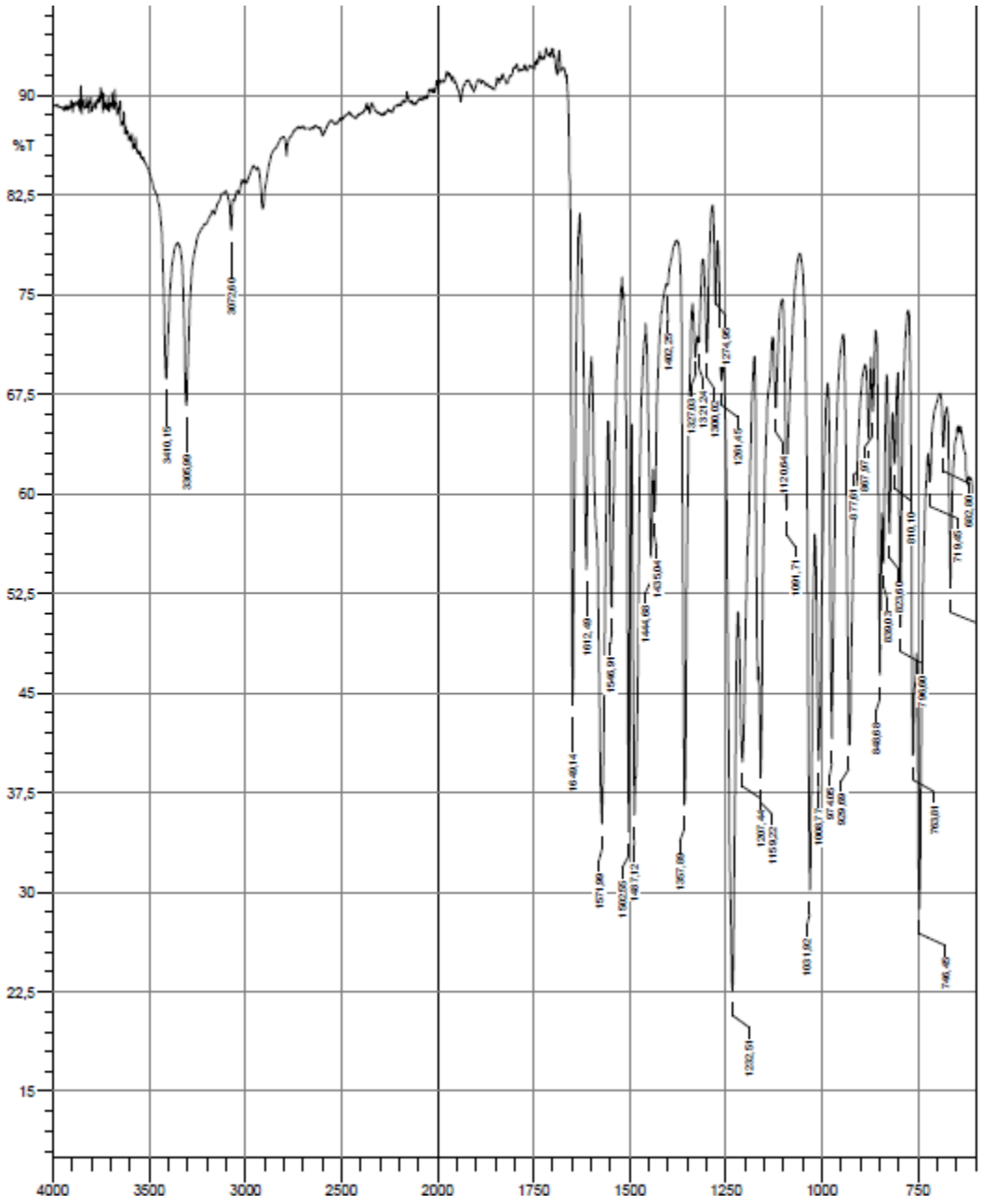

Figure S3. IR spectrum of chalcone **3**.

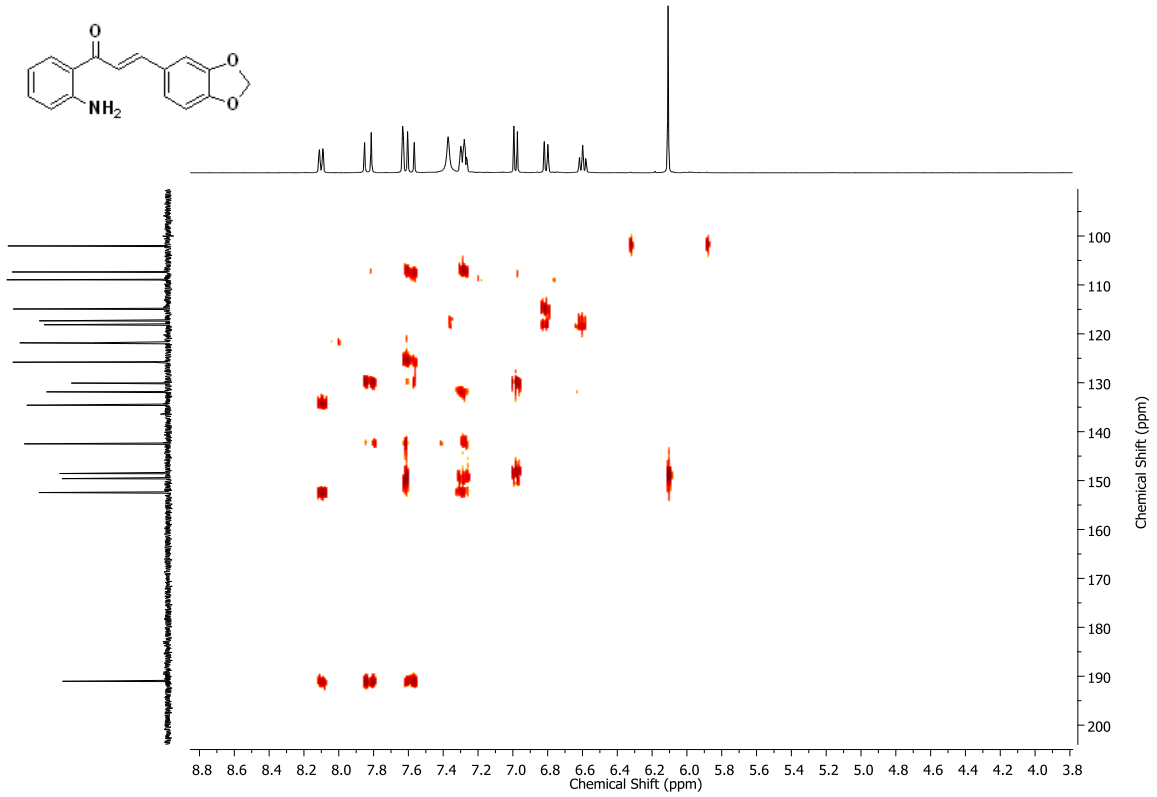

Figure S4. HMBC experiment of chalcone **3**.

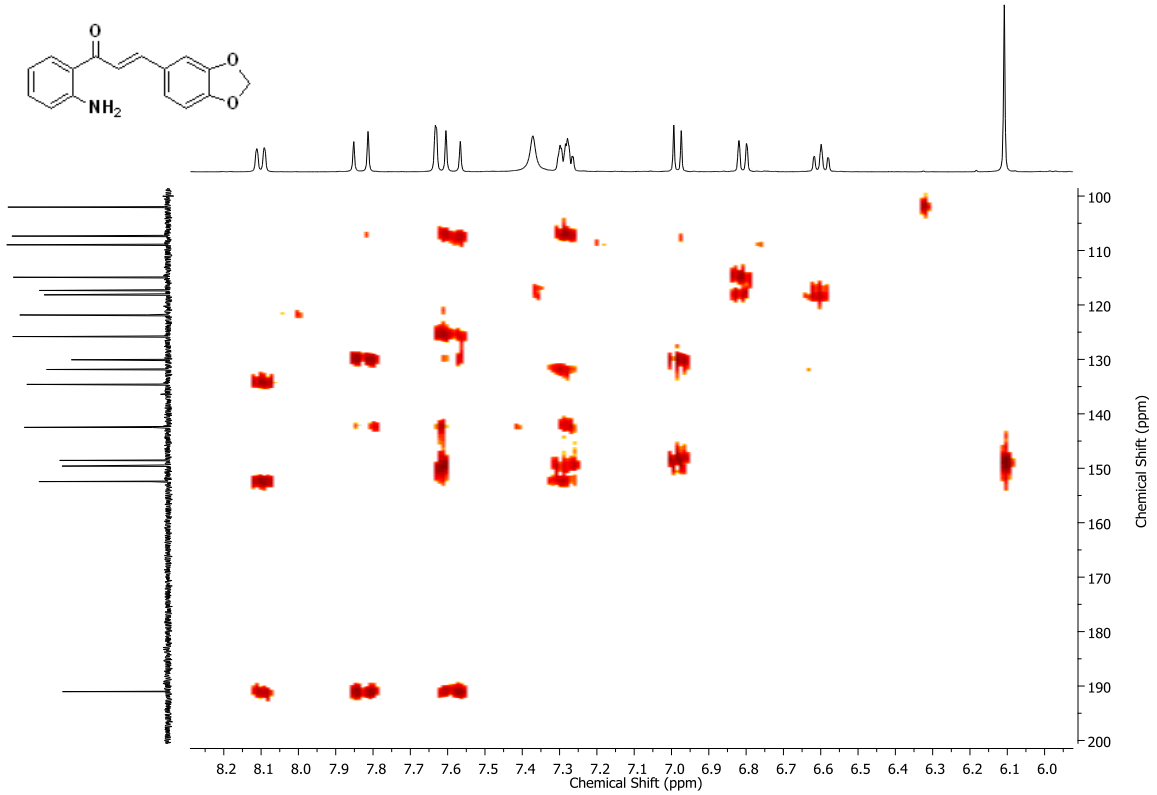

Figure S5. Expansion 1 HMBC experiment of chalcone **3**.

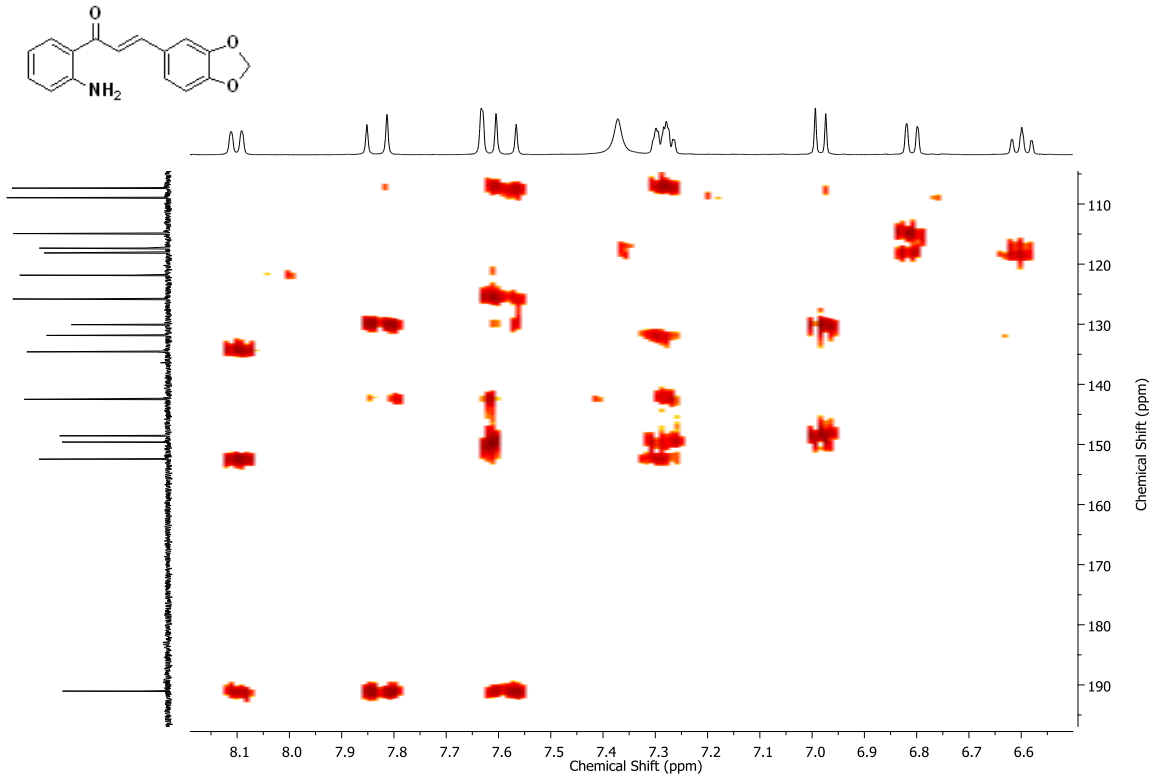

Figure S6. Expansion 2 HMBC experiment of chalcone **3**.

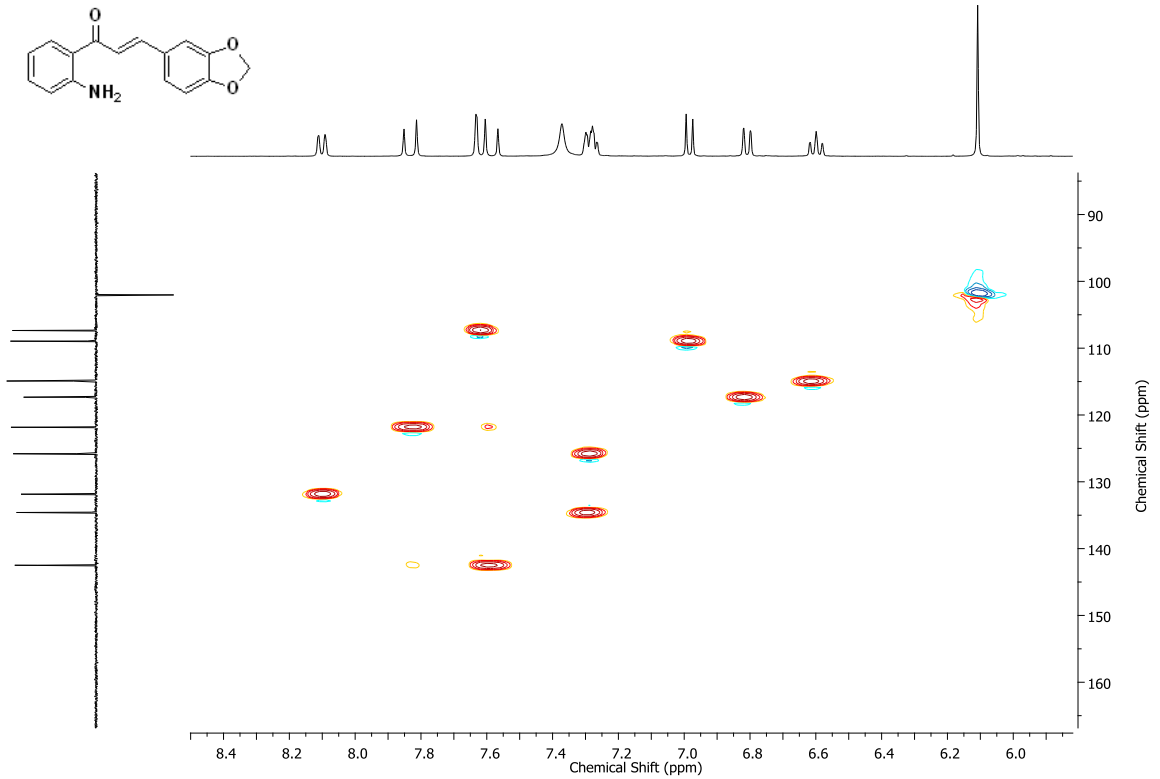

Figure S7. HSQC experiment of chalcone **3**.

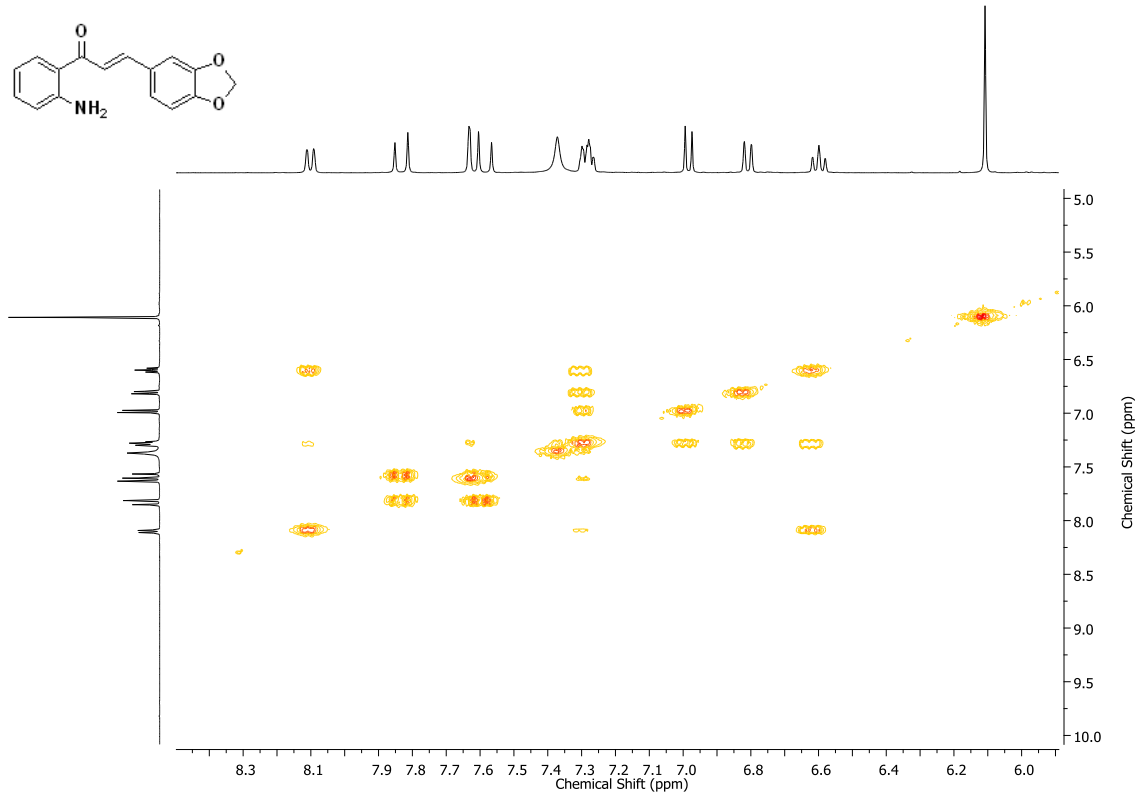

Figure S8. COSY experiment of chalcone **3**.

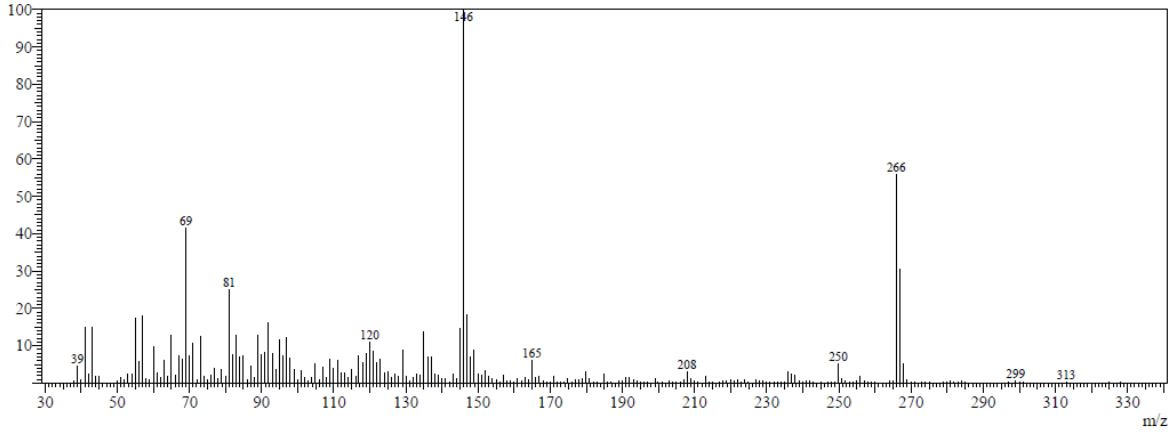

Figure S9. Mass spectrum of chalcone **3**.

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait **.**

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) shelx

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary

Please wait while processing .... Interpreting this report

Structure factor report

Datablock: shelx

Bond precision: C-C = 0.0020 A Wavelength=0.71073

Cell: a=7.7323(3) b=11.2145(5) c=15.1819(7)
alpha=87.527(4) beta=89.369(4) gamma=76.032(4)

Temperature: 123 K

	Calculated	Reported
Volume	1276.36(10)	1276.36(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H13 N O3	?
Sum formula	C16 H13 N O3	C16 H13 N O3
Mr	267.27	267.27
Dx,g cm-3	1.391	1.391
Z	4	4
Mu (mm-1)	0.097	0.097
F000	560.0	560.0
F000'	560.28	
h,k,lmax	10,14,19	9,14,19
Nref	5853	5794
Tmin,Tmax	0.977,0.986	
Tmin'	0.967	

Correction method= Not given

Data completeness= 0.990 Theta(max)= 27.497

R(reflections)= 0.0413(4581) wR2(reflections)= 0.1075(5794)
S = 1.032 Npar= 377

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O2 Check
PLAT410_ALERT_2_C Short Intra H...H Contact H6 .. H8 .. 1.98 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H22 .. H24 .. 1.98 Ang.
PLAT430_ALERT_2_C Short Inter D...A Contact O2 .. O6 .. 2.89 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C16 H13 N O3
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min) 7 Note
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 2 Report

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Alert level G

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.004 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact O6 .. C16 .. 2.96 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 1 Check
O1 -O1 -C7 1.000 1.555 1.555 0.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 30 Check
O1 -C7 -O1 1.000 1.555 1.555 0.00 Deg.
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 44 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density 17 Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

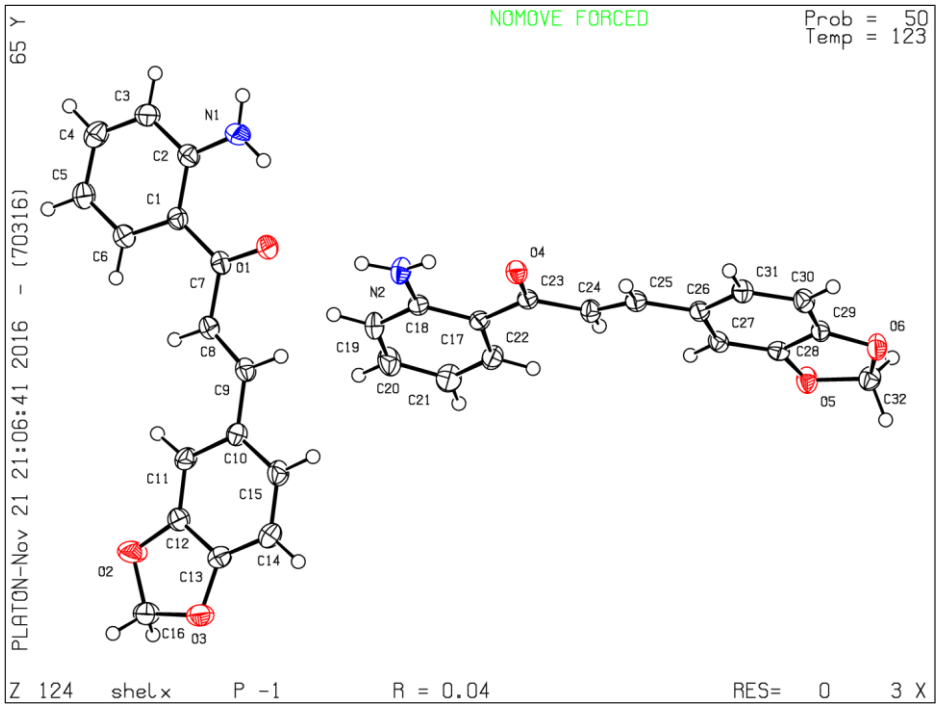
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 11/08/2016; check.def file version of 04/08/2016

Datablock shelx - ellipsoid plot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65 Y
PLATON-Nov 21 21:06:41 2016 - (70316)
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C4
C2
C5
C1
C6
O1
C7
C8
C9
C10
C11
C15
C12
C14
O2
C13
C16
O3
O4
C23
C24
C25
C26
C31
C30
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C28
O5
C32
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C18
C17
C22
C19
C20
C21
Z 124 shelx P -1 R = 0.04 RES= 0 3 X