Supplementary Material: (*E*)-1-(2-Aminophenyl)-3-(4-chlorophenyl)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 mass spectrum for aldehyde **2.**
- Copy of the checkCIF file for compound **3**.

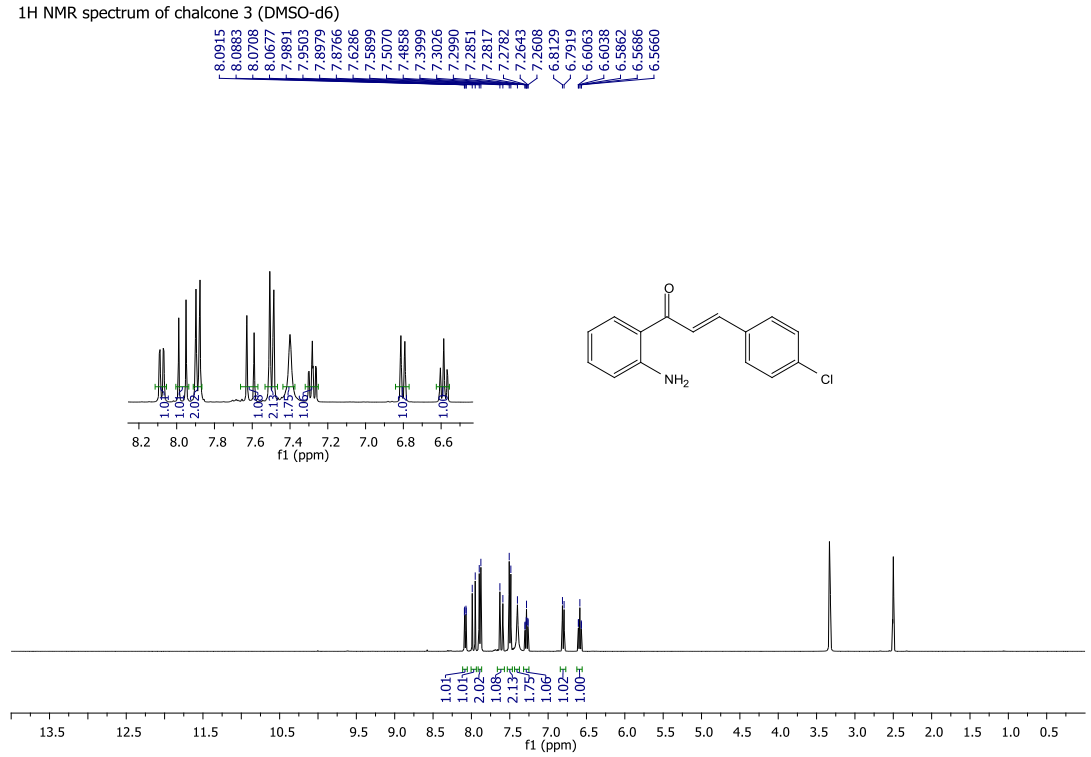

Figure S1. [1]H-NMR spectrum of chalcone **3**.

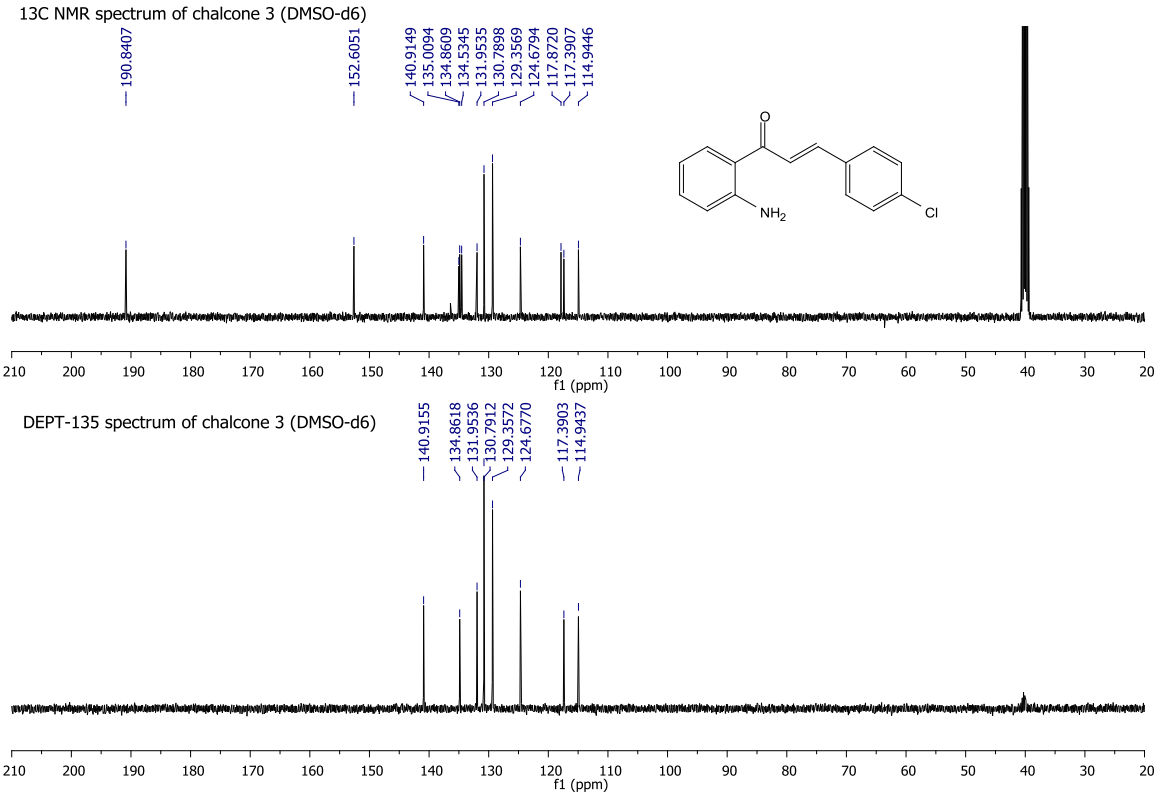

Figure S2. [13]C-NMR and DEPT-135 spectra of chalcone **3**.

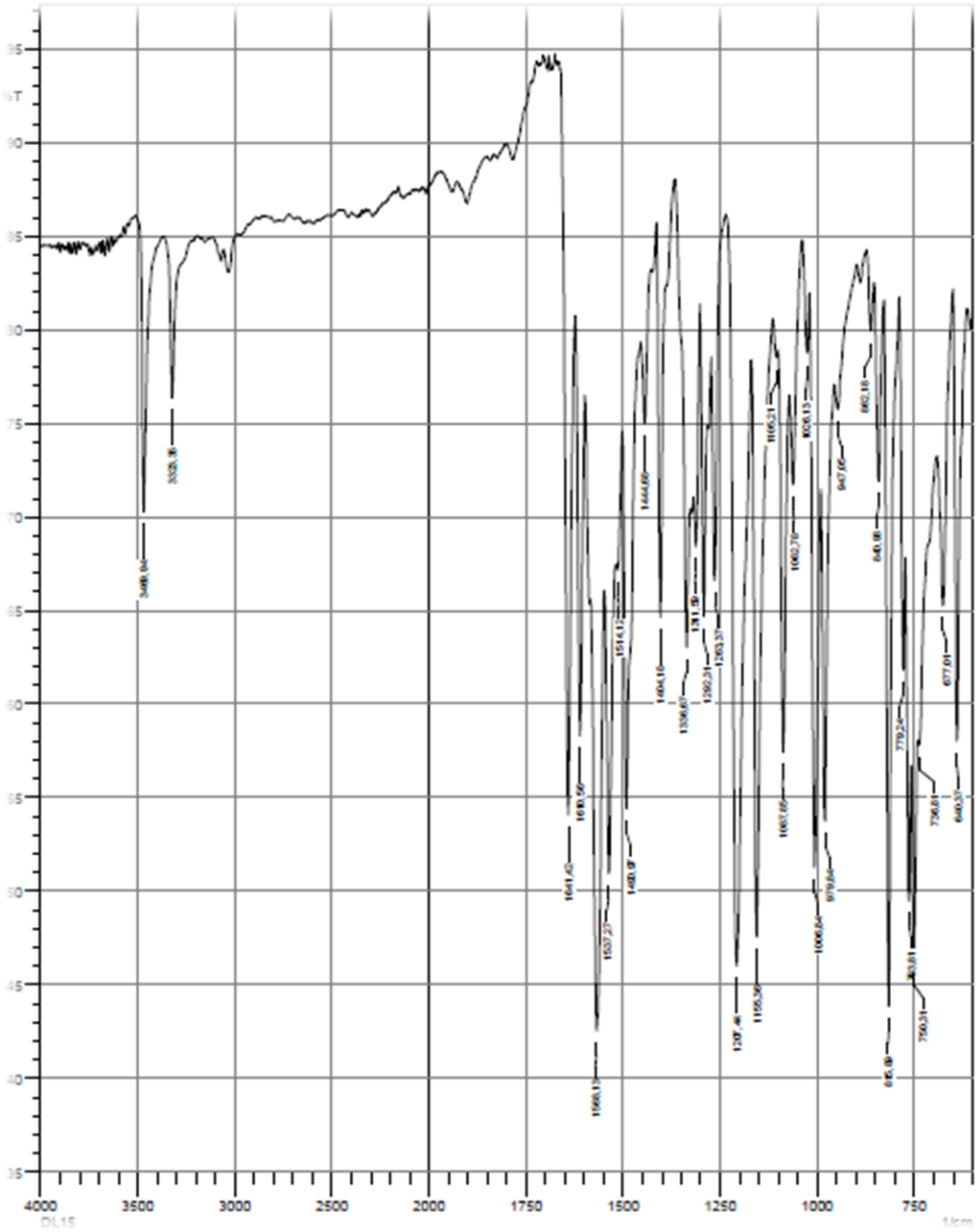

Figure S3. IR spectrum of chalcone **3**.

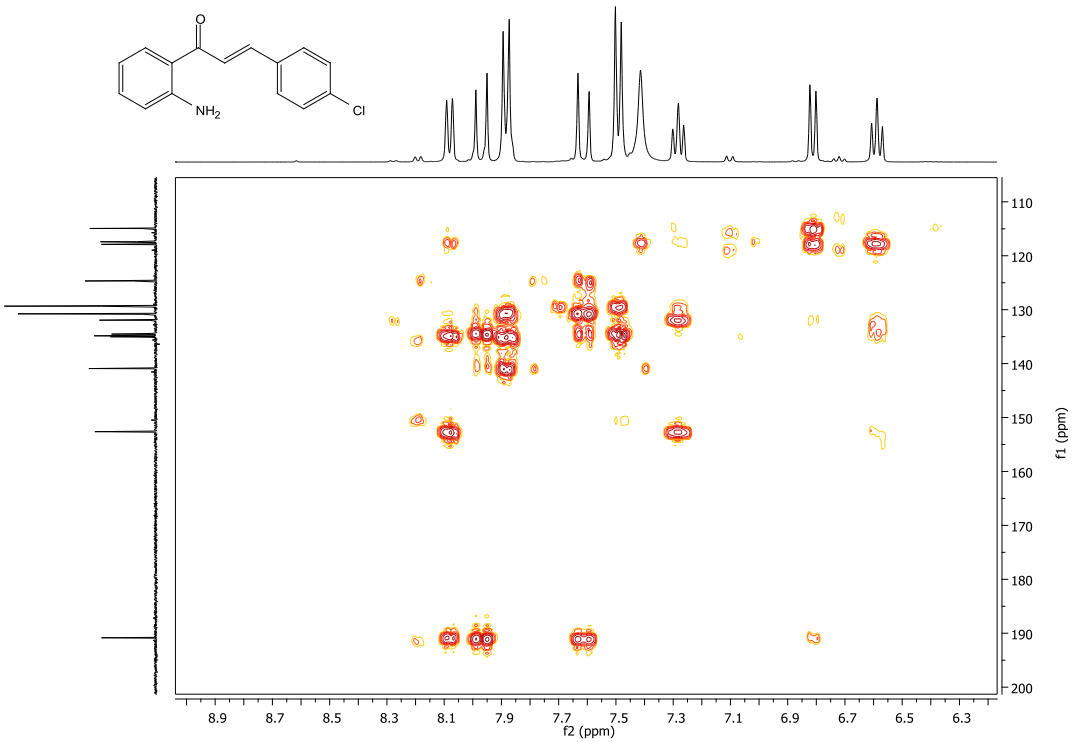

Figure S4. HMBC experiment of chalcone **3**.

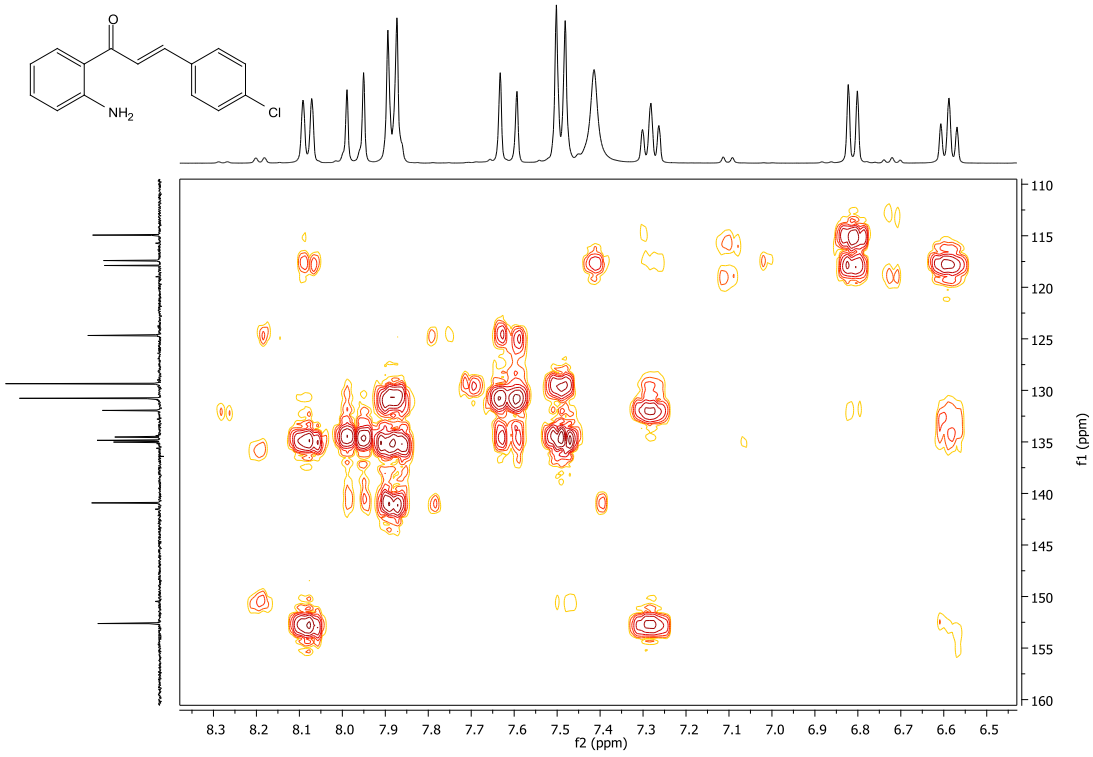

Figure S5. Expansion 1 HMBC experiment of chalcone **3**.

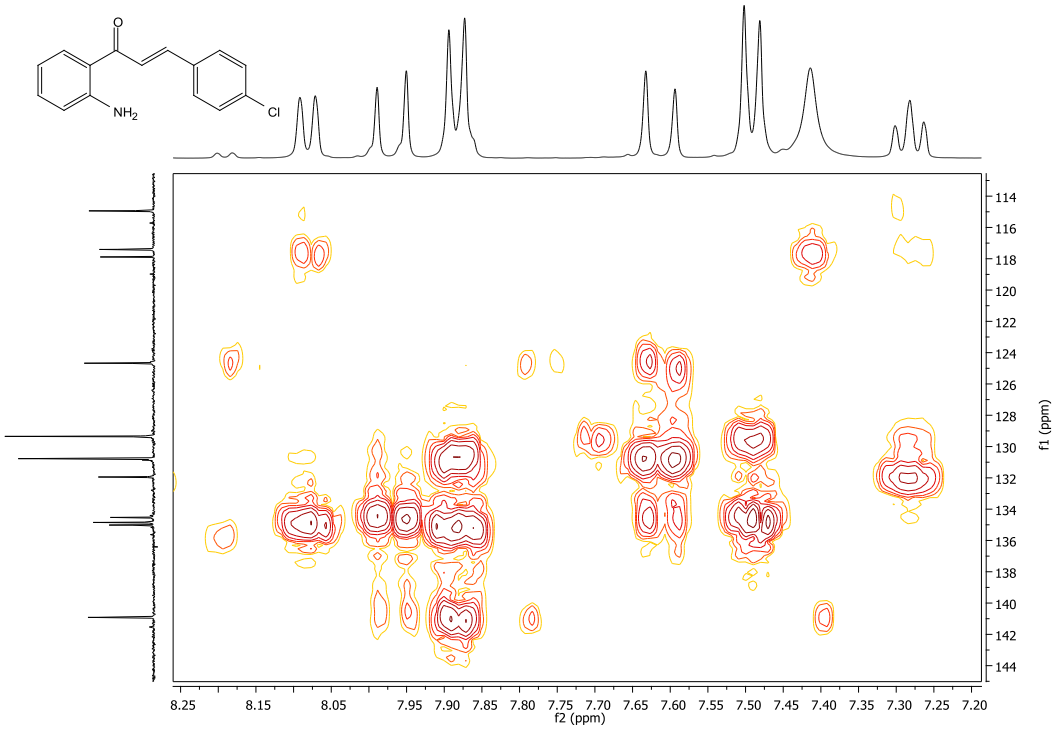

Figure S6. Expansion 2 HMBC experiment of chalcone **3**.

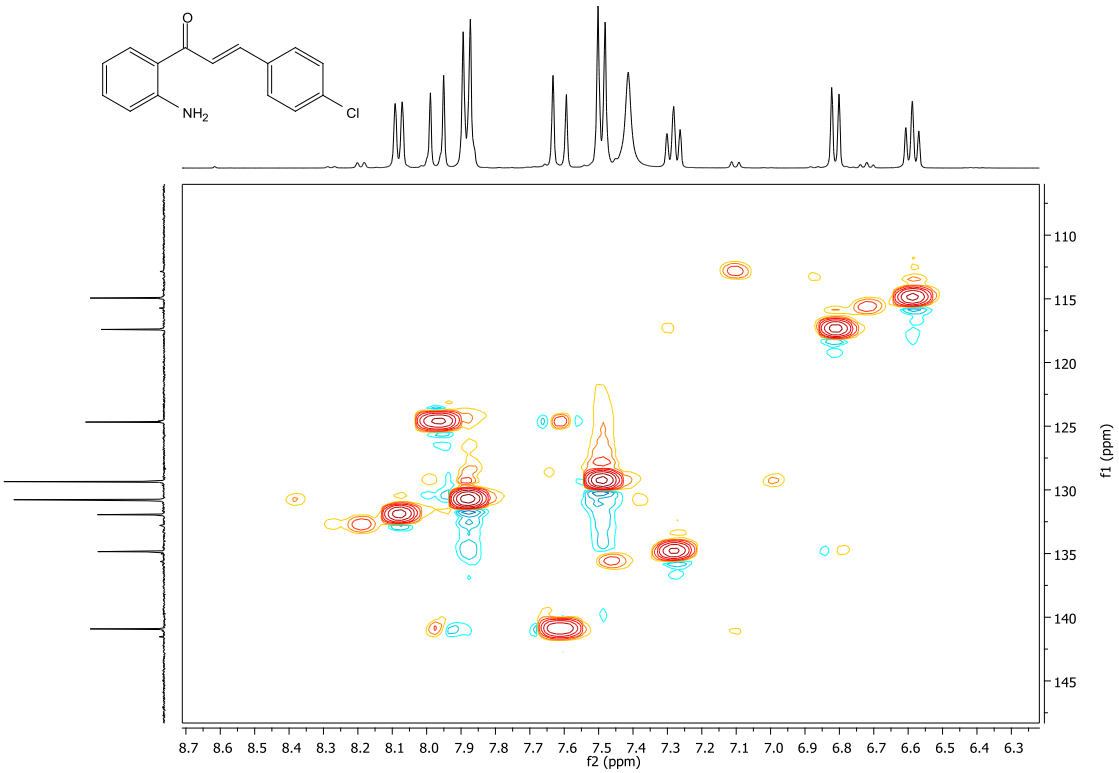

Figure S7. HSQC experiment of chalcone **3**.

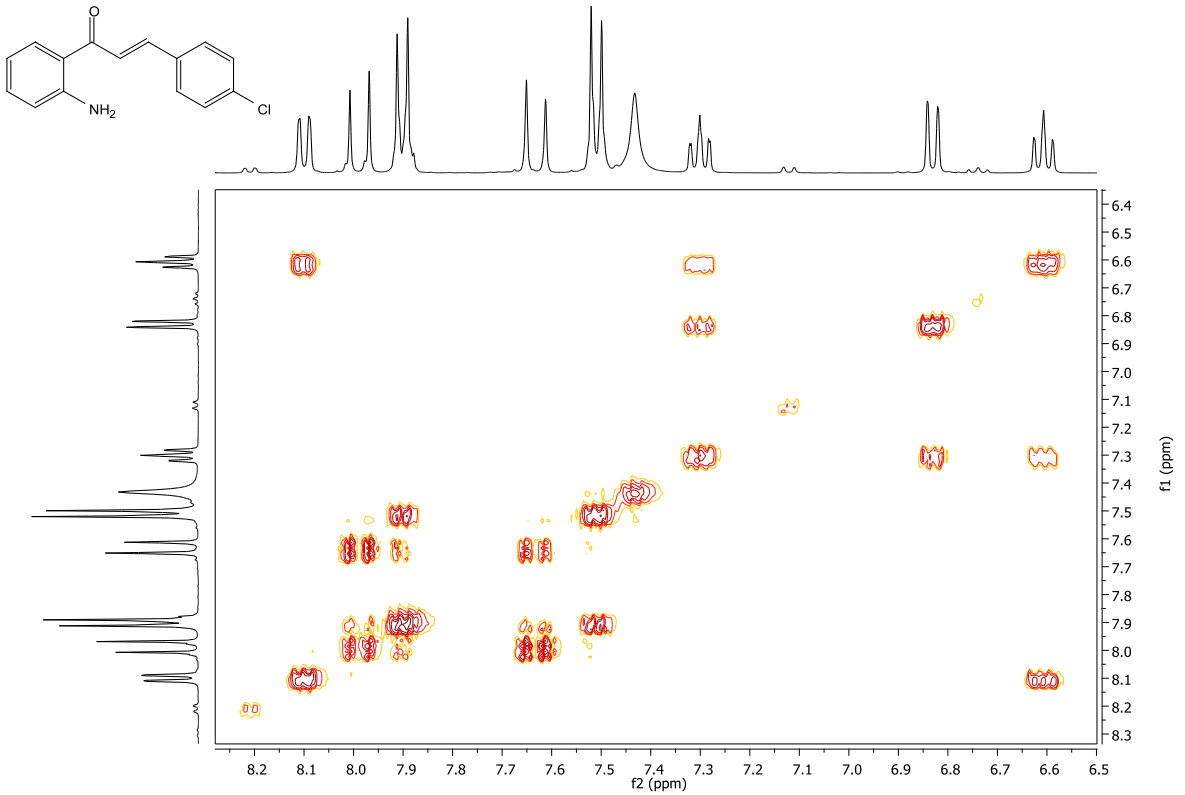

Figure S8. COSY experiment of chalcone **3**.

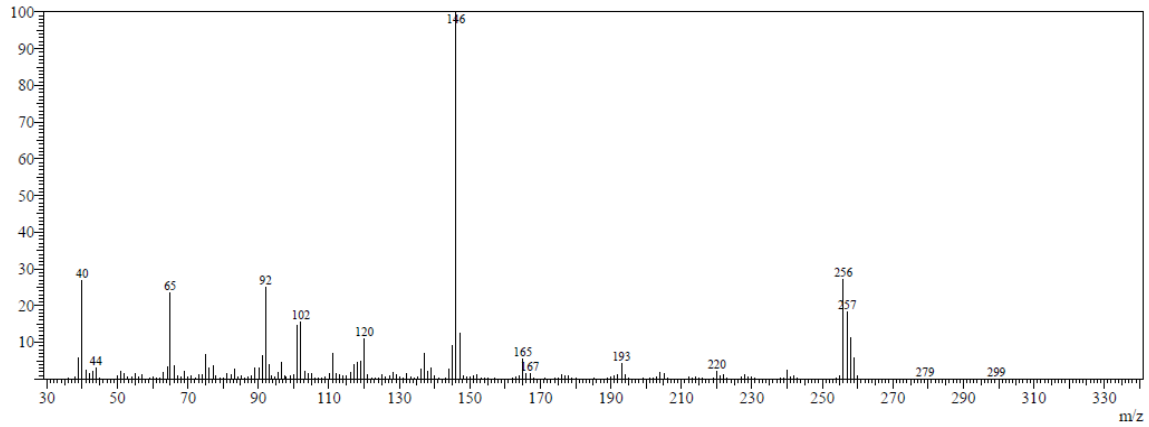

Figure S9. Mass spectrum of chalcone **3**.

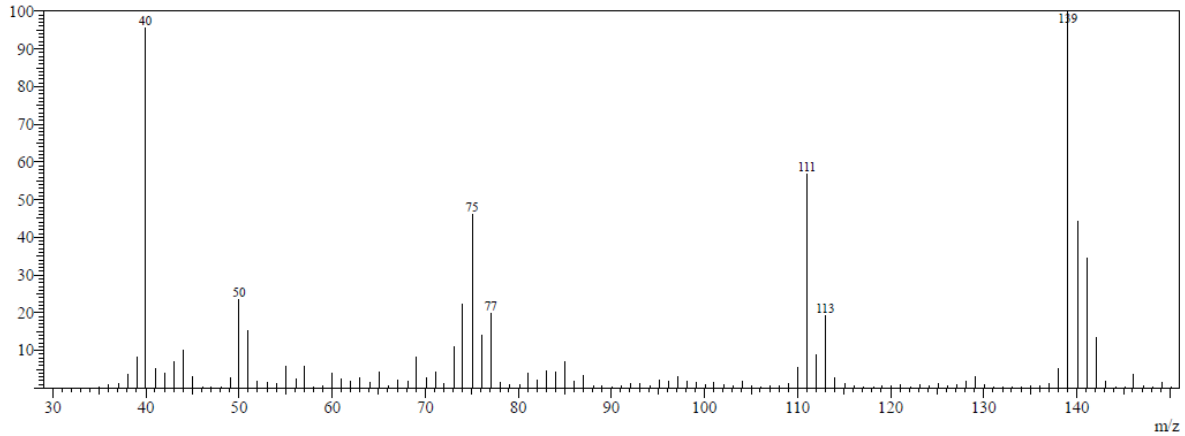

Figure S10. Mass spectrum of aldehyde **2**.

CheckCIF (full publication 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 (full publication check)

Structure factors have been supplied for datablock(s) I

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: I

Bond precision: C-C = 0.0033 A Wavelength=0.71073

Cell: a=7.2156(2) b=11.2733(3) c=30.0334(7)

alpha=90 beta=90 gamma=90

Temperature: 123 K

	Calculated	Reported
Volume	2443.03(11)	2443.03(11)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C15 H12 Cl N O	?
Sum formula	C15 H12 Cl N O	C15 H12 Cl N O
Mr	257.71	257.71
Dx,g cm-3	1.401	1.401
Z	8	8
Mu (mm-1)	0.298	0.298
F000	1072.0	1072.0
F000'	1073.57	
h,k,lmax	9,15,40	9,15,39
Nref	6419[3654]	5488
Tmin,Tmax	0.938,0.953	1.000,0.994
Tmin'	0.901	

Correction method= # Reported T Limits: Tmin=1.000 Tmax=0.994 AbsCorr = NONE

Data completeness= 1.50/0.85 Theta(max)= 28.869

R(reflections)= 0.0379(5041) wR2(reflections)= 0.0817(5488)

S = 1.079 Npar= 341

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

PLAT048_ALERT_1_C MoietyFormula Not Given (or Incomplete) ..... Please Check

PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min) 7 Note

PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage 74 %

Alert level G

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 211 Note

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density 12 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

3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

2 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

1 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

1 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check
