Supporting information

Design a novel sonophotoreactor for green and sustainable organic synthesis: Explorative sonophotocatalytic study of C-H arylation reaction of pyrazoles

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S1. Experimental

S1.1. The synthesized compounds with their physical data

phenyl(1,3,5-triphenyl-1H-pyrazol-4-yl)methanone (3a)

White solid, IR (KBr): 1719 (CO), 1596 (C=N) cm^{-1}; ^{1}H NMR (400MHz, DMSO,d_6) δ: 7.39-7.43 (m, 3H, ArH), 7.49-7.55 (m, 5H, ArH), 7.57-7.61 (m, 6H, ArH), 7.61-7.67 (m, 5H, ArH), 7.78-7.81 (m, 1H, ArH); ^{13}C NMR (100.62 MHz, DMSO-d6) d:116.1, 122.3, 125.6, 126.1, 126.2, 128.35, 128.36, 129.5, 129.8, 133.37, 133.38, 133.5, 140.9, 141.0, 152.8, 193.4. MS (m/z): 400 (M^+). (Found: C, 83.84; H, 4.95; N, 6.91; $C_{28}H_{20}N_2O$ requires C, 83.98; H, 5.03; N, 7.00).

1-(4-benzoyl-1,5-diphenyl-1H-pyrazol-3-yl)ethan-1-one (3b)

Off White solid, IR (KBr): 1716, 1705 (2CO), 1591 (C=N) cm^{-1}; ^{1}H NMR (400MHz, DMSO,d_6) δ: 2.55 (s, 3H, CH_3), 7.15-7.17 (m, 2H, ArH), 7.24-7.29 (m, 3H, ArH), 7.42-7.47 (m, 7H, ArH), 7.59 (t, 1H, *J* = 7.32 Hz, ArH), 7.77 (d, 2H, *J* = 7.24 Hz, ArH); ^{13}C NMR (100.62 MHz, DMSO-d6) d: 26.8, 121.7, 126.3, 128.1, 128.9, 129.1, 129.4, 129.6, 129.8, 129.9, 133.9, 137.9, 139.0, 143.8, 149.0, 191.5, 193.1. MS (m/z): 366 (M^+). (Found: C, 78.91; H, 4.86; N, 7.54; $C_{24}H_{18}N_2O_2$ requires C, 78.67; H, 4.95; N, 7.65).

1-(4-Benzoyl-1-(4-fluorophenyl)-5-phenyl-1H-pyrazol-3-yl)ethan-1-one (3c)

Off White solid, IR (KBr): 1719, 1711 (2CO), 1591 (C=N) cm^{-1}; ^{1}H NMR (400MHz, DMSO,d_6) δ: 2.54 (s, 3H, CH_3), 7.17 (d, 2H, *J* = 7.7 Hz, ArH), 7.27-7.33 (m, 5H, ArH), 7.43-7.57 (m, 4H, ArH), 7.57-7.60 (m, 1H, ArH), 7.78 (d, 2H, J = 7.4 Hz, ArH); ^{13}C NMR (100.62 MHz, DMSO-d6) d:26.8, 116.5 (d, $^{2}J_{CF}$ = 21.2 Hz), 121.7, 127.9, 128.7(d, $^{3}J_{CF}$ = 8.6Hz), 128.8, 129.4, 129.9, 130.0, 133.9, 135.40, 135.43, 137.9, 144.0, 149.0, 161.0 (d, $^{1}J_{CF}$ = 243.1 Hz), 191.5, 193.1. MS (m/z): 384 (M^+). (Found: C, 75.24; H, 4.41; N, 7.17; $C_{24}H_{17}FN_2O_2$ requires C, 74.99; H, 4.46; N, 7.29).

1-(4-benzoyl-5-phenyl-1-(p-tolyl)-1H-pyrazol-3-yl)ethan-1-one (3d)

Beige solid, IR (KBr): 1714, 1710 (2CO), 1595 (C=N) cm^{-1}; ^1H NMR (400MHz, DMSO,d_6) δ: 2.36 (s, 3H, CH_3), 2.57 (s, 3H, CH_3), 7.19-7.21 (m, 2H, ArH), 7.27-7.35 (m, 7H, ArH), 7.49 (t, 2H, *J* = 7.64 Hz, ArH), 7.62 (t, 1H, *J* = 7.32 Hz, ArH), 7.80 (d, 2H, *J* = 7.44 Hz, ArH); ^{13}C NMR (100.62 MHz, DMSO-d6) d: 21.1, 26.8, 121.7, 126.1, 128.9, 129.1, 129.4, 129.8, 129.9, 130.1, 133.9, 136.6, 137.9, 139.0, 143.8, 148.9, 191.5, 193.1. MS (m/z): 380 (M^+). (Found: C, 79.18; H, 5.22; N, 7.23; $C_{25}H_{20}N_2O_2$ requires C, 78.93; H, 5.30; N, 7.36).

1-(4-Benzoyl-5-phenyl-1-(4-(trifluoromethyl)phenyl)-1H-pyrazol-3-yl)ethan-1-one (3e)

Puff solid, IR (KBr): 1715, 1711 (2 CO), 1599(C=N) cm^{-1}; ^1H NMR (400MHz, DMSO,d_6) δ: 2.56 (s, 3H, CH_3), 7.21 (d, 2H, *J* = 7.2 Hz, ArH), 7.28-7.33 (m, 3H, ArH), 7.44-7.48 (m, 2H, ArH), 7.57-7.66 (m, 3H, ArH), 7.79 (d, 2H, J = 7.8 Hz, ArH), 7.84-7.86 (m, 2H, ArH); ^{13}C NMR (100.62 MHz, DMSO-d6) d:26.83, 122.3, 122.8, 125.5 5 (q, $^1J_{CF}$ = 274.3 Hz), 126.86, 126.89, 127.7, 129.15, 129.2, 129.4, 129.5, 130.0, 133.9, 137.8, 142.1, 143.9, 149.5, 191.3, 193.1. MS (m/z): 434 (M^+). (Found: C, 69.34; H, 3.87; N, 6.36; $C_{25}H_{17}F_3N_2O_2$ requires C, 69.12; H, 3.94; N, 6.45.)

ethyl 4-benzoyl-1,5-diphenyl-1H-pyrazole-3-carboxylate (3f)

Off White solid, IR (KBr): 1739, 1710 (2CO), 1603 (C=N) cm^{-1}; ^1H NMR (400 MHz, DMSO-d6) d: 0.95 (t, 3H, *J* = 7.08Hz, CH_3 ester), 4.05 (q, 2H, *J* = 7.08Hz, CH_2 ester), 7.18 (d, 2H, *J* = 6.8 Hz, ArH), 7.25-7.30 (m, 3H, ArH), 7.39-7.50 (m, 7H, ArH), 7.62 (t, 1H, *J* = 7.62 Hz, ArH), 7.79 (d, 2H, *J* = 7.48 Hz, ArH); ^{13}C NMR (100.62 MHz, DMSO-d6) d:13.9, 61.3, 123.1, 126.4, 128.0, 128.9, 129.2, 129.4, 129.6, 129.8, 130.2, 134.0, 138.2, 138.9, 141.9, 143.9, 161.2, 190.9. MS (m/z): 396 (M^+). (Found: C, 75.96; H, 4.99; N, 6.98; $C_{25}H_{20}N_2O_3$ requires C, 75.74; H, 5.09; N, 7.07.)

Ethyl 4-benzoyl-1-(4-fluorophenyl)-5-phenyl-1H-pyrazole-3-carboxylate (3g)

Off White solid, IR (KBr): 1742, 1712 (2CO), 1601 (C=N) cm^{-1}; ^1H NMR (400 MHz, DMSO-d6) d: 0.95 (t, 3H, *J* = 7.08Hz, CH_3 ester), 4.05 (q, 2H, *J* = 7.08Hz, CH_2 ester), 7.19 (d, 2H, *J* = 6.6 Hz, ArH), 7.26-7.31 (m, 5H, ArH), 7.48(t, 4H, *J* = 7.76Hz, ArH), 7.61 (t, 1H, *J* = 7.4Hz, ArH), 7.80 (d, 2H, *J* = 7.52 Hz, ArH); ^{13}C NMR (100.62 MHz, DMSO-d6) d:13.9, 61.3, 116.4(d, $^2J_{CF}$ = 22.8 Hz), 116.6, 123.0, 127.9, 128.8(d, $^3J_{CF}$ = 9.2Hz), 128.9, 129.2, 130.2, 134.0, 135.4(d, $^4J_{CF}$ = 2.4 Hz), 138.2, 141.9, 144.1, 162.2 (d, $^1J_{CF}$ = 247.5 Hz), 190.9. MS (m/z): 414 (M^+). (Found: C, 72.68; H, 4.54; N, 6.65; $C_{25}H_{19}FN_2O_3$ requires C, 72.45; H, 4.62; N, 6.76.)

ethyl 4-benzoyl-5-phenyl-1-(p-tolyl)-1H-pyrazole-3-carboxylate (3h)

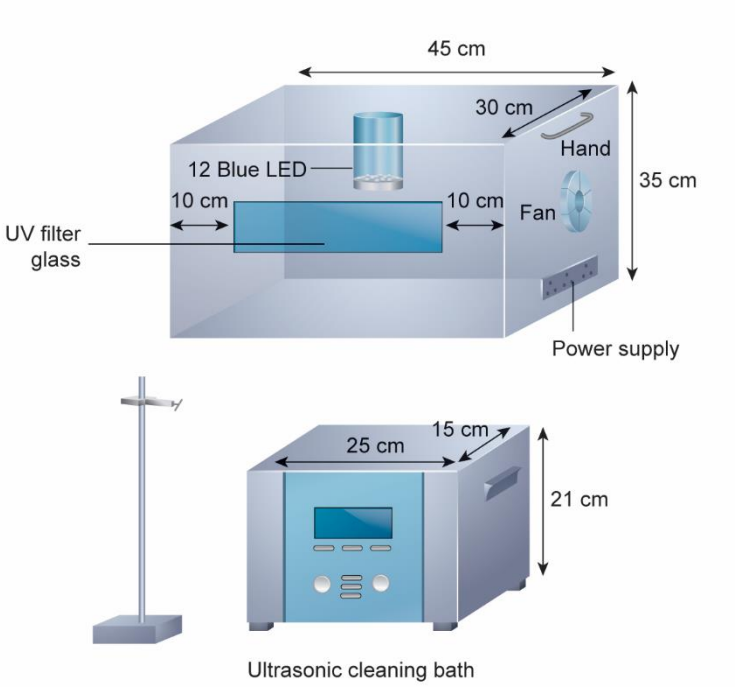
Off White solid, IR (KBr): 1744, 1710 (2CO), 1601 (C=N) cm^{-1}; ^1H NMR (400 MHz, DMSO-d6) d: 0.94 (t, 3H, *J* = 7.04 Hz, CH_3 ester), 2.30 (s, 3H, CH_3), 4.04 (q, 2H, *J* = 7.04 Hz, CH_2 ester), 7.18-7.28 (m, 9H, ArH), 7.47 (t, 2H, *J* = 7.68 Hz, ArH), 7.61 (t, 1H, *J* = 7.36 Hz, ArH), 7.79 (d, 2H, *J* = 7.28 Hz, ArH); ^{13}C NMR (100.62 MHz, DMSO-d6) d:13.9, 21.1, 61.2, 123.0, 126.1, 128.1, 128.9, 129.2, 129.5, 129.8, 129.9, 130.2, 133.9, 136.6, 138.2, 139.0, 141.7, 143.8, 161.2, 190.9. MS (m/z): 410 (M^+). (Found: C, 76.30; H, 5.32; N, 6.71; $C_{26}H_{22}N_2O_3$ requires C, 76.08; H, 5.40; N, 6.82.)

S1.2. Single-crystal X-ray determination

The compounds **3c** and **3e** were synthesized through slow evaporation of solvent to give single crystals suitable for single-crystal X-ray diffraction studies. The crystals were viewed under the microscope for the selection of suitable samples for data collection. The certain selected sample was fixed on the tip of thin glass fiber, which was interleaved in the wax. This sample was mounted on Agilent Supernova (Dual source) Agilent Technologies Diffractometer for each sample, equipped with microfocus Cu/Mo Ka radiation for data collection. The data collection was accomplished using CrysAlisPro software [62] at 296 K under the Mo Ka radiation. The structure solution was performed using SHELXSe2013 method [63] and refined by full-matrix least-squares methods on F2 using the SHELXLe2013 method [64], in-built with WinGX [64]. All non-hydrogen atoms were refined aniso tropically by full-matrix least-squares methods [63].

S2: An illustration of our design

1. A schematic illustration of our design with dimensions



2. <u>The Designed Reactor</u>

<u>The Light Source</u>

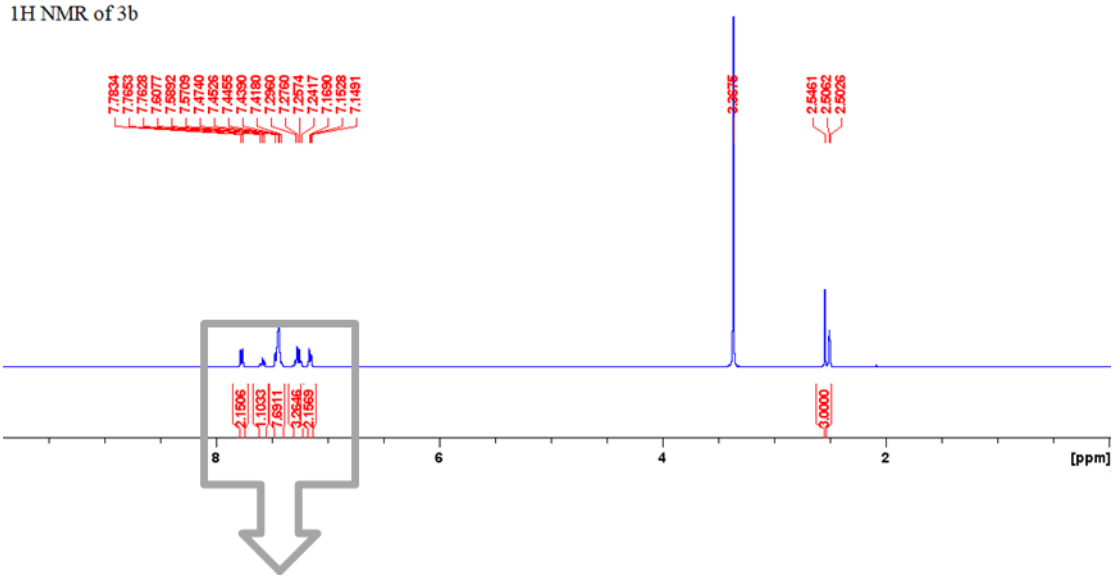
<u>Lateral View</u>

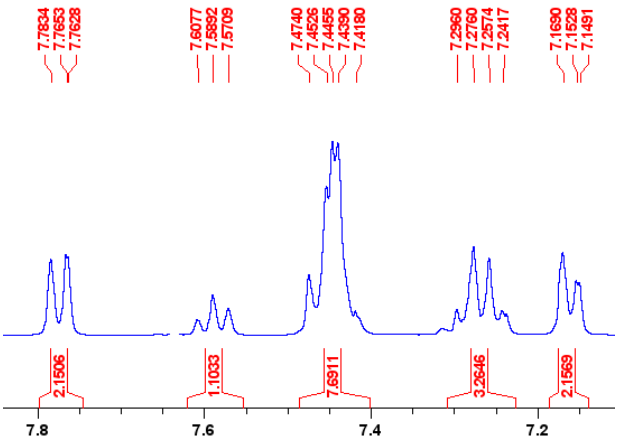
<u>The Sonicator</u>

<u>Front View</u>

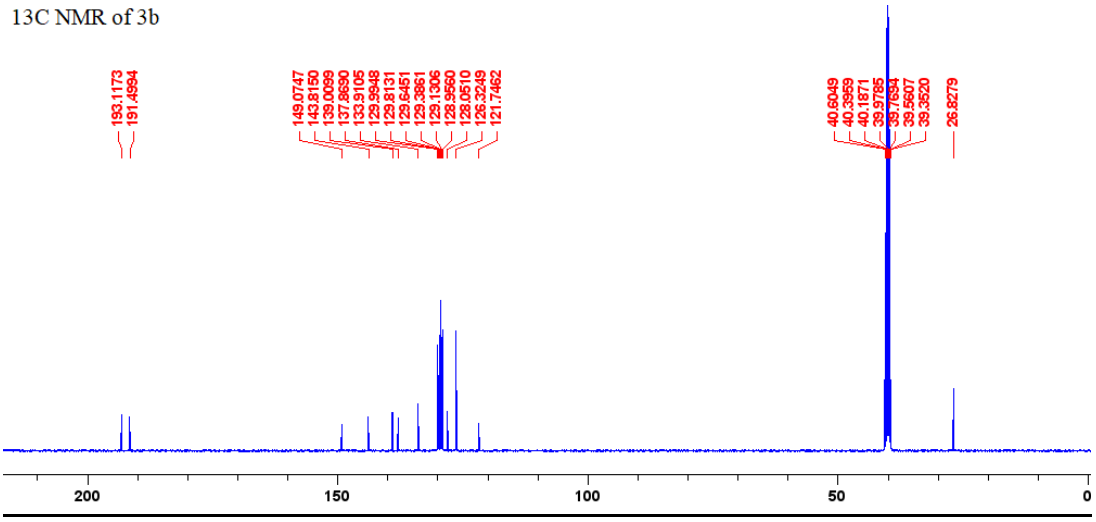
S3: Copies of NMR Data

1H NMR of 3b

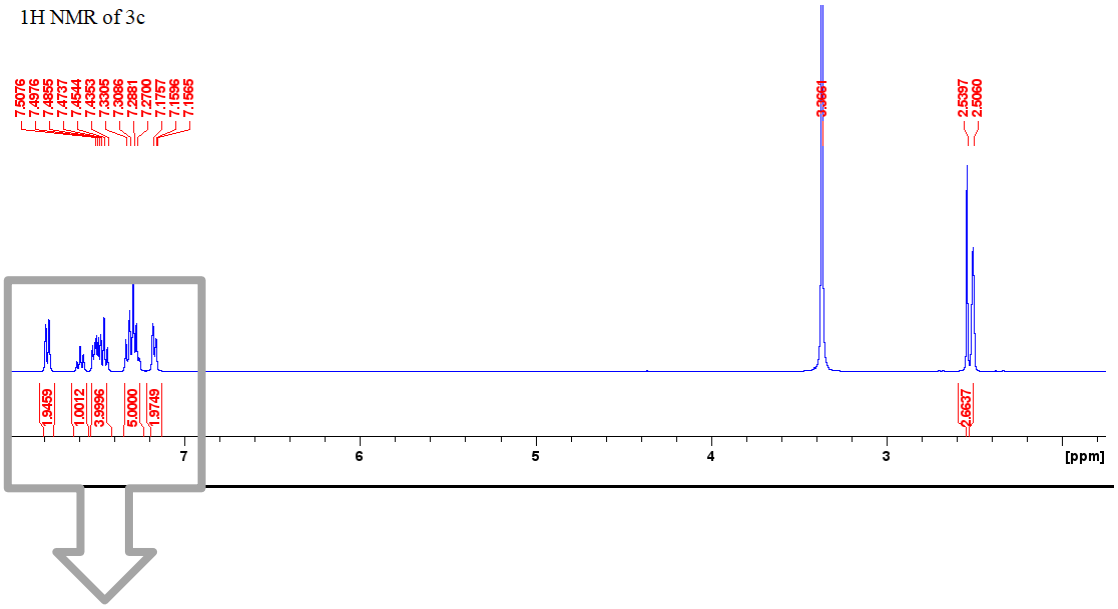


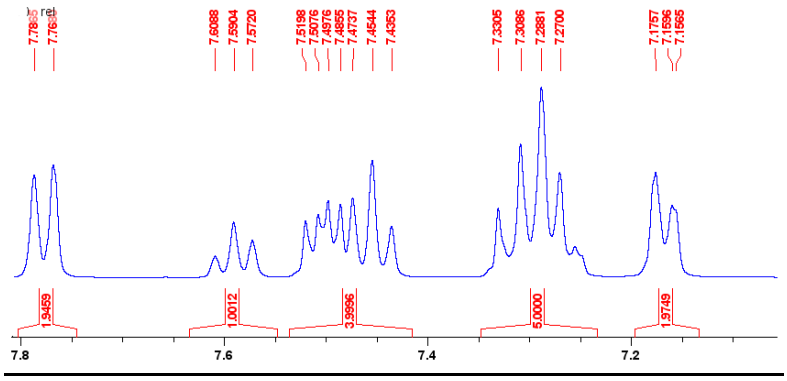


13C NMR of 3b

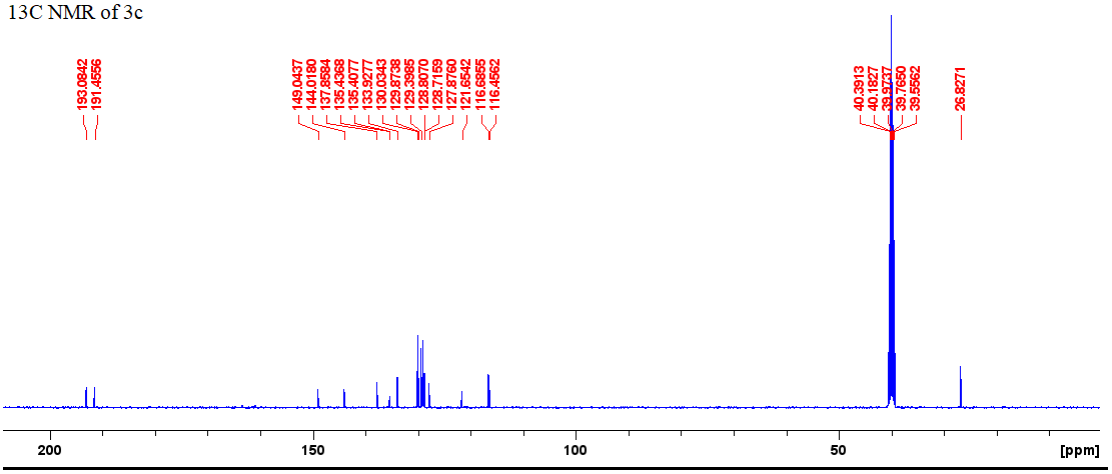


1H NMR of 3c

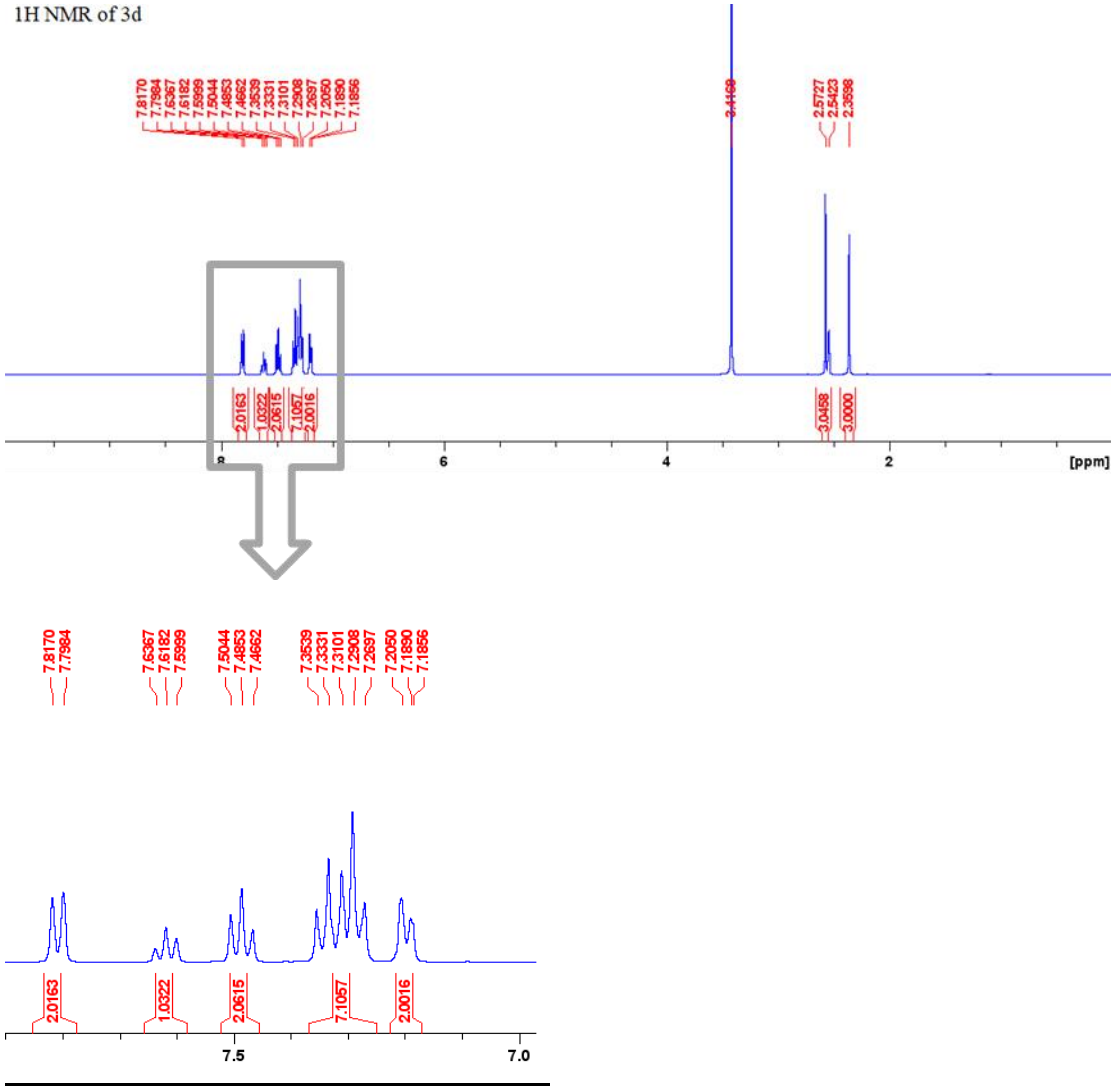




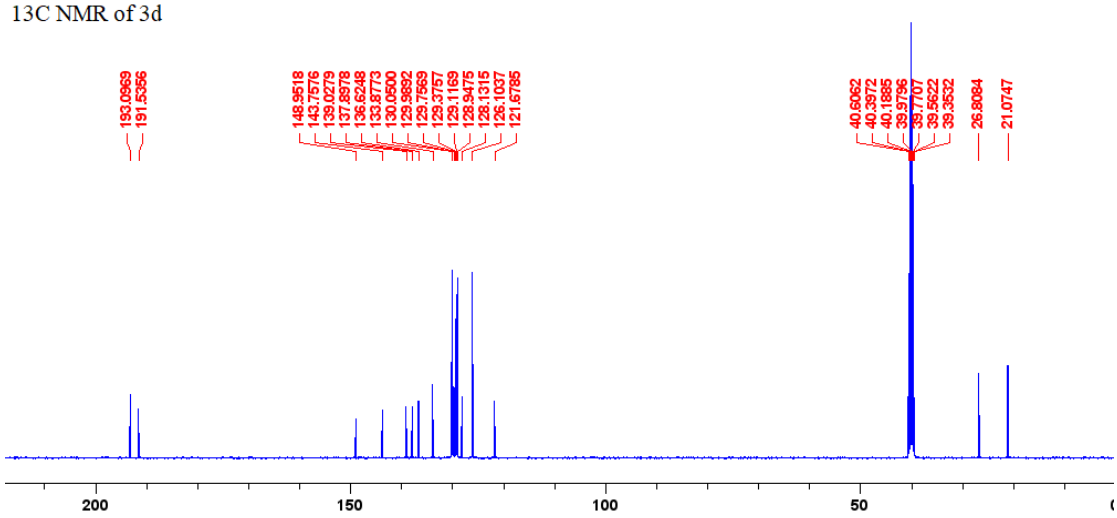
13C NMR of 3c



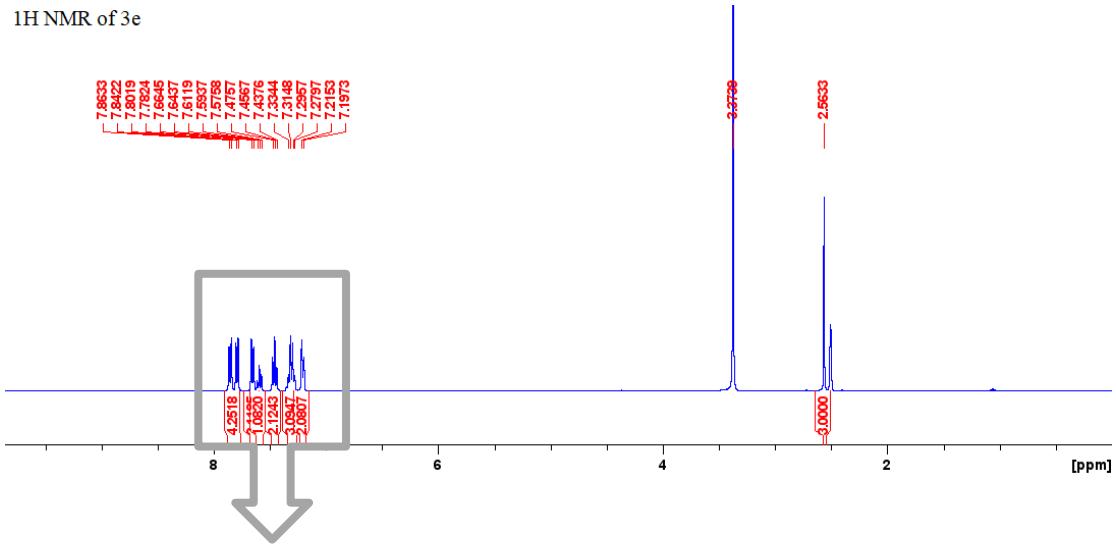
1H NMR of 3d

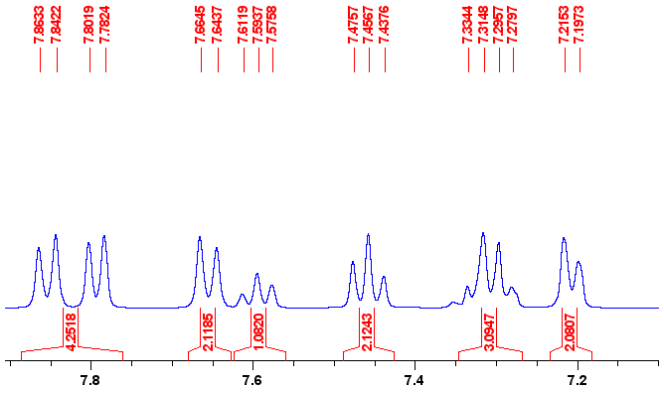


13C NMR of 3d

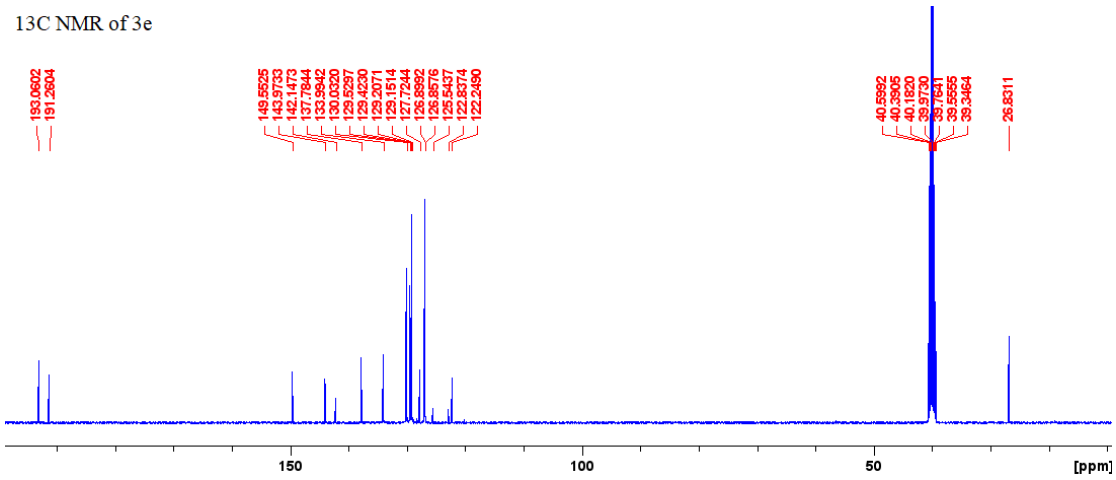


1H NMR of 3e

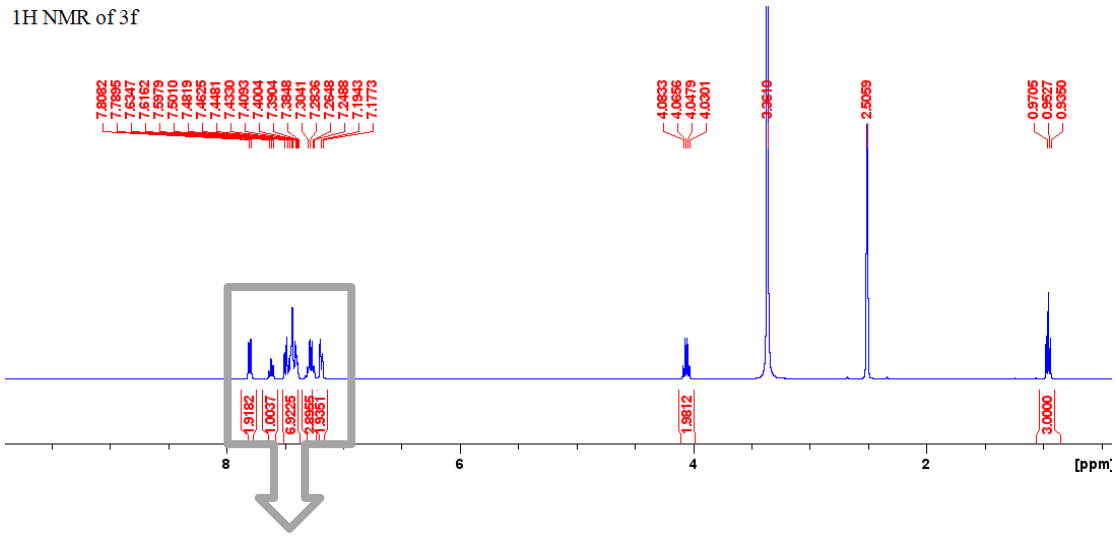


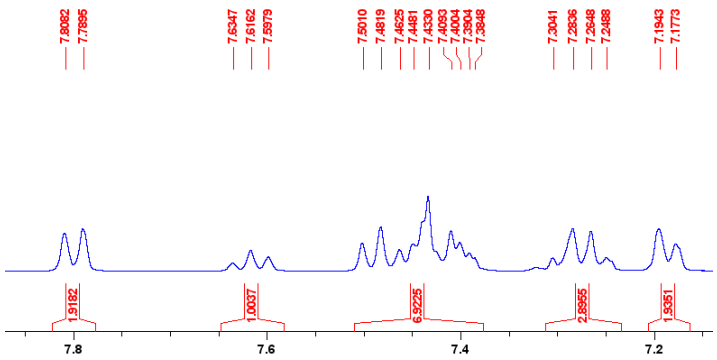


13C NMR of 3e

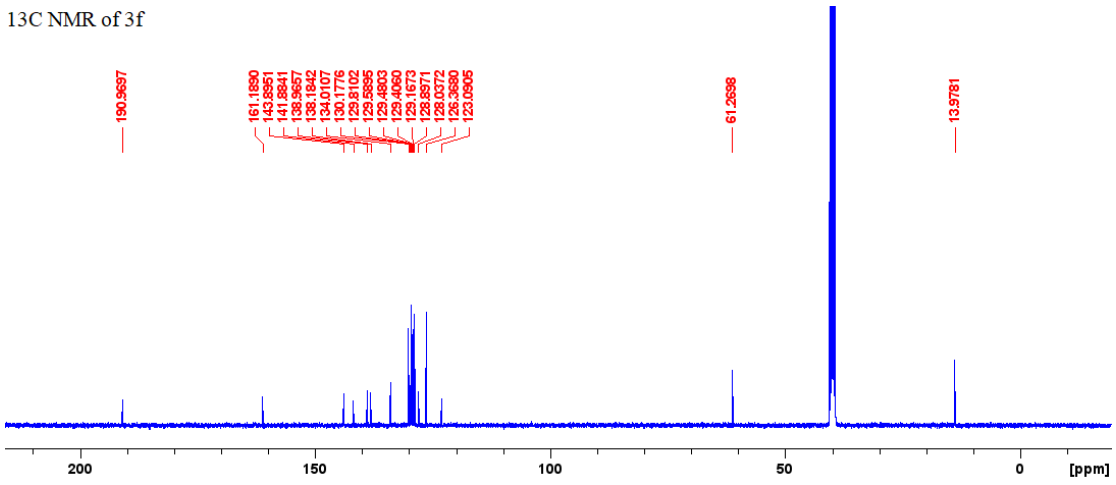


1H NMR of 3f

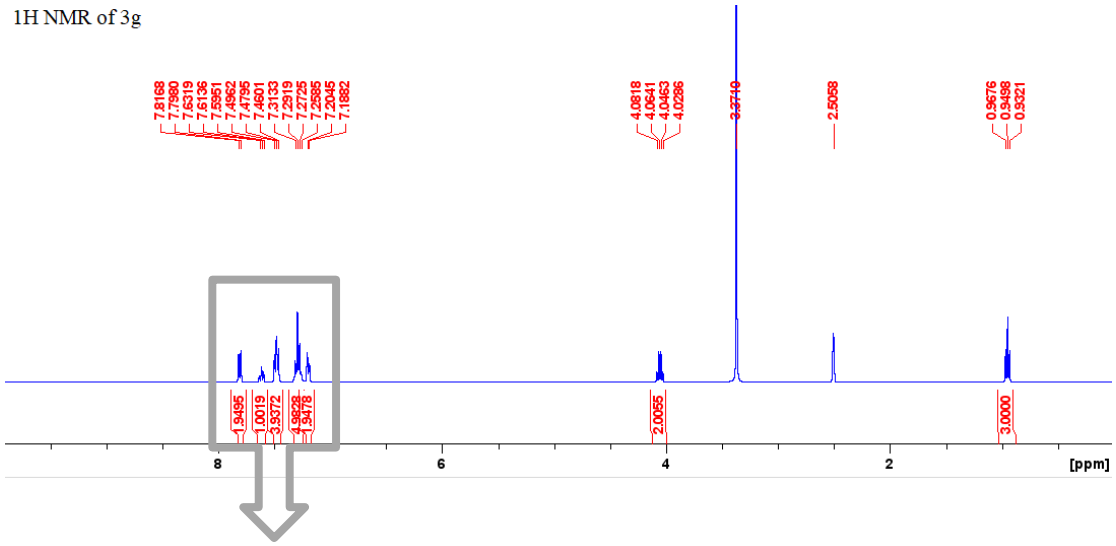


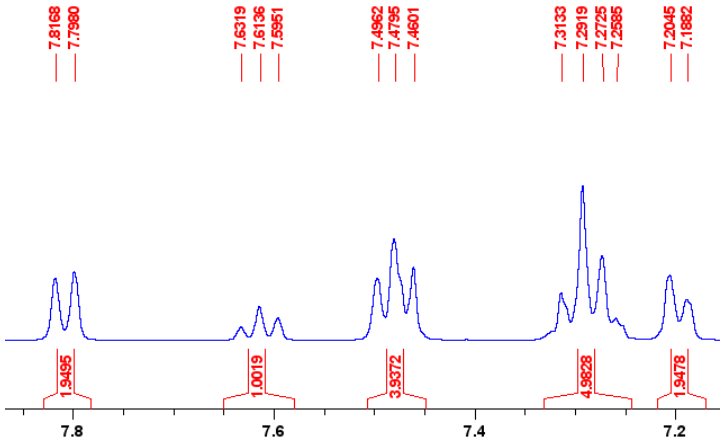


13C NMR of 3f

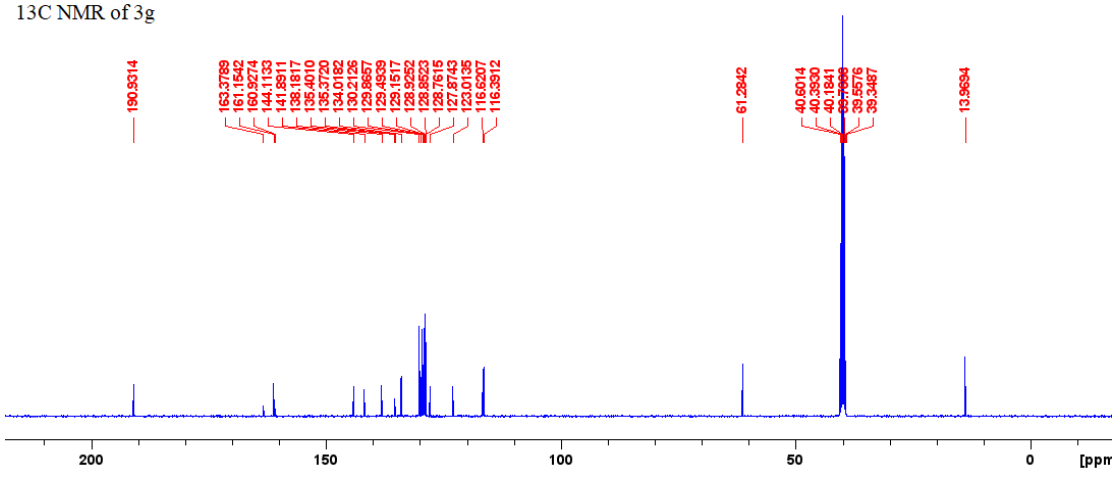


1H NMR of 3g

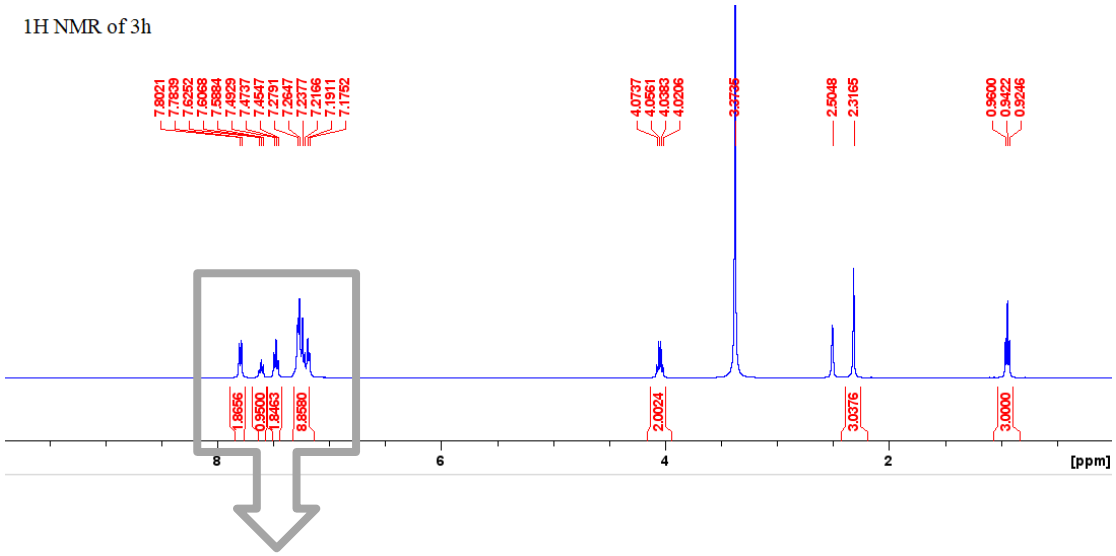


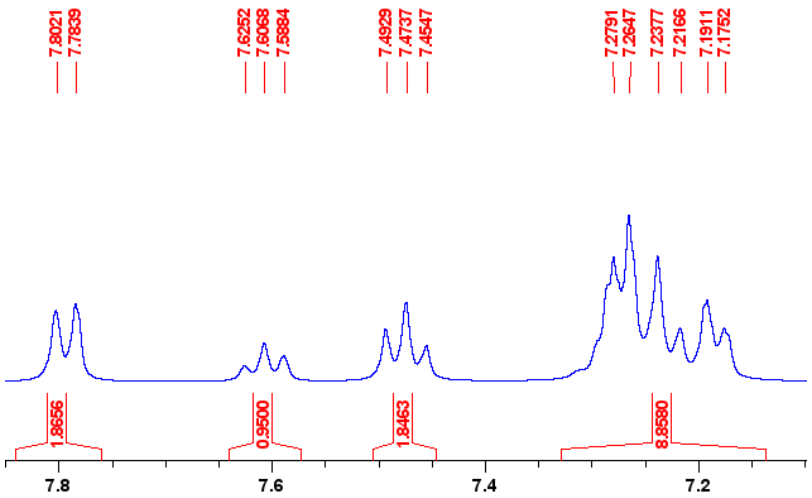


13C NMR of 3g

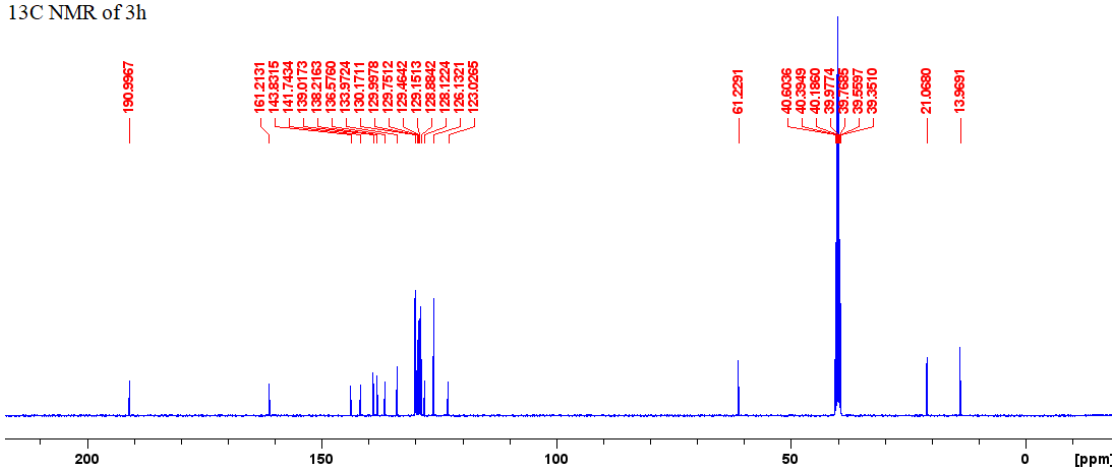


1H NMR of 3h





13C NMR of 3h



S4: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 = 0.0047 A Wavelength=0.71073
Cell: a=10.2905(5) b=11.9920(7) c=16.5715(10)
alpha=78.698(5) beta=81.660(5) gamma=80.197(4)
Temperature: 293 K

	Calculated	Reported
Volume	1962.8(2)	1962.8(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 H17 F N2 O2	?
Sum formula	C24 H17 F N2 O2	C24 H17 F N2 O2
Mr	384.40	384.39
Dx,g cm-3	1.301	1.301
Z	4	4
Mu (mm-1)	0.090	0.090
F000	800.0	800.0
F000'	800.39	
h,k,lmax	14,16,22	13,16,22
Nref	10678	9674
Tmin,Tmax		
Tmin'		

Correction method= Not given
Data completeness= 0.906 Theta(max)= 29.244

R(reflections)= 0.0741(4481) wR2(reflections)= 0.2682(9674)

S = 1.055 Npar= 524

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

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 46% Check

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check

PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check

PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.27 Report

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C21 Check

PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C18 -C23 1.37 Ang.

PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C41 -C46 1.37 Ang.

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00468 Ang.

PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -1.929 Report

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Alert level G

PLAT199_ALERT_1_G Reported _cell_measurement_temperature.....(K) 293 Check

PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature.....(K) 293 Check

PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C24 Check

PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C48 Check

PLAT480_ALERT_4_G Long H...A H-Bond Reported H42 ..F1 . 2.58 Ang.

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 968 Note

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.1 Low

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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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

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  11 ALERT level C = Check. Ensure it is not caused by an omission or
oversight
   9 ALERT level G = General information/check it is not something
unexpected

  13 ALERT type 1 CIF construction/syntax error, inconsistent or
missing data
   4 ALERT type 2 Indicator that the structure model may be wrong or
deficient
   7 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
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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

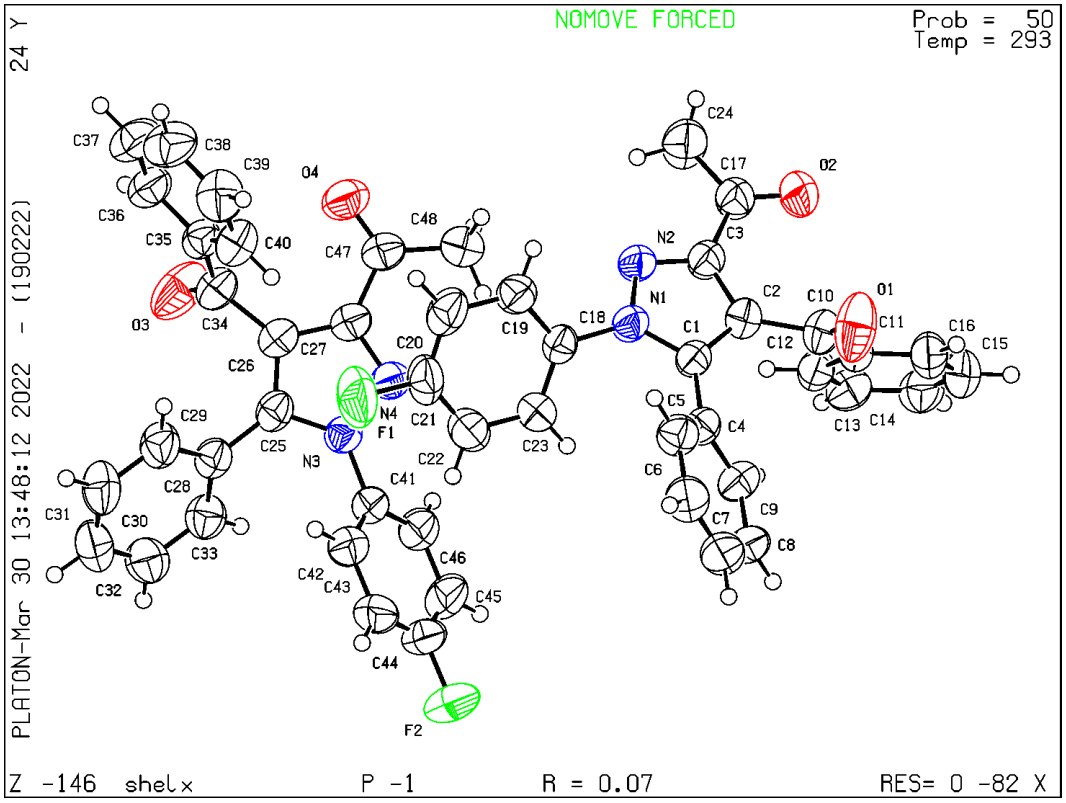
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 19/02/2022; check.def file version of 19/02/2022

Datablock shelx - ellipsoid plot


NOMOVE FORCED
Prob = 50
Temp = 293
24 Y
PLATON-Mar 30 13:48:12 2022 - (190222)
C24
C17
O2
C3
N2
C37
C38
C39
O4
C48
C36
C35
C40
C47
N1
C2
C10
O1
O3
C34
C27
C20
C19
C18
C1
C11
C16
C12
C15
C26
C5
C4
C29
N4
F1
C21
C25
N3
C22
C23
C13
C14
C6
C28
C41
C7
C9
C31
C30
C33
C46
C8
C42
C43
C45
C32
C44
F2
Z -146 shelx
P -1
R = 0.07
RES= 0 -82 X

S:5 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 = 0.0031 A Wavelength=0.71073
Cell: a=11.4370(6) b=8.8132(4) c=21.0108(12)
alpha=90 beta=92.604(5) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	2115.63(19)	2115.63(19)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C25 H17 F3 N2 O2	?
Sum formula	C25 H17 F3 N2 O2	C25 H17 F3 N2 O2
Mr	434.41	434.40
Dx,g cm-3	1.364	1.364
Z	4	4
Mu (mm-1)	0.105	0.105
F000	896.0	896.0
F000'	896.53	
h,k,lmax	15,12,28	15,11,28
Nref	5673	5109
Tmin,Tmax		
Tmin'		

Correction method= Not given
Data completeness= 0.901 Theta(max)= 29.097

R(reflections)= 0.0545(3133) wR2(reflections)= 0.1617(5109)

S = 1.023 Npar= 316

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 !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...
Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ...
Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...
Please Check
PLAT213_ALERT_2_C Atom F3A has ADP max/min Ratio .....
3.3 prolat
PLAT213_ALERT_2_C Atom F3B has ADP max/min Ratio .....
3.1 prolat
PLAT234_ALERT_4_C Large Hirshfeld Difference F3A --C25 .
0.18 Ang.

Alert level G

PLAT199_ALERT_1_G Reported _cell_measurement_temperature.....(K)
293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature.....(K)
293 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of
C25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1A Constrained at
0.6 Check
And 5 other PLAT300 Alerts
More ...
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1)
9% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....
C24 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .
Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).
4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600
553 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....
3.4 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.
1 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by
3 Check

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully

```
   7 ALERT level C = Check. Ensure it is not caused by an omission or
oversight
  17 ALERT level G = General information/check it is not something
unexpected

    13 ALERT type 1 CIF construction/syntax error, inconsistent or
  missing data
     4 ALERT type 2 Indicator that the structure model may be wrong or
deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   9 ALERT type 4 Improvement, methodology, query or suggestion
   1 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.

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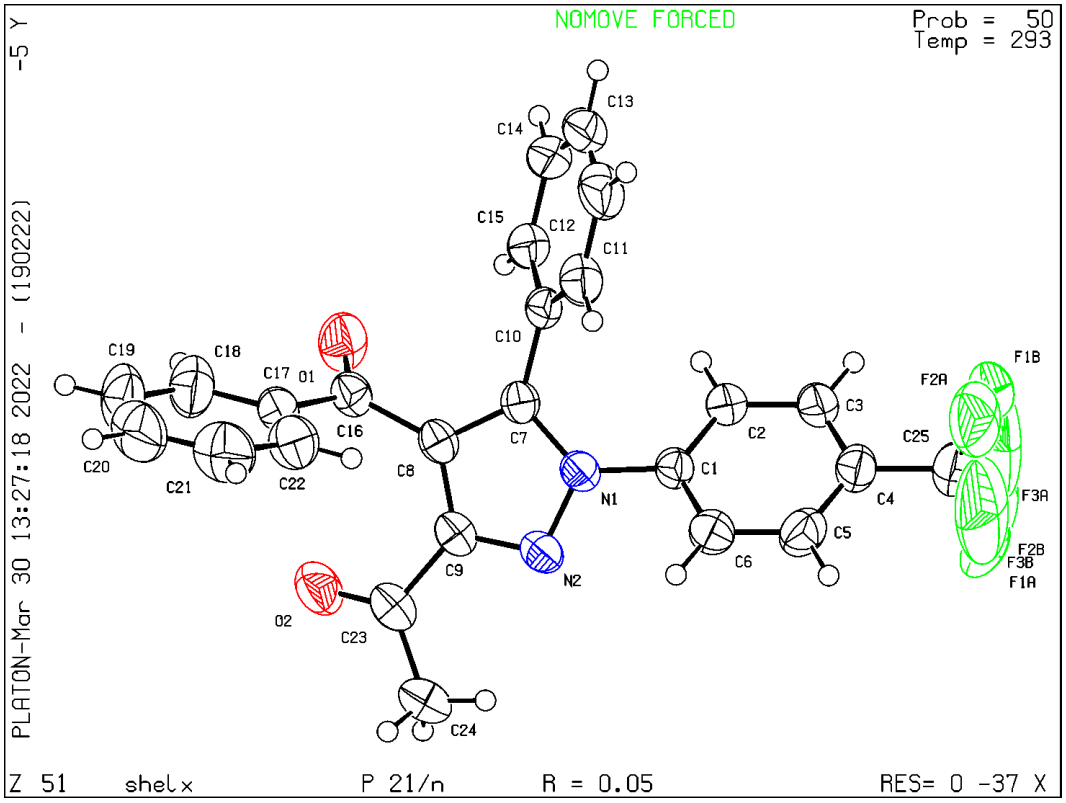
Datablock shelx - ellipsoid plot


NOMOVE FORCED
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Temp = 293
-5 Y
PLATON-Mar 30 13:27:18 2022 - (190222)
C13
C14
C15
C12
C11
C10
C19
C18
C17
O1
C16
C7
C8
C20
C21
C22
C2
C3
C1
C25
F1B
F2A
C4
F3A
N1
C5
C9
N2
C6
F2B
F3B
F1A
O2
C23
C24
Z 51
shelx
P 21/n
R = 0.05
RES= 0 -37 X