Electronic Supplementary Information for

**Acceptorless dehydrogenative condensation of o-aminobenzamides with aldehydes to quinazolinones in water catalyzed by a water-soluble iridium complex [Cp*Ir(H_2O)_3][OTf]_2**

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Copies of ^1^H NMR and ^1^3^C NMR spectra of products S2-S57

A characteristic signal of [Ir-H] (species C in Scheme 3) S58
2-phenylquinazolin-4(3H)-one

PROTON  CDCl3

![NMR spectrum of 2-phenylquinazolin-4(3H)-one](image)

3aa
2-phenylquinazolin-4(3H)-one
C13CPD    CDC13
2-o-tolylquinazolin-4(3H)-one

PROTON  DMSO-d6

12.443

8.172 8.160 8.172
7.835 7.694 7.835
7.430 7.511 7.430
7.500 7.540 7.500
7.342 7.342 7.342
2.499 2.383 2.499

3ab
2-o-tolylquinazolin-4(3H)-one
C13CPD  DMSO-d6

\[ \text{3ab} \]
2-p-tolylquinazolin-4(3H)-one

PROTON  CDCl3
2-p-tolylquinazolin-4(3H)-one
C13CPD   CDCl3

O

3ac

163.973  151.821  149.649
 142.122  134.769  129.993
 129.701  129.993  127.884
 127.362  127.884  126.490
 126.490  126.931  120.783
 120.783  127.362  76.999

21.505
2-(3,4-dimethylphenyl)quinazolin-4(3H)-one

PROTON DMSO-d6

3ad
2-(3,4-dimethylphenyl)quinazolin-4(3H)-one
C13CPD  DMSO-d6

3ad
2-(4-isopropylphenyl)quinazolin-4(3H)-one

PROTON DMSO-d6

3ae
2-(4-isopropylphenyl)quinazolin-4(3H)-one
C13CPD  DMSO-d6

3ae
2-(4-methoxyphenyl)quinazolin-4(3H)-one

PROTON DMSO-d6
2-(4-methoxyphenyl)quinazolin-4(3H)-one
C13CPD DMSO-d6

3af

\[
\text{O}
\]

\[
\text{N}
\]

\[
\text{OMe}
\]
2-(3,4-dimethoxyphenyl)quinazolin-4(3H)-one

PROTON  DMSO-d6
2-(3,4-dimethoxyphenyl)quinazolin-4(3H)-one
C13CPD DMSO-d6
2-(2-fluorophenyl)quinazolin-4(3H)-one
PROTON   DMSO-d6
2-(2-fluorophenyl)quinazolin-4(3H)-one

PROTON  DMSO-d6
2-(2-chlorophenyl)quinazolin-4(3H)-one
PROTON  DMSO-d6

3ai
2-(2-chlorophenyl)quinazolin-4(3H)-one
C13CPD  DMSO-d6
2-(4-chlorophenyl)quinazolin-4(3H)-one
PROTON  DMSO-d$_6$
2-(4-chlorophenyl)quinazolin-4(3H)-one
C13CPD  DMSO-d6
2-(4-bromophenyl)quinazolin-4(3H)-one

PROTON  DMSO-d6
2-(4-bromophenyl)quinazolin-4(3H)-one
C13CPD  DMSO-d6

3ak
2-(4-(trifluoromethyl)phenyl)quinazolin-4(3H)-one

PROTON  DMSO-d6

S24
2-(4-(trifluoromethyl)phenyl)quinazolin-4(3H)-one

C13CPD    DMSO-d6
2-(4-(trifluoromethoxy)phenyl)quinazolin-4(3H)-one
PROTON    DMSO-d6

3am
2-(4-(trifluoromethoxy)phenyl)quianzolin-4(3H)-one
C13CPD  DMSO-d6
2-(naphthalen-1-yl)quinazolin-4(3H)-one

PROTON  DMSO-d6

3an
2-(naphthalen-1-yl)quinazolin-4(3H)-one
C13CPD  DMSO-d6
2-(naphthalen-2-yl)quinazolin-4(3H)-one

PROTON    DMSO-d6

\[ \text{S30} \]
2-(naphthalen-2-yl)quinazolin-4(3H)-one
C13CPD   DMSO-d6

3ao
2-(thiophen-2-yl)quinazolin-4(3H)-one

PROTON  DMSO-d6

3ap
2-(thiophen-2-yl)quinazolin-4(3H)-one
C13CPD  DMSO-d6
2-phenethylquinazolin-4(3H)-one

PROTON DMSO-d$_6$

3aq
2-phenethylquinazolin-4(3H)-one
C13CPD  DMSO-d6

3aq
2-propylquinazolin-4(3H)-one

PROTON  DMSO-d6

![NMR Spectrum of 2-propylquinazolin-4(3H)-one](image)

**Chemical Structure**

![Structure of 2-propylquinazolin-4(3H)-one](image)

**Peak Assignments**

- 12.157 ppm
- 8.080, 7.796, 7.570, 7.365, 7.345, 7.330
- 7.597, 7.581, 7.750, 7.765, 7.779
- 8.065, 8.080, 8.085
- 2.500, 2.556, 2.571, 2.586
- 2.500, 2.000, 1.000, 1.000
- 0.917
2-propylquinazolin-4(3H)-one
C13CPD   DMSO-d6
2-cyclohexylquinazolin-4(3H)-one

PROTON   DMSO-d6

S38
2-cyclohexylquinazolin-4(3H)-one
C13CPD DMSO-d6

\[ \text{3as} \]
7-methyl-2-phenylquinazolin-4(3H)-one
PROTON  DMSO-d6

3ba
7-methyl-2-phenylquinazolin-4(3H)-one
C13CPD  DMSO-d6
6,7-dimethoxy-2-phenylquinazolin-4(3H)-one

PROTON  DMSO-d6

$3ca$
6,7-dimethoxy-2-phenylquinazolin-4(3H)-one
C13CPD DMSO-d6

![Graphical representation of the chemical structure of 6,7-dimethoxy-2-phenylquinazolin-4(3H)-one](image_url)
5-fluoro-2-phenylquinazolin-4(3H)-one

PROTON   DMSO-d6

![NMR spectrum diagram]

3da
5-fluoro-2-phenylquinazolin-4(3H)-one
C13CPD   DMSO-d6
6-fluoro-2-phenylquinazolin-4(3H)-one

PROTON  DMSO-d6

3ea
6-fluoro-2-phenylquinazolin-4(3H)-one

C13CPD    DMSO-d6

3ea
5-bromo-2-phenylquinazolin-4(3H)-one

PROTON DMSO-d$_6$

![NMR Spectrum of 5-bromo-2-phenylquinazolin-4(3H)-one in DMSO-d$_6$](image-url)

**Chemical Structure:**

![Chemical Structure of 5-bromo-2-phenylquinazolin-4(3H)-one](image-url)

**NMR Data:**

- 8.214 ppm
- 8.200 ppm
- 8.184 ppm
- 8.159 ppm
- 7.599 ppm
- 7.585 ppm
- 7.562 ppm
- 7.547 ppm
- 7.533 ppm
- 7.503 ppm
- 7.484 ppm
- 7.382 ppm
- 7.368 ppm
- 7.351 ppm

**Peak Assignments:**

- 3fa: 0.69 ppm
- Other peaks: 1.00, 2.00, 3.00 ppm

**Remarks:**

- The spectrum was recorded in DMSO-d$_6$ solvent.
- The structure includes a fluoro-substituted aromatic ring and a quinazolinone heterocycle.

**References:**

- [Chemical Structure Image]
- [NMR Spectrum Image]
7-fluoro-2-phenylquinazolin-4(3H)-one
C13CPD  DMSO-d6
6-chloro-2-phenylquinazolin-4(3H)-one

PROTON  DMSO-d6

PROTON  DMSO-d6
6-chloro-2-phenylquinazolin-4(3H)-one
C13CPD  DMSO-d6
7-chloro-2-phenylquinazolin-4(3H)-one

PROTON DMSO-d6

3ha

0 ppm
7-chloro-2-phenylquinazolin-4(3H)-one

C13CPD  DMSO-d6

3ha
5-bromo-2-phenylquinazolin-4(3H)-one
PROTON  DMSO-d$_6$
5-bromo-2-phenylquinazolin-4(3H)-one
C13CPD  DMSO-d6
3-Phenyl-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide

PROTON    DMSO-d6
3-Phenyl-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide
C13CPD DMSO-d6

3-Phenyl-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide
C13CPD DMSO-d6

3ja