#### **Supporting Information (SI)**

## Oxalic acid as a dual C1 surrogate for heterogeneous palladium-catalyzed tandem fourcomponent quinazolinones synthesis

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#### **Contents:**

General Information	2
Optimization studies	2-4
General procedure, ESI-MS and NMR data	4-44
Recyclability experiments for Pd/C Catalyst	44
Hot filtration test for Pd/C catalyst	45
Control Experiments	45-46
Schematic Diagram of Double Layer Vial (DLV) System	46
Time-based study of the reaction between 2-iodoaniline and iodobenzene	47-48
Computational Details	49-68
References	68

#### **General Information:**

High-quality reagents were purchased from Sigma Aldrich, Tokyo Chemical Industry (TCI), Loba Chemie, SD Fine-chem Ltd and Alfa Aesar. Pd/C and Pd/Al<sub>2</sub>O<sub>3</sub> have been purchased from Sd fine Chem Ltd. and TCI Chemicals respectively. Analytical grade solvents were used. Reactions were monitored by thin layer chromatography which was performed using precoated silica gel plates 60F254 (Merck) in a UV light detector. Silica gel (60-120 and 230-400 mesh size) for column chromatography was purchased from SD Fine-chem Ltd. ESI-MS spectra were recorded using a Waters micro mass Q-TOF Ultima Spectrometer. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded using a Bruker Avance 600 spectrometer operating at 600 MHz (<sup>1</sup>H) and 150 MHz (13C), JNM ECX -500 spectrometer operating at 500 MHz (1H) and 125 (13C). All the Spectra were recorded at 25 °C in DMSO- $d_6$  [residual DMSO- $d_6$  ( $\delta$ H 2.50, 3.39ppm) or DMSO- $d_6$  ( $\delta$ C 39.51 ppm)] with TMS as the internal standard. Chemical shifts were recorded in  $\delta$  (ppm) relative to the TMS and NMR solvent signal. Coupling constants (J) are given in Hz and multiplicities of signals are reported as follows: s, singlet; d, doublet; t, triplet; m, multiplet; brs, broad singlet; q, quartet. All the reactions were carried out by using a doublelayer vial system (DLV) consisting of an inner vial (diameter = 12 mm, height = 32 mm) placed inside an outer vial (diameter = 20 mm, height = 65 mm) tightened with solid PTFE cap.

#### **Optimization studies:**

To check the effect of catalyst, various homogeneous and heterogeneous metal catalysts were further screened, however, no significant enhancement in desired product yield was observed (Table 1S entries 16-19). The implementation of paraformaldehyde as well as formic acid as CO surrogate or decreasing the equivalency (eq.) of  $(CO_2H)_2$  also resulted in decreased desired product yield (Table 1S, entries 20-22) and  $(CO_2H)_2$  (7 eq.) in DMF in outer vial of DLV system was found to the best-suited condition. Finally, the reaction temperature, as well as time, were also optimized (Table 1S, entries 23-24) and 130 °C for 24 h delivered the highest desired product yield. In addition, no desired product formation was observed in the absence of either base,  $(CO_2H)_2$  or NH<sub>2</sub>COONH<sub>4</sub>, whereas the elimination of KI from the standard reaction condition resulted in lower desired product yield (Table 1S, entries 25-28).

		(CO <sub>2</sub> H Cat	<mark>)₂/</mark> DMF alyst <mark>O₂NH₄</mark>		
	▼ NH <sub>2</sub>	∣ base, OCH <sub>3</sub> sol	additive vent		
	1a - 2	<b>2a</b> 130 °	C, 24h	Ja (	JCH <sub>3</sub>
S.No.	Catalyst (mol%)	Base (equiv)	Additive	Solvent	/ield (%) <sup>[b]</sup>
1.	Pd/C (5 mol%)	K <sub>3</sub> PO <sub>4</sub> (2.5)	KI (1.5)	DMSO	23
2.	Pd/C (5 mol%)	KO <sup>t</sup> Bu (2.5)	KI (1.5)	DMSO	16
3.	Pd/C (5 mol%)	K <sub>2</sub> CO <sub>3</sub> (2.5)	KI (1.5)	DMSO	26
4.	Pd/C (5 mol%)	Cs <sub>2</sub> CO <sub>3</sub> (2.5)	KI (1.5)	DMSO	13
5.	Pd/C (5 mol%)	NEt <sub>3</sub> (2.5)	KI (1.5)	DMSO	traces
6.	Pd/C (5 mol%)	K <sub>2</sub> CO <sub>3</sub> (3.5)	KI (1.5)	DMSO	33
7.	Pd/C (5 mol%)	$K_2CO_3(4.5)$	KI (1.5)	DMSO	29
8.	Pd/C (5 mol%)	$K_2CO_3(3.5)$	TBAI (1.5)	DMSO	22
9.	Pd/C (5 mol%)	$K_2CO_3(3.5)$	Lil (1.5)	DMSO	28
10.	Pd/C (5 mol%)	$K_2CO_3(3.5)$	KI (2)	DMSO	38
11.	Pd/C (5 mol%)	K <sub>2</sub> CO <sub>3</sub> (3.5)	KI (2)	DMF	35
12.	Pd/C (5 mol%)	$K_2CO_3(3.5)$	KI (2)	Dioxane	15
13.	Pd/C (5 mol%)	$K_2CO_3(3.5)$	KI (2)	PEG-400	traces
14.	Pd/C (5 mol%)	$K_2CO_3(3.5)$	KI (2)	DMSO/Dioxane (1:1)	57
15.	Pd/C (5 mol%)	$K_2CO_3(3.5)$	KI (2)	DMSO/Dioxane (1:2)	68
16.	Pd@PS (5 mol%)	K <sub>2</sub> CO <sub>3</sub> (3.5)	KI (2)	DMSO/Dioxane (1:2)	53
17.	Pd/Al <sub>2</sub> O <sub>3</sub> (5 mol%)	K <sub>2</sub> CO <sub>3</sub> (3.5)	KI (2)	DMSO/Dioxane (1:2)	59
18.	Pd(OAc) <sub>2</sub> (5 mol%)	K <sub>2</sub> CO <sub>3</sub> (3.5)	KI (2)	DMSO/Dioxane (1:2)	48
19.	Pd/C (8 mol%)	K <sub>2</sub> CO <sub>3</sub> (3.5)	KI (2)	DMSO/Dioxane (1:2)	70
20. <sup>[c]</sup>	Pd/C (5 mol%)	K <sub>2</sub> CO <sub>3</sub> (3.5)	KI (2)	DMSO/Dioxane (1:2)	nd
21. <sup>[d]</sup>	Pd/C (5 mol%)	$K_2CO_3(3.5)$	KI (2)	DMSO/Dioxane (1:2)	traces
22. <sup>[e]</sup>	Pd/C (5 mol%)	$K_2CO_3(3.5)$	KI (2)	DMSO/Dioxane (1:2)	59
23. <sup>[f]</sup>	Pd/C (5 mol%)	$K_2CO_3(3.5)$	KI (2)	DMSO/Dioxane (1:2)	67
24. <sup>[g]</sup>	Pd/C (5 mol%)	K <sub>2</sub> CO <sub>3</sub> (3.5)	KI (2)	DMSO/Dioxane (1:2)	65
25.	Pd/C (5 mol%)	-	KI (2)	DMSO/Dioxane (1:2)	nd
26. <sup>[h]</sup>	Pd/C (5 mol%)	$K_2CO_3(3.5)$	KI (2)	DMSO/Dioxane (1:2)	nd
27. <sup>[i]</sup>	Pd/C (5 mol%)	$K_2CO_3(3.5)$	KI (2)	DMSO/Dioxane (1:2)	nd
28.	Pd/C (5 mol%)	K <sub>2</sub> CO <sub>3</sub> (3.5)	-	DMSO/Dioxane (1:2)	52

Table 1S. Optimization studies for 2-aryl quinazolinones synthesis<sup>a</sup>

<sup>a</sup>**1a** (0.23 mmol, 1 eq.), **2a** (1.5 eq.), 5 wt% Pd/C (5 mol%), NH<sub>2</sub>COONH<sub>4</sub> (3 eq.), K<sub>2</sub>CO<sub>3</sub> (3.5 eq.), KI (2 eq.) in DMSO/Dioxane (1:2) (1.5 mL) in an inner vial and  $(CO_2H)_2$  (7 eq.) in DMF (0.5 mL) in outer vial at 130 °C for 24 h; <sup>b</sup>Isolated yield; <sup>c</sup>Paraformaldehyde (7 eq); <sup>d</sup>HCOOH (7 eq.); <sup>e</sup>(CO<sub>2</sub>H)<sub>2</sub> (5 eq.); <sup>f</sup>30 h; <sup>g</sup>140 °C; <sup>h</sup>Without (CO<sub>2</sub>H)<sub>2</sub>; <sup>i</sup>Without NH<sub>2</sub>COONH<sub>4</sub>.

Also, various N-atom surrogates and their equivalencies were also examined as shown in Table 2S. Herein, the implementation of ammonium carbonate and ammonium formate as N-atom surrogate resulted in comparatively less desired product yield (Table 2S, entries 1-2), whereas no desired product formation was observed in case of ammonium acetate (Table 2S, entry 3). Further, the replacement of ammonium carbamate with liquid ammonia resulted in only the traces of expected product (Table 2S, entry 4). Moreover, the employement of ammonium bicarbonate, urea or ammonium chloride as N-atom surrogate as well as changing the equivalency of ammonium carbamate also didn't have any positive effect on anticipated product yield (Table 2S, entries 5-9). Hence, **1a** (1 eq.), **2a** (1.5 eq.), 5 wt% Pd/C (5 mol%), ammonium carbamate (3 eq.),  $K_2CO_3$  (3.5 eq.), KI (2 eq.) in DMSO/Dioxane (1:2) in an inner vial and (COOH)<sub>2</sub> (7 eq.) in DMF in the outer vial were turned out to be the most suited conditions for the synthesis of targeted product **3a**.

$\mathbf{\mathbf{U}}_{\mathbf{NH}_{2}}^{\mathbf{I}}$	(CO <sub>2</sub> H) <sub>2</sub> /DMF Pd/C (5 mol%) N-atom surrogate K <sub>2</sub> CO <sub>3</sub> , KI OCH <sub>3</sub> Dioxane/DMSO 130 °C, 24h	
S.No.	N-atom surrogate (equiv)	yield (%) <sup>[b]</sup>
1.	(NH <sub>4</sub> ) <sub>2</sub> CO <sub>3</sub> (3)	52
2.	HCOONH <sub>4</sub> (3)	29
3.	$CH_3CO_2NH_4(3)$	n.d.
4.	liq. NH <sub>3</sub> (3)	traces
5.	$NH_4HCO_3$ (3)	32
6.	$NH_2CONH_2(3)$	54
7.	NH <sub>4</sub> Cl (3)	31
8.	$NH_2CO_2NH_4$ (2)	63
9.	$NH_2CO_2NH_4$ (4)	69

<b>I apic</b> 20. Optimization of it atom sunogates	Table 2	2 <b>S</b> . O	ptimiz	ation	of N-atom	surrogates
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<sup>a</sup>1a (0.23 mmol, 1 eq.), 2a (1.5 eq.), 5 wt% Pd/C (5 mol%), NH<sub>2</sub>CO2NH4 (3 eq.), K<sub>2</sub>CO<sub>3</sub> (3.5 eq.), KI (2 eq.) in DMSO/dioxane (1:2) (1.5 mL) in an inner vial and  $(CO_2H)_2$  (7 eq.) in DMF (0.5 mL) in outer vial at 130 °C for 24 h; bIsolated yield.

#### Typical Experimental procedure and characterization:



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

With the DLV system, 2-iodoaniline (50 mg, 0.23 mmol), 1-iodo-4-methoxybenzene (80.1 mg, 0.34mmol), 5 wt% of Pd/C (5 mol%), ammonium carbamate (53.4 mg, 0.68 mmol), K<sub>2</sub>CO<sub>3</sub> (110 mg, 0.80 mmol) and KI (75.78 mg, 0.47 mmol) in dioxane/DMSO (2:1) solvent system were taken in the inner vial and this vial was placed inside the outer reaction vial containing oxalic acid (1.60 mmol, 143.8 mg) and 0.5 mL of DMF. The 5 mL reaction vessel was tightened under air with solid PTFE cap and stirred on a heating metal block at 130 °C for 24 h. The progress of the reaction was monitored with the help of TLC. After the completion of the reaction, the inner vial was taken out. The reaction was quenched with water and the organic layer was extracted with ethyl acetate. The extracted organic layer was dried over anhydrous sodium sulphate and concentrated over a rotary evaporator. The crude mixture was further purified by column chromatography using hexane: ethyl acetate (80:20) as eluent, afforded compound **3a** as white solid (39.3 mg); yield: 68%; <sup>1</sup>H (600 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 12.40 (brs, 1H), 8.19 (d, J = 8.8 Hz, 2H), 8.13 (d, J = 7.8 Hz, 1H), 7.82 - 7.80 (m, 1H), 7.70 (d, J = 8.1 Hz, 1H), 7.49 - 7.47 (m, 1H), 7.09 (d, J = 8.8 Hz, 2H), 3.85 (s, 3H); <sup>13</sup>C (150 MHz, DMSO $d_6$ )  $\delta$  (ppm) = 162.27, 161.85, 151.84, 148.92, 134.52, 129.43, 127.27, 126.10, 125.80, 124.79,120.68,113.98, 55.44.

ESI-MS(M+H)<sup>+</sup> calculated for  $C_{15}H_{13}N_2O_2^+$  is 253.0972 and observed is 253.0973.

#### 2-phenylquinazolin-4(3H)-one



Prepared as the general procedure described for **3a** starting from 2-iodoaniline (50 mg, 0.23 mmol) and iodobenzene (70 mg, 0.34 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3b** as white solid (37.5 mg); yield: 74%; <sup>1</sup>H (600 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  (ppm) = 12.54 (brs, 1H), 8.19 - 8.15 (m, 3H), 7.85 - 7.83 (m, 1H), 7.75 (d, J = 8.1 Hz, 1H), 7.61 - 7.51 (m, 4H); <sup>13</sup>C (150 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  (ppm) = 162.20, 152.29, 148.72, 134.58, 132.70, 131.37, 128.58, 127.74, 127.49, 126.57, 125.83, 120.97. ESI-MS(M+H)<sup>+</sup> calculated for C<sub>14</sub>H<sub>11</sub>N<sub>2</sub>O<sup>+</sup> is 223.0866 and observed is 223.0866.

#### 2-(p-tolyl)quinazolin-4(3H)-one



Prepared as the general procedure described for **3a** starting from 2-iodoaniline (50 mg, 0.23 mmol) and 1-iodo-4-methylbenzene (74.7 mg, 0.34 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3c** as white solid (41.2 mg); yield: 76%; <sup>1</sup>H (600 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 12.45 (brs, 1H), 8.15 (dd,  $J_{1-3} = 7.9$  Hz,  $J_{1-2} = 1.2$  Hz, 1H), 8.09 (d, J = 8.2 Hz, 2H), 7.83 -7.80 (m, 1H), 7.72 (d, J = 8.0 Hz, 1H), 7.51 - 7.49 (m, 1H), 7.34 (d, J = 8.0 Hz, 2H), 2.38 (s, 3H); <sup>13</sup>C (150 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 162.29, 152.25, 148.81, 141.44, 134.54, 129.89, 129.17, 127.67, 127.36, 126.36, 125.83, 120.88, 20.97. ESI-MS(M+H)<sup>+</sup> calculated for C<sub>15</sub>H<sub>13</sub>N<sub>2</sub>O<sup>+</sup> is 237.1022 and observed is 237.1029.

#### 2-(m-tolyl)quinazolin-4(3H)-one



Prepared as the general procedure described for **3a** starting from 2-iodoaniline (50 mg, 0.23 mmol) and 1-iodo-3-methylbenzene (74.7 mg, 0.34 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3d** as white solid (39.7 mg); yield: 74%; <sup>1</sup>H (600 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 12.47 (brs, 1H), 8.15 (d, J = 7.86 Hz, 1H), 8.02 (s, 1H), 7.97 (d, J = 7.5 Hz, 1H), 7.85 - 7.82 (m, 1H), 7.74 (d, J = 8.1 Hz, 1H), 7.53 - 7.51 (m, 1H), 7.44 - 7.39 (m, 2H), 2.41 (s, 3H); <sup>13</sup>C (150 MHz, DMSO- $d_6$ )  $\delta$  (ppm) =162.21, 152.40,

148.78, 137.94, 134.62, 132.65, 132.02, 128.52, 128.29, 127.49, 126.56, 125.85, 124.89, 120.98, 20.97.

ESI-MS(M+H)<sup>+</sup> calculated for  $C_{15}H_{13}N_2O^+$  is 237.1022 and observed is 237.1025.

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



Prepared as the general procedure described for **3a** starting from 2-iodoaniline (50 mg, 0.23 mmol) and 1-iodo-3-methoxybenzene (80.1 mg, 0.34 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (80:20) **3e** as white solid (36.4 mg); yield: 63%; <sup>1</sup>H (600 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  (ppm) = 12.53 (brs, 1H), 8.16 (d, *J* = 7.8 Hz, 1H), 7.84 - 7.73 (m, 4H), 7.53 - 7.50 (m, 1H), 7.46 - 7.43 (m, 1H), 7.14 (d, *J* = 8.1 Hz, 1H), 3.86 (s, 3H); <sup>13</sup>C (150 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  (ppm) = 162.31, 159.35, 152.09, 148.61, 134.58, 134.04, 129.73, 127.46, 126.60, 125.85, 121.01, 120.13, 117.58, 112.54, 55.38. ESI-MS(M+H)<sup>+</sup> calculated for C<sub>15</sub>H<sub>13</sub>N<sub>2</sub>O<sub>2</sub><sup>+</sup> is 253.0972 and observed is 253.0975.

#### 2-(o-tolyl)quinazolin-4(3H)-one



Prepared as the general procedure described for **3a** starting from 2-iodoaniline (50 mg, 0.23 mmol) and 1-iodo-2-methylbenzene (74.7 mg, 0.34 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3f** as white solid (32.1 mg); yield: 60%; <sup>1</sup>H (600 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  (ppm) = 12.45 (brs, 1H), 8.18 (dd, *J*<sub>1-3</sub> = 7.9 Hz, *J*<sub>1-2</sub> = 1.1 Hz, 1H), 7.84 - 7.81 (m, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.55 - 7.50 (m, 2H), 7.44 - 7.41 (m, 1H), 7.35 - 7.31 (m, 2H), 2.39 (s, 3H); <sup>13</sup>C (150 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  (ppm) = 161.79, 154.38, 148.75, 136.13, 134.45, 134.24, 130.53, 129.88, 129.12, 127.37, 126.63, 125.79, 125.69, 120.99. 19.56. ESI-MS(M+H)<sup>+</sup> calculated for C<sub>15</sub>H<sub>13</sub>N<sub>2</sub>O<sup>+</sup> is 237.1022 and observed is 237.1024.

#### 2-(2-ethylphenyl)quinazolin-4(3H)-one



Prepared as the general procedure described for **3a** starting from 2-iodoaniline (50 mg, 0.23 mmol) and 1-ethyl-2-iodobenzene (79.5 mg, 0.34 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3g** as white solid (29.3 mg); yield: 51%; <sup>1</sup>H (600 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 12.48 (brs, 1H), 8.17 (dd,  $J_{1-3} = 7.9$  Hz,  $J_{1-2} = 1.3$  Hz, 1H), 7.85 - 7.82 (m, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.56 - 7.53 (m, 1H), 7.48 - 7.46 (m, 2H), 7.39 (d, J = 7.4 Hz, 1H), 7.35 - 7.32 (m, 1H), 2.76 - 2.72 (m, 2H), 1.13 - 1.10 (m, 3H); <sup>13</sup>C (150 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 161.72, 154.36, 148.63, 142.16, 134.48, 133.84, 129.98, 129.11, 128.94, 127.35, 126.63, 125.77, 125.65, 120.95, 25.71, 15.40.

ESI-MS(M+H)<sup>+</sup> calculated for  $C_{16}H_{15}N_2O^+$  is 251.1179 and observed is 251.1179.

#### 2-(4-(tert-butyl)phenyl)quinazolin-4(3H)-one



Prepared as the general procedure described for **3a** starting from 2-iodoaniline (50 mg, 0.23 mmol) and 1-(tert-butyl)-4-iodobenzene (89.1mg, 0.34 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3h** as a white solid (35.4 mg); yield: 66%; <sup>1</sup>H (500 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 12.42 (s, 1H), 8.16 - 8.12 (m, 3H), 7.84 - 7.81 (m, 1H), 7.73 (d, J = 7.75 Hz, 1H), 7.58 - 7.55 (m, 2H), 7.52 - 7.49 (m, 1H), 1.33 (s, 9H); <sup>13</sup>C (125 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 162.15, 154.25, 152.12, 148.78, 134.46, 129.89, 127.48, 127.36, 126.31, 125.76, 125.33, 120.86, 34.59, 30.83. ESI-MS(M+H)<sup>+</sup> calculated for C<sub>18</sub>H<sub>19</sub>N<sub>2</sub>O<sup>+</sup> is 279.1492 and observed is 279.1492.

#### 2-(3,5-dimethylphenyl)quinazolin-4(3H)-one



Prepared as the general procedure described for **3a** starting from 2-iodoaniline (50 mg, 0.23 mmol) and 1-iodo-3,5-dimethylbenzene (79.5mg, 0.34 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3i** as white solid (40.7 mg); yield: 71%; <sup>1</sup>H (600 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 12.39 (brs, 1H), 8.15 (d, J = 7.8 Hz, 1H), 7.84 - 7.81 (m, 3H), 7.74 (d, J = 8.1 Hz, 1H), 7.51 (t, J = 7.4 Hz, 1H), 7.20 (s, 1H), 2.36 (s, 6H); <sup>13</sup>C (150 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 162.15, 152.45, 148.79, 137.74, 134.54, 132.71, 132.57, 127.43, 126.44, 125.83, 125.47, 120.96, 20.85.

ESI-MS(M+H)<sup>+</sup> calculated for  $C_{16}H_{15}N_2O^+$  is 251.1179 and observed is 251.1179.

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



Prepared as the general procedure described for **3a** starting from 2-iodoaniline (50 mg, 0.23 mmol) and 1-iodo-2,4-dimethylbenzene (79.5 mg, 0.34 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3j** as white solid (34.2 mg); yield: 60%; <sup>1</sup>H (500 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 12.37 (brs, 1H), 8.17 (dd,  $J_{1-3}$  = 7.95 Hz,  $J_{1-2}$  = 1.55 Hz, 1H), 7.84 - 7.81 (m, 1H), 7.68 - 7.67 (m, 1H), 7.54 - 7.51 (m, 1H), 7.41 (d, J = 7.75 Hz, 1H), 7.16 - 7.12 (m, 2H), 2.37 (d, J = 12.3 Hz, 6H); <sup>13</sup>C (125 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 161.85, 154.39, 148.79, 139.47, 136.06, 134.42, 131.41, 131.19, 129.17, 127.32, 126.50, 126.23, 125.75, 120.89, 20.84, 19.58.

ESI-MS(M+H)<sup>+</sup> calculated for  $C_{16}H_{15}N_2O^+$  is 251.1179 and observed is 251.1177

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



Prepared as the general procedure described for **3a** starting from 2-iodoaniline (50 mg, 0.23 mmol) and 4-iodo-1,2-dimethylbenzene (79.5 mg, 0.34 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3k** as white solid (47.9 mg); yield: 84%; <sup>1</sup>H (500 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 12.39 (brs, 1H), 8.15 (d, J = 8.3 Hz, 1H), 8.0 (s, 1H), 7.93 (d, J = 7.6 Hz, 1H), 7.84 – 7.80 (m, 1H), 7.73 (d, J = 8.3 Hz, 1H), 7.51 – 7.48 (m, 1H), 7.31 (d, J = 8.3 Hz, 1H), 2.32 (d, J = 7.6 Hz, 6H); <sup>13</sup>C (125 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 162.33, 152.40, 148.79, 140.23,136.58, 134.52, 130.17, 129.68, 128.61, 127.28, 126.30, 125.83, 125.16, 120.87, 19.40.

ESI-MS(M+H)<sup>+</sup> calculated for  $C_{16}H_{15}N_2O^+$  is 251.1179 and observed is 251.1182.

#### 2-(4-chlorophenyl)quinazolin-4(3H)-one



Prepared as the general procedure described for **3a** starting from 2-iodoaniline (50 mg, 0.23 mmol) and 1-chloro-4-iodobenzene (81.7 mg, 0.34 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3l** as white solid (35.2 mg); yield: 60%; <sup>1</sup>H (600 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 12.61 (brs, 1H), 8.21 (d, J = 8.6 Hz, 2H), 8.16 (d, J = 7.6 Hz, 1H), 7.86 - 7.84 (m, 1H), 7.75 (d, J = 8.1 Hz, 1H), 7.63 (d, J = 8.5 Hz, 2H), 7.55 - 7.53 (m, 1H); <sup>13</sup>C (150 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 162.59, 151.75, 148.69, 136.52, 134.94, 131.79, 129.82, 128.92, 127.60, 127.04, 126.08, 121.09.

ESI-MS(M+H)<sup>+</sup> calculated for  $C_{14}H_{10}ClN_2O^+$  is 257.0476 and observed is 257.0476.

#### 2-(3-fluorophenyl)quinazolin-4(3H)-one



Prepared as the general procedure described for **3a** starting from 2-iodoaniline (50 mg, 0.23 mmol) and 1-fluoro-3-iodobenzene (76.0 mg, 0.34 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3m** as white solid (30.3 mg); yield: 55%; <sup>1</sup>H (600 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 12.58 (brs, 1H), 8.16 - 8.14 (m, 1H), 8.04 (d, J = 7.9 Hz, 1H), 8.00 - 7.98 (m, 1H), 7.85 - 7.82 (m, 1H), 7.75 (d, J = 7.9 Hz, 1H), 7.61 - 7.57 (m, 1H), 7.54 - 7.52 (m, 1H), 7.44 - 7.41 (m, 1H); <sup>13</sup>C (150 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 162.92, 162.18, 161.31, 151.06, 148.46, 135.05, 135.00, 134.69, 130.78, 130.73, 127.60, 126.92, 125.90, 123.95, 123.93, 121.12, 118.33, 118.19, 114.63, 114.47; <sup>19</sup>F (DMSO- $d_6$ , 471 MHz)  $\delta$  (*ppm*) - 112.24 (s).

ESI-MS(M+H)<sup>+</sup> calculated for  $C_{14}H_{10}FN_2O^+$  is 241.0772 and observed is 241.0770.

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



Prepared as the general procedure described for **3a** starting from 2-iodoaniline (50 mg, 0.23 mmol) and 1-iodo-3-(trifluoromethyl)benzene (93.1 mg, 0.34 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3n** as a white solid (54.7 mg); yield: 83%; <sup>1</sup>H (500 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 12.72 (brs, 1H), 8.55 – 8.54 (m, 1H), 8.50 – 8.48 (m, 1H), 8.18 – 8.16 (m, 1H), 7.95 (dd,  $J_{1-3}$  = 7.75 Hz,  $J_{1-2}$  = 1.8 Hz, 1H), 7.87 – 7.84 (m, 1H), 7.81 – 7.78 (m, 2H), 7.57 – 7.53 (m, 1H); <sup>13</sup>C (150 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 162.05, 150.94, 148.36, 134.58, 133.68, 131.68, 129.75, 129.52, 129.25, 127.71, 127.55, 126.90, 125.80, 125.00, 124.40, 122.83, 121.11; <sup>19</sup>F (DMSO- $d_6$ , 471 MHz)  $\delta$  (*ppm*) -61.12 (s). ESI-MS(M+H)<sup>+</sup> calculated for C<sub>15</sub>H<sub>10</sub>F<sub>3</sub>N<sub>2</sub>O<sup>+</sup> is 291.0740 and observed is 291.0744.

#### 2-(naphthalen-1-yl)quinazolin-4(3H)-one



Prepared as the general procedure described for **3a** starting from 2-iodoaniline (50 mg, 0.23 mmol) and 1-iodonaphthalene (87.0 mg, 0.34 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3o** as white solid (33.1 mg); yield: 53%; <sup>1</sup>H (600 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 12.66 (brs, 1H), 8.22 (dd, J<sub>1-3</sub> = 8.0 Hz, J<sub>1-2</sub> = 1.3 Hz, 1H), 8.17 – 8.16 (m, 1H), 8.12 (d, J = 8.2 Hz, 1H), 8.06 -m8.04 (m, 1H), 7.88 – 7.86 (m, 1H), 7.79 (d, J<sub>1-3</sub> = 7.0 Hz, J<sub>1-2</sub> = 1.0 Hz, 1H), 7.74 (d, J = 7.9 Hz, 1H), 7.66 – 7.64 (m, 1H), 7.61 – 7.57 (m, 3H); <sup>13</sup>C (150 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 161.90, 153.67, 148.72, 134.53, 133.13, 131.72, 130.37, 130.25, 128.33, 127.67, 127.46, 127.07, 126.80, 126.36, 125.85, 125.19, 125.07, 121.23.

ESI-MS(M+H)<sup>+</sup> calculated for  $C_{18}H_{13}N_2O^+$  is 273.1022 and observed is 273.1020.

#### 7-methyl-2-phenylquinazolin-4(3H)-one



Prepared as the general procedure described for **3a** starting from 2-iodo-5-methylaniline (50 mg, 0.22 mmol) and iodobenzene (65.7 mg,0.32 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3p** as white solid (30.9 mg); yield: 61%; <sup>1</sup>H (500 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 12.44 (brs, 1H), 8.18 - 8.16 (m, 2H), 8.04 (d, J = 8.04 Hz, 1H), 7.60 - 7.52 (m, 4H), 7.35 - 7.33 (m 1H), 2.47 (s, 3H); <sup>13</sup>C (125 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 162.10, 152.31, 148.86, 145.07, 132.78, 131.32, 128.59, 128.02, 127.69, 127.15, 125.70, 118.59, 21.35.

ESI-MS(M+H)<sup>+</sup> calculated for  $C_{15}H_{13}N_2O^+$  is 237.1022 and observed is 237.1029.

#### 6-methyl-2-phenylquinazolin-4(3H)-one



Prepared as the general procedure described for **3a** starting from 2-iodo-4-methylaniline (50 mg, 0.22 mmol) and iodobenzene (65.7 mg,0.32 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3q** as white solid (24.2 mg); yield: 48%; <sup>1</sup>H (500 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 12.45 (brs, 1H), 8.18 - 8.15 (m, 2H), 7.96 - 7.95 (m, 1H), 7.67 - 7.63 (m, 2H), 7.60 - 7.52 (m, 3H), 2.46 (s, 3H); <sup>13</sup>C (125 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 162.14, 151.46, 146.74, 136.30, 135.87, 132.78, 131.22, 128.58, 127.63, 127.38, 125.23, 120.72, 20.83.

ESI-MS(M+H)<sup>+</sup> calculated for  $C_{15}H_{13}N_2O^+$  is 237.1022 and observed is 273.1026.

#### 6-bromo-2-phenylquinazolin-4(3H)-one



Prepared as the general procedure described for **3a** starting from 4-bromo-2-iodoaniline (50 mg, 0.17 mmol) and iodobenzene (51.4 mg, 0.25 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3r** as white solid (21.4 mg); yield: 42%; <sup>1</sup>H (400 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 12.71 (brs, 1H), 8.23 (d, J = 2.32 Hz, 1H), 8.19 – 8.16 (m, 2H), 7.98 (dd,  $J_{1-3} = 8.8$  Hz,  $J_{1-2} = 2.4$  Hz, 1H), 7.70 (d, J = 8.4 Hz, 1H), 7.63 – 7.54 (m, 3H);<sup>13</sup>C (100 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 161.72, 153.48, 148.16, 137.91, 132.90, 132.11, 130.34, 129.13, 128.45, 128.30, 123.00, 119.42.

ESI-MS(M+H)<sup>+</sup> calculated for  $C_{14}H_{10}BrN_2O^+$  is 300.9971 and observed is 300.9973.

#### 7-chloro-2-phenylquinazolin-4(3H)-one



Prepared as the general procedure described for **3a** starting from 5-chloro-2-iodoaniline (50 mg, 0.20 mmol) and iodobenzene (60.4 mg, 0.30 mmol), gave after purification with silica gel column chromatography in hexane: ethyl acetate (85:15) **3s** as white solid (28.7 mg); yield: 57%; <sup>1</sup>H (500 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 12.66 (brs, 1H), 8.19 – 8.13 (m, 3H), 7.80 – 7.78 (m, 1H), 7.63 – 7.53 (m, 4H); <sup>13</sup>C (125 MHz, DMSO- $d_6$ )  $\delta$  (ppm) = 161.69, 153.81, 139.16, 132.39, 131.70, 128.63, 127.95, 127.91, 126.79, 126.54, 119.81.

ESI-MS(M+H)<sup>+</sup> calculated for  $C_{14}H_{10}ClN_2O^+$  is 257.0476 and observed is 257.0471.

## <sup>1</sup>H, <sup>13</sup>C NMR and ESI-MS spectra





































190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm













![](_page_31_Figure_0.jpeg)

![](_page_31_Figure_1.jpeg)

![](_page_32_Figure_0.jpeg)

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

![](_page_33_Figure_0.jpeg)

200	180	160	140	120	100	80	60	40	20	0 f1 (pp	-20 m)	-40	-60	-80	-100	-120	-140	-160	-180	-20(

![](_page_33_Figure_2.jpeg)

![](_page_34_Figure_0.jpeg)

![](_page_34_Figure_1.jpeg)

f1 (ppm) 

![](_page_35_Figure_0.jpeg)

200	180	160	140	120	100	80	60	40	20 f	0 1 (ppm	-20 i)	-40	-60	-80	-100	-120	-140	-160	-180	-20(

![](_page_35_Figure_2.jpeg)

![](_page_36_Figure_0.jpeg)

![](_page_37_Figure_0.jpeg)

![](_page_38_Figure_0.jpeg)

![](_page_38_Figure_1.jpeg)

![](_page_39_Figure_0.jpeg)

![](_page_40_Figure_0.jpeg)

![](_page_40_Figure_1.jpeg)

![](_page_41_Figure_0.jpeg)

![](_page_41_Figure_1.jpeg)

![](_page_42_Figure_0.jpeg)

![](_page_43_Figure_0.jpeg)

#### **Recyclability experiments for Pd/C Catalyst:**

The recyclability experiment of Pd/C (5 wt%) catalyst was further performed under the developed reaction conditions employing 2-iodoaniline (1a) and iodobenzene (2b) as a model substrate (Figure S1). After completion of the reaction, the given reaction mixture was left aside for some time and the cooled reaction mixture was then subjected to centrifugation to separate the Pd/C catalyst from the reaction mixture. The catalyst was then washed properly with distilled water followed by acetone and was dried completely under reduced pressure for further use. The Pd/C catalyst showed high recyclability up to five cycles with a small decrease in desired product yield.

![](_page_43_Figure_3.jpeg)

Figure S1. Recyclability experiment of Pd/C (5 wt%) catalyst

#### Hot Filtration Test for Pd/C Catalyst:

The reaction between 2-iodoaniline (1a) and iodobenzene (2b) was carried out under standard reaction conditions and after 22% of the product (3b) formation, the solid catalyst (Pd/C) was filtered off, and the reaction was further continued with the addition of 5 equiv. of oxalic acid to realize the total time of 24 h. There is no increase in the yield of the product was observed, hence indicating the absence of catalytic active species in the solution for fruitful conversion. While the same reaction when performed unperturbed under standard reaction conditions, gave **3b** in 74% yield. On the basis of these experiments, we concluded that the reaction takes place in truly heterogeneous manner and the catalytically active species involved in the reaction is Pd(0).

![](_page_44_Figure_2.jpeg)

Figure S2. Hot filtration test for Pd/C catalyst.

#### **Control Experiments:**

Further, several other control experiments were also performed to depict the utility of DLV system as well as the role of  $(COOH)_2$  as C1 surrogate. Herein, no product formation was detected under single vial system with DMF as solvent, whereas traces of **3b** were obtained on employing DMSO/dioxane (1:2) solvent system (Scheme 1Sa-1Sb). These control experiments clearly indicates the essential need of DLV system in carrying out given transformation. Thereafter, to confirm the role of oxalic acid the given reaction was also carried out under acetic acid conditions, wherein the oxalic acid in the outer vial of DLV system was replaced with acetic acid, however, no desired product formation was obtained under these conditions (Scheme 1Sc). It clearly indicates the role of oxalic acid as a CO surrogate rather than just as an acid additive to facilitate the DMF decomposition. Furthermore, the desired product

formation was also observed in 67% yield with PEG-200 as external solvent and hence eliminating the possibility of DMF acting as CO surrogate (Scheme 1Sd).

a) Standard reaction under single vial system with DMF as solvent  $(CO_2H)_2$ NH<sub>2</sub>CO<sub>2</sub>NH<sub>4</sub> NH K<sub>2</sub>CO<sub>3</sub>, KI 12 DMF, 130 °C, 24h 1a 2b Single vial 3b, nd b) Standard reaction under single vial system with DMSO/Dioxane (1:2) as solvent  $CO_2H)_2$ NH<sub>2</sub>CO<sub>2</sub>NH<sub>4</sub> NH K<sub>2</sub>CO<sub>3</sub>, KI DMSO/Dioxane 1a 2b 130 °C, 24h 3b, traces Single vial c) Implementation of acetic acid instead of oxalic acid in outer vial of DLV system CH<sub>3</sub>COOH/DMF NH<sub>2</sub>CO<sub>2</sub>NH<sub>4</sub> K<sub>2</sub>CO<sub>3</sub>, KI H<sub>2</sub> DMSO/Dioxane 1a 2b 130 °C, 24h 3b, nd d) Implementation of PEG-200 as external solvent in outer vial of DLV system (CO<sub>2</sub>H)<sub>2</sub>/PEG-200 NH<sub>2</sub>CO<sub>2</sub>NH<sub>4</sub> K<sub>2</sub>CO<sub>3</sub>, KI  $H_2$ DMSO/Dioxane 1a 2b 130 °C, 24h **3b**, 67%

Scheme 1S. Control experiments

#### Schematic Diagram of Double Layer Vial (DLV) System

![](_page_45_Picture_4.jpeg)

![](_page_46_Figure_0.jpeg)

![](_page_46_Figure_1.jpeg)

**Figure S3.** LCMS chromatogram for the reaction between 2-iodoaniline and iodobenzene a) after 5h; b) after 10h; c) after 15h; d) after 20h; e) after 24h.

![](_page_46_Figure_3.jpeg)

Figure S4. LCMS chromatogram for a) intermediate 4a; b) intermediate 4b.

a) Mass spectra for intermediate 4a:

![](_page_47_Figure_0.jpeg)

b) Mass spectra for intermediate 4b:

![](_page_47_Figure_2.jpeg)

#### **Computational Details**

All calculations were performed using the ORCA 5.0.3 software.<sup>1,2</sup> The density functional theoretical method was used in conjunction with the PBE0 functional,<sup>3</sup> with the dispersion corrections based on tight binding partial charges (D4)<sup>4,5</sup> and the balanced polarized double zeta basis set of Ahlrichs and coworkers.<sup>6</sup> The RIJCOSX<sup>7</sup> approximation was utilized throughout to expedite the computations. Transition states were computed using the nudged-elastic-band method.<sup>8</sup> Additionally, to further refine the outcome, the single point-energy of the entire system was computed using the PBE0 functional and a higher valance polarised triple zeta basis set (def2-tzvp). Using the same degree of theory, all of the minima and transition states on the potential energy surface were confirmed. The conductor-like polarizable continuum model<sup>9</sup> was used to describe the solute-solvent interaction. The dielectric constant and refractive index of the solvent were taken as 17.0585 and 1.4437, respectively.

![](_page_48_Figure_2.jpeg)

**Figure S5.** DFT calculations for desired product formation a) via the formation of N-(2iodophenyl)benzamide as reaction intermediate b) via the formation of 2-aminobenzamide as reaction intermediate

## Energies

## All energies are in hartee

CDECIEC	Б	C	тт
SPECIES	E <sub>elec</sub>	G <sub>solv</sub>	H <sub>solv</sub>
<u>la</u>	-584.50339424	-584.44476791	-584.38391352
2b	-529.18466560	-529.14014464	-529.08293974
3b	-723.75496374	-723.60111653	-723.52073929
4a	-456.00037233	-455.90450615	-455.83866658
4b	-928.65667167	-928.51926719	-928.43329321
4c	-800.14213161	-799.96755717	-799.87811921
CO	-113.23209685	-113.25420004	-113.22253277
Ι	-657.09514938	-657.05598408	-656.99323136
II	-770.41247375	-770.36733415	-770.29391287
III	-1056.55482419	-1056.42431468	-1056.33001816
IV	-1056.60538200	-1056.47113321	-1056.37827562
V	-1169.90177925	-1169.76054233	-1169.66121985
VI	-928.02293570	-927.85634803	-927.75805658
VII	-712.45106865	-712.39974356	-712.32742005
VIII	-825.74435952	-825.68522296	-825.60683739
IX	-583.87545267	-583.78838512	-583.71265876
Χ	-928.03497171	-927.86563450	-927.76860278
TS2_1	-882.19583981	-882.11227957	-882.02269469
TS2_2	-1226.36851758	-1226.19991152	-1226.09229312
KI	-897.58676182	-897.62272010	-897.58098942
KHCO <sub>3</sub>	-864.09839042	-864.11336225	-864.06099355
K <sub>2</sub> CO <sub>3</sub>	-1463.308014018	-1463.33902444	-1463.27984468
Pd	-127.85736603	-127.88077320	-127.85417426
NH <sub>3</sub>	-56.52138052	-56.51305582	-56.48184992
H <sub>2</sub> O	-76.38778668	-76.39189549	-76.36136048

# Optimized geometries

![](_page_50_Figure_1.jpeg)

TS\_2\_1

TS\_2\_2

K<sub>2</sub>CO<sub>3</sub>

![](_page_51_Figure_0.jpeg)

## Coordinates

1a			
С	-0.52046072890719	0.81830433960681	0.00035457779764
С	0.86740134268250	0.81656573173316	0.00041931124228
С	1.55663039031574	2.01834063616355	-0.00030103456615
С	0.85336667756079	3.21619292975393	-0.00098194400655
С	-0.54044407627414	3.24634485331450	-0.00112169614319
С	-1.20742336048079	2.02057338240322	-0.00048491686425
Η	-1.06852301521944	-0.11682656578409	0.00088672623570
Η	1.41842021914509	-0.11674219331759	0.00104749323674
Η	2.63953208162486	2.02526355355312	-0.00024286218238
Η	-2.29250417531096	2.02889200309102	-0.00061694715809
Ι	1.94331567080651	4.99933438901656	-0.00204982845472
N	-1.24505457058282	4.48379340374633	-0.00170064801205
Η	-1.84973446548360	4.53859220824906	-0.81456239211728
Н	-1.85633968987657	4.53539477847041	0.80640434099232

### 2b

С	-0.52289585749555	0.81622238029333	0.00001220216944
С	0.86487159040550	0.81791408581916	0.00048752960315
С	1.56626886575658	2.01622242463705	0.00000725404947
С	0.85851618975413	3.20885508483728	-0.00095412639926
С	-0.52838103260956	3.22587123865648	-0.00143130418255

С	-1.21517321456539	2.01904680747184	-0.00093986137731
Η	-1.06476175132965	-0.12231026211186	0.00039071102489
Η	1.41274675946823	-0.11754403931765	0.00124505068566
Η	2.64917857479302	2.01589553317901	0.00038762944972
Η	-1.07042230504637	4.16337281986645	-0.00217442268264
Η	-2.29932486335625	2.02552714254869	-0.00131176470663
Ι	1.90545557422532	5.01955070412021	-0.00168356763395

3b

С	-1.20035739860011	1.03142703272465	0.19030343051345
С	-0.18728100900449	1.98975152845405	0.04525201908254
С	-0.55448186098911	3.33670254536842	-0.12569295300169
С	-1.89941409569711	3.70924490547531	-0.14642443329079
С	-2.88042561495014	2.75442280887842	0.00061908205676
С	-2.52338445494224	1.41160150323773	0.16783551835421
Н	-0.91548626648851	-0.00570926992215	0.32261228857529
Н	-2.14966832638890	4.75501306200520	-0.27887490721566
Н	-3.92559703062431	3.03950649067850	-0.01222706099381
Н	-3.29794445554184	0.66171914367188	0.28294297221650
С	3.83373706419529	0.80665278104686	-0.38967895291322
С	5.16210924143640	0.42115505534253	-0.34740217695707
С	6.13262008275746	1.31010104515383	0.09857418601611
С	5.76801657135972	2.58655277700696	0.50183718465952
С	4.43983106052302	2.97967472042036	0.45221917879689
С	3.46283557088573	2.09117689992498	0.00504317471120
Н	3.07027298525559	0.12200557553876	-0.73735811672833
Н	5.44336018127614	-0.57581989578652	-0.66632355041327
Η	7.17264555309670	1.00641387660261	0.13371219593807
Η	6.51913592571527	3.27970383375520	0.86213152998718
Н	4.17222542560320	3.97239847898903	0.79729705083434

С	0.49340042644293	4.33015598984513	-0.29391759310086
С	2.04162218654635	2.47314826898507	-0.04774290035492
N	1.76196789899045	3.79497809512556	-0.24288998644608
N	1.12280532031339	1.57594022736924	0.08861198725693
0	0.32825163963556	5.52658515699408	-0.47672720409655
Η	2.52034139919352	4.44331525311427	-0.40519785348674

4a

С	-1.61533007343459	1.46088719425409	-0.37727105407989
С	-0.24233518208750	1.44769958317649	-0.24209743491951
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Η	2.01523489651692	6.28756579710751	-0.04217656628826
Н	2.05464388013944	4.70239753124369	-0.73211794318643

4b

С	-1.15013730196404	-0.15342600926163	0.51991299176207
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Η	2.24962463867628	-1.93012202701110	0.55841158763161
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### 4c

С	-0.64097570915032	-1.46677844771664	-0.78072963963522
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Η	-1.26868290885610	-2.25264929966598	-0.37834432010316
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Η	3.85775162857092	-4.07330364410819	2.53265682368080
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Ι

C -2.38008408694202 0.59746868859193 0.16235528431595

С	-0.98660257352311	0.57913402010683	0.12199455732453
С	-0.34758251248669	1.79697453411509	0.09537067478072
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Η	-2.92225400697500	-0.34108831450099	0.18609930331712
Η	-0.43827842727767	-0.35948399648825	0.11313882345183
Η	-0.42323661382391	3.95402611519776	0.07451735555792
Η	-2.90735454171559	3.95415859204855	0.14747590716550
Η	-4.14487623644823	1.81117332460810	0.20363056002540
Po	1 1.54874820683493	1.79098861031719	0.06641505827608
Ι	4.27665653113044	1.78924412962329	0.02606363178992

II

С	-1.76971692125370	0.45985724043777	0.11216684621434
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C       -0.70982250993823       0.41796894111373       0.104865         C       -0.19361496626782       1.72377989565948       0.233994         C       -1.18344696795923       2.70634300431997       0.503506         C       -2.51897361772664       2.38922777342531       0.625262         C       -2.97324953751253       1.07690728827191       0.487053         H       -2.36021415221552       -0.94958105790416       0.111243         H       -0.85514411263042       3.73526685265475       0.616936         H       -3.22867243257867       3.18282193134823       0.835212         H       -4.02343068118158       0.83218866258576       0.584536         I       0.70477680410194       -1.08191021176489       -0.2798524         N       1.11557142941880       1.99506854505960       0.1117225         Pd       2.61640310687169       0.60571118891355       -0.2300909         C       4.32093258616486       -0.18119428193799       -0.4773836         O       4.81971331514910       0.92526052442560       -0.3529274         C       6.35440794358490       -3.82622226944817       -1.0909035         C       5.01241426231055       -1.44030463570572       -0.6684725         C </td <td>С</td> <td>-2.04435042411077</td> <td>0.08186179830407</td> <td>0.22263043827165</td>	С	-2.04435042411077	0.08186179830407	0.22263043827165
C       -0.19361496626782       1.72377989565948       0.233994         C       -1.18344696795923       2.70634300431997       0.503506         C       -2.51897361772664       2.38922777342531       0.625262         C       -2.97324953751253       1.07690728827191       0.487053         H       -2.36021415221552       -0.94958105790416       0.111243         H       -0.85514411263042       3.73526685265475       0.616936         H       -3.22867243257867       3.18282193134823       0.835212         H       -4.02343068118158       0.83218866258576       0.584536         I       0.70477680410194       -1.08191021176489       -0.2798524         N       1.11557142941880       1.99506854505960       0.1117225         Pd       2.61640310687169       0.60571118891355       -0.2300909         C       4.32093258616486       -0.18119428193799       -0.4773836         O       4.81971331514910       0.92526052442560       -0.3529274         C       4.96583315156540       -3.80366774144062       -1.1192049         C       6.35440794358490       -3.82622226944817       -1.0909039         C       5.01241426231055       -1.44030463570572       -0.6927507         C	С	-0.70982250993823	0.41796894111373	0.10486521952189
C       -1.18344696795923       2.70634300431997       0.503506         C       -2.51897361772664       2.38922777342531       0.625262         C       -2.97324953751253       1.07690728827191       0.487053         H       -2.36021415221552       -0.94958105790416       0.111243         H       -0.85514411263042       3.73526685265475       0.616936         H       -3.22867243257867       3.18282193134823       0.835212         H       -4.02343068118158       0.83218866258576       0.584536         I       0.70477680410194       -1.08191021176489       -0.2798524         N       1.11557142941880       1.99506854505960       0.1117225         Pd       2.61640310687169       0.60571118891355       -0.2300909         C       4.32093258616486       -0.18119428193799       -0.4773836         O       4.81971331514910       0.92526052442560       -0.3529274         C       6.35440794358490       -3.82622226944817       -1.0909039         C       6.35440794358490       -3.82622226944817       -1.0909039         C       5.01241426231055       -1.44030463570572       -0.6927507         C       6.41084224419140       -1.46435448350644       -0.6684723 <td< td=""><td>С</td><td>-0.19361496626782</td><td>1.72377989565948</td><td>0.23399429178929</td></td<>	С	-0.19361496626782	1.72377989565948	0.23399429178929
C       -2.51897361772664       2.38922777342531       0.625262         C       -2.97324953751253       1.07690728827191       0.487053         H       -2.36021415221552       -0.94958105790416       0.111243         H       -0.85514411263042       3.73526685265475       0.616936         H       -3.22867243257867       3.18282193134823       0.835212         H       -4.02343068118158       0.83218866258576       0.584536         I       0.70477680410194       -1.08191021176489       -0.2798524         N       1.11557142941880       1.99506854505960       0.1117225         Pd       2.61640310687169       0.60571118891355       -0.2300909         C       4.32093258616486       -0.18119428193799       -0.4773836         O       4.81971331514910       0.92526052442560       -0.3529274         C       6.35440794358490       -3.82622226944817       -1.0909039         C       7.07643491794255       -2.65888373277361       -0.8644282         C       6.41084224419140       -1.46435448350644       -0.6684722         C       5.01241426231055       -1.44030463570572       -0.6927507         C       4.29386463281534       -2.61166920888298       -0.9160744         <	С	-1.18344696795923	2.70634300431997	0.50350656724726
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N       1.11557142941880       1.99506854505960       0.1117225         Pd       2.61640310687169       0.60571118891355       -0.2300909         C       4.32093258616486       -0.18119428193799       -0.4773836         O       4.81971331514910       0.92526052442560       -0.3529274         C       4.96583315156540       -3.80366774144062       -1.1192049         C       6.35440794358490       -3.82622226944817       -1.0909039         C       7.07643491794255       -2.65888373277361       -0.8644282         C       6.41084224419140       -1.46435448350644       -0.6684723         C       5.01241426231055       -1.44030463570572       -0.6927507         C       4.29386463281534       -2.61166920888298       -0.9160747         H       4.40970493169257       -4.71601140531648       -1.2975393         H       6.88026817582226       -4.76153572171750       -1.2460874         H       8.15949031358618       -2.68533174970082       -0.8423383         H       6.95705843882512       -0.54561742383363       -0.4913472         H       3.21173305504052       -2.58204277678873       -0.9387194         H       1.31432169303812       2.97734532463980       0.2400305 <td>Ι</td> <td>0.70477680410194</td> <td>-1.08191021176489</td> <td>-0.27985243026620</td>	Ι	0.70477680410194	-1.08191021176489	-0.27985243026620
Pd2.616403106871690.60571118891355-0.2300909C4.32093258616486-0.18119428193799-0.4773836O4.819713315149100.92526052442560-0.3529274C4.96583315156540-3.80366774144062-1.1192049C6.35440794358490-3.82622226944817-1.0909039C7.07643491794255-2.65888373277361-0.8644282C6.41084224419140-1.46435448350644-0.6684722C5.01241426231055-1.44030463570572-0.6927507C4.29386463281534-2.61166920888298-0.9160747H4.40970493169257-4.71601140531648-1.2975392H6.88026817582226-4.76153572171750-1.2460874H8.15949031358618-2.68533174970082-0.8423389H6.95705843882512-0.54561742383363-0.4913472H3.21173305504052-2.58204277678873-0.9387194H1.314321693038122.977345324639800.2400305	N	1.11557142941880	1.99506854505960	0.11172259840816
<ul> <li>C 4.32093258616486 -0.18119428193799 -0.4773836</li> <li>O 4.81971331514910 0.92526052442560 -0.3529274</li> <li>C 4.96583315156540 -3.80366774144062 -1.1192049</li> <li>C 6.35440794358490 -3.82622226944817 -1.0909039</li> <li>C 7.07643491794255 -2.65888373277361 -0.8644282</li> <li>C 6.41084224419140 -1.46435448350644 -0.6684723</li> <li>C 5.01241426231055 -1.44030463570572 -0.6927503</li> <li>C 4.29386463281534 -2.61166920888298 -0.9160747</li> <li>H 4.40970493169257 -4.71601140531648 -1.2975393</li> <li>H 6.88026817582226 -4.76153572171750 -1.2460874</li> <li>H 8.15949031358618 -2.68533174970082 -0.8423389</li> <li>H 6.95705843882512 -0.54561742383363 -0.4913477</li> <li>H 3.21173305504052 -2.58204277678873 -0.9387194</li> <li>H 1.31432169303812 2.97734532463980 0.2400305</li> </ul>	Pd	2.61640310687169	0.60571118891355	-0.23009091731202
<ul> <li>O 4.81971331514910 0.92526052442560 -0.3529274</li> <li>C 4.96583315156540 -3.80366774144062 -1.1192049</li> <li>C 6.35440794358490 -3.82622226944817 -1.0909039</li> <li>C 7.07643491794255 -2.65888373277361 -0.8644282</li> <li>C 6.41084224419140 -1.46435448350644 -0.6684723</li> <li>C 5.01241426231055 -1.44030463570572 -0.6927503</li> <li>C 4.29386463281534 -2.61166920888298 -0.9160744</li> <li>H 4.40970493169257 -4.71601140531648 -1.2975393</li> <li>H 6.88026817582226 -4.76153572171750 -1.2460874</li> <li>H 8.15949031358618 -2.68533174970082 -0.8423383</li> <li>H 6.95705843882512 -0.54561742383363 -0.4913472</li> <li>H 3.21173305504052 -2.58204277678873 -0.9387194</li> <li>H 1.31432169303812 2.97734532463980 0.2400305</li> </ul>	С	4.32093258616486	-0.18119428193799	-0.47738360739818
<ul> <li>C 4.96583315156540 -3.80366774144062 -1.1192049</li> <li>C 6.35440794358490 -3.82622226944817 -1.0909039</li> <li>C 7.07643491794255 -2.65888373277361 -0.8644282</li> <li>C 6.41084224419140 -1.46435448350644 -0.6684725</li> <li>C 5.01241426231055 -1.44030463570572 -0.6927503</li> <li>C 4.29386463281534 -2.61166920888298 -0.9160747</li> <li>H 4.40970493169257 -4.71601140531648 -1.2975395</li> <li>H 6.88026817582226 -4.76153572171750 -1.2460874</li> <li>H 8.15949031358618 -2.68533174970082 -0.8423385</li> <li>H 6.95705843882512 -0.54561742383363 -0.4913477</li> <li>H 3.21173305504052 -2.58204277678873 -0.9387194</li> <li>H 1.31432169303812 2.97734532463980 0.2400305</li> </ul>	0	4.81971331514910	0.92526052442560	-0.35292749466369
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C7.07643491794255-2.65888373277361-0.8644282C6.41084224419140-1.46435448350644-0.6684723C5.01241426231055-1.44030463570572-0.6927503C4.29386463281534-2.61166920888298-0.9160747H4.40970493169257-4.71601140531648-1.2975393H6.88026817582226-4.76153572171750-1.2460874H8.15949031358618-2.68533174970082-0.8423383H6.95705843882512-0.54561742383363-0.4913472H3.21173305504052-2.58204277678873-0.9387194H1.314321693038122.977345324639800.2400305	С	6.35440794358490	-3.82622226944817	-1.09090397926044
C6.41084224419140-1.46435448350644-0.6684724C5.01241426231055-1.44030463570572-0.6927504C4.29386463281534-2.61166920888298-0.9160744H4.40970493169257-4.71601140531648-1.2975394H6.88026817582226-4.76153572171750-1.2460874H8.15949031358618-2.68533174970082-0.8423384H6.95705843882512-0.54561742383363-0.4913472H3.21173305504052-2.58204277678873-0.9387194H1.314321693038122.977345324639800.2400305	С	7.07643491794255	-2.65888373277361	-0.86442827460577
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C4.29386463281534-2.61166920888298-0.9160747H4.40970493169257-4.71601140531648-1.2975393H6.88026817582226-4.76153572171750-1.2460874H8.15949031358618-2.68533174970082-0.8423383H6.95705843882512-0.54561742383363-0.4913472H3.21173305504052-2.58204277678873-0.9387194H1.314321693038122.977345324639800.2400305	С	5.01241426231055	-1.44030463570572	-0.69275012264822
H4.40970493169257-4.71601140531648-1.2975393H6.88026817582226-4.76153572171750-1.2460874H8.15949031358618-2.68533174970082-0.8423383H6.95705843882512-0.54561742383363-0.4913472H3.21173305504052-2.58204277678873-0.9387194H1.314321693038122.977345324639800.2400305	С	4.29386463281534	-2.61166920888298	-0.91607471210857
H6.88026817582226-4.76153572171750-1.2460874H8.15949031358618-2.68533174970082-0.8423389H6.95705843882512-0.54561742383363-0.4913472H3.21173305504052-2.58204277678873-0.9387194H1.314321693038122.977345324639800.2400305	Η	4.40970493169257	-4.71601140531648	-1.29753951320228
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Н 1.31432169303812 2.97734532463980 0.2400305	Η	3.21173305504052	-2.58204277678873	-0.93871942306805
	Η	1.31432169303812	2.97734532463980	0.24003050042479

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V

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VI

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Н	0.02470051854334	-3.57603130393234	-0.49439758128237

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С	-2.08837809745776	1.69665353016232	-0.07150945962216
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Н	1.86539873010663	1.62201952641448	0.08905300339581
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Ι	2.47069884363518	5.91491303126650	0.04850528139655

VIII

С	-2.26128025161057	1.13744096009969	-0.28317752695884
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N	1.06953905996099	2.48978854553258	0.22004973445279
Η	1.60662326011123	1.66394550150954	0.01680520947753
Η	1.57349355783206	3.36098586593534	0.28648596696152
Ι	3.15537733316424	5.27982301437508	-0.89148444414186
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Ν	1.06392858835652	2.72856038012940	-0.13572553697486
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С	-1.54105001600362	2.90401781686214	0.05358959219867
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Ν	3.39888476932787	3.41189825468186	1.09179689334275
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Pd	3.68836970945424	1.38588183828011	0.76035842653912
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CO

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С	-1.36929212673541	-2.22324957029106	-1.71924287430344
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Kł	HCO <sub>3</sub>		
С	-1.39128418842014	-2.33617034640655	-1.70590851344620
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KI

K	-0.62905577247081	0.88047080000000	0.15021488000000
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N	-2.65325919493804	1.65262589713872	0.0000000544584
Η	-2.26296039075569	0.71642965138457	-0.0000002368020
Η	-2.26294312183103	2.12072898467791	0.81081084729601
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0	0.15538994557158	0.67750594663781	-0.01134225000000
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Pd	2.06875249597706	-1.50275883498584	0.57566358060456
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Ι	0.07112293607802	5.69962753968511	0.25090042440877
Pd	0.62982684528626	3.11977468130052	-0.20209509505514
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Η	1.62260729110434	-3.13797193315409	0.32897091810051
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Н	0.98653345576770	-2.77846172956256	-3.04269744010481

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