# Supplementary Information 

# $\mathrm{CO}_{2}$-Mediated Isomerization of Enamides 

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## General Remarks

The reactions were carried out in undivided electrochemical cells ( 15 mL ) using predried glassware, if not noted otherwise. The substrates were obtained from commercial sources (J\&K Scientific, Bidepharm, Energy Chemical) or synthesized according to literature methods. ${ }^{[1-2]}$ Solvents were obtained from commercial sources. Magnesium plates electrodes $(0.1 \mathrm{~mm} \times 10.0 \mathrm{~mm} \times 20.0 \mathrm{~mm}, 99.95 \%$; obtained from Bochuang scientific research metal materials, Guangdong, China) and Platinum electrodes ( 0.25 $\mathrm{mm} \times 10 \mathrm{~mm} \times 15 \mathrm{~mm}, 99.9 \%$; obtained from Chuxi, Shanghai, China) were connected using stainless steel adapters. Electrocatalysis was conducted using an HSPY-36-03 potentiostat in constant current mode. Cyclic Voltammetry studies were performed using a Shanghai Chenhua CHI760E workstation. Yields refer to isolated compounds, estimated to be $>95 \%$ purity as determined by ${ }^{1} \mathrm{H}$ NMR. Flash chromatography was performed using Silica gel (200 - 300 mesh) purchased from Qingdao Haiyang Chemical Co., China. NMR spectra were recorded on Bruker AVANCE AV 400 or 600 in the solvent indicated; using $\mathrm{CDCl}_{3}$ or DMSO- $d_{6}$ as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature, chemical shifts ( $\delta$ ) are given in ppm relative to the residual solvent peak, coupling constants (J) are reported in Hertz $(\mathrm{Hz})$. Multiplicities are recorded as: $\mathrm{s}=$ singlet, $\mathrm{d}=$ doublet, $\mathrm{t}=$ triplet, $\mathrm{q}=$ quadruplet, $\mathrm{dd}=$ doublet of doublets, $\mathrm{m}=$ multiplet. The High-resolution mass spectrometry (HRMS) data were collected on a Micro TOF mass spectrometer with ESI mass analyzer. Melting points were recorded on Shanghai ShenGuang WRS-2 apparatus. Visualization was achieved under a UV lamp ( 254 nm and 365 nm ).

## Optimization of the Reaction Conditions ${ }^{\text {a }}$

## Table S1:



1a, (Z)-N-styrylbenzamide

$\mathrm{Cs}_{2} \mathrm{CO}_{3}$ (1.0 equiv.)
$\mathrm{TBABF}_{4}$ (1.0 equiv.)
DMF ( 4 mL ), $60^{\circ} \mathrm{C}, 2 \mathrm{~h} \quad \mathbf{1 ,}(E)-N$-styrylbenzamide


| Entry | Alteration | $(\mathbf{1 a + 1})$ Yield (\%) ${ }^{b}$ | $\mathbf{1 - E}$ |
| :---: | :---: | :---: | :---: |
| 1 | None | 99 | 98 |

$2 \quad \mathrm{Fe}(+)$ instead of $\operatorname{Mg}(+) \quad 90 \quad 90$
$3 \quad \mathrm{CF}(-)$ instead of $\operatorname{Pt}(-) \quad 62 \quad 62$

3 DMA/MeCN/NMP instead of DMF 85/-/- 85/76/83
$4 \quad \mathrm{TBAI} / \mathrm{TBAClO}_{4}$ instead of $\mathrm{TBABF}_{4} \quad 94 /-\quad 94 / 59$

4
$\mathrm{Li}_{2} \mathrm{CO}_{3} / \mathrm{Na}_{2} \mathrm{CO}_{3} / \mathrm{K}_{2} \mathrm{CO}_{3}$ instead of
90/88/93
trace/27/87 $\mathrm{Cs}_{2} \mathrm{CO}_{3}$
0.5 equiv. of $\mathrm{Cs}_{2} \mathrm{CO}_{3}$

94
$40^{\circ} \mathrm{C} / 50^{\circ} \mathrm{C} / 70{ }^{\circ} \mathrm{C} / 80^{\circ} \mathrm{C}$
81/85/97/99
68/85/98/99

6
No Cs2 $\mathrm{CO}_{3} \quad 79$
23

7
No current 90
89

8
No $\mathrm{CO}_{2}$
97
16

9
No current and $\mathrm{CO}_{2}$
90
$<10$
${ }^{a}$ Reaction conditions: undivided cell, $\mathbf{1}(0.2 \mathrm{mmol}), \mathrm{Cs}_{2} \mathrm{CO}_{3}$ ( $0.2 \mathrm{mmol}, 1.0$ equiv.), $\mathrm{TBABF}_{4}$ ( 0.2 mmol , 1.0 equiv.) in DMF ( 4.0 mL ), $60^{\circ} \mathrm{C}, 2 \mathrm{~h}$, under $\mathrm{CO}_{2}$ ( 1 atm ), Mg plate as the anode, and platinum plate as the cathode, $\mathrm{CCE}=5.0 \mathrm{~mA} .{ }^{b}$ Yield of isolated products. $\mathrm{CCE}=$ constant current electrolysis;DMA $=$ $N, N$-Dimethylacetamide; DMF = N, N-dimethylformamide; NMP = 1-Methyl-2-pyrrolidinone; MeCN $=$ Acetonitrile; $\mathrm{TBABF}_{4}=$ tetrabutylammonium tetrafluoroborate; $\mathrm{TBAI}=$ tetrabutylammonium iodide; $\mathrm{TBAClO}_{4}=$ tetrabutylammonium perchlorate.

## Synthesis of starting materials

## General procedure for the preparation of substrates



Method A: A 100 mL schlenk flask was charged with amide (1.2 equiv.), copper(I) iodide ( 0.5 equiv.), and $\mathrm{Cs}_{2} \mathrm{CO}_{3}$ ( 2.0 equiv.). The flask was backfilled with argon, and closed with a rubber bung. Vinyl bromide ( 1.0 equiv.) and $N, N-$ dimethylethylenediamine ( 1.0 equiv.) in dry and degassed THF ( 25 mL ) were next added. The mixture was stirred at $65^{\circ} \mathrm{C}$ overnight. The reaction mixture was cooled to room temperature, filtered, the solution layer was extracted with EtOAc and concentrated under vacuo. The crude residue was purified by flash chromatography on silica gel to give the desired enamides (1a-21a). Physical and spectral data were in accordance with literature data. ${ }^{[1]}$


Figure S1: Starting materials synthesized according to Method A.


Method B: A dried 100 mL schlenk flask was charged with the amide ( 1.0 equiv.), bis(2-methallyl)-cycloocta-1,5-diene-ruthenium (II) (5 mol\%), 1,4bis(dicyclohexylphosphino)butane ( $6 \mathrm{~mol} \%$ ) and ytterbium triflate ( $4 \mathrm{~mol} \%$ ) and flushed with argon. Subsequently, dry DMF ( 0.5 M ), alkyne ( 2.0 equiv.) and water $(0.017 \mathrm{M})$ were added via syringe. The resulting solution was stirred for 6 h at $60^{\circ} \mathrm{C}$, then poured into an aqueous sodium bicarbonate solution ( 30 mL ). The resulting mixture was extracted three times with EtOAc $(20 \mathrm{~mL} \times 3)$, the combined organic layers were washed with water and brine, dried with anhydrous $\mathrm{Na}_{2} \mathrm{SO}_{4}$, filtered, and the volatiles were removed under vacuo. The residue was purified by column chromatography (silica gel, ethyl acetate/ petroleum ether) to yield the Z-enamides. Physical and spectral data were in accordance with literature data. ${ }^{[2]}$


Figure S2: Starting materials synthesized according to Method B.


## Method C:

Step1: A dried 50 mL round bottom flask was charged with the carboxylic acid (10 mmol, 1.0 equiv.) and 1,1 '-carbonyldiimidazole (CDI) ( $10 \mathrm{mmol}, 1.0$ equiv.). Subsequently, EtOAc ( $2.0 \mathrm{~mL} / \mathrm{mmol}$ ) were added via syringe. The resulting solution was stirred for 2 h at room temperature, then, ammonium hydroxide ( $0.8 \mathrm{~mL} / \mathrm{mmol}$ ) was added slowly under vigorous stirring. The mixture stirred for 2 h at $45^{\circ} \mathrm{C}$. The
resulting mixture was extracted three times with EtOAc $(20 \mathrm{~mL} \times 3)$ the combined organic layers were washed with water and brine, dried with anhydrous $\mathrm{Na}_{2} \mathrm{SO}_{4}$, filtered, and the volatiles were removed under vacuo. The residue was used for step 2 without further purification.

## Step2: see Method A.



Figure S3: Starting materials synthesized according to Method C.

## unsuccessful examples:








## Graphical Guide

Pictures of the reaction setups


Figure S4. General reaction apparatus.

## General Procedure

The reaction was carried out in an undivided cell with magnesium plates anodes ( 0.1 $\mathrm{mm} \times 10.0 \mathrm{~mm} \times 20.0 \mathrm{~mm}$ ) and platinum cathodes $(0.25 \mathrm{~mm} \times 10 \mathrm{~mm} \times 15 \mathrm{~mm})$. To a 15.0 mL oven-dried undivided cell equipped with a magnetic bar was added substrates $Z$-enamide 1a ( $0.2 \mathrm{mmol}, 1.0$ equiv.), $\mathrm{Cs}_{2} \mathrm{CO}_{3}$ ( 0.2 mmol , 1.0 equiv.), $\mathrm{TBABF}_{4}$ ( 0.2 mmol, 1.0 equiv.). Then the tube was evacuated and back-filled under $\mathrm{CO}_{2}$ flow (this procedure was repeated three times), and DMF ( 4.0 mL ) was added via a syringe. The electrocatalysis was performed under $\mathrm{CO}_{2}$ balloon at $60^{\circ} \mathrm{C}$ with a constant current of 5.0 mA maintained for 2 h . After that, the reaction mixture was acidized with HCl aqueous ( $1.0 \mathrm{~N}, 5 \mathrm{~mL}$ ). The aqueous layer was extracted with $\mathrm{EtOAc}(2 \times 10 \mathrm{~mL})$ and the combined organic phase was washed with brine, dried by anhydrous $\mathrm{MgSO}_{4}$, filtered, and concentrated under vacuo. The crude product was purified by column chromatography to furnish the desired product.

## Characterization Data of Products


(E)- N -Styrylbenzamide (1)

Compound 1 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $\mathbf{1}(43.9 \mathrm{mg}, 98 \%)$ as a pale-yellow solid. ${ }^{1} \mathrm{H}$ NMR ( $400 \mathrm{MHz}, \mathrm{DMSO}-d_{6}$ ) $\delta 10.64(\mathrm{~d}, J=9.2 \mathrm{~Hz}, 1 \mathrm{H})$, $7.98(\mathrm{~d}, J=6.8 \mathrm{~Hz}, 2 \mathrm{H}), 7.74-7.45(\mathrm{~m}, 4 \mathrm{H}), 7.40(\mathrm{~d}, J=8.0 \mathrm{~Hz}, 2 \mathrm{H}), 7.32(\mathrm{t}, J=7.6$ $\mathrm{Hz}, 2 \mathrm{H}), 7.18(\mathrm{t}, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 6.48(\mathrm{~d}, J=14.8 \mathrm{~Hz}, 1 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , DMSO- $d_{6}$ ) $\delta 164.5,137.1,133.8,132.4,129.2,129.0,128.1,126.7,125.7,124.6,113.4$. Spectroscopic data match those previously reported in the literature. ${ }^{[1]}$


## (E)-N-Styrylpropionamide (2)

Compound 2 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $2(29.8 \mathrm{mg}, 85 \%)$ as a white solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 7.66(\mathrm{~d}, J=10.0 \mathrm{~Hz}, 1 \mathrm{H}), 7.54$ (dd, $J=14.8,10.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.31-7.23(\mathrm{~m}, 4 \mathrm{H}), 7.19-7.13(\mathrm{~m}, 1 \mathrm{H}), 6.10(\mathrm{~d}, J=14.4$ $\mathrm{Hz}, 1 \mathrm{H}), 2.33(\mathrm{q}, J=7.2 \mathrm{~Hz}, 2 \mathrm{H}), 1.22(\mathrm{t}, J=7.6 \mathrm{~Hz}, 3 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform-d) $\delta 171.4,136.2,128.7,126.6,125.5,122.8,112.4,29.7,9.6$. Spectroscopic data match those previously reported in the literature. ${ }^{[1]}$


## (E)-N-Styrylpentanamide (3)

Compound $\mathbf{3}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=15: 1$ ) yielded $\mathbf{3}(29.7 \mathrm{mg}, 73 \%)$ as a white solid. M.p.: $100-101{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform-d) $\delta 7.59-7.46$ $(\mathrm{m}, 2 \mathrm{H}), 7.32-7.23(\mathrm{~m}, 4 \mathrm{H}), 7.16(\mathrm{~m}, 1 \mathrm{H}), 6.09(\mathrm{~d}, J=14.0 \mathrm{~Hz}, 1 \mathrm{H}), 2.30(\mathrm{t}, J=7.6$
$\mathrm{Hz}, 2 \mathrm{H}), 1.68(\mathrm{p}, J=7.6 \mathrm{~Hz}, 2 \mathrm{H}), 1.43-1.34(\mathrm{~m}, 2 \mathrm{H}), 0.93(\mathrm{t}, J=7.2 \mathrm{~Hz}, 3 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform-d) $\delta$ 170.7, 136.1, 128.7, 126.6, 125.5, 122.7, 112.4, 36.5, 27.6, 22.4, 13.8. HRMS (ESI, m/z): Calculated $\mathrm{C}_{13} \mathrm{H}_{17} \mathrm{NO}[\mathrm{M}+\mathrm{H}]^{+}$: 204.1388, found 204.1390.


## (E)-N-Styrylhexanamide (4)

Compound $\mathbf{4}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $\mathbf{4}(34.3 \mathrm{mg}, 79 \%)$ as a white solid. M.p.: $95-96^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 7.54(\mathrm{dd}, J=$ $14.4,10.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.48-7.39(\mathrm{~d}, J=9.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.34-7.23(\mathrm{~m}, 4 \mathrm{H}), 7.17(\mathrm{t}, J=7.2$ $\mathrm{Hz}, 1 \mathrm{H}), 6.09(\mathrm{~d}, J=14.4 \mathrm{~Hz}, 1 \mathrm{H}), 2.29(\mathrm{t}, J=7.6 \mathrm{~Hz}, 2 \mathrm{H}), 1.70(\mathrm{~m}, 2 \mathrm{H}), 1.40-1.27$ $(\mathrm{m}, 4 \mathrm{H}), 0.91(\mathrm{t}, J=6.4 \mathrm{~Hz}, 3 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta$ 170.7, 136.1, 128.7, 126.6, 125.5, 122.7, 112.4, 36.8, 31.4, 25.2, 22.4, 13.9. HRMS (ESI, m/z): Calculated $\mathrm{C}_{14} \mathrm{H}_{19} \mathrm{NO}[\mathrm{M}+\mathrm{H}]^{+}: 218.1545$, found 218.1549.


## (E)-N-Styrylisobutyramide (5)

Compound 5 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $5(34.1 \mathrm{mg}, 90 \%)$ as a yellow solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 7.81(\mathrm{~d}, J=10.4 \mathrm{~Hz}, 1 \mathrm{H}), 7.54$ (dd, $J=14.8,10.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.32-7.22(\mathrm{~m}, 4 \mathrm{H}), 7.15(\mathrm{t}, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 6.15(\mathrm{~d}, J=$ $14.8 \mathrm{~Hz}, 1 \mathrm{H}), 2.49(\mathrm{~m}, 1 \mathrm{H}), 1.22(\mathrm{~d}, \mathrm{~J}=6.8 \mathrm{~Hz}, 6 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroformd) $\delta 174.8,136.2,128.7,126.6,125.5,122.9,112.7,35.7,19.5$. Spectroscopic data match those previously reported in the literature. ${ }^{[2]}$

(E)-N-Styrylpivalamide (6)

Compound 6 as prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=15: 1$ ) yielded $\mathbf{6}(39.8 \mathrm{mg}, 98 \%)$ as a white solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 7.54(\mathrm{dd}, J=14.0,10.4 \mathrm{~Hz}, 1 \mathrm{H})$, $7.46(\mathrm{~d}, J=10.0 \mathrm{~Hz}, 1 \mathrm{H}), 7.27(\mathrm{~m}, 4 \mathrm{H}), 7.19-7.13(\mathrm{~m}, 1 \mathrm{H}), 6.13(\mathrm{~d}, J=14.4 \mathrm{~Hz}, 1 \mathrm{H})$, 1.27 (s, 9H). ${ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta$ 175.7, 136.2, 128.7, 126.6, 125.5, 123.2, 112.6, 38.9, 27.5. Spectroscopic data match those previously reported in the literature. ${ }^{[2]}$


## (E)-N-Styrylcyclobutanecarboxamide (7)

Compound 7 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $7(34.6 \mathrm{mg}, 86 \%)$ as a white solid. M.p.: $126-127^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 7.54$ (dd, $J$ $=14.0,10.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.44(\mathrm{~d}, J=10.0 \mathrm{~Hz}, 1 \mathrm{H}), 7.32-7.24(\mathrm{~m}, 4 \mathrm{H}), 7.13-7.19(\mathrm{~m}$, $1 \mathrm{H}), 6.10(\mathrm{~d}, J=14.4 \mathrm{~Hz}, 1 \mathrm{H}), 3.10(\mathrm{p}, J=8.4 \mathrm{~Hz}, 1 \mathrm{H}), 2.41-2.31(\mathrm{~m}, 2 \mathrm{H}), 2.24-$ $2.15(\mathrm{~m}, 2 \mathrm{H}), 2.05-1.87(\mathrm{~m}, 2 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta 172.5,136.2$, 128.7, 126.6, 125.5, 122.8, 112.4, 39.9, 25.6, 18.2. HRMS (ESI, m/z): Calculated $\mathrm{C}_{13} \mathrm{H}_{15} \mathrm{NO}[\mathrm{M}+\mathrm{H}]^{+}: 202.1232$, found 202.1235.

tert-Butyl (E)-2-(styrylcarbamoyl)azetidine-1-carboxylate (8)
Compound $\mathbf{8}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=8: 1)$ yielded $\mathbf{8}(49.0 \mathrm{mg}, 81 \%)$ as a white solid. M.p.: $121-123{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform-d) $\delta 7.50(\mathrm{dd}, J$ $=14.8,10.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.39-7.24(\mathrm{~m}, 4 \mathrm{H}), 7.13-7.21(\mathrm{~m}, 1 \mathrm{H}), 6.17(\mathrm{~d}, J=14.4 \mathrm{~Hz}$, $1 \mathrm{H}), 4.75(\mathrm{t}, J=8.0 \mathrm{~Hz}, 1 \mathrm{H}), 3.94(\mathrm{q}, J=8.0 \mathrm{~Hz}, 1 \mathrm{H}), 3.76-3.86(\mathrm{~m}, 1 \mathrm{H}), 2.65-2.30$ $(\mathrm{m}, 2 \mathrm{H}), 1.49(\mathrm{~s}, 9 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta$ 169.1, 136.2, 128.7, 126.7, 125.6, 122.2, 113.8, 81.4, 62.1, 47.3, 28.3. HRMS (ESI, m/z): Calculated $\mathrm{C}_{17} \mathrm{H}_{22} \mathrm{~N}_{2} \mathrm{O}_{3}$
$[\mathrm{M}+\mathrm{Na}]^{+}: 325.1528$, found 325.1522.

(E)-N-Styrylcyclohexanecarboxamide (9)

Compound 9 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1)$ yielded $9(36.7 \mathrm{mg}, 80 \%)$ as a yellow solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 7.54(\mathrm{dd}, J=14.4,10.8 \mathrm{~Hz}$, $1 \mathrm{H}), 7.34-7.25(\mathrm{~m}, 5 \mathrm{H}), 7.20-7.14(\mathrm{~m}, 1 \mathrm{H}), 6.09(\mathrm{~d}, J=14.4 \mathrm{~Hz}, 1 \mathrm{H}), 2.17(\mathrm{tt}, J=$ 11.6, $3.6 \mathrm{~Hz}, 1 \mathrm{H}), 1.87-1.96(\mathrm{~m}, 2 \mathrm{H}), 1.79-1.86(\mathrm{~m}, 2 \mathrm{H}), 1.66-1.73(\mathrm{~m}, 1 \mathrm{H}), 1.55$ $-1.45(\mathrm{~m}, 2 \mathrm{H}), 1.35-1.23(\mathrm{~m}, 3 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform-d) $\delta 173.4,136.2$, 128.7, 126.6, 125.5, 122.9, 112.3, 45.5, 29.5, 25.7, 25.6. Spectroscopic data match those previously reported in the literature. ${ }^{[2]}$


## ( $E$ )- $N$-Styryladamantane-1-carboxamide (10)

Compound $\mathbf{1 0}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) yielded $10(54.6 \mathrm{mg}$, $97 \%$ ) as a white solid. M.p.: $173-174{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform-d) $\delta 7.66$ $-7.51(\mathrm{~m}, 2 \mathrm{H}), 7.33-7.21(\mathrm{~m}, 4 \mathrm{H}), 7.10-7.18(\mathrm{~m}, 1 \mathrm{H}), 6.15(\mathrm{~d}, J=14.4 \mathrm{~Hz}, 1 \mathrm{H})$, 2.07 (s, 3H), 1.93 (s, 6H), 1.66 - $1.80(\mathrm{~m}, 6 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta$ 175.4, 136.3, 128.7, 126.5, 125.5, 123.2, 112.6, 40.8, 39.1, 36.4, 28.0. HRMS (ESI, $\mathrm{m} / \mathrm{z})$ : Calculated $\mathrm{C}_{19} \mathrm{H}_{23} \mathrm{NO}[\mathrm{M}+\mathrm{H}]^{+}: 282.1858$, found 282.1861.

(E)-N-Styrylmethacrylamide (11)

Compound $\mathbf{1 1}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=15: 1$ ) yielded $11(30.7 \mathrm{mg}$, $82 \%)$ as a white solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 7.70(\mathrm{~d}, J=10.8 \mathrm{~Hz}, 1 \mathrm{H})$,
7.59 (dd, $J=14.8,10.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.37-7.26(\mathrm{~m}, 4 \mathrm{H}), 7.13-7.22(\mathrm{~m}, 1 \mathrm{H}), 6.19(\mathrm{~d}, J=$ $14.8 \mathrm{~Hz}, 1 \mathrm{H}), 5.82(\mathrm{~s}, 1 \mathrm{H}), 5.48(\mathrm{~s}, 1 \mathrm{H}), 2.04(\mathrm{~s}, 3 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroformd) $\delta 165.3,139.4,136.0,128.7,126.8,125.6,122.8,120.9,113.5,18.6$. Spectroscopic data match those previously reported in the literature. ${ }^{[3]}$


## Benzyl (E)-styrylcarbamate (12)

Compound $\mathbf{1 2}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1)$ yielded $12(36.0 \mathrm{mg}$, $71 \%$ ) as a white solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 7.37-7.45$ (m, 5H), 7.28 $-7.34(\mathrm{~m}, 5 \mathrm{H}), 7.18-7.24(\mathrm{~m}, 1 \mathrm{H}), 6.84(\mathrm{~d}, J=10.8 \mathrm{~Hz}, 1 \mathrm{H}), 6.01(\mathrm{~d}, J=14.4 \mathrm{~Hz}$, 1H), 5.23 (s, 2H). ${ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta$ 153.6, 136.2, 135.9, 128.7, $128.7,128.5,128.4,126.4,125.4,124.0,111.0,67.5$. Spectroscopic data match those previously reported in the literature. ${ }^{[4]}$


## ( $E$ )-4-Fluoro- N -styrylbenzamide (13)

Compound $\mathbf{1 3}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=8: 1$ ) yielded $\mathbf{1 3}(45.8 \mathrm{mg}, 95 \%)$ as a yellow solid. ${ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}\right.$, DMSO- $\left.d_{6}\right) \delta 10.67(\mathrm{~d}, J=10.0 \mathrm{~Hz}, 1 \mathrm{H}), 8.01-$ 8.10 (m, 2H), 7.65 (dd, $J=14.8,9.6 \mathrm{~Hz}, 1 \mathrm{H}), 7.42-7.35$ (m, 4H), 7.32 (t, $J=8.0 \mathrm{~Hz}$, $1 \mathrm{H}), 7.22-7.13(\mathrm{~m}, 1 \mathrm{H}), 6.47$ (d, $J=14.4 \mathrm{~Hz}, 1 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , DMSO- $d_{6}$ ) $\delta 166.0,163.5\left({ }^{1} J_{\mathrm{C}-\mathrm{F}}=248.1 \mathrm{~Hz}\right), 163.5,137.0,130.9,130.8\left({ }^{3} J_{\mathrm{C}-\mathrm{F}}=9.2 \mathrm{~Hz}\right), 130.3$, $130.3\left({ }^{4} J_{\mathrm{C}-\mathrm{F}}=3.1 \mathrm{~Hz}\right), 129.2,126.8,125.7,124.6,116.1,115.8\left({ }^{2} J_{\mathrm{C}-\mathrm{F}}=21.9 \mathrm{~Hz}\right), 113.5$. ${ }^{19}$ F NMR ( 375 MHz , Chloroform-d) $\delta$-103.45. Spectroscopic data match those previously reported in the literature. ${ }^{[5]}$


## ( $E$ )-4-Chloro- $N$-styrylbenzamide (14)

Compound $\mathbf{1 4}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $14(50.0 \mathrm{mg}$, $97 \%$ ) as a yellow solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz, DMSO- $d_{6}$ ) $\delta 10.72(\mathrm{~d}, J=9.6 \mathrm{~Hz}, 1 \mathrm{H})$, $8.04-7.97(\mathrm{~m}, 2 \mathrm{H}), 7.69-7.59(\mathrm{~m}, 3 \mathrm{H}), 7.37-7.43(\mathrm{~m}, 2 \mathrm{H}), 7.31(\mathrm{t}, J=7.6 \mathrm{~Hz}, 2 \mathrm{H})$, $7.21-7.15(\mathrm{~m}, 1 \mathrm{H}), 6.48(\mathrm{~d}, J=14.4 \mathrm{~Hz}, 1 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , DMSO- $d_{6}$ ) $\delta 163.5$, $137.2,136.9,132.5,130.0,129.2,129.1,126.8,125.8,124.5,113.8$. Spectroscopic data match those previously reported in the literature. ${ }^{[6]}$


## ( $E$ )-4-Methyl- $N$-styrylbenzamide (15)

Compound 15 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $15(44.6 \mathrm{mg}$, $94 \%$ ) as a white solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz, DMSO- $d_{6}$ ) $\delta 10.56(\mathrm{~d}, J=10.0 \mathrm{~Hz}, 1 \mathrm{H}$ ), 7.89 (d, $J=8.4 \mathrm{~Hz}, 2 \mathrm{H}), 7.65(\mathrm{dd}, J=14.4,10.0 \mathrm{~Hz}, 1 \mathrm{H}), 7.41-7.28(\mathrm{~m}, 6 \mathrm{H}), 7.13-$ $7.21(\mathrm{~m}, 1 \mathrm{H}), 6.45(\mathrm{~d}, J=14.8 \mathrm{~Hz}, 1 \mathrm{H}), 2.38(\mathrm{~s}, 3 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , DMSO- $d_{6}$ ) $\delta 164.4,142.5,137.1,131.0,129.5,129.2,128.2,126.7,125.7,124.7,113.1,21.5$. Spectroscopic data match those previously reported in the literature. ${ }^{[7]}$


## ( E)-N-Styryl-[1,1'-biphenyl]-4-carboxamide (16)

Compound 16 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1)$ yielded $16(47.9 \mathrm{mg}$, $80 \%$ ) as a white solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 8.35(\mathrm{~d}, J=10.0 \mathrm{~Hz}, 1 \mathrm{H}$ ), $7.75(\mathrm{~d}, J=8.4 \mathrm{~Hz}, 2 \mathrm{H}), 7.59(\mathrm{~d}, J=8.4 \mathrm{~Hz}, 2 \mathrm{H}), 7.52(\mathrm{~d}, J=6.8 \mathrm{~Hz}, 2 \mathrm{H}), 7.41-7.26$
$(\mathrm{m}, 7 \mathrm{H}), 7.24-7.18(\mathrm{~m}, 1 \mathrm{H}), 7.18-7.10(\mathrm{~m}, 1 \mathrm{H}), 5.82(\mathrm{~d}, J=9.6 \mathrm{~Hz}, 1 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta 164.1,145.0,139.8,135.9,132.0,129.3,129.0,128.2$, $127.9,127.7,127.5,127.2,127.1,122.5,111.0$. Spectroscopic data match those previously reported in the literature. ${ }^{[7]}$


## ( $E$ )-3-Methyl- $N$-styrylbenzamide (17)

Compound $\mathbf{1 7}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1)$ yielded $17(45.6 \mathrm{mg}$, $96 \%$ ) as a white solid. M.p.: $128-131^{\circ} \mathrm{C}$. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform-d) $\delta 8.49$ $(\mathrm{d}, J=10.4 \mathrm{~Hz}, 1 \mathrm{H}), 7.78-7.61(\mathrm{~m}, 3 \mathrm{H}), 7.32-7.22(\mathrm{~m}, 6 \mathrm{H}), 7.12-7.19(\mathrm{~m}, 1 \mathrm{H})$, $6.31(\mathrm{~d}, J=14.8 \mathrm{~Hz}, 1 \mathrm{H}), 2.35(\mathrm{~s}, 3 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta 165.0$, 138.7, 136.1, 133.4, 132.9, 128.7, 128.6, 128.1, 126.7, 125.7, 124.2, 123.2, 113.8, 21.4. HRMS (ESI, m/z): Calculated $\mathrm{C}_{16} \mathrm{H}_{15} \mathrm{NO}[\mathrm{M}+\mathrm{Na}]^{+}: 260.1051$, found 260.1047.


## (E)-2-Chloro- N -styrylbenzamide (18)

Compound 18 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $\mathbf{1 8}(36.1 \mathrm{mg}$, $70 \%)$ as a yellow solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 8.54(\mathrm{~d}, J=11.2 \mathrm{~Hz}, 1 \mathrm{H})$, $7.81(\mathrm{~d}, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.42-7.32(\mathrm{~m}, 7 \mathrm{H}), 7.28-7.14(\mathrm{~m}, 2 \mathrm{H}), 5.93(\mathrm{~d}, J=9.6 \mathrm{~Hz}$, 1H). ${ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta$ 163.5, 135.4, 133.4, 132.2, 131.3, 130.6, $130.5,129.1,128.0,127.4,127.2,121.8,111.8$. Spectroscopic data match those previously reported in the literature. ${ }^{[7]}$

(E)-6-Chloro- $N$-styrylnicotinamide (19)

Compound 19 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=5: 1$ ) yielded $19(46.0 \mathrm{mg}, 89 \%)$ as a pale-yellow solid. M.p.: $188-190{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR $\left(400 \mathrm{MHz}\right.$, DMSO- $\left.d_{6}\right) \delta 10.86(\mathrm{~d}$, $J=9.6 \mathrm{~Hz}, 1 \mathrm{H}), 8.96(\mathrm{~d}, J=2.8 \mathrm{~Hz}, 1 \mathrm{H}), 8.36(\mathrm{dd}, J=8.0,2.4 \mathrm{~Hz}, 1 \mathrm{H}), 7.70(\mathrm{~d}, J=$ $8.4 \mathrm{~Hz} 2 \mathrm{H}), 7.64(\mathrm{dd}, J=14.8,10.0 \mathrm{~Hz}, 1 \mathrm{H}), 7.41(\mathrm{~d}, J=7.2 \mathrm{~Hz}, 2 \mathrm{H}), 7.31(\mathrm{t}, J=8.0$ $\mathrm{Hz}, 2 \mathrm{H}), 7.16-7.21(\mathrm{~m}, 1 \mathrm{H}), 6.48(\mathrm{~d}, J=14.8 \mathrm{~Hz}, 1 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , DMSO$\left.d_{6}\right) \delta 162.0,153.5,149.8,139.4,136.7,129.2,128.9,127.0,125.9,124.7,124.0,114.4$. HRMS (ESI, m/z): Calculated $\mathrm{C}_{14} \mathrm{H}_{11} \mathrm{~N}_{2} \mathrm{O}^{35} \mathrm{Cl}[\mathrm{M}+\mathrm{H}]^{+}: 259.0638$, found 259.0636.

tert-Butyl (E)-(1-(styrylcarbamoyl)cyclobutyl)carbamate (20)
Compound 20 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=8: 1$ ) yielded $20(58.2 \mathrm{mg}, 88 \%)$ as a pale-yellow solid. M.p.: $158-162{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 8.99$ $(\mathrm{s}, 1 \mathrm{H}), 7.62-7.43(\mathrm{~m}, 1 \mathrm{H}), 7.36-7.22(\mathrm{~m}, 4 \mathrm{H}), 7.16(\mathrm{t}, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 6.13(\mathrm{~d}, J=$ $14.4 \mathrm{~Hz}, 1 \mathrm{H}), 2.82-2.63(\mathrm{~m}, 2 \mathrm{H}), 2.28-1.83(\mathrm{~m}, 4 \mathrm{H}), 1.45(\mathrm{~s}, 9 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR (100 MHz , Chloroform- $d$ ) $\delta 171.3,155.5,136.3,128.6,126.5,125.5,123.1,113.0,81.1$, 59.1, 30.9, 28.3, 15.2. HRMS (ESI, m/z): Calculated $\mathrm{C}_{18} \mathrm{H}_{24} \mathrm{~N}_{2} \mathrm{O}_{3}[\mathrm{M}+\mathrm{Na}]^{+}: 339.1685$, found 339.1682 .


## (E)-N-Styryl-1-naphthamide (21)

Compound 21 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $21(54.1 \mathrm{mg}$, $99 \%)$ as a white solid. M.p.: $177-178{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , DMSO- $d_{6}$ ) $\delta 10.86(\mathrm{~d}$, $J=10.0 \mathrm{~Hz}, 1 \mathrm{H}), 8.32-8.23(\mathrm{~m}, 1 \mathrm{H}), 8.10(\mathrm{~d}, J=8.4 \mathrm{~Hz}, 1 \mathrm{H}), 8.06-7.99(\mathrm{~m}, 1 \mathrm{H}), 7.81$ $-7.70(\mathrm{~m}, 2 \mathrm{H}), 7.65-7.57(\mathrm{~m}, 3 \mathrm{H}), 7.43(\mathrm{~d}, J=7.6 \mathrm{~Hz}, 2 \mathrm{H}), 7.33(\mathrm{t}, J=7.6 \mathrm{~Hz}, 2 \mathrm{H})$,
$7.20(\mathrm{t}, J=7.6 \mathrm{~Hz}, 1 \mathrm{H}), 6.40(\mathrm{~d}, J=14.8 \mathrm{~Hz}, 1 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz, DMSO- $d_{6}$ ) $\delta$ $166.6,137.0,133.8,133.7,131.1,130.3,129.2,128.9,127.6,126.9,126.8,126.4,125.8$, 125.7, 125.4, 124.4, 113.5. HRMS (ESI, m/z): Calculated $\mathrm{C}_{19} \mathrm{H}_{15} \mathrm{NO}[\mathrm{M}+\mathrm{H}]^{+}: 274.1232$, found 274.1222.

(E)-N-Styryl-2-naphthamide (22)

Compound 22 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $22(49.2 \mathrm{mg}$, $90 \%$ ) as a white solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz, DMSO- $d_{6}$ ) $\delta 10.84(\mathrm{~d}, J=10.0 \mathrm{~Hz}, 1 \mathrm{H})$, $8.62(\mathrm{~s}, 1 \mathrm{H}), 8.12-8.00(\mathrm{~m}, 4 \mathrm{H}), 7.74(\mathrm{dd}, J=14.4,10.0 \mathrm{~Hz}, 1 \mathrm{H}), 7.69-7.61(\mathrm{~m}, 2 \mathrm{H})$, 7.43 (d, $J=8.0 \mathrm{~Hz}, 2 \mathrm{H}), 7.33(\mathrm{t}, J=8.0 \mathrm{~Hz}, 2 \mathrm{H}), 7.23-7.16(\mathrm{~m}, 1 \mathrm{H}), 6.53(\mathrm{~d}, J=14.8$ $\mathrm{Hz}, 1 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz, DMSO- $d_{6}$ ) $\delta$ 164.6, 137.1, 134.9, 132.6, 131.1, 129.5, 129.2, 128.7, 128.6, 128.5, 128.2, 127.4, 126.8, 125.8, 124.7, 113.5. Spectroscopic data match those previously reported in the literature. ${ }^{[8]}$

(E)-N-(4-Fluorostyryl) benzamide (23)

Compound $\mathbf{2 3}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $23(44.4 \mathrm{mg}$, $92 \%$ ) as a white solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz, DMSO- $d_{6}$ ) $\delta 10.64(\mathrm{~d}, J=10.0 \mathrm{~Hz}, 1 \mathrm{H})$, 7.98 (d, J=7.2 Hz, 2H), 7.66-7.51 (m, 4H), 7.49-7.40 (m, 2H), 7.19-7.09 (m, 2H), $6.48(\mathrm{~d}, J=14.8 \mathrm{~Hz}, 1 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( $\left.100 \mathrm{MHz}, \mathrm{DMSO}-d_{6}\right) \delta 164.5,162.5,160.1\left({ }^{1} J_{\mathrm{C}}-\right.$ $\mathrm{F}=241.6 \mathrm{~Hz}), 133.8,133.6,133.6\left({ }^{3} \mathrm{~J}_{\mathrm{C}-\mathrm{F}}=3.0 \mathrm{~Hz}\right), 132.4,128.9,128.1,127.5,127.4$, $124.6,124.6\left({ }^{4} J_{\mathrm{C}-\mathrm{F}}=1.2 \mathrm{~Hz}\right), 116.1,115.9\left({ }^{2} J_{\mathrm{C}-\mathrm{F}}=21.4 \mathrm{~Hz}\right), 112.4 .{ }^{19} \mathrm{~F}$ NMR ( 375 MHz , DMSO- $d_{6}$ ) $\delta-116.24$. Spectroscopic data match those previously reported in the literature. ${ }^{[9]}$


## (E)-N-(4-Chlorostyryl) benzamide (24)

Compound 24 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $24(46.4 \mathrm{mg}$, $90 \%$ ) as a light pink solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz, DMSO- $d_{6}$ ) $\delta 10.55(\mathrm{~d}, J=10.0 \mathrm{~Hz}, 1 \mathrm{H})$, 7.96 (d, $J=7.6 \mathrm{~Hz}, 2 \mathrm{H}), 7.63-7.48(\mathrm{~m}, 5 \mathrm{H}), 7.39-7.29(\mathrm{~m}, 2 \mathrm{H}), 6.52(\mathrm{~d}, J=14.8 \mathrm{~Hz}$, 1H). ${ }^{13} \mathrm{C}$ NMR (100 MHz, DMSO- $d_{6}$ ) $\delta$ 164.4, 138.9, 133.9, 132.3, 128.9, 128.1, 127.2, $125.2,124.6,120.6,108.7$. Spectroscopic data match those previously reported in the literature. ${ }^{[10]}$

(E)-N-(4-bromostyryl) benzamide (25)

Compound 25 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=5: 1$ ) yielded $25(51.4 \mathrm{mg}, 85 \%)$ as a white solid. ${ }^{1} \mathrm{H}$ NMR ( $400 \mathrm{MHz}, \mathrm{DMSO}-\mathrm{d}_{6}$ ) $\delta 10.70(\mathrm{~d}, \mathrm{~J}=9.6 \mathrm{~Hz}, 1 \mathrm{H}$ ), 7.98 (d, J $=7.2 \mathrm{~Hz}, 2 \mathrm{H}), 7.70(\mathrm{dd}, \mathrm{J}=14.8,9.6 \mathrm{~Hz}, 1 \mathrm{H}), 7.60(\mathrm{t}, \mathrm{J}=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.54(\mathrm{t}, \mathrm{J}=7.6$ $\mathrm{Hz}, 2 \mathrm{H}), 7.49(\mathrm{~d}, \mathrm{~J}=8.4 \mathrm{~Hz}, 2 \mathrm{H}), 7.38(\mathrm{~d}, \mathrm{~J}=8.4 \mathrm{~Hz}, 2 \mathrm{H}), 6.44(\mathrm{~d}, \mathrm{~J}=14.8 \mathrm{~Hz}, 1 \mathrm{H})$. ${ }^{13}$ C NMR ( 100 MHz, DMSO- $d_{6}$ ) $\delta 164.6,136.5,133.7,132.5,132.0,129.0,128.1$, 127.7, 125.5, 119.3, 112.1. Spectroscopic data match those previously reported in the literature. ${ }^{[10]}$

( $E$ )- N -(4-Methoxystyryl) benzamide (26)
Compound 26 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=5: 1$ ) yielded $26(40.5 \mathrm{mg}, 80 \%)$ as a brown solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 8.31(\mathrm{~d}, J=11.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.83$

- 7.68 (m, 2H), $7.56-7.50(\mathrm{~m}, 1 \mathrm{H}), 7.49-7.40(\mathrm{~m}, 2 \mathrm{H}), 7.33-7.22(\mathrm{~m}, 2 \mathrm{H}), 7.13$ (dd, $J=10.8,9.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.01-6.89(\mathrm{~m}, 2 \mathrm{H}), 5.84(\mathrm{~d}, J=9.2 \mathrm{~Hz}, 1 \mathrm{H}), 3.83(\mathrm{~s}, 3 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR (100 MHz, Chloroform-d) $\delta 164.3,158.6,133.5,132.1,129.1,128.9,128.1$, 127.1, 121.4, 114.7, 110.8, 55.4. Spectroscopic data match those previously reported in the literature. ${ }^{[9]}$

(E)-N-(4-Methylstyryl) pivalamide (27)

Compound 27 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $27(39.1 \mathrm{mg}$, $90 \%$ ) as a brown solid. M.p.: $150-153{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 7.55$ - $7.40(\mathrm{~m}, 2 \mathrm{H}), 7.21(\mathrm{~d}, J=8.0 \mathrm{~Hz}, 2 \mathrm{H}), 7.09(\mathrm{~d}, J=8.0 \mathrm{~Hz}, 2 \mathrm{H}), 6.11(\mathrm{~d}, J=14.0 \mathrm{~Hz}$, $1 \mathrm{H}), 2.31(\mathrm{~s}, 3 \mathrm{H}), 1.26(\mathrm{~s}, 9 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform-d) $\delta$ 175.7, 136.3, 133.3, 129.4, 125.4, 122.4, 112.6, 38.8, 27.5, 21.1. HRMS (ESI, m/z): Calculated $\mathrm{C}_{14} \mathrm{H}_{19} \mathrm{NO}[\mathrm{M}+\mathrm{H}]^{+}: 218.1545$, found 218.1555.

( $E$ )-N-(4-ethylstyryl) benzamide (28)
Compound 28 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $28(45.0 \mathrm{mg}$, $90 \%$ ) as a white solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , DMSO- $d_{6}$ ) $\delta 10.59(\mathrm{~d}, \mathrm{~J}=10.0 \mathrm{~Hz}, 1 \mathrm{H}$ ), $7.98(\mathrm{~d}, \mathrm{~J}=7.6 \mathrm{~Hz}, 2 \mathrm{H}), 7.67-7.49(\mathrm{~m}, 4 \mathrm{H}), 7.31(\mathrm{~d}, \mathrm{~J}=8.0 \mathrm{~Hz}, 2 \mathrm{H}), 7.15(\mathrm{~d}, \mathrm{~J}=7.8$ $\mathrm{Hz}, 2 \mathrm{H}), 6.46(\mathrm{~d}, \mathrm{~J}=14.8 \mathrm{~Hz}, 1 \mathrm{H}), 2.58(\mathrm{q}, \mathrm{J}=7.6 \mathrm{~Hz}, 2 \mathrm{H}), 1.17(\mathrm{t}, \mathrm{J}=7.6 \mathrm{~Hz}, 3 \mathrm{H})$. ${ }^{13} \mathrm{C}$ NMR (100 MHz, DMSO- $d_{6}$ ) $\delta 164.4,142.4,134.5,133.9,132.3,128.9,128.6$, 128.1, 125.7, 123.8, 113.4, 28.3, 16.0. Spectroscopic data match those previously reported in the literature. ${ }^{[9]}$


## ( $E$ )- $N$-(3-fluorostyryl) benzamide (29)

Compound 29 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=8: 1$ ) yielded $29(43.9 \mathrm{mg}, 91 \%)$ as a white solid. ${ }^{1} \mathrm{H}$ NMR ( $400 \mathrm{MHz}, \mathrm{DMSO}-d_{6}$ ) $\delta 10.71(\mathrm{~d}, J=10.0 \mathrm{~Hz}, 1 \mathrm{H}), 7.99(\mathrm{~d}$, $J=7.6 \mathrm{~Hz}, 2 \mathrm{H}), 7.73(\mathrm{dd}, J=14.8,10.0 \mathrm{~Hz}, 1 \mathrm{H}), 7.65-7.48(\mathrm{~m}, 3 \mathrm{H}), 7.39-7.18(\mathrm{~m}$, $3 \mathrm{H}), 7.03-6.92(\mathrm{~m}, 1 \mathrm{H}), 6.47(\mathrm{~d}, J=14.8 \mathrm{~Hz}, 1 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz, DMSO- $d_{6}$ ) $\delta$ 164.7, 164.4, 161.9 $\left({ }^{1} J_{\mathrm{C}-\mathrm{F}}=241.2 \mathrm{~Hz}\right), 139.9,139.8,133.7,132.5,131.0,130.9\left({ }^{3} J_{\mathrm{C}-\mathrm{F}}=\right.$ $8.1 \mathrm{~Hz}), 129.0,128.1,126.1,121.9,121.9\left({ }^{4} J_{\mathrm{C}-\mathrm{F}}=2.4 \mathrm{~Hz}\right), 113.3,113.1\left({ }^{2} J_{\mathrm{C}-\mathrm{F}}=21.1 \mathrm{~Hz}\right)$, 112.3, 112.2, 112.0. ${ }^{19}$ F NMR ( 375 MHz, DMSO- $d_{6}$ ) $\delta$-113.40.

(E)-N-(3-Chlorostyryl) pivalamide (30)

Compound $\mathbf{3 0}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1)$ yielded $30(45.2 \mathrm{mg}$, $95 \%$ ) as a yellow solid. M.p.: $126-130^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform-d) $\delta 7.60$ $-7.46(\mathrm{~m}, 2 \mathrm{H}), 7.28-7.24(\mathrm{~m}, 1 \mathrm{H}), 7.21-7.16(\mathrm{~m}, 2 \mathrm{H}), 7.14-7.08(\mathrm{~m}, 1 \mathrm{H}), 6.06(\mathrm{~d}$, $J=14.0 \mathrm{~Hz}, 1 \mathrm{H}$ ), $1.27(\mathrm{~s}, 9 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta 175.9,138.2$, 134.6, 129.9, 126.4, 125.5, 124.4, 123.4, 111.1, 38.9, 27.4. HRMS (ESI, m/z): Calculated $\mathrm{C}_{13} \mathrm{H}_{16} \mathrm{NO}^{35} \mathrm{Cl}[\mathrm{M}+\mathrm{H}]^{+}: 238.0999$, found 238.1001.

(E)-N-(2-fluorostyryl) pivalamide (31)

Compound $\mathbf{3 1}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=8: 1$ ) yielded $31(35.4 \mathrm{mg}, 80 \%)$ as a white solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 7.84-7.70(\mathrm{~m}, 2 \mathrm{H}), 7.60(\mathrm{t}, J=$ $7.6 \mathrm{~Hz}, 1 \mathrm{H}), 7.36-7.28(\mathrm{~m}, 1 \mathrm{H}), 7.27-7.15(\mathrm{~m}, 2 \mathrm{H}), 6.45(\mathrm{~d}, J=14.0 \mathrm{~Hz}, 1 \mathrm{H}), 1.46$ (s, 9H). ${ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta 175.8,160.9,158.4(\mathrm{~J}=246.3 \mathrm{~Hz}), 127.7$, $127.6(J=8.0 \mathrm{~Hz}), 126.3,126.2(J=3.0 \mathrm{~Hz}), 125.1,125.0(J=5.0 \mathrm{~Hz}), 124.2,124.2$
$(J=3.0 \mathrm{~Hz}), 124.1,124.0(J=13.0 \mathrm{~Hz}), 115.7,115.5(J=8.0 \mathrm{~Hz}), 104.9,104.9(J=$ 7.0 Hz ), 38.9, 27.4. ${ }^{19}$ F NMR ( 375 MHz , Chloroform- $d$ ) $\delta-118.55$.

(E)-N-(2-Chlorostyryl) benzamide (32)

Compound $\mathbf{3 2}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $32(44.8 \mathrm{mg}$, $87 \%$ ) as a brown solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 8.44(\mathrm{~d}, J=11.2 \mathrm{~Hz}, 1 \mathrm{H}$ ), $7.94-7.81(\mathrm{~m}, 2 \mathrm{H}), 7.78-7.68(\mathrm{~m}, 1 \mathrm{H}), 7.58-7.40(\mathrm{~m}, 4 \mathrm{H}), 7.36-7.28(\mathrm{~m}, 1 \mathrm{H})$, $7.22-7.06(\mathrm{~m}, 2 \mathrm{H}), 6.68(\mathrm{~d}, J=14.4 \mathrm{~Hz}, 1 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta$ $164.8,134.1,133.2,132.4,132.3,129.7,128.8,127.8,127.3,127.0,125.8,125.1,109.8$. Spectroscopic data match those previously reported in the literature. ${ }^{[1]}$

(E)-N-(2-(Thiophen-3-yl)vinyl) benzamide (33)

Compound $\mathbf{3 3}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $33(43.1 \mathrm{mg}$, $94 \%)$ as white solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz, DMSO- $d_{6}$ ) $\delta 10.54(\mathrm{~d}, J=10.0 \mathrm{~Hz}, 1 \mathrm{H}), 7.96$ (d, $J=7.2 \mathrm{~Hz}, 2 \mathrm{H}), 7.62-7.49(\mathrm{~m}, 5 \mathrm{H}), 7.40-7.29(\mathrm{~m}, 2 \mathrm{H}), 6.52(\mathrm{~d}, J=14.4 \mathrm{~Hz}, 1 \mathrm{H})$. ${ }^{13} \mathrm{C}$ NMR ( 100 MHz, DMSO- $d_{6}$ ) $\delta$ 164.4, 138.9, 133.9, 132.3, 128.9, 128.1, 127.2, $125.2,124.6,120.6,108.7$. Spectroscopic data match those previously reported in the literature. ${ }^{[11]}$

(E)-N-(2-(Naphthalen-2-yl)vinyl) benzamide (34)

Compound $\mathbf{3 4}$ was prepared following the general procedure, purification by column
chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $34(48.6 \mathrm{mg}$, $89 \%$ ) as a pale yellow solid. M.p.: $183-184^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , DMSO- $d_{6}$ ) $\delta$ $10.77(\mathrm{~d}, J=9.6 \mathrm{~Hz}, 1 \mathrm{H}), 8.02(\mathrm{~d}, J=8.4 \mathrm{~Hz}, 2 \mathrm{H}), 7.90-7.79(\mathrm{~m}, 5 \mathrm{H}), 7.69(\mathrm{~d}, J=$ $8.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.64-7.52(\mathrm{~m}, 3 \mathrm{H}), 7.51-7.40(\mathrm{~m}, 2 \mathrm{H}), 6.66(\mathrm{~d}, J=14.8 \mathrm{~Hz}, 1 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR (10 MHz, DMSO- $d_{6}$ ) $\delta 164.6,134.7,134.0,133.8,132.4,132.3,129.0,128.7$, $128.2,128.0,128.0,126.8,125.8,125.2,124.7,123.6,113.5$. HRMS (ESI, m/z): Calculated $\mathrm{C}_{19} \mathrm{H}_{15} \mathrm{NO}[\mathrm{M}+\mathrm{Na}]^{+}: 296.1051$, found 296.1050.

(E)-N-(4-Phenylbut-1-en-1-yl) pivalamide (35)

Compound 35 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $35(33.8 \mathrm{mg}$, $73 \%$ ) as a white solid. M.p.: $127-128{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform-d) $\delta 7.35$ - $7.29(\mathrm{~m}, 2 \mathrm{H}), 7.25-7.19(\mathrm{~m}, 3 \mathrm{H}), 7.14(\mathrm{~d}, J=10.4 \mathrm{~Hz}, 1 \mathrm{H}), 6.93-6.79(\mathrm{~m}, 1 \mathrm{H}), 5.20$ (dt, $J=14.4,6.8 \mathrm{~Hz}, 1 \mathrm{H}), 2.78-2.68(\mathrm{t}, J=8.0 \mathrm{~Hz}, 2 \mathrm{H}), 2.47-2.33(\mathrm{~m}, 2 \mathrm{H}), 1.25(\mathrm{~s}$, 9H). ${ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta$ 175.5, 141.6, 128.4, 128.4, 125.9, 123.4, 111.9, 38.6, 36.4, 31.6, 27.4. HRMS (ESI, m/z): Calculated $\mathrm{C}_{15} \mathrm{H}_{21} \mathrm{NO}[\mathrm{M}+\mathrm{Na}]^{+}$: 254.1521, found 254.1516 .


## ( $\boldsymbol{E}$ )-N-(5-Phenylpent-1-en-1-yl) pivalamide (36)

Compound 36 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=15: 1$ ) yielded $36(24.5 \mathrm{mg}$, $50 \%)$ as a white solid. M.p.: $88-89^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 7.28(\mathrm{~d}$, $J=2.0 \mathrm{~Hz}, 1 \mathrm{H}), 7.25-7.22(\mathrm{~m}, 1 \mathrm{H}), 7.19-7.11(\mathrm{~m}, 4 \mathrm{H}), 6.78(\mathrm{dd}, J=14.0,10.4 \mathrm{~Hz}$, $1 \mathrm{H}), 5.17(\mathrm{dt}, J=14.0,7.2 \mathrm{~Hz}, 1 \mathrm{H}), 2.60(\mathrm{t}, J=7.6 \mathrm{~Hz}, 2 \mathrm{H}), 2.05(\mathrm{q}, J=6.8 \mathrm{~Hz}, 2 \mathrm{H})$, $1.68(\mathrm{p}, J=7.6 \mathrm{~Hz}, 2 \mathrm{H}), 1.21(\mathrm{~s}, 9 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta 175.5$, $142.3,128.5,128.3,125.7,123.3,112.5,38.6,35.3,31.6,29.4,27.5$.

tert-Butyl (S, E)-(3-methyl-1-oxo-1-(styrylamino)butan-2-yl)carbamate (37)
Compound 37 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=8: 1)$ yielded $37(59.9 \mathrm{mg}, 94 \%)$ as a white solid. M.p.: $156-157{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR $(400 \mathrm{MHz}$, Chloroform- $d) \delta 8.81(\mathrm{~d}, J=$ $8.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.43(\mathrm{dd}, J=14.8,10.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.25-7.16(\mathrm{~m}, 4 \mathrm{H}), 7.15-7.08(\mathrm{~m}, 1 \mathrm{H})$, $6.11(\mathrm{~d}, J=14.8 \mathrm{~Hz}, 1 \mathrm{H}), 5.42(\mathrm{~d}, J=8.8 \mathrm{~Hz}, 1 \mathrm{H}), 4.07(\mathrm{t}, J=8.0 \mathrm{~Hz}, 1 \mathrm{H}), 2.20-2.07$ $(\mathrm{m}, 1 \mathrm{H}), 1.47(\mathrm{~s}, 9 \mathrm{H}), 1.01(\mathrm{~d}, J=6.8 \mathrm{~Hz}, 6 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR (100 MHz, Chloroform-d) $\delta$ $169.8,156.4,136.1,128.6,126.6,125.6,122.4,113.8,60.4,30.8,28.4,19.3,18.4$. HRMS (ESI, m/z): Calculated $\mathrm{C}_{18} \mathrm{H}_{26} \mathrm{~N}_{2} \mathrm{O}_{3}[\mathrm{M}+\mathrm{Na}]^{+}: 341.1841$, found 341.1840.

tert-Butyl (R, E)-(3,3-dimethyl-1-oxo-1-(styrylamino)butan-2-yl)carbamate (38)
Compound 38 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=8: 1)$ yielded $\mathbf{3 8}(63.2 \mathrm{mg}, 95 \%)$ as a yellow liquid. ${ }^{1} \mathrm{H}$ NMR $(400 \mathrm{MHz}$, Chloroform- $d) \delta 9.02(\mathrm{~d}, J=10.4 \mathrm{~Hz}, 1 \mathrm{H}), 7.39$ $(\mathrm{dd}, J=14.4,10.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.15(\mathrm{~d}, J=4.0 \mathrm{~Hz}, 4 \mathrm{H}), 7.09(\mathrm{~m}, 1 \mathrm{H}), 6.06(\mathrm{~d}, J=14.8$ $\mathrm{Hz}, 1 \mathrm{H}), 5.63(\mathrm{~d}, J=9.2 \mathrm{~Hz}, 1 \mathrm{H}), 4.09(\mathrm{~d}, J=9.2 \mathrm{~Hz}, 1 \mathrm{H}), 1.46(\mathrm{~s}, 9 \mathrm{H}), 1.07(\mathrm{~s}, 9 \mathrm{H})$. ${ }^{13} \mathrm{C}$ NMR (100 MHz, Chloroform-d) $\delta 169.3,156.6,136.2,128.5,126.4,125.6,122.4$, 113.8, 62.7, 34.4, 28.5, 26.6.

tert-Butyl $\quad(R, \quad E)$-(3,3-dimethyl-1-((4-methylstyryl)amino)-1-oxobutan-2-yl)
carbamate (39)
Compound 39 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $39(61.0 \mathrm{mg}$, $88 \%$ ) as a white solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 8.99(\mathrm{~d}, J=9.6 \mathrm{~Hz}, 1 \mathrm{H}$ ), $7.43-7.31(\mathrm{~m}, 1 \mathrm{H}), 7.10-6.89(\mathrm{~m}, 4 \mathrm{H}), 6.04(\mathrm{~d}, J=14.8 \mathrm{~Hz}, 1 \mathrm{H}), 5.67(\mathrm{~d}, J=8.0 \mathrm{~Hz}$, $1 \mathrm{H}), 4.10(\mathrm{~d}, J=9.2 \mathrm{~Hz}, 1 \mathrm{H}), 2.26(\mathrm{~s}, 3 \mathrm{H}), 1.45(\mathrm{~s}, 9 \mathrm{H}), 1.07(\mathrm{~s}, 9 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR (100 MHz , Chloroform- $d$ ) $\delta 169.2,156.5,136.0,133.3,129.2,125.5,121.6,113.9,62.6$, 34.4, 28.5, 26.7, 21.1.

tert-Butyl (R, E)-(3, 3-dimethyl-1-((3-methylstyryl)amino)-1-oxobutan-2-yl)
carbamate (40)
Compound $\mathbf{4 0}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1)$ yielded $40(62.4 \mathrm{mg}$, $90 \%$ ) as a white solid. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 9.19$ (d, $J=9.6 \mathrm{~Hz}, 1 \mathrm{H}$ ), $7.51-7.37(\mathrm{~m}, 1 \mathrm{H}), 7.09-6.88(\mathrm{~m}, 4 \mathrm{H}), 6.07(\mathrm{~d}, J=14.8 \mathrm{~Hz}, 1 \mathrm{H}), 5.74(\mathrm{~d}, J=9.2 \mathrm{~Hz}$, $1 \mathrm{H}), 4.16(\mathrm{~d}, J=6.8 \mathrm{~Hz}, 1 \mathrm{H}), 2.18(\mathrm{~s}, 3 \mathrm{H}), 1.50(\mathrm{~s}, 9 \mathrm{H}), 1.11(\mathrm{~s}, 9 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR (100 MHz , Chloroform- $d$ ) $\delta 169.3,156.6,137.9,136.1,128.3,127.2,126.2,122.8,122.2$, 113.9, 62.7, 34.4, 28.5, 26.7, 21.3.

tert-Butyl (S, E)-(1-oxo-1-(styrylamino)pentan-2-yl)carbamate (41)
Compound $\mathbf{4 1}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $41(58.6 \mathrm{mg}$, $92 \%$ ) as a white solid. M.p.: $140-141{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 8.78$
(d, $J=8.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.43(\mathrm{dd}, J=12.0,11.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.26-7.19(\mathrm{~m}, 4 \mathrm{H}), 7.17-7.11$ $(\mathrm{m}, 1 \mathrm{H}), 6.12(\mathrm{~d}, J=14.4 \mathrm{~Hz}, 1 \mathrm{H}), 5.28(\mathrm{~d}, J=8.0 \mathrm{~Hz}, 1 \mathrm{H}), 4.30-4.17(\mathrm{~m}, 1 \mathrm{H}), 1.87$ $-1.77(\mathrm{~m}, 1 \mathrm{H}), 1.69-1.58(\mathrm{~m}, 1 \mathrm{H}), 1.47(\mathrm{~s}, 9 \mathrm{H}), 1.44-1.36(\mathrm{~m}, 2 \mathrm{H}), 0.94(\mathrm{t}, J=7.2$ $\mathrm{Hz}, 3 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform-d) $\delta 170.2,156.2,136.1,128.6,126.6,125.6$, 122.5, 113.7, 54.5, 34.3, 28.4, 19.0, 13.7. HRMS (ESI, m/z): Calculated $\mathrm{C}_{18} \mathrm{H}_{26} \mathrm{~N}_{2} \mathrm{O}_{3}$ $[\mathrm{M}+\mathrm{Na}]^{+}: 341.1841$, found 341.1843 .

tert-Butyl (S, E)-(2-oxo-1-phenyl-2-(styrylamino)ethyl)carbamate (42)
Compound $\mathbf{4 2}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=8: 1$ ) yielded $42(63.4 \mathrm{mg}, 90 \%)$ as a white solid. M.p.: $164-166{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform-d) $\delta 8.09(\mathrm{~s}, 1 \mathrm{H})$, $7.44-7.32(\mathrm{~m}, 6 \mathrm{H}), 7.27-7.21(\mathrm{~m}, 4 \mathrm{H}), 7.18-7.12(\mathrm{~m}, 1 \mathrm{H}), 6.03(\mathrm{~d}, J=14.8 \mathrm{~Hz}$, $1 \mathrm{H}), 5.83(\mathrm{~s}, 1 \mathrm{H}), 5.33(\mathrm{~s}, 1 \mathrm{H}), 1.44(\mathrm{~s}, 9 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta$ 167.8, 137.3, 135.8, 129.2, 128.7, 128.6, 127.4, 126.8, 125.6, 122.2, 114.1, 28.3. HRMS (ESI, m/z): Calculated $\mathrm{C}_{21} \mathrm{H}_{24} \mathrm{~N}_{2} \mathrm{O}_{3}[\mathrm{M}+\mathrm{Na}]^{+}: 375.1685$, found 375.1683.

tert-Butyl ((2S,3S)-3-methyl-1-oxo-1-(((E)-styryl)amino)pentan-2-yl)carbamate (43)

Compound $\mathbf{4 3}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $43(60.5 \mathrm{mg}$, $91 \%$ ) as a white solid. M.p.: $140-141{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz, DMSO- $d_{6}$ ) $\delta 10.24$ (d, $J=9.6 \mathrm{~Hz}, 1 \mathrm{H}), 7.46-7.32(\mathrm{~m}, 3 \mathrm{H}), 7.28(\mathrm{t}, J=7.6 \mathrm{~Hz}, 2 \mathrm{H}), 7.15(\mathrm{t}, J=7.2 \mathrm{~Hz}, 1 \mathrm{H})$, $6.95(\mathrm{~d}, J=8.4 \mathrm{~Hz}, 1 \mathrm{H}), 6.22(\mathrm{~d}, J=14.7 \mathrm{~Hz}, 1 \mathrm{H}), 3.87(\mathrm{t}, J=8.0 \mathrm{~Hz}, 1 \mathrm{H}), 1.80-1.66$ $(\mathrm{m}, 1 \mathrm{H}), 1.52-1.42(\mathrm{~m}, 1 \mathrm{H}), 1.39(\mathrm{~s}, 9 \mathrm{H}), 1.23-1.07(\mathrm{~m}, 1 \mathrm{H}), 0.89-0.78(\mathrm{~m}, 6 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR (100 MHz, DMSO- $d_{6}$ ) $\delta 170.5,155.9,136.9,129.1,126.6,125.6,123.8,112.5$,
78.5, 59.4, 36.6, 28.7, 25.1, 15.8, 11.3. HRMS (ESI, m/z): Calculated $\mathrm{C}_{19} \mathrm{H}_{28} \mathrm{~N}_{2} \mathrm{O}_{3}$ $[\mathrm{M}+\mathrm{H}]^{+}: 333.2178$, found 333.2147.

tert-Butyl (S, E)-(1-cyclopropyl-2-oxo-2-(styrylamino)ethyl)carbamate (44)
Compound 44 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=8: 1$ ) yielded $44(55.7 \mathrm{mg}, 88 \%)$ a white solid. M.p.: $150-151{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform-d) $\delta 8.69(\mathrm{~d}, J=$ $12.0 \mathrm{~Hz}, 1 \mathrm{H}), 7.49-7.38(\mathrm{~m}, 1 \mathrm{H}), 7.29-7.19(\mathrm{~m}, 4 \mathrm{H}), 7.18-7.12(\mathrm{~m}, 1 \mathrm{H}), 6.12$ (d, J $=14.4 \mathrm{~Hz}, 1 \mathrm{H}), 5.23(\mathrm{~d}, J=8.0 \mathrm{~Hz}, 1 \mathrm{H}), 4.21(\mathrm{~s}, 1 \mathrm{H}), 1.90-1.78(\mathrm{~m}, 2 \mathrm{H}), 1.69-1.58$ $(\mathrm{m}, 1 \mathrm{H}), 1.47(\mathrm{~s}, 9 \mathrm{H}), 1.44-1.35(\mathrm{~m}, 2 \mathrm{H}), 0.95(\mathrm{t}, J=7.6 \mathrm{~Hz}, 3 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR (100 MHz , Chloroform- $d$ ) $\delta 170.2,136.1,128.6,126.6,125.6,122.5,113.7,54.5,34.3,28.3$, 19.0, 13.7. HRMS (ESI, m/z): Calculated $\mathrm{C}_{18} \mathrm{H}_{24} \mathrm{~N}_{2} \mathrm{O}_{3}[\mathrm{M}+\mathrm{Na}]^{+}: 339.1685$, found 339.1682.

tert-Butyl (S, E)-(1-oxo-1-(styrylamino)pent-4-en-2-yl)carbamate (45)
Compound $\mathbf{4 5}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $45(59.5 \mathrm{mg}$, $94 \%)$ as a white solid. M.p.: $143-144{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform-d) $\delta 8.42$ $(\mathrm{s}, 1 \mathrm{H}), 7.44(\mathrm{dd}, J=14.4,10.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.31-7.22(\mathrm{~m}, 4 \mathrm{H}), 7.20-7.14(\mathrm{~m}, 1 \mathrm{H}), 6.13$ $(\mathrm{d}, J=14.4 \mathrm{~Hz}, 1 \mathrm{H}), 5.85-5.71(\mathrm{~m}, 1 \mathrm{H}), 5.22-5.15(\mathrm{~m}, 2 \mathrm{H}), 5.09(\mathrm{~s}, 1 \mathrm{H}), 4.27(\mathrm{~s}$, 1H), $2.63-2.45(\mathrm{~m}, 2 \mathrm{H}), 1.47(\mathrm{~s}, 9 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform-d) $\delta 169.6$, 156.2, 136.1, 132.8, 128.6, 126.6, 125.6, 122.4, 119.2, 114.0, 54.1, 36.8, 28.4. HRMS (ESI, m/z): Calculated $\mathrm{C}_{18} \mathrm{H}_{24} \mathrm{~N}_{2} \mathrm{O}_{3}[\mathrm{M}+\mathrm{Na}]^{+}: 339.1685$, found 339.1683.

tert-Butyl (S, E)-(1-oxo-3-phenyl-1-(styrylamino)propan-2-yl)carbamate (46)
Compound 46 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $46(70.4 \mathrm{mg}$, $96 \%$ ) as a yellow solid. M.p.: $156-157{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform-d) $\delta 8.42$ $(\mathrm{s}, 1 \mathrm{H}), 7.40(\mathrm{dd}, J=14.8,10.4 \mathrm{~Hz}, 1 \mathrm{H}), 7.30-7.17(\mathrm{~m}, 10 \mathrm{H}), 5.99(\mathrm{~d}, J=14.4 \mathrm{~Hz}$, $1 \mathrm{H}), 5.36(\mathrm{~d}, J=8.4 \mathrm{~Hz}, 1 \mathrm{H}), 4.52(\mathrm{~s}, 1 \mathrm{H}), 3.19-2.94(\mathrm{~m}, 2 \mathrm{H}), 1.41(\mathrm{~s}, 9 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR (100 MHz, Chloroform-d) $\delta 169.2,155.9,136.5,136.0,129.3,128.7,128.6,127.1$, $126.7,125.6,122.2,114.1,56.0,38.6,28.3$. HRMS (ESI, m/z): Calculated $\mathrm{C}_{22} \mathrm{H}_{26} \mathrm{~N}_{2} \mathrm{O}_{3}$ $[\mathrm{M}+\mathrm{Na}]^{+}: 389.1841$, found 389.1838.

tert-Butyl (S, E)-(4-methyl-1-oxo-1-(styrylamino)pentan-2-yl)carbamate (47)
Compound 47 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $47(46.5 \mathrm{mg}$, $70 \%$ ) as a white solid. M.p.: $135-137{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR (400 MHz, Chloroform-d) $\delta 9.27$ $(\mathrm{d}, J=9.6 \mathrm{~Hz}, 1 \mathrm{H}), 7.45(\mathrm{dd}, J=14.0,10.4 \mathrm{~Hz} 1 \mathrm{H}), 7.27-7.09(\mathrm{~m}, 5 \mathrm{H}), 6.15(\mathrm{~d}, J=$ $14.4 \mathrm{~Hz}, 1 \mathrm{H}), 5.52(\mathrm{~d}, J=8.0 \mathrm{~Hz}, 1 \mathrm{H}), 4.38(\mathrm{dd}, J=15.6,8.0 \mathrm{~Hz}, 1 \mathrm{H}), 1.83-1.73(\mathrm{~m}$, $1 \mathrm{H}), 1.72-1.61(\mathrm{~m}, 2 \mathrm{H}), 1.49(\mathrm{~s}, 9 \mathrm{H}), 0.99(\mathrm{dd}, J=9.2,6.4 \mathrm{~Hz}, 6 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR (100 MHz, Chloroform-d) $\delta 170.9,156.4,136.2,128.6,126.5,125.6,122.7,113.9,53.3$, $41.2,28.4,24.8,23.0,21.9$. HRMS (ESI, m/z): Calculated $\mathrm{C}_{19} \mathrm{H}_{28} \mathrm{~N}_{2} \mathrm{O}_{3}[\mathrm{M}+\mathrm{Na}]^{+}$: 355.1998, found 355.1993.

tert-Butyl ( $R, E$ )-(4-(methylthio)-1-oxo-1-(styrylamino)butan-2-yl)carbamate (48) Compound 48 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $48(59.9 \mathrm{mg}$, $89 \%$ ) as a pale-yellow solid. M.p.: $104-106{ }^{\circ}$ C. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform-d) $\delta$ 8.91 (d, $J=9.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.47$ (dd, $J=14.4,10.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.30-7.22$ (m, 4H), $7.21-$ $7.15(\mathrm{~m}, 1 \mathrm{H}), 6.19(\mathrm{~d}, J=14.8 \mathrm{~Hz}, 1 \mathrm{H}), 5.58(\mathrm{~d}, J=8.0 \mathrm{~Hz}, 1 \mathrm{H}), 4.48(\mathrm{~d}, J=8.0 \mathrm{~Hz}$, $1 \mathrm{H}), 2.63(\mathrm{t}, J=7.2 \mathrm{~Hz}, 2 \mathrm{H}), 2.20(\mathrm{~m}, 1 \mathrm{H}), 2.13(\mathrm{~s}, 3 \mathrm{H}), 2.03(\mathrm{~m}, 1 \mathrm{H}), 1.49(\mathrm{~s}, 9 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR (100 MHz, Chloroform-d) $\delta 169.6,156.2,135.9,128.6,126.7,125.6,122.3$, 114.1, 53.6, 31.5, 30.3, 28.4, 15.4. HRMS (ESI, m/z): Calculated $\mathrm{C}_{18} \mathrm{H}_{26} \mathrm{~N}_{2} \mathrm{O}_{3} \mathrm{~S}$ $[\mathrm{M}+\mathrm{Na}]^{+}: 373.1562$, found 373.1558 .

$N$-((E)-Styryl) cinnamamide (49)
Compound 49 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1)$ yielded $49(44.9 \mathrm{mg}$, $90 \%$ ) as a yellow solid. ${ }^{1} \mathrm{H}$ NMR ( $400 \mathrm{MHz}, \mathrm{DMSO}-d_{6}$ ) $\delta 10.50(\mathrm{~d}, J=10.0 \mathrm{~Hz}, 1 \mathrm{H})$, $7.68-7.53(\mathrm{~m}, 4 \mathrm{H}), 7.37-7.48(\mathrm{~m}, 5 \mathrm{H}), 7.30(\mathrm{t}, J=7.6 \mathrm{~Hz}, 2 \mathrm{H}), 7.17(\mathrm{t}, J=7.6 \mathrm{~Hz}$, $1 \mathrm{H}), 6.73(\mathrm{~d}, J=16.0 \mathrm{~Hz}, 1 \mathrm{H}), 6.26(\mathrm{~d}, J=14.8 \mathrm{~Hz}, 1 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , DMSO$\left.d_{6}\right) \delta 163.1,141.1,137.0,135.1,130.4,129.5,129.2,128.3,126.7,125.7,124.2,121.3$, 112.7. Spectroscopic data match those previously reported in the literature. ${ }^{[12]}$

(E)-2-(4-Isobutylphenyl)- $N$-styrylpropanamide (50)

Compound $\mathbf{5 0}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) yielded $50(43.0 \mathrm{mg}$, $70 \%$ ) as a white solid. M.p.: $136-139{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform-d) $\delta 7.49$ (dd, $J=14.8,10.4 \mathrm{~Hz}, 1 \mathrm{H}), 7.32(\mathrm{~d}, J=10.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.26-7.19(\mathrm{~m}, 6 \mathrm{H}), 7.14(\mathrm{~d}, J=$
$7.6 \mathrm{~Hz}, 3 \mathrm{H}), 5.95(\mathrm{~d}, J=14.8 \mathrm{~Hz}, 1 \mathrm{H}), 3.63(\mathrm{q}, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 2.46(\mathrm{~d}, J=7.2 \mathrm{~Hz}$, $2 \mathrm{H}), 1.93-1.80(\mathrm{~m}, 1 \mathrm{H}), 1.55(\mathrm{~d}, J=7.2 \mathrm{~Hz}, 3 \mathrm{H}), 0.90(\mathrm{~d}, J=6.6 \mathrm{~Hz}, 6 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR (100 MHz, Chloroform-d) $\delta 171.9,141.2,137.7,136.1,129.9,128.7,127.5,126.6$, 125.5, 122.8, 112.8, 46.8, 45.0, 30.2, 22.4, 18.5. HRMS (ESI, m/z): Calculated $\mathrm{C}_{21} \mathrm{H}_{25} \mathrm{NO}[\mathrm{M}+\mathrm{H}]^{+}: 308.2014$, found 308.2010.

(E)-2-(4-(4-Chlorobenzoyl)phenoxy)-2-methyl- $N$-styrylpropanamide (51)

Compound $\mathbf{5 1}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $51(67.2 \mathrm{mg}$, $80 \%$ ) as a yellow solid. M.p.: $128-131{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 8.95$ $(\mathrm{d}, J=10.4 \mathrm{~Hz}, 1 \mathrm{H}), 7.72(\mathrm{~d}, J=8.4 \mathrm{~Hz}, 2 \mathrm{H}), 7.66(\mathrm{~d}, J=8.4 \mathrm{~Hz}, 2 \mathrm{H}), 7.58(\mathrm{dd}, J=$ $14.8,10.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.40(\mathrm{~d}, J=8.8 \mathrm{~Hz}, 2 \mathrm{H}), 7.29-7.18(\mathrm{~m}, 4 \mathrm{H}), 7.15-7.09(\mathrm{~m}, 1 \mathrm{H})$, $7.00(\mathrm{~d}, J=8.8 \mathrm{~Hz}, 2 \mathrm{H}), 6.27(\mathrm{~d}, J=14.4 \mathrm{~Hz}, 1 \mathrm{H}), 1.66(\mathrm{~s}, 6 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform-d) $\delta 194.1,171.8,158.5,138.6,136.0,132.0,131.7,131.2,128.7,128.6$, 126.8, 125.6, 122.3, 119.8, 114.4, 81.8, 25.1. HRMS (ESI, m/z): Calculated $\mathrm{C}_{25} \mathrm{H}_{22} \mathrm{NO}_{3}{ }^{35} \mathrm{Cl} \quad[\mathrm{M}+\mathrm{Na}]^{+}: \quad 442.1186$, found 442.1186 .

( $\boldsymbol{E}$ )-5-(2,5-Dimethylphenoxy)-2,2-dimethyl- $N$-styrylpentanamide (52)
Compound 52 was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=10: 1$ ) yielded $52(40.1 \mathrm{mg}$, $57 \%$ ) as a pale-yellow solid. M.p.: $90-92{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform-d) $\delta$ 7.55 (d, $J=9.2 \mathrm{~Hz}, 2 \mathrm{H}), 7.31-7.22(\mathrm{~m}, 4 \mathrm{H}), 7.18-7.12(\mathrm{~m}, 1 \mathrm{H}), 6.99(\mathrm{~d}, J=7.2 \mathrm{~Hz}$, $1 \mathrm{H}), 6.65(\mathrm{~d}, J=7.6 \mathrm{~Hz}, 1 \mathrm{H}), 6.60(\mathrm{~s}, 1 \mathrm{H}), 6.14-6.06(\mathrm{~m}, 1 \mathrm{H}), 3.91(\mathrm{~s}, 2 \mathrm{H}), 2.28(\mathrm{~s}$, 3 H ), $2.18(\mathrm{~s}, 3 \mathrm{H}), 1.77(\mathrm{~s}, 4 \mathrm{H}), 1.28(\mathrm{~s}, 6 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta$ $175.0,156.9,136.6,136.2,130.4,128.7,126.6,125.6,123.5,123.1,120.9,112.8,112.2$,
67.8, 42.2, 37.5, 25.5, 25.1, 21.5, 15.9. HRMS (ESI, m/z): Calculated $\mathrm{C}_{23} \mathrm{H}_{29} \mathrm{NO}_{2}$ $[\mathrm{M}+\mathrm{H}]^{+}: 352.2277$, found 352.2274.


## ( $\boldsymbol{E}$ )-3-(4,5-Diphenyloxazol-2-yl)- $N$-styrylpropanamide (53)

Compound $\mathbf{5 3}$ was prepared following the general procedure, purification by column chromatography on silica gel (petroleum ether/EtOAc $=8: 1$ ) yielded $53(45.0 \mathrm{mg}, 60 \%)$ as a white solid. M.p.: $151-152{ }^{\circ} \mathrm{C} .{ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform- $d$ ) $\delta 8.80(\mathrm{~d}, \mathrm{~J}=$ $10.4 \mathrm{~Hz}, 1 \mathrm{H}), 7.66-7.61(\mathrm{~m}, 2 \mathrm{H}), 7.58-7.49(\mathrm{~m}, 3 \mathrm{H}), 7.40-7.31(\mathrm{~m}, 6 \mathrm{H}), 7.27-$ 7.22 (m, 4H), 7.18 - 7.11 (m, 1H), 6.05 (d, $J=14.8 \mathrm{~Hz}, 1 \mathrm{H}), 3.23(\mathrm{t}, J=6.8 \mathrm{~Hz}, 2 \mathrm{H})$, $2.86(\mathrm{t}, J=6.8 \mathrm{~Hz}, 2 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta$ 169.0, 162.4, 145.7, $136.1,134.8,132.2,128.7,128.7,128.3,127.9,126.6,126.5,125.6,122.8,112.9,33.0$, 23.9. HRMS (ESI, m/z): Calculated $\mathrm{C}_{26} \mathrm{H}_{22} \mathrm{~N}_{2} \mathrm{O}_{2}[\mathrm{M}+\mathrm{Na}]^{+}: 417.1579$, found 417.1575 .

## Mechanistic Studies

(a) Influence of the concentration of $\mathrm{CO}_{2}$ atmosphere on reaction yield


The reaction was carried out in an undivided cell with magnesium plates electrodes ( 0.1 $\mathrm{mm} \times 10.0 \mathrm{~mm} \times 20.0 \mathrm{~mm})$ and platinum electrodes $(0.25 \mathrm{~mm} \times 10 \mathrm{~mm} \times 15 \mathrm{~mm})$. To a 15.0 mL oven-dried undivided cell equipped with a magnetic bar was added substrates $Z$-enamide $6 \mathbf{a}$ ( $0.2 \mathrm{mmol}, 1.0$ equiv.), $\mathrm{Cs}_{2} \mathrm{CO}_{3}$ ( $0.2 \mathrm{mmol}, 1.0$ equiv.), TBABF 4 ( 0.2 mmol, 1.0 equiv.). Then the tube was evacuated and back-filled under $\mathrm{CO}_{2}$ ( $\mathrm{V} \% \mathrm{in} \mathrm{Ar}$ ) flow (this procedure was repeated three times), and anhydrous DMF ( 4.0 mL ) was added via a syringe. The electrocatalysis was performed under $\mathrm{CO}_{2}(\mathrm{~V} \%$ in Ar$)$ balloon at $60^{\circ} \mathrm{C}$ with a constant current of 5.0 mA maintained for 2 h . After that, the reaction mixture was acidized with HCl aqueous ( $1.0 \mathrm{~N}, 5 \mathrm{~mL}$ ). The aqueous layer was extracted with EtOAc $(2 \times 10 \mathrm{~mL})$ and the combined organic phase was washed with brine, dried
by anhydrous $\mathrm{MgSO}_{4}$, filtered, and concentrated under vacuo. The residue was detected by ${ }^{1}$ HNMR ( 0.2 mmol of dibromomethane was added as an internal standard) and the ${ }^{1} \mathrm{HNMR}$ yields were reported.

## (b) Monitoring the reaction process of 2



| Time $/ \mathrm{min}$ | 20 | 40 | 60 | 80 | 100 | 120 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{2}$ | 17 | 22 | 72 | 88 | 91 | 92 |
| $\mathbf{2 a}$ | 65 | 63 | 13 | 3 | 2 | 1 |



The reaction was carried out in six undivided cells with magnesium plates electrodes $(0.1 \mathrm{~mm} \times 10.0 \mathrm{~mm} \times 20.0 \mathrm{~mm})$ and platinum electrodes $(0.25 \mathrm{~mm} \times 10 \mathrm{~mm} \times 15 \mathrm{~mm})$, respectively. To six 15.0 mL oven-dried undivided cells equipped with magnetic bars were added substrates $Z$-enamide 2a ( 0.2 mmol , 1.0 equiv.), $\mathrm{Cs}_{2} \mathrm{CO}_{3}(0.2 \mathrm{mmol}, 1.0$ equiv.), $\mathrm{TBABF}_{4}$ ( $0.2 \mathrm{mmol}, 1.0$ equiv.), parallelly. Then the tubes were evacuated and back-filled under $\mathrm{CO}_{2}$ flow (this procedure was repeated three times), and anhydrous

DMF ( 4.0 mL ) was added via a syringe. The electrocatalysis were performed under $\mathrm{CO}_{2}$ balloon at $60{ }^{\circ} \mathrm{C}$ with a constant current of 5.0 mA . Six tubes maintained for incremental time, respectively. After that, every reaction mixture was acidized with HCl aqueous ( $1.0 \mathrm{~N}, 5 \mathrm{~mL}$ ). The aqueous layer was extracted with $\mathrm{EtOAc}(2 \times 10 \mathrm{~mL})$ and the combined organic phase was washed with brine, dried by anhydrous $\mathrm{MgSO}_{4}$, filtered, and concentrated under vacuo. The residue was detected by ${ }^{1} \mathrm{HNMR}(0.2 \mathrm{mmol}$ of dibromomethane was added as an internal standard) and the ${ }^{1} \mathrm{HNMR}$ yields were reported.
(d) Radical probe experiment


The reaction was carried out in an undivided cell with magnesium plates electrodes ( 0.1 $\mathrm{mm} \times 10.0 \mathrm{~mm} \times 20.0 \mathrm{~mm})$ and platinum electrodes $(0.25 \mathrm{~mm} \times 10 \mathrm{~mm} \times 15 \mathrm{~mm})$. To a 15.0 mL oven-dried undivided cell equipped with a magnetic bar was added substrates $Z$-enamide 54a ( $0.2 \mathrm{mmol}, 1.0$ equiv.), $\mathrm{Cs}_{2} \mathrm{CO}_{3}$ ( $0.2 \mathrm{mmol}, 1.0$ equiv.), $\mathrm{TBABF}_{4}$ ( 0.2 mmol, 1.0 equiv.). Then the tube was evacuated and back-filled under $\mathrm{CO}_{2}$ flow (this procedure was repeated three times), and DMF ( 4.0 mL ) was added via a syringe. The electrocatalysis was performed under $\mathrm{CO}_{2}$ balloon at $60^{\circ} \mathrm{C}$ with a constant current of 5.0 mA maintained for 10 h . After that, the reaction mixture was acidized with HCl aqueous ( $1.0 \mathrm{~N}, 5 \mathrm{~mL}$ ). The aqueous layer was extracted with EtOAc $(2 \times 10 \mathrm{~mL})$ and the combined organic phase was washed with brine, dried by anhydrous $\mathrm{MgSO}_{4}$, filtered, and concentrated under vacuo. The crude product was purified by column chromatography to furnish the desired product 54 in $32 \%$ yield. ${ }^{1} \mathrm{H}$ NMR ( 400 MHz , Chloroform-d) $\delta 7.45(\mathrm{~d}, \mathrm{~J}=9.6 \mathrm{~Hz}, 1 \mathrm{H}), 6.52(\mathrm{dd}, \mathrm{J}=14.4,10.0 \mathrm{~Hz}, 1 \mathrm{H}), 4.66(\mathrm{dd}, \mathrm{J}$ $=14.0,8.0 \mathrm{~Hz}, 1 \mathrm{H}), 1.08-0.99(\mathrm{~m}, 1 \mathrm{H}), 0.92(\mathrm{~s}, 9 \mathrm{H}), 0.39-0.32(\mathrm{~m}, 2 \mathrm{H}), 0.01-0.05$
(m, 2H). ${ }^{13} \mathrm{C}$ NMR ( 100 MHz , Chloroform- $d$ ) $\delta 175.4,121.7,116.7,38.5,27.3,11.2$, 6.3. HRMS (ESI, m/z): Calculated $\mathrm{C}_{10} \mathrm{H}_{17} \mathrm{NO}[\mathrm{M}+\mathrm{H}]^{+}: 168.1388$, found 168.1390 .
(e) Deuteration experiments at room temperature.


The reaction was carried out in an undivided cell with magnesium plates electrodes ( 0.1 $\mathrm{mm} \times 10.0 \mathrm{~mm} \times 20.0 \mathrm{~mm}$ ) and platinum electrodes $(0.25 \mathrm{~mm} \times 10 \mathrm{~mm} \times 15 \mathrm{~mm})$. To a 15.0 mL oven-dried undivided cell equipped with a magnetic bar was added substrates Z-enamide 1a-D or $\mathbf{6 a - D}$ ( $0.2 \mathrm{mmol}, 1.0$ equiv.), $\mathrm{Cs}_{2} \mathrm{CO}_{3}$ ( $0.2 \mathrm{mmol}, 1.0$ equiv.), $\mathrm{TBABF}_{4}$ ( 0.2 mmol, 1.0 equiv.). Then the tube was evacuated and back-filled under $\mathrm{CO}_{2}$ flow (this procedure was repeated three times), and DMF ( 4.0 mL ) was added via a syringe. The electrocatalysis was performed under $\mathrm{CO}_{2}$ balloon at room temperature with a constant current of 5.0 mA maintained for 2 h . After that, the reaction mixture was acidized with HCl aqueous ( $1.0 \mathrm{~N}, 5 \mathrm{~mL}$ ). The aqueous layer was extracted with EtOAc $(2 \times 10 \mathrm{~mL})$ and the combined organic phase was washed with brine, dried by anhydrous $\mathrm{MgSO}_{4}$, filtered, and concentrated under vacuo. The crude product was purified by column chromatography to furnish the desired product 1-D and 6-D in 35\% and $11 \%$ yield, respectively.

##  <br> 囍







##  <br> NNNNNNNかNNから


6－D，11\％


## （f）Influence of $\boldsymbol{N}$－protected groups



49a or 49a'



R=H, 49, 90\%
$\mathrm{R}=\mathrm{Me}, \mathrm{N} . \mathrm{R}$.

The reaction was carried out in an undivided cell with magnesium plates electrodes ( 0.1 $\mathrm{mm} \times 10.0 \mathrm{~mm} \times 20.0 \mathrm{~mm}$ ) and platinum electrodes $(0.25 \mathrm{~mm} \times 10 \mathrm{~mm} \times 15 \mathrm{~mm})$. To a 15.0 mL oven-dried undivided cell equipped with a magnetic bar was added substrates Z-enamide 49a and $N$-Me-protected 49a' ( 0.2 mmol , 1.0 equiv.), $\mathrm{Cs}_{2} \mathrm{CO}_{3}$ ( 0.2 mmol , 1.0 equiv.), $\mathrm{TBABF}_{4}$ ( $0.2 \mathrm{mmol}, 1.0$ equiv.). Then the tube was evacuated and backfilled under $\mathrm{CO}_{2}$ flow (this procedure was repeated three times), and DMF ( 4.0 mL ) was added via a syringe. The electrocatalysis was performed under $\mathrm{CO}_{2}$ balloon at $80^{\circ} \mathrm{C}$ with a constant current of 5.0 mA maintained for 2 h . After that, the reaction mixture was acidized with HCl aqueous ( $1.0 \mathrm{~N}, 5 \mathrm{~mL}$ ). The aqueous layer was extracted with EtOAc $(2 \times 10 \mathrm{~mL})$ and the combined organic phase was washed with brine, dried by anhydrous $\mathrm{MgSO}_{4}$, filtered, and concentrated under vacuo. The crude product was purified by column chromatography to furnish the desired product 49 in $90 \%$ and no target product was detected when using $N$-Me-protected 49a' as starting material.


The reaction was carried out in an undivided cell with magnesium plates electrodes ( 0.1 $\mathrm{mm} \times 10.0 \mathrm{~mm} \times 20.0 \mathrm{~mm}$ ) and platinum electrodes $(0.25 \mathrm{~mm} \times 10 \mathrm{~mm} \times 15 \mathrm{~mm})$. To a 15.0 mL oven-dried undivided cell equipped with a magnetic bar was added substrates $Z$-enamide 2a and $N$-Boc-protected 2a' ( $0.2 \mathrm{mmol}, 1.0$ equiv.), $\mathrm{Cs}_{2} \mathrm{CO}_{3}$ ( $0.2 \mathrm{mmol}, 1.0$ equiv.), $\mathrm{TBABF}_{4}$ ( $0.2 \mathrm{mmol}, 1.0$ equiv.). Then the tube was evacuated and back-filled under $\mathrm{CO}_{2}$ flow (this procedure was repeated three times), and DMF ( 4.0 mL ) was added via a syringe. The electrocatalysis was performed under $\mathrm{CO}_{2}$ balloon at $60^{\circ} \mathrm{C}$ with a constant current of 5.0 mA maintained for 2 h . After that, the reaction mixture
was acidized with HCl aqueous ( $1.0 \mathrm{~N}, 5 \mathrm{~mL}$ ). The aqueous layer was extracted with EtOAc $(2 \times 10 \mathrm{~mL})$ and the combined organic phase was washed with brine, dried by anhydrous $\mathrm{MgSO}_{4}$, filtered, and concentrated under vacuo. The crude product was purified by column chromatography to furnish the desired product $\mathbf{2}$ in $85 \%$ and no target product was detected when using $N$-Boc-protected $\mathbf{2 a}{ }^{\prime}$ as starting material.
(g) Control experiments at room temperature


The reaction was carried out in an undivided cell with magnesium plates electrodes ( 0.1 $\mathrm{mm} \times 10.0 \mathrm{~mm} \times 20.0 \mathrm{~mm})$ and platinum electrodes $(0.25 \mathrm{~mm} \times 10 \mathrm{~mm} \times 15 \mathrm{~mm})$. To a 15.0 mL oven-dried undivided cell equipped with a magnetic bar was added substrates $Z$-enamide 1a ( 0.2 mmol , 1.0 equiv.), $\mathrm{Cs}_{2} \mathrm{CO}_{3}$ ( 0.2 mmol , 1.0 equiv.), $\mathrm{TBABF}_{4}$ ( 0.2 mmol, 1.0 equiv.). Then the tube was evacuated and back-filled under $\mathrm{CO}_{2}$ flow (this procedure was repeated three times), and DMF ( 4.0 mL ) was added via a syringe. The electrocatalysis was performed under $\mathrm{CO}_{2}$ balloon at room temperature with a constant current of 5.0 mA maintained for 2 h . After that, the reaction mixture was acidized with HCl aqueous ( $1.0 \mathrm{~N}, 5 \mathrm{~mL}$ ). The aqueous layer was extracted with $\mathrm{EtOAc}(2 \times 10 \mathrm{~mL}$ ) and the combined organic phase was washed with brine, dried by anhydrous $\mathrm{MgSO}_{4}$, filtered, and concentrated under vacuo. The crude product was purified by column chromatography to furnish the desired product.
(h) Control experiments with/without current on standard conditions
(
(i) The differences between $Z$-enaimdes and $E$-enamides by ${ }^{1} \mathrm{H}$ NMR spectrum (substrates 1 and 6 as examples)


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## Cyclic Voltammetry Studies

The cyclic voltammetry was carried out with a Shanghai Chenhua CHI760E workstation. A glassy-carbon electrode ( 5 mm -diameter, disc-electrode) was used as the working electrode, a Pt plate was used as the auxiliary electrode and an $\mathrm{Ag} / \mathrm{AgNO}_{3}$ electrode was used as a reference electrode. The sample should be bubbled with Ar or $\mathrm{CO}_{2}$ for 5 min before testing. The measurements were carried out at a scan rate of 100 $\mathrm{mV} \mathrm{s}^{-1}$ in $\mathrm{DMF}^{n} \mathrm{Bu}_{4} \mathrm{NBF}_{4}$ (0.1 M).


Figure S5. Cyclic voltammograms of $\mathbf{6}$ under Ar atmosphere (blue line), $\mathbf{6}$ under $\mathrm{CO}_{2}$ atmosphere (green line), $\mathbf{6}$ with $\mathrm{Cs}_{2} \mathrm{CO}_{3}$ under $\mathrm{CO}_{2}$ atmosphere (purple line) in DMF with ${ }^{n} \mathrm{Bu}_{4} \mathrm{NBF}_{4}(0.1 \mathrm{M})$.


Figure S6. Cyclic voltammograms of different concentrations of 6 under Ar atmosphere in DMF with ${ }^{n} \mathrm{Bu}_{4} \mathrm{NBF}_{4}$ (0.1 M).


Figure S7. Cyclic voltammograms of different concentrations of 6 under $\mathrm{CO}_{2}$ atmosphere in DMF with ${ }^{n} \mathrm{Bu}_{4} \mathrm{NBF}_{4}$ (0.1 M).


Figure S8. Cyclic voltammograms of $\mathbf{1}$ under Ar atmosphere (blue line), $\mathbf{1}$ under $\mathrm{CO}_{2}$ atmosphere (green line) in DMF with ${ }^{n} \mathrm{Bu}_{4} \mathrm{NBF}_{4}$ ( 0.1 M ).


Figure S9. Cyclic voltammograms of $\mathbf{2}$ under Ar atmosphere (blue line), $\mathbf{2}$ under $\mathrm{CO}_{2}$ atmosphere (green line) in DMF with ${ }^{n} \mathrm{Bu}_{4} \mathrm{NBF}_{4}$ ( 0.1 M ).

## DFT Calculations

## General Information of DFT Computational Studies

For single-point energy (SPE) calculation of optimized geometries:
$>$ Calculation software: Gaussian 16, Rev. A $03{ }^{[13]}$
$>$ DFT functional: M06-2X-D3 (Hybrid functional M06-2X ${ }^{[14]}$ with dispersioncorrection DFT-D3 ${ }^{[15]}$ )
> Basis sets: ma-TZVP ${ }^{[16]}$
$>$ Solvation model: $\mathrm{SMD},{ }^{[17]}$ an implicit solvation model. The keyword scrf=solvent=N,N-dimethylformamide was input to set up solvent parameters.
$>$ Other information: The keyword $\mathrm{SCF}=$ conver $=6$ was implemented to loosen the convergence criteria of SCF iterations, and reduce the running time. Other settings were kept default.

For geometry optimization and frequency analysis:
$>$ Calculation software: Gaussian 16 , Rev. A $03{ }^{[13]}$
$>$ DFT functional: M06-2X-D3 (Hybrid functional M06-2X ${ }^{[14]}$ with dispersioncorrection DFT-D3 ${ }^{[15]}$ )
$>$ Basis sets: def2-SVP ${ }^{[18]}$
$>$ Solvation model: IEFPCM, ${ }^{[19]}$ an implicit solvation model. The keyword scrf=solvent=N,N-dimethylformamide was input to set up solvent parameters.
$>$ Other information: The keyword "Opt=(TS, CalcFC, NoEigen)" was implemented while searching transition states. Each intermediate does not have any imaginary frequency, and each transition state only has a sole imaginary frequency. Most other settings, like the accuracy of integration grids, and criteria of convergence, were kept default.

For the calculation of thermodynamic properties:
$>$ Calculation software: Shermo $2.3,{ }^{[20]}$ the calculated harmonic frequencies
from frequency analysis are required for a certain geometry. Thermal corrections, including the thermal correction to Gibbs free energy (TCG), are the output.
$>$ Environment parameters: $T=333.15 \mathrm{~K}$ and $p=1 \mathrm{~atm}$
$>$ Treatment for low frequencies: Grimme's interpolation for entropy ${ }^{[21]}$
$>$ Harmonic vibrational frequency scale factors for zero-point energy (ZPE), thermal energy ( U ), and entropy ( S ) were set to $0.977,0.948$, and 0.952 , respectively. To see how these scale factors are obtained, please check the supporting information of Feng's work. ${ }^{[22]}$

In this work, we adopted the same method ${ }^{[22]}$ to calculate the harmonic vibrational frequency scale factors. The procedure and test sets remained the same, however, while performing geometry optimization to molecules in test sets, M06-2X/def2-SVP was applied instead. To check test sets and source codes, please access:
https://github.com/TMSCN/Computational_Chemistry_Utils/tree/main/Scale _Factor_Generator

The level of DFT computation can be noted as SMD(DMF) / M06-2X-D3 / ma-
TZVP // IEFPCM(DMF) / M06-2X-D3 / def2-SVP.

## Computed Energies of Stationary Points




Table S2. Single-point energies (SPE) and thermal corrections to Gibbs free energies (TCG). 1 Hartree $=627.51 \mathrm{kcal} / \mathrm{mol}=2625.5 \mathrm{~kJ} / \mathrm{mol}$.

| Structures | SPE (Hartree) | TCG (Hartree) |
| :---: | :---: | :---: |
| $1 \_Z$ | -709.396836 | 0.192354 |
| $1-\_Z$ | -708.908438 | 0.179233 |
| CO $_{2}$ | -188.599399 | -0.01184 |
| CO_2- $_{3}$ | -264.039294 | -0.0126 |
| 1_E | -709.399010 | 0.191705 |
| 1-_E | -708.908813 | 0.178694 |
| HCO3- | -264.572060 | -0.00265 |
| INT-1 | -897.517087 | 0.191063 |
| INT-2 | -896.967820 | 0.177695 |
| INT-3 | -896.969377 | 0.175525 |
| INT-4 | -897.521577 | 0.190089 |
| INT-5 | -897.506038 | 0.189153 |
| INT-6 | -897.504402 | 0.18809 |
| TS-1 | -897.504105 | 0.187999 |
| TS-2 | -1161.536706 | 0.194968 |
| TS-3 | -896.953289 | 0.17595 |
| TS-4 | -1161.536111 | 0.195011 |
| TS-5 | -897.504213 | 0.186686 |
| TS-6 | -897.493523 | 0.187232 |
| TS-7 | -897.504376 | 0.190084 |
| TS-8 | -897.492183 | 0.186773 |
| TS-9 | -708.844750 | 0.175379 |

Cartesian Coordinates of Stationary Points (Unit: Å) 1-_E
Charge $=-1 \quad$ Spin Multiplicity $=1$

| C | -4.63771146 | -1.58977574 | 0.01832857 |
| :--- | ---: | ---: | ---: |
| C | -3.30567953 | -1.17800742 | 0.01223981 |
| C | -2.98350922 | 0.18438335 | -0.01722193 |
| C | -4.01867044 | 1.12576033 | -0.04046761 |
| C | -5.35195264 | 0.71716665 | -0.03445627 |
| C | -5.66498776 | -0.64321539 | -0.00499865 |
| H | -4.87869738 | -2.65432366 | 0.04138088 |
| H | -2.48682342 | -1.89661630 | 0.03002122 |
| H | -3.74952268 | 2.18243119 | -0.06328043 |
| H | -6.15130332 | 1.46046015 | -0.05276601 |
| H | -6.70771133 | -0.96589783 | -0.00021572 |
| C | -1.54584831 | 0.67251946 | -0.02471662 |
| O | -1.35018829 | 1.90034282 | -0.05154116 |
| N | -0.62924480 | -0.30803791 | -0.00079753 |
| C | 0.66930785 | 0.09213476 | -0.00670472 |
| H | 0.85663195 | 1.17680348 | -0.03052350 |
| C | 1.73136415 | -0.76126754 | 0.01478512 |
| H | 1.51633887 | -1.83426601 | 0.03830698 |
| C | 3.14107460 | -0.38219677 | 0.00950638 |
| C | 3.59418984 | 0.95586745 | -0.01957302 |
| C | 4.12914270 | -1.38890410 | 0.03448007 |
| C | 4.95173203 | 1.26026926 | -0.02324991 |
| H | 2.86987521 | 1.77158868 | -0.03965510 |
| C | 5.48819884 | -1.08277924 | 0.03076286 |
| H | 3.81118625 | -2.43419035 | 0.05727499 |
| C | 5.91377621 | 0.24609287 | 0.00184395 |
| H | 5.26468563 | 2.30628477 | -0.04607543 |
| H | 6.22201241 | -1.89126035 | 0.05067894 |
| H | 6.97709901 | 0.48982140 | -0.00115515 |
|  |  |  |  |

1-_Z
Charge $=-1 \quad$ Spin Multiplicity $=1$
C $\quad 3.71157654 \quad-0.49925726 \quad-0.64667160$
C $\quad 2.43164139-0.14327048 \quad-0.22255636$
$\begin{array}{lllll}\text { C } & 2.25574075 & 0.85265838 & 0.74586749\end{array}$
$\begin{array}{llll}\text { C } & 3.38469278 & 1.48383401 & 1.28066386\end{array}$
C $\quad 4.66577318 \quad 1.13005345 \quad 0.85909078$
$\begin{array}{llll}\text { C } & 4.83247098 & 0.13621288 & -0.10720400\end{array}$
H 3.83760176 -1.27733105 -1.40189443

| H | 1.54852124 | -0.63259519 | -0.63324229 |
| :--- | ---: | ---: | ---: |
| H | 3.22819345 | 2.25675705 | 2.03399650 |
| H | 5.53836511 | 1.62974970 | 1.28409776 |
| H | 5.83386660 | -0.14346784 | -0.43943984 |
| C | 0.88286334 | 1.27291908 | 1.24181240 |
| O | 0.82919348 | 2.15963862 | 2.10957475 |
| N | -0.14109978 | 0.61859278 | 0.66683861 |
| C | -1.38186572 | 0.95642529 | 1.10719246 |
| H | -1.43282726 | 1.71323077 | 1.90553339 |
| C | -2.57956750 | 0.45940008 | 0.67420857 |
| H | -3.47091997 | 0.85760730 | 1.16675556 |
| C | -2.84083179 | -0.53809308 | -0.35978999 |
| C | -1.83141683 | -1.15899299 | -1.12963695 |
| C | -4.17577057 | -0.91716813 | -0.62197216 |
| C | -2.15143043 | -2.10518922 | -2.10154072 |
| H | -0.79887667 | -0.87172427 | -0.93798889 |
| C | -4.49072861 | -1.86260730 | -1.59369006 |
| H | -4.97768784 | -0.45216232 | -0.04262903 |
| C | -3.47872506 | -2.46721239 | -2.34364129 |
| H | -1.34942054 | -2.56826386 | -2.68099455 |
| H | -5.53493603 | -2.13081718 | -1.76789021 |
| H | -3.72172901 | -3.20914483 | -3.10600276 |


| 1_E |  |  |  |
| :--- | :---: | :---: | :---: |
| Charge $=0$ |  |  |  |
| C | Spin Multiplicity $=1$ |  |  |
| C | -7.44839569 | 1.55009501 | 0.80719862 |
| C | -6.27016535 | 0.80511097 | 0.82299095 |
| C | -6.10378799 | -0.26157438 | -0.06812788 |
| C | -7.11776200 | -0.56247024 | -0.98451498 |
| C | -8.29696880 | 0.17726983 | -0.99322902 |
| C | -8.46394742 | 1.23383490 | -0.09560878 |
| H | -7.56942497 | 2.38494420 | 1.49840503 |
| H | -5.47625372 | 1.08684705 | 1.51707187 |
| H | -6.96322896 | -1.38543403 | -1.68319773 |
| H | -9.08812905 | -0.06811113 | -1.70285615 |
| H | -9.38615658 | 1.81667683 | -0.10382407 |
| C | -4.85897639 | -1.09655472 | -0.12493305 |
| O | -4.54933054 | -1.72557445 | -1.11984352 |
| H | -4.44995383 | -0.66227969 | 1.85139195 |
| N | -4.09999024 | -1.11952669 | 1.01686363 |
| C | -2.90728464 | -1.82414648 | 1.10070961 |
| H | -2.63173626 | -2.30146115 | 0.15926728 |


| C | -2.16913260 | -1.91216783 | 2.21915680 |
| :--- | ---: | ---: | :--- |
| H | -2.52558056 | -1.40843943 | 3.12315398 |
| C | -0.89976158 | -2.64105866 | 2.34882920 |
| C | -0.28467118 | -3.31384882 | 1.27707649 |
| C | -0.26219039 | -2.67219868 | 3.59993647 |
| C | 0.91722100 | -3.99126702 | 1.45653532 |
| H | -0.74668309 | -3.30830363 | 0.28858330 |
| C | 0.94244439 | -3.35058764 | 3.77935897 |
| H | -0.72394215 | -2.15448377 | 4.44358854 |
| C | 1.53881772 | -4.01454207 | 2.70819519 |
| H | 1.37546239 | -4.50587722 | 0.61030642 |
| H | 1.41656594 | -3.35940082 | 4.76219450 |
| H | 2.48154590 | -4.54627676 | 2.84424473 |


| 1_Z |  |  |  |
| :--- | ---: | ---: | ---: |
| Charge $=0$ |  |  |  |
| Spin Multiplicity $=1$ |  |  |  |
| C | 2.99880946 | -2.04783687 | 0.78695632 |
| C | 2.07487411 | -1.00931486 | 0.68110975 |
| C | 2.45370210 | 0.21014601 | 0.10663571 |
| C | 3.76720577 | 0.38261450 | -0.34473830 |
| C | 4.68636762 | -0.65790239 | -0.24493829 |
| C | 4.30223826 | -1.87552574 | 0.32031583 |
| H | 2.69966017 | -2.99241870 | 1.24258382 |
| H | 1.06946768 | -1.15956548 | 1.07912881 |
| H | 4.04843551 | 1.34410971 | -0.77559185 |
| H | 5.70600007 | -0.51993994 | -0.60692444 |
| H | 5.02233618 | -2.69095780 | 0.40254536 |
| C | 1.52582496 | 1.38183887 | -0.03143326 |
| O | 1.93813580 | 2.51625308 | -0.18314772 |
| N | 0.18588507 | 1.09076264 | 0.00091615 |
| C | -0.79099469 | 2.07831544 | -0.02745765 |
| H | -0.37761490 | 3.08614202 | 0.02120542 |
| C | -2.11900061 | 1.87267438 | -0.06925339 |
| H | -2.74706633 | 2.76236577 | 0.00898874 |
| C | -2.81582619 | 0.57517744 | -0.14534896 |
| C | -2.32502024 | -0.50663373 | -0.89778842 |
| C | -4.03557811 | 0.41013952 | 0.53319965 |
| C | -3.01087369 | -1.72040401 | -0.93697326 |
| H | -1.41733605 | -0.38907541 | -1.49363051 |
| C | -4.72039262 | -0.80155751 | 0.49318948 |
| H | -4.44253662 | 1.24719824 | 1.10451433 |
| C | -4.20681336 | -1.87581806 | -0.23655579 |


| H | -2.61248556 | -2.54498115 | -1.53028713 |
| :--- | ---: | ---: | ---: |
| H | -5.66218608 | -0.90872233 | 1.03385188 |
| H | -4.74287971 | -2.82535423 | -0.26842402 |
| H | -0.10479477 | 0.12247198 | 0.06868029 |

$\mathrm{CO}_{2}$
Charge $=0 \quad$ Spin Multiplicity $=1$
C $-0.538415420 .06153846-0.00704824$
$\begin{array}{llll}\text { O } & -1.69452363 & 0.06153846 & -0.00704824\end{array}$
O $\quad 0.61769279 \quad 0.06153846-0.00704824$
$\mathrm{CO}_{3}$ 2-
Charge $=-2 \quad$ Spin Multiplicity $=1$
C -4.33485909
$1.66235897-0.40597931$
$\begin{array}{llll}\text { O } & -3.69242930 & 2.78109323 & -0.40597931\end{array}$
O $\quad-5.62539401 \quad 1.66235899-0.40597931$
O $\quad-3.69242934 \quad 0.54362468$-0.40597931

| $\mathrm{HCO}_{3}-$ |  |  |  |
| :---: | :---: | :---: | :---: |
| C | -0.58295426 | 0.09719327 | -0.15780655 |
| O | -0.63989493 | 0.43277333 | 1.03754480 |
| O | -1.16860979 | -0.80391778 | -0.76771144 |
| O | 0.28624600 | 0.85929784 | -0.94987339 |
| H | 0.66449433 | 1.51552592 | -0.35215531 |

INT-1
Charge $=-1 \quad$ Spin Multiplicity $=1$
C $\quad 3.95106217-1.59206342 \quad 1.07278644$
C $\quad 2.78330662-0.83911049 \quad 0.97403725$
C $\quad 2.59428414 \quad 0.02104998 \quad-0.11386909$
C $\quad 3.590827440 .13312672 \quad-1.08689916$
C $\quad 4.75041025-0.63578177-0.99835182$
C 4.93217488 -1.49871838 0.08296036
$\begin{array}{llll}\mathrm{H} & 4.09723763 & -2.25570386 & 1.92637878\end{array}$
$\begin{array}{llll}\mathrm{H} & 2.01755651 & -0.91303731 & 1.74899297\end{array}$
H $\quad 3.44410566$ 0.82984568 $\quad-1.91350599$
H $\quad 5.51734415$-0.55593865 -1.77023570
$\begin{array}{llll}\mathrm{H} & 5.84242947 & -2.09574864 & 0.15900111\end{array}$
C $\quad 1.41554367 \quad 0.95046430 \quad-0.20174026$
$\begin{array}{lllll}\text { O } & 1.57465644 & 2.08520287 & -0.62785053\end{array}$
$\begin{array}{lllll}\mathrm{N} & 0.20219309 & 0.52589211 & 0.28540729\end{array}$

| C | -0.69722728 | 1.53111475 | 0.65778171 |
| :--- | ---: | ---: | ---: |
| H | -0.20353321 | 2.44853025 | 0.98931035 |
| C | -2.04262292 | 1.50084690 | 0.66945824 |
| H | -2.51570876 | 2.37898543 | 1.11729666 |
| C | -2.97976068 | 0.48551077 | 0.16491946 |
| C | -2.66401796 | -0.40104588 | -0.87969348 |
| C | -4.28125068 | 0.44517522 | 0.69392136 |
| C | -3.60929541 | -1.30765729 | -1.35424250 |
| H | -1.67080193 | -0.38175936 | -1.32846385 |
| C | -5.22533024 | -0.46459111 | 0.22235823 |
| H | -4.55055066 | 1.14110160 | 1.49186497 |
| C | -4.89208757 | -1.34913857 | -0.80426944 |
| H | -3.34181792 | -1.98625717 | -2.16630654 |
| H | -6.22710252 | -0.47970619 | 0.65528620 |
| H | -5.62927858 | -2.06072799 | -1.17945143 |
| C | -0.10796618 | -0.95179200 | 0.50586720 |
| O | 0.26404835 | -1.67385768 | -0.41765170 |
| O | -0.67875373 | -1.18949834 | 1.56584913 |

INT-2
Charge $=-2 \quad$ Spin Multiplicity $=1$
C $\quad-4.66608311 \quad-0.467879141 .65442799$
C $-3.35866682-0.60545362 \quad 1.19206222$
C $\quad-3.08886333-0.56368455-0.18083175$
C $\quad-4.14574060 ~-0.40278772-1.08065990$
C $-5.45195521-0.24368958-0.61847702$
C $\quad-5.71490597-0.27810942 \quad 0.75156004$
H $\quad-4.86916729-0.50899455 \quad 2.72600864$
$\begin{array}{llll}\mathrm{H} & -2.53751357 & -0.74710418 & 1.89803772\end{array}$
H $\quad-3.92762800 ~-0.40616176-2.14971010$
H $-6.26818434-0.10101772-1.32880575$
H $\quad-6.73701003-0.16342736 \quad 1.11661004$
C $-1.71110378 \quad-0.83458953-0.74084216$
O $-1.62567813-1.51105820 \quad-1.76767258$
N $-0.63430899-0.40077450-0.05042586$
C $\quad 0.66054348$-0.96580546 -0.38768085
H $\quad 0.57241090$-2.05363452 -0.52766591
C $\quad 1.81250196$-0.30270130 -0.53377639
C $\quad 1.89144093 \quad 1.13622723-0.47253371$
C $\quad 1.51088995 \quad 1.94988734-1.57425524$
$\begin{array}{llll}\text { C } & 2.44746687 & 1.82487116 & 0.63961353\end{array}$
C $\quad 1.66414808 \quad 3.33341967 \quad-1.55821245$

| H | 1.08393732 | 1.46325424 | -2.45565102 |
| :--- | ---: | ---: | ---: |
| C | 2.58631494 | 3.20780997 | 0.65518664 |
| H | 2.75934318 | 1.23949450 | 1.50759986 |
| C | 2.20065046 | 3.98573968 | -0.44376599 |
| H | 1.35165326 | 3.91599409 | -2.42933867 |
| H | 3.00757622 | 3.69234891 | 1.54039061 |
| H | 2.31935020 | 5.07033263 | -0.43158827 |
| C | -0.73284655 | 0.65477648 | 1.01088203 |
| O | -1.39590176 | 1.64783829 | 0.69479934 |
| O | -0.15756727 | 0.37975791 | 2.06928196 |

## INT-3

Charge $=-2 \quad$ Spin Multiplicity $=1$
C $\quad 4.66627387 \quad 0.97757473-0.65812618$
C $\quad 3.29257245 \quad 0.74093264-0.61308791$
C $\quad 2.80687999-0.50921924-0.21120163$
C $\quad 3.71556158$-1.51856965 $\quad 0.12411101$
C $\quad 5.08789660-1.27679472 \quad 0.09634781$
C $\quad 5.56691795-0.02613120 \quad-0.29753024$
H $\quad 5.03639267 \quad 1.95270730 \quad-0.97967848$
H 2.59049196 1.52958345 -0.88857307
H $\quad 3.32499064-2.498250330 .40282087$
H $\quad 5.78662993-2.06758687 \quad 0.37479522$
H $\quad 6.64106346 \quad 0.16438127-0.32938614$
C $\quad 1.33953154-0.87335579-0.23828089$
$\begin{array}{lllll}\text { O } & 1.03256347 & -2.02691484 & -0.55179994\end{array}$
$\begin{array}{lllll}\mathrm{N} & 0.43717803 & 0.09232008 & 0.03269115\end{array}$
C $-0.96013350-0.17851293-0.15585649$
H -1.10234317 -0.95366654 -0.92788012
C $-1.93774659 \quad 0.421317940 .53278290$
C $-3.30860556 \quad 0.11918719 \quad 0.19854236$
C $-3.94272261 \quad 0.63011452 \quad-0.96650665$
C $-4.13253961-0.66425396 \quad 1.05295301$
C -5.28229948 0.37510442 -1.25201271
H $\quad-3.35071489 \quad 1.24376927-1.65046851$
C $-5.46584317-0.927061330 .75747526$
H $\quad-3.69017564-1.06933969 \quad 1.96717054$
C $-6.06382747-0.40722301 \quad-0.39706964$
H $\quad-5.723019670 .78926916-2.16297542$
H $\quad-6.05346661-1.54599084 \quad 1.44085731$
H $\quad-7.11301787-0.60537413-0.62157041$
C $\quad 0.81048771 \quad 1.36753605 \quad 0.74826259$

| O | 1.31846655 | 1.19461837 | 1.85898144 |
| :--- | :--- | :--- | :--- |
| O | 0.58189069 | 2.40469149 | 0.11931089 |


| INT-4 |  |  |  |
| :--- | ---: | ---: | ---: |
| Charge $=-1$ | Spin Multiplicity $=1$ |  |  |
| C | -4.72771012 | -1.10950673 | 0.96098007 |
| C | -3.37978326 | -0.86999133 | 0.70251168 |
| C | -3.00878414 | 0.09338623 | -0.24272502 |
| C | -3.99627548 | 0.82469310 | -0.90883078 |
| C | -5.34453163 | 0.57243582 | -0.66202396 |
| C | -5.71172386 | -0.39494480 | 0.27452998 |
| H | -5.01227042 | -1.85660890 | 1.70336166 |
| H | -2.61186309 | -1.42886839 | 1.24106396 |
| H | -3.69110308 | 1.59187758 | -1.62172016 |
| H | -6.11092771 | 1.13593332 | -1.19625212 |
| H | -6.76668844 | -0.58897694 | 0.47487743 |
| C | -1.57394692 | 0.47200188 | -0.48052903 |
| O | -1.28975730 | 1.62828963 | -0.75099238 |
| N | -0.61890937 | -0.50553343 | -0.29586205 |
| C | 0.70652708 | -0.09814968 | -0.18779754 |
| H | 0.80357601 | 0.98911506 | -0.18028381 |
| C | 1.79177905 | -0.89257354 | -0.11745424 |
| H | 1.65975646 | -1.97487491 | -0.12214135 |
| C | 3.17367704 | -0.40441161 | -0.00593077 |
| C | 3.52045370 | 0.95756380 | 0.08222049 |
| C | 4.21890559 | -1.34473881 | 0.01457359 |
| C | 4.85065322 | 1.35392350 | 0.18261673 |
| H | 2.74212371 | 1.72227909 | 0.07680810 |
| C | 5.55153907 | -0.94841952 | 0.11527025 |
| H | 3.97309082 | -2.40705966 | -0.05121242 |
| C | 5.87670297 | 0.40503683 | 0.19968747 |
| H | 5.09002595 | 2.41673596 | 0.25034423 |
| H | 6.33999537 | -1.70311379 | 0.12809285 |
| H | 6.91811057 | 0.72009672 | 0.27935878 |
| C | -0.95497836 | -1.98161136 | -0.49210902 |
| O | -0.46543932 | -2.72744722 | 0.35490736 |
| O | -1.65714955 | -2.19462592 | -1.47600628 |
|  |  |  |  |

INT-5
Charge $=-1 \quad$ Spin Multiplicity $=1$
C $\quad 2.60612767-1.19597858 \quad 1.77592558$
C $\quad 1.78830690 \quad-0.44270893 \quad 0.93152347$

| C | 2.28633589 | -0.02128634 | -0.30844372 |
| :--- | ---: | ---: | ---: |
| C | 3.59031429 | -0.35553435 | -0.69459636 |
| C | 4.39588650 | -1.11402148 | 0.14886673 |
| C | 3.90218567 | -1.53514553 | 1.38669243 |
| H | 2.22623581 | -1.52084321 | 2.74574827 |
| H | 0.77799835 | -0.16608410 | 1.25023026 |
| H | 3.95375662 | -0.01009927 | -1.66330025 |
| H | 5.40988962 | -1.37805818 | -0.15486685 |
| H | 4.53292353 | -2.12896805 | 2.05045387 |
| C | 1.47020360 | 0.81416118 | -1.25278106 |
| O | 1.95028774 | 1.32221748 | -2.24396739 |
| N | 0.11316018 | 0.88029278 | -0.97497689 |
| C | -0.40132560 | 1.74632231 | -0.20648703 |
| H | 0.22619658 | 2.51601951 | 0.27828983 |
| C | -1.84876826 | 1.79152184 | 0.16721470 |
| H | -2.20916993 | 2.82263297 | 0.04043987 |
| C | -2.72429907 | 0.84579957 | -0.61710763 |
| C | -3.68594658 | 1.32382993 | -1.51213242 |
| C | -2.59029799 | -0.54035758 | -0.45030473 |
| C | -4.49824864 | 0.44108655 | -2.22801494 |
| H | -3.80084932 | 2.40153554 | -1.65002849 |
| C | -3.39669184 | -1.42281224 | -1.16501793 |
| H | -1.84613714 | -0.91104865 | 0.25758123 |
| C | -4.35454227 | -0.93499105 | -2.05820268 |
| H | -5.24559941 | 0.83248743 | -2.92055546 |
| H | -3.28044229 | -2.49901218 | -1.02407200 |
| H | -4.98737772 | -1.62660163 | -2.61684003 |
| C | -1.95479176 | 1.45205871 | 1.71040254 |
| O | -1.05307146 | 0.70925801 | 2.15322232 |
| O | -2.93574764 | 1.92000794 | 2.29960679 |
|  | -1593 |  |  |

## INT-6

Charge $=-1 \quad$ Spin Multiplicity $=1$
C $\quad-3.70420214-0.99835189 \quad 1.68706655$
C $\quad-2.56503569-0.58701086 \quad 0.99653904$
C $\quad-2.68058042 \quad 0.32589414-0.05823475$
$\begin{array}{llll}\text { C } & -3.93933231 & 0.82598300 & -0.41391600\end{array}$
C $\quad-5.07489865 \quad 0.41378066 \quad 0.27682695$
C $\quad-4.95707235-0.49920233 \quad 1.32834681$
$\begin{array}{llll}\mathrm{H} & -3.61407100 & -1.70864315 & 2.51003267\end{array}$
H $\quad-1.57931817-0.96286742 \quad 1.26977097$
$\begin{array}{llll}\mathrm{H} & -4.00660789 & 1.53714389 & -1.23819254\end{array}$

| H | -6.05509968 | 0.80284944 | -0.00206232 |
| :--- | ---: | ---: | ---: |
| H | -5.84714784 | -0.82186468 | 1.87098777 |
| C | -1.48700700 | 0.78258595 | -0.83729168 |
| O | -1.56613428 | 1.63464689 | -1.69603772 |
| N | -0.27394778 | 0.17927030 | -0.46644960 |
| C | 0.53716666 | -0.11780215 | -1.40480346 |
| H | 0.26258977 | 0.04511823 | -2.46118590 |
| C | 1.89505324 | -0.67420088 | -1.15885901 |
| H | 2.04563272 | -0.80211840 | -0.07999714 |
| C | 2.04830939 | -2.01076639 | -1.85959161 |
| C | 2.14694614 | -3.19639401 | -1.12306812 |
| C | 2.07424120 | -2.08215318 | -3.26005606 |
| C | 2.27577020 | -4.42755070 | -1.76826859 |
| H | 2.12399798 | -3.15248918 | -0.03192531 |
| C | 2.19617919 | -3.31190323 | -3.90471965 |
| H | 2.01828768 | -1.15340133 | -3.83157017 |
| C | 2.29800807 | -4.48980795 | -3.16143425 |
| H | 2.35687519 | -5.34211450 | -1.17814308 |
| H | 2.21694786 | -3.35116884 | -4.99533606 |
| H | 2.39606564 | -5.45184989 | -3.66689117 |
| C | 2.98083820 | 0.33230400 | -1.71923449 |
| O | 2.63329029 | 0.97891385 | -2.72631211 |
| O | 4.06012974 | 0.33491460 | -1.11509777 |

TS-1
Charge $=-1 \quad$ Spin Multiplicity $=1$
C $\quad 3.88333984-1.29617852 \quad 1.02490729$
C $\quad 2.76060668$-0.47104443 $\quad 0.95914821$
C $\quad 2.57861686 \quad 0.39456737-0.12432870$
C $\quad 3.55057782 \quad 0.43833769-1.12967685$
C $4.66344714-0.39945384-1.07804991$
C $4.83179861-1.26961372 \quad 0.00110623$
H 4.02030362 -1.96071434 1.87972695
H $\quad 2.02561138$-0.48018954 1.76667856
H $\quad 3.41714684 \quad 1.14203735-1.95290754$
H $\quad 5.40624875-0.37020526-1.87717341$
H $\quad 5.70619501$-1.92097021 $\quad 0.04823978$
C $\quad 1.41938558 \quad 1.36292403 \quad-0.19587318$
$\begin{array}{lllll}\text { O } & 1.64371045 & 2.49651460 & -0.64250529\end{array}$
$\begin{array}{lllll}\mathrm{N} & 0.22632722 & 0.91193780 & 0.23167039\end{array}$
C $\quad-0.70805199 \quad 1.87836042 \quad 0.51216926$
$\begin{array}{llll}\mathrm{H} & -0.29866390 & 2.85863735 & 0.79860417\end{array}$

| C | -2.06013527 | 1.76043115 | 0.53554762 |
| :--- | :---: | :---: | :---: |
| H | -2.61171325 | 2.61456076 | 0.93777899 |
| C | -2.88548476 | 0.63514390 | 0.08596202 |
| C | -2.45494151 | -0.28377012 | -0.89045968 |
| C | -4.19030641 | 0.48160554 | 0.59413447 |
| C | -3.28014966 | -1.32593328 | -1.30964944 |
| H | -1.46061262 | -0.16937874 | -1.32155031 |
| C | -5.01553050 | -0.55820728 | 0.17293811 |
| H | -4.55403907 | 1.19455358 | 1.33818766 |
| C | -4.56287567 | -1.47475166 | -0.77895419 |
| H | -2.91837877 | -2.02603212 | -2.06557451 |
| H | -6.01979974 | -0.65479085 | 0.59020770 |
| H | -5.20679013 | -2.29123535 | -1.10953860 |
| C | -0.20765673 | -1.11215200 | 0.83611755 |
| O | 0.16525465 | -1.74378862 | -0.08051365 |
| O | -0.67122406 | -0.92569757 | 1.89891184 |

TS-2
Charge $=-3 \quad$ Spin Multiplicity $=1$
C $\quad-4.75129700 \quad-0.42906010 \quad 1.41255354$
C $\quad-3.40421110 \quad-0.521689331 .06887036$
C $\quad-3.02940889-0.70201893-0.26770586$
C $\quad-4.01915467-0.80596354-1.24829684$
C $\quad-5.36702057-0.69204498 \quad-0.90844648$
C $\quad-5.73566827-0.50544506 \quad 0.42427869$
$\begin{array}{llll}\mathrm{H} & -5.03628285 & -0.29622626 & 2.45762824\end{array}$
H
H $\quad-3.71709847-0.97841421 \quad-2.28244307$
H -6.13210600 -0.75771231 -1.68392504
H $\quad-6.78989977-0.42533975 \quad 0.69497722$
C $-1.59513670-0.94101907-0.67499930$
O $-1.36875541 \quad-1.77730669 \quad-1.54757386$
N $\quad-0.60908918$-0.29462178 -0.00261681
C $\quad 0.71496544-0.84080027-0.09381706$
H $\quad 0.72295408$-1.93640675 -0.09688348
C $\quad 1.88245736-0.18238530 \quad-0.14115723$
H $\quad 3.06952913-0.95291699 \quad-0.01617292$
C $\quad 1.96934282 \quad 1.28051820 \quad-0.24690672$
C $\quad 1.25512749 \quad 2.02060556-1.21262588$
$\begin{array}{lllll}\text { C } & 2.87284929 & 1.99913431 & 0.56568120\end{array}$
C $\quad 1.42451758 \quad 3.39779731 \quad-1.34808615$
H $\quad 0.55088289 \quad 1.49274704 \quad-1.85981673$

| C | 3.02983132 | 3.37795024 | 0.44569684 |
| :--- | ---: | ---: | ---: |
| H | 3.45977619 | 1.44386336 | 1.30186464 |
| C | 2.30729582 | 4.09002529 | -0.51592910 |
| H | 0.85621671 | 3.93957773 | -2.10800990 |
| H | 3.73019510 | 3.90250434 | 1.09994441 |
| H | 2.43678318 | 5.16876012 | -0.62024670 |
| C | -0.87814441 | 0.94486338 | 0.80490323 |
| O | -1.62703424 | 1.75978873 | 0.25665436 |
| O | -0.32889555 | 0.97269851 | 1.90883494 |
| C | 4.01439987 | -2.84052116 | 0.34190933 |
| O | 5.06900204 | -3.47305514 | 0.62604819 |
| O | 2.87328157 | -3.37616985 | 0.22302364 |
| O | 4.12442838 | -1.52170573 | 0.15245225 |

TS-3
Charge $=-2 \quad$ Spin Multiplicity $=1$
C $\quad-3.72241397-1.57517846-0.69666833$
C $-2.60058078-0.75016008-0.76014291$
C $\quad-2.50588348 \quad 0.37298205 \quad 0.07006283$
C $\quad-3.55453871 \quad 0.66618537 \quad 0.94708036$
C $\quad-4.66836825-0.16856752 \quad 1.02395287$
C $\quad-4.75496878-1.29138498 \quad 0.19948793$
H $\quad-3.79260562-2.44448920 \quad-1.35265989$
H $\quad-1.79293484-0.97510950-1.45923682$
$\begin{array}{llll}\mathrm{H} & -3.48180026 & 1.56210498 & 1.56509310\end{array}$
H $\quad-5.47464792 \quad 0.06101024 \quad 1.72265010$
H $\quad-5.62943990-1.94232477 \quad 0.25041329$
C $\quad-1.37155178 \quad 1.36667358 \quad-0.02417496$
$\begin{array}{llll}\text { O } & -1.61804843 & 2.55815574 & 0.16736688\end{array}$
$\begin{array}{llll}\mathrm{N} & -0.14981144 & 0.90757890 & -0.38038706\end{array}$
C $\quad 0.88093690 \quad 1.86165740 \quad-0.71086480$
H $0.42243105 \quad 2.80336264 \quad-1.05212653$
C $2.16912166 \quad 1.63757630 \quad-0.61419315$
C $\quad 3.51755920 \quad 1.46885046 \quad-0.62635445$
C $4.38071219 \quad 1.80590795 \quad 0.49412280$
C $4.22192587 \quad 0.91528759-1.77293009$
C $5.74914540 \quad 1.60955056 \quad 0.45057836$
$\begin{array}{llll}\mathrm{H} & 3.92143462 & 2.22207666 & 1.39406900\end{array}$
C $\quad 5.59263100 \quad 0.73561703-1.77556311$
H $3.63198422 \quad 0.62685542$-2.64632861
C $\quad 6.40073573 \quad 1.07378370 \quad-0.67450831$
H $6.33871119 \quad 1.88493640 \quad 1.33145125$

| H | 6.05672327 | 0.31151211 | -2.67231728 |
| :--- | ---: | ---: | ---: |
| H | 7.48049399 | 0.92479233 | -0.69183678 |
| C | 0.25238688 | -0.54009002 | -0.23925443 |
| O | 0.03996836 | -1.01662336 | 0.87841715 |
| O | 0.72483258 | -1.04914343 | -1.25851081 |

TS-4
Charge $=-3 \quad$ Spin Multiplicity $=1$
C $\quad-5.18367473-0.13370508 \quad 1.12057218$
C $\quad-3.82357444-0.37572019 \quad 0.93341284$
C $\quad-3.32350601-0.61967734-0.35122760$
C $\quad-4.20489420-0.63625054-1.43683331$
C $\quad-5.56191684-0.37649127-1.25221038$
C $\quad-6.05468098$-0.12601782 0.02929786
$\begin{array}{llll}\mathrm{H} & -5.56688756 & 0.04970884 & 2.12580170\end{array}$
H $\quad-3.14437592-0.37457612 \quad 1.78784797$
$\begin{array}{llll}\mathrm{H} & -3.80759301 & -0.85684668 & -2.42856756\end{array}$
H $\quad-6.23798078-0.37559046-2.10887905$
H $\quad-7.11772166 \quad 0.07050573 \quad 0.17880678$
C $\quad-1.88446751-0.99262146-0.61506776$
O $-1.64450624-1.81444590-1.49968721$
N $\quad-0.92393038-0.44864923 \quad 0.17200322$
C $0.39781129 \quad-0.96017401 \quad 0.07342492$
H $0.40076106-2.00878740 \quad-0.25718291$
C $\quad 1.51714616 \quad-0.25086368 \quad 0.29627449$
H $\quad 1.73189659 \quad 1.12060262 \quad 0.47595523$
C $\quad 2.79893875-0.96552199 \quad 0.18383357$
C $\quad 3.03126159 \quad-2.25444585 \quad 0.70674444$
C $3.88149269-0.31420713-0.45088325$
C $4.27567102-2.87509037 \quad 0.58451031$
H 2.22016689 -2.76444932 1.23273307
C $\quad 5.11969464-0.93996364-0.57705743$
H 3.689226220 .68619476 -0.85606989
C $5.32840219-2.22384148 \quad-0.06037103$
H $4.42639673-3.873392931 .00253974$
H $5.93910168 \quad-0.42196357-1.08200361$
H $6.30309652-2.70684889-0.15251910$
C $\quad-1.17291124 \quad 0.78375859 \quad 1.01686318$
O $\quad-1.62394127 \quad 1.74283641 \quad 0.38904736$
$\begin{array}{llll}\text { O } & -0.91920754 & 0.64190032 & 2.21495974\end{array}$
C $\quad 2.34744200 \quad 3.00715840 \quad-0.40375795$
$\begin{array}{llll}\text { O } & 2.50353899 & 4.25072479 & -0.25944442\end{array}$

| O | 2.46020377 | 2.40422720 | -1.51600531 |
| :--- | :--- | :--- | :--- |
| O | 2.06166472 | 2.28951183 | 0.68267543 |

TS-5
Charge $=-1 \quad$ Spin Multiplicity $=1$
C $\quad 2.92939641-2.81169470 \quad 0.36824942$
C $\quad 1.76327342-2.094349470 .63302470$
C $\quad 1.54551623-0.84412047 \quad 0.04468156$
C $\quad 2.50429314-0.33379433-0.83821146$
C $\quad 3.66482929-1.05433454-1.11656176$
C $\quad 3.88361247-2.29265642-0.50859065$
H 3.09386360 -3.78065114 0.84309158
H $\quad 0.99749978$-2.49080816 1.30111023
H $2.32119242 \quad 0.63065136-1.31486724$
H $4.40215613-0.65023640-1.81255417$
H $\quad 4.79453571-2.85442847-0.72265611$
C $\quad 0.24641852-0.11892911 \quad 0.33723886$
$\begin{array}{llll}\text { O } & -0.71070929 & -0.79120089 & 0.74403590\end{array}$
C $-0.853882671 .97457174 \quad 0.16884080$
$\begin{array}{lllll}\mathrm{H} & -0.62855436 & 3.02878989 & -0.04416619\end{array}$
C $\quad-2.15254684 \quad 1.65741475 \quad 0.43289697$
C $\begin{array}{llll}-3.25752388 & 2.62149251 & 0.42631775\end{array}$
$\begin{array}{llll}\text { C } & -3.13334791 & 3.97391562 & 0.04244687\end{array}$
$\begin{array}{llll}\text { C } & -4.53796541 & 2.18577931 & 0.82356391\end{array}$
C $\quad-4.22558751 \quad 4.83629440 \quad 0.06869000$
H $\quad-2.16832649 \quad 4.35980160-0.28958656$
C $-5.63221872 \quad 3.04795371 \quad 0.84715547$
$\begin{array}{llll}\mathrm{H} & -4.66572675 & 1.14235046 & 1.12172642\end{array}$
C $\quad-5.48522660$ 4.38370796 0.47137999
$\begin{array}{llll}\mathrm{H} & -4.09306484 & 5.87680729 & -0.23488715\end{array}$
H $-6.60795296 \quad 2.67249786 \quad 1.16219305$
$\begin{array}{llll}\mathrm{H} & -6.33884430 & 5.06285685 & 0.48761872\end{array}$
$\begin{array}{llll}\mathrm{H} & -2.40731949 & 0.62978831 & 0.68174345\end{array}$
$\begin{array}{llll}\mathrm{N} & 0.27557053 & 1.20460940 & 0.10083120\end{array}$
$\begin{array}{llll}\text { C } & 2.02348104 & 2.46541302 & 0.61243794\end{array}$
$\begin{array}{llll}\text { O } & 1.80431899 & 3.37895375 & -0.08727612\end{array}$
$\begin{array}{llll}\text { O } & 2.55543298 & 1.80584262 & 1.41895876\end{array}$

TS-6
Charge $=-1 \quad$ Spin Multiplicity $=1$
C $\quad-3.45840253 \quad 0.62940597 \quad 2.16056543$
C $\begin{array}{llll}-2.47524845 & 0.41738872 & 1.19444557\end{array}$

| C | -2.83651533 | 0.04387063 | -0.10537778 |
| :--- | :---: | :---: | :---: |
| C | -4.19003455 | -0.11442574 | -0.42580315 |
| C | -5.17201259 | 0.09728872 | 0.53904101 |
| C | -4.80654012 | 0.46963199 | 1.83493721 |
| H | -3.17249206 | 0.92031848 | 3.17268210 |
| H | -1.41786248 | 0.53815484 | 1.42940747 |
| H | -4.45137041 | -0.40588533 | -1.44381847 |
| H | -6.22540543 | -0.02788168 | 0.28324881 |
| H | -5.57454839 | 0.63539385 | 2.59244014 |
| C | -1.80631724 | -0.18843137 | -1.18137583 |
| O | -2.16555832 | -0.51255662 | -2.30648525 |
| N | -0.50354026 | -0.02262330 | -0.76477424 |
| C | 0.40355712 | 0.02887069 | -1.71195370 |
| H | 0.06418709 | 0.01975893 | -2.76220396 |
| C | 1.80702624 | 0.02878582 | -1.52878889 |
| H | 2.36528358 | 0.36955685 | -2.40318954 |
| C | 2.48533450 | 0.26453774 | -0.24158832 |
| C | 3.75475109 | 0.87135195 | -0.24284591 |
| C | 1.94578875 | -0.12726492 | 0.99792246 |
| C | 4.45290605 | 1.09705434 | 0.94125526 |
| H | 4.19510879 | 1.17469636 | -1.19604449 |
| C | 2.64689695 | 0.09926614 | 2.18218867 |
| H | 0.97180455 | -0.61127251 | 1.01233373 |
| C | 3.90026450 | 0.71368659 | 2.16489399 |
| H | 5.43376114 | 1.57532396 | 0.90848002 |
| H | 2.20820713 | -0.21196948 | 3.13262992 |
| H | 4.44299883 | 0.88917929 | 3.09519854 |
| C | 1.96127328 | -1.93060337 | -1.94130480 |
| O | 1.79444968 | -2.54181134 | -0.92835920 |
| O | 2.20396037 | -2.01861458 | -3.11108947 |
|  |  |  |  |
|  |  |  |  |

TS-7
Charge $=-1 \quad$ Spin Multiplicity $=1$
C $\quad-4.75726301 \quad 0.37538041 \quad 0.49174782$
C $\quad-3.94212883-0.71809515 \quad 0.21467289$
C $-2.60689065-0.52297830-0.15778052$
C $\quad-2.09268416 \quad 0.77615895-0.25591685$
C $\quad-2.91116691 \quad 1.86949600 \quad 0.02510342$
C $\quad-4.24097253 \quad 1.67040935 \quad 0.39795381$
$\begin{array}{llll}\mathrm{H} & -5.79717083 & 0.22118795 & 0.78284021\end{array}$
$\begin{array}{llll}\mathrm{H} & -4.32112141 & -1.73847559 & 0.28456201\end{array}$
H $\quad-1.05491390 \quad 0.93395878$-0.55468013

| H | -2.50829505 | 2.88040376 | -0.04989027 |
| :--- | ---: | ---: | ---: |
| H | -4.87932558 | 2.52812478 | 0.61593844 |
| C | -1.76313275 | -1.73838541 | -0.41775998 |
| O | -2.19844594 | -2.86330032 | -0.30611908 |
| N | -0.47479390 | -1.47689277 | -0.86998707 |
| C | 0.50846934 | -1.38292330 | -0.07294675 |
| H | 0.40090241 | -1.51936750 | 1.01752295 |
| C | 1.88381004 | -1.01058852 | -0.52566779 |
| C | 2.01912947 | 0.48265639 | -0.26491518 |
| C | 1.85044238 | 1.39755558 | -1.31153716 |
| C | 2.22879436 | 0.96977359 | 1.03260233 |
| C | 1.90084139 | 2.77116227 | -1.07102208 |
| H | 1.67619061 | 1.02683987 | -2.32428283 |
| C | 2.27585482 | 2.34280088 | 1.27282524 |
| H | 2.36041153 | 0.25121877 | 1.84385099 |
| C | 2.11175243 | 3.24838973 | 0.22328677 |
| H | 1.77385884 | 3.47106603 | -1.89878558 |
| H | 2.44169448 | 2.70838059 | 2.28782619 |
| H | 2.14889139 | 4.32224391 | 0.41299456 |
| C | 2.99061597 | -1.80949305 | 0.24217500 |
| O | 4.03148910 | -2.02726666 | -0.39500974 |
| O | 2.71872405 | -2.10601109 | 1.42427871 |
| H | 1.97200782 | -1.19064295 | -1.60462836 |

TS-8
Charge $=-1 \quad$ Spin Multiplicity $=1$
C $\quad 4.83949991 \quad 0.14313138-1.60344746$
C $\quad 3.54938017-0.06044054-1.11505896$
C $\quad 3.32011411 \quad-0.10774562 \quad 0.26511579$
$\begin{array}{llll}\text { C } & 4.39438276 & 0.04887496 & 1.14866887\end{array}$
$\begin{array}{lllll}\text { C } & 5.68387382 & 0.24761859 & 0.66078368\end{array}$
$\begin{array}{lllll}\text { C } & 5.90768068 & 0.29532867 & -0.71737525\end{array}$
$\begin{array}{llll}\mathrm{H} & 5.01378952 & 0.18282922 & -2.67995902\end{array}$
H $\quad 2.70019130$-0.18035198 -1.78732609
$\begin{array}{llll}\mathrm{H} & 4.19476939 & 0.01147803 & 2.22030224\end{array}$
$\begin{array}{llll}\mathrm{H} & 6.51820856 & 0.36669989 & 1.35393563\end{array}$
H $\quad 6.91722678$ 0.45232489 -1.10120363
C $1.93666723-0.30589742 \quad 0.83039338$
$\begin{array}{llll}\text { O } & 1.76489488 & -0.27029002 & 2.04332695\end{array}$
N $\quad 0.96753688$-0.53851752 -0.11883496
C $\quad-0.27753016-0.47444082 \quad 0.29095864$
H $\quad-0.47287310-0.19099471 \quad 1.34005581$

| C | -1.38958540 | -0.68293114 | -0.55588098 |
| :--- | ---: | ---: | ---: |
| H | -1.16040114 | -1.20032017 | -1.49201023 |
| C | -2.73381880 | -0.92898761 | -0.00301179 |
| C | -3.61700859 | -1.79603916 | -0.66872069 |
| C | -3.19552653 | -0.29470078 | 1.16444116 |
| C | -4.90005411 | -2.03835664 | -0.18039147 |
| H | -3.28229129 | -2.29216362 | -1.58294813 |
| C | -4.47492471 | -0.54199019 | 1.65685925 |
| H | -2.54948334 | 0.41589690 | 1.68224554 |
| C | -5.33652637 | -1.41617221 | 0.98998892 |
| H | -5.56205697 | -2.72075905 | -0.71708604 |
| H | -4.80703197 | -0.03903416 | 2.56725840 |
| H | -6.33925690 | -1.60526093 | 1.37624812 |
| C | -1.40916899 | 1.18617575 | -1.32435803 |
| O | -2.21806458 | 1.83232322 | -0.72771396 |
| O | -0.61254686 | 1.18765474 | -2.21499420 |

## TS-9

Charge $=-1 \quad$ Spin Multiplicity $=1$
C $\quad 3.03781693-1.02809336-1.48714598$
C $\quad 2.16041792-0.76879415 \quad-0.43500592$
$\begin{array}{llll}\text { C } & 2.53548979 & 0.11330770 & 0.58522859\end{array}$
$\begin{array}{llll}\text { C } & 3.79295320 & 0.72685504 & 0.54946544\end{array}$
C $\quad 4.66831574 \quad 0.46486688 \quad-0.50083737$
C $\quad 4.29015339-0.41276586-1.52022285$
H $\quad 2.74485052-1.71488102 \quad-2.28240189$
H $\quad 1.18183347-1.24859456-0.39436587$
H $4.06420149 \quad 1.41041156 \quad 1.35513196$
H $\quad 5.64767103 ~ 0.94468560 \quad-0.52825184$
H $\quad 4.97592032$-0.61806652 -2.34385975
$\begin{array}{lllll}\text { C } & 1.61059368 & 0.44354024 & 1.71934628\end{array}$
$\begin{array}{llll}\text { O } & 1.94625593 & 1.17247294 & 2.63044381\end{array}$
N $\quad 0.37236222 \quad-0.19053683 \quad 1.67245378$
C $\quad-0.69770706 \quad 0.51306012 \quad 1.66237282$
H $\quad-0.55613065 \quad 1.62052945 \quad 1.63312607$
C $-2.05804863-0.03664532 \quad 1.65035101$
H $\quad-2.58458939-0.09322723 \quad 2.60729635$
C $\quad-2.74287941-0.25647886 \quad 0.45448934$
C $\quad-2.14087281 \quad-0.08416238 \quad-0.84756352$
C $\quad-4.12200852-0.68221960 \quad 0.41522575$
C $\quad-2.84107209 \quad-0.31320702 \quad-2.02313530$
H $\quad-1.09447077 \quad 0.22977907 \quad-0.90774499$
C $\quad-4.79578628-0.90813008 \quad-0.77207279$

| H | -4.64309437 | -0.83137037 | 1.36574814 |
| :--- | ---: | ---: | ---: |
| C | -4.18022683 | -0.73023537 | -2.02408335 |
| H | -2.32332849 | -0.16274520 | -2.97588684 |
| H | -5.84030825 | -1.23265220 | -0.72723955 |
| H | -4.71981244 | -0.91122848 | -2.95409028 |

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Copies of ${ }^{1} \mathrm{H},{ }^{13} \mathrm{C}$ and ${ }^{19} \mathrm{~F}$ NMR Spectra for Compounds
${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{1}\left(\mathbf{4 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{1}\left(\mathbf{1 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$

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[^1]${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{2}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)



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${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{2}(\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d})$





${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{3}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d}$ )



${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{3}(\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d})$





${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{4}(\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{4}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d}$ )

-36.747
-31.438
-25.221
-22.415
-13.938



${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{5}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)


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${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{5}(\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d})$



${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{6}(\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)



${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{6}(\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d})$

${ }^{1} \mathrm{H}$ NMR spectrum of $7(\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)



${ }^{13} \mathrm{C}$ NMR spectrum of $7(\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d $)$

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${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{8}(\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)




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${ }^{1} \mathrm{H}$ NMR spectrum of 9 ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d}$ )

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{9}(\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d})$




${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{1 0 ( 4 0 0 ~ M H z , ~ C h l o r o f o r m - d ) ~}$


${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{1 0}(\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d})$



${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{1 1}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)


${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{1 1}(\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)



${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{1 2 ( 4 0 0 ~ M H z , ~ C h l o r o f o r m - d ) ~}$ ジ


${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{1 2}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d}$ )
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${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{1 3}\left(\mathbf{4 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$


${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{1 3}\left(\mathbf{1 0 0} \mathbf{M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$

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[^2]${ }^{19}$ F NMR spectrum of $\mathbf{1 3}$ ( $\mathbf{3 7 5} \mathbf{~ M H z}$ DMSO- $\boldsymbol{d}_{6}$ )


${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{1 4}\left(\mathbf{4 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$


${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{1 4}\left(\mathbf{1 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$



${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{1 5}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, DMSO- $\boldsymbol{d}_{6}$ )




${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{1 5}\left(\mathbf{1 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$

${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{1 6}(\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{1 6}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d}$ )

${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{1 7}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)


${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{1 7}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)

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${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{1 8}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{1 8}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)
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${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{1 9}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, DMSO- $\boldsymbol{d}_{6}$ )



${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{1 9}\left(\mathbf{1 0 0} \mathbf{M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$




${ }^{1} \mathrm{H}$ NMR spectrum of $20(\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)

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${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{2 0}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d}$ )

${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{2 1}\left(\mathbf{4 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$

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${ }^{13} \mathrm{C}$ NMR spectrum of $21\left(\mathbf{1 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$



${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{2 2}\left(\mathbf{4 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$


${ }^{13} \mathrm{C}$ NMR spectrum of $22\left(\mathbf{1 0 0} \mathbf{M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$



${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{2 3}\left(\mathbf{4 0 0} \mathbf{~ M H z}, ~ D M S O-\boldsymbol{d}_{6}\right)$


${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{2 3}\left(\mathbf{1 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$

${ }^{19}$ F NMR spectrum of $\mathbf{2 3}$ ( $\mathbf{3 7 5} \mathbf{~ M H z}$ DMSO- $\boldsymbol{d}_{6}$ )




${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{2 4}\left(\mathbf{4 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{2 4}\left(\mathbf{1 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$

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${ }^{1} \mathrm{H}$ NMR spectrum of $25\left(400 \mathrm{MHz}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$



${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{2 5}\left(\mathbf{1 0 0} \mathbf{M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$




${ }^{1} \mathrm{H}$ NMR spectrum of $26(400 \mathrm{MHz}$, Chloroform-d)



${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{2 6}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)


[^3]${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{2 7}(\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{2 7}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)


[^4]${ }^{1} \mathrm{H}$ NMR spectrum of $28\left(\mathbf{4 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$



${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{2 8}\left(\mathbf{1 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$


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${ }^{1} \mathrm{H}$ NMR spectrum of $29\left(\mathbf{4 0 0} \mathbf{~ M H z}\right.$, DMSO－ $\left.\boldsymbol{d}_{6}\right)$

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{2 9}\left(\mathbf{1 0 0} \mathbf{M H z}\right.$ ，DMSO－ $\left.\boldsymbol{d}_{6}\right)$

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${ }^{19}$ F NMR spectrum of 29 ( $\mathbf{3 7 5} \mathbf{~ M H z}$ DMSO- $\boldsymbol{d}_{6}$ )


${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{3 0}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{3 0}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d}$ )

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${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{3 1}(\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{3 1}(\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)

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${ }^{19}$ F NMR spectrum of $\mathbf{3 1}$ ( $\mathbf{3 7 5} \mathbf{~ M H z}$ Chloroform-d)
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${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{3 2}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d}$ )



| ${ }_{190}$ | 180 | ${ }_{170}$ | ${ }_{160}$ | ${ }_{150}$ | $\stackrel{1}{140}$ | ${ }_{130}$ | ${ }_{120}$ | ${ }_{110}^{10}$ | ${ }_{100}^{10}$ | ${ }_{90}$ | ${ }_{80}$ | ${ }_{70}$ | 60 | ${ }_{50}$ | 40 | ${ }_{30}$ | ${ }_{20}^{10}$ |
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${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{3 3}\left(\mathbf{4 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{3 3}\left(\mathbf{1 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$
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| ${ }^{1} 00$ | 190 | 180 | 170 | 160 | 150 | 140 | ${ }_{130}$ | 120 | 110 | 100 | 90 | 80 | 70 | ${ }_{6} 1$ | ${ }_{50}$ | 40 | ${ }^{1} 0$ | ${ }_{20}$ | 10 | ${ }_{0}$ |
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${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{3 4}\left(\mathbf{4 0 0} \mathbf{~ M H z}, \mathbf{D M S O}-\boldsymbol{d}_{6}\right)$

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{3 4}\left(\mathbf{1 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$



${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{3 5}$（ $\mathbf{4 0 0} \mathbf{~ M H z}$ ，Chloroform－d）

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${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{3 5} \mathbf{( 1 0 0} \mathbf{~ M H z}$ ，Chloroform－d）

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| ${ }_{190}$ | 180 | 170 | ${ }_{160}$ | ${ }_{150}^{1}$ | ${ }_{140}^{1 /}$ | 130 | ${ }_{120}^{1}$ | 110 | ${ }_{100}$ | 90 | ${ }_{80}$ | ${ }_{70}$ | $1{ }_{60}$ | ${ }_{50}$ | 10 | ${ }_{30}$ | 10 | 10 | ${ }_{0}$ |
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${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{3 6}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)




${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{3 6}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)






${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{3 7}(\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)




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${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{3 7}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d}$ )

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[^5]${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{3 8}(\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{3 8}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)

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${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{3 9}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)


${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{3 9} \mathbf{( 1 0 0 ~ M H z}$, Chloroform-d)





${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{4 0}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)

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${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{4 0}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d}$ )


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[^6]${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{4 1}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)


${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{4 1}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)


${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{4 2}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)




${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{4 2}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)




${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{4 3}\left(\mathbf{1 0 0} \mathbf{M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$



[^7]${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{4 4} \mathbf{( 4 0 0 ~ M H z}$, Chloroform-d)


${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{4 4}$ ( $\mathbf{1 5 0} \mathbf{~ M H z}$, Chloroform-d)

${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{4 5}$（ $\mathbf{4 0 0} \mathbf{~ M H z}$ ，Chloroform－d）

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{4 5}$（ $\mathbf{1 0 0} \mathbf{~ M H z}$ ，Chloroform－d）

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${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{4 6}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{4 6}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)


${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{4 7}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{4 7}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)

${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{4 8}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)


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${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{4 8}(\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)

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${ }^{1} \mathrm{H}$ NMR spectrum of $49\left(400 \mathrm{MHz}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$


${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{4 9}\left(\mathbf{1 0 0} \mathbf{~ M H z}\right.$, DMSO- $\left.\boldsymbol{d}_{6}\right)$



${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{5 0}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{5 0}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)

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${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{5 1}$ ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{5 1}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)
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${ }^{1} \mathrm{H}$ NMR spectrum of 52 ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)

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${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{5 2}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform- $\boldsymbol{d}$ )




${ }^{1} \mathrm{H}$ NMR spectrum of $\mathbf{5 3} \mathbf{( 4 0 0 ~ M H z}$, Chloroform-d)

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${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{5 3}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)

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${ }^{1} \mathrm{H}$ NMR spectrum of 54 ( $\mathbf{4 0 0} \mathbf{~ M H z}$, Chloroform-d)

${ }^{13} \mathrm{C}$ NMR spectrum of $\mathbf{5 4}$ ( $\mathbf{1 0 0} \mathbf{~ M H z}$, Chloroform-d)







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