SUPPORTING MATERIAL

1-(3,4-Dimethoxyphenyl)-3-(4-methoxyphenyl)-

-3-(1*H*-1,2,4-triazol-1-yl)propan-1-one

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1-(3,4-Dimethoxyphenyl)-3-(4-methoxyphenyl)prop-2-enone

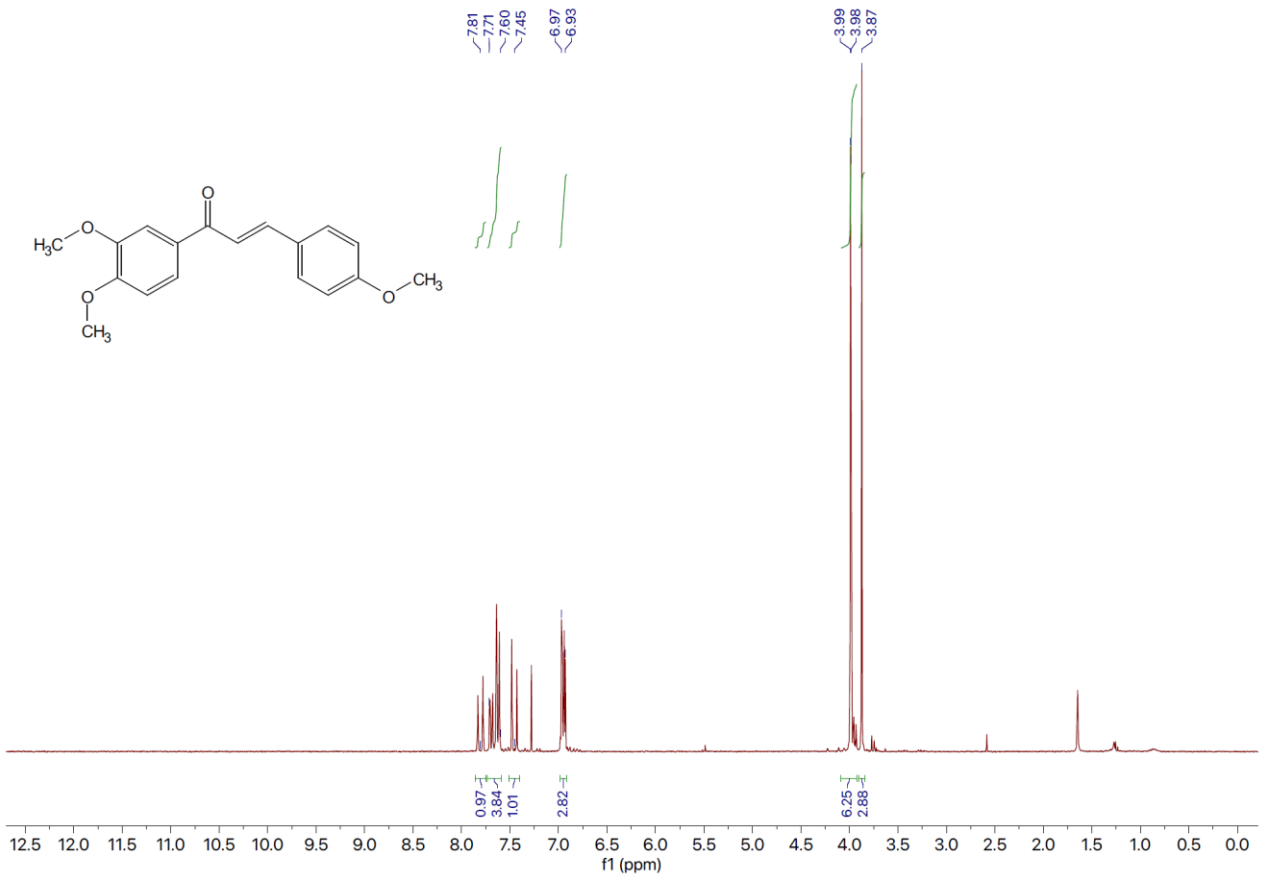


Figure S1. 1H-NMR spectrum of 1-(3,4-dimethoxyphenyl)-3-(4-methoxyphenyl)prop-2-enone.

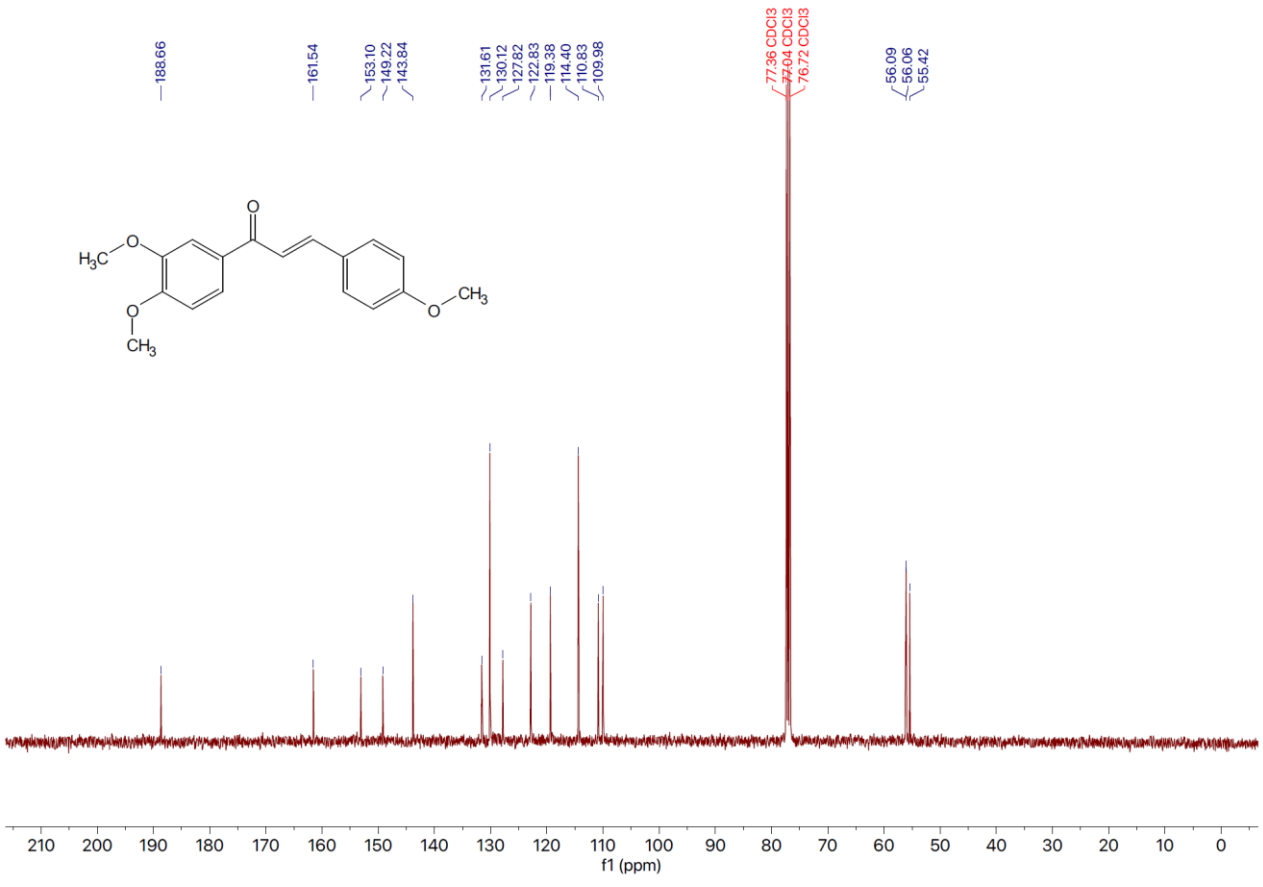


Figure S2. 13C-NMR spectrum of 1-(3,4-dimethoxyphenyl)-3-(4-methoxyphenyl)prop-2-enone.

1-(3,4-Dimethoxyphenyl)-3-(4-methoxyphenyl)-3-(1*H*-1,2,4-triazol-1-yl)propan-1-one

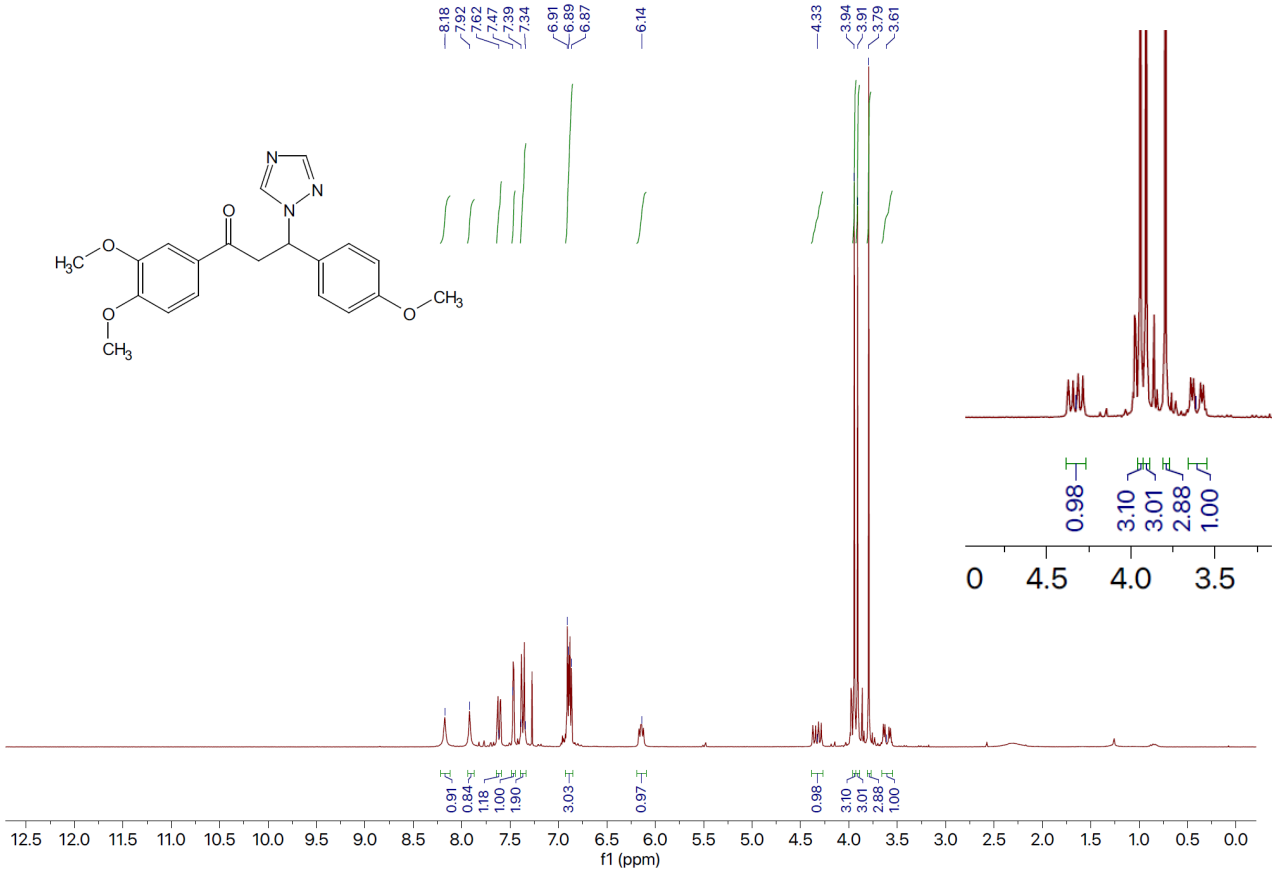


Figure S3. 1H-NMR spectrum of 1-(3,4-dimethoxyphenyl)-3-(1*H*-1,2,4-triazol-1-yl)propan-1-one.

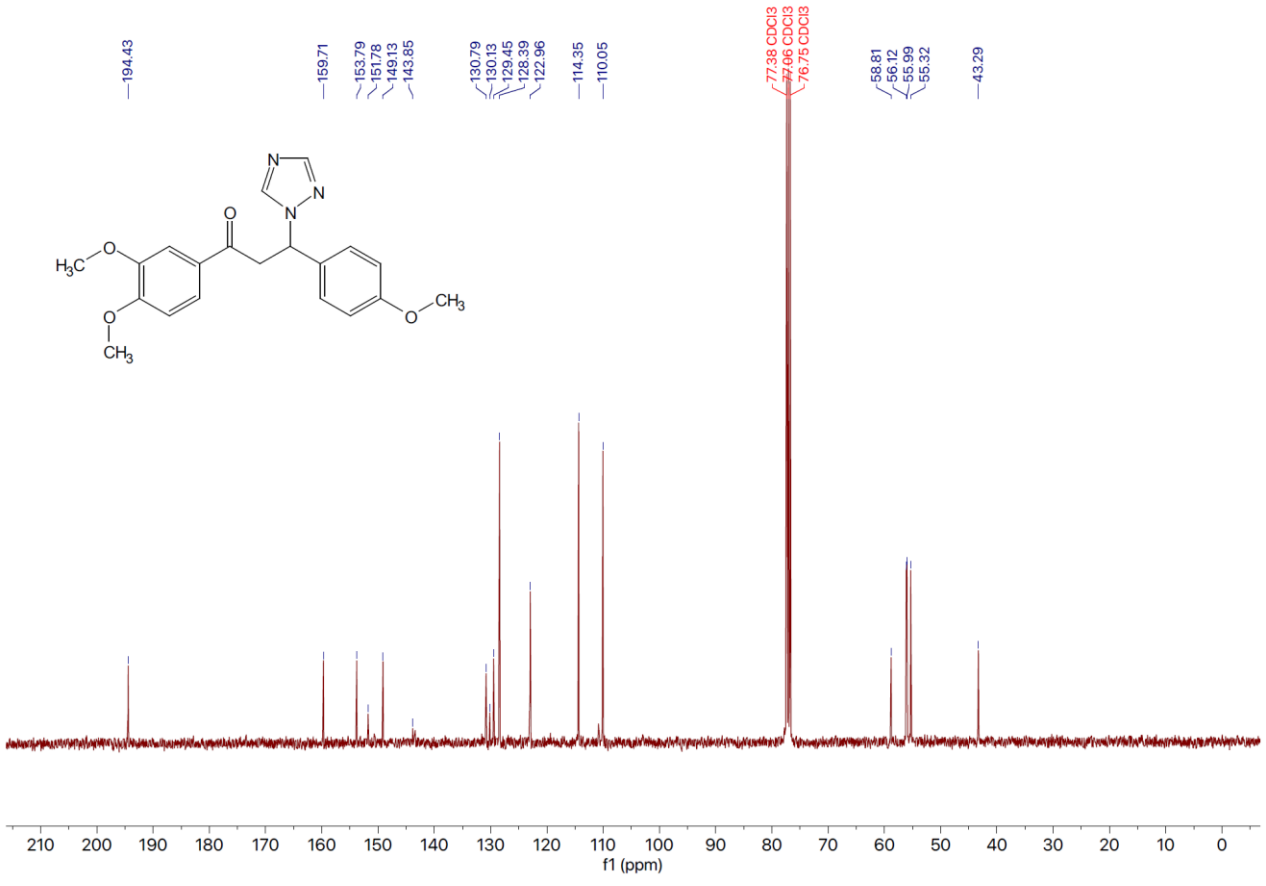


Figure S4. 13C-NMR spectrum of 1-(3,4-dimethoxyphenyl)-3-(1*H*-1,2,4-triazol-1-yl)propan-1-one.

Green Metrics – Synthesis of 1-(3,4-Dimethoxyphenyl)-3-(4-methoxyphenyl)-3-(1*H*-1,2,4-triazol-1-yl)propan-1-one

Reaction (balanced chemical equation)

4-Anisaldehyde 136.15 g/mol
3,4-Di(MeO)acetophenon 180.20 g/mol

References

Material Efficiency

PART ONE

Reactants	MW(g/mol)	Stoich. Coeff. (SC)	Adjusted MW (g/mol)	density (g/mL)	volume (mL)	mass used (g)	moles	comments		stoich. Moles	stoich. Mass (g)	mole ratio	mass ratio	excess mass (g)	mass kernel unreacted reagent (g)
4-Anisaldehyde	136.15	1	136.15			0.272	0.0020		limiting reagent	0.00	0.272	1	1	0	0.05
3,4-Di(MeO)acetophen	180.2	1	180.2			0.36	0.0020			0.00	0.360002938	0.999992	0.9999918	-2.93794E-06	0.06
		SUM	316.35			0.632	SUM				0.63		1.0000	0.00	0.11

Products	MW(g/mol)	Stoich. Coeff.	Adjusted MW (g/mol)
Chalcone, 3,4,4'-tri(MeO)	298.33	1	298.33
H2O	18.02	1	18.02
		1	0
		1	0
		SUM	316.35 chemical equation is balanced

Reaction Solvents	MW(g/mol)	density (g/mL)	volume (mL)	mass used (g)	comments
				0 SUM	

Catalysts	MW(g/mol)	density (g/mL)	volume (mL)	mass used (g)	moles	comments
NaOH	40			0.08	0.00	
					#¡DIV/0!	
					#¡DIV/0!	
				0.08 SUM		

Workup Materials	density (g/mL)	volume (mL)		mass used (g)	comments
EtOH	0.789		5	3.945	
				3.945 SUM	

Purification Materials	density (g/mL)	volume (mL)	mass used (g)	comments
[redacted]			0	
			0	
			0 SUM	

TOTAL INPUT MASS 4.657 g

Target Product	MW(g/mol)	moles collected		mass collected
Chalcone, 3,4,4'-tri(MeO)	298.33	0.00166	MASS OF TARGET PRODUCT	0.495 g

MASS RAW WASTE = TOTAL INPUT MASS - MASS OF TARGET PRODUCT 4.162 g

PART TWO

Recycling-Recovery of Materials

Item		mass recovered
EtOH	[redacted]	3.1 g
		g
		g
MASS RECOVERED MATERIALS		3.1 SUM

MASS ADJUSTED WASTE = MASS RAW WASTE - MASS RECOVERED MATERIALS 1.062 g

E-factor (E) = mass adjusted waste / mass product 2.145

Process Mass Intensity (PMI) = (total input mass - mass recovered materials) / mass product 3.145

Reaction Mass Efficiency (RME) = 100 * (mass product / (total input mass - mass recovered materials)) 31.8 %

Atom Economy (AE) = 100 * (MW product / sum of MWs of reactants) 94.3 %

Yield (Y) = 100 * (moles product / moles limiting reagent) * (SC limiting reagent / SC Product) 83.1 % SC product = 1

CHECK CALCULATIONS

PMI = 1 + E 3.145

RME = 1/(1 + E) 0.3

PART THREE

Metrics Report Summary

Actual Mass of Reagents	0.632	g
Stoichiometric Mass of Reagents	0.63	g
Stoichiometric Factor	0.999995351	
Materials Recovery Parameter	0.405908799	

Raw E-factor profile

E-kernel	0.276773612	
E-excess	-5.93522E-06	
E-rxn solvent	0	
E-catalyst	0.161616162	
E-work-up	7.96969697	
E-purification	0	
E-aux	8.13	
E-total	8.408080808	

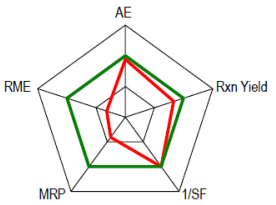
Yield	83.1	%
AE	94.3	%
PMI	3.145	
RME (global)	31.8	%

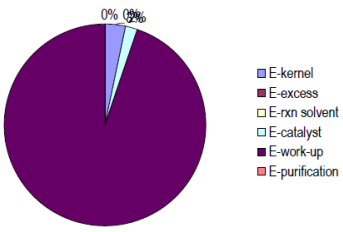
Use for synthesis plans only

target mass of product		g
scaling factor	0	
scaled mass of limiting reagent	0	g

Parameter	Actual	Ideal Limit
AE	0.943	1
Rxn Yield	0.831	1
1/SF	1.000	1
MRP	0.405908799	1
RME	0.318	1

VMR 0.754314189
(vector magnitude ratio)





Green Metrics – Synthesis of 1-(3,4-Dimethoxyphenyl)-3-(4-methoxyphenyl)prop-2-enone

Reaction (balanced chemical equation)

Chalcone, 3,4,4'-tri(MeO) 298.33 g/mol
1H-1,2,4-triazole 69.01 g/mol

References

Material Efficiency

PART ONE

Reactants	MW(g/mol)	Stoich. Coeff. (SC)	Adjusted MW (g/mol)	density (g/mL)	volume (mL)	mass used (g)	moles	comments		stoich. Moles	stoich. Mass (g)	mole ratio	mass ratio	excess mass (g)	mass kernel unreacted reagent (g)
Chalcone, 3,4,4'-tri(MeO)	298.33	1	298.33			0.15	0.0005		limiting reagent	0.00	0.15	1	1	0	0.09
1H-1,2,4-triazole	69.01	1	69.01			0.035	0.0005			0.00	0.034698153	1.008699	1.0086992	0.000301847	0.02
		SUM	367.34			0.185	SUM				0.18		1.0016	0.00	0.11

Products	MW(g/mol)	Stoich. Coeff.	Adjusted MW (g/mol)
Diaryl-azolyl-propanone	367.34	1	367.34
		1	0
		1	0
		1	0
		SUM	367.34 chemical equation is balanced

Reaction Solvents	MW(g/mol)	density (g/mL)	volume (mL)	mass used (g)	comments
				0 SUM	

Catalysts	MW(g/mol)	density (g/mL)	volume (mL)	mass used (g)	moles	comments
bcmim-Cl	220.45			0.011	0.00	
					#¡DIV/0!	
					#¡DIV/0!	
				0.011	SUM	

Workup Materials	density (g/mL)	volume (mL)	mass used (g)	comments
AcOEt	0.902	4	3.608	
			3.608	SUM

Purification Materials	density (g/mL)	volume (mL)	mass used (g)	comments
[redacted]			0	
			0	
			0	SUM

TOTAL INPUT MASS 3.804 g

Target Product	MW(g/mol)	moles collected		mass collected
Diaryl-azolyl-propanone	367.34	0.00019	MASS OF TARGET PRODUCT	0.07 g

MASS RAW WASTE = TOTAL INPUT MASS - MASS OF TARGET PRODUCT 3.734 g

PART TWO

Recycling-Recovery of Materials

Item	mass recovered
[redacted]	
AcOEt	3 g
bcmim-Cl	0.011 g
	g
MASS RECOVERED MATERIALS	3.011 SUM

MASS ADJUSTED WASTE = MASS RAW WASTE - MASS RECOVERED MATERIALS 0.723 g

E-factor (E) = mass adjusted waste / mass product 10.329

Process Mass Intensity (PMI) = (total input mass - mass recovered materials) / mass product 11.329

Reaction Mass Efficiency (RME) = 100 * (mass product / (total input mass - mass recovered materials)) 8.8 %

Atom Economy (AE) = 100 * (MW product / sum of MWs of reactants) 100.0 %

Yield (Y) = 100 * (moles product / moles limiting reagent) * (SC limiting reagent / SC Product) 37.9 % SC product = 1

CHECK CALCULATIONS

PMI = 1 + E 11.329

RME = 1/(1 + E) 0.1

PART THREE

Metrics Report Summary

Actual Mass of Reagents	0.185 g
Stoichiometric Mass of Reagents	0.18 g
Stoichiometric Factor	1.001634272
Materials Recovery Parameter	0.233291299

Raw E-factor profile

E-kernel	1.638545044
E-excess	0.004312099
E-rxn solvent	0
E-catalyst	0.157142857
E-work-up	51.54285714
E-purification	0
E-aux	51.70
E-total	53.34285714

Yield	37.9 %
AE	100.0 %
PMI	11.329
RME (global)	8.8 %

Use for synthesis plans only

target mass of product	g
scaling factor	0
scaled mass of limiting reagent	0 g

Parameter	Actual	Ideal Limit
AE	1.000	1
Rxn Yield	0.379	1
1/SF	0.998	1
MRP	0.233291299	1
RME	0.088	1

VMR 0.663716029
(vector magnitude ratio)