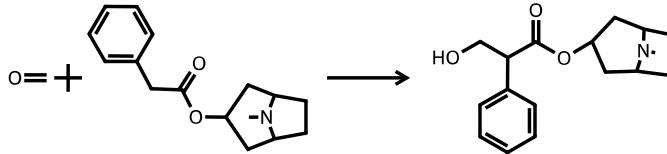
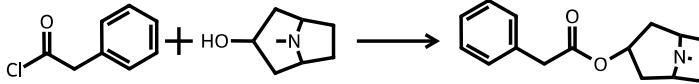
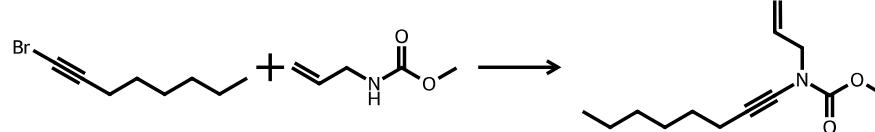
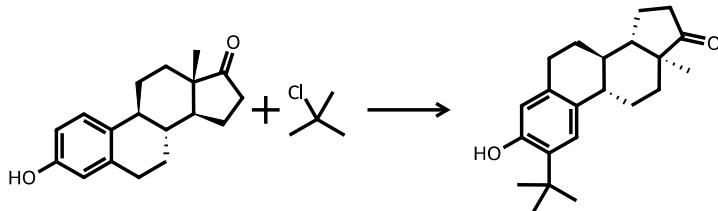
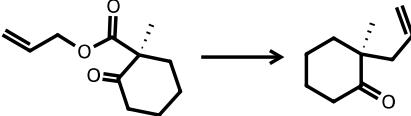
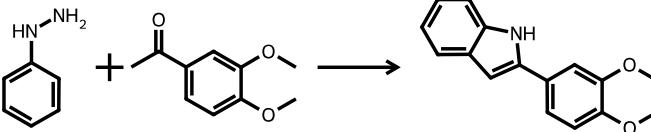


ID	Step	Yield	Scale	Reaction
CHEMIFY-0001	Step 1	98 %	8.8 mmol	<p>Reaction scheme for Step 1 of CHEMIFY-0001:</p> <p>Starting materials: 4-bromoaniline and 4-methylbenzenesulfonyl chloride.</p> <p>Product: N-(4-bromophenyl)-4-methylbenzenesulfonamide.</p>
CHEMIFY-0002	Step 1	56 %	20.0 mmol	<p>Reaction scheme for Step 1 of CHEMIFY-0002:</p> <p>Starting materials: Diisopropyl malonate and allyl bromide.</p> <p>Products: Two diisopropyl substituted products resulting from the addition of allyl bromide to the malonate.</p>
CHEMIFY-0004	Step 1	84 %	10.0 mmol	<p>Reaction scheme for Step 1 of CHEMIFY-0004:</p> <p>Starting materials: A cyclic amine, a borane reagent, and Li⁺.</p> <p>Product: A hydroxylated product where the nitrogen atom is negatively charged.</p>

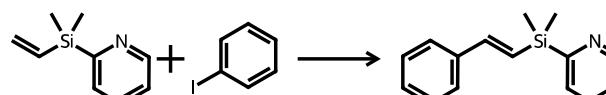
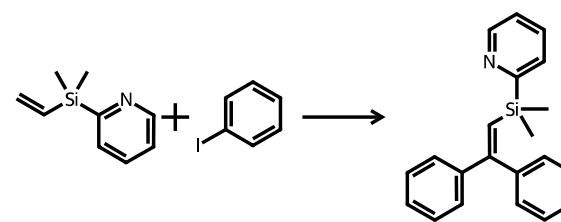
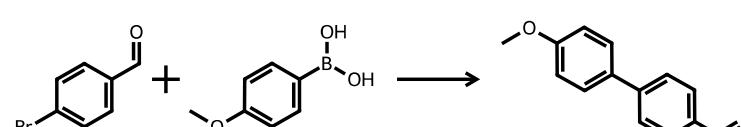
ID	Step	Yield	Scale	Reaction
CHEMIFY-0005	Step 1	37 %	13.0 mmol	
CHEMIFY-0006	Step 1	65 %	20.0 mmol	
CHEMIFY-0010	Step 1	43 %	10.0 mmol	

ID	Step	Yield	Scale	Reaction
CHEMIFY-0011	Step 1	94 %	5.0 mmol	
CHEMIFY-0012	Step 1	92 %	2.0 mmol	
CHEMIFY-0013	Step 1	62 %	15.0 mmol	

ID	Step	Yield	Scale	Reaction
CHEMIFY-0014	Step 1	60 %	25.1 mmol	
CHEMIFY-0015	Step 1	56 %	0.5 mmol	
CHEMIFY-0016	Step 1	64 %	12.0 mmol	

ID	Step	Yield	Scale	Reaction
CHEMIFY-0017	Step 1	86 %	5.0 mmol	<p>Reaction scheme for CHEMIFY-0017, Step 1:</p> <p>Reactants: 4-bromobiphenyl and 4-nitrophenyl acetate.</p> <p>Product: 4-(4-acetoxybiphenyl)-4-nitrophenol.</p>
CHEMIFY-0018	Step 1	36 %	100.0 mmol	<p>Reaction scheme for CHEMIFY-0018, Step 1:</p> <p>Reactants: Diethyl malonate and CO₂.</p> <p>Product: Diethyl 2-hydroxy-3-oxobutylmalonate.</p>
CHEMIFY-0020	Step 1		4.0 mmol	<p>Reaction scheme for CHEMIFY-0020, Step 1:</p> <p>Reactant: 2-fluorobiphenyl-2-carbonyl fluoride.</p> <p>Product: 2-(2-fluorophenyl)-2-hydroxypropane-1,1-difluoride.</p>

ID	Step	Yield	Scale	Reaction
CHEMIFY-0021	Step 1	68.8 %	2.64 mmol	<p>Detailed description: This reaction shows the formation of a cyclic boronate ester. On the left, there is a biphenyl ring with a hydroxyl group at the para position. To its right is a plus sign, followed by a 2-bromo-3-thienylboronic acid pinacol ester molecule. An arrow points to the right, leading to the final product, which is a cyclic boronate ester where the biphenyl ring is linked to the thienyl ring via the boron atom.</p>
CHEMIFY-0022	Step 1	32 %	1.86 mmol	<p>Detailed description: This reaction shows the cyclization of a complex organic molecule. The starting material is a linear molecule with an iodide group on one end and a chlorine atom on another. It also contains a cyclohexylamino group and a carbonyl group. An arrow points to the right, leading to the cyclized product, which is a substituted indole derivative where the iodide and chlorine atoms are now part of the indole ring system.</p>
CHEMIFY-0023	Step 1	35 %	6.0 mmol	<p>Detailed description: This reaction shows a multi-component synthesis. The starting materials are cyclohexylidenecyanoimidium, allylamine, 4-chlorobenzaldehyde, and 2-iodophenol. An arrow points to the right, leading to the final product, which is a substituted indole derivative formed through a series of reactions involving these components.</p>

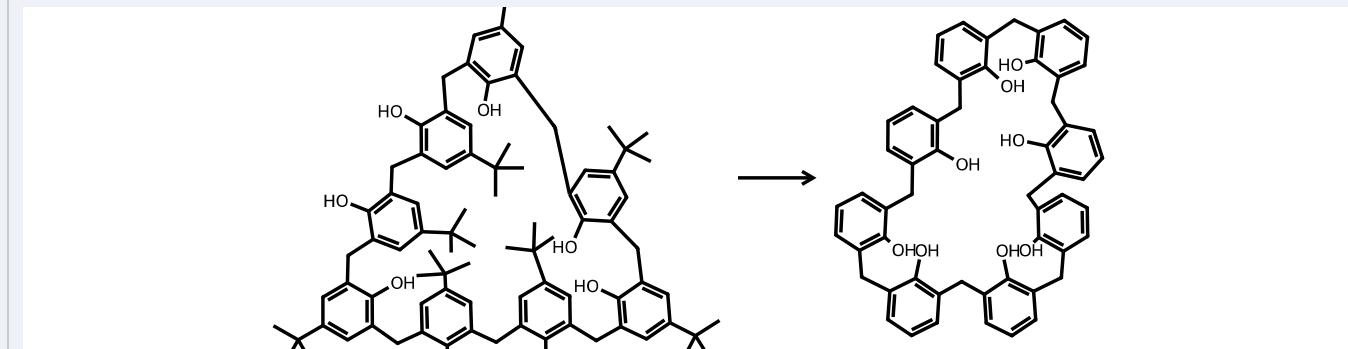
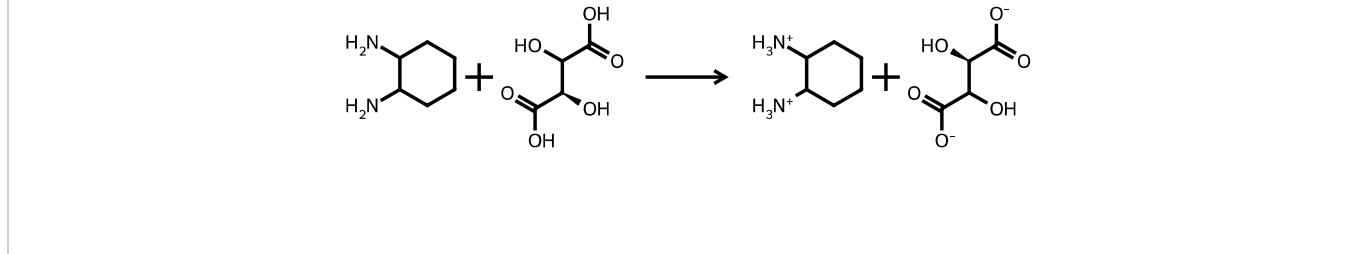
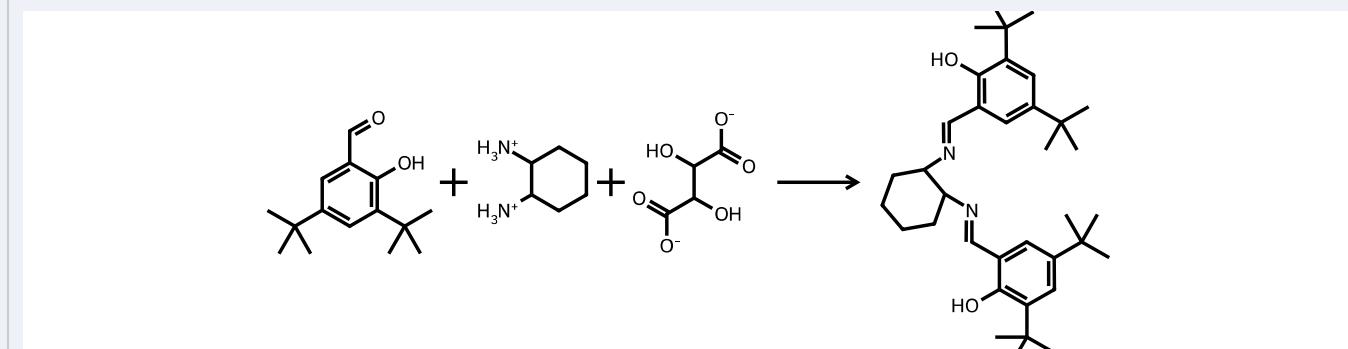
ID	Step	Yield	Scale	Reaction
CHEMIFY-0024	Step 1	65 %	3.10 mmol	
CHEMIFY-0025	Step 1	74 %	3.10 mmol	
CHEMIFY-0026	Step 1	61 %	5.02 mmol	

ID	Step	Yield	Scale	Reaction
CHEMIFY-0027	Step 1	84 %	5.0 mmol	<p>Reaction scheme for Step 1 of CHEMIFY-0027:</p> <p>Starting materials:</p> <ul style="list-style-type: none"> 4-nitroiodobiphenyl (a biphenyl ring with a nitro group at position 4 and an iodine atom at position 4') 2-hydroxypropanoic acid (propionic acid) <p>Product:</p> <p>2-(4-nitrophenyl)-2-hydroxypropanoic acid (a biphenyl ring with a nitro group at position 4, a carboxylic acid group (-COOH) at position 2, and a hydroxyl group (-OH) at position 2')</p>
CHEMIFY-0028	Step 1	66 %	50.0 mmol	<p>Reaction scheme for Step 1 of CHEMIFY-0028:</p> <p>Starting materials:</p> <ul style="list-style-type: none"> cyclohexene oxide Water (HO-OH) <p>Product:</p> <p>cyclohexanol (a cyclohexane ring with a hydroxyl group (-OH))</p>
CHEMIFY-0029	Step 1	62 %	25.0 mmol	<p>Reaction scheme for Step 1 of CHEMIFY-0029:</p> <p>Starting materials:</p> <ul style="list-style-type: none"> diethyl malonate (two ethyl ester groups attached to a central carbon atom) 1,2-dibromoethane (bromopropane) <p>Product:</p> <p>2,2-dihydroxy-1,3-dioxolan-4-one (a four-membered ring containing two carbonyl groups and two hydroxyl groups)</p>

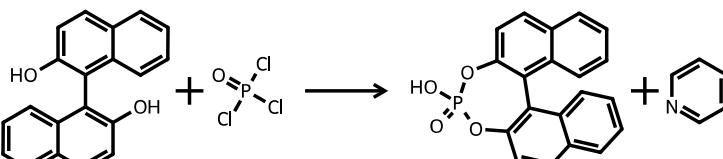
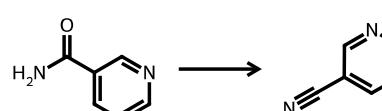
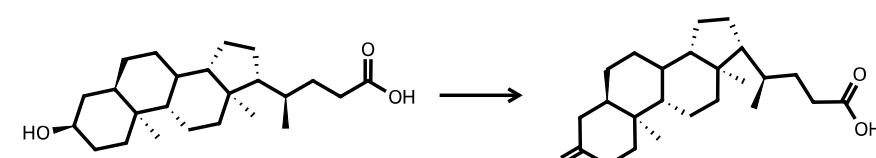
ID	Step	Yield	Scale	Reaction
CHEMIFY-0030	Step 1	88 %	5.0 mmol	<p>Reaction scheme for Step 1 of CHEMIFY-0030:</p> <p>Starting materials: 4-methoxybenzylamine and diisopropyl carbonic anhydride.</p> <p>Product: N,N-diisopropyl-4-methoxybenzylamine.</p>
CHEMIFY-0032	Step 1	36 %	40.0 mmol	<p>Reaction scheme for Step 1 of CHEMIFY-0032:</p> <p>Starting materials: 2-chloro-2-methylpropane and 2-hydroxypropane.</p> <p>Product: 2-(2-hydroxypropan-2-yl)-2-methylpropane and trifluoromethanesulfonic acid.</p>
CHEMIFY-0033	Step 1	59 %	33.8 mmol	<p>Reaction scheme for Step 1 of CHEMIFY-0033:</p> <p>Starting material: Ethyl chloroformate.</p> <p>Product: 2-(2-oxo-2,3-dimethyl-1,3-dioxolan-4-yl)-4,5-dimethylfuran.</p>

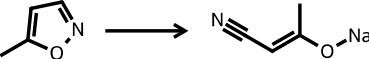
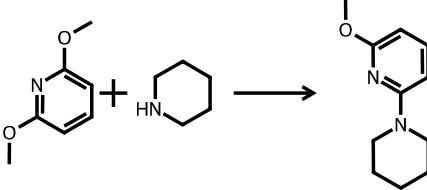
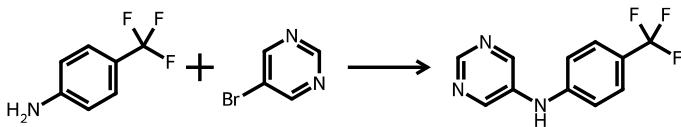
ID	Step	Yield	Scale	Reaction
CHEMIFY-0034	Step 1	81 %	90.5 mmol	<p>Reaction scheme for CHEMIFY-0034:</p> <p>Starting materials: Acrylic acid chloride (<chem>CC(=O)Cl</chem>) and allylamine (<chem>CC=CCN</chem>).</p> <p>Product: N-(allyl)acrylamide (<chem>CC=CCN(C(=O)C=O)C</chem>).</p>
CHEMIFY-0035	Step 1	91 %	10.0 mmol	<p>Reaction scheme for CHEMIFY-0035:</p> <p>Starting materials: Hex-5-yn-1-yl bromide (<chem>BrC#CCCCC</chem>) and 1-bromo-2-methylimidazolidin-2-one (<chem>BrN1C=CC2=C1C(=O)C(=O)C2</chem>).</p> <p>Product: 1-(hex-5-ynyl)-2-methylimidazolidin-2-one (<chem>BrC#CCCCC1C=CC2=C1C(=O)C(=O)C2</chem>).</p>
CHEMIFY-0037	Step 1	74 %	9.0 mmol	<p>Reaction scheme for CHEMIFY-0037:</p> <p>Starting materials: A bis(alkene acetoxy) compound (<chem>CC=CCOC(=O)CCCCCCOC(=O)CC=CC</chem>) and cyclopentadiene (<chem>c1ccccc1</chem>).</p> <p>Product: A bicyclic product formed by the Diels-Alder reaction between the alkene and cyclopentadiene.</p>

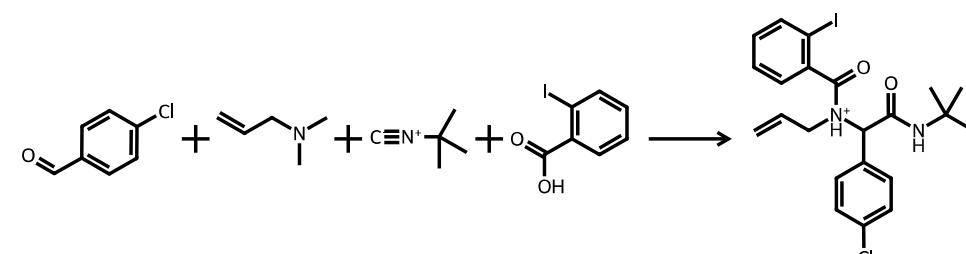
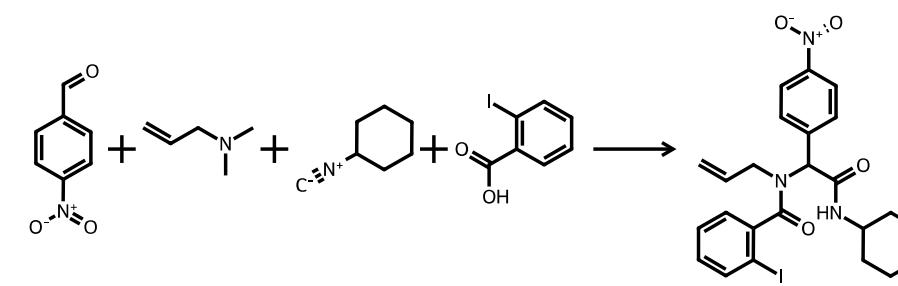
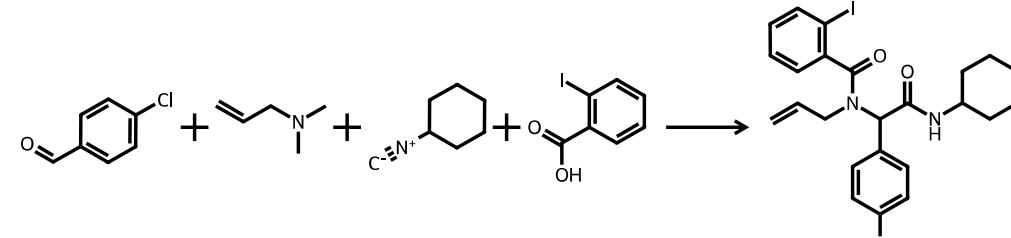
ID	Step	Yield	Scale	Reaction
CHEMIFY-0038	Step 1	52 %	45.0 mmol	<p>Reaction scheme for CHEMIFY-0038, Step 1:</p> <p>Starting materials: N-vinylcyclopentanone and phenyl chloroformate.</p> <p>Product: N-(phenylcarbamoyl)-N-vinylcyclopentanone.</p>
CHEMIFY-0040	Step 1	36 %	33.3 mmol	<p>Reaction scheme for CHEMIFY-0040, Step 1:</p> <p>Starting material: 4-hydroxy-2,6-diisopropylphenol.</p> <p>Product: Branched polymer chain formed by the polymerization of the starting material.</p>
CHEMIFY-0041	Step 1	65 %	25.6 mmol	<p>Reaction scheme for CHEMIFY-0041, Step 1:</p> <p>Starting materials: -OH and 2-carboxy-1-pyrrolidinecarboxylic acid.</p> <p>Product: Cyclic amide formed by the reaction of the hydroxyl group and the carboxylic acid group.</p>

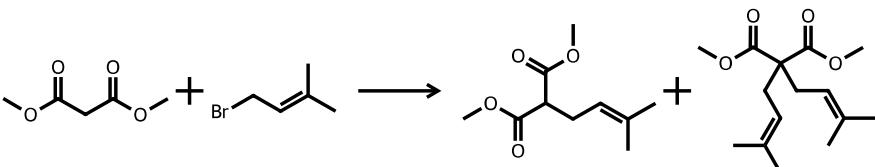
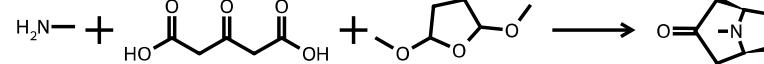
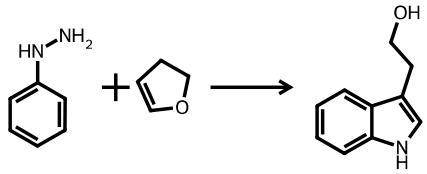
ID	Step	Yield	Scale	Reaction
CHEMIFY-0042	Step 1	58 %	0.77 mmol	
CHEMIFY-0043	Step 1	76 %	100.0 mmol	
CHEMIFY-0044	Step 1	85 %	11.2 mmol	

ID	Step	Yield	Scale	Reaction
CHEMIFY-0045	Step 1	70 %	1.5 mmol	
CHEMIFY-0046	Step 1	99 %	15.0 mmol	
CHEMIFY-0047	Step 1	71 %	5.00 mmol	

ID	Step	Yield	Scale	Reaction
CHEMIFY-0048	Step 1	40 %	34.9 mmol	
CHEMIFY-0049	Step 1		20.0 mmol	
CHEMIFY-0050	Step 1	65 %	1.35 mmol	

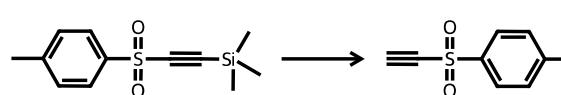
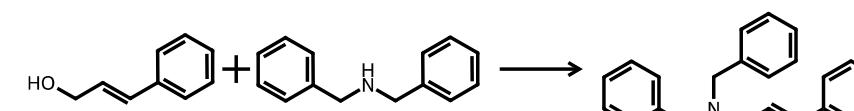
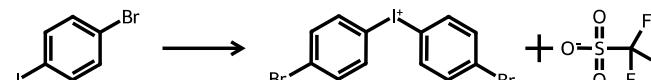
ID	Step	Yield	Scale	Reaction
CHEMIFY-0051	Step 1	76 %	33.0 mmol	
CHEMIFY-0052	Step 1	53 %	10.1 mmol	
CHEMIFY-0053	Step 1	75 %	5.0 mmol	

ID	Step	Yield	Scale	Reaction
CHEMIFY-0054	Step 1	56 %	12.0 mmol	
CHEMIFY-0055	Step 1	80 %	12.0 mmol	
CHEMIFY-0056	Step 1	78 %	12.0 mmol	

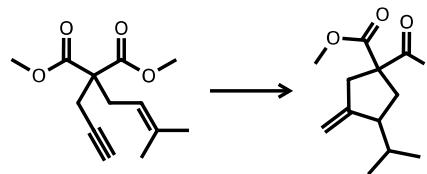
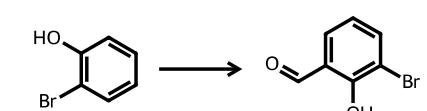
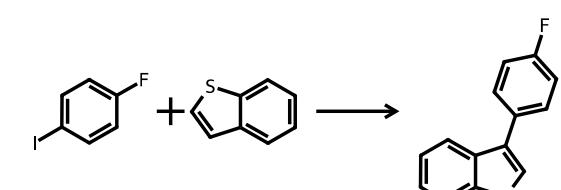
ID	Step	Yield	Scale	Reaction
CHEMIFY-0057	Step 1	31 %	20.0 mmol	 <p>Reaction scheme for Step 1 of CHEMIFY-0057. The reactants are a diisopropyl acetylacetate derivative and a substituted allyl bromide. The products are two isomeric compounds resulting from the addition reaction.</p>
CHEMIFY-0075	Step 1	56 %	20 mmol	 <p>Reaction scheme for Step 1 of CHEMIFY-0075. The reactants are a primary amine, a hydroxy acid, and a cyclic acetal. The product is a cyclic imide formed by the condensation of these components.</p>
CHEMIFY-0077	Step 1	33 %	30 mmol	 <p>Reaction scheme for Step 1 of CHEMIFY-0077. The reactants are a substituted benzyl amine and a cyclic ether. The product is a substituted indole formed by the condensation of these components.</p>

ID	Step	Yield	Scale	Reaction
CHEMIFY-0078	Step 1	64 %	40 mmol	<p>Reaction scheme for CHEMIFY-0078:</p> <p>Starting materials: Hexanedioic acid (HOOC(CH₂)₄COOH) and allyl alcohol (CH₂=CH-CH₂-OH).</p> <p>Product: Bis(allyl ester) formed by the condensation of two molecules of the diacid with one molecule of allyl alcohol.</p>
CHEMIFY-0079	Step 1	38 %	10 mmol	<p>Reaction scheme for CHEMIFY-0079:</p> <p>Starting material: A cyclic enone derivative (cyclic ketone with a vinyl group).</p> <p>Product: A bicyclic product formed by the cyclization of the enone.</p>
CHEMIFY-0080	Step 1			<p>Reaction scheme for CHEMIFY-0080:</p> <p>Starting materials: Chlorotriethylsilane (Cl-Si(CH₃)₃) and ethyl bromoformate (CH₃COBr).</p> <p>Product: Ethyl 2-(chlorotriethylsilyl)acetate (CH₃CO-O-CH₂-Si(CH₃)₃).</p>

ID	Step	Yield	Scale	Reaction
CHEMIFY-0081	Step 1			
CHEMIFY-0082	Step 1			
CHEMIFY-0084	Step 1			

ID	Step	Yield	Scale	Reaction
CHEMIFY-0085	Step 1			
CHEMIFY-0086	Step 1			
CHEMIFY-0087	Step 1			

ID	Step	Yield	Scale	Reaction
CHEMIFY-0088	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0088:</p> <p>Starting materials:</p> <ul style="list-style-type: none"> Benzaldehyde: <chem>O=Cc1ccccc1</chem> 4-(4-aminophenyl)-2-(4-fluorophenyl)-5-methylimidazole: <chem>Nc1ccc(cc1)N(c2ccccc2)c3cc(F)c(F)c(F)c3</chem> <p>Product:</p> <p>4-(4-(4-aminophenyl)-2-(4-fluorophenyl)-5-methylimidazol-1-yl)benzaldehyde: <chem>CC(=O)c1ccc(cc1)N(c2ccccc2)c3cc(F)c(F)c(F)c3</chem></p>
CHEMIFY-0089	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0089:</p> <p>Starting material:</p> <p>2-(4-methoxybutyl)phenol: <chem>CC(=O)c1ccc(O)cc(COC)c1</chem></p> <p>Product:</p> <p>2-(4-methoxybutyl)-3,4-dihydro-2H-pyran-4-one: <chem>CC(=O)c1ccc2c(c1)C(=O)NC(=O)C2OC</chem></p>
CHEMIFY-0090	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0090:</p> <p>Starting material:</p> <p>2,2,4,4-tetramethyl-2,4-pentadiene-1,5-dione: <chem>CC(=O)C(C(C)(C)C)=CC(C(C)(C)C)=O</chem></p> <p>Product:</p> <p>2,2,4,4-tetramethyl-2-((2,4-pentadienyl)ethynyl)-4,4-dimethyl-2H-pyran-4-one: <chem>CC(=O)C(C(C)(C)C)=CC(C(C)(C)C)=CC#CC(=O)C(C(C)(C)C)=O</chem></p>

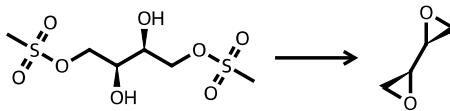
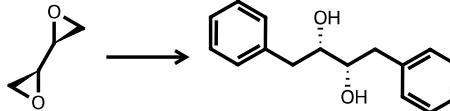
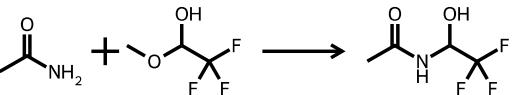
ID	Step	Yield	Scale	Reaction
CHEMIFY-0091	Step 1			
CHEMIFY-0092	Step 1			
CHEMIFY-0093	Step 1			

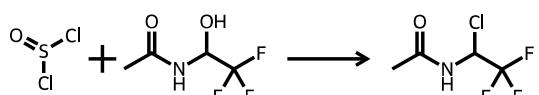
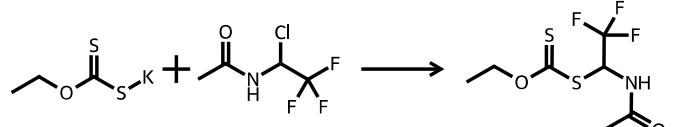
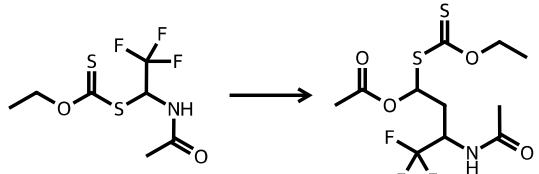
ID	Step	Yield	Scale	Reaction
CHEMIFY-0094	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0094:</p> <p>Starting materials: 1-phenylpropene and allyl phenyl ether.</p> <p>Product: 3-(2-methoxyphenyl)-2-phenylpropan-2-yl phenyl ether.</p>
CHEMIFY-0095	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0095:</p> <p>Starting material: 2-bromo-3-thiophenylmethanol.</p> <p>Product: 2-methyl-3-thiophenylmethanol.</p>
CHEMIFY-0096	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0096:</p> <p>Starting materials: Cyclopentanecarbohydrazide and phenylacetylene.</p> <p>Product: 2,4-diphenyl-4,5-dihydroimidazo[1,2-b]pyridine.</p>

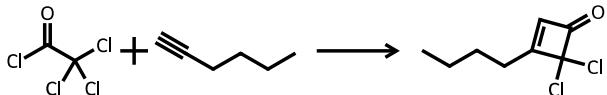
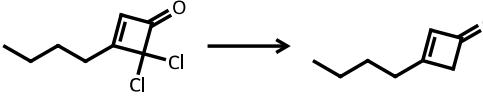
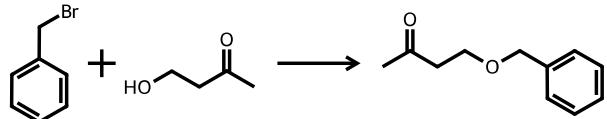
ID	Step	Yield	Scale	Reaction
CHEMIFY-0097	Step 1			<p>Reaction scheme for CHEMIFY-0097:</p> <p>Reagents: <chem>Brc1ccccc1</chem> + <chem>c1cc[nH]n1</chem></p> <p>Product: <chem>CN1C=CC=C1c2ccccc2Br</chem></p>
CHEMIFY-0098	Step 1			<p>Reaction scheme for CHEMIFY-0098:</p> <p>Reagents: <chem>CCOC(=O)C=C(COC)C(=O)OC</chem> + <chem>Nc1ccccc1</chem></p> <p>Product: <chem>CCOC(=O)c1cc(O)c2c(c1)Nc3ccccc3N2</chem></p>
CHEMIFY-0099	Step 1			<p>Reaction scheme for CHEMIFY-0099:</p> <p>Reagents: <chem>CC(=O)c1ccccc1</chem> + <chem>S8</chem> + <chem>N#Cc1ccccc1C(=O)N#N</chem></p> <p>Product: <chem>C1=c2sc3c(c2=C1)sc4ccccc43</chem></p>

ID	Step	Yield	Scale	Reaction
CHEMIFY-0100	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0100:</p> <p>Starting materials: 4-phenylazidomethylbenzene and phenylacetylene.</p> <p>Product: 1-(4-phenylazidomethyl)imidazole.</p>
CHEMIFY-0101	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0101:</p> <p>Starting material: N-(2-methylallyl)-N,N-dimethylacetamide.</p> <p>Product: 2-(dimethylamino)-2-methylpropan-1-oxepine.</p>
CHEMIFY-0102	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0102:</p> <p>Starting materials: Bis(diphenylphosphino)biphenyl, two equivalents of cyanogen ($N\equiv C$), and one equivalent of Pd^{Pd}_{Cl}.</p> <p>Products: Bis(diphenylphosphino)biphenyl and Pd^{Pd}_{Cl}.</p>

ID	Step	Yield	Scale	Reaction
CHEMIFY-0103	Step 1			
CHEMIFY-0104	Step 1			
CHEMIFY-0105	Step 1			

ID	Step	Yield	Scale	Reaction
CHEMIFY-0106	Step 1			
CHEMIFY-0107	Step 1			
CHEMIFY-0108	Step 1			

ID	Step	Yield	Scale	Reaction
CHEMIFY-0109	Step 1			
CHEMIFY-0110	Step 1			
CHEMIFY-0111	Step 1			

ID	Step	Yield	Scale	Reaction
CHEMIFY-0112	Step 1			
CHEMIFY-0113	Step 1			
CHEMIFY-0114	Step 1			

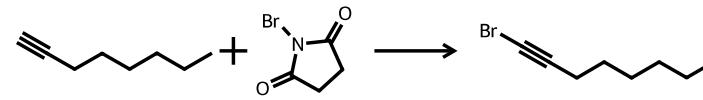
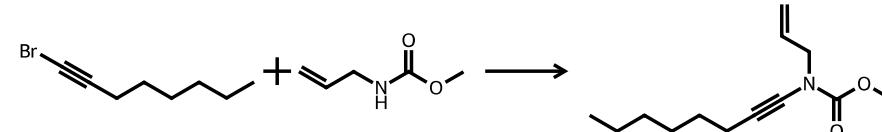
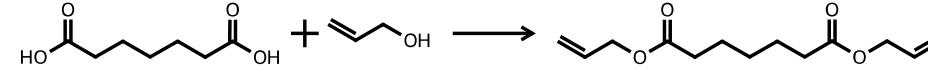
ID	Step	Yield	Scale	Reaction
CHEMIFY-0115	Step 1			<p>Detailed description: This reaction shows the condensation of a carboxylic acid derivative with a benzyl acetal. The reactants are a carboxylic acid derivative with a ¹³C label on the carbonyl carbon, and a benzyl acetal. The product is a substituted cyclohexane where the carboxylic acid group has been converted into a hydroxyl group, and the carbonyl carbon is now bonded to both the hydroxyl group and the original substituent.</p>
CHEMIFY-0116	Step 1			<p>Detailed description: This reaction scheme illustrates a multi-step synthesis. It begins with the reaction of a carboxylic acid chloride with a primary amine to form a diamine intermediate. This intermediate then reacts with a cyclic anhydride to form a complex heterocyclic product, likely a tricyclic system containing nitrogen and oxygen atoms.</p>
CHEMIFY-0117	Step 1			<p>Detailed description: This reaction shows the reduction of a complex heterocyclic compound. The starting material is a tricyclic system with multiple functional groups, including a carbamate group and a carbonyl group. The product is a substituted indole derivative where the carbonyl group has been reduced to a hydroxyl group.</p>

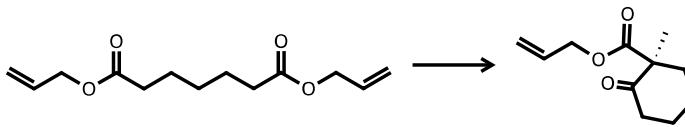
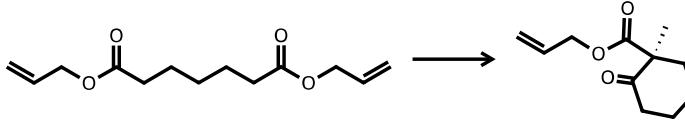
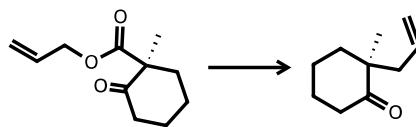
ID	Step	Yield	Scale	Reaction
CHEMIFY-0118	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0118:</p> <p>Starting materials: 4-carboxybutylbenzene (a benzene ring attached to a -CH₂-CH₂-CH₂-COOH group) and cyclopentylamine (a five-membered ring containing one nitrogen atom).</p> <p>Product: N-(4-carboxybutyl)cyclopentylamine (a cyclopentyl ring attached to the nitrogen atom of the amine, which is further attached to the 4-carboxybutyl group).</p>
CHEMIFY-0119	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0119:</p> <p>Starting materials: Phenylmethanethiol (a benzene ring attached to a -CH₂SH group) and N-(4-carboxybutyl)cyclopentylamine.</p> <p>Product: 1-(4-((cyclopentylamino)methyl)phenyl)ethanethiol (a benzene ring attached to a -CH₂CH₂SH group, which is further attached to the nitrogen atom of the cyclopentylamine ring).</p>
CHEMIFY-0120	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0120:</p> <p>Starting materials: 2-hydrosy-4-(trifluoromethyl)pyridine (a pyridine ring with a hydroxyl group at position 2 and a trifluoromethyl group at position 4) and allyl bromide (CH₂=CH-CH₂Br).</p> <p>Product: 2-allyl-4-(trifluoromethyl)sulfonypyridine (a pyridine ring with a hydroxyl group at position 2, a trifluoromethyl group at position 4, and an allylsulfone group at position 1).</p>

ID	Step	Yield	Scale	Reaction
CHEMIFY-0121	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0121:</p> <p>Starting materials:</p> <ul style="list-style-type: none"> 2-(2,2,2-trifluoroethylsulfonyl)-4-fluoropyridine 4-bromobiphenyl <p>Product:</p> <p>4-(4-biphenylmethyl)-2-fluoropyridine</p>
CHEMIFY-0122	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0122:</p> <p>Starting material:</p> <p>1,3-diphenylpropanone</p> <p>Product:</p> <p>1,3-diphenyl-2-(acetyloximino)propane</p>
CHEMIFY-0123	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0123:</p> <p>Starting material:</p> <p>1,3-diphenyl-2-(acetyloximino)propane</p> <p>Product:</p> <p>1-phenyl-2-phenylaziridine</p>

ID	Step	Yield	Scale	Reaction
CHEMIFY-0124	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0124:</p> <p>Starting materials: 4,4,4-trimethyl-2-methylbenzonitrile and propionaldehyde ($\text{CH}_3\text{CH}_2\text{CHO}$).</p> <p>Product: 4,4,4-trimethyl-2-(2-(propan-2-enyl)benzylidene)benzonitrile.</p>
CHEMIFY-0125	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0125:</p> <p>Starting material: 4,4,4-trimethyl-2-(2-(propan-2-enyl)benzylidene)benzonitrile.</p> <p>Reagent: $=\text{O}$ (oxygen).</p> <p>Product: 4,4,4-trimethyl-2-(2-(4,4,4-trimethyl-2-methylbenzylidene)imidazolin-2-yl)benzonitrile and Cl^-.</p>
CHEMIFY-0126	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0126:</p> <p>Starting materials: 4-chlorobiphenyl-4-carbonyl trifluoromethyl ether, 4-aminobiphenyl, diisopropylcarbamoyl chloride ($\text{H}_3\text{N}^+\text{OCH}_2\text{CH}_2\text{NH}_3^+$), and NaOAc.</p> <p>Product: 4-(4-(diisopropylcarbamoyloxy)biphenyl-4-yl)-N,N-diisopropylbenzyl carbamate.</p>

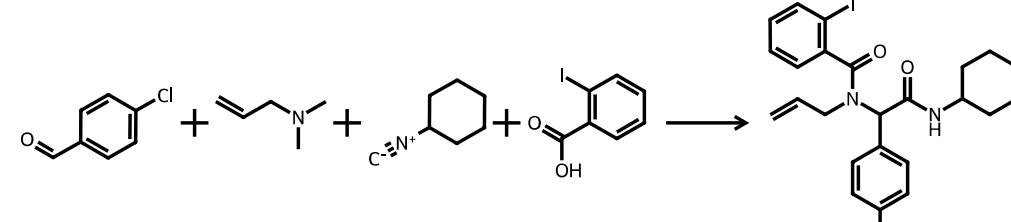
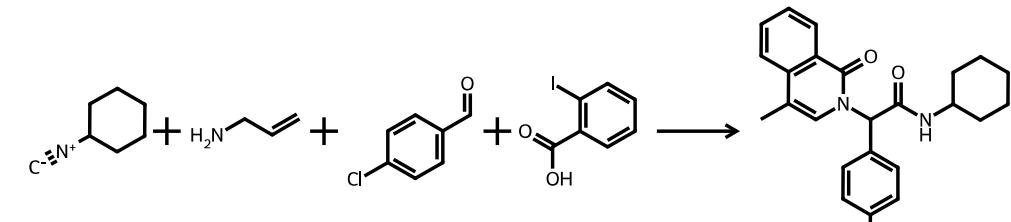
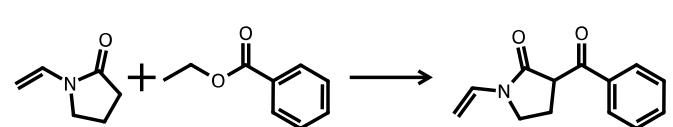
ID	Step	Yield	Scale	Reaction
CHEMIFY-0127	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0127:</p> <p>Starting materials: 4,4'-dibromobiphenyl-4,4'-diamine (a diamine with two bromine atoms at the para positions of each benzene ring).</p> <p>Product: 4,4'-dibromobiphenyl-4,4'-diphenylmethane (a diarylmethane where the two phenyl groups are linked by a methylene group).</p>
TwoStep-1 (0034+0010)	Step 1	81 %, 43 %	90.5 mmol, 10.0 mmol	<p>Reaction scheme for Step 1 of TwoStep-1:</p> <p>Starting materials: N-(2-chloroethyl)formamide (a chloromethyl formamide) and allylamine (an amine with a terminal alkene group).</p> <p>Product: N-(2-allyl-1-methylpropyl)formamide (a secondary amide formed by the condensation of the two starting materials).</p>
	Step 2			<p>Reaction scheme for Step 2 of TwoStep-1:</p> <p>Starting materials: The product from Step 1 (N-(2-allyl-1-methylpropyl)formamide) and 1-bromo-1-alkyne (a substituted alkene with a terminal alkyne group).</p> <p>Product: A substituted alkene where the alkyne group has been converted to an alkene group, resulting in a complex branched chain molecule.</p>

ID	Step	Yield	Scale	Reaction
TwoStep-2 (0035+0010)	Step 1	91 %, 43 %	10.0 mmol, 10.0 mmol	
	Step 2			
TwoStep-3 (0078+0037)	Step 1	64 %, 74 %	40 mmol, 9.0 mmol	

ID	Step	Yield	Scale	Reaction
	Step 2			
TwoStep-4 (0037+0012)	Step 1			
		74 %, 92 %	9.0 mmol, 2.0 mmol	
	Step 2			

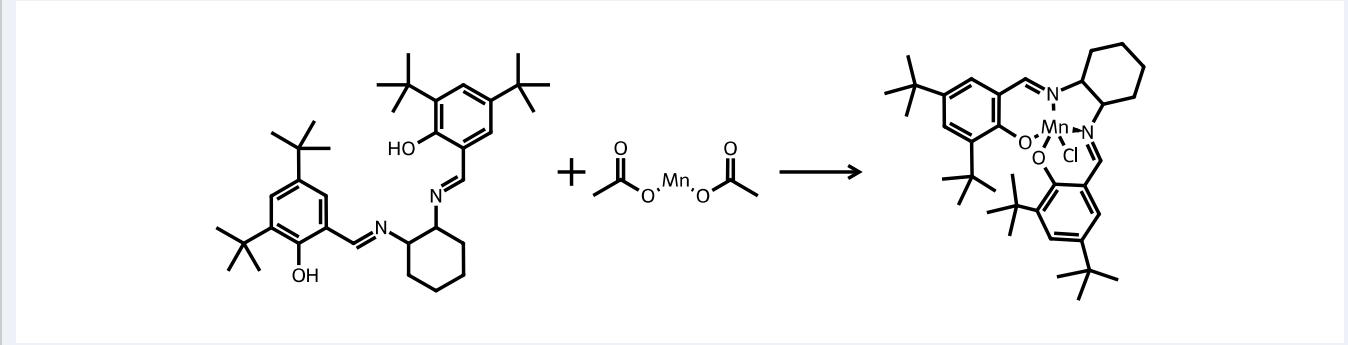
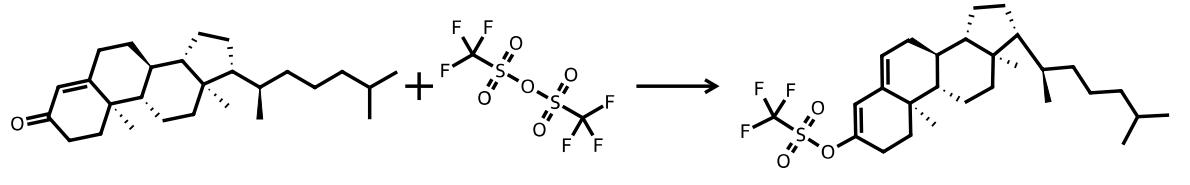
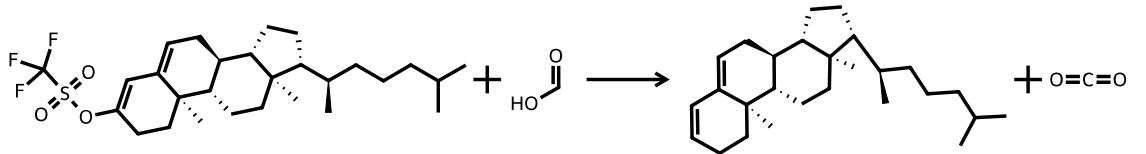
ID	Step	Yield	Scale	Reaction
TwoStep-5 (0075+0004)	Step 1	56 %, 84 %	20 mmol, 10.0 mmol	<p>Reaction scheme for Step 1:</p> $\text{H}_2\text{N}- + \text{HO}-\text{C}(=\text{O})-\text{CH}_2-\text{C}(=\text{O})-\text{CH}_2-\text{C}(=\text{O})-\text{OH} + -\text{O}-\text{C}(\text{O})-\text{CH}_2-\text{CH}_2-\text{O}- \longrightarrow \text{Product}$
	Step 2			<p>Reaction scheme for Step 2:</p> $\text{Product} + \text{BH}_3-\text{Et}_2\text{O} + \text{Li}^+ \longrightarrow \text{Product}$
TwoStep-6 (0004+0005)	Step 1	84 %, 37 %	10.0 mmol, 13.0 mmol	<p>Reaction scheme for Step 1:</p> $\text{Product} + \text{BH}_3-\text{Et}_2\text{O} + \text{Li}^+ \longrightarrow \text{Product}$

ID	Step	Yield	Scale	Reaction
	Step 2			
TwoStep-7 (0056+0022)	Step 1	78 %, 32 %	12.0 mmol, 1.86 mmol	
	Step 2			

ID	Step	Yield	Scale	Reaction
TwoStep-8 (0056+0023)	Step 1	78 %, 35 %	12.0 mmol, 6.0 mmol	
	Step 2			
TwoStep-9 (0038+0079)	Step 1	52 %, 38 %	45.0 mmol, 10 mmol	

ID	Step	Yield	Scale	Reaction
	Step 2			
TwoStep-10 (0040+0042)	Step 1	36 %, 58 %	33.3 mmol, 0.77 mmol	
	Step 2			

ID	Step	Yield	Scale	Reaction
TwoStep-11 (0043+0044)	Step 1	76 %, 85 %	100.0 mmol, 11.2 mmol	<p>Reaction scheme for Step 1:</p> <p>Reactants: 1,4-diaminobutane and dihydroxyacetone.</p> <p>Product: Ammonium salt of 1,4-diaminobutane where one amino group is protonated.</p>
	Step 2			<p>Reaction scheme for Step 2:</p> <p>Reactants: 2-hydroxy-4,4,6,6-tetramethyl-2H-1,3-bis(2,6-diisopropylphenyl)-1,3-dioxolene, Ammonium salt of 1,4-diaminobutane, and dihydroxyacetone.</p> <p>Product: A complex polycyclic compound formed by the condensation of the three reactants.</p>
TwoStep-12 (0044+0045)	Step 1	85 %, 70 %	11.2 mmol, 1.5 mmol	<p>Reaction scheme for Step 1:</p> <p>Reactants: 2-hydroxy-4,4,6,6-tetramethyl-2H-1,3-bis(2,6-diisopropylphenyl)-1,3-dioxolene, 1,4-diaminobutane, and dihydroxyacetone.</p> <p>Product: A complex polycyclic compound formed by the condensation of the three reactants.</p>

ID	Step	Yield	Scale	Reaction
TwoStep-13 (0046+0047)	Step 2			
	Step 1	99 %, 71 %	15.0 mmol, 5.00 mmol	
	Step 2			

ID	Step	Yield	Scale	Reaction
ThreeStep-1 (0034+0035+0010)	Step 1			<p>Reaction scheme for Step 1: Acrylic acid chloride (<chem>O=C(Cl)C(=O)O</chem>) reacts with allylamine (<chem>C=CCN</chem>) to form N-(allyl)acrylamide (<chem>C=CCN(C(=O)OC)C(=O)O</chem>).</p>
	Step 2	81 %, 91 %, 43 %	90.5 mmol, 10.0 mmol, 10.0 mmol	<p>Reaction scheme for Step 2: Prop-1-yn-1-yl bromide (<chem>BrC#CCCC#C</chem>) reacts with 1-bromo-2-methylimidazolidine-2,5-dione (<chem>BrC1=CC=CC2=C1C(=O)N2C=O</chem>) to form 1-(prop-1-ynyl)-2-methylimidazolidine-2,5-dione.</p>
	Step 3			<p>Reaction scheme for Step 3: The product from Step 2 (1-(prop-1-ynyl)-2-methylimidazolidine-2,5-dione) reacts with N-(allyl)acrylamide (<chem>C=CCN(C(=O)OC)C(=O)O</chem>) to form the final product.</p>

ID	Step	Yield	Scale	Reaction
ThreeStep-2 (0078+0037+0012)	Step 1			<p>Reaction scheme for Step 1: A linear diacid (hexanedioic acid) reacts with allyl alcohol to form a diester where the allyl group is attached to one of the carboxylic acid carbons.</p>
	Step 2	64 %, 74 %, 92 %	40 mmol, 9.0 mmol, 2.0 mmol	<p>Reaction scheme for Step 2: The product from Step 1 is cyclized to form a cyclohexane ring containing a ketone and a vinyl group.</p>
	Step 3			<p>Reaction scheme for Step 3: The product from Step 2 is further modified to form a substituted cyclohexene ring.</p>

ID	Step	Yield	Scale	Reaction
ThreeStep-3 (0075+0004+0005)	Step 1			<p>Reaction scheme for Step 1: $\text{H}_2\text{N}- + \text{HO}-\text{C}(=\text{O})-\text{CH}_2-\text{C}(=\text{O})-\text{CH}_2-\text{C}(=\text{O})-\text{OH} + -\text{O}-\text{C}(\text{O})-\text{CH}_2-\text{CH}_2-\text{O}-\text{Br} \rightarrow \text{Product}$</p>
	Step 2	56 %, 84 %, 37 %	20 mmol, 10.0 mmol, 13.0 mmol	<p>Reaction scheme for Step 2: $\text{Product} + \text{BH}_3-\text{Et}_2\text{O} + \text{Li}^+ \rightarrow \text{Product}$</p>
	Step 3			<p>Reaction scheme for Step 3: $\text{Product} + \text{Cl-C(=O)-CH}_2-\text{C}_6\text{H}_5 \rightarrow \text{Product}$</p>

ID	Step	Yield	Scale	Reaction
ThreeStep-4 (0043+0044+0045)	Step 1			<p>Reaction scheme for Step 1: 1,4-diaminocyclohexane reacts with dihydroxyacetone to form 1-(dihydroxyacetone)-1,4-diaminocyclohexane and a protonated intermediate.</p>
	Step 2	76 %, 85 %, 70 %	100.0 mmol, 11.2 mmol, 1.5 mmol	<p>Reaction scheme for Step 2: 1-(dihydroxyacetone)-1,4-diaminocyclohexane, 2,6-diisopropyl-4-hydroxy-2,3-dihydro-1H-pyran-3-one, and dihydroxyacetone react to form a tricyclic product.</p>
	Step 3			<p>Reaction scheme for Step 3: The tricyclic product from Step 2 reacts with Mn(OAc)₂ to form a manganese complex.</p>