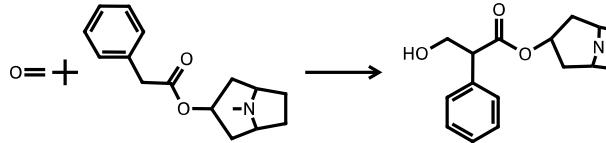
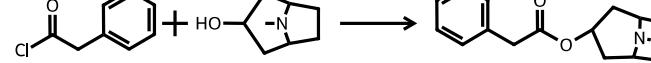
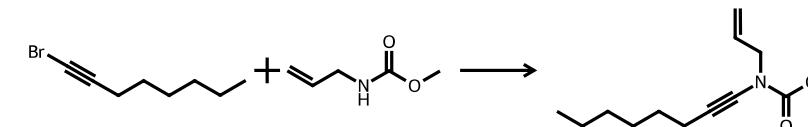
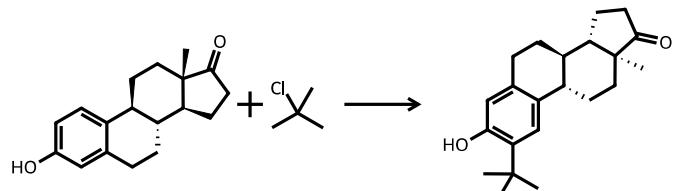
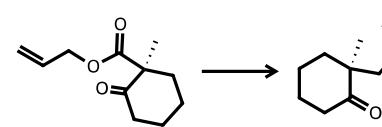
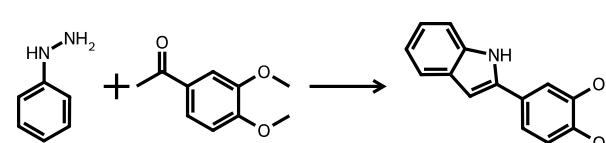
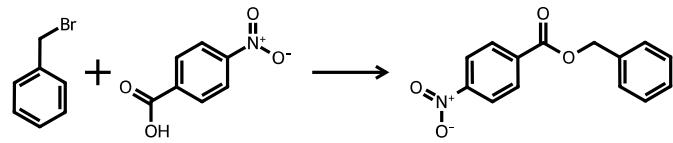
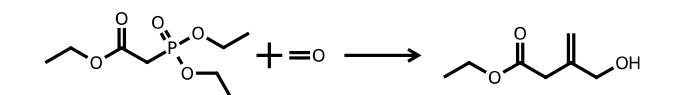
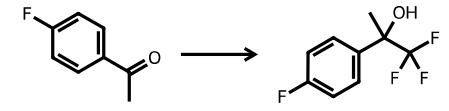


ID	Step	Yield	Scale	Reaction
CHEMIFY-0001	Step 1	98 %	8.8 mmol	<p>Detailed description: This reaction shows the substitution of the amino group in 4-bromobiphenyl with a methoxybenzenesulfonyl group. The starting materials are 4-bromobiphenyl (a biphenyl ring with a bromine at position 4) and 4-methoxybenzenesulfonyl chloride (a biphenyl ring with a methoxy group at position 4 and a sulfonyl chloride group at position 1). The product is N-(4-bromobiphenyl)-4-methoxybenzenesulfonamide, where the amino group of the starting material has been replaced by the sulfonyl group.</p>
CHEMIFY-0002	Step 1	56 %	20.0 mmol	<p>Detailed description: This reaction shows the addition of allyl bromide to diethyl malonate. Diethyl malonate is a dicarboxylic acid derivative with two methyl ester groups. Allyl bromide is an allylic bromide. The reaction yields two diastereomeric allylated malonates, where the allyl group is added at the same position on both carbonyls of the malonate.</p>
CHEMIFY-0004	Step 1	84 %	10.0 mmol	<p>Detailed description: This reaction shows the reduction of a cyclic imide. The starting material is a five-membered ring containing a nitrogen atom bonded to a carbonyl group. It reacts with a borane reagent (a trialkylborane with a hydride) and a lithium cation (Li+) to produce a hydroxylated product where the nitrogen is bonded to a hydroxyl group.</p>

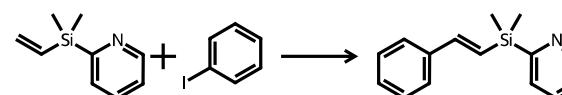
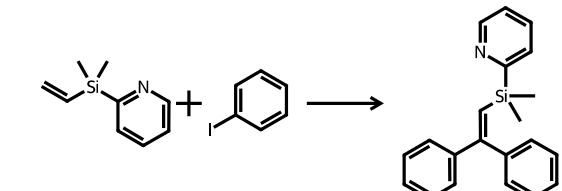
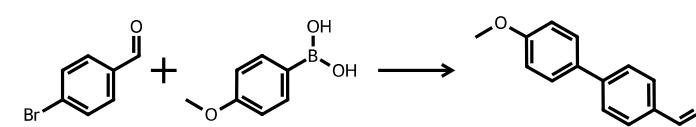
ID	Step	Yield	Scale	Reaction
CHEMIFY-0005	Step 1	37 %	13.0 mmol	
CHEMIFY-0006	Step 1	65 %	20.0 mmol	
CHEMIFY-0010	Step 1	43 %	10.0 mmol	

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	

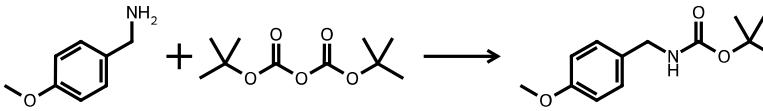
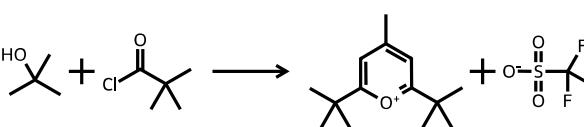
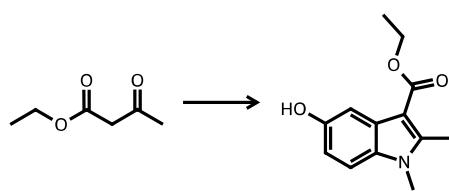
ID	Step	Yield	Scale	Reaction
CHEMIFY-0014	Step 1	60 %	25.1 mmol	<p>Detailed description: This reaction shows the formation of a bicyclic compound. It starts with cyclohexylamine reacting with allylbenzylamine, 2-hydroxyborylarene, and 2-hydroxypropanoic acid. The resulting product is a bicyclic structure where the allyl group from the first reactant is fused with the ring formed by the other three components.</p>
CHEMIFY-0015	Step 1	56 %	0.5 mmol	<p>Detailed description: This reaction involves a substituted benzyl amine, a benzyl bromide derivative, and a tin reagent. The products are highly substituted polycyclic compounds, likely formed through a series of nucleophilic attacks and cyclizations.</p>
CHEMIFY-0016	Step 1	64 %	12.0 mmol	<p>Detailed description: This reaction features a nitrophenol, an alkene, a nitrile, and a carboxylic acid. The final product is a complex molecule with multiple functional groups, including a nitro group, a carbamate-like group, and a carboxylic acid derivative.</p>

ID	Step	Yield	Scale	Reaction
CHEMIFY-0017	Step 1	86 %	5.0 mmol	
CHEMIFY-0018	Step 1	36 %	100.0 mmol	
CHEMIFY-0020	Step 1		4.0 mmol	

ID	Step	Yield	Scale	Reaction
CHEMIFY-0021	Step 1	68.8 %	2.64 mmol	
CHEMIFY-0022	Step 1	32 %	1.86 mmol	
CHEMIFY-0023	Step 1	35 %	6.0 mmol	

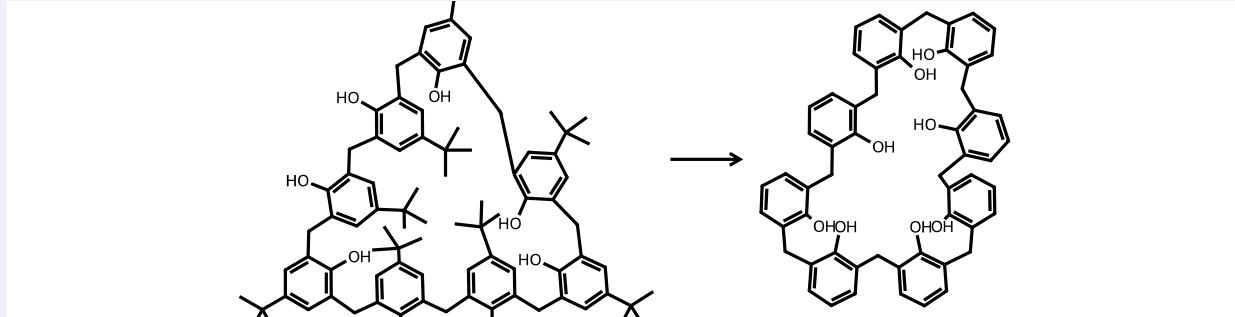
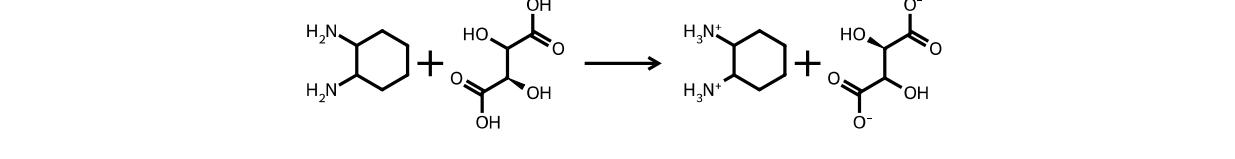
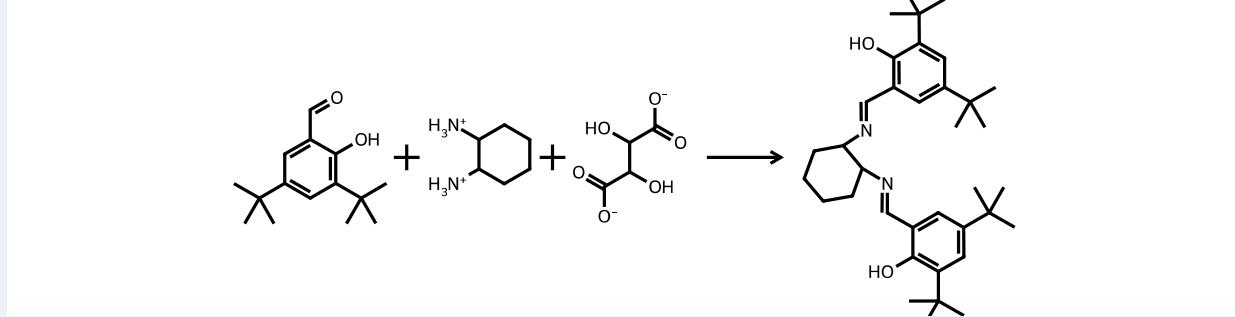
ID	Step	Yield	Scale	Reaction
CHEMIFY-0024	Step 1	65 %	3.10 mmol	 <p>Reaction scheme for CHEMIFY-0024: A substituted pyridine ring reacts with iodobenzene to form a substituted styrene product.</p>
CHEMIFY-0025	Step 1	74 %	3.10 mmol	 <p>Reaction scheme for CHEMIFY-0025: A substituted pyridine ring reacts with iodobenzene to form a bis(phenyl)alkene product.</p>
CHEMIFY-0026	Step 1	61 %	5.02 mmol	 <p>Reaction scheme for CHEMIFY-0026: 4-bromobiphenyl reacts with a boronic ester to form a substituted biphenyl product.</p>

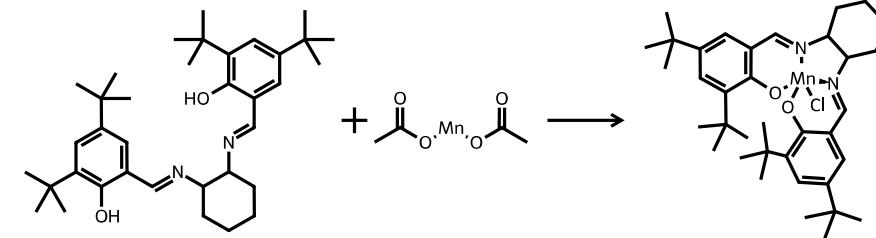
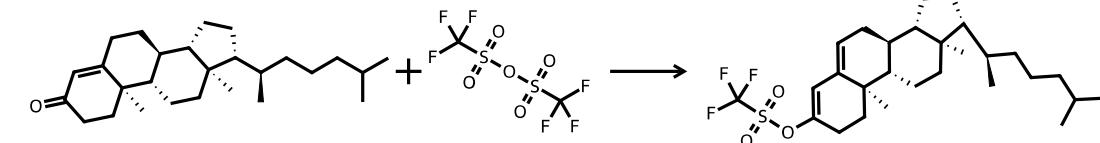
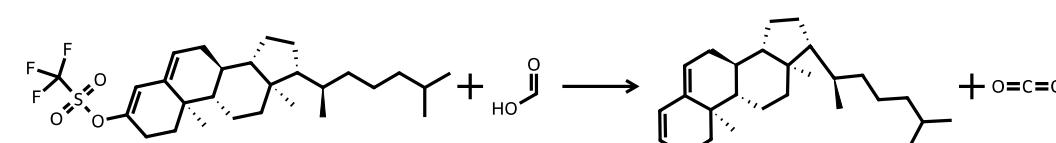
ID	Step	Yield	Scale	Reaction
CHEMIFY-0027	Step 1	84 %	5.0 mmol	<p>Reaction scheme for Step 1 of CHEMIFY-0027:</p> <p>Starting materials: 4-nitroiodobiphenyl and 2-hydroxypropanoic acid.</p> <p>Product: 2-(4-nitrophenyl)-3-hydroxypropanoic acid.</p>
CHEMIFY-0028	Step 1	66 %	50.0 mmol	<p>Reaction scheme for Step 1 of CHEMIFY-0028:</p> <p>Starting materials: Water (HO-OH) and Cyclooctene.</p> <p>Product: Cyclooctanediol.</p>
CHEMIFY-0029	Step 1	62 %	25.0 mmol	<p>Reaction scheme for Step 1 of CHEMIFY-0029:</p> <p>Starting materials: Diethyl malonate and 1,2-dibromoethane.</p> <p>Product: A bicyclic product formed by a Diels-Alder reaction.</p>

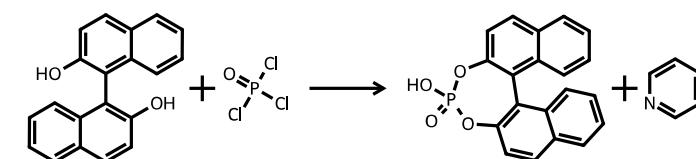
ID	Step	Yield	Scale	Reaction
CHEMIFY-0030	Step 1	88 %	5.0 mmol	
CHEMIFY-0032	Step 1	36 %	40.0 mmol	
CHEMIFY-0033	Step 1	59 %	33.8 mmol	

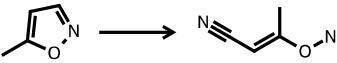
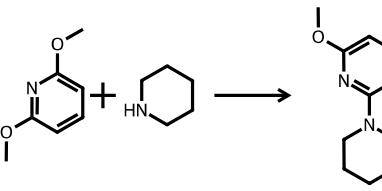
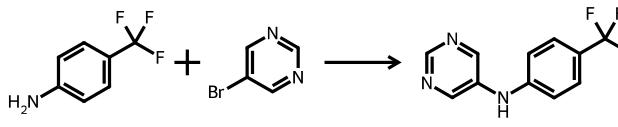
ID	Step	Yield	Scale	Reaction
CHEMIFY-0034	Step 1	81 %	90.5 mmol	<p>Reaction scheme for Step 1 of CHEMIFY-0034:</p> <p>Starting materials: 3-chloroacrylic acid (<chem>O=C(Cl)C(=O)O</chem>) and allylamine (<chem>CC=CCN</chem>).</p> <p>Product: N-(allyl)-3-chloroacrylamide (<chem>CC=CCNC(=O)C(Cl)=O</chem>).</p>
CHEMIFY-0035	Step 1	91 %	10.0 mmol	<p>Reaction scheme for Step 1 of CHEMIFY-0035:</p> <p>Starting materials: 1-pentyne (<chem>C#CCCC</chem>) and 1-bromo-4-pentyn-3-one (<chem>BrC(=O)C1CCCC1</chem>).</p> <p>Product: 1-(5-pentyne-1-yl)-1-bromo-4-pentyn-3-one (<chem>BrC(=O)C(C#CCCC)C(C#CCCC)C</chem>).</p>
CHEMIFY-0037	Step 1	74 %	9.0 mmol	<p>Reaction scheme for Step 1 of CHEMIFY-0037:</p> <p>Starting material: A long-chain diester with two terminal alkene groups (<chem>CC=CCOC(=O)CCCCCC(=O)OC=CC</chem>).</p> <p>Product: A cyclic dimer formed by the intramolecular cyclization of the diester.</p>

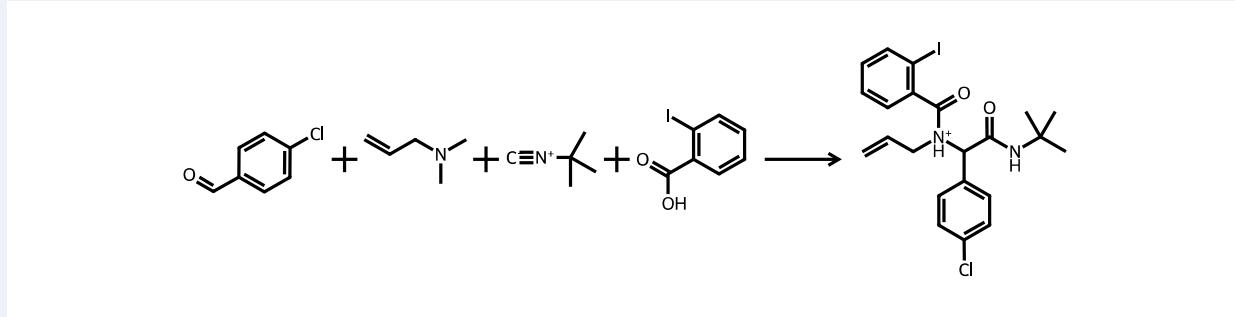
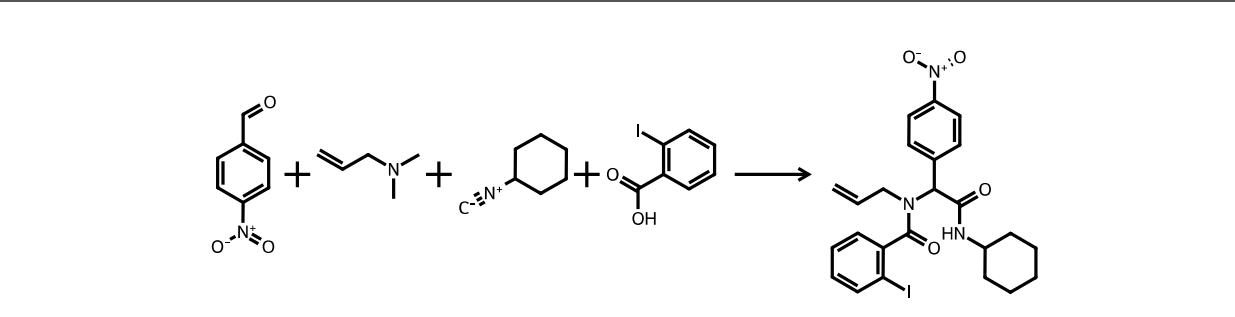
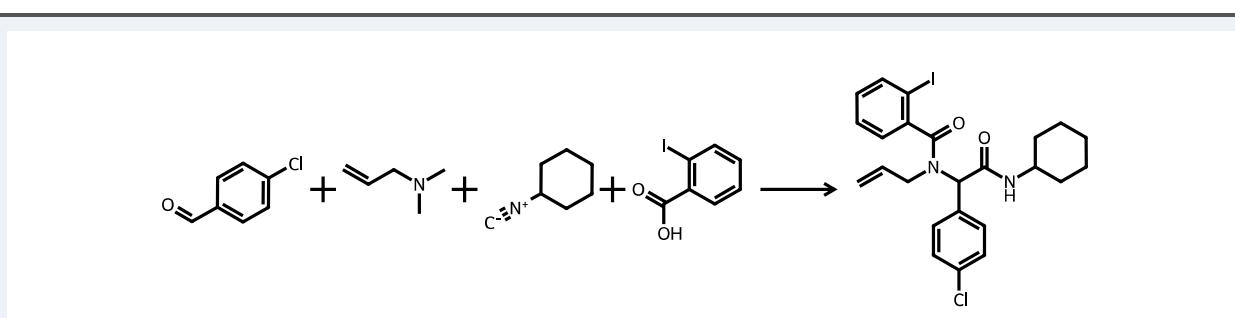
ID	Step	Yield	Scale	Reaction
CHEMIFY-0038	Step 1	52 %	45.0 mmol	<p>Reaction scheme for CHEMIFY-0038:</p> <p>Starting materials: N-vinyl-1-piperidin-4-one and phenyl chloroformate ($\text{C}_6\text{H}_5\text{COCl}$).</p> <p>Product: N-(phenylcarbamoyl)-N-vinylpiperidin-4-one.</p>
CHEMIFY-0040	Step 1	36 %	33.3 mmol	<p>Reaction scheme for CHEMIFY-0040:</p> <p>Starting material: 4-hydroxy-2,6-diisopropylphenol.</p> <p>Product: A complex polyphenol polymer formed by oxidative coupling.</p>
CHEMIFY-0041	Step 1	65 %	25.6 mmol	<p>Reaction scheme for CHEMIFY-0041:</p> <p>Starting materials: A hydroxyl group ($-\text{OH}$) and 2-oxo-2,3-dihydro-1H-imidazol-3-carboxylic acid.</p> <p>Product: A cyclic imide formed by the reaction of the hydroxyl group with the carboxylic acid.</p>

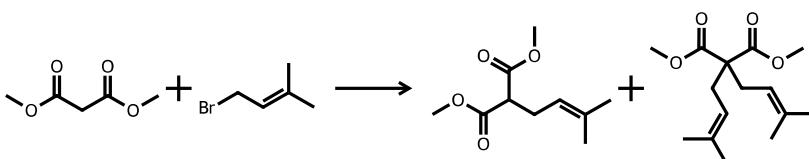
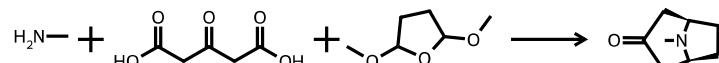
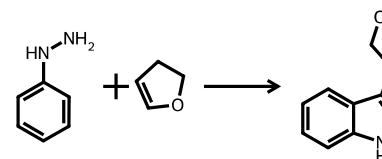
ID	Step	Yield	Scale	Reaction
CHEMIFY-0042	Step 1	58 %	0.77 mmol	
CHEMIFY-0043	Step 1	76 %	100.0 mmol	
CHEMIFY-0044	Step 1	85 %	11.2 mmol	

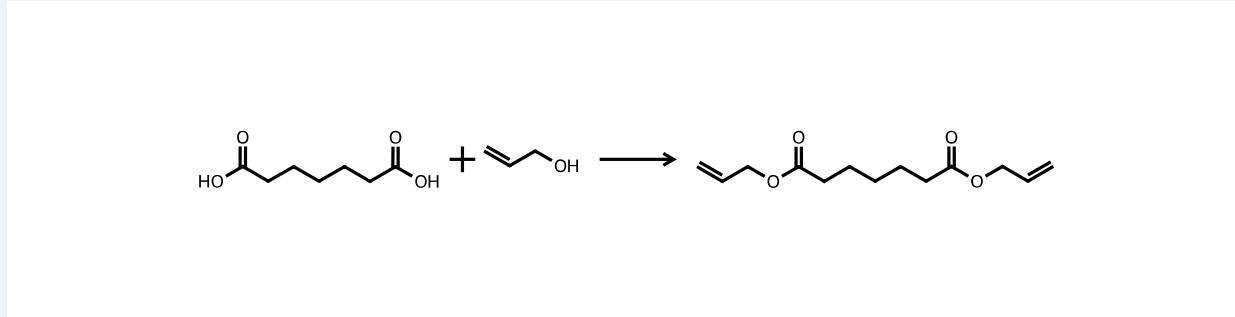
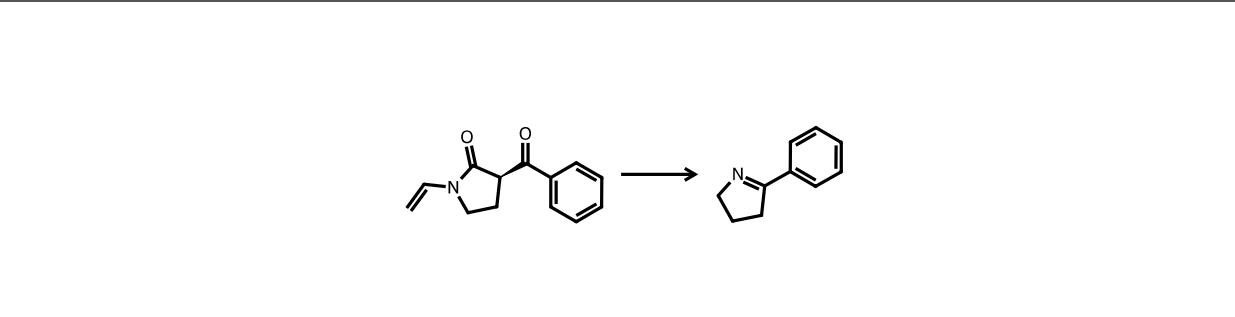
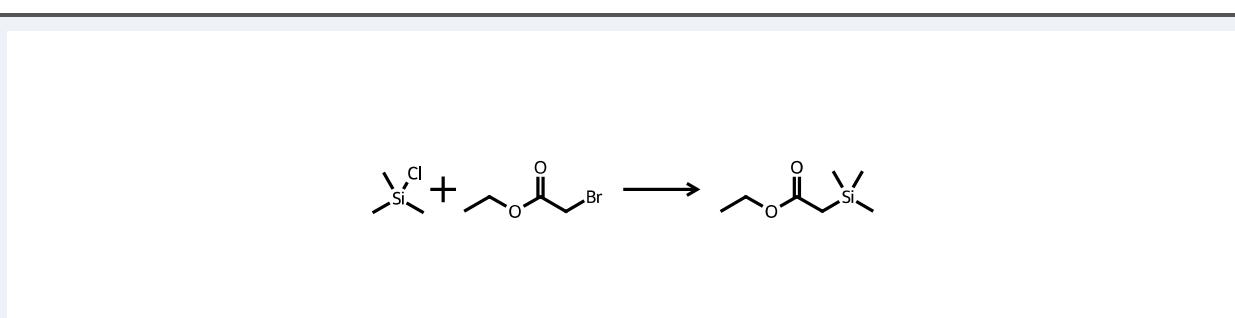
ID	Step	Yield	Scale	Reaction
CHEMIFY-0045	Step 1	70 %	1.5 mmol	
CHEMIFY-0046	Step 1	99 %	15.0 mmol	
CHEMIFY-0047	Step 1	71 %	5.00 mmol	

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	

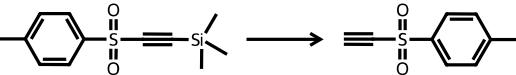
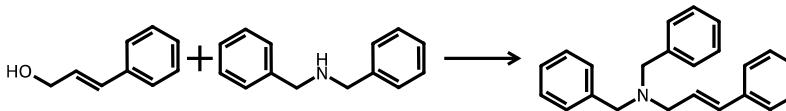
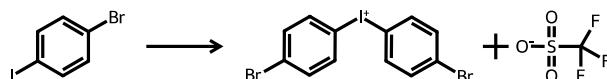
ID	Step	Yield	Scale	Reaction
CHEMIFY-0051	Step 1	76 %	33.0 mmol	
CHEMIFY-0052	Step 1	53 %	10.1 mmol	
CHEMIFY-0053	Step 1	75 %	5.0 mmol	

ID	Step	Yield	Scale	Reaction
CHEMIFY-0054	Step 1	56 %	12.0 mmol	 <p>Reaction scheme for CHEMIFY-0054:</p> <p>Starting materials: 4-chlorobenzaldehyde, allyltrimethylammonium iodide, 2-(triisopropylsilyl)acetonitrile, and 4-iodobenzoic acid.</p> <p>Product: A polymer where the aldehyde group of 4-chlorobenzaldehyde has been converted into a polymer-bound ammonium cation ($\text{C}_2\text{H}_5\text{CH}=\text{CH}-\text{N}^+(\text{CH}_3)_3$).</p>
CHEMIFY-0055	Step 1	80 %	12.0 mmol	 <p>Reaction scheme for CHEMIFY-0055:</p> <p>Starting materials: 4-nitrobenzaldehyde, allyltrimethylammonium iodide, 2-(triisopropylsilyl)acetonitrile, and 4-iodobenzoic acid.</p> <p>Product: A polymer where the aldehyde group of 4-nitrobenzaldehyde has been converted into a polymer-bound ammonium cation ($\text{C}_2\text{H}_5\text{CH}=\text{CH}-\text{N}^+(\text{CH}_3)_3$).</p>
CHEMIFY-0056	Step 1	78 %	12.0 mmol	 <p>Reaction scheme for CHEMIFY-0056:</p> <p>Starting materials: 4-chlorobenzaldehyde, allyltrimethylammonium iodide, 2-(triisopropylsilyl)acetonitrile, and 4-iodobenzoic acid.</p> <p>Product: A polymer where the aldehyde group of 4-chlorobenzaldehyde has been converted into a polymer-bound ammonium cation ($\text{C}_2\text{H}_5\text{CH}=\text{CH}-\text{N}^+(\text{CH}_3)_3$).</p>

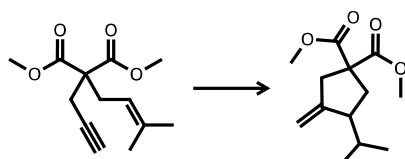
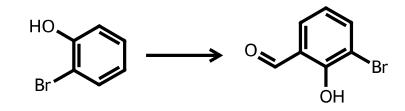
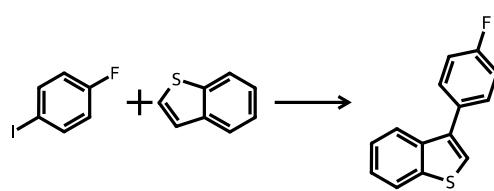
ID	Step	Yield	Scale	Reaction
CHEMIFY-0057	Step 1	31 %	20.0 mmol	
CHEMIFY-0075	Step 1	56 %	20 mmol	
CHEMIFY-0077	Step 1	33 %	30 mmol	

ID	Step	Yield	Scale	Reaction
CHEMIFY-0078	Step 1	64 %	40 mmol	 <p>Reaction scheme for CHEMIFY-0078:</p> <p>Starting materials: Hexanedioic acid (a diacid with two carboxylic acid groups at the ends of a six-carbon chain) and allyl alcohol (propene-1-ol).</p> <p>Product: A bis(ether) diester where the two carboxylic acid groups have been converted into ether linkages (-O-CH=CH2-O-) between the two ends of the hexane chain.</p>
CHEMIFY-0079	Step 1	38 %	10 mmol	 <p>Reaction scheme for CHEMIFY-0079:</p> <p>Starting material: A cyclic amide with an allyl group at the 2-position and a carbonyl group at the 5-position, which is further substituted with a phenyl group.</p> <p>Product: A cyclized product where the allyl group has participated in a cyclization reaction, forming a five-membered ring containing the nitrogen atom and the carbonyl group, resulting in a cyclopentenone derivative.</p>
CHEMIFY-0080	Step 1			 <p>Reaction scheme for CHEMIFY-0080:</p> <p>Starting materials: Chlorotriethylsilane (a silane with three methyl groups and one chlorine atom) and ethyl bromoformate (an ester with a bromine atom).</p> <p>Product: The formation of a silyl acetal, where the silane has replaced the bromine atom in the ester, resulting in a triethylsilyl ether.</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			

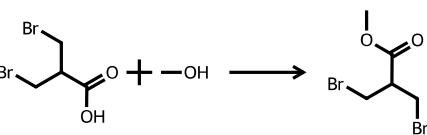
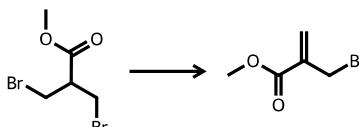
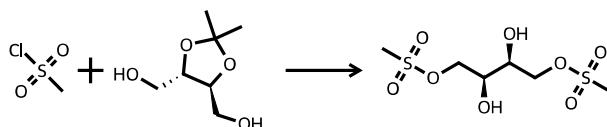
ID	Step	Yield	Scale	Reaction
CHEMIFY-0088	Step 1			
CHEMIFY-0089	Step 1			
CHEMIFY-0090	Step 1			

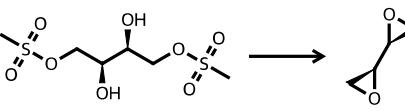
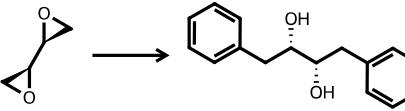
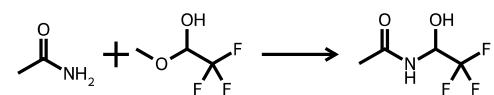
ID	Step	Yield	Scale	Reaction
CHEMIFY-0091	Step 1			
CHEMIFY-0092	Step 1			
CHEMIFY-0093	Step 1			

ID	Step	Yield	Scale	Reaction
CHEMIFY-0094	Step 1			
CHEMIFY-0095	Step 1			
CHEMIFY-0096	Step 1			

ID	Step	Yield	Scale	Reaction
CHEMIFY-0097	Step 1			<p>Reaction scheme for CHEMIFY-0097:</p> <p>Reagents: <chem>Brc1ccccc1</chem> + <chem>c1cc[nH]cn1</chem></p> <p>Product: <chem>c1cc[nH]c(Brc1ccccc1)c1</chem></p>
CHEMIFY-0098	Step 1			<p>Reaction scheme for CHEMIFY-0098:</p> <p>Reagents: <chem>CCOC(=O)C(COC)C(=O)OC(C)C + c1ccccc1N</chem></p> <p>Product: <chem>CCOC(=O)c1c(O)nc2c(c1)N(c1ccccc1)C(=O)N2C</chem></p>
CHEMIFY-0099	Step 1			<p>Reaction scheme for CHEMIFY-0099:</p> <p>Reagents: <chem>CC(=O)c1ccccc1 + SSSS + H2NC(=O)NH2</chem></p> <p>Product: <chem>c1ccccc1c2sc3c(c2)sc4c(c3)ccccc4</chem></p>

ID	Step	Yield	Scale	Reaction
CHEMIFY-0100	Step 1			<p>Detailed description: This reaction shows the formation of an alkene via a [3+2] cycloaddition. The reactants are 4-phenylazidomethylbenzene (a benzene ring with a phenyl group at position 4 and an azide group (-N=N+=N+) at position 1) and phenylacetylene (a benzene ring with a phenyl group at position 1 and a triple bond between positions 2 and 3). The product is 1-(4-phenylazidomethyl)prop-1-ene (a benzene ring with a phenyl group at position 1 and a double bond between positions 2 and 3, with an azide group at position 4).</p>
CHEMIFY-0101	Step 1			<p>Detailed description: This reaction shows the cyclization of a carbamate derivative. The reactant is N,N-dimethylallyl diisopropylcarbamate (a molecule with two allyl groups attached to a central nitrogen atom, which is further bonded to two isopropyl groups and a carbonyl group). The product is 1-methyl-1,2-dihydro-3H-pyrazole-3-carbonyldiisopropyl ether (a five-membered heterocyclic ring containing one nitrogen and one oxygen atom, with a methyl group, a carbonyl group, and two isopropyl groups).</p>
CHEMIFY-0102	Step 1			<p>Detailed description: This reaction shows the oxidative addition of a Pd(0) complex. The reactants are a Pd(0) complex (a macrocyclic ligand with two phenyl groups and a phosphine group, coordinated to a Pd atom), two equivalents of cyanide (N≡C), and one equivalent of a Pd(IV) salt (PdCl4^2-). The products are a Pd(IV) complex (a macrocyclic ligand with two phenyl groups and a phosphine group, coordinated to a Pd atom with four chlorine atoms) and a chloride ion (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			<p>Reaction scheme for Step 1 of CHEMIFY-0112:</p> <p>Starting materials:</p> <ul style="list-style-type: none"> 1,3-dichloro-2,2-dimethylpropan-1-one 1-pentyne <p>Product:</p> <p>1-(5-pentynyl)-2,2-dimethylcyclopropanecarboxylic acid</p>
CHEMIFY-0113	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0113:</p> <p>Starting material:</p> <p>1-(5-pentynyl)-2,2-dimethylcyclopropanecarboxylic acid</p> <p>Product:</p> <p>1-(5-pentynyl)cyclopropanecarboxylic acid</p>
CHEMIFY-0114	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0114:</p> <p>Starting materials:</p> <ul style="list-style-type: none"> 1-bromo-2-phenylethane 3-hydroxybutanal <p>Product:</p> <p>2-(2-phenylethoxy)-3-hydroxybutanal</p>

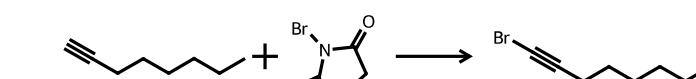
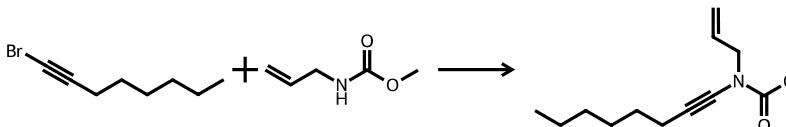
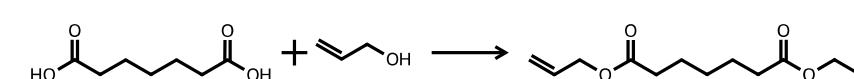
ID	Step	Yield	Scale	Reaction
CHEMIFY-0115	Step 1			<p>Detailed description: This reaction shows the condensation of 3-hydroxy-2-13C-propanal (an aldehyde with a 13C label at the beta position) with 4-(2-hydroxyethyl)benzyl alcohol. The product is 3-hydroxy-2-(4-(2-hydroxyethyl)benzyl)-2-13C-propanal, where the 13C label is retained at the beta position.</p>
CHEMIFY-0116	Step 1			<p>Detailed description: This reaction sequence starts with N,N-dimethylbenzylamine reacting with succinimidyl chloroformate to form a cyclic intermediate. This intermediate then reacts with 2-(2-methylacetoxy)indole to produce a complex heterocyclic product.</p>
CHEMIFY-0117	Step 1			<p>Detailed description: This reaction shows the reduction of the intermediate from Step 1 of CHEMIFY-0116. The starting material is a complex heterocyclic compound containing a benzyl group, which is reduced to a substituted indole derivative.</p>

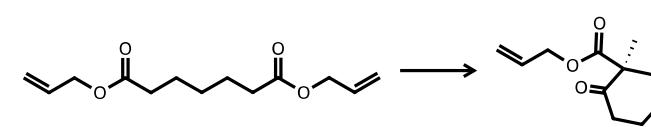
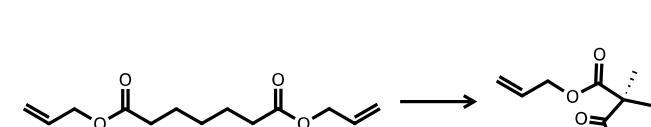
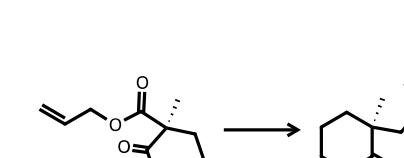
ID	Step	Yield	Scale	Reaction
CHEMIFY-0118	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0118:</p> <p>Starting materials: 4-phenylbutanoic acid (a benzene ring attached to a butanoate group) and pyrrolidine (a five-membered nitrogen-containing ring).</p> <p>Product: N-(4-phenylbutyl)pyrrolidine (a pyrrolidine ring attached to a butyl group, which is further attached to a phenyl ring).</p>
CHEMIFY-0119	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0119:</p> <p>Starting materials: Benzyl thiol (a benzene ring attached to a methylthio group) and N-(4-phenylbutyl)pyrrolidine.</p> <p>Product: A substituted benzyl thioether where the thiomethyl group is attached to the 4-phenylbutyl chain of the pyrrolidine.</p>
CHEMIFY-0120	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0120:</p> <p>Starting materials: 2-hydrosybenzyl trifluoromethyl sulfide (a benzene ring with a hydroxymethyl group at position 2 and a trifluoromethyl sulfide group at position 4) and allyl bromide (an allyl cation).</p> <p>Product: A substituted sulfone where the allyl group is attached to the hydroxymethyl group of the benzyl sulfide.</p>

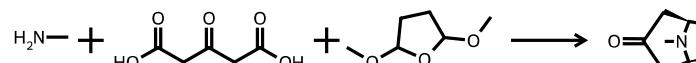
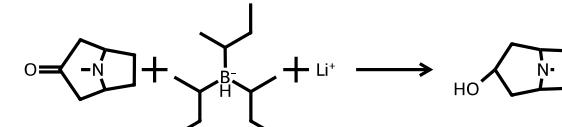
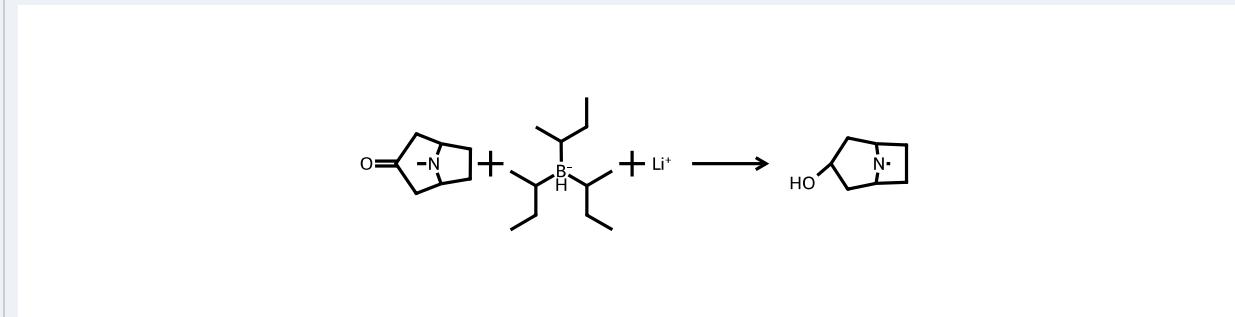
ID	Step	Yield	Scale	Reaction
CHEMIFY-0121	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0121:</p> <p>Starting materials: 2-(2,2,2-trifluoroethylsulfonyl)pyridine and 4-bromobiphenyl.</p> <p>Product: 4-(2,2,2-trifluoroethylsulfonyl)biphenyl.</p>
CHEMIFY-0122	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0122:</p> <p>Starting materials: N-phenyl-N-((2-phenylpropyl)nitroso)benzylamine and benzaldehyde.</p> <p>Product: N-((2-phenylpropyl)(4-phenylbutyl)nitroso)benzylamine.</p>
CHEMIFY-0123	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0123:</p> <p>Starting materials: N-((2-phenylpropyl)(4-phenylbutyl)nitroso)benzylamine and benzaldehyde.</p> <p>Product: N-((2-phenylpropyl)(4-phenylbutyl)nitroso)cyclopropane.</p>

ID	Step	Yield	Scale	Reaction
CHEMIFY-0124	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0124:</p> <p>Starting materials: 2-(2,6-diisopropylphenyl)benzylamine and acryloyl chloride ($\text{CH}_2=\text{CHCOCl}$).</p> <p>Product: 2-(2-(acryloyl)benzylidene)benzylidene-2,6-diisopropylphenylamine.</p>
CHEMIFY-0125	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0125:</p> <p>Starting material: The product from Step 1 of CHEMIFY-0124.</p> <p>Reagent: $=\text{O}$ (oxygen).</p> <p>Product: A cyclic iminium salt (a tricyclic compound with a pyrazole ring fused to the benzene rings) and a chloride ion (Cl^-).</p>
CHEMIFY-0126	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0126:</p> <p>Starting materials: 2-chloro-N-(2,6-difluorophenyl)benzoylamine, 4-aminobiphenyl, and tert-butyldimethylsilyl trifluoromethanesulfonate ($\text{NaO}(\text{C}_2\text{H}_5)_2\text{SO}_3\text{CF}_3$).</p> <p>Product: A substituted phenyl ring linked to a bis(tert-butylcarbamoyl) group via an amide linkage.</p>

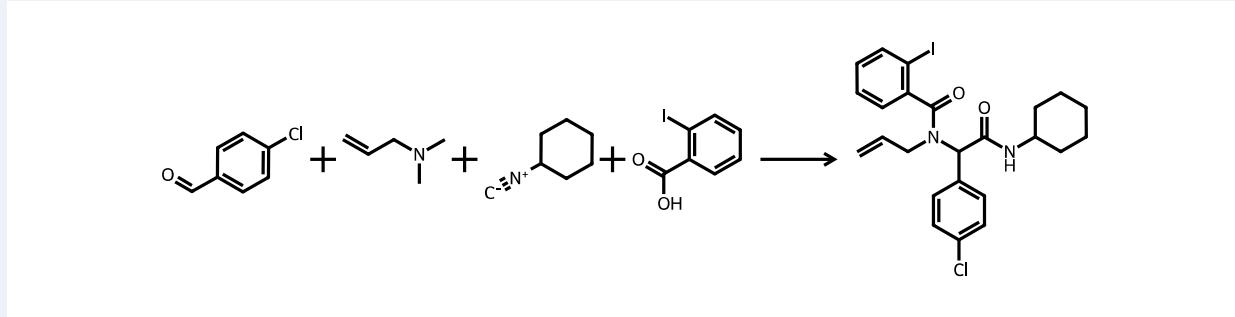
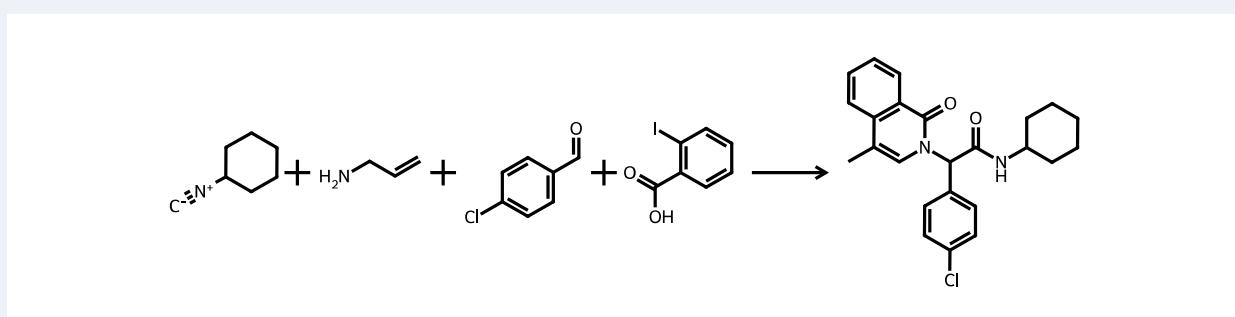
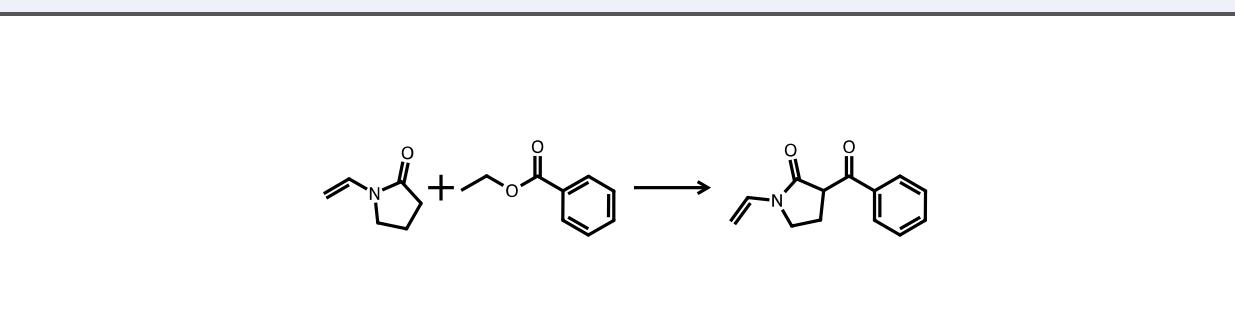
ID	Step	Yield	Scale	Reaction
CHEMIFY-0127	Step 1			<p>Reaction scheme for Step 1 of CHEMIFY-0127:</p> <p>Starting materials: 4-bromo-N-(4-bromophenyl)benzylamine and 4-bromobiphenyl.</p> <p>Product: 4-bromo-N-(4-bromobiphenyl-4-yl)benzylamine.</p>
TwoStep-1 (0034+0010)	Step 1	81 %, 43 %	90.5 mmol, 10.0 mmol	<p>Reaction scheme for Step 1 of TwoStep-1:</p> <p>Starting materials: Allylamine and Chloroacetic acid.</p> <p>Product: N-(allyl)acetoformamide.</p>
	Step 2			<p>Reaction scheme for Step 2 of TwoStep-1:</p> <p>Starting materials: N-(allyl)acetoformamide and a substituted alkene (with a bromine atom).</p> <p>Product: A substituted amide where the allyl group from Step 1 has reacted with the alkene.</p>

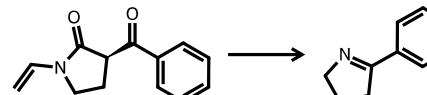
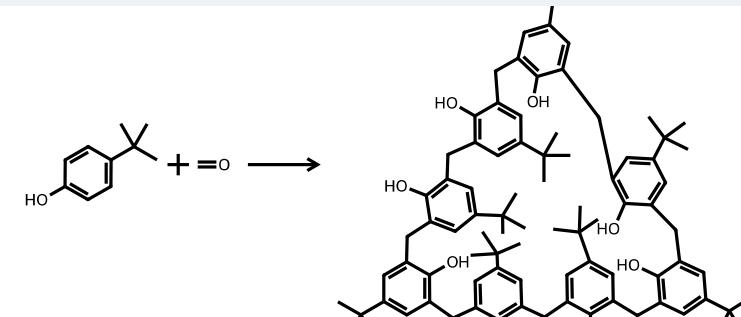
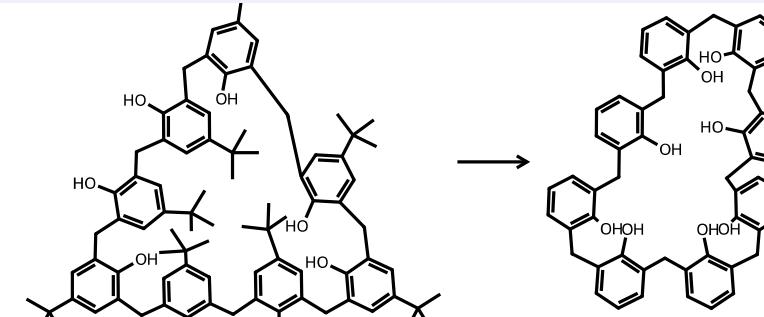
ID	Step	Yield	Scale	Reaction
TwoStep-2 (0035+0010)	Step 1	91 %, 43 %	10.0 mmol, 10.0 mmol	
	Step 2			
TwoStep-3 (0078+0037)	Step 1	64 %, 74 %	40 mmol, 9.0 mmol	

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

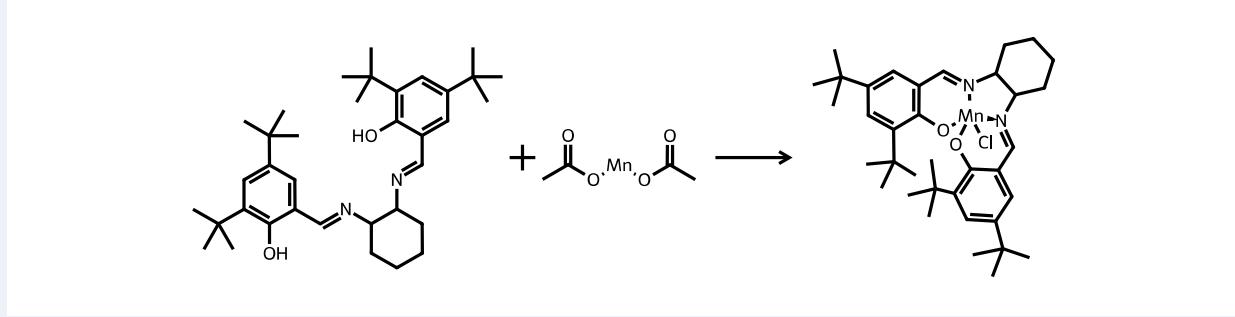
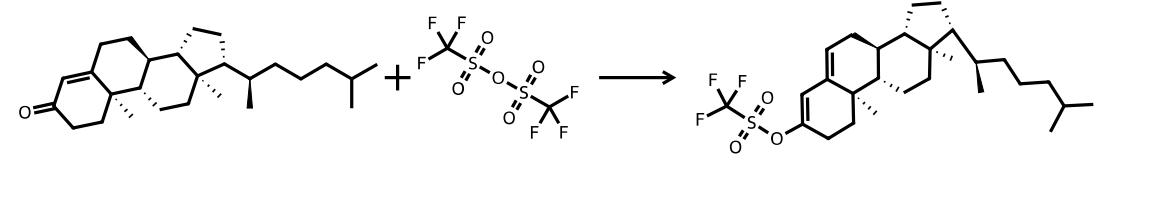
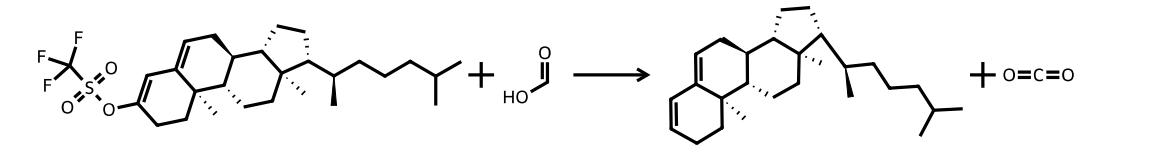
ID	Step	Yield	Scale	Reaction
TwoStep-5 (0075+0004)	Step 1	56 %, 84 %	20 mmol, 10.0 mmol	
	Step 2			
TwoStep-6 (0004+0005)	Step 1	84 %, 37 %	10.0 mmol, 13.0 mmol	

ID	Step	Yield	Scale	Reaction
	Step 2			<p>Reaction scheme for Step 2:</p> <p>Starting materials: A carboxylic acid derivative (benzyl ester) and a cyclic amine.</p> <p>Product: A substituted cyclopentane derivative where the carboxylic acid group has been converted to a hydroxyl group.</p>
TwoStep-7 (0056+0022)	Step 1	78 %, 32 %	12.0 mmol, 1.86 mmol	<p>Reaction scheme for Step 1:</p> <p>Starting materials: Benzaldehyde, allyltrimethylsilane, a cyclic carbonyl compound (e.g., cyclohexanone), and 2-iodophenylacetic acid.</p> <p>Product: A complex intermediate formed by the multi-step coupling of these four components.</p>
	Step 2			<p>Reaction scheme for Step 2:</p> <p>Starting material: The complex intermediate from Step 1.</p> <p>Product: A substituted indole derivative where the intermediate has undergone cyclization.</p>

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	

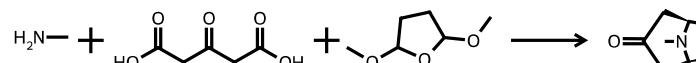
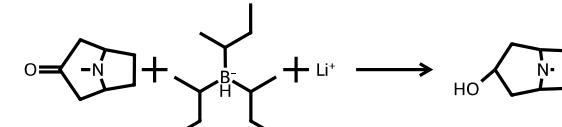
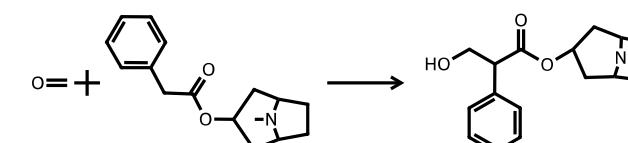
ID	Step	Yield	Scale	Reaction
TwoStep-10 (0040+0042)	Step 2			
	Step 1	36 %, 58 %	33.3 mmol, 0.77 mmol	
	Step 2			

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: A 1,4-diaminocyclohexane derivative reacts with L-lactate to form a protonated intermediate where one amino group is replaced by a protonated ammonium group.</p>
	Step 2			<p>Reaction scheme for Step 2: The intermediate from Step 1 reacts with a substituted benzaldehyde and a substituted cyclopentenone to form a complex polycyclic product.</p>
TwoStep-12 (0044+0045)	Step 1	85 %, 70 %	11.2 mmol, 1.5 mmol	<p>Reaction scheme for Step 1 of TwoStep-12: A substituted benzaldehyde, a substituted cyclopentenone, and L-lactate react to form a complex polycyclic product.</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: $\text{Cl}-\text{CH}_2-\text{COOH} + \text{CH}_2=\text{CH}-\text{NH}_2 \rightarrow \text{CH}_2=\text{CH}-\text{NH}-\text{COOCH}_2\text{CH}_3$</p>
	Step 2	81 %, 91 %, 43 %	90.5 mmol, 10.0 mmol, 10.0 mmol	<p>Reaction scheme for Step 2: $\text{CH}_2=\text{CH}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{C}\equiv\text{N} + \text{Br}-\text{C}(\text{O})-\text{N}(\text{C}_2\text{H}_5)-\text{C}(\text{O})-\text{Br} \rightarrow \text{CH}_2=\text{CH}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{C}\equiv\text{N}-\text{CH}_2-\text{CH}_2-\text{C}\equiv\text{N}$</p>
	Step 3			<p>Reaction scheme for Step 3: $\text{CH}_2=\text{CH}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{C}\equiv\text{N}-\text{CH}_2-\text{CH}_2-\text{C}\equiv\text{N} + \text{CH}_2=\text{CH}-\text{NH}-\text{COOCH}_2\text{CH}_3 \rightarrow \text{Product}$</p>

ID	Step	Yield	Scale	Reaction
ThreeStep-2 (0078+0037+0012)	Step 1			<p>Reaction scheme for Step 1: A diacid (hexanedioic acid) reacts with allyl alcohol to form a bis(allyl) ester.</p>
	Step 2	64 %, 74 %, 92 %	40 mmol, 9.0 mmol, 2.0 mmol	<p>Reaction scheme for Step 2: A bis(allyl) ester undergoes cyclization to form a cycloheptanone derivative.</p>
	Step 3			<p>Reaction scheme for Step 3: A cycloheptanone derivative undergoes further cyclization to form a bicyclic product.</p>

ID	Step	Yield	Scale	Reaction
ThreeStep-3 (0075+0004+0005)	Step 1			
	Step 2	56 %, 84 %, 37 %	20 mmol, 10.0 mmol, 13.0 mmol	
	Step 3			

ID	Step	Yield	Scale	Reaction
ThreeStep-4 (0043+0044+0045)	Step 1			
	Step 2	76 %, 85 %, 70 %	100.0 mmol, 11.2 mmol, 1.5 mmol	
	Step 3			