Synthesis of Multicyclic Organic Scaffolds Via An Intramolecular Ylide-Alkene Cycloaddition:

An Approach to Bioisosteric Morphine Analogs

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Abstract

Access to a diverse array of druglike organic molecules via efficient total synthesis is of critical importance for the exploration of new compounds of biological and medicinal interest. In particular, any viable synthetic route to such molecules must incorporate precise control of stereochemistry as well as the ability to tune medicinally relevant parameters such as acidity, lipophilicity, and the incorporation of bioisosteres. Synthesis of a bioisosteric analog of the opiate analgesic morphine was pursued using an intramolecular ylide-alkene cycloaddition as the key step which would establish the configuration of the six stereocenters of the molecule in a single operation. The novel structure of the target analog should produce a compound with compelling biological activity from a brief, diversifiable synthesis.
Acknowledgements

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Introduction

Opiate analgesic drugs such as the natural product morphine 1 represent a biologically potent and clinically important class of organic compounds. The clinical usefulness of several morphine analogs such as butorphanol 2, morphinan 3, and benzomorphan 4 indicates that the chemical synthesis of morphine analogs represents a promising route for the discovery of biologically active organic materials.

Of particular interest to our laboratory is the preparation of morphine analogs in which the catechol motif 5 present in morphine is replaced with bioisosteric1 benzoxazole groups 6 and 7 and benzothiazole group 8. Accordingly, synthetic targets 9, 10, and 11 are currently being pursued in our laboratory, with analog 9 being the subject of this study.

The complex, polycyclic structure of these analgesic analogs mandates a synthetic route displaying excellent regiochemical and stereochemical control. To this end, the total synthesis of
analog 9 was pursued via a photoinitiated intramolecular ylide-alkene cycloaddition reaction
developed in our laboratory, which allows for the construction of up to three rings and six chiral
centers in a single experimental operation.
Background

The basis for the synthesis of natural product analogs in this study lies in the heteroatom-directed photoarylation reaction of aryl vinyl ethers 12a and aryl vinyl sulfides 12b. This reaction was originally developed as a means of facile synthetic access to dihydrofuran 14a and dihydrothiophene 14b systems. Chemical and spectroscopic evidence supports the intermediacy of carbonyl ylide 13a and thiocarbonyl ylide 13b intermediates in this conversion.3-5

\[
\begin{align*}
\text{12a, } X &= O \\
\text{12b, } X &= S \\
\text{13a, } X &= O \\
\text{13b, } X &= S \\
\text{14a, } X &= O \\
\text{14b, } X &= S
\end{align*}
\]

The synthetic utility of such ylide systems for cycloaddition processes is widely recognized, and several methods for their generation have been reported.6-8 Nevertheless, the heteroatom-directed photoarylation reaction has received relatively little attention in the literature as a strategy for the formation of these ylides. Our laboratory has investigated the attachment of a pendant alkene to the photoarylation precursor that may react with the resulting ylide intermediate via an intramolecular [3+2] cycloaddition process. This concept is exemplified by the formation of generalized ylide 16 from precursor 15 to yield photoproducts 17a or 17b, depending on the length of the pendant alkene chain.
This strategy of photoarylation followed by intramolecular cycloaddition was viewed as a potentially rapid and powerful method for constructing multicyclic organic scaffolds.

Previous studies in our laboratory have established several factors controlling product formation in the photoinitiated intramolecular ylide-alkene cycloaddition. For example, low-temperature irradiation of a solution of 18 in toluene provided product 19, which is consistent with ylide formation and subsequent hydrogen shift.\(^9\)

\[
\begin{align*}
\text{hv, toluene} & \quad 25 \text{ to } -70 \degree C \\
18 & \quad \xrightarrow{} \quad 19
\end{align*}
\]

In contrast, high-temperature irradiation of 18 in toluene resulted in formation of unexpected intramolecular addition product 19 as a mixture of diastereomers 19a and 19b.\(^9\)

\[
\begin{align*}
\text{hv, toluene} & \quad 110 \degree C, 4h \\
18 & \quad \xrightarrow{} \quad 19a, 19b
\end{align*}
\]

Control experiments indicated that both light and heat are required for the formation of intramolecular addition products such as 19, suggesting that photochemical ylide formation is followed by a thermally induced intramolecular process. While valuable for determining the thermal requirement for such reactions, these studies of aryl vinyl sulfides failed to produce the desired [3+2] addition product, which motivated subsequent studies of aryl vinyl ether systems.
The temperature dependence of the ylide-alkene addition reaction was found to extend to aryl vinyl ethers, although the overall reactivity of such ether systems is generally quite different. For example, when aryl vinyl ether 20 was subjected to irradiation in toluene at room temperature, the major product 21 was consistent with photocyclization followed by hydrogen shift, and a minor product 22 was also formed that was analogous to aryl vinyl sulfide addition product 19. At this temperature, the desired [3+2] addition product was not observed.10

![Chemical structure of 20, 21, and 22](image)

However, at high temperature irradiation of 20 furnishes the desired [3+2] cycloaddition product 23 as the major product in addition to addition product 24. Thus, while aryl vinyl ether systems preserve the requirements for heat and light observed with aryl vinyl sulfides, changing the heteroatom to oxygen alters the reactivity to allow the formation of the desired [3+2] adduct, which was never observed for the sulfur analogs.11

![Chemical structure of 20, 23, and 24](image)

Additionally, it was observed that substitution of the pendant alkene with electron-withdrawing groups greatly favors formation of the [3+2] cycloaddition product. This is evidenced by the irradiation of aryl vinyl ether 25, which effected the high-yield preparation of [3+2] addition
product 26 even at room temperature, with trace amounts of addition product 27 occasionally observed.\textsuperscript{11}

Having studied the reactivity of naphthyl vinyl ethers, the potential for similar reactions of phenyl vinyl ethers was explored. Unfortunately, irradiation of phenyl-substituted precursor 28 at a variety of temperatures furnished only ring-closed product 29 and none of expected intramolecular addition product 30, nor of a [3+2] cycloaddition product.\textsuperscript{11}

The difference in reactivity for such phenyl-substituted systems could be rationalized by the loss of aromaticity upon formation of the ylide, reducing the resonance stabilization of the intermediate relative to the corresponding naphthyl system. Because they retain aromaticity to some extent during ylide formation, bicyclic aryl groups would be expected to favor intramolecular ylide-alkene cycloaddition.

Given these precedents, we expected that synthetic target 9 could be prepared from photoprecursor 31 via ylide intermediate 32.
Success with heterocyclic aromatic systems would further extend the utility of our methodology in the synthesis of natural product analogs. For example, the benzoxazole group, in addition to its intended use in this study as a bioisosteric replacement for a catechol motif, could be hydrolyzed to reveal a disubstituted aromatic ring with additional potential for interesting reactivity and biological activity.

The preparation of 31 is illustrated by the following synthesis, which is representative of many photoprecursor syntheses performed in our laboratory.
The aromatic alcohol 2-methylbenzo[d]oxazol-5-ol 37 required for this synthesis is not commercially available and was obtained synthetically. Several methods for the generation of benzoazole systems are available, and the Beckmann rearrangement of \( o \)-acylphenol oximes was selected as an appropriate and convenient approach to the desired hydroxy-substituted benzoazole.\(^{12}\) Accordingly, it was expected that 37 could be prepared by conversion of 40 to the corresponding oxime 41 followed by subsequent cyclization to yield 37.
Synthesis of the desired photoprecursor in this manner should provide an efficient route to morphine analog 9 via intramolecular ylide-alkene cycloaddition, and, further, could exhibit broad utility in natural products synthesis.
Results and Discussion

3-ethoxycyclohex-2-enone 33 was prepared from 1,3-cyclohexanedione 34 as shown.\textsuperscript{13} Subsequent Grignard reaction of 34 with \textit{in situ} prepared 4-bromomagnesium-1-butene afforded 35 in 73\% yield, which after epoxidation to 36 (59\% yield) completed the first branch of the convergent synthesis of photoprecursor 31.\textsuperscript{9}

![Diagram of synthesis](image)

Additionally, the synthesis of aromatic alcohol 37 was achieved to complete the second branch of the synthesis. Acetophenone derivative 40 was cleanly converted to oxime 41 as shown (87\% yield),\textsuperscript{14} which in turn was successfully subjected to conditions for Beckmann rearrangement to benzoxazole 37 in 65\% yield.\textsuperscript{12} Although such benzoxazoles reportedly precipitate from aqueous solution, precipitation of 37 was not observed. Extraction with ethyl acetate proved a superior method for its isolation, with a single recrystallization from acetonitrile providing a convenient purification method.

![Diagram of synthesis](image)
Coupling of 36 with benzoxazole 37 via nucleophilic epoxide opening, followed by elimination, was subsequently achieved. A preliminary run at room temperature with a catalytic quantity of KH indeed furnished coupled product 38, as indicated by LC/MS analysis of the reaction mixture. However, the rate of product formation under those conditions was impractically slow, due to the modest nucleophilicity of the hydroxyl oxygen atom of 37, and the reaction was incomplete after 5 days. The reaction is greatly facilitated by heat, as well as by the addition of N,N’-dimethylpropyleneurea (DMPU), which is notable for its ability to facilitate nucleophilic substitutions.15 Under these conditions, the reaction was complete in 48 hours, with coupled product 38 as the major product, which was successfully purified by flash chromatography on silica gel.

While the well-established conditions above remain the most reliable method to achieve the synthesis of coupled aryl vinyl ethers such as 38, the reaction was also attempted using a microwave reactor.16 In a pilot study, the reaction mixture was irradiated for two hours at 110 °C in fixed-temperature mode. Although the irradiation time and temperature have not been optimized, 38 was indeed observed by ¹H NMR analysis as a product of the microwave-assisted coupling reaction.
Modification of the pendant alkene group of 38 via ozonolysis, followed by Wittig addition, will complete the synthesis of photoprecursor 31.

Upon irradiation in toluene at reflux, photoprecursor 31 is expected to furnish photoproduct 9 via ylide formation and subsequent [3+2] cycloaddition. This preparation of 9 is notable for its brevity—with a longest linear sequence of 7 steps, this scheme will establish a multicyclic scaffold with precise stereocontrol in a remarkably brief synthesis.
Experimental

General Methods

$^1$H NMR spectra were recorded on a Bruker AVANCE III 500 (500 MHz) NMR spectrometer. Chemical shifts are reported in ppm ($\delta$) relative to tetramethylsilane at 0.00. $^{13}$C NMR spectra were recorded at 125.72 MHz. Infrared spectra (IR) were recorded on a Bruker Vertex 70 Infrared Spectrometer equipped with an ATR accessory, scanning from 4000 to 650 cm$^{-1}$ over 16 scans. Analytical thin-layer chromatography was performed on precoated silica gel plates (0.25 mm thickness) with a 254 nm fluorescent indicator and was visualized under ultraviolet light and/or with a $p$-anisaldehyde stain. Flash chromatography was performed on Thompson Single StEP pre-packed silica gel columns using an AnaLogix IntelliFlash 280 automated chromatography system. LC/MS data were obtained on an Agilent Technologies 6130 Quadrupole LC/MS using an SB-C18 Rapid Resolution 3.5 $\mu$m, 2.1x30 mm Zorbax HRLC cartridge column. Microwave-assisted reactions were performed using an Emrys Optimizer automated microwave synthesizer.
3-ethoxycyclohex-2-enone

(33, DJS-I-001, DJS-I-002, DJS-I-008)

To a 2-L three-neck flask fitted with a water-cooled reflux condenser and Dean Stark trap was added 1,3-cyclohexanediol 33 (57.54 g, 0.51 mmol) and ethanol (100 mL). To this solution was added toluene (900 mL) and p-toluenesulfonic acid monohydrate (2.32 g). The resulting solution was refluxed for 3 h with periodic removal of the distillate, and subsequently was concentrated under reduced pressure. The residue was taken up in toluene and washed with 10% aqueous NaOH solution saturated with NaCl (4 x 100 mL). The organic layer was washed with water until the aqueous washings were neutral, washed with brine, and dried (MgSO₄). The product was concentrated under reduced pressure and subsequently distilled under reduced pressure to furnish 34 as a light-yellow oil (25.49 g, 34%): bp 76-78 °C (1 mm Hg); ¹H NMR (CDCl₃, 500 MHz) δ 1.35 (t, 3 H, J = 7 Hz), 1.97 (m, 2 H), 2.33 (t, 2H, J = 6 Hz), 2.39 (t, 2H, J = 6 Hz), 3.89 (q, 2 H, J = 7 Hz), 5.33 (s, 1 H).
3-(3-butenyl)-2-cyclohexenone

(35, DJS-I-007, DJS-I-009, DJS-I-011)

\[
\begin{array}{c}
\text{OEt} \\
\text{34}
\end{array}
\xrightarrow{1. \text{BrMg}}, \text{THF}
\xrightarrow{2. \text{H}_2\text{O}^+}
\begin{array}{c}
\text{35}
\end{array}
\]

In a dry flask under nitrogen was added magnesium (0.140 g, 5.76 mmol) in dry THF (1 mL). 4-Bromo-1-butene (0.386 mL, 3.80 mmol) was added slowly with gentle heating. A vigorous exothermic reaction was observed. An additional portion of dry THF (0.9 mL) was added. The mixture was stirred until the exothermic reaction had subsided, followed by an additional 30 min at room temperature. 3-ethoxycyclohex-2-enone 34 (0.519 mL, 3.57 mmol) was added dropwise, followed by an additional portion of dry THF (1.8 mL). The mixture was stirred at room temperature for 18 h. The resulting solution was partitioned between dichloromethane and a saturated aqueous solution of ammonium chloride (10 mL). The organic layer was concentrated under reduced pressure. The residue was stirred for 1 h in a solution of HCl (1 M, 1 mL) and ethanol (2.5 mL). The solution was neutralized with saturated aqueous sodium bicarbonate and concentrated under reduced pressure. The residue was taken up in dichloromethane, washed with water, brine, and dried (MgSO\textsubscript{4}). The sample was concentrated under reduced pressure to yield 35 as an orange oil, (0.389 g, 73\%): \(^1\)H NMR (CDCl\textsubscript{3}, 500 MHz) \(\delta\) 1.99 (m, 2 H), 2.25-2.33 (m, 6 H), 2.36 (t, 2 H, \(J = 6\) Hz), 5.00 (d, 1 H, \(J = 10\) Hz), 5.05 (d, 1H, \(J = 17\) Hz), 5.79 (m, 1H), 5.88 (s, 1 H).
6-(3-butenyl)-7-oxabicyclo[4.1.0]heptan-2-one

(36, DJS-I-013, DJS-I-014, DJS-I-016)

Aqueous hydrogen peroxide (1.567 mL, 6.66 mmol) was added to a solution of 3-(3-butenyl)-2-cyclohexenone 35 (1.00 g, 6.66 mmol) in methanol (6.3 mL). The mixture was cooled to 0 °C, and a solution of sodium hydroxide (0.57 mL, 3.43 mmol) was added slowly. The mixture was stirred at room temperature for 2 h, after which solvent was removed under reduced pressure. The product was partitioned between dichloromethane and water, and the organic phase was washed with water, brine, and dried (MgSO4). Removal of solvent furnished 36 as a colorless oil (0.653 g, 59%): bp 100 °C (5 mm Hg); \(^1\)H NMR (CDCl\(_3\), 500 MHz) \(\delta\) 1.22-1.58 (m, 9H), 2.45 (d, 1H, \(J = 18\) Hz), 3.04 (s, 1H), 4.95 (d, 1H, \(J = 10\) Hz), 5.00 (d, 1H, \(J = 17\) Hz), 5.75 (m, 1H).
(E)-1-(2,5-dihydroxyphenyl)ethanone oxime

(41, DJS-I-018)

To a solution of hydroxylamine hydrochloride (1.53 mL, 36.8 mmol) and sodium acetate (1.779 g, 21.69 mmol) in water (4 mL) was added a solution of 1-(2,5-dihydroxyphenyl)ethanone 40 (1.00 g, 6.57 mmol) in boiling water (40 mL). The resulting solution was heated at reflux for 2 h and extracted with ethyl acetate. The organic phase was washed with water, brine, and dried (MgSO₄). Solvent was removed under reduced pressure to furnish 41 (0.954 g, 87%) as a crystalline, off-white solid: ¹H NMR (DMSO-d₆, 500 MHz) δ 2.20 (s, 3H), 6.68 (s, 2H) 6.85 (d, 1H, J = 2 Hz), 8.91 (s, 1H), 10.85 (s, 1H), 11.48 (s, 1H).
2-methylbenzo[d]oxazol-5-ol

(37, DJS-I-010, DJS-I-012, DJS-I-015, DJS-I-017, DJS-I-023)

(E)-1-(2,5-dihydroxyphenyl)ethanone oxime 41 (4.20 g, 25.1 mmol) was dissolved in dry N,N-dimethylacetamide (5.0 mL) and dry acetonitrile (15.0 mL). The solution was cooled to 0 °C, and phosphorus oxychloride (2.42 mL, 26.0 mmol) was added during 3 min. The solution was stirred at room temperature for 60 min, after which a solution of ice/water (200 mL) containing sodium acetate (6.00 g) was added. The product was extracted with ethyl acetate, and the combined organic phases were washed with water, brine, and dried (MgSO₄). The resulting solution was concentrated under reduced pressure to furnish 37 as a dark brown solid (crude yield: 2.438 g, 65%). The crude product was recrystallized from acetonitrile to furnish the analytical sample (isolated yield: 1.843 g, 49%): ¹H NMR (DMSO-d₆, 500 MHz) δ 2.54 (s, 3H), 6.75 (dd, 1H, J = 9 and 2 Hz), 6.95 (d, 1H, J = 2 Hz), 7.41 (d, 1H, J = 9 Hz), 9.39 (s, 1H).
**3-(but-3-enyl)-2-(2-methylbenzo[d]oxazol-5-yloxy)cyclohex-2-enone**

(38, DJS-I-019, DJS-I-020, DJS-I-021, DJS-I-024, DJS-I-025)

In a dry flask under nitrogen, 2-methylbenzo[d]oxazol-5-ol 37 (0.179 g, 1.203 mmol) was dissolved in dry THF (3 mL). A suspension of potassium hydride (30% in mineral oil, 0.074 g, 0.568 mmol) in THF (2 mL) was added. After 5 min, a solution of 6-(3-butenyl)-7-oxabicyclo[4.1.0]heptan-2-one 36 (0.200 g, 1.203 mmol) in dry THF (2 mL) was added. DMPU (0.19 mL, 1.600 mmol) was added and the mixture was heated at reflux for 48 h. Solvent was removed under reduced pressure, and the residue was partitioned between diethyl ether and water. The organic phase was washed with several portions of water, washed with brine, and dried (MgSO₄). Solvent was removed under reduced pressure to yield the crude product (0.260 g, 73%), which was purified by flash chromatography on silica gel (hexanes-ethyl acetate (3:2)) to furnish 38 (0.110 g, 30.7 %): IR 2943, 1681, 1576, 1472, 1272, 1150, 923, 846 cm⁻¹; ¹H NMR (CDCl₃, 500 MHz) δ 2.07 (m, 2H), 2.23 (q, 2H, J = 7 Hz), 2.40 (t, 2H, J = 7 Hz), 2.50-2.56 (m, 4 H), 2.59 (s, 3H), 4.96 (d, 1H, J = 10 Hz), 5.00 (dd, 1H, J = 17 and 2 Hz), 5.73 (m, 1H), 6.93 (dd, 1H, J = 9 and 2 Hz), 7.01 (d, 1H, J = 2 Hz), 7.33 (d, 1H, J = 9 Hz); ¹³C NMR (CDCl₃, 125.72 MHz) δ 14.6 (CH₃), 22.2 (CH₂), 29.6 (CH₂), 30.8 (CH₂), 31.2 (CH₂), 38.5 (CH₂), 104.3 (CH), 110.3 (CH), 112.8 (CH), 115.6 (CH₂), 137.1 (CH), 142.2 (C), 144.5 (C), 146.3 (C), 151.6 (C), 155.0 (C), 164.8 (C), 193.0 (C=O); LC/MS (ESI/APCI) m/z 298.2 (MH⁺).
Figure 1: $^1$H NMR Spectrum of 3-ethoxycyclohex-2-enone (34)
Figure 2: $^1$H NMR Spectrum of 3-(3-Butenyl)-2-cyclohexenone (35)
Figure 3: $^1$H NMR Spectrum of 6-(3-butenyl)-7-oxabicyclo[4.1.0]heptan-2-one (36)
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