

# Comparative Analysis of Raspberry Ketone and its 4-Methoxy Analogue: Synthesis, Properties, and Spectroscopic Characterization

## Introduction:

Raspberry ketone (4-(4-hydroxyphenyl)butan-2-one), a naturally occurring phenolic compound, is renowned as the primary aroma constituent of red raspberries.<sup>1</sup> Its significant role in the flavor and fragrance industries has led to extensive research into its synthesis, properties, and applications.<sup>3</sup> Beyond its sensory attributes, raspberry ketone has also garnered attention for its potential nutraceutical properties, including anti-obesity, antioxidant, and anti-inflammatory effects.<sup>7</sup> The modification of natural compounds to create structural analogues is a common practice in chemistry to tailor their properties for specific applications in fields ranging from flavor chemistry and perfumery to pharmaceuticals.<sup>3</sup> In this context, the synthesis of a raspberry ketone analogue using 4-methoxybenzaldehyde as the starting material, instead of the conventional 4-hydroxybenzaldehyde, presents an interesting case for investigating how subtle structural changes can influence the resulting compound's characteristics. This report aims to provide a comprehensive analysis of this novel raspberry ketone analogue, 4-(4-methoxyphenyl)butan-2-one (also known as anisylacetone), by comparing it with standard raspberry ketone. The analysis will cover established synthesis methods for raspberry ketone, potential synthetic routes for the analogue, detailed physical and chemical properties of 4-methoxybenzaldehyde, expected spectroscopic and thermal analysis data for all three compounds, and a comparative assessment highlighting the impact of the methoxy substitution.

The user's choice of 4-methoxybenzaldehyde as a starting material likely stems from an interest in modulating the properties of raspberry ketone by replacing the phenolic hydroxyl group with a methoxy group. This structural modification is anticipated to alter the intermolecular interactions, electronic properties, and consequently, the physical, chemical, and sensory characteristics of the molecule. The request for detailed spectroscopic and thermal analysis underscores the need for comprehensive characterization data to confirm the identity of the synthesized analogue and to understand its behavior in comparison to the well-established raspberry ketone. This comparative study will provide valuable insights into the structure-property relationships of these flavour compounds.

## Established Organic Synthesis of Raspberry Ketone from 4-Hydroxybenzaldehyde:

The most prevalent method for the organic synthesis of raspberry ketone involves a two-step process: aldol condensation followed by catalytic hydrogenation.<sup>1</sup> In the first step, 4-hydroxybenzaldehyde is condensed with acetone in the presence of a base, typically sodium hydroxide (NaOH), to yield an  $\alpha,\beta$ -unsaturated ketone,

4-(4-hydroxyphenyl)-3-buten-2-one, also known as p-hydroxybenzalacetone (PHBA).<sup>3</sup> This condensation reaction can be carried out at room temperature over a day, achieving yields in the range of 70-80%.<sup>17</sup> However, various catalysts have been explored to enhance the yield and selectivity of this step, including mixed oxide catalysts like Ni/Zn<sub>3</sub>La<sub>1</sub> and Ni/BNC, as well as noble metal-based catalysts such as Ni/La<sub>2</sub>O<sub>3</sub> and Pd/La<sub>2</sub>O<sub>3</sub>.<sup>3</sup> One-pot synthesis methods that combine the aldol condensation and subsequent hydrogenation in a single reaction vessel have also been developed, often utilizing bifunctional catalysts like Ni/Zn-La or Pd loaded Zn-La, achieving high conversions and selectivities.<sup>3</sup> These advancements aim to improve the efficiency and sustainability of raspberry ketone production.<sup>3</sup>

The second step in the synthesis involves the catalytic hydrogenation of the double bond in 4-(4-hydroxyphenyl)-3-buten-2-one to obtain the saturated ketone, raspberry ketone.<sup>14</sup> A variety of hydrogenation catalysts can be employed for this reduction, including rhodium on alumina, palladium, platinum, Raney nickel, and nickel boride.<sup>14</sup> Rhodium on alumina has been reported to provide clean hydrogenation with high yields (around 99%).<sup>14</sup> Nickel boride (Ni<sub>2</sub>B), prepared from nickel(II) salts and sodium borohydride, offers a cheaper alternative to the more expensive noble metal catalysts and can also provide good yields.<sup>15</sup> It is important to carefully control the reaction conditions when using nickel boride to prevent the reduction of the carbonyl function.<sup>15</sup> In some cases, the preparation of the catalyst and the hydrogenation step can be carried out in a one-pot reaction, significantly reducing reaction time.<sup>15</sup>

Besides the established two-step method, alternative synthetic routes for raspberry ketone exist. Friedel-Crafts alkylation of phenol with 4-hydroxybutan-2-one using solid acid catalysts, such as acid-activated Montmorillonite clay, provides an environmentally friendly approach.<sup>1</sup> This method has reported conversions of 35-55% with high selectivity.<sup>18</sup> Another early method involves the reaction of phenol with methyl vinyl ketone under acidic catalysis.<sup>5</sup> While this route utilizes cheaper raw materials, it typically suffers from lower yields.<sup>19</sup> Raspberry ketone can also be synthesized from anisylacetone (the methoxy analogue) via demethylation using hydrobromic acid in the presence of an alkyl phenol catalyst.<sup>7</sup> This method essentially reverses the methylation of the phenolic hydroxyl group. Enzymatic synthesis of raspberry ketone, mimicking the natural phenylpropanoid pathway in raspberries, involves the condensation of coumaroyl-CoA with malonyl-CoA by benzalacetone synthase (BAS) to form 4-hydroxybenzalacetone, followed by reduction by benzalacetone reductase (BAR) to yield raspberry ketone.<sup>5</sup> However, the yield of raspberry ketone from natural extraction is extremely low, making this route commercially challenging.<sup>3</sup> Current research focuses on improving yields through microbial and cell-free synthetic strategies.<sup>21</sup>

The aldol condensation followed by catalytic hydrogenation stands out as the most established and widely used method for raspberry ketone synthesis due to its relatively high yields and ease of implementation on both laboratory and industrial scales. The continuous development of more efficient and selective catalysts further solidifies its importance. While alternative methods offer advantages in specific contexts, the two-step approach remains a cornerstone in the production of this valuable flavor compound. The demethylation of anisylacetone is particularly relevant to the user's query, as it suggests a potential pathway to

synthesize raspberry ketone from the analogue if desired.

#### **Investigating Organic Synthesis Routes for the Raspberry Ketone Analogue from 4-Methoxybenzaldehyde:**

Given the structural similarity between 4-hydroxybenzaldehyde and 4-methoxybenzaldehyde, the most direct and likely route for synthesizing the raspberry ketone analogue, 4-(4-methoxyphenyl)butan-2-one (anisylacetone), involves an analogous two-step process of aldol condensation followed by catalytic hydrogenation.<sup>15</sup> In the first step, 4-methoxybenzaldehyde is condensed with acetone under basic conditions, similar to the synthesis of raspberry ketone, to form 4-(4-methoxyphenyl)-3-buten-2-one, also known as anisylidene acetone.<sup>15</sup> The reaction conditions for this condensation are expected to be comparable to those used for 4-hydroxybenzaldehyde, potentially involving a base catalyst like NaOH at room temperature.<sup>14</sup>

The second step involves the catalytic hydrogenation of the double bond in 4-(4-methoxyphenyl)-3-buten-2-one to yield the saturated ketone, 4-(4-methoxyphenyl)butan-2-one.<sup>15</sup> Hydrogenation catalysts commonly used for raspberry ketone, such as palladium (Pd) and nickel boride (Ni<sub>2</sub>B), are expected to be effective for this transformation as well.<sup>15</sup> Notably, a one-pot tandem synthesis of 4-(4-methoxyphenyl)butan-2-one directly from 4-methoxybenzyl alcohol and acetone using a multifunctional supported AuPd nanoalloy catalyst has been reported.<sup>27</sup> Furthermore, a telescoped flow system consisting of three micropacked bed reactors has been successfully employed for the synthesis of 4-(4-methoxyphenyl)butan-2-one from 4-methoxybenzyl alcohol, achieving increased yields compared to batch methods.<sup>26</sup>

Beyond the aldol condensation-hydrogenation route, other potential synthetic pathways for 4-(4-methoxyphenyl)butan-2-one exist. These include the alkylation of acetoacetic ester with methoxy-benzyl chloride followed by hydrolysis and decarboxylation, a method mentioned in the context of raspberry ketone synthesis.<sup>7</sup> Another possibility involves the reaction of methyl vinyl ketone with phenol, followed by methylation of the resulting raspberry ketone's hydroxyl group to yield the methoxy analogue.<sup>24</sup> Additionally, the three-step flow synthesis from 4-methoxybenzyl alcohol, involving oxidation to 4-methoxybenzaldehyde, C-C coupling with acetone, and subsequent reduction, presents an alternative approach.<sup>26</sup>

Given the well-established nature of the aldol condensation and hydrogenation sequence for synthesizing ketones with similar structural features, this route is the most likely and straightforward method for preparing the raspberry ketone analogue from 4-methoxybenzaldehyde. The literature on the synthesis of zingerone (using vanillin) via the same method further supports this expectation. The alternative routes offer valuable flexibility depending on the availability of starting materials and the specific requirements of the synthesis. The flow synthesis method, in particular, highlights the potential for optimizing the reaction process for improved efficiency and scalability.

#### **Physical and Chemical Properties of 4-Methoxybenzaldehyde:**

4-Methoxybenzaldehyde, also known as p-anisaldehyde or anisaldehyde, is a commercially important aromatic aldehyde with the chemical formula C<sub>8</sub>H<sub>8</sub>O<sub>2</sub> and a molecular weight of 136.15 g/mol.<sup>29</sup> Its CAS Registry Number is 123-11-5.<sup>29</sup> At room temperature, it typically

presents as a clear colorless to pale yellow liquid.<sup>31</sup> The odor of 4-methoxybenzaldehyde is often described as sweet, almond-like, and reminiscent of anise<sup>33</sup>, although some sources report it as odorless.<sup>29</sup> The compound has a relatively low melting point, generally reported between -1 °C and 2 °C.<sup>35</sup> Its boiling point is high, ranging from 247 °C to 249 °C at atmospheric pressure.<sup>29</sup> The density of 4-methoxybenzaldehyde is approximately 1.121 g/cm<sup>3</sup>.<sup>29</sup> It has a refractive index (n<sub>20/D</sub>) of around 1.573.<sup>29</sup>

In terms of solubility, 4-methoxybenzaldehyde is miscible with common organic solvents such as acetone, alcohol, ether, chloroform, and benzene, but it is immiscible with water.<sup>29</sup> The solubility of 4-methoxybenzaldehyde in water is reported to be low, around 2 g/L at 20°C.<sup>37</sup> It is also soluble in oils and slightly soluble in propylene glycol and glycerol.<sup>24</sup> The vapor pressure of 4-methoxybenzaldehyde is low, less than 1 hPa at 20 °C.<sup>30</sup> Its flash point, which indicates its flammability, is around 116 °C.<sup>29</sup> The autoignition temperature is reported to be 220 °C.<sup>30</sup> Chemically, 4-methoxybenzaldehyde is a versatile compound widely utilized in the fragrance and flavor industry due to its pleasant aroma.<sup>29</sup> It serves as a crucial intermediate in the synthesis of various other organic compounds, including perfumes, pharmaceuticals (like antihistamines), agrochemicals, dyes, and plastic additives.<sup>29</sup> A solution of 4-methoxybenzaldehyde in acid and ethanol is also employed as a stain in thin layer chromatography (TLC) for the easy identification of different compounds.<sup>29</sup> The aldehyde group in 4-methoxybenzaldehyde is electrophilic and readily undergoes nucleophilic addition reactions, including aldol condensation with ketones like acetone, under both basic and acidic conditions.<sup>25</sup> It can also be oxidized or reduced depending on the specific reagents and conditions used.<sup>5</sup> Furthermore, 4-methoxybenzaldehyde can react with various reagents to form derivatives such as hydrazones.<sup>42</sup>

The physical properties of 4-methoxybenzaldehyde are consistent with its molecular structure, featuring a polar aldehyde group and a methoxy substituent on an aromatic ring. Its moderate boiling point suggests it can be readily vaporized, contributing to its use in fragrances. The solubility profile indicates a preference for organic environments over aqueous ones. The chemical reactivity is characteristic of an aromatic aldehyde, making it a valuable building block in organic synthesis.

#### **Expected Spectroscopic Analysis of 4-Methoxybenzaldehyde:**

The Ultraviolet-Visible (UV-Vis) spectrum of 4-methoxybenzaldehyde is expected to exhibit characteristic absorption bands in the range of 225-350 nm, corresponding to  $\pi \rightarrow \pi^*$  and  $n \rightarrow \pi^*$  electronic transitions within the aromatic ring and the carbonyl group.<sup>44</sup> The exact wavelengths of maximum absorbance ( $\lambda_{\text{max}}$ ) and their intensities will be influenced by the solvent used for the analysis.<sup>46</sup> The presence of the electron-donating methoxy group is anticipated to cause a bathochromic shift (redshift) in the absorption bands compared to unsubstituted benzaldehyde, due to the increased conjugation and stabilization of the excited state.

The Infrared (IR) spectrum of 4-methoxybenzaldehyde should display several key characteristic peaks.<sup>48</sup> A strong absorption band corresponding to the stretching vibration of the aldehyde carbonyl group (C=O) is expected in the region of 1700-1725

$\text{cm}^{-1}$ .<sup>49</sup> Peaks associated with the aromatic ring will include C=C stretching vibrations around 1500-1600  $\text{cm}^{-1}$  and C-H stretching vibrations in the range of 3000-3100  $\text{cm}^{-1}$ .<sup>50</sup> The C-H stretching vibration of the aldehyde proton (CHO) will likely appear as a weak band around 2700-2800  $\text{cm}^{-1}$ . A prominent absorption band in the region of 1000-1300  $\text{cm}^{-1}$  will be due to the stretching vibration of the C-O bond in the methoxy group (OCH<sub>3</sub>).<sup>50</sup> Additionally, aromatic C-H bending vibrations are expected below 1000  $\text{cm}^{-1}$ .

In the <sup>1</sup>H Nuclear Magnetic Resonance (NMR) spectrum, the aldehyde proton (CHO) will give rise to a characteristic singlet around  $\delta$  9.8-10.0 ppm.<sup>49</sup> The four aromatic protons on the para-substituted benzene ring will typically appear as two doublets in the region of  $\delta$  6.8-7.9 ppm, with coupling patterns indicative of their relative positions.<sup>49</sup> The three protons of the methoxy group (OCH<sub>3</sub>) will show a singlet around  $\delta$  3.8-3.9 ppm.<sup>49</sup> The <sup>13</sup>C NMR spectrum will feature a signal for the carbonyl carbon (CHO) around  $\delta$  190-192 ppm.<sup>51</sup> The six carbons of the aromatic ring will exhibit signals in the range of  $\delta$  114-165 ppm, reflecting their different electronic environments.<sup>51</sup> The carbon atom of the methoxy group (OCH<sub>3</sub>) will appear around  $\delta$  55-56 ppm.<sup>51</sup>

High-Resolution Mass Spectrometry (HRMS) analysis of 4-methoxybenzaldehyde is expected to yield a protonated molecular ion [M+H]<sup>+</sup> with an exact mass of 137.05971 Da, based on its molecular formula C<sub>8</sub>H<sub>8</sub>O<sub>2</sub>.<sup>54</sup> The high resolution of the instrument will allow for precise determination of the mass, confirming the elemental composition of the compound. The expected spectroscopic data for 4-methoxybenzaldehyde is consistent with its structure. The UV-Vis spectrum will reveal its conjugated electronic system, while the IR spectrum will confirm the presence of the aldehyde and methoxy functional groups. The <sup>1</sup>H and <sup>13</sup>C NMR spectra will provide detailed structural information through the chemical shifts and coupling patterns of its constituent atoms. HRMS will offer precise molecular weight confirmation.

#### **Expected Thermal Analysis of 4-Methoxybenzaldehyde:**

Thermogravimetric Analysis (TGA) of 4-methoxybenzaldehyde is expected to show minimal mass loss at temperatures below its boiling point (around 248 °C). Above this temperature, a significant mass loss due to vaporization will be observed. The rate of mass loss will depend on the heating rate and the flow of the purge gas in the TGA instrument. The temperature at which complete vaporization occurs will provide an indication of its thermal stability under the experimental conditions. While specific TGA data for 4-methoxybenzaldehyde was not found in the provided snippets, TGA has been used to characterize catalysts in reactions involving this compound, suggesting its applicability for assessing its thermal behavior.<sup>55</sup>

Differential Scanning Calorimetry (DSC) of 4-methoxybenzaldehyde is expected to reveal endothermic transitions corresponding to its melting and boiling points.<sup>29</sup> An endothermic peak will be observed around its melting point (-1 °C to 2 °C), corresponding to the solid-to-liquid phase transition. Another endothermic peak will appear around its boiling point (around 248 °C), representing the liquid-to-gas phase transition. The area under these peaks will be proportional to the enthalpy of fusion and enthalpy of vaporization, respectively. DSC has been employed in various studies involving 4-methoxybenzaldehyde and its derivatives to

determine phase diagrams and analyze thermal stability, indicating its suitability for characterizing the thermal properties of this compound.<sup>65</sup>

Based on its physical properties, 4-methoxybenzaldehyde is expected to exhibit thermal stability up to its boiling point. TGA will likely show a significant mass loss above this temperature due to vaporization. DSC will provide precise values for its melting and boiling points, along with the associated enthalpy changes.

#### **Key Properties of Raspberry Ketone (4-(4-hydroxyphenyl)butan-2-one):**

Raspberry ketone (4-(4-hydroxyphenyl)butan-2-one) has a molecular formula of C<sub>10</sub>H<sub>12</sub>O<sub>2</sub> and a molecular weight of 164.20 g/mol.<sup>69</sup> Its CAS Registry Number is 5471-51-2.<sup>69</sup> It is characterized by a sweet, fruity, warm odor resembling that of raspberry preserves.<sup>69</sup>

Raspberry ketone is reported to be stable under recommended storage conditions but is incompatible with oxidizing agents.<sup>71</sup> It decomposes when heated.<sup>70</sup> This compound finds widespread use in perfumery, cosmetics, and as a food additive to impart a fruity odor.<sup>69</sup> It has also been investigated for its potential role in weight loss, as well as its antioxidant and anti-inflammatory properties.<sup>8</sup>

Spectroscopic analysis of raspberry ketone has yielded the following characteristic data: IR spectrum shows a broad O-H stretch around 3373 cm<sup>-1</sup> and a C=O stretch at 1691 cm<sup>-1</sup>.<sup>15</sup> In the <sup>1</sup>H NMR spectrum, key signals include a singlet at δ 2.14 ppm (methyl group), multiplets around δ 2.7-2.85 ppm (methylene groups), a broad singlet around δ 6.29 ppm (phenolic O-H), and multiplets around δ 6.75-7.09 ppm (aromatic protons).<sup>15</sup> The <sup>13</sup>C NMR spectrum shows characteristic peaks at δ 207.9 (carbonyl carbon), 154.9 (aromatic carbon with hydroxyl), and other signals for the remaining carbons.<sup>15</sup> High-Resolution Mass Spectrometry (HRMS) typically shows a molecular ion [M]<sup>+</sup> at m/z 164.<sup>15</sup>

Thermal analysis indicates that raspberry ketone has a melting point in the range of 82-83 °C<sup>15</sup>, and some sources report it as 81-85 °C.<sup>10</sup> The boiling point is reported to be above 200 °C, with decomposition occurring at higher temperatures.<sup>69</sup>

#### **Expected Properties of the Raspberry Ketone Analogue (4-(4-methoxyphenyl)butan-2-one):**

The raspberry ketone analogue, 4-(4-methoxyphenyl)butan-2-one (anisylacetone), has a molecular formula of C<sub>11</sub>H<sub>14</sub>O<sub>2</sub> and a molecular weight of 178.23 g/mol.<sup>13</sup> Its CAS Registry Number is 104-20-1.<sup>24</sup> The odor of this analogue is described as intensely sweet, floral, and fruity, often with cherry-raspberry notes.<sup>24</sup> It is reported to be stable under normal conditions but incompatible with oxidizing agents.<sup>75</sup> Applications of 4-(4-methoxyphenyl)butan-2-one include its use as an insect attractant, in organic synthesis, as a flavoring agent, and in perfume compositions, particularly as a modifier for Heliotropine.<sup>13</sup> It is also used as a pharmaceutical intermediate and has potential as a selective serotonin releasing agent.<sup>24</sup> Based on the structural change (methoxy group instead of hydroxyl), the expected spectroscopic data for 4-(4-methoxyphenyl)butan-2-one would show some differences compared to raspberry ketone. The IR spectrum is expected to exhibit a strong C=O stretch around 1715 cm<sup>-1</sup>, similar to raspberry ketone, but the O-H stretch will be absent.

Instead, C-O-C stretches for the methoxy group will be present in the 1000-1300  $\text{cm}^{-1}$  region. The  $^1\text{H}$  NMR spectrum is expected to show a singlet for the methyl ketone protons around  $\delta$  2.1 ppm, multiplets for the methylene protons around  $\delta$  2.7-2.9 ppm, and two doublets for the aromatic protons around  $\delta$  6.8-7.2 ppm. A key difference will be the presence of a singlet around  $\delta$  3.8 ppm for the methoxy group protons, instead of the phenolic O-H signal. The  $^{13}\text{C}$  NMR spectrum is expected to show a carbonyl carbon signal around  $\delta$  208 ppm, aromatic carbons in the range of  $\delta$  114-160 ppm, a methyl ketone carbon around  $\delta$  30 ppm, methylene carbons around  $\delta$  45 ppm, and a methoxy carbon around  $\delta$  55 ppm. The expected molecular ion  $[M]^+$  in HRMS would be at  $m/z$  178.0994 Da.

Thermal analysis of 4-(4-methoxyphenyl)butan-2-one suggests a melting point around 8-10  $^{\circ}\text{C}$ <sup>24</sup> and a boiling point around 152-153  $^{\circ}\text{C}$  at 15 mmHg<sup>24</sup>, or 269-271  $^{\circ}\text{C}$  at atmospheric pressure.<sup>13</sup> These values indicate a lower melting point compared to raspberry ketone, likely due to the absence of intermolecular hydrogen bonding through a hydroxyl group.

### **Comparative Spectroscopic and Thermal Analysis of Raspberry Ketone and its Analogue:**

The substitution of a hydroxyl group in raspberry ketone with a methoxy group in its analogue, 4-(4-methoxyphenyl)butan-2-one, leads to notable differences in their expected spectroscopic and thermal properties.

In terms of spectroscopic data, the UV-Vis spectrum of the analogue is expected to show a slight shift in  $\lambda_{\text{max}}$  compared to raspberry ketone due to the altered electronic environment of the aromatic ring. The most significant difference in the IR spectra will be the presence of a characteristic O-H stretch in raspberry ketone (around 3300-3400  $\text{cm}^{-1}$ ) that will be absent in the analogue. Conversely, the analogue will exhibit C-O-C stretches for the methoxy group in the 1000-1300  $\text{cm}^{-1}$  region, which will not be present in raspberry ketone. The  $^1\text{H}$  NMR spectra will differ by the presence of a phenolic O-H signal in raspberry ketone (around  $\delta$  6-7 ppm) and a methoxy methyl signal in the analogue (around  $\delta$  3.8 ppm). Minor shifts in the aromatic proton signals might also be observed. Similarly, the  $^{13}\text{C}$  NMR spectra will show a phenolic carbon signal in raspberry ketone (around  $\delta$  155 ppm) and an aromatic carbon bonded to methoxy around  $\delta$  160-165 ppm in the analogue, along with the methoxy carbon signal around  $\delta$  55 ppm. The HRMS will clearly distinguish the two compounds based on their different molecular weights: 164.0837 Da for raspberry ketone and 178.0994 Da for the analogue. The fragmentation patterns in mass spectrometry are also likely to differ due to the different functional groups present.

The thermal analysis data also highlights the impact of the structural modification. Raspberry ketone has a melting point around 82-83  $^{\circ}\text{C}$ , while the analogue melts significantly lower, around 8-10  $^{\circ}\text{C}$ . This substantial difference is primarily attributed to the absence of intermolecular hydrogen bonding in the analogue, which is possible in raspberry ketone through its phenolic hydroxyl group. The boiling points might also vary, with the analogue potentially exhibiting different volatility characteristics.

### **Conclusion:**

The raspberry ketone analogue synthesized using 4-methoxybenzaldehyde,

4-(4-methoxyphenyl)butan-2-one, exhibits distinct properties compared to raspberry ketone derived from 4-hydroxybenzaldehyde. While both compounds share a similar structural motif, the replacement of the hydroxyl group with a methoxy group in the analogue results in significant differences in their odor profiles, potential applications, and spectroscopic and thermal characteristics. The analogue presents a sweet, floral, and fruity aroma, contrasting with the pure raspberry scent of raspberry ketone. Its applications extend beyond flavor and fragrance to include insect attractants and pharmaceutical intermediates. Spectroscopically, the absence of the O-H functionality and the presence of the methoxy group in the analogue lead to clear distinctions in the IR and NMR spectra. Thermally, the most notable difference is the significantly lower melting point of the analogue, likely due to the lack of intermolecular hydrogen bonding. These findings underscore how subtle structural modifications can profoundly influence the properties of organic molecules, potentially making the raspberry ketone analogue suitable for specific applications where its unique characteristics offer advantages over the parent compound. Further research into the specific sensory properties and biological activities of this analogue would be beneficial.

Property	Raspberry Ketone	4-(4-methoxyphenyl)butan-2-one
Molecular Weight (g/mol)	164.20	178.23
Odor	Sweet, fruity, raspberry	Sweet, floral, fruity
Melting Point (°C)	82-83	8-10
IR (O-H stretch, cm <sup>-1</sup> )	~3373	Absent
IR (C-O-C stretch, cm <sup>-1</sup> )	Absent	1000-1300
<sup>1</sup> H NMR (Phenolic OH, ppm)	~6-7	Absent
<sup>1</sup> H NMR (Methoxy CH <sub>3</sub> , ppm)	Absent	~3.8
HRMS [M] <sup>+</sup> (Da)	164.0837	178.0994

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