HNUE JOURNAL OF SCIENCE DOI: 10.18173/2354-1059.2019-0039
Natural Sciences, 2019, Volume 64, Issue 6, pp. 121-129
This paper is available online at http://stdb.hnue.edu.vn

PREPARATION OF SOME BENZO[*d*]THIAZOLE-CONTAINING ACETOHYDRAZIDE DERIVATIVES

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Abstract. Four benzo[*d*]thiazole-containing acetohydrazide derivatives **1c**, **2c**, **3e**, and **4e** were prepared via condensation reaction of esters and hydrazine hydrate up to 89% yield. These processes involved in some modification of some known compounds in ether synthesis and acetylation of amino groups. Structures of these derivatives were elucidated by IR, NMR and MS analysis that referred a strong agreement between spectral data and structures.

Keywords: Benzo[*d*]thiazole, acetohydrazide, anticancer, hydrazine derivative**.**

I. Introduction

Benzo[*d*]thiazole derivatives show remarkable bioactivities such as: anti-cancer [1, 2], antimicrobial [3] activities. For example, 2-(4-aminophenyl) benzo[*d*]thiazole (**1**), an amino aromatic compound, and their corresponding *N*-acetylated derivatives (**2**) and (**4**) have showed surprisingly remarkable anticancer activity against breast, colon and ovarian cell lines *in vitro* [4-6]. J. Pan *et al.* showed that complexes **3** containing benzo[*d*]thiazole exhibited the lipophilicities in range of $\log P_{C18}$ = 1-4, their binding affinities (K_i = 30 - 617 nM) to $A\beta_{1\text{-}40}$ fibrils [7].

Received April 28, 2019. Revised June 3, 2019. Accepted June10, 2019.
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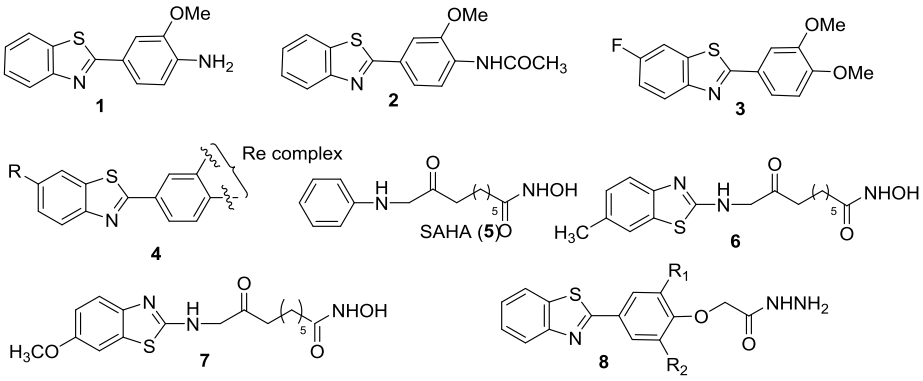


Figure 1. Some examples of benzo[d]thiazole-containing derivatives [1-6]

Recently, Oanh, D. T and *et al.* have modified structure of SAHA (**5**, an active agent in anti-cancer drug) to make compounds **6** and **7**. They exhibited a significant cytotoxic activity on cancer cell lines. Picture A and B in the Figure 2 animated the interaction of compound **6** and **7** interacting with enzyme histone deacetylases (HDAC) and also indicating that the side chains and benzo[*d*]thiazole ring played an important role in improving the anticancer activity [8].

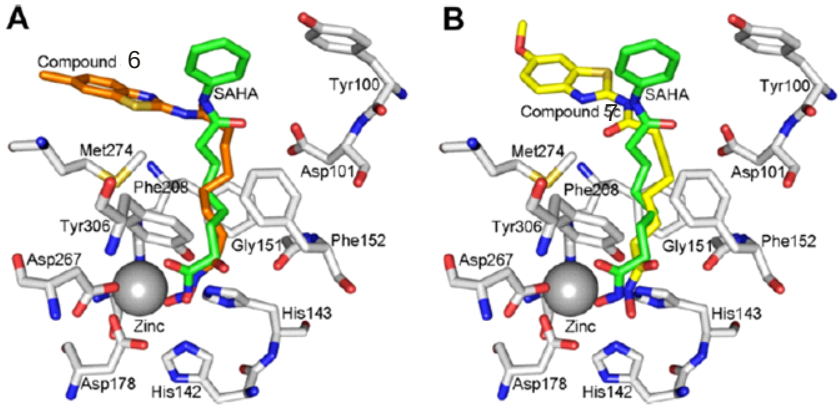


Figure 2. Compound 6 and 7 bind to HDAC [7]

In this work, benzo[*d*]thiazole derivatives **8** were designed by retaining structure of benzo[*d*]thiazole ring and modification of the "left" side into acetohydrazide, and variety of R1 and R2 to make four new acetohydrazide compounds which were ready for preparing more benzo[*d*]thiazole derivatives.

2. Content

2.1. Experimental

2.1.1. Chemicals and equipment

Solvents and other chemicals were purchased from Sigma-Aldrich, Merck Corp, Aladdin, Vietnam or other China's companies were used as received, unless indicated. The NMR spectra were recorded on the BrukerAvance 500 NMR spectrometer in DMSO-d_6; IRs was taken on FT-IR 4700 in The Vietnam Academy of Science and

Technology. Chemical-shift data for each signal was reported in ppm. A domestic Sanyo microwave oven (made in Thailand, 2005) was used to carry out the reactions.

2.1.2. Synthetic procedure

** General procedure for synthesis of 4-(benzo[d]thiazol-2-yl)phenol (**1a**); 4-(benzo [d]thiazol-2-yl)-2-methoxyphenol (**2a**); 4-(benzo[d]thiazol-2-yl)-2-nitrophenol (**3a**); 4-(benzo[d]thiazol-2-yl)-2-methoxy-6-nitrophenol (**4a**).*

A mixture of *o*-aminothiophenol (0.34 mL, 2.1 mmol, 152 g/mol) and an aldehyde (2.0 mmol) in a 250 mL beaker was irradiated 3 - 4 min at 400W power level. The progress of reaction was monitored with TLC in every 30 seconds. The mixture was then dissolved in ethyl acetate, *n*-hexane or ethanol and stood at room temperature to form solid. The crystals were collected and dried over to calculate yields. The yields of the reaction were up to 98% (1a: mp. = 226°C, 2a: mp. = 164°C, 3a: mp. =137°C, 4a: mp. = 178°C) [9].

** Synthesis of 2-amino-4-(benzo[d]thiazol-2-yl)phenol hydrochloride (**3b**) and 2-amino-4-(benzo[d]thiazol-2-yl)-6-methoxyphenol hydrochloride (**4b**) [9-11]*

Iron powder (8 g, 140 mmol) was added portion wise with stirring to a warm mixture (at 70 °C) of **3a** or **4a** (20 mmol) in absolute ethanol (20 mL) and concentrated hydrochloric acid (30 mL) at reflux temperature. After completion of the addition, the refluxing was continued for 6 hours. Upon cooling a yellow precipitate formed, which was filtered off, washed with methanol, dried to yield the title product as a yellow powder of compound **3b** (80% yield, mp. = 262°C) or **4b** (80% yield, mp. = 217°C).

** Synthesis of 2-acetamido-4-(benzo[d]thiazol-2-yl)-phenol (**3c**) and2-acetamido-4-(benzo[d] thiazol2-yl)-6-methoxyphenol(**4c**)*

General procedure: Mixture of **3b** or **4b** and acetic acid (15 mL) was refluxed at 70 °C for 6 hours. The progress of reaction was monitored with TLC in eluent ethyl acetate and *n*-hexane (v/v, 1:1). The acid acetic was distilled and saved for next use. The residue was diluted with ice water (15 mL) for crystallizing. The obtained solid was re-crystallized in ethanol to obtain compounds **3c** (76% yield) and **4c** (76% yield), respectively.

*Synthesis of 2-acetamido-4-(benzo[d]thiazol-2-yl)-phenol (**3c**)*

Following the general procedure from **3b** (0.6 g, 2mmol) and acetic acid (15 mL) to give a yellow needle of **3c**, (0.41g, 76%, mp.= 246°C)

*Synthesis 2-acetamido-4-(benzo[d]thiazol-2-yl)-6-methoxyphenol(**4c**)*

Following the general procedure from **4b** (0.7 g, 2mmol) and acetic acid (15 mL) to give a yellow needle of **4c**, (0.47g, 78%, mp.= 211°C)

** Synthesis of ethyl 2-(4-(benzo[d]thiazol-2-yl)phenol)acetate (**1b**), ethyl 2-(4-(benzo[d]thiazol-2-yl)-2-methoxyphenoxy)acetate (**2b**), ethyl-2-acetamido-(4-(benzo[d] thiazol-2-yl)-phenoxy) acetate (**3d**) and ethyl-2-acetamido-(4-(benzo[d]thiazol-2-yl)-6-methoxyphenoxy) acetate (**4d**)*

A mixture of anhydrous potassium carbonate (0.2 g, 1.5 mmol), ethyl monochloroacetate (1 mmol) and NaI (0.15g, 1 mmol) were added into a round bottom flask containing **1a**, **2a**, **3c** or **4c** (0.5 mmol) in DMF (3 mL). The resulting mixture was refluxed for 2 h at room temperature. The progress of reaction was monitored with TLC

in eluent ethyl acetate and *n*-hexane (v/v, 1:1). Solution was collected. After removal of DMF, the residue was re-crystallized in ethanol 96 to give **1b**, **2b**, **3d (**mp. = 161°C) or **4d** (mp.= 163°C) in about 82 % yield, respectively.

** Synthesis of acetohydrazides*

General procedure: Hydrazine hydrate (4 mL, 80%) was added into solution of **1b**, **2b**, **3d** or **4d** in absolute ethanol (10 mL). The resulting solution was refluxed for 2 hours. The mixture was gradually cooled down at r.t then ice water for 10 minutes. The white precipitate was collected and washed with cold ethanol (5 × 5 mL), then dried in oven to give acetohydrides **1c**, **2c**, **3e** or **4e** respectively.

*Synthesis of 2-(4-(benzo[d]thiazol-2-yl)phenoxy)acetohydrazide (**1c**)*

Following the general procedure from **1b** (0.32 g, 1 mmol), hydrazine hydrate (4mL, 80%) and absolute ethanol (10 mL) gave 2-(4-(benzo[*d*]thiazol-2-yl)phenoxy)acetohydrazide ***(1c)***, (0.26g, 87%, mp. = 242 °C); IR v (cm^{-1}): 3248, 3200, 3050, 2982, 2810, 1678, 1590, 1510, 1498, 1312, 1110; ^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm): 9.39 (s,1H), 8.11 (dd, *J* = 8.0, 0.5 Hz, 1H), 8.13 (d, *J* = 9.0 Hz, 2H), 8.01 (d, *J* = 8.0 Hz, 1H), 7.52 (td, *J* = 8.5, 1.5 Hz, 1H), 7.43 (td, *J* = 8.5, 1.5 Hz, 1H), 7.14 (td, *J* = 9.0 Hz, 2H), 4.60 (s, 2H), 4.34 (s, 2H);^{13}C NMR (125 MHz, DMSO-d_6)δ (ppm): 169.2, 166.8, 166.1, 153.5, 134.2, 128.7, 126.4, 126.0, 125.0, 122.4, 122.1, 115.4, 66.2; EI-MS m/z:$[M+H]^+$ calcd.for $C_{16}H_{16}N_3O_3S$ 330, found 329.9

*Synthesis of 2-(4-(benzo[d]thiazol-2-yl)-2-methoxyphenoxy)acetohydrazide (**2c**)*

Following the general procedure from **2b** (0.34 g, 1mmol), hydrazine hydrate (4 mL, 80%) and absolute ethanol (10 mL) gave 2-(4-(benzo[*d*]thiazol-2-yl)-2-methoxyphenoxy)acetohydrazide (**2c**), (0.3 g, 89%, mp. = 270 °C). IR v (cm^{-1}): 3250, 3220, 3080, 2980, 2810, 1676, 1590, 1510, 1490, 1321, 1110; ^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm): 9.23 (s, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 7.0 Hz, 1H), 7.58 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.52 (td, *J* = 7.0, 1.0 Hz, 1H), 7.43 (td, *J* = 8.0, 1.5 Hz, 1H), 7.07 (d, *J* = 8.5 Hz, 1H), 4.57 (s, 2H), 4.34 (s, 2H), 3.90 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6)δ (ppm): 167.1, 166.3, 153.5, 150.2, 149.4, 134.3, 126.6, 126.5 125.2, 122.2, 120.7, 113.9, 109.9, 67.0, 55.8. EI-MS m/z:$[M+H]^+$calcd. for $C_{15}H_{14}N_3O_2S$ 300, found 299.9.

*Synthesis of N-(5-(benzo[d]thiazol-2-yl)-2-(2-hydrazinyl-2-oxoethoxy)phenyl)acetamide (**3e**)*

Following the general procedure from **3d** (0.37 g, 1mmol), hydrazine hydrate (4 mL, 80%) and absolute ethanol (10 mL) gave *N*-(5-(benzo[*d*]thiazol-2-yl)-2-(2-hydrazinyl-2-oxoethoxy) phenyl)acetamide (**3e**), (0.3 g, 85%, mp.= 252 °C).IR v (cm^{-1}): 3242, 3236, 3052, 2982, 2820, 1680, 1594, 1516, 1498, 1315, 1110; ^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm): 9.62 (s,1H), 9.55 (s, 1H), 8.79 (s, 1H), 8.11 (d, *J* = 8.0Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.77 (dd, *J* = 8.0, 2.5 Hz, 1H), 7.52 (td, *J* = 8.5, 1.0 Hz, 1H), 7.43 (td, *J* = 8.0, 1.0 Hz, 1H), 7.20 (d, *J* = 9.0 Hz, 1H), 4.70 (s, 2H), 4.41 (s, 2H), 2.18 (s, 3H);^{13}C NMR (125 MHz, DMSO-d_6) δ (ppm): 168.7, 166.8, 166.1, 153.6, 149.9, 134.2, 128.1, 126.5, 125.9, 125.1, 123.3, 122.5, 120.6, 112.9, 67.1, 23.9. EI-MS m/z:$[M-H]^-$calcd. for $C_{17}H_{15}N_4O_3S$ 355, found 354.8, $[M+H]^+$ calcd. for $C_{17}H_{18}N_4O_3S$ 357, found 356.9.

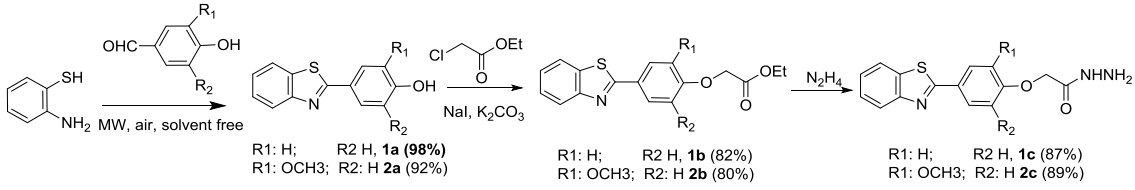
*Synthesis of N-(5-(benzo[d]thiazol-2-yl)-2-(2-hydrazinyl-2-oxoethoxy)-3-methoxyphenyl) acetamide (**4e**)*

Following the general procedure from **4d** (0.40 g, 1 mmol), hydrazine hydrate (4 mL, 80%) and absolute ethanol (10 mL) gave *N*-(5-(benzo[*d*]thiazol-2-yl)-2-(2-hydrazinyl-2-oxoethoxy)-3-methoxyphenyl)acetamide (**4e**), (0.33 g, 85%, mp.= 260 °C). IR v (cm^{-1}): 3330, 3200, 3070, 2900, 2810, 1675, 1590, 1510, 1489, 1312, 110; ^1H NMR (500 MHz, DMSO-d_6) δ 10.43 (s, 1H, Ha), 9.45 (s, 1H, Hb), 8.57 (s, 1H, H13), 8.13 (d, J = 8.0 Hz, 1H, H2), 8.06 (d, J = 8.0 Hz, 1H, H5), 7.54 (t, J = 7.5Hz, 1H, H5), 7.47 (s, 1H, H9), 7.45 (t, J = 7.5 Hz, 1H, H3), 4.56 (s, 2H, H17), 4.43 (s, 2H, Hc), 3.95 (s, 3H, H14), 2.19 (s, 3H, H16);^{13}C NMR (125 MHz, DMSO-d_6)δ 168.6 (C18, C15), 167.0(C7), 153.4 (C6), 152.3(C10), 139.3(C11), 134.4 (C1), 133.3(C12), 128.8(C8), 126.6 (C4), 125.4 (C3), 122.7 (C5), 122.2 (C2), 112.0(C13), 105.4 (C9), 70.9 (C17), 56.1 (C14), 24.1 (C16); EI-MS m/z: $[M+H]^+$ calcd. for $C_{18}H_{19}N_4O_4S$ 387, found 386.9; $[M-H]^-$ calcd. for $C_{18}H_{17}N_4O_4S$ 385, found 384.8.

2.2. Results and discussion

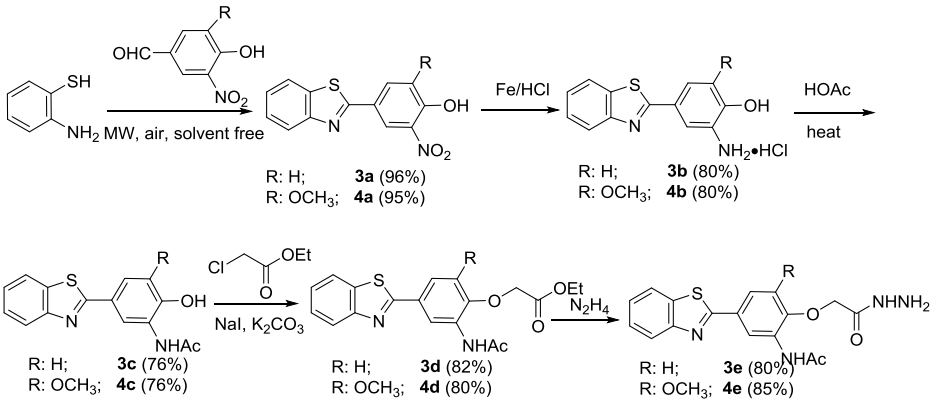
2.2.1. Synthesis

Synthesis of acetohydrazides was completed following Schemes 1 and 2. The benzo[*d*]thiazole cyclization was carried out based on our protocol using a domestic microwave oven to give **1a**, **2a**, **3a** and **4a** in high yield [11]. Reduction of nitro compounds **3b** and **4b** was followed our protocol without modification.



Scheme 1. Synthesis of acetohydrazides 1c and 2c

In contrast, conversion of amines **3b** and **4b** to acetamides**3c** and **4c** now was shortened in one step instead of two (30% yield) [12] in 82% yield when the salt form of amines was treated with acetic acid. The procedure of ether synthesis of **1b**, **2b**, **3d** and **4d** also was changed. Instead of using acetone solvent [13], in this paper, DMF was used. It seemed that acetone has lower boiling point than that of DMF, therefore, there was not enough heat for this transformation. In the final step, because of the strong nucleophilic property of hydrazine, as soon as added, acetohydrazides were formed and precipitated out. The precipitate was washed with ethanol several times to give pure enough products; otherwise, it could be re-crystallized in mixture solvent DMF and ethanol (v/v, 1:1) for further purification.



Scheme 2. Synthesis of acetohydrazides 3e and 4e

2.2.2. Structural determination

In order to analyze structures of acetohydrazides **1c**, **2c**, **3e** and **4e**, they were recorded IR, ^{1}H and ^{13}C NMR, MS spectra, exception of compound **4e** that was recorded HMBC also since its structure is the most complicated of all and its ^{13}C NMR spectrum lacked of one carbon that belongs to one of >C=O groups. IR, ^{1}H and ^{13}C NMR, MS spectrum analysis of acetohydrazides **1c**, **2c**, **3e** and **4e** was addressed in detail in the experimental section, except acetohydrazide **4e** was selected to show here. The structure of acetohydrazide **4e** had two amide groups that could let compound **4e** to exist in some conformers due to the rotation around the C-N single bond restricted based on the conjugation of nitrogen atom and >C=O group. Figure 3 showed two conformers of **4e** as examples. The right conformer **II** is less favoured than **I** because of the steric effect. Hydrogen bonding also gave some forms of compound **4e** such as **III**, **IV** and **V**.

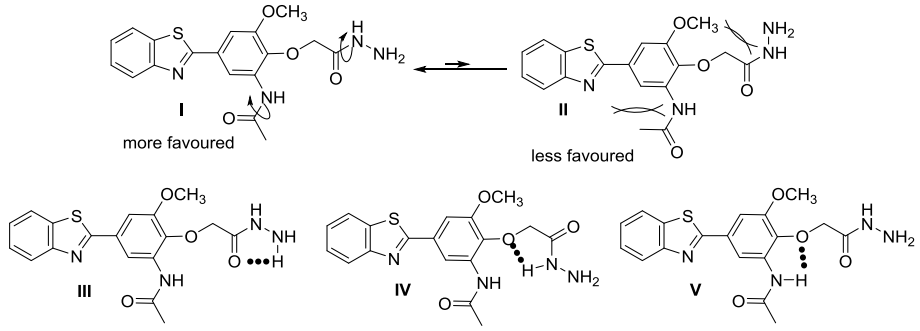


Figure 3.Some examples of conformers resulted from C-N rotation and hydrogen bonds of compound 4e

IR spectra of acetohydrazides **1c**, **2c**, **3e** and **4e** showed two sharp bands at about 3300 - 3200 cm^{-1} that indicated the vibration of N-H bond of –NH- and $–NH_2$. They also had band at about 1700 cm^{-1} expressing the stretching vibration of >C=O bonds. Thus, IR spectra indicated all expected functional groups of compound **4e**.

Interestingly, almost all signals showed two parts each in ^{1}H NMR spectrum. For example, Ha appeared two parts at 11.10 (smaller) and 10.43 (bigger) ppm; Hbat 9.45

(bigger) and 8.95 (smaller); H17 at 4.95 (smaller) and 4.56 (bigger) ppm. H14 and H16 had two parts but they were close to each other. Calculating the ratio of smaller signal/ bigger signal was about 1/9 ratio. These observations were matched with structural analysis mentioned above (Figure 3). The assignment of carbons and protons of benzo[*d*]thiazole ring was done in our papers [9, 11-13]. So, in this part, it was worth indicating the carbons and protons from position 8 to 18 (Figure 4). Firstly, it needed to get started at "known" signals on HMBC spectrum those were H16/C16 at 2.19/24.1 ppm; H14/C14 at 3.95/56.1 ppm and H17/C17 at 4.56/70.9 ppm. It also showed the peak at 4.43 ppm of two protons which was assigned for NH_2 group. Structure of acetohydrazide **4e** confirmed that H17 could have a correlation peak with C18; H16 with C15; Ha with C15; Hb with C18 respectively. Unfortunately, there were four correlation peaks *a2*, *a3*, *b2* and *b3* that confirmed C18 and C15 randomly appeared in same place at 168.6ppm that gave rise to an impossibility to identify Ha with Hb. Luckily, Ha (at 11.10 (smaller) and 10.43 (bigger) ppm) had a correlation *a7* with C11 and *a12* with C13. That helped to confirm Hb at 9.45 (bigger) and 8.95 (smaller) ppm and small part of C18 at 174.0 ppm through *a1* correlation peak accompanying with the bigger part at 168.6 ppm, picture A (Figure 4). C11 was assigned through peaks *b5* and *b6*; C10 was also confirmed through *b4*. H9/C9 and H13/C13 were distinguished each other through *a4*, *a5*, *a6*, *a8*, *a9*, *a10*, *a11*, *a13* and *a14*. Correlation peaks *a10* and *a11* referred C12 and C8 as well.

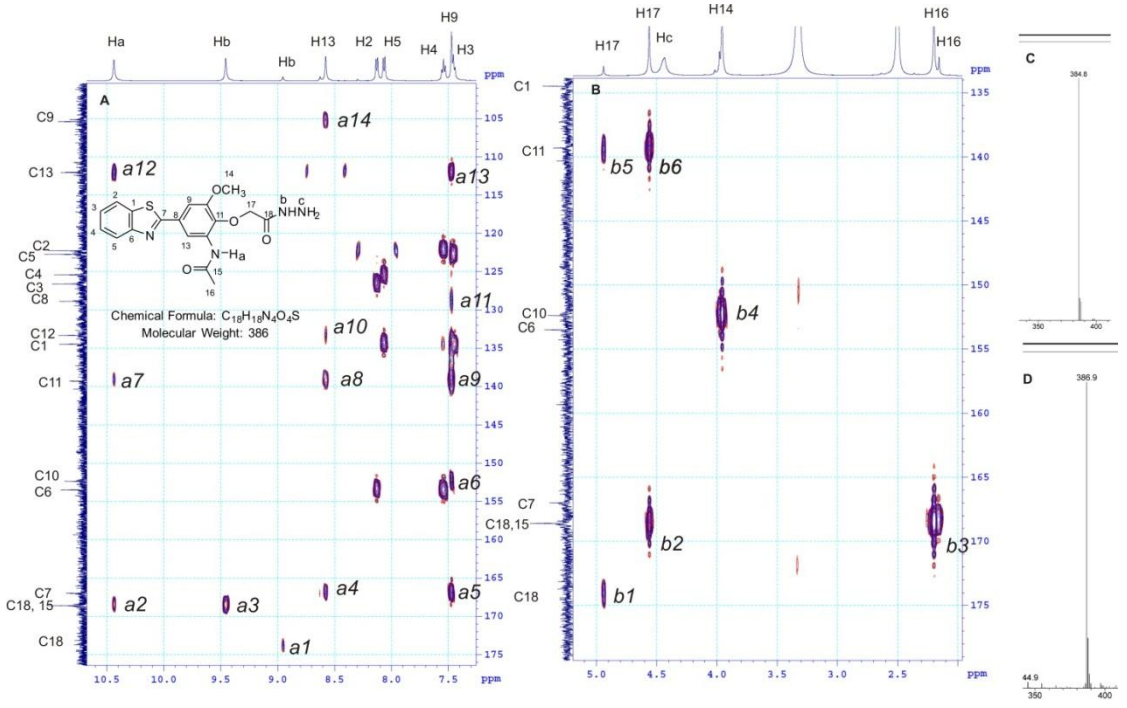


Figure 4. Parts of HMBC (A, B) andMS spectra (C, D) of compound 4e

Because acetohydrazides had some heteroatoms, mass spectral method was a good one for the final check. EI-MS spectrum analysis of all was detailed in the experimental section. In Figure 4, pictures C and D showed *pseudo* molecular peak at m/z 384.8 au (100%) in –MS method; m/z at 386.9 au (100%) in +MS method with strong agreement

with isotopic effects and nitrogen rule that referred compound **4e** had molecular weight of 386 g/mol and molecular formula was $C_{18}H_{18}N_4O_4S$.

3. Conclusions

Synthesis of acetohydrazides **1c** and **2c** has been done in three-step root in about 70% yield over all and the other two acetohydrazides **3e** and **4e** was via 5 steps in 38%. Structures of them were elucidated carefully and their carbons and protons were assigned exactly. The solvent of etherification step was replaced with DMF increasing the yield up to 82%. Acetylation of amino groups was carried out directly with acetic acid under refluxed condition in 76% yield. The structures of these new four acetohydrazides **1c**, **2c**, **3e** and **4e** were confirmed with IR, NMR and MS methods.

Acknowledgements: This research is supported by The Ministry of Education and Training of Vietnam under the project code B2019-SPH-09.

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