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Synthesis, spectral analysis and anti cancer activity of (E)-2-(4-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methoxy)phenyl)-1-(benzo[d]thiazol-2-yl)diazene

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The present work provides a comprehensive guide to the design and high-yield synthesis of 1,2,3-triazole derivatives employing a wide range of chemicals, bases, and catalysts. The methodology is simple, efficient, and effective. Amide coupling reagents have been developed that are more convenient, milder, and allow for higher selectivity under mild reaction conditions. Benzo[d]thiazol-2-amine (I) treated with $NaNO_2$/HCl gives diazonium salt (II) and compound (II) reacts with phenol to give intermediate (III). To get phenoxide compound (IV) compound (III) is treated with K_2CO_3/DMF. To get (E)-1-(benzo[d]thiazol-2-yl)-2-(4-(prop-2-ynyloxy)phenyl)diazene (V), compound (IV) is treated with 3-bromoprop-1-yne. Derivatives of (VIa-p) are obtained when compound (V) is treated with aniline and CuI/THF. The derivatives of (VIa-p) have shown moderate to excellent efficacy when tested for anticancer properties against several cancer cell lines. The MCF-7 cell line is the most resistant to compounds **6a** and **6e**, with an IC_{50} value of 1.92 and 1.99 µM respectively. The structures of the newly synthesized compounds have been established by ^1H and ^{13}C NMR, IR, and ESI-HRMS.

Keywords: Triazole, Benzothiazol, Molecular docking, Anticancer activity

Among heterocyclic compounds, N-heterocyclic compounds are among the most important in drug design[1]. This class of compounds is characterized by a wide variety of properties such as cytotoxic, antiviral, antibacterial, and anticancer[2-5] As a result, our primary objective was to identify innovative, stable, cost-effective, and physiologically active compounds for the synthesis of 1,2,3-triazoles[6-9]. This characteristic continues to grab the attention of scholars. In recent years, the synthesis of new compounds has gained prominence in organic synthesis due to their biological activity under moderate and accessible conditions[10], resulting in products with good selectivity and outstanding yields. Unfortunately, studies on the synthesis of these molecules are few[11]. There has been no publication in the open literature on the synthesis of 1,2,3-triazole derivatives[12].

Because of their synthesis and appealing properties, as well as numerous biological activities such as antibacterial, antifungal, antiallergic, antitubercular, antiinflammatory, analgesic, anticonvulsant, and antimalarial activities, 1,2,3-triazoles have had a significant impact not only in organic chemistry but also in medicinal chemistry[13-17]. They've also been used as herbicides, light stabilizers, optical brightening agents, and corrosion inhibitors. Certain 1,2,3-triazole derivatives have demonstrated strong antibacterial, cytostatic, virostatic, and anti-inflammatory effects, as well as anticancer, antihistamine, and muscarinic agonist activity in the treatment of Alzheimer's disease. Since they are resistant to metabolic degradation, 1,2,3-triazole moieties are appealing connecting units because they promote not only the binding of bimolecular medicines to the target *via* hydrogen bonding but also their solubility[18].

In accordance with our interest in the synthesis of new compounds, we provide here a simple, easy, and effective technique for the synthesis of physiologically active 1,2,3-triazole derivatives employing diverse reagents. Therefore, the purpose of the current work is to make an effort to synthesize compounds that comprise both the benzothiazole and the triazole systems. In addition, a series of novel derivatives **6a–p** of hybrid molecules were synthesized, and the insecticidal activity of these molecules was examined[19].

Results and Discussion

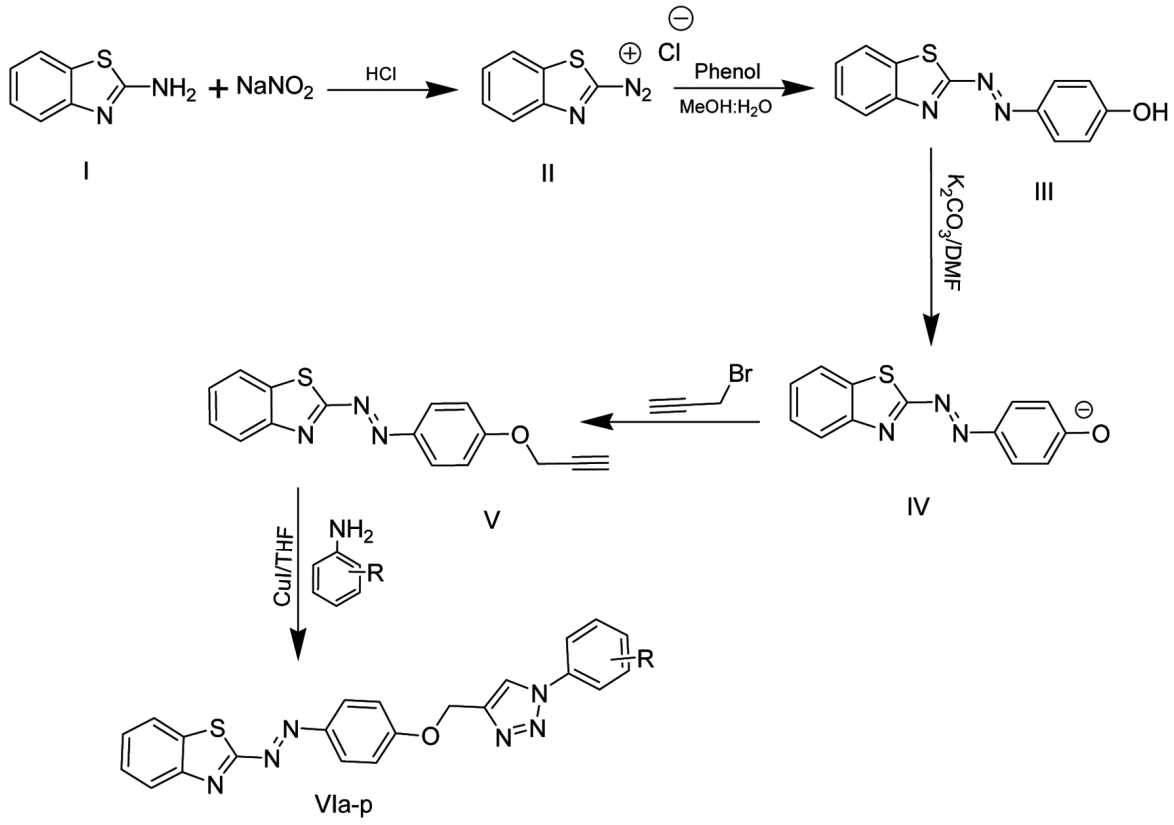
Benzo[d]thiazol-2-amine reacted with Sodium nitrite and Hydrogen chloride at 0-5°C will give benzo[d]thiazole diazonium chloride (**II**). Compound (**II**) is reacted with phenol in presence of KOH/MeOH and H_2O 2:1 ratio at 0-5°C will give

compound (**III**). The phenoxide compound (**IV**) was formed when reacts with Potassium carbonate and Dimetyl formamide. Phenoxide compound was treated with 3-bromoprop-1-yne will get compound (E)-1-(benzo[d]thiazol-2-yl)-2-(4-(prop-2-ynyloxy)phenyl) diazene (**V**). The compound (**VI**) (E)-2-(4-((1-phenyl-1H-1,2,3-triazol-4-yl)methoxy)phenyl)-1-(benzo[d] thiazol-2-yl)diazene was formed in presence of alkyl aniline and CuI/THF (Scheme 1).

The efficiency of compounds **VIa-p** to inhibit the growth of tumor cell lines in 96-well plates was evaluated to determine whether or not they were effective anticancer agents. The formation of these crystals was monitored by measuring the amount of tetrazolium salt that was reduced by the cells. Doxorubicin was used as a standard medication. MTT tests were used to determine the cytotoxic effects on a few human tumor cell lines: HEK 293 (normal human embryonic kidney cell line), A549 (human alveolar adenocarcinoma epithelial cells), Hela (human cervical cancer cells), and MDA-MB-231 (human breast adenocarcinoma cells). Through the analysis of absorbance data for dose-response curves, the concentrations at which inhibition occurred (IC50 values) were found. IC50 values (in μM) and standard deviations from three independent triplicate experiments are given. The MCF-7 cell line confirmed the highest sensitivity to the medicines (IC50values for VIa and VIe were 1.92 and 1.99 μM, accordingly), whereas the MDA-MB-231 and Hela cell lines showed the most promise (**VIb**, **VIc**, **VId**, **VIf**, **VIj**, **VIh**, **VIi**, **VIk**, **VIl**, **VIm**, **VIn**, **VIo**, and **VIp**).

Anticancer activity

The anticancer potential of the compounds **VIa-p** was investigated by evaluating their capacity to inhibit the growth of tumor cell lines in 96-well plates by cell-mediated inhibition of tetrazolium salt to water-insoluble crystal formation; doxorubicin was used as a reference. Four different human tumor cell lines (A549), Hela (human cervical cancer cells), MDA-MB-231 (human breast adenocarcinoma cells), and HEK 293 (normal human embryonic kidney cell line) were used in the MTT assays to determine cytotoxicity. Using dose-response curves based on absorbance data, inhibitory concentration (IC50) values were calculated. The median (and standard deviation) IC50 values (in μM) from three



Scheme 1 — Synthetic pathway to derivatives of triazole VIa-p

independent experiments are shown. As can be shown in Table 1, the majority of the synthesized compounds showed a significant cytotoxic effect on all the cell lines tested, with some compounds having potencies equal to the gold standard doxorubicin. The most potent activity of the compounds examined was shown against the MCF-7 cell line (IC50values of 1.92 and 1.99 M for VIa and VIe, respectively), while the MDA-MB-231 and Hela cell lines responded favorably to compounds **VIb**, **VIc**, **VId**, **VIf**, **VIh**, **VIi**, **VIk**, **VIl**, **VIm**, **VIn**, **VIo** and **VIp**.

Molecular Docking

Molecular docking studies using EGFR as the target revealed strong associations between compound a and the enzyme's active site[20] could be seen in Fig. 1. **VIk** shows Binding Energy -10.54 Kcal/mol and Inhibition Constant 18.68nM. **VIo** shows with Binding Energy -

Table 1 — *In vitro* anticancer activity of compounds

Compd	IC_{50} Values in μM				HEK 293
	A549	Hela	MDAMB231	MCF-7	>100
VIa	7.02	2.32	7.29	1.92	>100
VIb	7.08	3.72	4.11	10.27	>100
VIc	>100	3.66	4.13	4.13	>100
VId	13.09	3.88	4.87	>100	>100
VIe	5.01	2.15	6.45	1.99	>100
VIf	7.06	3.62	4.10	10.26	>100
VIg	>100	3.64	4.11	>100	>100
VIh	11.05	2.85	2.85	>100	>100
VIi	7.06	2.72	4.10	10.25	>100
VIj	>100	3.65	4.12	>100	>100
VIk	6.06	3.62	4.10	9.26	>100
VIl	>100	3.64	4.11	>100	>100
VIm	10.05	2.85	2.85	>100	>100
VIn	7.06	2.72	4.10	11.25	>100
VIo	>100	2.65	3.12	>100	>100
VIp	8.06	2.62	3.10	8.26	>100
Doxorubicin	0.449	0.519	0.81	1.17	>100

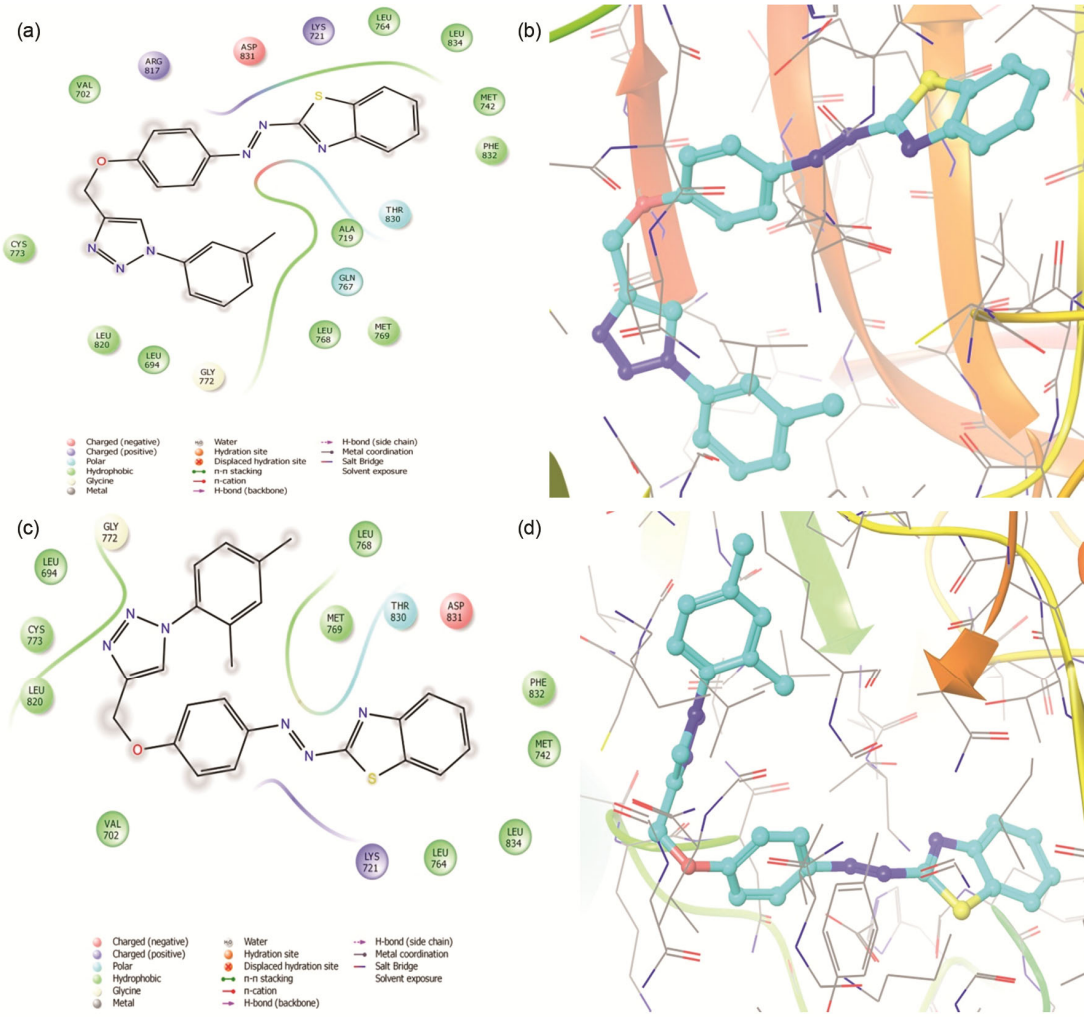


Fig. 1 — (a) Represents 2D interactions of compound VIk, (b) Represents 3D Surface area interactions of compound VIk, (c) Represents 2D interactions of compound VIp, (d) Represents 3D Surface area interactions of compound 6VI.

10.75 Kcal/mol and Inhibition Constant 13.22nM. **VIp** shows Binding Energy -10.14Kcal/mol and Inhibition Constant 37.00nM. Schrodinger's maestro v9.5 vizualizer was used to create the visuals, and AUTODOCK 4.2 was used for the docking analysis. Some of the docked molecules are shown below.

Experimental Section

To obtain a precise result, we utilized Electrothermal 9002 melting point equipment. The FTS-6000 BIO-RAD equipment may also record infrared spectra. A Bruker AC-300 was used to record ^{1}H and ^{13}C NMR spectra in $CdCl_3$. Chemical shifts (ppm) and coupling constants (*J*) were both measured in hertz (Hz). We used micromass LCT (electrospray ionization, positive mode) spectrometers for mass spectrometry (HRES-MS). TLC was employed to monitor the progress of all reactions on aluminum sheets of sds silica gel 60 F254,0.2 mm 4-Dimethylaminopiridinium.

Spectral data of synthesized compounds

(E)-2-(4-((1-Phenyl-1*H*-1,2,3-triazol-4-yl)methoxy) phenyl)-1-(benzo[d]thiazol-2-yl)diazene, Via: Yield 69%. m.p.172°-174°C. IR (KBr): 1480-1440 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.17 (s, 2H, CH_2), 7.31 (m, 3H, Ar-H), 7.43 (m, 4H, Ar-H), 7.92 (m, 3H, Ar-H), 8.14 (m, 4H, Ar-H); ^{13}C NMR (100MHz, $CDCl_3$): δ 56.97, 116.50, 119.40, 119.90, 121.48, 121.81, 123.85, 125.44, 127.60, 129.38, 135.36, 137.08, 147.86, 148.25, 152.04, 162.91, 166.72; MS: (M+H): *m/z* 412.11. Found: 412.68. Anal. Cacld for $C_{22}H_{16}N_6OS$: C, 64.06; H, 3.91; N, 20.38. Found: C, 64.09; H, 3.93; N, 20.42%.

(E)-2-(4-((1-(4-Chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)phenyl)-1-(benzo[d]thiazol-2-yl) diazene, VIb: Yield 70%. m.p.175°-176°C. IR (KBr): 1470-1442 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.16 (s, 2H, CH_2), 7.30 (m, 4H, Ar-H), 7.53 (d, *J*=7.1Hz, 2H, Ar-H), 7.89 (m, 2H, Ar-H), 8.14 (m, 5H, Ar-H); ^{13}C NMR (100MHz, $CDCl_3$): δ 56.97, 116.50, 119.40, 119.90, 121.81, 123.12, 123.35, 125.44, 129.20, 132.65, 135.36, 136.01, 147.86, 148.25, 152.04, 162.91, 166.72; MS: (M+H): *m/z* 446.07. Found: 446.91. Anal. Cacld for $C_{22}H_{15}ClN_6OS$: C, 59.12; H, 3.38; N, 18.80. Found: C, 59.15; H, 3.42; N, 18.84%.

(E)-2-(4-((1-(4-Fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)phenyl)-1-(benzo[d]thiazol-2-yl) diazene, VIc: Yield 72%. m.p.176°-178°C. IR (KBr): 1470-1442 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.14 (s, 2H, CH_2), 7.22 (m, 4H, Ar-H), 7.55 (d, *J*=7.1Hz, 2H, Ar-H), 7.86 (m, 2H, Ar-H), 8.14 (m, 5H, Ar-H); ^{13}C NMR (100MHz, $CDCl_3$): δ 56.97, 116.50, 119.40, 119.90, 121.81, 123.35, 124.19, 125.44, 133.22, 135.36, 147.86, 148.25, 152.04, 159.95, 162.91, 166.72; MS: (M+H): *m/z* 430.10. Found: 430.46. Anal. Cacld for $C_{22}H_{15}FN_6OS$: C, 61.38; H, 3.51; N, 19.52. Found: C, 61.42; H, 3.53; N, 19.54%.

(E)-2-(4-((1-(4-Methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)phenyl)-1-(benzo[d]thiazol-2-yl)diazene, VId: Yield 73%. m.p.175°-176°C. IR (KBr): 1470-1442 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.81 (s, 2H, OCH_3), 5.17 (s, 2H, CH_2), 7.08 (m, 4H, Ar-H), 7.53 (d, *J*=6.9HZ, 2H, Ar-H), 7.82 (m, 2H, Ar-H), 8.14 (m, 5H, ArH); ^{13}C NMR (100MHz, $CDCl_3$): δ 56.04, 56.97, 114.81, 116.50, 119.40, 119.90, 121.81, 123.35, 124.00, 125.44, 131.16, 135.36, 147.86, 148.25, 152.04, 157.83, 162.91, 166.72; MS: (M+H): *m/z* 442.49. Found: 442.12. Anal. Cacld for $C_{23}H_{18}N_6O_2S$: C, 62.43; H, 4.10; N, 18.96. Found: C, 62.46; H, 4.15; N, 18.99%.

(E)-2-(4-((1-(4-Nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)phenyl)-1-(benzo[d]thiazol-2-yl)diazene, VIe: Yield 74%. m.p.176°-178°C. IR (KBr): 1470-1442 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.15 (s, 2H, CH_2), 7.30 (s, 2H, ArH), 7.53 (d, *J*=6.8HZ, 2H, Ar-H), 8.23 (m, 7H, Ar-H), 8.41 (m, 2H, ArH); ^{13}C NMR (100MHz, $CDCl_3$): δ 56.97, 116.50, 119.40, 119.90, 121.81, 122.57, 123.35, 125.44, 126.22, 135.36, 140.69, 146.86, 147.86, 148.25, 152.04, 162.91, 166.72; MS: (M+H): *m/z* 457.12. Found: 457.71. Anal. Cacld for $C_{22}H_{15}N_7O_3S$: C, 57.76; H, 3.30; N, 21.43. Found: C,57.78; H, 3.35; N, 21.45%.

(E)-2-(4-((1-*p*-Tolyl-1*H*-1,2,3-triazol-4-yl) methoxy)phenyl)-1-(benzo[d]thiazol-2-yl)diazene, VIf: Yield 78%. m.p.182°-183°C. IR (KBr): 1470-1442 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.34 (s, 3H, CH_3), 5.12 (s, 2H, CH_2), 7.34 (m, 4H, ArH), 7.53 (d, *J*=7.1HZ, 2H, Ar-H), 7.88 (m, 2H, Ar-H), 8.14 (m, 5H, ArH); ^{13}C NMR (100MHz, $CDCl_3$): δ 21.13, 56.97, 116.50, 119.40, 119.90, 121.81, 123.35, 124.36, 125.44, 129.24, 135.36, 136.91, 137.81, 147.86, 148.25, 152.04, 162.91, 166.72; MS: (M+H): *m/z* 457.12. Found: 457.10. Anal. Cacld for $C_{22}H_{15}N_7O_3S$: C, 57.76; H, 3.30; N, 21.43. Found: C,57.78; H, 3.35; N, 21.45%.

(E)-2-(4-((1-(2,4-Dinitrophenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)phenyl)-1-(benzo[d]thiazol-2-yl)diazene, VIg: Yield 75%. m.p.185°-186°C. IR (KBr): 1470-1442 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.19 (s, 2H, CH_2), 7.31 (m, 2H, ArH), 7.53 (d,

J=7.6HZ, 2H, Ar-H), 8.21 (m, 5H, Ar-H), 8.16 (m, 3H, ArH); ^{13}C NMR (100MHz, $CDCl_3$): δ 56.97, 116.50, 119.40, 120.91, 121.81, 123.35, 124.70, 125.44, 127.60, 130.70, 135.00, 135.36, 145.60, 147.09, 148.25, 152.04, 162.91, 166.72; MS: (M+H): *m/z* 457.12. Found: 457.10. Anal. Cacld for $C_{22}H_{14}N_8O_5S$: C, 52.59; H, 2.81; N, 22.30. Found: C, 52.62; H, 2.84; N, 21.35%.

(E)-2-(4-((1-(4-Iodophenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)phenyl)-1-(benzo[d]thiazol-2-yl)diazene, VIh: Yield 74%. m.p.182°-183°C. IR (KBr): 1470-1442 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.18 (s, 2H, CH_2), 7.31 (m, 2H, ArH), 7.77 (m, 6H, Ar-H), 8.15 (m, 5H, Ar-H); ^{13}C NMR (100MHz, $CDCl_3$): δ 56.97, 93.16, 116.50, 119.40, 119.90, 121.80, 123.35, 123.80, 125.44, 135.36, 137.02, 140.21, 147.86, 148.25, 152.04, 162.91, 166.72; MS: (M+H): *m/z* 457.12. Found: 457.68. Anal. Cacld for $C_{22}H_{15}IN_8O_5S$: C, 49.08; H, 2.81; N, 15.61. Found: C, 49.12; H, 2.85; N, 15.65%.

(E)-2-(4-((1-(4-Bromo-2-(trifluoromethyl) phenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)phenyl)-1-(benzo[d]thiazol-2-yl)diazene, VIi: Yield 76%. m.p.175°-176°C. IR (KBr): 1470-1442 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.17 (s, 2H, CH_2), 7.30 (m, 3H, ArH), 7.53 (d, J=7.6Hz, 2H, Ar-H), 8.23 (m, 7H, Ar-H); ^{13}C NMR (100MHz, $CDCl_3$): δ 56.97, 116.50, 119.40, 120.91. 121.70, 123.35,132.60, 133.36, 135.45, 147.65, 148.25, 152.04, 162.91, 166.72; MS: (M+H): *m/z* 558.01. Found: 558.12. Anal. Cacld for $C_{23}H_{14}BrF_3N_6OS$: C, 49.39; H, 2.52; N, 15.02. Found: C, 49.42; H, 2.55; N, 15.05%.

(E)-2-(4-((1-(4-(Trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)phenyl)-1-(benzo[d]thiazol-2-yl)diazene, VIj: Yield 78%. m.p.176°-178°C. IR (KBr): 1470-1442 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.12 (s, 2H, CH_2), 7.30 (m, 2H, ArH), 7.53 (d, J=6.9Hz, 2H, Ar-H), 7.97 (m, 4H, ArH), 8.15 (m, 5H, Ar-H); ^{13}C NMR (100MHz, $CDCl_3$): δ 56.97, 116.50, 119.40, 119.90, 121.91, 123.35, 123.93, 125.44, 126.80, 135.36, 142.40, 147.86, 148.25, 152.04, 162.91, 166.72; MS: (M+H): *m/z* 480.81. Found: 480.12. Anal. Cacld for $C_{23}H_{15}F_3N_6OS$: C, 57.50; H, 3.15; N, 17.49. Found: C, 57.52; H, 3.18; N, 17.52%.

(E)-2-(4-((1-*m*-Tolyl-1*H*-1,2,3-triazol-4-yl) methoxy)phenyl)-1-(benzo[d]thiazol-2-yl)diazene, VIk: Yield 75%. m.p.172°-173°C. IR (KBr): 1470-1442 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.36 (s, 3H, CH_3), 5.14 (s, 2H, CH_2), 7.26 (m, 5H, ArH), 7.75 (m, 5H, ArH), 8.14 (m, 5H, Ar-H); ^{13}C NMR (100MHz, $CDCl_3$): δ 21.21, 56.97, 116.19, 116.50, 119.90, 121.81, 124.15, 125.44, 126.49, 128.42, 135.36, 138.72, 139.18, 147.86, 148.25, 152.04, 162.91, 166.72; MS: (M+H): *m/z* 426.13. Found: 426.49. Anal. Cacld for $C_{23}H_{18}N_6OS$: C, 64.77; H, 4.25; N, 19.70. Found: C, 64.79; H, 4.28; N, 19.72%.

(E)-2-(4-((1-(4-(Trifluoromethyl)-2-nitrophenyl) -1*H*-1,2,3-triazol-4-yl)methoxy)phenyl)-1-(benzo[d]thiazol-2-yl)diazene, VIl: Yield 77%. m.p.183°-184°C. IR (KBr): 1470-1442 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.15 (s, 3H, CH_2), 7.29 (m, 3H, ArH), 7.53 (d, *J*=7.6Hz, 2H, ArH), 8.12 (m, 4H, Ar-H), 8.21 (m, 3H, ArH); ^{13}C NMR (100MHz, $CDCl_3$): δ 56.97, 116.19, 119.40, 120.91, 121.81, 123.35, 124.14, 125.44, 125.71, 127.29, 128.22, 135.36, 139.27, 147.05, 147.65, 148.25, 152.05, 162.91, 166.72; MS: (M+H): *m/z* 525.08. Found: 525.46. Anal. Cacld for $C_{23}H_{14}F_3N_7O_3S$: C, 52.57; H, 2.69; N, 18.66. Found: C, 52.59; H, 2.69; N, 18.69%.

(E)-2-(4-((1-(4-Chloro-2-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)phenyl)-1-(benzo[d]thiazol-2-yl)diazene, VIm: Yield 79%. m.p.186°-187°C. IR (KBr): 1470-1442 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.18 (s, 3H, CH_2), 7.29 (m, 2H, ArH), 7.77 (m, 4H, ArH), 8.14 (m, 3H, ArH), 8.21 (m, 3H, ArH); ^{13}C NMR (100MHz, $CDCl_3$): δ 56.97, 116.19, 119.40, 120.91, 121.81, 123.35, 125.44, 127.53,129.03, 132.24, 133.57, 135.36, 144.08, 147.65, 148.25, 152.04, 162.91, 166.72; MS: (M+H): *m/z* 491.06. Found: 491.91. Anal. Cacld for $C_{22}H_{14}ClN_7O_3S$: C, 53.72; H, 2.87; N, 19.93. Found: C, 53.75; H, 2.89; N, 19.96%.

(E)-2-(4-((1-(4-Chloro-3-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)phenyl)-1-(benzo[d]thiazol-2-yl)diazene, VIn: Yield 75%. m.p.182°-183°C. IR (KBr): 1470-1442 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.14 (s, 2H, CH_2), 7.45 (m, 3H, ArH), 7.52 (t, *J*=6.1Hz, 3H, ArH), 8.15 (m, 3H, ArH), 8.22 (m, 3H, ArH); ^{13}C NMR (100MHz, $CDCl_3$): δ 56.97, 115.30, 116.50, 119.40, 119.90, 121.75, 123.35, 125.44, 129.23, 135.36, 135.98, 147.86, 148.25, 152.04, 158.95, 162.91, 166.72; MS: (M+H): *m/z* 465.06. Found: 465.91. Anal. Cacld for $C_{22}H_{14}ClFN_6O_3S$: C, 56.84; H, 3.04; N, 18.08. Found: C, 56.92; H, 3.09; N, 18.12%.

(E)-2-(4-((1-(2,4-Dichlorophenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)phenyl)-1-(benzo[d]thiazol-2-yl)diazene, VIo: Yield 77%. m.p.188°-189°C. IR (KBr): 1470-1442 cm^{-1}; ^{1}H NMR (400 MHz $CDCl_3$): δ

5.17 (s, 2H, CH_2), 7.29 (m, 2H, ArH), 7.50 (t, *J*=9.4Hz, 3H, ArH), 8.14 (m, 6H, ArH); ^{13}C NMR (100MHz, $CDCl_3$): δ 56.97, 116.50, 119.40, 120.91, 121.81, 123.35, 125.44, 128.06, 128.28, 130.46, 132.49, 133.30, 135.36, 137.15, 147,65, 148.25, 152.04, 162.91, 166.72; MS: (M+H): *m/z* 480.03. Found: 480.36. Anal. Cacld for $C_{22}H_{14}Cl_2N_6OS$: C, 54.89; H, 2.93; N, 17.46. Found: C, 54.91; H, 2.95; N, 17.50%.

(E)-2-(4-((1-(2,4-Dimethylphenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)phenyl)-1-(benzo[d]thiazol-2-yl)diazene, VIp: Yield 75%. m.p.178°-179°C. IR (KBr): 1470-1442 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.35 (s, 3H, CH_3), 2.41 (s, 3H, CH_3), 5.14 (s, 2H, CH_2), 7.07 (m, 4H, ArH), 7.53 (d, *J*=7.1Hz, 2H, ArH), 8.14 (m, 6H, ArH); ^{13}C NMR (100MHz, $CDCl_3$): δ 18.09, 21.21, 56.97, 116.50, 119.40, 120.91, 121.81, 123.35, 123.80, 125.09, 125.44,130.05, 131.36, 134.92, 135.41, 147.65, 148.25, 152.04, 162.91, 166.72; MS: (M+H): *m/z* 440.14. Found: 440.52. Anal. Cacld for $C_{24}H_{20}N_6OS$: C, 65.44; H, 4.58; N, 19.08. Found: C, 65.46; H, 4.60; N, 19.12%.

Conclusion

We conclude by describing a new, straightforward synthesis of the chemical-based in discussion using click chemistry. And analyzed for their potential to prevent cancer. The MCF-7 cell line was most sensitive to compounds 1a and 1e, with IC50values of 1.82 and 1.90 M, respectively. Promising action against MDA- MB-231 and Hela cell lines was shown with compounds **6b**, **6c**, and **6d**. Significant links were discovered by molecular modeling studies in which a fragment of drug A was docked into the active site with EGFR as the target.

Supplementary Information

Supplementary information is available in the website http://nopr.niscpr.res.in/handle/123456789/58776.

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Conflict of Interest

The authors state unequivocally that there are no possible conflicts of interest to declare.

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