# Supporting information

## An efficient synthesis of novel triazoles incorporating barbituric motifs *via* [3+2] cycloaddition reaction: Expermimental and theoretical study

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## Supplementary Material

Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI:WWW under http://dx.doi.org/10.1002/MS-number.

## Experimental:

**General information and apparatus**

Melting points were measured on an Electrothermal 9100 apparatus. NMR spectra were recorded with a Bruker DRX-400 AVANCE instrument (400.1 MHz for $^{1}H$, 100.6 MHz for 13C) with $CDCl_3$ as solvent. IR spectra were recorded on an FT-IR Bruker vector 22 spectrometer. Mass spectra were recorded on a Finnigan-Matt 8430 mass spectrometer operating at an ionization potential of 70 eV. Elemental analyses were carried with a Perkin-Elmer 2400II CHNS/O Elemental Analyzer

**Propargylation of hydroxybenzaldehyde derivatives 2a – b**

To a stirred solution of hydroxyl benaldehyde derivative 1a (5 mmol) and potassium carbonate (5mmol) in DMF (15ml) was added propargyl bromide (6mmol). After stirring for4–24 h, water was added and the precipitated solid was filtered and washed with water.

**2-(prop-2-yn-1-yloxy) benzaldehyde (2a).** [78] White solid, Yield: (93%), m.p. 69-70 ˚C;

**4-(prop-2-yn-1-yloxy) benzaldehyde (2b).** White solid, Yield: (90%), m.p. 68-69.5 ˚C; $^{1}$H NMR (400 MHz, DMSO-d6): 2.59 (s 1H), 4.86 (s, 2H), 7.11 (d, J = 7.7 Hz, 2H), 7.9 (d, J =7.7 Hz, 2H), 10.5 (s, 1H) ppm.

**General procedure for Knoevenagel condensation**

**Preparation of (4a-d):** To a stirred solution of barbituric acid derivatives (1.2 mmol) in aqueous HCl (25 ml, 10%) were added propargylated aldehydes 2a–b (1 mmol) at room temperature. After stirring for 2–15 h, the pure substances was collected by filtration, and washing with hot ethanol. [78]

To a stirred solution of N,N-dimethylbarbituric acid (**3c**) (1.2 mmol) in water (20 ml) containing $(NH_4)_2HPO_4$ (20 mol%) was added propargylated aldehydes **2a–b**(1 mmol) at room temperature. After stirring for 4–12 h, the yellow precipitated was filtered and washed with water and ethanol.

**5-(2-(prop-2-yn-1-yloxy)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione (4a)**:[78] Yellow solid, yield 85%; mp 207–208.3 °C; IR (KBr, cm$^{-1}$) ν =3310, 3155, 3010, 1771, 1642.

**5-(4-(prop-3-yn-1- yloxy)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione (4b):** Yellow solid, yield. 90%; mp 217.5–219.4 °C., IR (KBr, cm$^{-1}$) ν =3262, 2091, 1751, 1666. $^{1}$H NMR (400 MHz, DMSO-d6): 11.17(s, 1H, NH), 10.97 (s, 1H, NH), 8.32 (m, 2H, ArH), 8.30 (s, 1H, CH), 7.10 (d, J= 8.4 Hz, 2H), 4.96 (s, 2H, CH2), 3.66 (s, 1H, CH) ppm. ; $^{13}$C NMR (100 MHz, DMSO-d6):161.02, 160.58, 159.21, 149.33, 136.58, 133.32, 128.28, 117.45, 115.06, 79.07, 56.21.

**5-(2-(prop-2-yn-1-yloxy) benzylidene)-2-thioxodihydropyrimidine-4,6(1H,5H)-dione (4c):** Yellow solid, yield. 80%; mp 228–230°C., IR (KBr, cm$^{-1}$) ν =3249, 2095, 1670; $^{1}$H NMR (400 MHz, DMSO-d6): 11.41(1H, s, NH), 11.36 (1H, s, NH), 8.30 (s, 1H, CH), 7.71 (d, J=8.4 Hz, 2H, ArH), 7.21 (d, J= 8.4 Hz, 2H, ArH), 4.91 (s, 2H, CH2), 3.66 (s, 1H, CH) ppm. ; $^{13}$C NMR (100 MHz, DMSO-d6):173.02, 164.58, 162.21, 151.93, 150.58, 137.32, 126.28, 117.45, 115.06, 79.07, 56.21.

**5-(4-(prop-3-yn-1- yloxy)benzylidene)-2-thioxodihydropyrimidine-4,6(1H,5H)-dione (4d)**: Yellow solid, yield 87%; mp 196–198 °C. IR (KBr, cm$^{-1}$) ν =3230, 2119, 1678; $^{1}$H NMR (400 MHz, DMSO-d6): 11.37(1H, s, NH), 11.17 (1H, s, NH), 8.25 (s, 1H, CH), 7.83-7.80 (m, 2H, ArH), 7.22 (d, J= 8.4 Hz, 2H), 4.90 (s, 2H, CH2), 3.66 (s, 1H, CH) ppm. ; $^{13}$C NMR (100 MHz, DMSO-d6):173.02, 164.58, 162.21, 151.93, 150.58, 137.32, 126.28, 117.45, 115.06, 79.07, 56.21.;

**1,3-dimethyl-5-(2-(prop-2-yn-1-yloxy)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione (4e)**:[78] Yellow solid, yield 84%; mp, 141.5–143.0° C; IR (KBr, cm$^{-1}$) ν =3345, 1770, 1684.

**5-(4-(prop-3-yn-1- yloxy)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (4f)**: Yellow solid, yield 79%; mp: 172.5–173.8°C; IR (KBr, cm$^{-1}$) ν =3245, 2115, 16 84; $^{1}$H NMR (400 MHz, DMSO-d6): δ= 8.33 (d, 2H, ArH), 8.30 (s, 1H, CH), 7.11 (d, J= 8.4 Hz, 2H, 2H), 4.95 (s, 2H, CH2), 3.66 (s, 1H, CH), 3.25 (s, 3H, CH3), 3.21 (s, 3H, CH3) ppm. $^{13}$C

NMR (100 MHz, DMSO-d6): δ= 163.02, 161.58, 161.21, 155.93, 151.58, 137.36, 126.26, 116.45, 115.06, 79.34, 56.29, 29.10, 28.49.

**Preparation of alkyl azide 6a-c**

Sodium azide (1.2 mmol) was added to a solution of benzyl bromide derivatives **5a-c** (1 mmol) in DMF. The mixture was heated at 100° C and, after completion (3h), was quenched with an aqueous solution of $NH_4Cl$ (15 mL) and extracted with ethyl acetate (3 -20 mL). The organic extracts were washed with an aqueous solution of brine (3 -20 mL) and dried over $MgSO_4$. After evaporation of the solvent at reduced pressure, pure azides were isolate. [42]

**General procedure for click cycloaddition reaction**

Alkyne **4a-f** (1.2 mmol) and benzyl azide **6a-c** (1 mmol) were added at room temperature to a solution of $CuSO_4$ (0.2 equiv) DMSO (10 mL) in a capped flask. The reaction mixture was stirred at 80°C and, after completion (12h), the reaction was quenched with a saturated aqueous solution of $NH_4Cl$ (30 mL) and extracted with ethyl acetate (3- 40 mL). The organic extracts were washed with an aqueous solution of brine (3 -30 mL), dried over $Na_2SO_4$ and concentrated under vacuum.

**5-(2-((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy) benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione (7a)**: Yellow solid. Mp: 281.3-283.2 °C. IR (KBr, $cm^{-1}$) ν = 3438, 2925, 1677, 1597, 1159.$^1$H NMR (400 MHz, DMSO): δ= 10.99 (s, 1H, NH), 10.75 (s, 1H, NH), 8.32 (s, 1H, CH), 8.07 (s, 1H, CH), 7.86 (bs, 1H, ArH), 7.51-7.06 (m, 7H, ArH), 5.62 (s, 2H, $OCH_2$), 5.27 (s, 2H, $CH_2$) ppm. $^{13}$C NMR (100 MHz, DMSO): δ= 163.39, 162.79, 159.23, 148.05, 143.09, 136.41, 132.23, 131.71, 130.33, 129.24, 128.65, 128.27, 126.47, 125.43, 115.68, 115.44, 115.14, 61.92, 53.34 ppm. MS: m/z = 402.1 ($M^+$). Anal. calcd. for $C_{21}H_{17}N_5O_4$ (403.4): C, 62.53; H, 4.25; N, 17.36; Found: C, 62.48; H, 4.22; N, 17.38.

**5-(2-((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione (7b)**: Yellow solid. Mp: 279.2-280.3 °C. IR (KBr, $cm^{-1}$) ν = 3438, 2926, 1715, 1685, 1598, 1161. $^1$H NMR (400 MHz, DMSO): δ= 11.20 (s, 1H, NH), 10.99 (s, 1H, NH), 8.35 (s, 1H, CH), 8.07 (s, 1H, CH), 7.87 (d, J=8Hz, 1H, ArH), 7.53-7.21 (m, 5H, ArH), 7.15-7.01 (m, 2H, ArH), 5.67 (s, 2H, $OCH_2$), 5.28 (s, 2H, $CH_2$) ppm. $^{13}$C NMR (100 MHz, DMSO): δ= 164.59, 163.37, 161.08, 148.08, 135.19, 132.23, 130.34, 129.87, 129.33, 129.25, 128.90, 128.79, 128.46, 128.06, 125.54, 115.73, 115.67, 61.89, 53.41 ppm. MS: m/z = 483.3 ($M^+$). Anal. calcd. for $C_{21}H_{16}BrN_5O_4$ (482.3): C, 52.30; H, 3.34; N, 14.52; Found: C, 52.37; H, 3.37; N, 14.48.

**5-(2-((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (7c)**: Cream solid. Mp: 289-290.5 °C. IR (KBr, $cm^{-1}$) ν = 3439, 2956, 1629, 1524, 1144. $^1$H NMR (400 MHz, DMSO): δ= 8.37 (s, 1H, CH), 8.07 (s, 1H, CH), 7.87 (d, J=8.8 Hz, 2H, ArH), 7.52 (t, J=8.8 Hz, 1H, ArH), 7.42 (m, 1H, ArH), 7.23 (d, J=8.4 Hz, 1H, ArH), 7.18-7.11 (m, 2H, ArH),7.10-7.06 (m, 1H, ArH), 7.01 (m, 1H, ArH), 5.65 (s, 2H, $OCH_2$), 5.28 (s, 2H, $CH_2$), 3.23 (s, 3H, $CH_3$), 3.21 (s, 3H, $CH_3$) ppm. $^{13}$C NMR (100 MHz, DMSO): δ= 163.37, 161.58, 161.21, 155.95, 137.64, 132.22, 131.30, 130.35, 128.27, 126.27, 125.60, 124.52, 116.45, 115.69, 115.19, 115.06, 61.91, 52.63, 29.09, 28.49 ppm. MS: m/z = 430.0 ($M^+$). Anal. calcd. for $C_{23}H_{21}N_5O_4$ (431.5): C, 64.03; H, 4.91; N, 16.23; Found: C, 64.08; H, 4.93; N, 16.25.

**5-(2-((1-(3-fluorobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-1,3-dimethyl pyrimidine-2,4,6(1H,3H,5H)-trione (7d)**: Yellow solid. Mp: 273.2-274.9 °C. IR (KBr, $cm^{-1}$) ν = 3427, 2926, 1602, 1485, 1127. $^{1}H$ NMR (400 MHz, DMSO): δ= 8.37 (s, 1H, CH), 8.06(s,1H, CH), 7.96 (s, 1H, ArH), 7.87 (bs, 2H, ArH), 7.36- 7.33 (m, 3H, ArH), 7.23-7.16 (m, 2H, ArH), 5.67 (s, 2H, $OCH_2$), 5.29 (s, 2H, $CH_2$), 2.88 (s, 3H, $CH_3$), 2.72(s, 3H, $CH_3$) ppm. $^{13}C$ NMR (100 MHz, DMSO): δ= 163.01, 161.58, 161.21, 148.46, 136.32, 135.60, 132.23, 130.48, 130.34, 129.25, 128.68, 128.61, 128.47, 127.99, 115.75, 115.68, 115.44, 62.39, 56.57, 36.25, 31.23 ppm. MS: m/z = 451.0 ($M^+$). Anal. calcd. for $C_{23}H_{20}FN_5O_4$ (449.4): C, 61.47; H, 4.49; N, 15.58; Found: C, 61.50; H, 4.53; N, 15.54.

**5-(2-((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-2-thioxodihydro pyrimidine-4,6(1H,5H)-dione (7e)**: Yellow solid. Mp: 251.6-252.9 °C. IR (KBr, $cm^{-1}$) ν = 3439, 2924, 1710, 1660, 1597, 1220, 1166. $^{1}H$ NMR (400 MHz, DMSO): δ= 11.22 (s, 1H, NH), 11.08 (s, 1H, NH), 8.39 (s, 1H, CH), 8.24 (s, 1H, CH), 7.66 (d, J=7.6 Hz, 1H, ArH), 7.37-7.34 (m, 3H, ArH), 7.32-7.29 (m, 2H, ArH), 7.29-7.24 (m, 2H, ArH), 6.98 (t, J=7.2 Hz, 1H, ArH), 5.62 (s, 2H, $OCH_2$), 5.21 (s, 2H, $CH_2$) ppm. $^{13}C$ NMR (100 MHz, DMSO): δ= 168.04, 163.37, 156.06, 143.85, 137.39, 136.46, 131.13, 129.22, 128.60, 128.34, 126.83, 125.93, 125.22, 121.90, 121.61, 115.73, 113.88, 62.31, 53.32 ppm. MS: m/z = 420.1 ($M^+$). Anal. calcd. for $C_{21}H_{17}N_5O_3S$ (419.4): C, 60.13; H, 4.09; N, 16.70; Found: C, 60.08; H, 4.07; N, 16.72.

**5-(2-((1-(3-fluorobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-2-thioxodihydropyrimidine-4,6(1H,5H)-dione (7f)**: Yellow solid. Mp: 271.7-273.2 °C. IR (KBr, $cm^{-1}$) ν = 3441, 2920, 1726, 1627, 1597, 1250, 1166. $^{1}H$ NMR (400 MHz, DMSO): δ= 11.82 (s,1H, NH), 11.22 (s, 1H, NH), 8.35 (s, 1H, CH), 8.24 (s, 1H, CH), 7.66 (d, J=7.6 Hz, 1H, ArH), 7.43-7.31 (m, 2H, ArH), 7.25 (d, J=8.0 Hz, 1H, ArH), 7.19-7.08 (m, 3H, ArH), 6.98 (t, J=7.6 Hz, 1H, ArH), 5.65 (s, 2H, $OCH_2$), 5.22 (s, 2H, $CH_2$) ppm. $^{13}C$ NMR (100 MHz, DMSO): δ= 163.10, 159.28, 156.69, 154.10, 146.84, 137.83, 136.45, 131.13, 125.92, 125.41, 124.44, 121.62, 120.78, 119.89, 115.61, 115.34, 115.12, 114.96, 113.88, 113.23, 63.49, 52.63 ppm. MS: m/z = 438.1 ($M^+$). Anal. calcd. for $C_{21}H_{16}FN_5O_3S$ (437.5): C, 57.66; H, 3.69; N, 16.01; Found: C, 57.70; H, 3.71; N, 15.97.

**5-(2-((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-2-thioxodihydro pyrimidine-4,6(1H,5H)-dione (7g)**: Yellow solid. Mp: 275.0 -276.9 °C. IR (KBr, $cm^{-1}$) ν = 3439, 2925, 1729, 1627, 1485, 1238, 1166. $^{1}H$ NMR (400 MHz, DMSO): δ= 11.47 (s, 1H, NH), 11.10 (s, 1H, NH), 8.40 (s, 1H, CH), 8.23 (s, 1H, CH), 7.84 (d, J=8.8Hz, 2H, ArH), 7.44-7.41 (m, 1H, ArH), 7.39-7.27 (m, 2H, ArH), 7.18 (d, J-8.8Hz, 2H, ArH), 7.07 (m, 1H, ArH), 5.60 (s, 2H, $OCH_2$), 5.20 (s, 2H, $CH_2$) ppm. $^{13}C$ NMR (100 MHz, DMSO): δ= 167.53, 161.35, 159.73, 138.82, 131.37, 131.29, 130.29, 126.51, 125.71, 125.51, 125.48, 124.45, 124.42, 117.69, 115.60, 115.40, 115.34, 115.12, 113.50, 63.13, 52.67 ppm. MS: m/z = 497.4 ($M^+$). Anal. calcd. for $C_{21}H_{16}BrN_5O_3S$ (498.3): C, 50.61; H, 3.24; N, 14.05. Found: C, 50.67; H, 3.27; N, 14.02.

**5-(4-((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione (8a):** Yellow solid. Mp: 254-255.1 °C. IR (KBr, $cm^{-1}$) ν = 3439, 2924, 1718, 1680, 1597, 1166. $^{1}H$ NMR (400 MHz, DMSO): δ= 10.99 (s, 1H, NH), 10.97 (s, 1H, NH), 8.37 (s, 1H, CH), 8.06 (s, 1H, CH), 7.87 (d, J=8.8 Hz, 2H, ArH), 7.72 (d, J=8.8 Hz, 2H, ArH), 7.39-7.25 (m, 3H, ArH), 7.22 (d, J=8.8 Hz, 2H, ArH), 5.71 (s, 2H, $OCH_2$), 5.22 (s, 2H, $CH_2$) ppm. $^{13}C$ NMR (100 MHz, DMSO): δ= 163.32, 162.79, 159.23, 148.03, 137.39, 137.23, 132.22, 131.36, 130.20, 129.12, 128.29, 126.47, 115.76, 115.68, 61.89, 52.04

ppm. MS: m/z = 402.2 ($M^+$) Anal. calcd. for $C_{21}H_{17}N_5O_4$ (403.4): C, 62.53; H, 4.25; N, 17.36; Found: C, 62.41; H, 4.15; N, 17.46.

**5-(4-((1-(2-chlorobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione. (8b)**: Yellow solid. Mp: 241.5-243.2 °C. IR (KBr, $cm^{-1}$) ν = 3503, 2923, 1715, 1628, 1593, 1170. $^1H$ NMR (400 MHz, DMSO): δ= 11.02 (s, 1H, NH), 10.97 (s, 1H, NH), 8.35 (s, 1H, CH), 8.06 (s, 1H, CH), 7.87 (d, J=8.0 Hz, 2H, ArH), 7.52 (d, J=7.2 Hz, 1H, ArH), 7.35-7.42 (m, 1H, ArH), 7.24 (d.d, J=12.8, 8.0 Hz, 2H, ArH), 6.99-7.05 (m, 2H, ArH), 5.74 (s, 2H, $OCH_2$), 5.32 (s, 2H, $CH_2$) ppm. $^{13}C$ NMR (100 MHz, DMSO): δ= 163.49, 162.21, 159.37, 159.28, 133.49, 133.14, 132.06, 131.87, 131.05, 130.84, 130.55, 130.13, 128.27, 128.22, 128.15, 115.71, 115.49, 62.49, 51.32 ppm. MS: m/z = 437.0 ($M^+$) Anal. calcd. for $C_{21}H_{16}ClN_5O_4$ (437.9): C, 57.61; H, 3.68; N, 16.00; Found: C, 57.65; H, 3.71; N, 16.05.

**5-(4-((1-(3-fluorobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione. (8c)**: Yellow solid. Mp: 259.2-260.1 °C. IR (KBr, $cm^{-1}$) ν = 3461, 2932, 1684, 1502, 1159. $^1H$ NMR (400 MHz, DMSO): δ= 11.07 (s, 1H, NH), 10.97 (s, 1H, NH), 8.37 (s, 1H, CH), 8.08 (s, 1H, CH), 7.87 (d, J=8.4 Hz, 2H, ArH), 7.43-7.35 (m, 1H, ArH), 7.23 (d, J=8.8 Hz, 2H, ArH), 7.20-7.14 (m, 3H, ArH), 5.65 (s, 2H, $OCH_2$), 5.29 (s, 2H, $CH_2$) ppm. $^{13}C$ NMR (100 MHz, DMSO): δ= 163.80, 163.36, 161.37, 142.93, 139.07, 138.99, 132.24, 131.39, 131.31, 125.60, 124.55, 124.52, 116.30, 115.68, 115.64, 115.42, 61.88, 52.65 ppm. MS: m/z = 421.2 ($M^+$). Anal. calcd. for $C_{21}H_{16}FN_5O_4$ (421.4): C, 59.86; H, 3.83; N, 16.62; Found: C, 59.91; H, 3.88; N, 16.56.

**5-(4-((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione. (8d)**: Yellow solid. Mp: 235.5-237 °C. IR (KBr, $cm^{-1}$) ν = 3440, 2918, 1761, 1650, 1156. $^1H$ NMR (400 MHz, DMSO): δ= 11.23 (s, 1H, NH), 11.19(s, 1H, NH), 8.33 (s, 1H, CH), 8.23 (s, 1H, CH), 7.67 (d, J=8.4 Hz, 2H, ArH), 7.58 (d, J=8.0 Hz, 2H, ArH), 7.34 (d, J=8.0 Hz, 2H, ArH), 7.26 (d, J=8.4 Hz, 2H, ArH), 5.61 (s, 2H, $OCH_2$), 5.33 (s, 2H, $CH_2$) ppm. $^{13}C$ NMR (100 MHz, DMSO): δ= 168.53, 164.90, 163.37, 149.86, 138.90, 135.19, 132.23, 130.34, 129.06, 128.46, 128.05, 125.54, 125.06, 115.73, 115.57, 63.03, 52.64 ppm. MS: m/z = 481.3 ($M^+$). Anal. calcd. for $C_{21}H_{16}BrN_5O_4$ (482.3): C, 52.30; H, 3.34; N, 14.52; Found: C, 52.24; H, 3.41; N, 14.58.

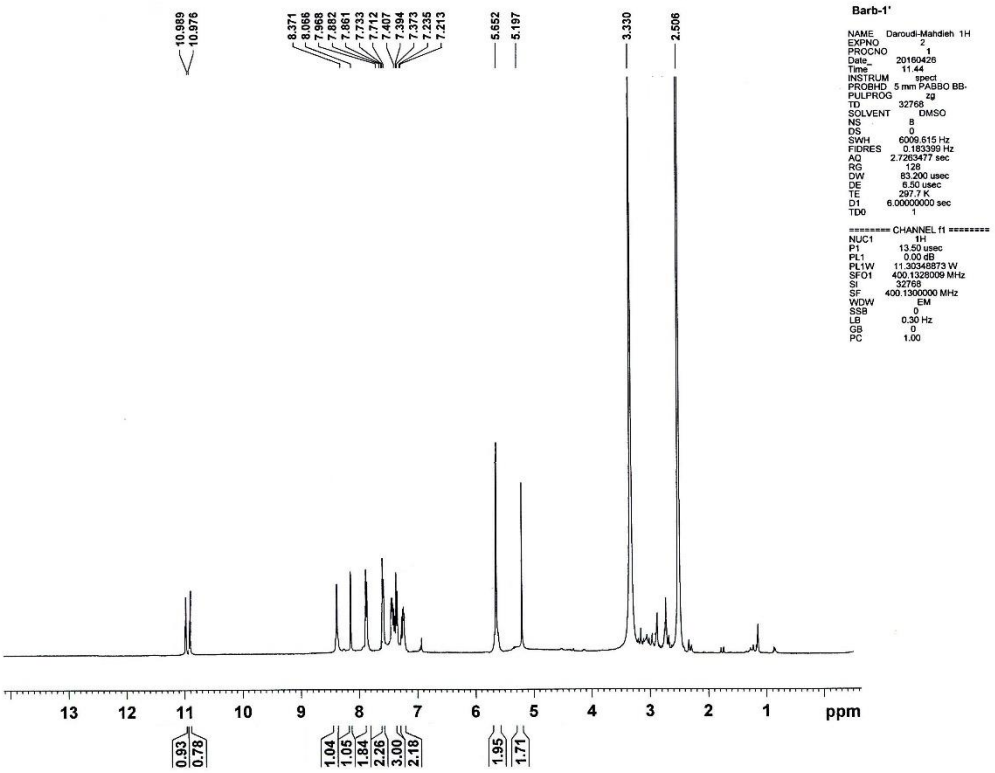
**5-(4-((1-(2-chlorobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-1,3-dimethylpyrimidine-2,4,6 (1H,3H,5H)-trione (8e)**: Yellow solid. Mp: 246.5-248.2 °C. IR (KBr, $cm^{-1}$) ν = 3447, 2923, 1670, 1597, 1178. $^1H$ NMR (400 MHz, DMSO): δ= 8.38 (s, 1H, CH), 7.97 (s, 1H, CH), 7.87 (m, 2H, ArH), 7.28-7.15 (m, 4H, ArH), 7.06-6.88 (m, 2H, ArH), 5.66 (s, 2H, $OCH_2$), 5.10 (s, 2H, $CH_2$), 2.87 (s, 3H, $CH_3$), 2.71 (s, 3H, $CH_3$) ppm. $^{13}C$ NMR (100 MHz, DMSO): δ= 162.79, 161.24 159.45, 147.39, 137.39, 132.23, 131.96, 131.36, 130.68, 129.19, 128.97, 128.28, 126.47, 115.91, 115.76, 61.59, 52.51, 35.25, 33.21 ppm. MS: m/z = 465.3 ($M^+$). Anal. calcd. for $C_{23}H_{20}ClN_5O_4$ (465.9): C, 59.30; H, 4.33; N, 15.03; Found C, 59.21; H, 4.30; N, 15.11.

**5-(4-((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-2-thioxodihydro pyrimidine-4,6(1H,5H)-dione (8f)**: Yellow solid. Mp: 229.9-231.5 °C. IR (KBr, $cm^{-1}$) ν = 3438, 2925, 1677, 1597, 1159. $^1H$ NMR (400 MHz, DMSO): δ= 11.06 (s, 1H, NH), 10.98 (s, 1H, NH), 8.34 (s, 1H, CH), 8.06 (s, 1H, CH), 7.87 (d, J=8.4 Hz, 2H, ArH), 7.57 (d, J=8.0 Hz, 2H, ArH), 7.51 (t, J=8.4 Hz, 1H, ArH), 7.22 (d, J=8.0 Hz, 2H, ArH), 7.04 (d, J=8.4 Hz, 2H, ArH), 5.60 (s, 2H, $OCH_2$), 5.27 (s, 2H, $CH_2$) ppm. $^{13}C$ NMR (100 MHz, DMSO): δ= 176.80, 163.37, 159.28, 148.04, 135.83, 135.79, 132.23, 132.17, 130.71, 130.69 130.33,

128.27, 126.42, 121.94, 115.67, 61.91, 52.60 ppm. MS: m/z = 421.1 ($M^+$). Anal. calcd. for $C_{21}H_{17}N_5O_4$ (419.4): C, 60.13; H, 4.09; N, 16.70; Found: C, 60.19 ; H, 4.13; N, 16.81.

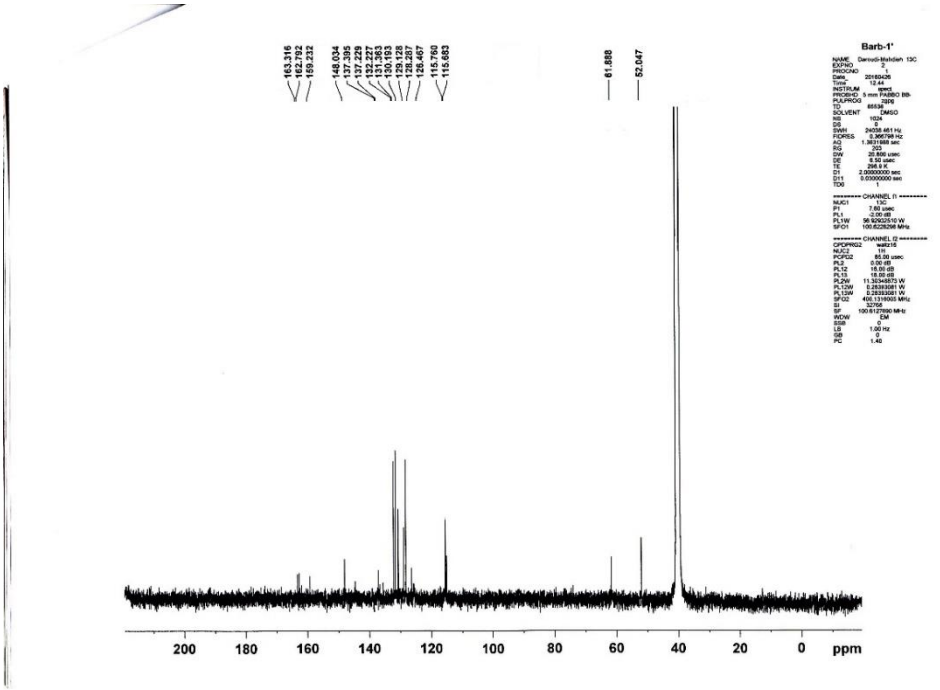
**5-(4-((1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-2-thioxodihydropyrimidine-4,6(1H,5H)-dione (8g)**: Yellow solid. Mp: 267.3-269.5 °C. IR (KBr, $cm^{-1}$) $\nu$ = 3439, 2925, 1728, 1627, 1238, 1130. $^1$H NMR (400 MHz, DMSO): δ= 11.47 (s, 1H, NH), 11.44(s, 1H, NH), 8.37 (s, 1H, CH), 8.16 (s, 1H, CH), 7.74 (d, J=8.0 Hz, 2H, ArH), 7.57 (d, J=8.0 Hz, 2H, ArH), 7.45-7.42 (m, 2H, ArH), 7.26 (d, J=8.8 Hz, 2H, ArH), 5.61 (s, 2H, $OCH_2$), 5.23 (s, 2H, $CH_2$) ppm. $^{13}$C NMR (100 MHz, DMSO): δ= 177.41, 162.19, 155.72, 142.69, 138.88, 136.85, 133.36, 132.15, 131.77, 130.59, 127.94, 125.35, 124.25, 121.89, 116.52, 113.50, 62.68, 52.56 ppm. MS: m/z = 497.0 ($M^+$). Anal. calcd. for $C_{21}H_{16}BrN_5O_3S$ (498.3): C, 50.61; H, 3.24; N, 14.05; Found: C, 50.55; H, 3.18; N, 14.13.

Index




210

211 $^{1}$H-NMR spectrum of 8a




212

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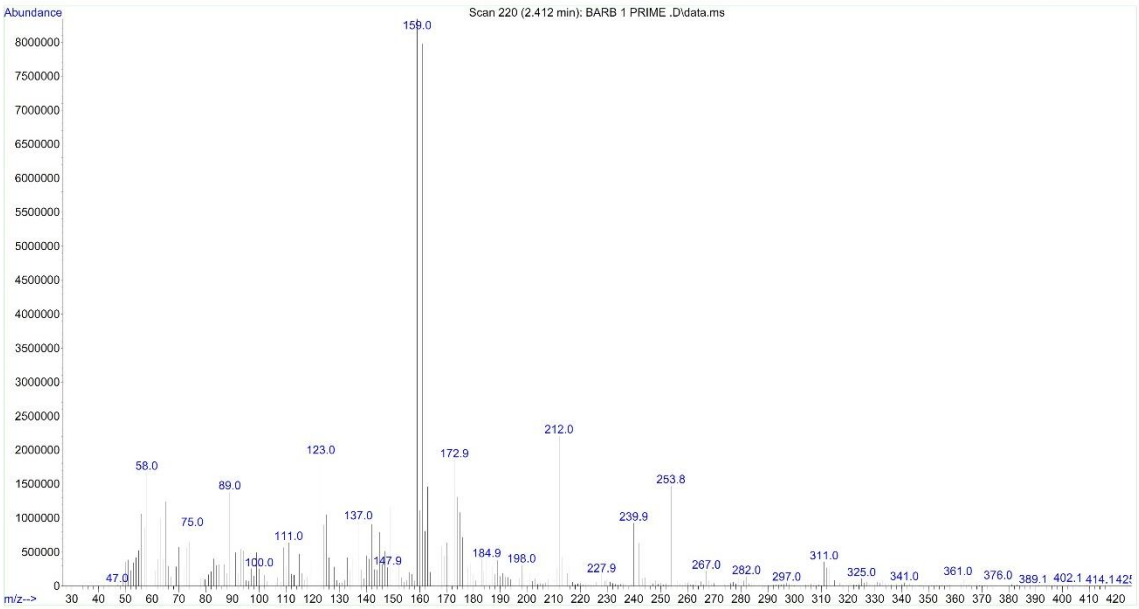
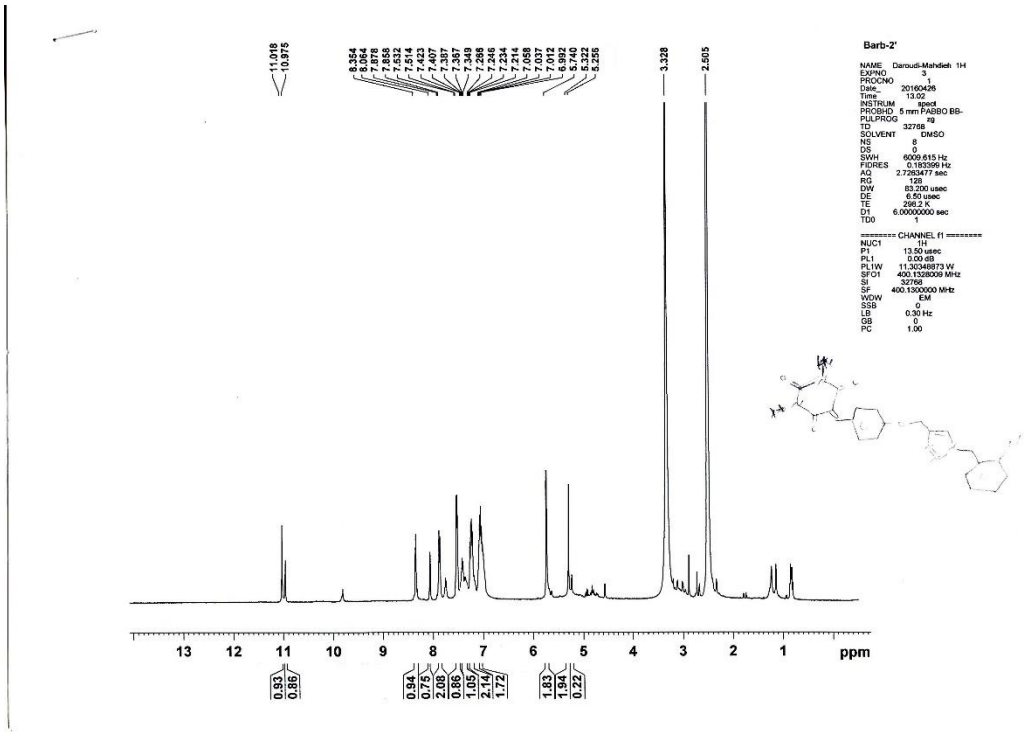



214

215 Mass spectrum of 8a




216

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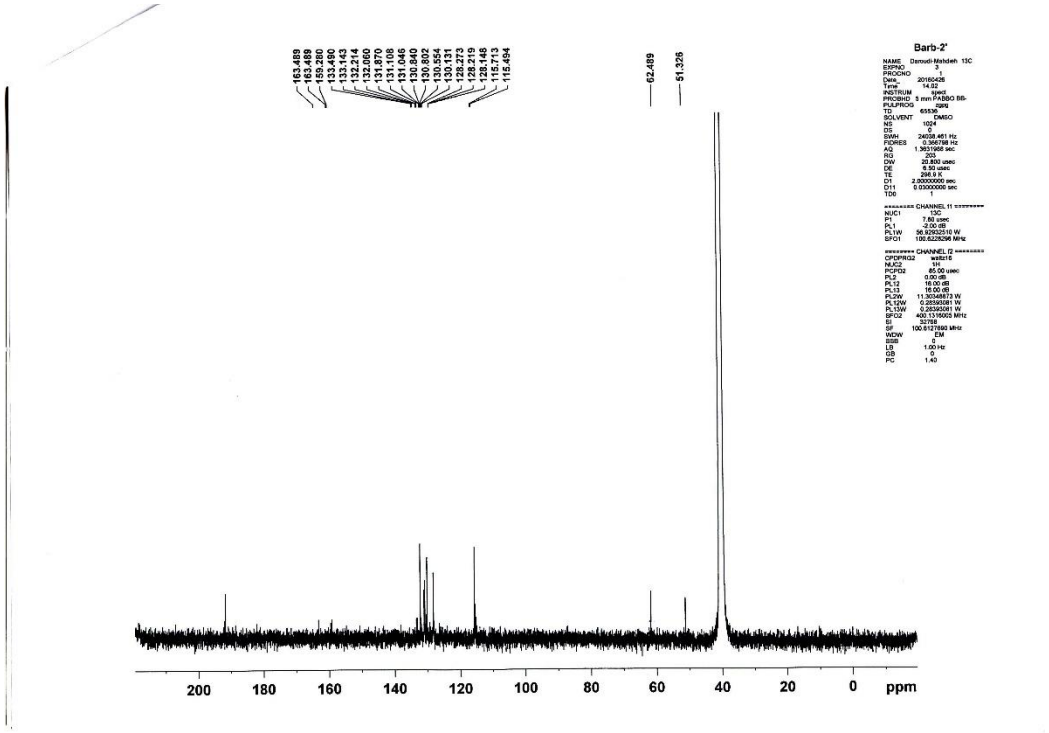


218

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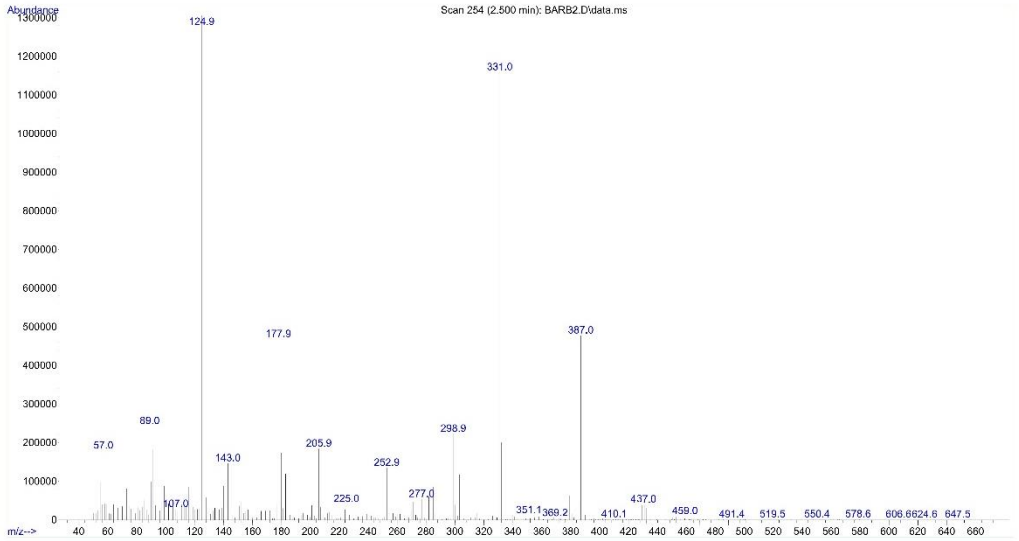


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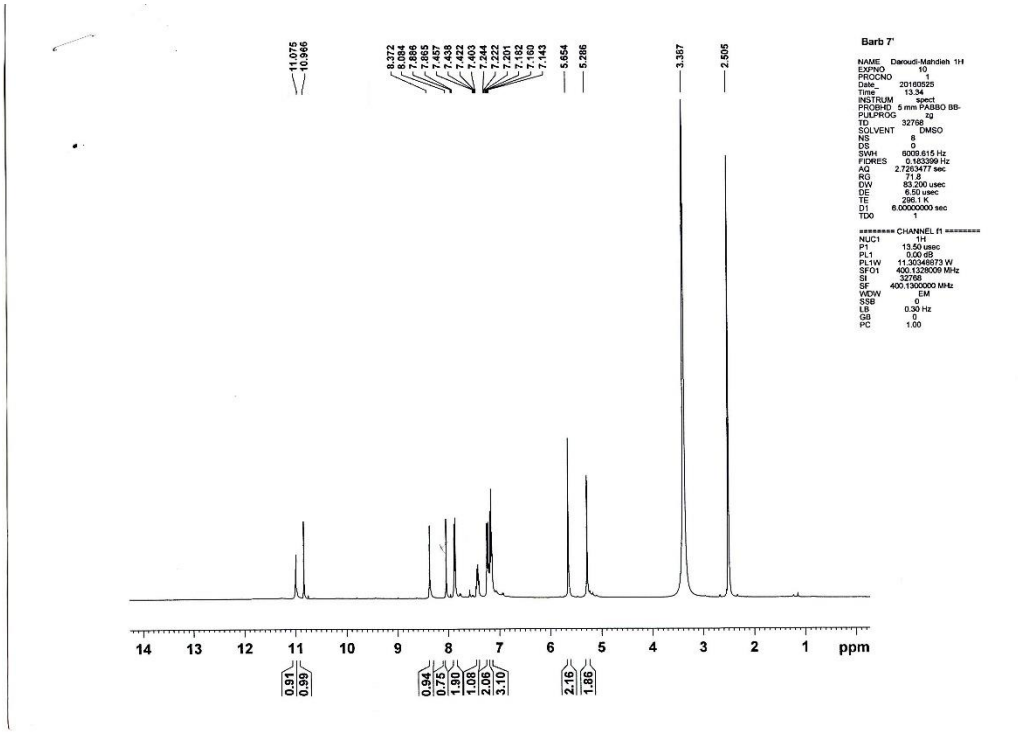
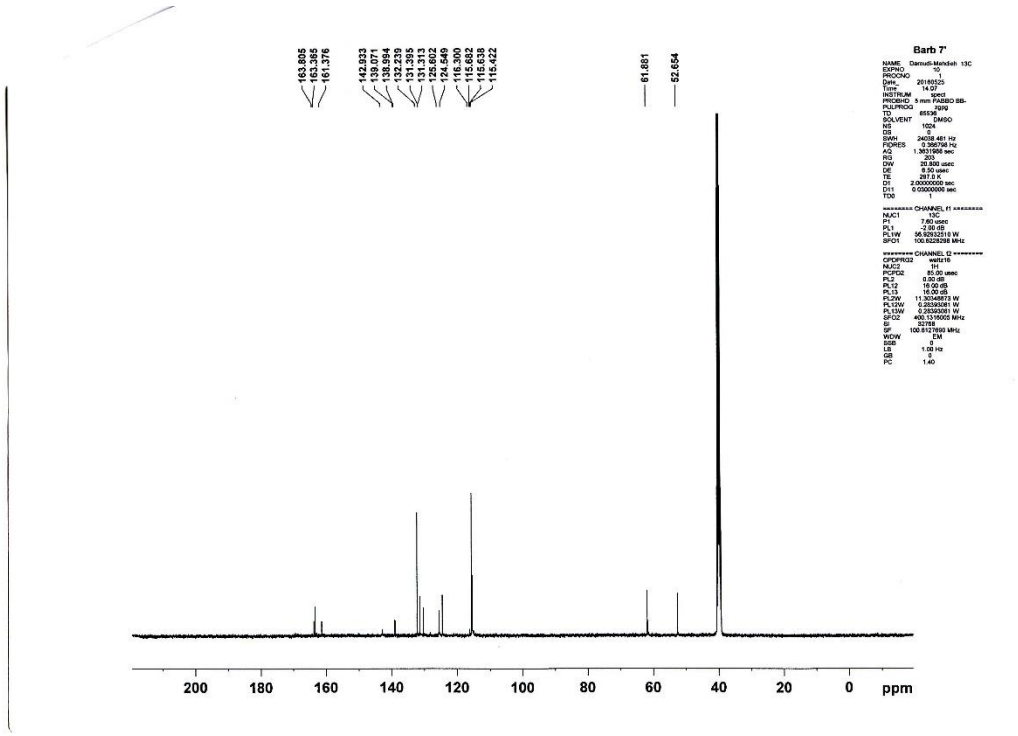



222

223 $^{1}$H-NMR spectrum of 8c

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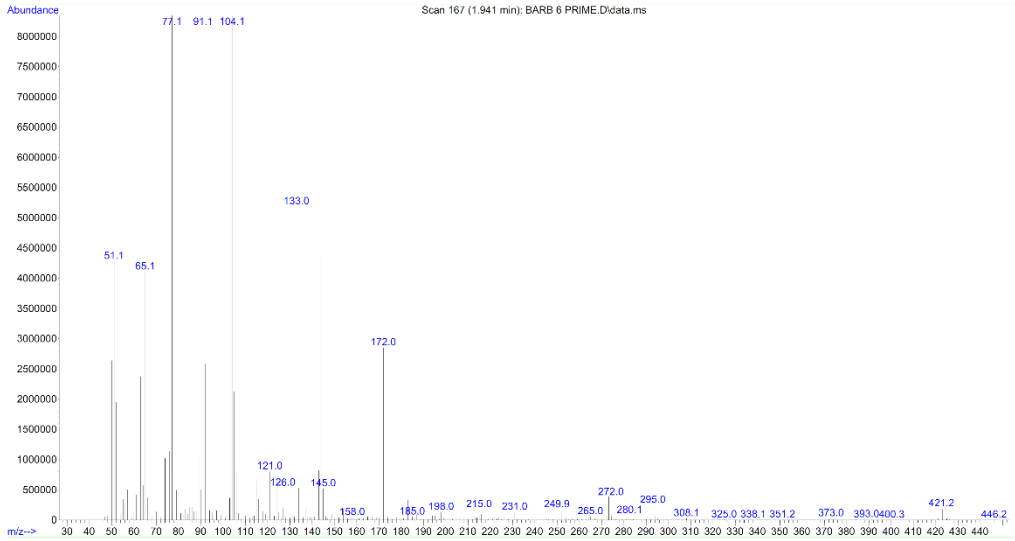


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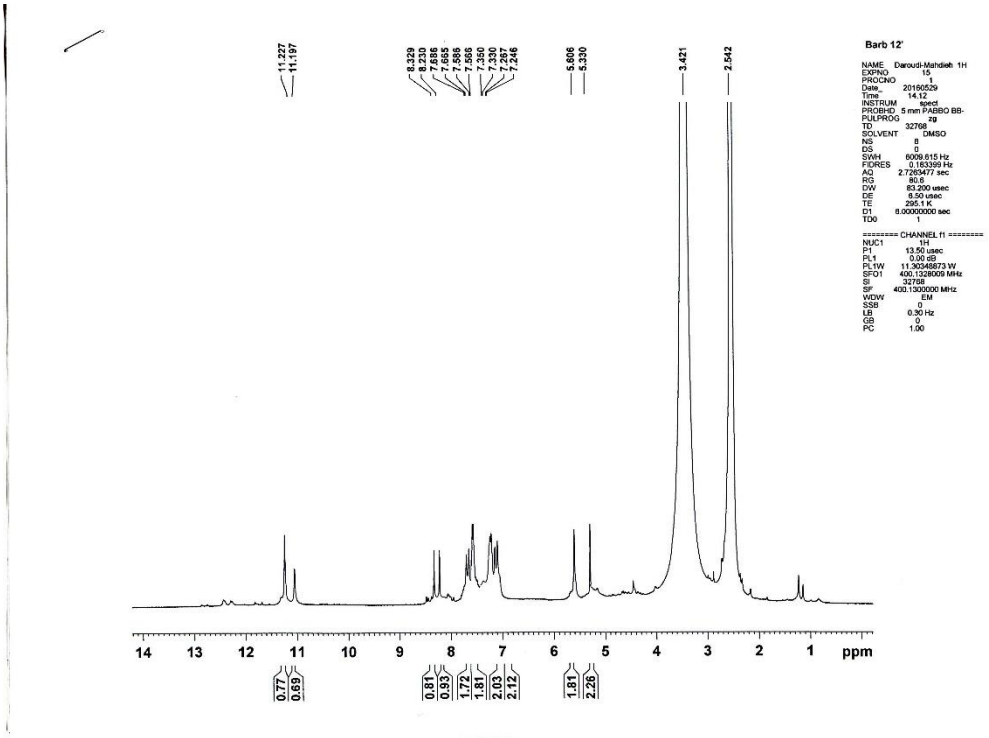
227 Mass spectrum of 8c

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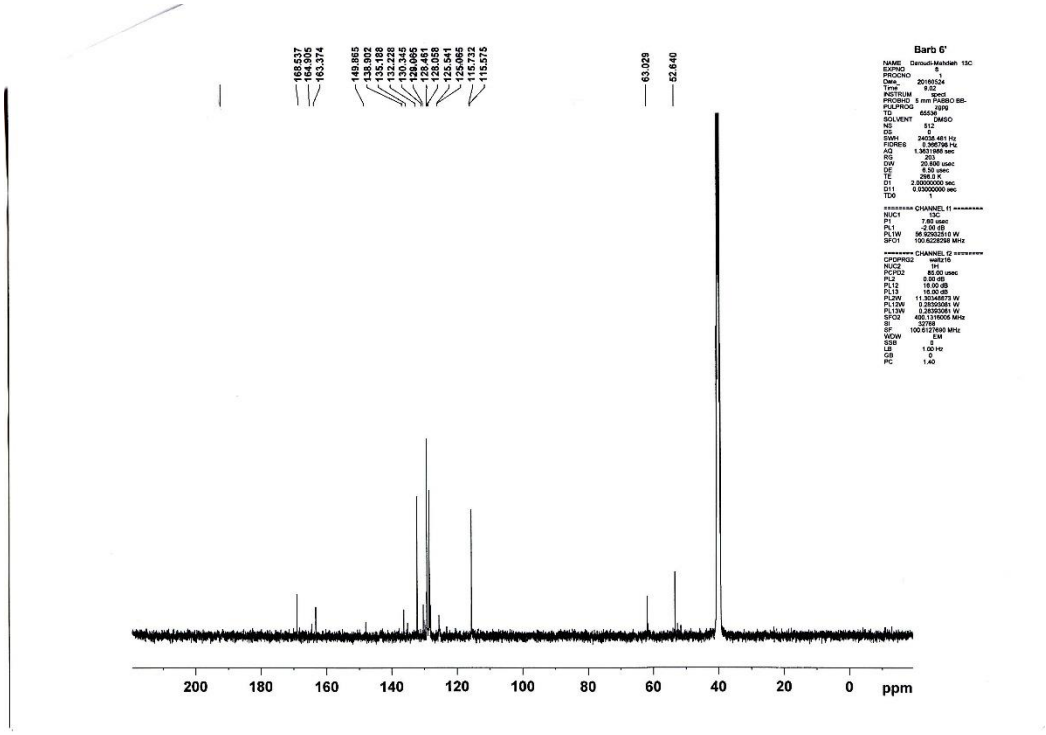


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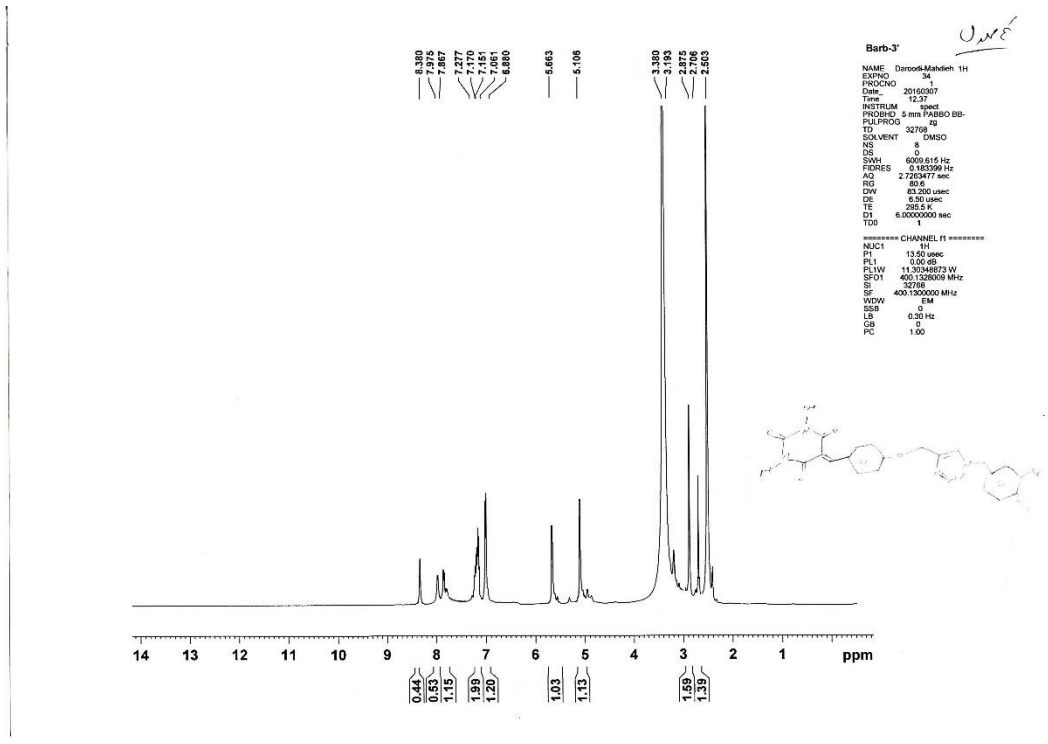
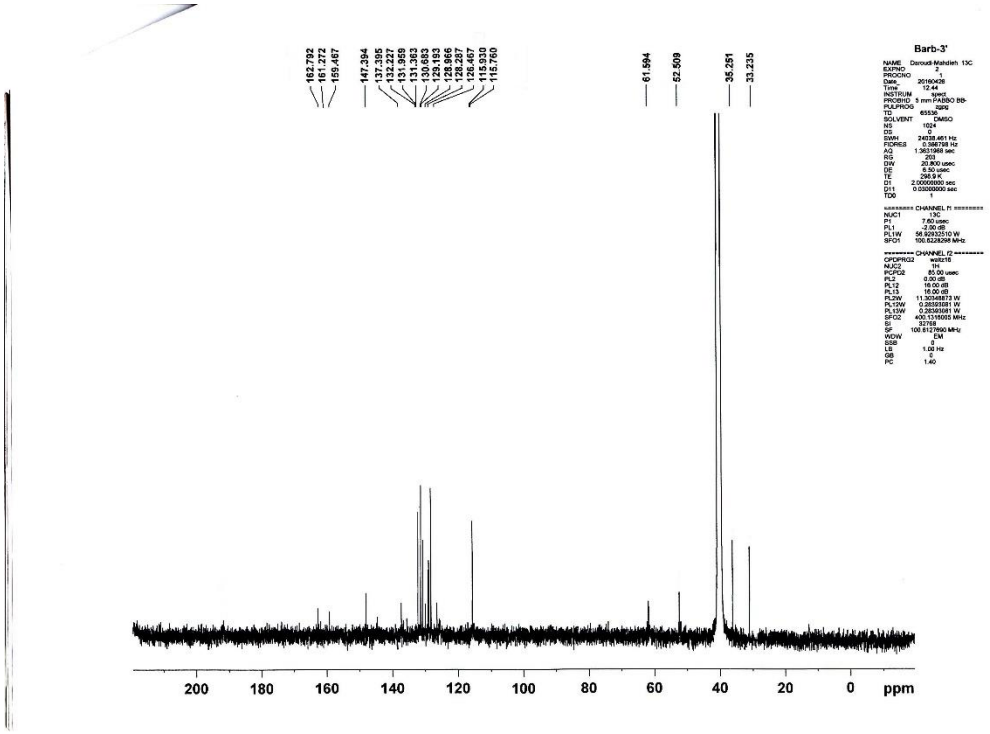



232

233 $^{1}$H-NMR spectrum of 8e

234




235

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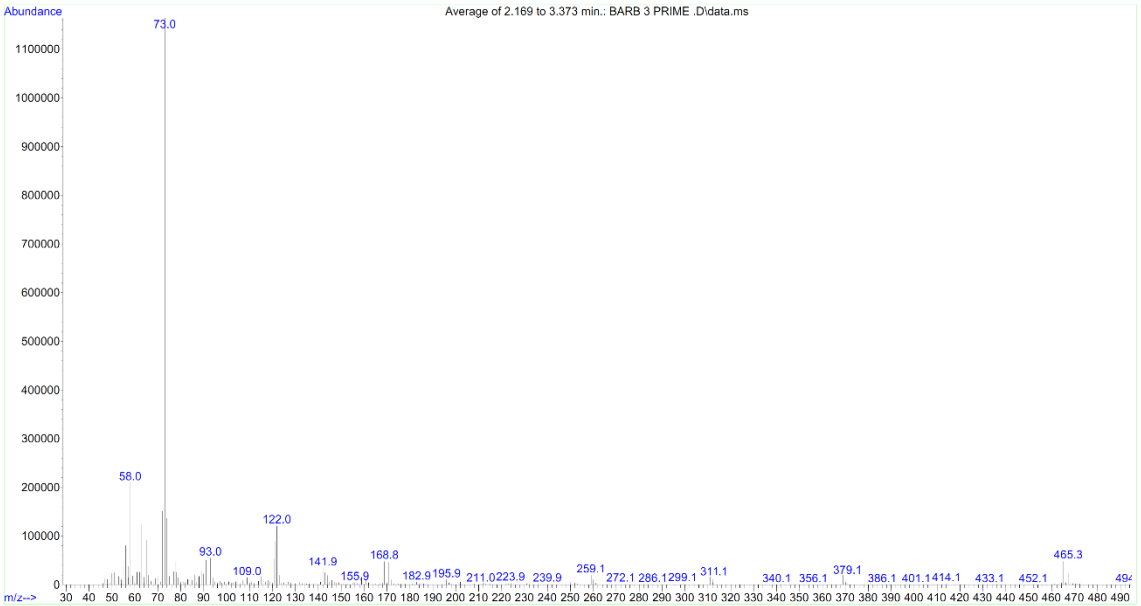
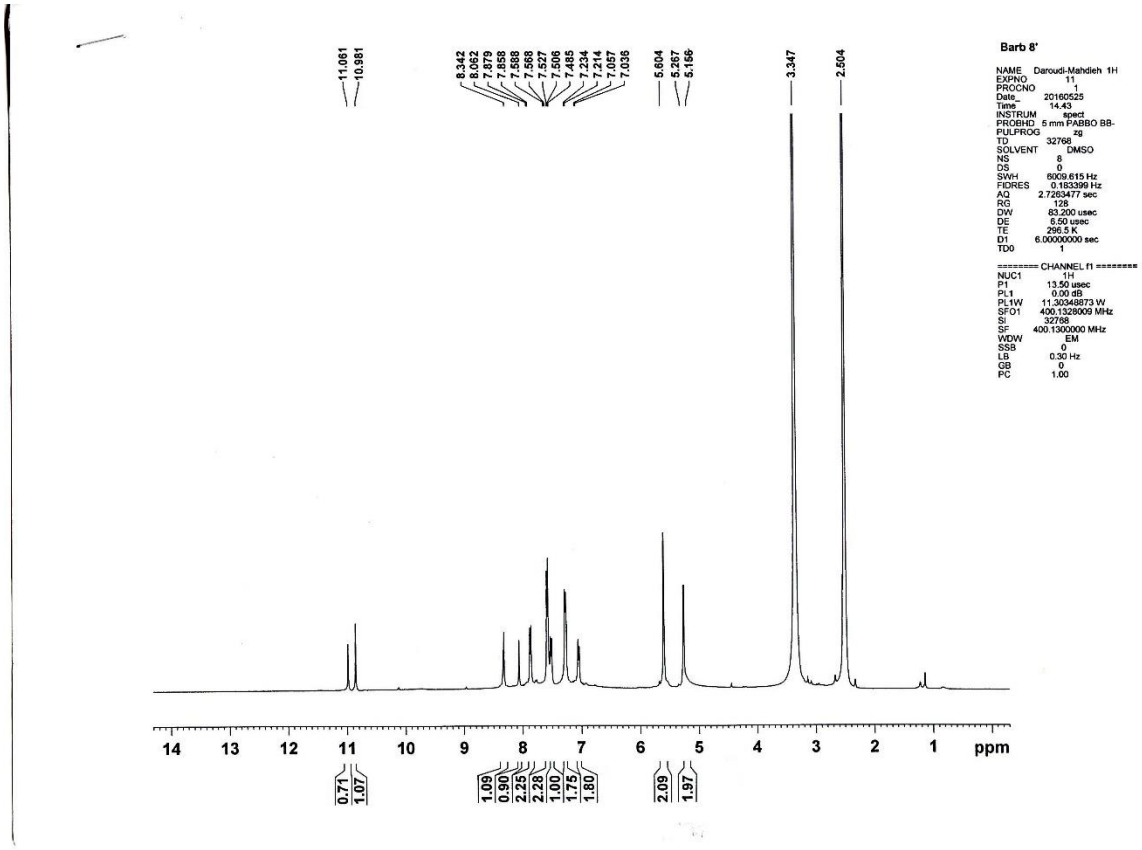


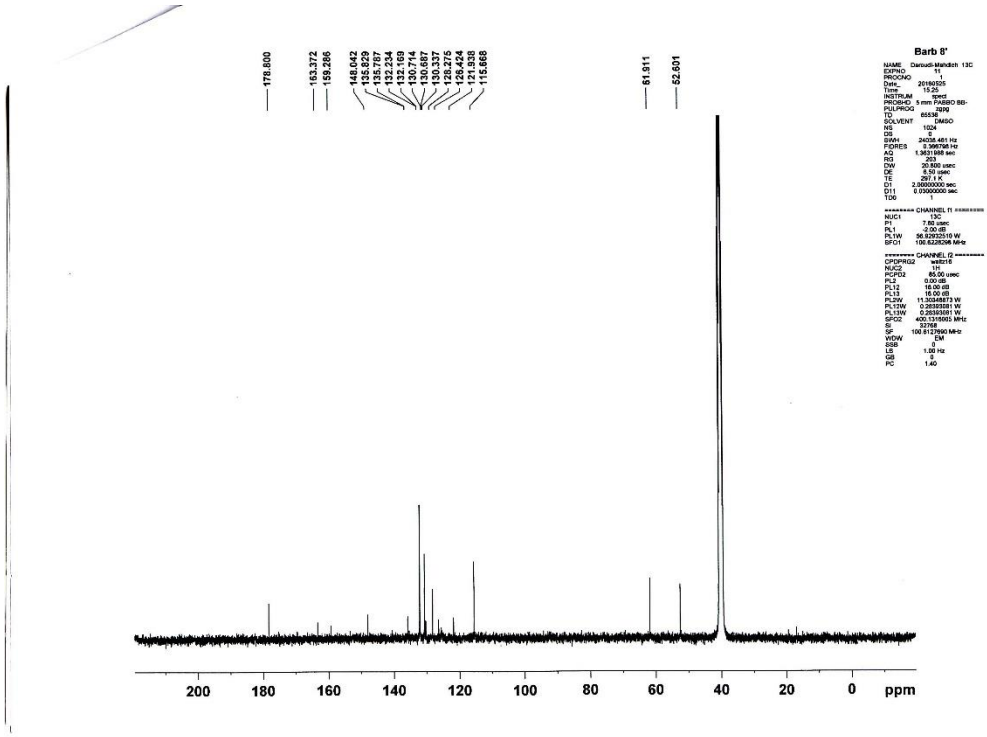

237

238 Mass spectrum of 8e




239

240 $^{1}$H-NMR spectrum of 8f

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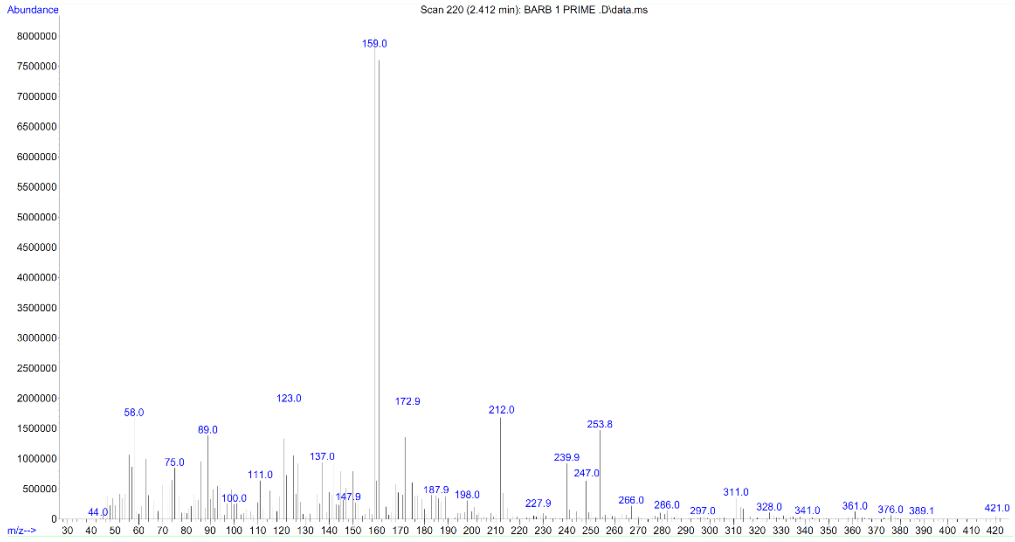
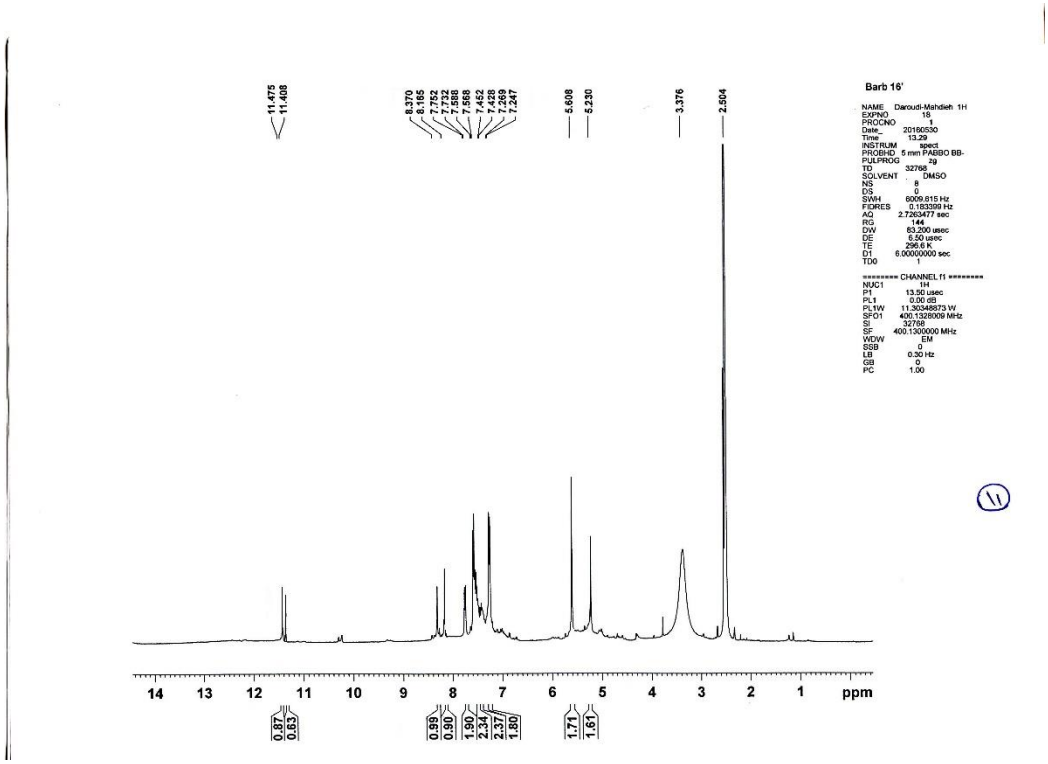



243

244 Mass spectrum of 8f




245

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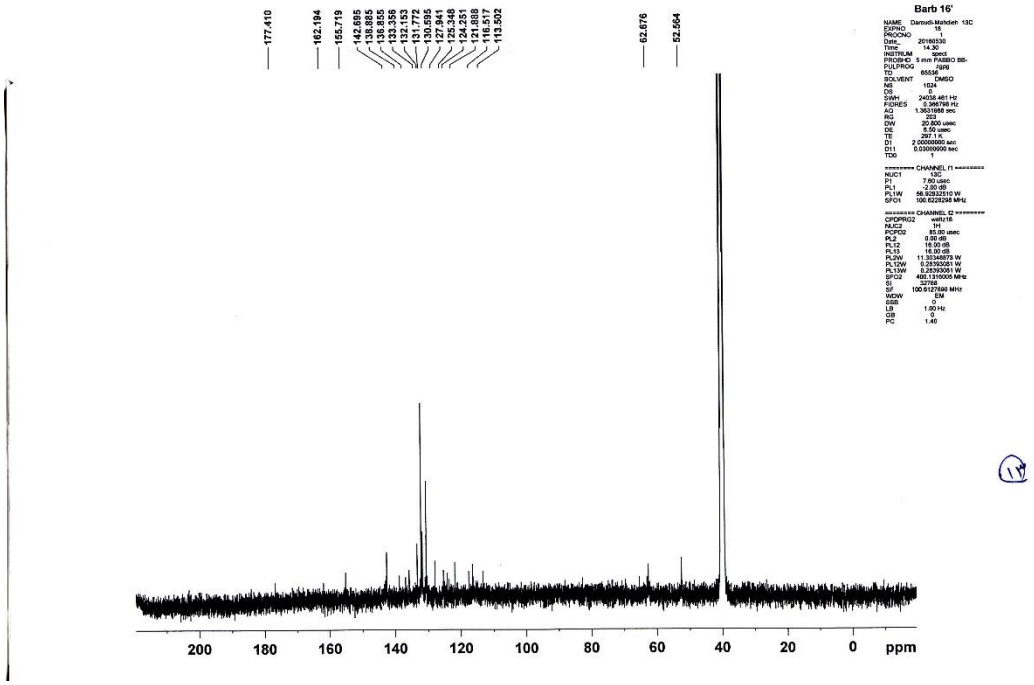


247

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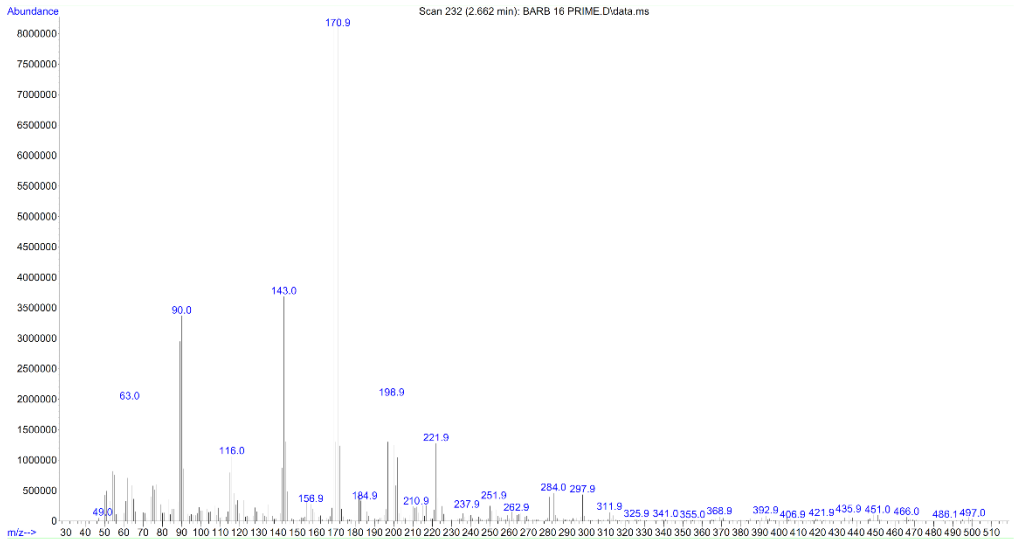
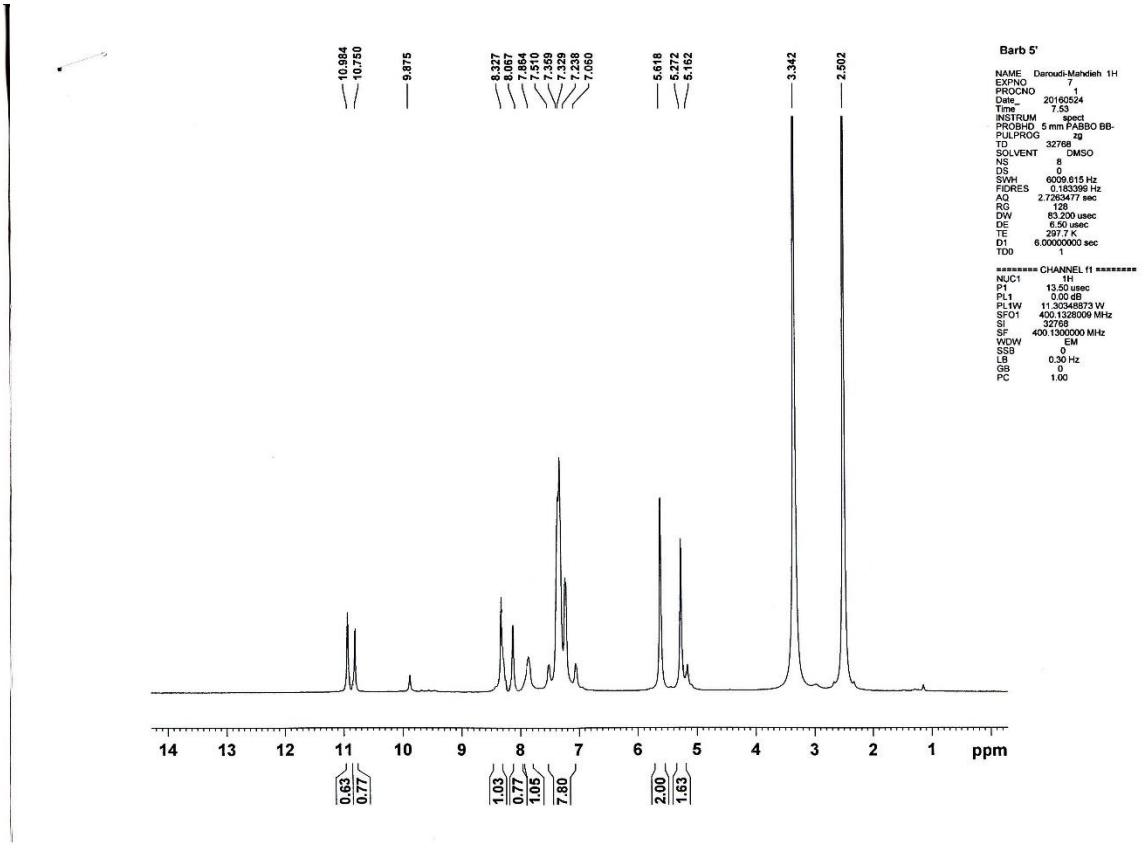


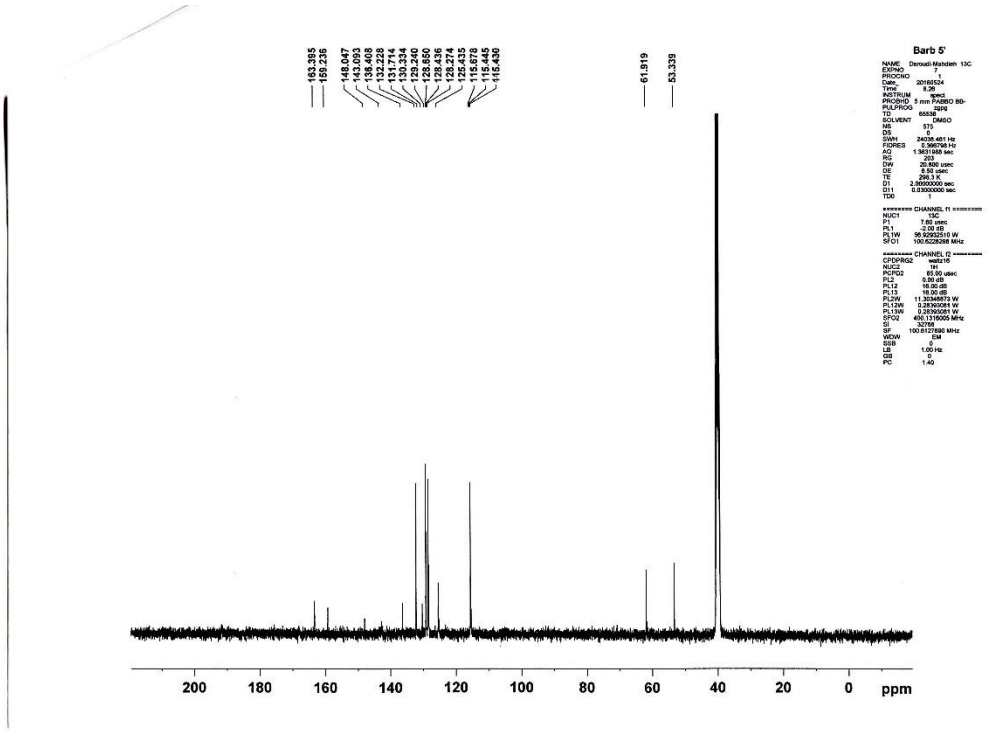

249

250 Mass spectrum of 8g




251

252 $^{1}$H-NMR spectrum of 7a




253

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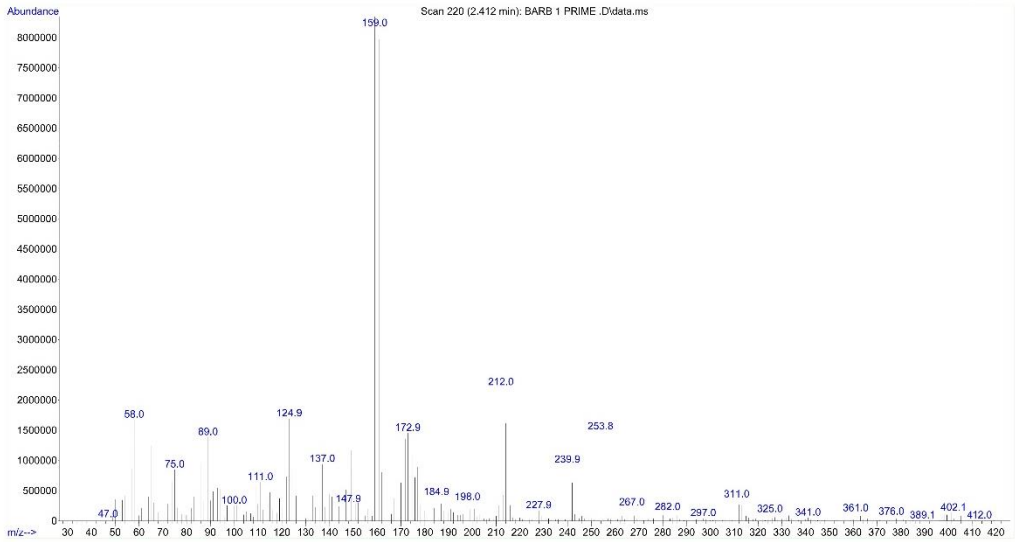
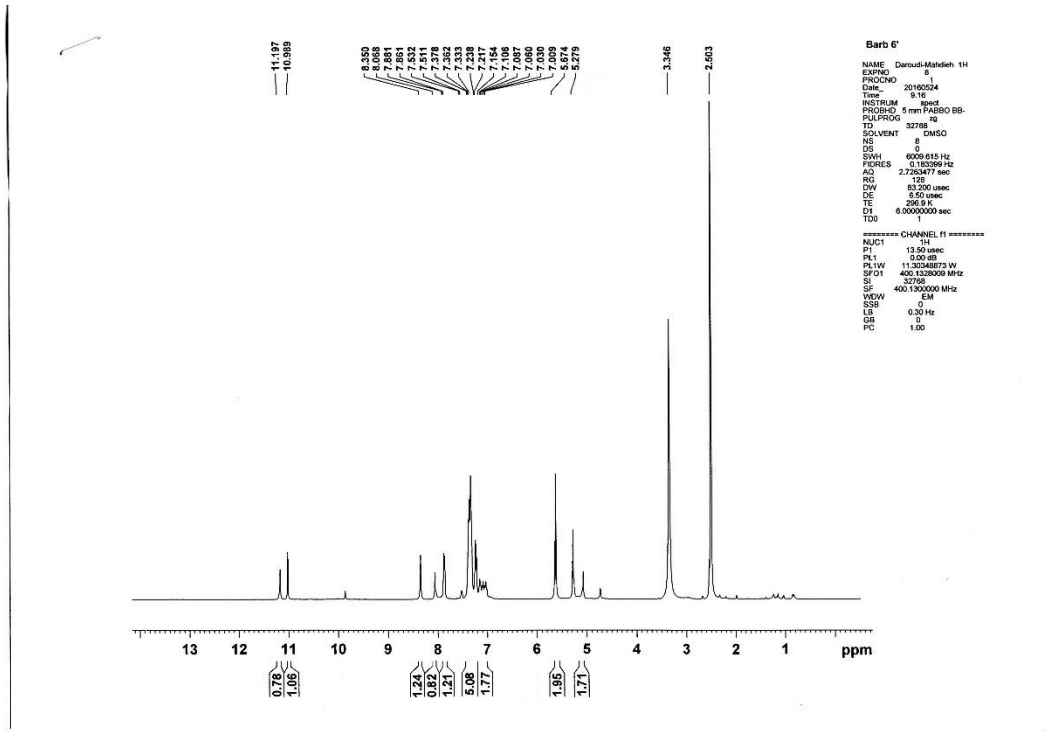



255

256 Mass spectrum of 7a




257

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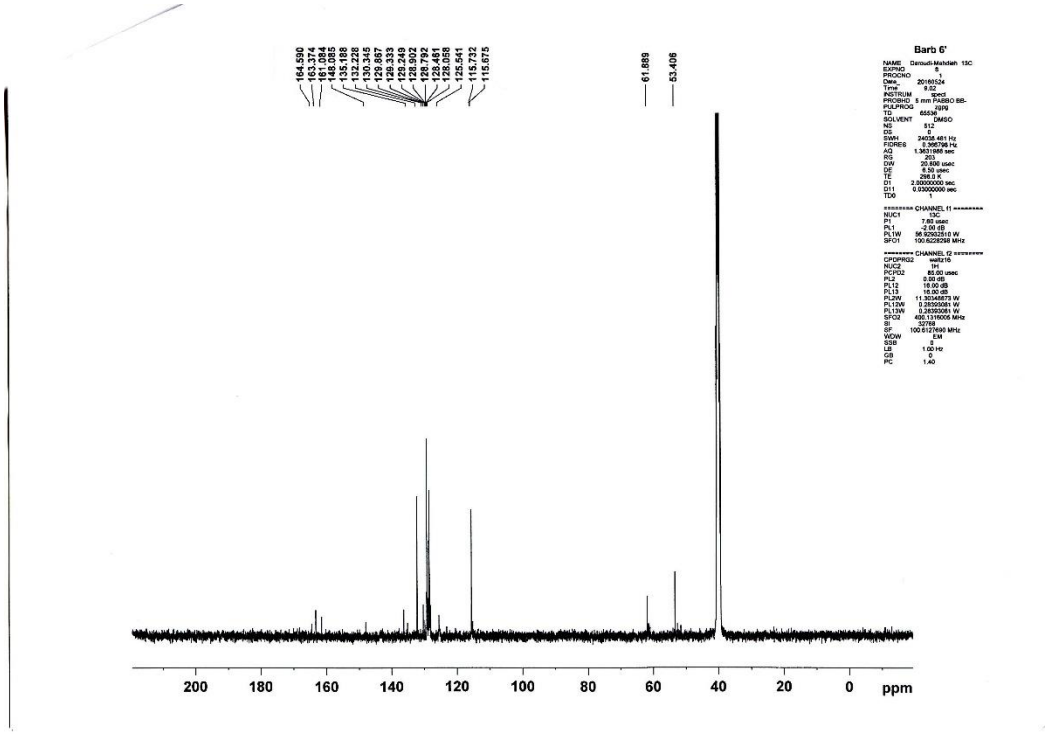
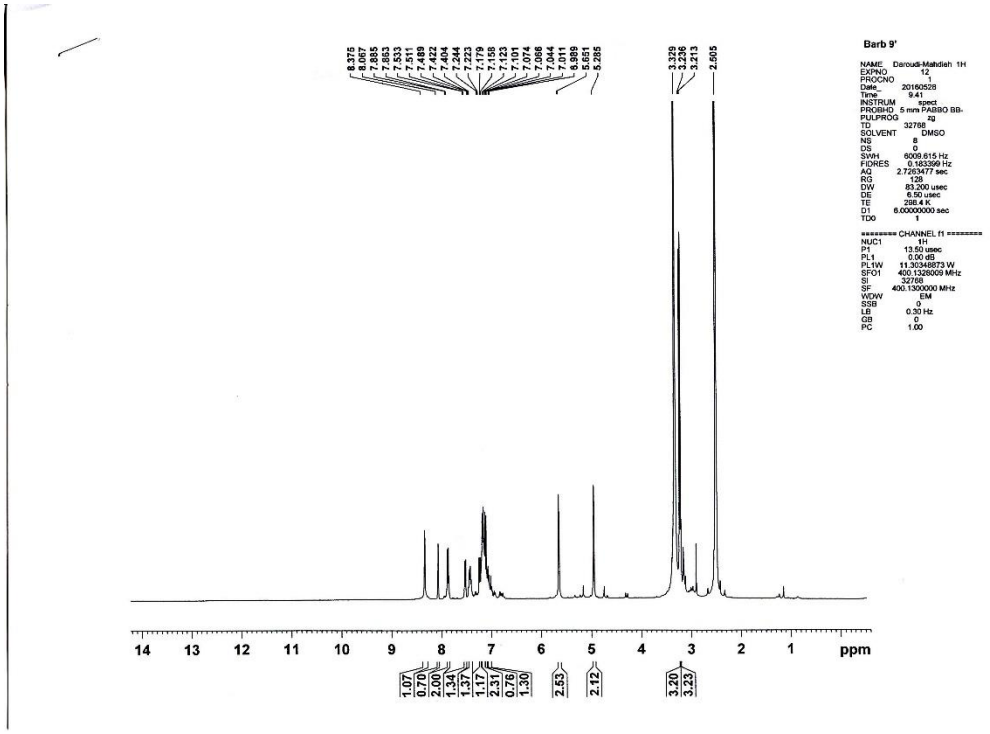



259

260 $^{13}C$ -NMR spectrum of 7b

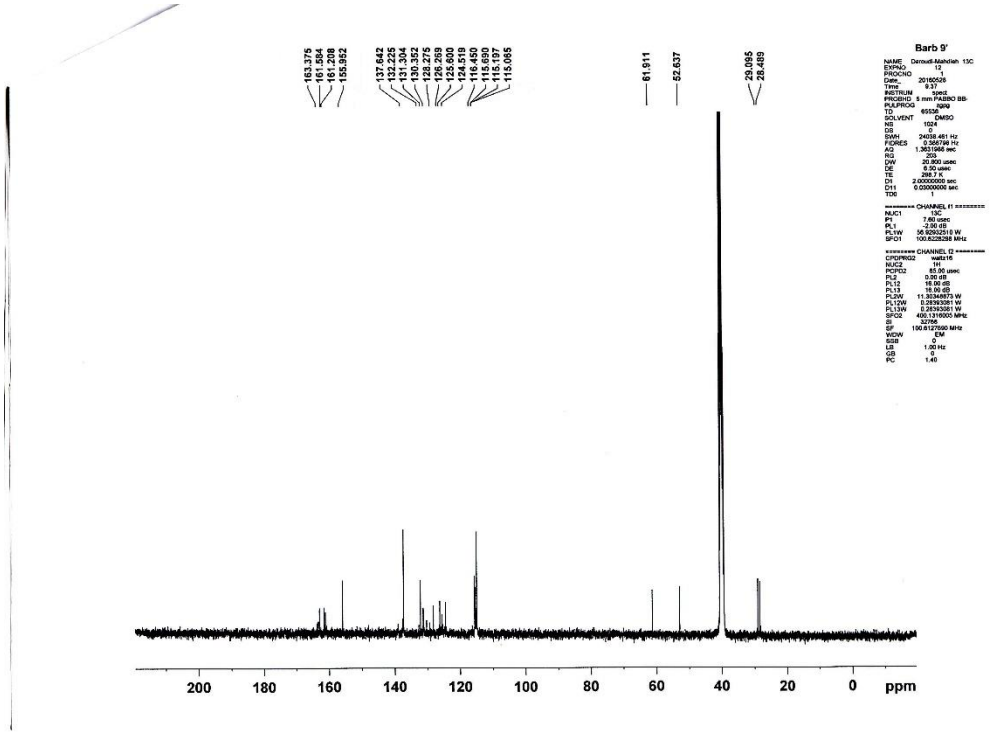

261

262 Mass spectrum of 7b



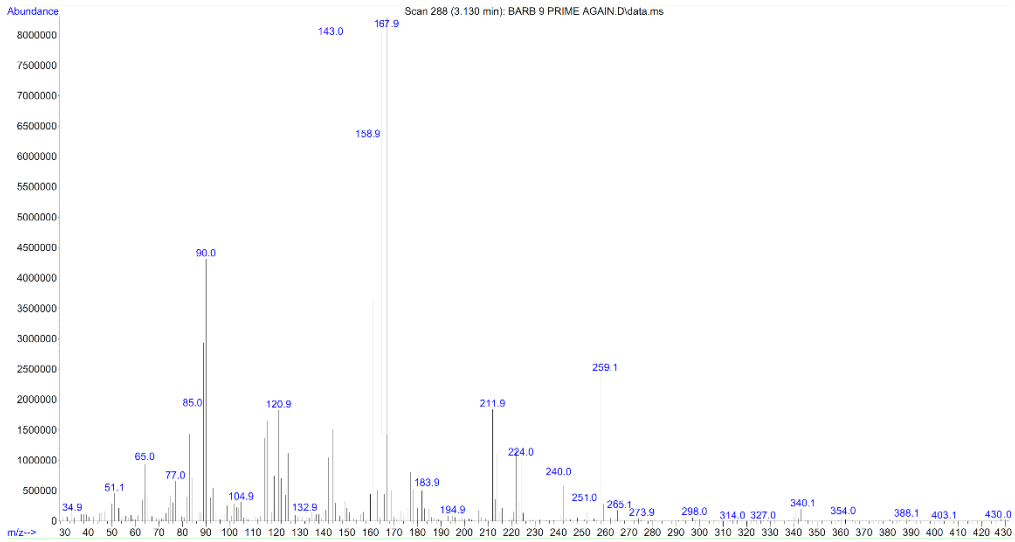

263

264 $^{1}$H-NMR spectrum of 7c



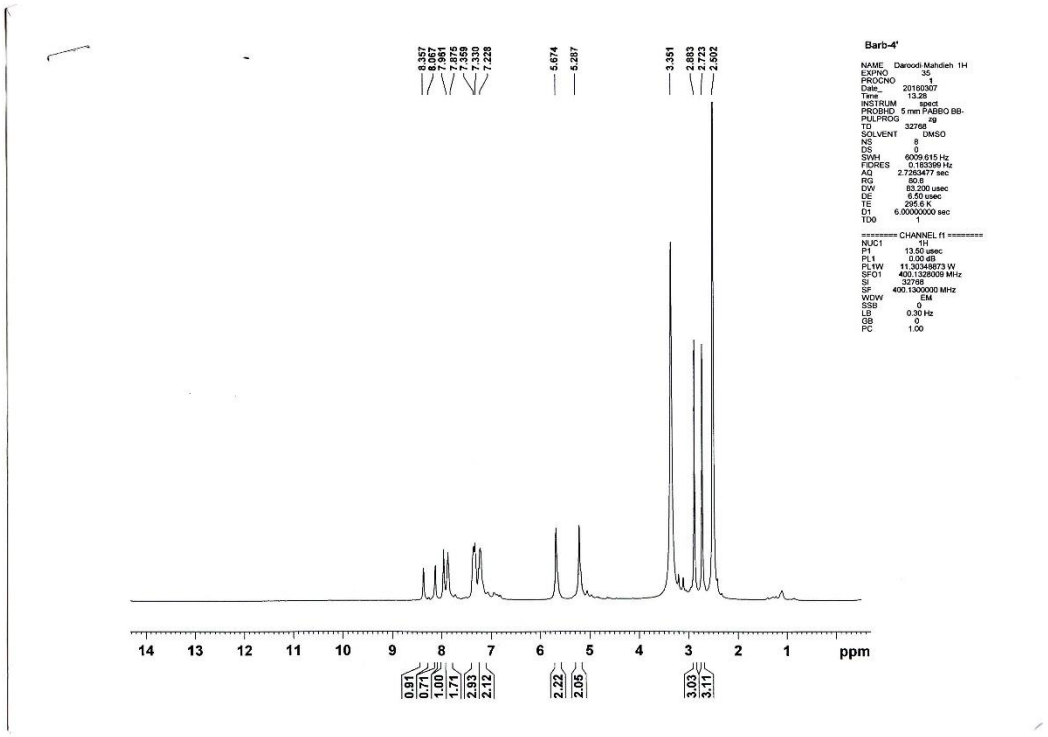

265

266 $^{13}$C-NMR spectrum of 7c



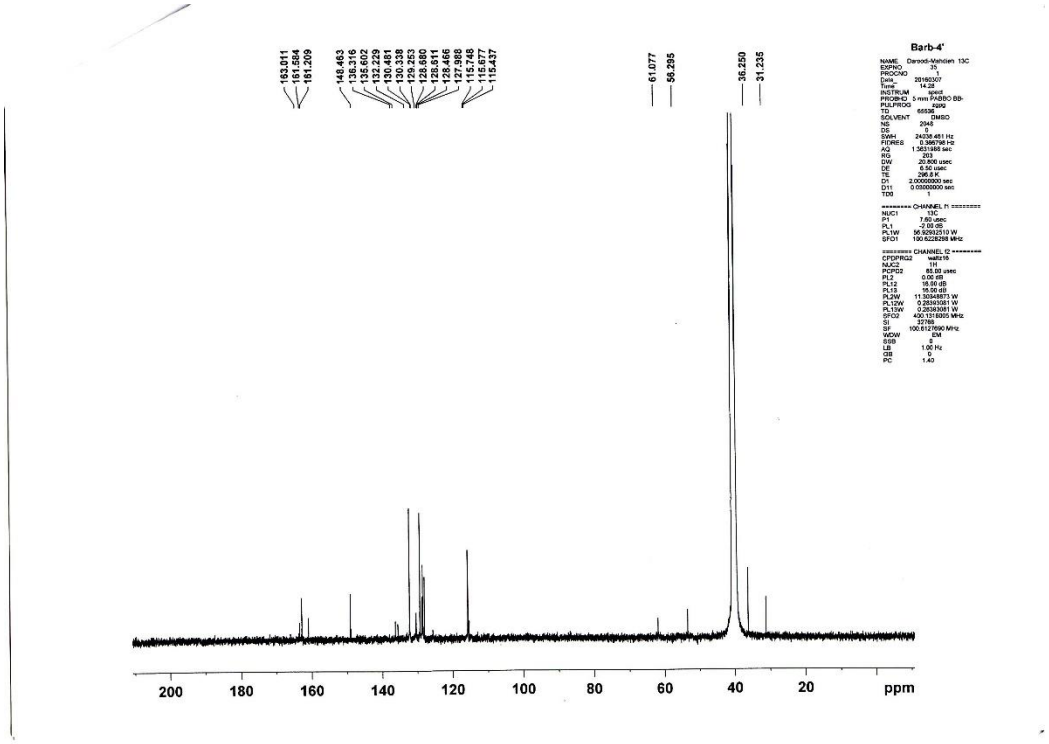

267

268 Mass spectrum of 7c




269

270 $^{1}$H-NMR spectrum of 7d

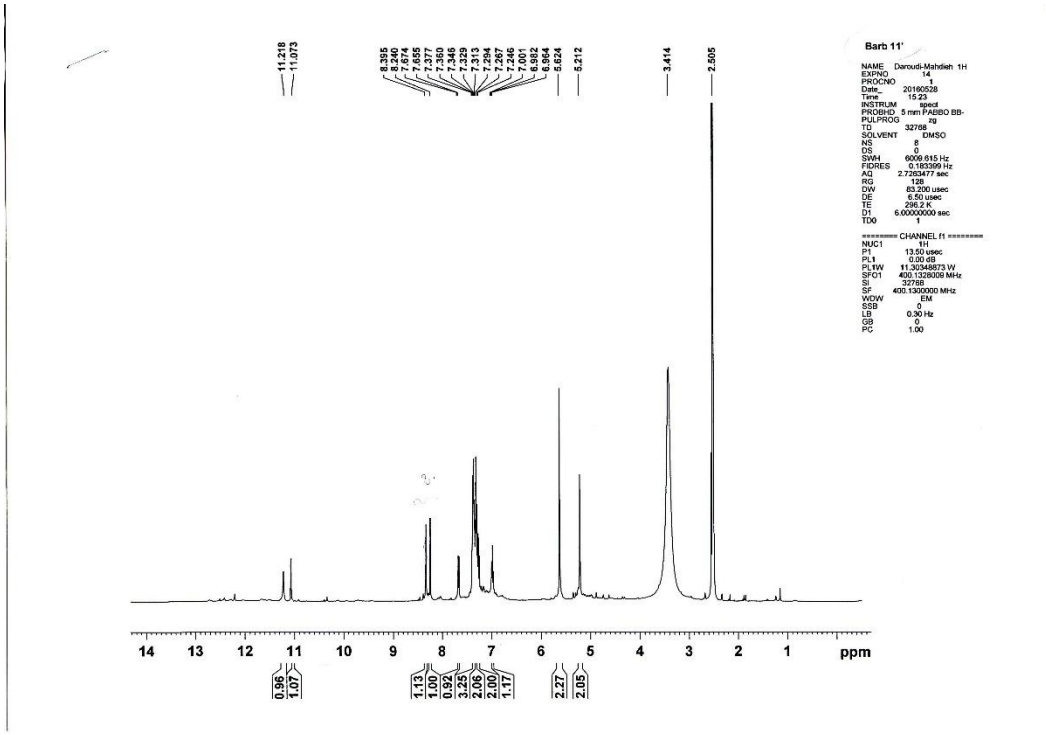



271

272 $^{13}$C -NMR spectrum of 7d


273

274 Mass spectrum of 7d




275

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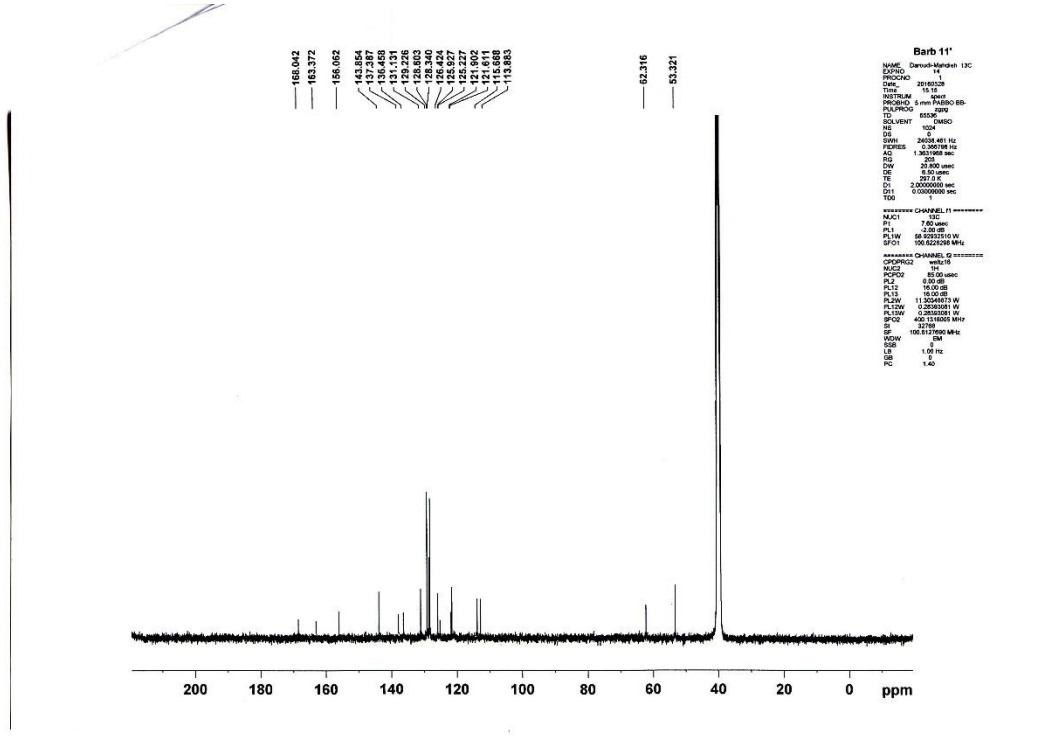


277

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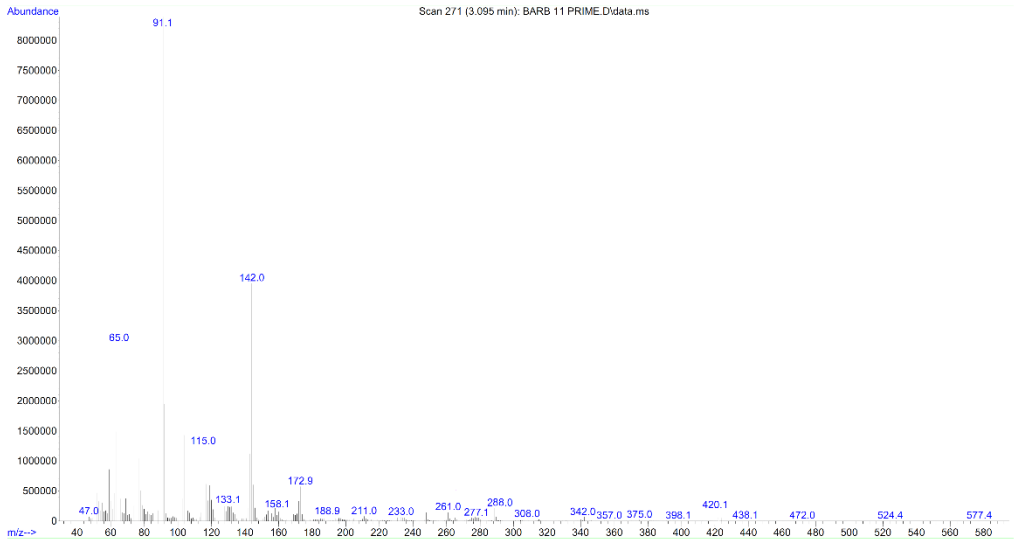
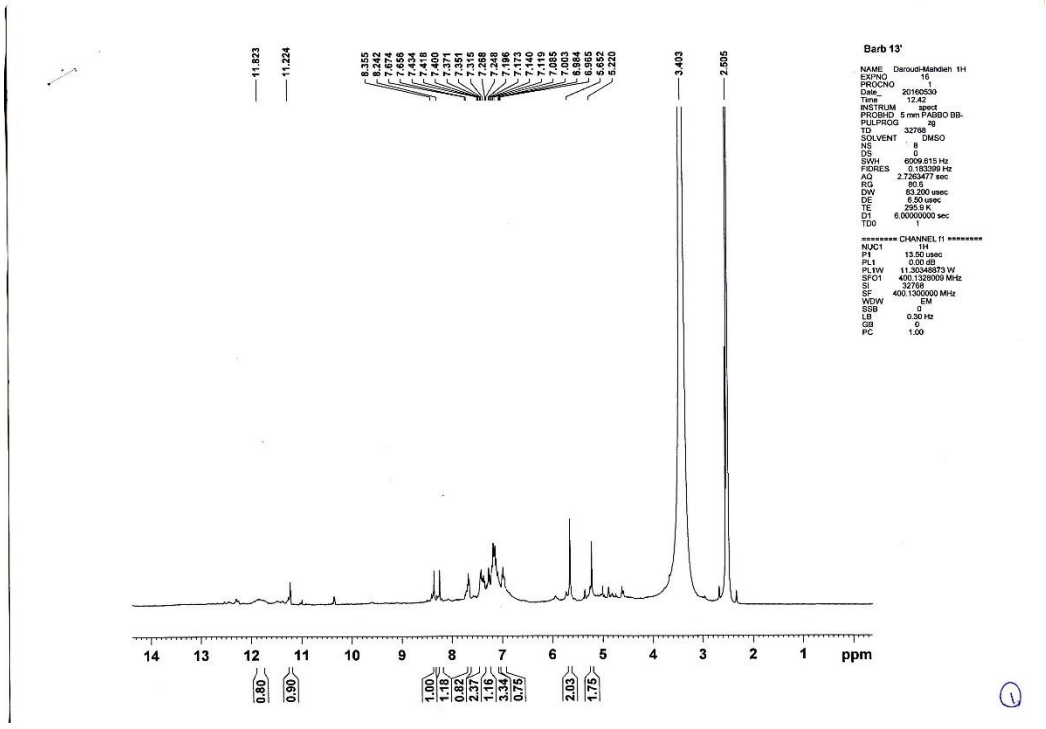



279

280 Mass spectrum of 7e




281

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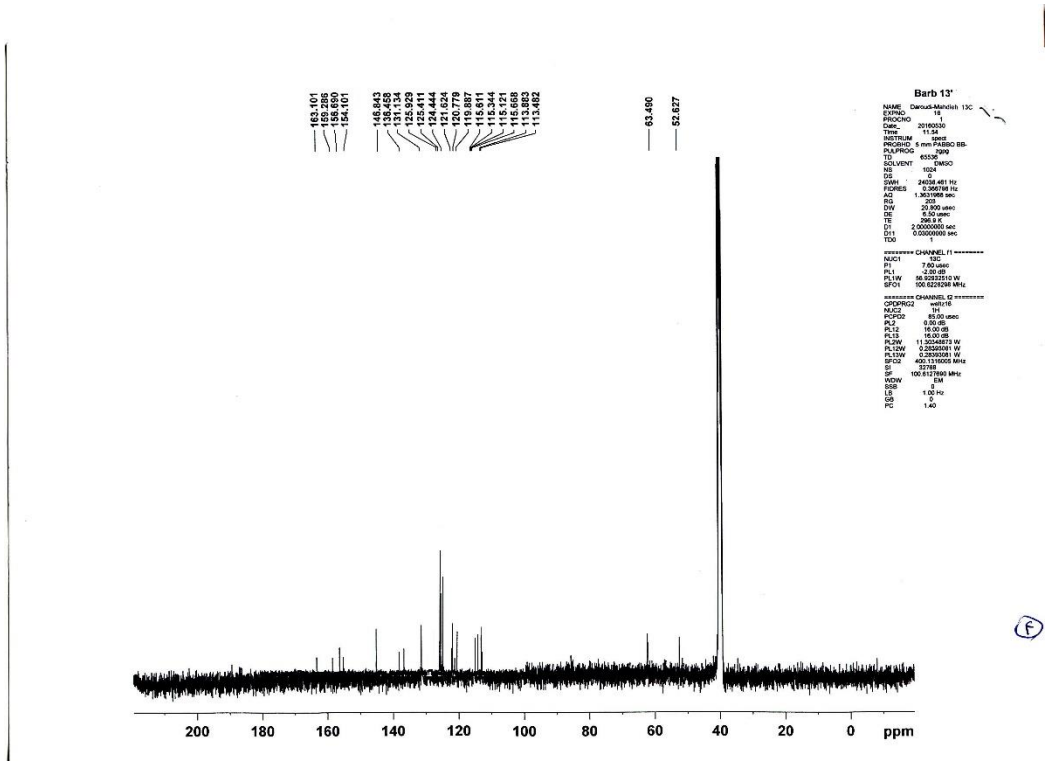


283

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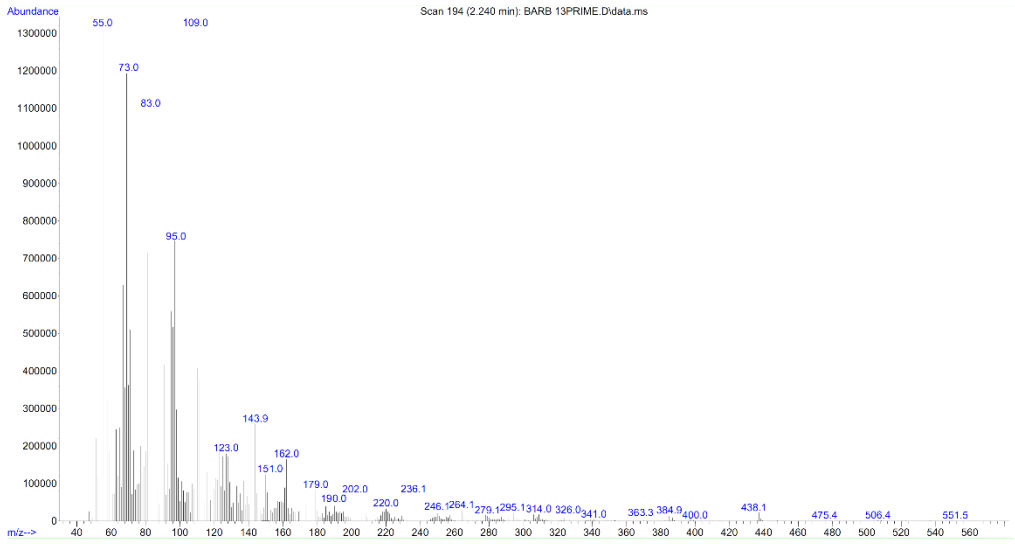
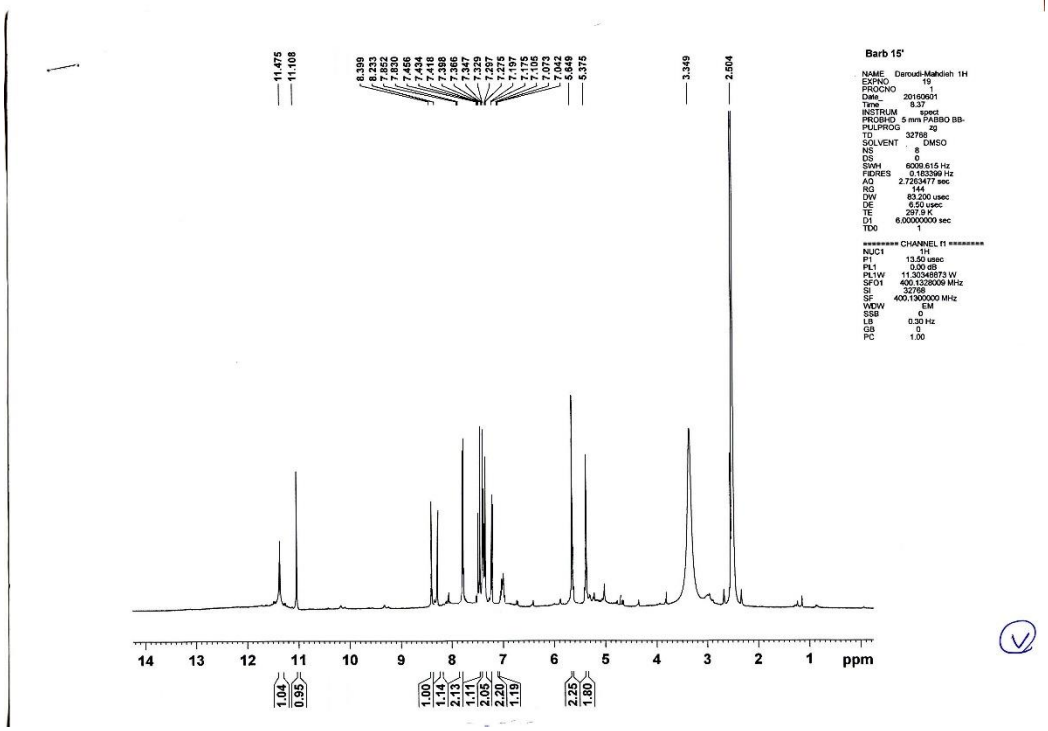



285

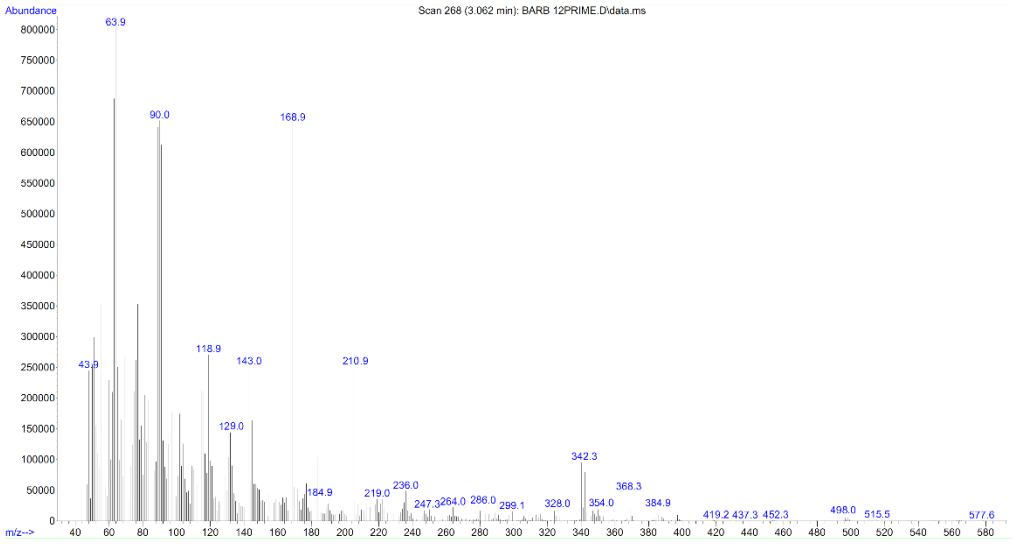
286 Mass spectrum of 7f




287

288 $^{1}$H-NMR spectrum of 7g

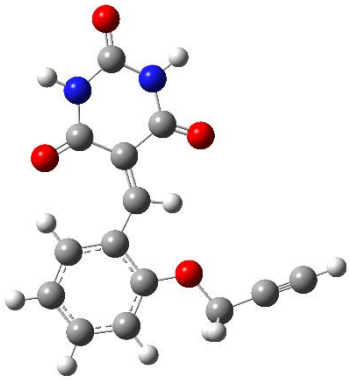
289




290

291 Mass spectrum of 7g

292



**4**

Input orientation:

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| 9 | 8 | 0 | 4.823413 | 2.304858 | 1.256785 |
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| 12 | 6 | 0 | -0.028144 | 0.264400 | 0.191033 |
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| 19 | 6 | 0 | -2.905448 | -2.274623 | 0.080035 |
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| 321 | 22 | 1 | 0 | -3.975141 | -2.271665 | 0.054564 |
| 322 | 23 | 1 | 0 | -2.744861 | -4.415071 | 0.048169 |
| 323 | 24 | 8 | 0 | -2.913941 | 0.177131 | 0.120725 |
| 324 | 25 | 6 | 0 | -4.319375 | -0.078986 | 0.057020 |
| 325 | 26 | 1 | 0 | -4.616229 | -0.653456 | 0.909524 |
| 326 | 27 | 1 | 0 | -4.542365 | -0.624630 | -0.835979 |
| 327 | 28 | 6 | 0 | -5.084733 | 1.257323 | 0.046701 |
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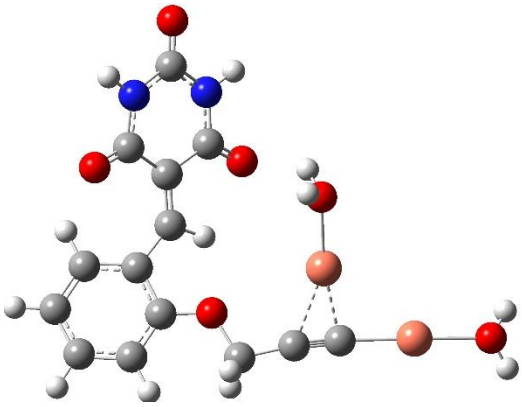
331 

332 **4a**

333 Input orientation:

334 ---

| 335 Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|---|---|
| 336 Number | Number | Type | X | Y | Z |

337 ---

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| 340 3 | 6 | 0 | 2.563484 | -1.829383 | -0.443948 |
| 341 4 | 6 | 0 | 4.224615 | -2.962477 | 0.956830 |
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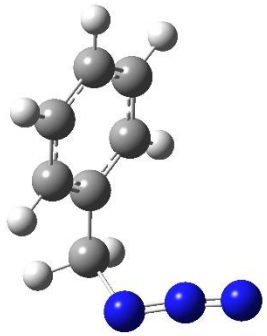
| 350 | 13 | 1 | 0 | 1.550263 | 0.317872 | -1.030037 |
| 351 | 14 | 6 | 0 | 2.607720 | 2.006682 | -0.266439 |
| 352 | 15 | 6 | 0 | 3.860317 | 2.617173 | -0.291641 |
| 353 | 16 | 6 | 0 | 1.460126 | 2.819493 | -0.220224 |
| 354 | 17 | 6 | 0 | 3.983867 | 3.995246 | -0.258537 |
| 355 | 18 | 1 | 0 | 4.738627 | 2.008710 | -0.357164 |
| 356 | 19 | 6 | 0 | 1.578481 | 4.200553 | -0.159494 |
| 357 | 20 | 6 | 0 | 2.841118 | 4.777031 | -0.181438 |
| 358 | 21 | 1 | 0 | 4.956031 | 4.450873 | -0.291367 |
| 359 | 22 | 1 | 0 | 0.712885 | 4.830154 | -0.100858 |
| 360 | 23 | 1 | 0 | 2.923961 | 5.848098 | -0.141786 |
| 361 | 24 | 8 | 0 | 0.283770 | 2.165599 | -0.217357 |
| 362 | 25 | 6 | 0 | -0.931772 | 2.883182 | -0.220973 |
| 363 | 26 | 1 | 0 | -0.976049 | 3.545971 | -1.075709 |
| 364 | 27 | 1 | 0 | -1.017746 | 3.469049 | 0.684516 |
| 365 | 28 | 6 | 0 | -2.035232 | 1.909384 | -0.306676 |
| 366 | 29 | 6 | 0 | -3.013164 | 1.200801 | -0.451469 |
| 367 | 30 | 29 | 0 | -1.906696 | -0.069816 | 0.916000 |
| 368 | 31 | 29 | 0 | -4.669058 | 0.170679 | -0.822115 |
| 369 | 32 | 8 | 0 | -1.114206 | -1.505982 | 2.171005 |
| 370 | 33 | 1 | 0 | -0.887531 | -1.260512 | 3.062233 |
| 371 | 34 | 8 | 0 | -6.388126 | -0.858909 | -1.217864 |
| 372 | 35 | 1 | 0 | -7.094160 | -0.420015 | -1.681861 |
| 373 | 36 | 1 | 0 | -0.396840 | -2.042638 | 1.848933 |
| 374 | 37 | 1 | 0 | -6.329401 | -1.736010 | -1.583455 |

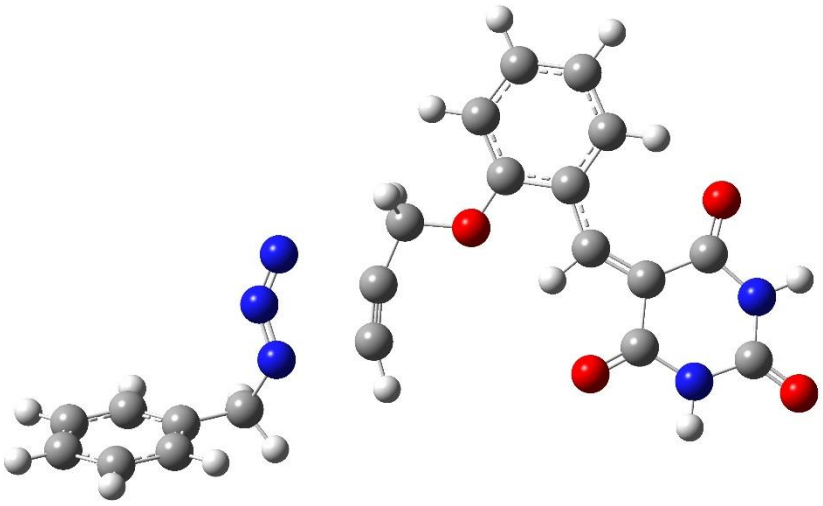
375 ----------



**6a**

Input orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.667601 | -0.152009 | -0.210094 |
| 2 | 6 | 0 | -1.304931 | -0.150994 | 0.117125 |
| 3 | 6 | 0 | -0.610319 | 1.061650 | 0.221618 |
| 4 | 6 | 0 | -1.278371 | 2.273273 | -0.001065 |
| 5 | 6 | 0 | -2.641037 | 2.272253 | -0.328252 |
| 6 | 6 | 0 | -3.335649 | 1.059615 | -0.432786 |
| 7 | 1 | 0 | -3.197964 | -1.077886 | -0.289903 |
| 8 | 1 | 0 | -0.794866 | -1.076096 | 0.287190 |
| 9 | 1 | 0 | -0.748026 | 3.199151 | 0.078727 |
| 10 | 1 | 0 | -3.151111 | 3.197351 | -0.498254 |
| 11 | 1 | 0 | -4.376072 | 1.058845 | -0.682637 |
| 12 | 6 | 0 | 0.887125 | 1.062781 | 0.581143 |
| 13 | 1 | 0 | 1.125855 | 1.960761 | 1.111738 |
| 14 | 1 | 0 | 1.106763 | 0.215642 | 1.196778 |
| 15 | 7 | 0 | 1.686782 | 0.994030 | -0.650414 |
| 16 | 7 | 0 | 2.281290 | 0.942967 | -1.564991 |
| 17 | 7 | 0 | 3.043473 | 0.877503 | -2.737505 |



**A**

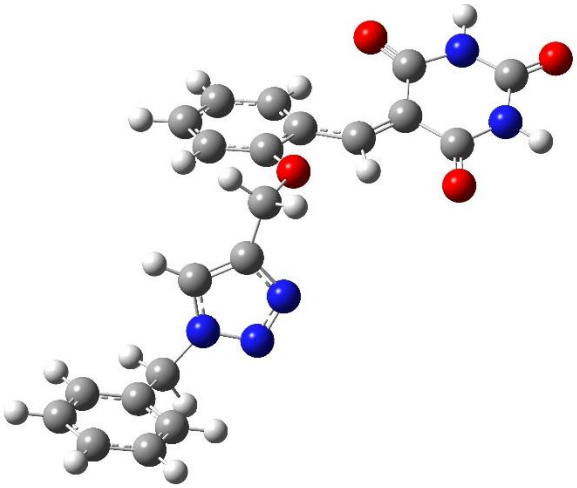
Input orientation:

| enter umber | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.517226 | 0.749869 | -0.219263 |
| 2 | 7 | 0 | -3.413687 | 1.968669 | -0.181507 |
| 3 | 7 | 0 | -4.120746 | 1.044465 | -0.282906 |
| 4 | 7 | 0 | -4.083387 | -0.211455 | -0.260570 |
| 5 | 6 | 0 | -0.594812 | 1.880843 | -0.119967 |
| 6 | 8 | 0 | 0.756912 | 1.372573 | -0.126750 |
| 7 | 1 | 0 | -0.768955 | 2.445544 | 0.803504 |
| 8 | 6 | 0 | 1.787053 | 2.234570 | 0.058533 |
| 9 | 6 | 0 | 3.092514 | 1.649853 | 0.177405 |
| 10 | 6 | 0 | 1.622573 | 3.622704 | 0.117659 |
| 11 | 6 | 0 | 3.153114 | 0.207203 | 0.193353 |
| 12 | 6 | 0 | 4.187504 | 2.525660 | 0.358547 |
| 13 | 6 | 0 | 2.733055 | 4.445064 | 0.301437 |
| 14 | 1 | 0 | 0.641580 | 4.069413 | 0.017016 |
| 15 | 6 | 0 | 4.122003 | -0.763728 | 0.103557 |
| 16 | 1 | 0 | 2.170839 | -0.242019 | 0.313971 |
| 17 | 6 | 0 | 4.014747 | 3.900830 | 0.426670 |
| 18 | 1 | 0 | 5.173574 | 2.094328 | 0.448123 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 426 | 19 | 1 | 0 | 2.590119 | 5.521125 | 0.344415 |
| 427 | 20 | 6 | 0 | 5.556703 | -0.581335 | -0.188413 |
| 428 | 21 | 6 | 0 | 3.598103 | -2.152588 | 0.259507 |
| 429 | 22 | 1 | 0 | 4.872639 | 4.548695 | 0.576200 |
| 430 | 23 | 7 | 0 | 6.308735 | -1.755004 | -0.269594 |
| 431 | 24 | 8 | 0 | 6.132879 | 0.485146 | -0.378965 |
| 432 | 25 | 7 | 0 | 4.529030 | -3.179201 | 0.144301 |
| 433 | 26 | 8 | 0 | 2.425972 | -2.434230 | 0.483476 |
| 434 | 27 | 6 | 0 | 5.881404 | -3.060932 | -0.116525 |
| 435 | 28 | 1 | 0 | 7.294455 | -1.633426 | -0.474686 |
| 436 | 29 | 1 | 0 | 4.176442 | -4.123109 | 0.257844 |
| 437 | 30 | 8 | 0 | 6.629595 | -4.020484 | -0.204808 |
| 438 | 31 | 1 | 0 | -0.733920 | 2.564142 | -0.965789 |
| 439 | 32 | 6 | 0 | -1.947741 | -0.404112 | -0.314976 |
| 440 | 33 | 1 | 0 | -1.957652 | -1.471378 | -0.385399 |
| 441 | 34 | 6 | 0 | -5.084320 | -0.993408 | -1.017296 |
| 442 | 35 | 6 | 0 | -6.459800 | -0.975328 | -0.380216 |
| 443 | 36 | 1 | 0 | -5.131727 | -0.647358 | -2.055800 |
| 444 | 37 | 6 | 0 | -6.684715 | -1.614070 | 0.847447 |
| 445 | 38 | 6 | 0 | -7.521135 | -0.313383 | -1.007139 |
| 446 | 39 | 6 | 0 | -7.948483 | -1.589233 | 1.436619 |
| 447 | 40 | 1 | 0 | -5.865363 | -2.130044 | 1.342283 |
| 448 | 41 | 6 | 0 | -8.789471 | -0.290316 | -0.420185 |
| 449 | 42 | 1 | 0 | -7.356888 | 0.184187 | -1.960014 |
| 450 | 43 | 6 | 0 | -9.005117 | -0.927030 | 0.803041 |
| 451 | 44 | 1 | 0 | -8.111192 | -2.089772 | 2.387293 |
| 452 | 45 | 1 | 0 | -9.605616 | 0.224907 | -0.919325 |
| 453 | 46 | 1 | 0 | -9.990346 | -0.910307 | 1.260886 |
| 454 | 47 | 1 | 0 | -4.676178 | -2.008096 | -1.020990 |

455 ----------

456



**B**

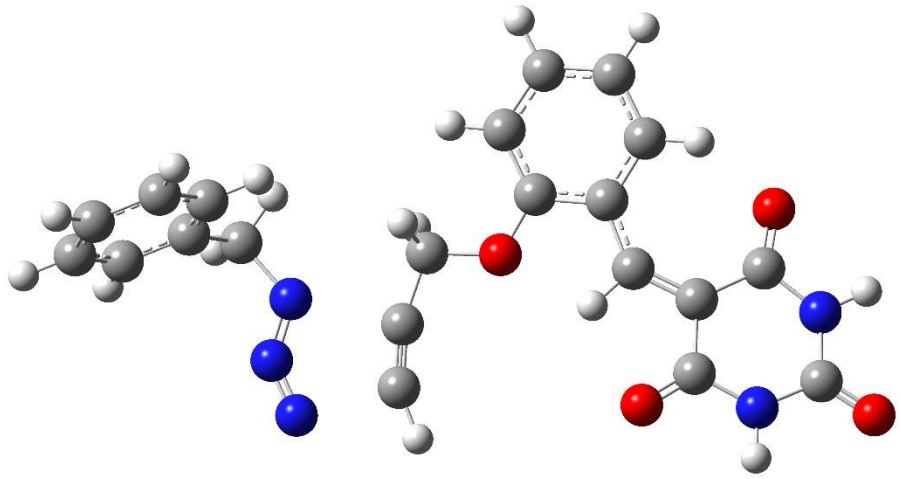
Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.979199 | 0.419689 | 0.317463 |
| 2 | 6 | 0 | -1.859264 | -0.278925 | 0.722211 |
| 3 | 6 | 0 | -0.897704 | -0.002710 | 1.834919 |
| 4 | 8 | 0 | 0.455778 | 0.199544 | 1.376364 |
| 5 | 1 | 0 | -1.227715 | 0.842815 | 2.444923 |
| 6 | 6 | 0 | 0.807994 | 1.330769 | 0.712349 |
| 7 | 6 | 0 | 2.106368 | 1.317633 | 0.109336 |
| 8 | 6 | 0 | 0.004804 | 2.473027 | 0.637977 |
| 9 | 6 | 0 | 2.819139 | 0.059636 | 0.128008 |
| 10 | 6 | 0 | 2.536860 | 2.486412 | -0.557543 |
| 11 | 6 | 0 | 0.468462 | 3.603224 | -0.033071 |
| 12 | 1 | 0 | -0.972876 | 2.495658 | 1.101147 |
| 13 | 6 | 0 | 4.121981 | -0.338057 | -0.036161 |
| 14 | 1 | 0 | 2.164860 | -0.788651 | 0.313374 |
| 15 | 6 | 0 | 1.729568 | 3.612256 | -0.637471 |
| 16 | 1 | 0 | 3.513264 | 2.484450 | -1.019183 |
| 17 | 1 | 0 | -0.165641 | 4.484003 | -0.081016 |
| 18 | 6 | 0 | 5.309194 | 0.535182 | -0.124658 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 482 | 19 | 6 | 0 | 4.318931 | -1.815832 | -0.016923 |
| 483 | 20 | 1 | 0 | 2.076364 | 4.493036 | -1.168502 |
| 484 | 21 | 7 | 0 | 6.535610 | -0.127066 | -0.207181 |
| 485 | 22 | 8 | 0 | 5.310491 | 1.761244 | -0.108796 |
| 486 | 23 | 7 | 0 | 5.632408 | -2.260925 | -0.120747 |
| 487 | 24 | 8 | 0 | 3.414124 | -2.637702 | 0.075559 |
| 488 | 25 | 6 | 0 | 6.776019 | -1.488975 | -0.213933 |
| 489 | 26 | 1 | 0 | 7.355930 | 0.466875 | -0.261007 |
| 490 | 27 | 1 | 0 | 5.770862 | -3.265437 | -0.117098 |
| 491 | 28 | 8 | 0 | 7.895968 | -1.965862 | -0.294511 |
| 492 | 29 | 1 | 0 | -0.809495 | -0.874758 | 2.485855 |
| 493 | 30 | 7 | 0 | -3.467149 | -0.292279 | -0.724010 |
| 494 | 31 | 7 | 0 | -2.697724 | -1.378675 | -0.960329 |
| 495 | 32 | 7 | 0 | -1.726593 | -1.373106 | -0.086018 |
| 496 | 33 | 1 | 0 | -3.449254 | 1.322198 | 0.677150 |
| 497 | 34 | 6 | 0 | -4.671083 | -0.048952 | -1.529028 |
| 498 | 35 | 6 | 0 | -5.954225 | -0.320119 | -0.768499 |
| 499 | 36 | 1 | 0 | -4.570830 | -0.707278 | -2.395489 |
| 500 | 37 | 6 | 0 | -6.250306 | -1.613572 | -0.315615 |
| 501 | 38 | 6 | 0 | -6.860388 | 0.715671 | -0.518266 |
| 502 | 39 | 6 | 0 | -7.433295 | -1.863717 | 0.378721 |
| 503 | 40 | 1 | 0 | -5.549754 | -2.423135 | -0.505402 |
| 504 | 41 | 6 | 0 | -8.048860 | 0.465151 | 0.173445 |
| 505 | 42 | 1 | 0 | -6.638699 | 1.721422 | -0.866878 |
| 506 | 43 | 6 | 0 | -8.336272 | -0.823985 | 0.624059 |
| 507 | 44 | 1 | 0 | -7.653392 | -2.869612 | 0.725447 |
| 508 | 45 | 1 | 0 | -8.745489 | 1.277615 | 0.360406 |
| 509 | 46 | 1 | 0 | -9.258917 | -1.020233 | 1.163182 |
| 510 | 47 | 1 | 0 | -4.638319 | 0.984743 | -1.881766 |

511 ----------

512



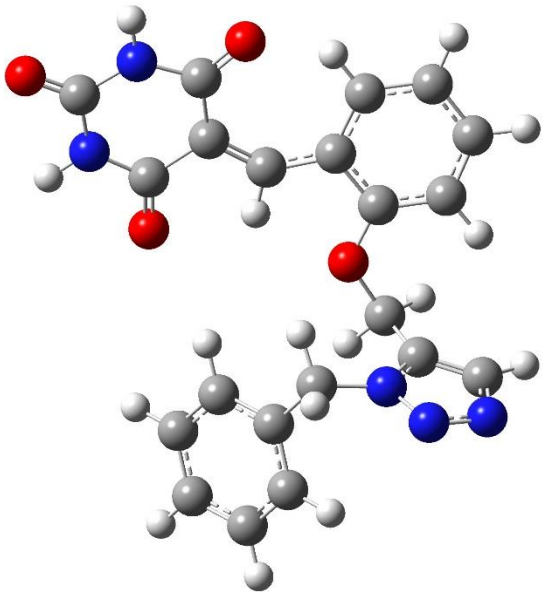
**C**

Input orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.559039 | -1.218181 | -0.690037 |
| 2 | 7 | 0 | -3.767715 | -0.928762 | -1.078410 |
| 3 | 7 | 0 | -4.026079 | -2.154836 | -1.069743 |
| 4 | 7 | 0 | -3.447758 | -3.171173 | -0.928999 |
| 5 | 6 | 0 | -1.209454 | 0.205303 | -0.682716 |
| 6 | 8 | 0 | 0.213421 | 0.299552 | -0.482619 |
| 7 | 1 | 0 | -1.733674 | 0.729658 | 0.124668 |
| 8 | 6 | 0 | 0.778556 | 1.527036 | -0.348389 |
| 9 | 6 | 0 | 2.179888 | 1.546960 | -0.048579 |
| 10 | 6 | 0 | 0.067744 | 2.720587 | -0.508312 |
| 11 | 6 | 0 | 2.808974 | 0.269211 | 0.198139 |
| 12 | 6 | 0 | 2.802819 | 2.808062 | 0.085087 |
| 13 | 6 | 0 | 0.725242 | 3.941744 | -0.363979 |
| 14 | 1 | 0 | -0.988228 | 2.711420 | -0.747389 |
| 15 | 6 | 0 | 4.092443 | -0.213339 | 0.268781 |
| 16 | 1 | 0 | 2.084953 | -0.521074 | 0.379571 |
| 17 | 6 | 0 | 2.089253 | 3.989559 | -0.062621 |
| 18 | 1 | 0 | 3.857852 | 2.834759 | 0.313885 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 538 | 19 | 1 | 0 | 0.161350 | 4.861510 | -0.490943 |
| 539 | 20 | 6 | 0 | 5.337101 | 0.505676 | -0.067270 |
| 540 | 21 | 6 | 0 | 4.179887 | -1.653434 | 0.649098 |
| 541 | 22 | 1 | 0 | 2.590671 | 4.944721 | 0.056725 |
| 542 | 23 | 7 | 0 | 6.509362 | -0.246549 | 0.026356 |
| 543 | 24 | 8 | 0 | 5.426335 | 1.673048 | -0.432809 |
| 544 | 25 | 7 | 0 | 5.456356 | -2.203806 | 0.684347 |
| 545 | 26 | 8 | 0 | 3.217464 | -2.358717 | 0.930444 |
| 546 | 27 | 6 | 0 | 6.651020 | -1.573718 | 0.388168 |
| 547 | 28 | 1 | 0 | 7.366684 | 0.241288 | -0.209433 |
| 548 | 29 | 1 | 0 | 5.520024 | -3.180251 | 0.950393 |
| 549 | 30 | 8 | 0 | 7.731900 | -2.136709 | 0.440685 |
| 550 | 31 | 1 | 0 | -1.479333 | 0.677031 | -1.634355 |
| 551 | 32 | 6 | 0 | -1.515738 | -2.451383 | -0.633577 |
| 552 | 33 | 6 | 0 | -4.830437 | 0.072337 | -1.305885 |
| 553 | 34 | 6 | 0 | -5.850848 | 0.140537 | -0.187084 |
| 554 | 35 | 1 | 0 | -5.318582 | -0.123803 | -2.267117 |
| 555 | 36 | 6 | 0 | -7.089273 | -0.499187 | -0.319750 |
| 556 | 37 | 6 | 0 | -5.561733 | 0.822379 | 1.002772 |
| 557 | 38 | 6 | 0 | -8.023180 | -0.461242 | 0.718550 |
| 558 | 39 | 1 | 0 | -7.325687 | -1.026434 | -1.241130 |
| 559 | 40 | 6 | 0 | -6.492162 | 0.860765 | 2.041952 |
| 560 | 41 | 1 | 0 | -4.604850 | 1.327195 | 1.114152 |
| 561 | 42 | 6 | 0 | -7.725699 | 0.217797 | 1.901989 |
| 562 | 43 | 1 | 0 | -8.982035 | -0.958725 | 0.600893 |
| 563 | 44 | 1 | 0 | -6.257266 | 1.395765 | 2.958131 |
| 564 | 45 | 1 | 0 | -8.451811 | 0.249958 | 2.709671 |
| 565 | 46 | 1 | 0 | -4.296908 | 1.021758 | -1.397708 |
| 566 | 47 | 1 | 0 | -1.057439 | -3.411108 | -0.518504 |

567 ----------



**D**

Input orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 4.092263 | 2.284715 | 0.131647 |
| 2 | 6 | 0 | 3.117946 | 1.332882 | -0.098419 |
| 3 | 6 | 0 | 2.211225 | 1.093983 | -1.264472 |
| 4 | 8 | 0 | 0.824449 | 1.010230 | -0.892762 |
| 5 | 1 | 0 | 2.366882 | 1.862596 | -2.025733 |
| 6 | 6 | 0 | 0.069830 | 2.128842 | -0.712165 |
| 7 | 6 | 0 | -1.324822 | 1.912070 | -0.449117 |
| 8 | 6 | 0 | 0.590031 | 3.423691 | -0.766682 |
| 9 | 6 | 0 | -1.772744 | 0.539319 | -0.452506 |
| 10 | 6 | 0 | -2.139280 | 3.053630 | -0.266746 |
| 11 | 6 | 0 | -0.254068 | 4.518288 | -0.584382 |
| 12 | 1 | 0 | 1.645316 | 3.590997 | -0.937287 |
| 13 | 6 | 0 | -2.908198 | -0.166209 | -0.131549 |
| 14 | 1 | 0 | -0.998695 | -0.136334 | -0.803789 |
| 15 | 6 | 0 | -1.618174 | 4.337607 | -0.339354 |
| 16 | 1 | 0 | -3.189760 | 2.898134 | -0.068776 |
| 17 | 1 | 0 | 0.165509 | 5.519146 | -0.630120 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 592 | 18 | 6 | 0 | -4.166660 | 0.347882 | 0.442606 |
| 593 | 19 | 6 | 0 | -2.782434 | -1.635905 | -0.365344 |
| 594 | 20 | 1 | 0 | -2.268296 | 5.195761 | -0.201398 |
| 595 | 21 | 7 | 0 | -5.147099 | -0.611407 | 0.702281 |
| 596 | 22 | 8 | 0 | -4.421849 | 1.516599 | 0.716542 |
| 597 | 23 | 7 | 0 | -3.889841 | -2.409621 | -0.042269 |
| 598 | 24 | 8 | 0 | -1.783536 | -2.188064 | -0.817256 |
| 599 | 25 | 6 | 0 | -5.090014 | -1.976484 | 0.492063 |
| 600 | 26 | 1 | 0 | -6.012054 | -0.260402 | 1.098862 |
| 601 | 27 | 1 | 0 | -3.806406 | -3.407317 | -0.203292 |
| 602 | 28 | 8 | 0 | -6.012765 | -2.729857 | 0.753674 |
| 603 | 29 | 1 | 0 | 2.415039 | 0.120972 | -1.717746 |
| 604 | 30 | 7 | 0 | 4.678744 | 2.038973 | 1.333333 |
| 605 | 31 | 7 | 0 | 4.115212 | 0.982379 | 1.866513 |
| 606 | 32 | 7 | 0 | 3.171509 | 0.540652 | 1.009571 |
| 607 | 33 | 1 | 0 | 4.394347 | 3.112386 | -0.494701 |
| 608 | 34 | 6 | 0 | 2.399593 | -0.664646 | 1.338658 |
| 609 | 35 | 6 | 0 | 2.788730 | -1.868582 | 0.500552 |
| 610 | 36 | 1 | 0 | 1.339721 | -0.434476 | 1.217526 |
| 611 | 37 | 6 | 0 | 4.124637 | -2.289282 | 0.437117 |
| 612 | 38 | 6 | 0 | 1.809968 | -2.588234 | -0.194816 |
| 613 | 39 | 6 | 0 | 4.475374 | -3.412500 | -0.311112 |
| 614 | 40 | 1 | 0 | 4.889538 | -1.734136 | 0.974157 |
| 615 | 41 | 6 | 0 | 2.162026 | -3.718018 | -0.939757 |
| 616 | 42 | 1 | 0 | 0.769910 | -2.273273 | -0.155478 |
| 617 | 43 | 6 | 0 | 3.493365 | -4.130916 | -1.000817 |
| 618 | 44 | 1 | 0 | 5.513686 | -3.729542 | -0.354596 |
| 619 | 45 | 1 | 0 | 1.394023 | -4.269382 | -1.475081 |
| 620 | 46 | 1 | 0 | 3.767239 | -5.006616 | -1.582794 |
| 621 | 47 | 1 | 0 | 2.592377 | -0.839419 | 2.400230 |

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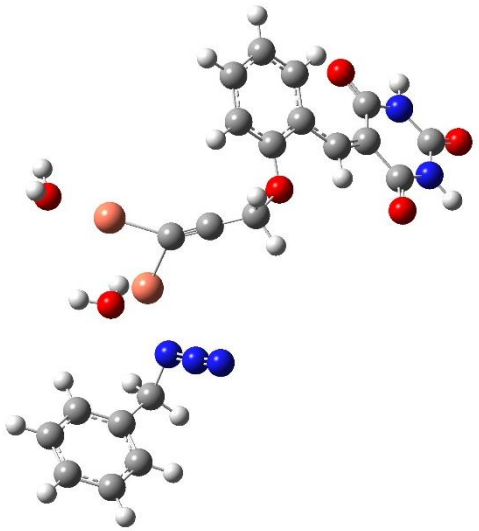
623



**E**

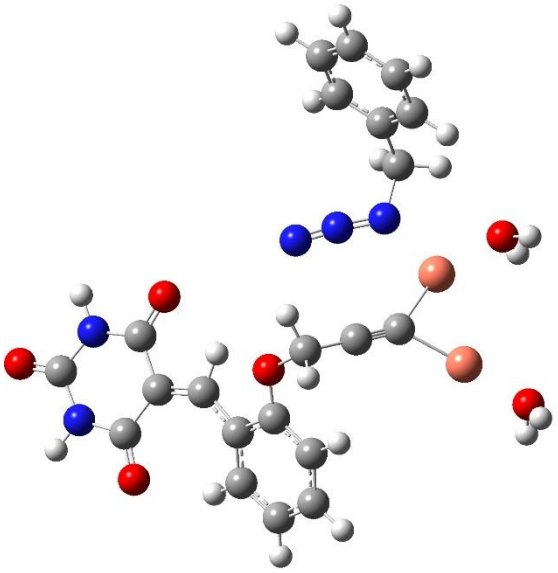
Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.291851 | 1.298692 | -0.401535 |
| 2 | 6 | 0 | 0.401186 | 0.947998 | -1.179051 |
| 3 | 7 | 0 | 3.497501 | -1.464053 | 0.036791 |
| 4 | 7 | 0 | 3.344964 | -1.783368 | -1.155502 |
| 5 | 7 | 0 | 3.140556 | -2.006065 | -2.251824 |
| 6 | 29 | 0 | 2.485515 | 0.236492 | 0.772913 |
| 7 | 29 | 0 | 2.181417 | 2.787674 | 0.400908 |
| 8 | 8 | 0 | 3.052631 | -0.031058 | 2.772937 |
| 9 | 1 | 0 | 3.644231 | 0.680501 | 3.073532 |
| 10 | 1 | 0 | 2.283045 | 0.014366 | 3.366508 |
| 11 | 8 | 0 | 3.042931 | 4.361779 | 1.176632 |
| 12 | 1 | 0 | 2.452458 | 4.912366 | 1.720802 |
| 13 | 1 | 0 | 3.436820 | 4.964525 | 0.521239 |
| 14 | 6 | 0 | -0.648266 | 0.509156 | -2.094769 |
| 15 | 8 | 0 | -1.932794 | 0.352604 | -1.461860 |
| 16 | 1 | 0 | -0.733146 | 1.187184 | -2.952877 |
| 17 | 6 | 0 | -2.706672 | 1.444604 | -1.218465 |
| 18 | 6 | 0 | -4.034952 | 1.181772 | -0.749198 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 649 | 19 | 6 | 0 | -2.260196 | 2.758547 | -1.390188 |
| 650 | 20 | 6 | 0 | -4.441331 | -0.204663 | -0.694011 |
| 651 | 21 | 6 | 0 | -4.867702 | 2.292380 | -0.482076 |
| 652 | 22 | 6 | 0 | -3.119547 | 3.823044 | -1.118723 |
| 653 | 23 | 1 | 0 | -1.248603 | 2.962395 | -1.717938 |
| 654 | 24 | 6 | 0 | -5.460780 | -0.926051 | -0.123168 |
| 655 | 25 | 1 | 0 | -3.772300 | -0.853786 | -1.253024 |
| 656 | 26 | 6 | 0 | -4.424074 | 3.594183 | -0.670564 |
| 657 | 27 | 1 | 0 | -5.871166 | 2.104886 | -0.129971 |
| 658 | 28 | 1 | 0 | -2.759654 | 4.838649 | -1.257324 |
| 659 | 29 | 6 | 0 | -6.481871 | -0.437348 | 0.824399 |
| 660 | 30 | 6 | 0 | -5.442510 | -2.377997 | -0.467908 |
| 661 | 31 | 1 | 0 | -5.088215 | 4.428489 | -0.468514 |
| 662 | 32 | 7 | 0 | -7.369034 | -1.403355 | 1.302684 |
| 663 | 33 | 8 | 0 | -6.603689 | 0.712943 | 1.233284 |
| 664 | 34 | 7 | 0 | -6.429302 | -3.162033 | 0.119446 |
| 665 | 35 | 8 | 0 | -4.632869 | -2.903651 | -1.224041 |
| 666 | 36 | 6 | 0 | -7.410596 | -2.753345 | 1.004310 |
| 667 | 37 | 1 | 0 | -8.068971 | -1.073942 | 1.958563 |
| 668 | 38 | 1 | 0 | -6.425200 | -4.147508 | -0.119418 |
| 669 | 39 | 8 | 0 | -8.237572 | -3.514148 | 1.479469 |
| 670 | 40 | 1 | 0 | -0.418966 | -0.487119 | -2.483001 |
| 671 | 41 | 6 | 0 | 4.497487 | -2.292731 | 0.805189 |
| 672 | 42 | 6 | 0 | 5.912717 | -2.103235 | 0.314400 |
| 673 | 43 | 1 | 0 | 4.191327 | -3.342112 | 0.749362 |
| 674 | 44 | 6 | 0 | 6.638829 | -0.956252 | 0.669550 |
| 675 | 45 | 6 | 0 | 6.511503 | -3.059809 | -0.515802 |
| 676 | 46 | 6 | 0 | 7.938240 | -0.768471 | 0.198466 |
| 677 | 47 | 1 | 0 | 6.185289 | -0.212195 | 1.320080 |
| 678 | 48 | 6 | 0 | 7.813980 | -2.873603 | -0.986761 |
| 679 | 49 | 1 | 0 | 5.961749 | -3.957704 | -0.787510 |
| 680 | 50 | 6 | 0 | 8.528061 | -1.727433 | -0.631776 |
| 681 | 51 | 1 | 0 | 8.493031 | 0.121260 | 0.482943 |
| 682 | 52 | 1 | 0 | 8.269231 | -3.624765 | -1.626035 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 683 | 53 | 1 | 0 | 9.541493 | -1.582597 | -0.995530 |
| 684 | 54 | 1 | 0 | 4.372483 | -1.945981 | 1.830847 |

685 ---



686

687 **F**

688 Standard orientation:

689 ---

| 690 Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|---|---|
| 691 Number | Number | Type | X | Y | Z |

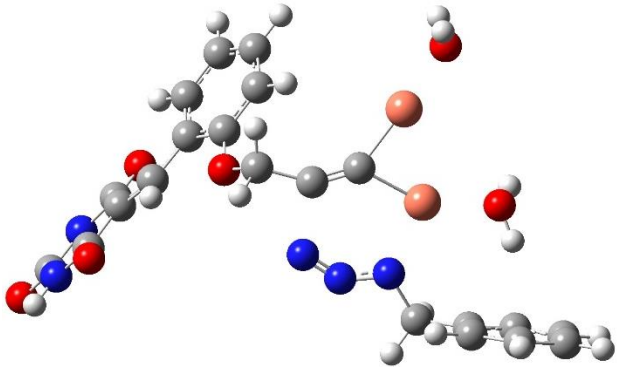
692 ---

| | | | | | |
|---|---|---|---|---|---|
| 693 1 | 6 | 0 | 1.828151 | -1.716749 | 0.575559 |
| 694 2 | 6 | 0 | 0.915357 | -1.448621 | 1.360346 |
| 695 3 | 7 | 0 | 2.697589 | 1.194375 | -0.936899 |
| 696 4 | 7 | 0 | 1.628680 | 1.613681 | -0.461657 |
| 697 5 | 7 | 0 | 0.624293 | 1.878112 | 0.002625 |
| 698 6 | 29 | 0 | 3.166204 | -0.869967 | -0.594047 |
| 699 7 | 29 | 0 | 2.616042 | -3.326139 | -0.121204 |
| 700 8 | 8 | 0 | 4.905342 | -0.830931 | -1.704881 |
| 701 9 | 1 | 0 | 5.624530 | -1.331070 | -1.281343 |
| 702 10 | 1 | 0 | 4.787837 | -1.245807 | -2.577322 |
| 703 11 | 8 | 0 | 3.325621 | -5.032176 | -0.775267 |
| 704 12 | 1 | 0 | 2.717074 | -5.519009 | -1.358973 |
| 705 13 | 1 | 0 | 3.576399 | -5.658376 | -0.073363 |
| 706 14 | 6 | 0 | -0.158866 | -1.112591 | 2.292053 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 707 | 15 | 8 | 0 | -1.416379 | -0.837567 | 1.646446 |
| 708 | 16 | 1 | 0 | -0.289316 | -1.897973 | 3.045778 |
| 709 | 17 | 6 | 0 | -2.127104 | -1.850155 | 1.080322 |
| 710 | 18 | 6 | 0 | -3.317616 | -1.463788 | 0.384124 |
| 711 | 19 | 6 | 0 | -1.767335 | -3.197861 | 1.179380 |
| 712 | 20 | 6 | 0 | -3.551617 | -0.044465 | 0.233721 |
| 713 | 21 | 6 | 0 | -4.104695 | -2.487347 | -0.190340 |
| 714 | 22 | 6 | 0 | -2.573967 | -4.174022 | 0.594614 |
| 715 | 23 | 1 | 0 | -0.867164 | -3.497031 | 1.701127 |
| 716 | 24 | 6 | 0 | -4.616797 | 0.758716 | -0.089320 |
| 717 | 25 | 1 | 0 | -2.657843 | 0.546089 | 0.417694 |
| 718 | 26 | 6 | 0 | -3.739186 | -3.823157 | -0.094176 |
| 719 | 27 | 1 | 0 | -5.004061 | -2.206220 | -0.717796 |
| 720 | 28 | 1 | 0 | -2.284324 | -5.217451 | 0.681863 |
| 721 | 29 | 6 | 0 | -6.026671 | 0.348758 | -0.246295 |
| 722 | 30 | 6 | 0 | -4.277404 | 2.208112 | -0.190700 |
| 723 | 31 | 1 | 0 | -4.355102 | -4.589100 | -0.554523 |
| 724 | 32 | 7 | 0 | -6.929478 | 1.385541 | -0.489371 |
| 725 | 33 | 8 | 0 | -6.464783 | -0.793784 | -0.161762 |
| 726 | 34 | 7 | 0 | -5.336520 | 3.070296 | -0.451658 |
| 727 | 35 | 8 | 0 | -3.148133 | 2.669339 | -0.065776 |
| 728 | 36 | 6 | 0 | -6.670552 | 2.739291 | -0.606057 |
| 729 | 37 | 1 | 0 | -7.900742 | 1.110949 | -0.588620 |
| 730 | 38 | 1 | 0 | -5.108967 | 4.055515 | -0.527588 |
| 731 | 39 | 8 | 0 | -7.540318 | 3.566078 | -0.825982 |
| 732 | 40 | 1 | 0 | 0.073924 | -0.185573 | 2.822860 |
| 733 | 41 | 6 | 0 | 3.631302 | 2.245321 | -1.478710 |
| 734 | 42 | 6 | 0 | 4.143647 | 3.179086 | -0.408255 |
| 735 | 43 | 1 | 0 | 3.113514 | 2.791949 | -2.273287 |
| 736 | 44 | 6 | 0 | 5.177041 | 2.773135 | 0.449681 |
| 737 | 45 | 6 | 0 | 3.580227 | 4.451307 | -0.244503 |
| 738 | 46 | 6 | 0 | 5.634718 | 3.623799 | 1.456129 |
| 739 | 47 | 1 | 0 | 5.625076 | 1.790215 | 0.323364 |
| 740 | 48 | 6 | 0 | 4.039078 | 5.304829 | 0.762421 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 741 | 49 | 1 | 0 | 2.786710 | 4.779089 | -0.911841 |
| 742 | 50 | 6 | 0 | 5.065278 | 4.891630 | 1.614611 |
| 743 | 51 | 1 | 0 | 6.438390 | 3.301566 | 2.112376 |
| 744 | 52 | 1 | 0 | 3.597549 | 6.290782 | 0.877113 |
| 745 | 53 | 1 | 0 | 5.424262 | 5.555179 | 2.396409 |
| 746 | 54 | 1 | 0 | 4.436414 | 1.660285 | -1.922768 |

747 ---



748

749 **G**

750 Standard orientation:

751 ---

| 752 Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|---|---|
| 753 Number | Number | Type | X | Y | Z |

754 ---

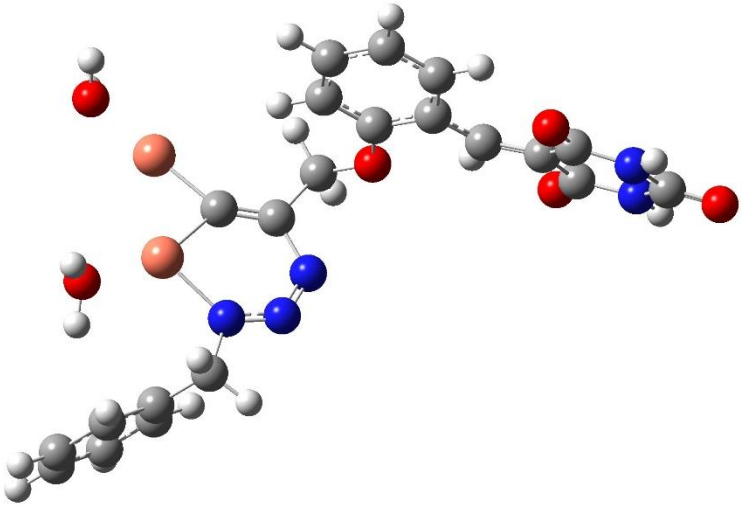
| | | | | | |
|---|---|---|---|---|---|
| 755 1 | 6 | 0 | 1.718796 | 1.201375 | 0.758062 |
| 756 2 | 6 | 0 | 0.686396 | 0.834255 | 1.386924 |
| 757 3 | 7 | 0 | 2.340869 | -1.579531 | 0.099843 |
| 758 4 | 7 | 0 | 1.288639 | -1.701351 | 0.797052 |
| 759 5 | 7 | 0 | 0.494777 | -1.071783 | 1.404672 |
| 760 6 | 29 | 0 | 3.072206 | 0.290087 | -0.255132 |
| 761 7 | 29 | 0 | 2.731811 | 2.770318 | 0.317142 |
| 762 8 | 8 | 0 | 4.730495 | 0.199345 | -1.398056 |
| 763 9 | 1 | 0 | 5.076248 | -0.709763 | -1.506762 |
| 764 10 | 1 | 0 | 4.604112 | 0.546579 | -2.298239 |
| 765 11 | 8 | 0 | 3.683438 | 4.439115 | -0.050265 |
| 766 12 | 1 | 0 | 3.210958 | 5.062926 | -0.629526 |
| 767 13 | 1 | 0 | 3.935804 | 4.947733 | 0.740673 |
| 768 14 | 6 | 0 | -0.524301 | 1.214290 | 2.164729 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 769 | 15 | 8 | 0 | -1.741970 | 0.935900 | 1.462590 |
| 770 | 16 | 1 | 0 | -0.593646 | 0.609577 | 3.070083 |
| 771 | 17 | 6 | 0 | -2.184533 | 1.768778 | 0.482169 |
| 772 | 18 | 6 | 0 | -3.444338 | 1.423563 | -0.106709 |
| 773 | 19 | 6 | 0 | -1.481333 | 2.895811 | 0.045814 |
| 774 | 20 | 6 | 0 | -4.149145 | 0.302361 | 0.474861 |
| 775 | 21 | 6 | 0 | -3.945482 | 2.264749 | -1.125804 |
| 776 | 22 | 6 | 0 | -2.017600 | 3.699572 | -0.960241 |
| 777 | 23 | 1 | 0 | -0.519071 | 3.149655 | 0.471170 |
| 778 | 24 | 6 | 0 | -5.192131 | -0.514053 | 0.114191 |
| 779 | 25 | 1 | 0 | -3.763032 | 0.031594 | 1.454168 |
| 780 | 26 | 6 | 0 | -3.249779 | 3.391009 | -1.544153 |
| 781 | 27 | 1 | 0 | -4.895799 | 2.014957 | -1.573653 |
| 782 | 28 | 1 | 0 | -1.461094 | 4.573015 | -1.288494 |
| 783 | 29 | 6 | 0 | -5.872815 | -0.567420 | -1.194918 |
| 784 | 30 | 6 | 0 | -5.586684 | -1.496130 | 1.166204 |
| 785 | 31 | 1 | 0 | -3.662567 | 4.026595 | -2.321065 |
| 786 | 32 | 7 | 0 | -6.858195 | -1.548380 | -1.319400 |
| 787 | 33 | 8 | 0 | -5.637991 | 0.144700 | -2.165747 |
| 788 | 34 | 7 | 0 | -6.604869 | -2.381262 | 0.829835 |
| 789 | 35 | 8 | 0 | -5.082380 | -1.560807 | 2.281929 |
| 790 | 36 | 6 | 0 | -7.276353 | -2.469522 | -0.376085 |
| 791 | 37 | 1 | 0 | -7.324115 | -1.594781 | -2.219049 |
| 792 | 38 | 1 | 0 | -6.881665 | -3.044710 | 1.545012 |
| 793 | 39 | 8 | 0 | -8.157347 | -3.286128 | -0.589386 |
| 794 | 40 | 1 | 0 | -0.473911 | 2.269900 | 2.447464 |
| 795 | 41 | 6 | 0 | 2.885960 | -2.813709 | -0.521666 |
| 796 | 42 | 6 | 0 | 4.394366 | -2.866220 | -0.399112 |
| 797 | 43 | 1 | 0 | 2.592169 | -2.833778 | -1.576700 |
| 798 | 44 | 6 | 0 | 5.195000 | -2.985097 | -1.545556 |
| 799 | 45 | 6 | 0 | 5.013479 | -2.804649 | 0.858645 |
| 800 | 46 | 6 | 0 | 6.590436 | -3.040805 | -1.437047 |
| 801 | 47 | 1 | 0 | 4.725752 | -3.048627 | -2.524898 |
| 802 | 48 | 6 | 0 | 6.403392 | -2.860663 | 0.966510 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 803 | 49 | 1 | 0 | 4.403635 | -2.712448 | 1.753490 |
| 804 | 50 | 6 | 0 | 7.195791 | -2.976812 | -0.180640 |
| 805 | 51 | 1 | 0 | 7.196753 | -3.134107 | -2.333301 |
| 806 | 52 | 1 | 0 | 6.869606 | -2.814367 | 1.946604 |
| 807 | 53 | 1 | 0 | 8.277595 | -3.018457 | -0.093918 |
| 808 | 54 | 1 | 0 | 2.428539 | -3.678203 | -0.030938 |

809 ---

810



811

812 **H**

813 Standard orientation:

814 ---

| 815 Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|---|---|
| 816 Number | Number | Type | X | Y | Z |

817 ---

| | | | | | | |
|---|---|---|---|---|---|---|
| 818 | 1 | 6 | 0 | -2.929099 | -0.379280 | 0.196293 |
| 819 | 2 | 6 | 0 | -1.730852 | 0.151193 | 0.424685 |
| 820 | 3 | 7 | 0 | -3.116810 | 1.408074 | -1.551761 |
| 821 | 4 | 7 | 0 | -2.009687 | 1.804129 | -1.249211 |
| 822 | 5 | 7 | 0 | -1.250867 | 1.302847 | -0.278378 |
| 823 | 6 | 29 | 0 | -4.358228 | 0.083493 | -0.927552 |
| 824 | 7 | 29 | 0 | -3.973369 | -1.799603 | 0.917307 |
| 825 | 8 | 8 | 0 | -6.199297 | -0.004958 | -1.730719 |
| 826 | 9 | 1 | 0 | -6.741545 | 0.786336 | -1.566677 |
| 827 | 10 | 1 | 0 | -6.209188 | -0.134762 | -2.695239 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 828 | 11 | 8 | 0 | -5.062976 | -3.252720 | 1.647843 |
| 829 | 12 | 1 | 0 | -4.718899 | -4.145610 | 1.467636 |
| 830 | 13 | 1 | 0 | -5.199325 | -3.209138 | 2.610977 |
| 831 | 14 | 6 | 0 | -0.791866 | -0.413174 | 1.485188 |
| 832 | 15 | 8 | 0 | 0.512743 | -0.732902 | 0.985349 |
| 833 | 16 | 1 | 0 | -0.607892 | 0.329872 | 2.265548 |
| 834 | 17 | 6 | 0 | 0.771119 | -1.924888 | 0.375399 |
| 835 | 18 | 6 | 0 | 2.144337 | -2.173407 | 0.061649 |
| 836 | 19 | 6 | 0 | -0.215144 | -2.857462 | 0.046108 |
| 837 | 20 | 6 | 0 | 3.111165 | -1.204812 | 0.533443 |
| 838 | 21 | 6 | 0 | 2.462510 | -3.394424 | -0.573021 |
| 839 | 22 | 6 | 0 | 0.145096 | -4.052928 | -0.576619 |
| 840 | 23 | 1 | 0 | -1.258213 | -2.656952 | 0.253495 |
| 841 | 24 | 6 | 0 | 4.404904 | -0.873566 | 0.223330 |
| 842 | 25 | 1 | 0 | 2.725143 | -0.581678 | 1.336250 |
| 843 | 26 | 6 | 0 | 1.481406 | -4.327708 | -0.881183 |
| 844 | 27 | 1 | 0 | 3.496949 | -3.596537 | -0.808309 |
| 845 | 28 | 1 | 0 | -0.631335 | -4.769888 | -0.828294 |
| 846 | 29 | 6 | 0 | 5.199185 | -1.374409 | -0.917043 |
| 847 | 30 | 6 | 0 | 4.993403 | 0.180369 | 1.100387 |
| 848 | 31 | 1 | 0 | 1.753617 | -5.264195 | -1.357389 |
| 849 | 32 | 7 | 0 | 6.466930 | -0.807795 | -1.058041 |
| 850 | 33 | 8 | 0 | 4.838002 | -2.207348 | -1.741172 |
| 851 | 34 | 7 | 0 | 6.283212 | 0.591062 | 0.784005 |
| 852 | 35 | 8 | 0 | 4.421186 | 0.684913 | 2.060036 |
| 853 | 36 | 6 | 0 | 7.069747 | 0.153762 | -0.266765 |
| 854 | 37 | 1 | 0 | 7.015257 | -1.140774 | -1.843637 |
| 855 | 38 | 1 | 0 | 6.691145 | 1.302049 | 1.381001 |
| 856 | 39 | 8 | 0 | 8.193899 | 0.578080 | -0.477471 |
| 857 | 40 | 1 | 0 | -1.249252 | -1.284123 | 1.954459 |
| 858 | 41 | 6 | 0 | 0.046100 | 2.001412 | -0.082427 |
| 859 | 42 | 6 | 0 | -0.115252 | 3.500056 | 0.064857 |
| 860 | 43 | 1 | 0 | 0.698184 | 1.762588 | -0.927538 |
| 861 | 44 | 6 | 0 | -0.828063 | 4.043723 | 1.143716 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 45 | 6 | 0 | 0.476309 | 4.363168 | -0.864100 |
| 46 | 6 | 0 | -0.950810 | 5.426012 | 1.284354 |
| 47 | 1 | 0 | -1.289962 | 3.384201 | 1.874381 |
| 48 | 6 | 0 | 0.360356 | 5.748724 | -0.720595 |
| 49 | 1 | 0 | 1.030754 | 3.950551 | -1.703323 |
| 50 | 6 | 0 | -0.355091 | 6.282719 | 0.352475 |
| 51 | 1 | 0 | -1.505754 | 5.835410 | 2.123944 |
| 52 | 1 | 0 | 0.825671 | 6.406943 | -1.449023 |
| 53 | 1 | 0 | -0.448718 | 7.359280 | 0.464643 |
| 54 | 1 | 0 | 0.505024 | 1.574412 | 0.806187 |

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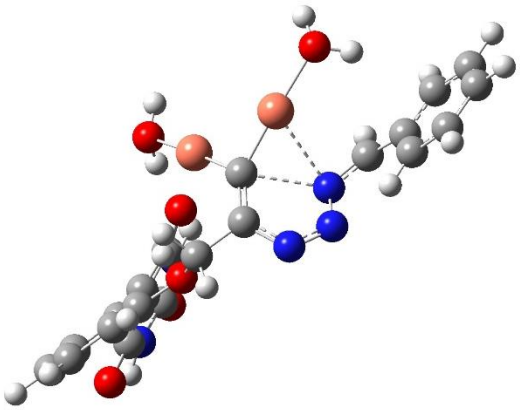

**I**

Standard orientation:

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 29 | 0 | -3.205964 | 0.299240 | 1.328498 |
| 2 | 6 | 0 | -1.497175 | 0.774336 | 0.652759 |
| 3 | 6 | 0 | -1.154679 | 1.659959 | -0.344371 |
| 4 | 29 | 0 | -0.270564 | -0.073280 | 1.811235 |
| 5 | 7 | 0 | -1.770804 | 1.718327 | -1.573926 |
| 6 | 7 | 0 | -2.570559 | -0.329638 | -1.086700 |
| 7 | 7 | 0 | -2.555500 | 0.738526 | -1.888536 |
| 8 | 6 | 0 | 0.015788 | 2.613224 | -0.242437 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 889 | 9 | 8 | 0 | 1.246358 | 1.869150 | -0.453884 |
| 890 | 10 | 1 | 0 | -0.081813 | 3.380721 | -1.017091 |
| 891 | 11 | 6 | 0 | 2.429792 | 2.507497 | -0.317541 |
| 892 | 12 | 6 | 0 | 3.596404 | 1.677296 | -0.236952 |
| 893 | 13 | 6 | 0 | 2.553292 | 3.902662 | -0.284210 |
| 894 | 14 | 6 | 0 | 3.381999 | 0.260122 | -0.084217 |
| 895 | 15 | 6 | 0 | 4.858081 | 2.312573 | -0.147850 |
| 896 | 16 | 6 | 0 | 3.815378 | 4.484020 | -0.185133 |
| 897 | 17 | 1 | 0 | 1.676528 | 4.534467 | -0.348946 |
| 898 | 18 | 6 | 0 | 4.153111 | -0.868303 | -0.253660 |
| 899 | 19 | 1 | 0 | 2.378427 | 0.027211 | 0.262970 |
| 900 | 20 | 6 | 0 | 4.969783 | 3.693997 | -0.115315 |
| 901 | 21 | 1 | 0 | 5.742204 | 1.695677 | -0.083071 |
| 902 | 22 | 1 | 0 | 3.896255 | 5.567250 | -0.166177 |
| 903 | 23 | 6 | 0 | 5.450451 | -0.934182 | -0.957119 |
| 904 | 24 | 6 | 0 | 3.536763 | -2.130510 | 0.210703 |
| 905 | 25 | 1 | 0 | 5.946698 | 4.158587 | -0.028244 |
| 906 | 26 | 7 | 0 | 5.971929 | -2.218419 | -1.136276 |
| 907 | 27 | 8 | 0 | 6.074585 | 0.016186 | -1.413729 |
| 908 | 28 | 7 | 0 | 4.217666 | -3.297614 | -0.071111 |
| 909 | 29 | 8 | 0 | 2.467249 | -2.215027 | 0.828975 |
| 910 | 30 | 6 | 0 | 5.430769 | -3.422873 | -0.734821 |
| 911 | 31 | 1 | 0 | 6.853729 | -2.271678 | -1.634827 |
| 912 | 32 | 1 | 0 | 3.799486 | -4.160497 | 0.260191 |
| 913 | 33 | 8 | 0 | 5.962765 | -4.500649 | -0.935664 |
| 914 | 34 | 1 | 0 | 0.075258 | 3.089759 | 0.740890 |
| 915 | 35 | 8 | 0 | -4.985737 | -0.303788 | 1.966964 |
| 916 | 36 | 1 | 0 | -4.948284 | -0.903637 | 2.733017 |
| 917 | 37 | 8 | 0 | 1.088670 | -1.050093 | 2.843207 |
| 918 | 38 | 1 | 0 | 0.726183 | -1.760706 | 3.400000 |
| 919 | 39 | 1 | 0 | 1.677684 | -1.490777 | 2.177029 |
| 920 | 40 | 1 | 0 | -5.434840 | -0.806570 | 1.256469 |
| 921 | 41 | 6 | 0 | -3.542132 | -1.229578 | -1.092307 |
| 922 | 42 | 6 | 0 | -4.963615 | -1.005573 | -1.264562 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 43 | 1 | 0 | -3.248497 | -2.199151 | -0.693161 |
| 44 | 6 | 0 | -5.858186 | -2.046367 | -0.896766 |
| 45 | 6 | 0 | -5.531089 | 0.215400 | -1.709245 |
| 46 | 6 | 0 | -7.238816 | -1.881515 | -0.988824 |
| 47 | 1 | 0 | -5.449835 | -2.993247 | -0.549257 |
| 48 | 6 | 0 | -6.914236 | 0.369271 | -1.796458 |
| 49 | 1 | 0 | -4.874384 | 1.025782 | -2.002987 |
| 50 | 6 | 0 | -7.778876 | -0.671785 | -1.442143 |
| 51 | 1 | 0 | -7.895876 | -2.699308 | -0.704019 |
| 52 | 1 | 0 | -7.321747 | 1.314072 | -2.148056 |
| 53 | 1 | 0 | -8.854939 | -0.543331 | -1.515275 |

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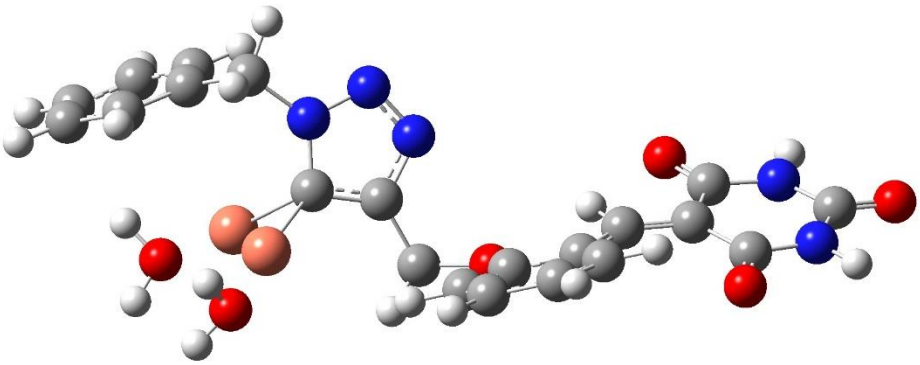

**J**

Standard orientation:

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.012312 | 0.030385 | -0.163792 |
| 2 | 6 | 0 | -0.693736 | -0.357935 | 0.132066 |
| 3 | 6 | 0 | 0.133159 | -0.040044 | 1.348285 |
| 4 | 8 | 0 | 1.523066 | 0.146575 | 1.047716 |
| 5 | 1 | 0 | -0.273949 | 0.820114 | 1.888819 |
| 6 | 6 | 0 | 1.950352 | 1.240766 | 0.363623 |
| 7 | 6 | 0 | 3.296700 | 1.186904 | -0.115768 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 950 | 8 | 6 | 0 | 1.171471 | 2.384168 | 0.163184 |
| 951 | 9 | 6 | 0 | 3.985731 | -0.077863 | 0.023029 |
| 952 | 10 | 6 | 0 | 3.802539 | 2.319651 | -0.792062 |
| 953 | 11 | 6 | 0 | 1.708135 | 3.478496 | -0.514249 |
| 954 | 12 | 1 | 0 | 0.156522 | 2.434213 | 0.536191 |
| 955 | 13 | 6 | 0 | 5.291642 | -0.496560 | 0.002479 |
| 956 | 14 | 1 | 0 | 3.303149 | -0.910082 | 0.176521 |
| 957 | 15 | 6 | 0 | 3.020103 | 3.447820 | -0.998257 |
| 958 | 16 | 1 | 0 | 4.817347 | 2.287807 | -1.160414 |
| 959 | 17 | 1 | 0 | 1.092796 | 4.361936 | -0.660657 |
| 960 | 18 | 6 | 0 | 6.495174 | 0.359155 | -0.008518 |
| 961 | 19 | 6 | 0 | 5.462672 | -1.974635 | 0.102781 |
| 962 | 20 | 1 | 0 | 3.426068 | 4.299768 | -1.534203 |
| 963 | 21 | 7 | 0 | 7.713220 | -0.319477 | 0.062030 |
| 964 | 22 | 8 | 0 | 6.512829 | 1.584616 | -0.050465 |
| 965 | 23 | 7 | 0 | 6.772786 | -2.438361 | 0.149846 |
| 966 | 24 | 8 | 0 | 4.539791 | -2.780916 | 0.139150 |
| 967 | 25 | 6 | 0 | 7.931801 | -1.683436 | 0.137811 |
| 968 | 26 | 1 | 0 | 8.544187 | 0.262012 | 0.063431 |
| 969 | 27 | 1 | 0 | 6.895047 | -3.443228 | 0.209078 |
| 970 | 28 | 8 | 0 | 9.046882 | -2.175791 | 0.189982 |
| 971 | 29 | 1 | 0 | 0.136523 | -0.889059 | 2.036868 |
| 972 | 30 | 7 | 0 | -2.216471 | -0.626775 | -1.367994 |
| 973 | 31 | 7 | 0 | -1.145907 | -1.323997 | -1.755673 |
| 974 | 32 | 7 | 0 | -0.210839 | -1.167920 | -0.845360 |
| 975 | 33 | 29 | 0 | -3.481578 | -0.289786 | 1.149093 |
| 976 | 34 | 8 | 0 | -4.874875 | -0.881941 | 2.408901 |
| 977 | 35 | 1 | 0 | -5.257030 | -0.165027 | 2.945458 |
| 978 | 36 | 1 | 0 | -5.624998 | -1.282455 | 1.925210 |
| 979 | 37 | 29 | 0 | -2.703085 | 1.860873 | 0.105910 |
| 980 | 38 | 8 | 0 | -3.197321 | 3.751967 | 0.259603 |
| 981 | 39 | 1 | 0 | -3.645310 | 4.114791 | -0.525156 |
| 982 | 40 | 1 | 0 | -3.779422 | 3.953247 | 1.013708 |
| 983 | 41 | 6 | 0 | -3.435643 | -0.665423 | -2.190798 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 984 | 42 | 6 | 0 | -4.628323 | -1.211412 | -1.428744 |
| 985 | 43 | 1 | 0 | -3.184810 | -1.296243 | -3.046835 |
| 986 | 44 | 6 | 0 | -4.613169 | -2.526259 | -0.932792 |
| 987 | 45 | 6 | 0 | -5.760159 | -0.412847 | -1.214461 |
| 988 | 46 | 6 | 0 | -5.707228 | -3.026905 | -0.225530 |
| 989 | 47 | 1 | 0 | -3.744115 | -3.156548 | -1.103206 |
| 990 | 48 | 6 | 0 | -6.859315 | -0.914728 | -0.509599 |
| 991 | 49 | 1 | 0 | -5.781280 | 0.603792 | -1.597823 |
| 992 | 50 | 6 | 0 | -6.834199 | -2.221121 | -0.010233 |
| 993 | 51 | 1 | 0 | -5.686641 | -4.045454 | 0.150666 |
| 994 | 52 | 1 | 0 | -7.731456 | -0.287212 | -0.351769 |
| 995 | 53 | 1 | 0 | -7.691002 | -2.616097 | 0.528314 |
| 996 | 54 | 1 | 0 | -3.641260 | 0.342748 | -2.559063 |
| 997 | ---------- | | | | | |
| 998 | | | | | | |