**Supporting information**

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

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Contents:

experimental and spectral data

Spectra of products:

Cartesian coordinates for all optimized geometries

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 1H, 100.6 MHz for 13C) with CDCl3 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; 1H 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 (NH4)2HPO4 (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. 1H 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. ; 13C 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; 1H 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. ; 13C 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; 1H 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. ; 13C 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; 1H 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. 13C 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 NH4Cl (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 MgSO4. 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 CuSO4 (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 NH4Cl (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 Na2SO4 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, 1159.1H 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, OCH2), 5.27 (s, 2H, CH2) ppm. 13C 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 C21H17N5O4 (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. 1H 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, OCH2), 5.28 (s, 2H, CH2) ppm. 13C 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 C21H16BrN5O4 (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. 1H 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, OCH2), 5.28 (s, 2H, CH2), 3.23 (s, 3H, CH3), 3.21 (s, 3H, CH3) ppm. 13C 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 C23H21N5O4 (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. 1H 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, OCH2), 5.29 (s, 2H, CH2), 2.88 (s, 3H, CH3), 2.72(s, 3H, CH3) ppm. 13C 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 C23H20FN5O4 (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. 1H 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, OCH2), 5.21 (s, 2H, CH2) ppm. 13C 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 C21H17N5O3S (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. 1H 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, OCH2), 5.22 (s, 2H, CH2) ppm. 13C 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 C21H16FN5O3S (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. 1H 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, OCH2), 5.20 (s, 2H, CH2) ppm. 13C 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 C21H16BrN5O3S (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. 1H 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, OCH2), 5.22 (s, 2H, CH2) ppm. 13C 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 C21H17N5O4 (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, OCH2), 5.32 (s, 2H, CH2) ppm. 13C 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 C21H16ClN5O4 (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, OCH2), 5.29 (s, 2H, CH2) ppm. 13C 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 C21H16FN5O4 (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, OCH2), 5.33 (s, 2H, CH2) ppm. 13C 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 C21H16BrN5O4 (482.3): C, 52.30; H, 3.34; N, 14.52; Found: C, 52.24; H, 3.41; N, 14.58.

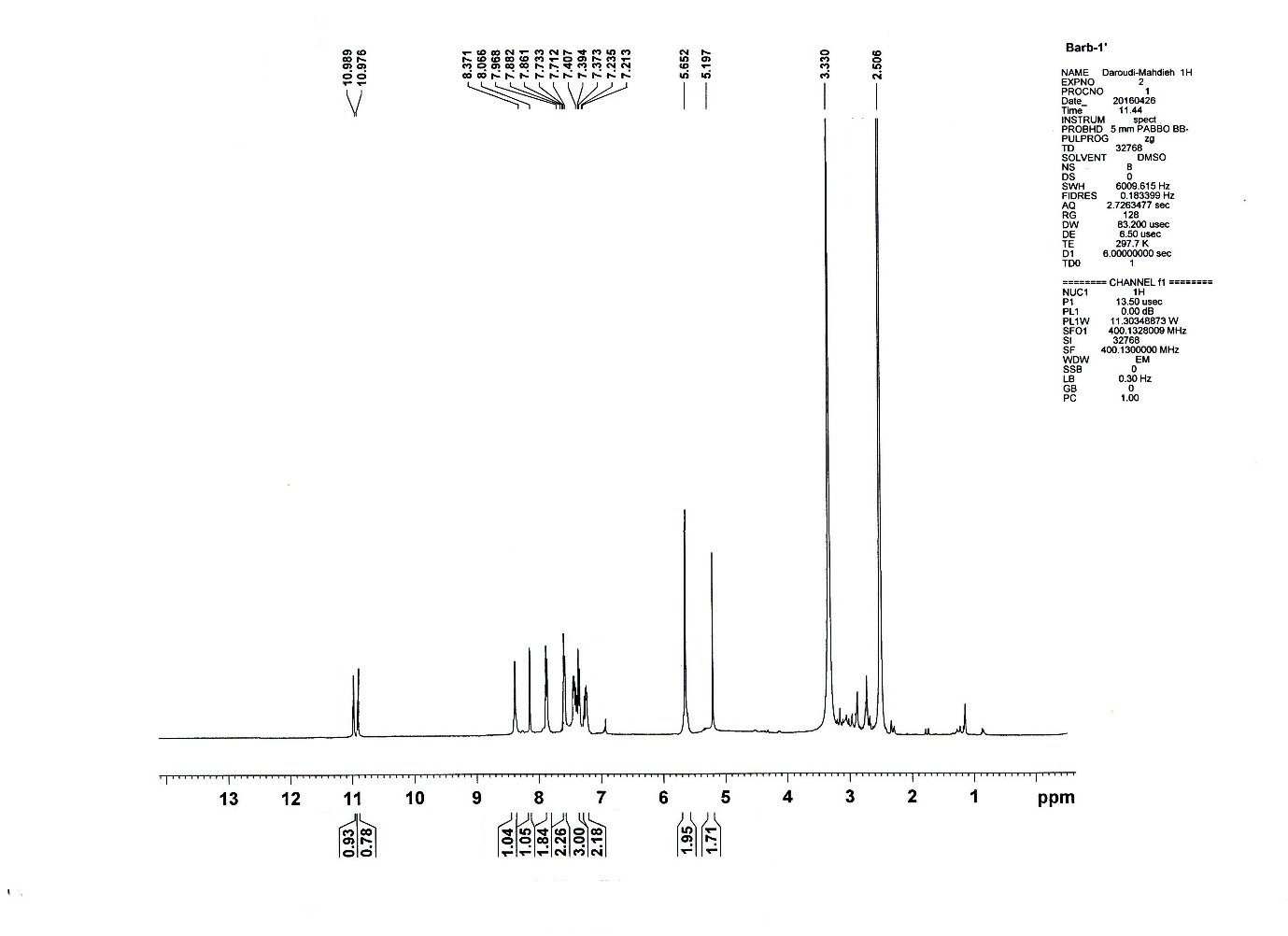
**5-(4-((1-(2-chlorobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-1,3-dimethylpyrimidine-2,4,6 (1H,3H,5H)-trione (8e)**: Yellow solid. Mp: 246.5-248.2 °C. IR (KBr, cm-1) ν = 3447, 2923, 1670, 1597, 1178. 1H NMR (400 MHz, DMSO): δ= 8.38 (s, 1H, CH), 7.97 (s, 1H, CH), 7.87 (m, 2H, ArH), 7.28-7.15 (m, 4H, ArH), 7.06-6.88 (m, 2H, ArH), 5.66 (s, 2H, OCH2), 5.10 (s, 2H, CH2), 2.87 (s, 3H, CH3), 2.71 (s, 3H, CH3) ppm. 13C 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 C23H20ClN5O4 (465.9): C, 59.30; H, 4.33; N, 15.03; Found C, 59.21; H, 4.30; N, 15.11.

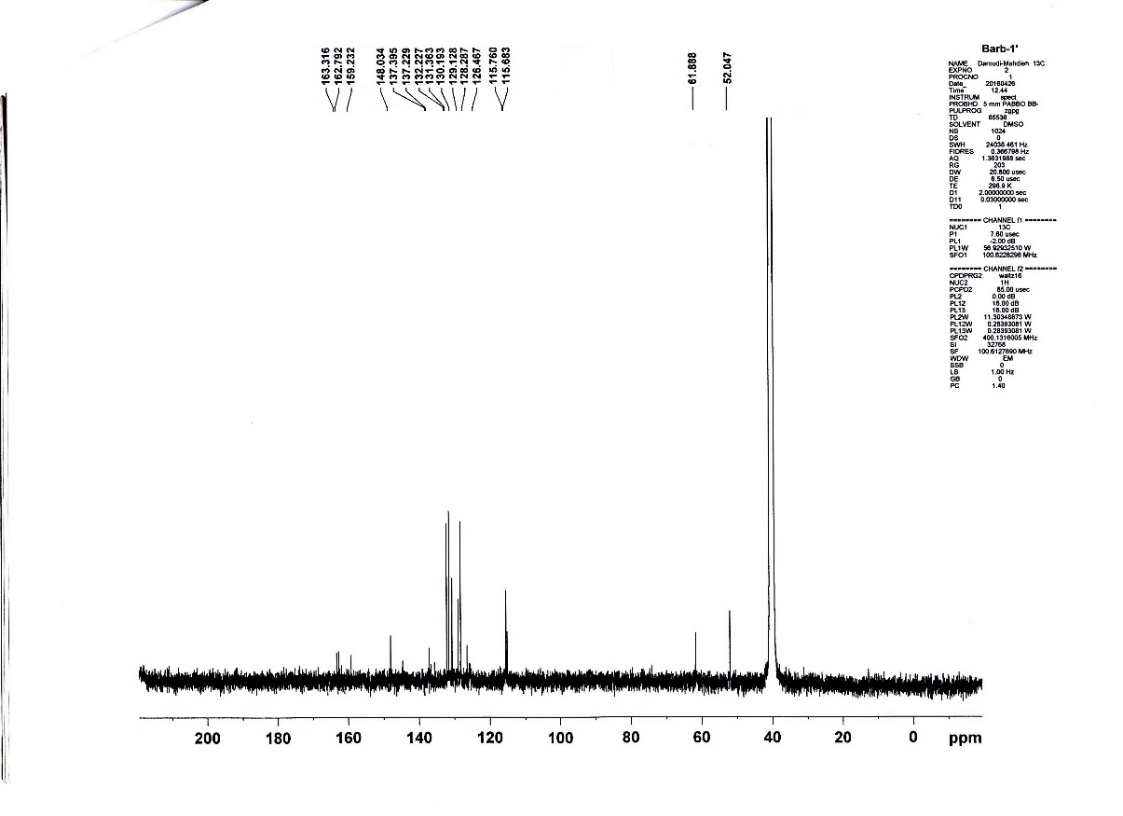
**5-(4-((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-2-thioxodihydro pyrimidine-4,6(1H,5H)-dione (8f)**: Yellow solid. Mp: 229.9-231.5 °C. IR (KBr, cm-1) ν = 3438, 2925, 1677, 1597, 1159. 1H NMR (400 MHz, DMSO): δ= 11.06 (s, 1H, NH), 10.98 (s, 1H, NH), 8.34 (s, 1H, CH), 8.06 (s, 1H, CH), 7.87 (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, OCH2), 5.27 (s, 2H, CH2) ppm. 13C 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 C21H17N5O4 (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) ν = 3439, 2925, 1728, 1627, 1238, 1130. 1H 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, OCH2), 5.23 (s, 2H, CH2) ppm. 13C 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 C21H16BrN5O3S (498.3): C, 50.61; H, 3.24; N, 14.05; Found: C, 50.55; H, 3.18; N, 14.13.

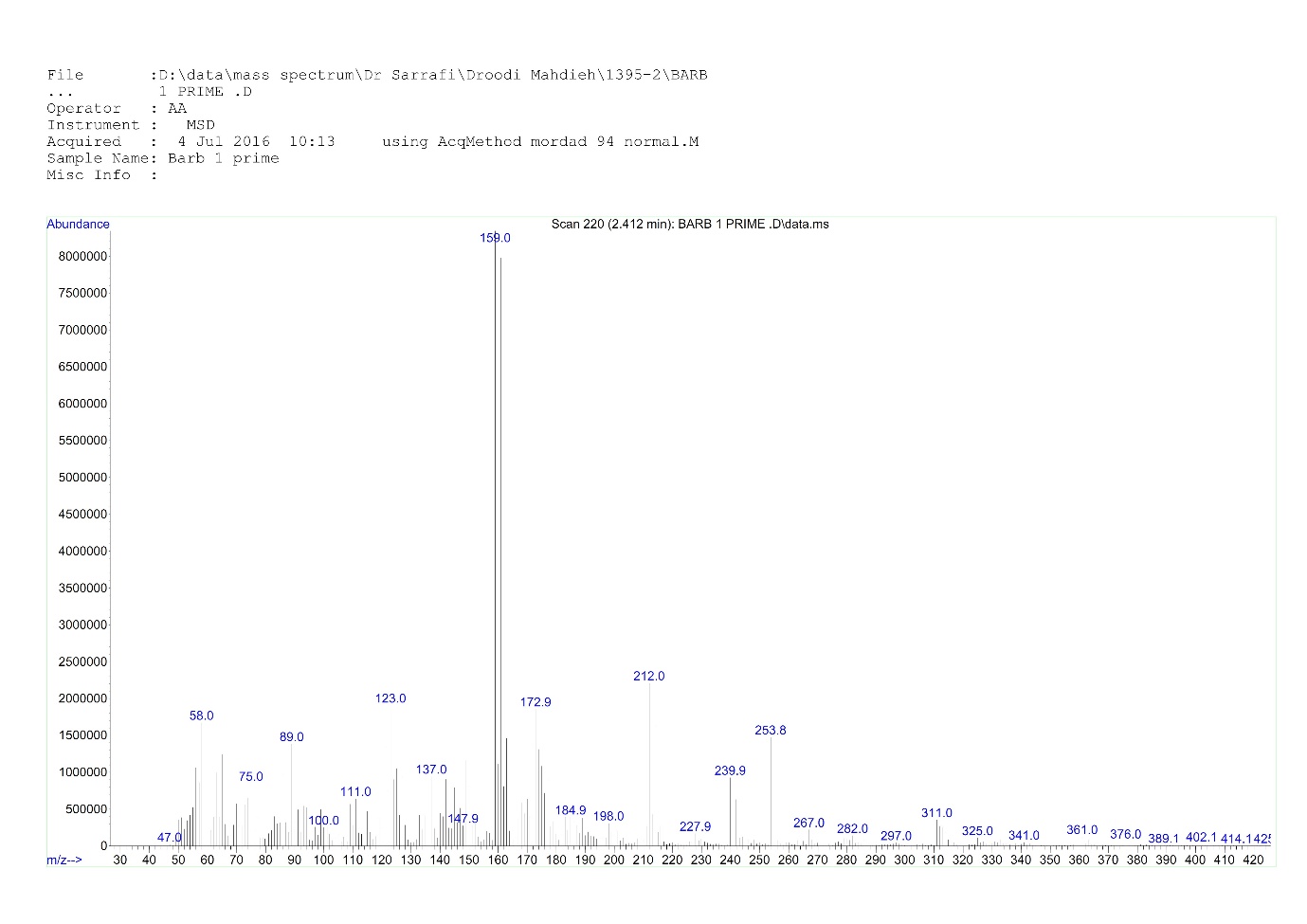
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3. Mass spectrum of 8a
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6. Mass spectrum of 8b
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34. 13C-NMR spectrum of 7e
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36. 1H-NMR spectrum of 7f
37. 13C-NMR spectrum of 7f
38. Mass spectrum of 7f
39. 1H-NMR spectrum of 7g
40. Mass spectrum of 7g

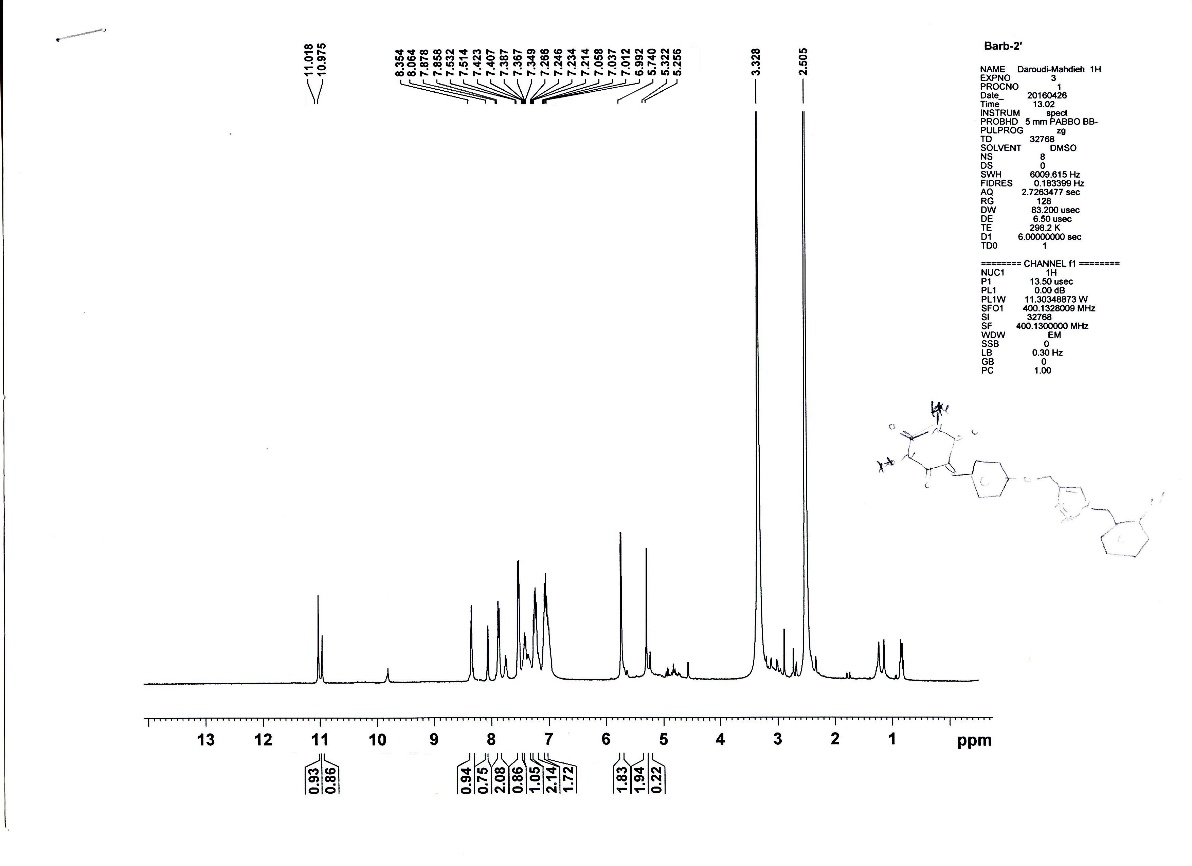


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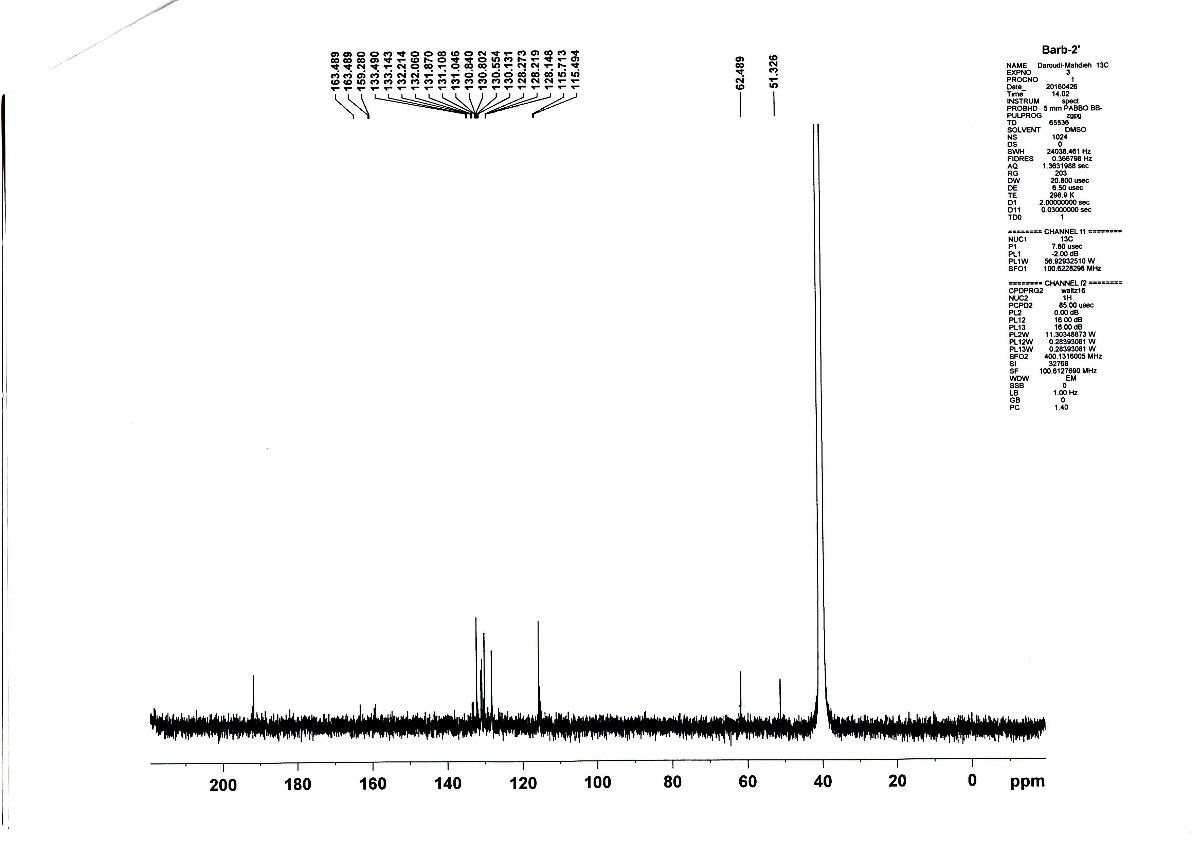
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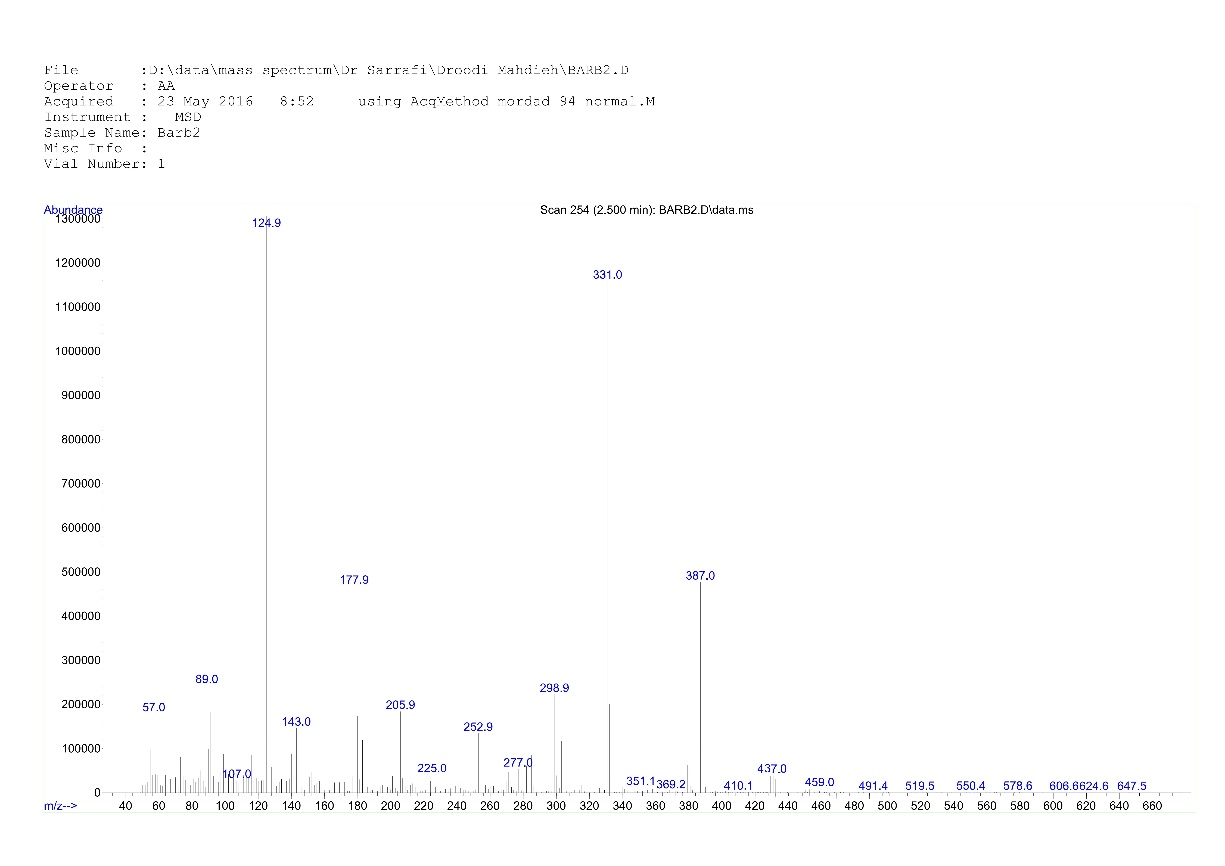
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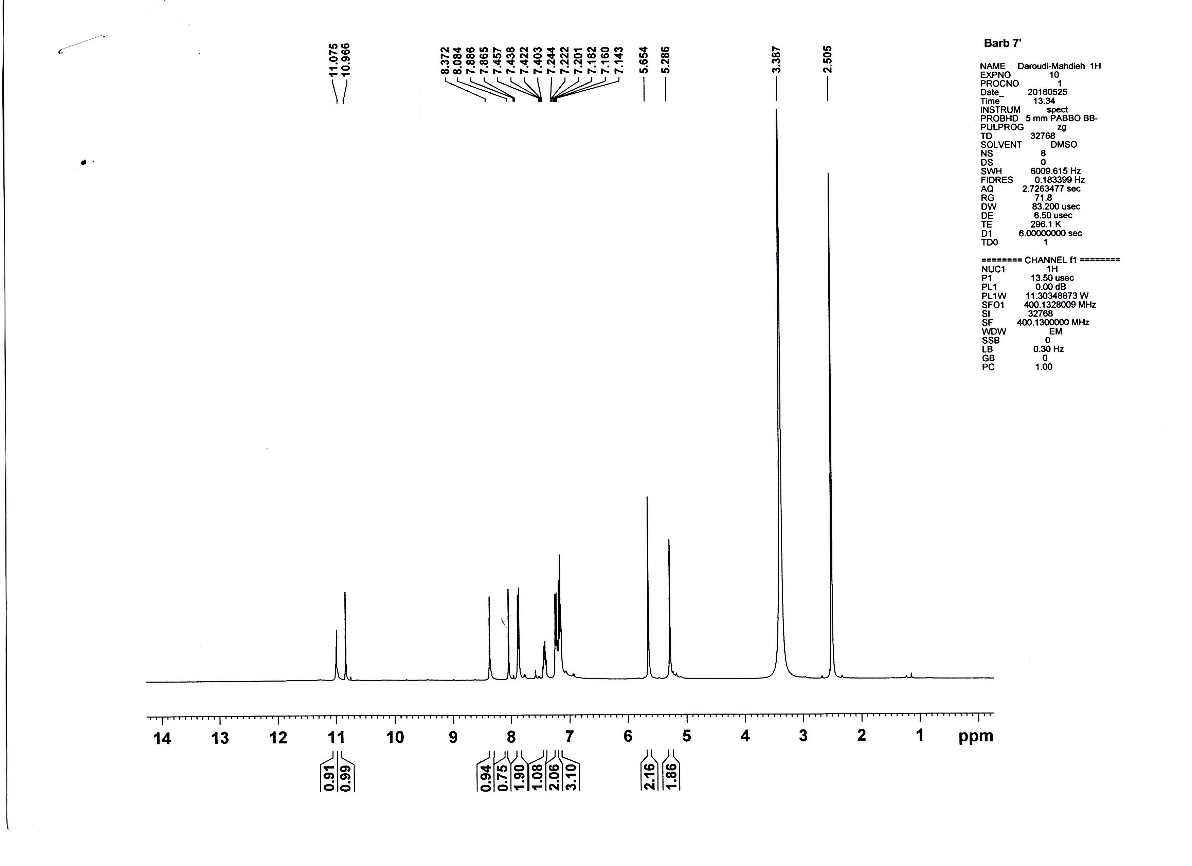
1H-NMR spectrum of 8b



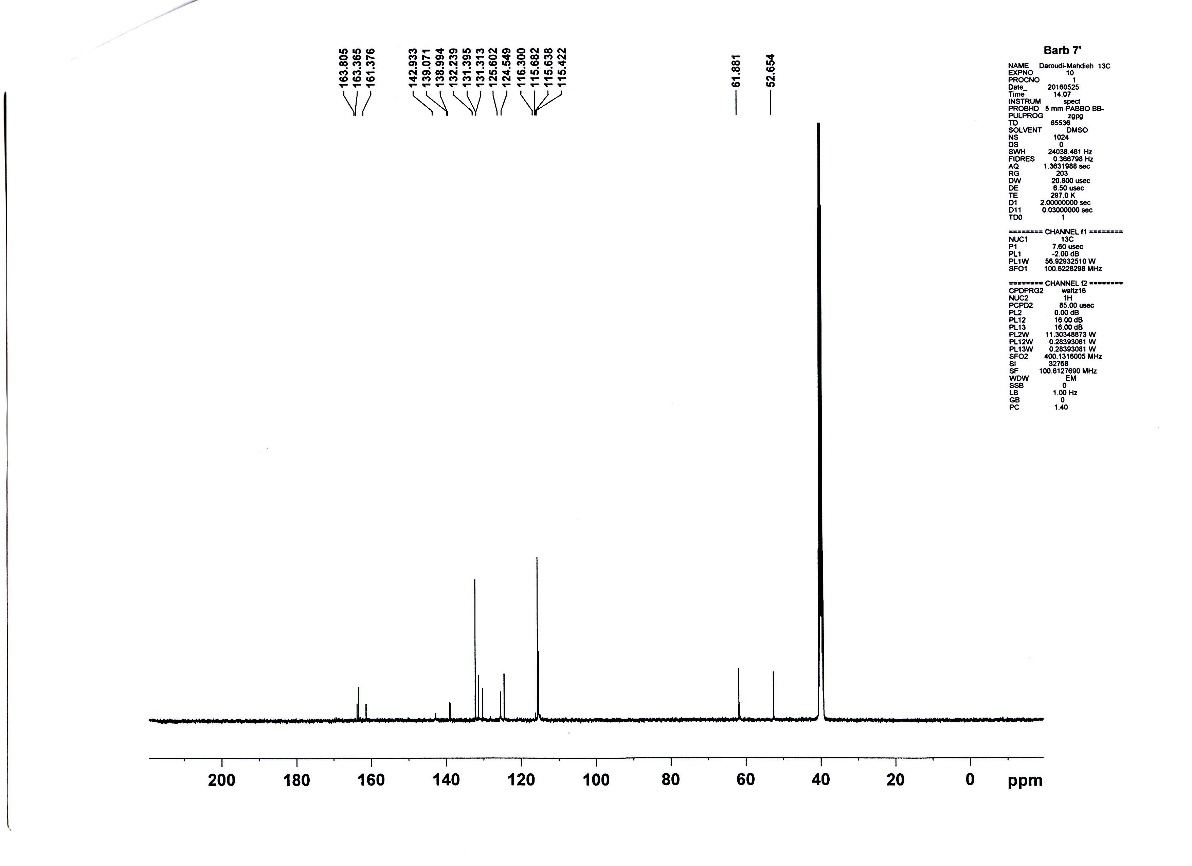
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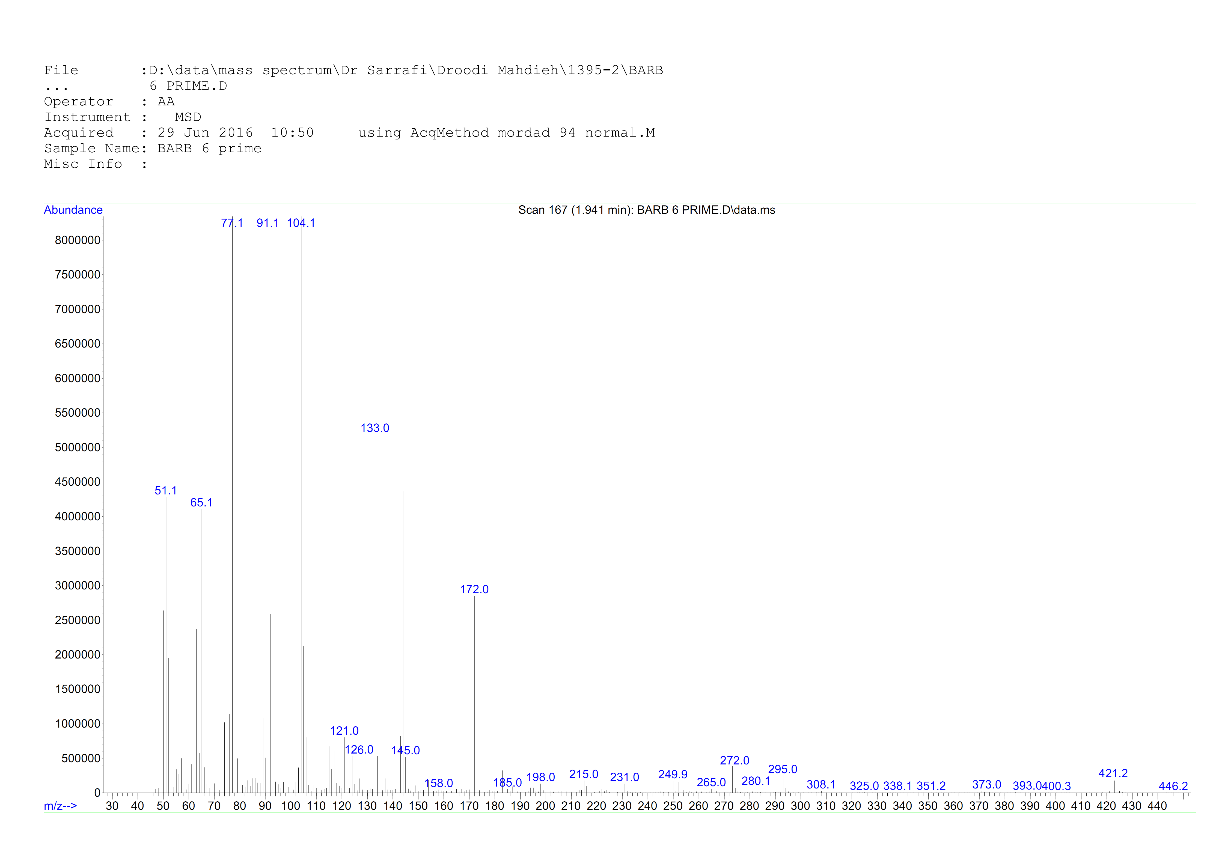
Mass spectrum of 8b



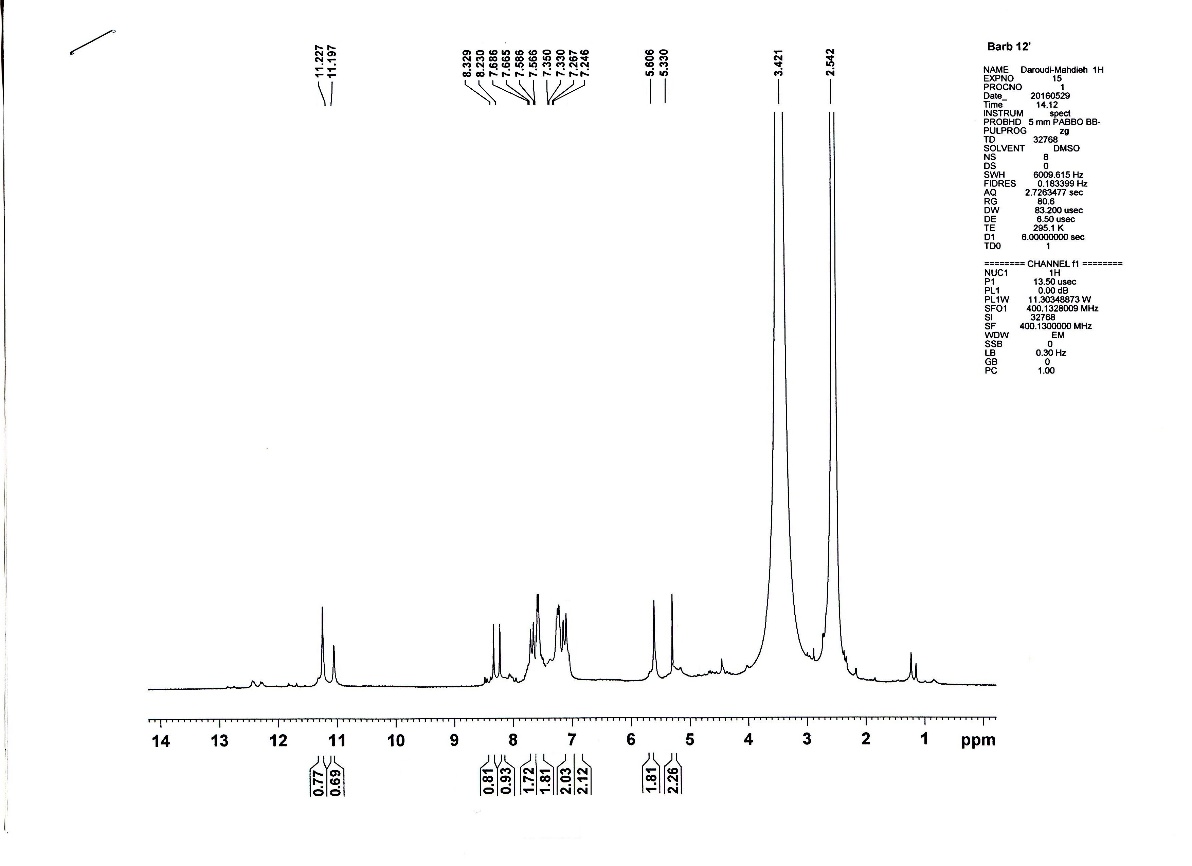
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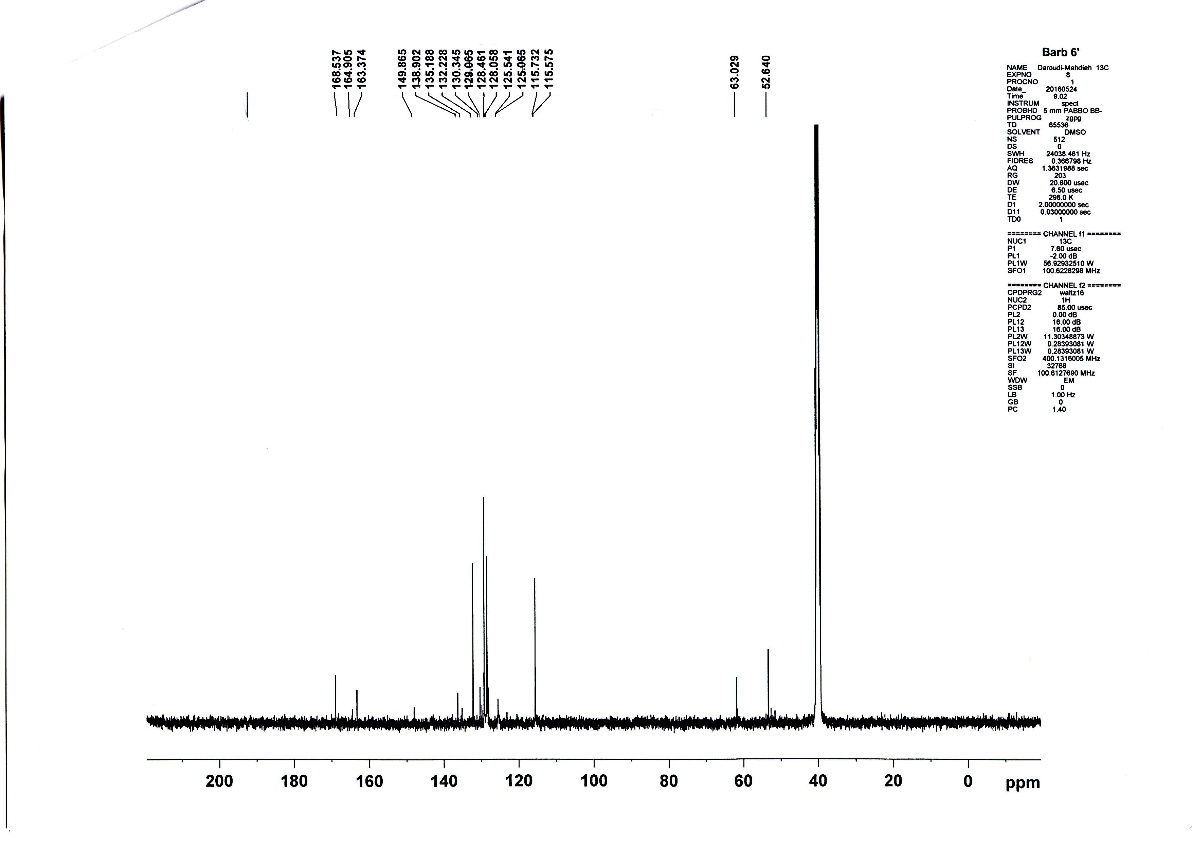
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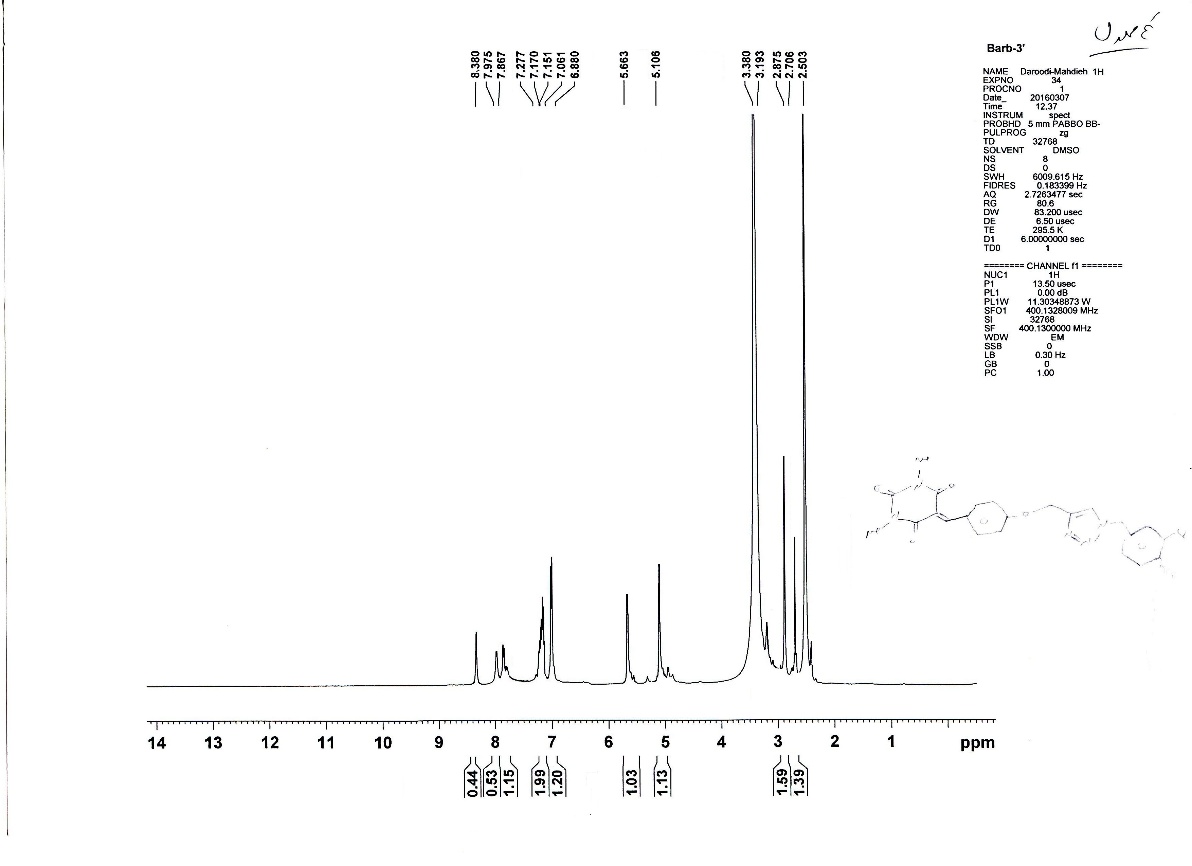
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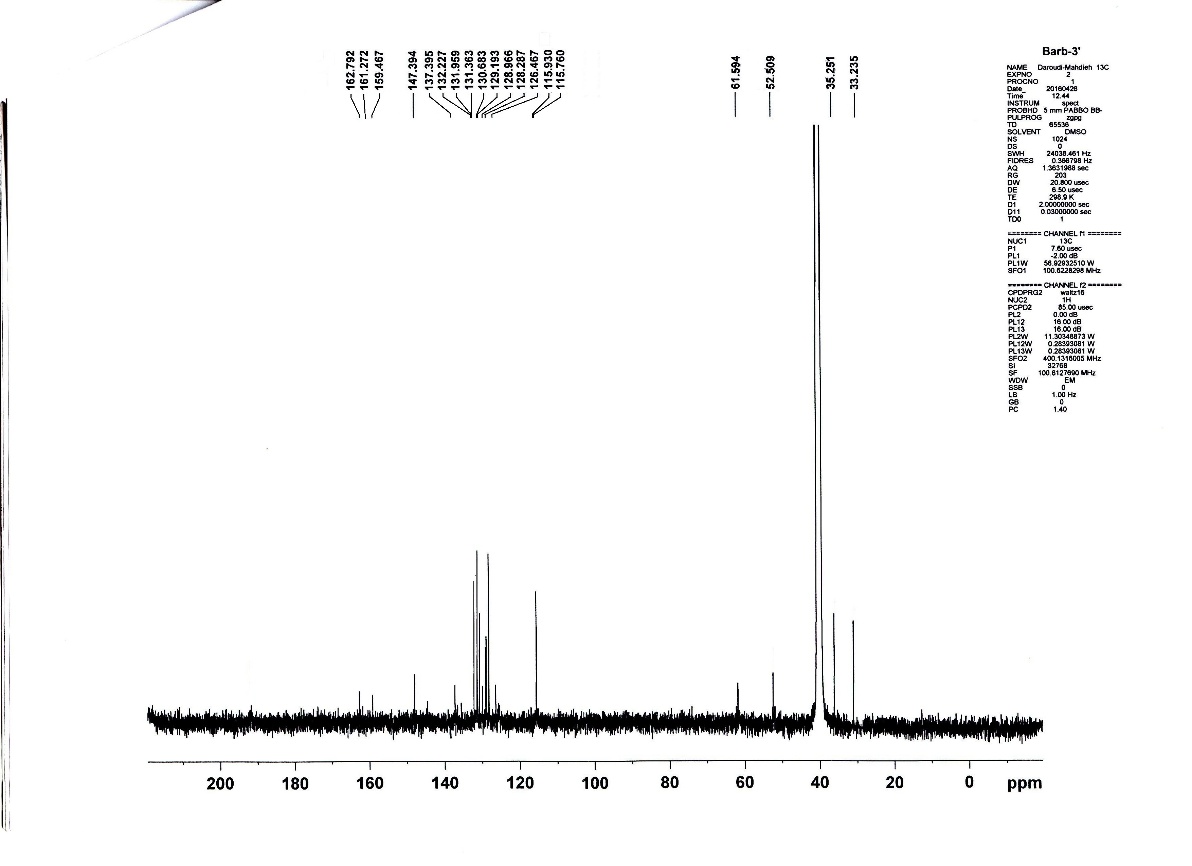
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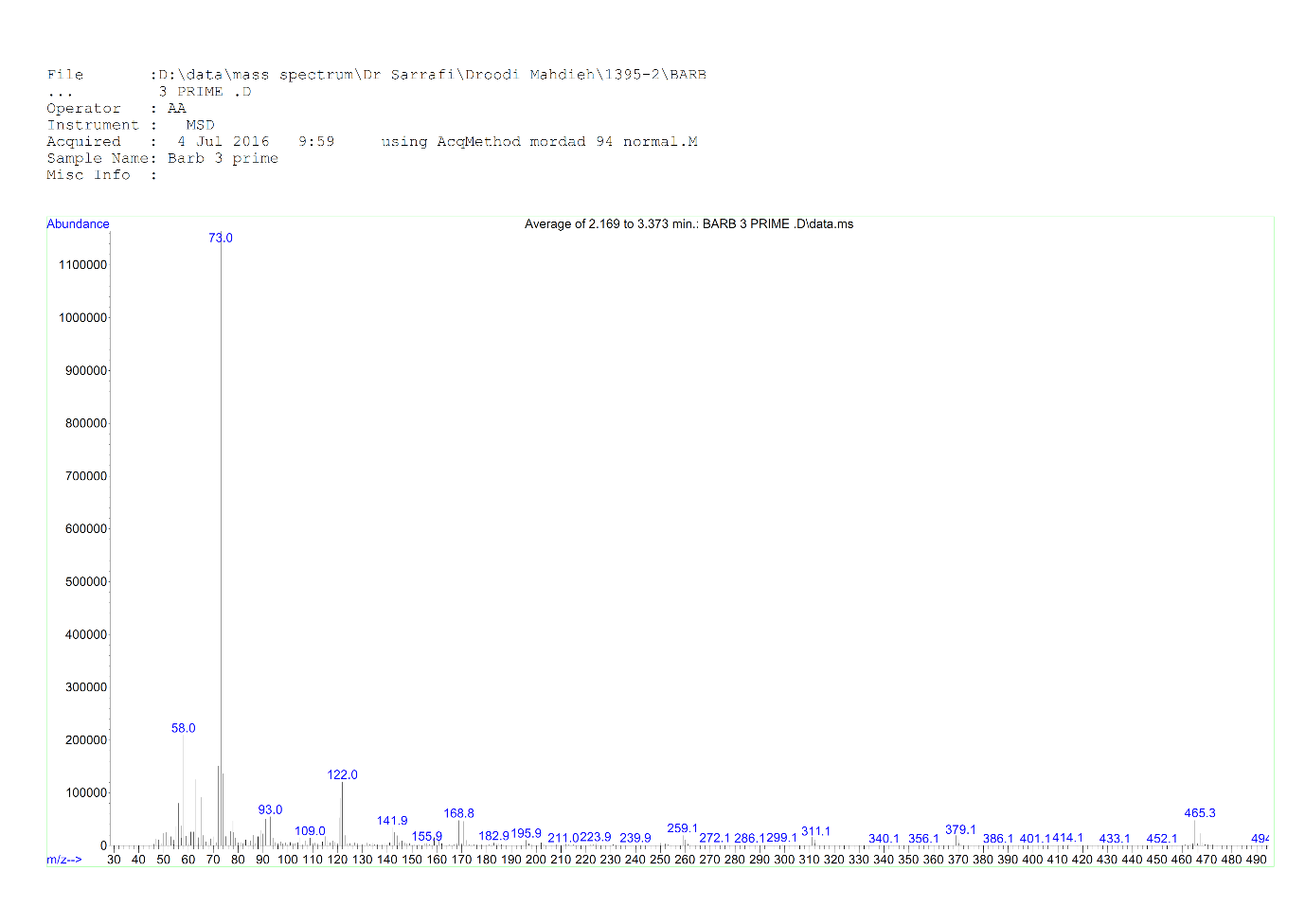
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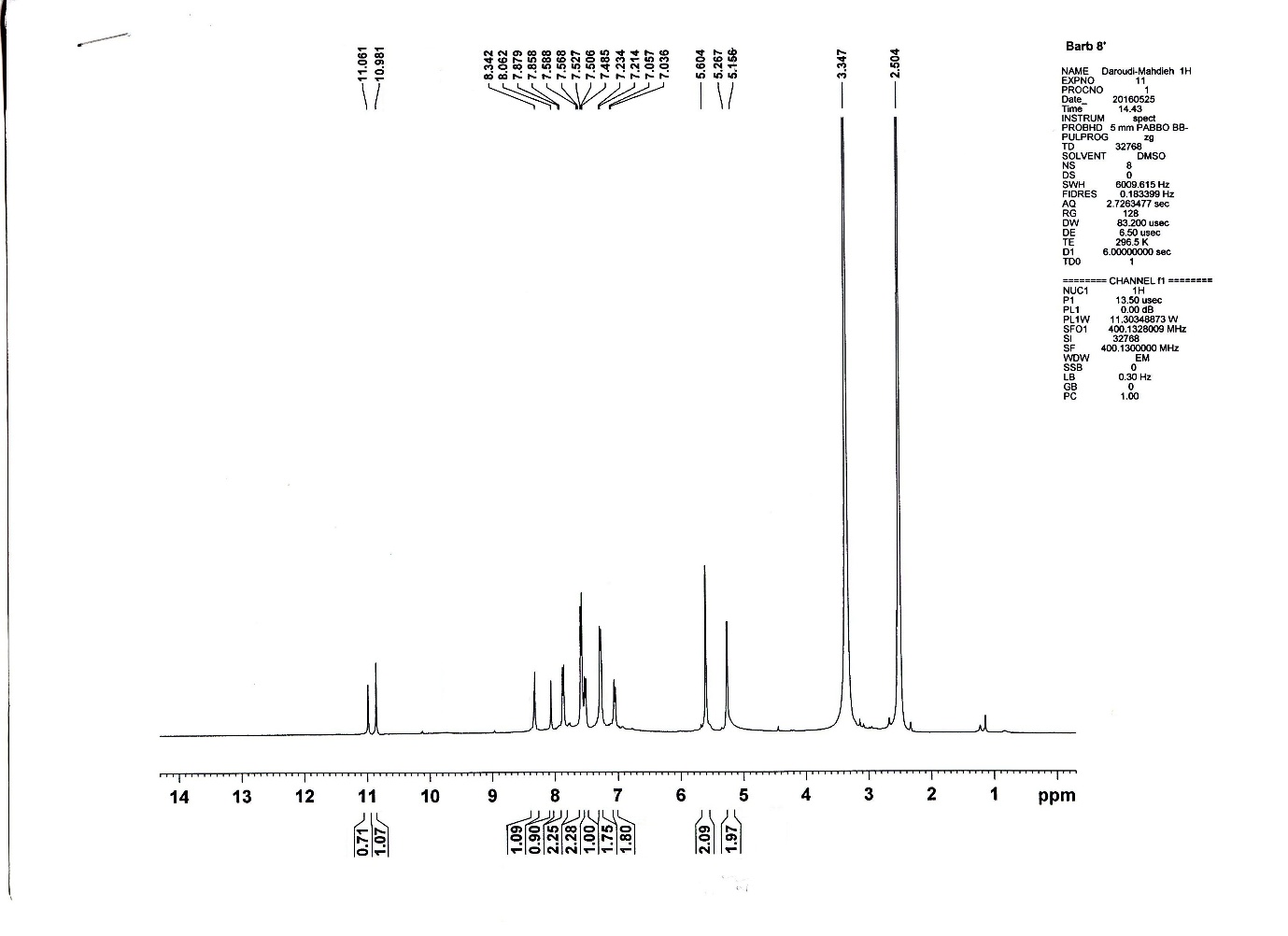
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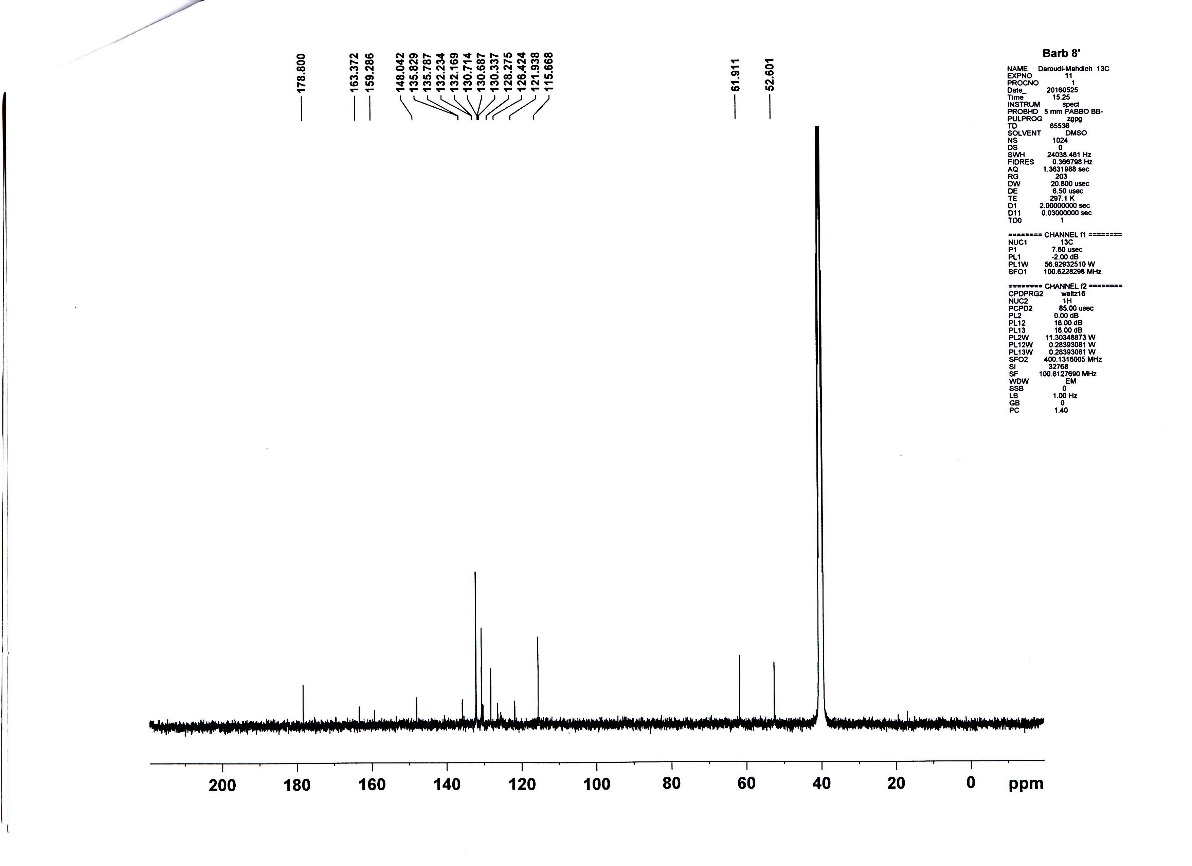
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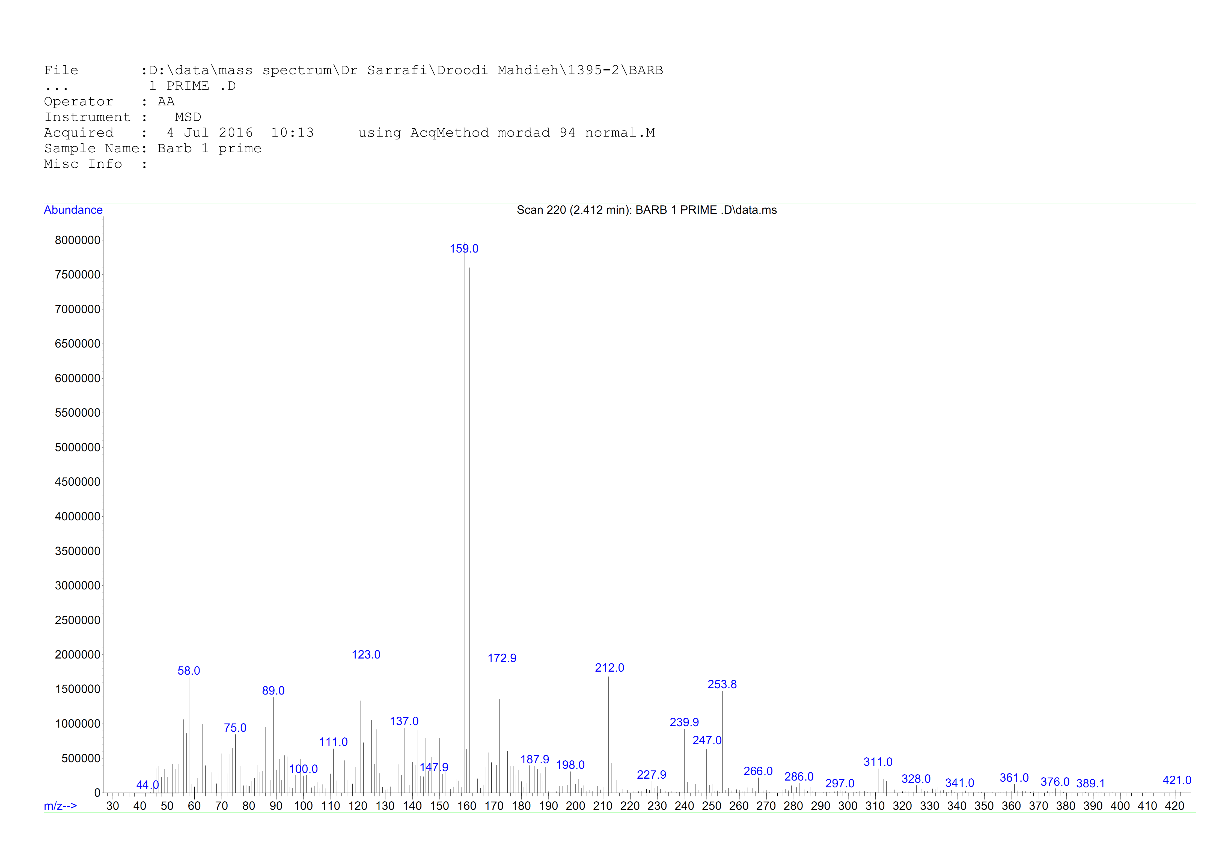
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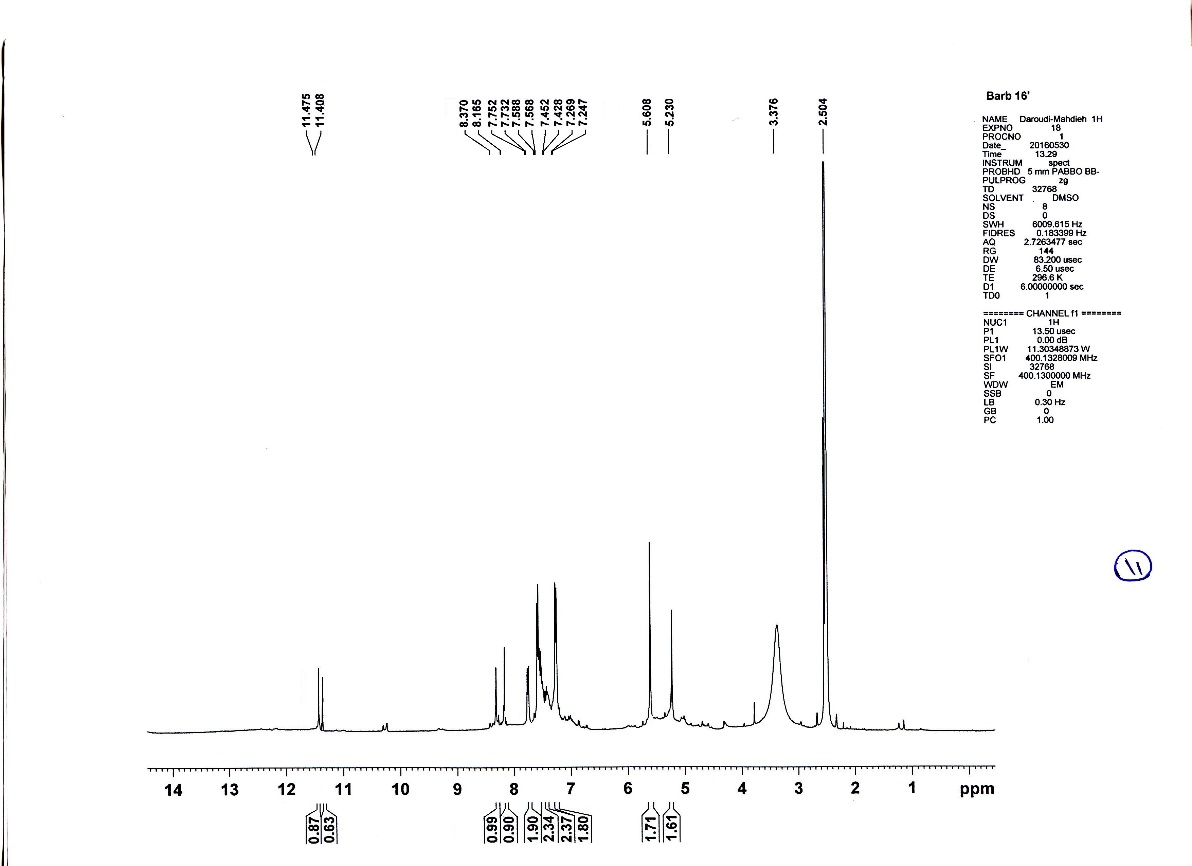
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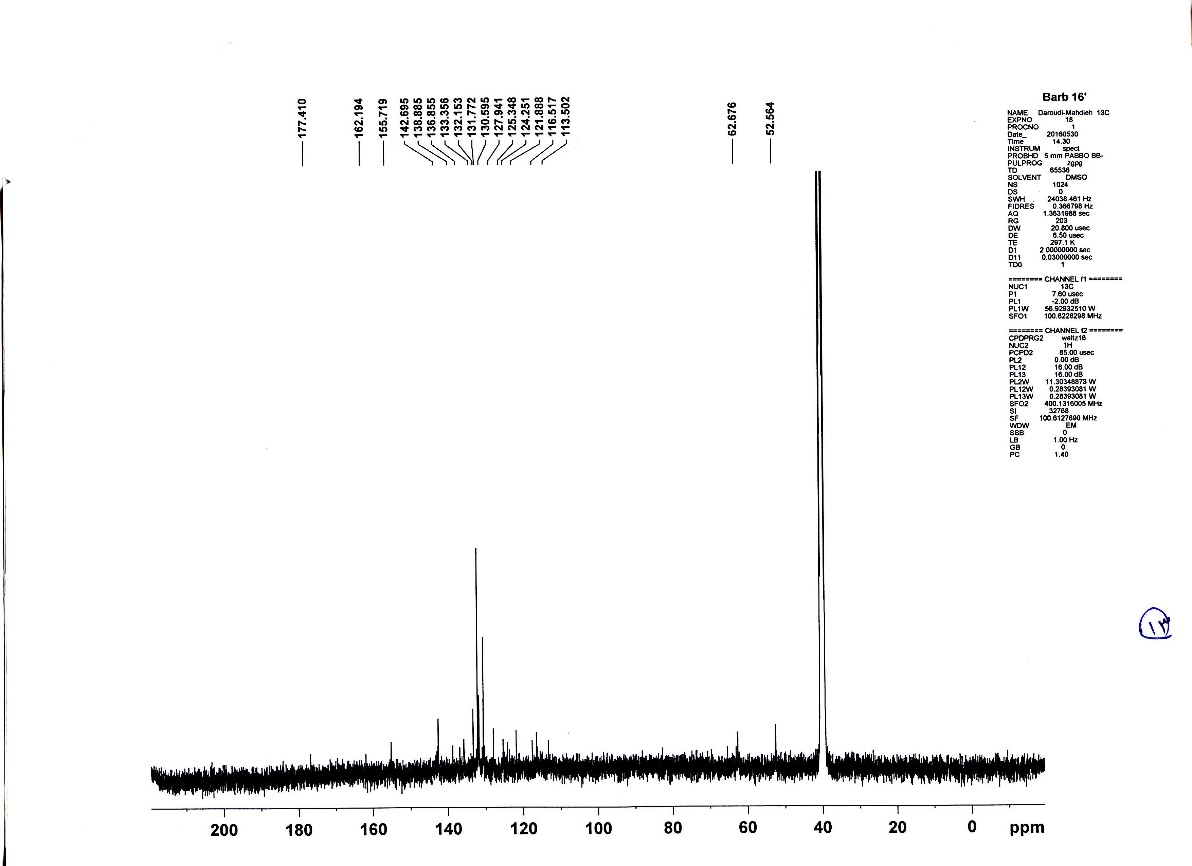
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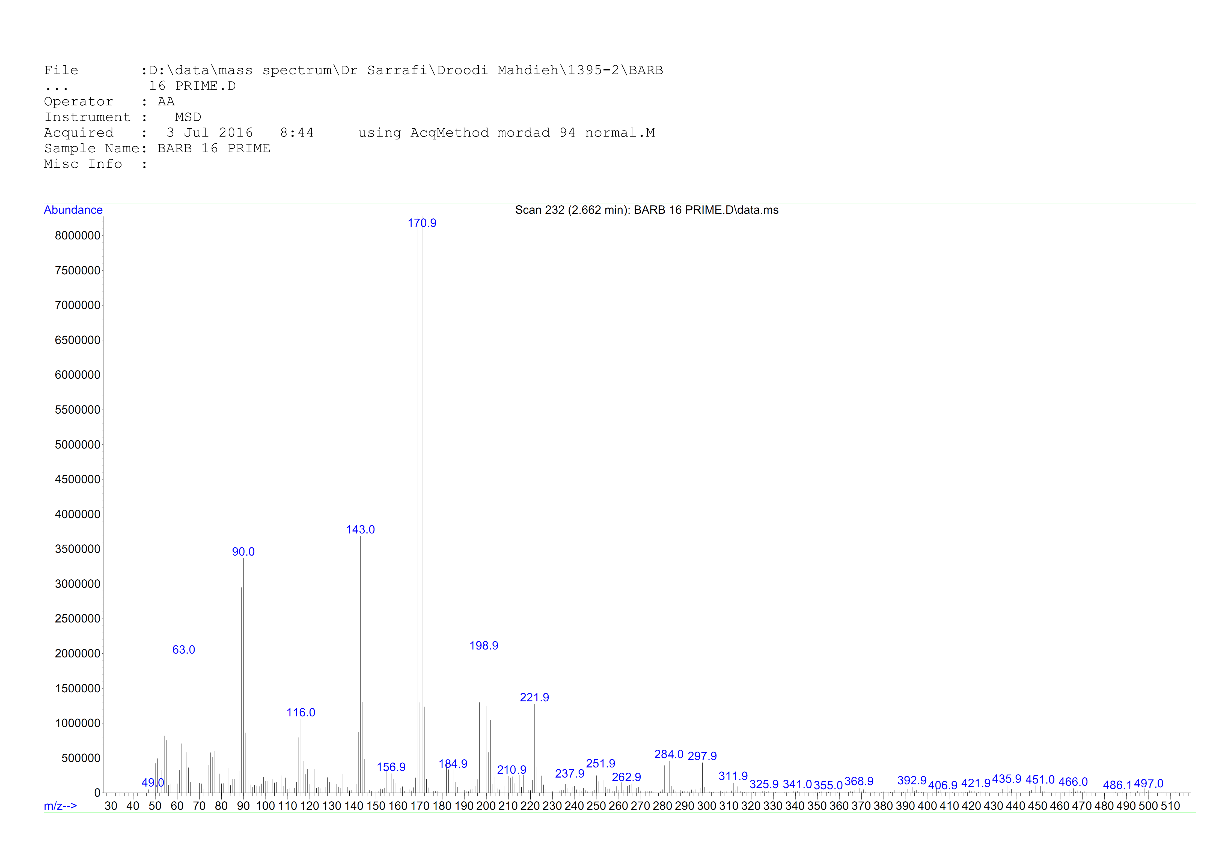
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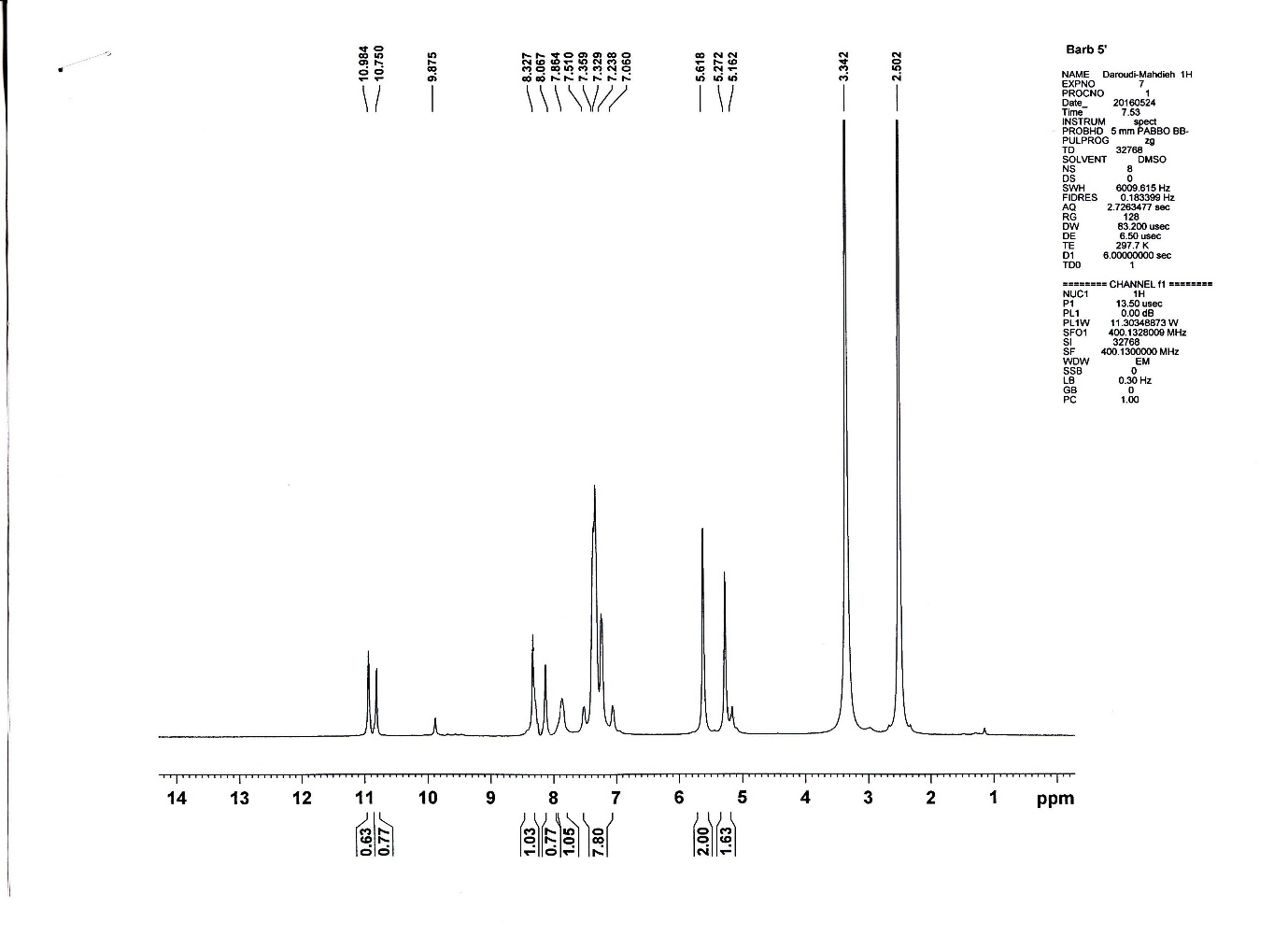
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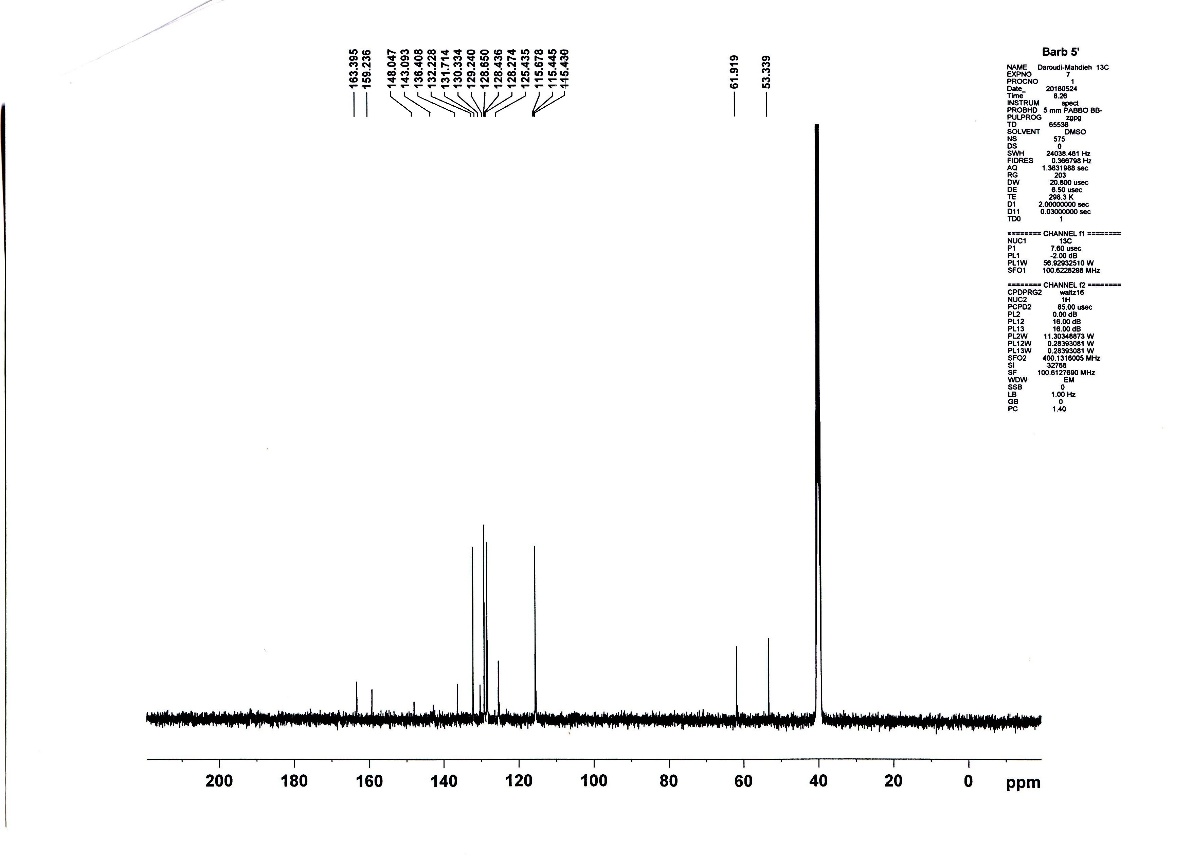
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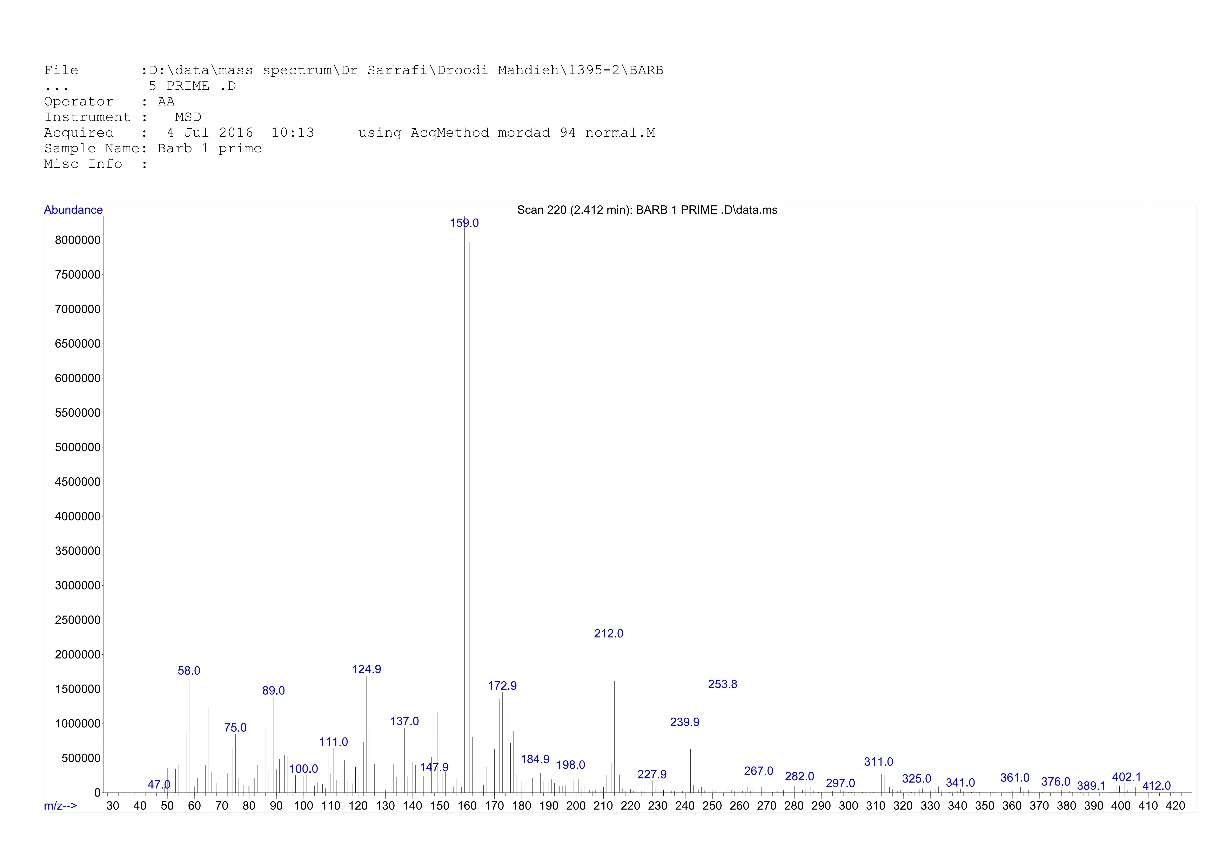
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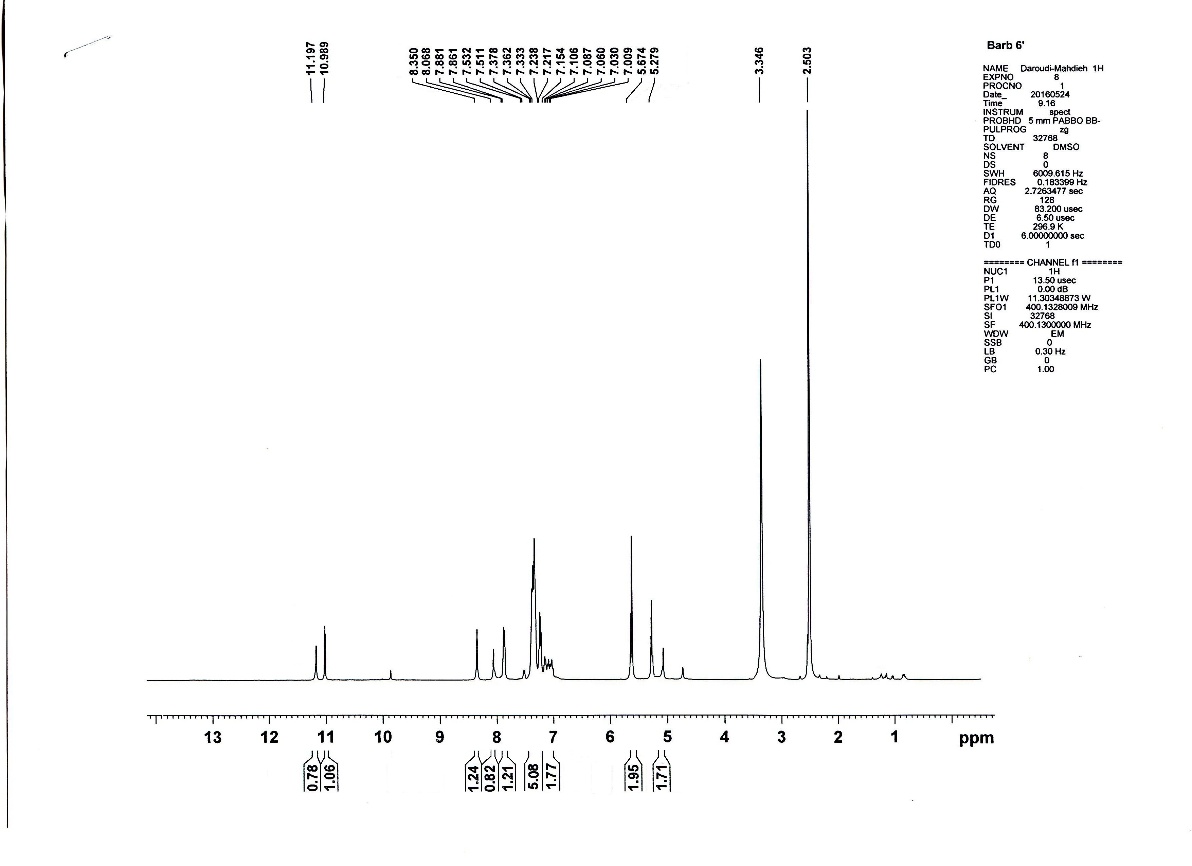
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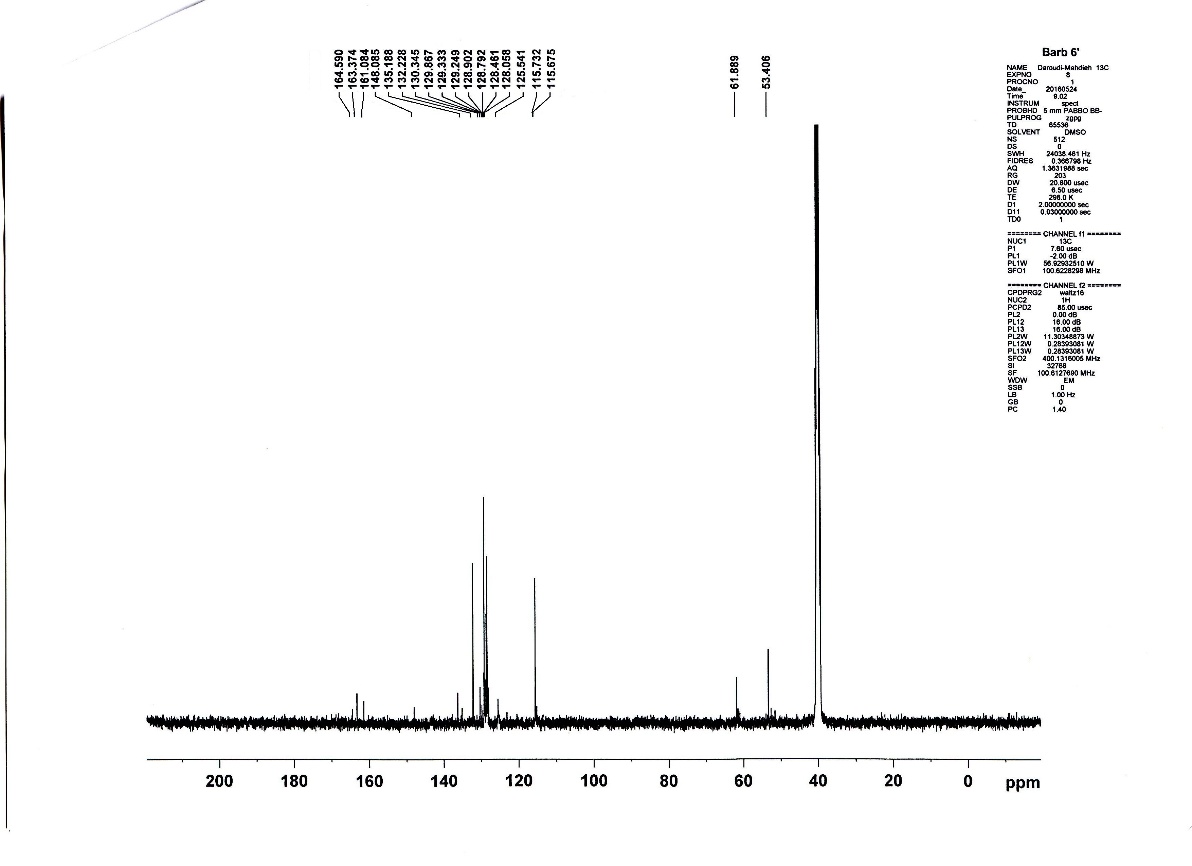
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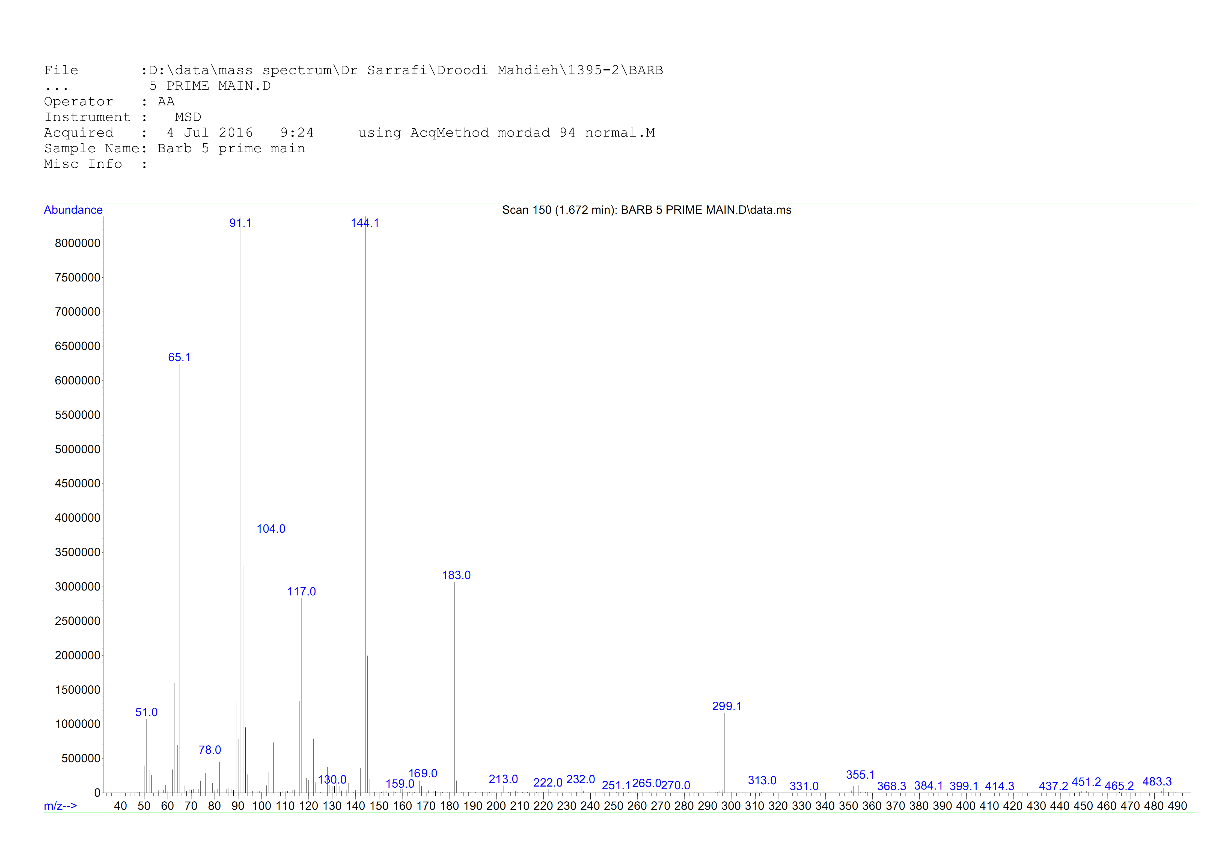
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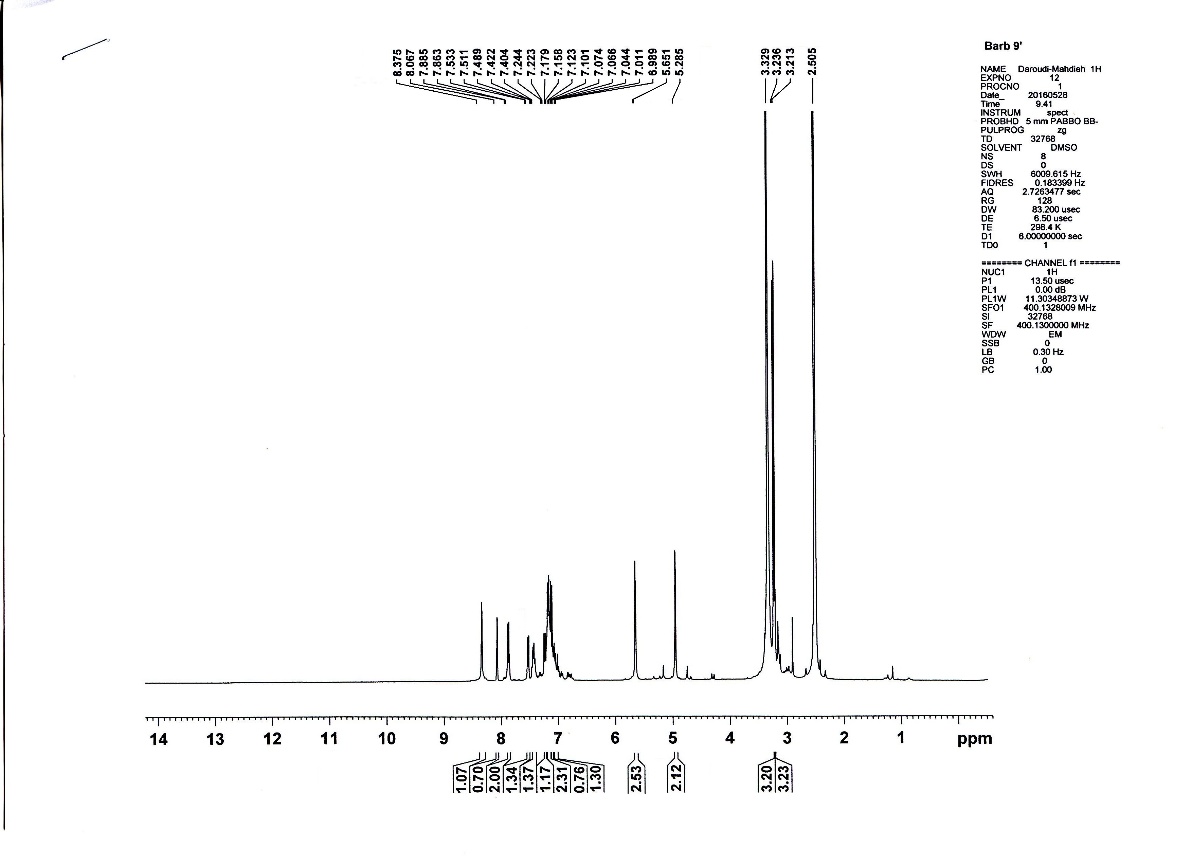
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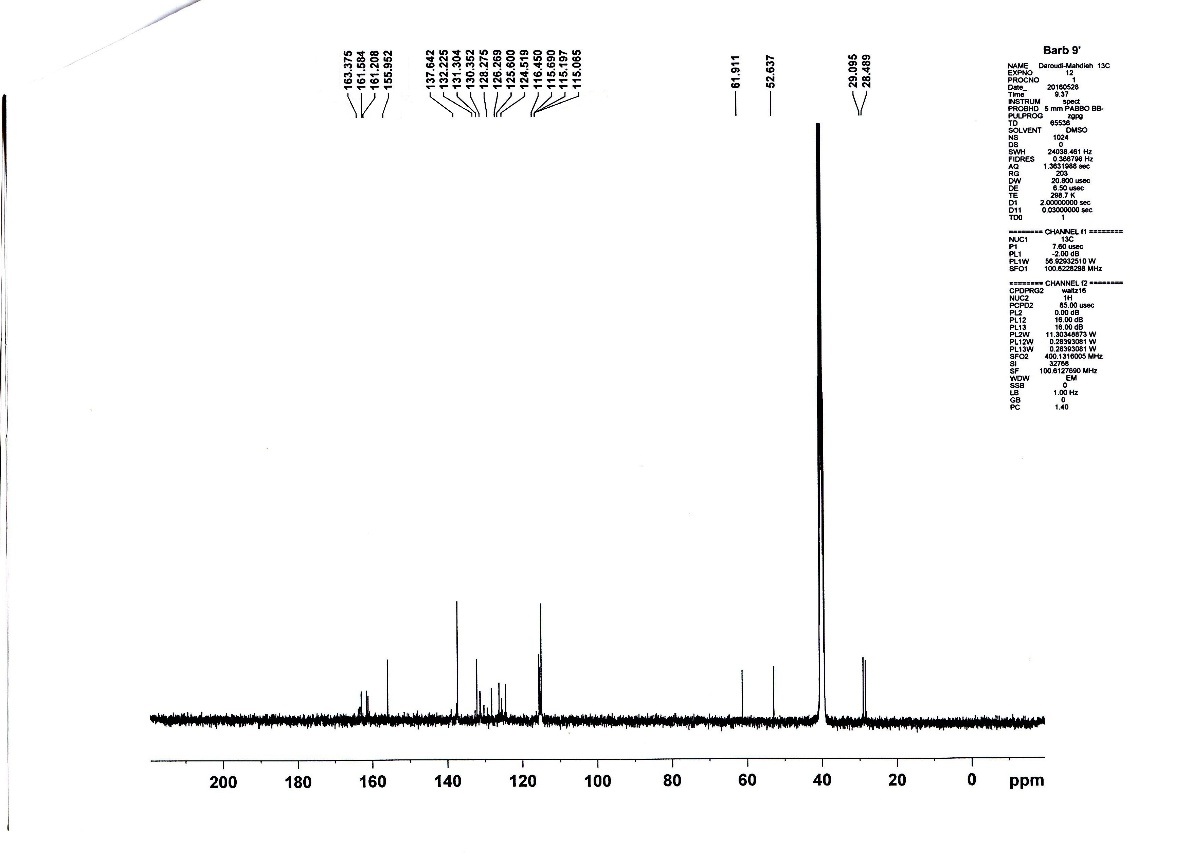
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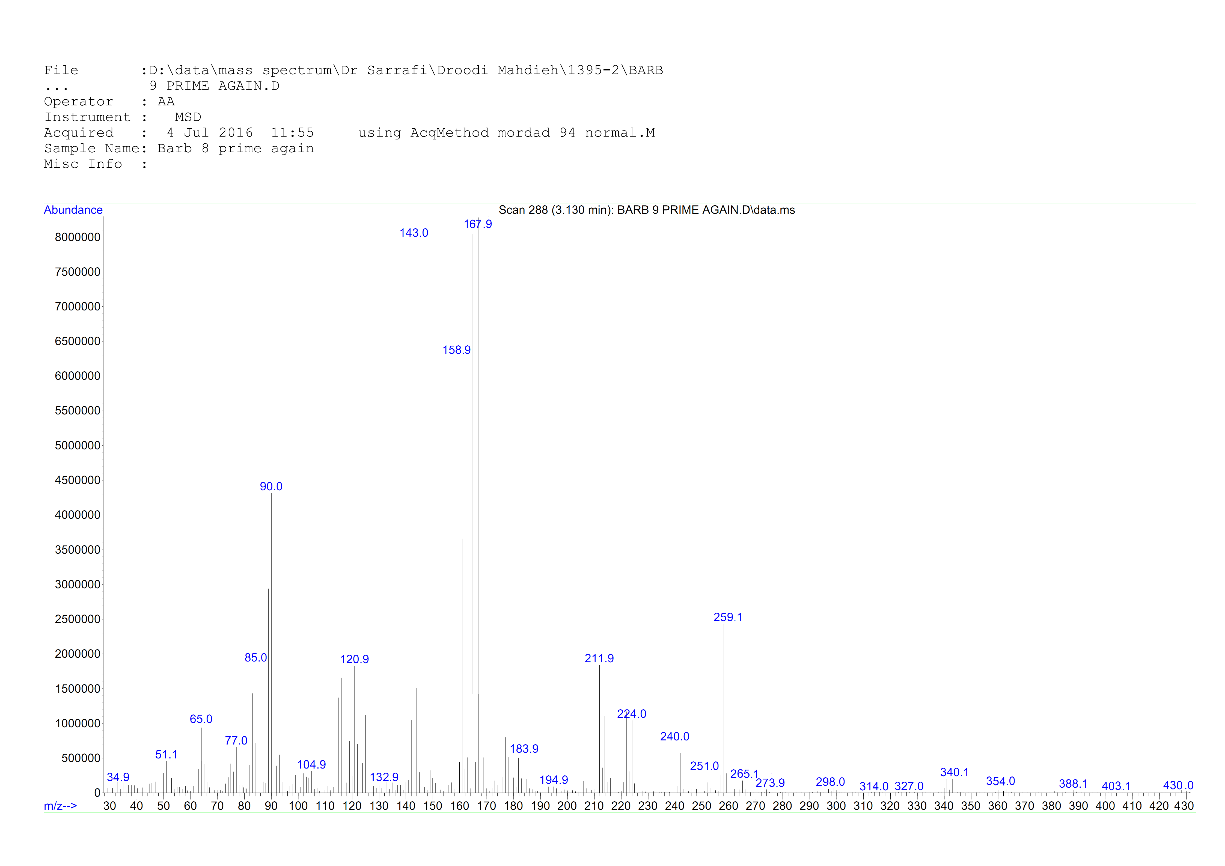
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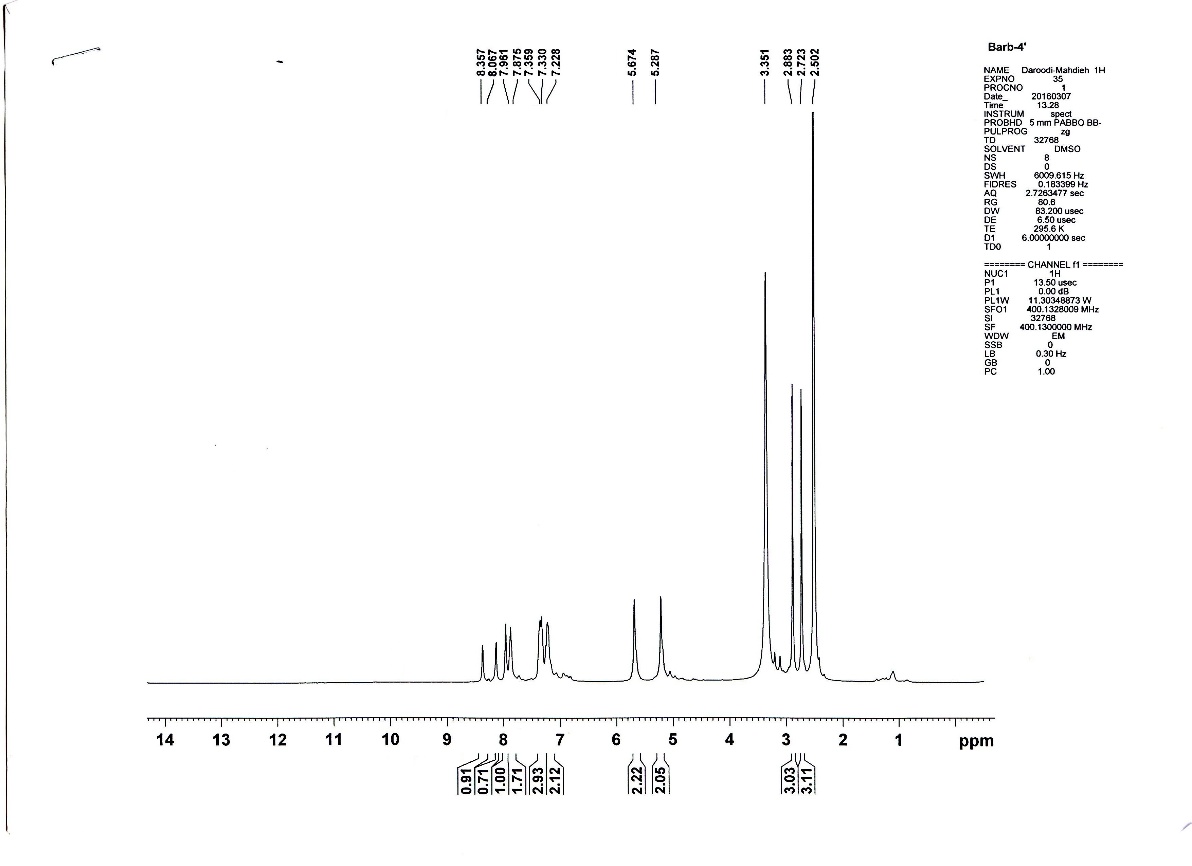
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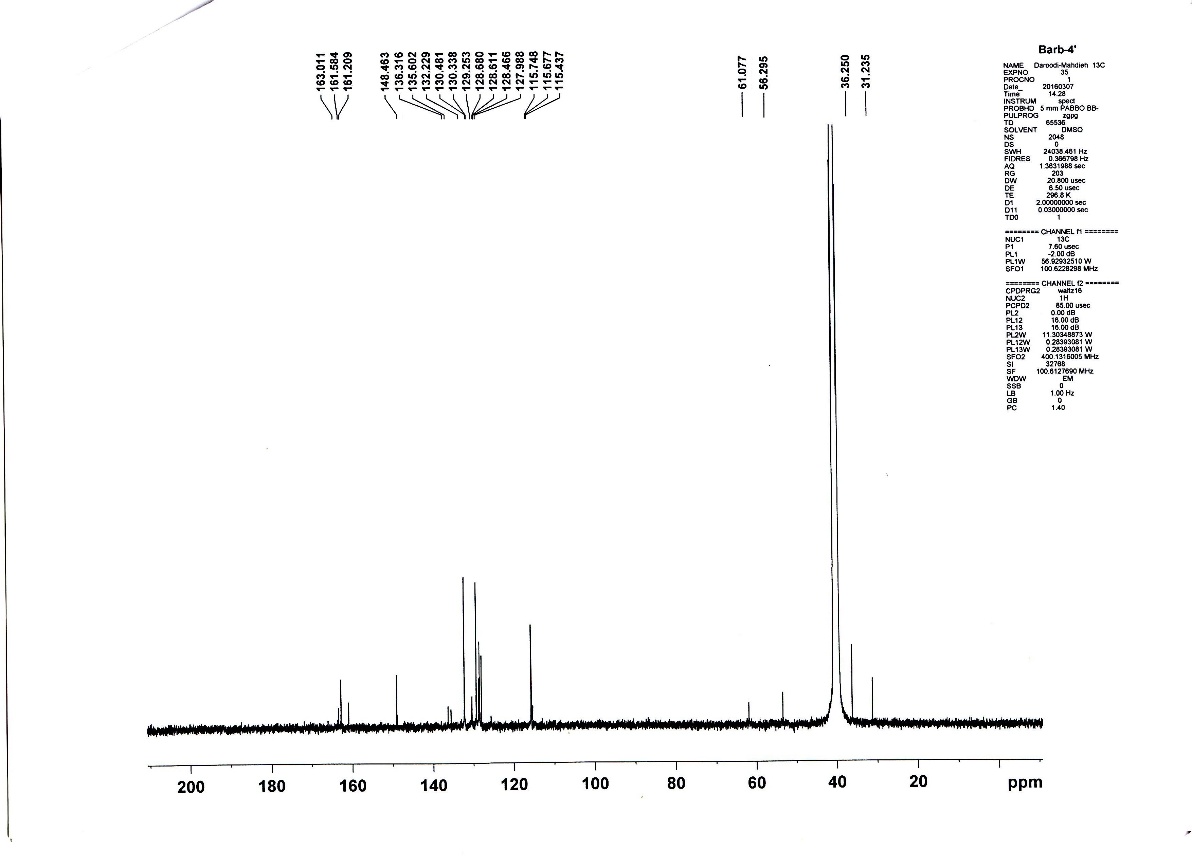
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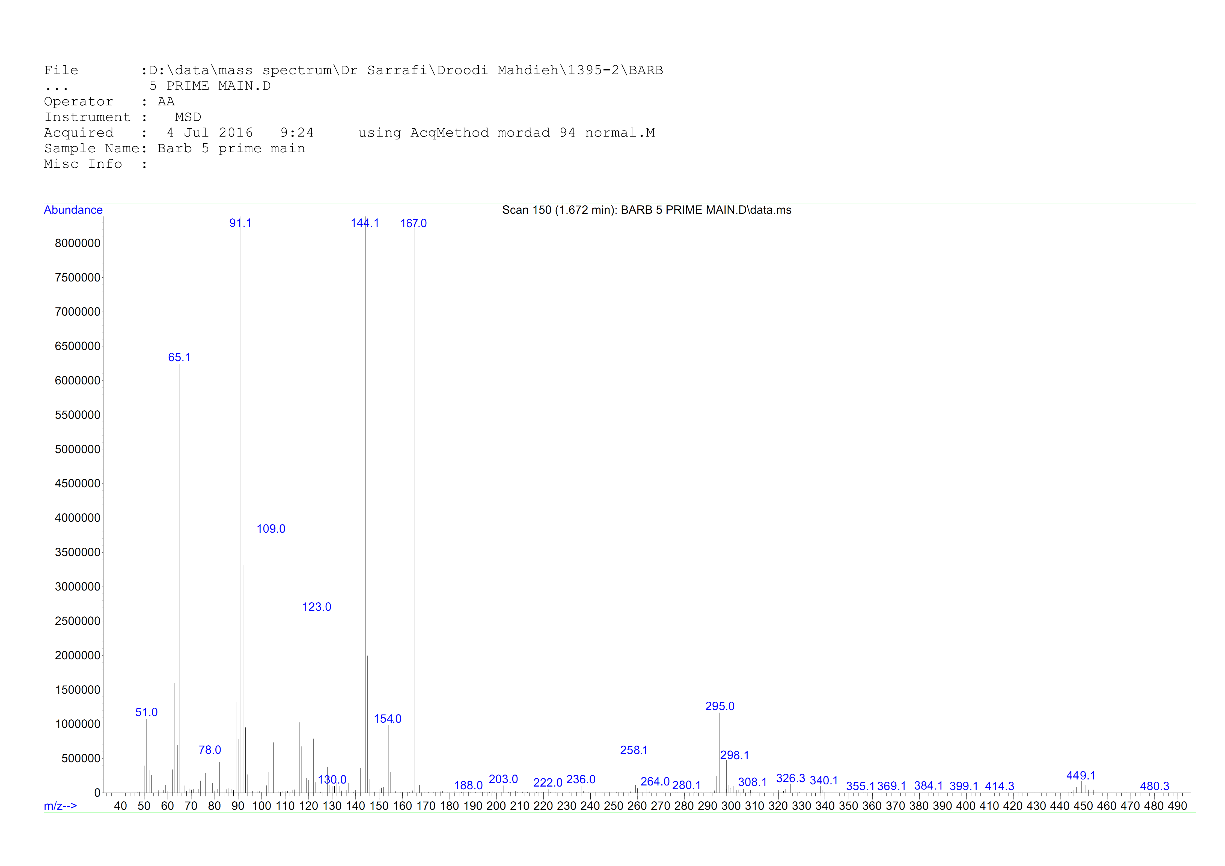
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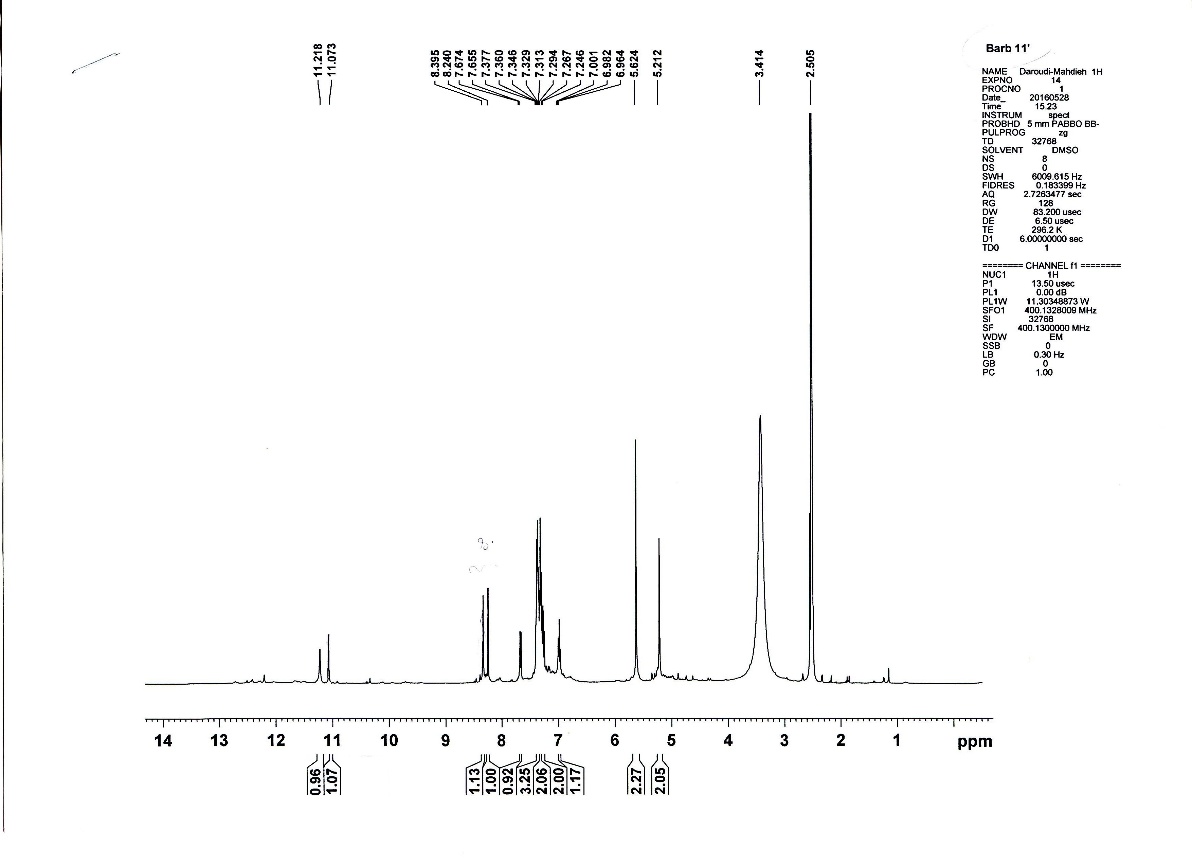


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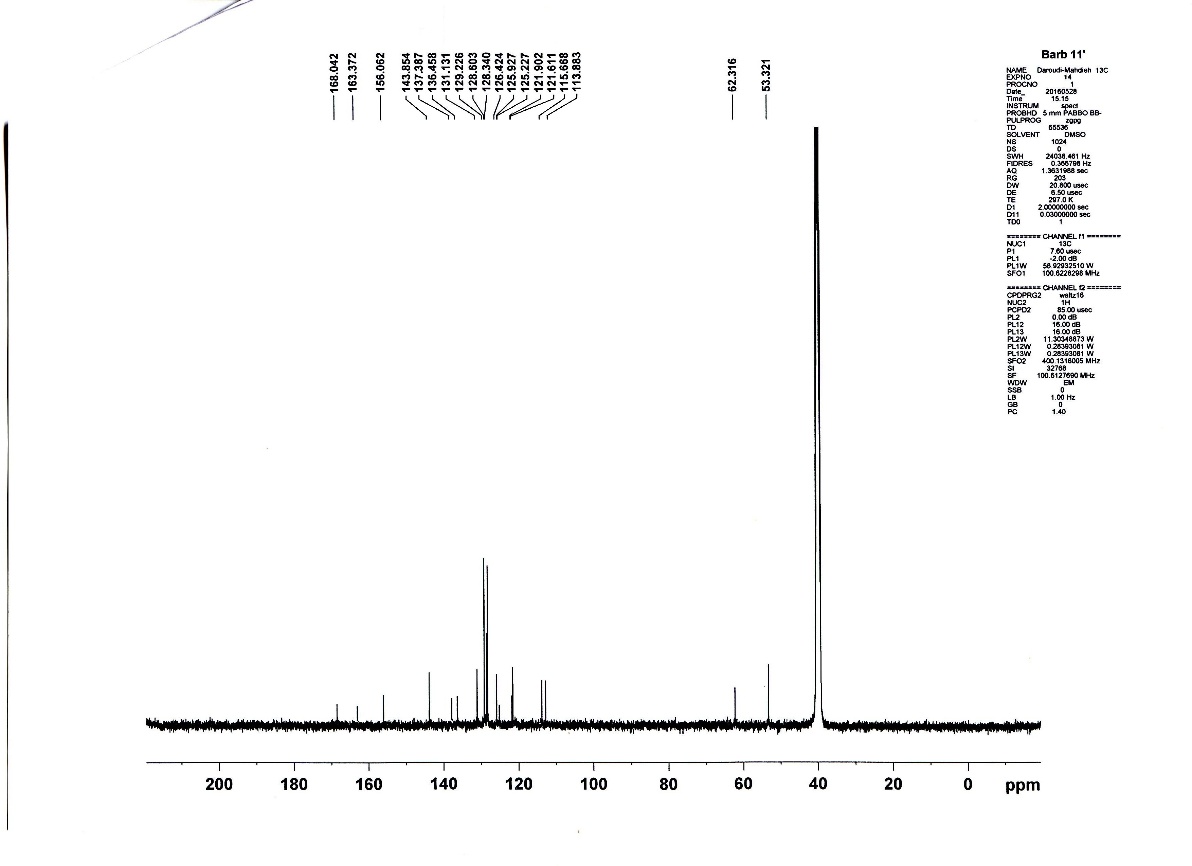


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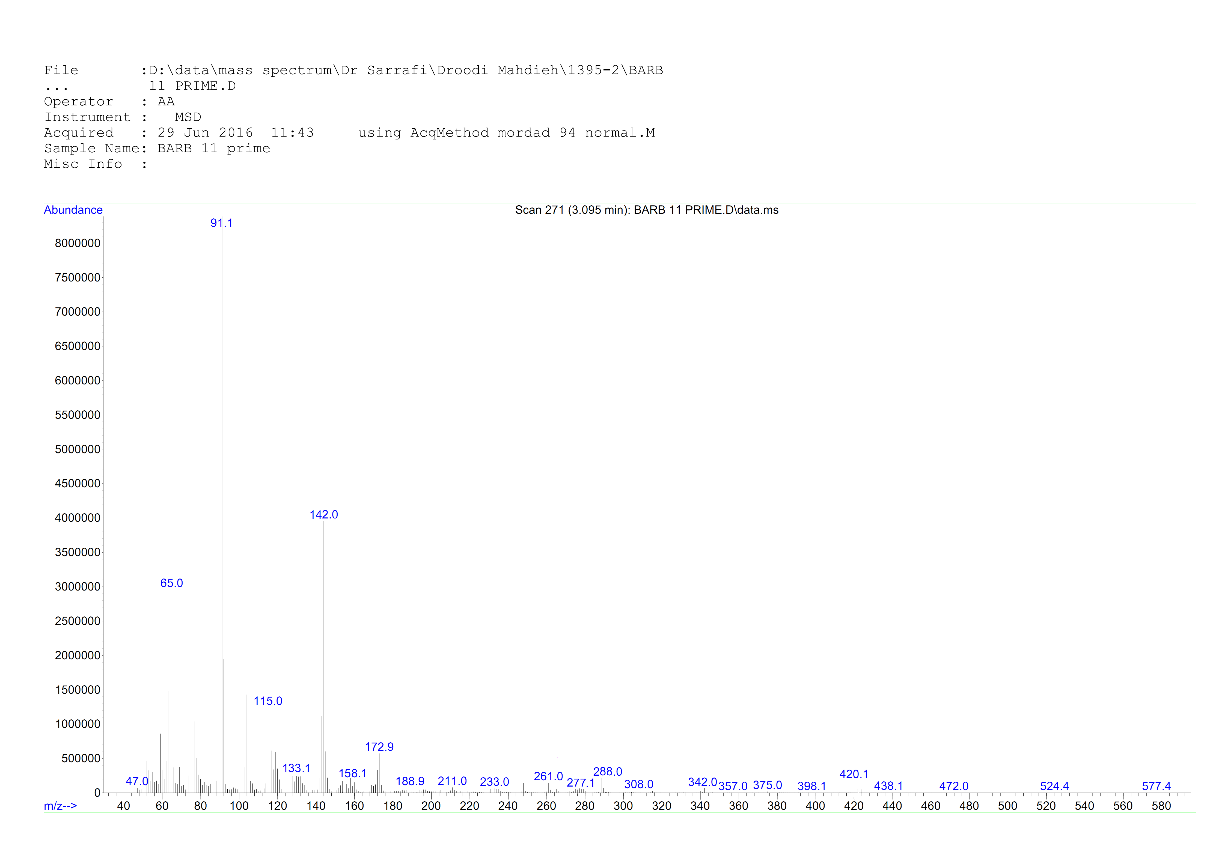
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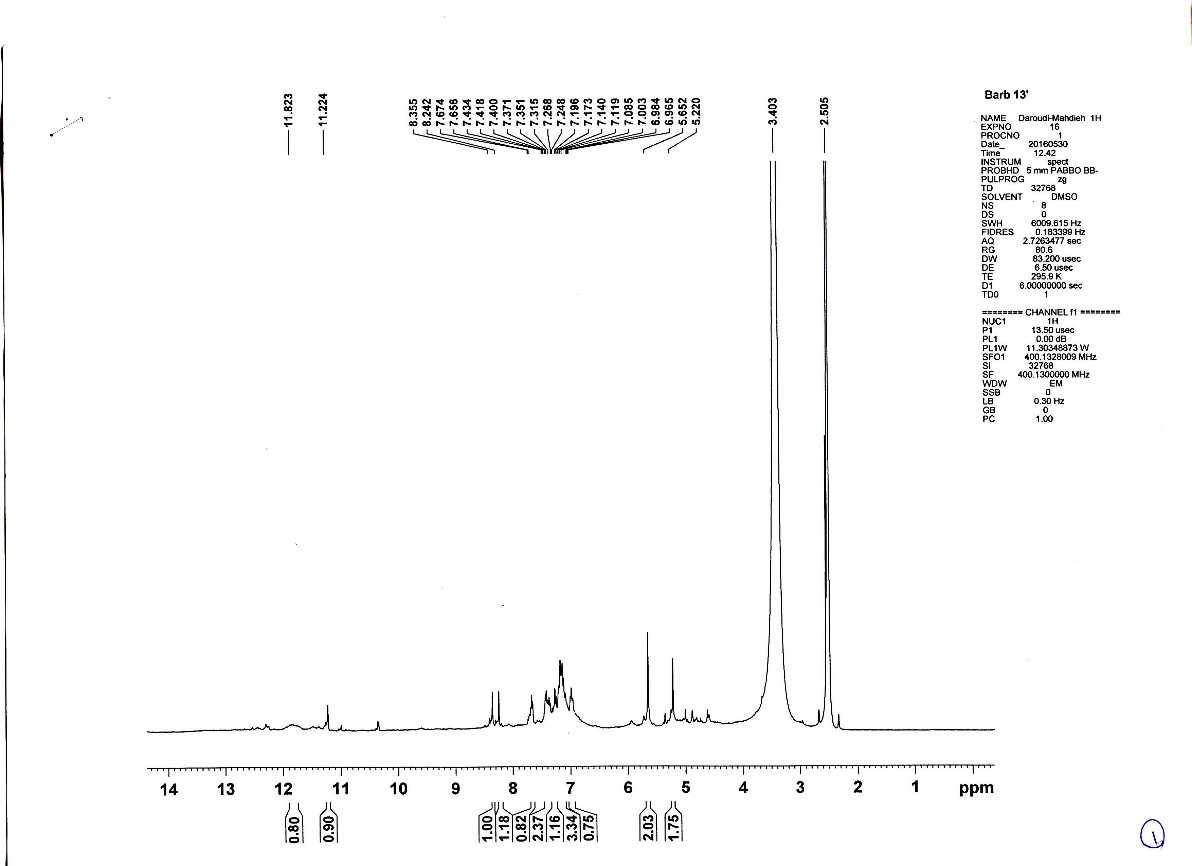
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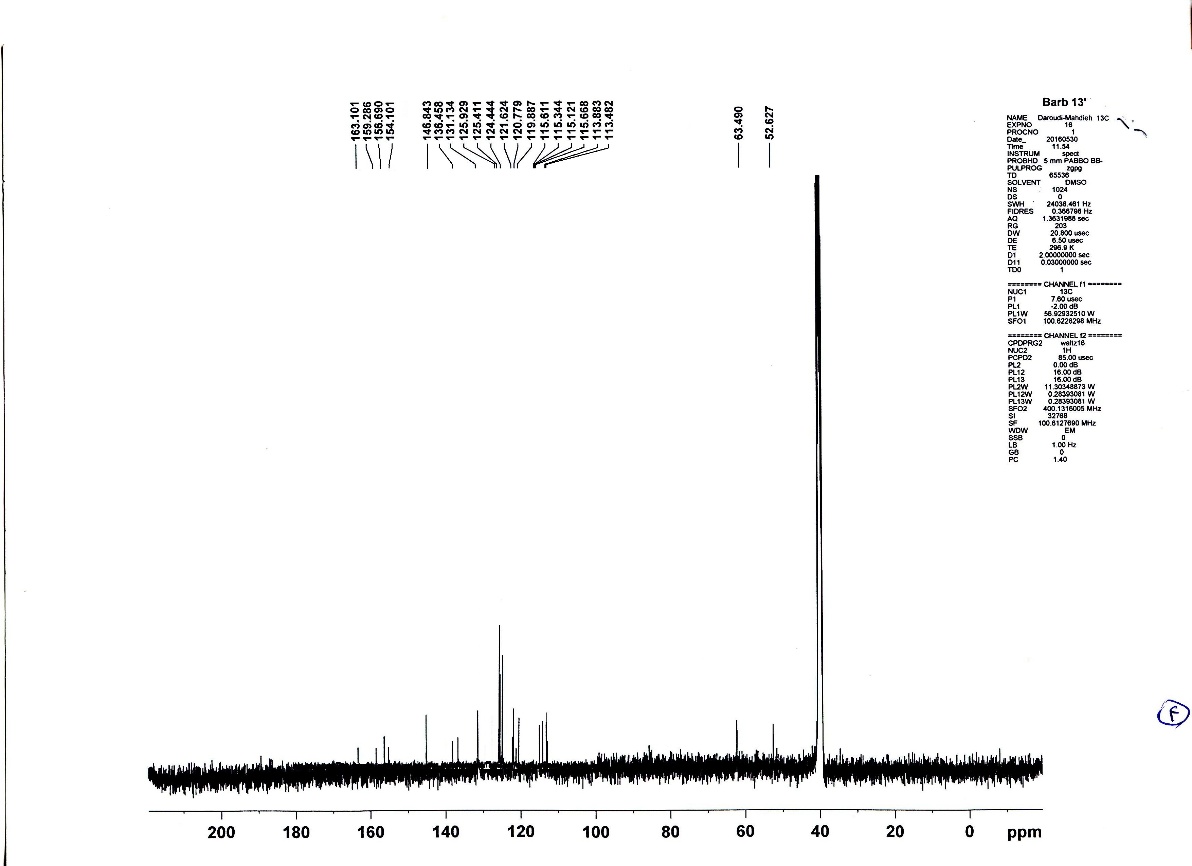
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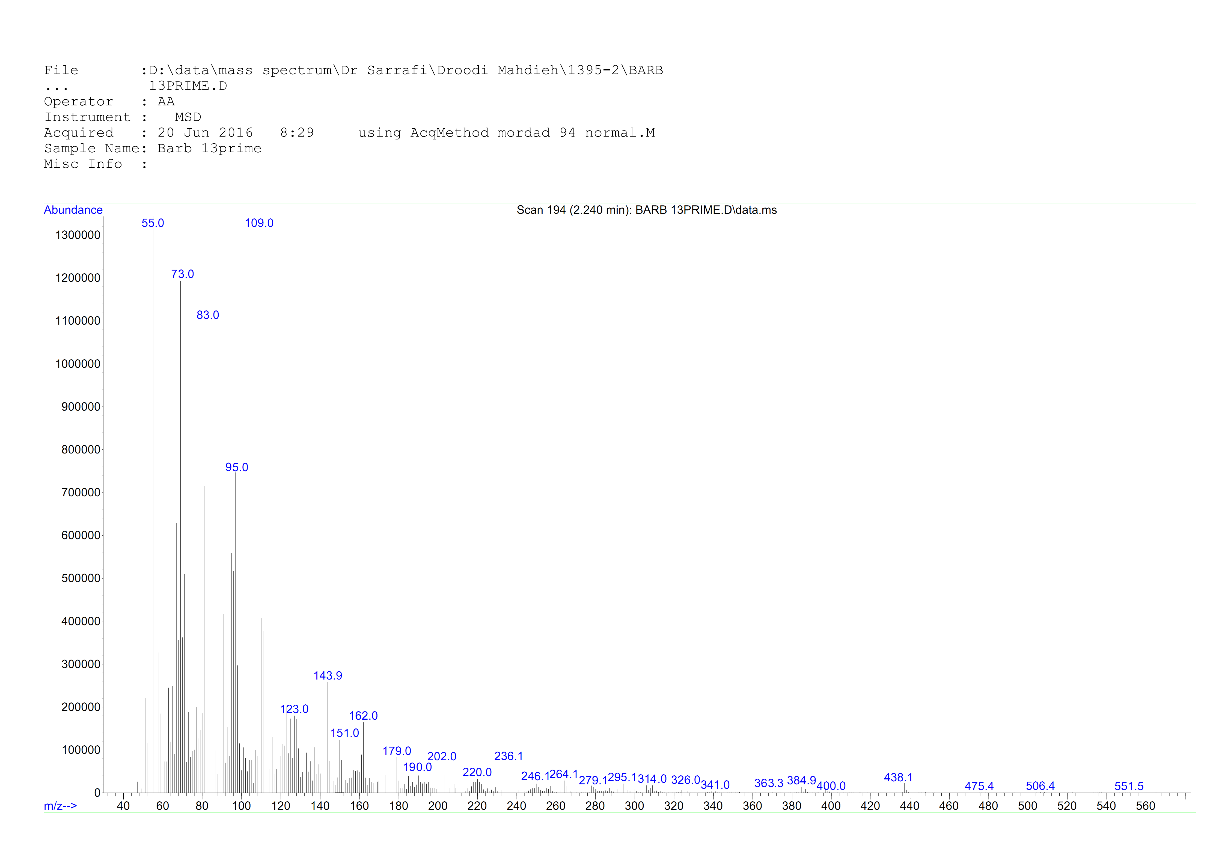
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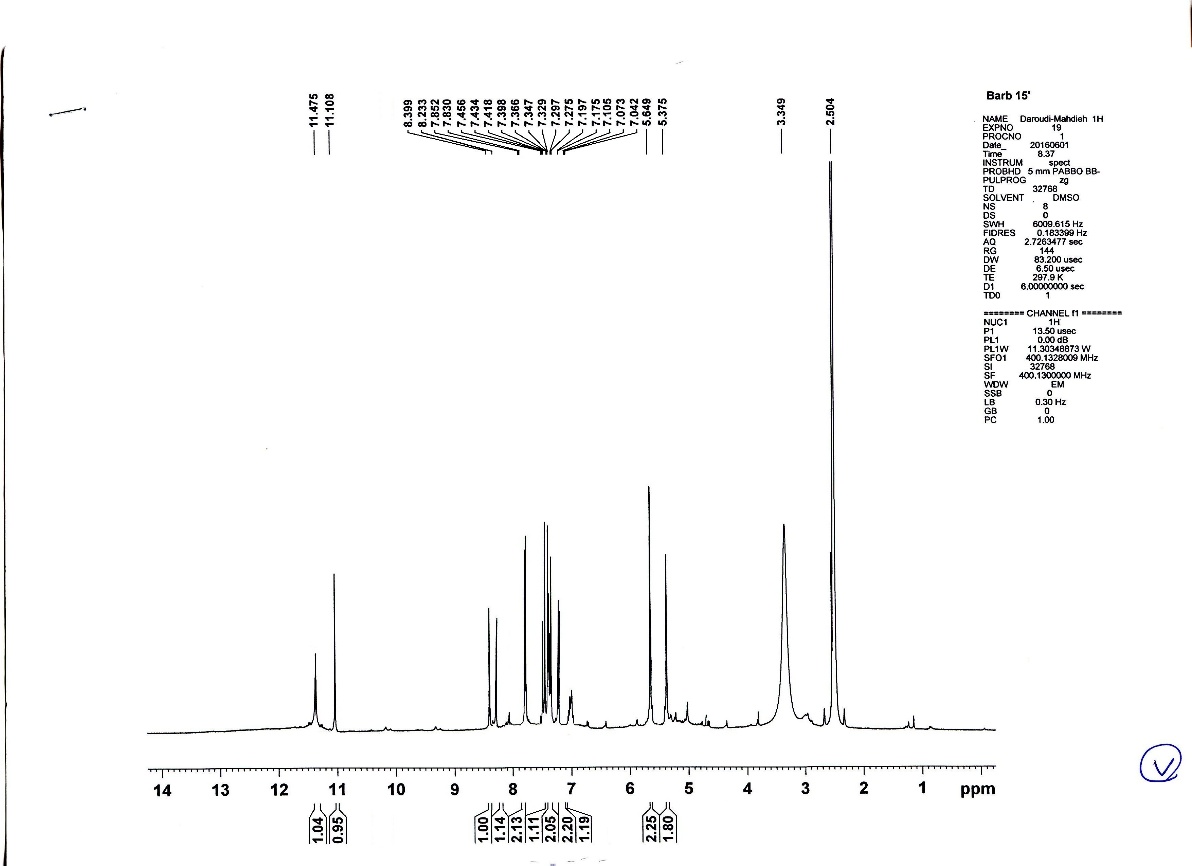
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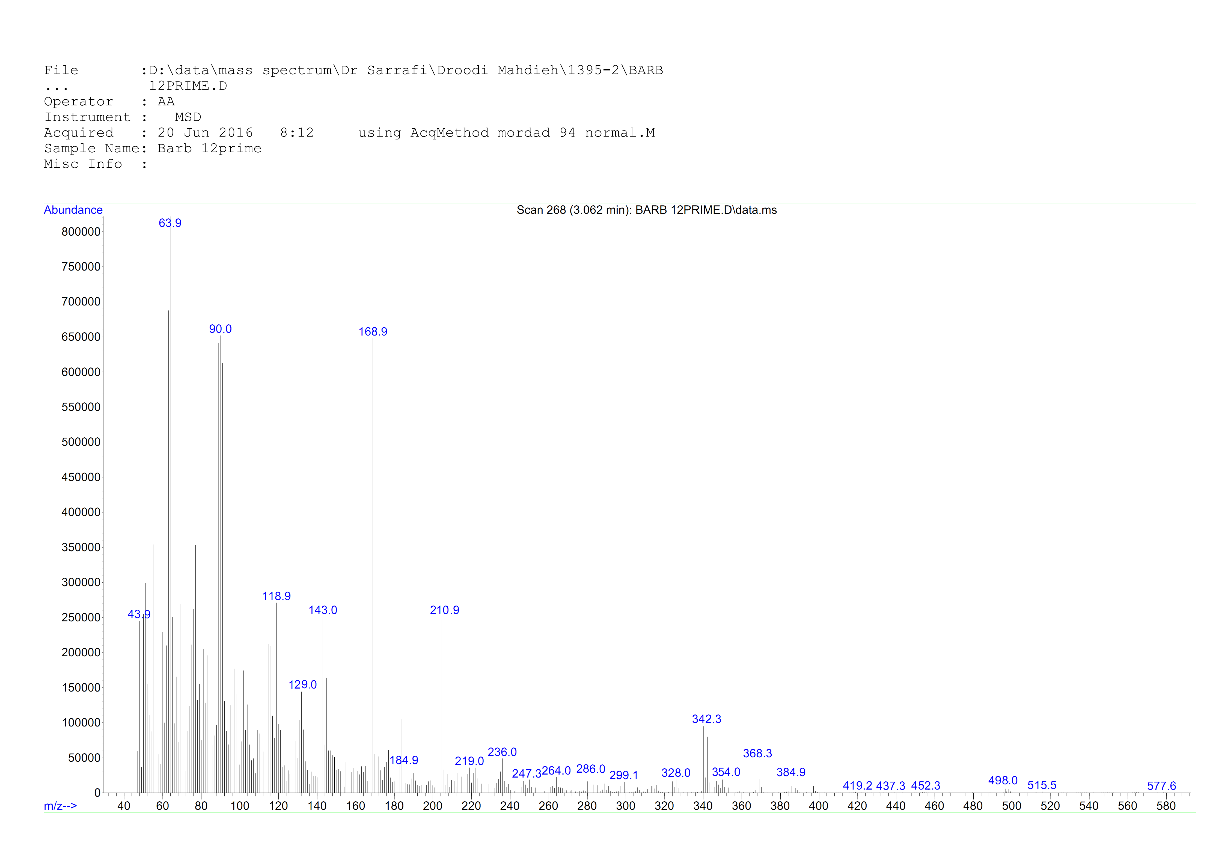
13C-NMR spectrum of 7f



Mass spectrum of 7f



1H-NMR spectrum of 7g



Mass spectrum of 7g

C:\Users\user\Desktop\4.tif

**4**

Input orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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4 6 0 3.835253 1.892306 0.595793

5 7 0 2.780049 2.870306 0.218750

6 1 0 2.806734 3.644736 0.850846

7 7 0 3.797997 0.458488 0.202275

8 1 0 4.144078 0.395078 -0.733784

9 8 0 4.823413 2.304858 1.256785

10 8 0 0.430087 3.063134 0.358360

11 8 0 2.297582 -1.361279 0.329507

12 6 0 -0.028144 0.264400 0.191033

13 1 0 -0.881205 0.910229 0.181456

14 6 0 -0.801079 -1.066960 0.150383

15 6 0 -0.103453 -2.282372 0.146754

16 6 0 -2.202077 -1.063085 0.117024

17 6 0 -0.806824 -3.493909 0.109765

18 1 0 0.966240 -2.285330 0.172222

19 6 0 -2.905448 -2.274623 0.080035

20 6 0 -2.207822 -3.490035 0.076407

21 1 0 -0.274171 -4.421903 0.106995

22 1 0 -3.975141 -2.271665 0.054564

23 1 0 -2.744861 -4.415071 0.048169

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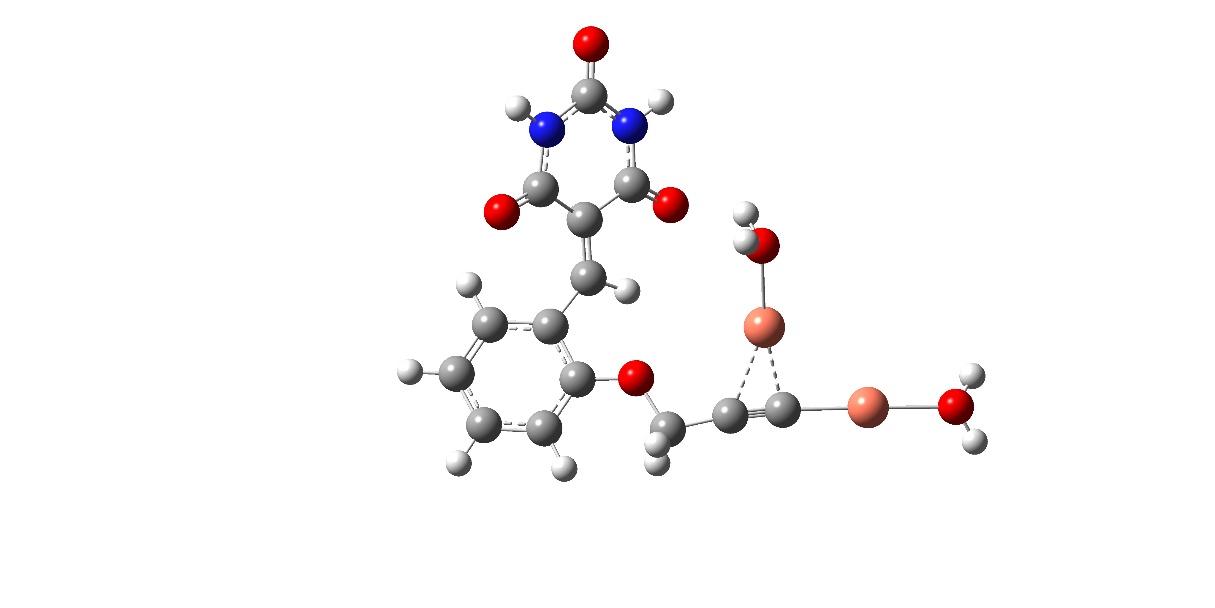
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28 6 0 -5.084733 1.257323 0.046701

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30 1 0 -6.213486 3.228118 0.031481

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**4a**

Input orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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4 6 0 4.224615 -2.962477 0.956830

5 7 0 3.198391 -2.940420 0.055192

6 1 0 2.876781 -3.829830 -0.269528

7 7 0 4.646383 -1.738777 1.392002

8 1 0 5.383321 -1.744744 2.067984

9 8 0 4.718223 -3.986029 1.341787

10 8 0 1.660012 -1.965766 -1.225276

11 8 0 4.624858 0.479420 1.535991

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13 1 0 1.550263 0.317872 -1.030037

14 6 0 2.607720 2.006682 -0.266439

15 6 0 3.860317 2.617173 -0.291641

16 6 0 1.460126 2.819493 -0.220224

17 6 0 3.983867 3.995246 -0.258537

18 1 0 4.738627 2.008710 -0.357164

19 6 0 1.578481 4.200553 -0.159494

20 6 0 2.841118 4.777031 -0.181438

21 1 0 4.956031 4.450873 -0.291367

22 1 0 0.712885 4.830154 -0.100858

23 1 0 2.923961 5.848098 -0.141786

24 8 0 0.283770 2.165599 -0.217357

25 6 0 -0.931772 2.883182 -0.220973

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27 1 0 -1.017746 3.469049 0.684516

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29 6 0 -3.013164 1.200801 -0.451469

30 29 0 -1.906696 -0.069816 0.916000

31 29 0 -4.669058 0.170679 -0.822115

32 8 0 -1.114206 -1.505982 2.171005

33 1 0 -0.887531 -1.260512 3.062233

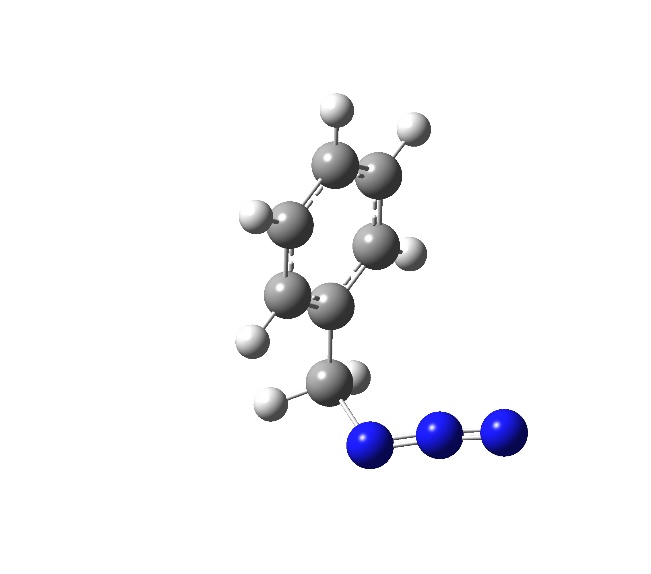
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**6a**

Input orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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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

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13 1 0 1.125855 1.960761 1.111738

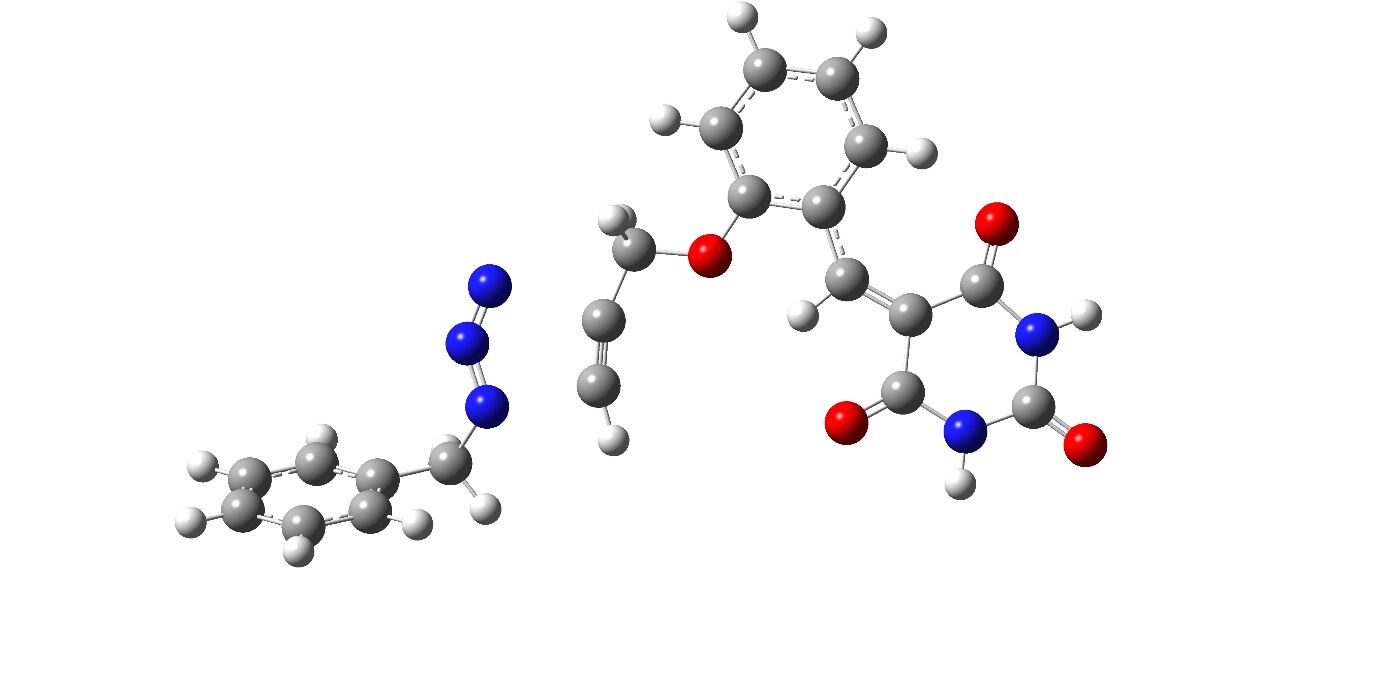
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17 7 0 3.043473 0.877503 -2.737505

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**A**

Input orientation:

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enter Atomic Atomic Coordinates (Angstroms)

umber Number Type X Y Z

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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

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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

19 1 0 2.590119 5.521125 0.344415

20 6 0 5.556703 -0.581335 -0.188413

21 6 0 3.598103 -2.152588 0.259507

22 1 0 4.872639 4.548695 0.576200

23 7 0 6.308735 -1.755004 -0.269594

24 8 0 6.132879 0.485146 -0.378965

25 7 0 4.529030 -3.179201 0.144301

26 8 0 2.425972 -2.434230 0.483476

27 6 0 5.881404 -3.060932 -0.116525

28 1 0 7.294455 -1.633426 -0.474686

29 1 0 4.176442 -4.123109 0.257844

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32 6 0 -1.947741 -0.404112 -0.314976

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37 6 0 -6.684715 -1.614070 0.847447

38 6 0 -7.521135 -0.313383 -1.007139

39 6 0 -7.948483 -1.589233 1.436619

40 1 0 -5.865363 -2.130044 1.342283

41 6 0 -8.789471 -0.290316 -0.420185

42 1 0 -7.356888 0.184187 -1.960014

43 6 0 -9.005117 -0.927030 0.803041

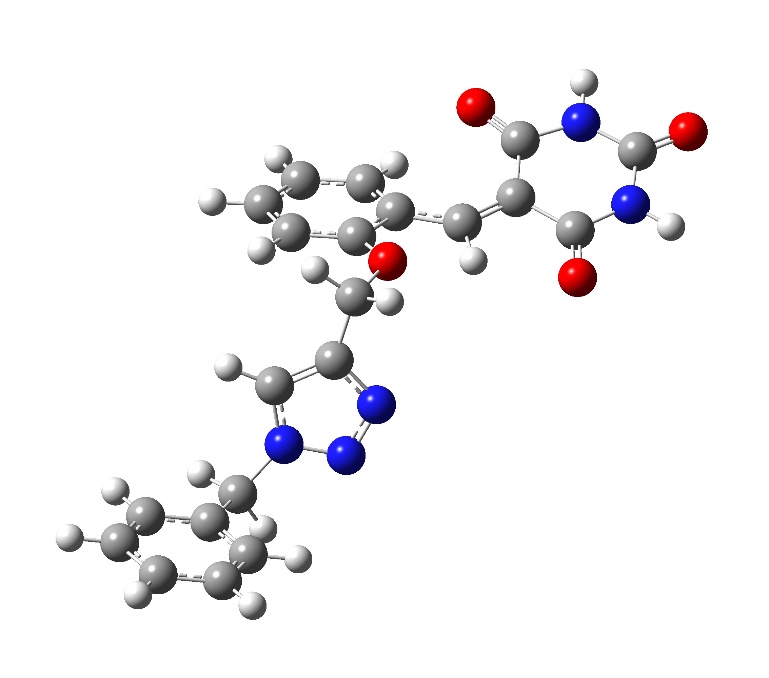
44 1 0 -8.111192 -2.089772 2.387293

45 1 0 -9.605616 0.224907 -0.919325

46 1 0 -9.990346 -0.910307 1.260886

47 1 0 -4.676178 -2.008096 -1.020990

--------------------------------------------------------------------



**B**

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type 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

19 6 0 4.318931 -1.815832 -0.016923

20 1 0 2.076364 4.493036 -1.168502

21 7 0 6.535610 -0.127066 -0.207181

22 8 0 5.310491 1.761244 -0.108796

23 7 0 5.632408 -2.260925 -0.120747

24 8 0 3.414124 -2.637702 0.075559

25 6 0 6.776019 -1.488975 -0.213933

26 1 0 7.355930 0.466875 -0.261007

27 1 0 5.770862 -3.265437 -0.117098

28 8 0 7.895968 -1.965862 -0.294511

29 1 0 -0.809495 -0.874758 2.485855

30 7 0 -3.467149 -0.292279 -0.724010

31 7 0 -2.697724 -1.378675 -0.960329

32 7 0 -1.726593 -1.373106 -0.086018

33 1 0 -3.449254 1.322198 0.677150

34 6 0 -4.671083 -0.048952 -1.529028

35 6 0 -5.954225 -0.320119 -0.768499

36 1 0 -4.570830 -0.707278 -2.395489

37 6 0 -6.250306 -1.613572 -0.315615

38 6 0 -6.860388 0.715671 -0.518266

39 6 0 -7.433295 -1.863717 0.378721

40 1 0 -5.549754 -2.423135 -0.505402

41 6 0 -8.048860 0.465151 0.173445

42 1 0 -6.638699 1.721422 -0.866878

43 6 0 -8.336272 -0.823985 0.624059

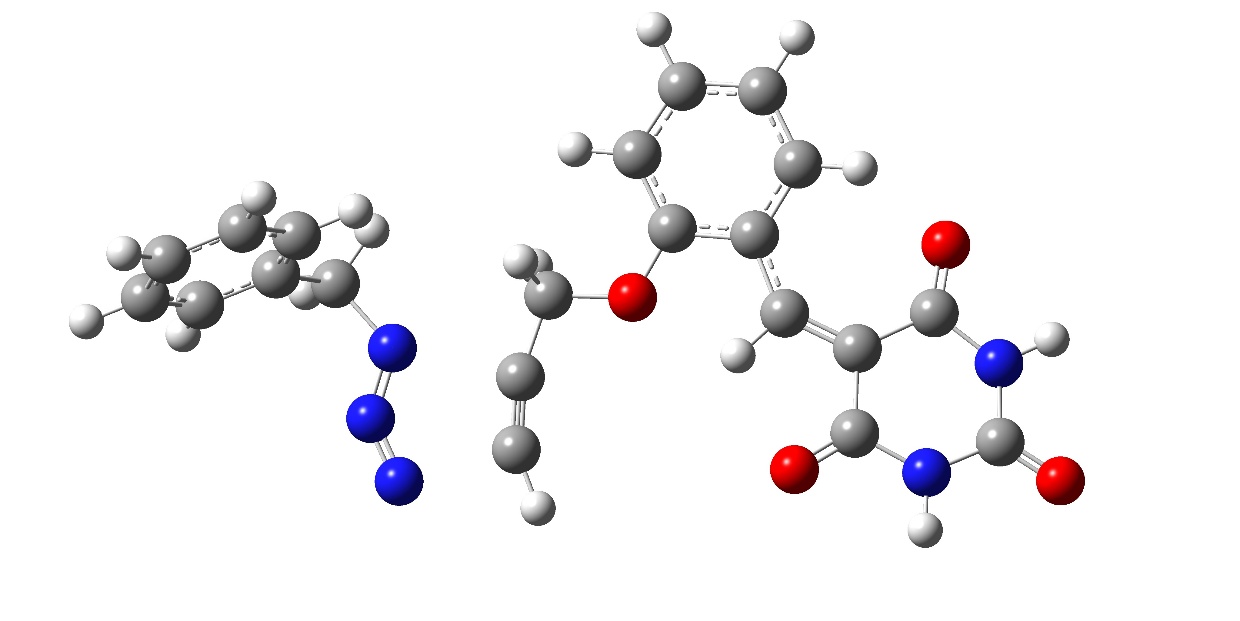
44 1 0 -7.653392 -2.869612 0.725447

45 1 0 -8.745489 1.277615 0.360406

46 1 0 -9.258917 -1.020233 1.163182

47 1 0 -4.638319 0.984743 -1.881766

---------------------------------------------------------------------



**C**

Input orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type 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

19 1 0 0.161350 4.861510 -0.490943

20 6 0 5.337101 0.505676 -0.067270

21 6 0 4.179887 -1.653434 0.649098

22 1 0 2.590671 4.944721 0.056725

23 7 0 6.509362 -0.246549 0.026356

24 8 0 5.426335 1.673048 -0.432809

25 7 0 5.456356 -2.203806 0.684347

26 8 0 3.217464 -2.358717 0.930444

27 6 0 6.651020 -1.573718 0.388168

28 1 0 7.366684 0.241288 -0.209433

29 1 0 5.520024 -3.180251 0.950393

30 8 0 7.731900 -2.136709 0.440685

31 1 0 -1.479333 0.677031 -1.634355

32 6 0 -1.515738 -2.451383 -0.633577

33 6 0 -4.830437 0.072337 -1.305885

34 6 0 -5.850848 0.140537 -0.187084

35 1 0 -5.318582 -0.123803 -2.267117

36 6 0 -7.089273 -0.499187 -0.319750

37 6 0 -5.561733 0.822379 1.002772

38 6 0 -8.023180 -0.461242 0.718550

39 1 0 -7.325687 -1.026434 -1.241130

40 6 0 -6.492162 0.860765 2.041952

41 1 0 -4.604850 1.327195 1.114152

42 6 0 -7.725699 0.217797 1.901989

43 1 0 -8.982035 -0.958725 0.600893

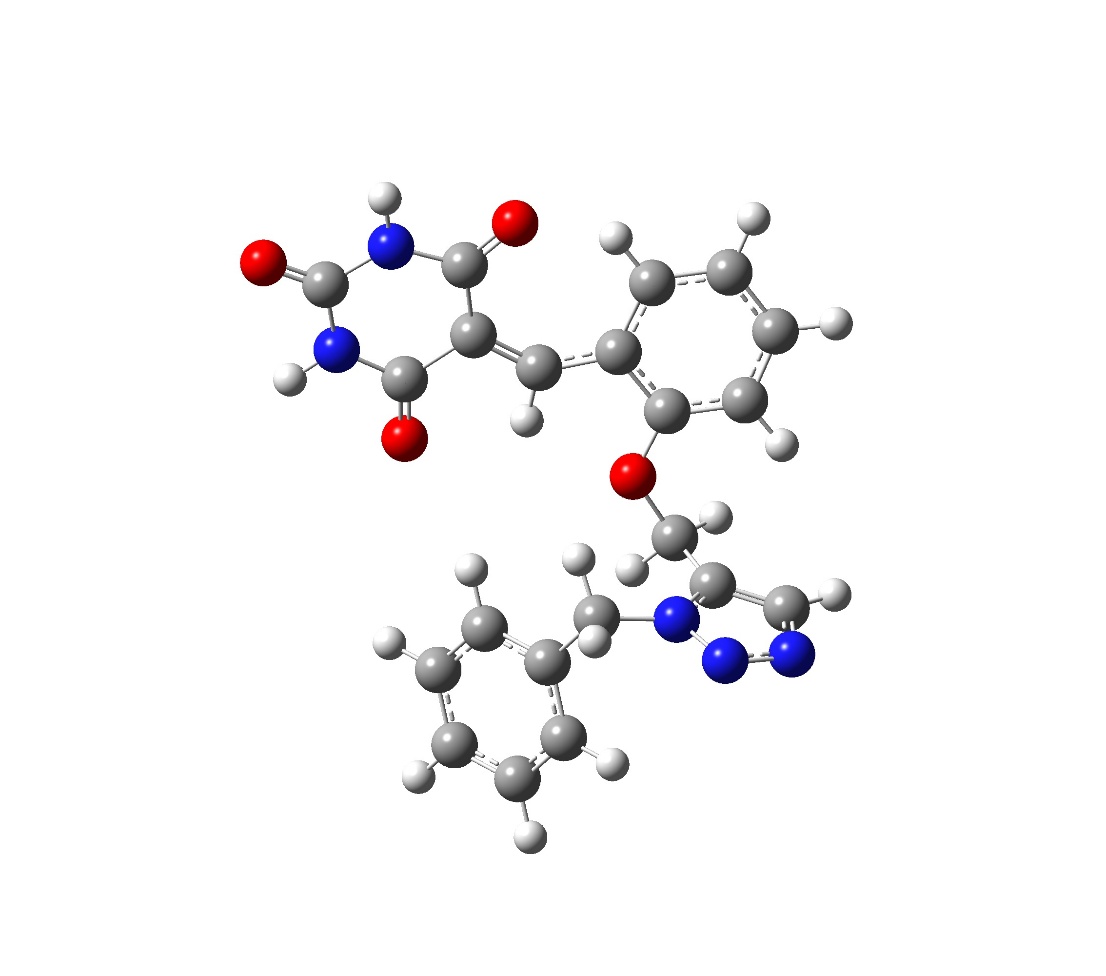
44 1 0 -6.257266 1.395765 2.958131

45 1 0 -8.451811 0.249958 2.709671

46 1 0 -4.296908 1.021758 -1.397708

47 1 0 -1.057439 -3.411108 -0.518504

---------------------------------------------------------------------



**D**

Input orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type 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

18 6 0 -4.166660 0.347882 0.442606

19 6 0 -2.782434 -1.635905 -0.365344

20 1 0 -2.268296 5.195761 -0.201398

21 7 0 -5.147099 -0.611407 0.702281

22 8 0 -4.421849 1.516599 0.716542

23 7 0 -3.889841 -2.409621 -0.042269

24 8 0 -1.783536 -2.188064 -0.817256

25 6 0 -5.090014 -1.976484 0.492063

26 1 0 -6.012054 -0.260402 1.098862

27 1 0 -3.806406 -3.407317 -0.203292

28 8 0 -6.012765 -2.729857 0.753674

29 1 0 2.415039 0.120972 -1.717746

30 7 0 4.678744 2.038973 1.333333

31 7 0 4.115212 0.982379 1.866513

32 7 0 3.171509 0.540652 1.009571

33 1 0 4.394347 3.112386 -0.494701

34 6 0 2.399593 -0.664646 1.338658

35 6 0 2.788730 -1.868582 0.500552

36 1 0 1.339721 -0.434476 1.217526

37 6 0 4.124637 -2.289282 0.437117

38 6 0 1.809968 -2.588234 -0.194816

39 6 0 4.475374 -3.412500 -0.311112

40 1 0 4.889538 -1.734136 0.974157

41 6 0 2.162026 -3.718018 -0.939757

42 1 0 0.769910 -2.273273 -0.155478

43 6 0 3.493365 -4.130916 -1.000817

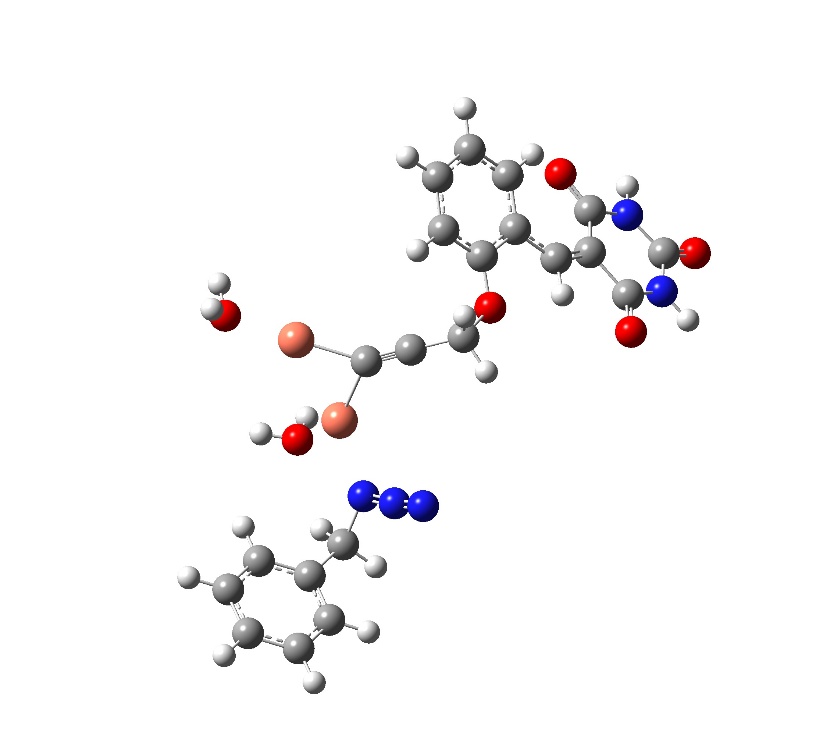
44 1 0 5.513686 -3.729542 -0.354596

45 1 0 1.394023 -4.269382 -1.475081

46 1 0 3.767239 -5.006616 -1.582794

47 1 0 2.592377 -0.839419 2.400230

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**E**

Standard orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type 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

19 6 0 -2.260196 2.758547 -1.390188

20 6 0 -4.441331 -0.204663 -0.694011

21 6 0 -4.867702 2.292380 -0.482076

22 6 0 -3.119547 3.823044 -1.118723

23 1 0 -1.248603 2.962395 -1.717938

24 6 0 -5.460780 -0.926051 -0.123168

25 1 0 -3.772300 -0.853786 -1.253024

26 6 0 -4.424074 3.594183 -0.670564

27 1 0 -5.871166 2.104886 -0.129971

28 1 0 -2.759654 4.838649 -1.257324

29 6 0 -6.481871 -0.437348 0.824399

30 6 0 -5.442510 -2.377997 -0.467908

31 1 0 -5.088215 4.428489 -0.468514

32 7 0 -7.369034 -1.403355 1.302684

33 8 0 -6.603689 0.712943 1.233284

34 7 0 -6.429302 -3.162033 0.119446

35 8 0 -4.632869 -2.903651 -1.224041

36 6 0 -7.410596 -2.753345 1.004310

37 1 0 -8.068971 -1.073942 1.958563

38 1 0 -6.425200 -4.147508 -0.119418

39 8 0 -8.237572 -3.514148 1.479469

40 1 0 -0.418966 -0.487119 -2.483001

41 6 0 4.497487 -2.292731 0.805189

42 6 0 5.912717 -2.103235 0.314400

43 1 0 4.191327 -3.342112 0.749362

44 6 0 6.638829 -0.956252 0.669550

45 6 0 6.511503 -3.059809 -0.515802

46 6 0 7.938240 -0.768471 0.198466

47 1 0 6.185289 -0.212195 1.320080

48 6 0 7.813980 -2.873603 -0.986761

49 1 0 5.961749 -3.957704 -0.787510

50 6 0 8.528061 -1.727433 -0.631776

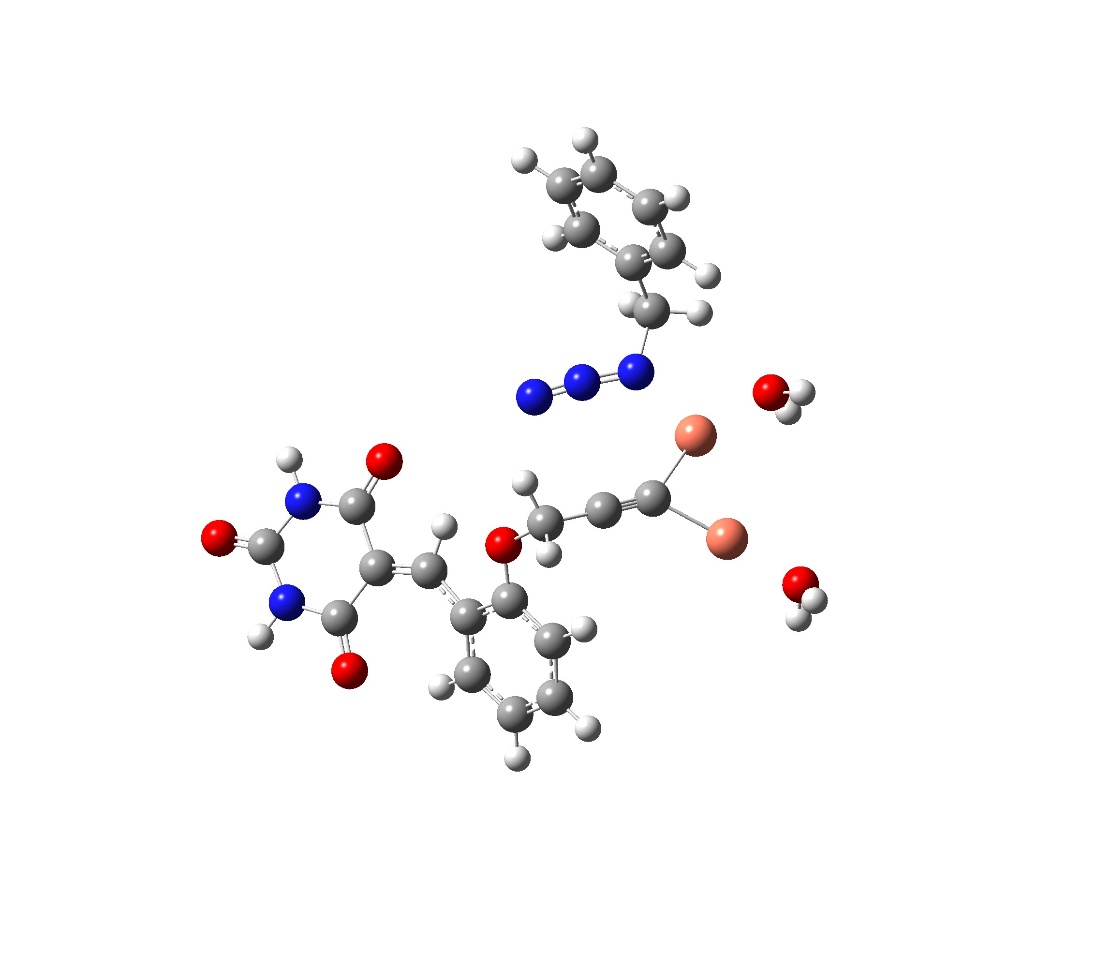
51 1 0 8.493031 0.121260 0.482943

52 1 0 8.269231 -3.624765 -1.626035

53 1 0 9.541493 -1.582597 -0.995530

54 1 0 4.372483 -1.945981 1.830847

---------------------------------------------------------------------



**F**

Standard orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 1.828151 -1.716749 0.575559

2 6 0 0.915357 -1.448621 1.360346

3 7 0 2.697589 1.194375 -0.936899

4 7 0 1.628680 1.613681 -0.461657

5 7 0 0.624293 1.878112 0.002625

6 29 0 3.166204 -0.869967 -0.594047

7 29 0 2.616042 -3.326139 -0.121204

8 8 0 4.905342 -0.830931 -1.704881

9 1 0 5.624530 -1.331070 -1.281343

10 1 0 4.787837 -1.245807 -2.577322

11 8 0 3.325621 -5.032176 -0.775267

12 1 0 2.717074 -5.519009 -1.358973

13 1 0 3.576399 -5.658376 -0.073363

14 6 0 -0.158866 -1.112591 2.292053

15 8 0 -1.416379 -0.837567 1.646446

16 1 0 -0.289316 -1.897973 3.045778

17 6 0 -2.127104 -1.850155 1.080322

18 6 0 -3.317616 -1.463788 0.384124

19 6 0 -1.767335 -3.197861 1.179380

20 6 0 -3.551617 -0.044465 0.233721

21 6 0 -4.104695 -2.487347 -0.190340

22 6 0 -2.573967 -4.174022 0.594614

23 1 0 -0.867164 -3.497031 1.701127

24 6 0 -4.616797 0.758716 -0.089320

25 1 0 -2.657843 0.546089 0.417694

26 6 0 -3.739186 -3.823157 -0.094176

27 1 0 -5.004061 -2.206220 -0.717796

28 1 0 -2.284324 -5.217451 0.681863

29 6 0 -6.026671 0.348758 -0.246295

30 6 0 -4.277404 2.208112 -0.190700

31 1 0 -4.355102 -4.589100 -0.554523

32 7 0 -6.929478 1.385541 -0.489371

33 8 0 -6.464783 -0.793784 -0.161762

34 7 0 -5.336520 3.070296 -0.451658

35 8 0 -3.148133 2.669339 -0.065776

36 6 0 -6.670552 2.739291 -0.606057

37 1 0 -7.900742 1.110949 -0.588620

38 1 0 -5.108967 4.055515 -0.527588

39 8 0 -7.540318 3.566078 -0.825982

40 1 0 0.073924 -0.185573 2.822860

41 6 0 3.631302 2.245321 -1.478710

42 6 0 4.143647 3.179086 -0.408255

43 1 0 3.113514 2.791949 -2.273287

44 6 0 5.177041 2.773135 0.449681

45 6 0 3.580227 4.451307 -0.244503

46 6 0 5.634718 3.623799 1.456129

47 1 0 5.625076 1.790215 0.323364

48 6 0 4.039078 5.304829 0.762421

49 1 0 2.786710 4.779089 -0.911841

50 6 0 5.065278 4.891630 1.614611

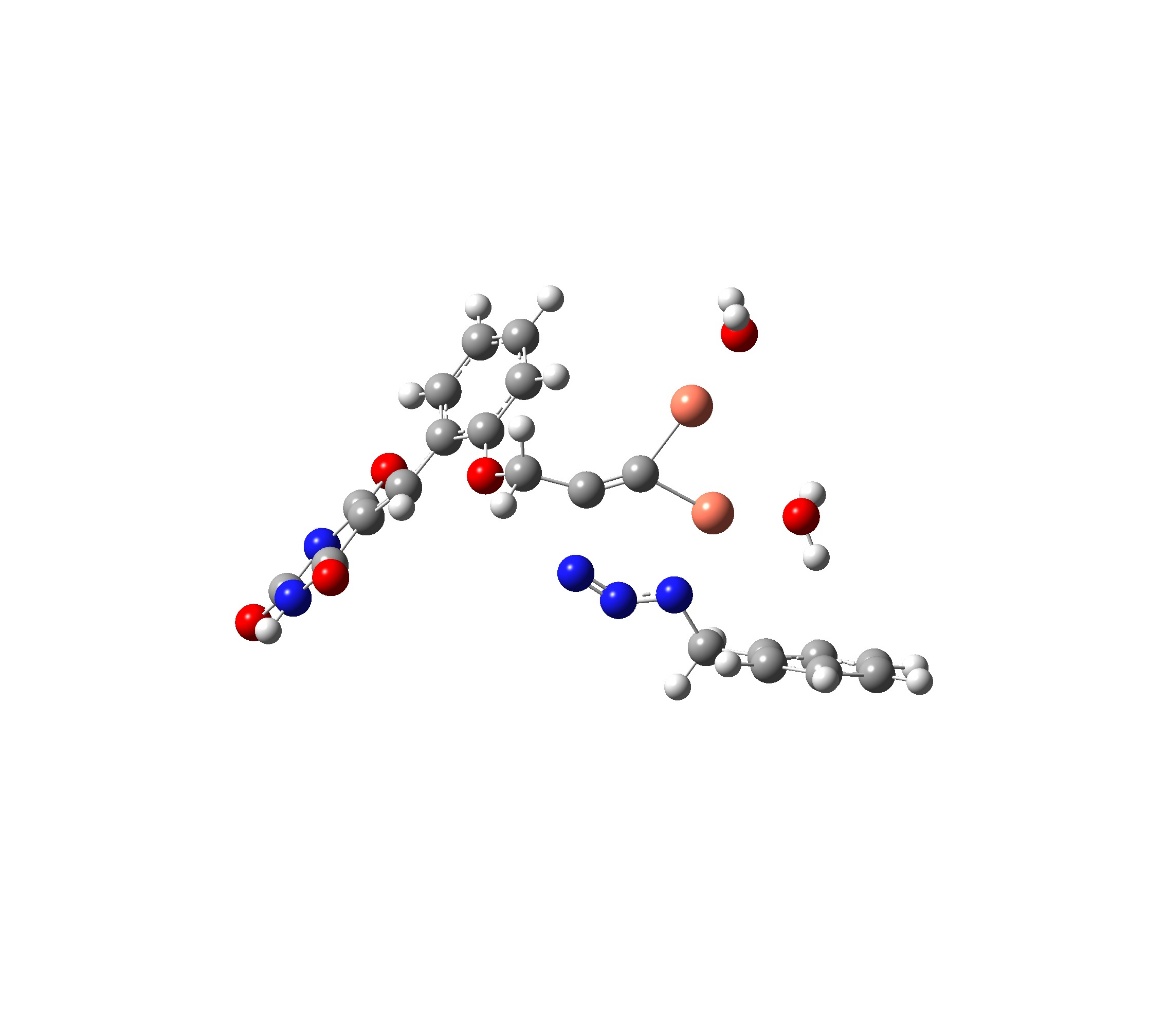
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52 1 0 3.597549 6.290782 0.877113

53 1 0 5.424262 5.555179 2.396409

54 1 0 4.436414 1.660285 -1.922768

---------------------------------------------------------------------



**G**

Standard orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 1.718796 1.201375 0.758062

2 6 0 0.686396 0.834255 1.386924

3 7 0 2.340869 -1.579531 0.099843

4 7 0 1.288639 -1.701351 0.797052

5 7 0 0.494777 -1.071783 1.404672

6 29 0 3.072206 0.290087 -0.255132

7 29 0 2.731811 2.770318 0.317142

8 8 0 4.730495 0.199345 -1.398056

9 1 0 5.076248 -0.709763 -1.506762

10 1 0 4.604112 0.546579 -2.298239

11 8 0 3.683438 4.439115 -0.050265

12 1 0 3.210958 5.062926 -0.629526

13 1 0 3.935804 4.947733 0.740673

14 6 0 -0.524301 1.214290 2.164729

15 8 0 -1.741970 0.935900 1.462590

16 1 0 -0.593646 0.609577 3.070083

17 6 0 -2.184533 1.768778 0.482169

18 6 0 -3.444338 1.423563 -0.106709

19 6 0 -1.481333 2.895811 0.045814

20 6 0 -4.149145 0.302361 0.474861

21 6 0 -3.945482 2.264749 -1.125804

22 6 0 -2.017600 3.699572 -0.960241

23 1 0 -0.519071 3.149655 0.471170

24 6 0 -5.192131 -0.514053 0.114191

25 1 0 -3.763032 0.031594 1.454168

26 6 0 -3.249779 3.391009 -1.544153

27 1 0 -4.895799 2.014957 -1.573653

28 1 0 -1.461094 4.573015 -1.288494

29 6 0 -5.872815 -0.567420 -1.194918

30 6 0 -5.586684 -1.496130 1.166204

31 1 0 -3.662567 4.026595 -2.321065

32 7 0 -6.858195 -1.548380 -1.319400

33 8 0 -5.637991 0.144700 -2.165747

34 7 0 -6.604869 -2.381262 0.829835

35 8 0 -5.082380 -1.560807 2.281929

36 6 0 -7.276353 -2.469522 -0.376085

37 1 0 -7.324115 -1.594781 -2.219049

38 1 0 -6.881665 -3.044710 1.545012

39 8 0 -8.157347 -3.286128 -0.589386

40 1 0 -0.473911 2.269900 2.447464

41 6 0 2.885960 -2.813709 -0.521666

42 6 0 4.394366 -2.866220 -0.399112

43 1 0 2.592169 -2.833778 -1.576700

44 6 0 5.195000 -2.985097 -1.545556

45 6 0 5.013479 -2.804649 0.858645

46 6 0 6.590436 -3.040805 -1.437047

47 1 0 4.725752 -3.048627 -2.524898

48 6 0 6.403392 -2.860663 0.966510

49 1 0 4.403635 -2.712448 1.753490

50 6 0 7.195791 -2.976812 -0.180640

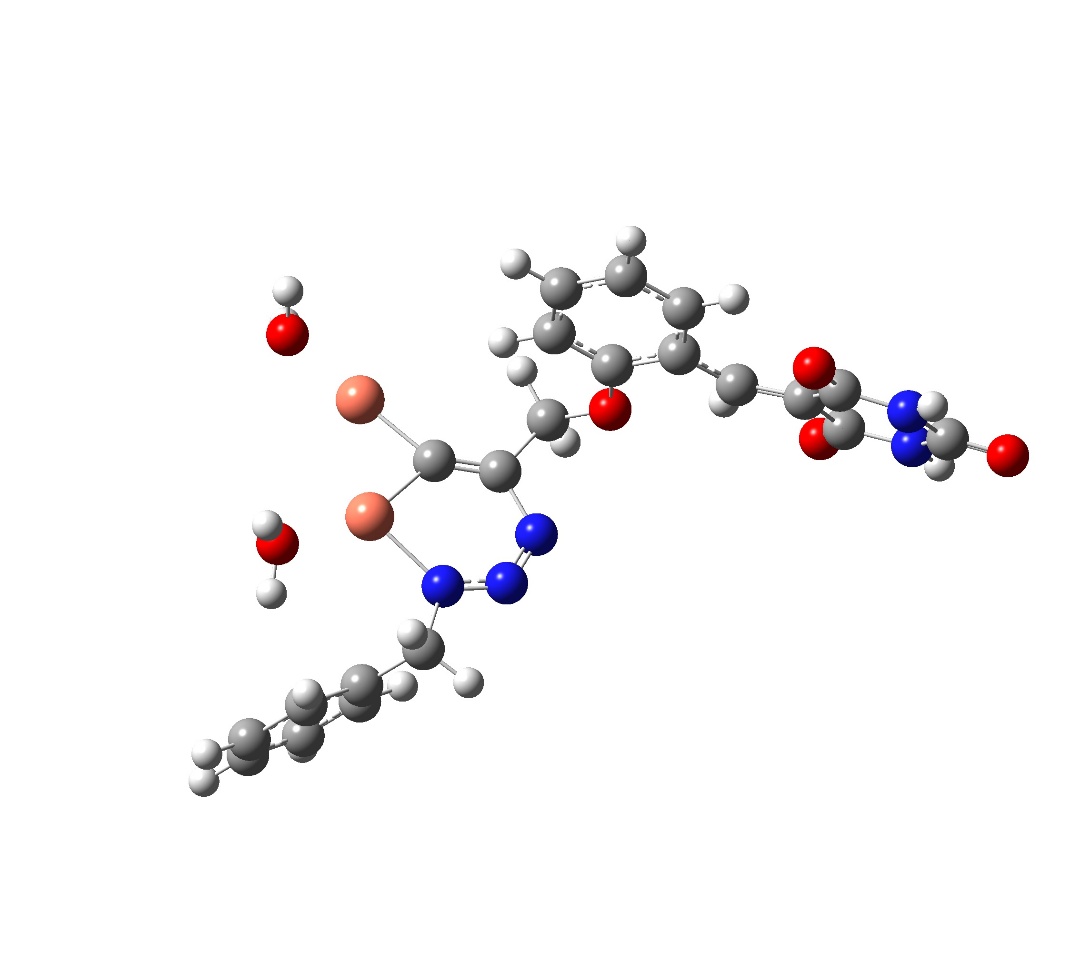
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52 1 0 6.869606 -2.814367 1.946604

53 1 0 8.277595 -3.018457 -0.093918

54 1 0 2.428539 -3.678203 -0.030938

---------------------------------------------------------------------



**H**

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -2.929099 -0.379280 0.196293

2 6 0 -1.730852 0.151193 0.424685

3 7 0 -3.116810 1.408074 -1.551761

4 7 0 -2.009687 1.804129 -1.249211

5 7 0 -1.250867 1.302847 -0.278378

6 29 0 -4.358228 0.083493 -0.927552

7 29 0 -3.973369 -1.799603 0.917307

8 8 0 -6.199297 -0.004958 -1.730719

9 1 0 -6.741545 0.786336 -1.566677

10 1 0 -6.209188 -0.134762 -2.695239

11 8 0 -5.062976 -3.252720 1.647843

12 1 0 -4.718899 -4.145610 1.467636

13 1 0 -5.199325 -3.209138 2.610977

14 6 0 -0.791866 -0.413174 1.485188

15 8 0 0.512743 -0.732902 0.985349

16 1 0 -0.607892 0.329872 2.265548

17 6 0 0.771119 -1.924888 0.375399

18 6 0 2.144337 -2.173407 0.061649

19 6 0 -0.215144 -2.857462 0.046108

20 6 0 3.111165 -1.204812 0.533443

21 6 0 2.462510 -3.394424 -0.573021

22 6 0 0.145096 -4.052928 -0.576619

23 1 0 -1.258213 -2.656952 0.253495

24 6 0 4.404904 -0.873566 0.223330

25 1 0 2.725143 -0.581678 1.336250

26 6 0 1.481406 -4.327708 -0.881183

27 1 0 3.496949 -3.596537 -0.808309

28 1 0 -0.631335 -4.769888 -0.828294

29 6 0 5.199185 -1.374409 -0.917043

30 6 0 4.993403 0.180369 1.100387

31 1 0 1.753617 -5.264195 -1.357389

32 7 0 6.466930 -0.807795 -1.058041

33 8 0 4.838002 -2.207348 -1.741172

34 7 0 6.283212 0.591062 0.784005

35 8 0 4.421186 0.684913 2.060036

36 6 0 7.069747 0.153762 -0.266765

37 1 0 7.015257 -1.140774 -1.843637

38 1 0 6.691145 1.302049 1.381001

39 8 0 8.193899 0.578080 -0.477471

40 1 0 -1.249252 -1.284123 1.954459

41 6 0 0.046100 2.001412 -0.082427

42 6 0 -0.115252 3.500056 0.064857

43 1 0 0.698184 1.762588 -0.927538

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

---------------------------------------------------------------------



**I**

Standard orientation:

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type 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

9 8 0 1.246358 1.869150 -0.453884

10 1 0 -0.081813 3.380721 -1.017091

11 6 0 2.429792 2.507497 -0.317541

12 6 0 3.596404 1.677296 -0.236952

13 6 0 2.553292 3.902662 -0.284210

14 6 0 3.381999 0.260122 -0.084217

15 6 0 4.858081 2.312573 -0.147850

16 6 0 3.815378 4.484020 -0.185133

17 1 0 1.676528 4.534467 -0.348946

18 6 0 4.153111 -0.868303 -0.253660

19 1 0 2.378427 0.027211 0.262970

20 6 0 4.969783 3.693997 -0.115315

21 1 0 5.742204 1.695677 -0.083071

22 1 0 3.896255 5.567250 -0.166177

23 6 0 5.450451 -0.934182 -0.957119

24 6 0 3.536763 -2.130510 0.210703

25 1 0 5.946698 4.158587 -0.028244

26 7 0 5.971929 -2.218419 -1.136276

27 8 0 6.074585 0.016186 -1.413729

28 7 0 4.217666 -3.297614 -0.071111

29 8 0 2.467249 -2.215027 0.828975

30 6 0 5.430769 -3.422873 -0.734821

31 1 0 6.853729 -2.271678 -1.634827

32 1 0 3.799486 -4.160497 0.260191

33 8 0 5.962765 -4.500649 -0.935664

34 1 0 0.075258 3.089759 0.740890

35 8 0 -4.985737 -0.303788 1.966964

36 1 0 -4.948284 -0.903637 2.733017

37 8 0 1.088670 -1.050093 2.843207

38 1 0 0.726183 -1.760706 3.400000

39 1 0 1.677684 -1.490777 2.177029

40 1 0 -5.434840 -0.806570 1.256469

41 6 0 -3.542132 -1.229578 -1.092307

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

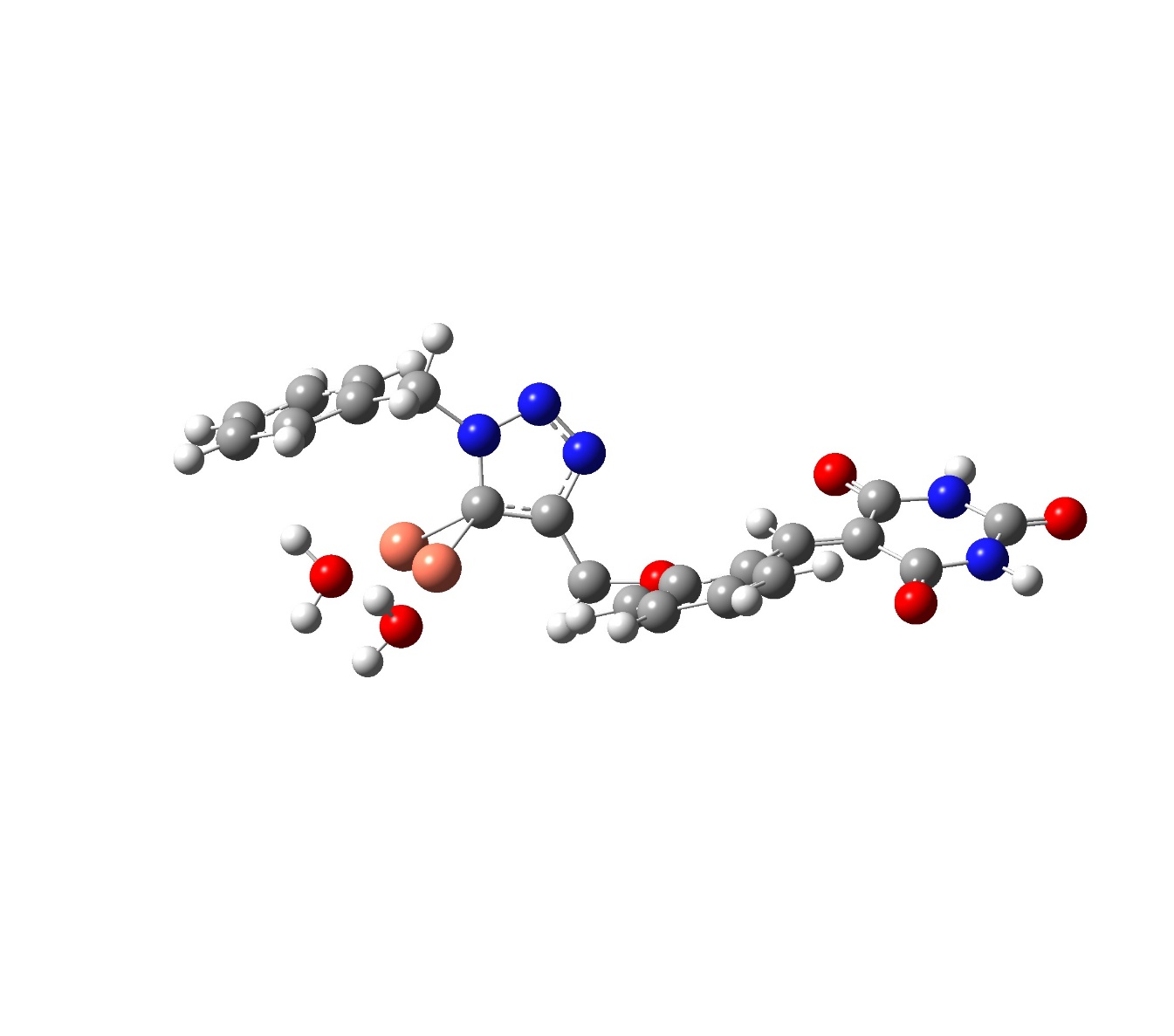
50 6 0 -7.778876 -0.671785 -1.442143

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 Atomic Atomic Coordinates (Angstroms)

Number Number Type 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

8 6 0 1.171471 2.384168 0.163184

9 6 0 3.985731 -0.077863 0.023029

10 6 0 3.802539 2.319651 -0.792062

11 6 0 1.708135 3.478496 -0.514249

12 1 0 0.156522 2.434213 0.536191

13 6 0 5.291642 -0.496560 0.002479

14 1 0 3.303149 -0.910082 0.176521

15 6 0 3.020103 3.447820 -0.998257

16 1 0 4.817347 2.287807 -1.160414

17 1 0 1.092796 4.361936 -0.660657

18 6 0 6.495174 0.359155 -0.008518

19 6 0 5.462672 -1.974635 0.102781

20 1 0 3.426068 4.299768 -1.534203

21 7 0 7.713220 -0.319477 0.062030

22 8 0 6.512829 1.584616 -0.050465

23 7 0 6.772786 -2.438361 0.149846

24 8 0 4.539791 -2.780916 0.139150

25 6 0 7.931801 -1.683436 0.137811

26 1 0 8.544187 0.262012 0.063431

27 1 0 6.895047 -3.443228 0.209078

28 8 0 9.046882 -2.175791 0.189982

29 1 0 0.136523 -0.889059 2.036868

30 7 0 -2.216471 -0.626775 -1.367994

31 7 0 -1.145907 -1.323997 -1.755673

32 7 0 -0.210839 -1.167920 -0.845360

33 29 0 -3.481578 -0.289786 1.149093

34 8 0 -4.874875 -0.881941 2.408901

35 1 0 -5.257030 -0.165027 2.945458

36 1 0 -5.624998 -1.282455 1.925210

37 29 0 -2.703085 1.860873 0.105910

38 8 0 -3.197321 3.751967 0.259603

39 1 0 -3.645310 4.114791 -0.525156

40 1 0 -3.779422 3.953247 1.013708

41 6 0 -3.435643 -0.665423 -2.190798

42 6 0 -4.628323 -1.211412 -1.428744

43 1 0 -3.184810 -1.296243 -3.046835

44 6 0 -4.613169 -2.526259 -0.932792

45 6 0 -5.760159 -0.412847 -1.214461

46 6 0 -5.707228 -3.026905 -0.225530

47 1 0 -3.744115 -3.156548 -1.103206

48 6 0 -6.859315 -0.914728 -0.509599

49 1 0 -5.781280 0.603792 -1.597823

50 6 0 -6.834199 -2.221121 -0.010233

51 1 0 -5.686641 -4.045454 0.150666

52 1 0 -7.731456 -0.287212 -0.351769

53 1 0 -7.691002 -2.616097 0.528314

54 1 0 -3.641260 0.342748 -2.559063

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