Supporting Information for

Parallel Synthesis of Aurones Using a Homogeneous Scavenger

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General Information:

Supported scavengers were obtained from Aldrich. NMR spectra were recorded on either a JEOL ECA-500 or ECX-300 MHz instrument as indicated. Infrared spectroscopy were recorded on an Aligent Cary 630 FTIR using an ATR attachment as neat films. Mass Spectra were recorded on a Waters Synapt HRMS. All gas chromatography was performed on an HP G1530A under the conditions found in Table 1 of the supporting information.

Summary of Spectral Data for Aurone Products:

(*Z*)-4-((3-oxobenzofuran-2(3*H*)-ylidene)methyl)benzonitrile[1]

Yellow solid. (MP = 181-184 °C). IR (neat; thin film): 1703, 1650, 1602, 1475, 1461, 1302, 1190, 1130, 1108, 885, 833, 755, 734, 699, 664, 645, 626 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): 6.79 (s, 1H), 7.24 (t, J = 6.85 Hz, 1H), 7.32 (d, J = 8.6 Hz, 1H), 7.65-7.70 (m, 3H), 7.79 (d, J = 7.45, 1H), 7.97 (d, J = 8.55 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 110.09, 112.65, 113.10, 118.65, 121.20, 124.17, 125.04, 131.61, 132.56, 136.83, 137.64, 148.21, 166.34, 184.65.

(*Z*)-2-(4-(trifluoromethyl)benzylidene)benzofuran-3(2*H*)-one[2]

Orange-yellow solid (MP = 98-102 °C). IR (neat, thin film): 3020, 1700, 1600, 1320, 1110, 1080, 750 cm^{-1}; ^{1}H NMR ($CDCl_3$, 500 MHz): 8.01 (d, J = 8.0 Hz, 2H), 7.82 (d, J = 8.0 Hz, 1H), 7.72-7.66 (m, 3H), 7.35 (d, J = 8.5 Hz, 1H), 7.29-7.25 (m, 1H), 6.87 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz) 184.76, 166.32, 147.80, 137.48, 135.74, 131.50, 131.00 (q, J = 32 Hz), 129.03, 125.78 (q, J = 4 Hz), 123.52 (q, J = 270 Hz), 122.17, 121.27, 113.06, 110.82

(*Z*)-2-(4-(dimethylamino)benzylidene)benzofuran-3(2*H*)-one[3]

Red solid (MP = 168-170 °C). IR (neat, thin film): 3020, 1700, 1650, 1600, 1110, 750, 690 cm^{-1}; ^{1}H NMR ($CDCl_3$, 300 MHz): 7.85 (d, J = 5.4 Hz, 2H), 7.80 (d, J = 3.9 Hz, 1H), 7.60 (t, J = 4.2 Hz, 1H),

7.31 (d, J = 5.1 Hz, 1H), 7.18 (t, J = 4.5 Hz, 1H), 6.92 (s, 1H), 6.75 (d, J = 5.4 Hz, 2H), 3.07 (s, 6H); ^{13}C NMR ($CDCl_3$, 75 MHz): 184.09, 165.36, 151.43, 145.10, 135.92, 133.74, 124.40, 122.97, 122.54, 120.07, 115.46, 112.86, 112.02, 40.16.

(*Z*)-2-(4-methylbenzylidene)benzofuran-3(2*H*)-one[3]

Tan solid (MP = 75-76 °C). IR (neat, thin film): 3020, 2920, 1700, 1650, 1600, 1490, 1300, 1200, 1110, 900, 750 cm^{-1}; ^{1}H NMR ($CDCl_3$, 300 MHz): 7.85-7.75 (m, 3H), 7.64 (ddd, J = 8.6, 7.3, 1.4 Hz, 1H), 7.32 (d, J = 8.3 Hz, 1H), 7.30-7.19 (m, 3H), 6.89 (s, 1H), 2.40 (s, 3H); ^{13}C NMR ($CDCl_3$, 75 MHz): 184.88, 166.12, 146.61, 140.63, 136.86, 131.70, 129.81, 129.60, 124.71, 123.46, 121.85, 113.53, 113.03, 21.75.

(*Z*)-2-(4-methoxybenzylidene)benzofuran-3(2*H*)-one[4]

Red-orange solid (MP = 135-138 °C). IR (neat, thin film): 3020, 3000, 1700, 1670, 1600, 1510, 1240, 900, 820, 750 cm^{-1}; ^{1}HNMR ($CDCl_3$, 300 MHz) 7.90 (d, J = 8.91Hz, 2H), 7.80 (d, J = 6.87Hz, 1H), 7.65 (t, J = 7.2Hz. 1H), 7.31 (d, J = 8.25Hz, 1H), 7.21 (t, J = 7.2Hz, 1H), 7.00 (d, J = 8.94Hz, 2H), 6.89 (s, 1H), 3.87 (s, 3H); ^{13}C NMR ($CDCl_3$, 75 MHz): 184.67, 165.92, 161.16, 145.97, 136.64, 133.55, 125.14, 124.65, 123.37, 122.03, 114.59, 113.52, 112.97, 55.49.

Methyl (*Z*)-4-((3-oxobenzofuran-2(3*H*)-ylidene)methyl)benzoate[2]

Yellow solid (MP = 144-147 °C). IR (neat, thin film): 2980, 1700, 1650, 1280, 1050, 1020 cm^{-1}; ^{1}H NMR ($CDCl_3$, 300 MHz): 8.10 (d, J = 8.5 Hz, 2H), 7.96 (d, J = 8.3 Hz, 2H), 7.81 (ddd, J = 7.7 Hz, J = 1.4 Hz, J = 0.6 Hz, 1H), 7.68 (ddd, J = 8.6 Hz, J = 7.3 Hz, J = 1.4 Hz, 1H), 7.35 (d, J = 8.3 Hz, 1H), 7.24 (td, J = 7.7 Hz, J = 0.8 Hz, 1H), 6.87 (s, 1H), 3.94 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): 184.85, 166.63, 166.36, 147.82, 137.38, 136.71, 131.29, 130.69, 130.06, 124.93, 123.91, 121.42, 113.12, 111.36, 52.34.

(*Z*)-2-(2-bromobenzylidene)benzofuran-3(2*H*)-one[5]

Yellow solid (MP = 134-140 °C). IR (neat, thin film): 2980, 1700, 1600, 1450, 780 cm^{-1}; ^{1}H NMR ($CDCl_3$, 300 MHz): 8.34 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.82 (ddd, *J* = 7.6, 1.4, 0.6 Hz, 1H), 7.67-7.61 (m, 2H), 7.43-7.37 (m, 1H), 7.31 (d, *J* = 7.0 Hz, 2H), 7.23-7.17 (m, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz): 184.64, 166.26, 147.62, 137.22, 133.48, 132.45, 132.11, 130.86, 127.77, 126.64, 124.93, 123.81, 121.54, 113.03, 110.83.

(*Z*)-2-(3-bromobenzylidene)benzofuran-3(2*H*)-one[6]

Yellow solid (MP = 117-118 °C). IR (neat, thin film): 2980, 1705, 1610, 1445, 810, 785. ^{1}H NMR ($CDCl_3$, 500 MHz): 8.09 (s, 1H), 7.80 (t, J = 7.1 Hz, 2H), 7.67 (t, J = 7.6 Hz, 1H), 7.51 (d, J = 7.8 Hz, 1H), 7.36 (d, J = 8.6 Hz, 1H), 7.32 (t, J = 7.9 Hz, 1H), 7.24 (t, J = 7.5 Hz, 2H), 6.78 (s, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): 184.75, 166.29, 147.40, 137.29, 134.43, 133.91, 132.73, 130.42, 130.10, 124.88, 123.84, 123.05, 121.48, 113.14, 111.14.

(*Z*)-2-(4-bromobenzylidene)benzofuran-3(2*H*)-one[1]

Yellow solid (MP = 152-158 °C). IR: 1714, 1655, 1601, 1487, 1474, 1460, 1298, 1205, 1186, 1128, 1112, 1099, 1071, 1008, 884, 821, 756, 697, 653, 626 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): 6.81 (s, 1H), 7.24 (t, J = 7.45 Hz, 1H), 7.34 (d, J = 8 Hz, 1H), 7.58 (d, J = 8.6 Hz, 2H), 7.67 (t, J = 8.6 Hz, 1H), 7.78 (d, J = 8.6 Hz, 2H), 7.81 (d, J = 8.6 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 111.47, 112.87, 121.39, 123.57, 124.21, 124.66, 131.03, 132.07, 132.61, 136.99, 146.99, 165.99, 184.58.

(*Z*)-2-(thiophen-2-ylmethylene)benzofuran-3(2*H*)-one[1]

Brown solid (MP = 92-96 °C). IR: 1698, 1684, 1645, 1593, 1504, 1475, 1458, 1417, 1391, 1328, 1295, 1232, 1185, 1124, 1095, 992, 881, 846, 756, 710, 695, 625 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): 7.17 (t, J = 4 Hz, 1H), 7.20 (s, 1H), 7.24 (t, J = 7.45 Hz, 1H), 7.27 (s, 1H), 7.36 (d, J = 8.55 Hz, 1H),

7.57 (d, J = 3.45 Hz, 1H), 7.63 (d, J = 5.15 Hz, 1H), 7.66 (t, J = 8.55 Hz, 1H), 7.81 (d, J = 7.45 Hz, 1H); ^{13}C NMR (500 MHz, CDCl3): 107.12, 112.92, 122.25, 123.52, 124.58, 128.09, 131.54, 133.17, 135.55, 136.71, 145.33, 165.65, 183.85.

(*Z*)-2-(furan-2-ylmethylene)benzofuran-3(2*H*)-one[1]

Brown solid (MP = 66-68 °C). IR (Neat, thin film): 1730, 1650, 1610, 1480, 1300, 1190, 1105, 850, 760 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): 6.56 (br s, 1H), 6.85 (s, 1H), 7.10 (d, J = 3.45 Hz, 1H), 7.17 (t, J = 8.0 Hz, 1H), 7.27 (d, J = 8.6 Hz, 1H), 7.61-7.57 (m, 2H), 7.75 (d, J = 8.6 Hz, 1H); 13C NMR (500 MHz, CDCl3): 101.57, 112.81, 113.11, 117.24, 121.87, 123.39, 124.41, 136.62, 144.87, 145.34, 148.65, 165.59, 183.90.

(*Z*)-4-((4-chloro-3-oxobenzofuran-2(3*H*)-ylidene)methyl)benzonitrile[2]

Yellow solid (MP = 230-232). ^{1}H NMR (300 MHz, DMSO-D6) 8.12 (d, J = 8.5 Hz, 2H), 7.94 (d, J = 8.5 Hz, 2H), 7.90 (s, 1H), 7.77 (t, J = 8.1 Hz, 1H), 7.53 (d, J = 8.8 Hz, 1H), 7.33 (d, J = 8.4 Hz, 1H), 7.00 (s, 1H). ^{13}C NMR (75 MHz, DMSO-D6) 181.68, 166.77, 147.81, 139.10, 137.02, 133.37, 132.13, 131.20, 125.68, 119.20, 118.36, 112.64, 112.17, 110.56.

(*Z*)-4-((5-chloro-3-oxobenzofuran-2(3*H*)-ylidene)methyl)benzonitrile[2]

Yellow solid (213-215 °C). IR (neat, thin film): 2980, 2200, 1705, 1615. ^{1}H NMR (300 MHz, DMSO-D6) 8.12 (d, J = 8.6 Hz, 2H), 7.93 (d, J = 8.5 Hz, 2H), 7.84 (s, 1H), 7.81 (d, J = 2.4 Hz, 1H), 7.60 (dd, J = 8.2, 1.1 Hz, 1H), 7.02 (s, 1H).

(*Z*)-4-((5-fluoro-3-oxobenzofuran-2(3*H*)-ylidene)methyl)benzonitrile[2]

Yellow solid (MP = 200-202 °C). IR (neat, thin film): 2980, 2200, 1700, 1605. ^{1}H NMR (300 MHz, ACETONE-D6) 8.19 (d, J = 8.3 Hz, 2H), 7.89 (d, J = 8.5 Hz, 2H), 7.63 (d, J = 2.7 Hz, 1H), 7.61 – 7.58 (m, 1H), 7.52 (ddd, J = 6.9, 2.6, 0.7 Hz, 1H), 6.92 (s, 1H).

(*Z*)-4-((6-fluoro-3-oxobenzofuran-2(3*H*)-ylidene)methyl)benzonitrile

Yellow solid (MP = 190-193 °C). IR (neat, thin flim): 2980, 2200, 1705, 1615. HRMS: calcd for $C_{14}H_8FNO_2$ 241.0609, obsvd 241.0611. ^{1}H NMR (300 MHz, DMSO-D6) 8.09 (d, J = 8.3 Hz, 2H), 7.93 (d, J = 8.5 Hz, 2H), 7.87 (dd, J = 8.5, 5.8 Hz, 1H), 7.55 (dd, J = 9.3, 2.1 Hz, 1H), 7.17 (ddd, J = 9.4, 8.5, 2.2 Hz, 1H), 6.99 (s, 1H).

(*Z*)-4-((5-bromo-3-oxobenzofuran-2(3*H*)-ylidene)methyl)benzonitrile[2]

Yellow solid (MP = decomp 170 °C). IR (neat, thin flim): 3000, 2200, 1700, 1610. ^{1}H NMR (300 MHz, DMSO-D6) 8.13 (d, J = 8.6 Hz, 2H), 7.95 (d, J = 8.6 Hz, 2H), 7.65 (d, J = 7.3 Hz, 1H), 7.60 (d, J = 7.2 Hz, 1H), 7.22 (t, J = 7.5 Hz, 1H), 7.00 (s, 1H). ^{13}C NMR (75 MHz, DMSO-D6) 184.78, 164.80, 148.26, 139.33, 137.24, 133.34, 132.27, 124.77, 123.44, 122.33, 120.68, 119.24, 112.20, 110.22.

Table 1: Sample conditions for analysis of reaction kinetics of isoniazid and carbonyls via gas chromatography

	Temp. °C	Run Time (min)	Standard	Time between injections (s)
Benzaldehyde	90	2.98	Decane	240
4-Nitrobenzaldehyde	120	2.98	Decane	240
4-Cyanobenzaldehyde	120	2.98	Decane	240
4-Bromobenzaldehyde	120	2.98	Decane	240
4-Methylbenzaldehyde	100	2.98	Decane	240
4-Methoxybenzaldehyde	130	2.98	Decane	240
3-Methoxybenzaldehyde	120	2.98	Decane	240
2-Methoxybenzaldehyde	120	2.98	Decane	240
Trans-cinnamaldehdye	125	2.98	Decane	240
Dihydrocinnamaldehyde	130	2.98	Decane	240
Thiophene-2-carboxaldehyde	80	2.98	Decane	240
Furan-3-carboxaldehyde	80	2.98	Decane	240
2-Octanone	120	2.98	Dodecane	2010

Cyclohexanone	80	2.98	Decane	240
Acetophenone	100	2.98	Decane	2010
Benzophenone	150	6.98	Dodecane	2010
Ethyl Acetoacetate	80	2.98	Decane	720
Butyl acetate	75	2.98	Decane	2010
Methyl benzoate	100	2.98	Decane	2010

Protocol for determination of rate constant via linear regression

The concentration of aldehyde was determined according to the equations below. The natural log of the concentration was then plotted against time and linear regression calculated using the method of least squares to yield the rate constant.

$$Percent\ carbonyl\ remaining\ at\ t_x = \left(\frac{Area\ Carbonyl\ at\ t_x}{Area\ Standard\ at\ t_x}\right) \div \left(\frac{Area\ Carbonyl\ at\ t_0}{Area\ Standard\ at\ t_0}\right) \times 100\%$$

$$Concentration\ of\ carbonyl\ at\ t_x = \ Percent\ carbonyl\ remaining\ at\ t_x \times 0.05\ M$$

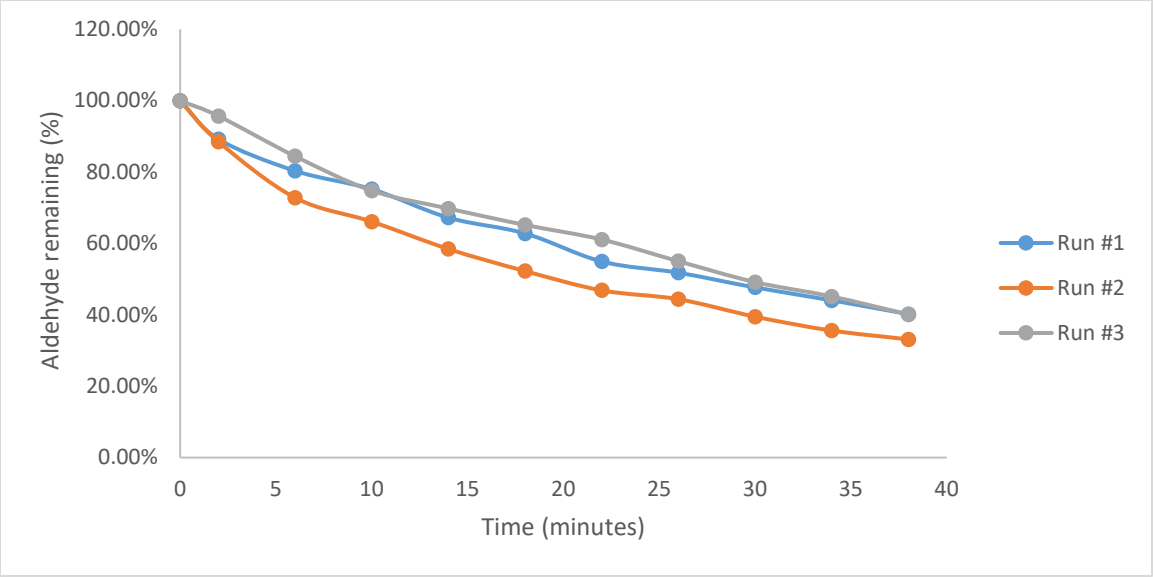


Figure 16: Percent decrease in concentration of benzaldehyde as it is consumed by isoniazid.

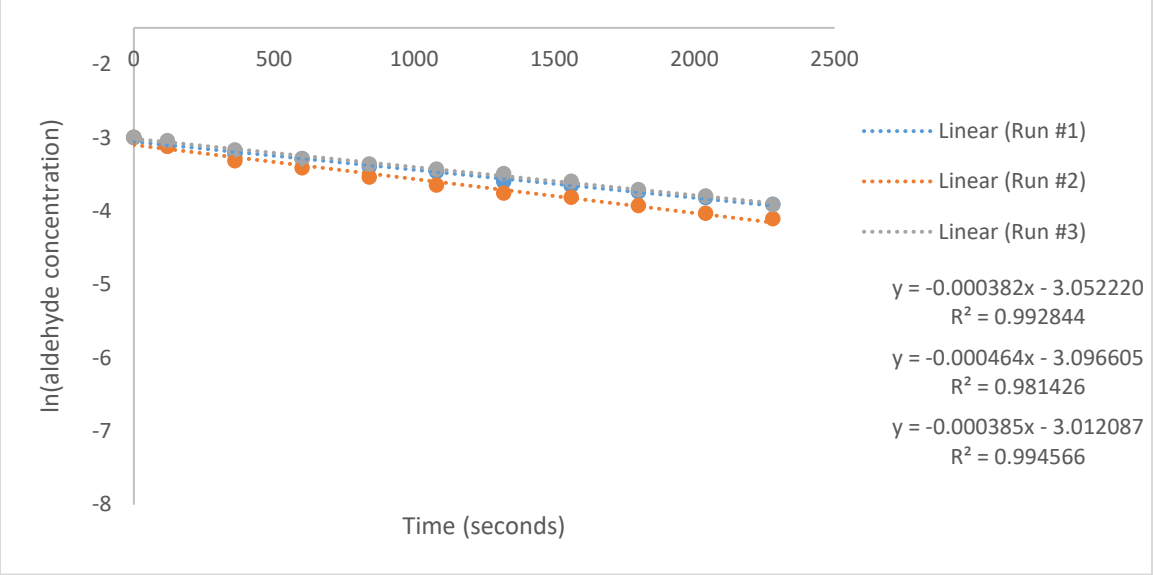


Figure 17: Linear regression of the decrease in concentration of benzaldehyde as it is consumed by isoniazid.

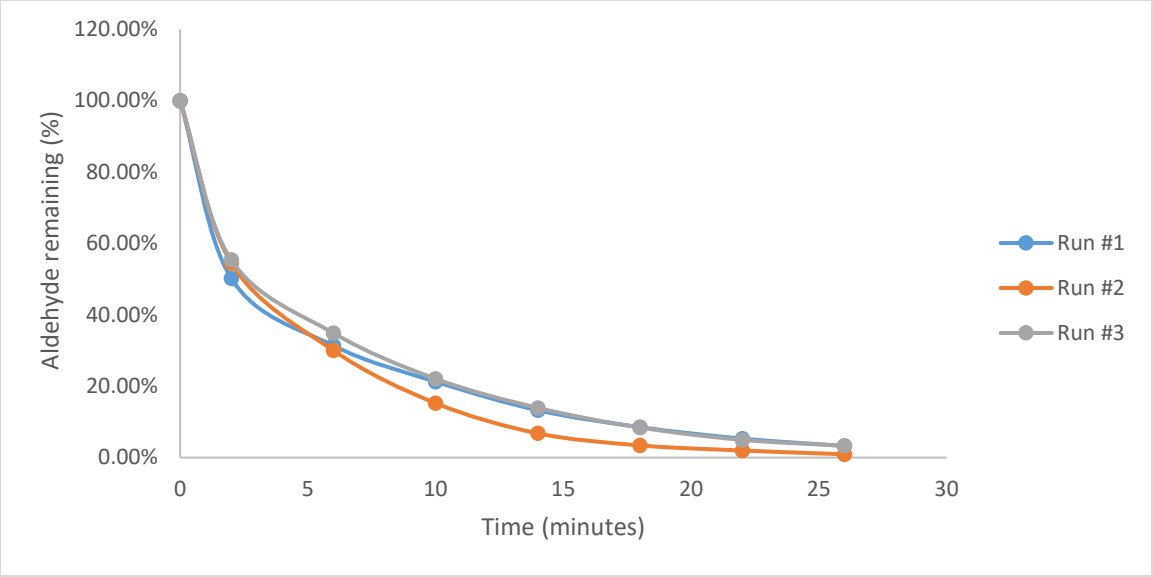


Figure 18: Percent decrease in concentration of 4-nitrobenzaldehyde as it is consumed by isoniazid.

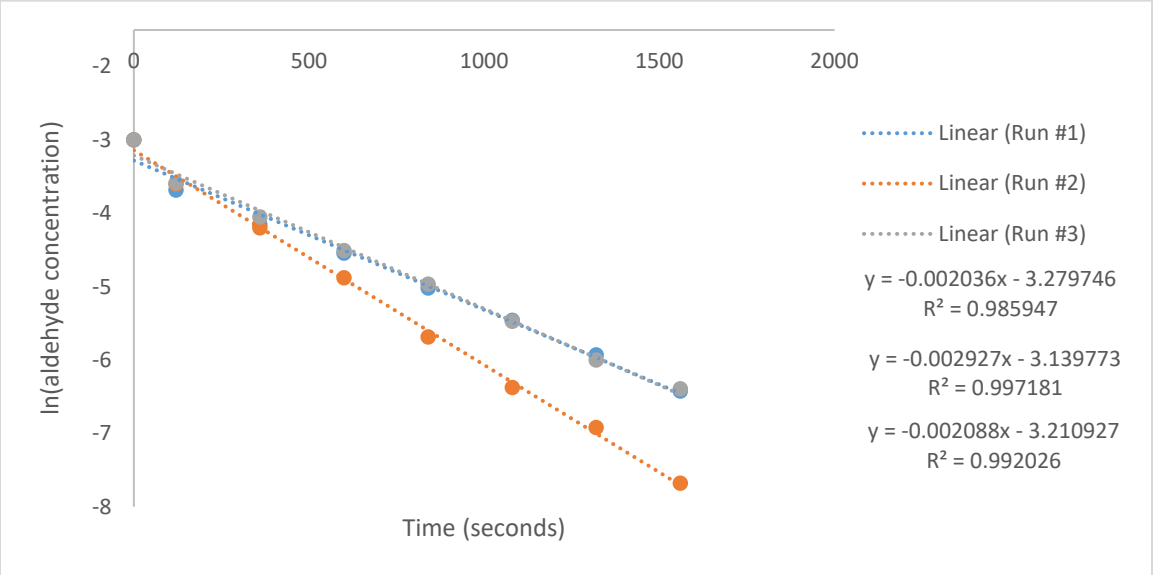


Figure 19: Linear regression of the decrease in concentration of 4-nitrobenzaldehyde as it is consumed by isoniazid.

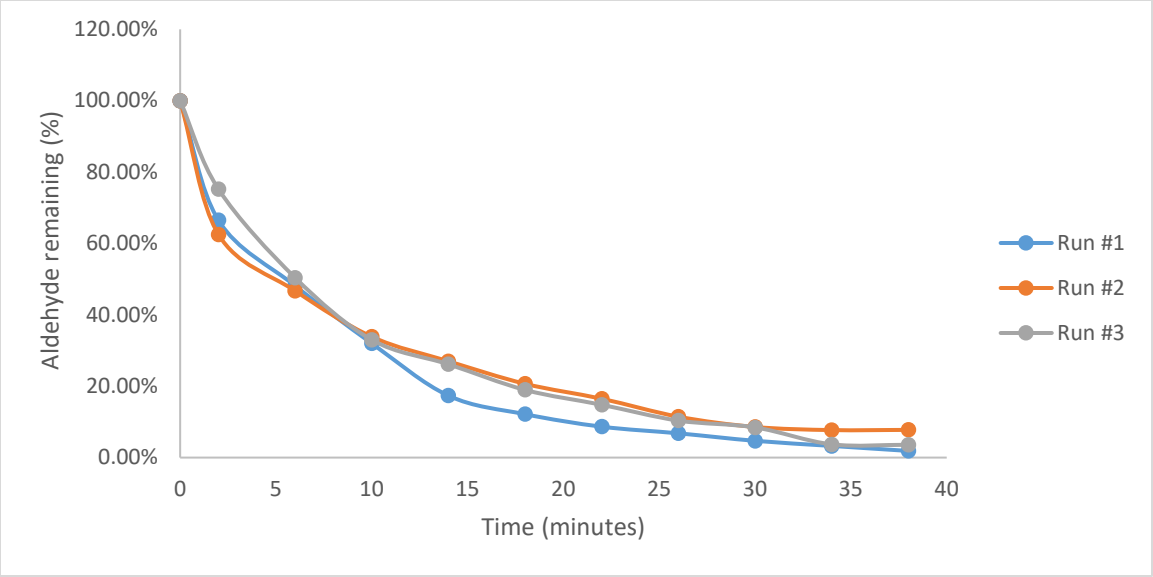


Figure 20: Percent decrease in concentration of 4-cyanobenzaldehyde as it is consumed by isoniazid.

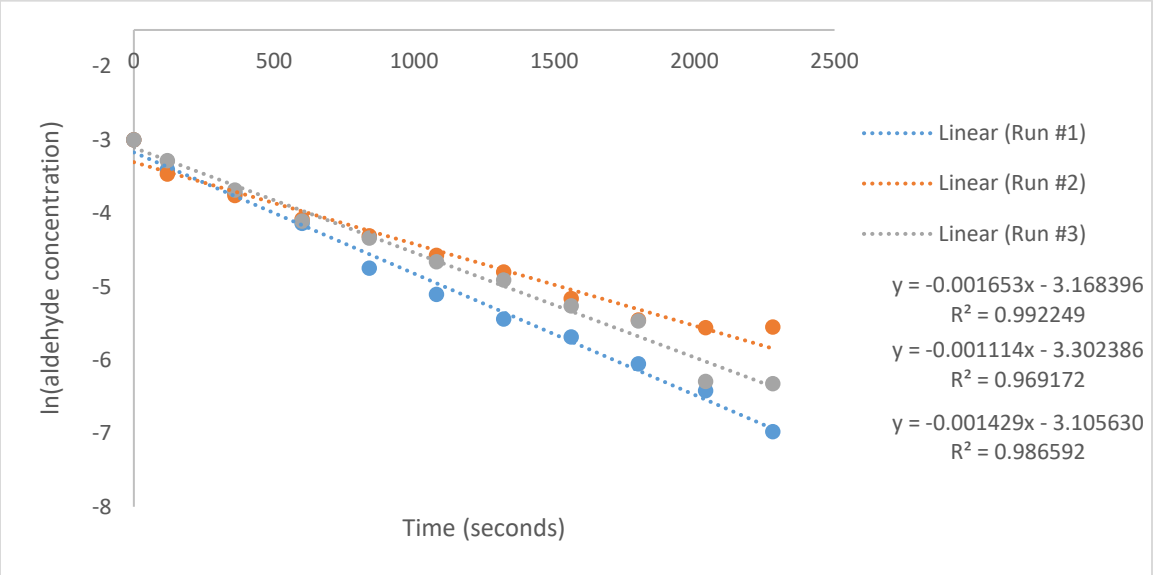


Figure 21: Linear regression of the decrease in concentration of 4-cyanobenzaldehyde as it is consumed by isoniazid.

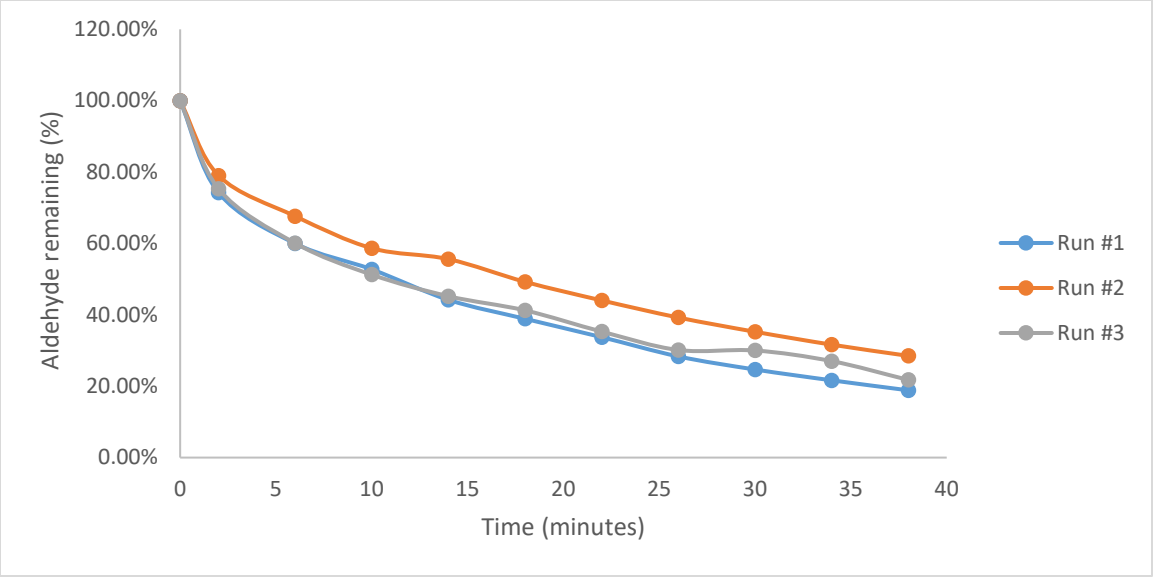


Figure 22: Percent decrease in concentration of 4-bromobenzaldehyde as it is consumed by isoniazid.

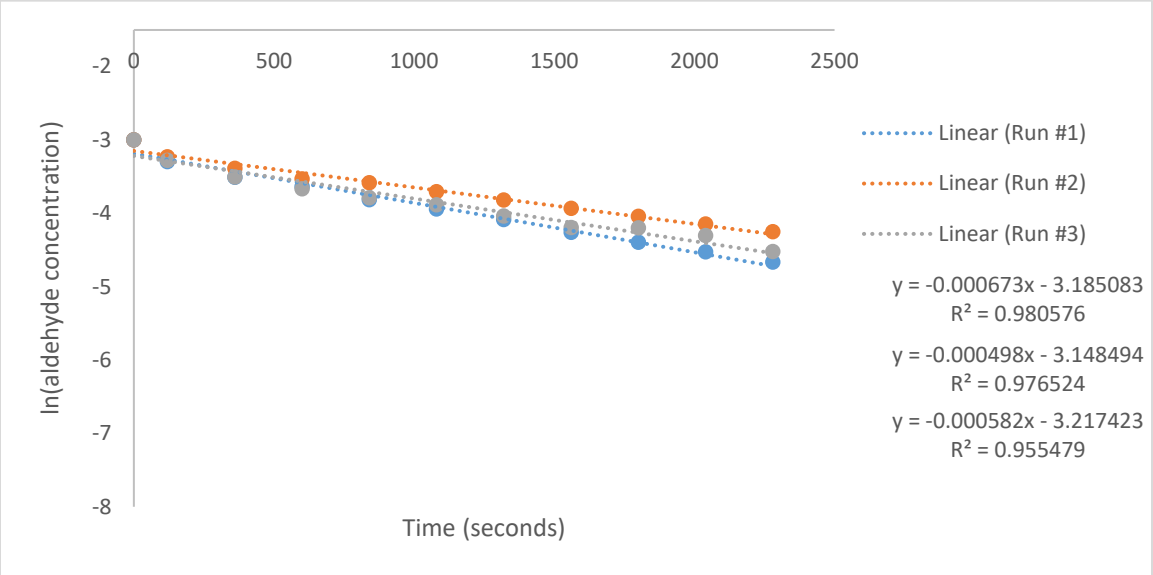


Figure 23: Linear regression of the decrease in concentration of 4-bromobenzaldehyde as it is consumed by isoniazid.

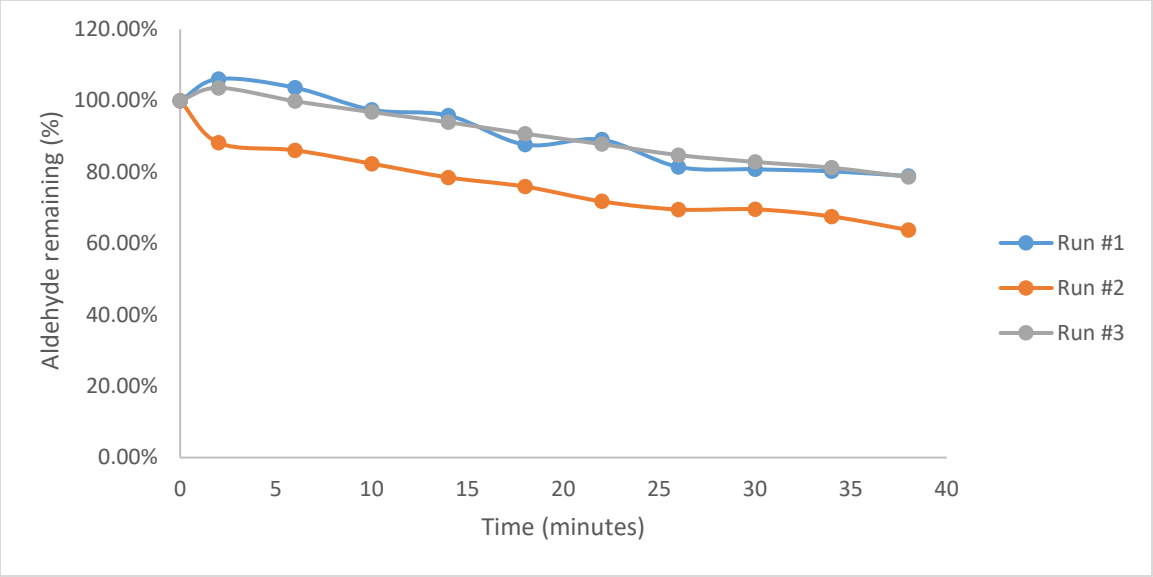


Figure 24: Percent decrease in concentration of 4-tolualdehyde as it is consumed by isoniazid.

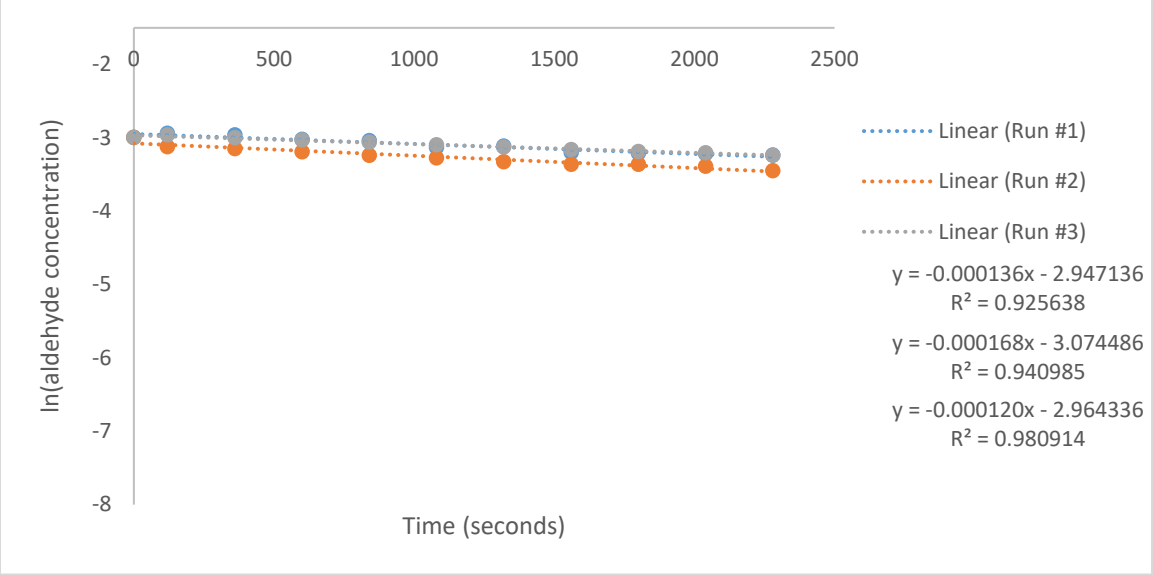


Figure 25: Linear regression of the decrease in concentration of 4-tolualdehyde as it is consumed by isoniazid.

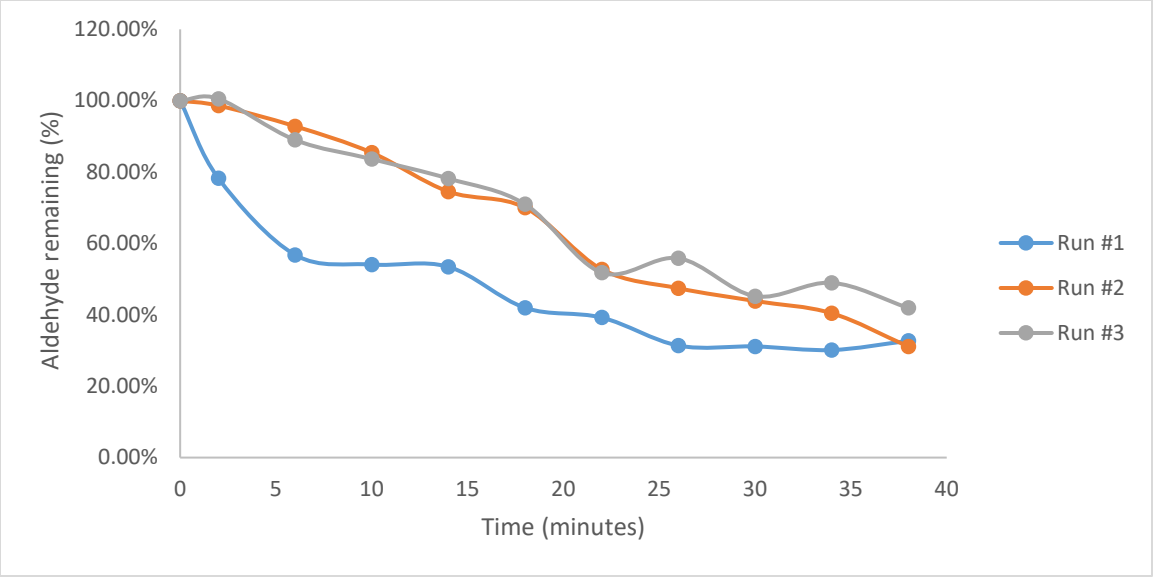


Figure 26: Percent decrease in concentration of 4-methoxybenzaldehyde as it is consumed by isoniazid.

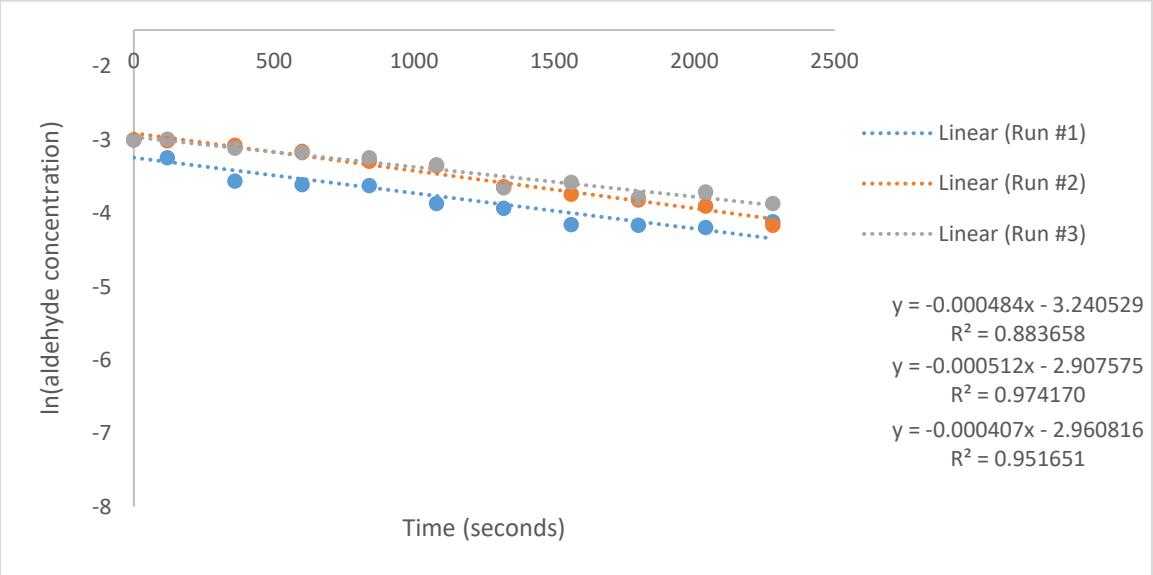


Figure 27: Linear regression of the decrease in concentration of 4-methoxybenzaldehyde as it is consumed by isoniazid.

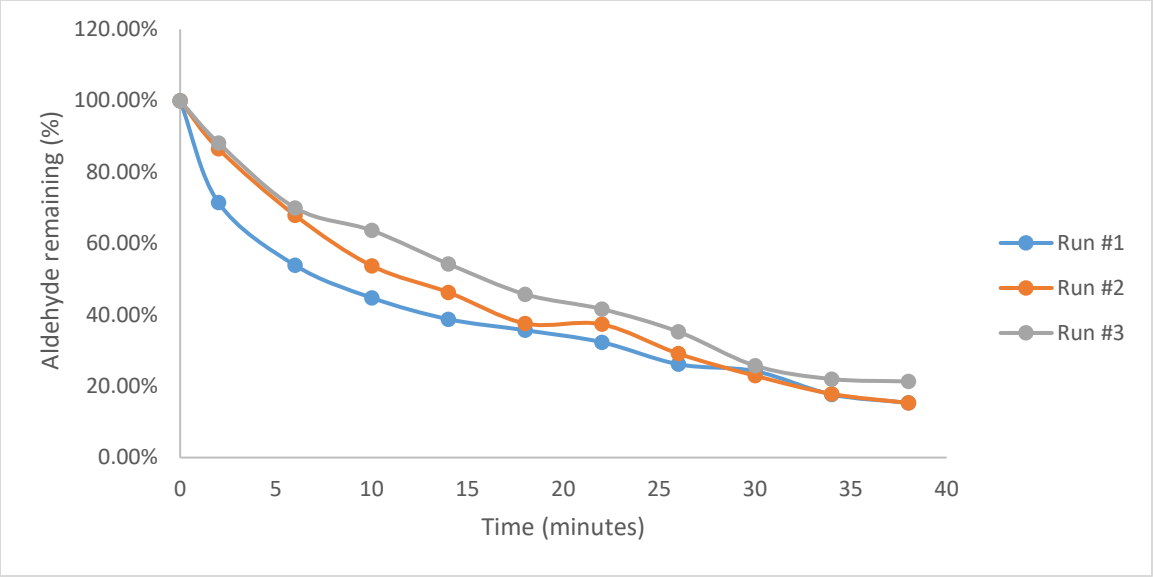


Figure 28: Percent decrease in concentration of 3-methoxybenzaldehyde as it is consumed by isoniazid.

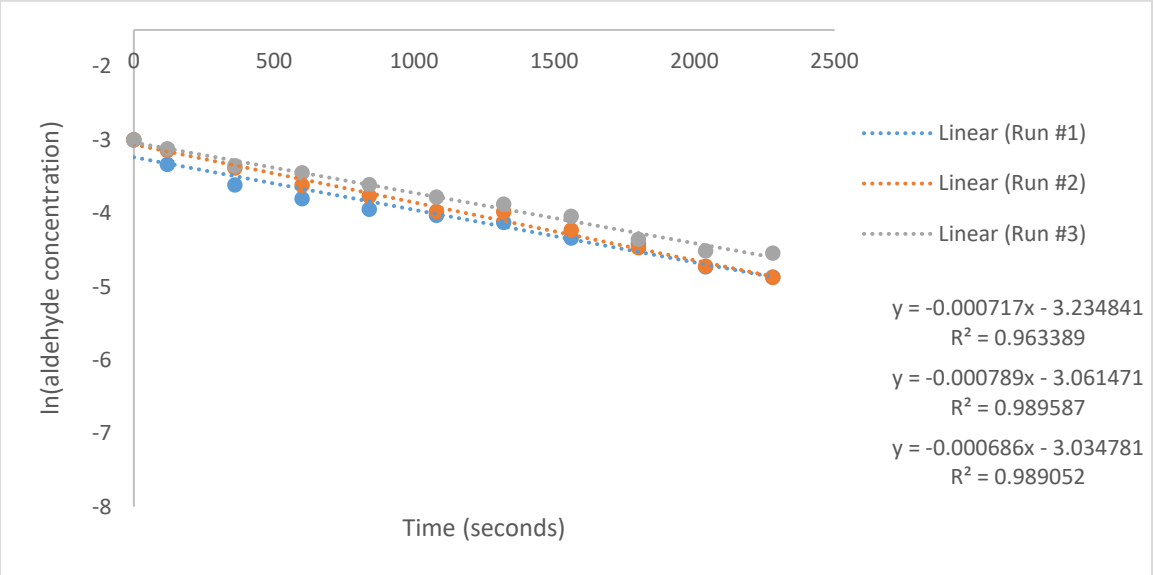


Figure 29: Linear regression of the decrease in concentration of 3-methoxybenzaldehyde as it is consumed by isoniazid.

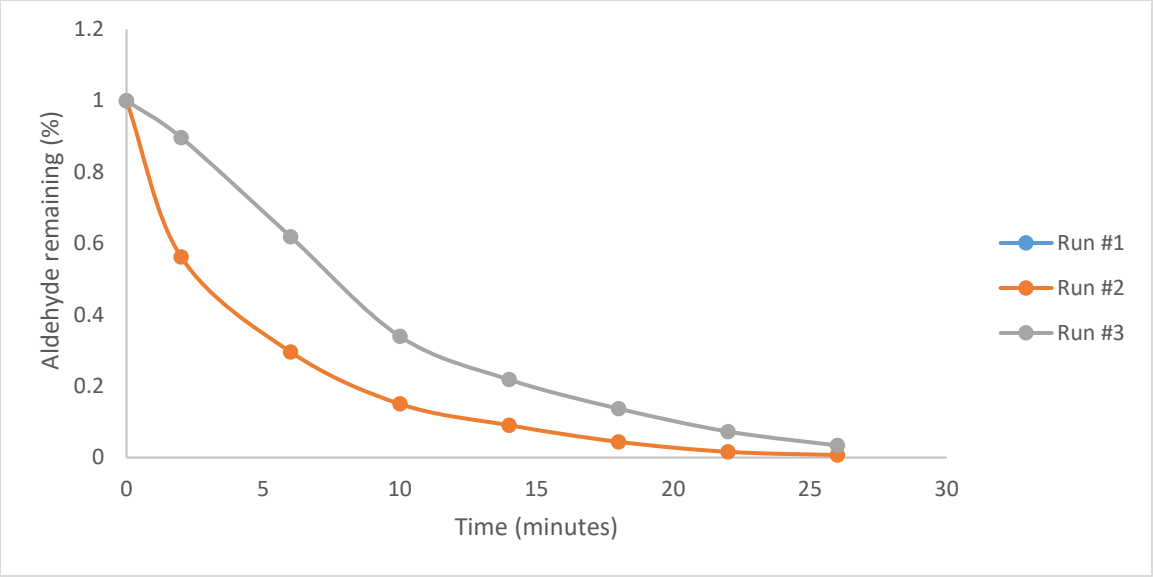


Figure 30: Percent decrease in concentration of 2-methoxybenzaldehyde as it is consumed by isoniazid.

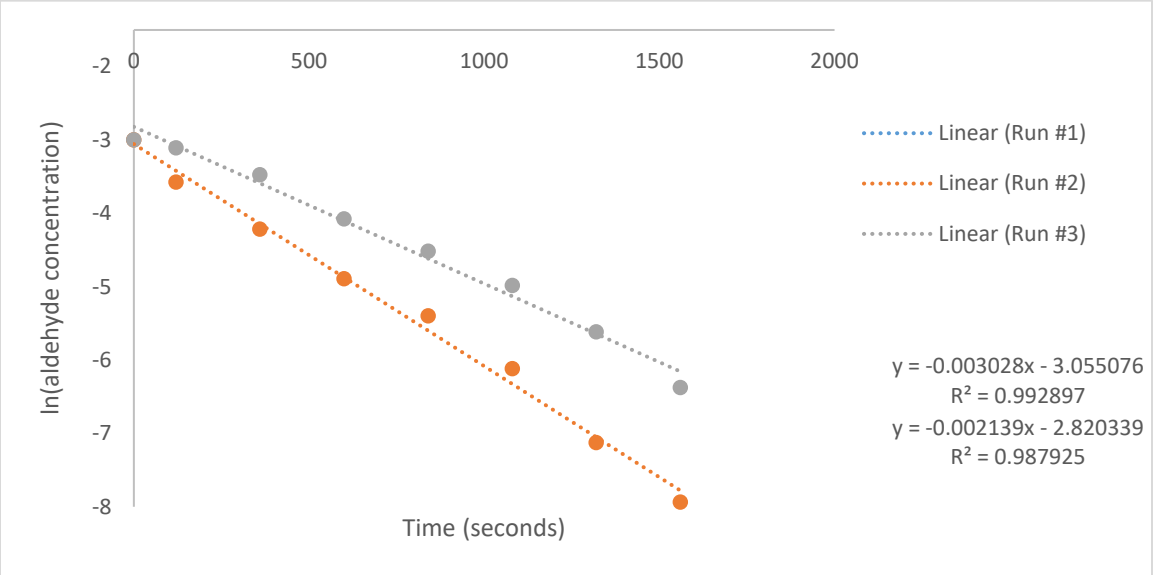


Figure 31: Linear regression of the decrease in concentration of 2-methoxybenzaldehyde as it is consumed by isoniazid.

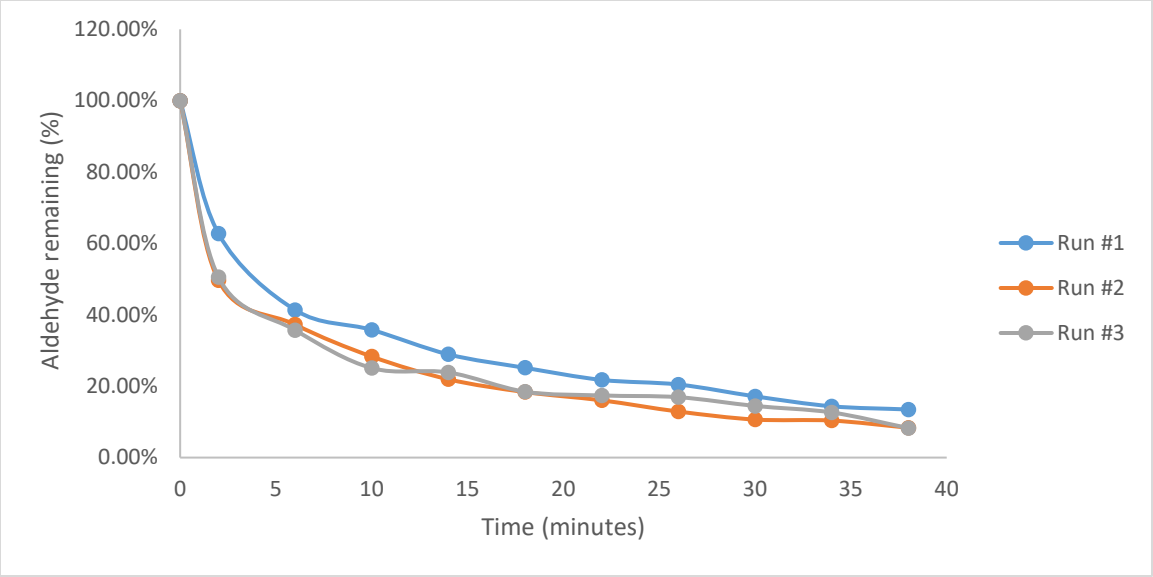


Figure 32: Percent decrease in concentration of trans-cinnamaldehdye as it is consumed by isoniazid.

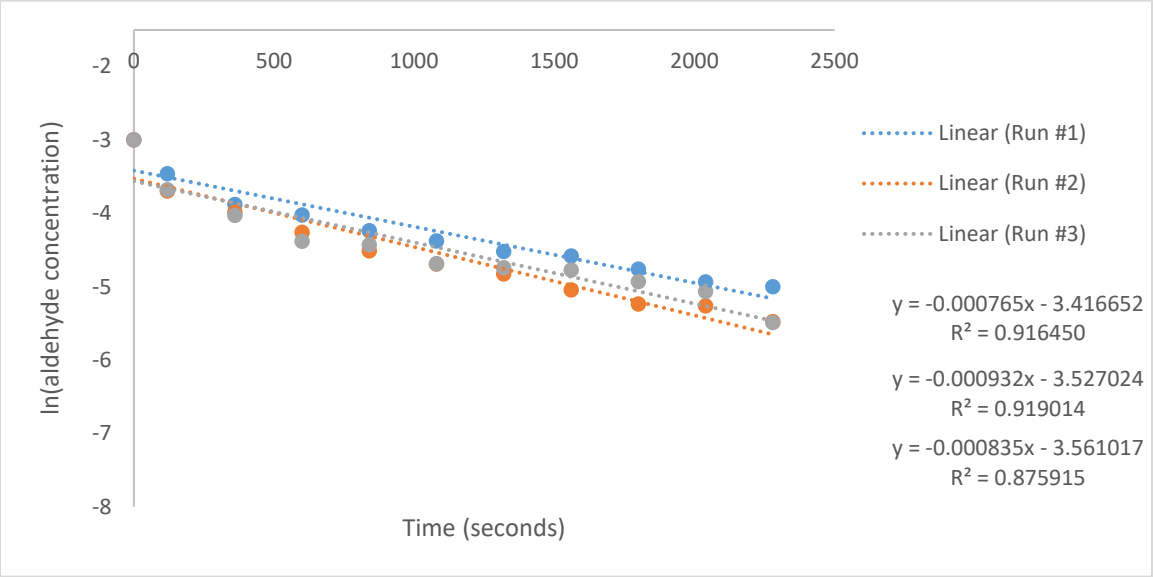


Figure 33: Linear regression of the decrease in concentration of trans-cinnamaldehyde as it is consumed by isoniazid.

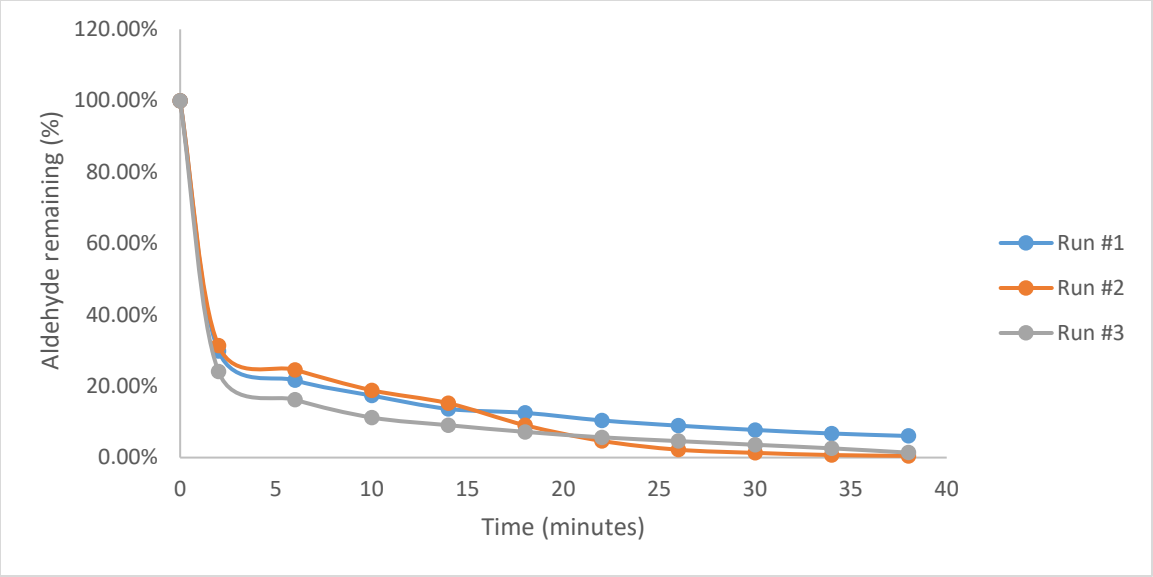


Figure 34: Percent decrease in concentration of dihydrocinnamaldehdye as it is consumed by isoniazid.

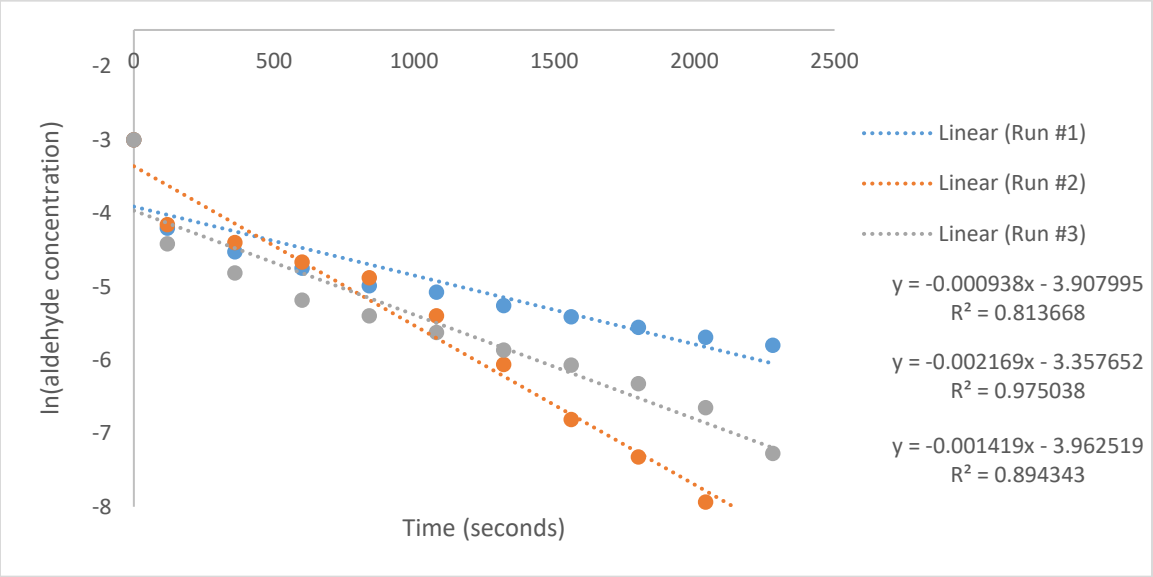


Figure 35: Linear regression of the decrease in concentration of dihydrocinnamaldehyde as it is consumed by isoniazid.

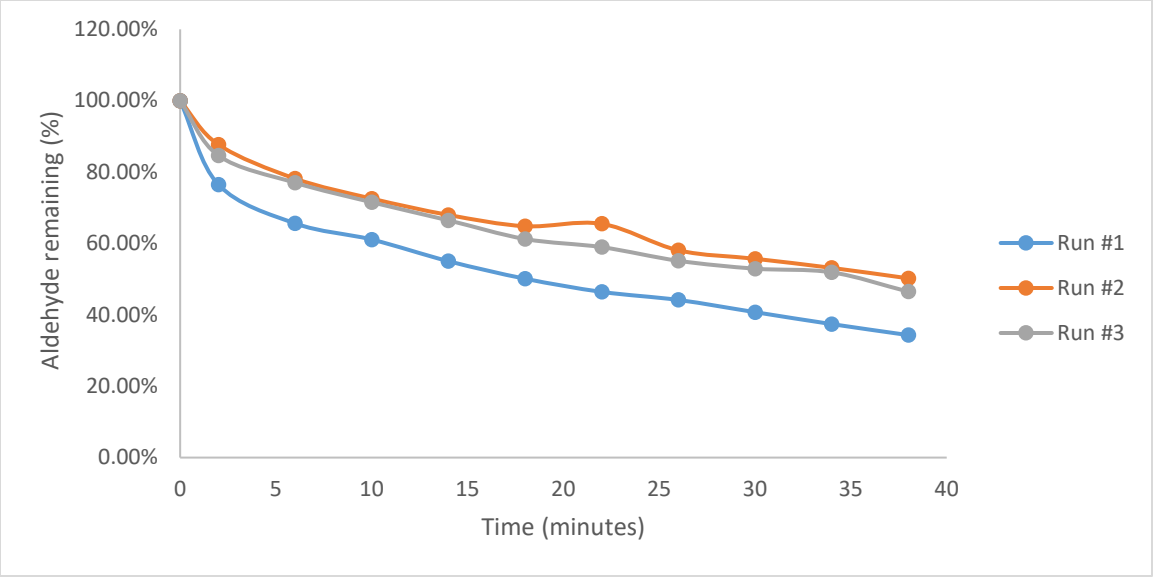


Figure 36: Percent decrease in concentration of thiophene-2-carboxaldehyde as it is consumed by isoniazid.

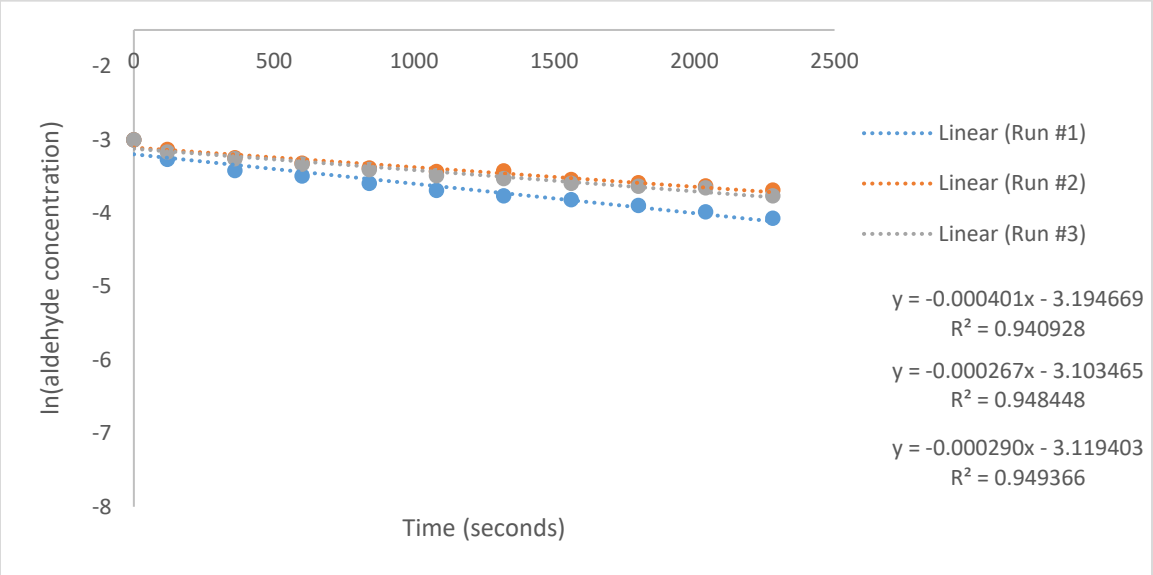


Figure 37: Linear regression of the decrease in concentration of thiophene-2-carboxaldehyde as it is consumed by isoniazid.

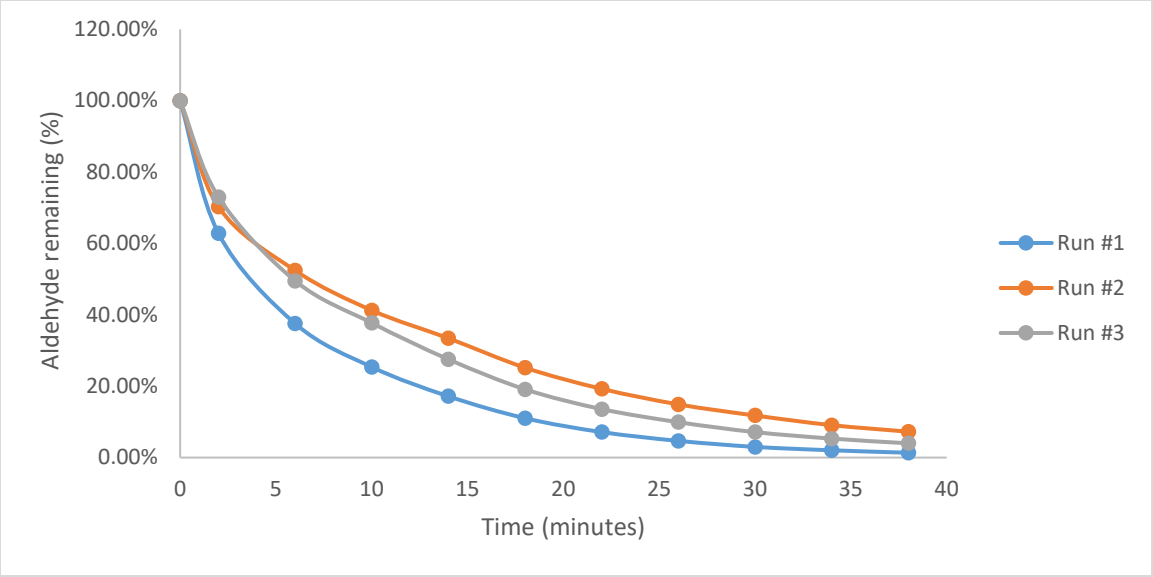


Figure 38: Percent decrease in concentration of furan-3-carboxaldehyde as it is consumed by isoniazid.

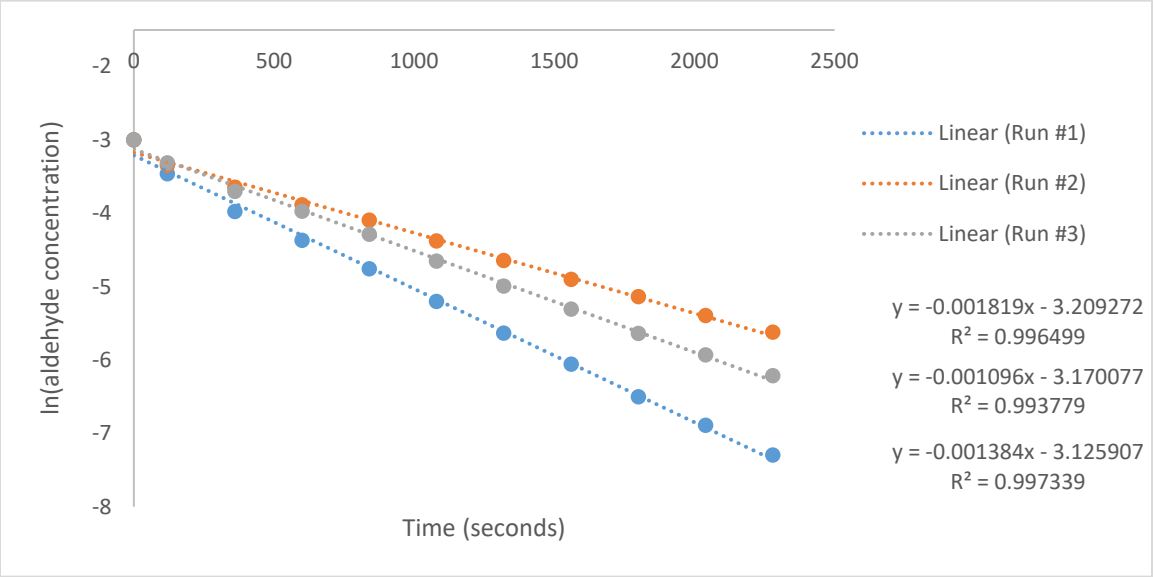


Figure 39: Linear regression of the decrease in concentration of furan-3-carboxaldehyde as it is consumed by isoniazid.

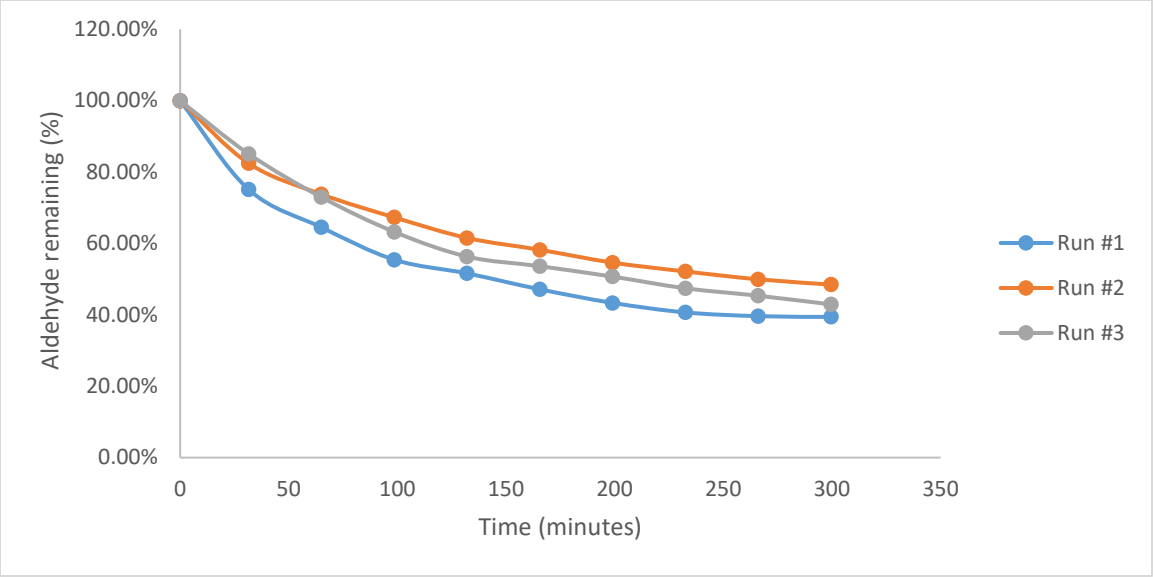


Figure 40: Percent decrease in concentration of 2-octanone as it is consumed by isoniazid.

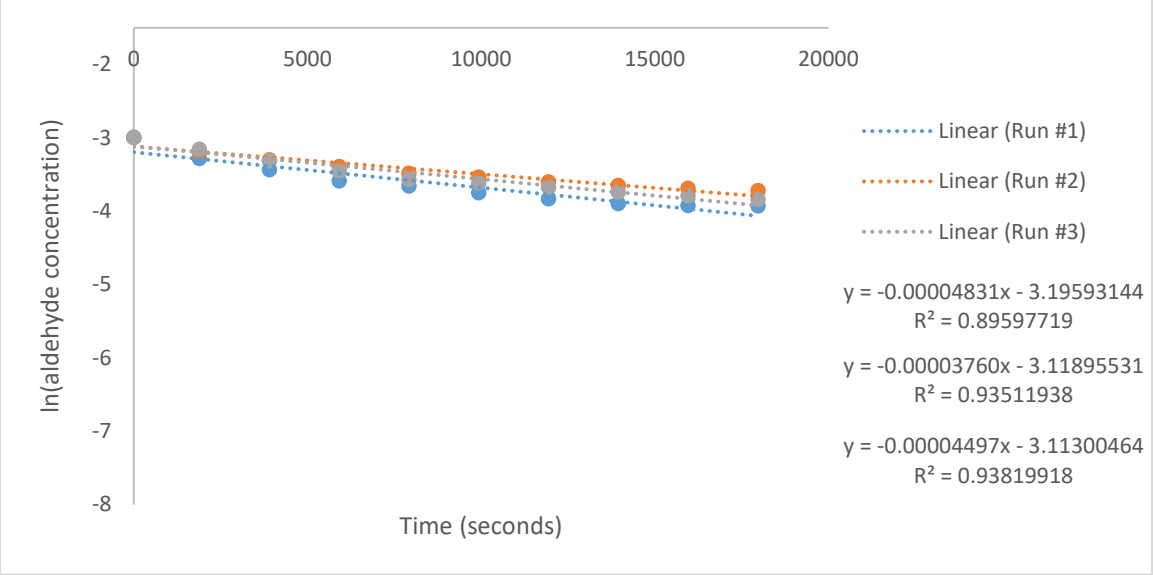


Figure 41: Linear regression of the decrease in concentration of 2-octanone as it is consumed by isoniazid.

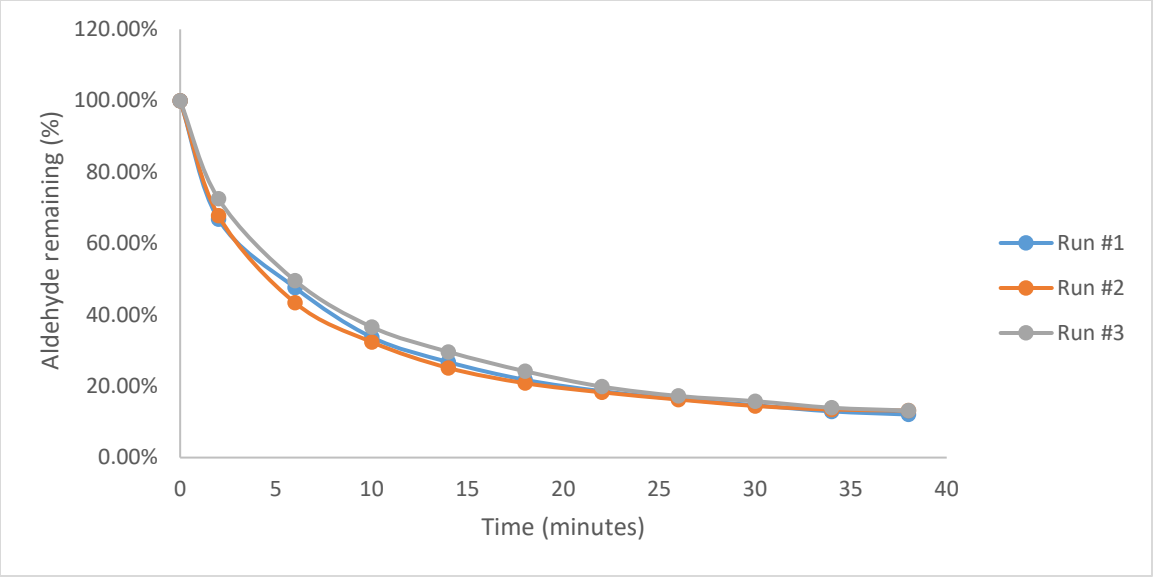


Figure 1: Percent decrease in concentration of cyclohexanone as it is consumed by isoniazid.

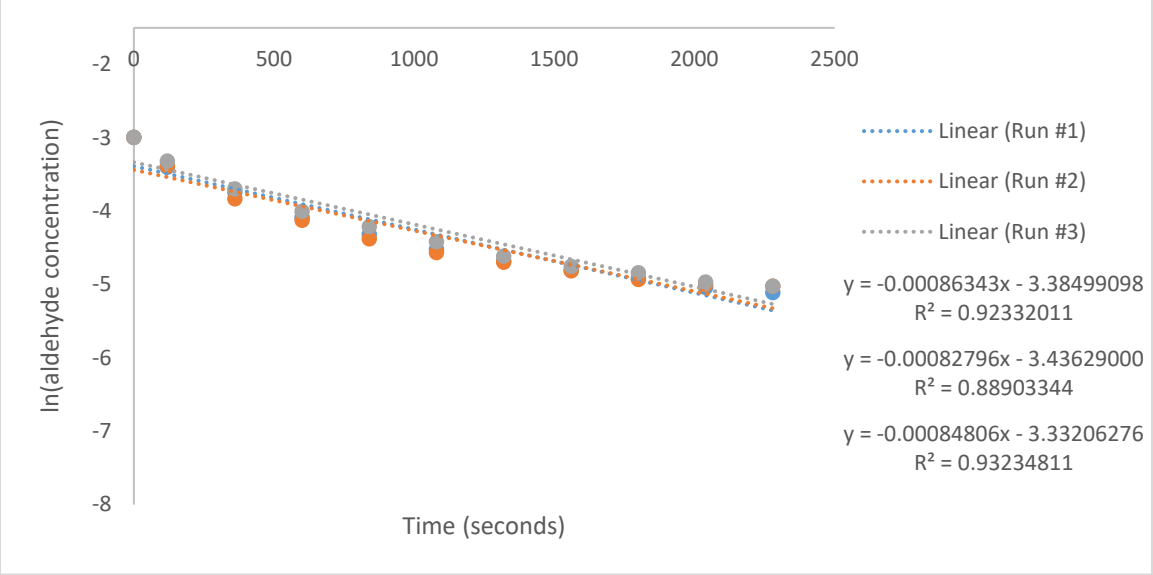


Figure 42: Linear regression of the decrease in concentration of cyclohexanone as it is consumed by isoniazid.

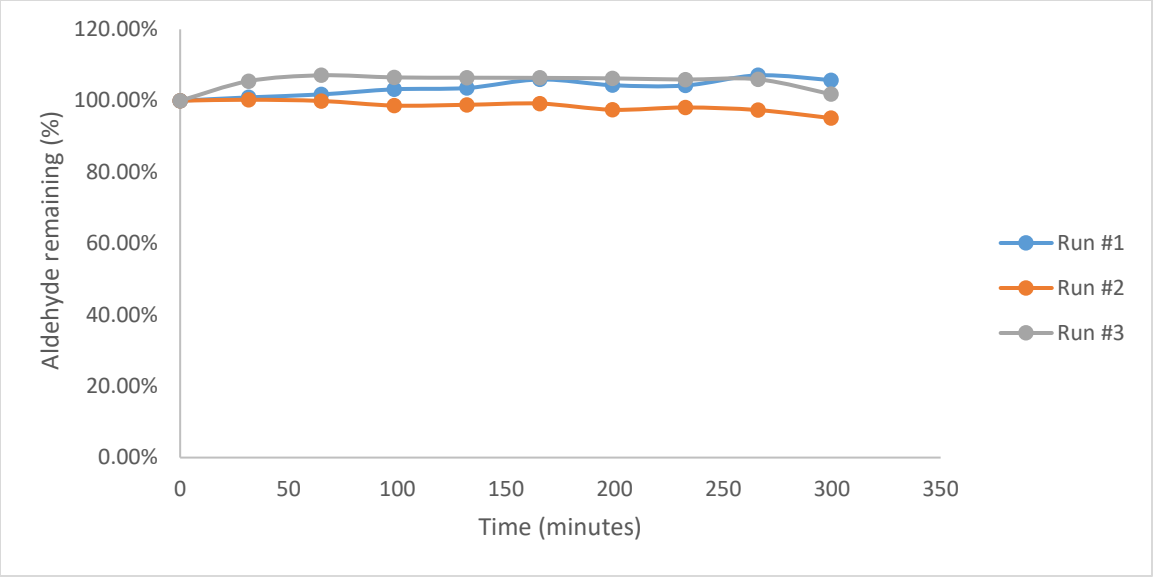


Figure 43: Percent decrease in concentration of acetopheone as it is consumed by isoniazid.

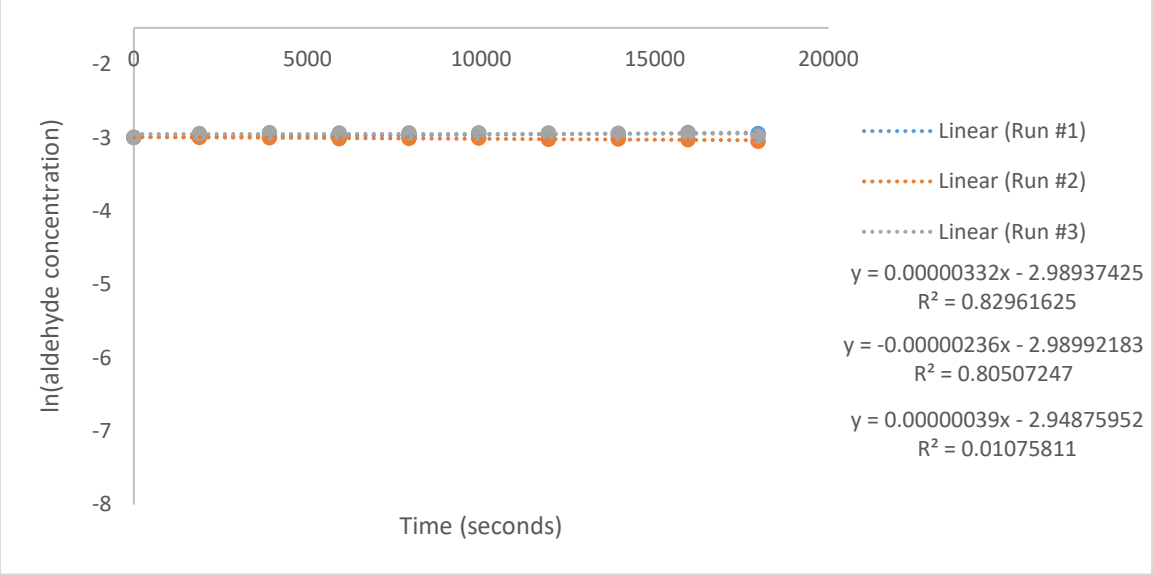


Figure 44: Linear regression of the decrease in concentration of acetophenone as it is consumed by isoniazid.

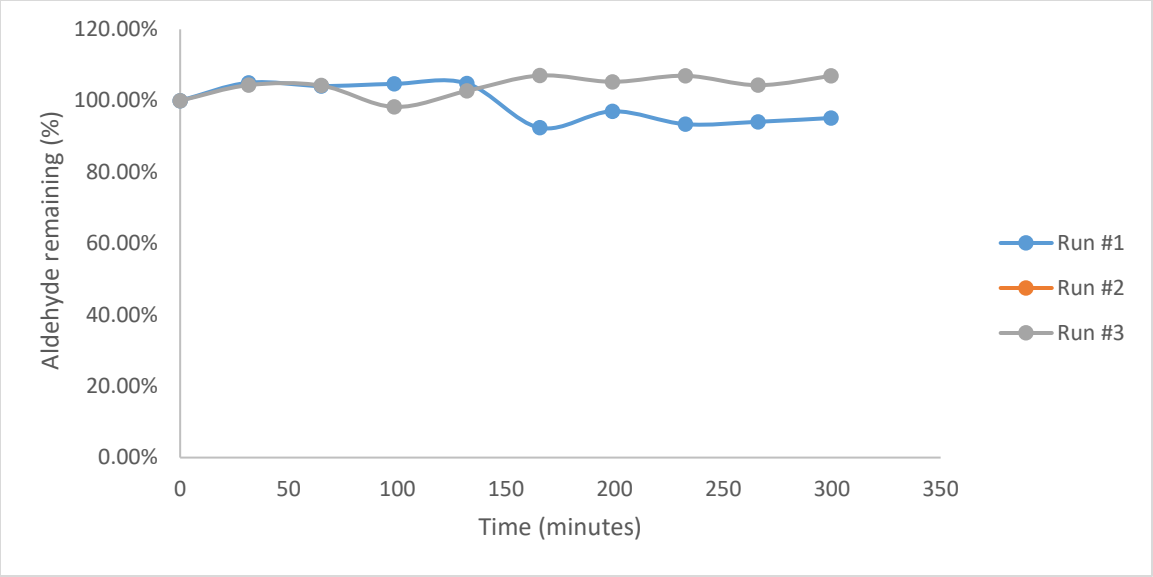


Figure 45: Percent decrease in concentration of benzophenone as it is consumed by isoniazid.

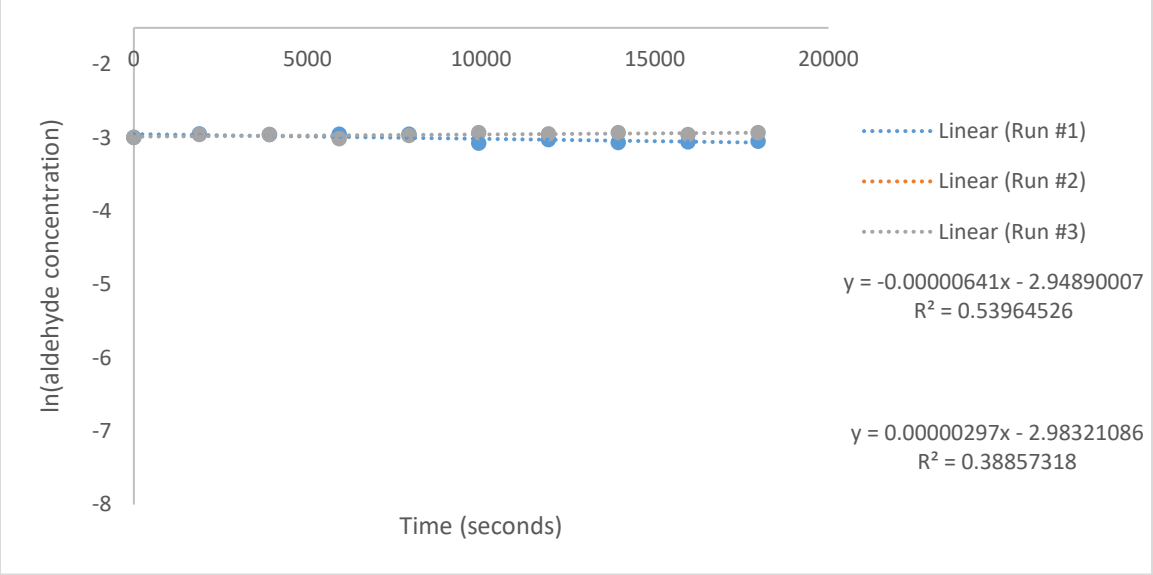


Figure 46: Linear regression of the decrease in concentration of benzophenone as it is consumed by isoniazid

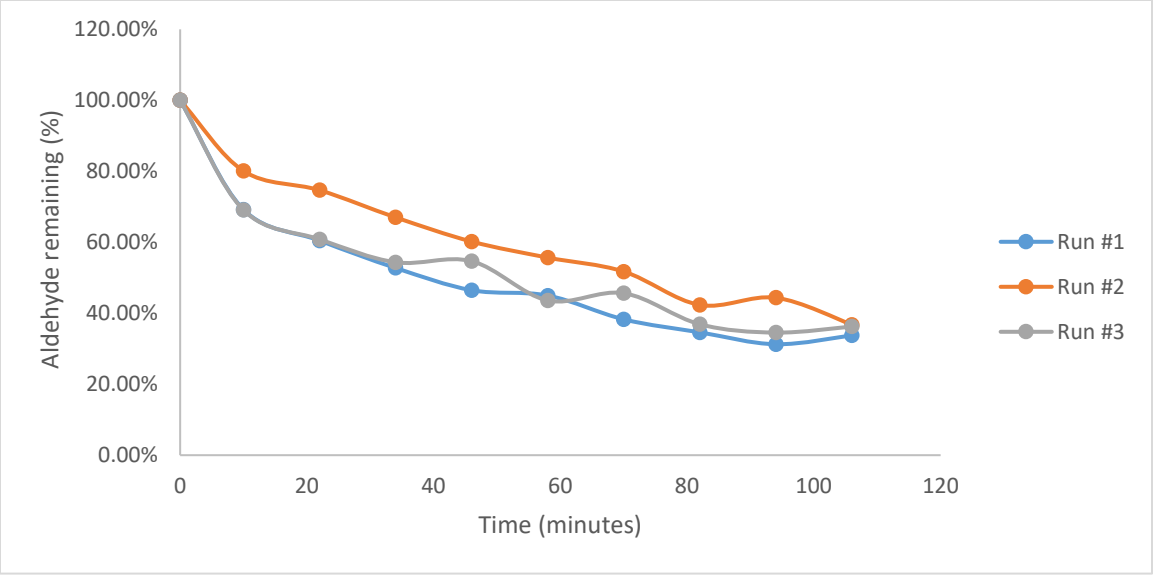


Figure 47: Percent decrease in concentration of ethyl acetoacetate as it is consumed by isoniazid.

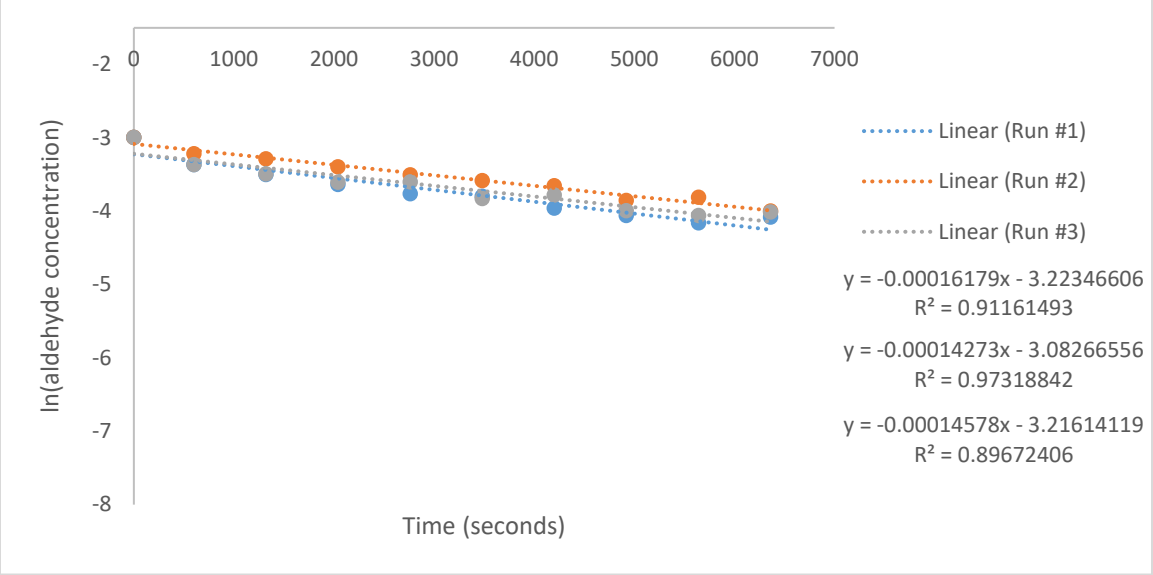


Figure 48: Linear regression of the decrease in concentration of ethyl acetoacetate as it is consumed by isoniazid.

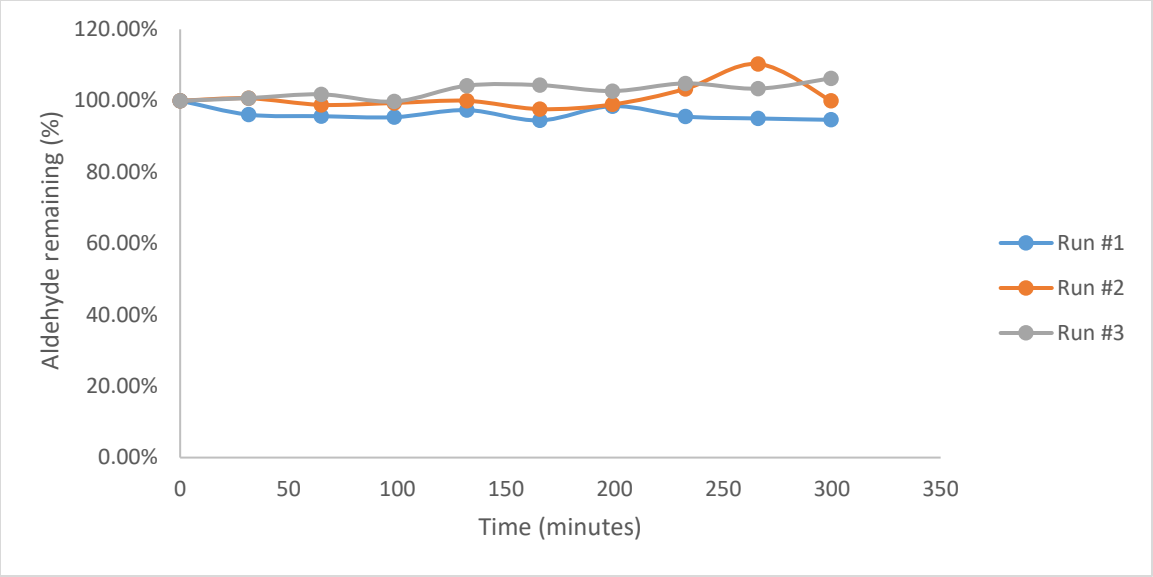


Figure 49: Percent decrease in concentration of butyl acetate as it is consumed by isoniazid.

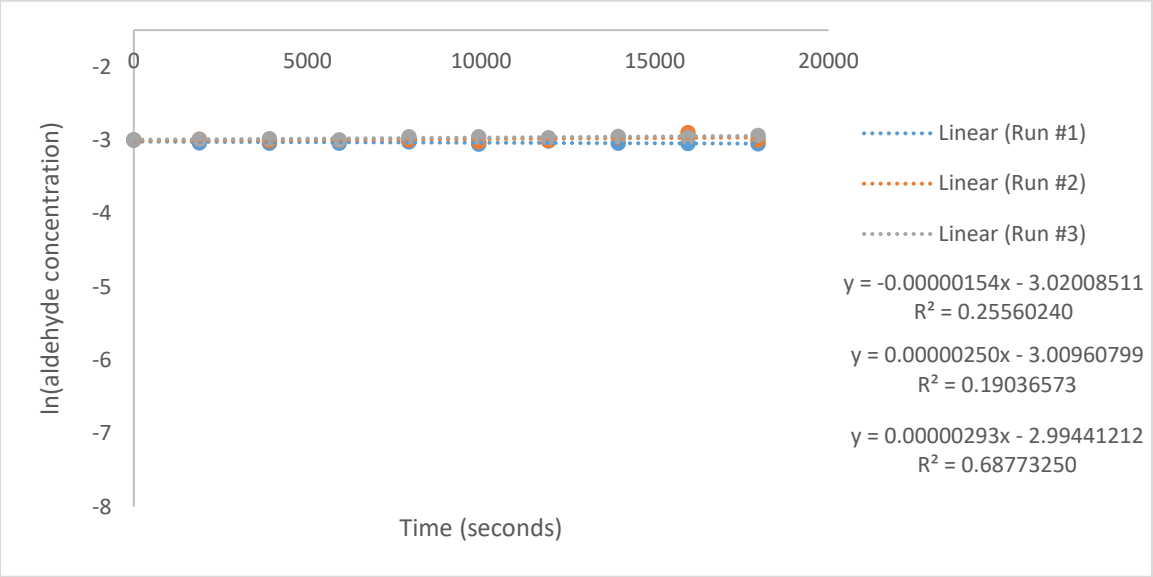


Figure 50: Linear regression of the decrease in concentration of butyl acetate as it is consumed by isoniazid

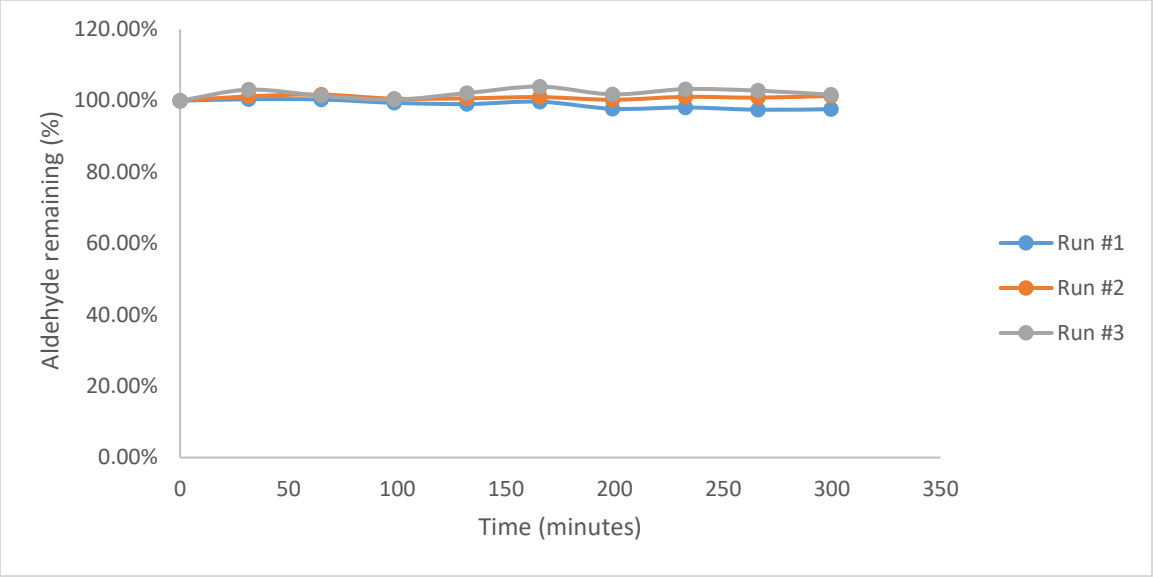


Figure 51: Percent decrease in concentration of methyl benzoate as it is consumed by isoniazid.

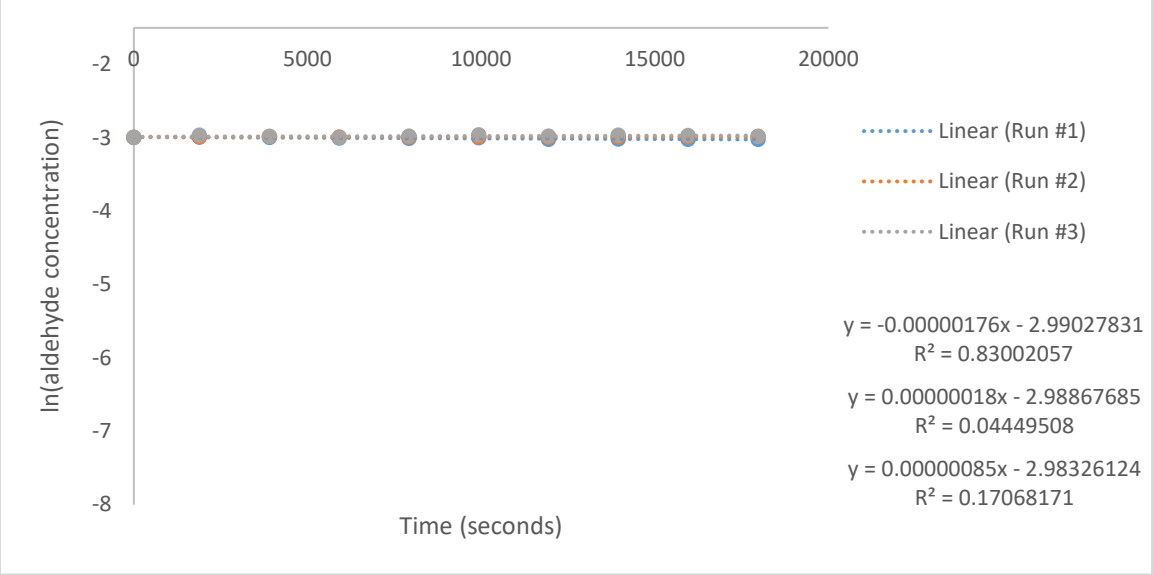
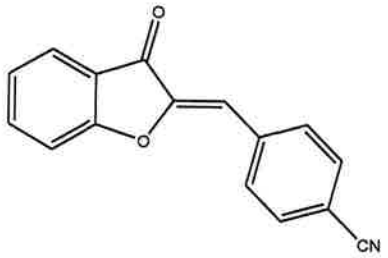


Figure 52: Linear regression of the decrease in concentration of methyl benzoate as it is consumed by isoniazid.

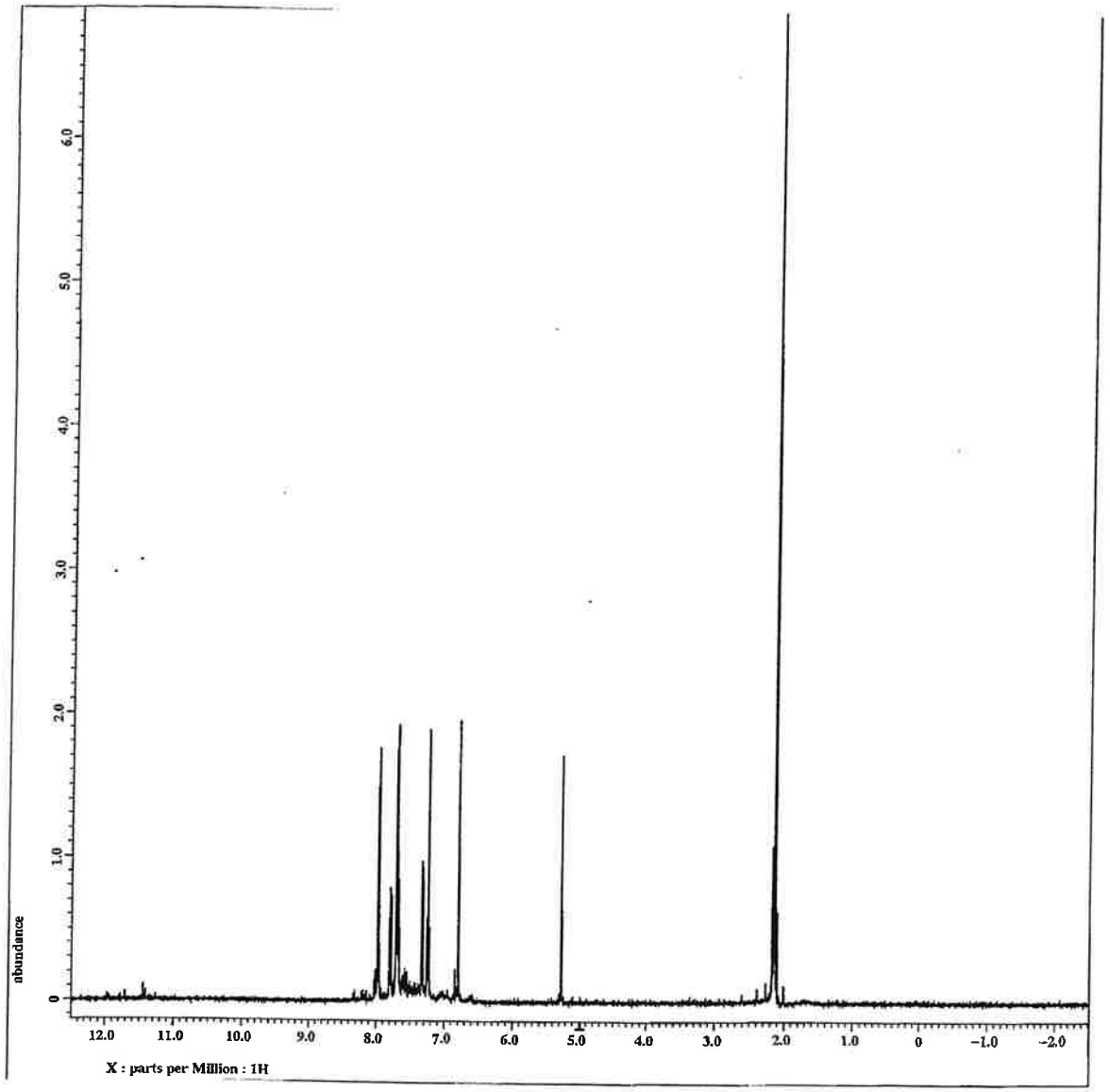
References:

1. Hawkins, I.; Handy, S.T. *Tetrahedron* **2013**, *69*, 9200-9204.
2. Kafle, A.; Bhatarai, S.; Handy, S.T. *Synthesis*, **2020**, 2337-2346.
3. Venkateswarlu, S.; Murty, G.N.; Satyanarayana, M. *ARKIVOC*, **2017**, *4*, 303-314.
4. Taylor, K.M.; Taylor, Z.E.; Handy, S.T. *Tetrahedron Lett.* **2017**, *58*, 240-241.
5. Varma, R.S.; Varma, M. *Tetrahedron Lett.* **1992**, *33*, 5937-5940.
6. Xu, H.; Ziao, H.; Hu, X.; Zuan, G.; Li, P.; Zhang, Z. *J. Org. Chem.* **2022**, *87*, 16204-16212.

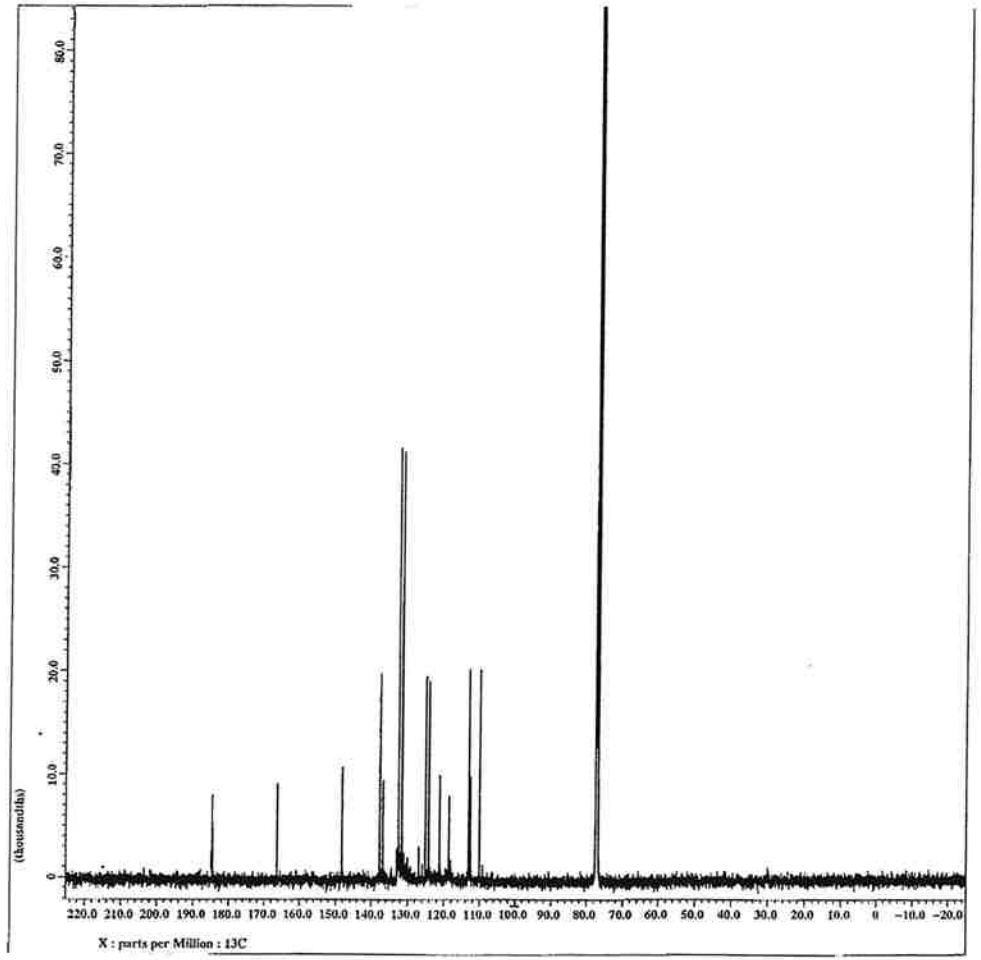
(Z)-4-((3-oxobenzofuran-2(3H)-ylidene)methyl)benzonitrile



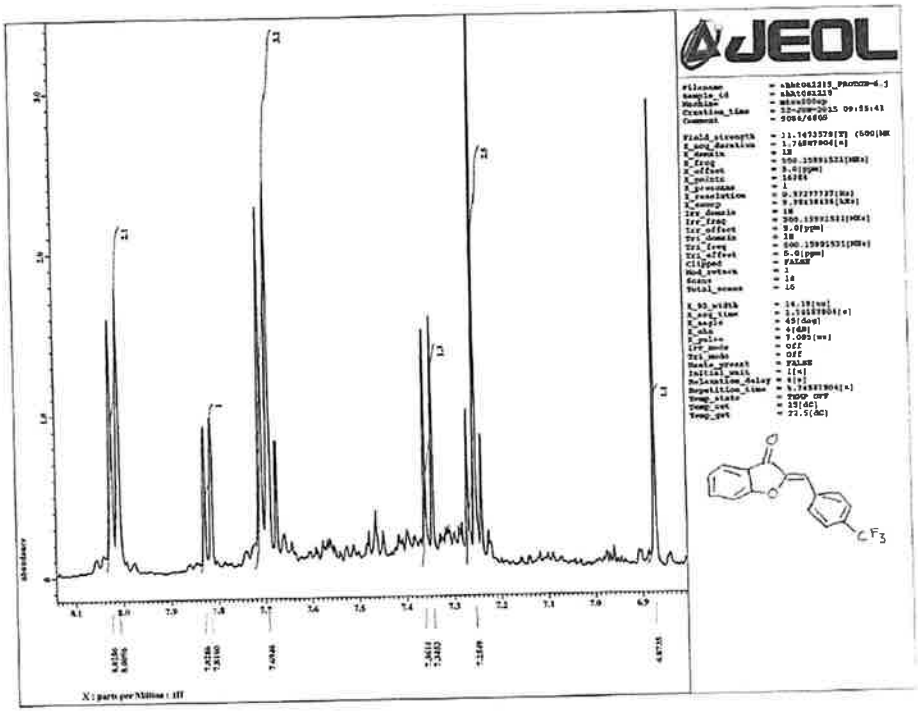
^{1}H-NMR

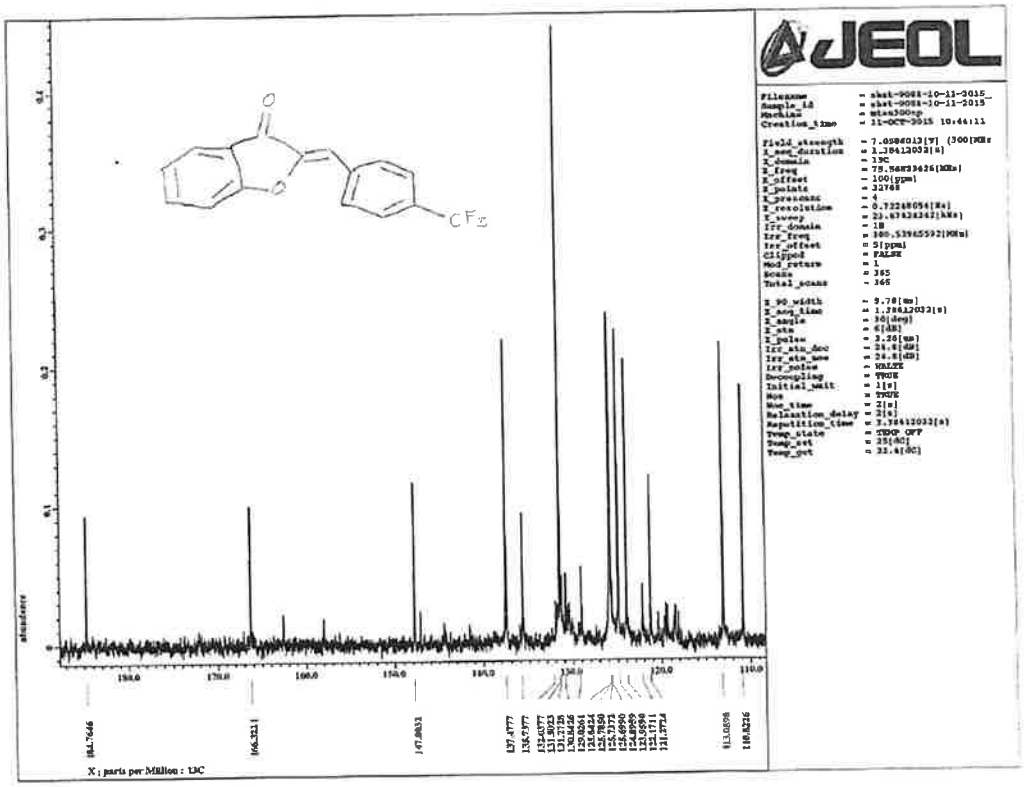


^{13}C-NMR

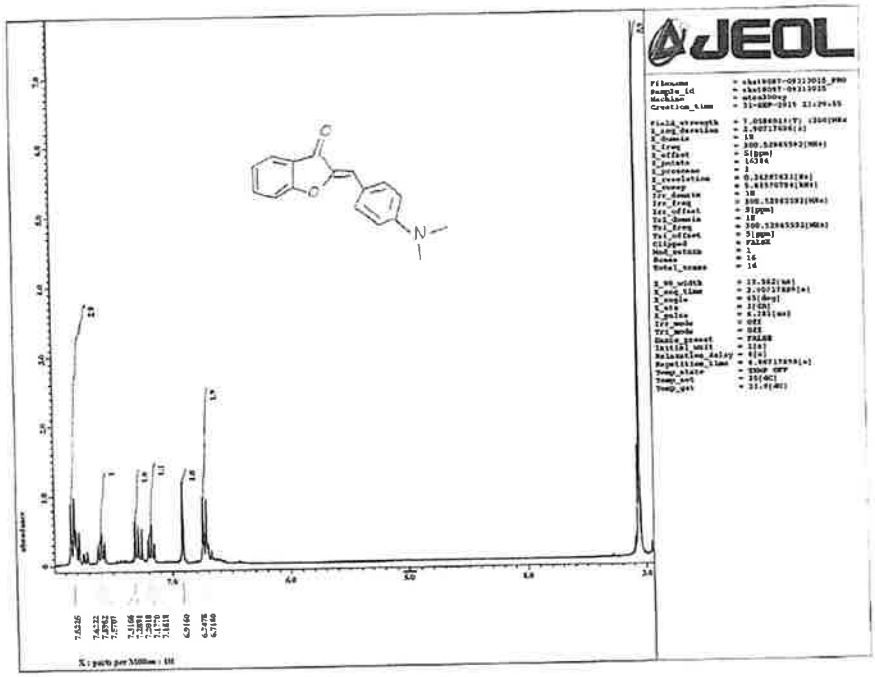

(thousandths)
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : 13C

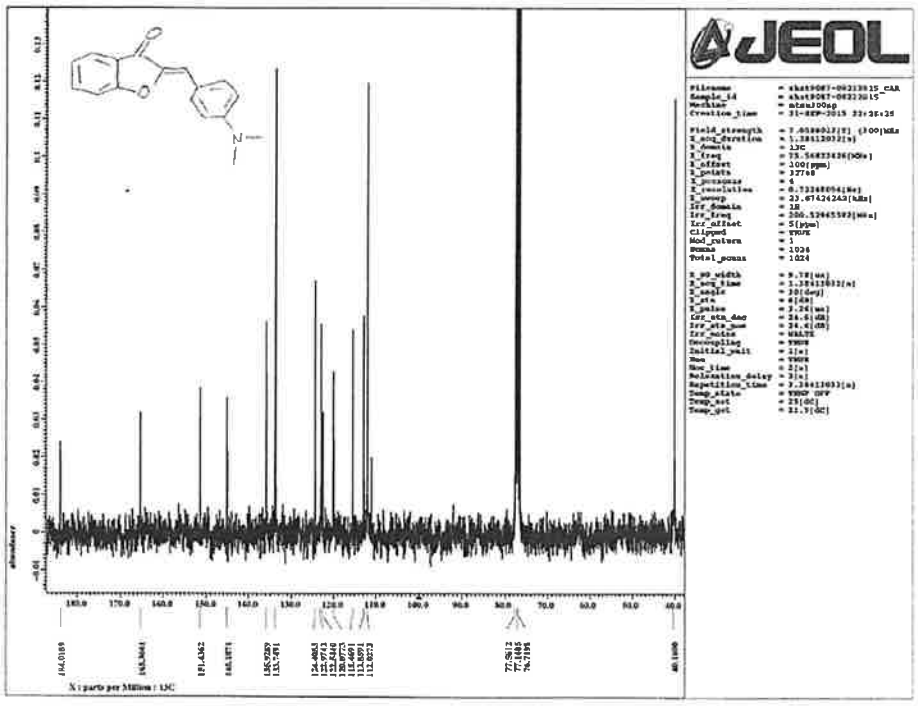
(Z)-2-(4-(trifluoromethyl)benzylidene)benzofuran-3(2H)-one



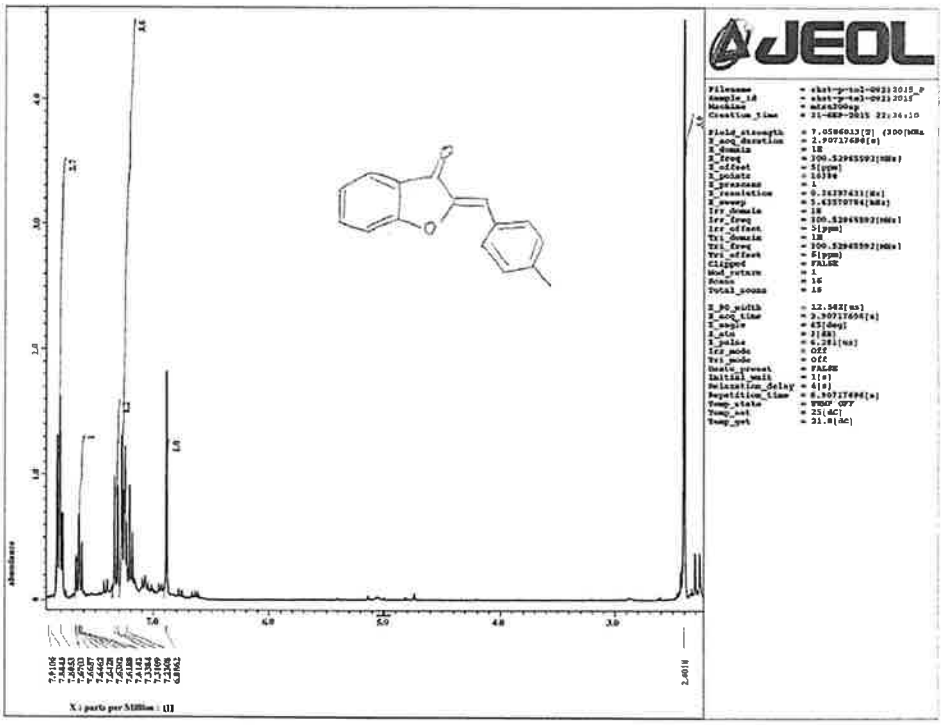


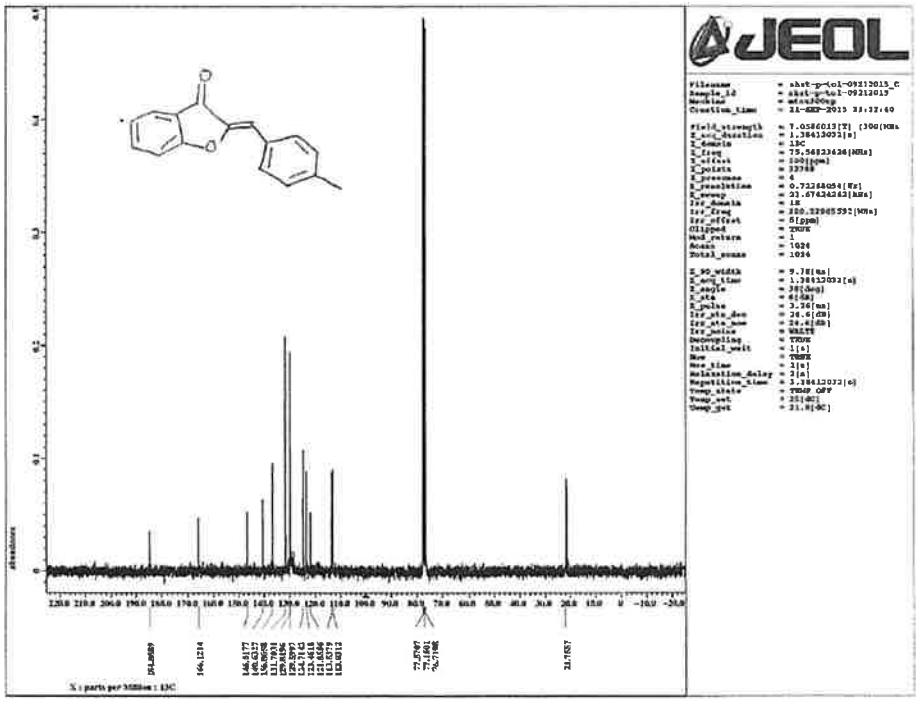
(Z)-2-(4-(dimethylamino)benzylidene)benzofuran-3(2H)-one



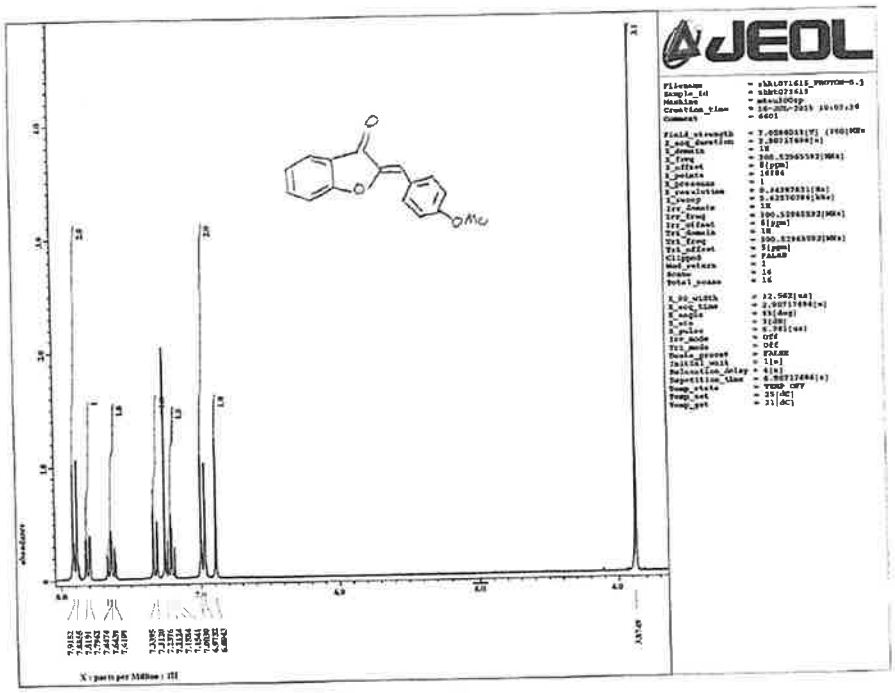


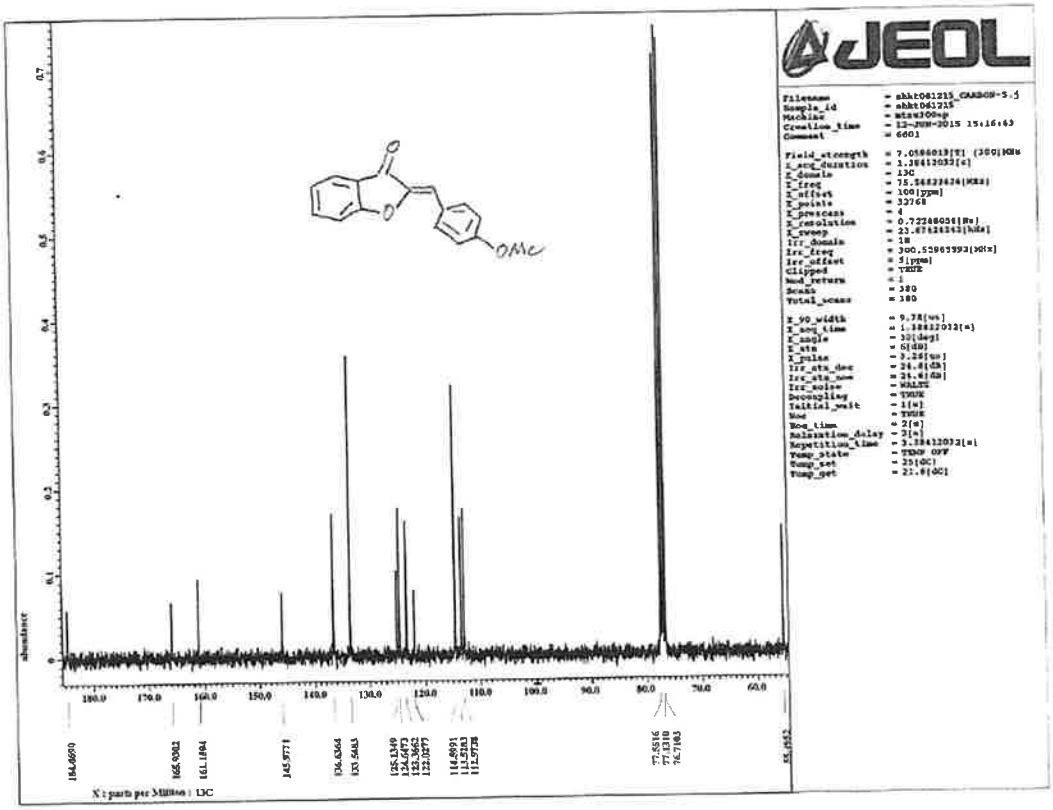
(Z)-2-(4-methylbenzylidene)benzofuran-3(2H)-one



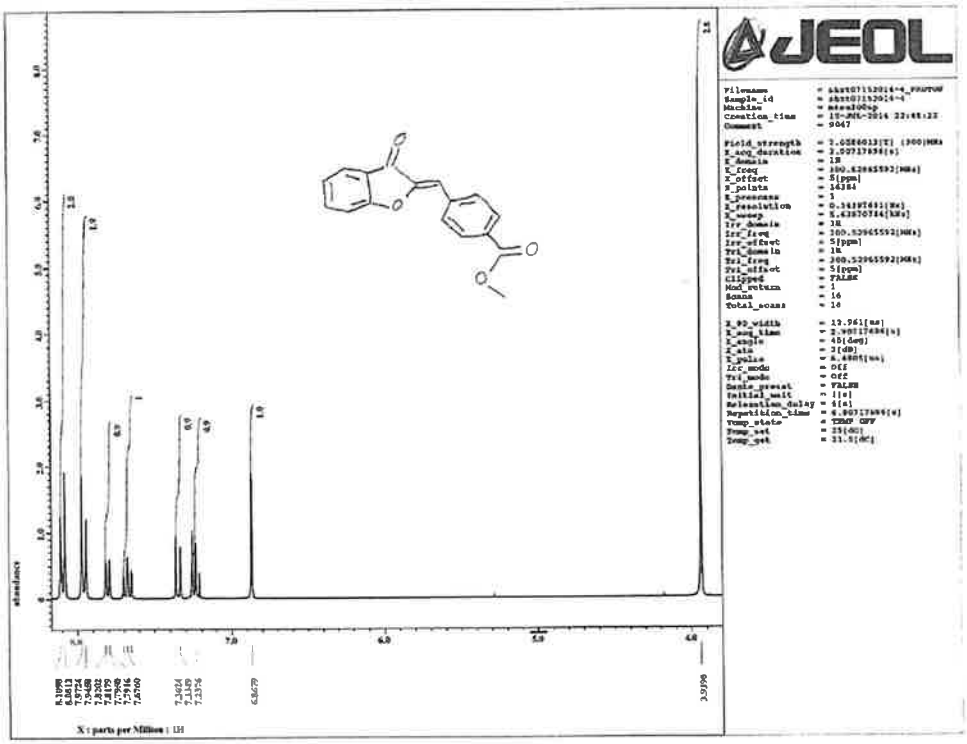


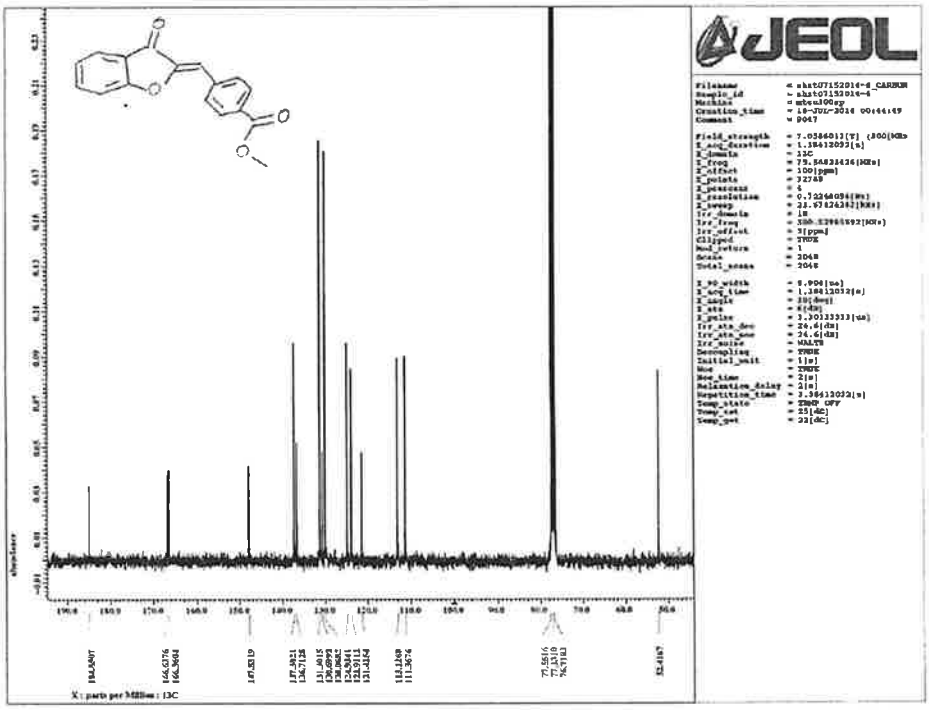
(Z)-2-(4-methoxybenzylidene)benzofuran-3(2H)-one



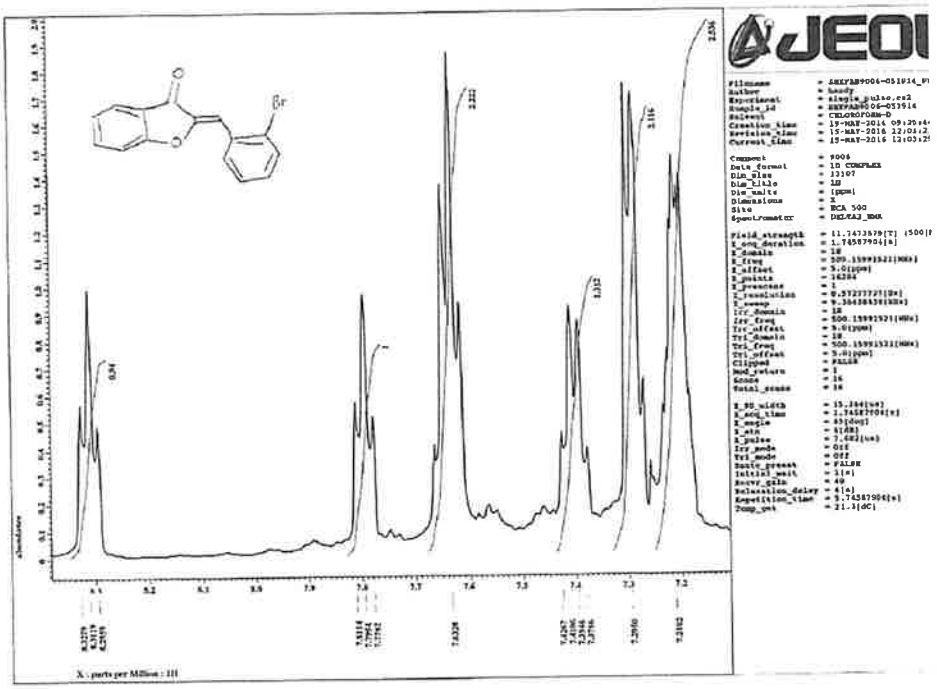


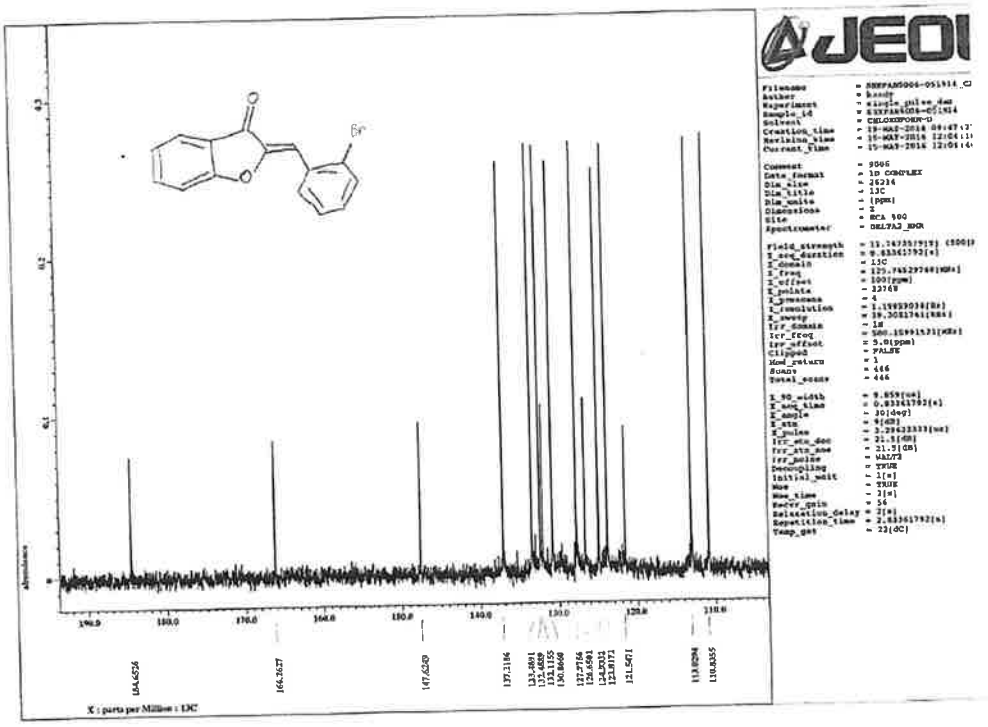
Methyl (Z)-4-((3-oxobenzofuran-2(3H)-ylidene)methyl)benzoate



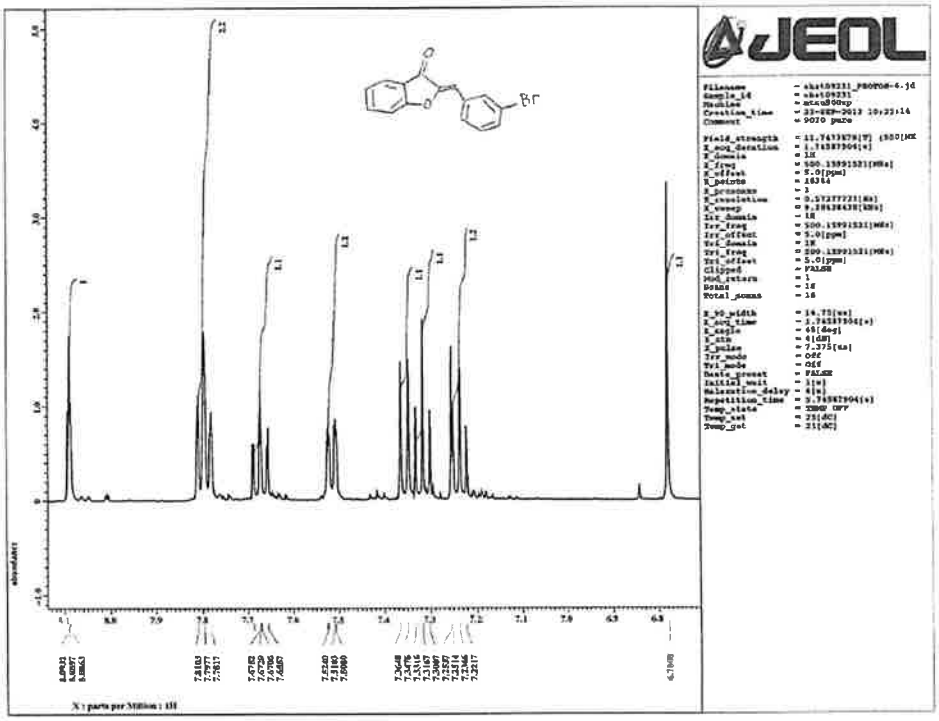


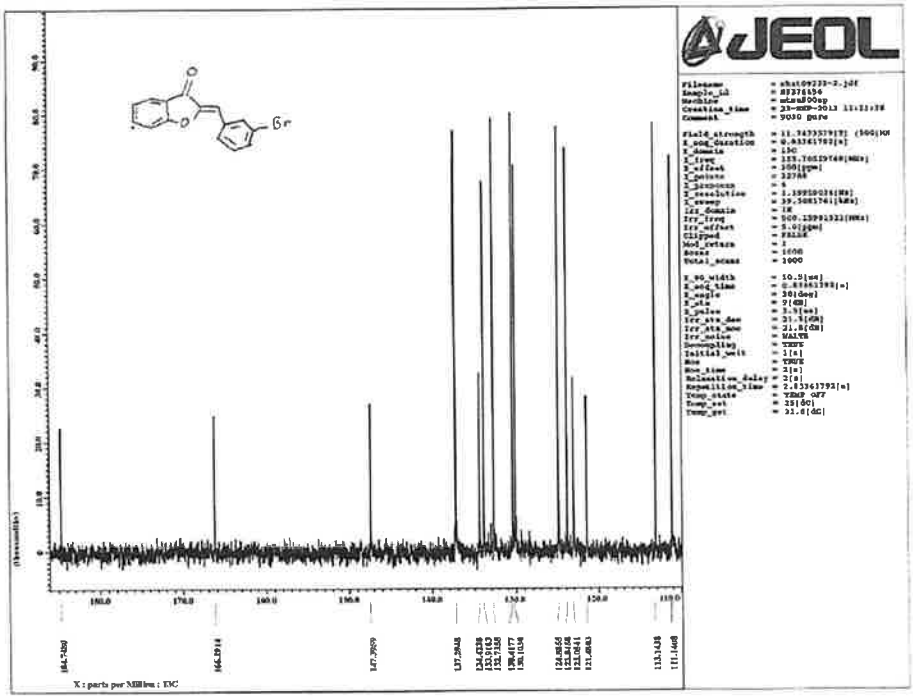
(Z)-2-(2-bromobenzylidene)benzofuran-3(2H)-one



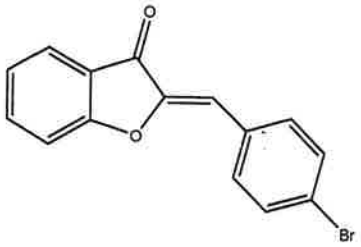


(Z)-2-(3-bromobenzylidene)benzofuran-3(2H)-one

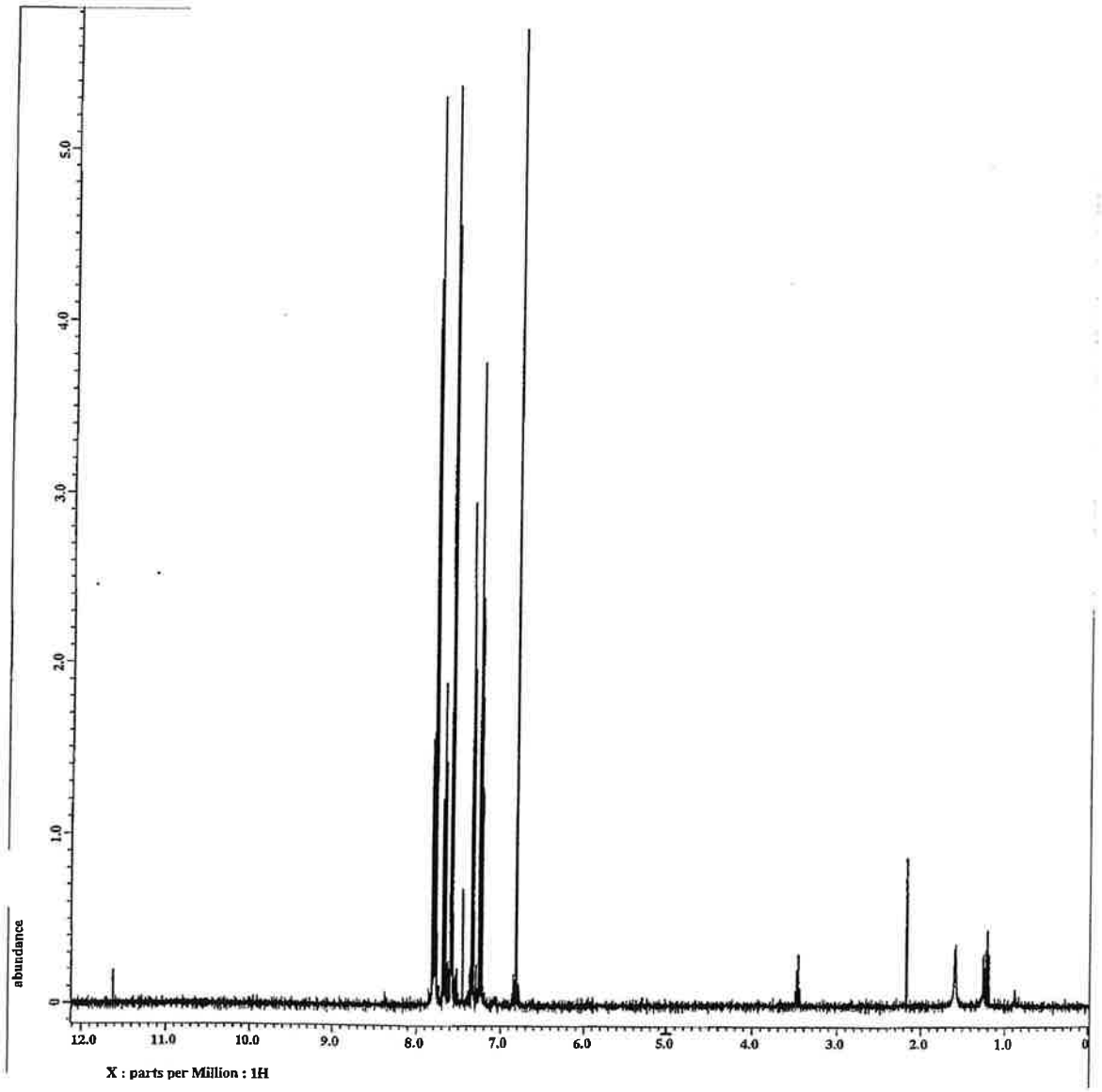




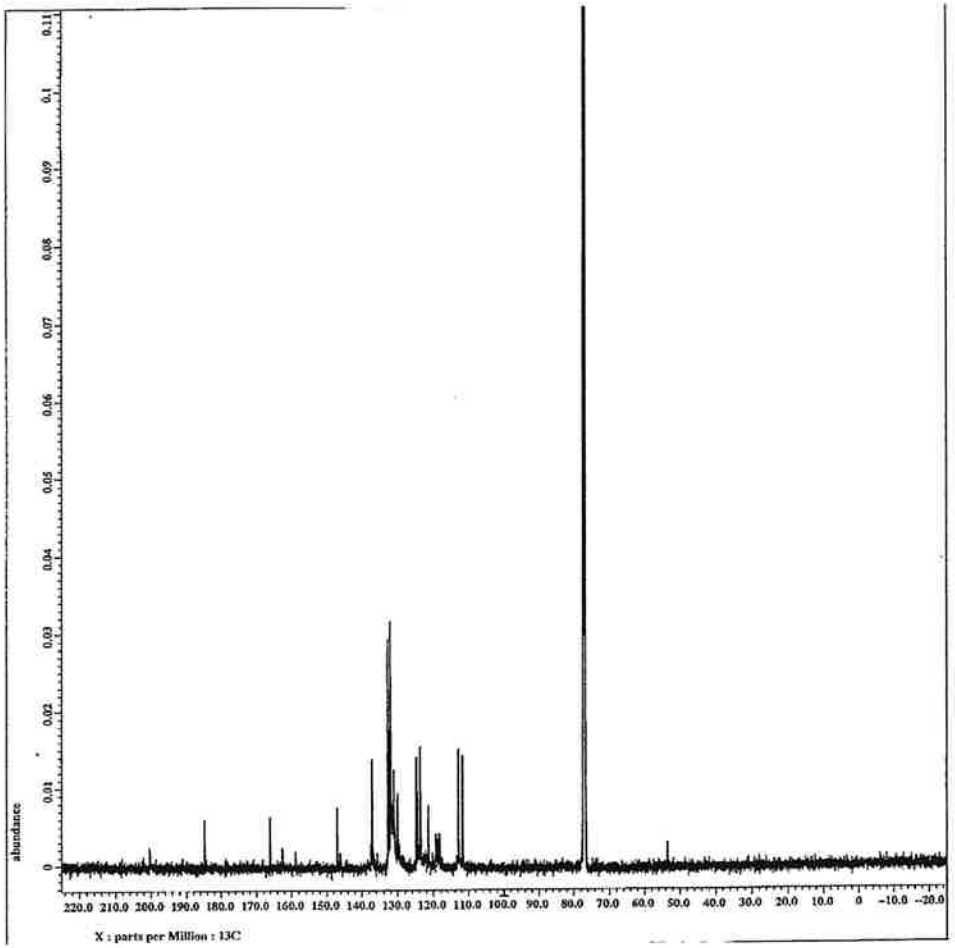
(Z)-2-(4-bromobenzylidene)benzofuran-3(2H)-one



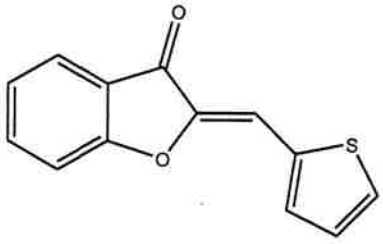
^{1}H-NMR



^{13}C-NMR


abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : 13C

2-(thiophen-2-ylmethylene)benzofuran-3(2H)-one



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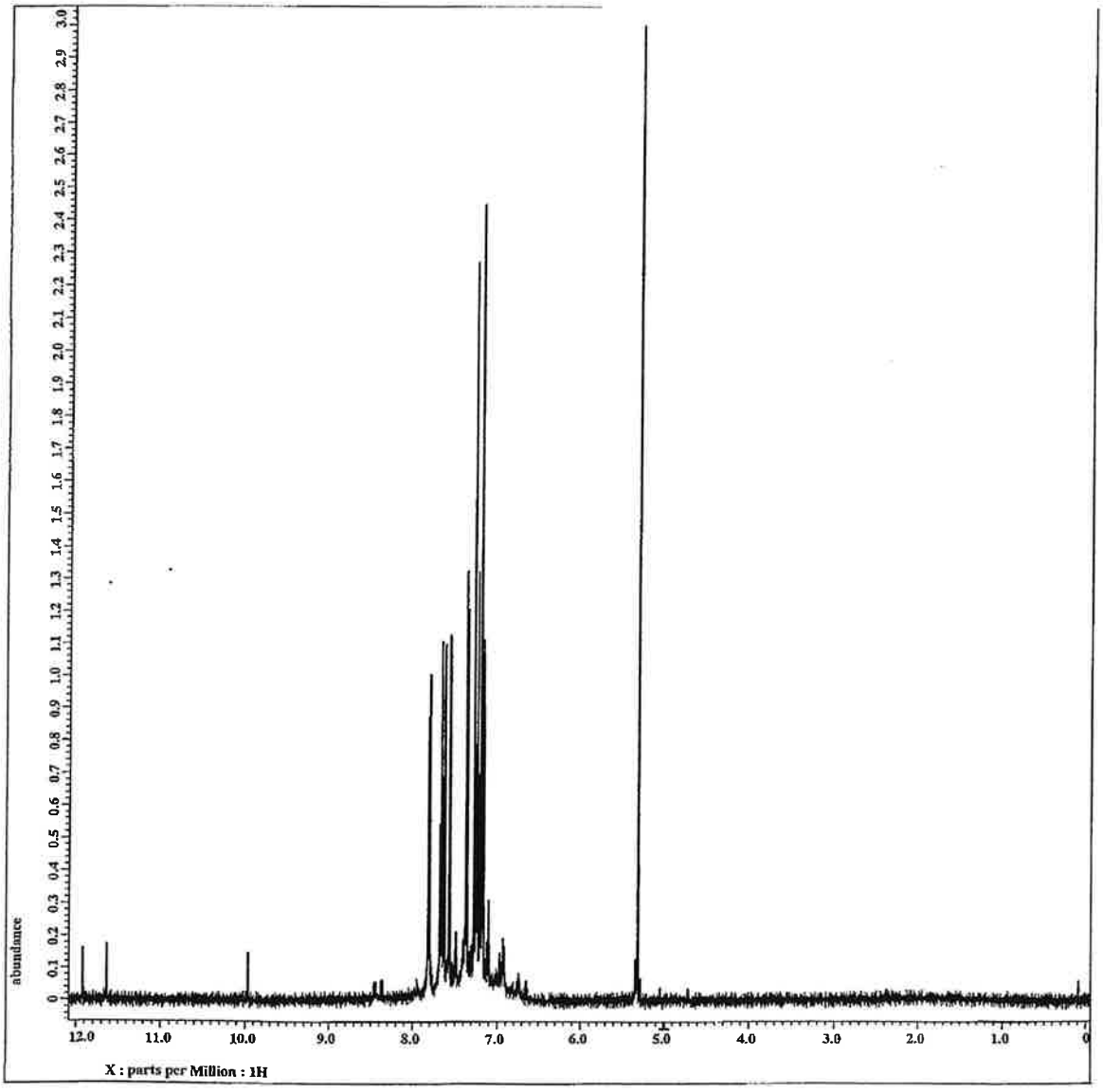
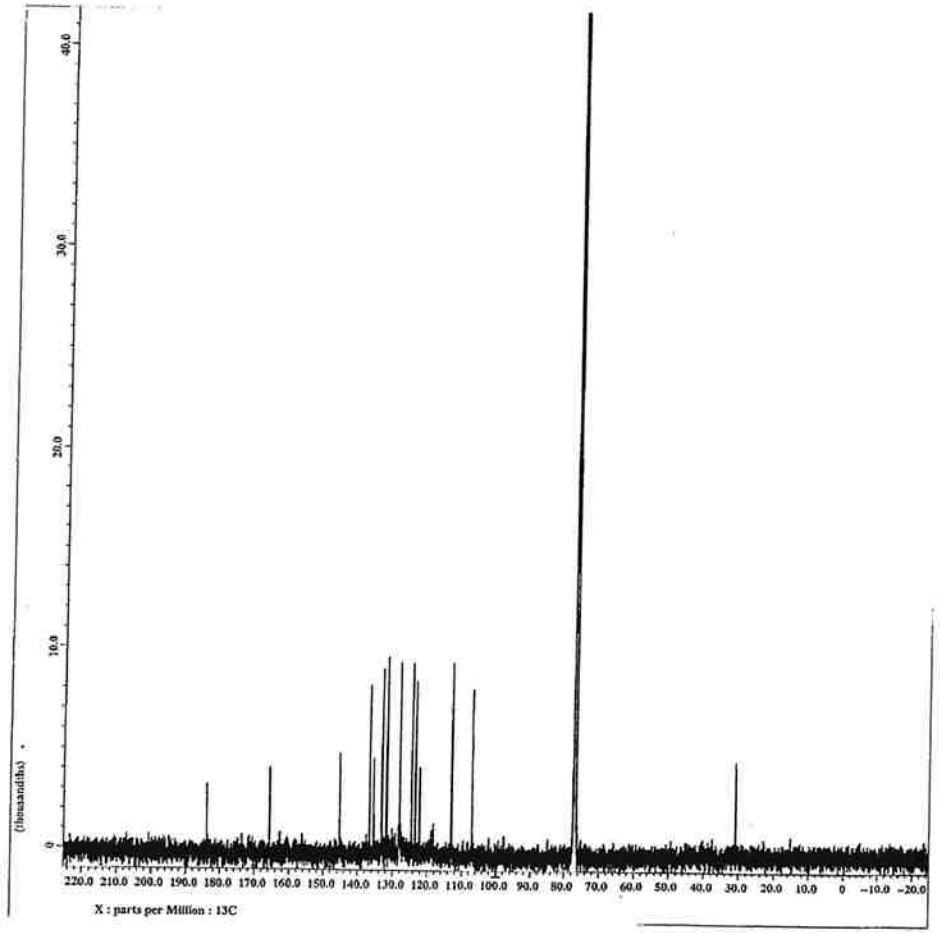
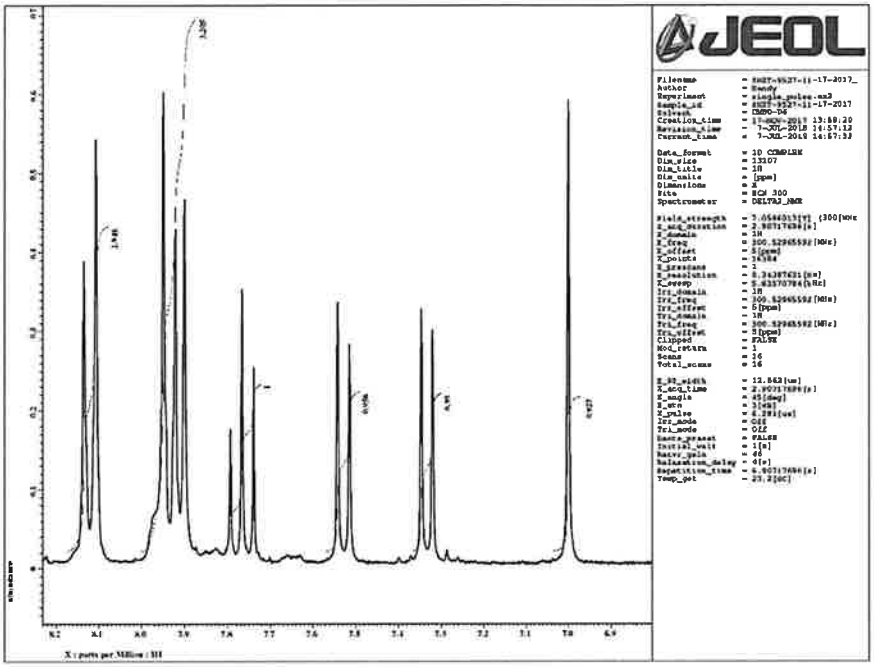
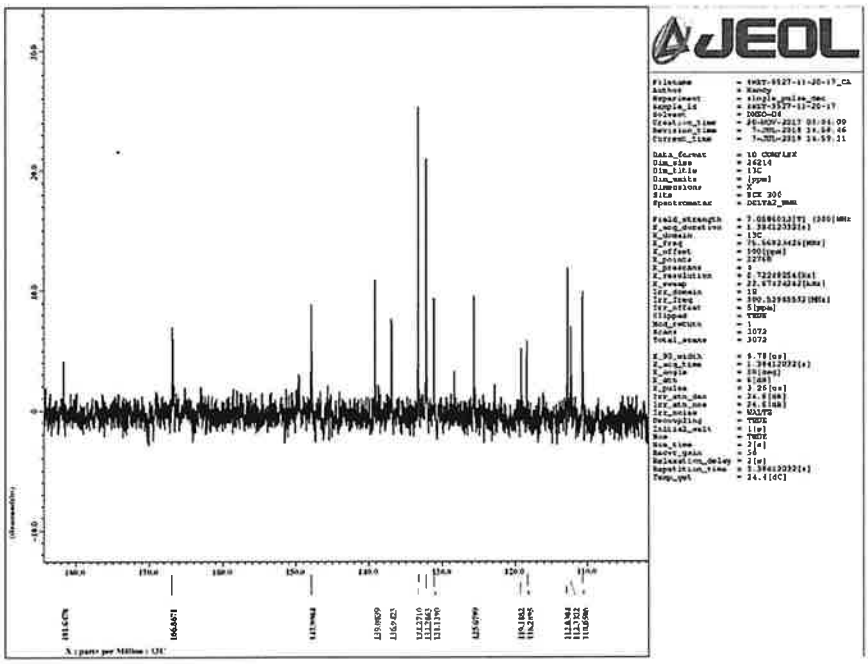


^{13}C-NMR

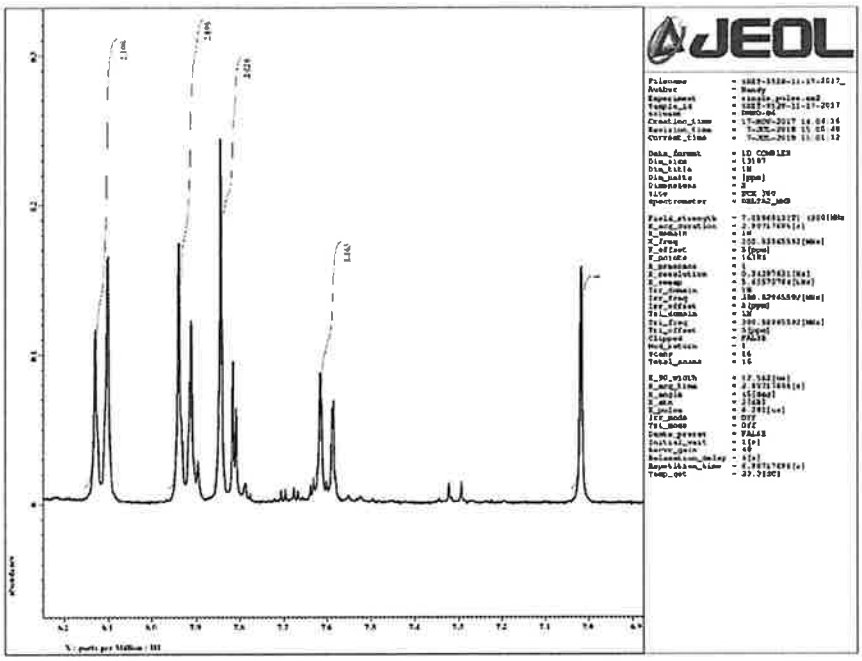

(thousandths)
40.0
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : 13C

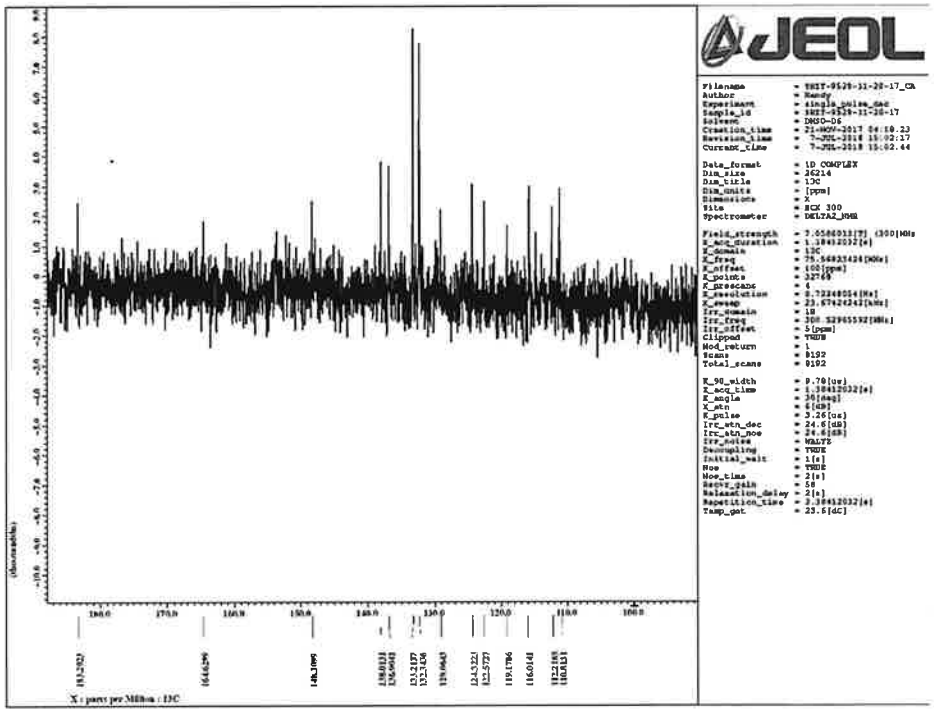
(Z)-4-((4-chloro-3-oxobenzofuran-2(3H)-ylidene)methyl)benzonitrile



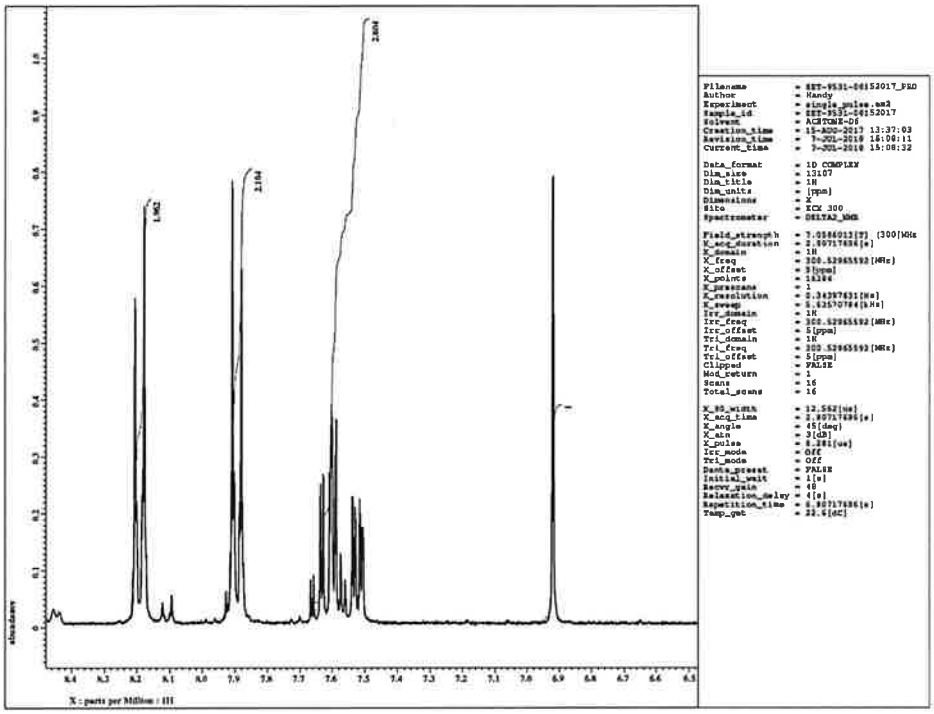


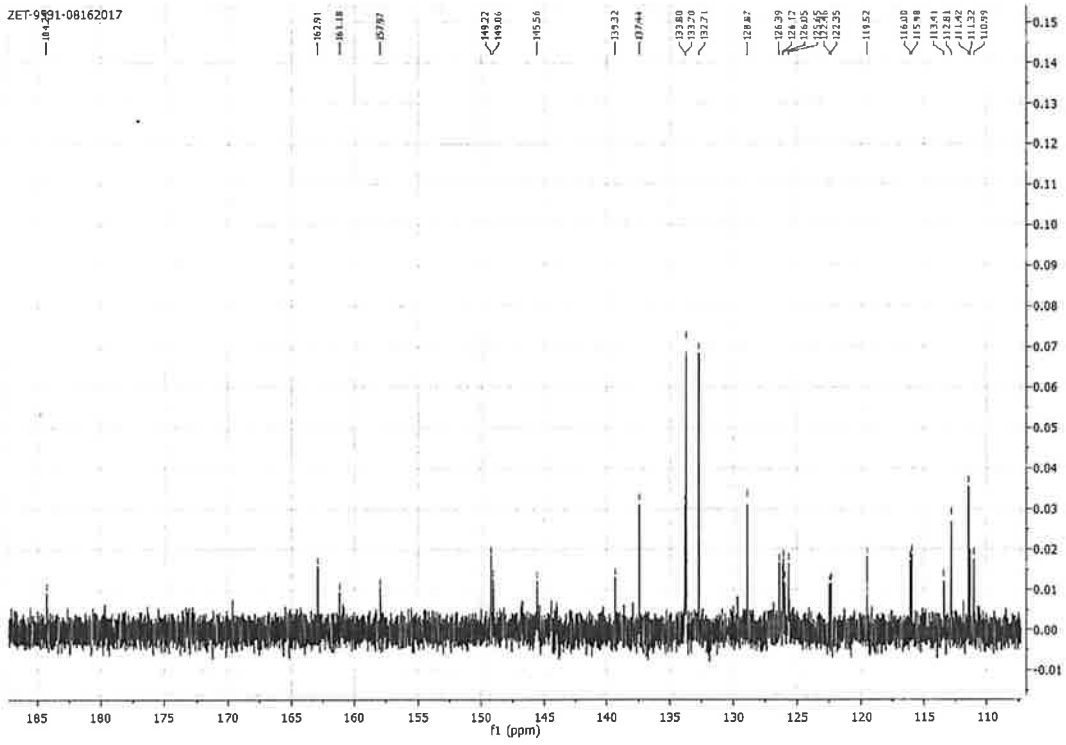
(Z)-4-((5-chloro-3-oxobenzofuran-2(3H)-ylidene)methyl)benzonitrile



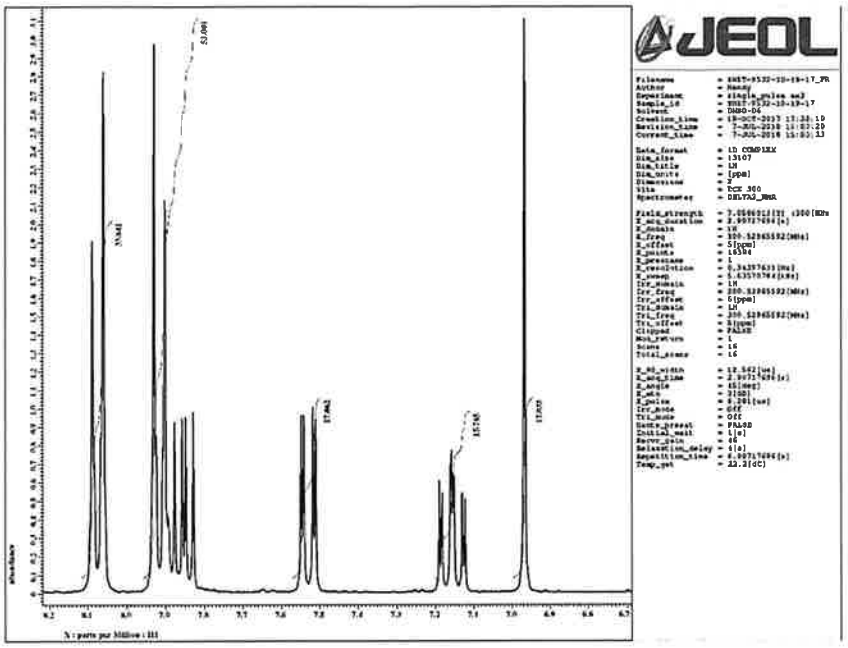


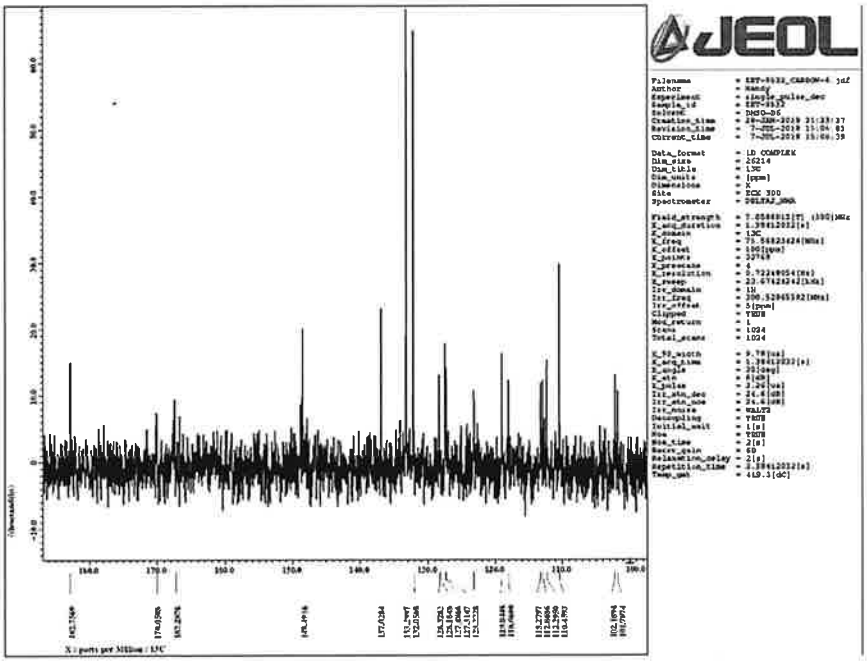
(Z)-4-((5-fluoro-3-oxobenzofuran-2(3H)-ylidene)methyl)benzonitrile





(Z)-4-((6-fluoro-3-oxobenzofuran-2(3H)-ylidene)methyl)benzonitrile





(Z)-4-((5-bromo-3-oxobenzofuran-2(3H)-ylidene)methyl)benzonitrile