

Spektri masa i NMR spektri (1H i 13C) sintetiziranih kumarina, rodanina i tiazolidindiona

Lončarić, Melita

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**SVEUČILIŠTE JOSIPA JURJA STROSSMAYERA U OSIJEKU
PREHRAMBENO-TEHNOLOŠKI FAKULTET OSIJEK**

Melita Lončarić

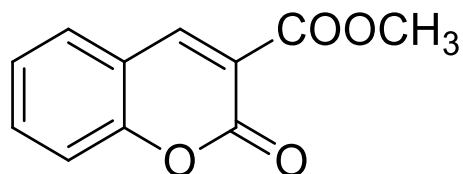
**INHIBICIJA LIPOOKSIGENAZE DERIVATIMA KUMARINA, RODANINA I
TIAZOLIDINDIONA**

DOKTORSKA DISERTACIJA

Osijek, ožujak, 2022.

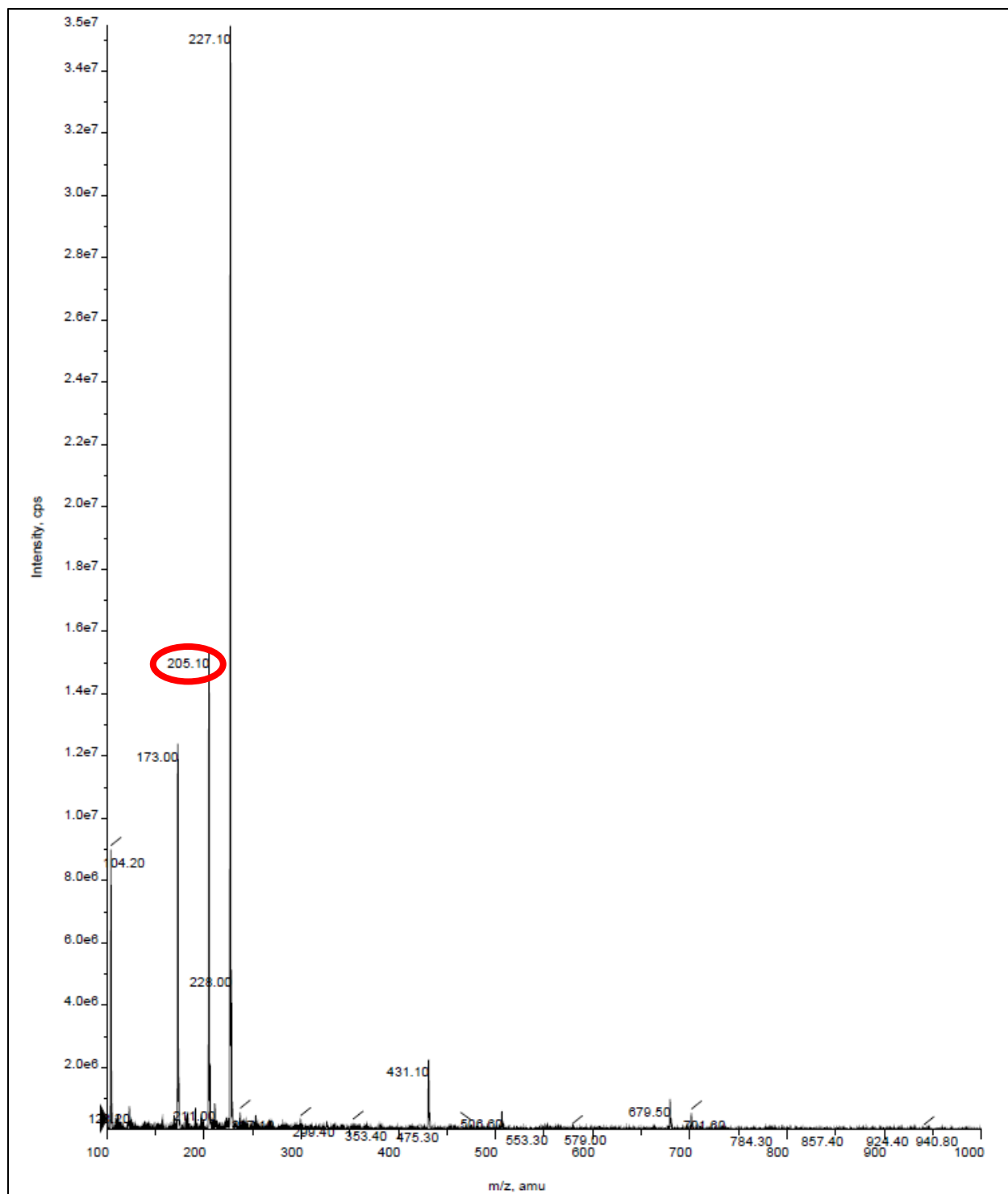
Prilog 1 Spektri masa i NMR spektri (^1H i ^{13}C) sintetiziranih kumarina, rodanina i tiazolidindiona.

metil 2-okso-2H-kromen-3-karboksilat (1a)

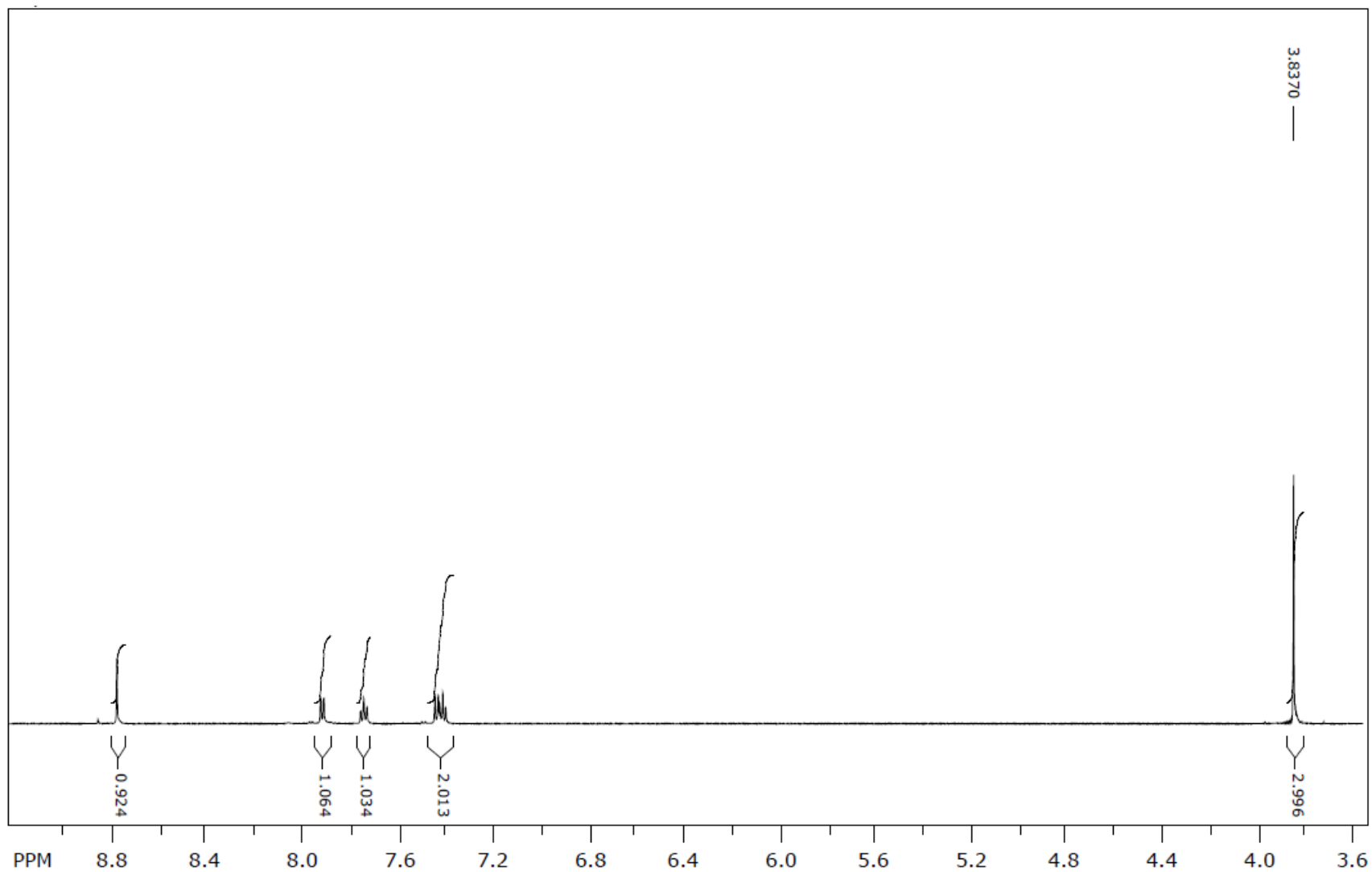


Reaktanti	Salicilaldehid (10 mmol) i dimetilmalonat (10 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola
Molekulska masa	204,18 g/mol
Molekulska formula	C ₁₁ H ₈ O ₄
Temperatura tališta	102 – 105 °C (lit. 119 – 120 °C, Saeed i sur., 2012)
Boja kristala	Svijetložuta
R_f	0,76
LC/MS/MS m/z (M⁺)	205,10
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,73 (s, 1H), 7,84 (d, <i>J</i> = 8,40 Hz, 1H, arom.), 7,01 (d, <i>J</i> = 13,20 Hz, 2H, arom.), 3,90 (s, 3H, -OCH ₃), 3,82 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 164,8; 163,4; 157,11; 156,2; 149,4; 131,6; 113,2; 111,4; 100,3; 56,2; 52,1.

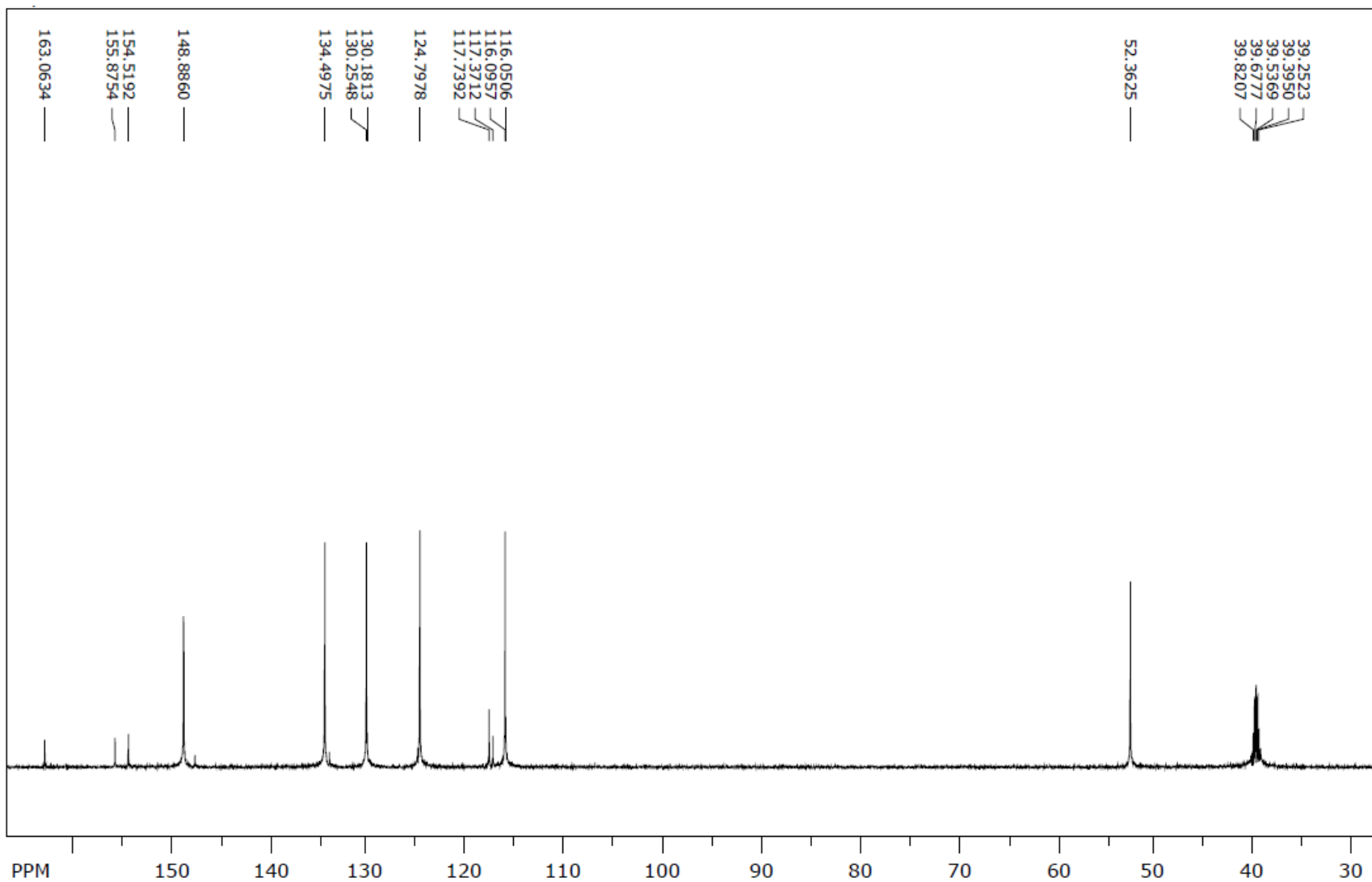
Maseni spektr (1a)



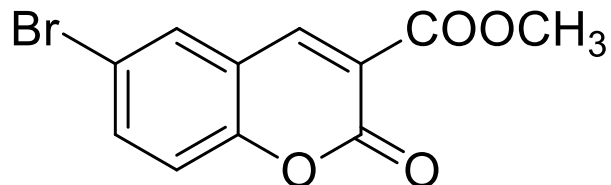
¹H NMR spektr (1a)



¹³C NMR spektr (1a)

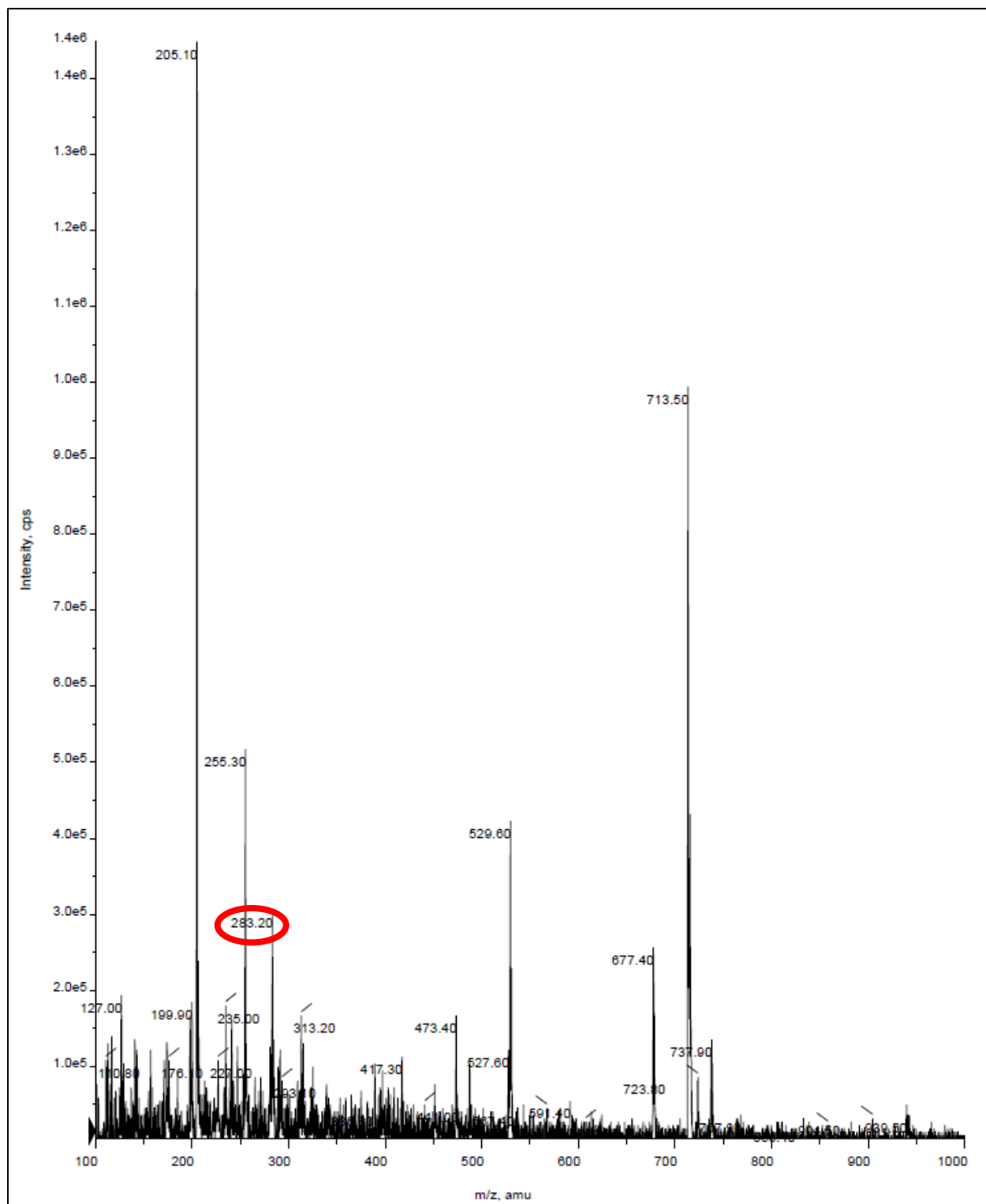


metil 6-brom-2-okso-2H-kromen-3-karboksilat (1b)

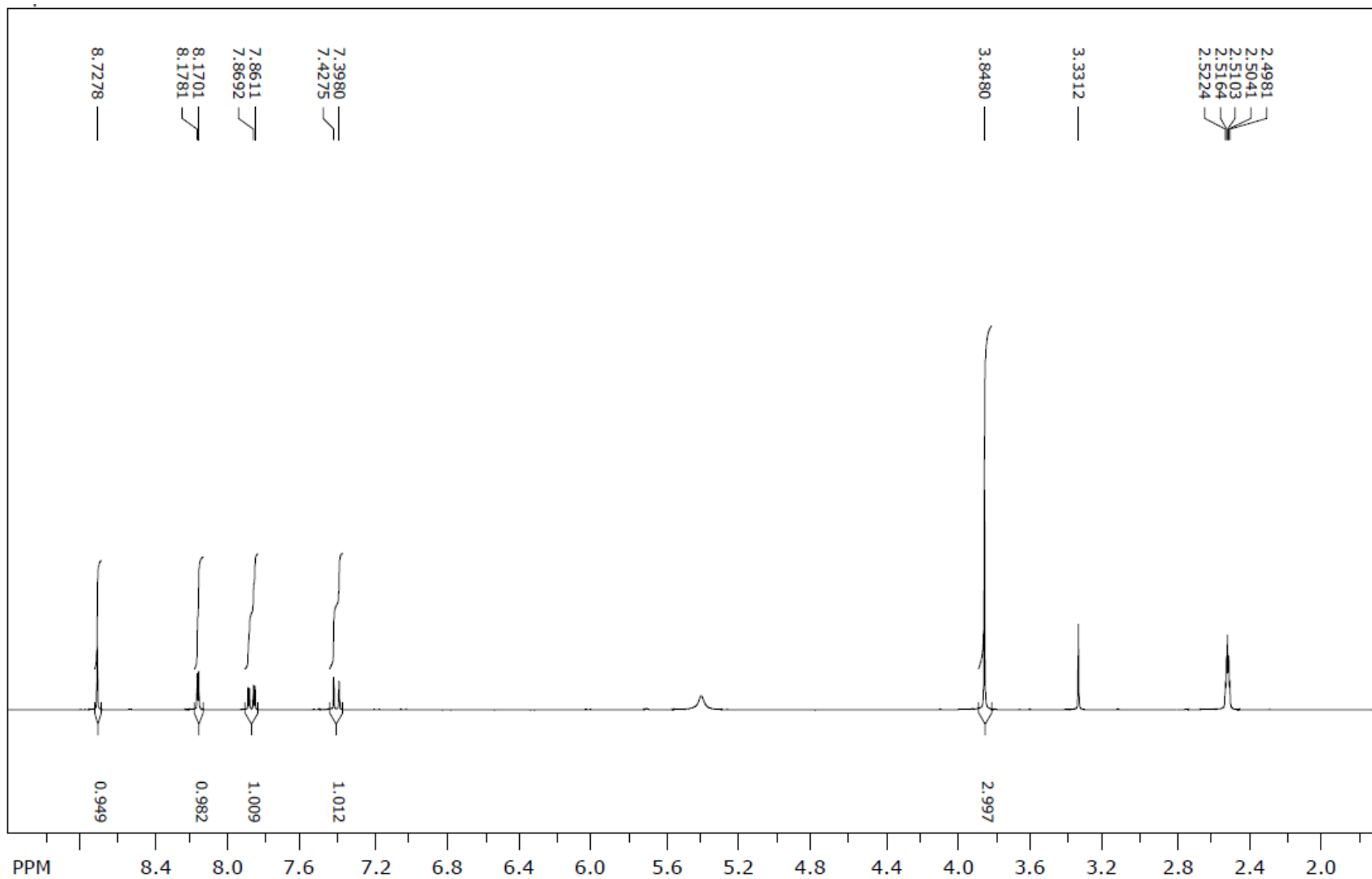


Reaktanti	5-bromosalicilaldehid (10 mmol) i dimetilmalonat (10 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola
Molekulska masa	283,07 g/mol
Molekulska formula	C ₁₁ H ₇ BrO ₄
Temperatura tališta	180 – 185 °C (lit. 180 – 182 °C, Keshavarzipour i Tavakol, 2016)
Boja kristala	Bijela
R_f	0,74
LC/MS/MS <i>m/z</i> (M⁻)	283,20
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 8,73 (s, 1H, arom.), 8,17 (d, <i>J</i> = 2,40 Hz, 1H, arom.), 7,87 (dd, <i>J</i> = 8,88, 2,45 Hz, 1H, arom.), 7,41 (d, <i>J</i> = 8,85 Hz, 1H, arom.), 3,84 (s, 3H, OCH ₃).
¹³C NMR	(75 MHz, DMSO- <i>d</i> ₆) δ 163,3; 154,0; 148,1; 137,1; 132,6; 120,1; 119,1; 116,7; 53,0.

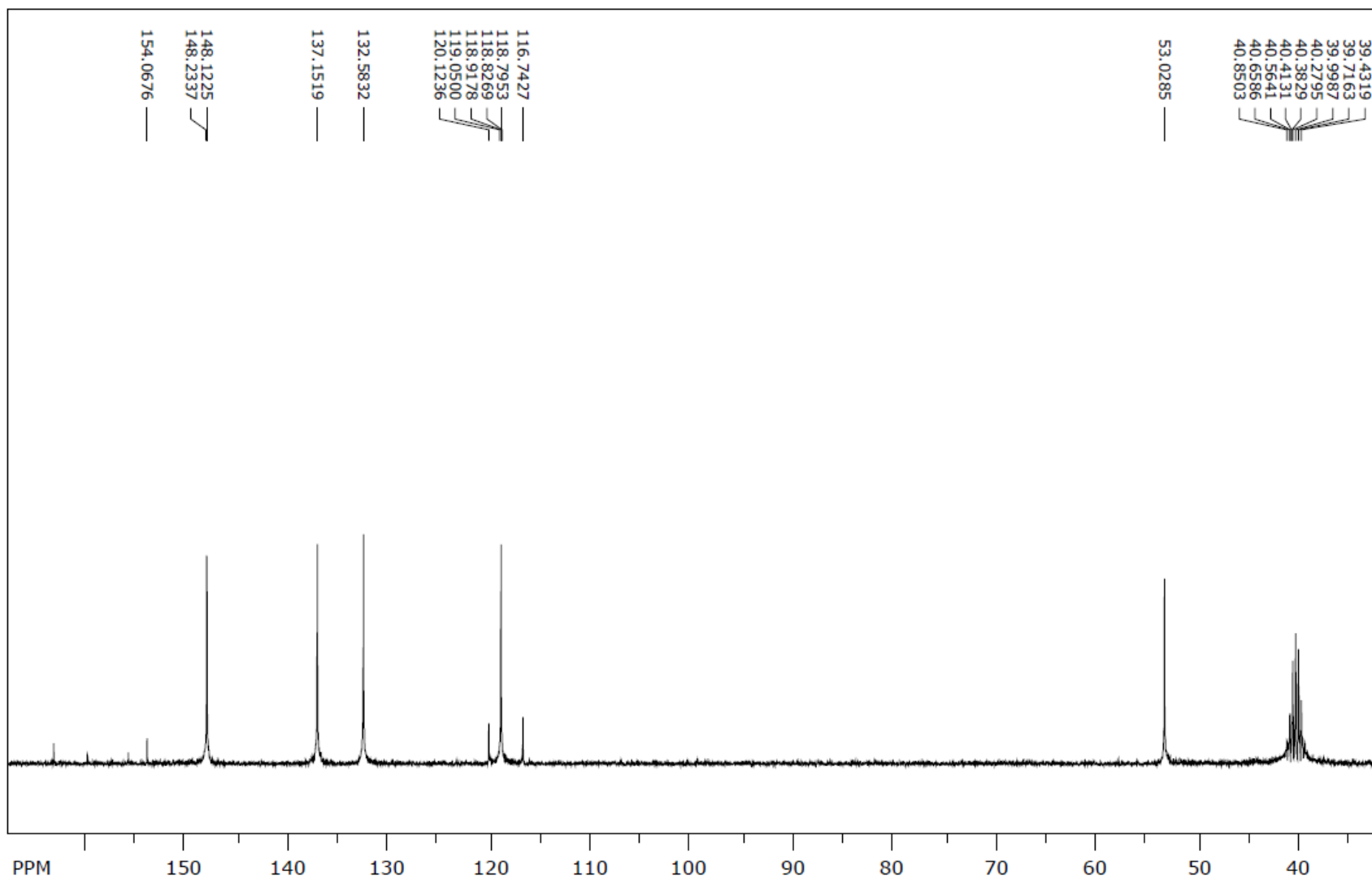
Maseni spektar (1b)



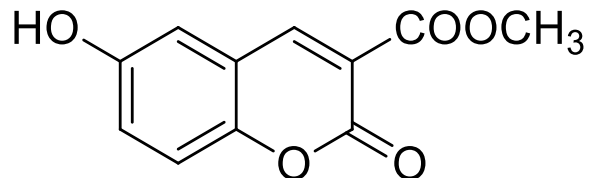
¹H NMR spektr (1b)



¹³C NMR spektr (1b)

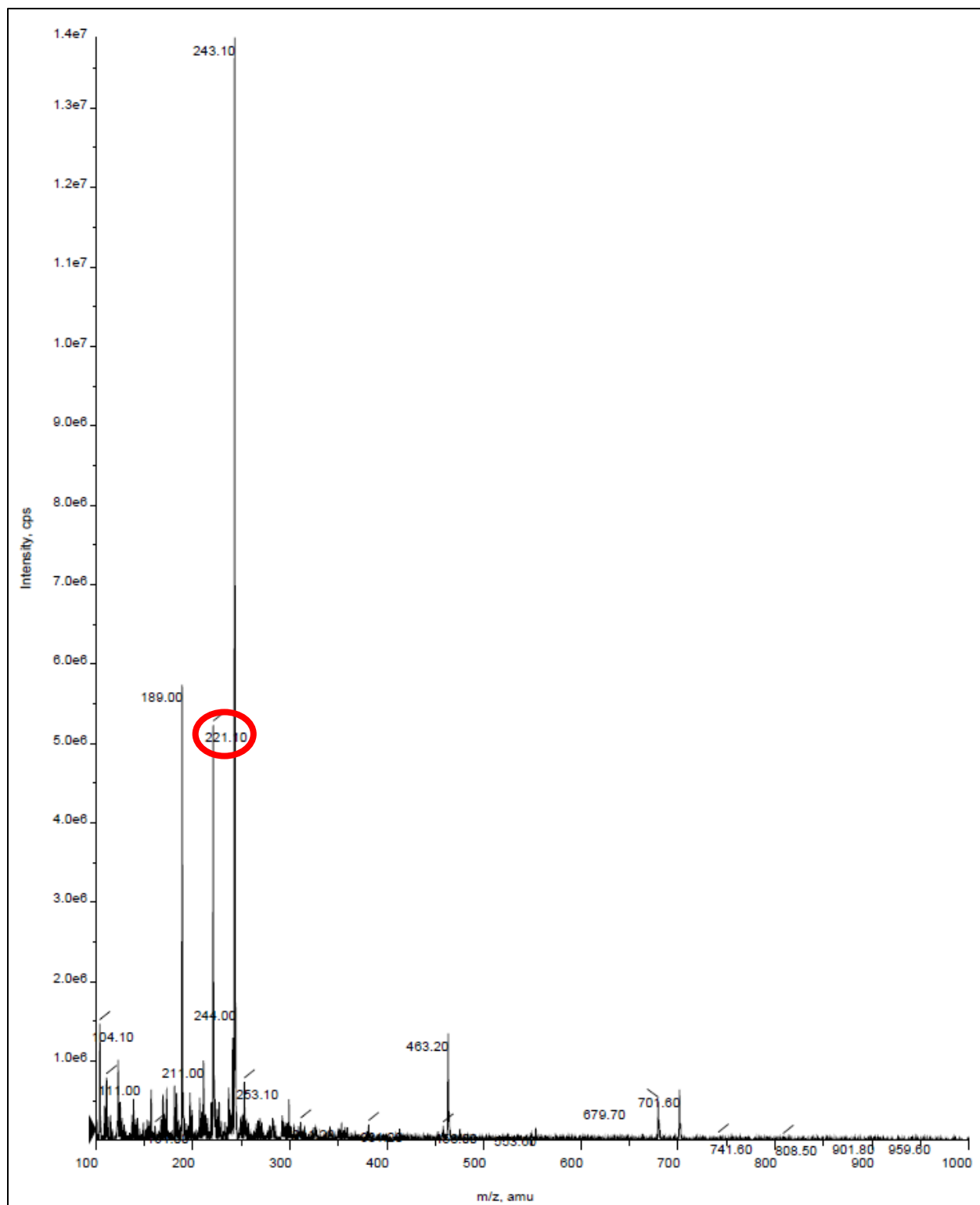


metil 6-hidroksi-2-okso-2H-kromen-3-karboksilat (1c)

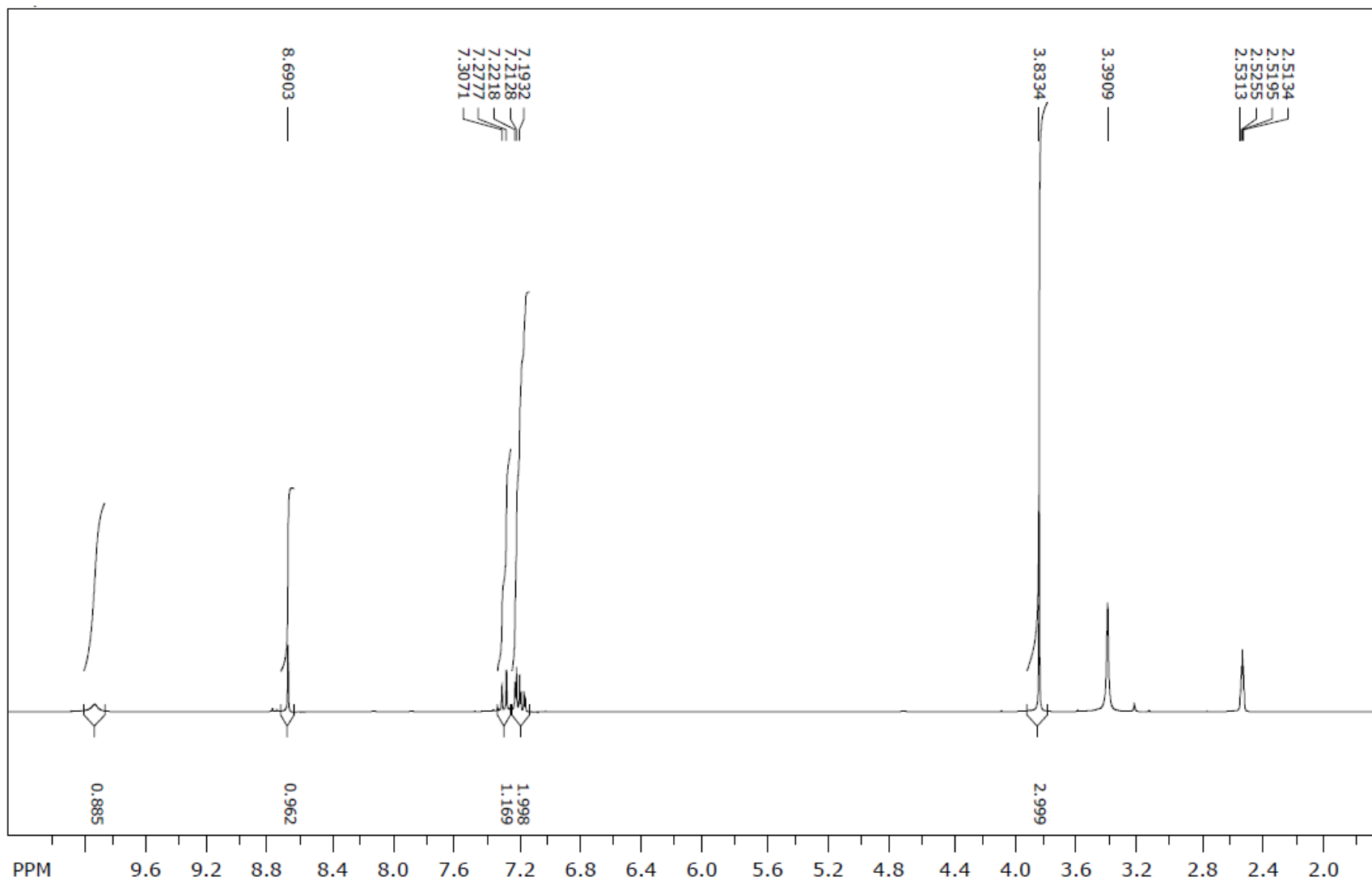


Reaktanti	2,5-dihidroksibenzaldehid (10 mmol) i dimetilmalonat (10 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	C ₁₁ H ₈ O ₅
Molekulska formula	220,18 g/mol
Temperatura tališta	185 – 190 °C (lit. 195 – 196 °C, Bisht i sur., 2017)
Boja kristala	Tamnocrvena
R_f	0,29
LC/MS/MS <i>m/z</i> (M⁺)	221,10
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 9,94 (s, 1H, OH), 8,69 (s, 1H, coum.), 7,29 (d, <i>J</i> = 8,82 Hz, 1H, arom.), 7,15 - 7,22 (m, 2H, arom.), 3,83 (s, 3H, OCH ₃).
¹³C NMR	(75 MHz, DMSO- <i>d</i> ₆) δ 163,8; 156,7; 154,4; 149,2; 148,4; 123,1; 118,7; 117,8; 117,5; 114,4; 52,8.

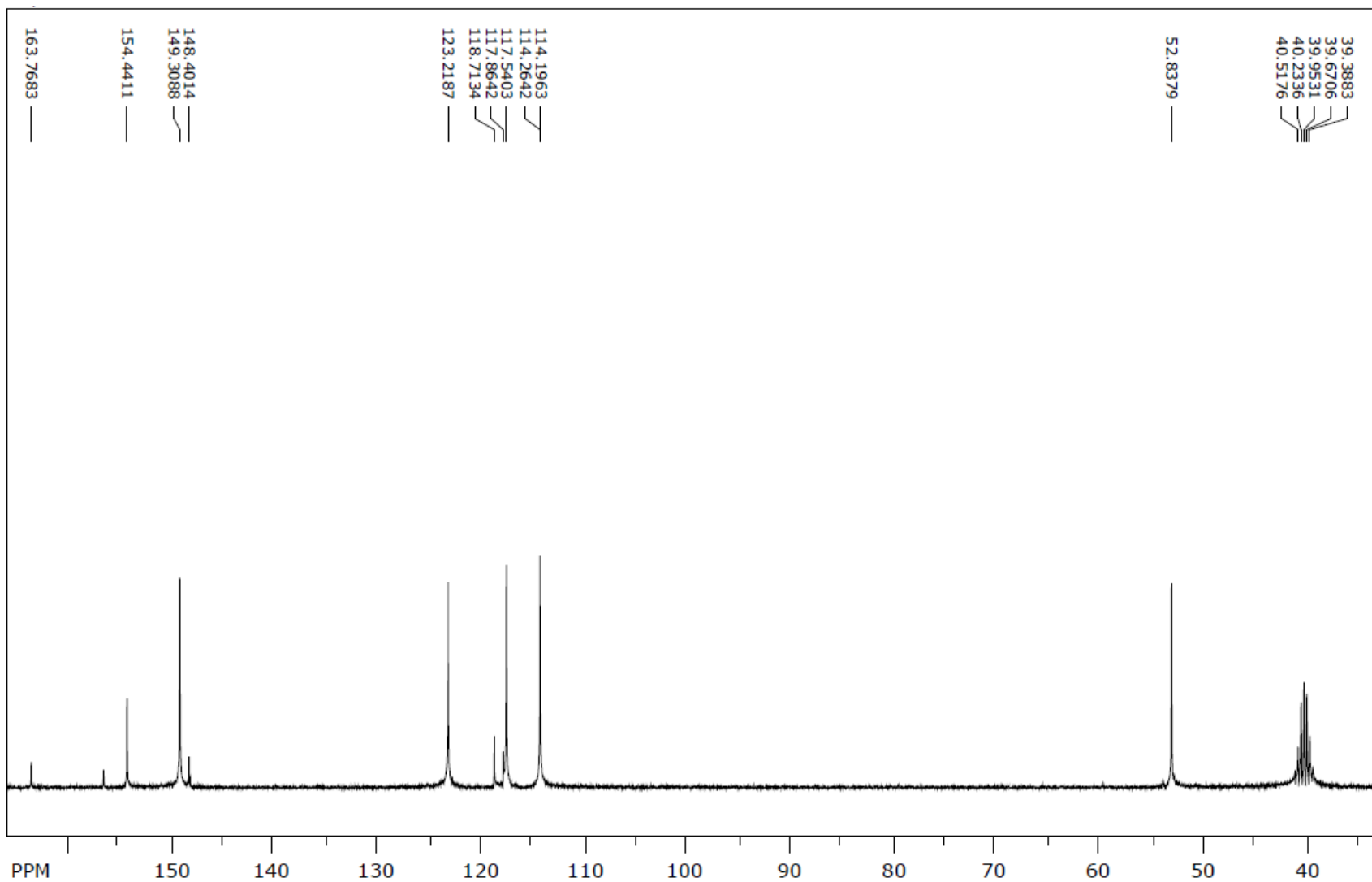
Maseni spektr (1c)



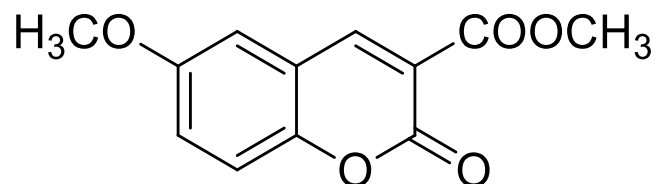
¹H NMR spektr (1c)



¹³C NMR spektr (1c)

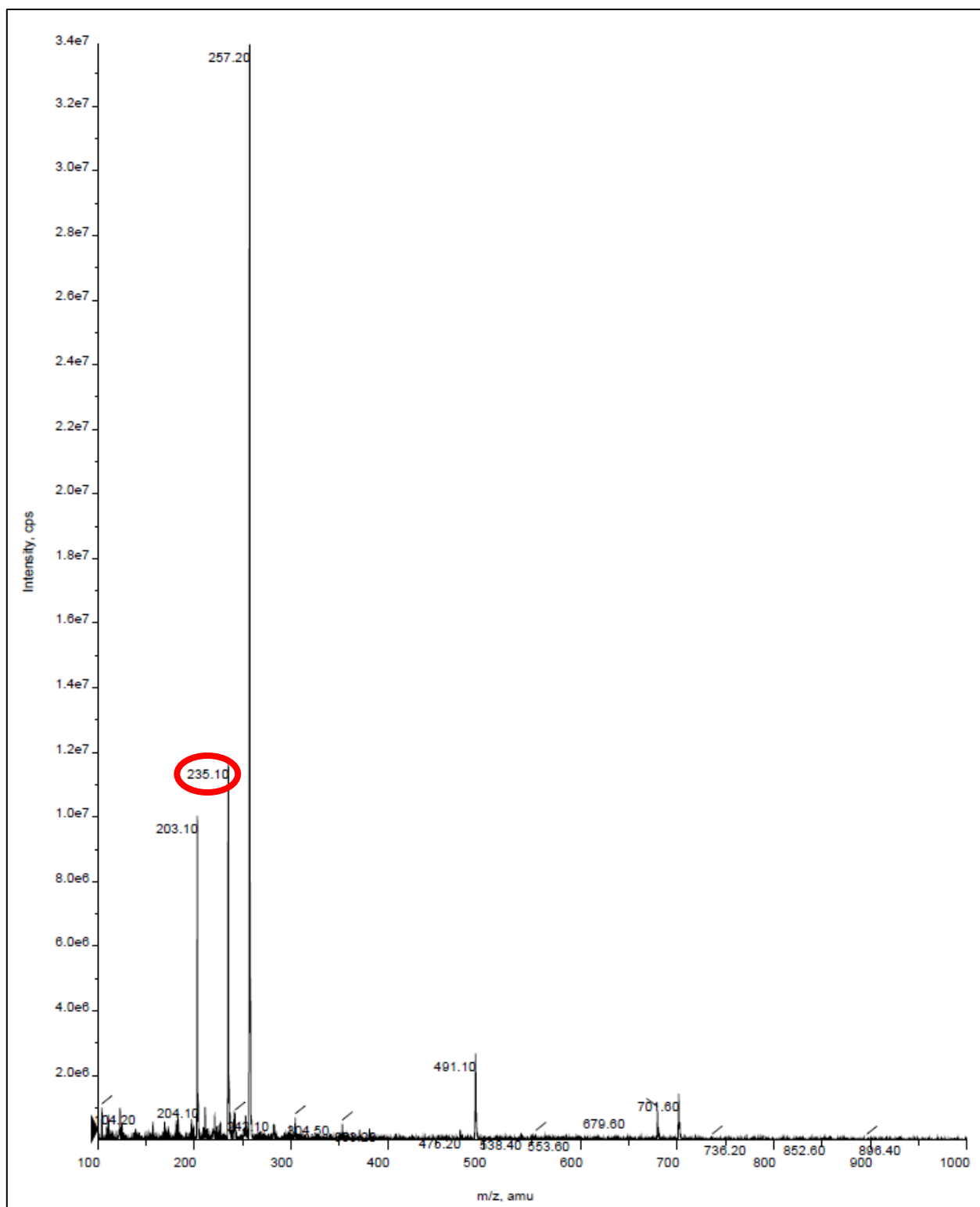


metil 6-metoksi-2-okso-2H-kromen-3-karboksilat (1d)

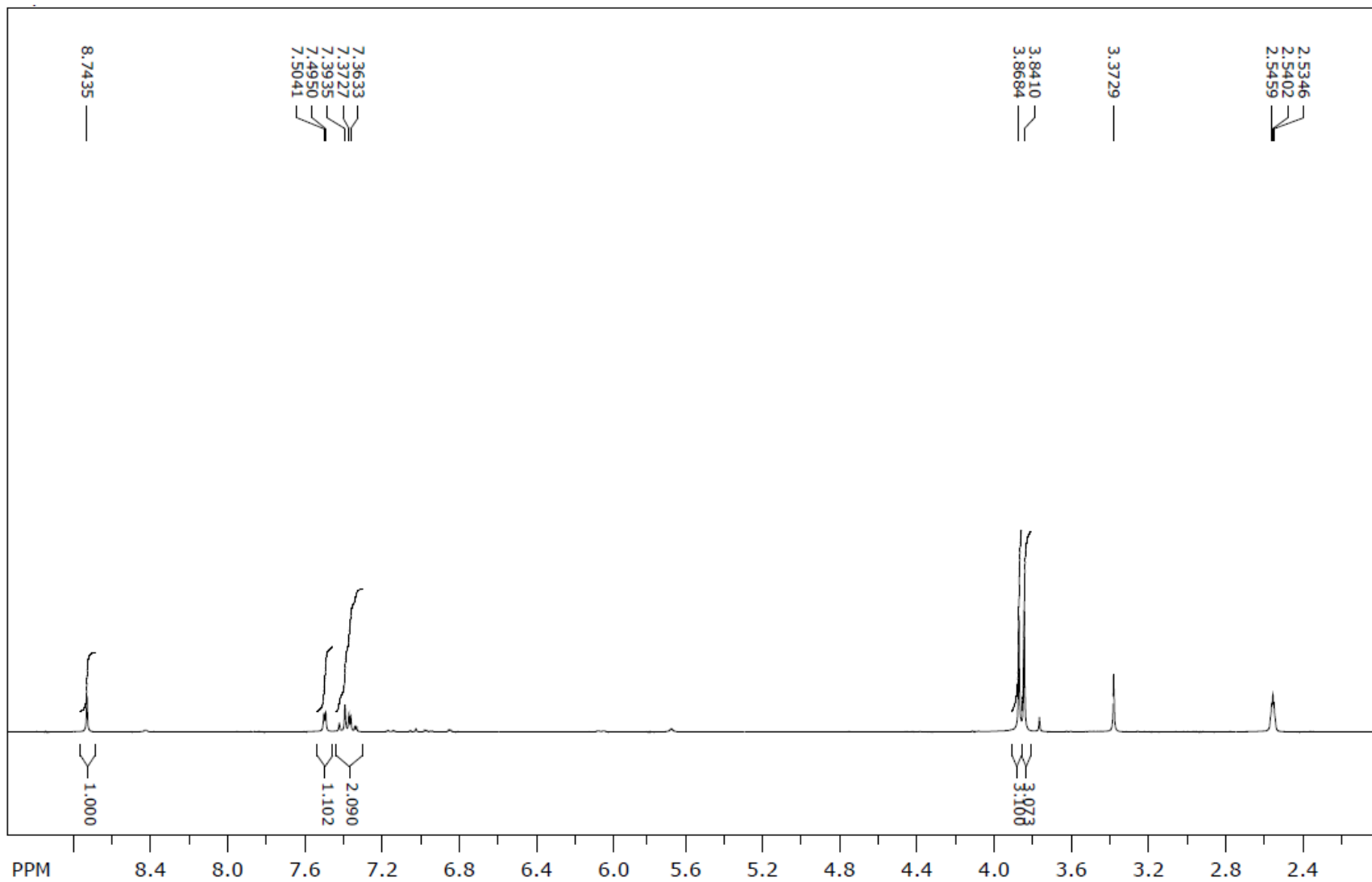


Reaktanti	5-metoksisalicilaldehid (3,2 mmol) i dimetilmalonat (3,2 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola
Molekulska masa	234,20 g/mol
Molekulska formula	C ₁₂ H ₁₀ O ₅
Temperatura tališta	155 -157 °C
Boja kristala	Žuta
R_f	0,66
LC/MS/MS m/z (M⁺)	235,10
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 8,74 (s, 1H, coum.), 7,50 (s, 1H, arom.), 7,36 - 7,40 (m, 2H, arom.), 3,87 (s, 3H, OCH ₃), 3,84 (s, 3H, OCH ₃).
¹³C NMR	(75 MHz, CDCl ₃) δ 163,6; 156,2; 149,2; 122,9; 118,6; 118,0; 117,7; 112,4; 111,4; 56,2; 52,9.

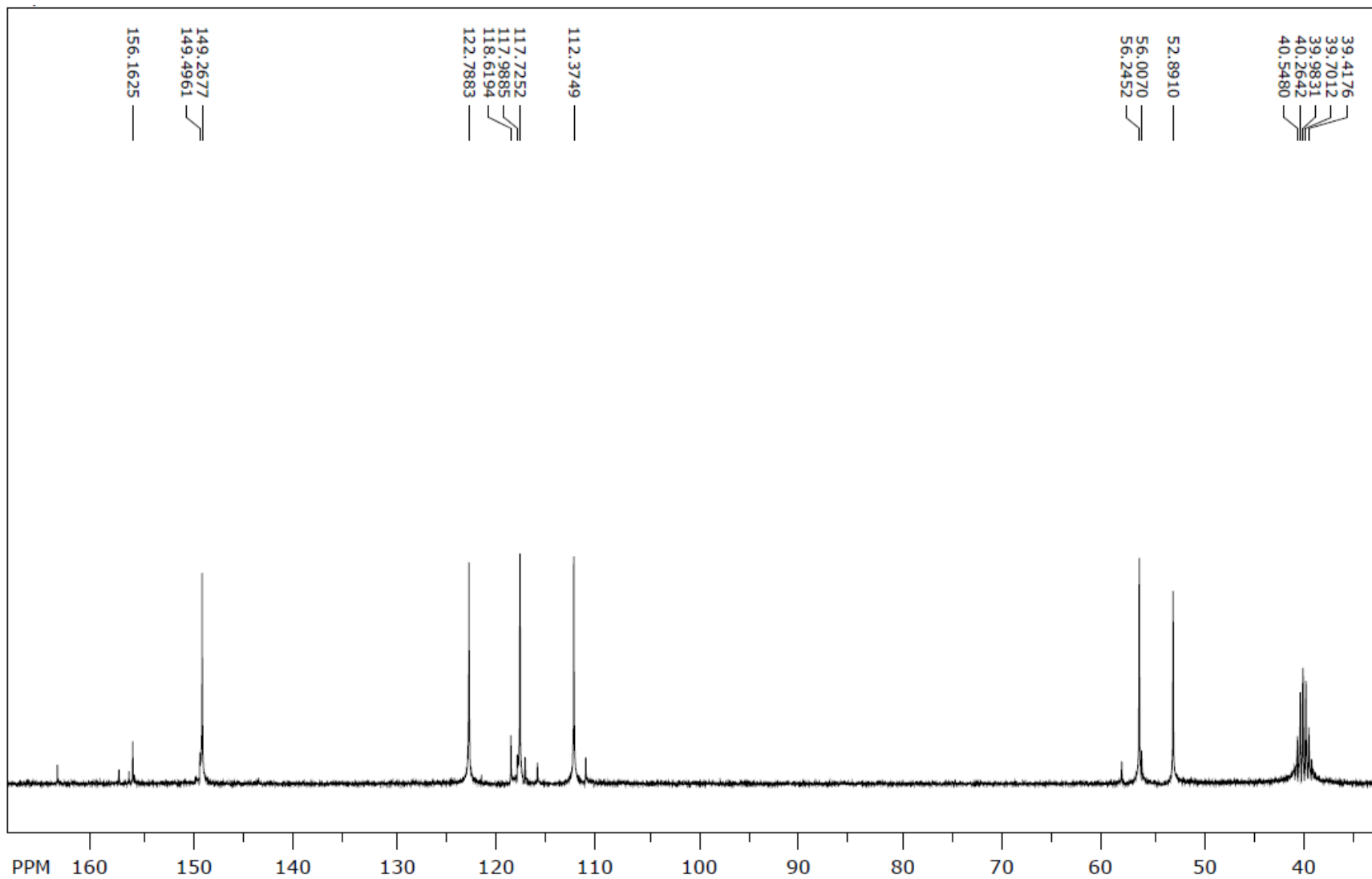
Maseni spektar (1d)



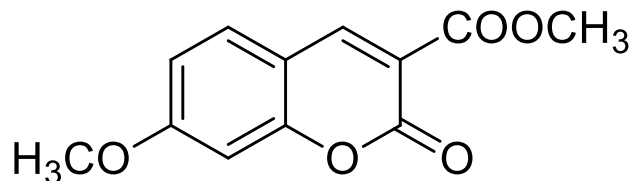
¹H NMR spektr (1d)



¹³C NMR spektr (1d)

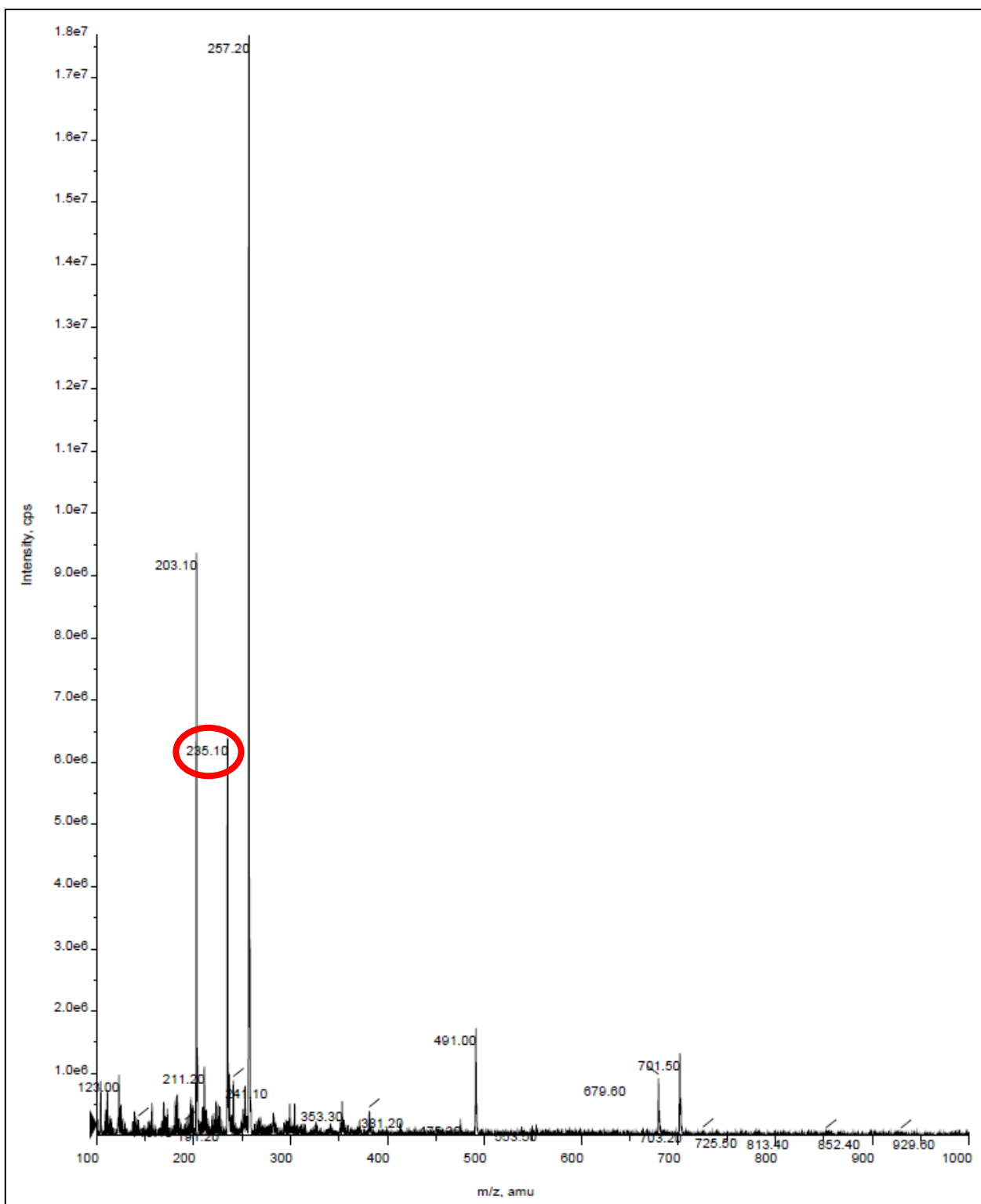


metil 7-metoksi-2-okso-2H-kromen-3-karboksilat (1e)

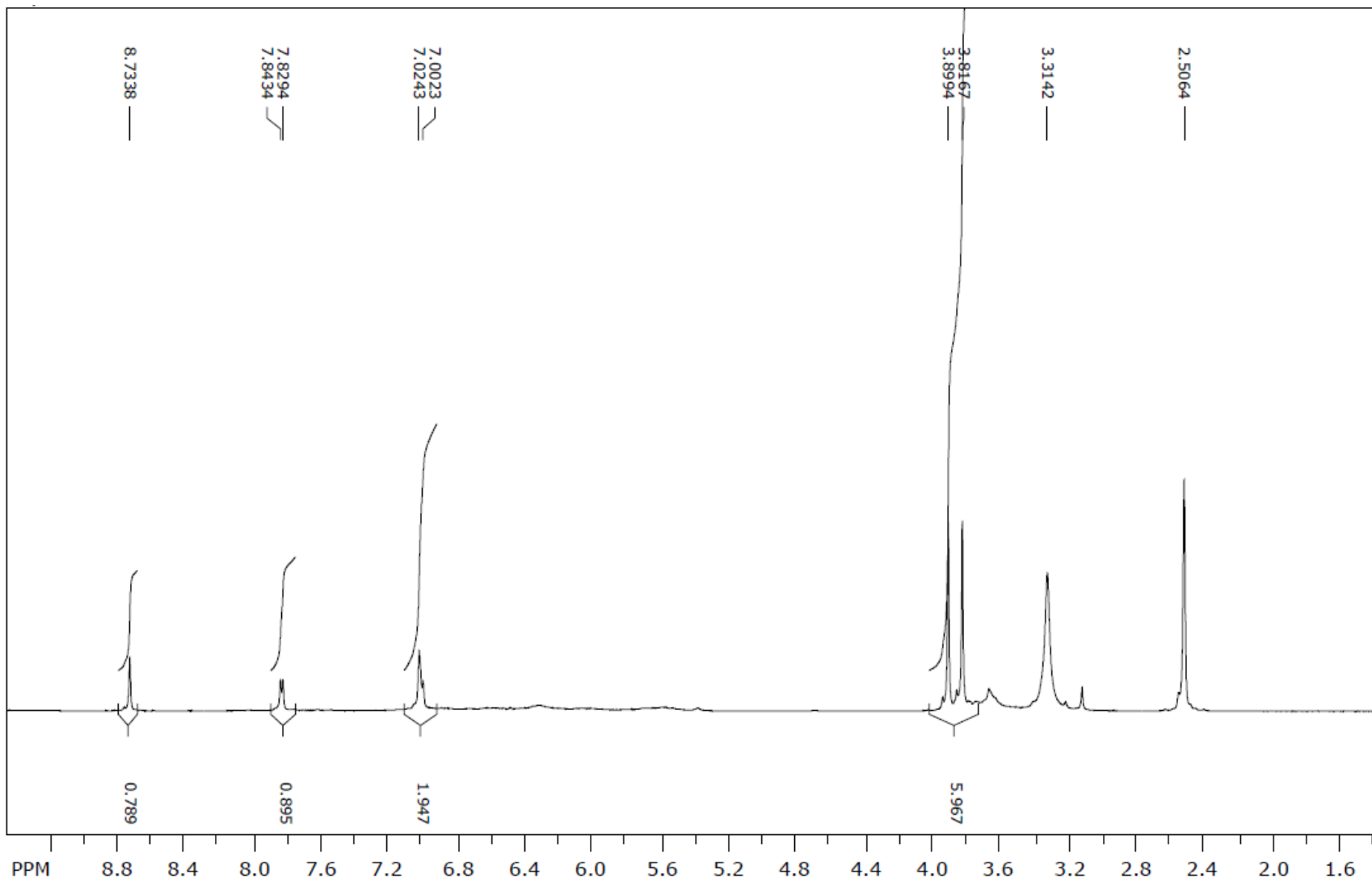


Reaktanti	4-metoksisalicilaldehid (3,3 mmol) i dimetilmalonat (3,3 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	234,20 g/mol
Molekulska formula	C ₁₂ H ₁₀ O ₅
Temperatura tališta	200 – 202 °C (lit. 201 – 203 °C, Shaabani i sur., 2009)
Boja kristala	Tamnožuta
R_f	0,64
LC/MS/MS <i>m/z</i> (M⁺)	235,10
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,73 (s, 1H), 7,84 (d, <i>J</i> = 8,40 Hz, 1H, arom.), 7,01 (d, <i>J</i> = 13,20 Hz, 2H, arom.), 3,90 (s, 3H, -OCH ₃), 3,82 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 164,8; 163,4; 157,11; 156,2; 149,4; 131,6; 113,2; 111,4; 100,3; 56,2; 52,1.

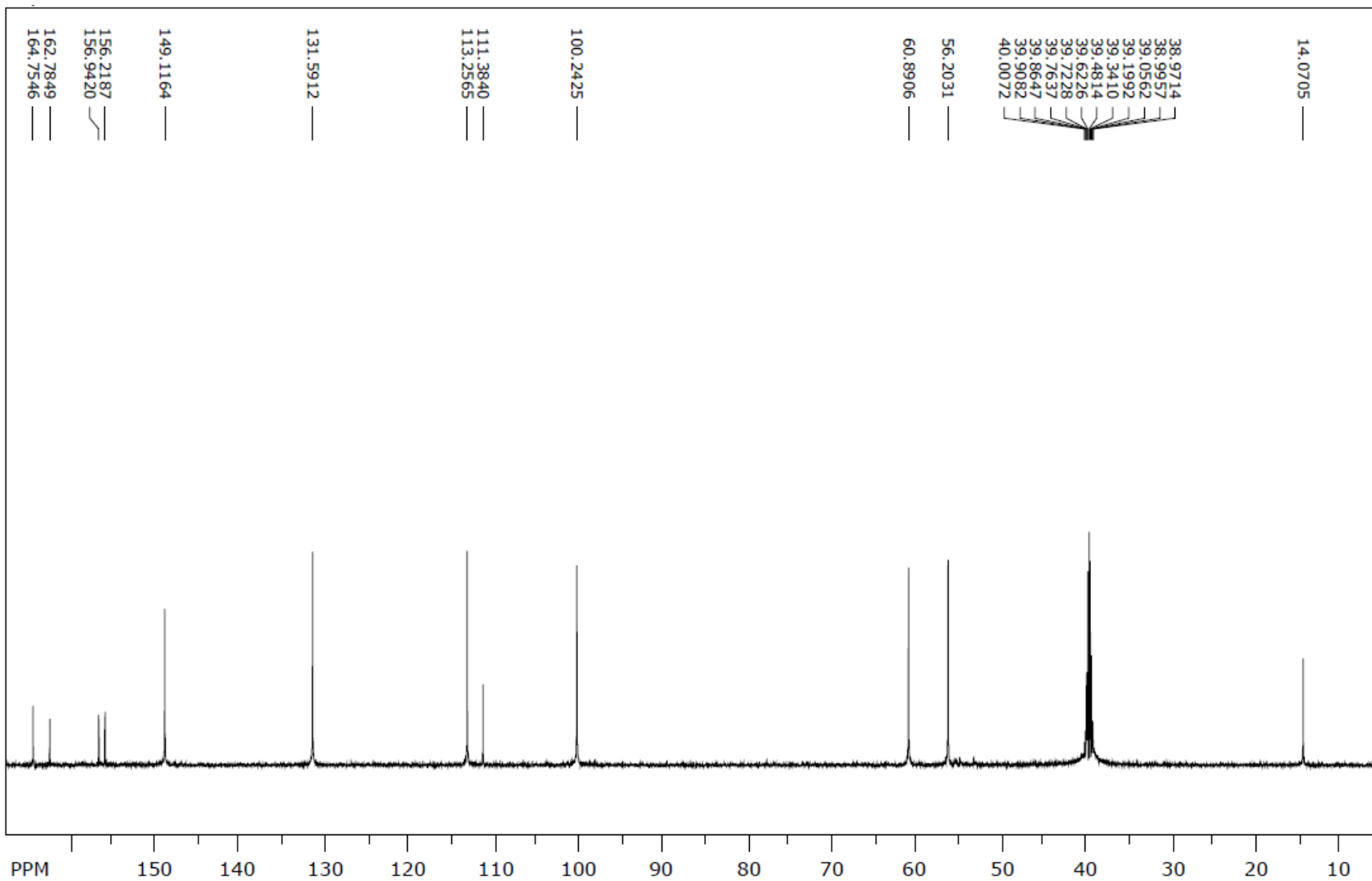
Maseni spektar (1e)



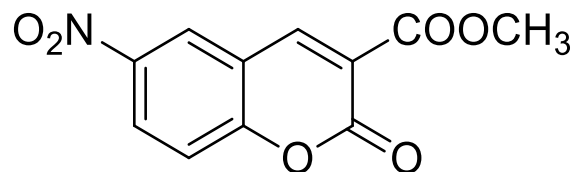
¹H NMR spektr (1e)



¹³C NMR spektr (1e)

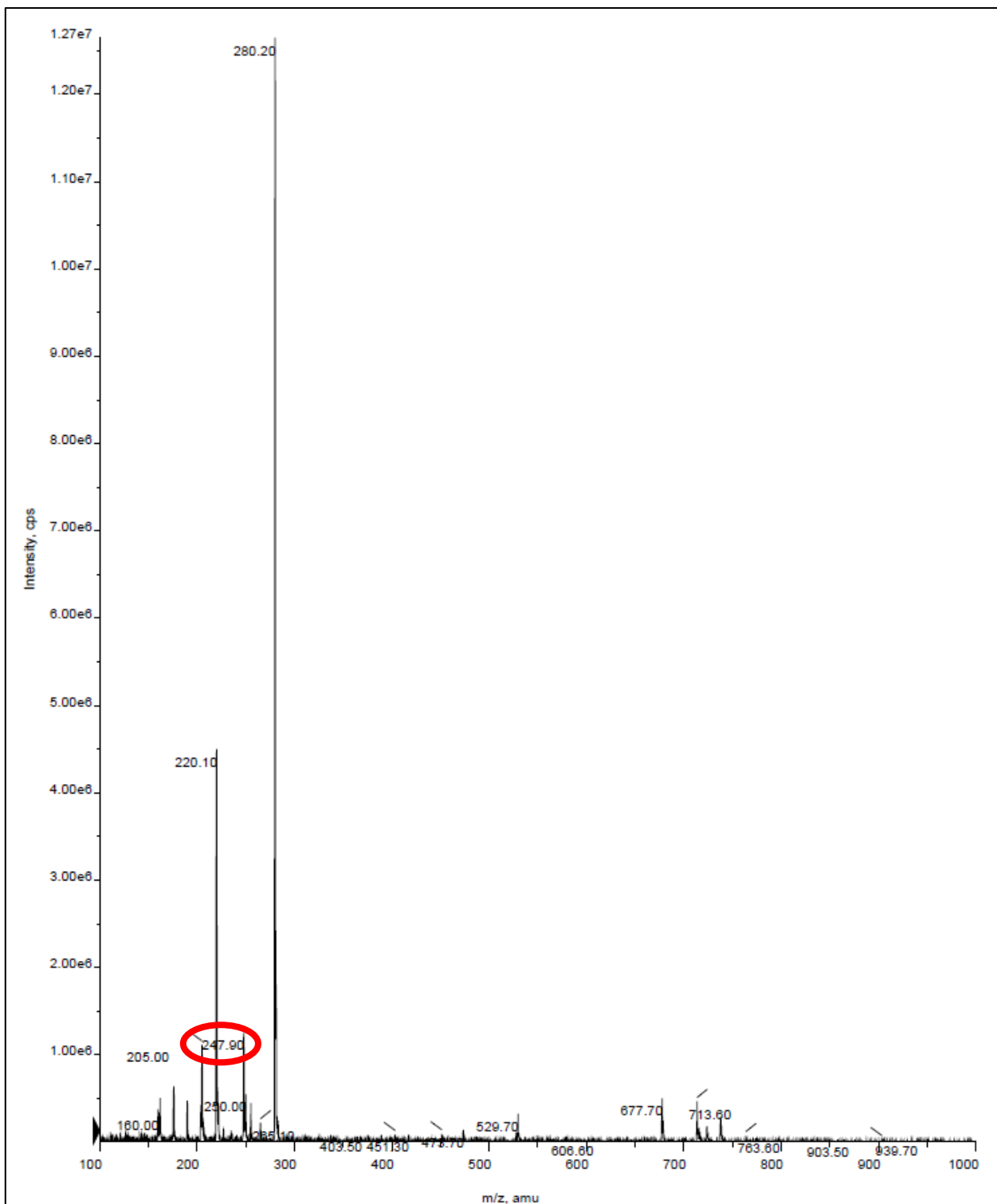


metil 6-nitro-2-okso-2H-kromen-3-karboksilat (1f)

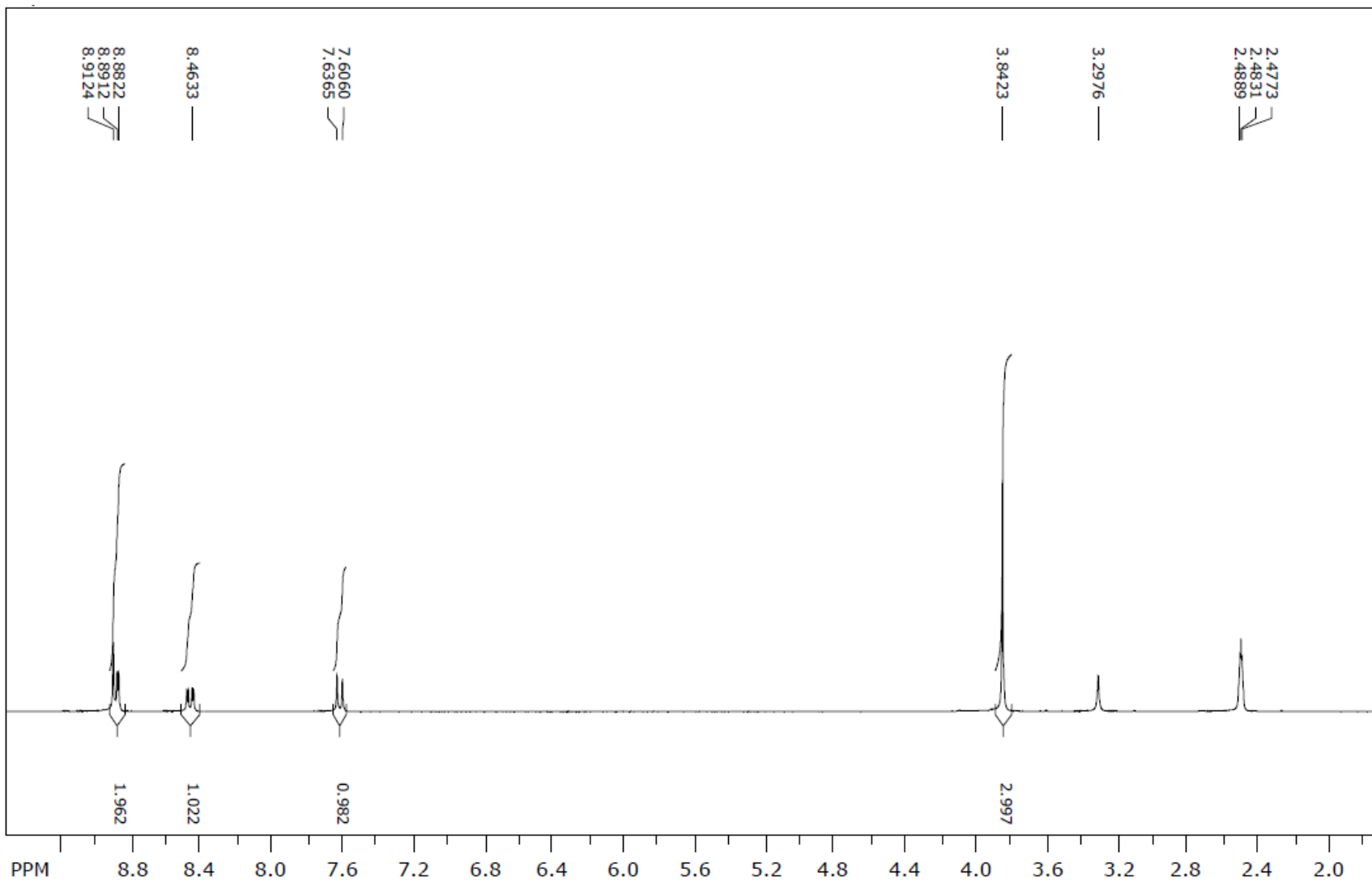


Reaktanti	5-nitrosalicilaldehid (3,1 mmol) i dimetilmalonat (3,1 mmol)
Metoda pročišćavanja	Ispran etanolom
Molekulska masa	249,17 g/mol
Molekulska formula	C ₁₁ H ₇ NO ₆
Temperatura tališta	210 – 213 °C
Boja kristala	Svijetlosmeđa
R_f	0,78
LC/MS/MS m/z (M-)	247,90
1H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 8,91 (s, 1H, coum.), 8,89 (d, <i>J</i> = 2,70 Hz, 1H, arom.), 8,47 (dd, <i>J</i> = 9,12, 2,76 Hz, 1H, arom.), 7,62 (d, <i>J</i> = 9,15 Hz, 1H, arom.), 3,84 (s, 3H, OCH ₃).
13C NMR	(75 MHz, DMSO- <i>d</i> ₆) δ 163,1; 158,5; 155,4; 148,4; 144,1; 129,1; 126,6; 119,7; 118,6; 118,2; 53,2.

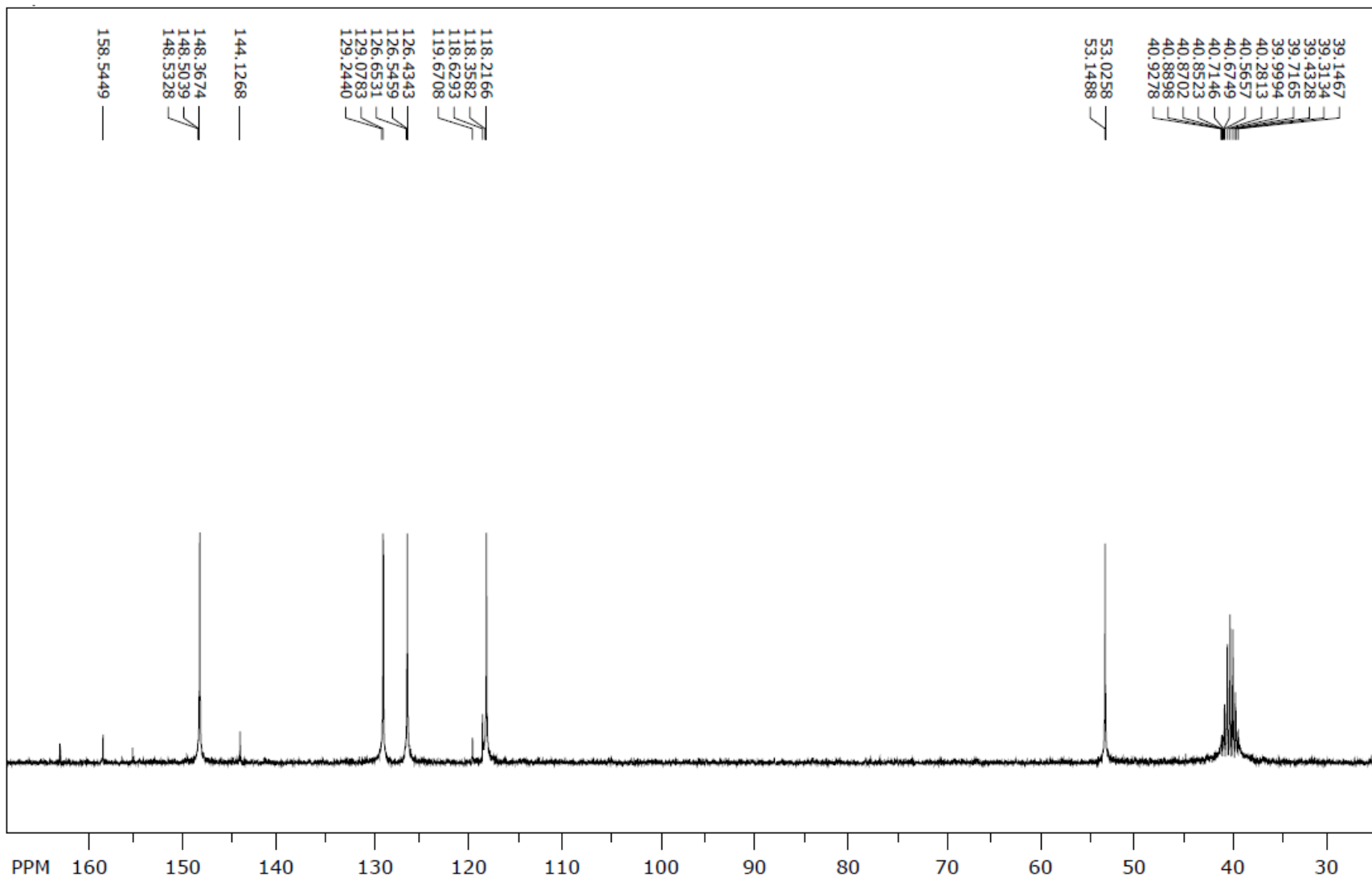
Maseni spektar (1f)



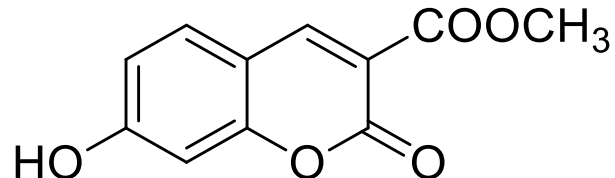
¹H NMR spektr (1f)



¹³C NMR spektr (1f)

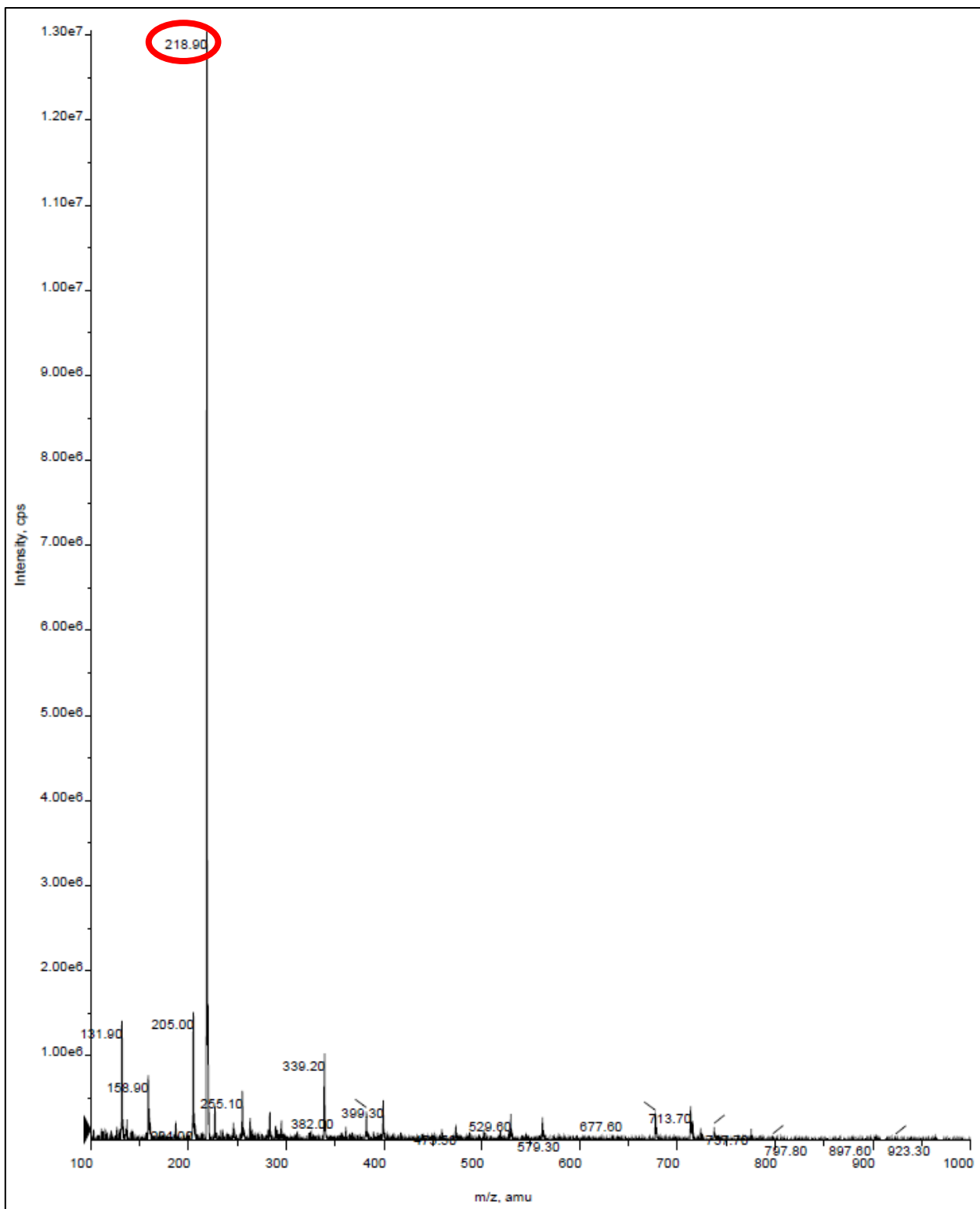


metil 7-hidroksi-2-okso-2H-kromen-3-karboksilat (1g)

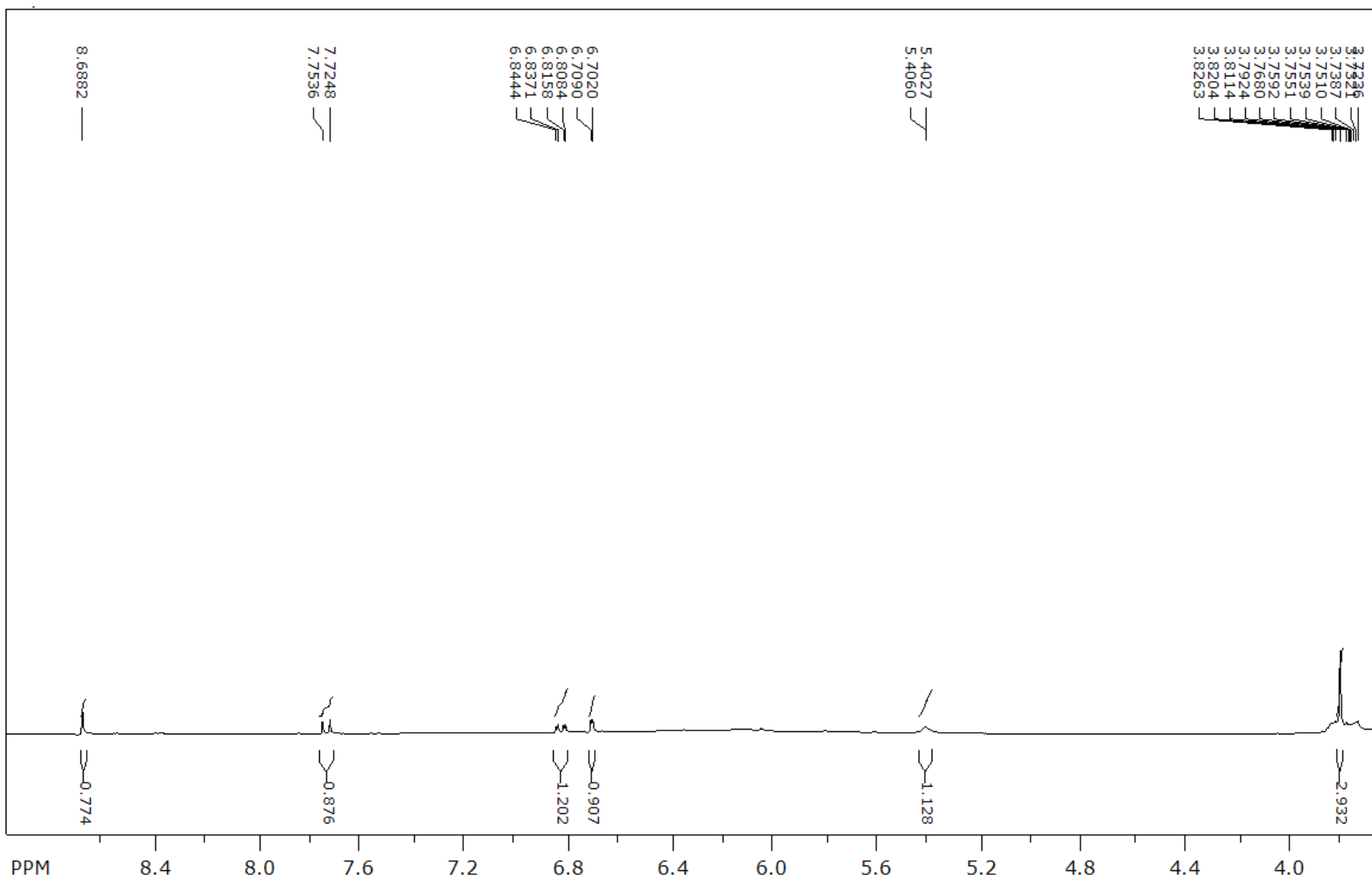


Reaktanti	2,4-dihidroksibenzaldehid (10 mmol) i dimetilmalonat (10 mmol)
Metoda pročišćavanja	Ispran etanolom
Molekulska masa	220,18 g/mol
Molekulska formula	C ₁₁ H ₈ O ₅
Temperatura tališta	>300 °C
Boja kristala	Smeđa
R_f	0,33
LC/MS/MS m/z (M-)	218,90
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,68 (s, 1H, OH), 7,74 (d, <i>J</i> = 17,28 Hz, 1H, arom.), 6,82 (dd, <i>J</i> = 17,16, 4,41 Hz, 1H, arom.), 6,70 (d, <i>J</i> = 4,20 Hz, 1H, arom.), 5,40 (s, 1H, arom.), 3,79 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 165,17; 164,01; 157,73; 156,91; 150,17; 132,62; 114,74; 111,78; 110,71; 102,29; 55,61.

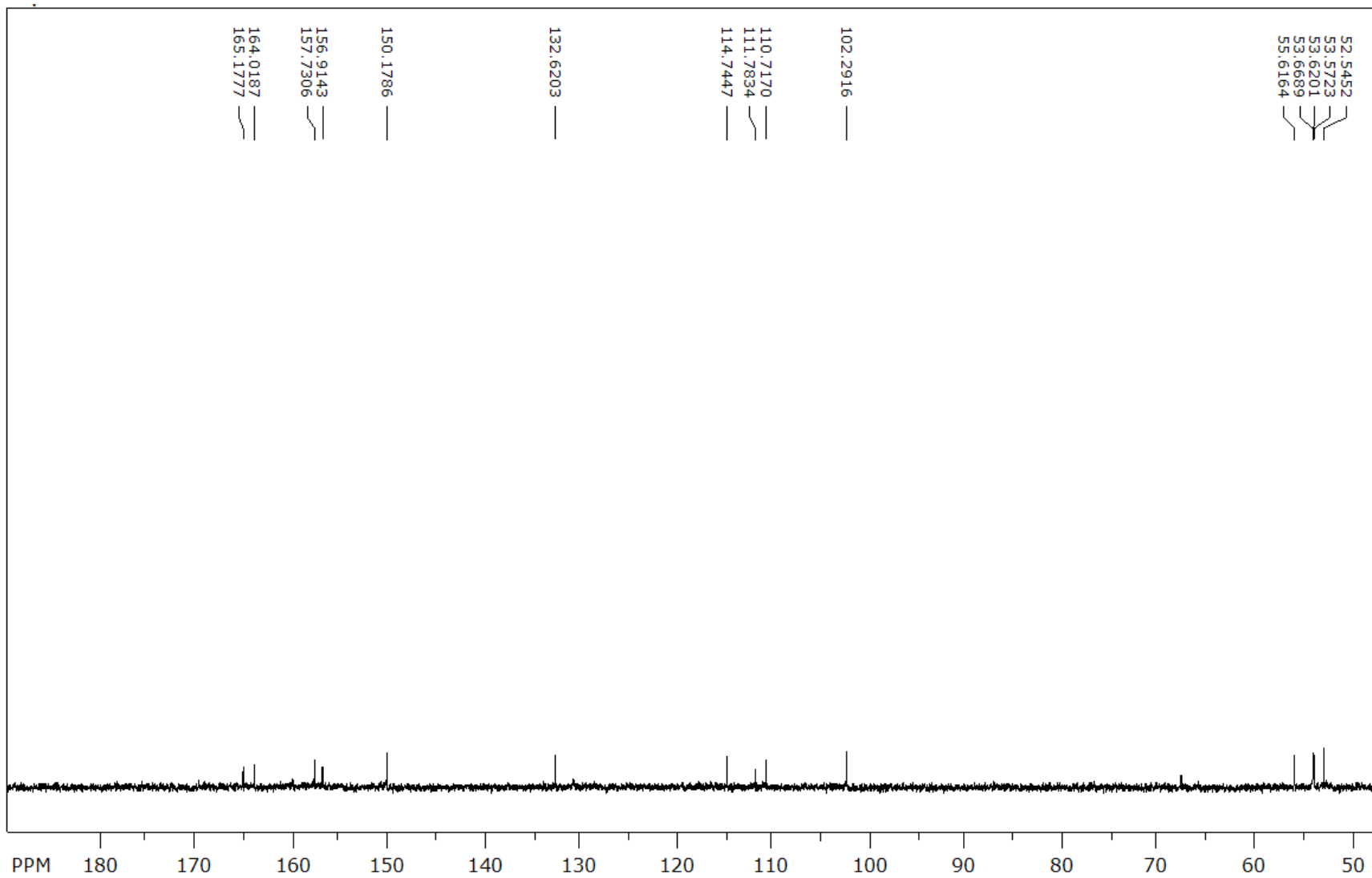
Maseni spektar (1g)



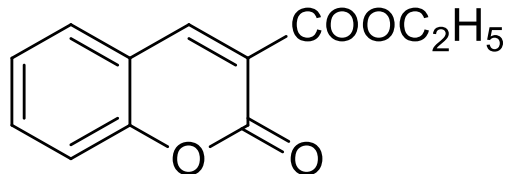
¹H NMR spektr (1g)



¹³C NMR spektar (1g)

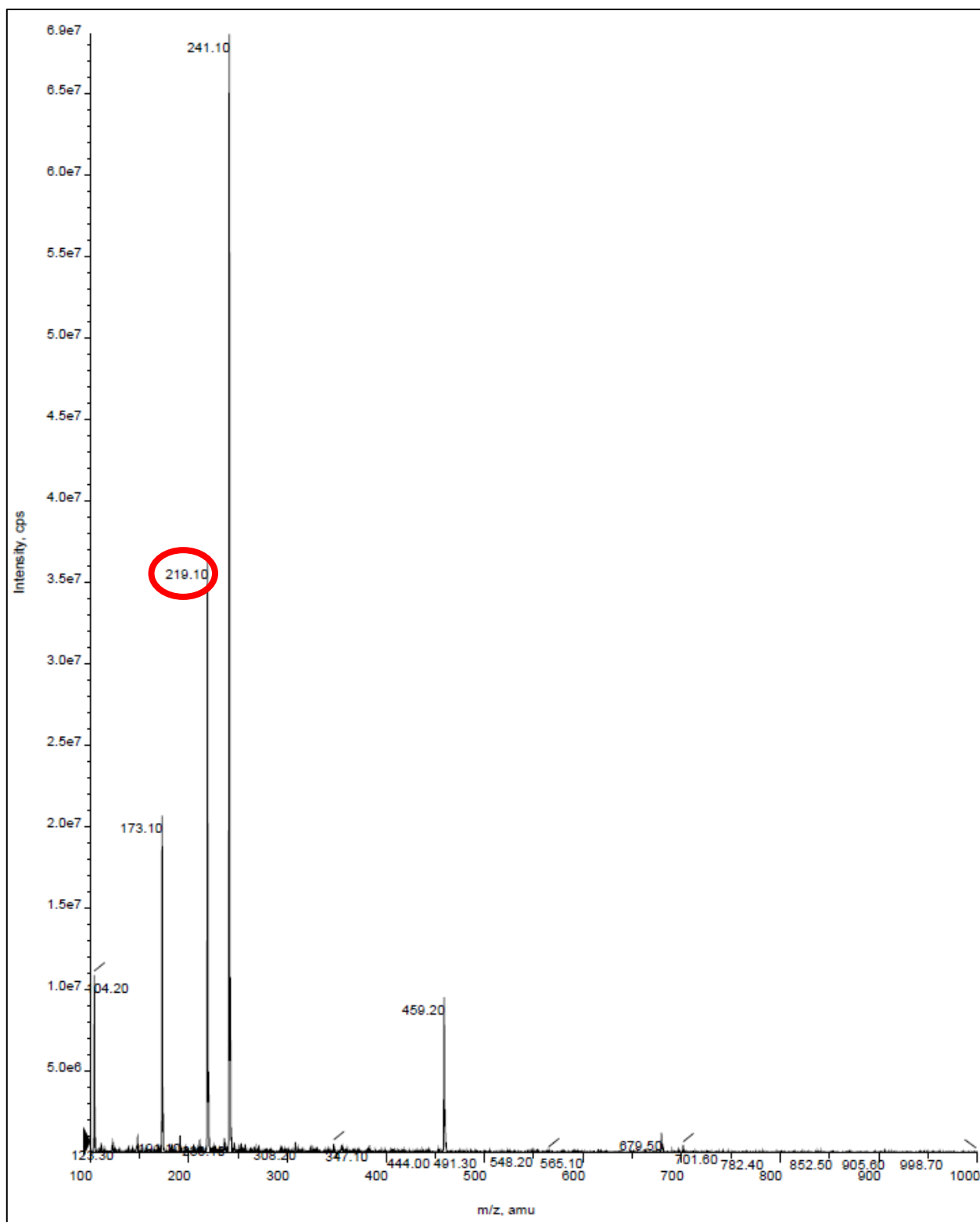


etil 2-okso-2H-kromen-3-karboksilat (2a)

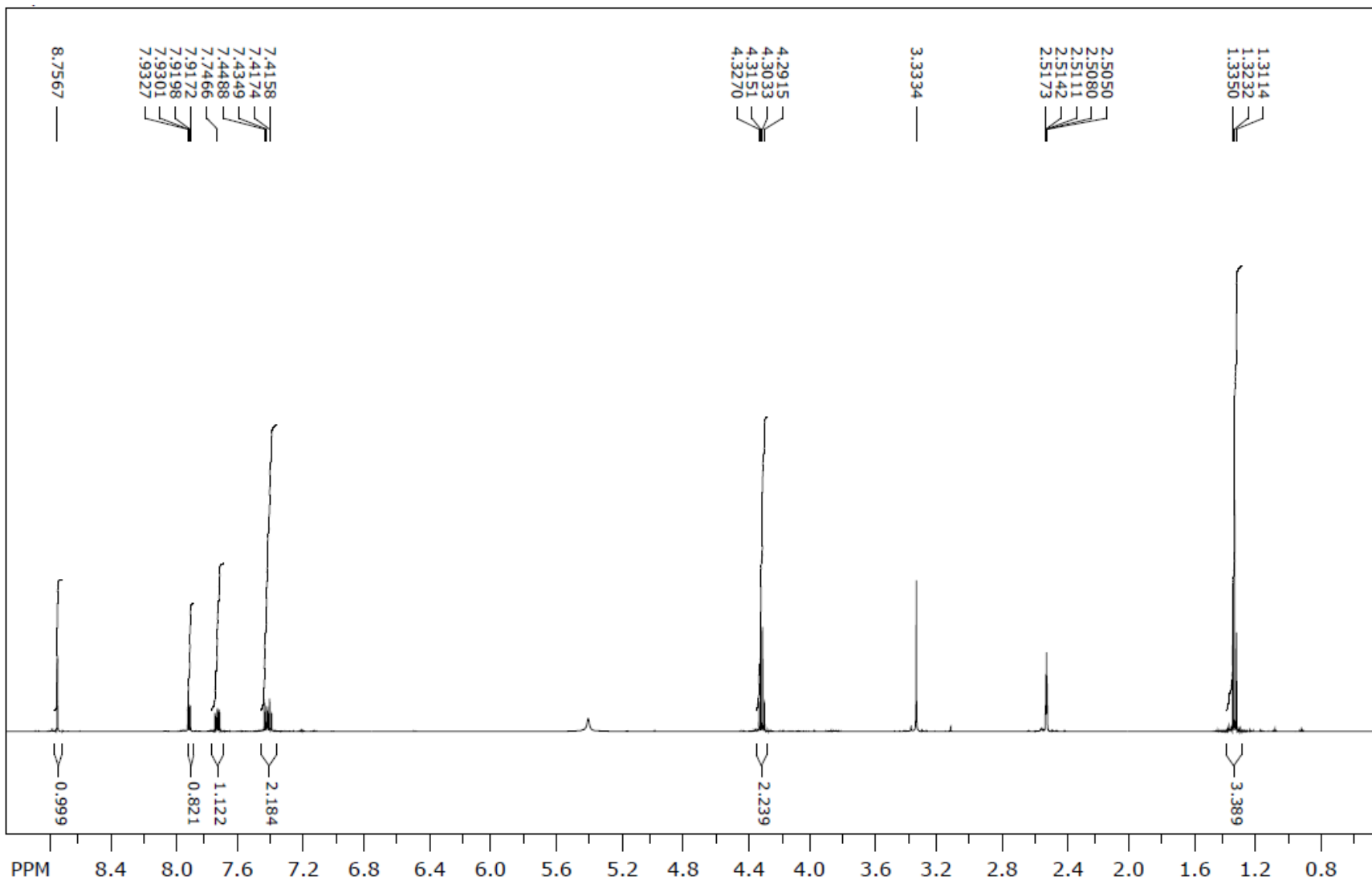


Reaktanti	Salicilaldehid (10 mmol) i dietilmalonat (10 mmol)
Metoda pročišćavanja	Ispran etanolom
Molekulska masa	218,20 g/mol
Molekulska formula	C ₁₂ H ₁₀ O ₄
Temperatura tališta	92 – 94 °C (lit. 90 – 91 °C, Shaabani i sur., 2009)
Boja kristala	Svijetložuta
R_f	0,67
LC/MS/MS <i>m/z</i> (M⁺)	219,10
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 8,76 (s, 1H, coum.), 7,92 (dd, <i>J</i> = 9,09, 1,40 Hz, 1H, arom.), 7,71 - 7,78 (m, 1H, arom.), 7,39 - 7,45 (m, 2H, arom.), 4,32 (q, <i>J</i> = 7,10 Hz, 2H, CH ₂ CH ₃), 1,33 (t, <i>J</i> = 7,10 Hz 3H, CH ₂ CH ₃).
¹³C NMR	(75 MHz, DMSO- <i>d</i> ₆) δ 162,6; 155,9; 154,5; 148,6; 134,4; 130,2; 124,8; 117,8; 116,1; 61,2; 14,0.

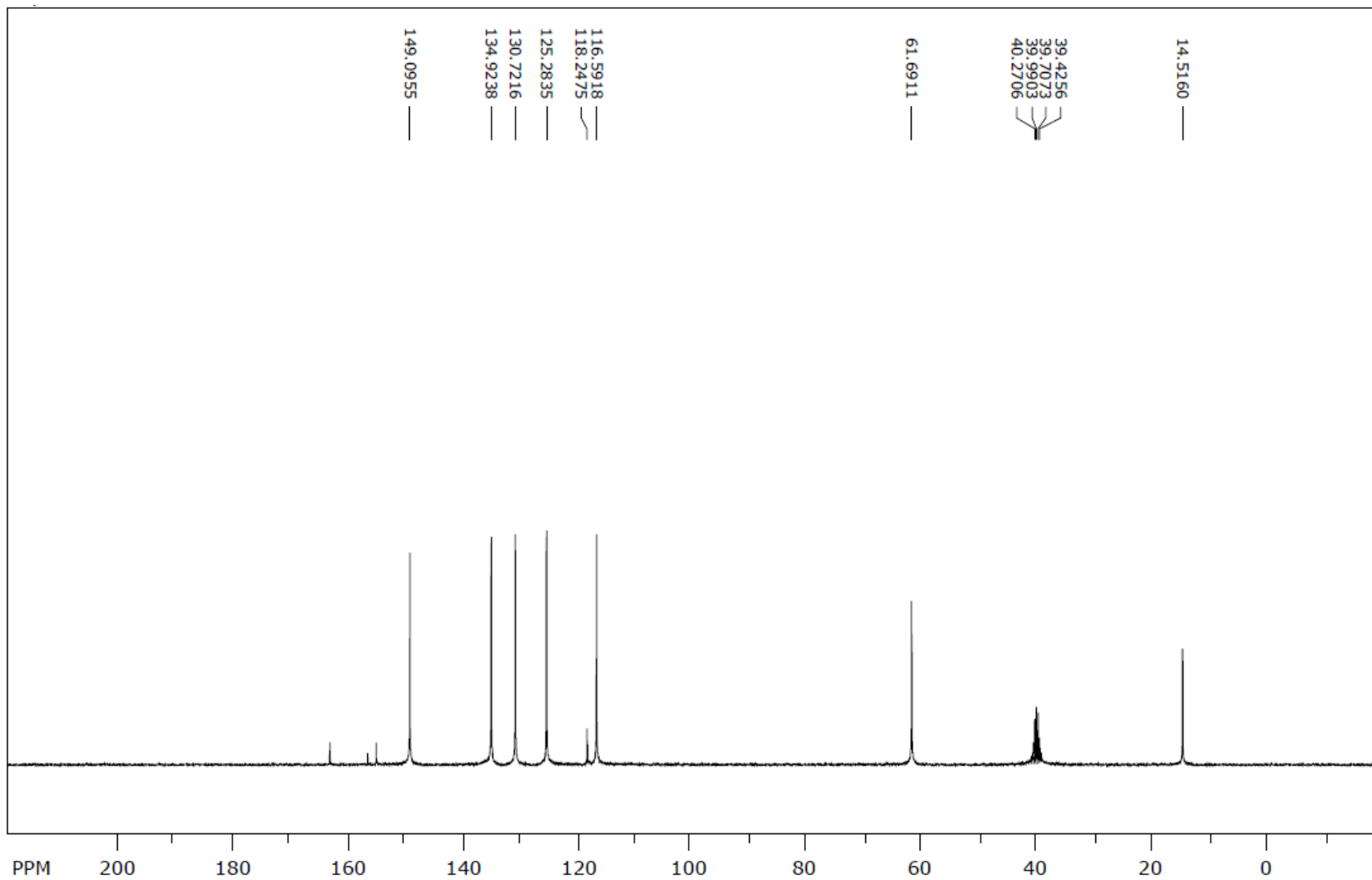
Maseni spektar (2a)



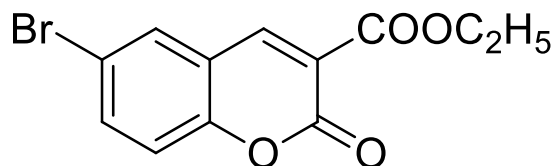
¹H NMR spektr (2a)



¹³C NMR spektr (2a)

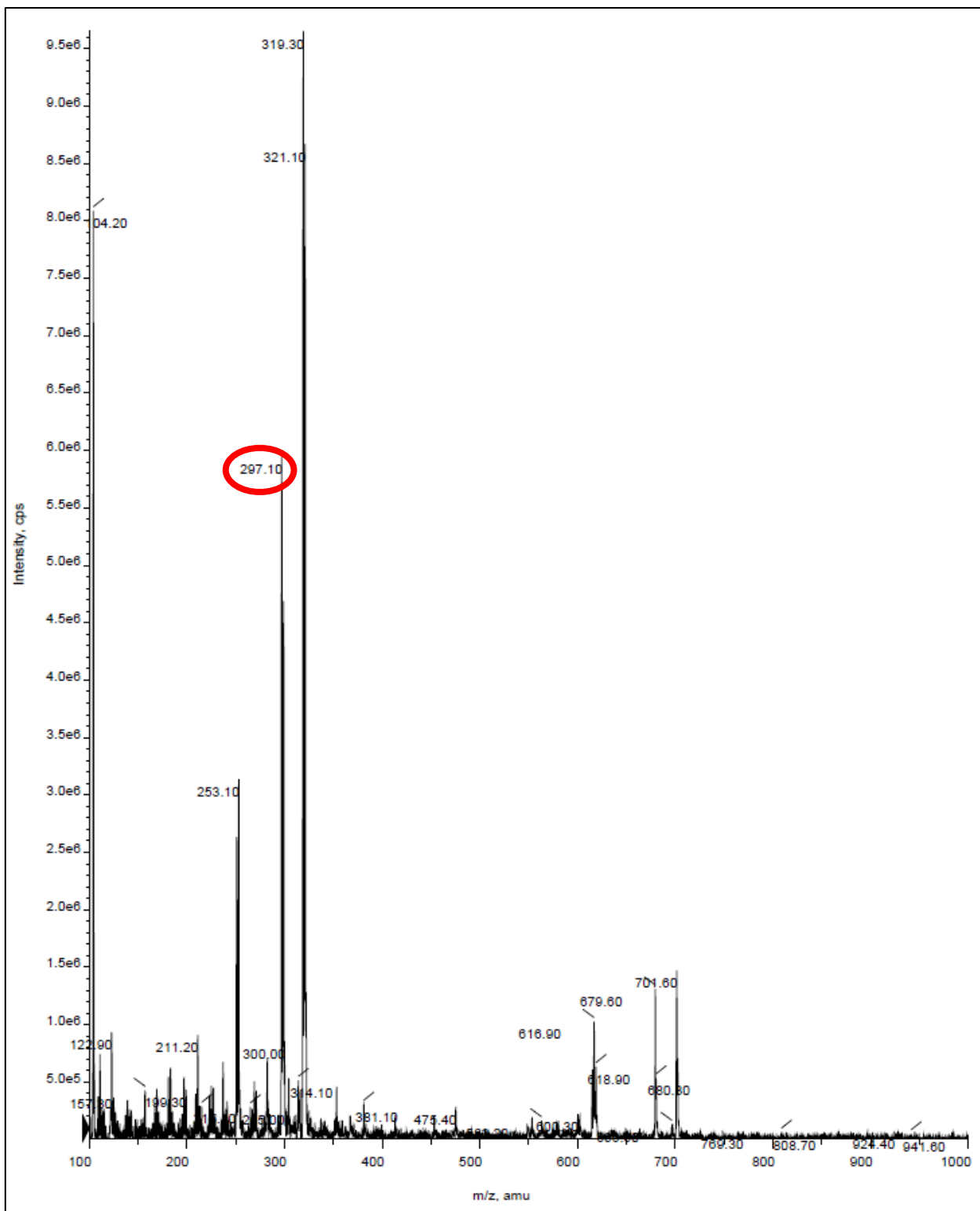


etil 6-brom-2-okso-2H-kromen-3-karboksilat (2b)

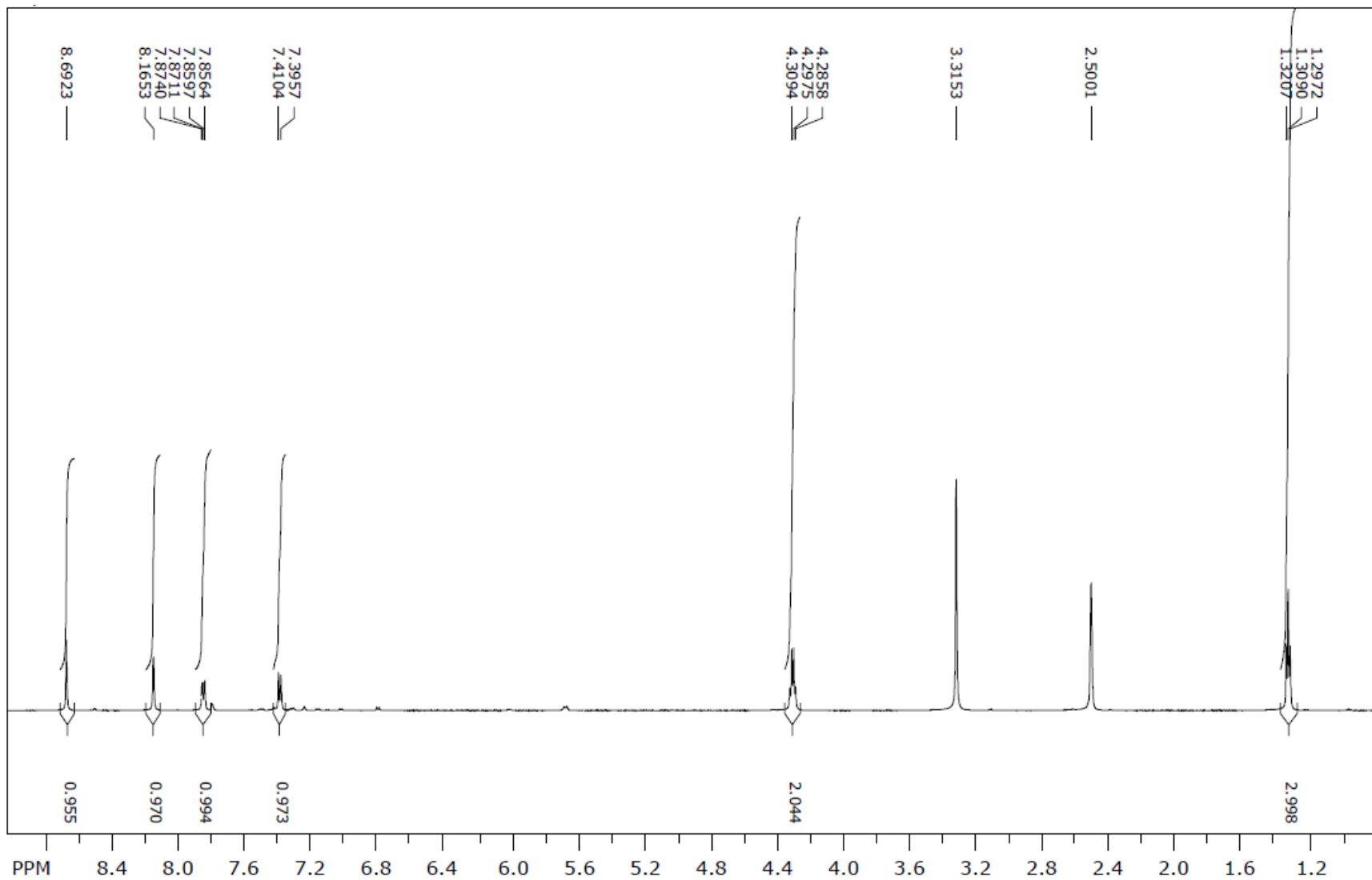


Reaktanti	5-bromsalicilaldehid (10 mmol) i dietilmalonat (10 mmol)
Metoda pročišćavanja	Ispran etanolom
Molekulska masa	297,1 g/mol
Molekulska formula	C ₁₂ H ₉ BrO ₄
Temperatura tališta	164 – 169 °C (lit. 164 – 166 °C, Srikrishna i sur., 2014; 171 °C, Santos-Contreras i sur., 2007; 175 – 177 °C, He i sur., 2015)
Boja kristala	Bijela
R_f	0,76
LC/MS/MS m/z (M⁺)	297,10
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,69 (s, 1H, coum.), 8,17 (s, 1H, arom.), 7,87 (dd, <i>J</i> = 8,58, 1,86 Hz, 1H, arom.), 7,40 (d, <i>J</i> = 8,82 Hz, 1H, arom.), 4,30 (q, 2H, <i>J</i> = 7,06 Hz, CH ₂ CH ₃), 1,31 (t, 3H, <i>J</i> = 7,05 Hz, CH ₂ CH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 162,3; 155,5; 153,5; 147,2; 136,6; 132,3; 119,6; 118,8; 118,4; 116,2; 61,4; 14,00.

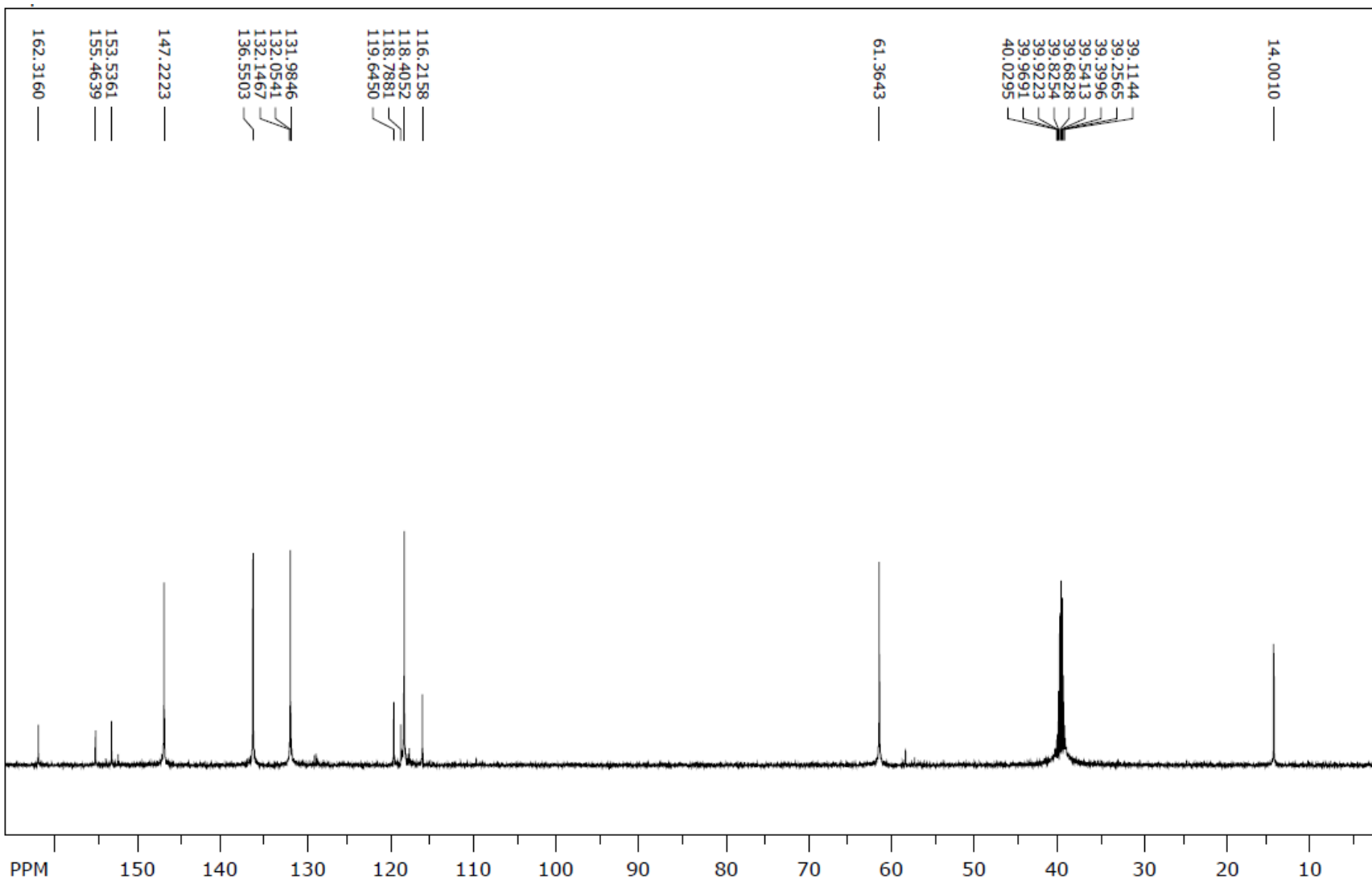
Maseni spektar (2b)



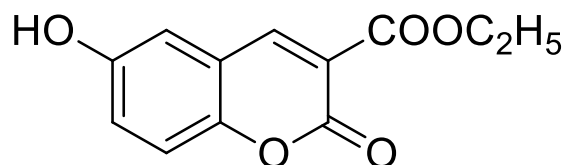
¹H NMR spektr (2b)



¹³C NMR spektr (2b)

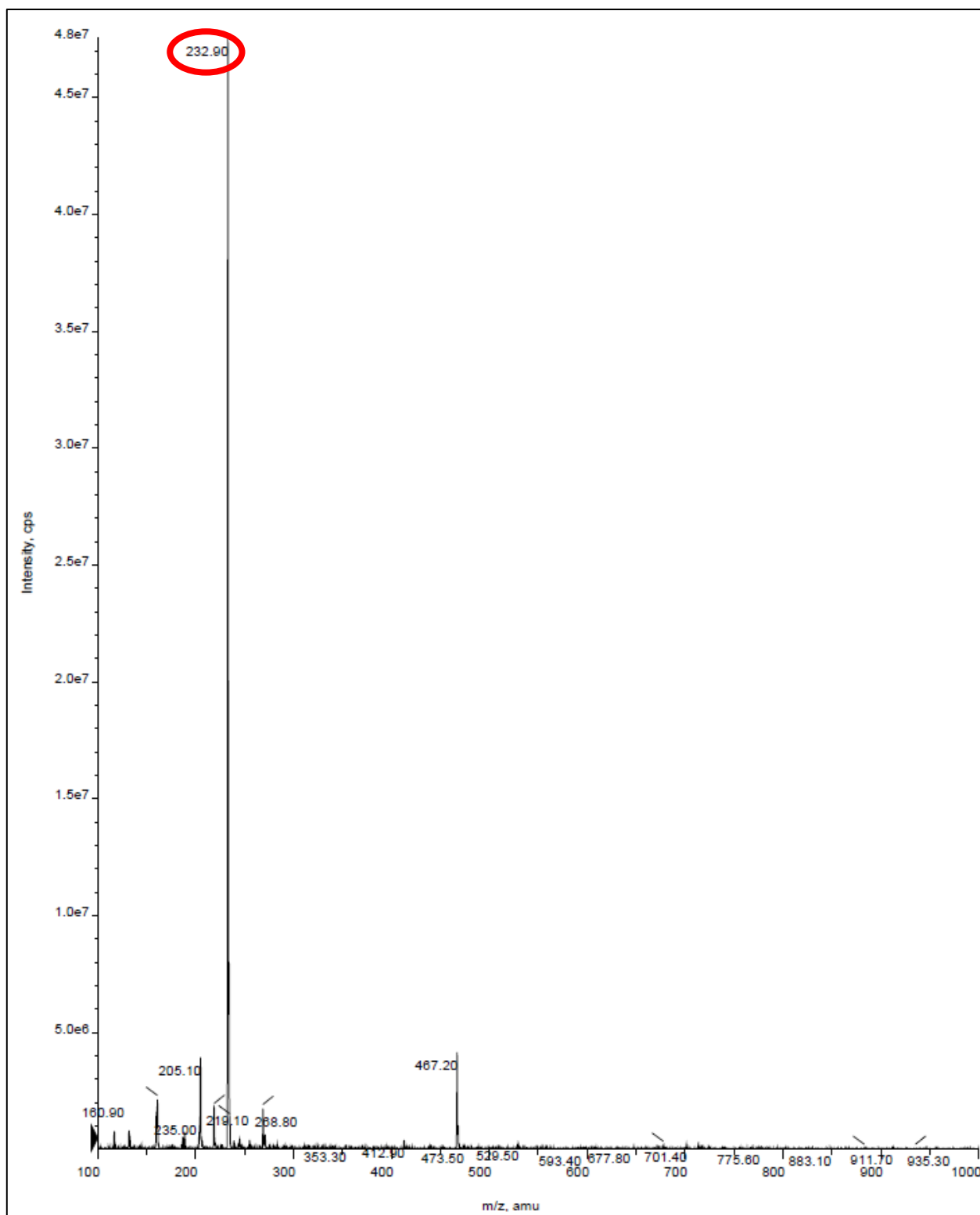


etil 6-hidroksi-2-okso-2H-kromen-3-karboksilat (2c)

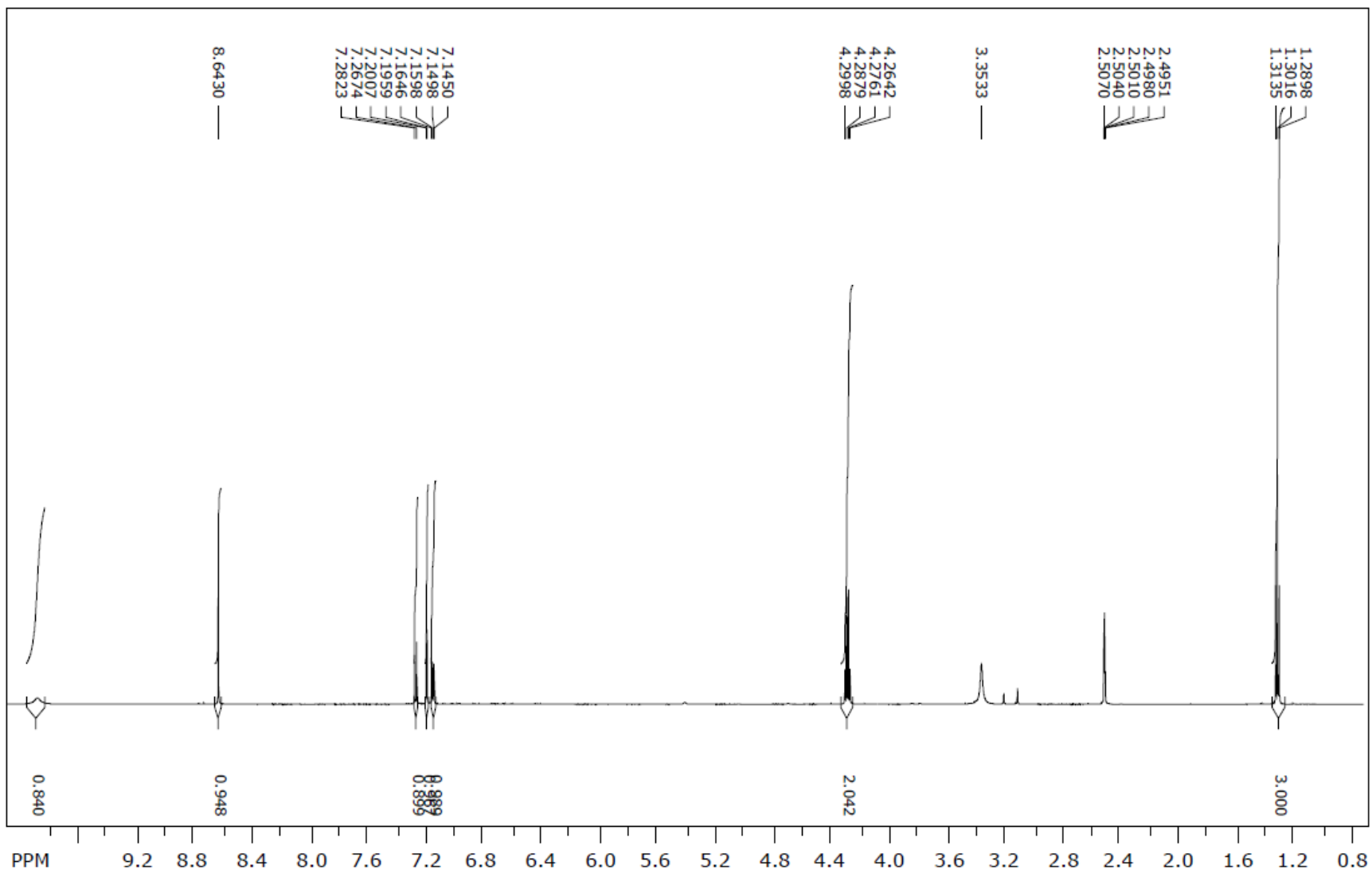


Reaktanti	2,5-dihidroksibenzaldehid (10 mmol) i dietilmalonat (10 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	234,20 g/mol
Molekulska formula	C ₁₂ H ₁₀ O ₅
Temperatura tališta	170 – 173 °C (lit. 174 – 175 °C, Bisht i sur., 2017)
Boja kristala	Crna
R_f	0,36
LC/MS/MS m/z (M-)	232,90
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 9,90 (s, 1H, OH), 8,64 (s, 1H, arom.), 7,28 (d, 1H, <i>J</i> = 8,94 Hz, arom.), 7,20 (d, <i>J</i> = 2,88 Hz, 1H, arom.), 7,15 (dd, <i>J</i> = 8,88, 2,88 Hz, 1H, arom.), 4,28 (q, 2H, <i>J</i> = 7,12 Hz, <u>CH</u> ₂ CH ₃), 1,30 (t, 3H, <i>J</i> = 7,11 Hz, CH ₂ <u>CH</u> ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 162,7; 156,3; 153,9; 148,4; 147,9; 122,6; 118,2; 117,8; 117,0; 113,7; 61,1; 14,0.

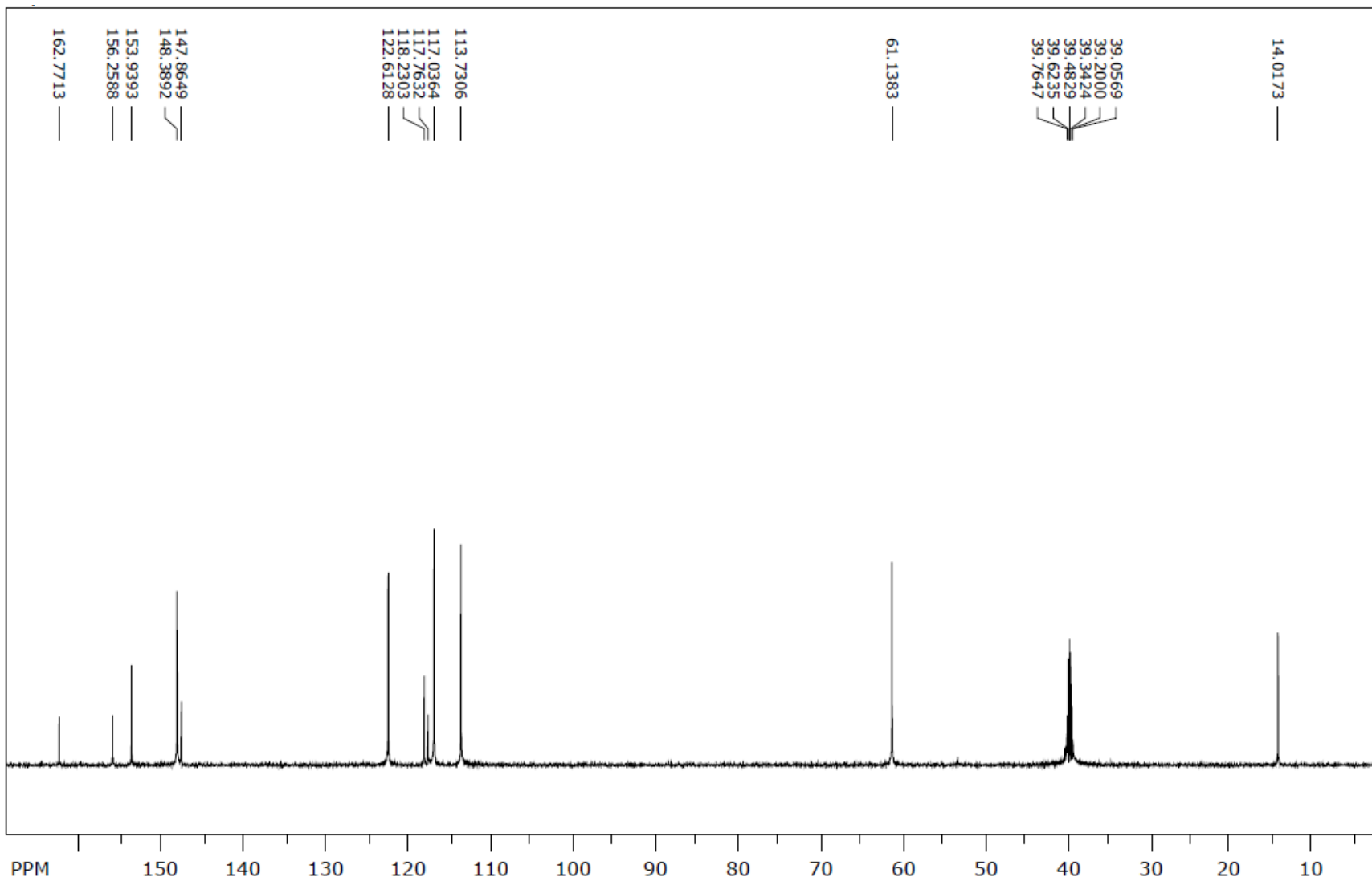
Maseni spektar (2c)



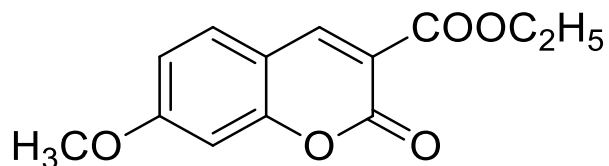
¹H NMR spektr (2c)



¹³C NMR spektr (2c)

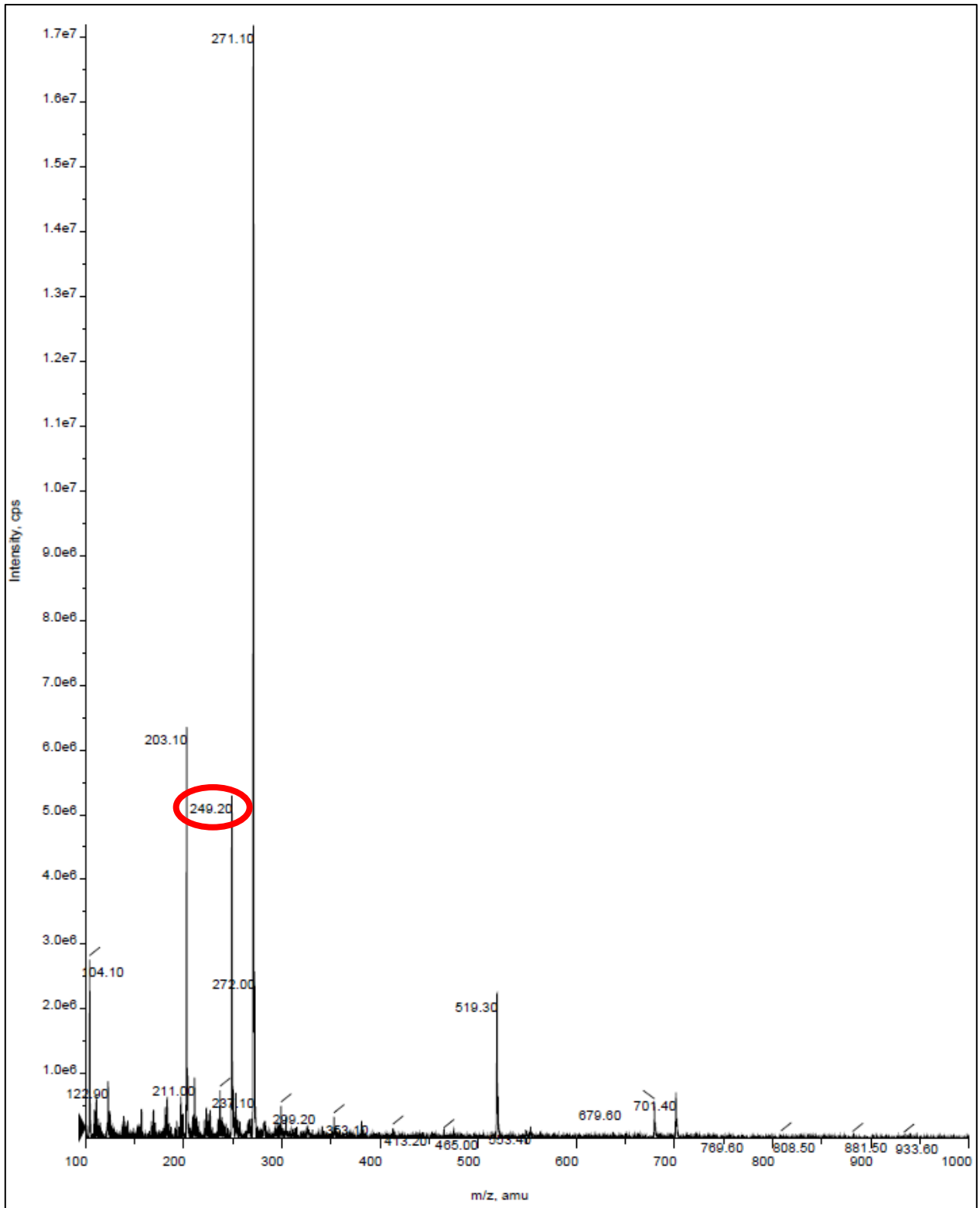


etil 7-metoksi-2-okso-2H-kromen-3-karboksilat (2d)

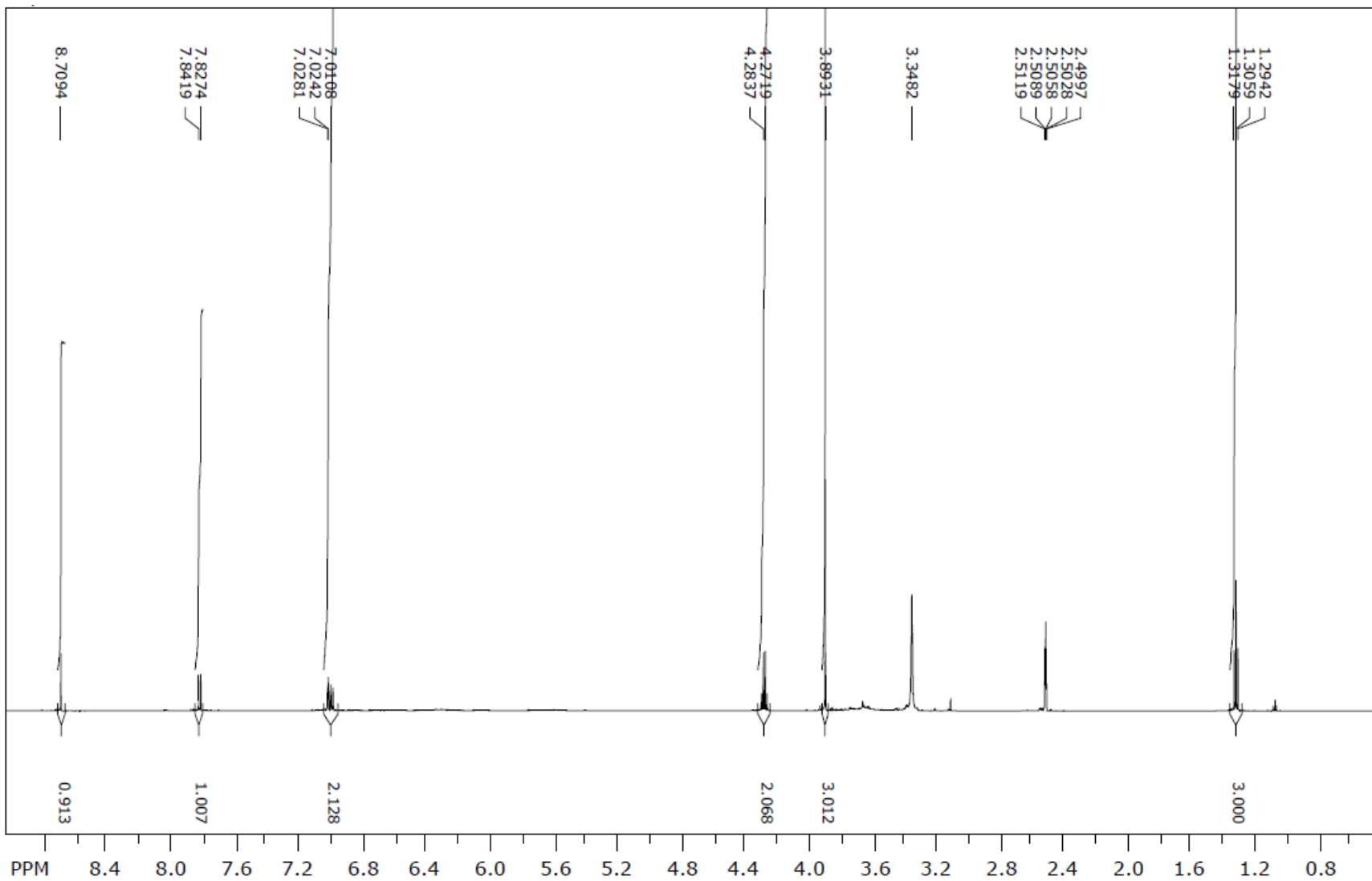


Reaktanti	4-metoksibenzaldehid (3,3 mmol) i dietilmalonat (3,3 mmol)
Metoda pročišćavanja	Ispran etanolom
Molekulska masa	248,23 g/mol
Molekulska formula	C ₁₃ H ₁₂ O ₅
Temperatura tališta	157 – 160 °C (lit. 125 – 126 °C, Shaabani i sur., 2009)
Boja kristala	Svijetlosmeđa
R_f	0,68
LC/MS/MS m/z (M⁺)	249,20
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,69 (s, 1H, coum.), 7,47 (d, 1H, <i>J</i> = 2,82 Hz, arom.), 7,37 (d, <i>J</i> = 9,06 Hz, 1H, arom.), 7,32 (dd, <i>J</i> = 9,06, 2,94 Hz, 1H, arom.), 4,30 (q, 2H, <i>J</i> = 7,10 Hz, <u>CH</u> ₂ CH ₃), 3,81 (s, 3H, OCH ₃), 1,32 (t, 3H, <i>J</i> = 7,08 Hz, CH ₂ <u>CH</u> ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 162,6; 155,7; 148,9; 122,2; 118,1; 117,2; 115,5; 111,9; 110,8; 61,2; 55,7; 14,00.

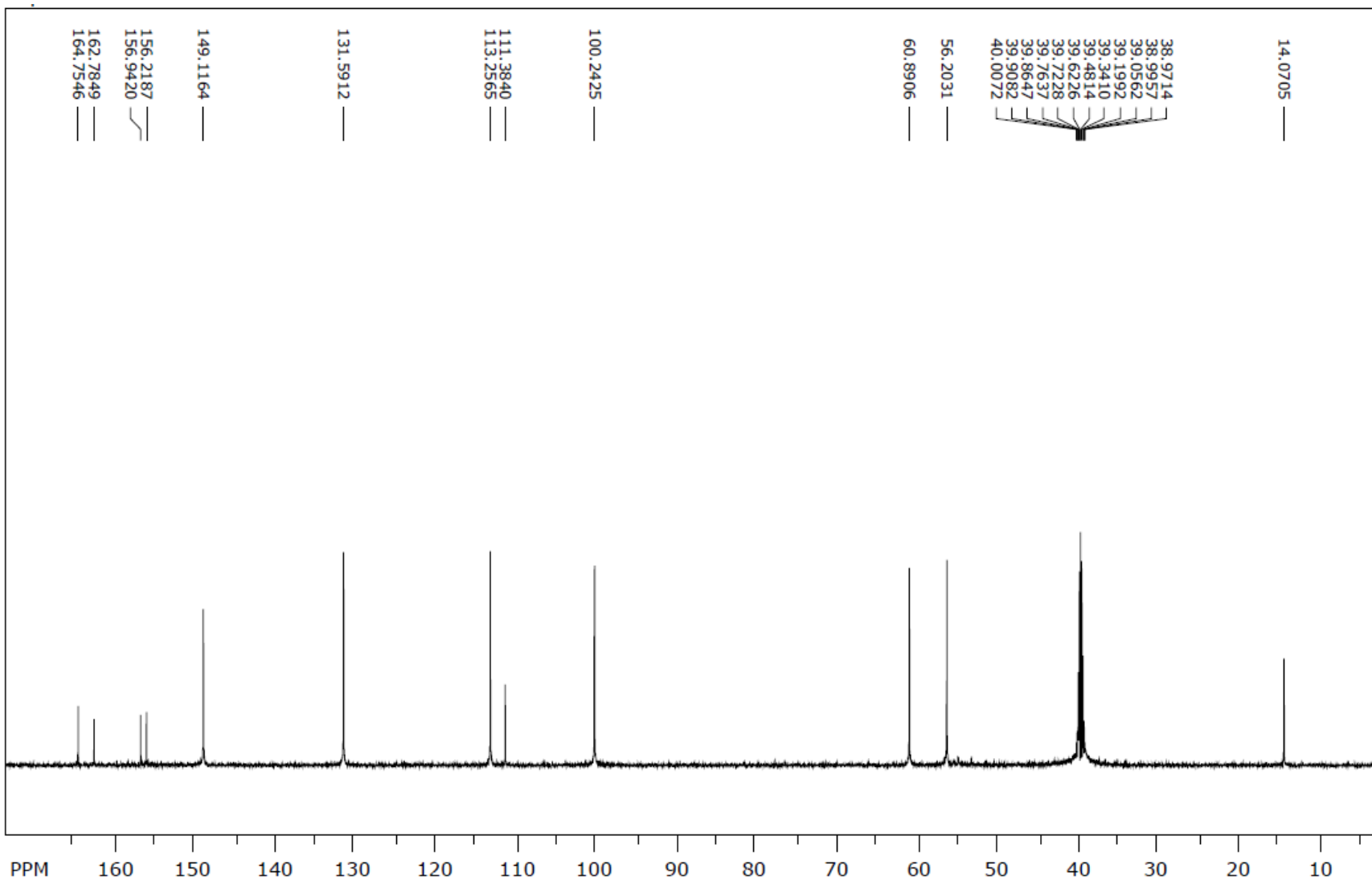
Maseni spektar (2d)



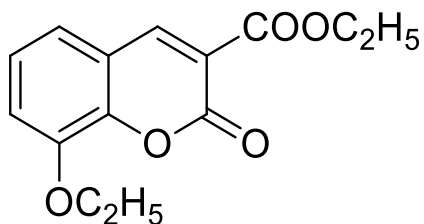
¹H NMR spektr (2d)



¹³C NMR spektr (2d)

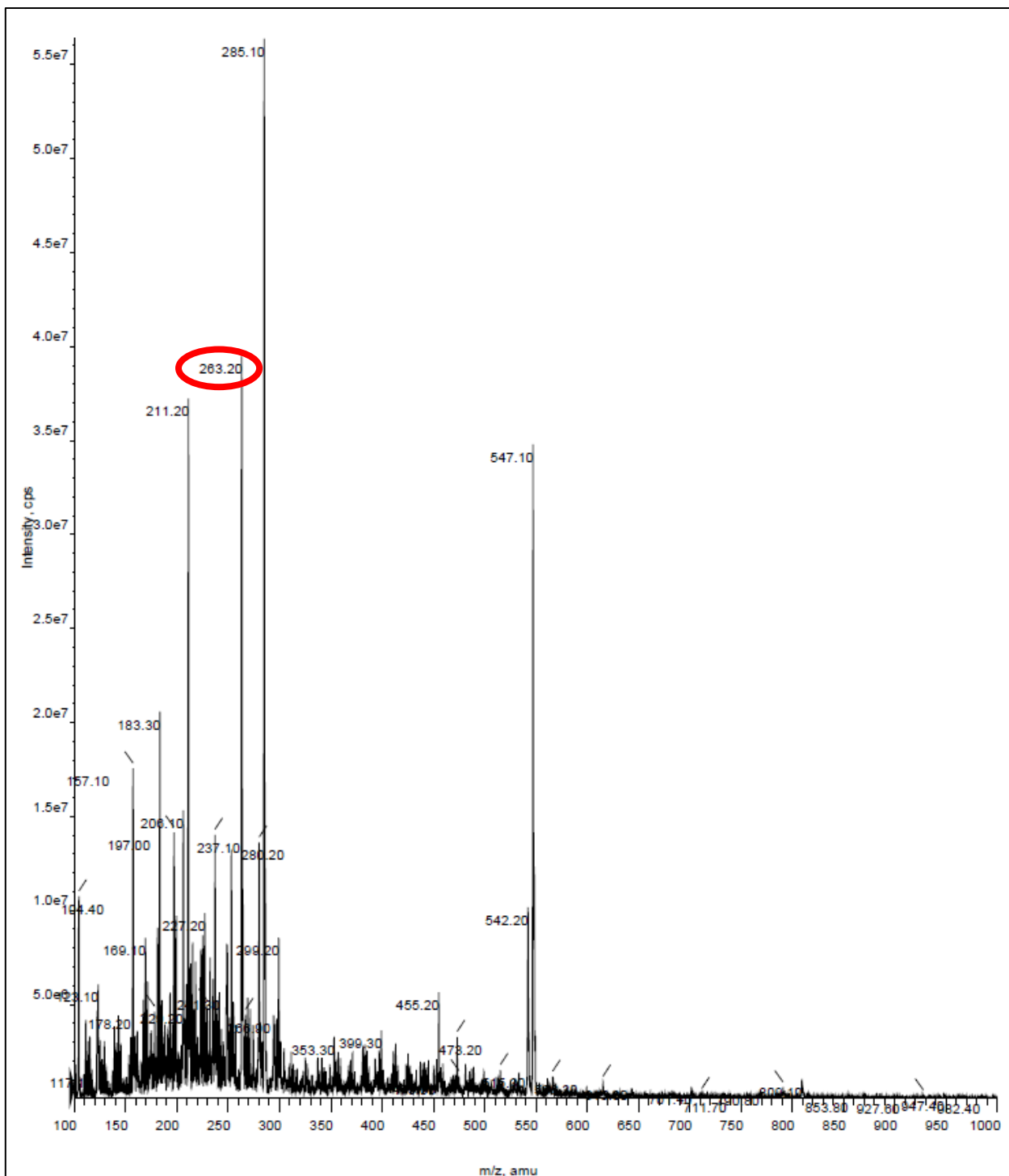


etil 8-etoksi-2-okso-2H-kromen-3-karboksilat (2e)

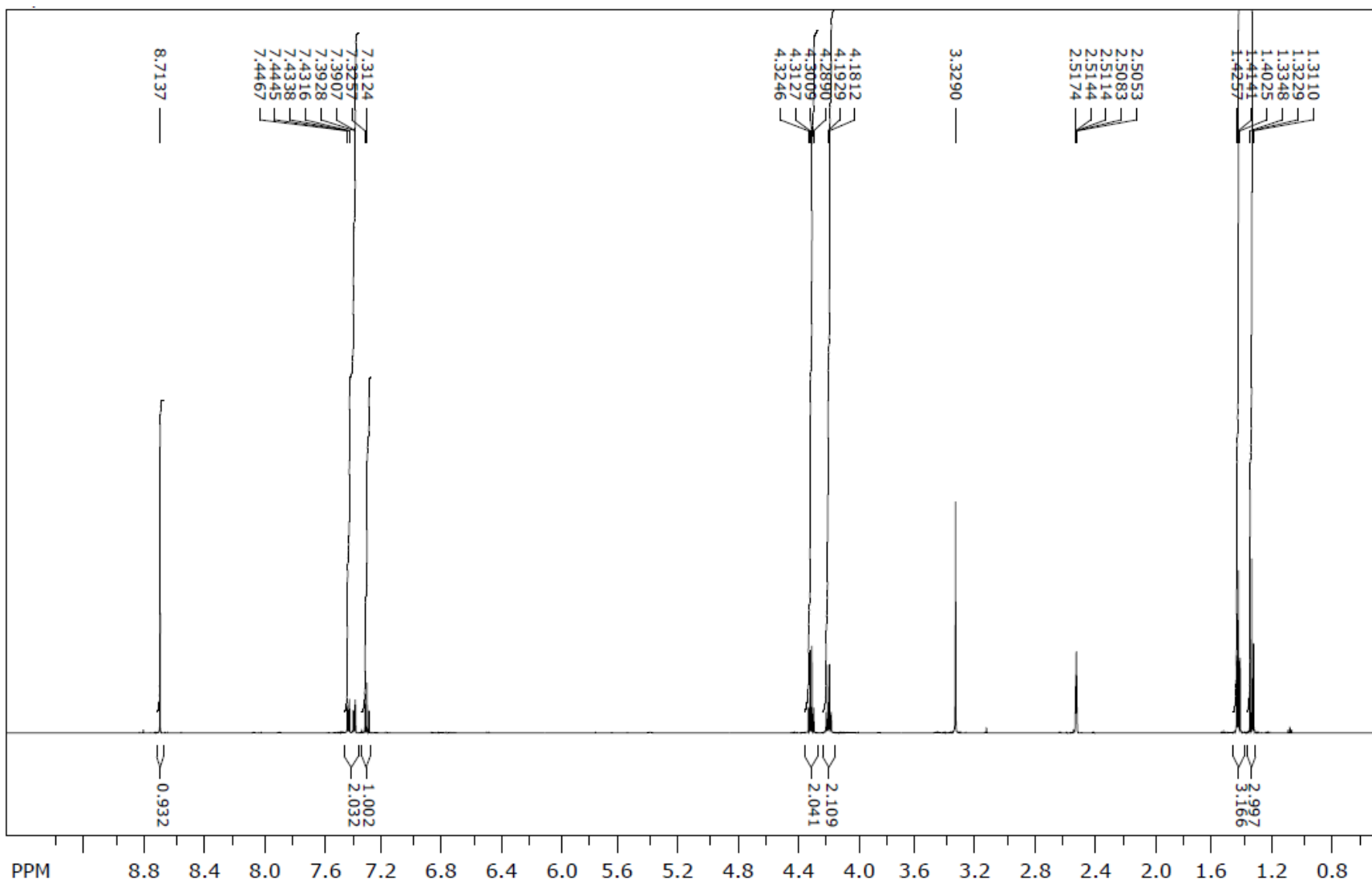


Reaktanti	3-etoksisalicilaldehid (10 mmol) i dietilmalonat (10 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola
Molekulska masa	262,25
Molekulska formula	C ₁₄ H ₁₄ O ₅
Temperatura tališta	98 – 100 °C
Boja kristala	Bijela
R_f	0,72
LC/MS/MS m/z (M⁺)	263,20
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,71 (s, 1H, coum.), 7,44 (dd, <i>J</i> = 7,74, 1,32 Hz, 1H, arom.), 7,40 (dd, <i>J</i> = 8,22, 1,29 Hz, 1H, arom.), 7,32 (d, <i>J</i> = 7,98 Hz, 1H, arom.), 4,31 (q, 2H, <i>J</i> = 7,12 Hz, <u>CH₂CH₃</u>), 4,19 (q, 2H, <i>J</i> = 6,98 Hz, <u>CH₂CH₃</u>), 1,41 (t, <i>J</i> = 6,96 Hz, 3H, <u>CH₂CH₃</u>), 1,32 (t, <i>J</i> = 7,14 Hz, 3H, <u>CH₂CH₃</u>).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 162,5; 155,7; 148,9; 145,4; 143,9; 124,7; 121,1; 118,4; 117,7; 117,3; 64,5; 61,2; 14,5; 14,0.

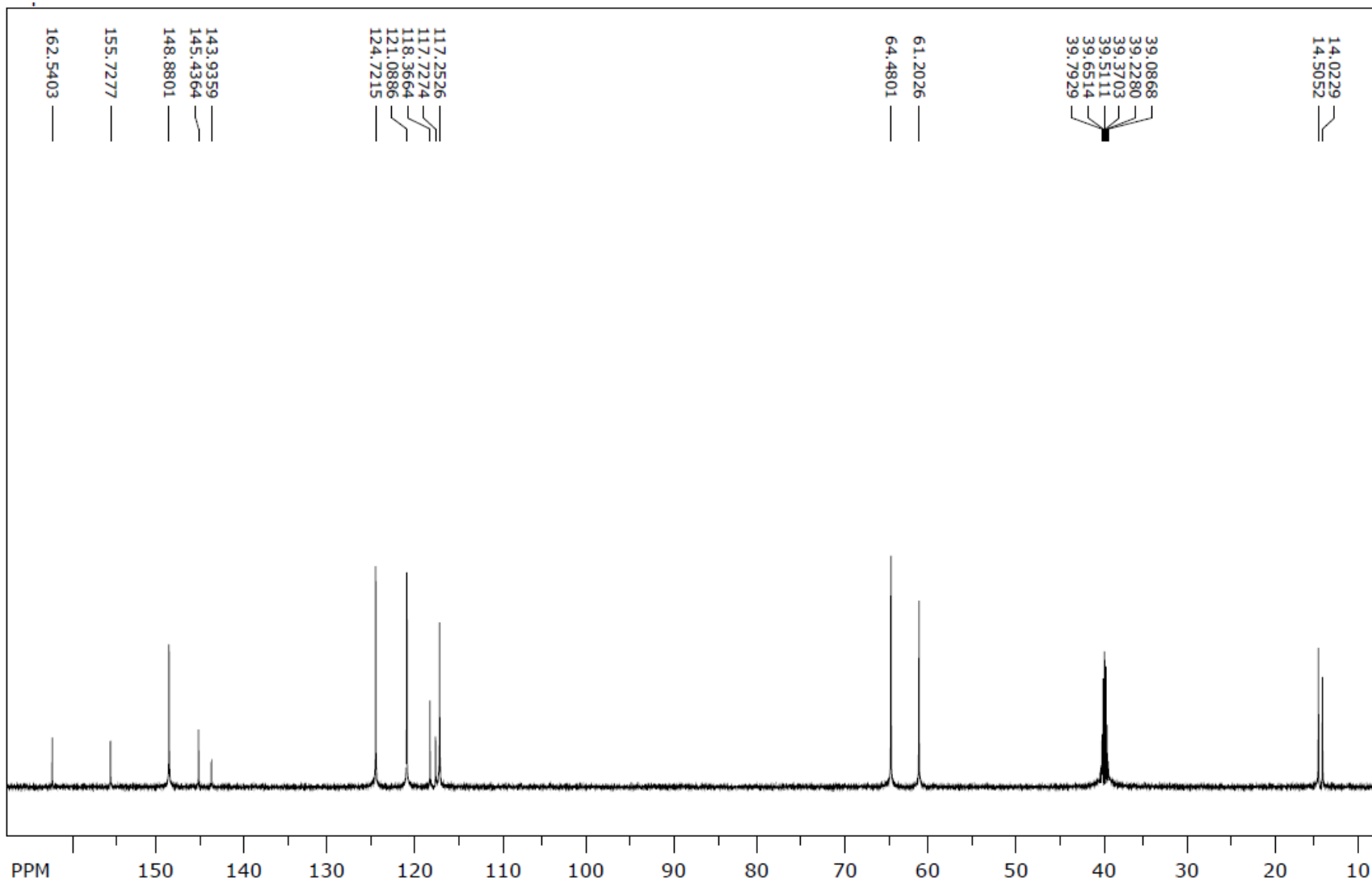
Maseni spektr (2e)



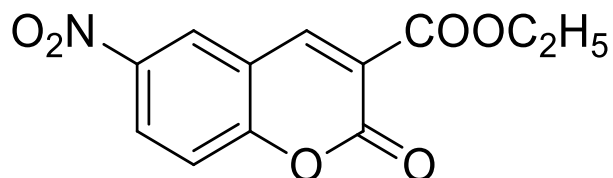
¹H NMR spektr (2e)



¹³C NMR spektr (2e)

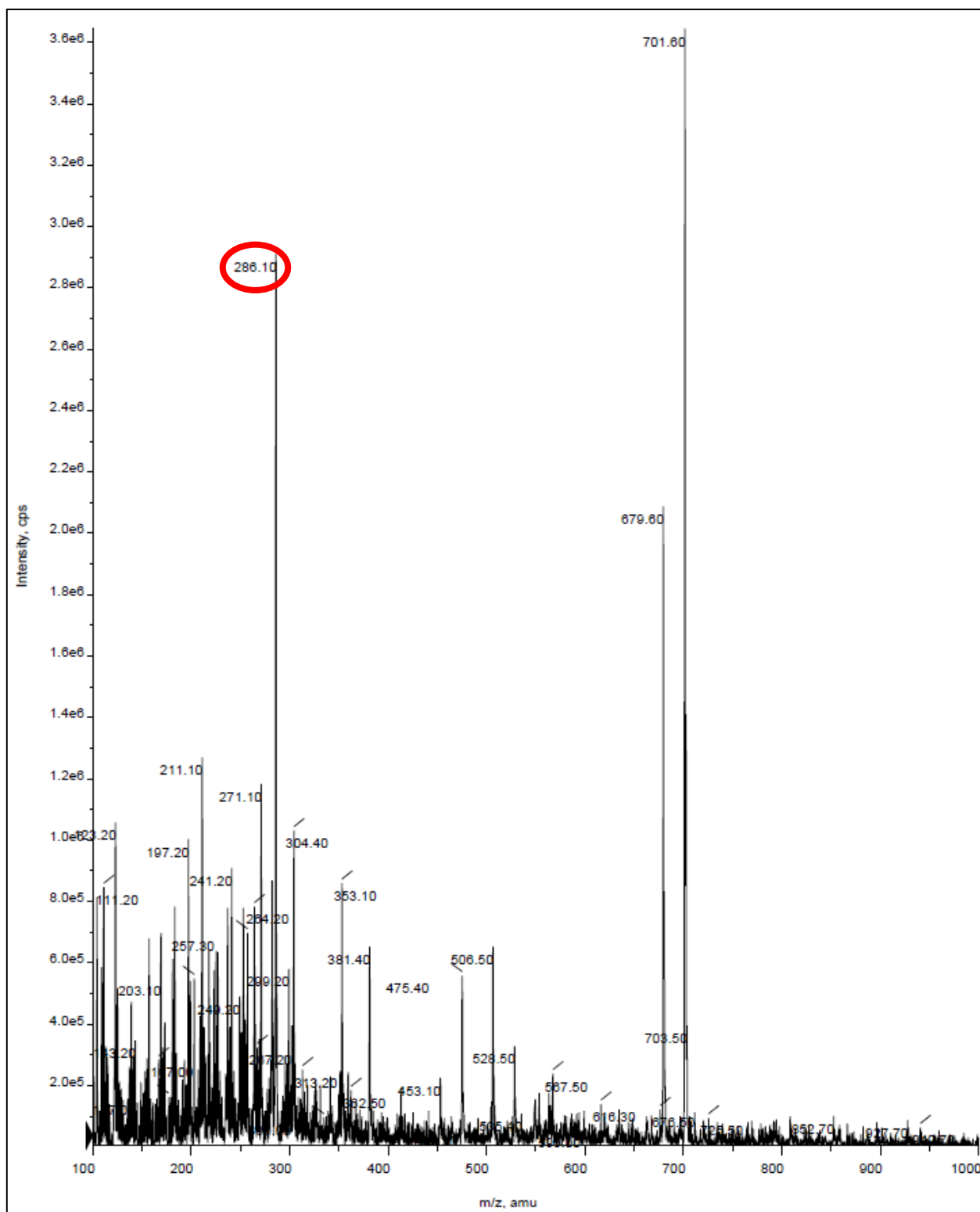


etil 6-nitro-2-okso-2H-kromen-3-karboksilat (2f)

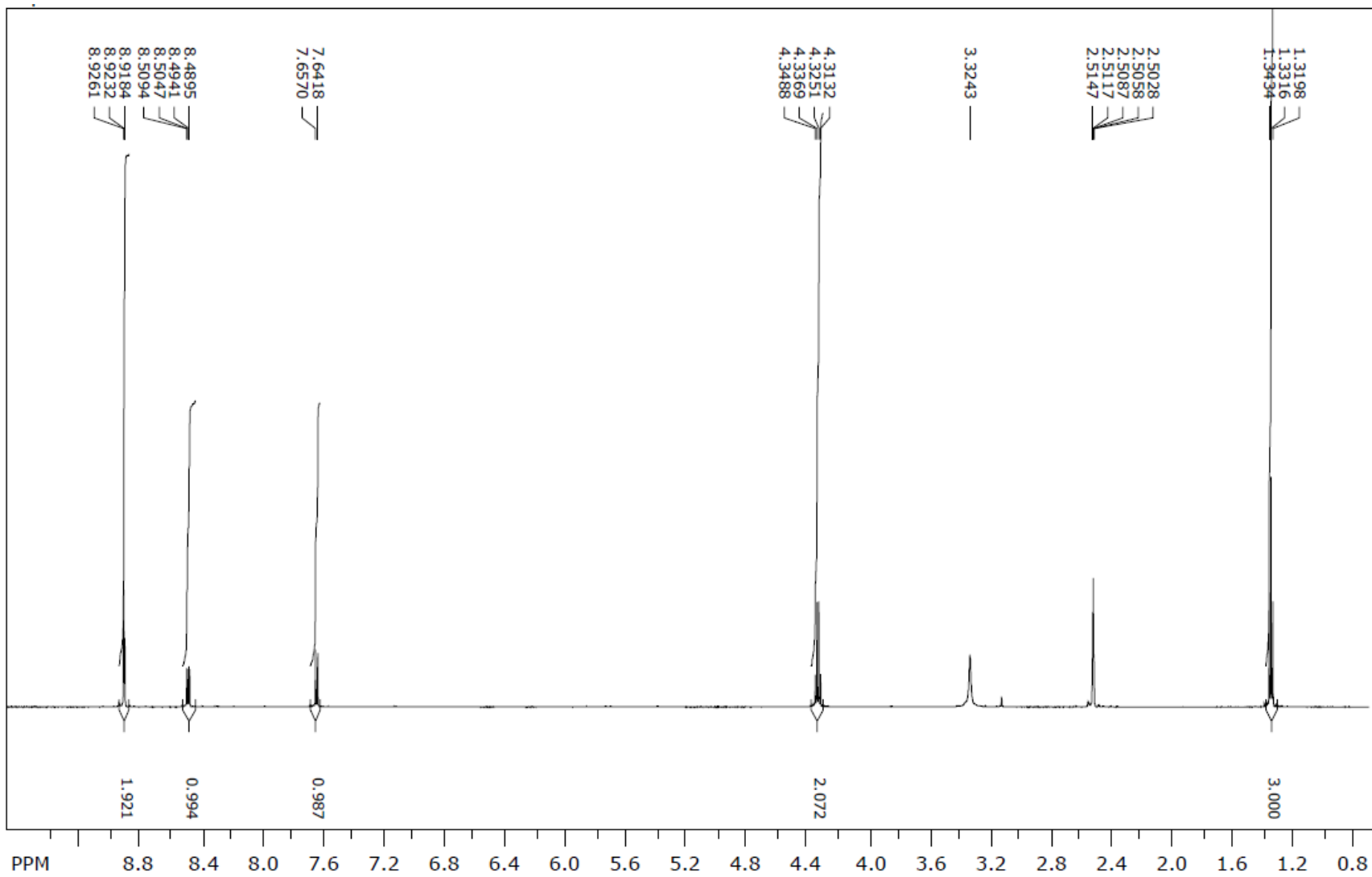


Reaktanti	5-nitrosalicilaldehid (3,1 mmol) i dietilmalonat (3,1 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	263,20 g/mol
Molekulska formula	C ₁₂ H ₉ NO ₆
Temperatura tališta	198 - 203 °C (lit. 192 - 193 °C, He i sur., 2015)
Boja kristala	Žuta
R_f	0,83
LC/MS/MS m/z (M+Na⁺)	286,10
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,92 (s, 2H, arom.), 8,50 (dd, <i>J</i> = 9,18, 2,79 Hz, 1H, arom.), 7,65 (d, <i>J</i> = 9,12 Hz, 1H, arom.), 4,33 (q, <i>J</i> = 7,12 Hz, 2H, CH ₂ CH ₃), 1,33 (t, <i>J</i> = 7,08 Hz, 3H, CH ₂ CH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 162,0; 158,0; 147,6; 143,6; 128,5; 126,0; 119,5; 118,2; 117,7; 61,5; 14,0.

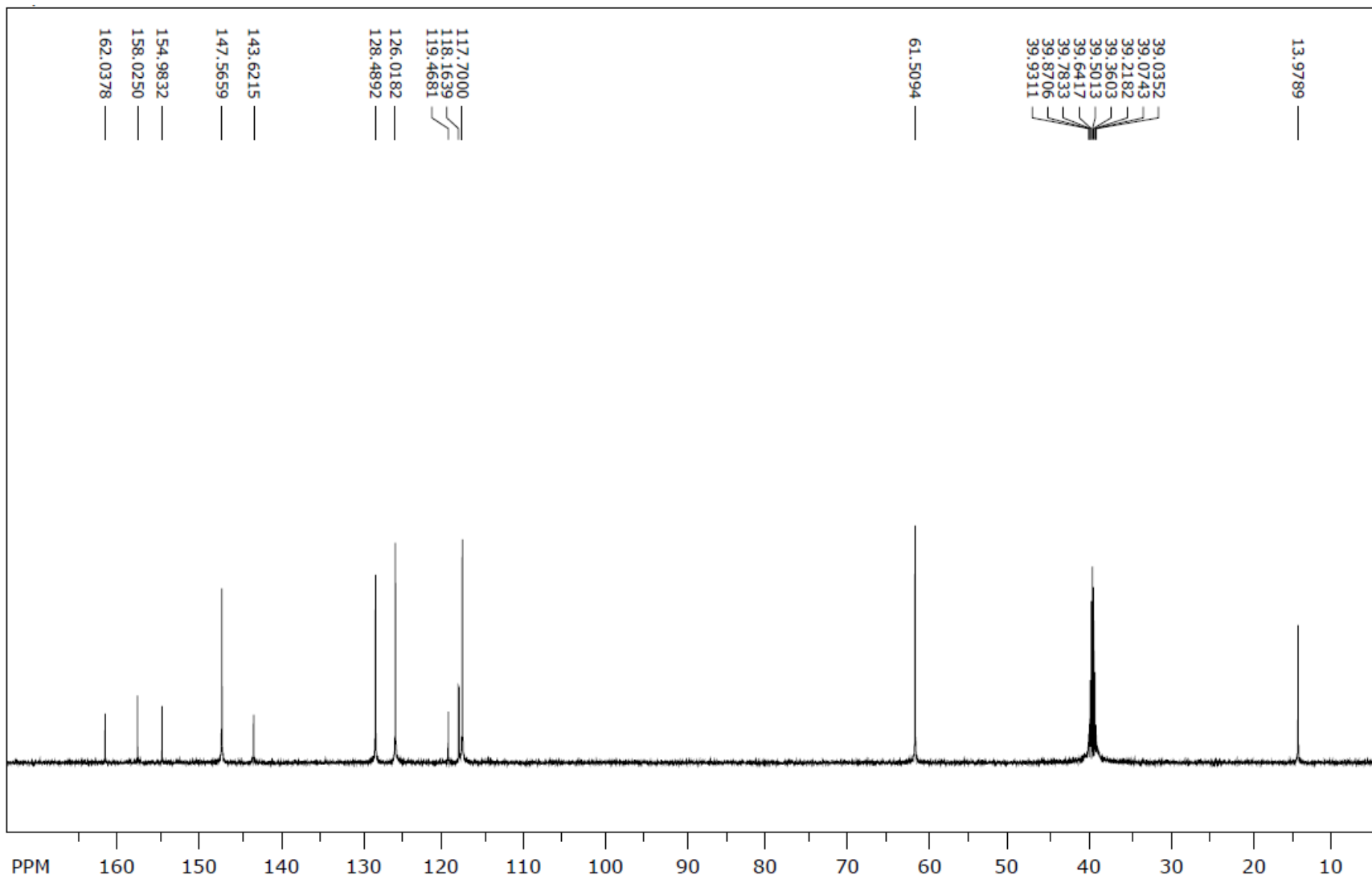
Maseni spektar (2f)



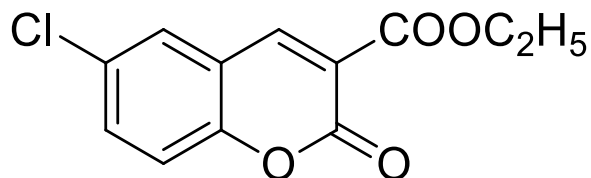
¹H NMR spektr (2f)



¹³C NMR spektr (2f)

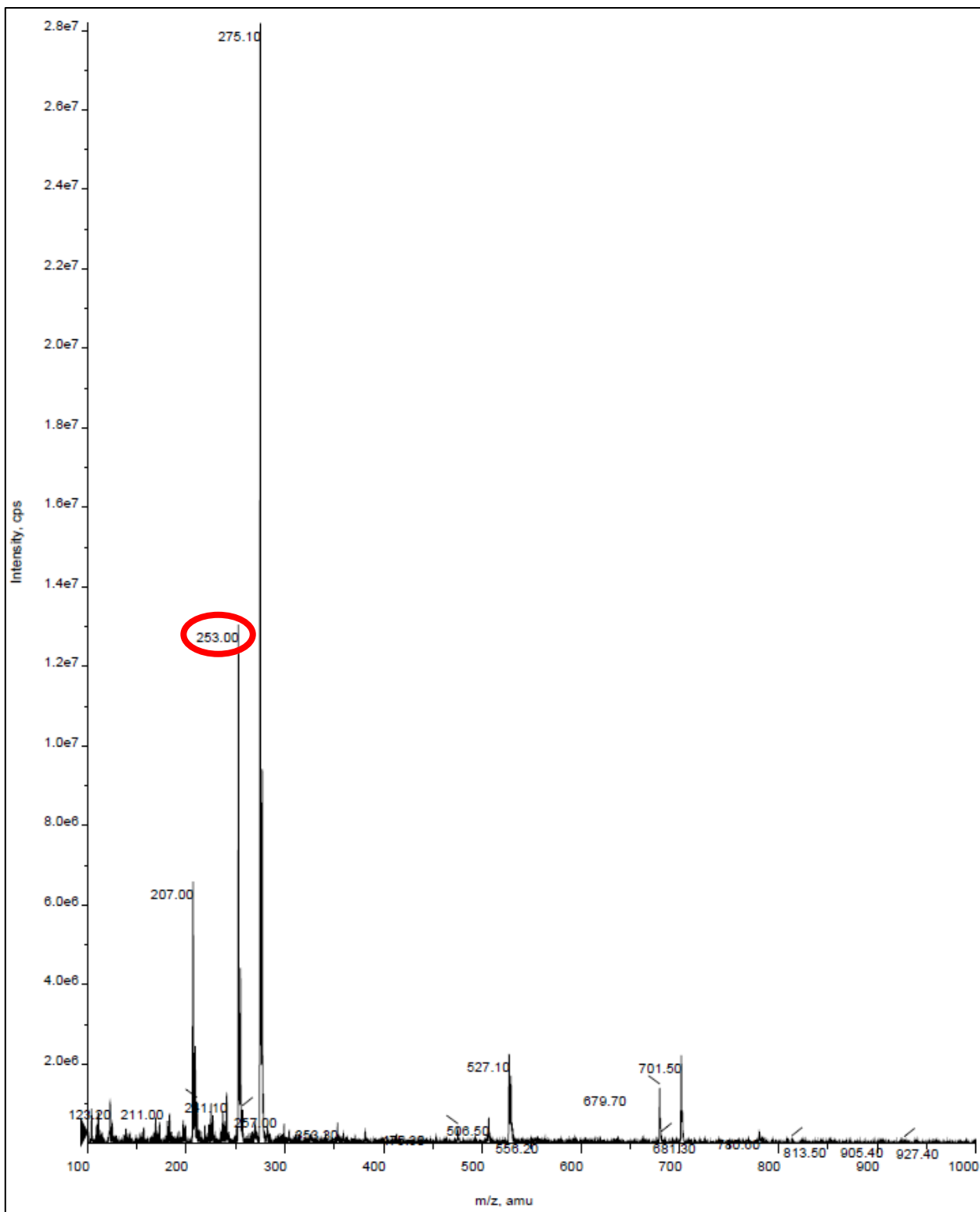


etil 6-klor-2-okso-2H-kromen-3-karboksilat (2g)

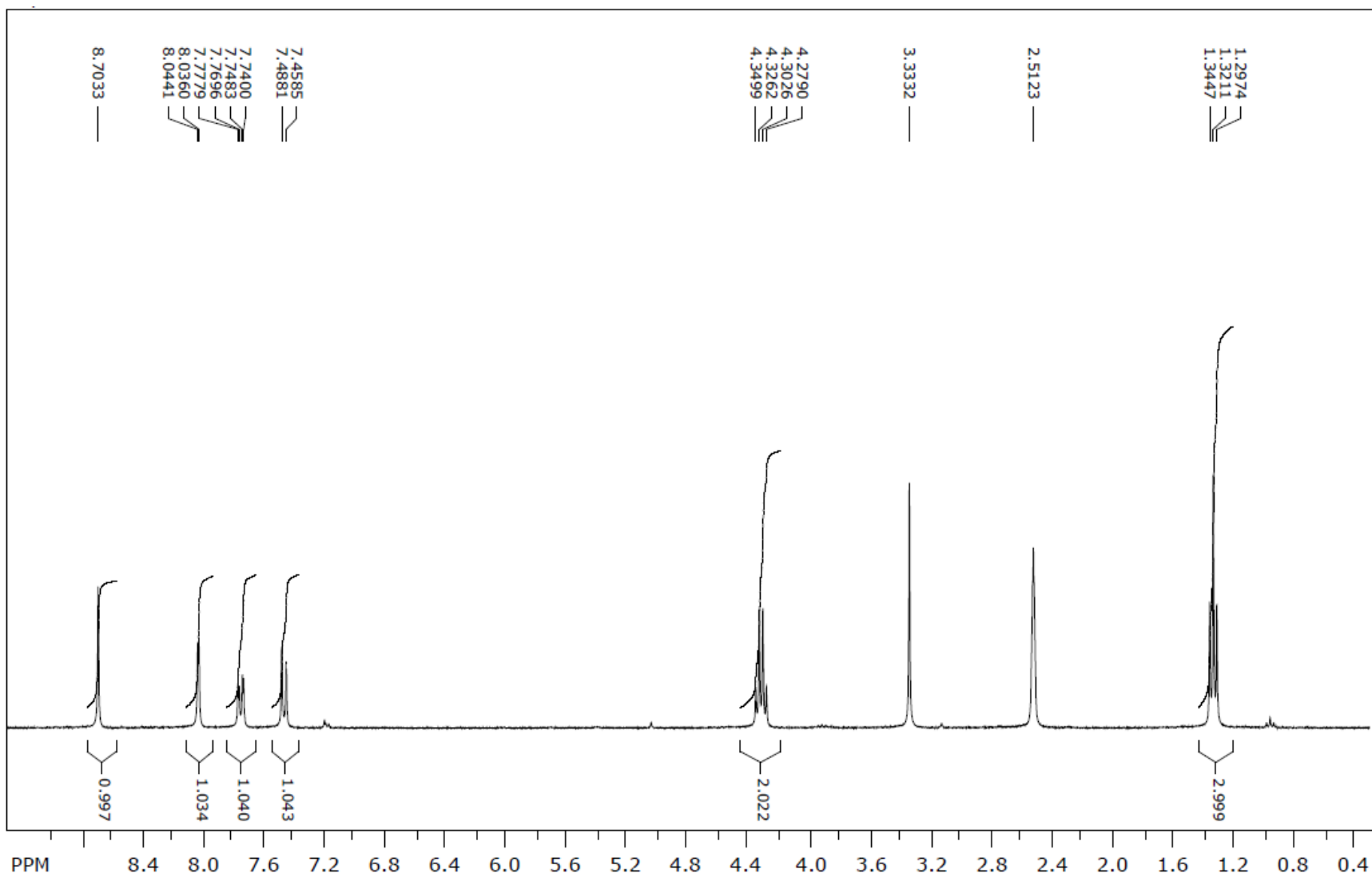


Reaktanti	5-klorosalicilaldehid (3,3 mmol) i dietilmalonat (3,3 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	252,65 g/mol
Molekulska formula	C ₁₂ H ₉ ClO ₄
Temperatura tališta	167 – 172 °C (lit. 174 – 175 °C, He i sur., 2015)
Boja kristala	Svijetložuta
R_f	0,76
LC/MS/MS m/z (M⁺)	253,0
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 8,70 (s, 1H, arom.), 8,04 (d, 1H, <i>J</i> = 2,43 Hz, arom.), 7,76 (dd, <i>J</i> = 8,88, 2,49 Hz, 1H, arom.), 7,47 (d, <i>J</i> = 8,88 Hz, 1H, arom.), 4,31 (q, 2H, <i>J</i> = 7,09 Hz, <u>CH₂</u> CH ₃), 1,32 (t, 3H, <i>J</i> = 7,10 Hz, CH ₂ <u>CH₃</u>).
¹³C NMR	(75 MHz, DMSO- <i>d</i> ₆) δ 162,8; 156,0; 153,6; 147,8; 134,3; 129,5; 128,9; 119,6; 118,7; 62,6; 14,5.

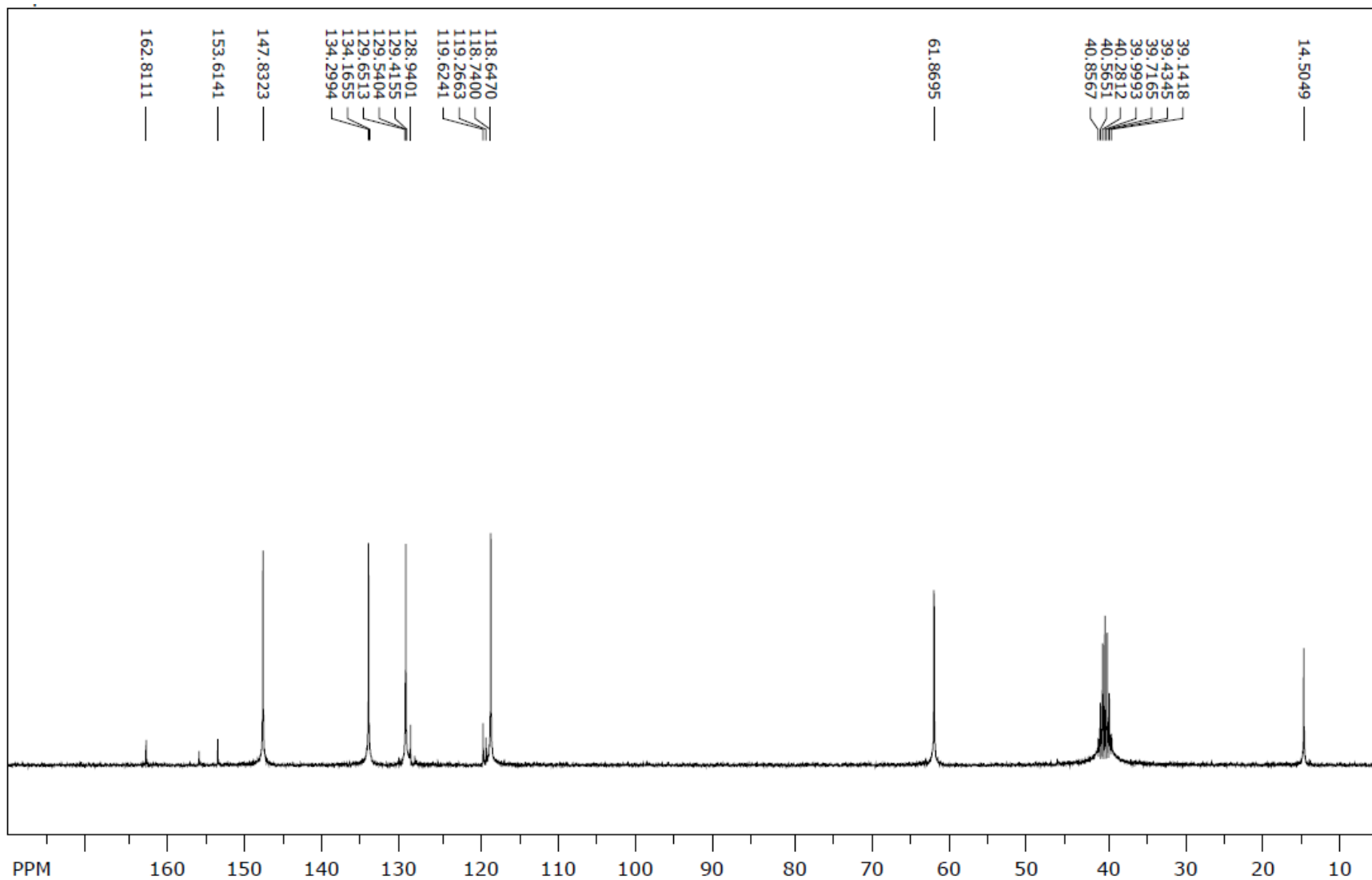
Maseni spektar (2g)



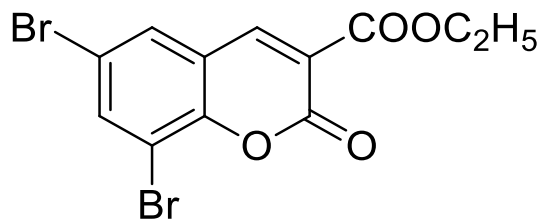
¹H NMR spektr (2g)



¹³C NMR spektr (2g)

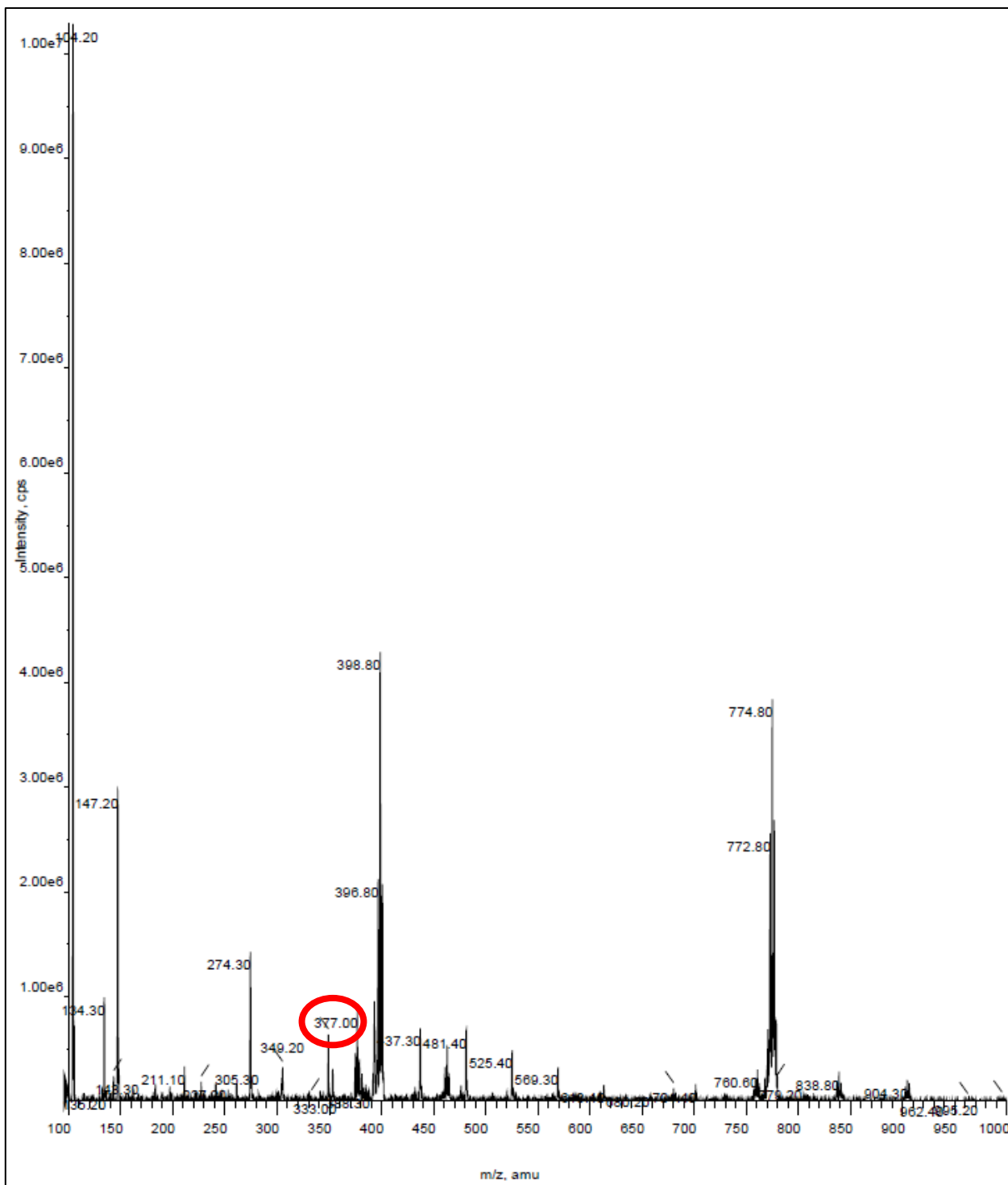


etil 6,8-dibrom-2-okso-2H-kromen-3-karboksilat (2h)

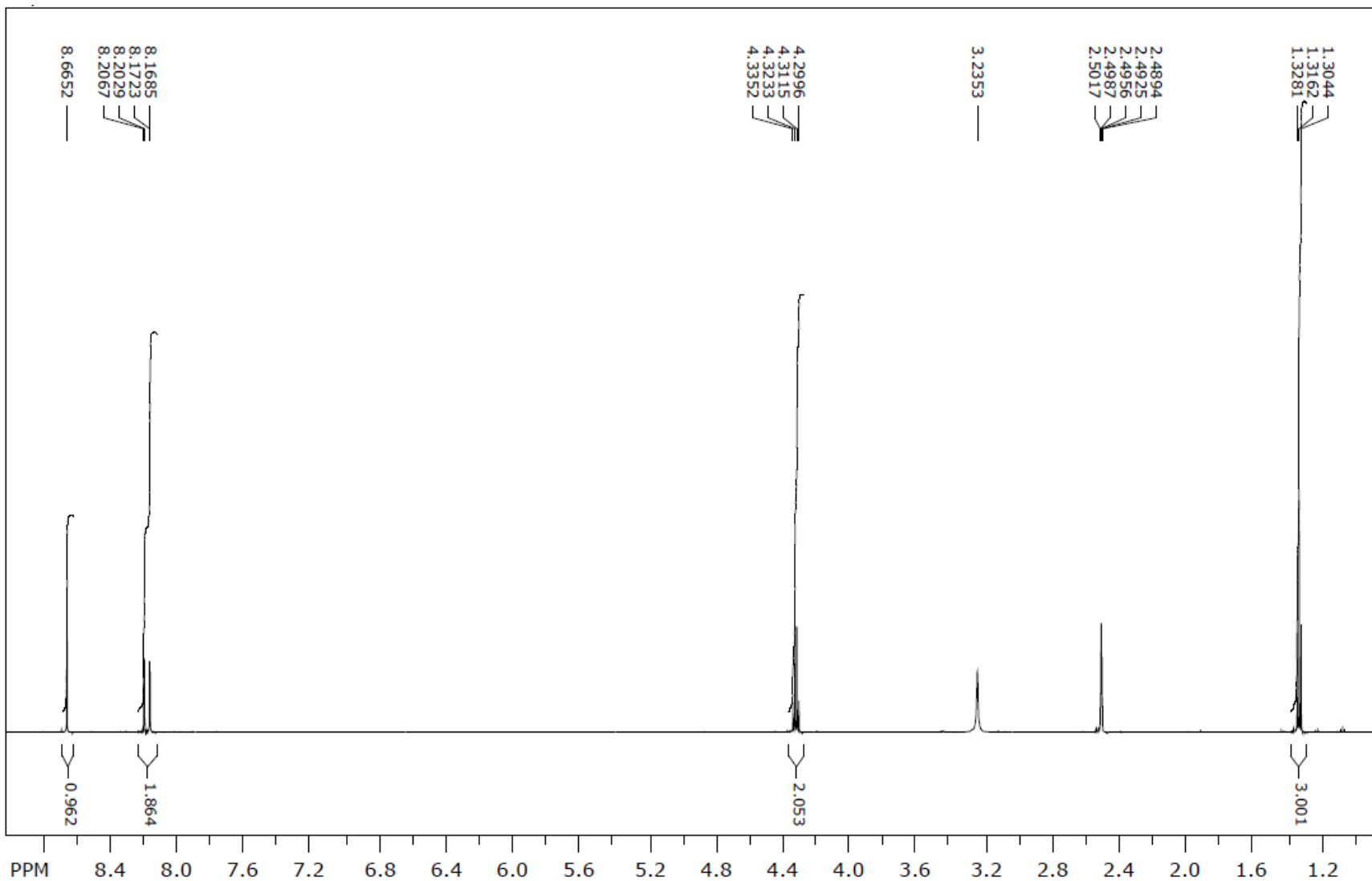


Reaktanti	3,5-dibromsalicilaldehid (2,8 mmol) i dietilmalonat (2,8 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	375,99 g /mol
Molekulska formula	C ₁₂ H ₈ Br ₂ O ₄
Temperatura tališta	170 – 173 °C
Boja kristala	Svijetlosmeđa
R_f	0,83
LC/MS/MS m/z (M⁺)	377,0
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,66 (s, 1H, arom.), 8,20 (d, <i>J</i> = 2,28 Hz, 1H, arom.), 8,17 (d, <i>J</i> = 2,28 Hz, 1H, arom.), 4,32 (q, <i>J</i> = 7,12 Hz, 2H, CH ₂ CH ₃), 1,32 (t, <i>J</i> = 7,11 Hz, 3H, CH ₂ CH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 161,9; 154,8; 150,4; 147,0; 138,4; 131,7; 120,7; 119,4; 116,2; 110,0; 61,5; 13,9.

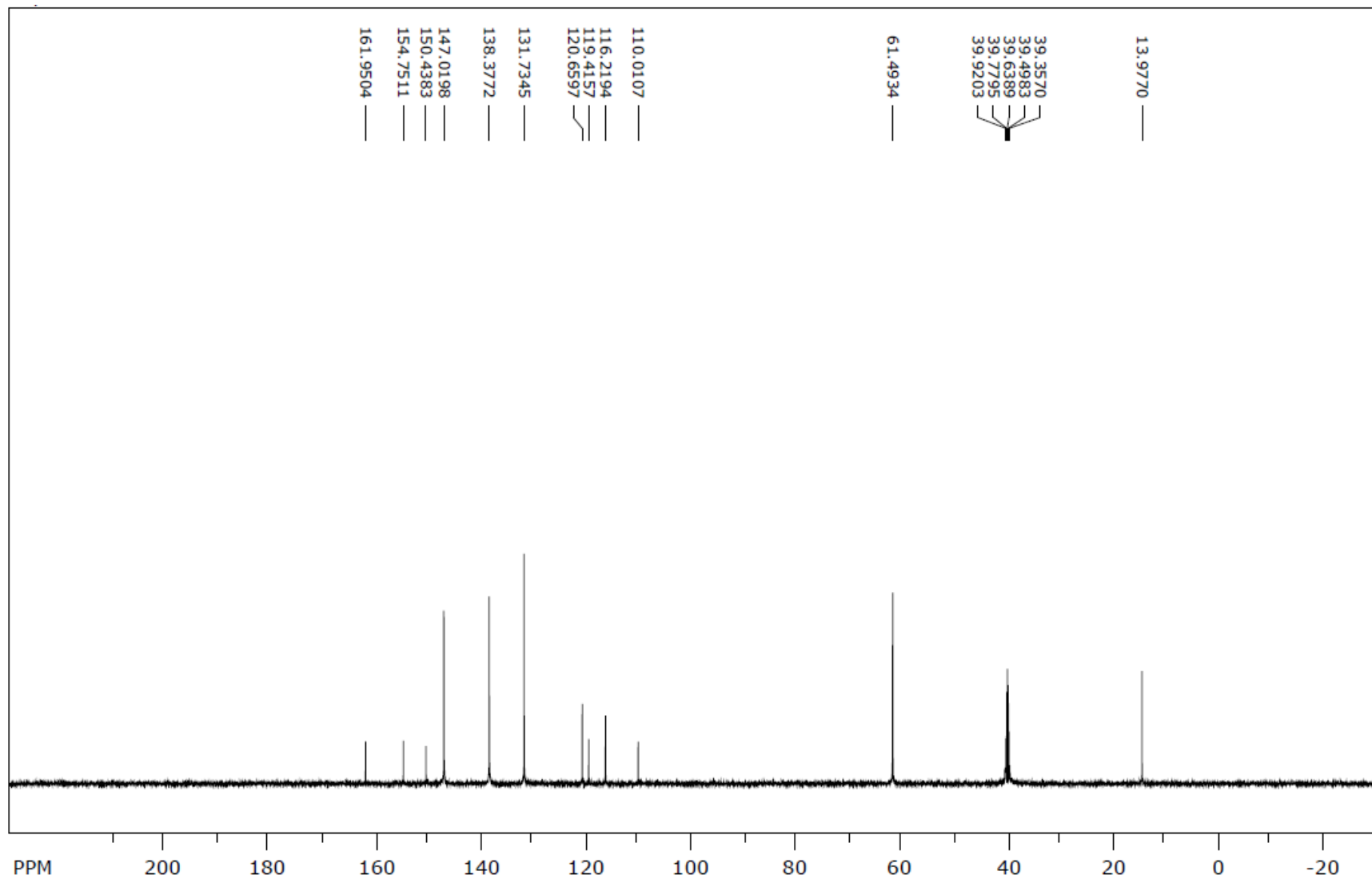
Maseni spektr (2h)



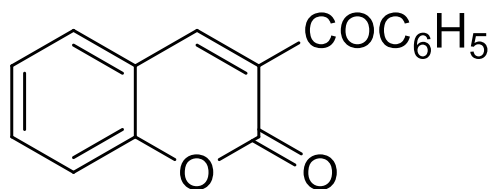
¹H NMR spektr (2h)



¹³C NMR spektr (2h)

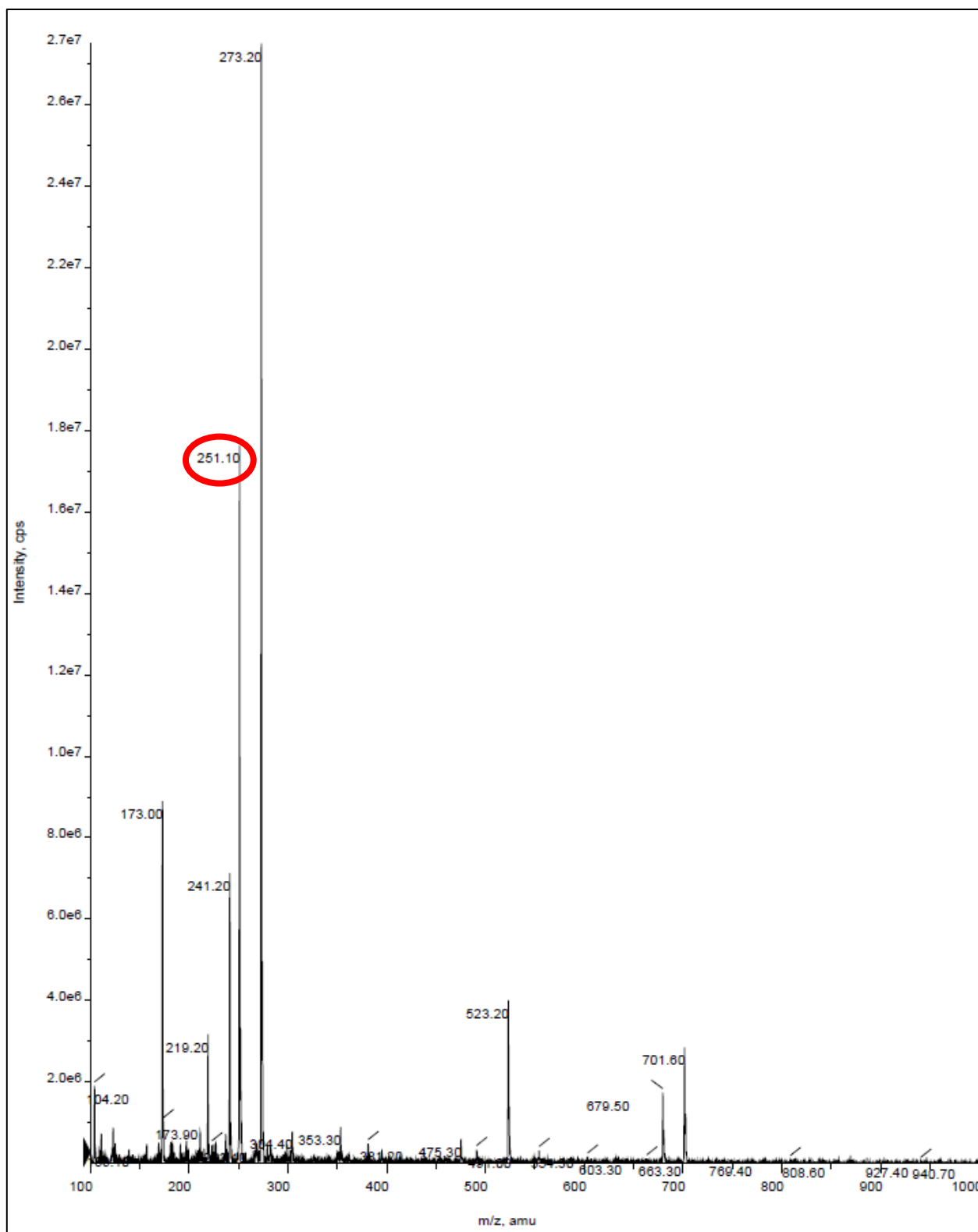


3-benzoil-2H-kromen-2-on (3a)

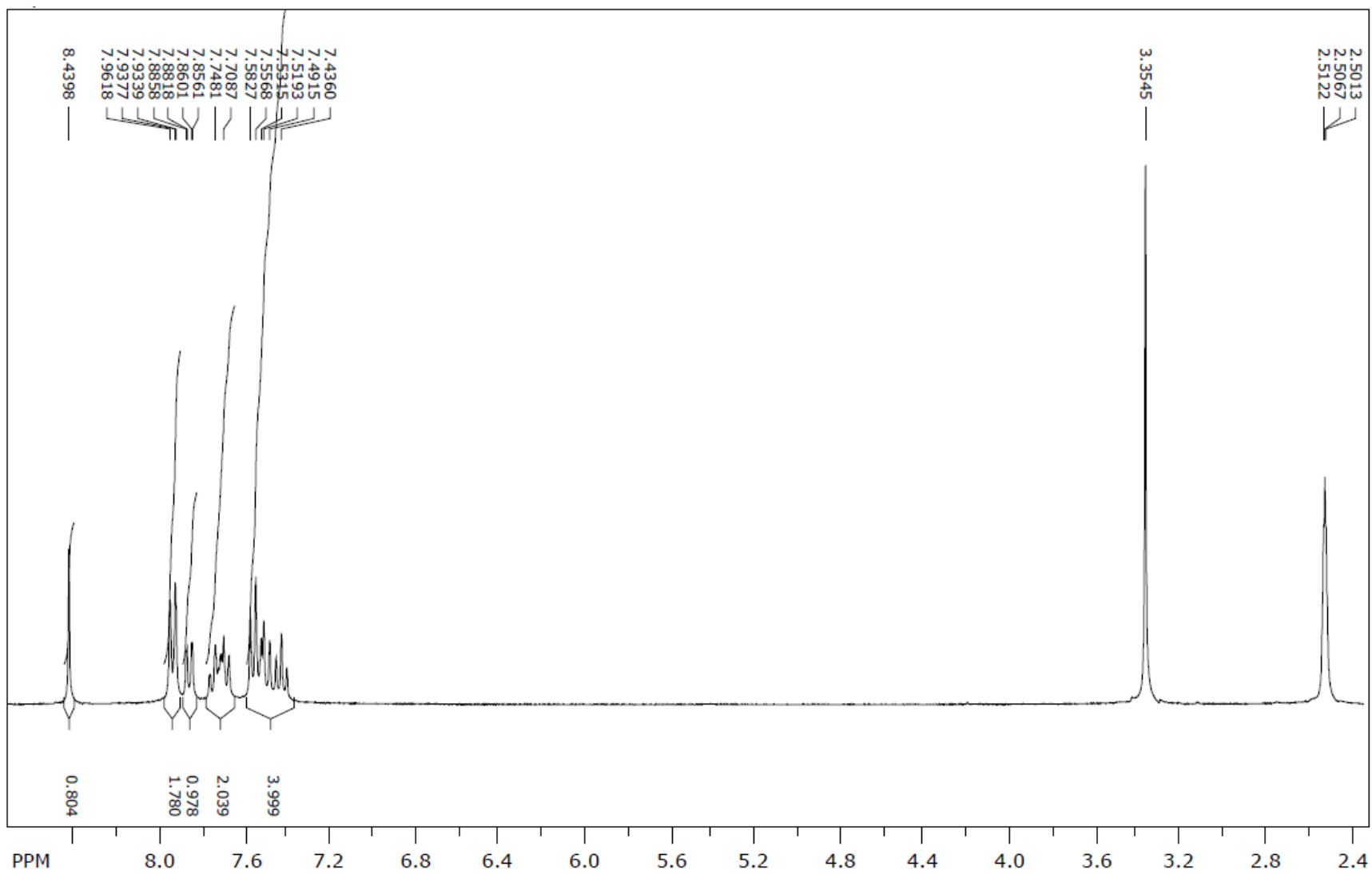


Reaktanti	Salicilaldehid (1,3 mmol) i etil benzoilacetat (1,3 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	250,24 g/mol
Molekulska formula	C ₁₆ H ₁₀ O ₃
Temperatura tališta	100 – 103 °C
Boja kristala	Svijetložuta
R_f	0,82
LC/MS/MS <i>m/z</i> (M⁺)	251,10
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 8,44 (s, 1H, arom.), 7,95 (d, <i>J</i> = 8,37 Hz, 2H, arom.), 7,86 (dd, <i>J</i> = 7,71, 1,2 Hz, 1H, arom.), 7,68 - 7,78 (m, 2H, arom.), 7,41 - 7,58 (m, 4H, arom.).
¹³C NMR	(75 MHz, DMSO- <i>d</i> ₆) δ 192,2; 158,5; 154,6; 145,8; 136,5; 134,4; 134,1, 130,4; 130,3; 129,2; 126,8; 125,4; 118,7; 116,8.

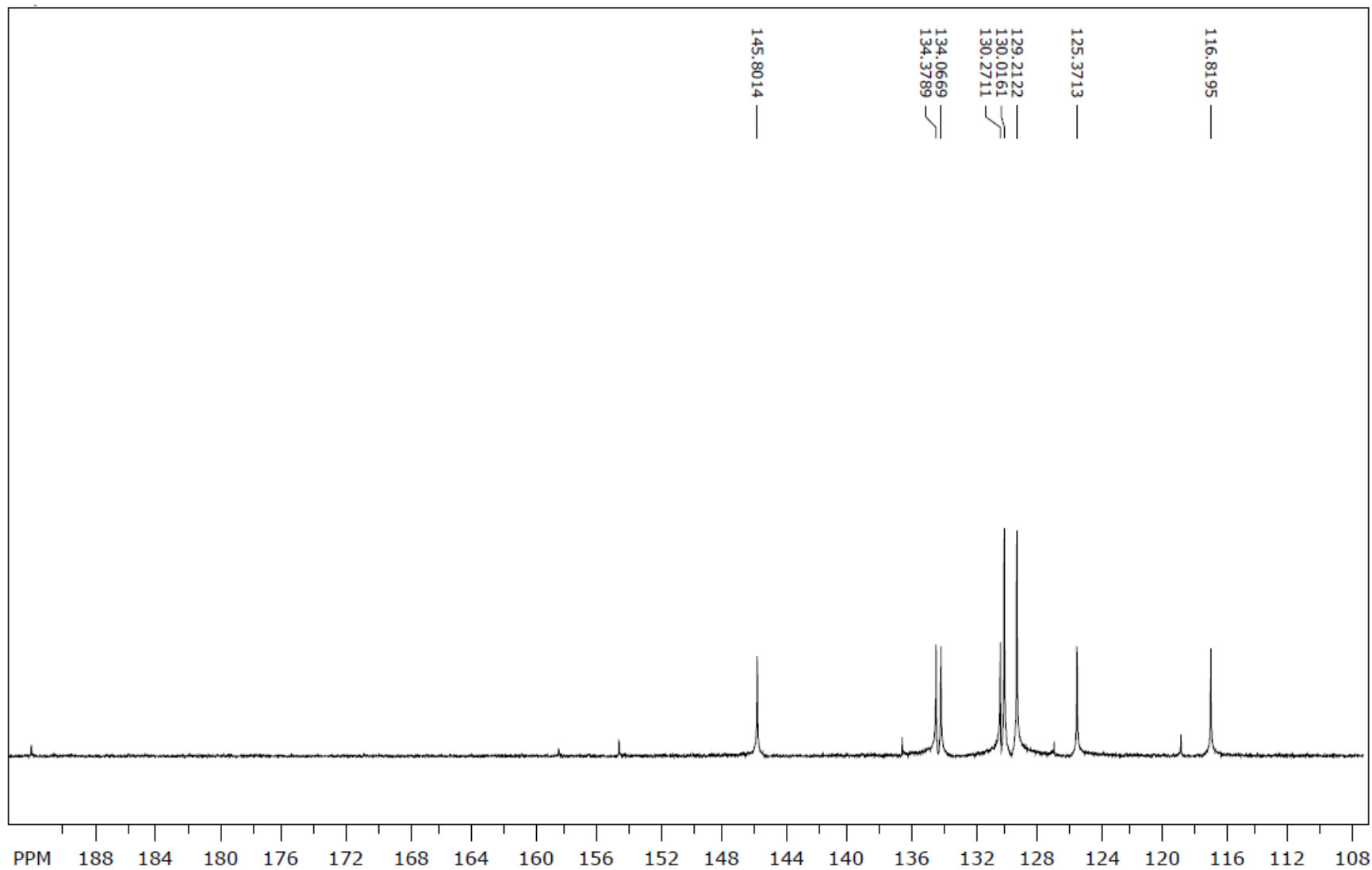
Maseni spektar (3a)



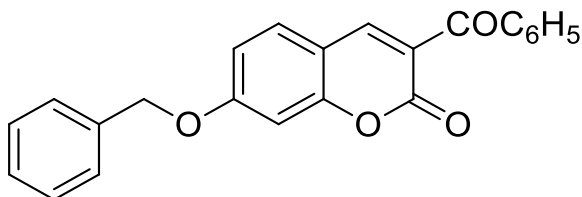
¹H NMR spektr (3a)



¹³C NMR spektr (3a)

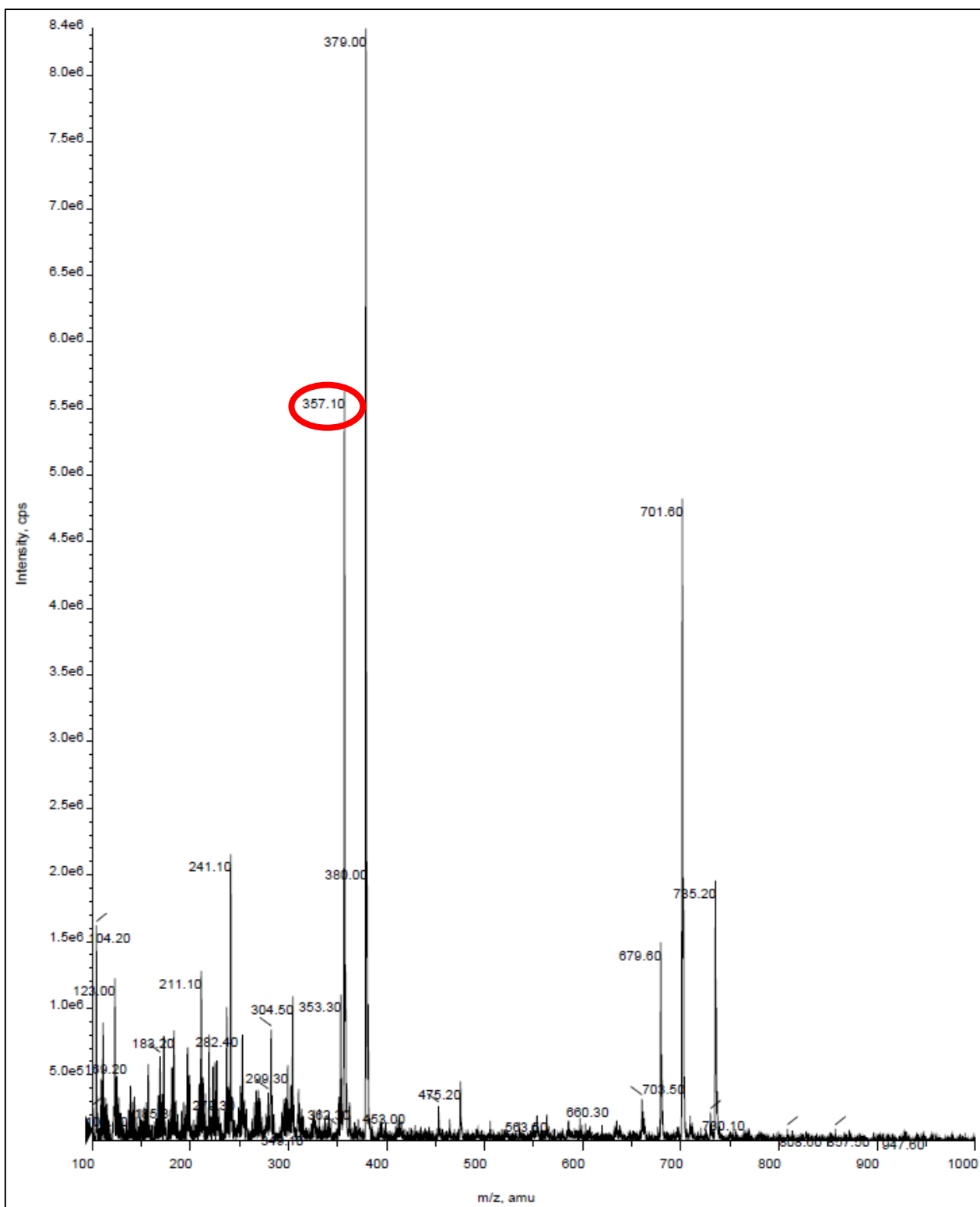


3-benzoil-7-(benziloksi)-2H-kromen-2-on (3b)

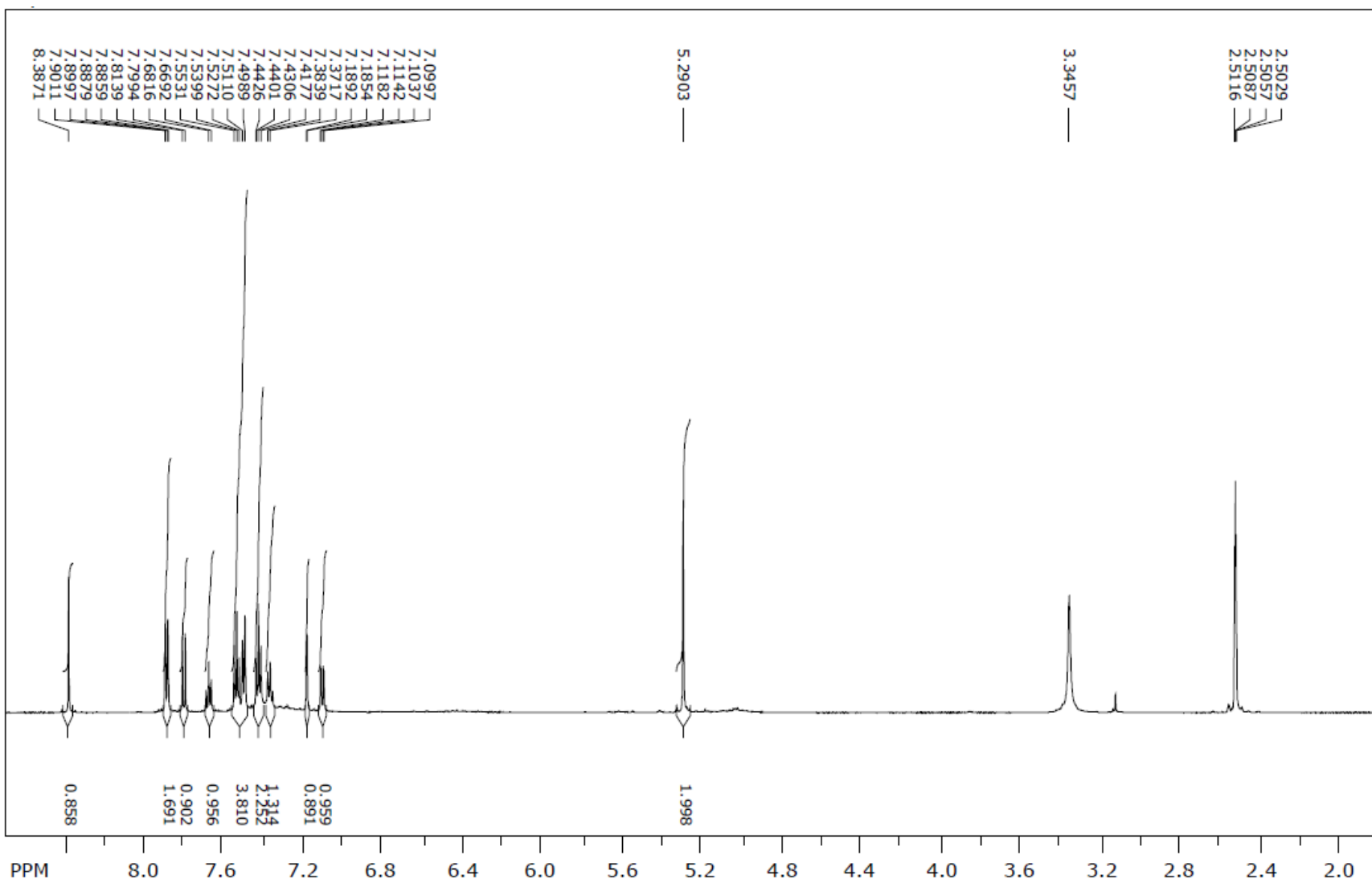


Reaktanti	4-(benziloksi)salicilaldehid (0,64 mmol) i etil benzoilacetat (0,64 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	356,37 g/mol
Molekulska formula	C ₂₃ H ₁₆ O ₄
Temperatura tališta	140 – 143 °C
Boja kristala	Smeđa
R_f	0,85
LC/MS/MS m/z (M⁺)	357,10
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,39 (s, 1H, coum.), 7,90 (dd, <i>J</i> = 7,92, 1,02 Hz, 2H, arom.), 7,81 (d, <i>J</i> = 8,70 Hz, 1H, arom.), 7,67 - 7,69 (m, 1H, arom.), 7,53 - 7,55 (m, 2H, arom.), 7,50 (d, <i>J</i> = 7,26 Hz, 2H, arom.), 7,41 - 7,44 (m, 2H, arom.), 7,36 - 7,38 (m, 1H, arom.), 7,19 (d, <i>J</i> = 2,28 Hz, 1H, arom.), 7,11 (dd, <i>J</i> = 8,70, 2,40 Hz, 1H, arom.), 5,29 (s, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 191,0; 163,0; 158,2; 156,3; 146,2; 136,5; 136,0; 133,5; 131,2; 129,4; 128,6; 128,5; 128,2; 127,9; 122,4; 113,7; 111,9; 101,5; 70,1.

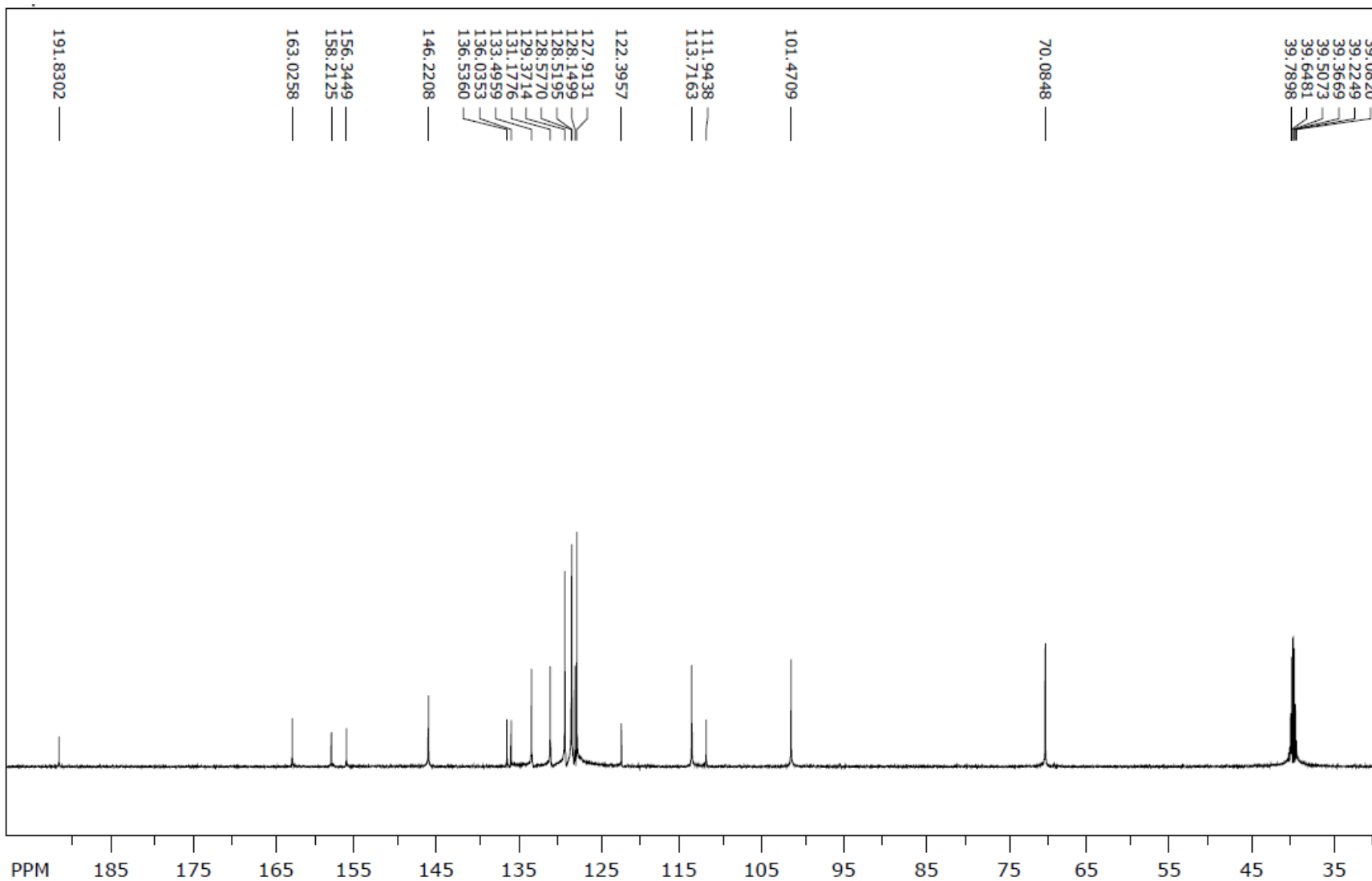
Maseni spektar (3b)



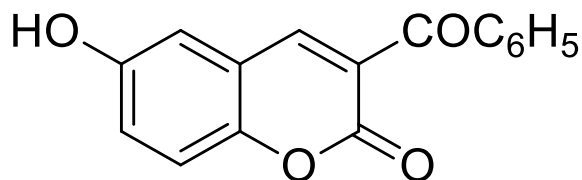
¹H NMR spektr (3b)



¹³C NMR spektr (3b)

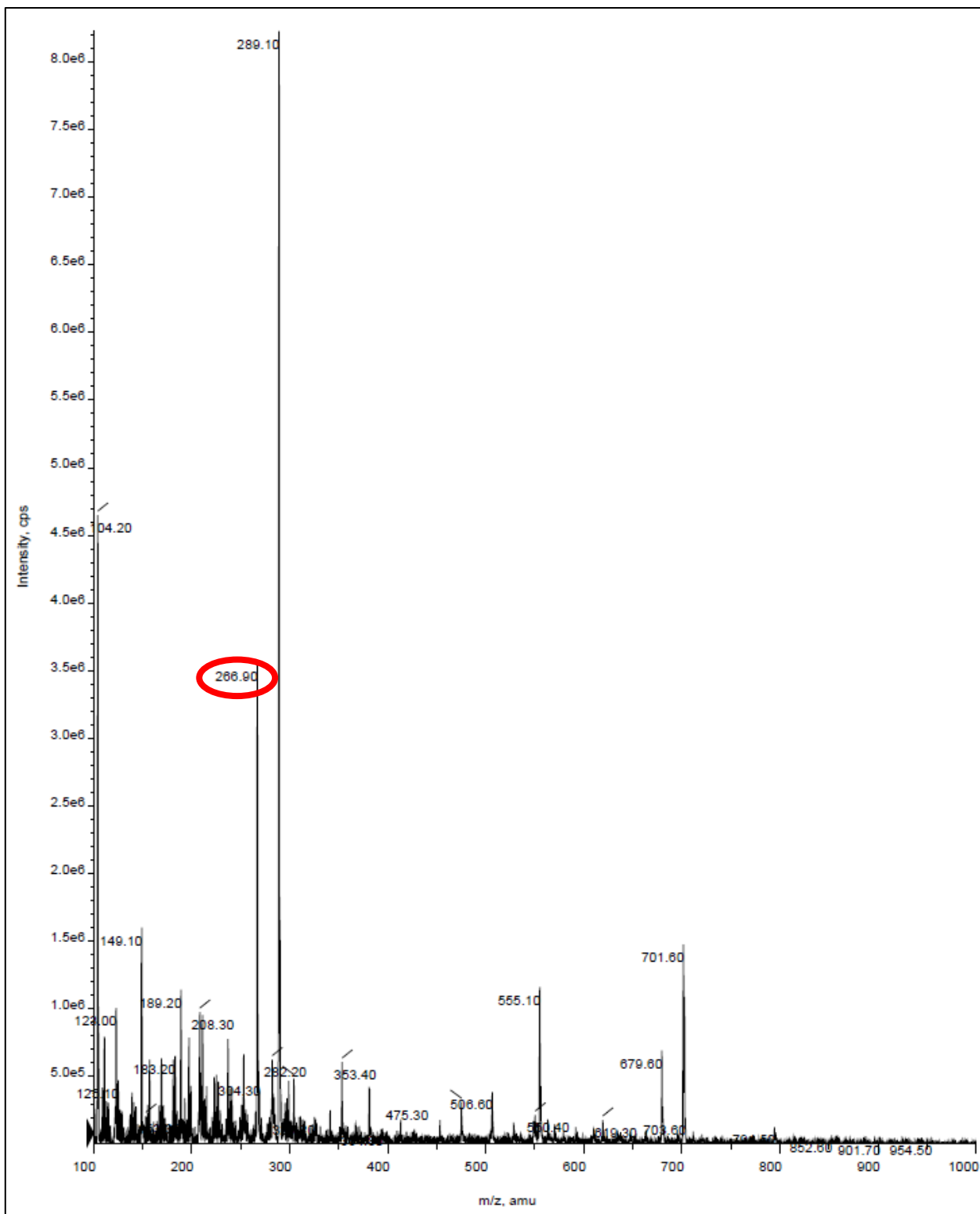


3-benzoil-6-hidroksi-2H-kromen-2-on (3c)

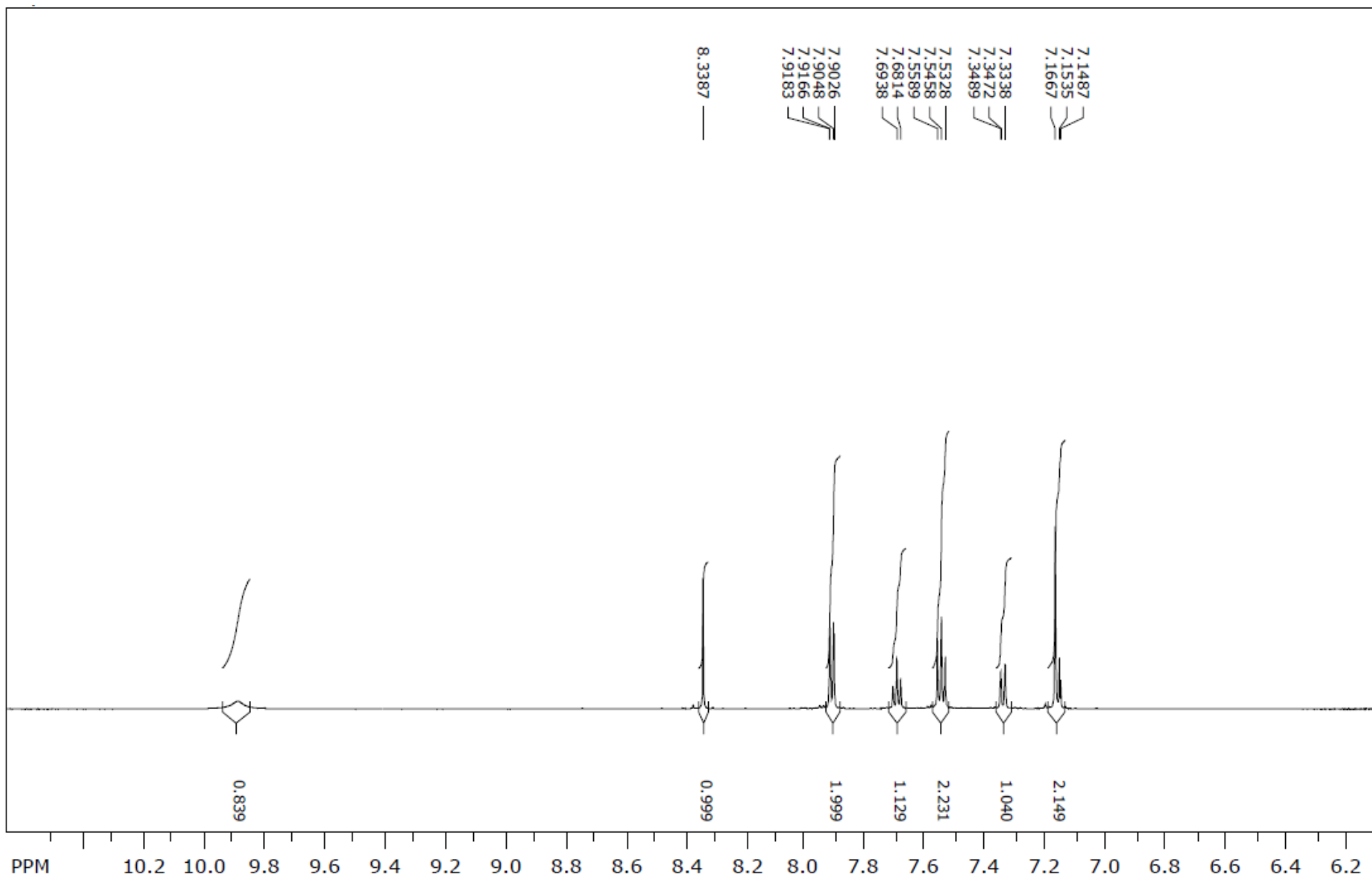


Reaktanti	2,5-dihidroksibenzaldehid (1,3 mmol) i etil benzoilacetat (1,3 mmol)
Metoda pročiščavanja	Ispran etanolom
Molekulska masa	266,24 g/mol
Molekulska formula	C ₁₆ H ₁₀ O ₄
Temperatura tališta	227 – 230 °C (lit. 224 – 225 °C, Secci i sur., 2011)
Boja kristala	Smeđa
R_f	0,52
LC/MS/MS <i>m/z</i> (M⁺)	266,90
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 9,88 (s, 1H, OH), 8,34 (s, 1H, coum.), 7,91 (dd, <i>J</i> = 8,10, 1,17 Hz, 2H, arom.), 7,68 - 7,71 (m, 1H, arom.), 7,53 - 7,56 (m, 2H, arom.), 7,34 (d, 1H, <i>J</i> = 9,06 Hz, arom.), 7,17 (s, 1H, arom.), 7,15 (d, <i>J</i> = 2,88 Hz, 1H, arom.).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 191,9; 158,2; 154,0; 145,1; 136,1; 133,9; 129,6; 128,7; 126,4; 121,6; 118,7; 117,2; 113,5.

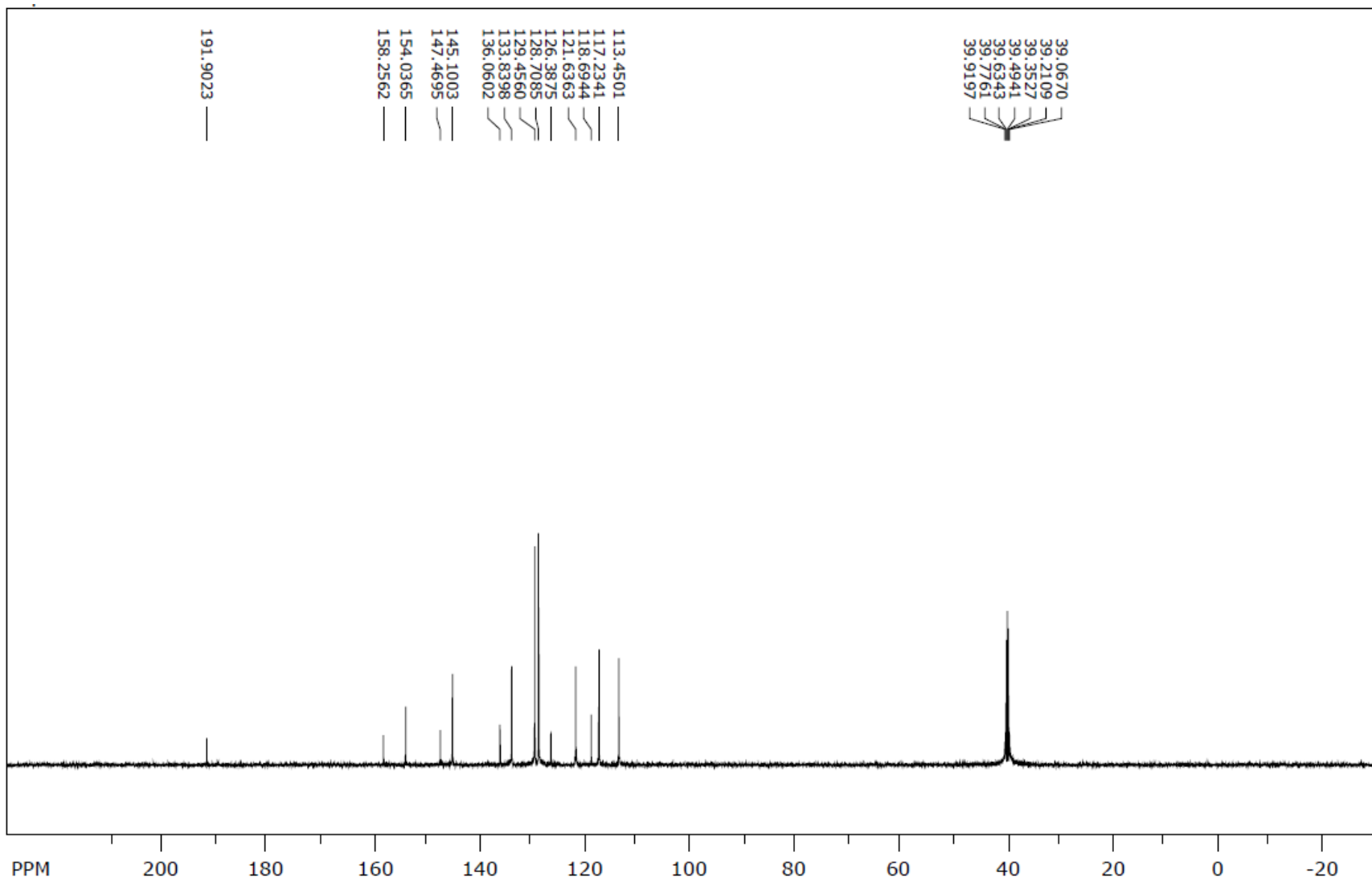
Maseni spektar (3c)



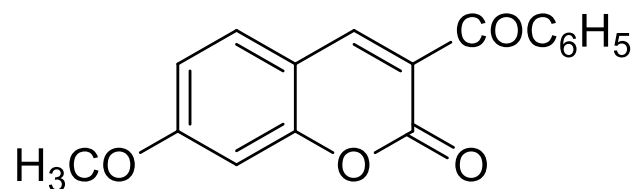
¹H NMR spektr (3c)



¹³C NMR spektr (3c)

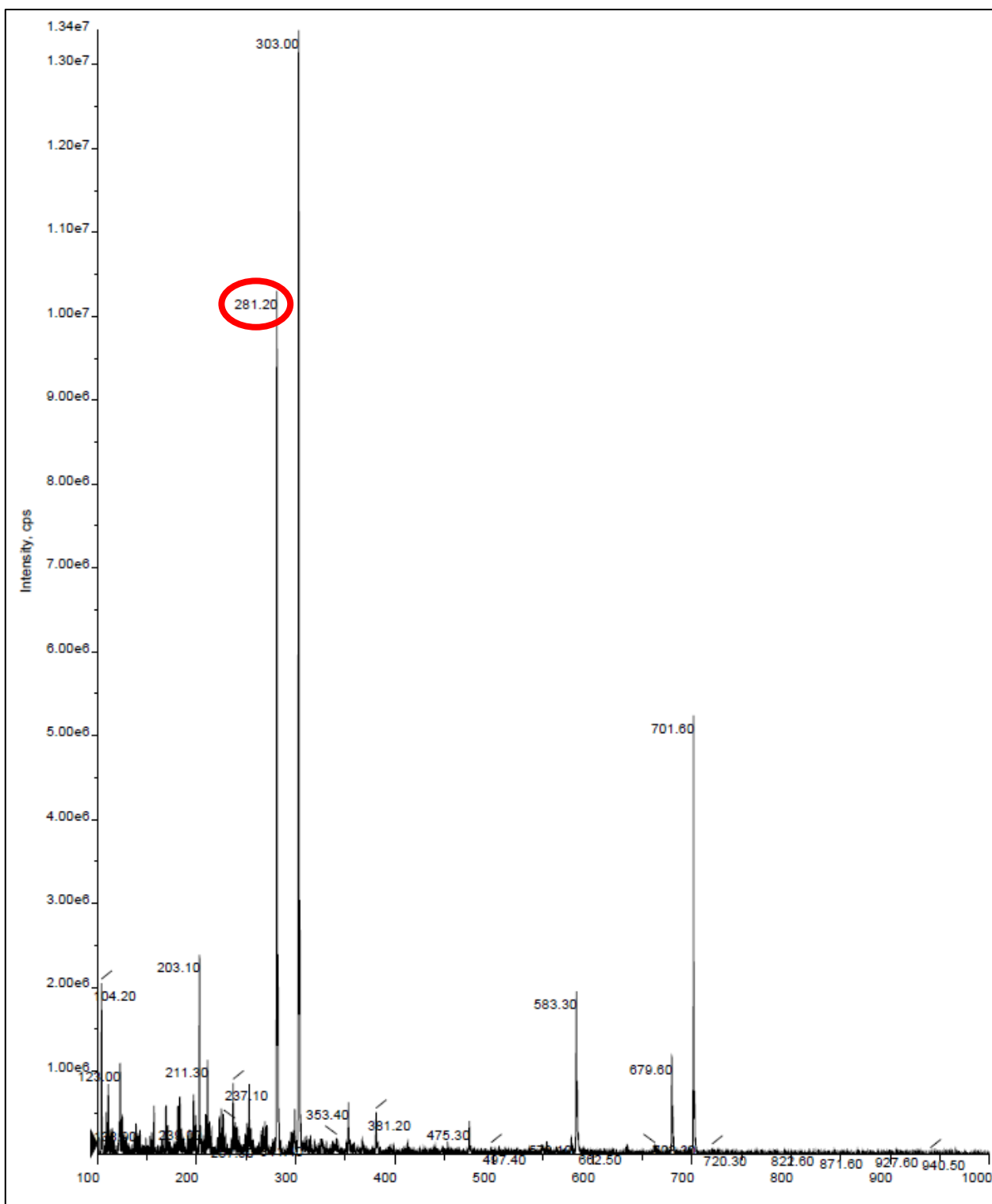


3-benzoil-7-metoksi-2H-kromen-2-on (3d)

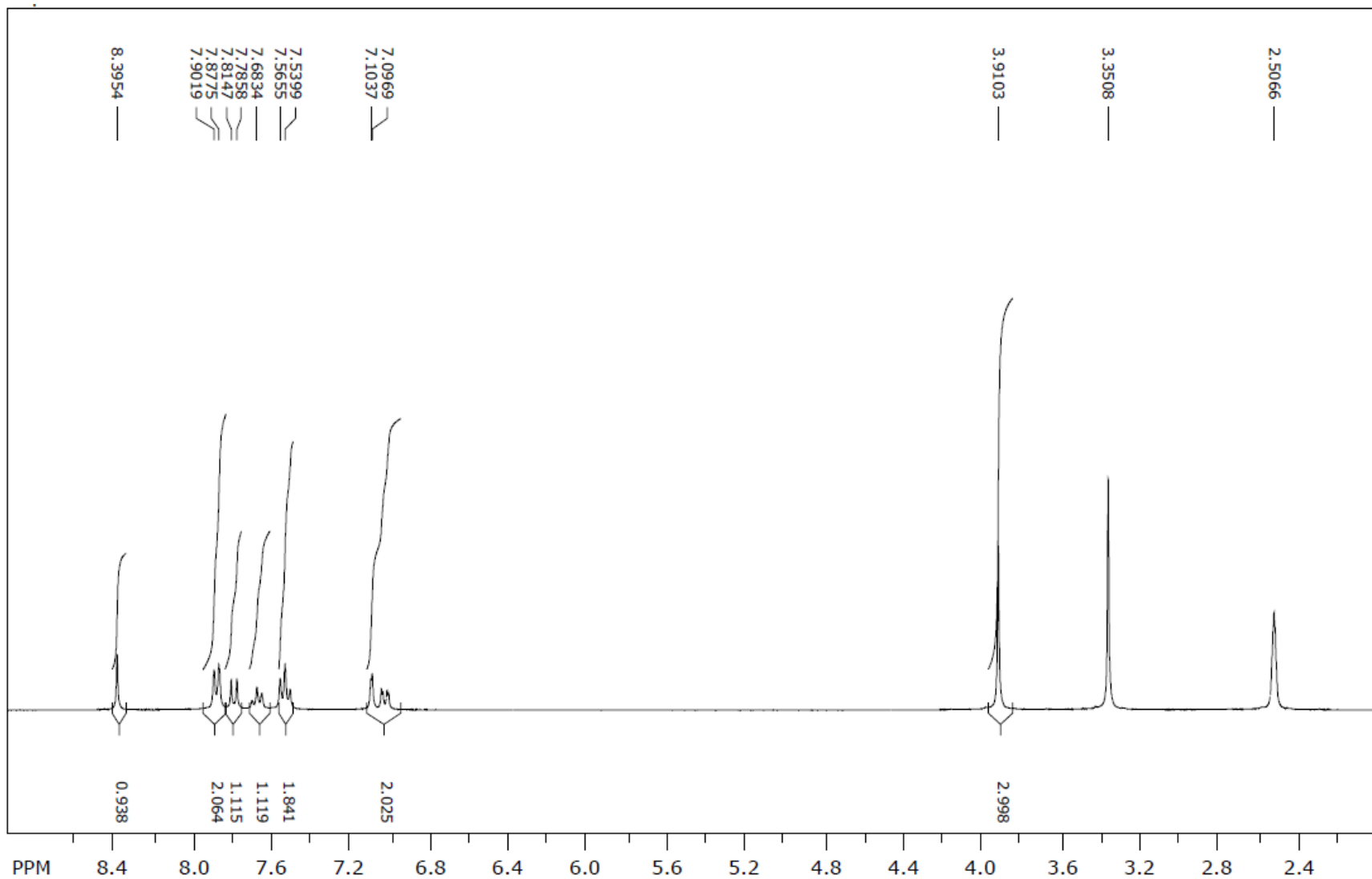


Reaktanti	4-metoksibenzaldehid (1,2 mmol) i etil benzoilacetat (1,2 mmol)
Metoda pročišćavanja	Ispran etanolom
Molekulska masa	280,27 g/mol
Molekulska formula	C ₁₇ H ₁₂ O ₄
Temperatura tališta	140 – 143 °C
Boja kristala	Bijela
R_f	0,75
LC/MS/MS <i>m/z</i> (M⁺)	281,20
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 8,40 (s, 1H, coum.), 7,89 (d, <i>J</i> = 7,32 Hz, 2H, arom.), 7,80 (d, <i>J</i> = 8,67 Hz, 1H, arom.), 7,68 (t, <i>J</i> = 7,29 Hz, 1H, arom.), 7,54 (t, <i>J</i> = 7,58 Hz, 2H, arom.), 7,10 (d, <i>J</i> = 2,04 Hz, 1H, arom.), 7,03 (dd, <i>J</i> = 8,64, 2,24 Hz, 1H, arom.), 3,91 (s, 3H, OCH ₃).
¹³C NMR	(75 MHz, DMSO- <i>d</i> ₆) δ 192,3; 164,6; 158,7; 156,9; 146,7; 137,0; 133,9; 131,8; 130,1; 129,1; 122,7; 113,6; 112,3; 101,1; 56,5.

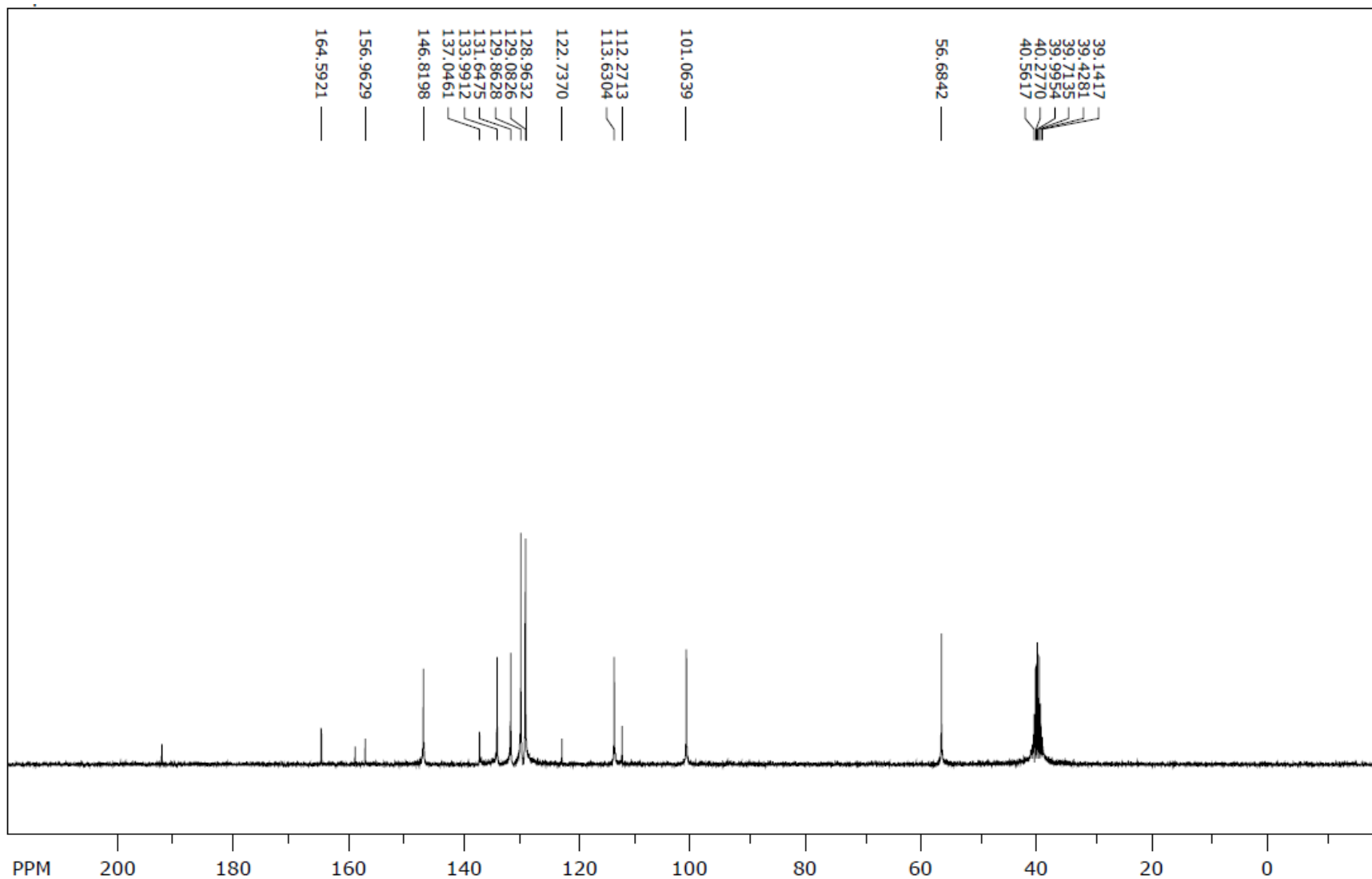
Maseni spektar (3d)



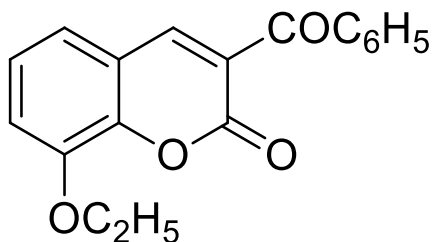
¹H NMR spektr (3d)



¹³C NMR spektr (3d)

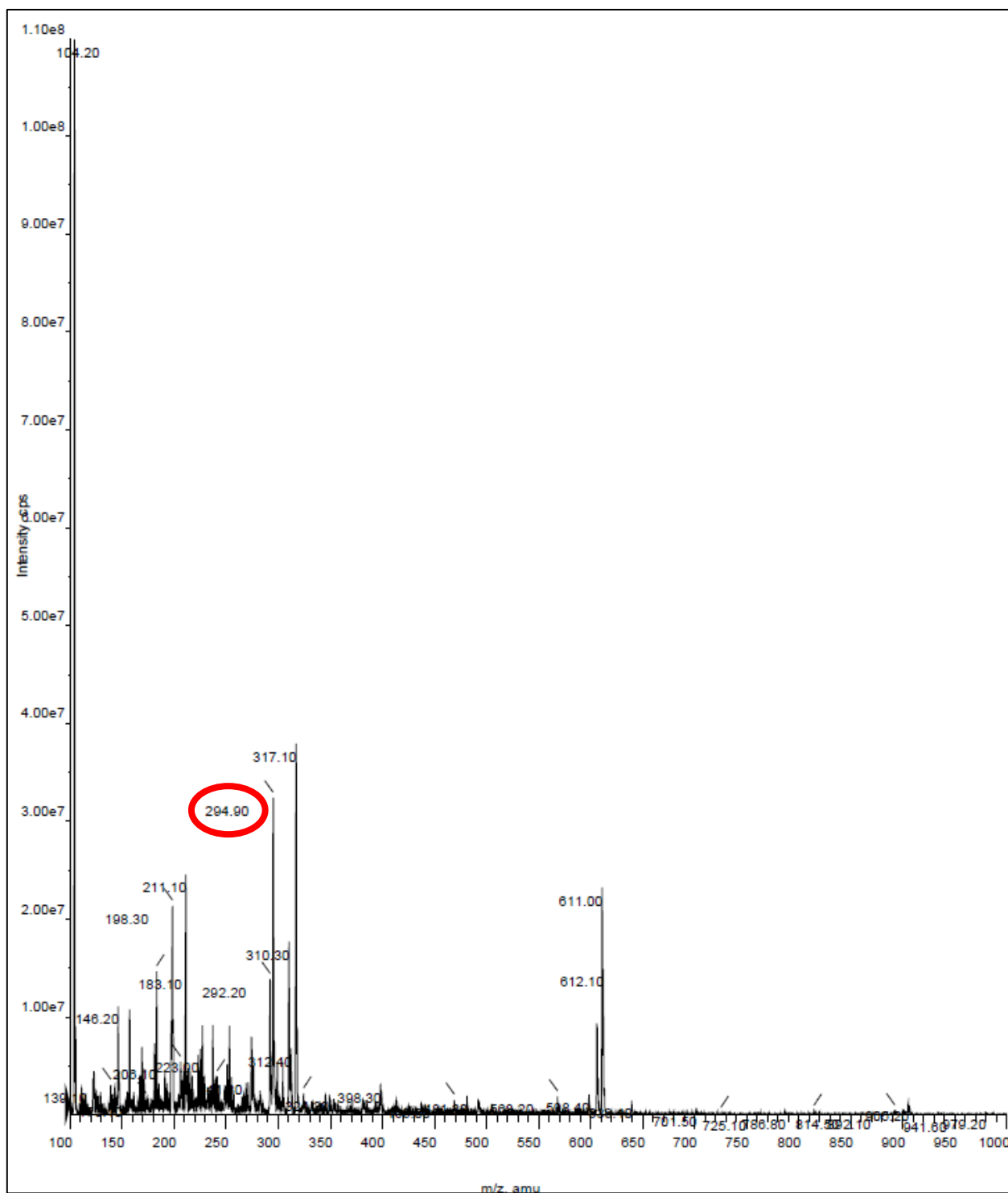


3-benzoil-8-etoksi-2H-kromen-2-on (3e)

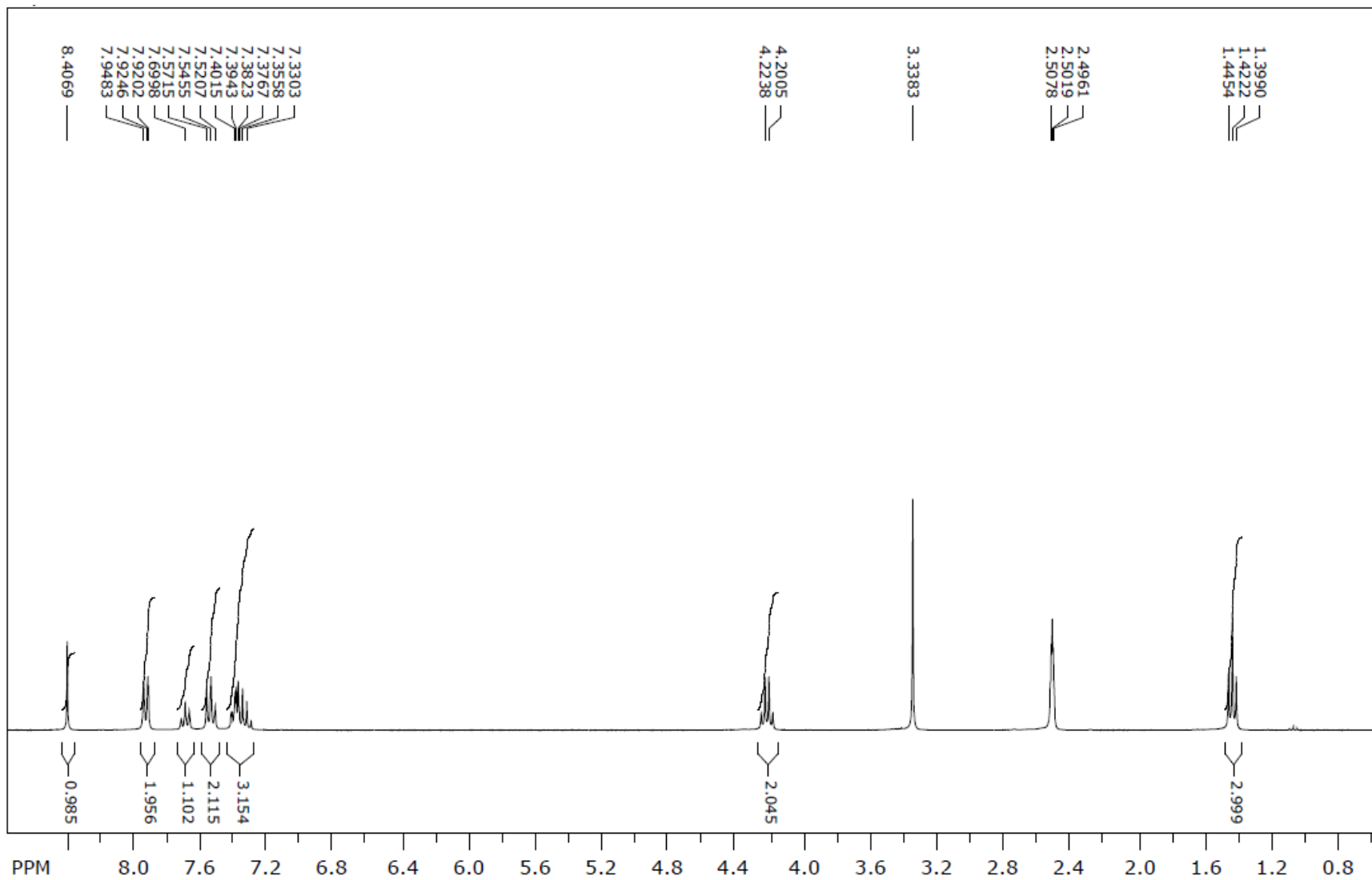


Reaktanti	3-etoksisalicilaldehid (1,2 mmol) i etil benzoilacetat (1,2 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola
Molekulska masa	294,30 g/mol
Molekulska formula	C ₁₈ H ₁₄ O ₄
Temperatura tališta	102-105 °C
Boja kristala	Svijetložuta
R_f	0,79
LC/MS/MS <i>m/z</i> (M⁺)	294,90
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 8,40 (s, 1H, coum.), 7,92 - 7,95 (m, 2H, arom.), 7,67 - 7,72 (m, 1H, arom.), 7,54 (t, <i>J</i> = 7,62 Hz, 2H, arom.), 7,30 - 7,42 (m, 3H, arom.), 4,21 (q, <i>J</i> = 6,96 Hz, 2H, CH ₂ CH ₃), 1,42 (t, <i>J</i> = 6,96 Hz, 3H, CH ₂ CH ₃).
¹³C NMR	(75 MHz, DMSO- <i>d</i> ₆) δ 192,2; 158,3; 146,1; 136,5; 134,4; 130,1; 130,0; 129,2; 126,9; 125,3; 121,2; 119,4; 117,0; 64,9; 15,1.

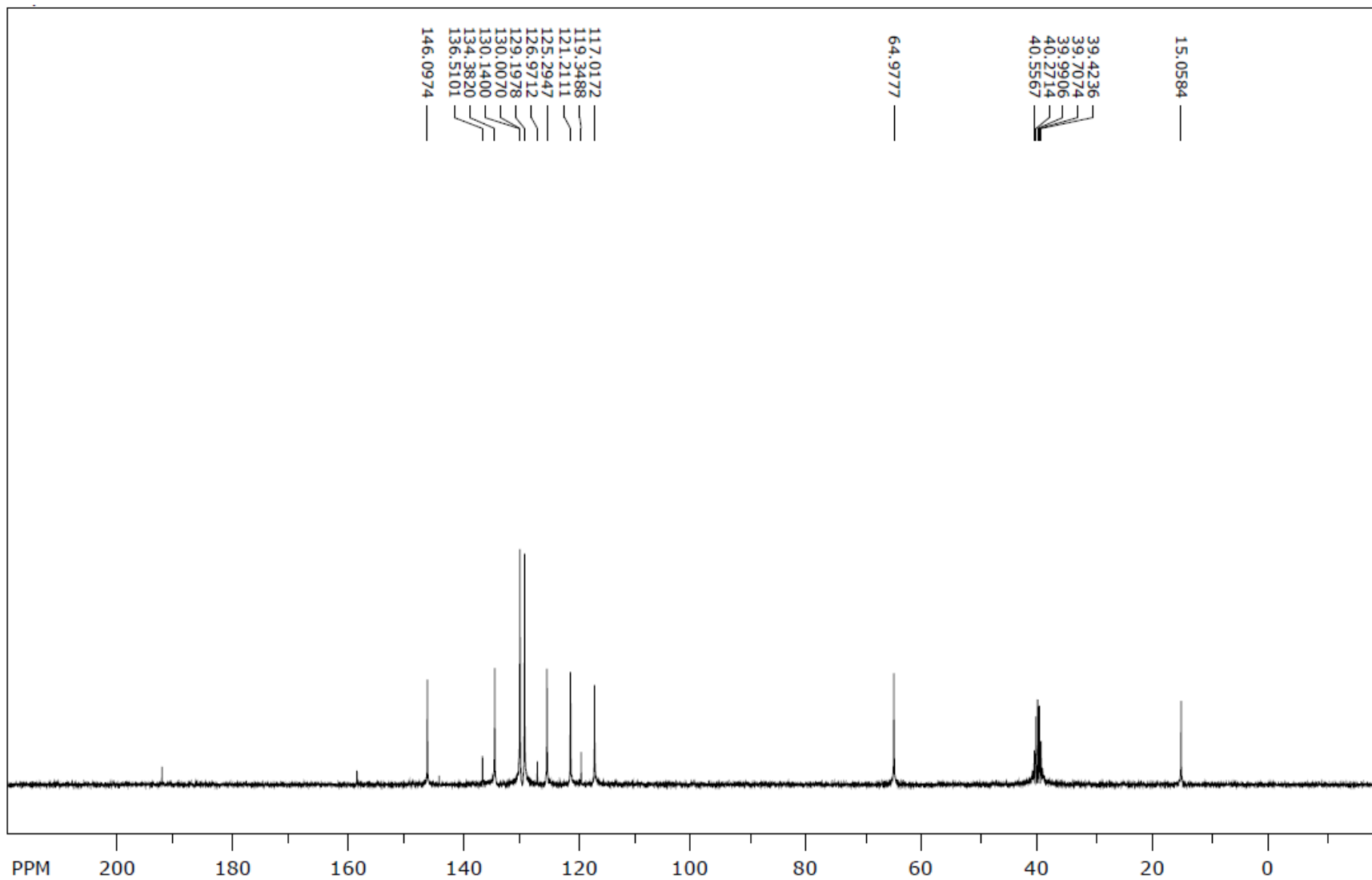
Maseni spektar (3e)



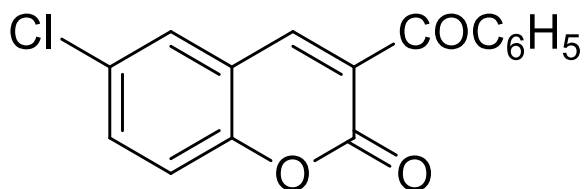
¹H NMR spektr (3e)



¹³C NMR spektr (3e)

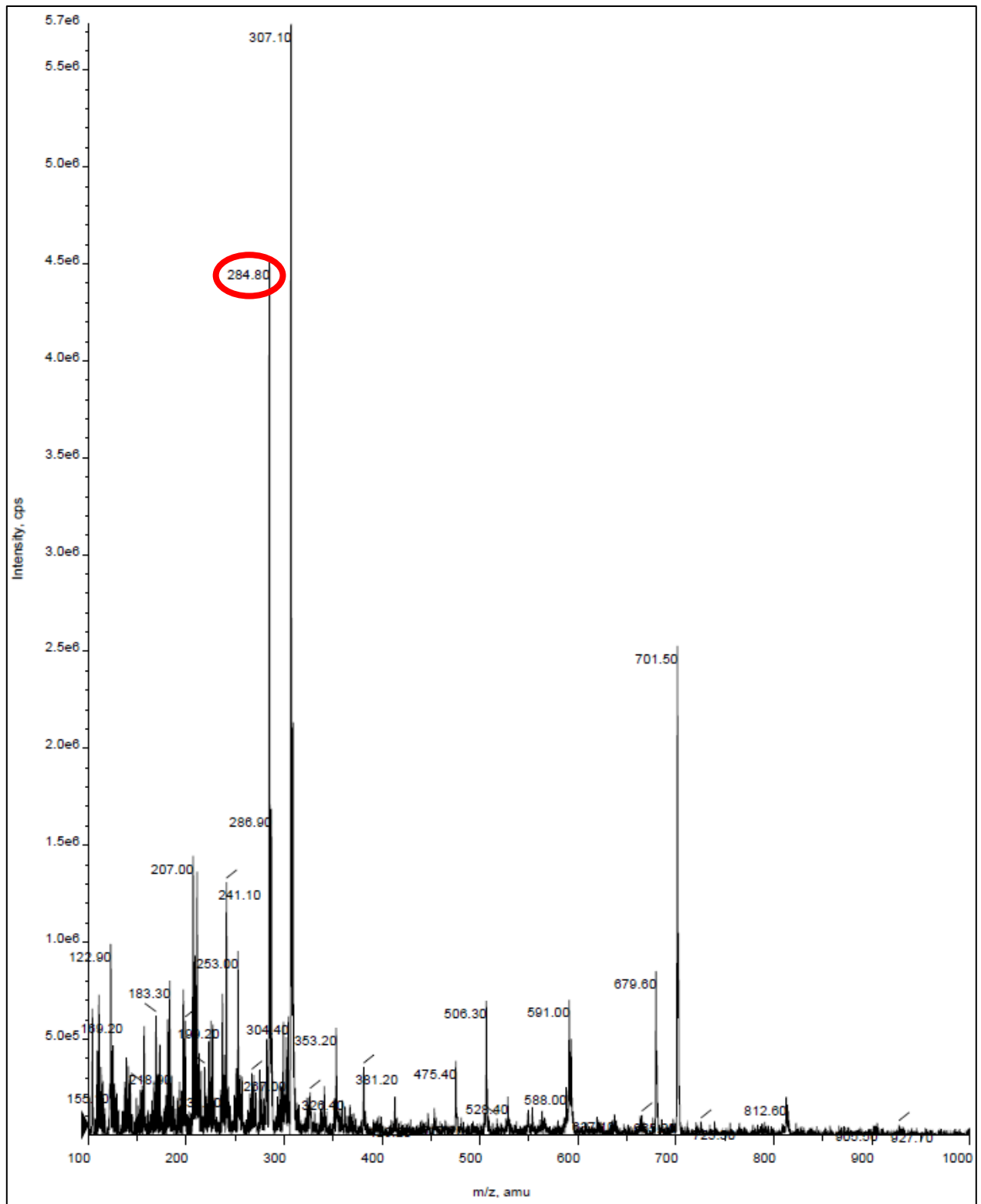


3-benzoil-6-klor-2H-kromen-2-on (3f)

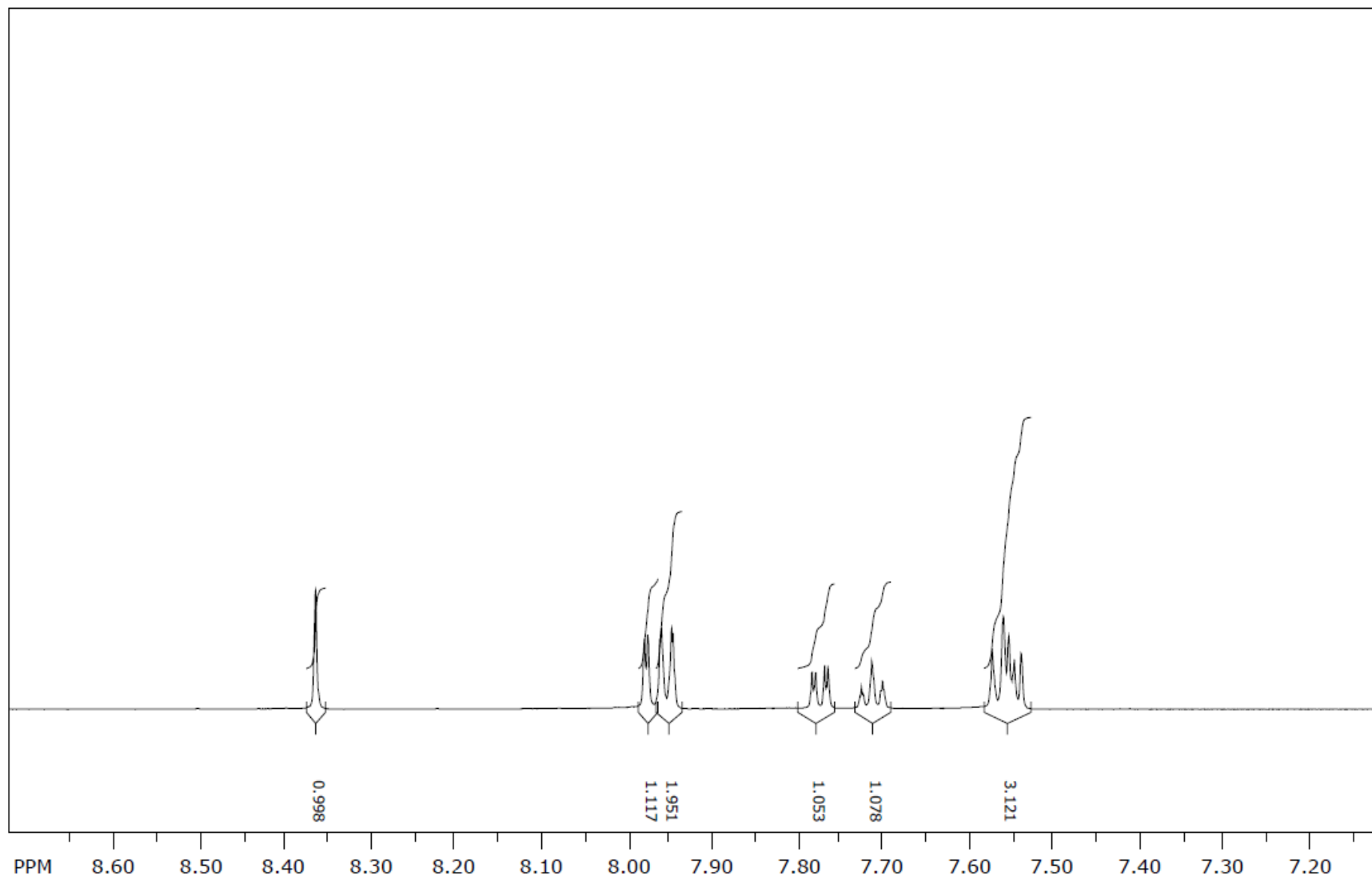


Reaktanti	5-klorosalicilaldehid (1,2 mmol) i etil benzoilacetat (1,2 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola
Molekulska masa	284,69 g/mol
Molekulska formula	C ₁₆ H ₉ ClO ₃
Temperatura tališta	150 -155 °C
Boja kristala	Bijela
R_f	0,88
LC/MS/MS m/z (M⁺)	284,90
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,37 (s, 1H, coum.), 7,98 (d, <i>J</i> = 2,52 Hz 1H, arom.), 7,95 (dd, <i>J</i> = 8,10, 1,02 Hz, 2H, arom.), 7,77 (dd, <i>J</i> = 8,94, 2,55 Hz, 1H, arom.), 7,70 – 7,72 (m, 1H, arom.), 7,54 – 7,57 (m, 3H, arom.).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 191,3; 157,6; 152,8; 143,9; 135,8; 134,0; 132,9; 129,6; 128,7; 128,6; 127,4; 119,6.

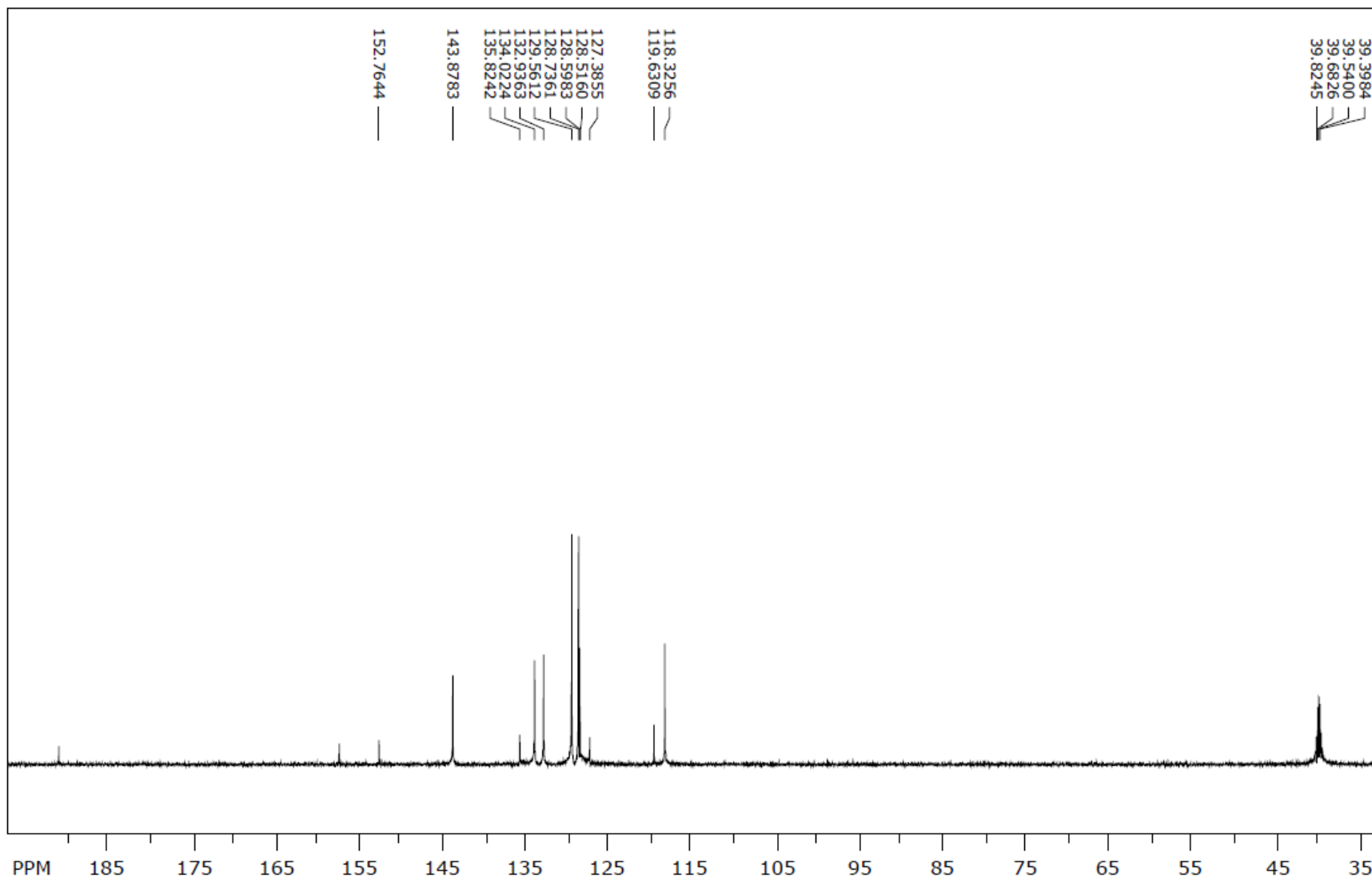
Maseni spektar (3f)



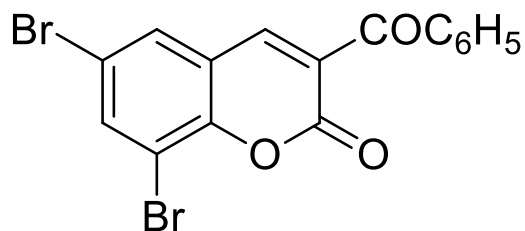
¹H NMR spektr (3f)



¹³C NMR spektr (3f)

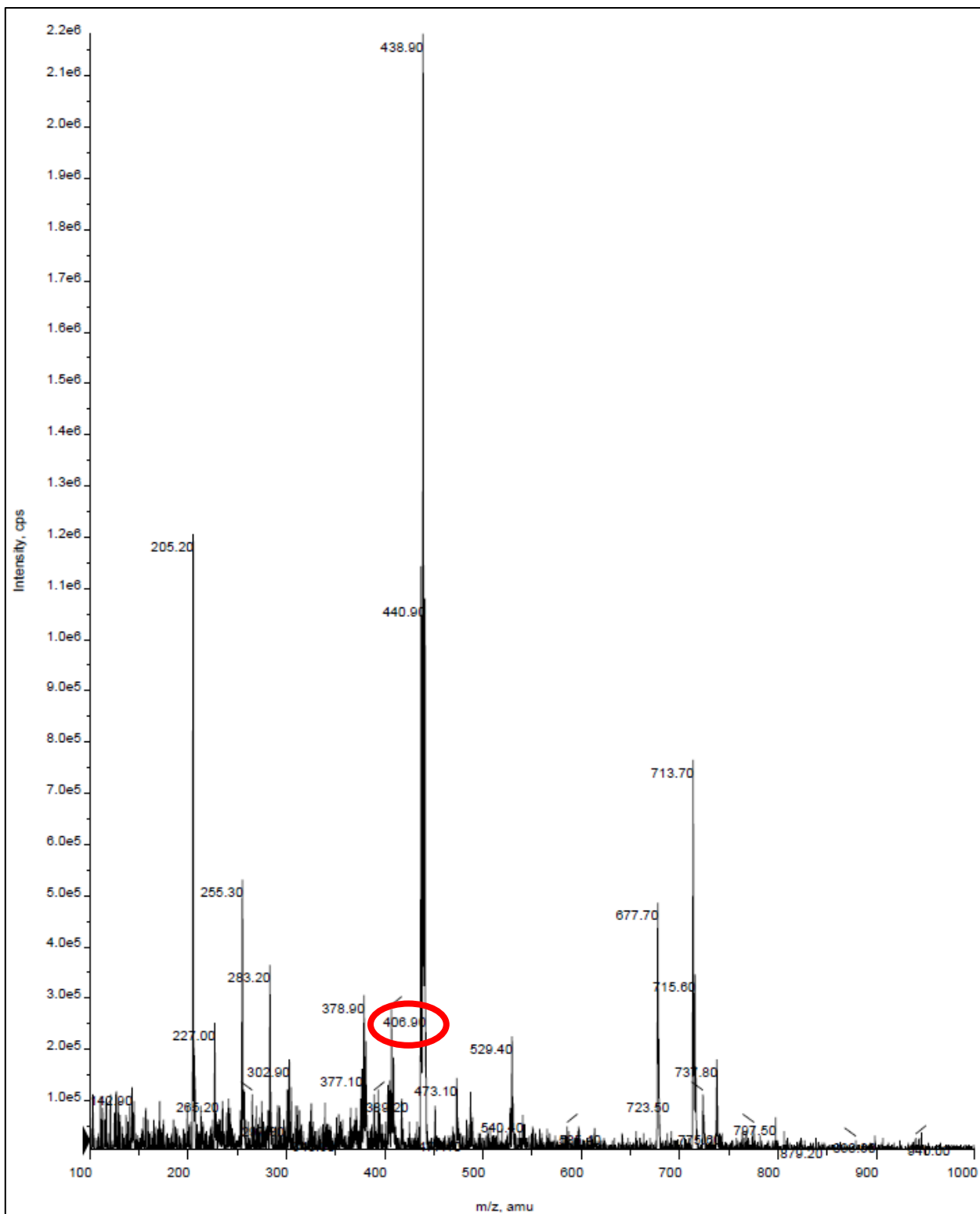


3-benzoil-6,8-dibrom-2H-kromen-2-on (3g)

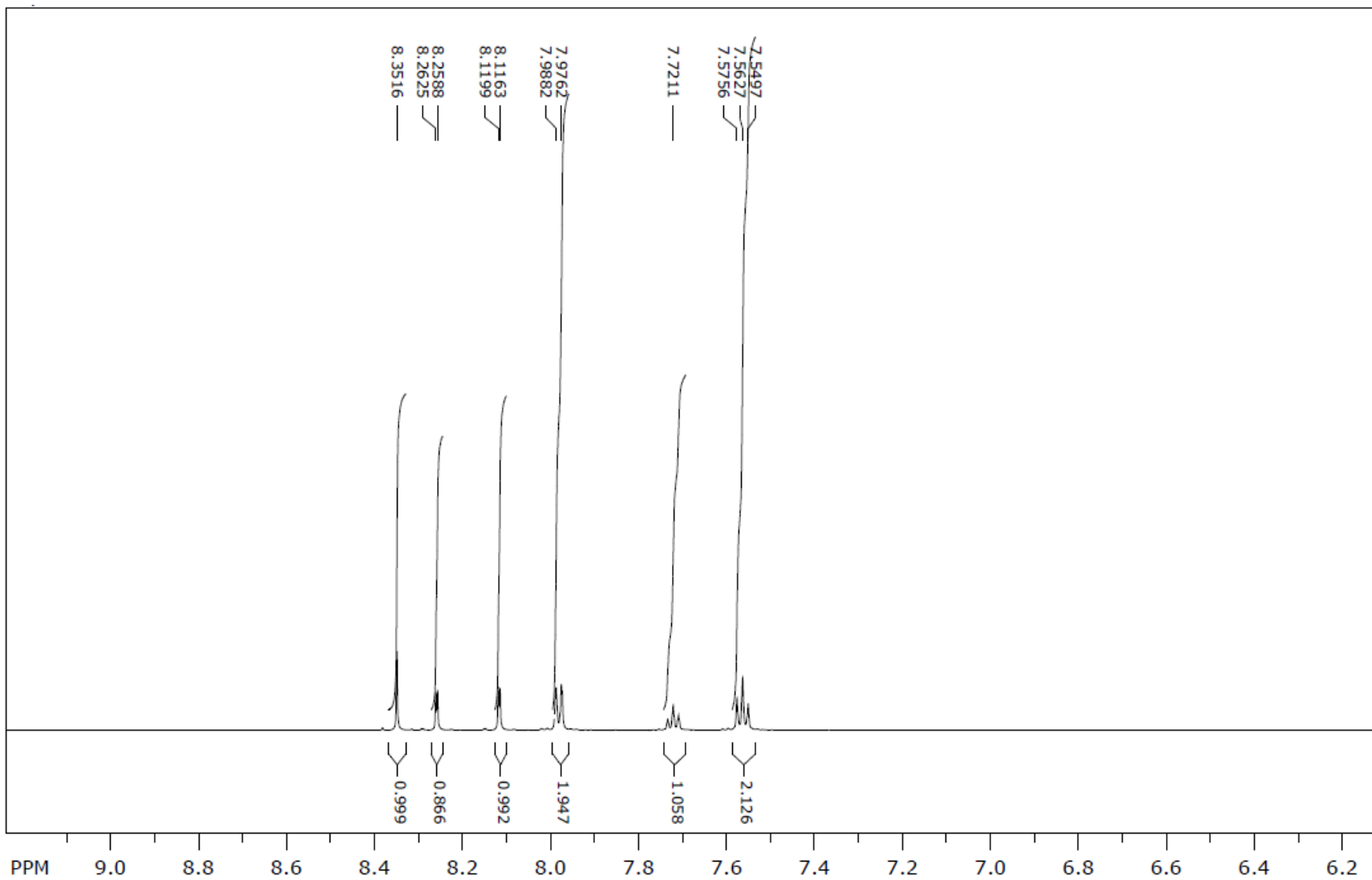


Reaktanti	3,5-dibromsalicilaldehid (1,2 mmol) i etil benzoilacetat (1,2 mmol)
Metoda pročišćavanja	Ispran etanolom
Molekulska masa	408,04 g/mol
Molekulska formula	C ₁₆ H ₈ Br ₂ O ₃
Temperatura tališta	200 – 202 °C
Boja kristala	Bijela
R_f	0,88
LC/MS/MS <i>m/z</i> (M⁻)	406,90
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,35 (s, 1H, coum.), 8,26 (d, <i>J</i> = 2,22 Hz, 1H, arom.), 8,12 (d, <i>J</i> = 2,16 Hz, 1H, arom.), 7,98 (d, <i>J</i> = 7,20 Hz, 2H, arom.), 7,72 (t, <i>J</i> = 7,41 Hz, 1H, arom.), 7,56 (t, <i>J</i> = 7,77 Hz, 1H, arom.).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 191,0; 157,0; 150,1; 143,6; 137,6; 135,7; 134,2; 131,2; 139,7; 128,8; 127,9; 121,2; 116,3; 110,3.

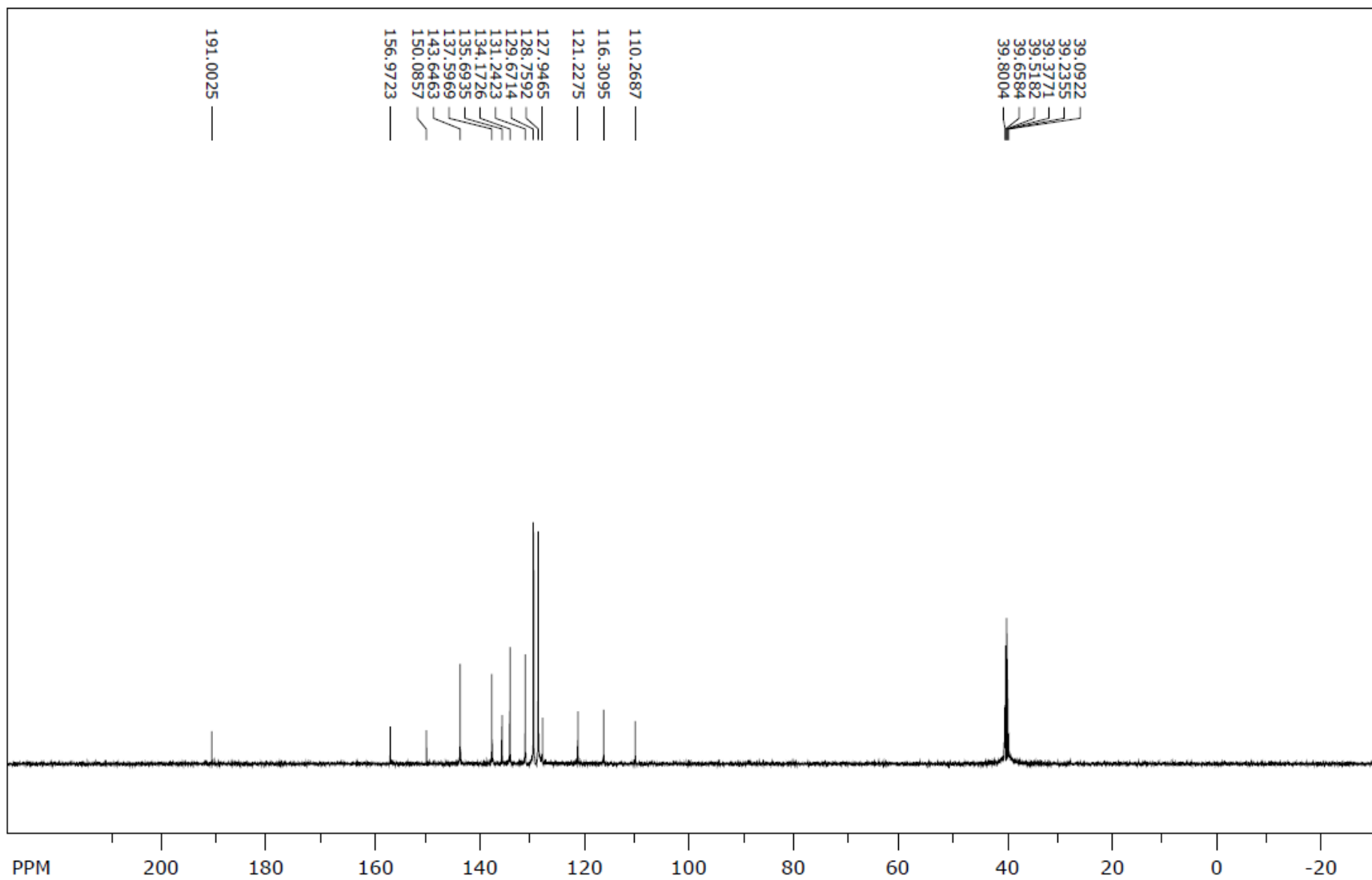
Maseni spektar (3g)



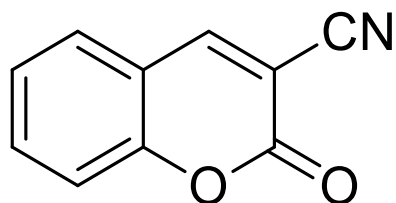
¹H NMR spektr (3g)



¹³C NMR spektr (3g)

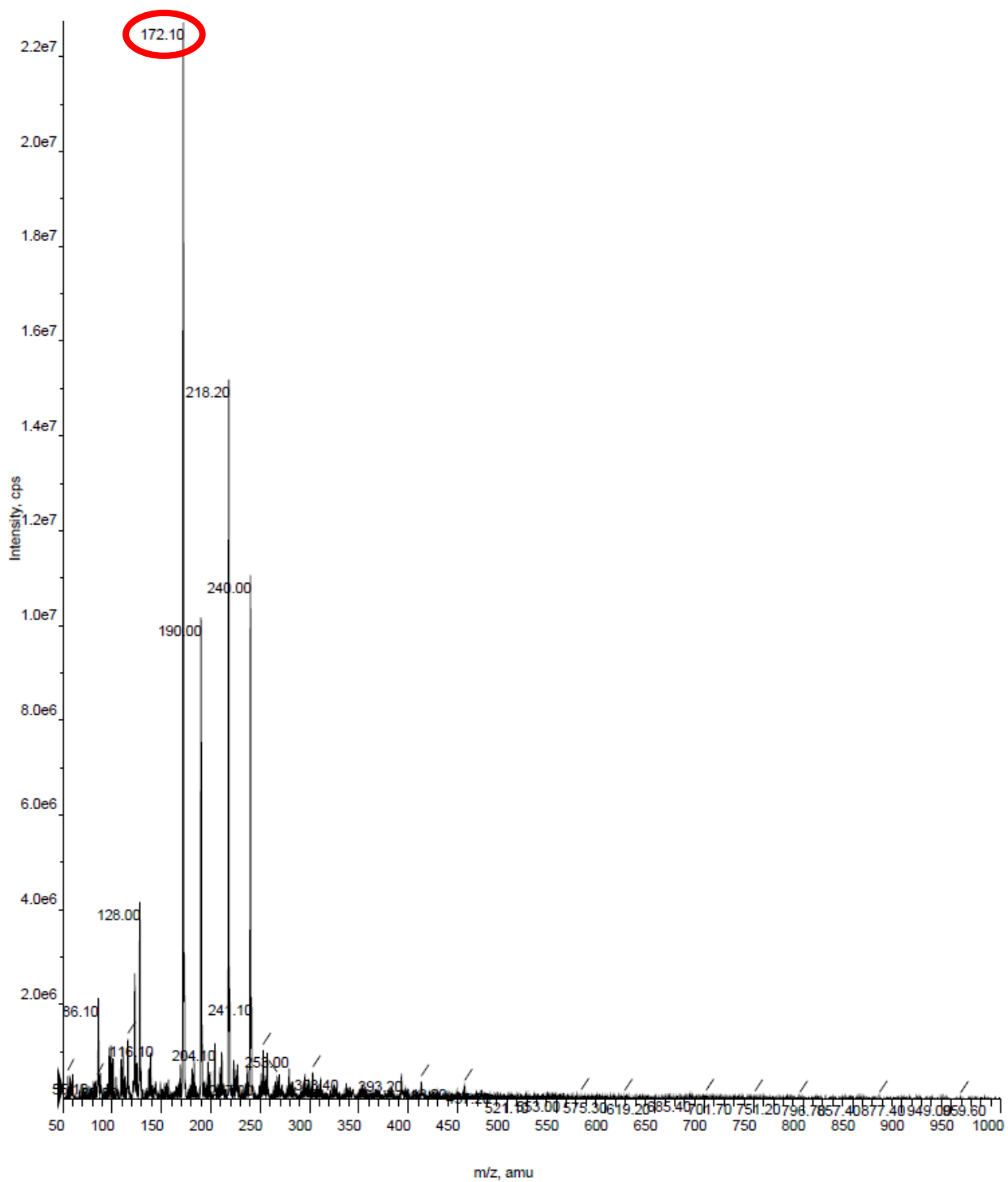


2-okso-2H-kromen-3-karbonitril (4a)

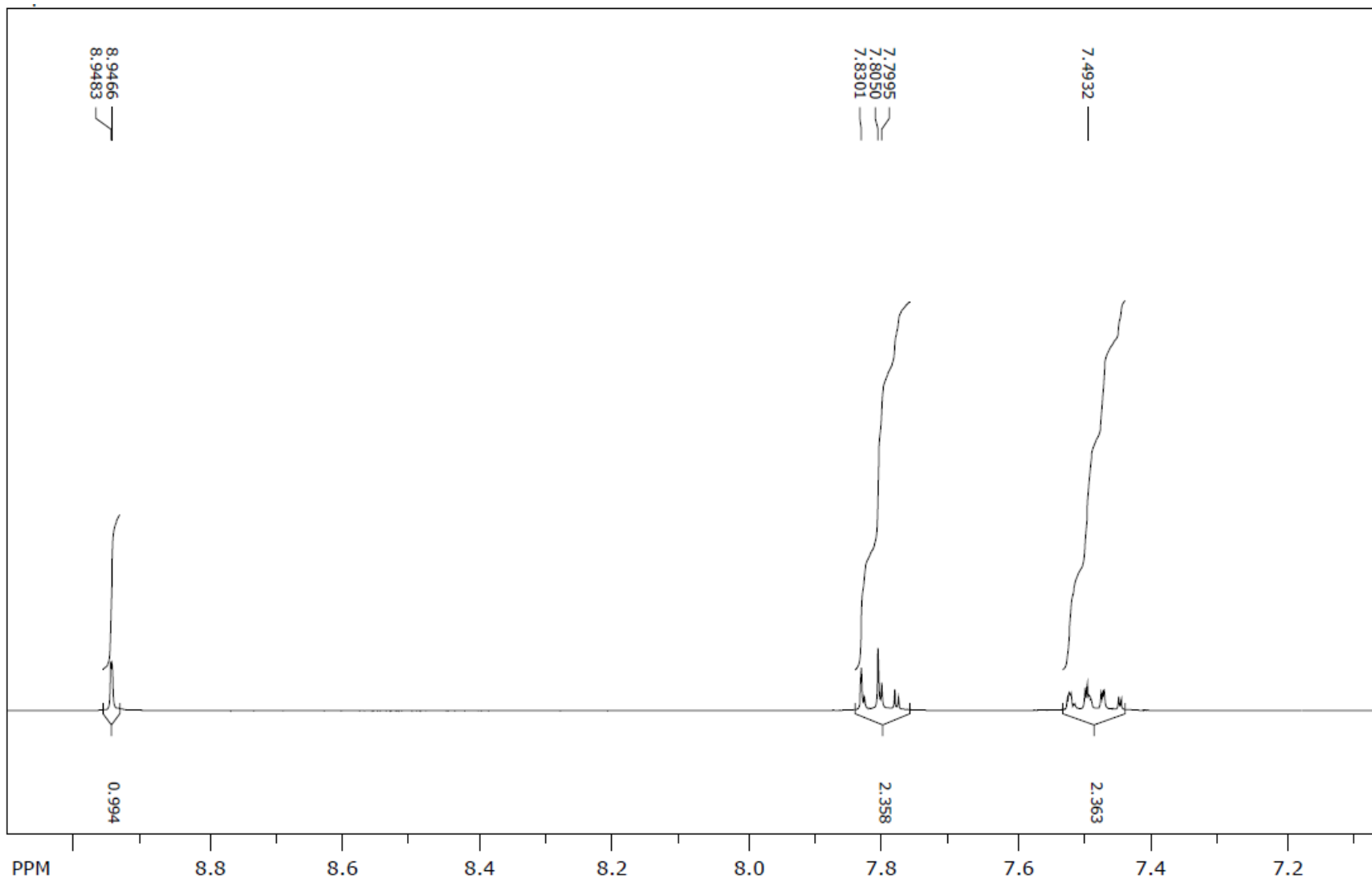


Reaktanti	Salicilaldehid (10 mmol) i etil cijanoacetat (10 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola
Molekulska masa	171,15 g/mol
Molekulska formula	C ₁₀ H ₅ NO ₂
Temperatura tališta	181 – 182 °C (lit. 175 – 176 °C, He i sur., 2014; 183 – 185 °C, Valizadeh i sur., 2011; 184 – 186 °C, Keshavarzipour i Tavakol, 2016)
Boja kristala	Žuta
R_f	0,42
LC/MS/MS <i>m/z</i> (M⁺)	172,10
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 8,95 (s, 1H, coum.), 7,77 - 7,83 (m, 2H, arom.), 7,44 – 7,52 (m, 2H, arom.).
¹³C NMR	(75 MHz, DMSO- <i>d</i> ₆) δ 157,3; 154,5; 135,9; 130,5; 125,9; 117,9; 117,3; 115,1; 102,6.

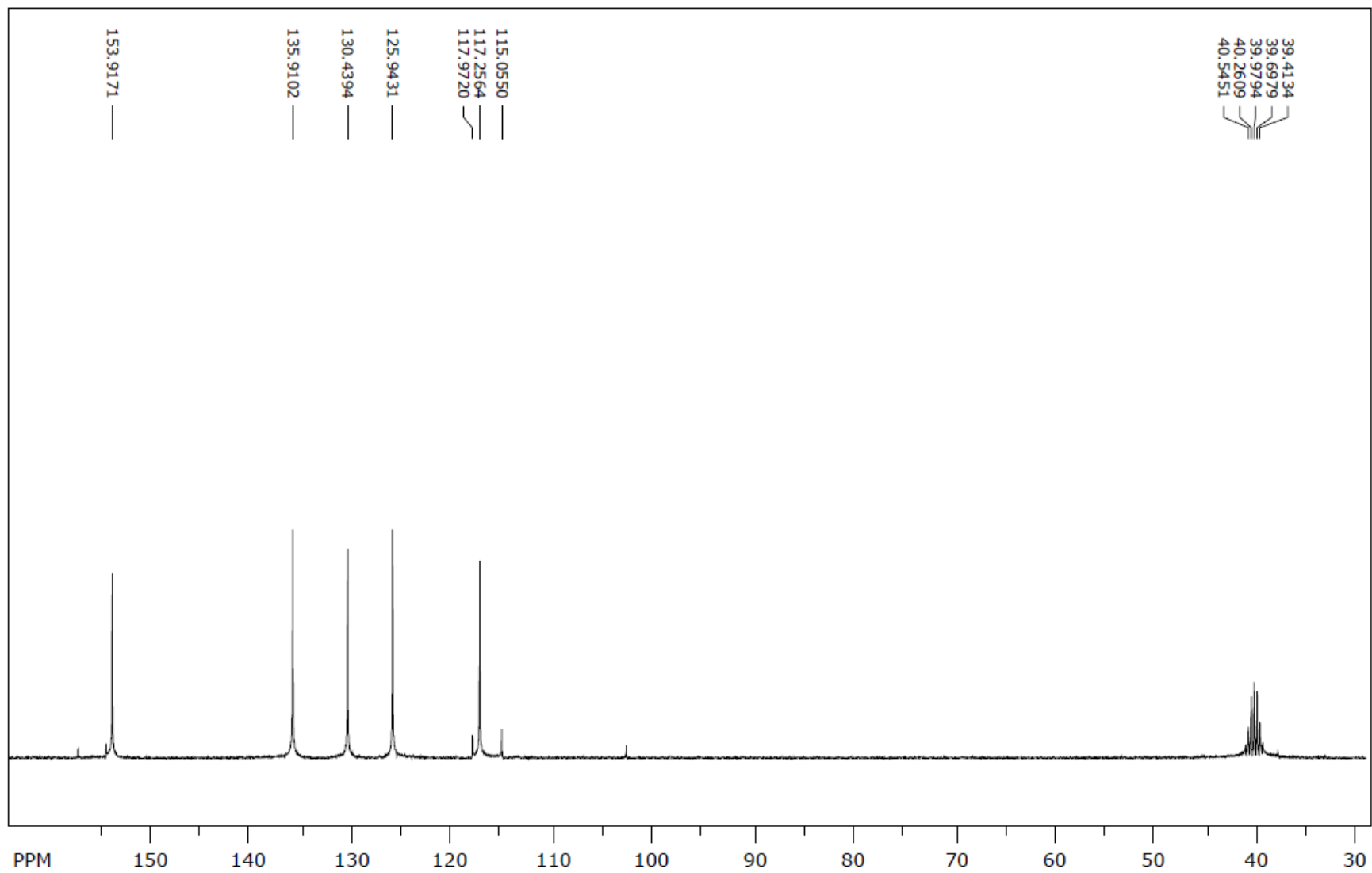
Maseni spektar (4a)



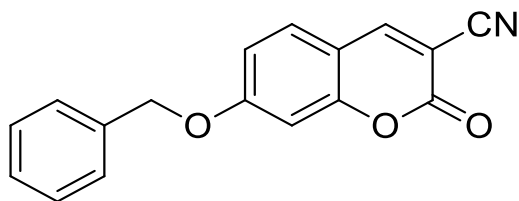
¹H NMR spektr (4a)



¹³C NMR spektr (4a)

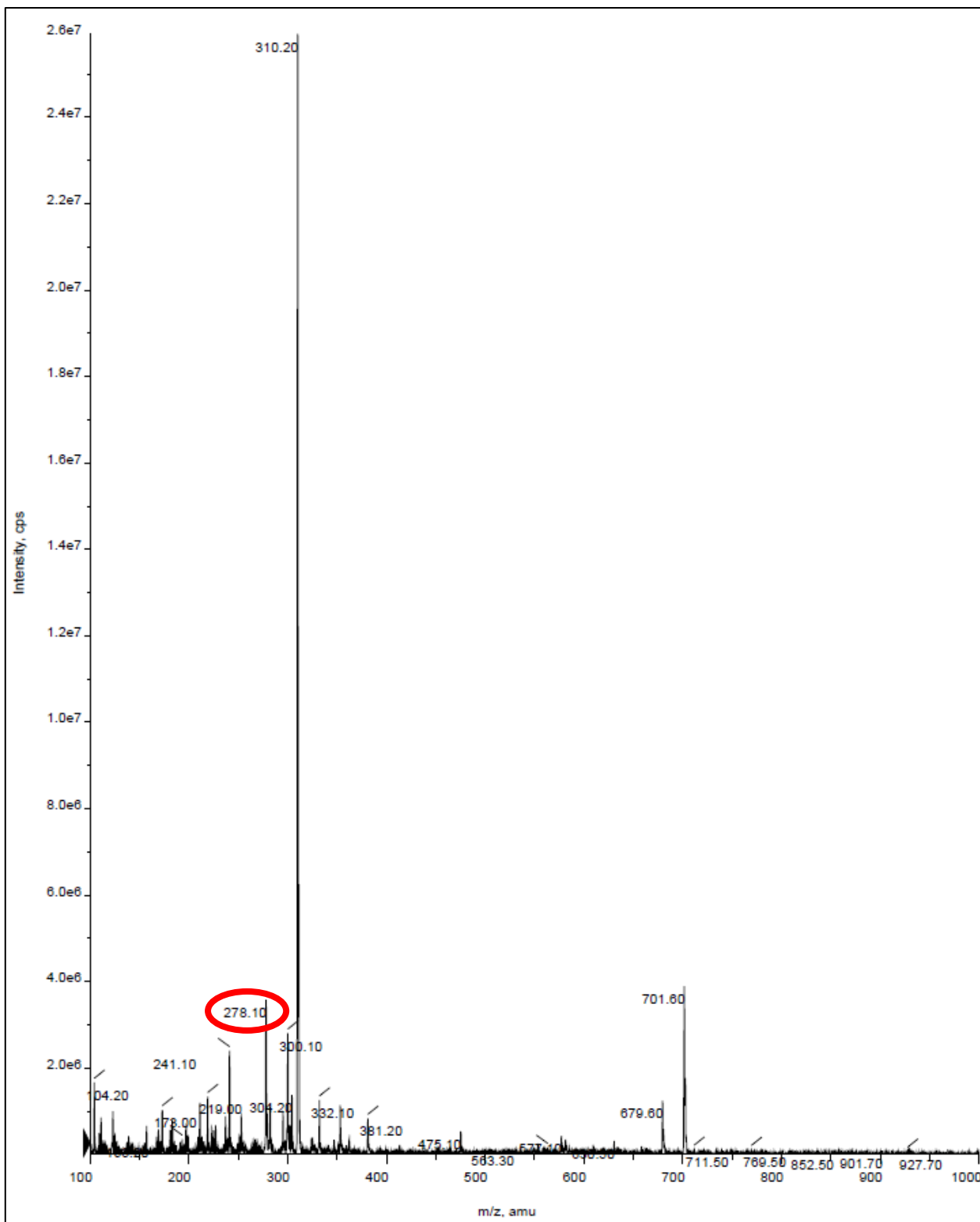


7-(benziloksi)-2-okso-2H-kromen-3-karbonitril (4b)

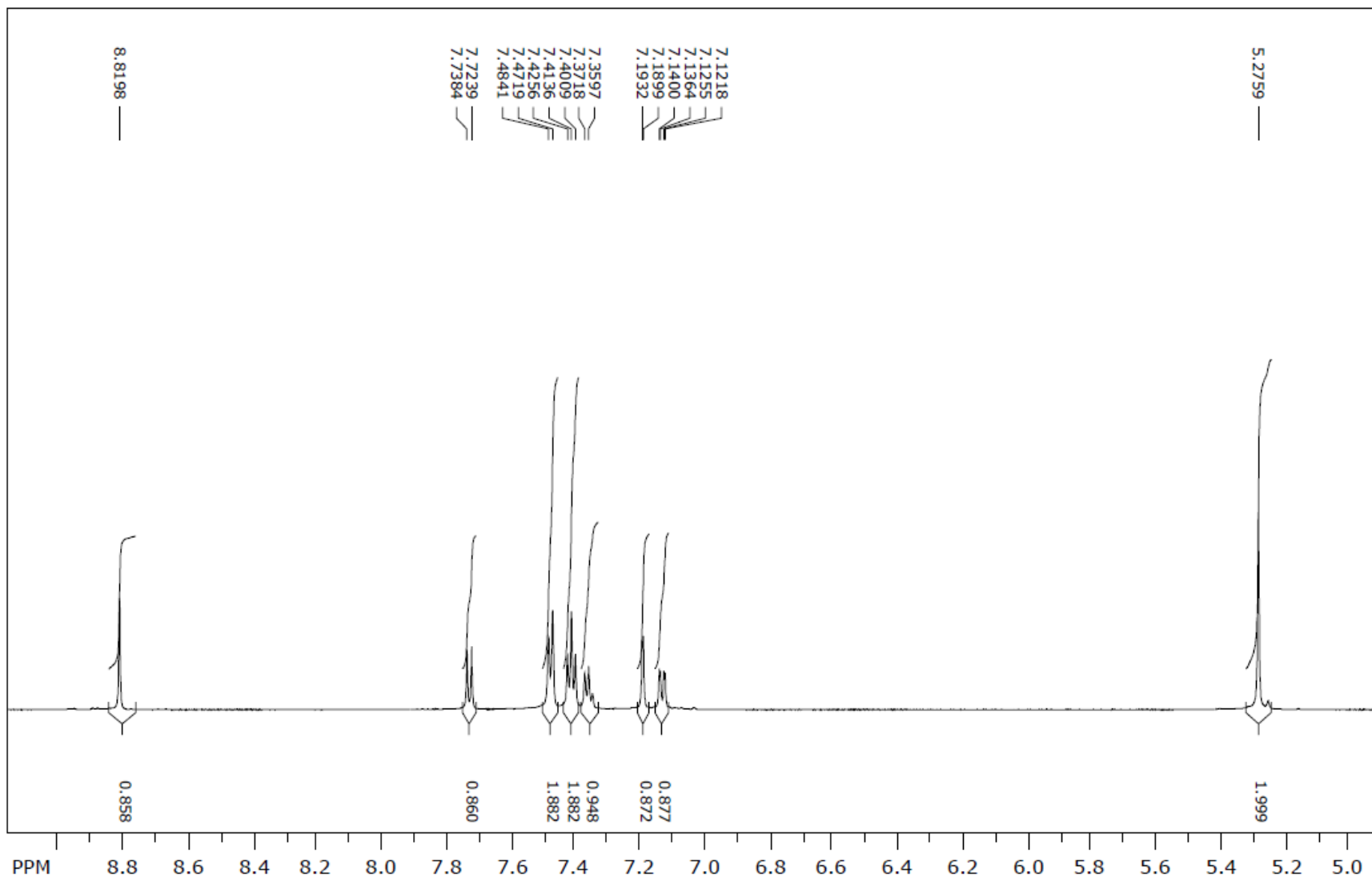


Reaktanti	4-(benziloksi)salicilaldehid (0,6 mmol) i etil cijanoacetat (0,6 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola
Molekulska masa	277,27 g/mol
Molekulska formula	C ₁₇ H ₁₁ NO ₃
Temperatura tališta	174 – 176 °C
Boja kristala	Žuta
R_f	0,88
LC/MS/MS <i>m/z</i> (M⁺)	278,10
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,82 (s, 1H, coum.), 7,73 (d, <i>J</i> = 8,70 Hz, 1H, arom.), 7,48 (d, <i>J</i> = 7,32 Hz, 2H, arom.), 7,41 (t, <i>J</i> = 7,41 Hz, 2H, arom.), 7,36 (t, <i>J</i> = 7,26 Hz, 1H, arom.), 7,19 (d, <i>J</i> = 1,98 Hz, 1H, arom.), 7,13 (dd, 1H, <i>J</i> = 8,70, 2,19 Hz, arom.), 5,28 (s, 2H, -CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 164,4; 157,3; 156,4; 153,1; 135,8; 131,3; 128,7; 128,2; 127,9; 114,9; 114,4; 111,4; 101,9; 97,6; 70,4.

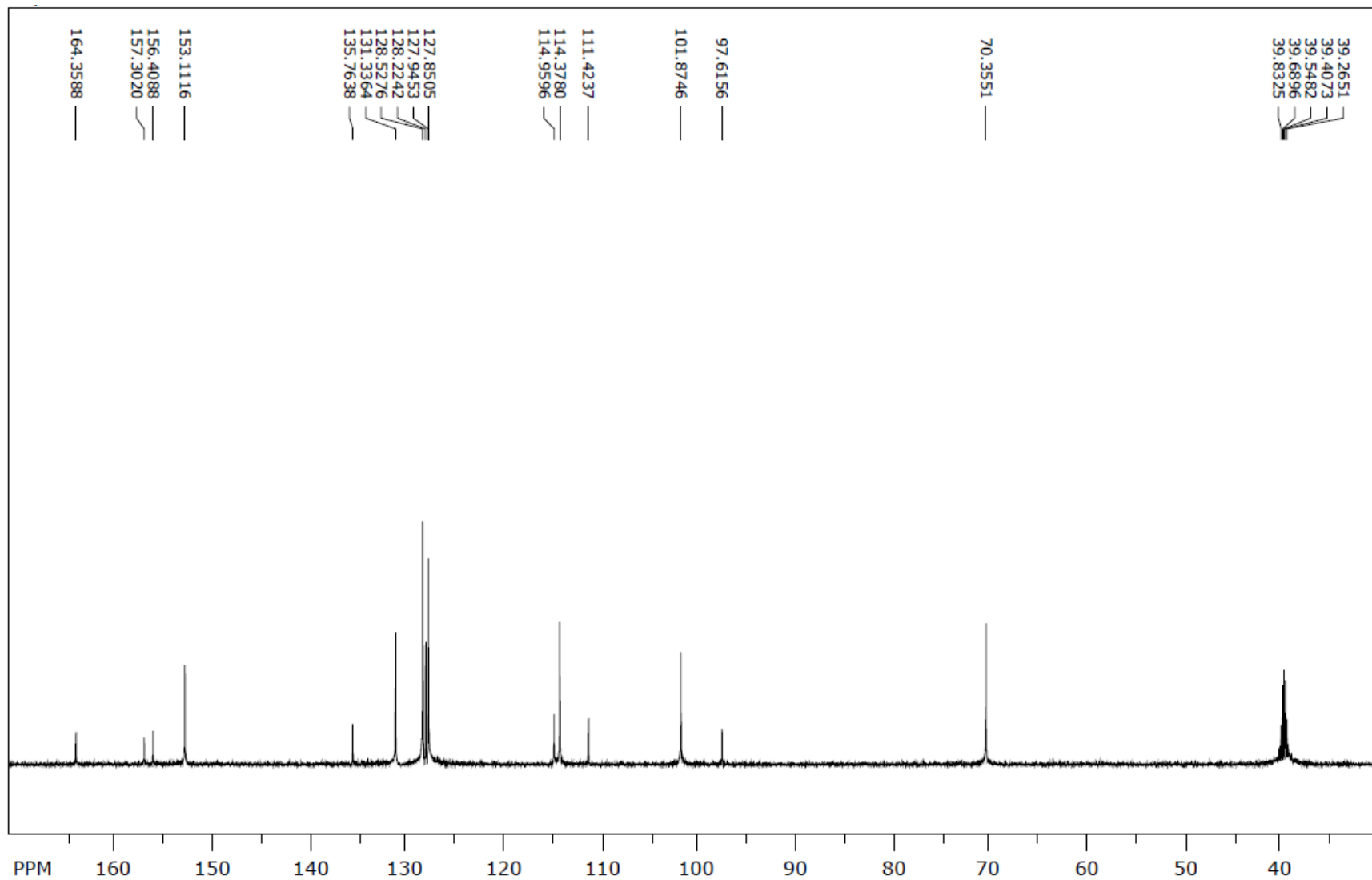
Maseni spektar (4b)



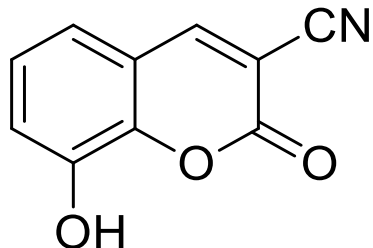
¹H NMR spektr (4b)



¹³C NMR spektr (4b)

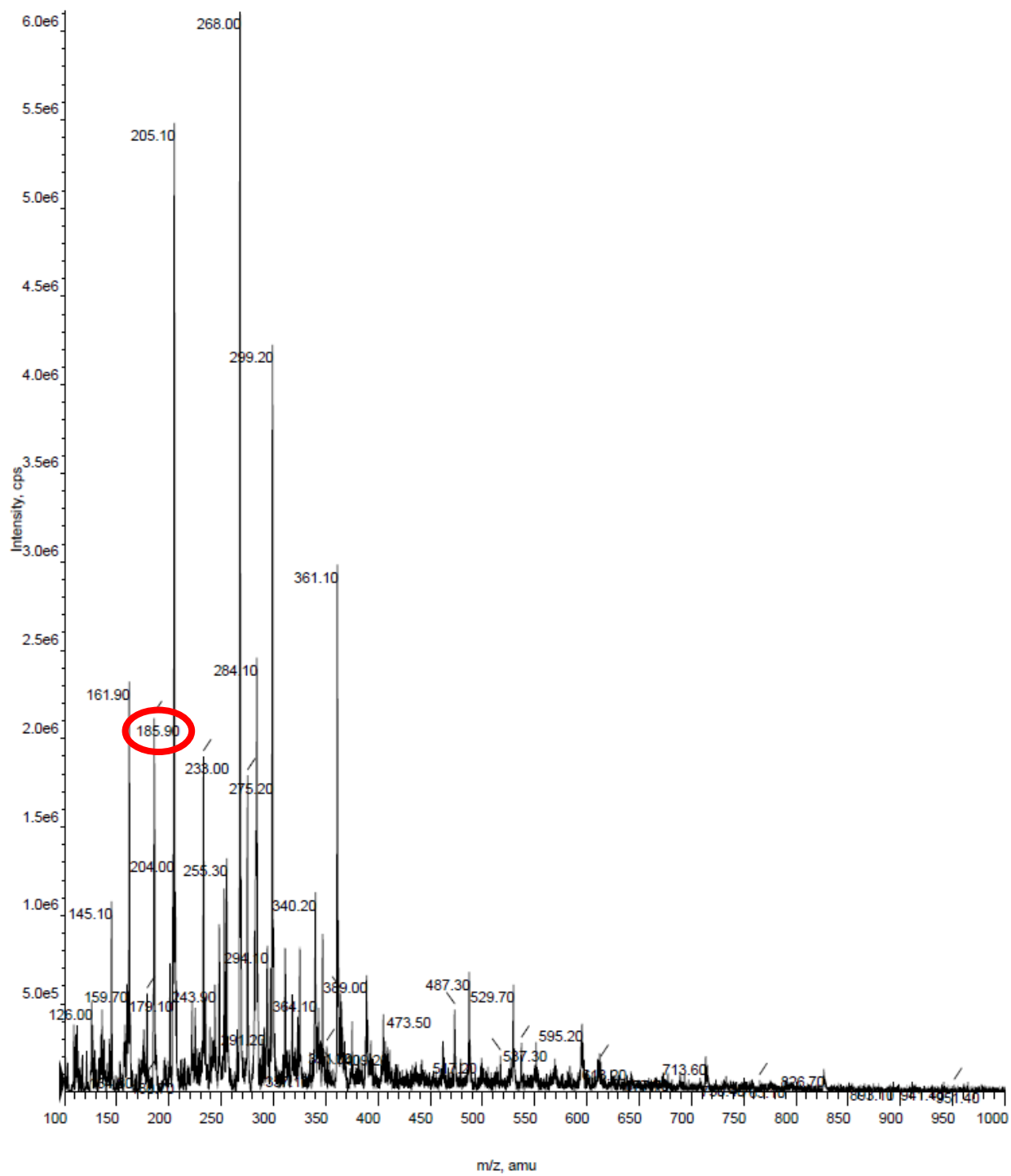


8-hidroksi-2-okso-2H-kromen-3-karbonitril (4c)

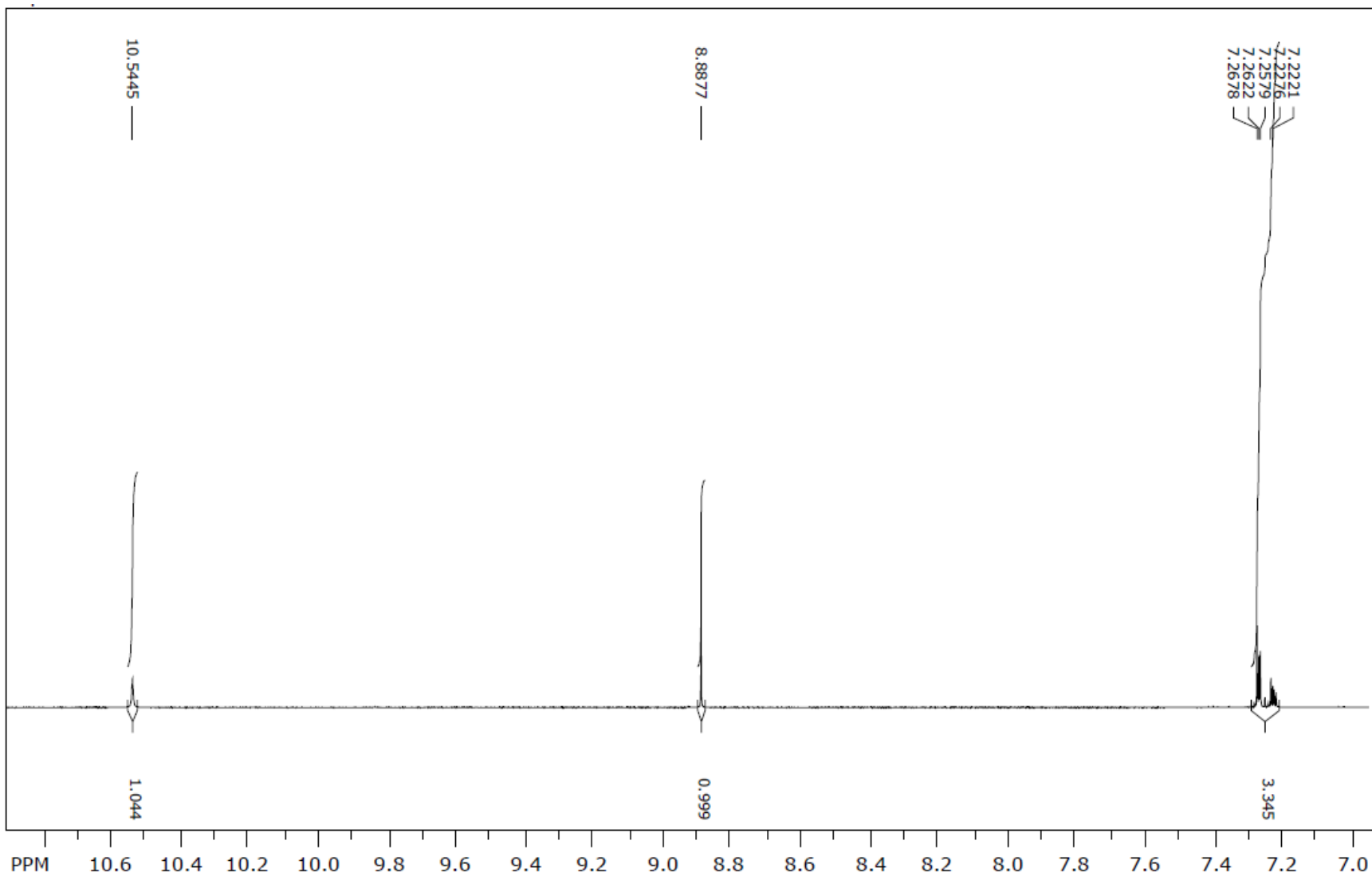


Reaktanti	2,3-dihidroksibenzaldehid (10 mmol) i etil cijanoacetat (10 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola
Molekulska masa	187,15 g/mol
Molekulska formula	C ₁₀ H ₅ NO ₃
Temperatura tališta	228 – 230 °C (lit. 228 – 230 °C, Valizadeh i sur., 2011)
Boja kristala	Tamno smeđa
R_f	0,69
LC/MS/MS m/z (M-)	185,90
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 10,55 (s, 1H, OH), 8,89 (s, 1H, arom.), 7,26 (t, <i>J</i> = 3,36, 2,58 Hz, 2H, arom.), 7,21 – 7,23 (m, 1H, arom.).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 156,8; 153,9; 144,8; 142,6; 125,4; 121,6; 119,8; 118,4; 114,7; 101,9.

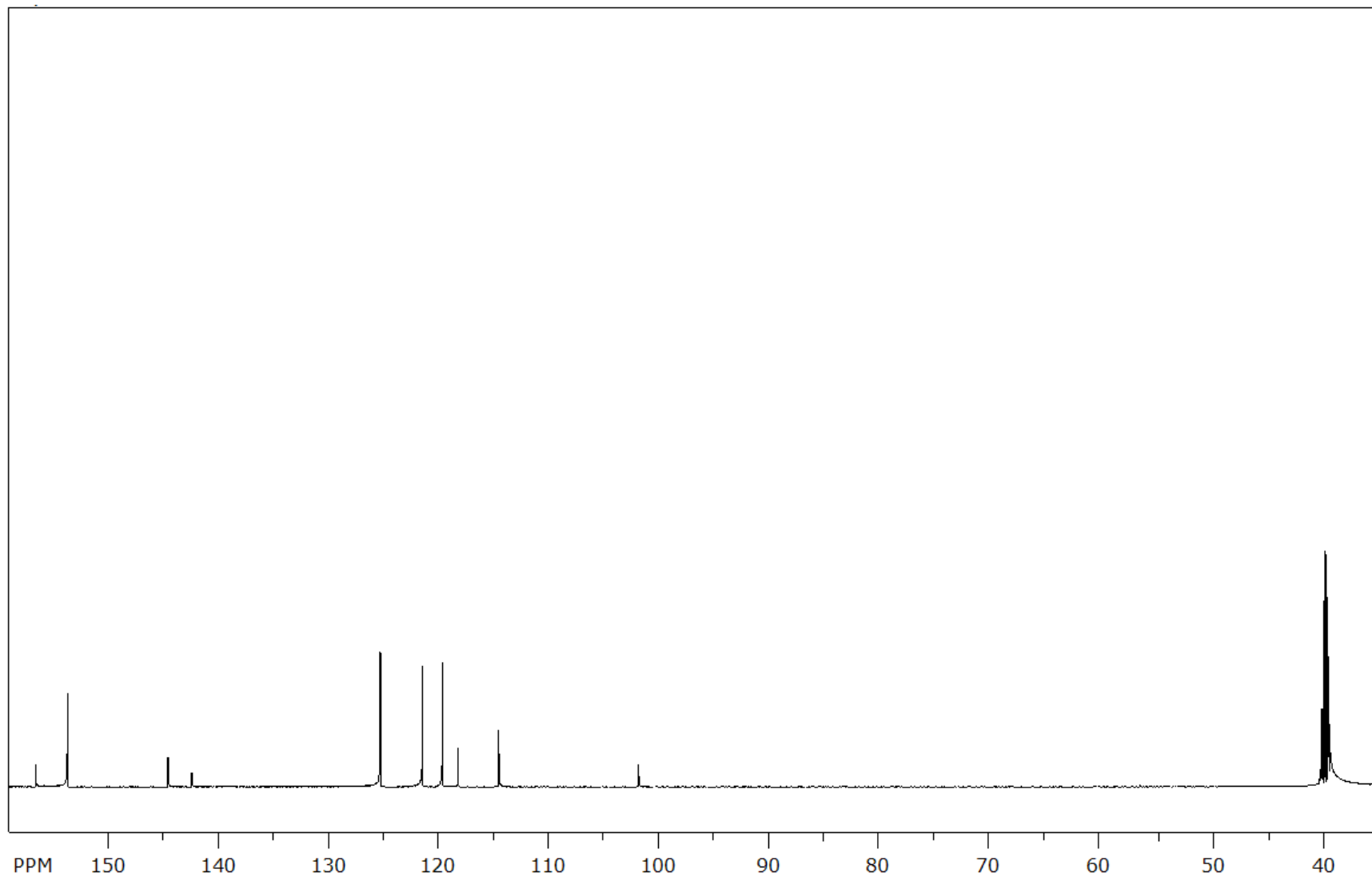
Maseni spektar (4c)



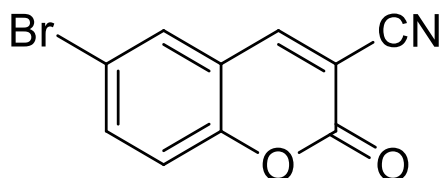
¹H NMR spektr (4c)



^{13}C NMR spektr (4c)

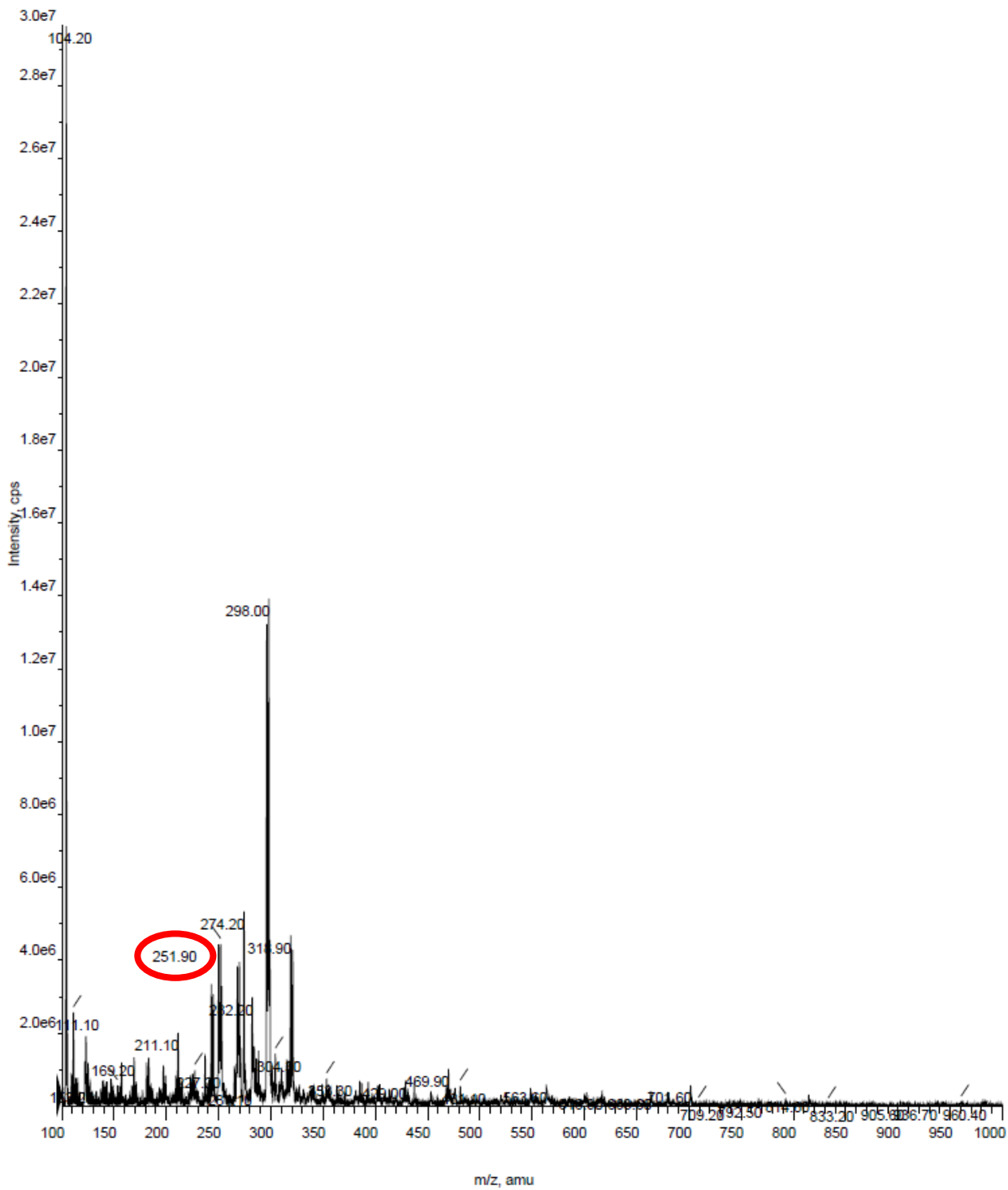


6-brom-2-okso-2H-kromen-3-karbonitril (4d)

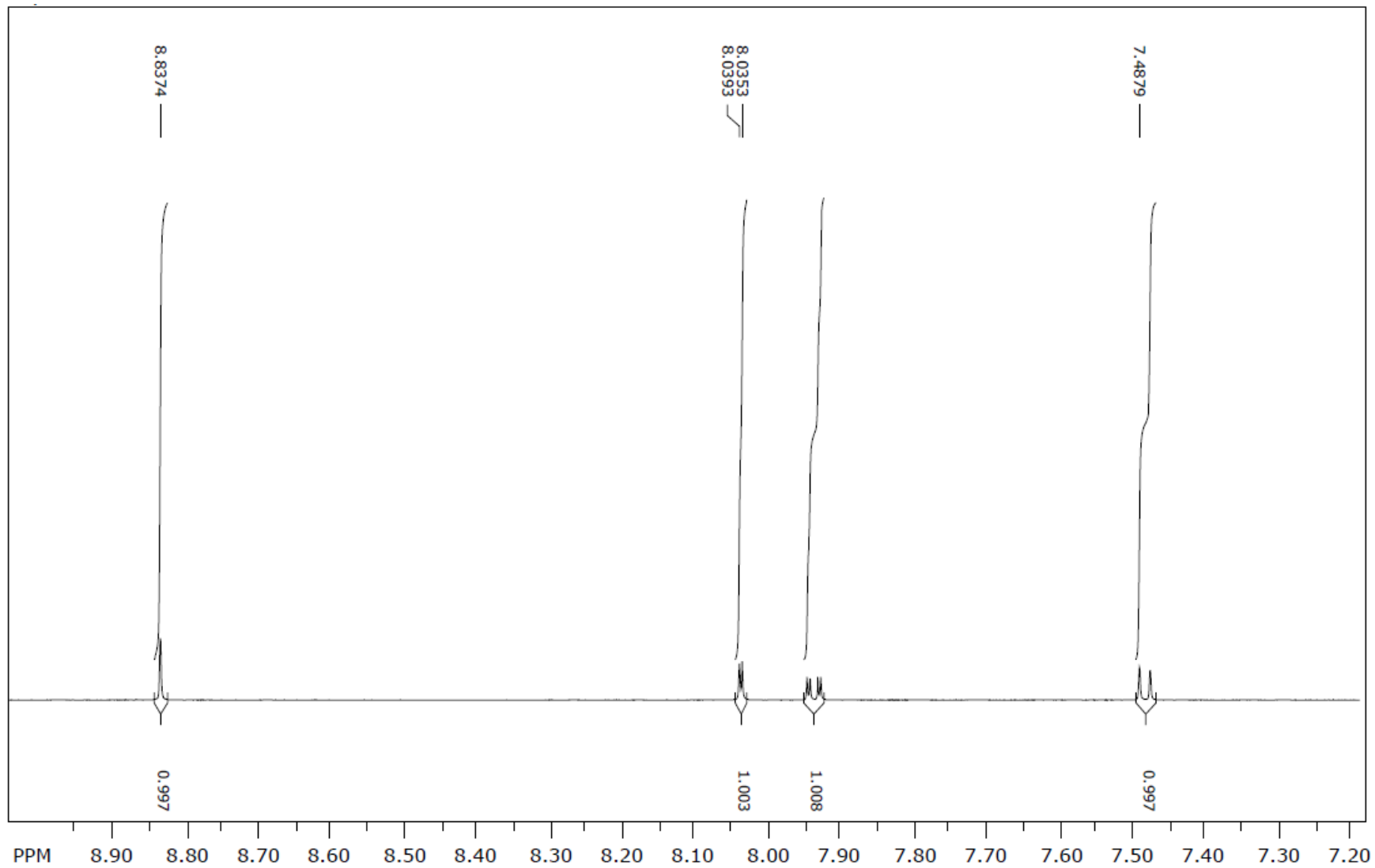


Reaktanti	5-bromsalicilaldehid (10 mmol) i etil cijanoacetat (10 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola
Molekulska masa	250,04 g/mol
Molekulska formula	C ₁₀ H ₄ BrNO ₂
Temperatura tališta	200 – 201 °C (lit. 200 – 201 °C, Keshavarzipour i Tavakol, 2016; 201 – 202 °C, Valizadeh i sur., 2011)
Boja kristala	Svijetlo žuta
R_f	0,84
LC/MS/MS <i>m/z</i> (M⁺)	251,90
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,84 (s, 1H, coum.), 8,04 (d, <i>J</i> = 2,40 Hz, 1H, arom.), 7,94 (dd, <i>J</i> = 8,88, 2,46 Hz, 1H, arom.) 7,48 (d, <i>J</i> = 8,88 Hz, 1H, arom.).
¹³C NMR	(150 MHz, CDCl ₃) δ 156,3; 153,1; 152,0; 137,5; 131,7; 119,0; 116,9; 114,3; 103,4.

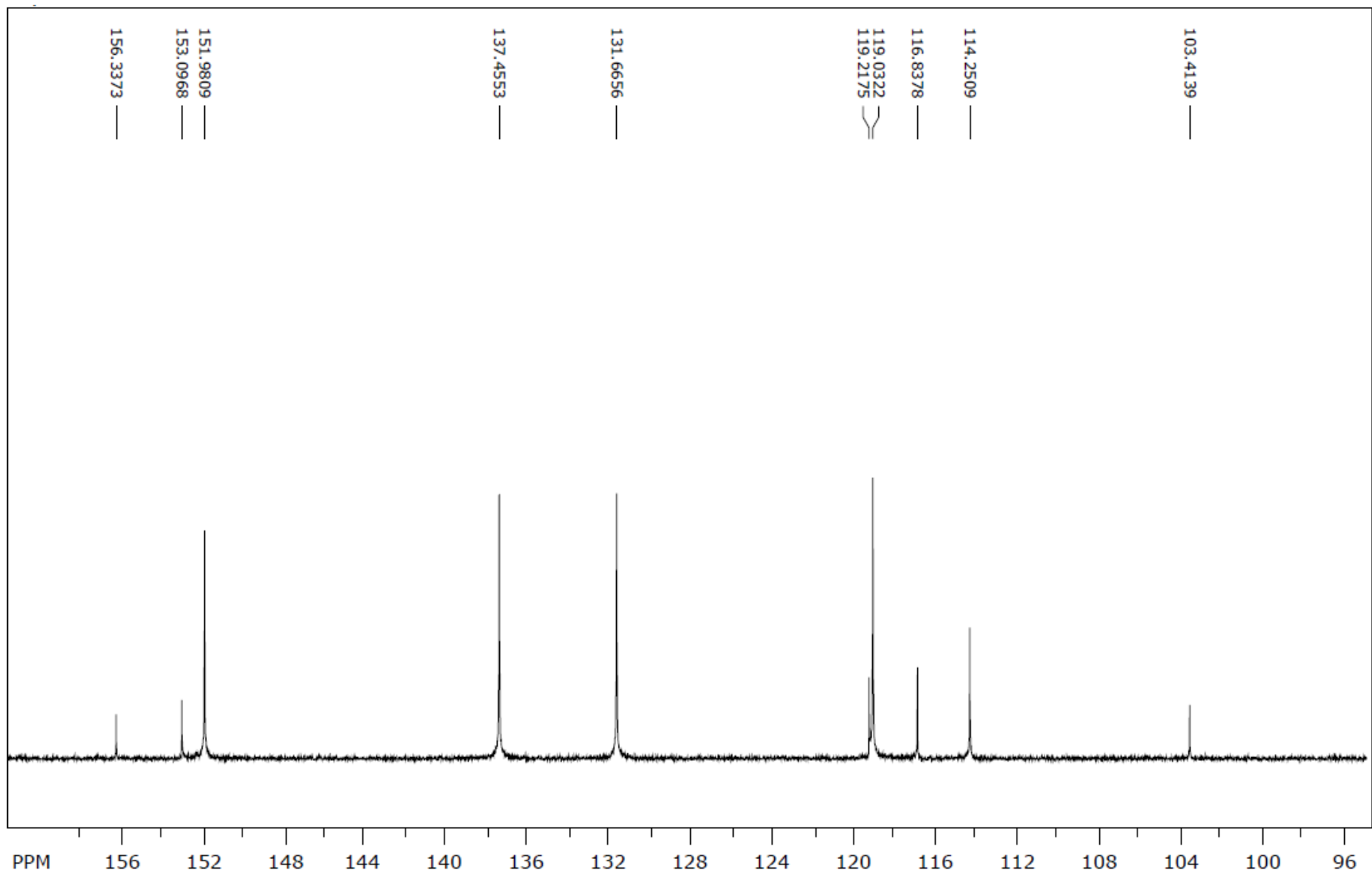
Maseni spektar (4d)



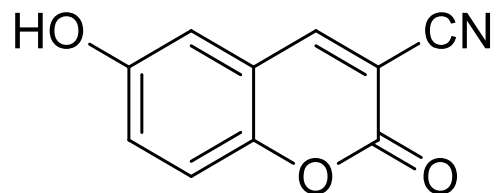
¹H NMR spektr (4d)



¹³C NMR spektr (4d)

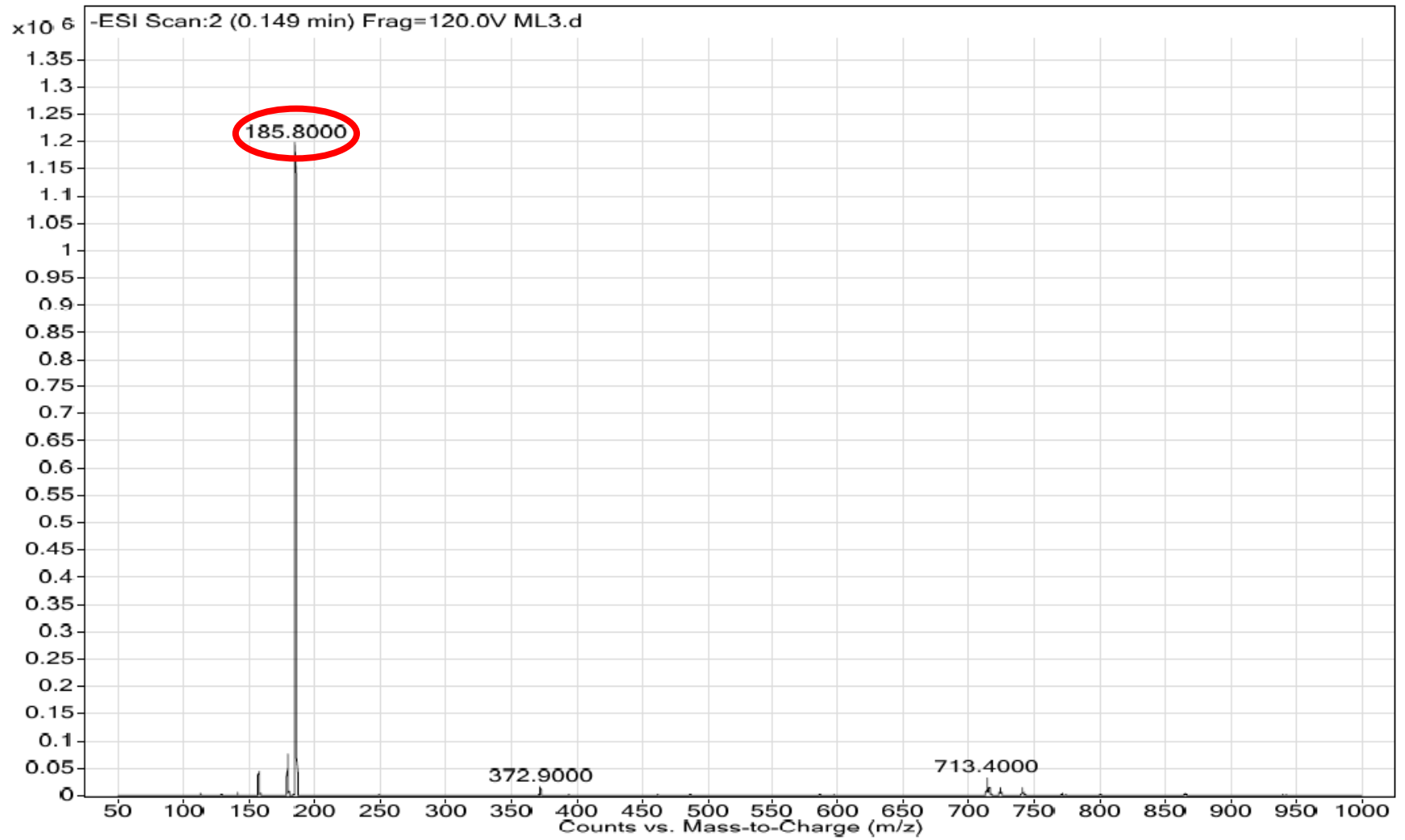


6-hidroksi-2-okso-2H-kromen-3-karbonitril (4e)

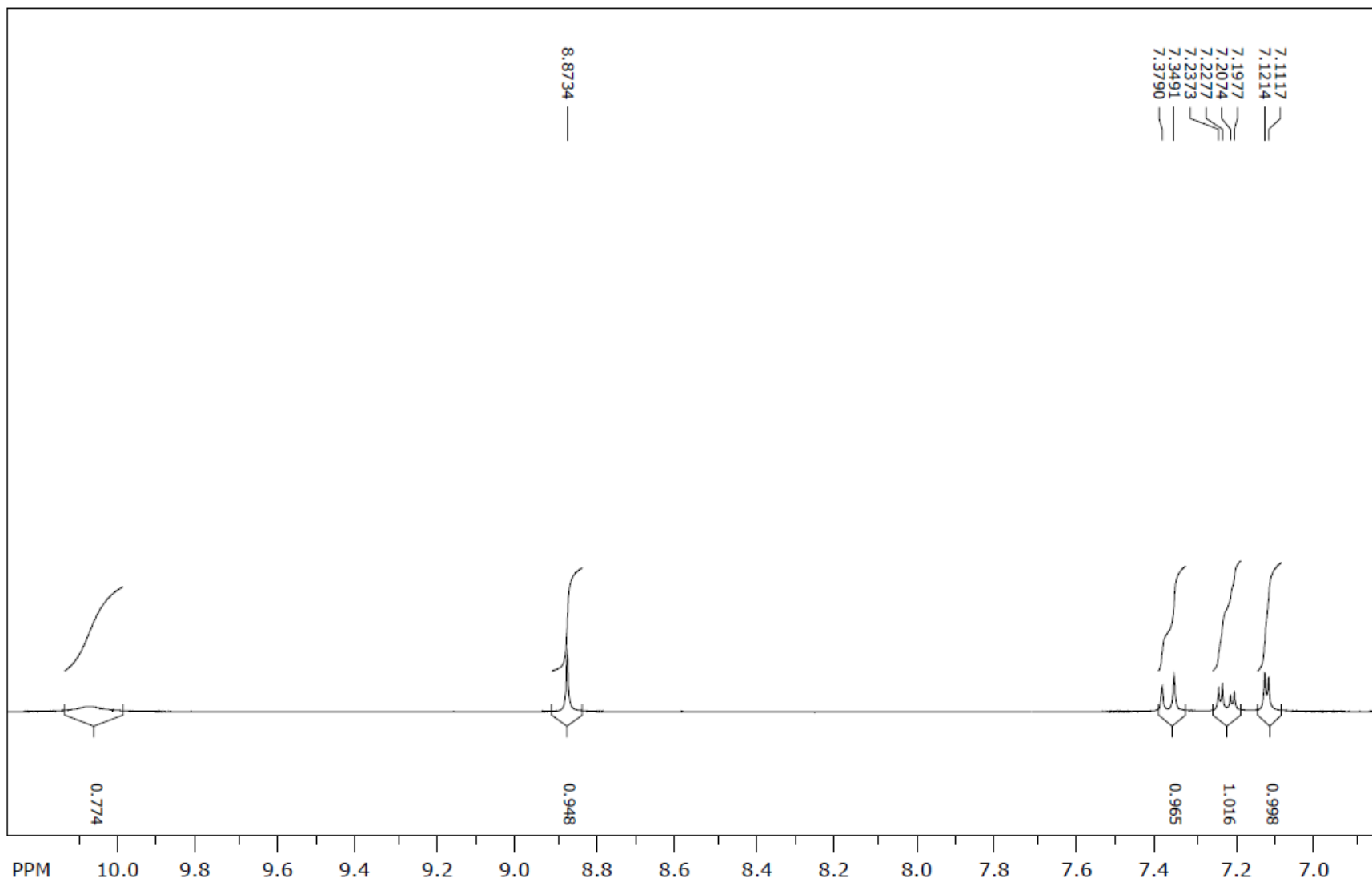


Reaktanti	2,5-dihidroksibenzaldehid (10 mmol) i etil cijanoacetat (10 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola
Molekulska masa	187,15 g/mol
Molekulska formula	C ₁₀ H ₅ NO ₃
Temperatura tališta	237 – 238 °C (lit. 236 – 239 °C, Valizadeh i sur., 2011)
Boja kristala	Svijetlo smeđa
R_f	0,50
LC/MS/MS <i>m/z</i> (M-)	185,80
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 10,07 (s, 1H, OH) 8,87 (s, 1H, C-4), 7,36 (d, <i>J</i> = 8,97 Hz, 1H, arom.) 7,21 (dd, <i>J</i> = 8,97, 2,90 Hz, 1H, arom.) 7,12 (d, <i>J</i> = 2,91 Hz, 1H, arom).
¹³C NMR	(75 MHz, CDCl ₃) δ 157,6; 154,9; 153,9; 147,9; 124,1; 118,3; 115,2; 113,8; 102,5.

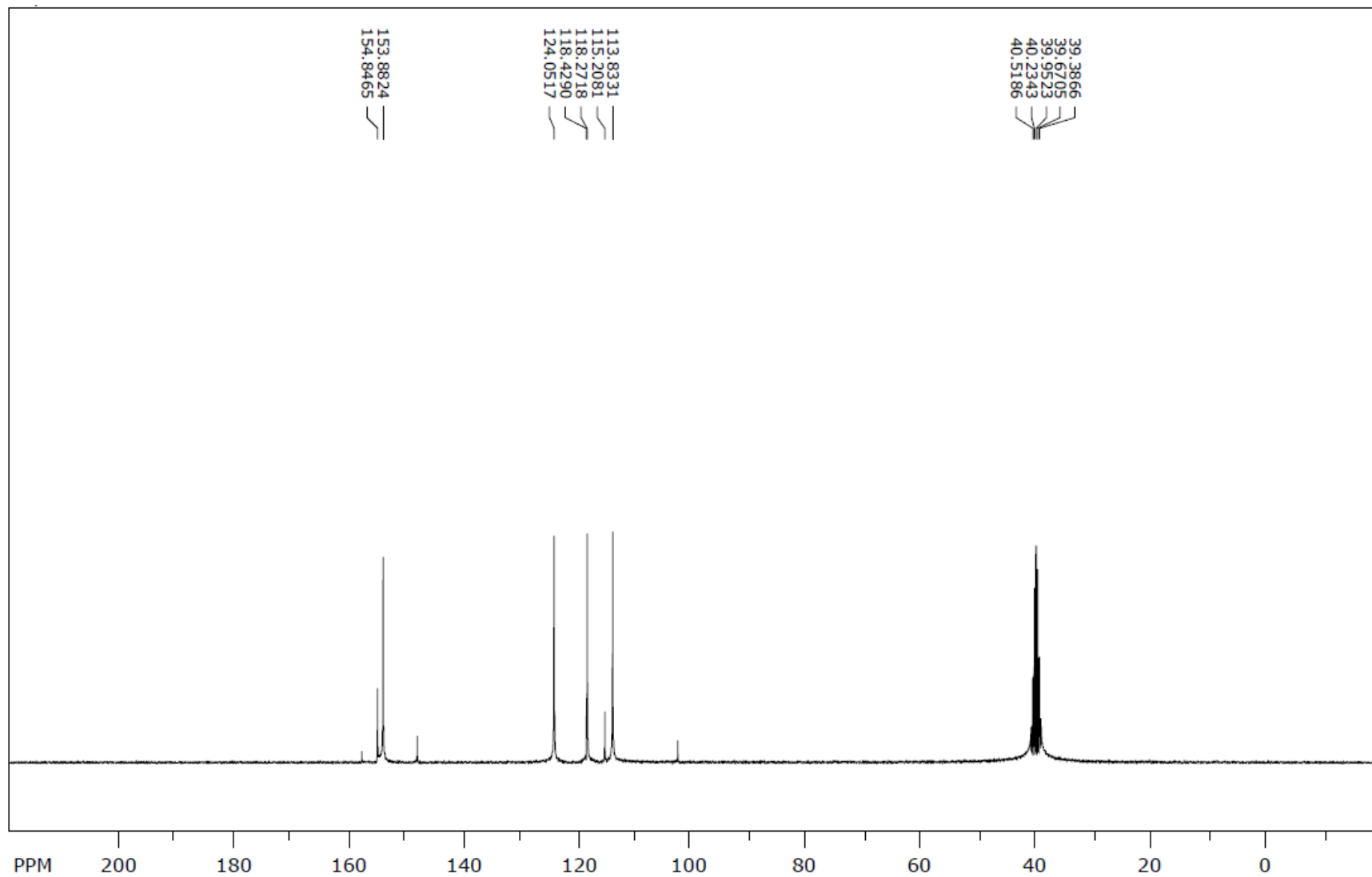
Maseni spektr (4e)



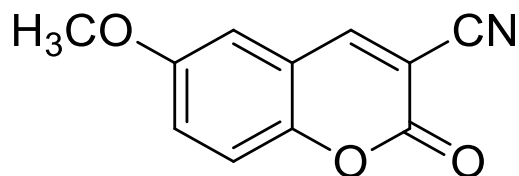
¹H NMR spektr (4e)



¹³C NMR spektr (4e)

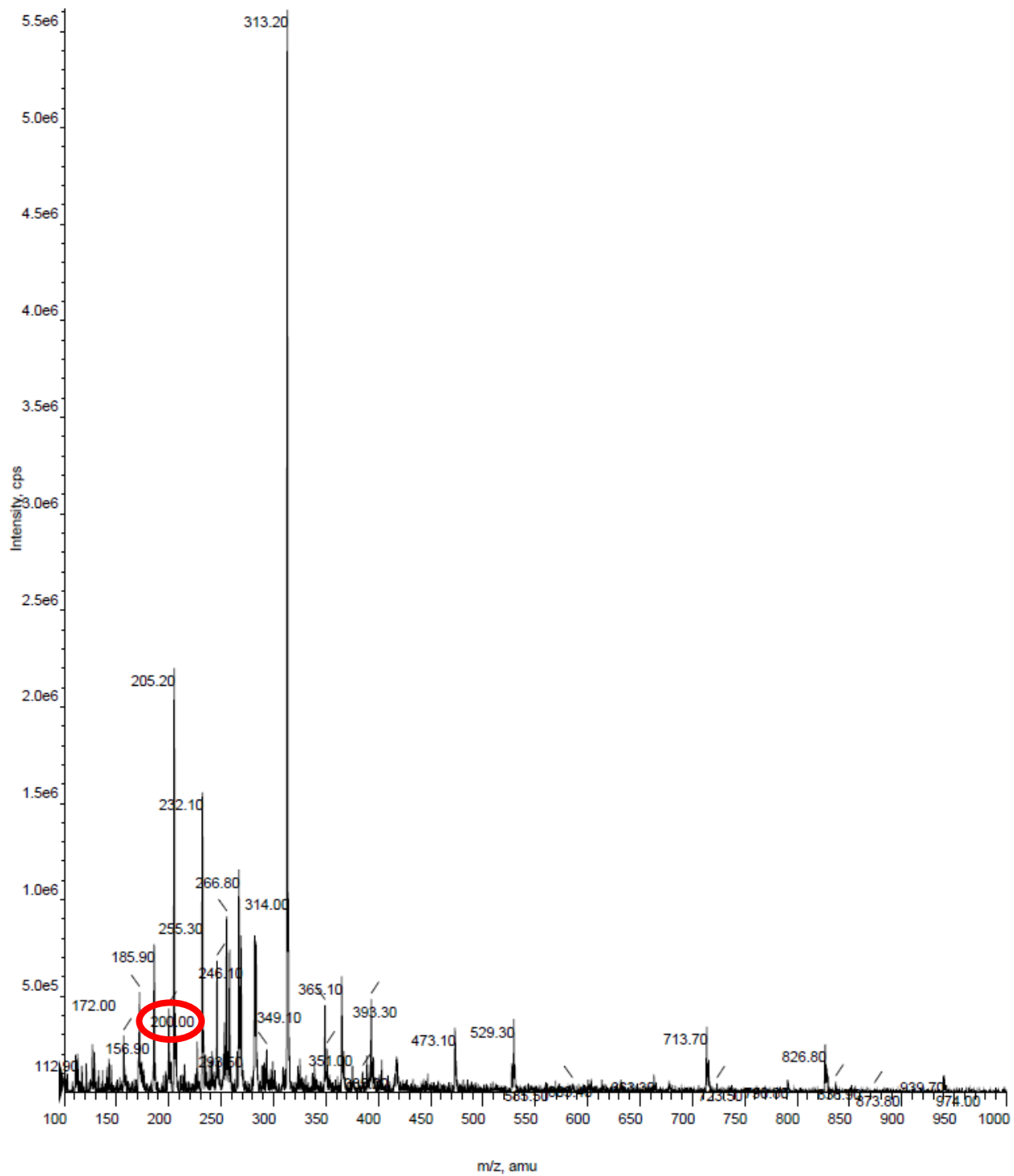


6-metoksi-2-okso-2H-kromen-3-karbonitril (4f)

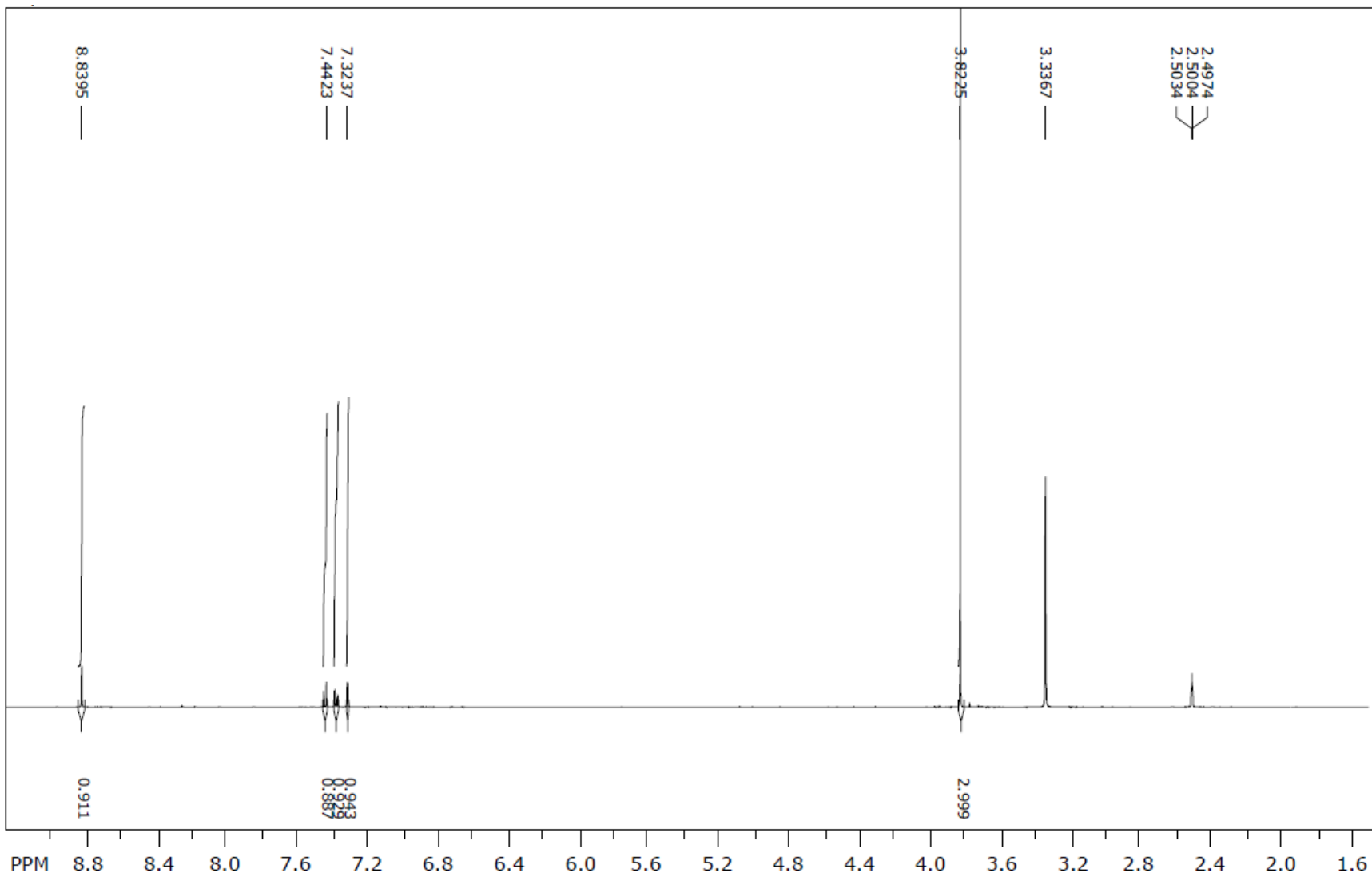


Reaktanti	5-metoksisalicilaldehid (3,2 mmol) i etil cijanoacetat (3,2 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola
Molekulska masa	201,17 g/mol
Molekulska formula	C ₁₁ H ₇ NO ₃
Temperatura tališta	230 – 232 °C
Boja kristala	Žuta
R_f	0,82
LC/MS/MS <i>m/z</i> (M⁻)	200,00
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,84 (s, 1H), 7,45 (d, <i>J</i> = 9,06 Hz, 1H, arom.) 7,39 (dd, <i>J</i> = 9,06, 3,06 Hz, 1H, arom.) 7,32 (d, <i>J</i> = 3,00 Hz, 1H, arom.), 3,82 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, CDCl ₃) δ 157,0; 156,1; 153,1; 148,5; 123,2; 117,9; 114,6; 111,4; 102,4; 55,9.

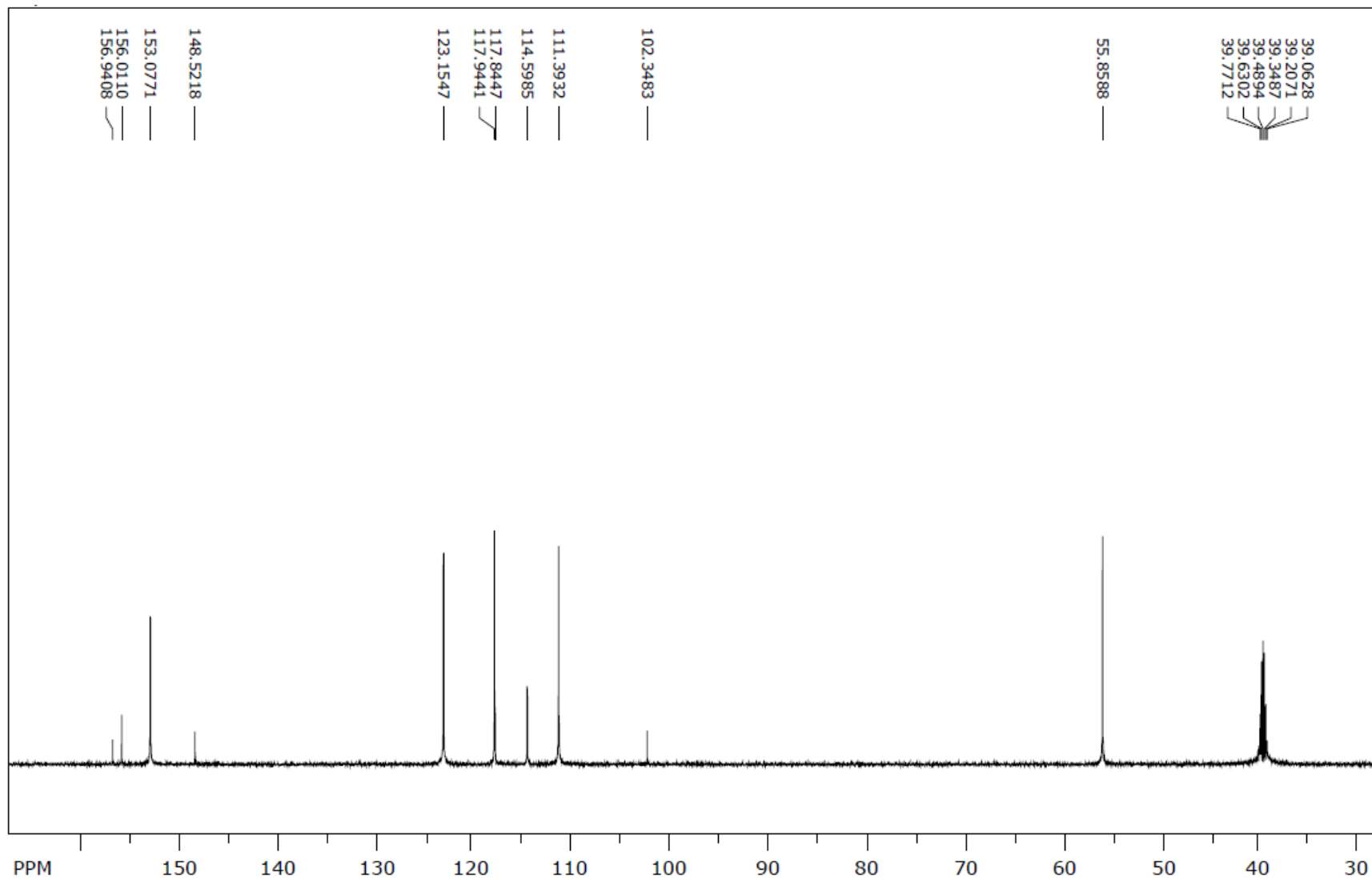
Maseni spektar (4f)



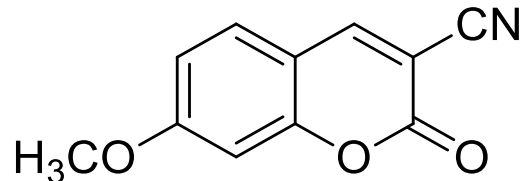
¹H NMR spektr (4f)



¹³C NMR spektr (4f)

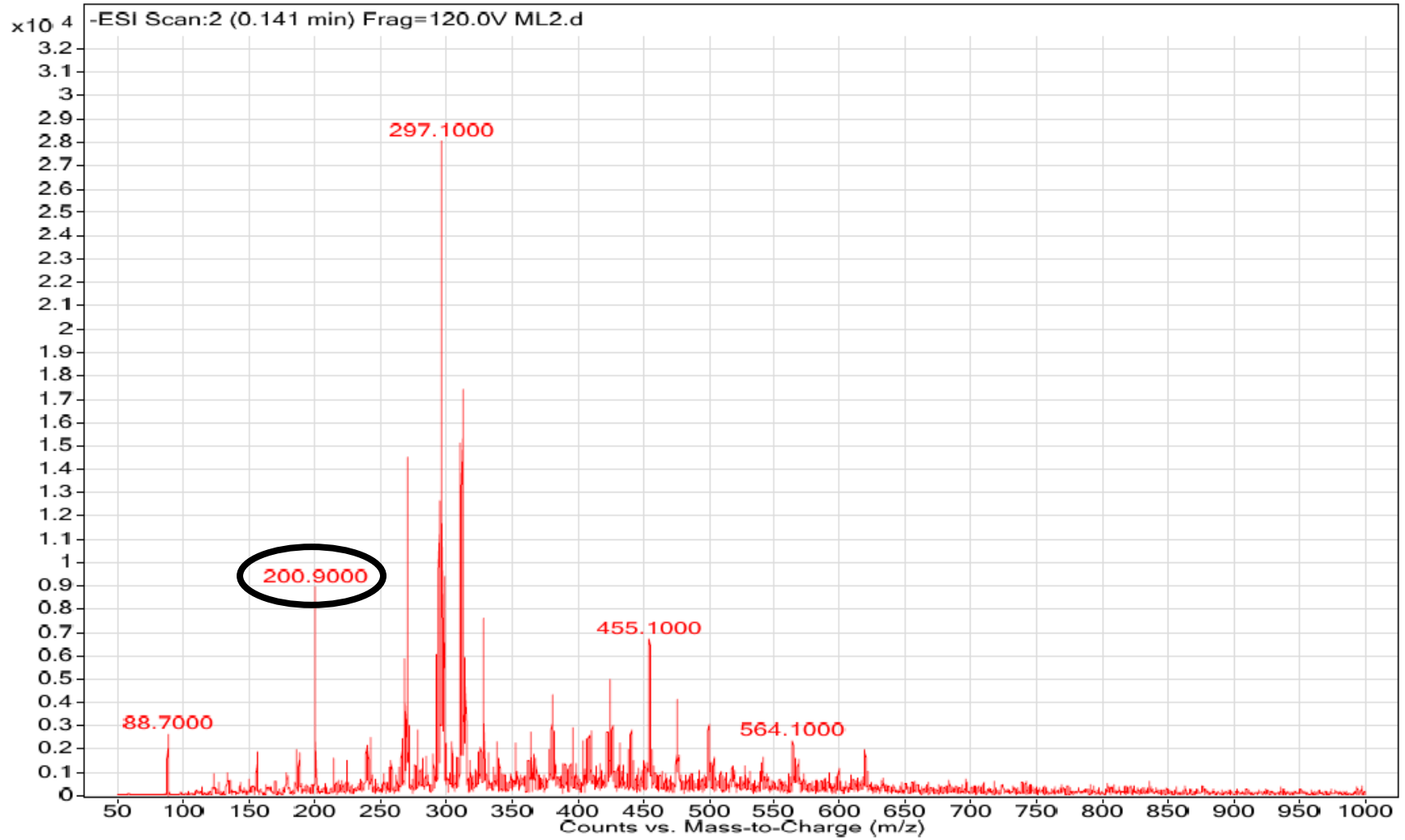


7-metoksi-2-okso-2H-kromen-3-karbonitril (4g)

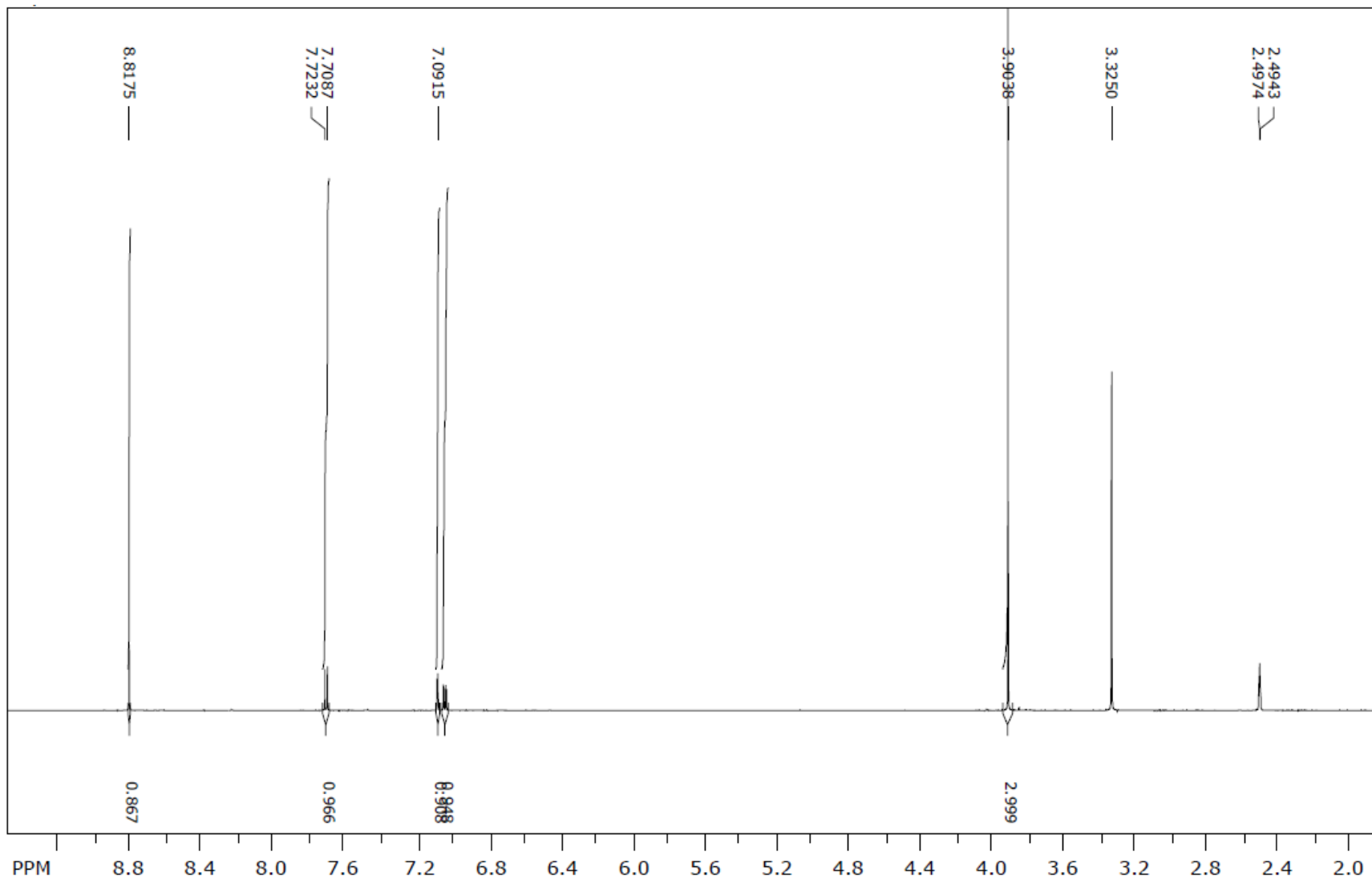


Reaktanti	4-metoksisalicilaldehid (3,3 mmol) i etil cijanoacetat (3,3 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola i metanola
Molekulska masa	201,18 g/mol
Molekulska formula	C ₁₁ H ₇ NO ₃
Temperatura tališta	221 – 223 °C (lit. 228 °C, Kumar i Makrandi, 2005; 224 – 226 °C, Valizadeh i sur., 2011)
Boja kristala	Svijetlo žuta
R_f	0,74
LC/MS/MS m/z (M-)	200,90
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,82 (s, 1H, coum.), 7,72 (d, <i>J</i> = 8,7 Hz, 1H, arom.), 7,09 (d, <i>J</i> = 2,34 Hz, 1H, arom.), 7,05 (dd, <i>J</i> = 8,76, 2,46 Hz, 1H, arom.), 3,90 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, CDCl ₃) δ 165,4; 157,3; 153,2; 131,3; 114,9; 113,9; 111,3; 101,0; 97,4; 56,4.

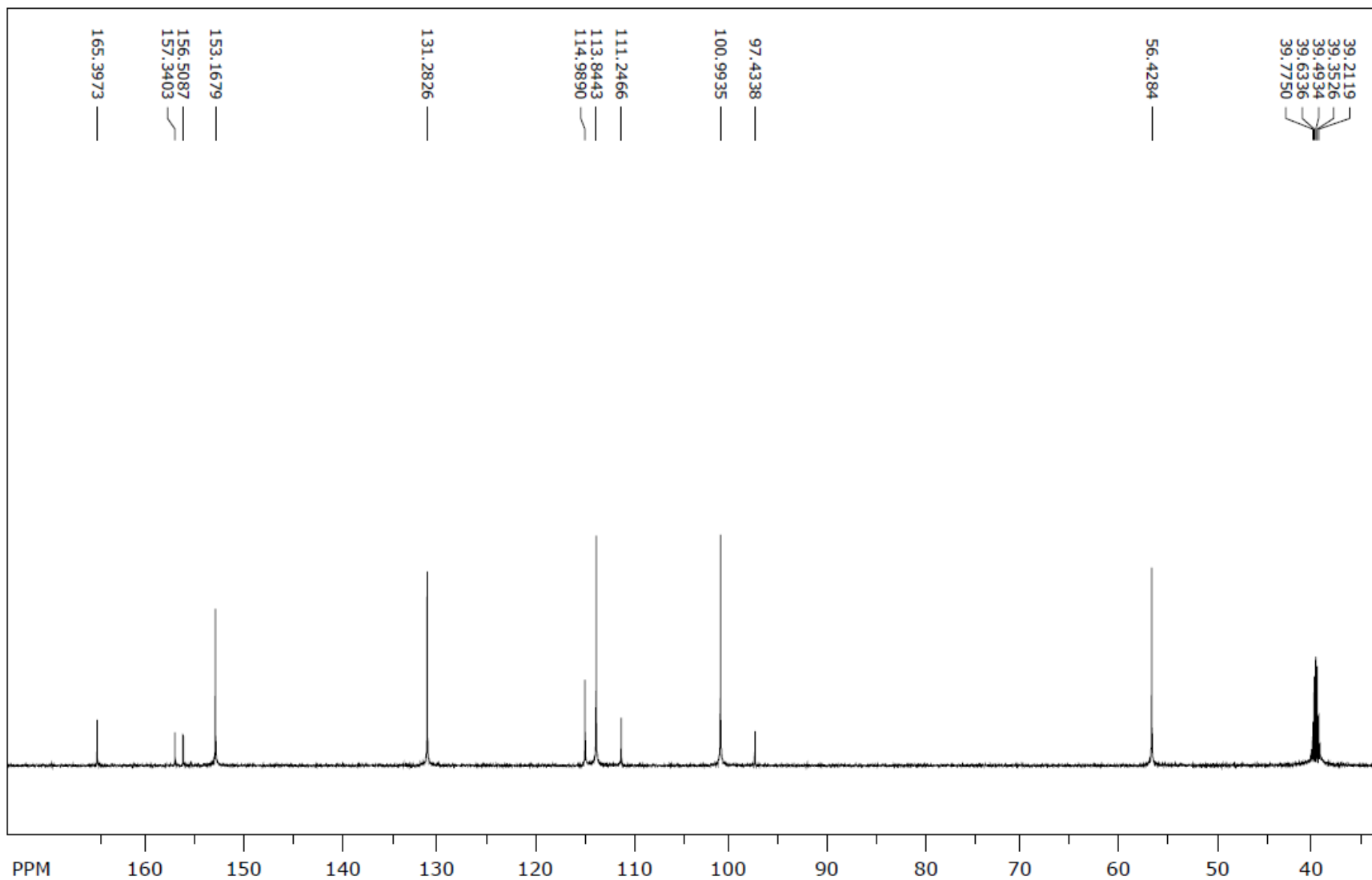
Maseni spektar (4g)



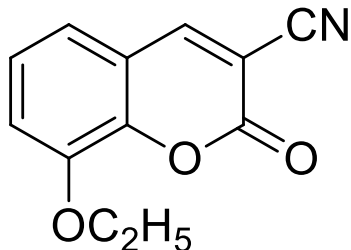
¹H NMR spektr (4g)



¹³C NMR spektr (4g)

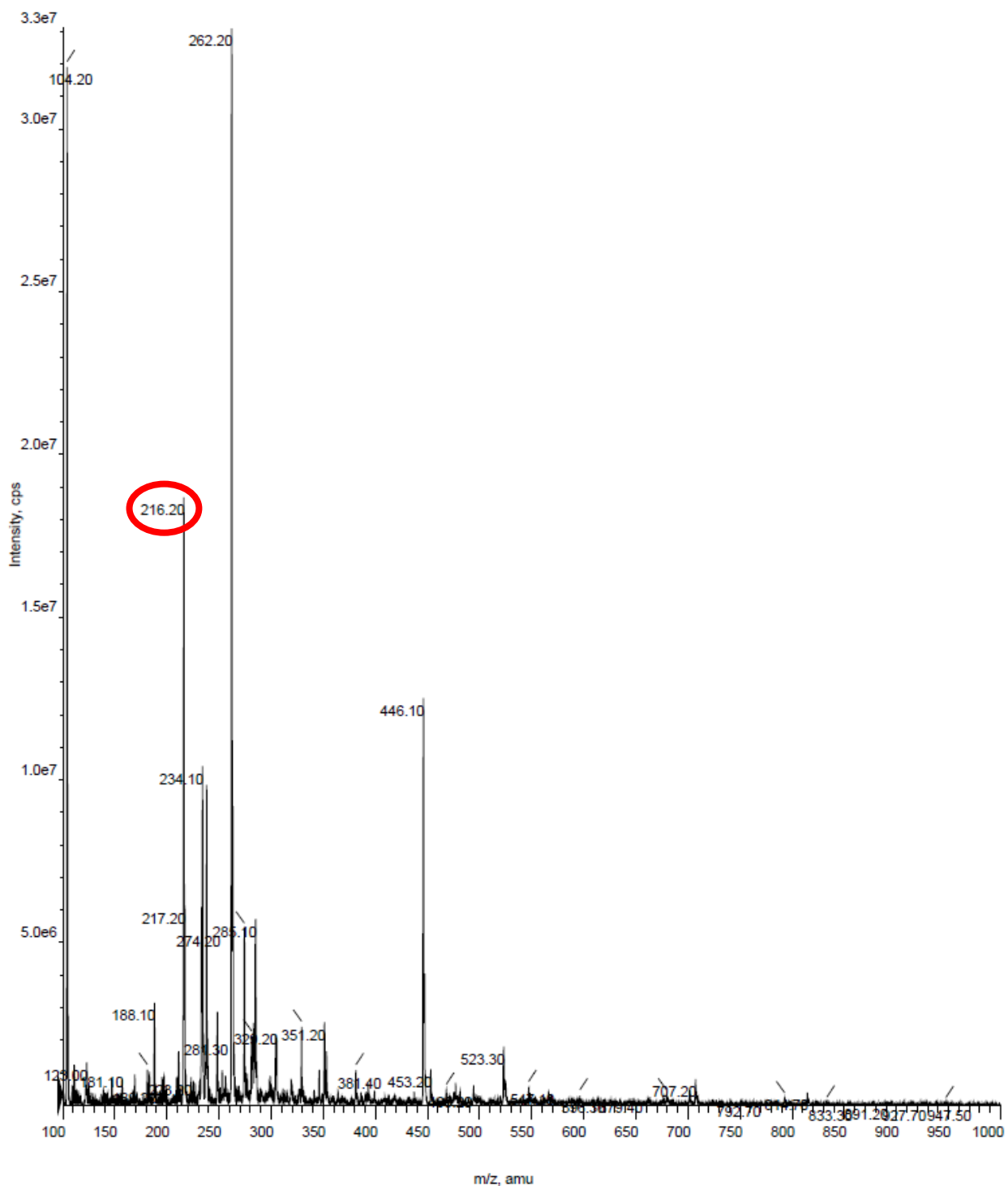


8-etoksi-2-okso-2H-kromen-3-karbonitril (4h)

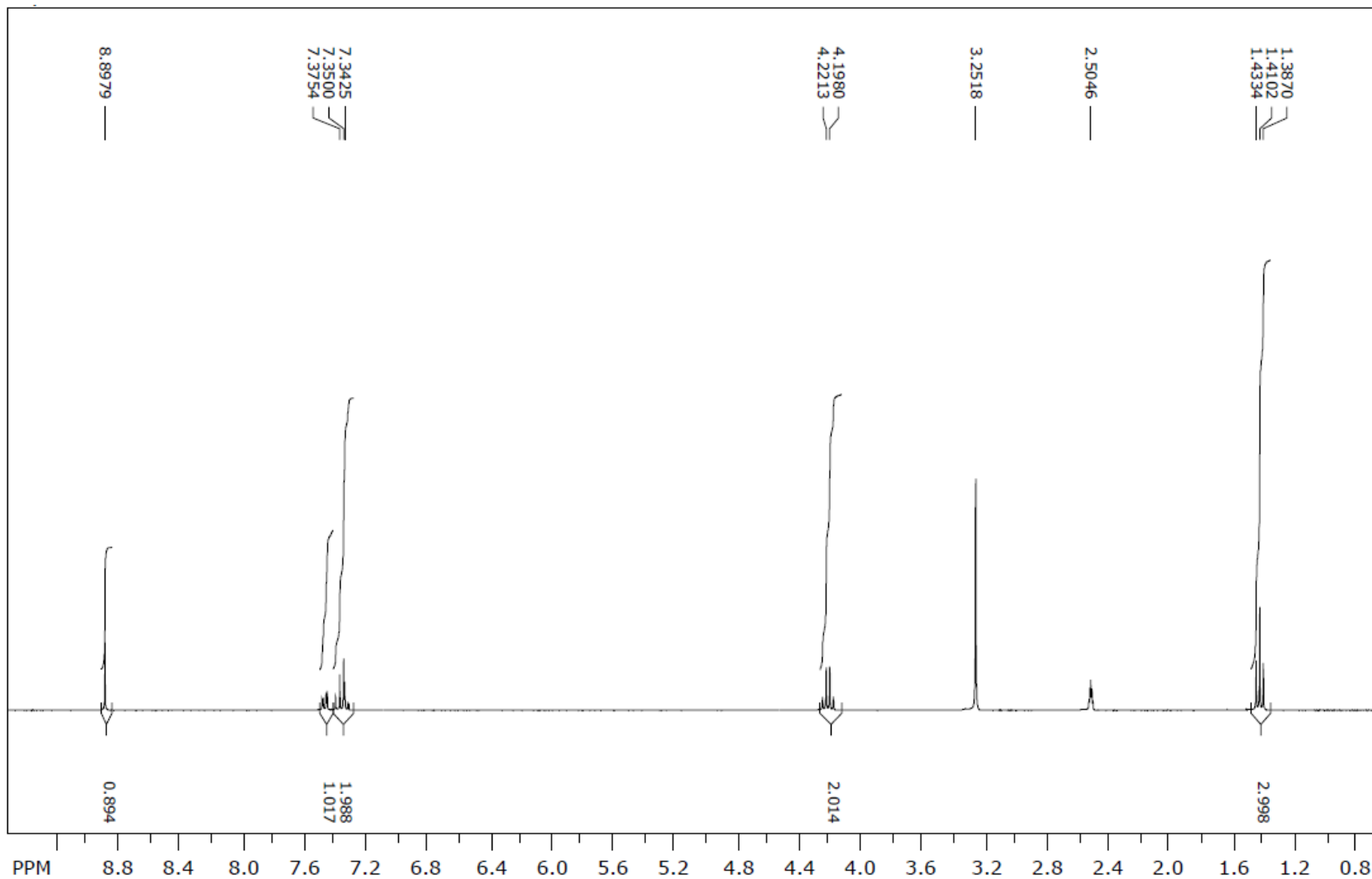


Reaktanti	3-etoksisalicilaldehid (10 mmol) i etil cijanoacetat (10 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola
Molekulska masa	215,20 g/mol
Molekulska formula	C ₁₂ H ₉ NO ₃
Temperatura tališta	185 -187 °C
Boja kristala	Žuta
R_f	0,49
LC/MS/MS m/z (M⁺)	216,20
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 8,90 (s, 1H, coum.), 7,47 (dd, <i>J</i> = 7,56, 2,07 Hz, 1H, arom.), 7,32 – 7,40 (m, 2H, arom.), 4,21 (q, <i>J</i> = 6,97 Hz, 2H, <u>CH</u> ₂ CH ₃), 1,41 (t, <i>J</i> = 6,96 Hz, 3H, CH ₂ <u>CH</u> ₃).
¹³C NMR	(75 MHz, CDCl ₃) δ 154,2; 125,9; 131,3; 119,1; 114,9; 102,7; 65,3; 14,9.

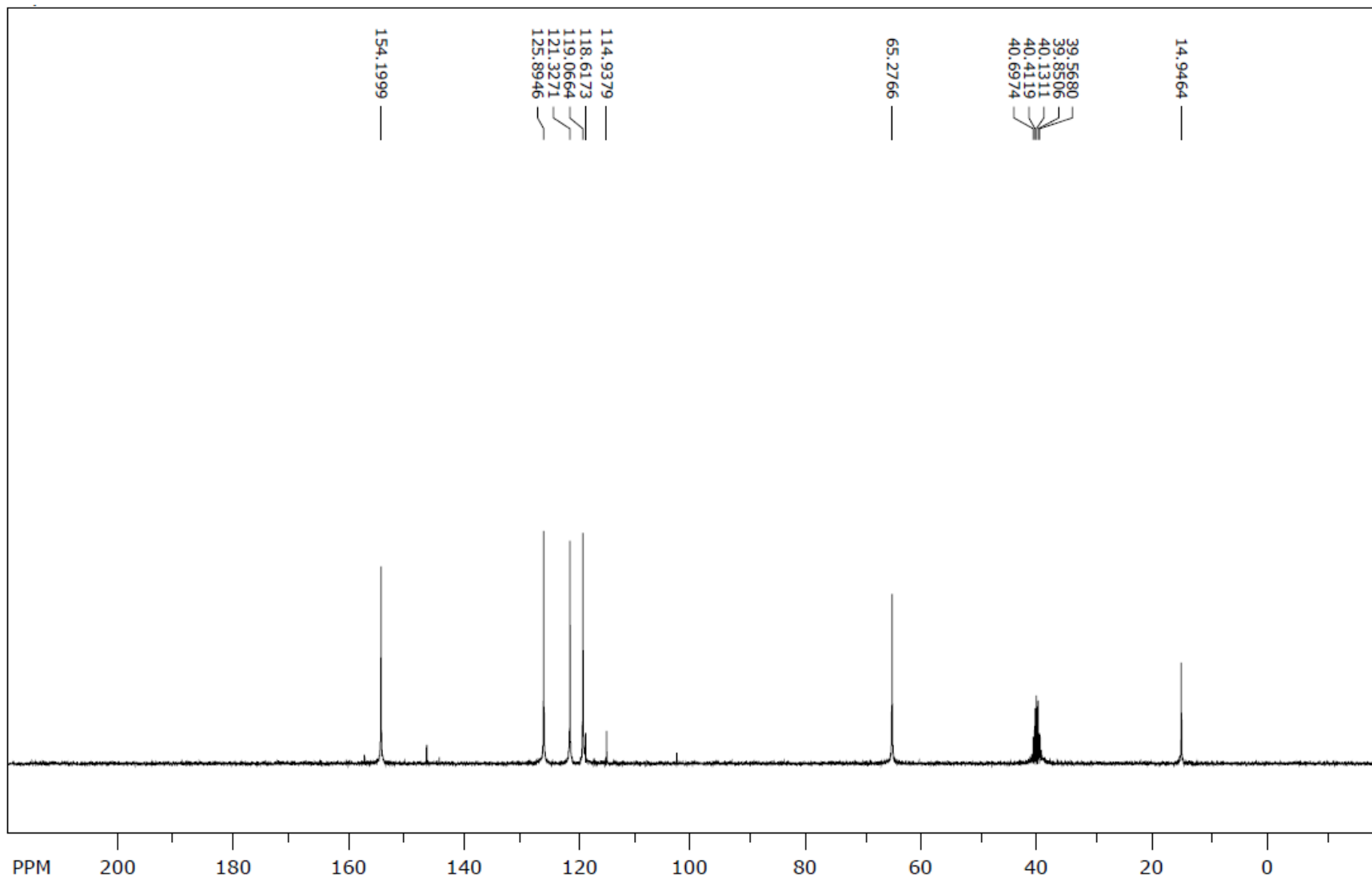
Maseni spektr (4h)



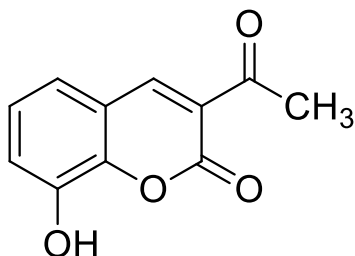
¹H NMR spektr (4h)



¹³C NMR spektr (4h)

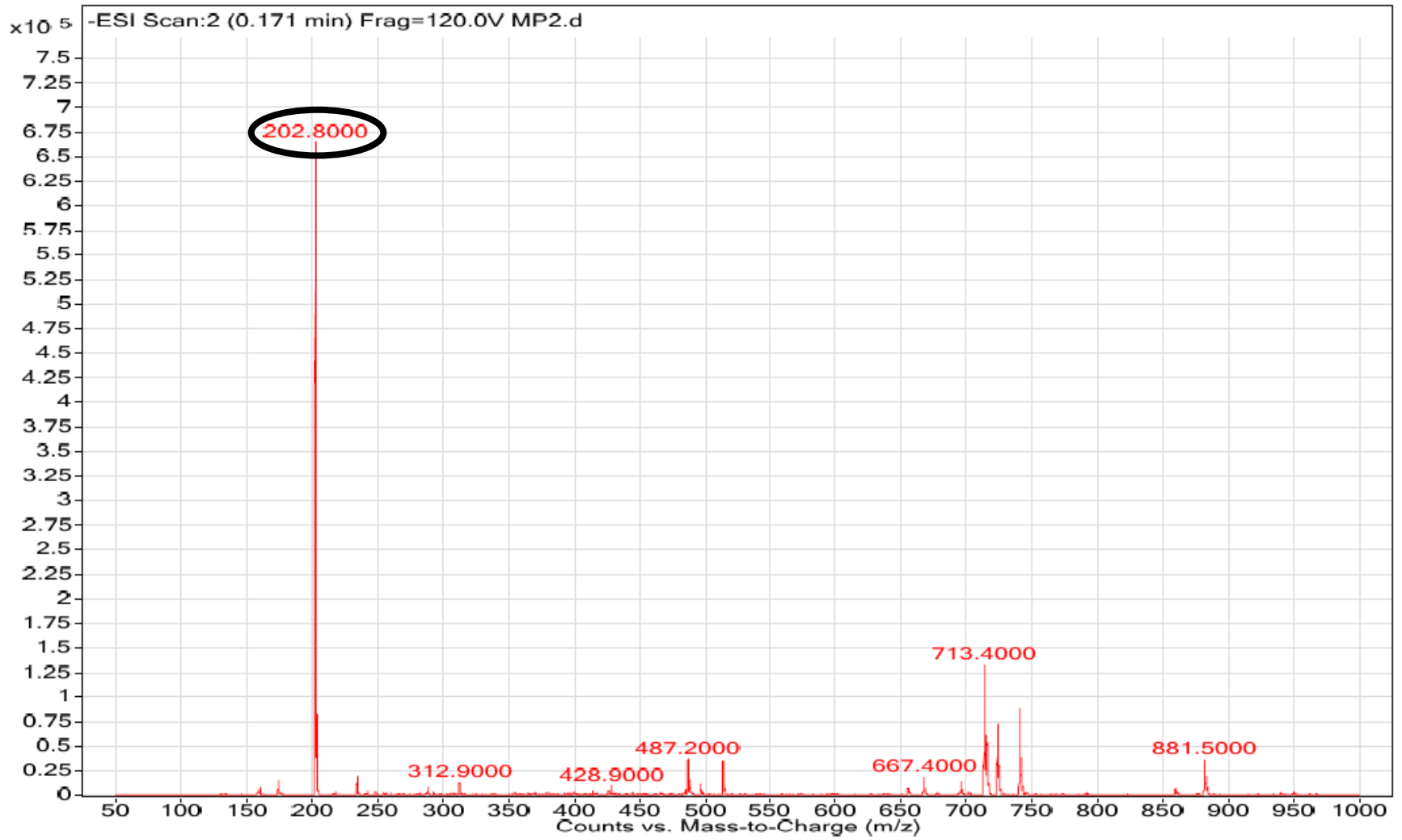


3-acetil-8-hidroksi-2H-kromen-2-on (5a)

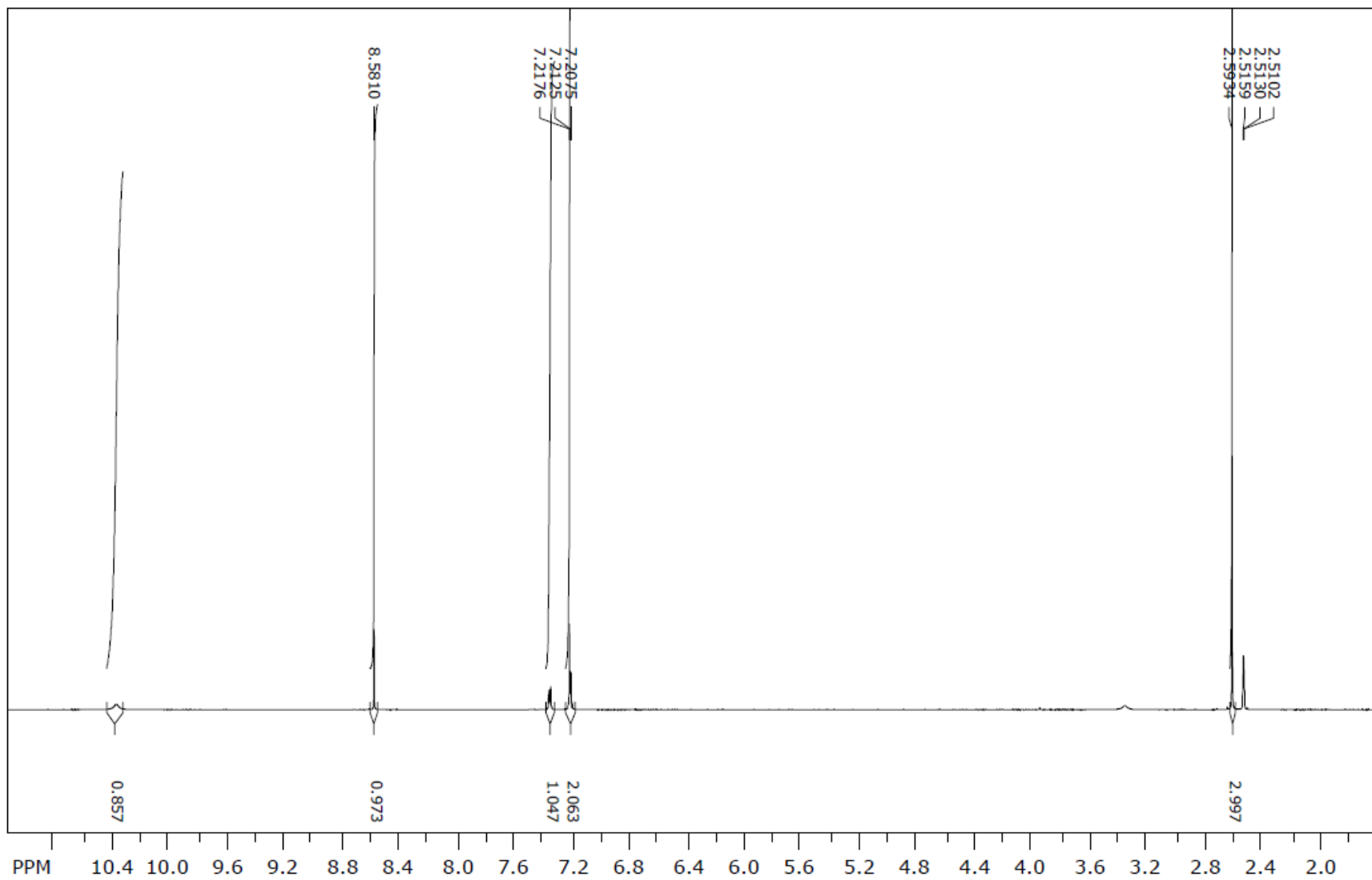


Reaktanti	2,3-dihidroksibenzaldehid (3,6 mmol) i etilacetoacetat (3,6 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola
Molekulska masa	204,17 g/mol
Molekulska formula	C ₁₁ H ₈ O ₄
Temperatura tališta	257 – 259 °C (lit. 249 – 251 °C, Zerangnasrabad i sur., 2021; 253 °C, la Pietra i sur., 2012)
Boja kristala	Bijela
R_f	0,66
LC/MS/MS <i>m/z</i> (M-)	202,8
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 10,38 (s, 1H, OH), 8,58 (s, 1H, coum.), 7,35 (dd, <i>J</i> = 5,94, 3,18 Hz, 1H, arom.), 7,19 - 7,23 (m, 2H, arom.), 2,59 (s, 3H, CH ₃).
¹³C NMR	(150 MHz, CDCl ₃) δ 195,2; 158,3; 147,4; 144,4; 143,2; 124,9; 124,3; 120,6; 119,0; 30,0.

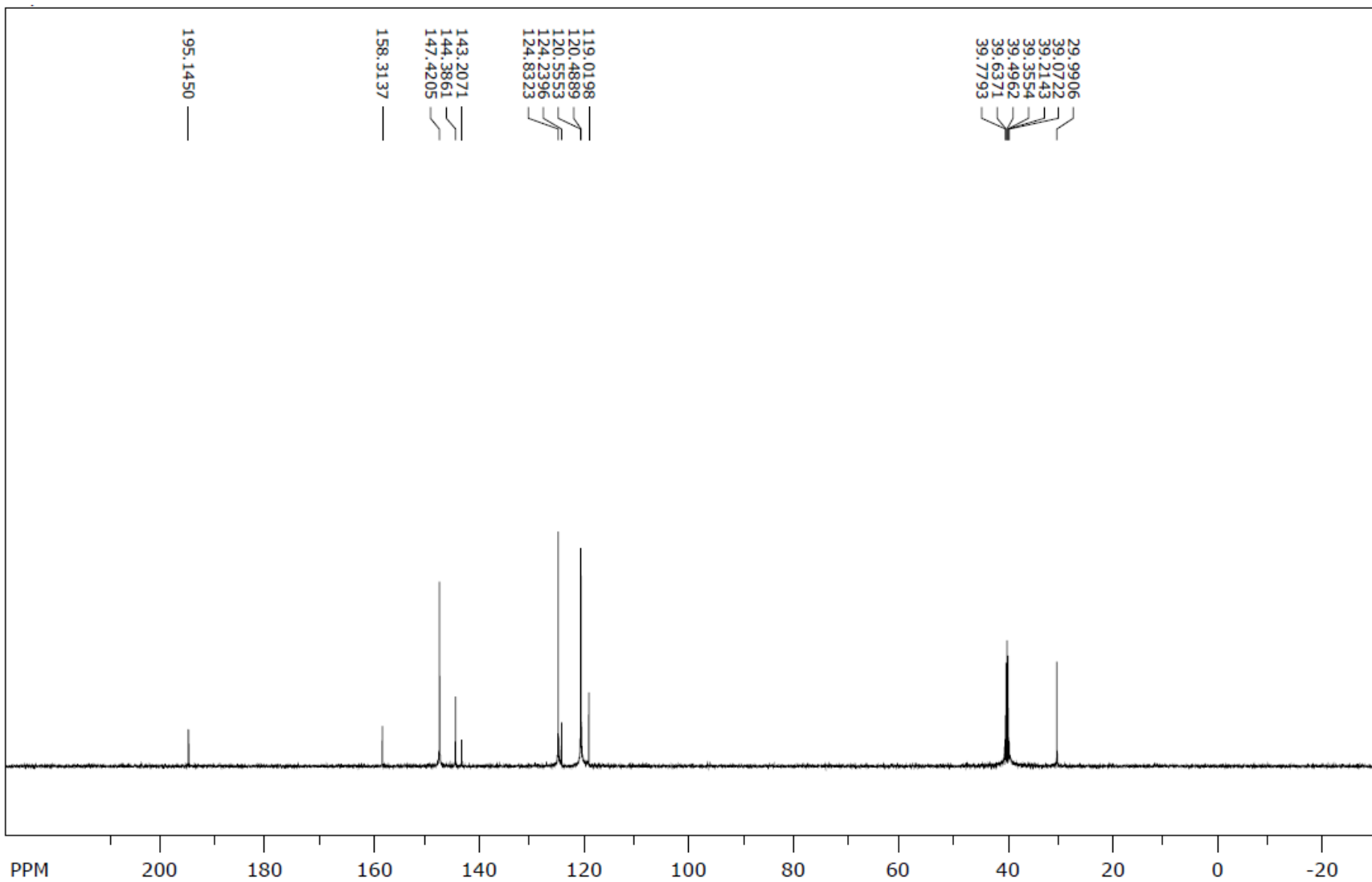
Maseni spektar (5a)



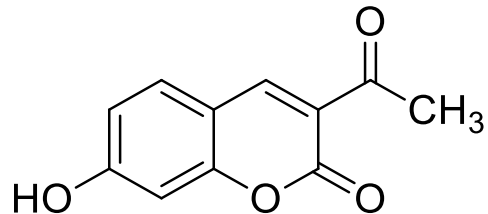
¹H NMR spektr (5a)



¹³C NMR spektr (5a)

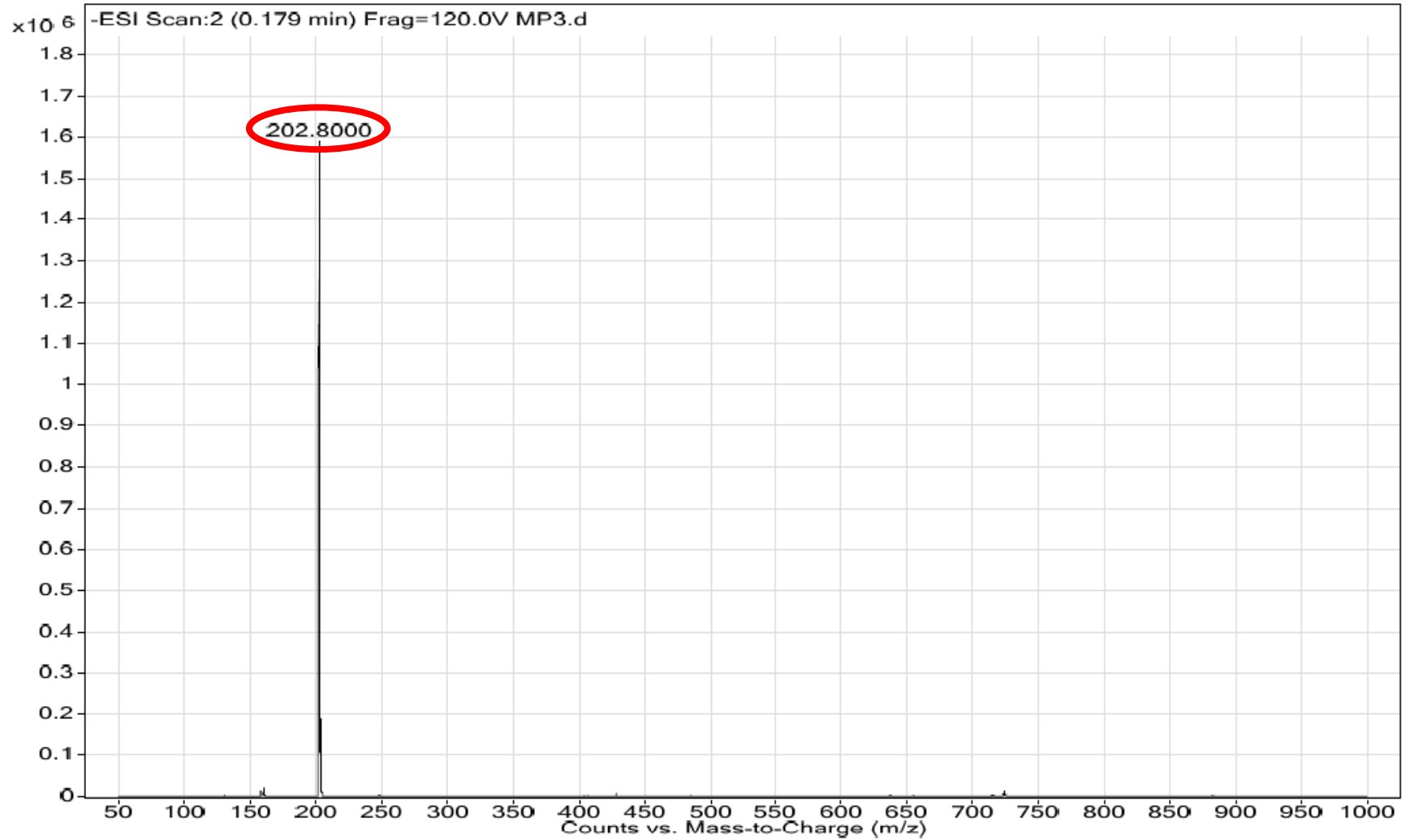


3-acetil-7-hidroksi-2*H*-kromen-2-on (5b)

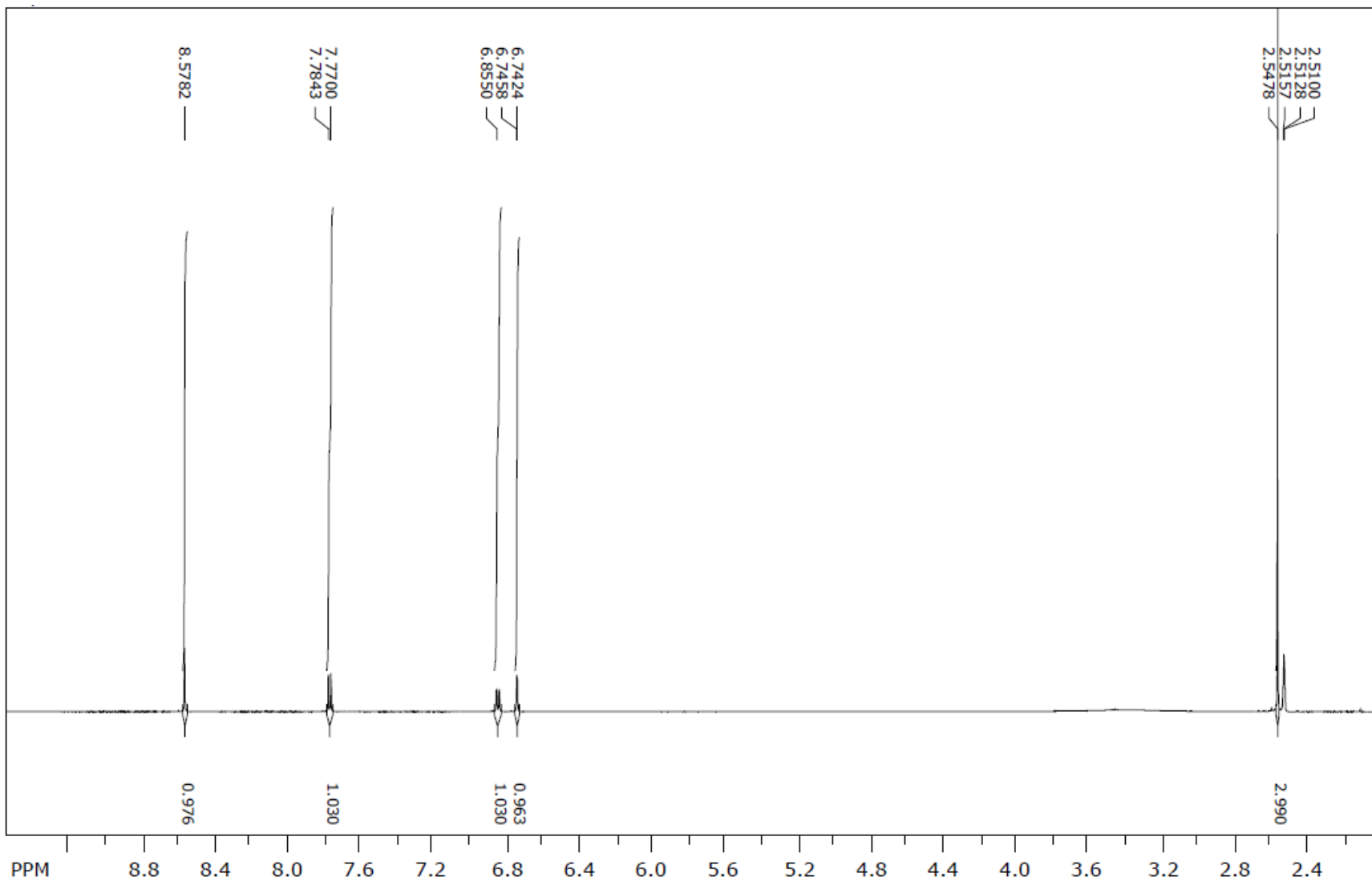


Reaktanti	2,4-dihidroksibenzaldehid (7,2 mmol) i etilacetoacetat (7,2 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola i metanola
Molekulska masa	204,17 g/mol
Molekulska formula	C ₁₁ H ₈ O ₄
Temperatura tališta	237 – 240 °C (lit. 226 – 228 °C, Zerangnasrabad i sur., 2021; 236 – 238 °C, Durgopal i sur., 2020)
Boja kristala	Svijetlo žuta
R_f	0,55
LC/MS/MS <i>m/z</i> (M-)	202,80
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,58 (s, 1H, coum.), 7,78 (d, <i>J</i> = 8,58 Hz, 1H, arom.), 6,85 (dd, <i>J</i> = 8,64, 2,16 Hz, 1H, arom.), 6,74 (d, <i>J</i> = 2,04 Hz, 1H, arom.), 2,55 (s, 3H, CH ₃).
¹³C NMR	(150 MHz, CDCl ₃) δ 194,6; 164,2; 159,0; 157,2; 147,8; 132,6; 119,2; 114,2; 110,8; 101,7; 30,0.

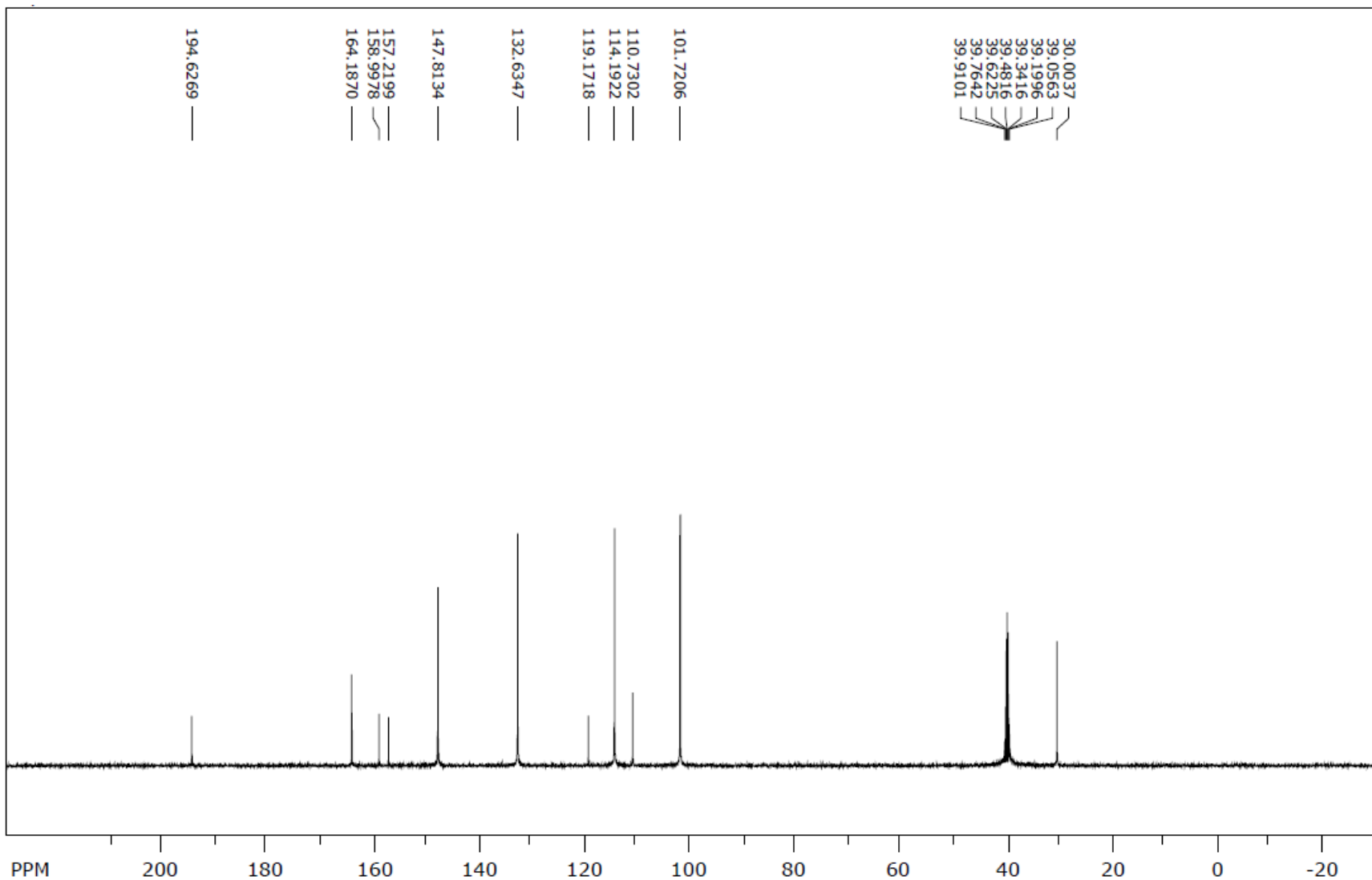
Maseni spektar (5b)



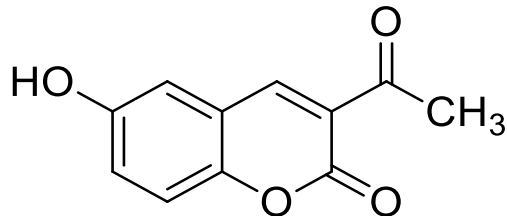
¹H NMR spektr (5b)



¹³C NMR spektr (5b)

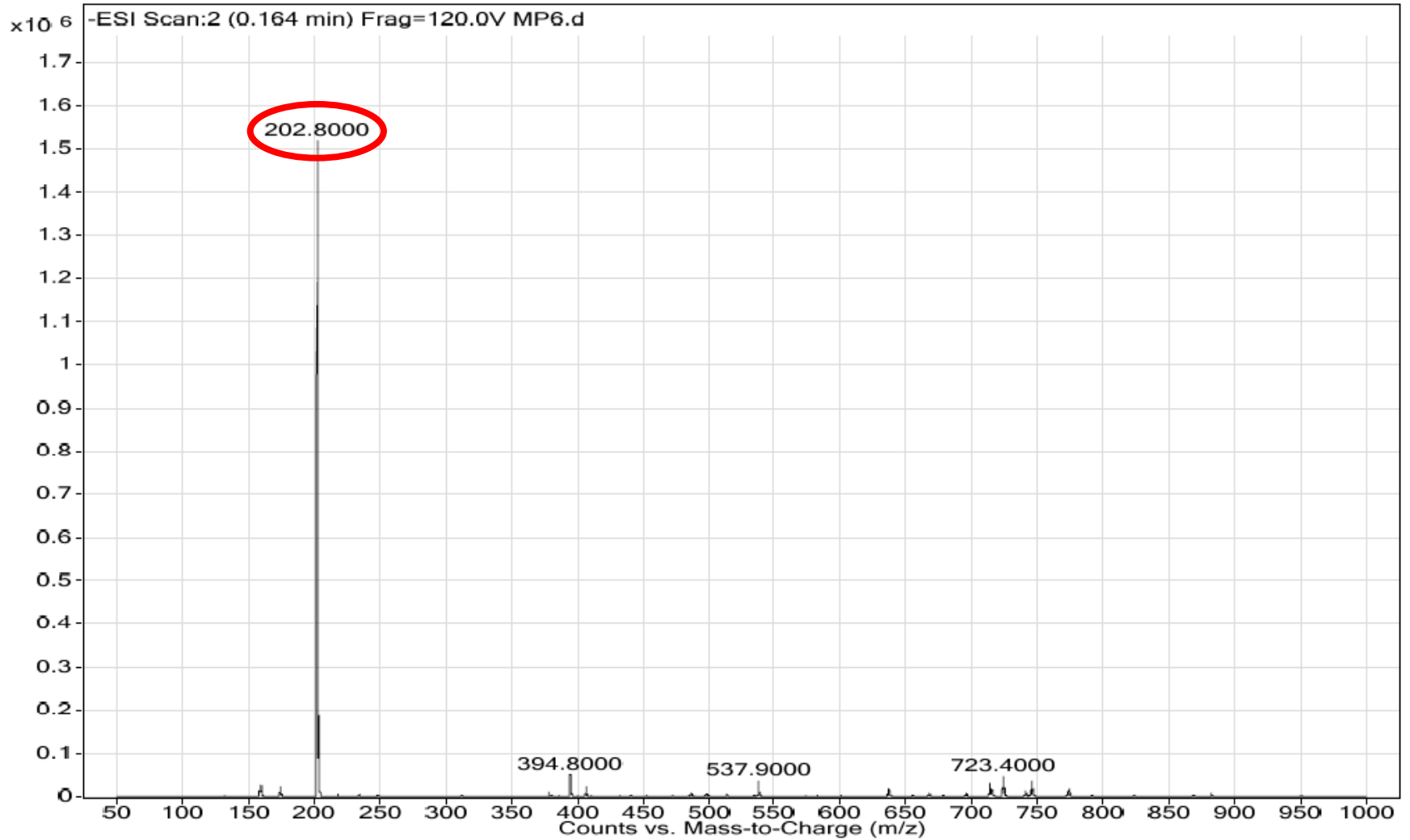


3-acetil-6-hidroksi-2H-kromen-2-on (5c)

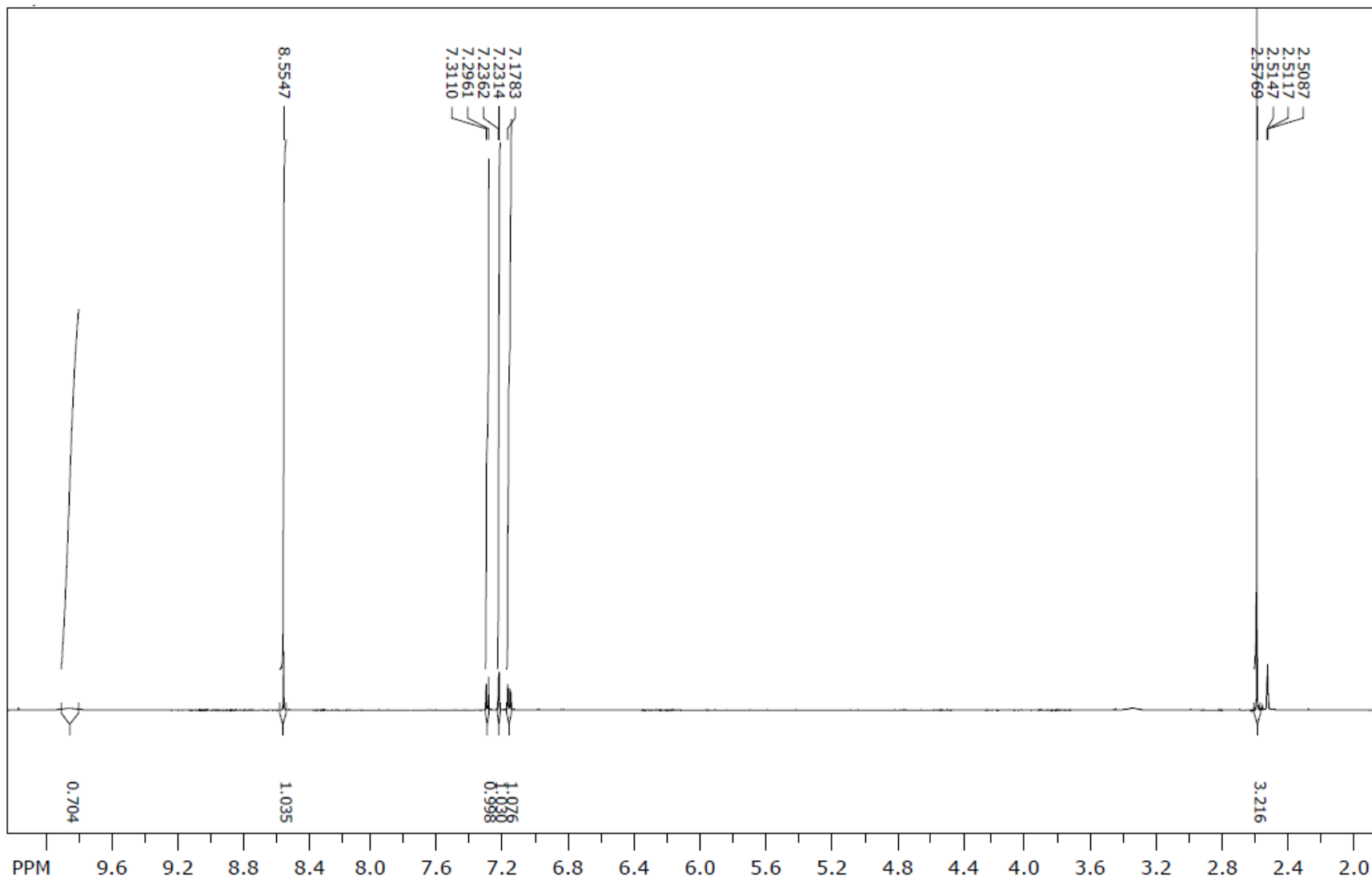


Reaktanti	2,5-dihidroksibenzaldehid (3,6 mmol) i etilacetoacetat (3,6 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola
Molekulska masa	204,18 g/mol
Molekulska formula	C ₁₁ H ₈ O ₄
Temperatura tališta	235 – 238 °C (lit. 246 – 249 °C, Zerangnasrabad i sur., 2021)
Boja kristala	Svijetlo smeđa
R_f	0,55
LC/MS/MS m/z (M-)	202,80
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,56 (s, 1H, coum.), 7,30 (d, <i>J</i> = 8,94 Hz, 1H, arom.), 7,23 (d, <i>J</i> = 2,88 Hz, 1H, arom.), 7,17 (dd, <i>J</i> = 8,88, 2,91 Hz, 1H, arom.), 2,58 (s, 3H, CH ₃).
¹³C NMR	(150 MHz, CDCl ₃) δ 195,3; 158,6; 154,0; 148,0; 146,9; 124,4; 122,7; 118,69; 117,0; 114,1; 30,0.

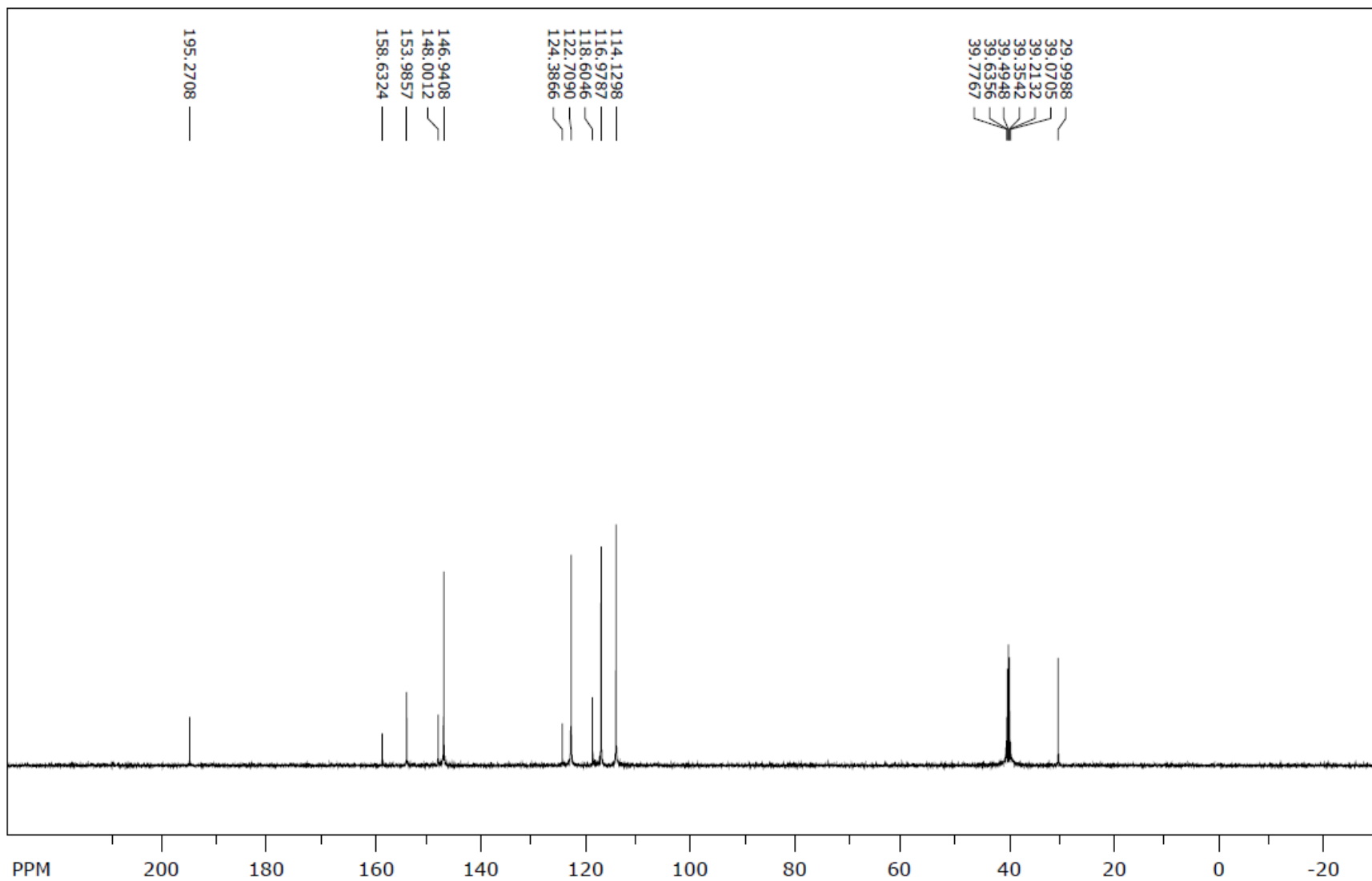
Maseni spektar (5c)



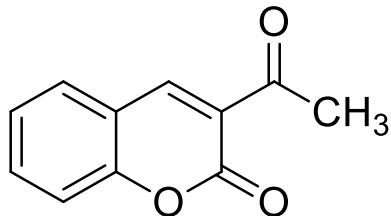
¹H NMR spektr (5c)



¹³C NMR spektr (5c)

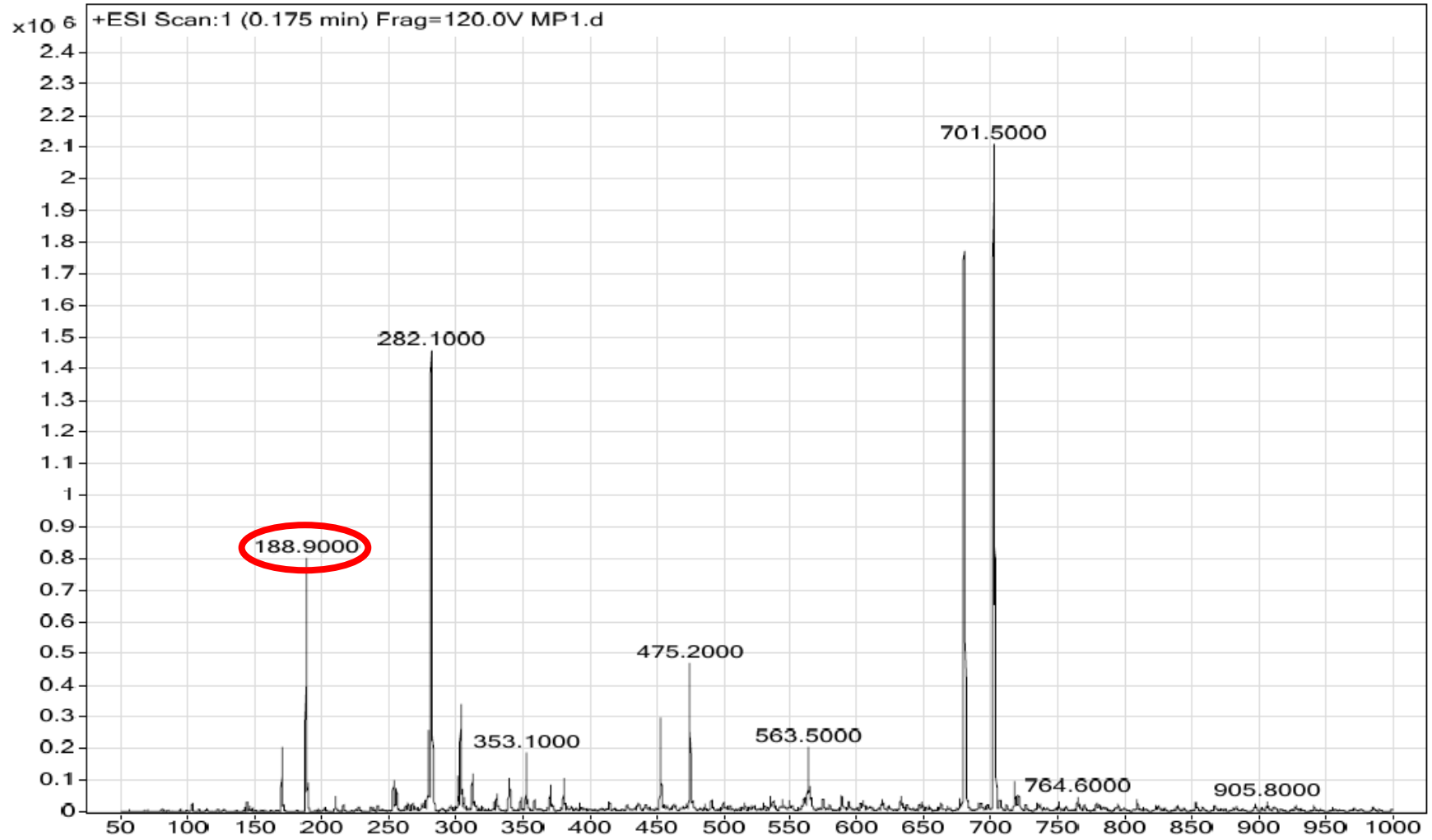


3-acetil-2H-kromen-2-on (5d)

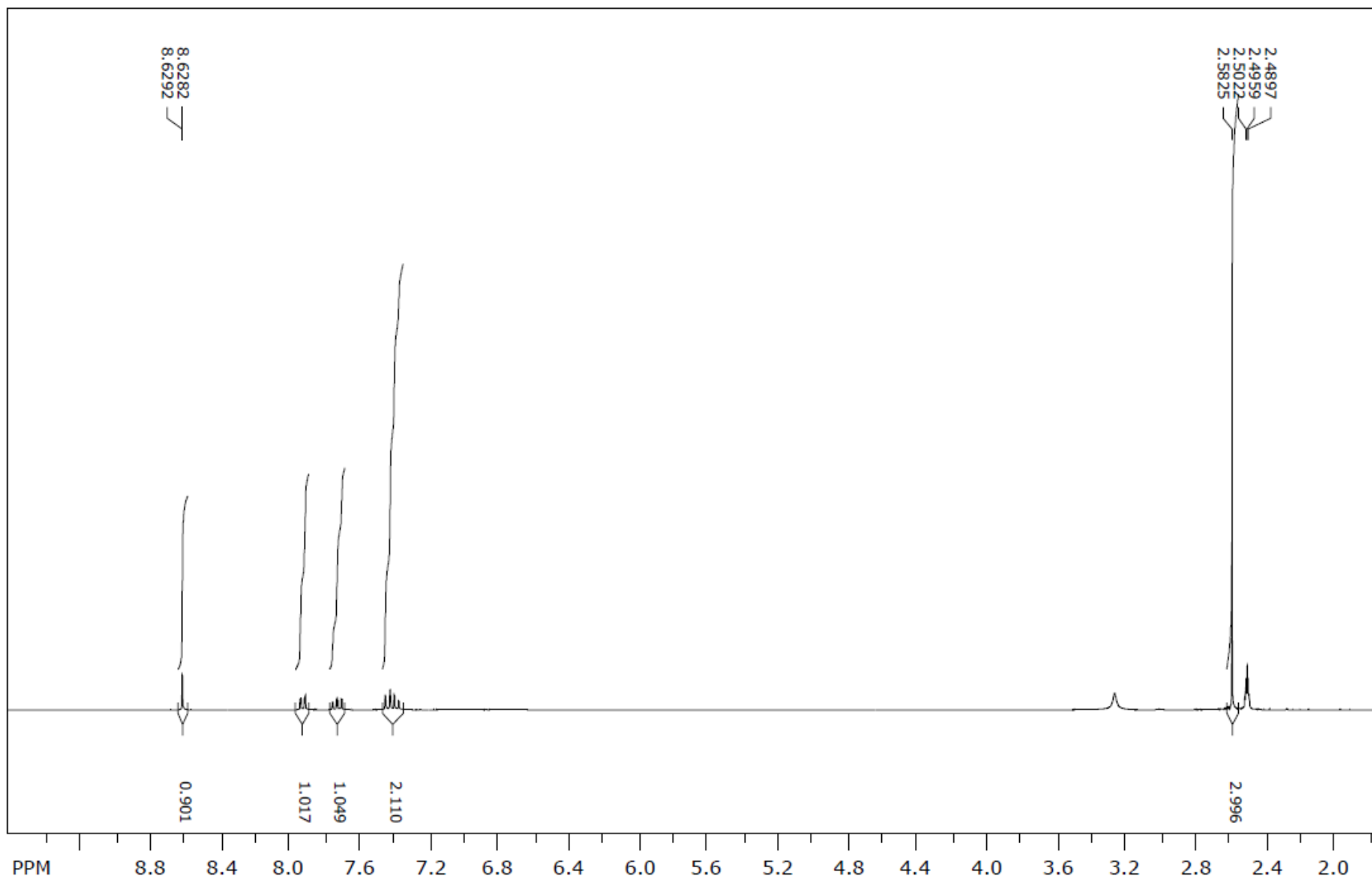


Reaktanti	Salicilaldehid (9,4 mmol) i etilacetoacetat (9,4 mmol)
Metoda pročišćavanja	Prekristalizacija iz etanola i metanola
Molekulska masa	188,17 g/mol
Molekulska formula	C ₁₁ H ₈ O ₃
Temperatura tališta	121 – 122 °C (lit. 118 °C, Phadtare i Shankarling, 2012)
Boja kristala	Žuta
R_f	0,79
LC/MS/MS <i>m/z</i> (M⁺)	188,90
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 8,63 (s, 1H, coum.), 7,94 (dd, <i>J</i> = 7,71, 1,58 Hz, 1H, arom.), 7,71 – 7,76 (m, 1H, arom.), 7,38 - 7,46 (m, 2H, arom.), 2,58 (s, 3H, CH ₃).
¹³C NMR	(75 MHz, CDCl ₃) δ 147,4; 134,9; 131,2; 125,4; 116,6; 30,4.

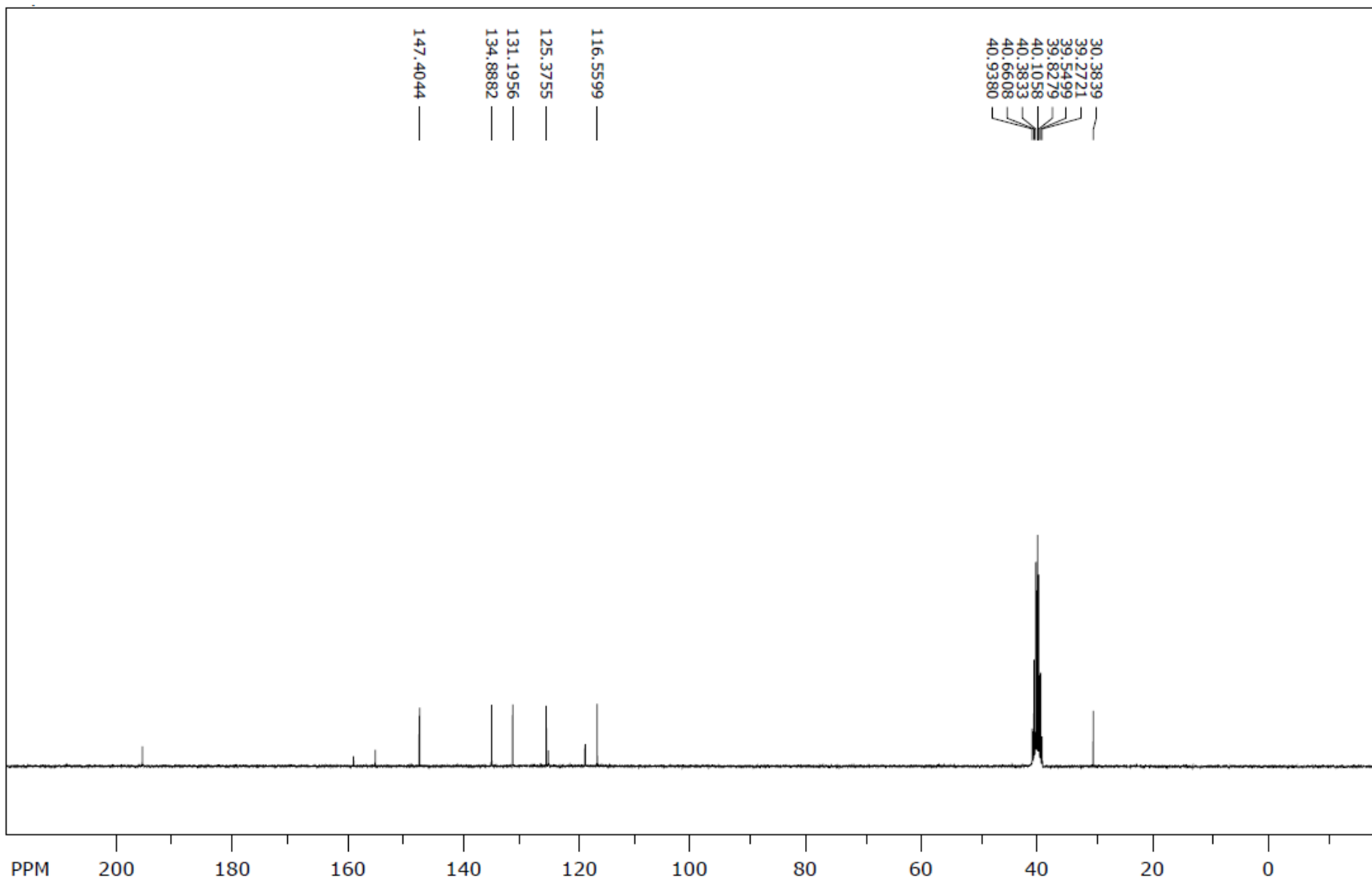
Maseni spektr (5d)



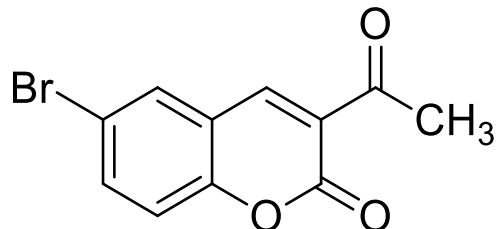
¹H NMR spektr (5d)



¹³C NMR spektr (5d)

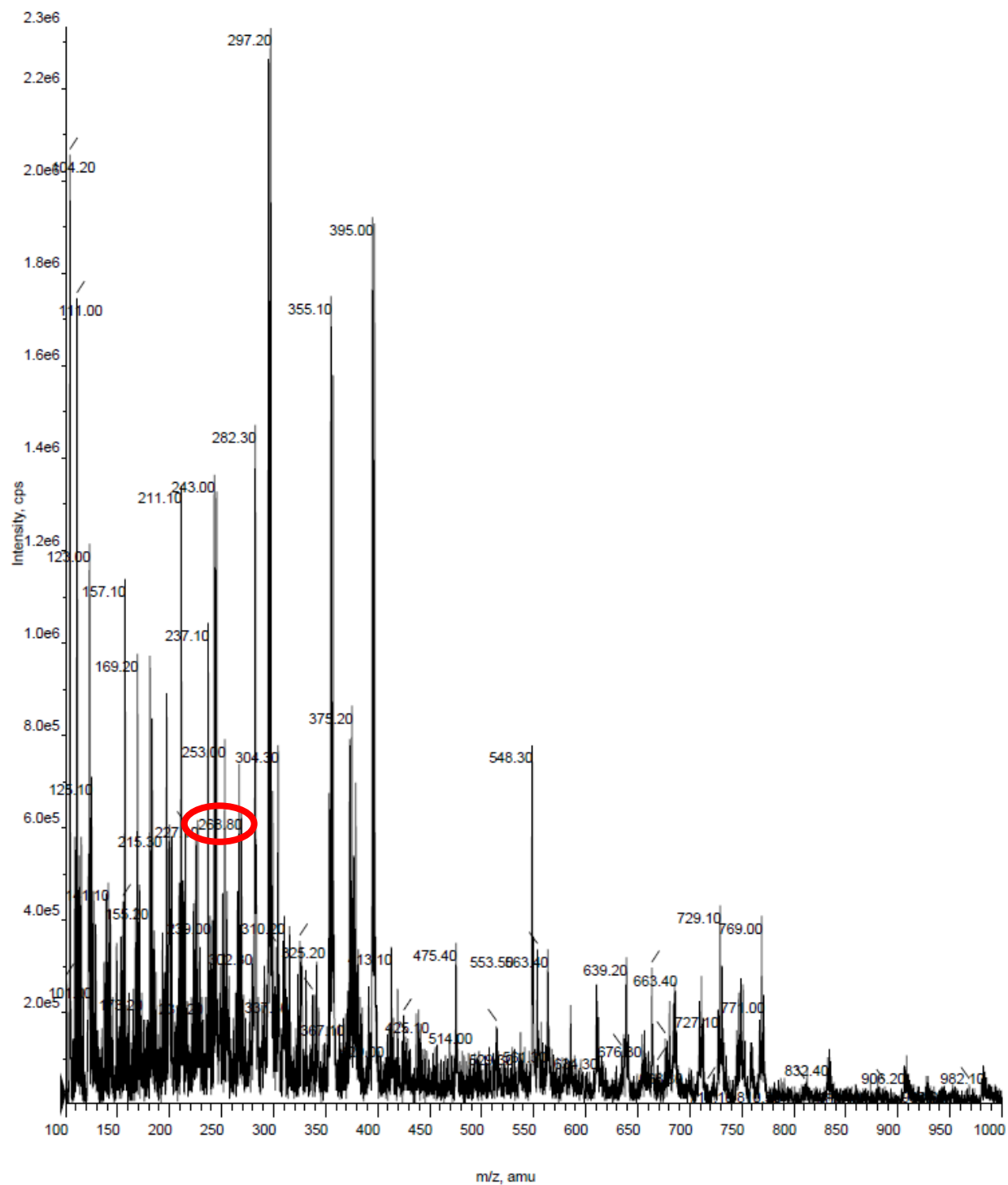


3-acetil-6-brom-2H-kromen-2-on (5e)

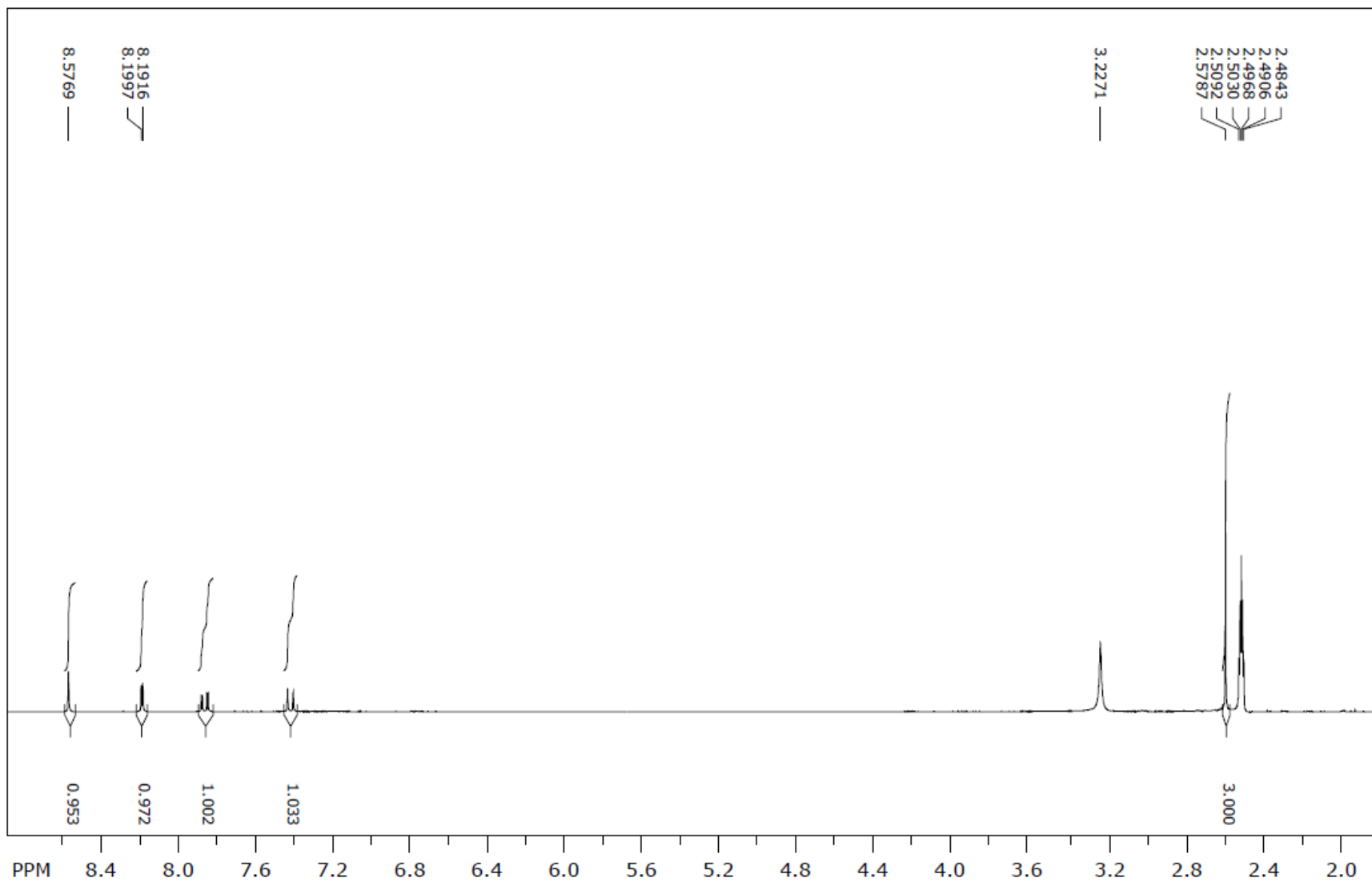


Reaktanti	5-bromsalicilaldehid (4,9 mmol) i etilacetoacetat (4,9 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	267,08 g/mol
Molekulska formula	C ₁₁ H ₇ BrO ₃
Temperatura tališta	229 – 232 °C (lit. 231 – 233 °C, Liu i sur., 2008)
Boja kristala	Bijela
R_f	0,84
LC/MS/MS <i>m/z</i> (M⁺)	268,80
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 8,58 (s, 1H, coum.), 8,20 (d, <i>J</i> = 2,43 Hz, 1H, arom.), 7,87 (dd, <i>J</i> = 8,85, 2,43 Hz, 1H, arom.), 7,43 (d, <i>J</i> = 8,85 Hz, 1H, arom.), 2,58 (s, 3H, CH ₃).
¹³C NMR	(75 MHz, CDCl ₃) δ 195,4; 158,4; 154,1; 146,0; 137,0; 133,0; 118,9; 116,8; 30,34.

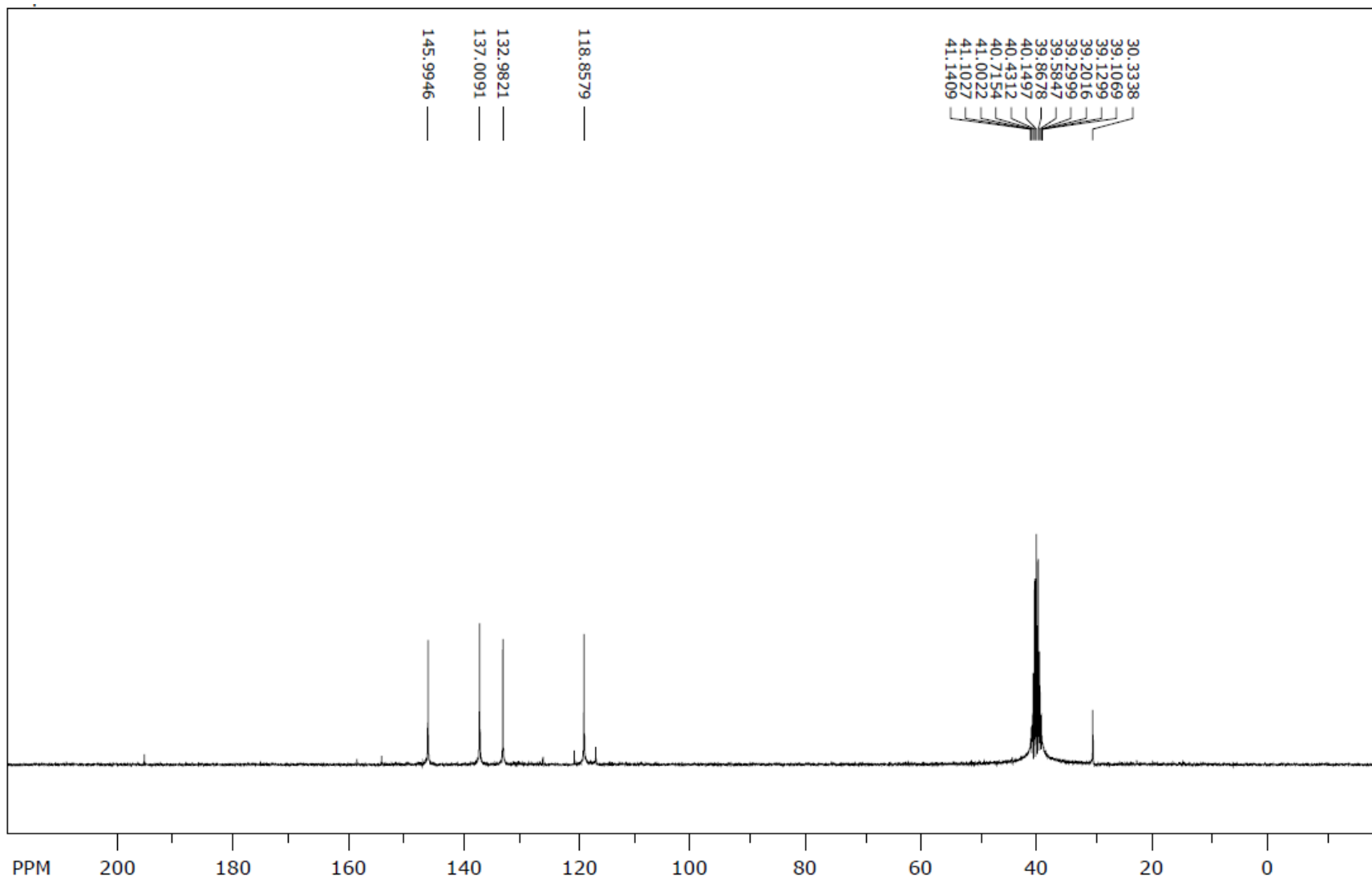
Maseni spektr (5e)



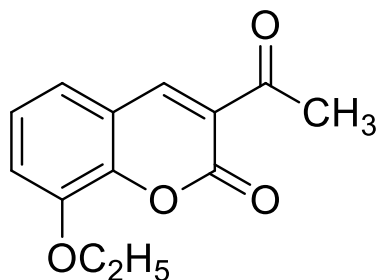
¹H NMR spektr (5e)



¹³C NMR spektr (5e)

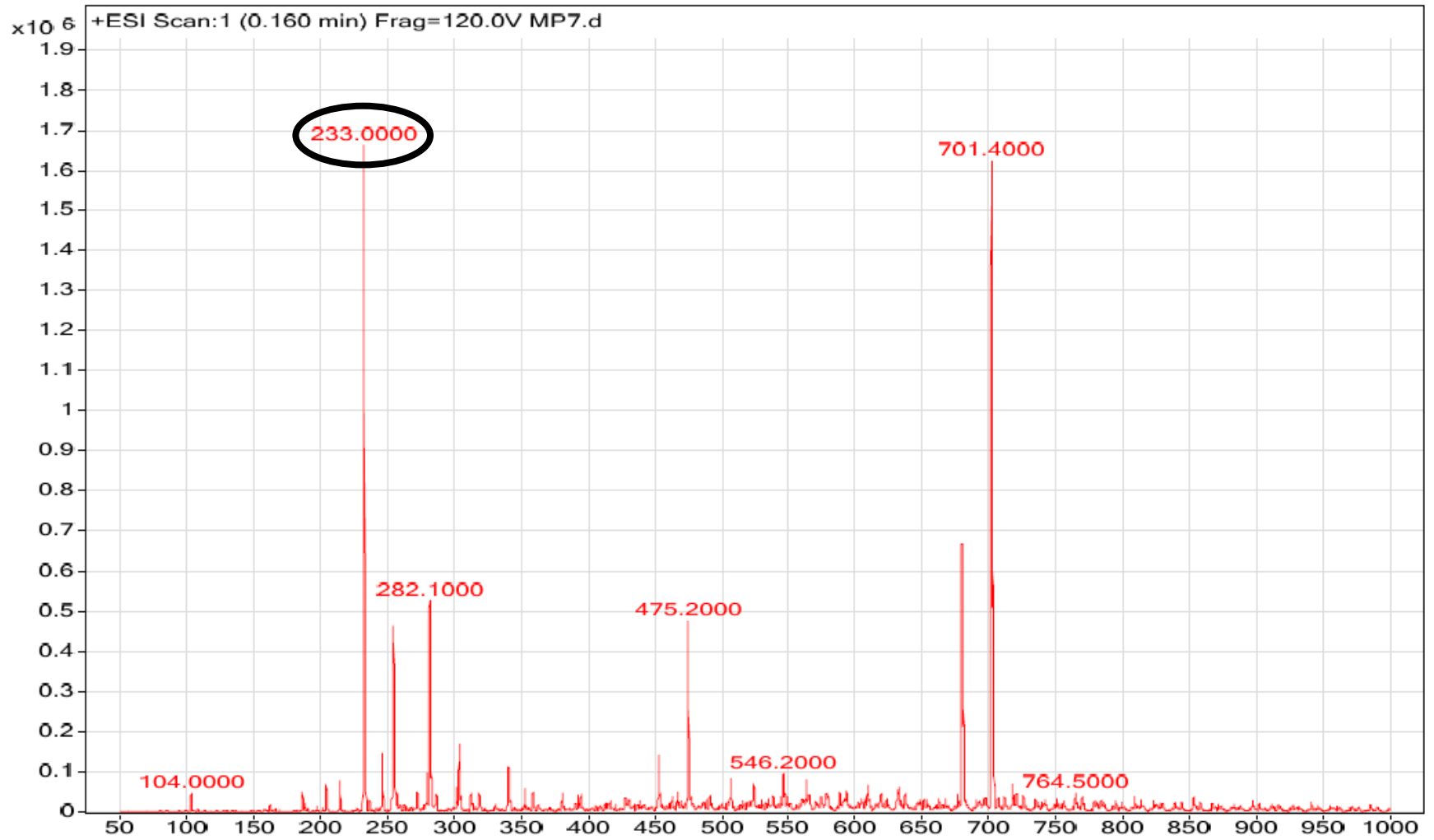


3-acetil-8-etoksi-2H-kromen-2-on (5f)

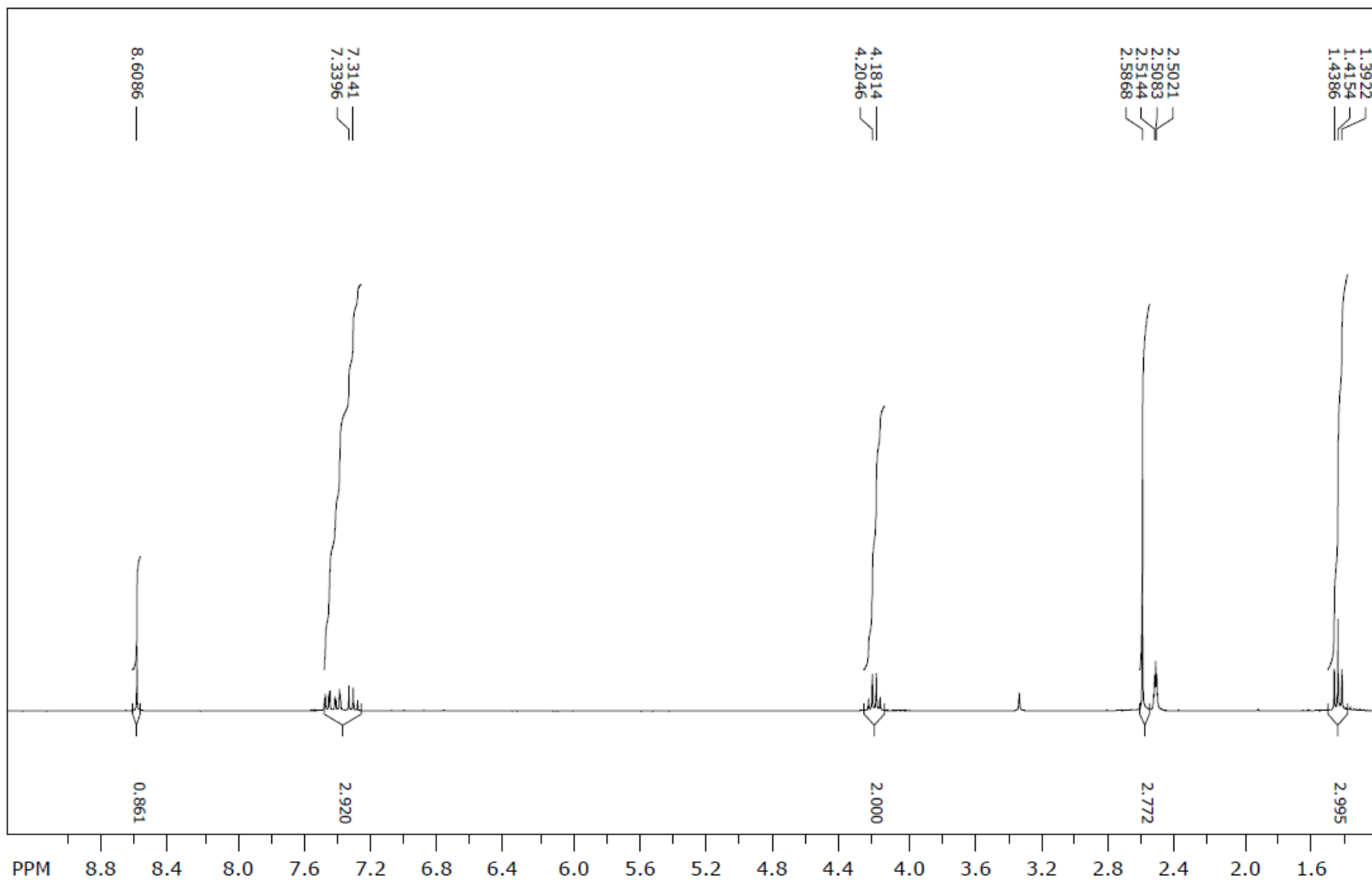


Reaktanti	3-etoksisalicilaldehid (6,0 mmol) i etilacetoacetat (6,0 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	232,23 g/mol
Molekulska formula	C ₁₃ H ₁₂ O ₄
Temperatura tališta	139 – 141 °C
Boja kristala	Svijetložuta
R_f	0,79
LC/MS/MS <i>m/z</i> (M⁺)	233,00
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 8,61 (s, 1H, coum.), 7,46 (dd, <i>J</i> = 7,65, 1,50 Hz, 1H, arom.), 7,41 (dd, <i>J</i> = 8,19, 1,53 Hz, 1H, arom.), 7,31 (t, <i>J</i> = 7,65, 8,10 Hz, 1H, arom.) 4,19 (q, <i>J</i> = 6,97 Hz, 2H, CH ₂ CH ₃), 2,59 (s, 3H, CH ₃), 1,42 (t, <i>J</i> = 6,96 Hz, 3H, CH ₂ CH ₃).
¹³C NMR	(75 MHz, CDCl ₃) δ 195,6; 158,7; 147,8; 145,9; 144,5; 125,3; 122,1; 119,3; 117,8; 64,9; 30,5; 15,0.

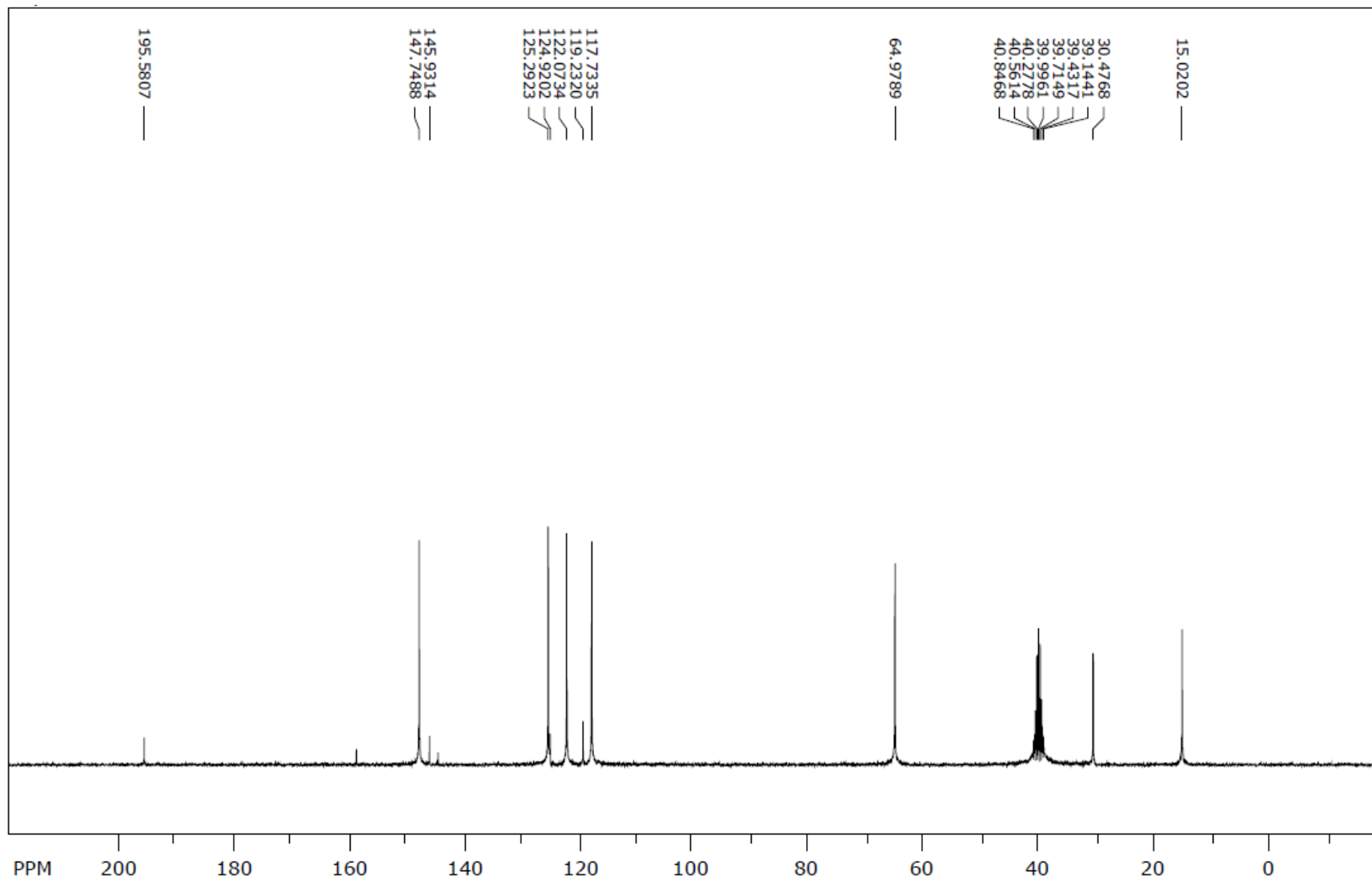
Maseni spektr (5f)



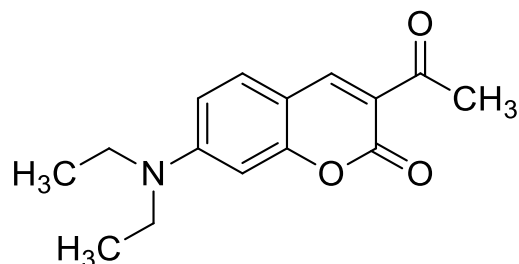
¹H NMR spektr (5f)



¹³C NMR spektr (5f)

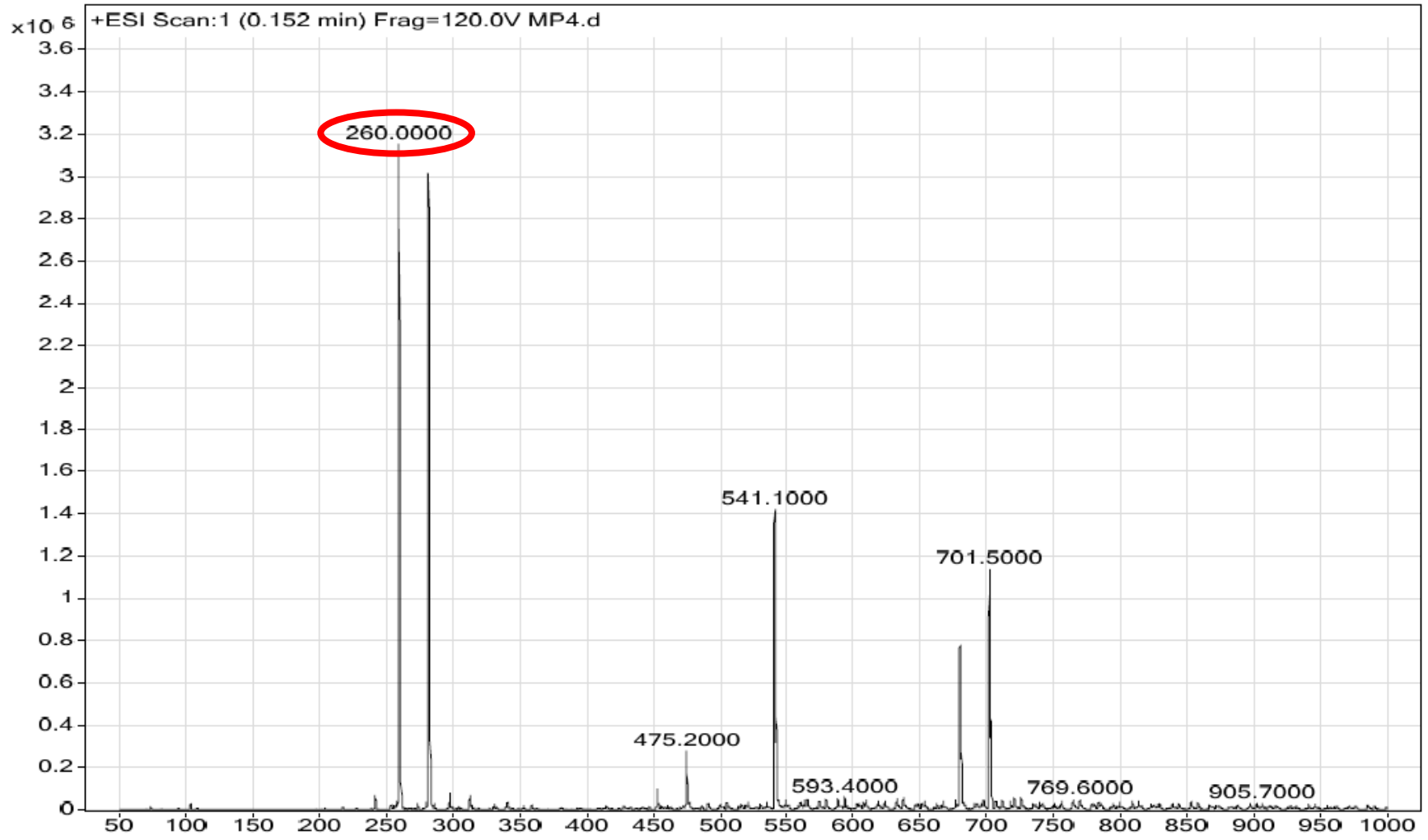


3-acetil-7-(dietilamino)-2H-kromen-2-on (5g)

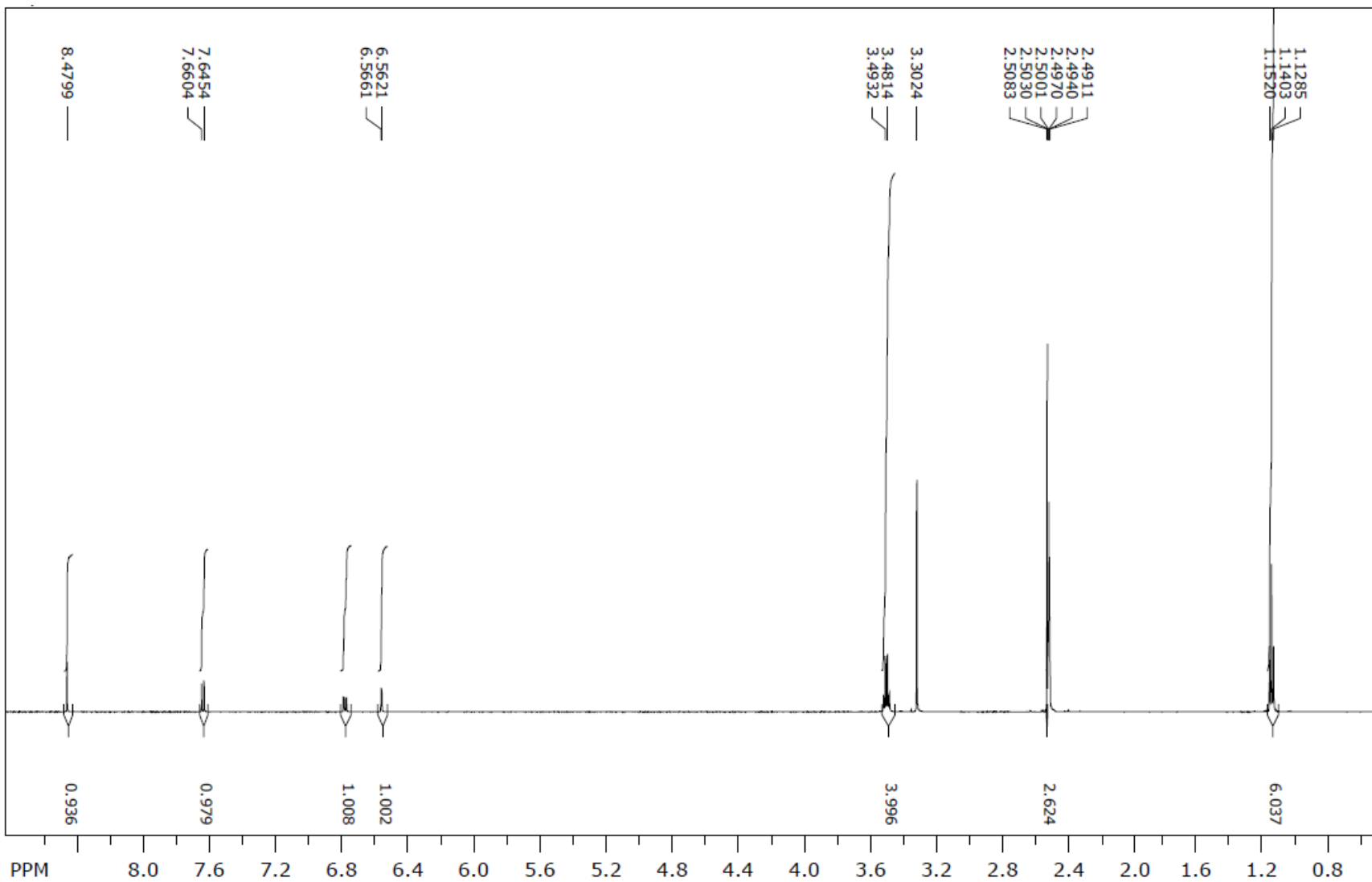


Reaktanti	4-(dietilamino)salicilaldehid (2,6 mmol) i etilacetoacetat (2,6 mmol)
Metoda pročiščavanja	Prekristalizacija iz etanola
Molekulska masa	259,30 g/mol
Molekulska formula	C ₁₅ H ₁₇ NO ₃
Temperatura tališta	153 – 156 °C (lit. 152 – 153 °C, Bogdač, 1998)
Boja kristala	Tamnožuta
R_f	0,72
LC/MS/MS m/z (M⁺)	260,00
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,48 (s, 1H, coum.), 7,65 (d, <i>J</i> = 9,00 Hz, 1H, arom.), 6,79 (dd, <i>J</i> = 9,06, 2,46 Hz, 1H, arom.), 6,56 (d, <i>J</i> = 2,40 Hz, 1H, arom.), 3,49 (q, <i>J</i> = 7,06 Hz, 4H, CH ₂ CH ₃), 2,49 - 2,51 (m, 3H, CH ₃), 1,14 (t, <i>J</i> = 7,05 Hz, 6H, CH ₂ CH ₃).
¹³C NMR	(150 MHz, CDCl ₃) δ 194,2; 147,6; 132,4; 110,1; 107,5; 95,8; 44,4; 30,1; 12,3.

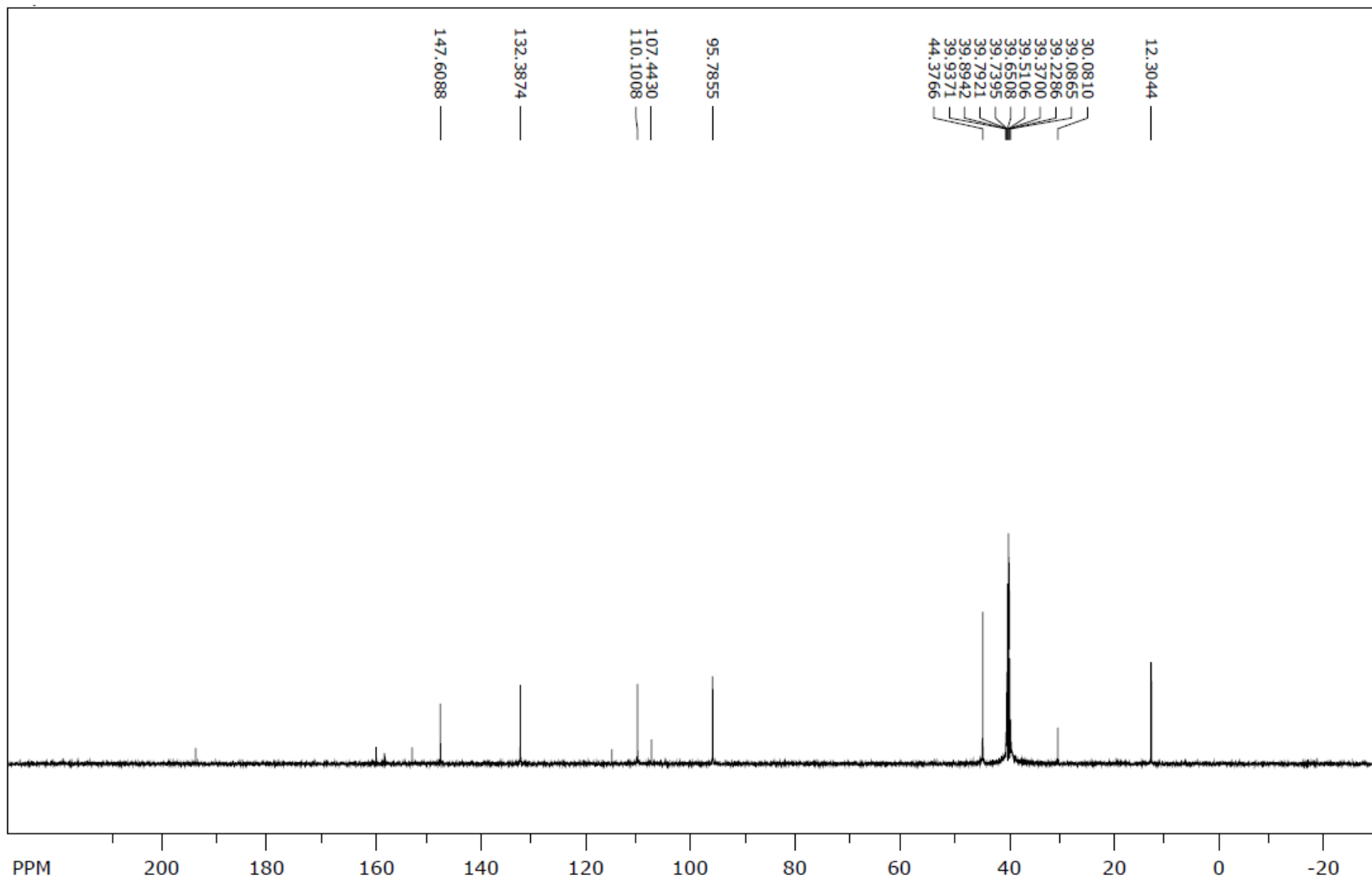
Maseni spektr (5g)



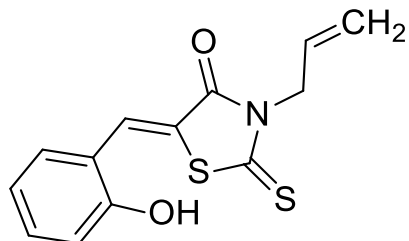
¹H NMR spektr (5g)



¹³C NMR spektar (5g)

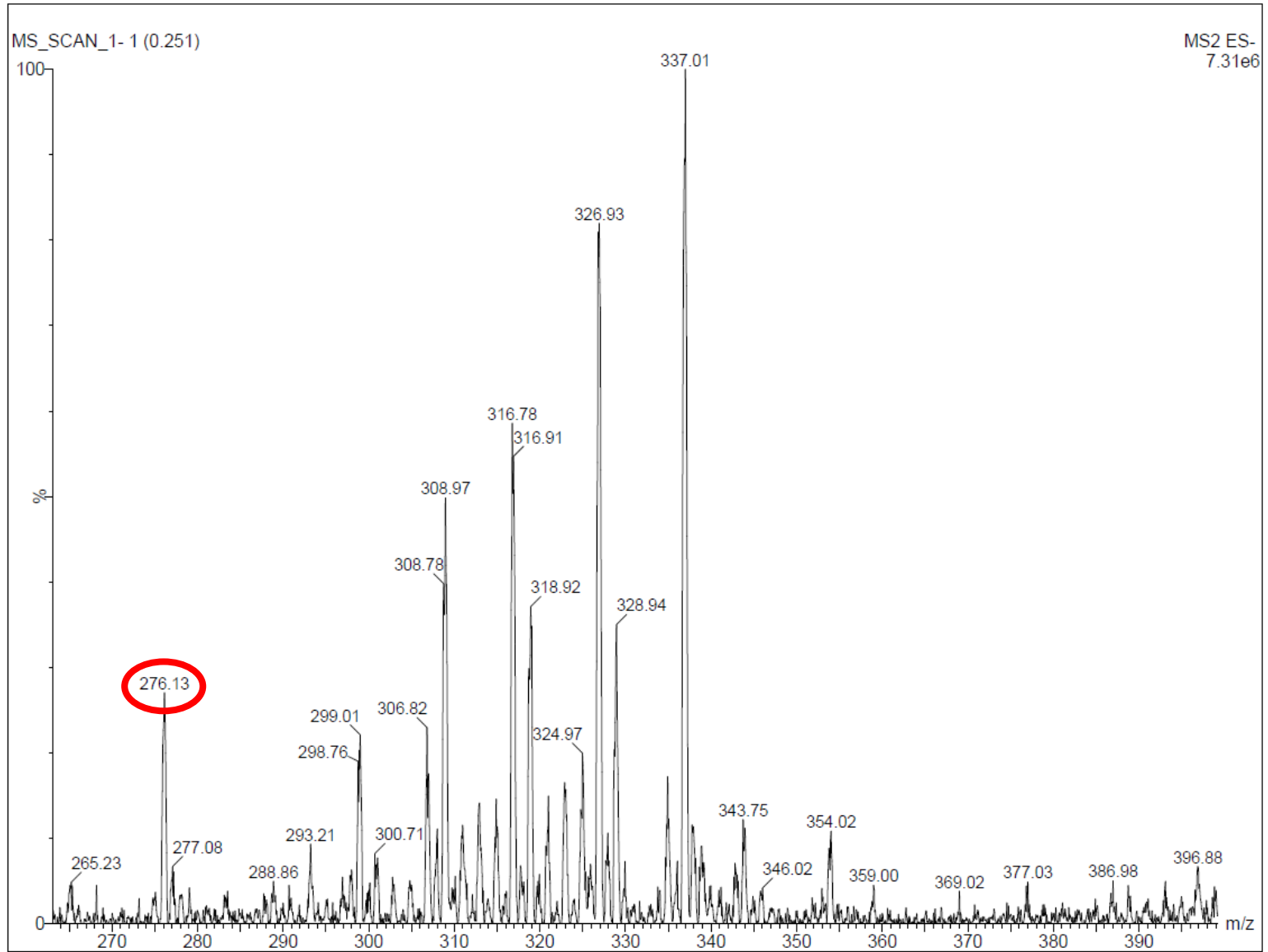


3-alil-5-(2-hidroksibenziliden)-2-tioksotiazolidin-4-on (6a)

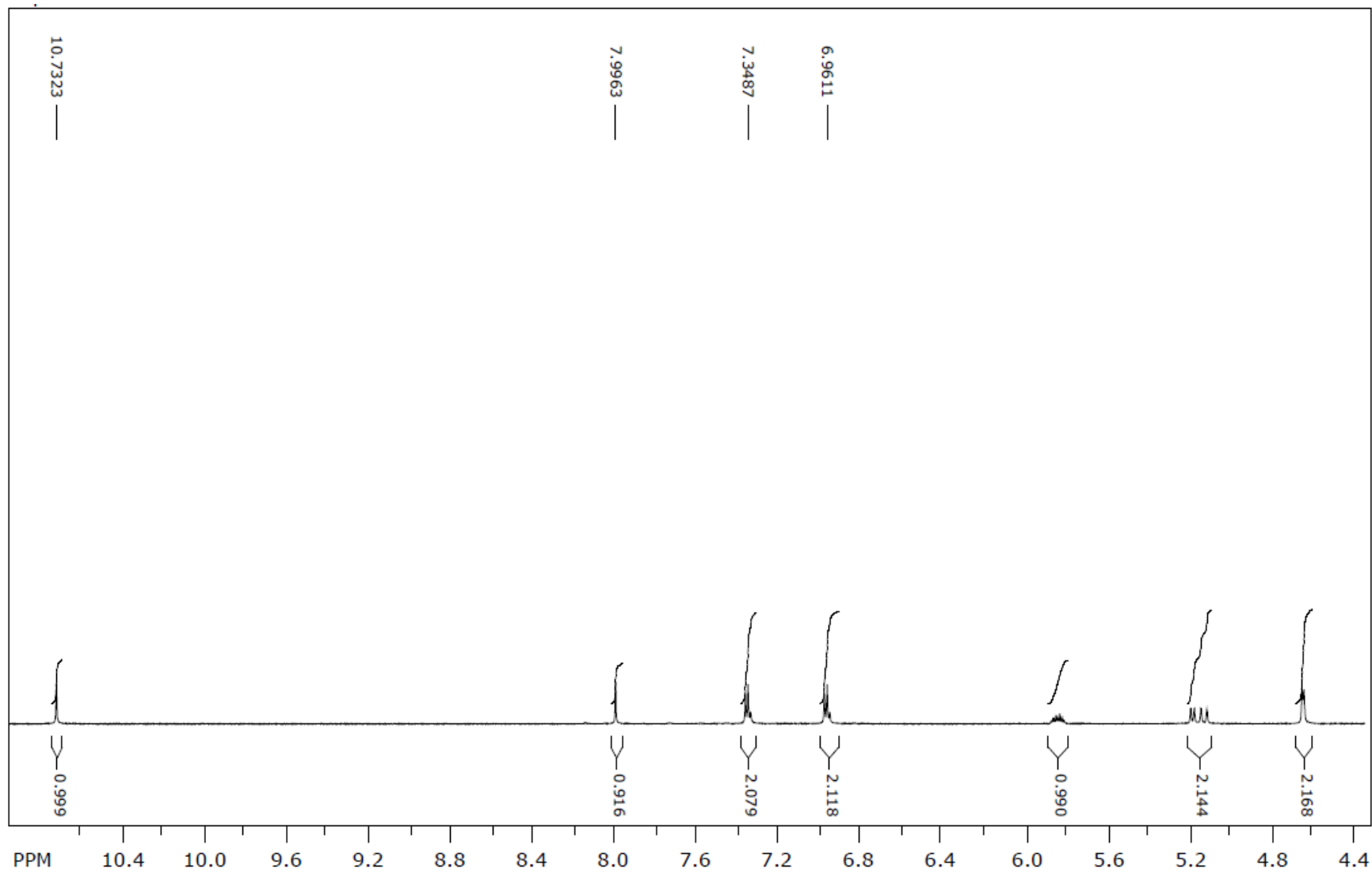


Reaktanti	Salicilaldehid (2 mmol) i 3-alilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	277,36 g/mol
Molekulska formula	C ₁₃ H ₁₁ NO ₂ S ₂
Temperatura tališta	180 – 182 °C
Boja kristala	Žuta
R_f	0,72
LC/MS/MS <i>m/z</i> (M-)	276,13
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 10,73 (s, 1H, OH), 7,96 (s, 1H, CH), 7,35 (t, <i>J</i> = 7,60 Hz, 2H, arom.), 6,95 (t, <i>J</i> = 8,04, 7,68 Hz, 2H, arom.), 5,81 – 5,87 (m, 1H, CH), 5,17 (dd, <i>J</i> = 10,32; 0,84 Hz, 1H, CH ₂), 5,12 (dd, <i>J</i> = 17,28; 0,84 Hz, 1H, CH ₂) 4,63 (d, <i>J</i> = 5,16 Hz, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,47; 166,69; 157,59; 133,1; 129,6; 128,6; 120,6; 117,7; 117,5; 116,28; 45,9.

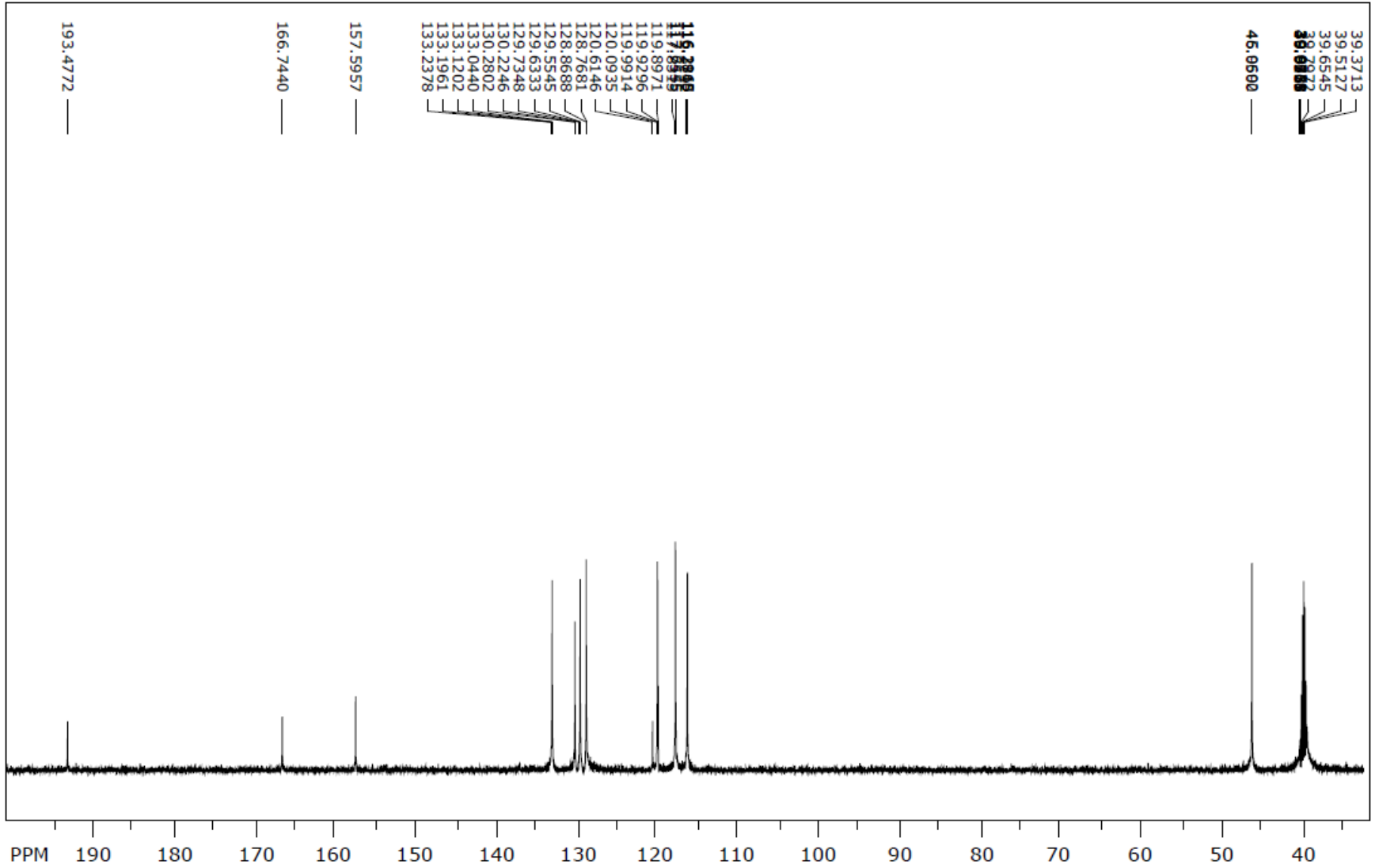
Maseni spektr (6a)



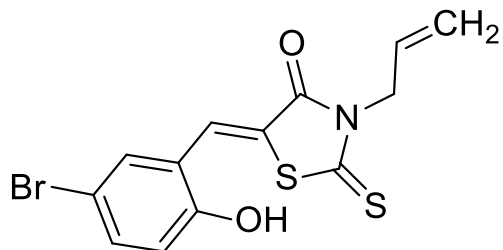
¹H NMR spektr (6a)



¹³C NMR spektr (6a)

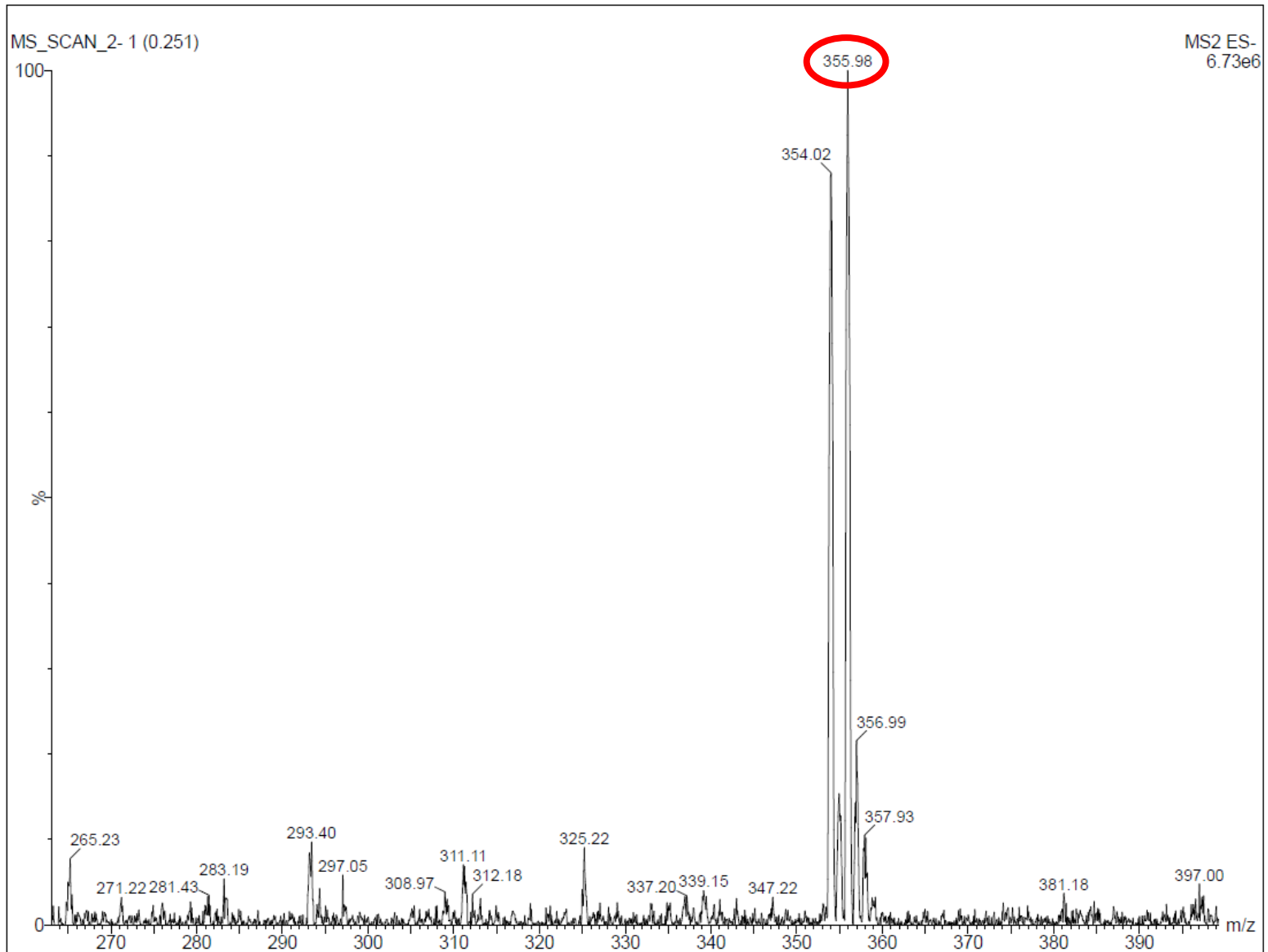


3-ailil-5-(5-brom-2-hidroksibenziliden)-2-tioksotiazolidin-4-on (6b)

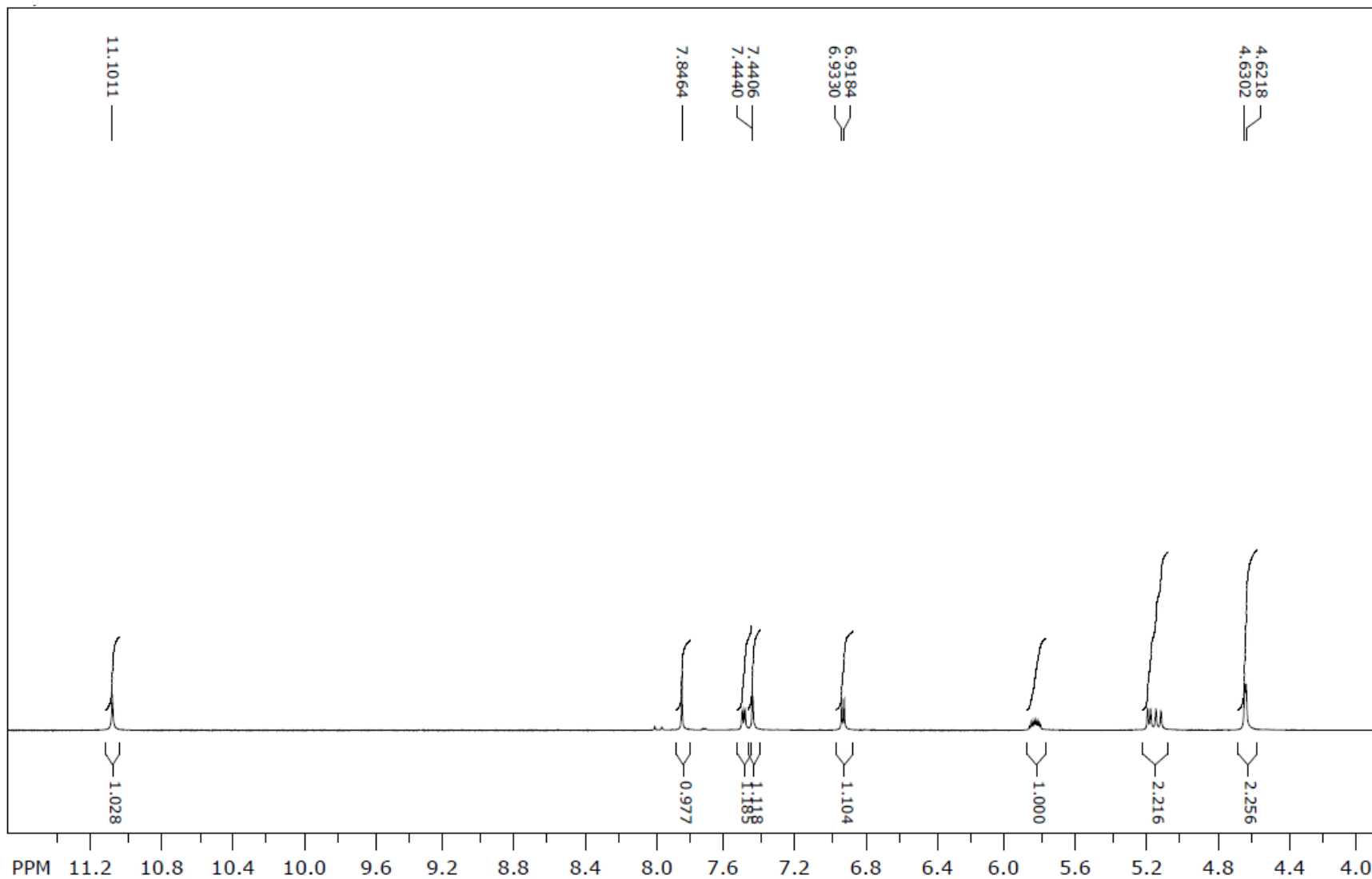


Reaktanti	5-bromsalicilaldehid (2 mmol) i 3-ailirodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	356,26 g/mol
Molekulska formula	C ₁₃ H ₁₀ BrNO ₂ S ₂
Temperatura tališta	203 – 204 °C
Boja kristala	Žuta
R_f	0,71
LC/MS/MS m/z (M-)	355,98
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 11,10 (s, 1H, OH), 7,84 (s, 1H, CH), 7,49 (dd, <i>J</i> = 8,70; 2,19 Hz, 1H, arom.), 7,44 (d, <i>J</i> = 2,04 Hz, 1H, arom.), 6,93 (d, <i>J</i> = 8,76 Hz, 1H, arom.), 5,81 – 5,85 (m, 1H, CH), 5,18 (d, <i>J</i> = 10,08 Hz, 1H, CH ₂), 5,12 (d, <i>J</i> = 17,22 Hz, 1H, CH ₂), 4,63 (d, <i>J</i> = 5,04 Hz, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,19; 166,57; 156,46; 135,18; 131,66; 130,20; 127,48; 122,57; 122,12; 118,4; 117,8; 110,72; 46,03.

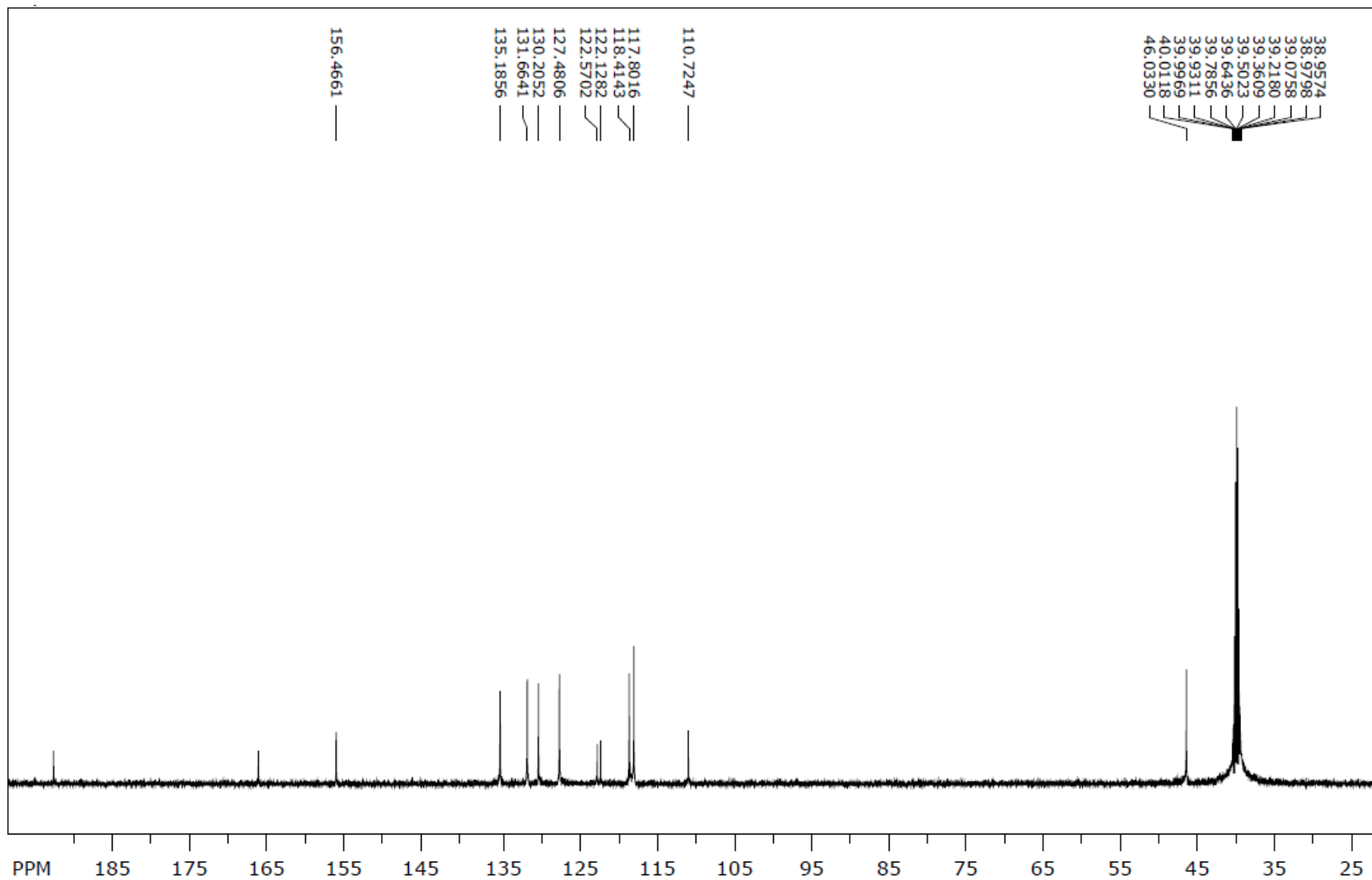
Maseni spektar (6b)



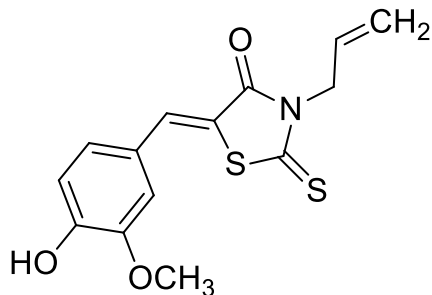
¹H NMR spektr (6b)



¹³C NMR spektr (6b)

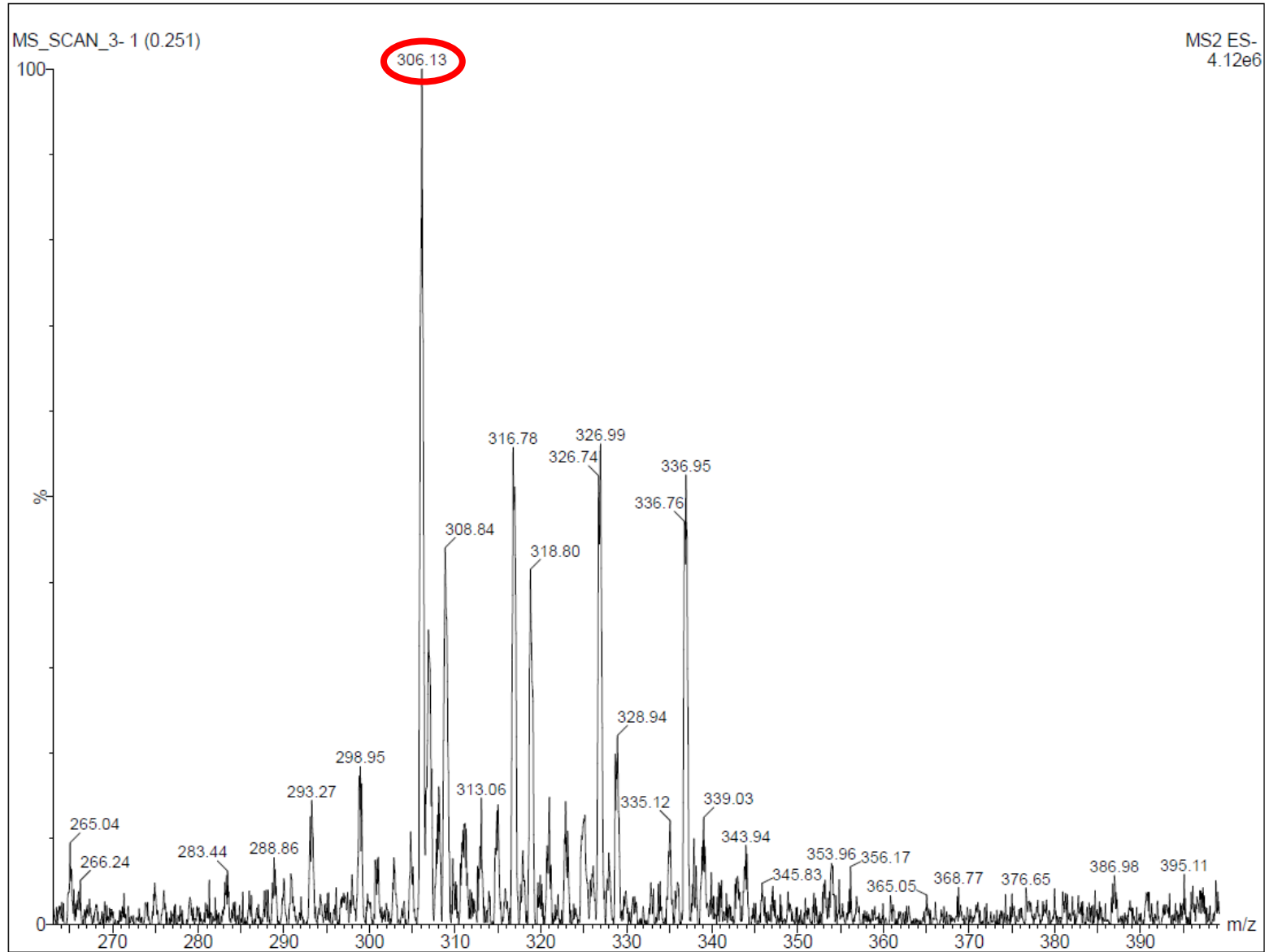


3-alil-5-(4-hidroksi-3-metoksibenziliden)-2-thioxothiazolidin-4-one (6c)

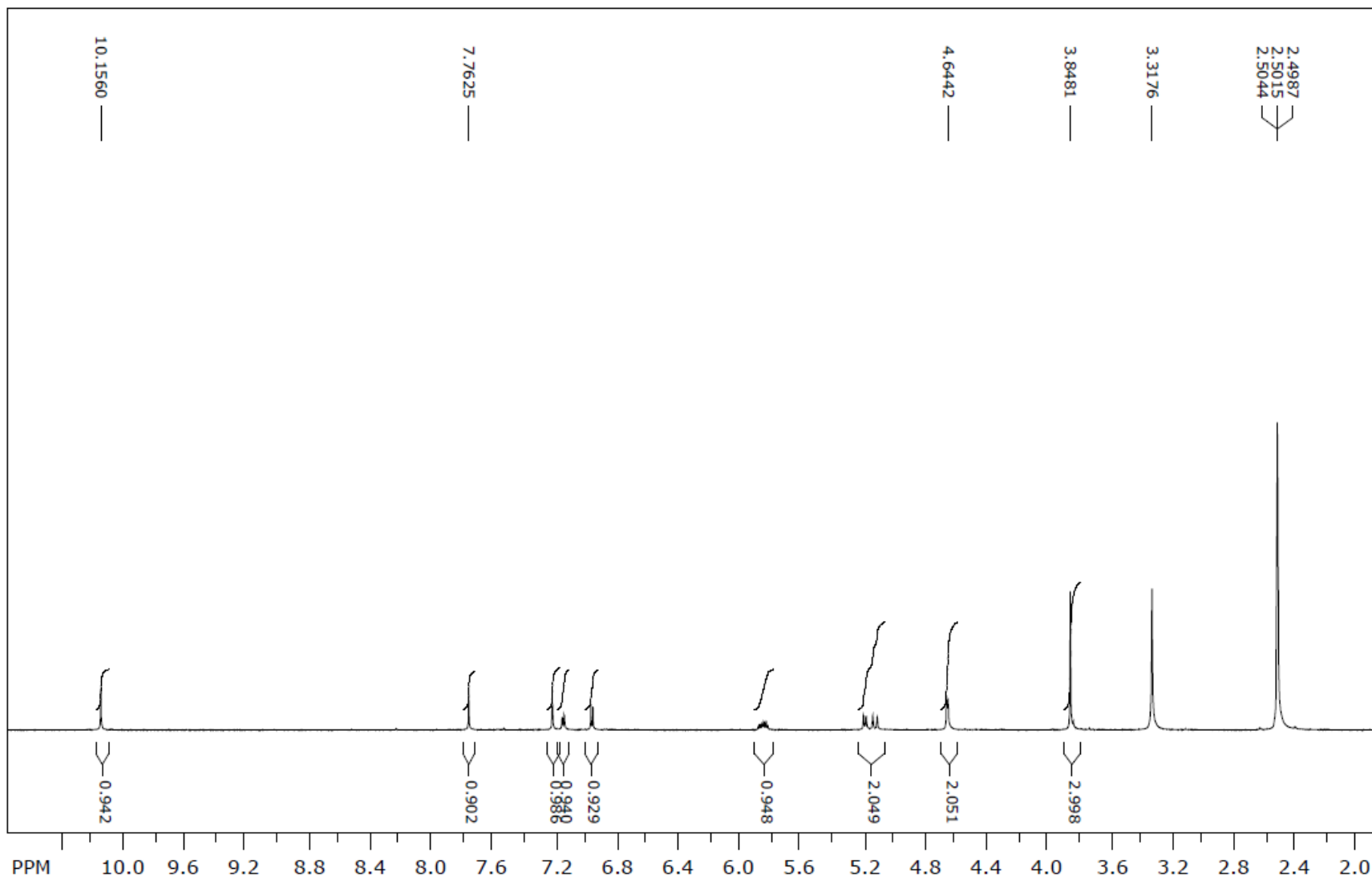


Reaktanti	3-metoksi-4-hidroksibenzaldehid (2 mmol) i 3-alilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	307,39 g/mol
Molekulska formula	C ₁₄ H ₁₃ NO ₃ S ₂
Temperatura tališta	143 – 144 °C
Boja kristala	Svijetlosmeđa
R_f	0,73
LC/MS/MS m/z (M-)	306,13
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 10,15 (s, 1H, OH), 7,76 (s, 1H, OH), 7,22 (d, <i>J</i> = 1,92 Hz, 1H, arom.), 7,15 (dd, <i>J</i> = 8,28; 1,92 Hz, 1H, arom.), 6,96 (d, <i>J</i> = 8,22 Hz, 1H, arom.), 5,82 – 5,88 (m, 1H, CH), 5,18 (dd, <i>J</i> = 10,32; 1,17 Hz, 1H, CH ₂), 5,12 (dd, <i>J</i> = 17,28; 1,14 Hz, 1H, CH ₂) 4,65 (d, <i>J</i> = 5,16 Hz, 1H, CH ₂), 3,85 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 192,80; 166,42; 135,07; 134,07; 131,30; 130,49; 130,13; 128,25; 124,15; 117, 84; 46,10.

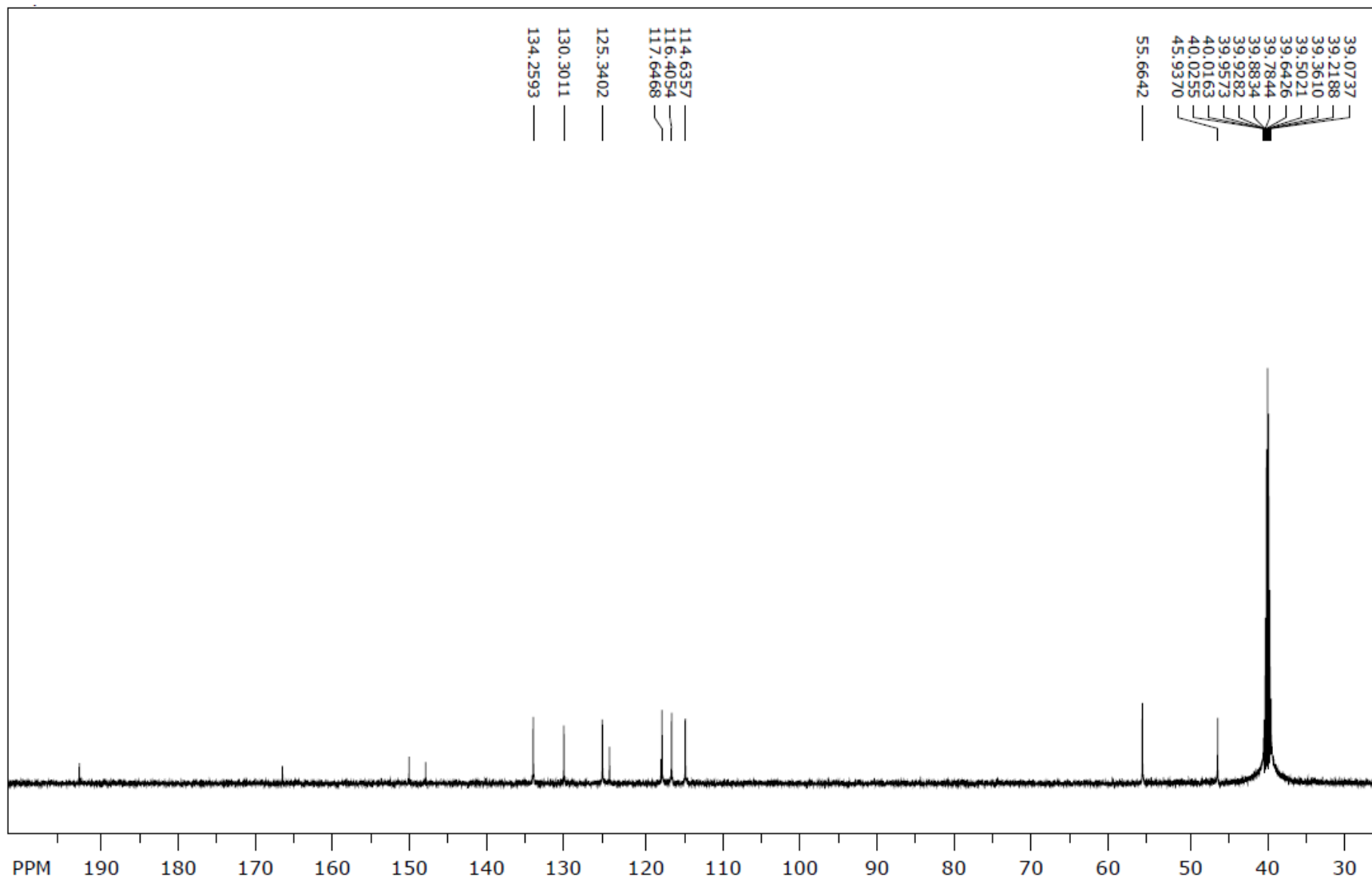
Maseni spektar (6c)



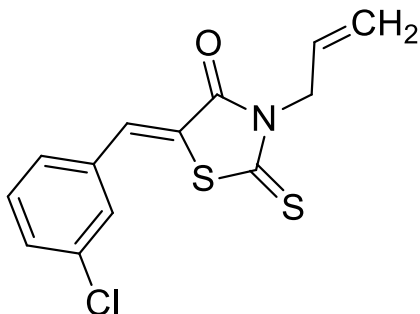
¹H NMR spektr (6c)



¹³C NMR spektr (6c)

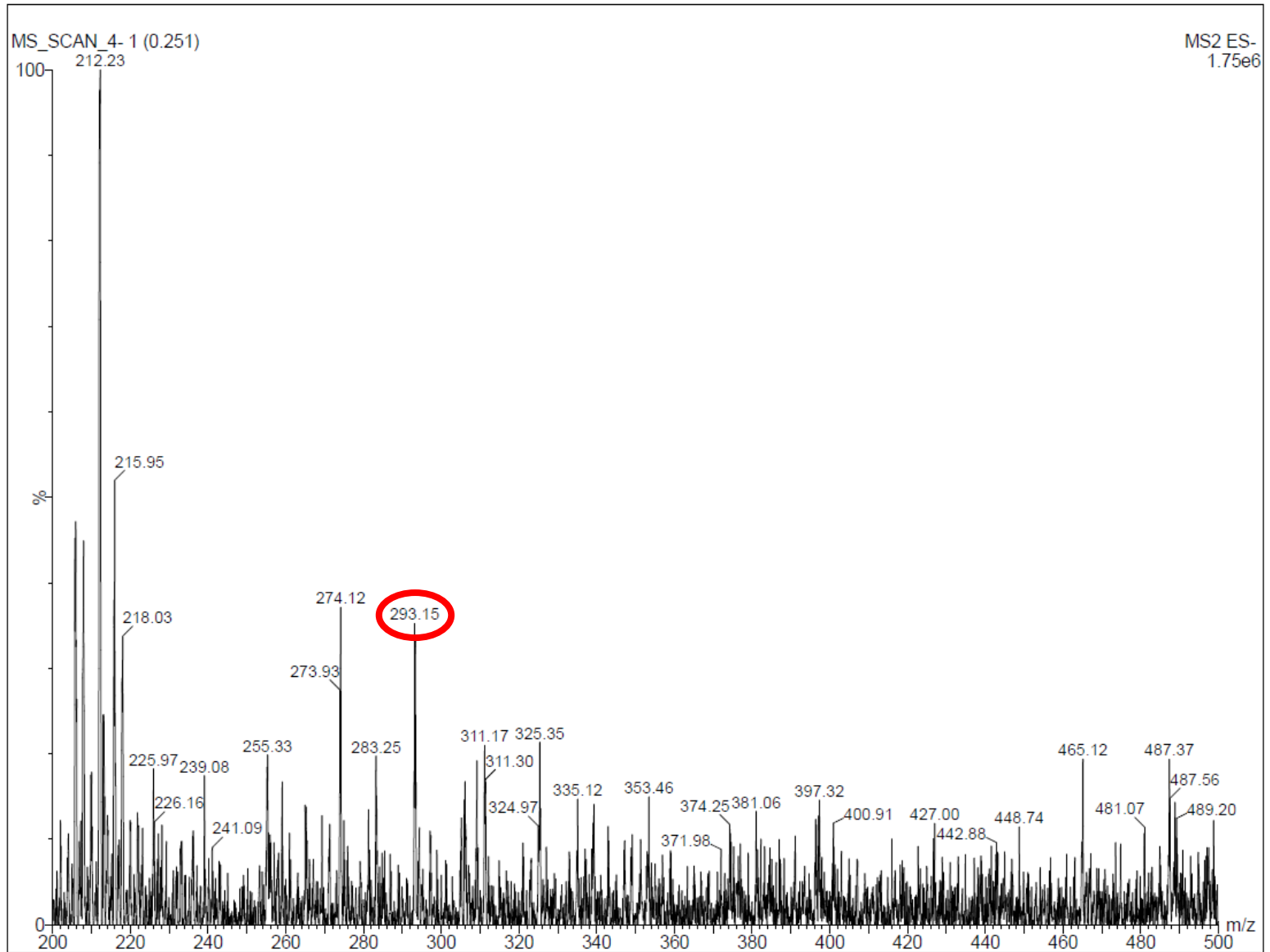


3-alil-5-(3-klorbenziliden)-2-tioksotiazolidin-4-on (6d)

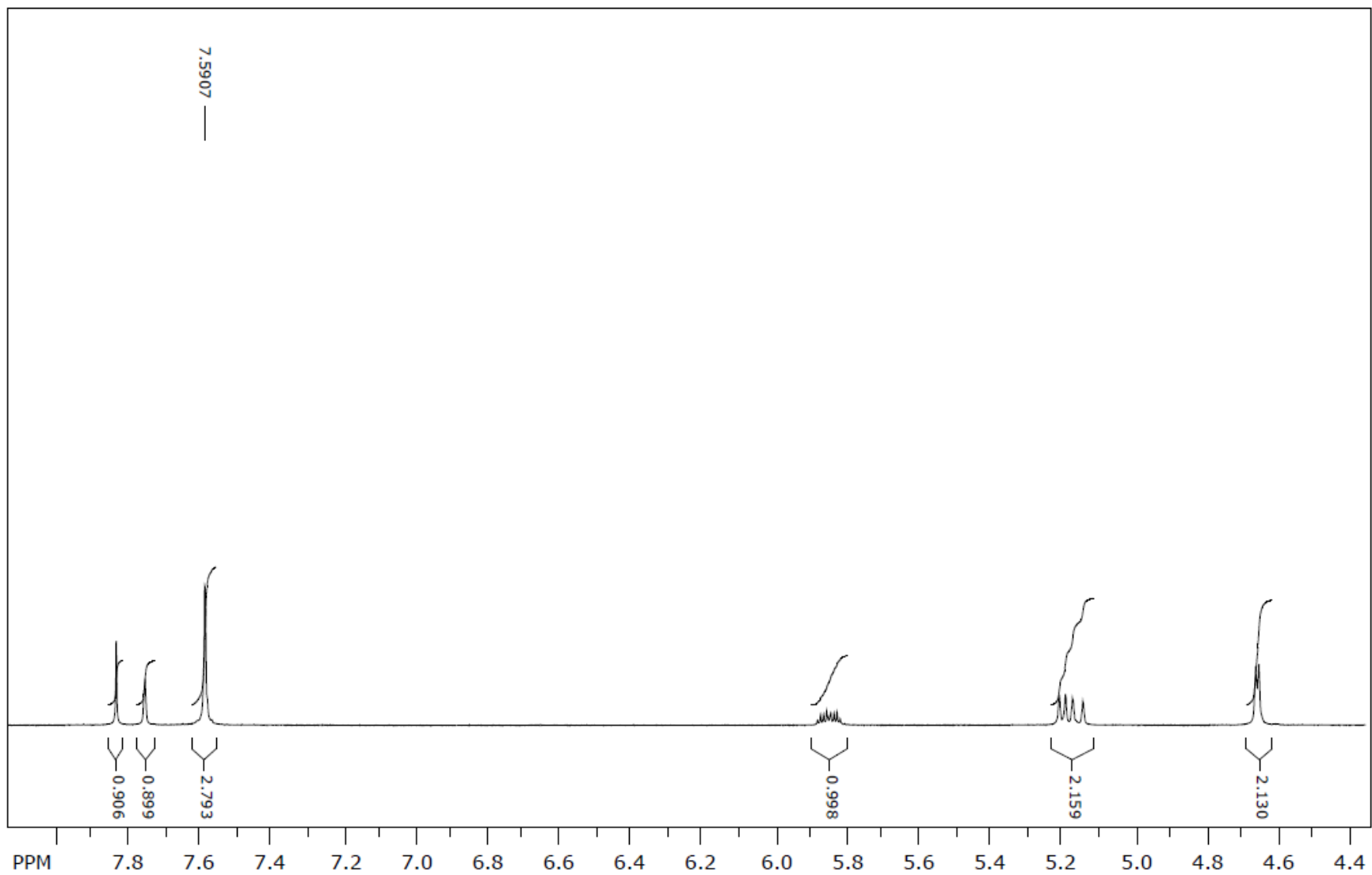


Reaktanti	3-klorbenzalhid (2 mmol) i 3-alilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	295,81 g/mol
Molekulska formula	C ₁₃ H ₁₀ ClNOS ₂
Temperatura tališta	106 -109 °C
Boja kristala	Tamnosmeđa
R_f	0,90
LC/MS/MS m/z (M⁻)	293,15
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,83 (s, 1H, CH), 7,75 (s, 1H, arom.), 7,59 (s, 3H, arom.), 5,82 – 5,88 (m, 1H, CH), 5,20 (dd, <i>J</i> = 10,38; 1,02 Hz, 1H, CH ₂), 5,15 (dd, <i>J</i> = 17,16; 1,11 Hz, 1H, CH ₂) 4,65 (d, <i>J</i> = 5,22 Hz, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 192,80; 166,42; 135,07; 134,07; 131,30; 130,49; 130,13; 128,25; 124,15; 117, 84; 46,10.

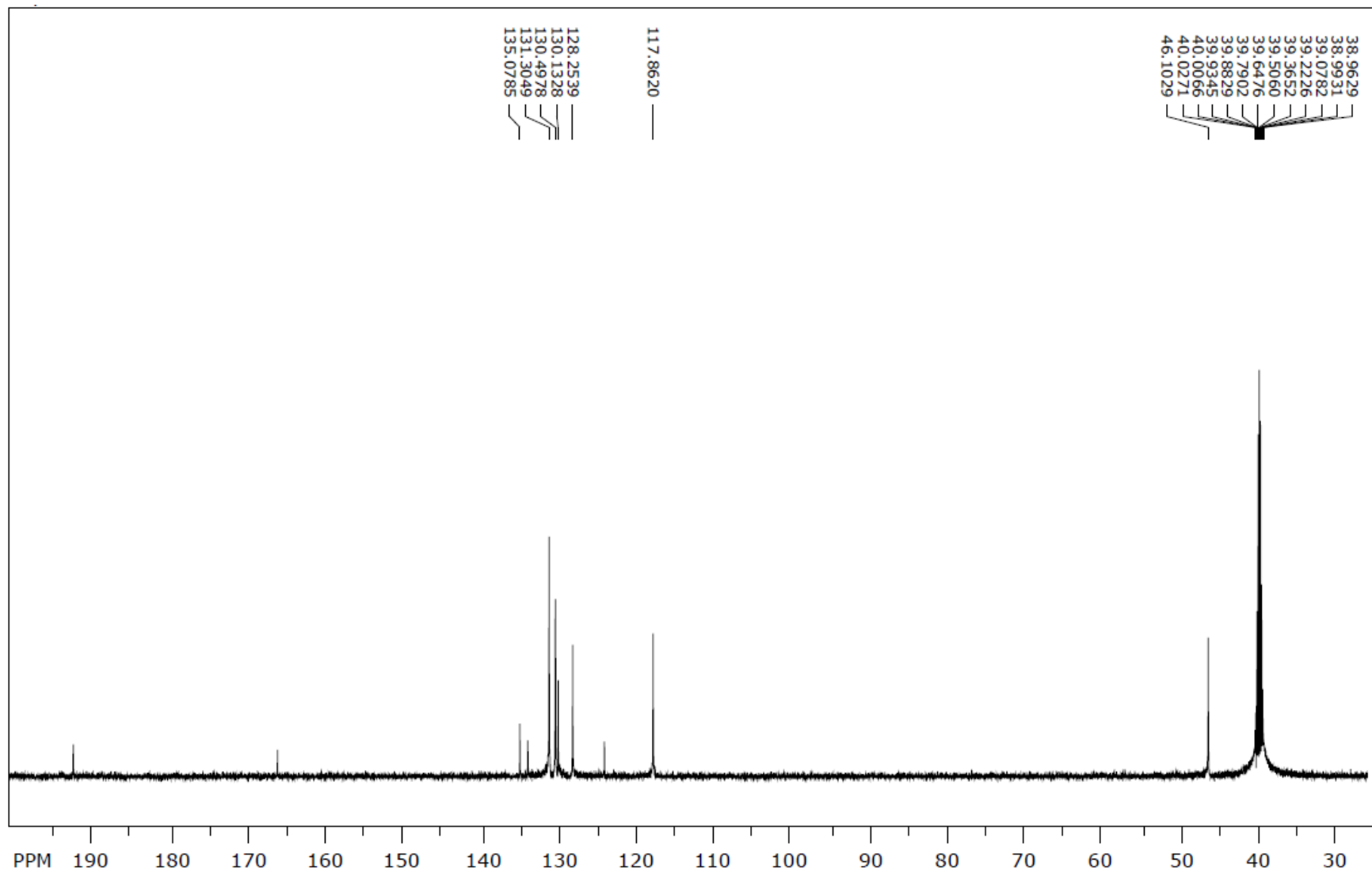
Maseni spektar (6d)



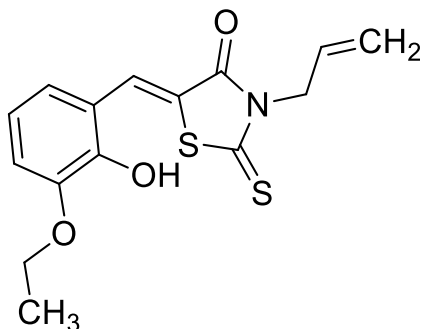
¹H NMR spektr (6d)



¹³C NMR spektr (6d)

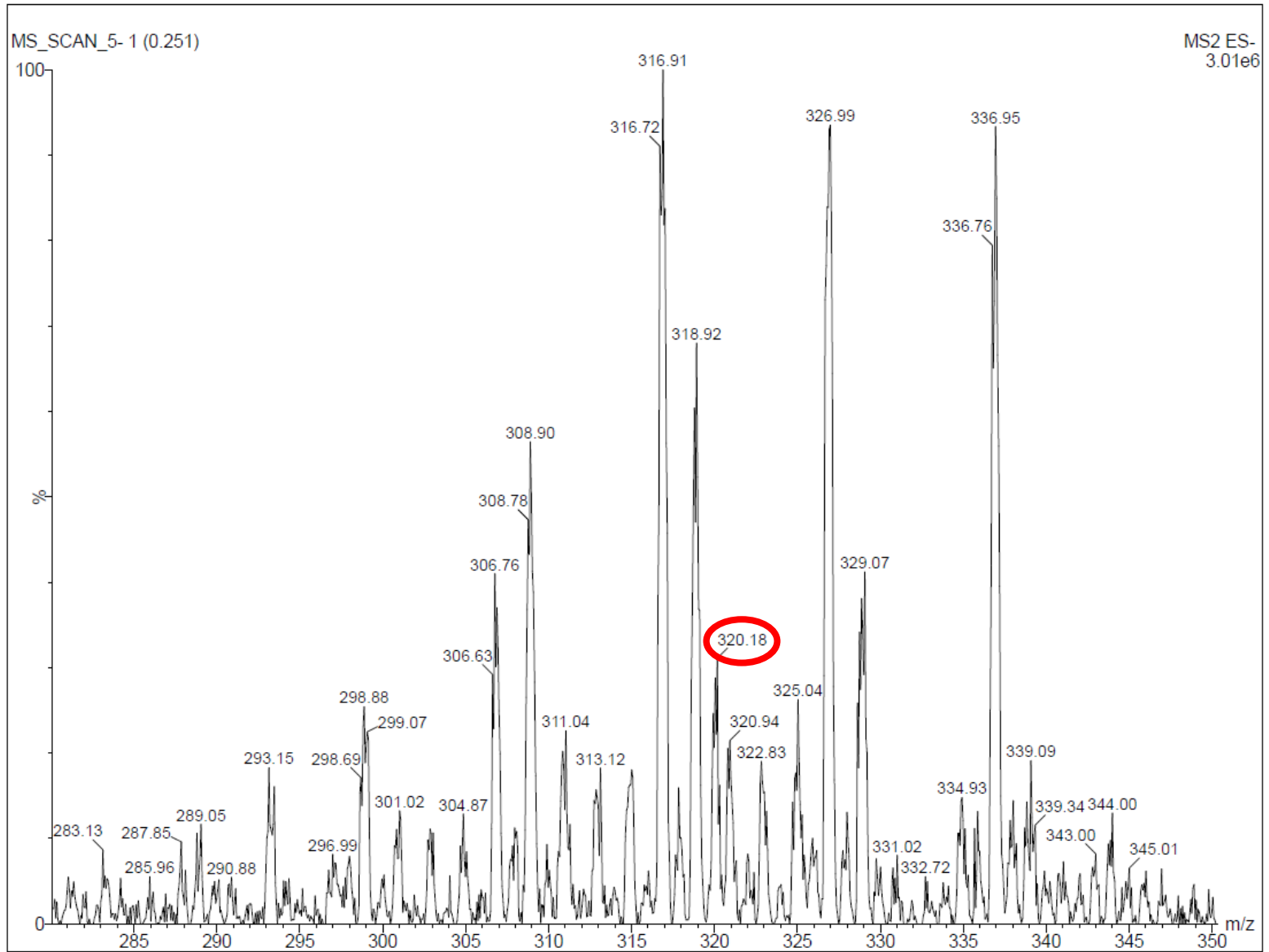


3-alil-5-(3-etoksi-2-hidroksibenziliden)-2-tioksotiazolidin-4-on (6e)

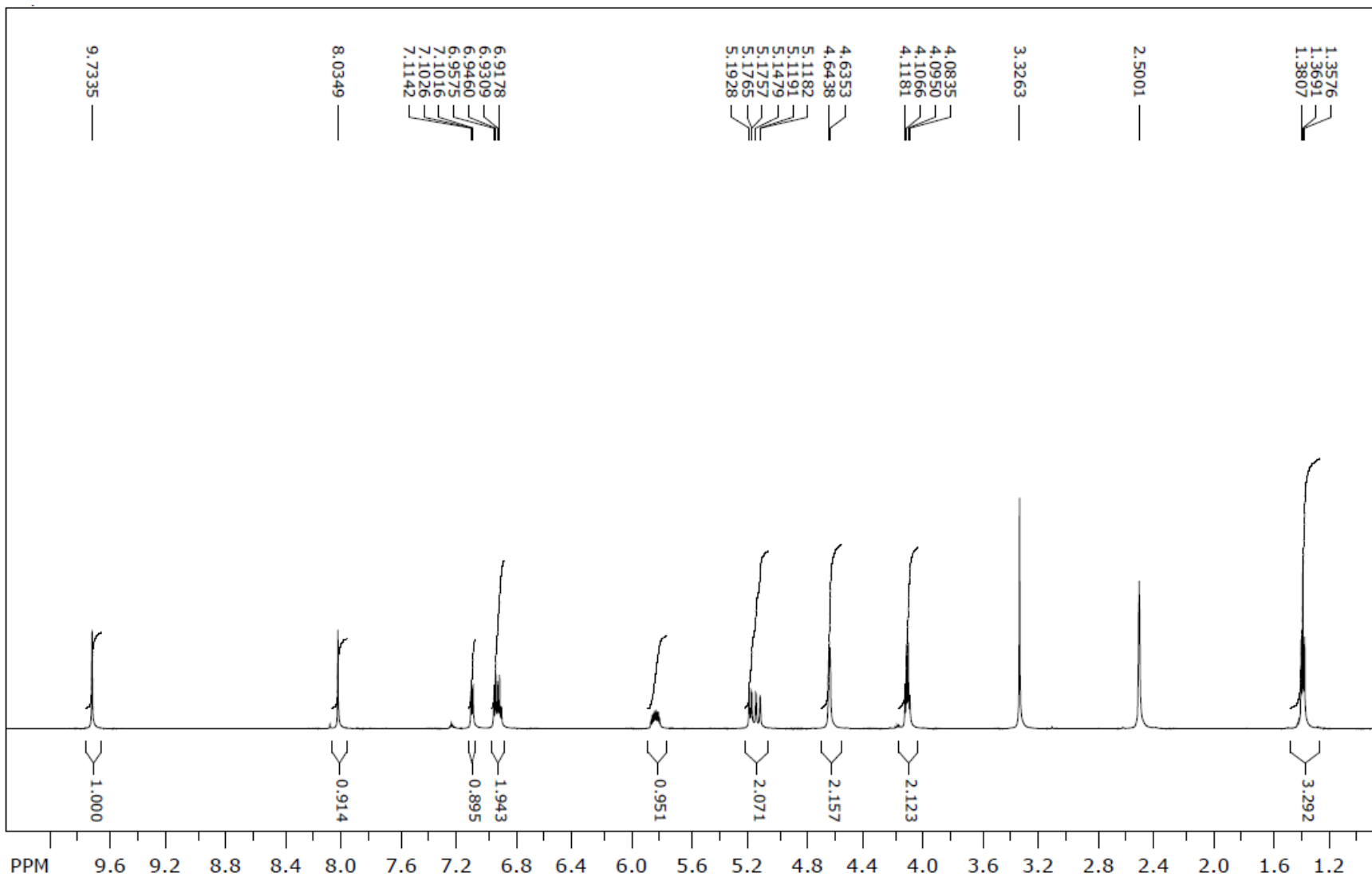


Reaktanti	3-etoksibenzaldehid (2 mmol) i 3-alilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	321,41 g/mol
Molekulska formula	C ₁₅ H ₁₅ NO ₃ S ₂
Temperatura tališta	172 – 174 °C
Boja kristala	Žuta
R_f	0,82
LC/MS/MS m/z (M-)	320,18
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 9,73 (s, 1H, OH), 8,03 (s, 1H, CH), 7,11 (d, <i>J</i> = 7,26 Hz, 1H, arom.), 6,90 – 6,96 (m, 2H, arom.), 5,81 – 5,87 (m, 1H, CH), 5,18 (d, <i>J</i> = 10,26 Hz, 1H, CH ₂), 5,13 (d, <i>J</i> = 17,82 Hz, 1H, CH ₂), 4,64 (d, <i>J</i> = 5,10 Hz, 2H, CH ₂), 4,10 (q, <i>J</i> = 6,92 Hz, 2H, CH ₂ CH ₃), 1,37 (t, <i>J</i> = 6,92 Hz, 3H, CH ₂ CH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,48; 166,72; 147,27; 147,18; 130,27; 128,77; 120,95; 120,54; 120,21; 119,90; 117,96; 115,69; 64,35; 45,97; 14,49.

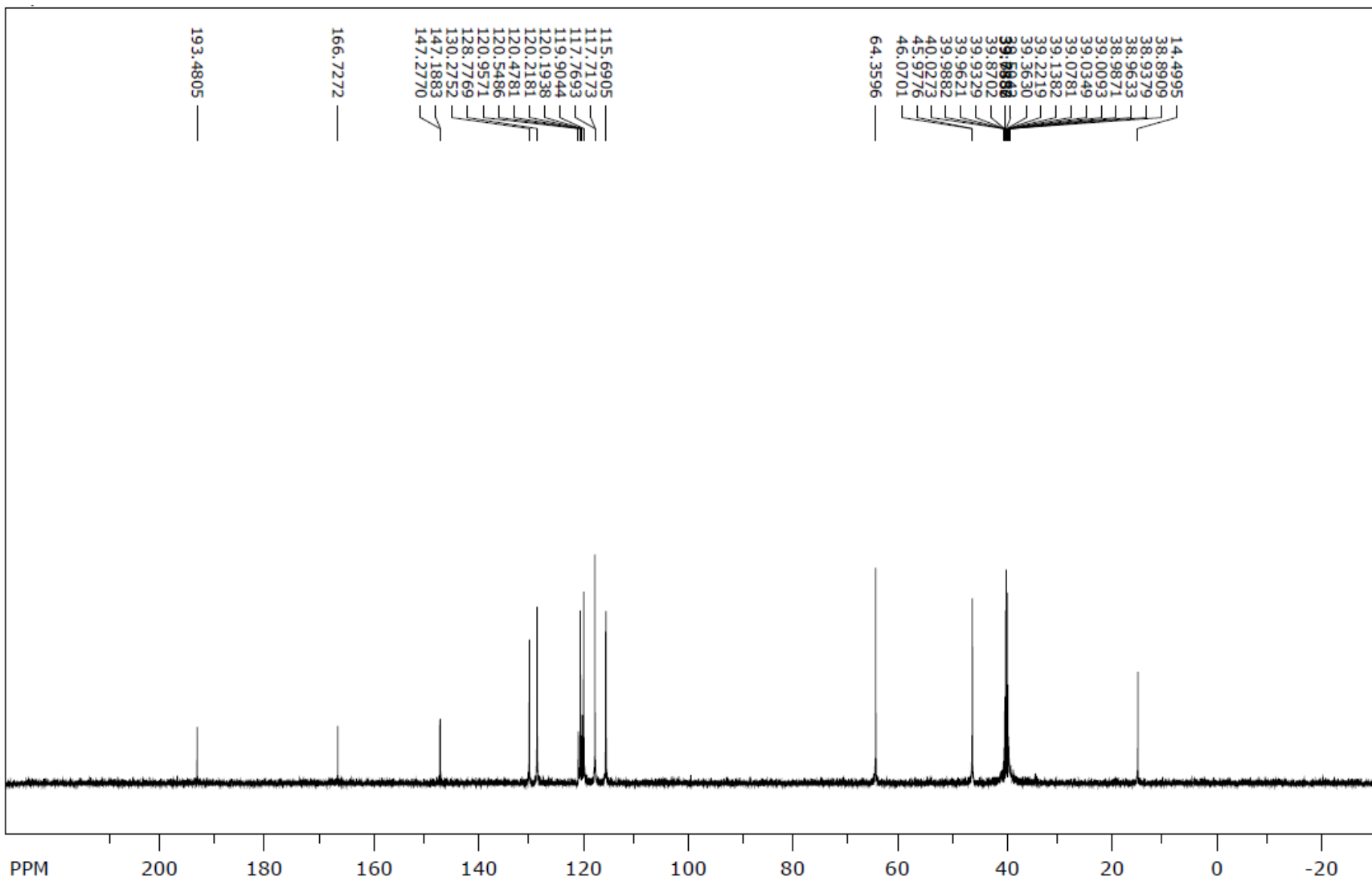
Maseni spektr (6e)



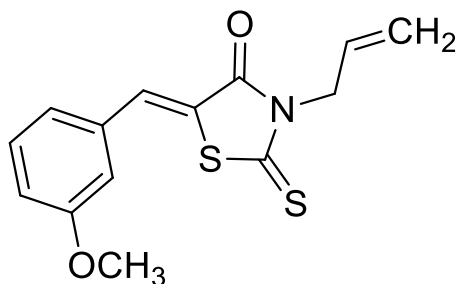
¹H NMR spektr (6e)



¹³C NMR spektr (6e)

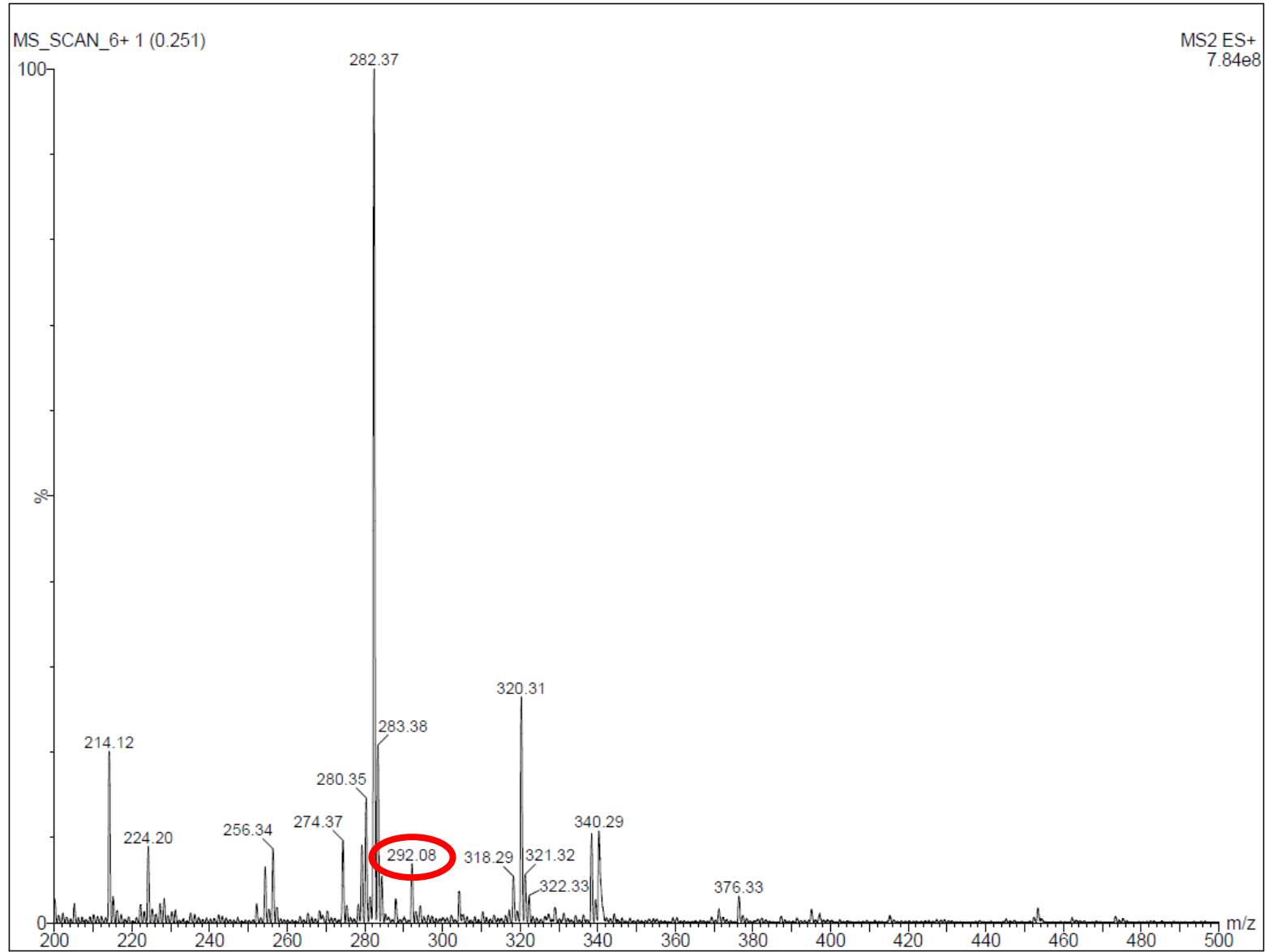


3-aliil-5-(3-metoksibenziliden)-2-tioksotiazolidin-4-on (6f)

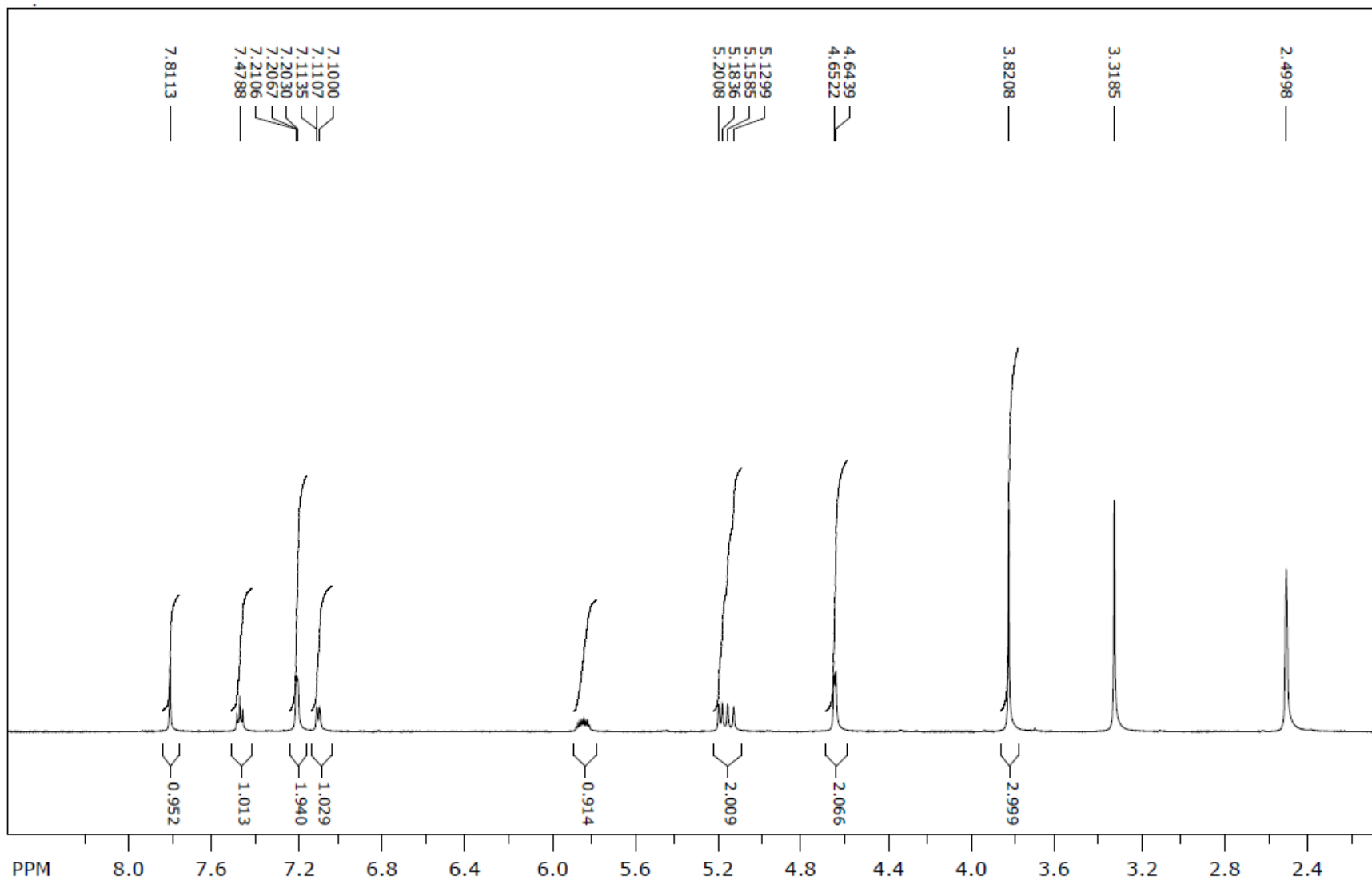


Reaktanti	3-metoksibenzaldehid (2 mmol) i 3-aliilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	291,39 g/mol
Molekulska formula	C ₁₄ H ₁₃ NO ₂ S ₂
Temperatura tališta	82 – 85 °C
Boja kristala	Narančasta
R_f	0,90
LC/MS/MS <i>m/z</i> (M⁺)	292,08
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,81 (s, 1H, CH), 7,48 (t, <i>J</i> = 8,16 Hz, 1H, arom.), 7,21 (t, <i>J</i> = 2,28 Hz, 2H, arom.), 7,10 (dd, <i>J</i> = 8,10; 1,65 Hz, 1H, arom.), 5,82 – 5,88 (m, 1H, CH), 5,19 (d, <i>J</i> = 10,32 Hz, 1H, CH ₂), 5,14 (d, <i>J</i> = 17,16 Hz, 1H, CH ₂), 4,65 (d, <i>J</i> = 4,98 Hz, 2H, CH ₂), 3,82 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,05; 166,50; 159,71; 134,28; 133,08; 130,62; 130,19; 122,46; 117,79; 117,01; 115,76; 55,32; 46,04.

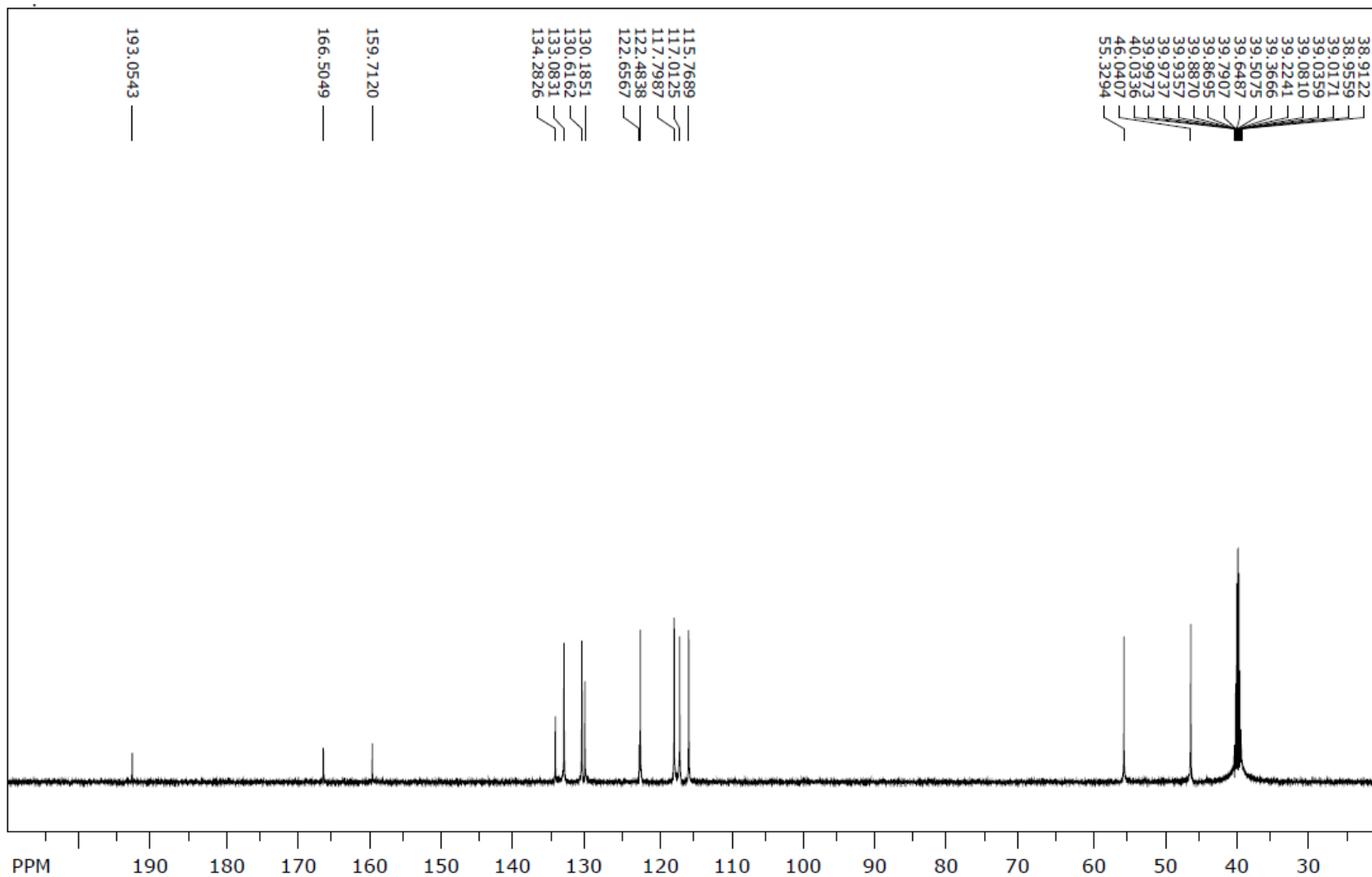
Maseni spektr (6f)



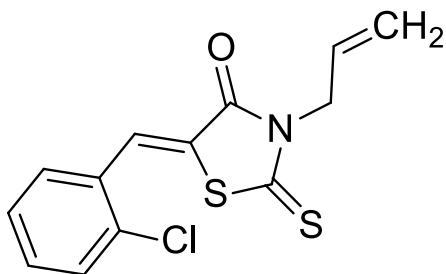
¹H NMR spektr (6f)



¹³C NMR spektr (6f)

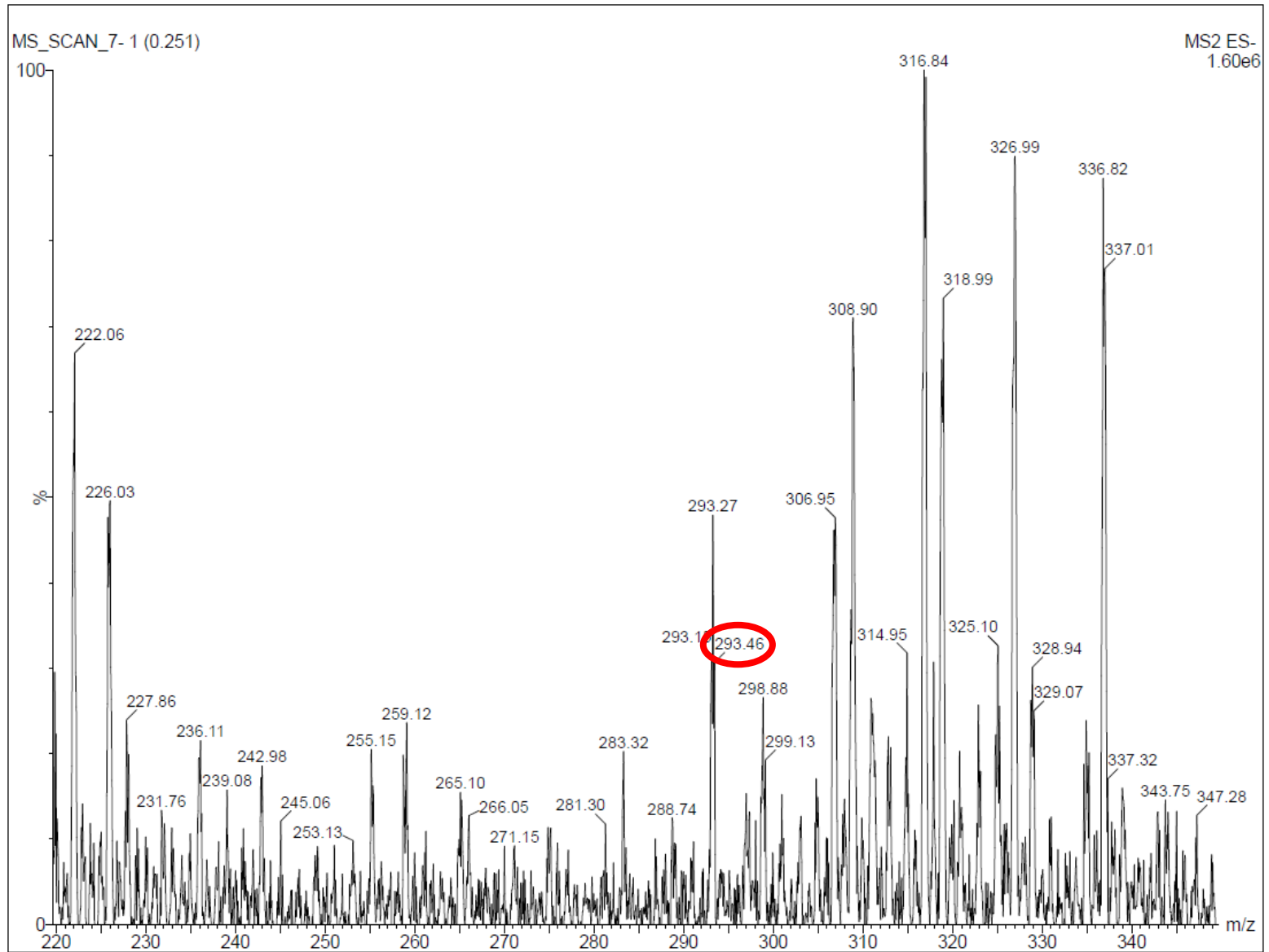


3-alil-5-(2-klorbenziliden)-2-tioksotiazolidin-4-on (6g)

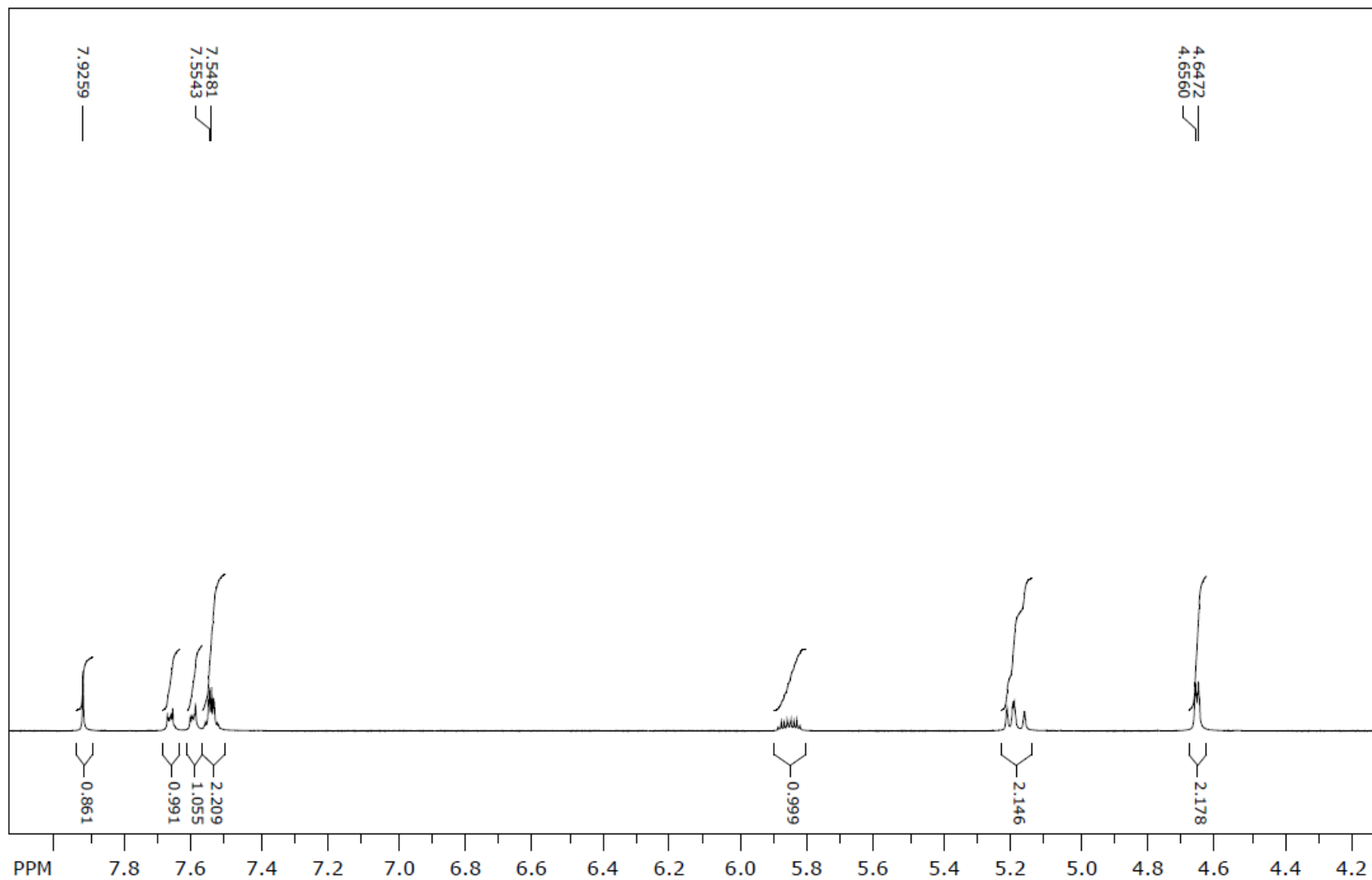


Reaktanti	2-klorbenzaldehyd (2 mmol) i 3-alilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	295,81 g/mol
Molekulska formula	C ₁₃ H ₁₀ ClNOS ₂
Temperatura tališta	95 – 98 °C
Boja kristala	Žuta
R_f	0,91
LC/MS/MS m/z (M-)	293,46
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,92 (s, 1H, CH), 7,56 - 7,68 (m, 1H, arom.), 7,60 – 7,61 (m, 1H, arom.), 7,53 – 7,57 (m, 2H, arom.), 5,82 – 5,88 (m, 1H, CH), 5,20 (dd, <i>J</i> = 10,38; 1,20 Hz, 1H, CH ₂), 5,17 (dd, <i>J</i> = 17,40; 1,23 Hz, 1H, CH ₂), 4,65 (d, <i>J</i> = 5,28 Hz, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,01; 166,31; 134,77; 132,35; 130,49; 130,02; 129,48; 128,34; 127,54; 125,98; 117,98; 50,68; 46,16.

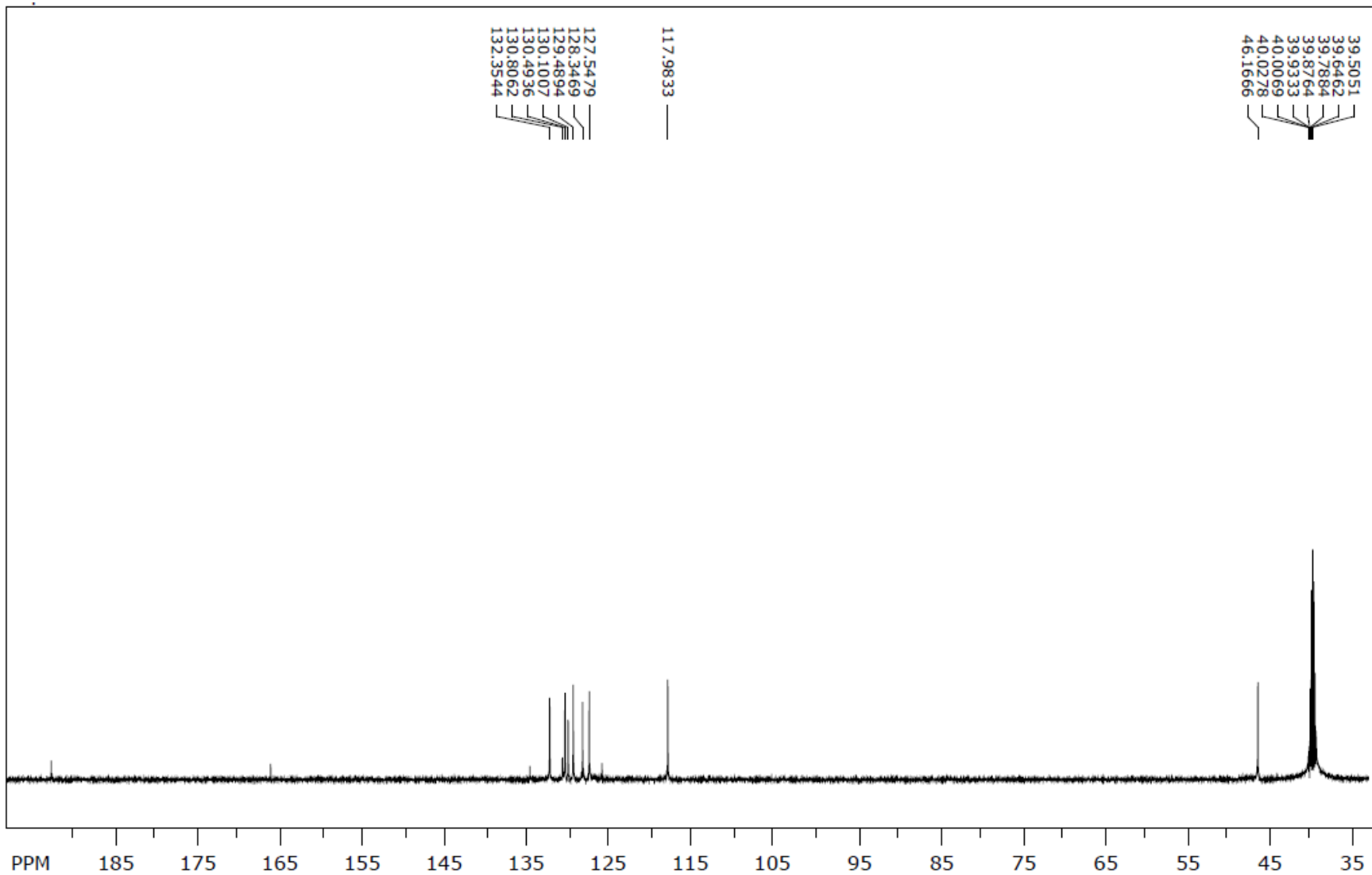
Maseni spektar (6g)



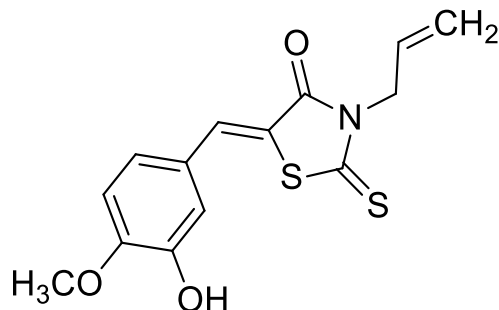
¹H NMR spektr (6g)



¹³C NMR spektr (6g)

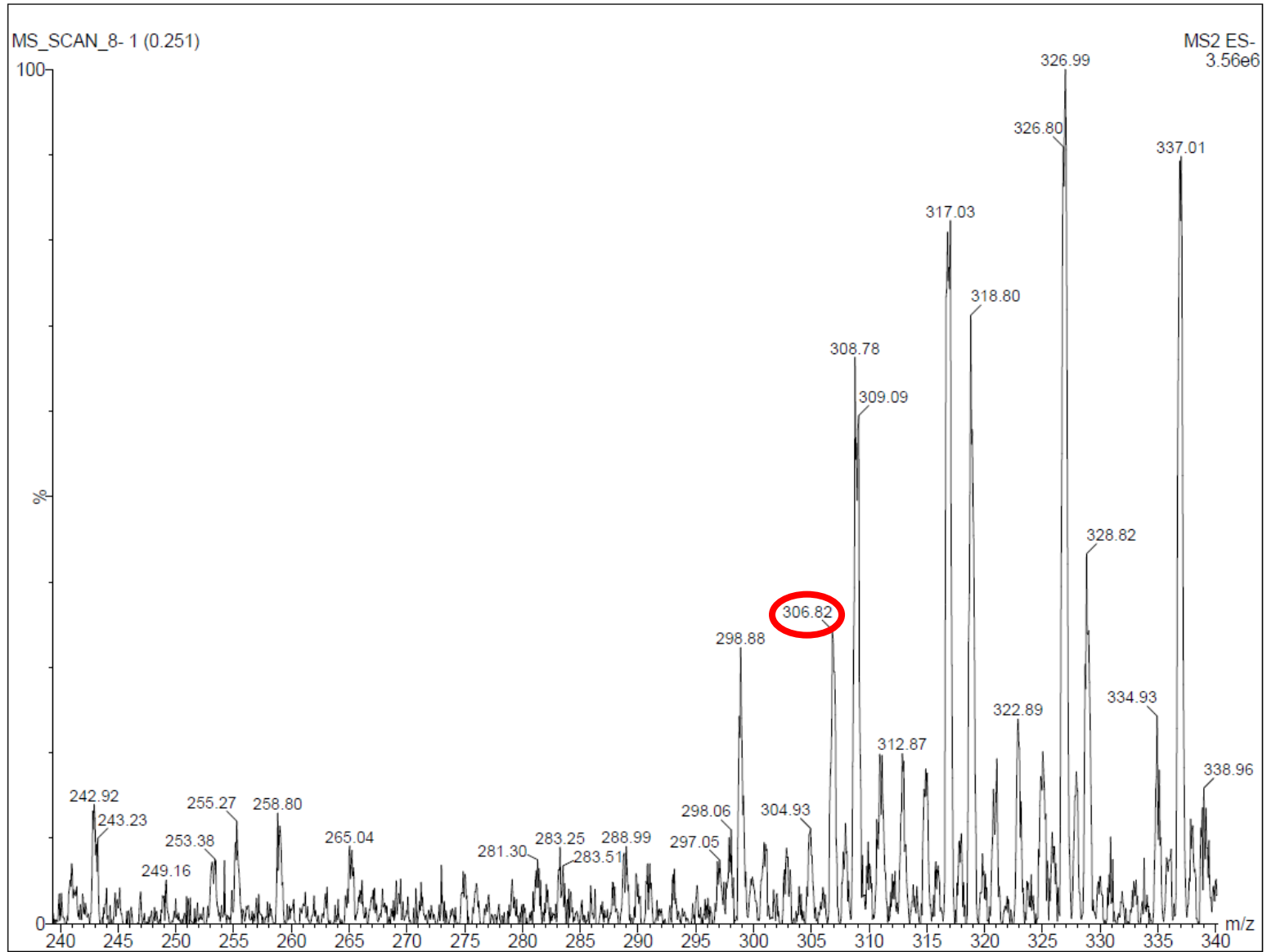


3-ailil-5-(3-hidroksi-4-metoksibenziliden)-2-tioksotiazolidin-4-on (6h)

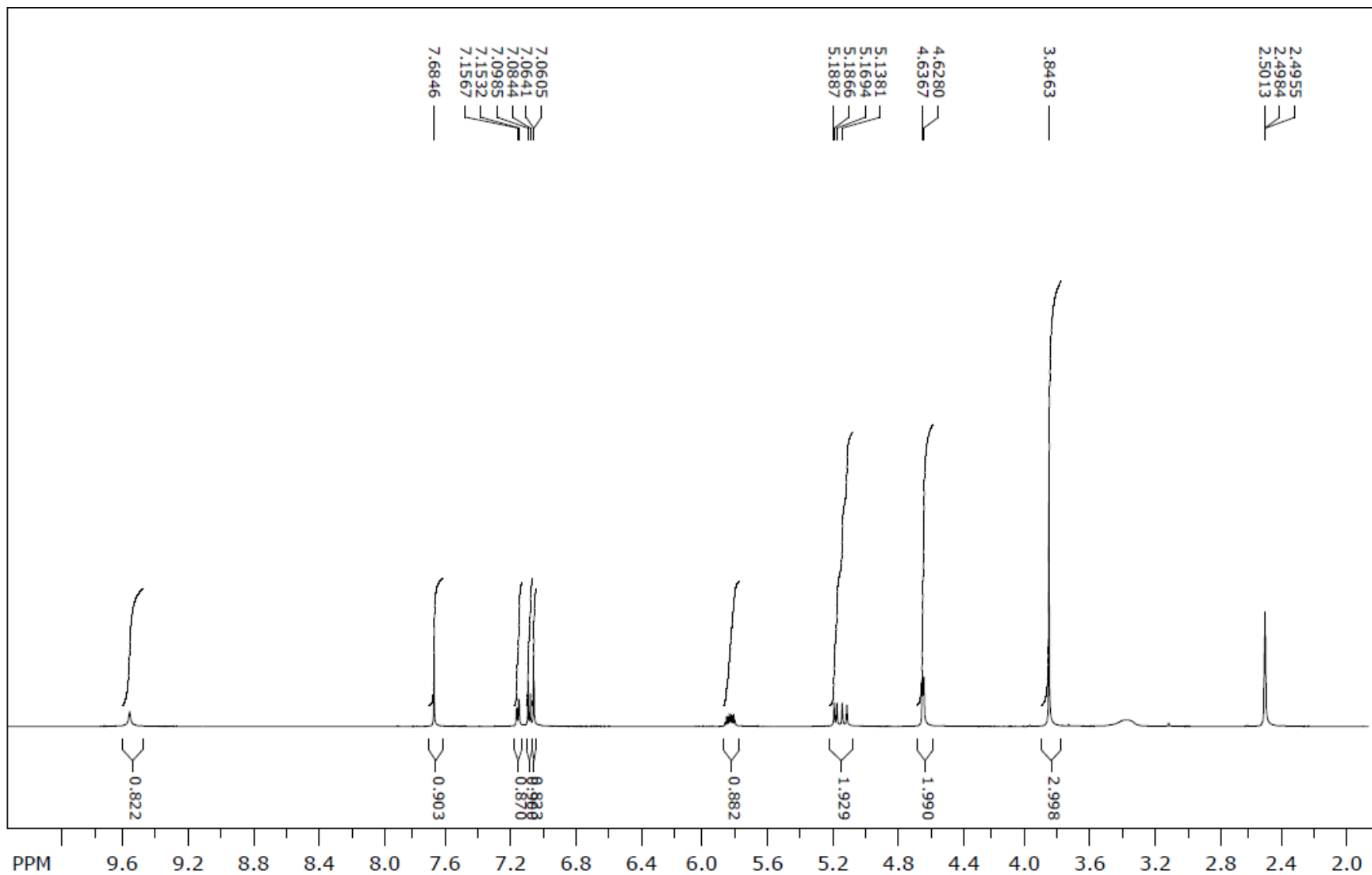


Reaktanti	3-hidroksi-4-metoksibenzaldehid (2 mmol) i 3-aililrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	307,39 g/mol
Molekulska formula	C ₁₄ H ₁₃ NO ₃ S ₂
Temperatura tališta	113 – 115 °C
Boja kristala	Svijetlosmeđa
R_f	0,73
LC/MS/MS m/z (M-)	306,82
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 9,58 (s, 1H, OH), 7,68 (s, 1H, CH), 7,16 (dd, <i>J</i> = 8,46; 2,10 Hz, 1H, arom.), 7,10 (d, <i>J</i> = 8,46 Hz, 1H, arom.), 7,06 (d, <i>J</i> = 2,16 Hz, 1H, arom.), 5,81 – 5,87 (m, 1H, CH), 5,18 (dd, <i>J</i> = 10,38; 1,23 Hz, 1H, CH ₂), 5,12 (dd, <i>J</i> = 17,22; 1,32 Hz, 1H, CH ₂) 4,63 (d, <i>J</i> = 5,22 Hz, 2H, CH ₂), 3,84 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 192,93; 166,58; 150,48; 147,13; 133,82; 130,27; 125,65; 124,77; 118,61; 117,72; 116,12; 112,54; 55,71; 45,93.

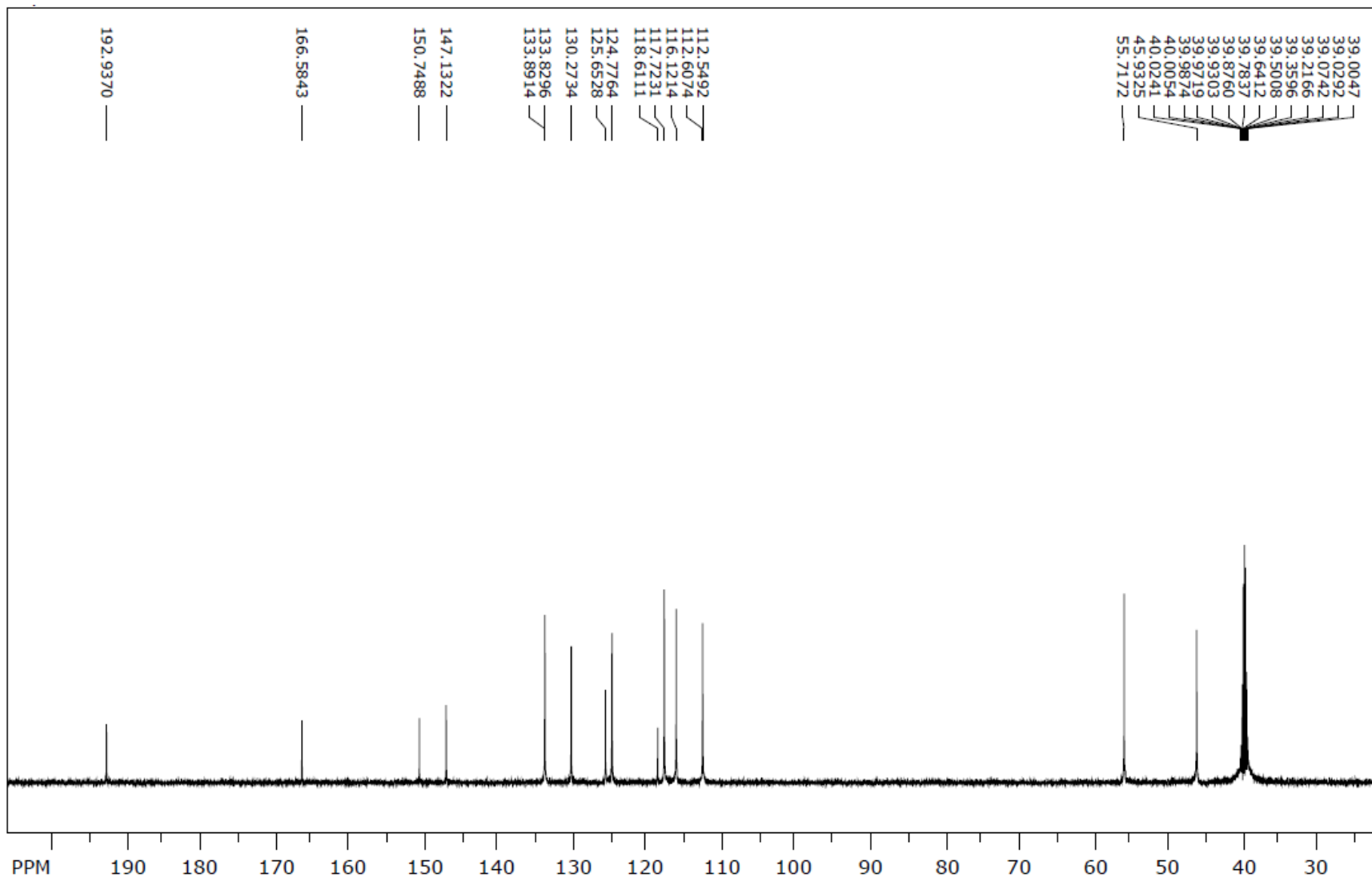
Maseni spektr (6h)



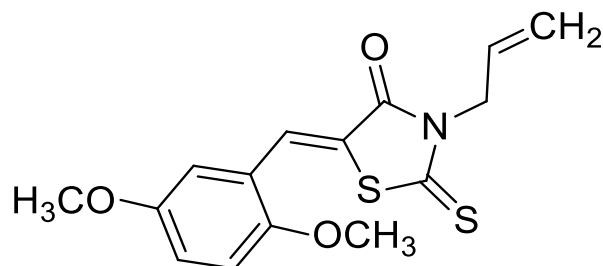
¹H NMR spektr (6h)



¹³C NMR spektr (6h)

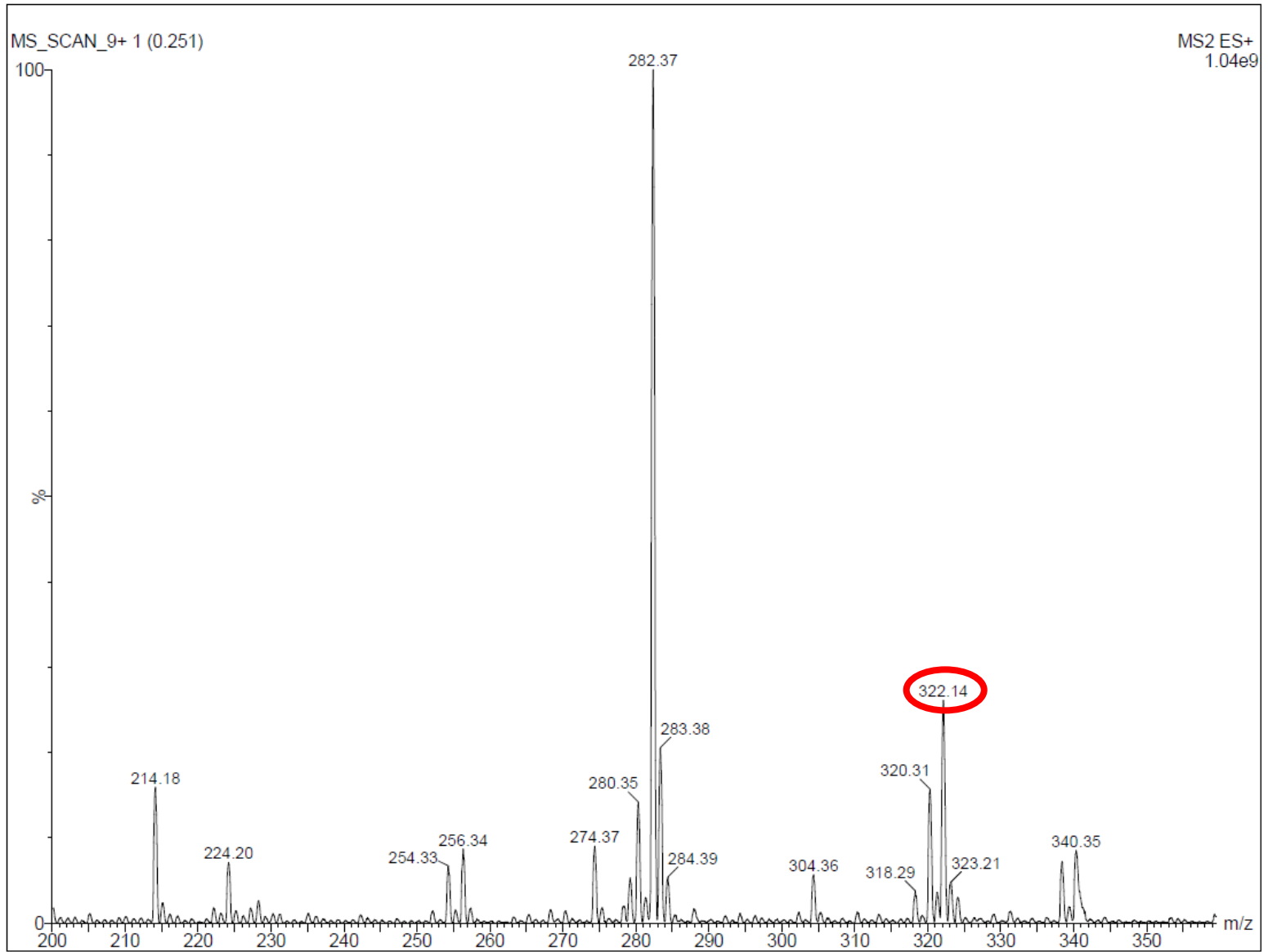


3-alil-5-(2,5-dimetoksibenziliden)-2-tioksotiazolidin-4-on (6i)

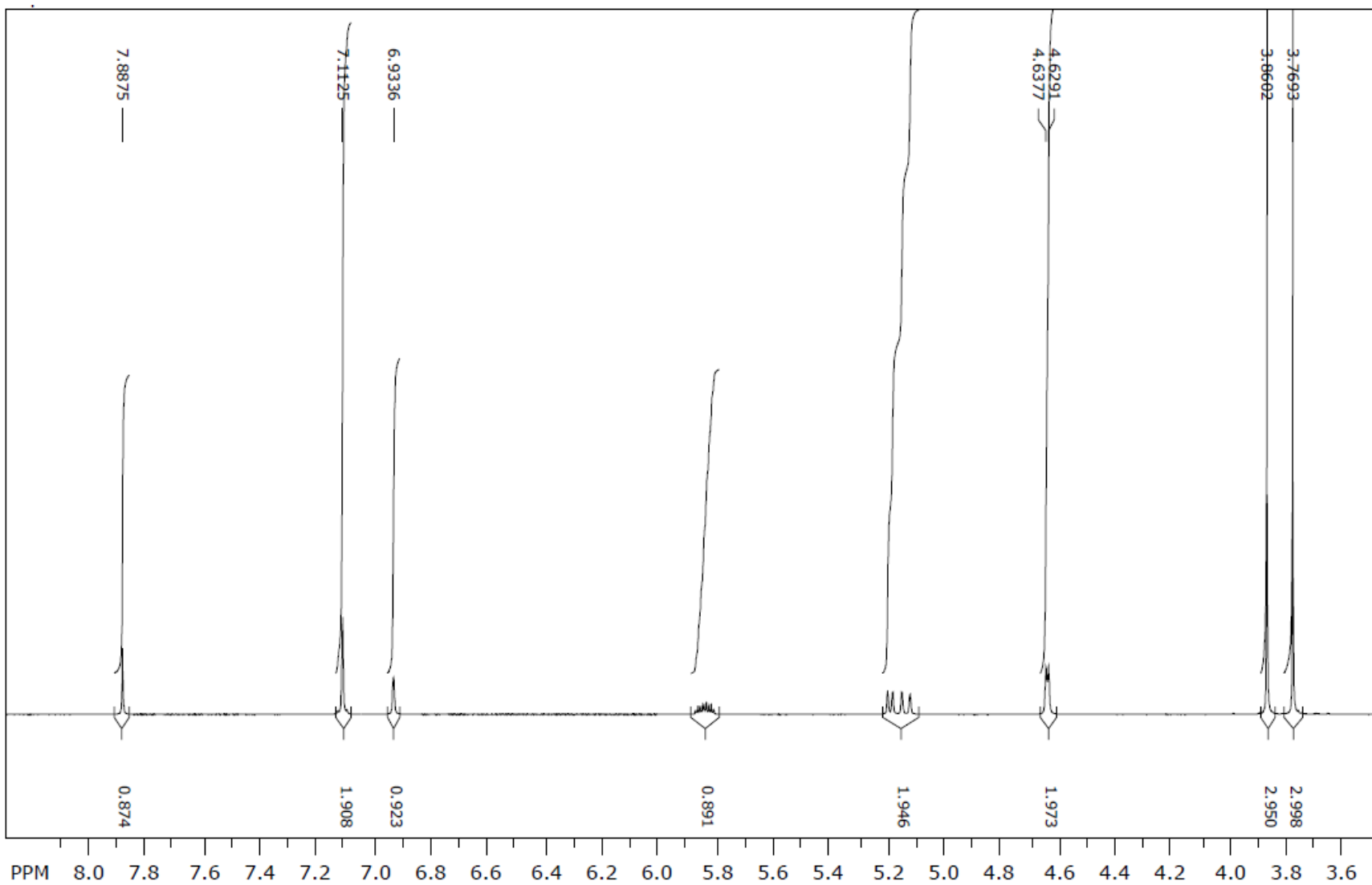


Reaktanti	2,5-dimetoksibenzaldehid (2 mmol) i 3-alilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	321,41 g/mol
Molekulska formula	C ₁₅ H ₁₅ NO ₃ S ₂
Temperatura tališta	93 – 96 °C
Boja kristala	Crvena
R_f	0,89
LC/MS/MS <i>m/z</i> (M⁺)	322,14
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,88 (s, 1H, CH), 7,11 (s, 2H, arom.), 6,93 (s, 1H, arom.), 5,81 – 5,87 (m, 1H, CH), 5,19 (d, <i>J</i> = 10,38 Hz, 1H, CH ₂), 5,13 (dd, <i>J</i> = 17,28; 0,66 Hz, 1H, CH ₂), 4,63 (d, <i>J</i> = 5,16 Hz, 2H, CH ₂), 3,86 (s, 3H, OCH ₃), 3,77 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,98; 166,59; 153,20; 152,53; 130,21; 118,92; 117,76; 114,25; 113,24; 56,06; 55,58; 46,00.

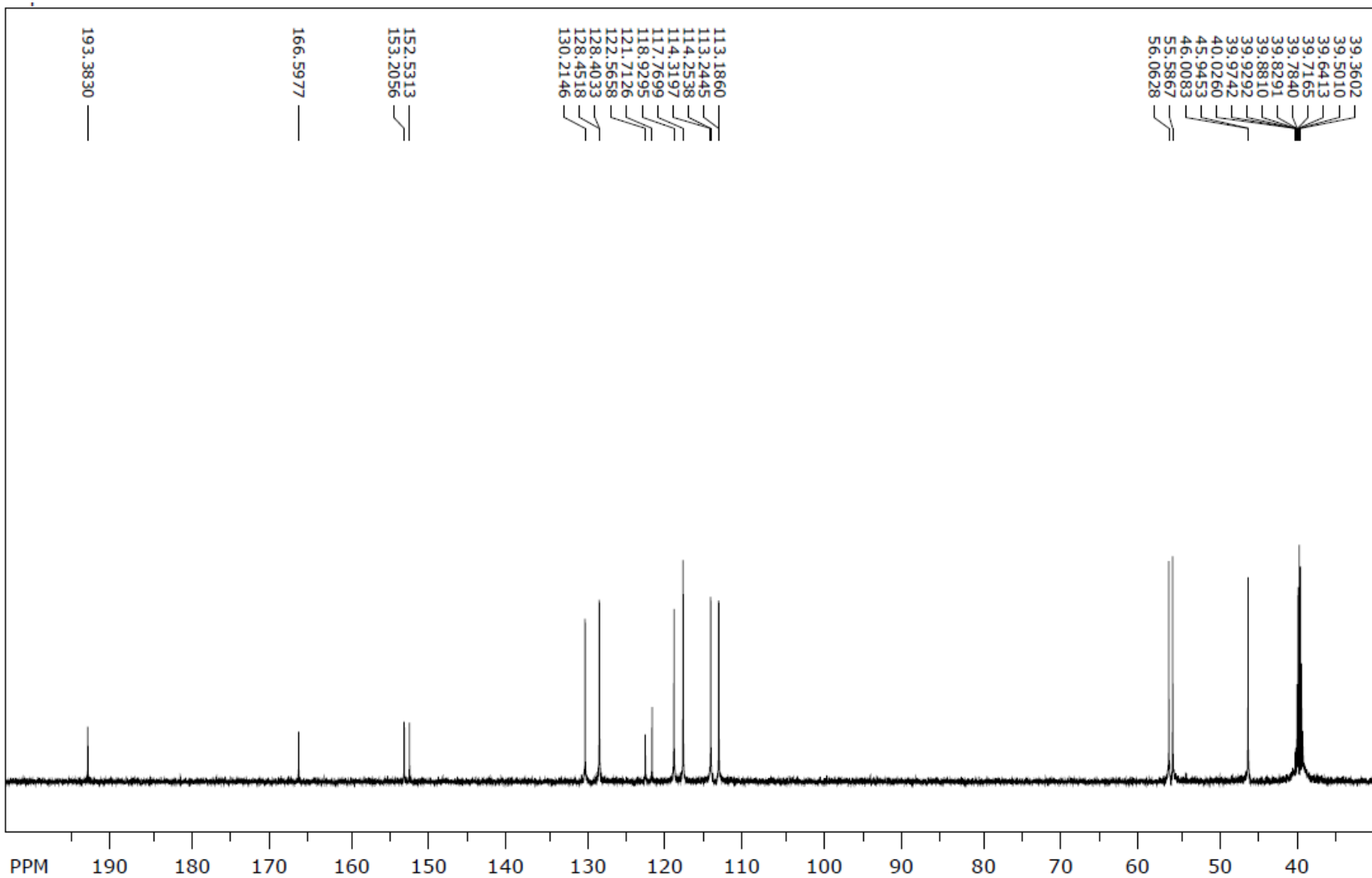
Maseni spektar (6i)



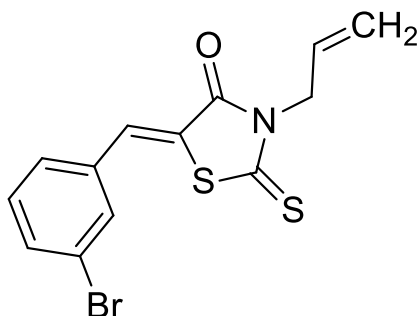
¹H NMR spektr (6i)



¹³C NMR spektr (6i)

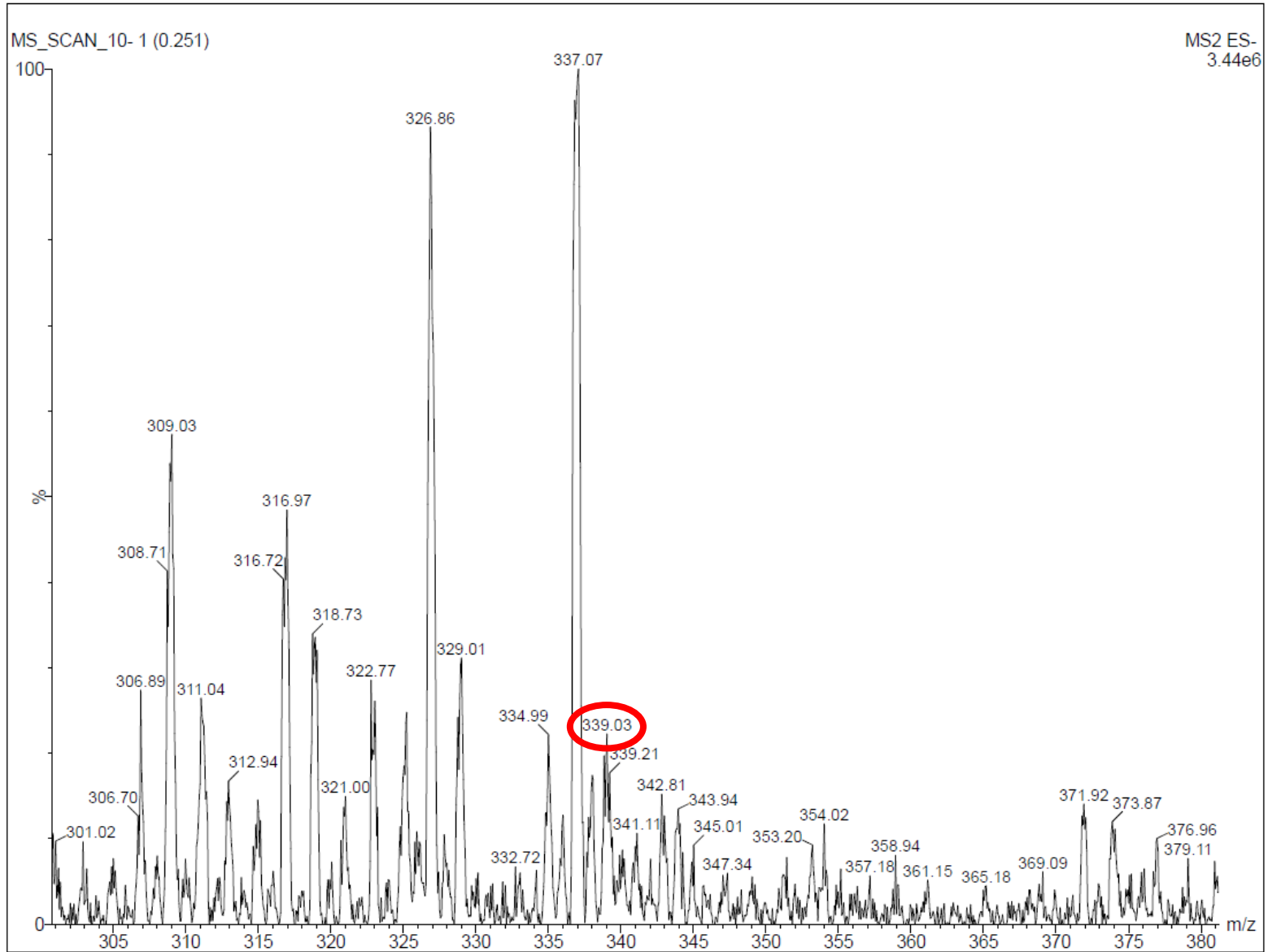


3-alil-5-(3-brombenziliden)-2-tioksotiazolidin-4-on (6j)

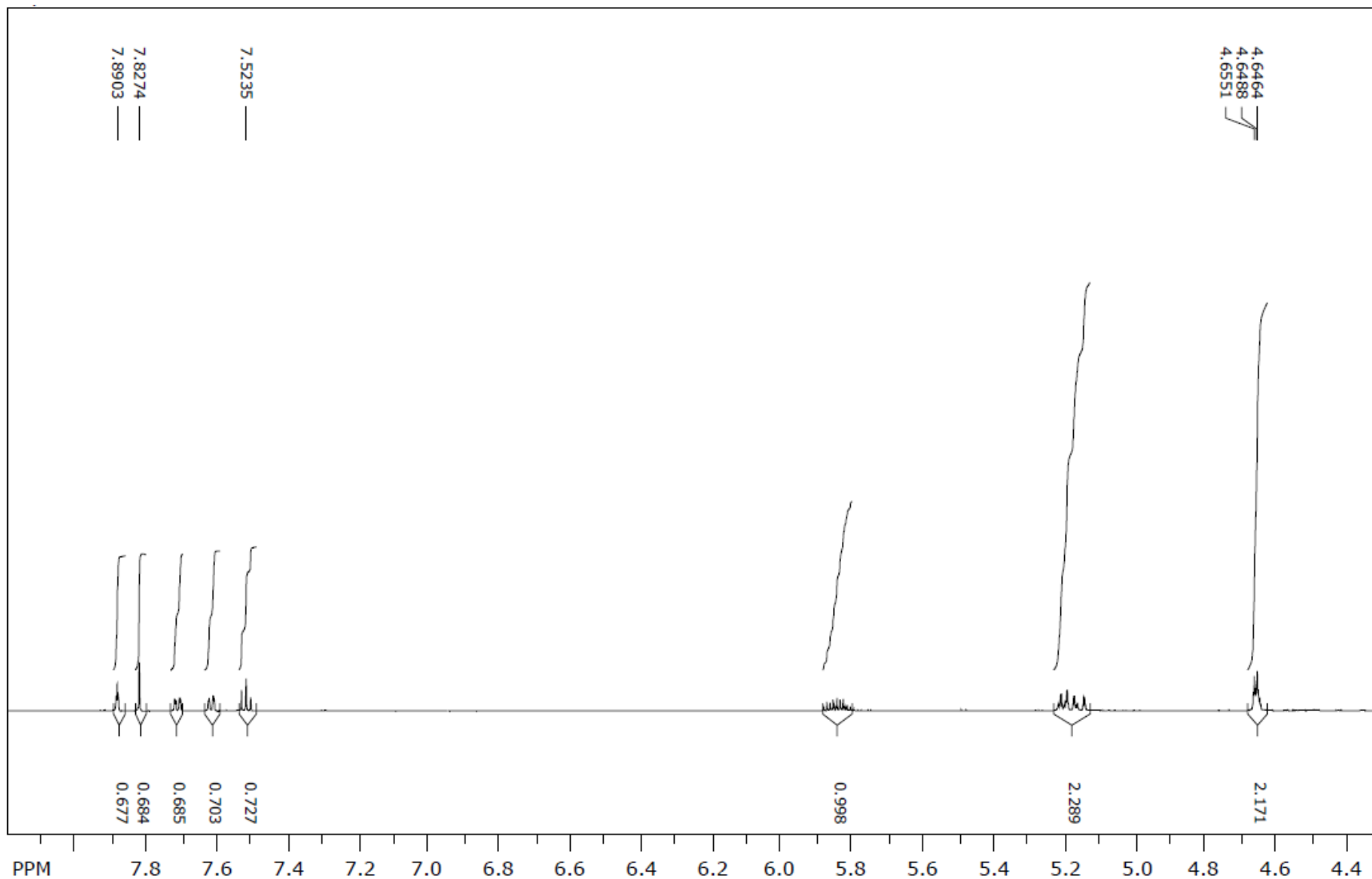


Reaktanti	3-brombenzalhid (2 mmol) i 3-alilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	340,26 g/mol
Molekulska formula	C ₁₃ H ₁₀ BrNOS ₂
Temperatura tališta	107 – 110 °C
Boja kristala	Tamnosmeđa
R_f	0,90
LC/MS/MS m/z (M-)	339,03
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,89 (t, <i>J</i> = 1,77 Hz, 1H, arom.), 7,82 (s, 1H, CH), 7,73 (dd, <i>J</i> = 1,86; 0,87 Hz, 1H, arom.), 7,71 (dd, <i>J</i> = 1,86; 0,81 Hz, 1H, arom.) 7,62 (dd, <i>J</i> = 7,02; 0,78 Hz, 1H, arom.), 7,52 (t, <i>J</i> = 7,89 Hz, 1H, arom.), 5,81 – 5,88 (m, 1H, CH), 5,14 – 5,22 (m, 2H, CH ₂), 4,64 – 4,66 (m, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 192,79; 166,40; 135,32; 133,37; 131,51; 130,13; 129,80; 128,58; 124,09; 122,56; 118,21; 117,86; 46,10.

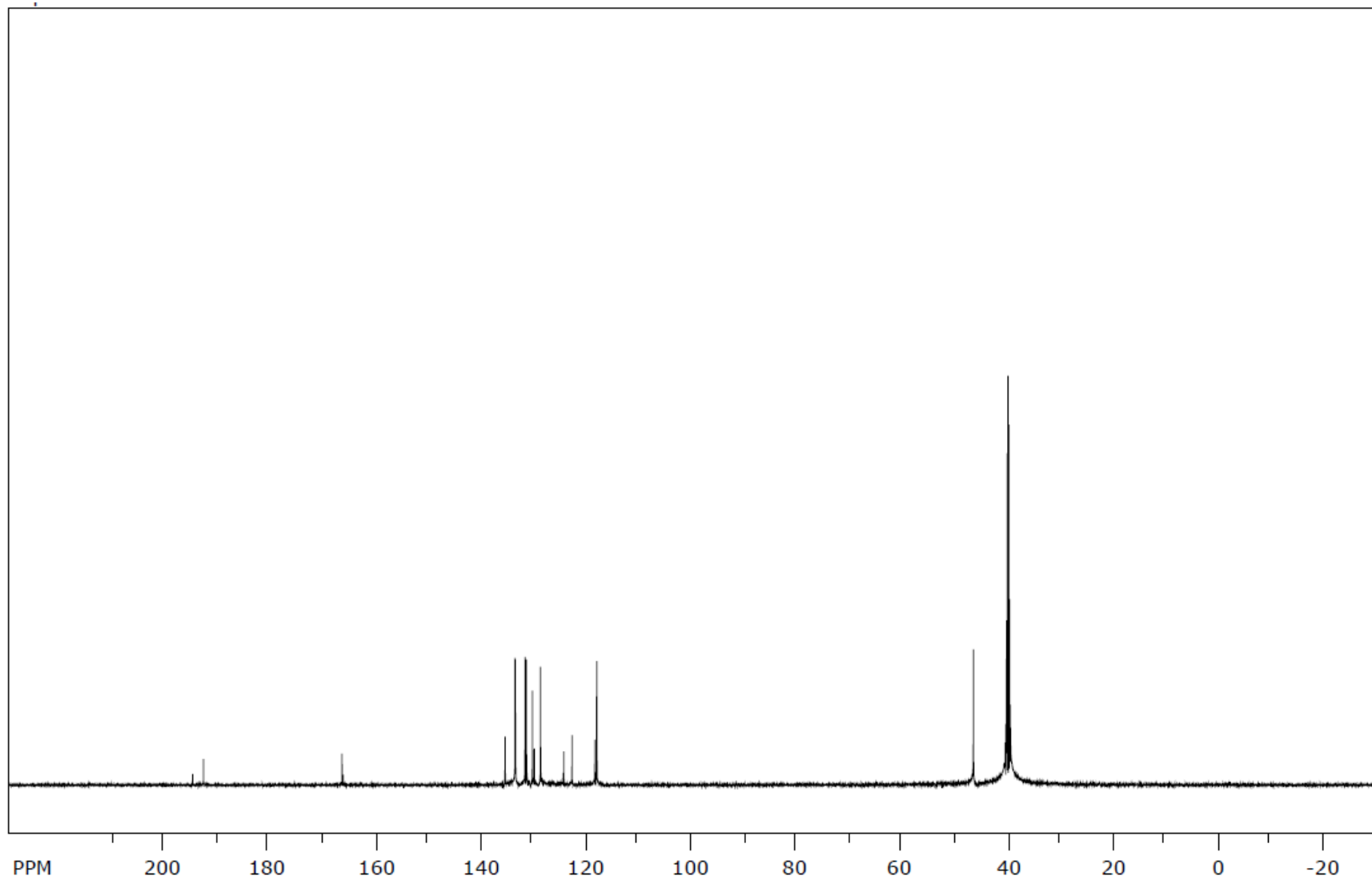
Maseni spektr (6j)



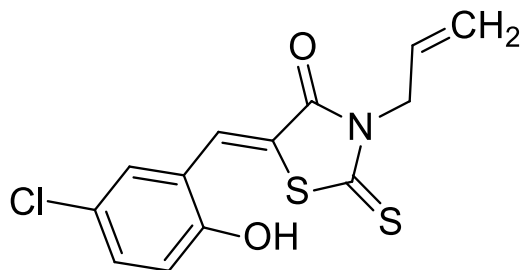
¹H NMR spektr (6j)



¹³C NMR spektr (6j)

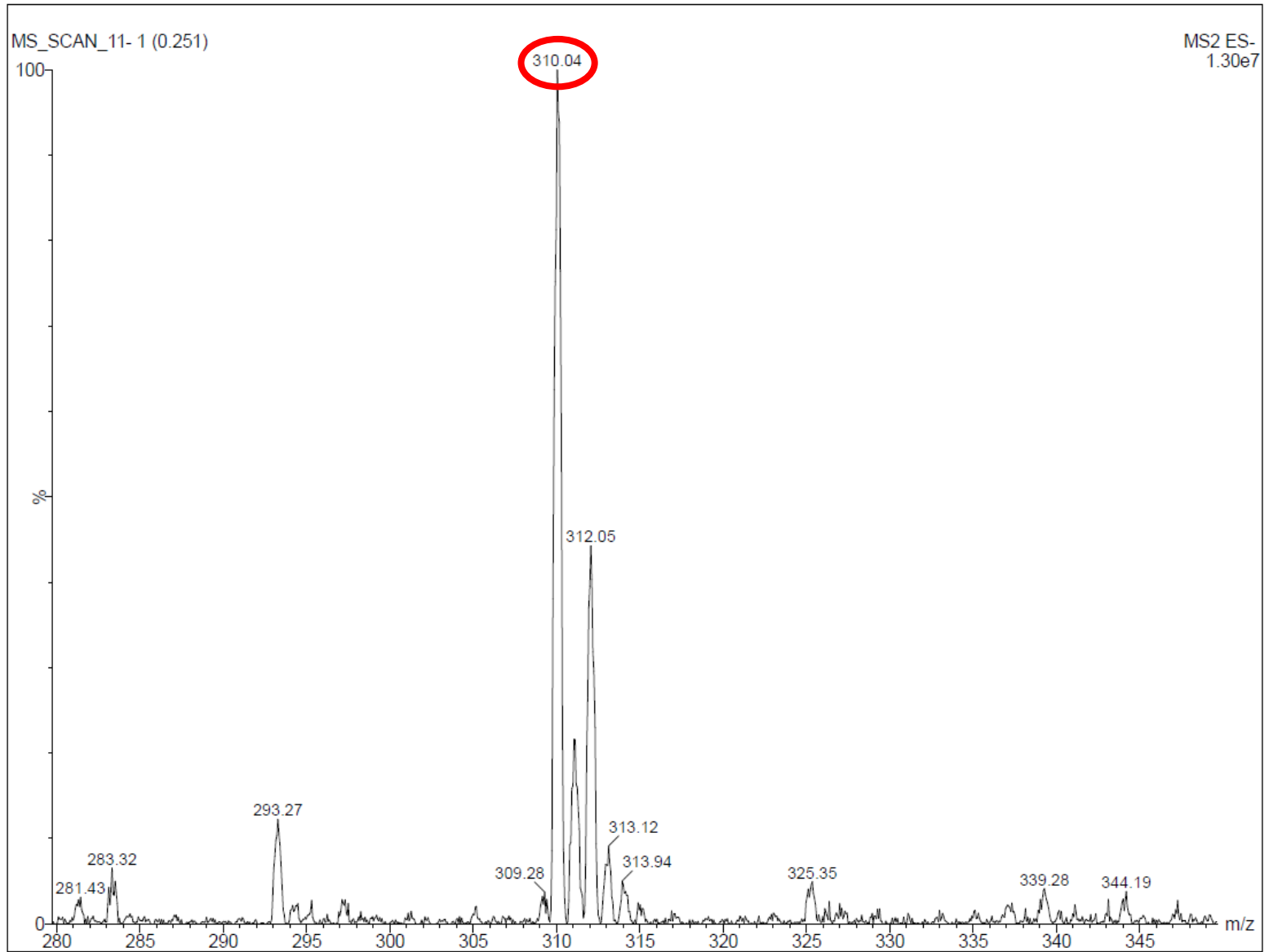


3-aliil-5-(5-Klor-2-hidroksibenziliden)-2-tioksotiazolidin-4-on (6k)

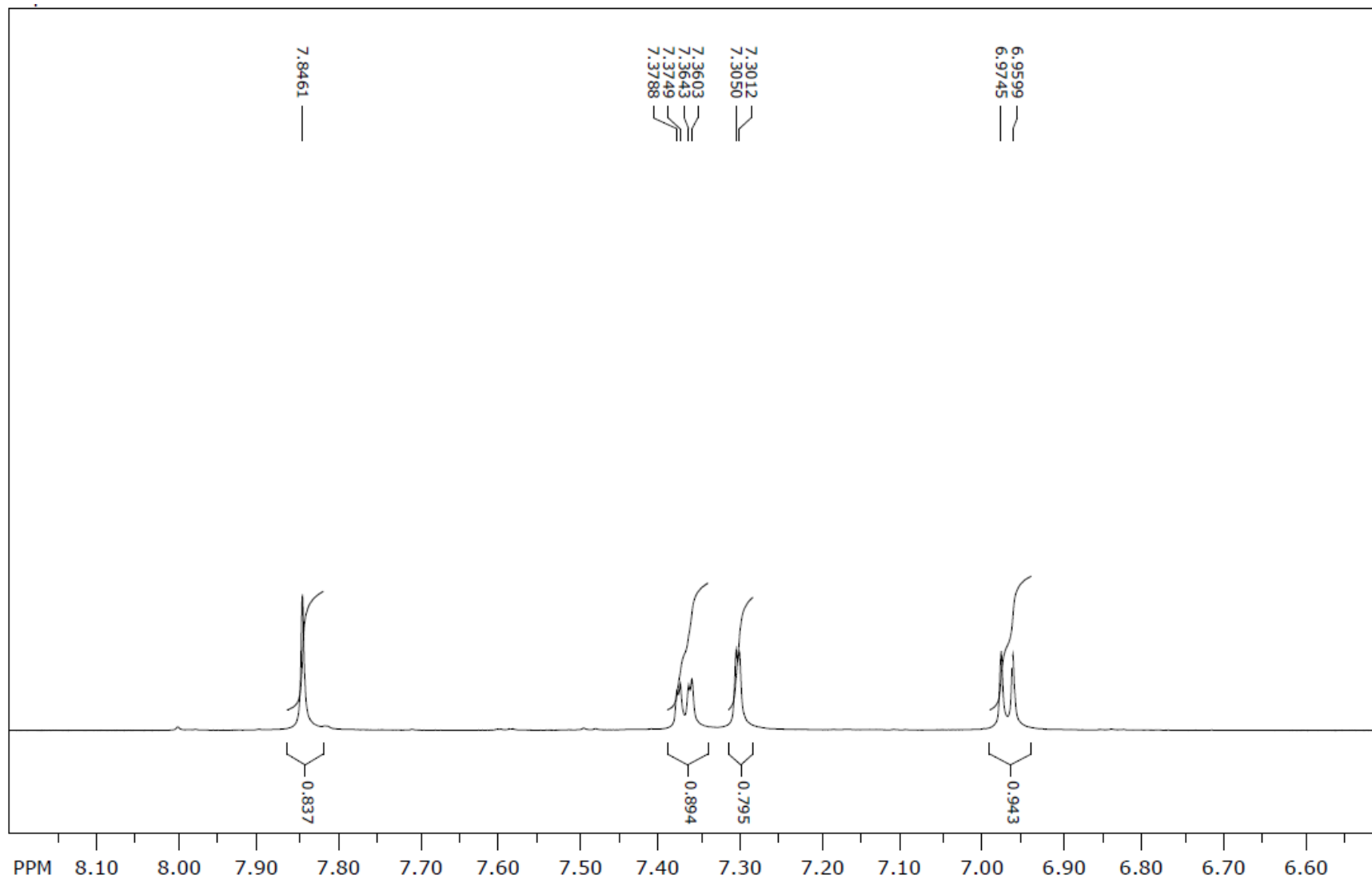


Reaktanti	5-klorsalicilaldehid (2 mmol) i 3-aliilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	311,81 g/mol
Molekulska formula	C ₁₃ H ₁₀ ClNO ₂ S ₂
Temperatura tališta	209 – 210 °C
Boja kristala	Tamnožuta
R_f	0,74
LC/MS/MS m/z (M-)	310,04
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 11,06 (s, 1H, OH), 7,84 (s, 1H, CH), 7,37 (dd, <i>J</i> = 8,70; 2,37 Hz, 1H, arom.), 7,30 (d, <i>J</i> = 2,28 Hz, 1H, arom.), 6,97 (d, <i>J</i> = 8,76 Hz, 1H, arom.), 5,79 – 5,85 (m, 1H, CH), 5,17 (d, <i>J</i> = 10,38 Hz, 1H, CH ₂), 5,12 (d, <i>J</i> = 17,22 Hz, 1H, CH ₂), 4,62 (d, <i>J</i> = 5,10 Hz, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,16; 166,58; 156,09; 132,36; 130,19; 128,71; 127,54; 123,31; 122,54; 121,49; 117,96; 117,82; 46,02.

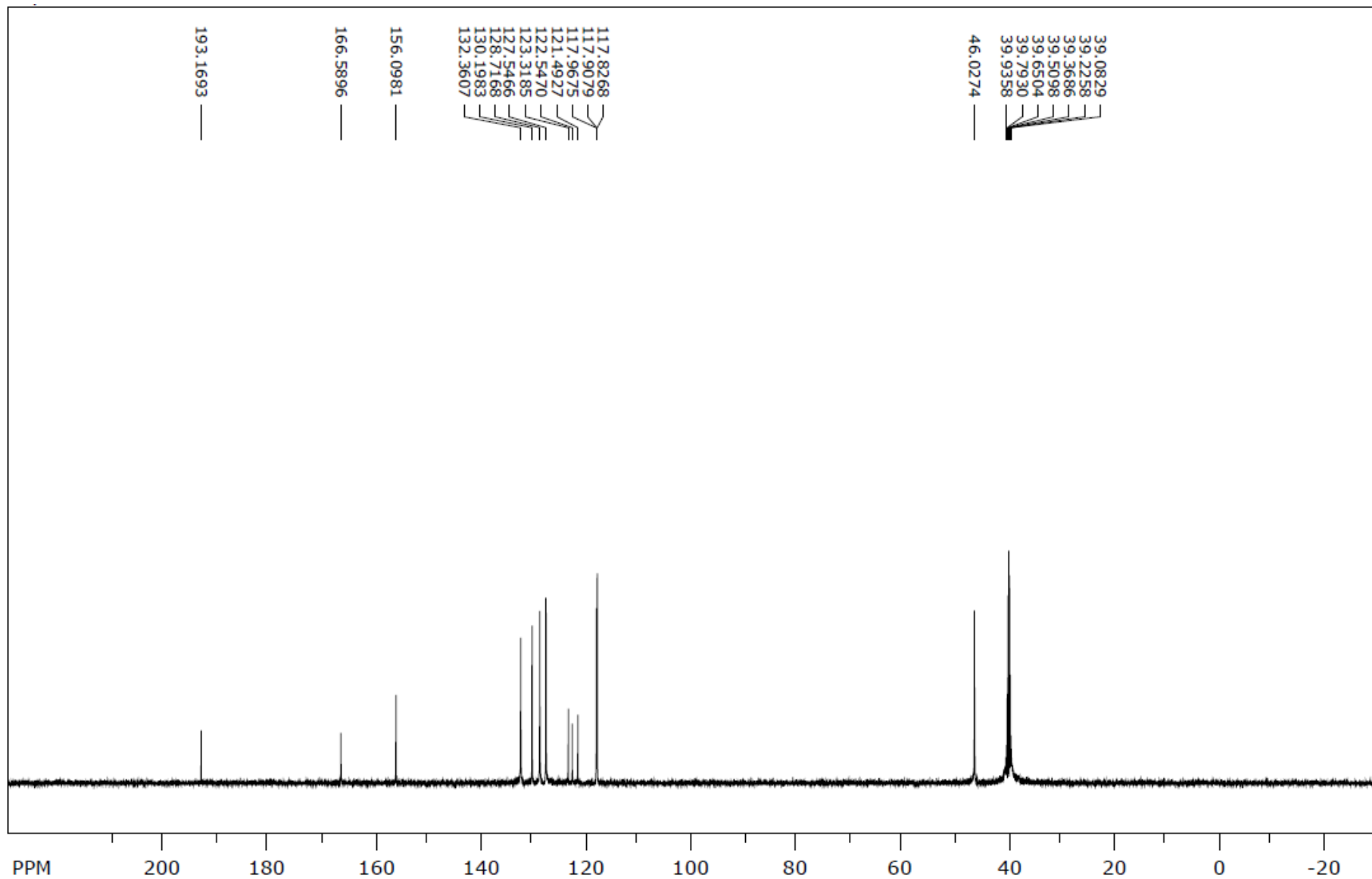
Maseni spektar (6k)



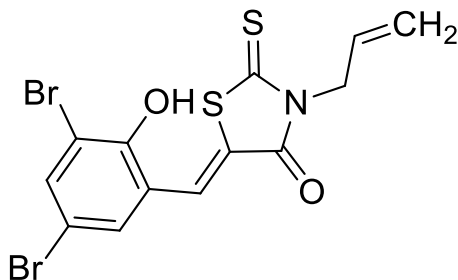
¹H NMR spektr (6k)



¹³C NMR spektr (6k)

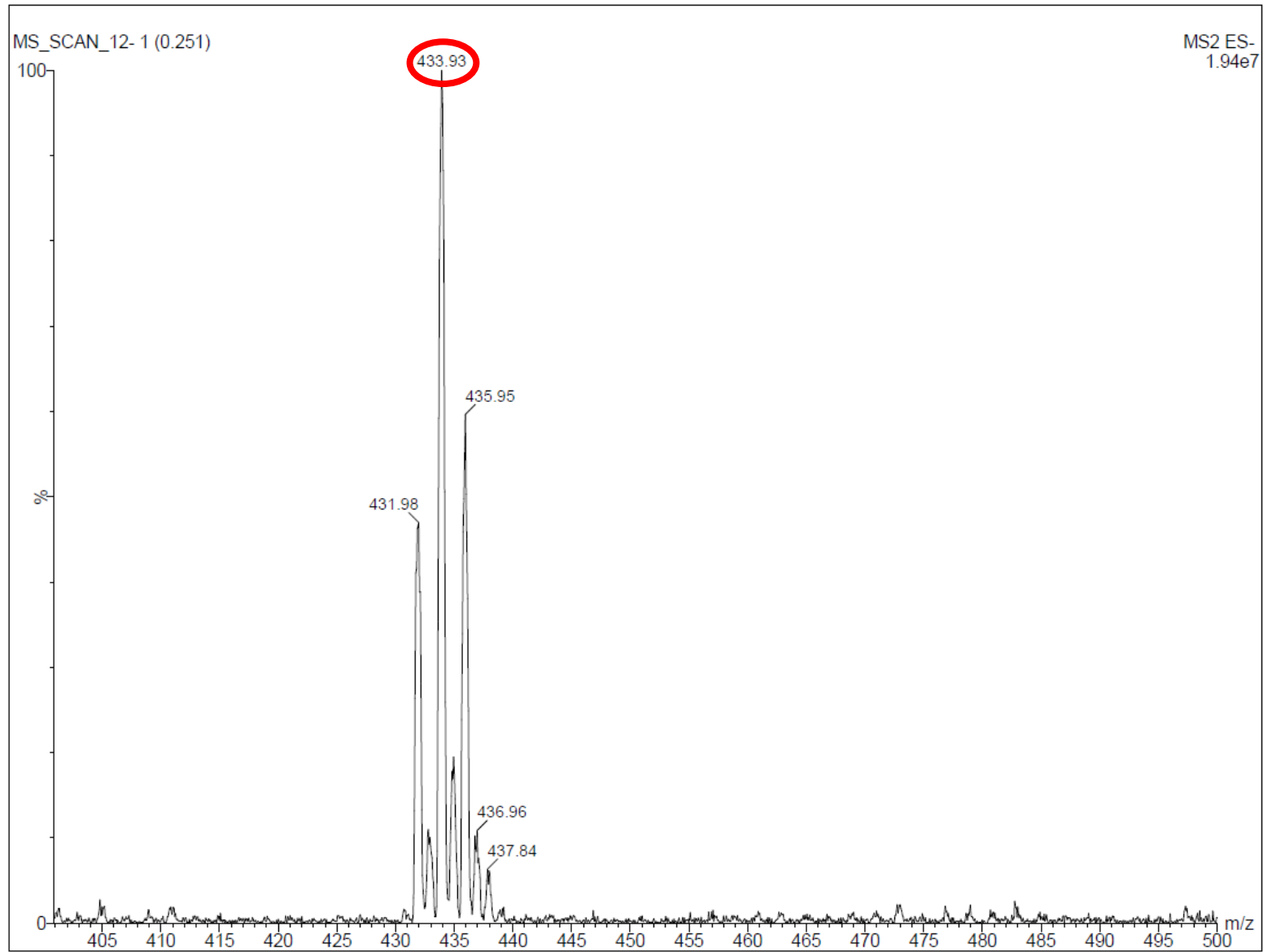


3-aliil-5-(3,5-dibrom-2-hidroksibenziliden)-2-tioksotiazolidin-4-on (6I)

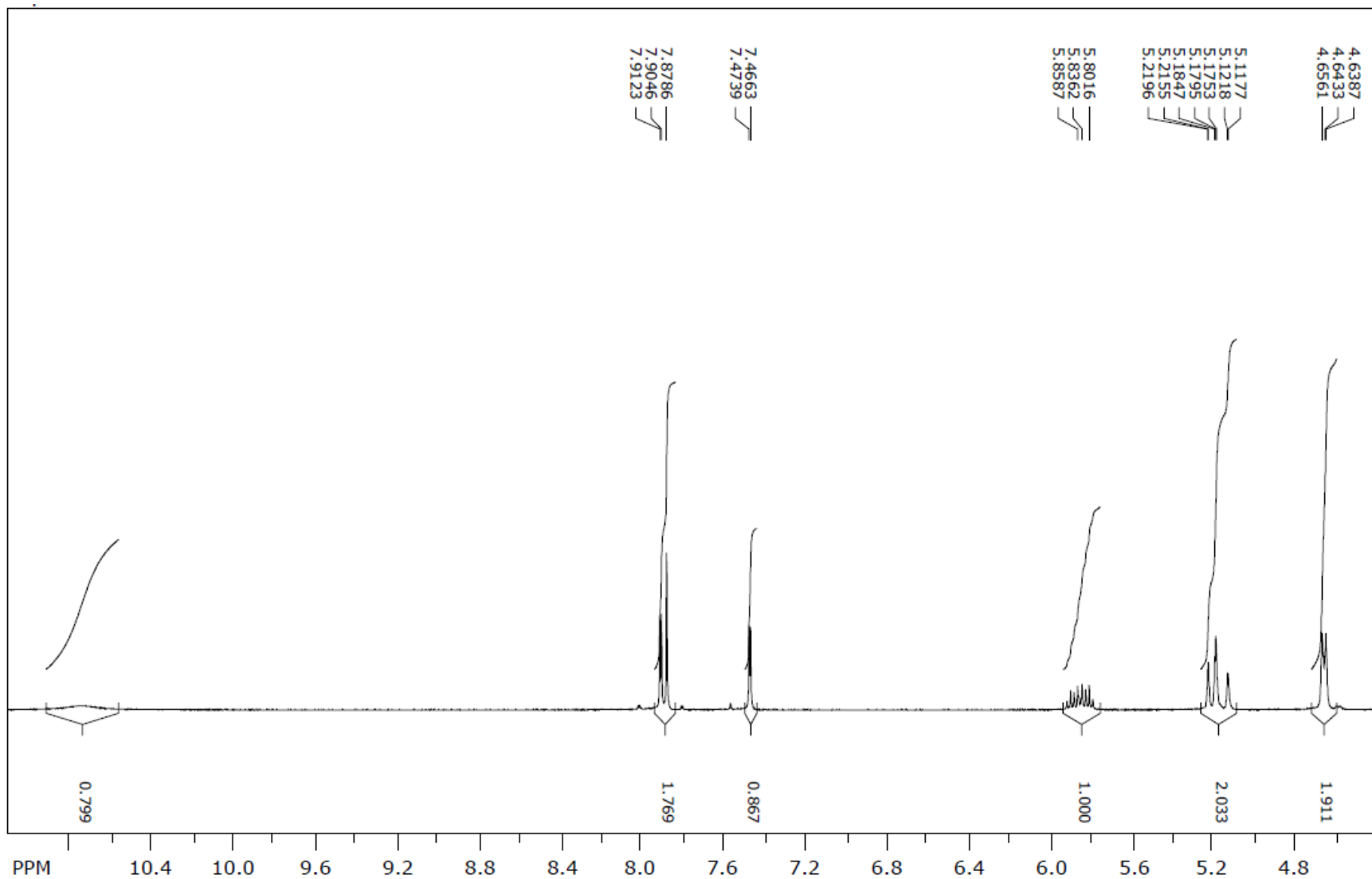


Reaktanti	3,5-dibromsalicilaldehid (2 mmol) i 3-aliilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	435,15 g/mol
Molekulska formula	C ₁₃ H ₉ Br ₂ NO ₂ S ₂
Temperatura tališta	215 – 218 °C
Boja kristala	Žuta
R_f	0,92
LC/MS/MS <i>m/z</i> (M-)	433,93
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 10,75 (s, 1H, OH), 7,91 (d, <i>J</i> = 4,25 Hz, 1H, arom.), 7,87 (s, 1H, CH), 7,47 (d, <i>J</i> = 2,28 Hz, 1H, arom.), 5,78 – 5,91 (m, 1H, CH), 5,17 (dtd, <i>J</i> = 1,23; 10,47; 8,40 Hz, 2H, CH ₂), 4,65 (d, <i>J</i> = 5,22 Hz, 2H, CH ₂).
¹³C NMR	(75 MHz, DMSO- <i>d</i> ₆) δ 193,48; 166,80; 153,22; 137,35; 131,25; 130,61; 127,69; 125,50; 118,39; 114,36; 112,28; 46,68.

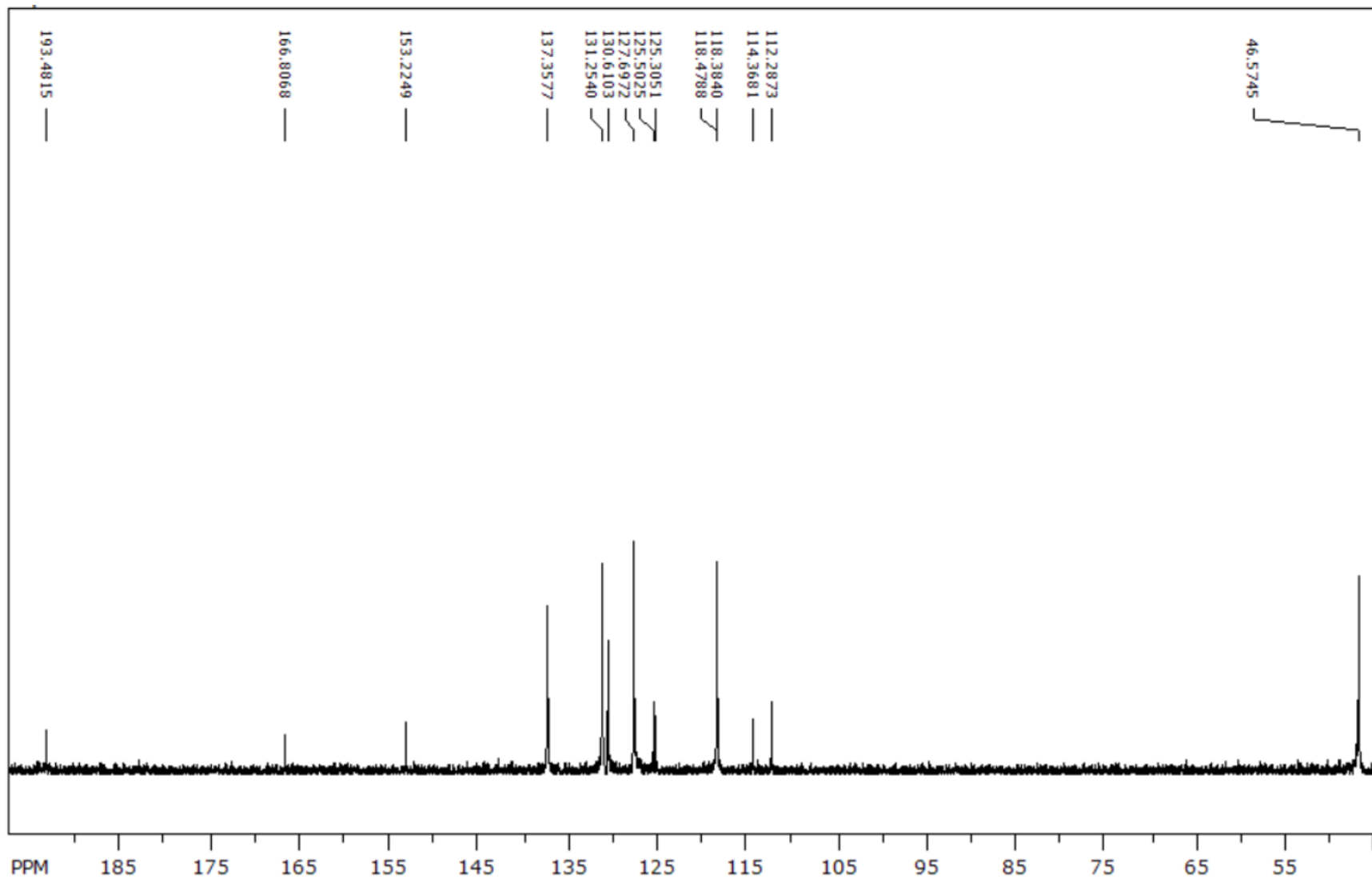
Maseni spektar (6I)



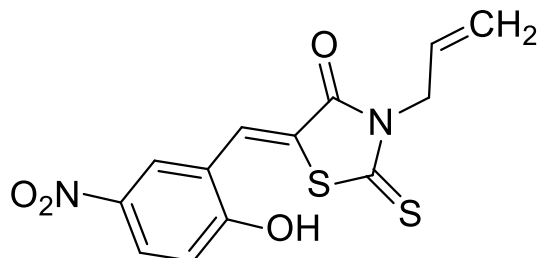
¹H NMR spektr (6I)



¹³C NMR spektr (6l)

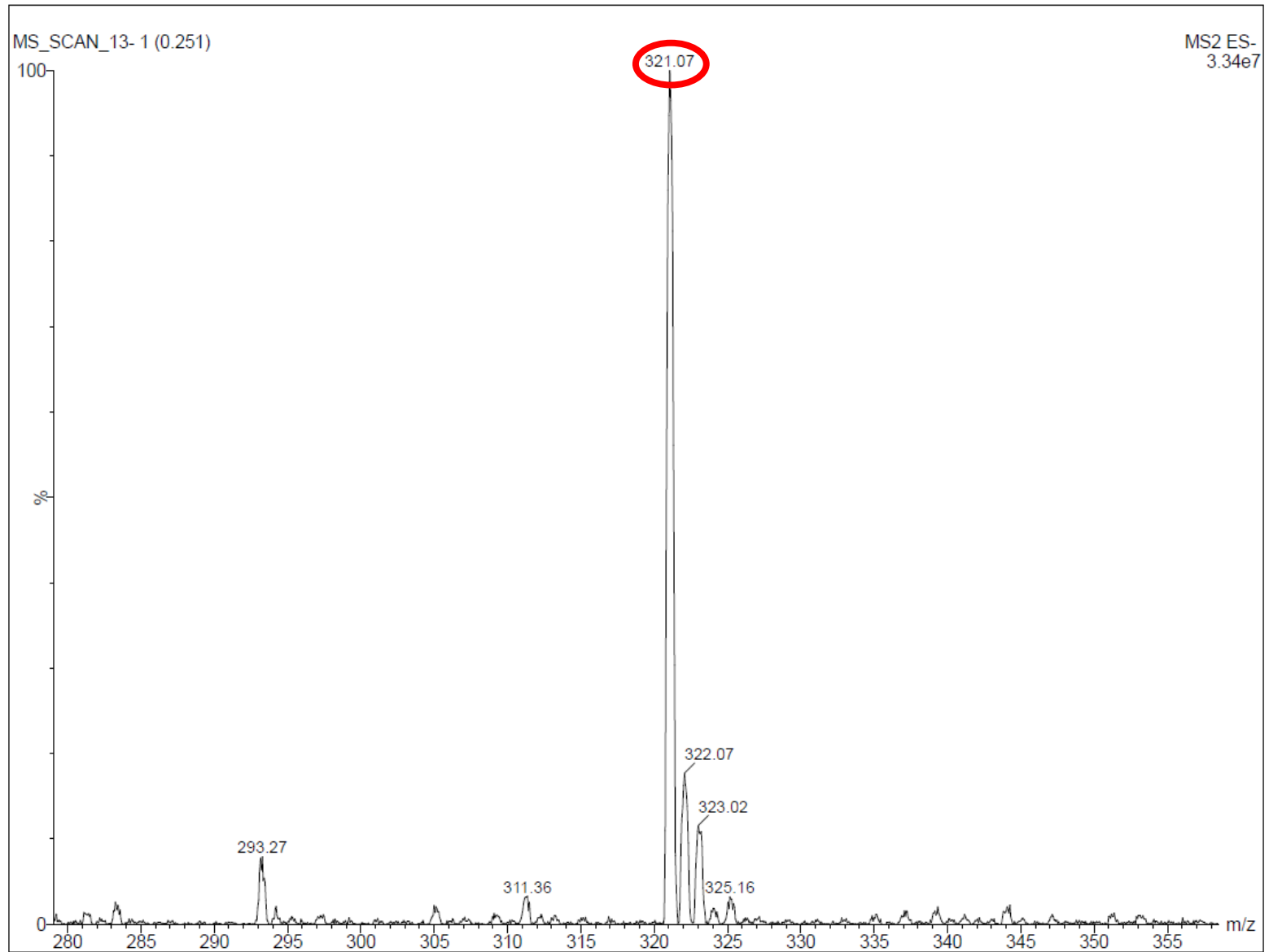


3-alil-5-(2-hidroksi-5-nitrobenziliden)-2-tioksotiazolidin-4-on (6m)

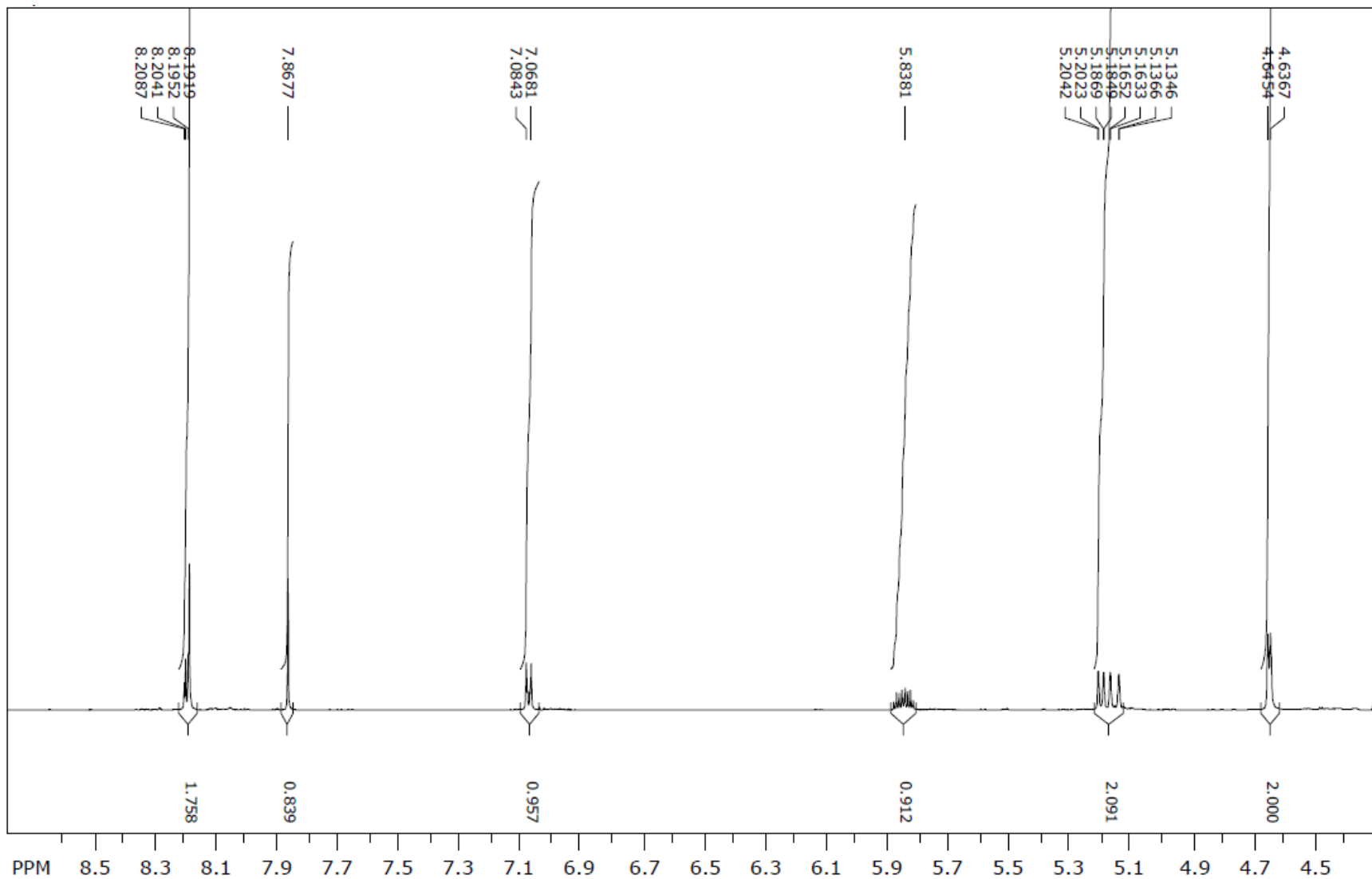


Reaktanti	5-nitrosalicilaldehid (2 mmol) i 3-alilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	322,36 g/mol
Molekulska formula	C ₁₃ H ₁₀ N ₂ O ₄ S ₂
Temperatura tališta	199 – 201 °C
Boja kristala	Narančasta
R_f	0,67
LC/MS/MS <i>m/z</i> (M⁻)	321,07
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,20 (dd, <i>J</i> = 8,10; 2,76; 1,98 Hz, 2H, arom.), 7,86 (s, 1H, CH), 7,08 (dd, <i>J</i> = 7,38; 2,31 Hz, 1H, arom.), 5,81 – 5,88 (m, 1H, CH), 5,19 (dd, <i>J</i> = 10,38; 1,14; 1,20 Hz, 1H, CH ₂), 5,15 (dd, <i>J</i> = 17,16; 1,14; 1,20 Hz, 1H, CH ₂), 4,64 (d, <i>J</i> = 5,22 Hz, 2H, CH ₂).
¹³C NMR	(150 MHz) δ 192,94; 166,51; 139,35; 130,15; 128,00; 126,74; 125,76; 123,62; 120,31; 117,85; 116,92; 46,08.

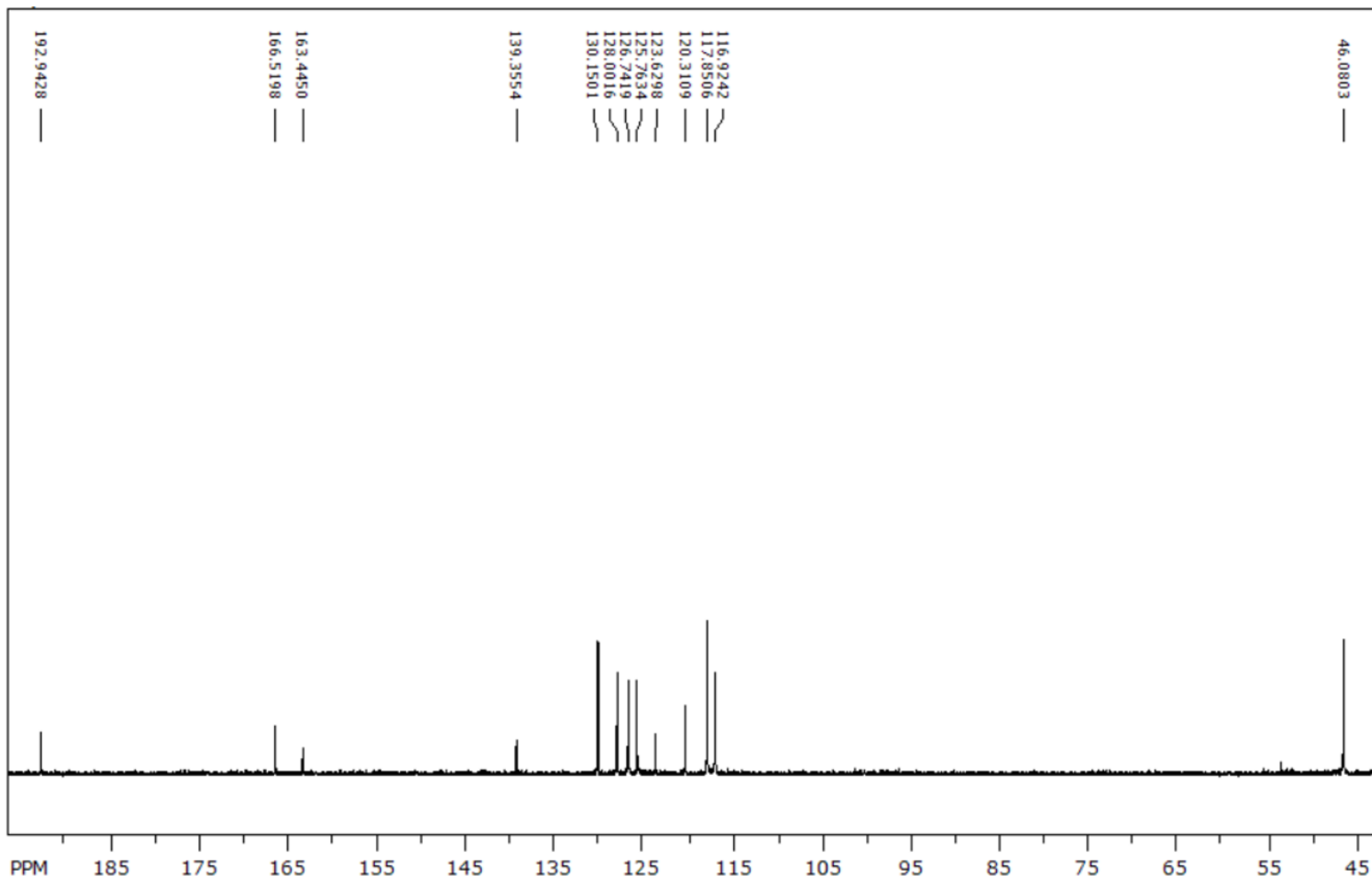
Maseni spektar (6m)



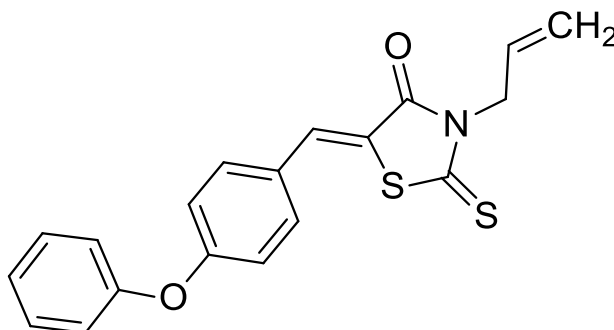
¹H NMR spektr (6m)



¹³C NMR spektr (6m)

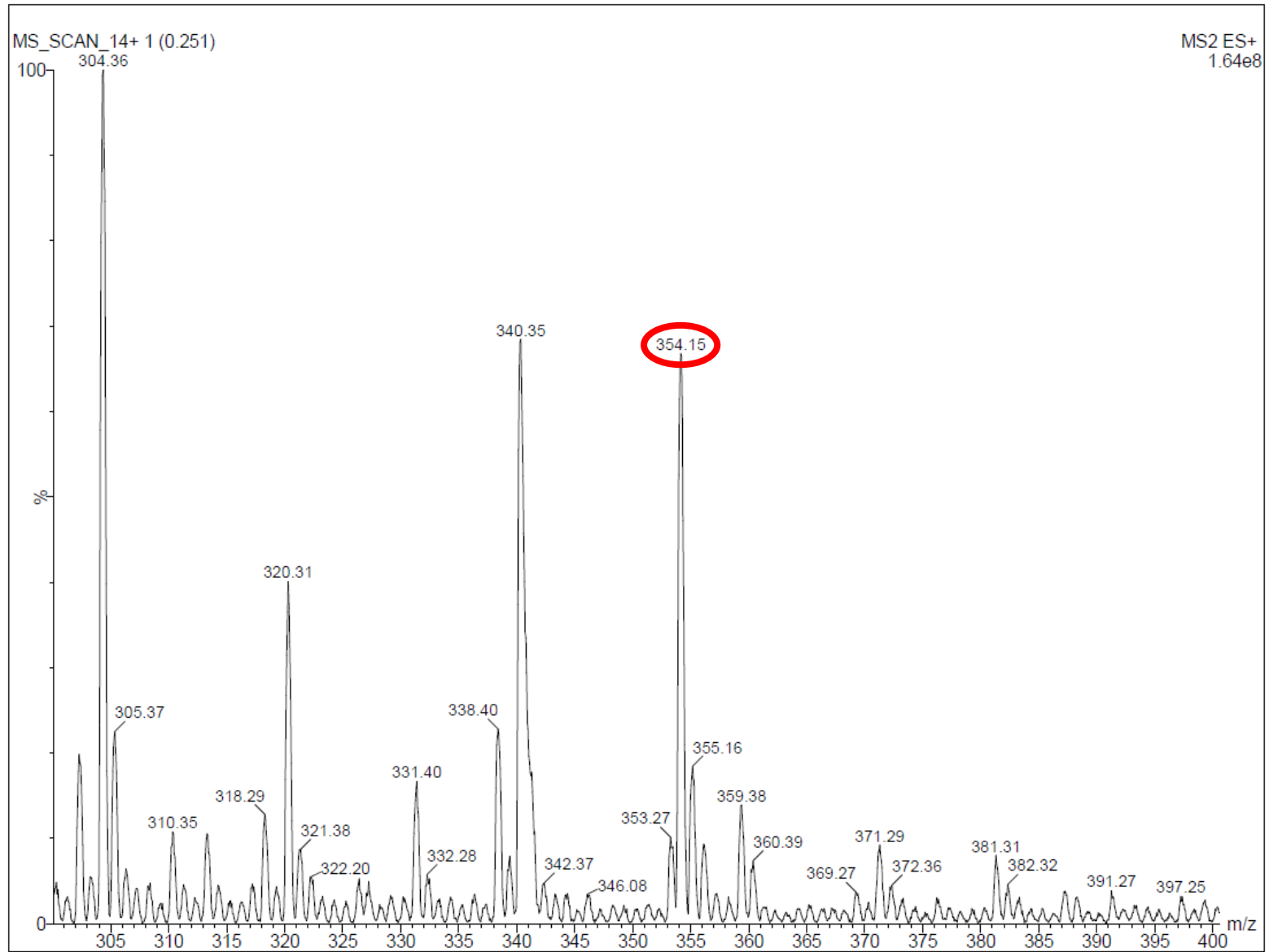


3-alil-5-(4-fenoksibenziliden)-2-tioksotiazolidin-4-on (6n)

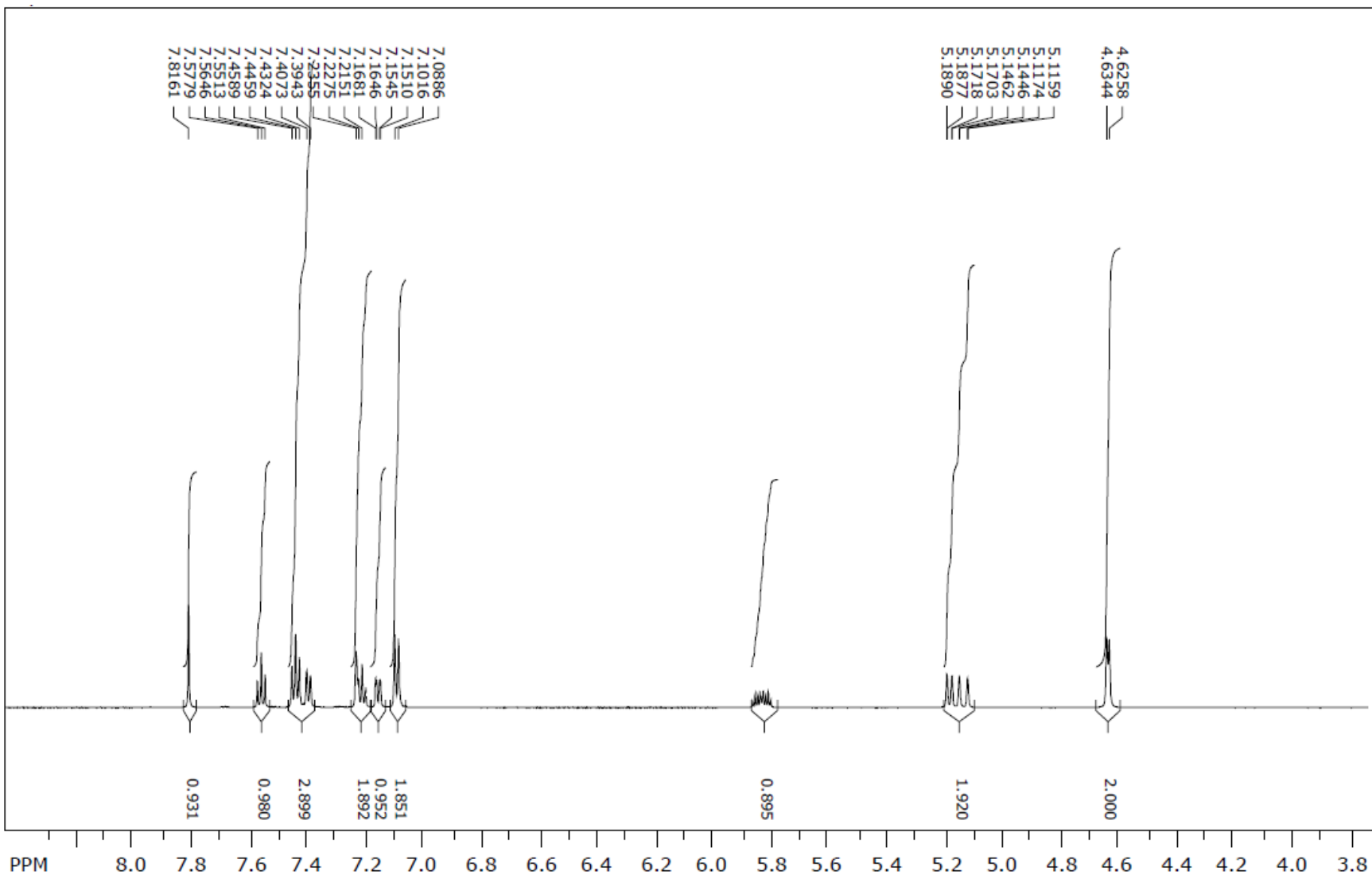


Reaktanti	3-fenoksibenzaldehid (2 mmol) i 3-alilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	353,46 g/mol
Molekulska formula	C ₁₉ H ₁₅ NO ₂ S ₂
Temperatura tališta	91 – 95 °C
Boja kristala	Narančasta
R_f	0,93
LC/MS/MS m/z (M⁺)	354,15
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,81 (s, 1H, CH), 7,56 (t, <i>J</i> = 7,98 Hz, 1H, arom.), 7,45 (t, <i>J</i> = 7,80; 8,10 Hz, 2H, arom.), 7,40 (d, <i>J</i> = 7,80 Hz, 1H, arom.), 7,22 (dd, <i>J</i> = 12,24; 4,80; 7,38 Hz, 2H, arom.), 7,16 (dd, <i>J</i> = 8,16; 2,10 Hz, 1H, arom.), 7,09 (d, <i>J</i> = 7,80 Hz, 2H, arom.), 5,80 – 5,85 (m, 1H, CH), 5,18 (dd, <i>J</i> = 10,32; 0,84 Hz, 1H, CH ₂), 5,13 (dd, <i>J</i> = 17,28; 0,93 Hz, 1H, CH ₂), 4,63 (d, <i>J</i> = 5,16 Hz, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 192,87; 166,42; 157,60; 134,81; 132,32; 131,19; 130,23; 125,21; 124,17; 123,28; 120,65; 119,55; 119,27; 117,78; 46,04.

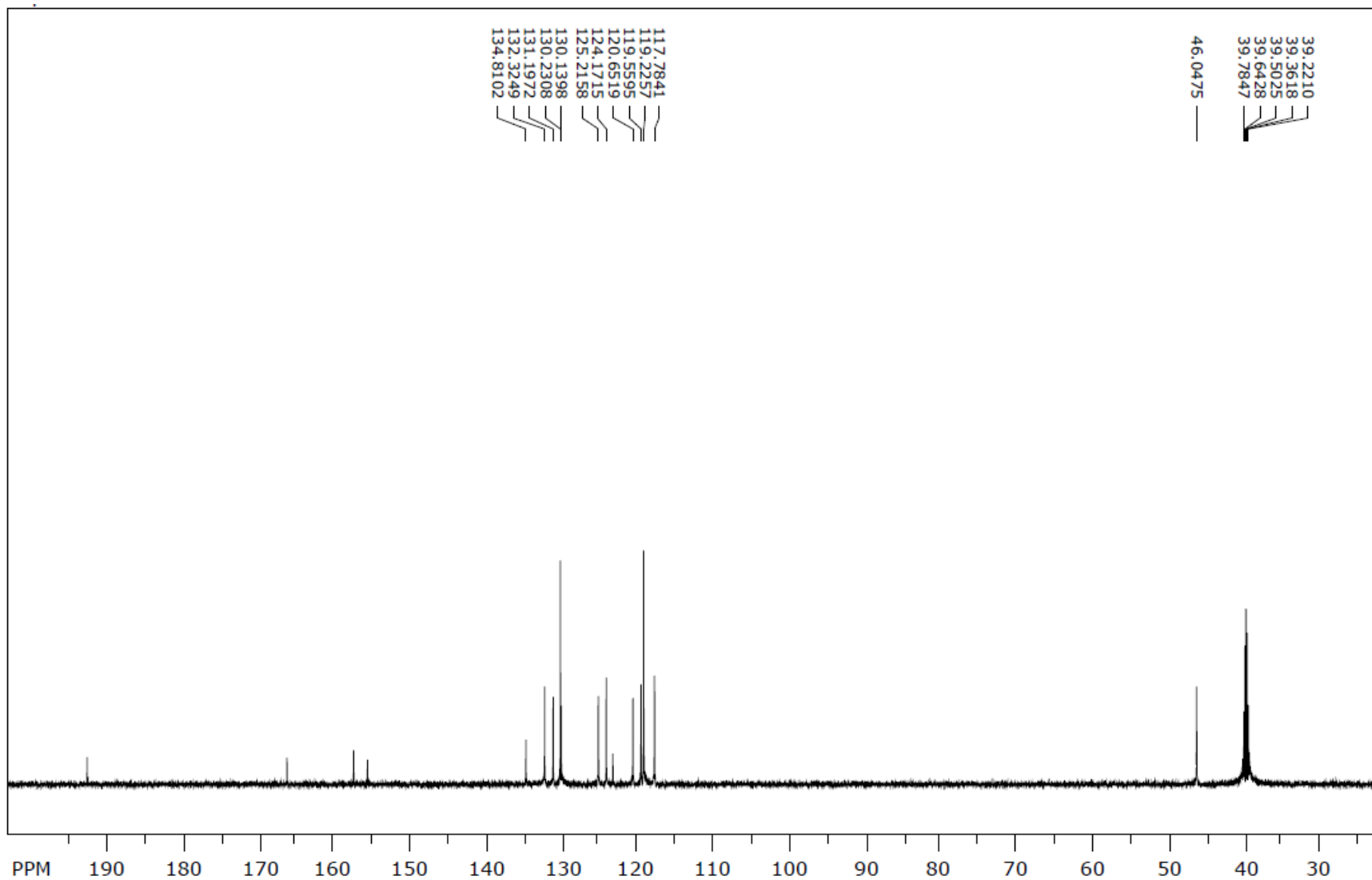
Maseni spektar (6n)



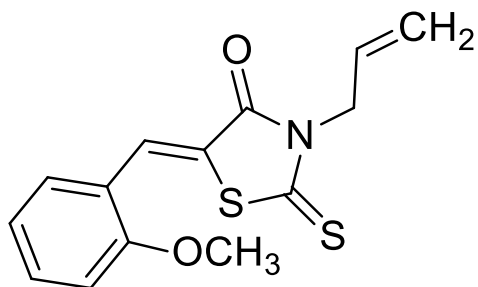
¹H NMR spektr (6n)



¹³C NMR spektr (6n)

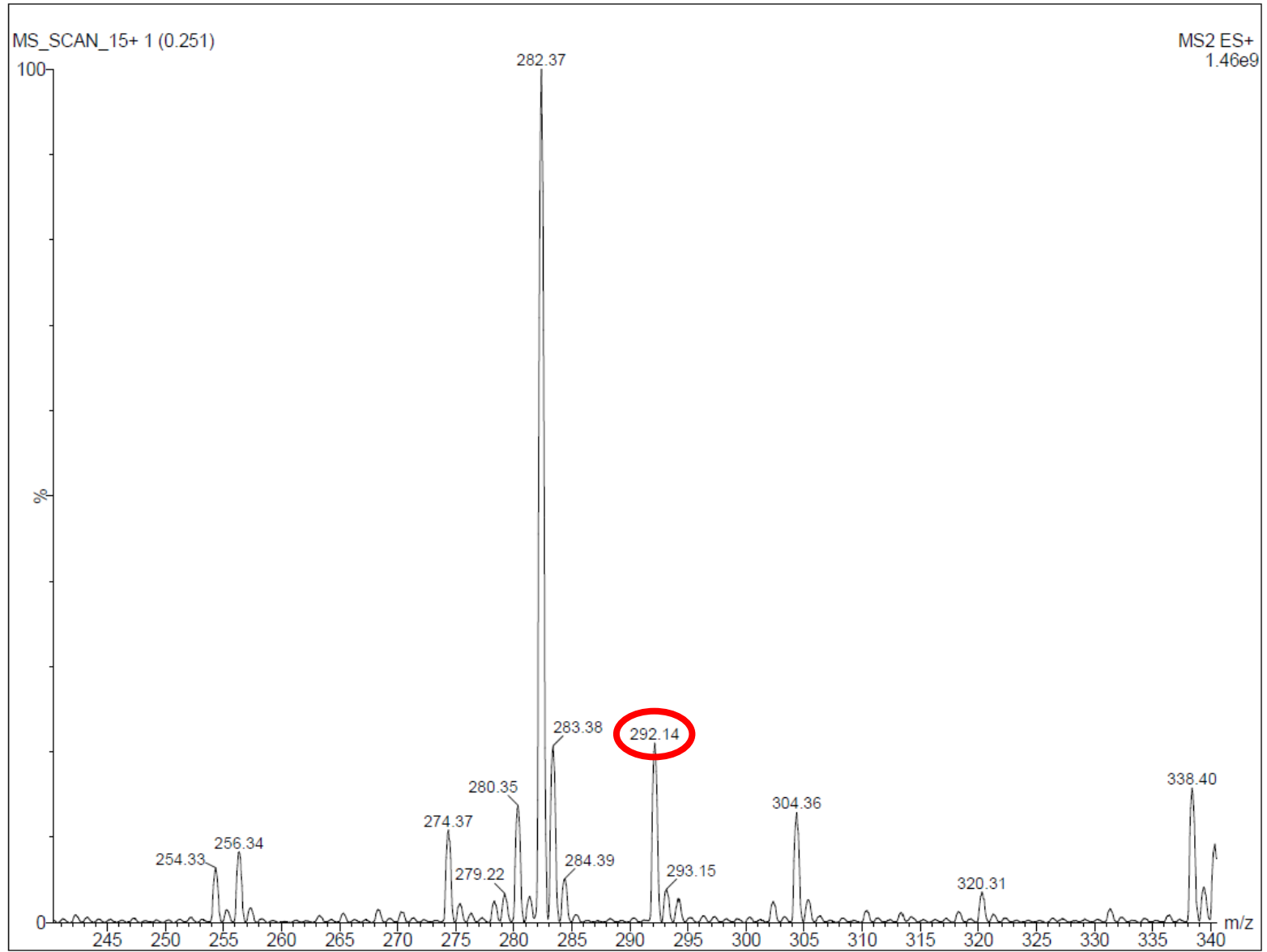


3-alil-5-(2-metoksibenziliden)-2-tioksotiazolidin-4-on (6o)

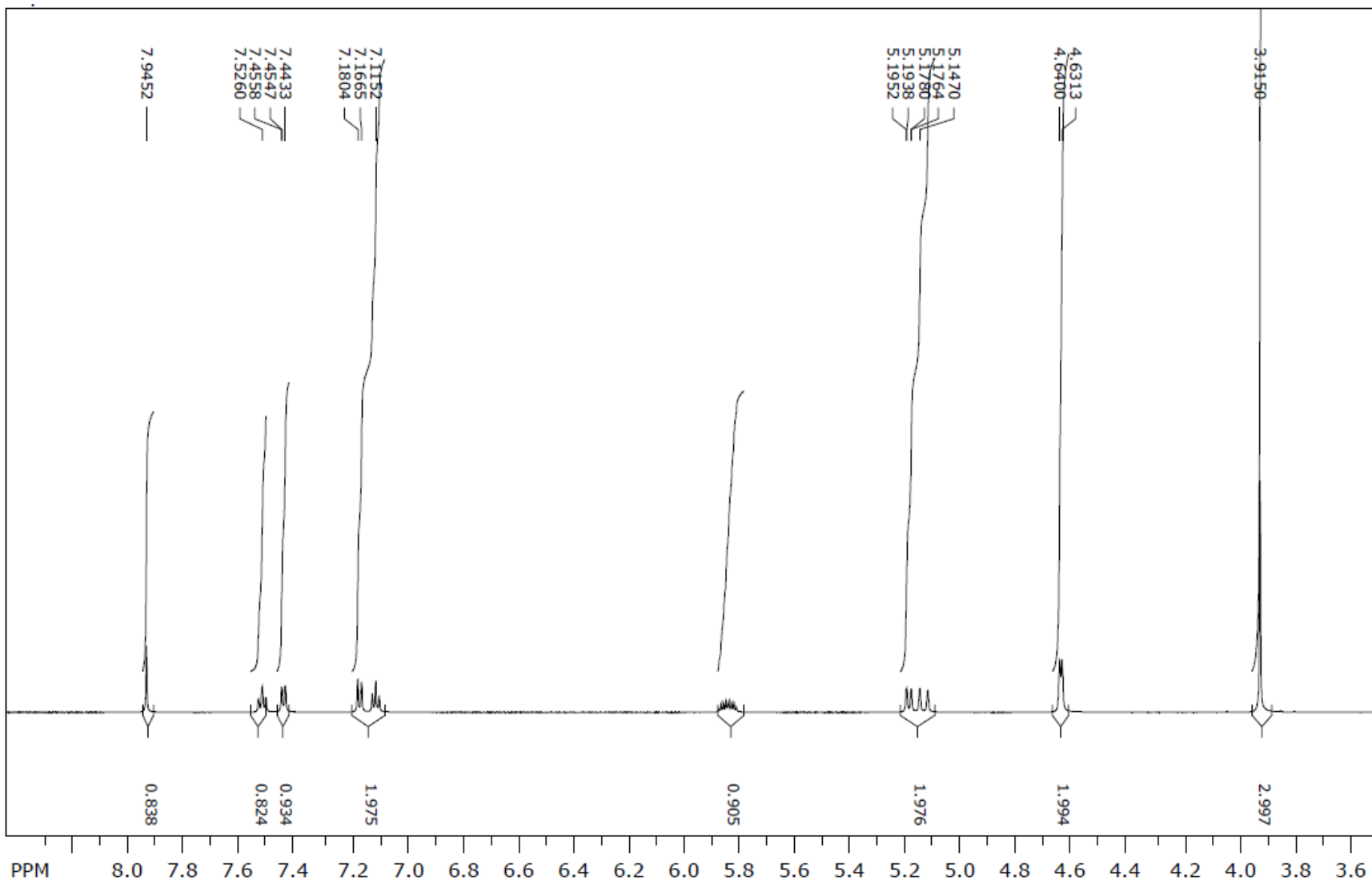


Reaktanti	2-metoksibenzaldehid (2 mmol) i 3-alilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	291,39 g/mol
Molekulska formula	C ₁₄ H ₁₃ NO ₂ S ₂
Temperatura tališta	102 – 104 °C
Boja kristala	Narančasta
R_f	0,90
LC/MS/MS <i>m/z</i> (M⁺)	292,14
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,94 (s, 1H, OH), 7,52 (t, <i>J</i> = 7,77 Hz, 1H, arom.), 7,44 (d, <i>J</i> = 7,20 Hz, 1H, arom.), 7,17 (d, <i>J</i> = 8,34 Hz, 1H, arom.), 7,12 (t, <i>J</i> = 7,50 Hz, 1H, arom.), 5,81 – 5,87 (m, H, CH), 5,19 (dd, <i>J</i> = 10,32; 0,90 Hz, 1H, CH ₂), 5,13 (dd, <i>J</i> = 17,22; 0,99 Hz, 1H, CH ₂), 4,64 (d, <i>J</i> = 5,22 Hz, 2H, CH ₂), 3,91 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,54; 166,65; 158,13; 133,28; 130,23; 130,09; 128,36; 122,17; 121,24; 117,77; 112,02; 55,76; 46,00.

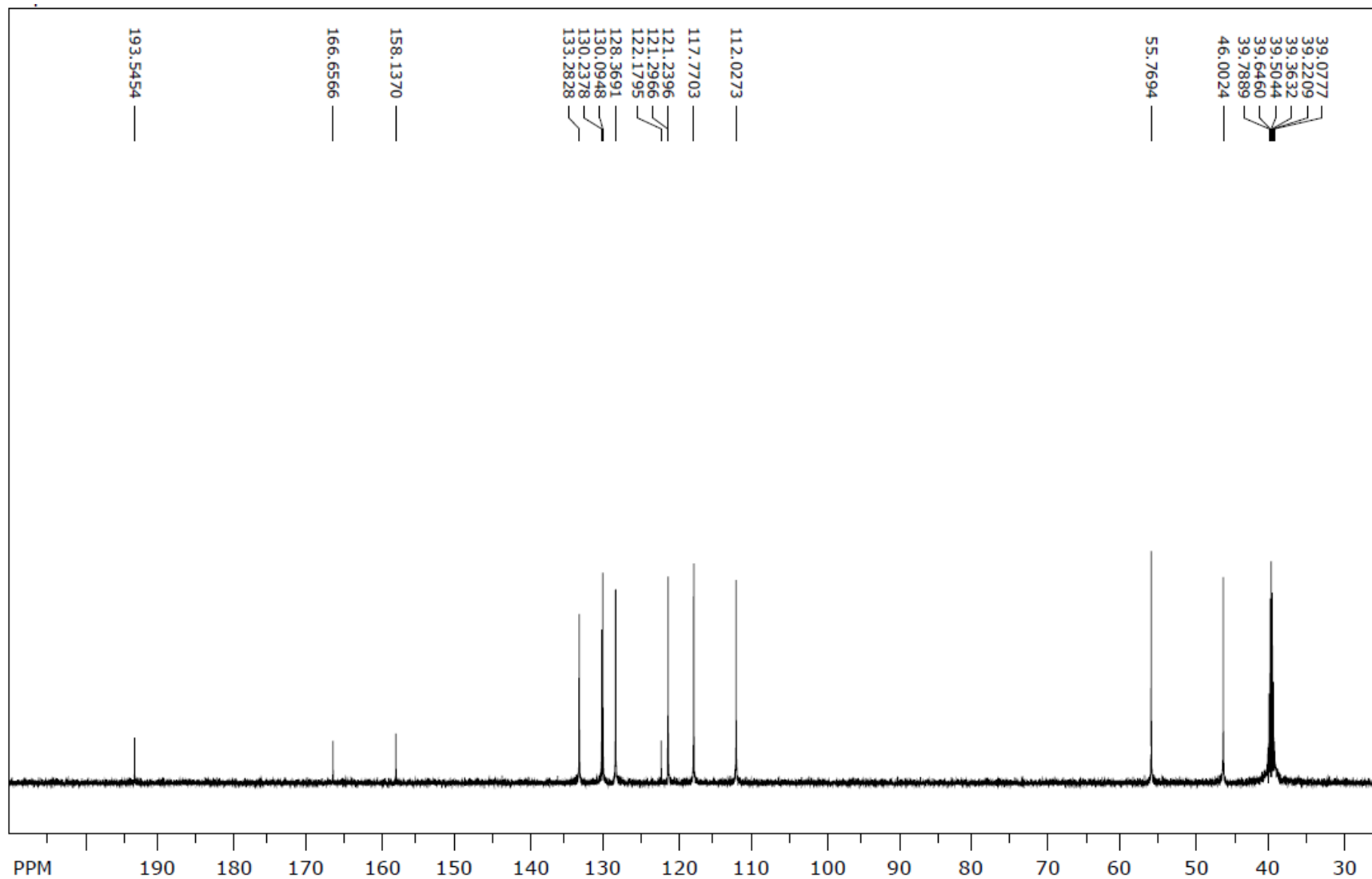
Maseni spektar (6o)



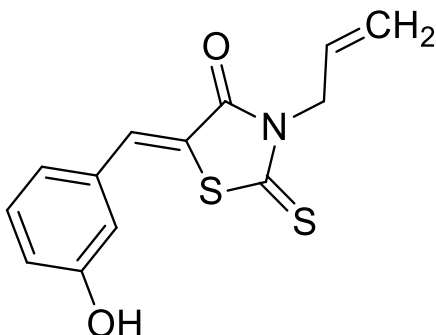
¹H NMR spektr (6o)



¹³C NMR spektr (6o)

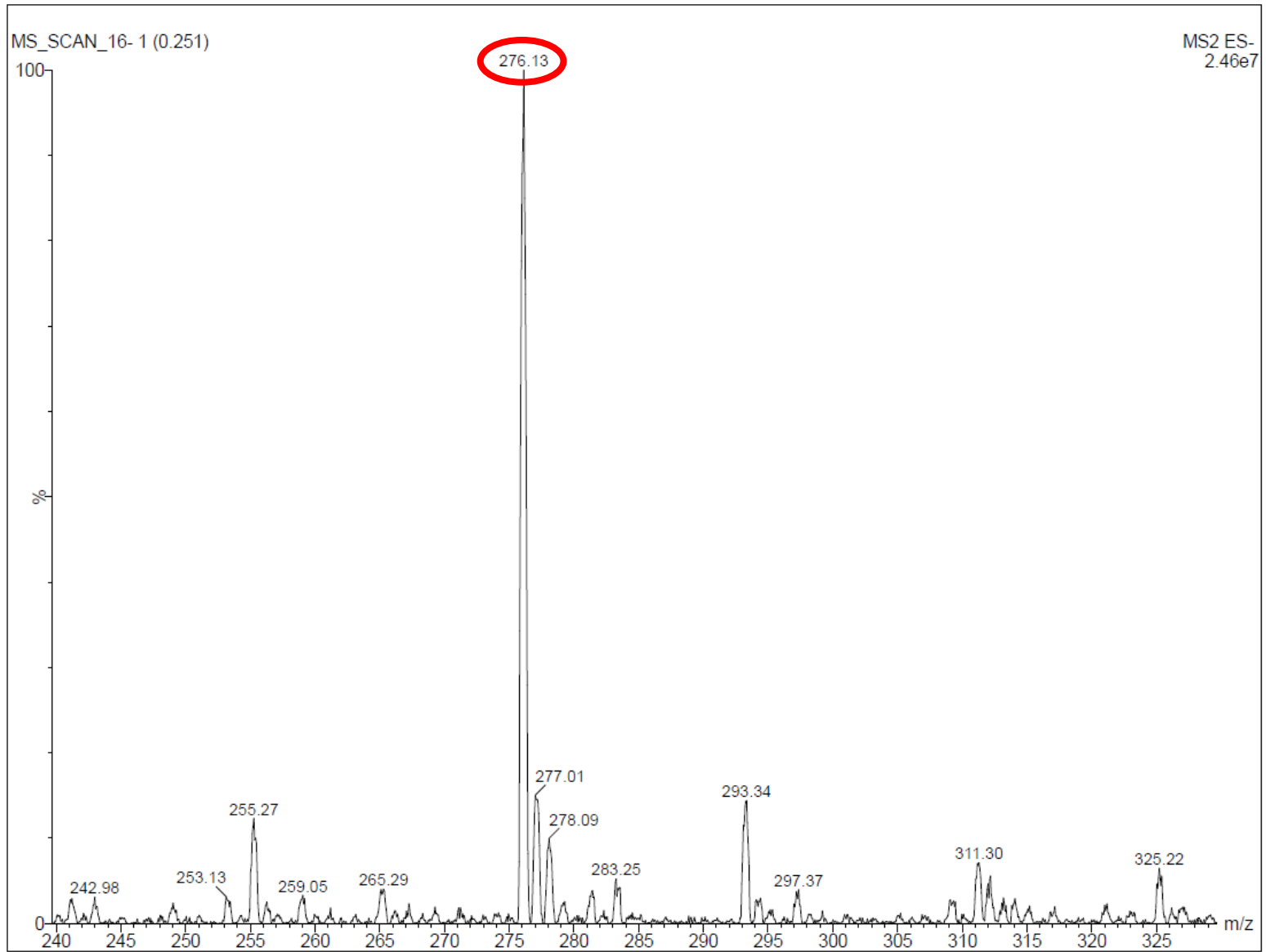


3-ailil-5-(3-hidroksibenziliden)-2-tioksotiazolidin-4-on (6p)

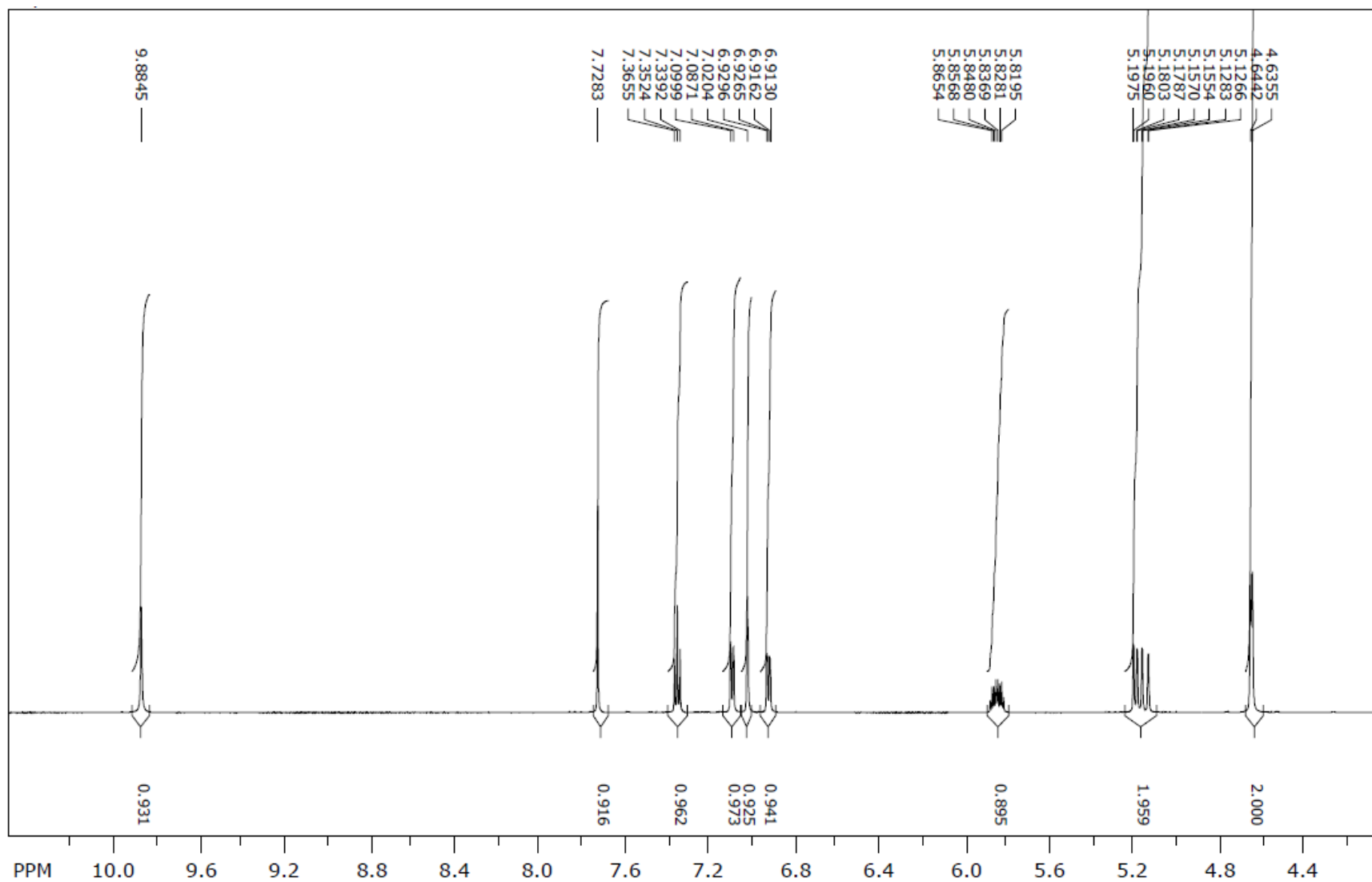


Reaktanti	3-hidroksibenzaldehid (2 mmol) i 3-aililrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	277,36 g/mol
Molekulska formula	C ₁₃ H ₁₁ NO ₂ S ₂
Temperatura tališta	142 – 145 °C
Boja kristala	Narančasta
R_f	0,73
LC/MS/MS <i>m/z</i> (M-)	276,13
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 9,88 (s, 1H, OH), 7,73 (s, 1H, CH), 7,35 (t, <i>J</i> = 7,89 Hz, 1H, arom.), 7,09 (d, <i>J</i> = 7,68 Hz, 1H, arom.), 7,02 (s, 1H, arom.), 6,92 (dd, <i>J</i> = 8,04; 1,89 Hz, 1H, arom.), 5,81 – 5,87 (m, 1H, CH), 5,19 (dd, <i>J</i> = 10,32; 0,93 Hz, Hz, 1H, CH ₂), 5,14 (dd, <i>J</i> = 17,22; 0,99 Hz, 1H, CH ₂), 4,64 (d, <i>J</i> = 5,22 Hz, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,15; 166,53; 157,98; 134,07; 133,32; 130,56; 130,19; 122,08; 118,37; 117,80; 116,28; 46,00.

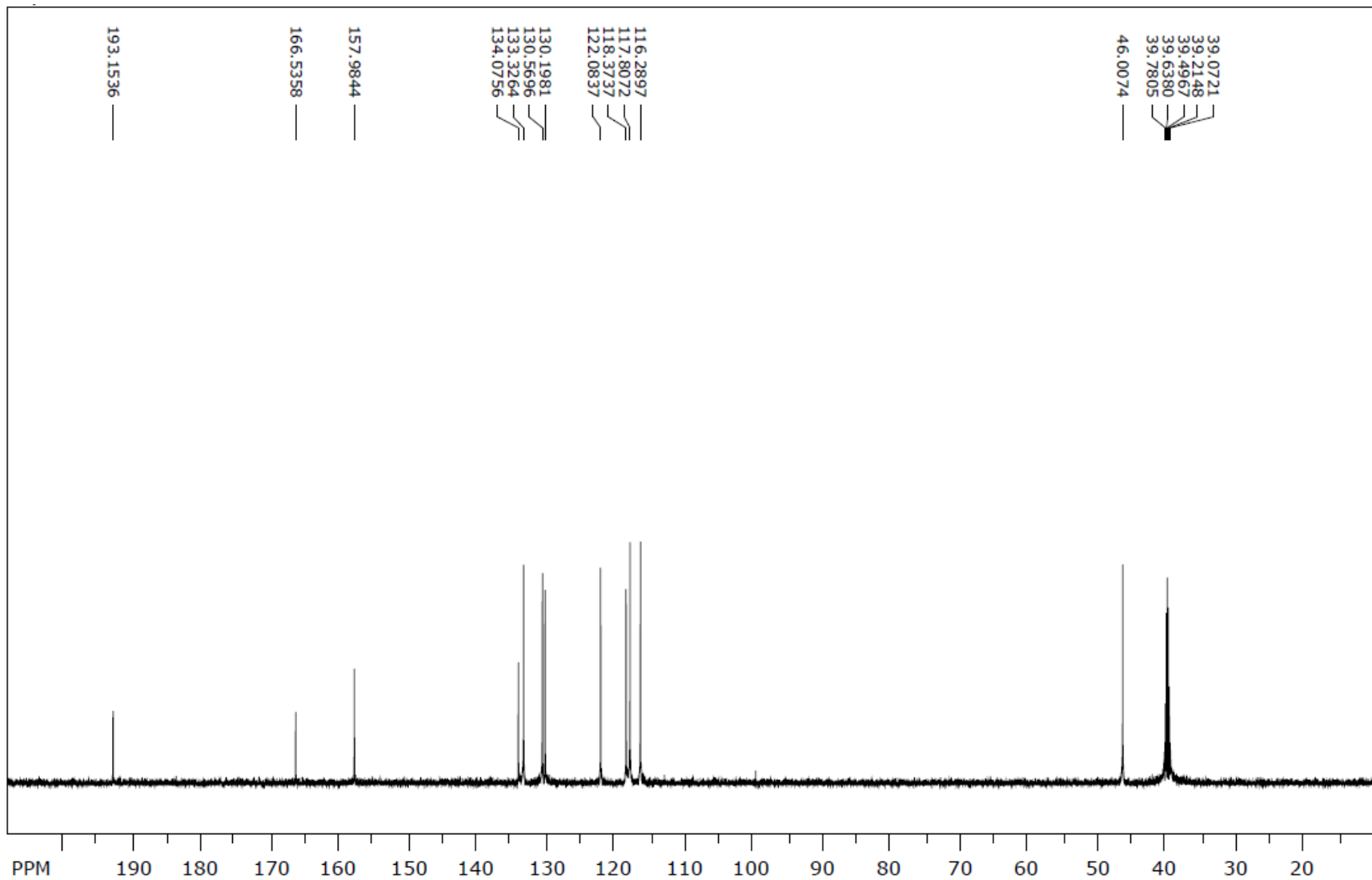
Maseni spektar (6p)



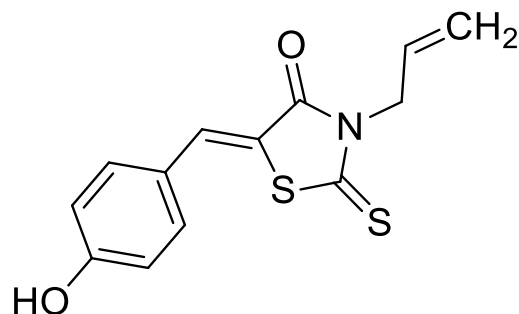
¹H NMR spektr (6p)



¹³C NMR spektr (6p)

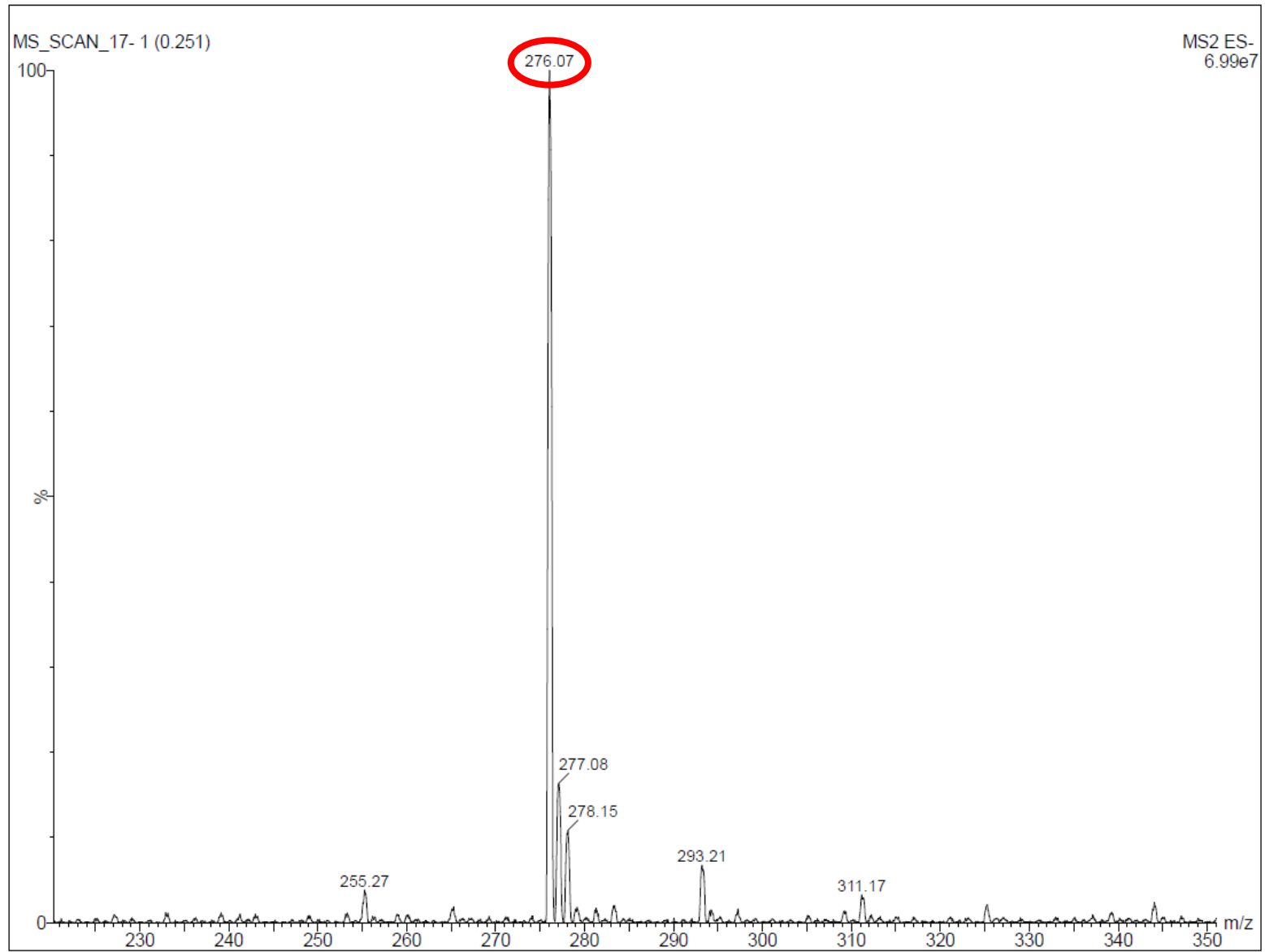


3-alil-5-(4-hidroksibenziliden)-2-tioksotiazolidin-4-on (6q)

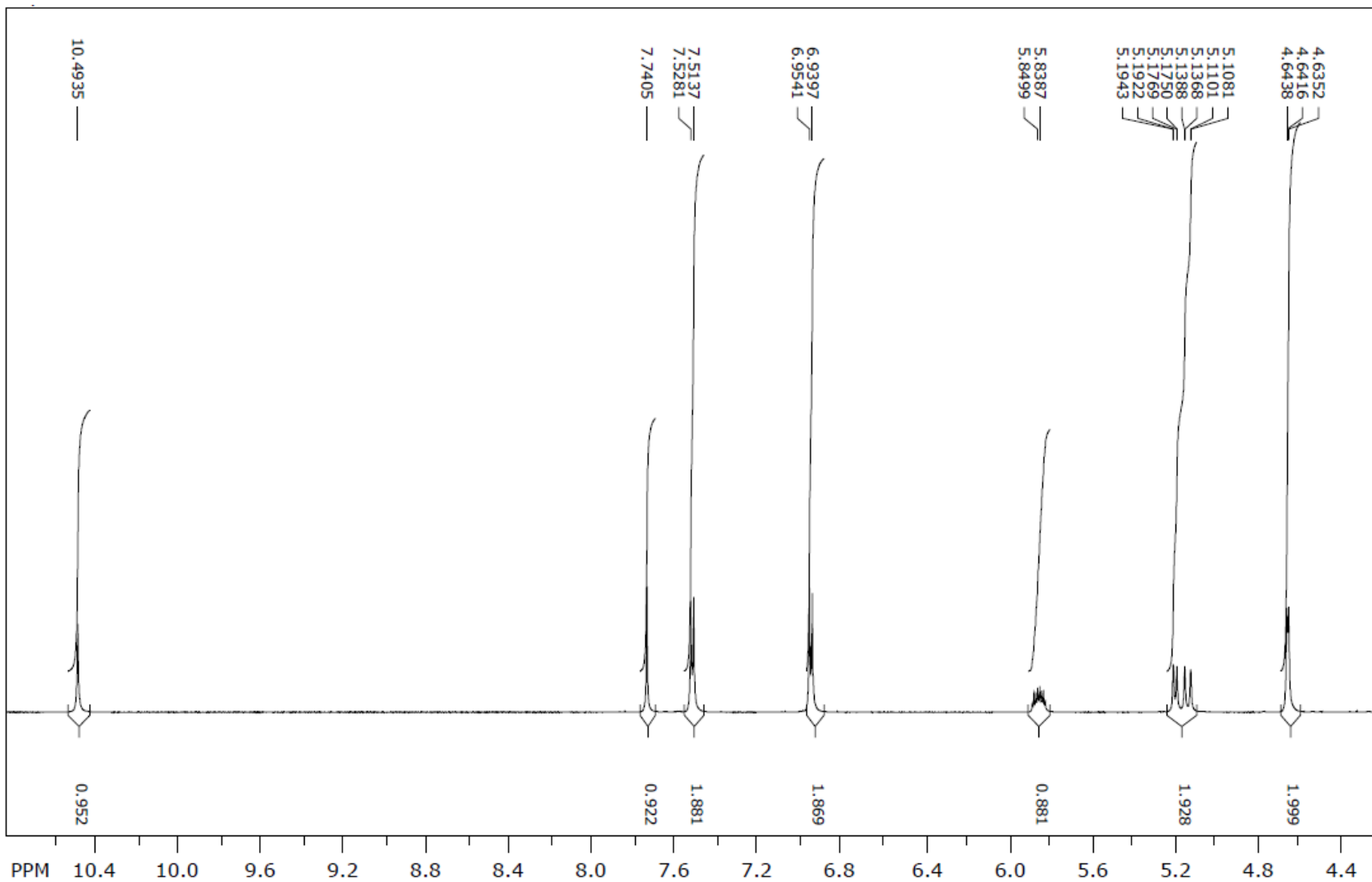


Reaktanti	4-hidroksibenzaldehid (2 mmol) i 3-alilrodanin (2 mmol)
Metoda pročiščavanja	Prekristalizacija iz etanola i metanola
Molekulska masa	277,36 g/mol
Molekulska formula	C ₁₃ H ₁₁ NO ₂ S ₂
Temperatura tališta	275 – 277 °C
Boja kristala	Narančasta
R_f	0,86
LC/MS/MS m/z (M-)	276,07
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 10,49 (s, 1H, OH), 7,74 (s, 1H, CH), 7,52 (d, <i>J</i> = 8,64 Hz, 2H, arom.), 6,95 (d, <i>J</i> = 8,64 Hz, 2H, arom.), 5,81 – 5,87 (m, 1H, CH), 5,18 (dd, <i>J</i> = 10,44; 1,20 Hz, 1H, CH ₂), 5,12 (dd, <i>J</i> = 17,22; 1,20 Hz, 1H, CH ₂), 4,64 (d, <i>J</i> = 5,16 Hz, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,37; 167,15; 161,14; 134,42; 133,84; 130,78; 124,47; 118,19; 118,06; 117,09; 46,42.

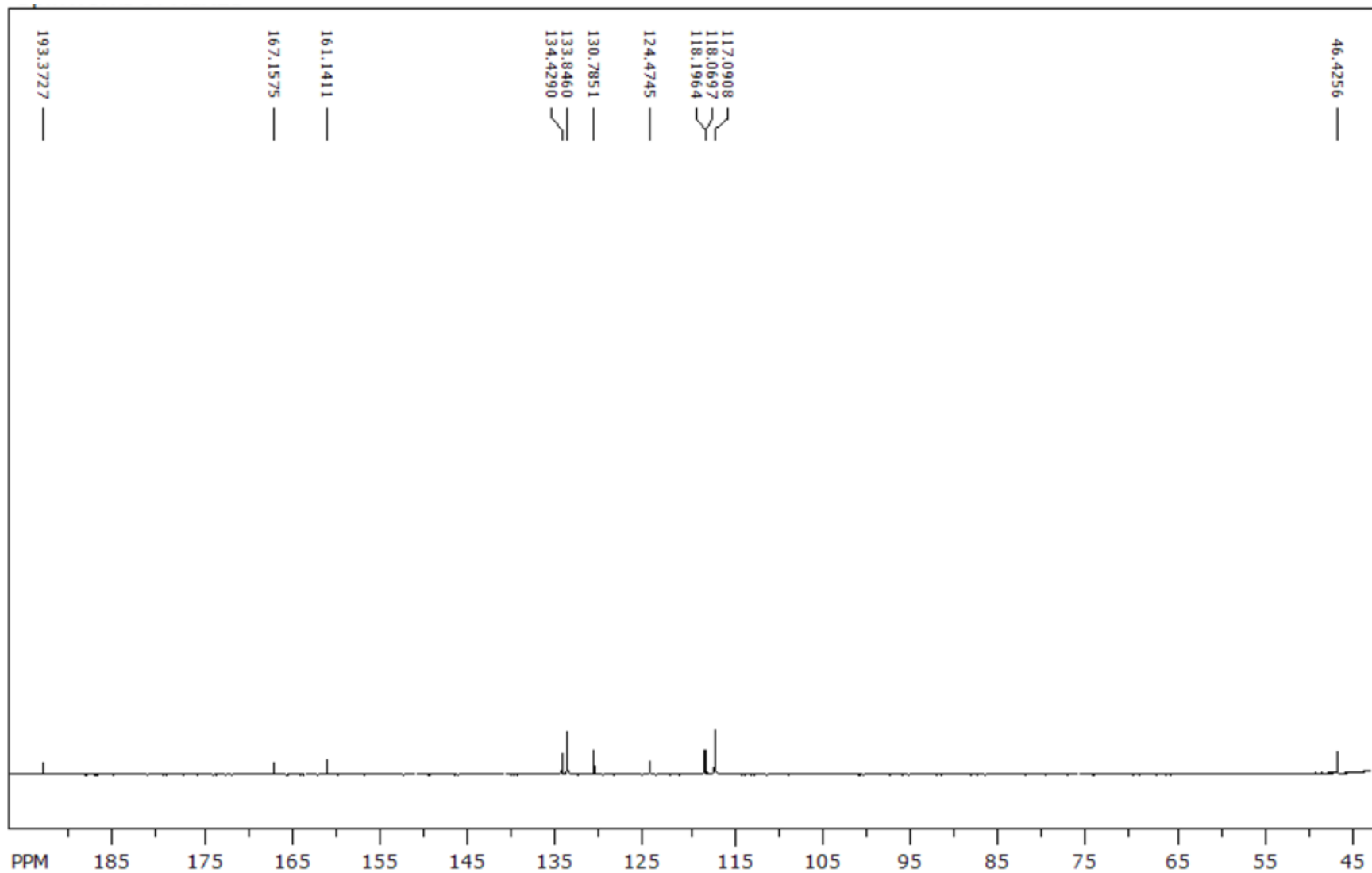
Maseni spektr (6q)



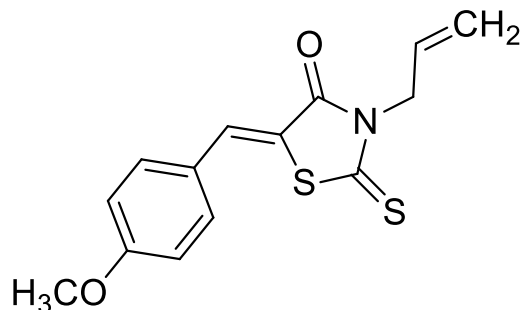
¹H NMR spektr (6q)



¹³C NMR spektar (6q)

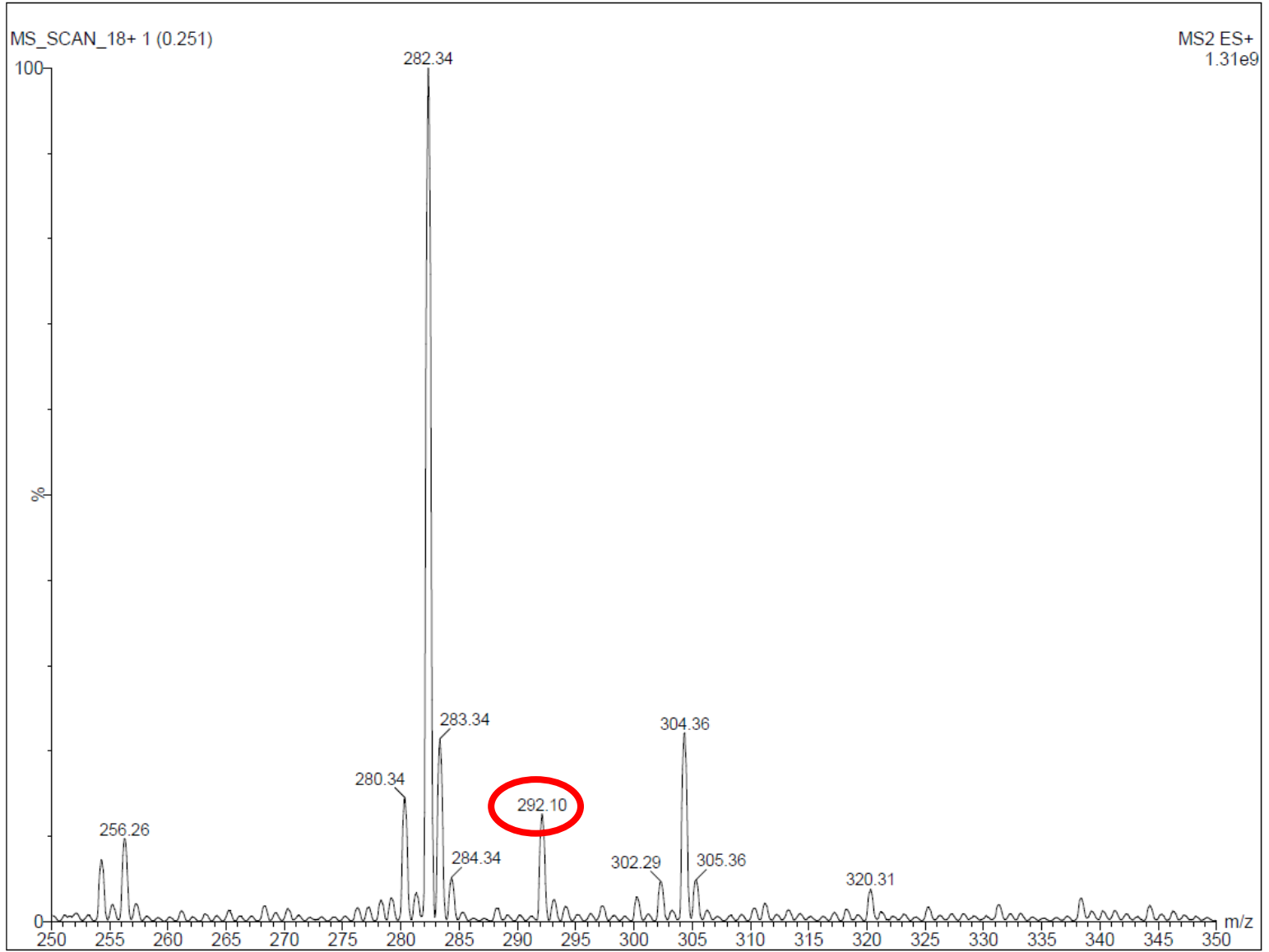


3-alil-5-(4-metoksibenzilidene)-2-tioksotiazolidin-4-on (6r)

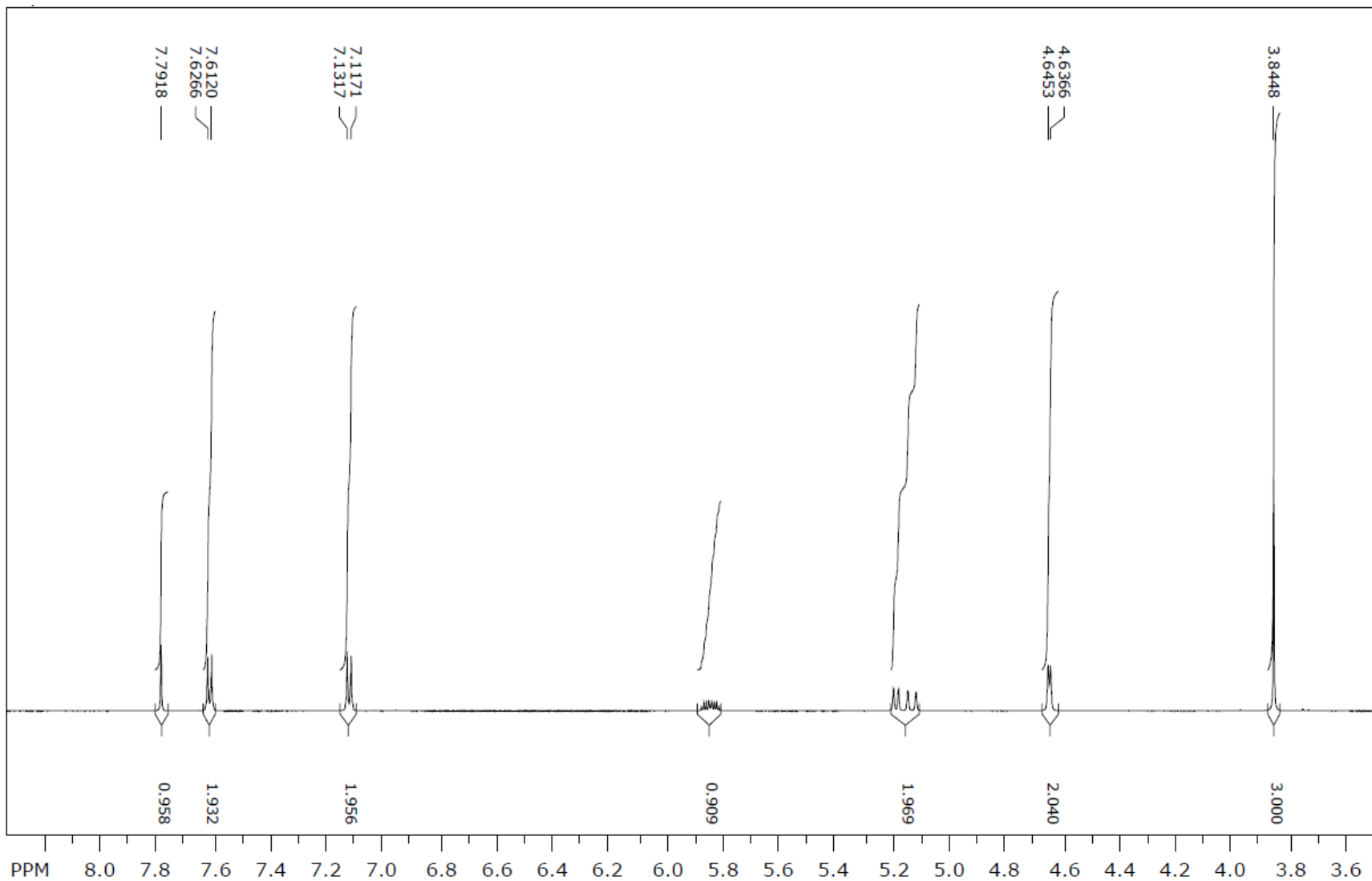


Reaktanti	4-metoksibenzaldehid (2 mmol) i 3-alilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	291,39 g/mol
Molekulska formula	C ₁₄ H ₁₃ NO ₂ S ₂
Temperatura tališta	109 – 111 °C
Boja kristala	Smeđa
R_f	0,90
LC/MS/MS m/z (M⁺)	292,10
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,79 (s, 1H, CH), 7,62 (d, <i>J</i> = 8,76 Hz, 2H, arom.), 7,12 (d, <i>J</i> = 8,76 Hz, 2H, arom.), 5,81 – 5,88 (m, 1H, CH), 5,18 (dd, <i>J</i> = 10,32; 1,08 Hz, 1H, CH ₂), 5,13 (dd, <i>J</i> = 17,22; 1,20 Hz, 1H, CH ₂), 4,64 (d, <i>J</i> = 5,22 Hz, 2H, CH ₂), 3,84 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 192,97; 166,62; 161,55; 133,37; 132,95; 130,25; 125,48; 118,90; 117,72; 115,14; 55,57; 45,96.

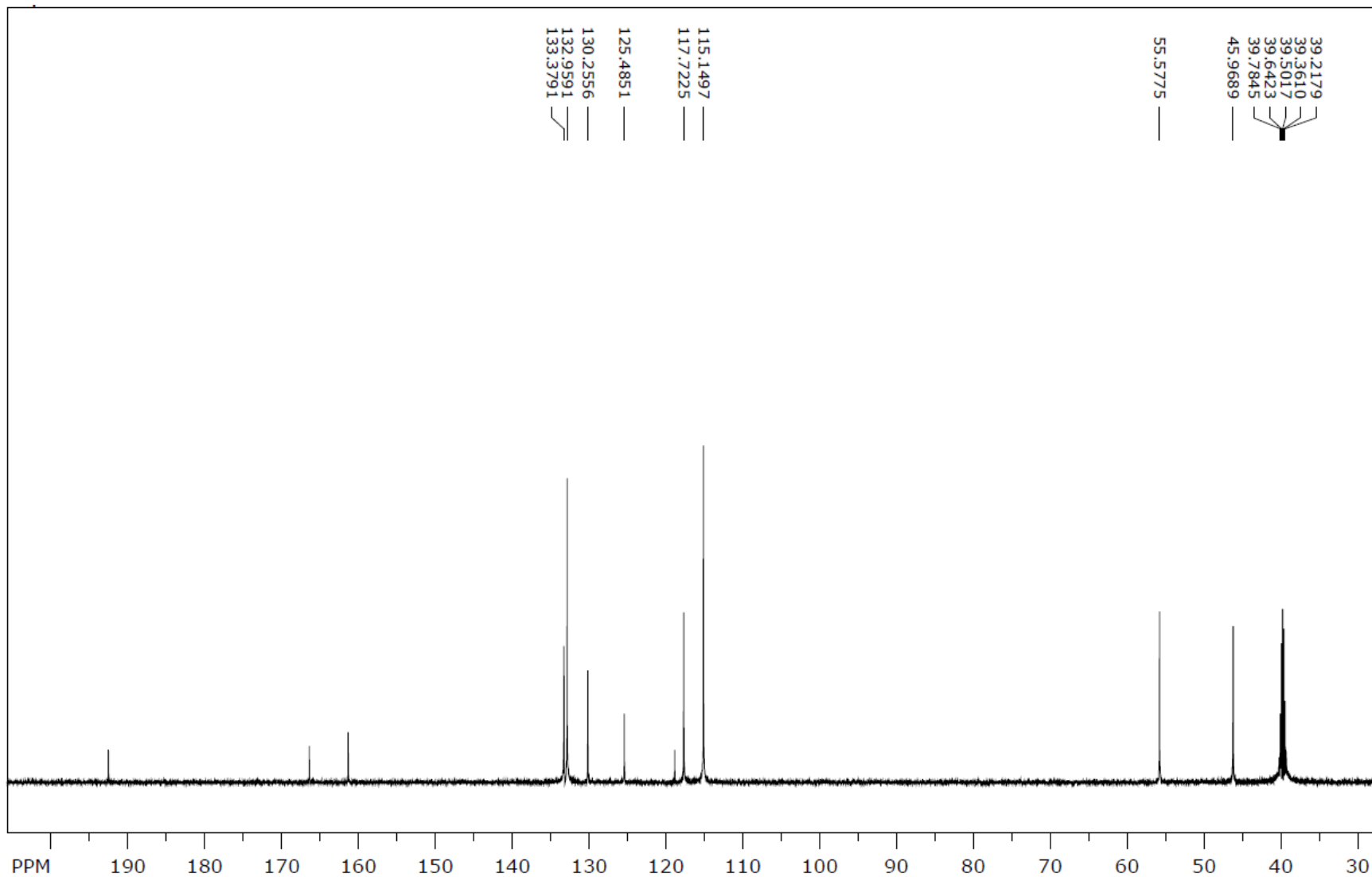
Maseni spektar (6r)



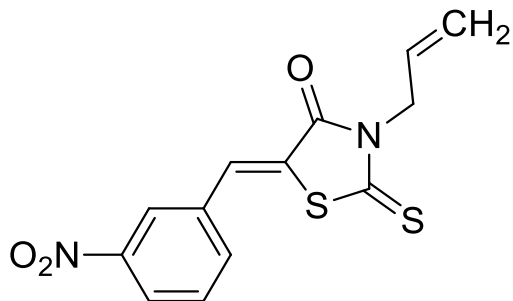
¹H NMR spektr (6r)



¹³C NMR spektr (6r)

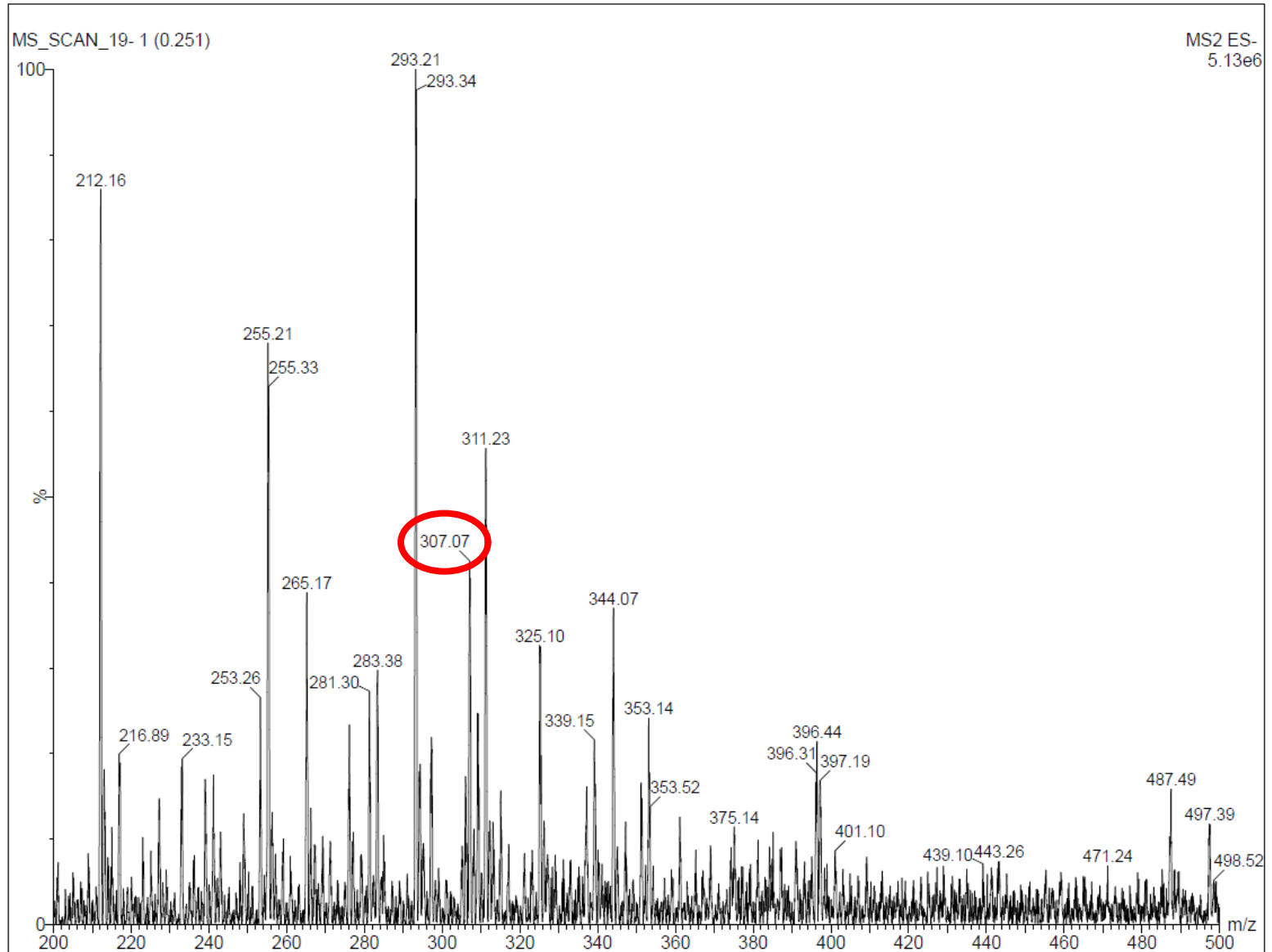


3-alil-5-(3-nitrobenziliden)-2-tioksotiazolidin-4-on (6s)

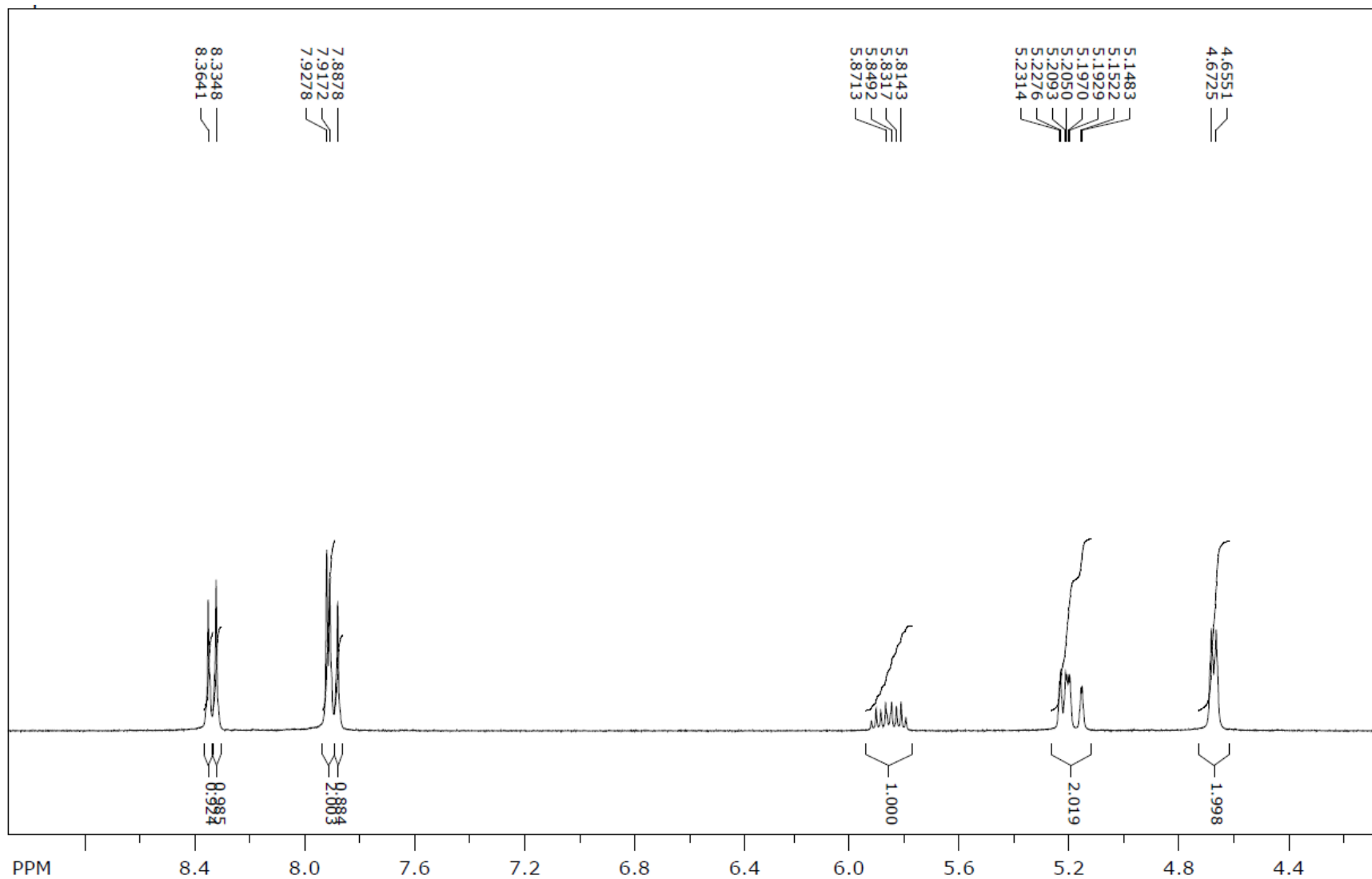


Reaktanti	3-nitrobenzaldehyd (2 mmol) i 3-alilrodanin (2 mmol)
Metoda pročiščavanja	Ispran heksan : etanol (4 : 1)
Molekulska masa	306,36 g/mol
Molekulska formula	C ₁₃ H ₁₀ N ₂ O ₃ S ₂
Temperatura tališta	161 – 163 °C
Boja kristala	Narančasta
R_f	0,92
LC/MS/MS <i>m/z</i> (M⁺)	307,07
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 8,36 (s, 1H, arom.), 8,33 (s, 1H, arom.), 7,92 (d, <i>J</i> = 3,18 Hz, 2H, arom.), 7,88 (s, 1H, CH), 5,80 – 5,92 (m, 1H, CH), 5,22 (dd, <i>J</i> = 6,63; 1,22 Hz, 1H, CH ₂), 5,17 (dd, <i>J</i> = 13,44; 1,20 Hz, 1H, CH ₂), 4,66 (d, <i>J</i> = 5,22 Hz, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,14; 166,87; 148,11; 139,52; 131,97; 130,52; 127,18; 124,84; 46,67.

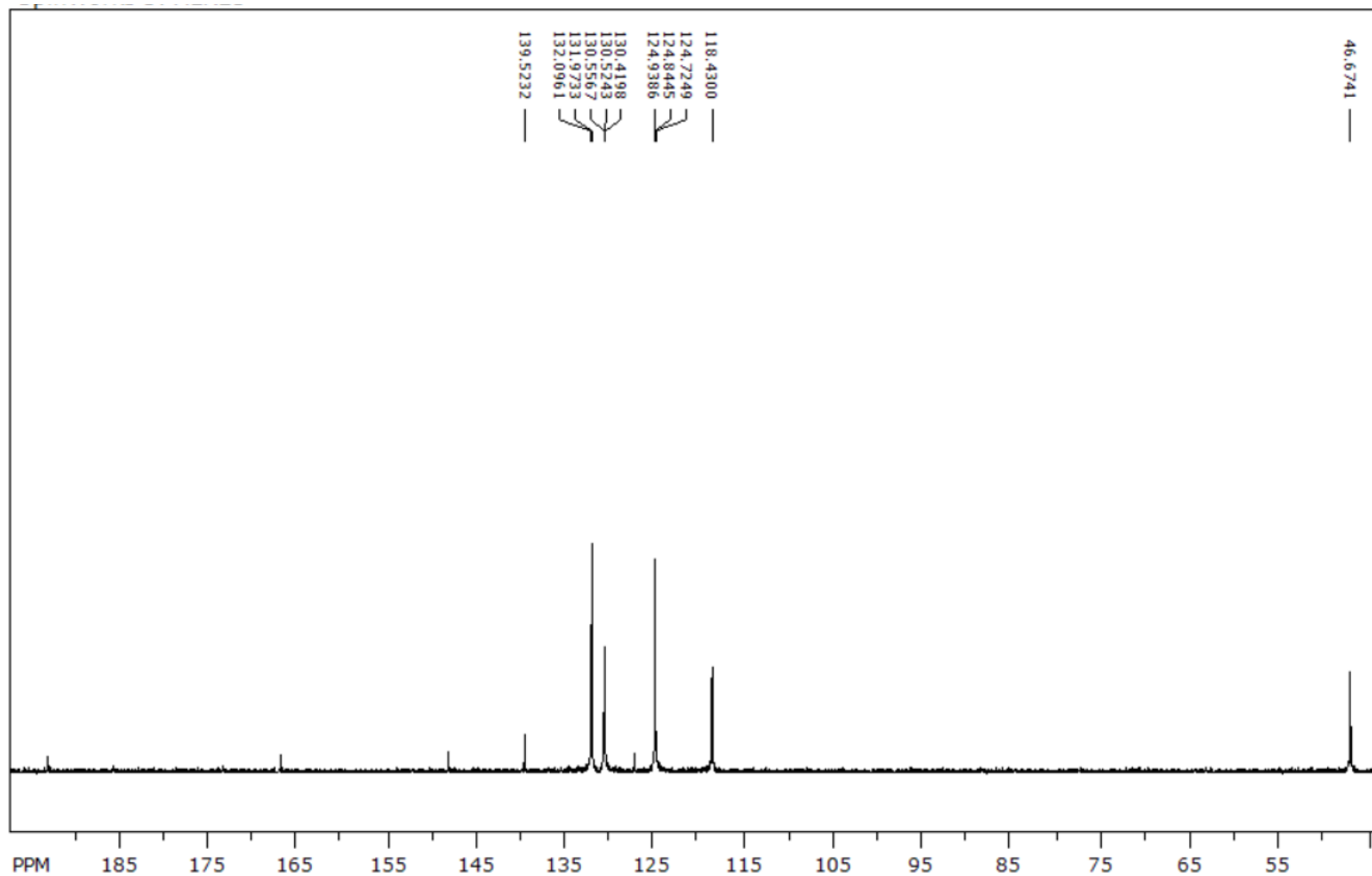
Maseni spektr (6s)



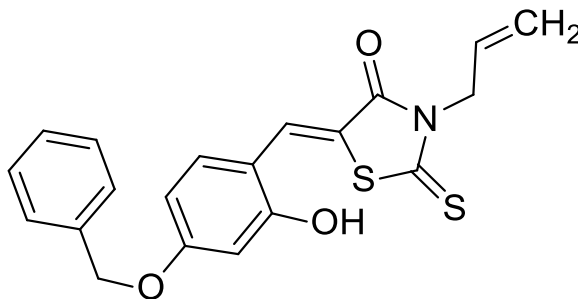
¹H NMR spektr (6s)



¹³C NMR spektr (6s)

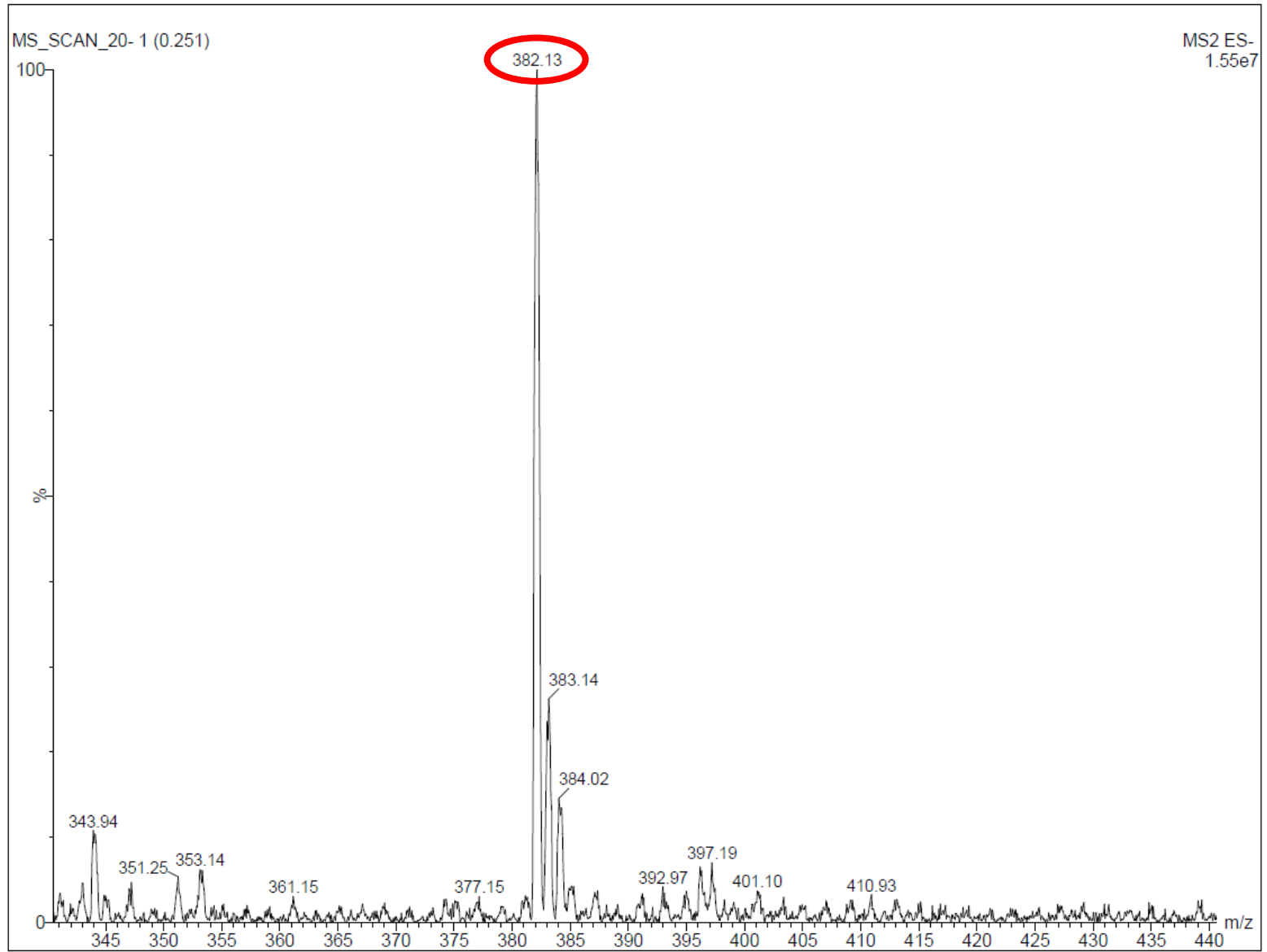


3-alil-5-(4-(benziloksi)-2-hidroksibenziliden)-2-tioksotiazolidin-4-on (6t)

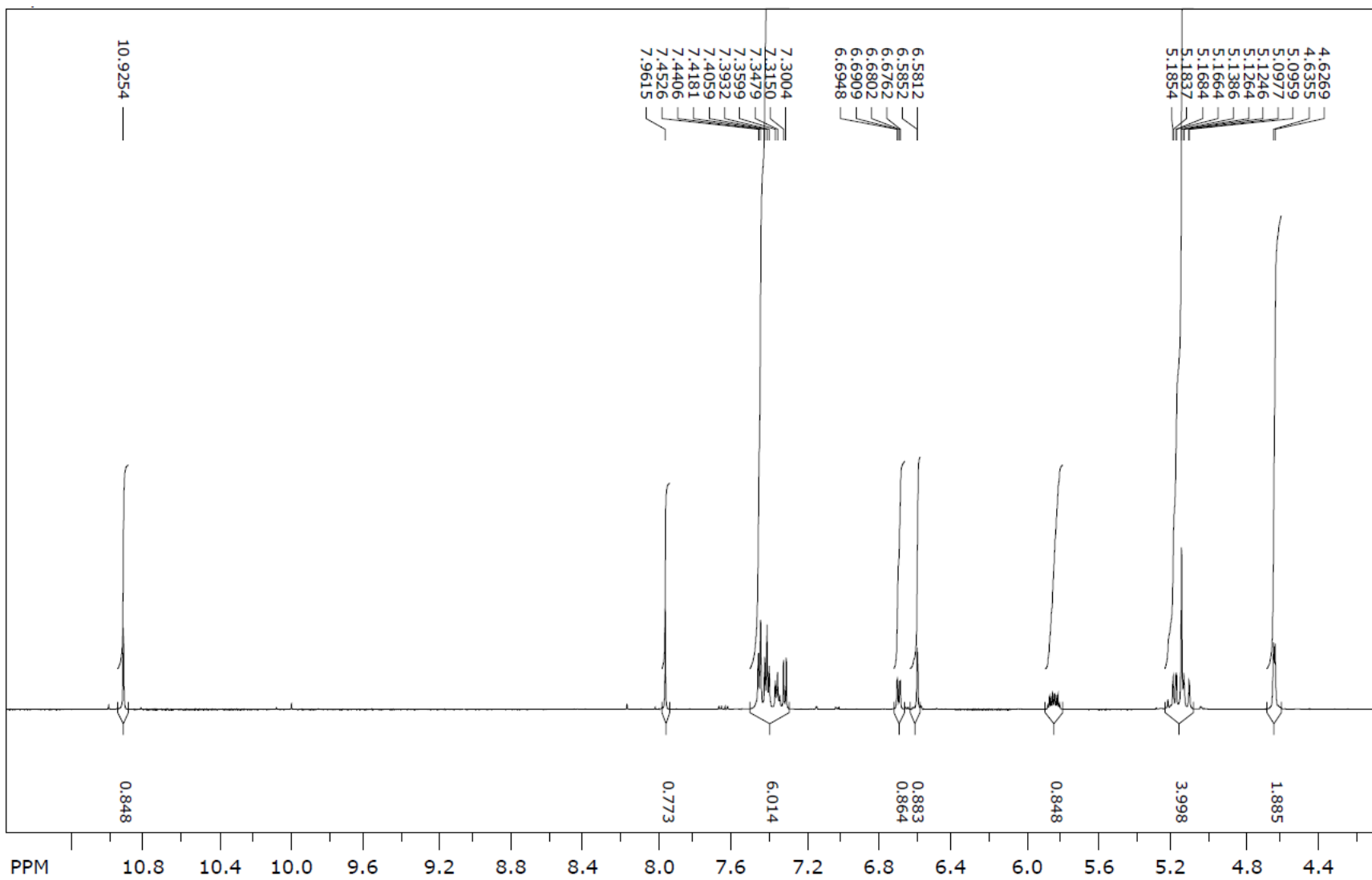


Reaktanti	4-(benziloksi) sakicilaldehid (1 mmol) i 3-alilrodanin (1 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	383,48 g/mol
Molekulska formula	C ₂₀ H ₁₇ NO ₃ S ₂
Temperatura tališta	182 -186 °C
Boja kristala	Tamnocrvena
R_f	0,77
LC/MS/MS m/z (M-)	382,13
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 10,92 (s, 1H, OH), 7,96 (s, 1H, CH), 7,45 (d, <i>J</i> = 7,20 Hz, 2H, arom.), 7,41 (t, <i>J</i> = 7,32; 7,62 Hz, 2H, arom.), 7,35 (t, <i>J</i> = 7,20 Hz, 1H, arom.), 7,31 (d, <i>J</i> = 8,76 Hz, 1H, arom.), 6,69 (dd, <i>J</i> = 8,76; 2,37 Hz, 1H, arom.), 6,58 (d, <i>J</i> = 2,40 Hz, 1H, arom.), 5,81 – 5,87 (m, 1H, CH), 5,18 (dd, <i>J</i> = 10,20; 1,02; 1,20 Hz, 1H, CH ₂), 5,13 (s, 2H, CH ₂), 5,11 (dd, <i>J</i> = 17,22; 1,08 Hz, 1H, CH ₂), 4,63 (d, <i>J</i> = 5,16 Hz, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,20; 166,82; 162,57; 159,59; 136,34; 131,35; 130,35; 129,02; 128,47; 128,01; 127,73; 117,66; 117,06; 113,44; 107,84; 101,97; 69,46; 45,90.

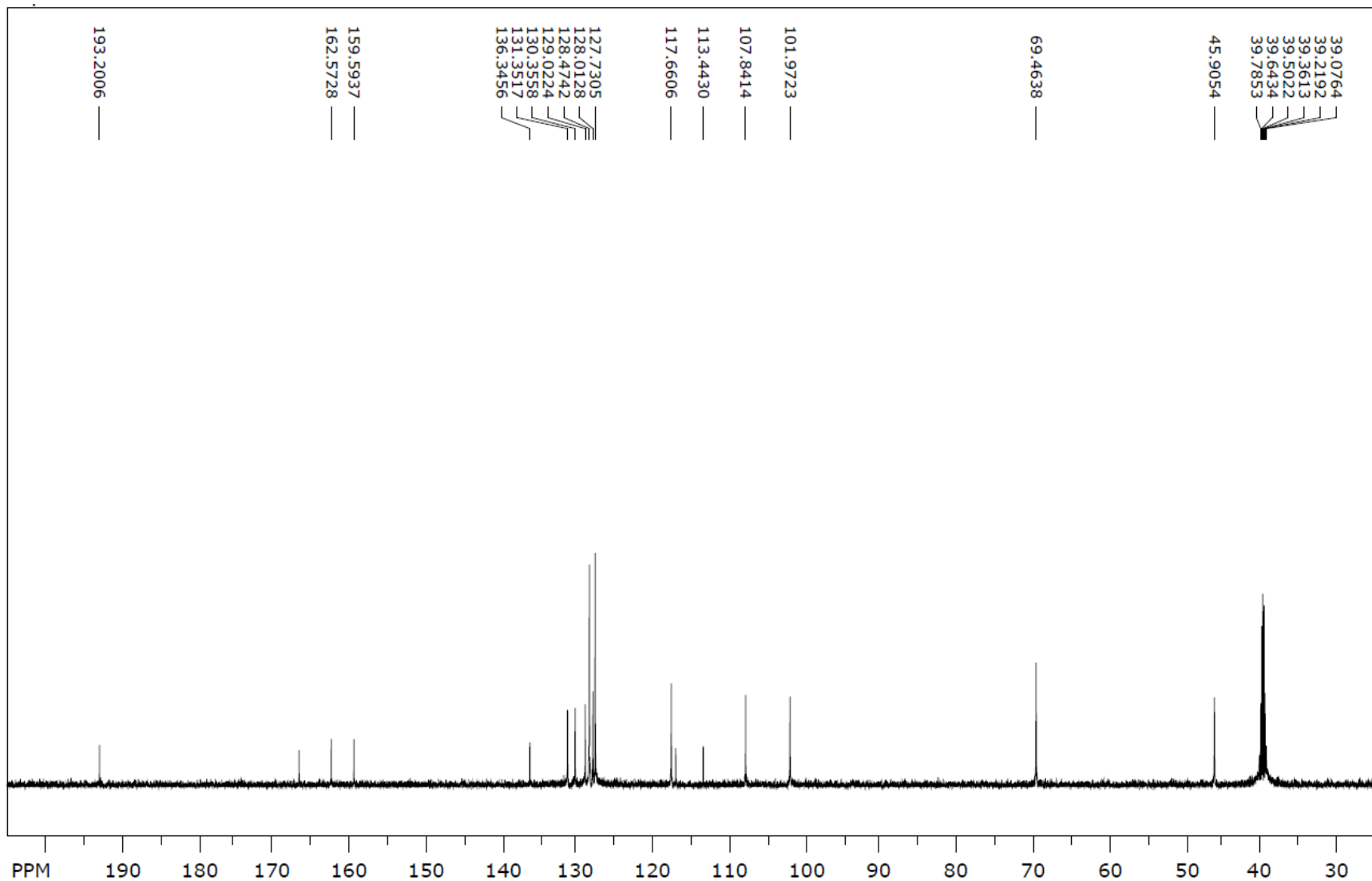
Maseni spektar (6t)



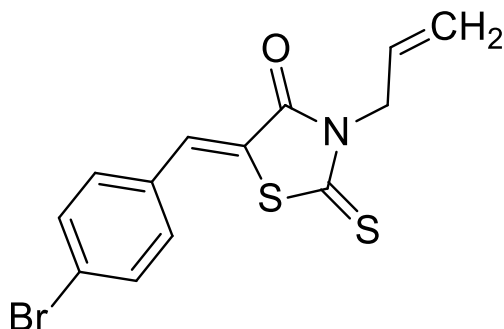
¹H NMR spektr (6t)



¹³C NMR spektr (6t)

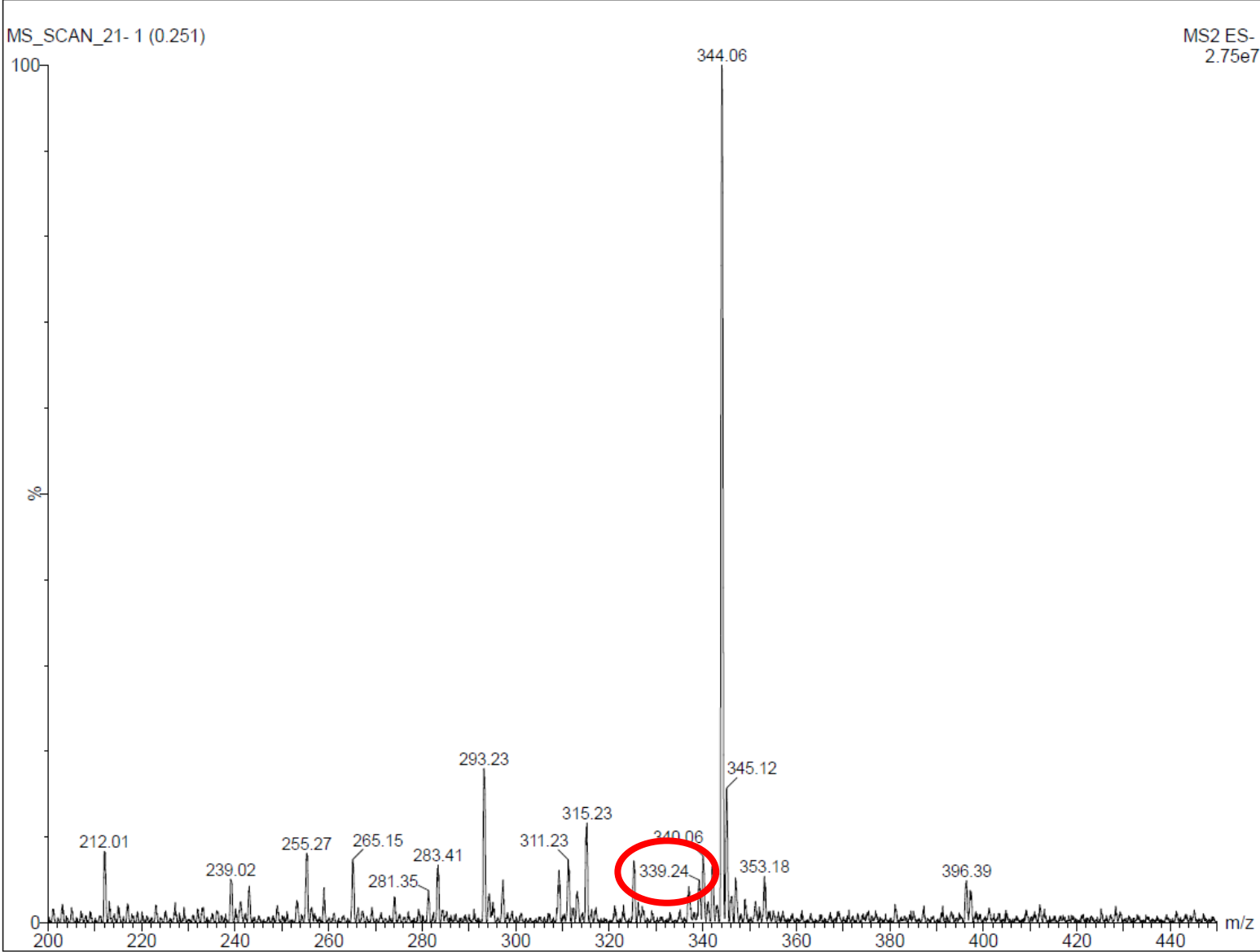


3-alil-5-(4-brombenziliden)-2-tioksotiazolidin-4-on (6u)

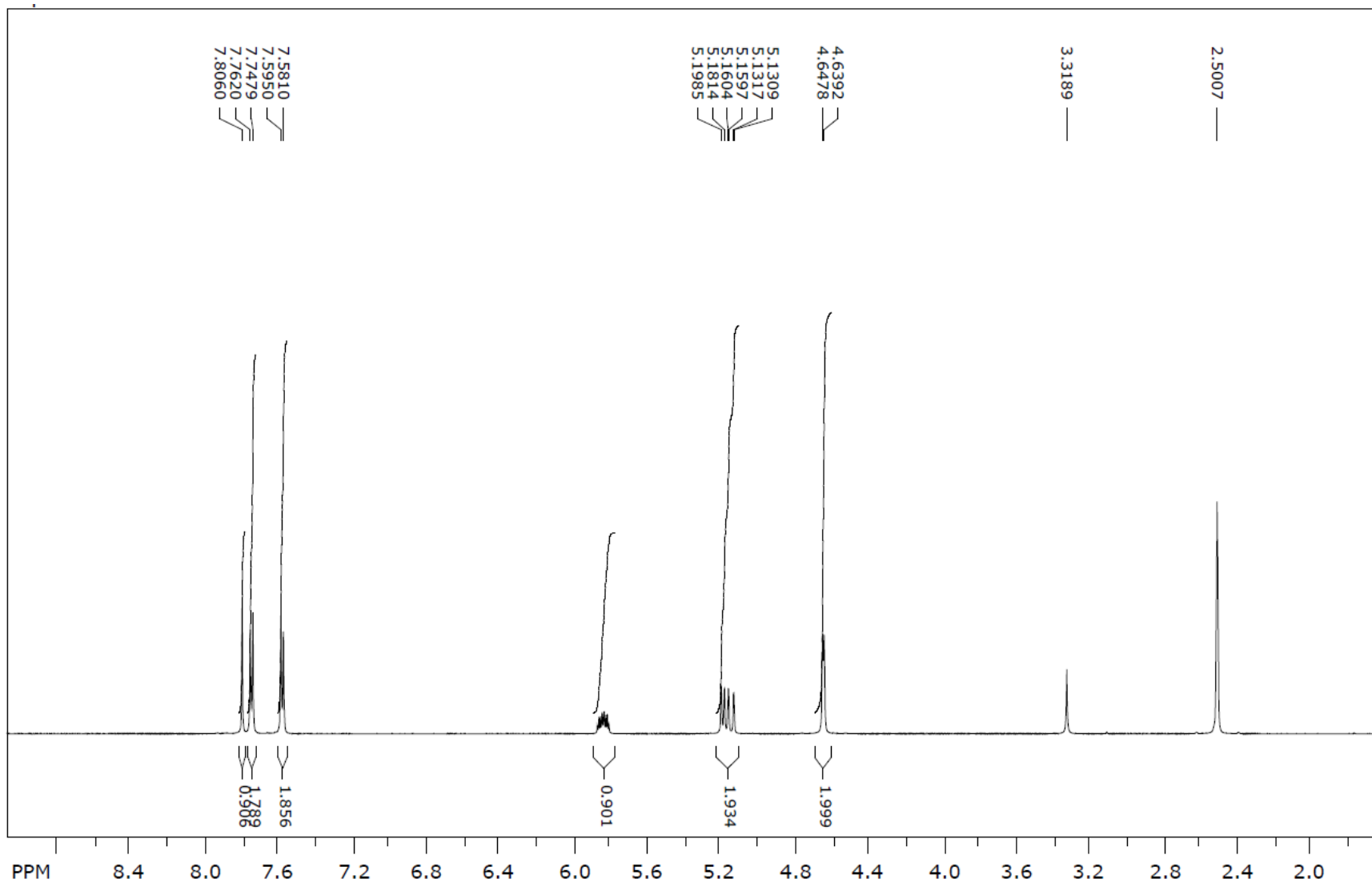


Reaktanti	3-brombenzaldehyd (2 mmol) i 3-alilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	340,26 g/mol
Molekulska formula	C ₁₃ H ₁₀ BrNOS ₂
Temperatura tališta	140 – 141 °C
Boja kristala	Narančasta
R_f	0,93
LC/MS/MS m/z (M-)	339,24
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,80 (s, 1H, CH), 7,75 (d, <i>J</i> = 8,46 Hz, 2H, arom.), 7,59 (d, <i>J</i> = 8,40 Hz, 2H, arom.), 5,81 – 5,87 (m, 1H, CH), 5,19 (d, <i>J</i> = 10,26 Hz, 1H, CH ₂), 5,15 (dd, <i>J</i> = 17,22; 0,45 Hz, 1H, CH ₂), 4,64 (d, <i>J</i> = 5,16 Hz, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 192,79; 166,51; 132,48; 132,36; 131,75; 130,14; 124,66; 123,14; 117, 83; 46,07.

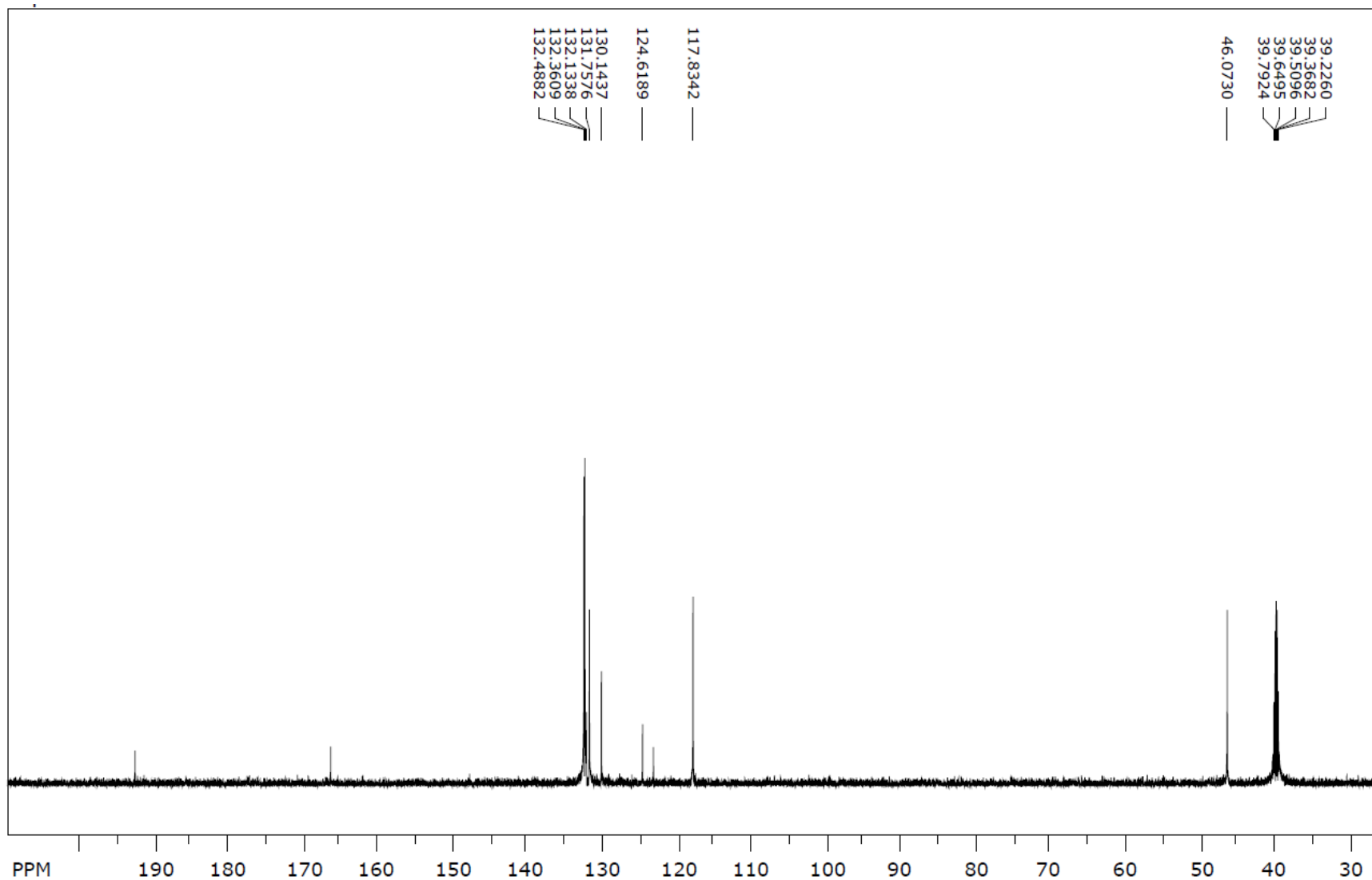
Maseni spektar (6u)



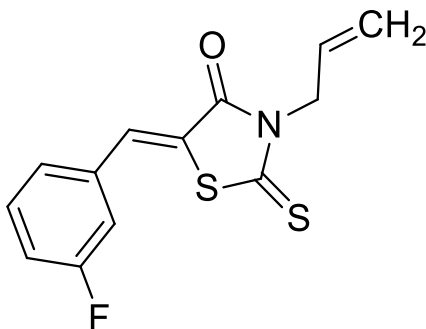
¹H NMR spektr (6u)



¹³C NMR spektr (6u)

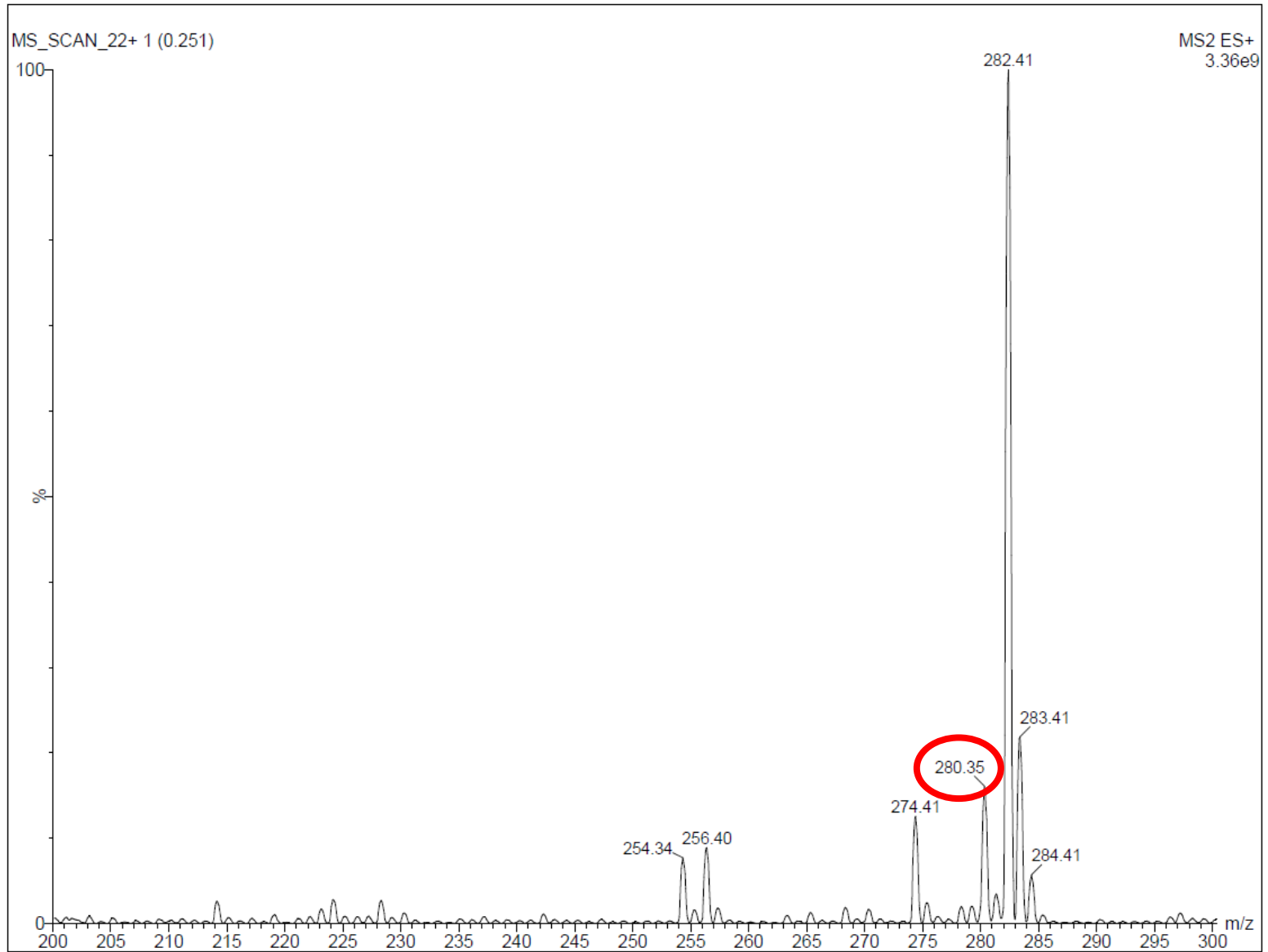


3-aliil-5-(3-fluorbenzilidene)-2-tioksoiazolidin-4-on (6v)

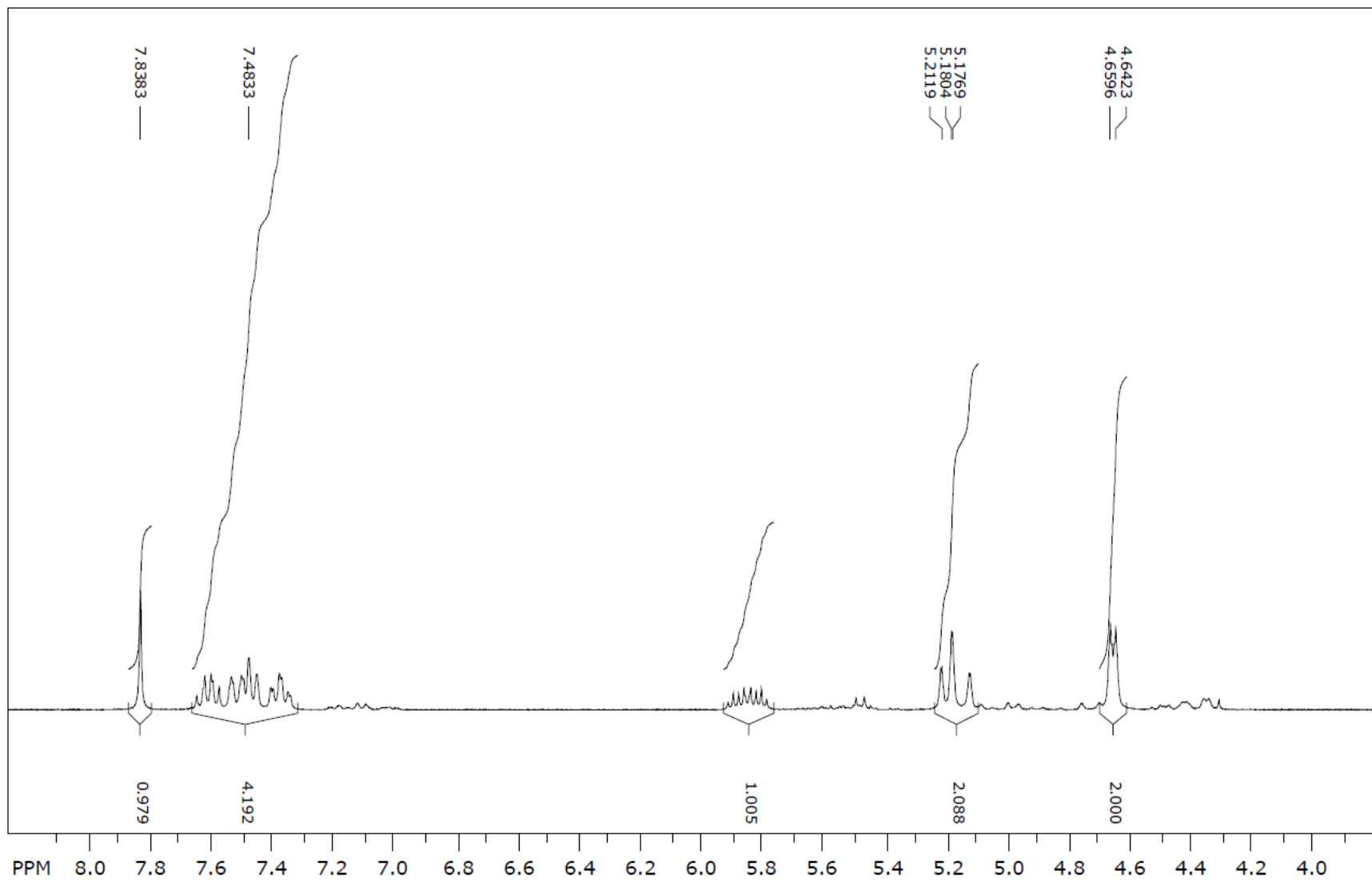


Reaktanti	3-fluorbenzaldehyd (2 mmol) i 3-aliilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	279,35 g/mol
Molekulska formula	C ₁₃ H ₁₀ FNOS ₂
Temperatura tališta	114 – 117 °C
Boja kristala	Žuta
R_f	0,91
LC/MS/MS <i>m/z</i> (M⁺)	280,35
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 7,83 (s, 1H, CH), 7,35 -7,65 (m, 4H, arom.), 5,79 – 5,91 (m, 1H, CH), 5,17 (ddd, <i>J</i> = 1,17; 10,62; 17,31 Hz, 2H, CH ₂), 4,65 (d, <i>J</i> = 5,19 Hz, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,36; 166,96; 164,41; 161,16; 135,58; 132,00; 126,58; 118,34; 117,95; 117,65; 55,29; 46,58.

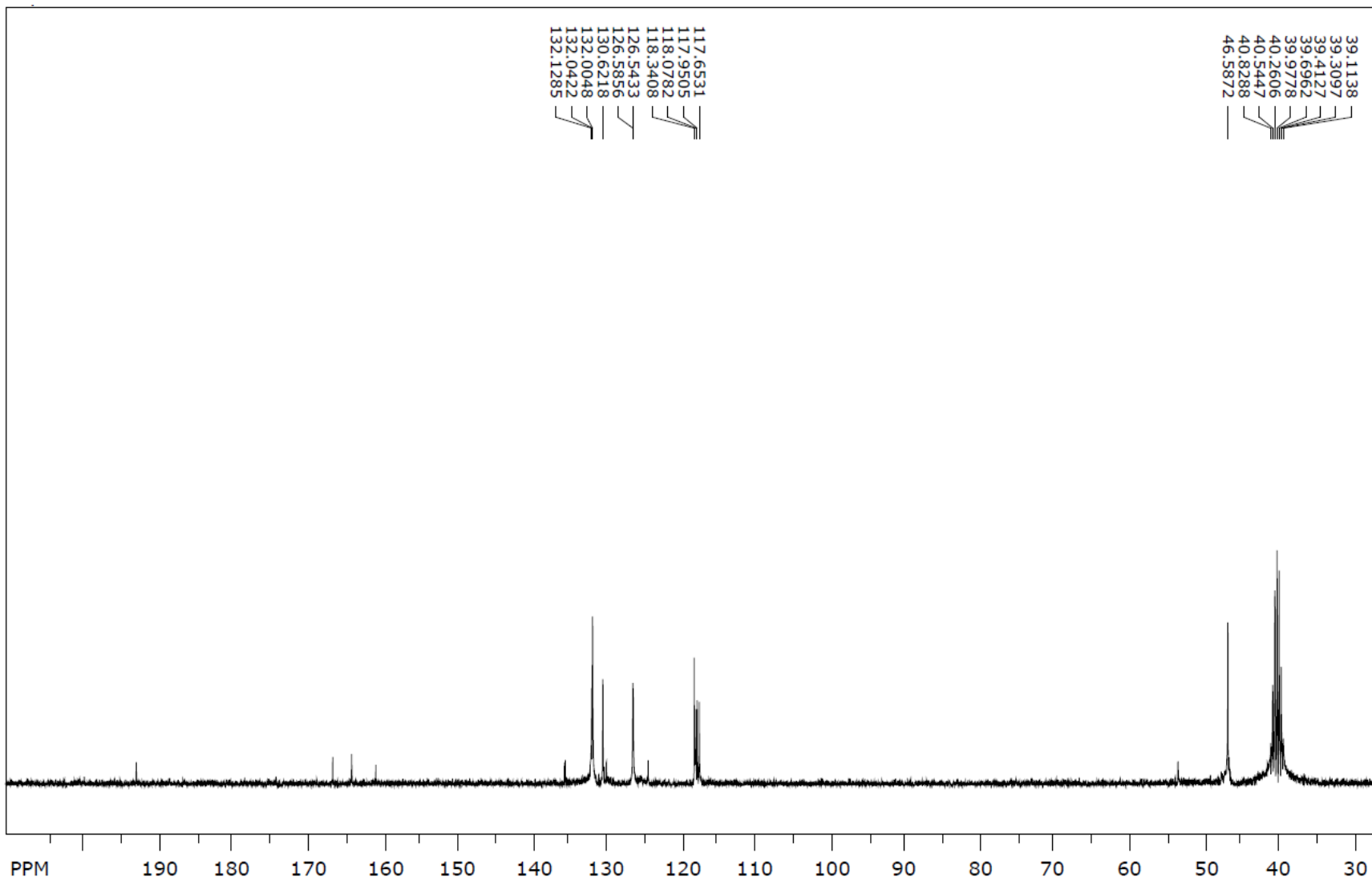
Maseni spektar (6v)



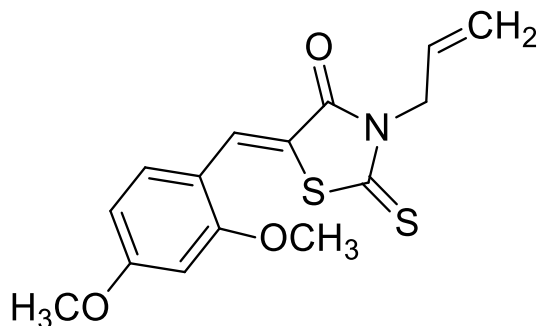
¹H NMR spektr (6v)



¹³C NMR spektar (6v)

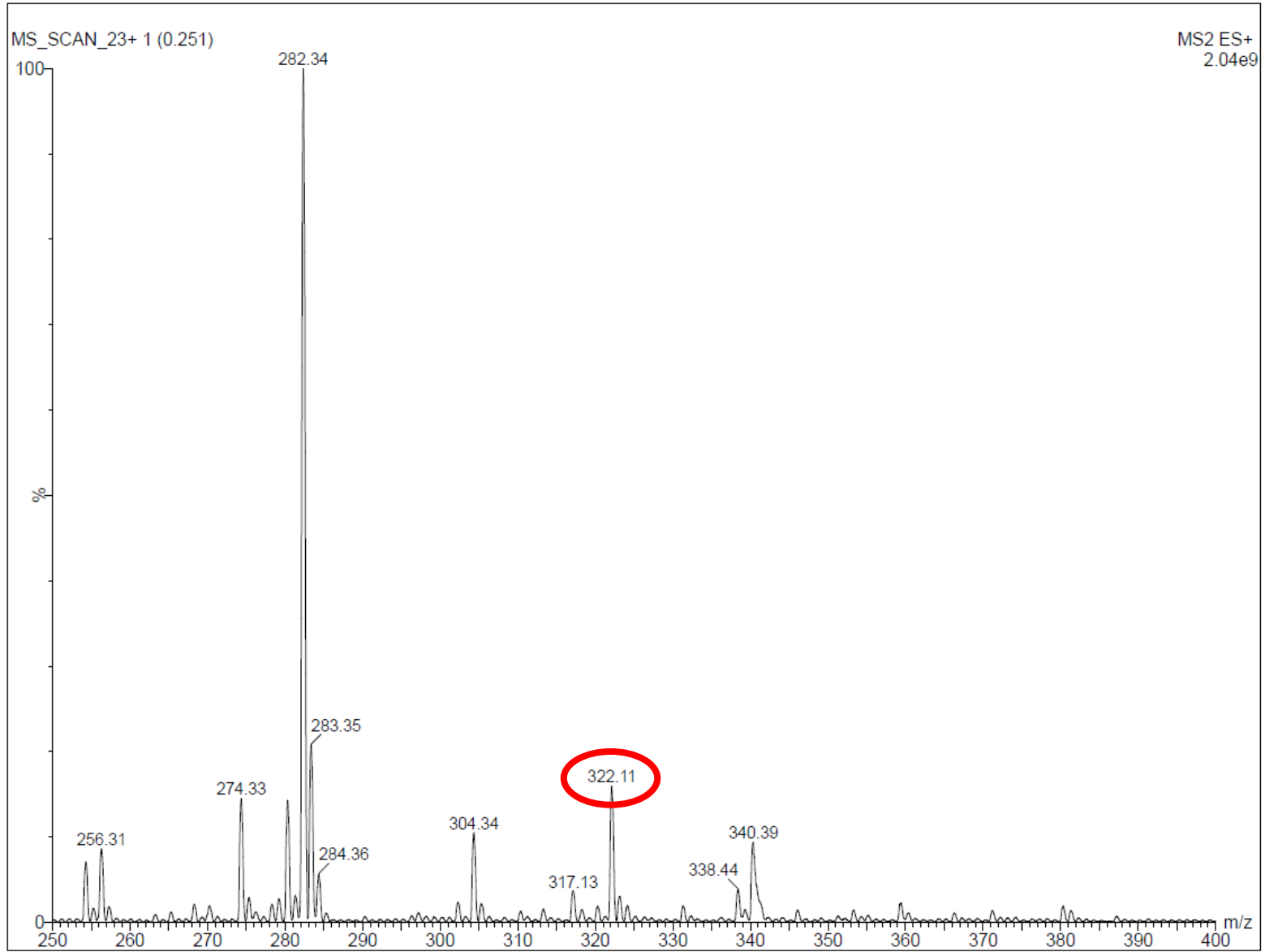


3-alil-5-(2,4-dimetoksibenziliden)-2-tioksotiazolidin-4-on (6w)

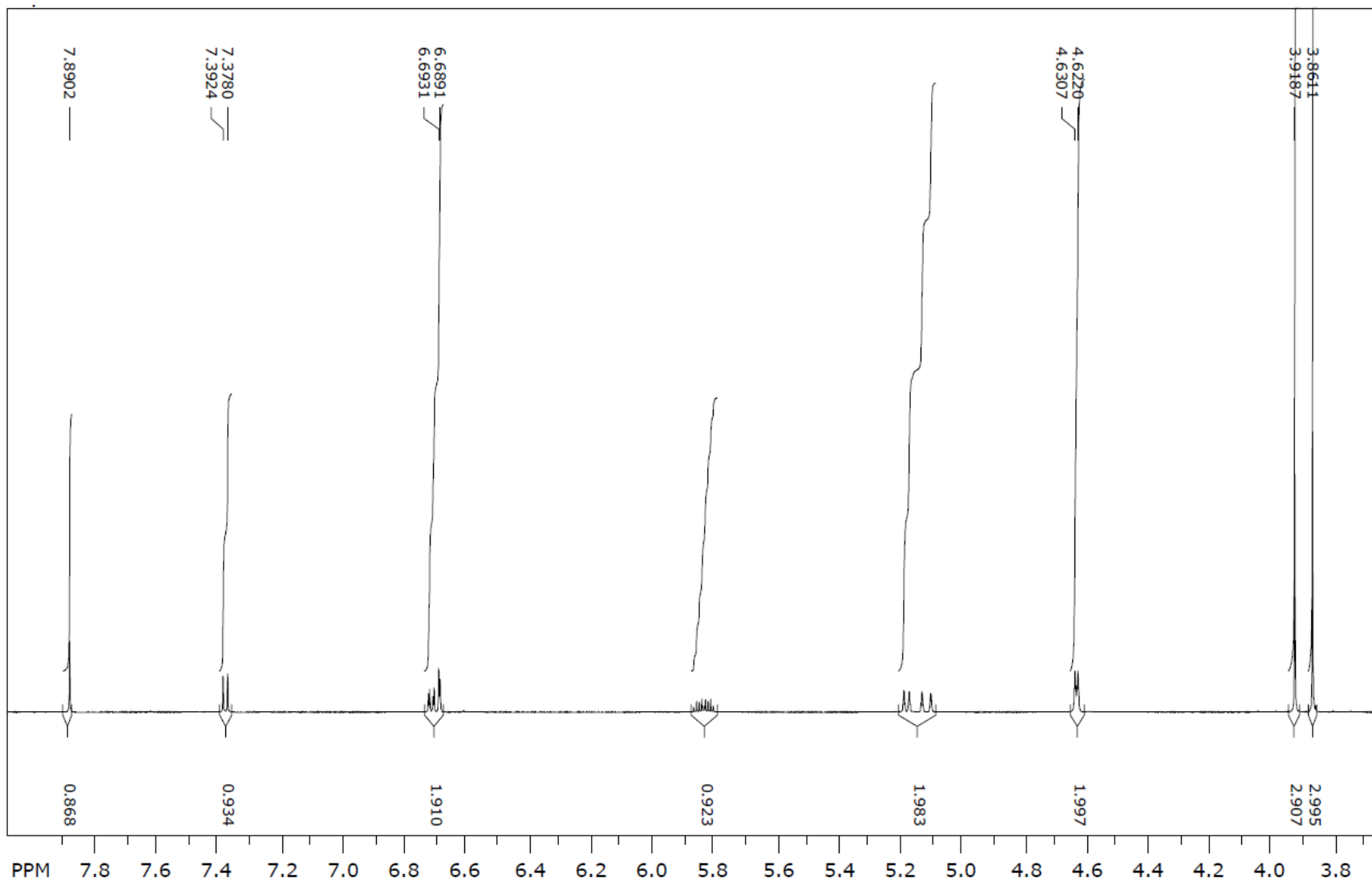


Reaktanti	2,4-dimetoksibenzaldehid (2 mmol) i 3-alilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	321,41 g/mol
Molekulska formula	C ₁₅ H ₁₅ NO ₃ S ₂
Temperatura tališta	126 – 130 °C
Boja kristala	Smeđa
R_f	0,90
LC/MS/MS <i>m/z</i> (M⁺)	322,11
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,89 (s, 1H, CH), 7,39 (d, <i>J</i> = 8,64 1H, arom.), 6,71 (dd, <i>J</i> = 8,70; 2,37 Hz, 1H, arom.), 6,69 (d, <i>J</i> = 2,40 Hz, 1H, arom.), 5,80 – 5,87 (m, 1H, CH), 5,17 (dd, <i>J</i> = 10,32; 1,32 Hz, 1H, CH ₂), 5,11 (dd, <i>J</i> = 17,16; 1,35 Hz, 1H, CH ₂), 4,63 (d, <i>J</i> = 5,22 Hz, 2H, CH ₂), 3,92 (s, 3H, OCH ₃), 3,86 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,31; 166,76; 160,09; 131,98; 130,31; 128,68; 118,36; 117,68; 114,31; 107,05, 96,62; 55,92; 55,76; 45,92.

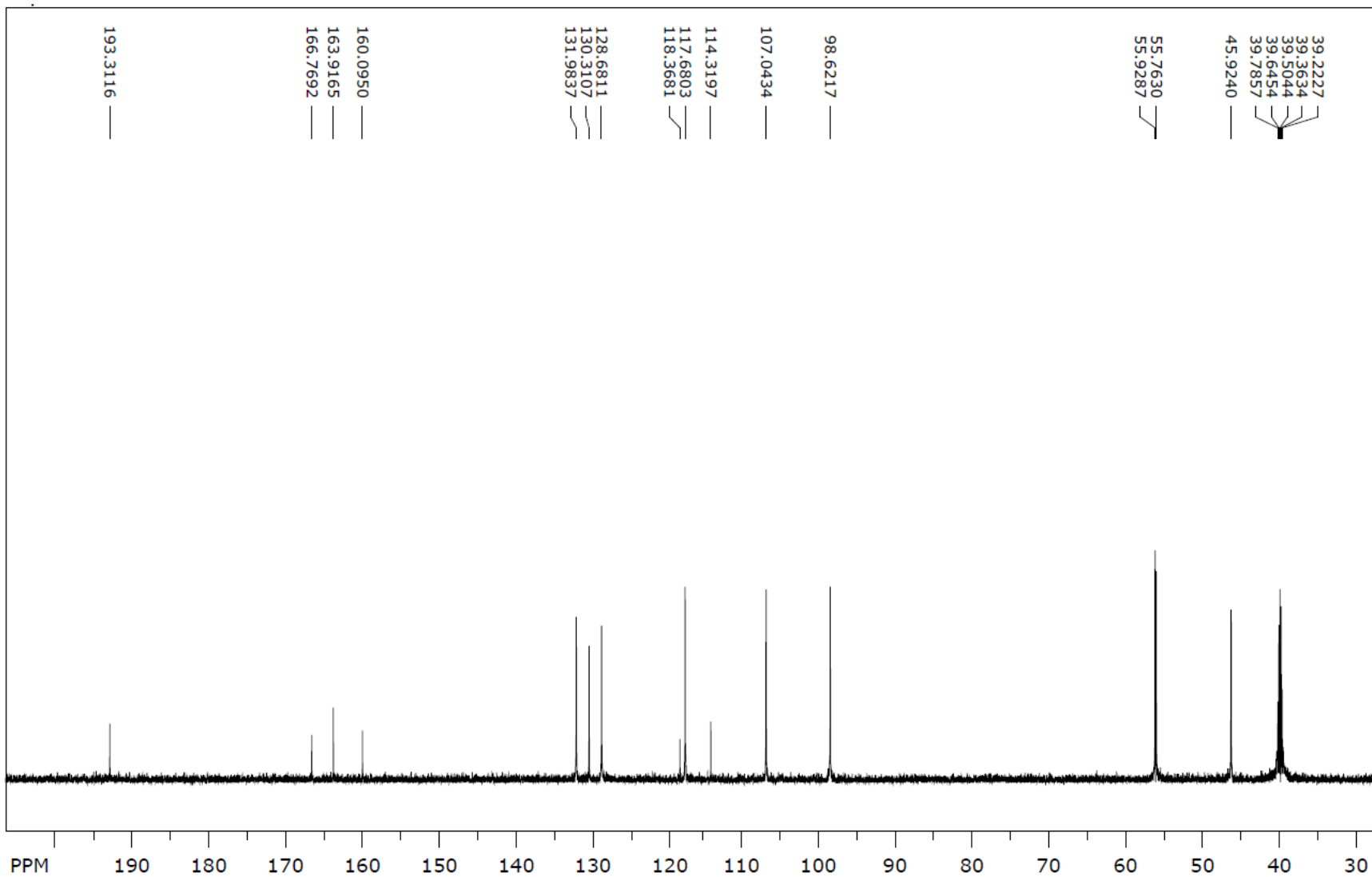
Maseni spektar (6w)



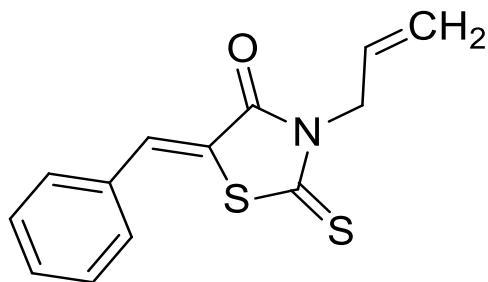
¹H NMR spektr (6w)



¹³C NMR spektr (6w)

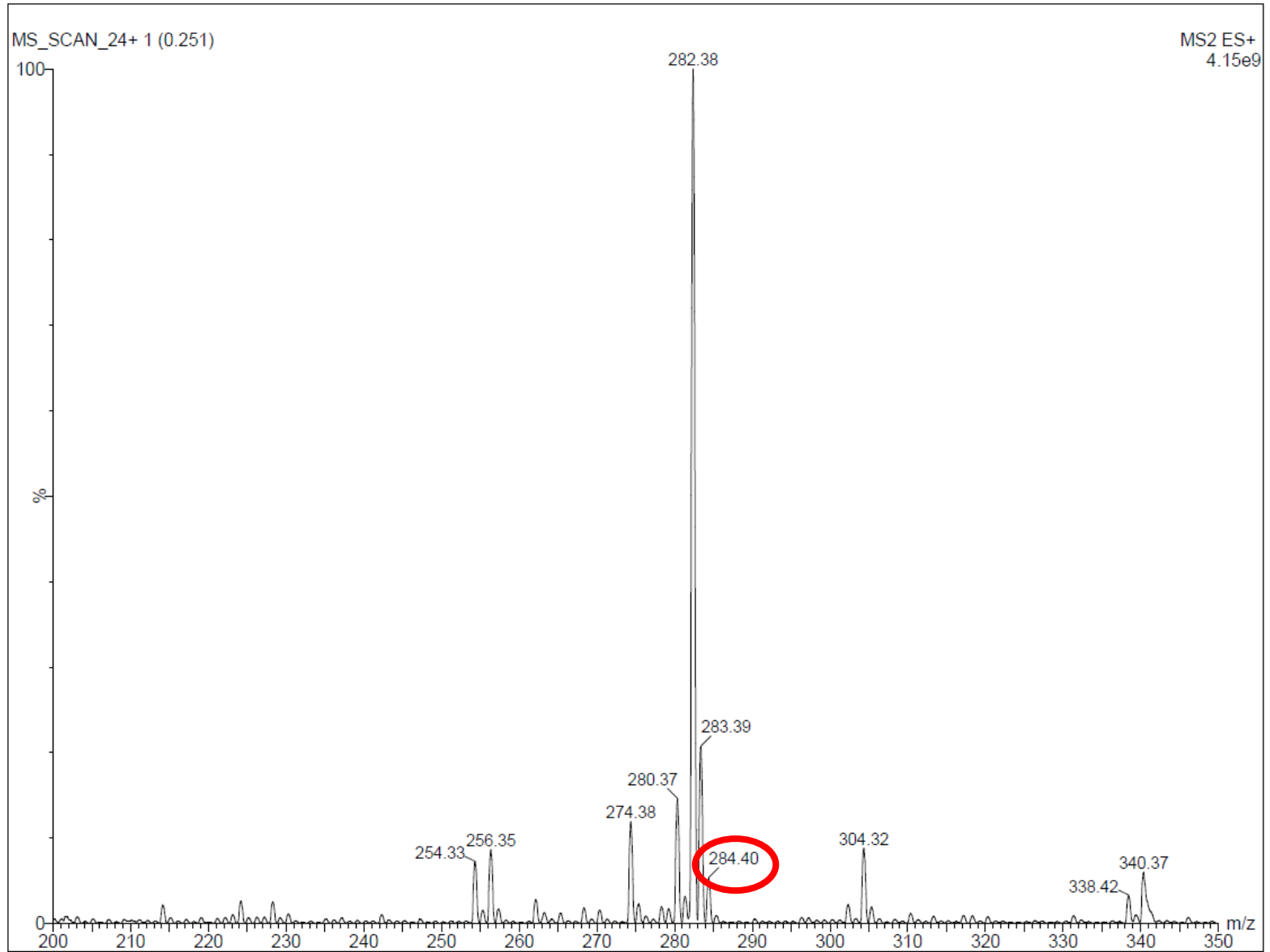


3-alil-5-benziliden-2-tioksotiazolidin-4-on (6x)

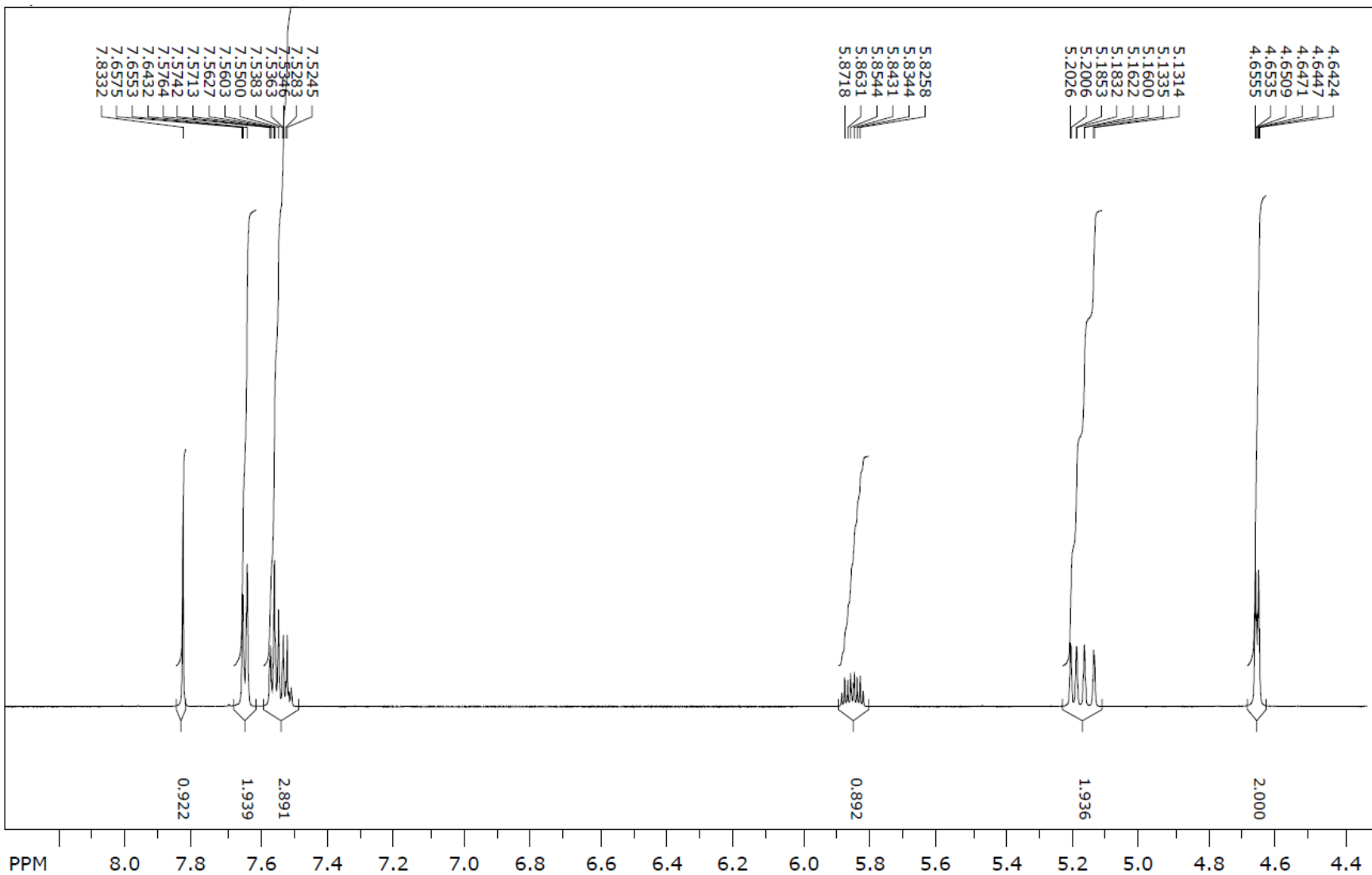


Reaktanti	Benzaldehid (2 mmol) i 3-alilrodanin (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	261,36 g/mol
Molekulska formula	C ₁₃ H ₁₁ NOS ₂
Temperatura tališta	139 -143 °C
Boja kristala	Smeđa
R_f	0,91
LC/MS/MS <i>m/z</i> (M+Na⁺)	284,40
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,83 (s, 1H, CH), 7,65 (d, <i>J</i> = 7,26 Hz, 2H, arom.), 7,51 – 7,58 (m, 3H, arom.), 5,81 – 5,88 (m, 1H, CH), 5,19 (dd, <i>J</i> = 10,38; 1,23 Hz, 1H, CH ₂), 5,15 (dd, <i>J</i> = 17,22; 1,29 Hz, 1H, CH ₂), 4,65 (d, <i>J</i> = 5,28 Hz, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,10; 166,55; 133,11; 130,98; 130,64; 129,48; 122,30; 117,81; 46,03.

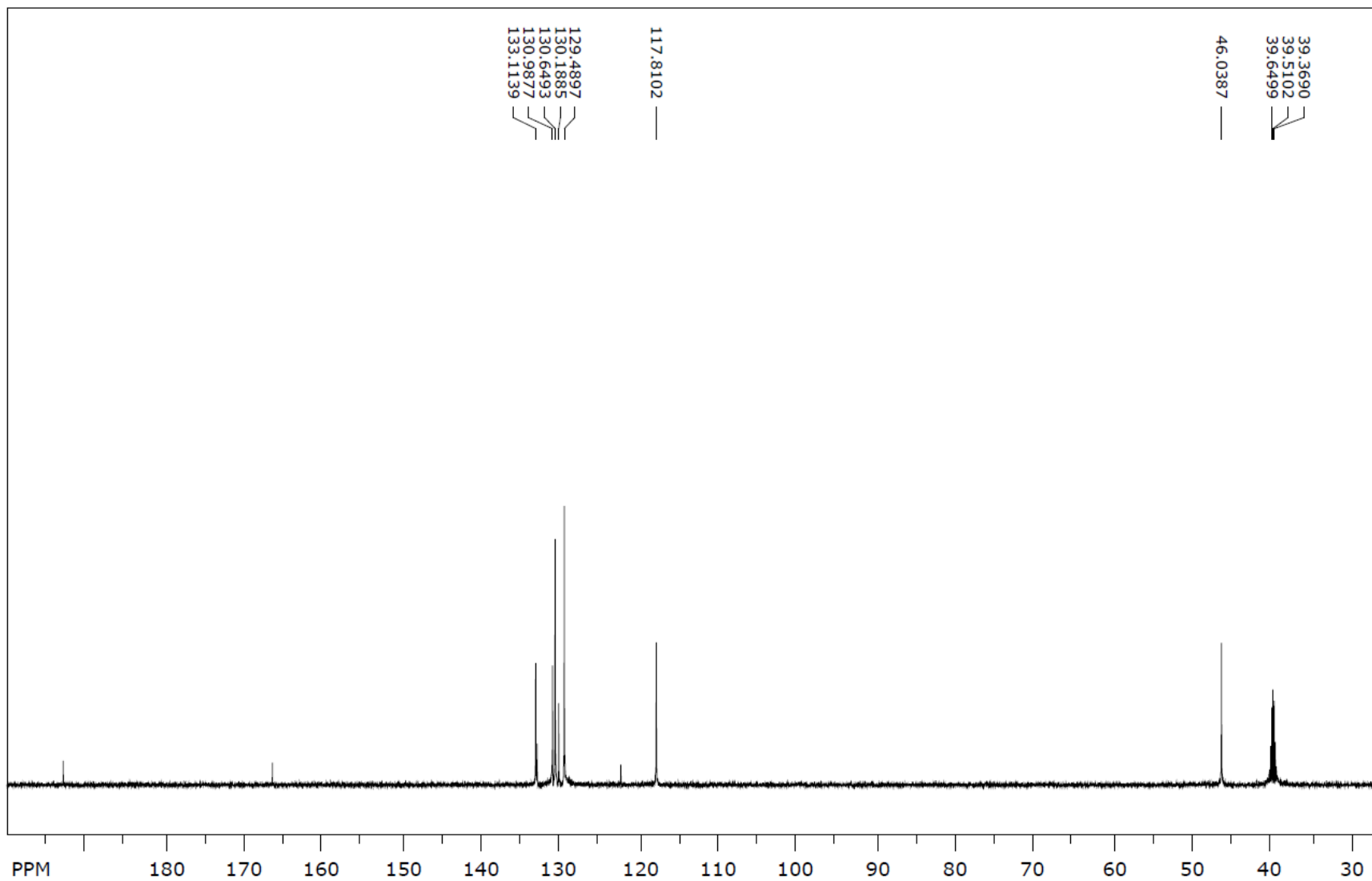
Maseni spektar (6x)



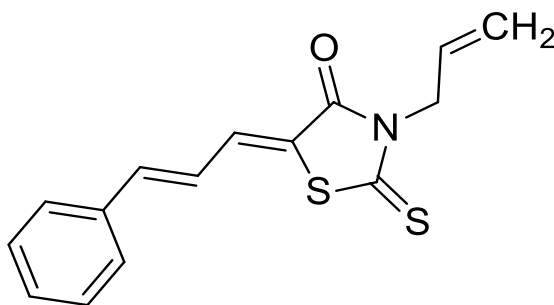
¹H NMR spektr (6x)



¹³C NMR spektr (6x)

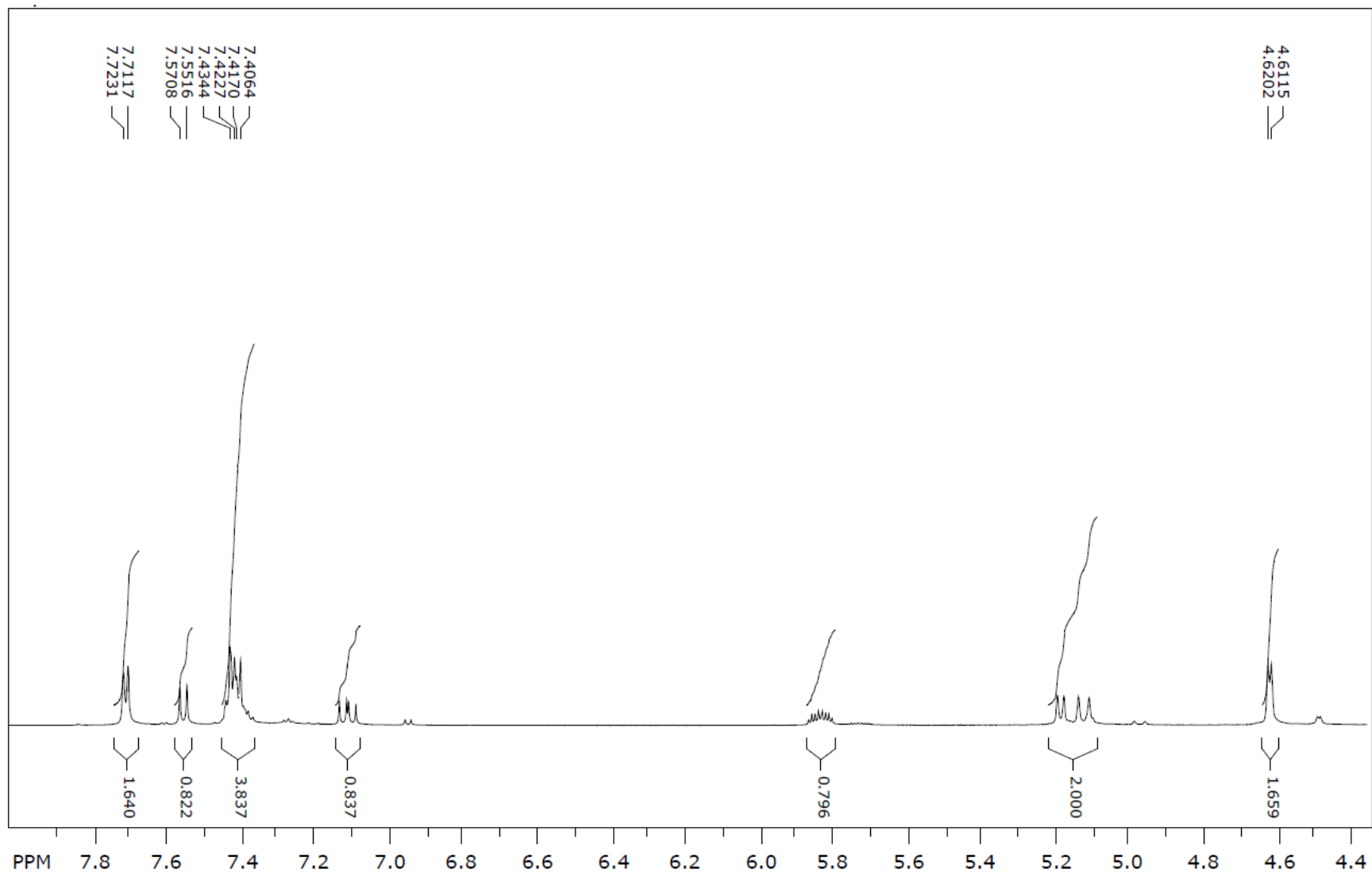


3-ailil-5-(3-fenilaliliden)-2-tioksotiazolidin-4-on (6y)

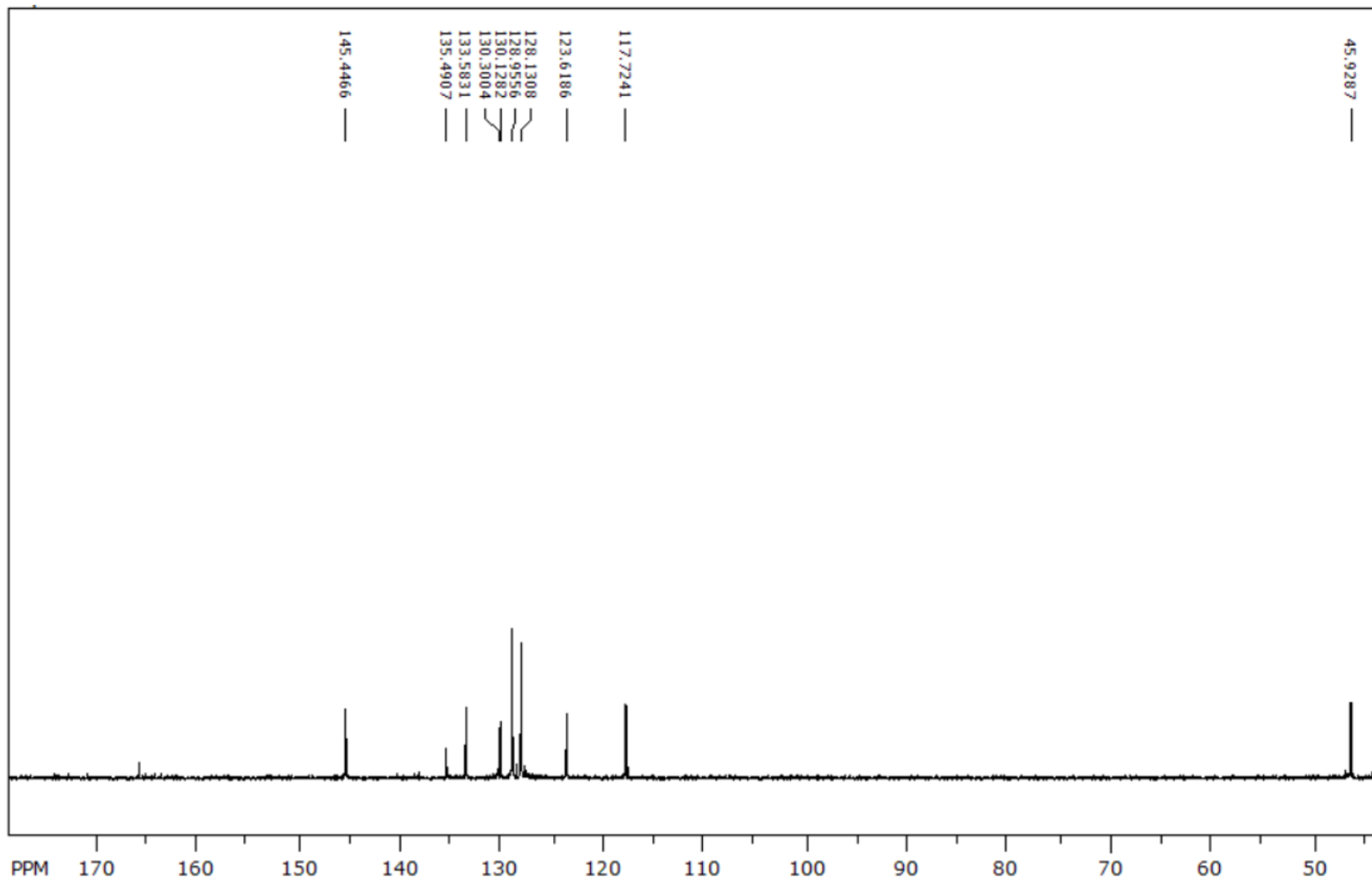


Reaktanti	Cimetaldhid (2 mmol) i 3-aililrodanin (2 mmol)
Metoda pročiščavanja	Nije pročiščavan
Molekulska masa	287,40 g/mol
Molekulska formula	C ₁₅ H ₁₃ NOS ₂
Temperatura tališta	167 -172 °C
Boja kristala	Tamnocrvena
R_f	0,91
LC/MS/MS <i>m/z</i> (M⁺)	288,05 (teor.)
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) 7,71 (d, <i>J</i> = 6,84 Hz, 2H, CH), 7,56 (d, <i>J</i> = 11,52 Hz, 1H, CH), 7,37 – 7,45 (m, 4H, arom.), 7,12 (q, <i>J</i> = 11,52; 3,54; 11,64 Hz, 1H, arom.), 5,80 – 5,86 (m, 1H, CH), 5,18 (dd, <i>J</i> = 10,32; 1,02 Hz, 1H, CH ₂), 5,12 (dd, <i>J</i> = 17,22; 1,02 Hz, 1H, CH ₂), 4,62 (d, <i>J</i> = 5,22 Hz, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 192,69; 165,92; 145,44; 135,49; 133,58; 130,30; 130,12; 129,03; 128,13; 123,61; 117,72; 45,92.

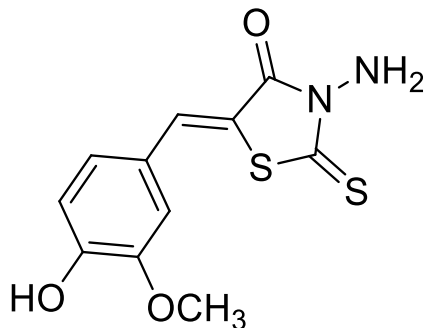
¹H NMR spektr (6y)



¹³C NMR spektr (6y)

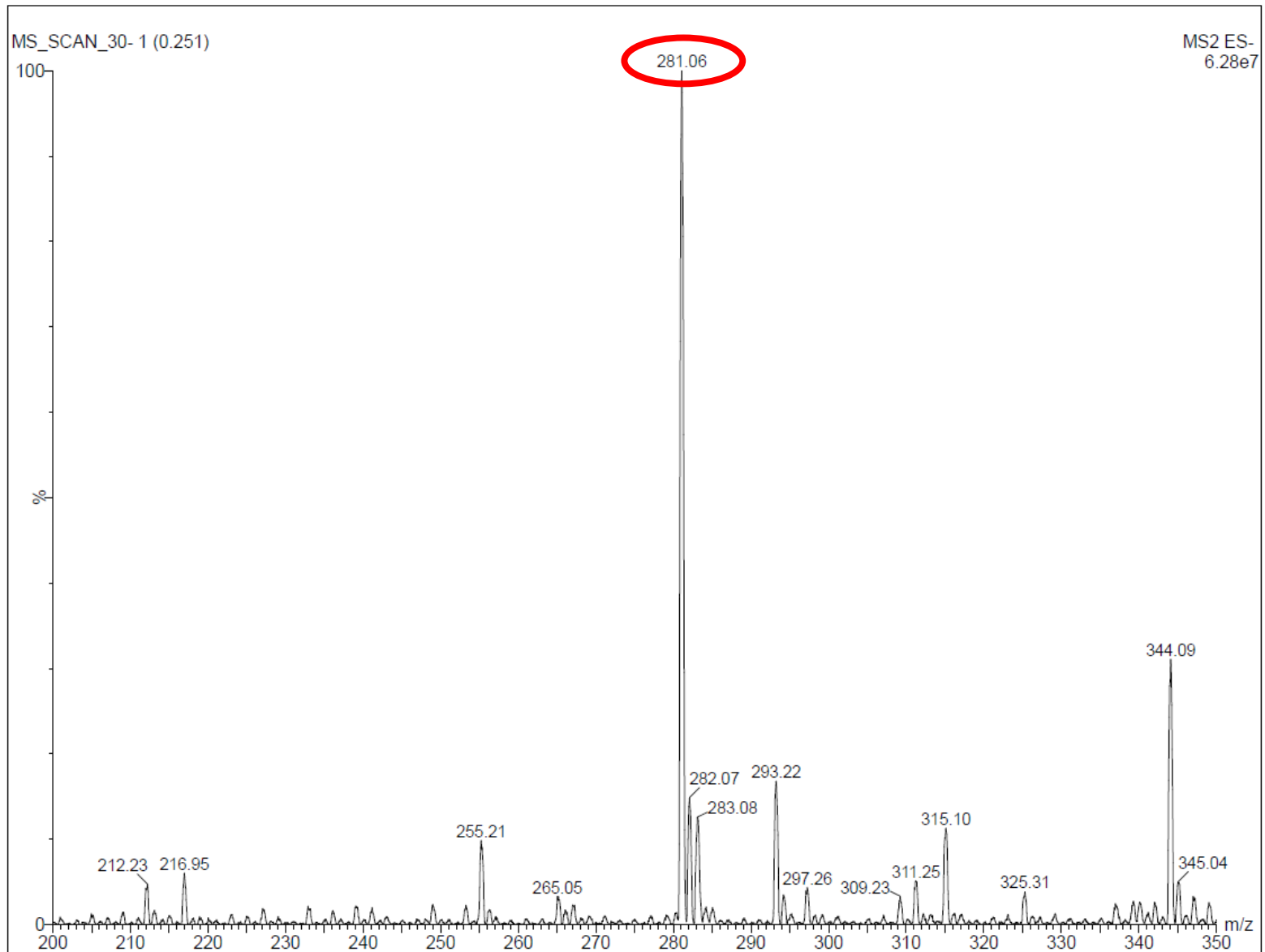


**3-amino-5-(4-hidroksi-3-metoksibenziliden)-2-tioksotiazolidin-4-on
(7a)**

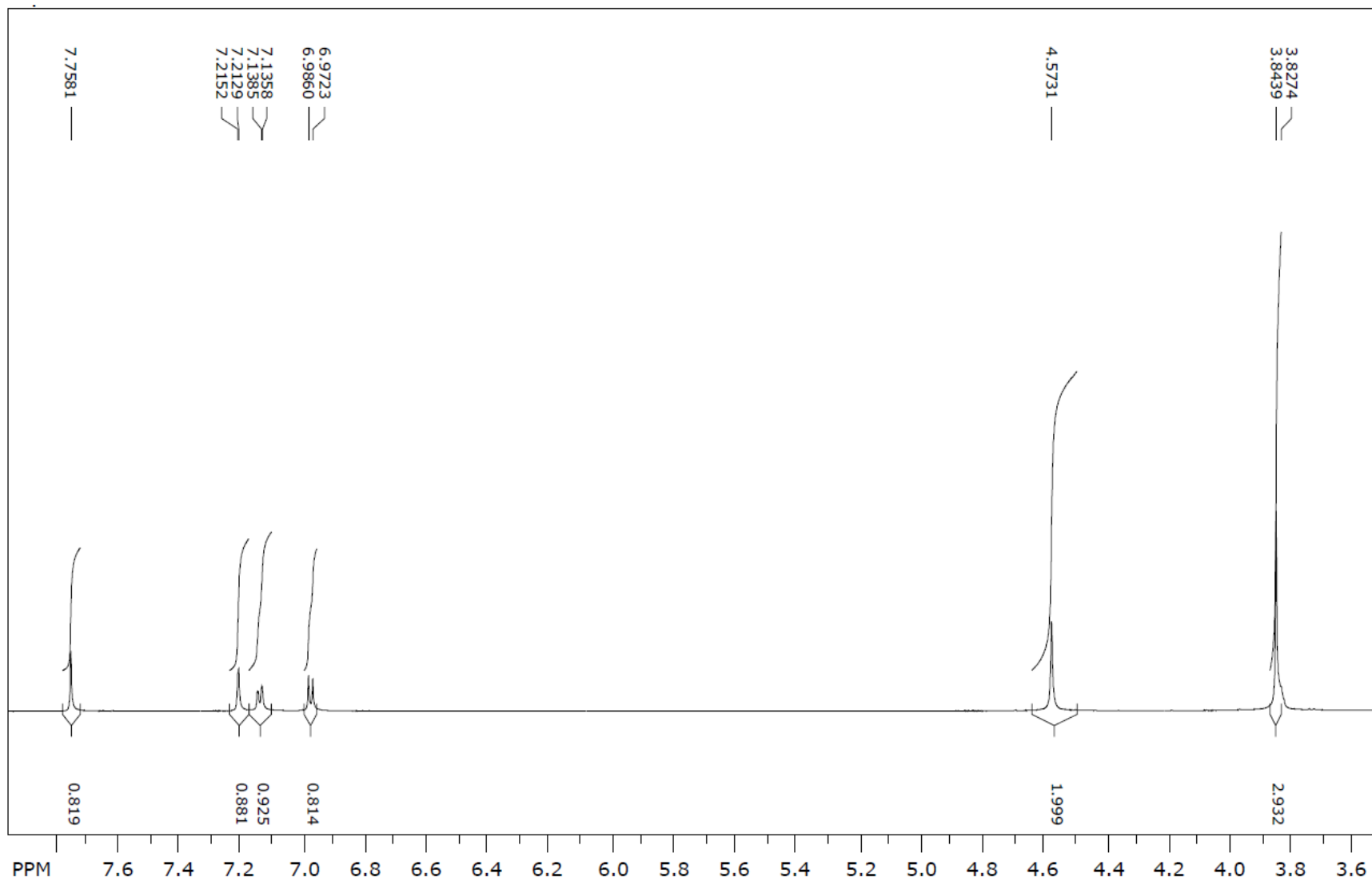


Reaktanti	3-metoksi-4-hidroksibenzaldehid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Ispran heksan : etanol (4 : 1), ispran heksanom
Molekulska masa	282,34 g/mol
Molekulska formula	C ₁₁ H ₁₀ N ₂ O ₃ S ₂
Temperatura tališta	182 – 185 °C
Boja kristala	Smeđa
R_f	0,67
LC/MS/MS <i>m/z</i> (M-)	281,06
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 10,17 (s, 1H, OH), 7,78 (s, 1H, CH), 7,22 (d, <i>J</i> = 2,04 Hz, 1H, arom.), 7,15 (dd, <i>J</i> = 8,31; 2,03 Hz, 1H, arom.), 6,96 (d, <i>J</i> = 8,25 Hz, 1H, arom.), 5,94 (s, 2H, NH ₂), 3,85 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,51; 164,23; 150,80; 148,62; 135,10; 125,92; 124,93; 116,89; 115,15; 56,13.

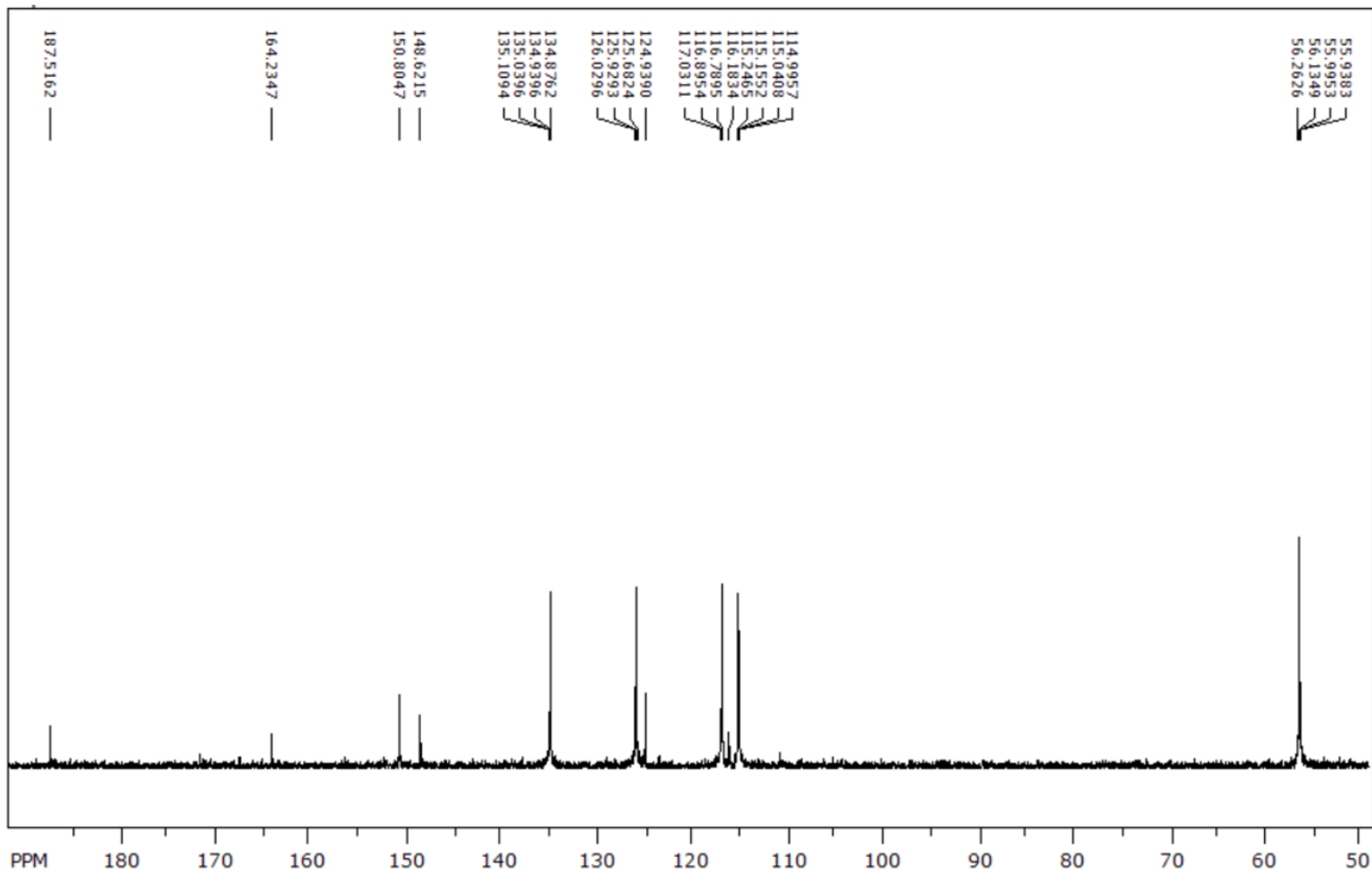
Maseni spektar (7a)



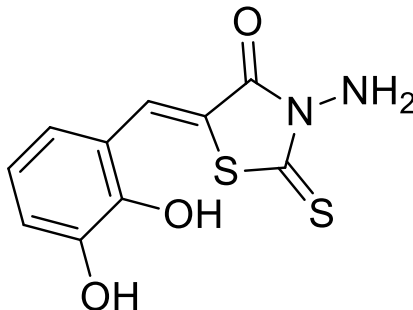
¹H NMR spektr (7a)



¹³C NMR spektar (7a)

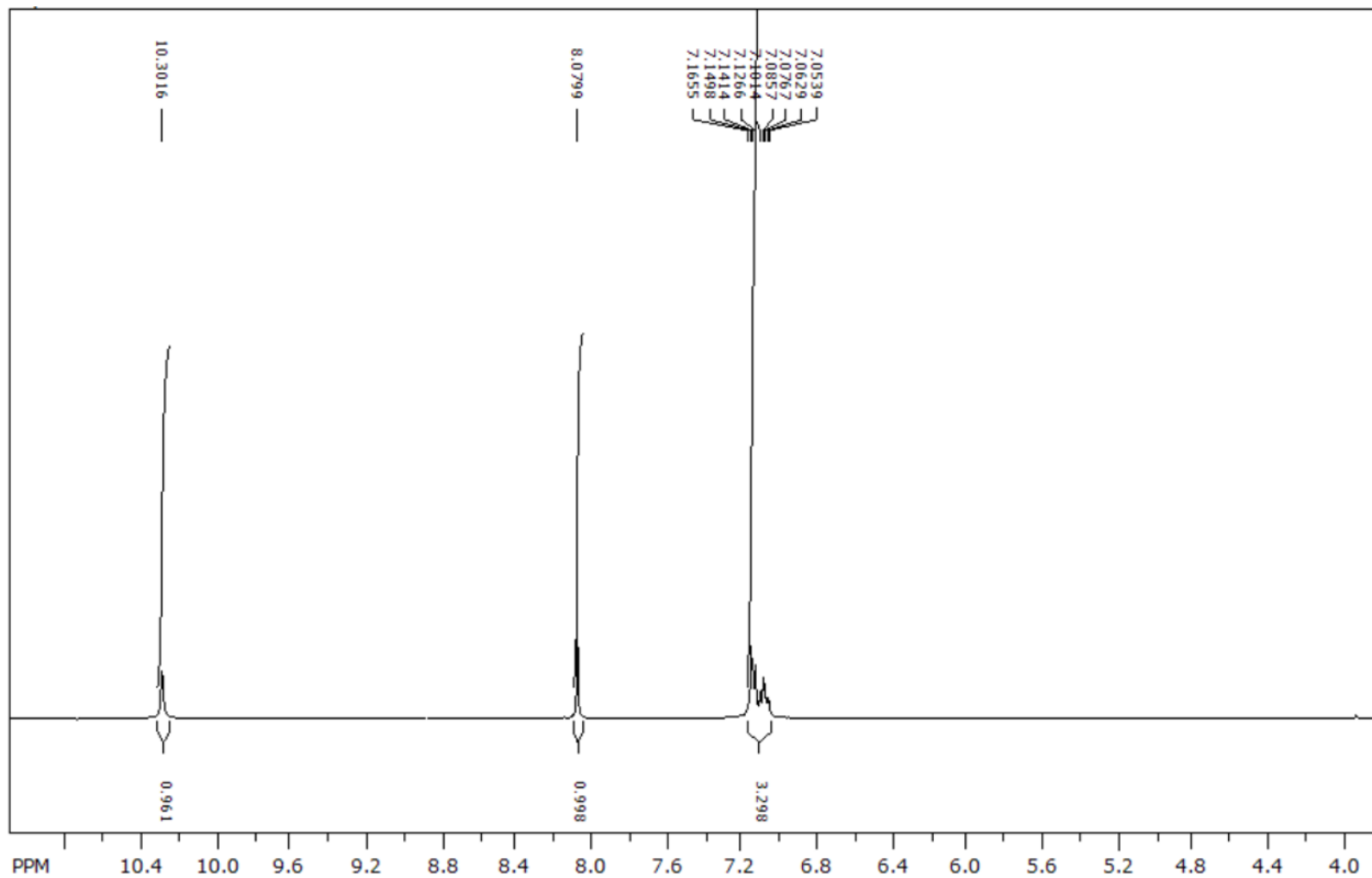


3-amino-5-(2,3-dihidroksibenziliden)-2-tioksotiazolidin-4-on (7b)

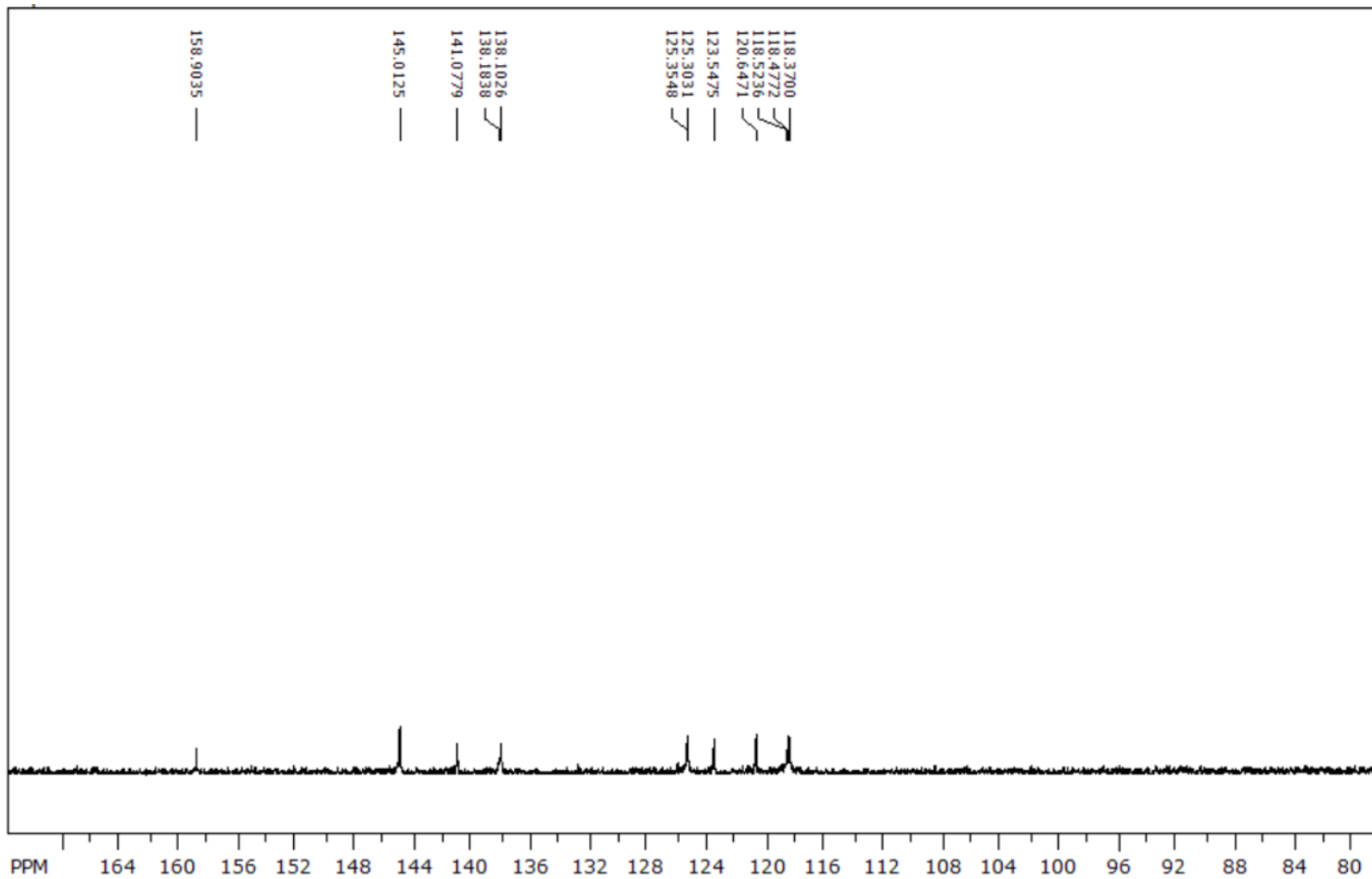


Reaktanti	2,3-dihidroksibenzaldehid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Ispran heksan : etanol (4 : 1), ispran heksanom
Molekulska masa	268,31 g/mol
Molekulska formula	C ₁₀ H ₈ N ₂ O ₃ S ₂
Temperatura tališta	296 – 299 °C
Boja kristala	Svijetlosmeđa
R_f	0,61
LC/MS/MS m/z (M-)	268,00 (teor.)
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 10,30 (s, 1H, OH), 8,07 (s, 1H, CH), 7,05 – 7,17 (m, 3H, arom.).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 158,90; 145,01; 141,07; 138,09; 125,35; 125,54; 120,64; 118,46; 118,37.

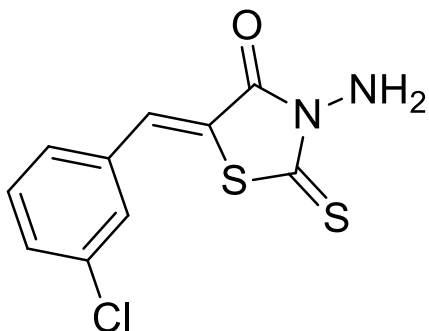
¹H NMR spektr (7b)



¹³C NMR spektr (7b)

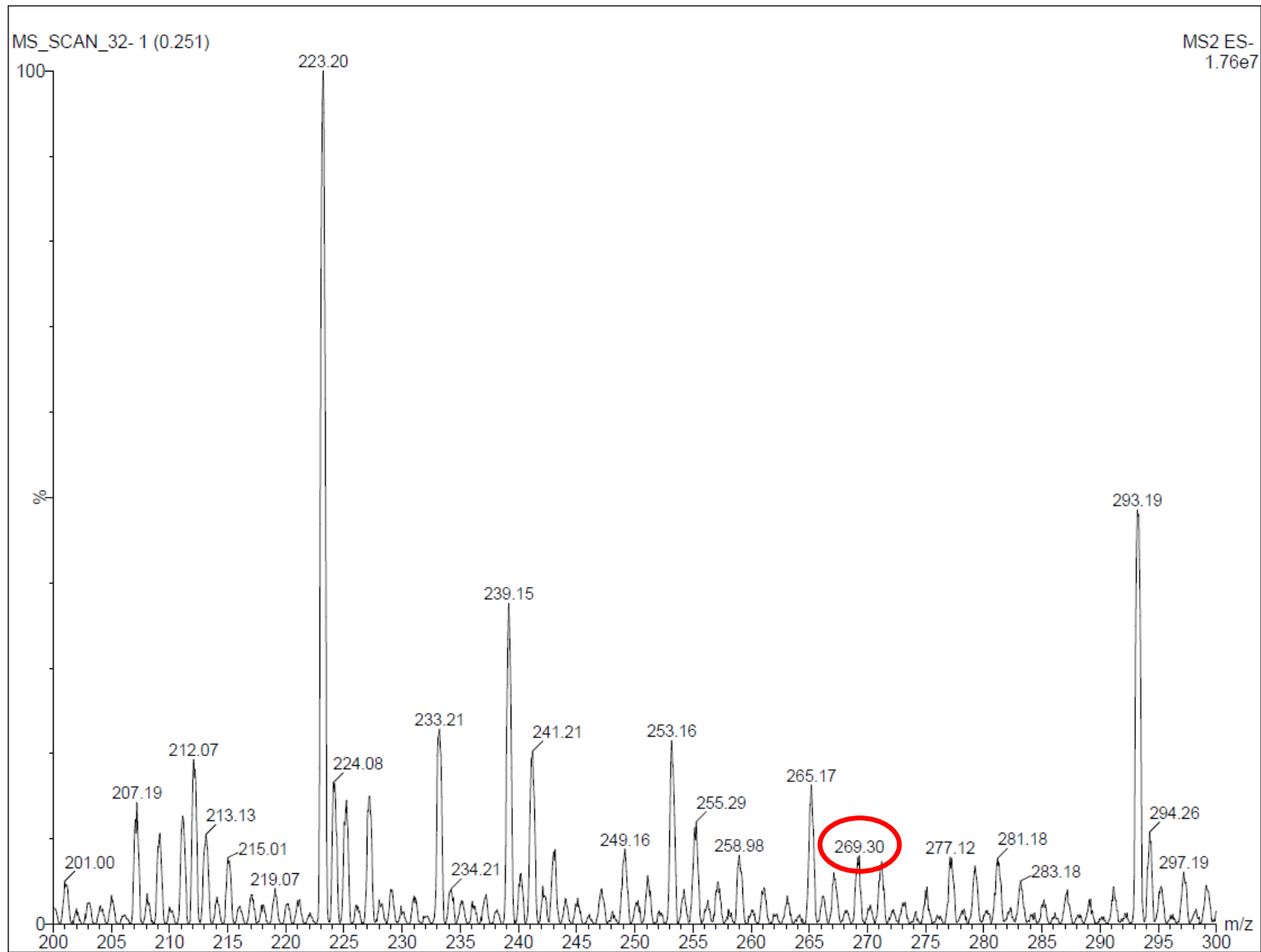


3-amino-5-(3-klorbenziliden)-2-tioksotiazolidin-4-on (7c)

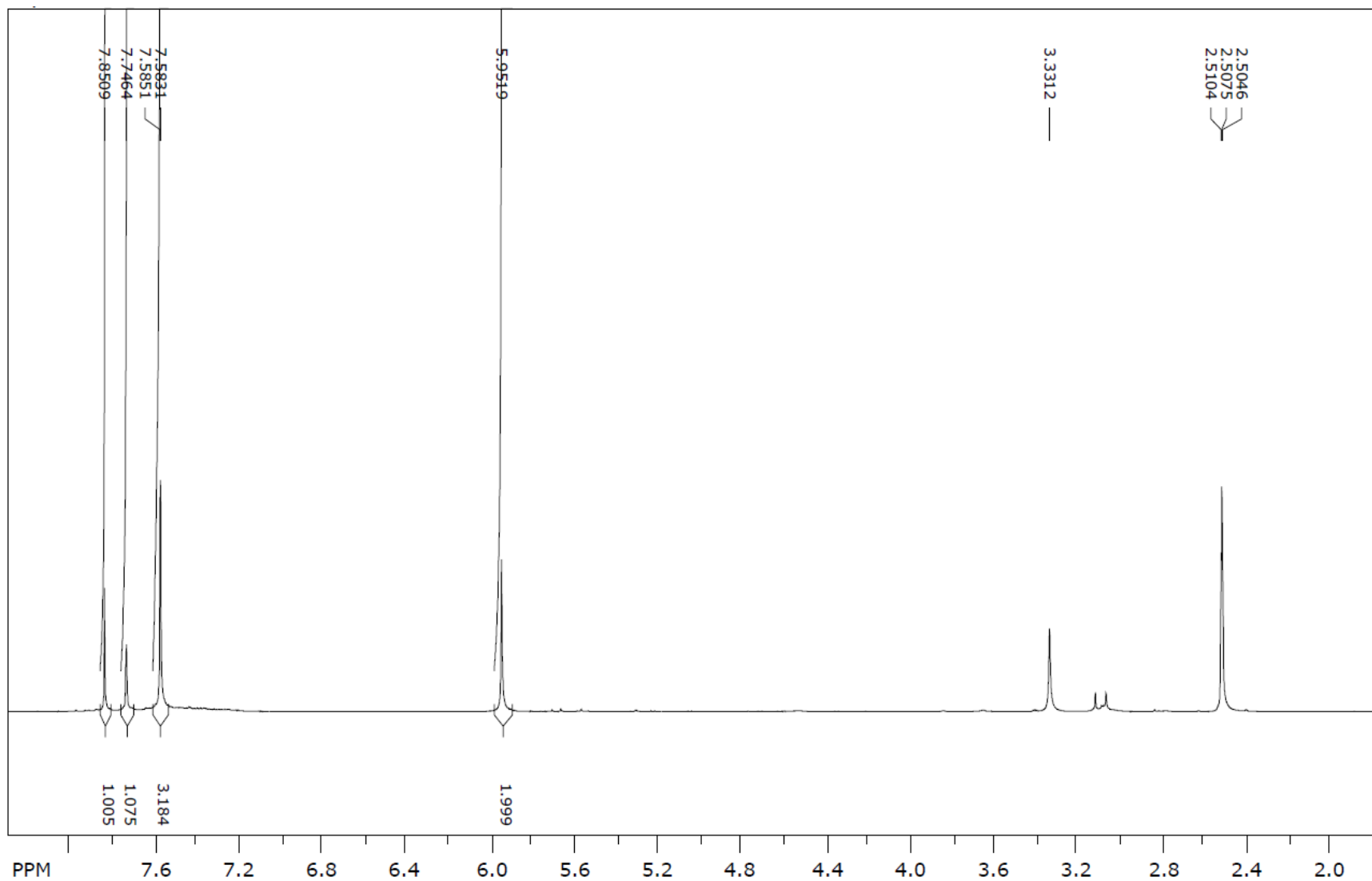


Reaktanti	3-klorbenzaldehyd (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Ispran heksan : etanol (4 : 1), ispran heksanom
Molekulska masa	270,76 g/mol
Molekulska formula	C ₁₀ H ₇ ClN ₂ OS ₂
Temperatura tališta	177 °C
Boja kristala	Žuto-smeđa
R_f	0,84; 0,78
LC/MS/MS m/z (M-)	269,30
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,85 (s, 1H, CH), 7,74 (s, 1H, arom.), 7,58 (s, 3H, arom.), 5,95 (s, 2H, NH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,51; 166,55; 135,04; 134,06; 131,50; 131,28; 130,50; 130,46; 128,32; 122,08.

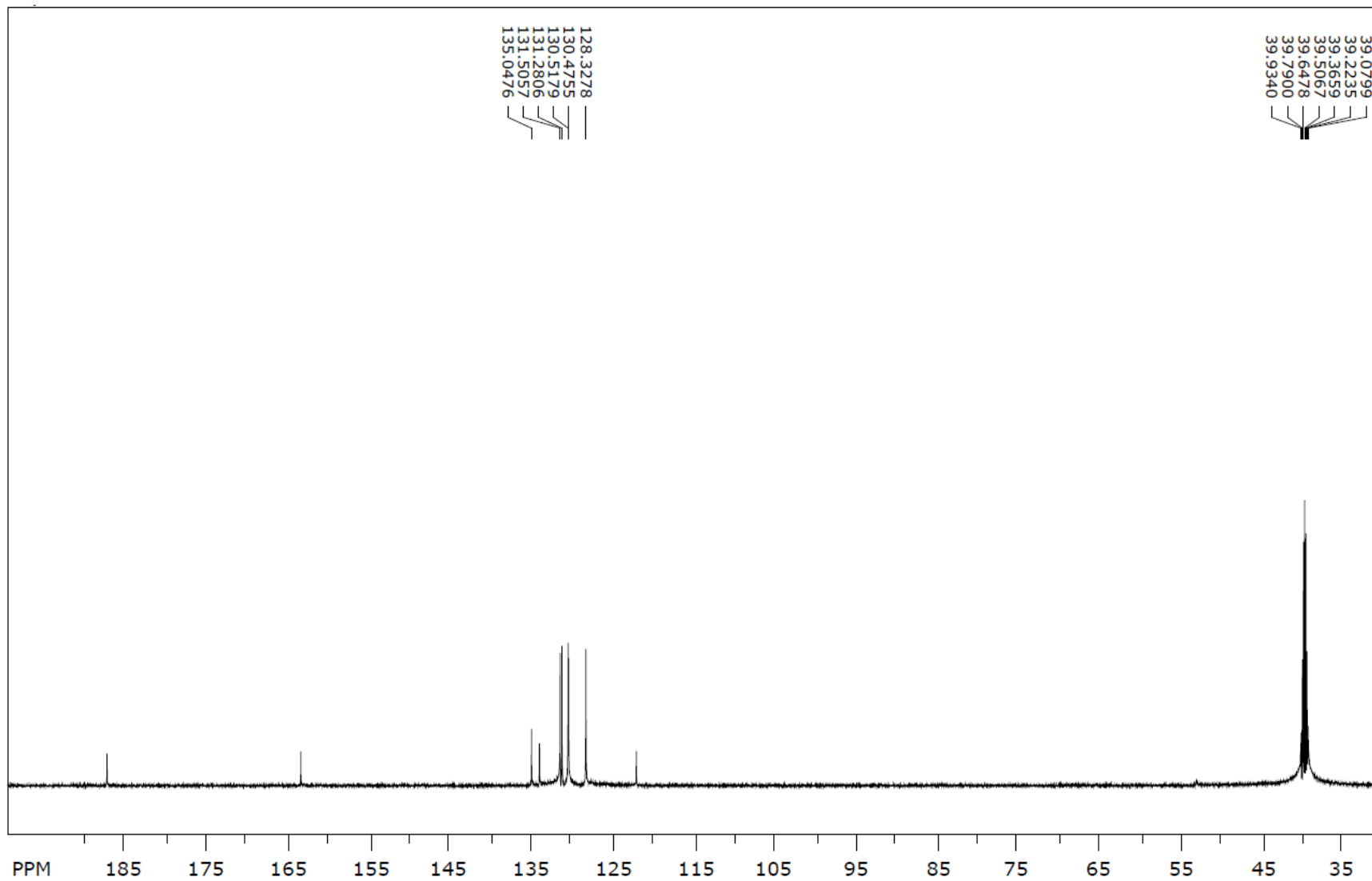
Maseni spektar (7c)



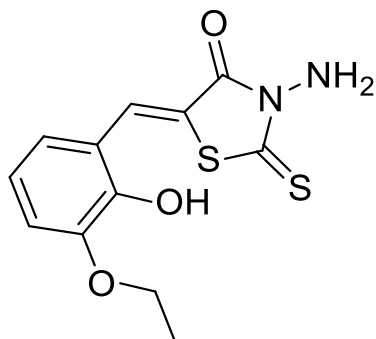
¹H NMR spektr (7c)



¹³C NMR spektr (7c)

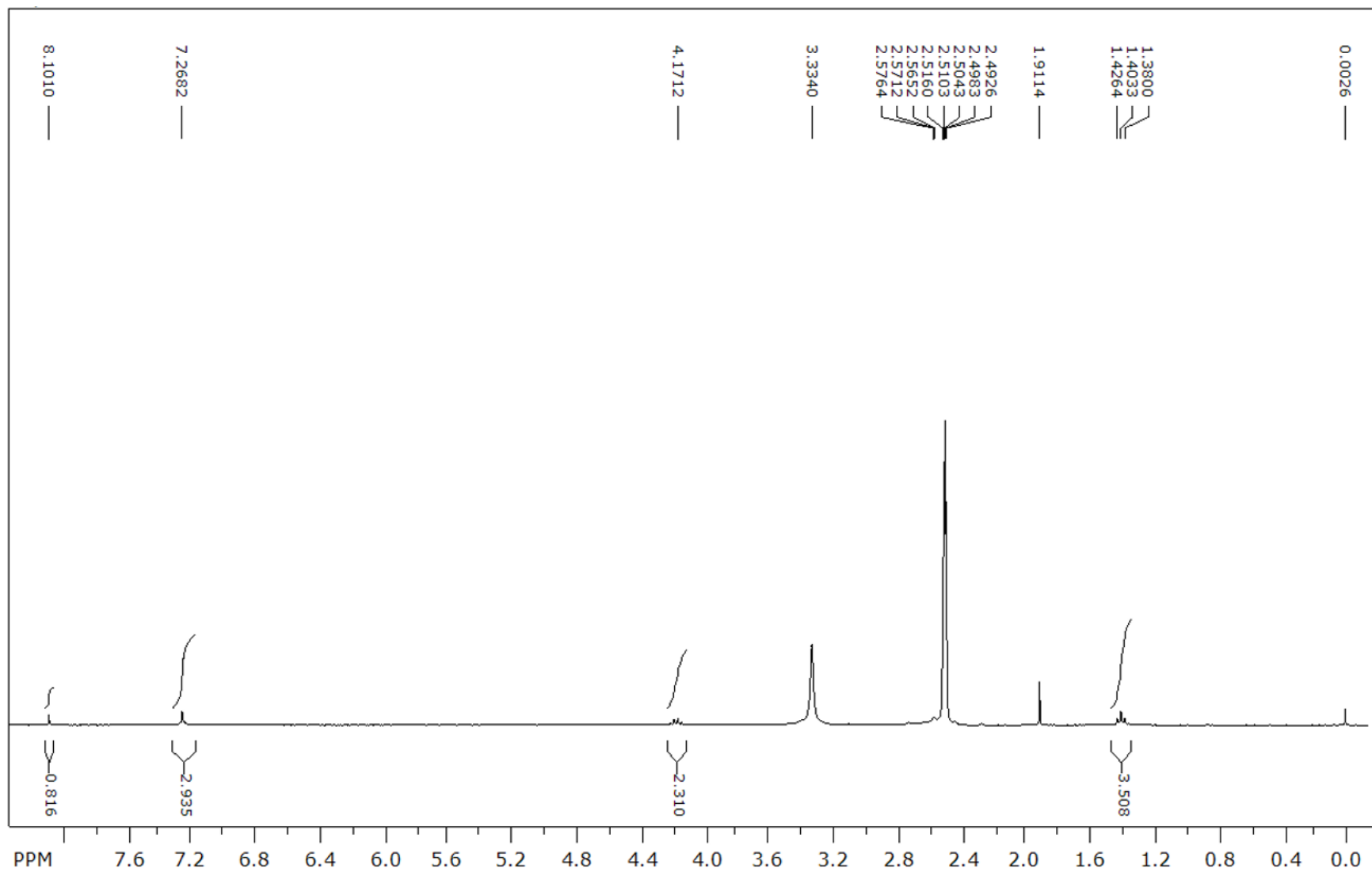


3-amino-5-(3-etoksi-2-hidroksibenziliden)-2-tioksotiazolidin-4-on (7d)

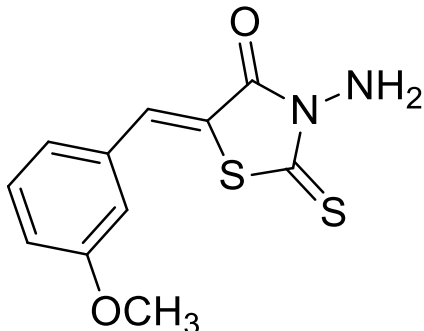


Reaktanti	3-etoksisalicilaldehid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Prekristalizacija iz octene kiseline
Molekulska masa	296,37 g/mol
Molekulska formula	C ₁₂ H ₁₂ N ₂ O ₃ S ₂
Temperatura tališta	229 – 233 °C
Boja kristala	Smeđa
R_f	0,81
LC/MS/MS m/z (M-)	296,03 (teor.)
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 8,10 (s, 1H, CH), 7,27 (t, <i>J</i> = 3,78; 4,44 Hz, 3H, arom.), 4,17 (q, <i>J</i> = 6,99 Hz, 2H, <u>CH</u> ₂ CH ₃), 1,40 (t, <i>J</i> = 6,96 Hz, 3H, CH ₂ <u>CH</u> ₃).
¹³C NMR	-

¹H NMR spektr (7d)

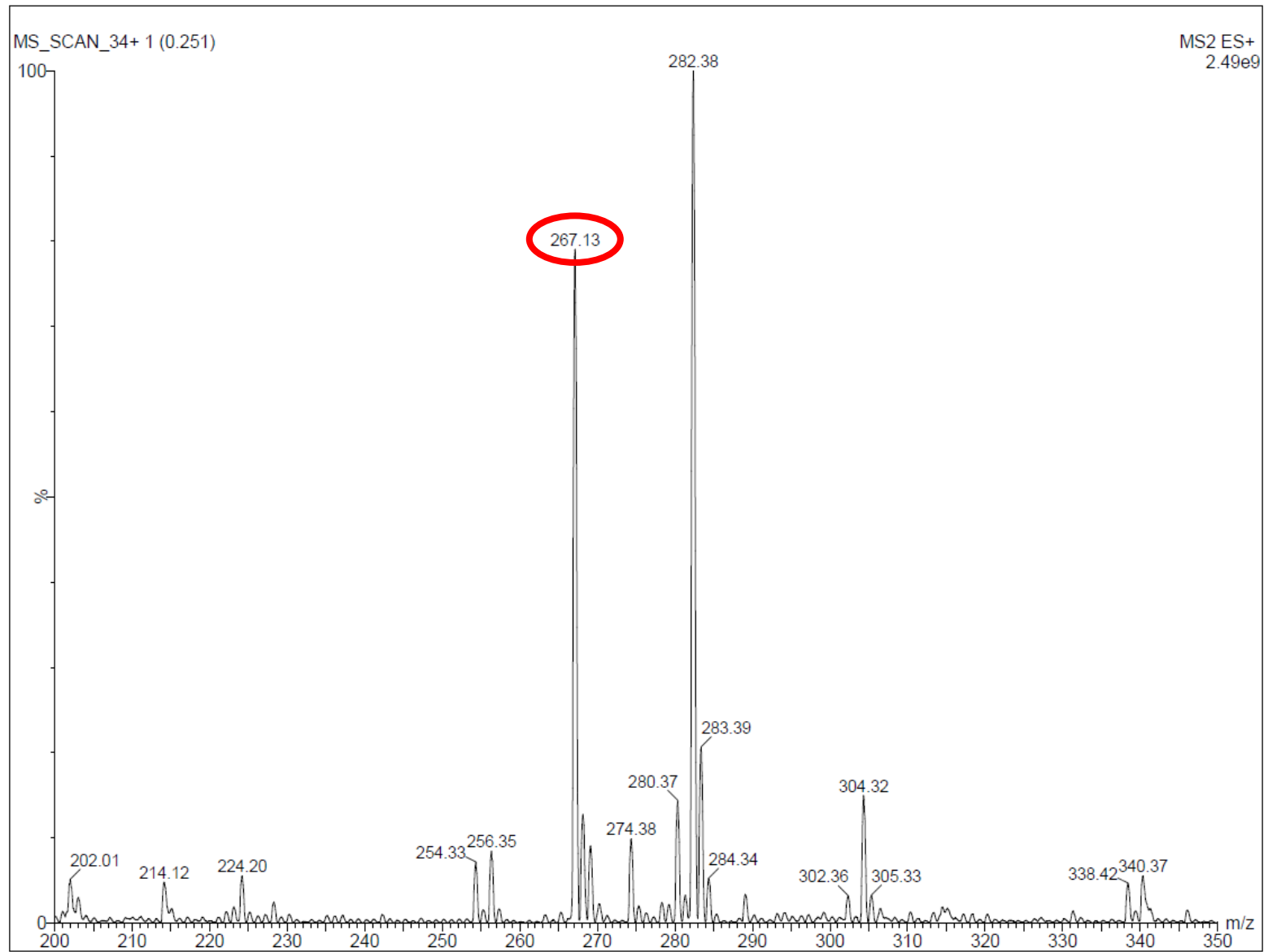


3-amino-5-(3-metoksibenziliden)-2-tioksotiazolidin-4-on (7e)

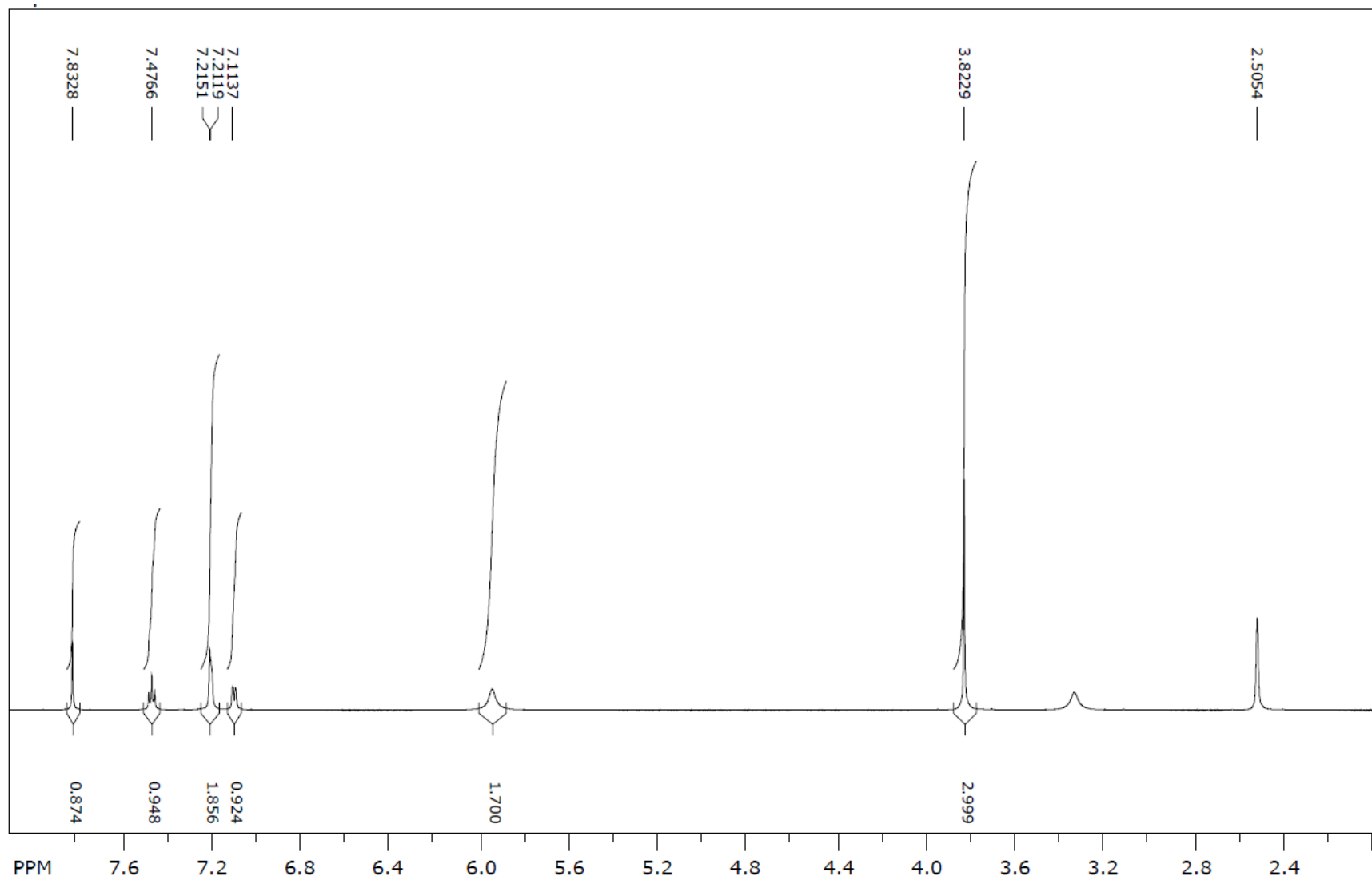


Reaktanti	3-metoksibenzaldehid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	266,34 g/mol
Molekulska formula	C ₁₁ H ₁₀ N ₂ O ₂ S ₂
Temperatura tališta	180 – 184 °C
Boja kristala	Svijetlosmeđa
R_f	0,78
LC/MS/MS <i>m/z</i> (M⁺)	267,13
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,82 (s, 1H, CH), 7,47 (t, <i>J</i> = 8,16 Hz, 1H, arom.), 7,21 (d, <i>J</i> = 1,92 Hz, 2H, arom.), 7,10 (dd, <i>J</i> = 8,04; 1,80 Hz, 1H, arom.), 5,94 (s, 2H, NH ₂), 3,82 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,65; 163,63; 132,23; 133,28; 130,60; 122,54; 120,58; 117,02; 115,81.

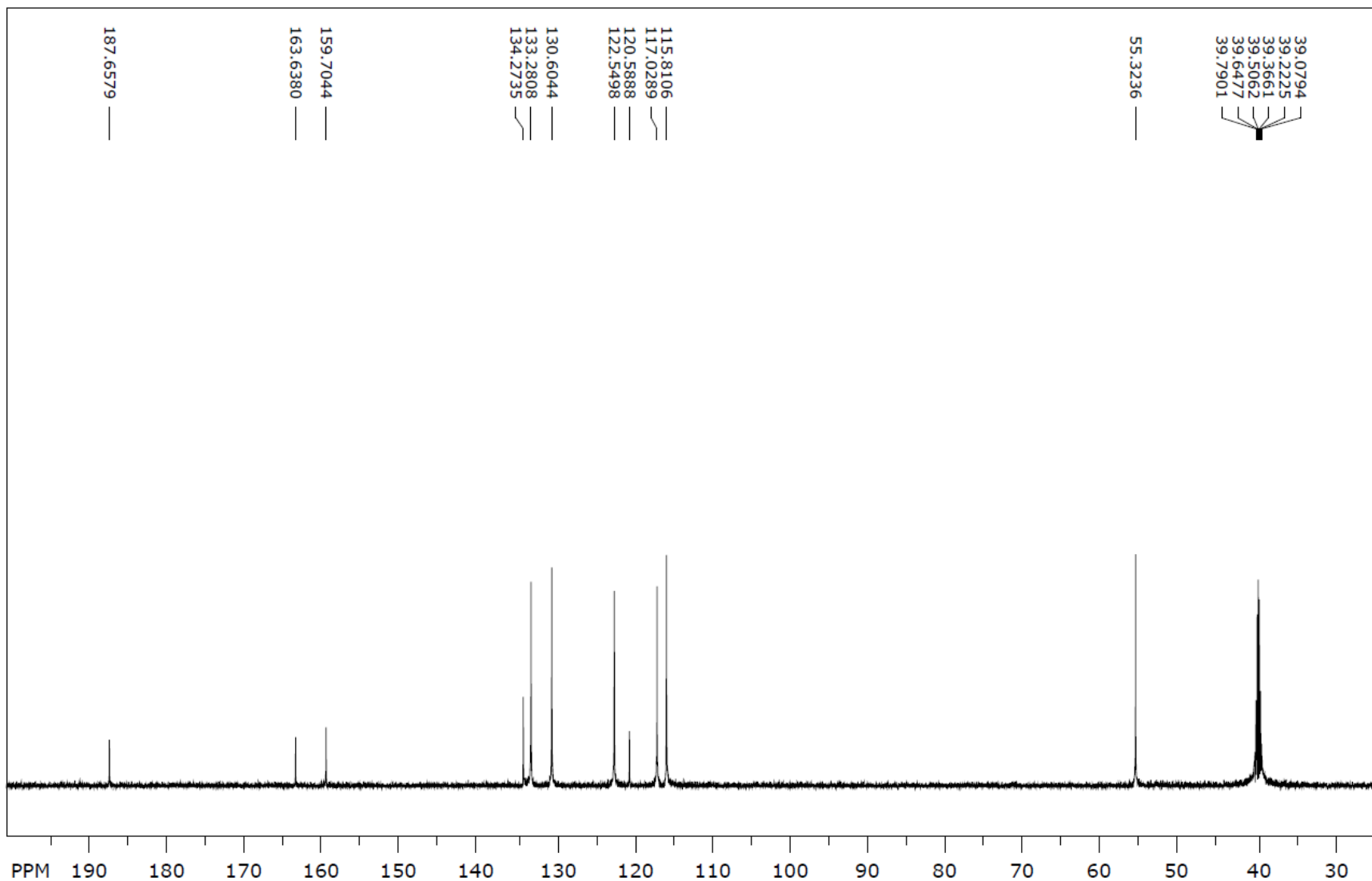
Maseni spektar (7e)



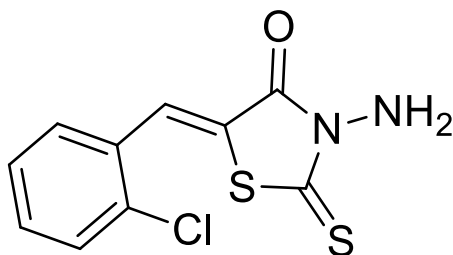
¹H NMR spektr (7e)



¹³C NMR spektr (7e)

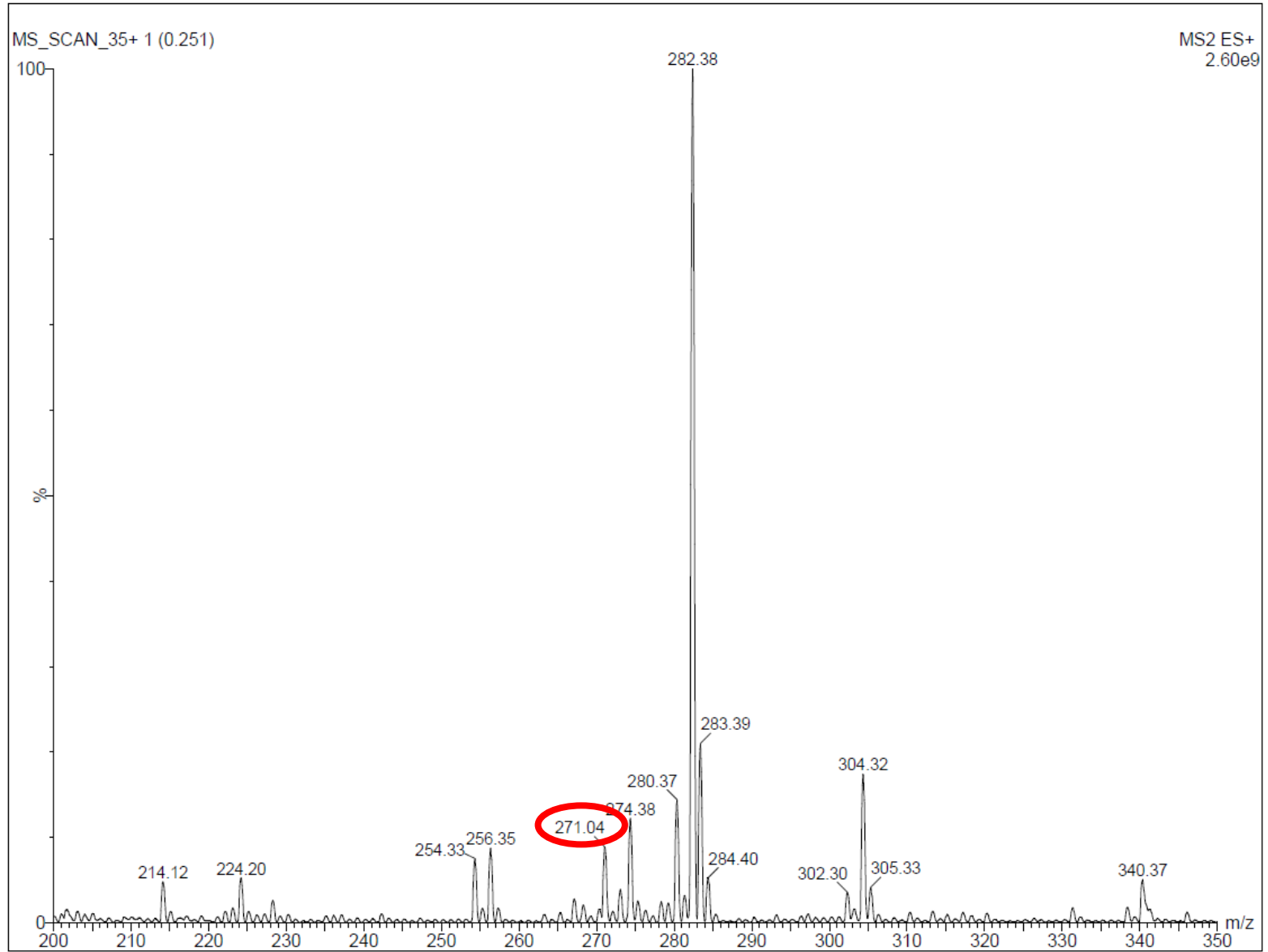


3-amino-5-(2-klorbenziliden)-2-tioksotiazolidin-4-on (7f)

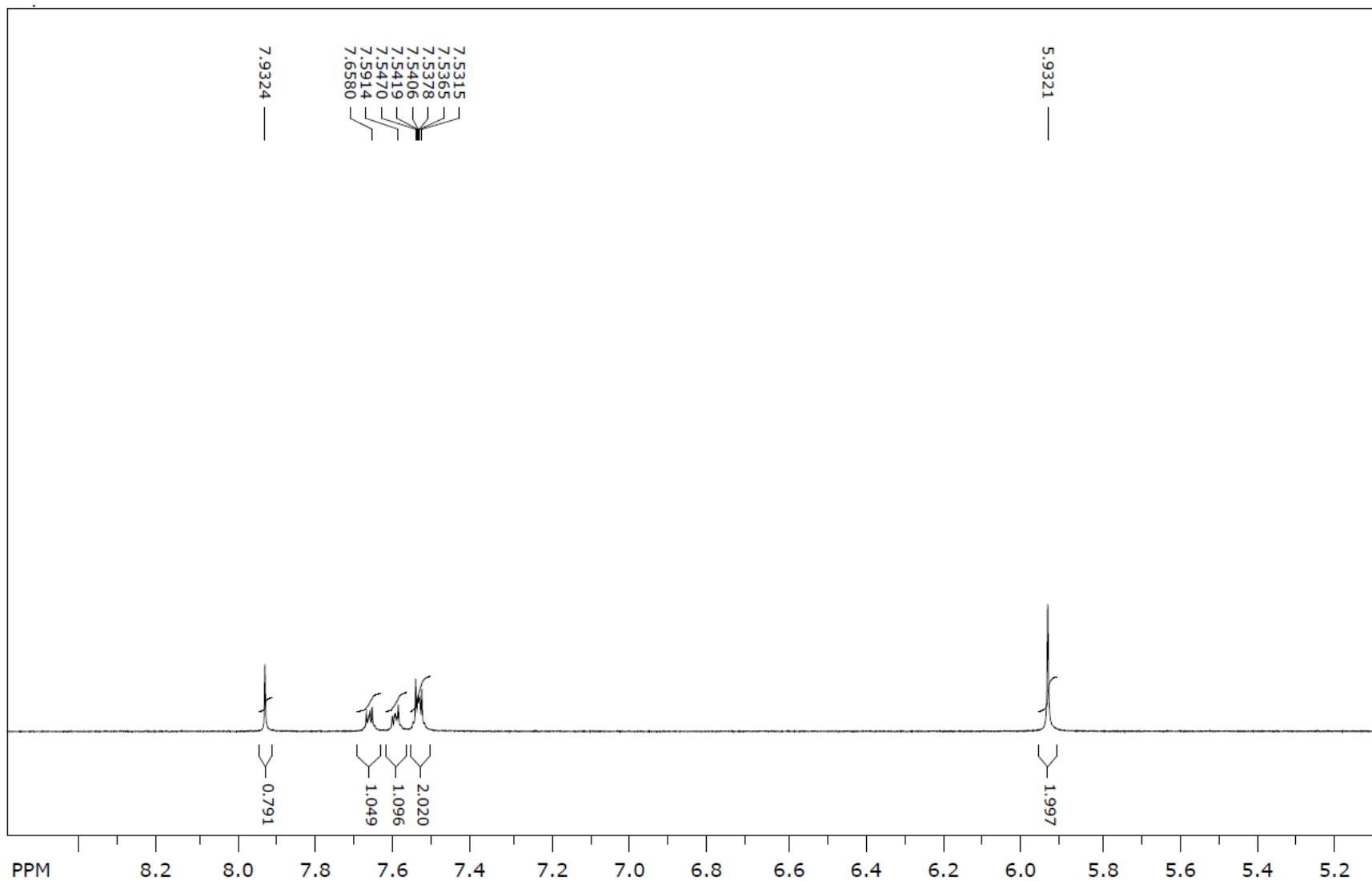


Reaktanti	2-klorbenzaldehyd (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	270,76 g/mol
Molekulska formula	C ₁₀ H ₇ ClN ₂ OS ₂
Temperatura tališta	160 – 162 °C
Boja kristala	Žuta
R_f	0,81
LC/MS/MS m/z (M⁺)	271,04
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,93 (s, 1H, CH), 7,66 – 7,67 (m, 1H, arom.), 7,59 – 7,60 (m, 1H, arom.), 7,53 – 7,55 (m, 2H, arom.), 5,93 (s, 2H, NH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,90; 163,44; 134,75; 132,33; 130,49, 129,56; 128,30; 127,81; 123,90.

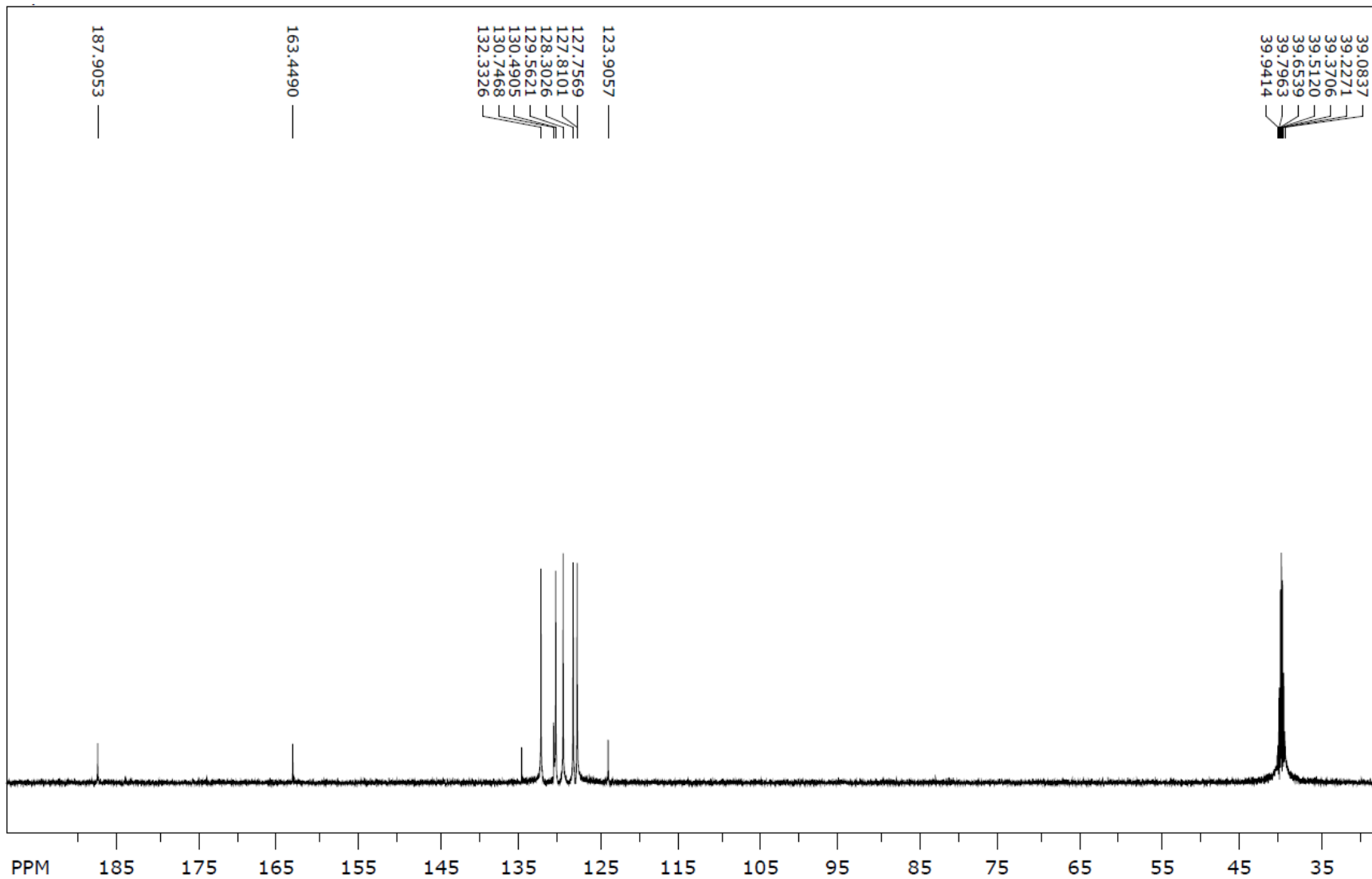
Maseni spektar (7f)



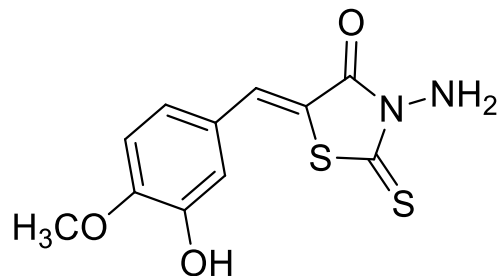
¹H NMR spektr (7f)



¹³C NMR spektr (7f)

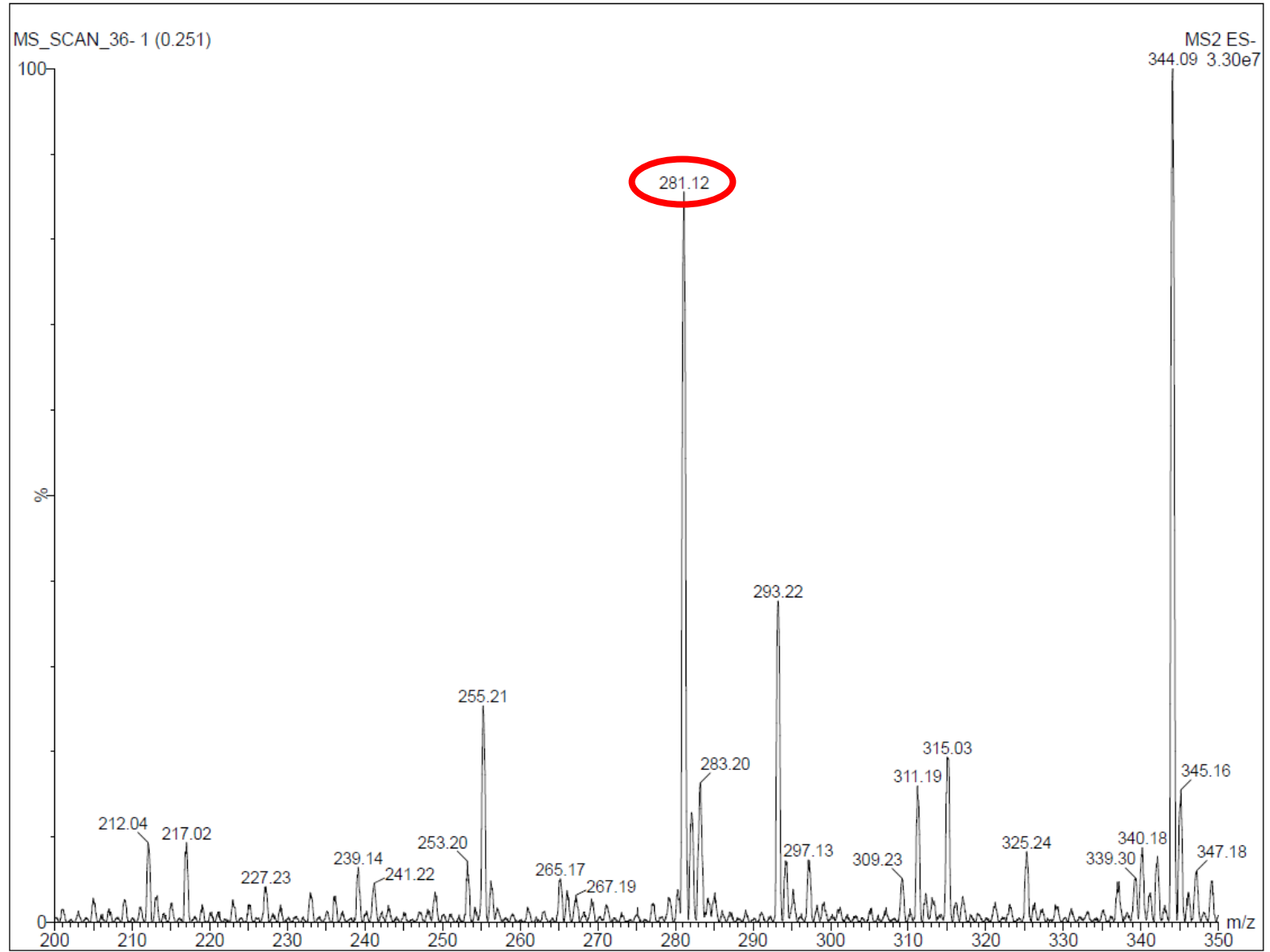


**3-amino-5-(3-hidroksi-4-metoksibenziliden)-2-tioksotiazolidin-4-on
(7g)**

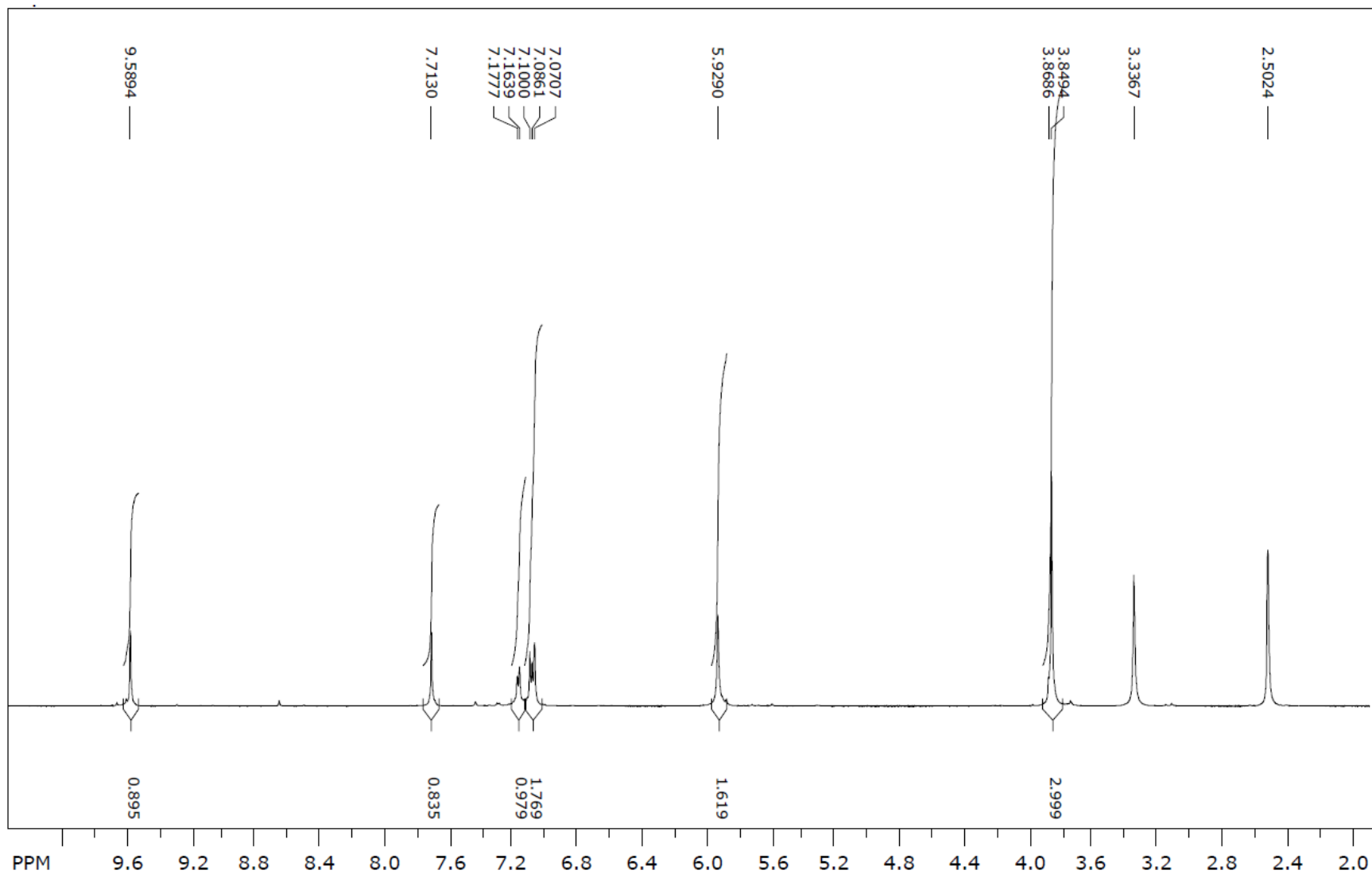


Reaktanti	3-hidroksi-4-metoksibenzaldehid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	282,34 g/mol
Molekulska formula	C ₁₁ H ₁₀ N ₂ O ₃ S ₂
Temperatura tališta	192 – 197 °C
Boja kristala	Smeđa
R_f	0,65
LC/MS/MS m/z (M⁻)	281,12
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 9,59 (s, 1H, OH), 7,71 (s, 1H, CH), 7,17 (d, <i>J</i> = 8,28 Hz, 1H, arom.), 7,09 (t, <i>J</i> = 8,34; 9,24 Hz, 2H, arom.), 5,29 (s, 2H, NH ₂), 3,84 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,20; 163,59; 150,76; 147,12; 134,03; 125,68; 124,84; 116,56; 116,17; 112,54, 55,72.

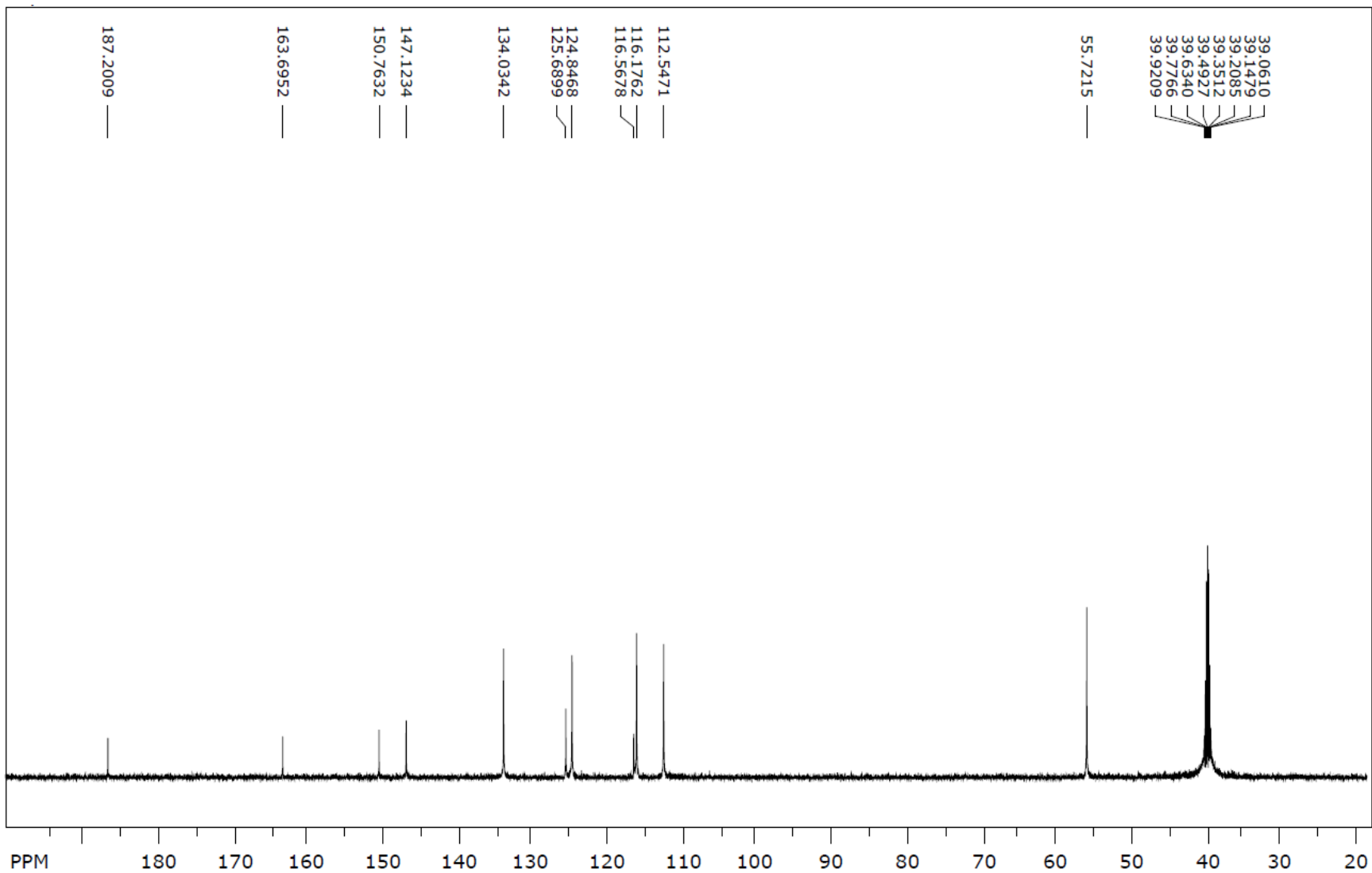
Maseni spektar (7g)



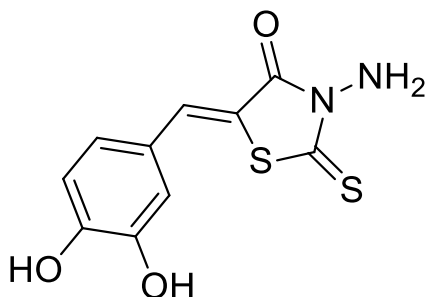
¹H NMR spektr (7g)



¹³C NMR spektr (7g)

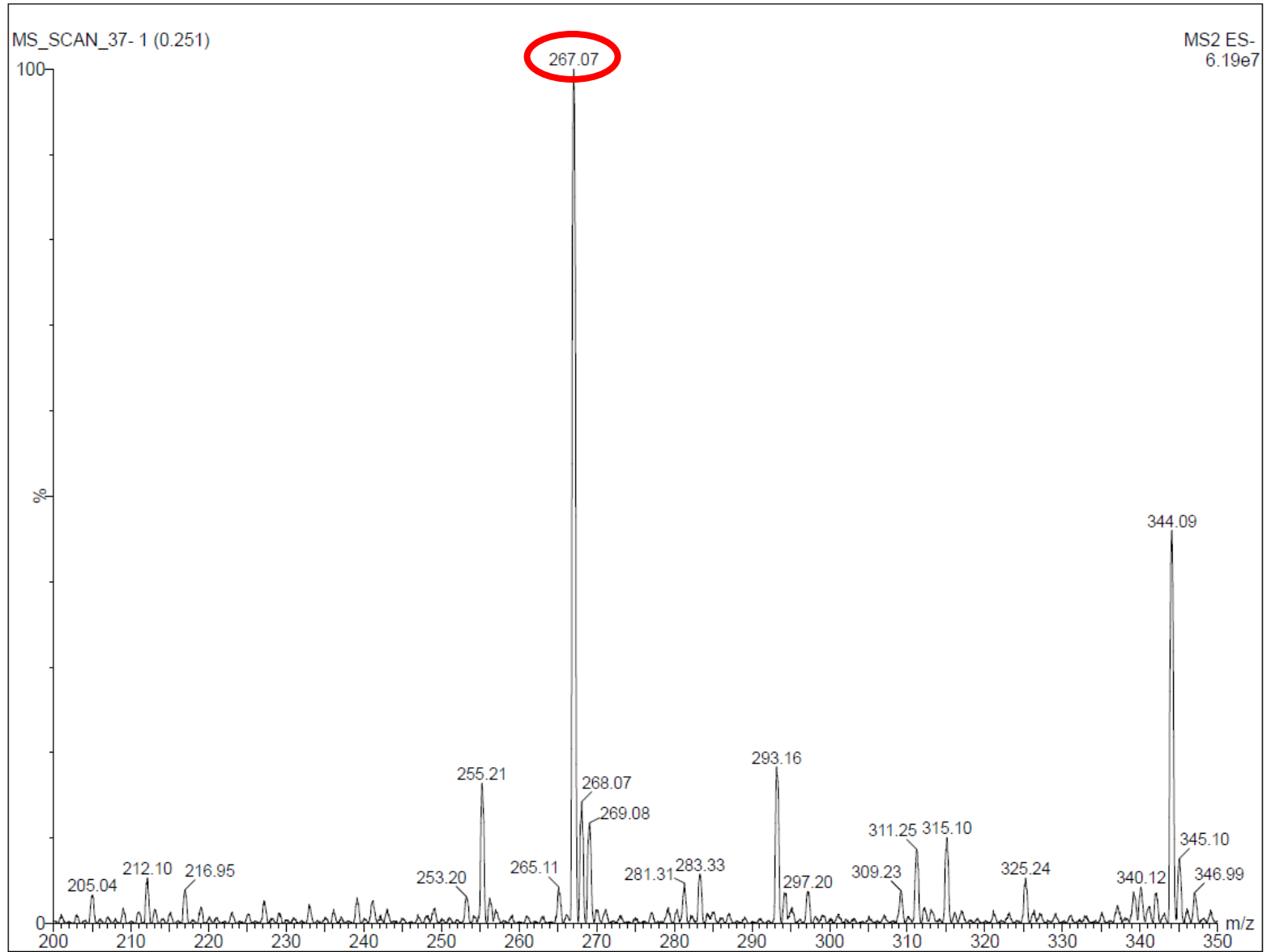


3-amino-5-(3,4-dihidroksibenziliden)-2-tioksotiazolidin-4-on (7h)

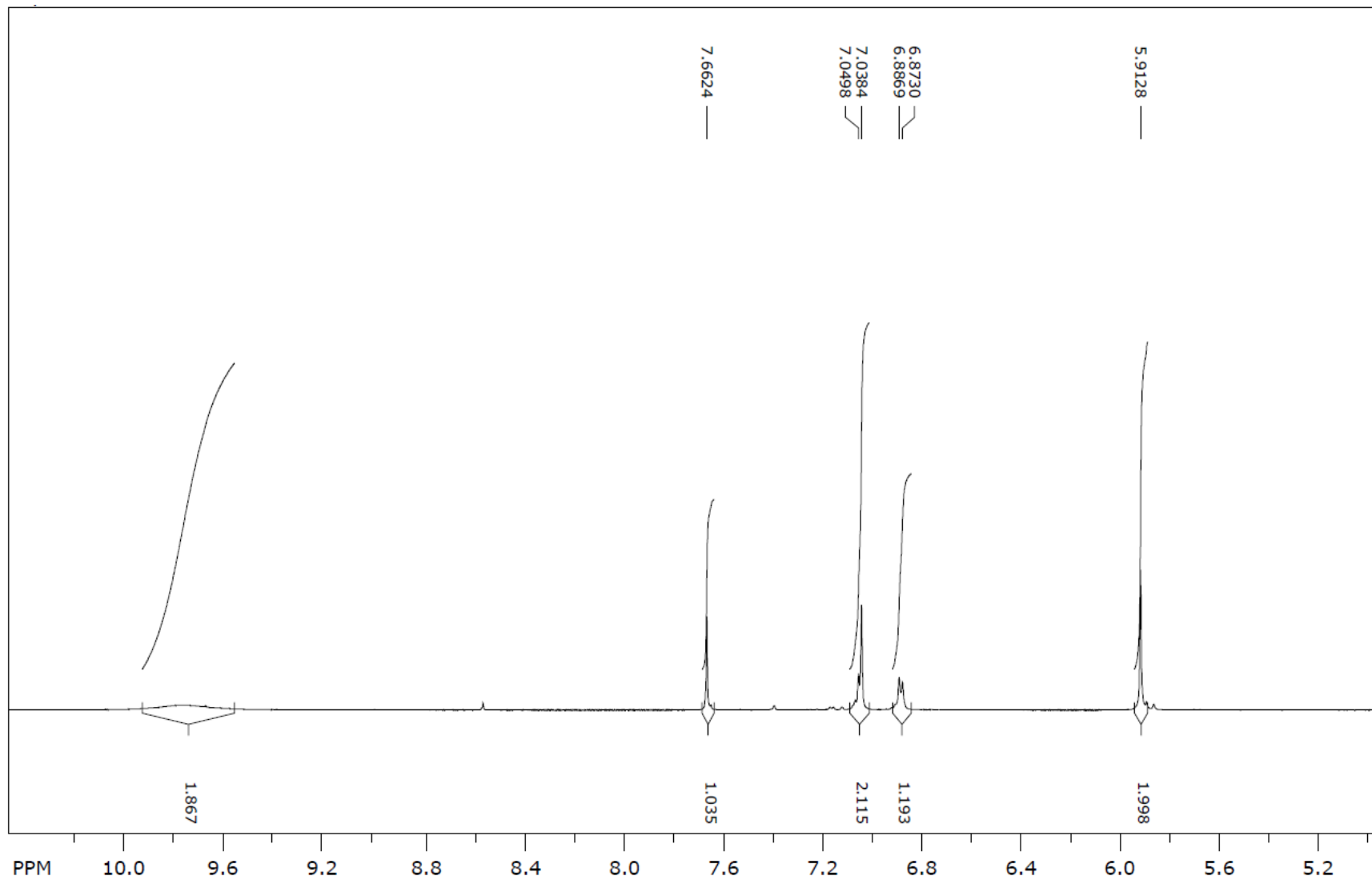


Reaktanti	3,4-dihidroksibenzaldehid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Ispran heksan : etanol (4 : 1), ispran heksanom
Molekulska masa	268,31 g/mol
Molekulska formula	C ₁₀ H ₈ N ₂ O ₃ S ₂
Temperatura tališta	257 – 258 °C
Boja kristala	Smeđa
R_f	0,51
LC/MS/MS <i>m/z</i> (M-)	267,07
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 9,78 (s, 1H, OH), 8,56 (s, 1H, OH), 7,66 (s, 1H, CH), 7,04 (d, <i>J</i> = 6,84 Hz, 2H, arom.), 6,88 (d, <i>J</i> = 8,34 Hz, 1H, arom.), 5,88 (s, 2H, NH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,04; 163,73; 149,58; 146,09; 134,52; 129,38; 124,40; 116,79; 116,49; 115,24.

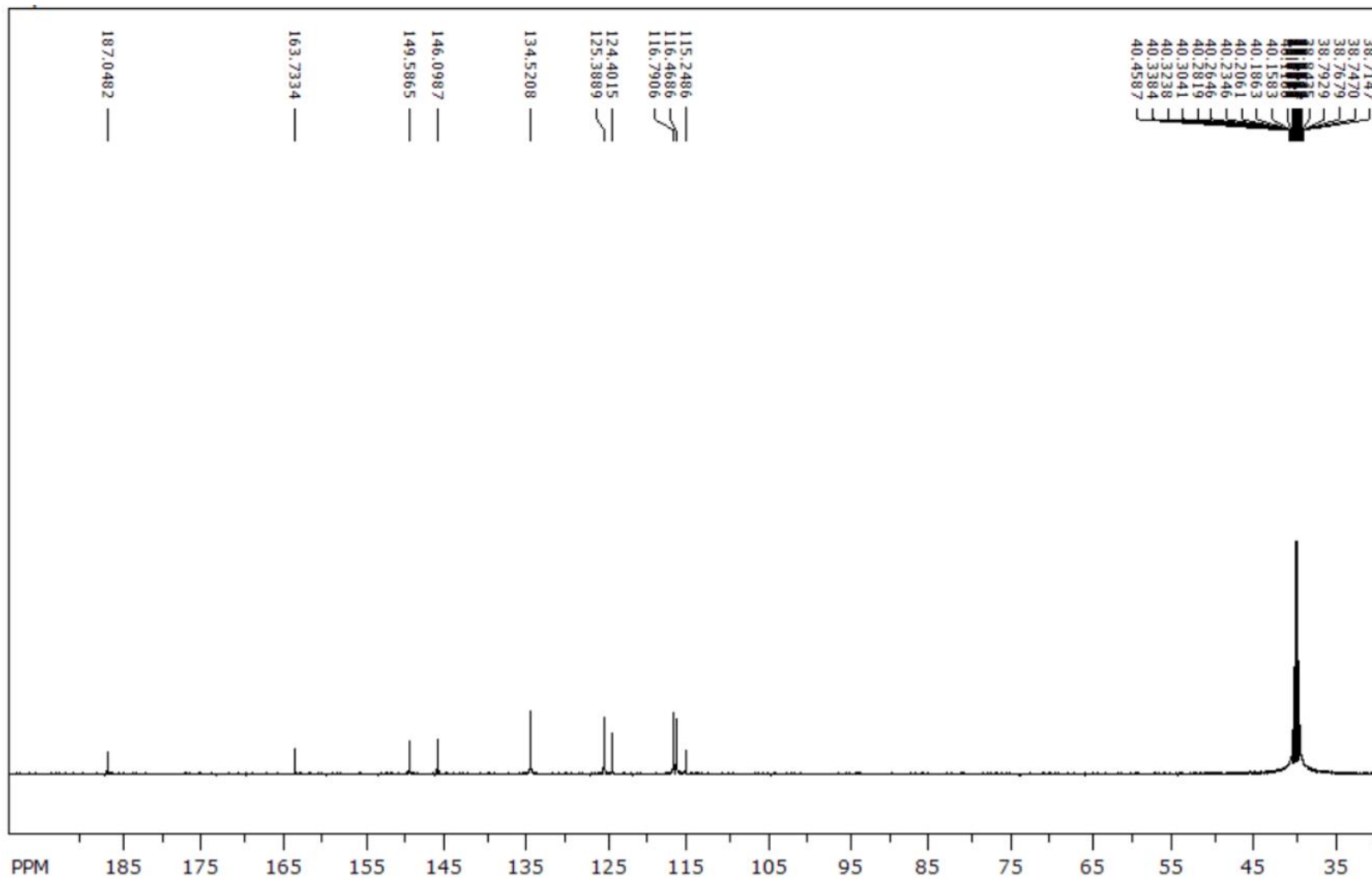
Maseni spektr (7h)



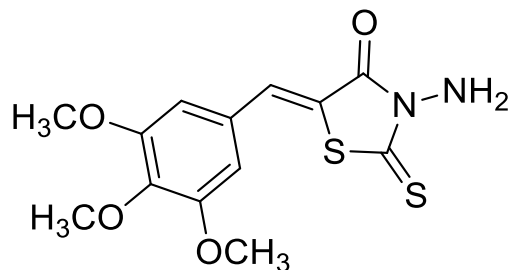
¹H NMR spektr (7h)



¹³C NMR spektar (7h)

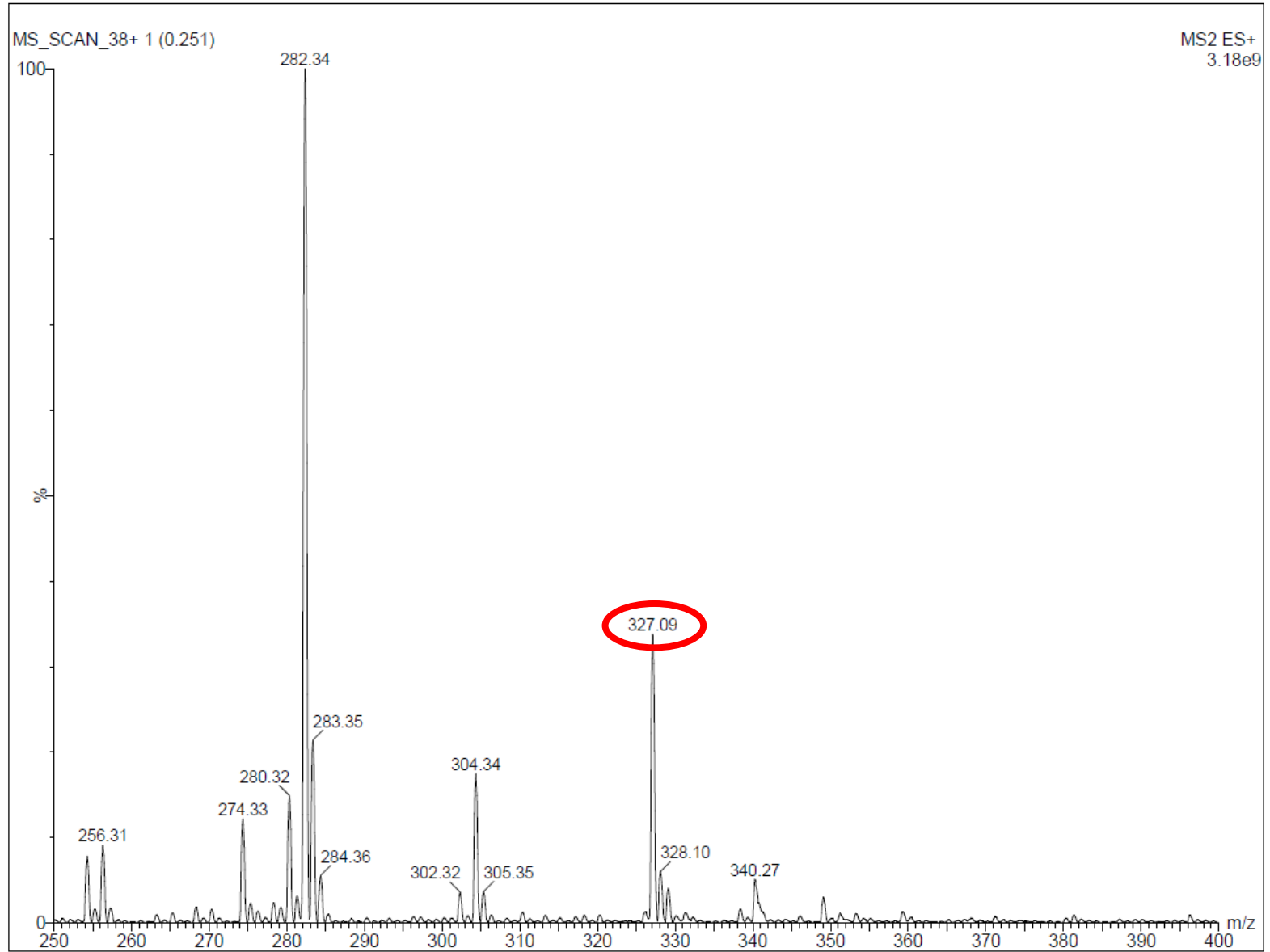


3-amino-2-tiokso-5-(3,4,5-trimetoksibenzilidene)tiazolidin-4-on (7i)

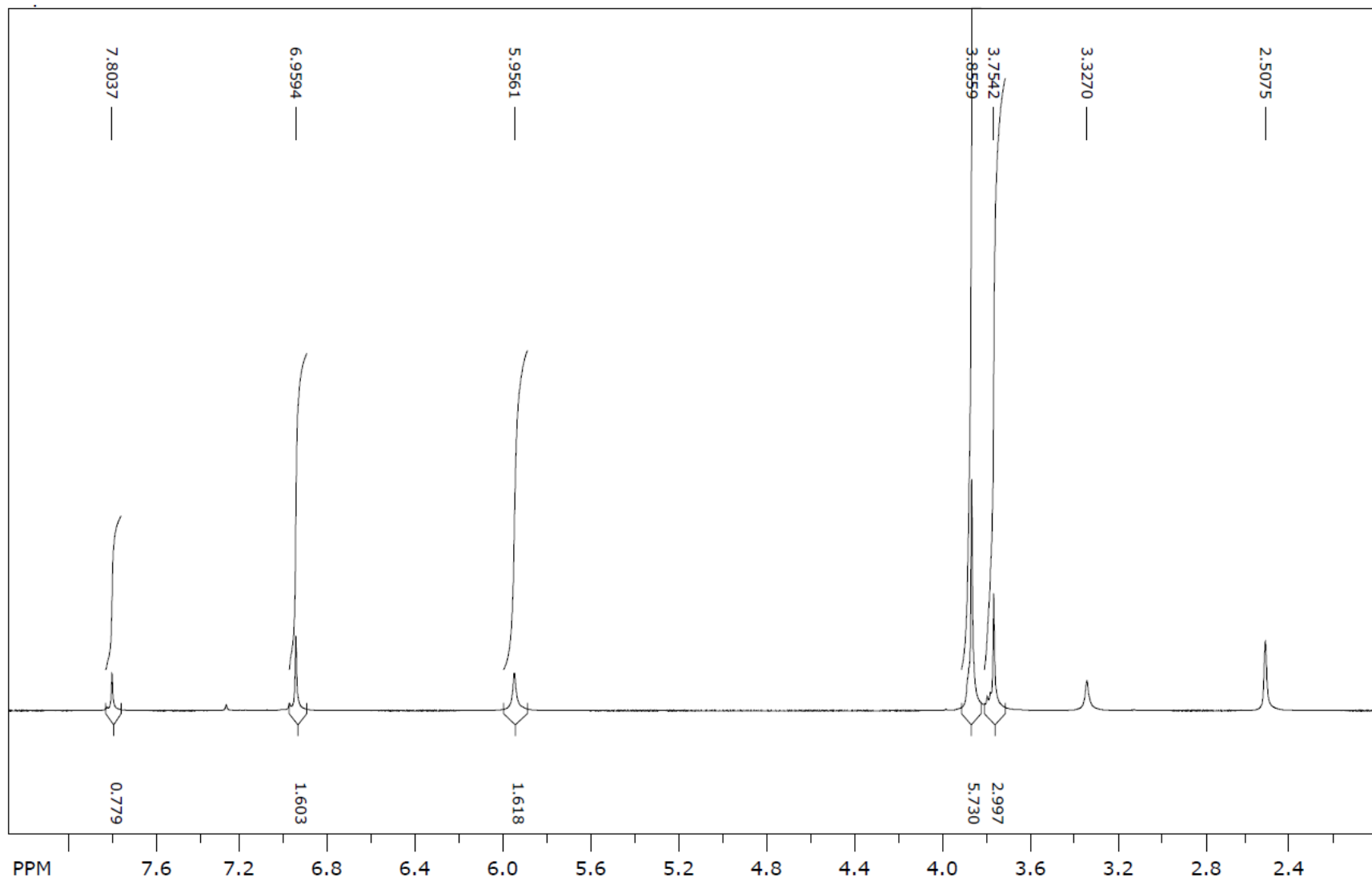


Reaktanti	3,4,5-trimetoksibenzaldehid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	326,39 g/mol
Molekulska formula	C ₁₃ H ₁₄ N ₂ O ₄ S ₂
Temperatura tališta	165 – 169 °C
Boja kristala	Smeđa
R_f	0,76
LC/MS/MS <i>m/z</i> (M⁺)	327,09
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,80 (s, 1H, CH), 6,95 (s, 2H, arom.), 5,95 (s, 2H, NH ₂), 3,85 (s, 6H, CH ₃ , OCH ₃), 3,75 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,32; 163,22; 153,27; 140,03; 133,68; 128,38; 118,99; 108,04; 60,22; 56,04.

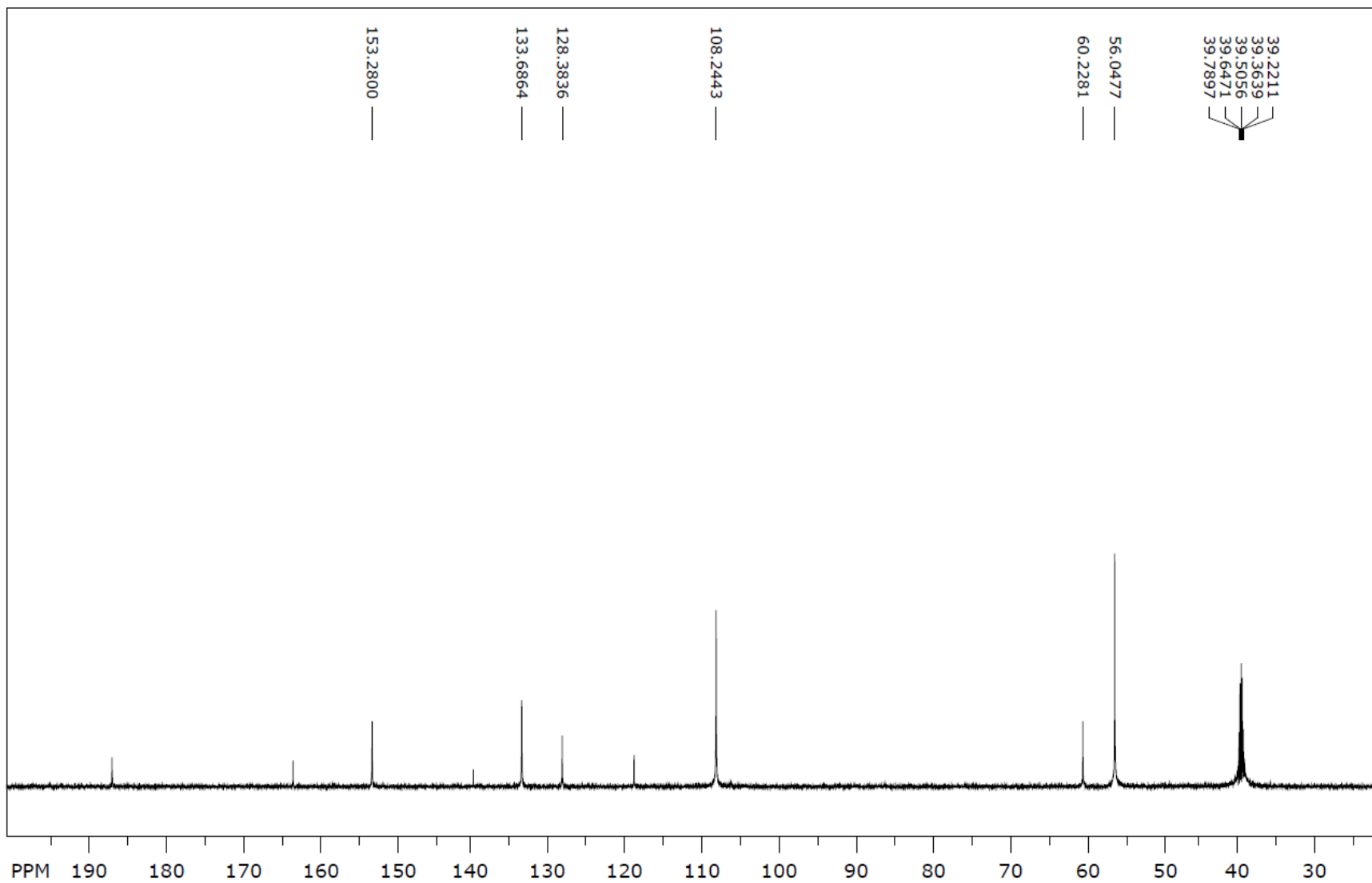
Maseni spektr (7i)



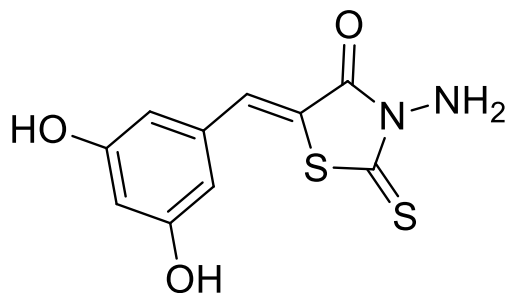
¹H NMR spektr (7i)



¹³C NMR spektr (7i)

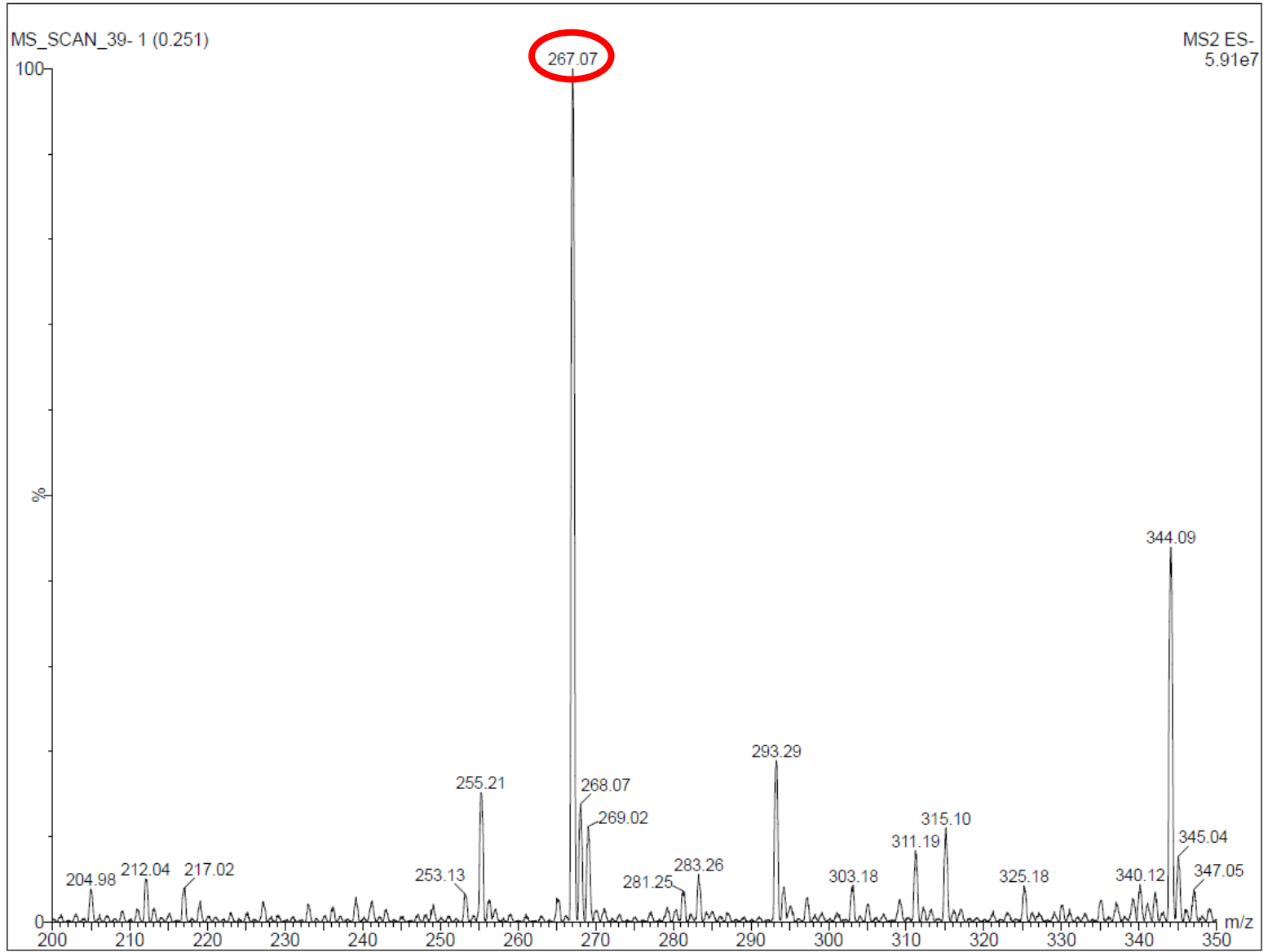


3-amino-5-(3,5-dihidroksibenziliden)-2-tioksotiazolidin-4-on (7j)

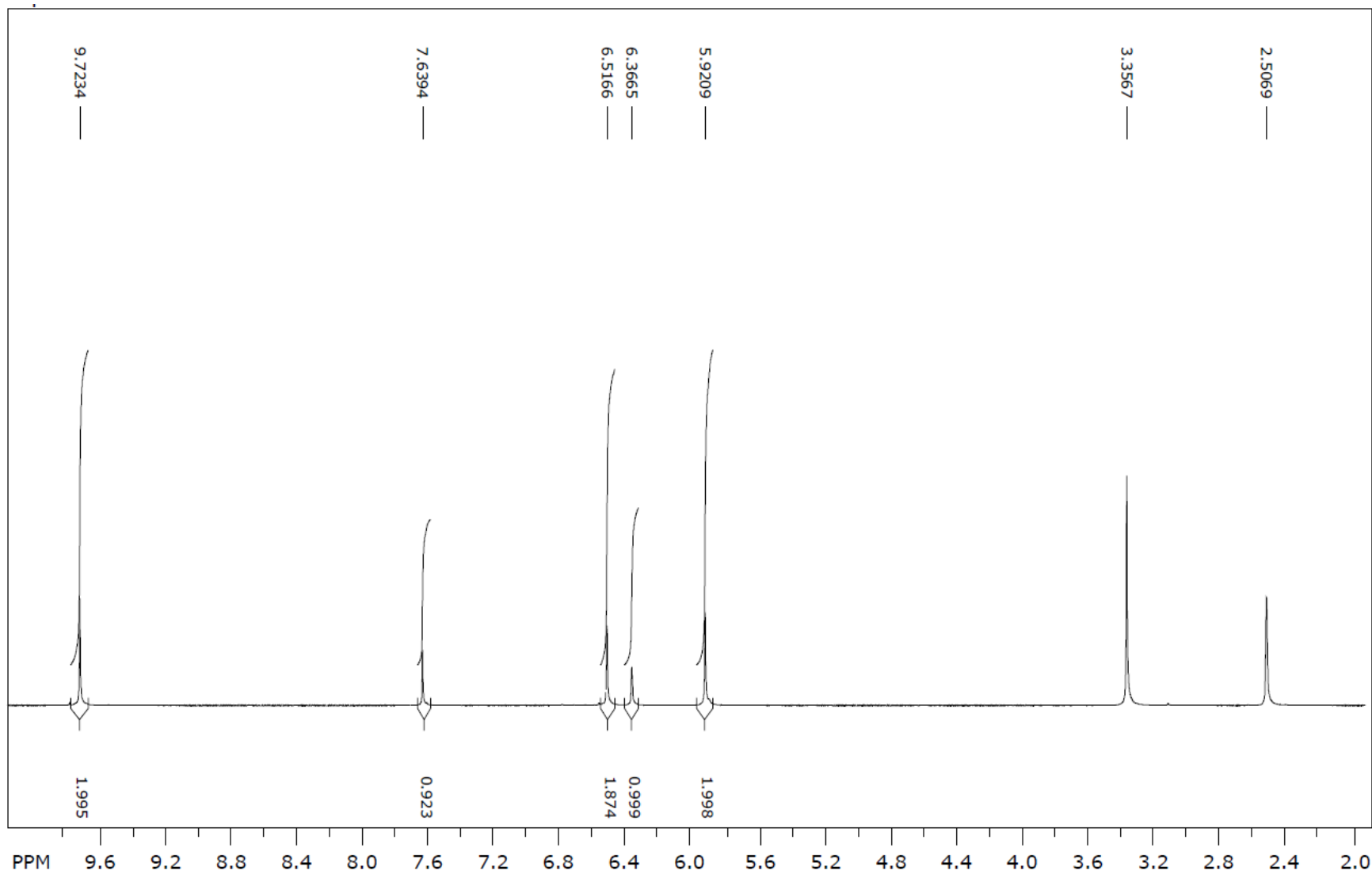


Reaktanti	3,5-dihidroksibenzaldehid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	268,31 g/mol
Molekulska formula	C ₁₀ H ₈ N ₂ O ₃ S ₂
Temperatura tališta	253 – 257 °C
Boja kristala	Smeđa
R_f	0,43
LC/MS/MS m/z (M-)	267,07
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 9,72 (s, 2H, OH), 7,63 (s, 1H, CH), 6,51 (s, 2H, arom.), 6,36 (s, 1H, arom.), 5,92 (s, 2H, NH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,82; 163,62; 159,06; 134,41; 133,92; 119,83; 108,60; 105,52.

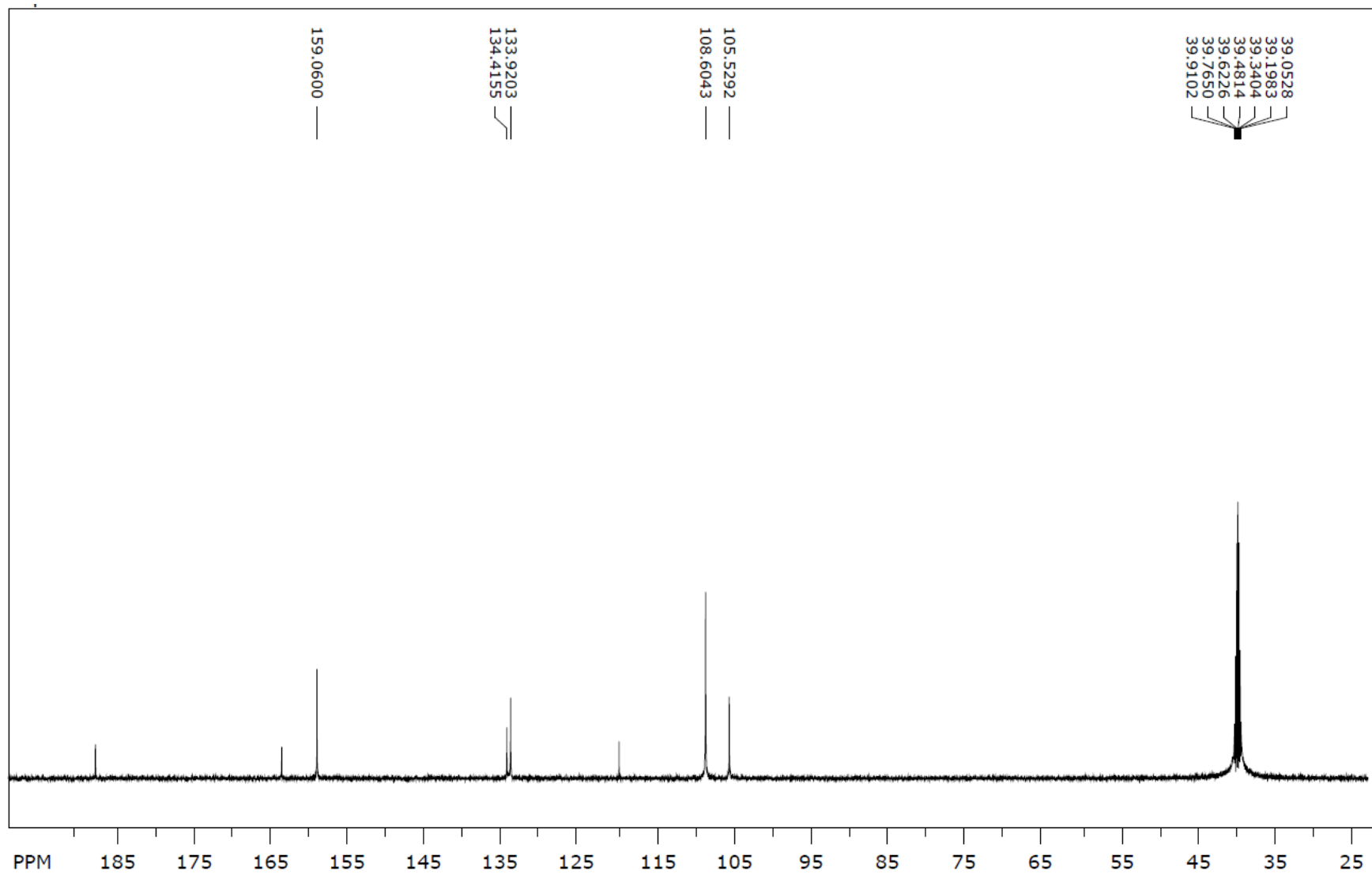
Maseni spektr (7j)



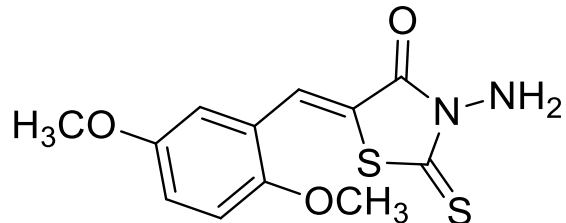
¹H NMR spektr (7j)



¹³C NMR spektr (7j)

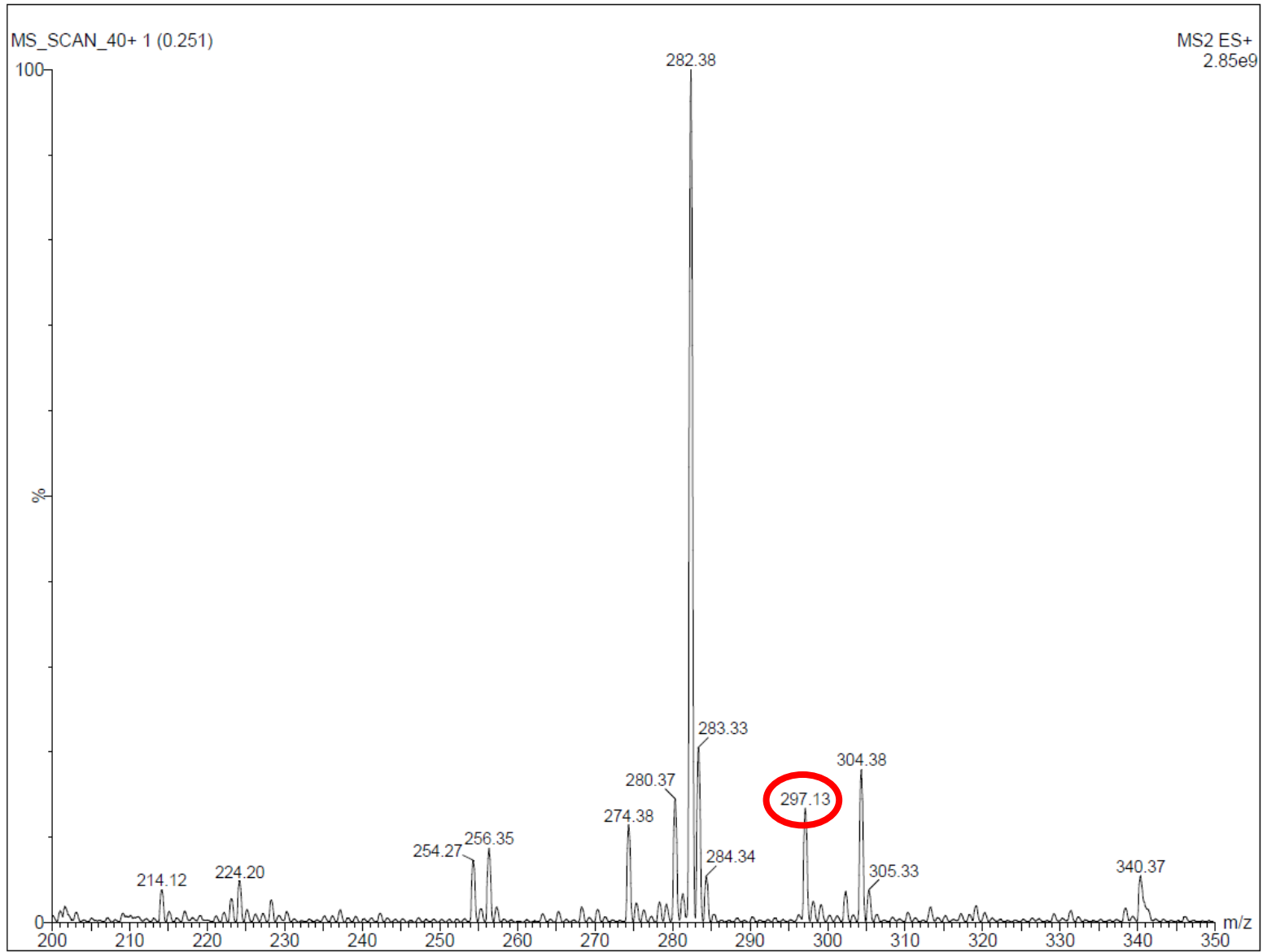


3-amino-5-(2,5-dimetoksibenziliden)-2-tioksotiazolidin-4-one (7k)

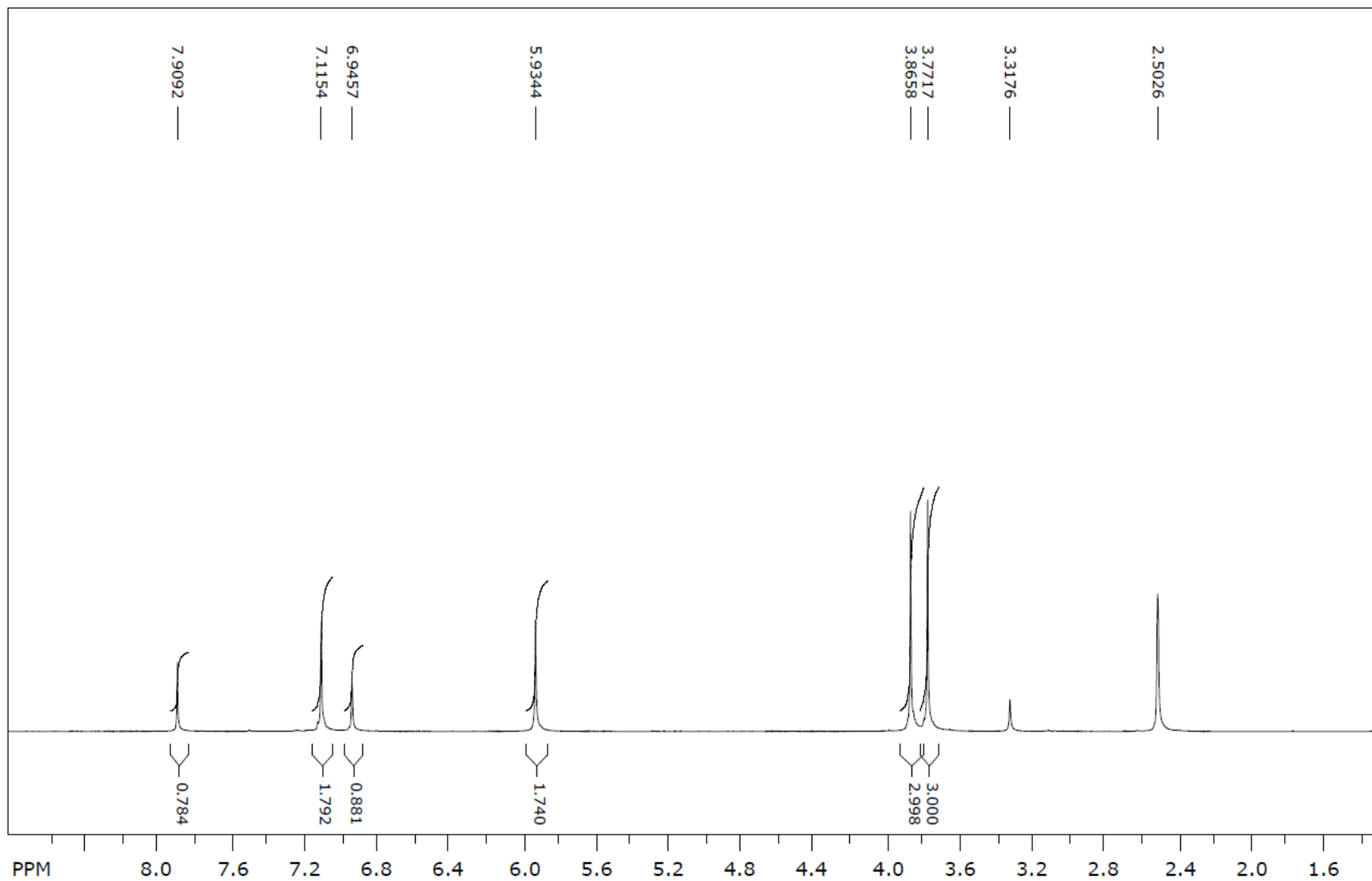


Reaktanti	2,5-dimetoksibenzaldehid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	296,37 g/mol
Molekulska formula	C ₁₂ H ₁₂ N ₂ O ₃ S ₂
Temperatura tališta	156 – 158 °C
Boja kristala	Narančasta
R_f	0,79; 0,74
LC/MS/MS <i>m/z</i> (M⁺)	297,13
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,90 (s, 1H, CH), 7,11 (s, 2H, arom.), 6,94 (s, 1H, arom.), 5,93 (s, 2H, NH ₂), 3,86 (s, 3H, OCH ₃), 3,77 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,96; 163,74; 153,21; 152,53; 128,57; 121,69; 120,49; 118,97; 114,37; 113,26; 56,07; 55,60.

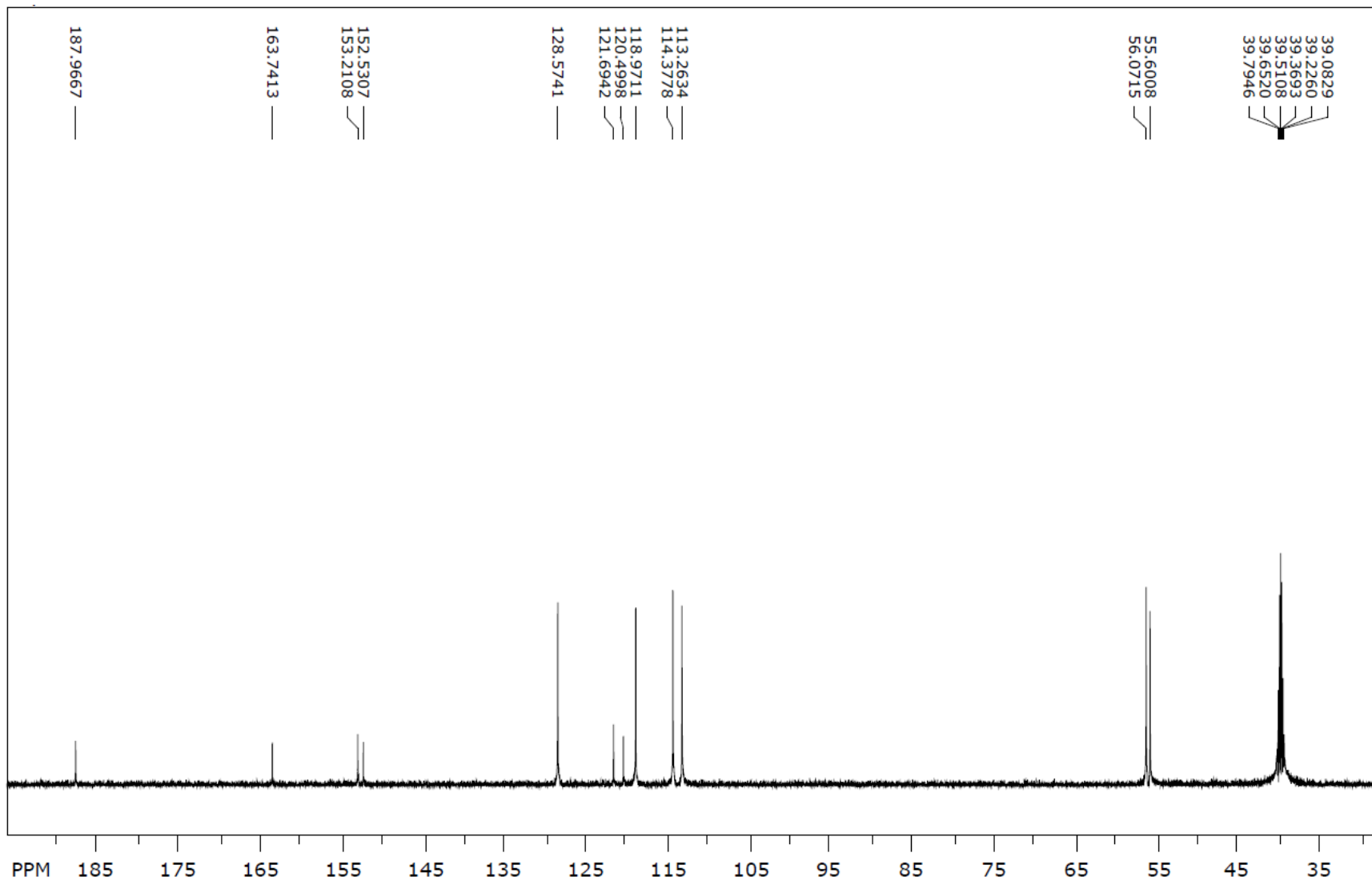
Maseni spektar (7k)



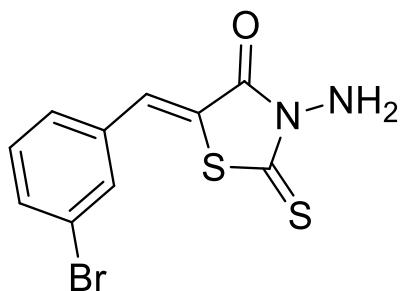
¹H NMR spektr (7k)



¹³C NMR spektr (7k)

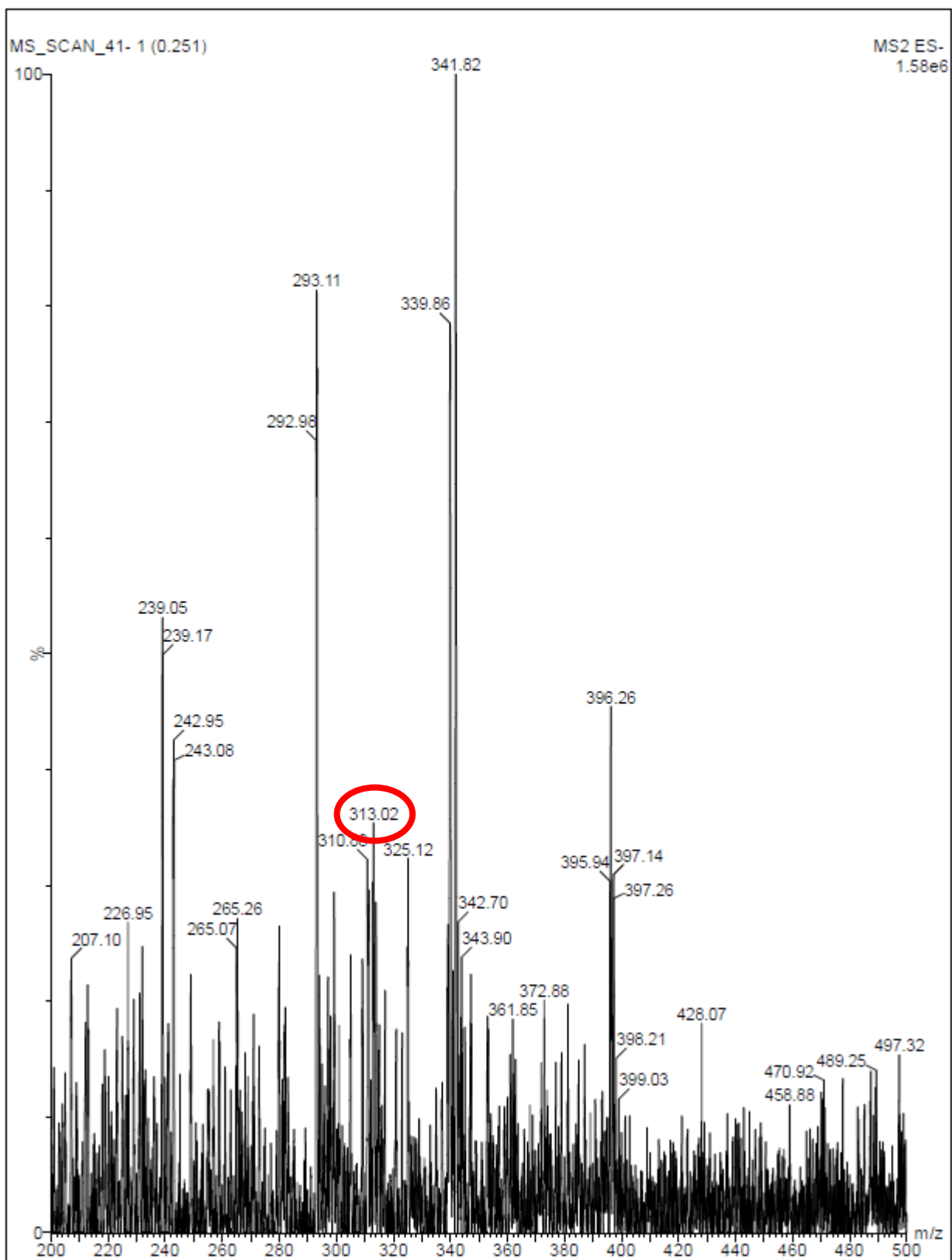


3-amino-5-(3-brombenziliden)-2-tioksotiazolidin-4-on (7I)

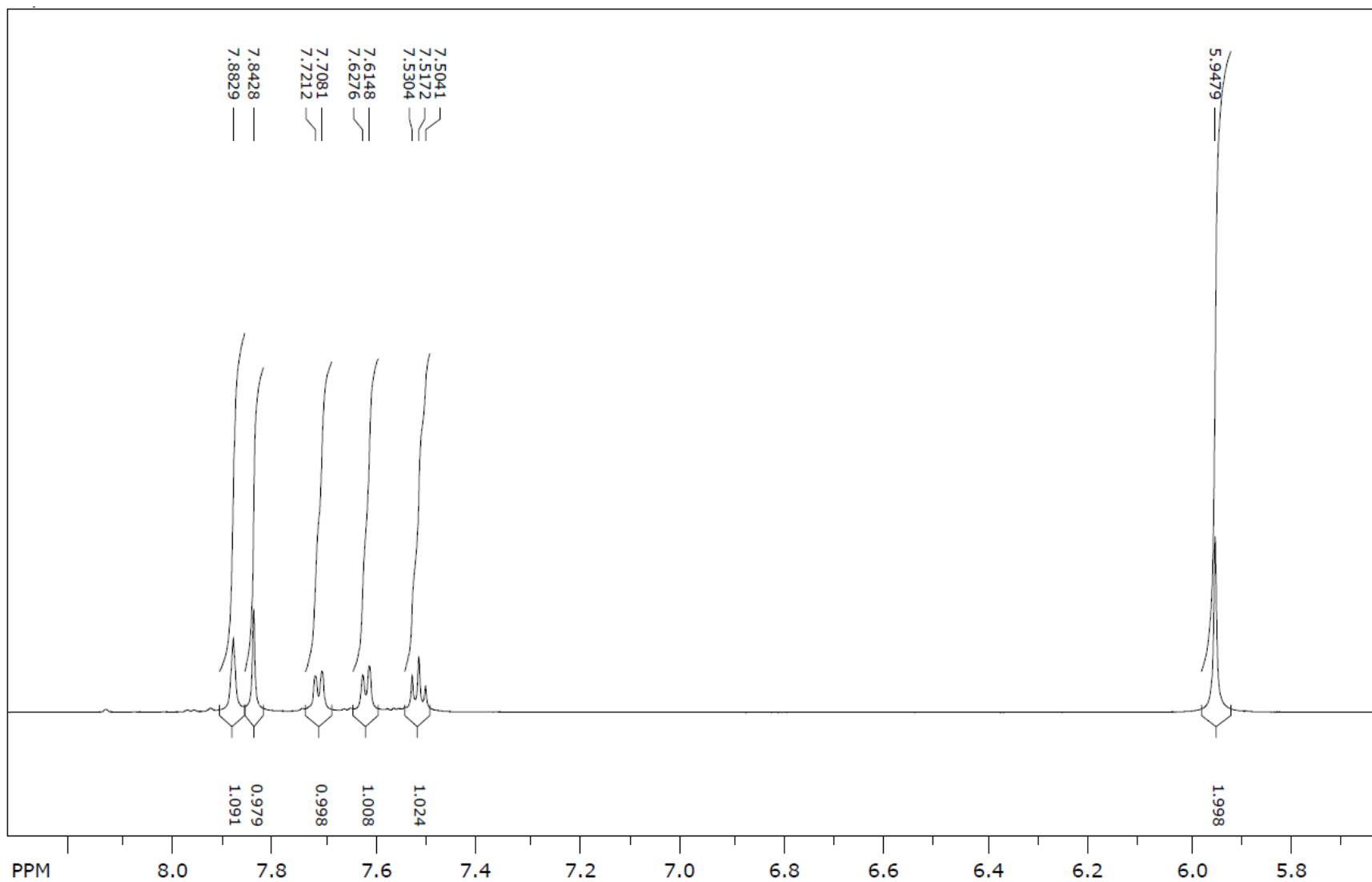


Reaktanti	3-brombenzaldehyd (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	315,21 g/mol
Molekulska formula	C ₁₀ H ₇ BrN ₂ OS ₂
Temperatura tališta	195 - 199 °C
Boja kristala	Žuta
R_f	0,78
LC/MS/MS <i>m/z</i> (M-)	313,02
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,88 (s, 1H, CH), 7,84 (s, 1H, arom.), 7,71 (d, <i>J</i> = 7,86 Hz, 1H, arom.), 7,62 (d, <i>J</i> = 7,68 Hz, 1H, arom.), 7,52 (t, <i>J</i> = 7,89 Hz, 1H, arom.), 5,94 (s, 2H, NH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,50; 163,54; 135,30; 133,40; 133,50; 131,48; 131,45; 128,66; 122,55; 122,04.

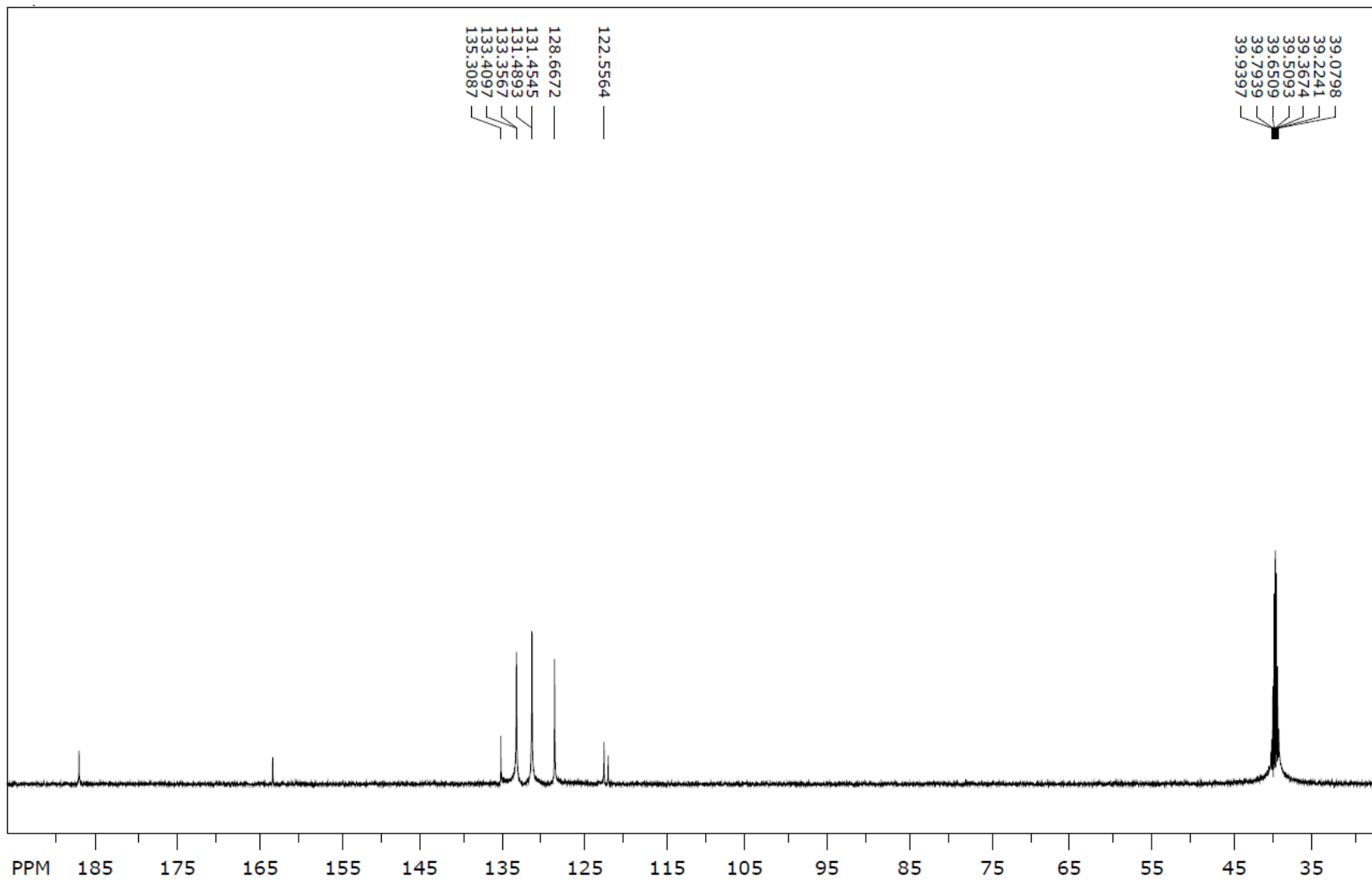
Maseni spektar (7I)



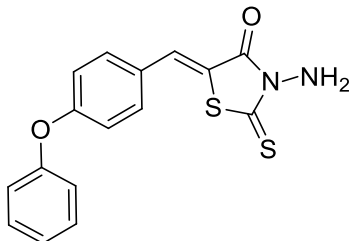
¹H NMR spektr (7I)



¹³C NMR spektr (7I)

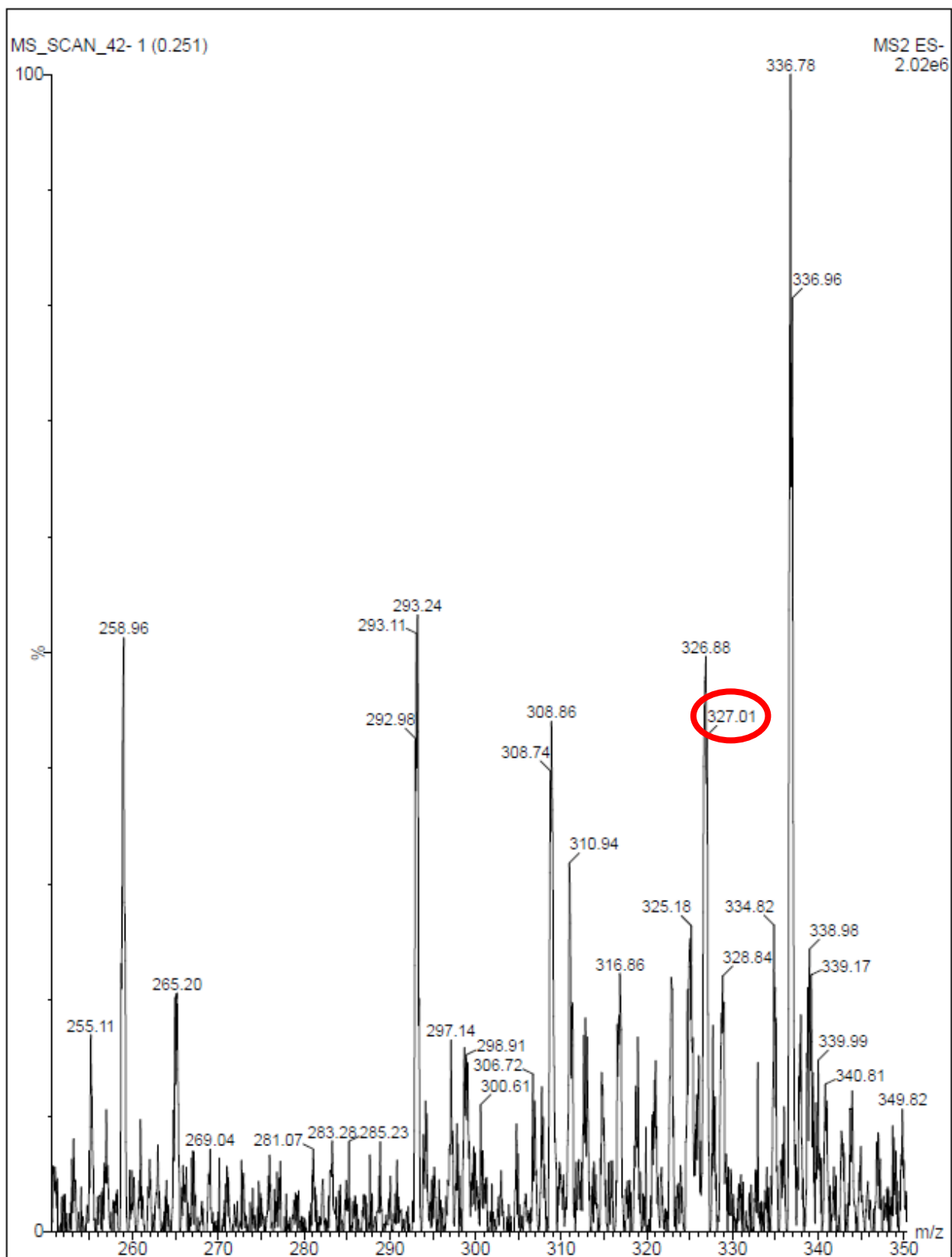


3-amino-5-(4-fenoksibenziliden)-2-tioksotiazolidin-4-on (7m)

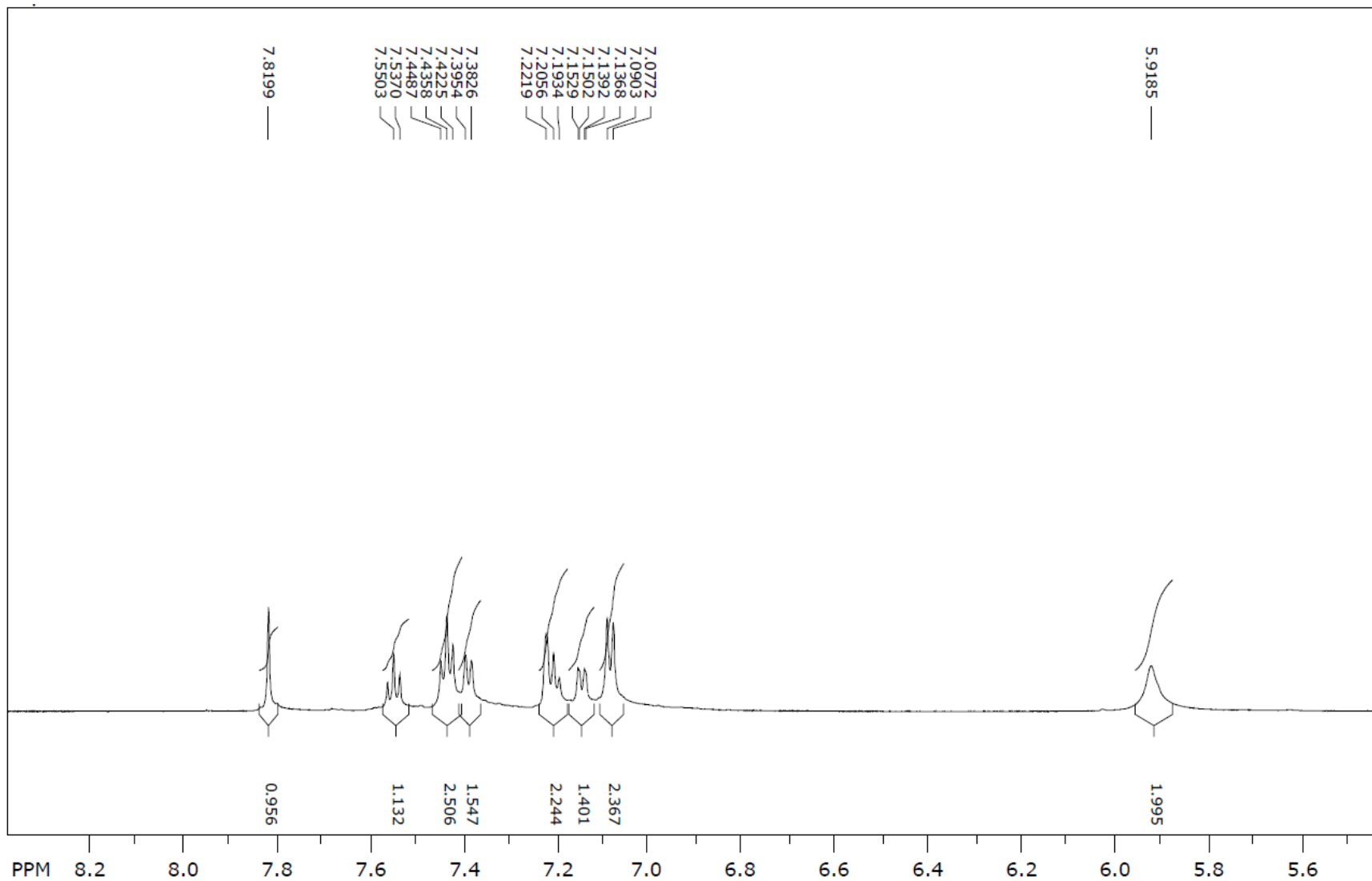


Reaktanti	3-fenoksialdehid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Ispran etanolom
Molekulska masa	328,41 g/mol
Molekulska formula	C ₁₆ H ₁₂ N ₂ O ₂ S ₂
Temperatura tališta	111 °C
Boja kristala	Smeđa
R_f	0,86; 0,80
LC/MS/MS <i>m/z</i> (M-)	327,01
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,82 (s, 1H, CH), 7,55 (t, <i>J</i> = 7,92 Hz, 1H, arom.), 7,44 (t, <i>J</i> = 7,86 Hz, 2H, arom.), 7,39 (d, <i>J</i> = 7,68 Hz, 1H, arom.), 7,21 (t, <i>J</i> = 9,78; 7,32 Hz, 2H, arom.), 7,14 (dd, <i>J</i> = 8,22; 1,53 Hz, 1H, arom.), 7,08 (d, <i>J</i> = 7,86 Hz, 2H, arom.), 5,91 (s, 2H, NH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,49; 163,55; 157,60; 155,74; 134,77; 132,53; 131,19; 130,22; 125,27; 124,17; 121,20; 120,65; 119,58; 119,22.

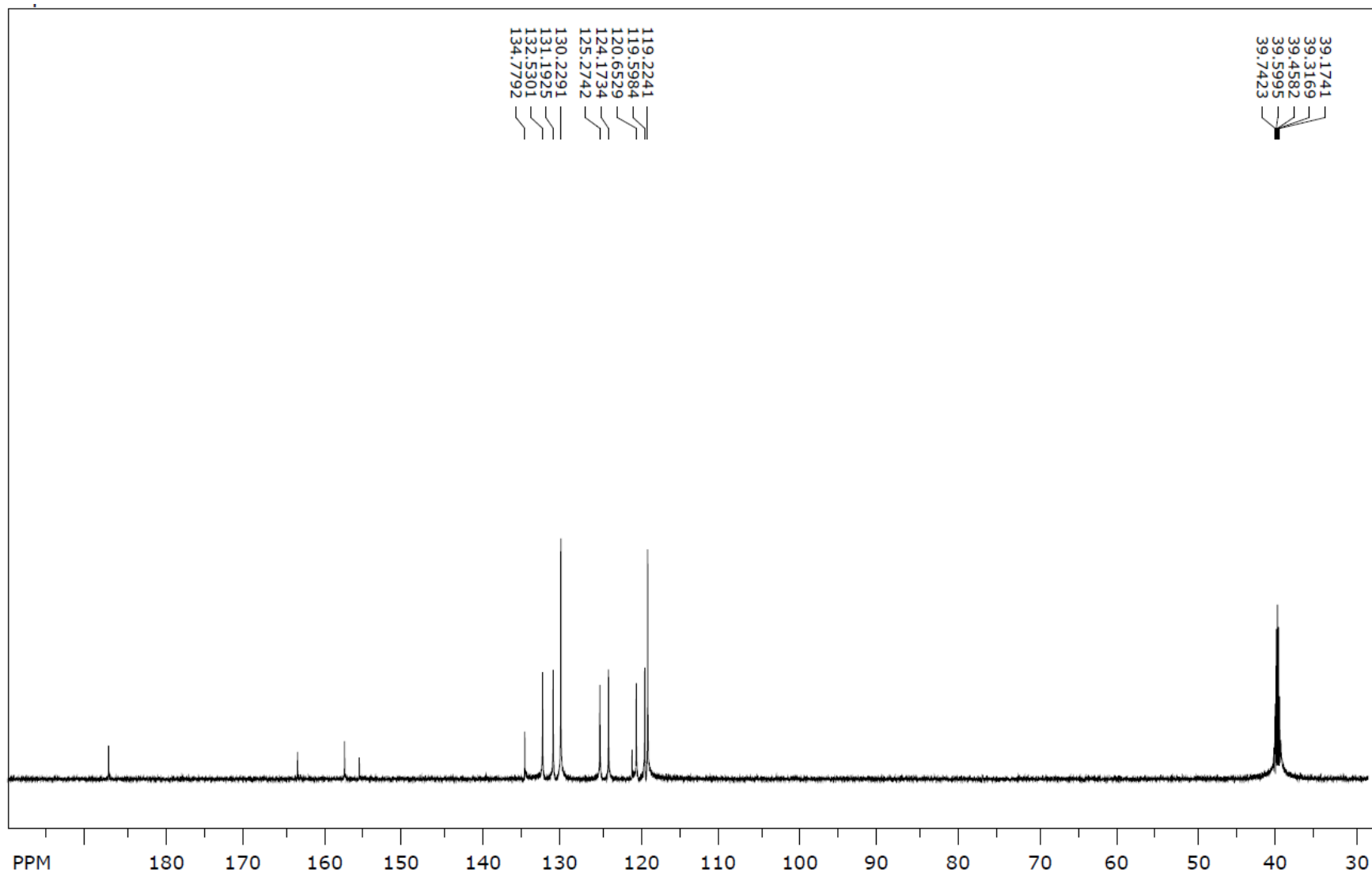
Maseni spektar (7m)



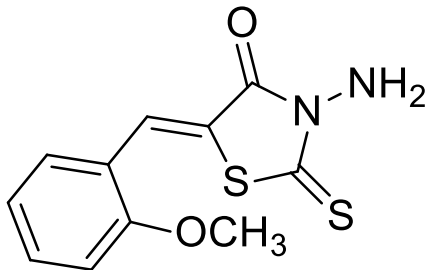
¹H NMR spektr (7m)



¹³C NMR spektr (7m)

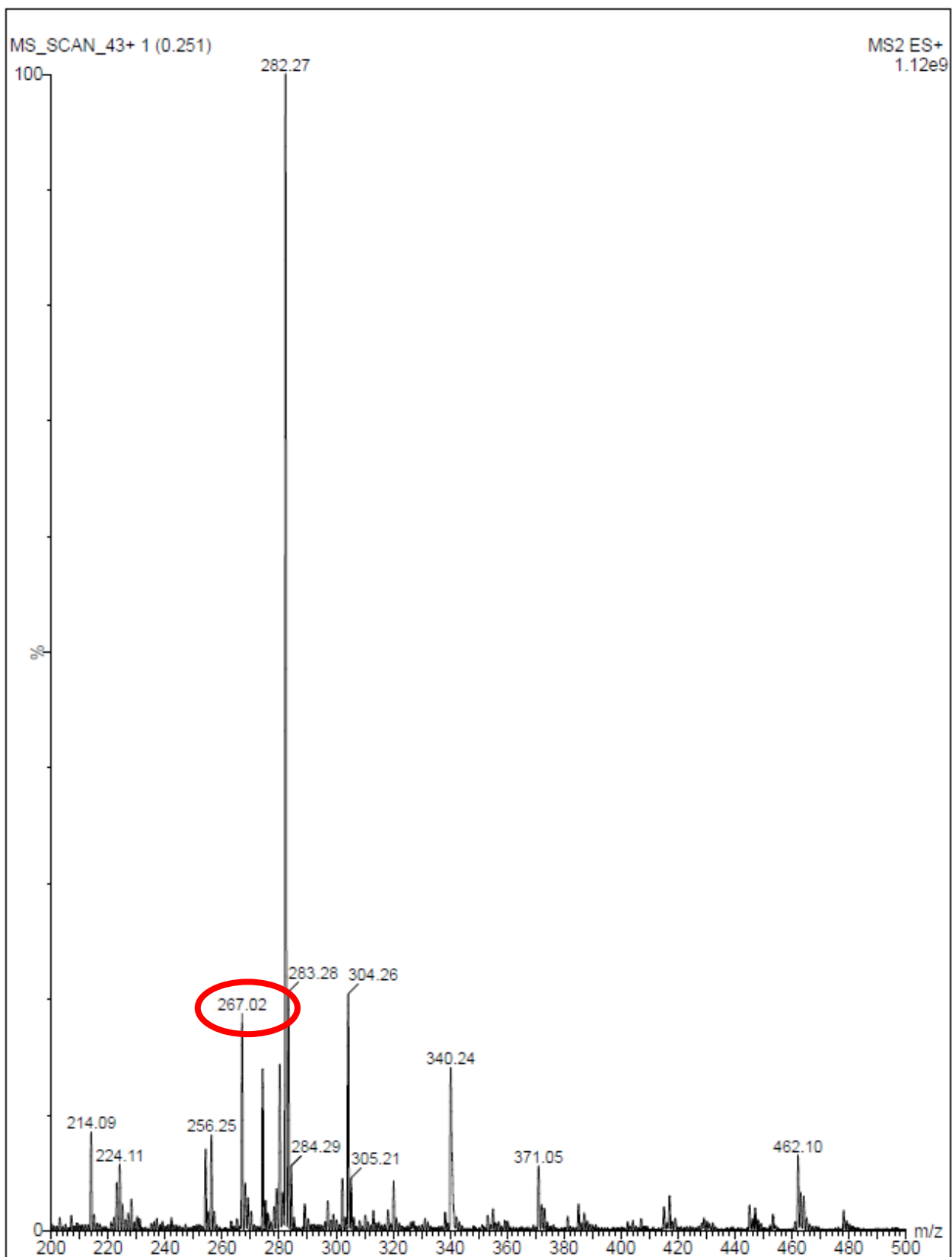


3-amino-5-(2-metoksibenziliden)-2-tioksotiazolidin-4-on (7n)

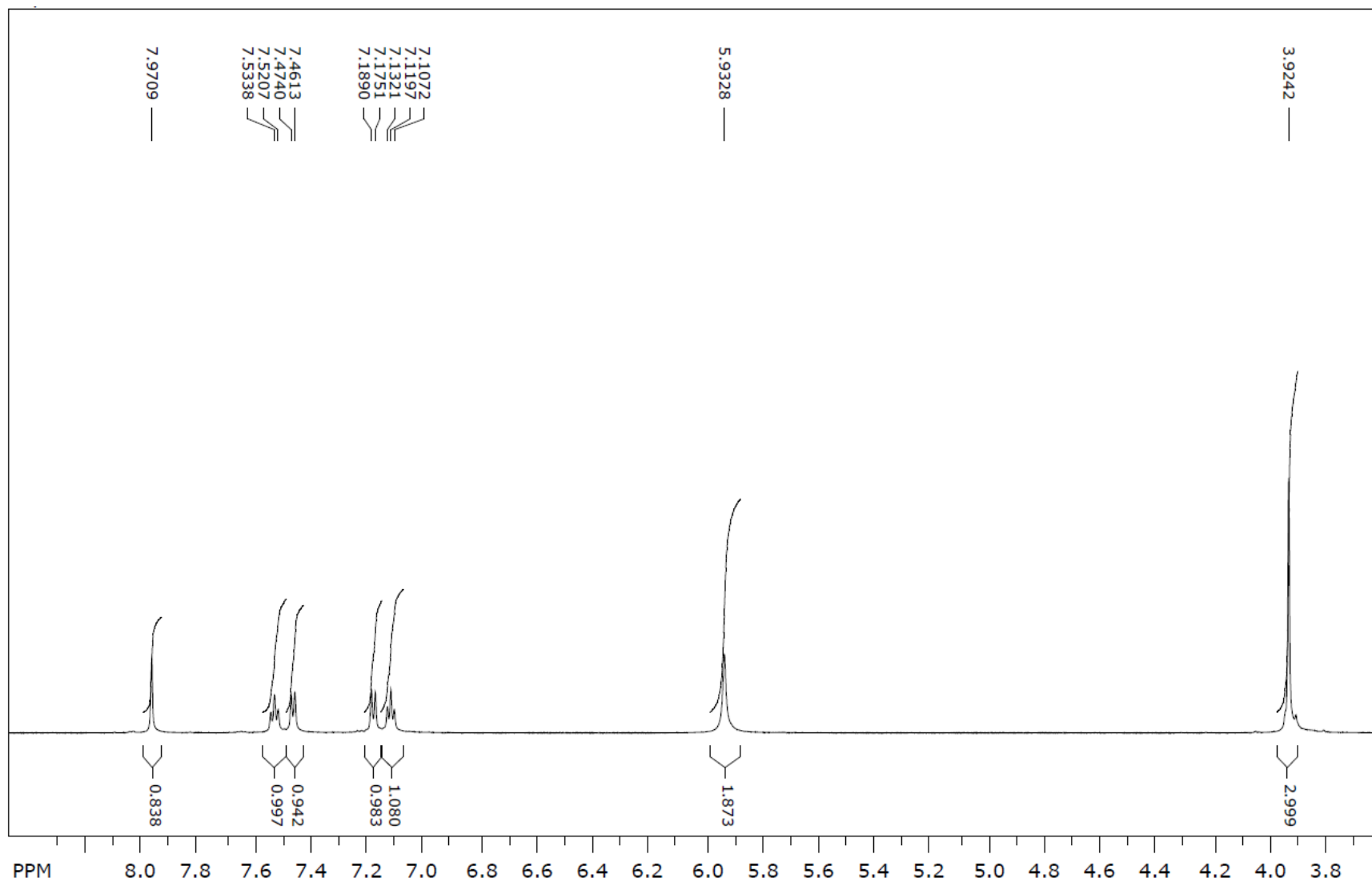


Reaktanti	2-metoksibenzaldehid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	266,34 g/mol
Molekulska formula	C ₁₁ H ₁₀ N ₂ O ₂ S ₂
Temperatura tališta	181 – 184 °C
Boja kristala	Žuto-smeđa
R_f	0,83; 0,78
LC/MS/MS <i>m/z</i> (M⁺)	267,02
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,97 (s, 1H, CH), 7,53 (t, <i>J</i> = 7,80 Hz, 1H, arom.), 7,47 (d, <i>J</i> = 7,62 Hz, 1H, arom.), 7,18 (d, <i>J</i> = 8,34 Hz, 1H, arom.), 7,12 (t, <i>J</i> = 7,47 Hz, 1H, arom.), 5,93 (s, 2H, NH ₂), 3,92 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 188,13; 163,81; 158,13; 133,31; 130,22; 128,55; 121,25; 120,13; 112,06; 55,78.

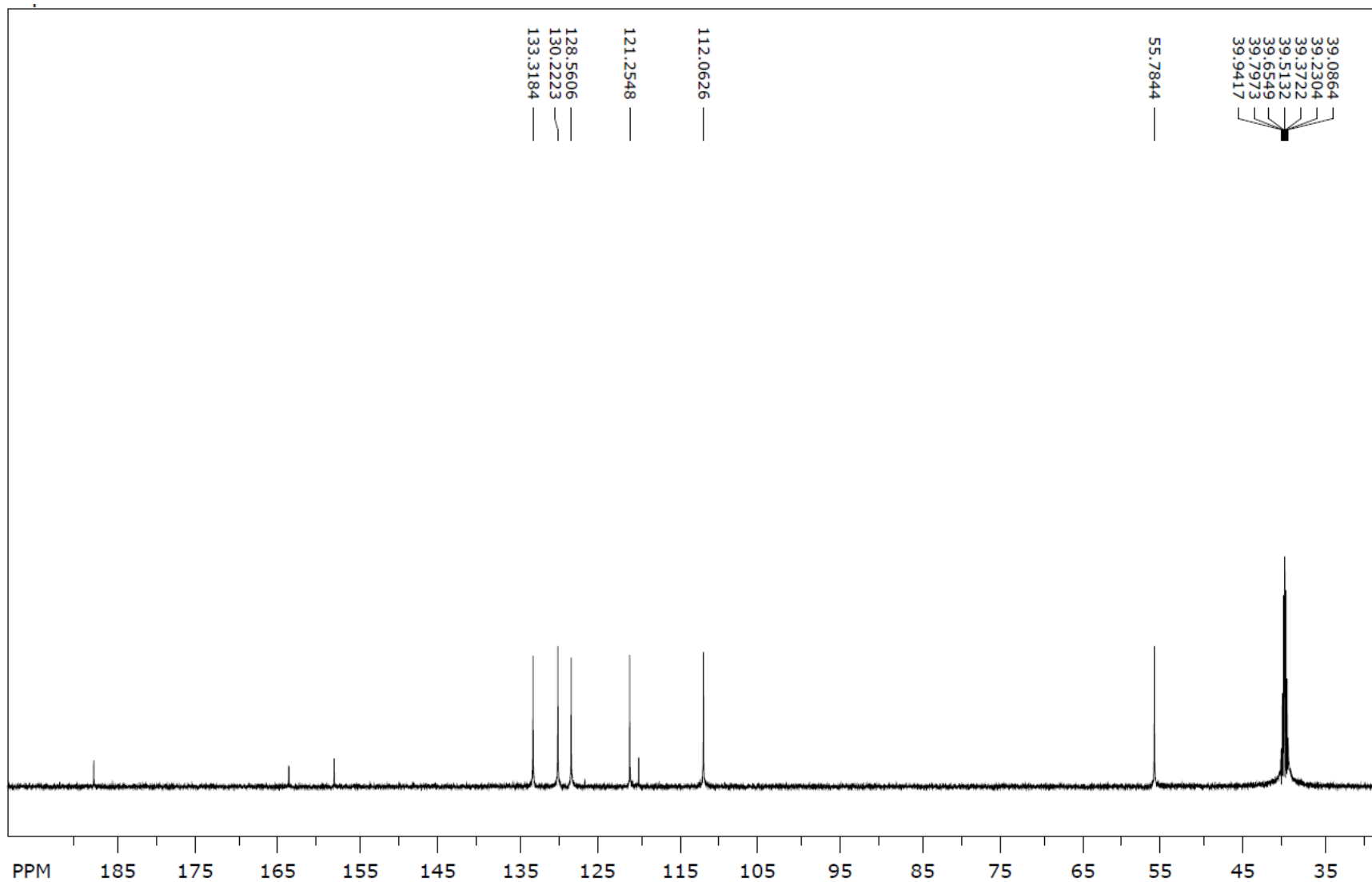
Maseni spektr (7n)



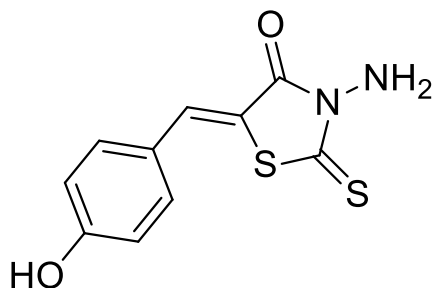
¹H NMR spektr (7n)



¹³C NMR spektr (7n)

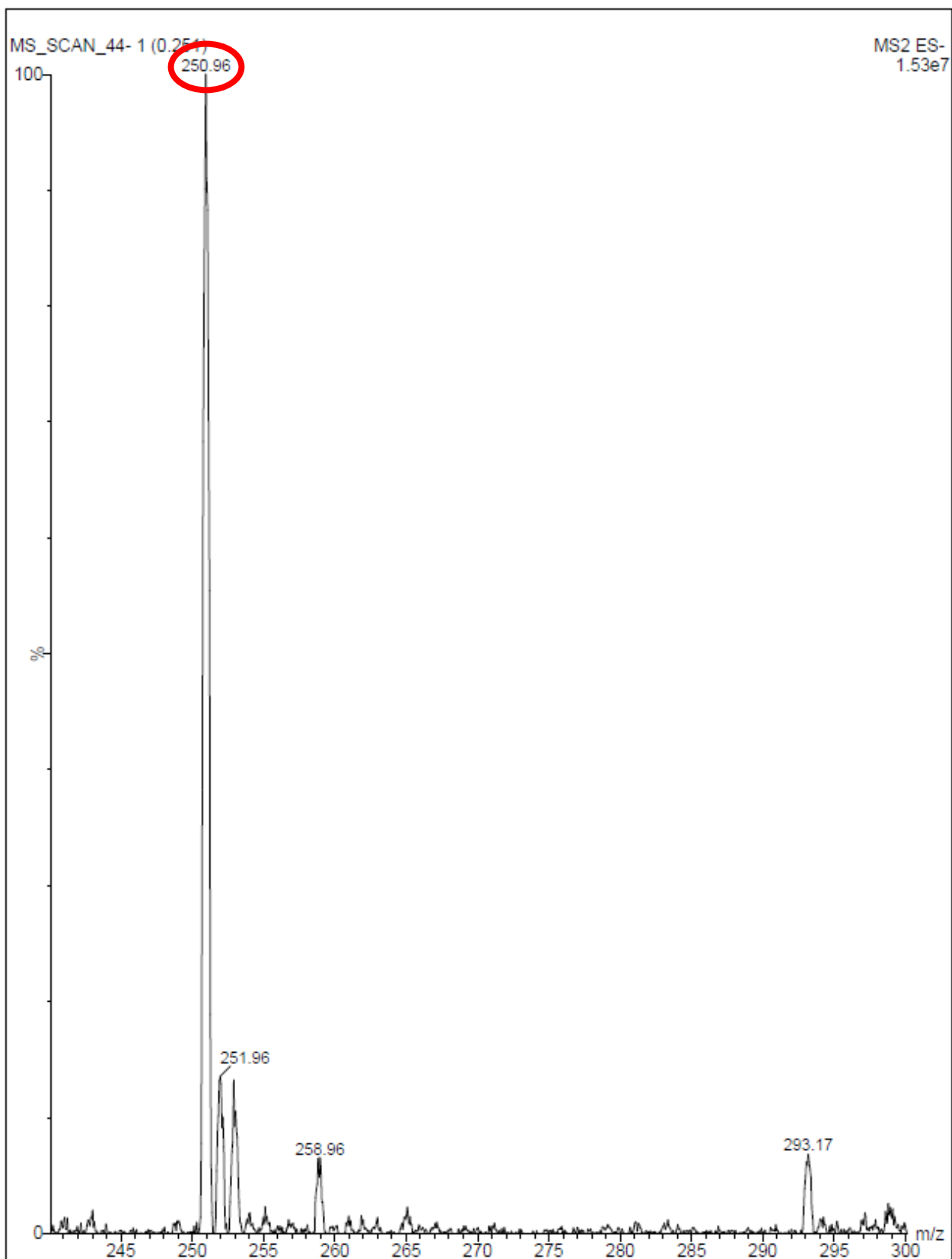


3-amino-5-(4-hidroksibenziliden)-2-tioksotiazolidin-4-on (7o)

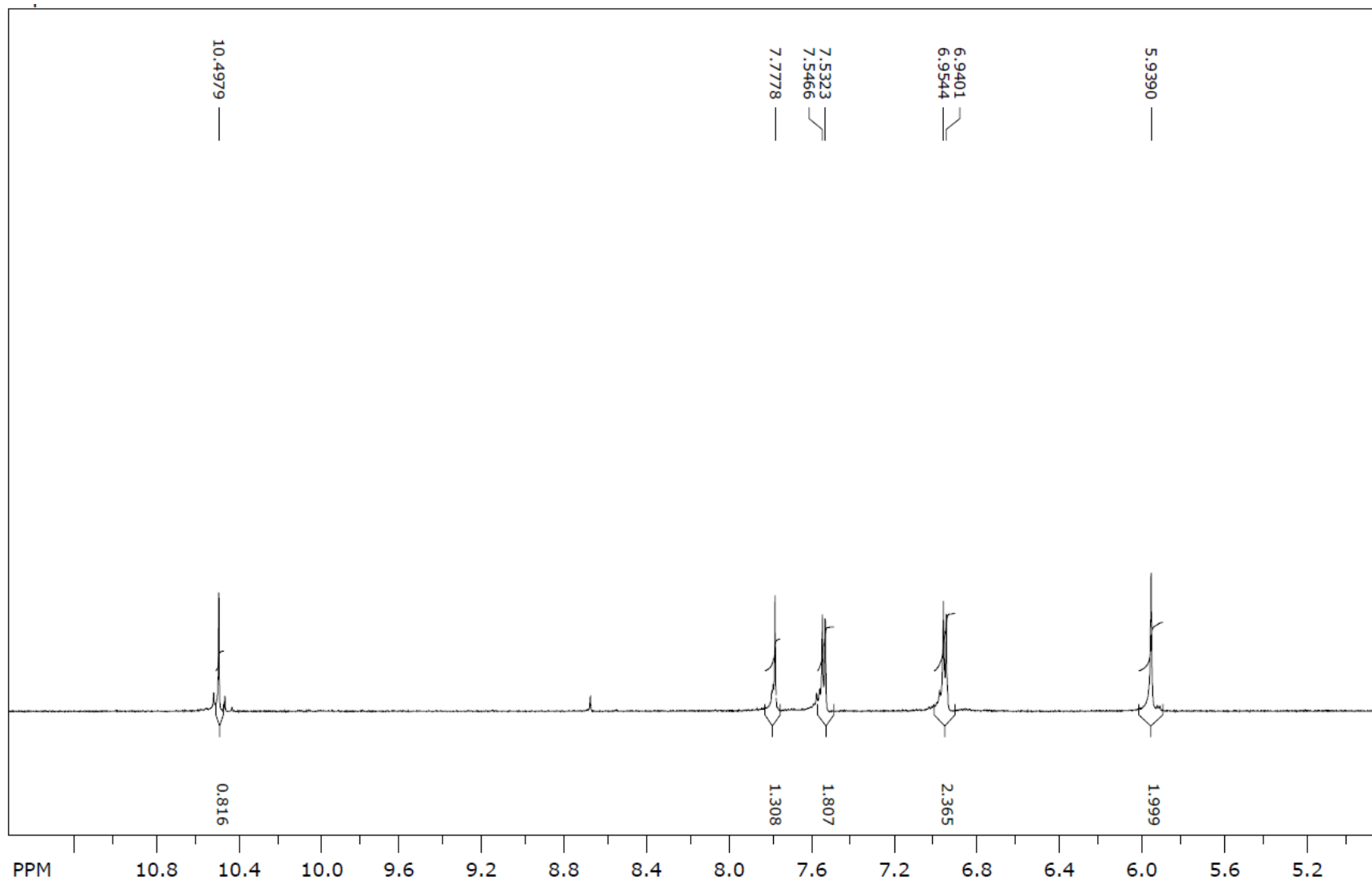


Reaktanti	4-hidroksibenzaldehid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Ispran etanolom
Molekulska masa	252,31 g/mol
Molekulska formula	C ₁₀ H ₈ N ₂ O ₂ S ₂
Temperatura tališta	262 – 264 °C
Boja kristala	Smeđa
R_f	0,66; 0,54
LC/MS/MS <i>m/z</i> (M-)	250,56
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 10,49 (s, 1H, OH), 7,77 (s, 1H, CH), 7,54 (d, <i>J</i> = 8,58 Hz, 2H, arom.), 6,95 (d, <i>J</i> = 8,58 Hz, 2H, arom.), 5,93 (s, 2H, NH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,09; 163,77; 160,65; 134,13; 133,42; 124,03; 116,59; 115,54.

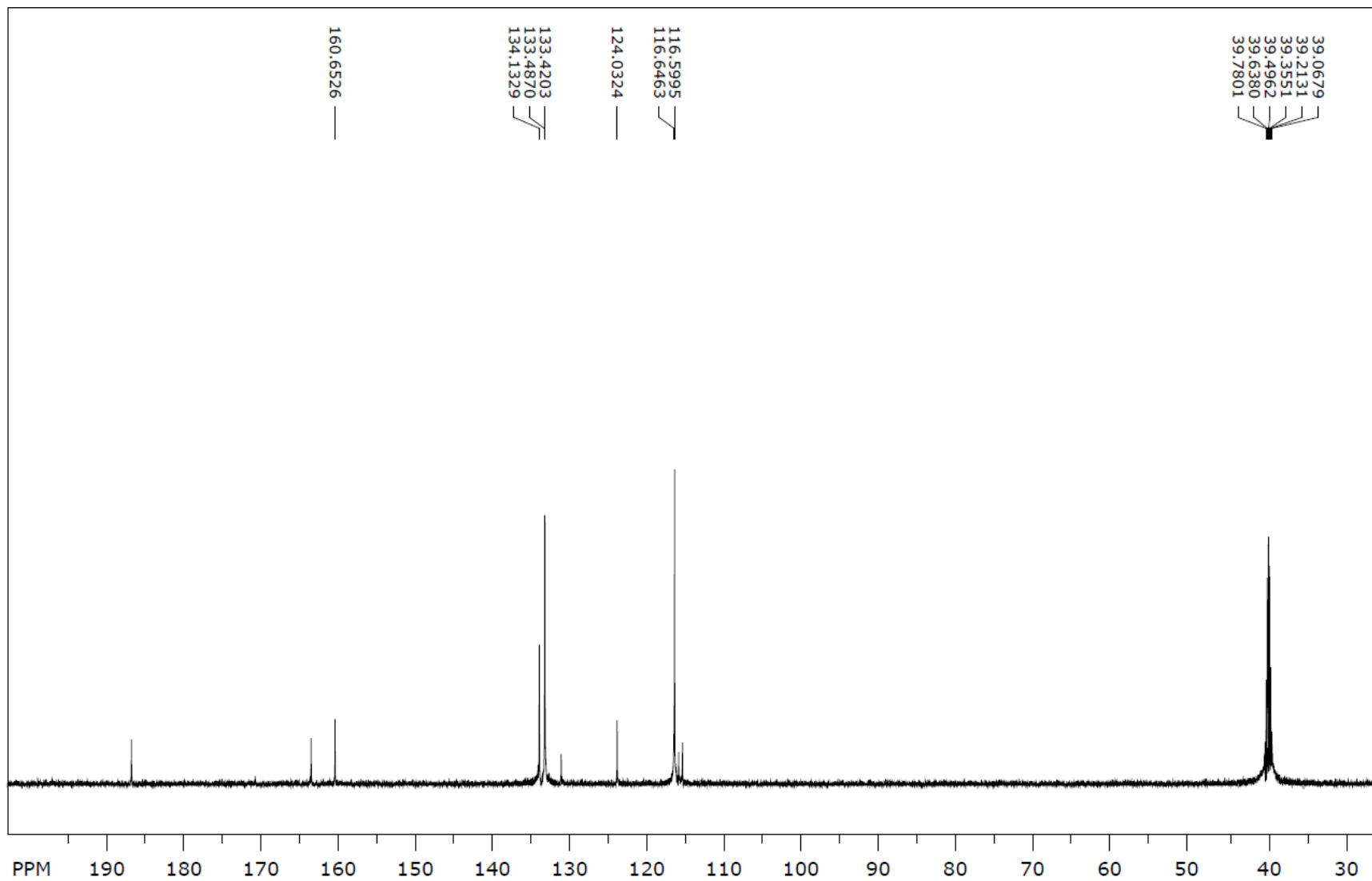
Maseni spektar (7o)



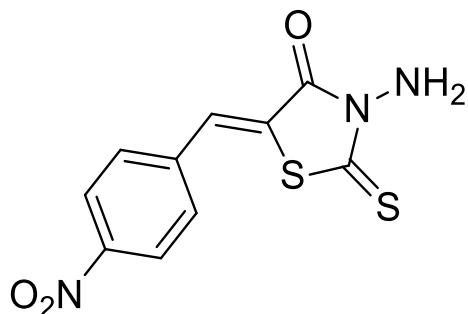
¹H NMR spektr (7o)



¹³C NMR spektr (7o)

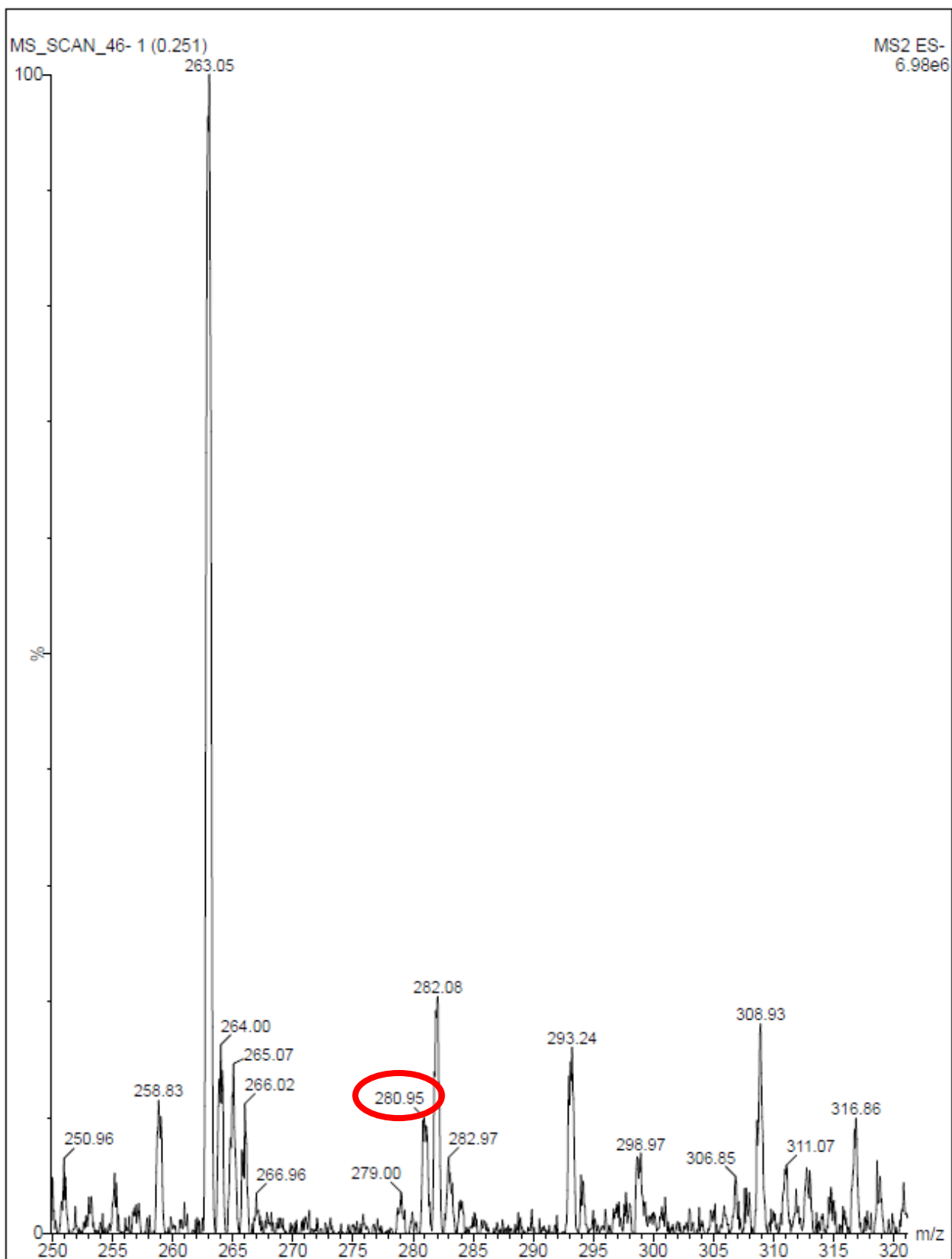


3-amino-5-(4-nitrobenziliden)-2-tioksotiazolidin-4-on (7p)

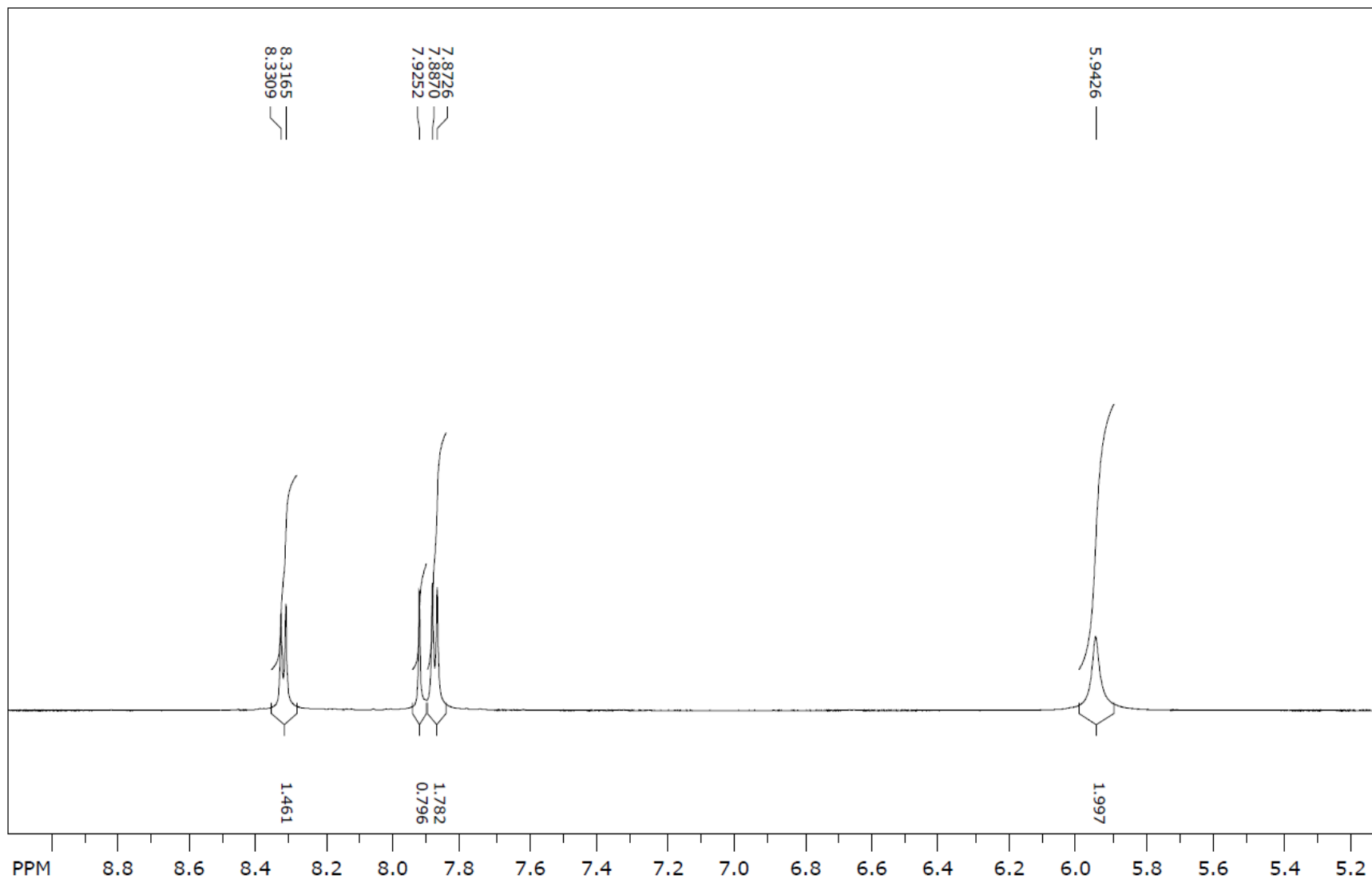


Reaktanti	4-nitrobenzalhid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	281,31 g/mol
Molekulska formula	C ₁₀ H ₇ N ₃ O ₃ S ₂
Temperatura tališta	234 – 238 °C
Boja kristala	Smeđa
R_f	0,84; 0,74
LC/MS/MS m/z (M-)	280,95
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,32 (d, <i>J</i> = 8,64 Hz, 2H, arom.), 7,92 (s, 1H, CH), 7,88 (d, <i>J</i> = 8,64 Hz, 2H, arom.), 5,94 (s, 2H, NH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,48; 163,53; 147,61; 139,02; 131,51; 130,25; 124,64; 124,33.

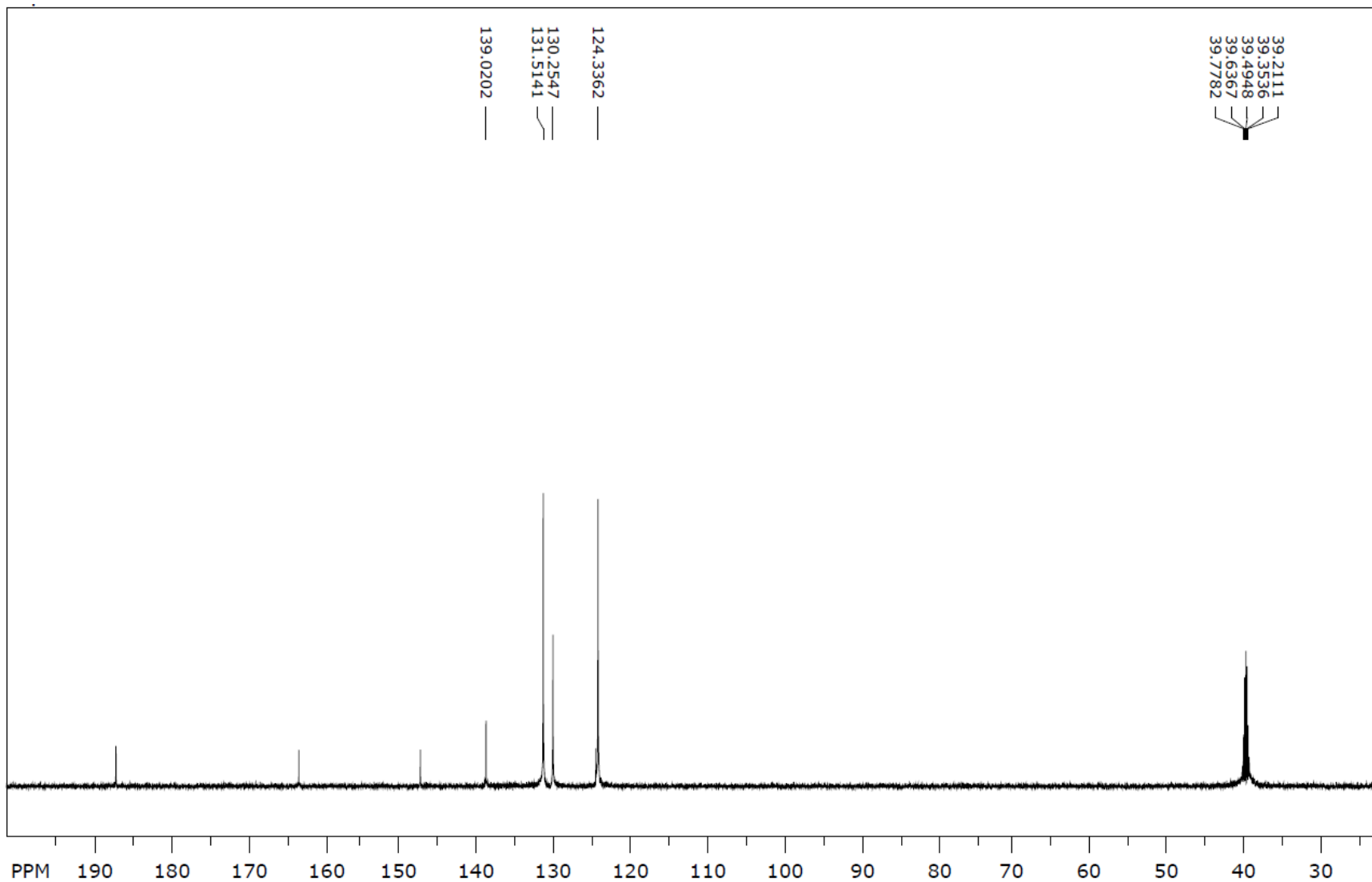
Masni spektar (7p)



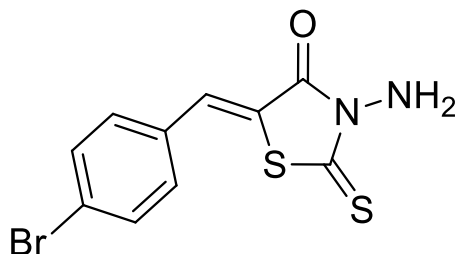
¹H NMR spektr (7p)



¹³C NMR spektr (7p)

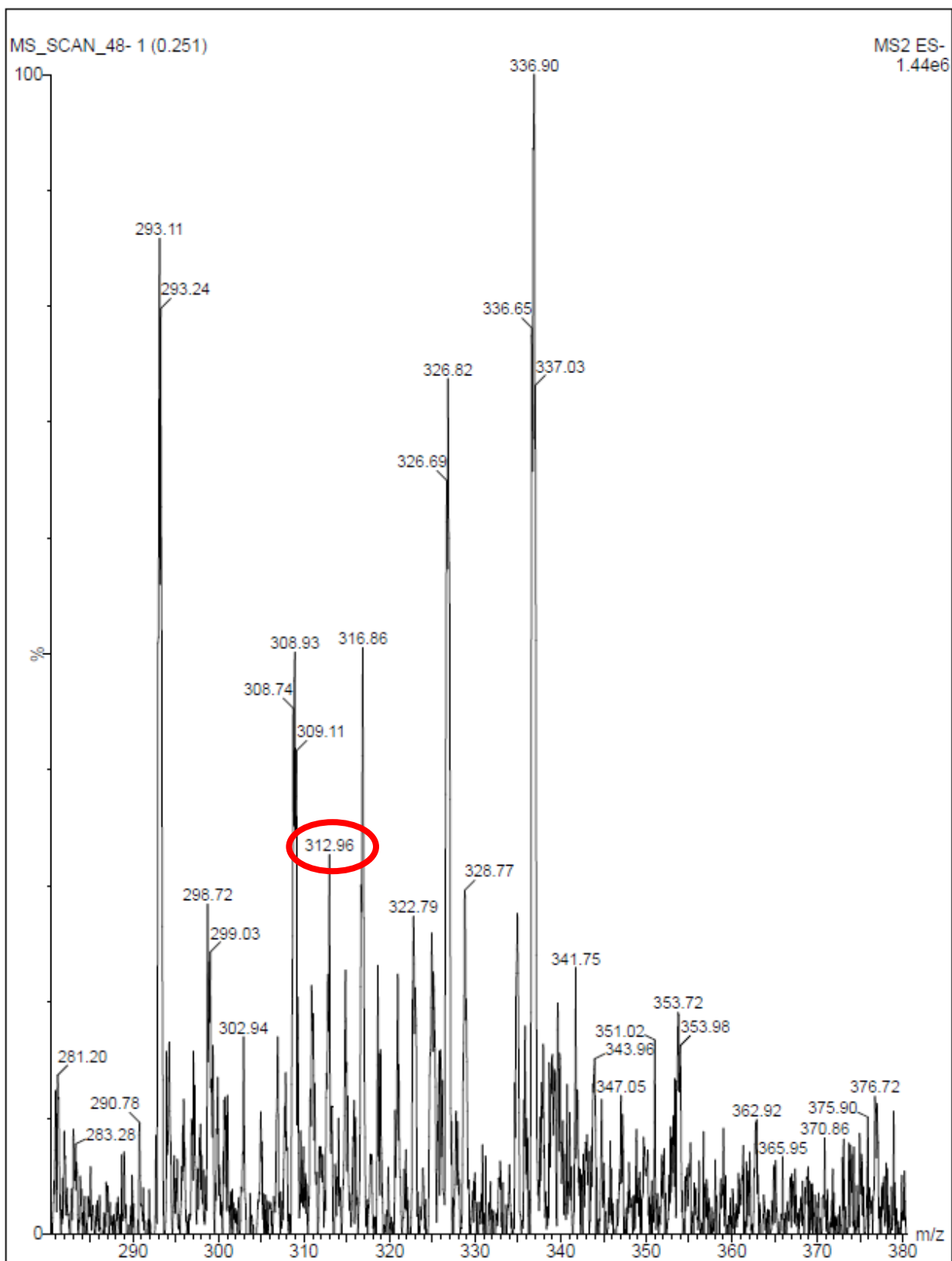


3-amino-5-(4-brombenziliden)-2-tioksotiazolidin-4-on (7q)

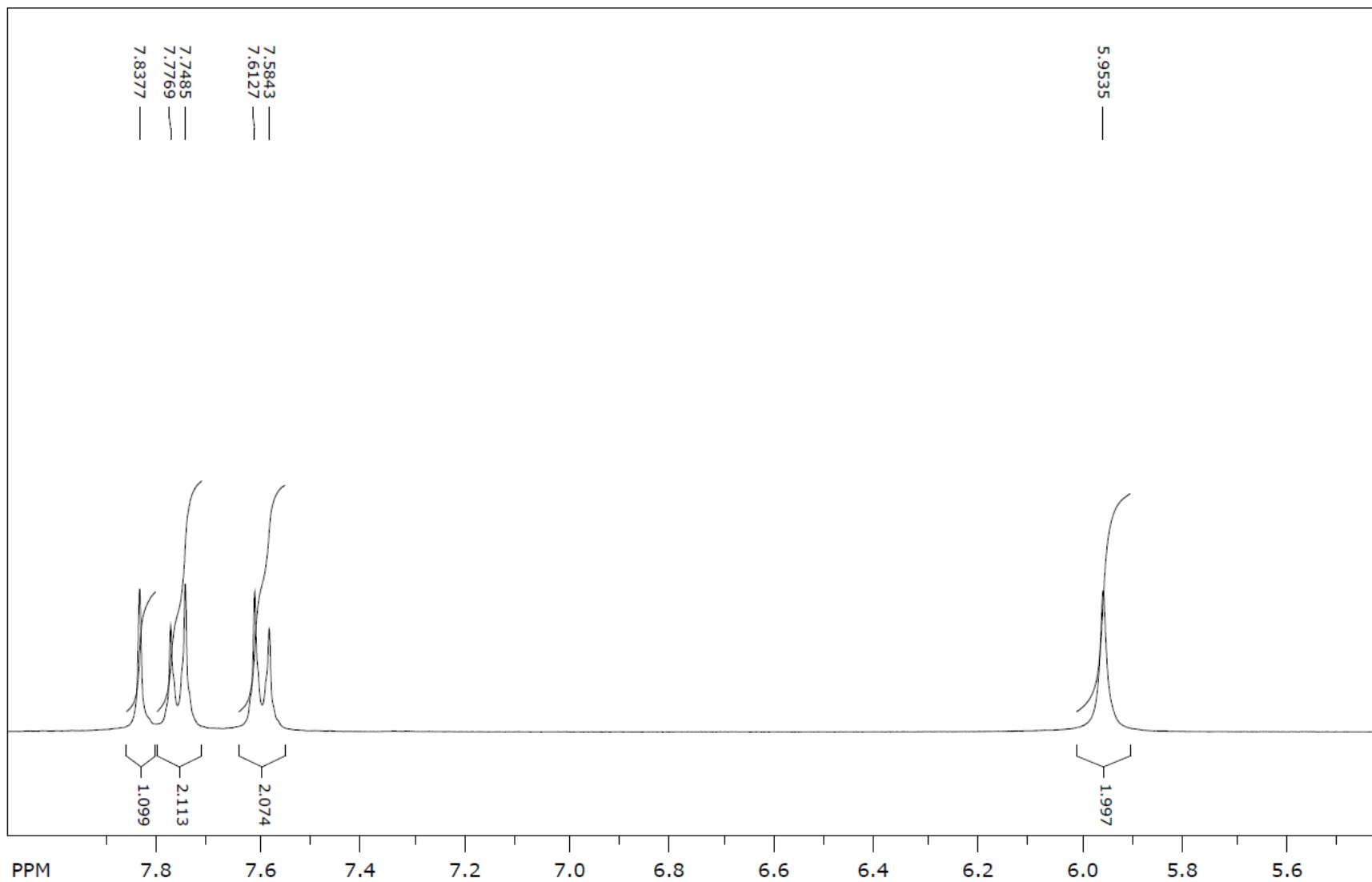


Reaktanti	4-brombenzalhid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Ispran etanolom
Molekulska masa	315,21 g/mol
Molekulska formula	C ₁₀ H ₇ BrN ₂ OS ₂
Temperatura tališta	227 – 229 °C
Boja kristala	Svijetlosmeđa
R_f	0,85; 0,79
LC/MS/MS <i>m/z</i> (M⁻)	312,96
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 7,83 (s, 1H, CH), 7,76 (d, <i>J</i> = 8,52 Hz, 2H, arom.), 7,60 (d, <i>J</i> = 8,52 Hz, 2H, arom.), 5,95 (s, 2H, NH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,95; 164,15; 132,98; 132,91; 132,46; 125,13; 121,58.

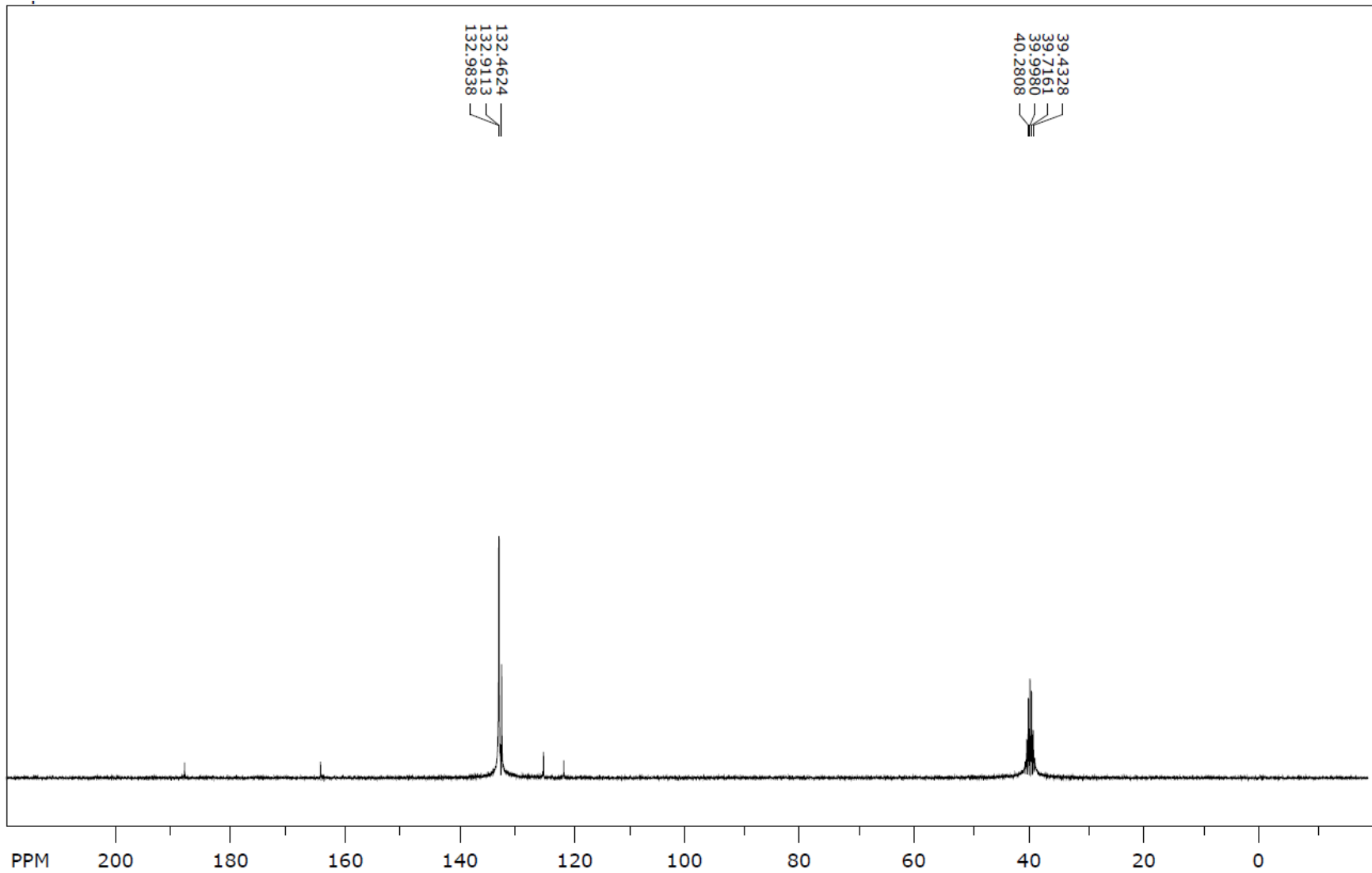
Maseni spektar (7q)



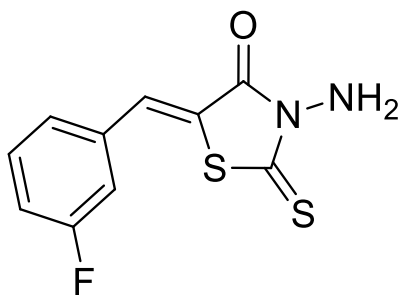
¹H NMR spektr (7q)



¹³C NMR spektr (7q)

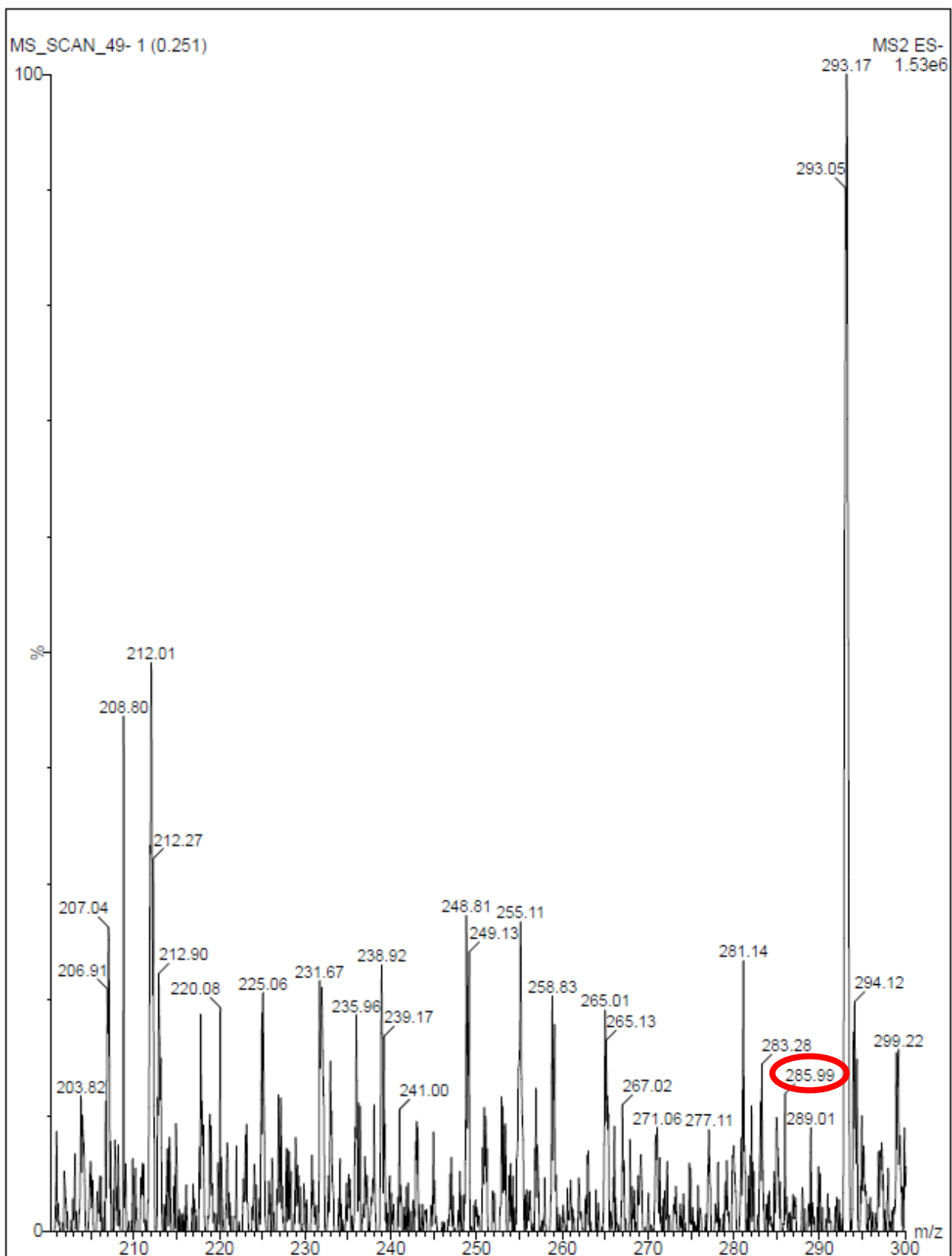


3-amino-5-(3-fluorbenziliden)-2-tioksotiazolidin-4-on (7r)

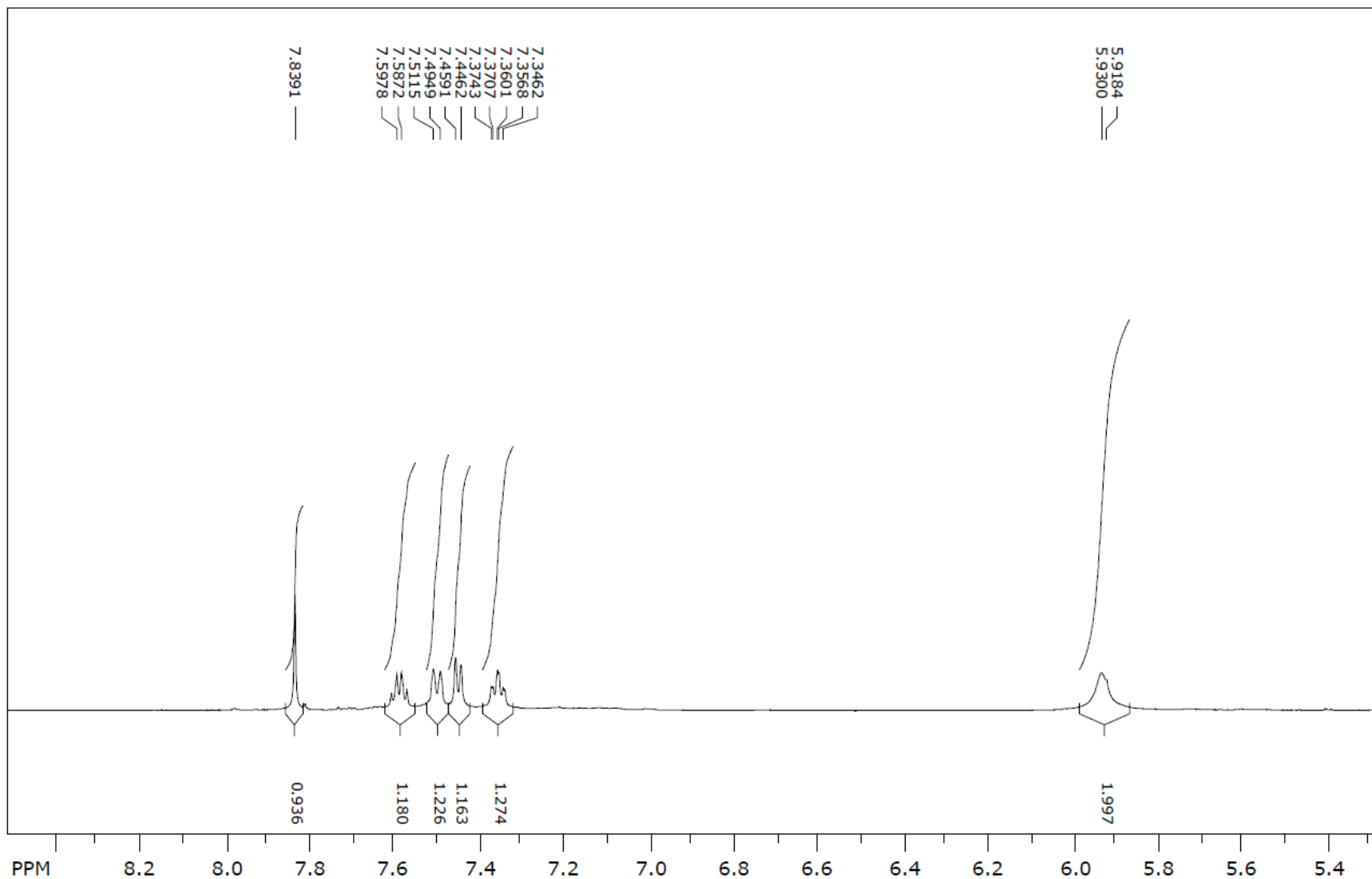


Reaktanti	3-fluorbenzalhid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročiščavanja	Ispran etanolom
Molekulska masa	254,30 g/mol
Molekulska formula	C ₁₀ H ₇ FN ₂ OS ₂
Temperatura tališta	169 – 171 °C
Boja kristala	Smeđa
R_f	0,85; 0,76
LC/MS/MS <i>m/z</i> (M-+MeOH)	285,99
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,83 (s, 1H, CH), 7,59 (q, <i>J</i> = 7,83; 6,36 Hz, 1H, arom.), 7,50 (d, <i>J</i> = 9,96 Hz, 1H, arom.), 7,45 (d, <i>J</i> = 7,74 Hz, 1H, arom.), 7,36 (ddd, <i>J</i> = 2,16; 8,52; 8,28 Hz, 1H, arom.), 5,93 (s, 2H, NH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,58; 131,71; 131,52; 126,13; 126,11; 117; 78; 117,64; 117,42; 117,27.

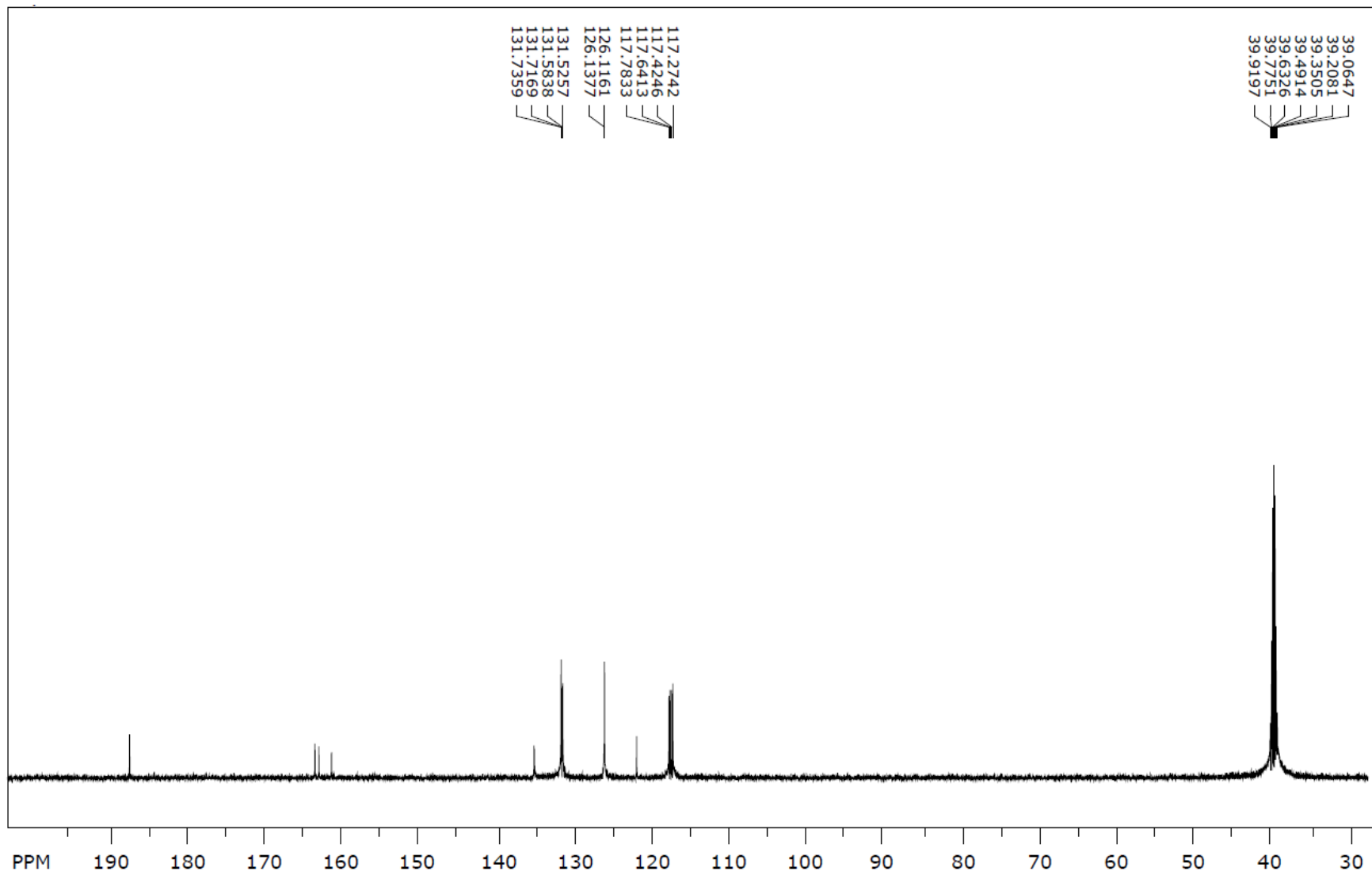
Maseni spektar (7r)



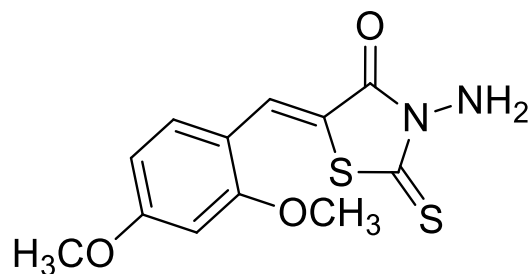
¹H NMR spektr (7r)



¹³C NMR spektr (7r)

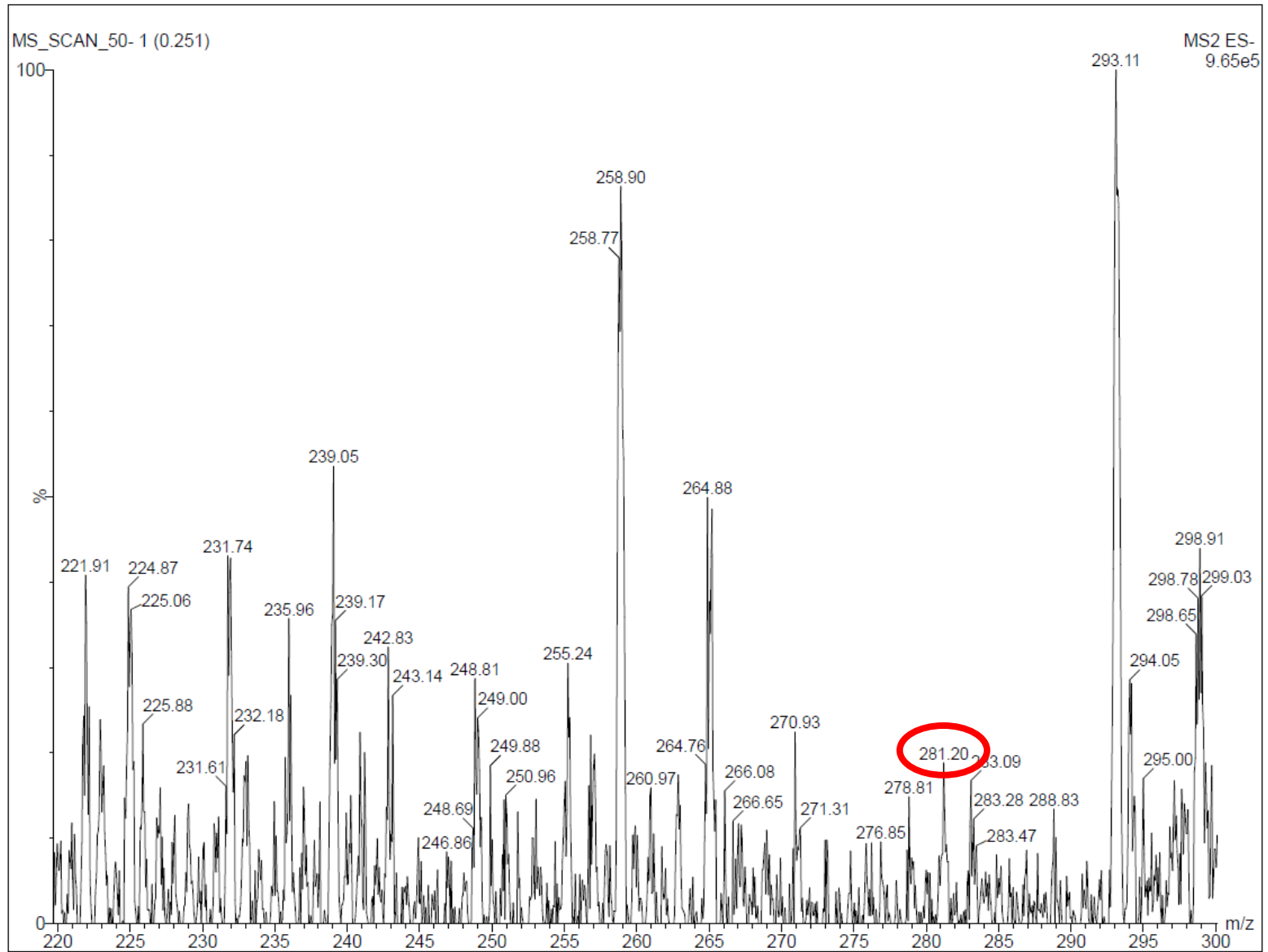


3-amino-5-(2,4-dimetoksibenziliden)-2-tioksotiazolidin-4-on (7s)

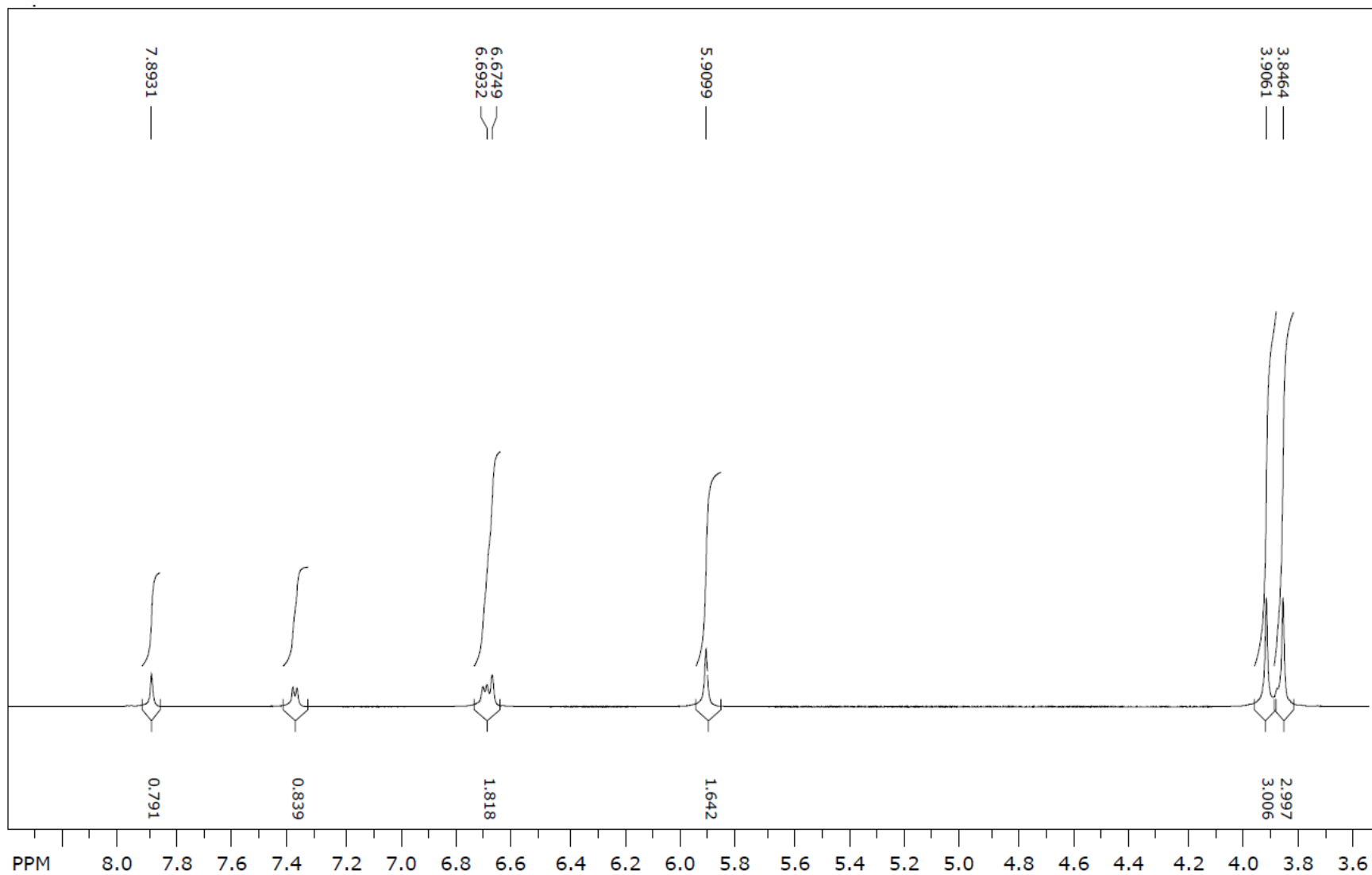


Reaktanti	2,4-dimetoksibenzaldehid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	282,34 g/mol
Molekulska formula	C ₁₂ H ₁₂ N ₂ O ₃ S ₂
Temperatura tališta	194 – 196 °C
Boja kristala	Smeđa
R_f	0,80
LC/MS/MS <i>m/z</i> (M⁻)	281,20
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,89 (s, 1H, CH), 7,38 (d, <i>J</i> = 8,46 Hz, 1H, arom.), 6,69 (t, <i>J</i> = 8,58; 10,98 Hz, 2H, arom.), 5,90 (s, 2H, NH ₂), 3,90 (s, 3H, OCH ₃), 3,84 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,51; 163,94; 163,87; 160,09; 132,10; 128,86; 116,28; 114,32; 107,06; 98,61; 55,92; 55,76.

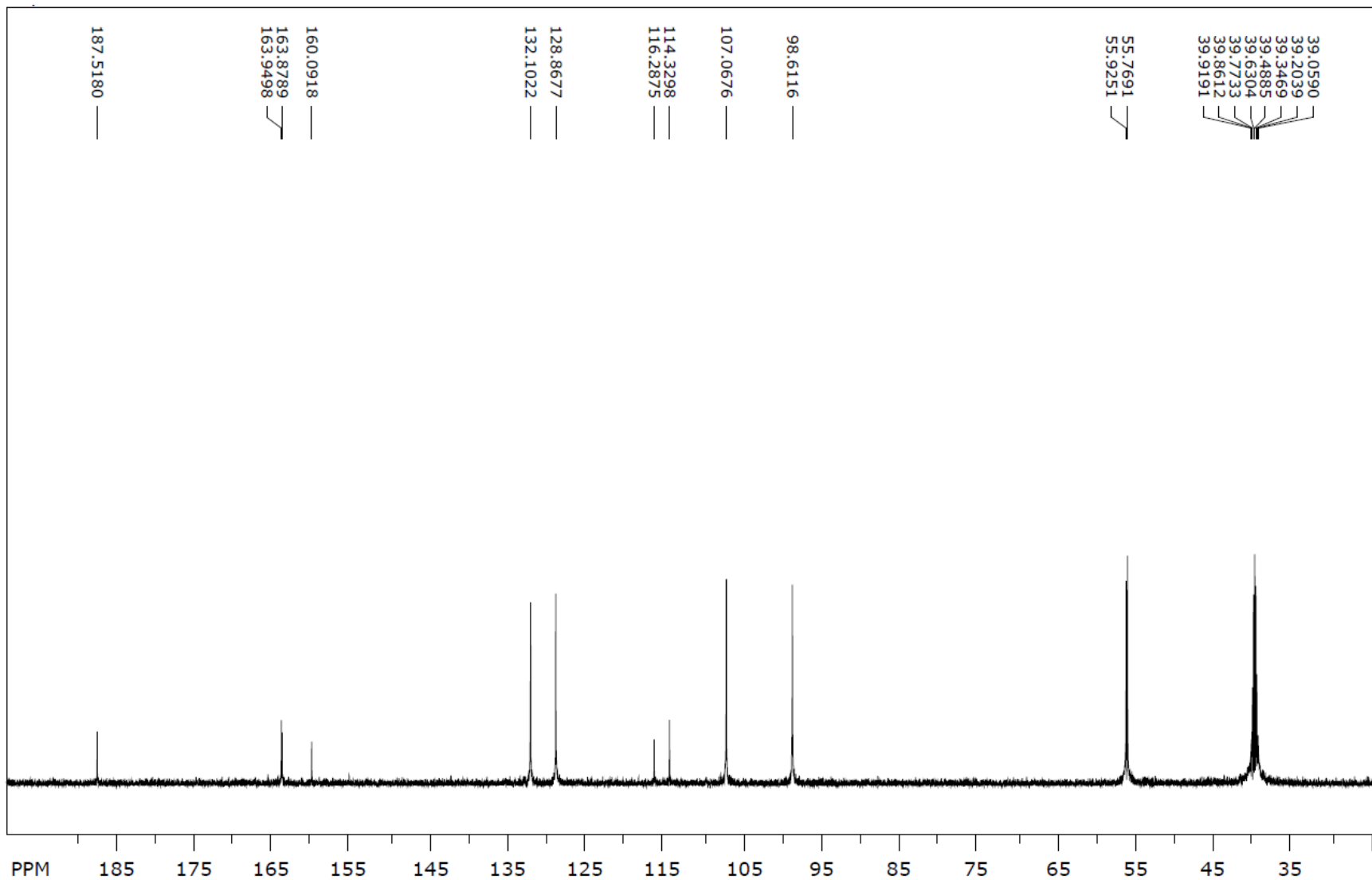
Maseni spektr (7s)



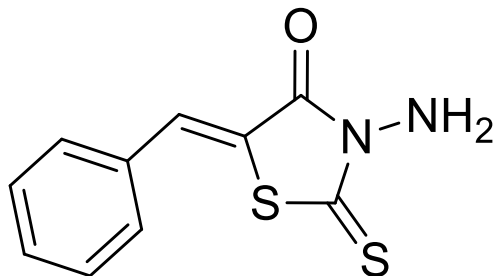
¹H NMR spektr (7s)



¹³C NMR spektr (7s)

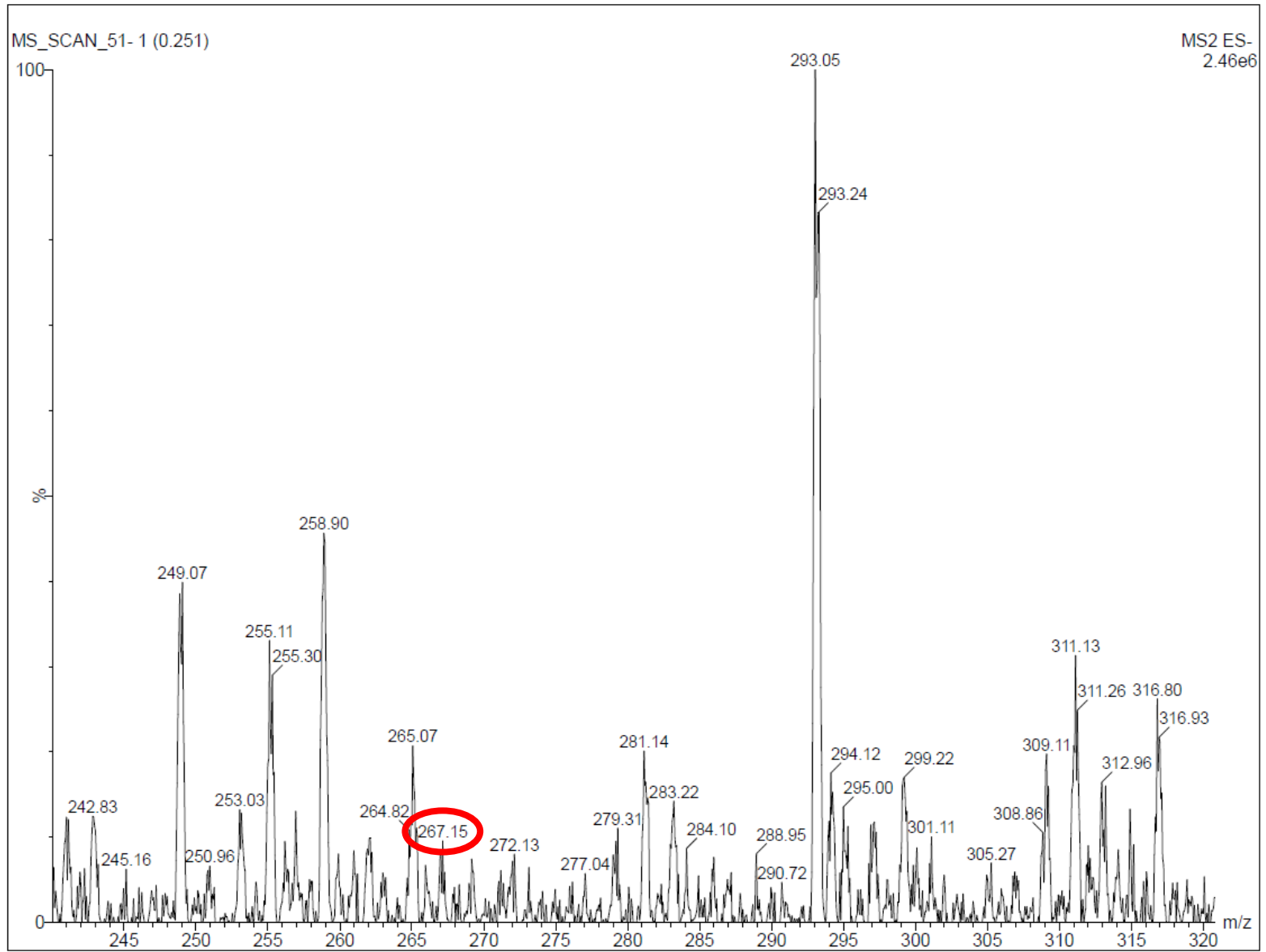


3-amino-5-benziliden-2-tioksotiazolidin-4-on (7t)

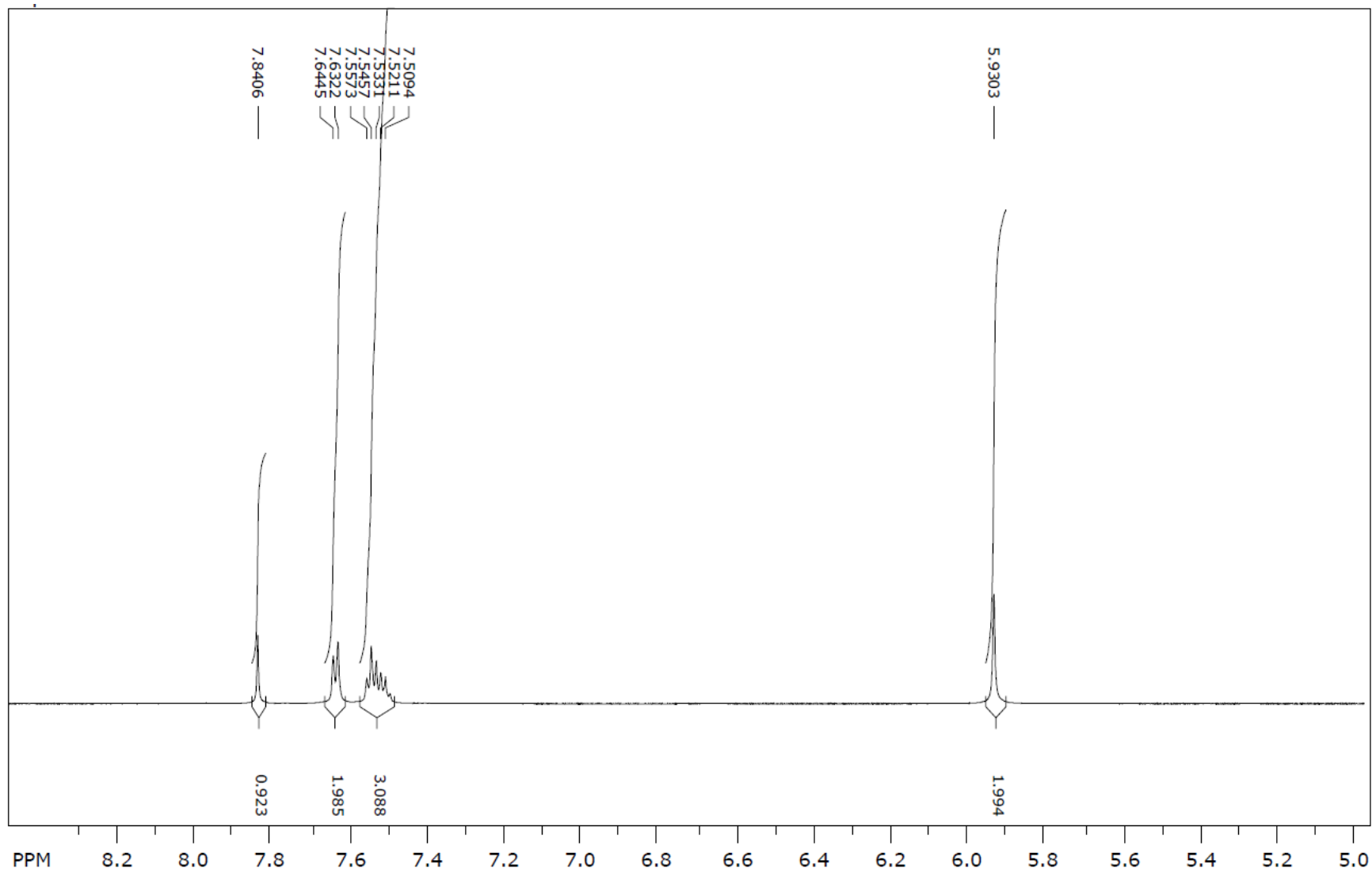


Reaktanti	Benzaldehid (1 mmol) i 3-aminorodanin (1 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	268,31 g/mol
Molekulska formula	C ₁₀ H ₈ N ₂ OS ₂
Temperatura tališta	199 – 201 °C
Boja kristala	Smeđa
R_f	0,84; 0,78
LC/MS/MS <i>m/z</i> (M-)	267,15
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,84 (s, 1H, CH), 7,64 (d, <i>J</i> = 7,38 Hz, 2H, arom.), 7,51 – 7,56 (m, 3H, arom.), 5,93 (s, 2H, NH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 187,71; 163,68; 133,31; 132,94; 130,99; 130,70; 129,48; 120,26.

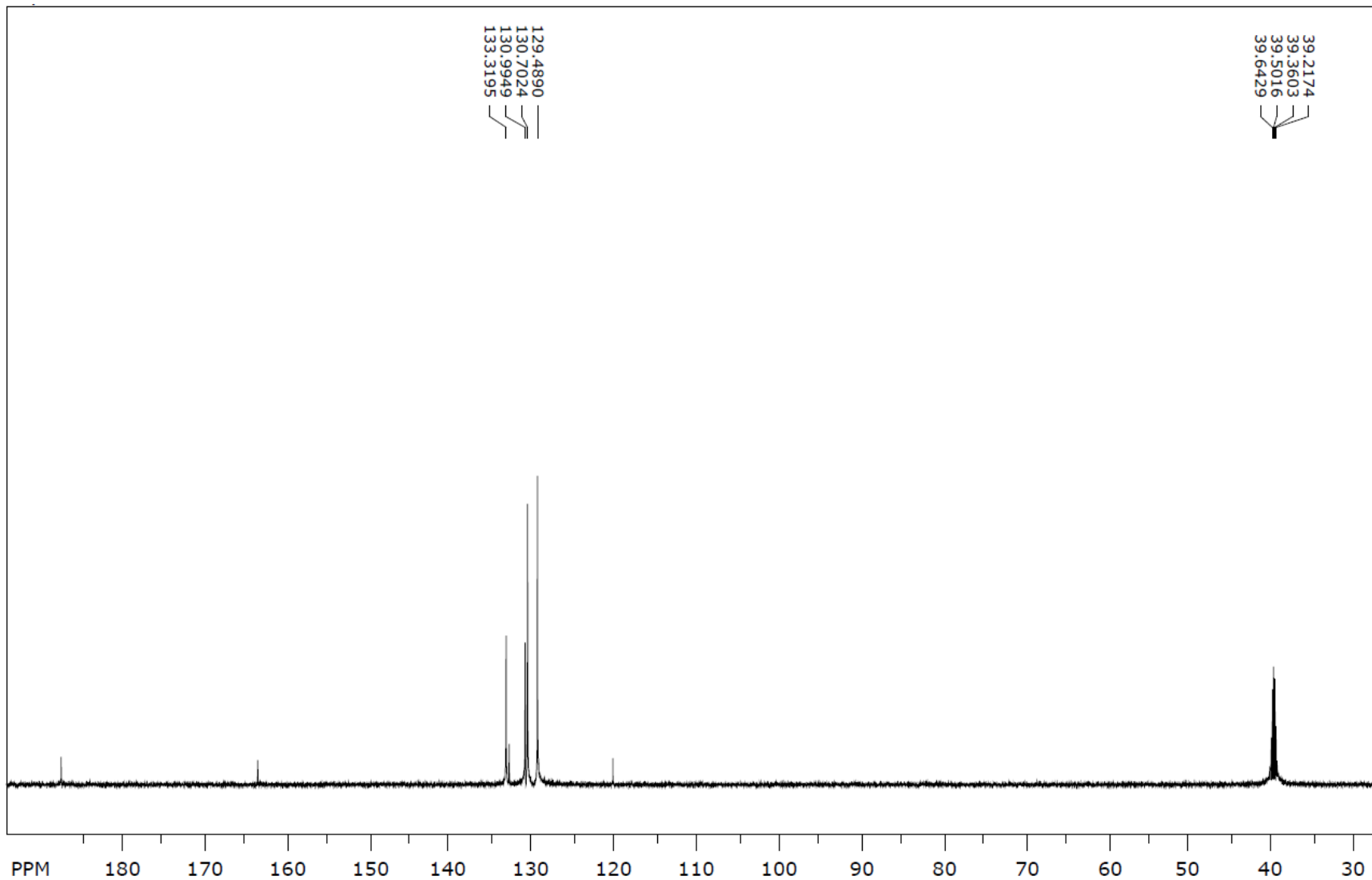
Maseni spektr (7t)



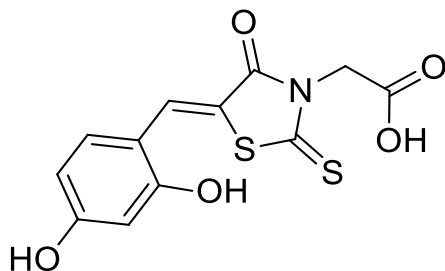
¹H NMR spektr (7t)



¹³C NMR spektr (7t)

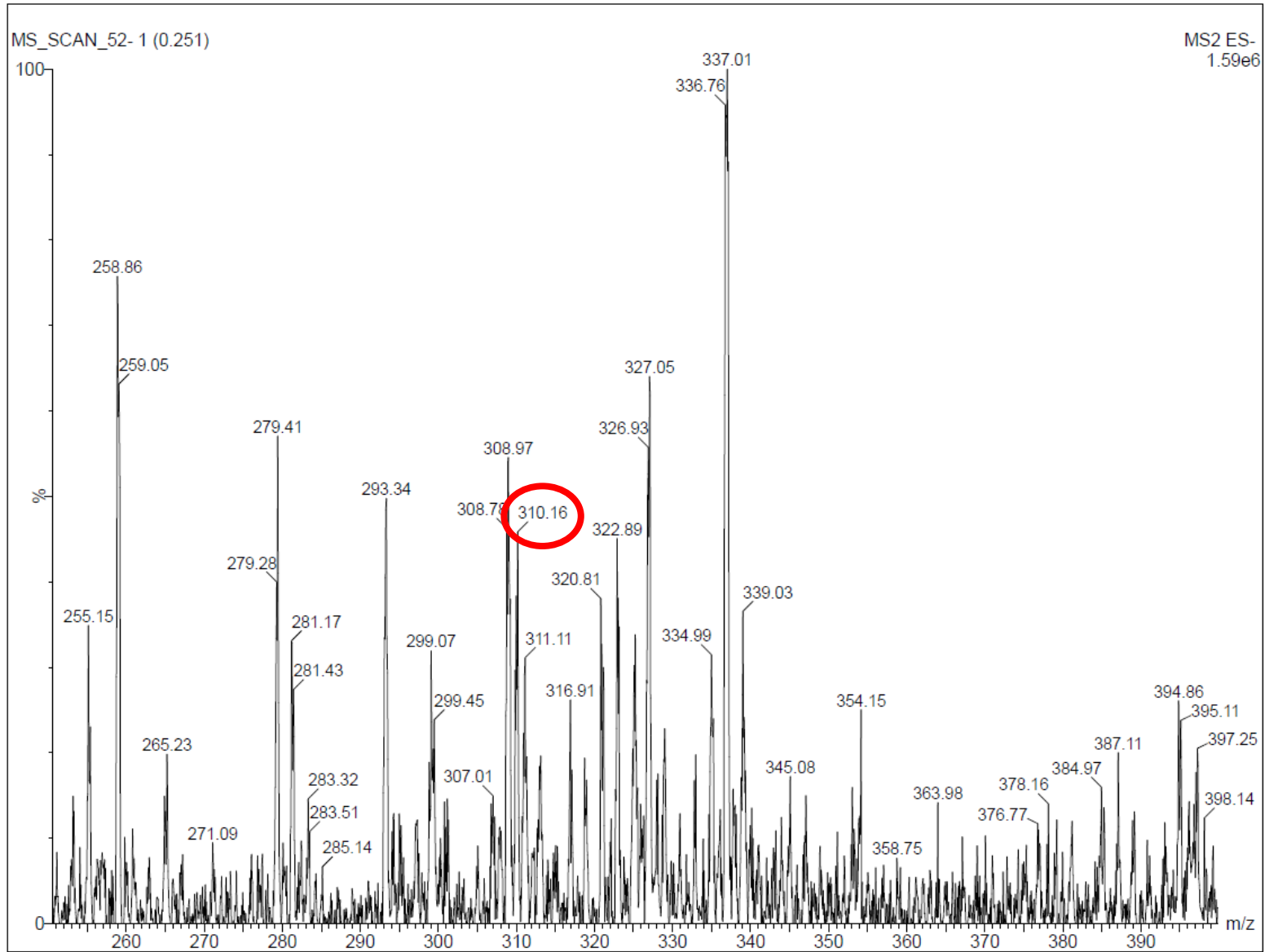


**2-(5-(2,4-dihidroksibenziliden)-4-okso-2-tioksotiazolidin-3-il) octena
kiselina (8a)**

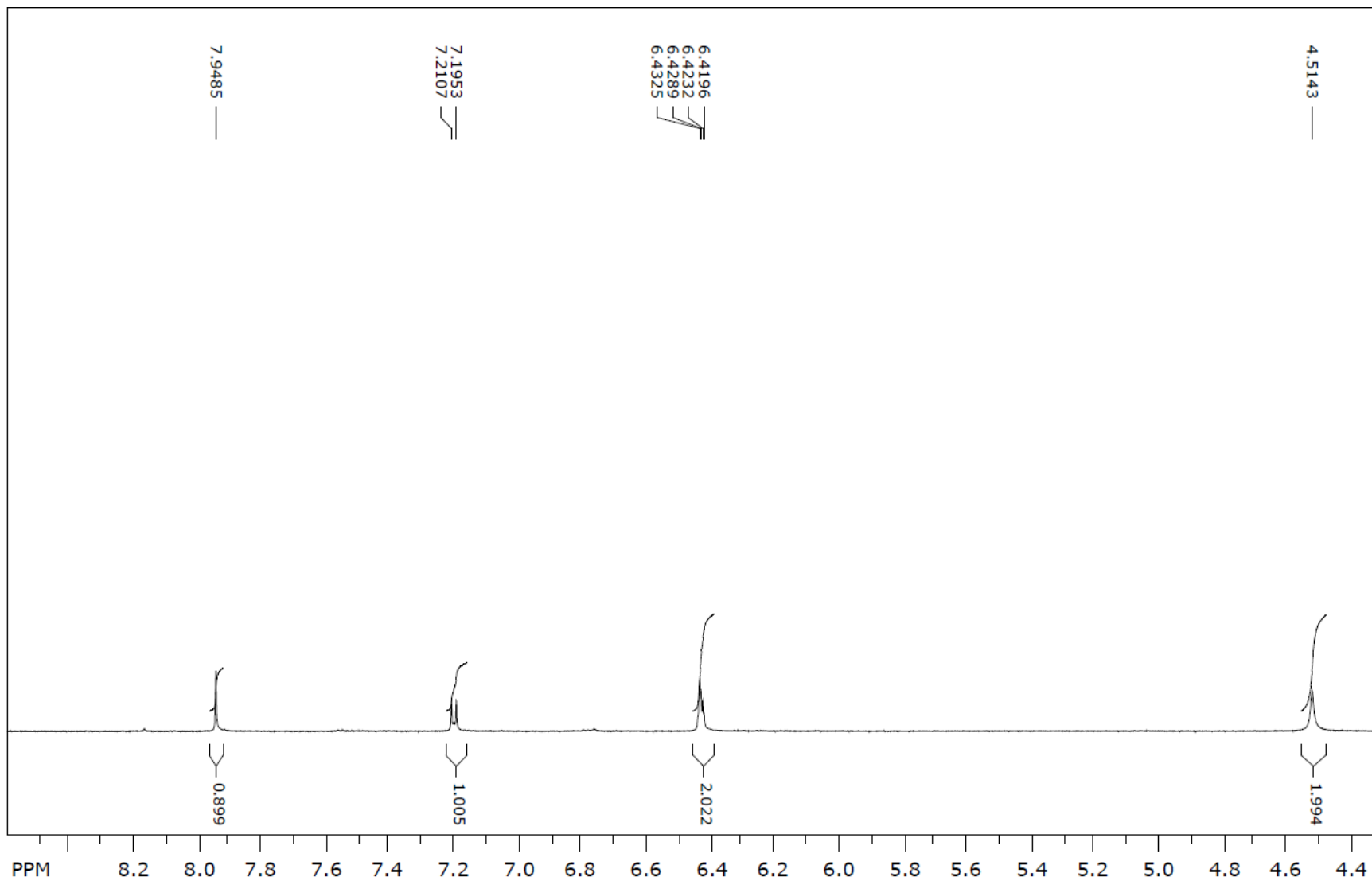


Reaktanti	2,4-dihidroksibenzaldehid (1 mmol) i 3-karboksimetilrodanin (1 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	311,33 g/mol
Molekulska formula	C ₁₂ H ₉ NO ₅ S ₂
Temperatura tališta	237 – 239 °C
Boja kristala	Smeđa
R_f	0,24
LC/MS/MS m/z (M-)	310,16
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 10,92 (s, 1H, OH), 10,49 (s, 1H, OH), 7,94 (s, 1H, CH), 7,20 (d, <i>J</i> = 9,24 Hz, 1H, arom.), 6,43 (q, <i>J</i> = 2,16; 3,42 Hz, 2H, arom.), 4,51 (s, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,37; 167,25; 166,91; 162,92; 160,36; 131,42; 129,64; 115,19; 111,88; 108,88; 102,58; 46,13.

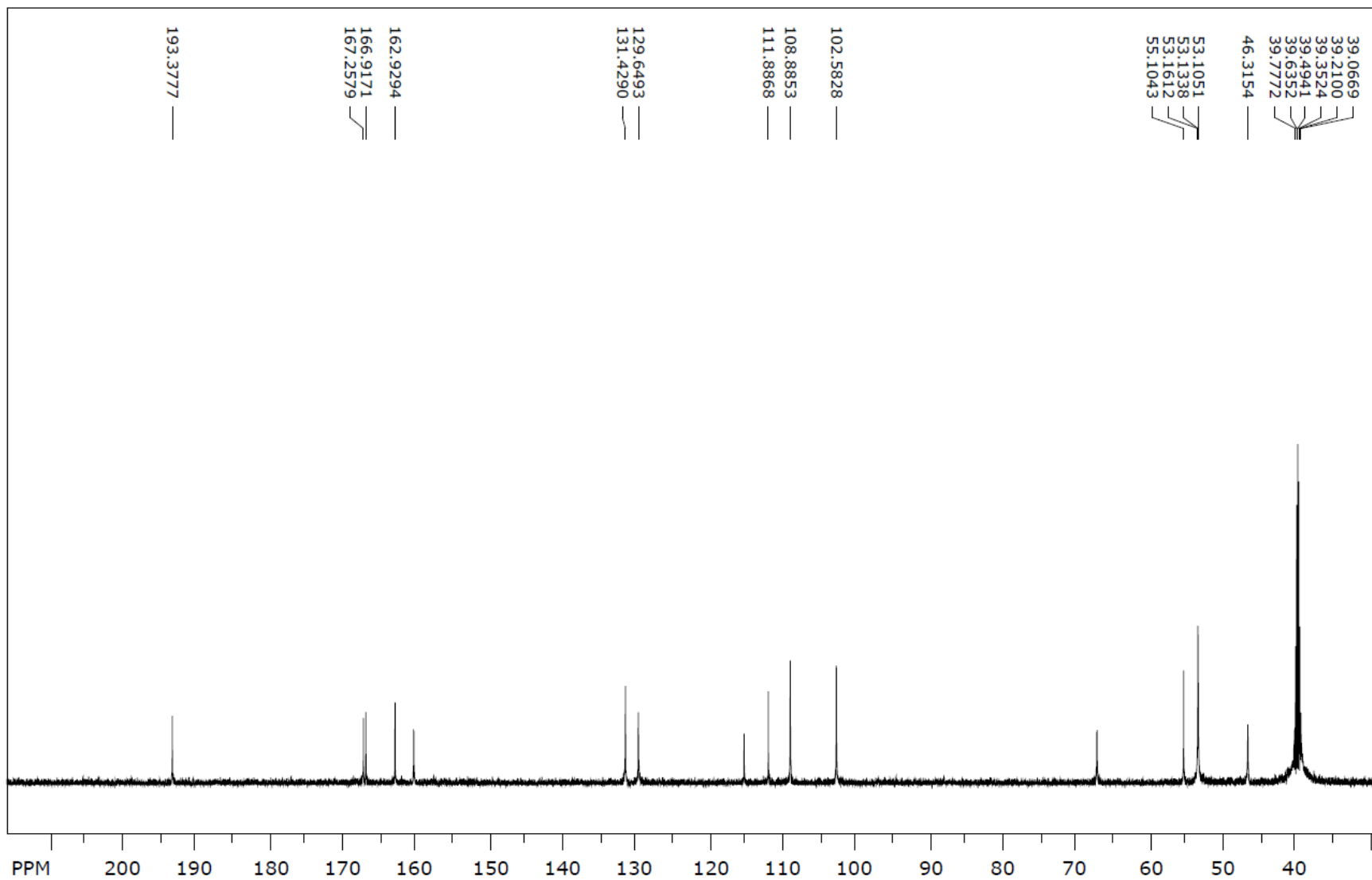
Maseni spektar (8a)



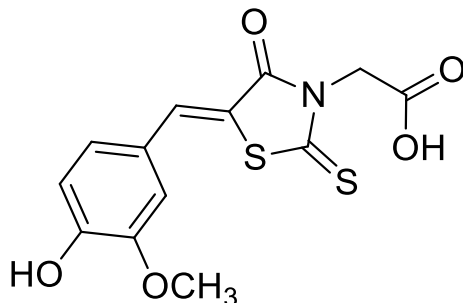
¹H NMR spektr (8a)



¹³C NMR spektr (8a)

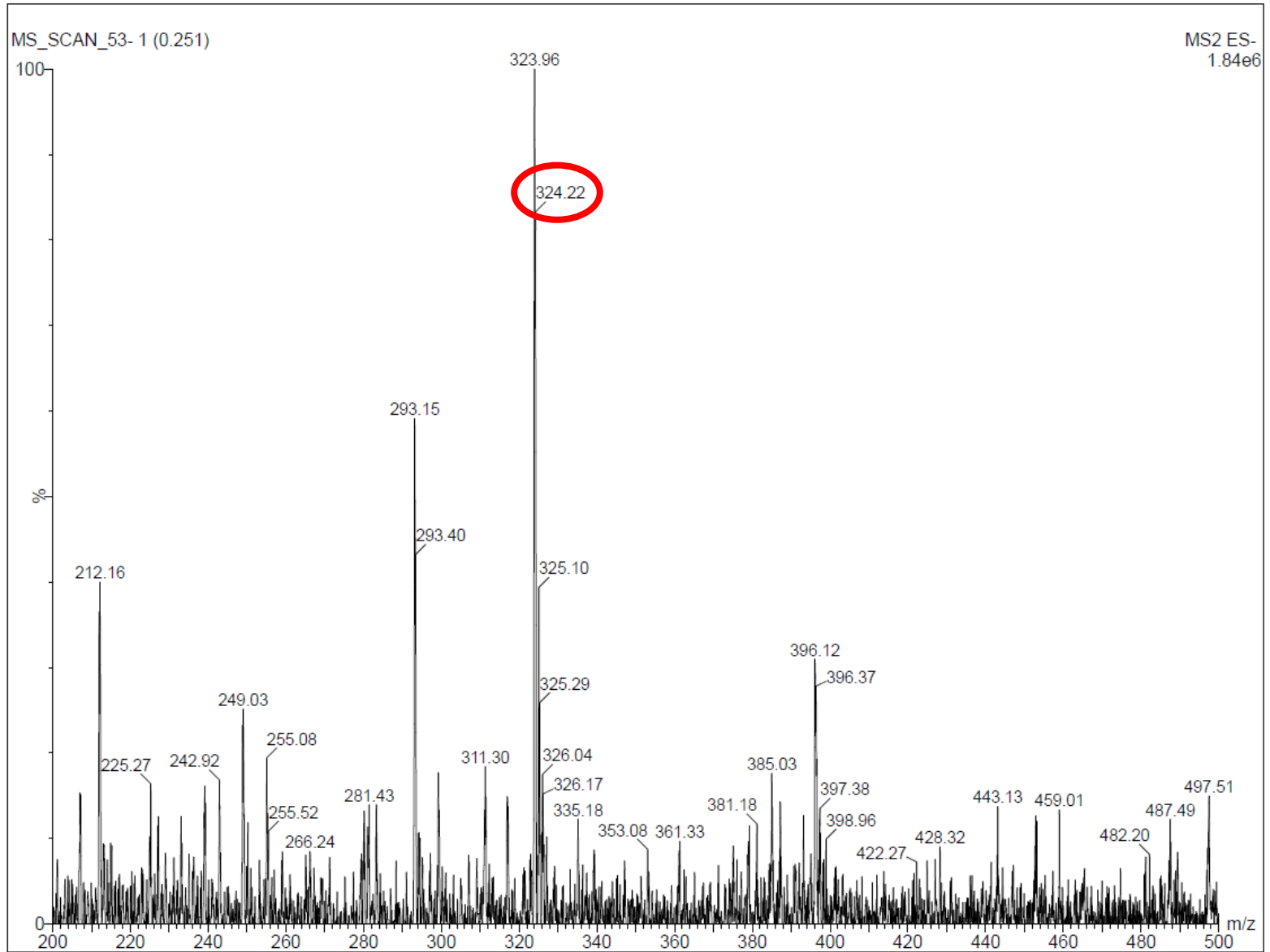


2-(5-(4-hidroksi-3-metoksibenziliden)-4-okso-2-tioksotiazolidin-3-il) octena kiselina (8b)

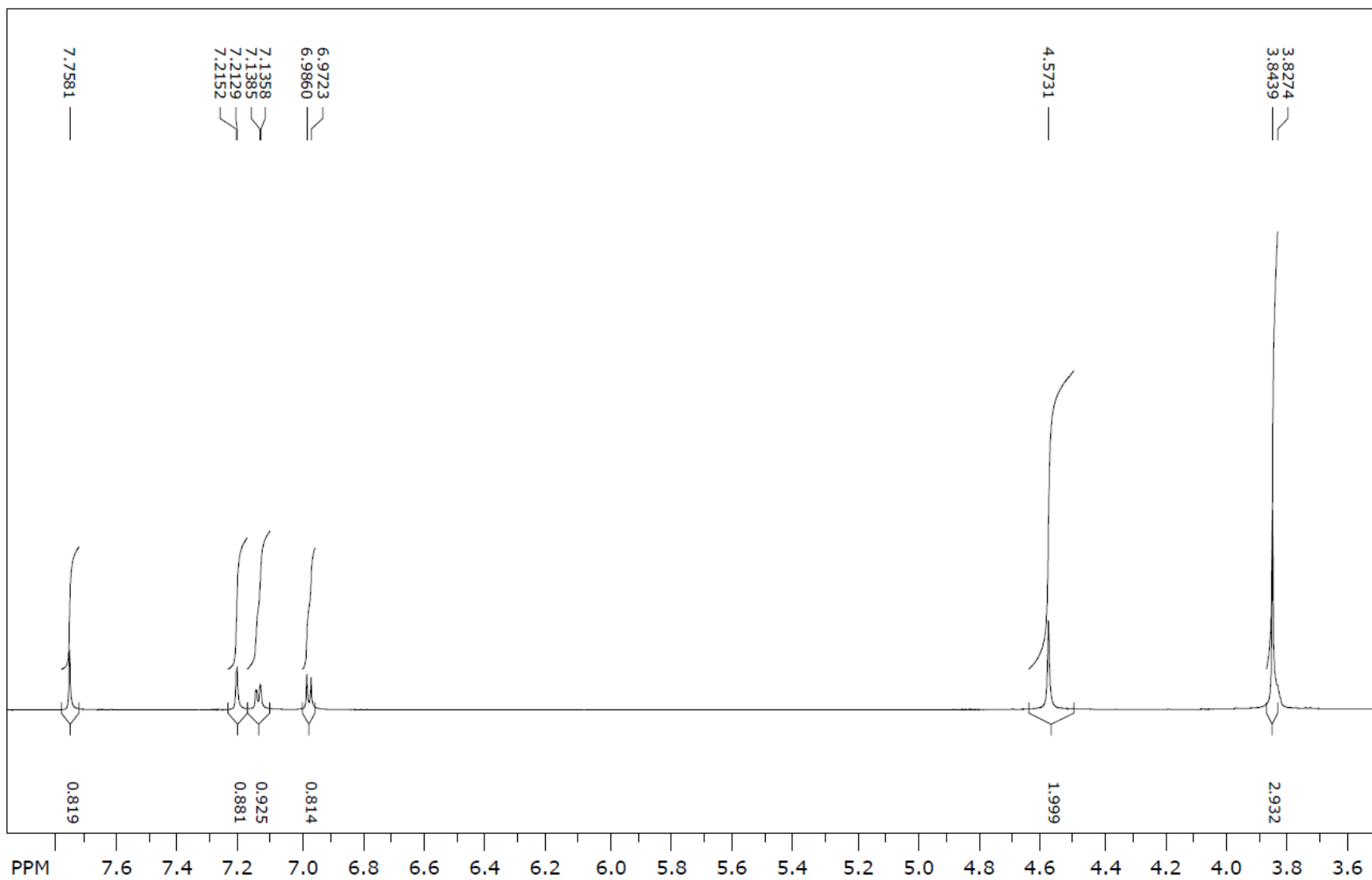


Reaktanti	3-metoksi-4-hidroksibenzaldehid (1 mmol) i 3-karboksimetilrodanin (1 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	325,36 g/mol
Molekulska formula	C ₁₃ H ₁₁ NO ₅ S ₂
Temperatura tališta	253 – 258 °C (lit. 233 °C, Abusetta i sur., 2020)
Boja kristala	Žuta
R_f	0,60
LC/MS/MS m/z (M-)	324,22
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,75 (s, 1H, CH), 7,21 (d, <i>J</i> = 1,38 Hz, 1H, arom.), 7,14 (dd, <i>J</i> = 8,22; 1,59 Hz, 1H, arom.), 6,97 (d, <i>J</i> = 8,22 Hz, 1H, arom.), 4,57 (s, 2H, CH ₂), 3,84 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 192,99; 166,99; 166,62; 150,53; 148,16; 134,22; 125,34; 124,26; 117,69; 116,42; 114,58; 55,62; 46,26.

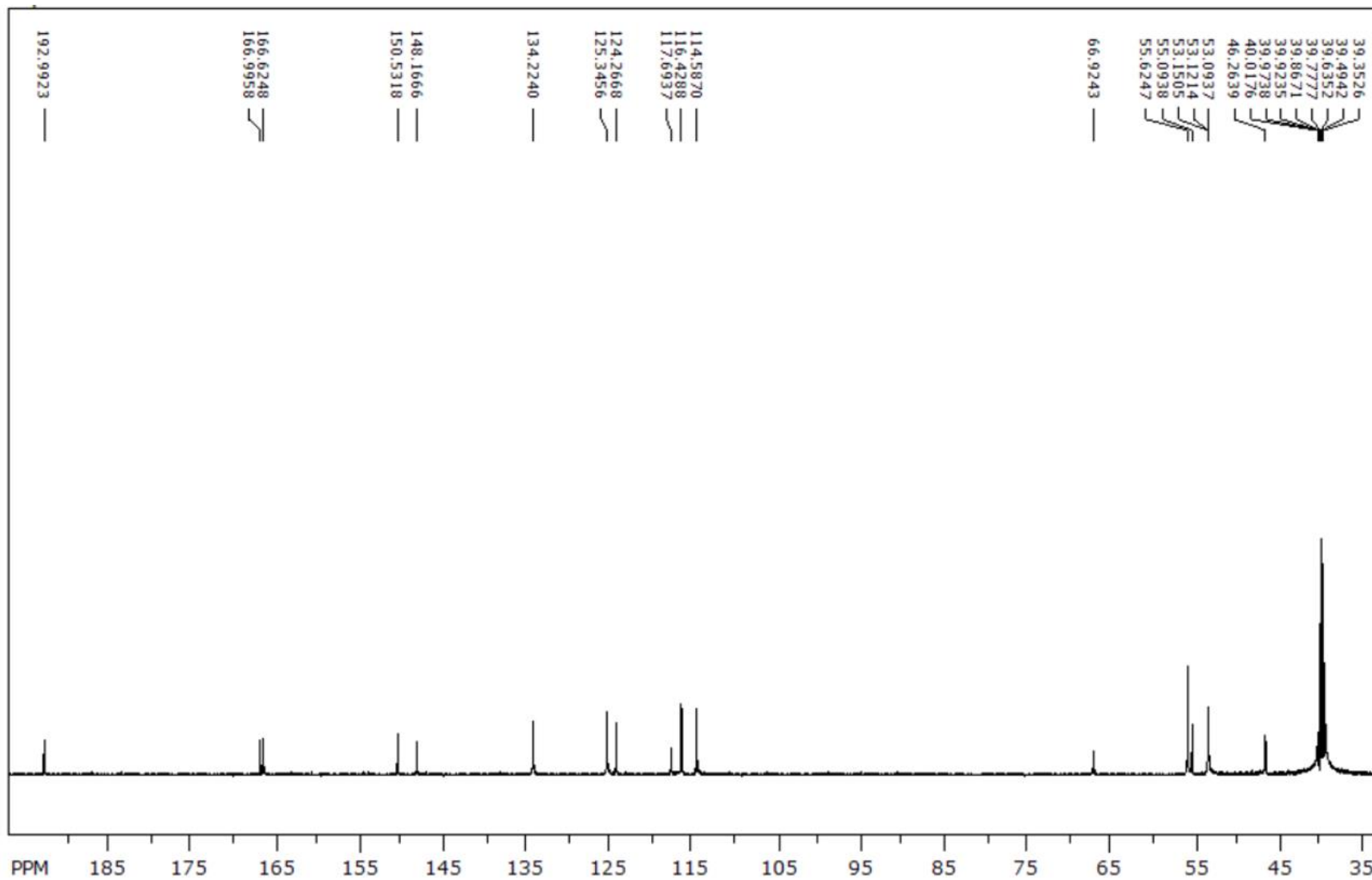
Maseni spektr (8b)



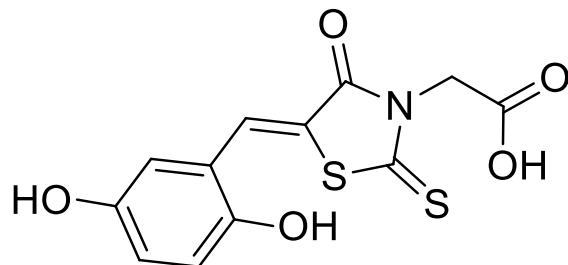
¹H NMR spektr (8b)



¹³C NMR spektr (8b)

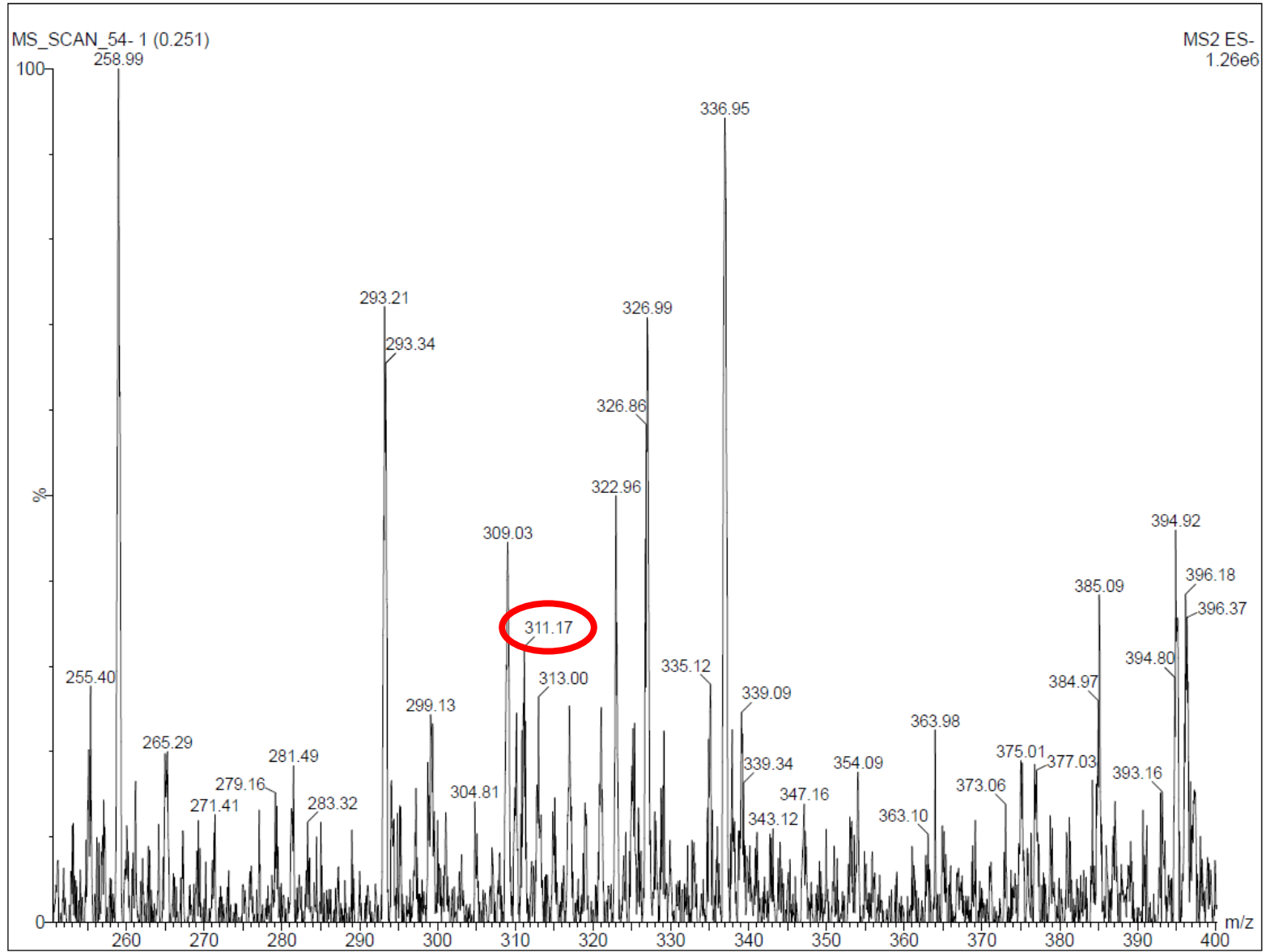


2-(5-(2,5-dihidroksibenziliden)-4-okso-2-tioksotiazolidin-3-il) octena kiselina (8c)

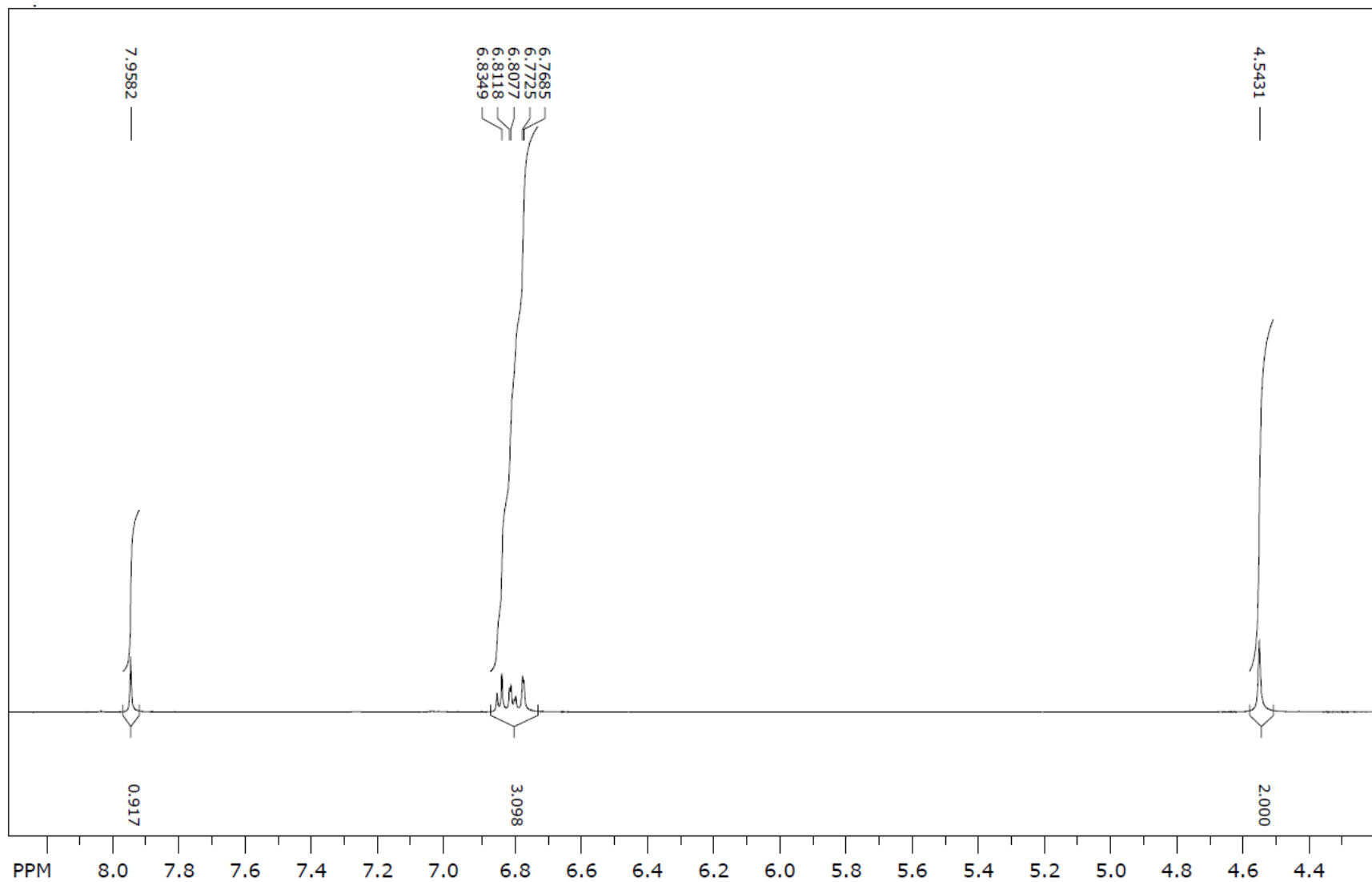


Reaktanti	2,5-dihidroksibenzaldehid (1 mmol) i 3-karboksimetilrodanin (1 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	311,33 g/mol
Molekulska formula	C ₁₂ H ₉ NO ₅ S ₂
Temperatura tališta	222 – 224 °C
Boja kristala	Crvena
R_f	0,40
LC/MS/MS <i>m/z</i> (M⁻)	311,17
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 10,38 (s, 1H, OH), 9,27 (s, 1H, OH), 7,95 (s, 1H, CH), 6,84 (d, <i>J</i> = 8,76 Hz, 1H, arom.), 6,80 (dd, <i>J</i> = 8,70; 2,52 Hz, 1H, arom.), 6,77 (d, <i>J</i> = 2,40 Hz, 1H, arom.), 4,54 (s, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,46; 167,06; 166,77; 151,26; 150,20; 128,69; 120,96; 119,95; 119,79; 117,35; 113,63; 46,44.

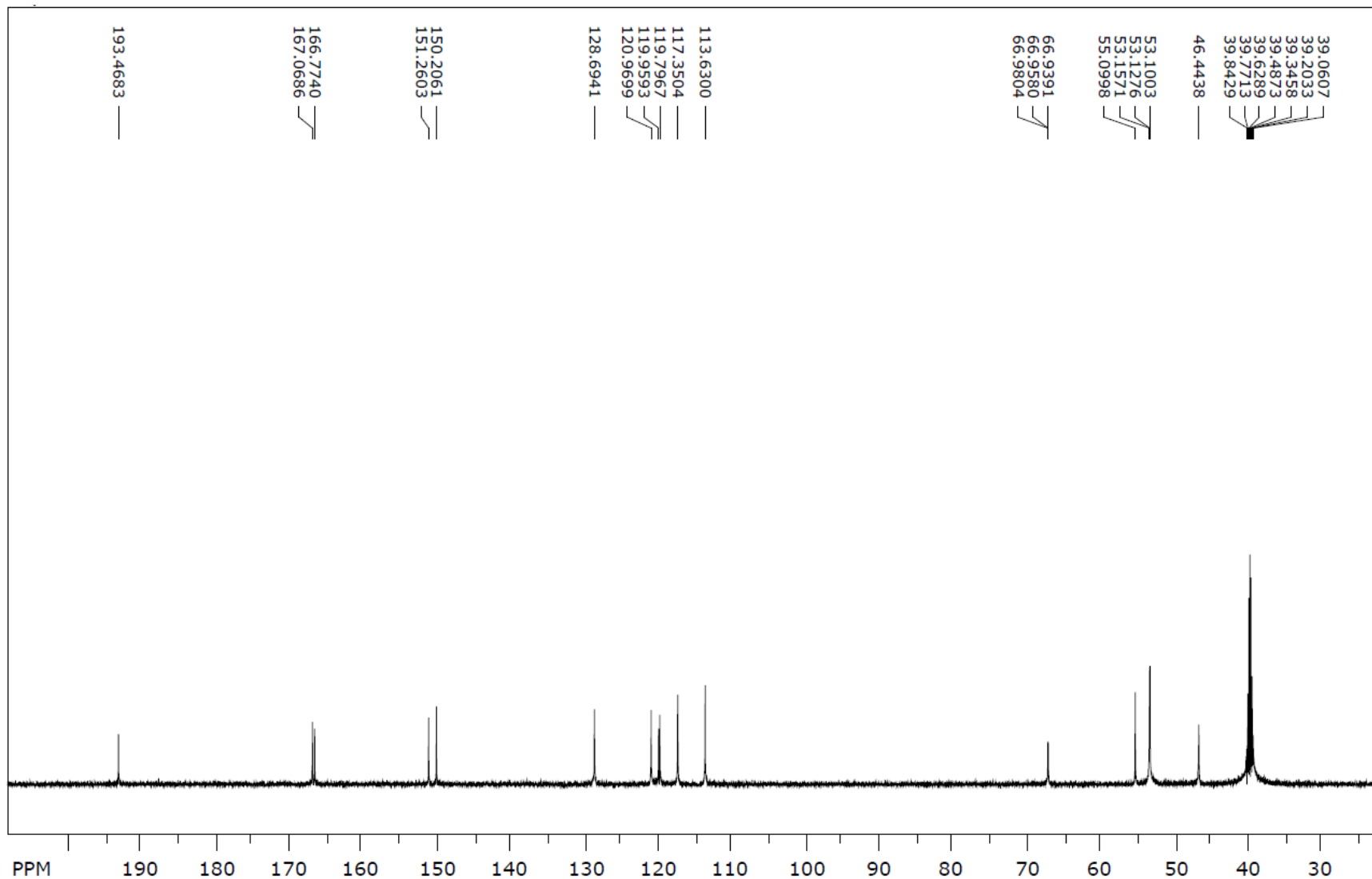
Maseni spektar (8c)



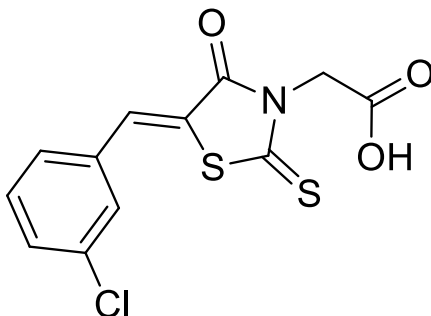
¹H NMR spektr (8c)



¹³C NMR spektr (8c)

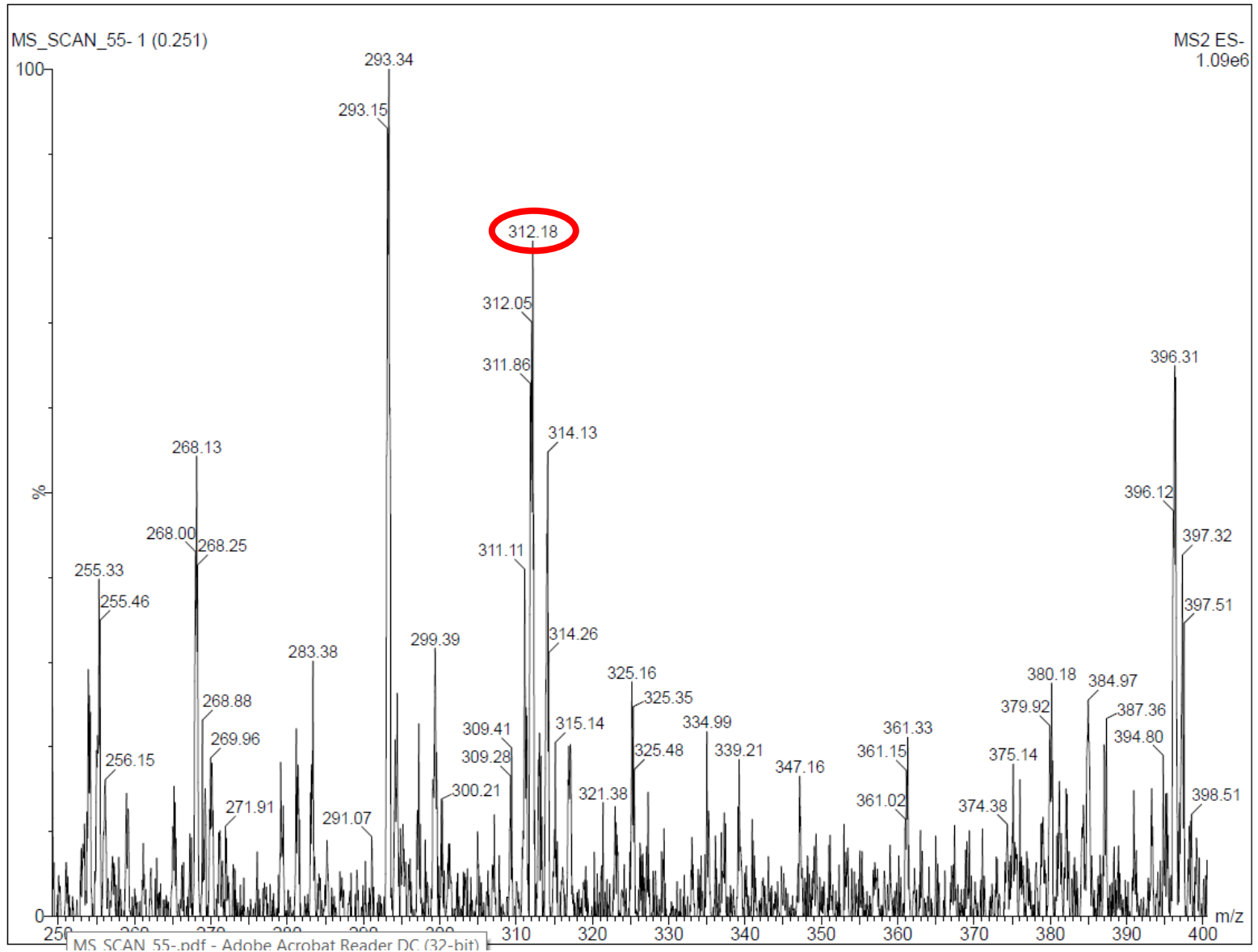


**2-(5-(3-klorbenziliden)-4-okso-2-tioksotiazolidin-3-il) octena kiselina
(8d)**

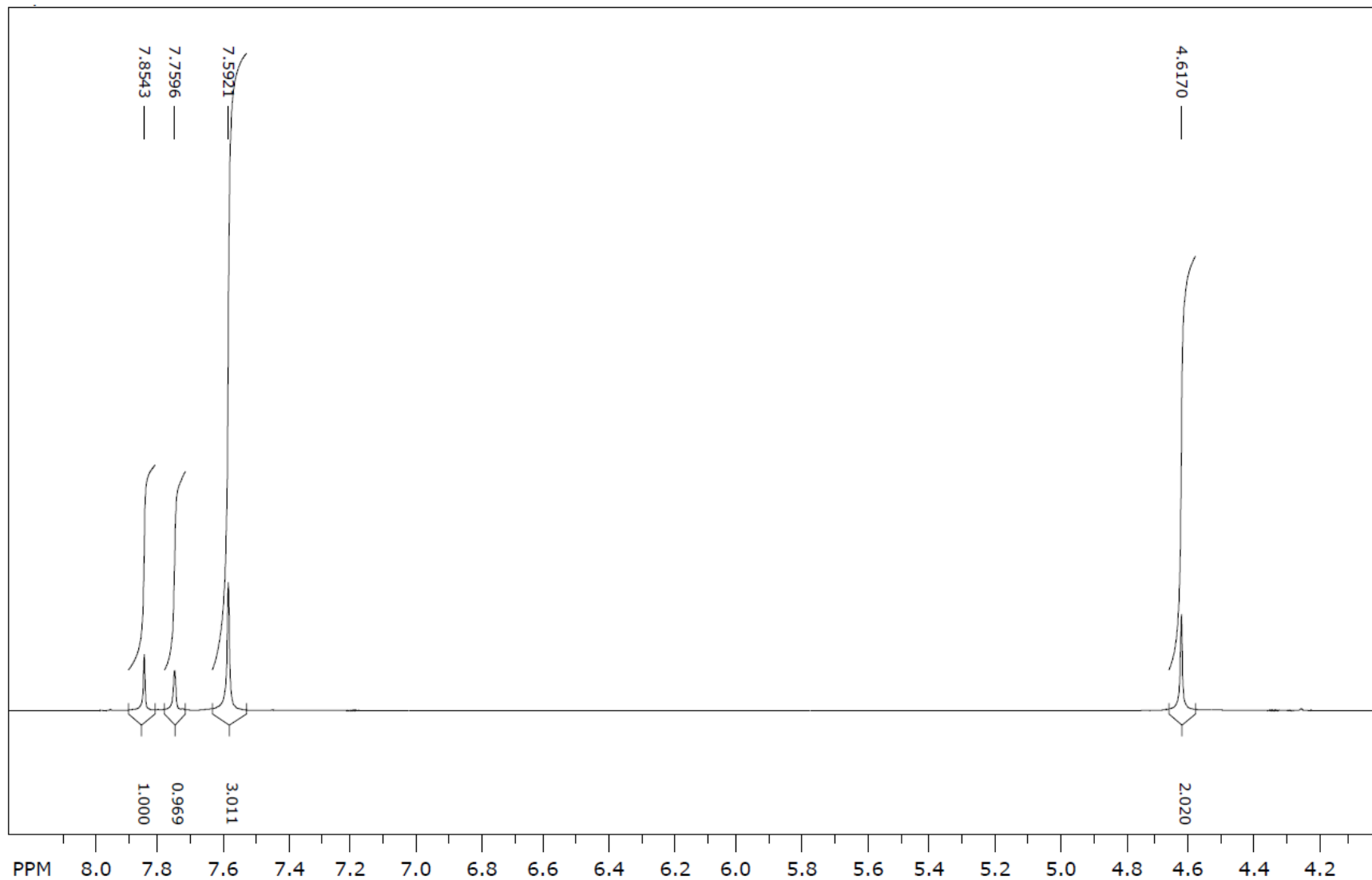


Reaktanti	3-klorbenzaldehyd (0,7 mmol) i 3-karboksimetilrodanin (0,7 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	313,78 g/mol
Molekulska formula	C ₁₂ H ₈ ClNO ₃ S ₂
Temperatura tališta	180 – 183 °C
Boja kristala	Tamnosmeđa
R_f	0,77
LC/MS/MS <i>m/z</i> (M⁻)	312,18
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,85 (s, 1H, CH), 7,75 (s, 1H, arom.), 7,59 (s, 3H, arom.), 4,61 (s, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 192,85; 166,96; 166,33; 135,02; 134,06; 131,53; 131,27; 130,53; 128,26; 123,98; 46,13.

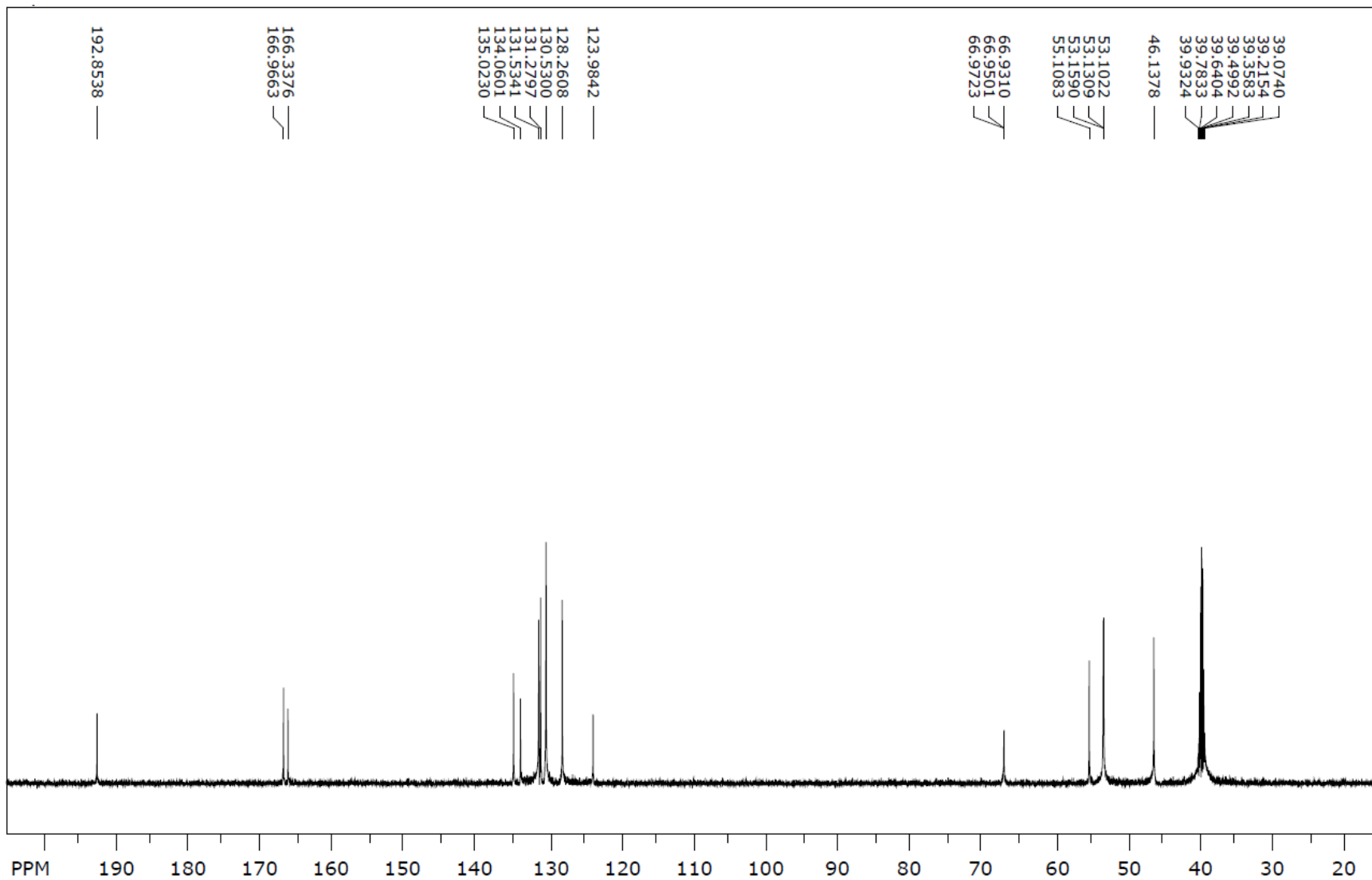
Maseni spektrar (8d)



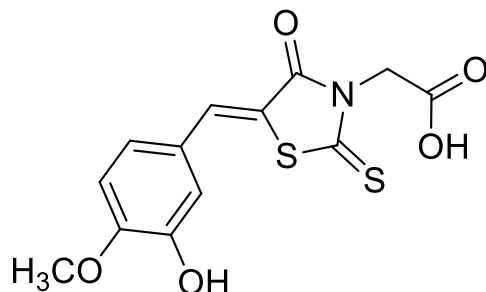
¹H NMR spektr (8d)



¹³C NMR spektr (8d)

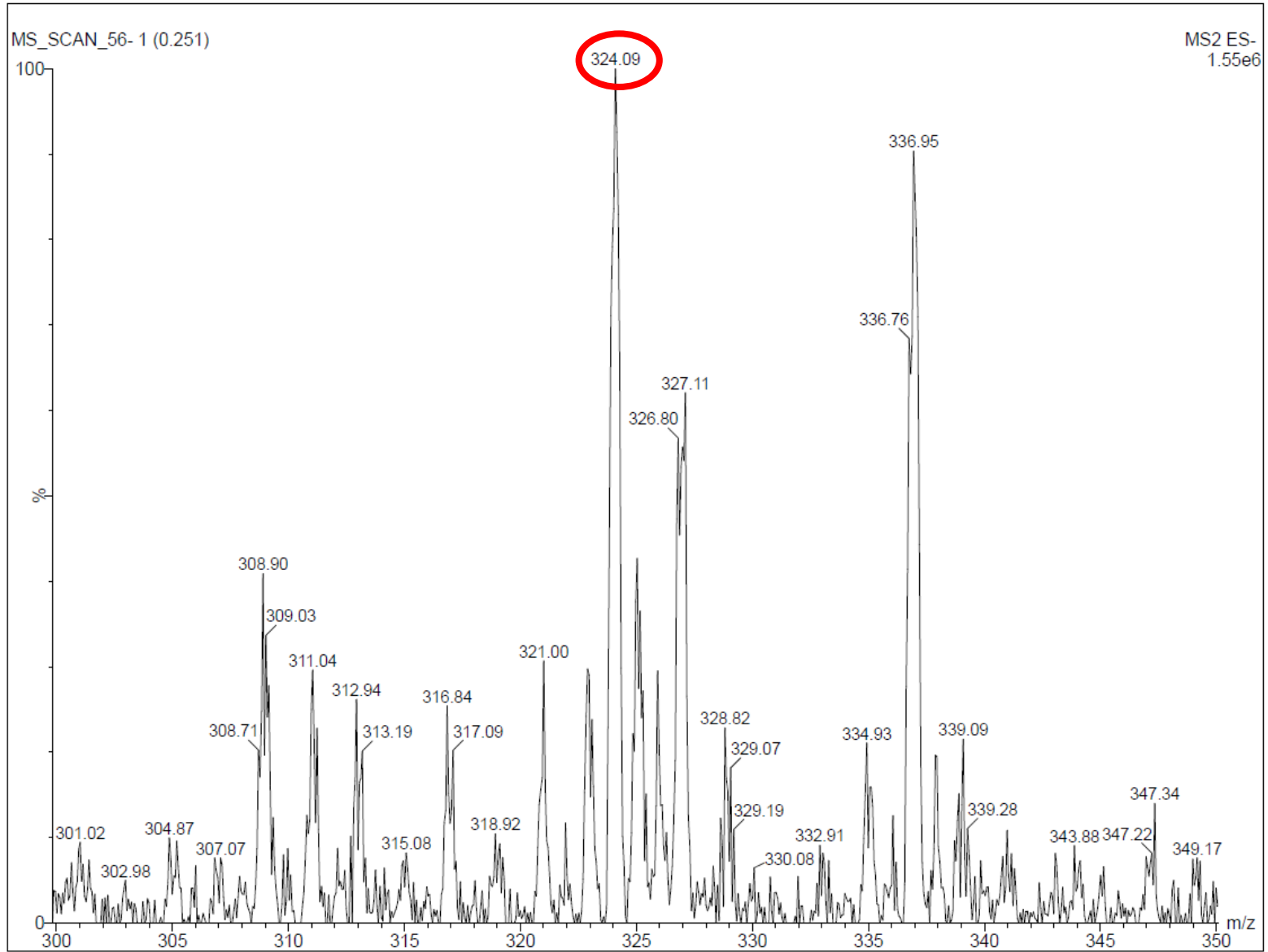


2-(5-(3-hidroksi-4-metoksibenziliden)-4-okso-2-tioksotiazolidin-3-il) octena kiselina (8e)

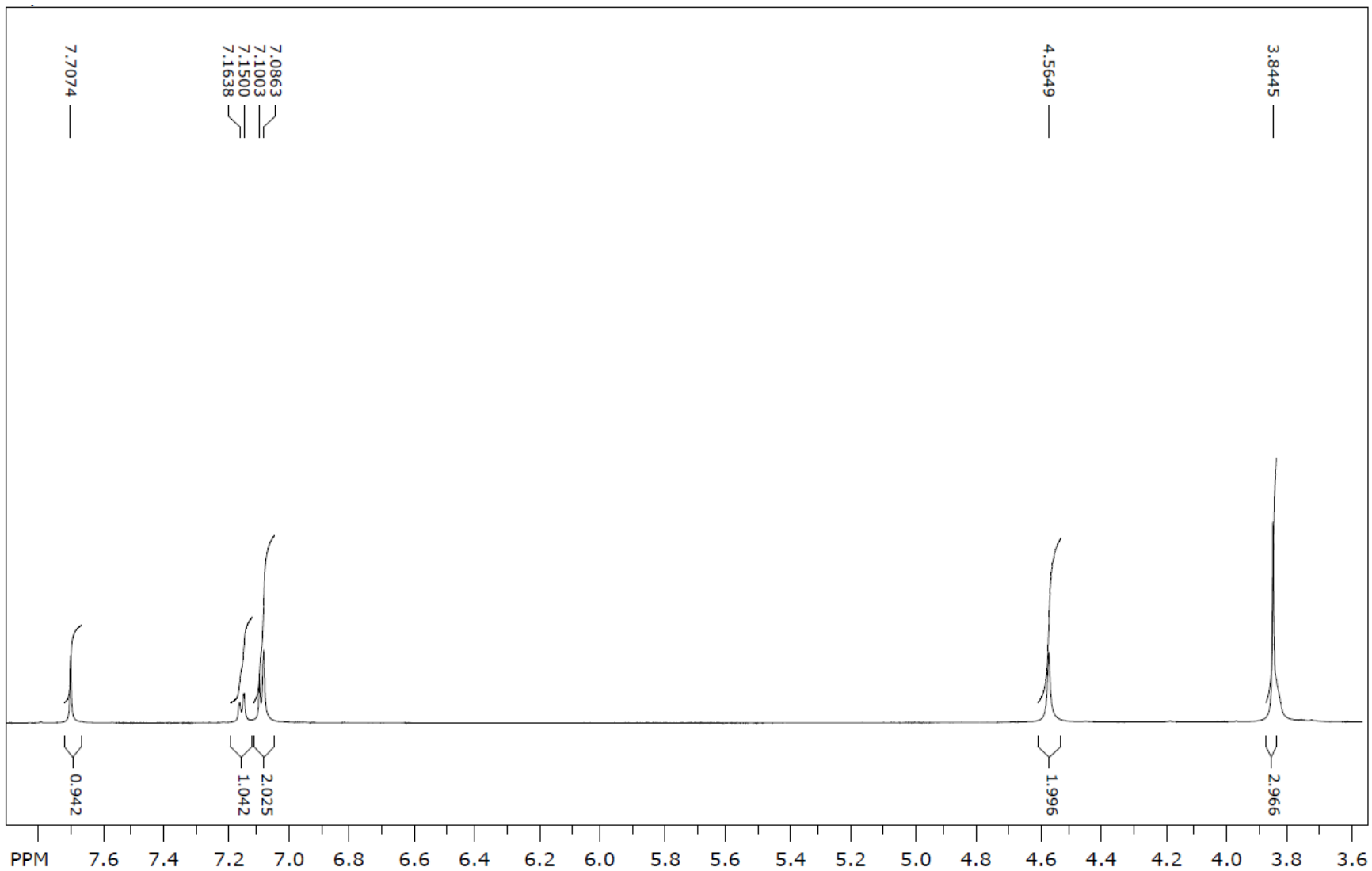


Reaktanti	3-hidroksi-4-metoksibenzaldehid (0,7 mmol) i 3-karboksimetilrodanin (0,7 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	325,36 g/mol
Molekulska formula	C ₁₃ H ₁₁ NO ₅ S ₂
Temperatura tališta	200 – 205 °C
Boja kristala	Smeđa
R_f	0,59
LC/MS/MS m/z (M-)	324,09
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 9,82 (s, 1H, OH), 7,70 (s, 1H, CH), 7,16 (d, <i>J</i> = 8,28 Hz, 1H, arom.), 7,09 (d, <i>J</i> = 8,40 Hz, 2H, arom.), 4,56 (s, 2H, CH ₂), 3,84 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,11; 166,63; 150,76; 147,27; 133,79; 125,67; 124,42; 118,66; 116,35; 112,57; 46,36.

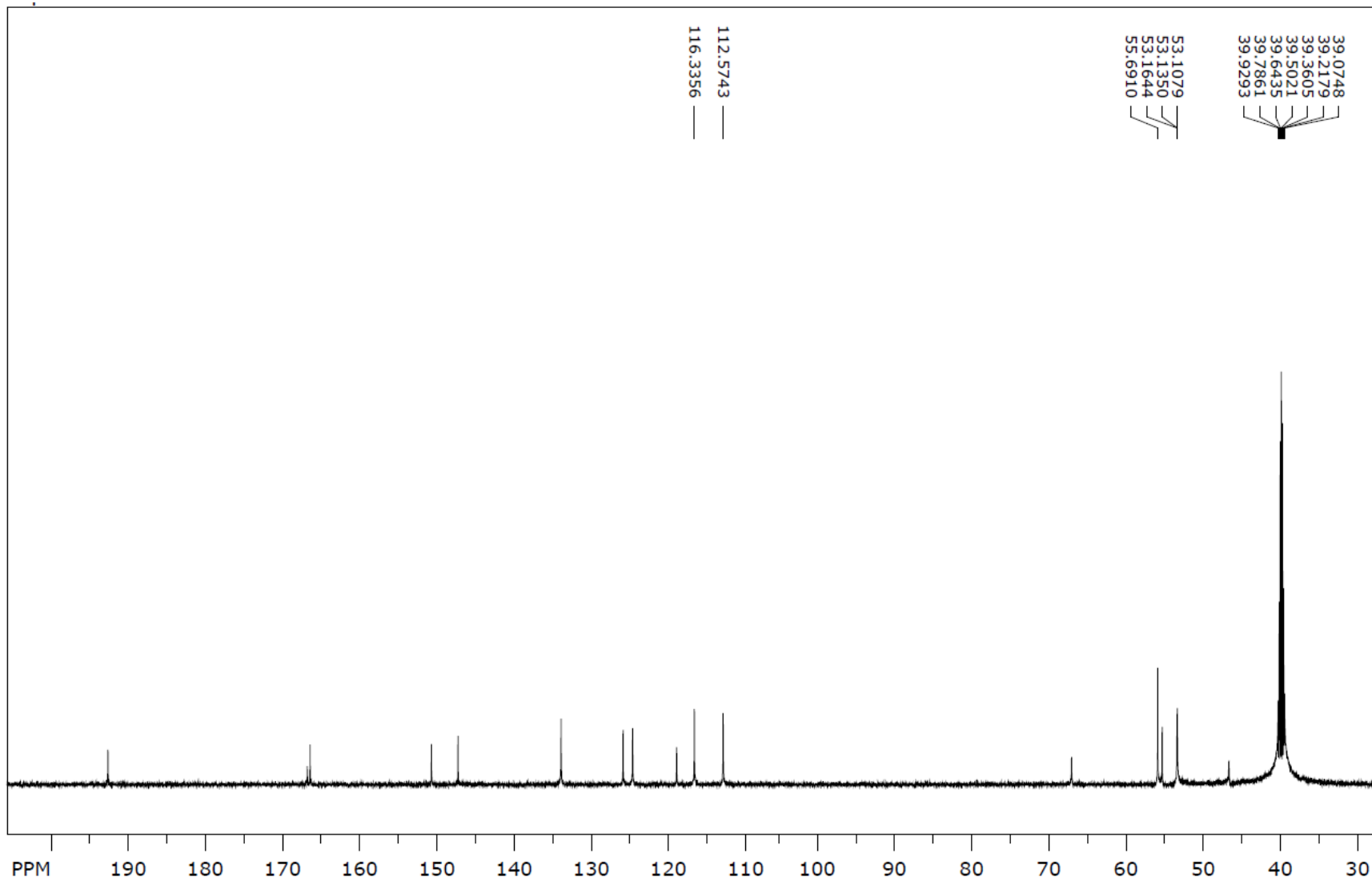
Maseni spektar (8e)



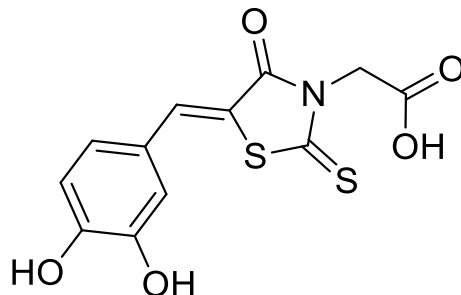
¹H NMR spektr (8e)



¹³C NMR spektr (8e)

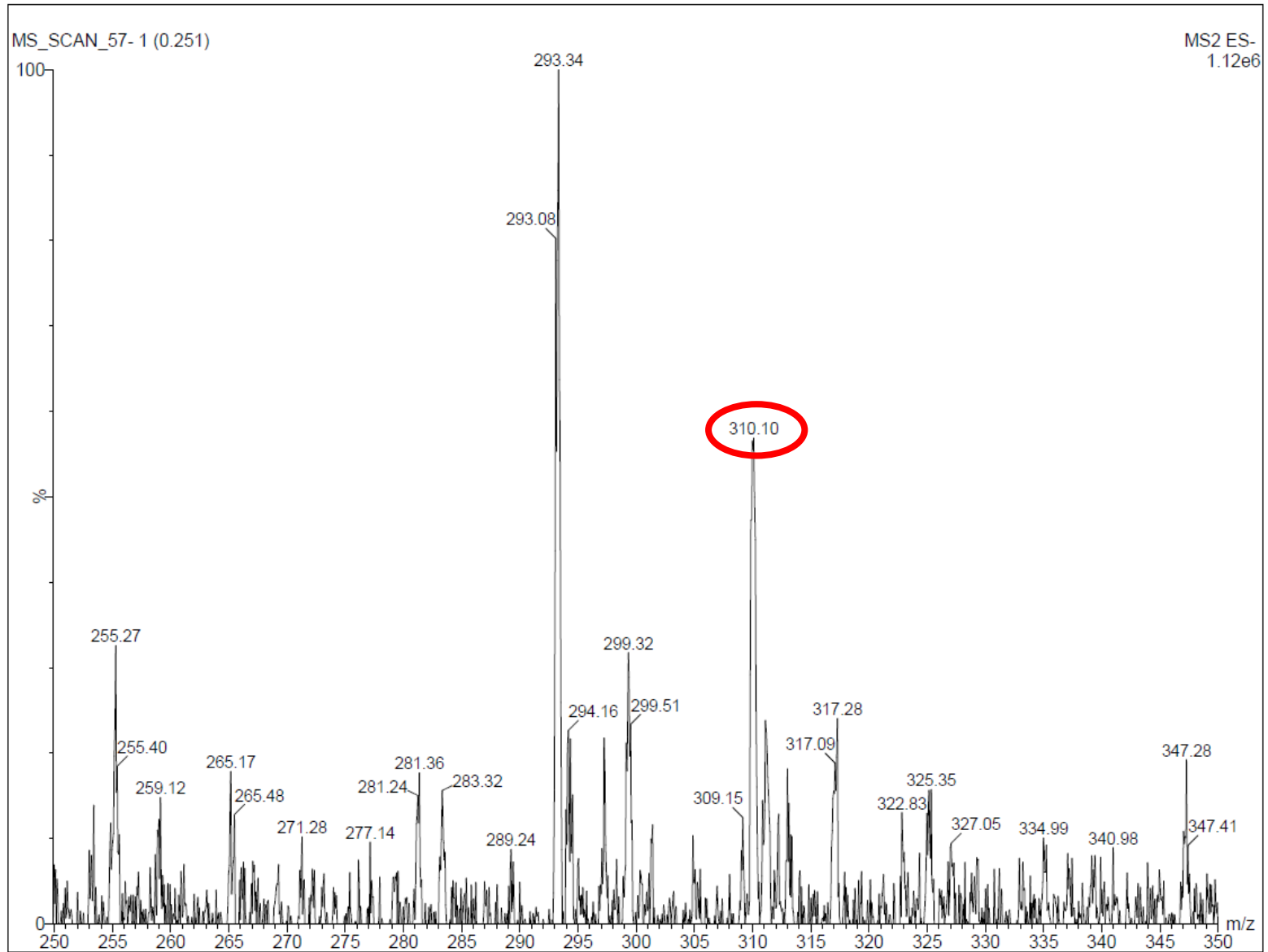


**2-(5-(3,4-dihidroksibenziliden)-4-okso-2-tioksotiazolidin-3-il) octena
kiselina (8f)**

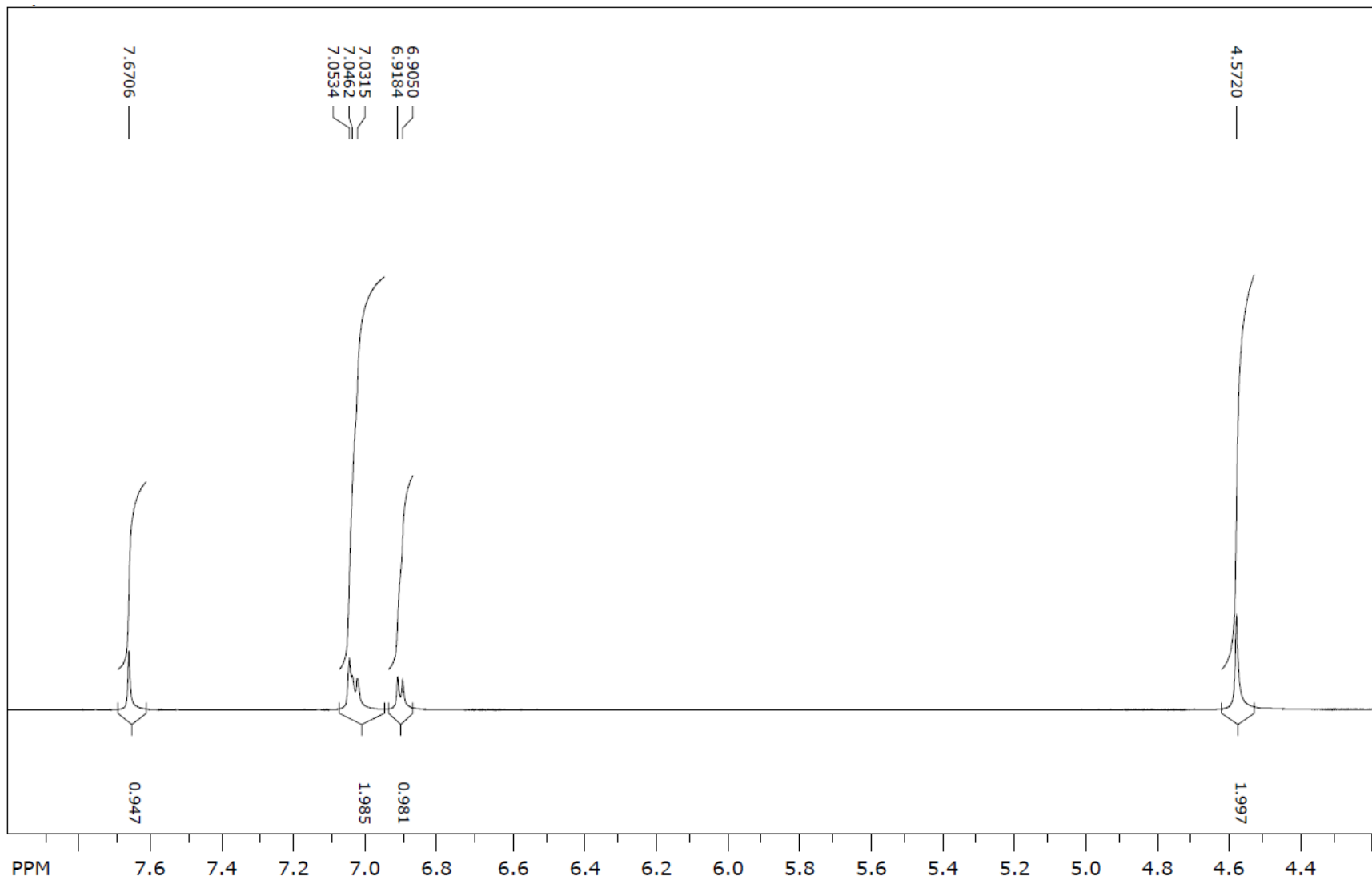


Reaktanti	3,4-dihidroksibenzaldehid (0,7 mmol) i 3-karboksimetilrodanin (0,7 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	311,33 g/mol
Molekulska formula	C ₁₂ H ₉ NO ₅ S ₂
Temperatura tališta	255 – 260 °C
Boja kristala	Smeđa
R_f	0,4
LC/MS/MS <i>m/z</i> (M-)	310,10
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,67 (s, 1H, CH), 7,04 (t, <i>J</i> = 4,32; 8,82 Hz, 2H, arom.), 6,91 (d, <i>J</i> = 8,04 Hz, 1H, arom.), 4,57 (s, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,08; 167,34; 166,67; 149,92; 146,28; 134,36; 125,07; 124,21; 117,04; 116,58; 46,30.

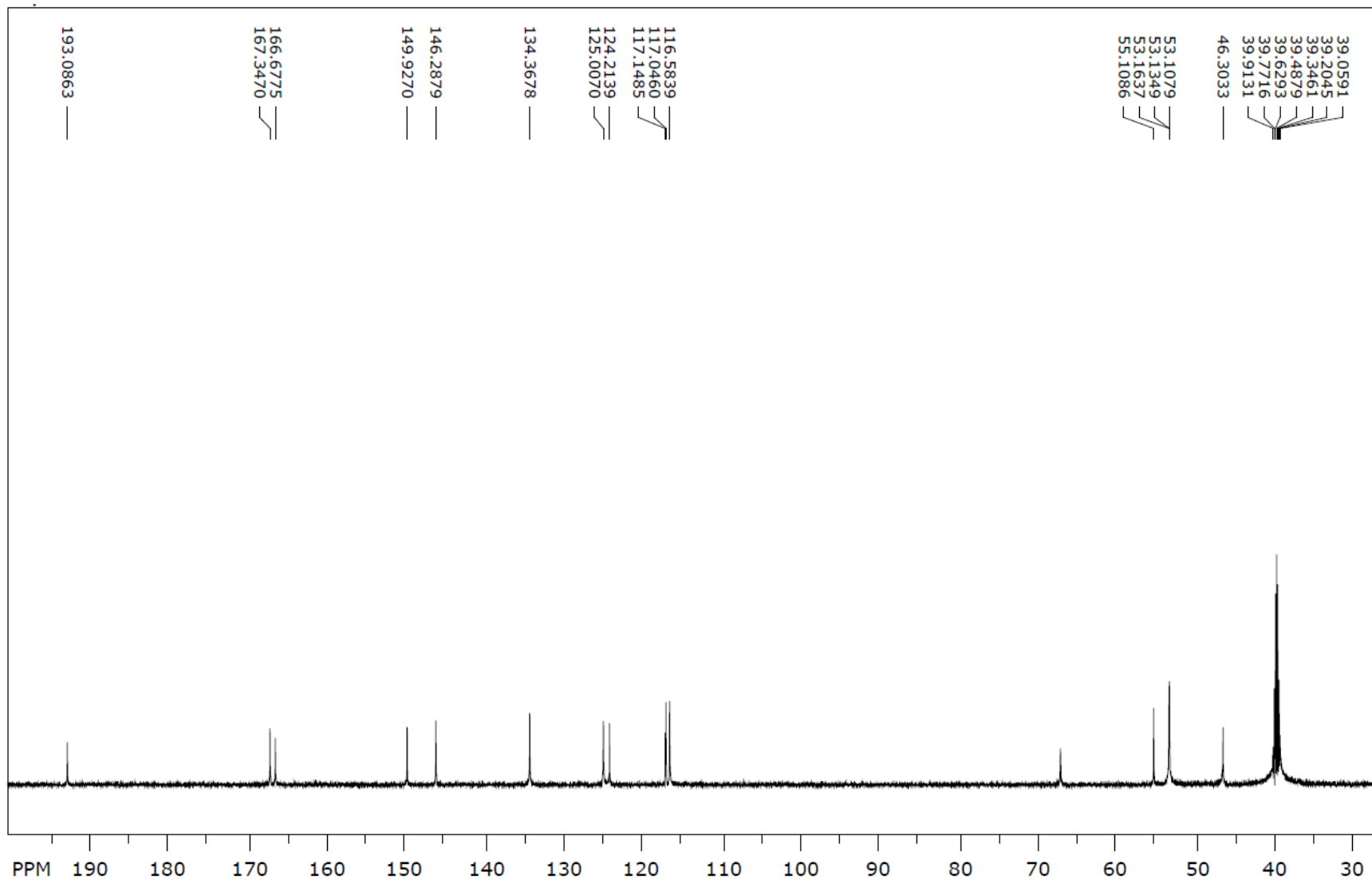
Maseni spektr (8f)



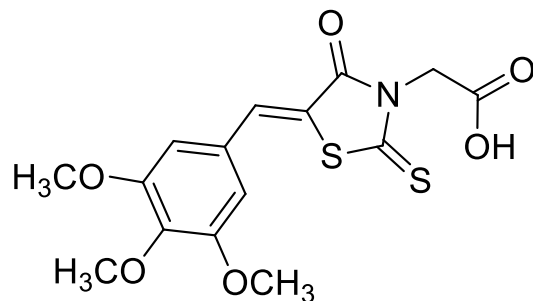
¹H NMR spektr (8f)



¹³C NMR spektr (8f)

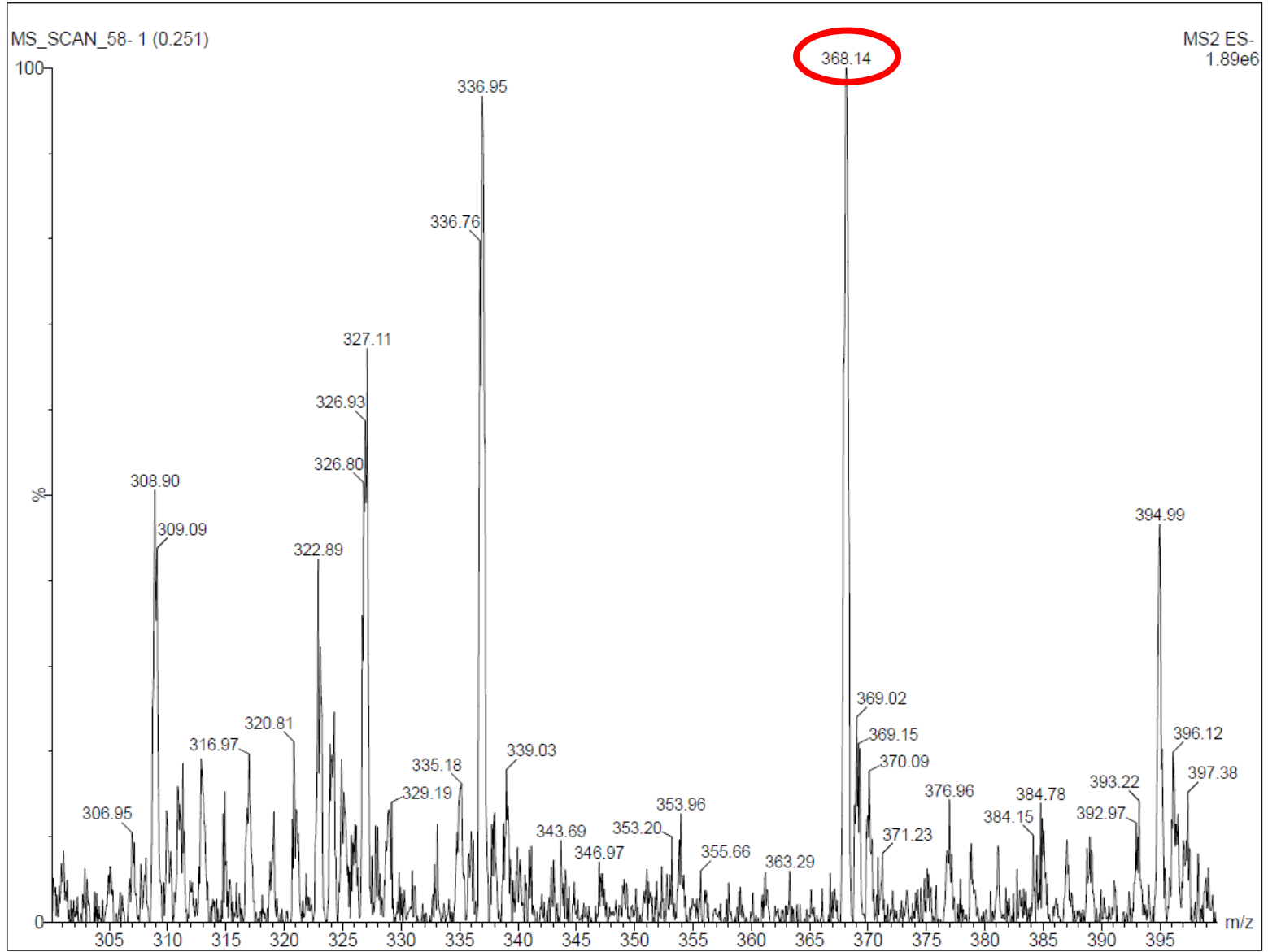


**2-(4-okso-2-tiokso-5-(3,4,5-trimetoksibenziliden) tiazolidin-3-il) octena
kiselina (8g)**

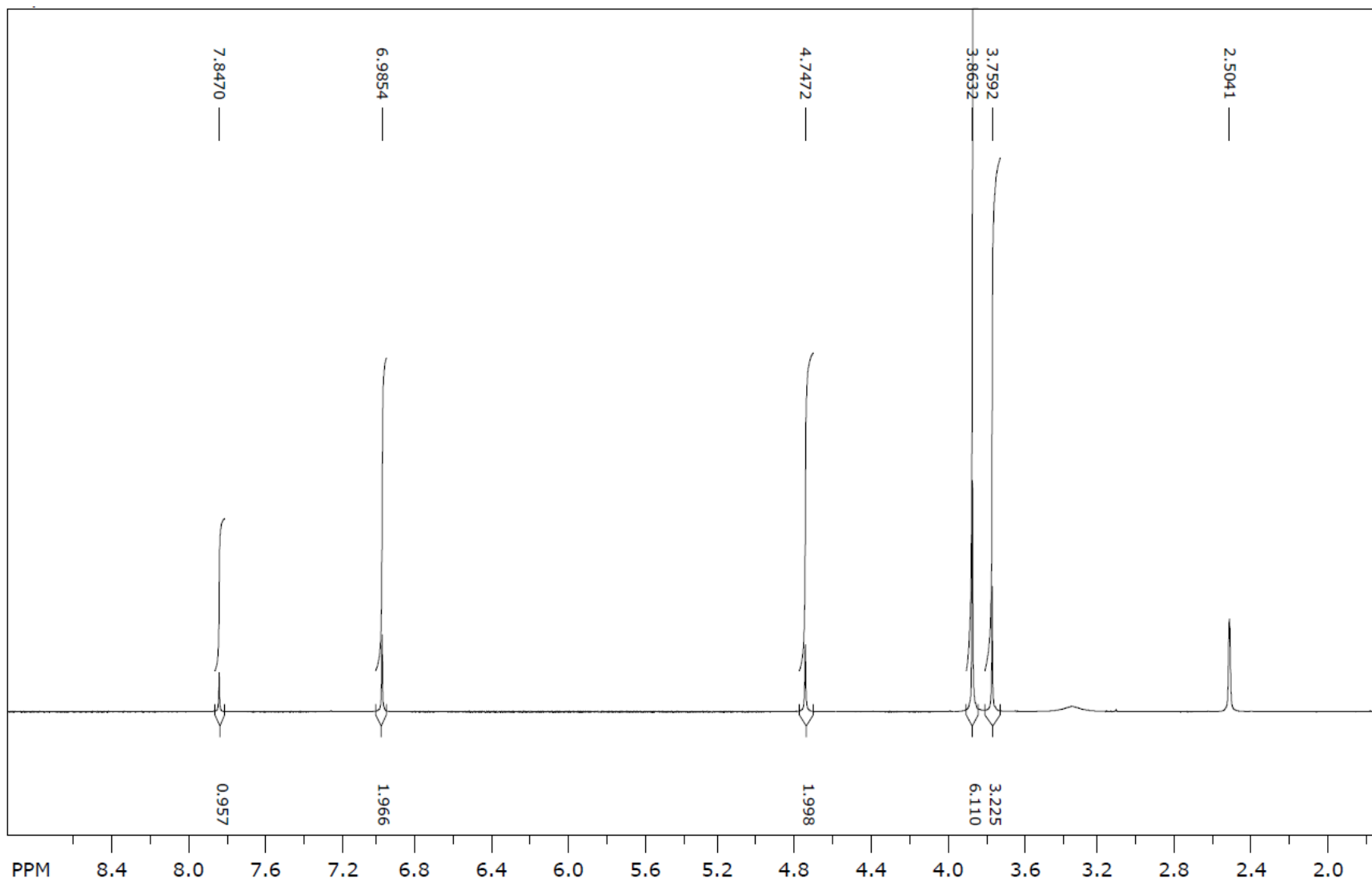


Reaktanti	3,4,5-trimetoksibenzaldehid (0,7 mmol) i 3-karboksimetilrodanin (0,7 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	369,41 g/mol
Molekulska formula	C ₁₅ H ₁₅ NO ₆ S ₂
Temperatura tališta	139 – 142 °C
Boja kristala	Smeđa
R_f	0,71
LC/MS/MS m/z (M-)	368,14
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,84 (s, 1H, CH), 6,95 (s, 2H, arom.), 4,74 (s, 2H, CH ₂), 3,86 (s, 6H, OCH ₃), 3,75 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 194,04; 167,23; 166,26; 153,29; 140,16; 134,28; 128,24; 120,63; 108,26; 60,23; 56,07; 44,99.

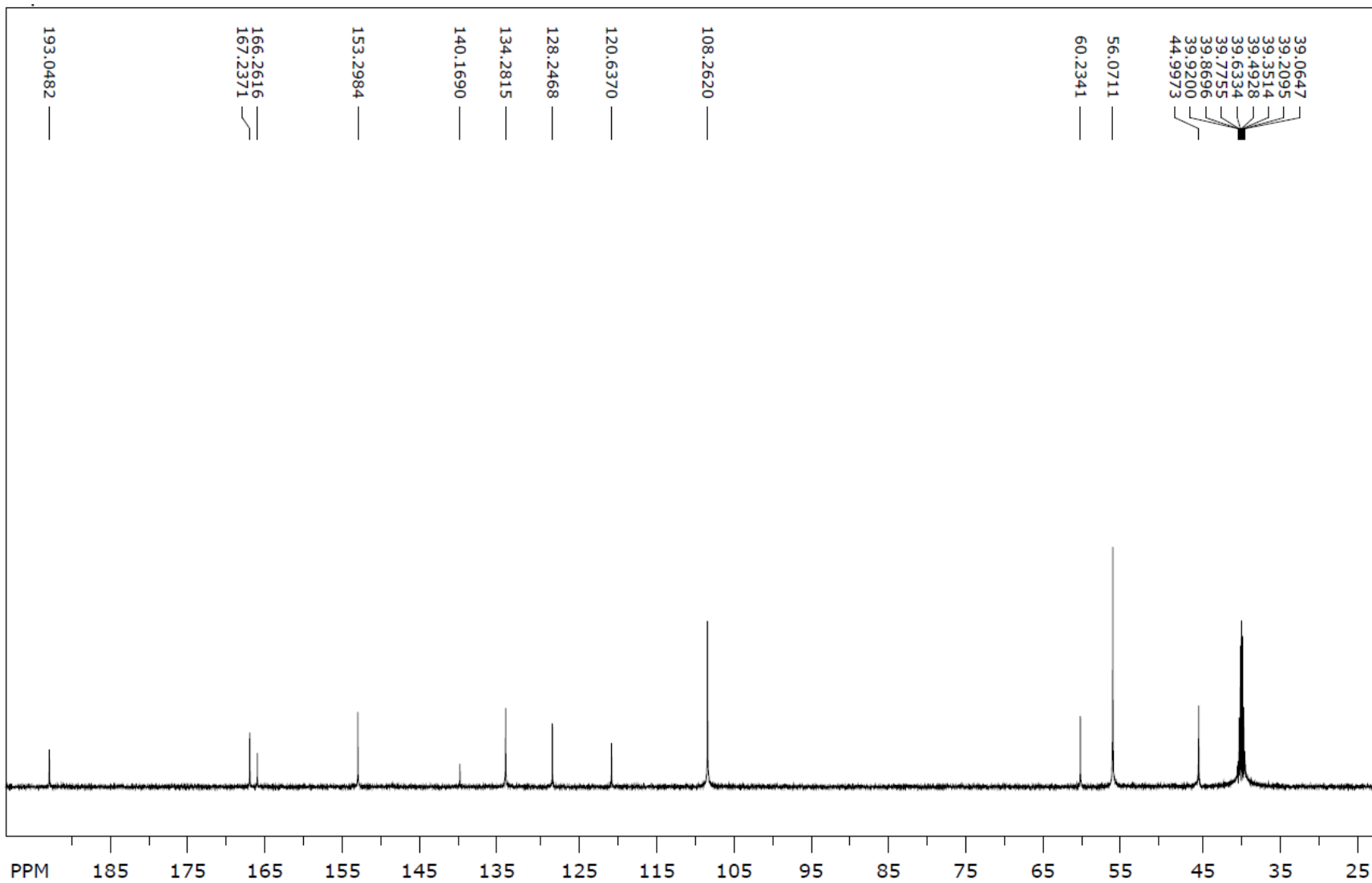
Maseni spektar (8g)



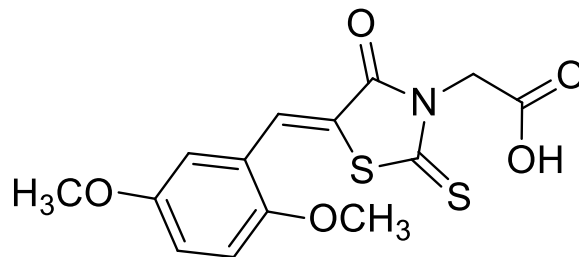
¹H NMR spektr (8g)



¹³C NMR spektr (8g)

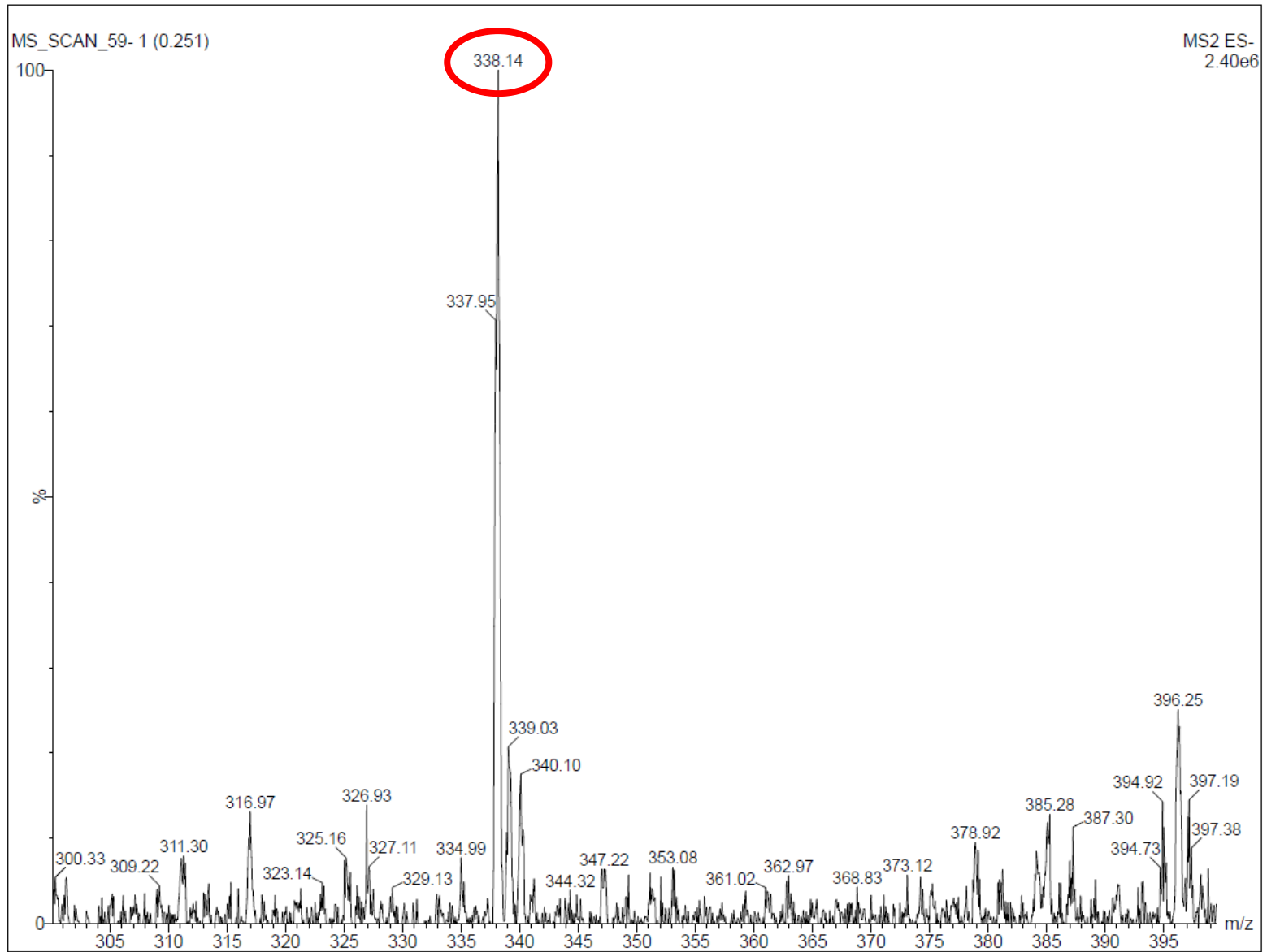


**2-(5-(2,5-dimetoksibenziliden)-4-okso-2-tioksotiazolidin-3-il) octena
kiselina (8h)**

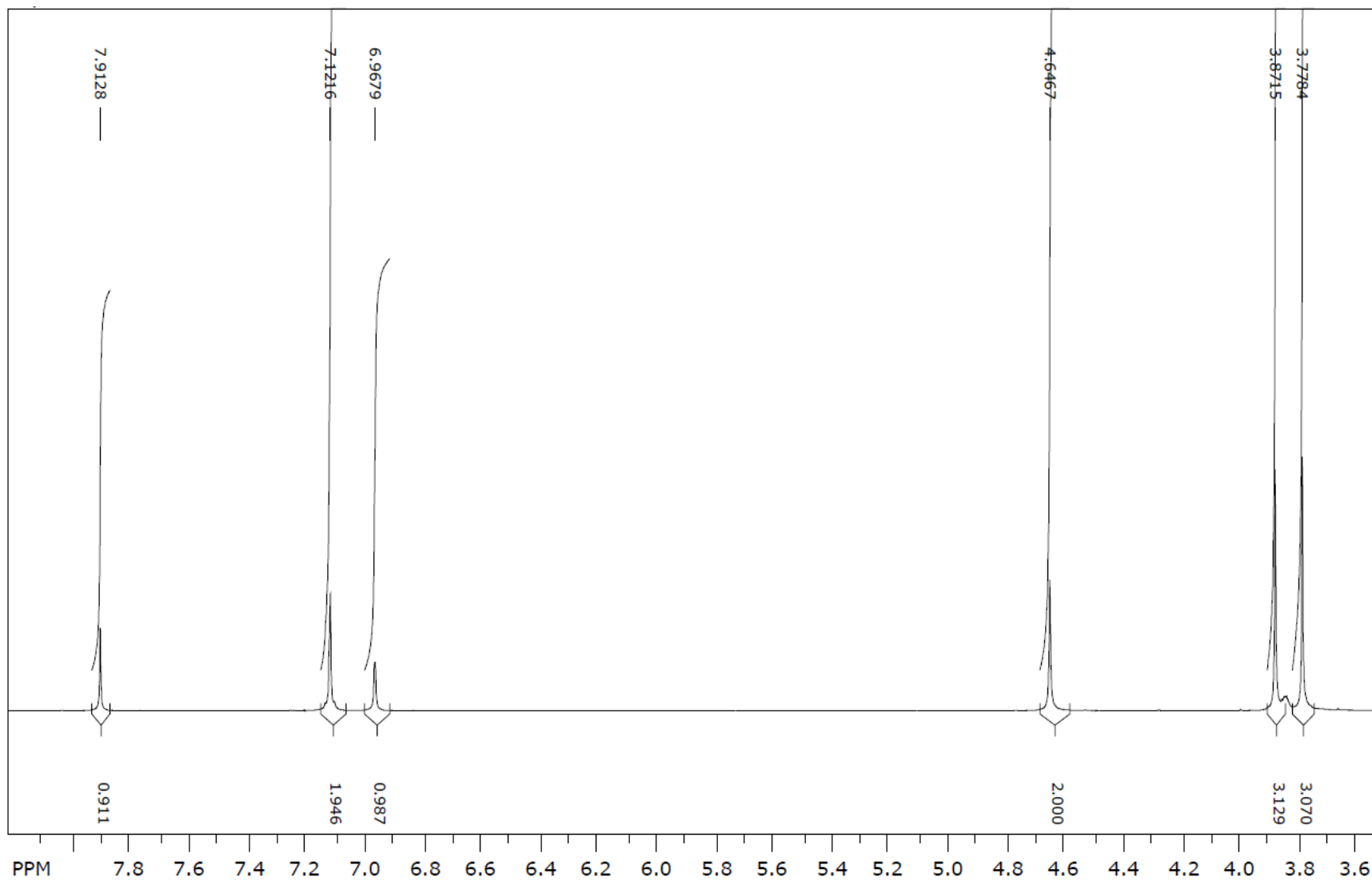


Reaktanti	2,5-dimetoksibenzaldehid (0,7 mmol) i 3-karboksimetilrodanin (0,7 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	339,39 g/mol
Molekulska formula	C ₁₄ H ₁₃ NO ₅ S ₂
Temperatura tališta	170 – 172 °C
Boja kristala	Žuta
R_f	0,73
LC/MS/MS m/z (M-)	338,14
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,91 (s, 1H, CH), 7,12 (s, 2H, arom.), 6,96 (s, 1H, arom.), 4,64 (s, 2H, CH ₂), 3,87 (s, 3H, OCH ₃), 3,77 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,58; 167,15; 166,50; 153,52; 152,21; 128,83; 122,46; 121,65; 119,05; 114,34; 113,26; 56,06; 55,58; 45,71.

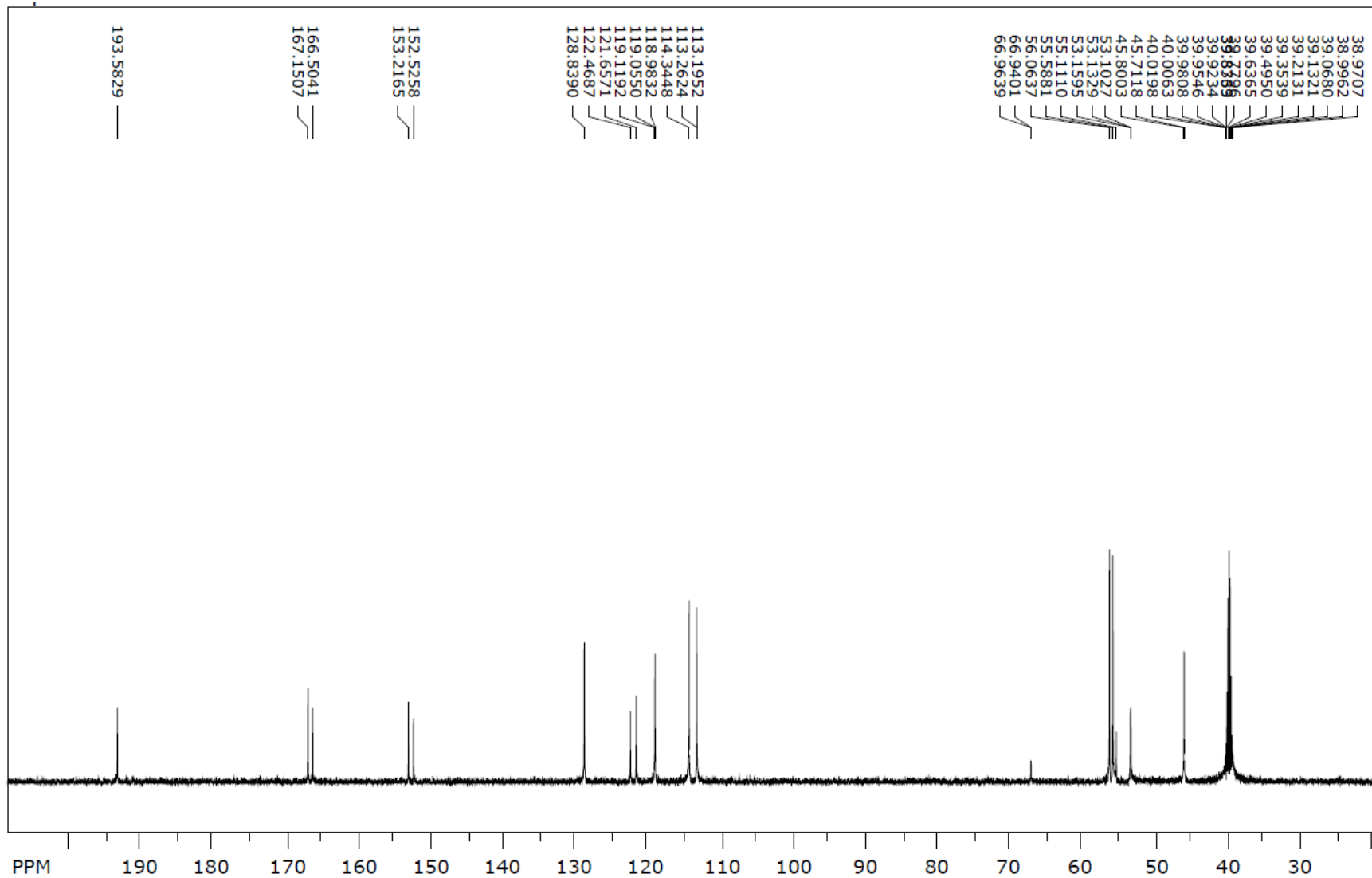
Maseni spektar (8h)



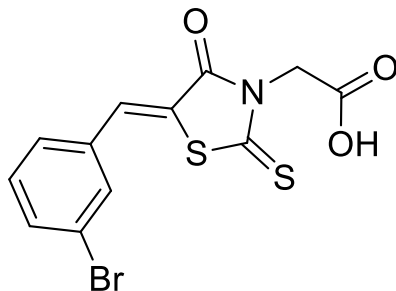
¹H NMR spektr (8h)



¹³C NMR spektr (8h)

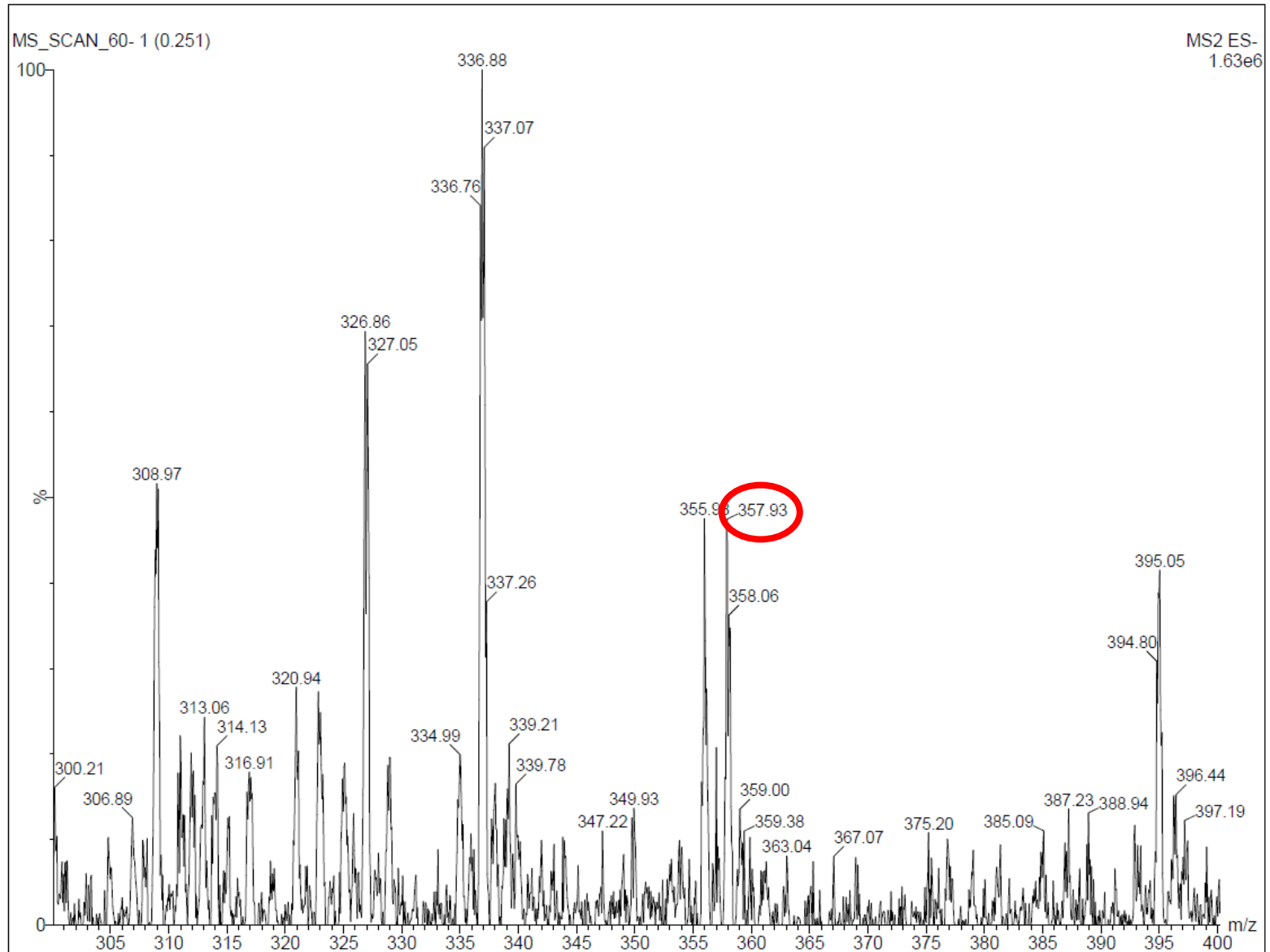


**2-(5-(3-brombenziliden)-4-okso-2-tioksotiazolidin-3-il) octena kiselina
(8i)**

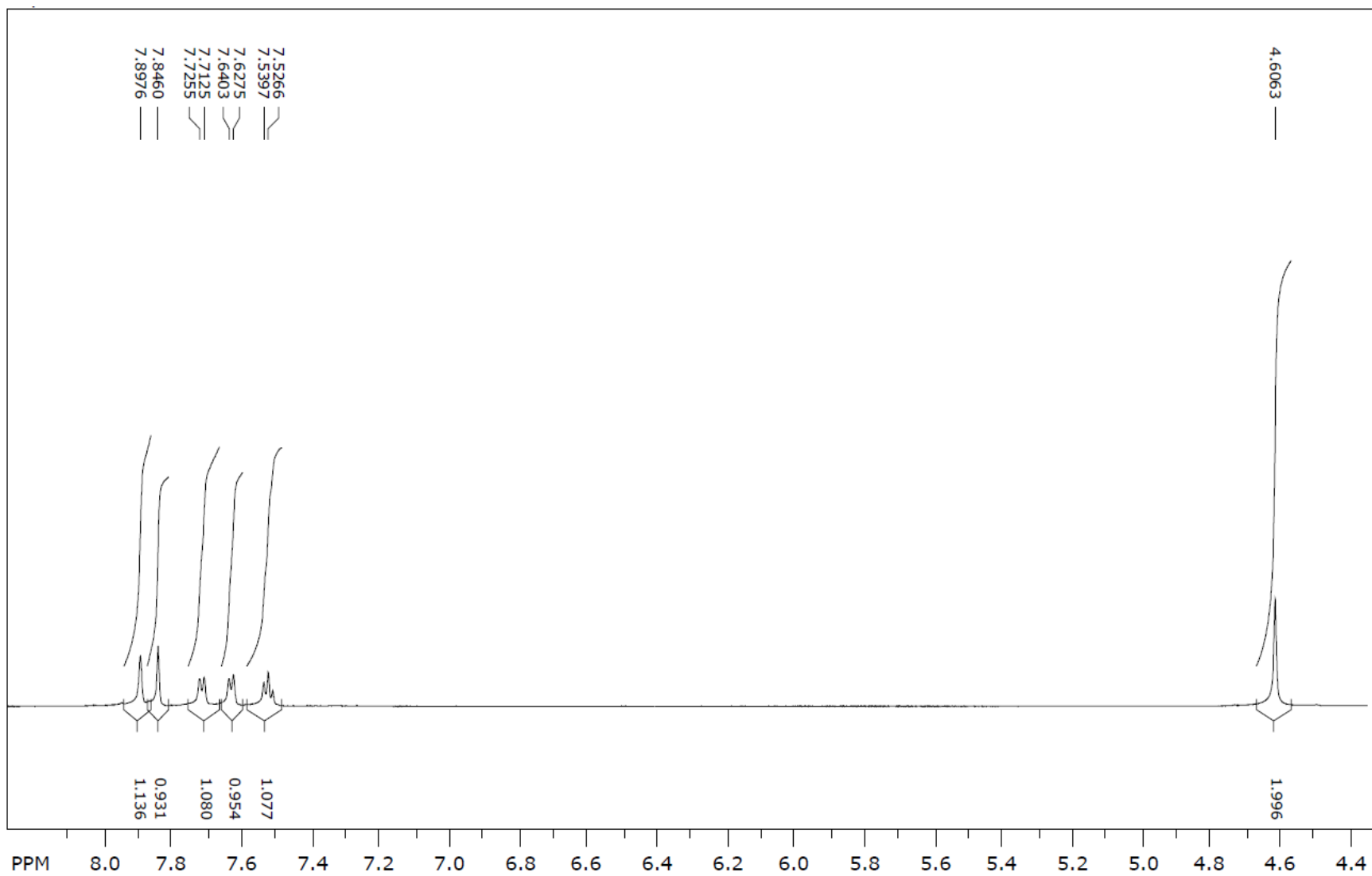


Reaktanti	3-brombenzaldehyd (0,7 mmol) i 3-karboksimetilrodanin (0,7 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	358,23 g/mol
Molekulska formula	C ₁₂ H ₈ BrNO ₃ S ₂
Temperatura tališta	176 – 180 °C
Boja kristala	Svijetlosmeđa
R_f	0,79
LC/MS/MS m/z (M-)	357,93
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,89 (s, 1H, CH), 7,84 (s, 1H, arom.), 7,72 (d, <i>J</i> = 7,80 Hz, 1H, arom.), 7,63 (d, <i>J</i> = 7,68 Hz, 1H, arom.), 7,53 (t, <i>J</i> = 7,83 Hz, 1H, arom.), 4,60 (s, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 192,84; 166,89; 166,32; 135,29; 133,42; 133,38; 131,458; 131,40; 128,56; 123,91; 122,56; 46,21.

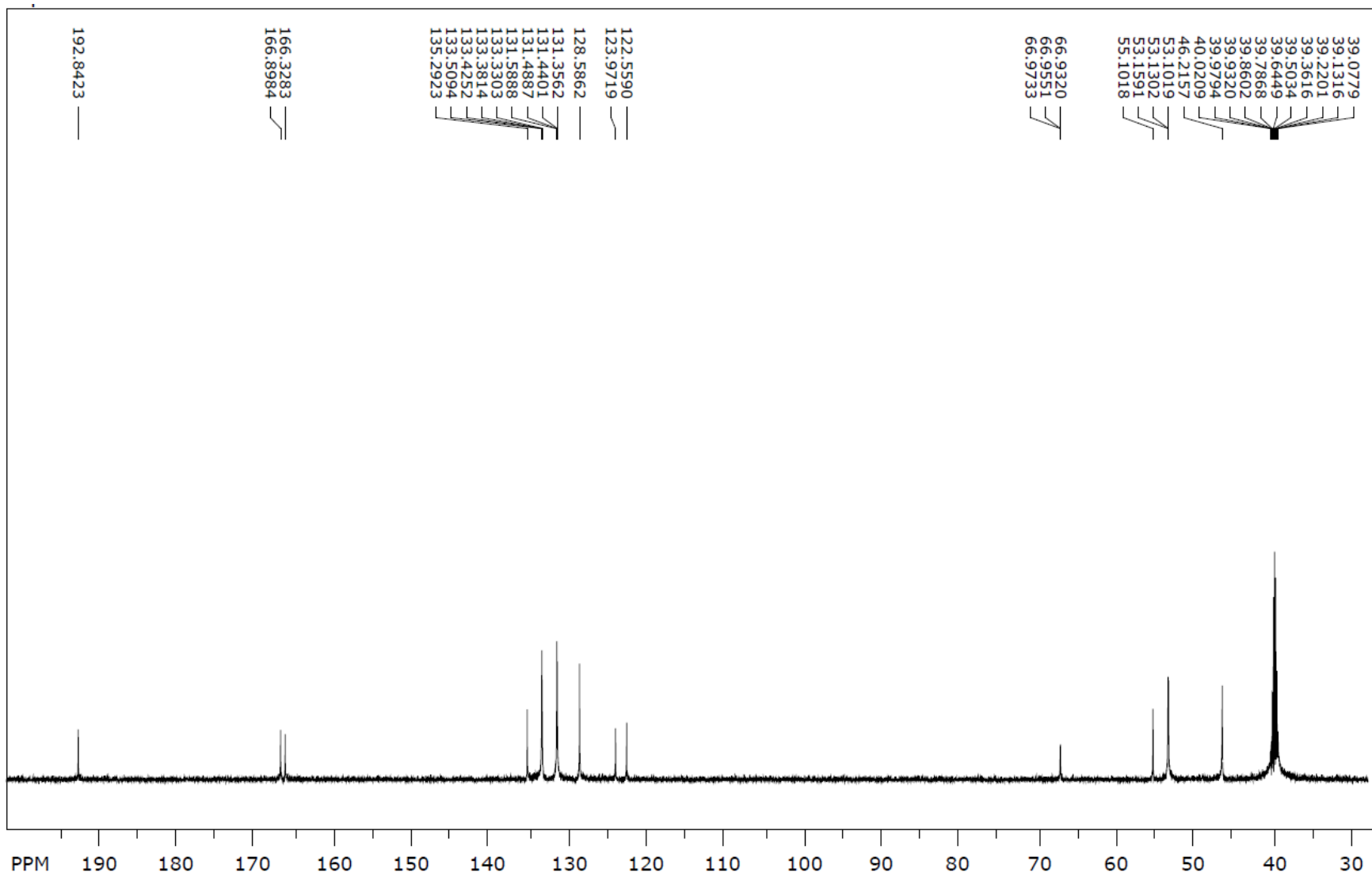
Maseni spektar (8i)



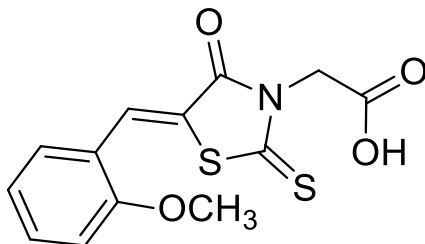
¹H NMR spektr (8i)



¹³C NMR spektr (8i)

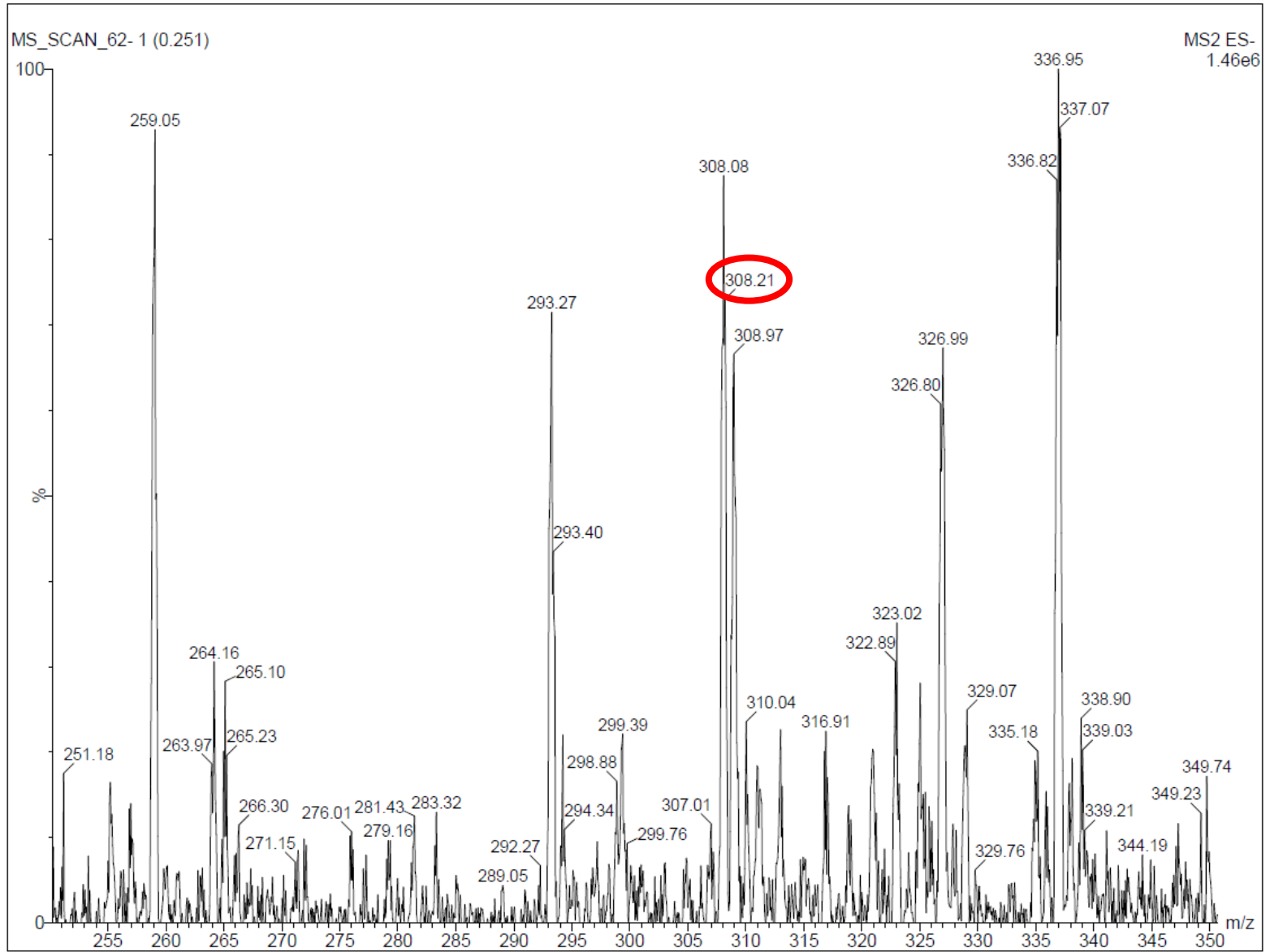


2-(5-(2-metoksibenziliden)-4-okso-2-tioksotiazolidin-3-il) octena kiselina (8j)

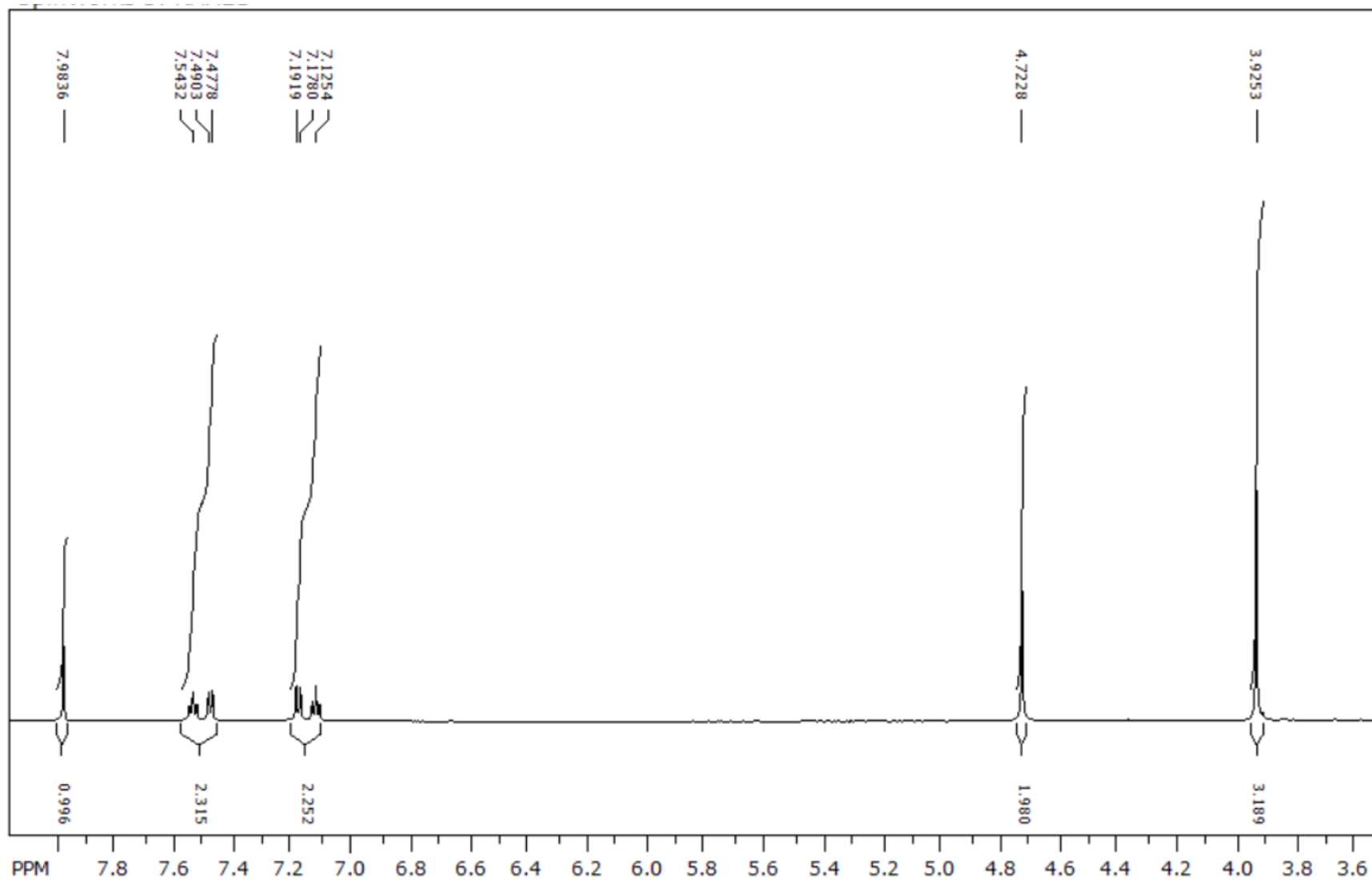


Reaktanti	2-metoksibenzaldehid (0,7 mmol) i 3-karboksimetilrodanin (0,7 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	309,36 g/mol
Molekulska formula	C ₁₃ H ₁₁ NO ₄ S ₂
Temperatura tališta	208 – 211 °C
Boja kristala	Smeđa
R_f	0,78
LC/MS/MS m/z (M-)	308,21
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,98 (s, 1H, CH), 7,54 (t, <i>J</i> = 7,35 Hz, 1H, arom.), 7,48 (d, <i>J</i> = 7,50 Hz, 1H, arom.), 7,18 (d, <i>J</i> = 8,34 Hz, 1H, arom.), 7,13 (t, <i>J</i> = 7,50 Hz, 1H, arom.), 4,72 (s, 2H, CH ₂), 3,92 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,76; 167,46; 166,27; 158,15; 133,50; 130,33; 129,23; 121,85; 121,27; 112,06; 55,77; 45,06.

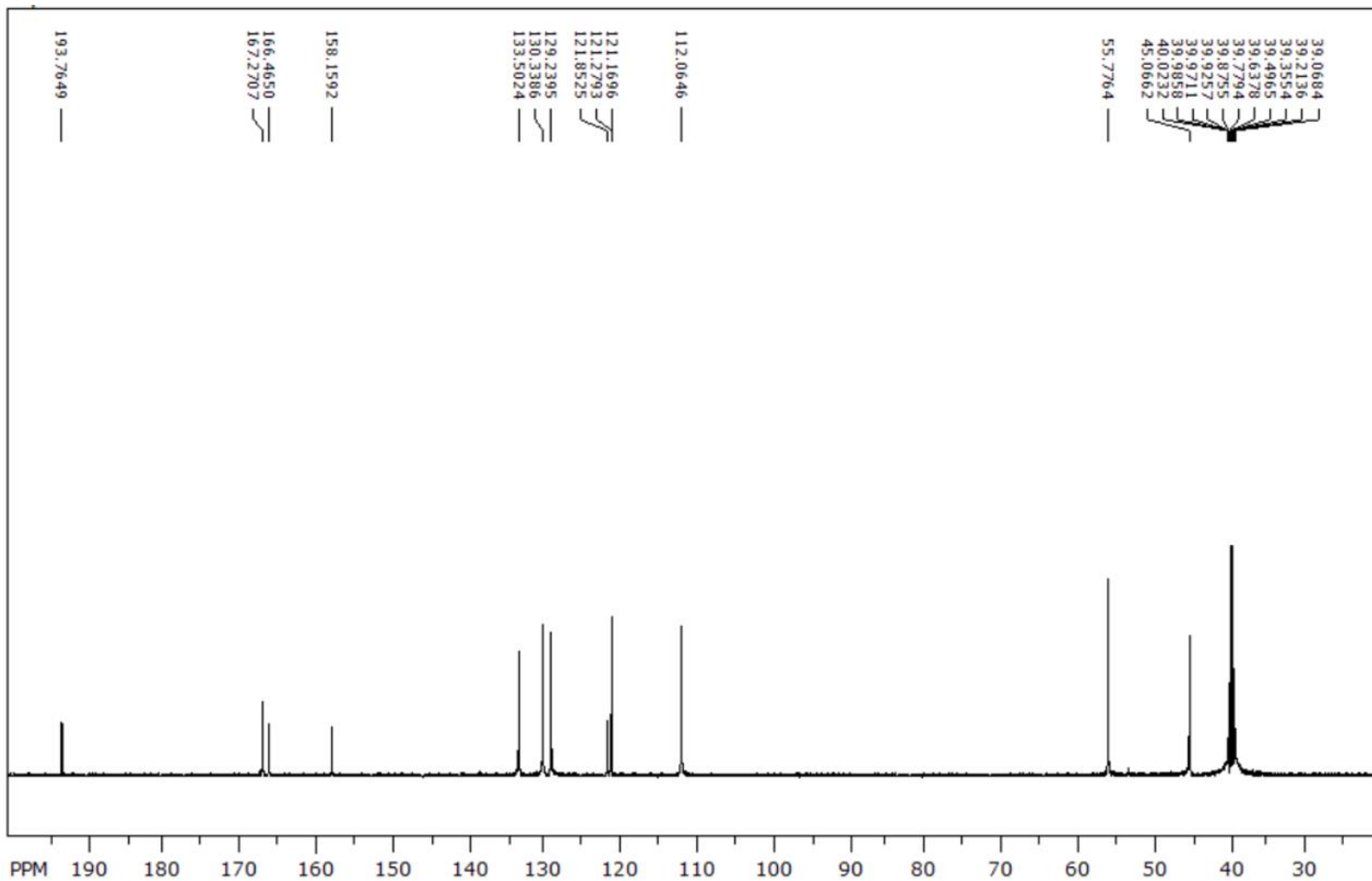
Maseni spektar (8j)



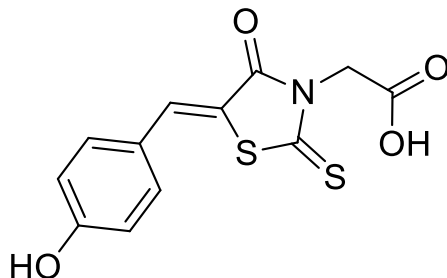
¹H NMR spektr (8j)



¹³C NMR spektr (8j)

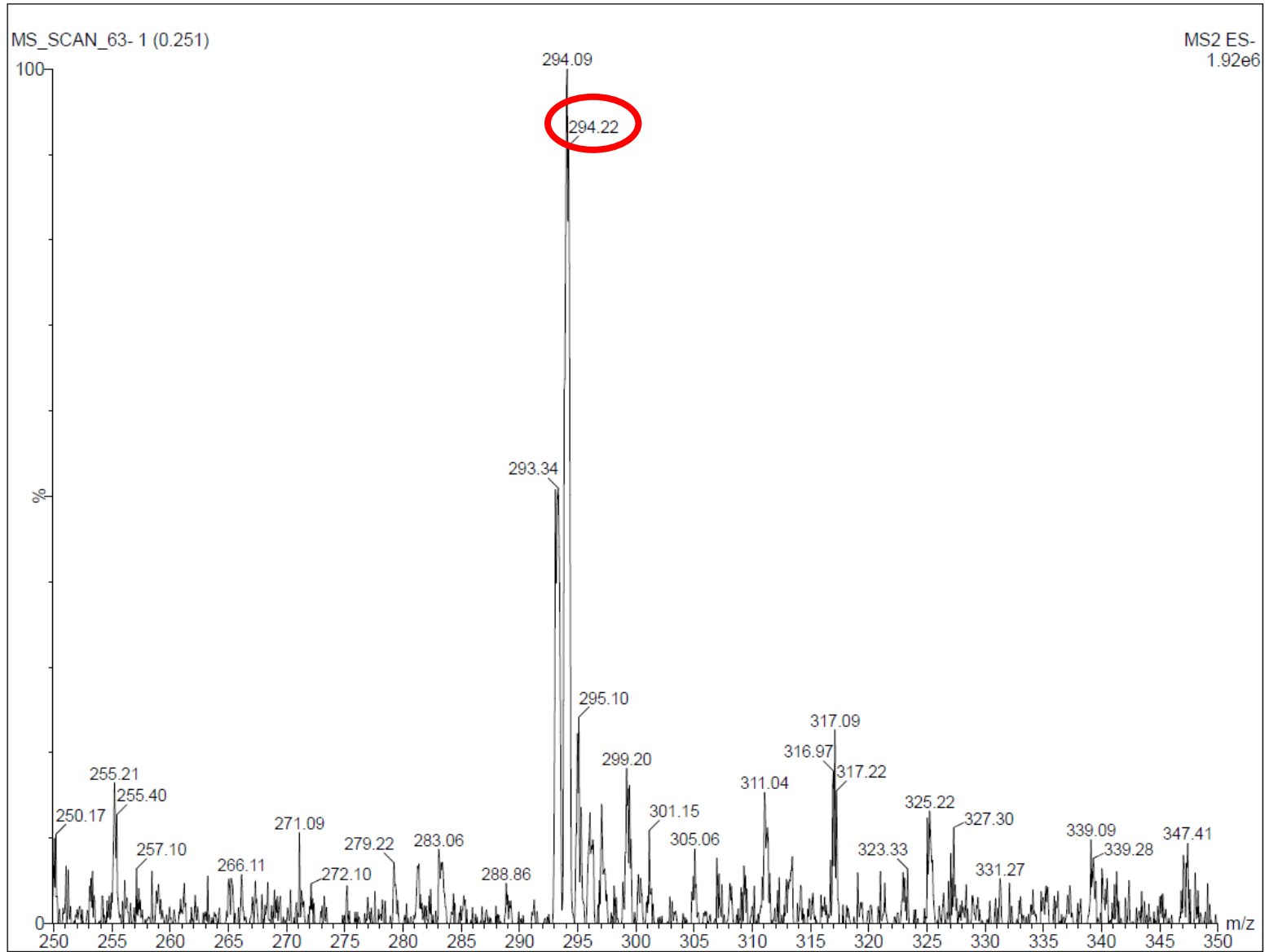


**2-(5-(4-hidroksibenziliden)-4-okso-2-tioksotiazolidin-3-il) octena
kiselina (8k)**

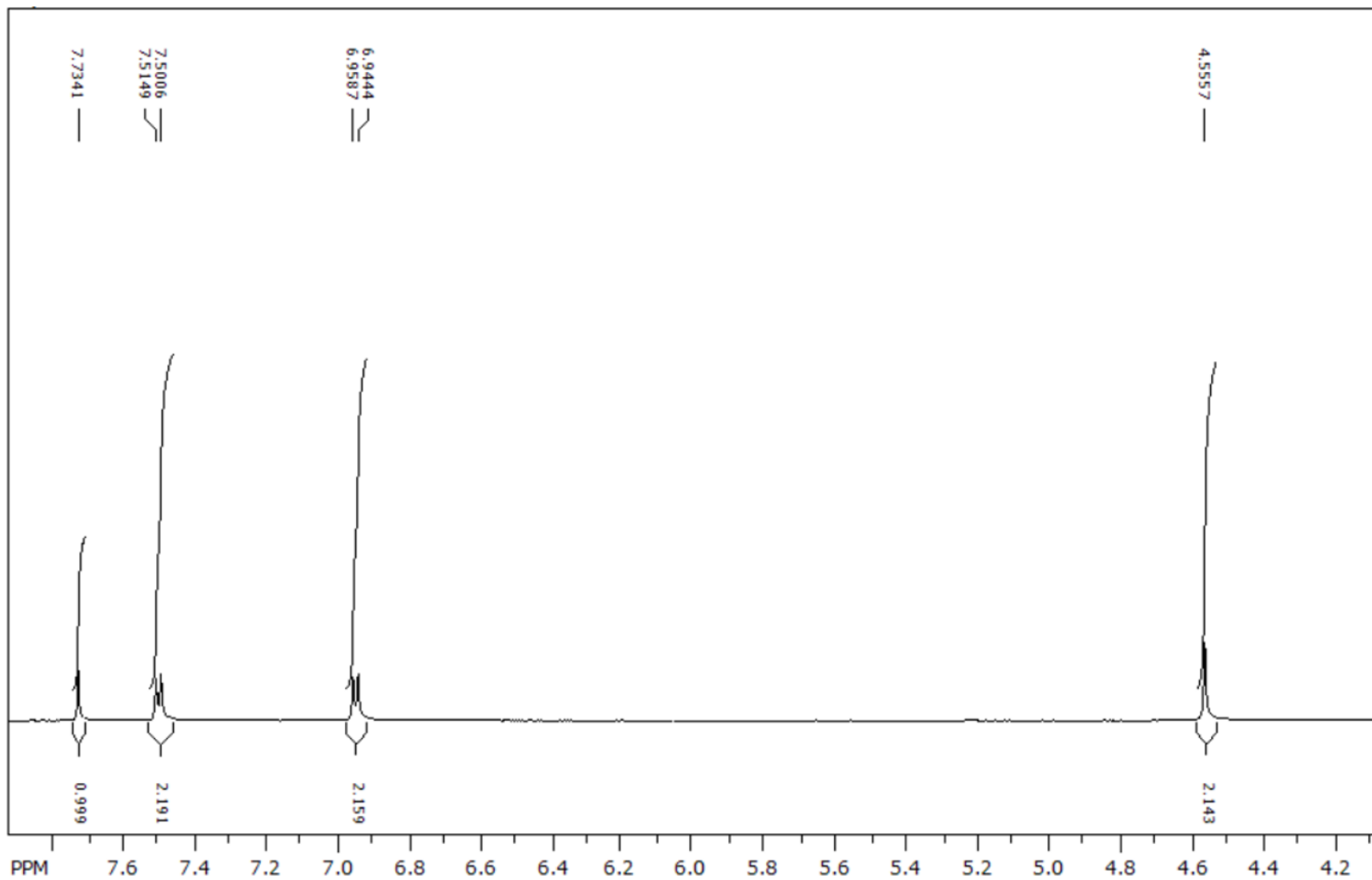


Reaktanti	4-hidroksibenzaldehid (0,7 mmol) i 3-karboksimetilrodanin (0,7 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	295,33 g/mol
Molekulska formula	C ₁₂ H ₉ NO ₄ S ₂
Temperatura tališta	>300 °C (lit. >300°C, Krátky i sur., 2017; >300°C, Zhou i sur., 2006)
Boja kristala	Smeđa
R_f	0,60
LC/MS/MS m/z (M-)	294,22
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,73 (s, 1H, CH), 7,51 (d, <i>J</i> = 8,58 Hz, 2H, arom.), 6,95 (d, <i>J</i> = 8,58 Hz, 2H, arom.), 4,55 (s, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,06; 167,13; 166,71; 161,06; 133,89; 133,28; 123,73; 117,44; 116,68; 46,41.

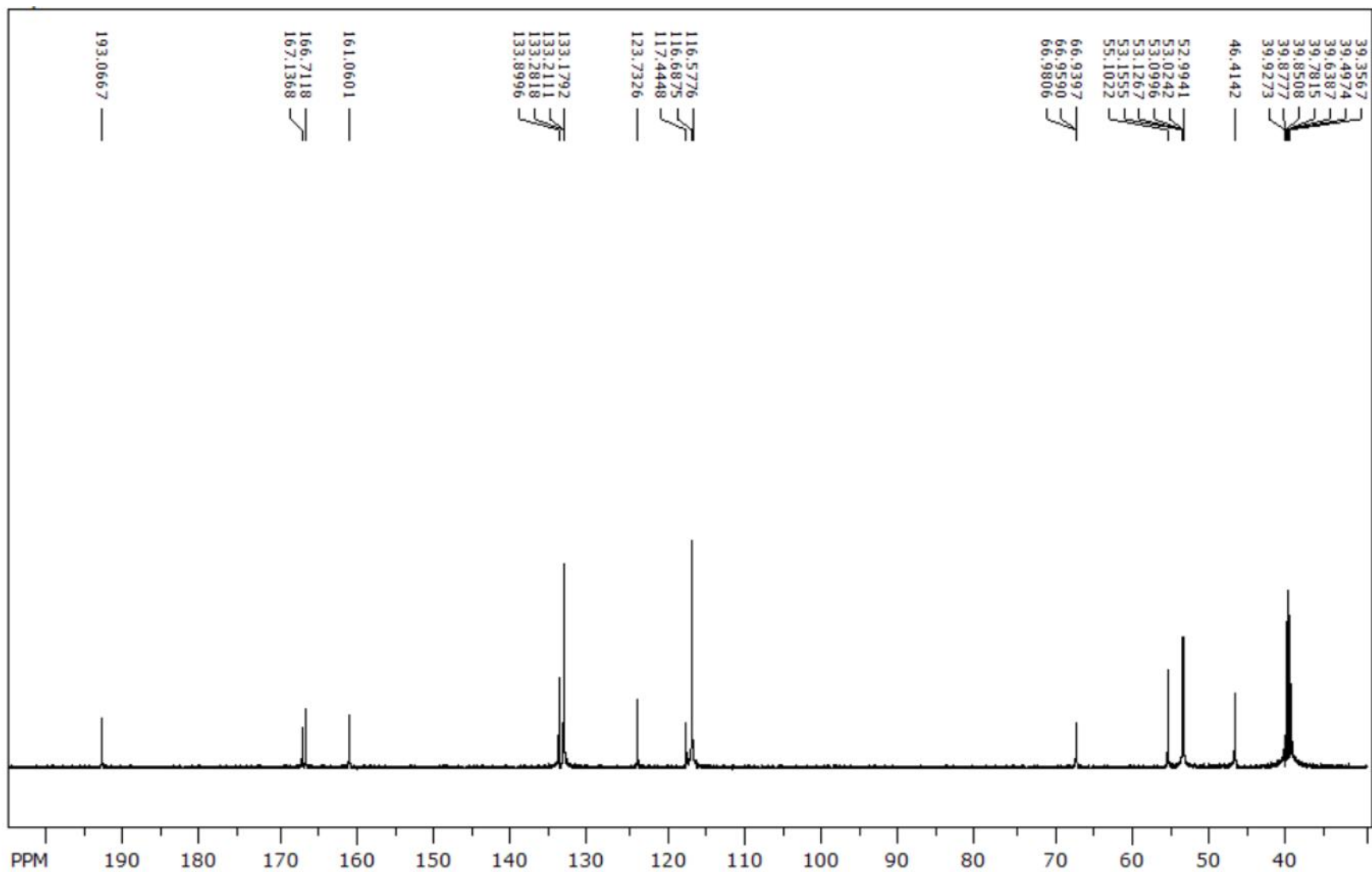
Maseni spektar (8k)



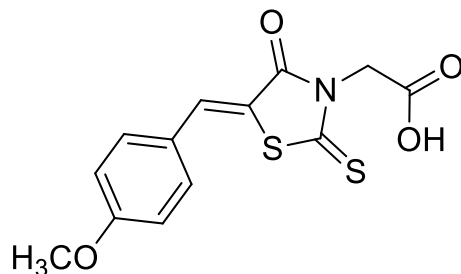
¹H NMR spektr (8k)



¹³C NMR spektar (8k)

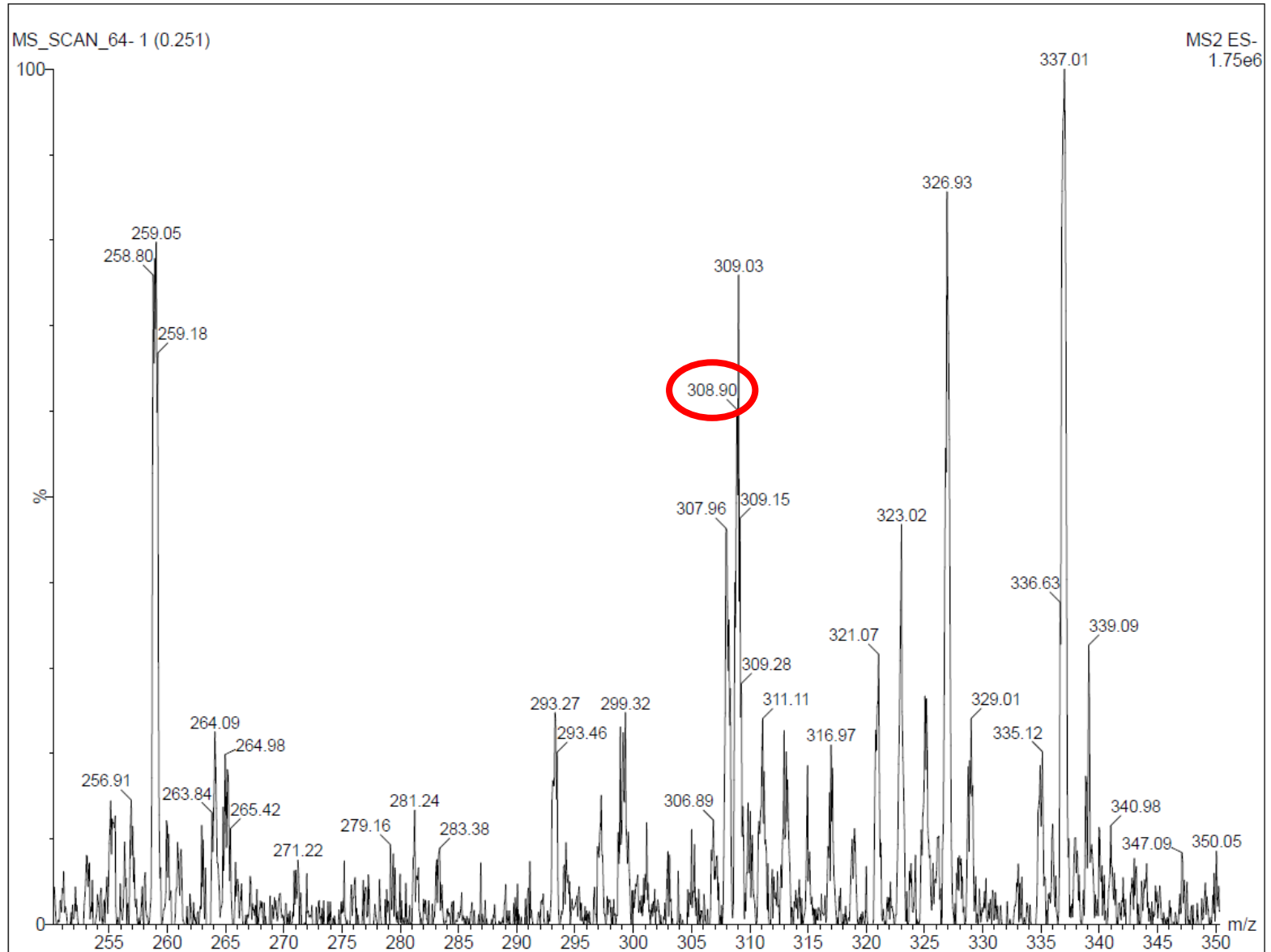


2-(5-(4-metoksibenziliden)-4-okso-2-tioksotiazolidin-3-il) octena kiselina (8l)

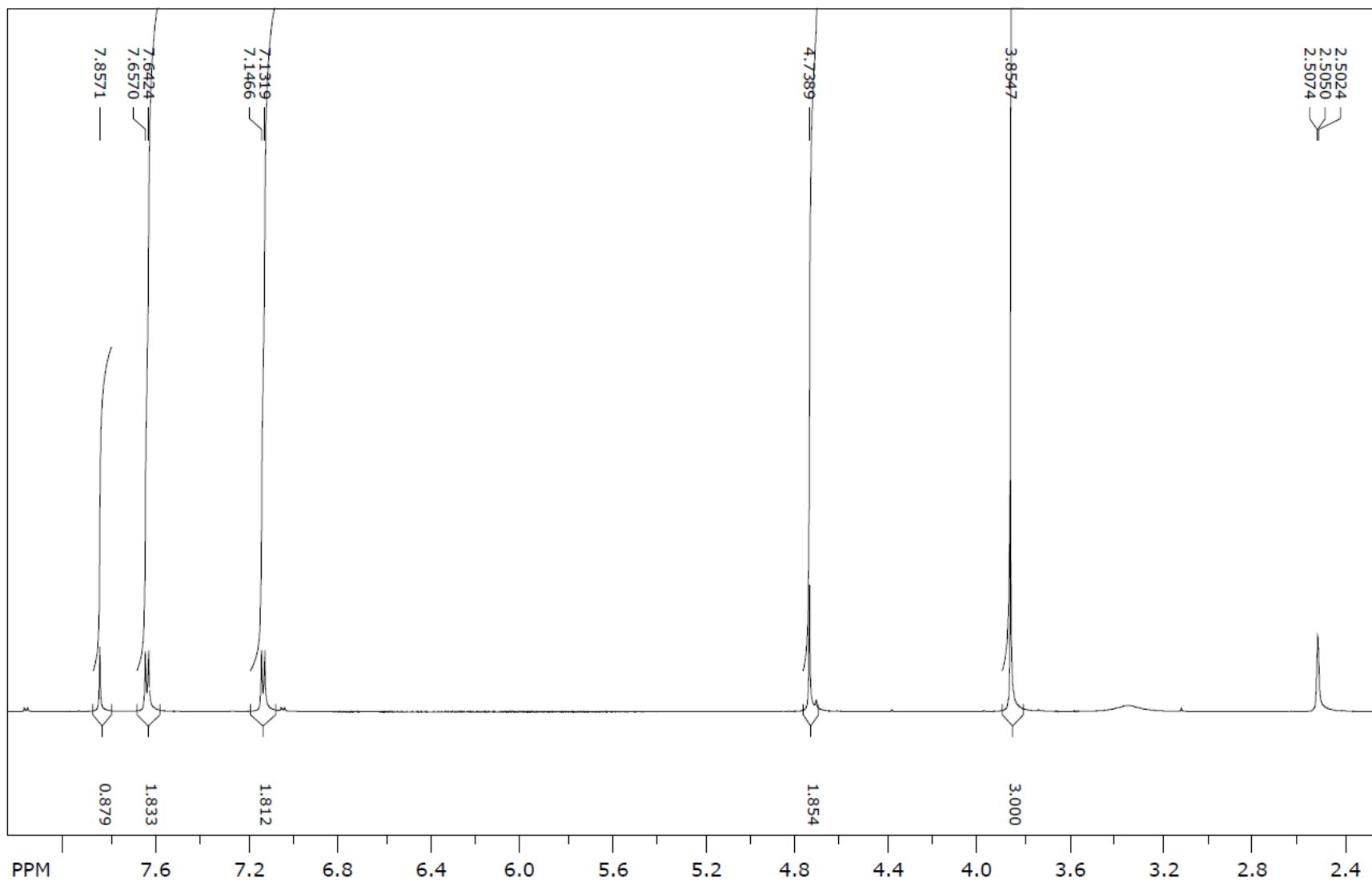


Reaktanti	4-metoksibenzaldehid (0,7 mmol) i 3-karboksimetilrodanin (0,7 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	309,36 g/mol
Molekulska formula	C ₁₃ H ₁₁ NO ₄ S ₂
Temperatura tališta	242 – 244 °C
Boja kristala	Svijetlosmeđa
R_f	0,78
LC/MS/MS <i>m/z</i> (M⁻)	308,90
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,85 (s, 1H, CH), 7,65 (d, <i>J</i> = 8,76 Hz, 2H, arom.), 7,14 (d, <i>J</i> = 8,82 Hz, 2H, arom.), 4,73 (s, 2H, CH ₂), 3,85 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,06; 167,29; 166,39; 161,73; 134,12; 133,08; 124,34; 118,43; 115,19; 55,59; 44,95.

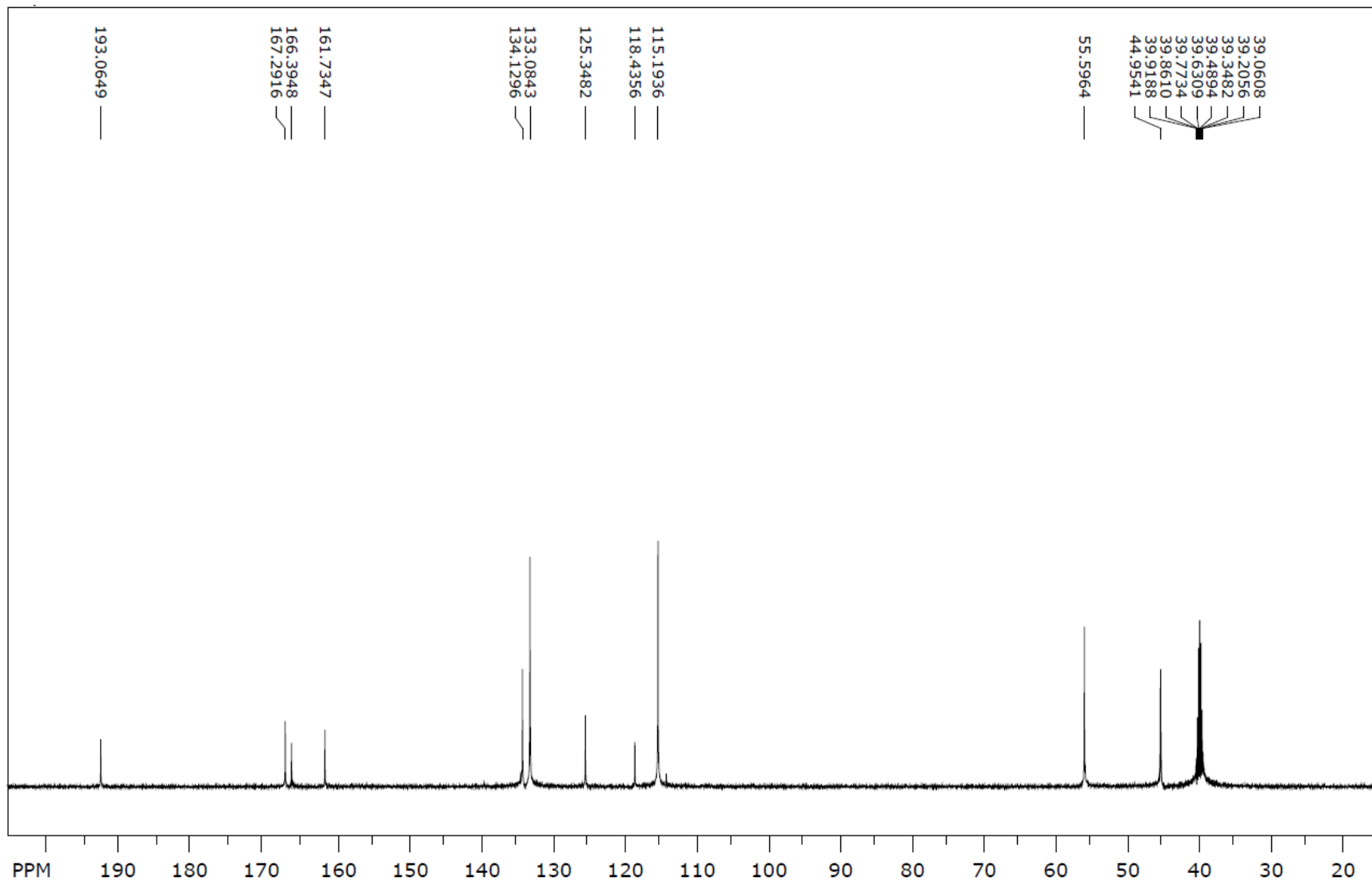
Maseni spektr (8l)



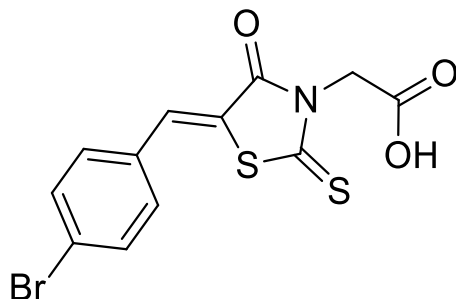
¹H NMR spektr (8I)



¹³C NMR spektr (8l)

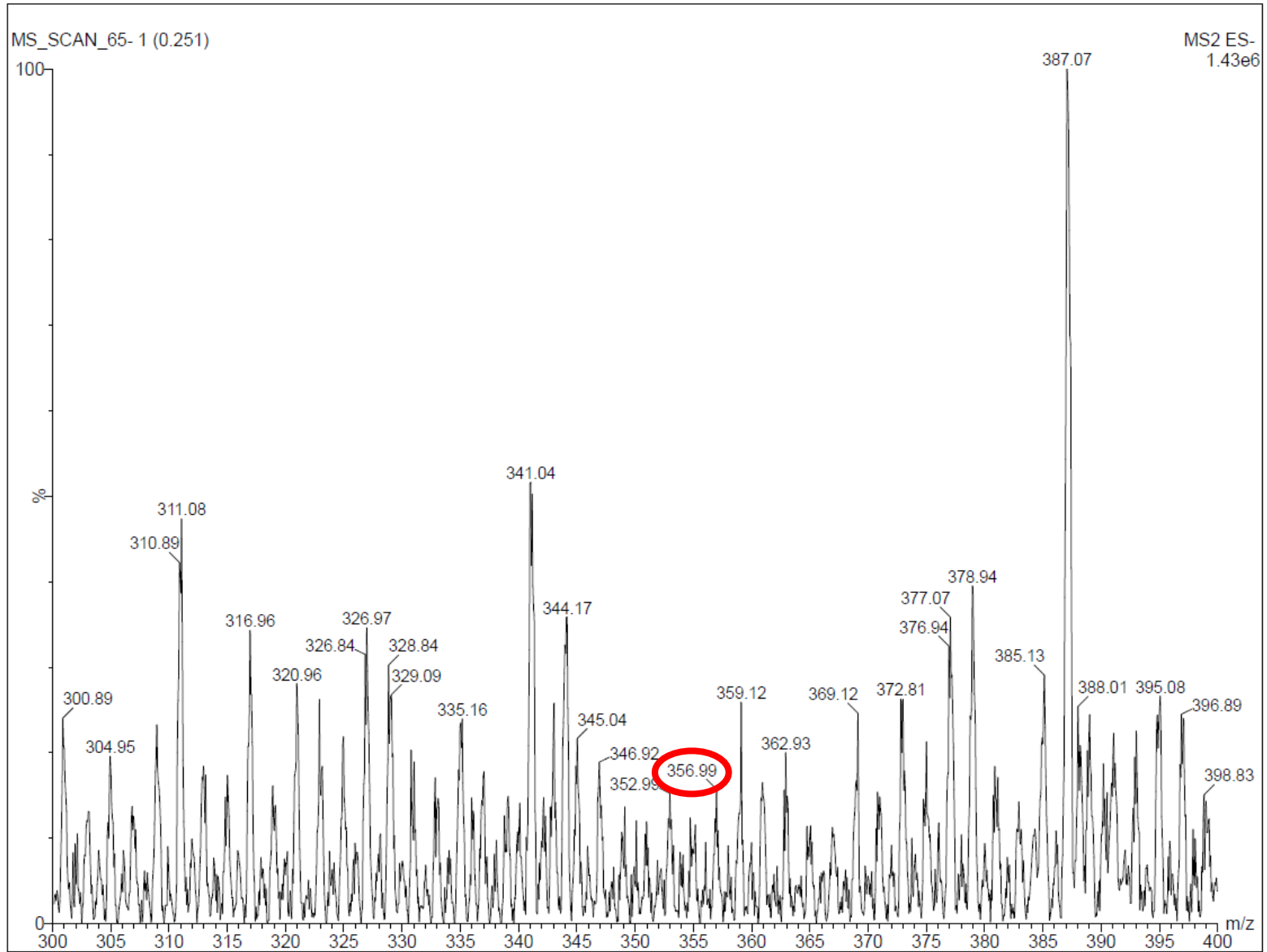


**2-(5-(4-brombenziliden)-4-okso-2-tioksotiazolidin-3-il) octena kiselina
(8m)**

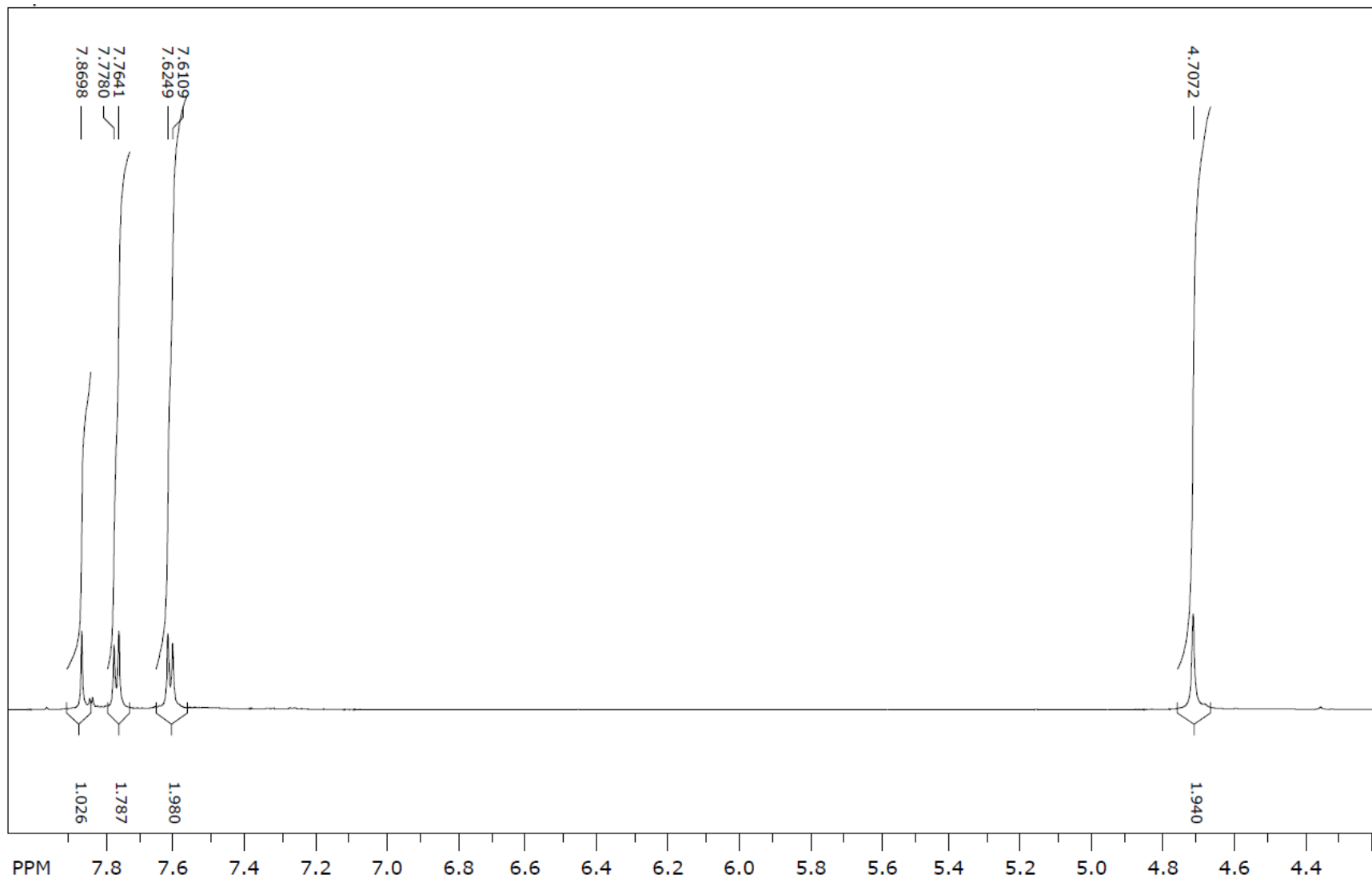


Reaktanti	4-brombenzalhid (0,7 mmol) i 3-karboksimetilrodanin (0,7 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	358,23 g/mol
Molekulska formula	C ₁₂ H ₈ BrNO ₃ S ₂
Temperatura tališta	228 – 231 °C
Boja kristala	Smeđa
R_f	0,79
LC/MS/MS <i>m/z</i> (M-)	356,99
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,86 (s, 1H, CH), 7,77 (d, <i>J</i> = 8,34 Hz, 2H, arom.), 7,62 (d, <i>J</i> = 8,40 Hz, 2H, arom.), 4,70 (s, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 192,92; 166,32; 132,51; 132,42; 132,03; 124,80; 122,76; 45,38.

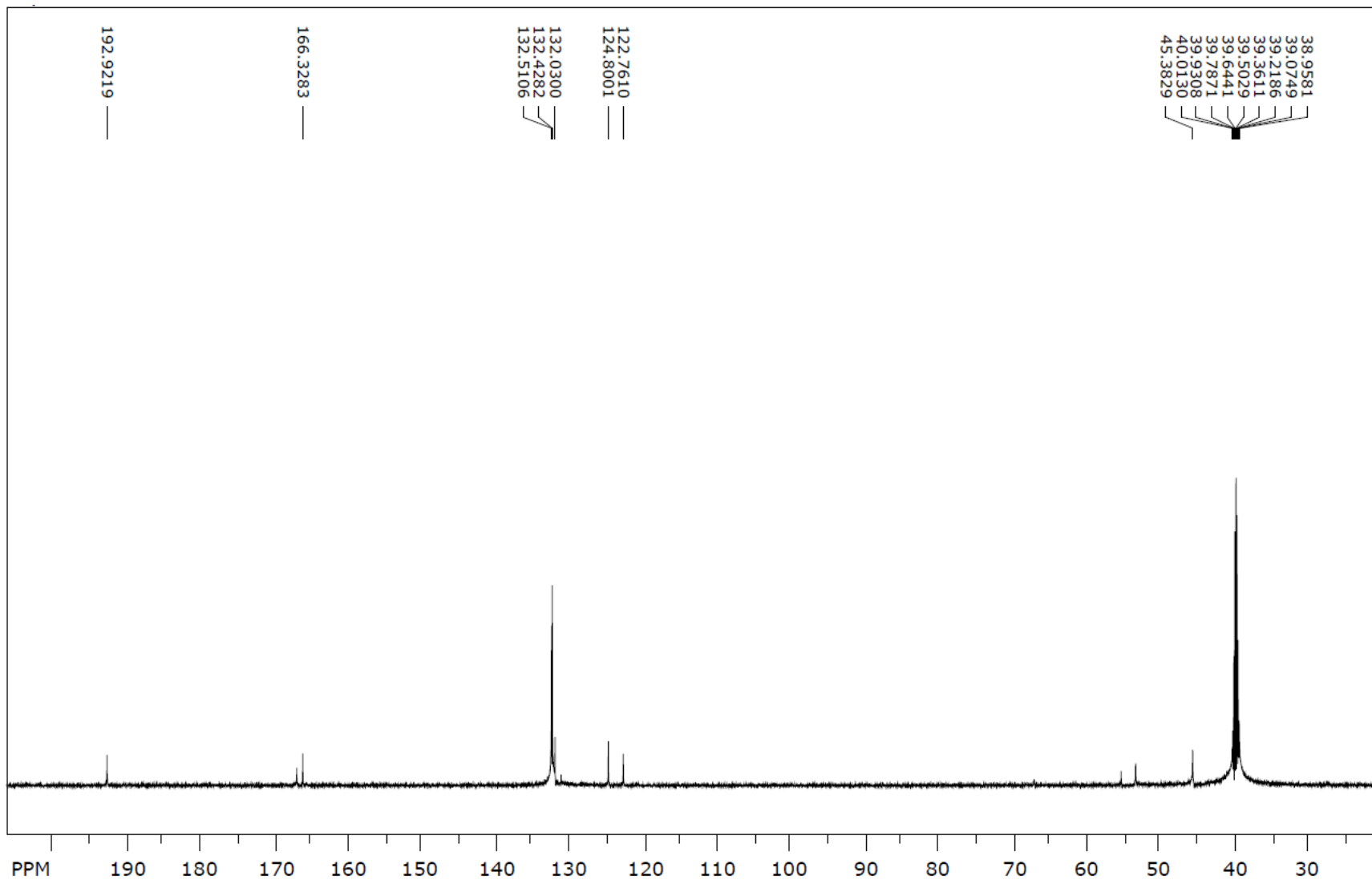
Maseni spektar (8m)



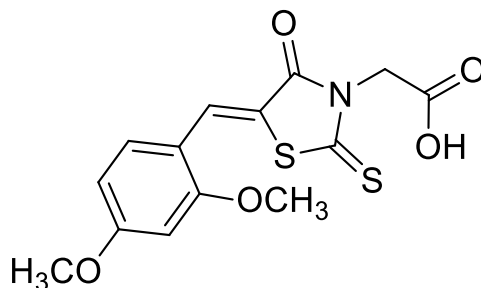
¹H NMR spektr (8m)



¹³C NMR spektr (8m)

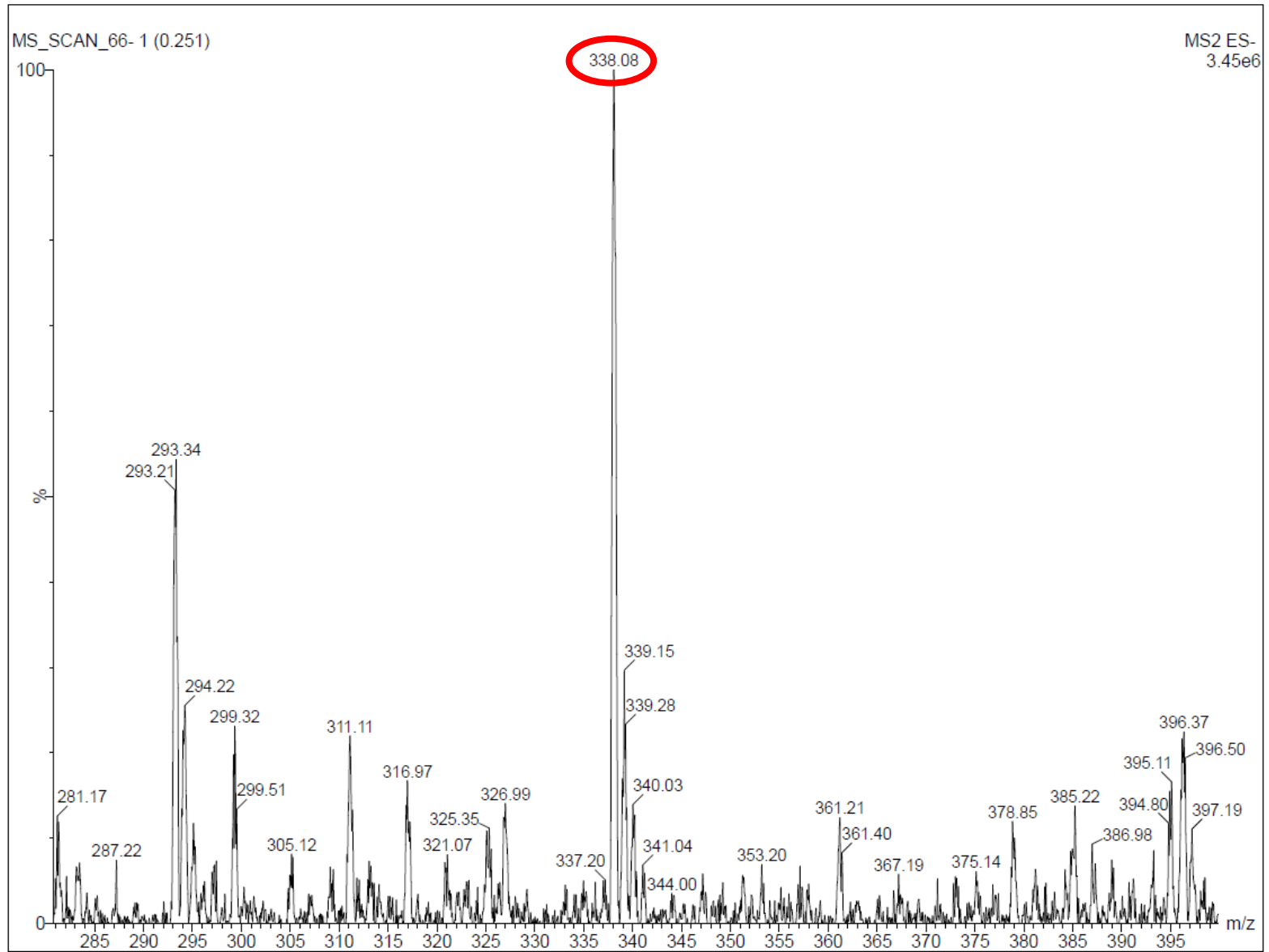


**2-(5-(2,4-dimetoksibenziliden)-4-okso-2-tioksotiazolidin-3-il) octena
kiselina (8n)**

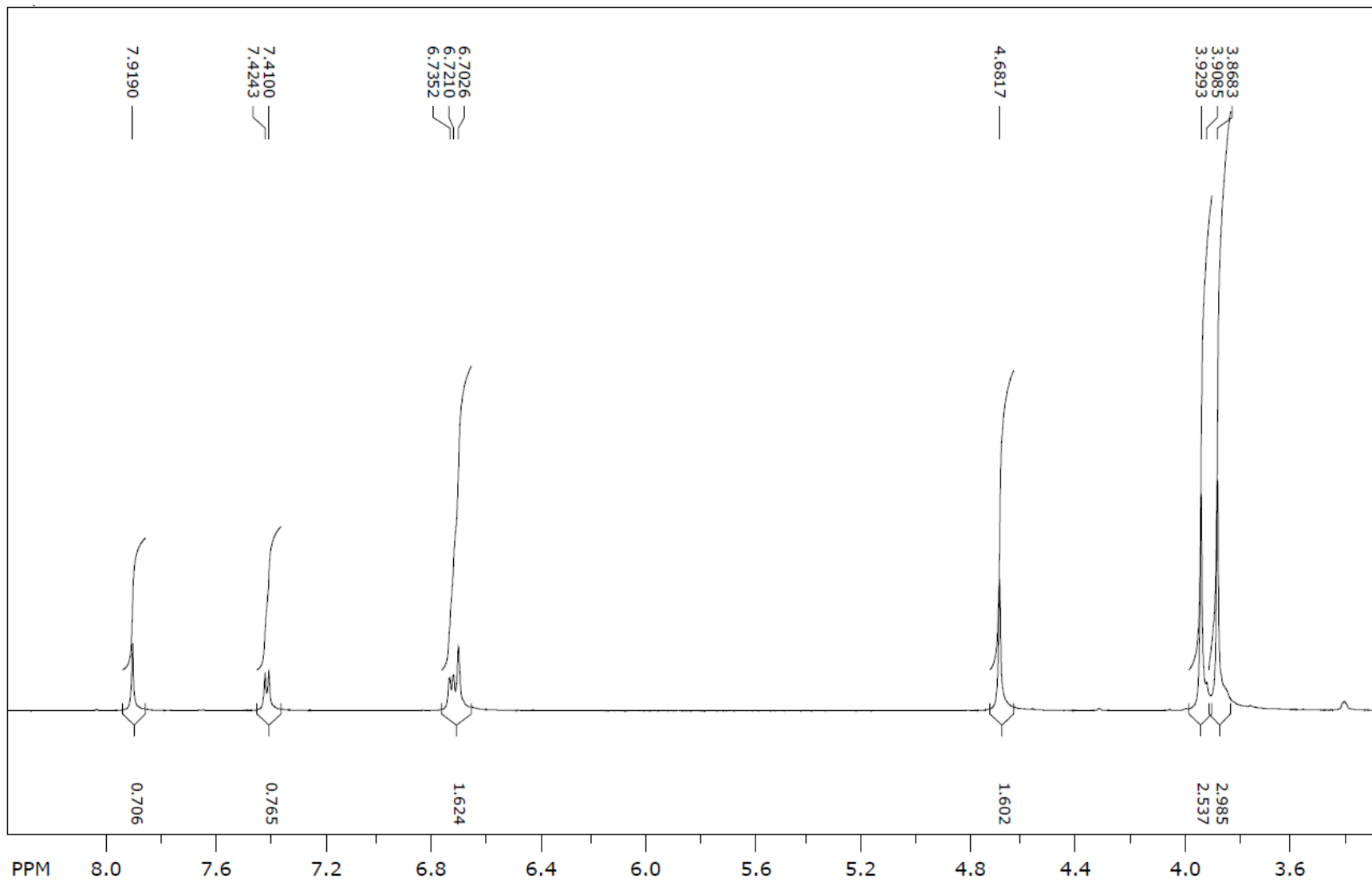


Reaktanti	2,4-dimetoksibenzaldehid (0,7 mmol) i 3-karboksimetilrodanin (0,7 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	339,39 g/mol
Molekulska formula	C ₁₄ H ₁₃ NO ₅ S ₂
Temperatura tališta	224 – 225 °C
Boja kristala	Crvena
R_f	0,71
LC/MS/MS m/z (M-)	338,09
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,91 (s, 1H, CH), 7,42 (d, <i>J</i> = 8,58 Hz, 1H, arom.), 6,72 (t, <i>J</i> = 8,52; 11,04 Hz, 2H, arom.), 4,68 (s, 2H, CH ₂), 3,92 (s, 3H, OCH ₃), 3,86 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,55; 167,30; 166,63; 164,05; 160,13; 132,18; 129,26; 118,12; 114,22; 107,10; 98,55; 55,93; 55,77; 45,25.

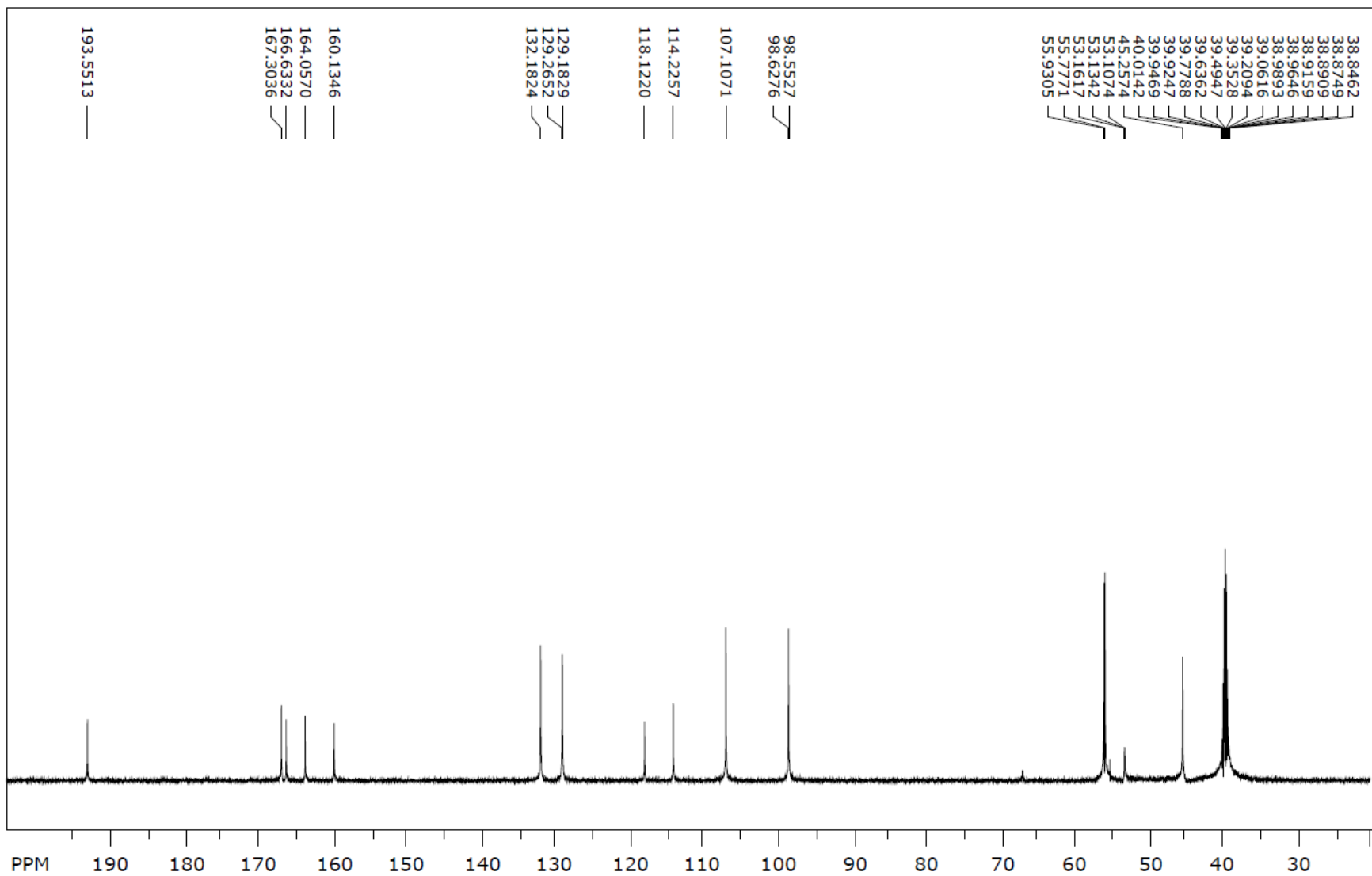
Maseni spektar (8n)



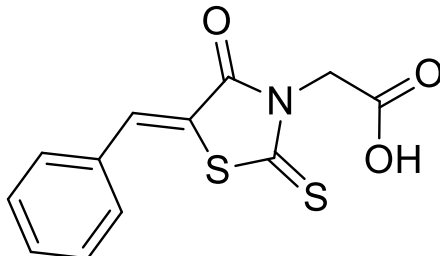
¹H NMR spektr (8n)



¹³C NMR spektr (8n)

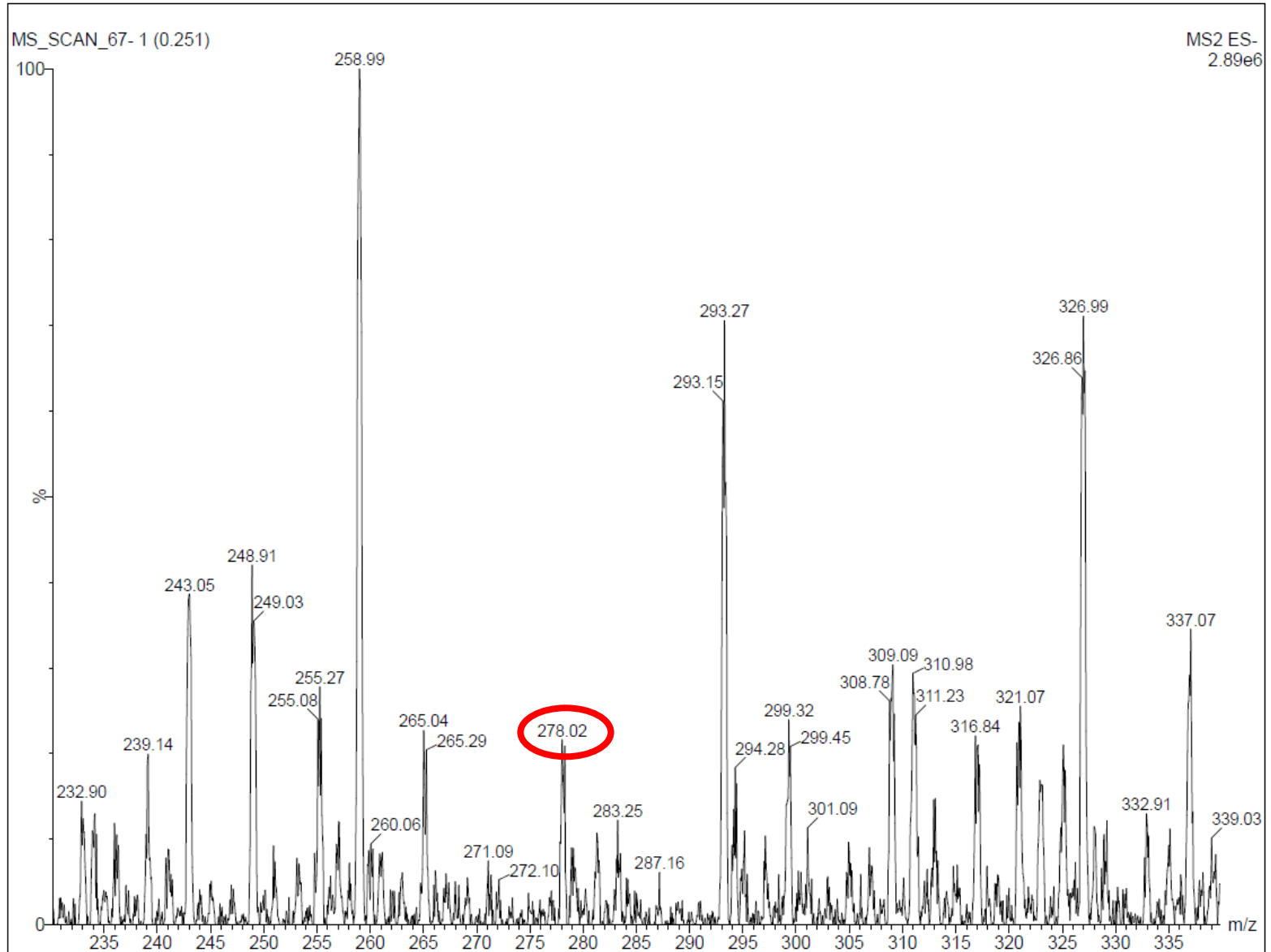


2-(5-benziliden-4-okso-2-tioksotiazolidin-3-il) octena kiselina (8o)

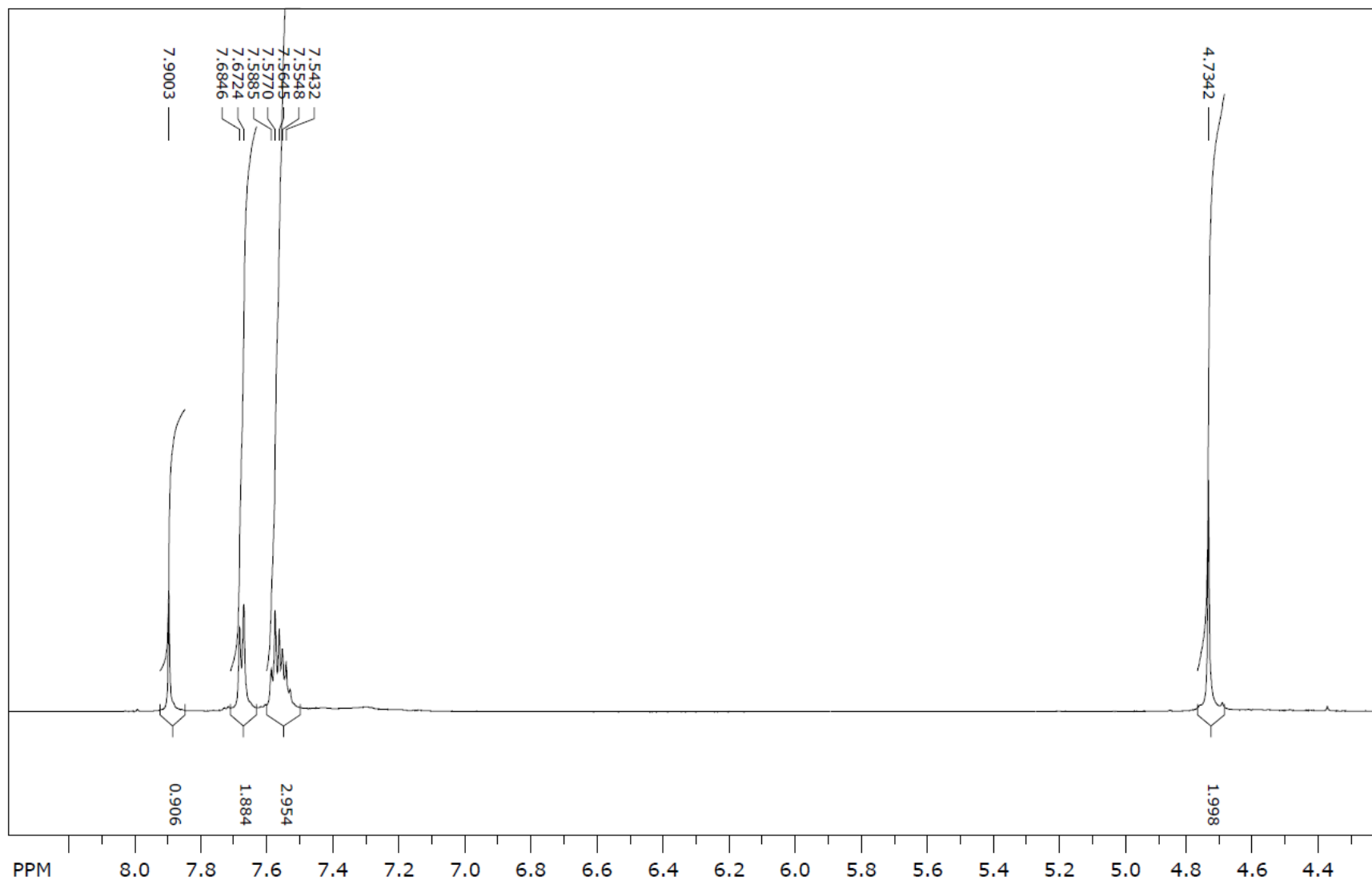


Reaktanti	Benzaldehid (0,7 mmol) i 3-karboksimetilrodanin (0,7 mmol)
Metoda pročišćavanja	Ispran etanolom
Molekulska masa	279,33 g/mol
Molekulska formula	C ₁₂ H ₉ NO ₃ S ₂
Temperatura tališta	217 – 219 °C (lit. 202 – 205 °C, Zhou i sur., 2006)
Boja kristala	Smeđa
R_f	0,72
LC/MS/MS m/z (M-)	278,02
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,90 (s, 1H, CH), 7,68 (d, <i>J</i> = 7,32 Hz, 2H, arom.), 7,54 – 7,59 (m, 3H, arom.), 4,73 (s, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 193,25; 167,22; 166,34; 133,85; 132,80; 131,17; 130,72; 129,52; 121,88; 45,15.

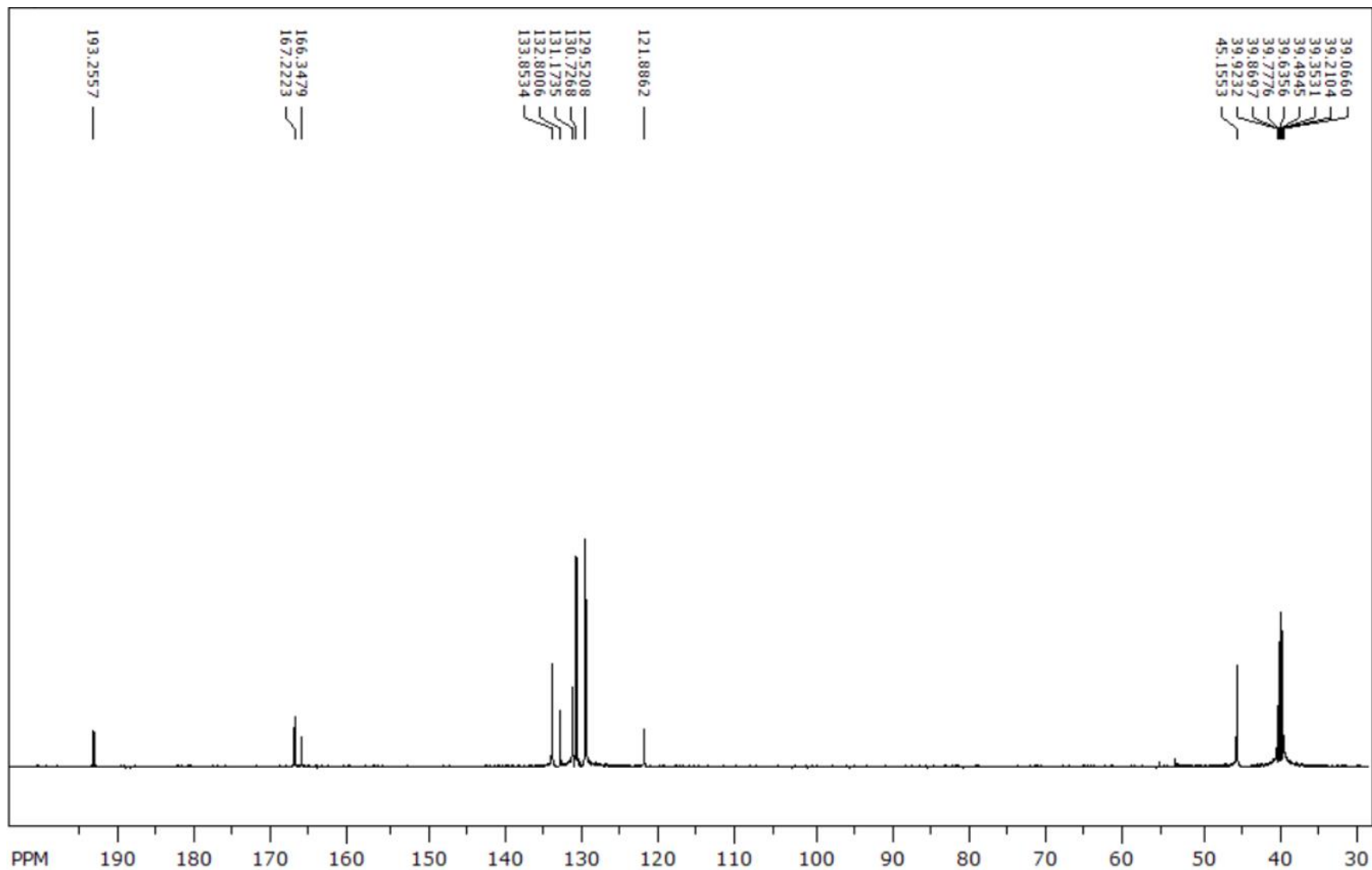
Maseni spektr (8o)



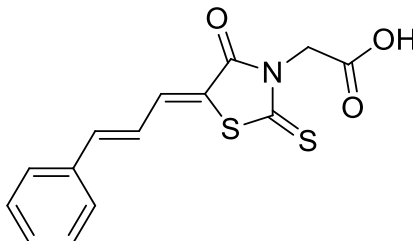
¹H NMR spektr (8o)



¹³C NMR spektr (8o)

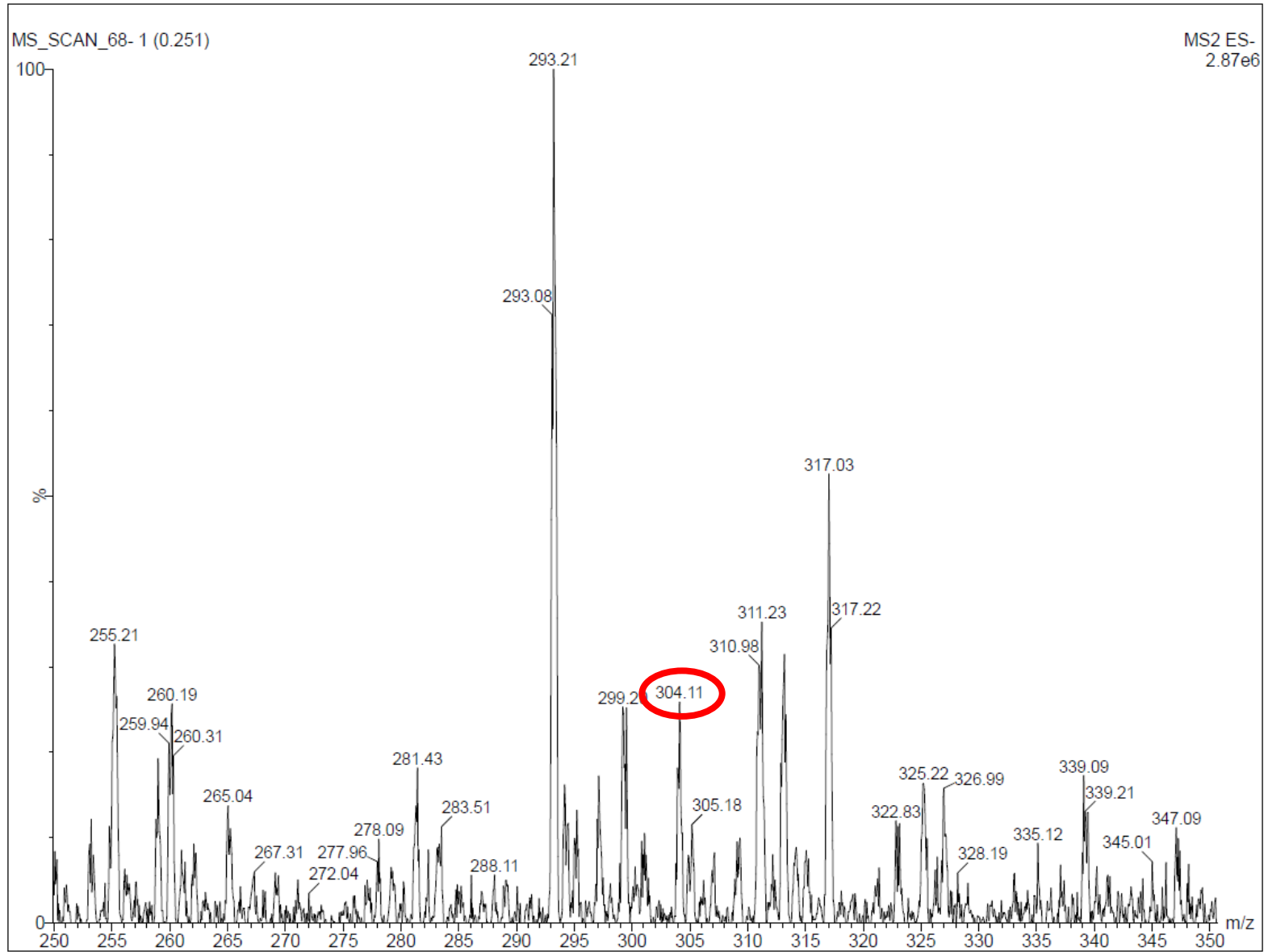


2-(4-okso-5-(3-fenilaliliden)-2-tioksotiazolidin-3-il) octena kiselina (8p)

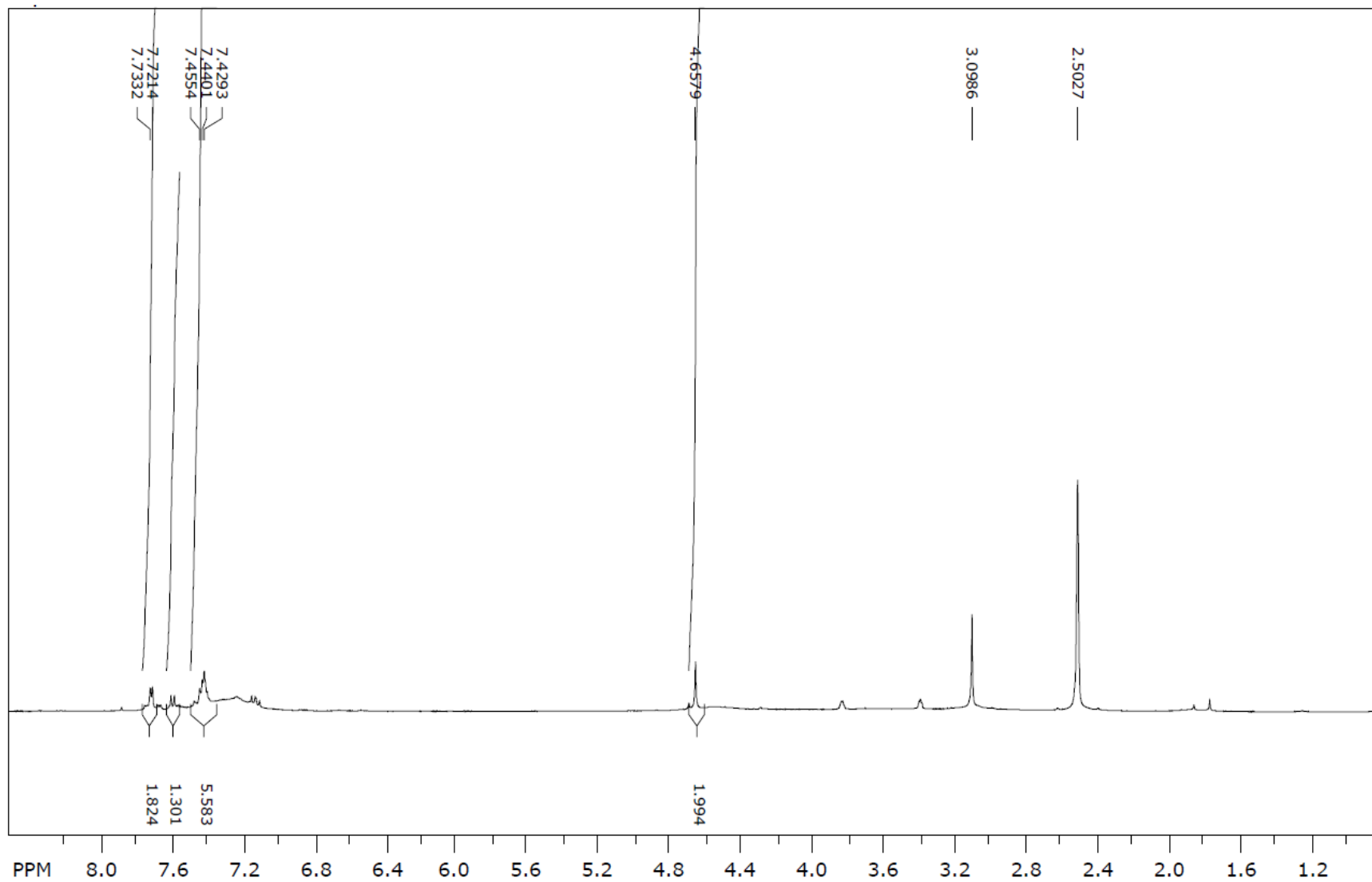


Reaktanti	Cimetaldhid (0,7 mmol) i 3-karboksimetilrodanin (0,7 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	305,37
Molekulska formula	C ₁₄ H ₁₁ NO ₃ S ₂
Temperatura tališta	189 – 194 °C
Boja kristala	Smeđa
R_f	0,73
LC/MS/MS m/z (M-)	304,11
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 7,73 (d, <i>J</i> = 7,08 Hz, 2H, CH), 7,61 (d, <i>J</i> = 11,46 Hz, 1H, CH), 7,41 – 7,46 (m, 5H, arom.), 4,65 (s, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 195,08; 169,46; 167,95; 148,04; 137,66; 136,34; 131,17; 130,40; 125,77; 47,43.

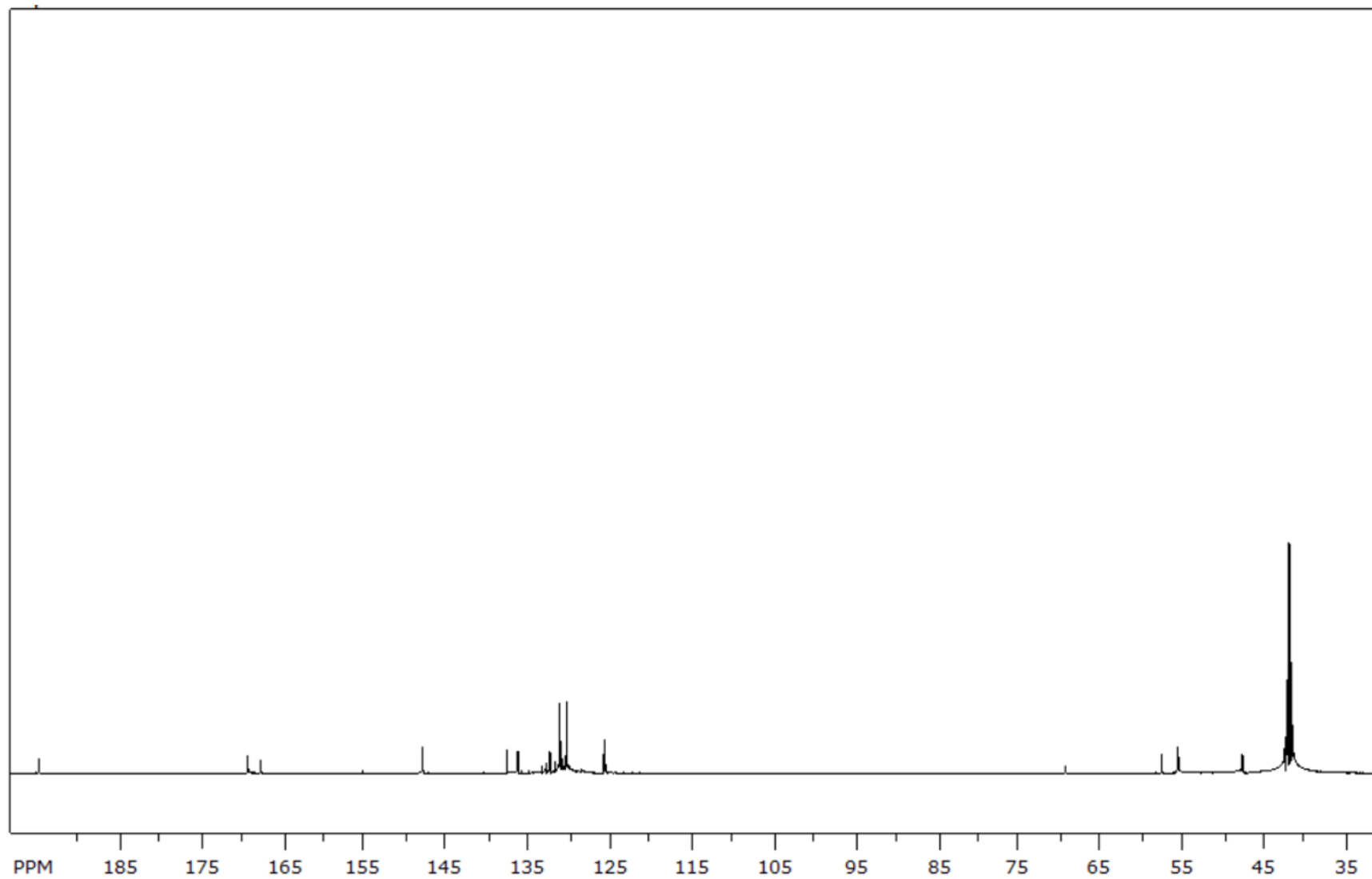
Maseni spektr (8p)



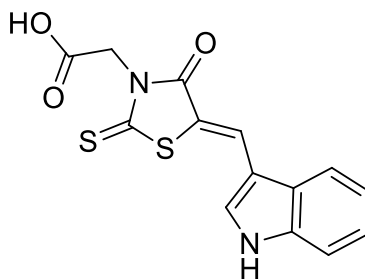
¹H NMR spektr (8p)



¹³C NMR spektr (8p)

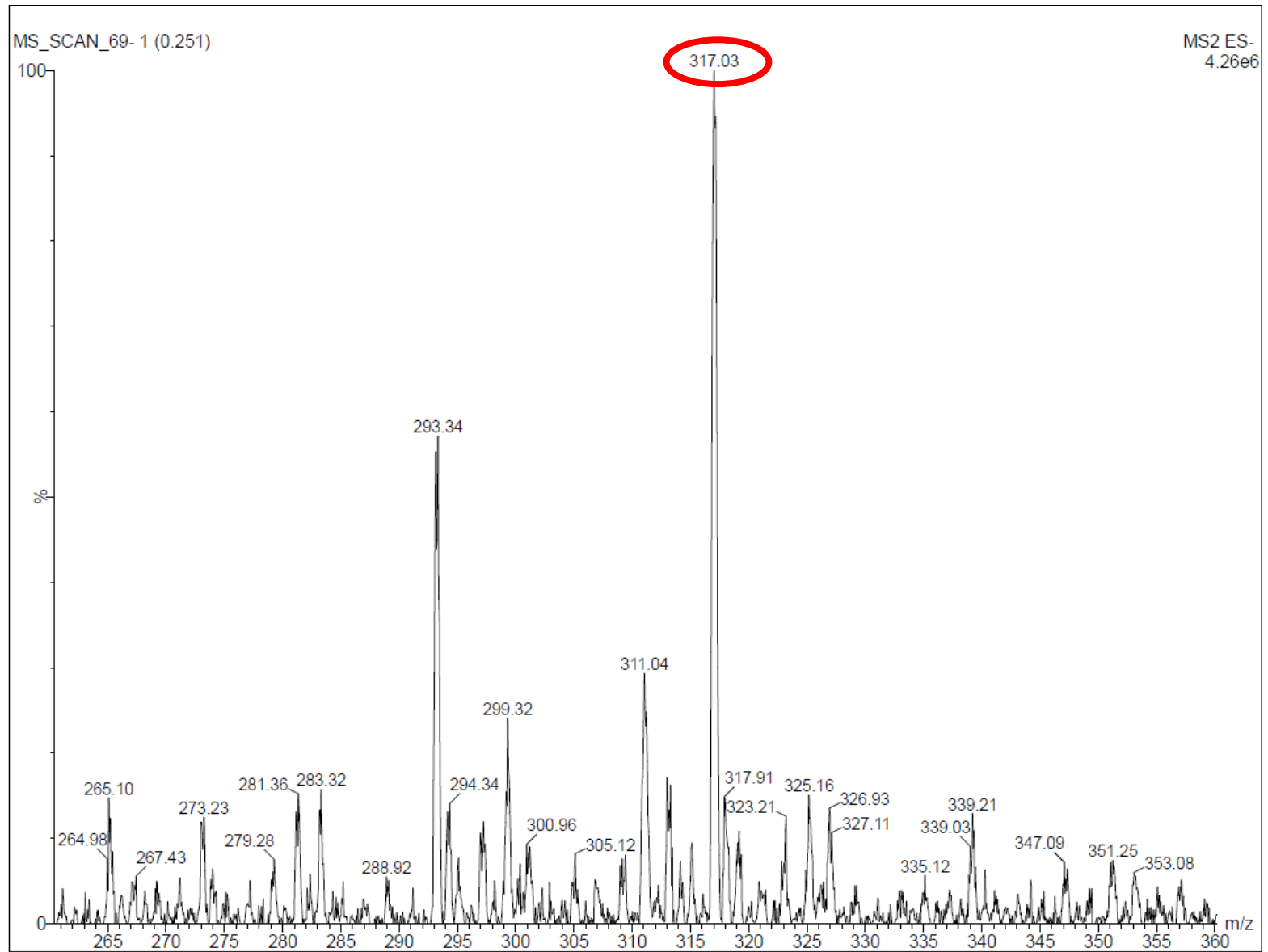


**2-(5-((1H-indol-3-il)metilen)-4-okso-2-tioksotiazolidin-3-il) octena
kiselina (8q)**

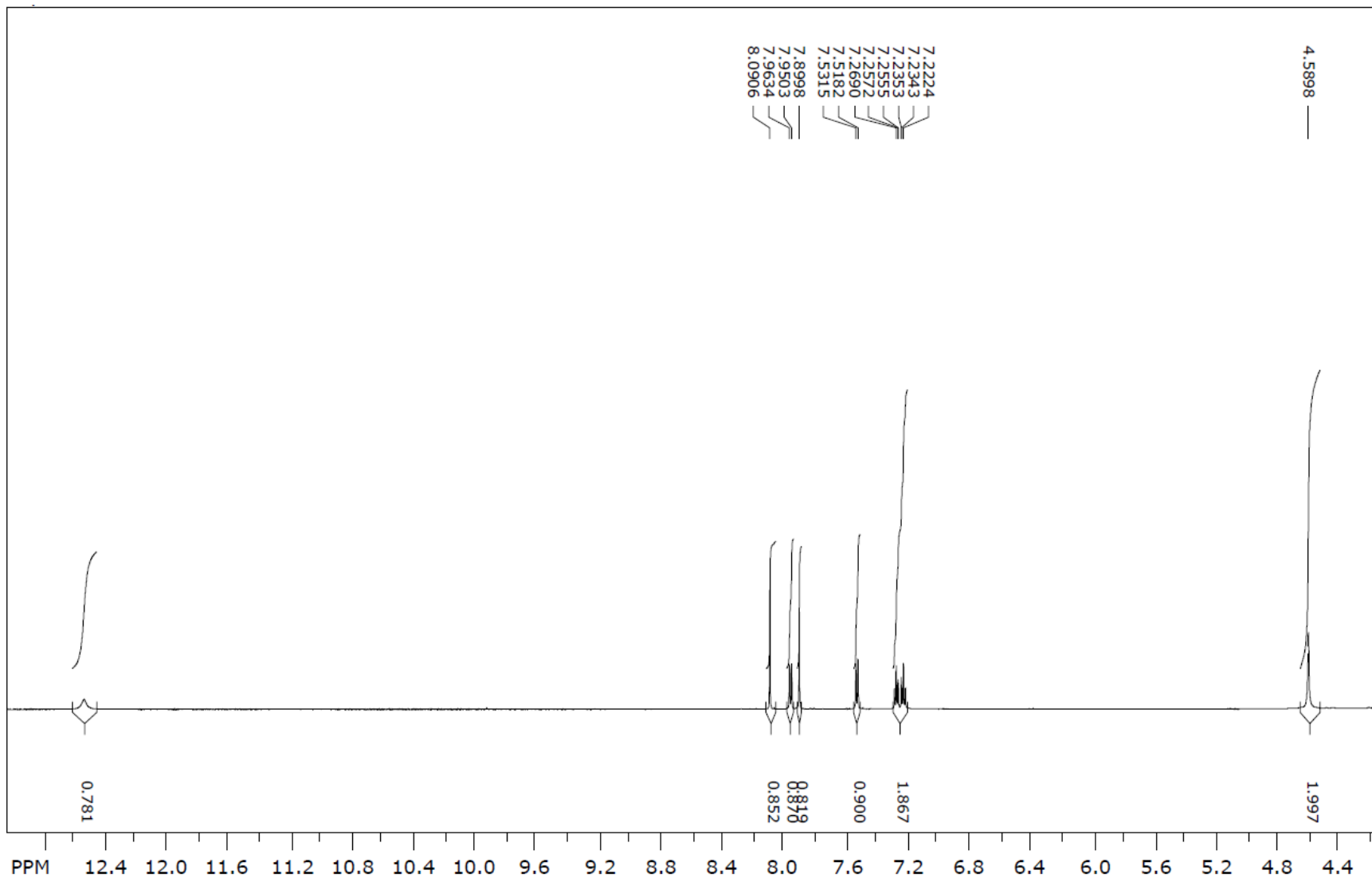


Reaktanti	Indol-3-karboksialdehid (0,7 mmol) i 3-karboksimetilrodanin (0,7 mmol)
Metoda pročišćavanja	Prekristalizacija iz octene kiseline
Molekulska masa	318,37
Molekulska formula	C ₁₄ H ₁₀ N ₂ O ₃ S ₂
Temperatura tališta	213 – 217 °C
Boja kristala	Svijetlo smeđa
R_f	0,55
LC/MS/MS m/z (M-)	317,03
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 12,54 (s, 1H, NH), 8,09 (s, 1H, CH), 7,96 (d, <i>J</i> = 7,86 Hz, 1H, arom.), 7,89 (s, 1H, arom.), 7,52 (d, <i>J</i> = 7,98 Hz, 1H, arom.), 7,27 (t, <i>J</i> = 7,05 Hz, 1H, arom.), 7,22 (t, <i>J</i> = 7,77 Hz, 1H, arom.), 4,59 (s, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 192,20; 167,24; 166,31; 136,43; 130,59; 126,75; 126,18; 123,26; 121,46; 118,49; 114,43; 112,58; 111,03; 46,31.

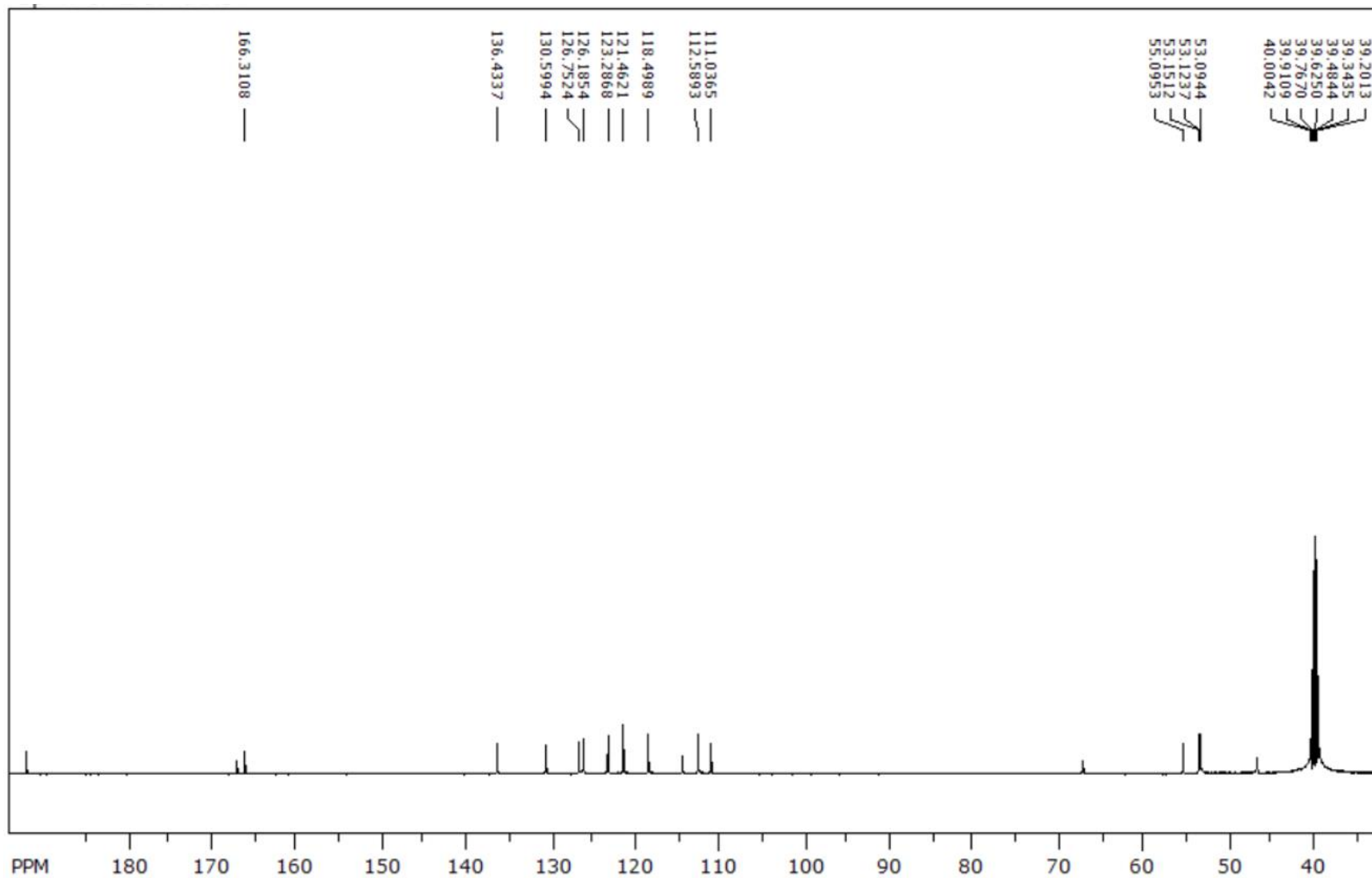
Maseni spektar (8q)



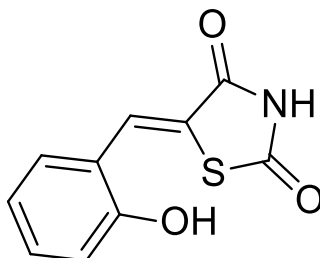
¹H NMR spektr (8q)



¹³C NMR spektr (8q)

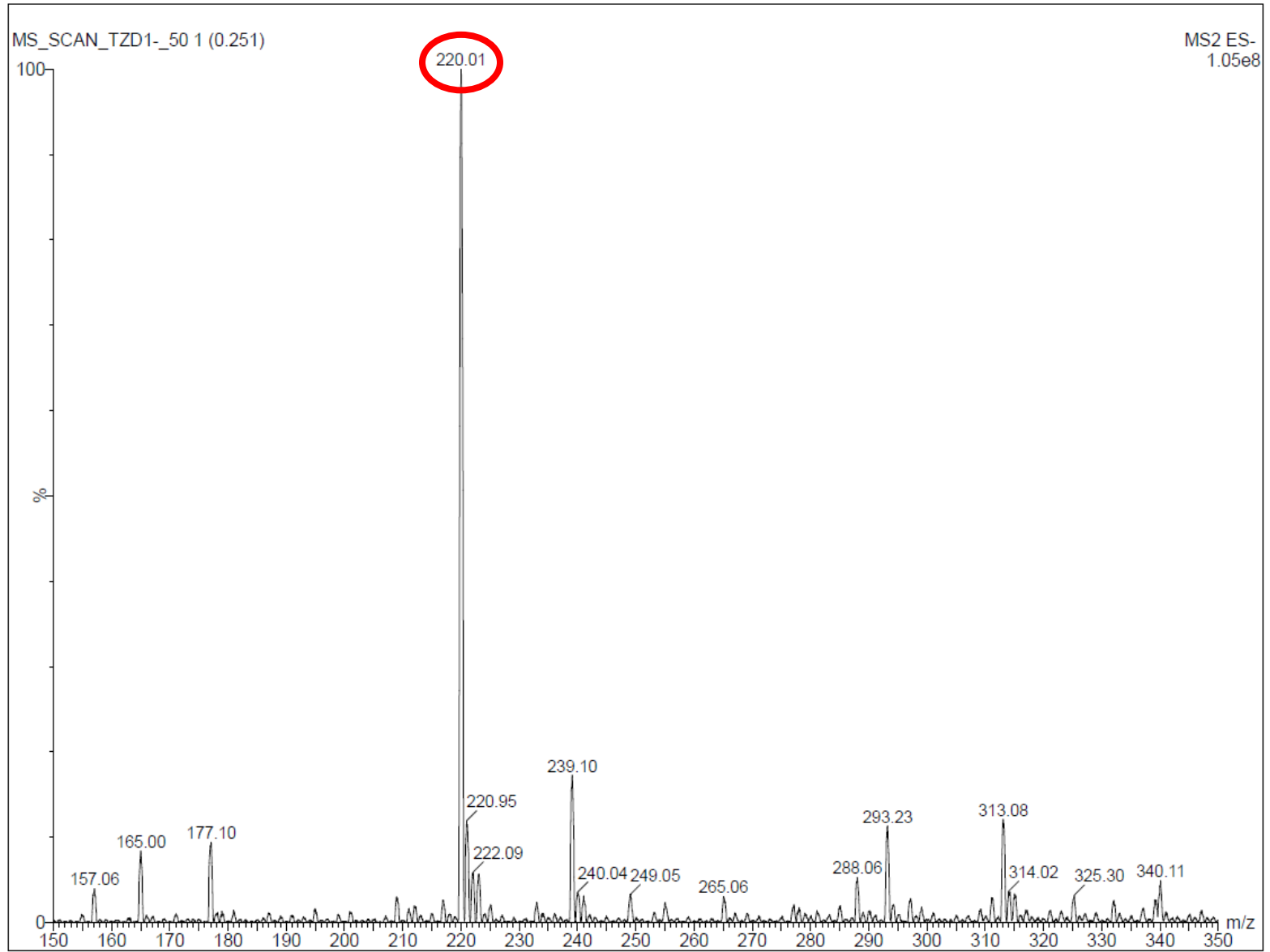


5-(2-hidroksibenziliden) tiazolidin-2,4-dion (9a)

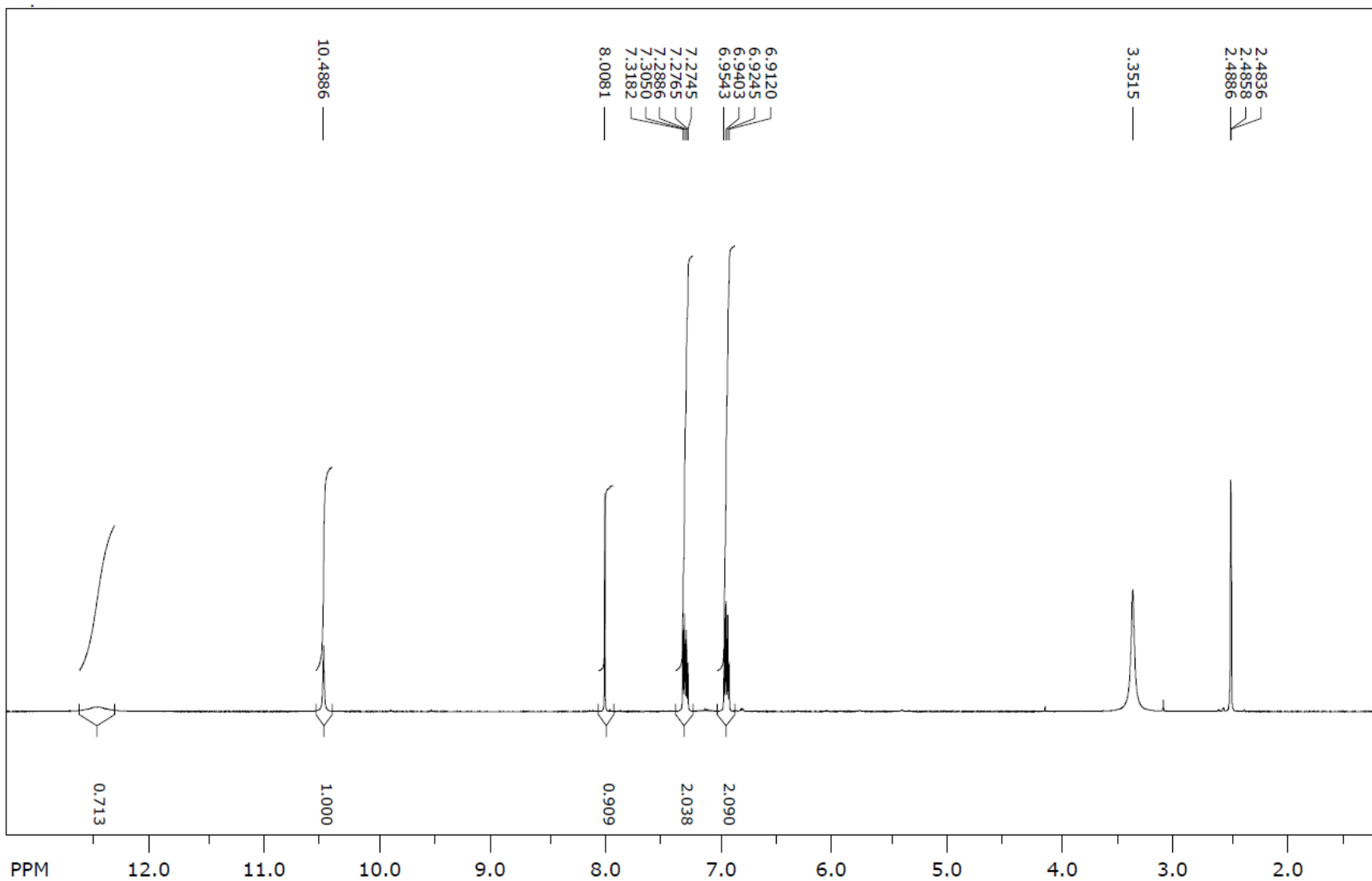


Reaktanti	Salicilaldehid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	221,23 g/mol
Molekulska formula	C ₁₀ H ₇ NO ₃ S
Temperatura tališta	269 – 272 °C (lit. 276 - 277 °C, Durai Ananda Kumar i sur., 2015; 254 – 256 °C, Ha i sur., 2012)
Boja kristala	Žuta
R_f	0,64
LC/MS/MS <i>m/z</i> (M-)	220,01
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 12,48 (s, 1H, NH), 10,48 (s, 1H, OH), 8,00 (s, 1H, CH), 7,30 (q, <i>J</i> = 7,92; 9,84; 7,26 Hz, 2H, arom.), 6,93 (q, <i>J</i> = 8,40; 9,48; 7,50 Hz, 2H, arom.).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 168,15; 167,50; 157,24; 132,20; 128,20; 126,27; 121,87; 119,64; 116,08.

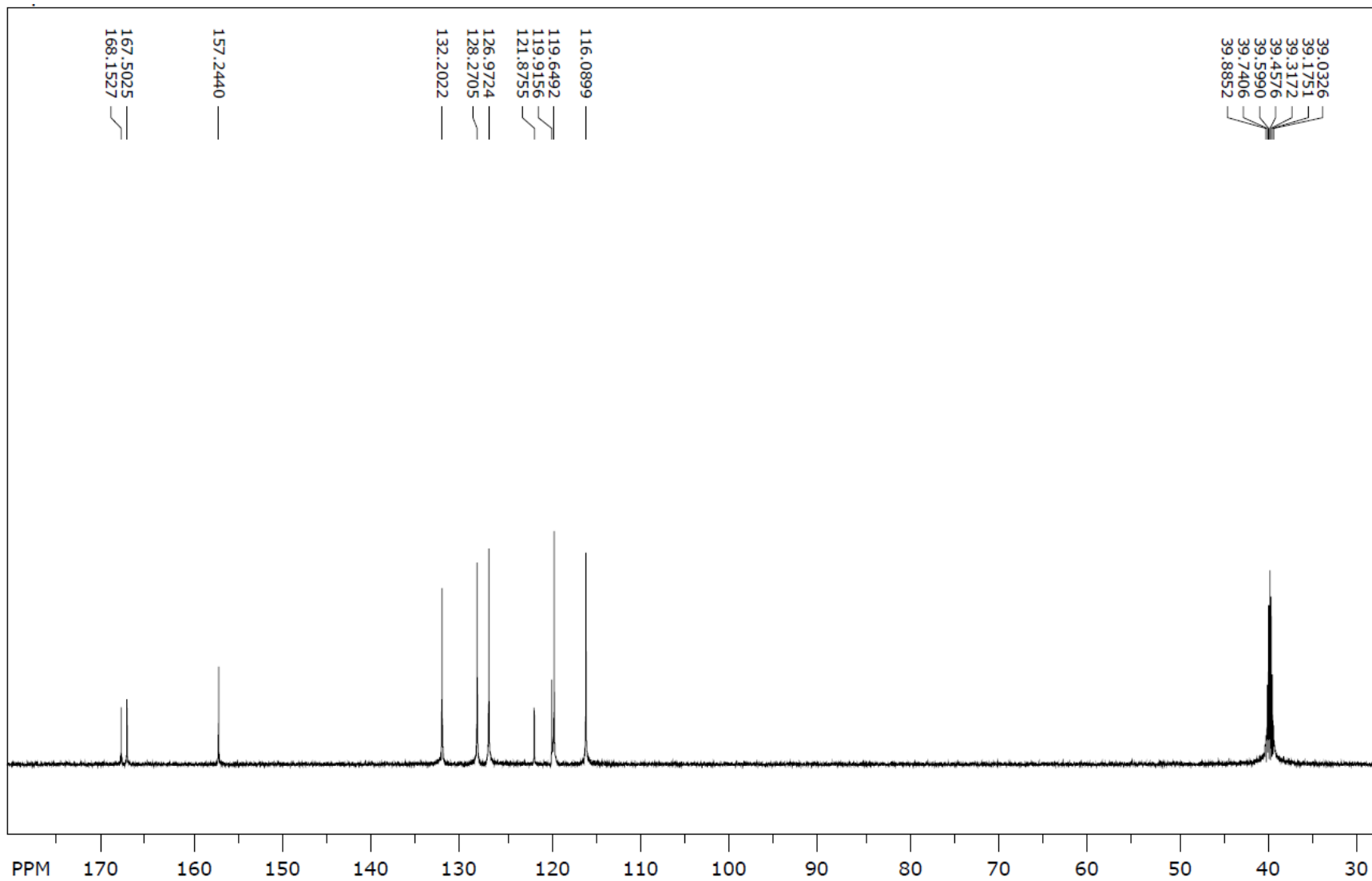
Maseni spektar (9a)



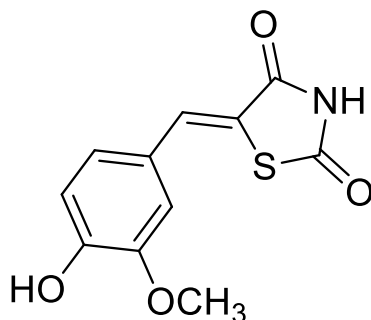
¹H NMR spektr (9a)



¹³C NMR spektr (9a)

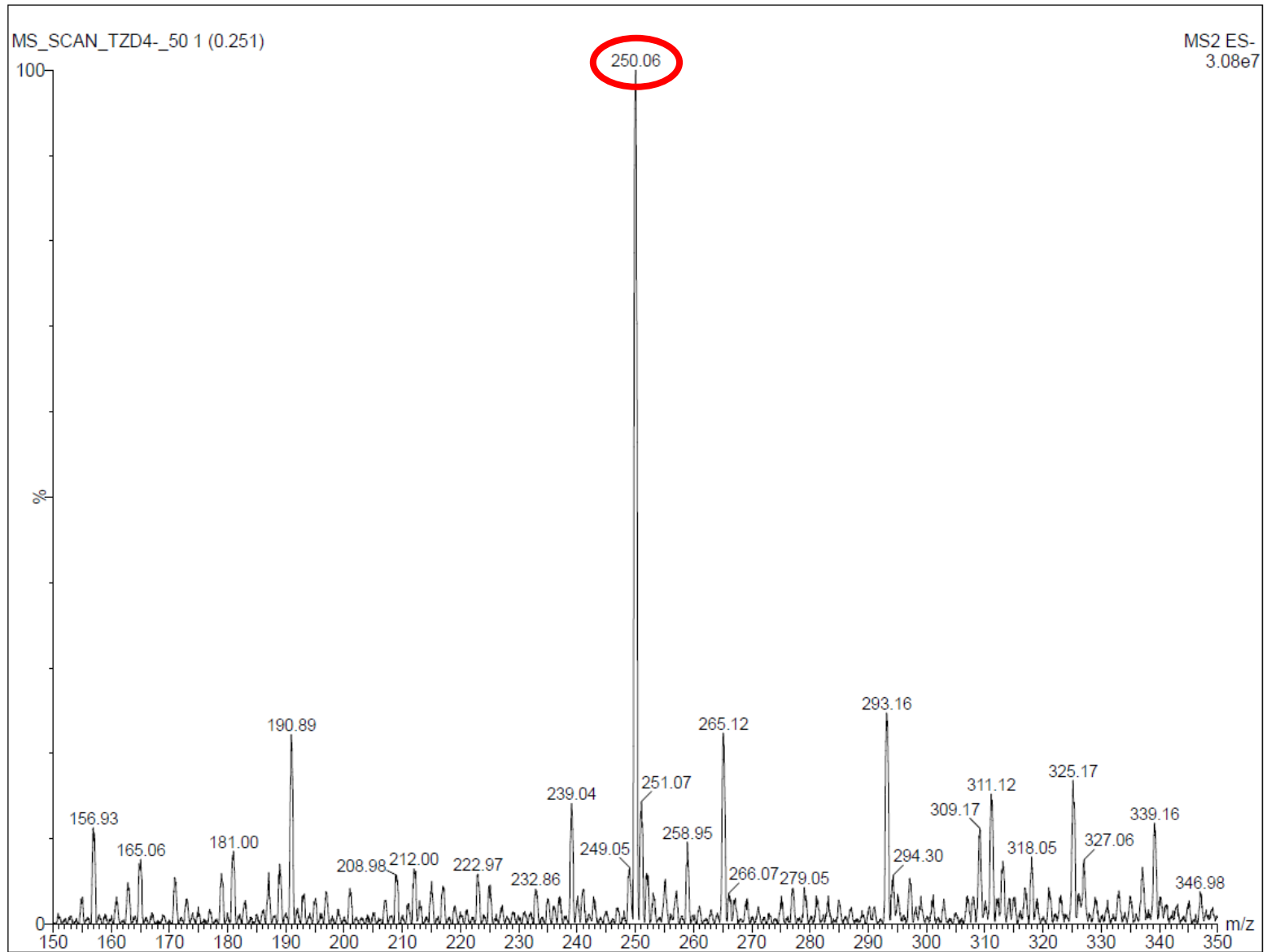


5-(4-hidroksi-3-metoksibenziliden)tiazolidin-2,4-dion (9b)

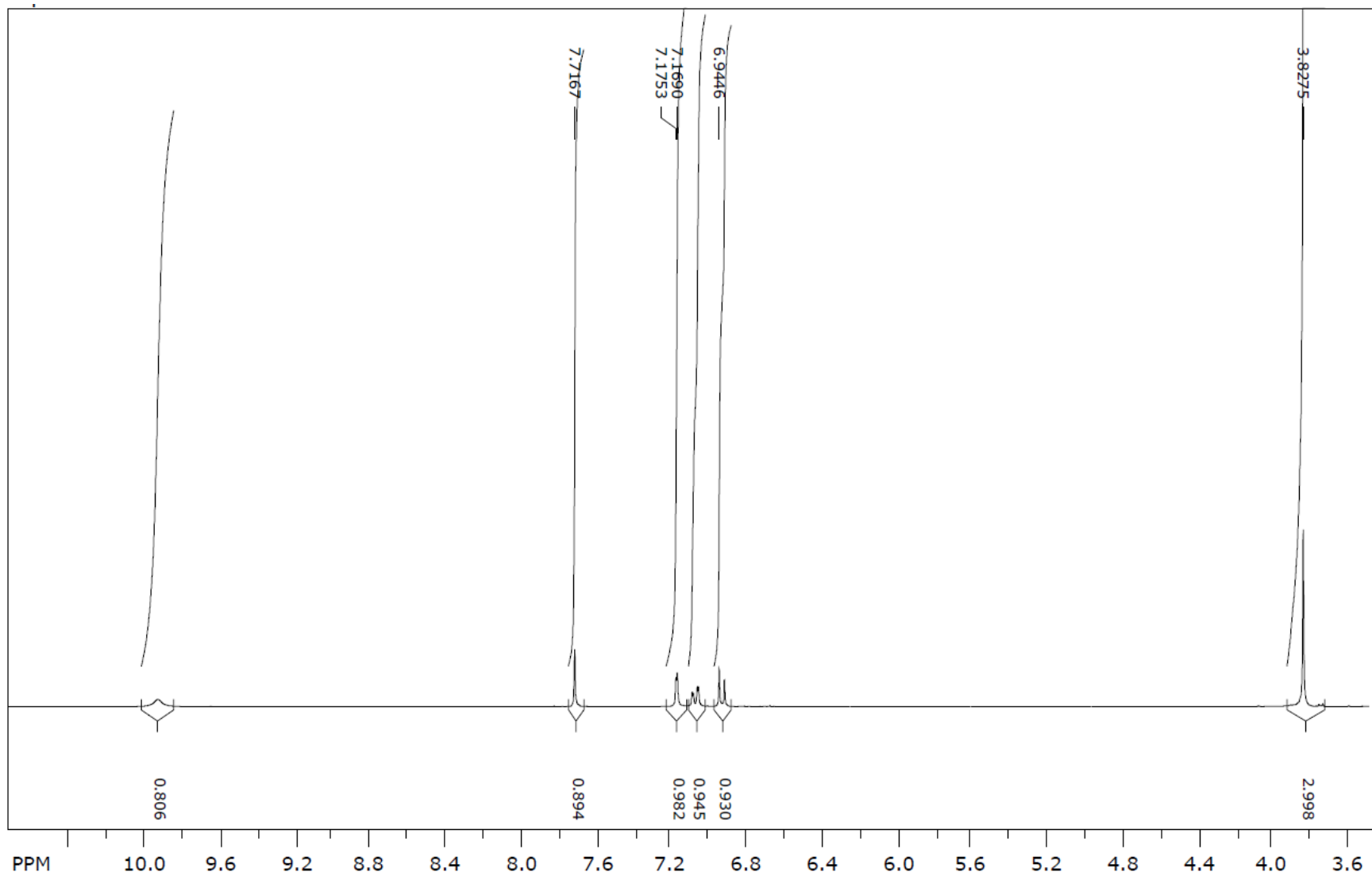


Reaktanti	3-metoksi-4-hidroksibenzaldehid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	251,26
Molekulska formula	C ₁₁ H ₉ NO ₄ S
Temperatura tališta	199 – 201 °C (lit. 194 – 195 °C, Durai Ananda Kumar i sur., 2015; 109 – 110 °C, Xiong i sur., 2011)
Boja kristala	Žuta
R_f	0,63
LC/MS/MS m/z (M⁻)	250,06
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 11,98 (s, 1H, NH), 9,94 (s, 1H, OH), 7,71 (s, 1H, CH), 7,17 (d, <i>J</i> = 1,89 Hz, 1H, arom.), 7,07 (dd, <i>J</i> = 8,34; 1,89 Hz, 1H, arom.), 6,93 (d, <i>J</i> = 8,25 Hz, 1H, arom.), 3,82 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 172,47; 168,52; 167,94; 149,89; 148,43, 130,06; 124,85; 124,59; 119,68; 116,71; 114,60.

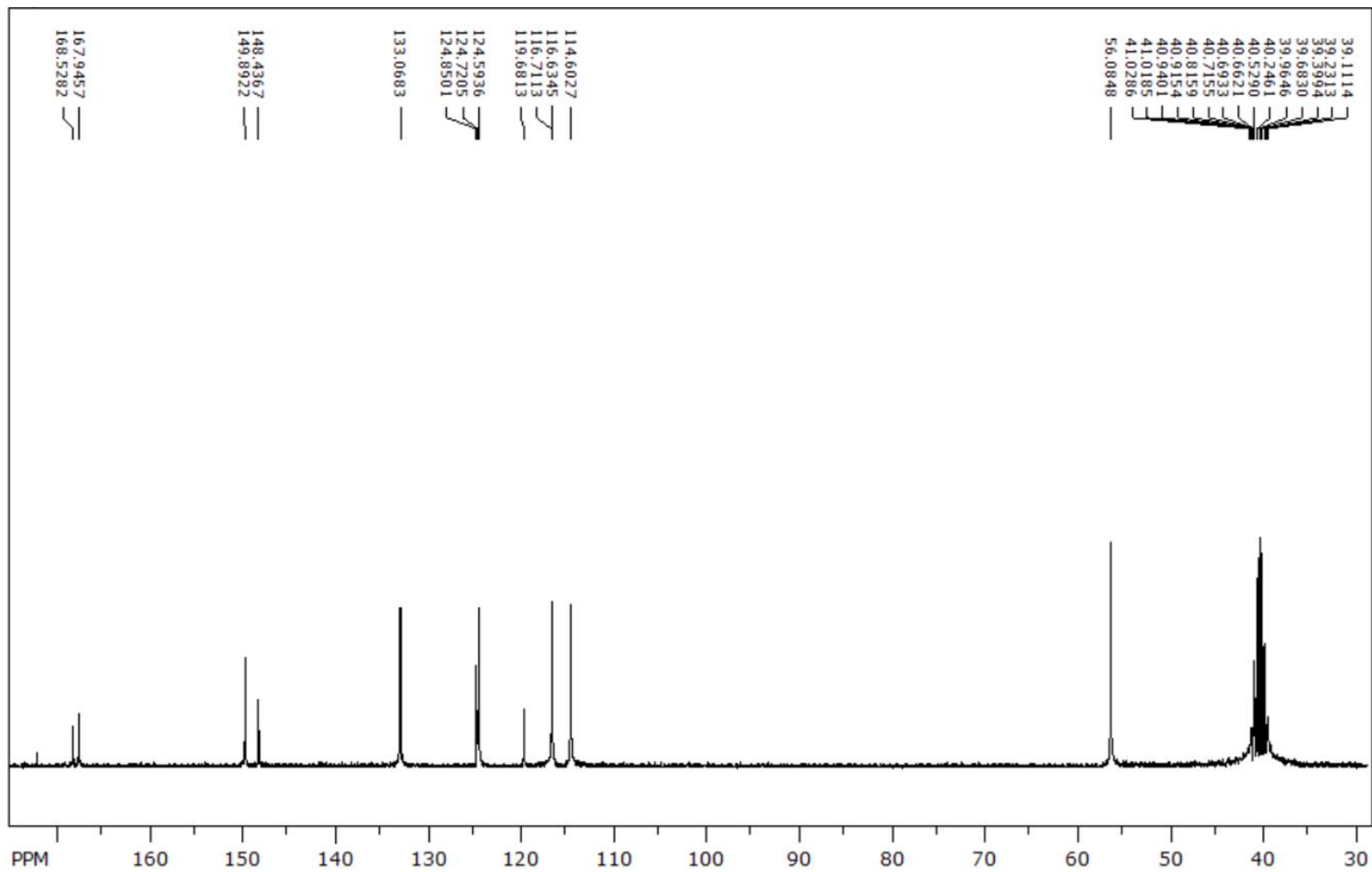
Maseni spektar (9b)



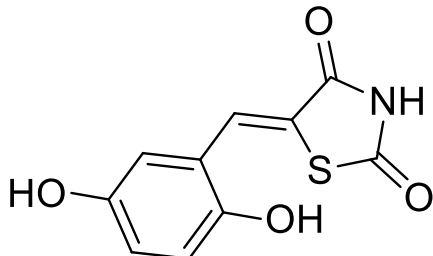
¹H NMR spektr (9b)



¹³C NMR spektar (9b)

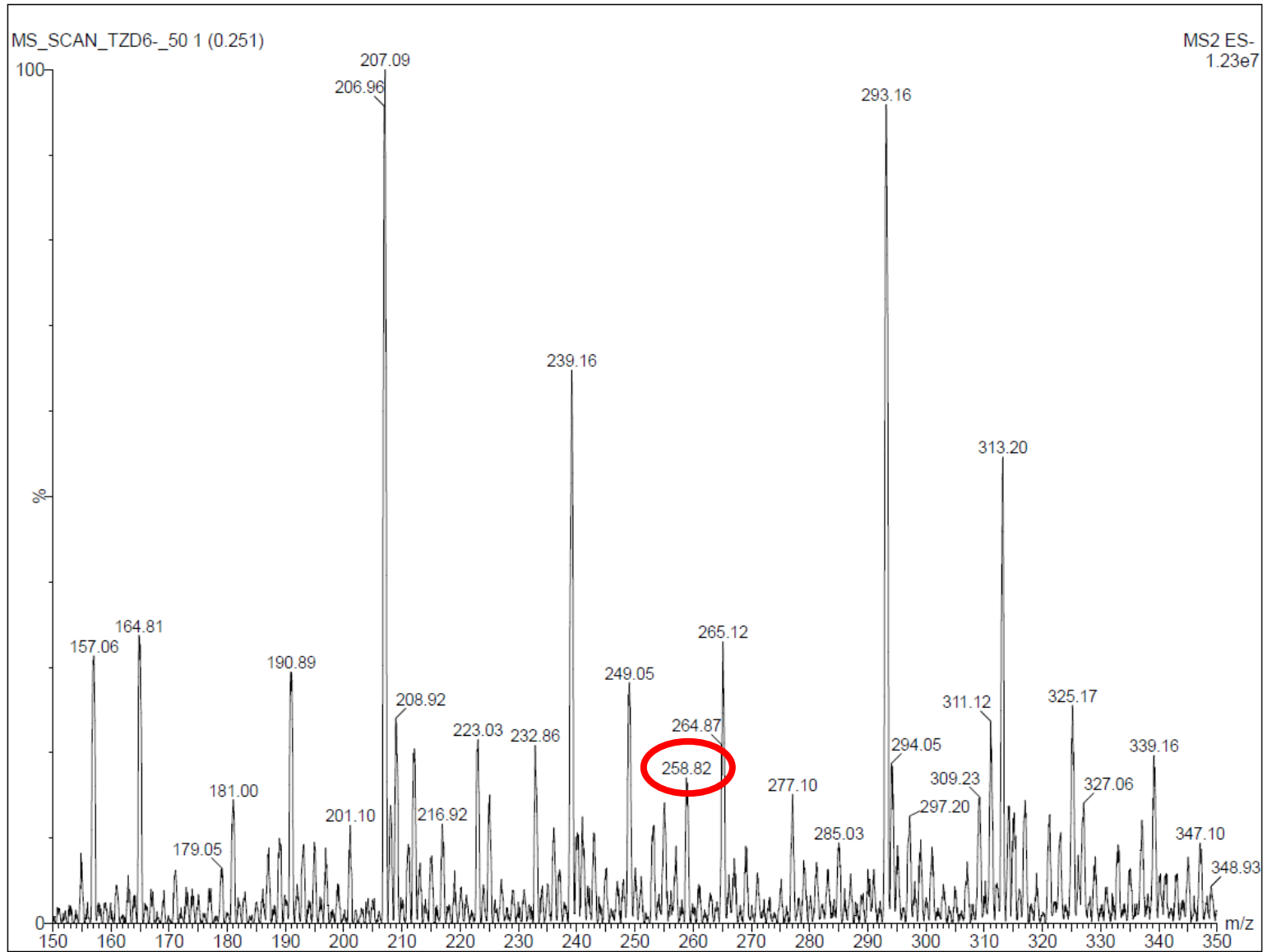


5-(2,5-dihidroksibenziliden) tiazolidin-2,4-dion (9c)

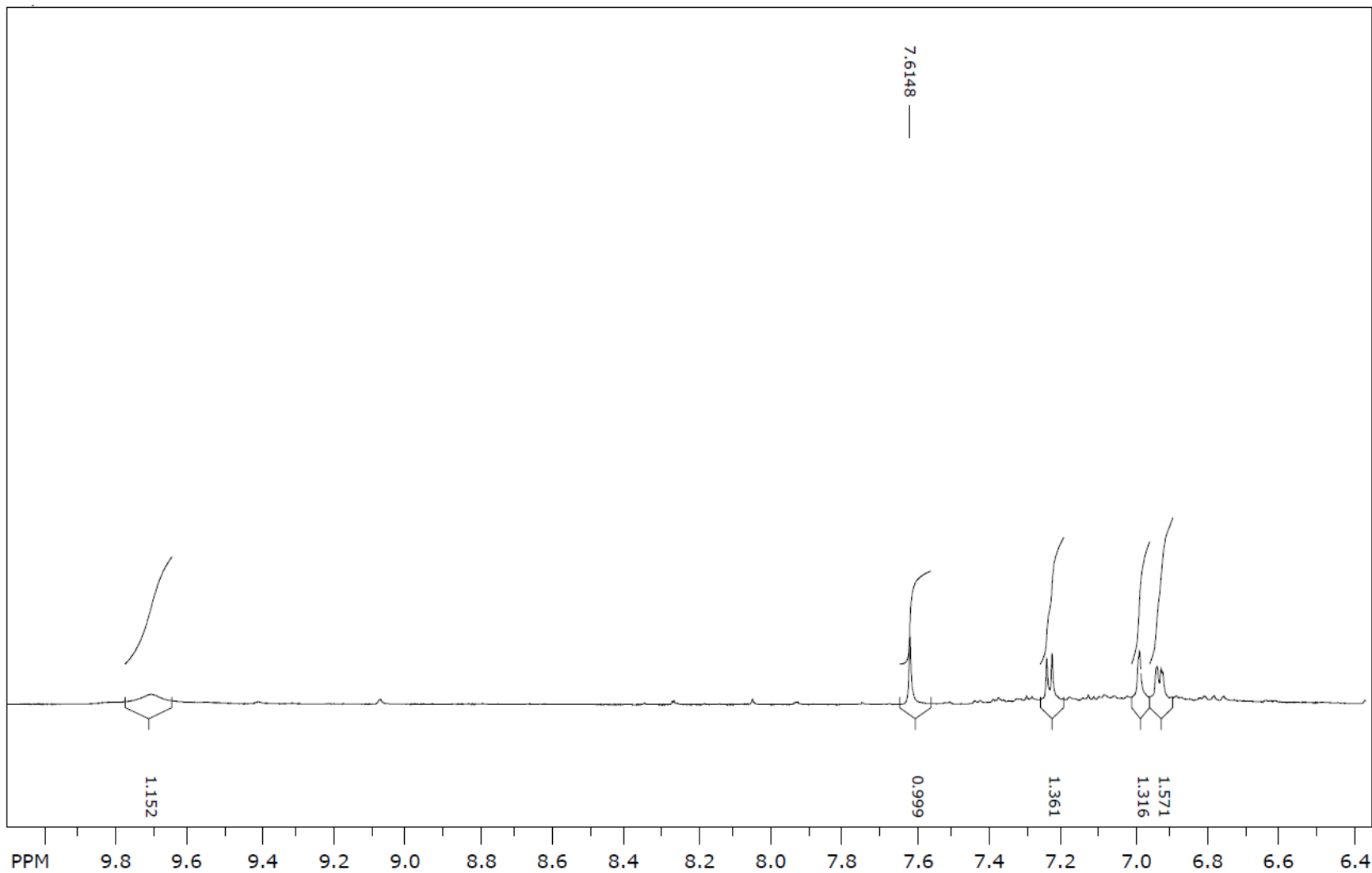


Reaktanti	2,5-dihidroksibenzaldehid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	237,23 g/mol
Molekulska formula	C ₁₀ H ₇ NO ₄ S
Temperatura tališta	194 – 198 °C
Boja kristala	Tamnosmeđa
R_f	0,58
LC/MS/MS <i>m/z</i> (M-+Na)	258,82
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 9,70 (s, 1H, OH), 7,61 (s, 1H, CH), 7,23 (d, <i>J</i> = 8,76 Hz, 1H, arom.), 6,98 (s, 1H, arom.), 6,91 – 6,93 (dd, <i>J</i> = 8,22; 1,68; 2,40 Hz, 1H, arom.).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 153,98; 144,08; 132,23; 128,61; 120,04; 117,85; 116,75; 110,91.

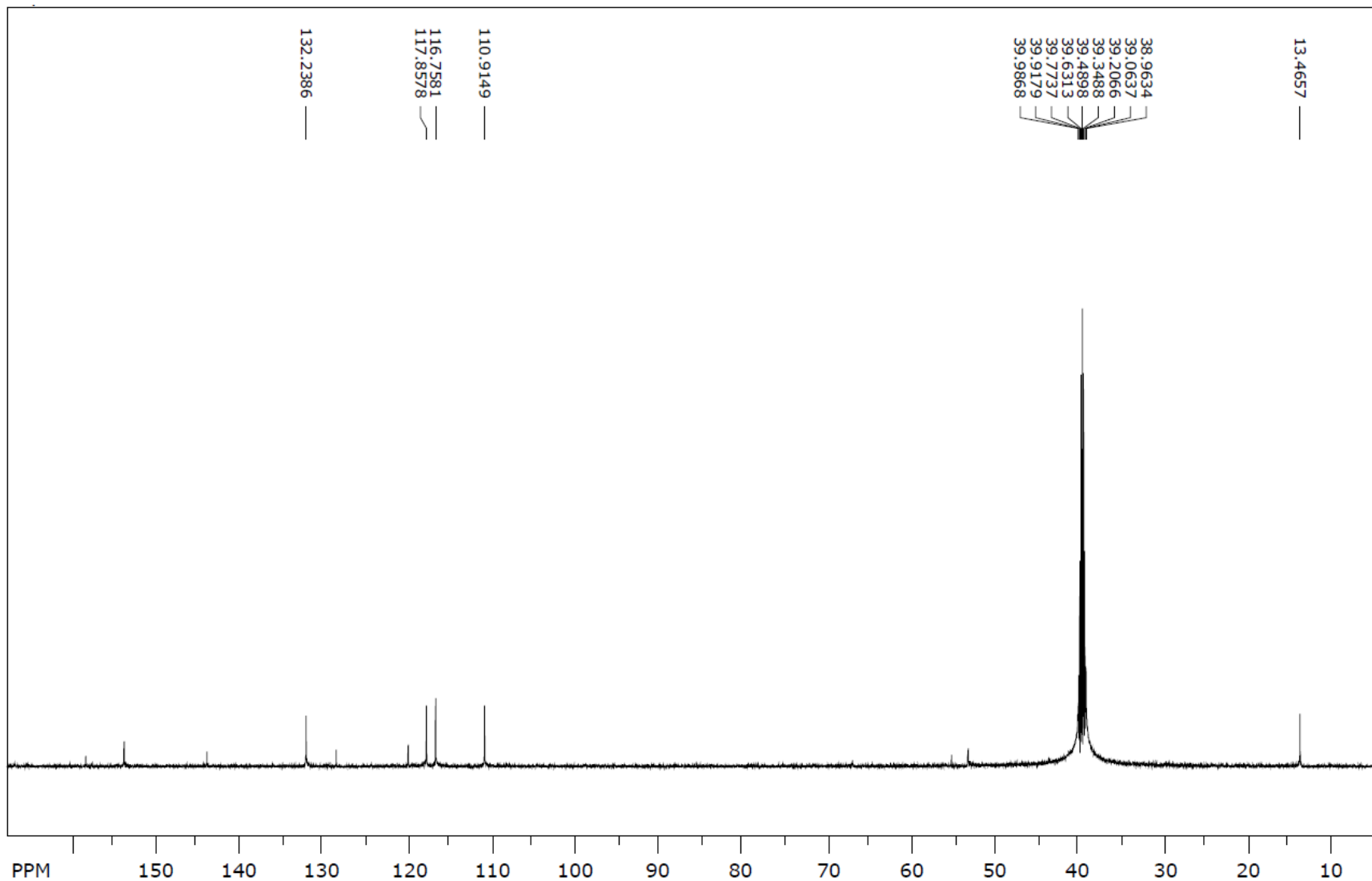
Maseni spektr (9c)



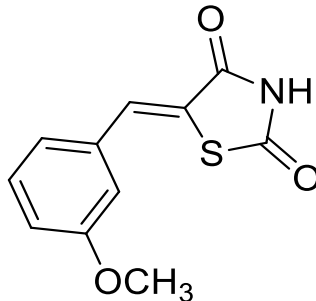
¹H NMR spektr (9c)



¹³C NMR spektr (9c)

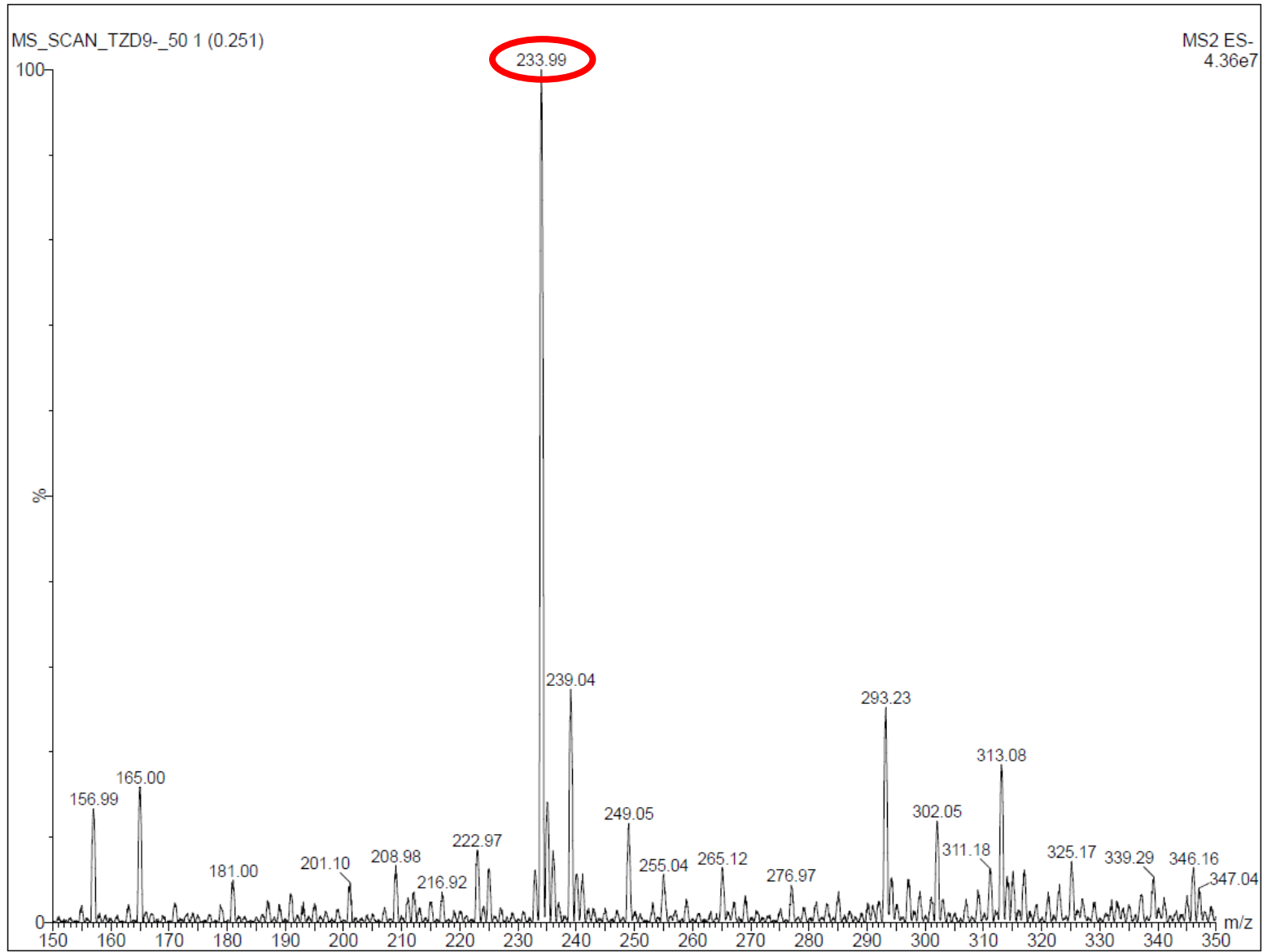


5-(3-metoksibenziliden) tiazolidin-2,4-dion (9d)

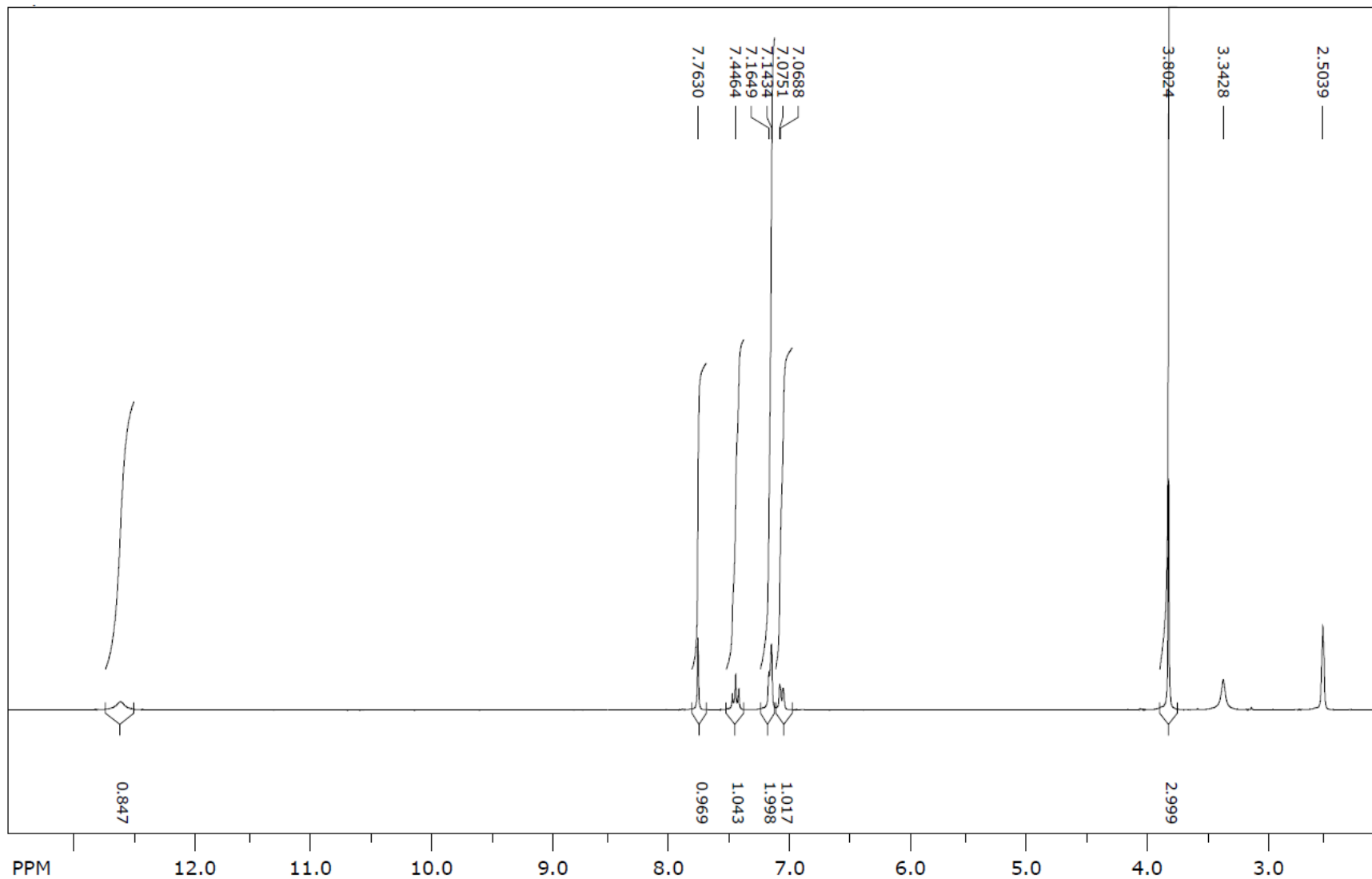


Reaktanti	3-metoksibenzaldehid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	235,26 g/mol
Molekulska formula	C ₁₁ H ₉ NO ₃ S
Temperatura tališta	194 – 197 °C
Boja kristala	Bijela
R_f	0,74
LC/MS/MS <i>m/z</i> (M-)	233,99
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 12,62 (s, 1H, NH), 7,76 (s, 1H, CH), 7,45 (t, <i>J</i> = 8,16 Hz, 1H, arom.), 7,15 (d, <i>J</i> = 6,45 Hz, 2H, arom.), 7,06 (dd, <i>J</i> = 8,34; 1,89; 0,30 Hz, 1H, arom.), 3,80 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 168,28; 167,70; 160,08; 134,85; 132,21; 130,86; 122,36; 116,74; 115,76; 55,73.

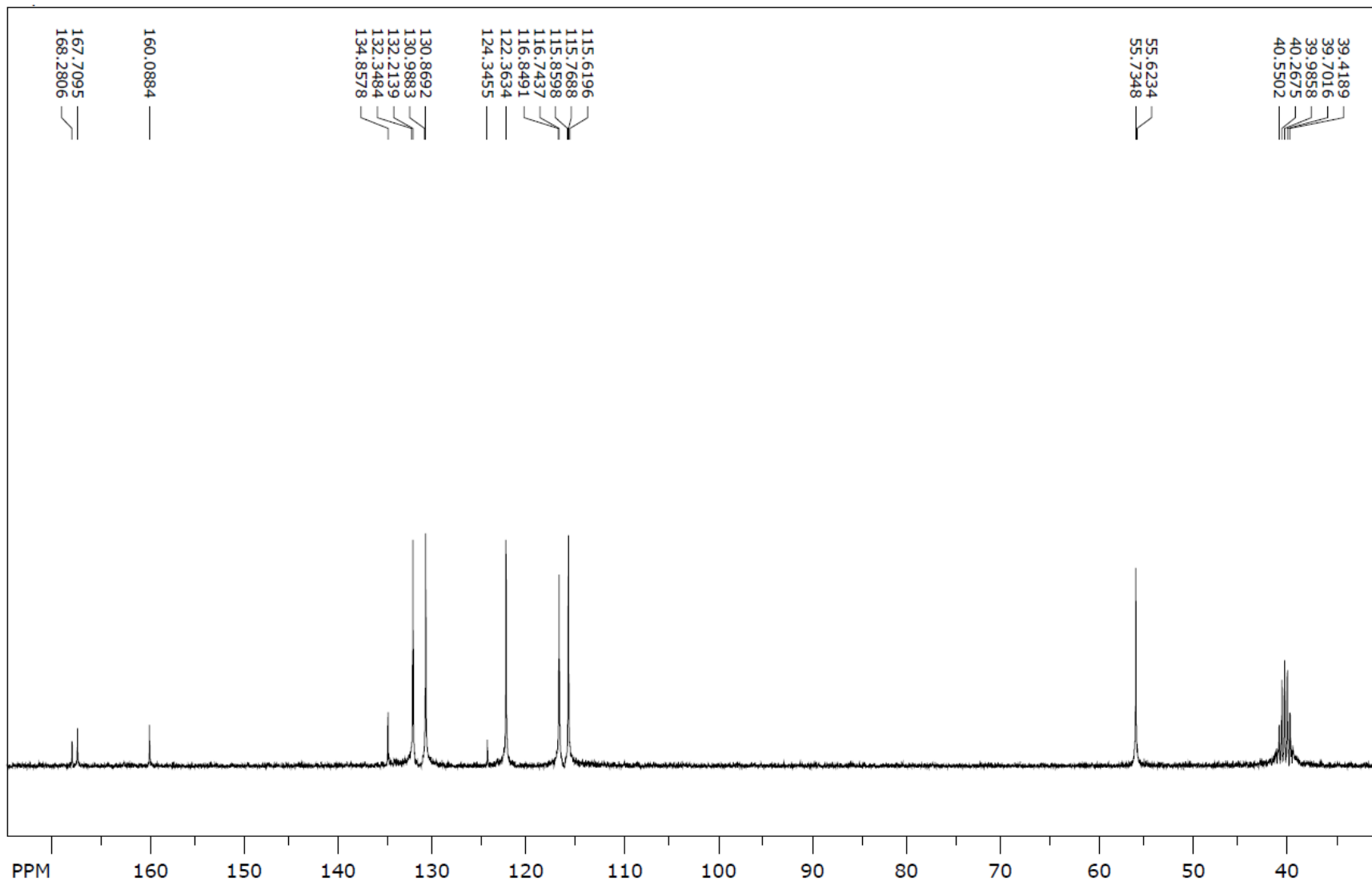
Maseni spektr (9d)



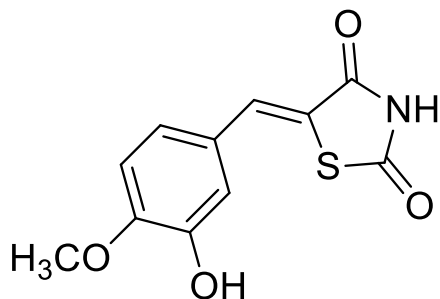
¹H NMR spektr (9d)



¹³C NMR spektr (9d)

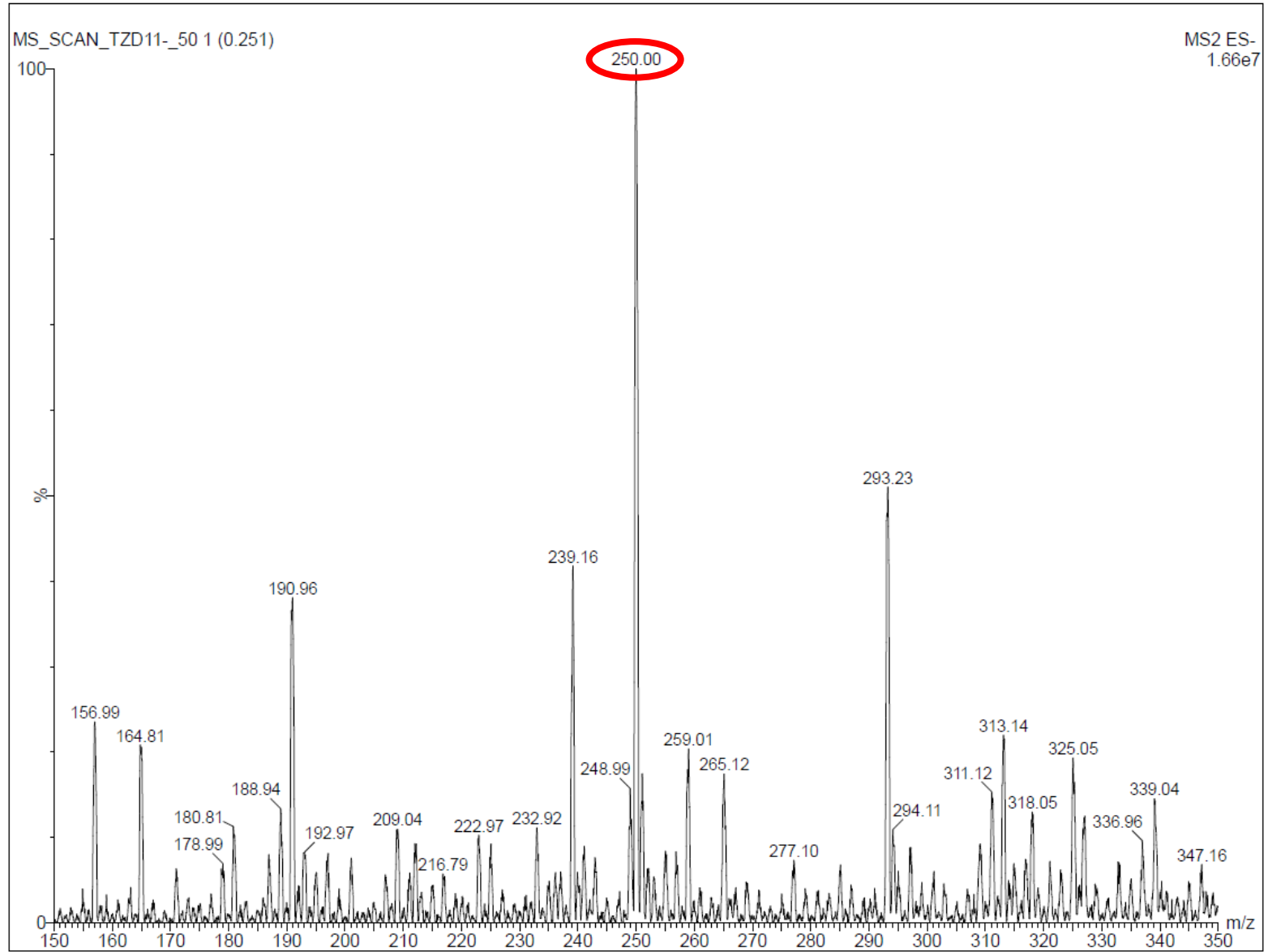


5-(3-hidroksi-4-metoksibenziliden) tiazolidin-2,4-dion (9e)

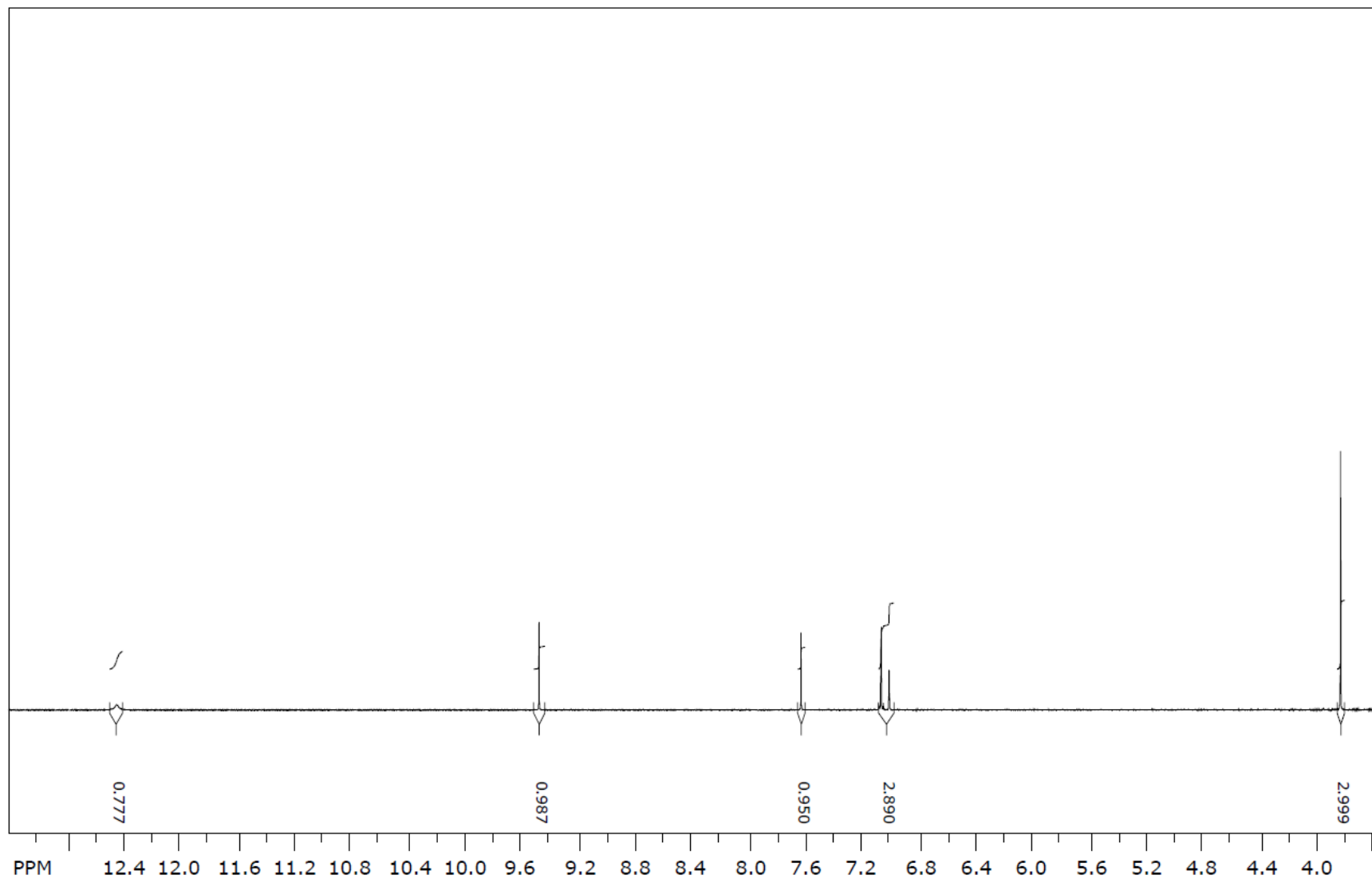


Reaktanti	3-hidroksi-4-metoksibenzaldehid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	251,26 g/mol
Molekulska formula	C ₁₁ H ₉ NO ₄ S
Temperatura tališta	254 – 257 °C (lit. 254 – 257 °C, Ha i sur., 2012)
Boja kristala	Žuta
R_f	0,58
LC/MS/MS m/z (M-)	250,00
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 12,46 (s, 1H, NH), 9,47 (s, 1H, OH), 7,62 (s, 1H, CH), 7,06 (d, <i>J</i> = 2,16 Hz, 2H, arom.), 7,00 (d, <i>J</i> = 1,56 Hz, 1H, arom.), 3,81 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 168,03; 167,40; 149,99; 146,89; 132,24; 125,63; 123,45; 119,96; 115,84; 112,37; 55,63.

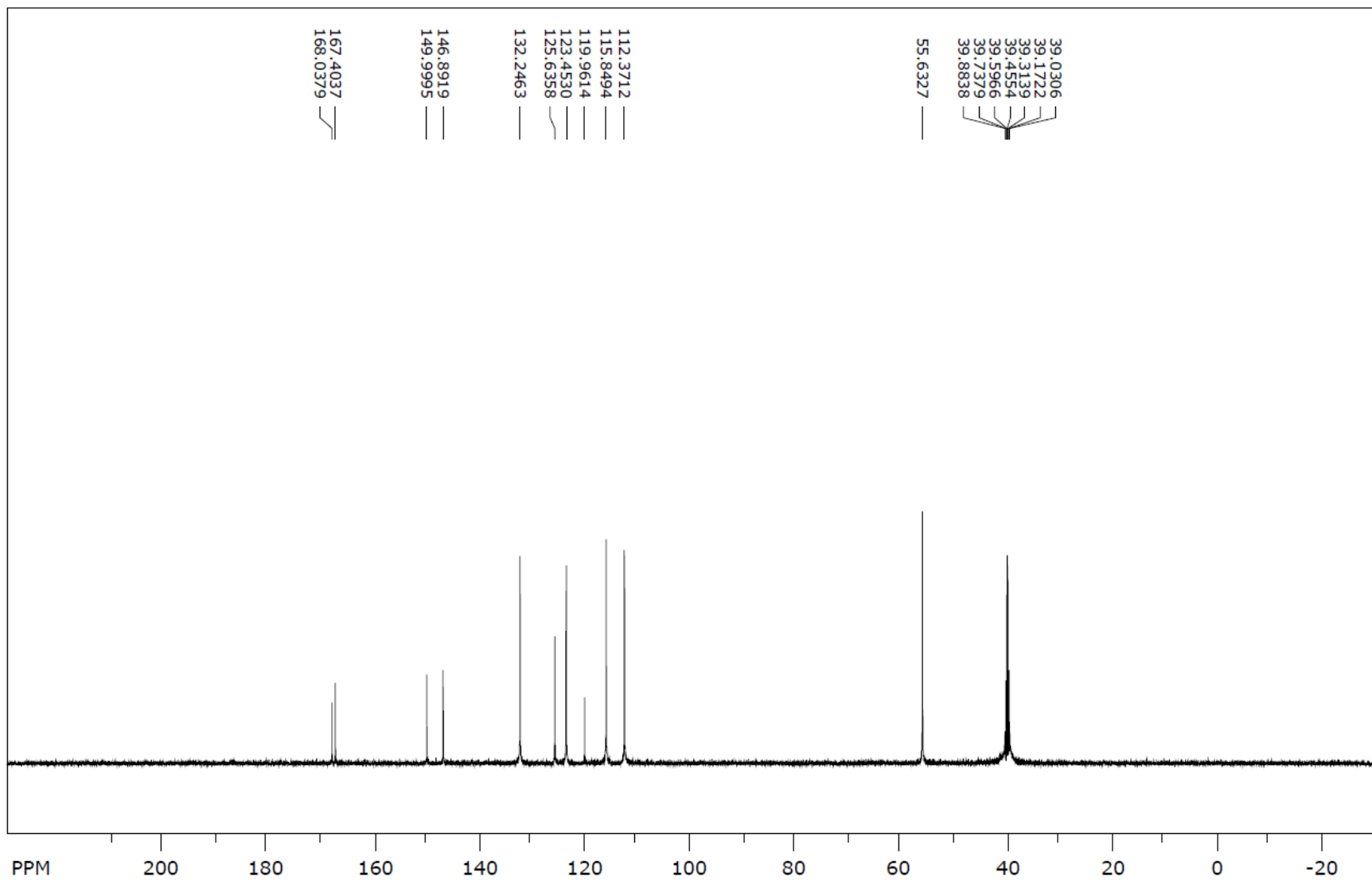
Maseni spektr (9e)



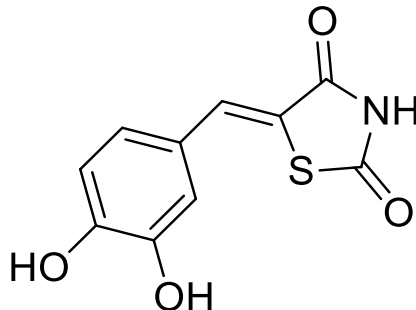
¹H NMR spektr (9e)



¹³C NMR spektr (9e)

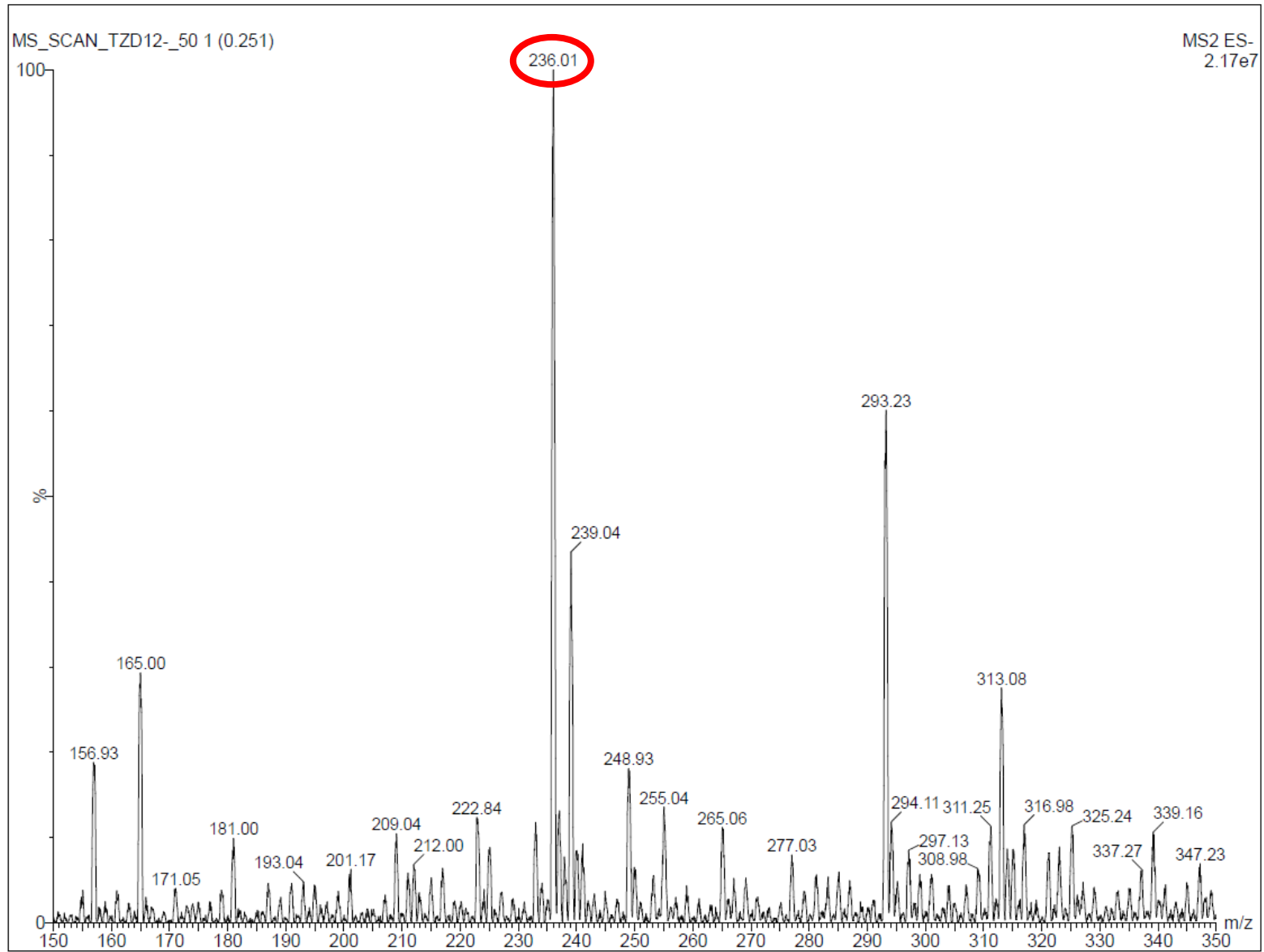


5-(3,4-dihidroksibenziliden) tiazolidin-2,4-dion (9f)

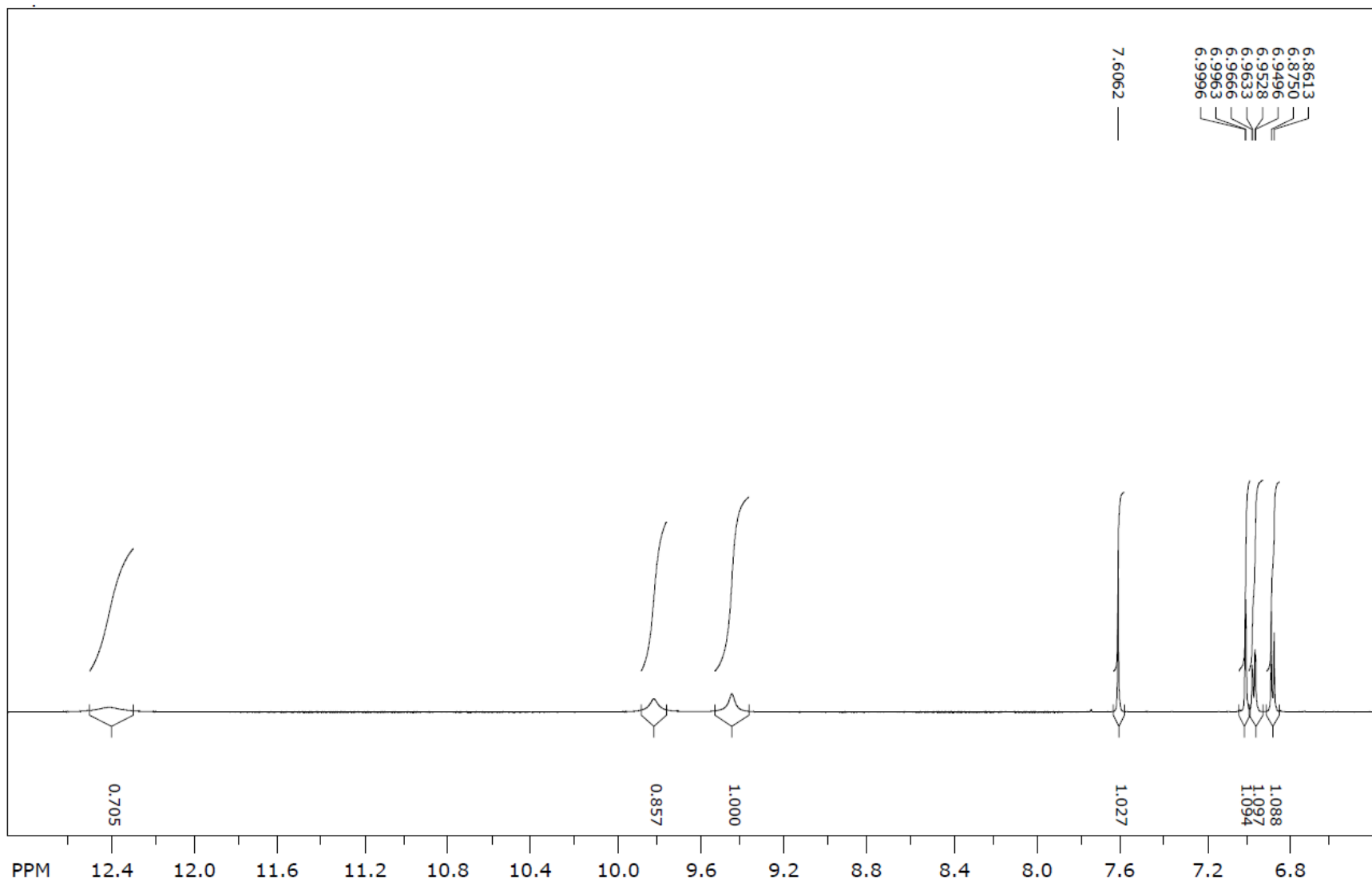


Reaktanti	3,4-dihidroksibenzaldehid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	237,23 g/mol
Molekulska formula	C ₁₀ H ₇ NO ₄ S
Temperatura tališta	270 - 271 °C (lit. 267 °C, Shelke i sur., 2011)
Boja kristala	Smeđa
R_f	0,35
LC/MS/MS m/z (M-)	236,01
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 12,42 (s, 1H, NH), 9,82 (s, 1H, OH), 9,44 (s, 1H, OH), 7,60 (s, 1H, CH), 6,99 (d, <i>J</i> = 1,98 Hz, 1H, arom.), 6,96 (q, <i>J</i> = 8,28; 1,95 Hz, 1H, arom.), 6,87 (d, <i>J</i> = 8,22 Hz, 1H, arom.).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 168,15; 166,53; 148,57; 145,82; 132,63; 124,28; 123,89; 118,72; 116,37; 116,22.

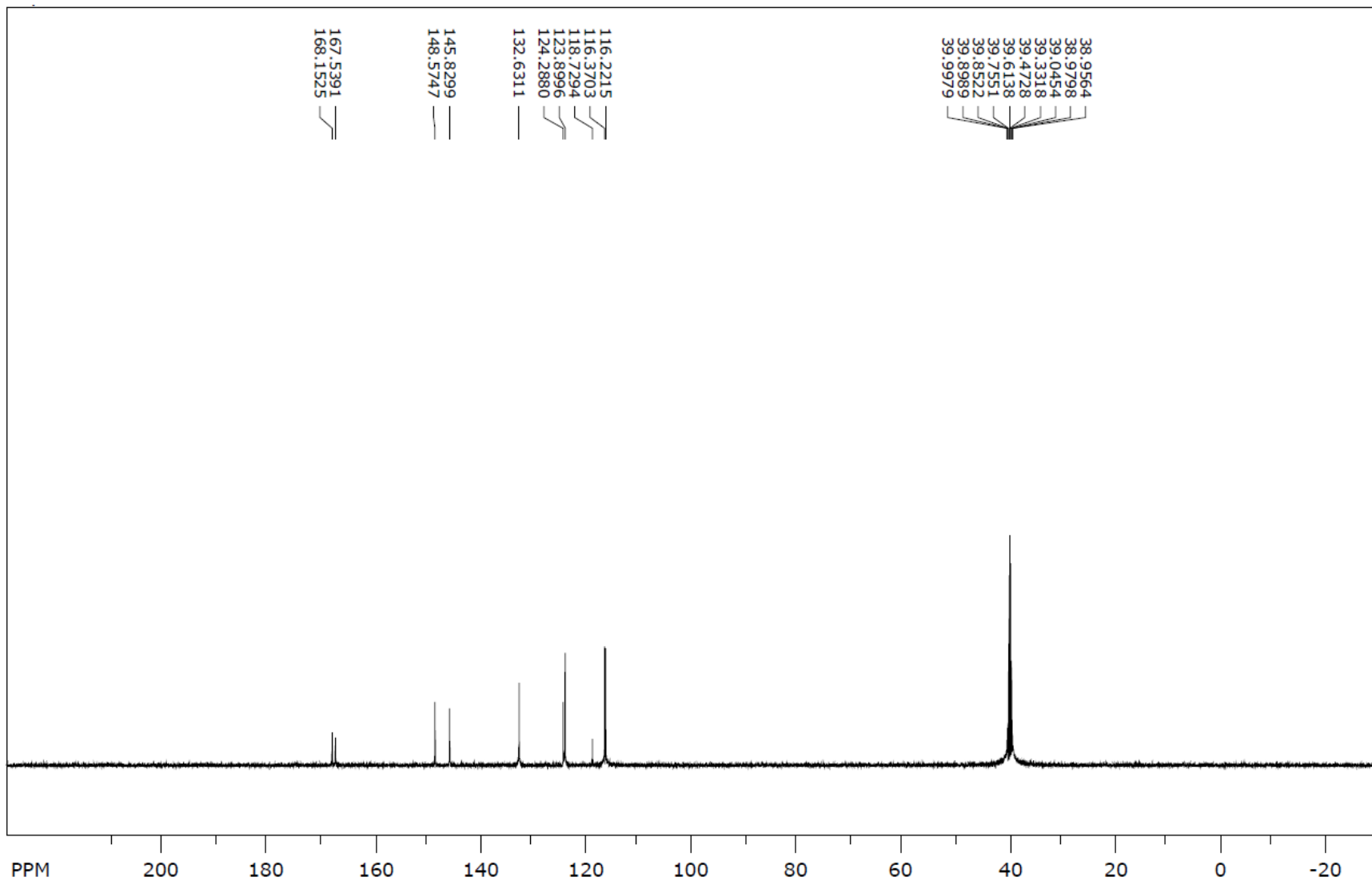
Maseni spektar (9f)



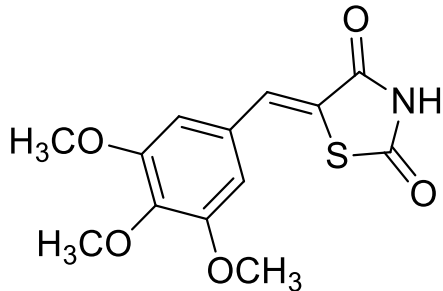
¹H NMR spektr (9f)



¹³C NMR spektr (9f)

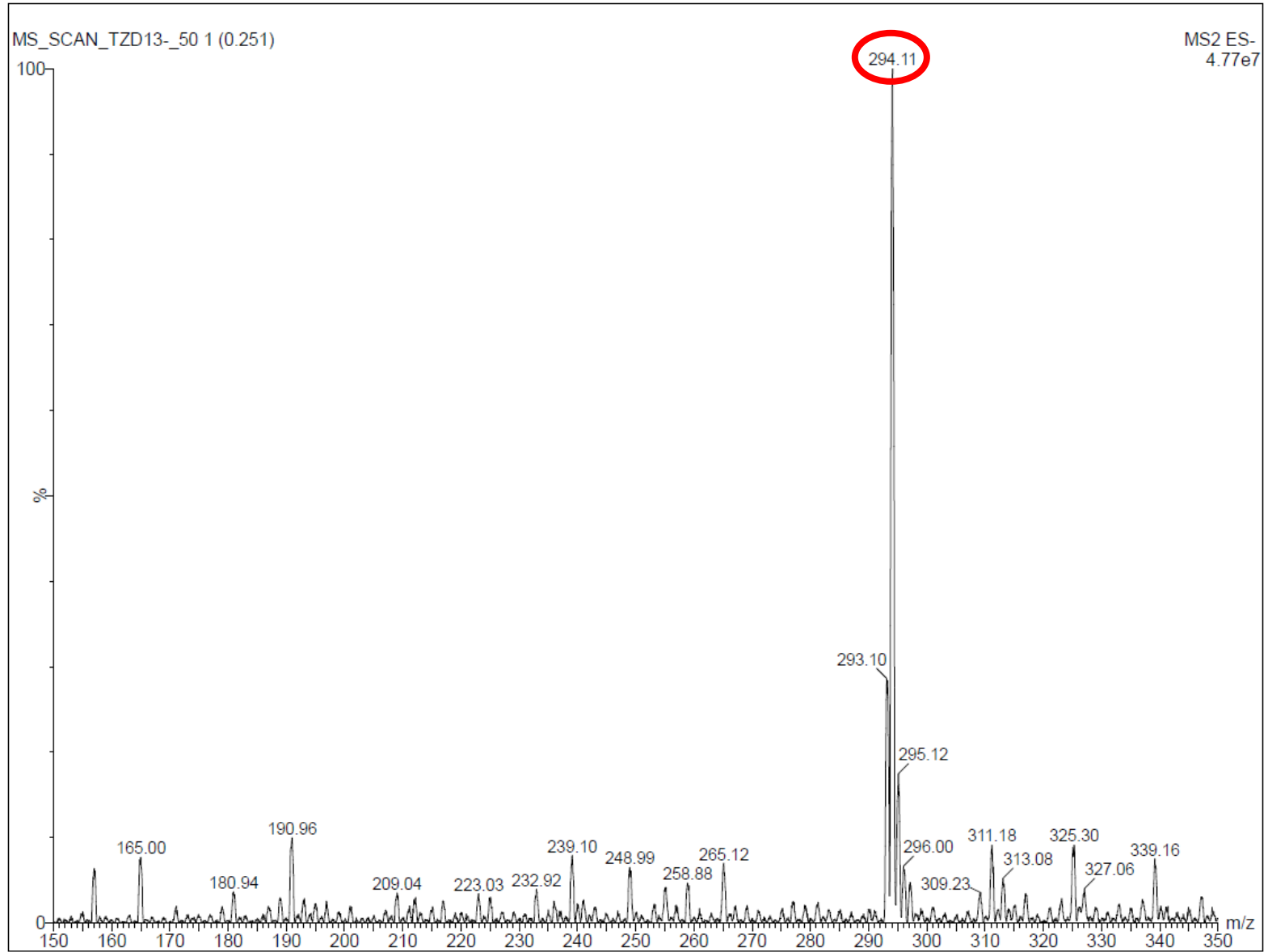


5-(3,4,5-trimetoksibenziliden) tiazolidin-2,4-dion (9g)

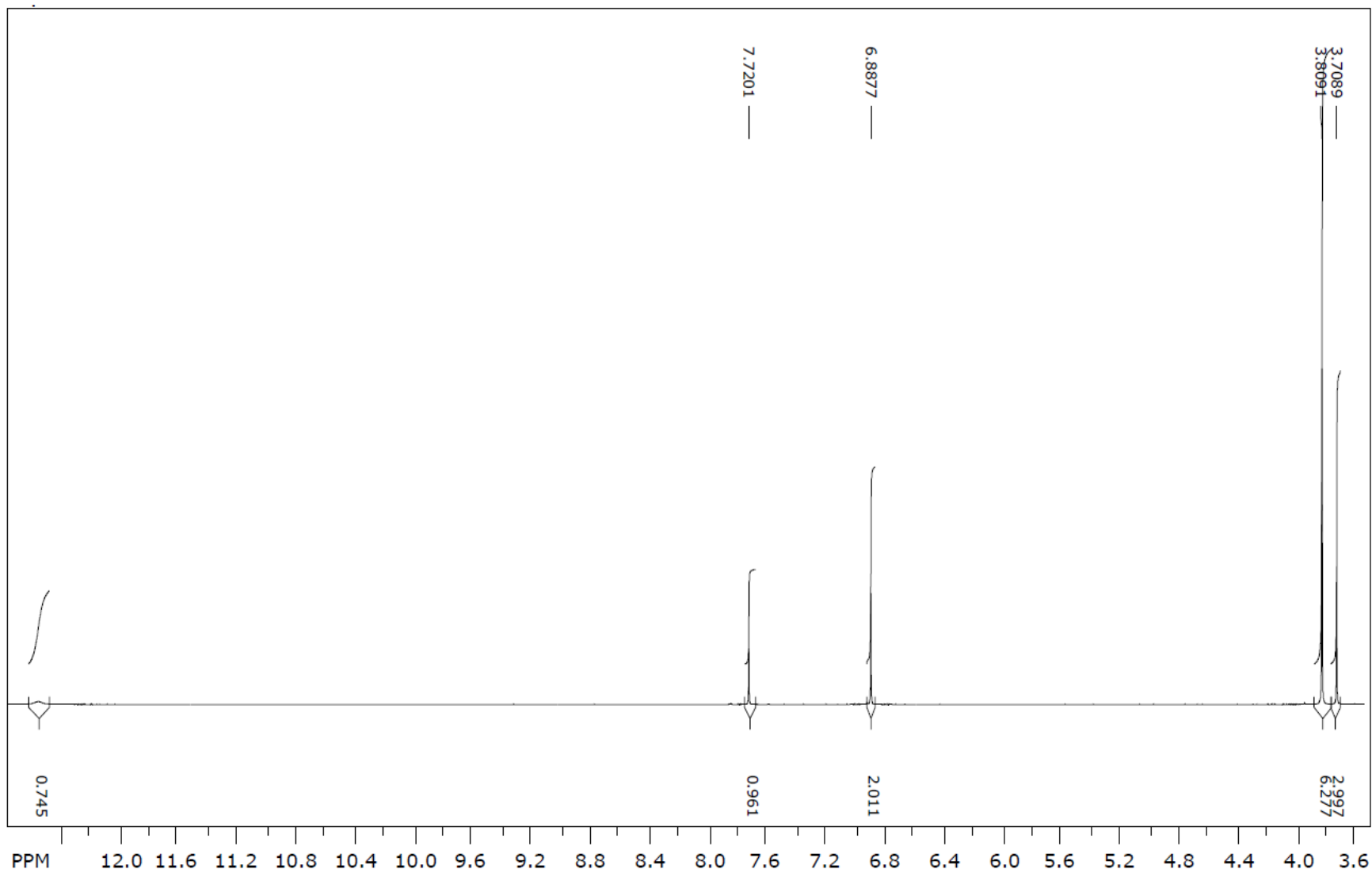


Reaktanti	3,4,5-trimetoksibenzaldehid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	295,31 g/mol
Molekulska formula	C ₁₃ H ₁₃ NO ₅ S
Temperatura tališta	172 – 174 °C (lit. 179 – 181 °C, Ha i sur., 2012)
Boja kristala	Žuta
R_f	0,71
LC/MS/MS m/z (M-)	294,11
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 12,59 (s, 1H, NH), 7,72 (s, 1H, CH), 6,88 (s, 2H, arom.), 3,80 (s, 6H, OCH ₃), 3,70 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 167,81; 167,20, 155,15; 139,35; 132,05; 128,49; 122,41; 107,48; 60,16; 55,96.

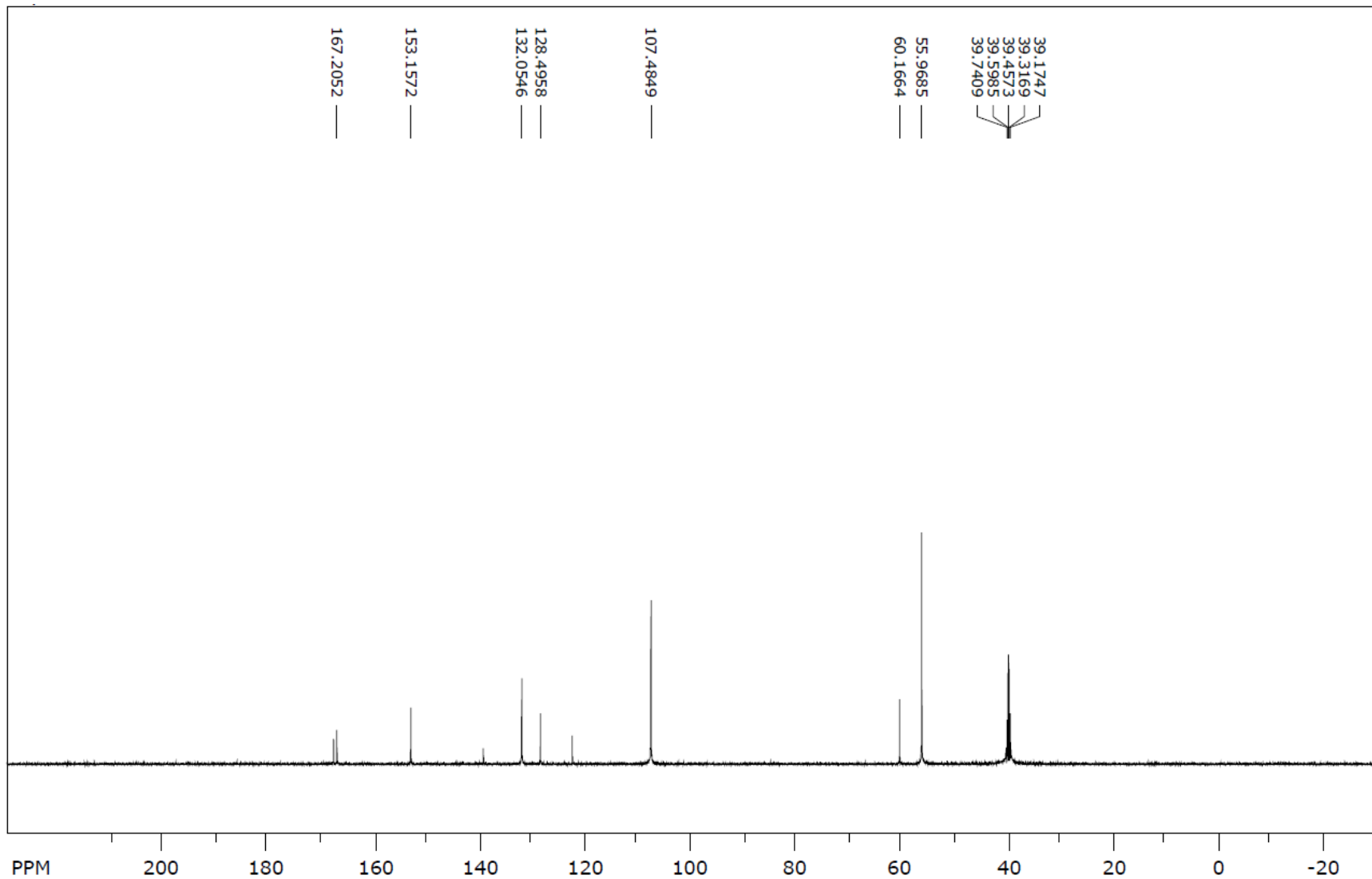
Maseni spektar (9g)



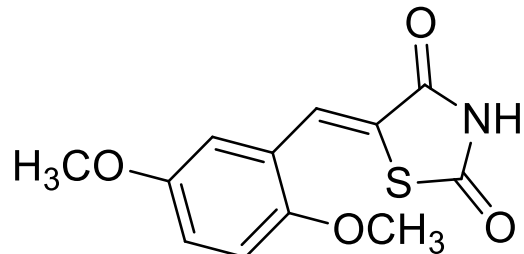
¹H NMR spektr (9g)



¹³C NMR spektr (9g)

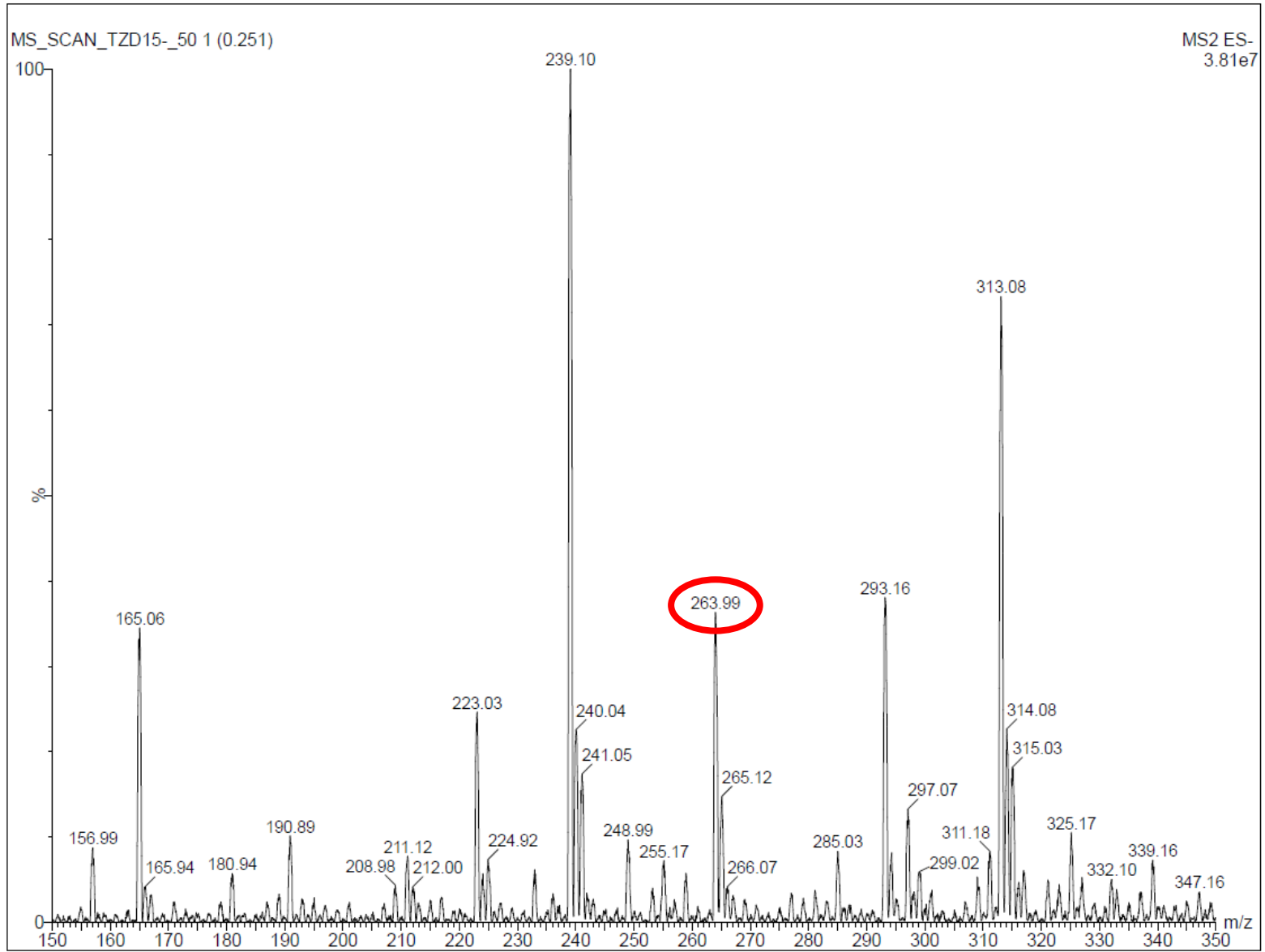


5-(2,5-dimetoksibenziliden) tiazolidin-2,4-dion (9h)

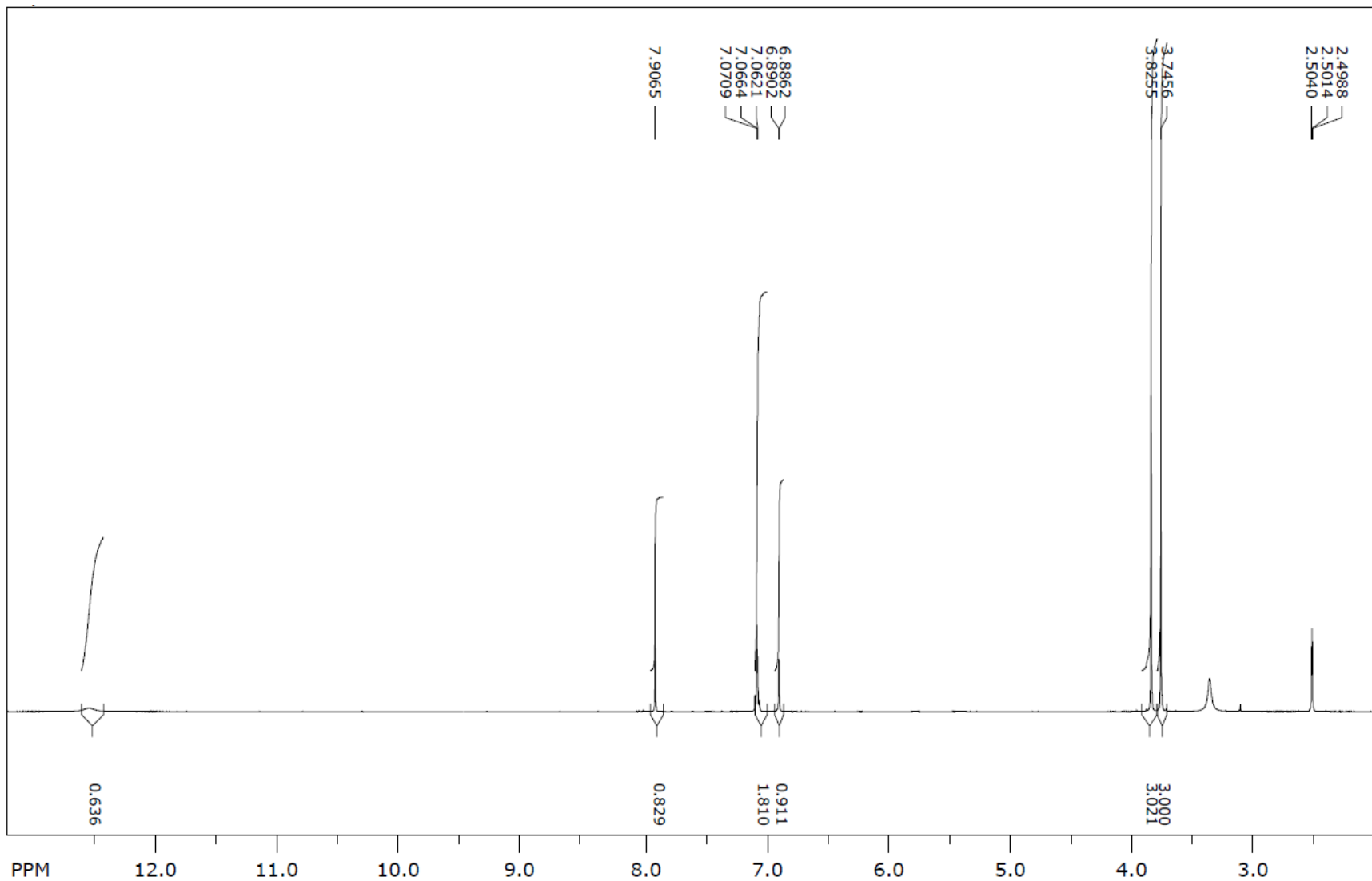


Reaktanti	2,5-dimetoksibenzaldehid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	265,29 g/mol
Molekulska formula	C ₁₂ H ₁₁ NO ₄ S
Temperatura tališta	220 – 223 °C (lit. 210 – 212 °C, Durai Ananda Kumar i sur., 2015)
Boja kristala	Žuta
R_f	0,74
LC/MS/MS m/z (M-)	263,99
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 12,56 (s, 1H, NH), 7,90 (s, 1H, CH), 7,07 (t, <i>J</i> = 2,64 Hz, 2H, arom.), 6,89 (d, <i>J</i> = 2,40 Hz, 1H, arom.), 3,82 (s, 3H, OCH ₃), 3,74 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 167,91; 167,28; 153,01; 152,36; 126,35; 123,79; 121,90; 117,57, 113,22; 113,00; 56,06: 55,47.

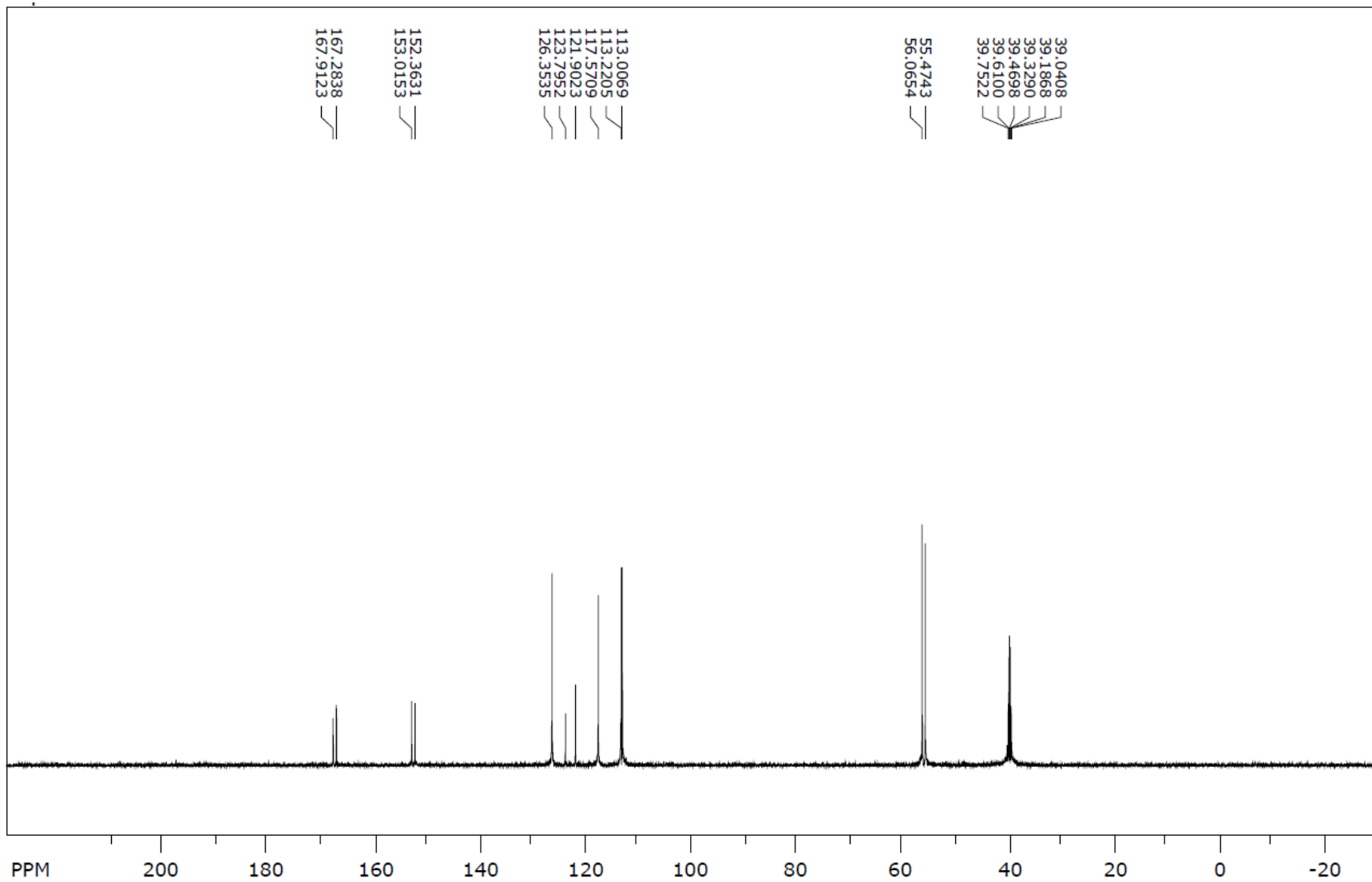
Maseni spektr (9h)



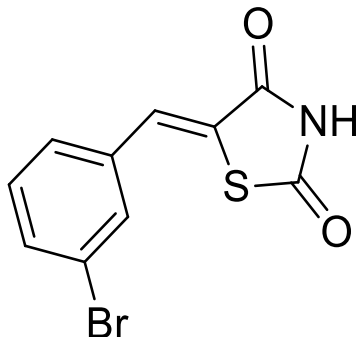
¹H NMR spektr (9h)



¹³C NMR spektr (9h)

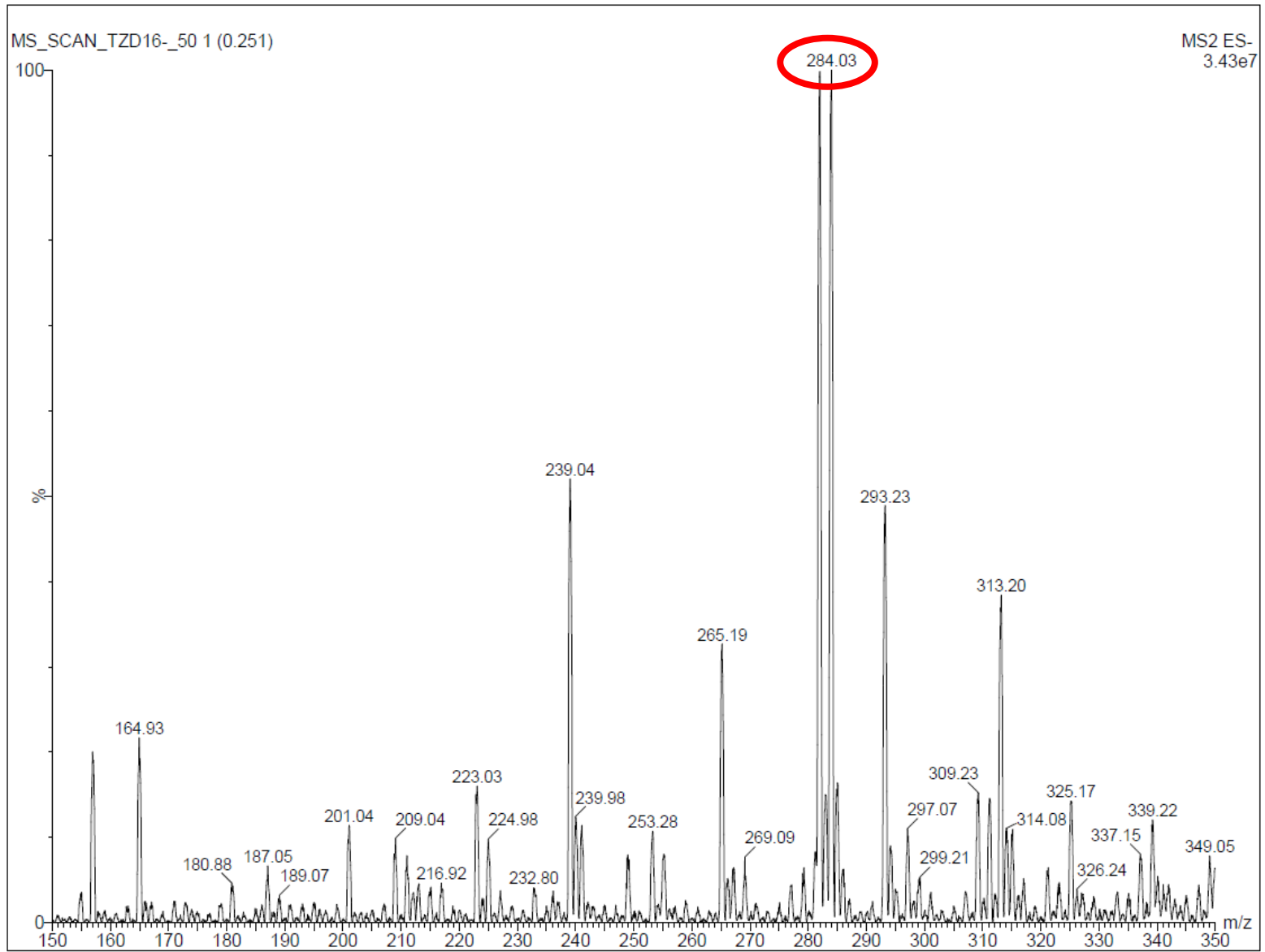


5-(3-brombenziliden) tiazolidin-2,4-dion (9i)

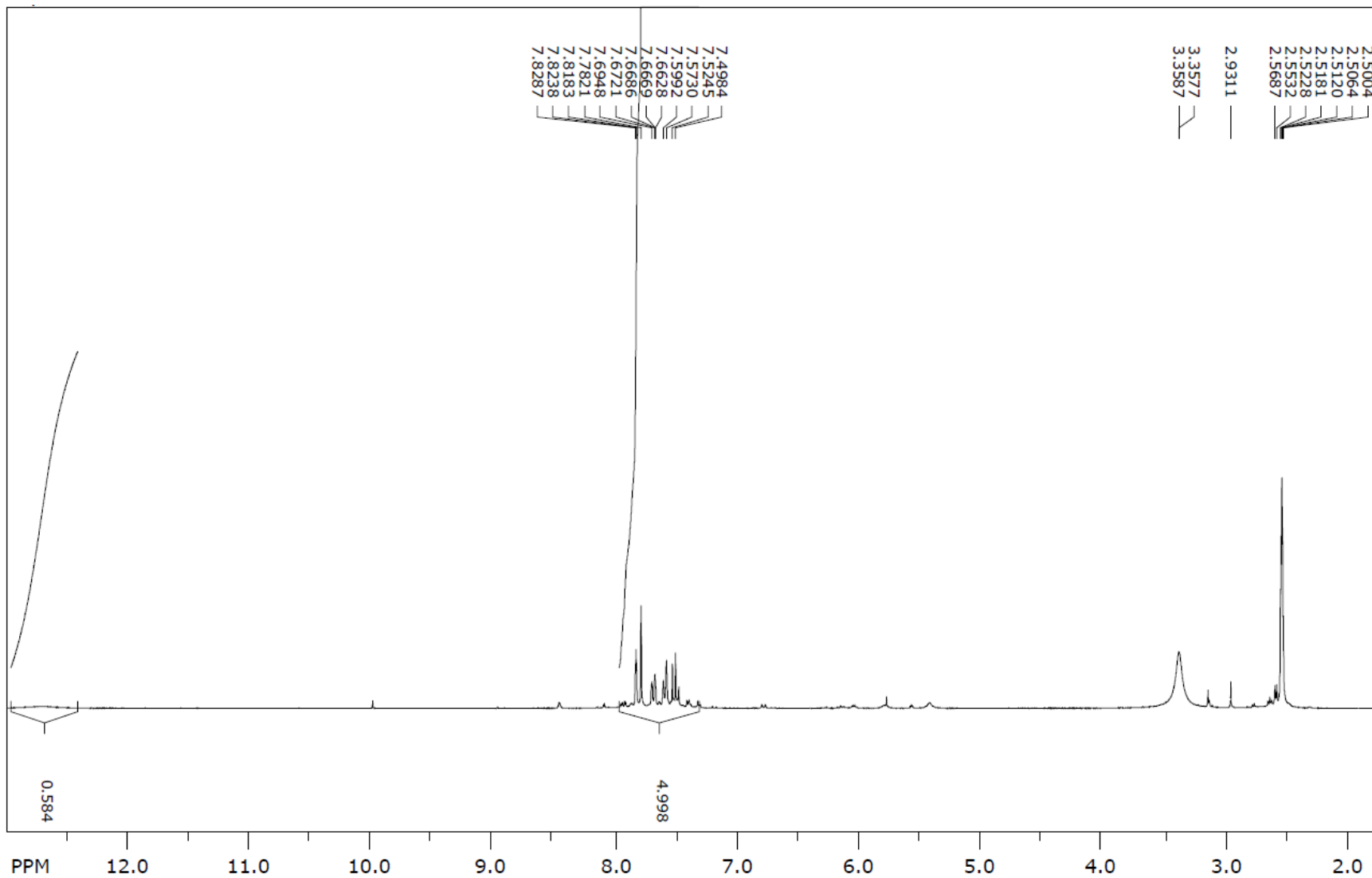


Reaktanti	3-brombenzaldehyd (2 mmol) i tiazolidindion (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	284,13 g/mol
Molekulska formula	C ₁₀ H ₆ BrNO ₂ S
Temperatura tališta	210 – 212 °C
Boja kristala	Bijela
R_f	0,76
LC/MS/MS <i>m/z</i> (M-)	284,03
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 12,69 (s, 1H, NH), 7,82 (t, <i>J</i> = 1,56 Hz, 1H, arom.), 7,78 (s, 1H, CH), 7,66 – 7,70 (m, 1H, arom.), 7,59 (d, <i>J</i> = 7,86 Hz, 1H, arom.), 7,50 (t, <i>J</i> = 7,82 Hz, 1H, arom.).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 168,05; 167,68; 135,98; 133,31; 133,23; 131,79; 130,46; 128,55; 125,92; 122,90.

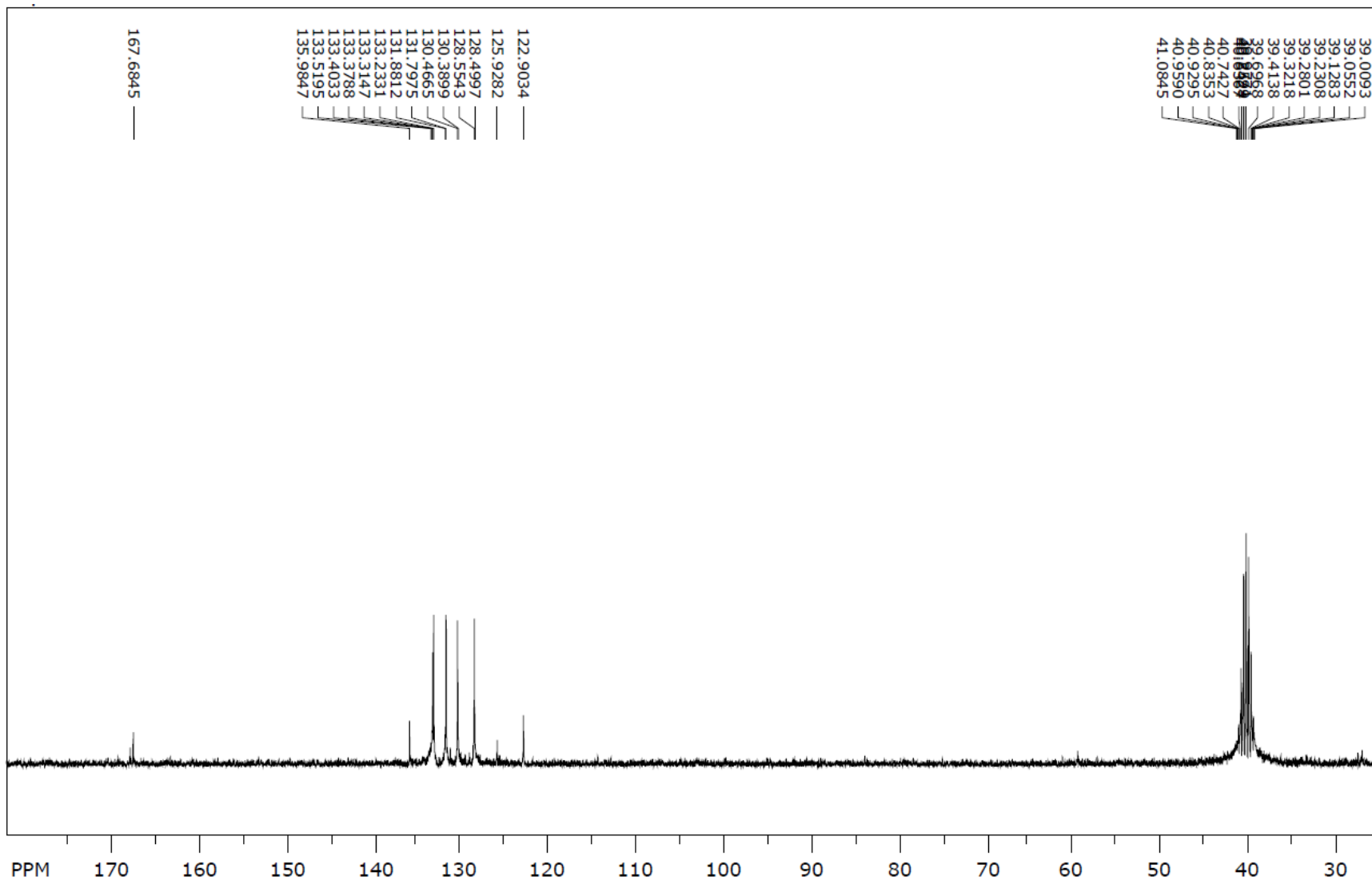
Maseni spektar (9i)



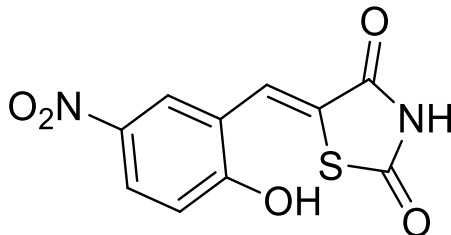
¹H NMR spektar (9i)



¹³C NMR spektr (9i)

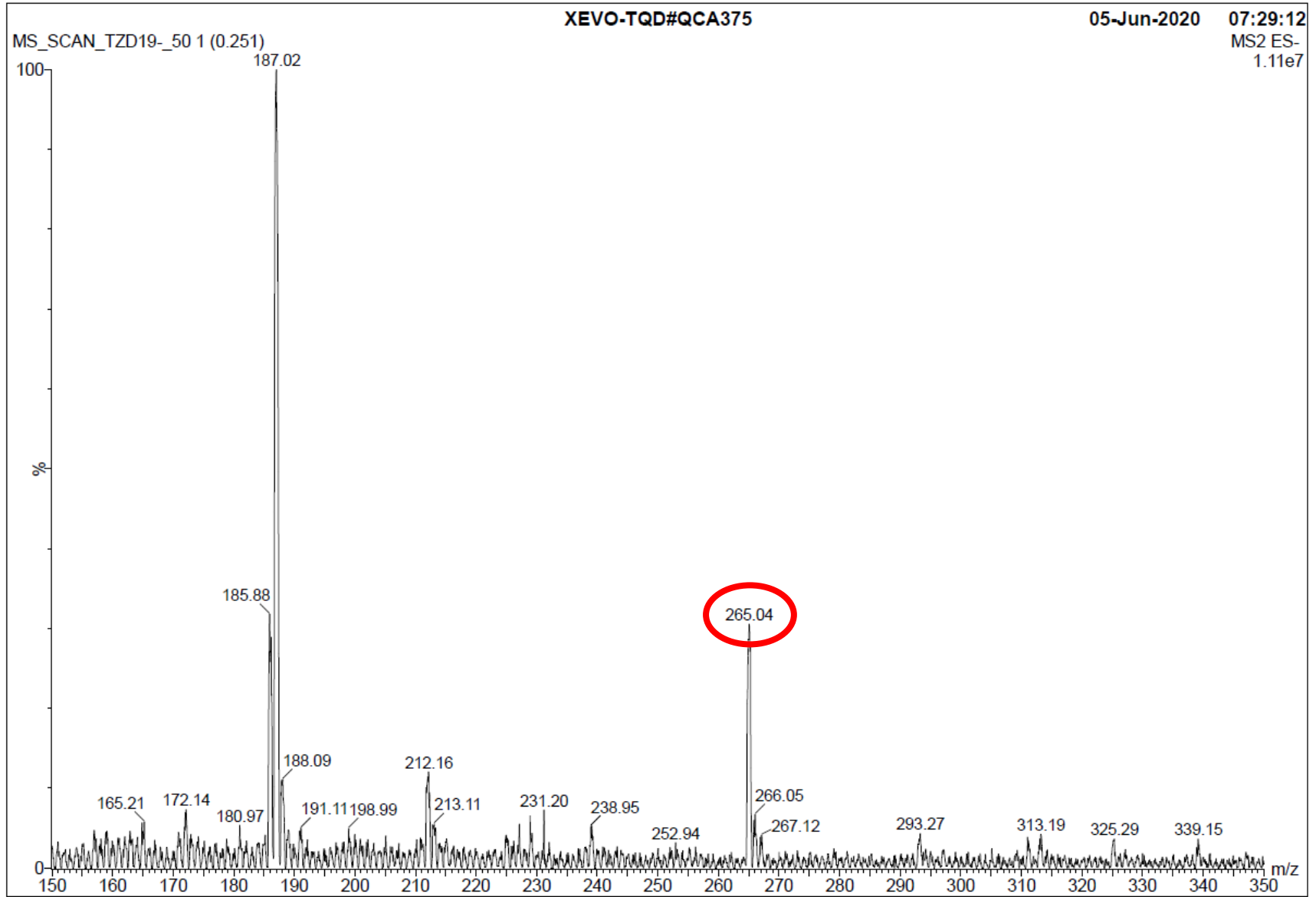


5-(2-hidroksi-5-nitrobenziliden) tiazolidin-2,4-dion (9j)

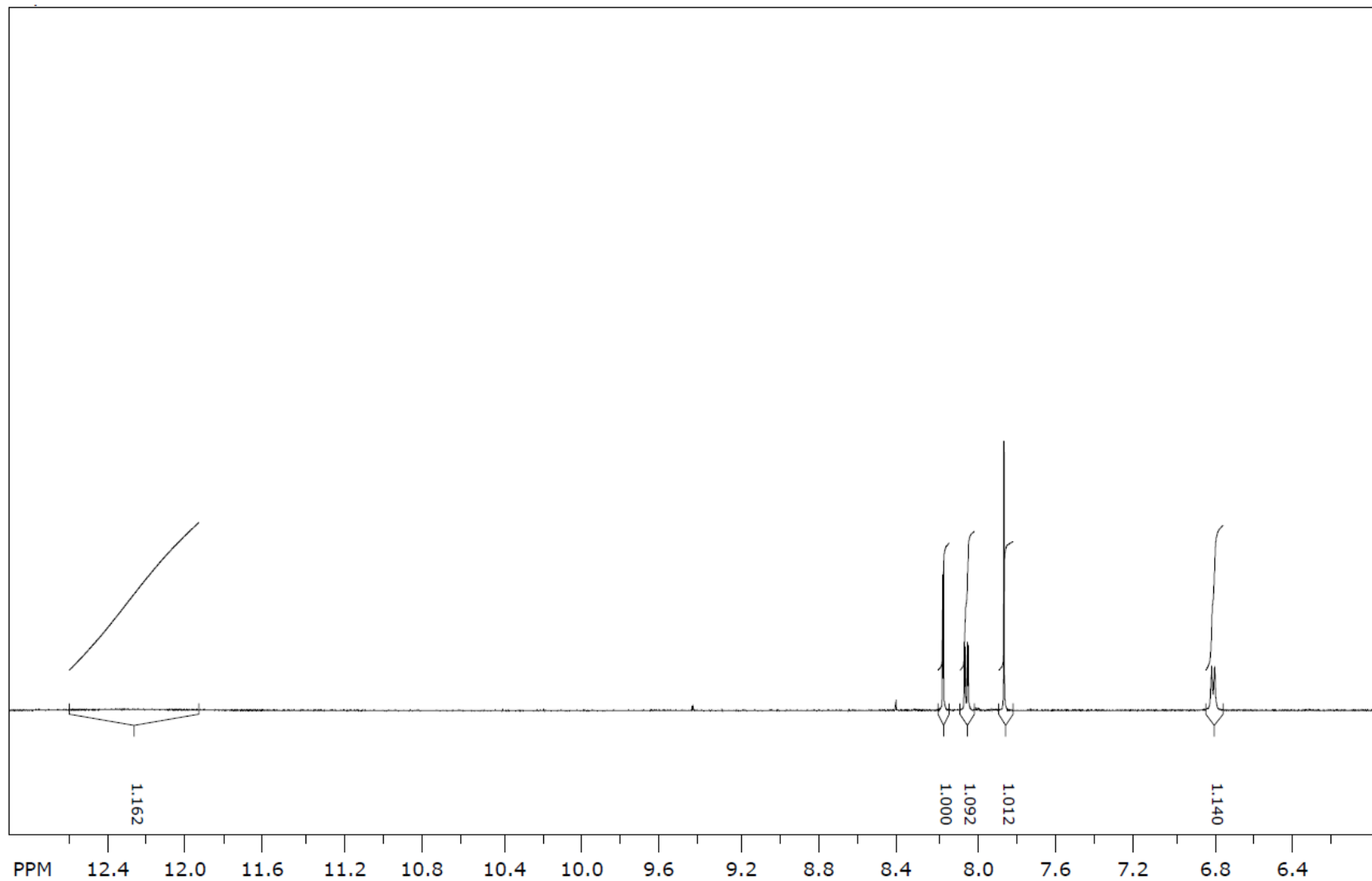


Reaktanti	5-nitrosalicilaldehid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	266,23 g/mol
Molekulska formula	C ₁₀ H ₆ N ₂ O ₅ S
Temperatura tališta	226 – 228 °C
Boja kristala	Crvena
R_f	0,49
LC/MS/MS <i>m/z</i> (M-)	265,04
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 8,40 (s, 1H, OH), 8,17 (d, <i>J</i> = 2,82 Hz, 1H, arom.), 8,04 (dd, <i>J</i> = 9,24; 2,82 Hz, 1H, arom.), 7,85 (s, 1H, arom.), 6,80 (d, <i>J</i> = 9,18 Hz, 1H, arom.).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 169,06; 127,19; 125,27; 125,07; 121,01; 117,88.

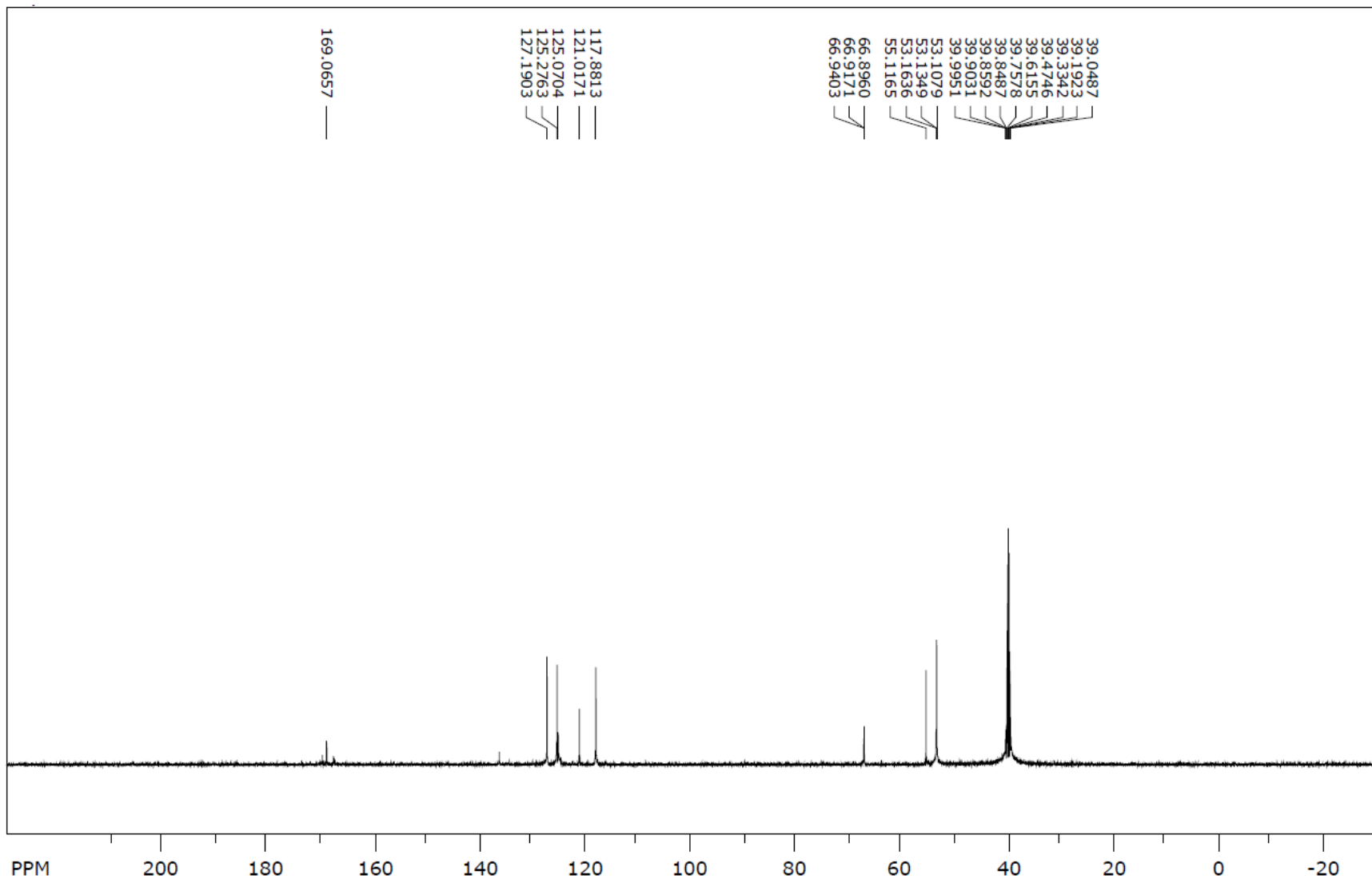
Maseni spektrar (9j)



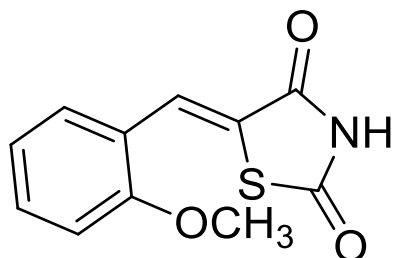
¹H NMR spektr (9j)



¹³C NMR spektr (9j)

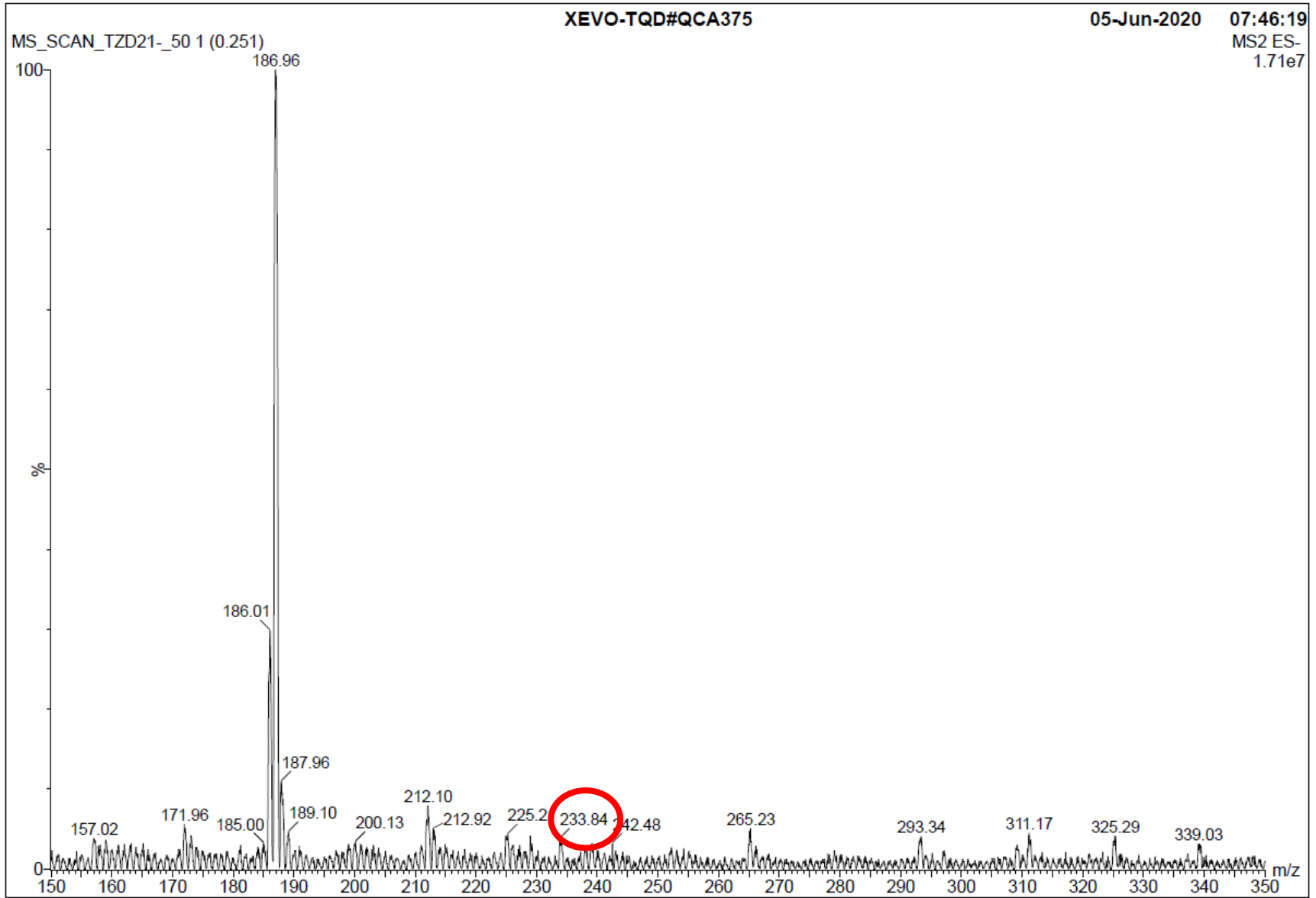


5-(2-metoksibenziliden) tiazolidin-2,4-dion (9k)

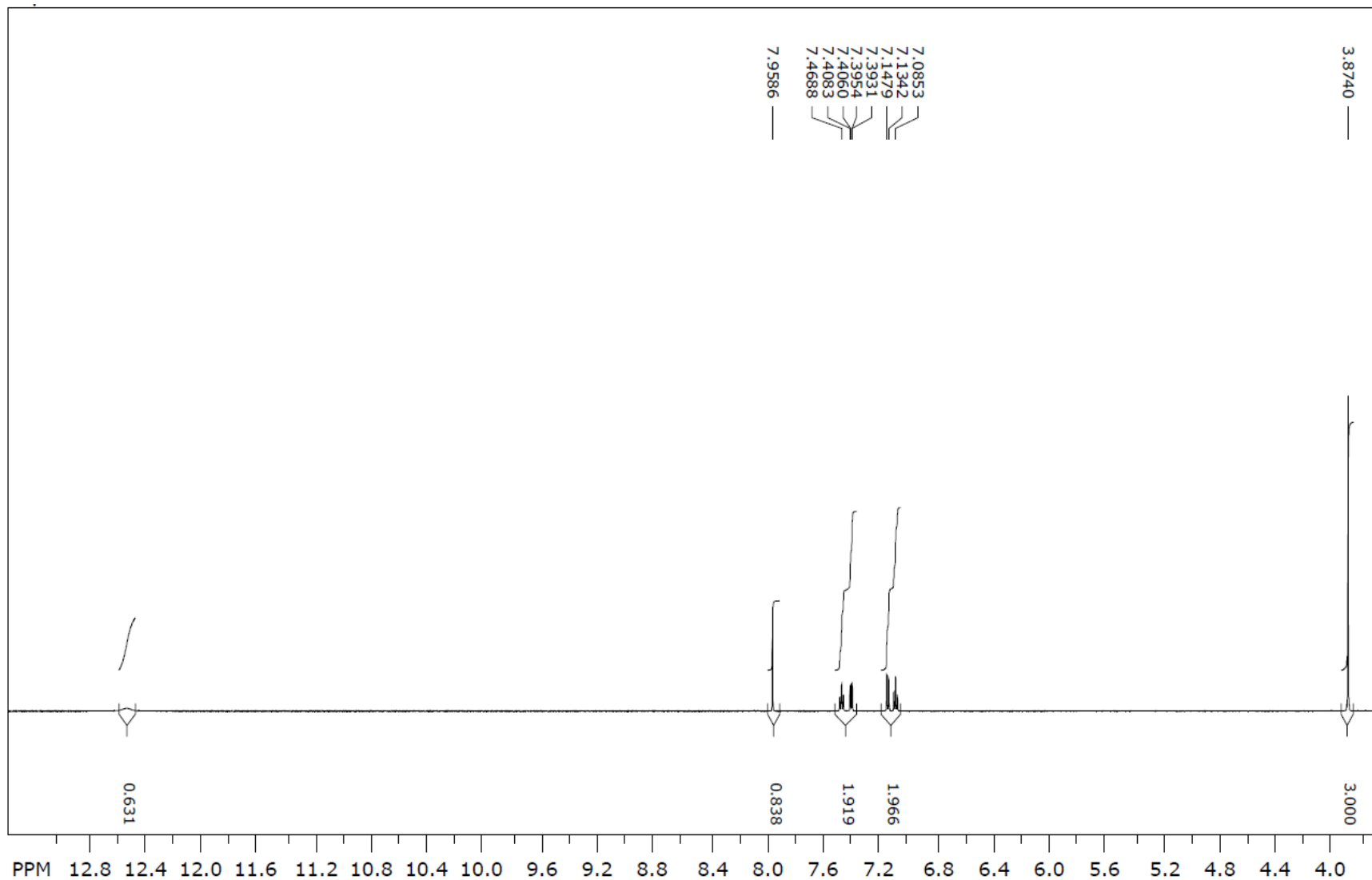


Reaktanti	2-metoksibenzaldehid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	235,26 g/mol
Molekulska formula	C ₁₁ H ₉ NO ₃ S
Temperatura tališta	240 – 241 °C
Boja kristala	Žuta
R_f	0,82
LC/MS/MS <i>m/z</i> (M⁻)	233,84
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 12,54 (s, 1H, NH), 7,95 (s, 1H, CH), 7,45 – 7,48 (m, 1H, arom.), 7,39 – 7,40 (dd, <i>J</i> = 7,74; 1,38 Hz, 1H, arom.), 7,14 (d, <i>J</i> = 8,22 Hz, 1H, arom.), 7,08 (t, <i>J</i> = 7,53 Hz, 1H, arom.), 3,87 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 168,09; 167,41; 132,36; 128,52; 126,42; 123,43; 121,41; 120,90; 111,82; 55,73.

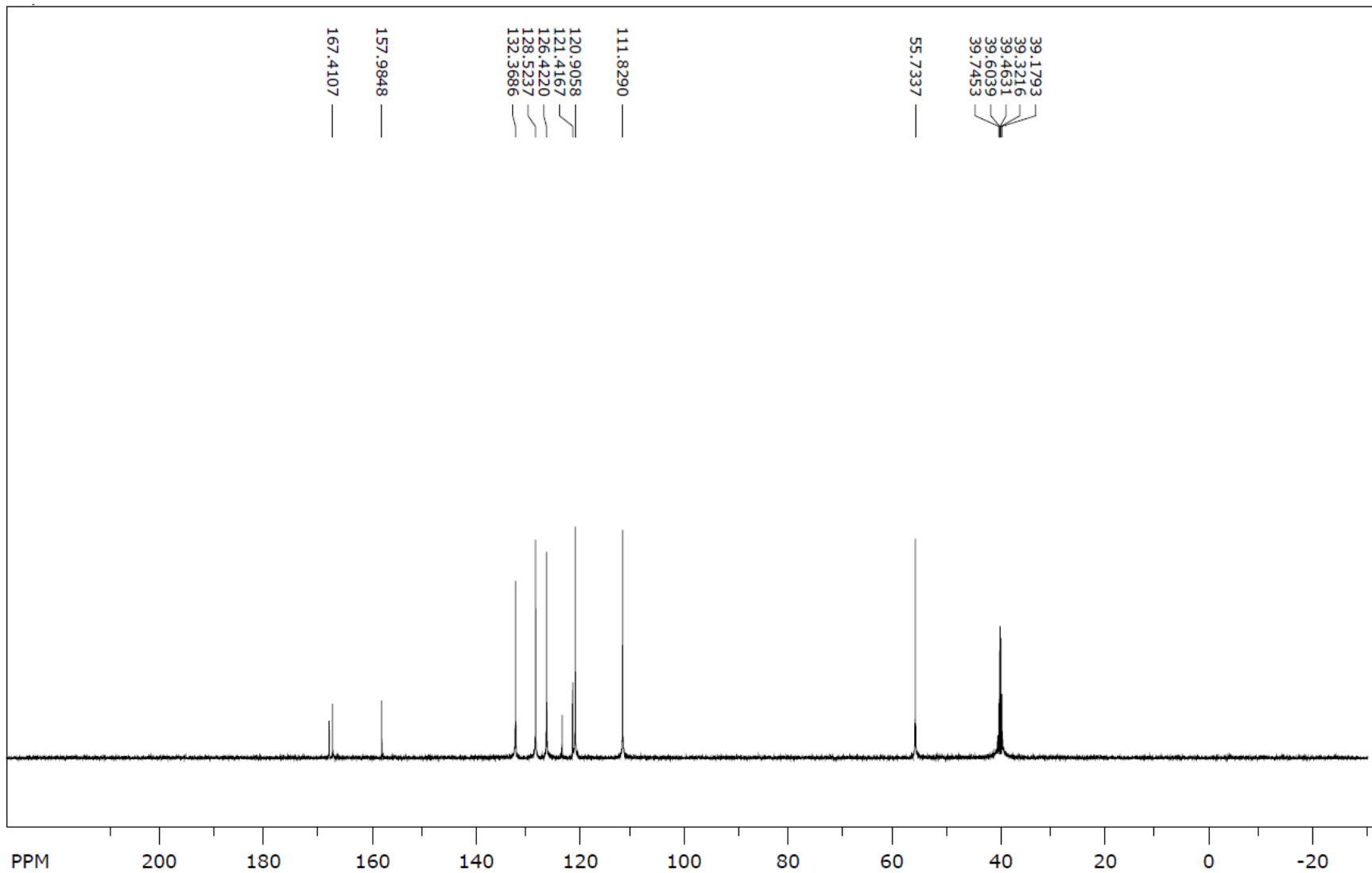
Maseni spektar (9k)



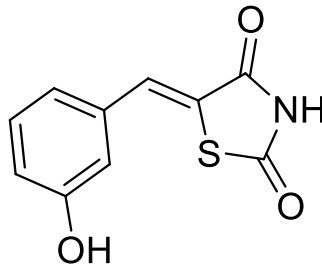
¹H NMR spektr (9k)



¹³C NMR spektr (9k)

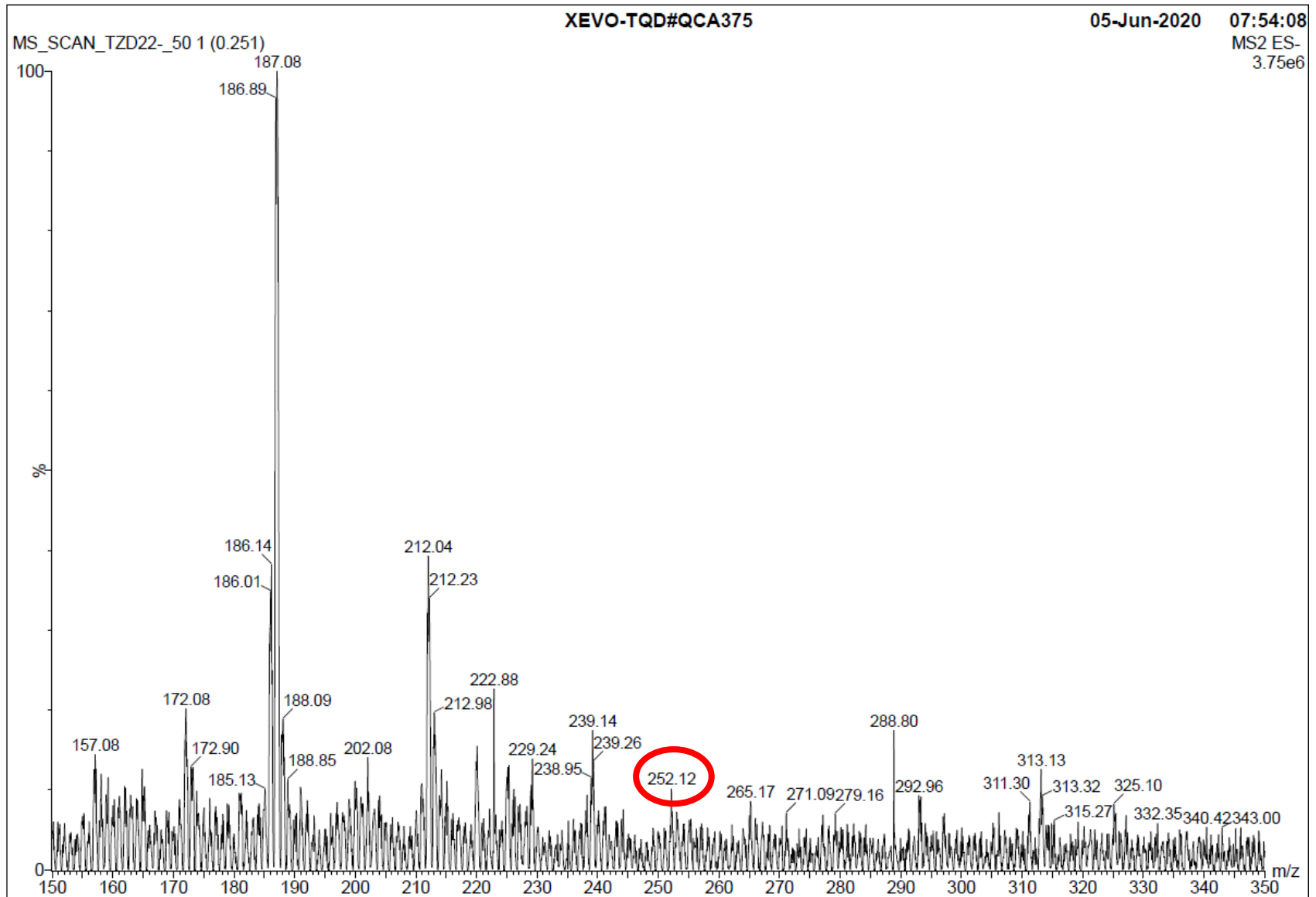


5-(3-hidroksibenziliden) tiazolidin-2,4-dion (9I)

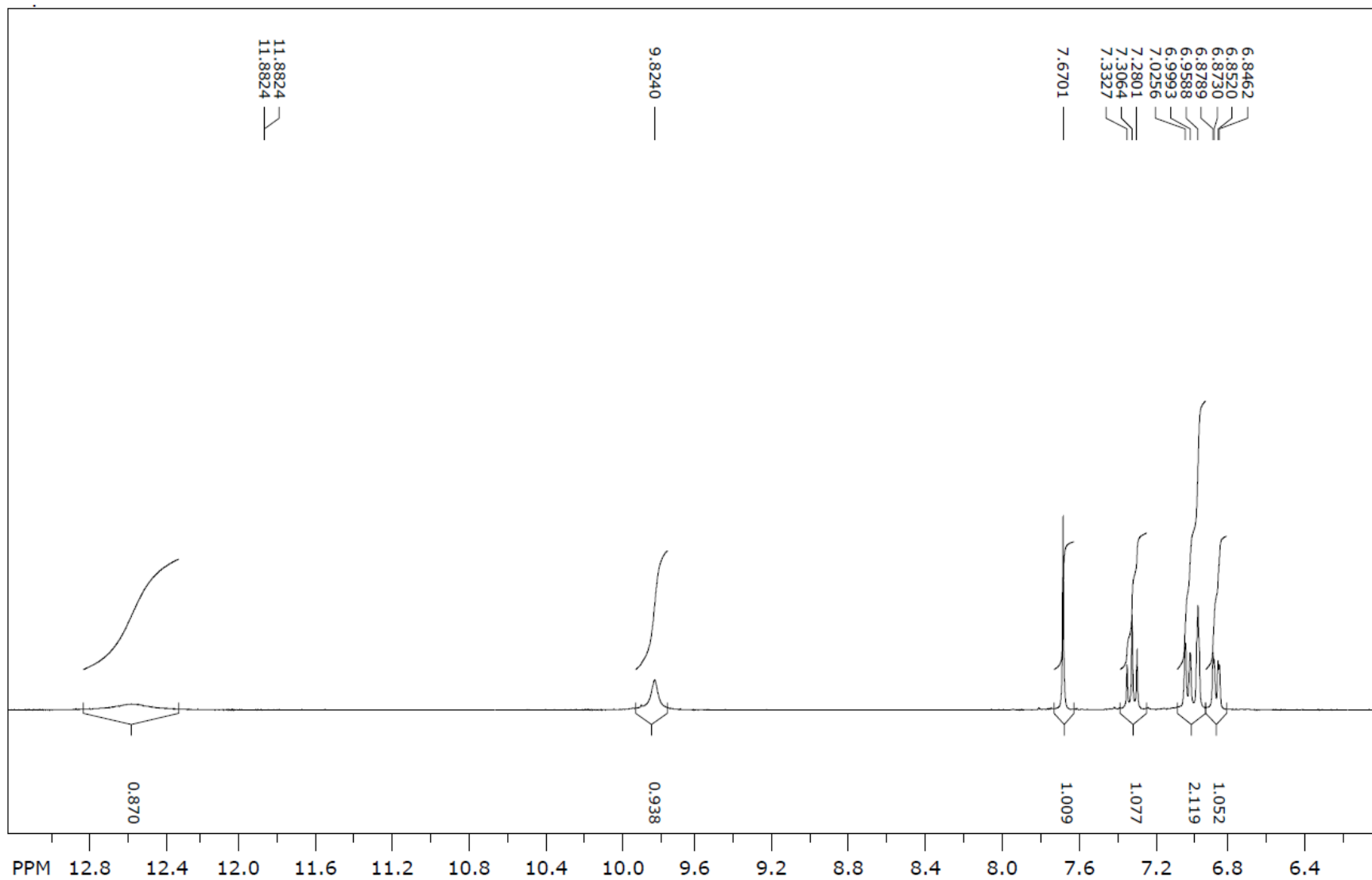


Reaktanti	3-hidroksibenzaldehid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	221,23 g/mol
Molekulska formula	C ₁₀ H ₇ NO ₃ S
Temperatura tališta	262 – 264 °C (lit. 246 – 248 °C, Durai Ananda Kumar i sur., 2015)
Boja kristala	Svijetlosmeđa
R_f	0,64
LC/MS/MS m/z (M-+MeOH)	252,12
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 12,58 (s, 1H, NH), 9,82 (s, 1H, OH), 7,67 (s, 1H, CH), 7,31 (t, <i>J</i> = 7,89 Hz, 1H, arom.), 7,01 (d, <i>J</i> = 7,89 Hz, 1H, arom.), 6,96 (s, 1H, arom.), 6,86 (dd, <i>J</i> = 8,07; 1,76 Hz, 1H, arom.).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 168,42; 167,80; 158,32; 134,65; 132,45; 130,83; 123,75; 121,78; 118,19; 116,37.

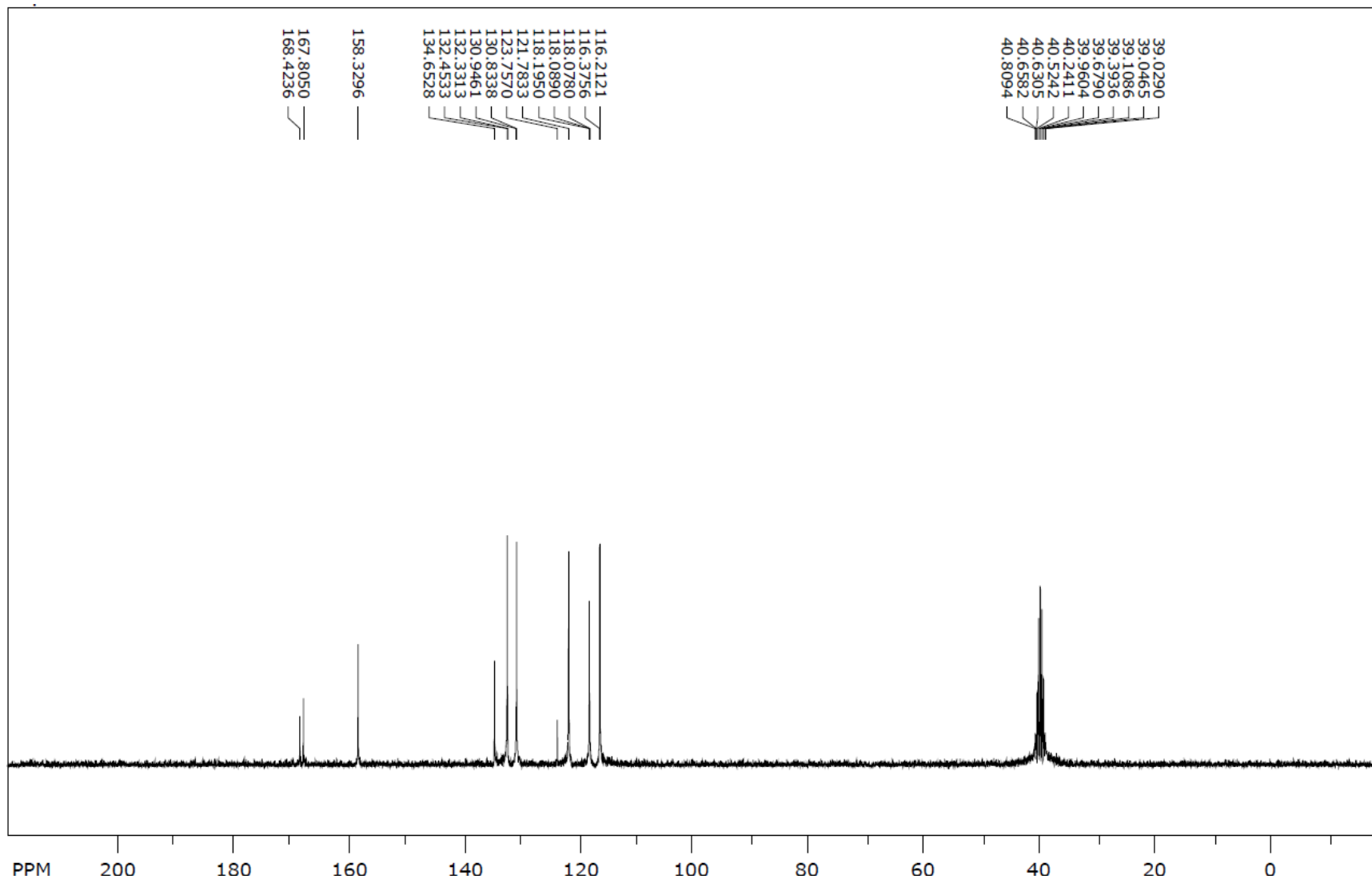
Maseni spektar (9I)



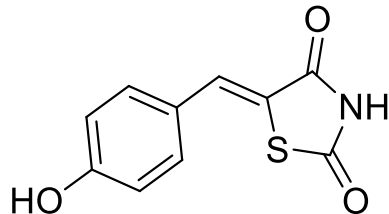
¹H NMR spektr (9I)



¹³C NMR spektr (9I)

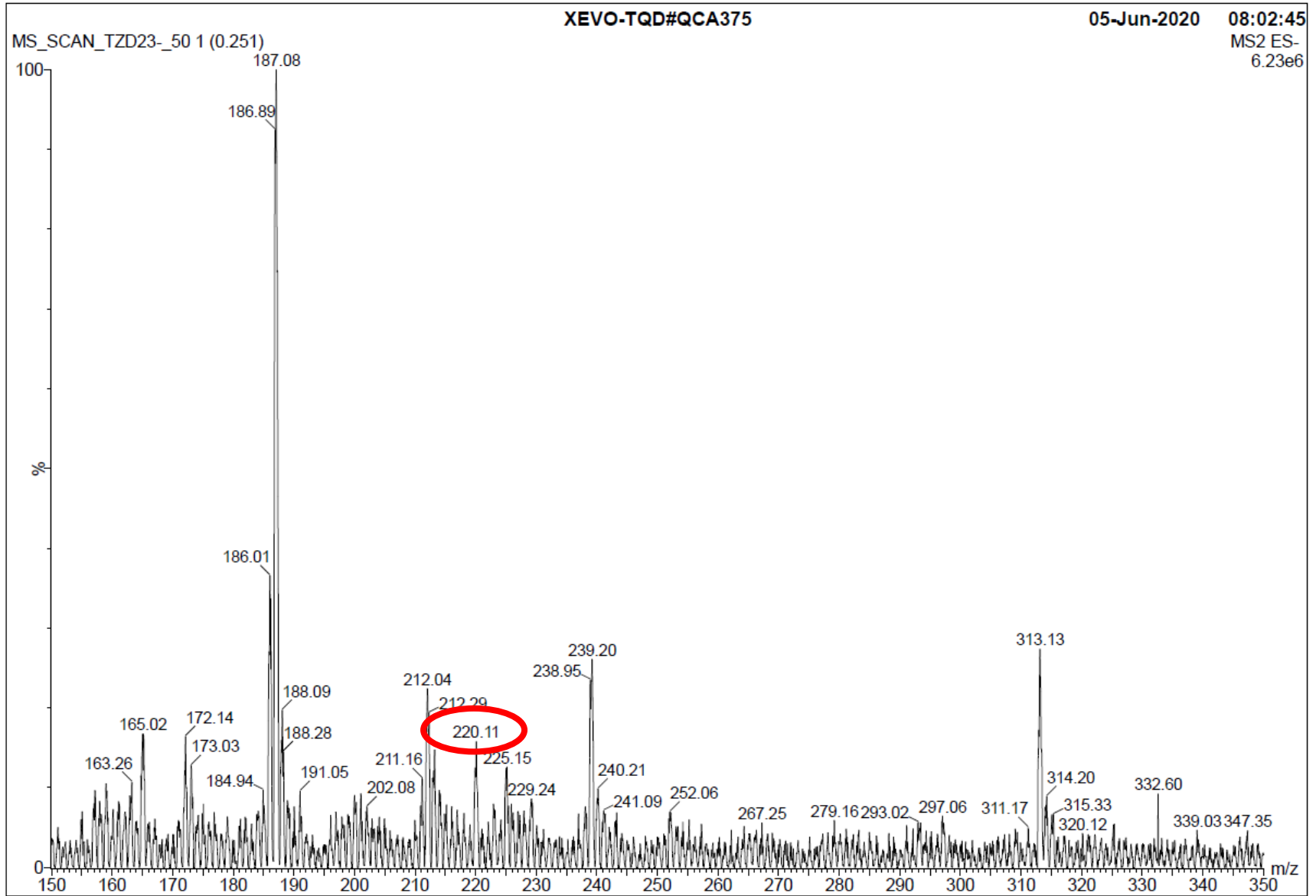


5-(4-hidroksibenziliden) tiazolidin-2,4-dion (9m)

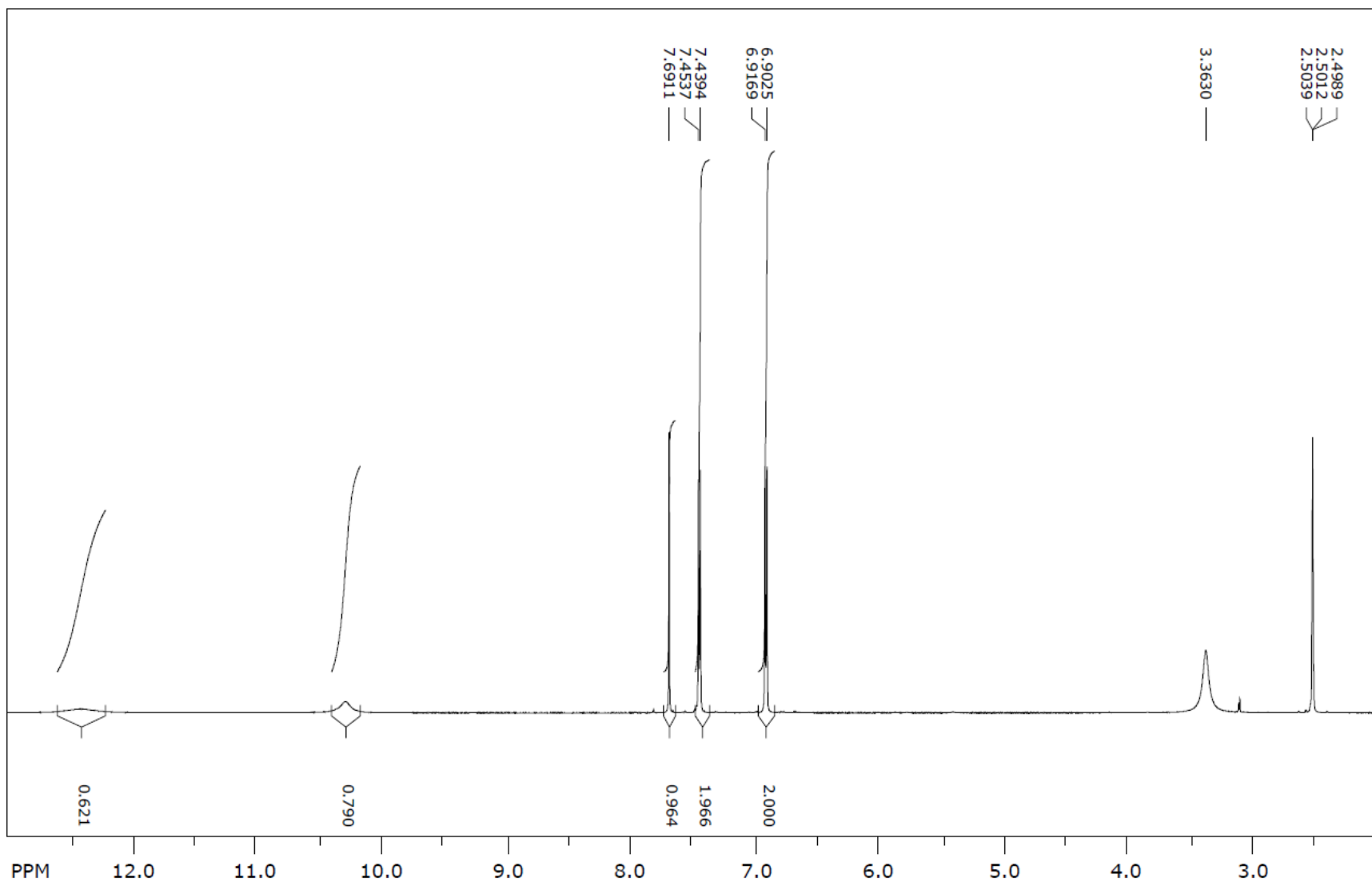


Reaktanti	4-hidroksibenzaldehid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	221,23 g/mol
Molekulska formula	C ₁₀ H ₇ NO ₃ S
Temperatura tališta	296 – 297 °C (lit. 280 – 281 °C, Durai Ananda Kumar i sur., 2015; 299 °C, Ha i sur., 2012; 322 °C, Metwally i sur., 2011; 311 – 313 °C, Yang i Yang, 2011)
Boja kristala	Žuta
R_f	0,62
LC/MS/MS <i>m/z</i> (M-)	220,11
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 12,43 (s, 1H, NH), 10,30 (s, 1H, OH), 7,69 (s, 1H, CH), 7,45 (d, <i>J</i> = 8,58 Hz, 2H, arom.), 6,91 (d, <i>J</i> = 8,64 Hz, 2H, arom.).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 168,05; 167,52; 159,84; 132,35; 132,24; 123,90; 118,97; 116,28.

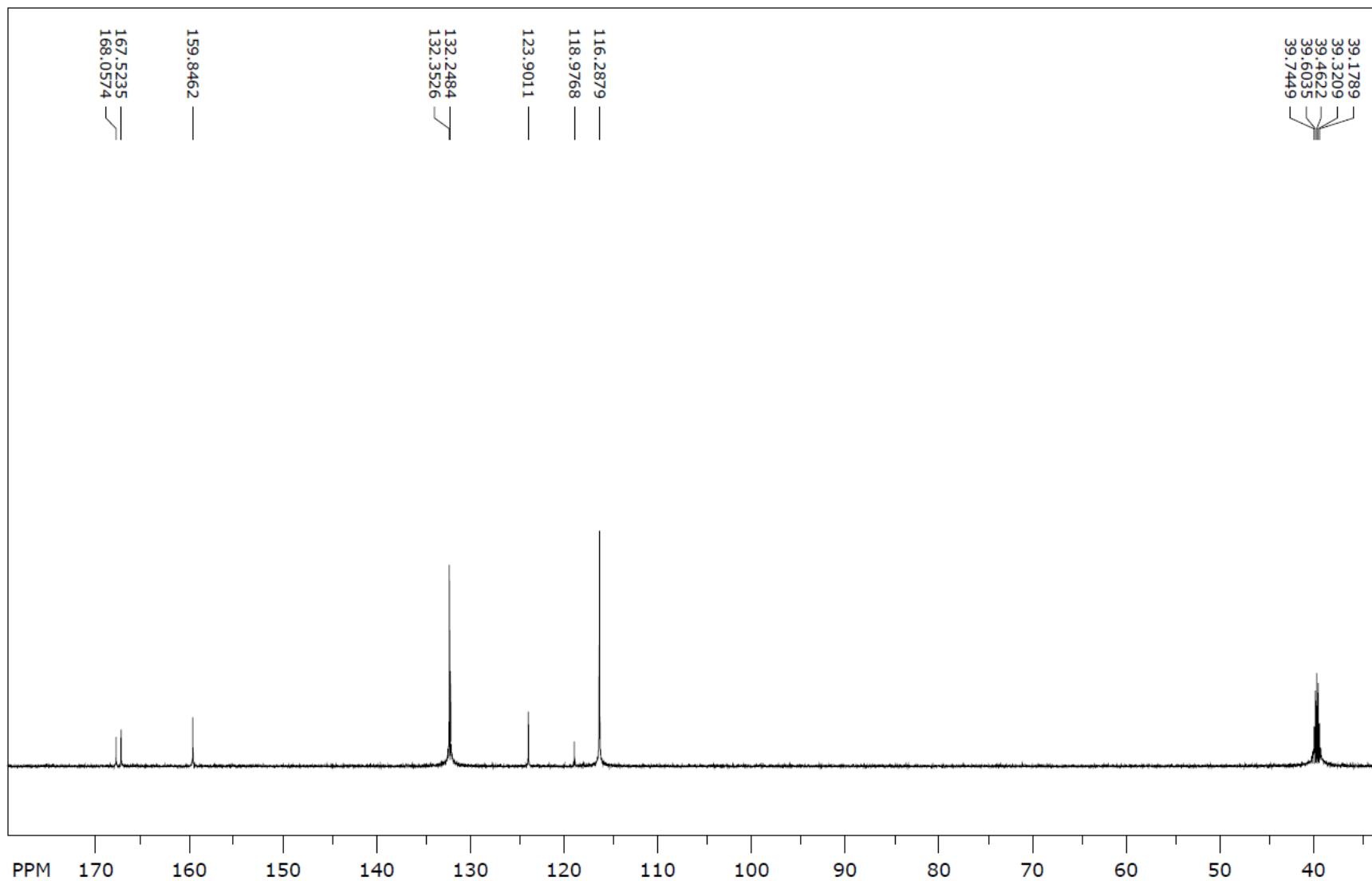
Maseni spektar (9m)



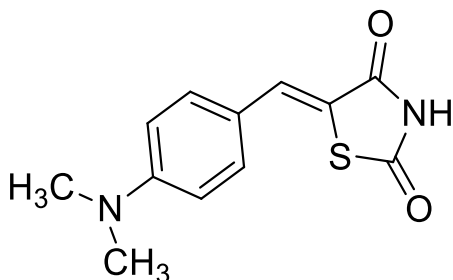
¹H NMR spektr (9m)



¹³C NMR spektr (9m)

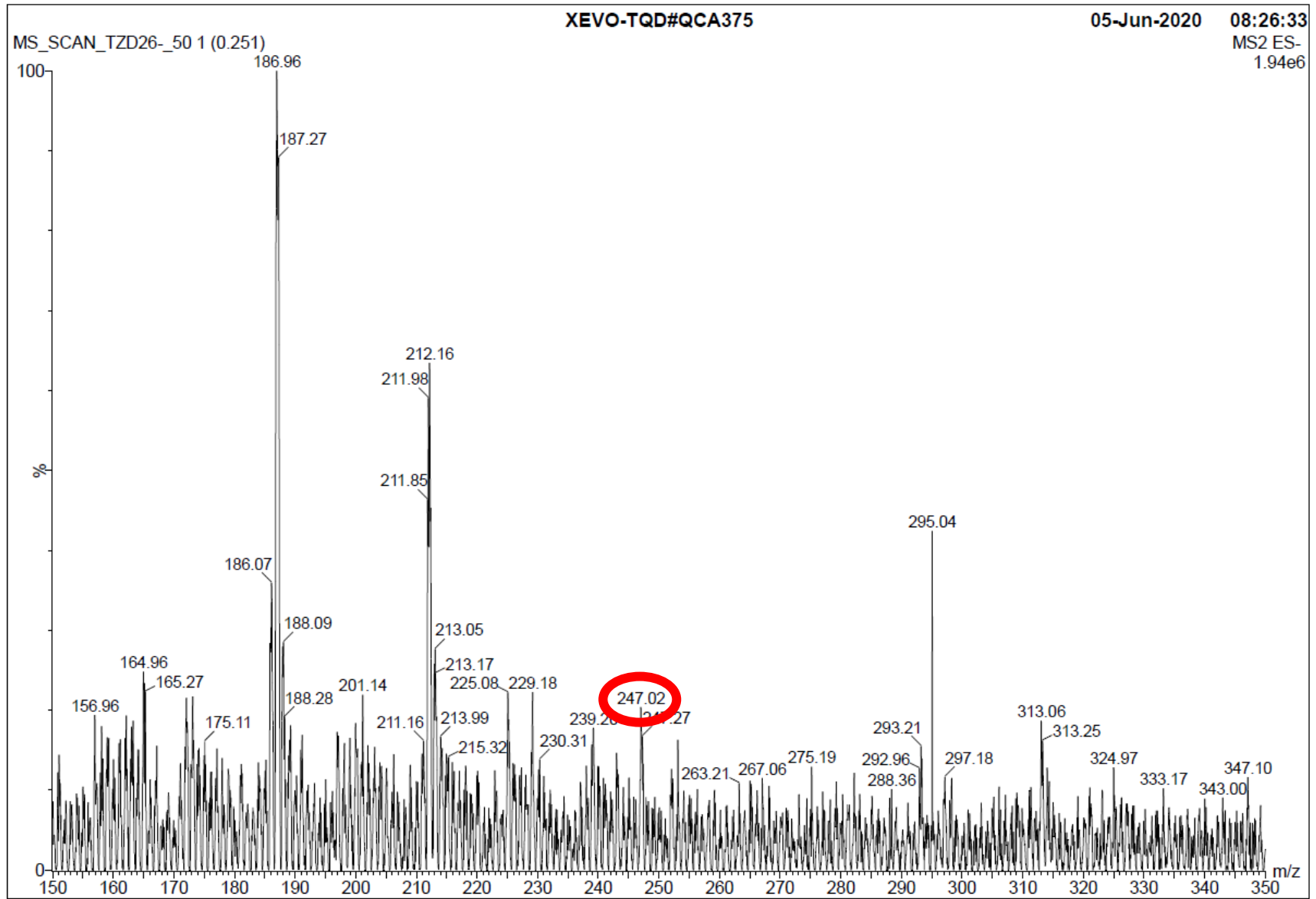


5-(4-(dimetilamino)benziliden) tiazolidin-2,4-dion (9n)

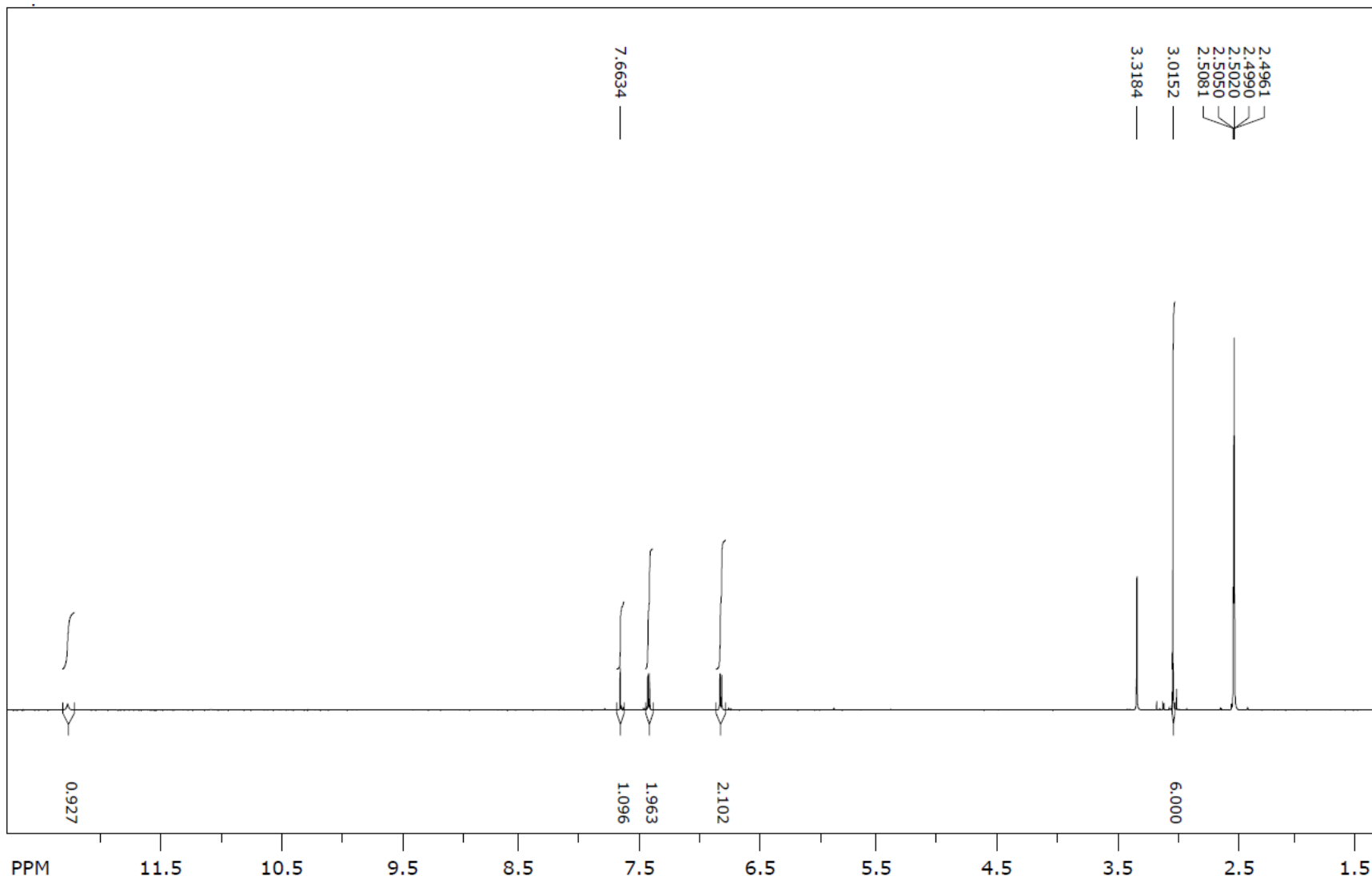


Reaktanti	4-dimetilaminobenzaldehid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročiščavanja	Ispran etanolom
Molekulska masa	248,30 g/mol
Molekulska formula	C ₁₂ H ₁₂ N ₂ O ₂ S
Temperatura tališta	286 – 289 °C (lit. 274 – 276 °C, Durai Ananda Kumar i sur., 2015; 282 – 283 °C, Shelke i sur., 2010)
Boja kristala	Narančasta
R_f	0,77
LC/MS/MS m/z (M-)	247,02
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 12,31 (s, 1H, NH), 7,66 (s, 1H, CH), 7,43 (d, <i>J</i> = 9,00 Hz, 2H, arom.), 6,82 (d, <i>J</i> = 9,00 Hz, 2H, arom.), 3,01 (s, 6H, CH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 168,15; 167,57; 151,39; 132,84; 132,08; 127,75; 119,79; 115,69; 111,99.

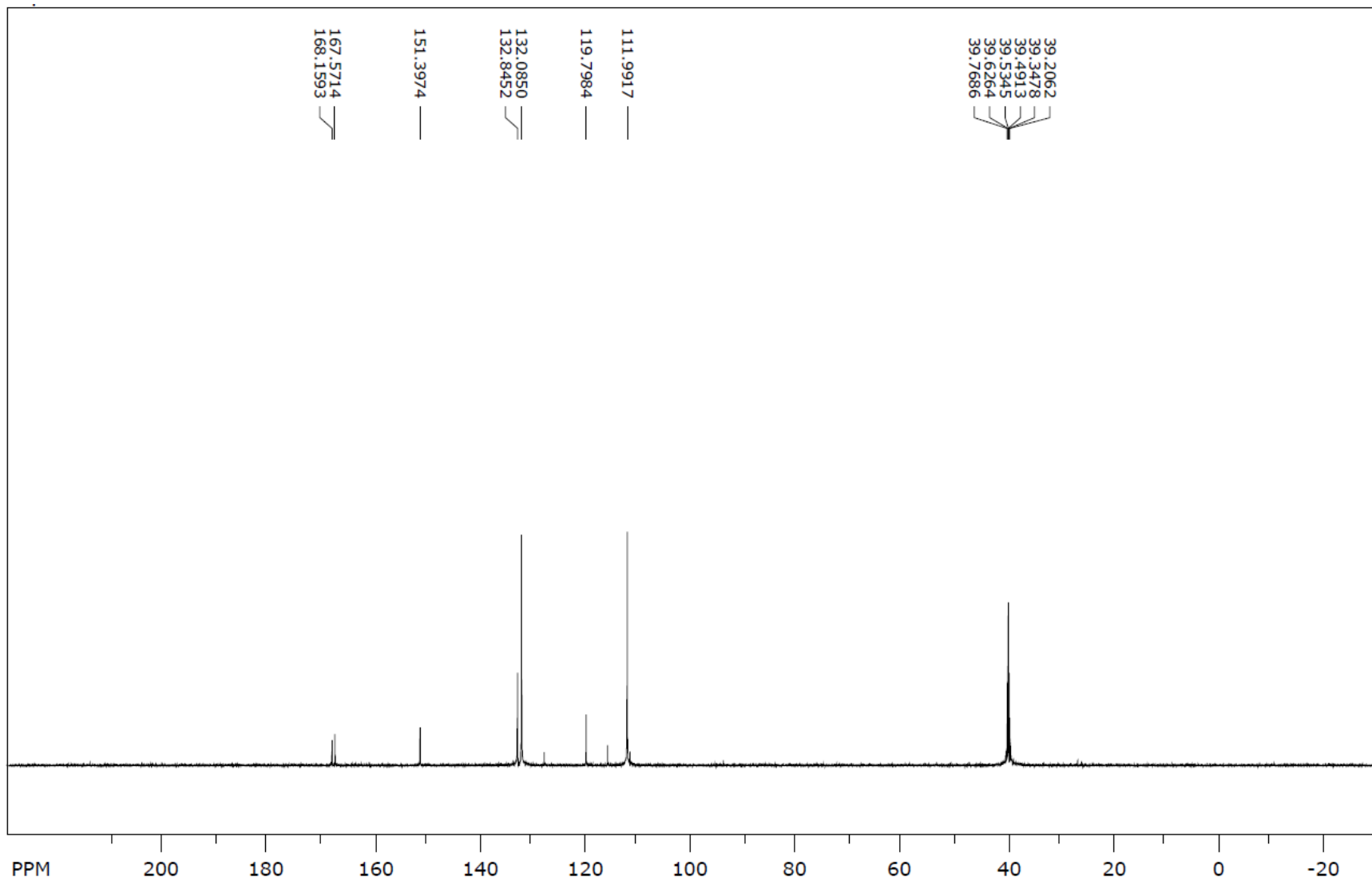
Maseni spektar (9n)



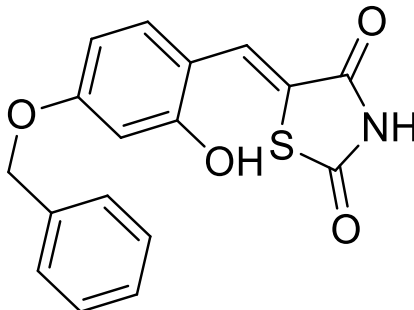
¹H NMR spektr (9n)



¹³C NMR spektr (9n)

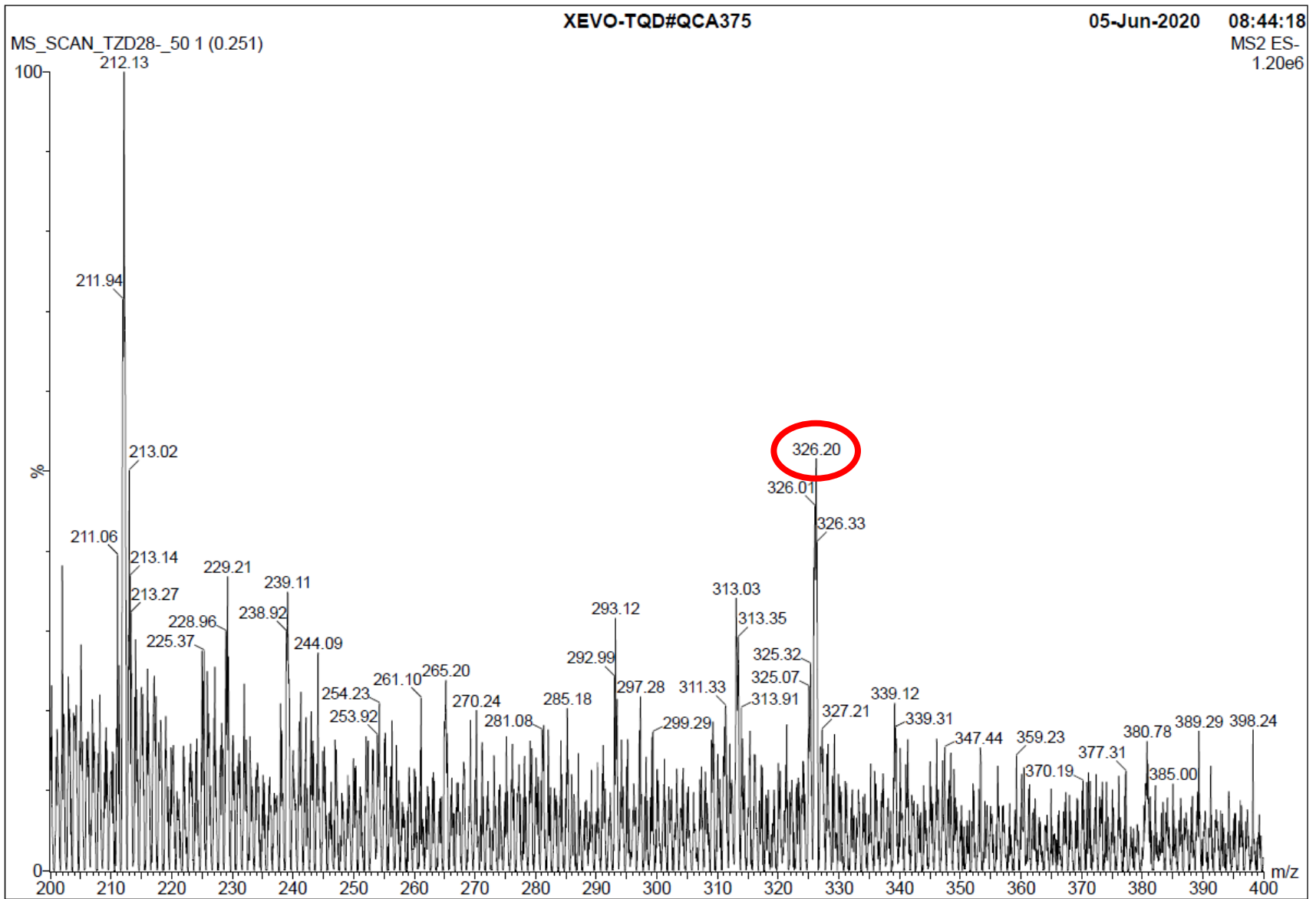


5-(4-(benziloksi)-2-hidroksibenziliden) tiazolidin-2,4-dion (9o)

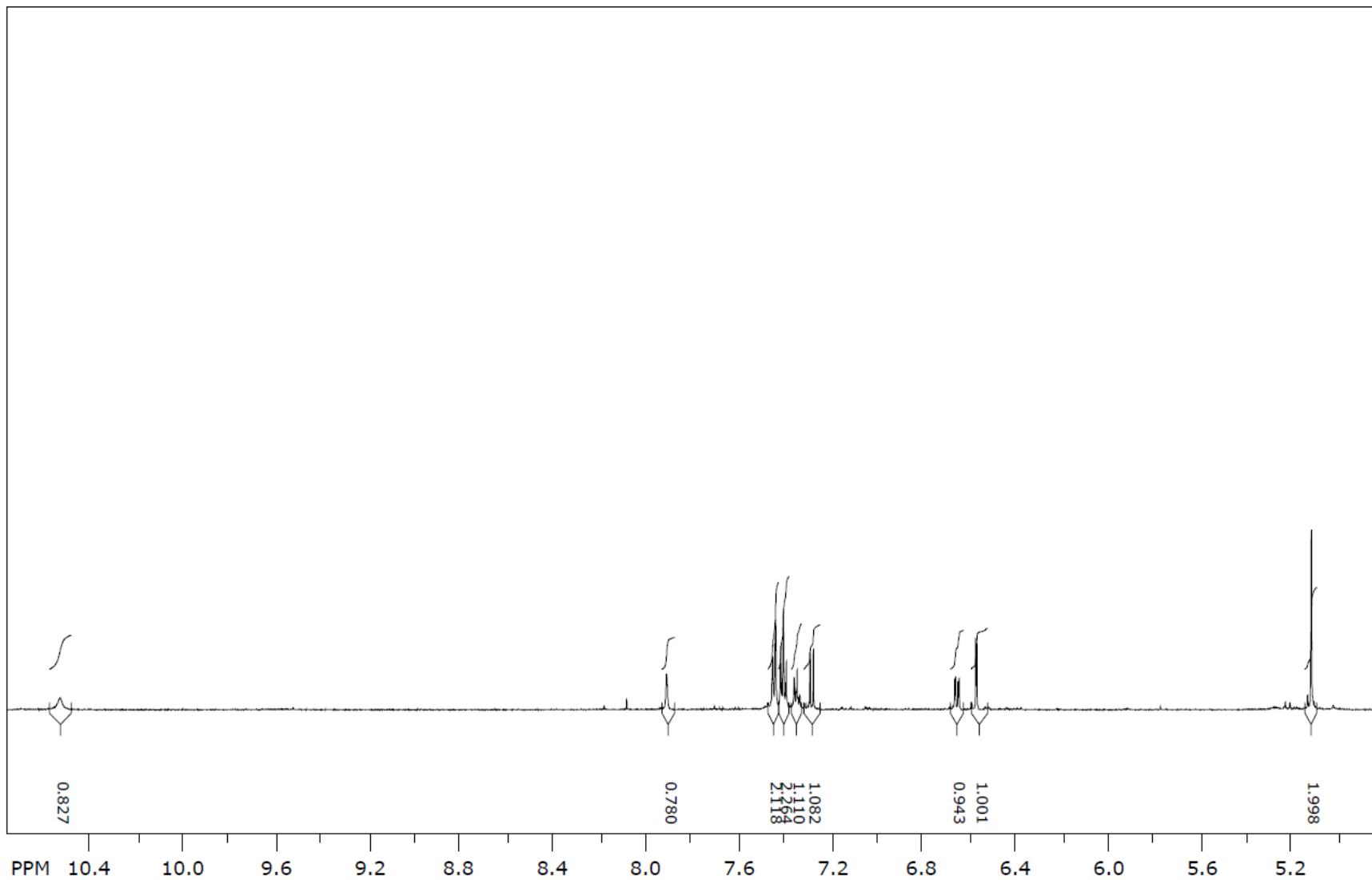


Reaktanti	4-(benziloksi) salicilaldehid (1 mmol) i tiazolidindion (1 mmol)
Metoda pročišćavanja	Ispran etanolom
Molekulska masa	327,35 g/mol
Molekulska formula	C ₁₇ H ₁₃ NO ₄ S
Temperatura tališta	184 – 188 °C
Boja kristala	Tamnožuta
R_f	0,63
LC/MS/MS <i>m/z</i> (M-)	326,20
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 12,39 (s, 1H, NH), 10,54 (s, 1H, OH), 7,91 (s, 1H, CH), 7,44 (d, <i>J</i> = 8,46 Hz, 2H, arom), 7,40 (t, <i>J</i> = 7,47 Hz, 2H, arom.), 7,33 – 7,36 (m, 1H, arom.), 7,28 (d, <i>J</i> = 8,76 Hz, 1H, arom.), 6,65 (dd, <i>J</i> = 8,76; 2,46 Hz, 1H, arom.), 6,57 (d, <i>J</i> = 2,52 Hz, 1H, arom.), 5,11 (s, 2H, CH ₂).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 161,08; 158,70; 136,57; 129,40; 128,44; 127,92; 127,69; 113,99; 106,85; 102,01; 69,28; 55,11; 53,13.

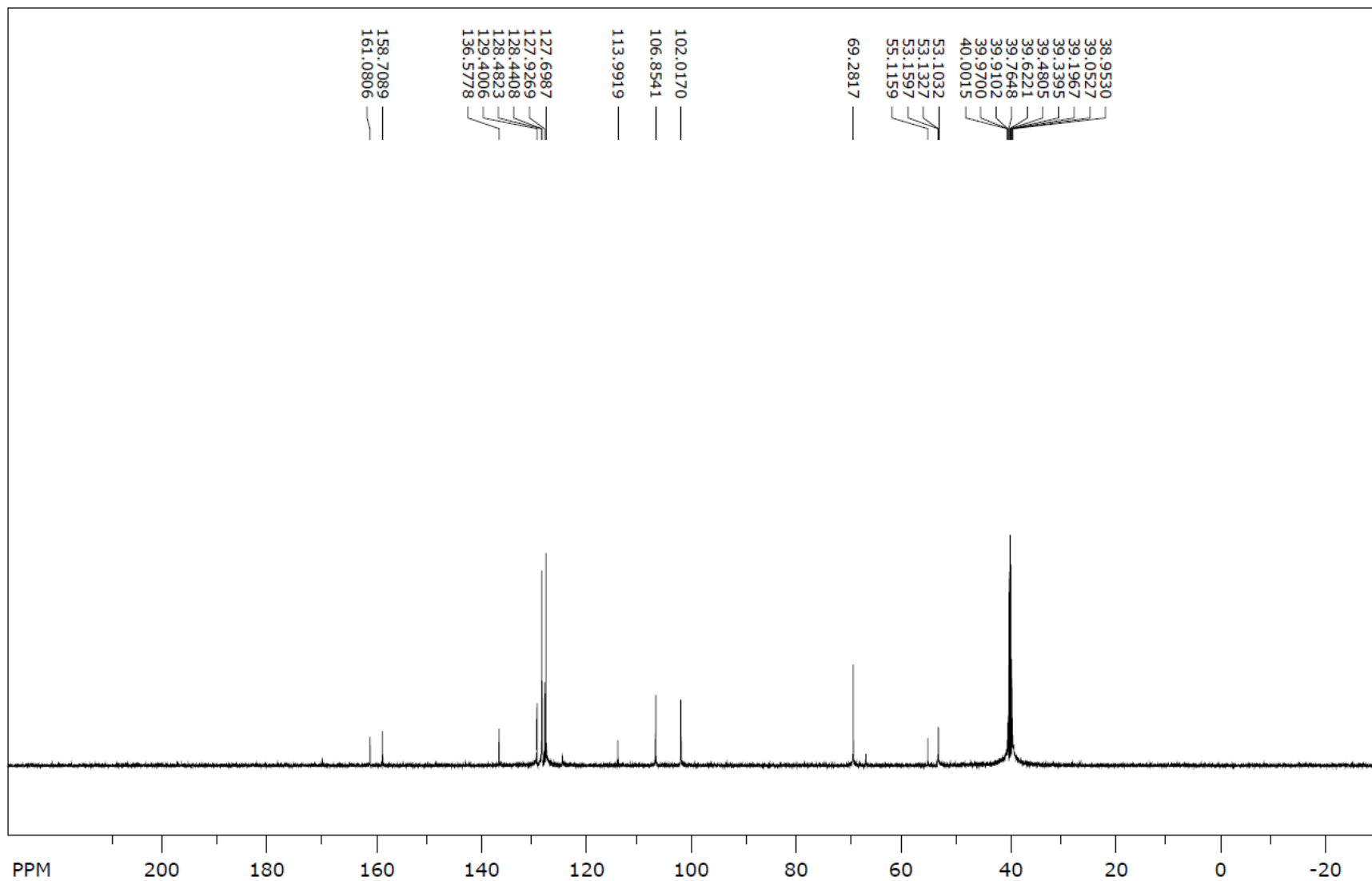
Maseni spektr (9o)



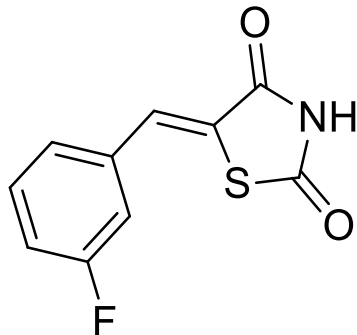
¹H NMR spektr (9o)



¹³C NMR spektr (9o)

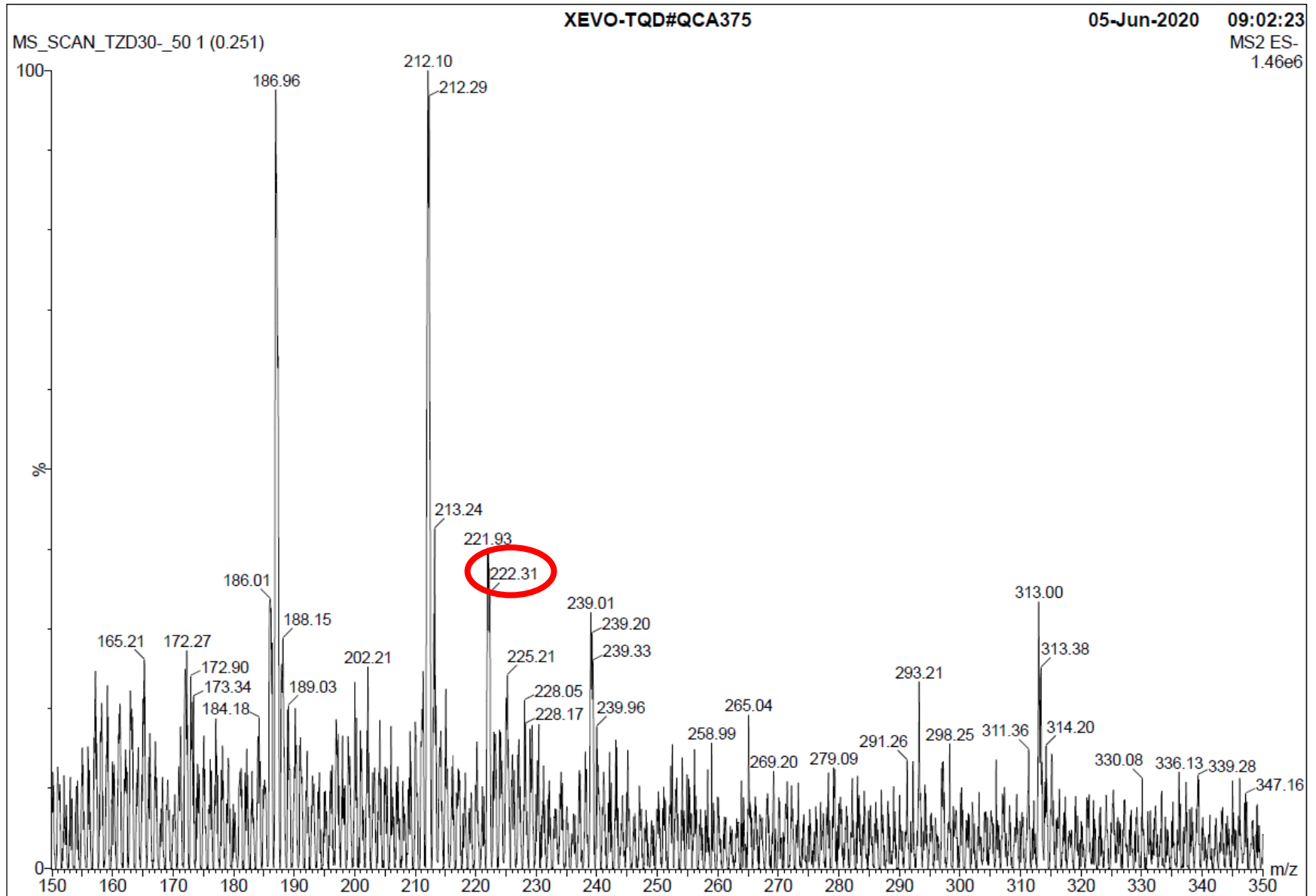


5-(3-fluorbenziliden) tiazolidin-2,4-dion (9p)

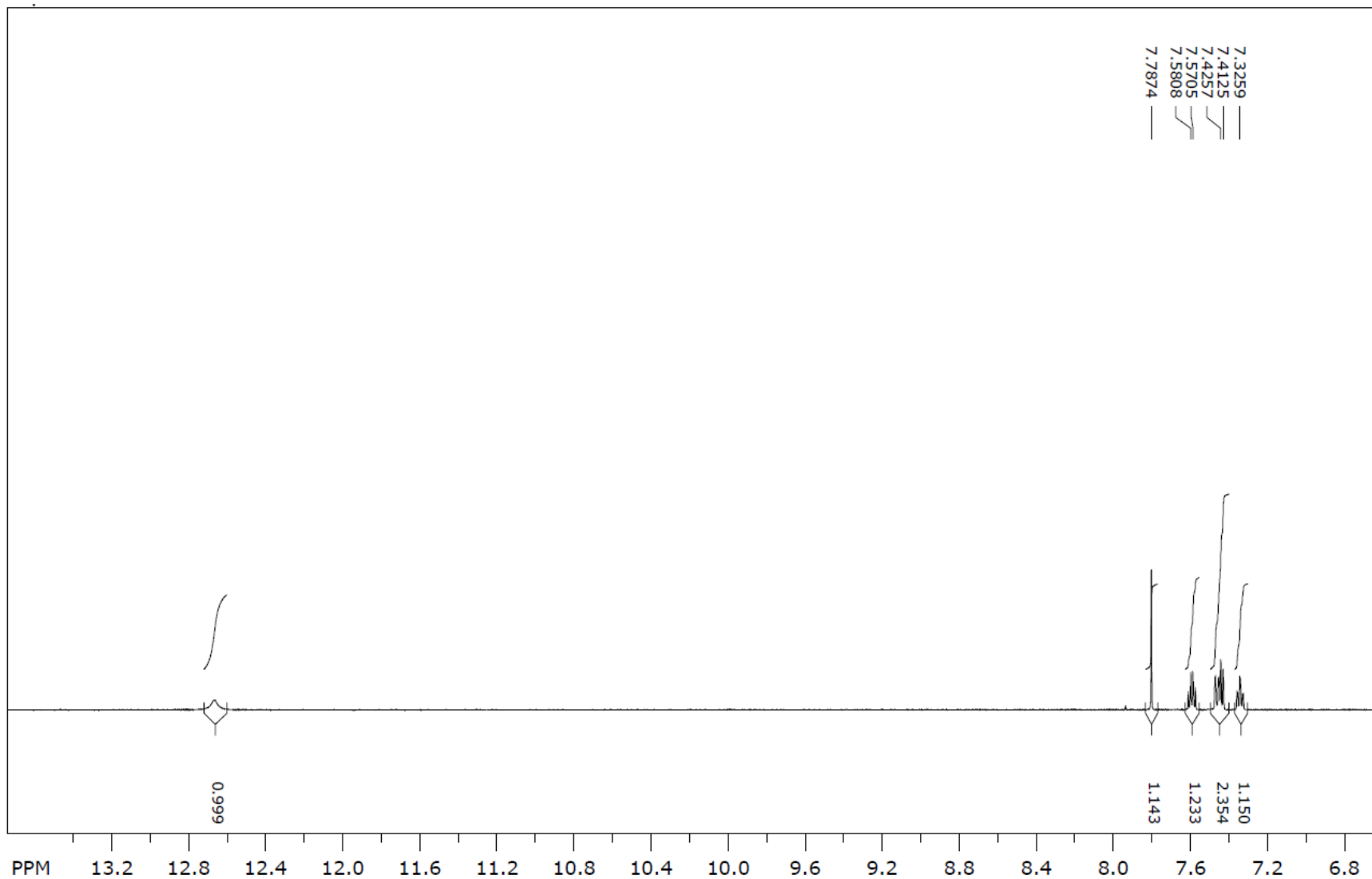


Reaktanti	3-fluorbenzalhid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	223,22 g/mol
Molekulska formula	C ₁₀ H ₆ FNO ₂ S
Temperatura tališta	169 – 171 °C (lit. 167 – 168 °C, Sun i sur., 2016)
Boja kristala	Bijela
R_f	0,78
LC/MS/MS <i>m/z</i> (M⁻)	222,31
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 12,67 (s, 1H, NH), 7,78 (s, 1H, CH), 7,58 (q, <i>J</i> = 7,98; 6,18 Hz, 1H, arom.), 7,44 (dd, <i>J</i> = 9,96; 1,98 Hz, 1H, arom.), 7,42 (d, <i>J</i> = 7,92 Hz, 1H, arom.), 7,32 (ddd, <i>J</i> = 2,16; 8,46; 8,70 Hz, 1H, arom.).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 167,54; 167,11; 163,03; 161,41; 135,35; 131,29; 130,31; 125,50; 119,97; 116,58.

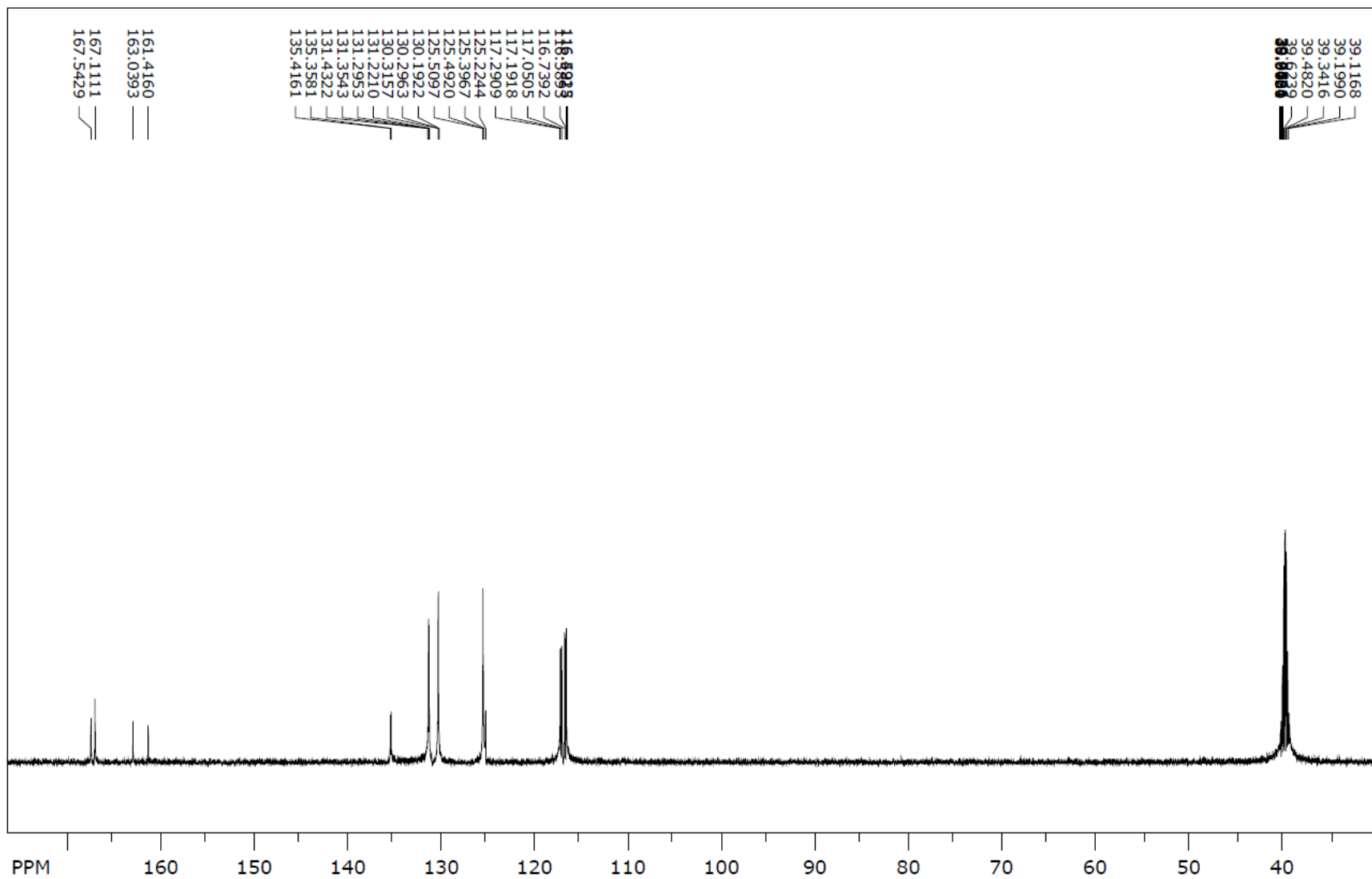
Maseni spektr (9p)



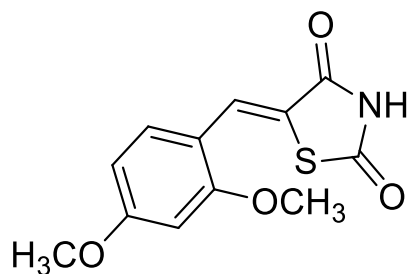
¹H NMR spektr (9p)



¹³C NMR spektar (9p)

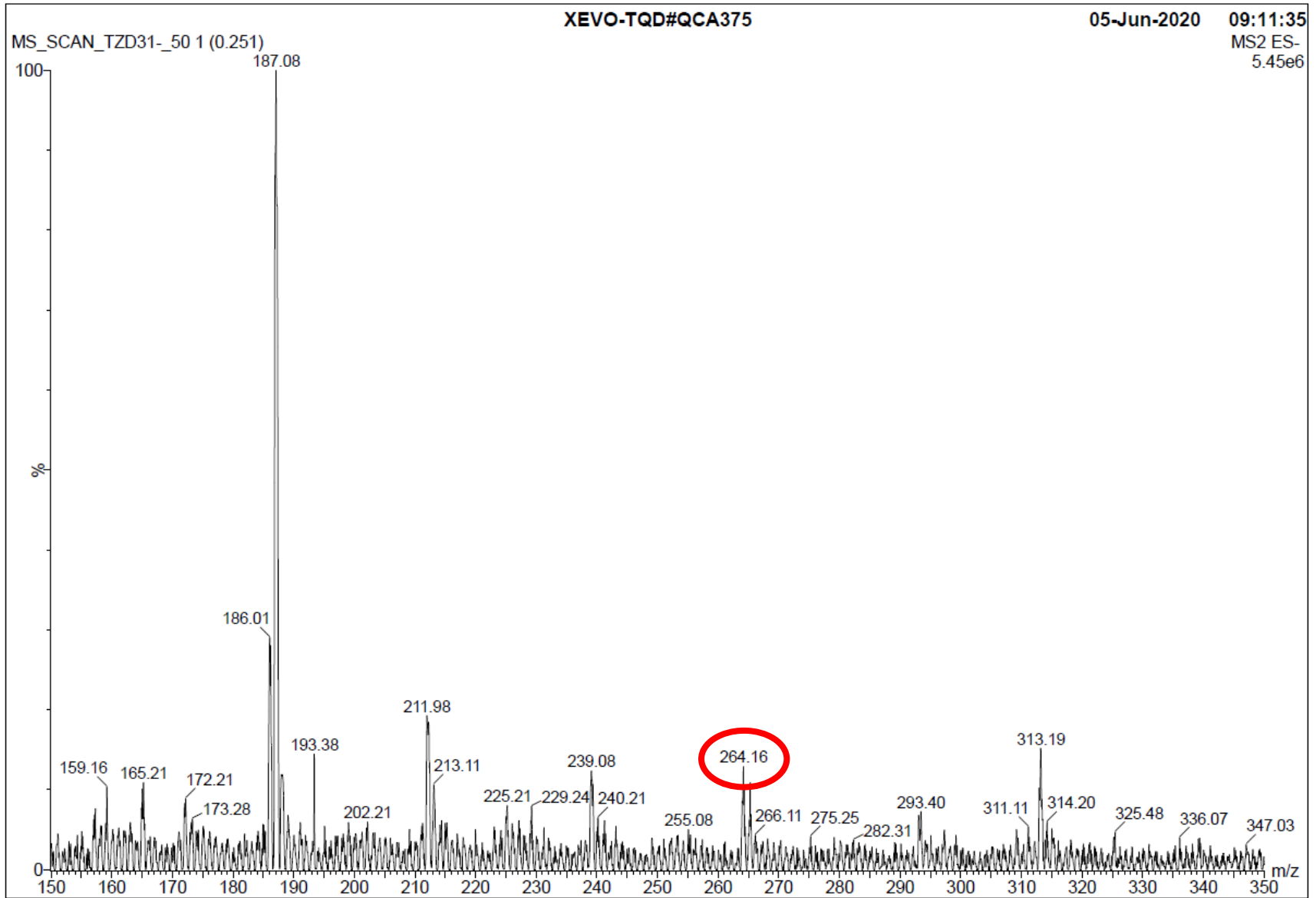


5-(2,4-dimetoksibenziliden) tiazolidin-2,4-dion (9q)

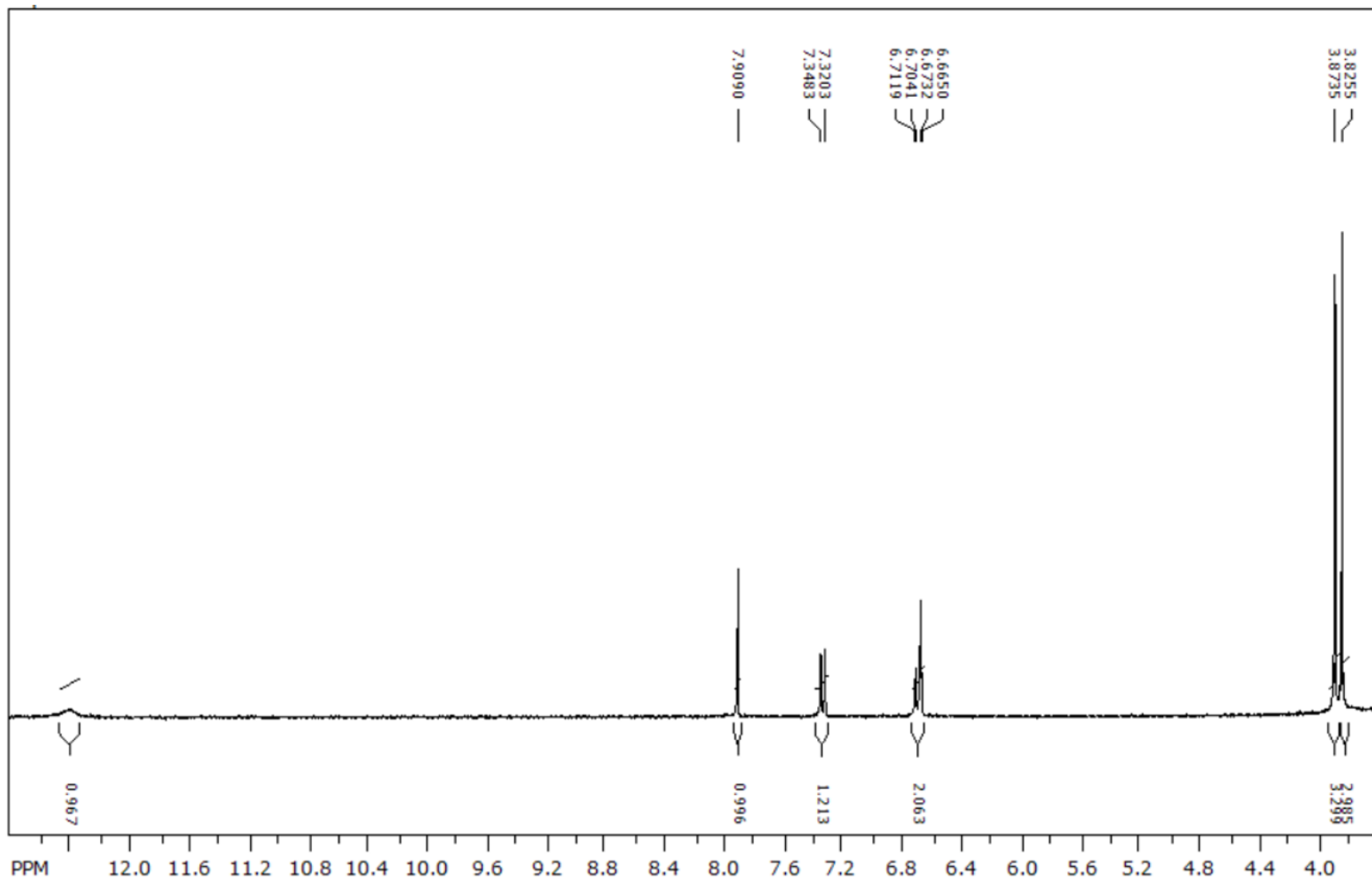


Reaktanti	2,4-dimetoksibenzaldehid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	265,29 g/mol
Molekulska formula	C ₁₂ H ₁₁ NO ₄ S
Temperatura tališta	251 – 253 °C (lit. 254 – 255 °C, Ha i sur., 2012)
Boja kristala	Žuta
R_f	0,77
LC/MS/MS m/z (M⁻)	264,16
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 12,42 (s, 1H, NH), 7,90 (s, 1H, CH), 7,33 (d, <i>J</i> = 8,40 Hz, 1H, arom.), 6,69 (dd, <i>J</i> = 11,61; 2,40 Hz, 2H, arom.), 3,87 (s, 3H, OCH ₃), 3,82 (s, 3H, OCH ₃).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 168,04; 163,52; 160,28; 130,52; 126,92; 120,34; 114,73; 106,74; 99,09; 56,38; 56,09.

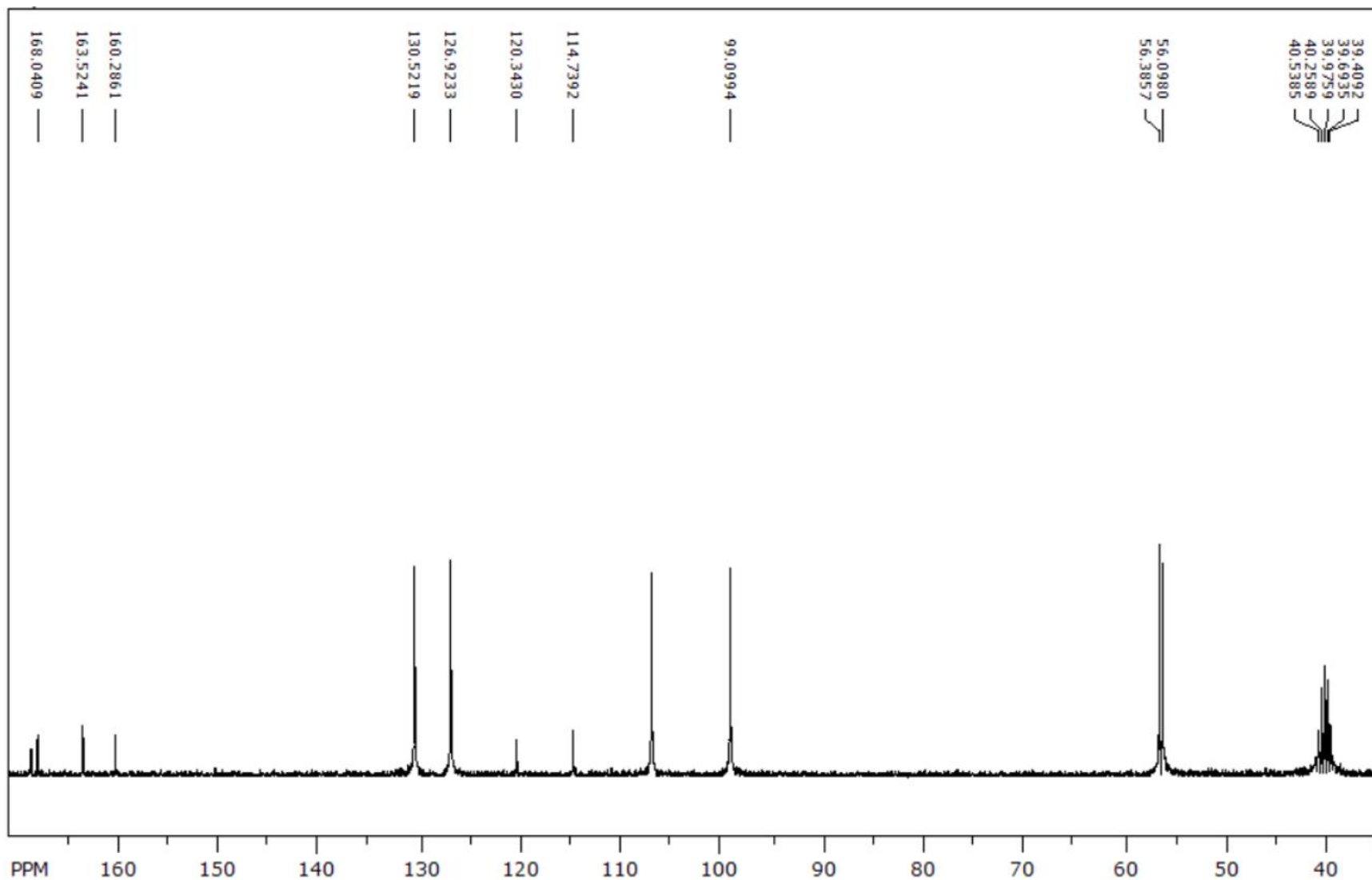
Maseni spektr (9q)



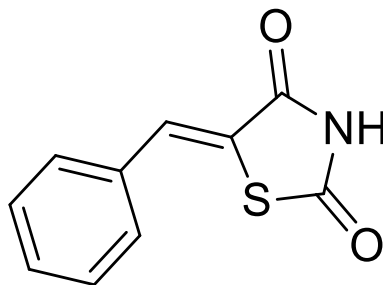
¹H NMR spektr (9q)



¹³C NMR spektr (9q)

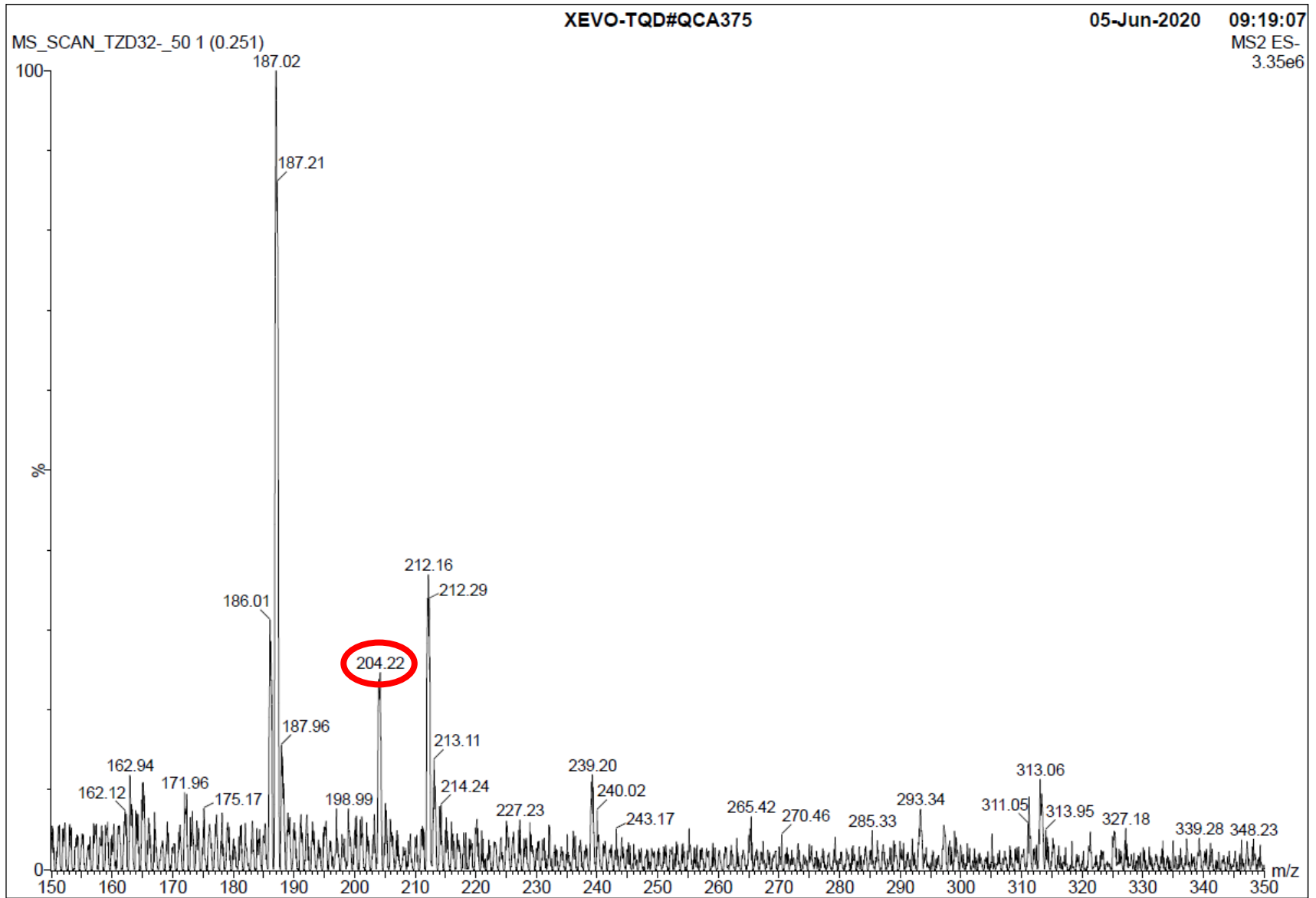


5-benziliden tiazolidin-2,4-dion (9r)

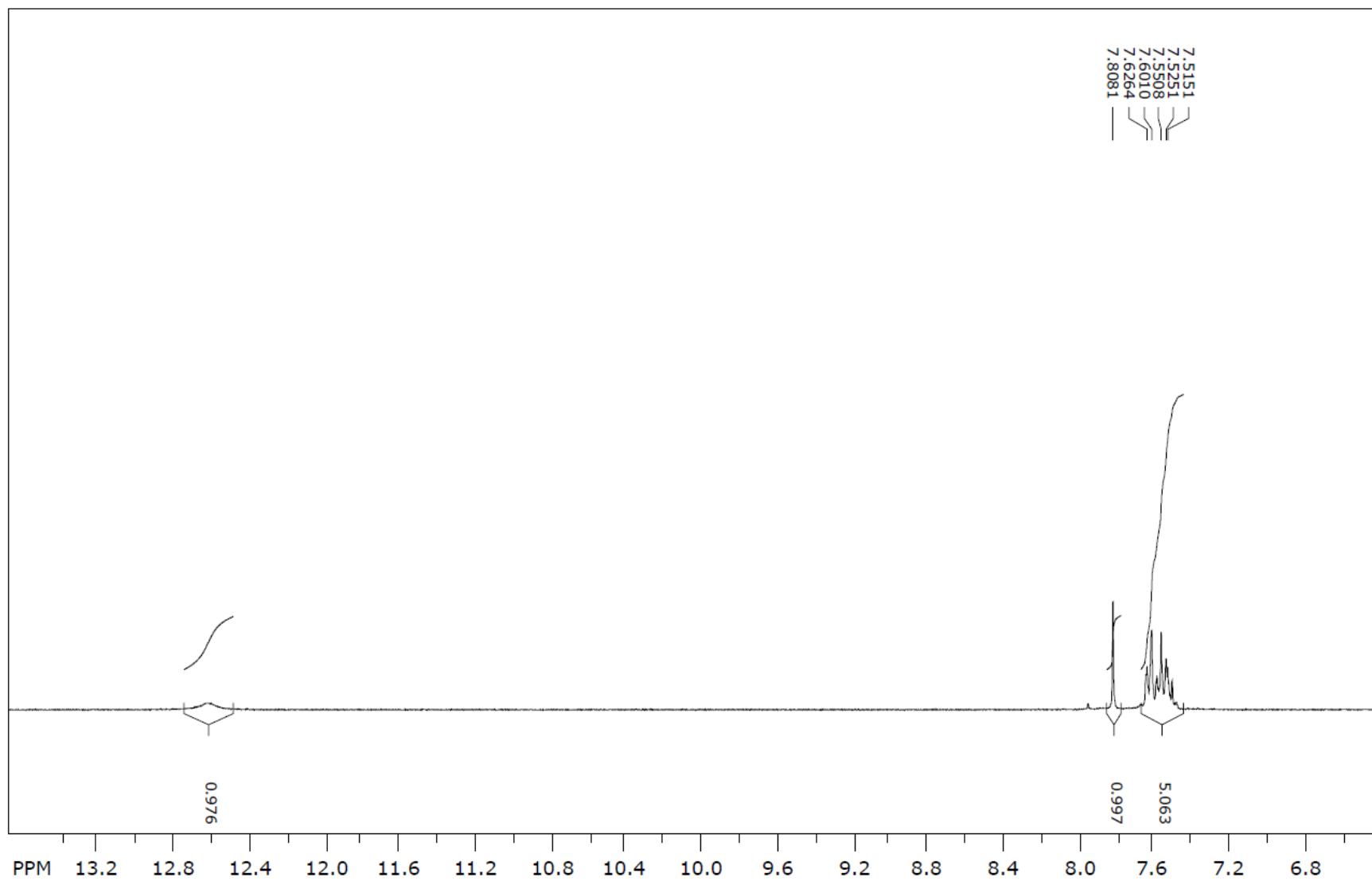


Reaktanti	Benzaldehid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročišćavanja	Nije pročišćavan
Molekulska masa	205,23 g/mol
Molekulska formula	C ₁₀ H ₇ NO ₂ S
Temperatura tališta	251 – 254 °C (lit. 240 °C, Metwally i sur., 2011; 245 – 247 °C. Ynag i Yang, 2011)
Boja kristala	Bijela
R_f	0,79
LC/MS/MS m/z (M-)	204,22
¹H NMR	(300 MHz, DMSO- <i>d</i> ₆) δ 12,62 (s, 1H, NH), 7,80 (s, 1H, CH), 7,46 – 7,65 (m, 6H, arom.).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 168,33; 167,77; 133,49; 132,24; 130,87; 130,46; 129,77; 124,01.

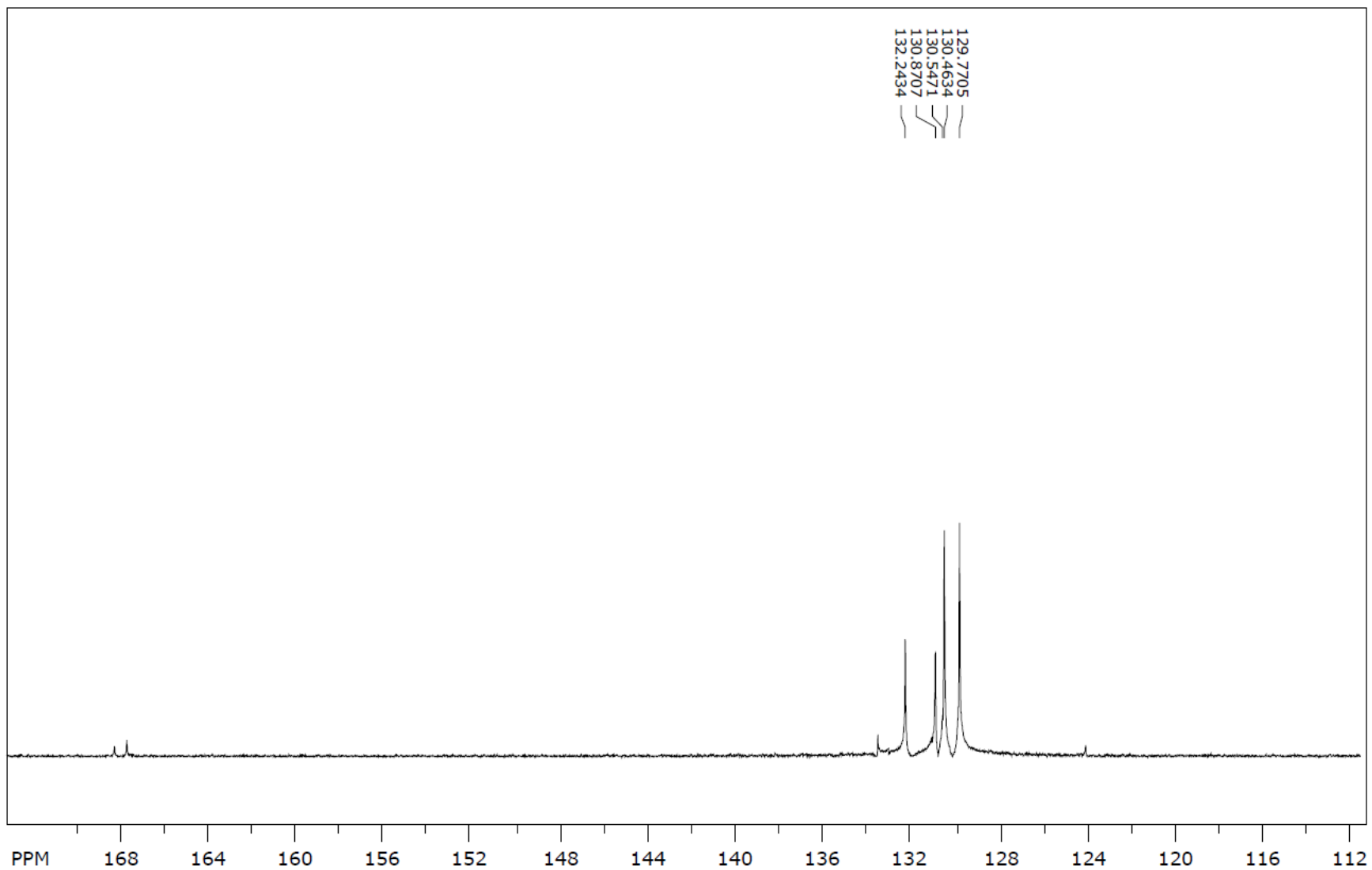
Maseni spektar (9r)



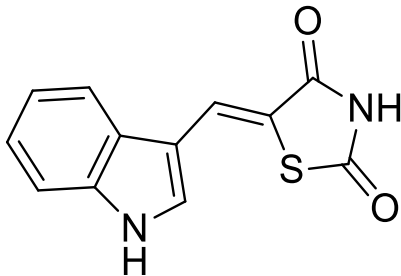
¹H NMR spektr (9r)



¹³C NMR spektr (9r)

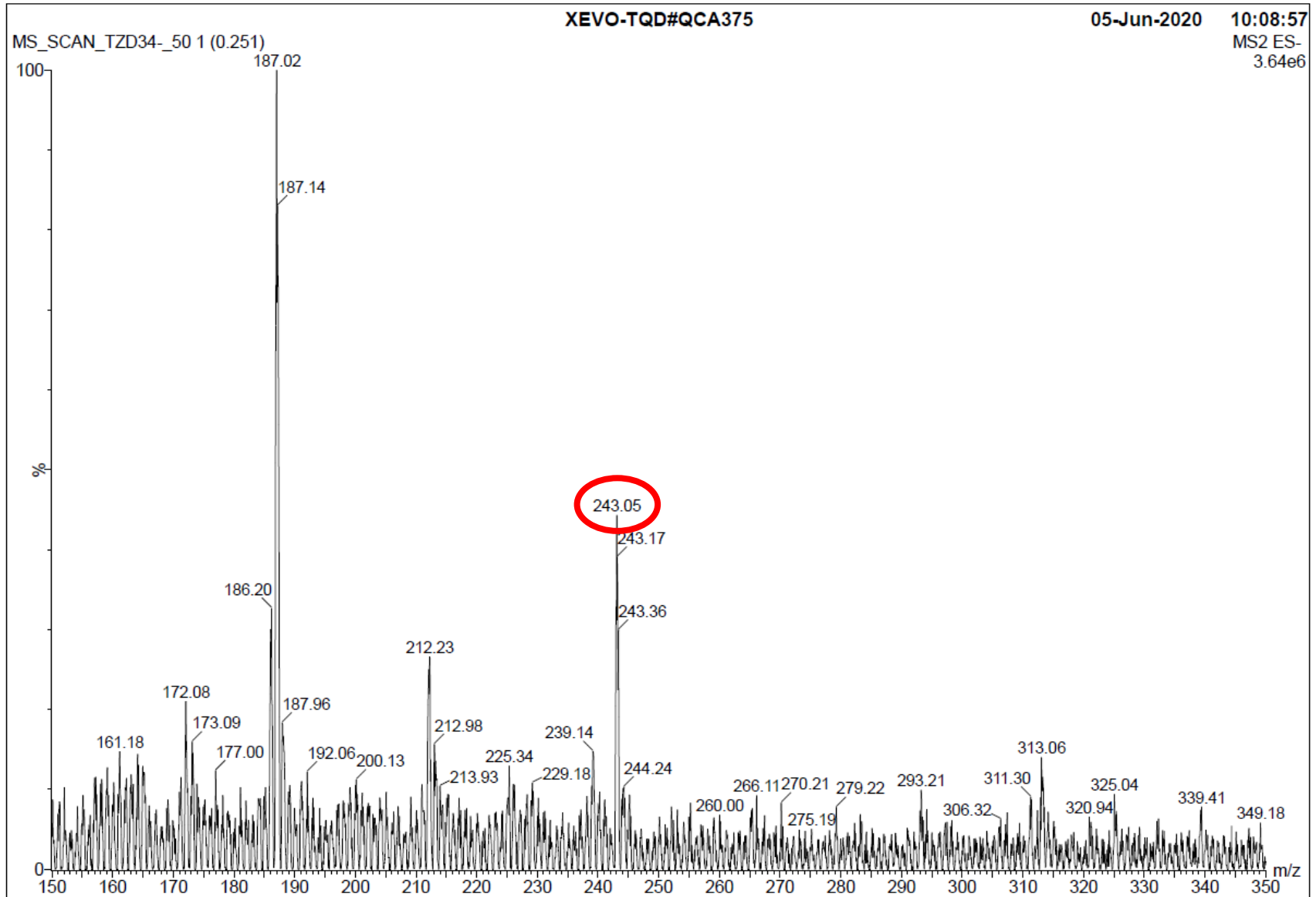


5-((1H-indol-3-il)metilen) tiazolidin-2,4-dion (9s)

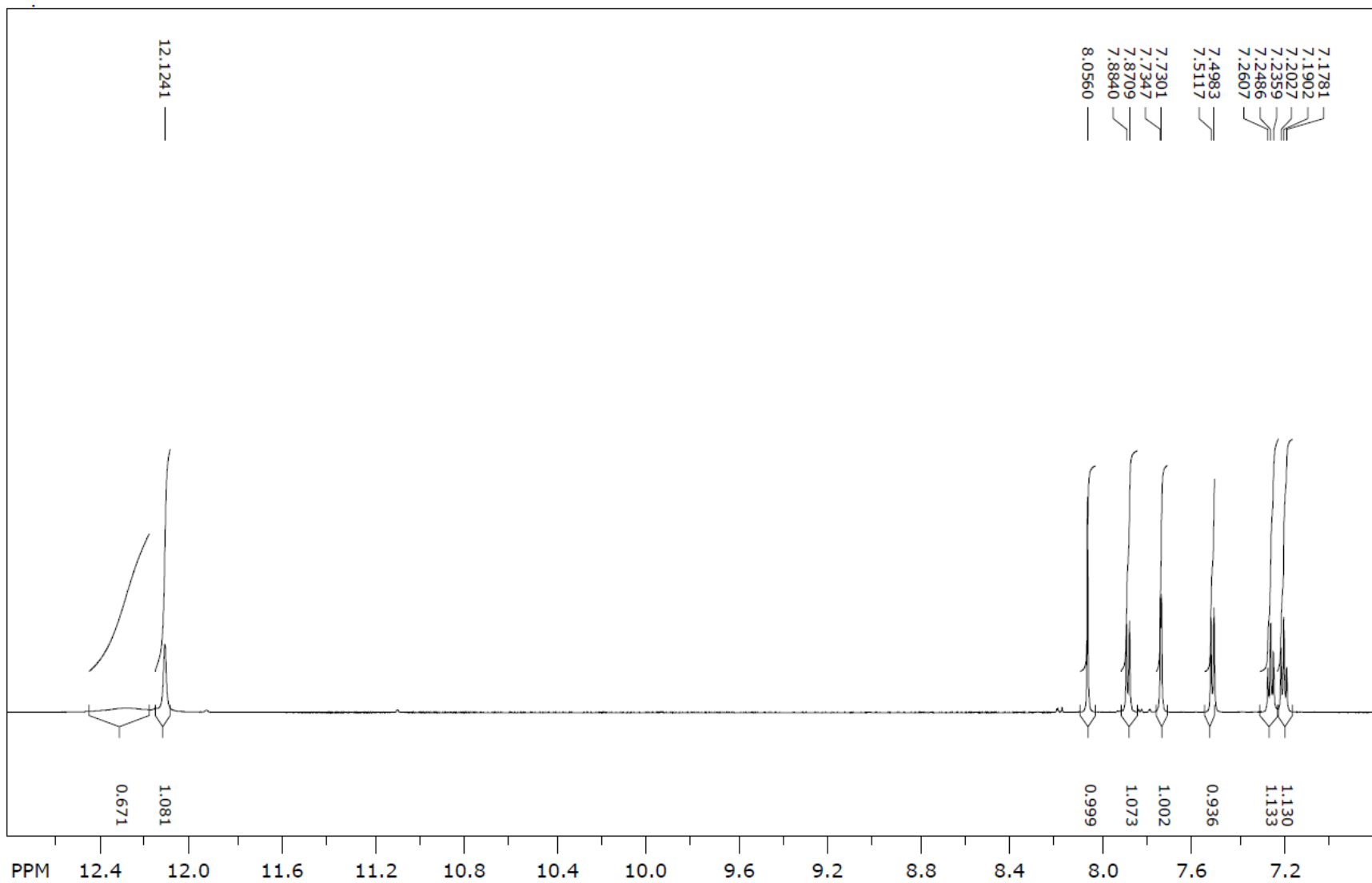


Reaktanti	Indol-3-karboksialdehid (2 mmol) i tiazolidindion (2 mmol)
Metoda pročiščavanja	Nije pročiščavan
Molekulska masa	244,27 g/mol
Molekulska formula	C ₁₂ H ₈ N ₂ O ₂ S
Temperatura tališta	> 300 °C
Boja kristala	Žuta
R_f	0,66
LC/MS/MS <i>m/z</i> (M-)	243,05
¹H NMR	(600 MHz, DMSO- <i>d</i> ₆) δ 12,31 (s, 1H, NH), 12,12 (s, 1H, NH), 7,88 (d, <i>J</i> = 7,86 Hz, 1H, arom.), 7,73 (d, <i>J</i> = 2,76 Hz, 1H, arom.), 7,51 (d, <i>J</i> = 8,04 Hz, 1H, arom.), 7,25 (t, <i>J</i> = 7,44 Hz, 1H, arom.), 7,19 (t, <i>J</i> = 7,38 Hz, 1H, arom.).
¹³C NMR	(150 MHz, DMSO- <i>d</i> ₆) δ 167,23; 136,16; 128,58; 126,75; 124,41; 123,02; 121,00; 118,29; 116,20; 112,36; 110,39.

Maseni spektr (9s)



¹H NMR spektr (9s)



¹³C NMR spektr (9s)

