Organometallic-erlotinib conjugates active against lung cancer cells and as emerging viruses entry inhibitors

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Authors of presented dataset: Przemysław Biegański[a] and Konrad Kowalski[a]

Dataset to Project NCN PRELUDIUM 20
UMO-2021/41/N/ST4/00059

Contents

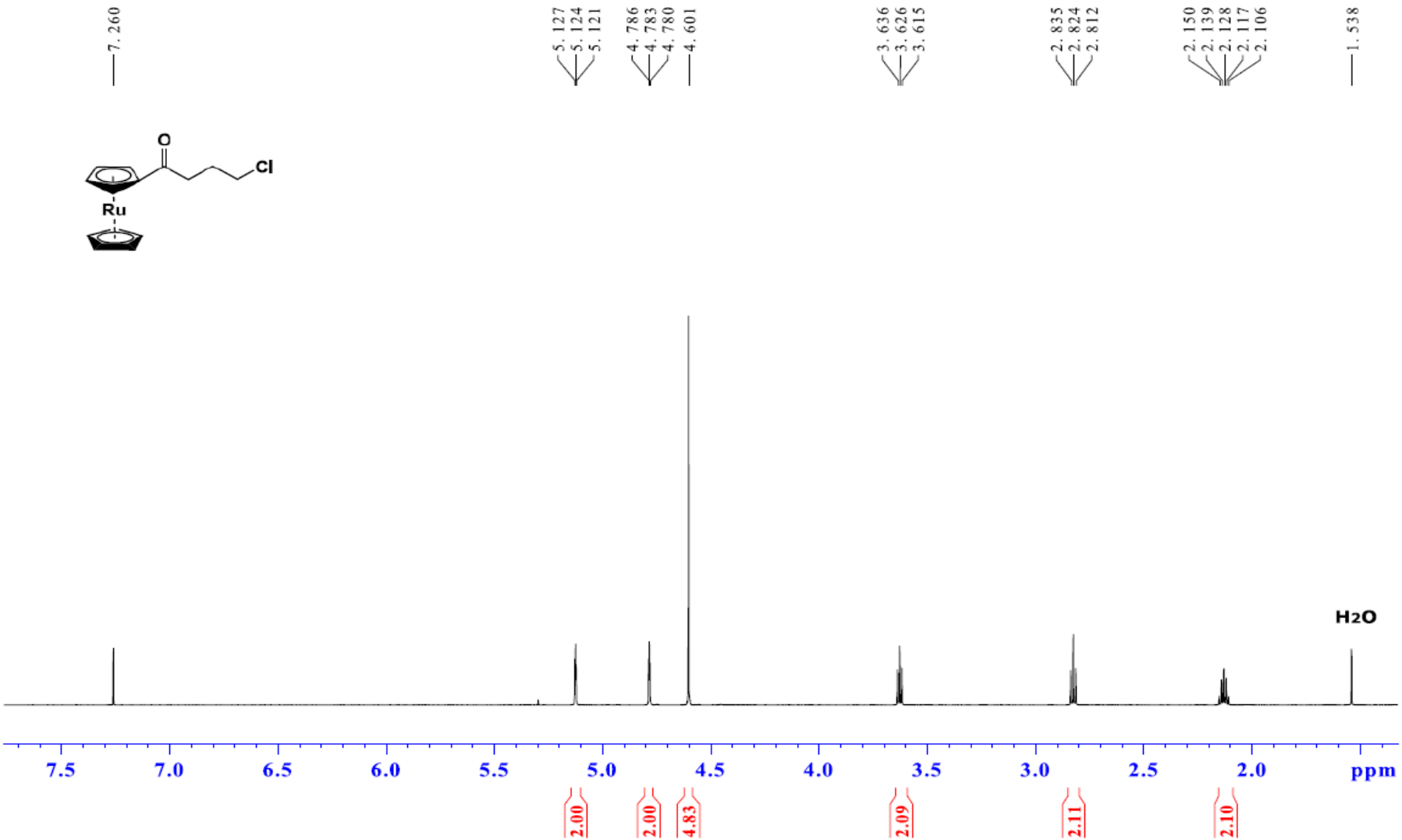


Fig S1 ^{1}H-NMR spectrum of **1** in $CDCl_3$ (600 MHz)

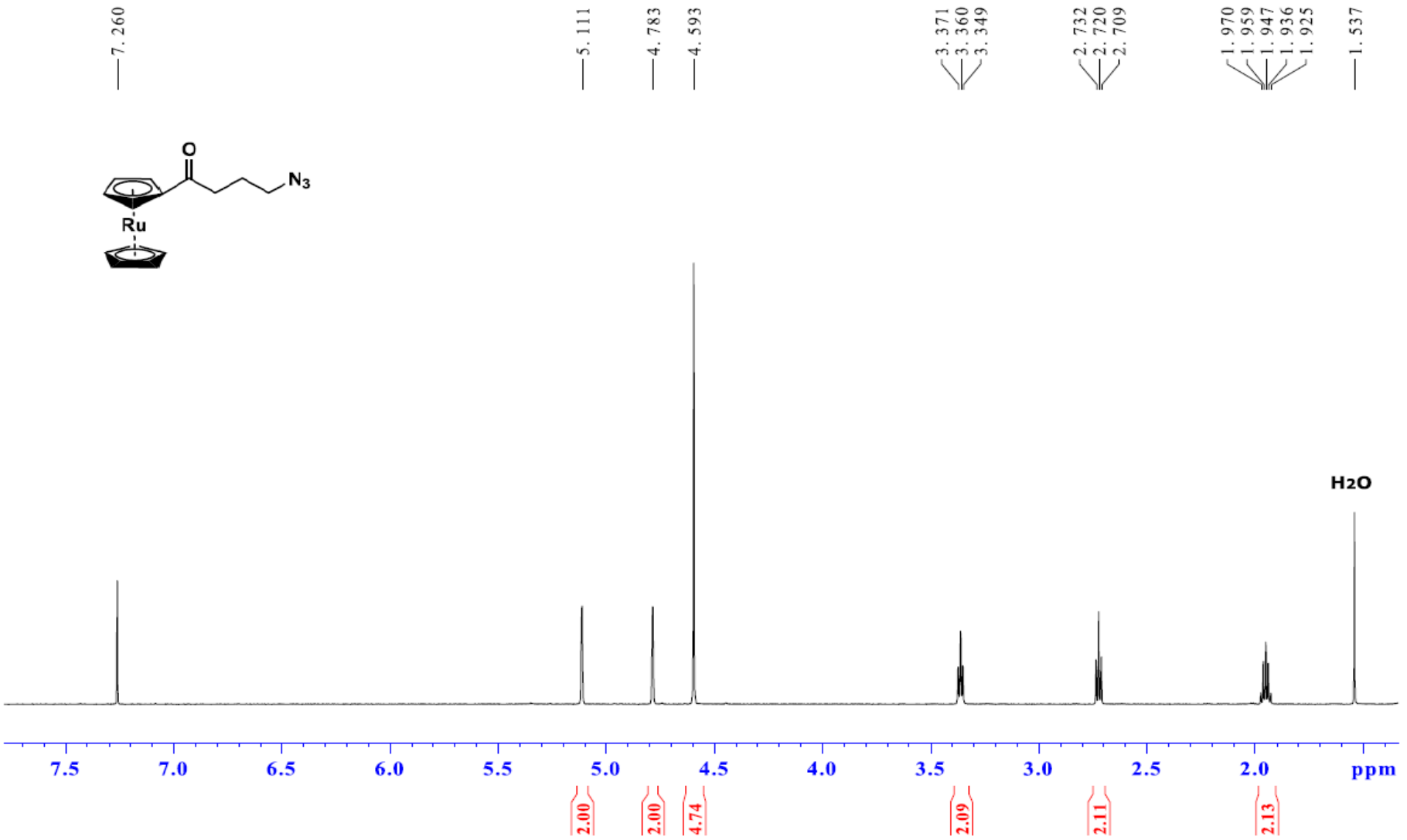


Fig S2 ^{1}H-NMR spectrum of **2** in $CDCl_3$ (600 MHz)

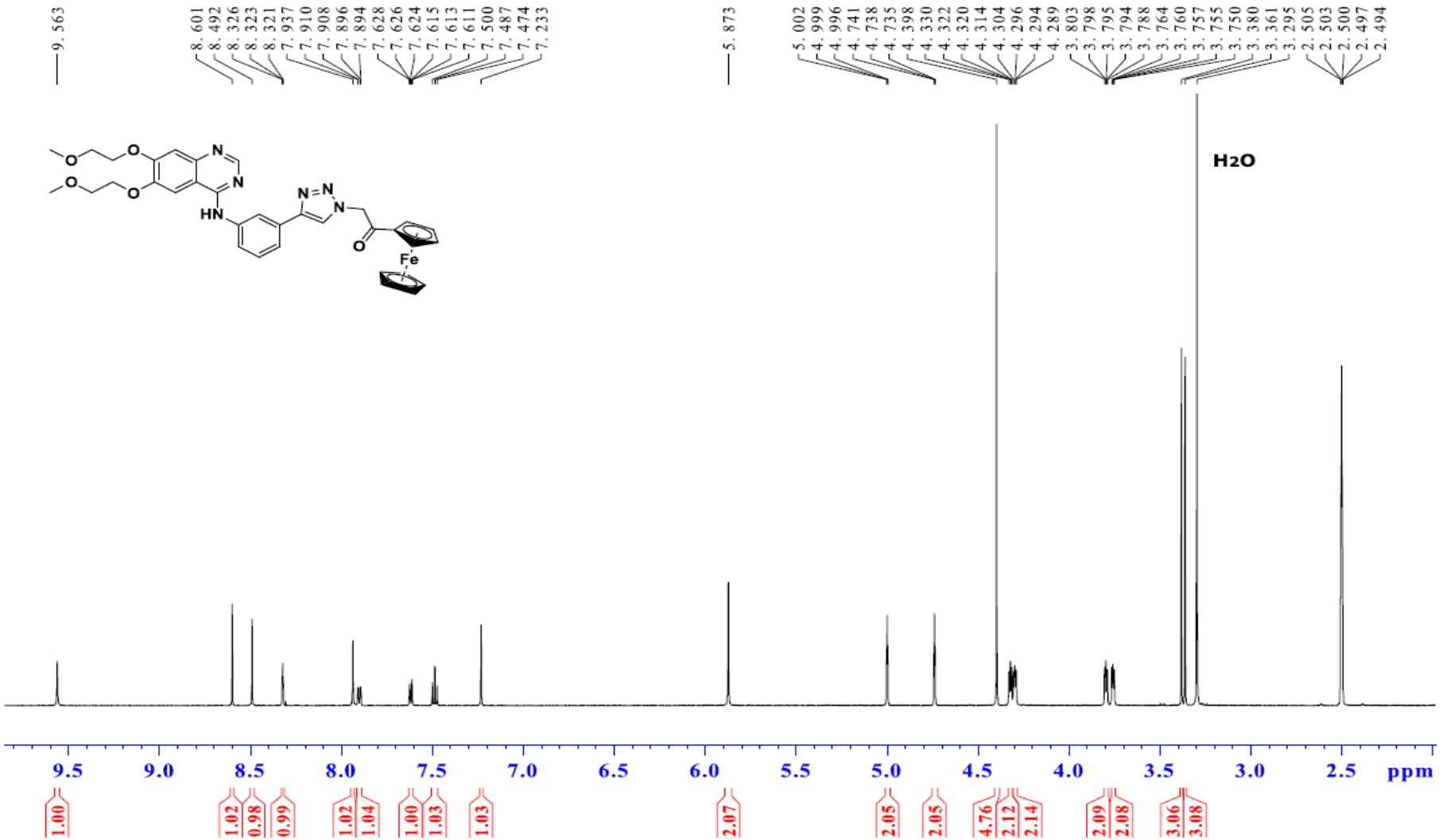


Fig S3 ^{1}H-NMR spectrum of **3** in DMSO-d_6 (600 MHz)

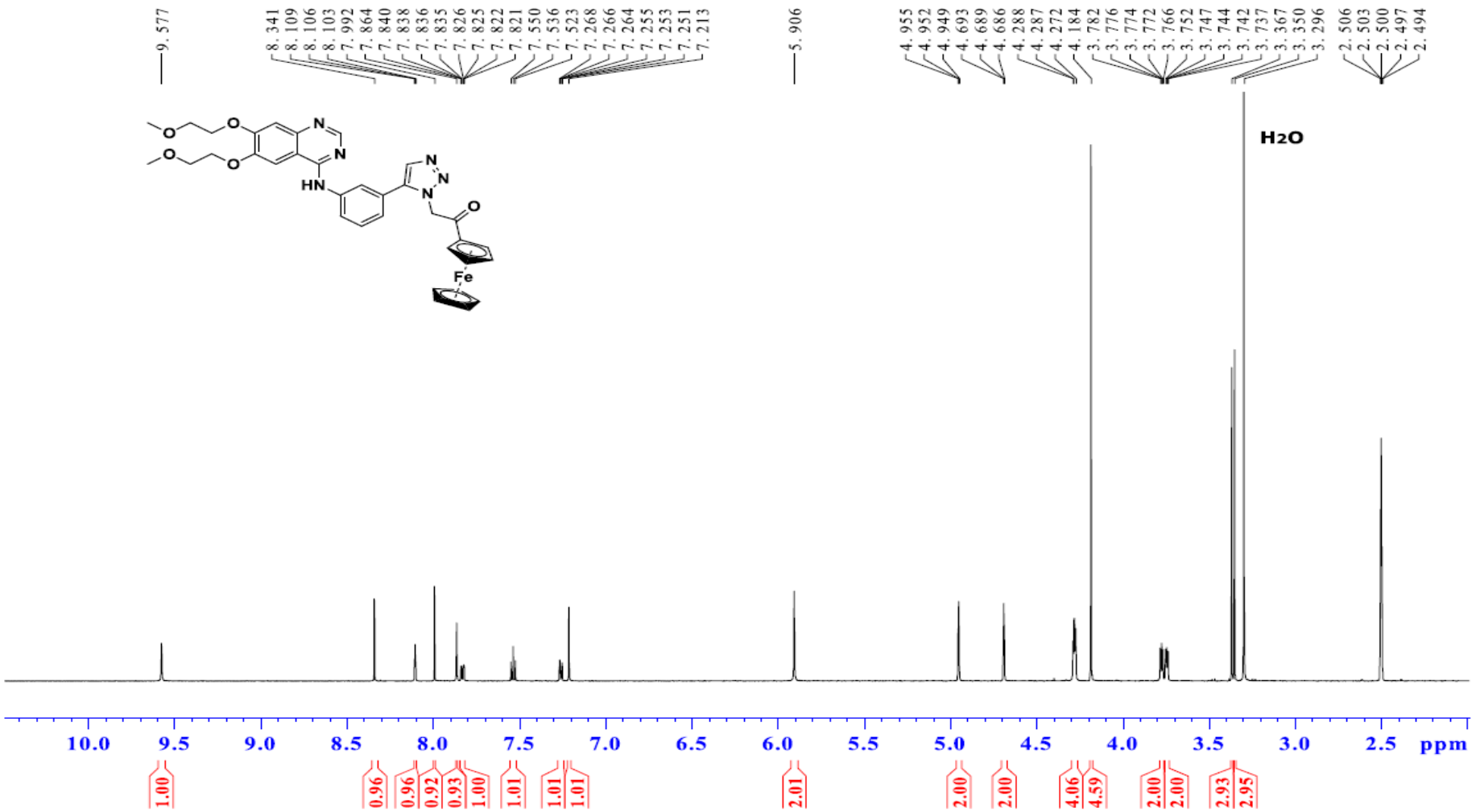


Fig S4 ^{1}H-NMR spectrum of **4** in DMSO-d_6 (600 MHz)

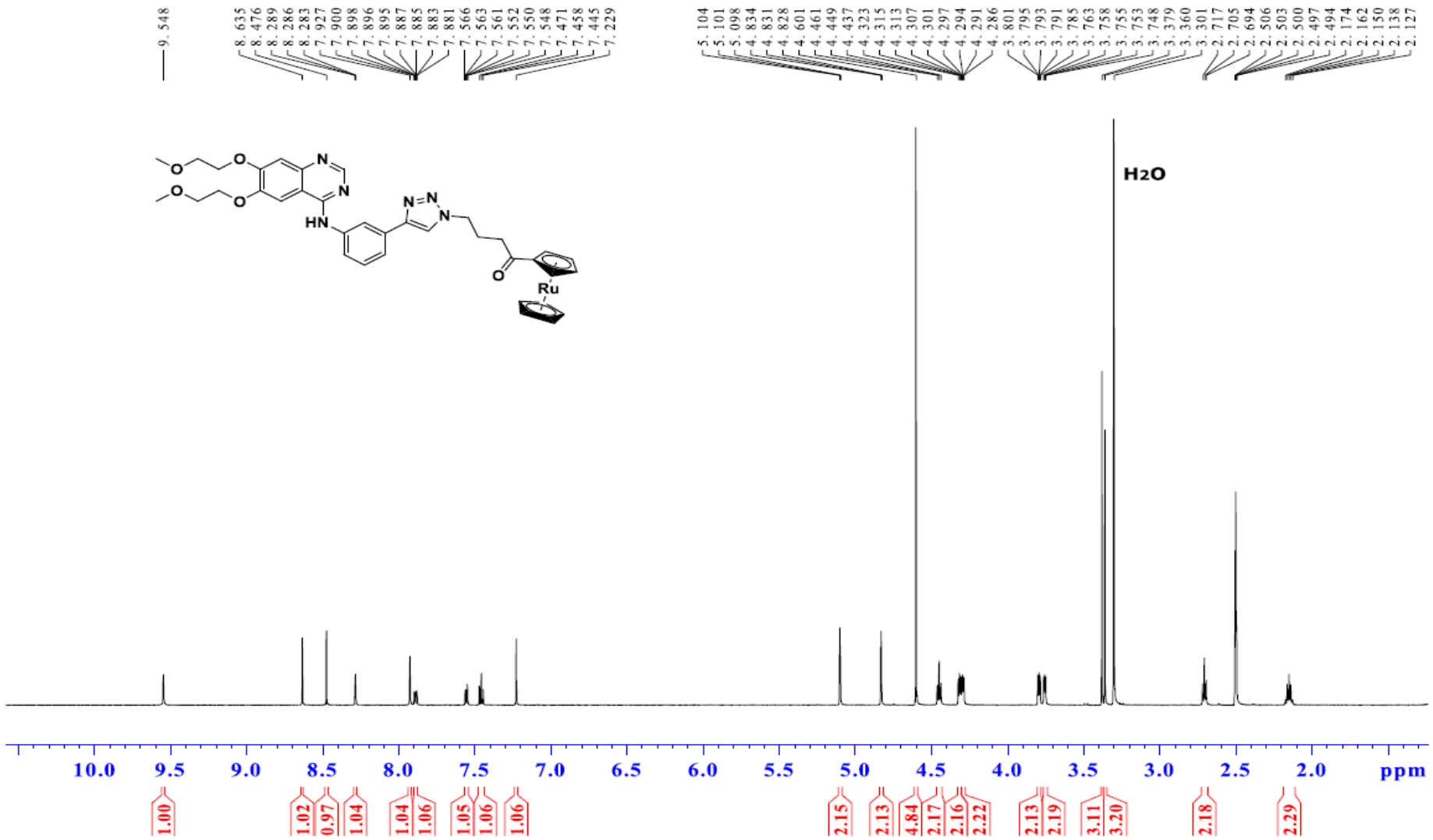


Fig S5 ^{1}H-NMR spectrum of **5** in DMSO-d_6 (600 MHz)

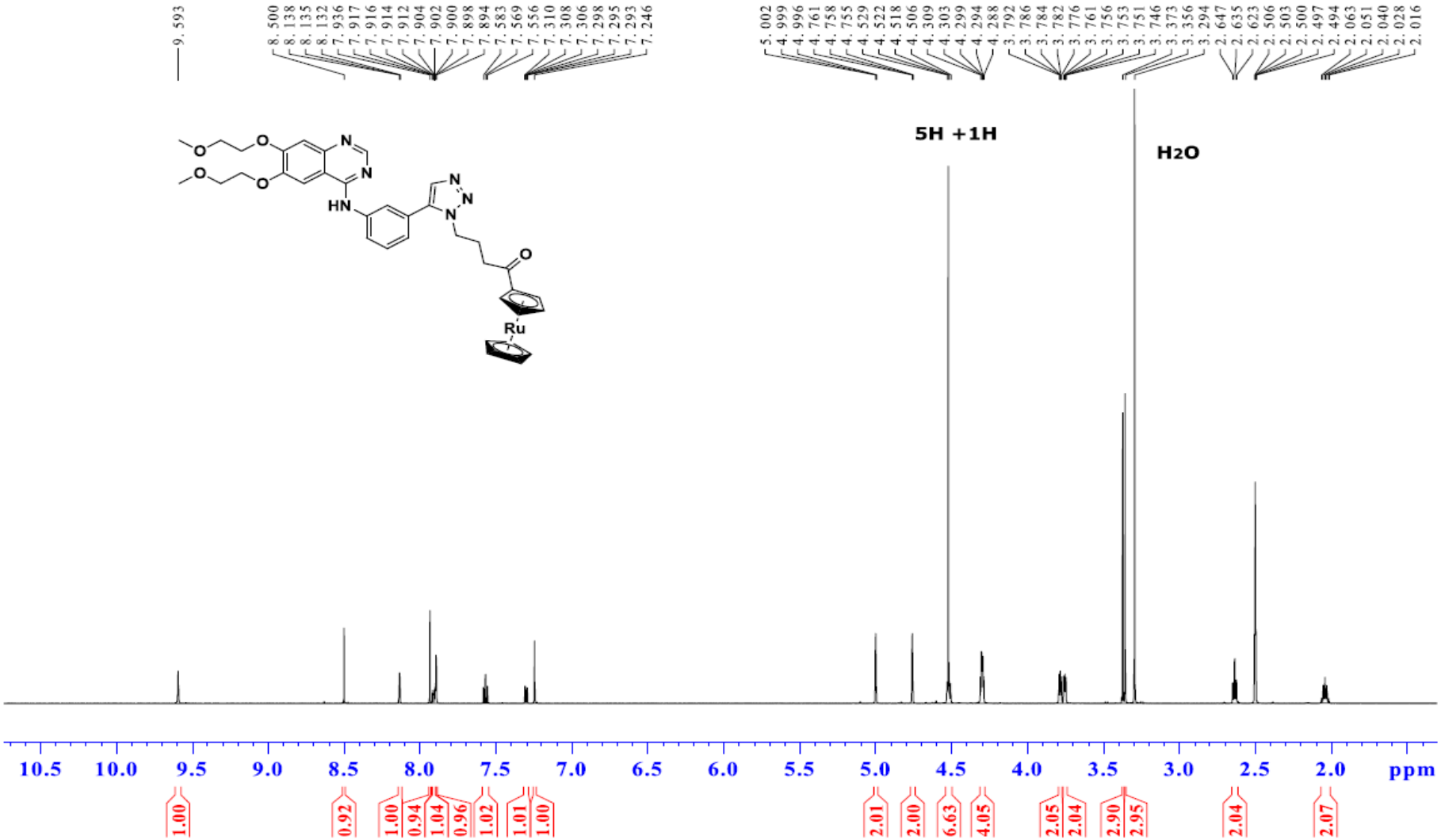


Fig S6 ^{1}H-NMR spectrum of **6** in DMSO-d_6 (600 MHz)

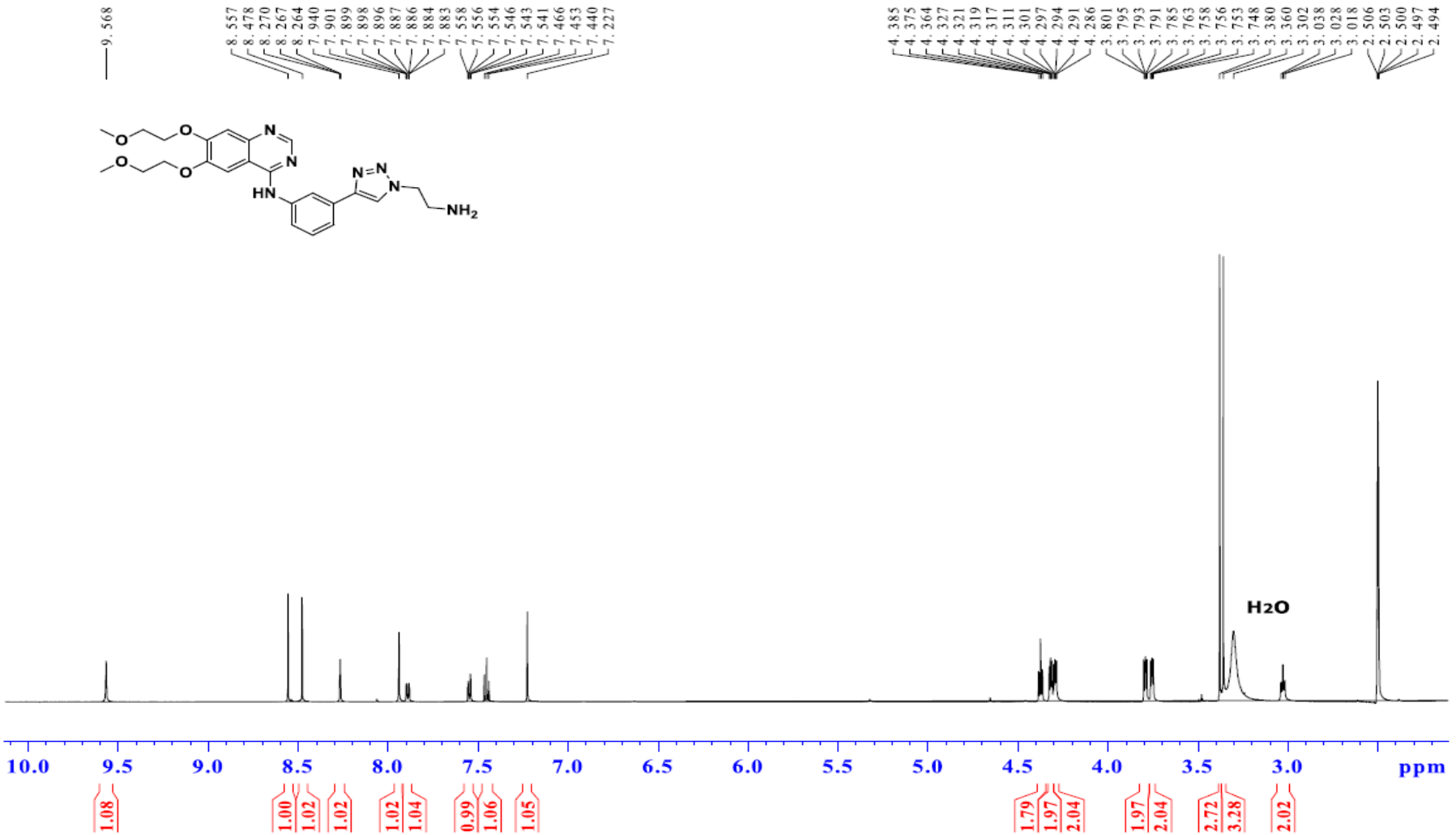


Fig S7 ^{1}H-NMR spectrum of **7** in DMSO-d_6 (600 MHz)

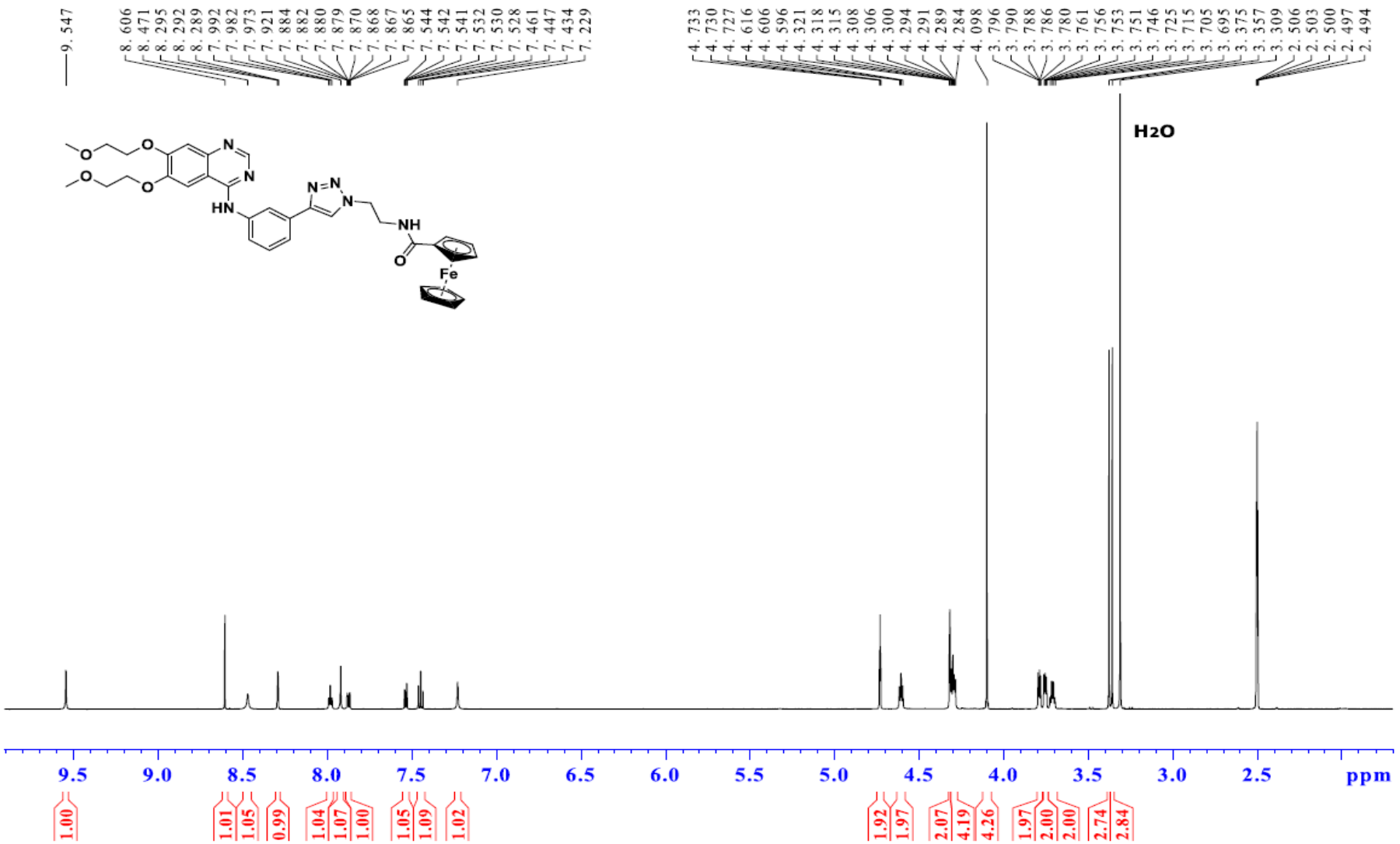


Fig S8 ^{1}H-NMR spectrum of **8** in DMSO-d_6 (600 MHz)

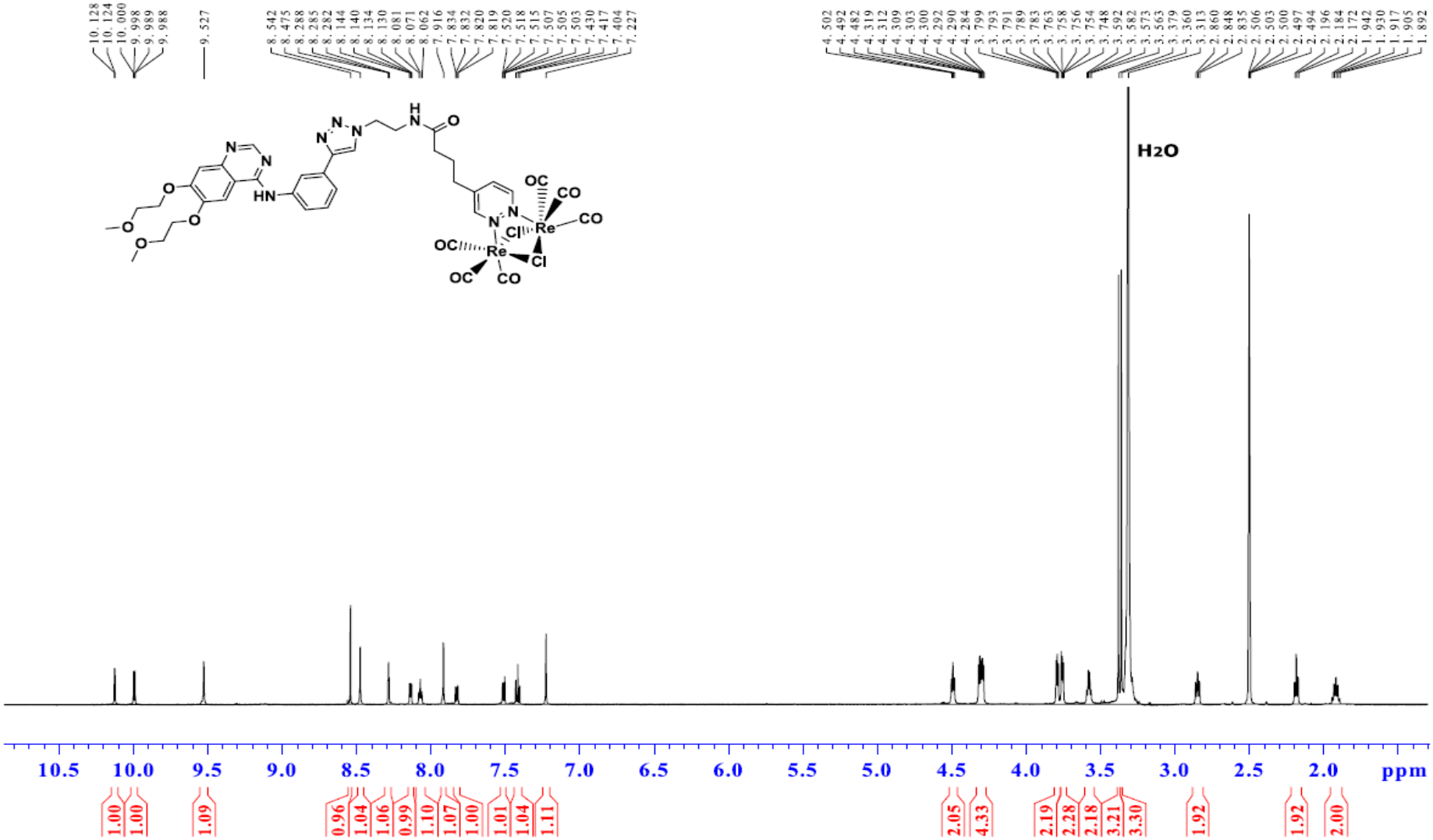


Fig S9 ^{1}H-NMR spectrum of **9** in DMSO-d_6 (600 MHz)

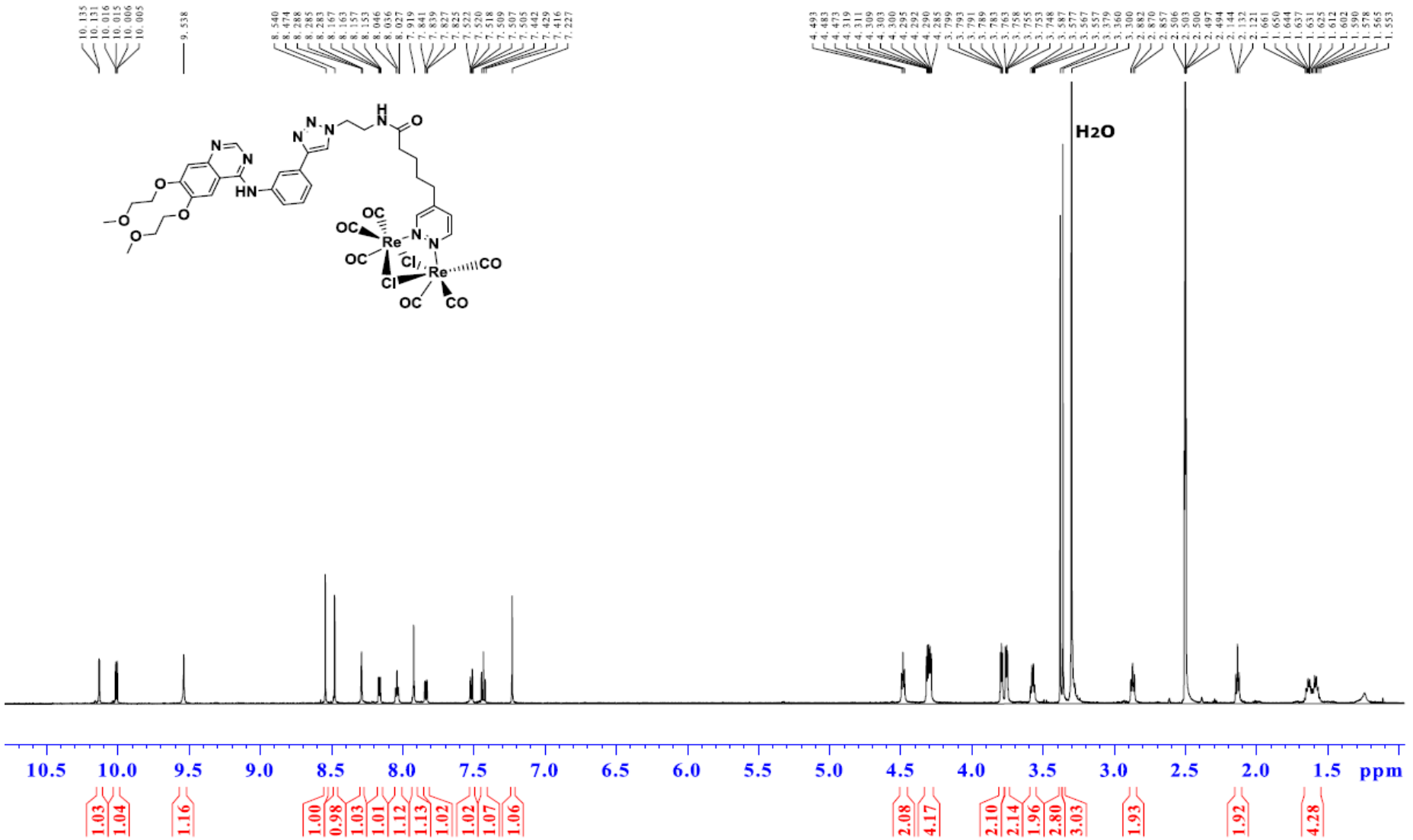


Fig S10 ^{1}H-NMR spectrum of **10** in DMSO-d_6 (600 MHz)

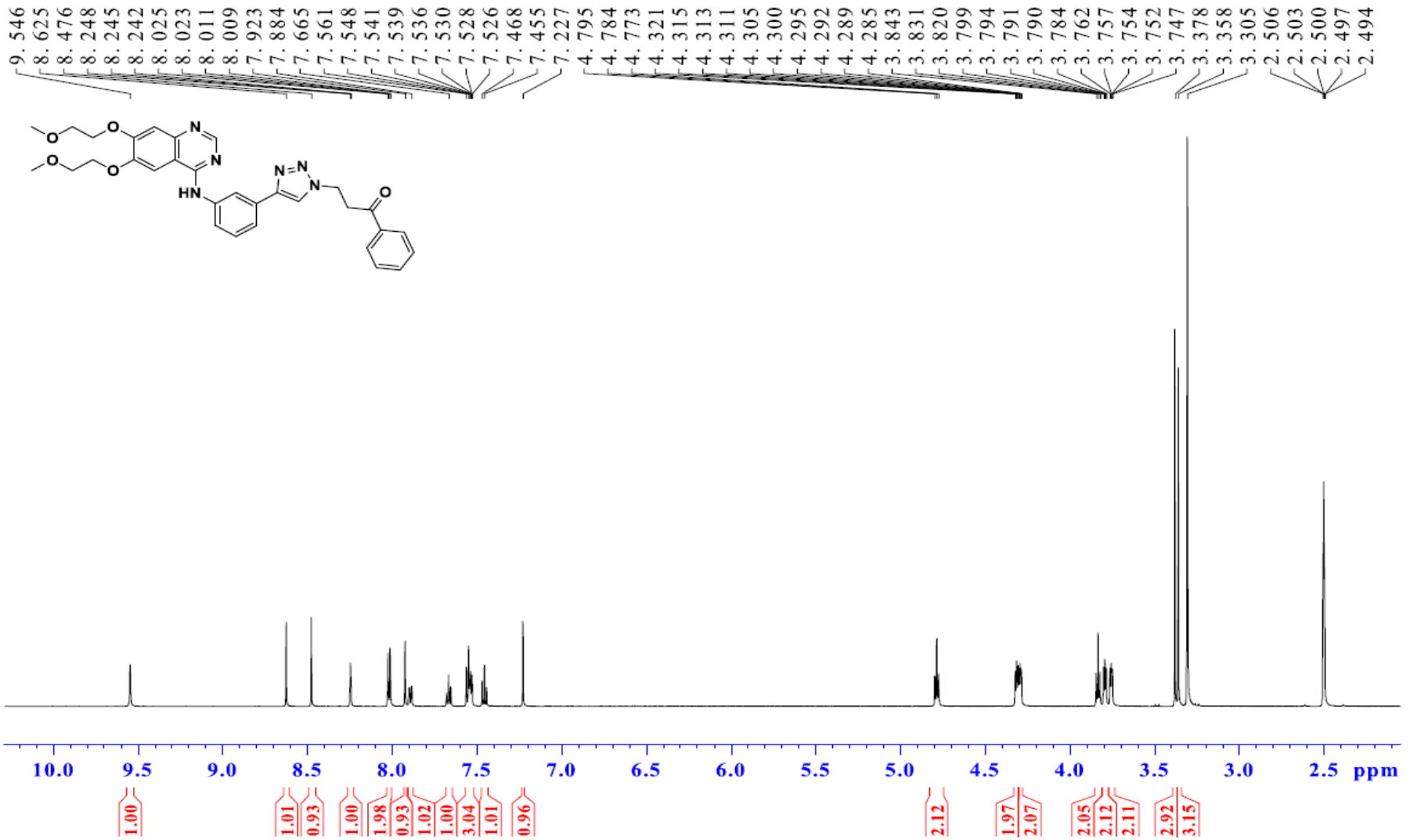


Fig S11 ^{1}H-NMR spectrum of **11** in DMSO-d_6 (600 MHz)

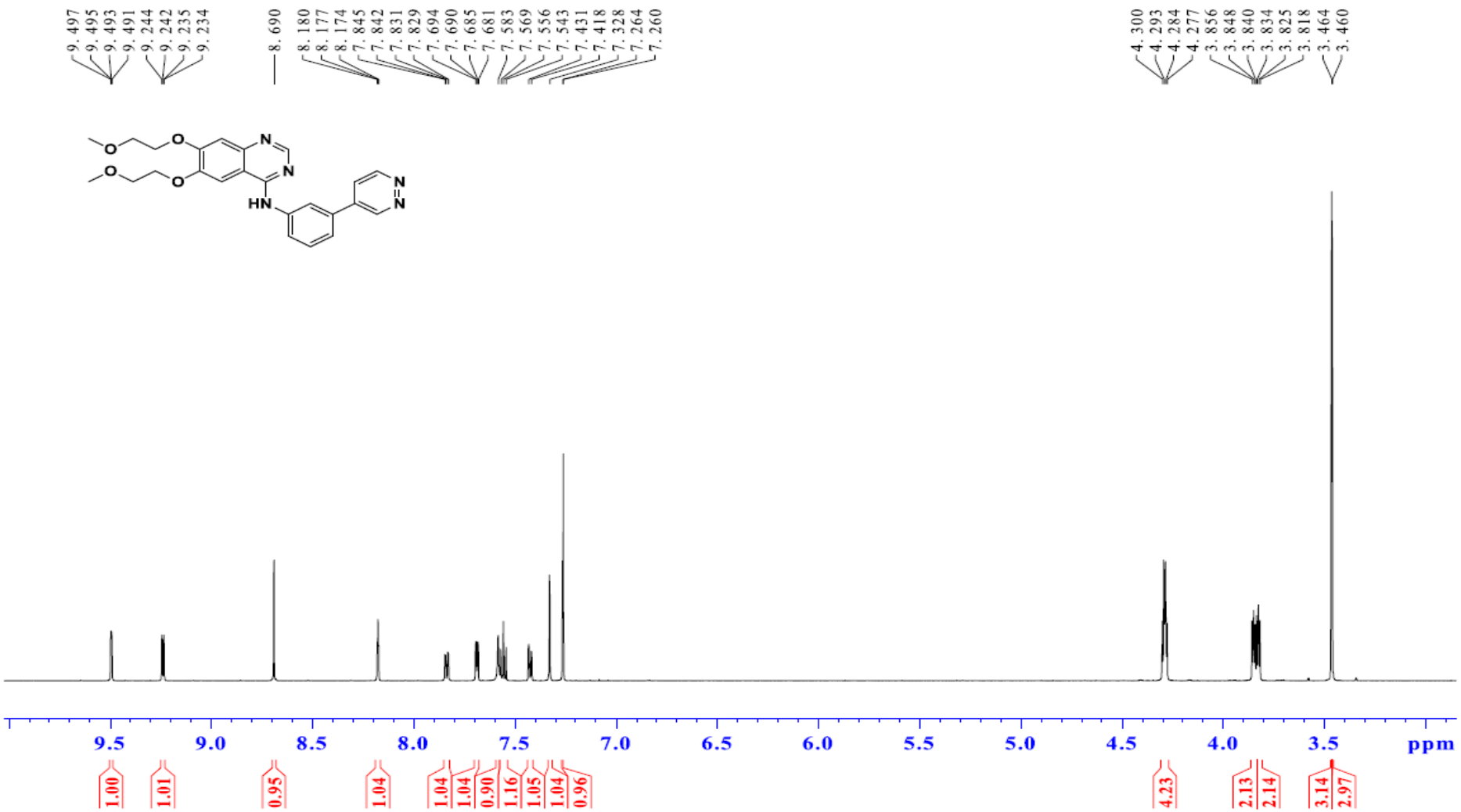


Fig S12 ^{1}H-NMR spectrum of **12** in $CDCl_3$ (600 MHz)

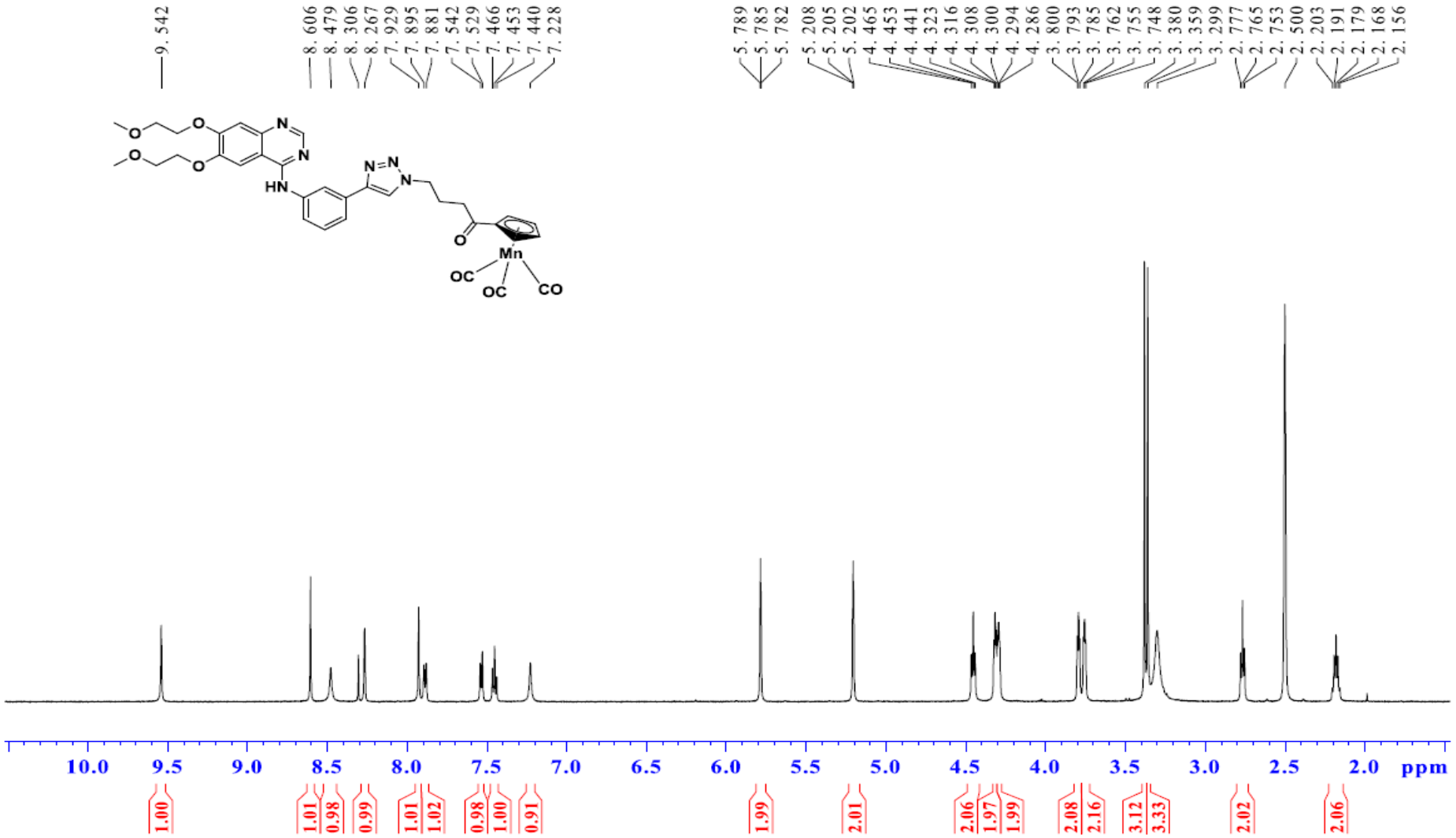


Fig S13 ^{1}H-NMR spectrum of **13** in DMSO-d_6 (600 MHz)

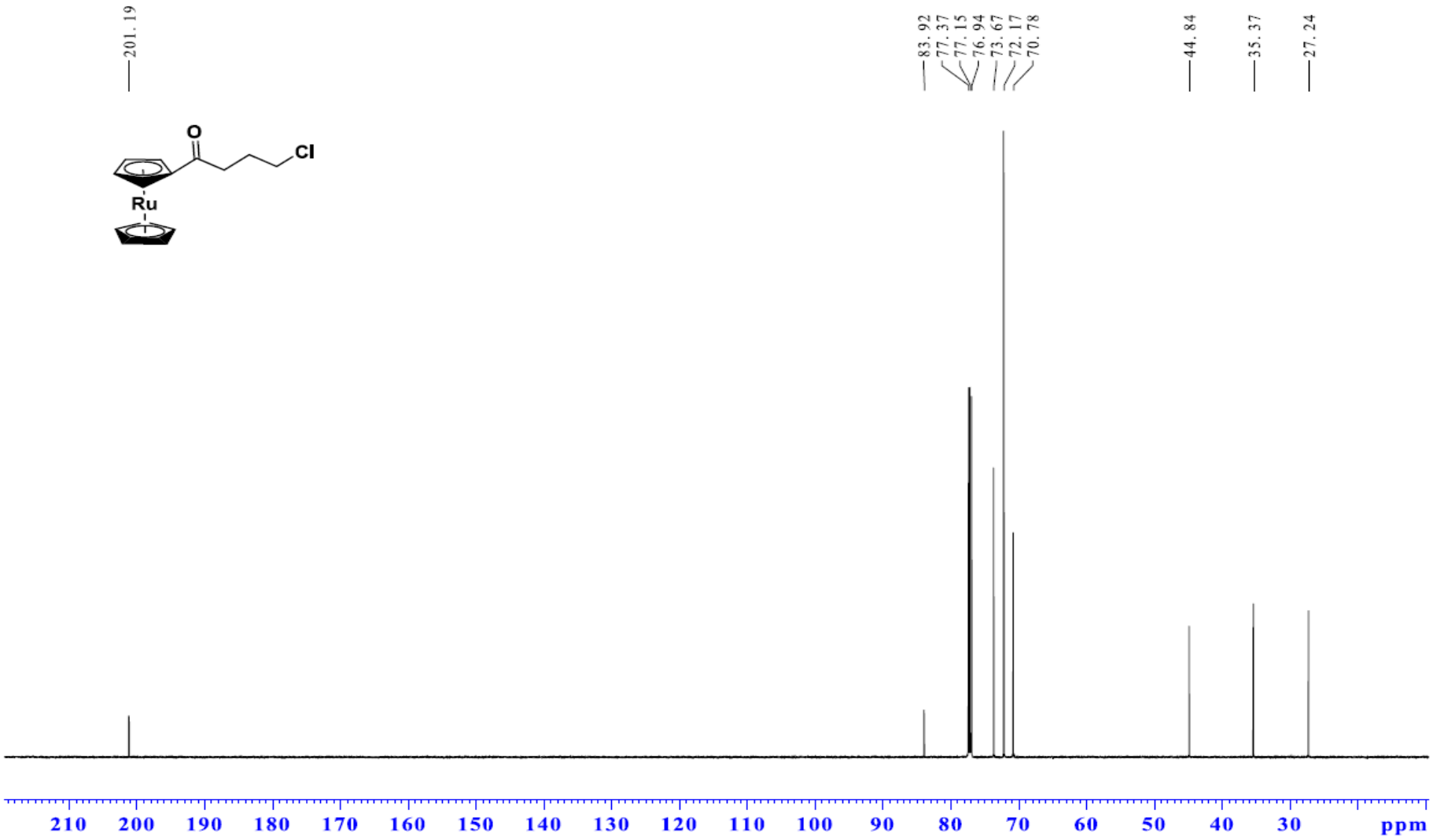


Fig S14 $^{13}C\{^{1}H\}$-NMR spectrum of **1** in $CDCl_3$ (150 MHz)

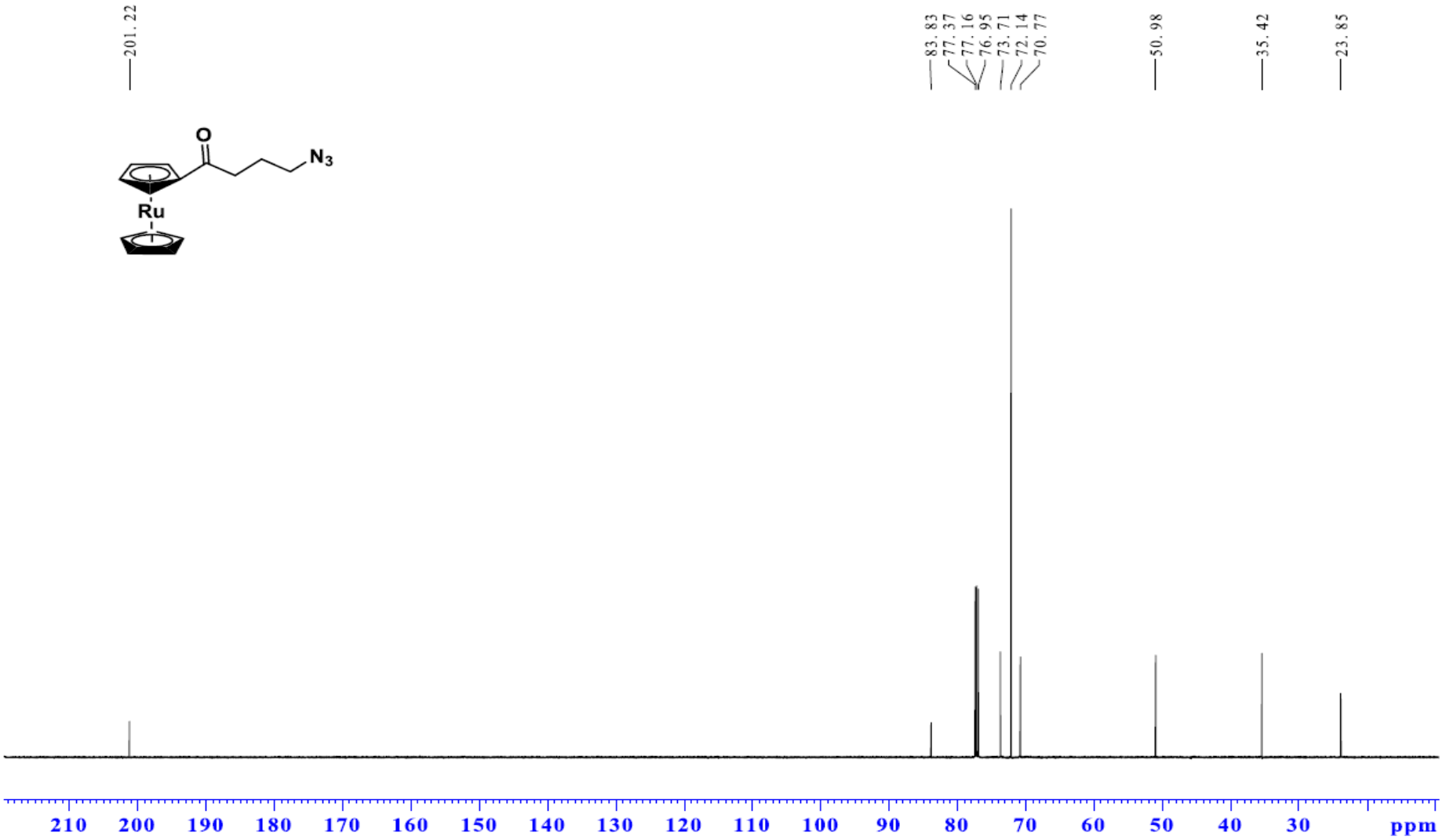


Fig S15 $^{13}C\{^{1}H\}$-NMR spectrum of **2** in $CDCl_3$ (150 MHz)

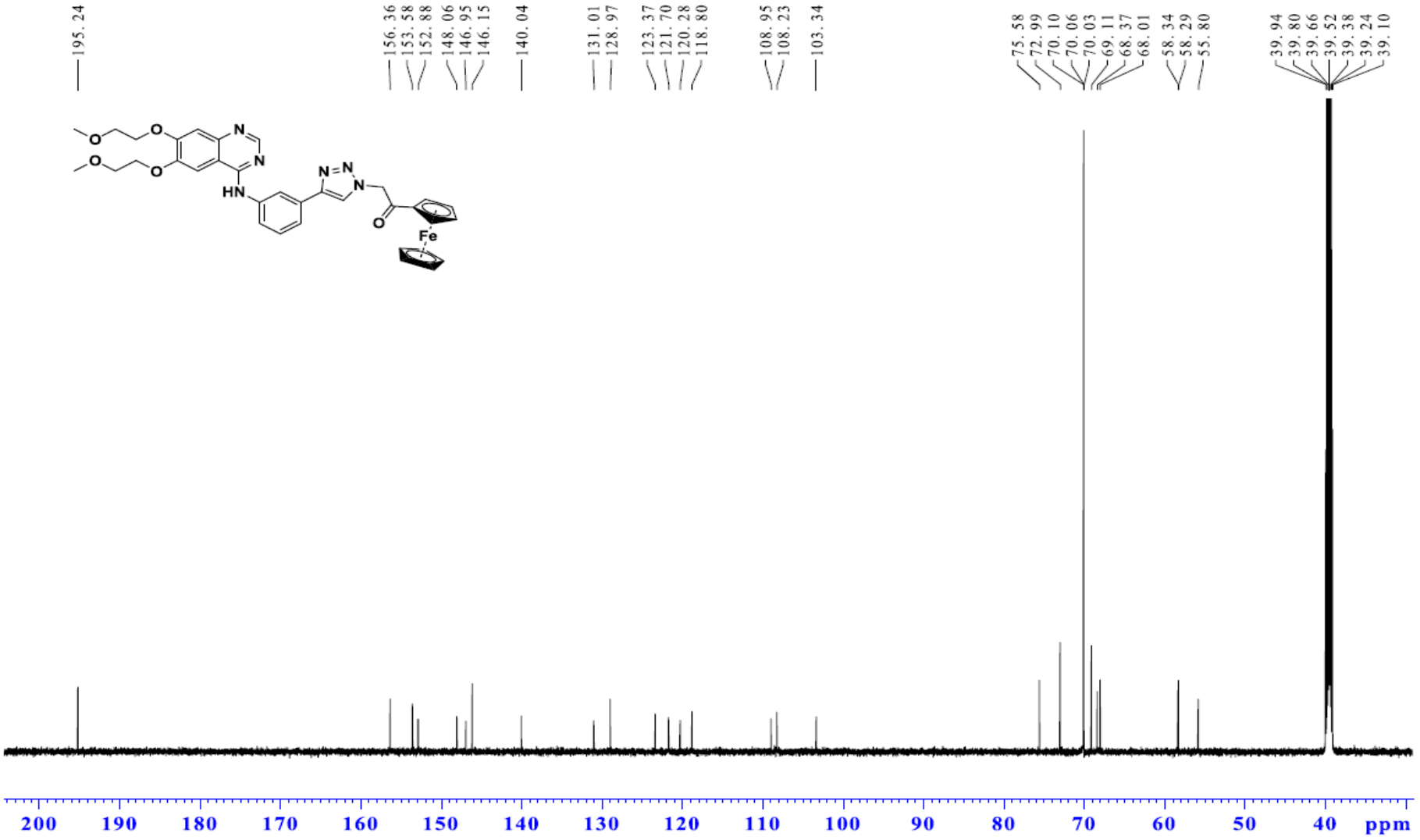


Fig S16 $^{13}C\{^{1}H\}$-NMR spectrum of **3** in DMSO-d_6 (150 MHz)

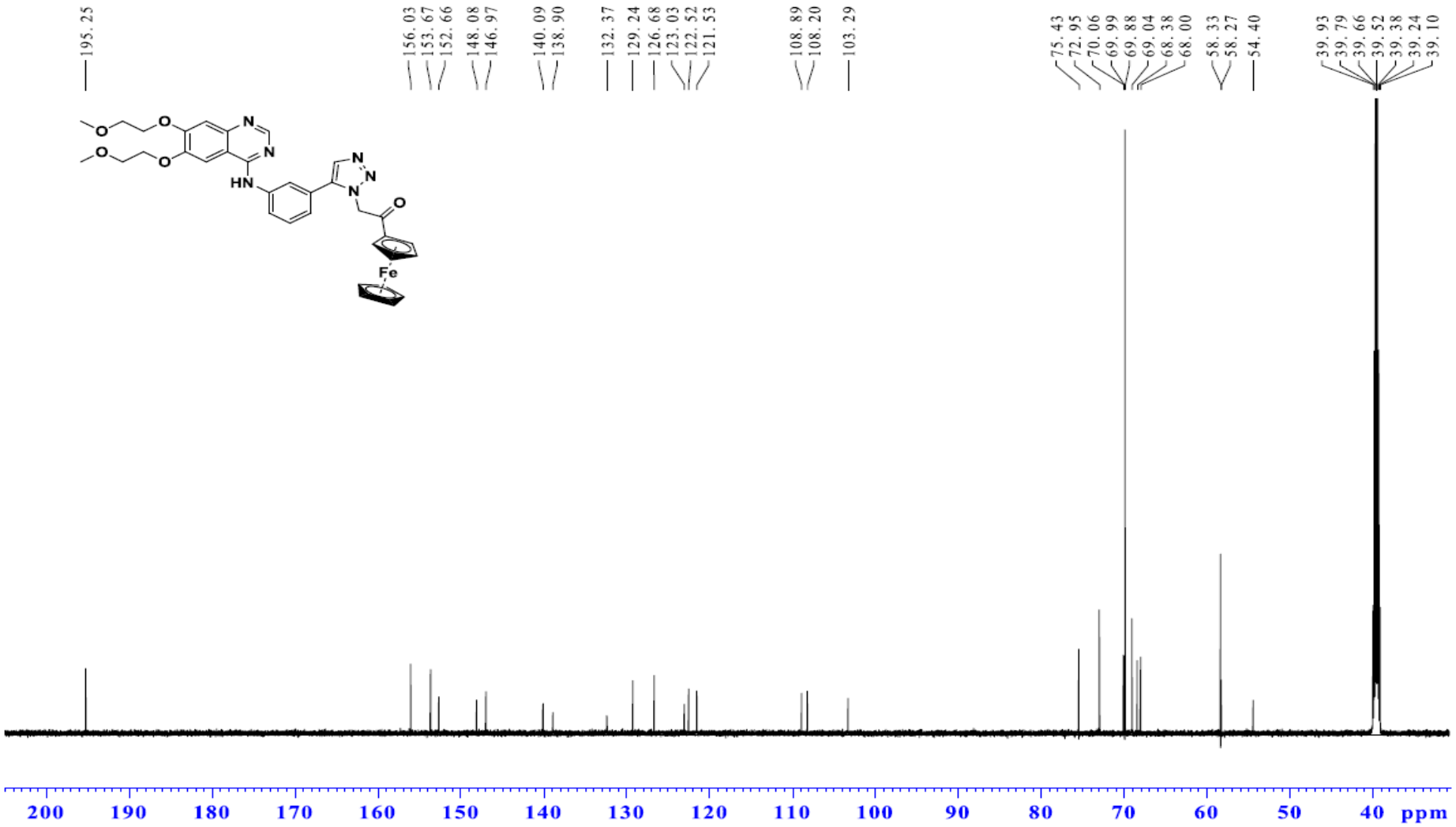


Fig S17 $^{13}C\{^{1}H\}$-NMR spectrum of **4** in DMSO-d_6 (150 MHz)

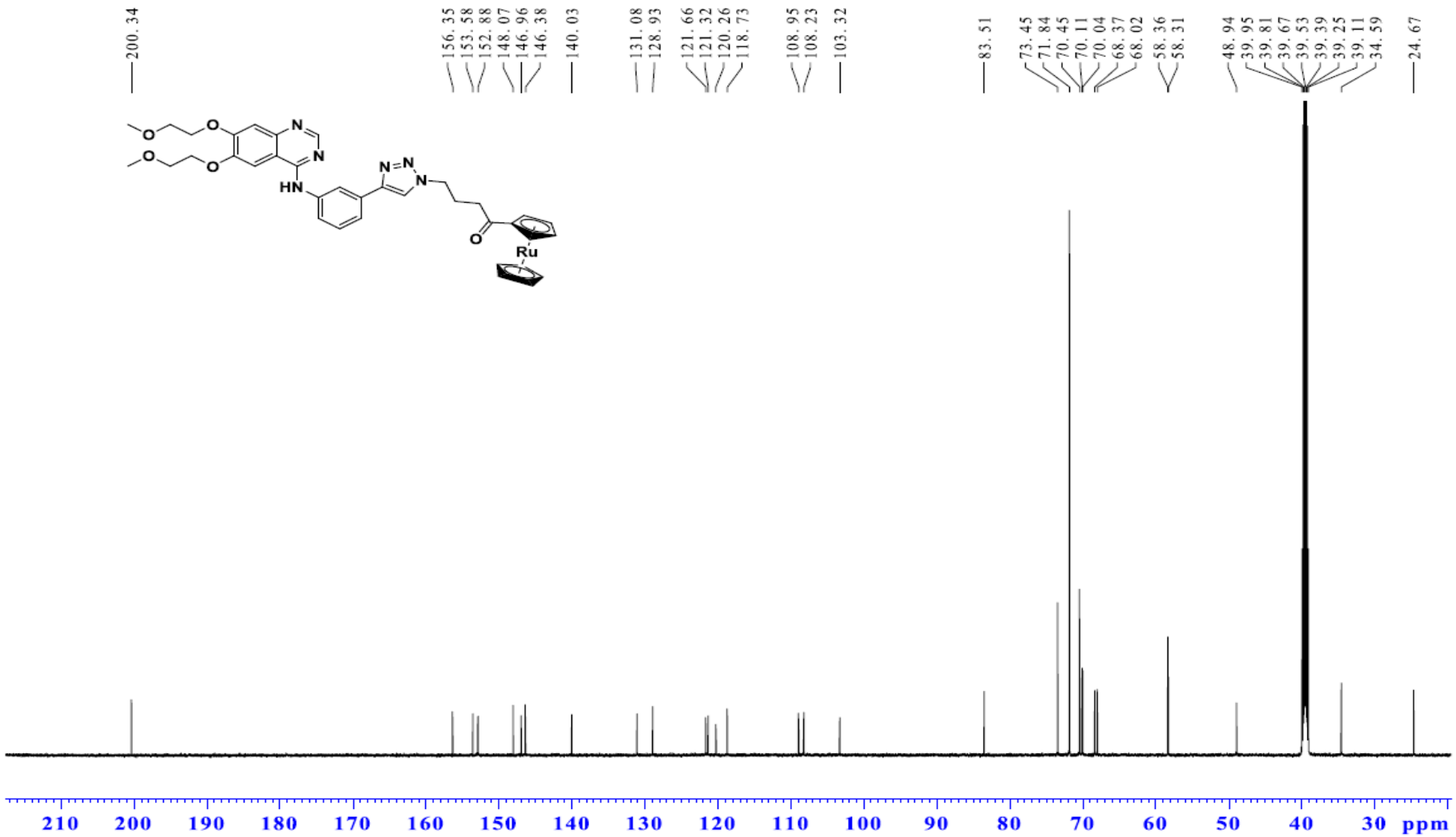


Fig S18 $^{13}C\{^{1}H\}$-NMR spectrum of **5** in DMSO-d_6 (150 MHz)

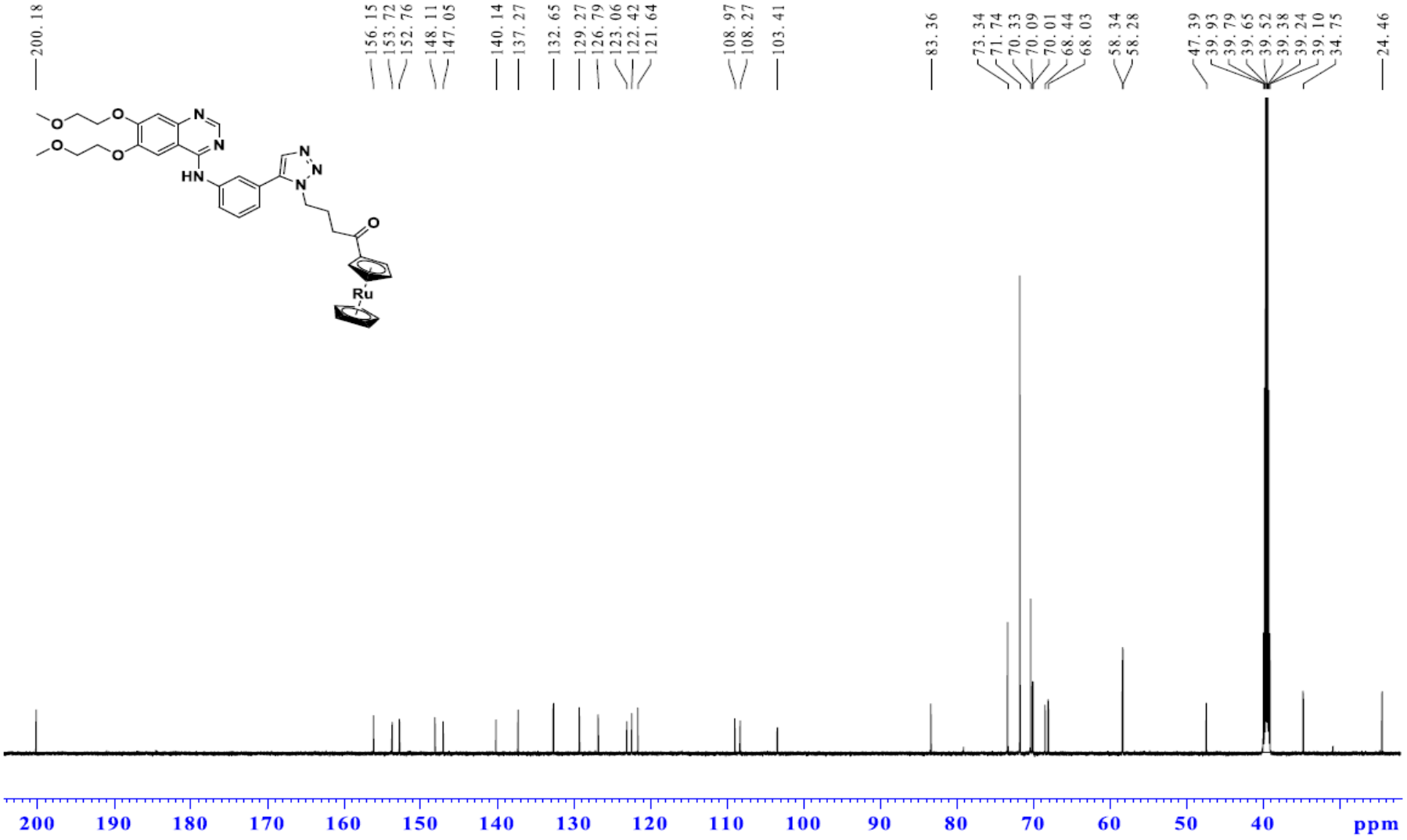


Fig S19 $^{13}C\{^{1}H\}$-NMR spectrum of **6** in DMSO-d_6 (150 MHz)

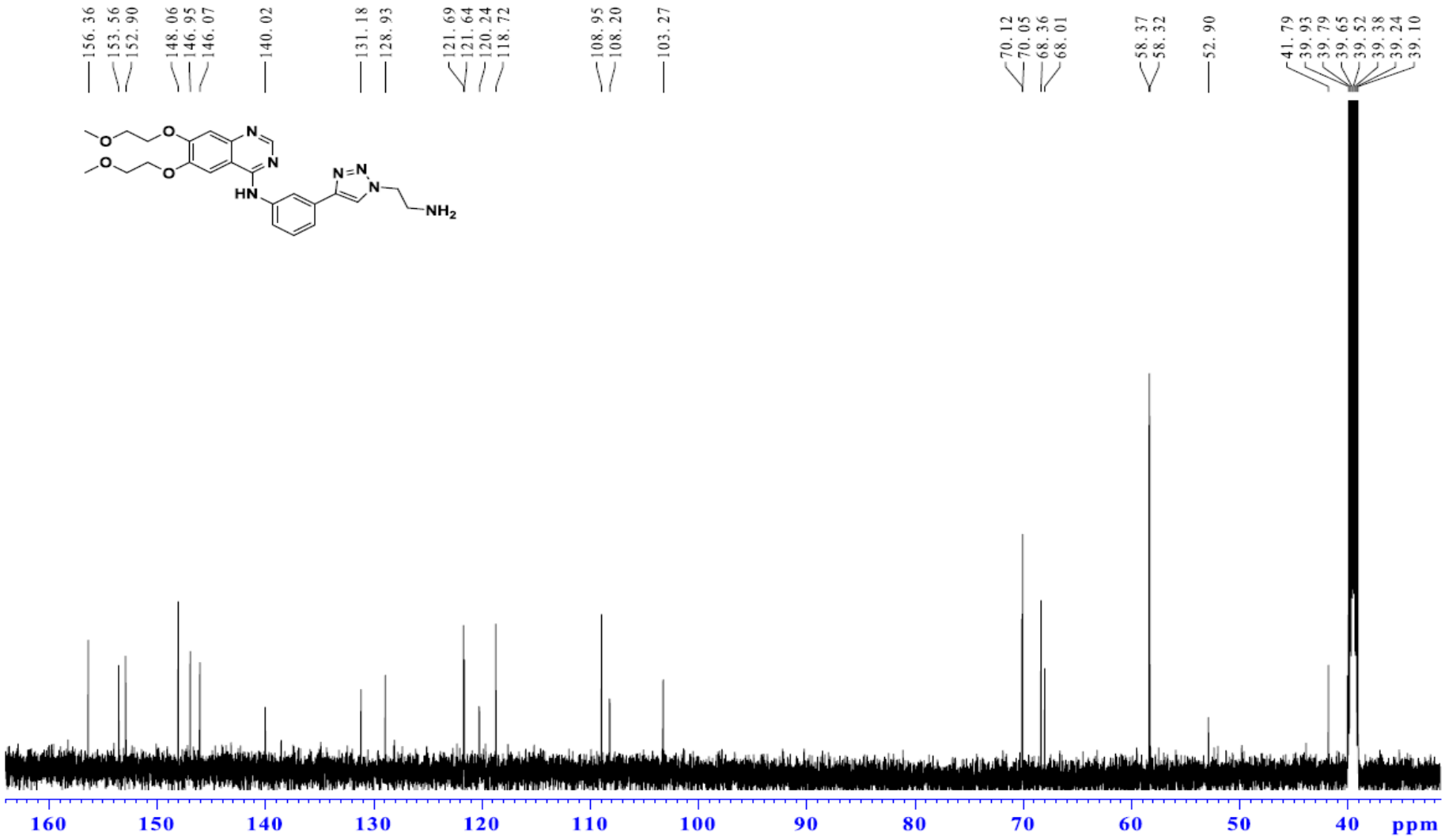


Fig S20 $^{13}C\{^{1}H\}$-NMR spectrum of **7** in DMSO-d_6 (150 MHz)

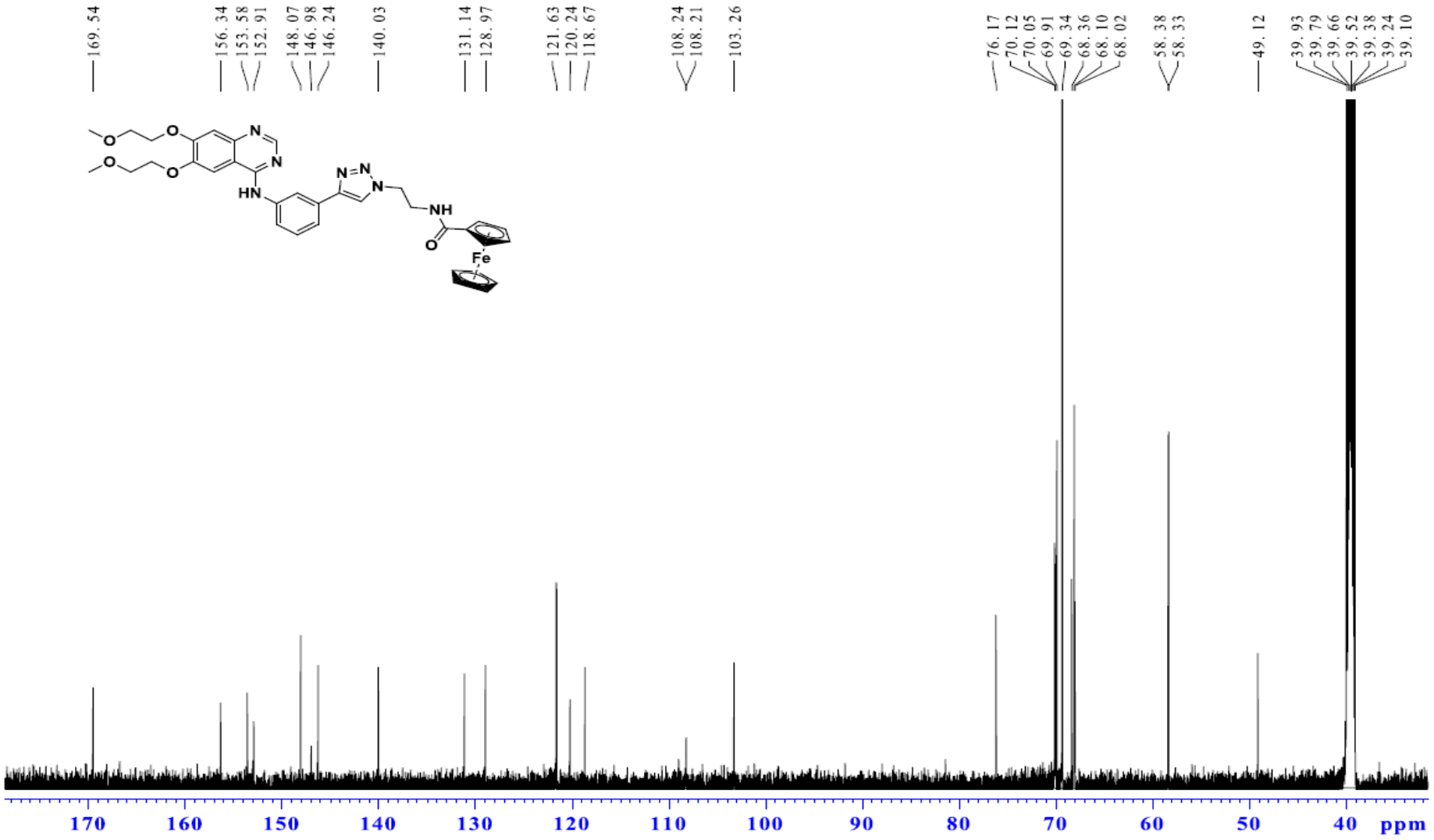


Fig S21 $^{13}C\{^{1}H\}$-NMR spectrum of **8** in DMSO-d_6 (150 MHz)

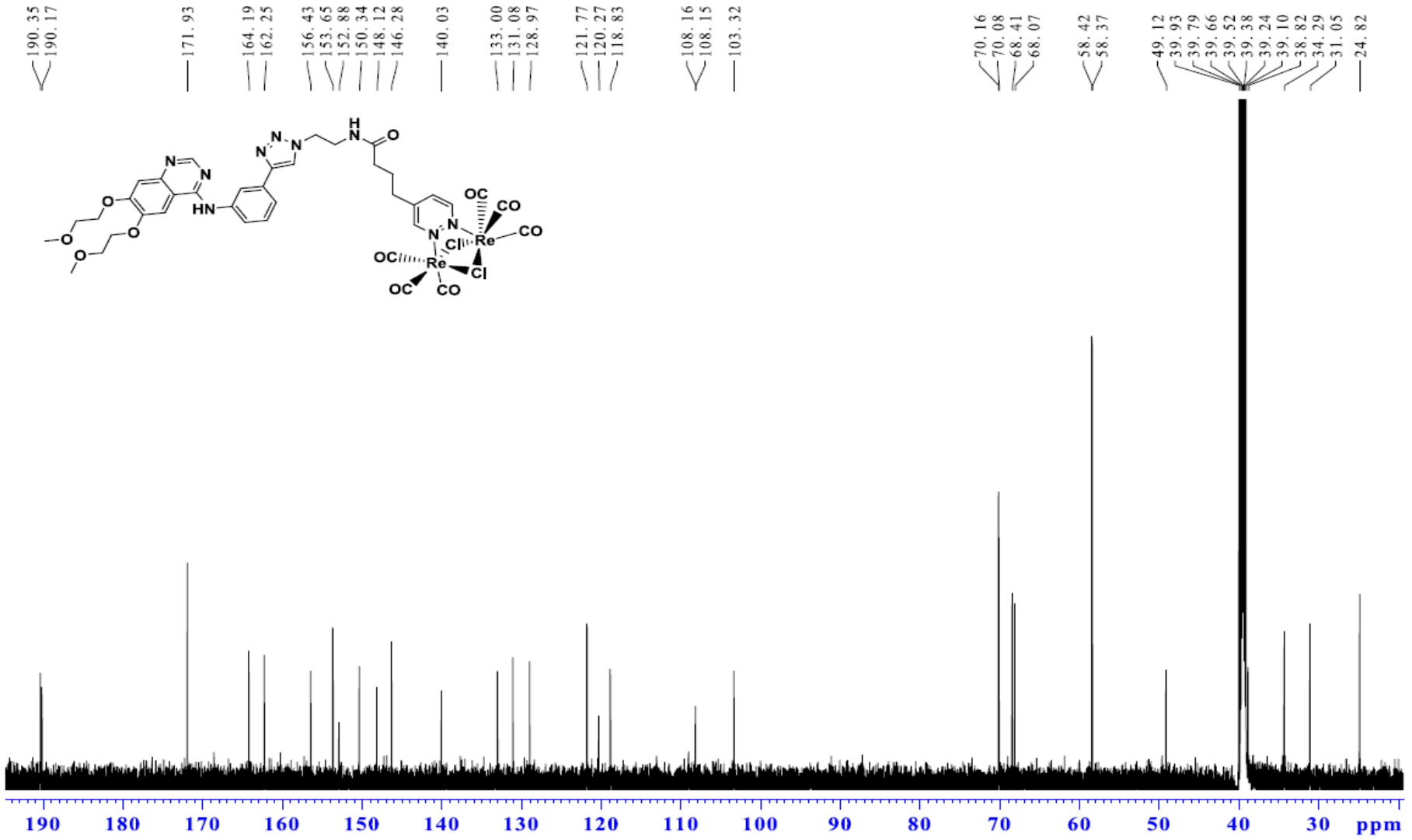


Fig S22 $^{13}C\{^{1}H\}$-NMR spectrum of **9** in DMSO-d_6 (150 MHz)

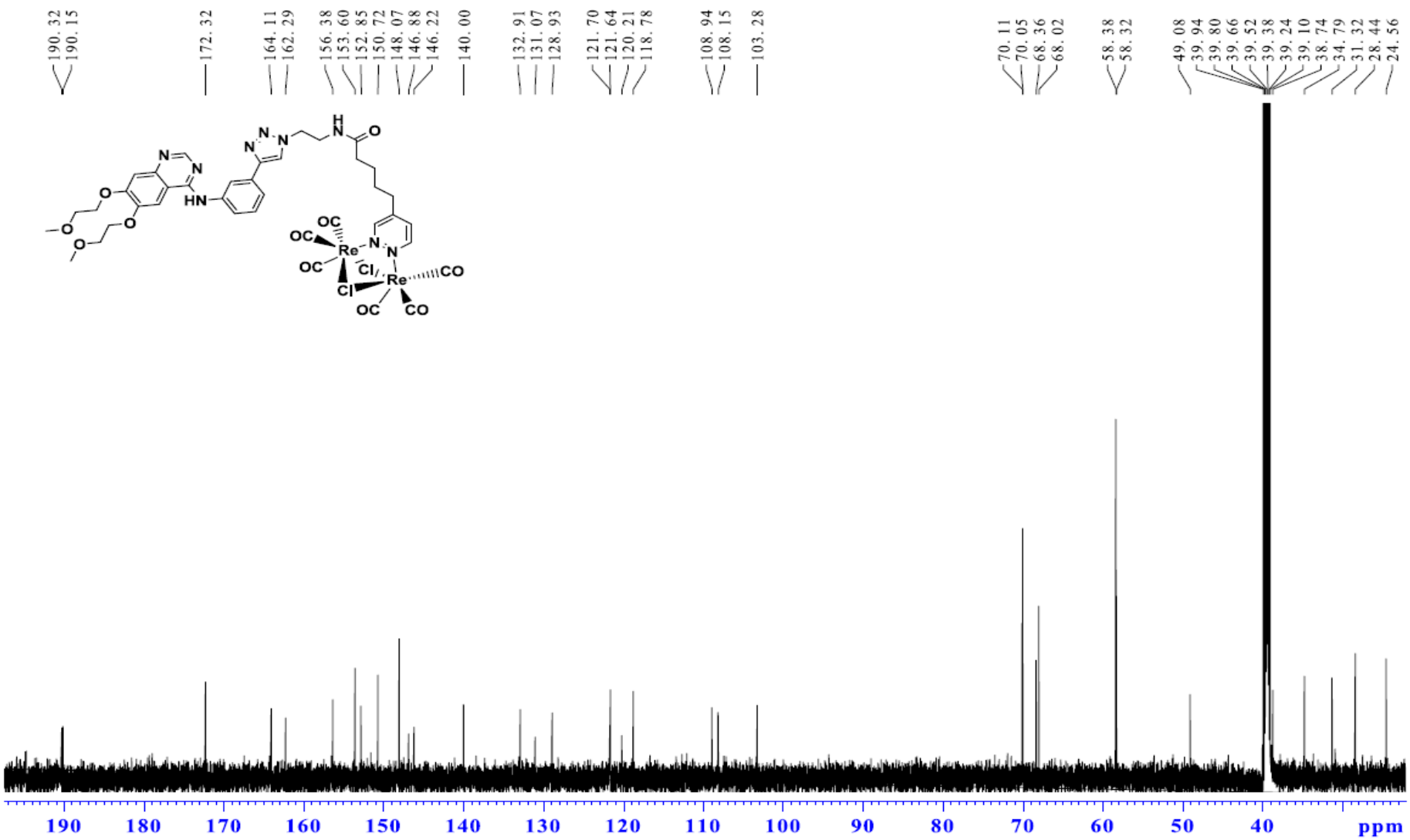


Fig S23 $^{13}C\{^{1}H\}$-NMR spectrum of **10** in DMSO-d_6 (150 MHz)

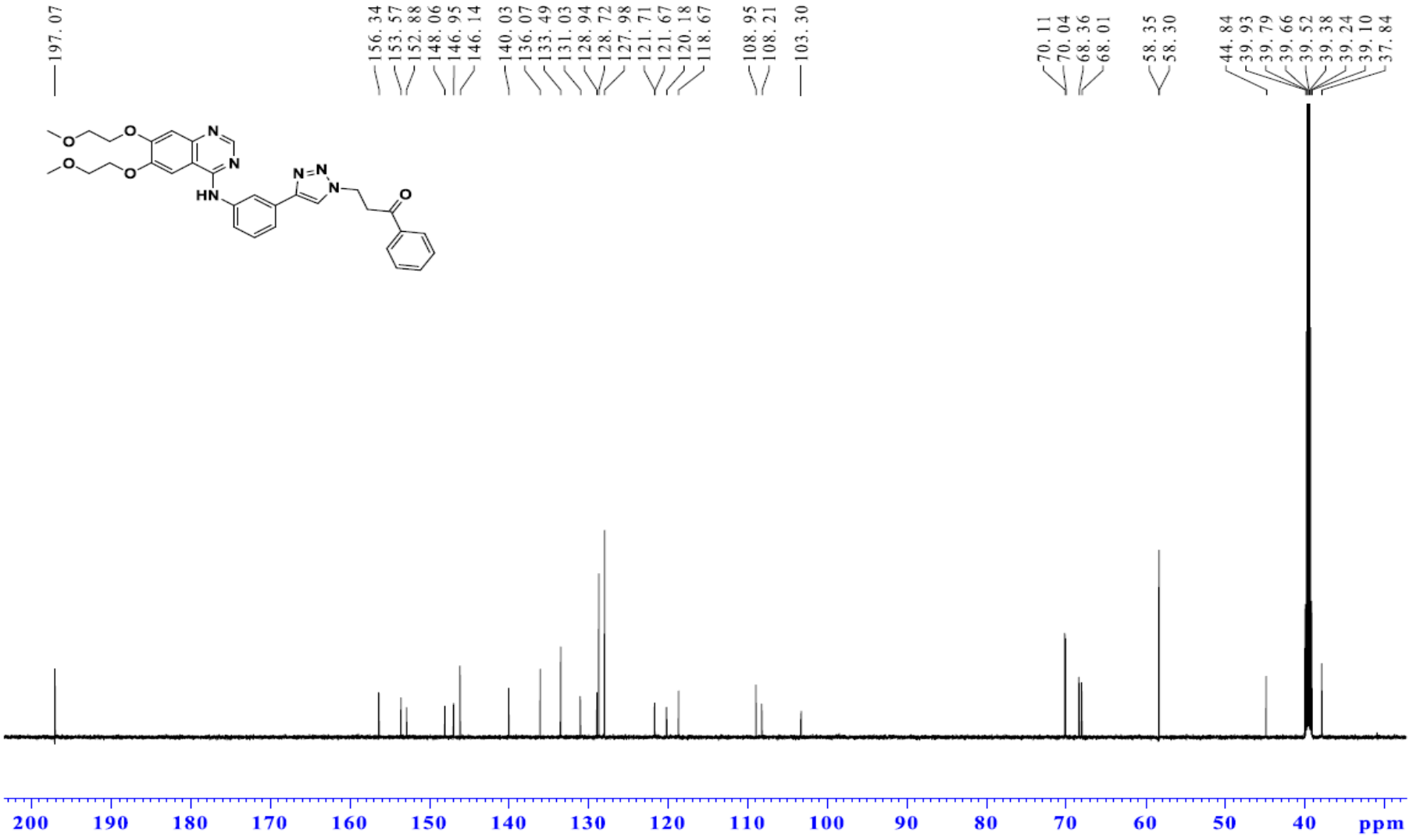


Fig S24 $^{13}C\{^{1}H\}$-NMR spectrum of **11** in DMSO-d_6 (150 MHz)

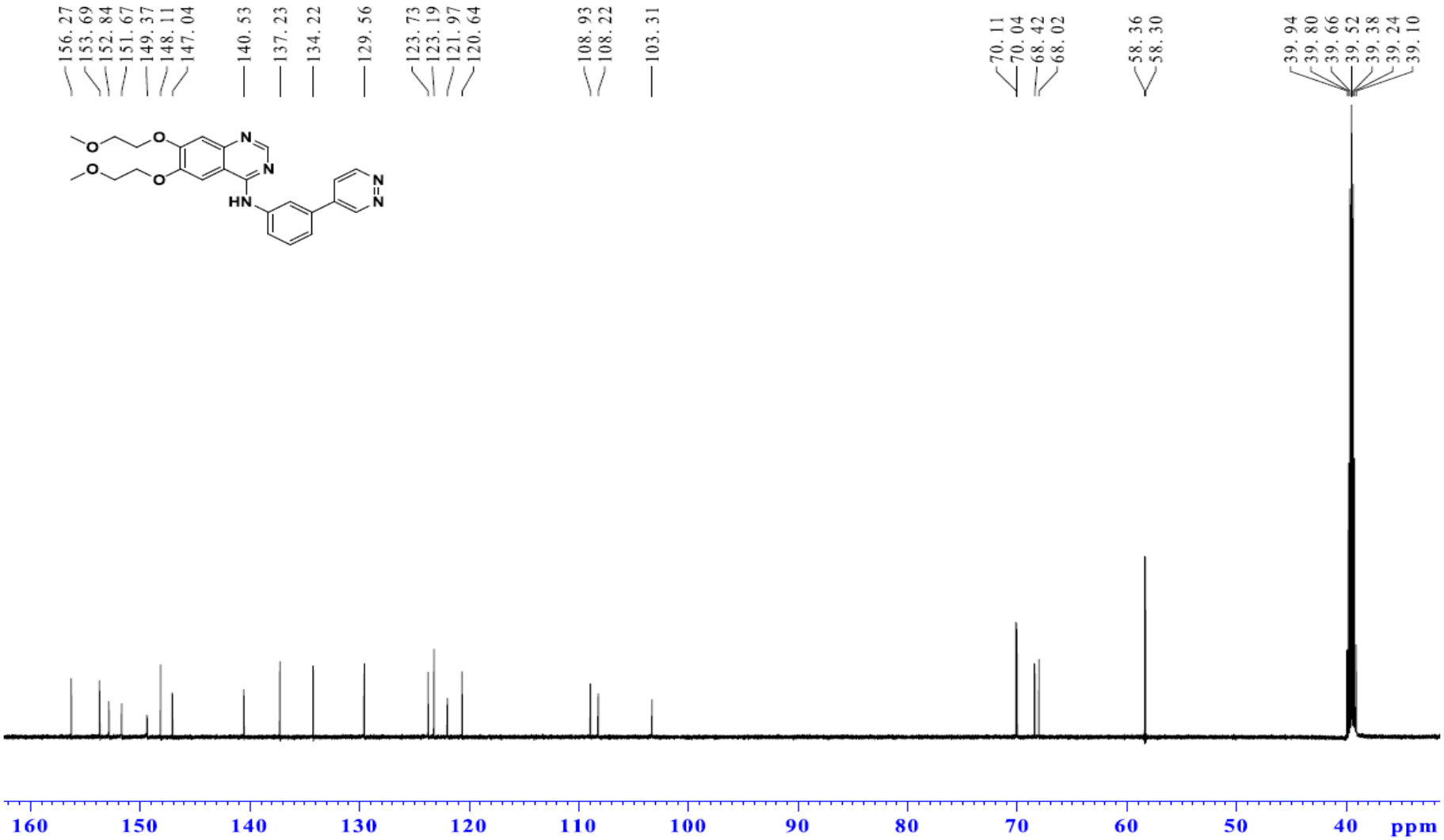


Fig S25 $^{13}C\{^{1}H\}$-NMR spectrum of **12** in DMSO-d_6 (150 MHz)

Elemental Composition Report

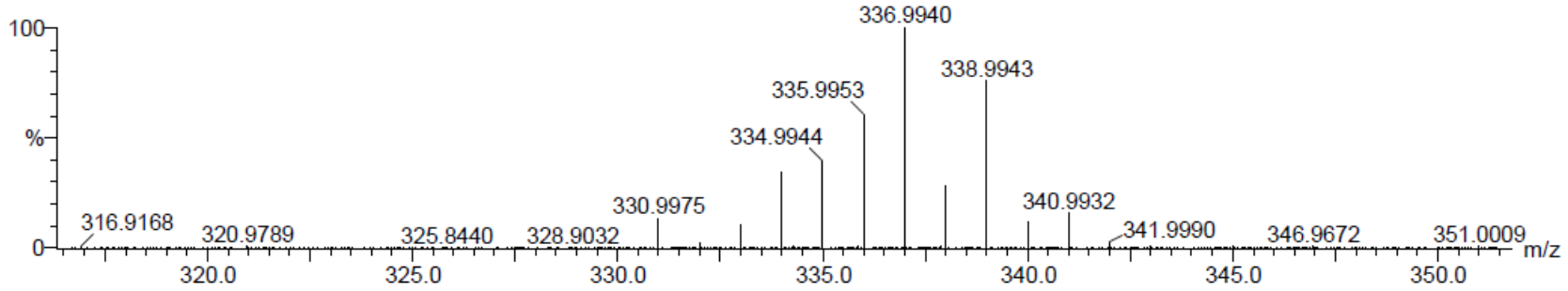
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 90.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-40 O: 0-2 Cl: 0-1 Ru: 1-1

221214_SPB_00127A 48 (0.497) Cm (47:48)

TOF MS ES+
2.08e+005



Minimum:				-1.5				
Maximum:		5.0	5.0	90.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
336.9940	336.9933	0.7	2.1	6.5	1069.3	n/a	n/a	C14 H16 O Cl Ru

Fig S26 HRMS spectrum of **1**

Elemental Composition Report

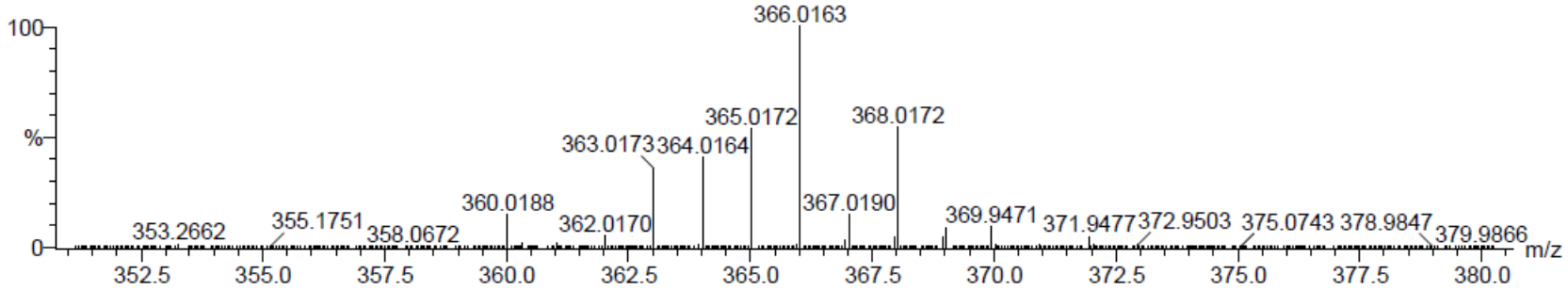
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 90.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
128 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-3 O: 0-2 Na: 0-3 Ru: 1-1

221214_SPB_00110XA 34 (0.365) Cm (34:45-4:8)

TOF MS ES+
1.11e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	90.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
366.0163	366.0156	0.7	1.9	8.5	1957.5	0.001	99.94	C14 H15 N3 O Na Ru
	366.0180	-1.7	-4.6	11.5	1965.0	7.432	0.06	C16 H14 N3 O Ru

Fig S27 HRMS spectrum of **2**

Elemental Composition Report

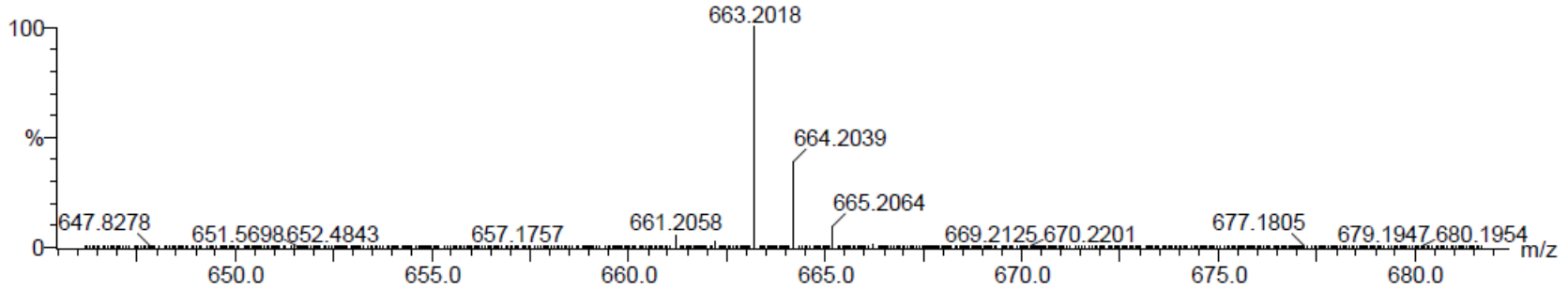
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 90.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
168 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-40 N: 1-7 O: 0-7 Fe: 0-1

221214_SPB_00101A 27 (0.294) Cm (27:34-4:6)

TOF MS ES+
4.29e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	90.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
663.2018	663.2018	0.0	0.0	20.5	1588.2	8.543	0.02	C34 H35 N6 O5 Fe
	663.1992	2.6	3.9	28.5	1579.7	0.000	99.98	C38 H27 N6 O6

Fig S28 HRMS spectrum of **3**

Elemental Composition Report

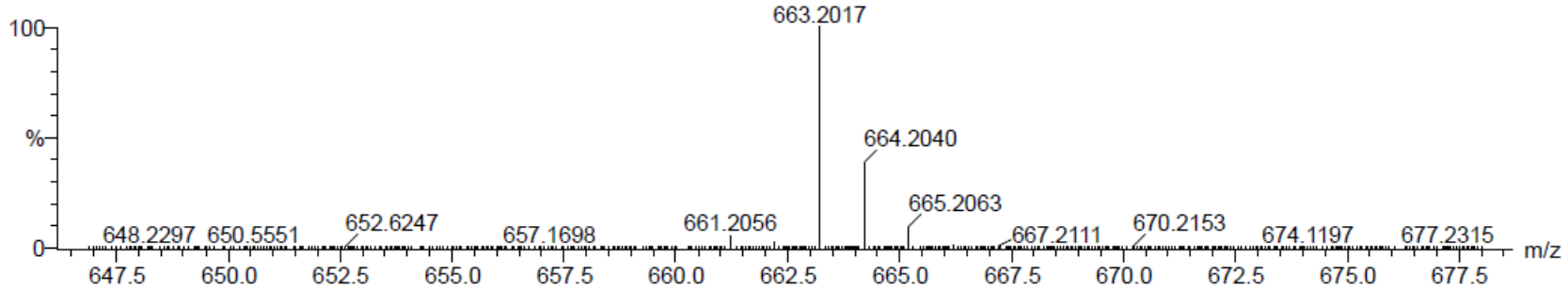
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 90.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
168 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-40 N: 1-7 O: 0-7 Fe: 0-1

221214_SPB_00107A 34 (0.366) Cm (34:36)

TOF MS ES+
2.78e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	90.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
663.2017	663.2018	-0.1	-0.2	20.5	1408.0	8.985	0.01	C34 H35 N6 O5 Fe
	663.1992	2.5	3.8	28.5	1399.0	0.000	99.99	C38 H27 N6 O6

Fig S29 HRMS spectrum of **4**

Elemental Composition Report

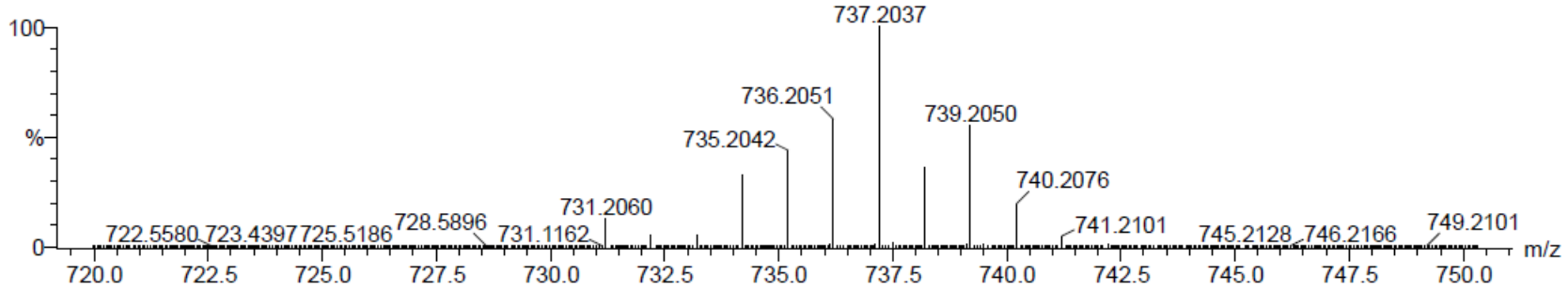
Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 90.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
82 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-60 N: 0-6 O: 0-6 Ru: 1-1

220316_SPB_00087A 17 (0.197) Cm (15:21)

TOF MS ES+
2.68e+007



Minimum:				-1.5				
Maximum:		5.0	10.0	90.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
737.2037	737.2025	1.2	1.6	20.5	2979.1	n/a	n/a	C36 H39 N6 O5 Ru

Fig S30 HRMS spectrum of **5**

Elemental Composition Report

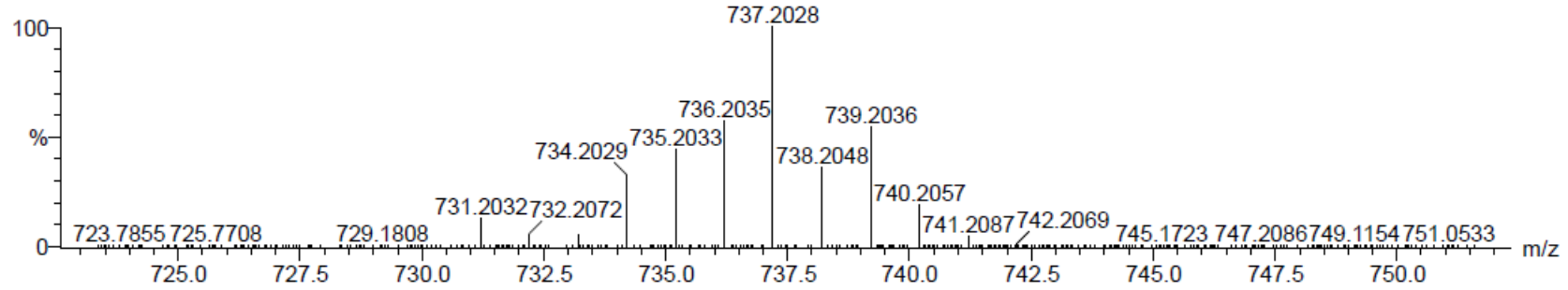
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 90.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
181 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-60 N: 0-7 O: 0-8 Ru: 1-1

221214_SPB_00110A 29 (0.311) Cm (29:35-3:8)

TOF MS ES+
1.12e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	90.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
737.2028	737.2025	0.3	0.4	20.5	1121.8	0.003	99.70	C36 H39 N6 O5 Ru
	737.2052	-2.4	-3.3	19.5	1127.6	5.800	0.30	C40 H43 O7 Ru

Fig S31 HRMS spectrum of **6**

Elemental Composition Report **Page 1**

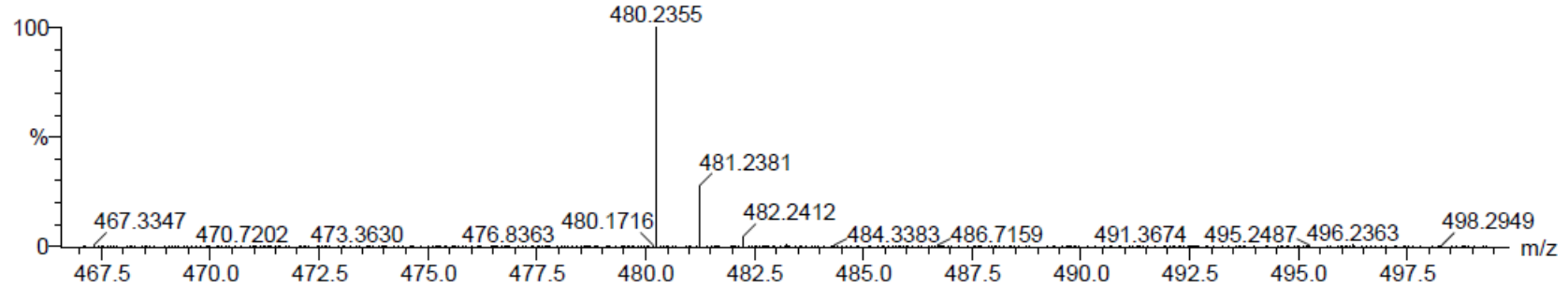
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 90.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
146 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-40 N: 1-7 O: 0-5

230215_SPB_00139B 24 (0.330) Cm (24:30-2:9)

TOF MS ES+
2.18e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	90.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
480.2355	480.2359	-0.4	-0.8	13.5	948.6	n/a	n/a	C24 H30 N7 O4

Fig S32 HRMS spectrum of **7**

Elemental Composition Report **Page 1**

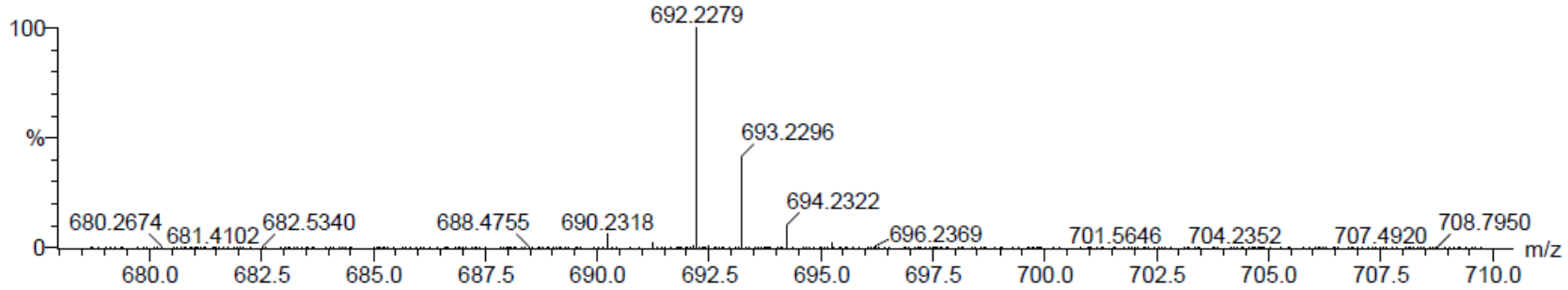
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 90.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
70 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-40 N: 1-7 O: 0-5 Fe: 0-1

230215_SPB_00141A 19 (0.287) Cm (19:28-43:54)

TOF MS ES+
5.27e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	90.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
692.2279	692.2284	-0.5	-0.7	20.5	1098.1	n/a	n/a	C35 H38 N7 O5 Fe

Fig S33 HRMS spectrum of **8**

Elemental Composition Report

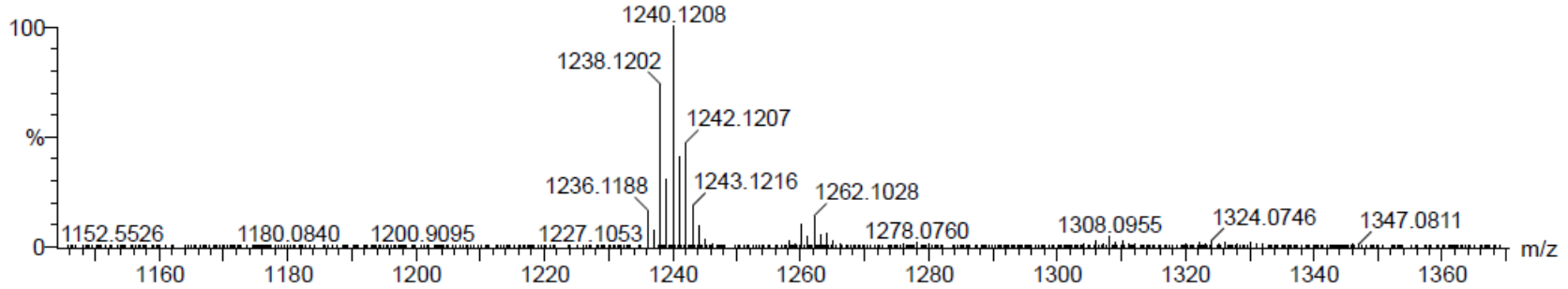
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 90.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
284 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-45 H: 0-45 N: 0-9 O: 0-12 Cl: 2-2 Re: 1-2

230421_SPB_00153_pos_A 11 (0.165) Cm (10:11)

TOF MS ES+
3.18e+005



Minimum:				-1.5				
Maximum:		5.0	5.0	90.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
1240.1208	1240.1183	2.5	2.0	23.5	289.0	0.188	82.82	C38 H38 N9 O11 Cl2 Re2
	1240.1223	-1.5	-1.2	27.5	290.5	1.762	17.18	C43 H38 N7 O9 Cl2 Re2

Fig S34 HRMS spectrum of **9**

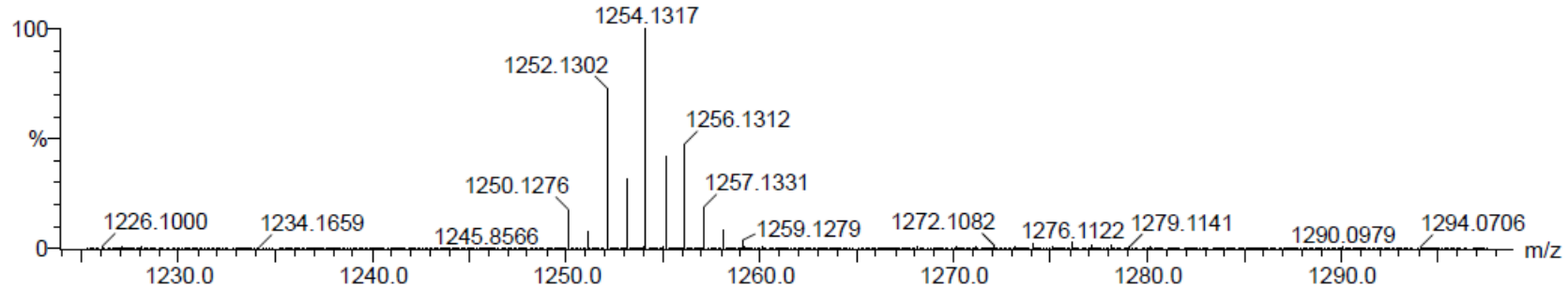
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 90.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
340 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-40 N: 0-9 O: 0-11 Cl: 0-2 Re: 2-2

230215_SPB_00145A 17 (0.197) Cm (13:17-3:7)

TOF MS ES+
4.36e+005



Minimum:				-1.5				
Maximum:		5.0	5.0	90.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
1254.1317	1254.1339	-2.2	-1.8	23.5	1077.0	n/a	n/a	C39 H40 N9 O11 Cl2 Re2

Fig S35 HRMS spectrum of **10**

Elemental Composition Report

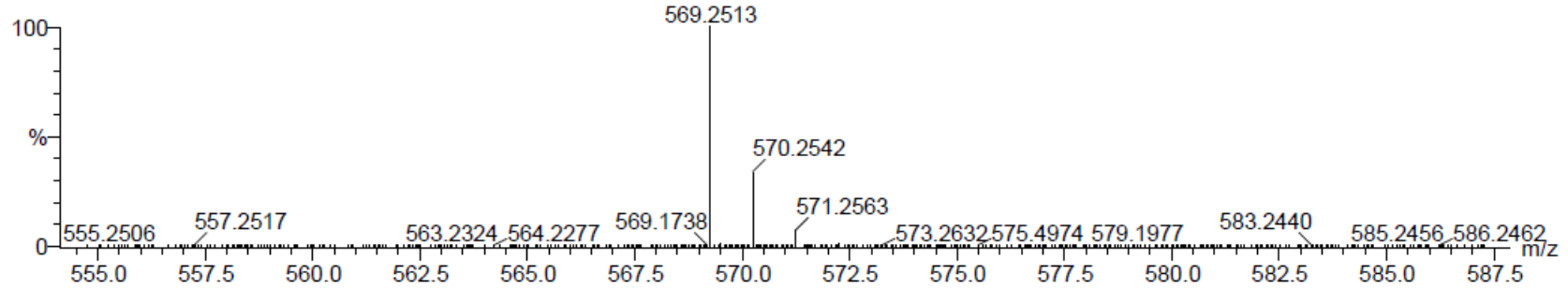
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 90.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
359 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-40 N: 1-7 O: 0-7 Fe: 0-1

221214_SPB_00112A 13 (0.151) Cm (11:13-(6+7))

TOF MS ES+
2.21e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	90.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
569.2513	569.2512	0.1	0.2	18.5	1174.4	n/a	n/a	C31 H33 N6 O5

Fig S36 HRMS spectrum of **11**

Elemental Composition Report

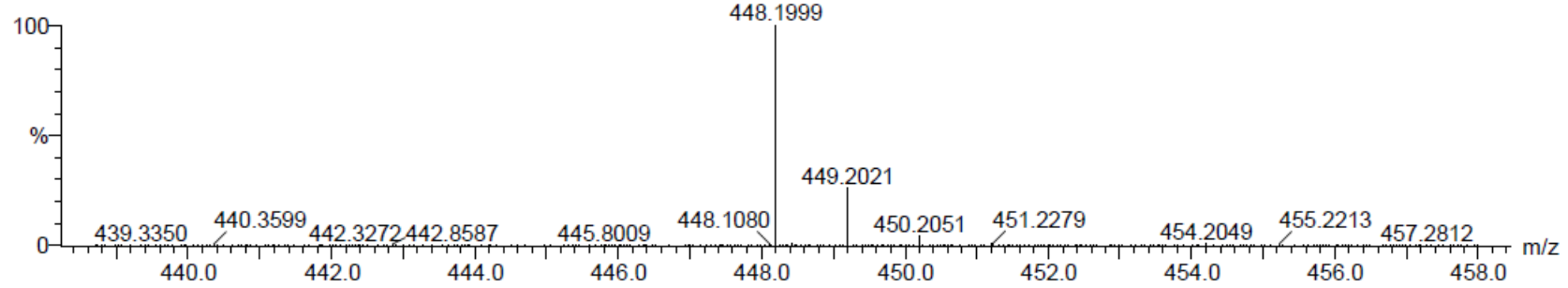
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 90.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
168 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-40 N: 1-6 O: 0-7

221214_SPB_00074 12 (0.143) Cm (11:12-5:6)

1: TOF MS ES+
7.42e+005



Minimum:				-1.5				
Maximum:		5.0	5.0	90.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
448.1999	448.1985	1.4	3.1	14.5	1131.0	n/a	n/a	C24 H26 N5 O4

Fig S37 HRMS spectrum of **12**

Elemental Composition Report

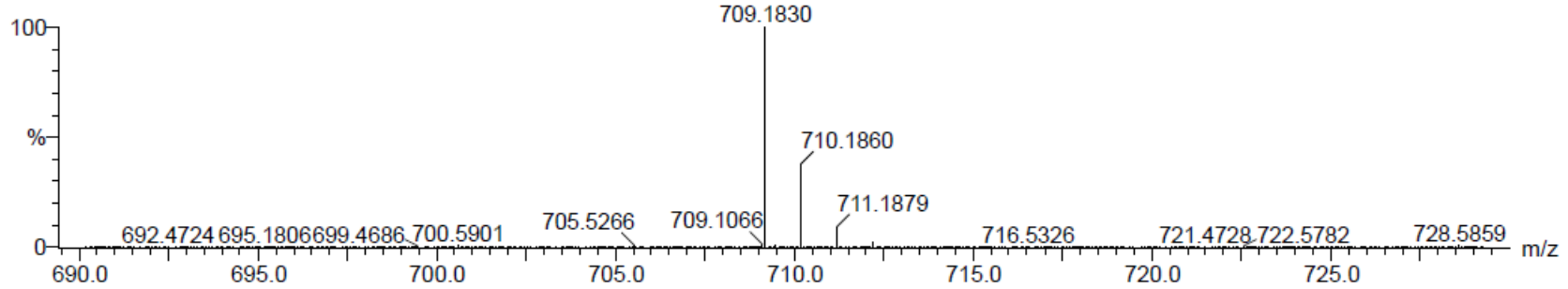
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 90.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Odd and Even Electron Ions
59 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-40 H: 0-40 N: 2-6 O: 0-8 Mn: 1-1

220304_SPB_00084A 37 (0.391) Cm (37:42-3:6)

TOF MS ES+
5.81e+006



Minimum:				-1.5				
Maximum:		5.0	5.0	90.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
709.1830	709.1819	1.1	1.6	21.0	1812.8	0.000	99.97	C34 H34 N6 O8 Mn
	709.1859	-2.9	-4.1	25.0	1820.9	8.089	0.03	C39 H34 N4 O6 Mn

Fig S38 HRMS spectrum of **13**

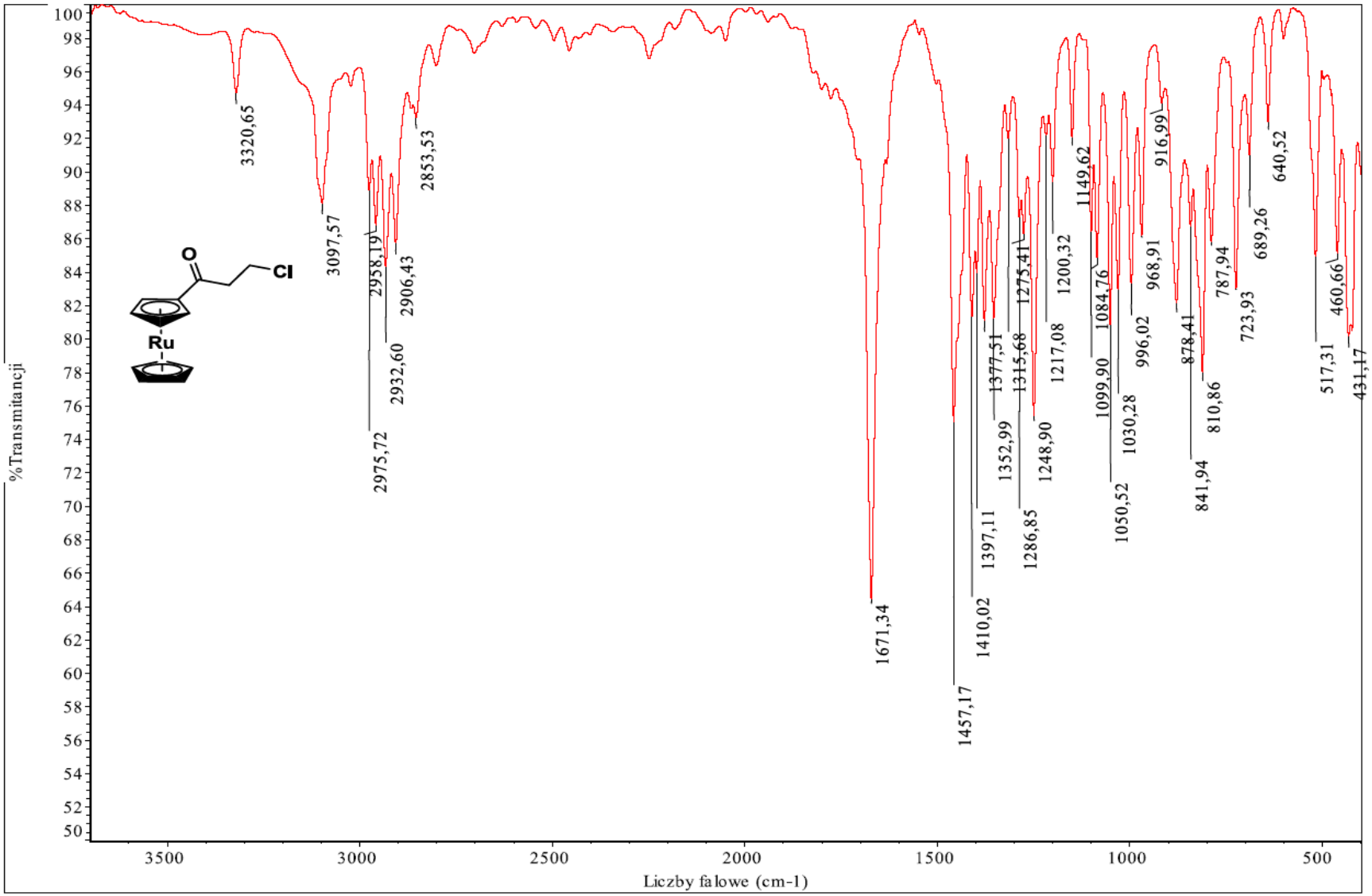


Fig S39 FTIR (KBr ν [cm^{-1}]) spectrum of **1**

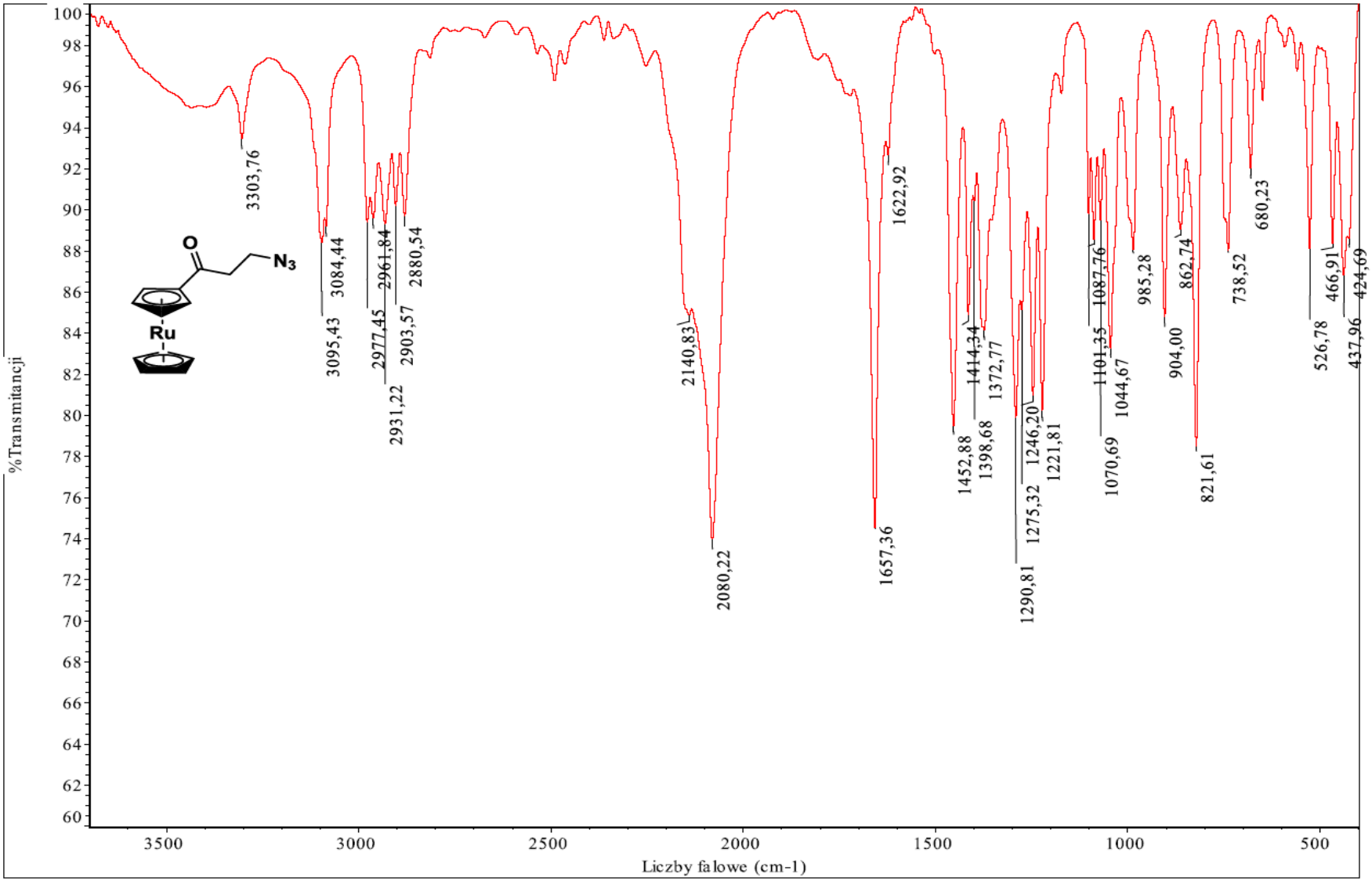


Fig S40 FTIR (KBr ν [cm^{-1}]) spectrum of **2**

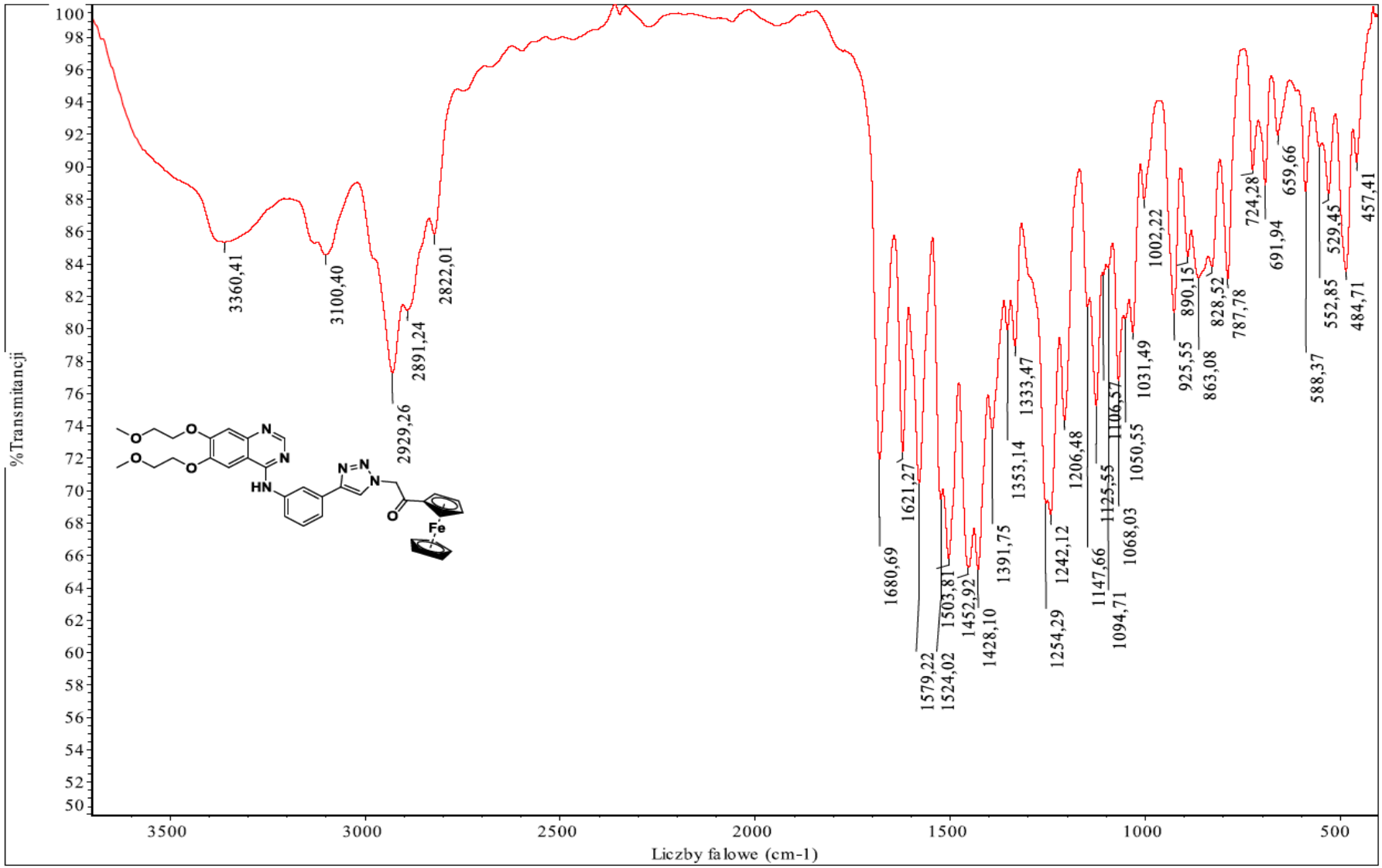


Fig S41 FTIR (KBr ν [cm^{-1}]) spectrum of **3**

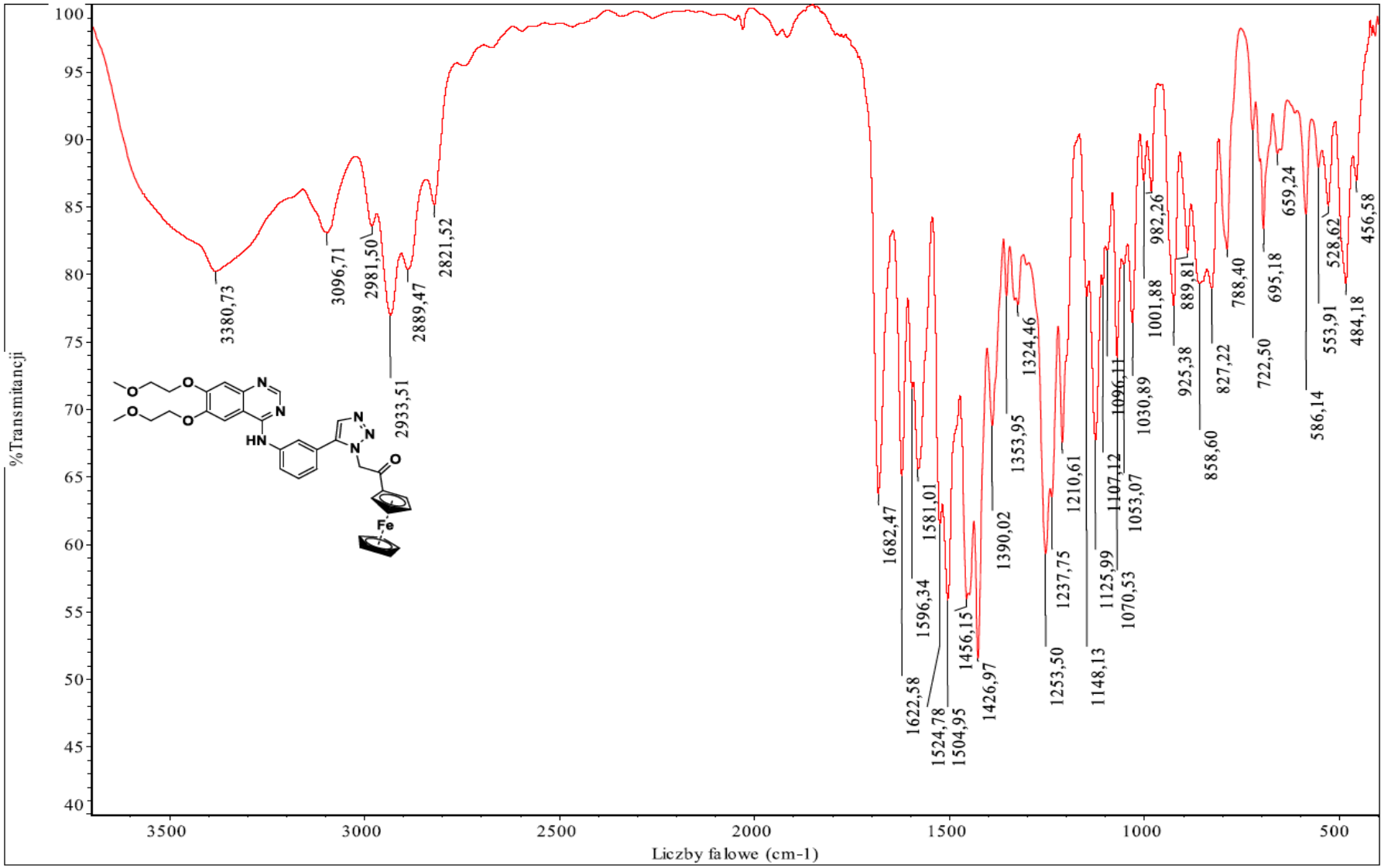


Fig S42 FTIR (KBr ν [cm^{-1}]) spectrum of **4**

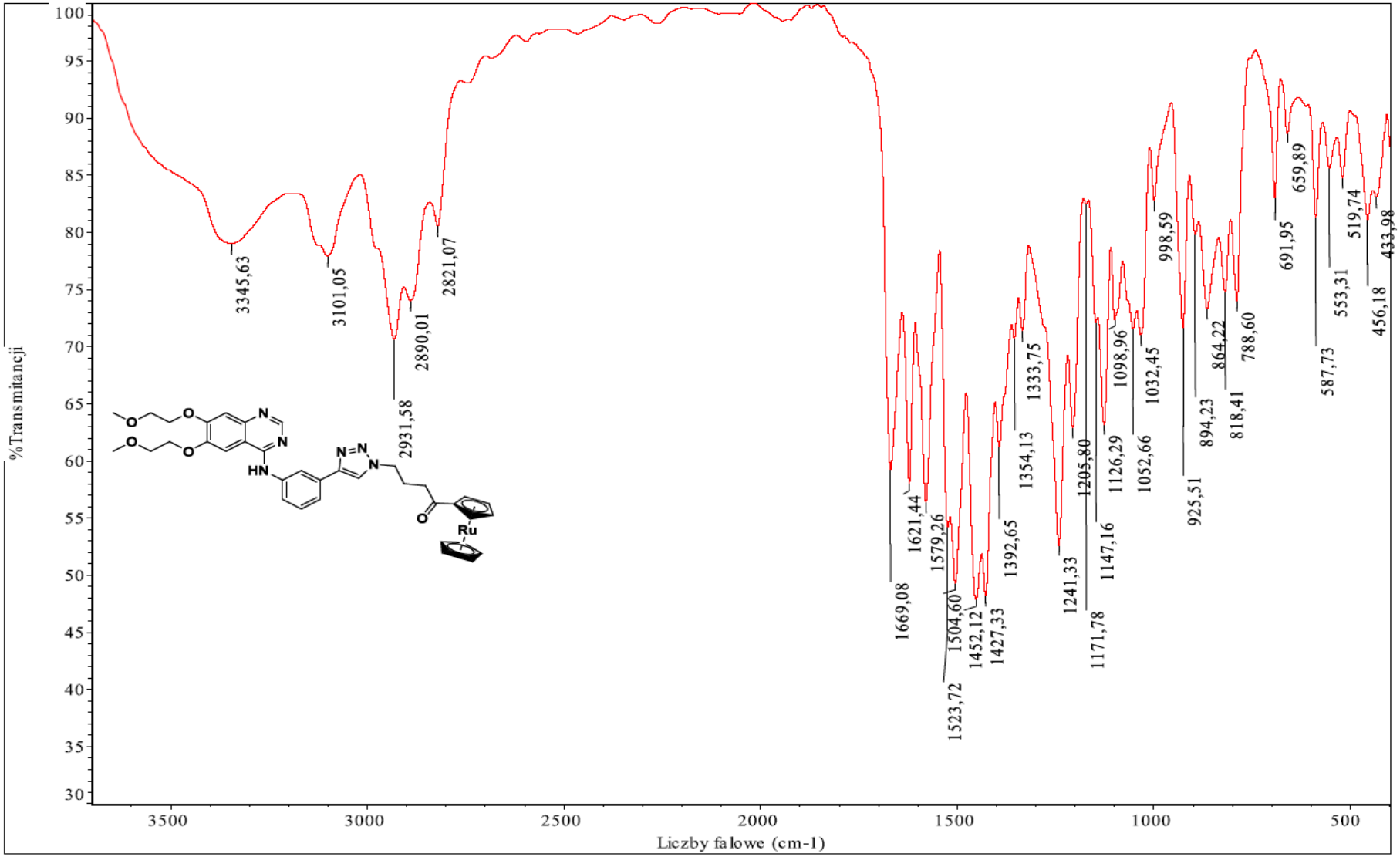


Fig S43 FTIR (KBr ν [cm^{-1}]) spectrum of **5**

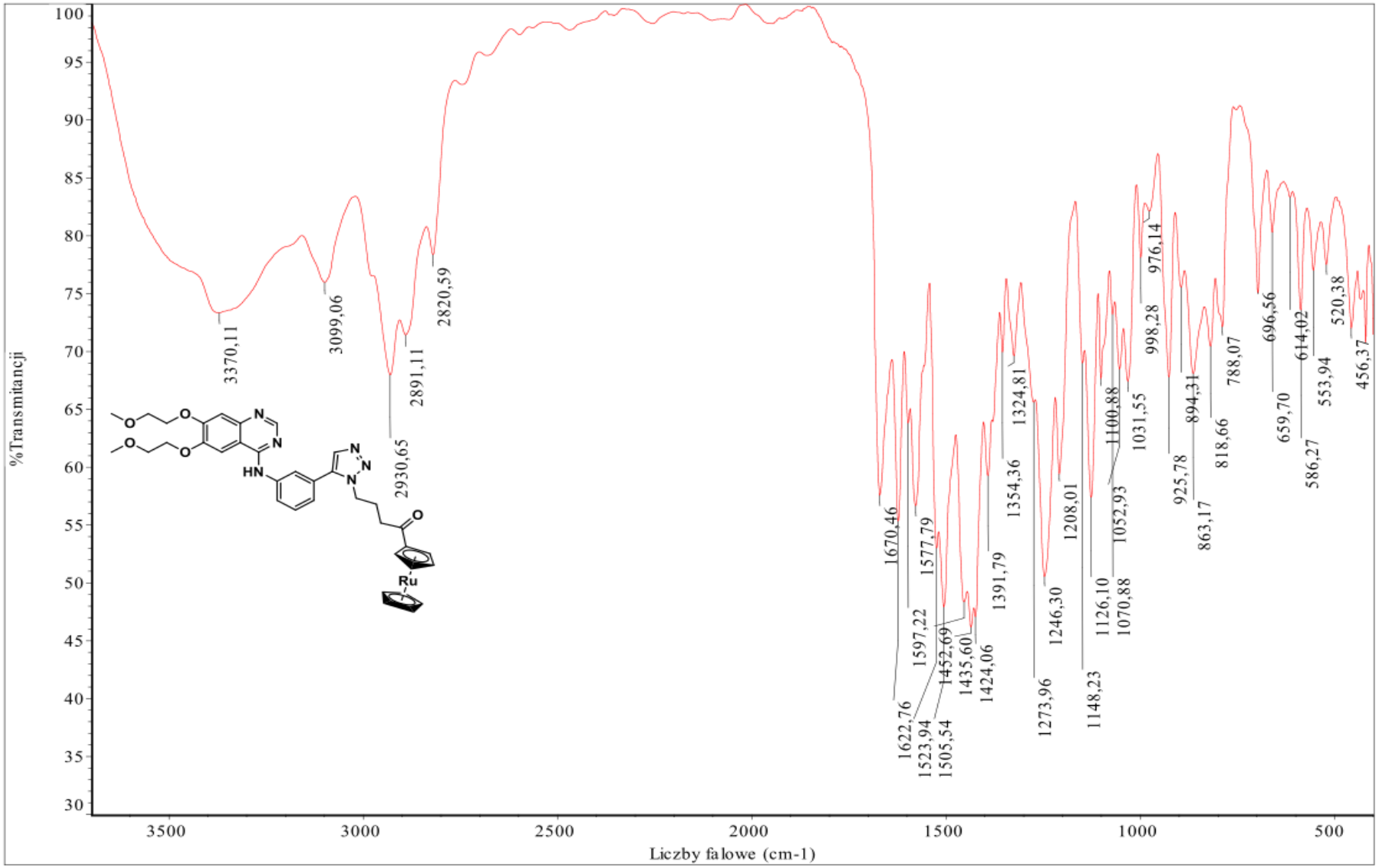


Fig S44 FTIR (KBr ν [cm^{-1}]) spectrum of **6**

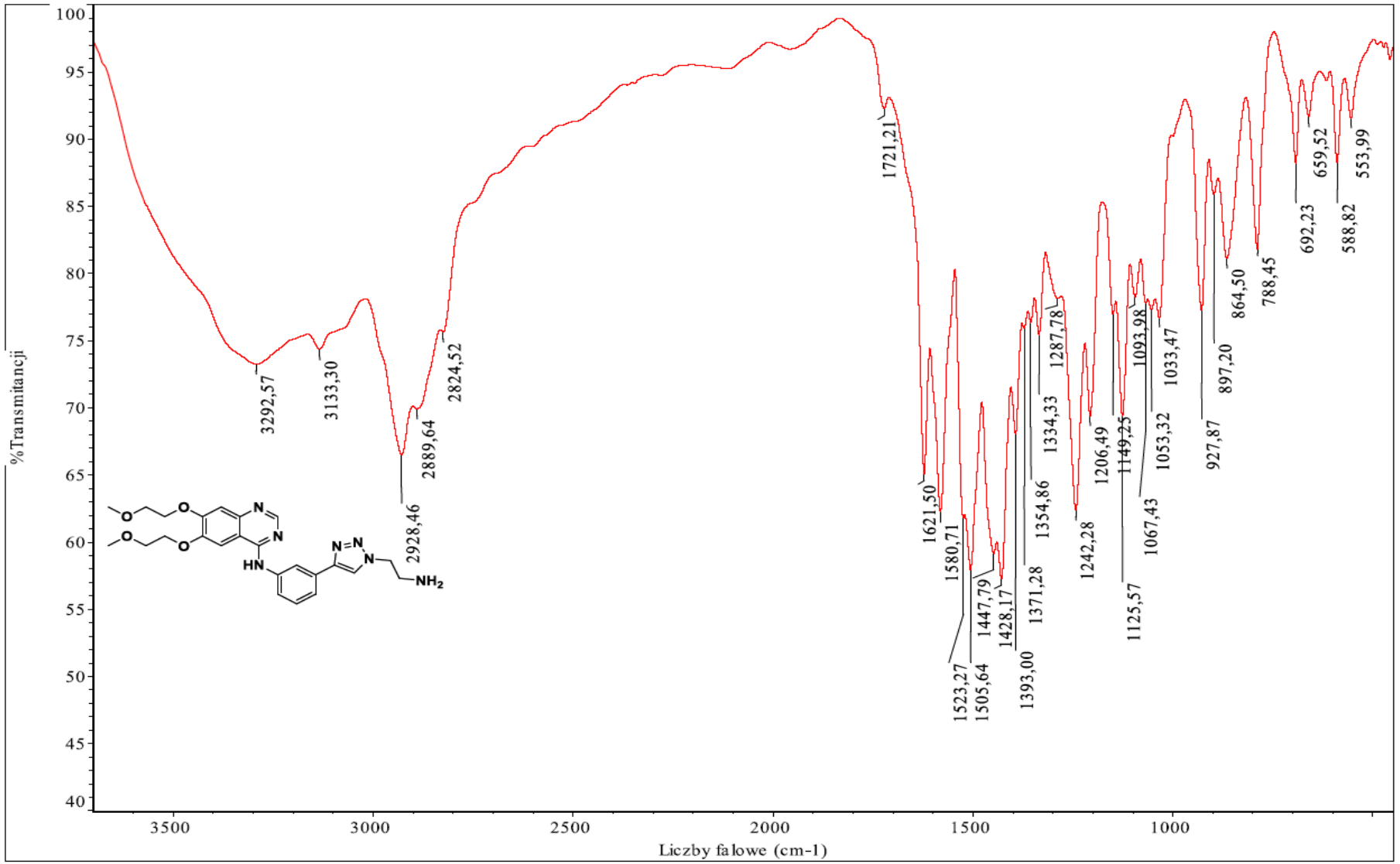


Fig S45 FTIR (KBr ν [cm^{-1}]) spectrum of **7**

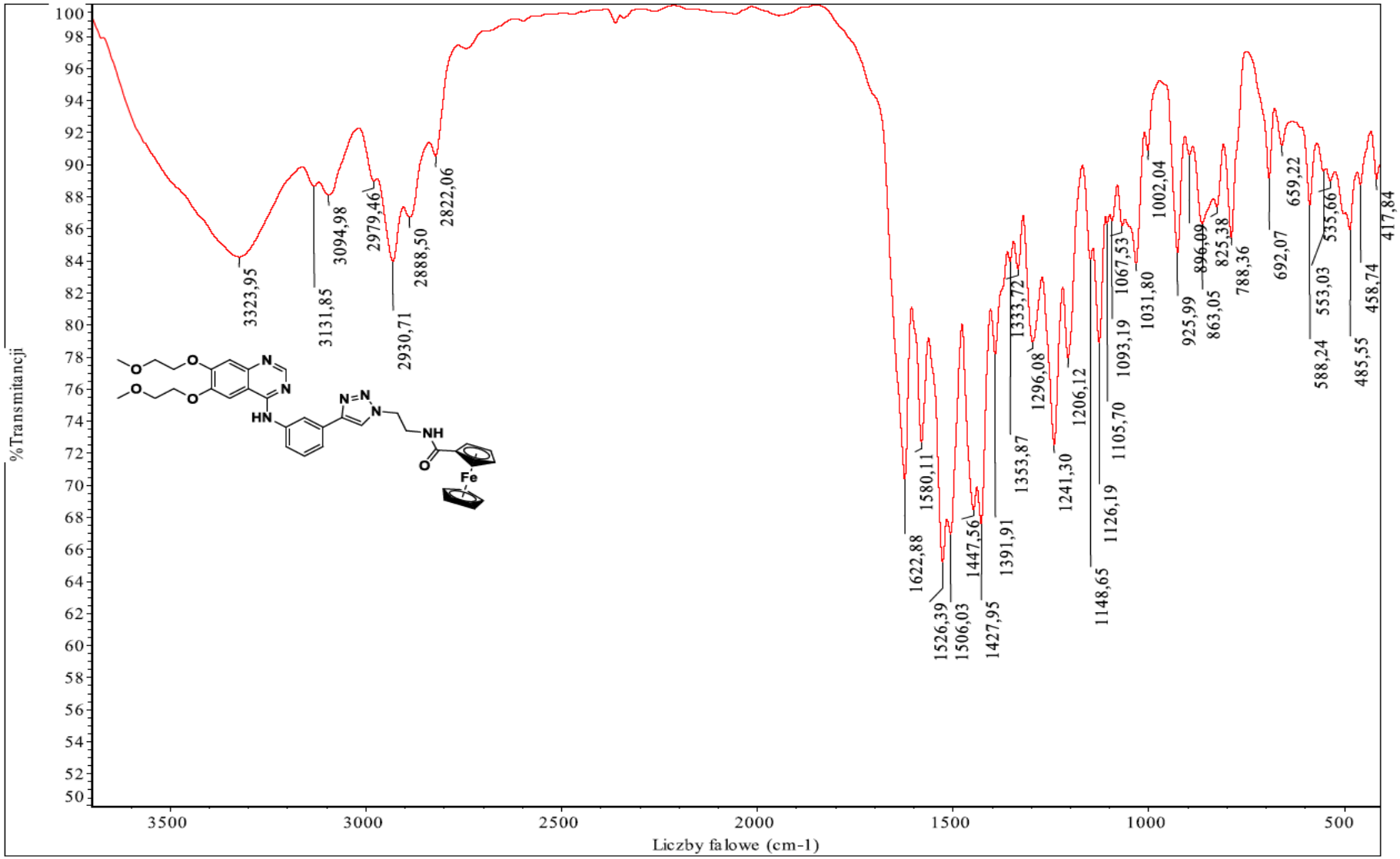


Fig S46 FTIR (KBr ν [cm^{-1}]) spectrum of **8**

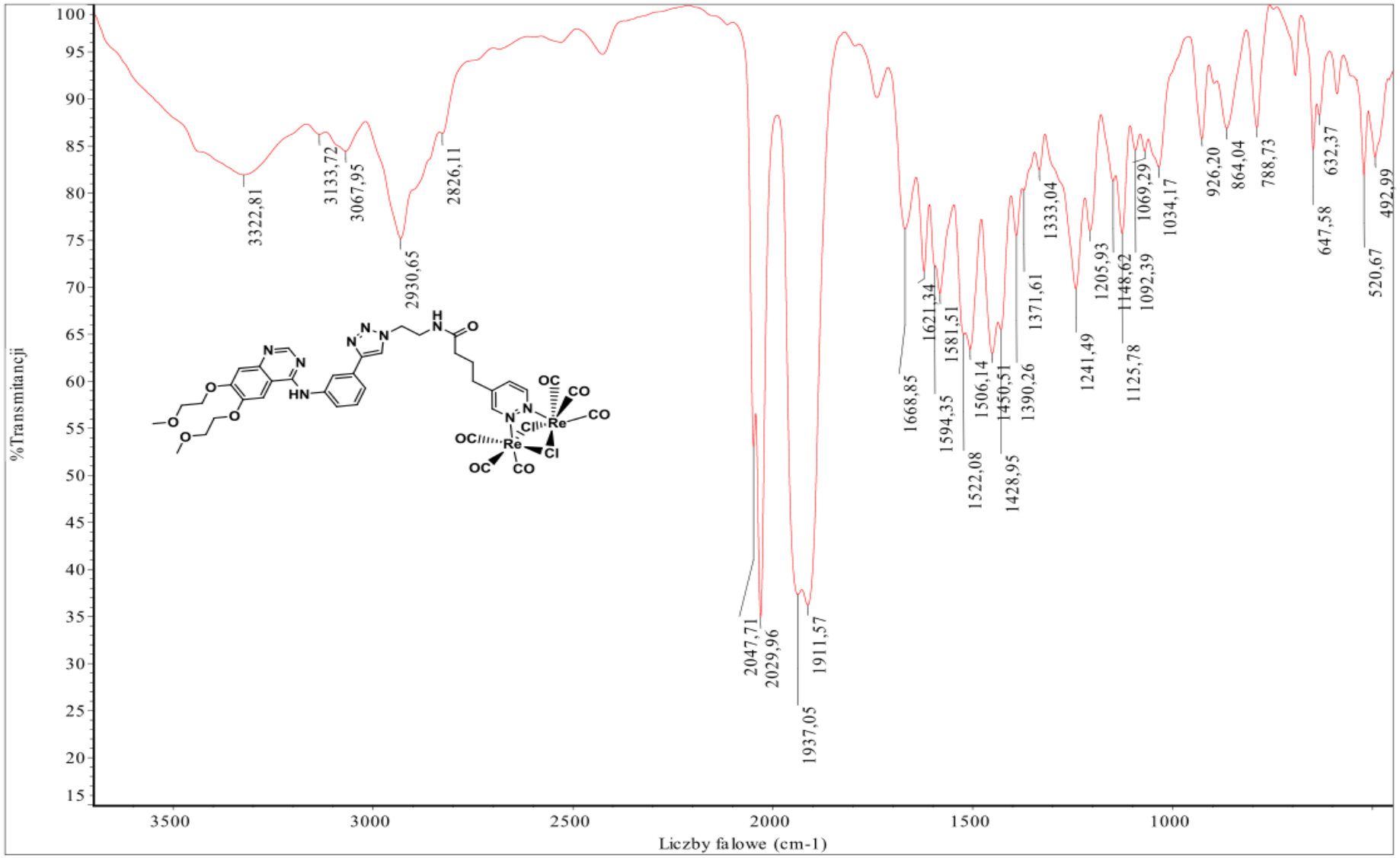


Fig S47 FTIR (KBr ν [cm^{-1}]) spectrum of **9**

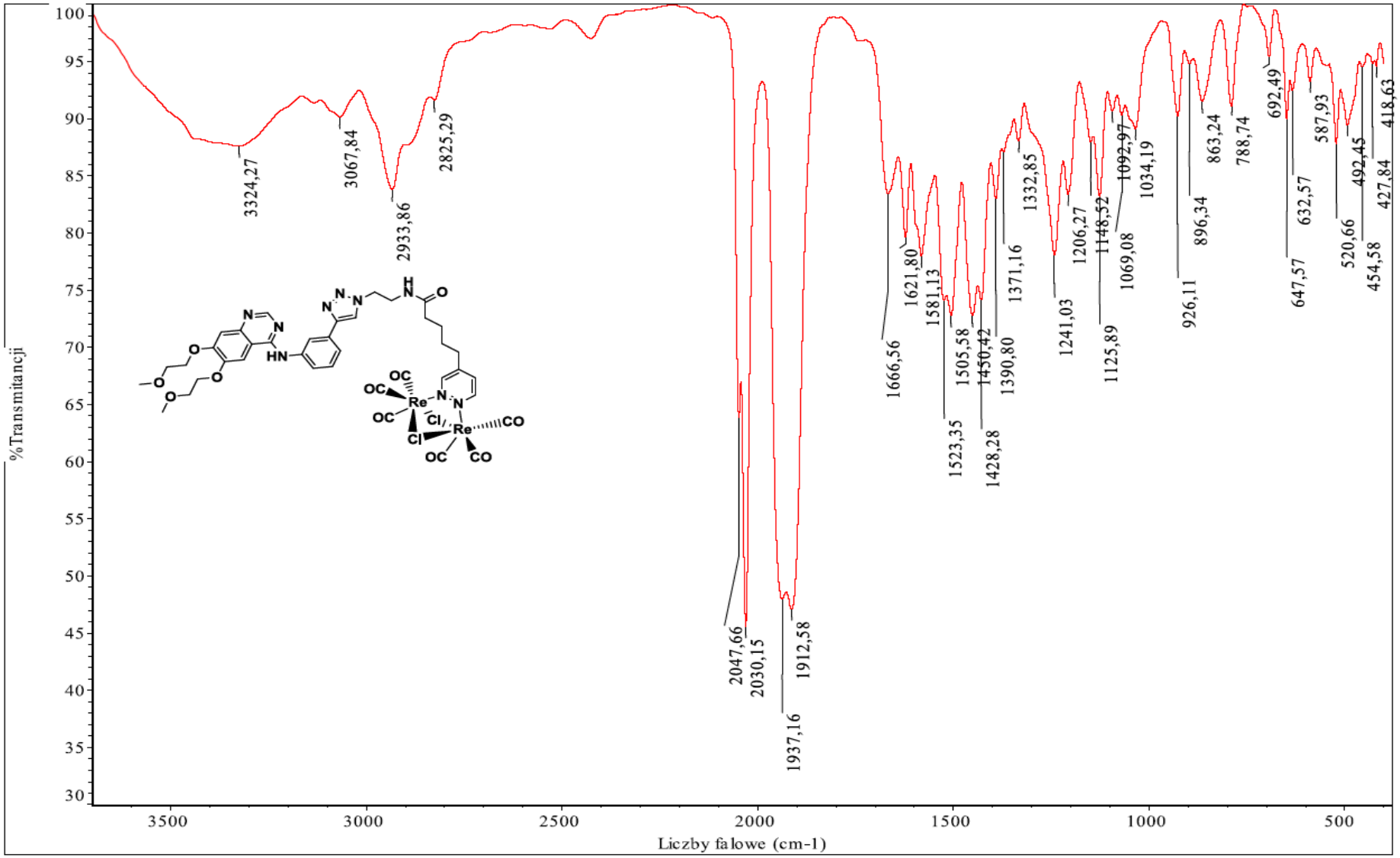


Fig S48 FTIR (KBr ν [cm^{-1}]) spectrum of **10**

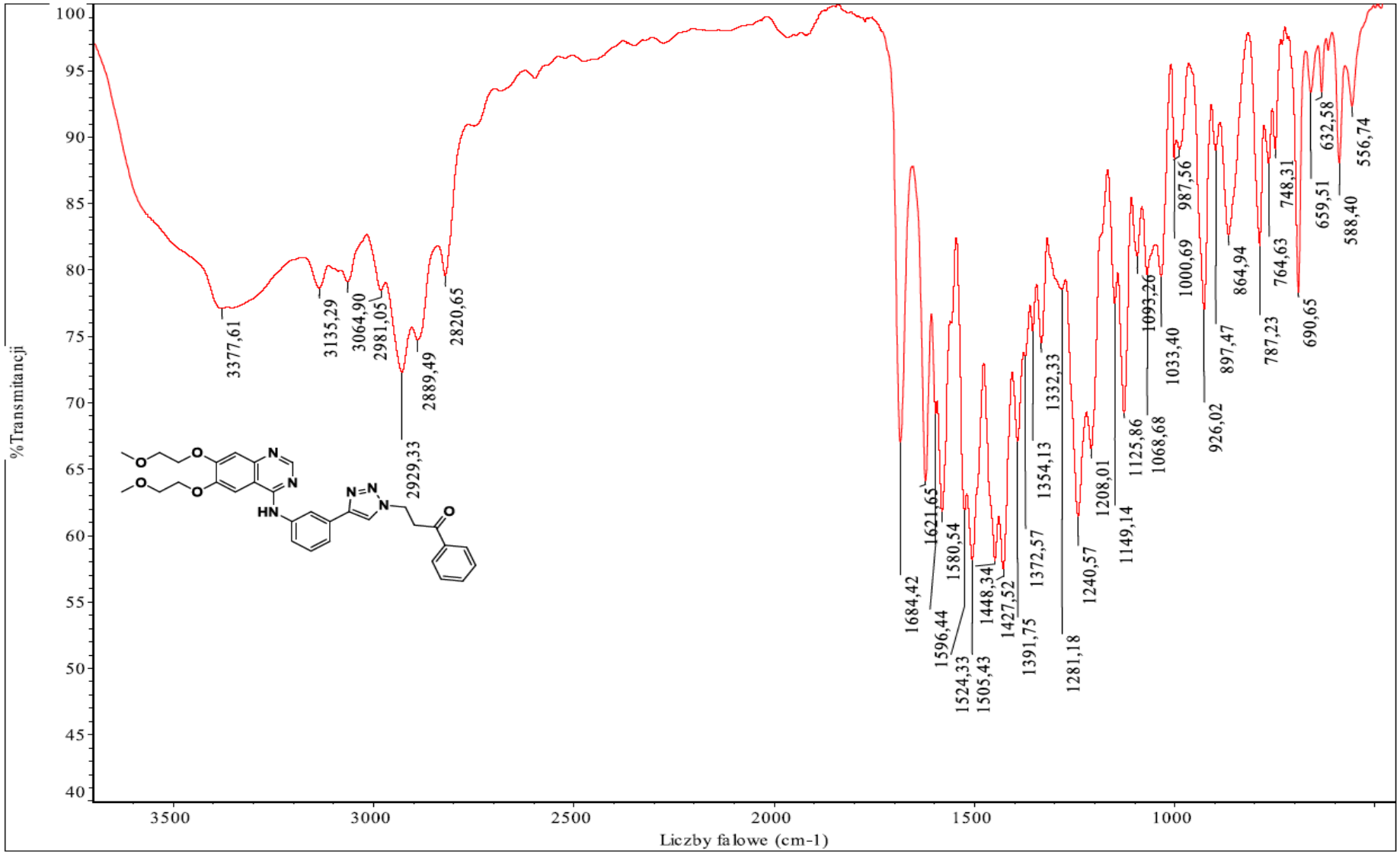


Fig S49 FTIR (KBr ν [cm^{-1}]) spectrum of **11**

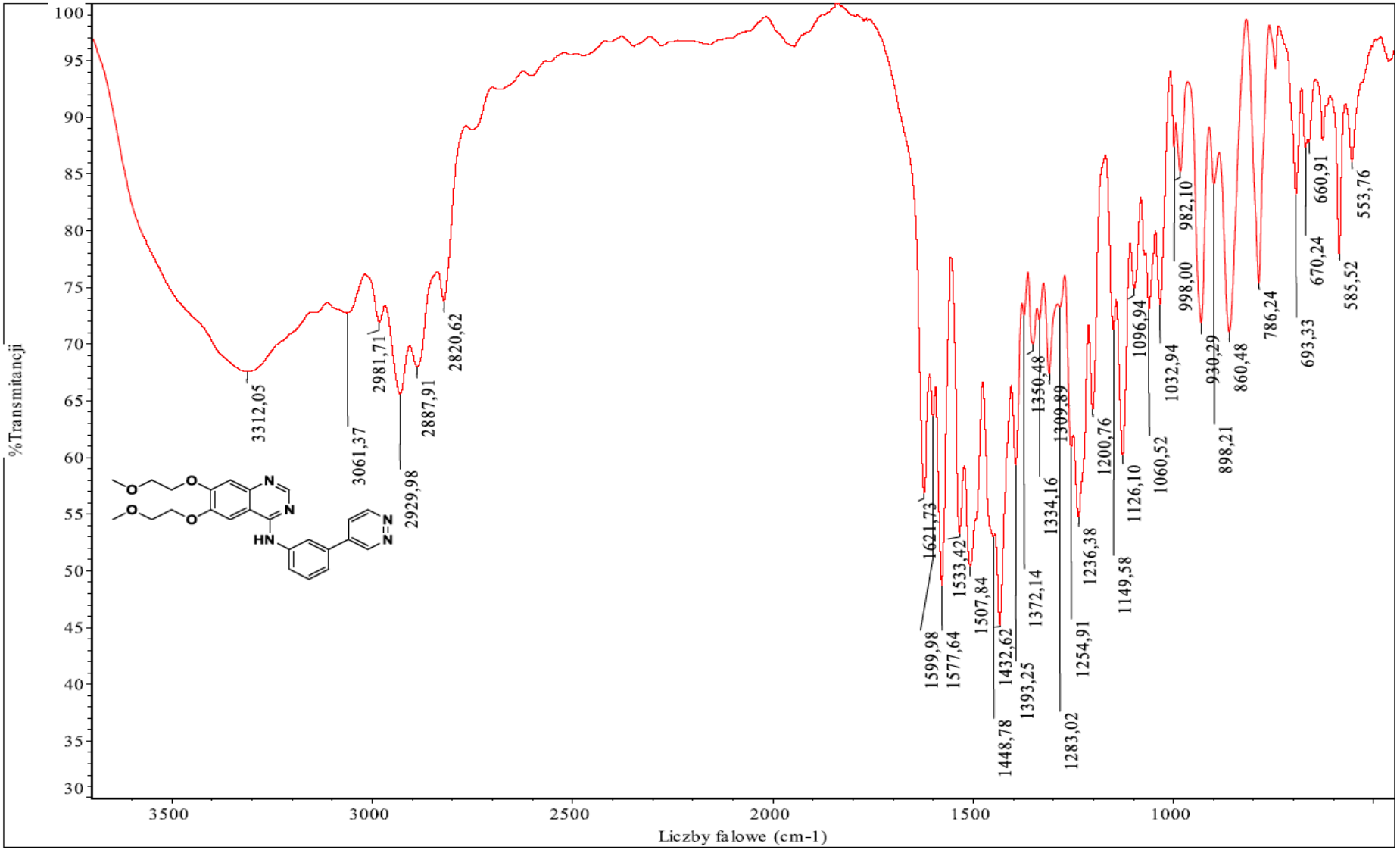


Fig S50 FTIR (KBr ν [cm^{-1}]) spectrum of **12**

Table 1. Elemental analysis result of **1**

$C_{14}H_{15}OClRu$	Theoretical value [%]	Sample [%]
C	50.08	50.03
H	4.50	4.68

Table 2. Elemental analysis result of **2**

$C_{14}H_{15}N_3ORu$	Theoretical value [%]	Sample [%]
C	49.12	49.13
H	4.42	4.24
N	12.27	12.06

Table 3. Elemental analysis result of **3**

$C_{34}H_{34}N_6O_5Fe$	Theoretical value [%]	Sample [%]
C	61.64	61.64
H	5.17	5.24
N	12.69	12.65

Table 4. Elemental analysis result of **4**

$C_{34}H_{34}N_6O_5Fe$	Theoretical value [%]	Sample [%]
C	61.64	61.45
H	5.17	5.12
N	12.69	12.50

Table 5. Elemental analysis result of **5**

$C_{36}H_{38}N_6O_5Ru$	Theoretical value [%]	Sample [%]
C	58.76	58.53
H	5.21	5.13
N	11.42	11.27

Table 6. Elemental analysis result of **6**

$C_{36}H_{38}N_6O_5Ru$	Theoretical value [%]	Sample [%]
C	58.76	58.71
H	5.21	5.11
N	11.42	11.40

Table 7. Elemental analysis result of **8**

$C_{35}H_{37}N_7O_5Fe$	Theoretical value [%]	Sample [%]
C	60.79	60.68
H	5.39	5.25
N	14.18	14.00

Table 8. Elemental analysis result of **9**

$C_{38}H_{37}N_9O_{11}Cl_2Re_2$	Theoretical value [%]	Sample [%]
C	36.84	36.77
H	3.01	3.11
N	10.17	10.02

Table 9. Elemental analysis result of **10**

$C_{39}H_{39}N_9O_{11}Cl_2Re_2$	Theoretical value [%]	Sample [%]
C	37.38	37.40
H	3.14	3.09
N	10.06	10.01

Table 10. Elemental analysis result of **11**

$C_{31}H_{32}N_6O_5$	Theoretical value [%]	Sample [%]
C	65.48	65.17
H	5.67	5.42
N	14.78	14.65

Table 11. Elemental analysis result of **12**

$C_{24}H_{25}N_5O_4$	Theoretical value [%]	Sample [%]
C	64.42	62.14
H	5.63	5.91
N	15.65	15.39