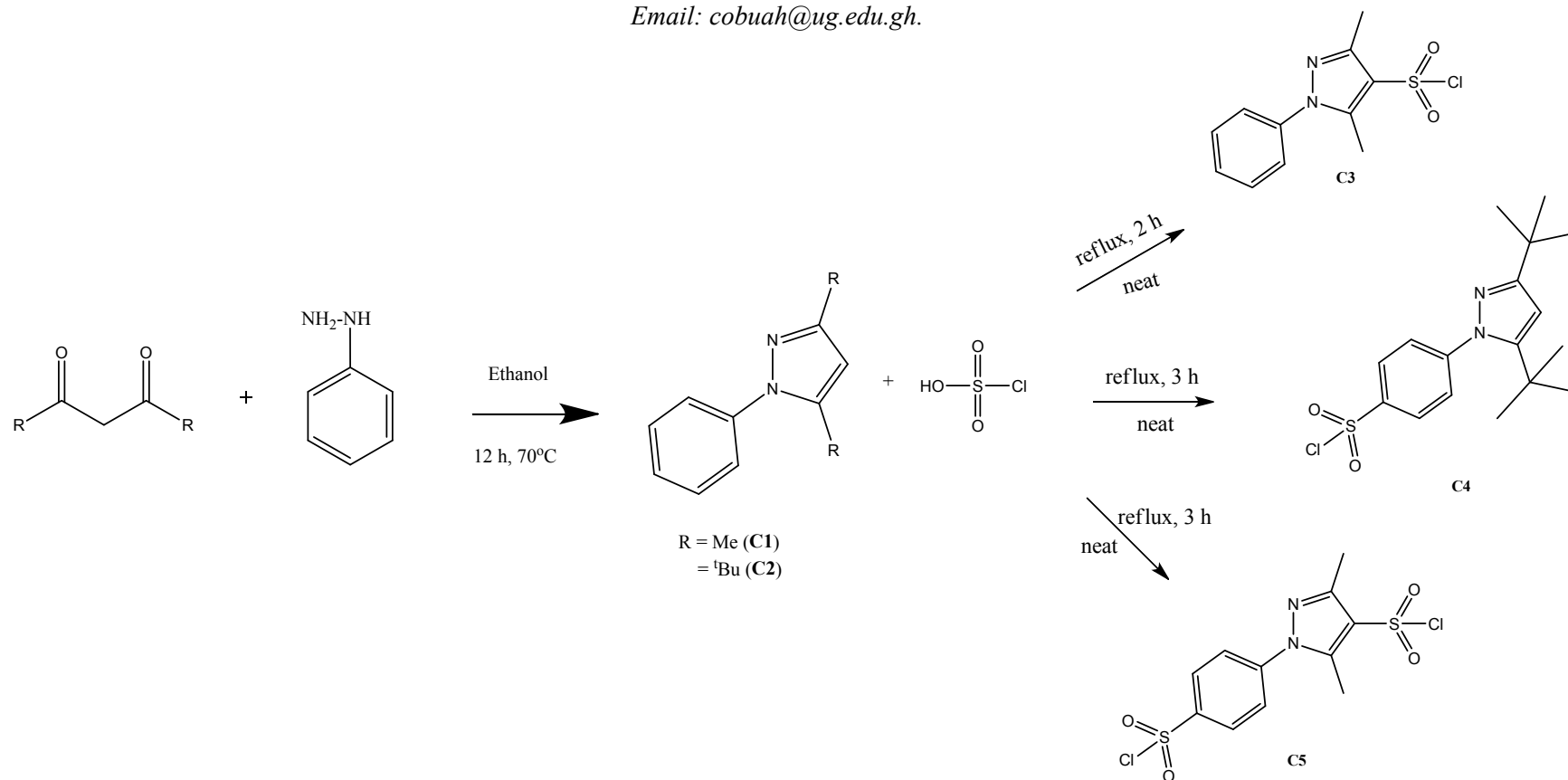


Supplementary information

Synthesis, Characterization and Antibacterial Applications of Pyrazolyl-Sulfonamides and their palladium Complexes

Cephas Amoah,^{a,b} Collins Obuah,^{a,b*} Michael K. Ainooson^{a,b} Christian K. Adokoh,^{c,b} and Alfred Muller^b

^aDepartment of Chemistry, University of Ghana, Legon, ^bDepartment of Chemical Sciences, University of Johannesburg, Auckland Park 2006, Johannesburg, South Africa; ^cDepartment of Forensic Sciences, School of Biological Sciences, University of Cape Coast, Cape Coast, Ghana.
Email: cobuah@ug.edu.gh.



Scheme S1: Synthesis of phenylpyrazolyl and phenylpyrazolyl sulfonyl chloride compounds

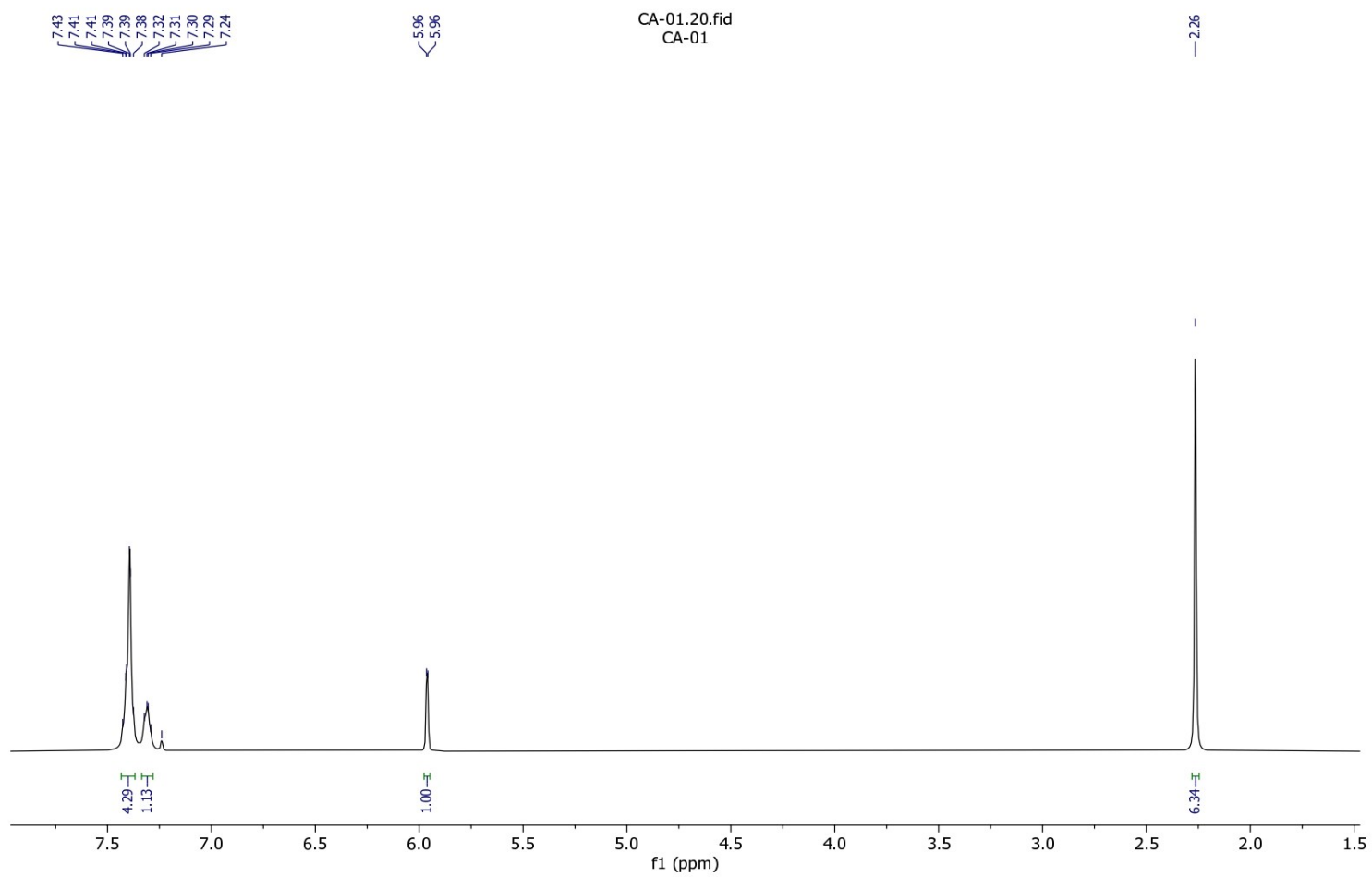


Figure S1 – ^1H -NMR spectrum of **C1**

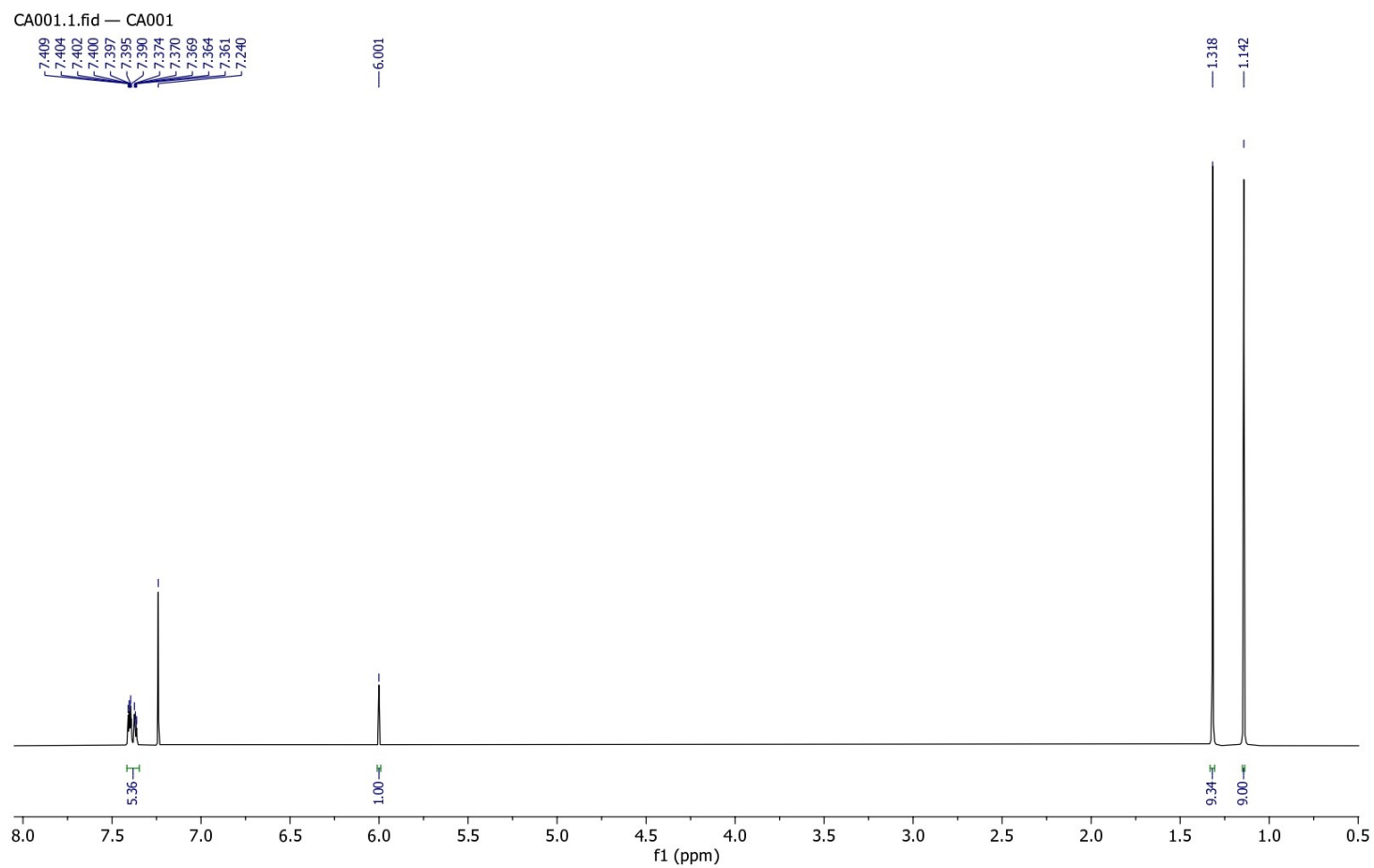


Figure S2 – ^1H -NMR spectrum of **C2**

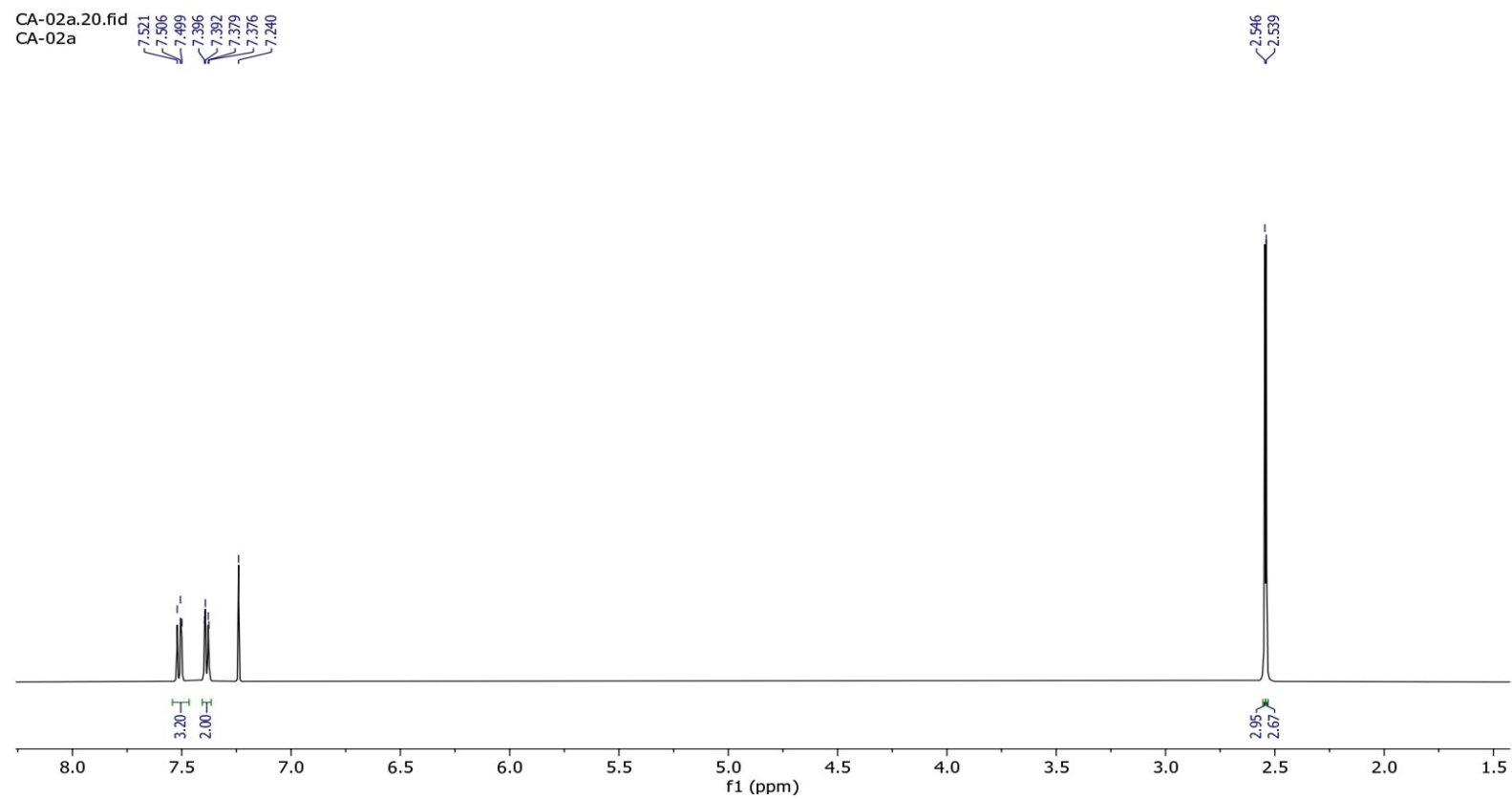


Figure S3 – ^1H -NMR spectrum of **C3**

CA10.1.fid — CA10

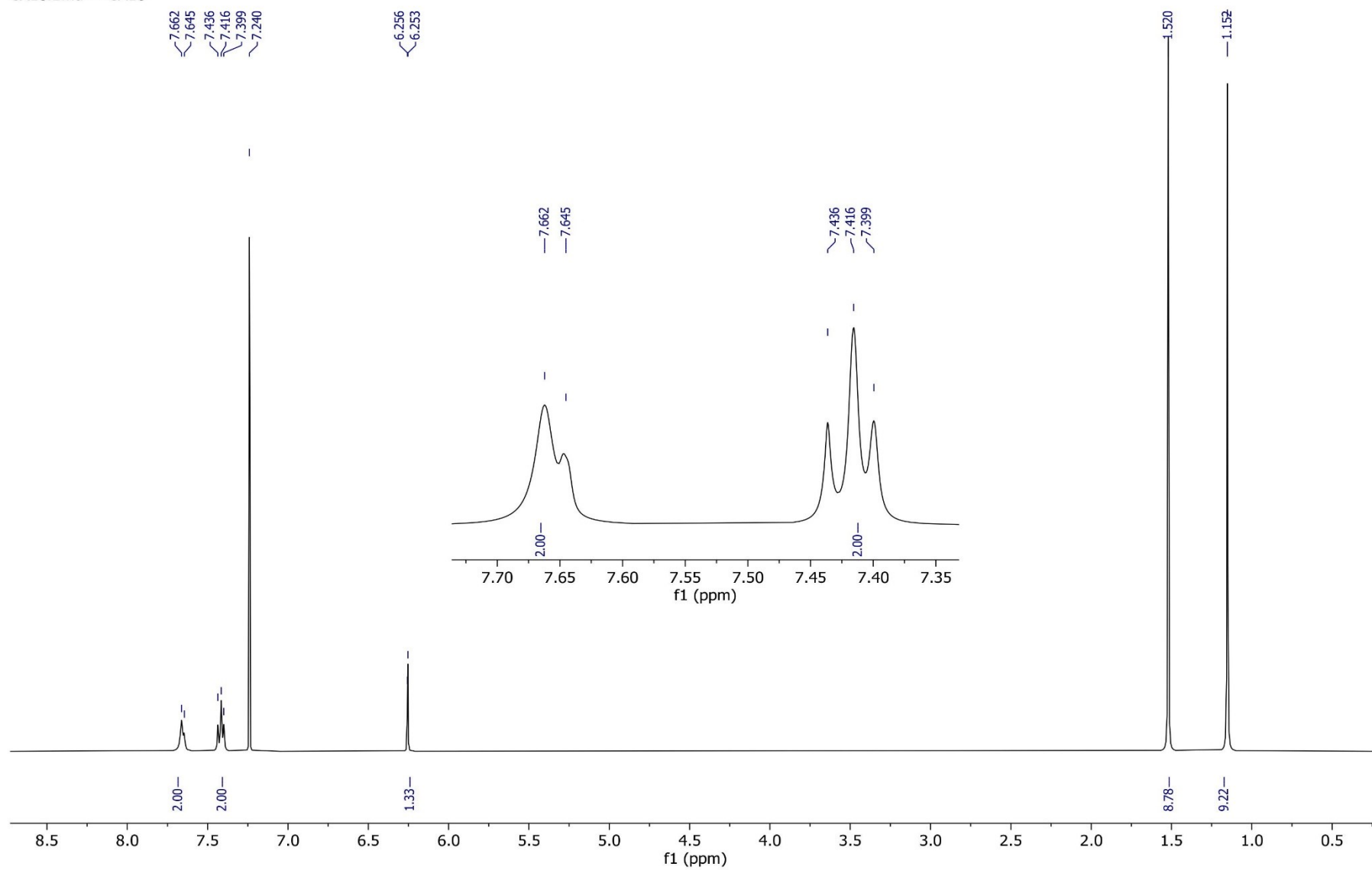


Figure S4 – ^1H -NMR spectrum of **C4**

CA14.20.fid — CA14

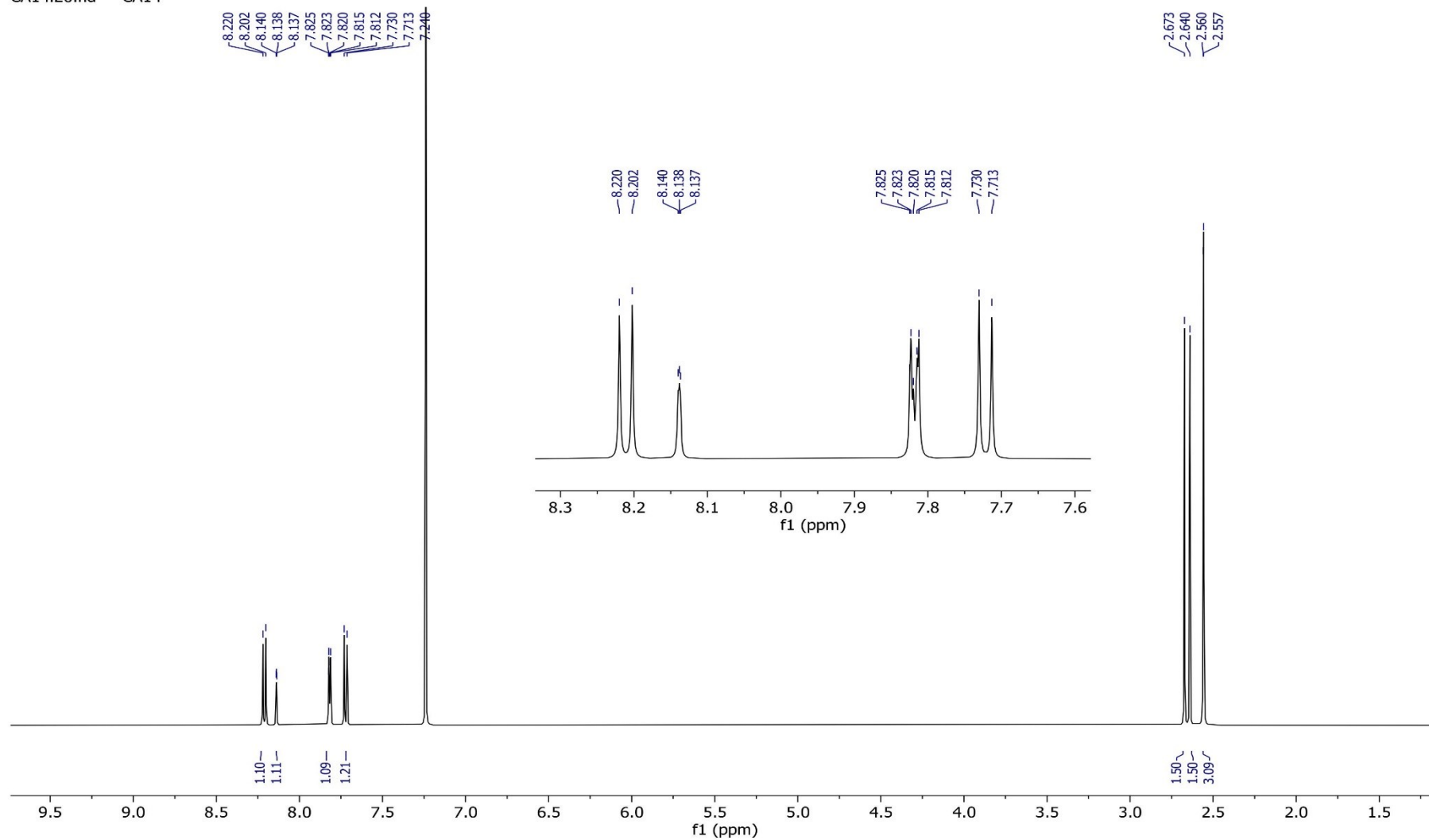


Figure S5 – ^1H -NMR spectrum of C5

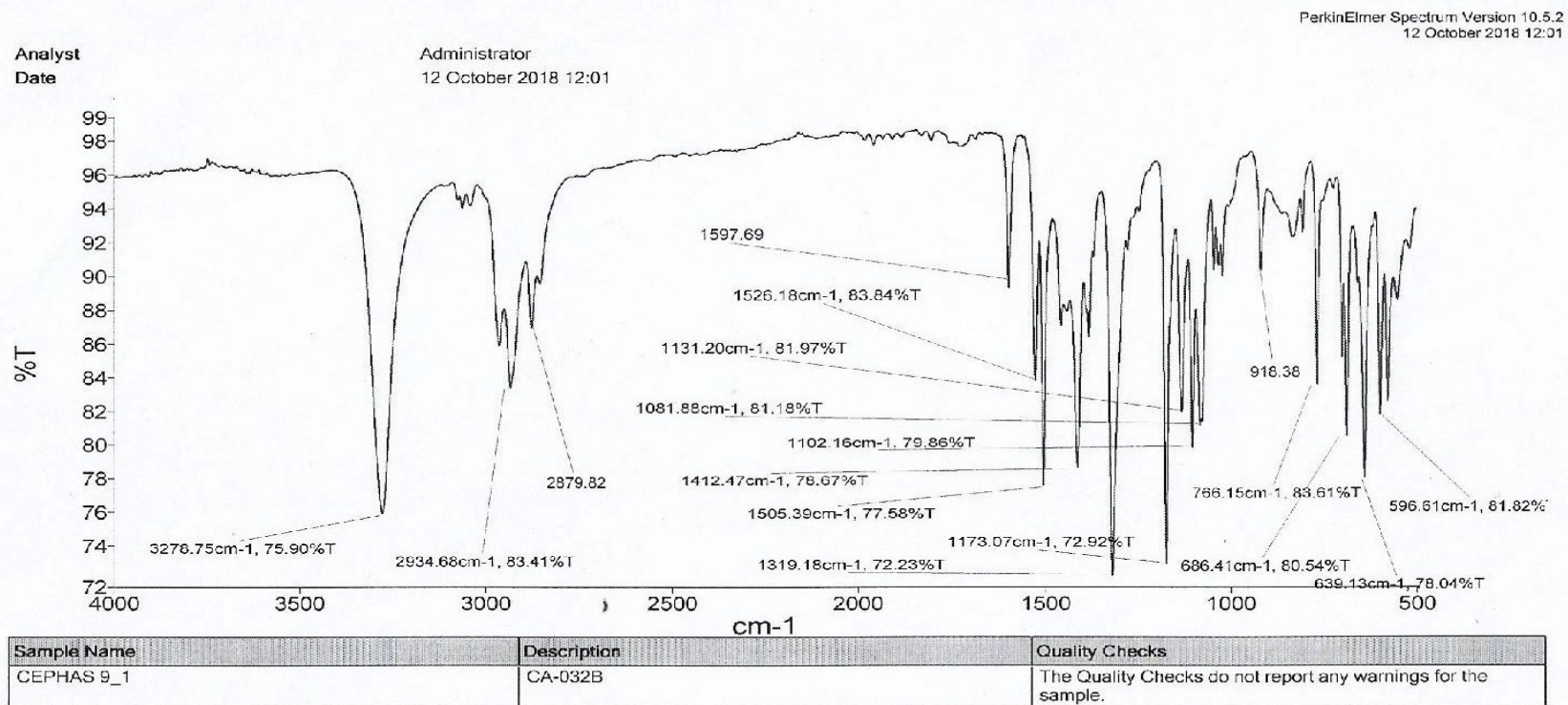


Figure S6-FT-IR of (L2)

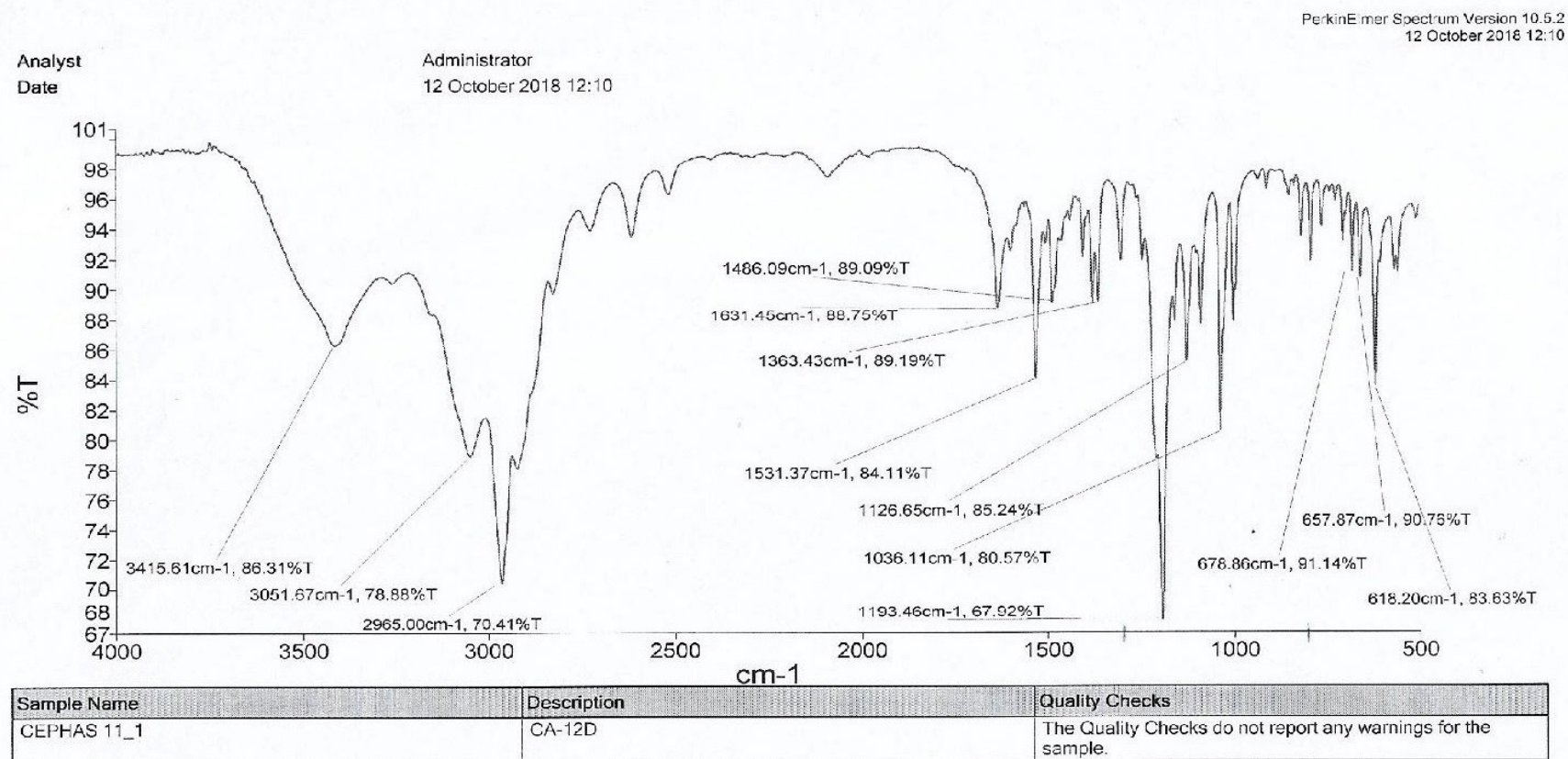


Figure S7-FT-IR of (L3)

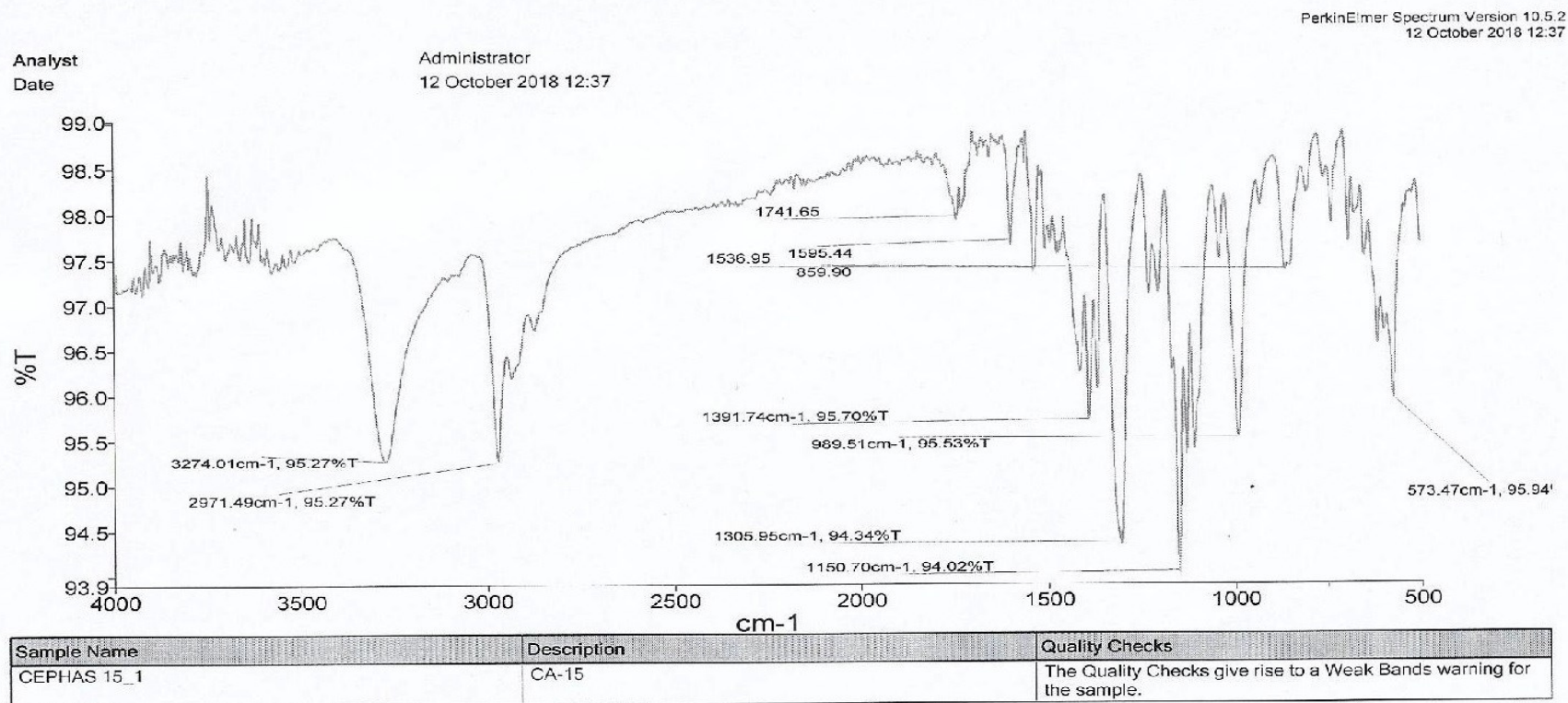


Figure S8-FT-IR of (L 5)

CA032a-1-new.10.fid — CA032a-1-new

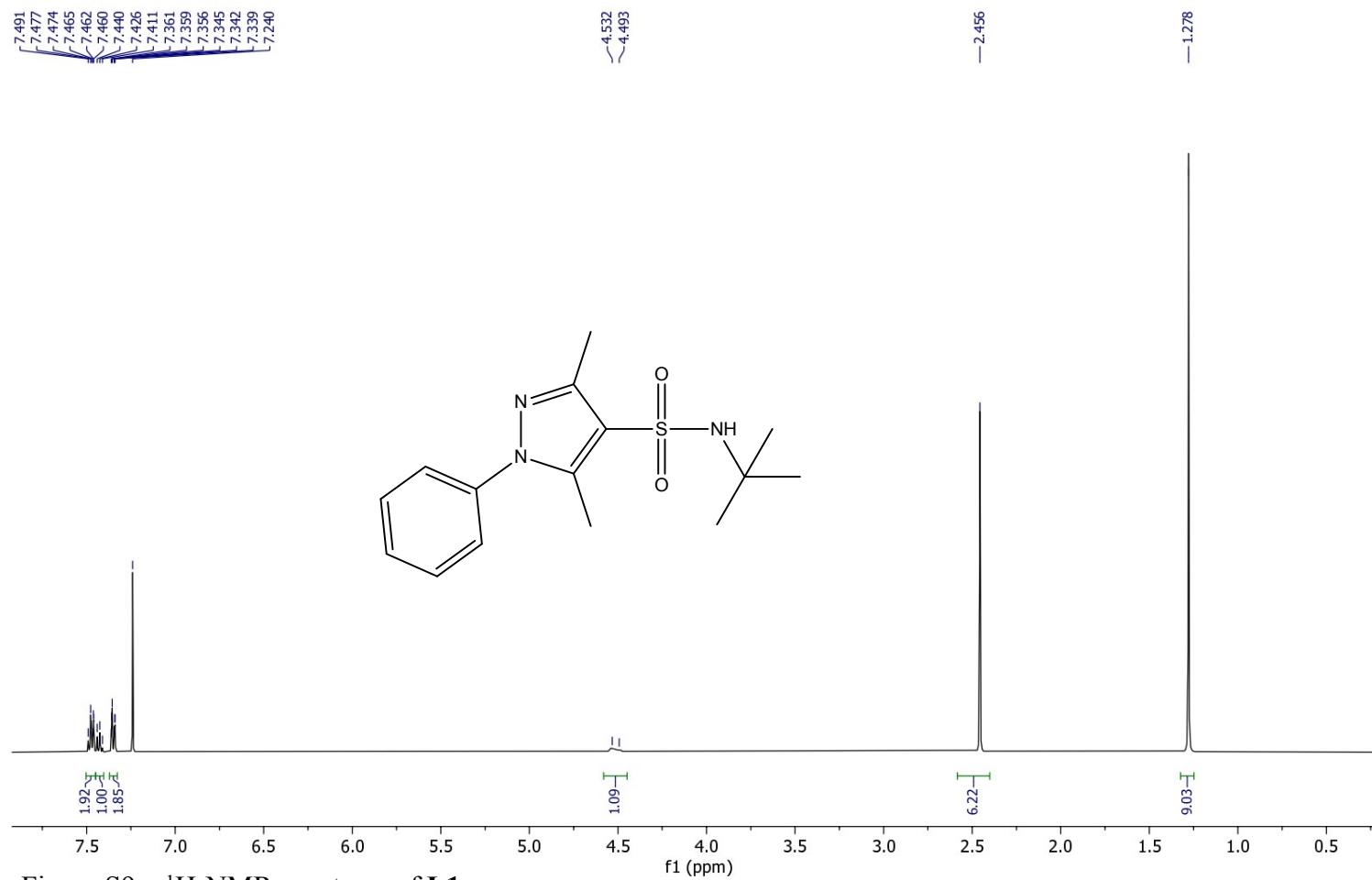


Figure S9 – ¹H-NMR spectrum of **L1**

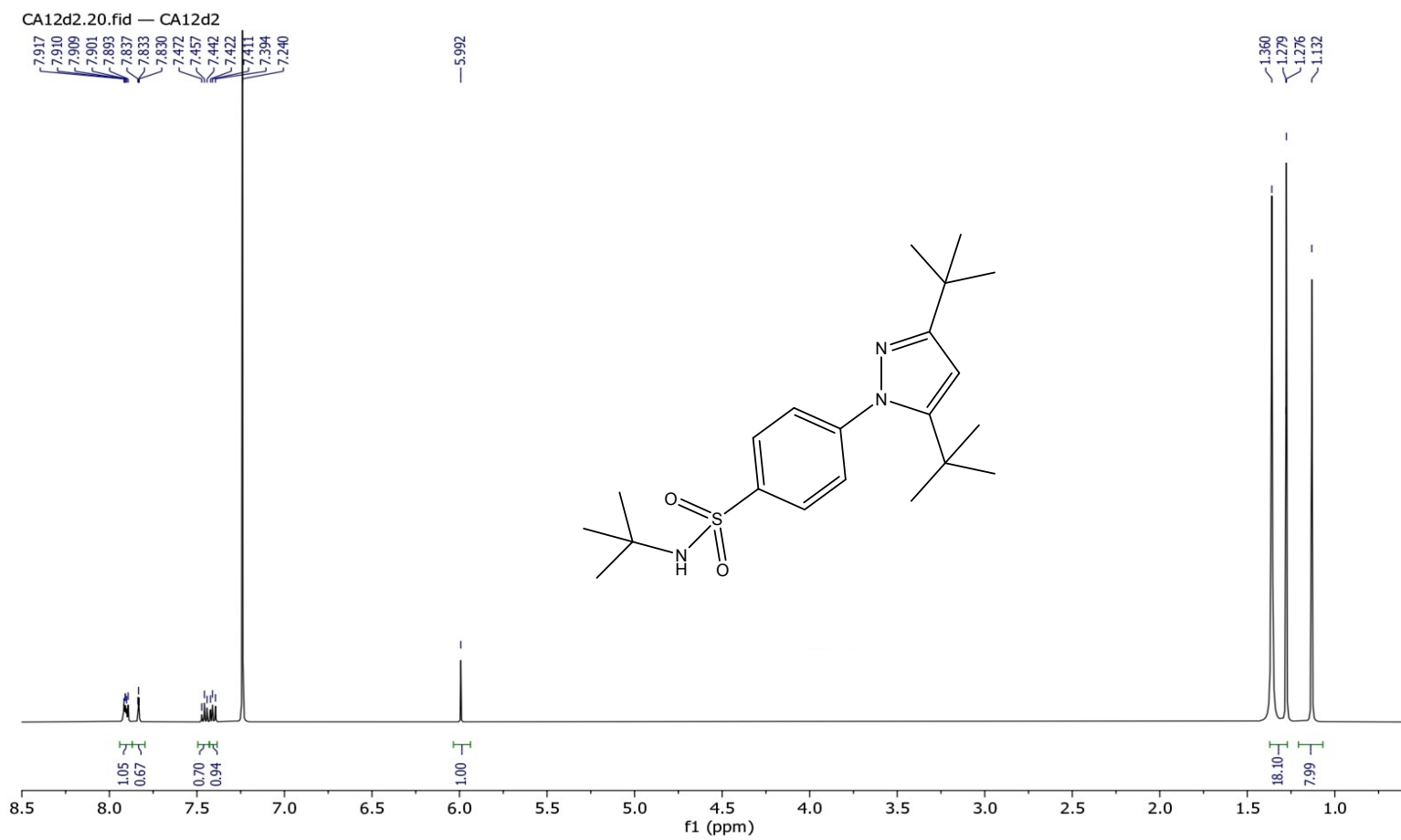


Figure S10 – ^1H -NMR spectrum of **L3**

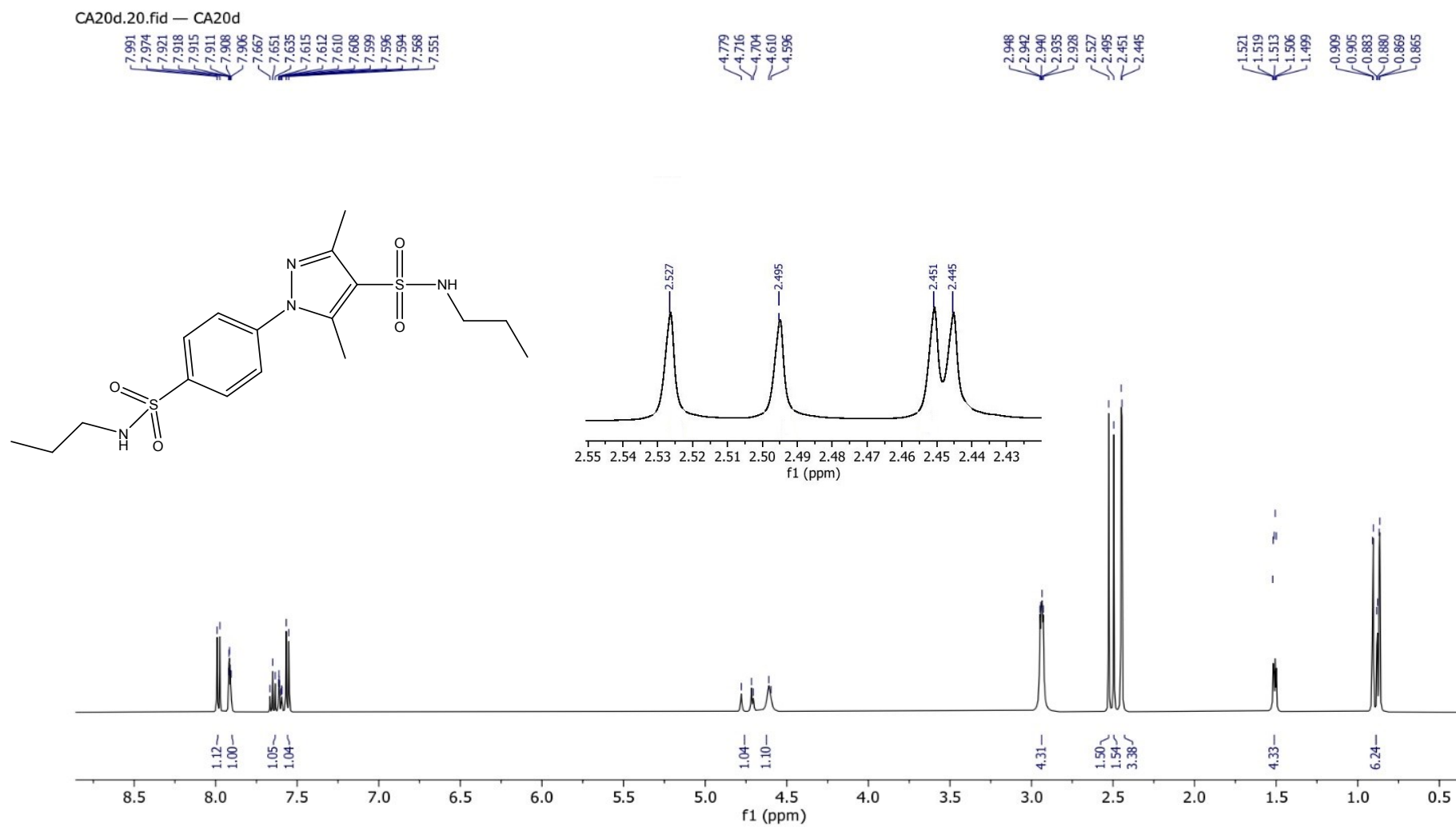


Figure S11 – ^1H -NMR spectrum of L6

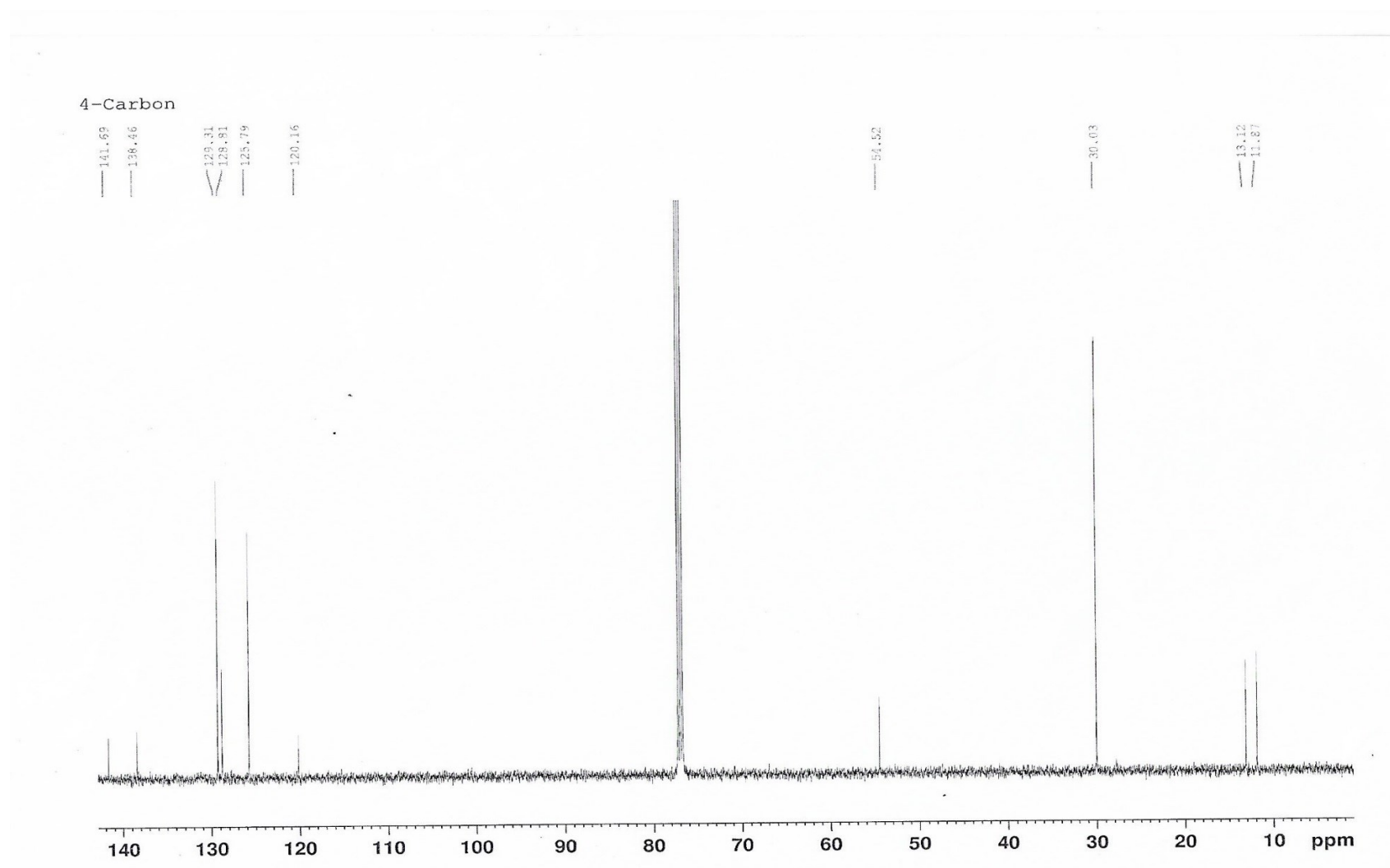


Figure S12 - $^{13}\text{C}\{^1\text{H}\}$ -NMR of **L1**

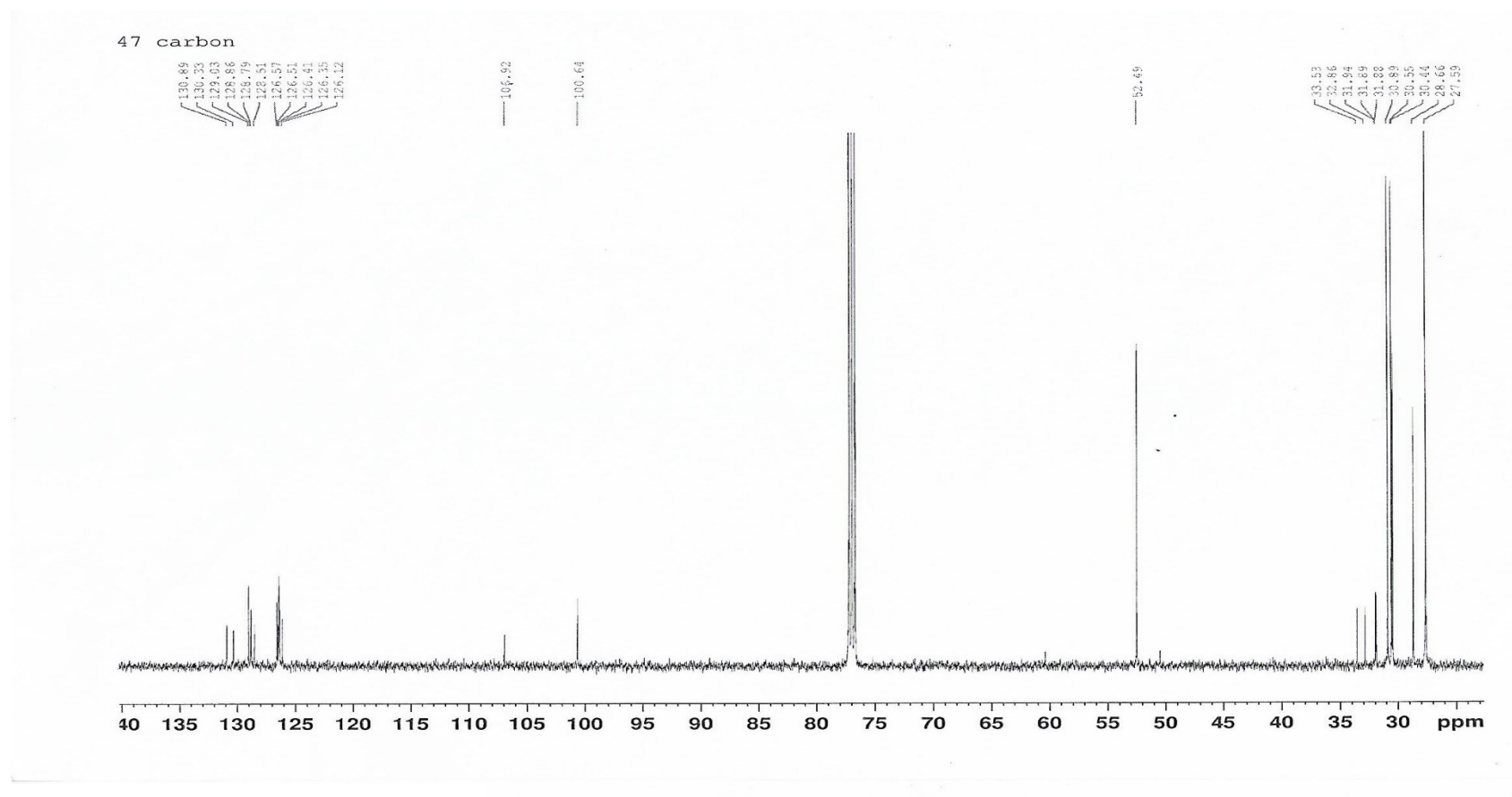


Figure S13 - $^{13}\text{C}\{^1\text{H}\}$ -NMR of **L3**

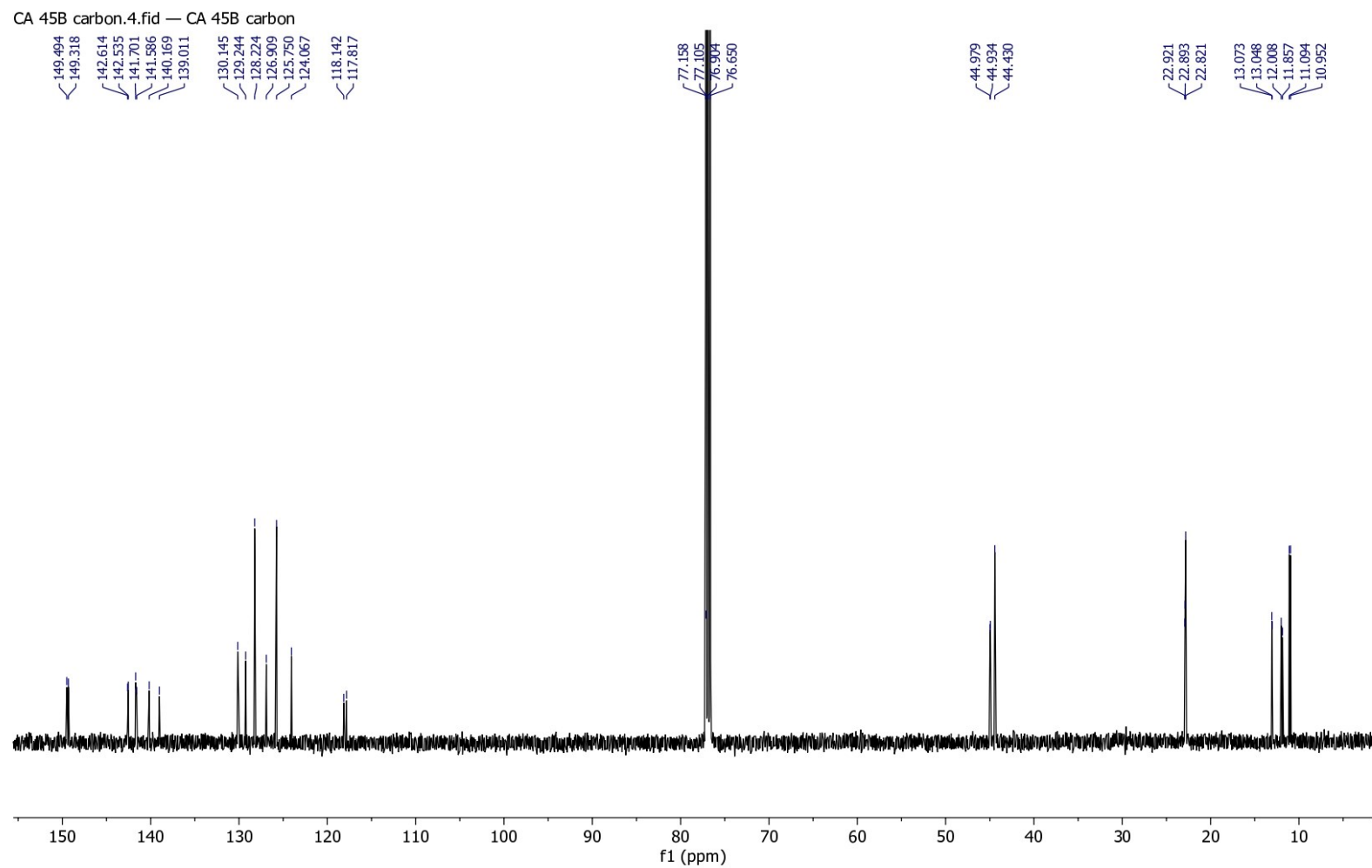


Figure S14 - $^{13}\text{C}\{^1\text{H}\}$ -NMR of **L6**

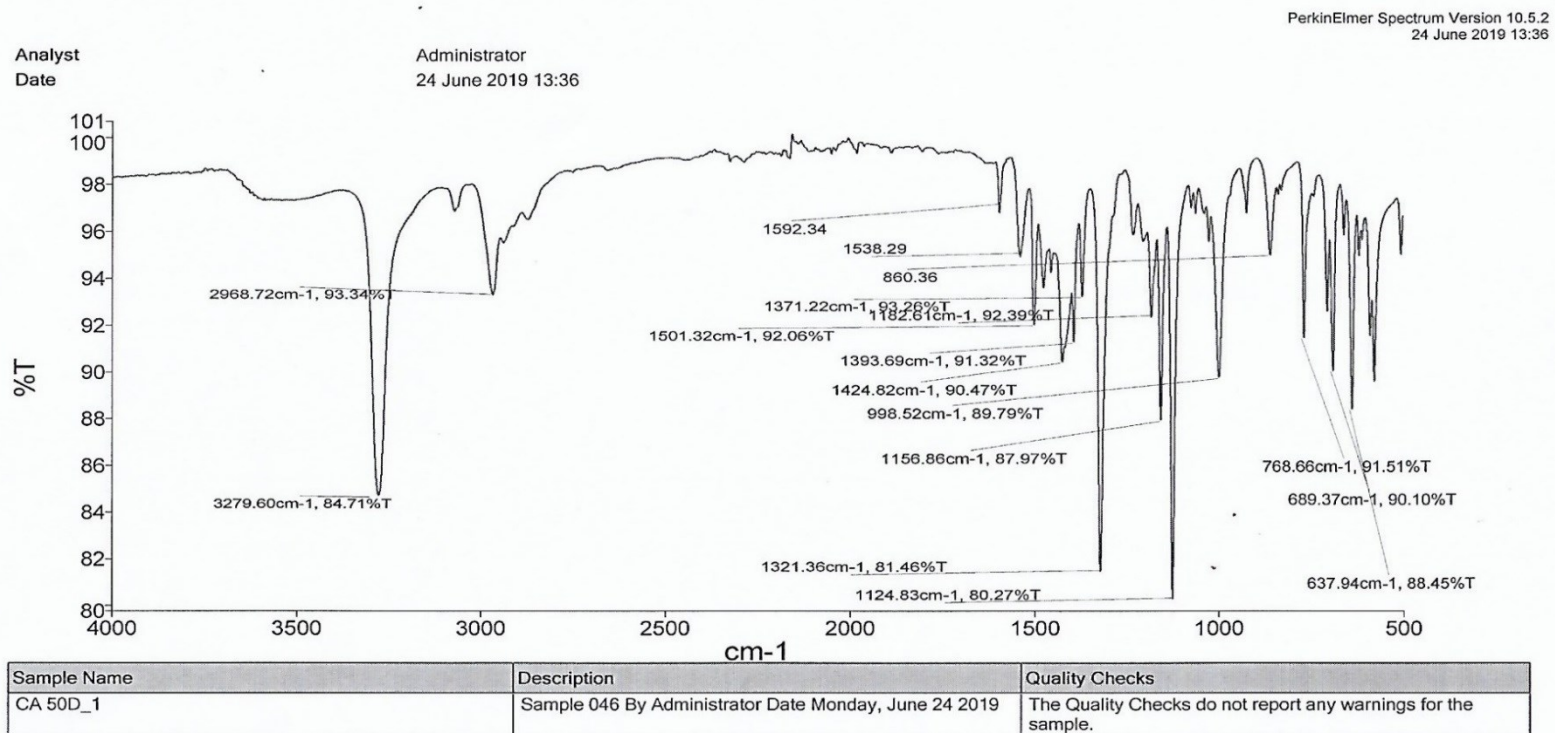


Figure S15-FT-IR of (1)

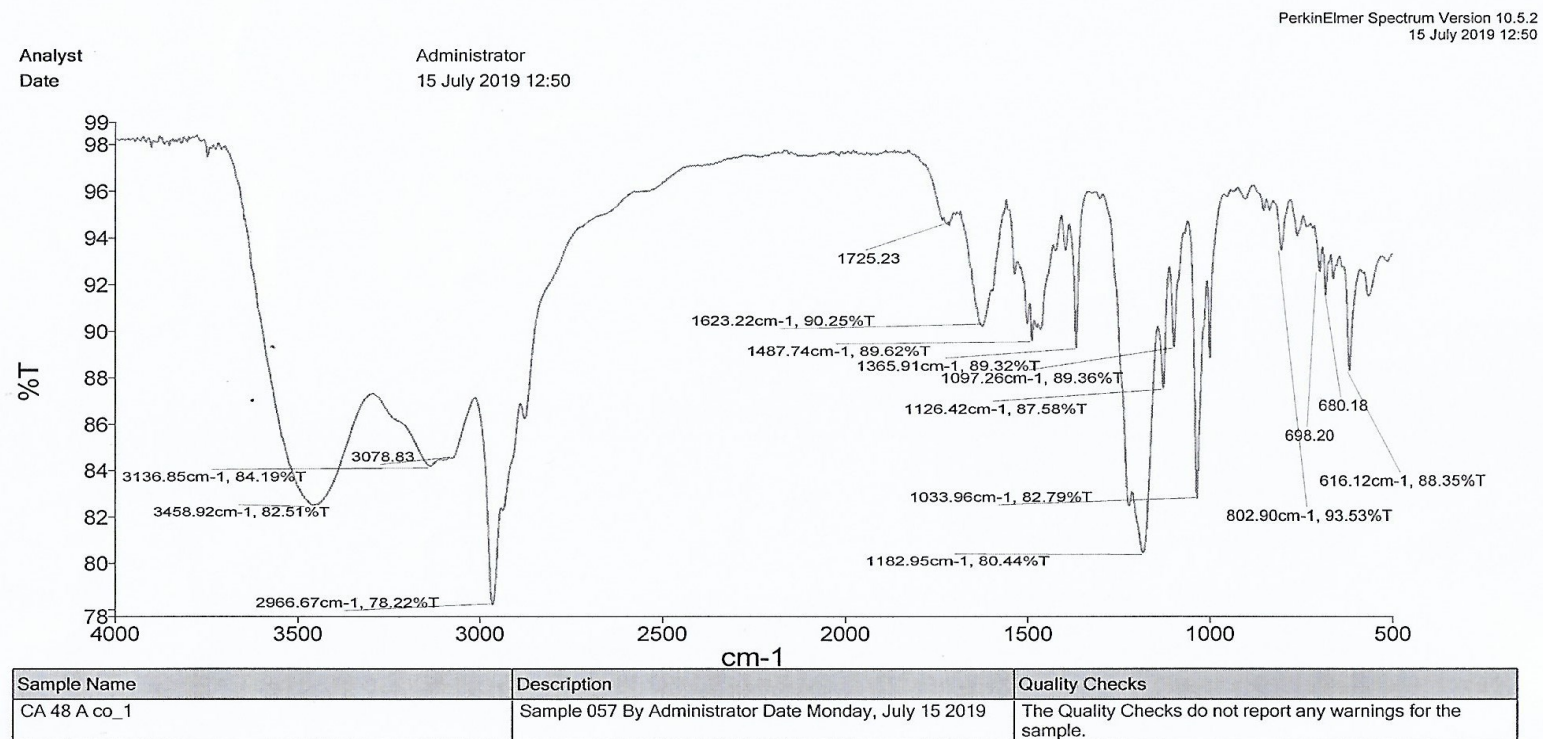


Figure S16-FT-IR of (4)

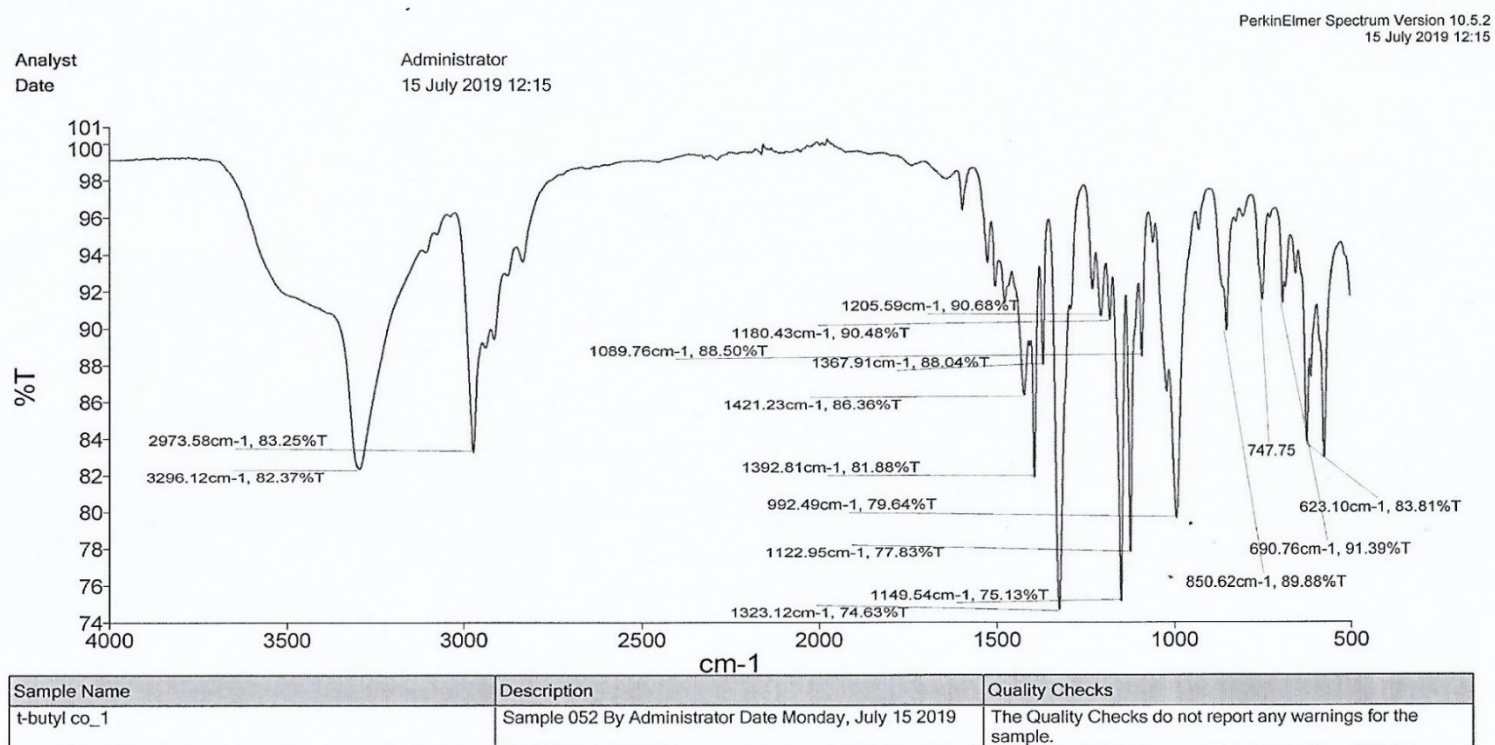


Figure S17-FT-IR of (5)

CA 50D new.5.fid — CA 50D new

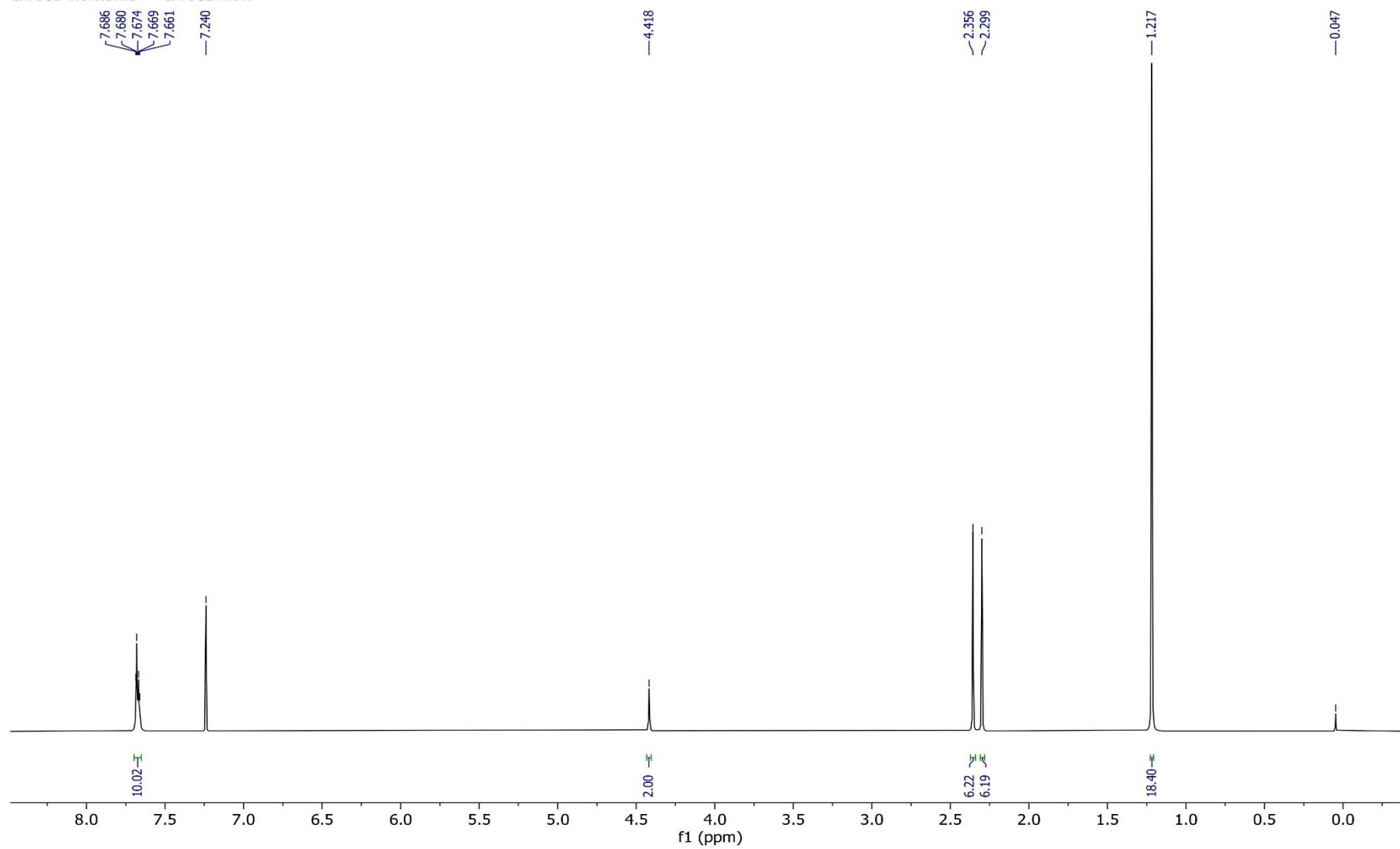


Figure S18 – ^1H -NMR spectrum of (1)

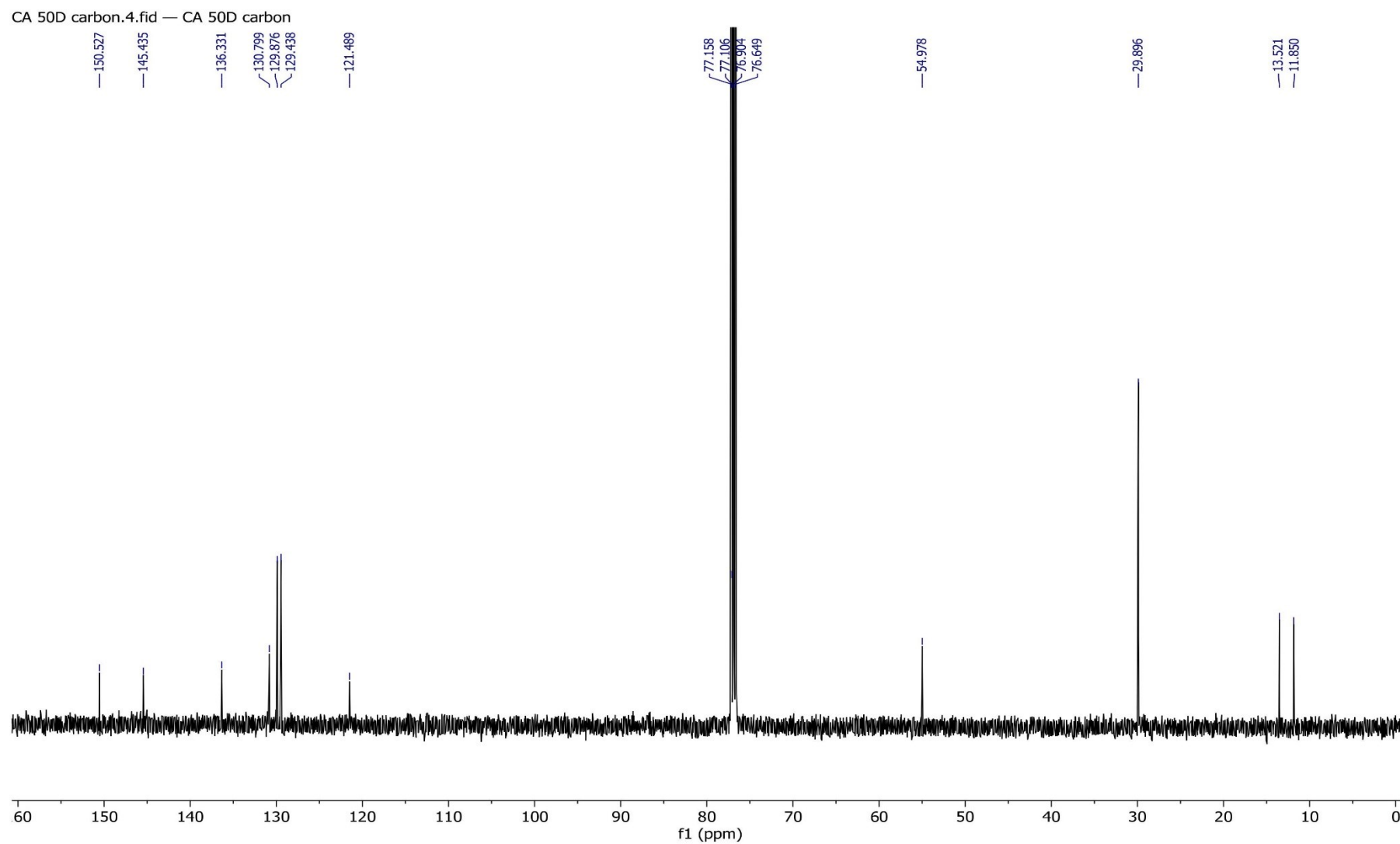


Figure S19 - $^{13}\text{C}\{^1\text{H}\}$ -NMR of **(1)**

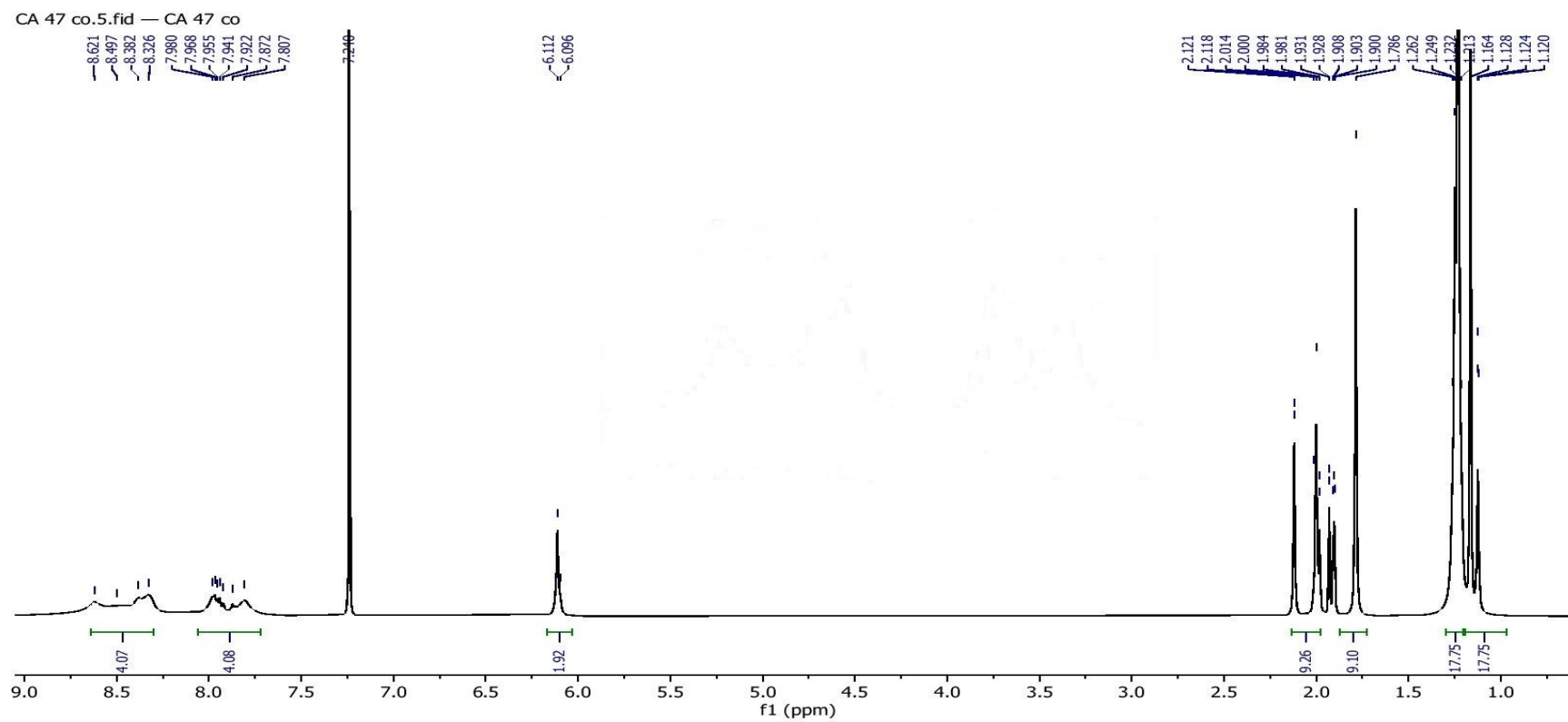


Figure S20 – ¹H-NMR spectrum of (3)

CA 47 aa carbon.4.fid — CA 47 aa carbon

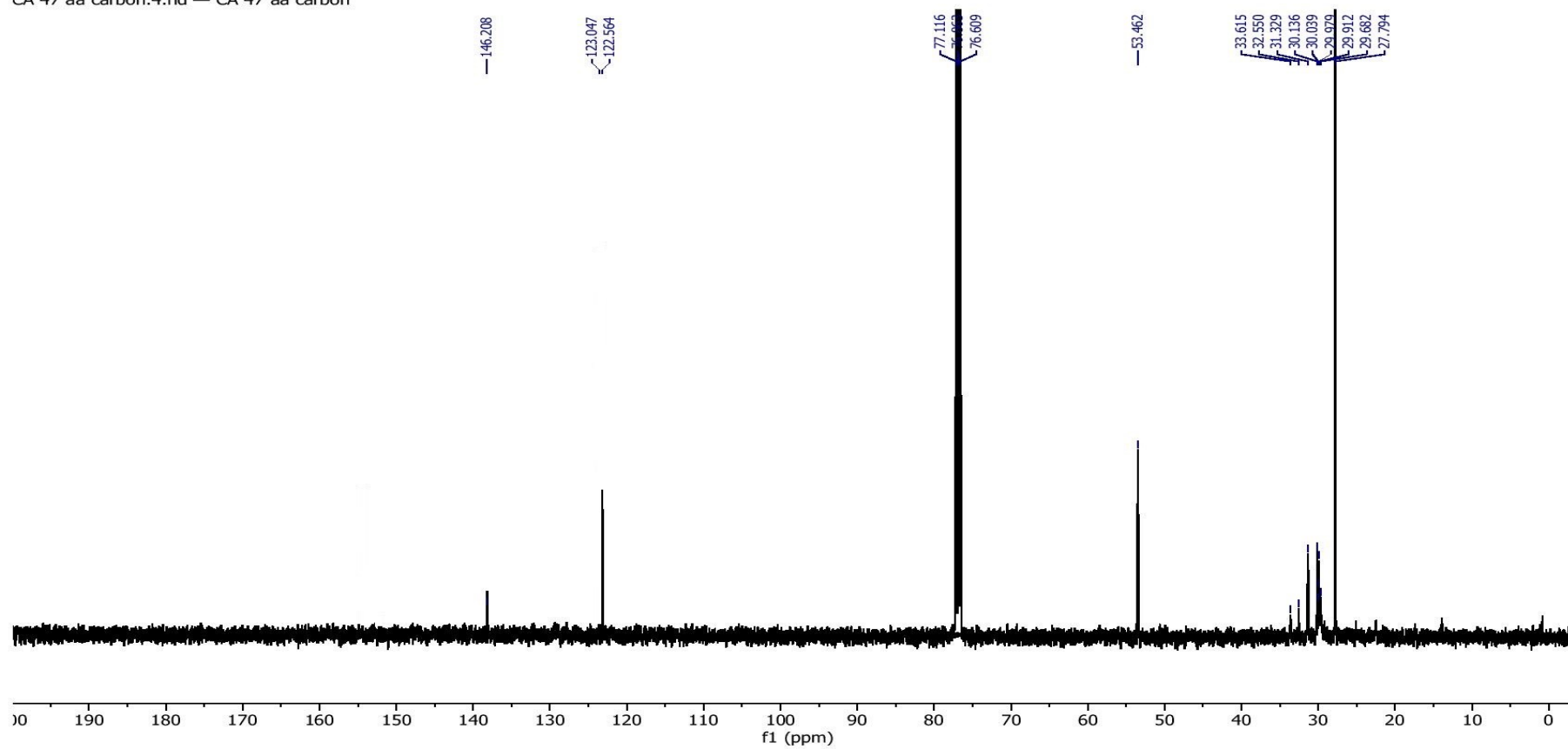


Figure S21- $^{13}\text{C}\{^1\text{H}\}$ -NMR of (3)

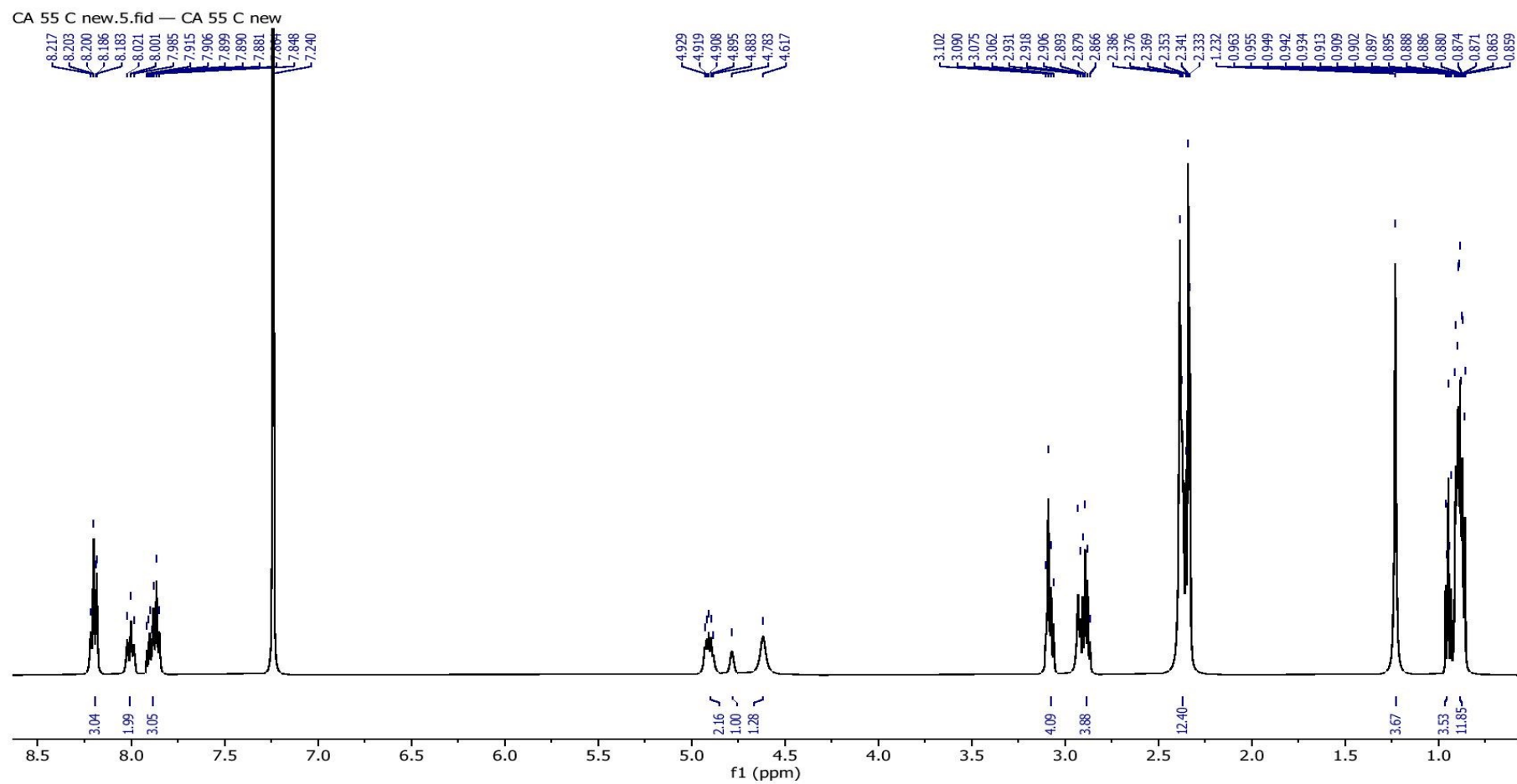


Figure S22 – ^1H -NMR spectrum of (6)

CA 55c carbon new 1.4.fid — CA 55c carbon new 1

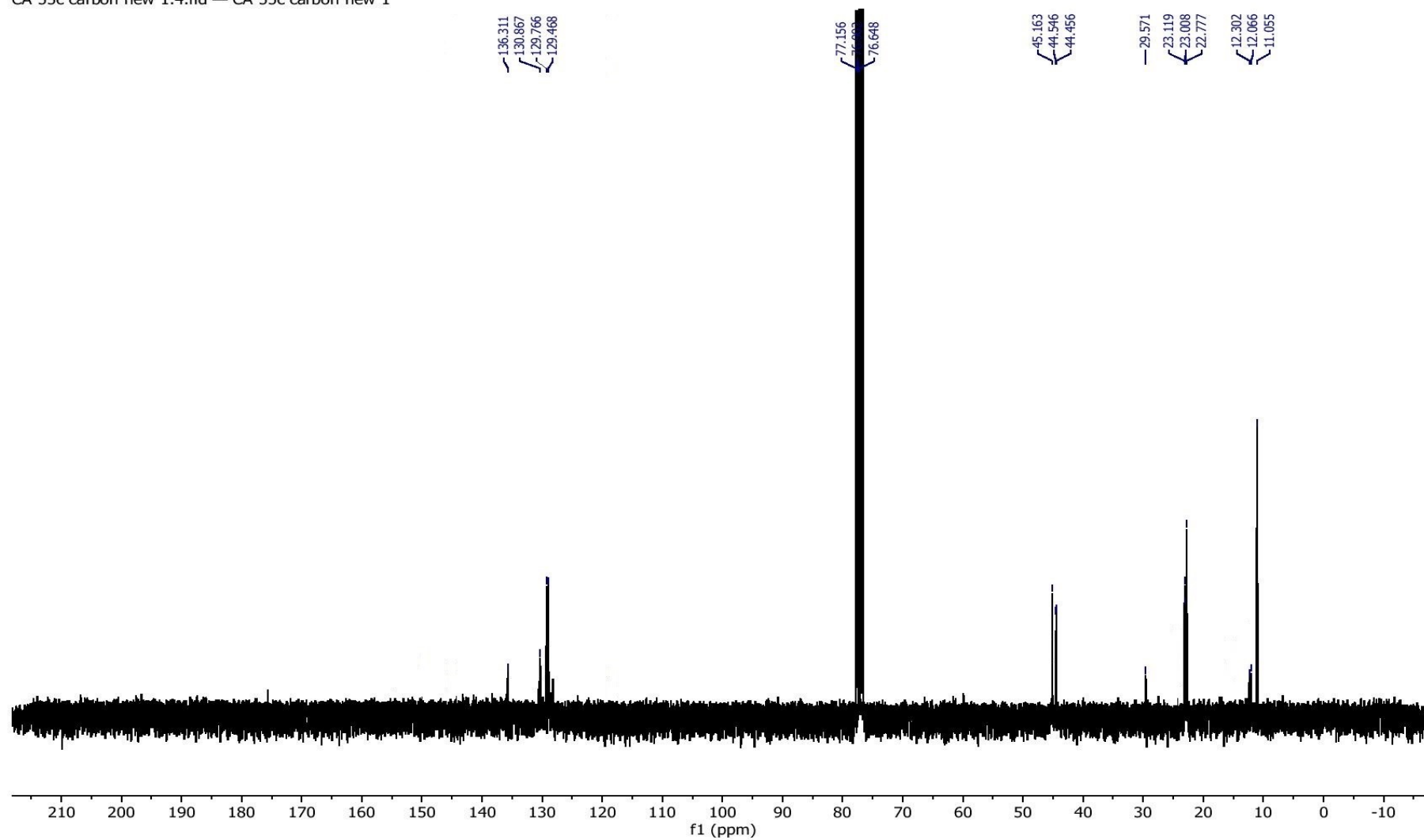


Figure S23- $^{13}\text{C}\{^1\text{H}\}$ -NMR of (6)

CA-032A (m/z =307.1354)

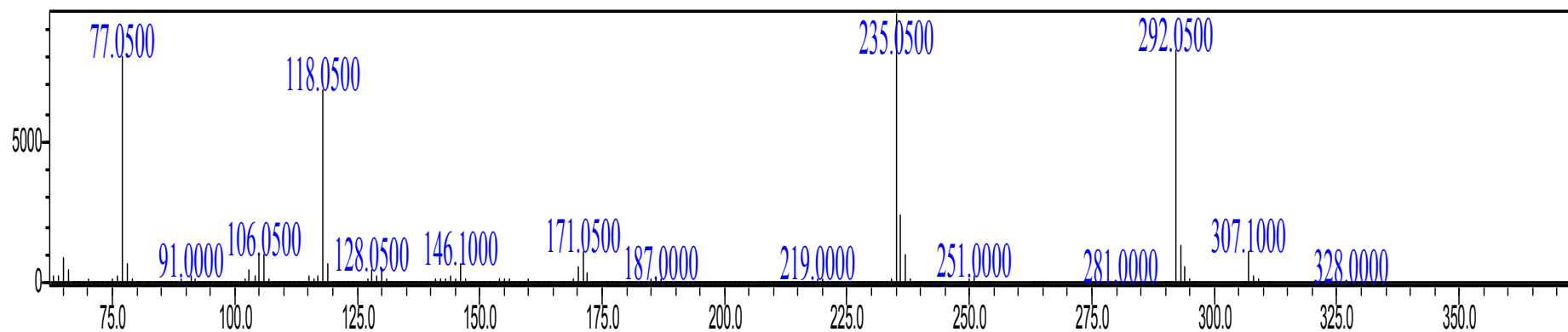
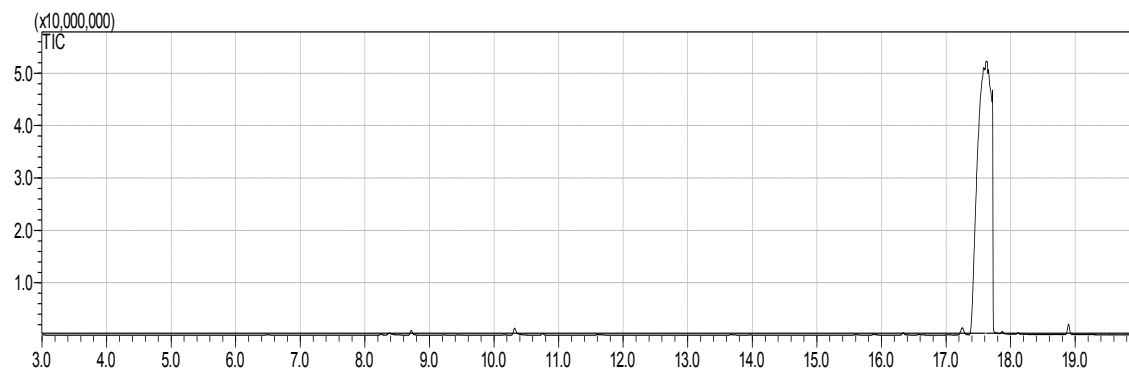


Figure S24 – GC-MS trace and mass spectra of **L1**

CA-032B (m/z = 293.1198)

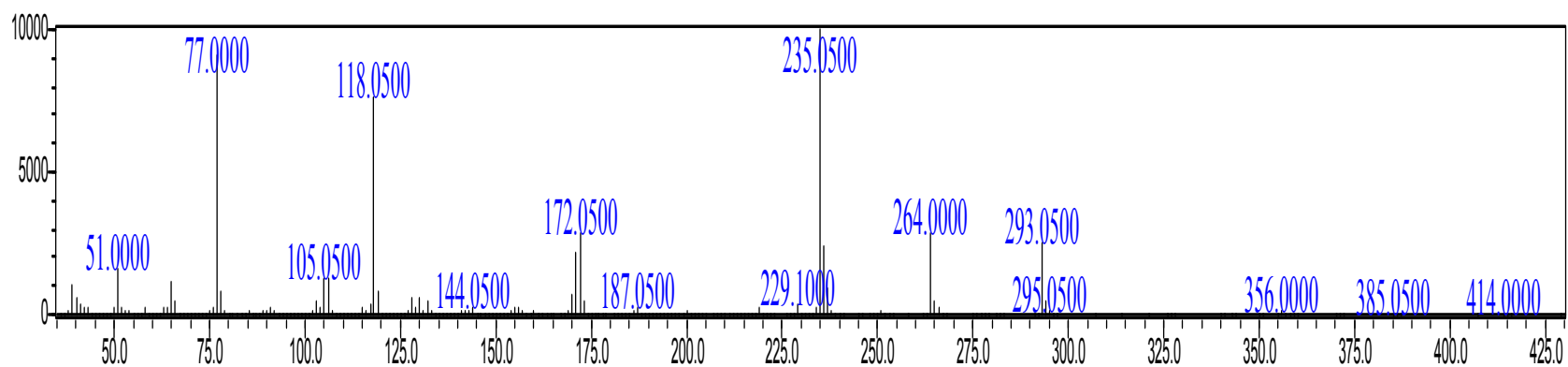
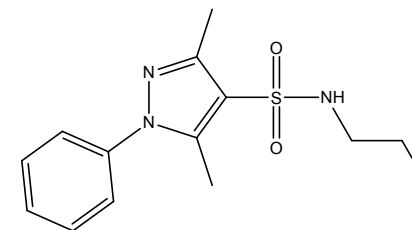
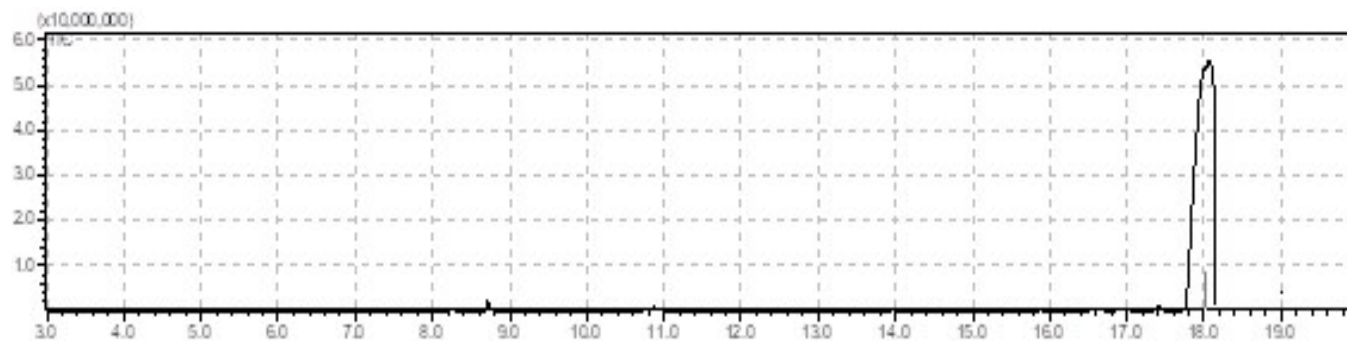


Figure S25- GC-MS trace and mass spectra of **L2**

CA12D2 (m/z = 391-Me) = 376.2500

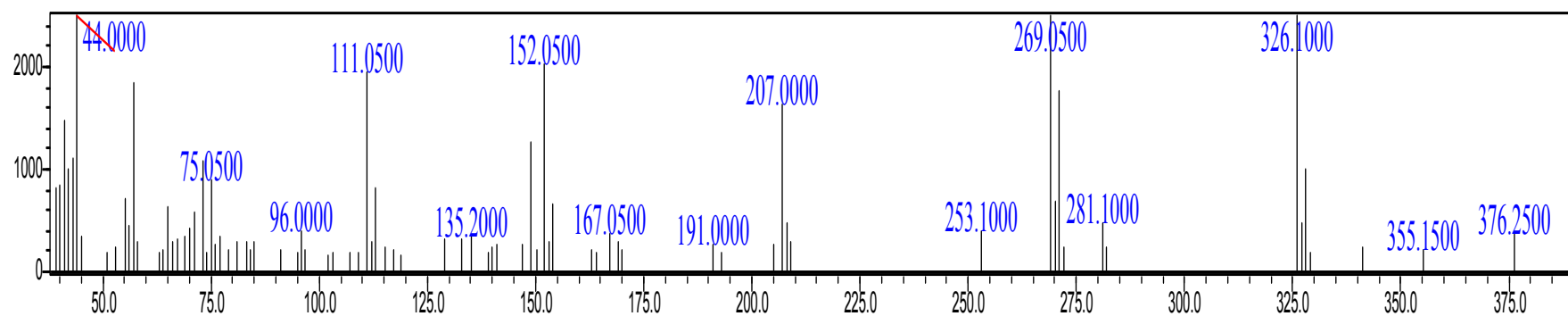
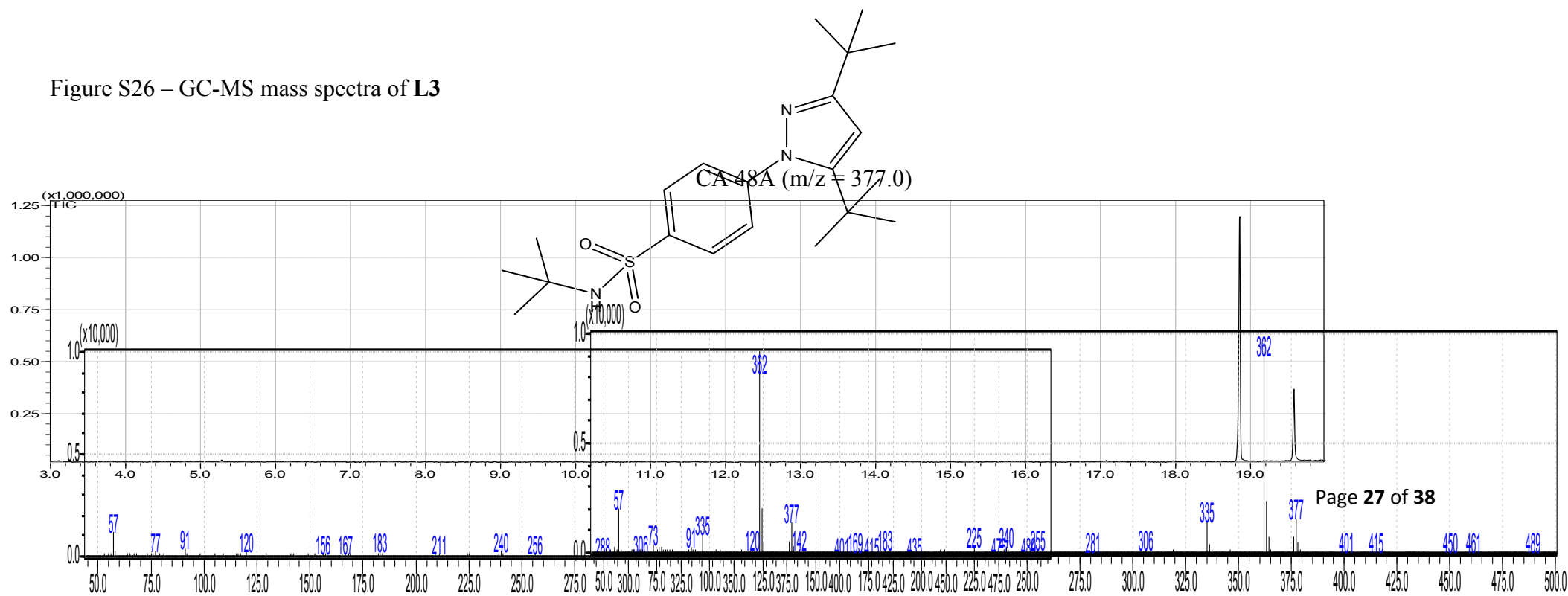
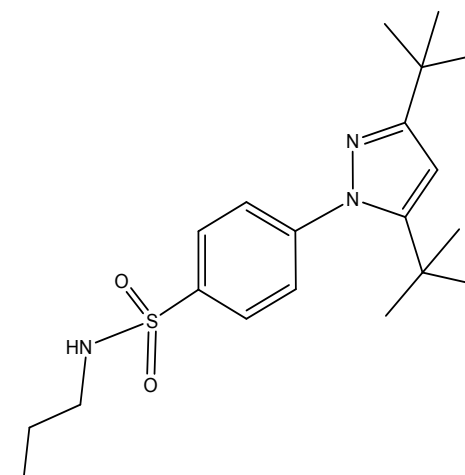


Figure S26 – GC-MS mass spectra of L3





CA 15 ($m/z = 442.3417$)
 Figure S27 - GC-MS trace and mass spectrum of L4

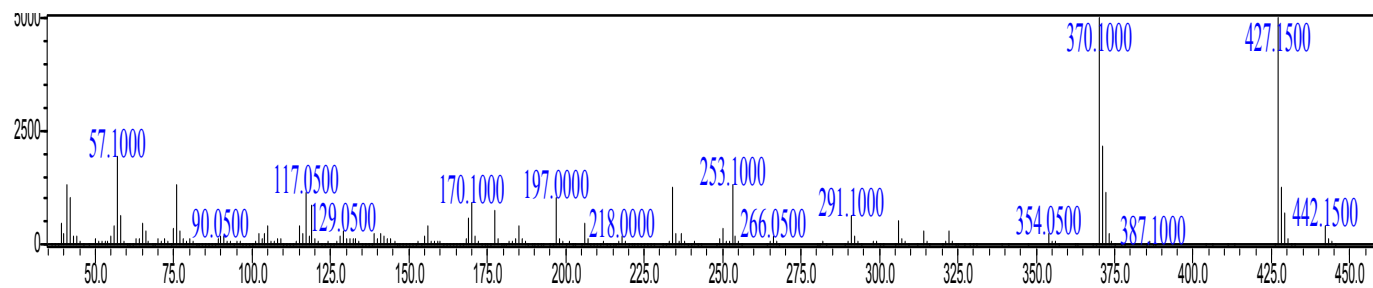


Figure S28 –GC-MS mass spectrum of **L5**

CA20D (m/z = 414.1395)

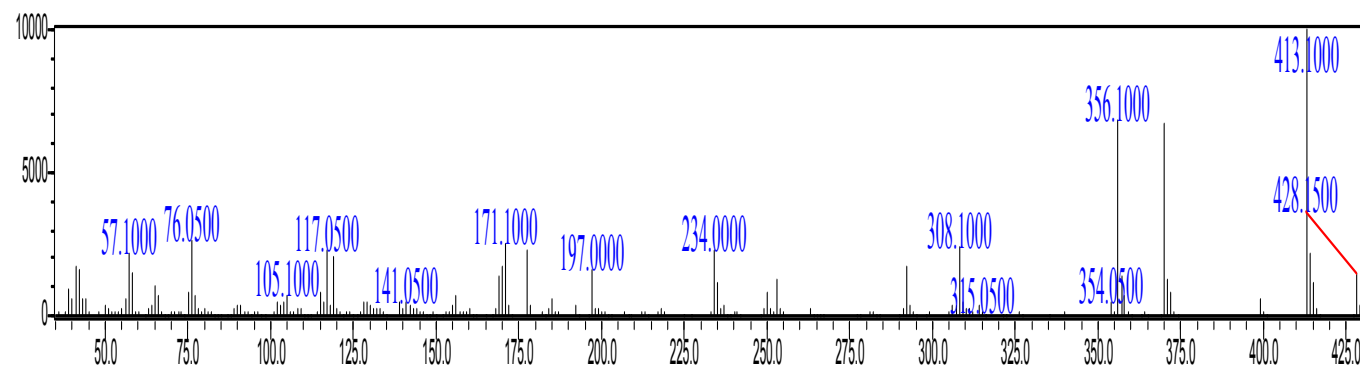


Figure S29 – GC-MS mass spectrum of **L6**

CA 45B HSQC.4.ser — CA 45B HSQC

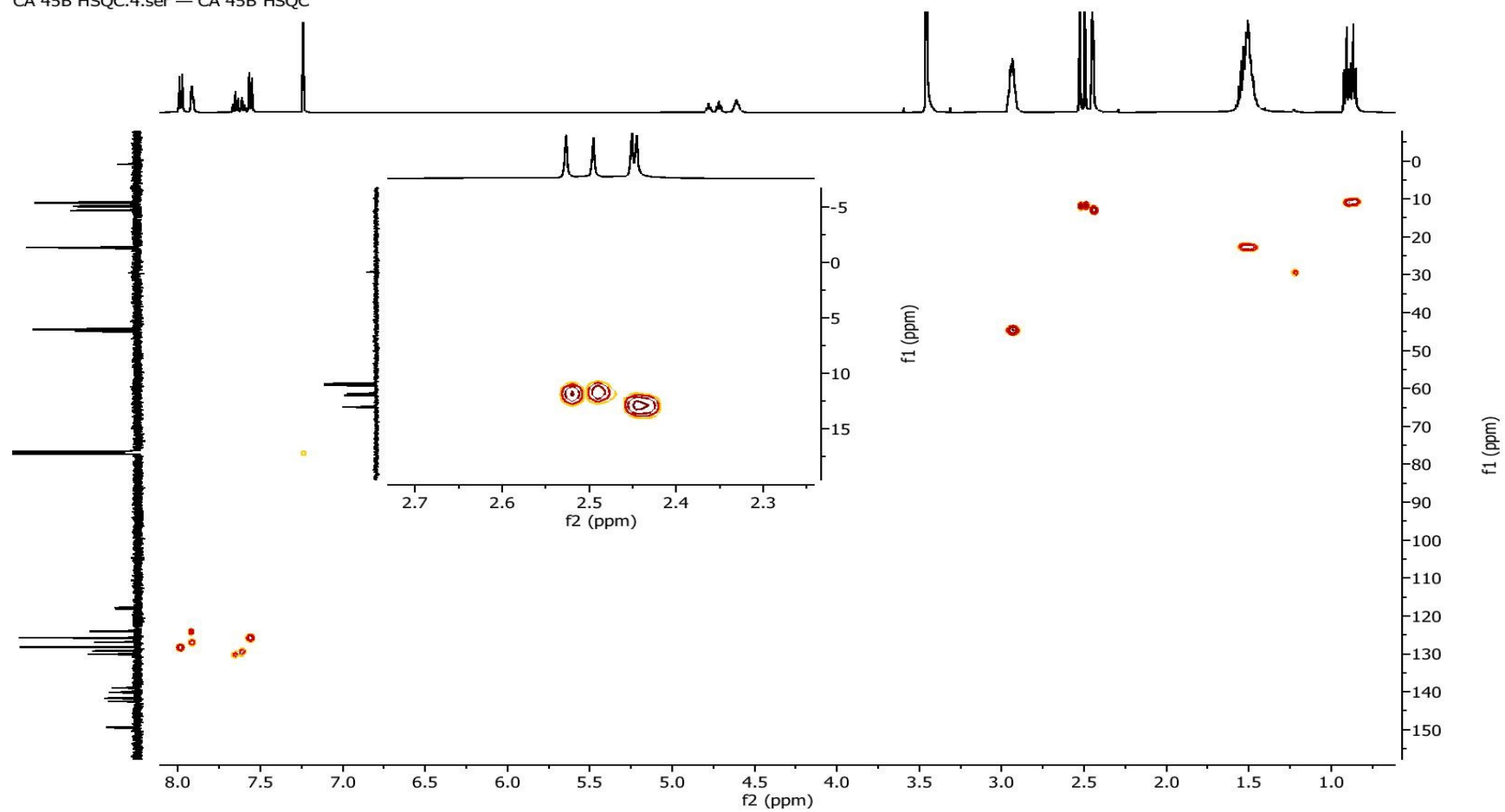


Figure S30 – HSQC of L11

Table S1: Inhibition zone diameter (mm) (n =3)

Entries	Compounds	Dose (µg/mL)	<i>S</i> <i>aereus</i>	<i>S</i> <i>epidermidis</i>	<i>E</i> <i>feacalis</i>	<i>E</i> <i>Coli</i>	<i>P</i> <i>aeruginosa</i>	<i>V</i> <i>cholerae</i>	<i>S</i> <i>typhii</i>	<i>C</i> <i>freundii</i>	<i>K</i> <i>pneumoniae</i>	<i>P</i> <i>mirabilis</i>
1	L1	1000	NA	19.00±0.47	NA	17.00±0.94	18.00±0.47	13.00±0.41	17.00±0.94	24.00±0.70	18.00±0.47	15.00±0.25
		500	NA	15.00±0.82	NA	18.00±0.25	19.00±0.82	17.00±0.25	16.00±0.47	23.00±0.82	14.00±0.94	15.00±0.47
		250	NA	14.00±0.47	NA	12.00±0.82	14.00±0.82	16.00±0.70	17.00±0.47	23.00±0.70	16.00±0.47	13.00±0.47
		125	NA	16.00±0.47	NA	10.00±0.25	13.00±0.47	15.00±0.41	14.00±0.82	21.00±0.47	13.00±0.47	11.00±0.25
		62.5	NA	11.00±0.25	NA	10.00±0.94	10.00±0.94	9.00±0.47	13.00±0.41	20.00±0.47	14.00±0.82	10.00±0.94
2	L2	1000	NA	25.00±0.63	NA	14.00±0.69	NA	13.00±0.62	16.00±0.81	25.00±0.63	16.00±0.20	NA
		500	NA	23.00±0.205	NA	12.00±0.82	NA	12.00±0.24	16.00±0.81	23.00±0.94	15.00±0.50	NA
		250	NA	21.00±0.88	NA	11.00±0.81	NA	11.00±0.87	15.00±0.81	21.00±0.63	14.00±0.20	NA
		125	NA	22.00±0.81	NA	13.00±0.90	NA	12.00±0.24	14.00±0.47	19.00±0.81	12.00±.50	NA
		62.5	NA	20.00±0.24	NA	11.00±0.81	NA	10.00±0.47	14.00±0.81	20.00±0.24	12.00±0.50	NA
3	L3	1000	NA	NA	NA	16.00±0.94	NA	16.00±0.25	14.00±0.82	17.00±0.47	15.00±0.47	NA
		500	NA	NA	NA	17.00±0.63	NA	16.00±0.41	15.00±0.94	15.00±0.47	13.00±0.82	NA
		250	NA	NA	NA	13.00±0.82	NA	17.00±0.47	11.00±0.25	15.00±0.47	10.00±0.50	NA
		125	NA	NA	NA	12.00±0.05	NA	13.00±0.47	11.00±0.82	13.00±0.47	11.00±0.94	NA
		62.5	NA	NA	NA	12.00±0.94	NA	14.00±0.47	12.00±0.25	10.00±0.25	10.00±0.82	NA
4	L4	1000	20.00 ±0.50	NA	NA	NA	NA	NA	NA	NA	18.00 ±0.10	NA
		500	17.00±0.20	NA	NA	NA	NA	NA	NA	NA	17.00±0.30	NA
		250	14.00±0.50	NA	NA	NA	NA	NA	NA	NA	15.00±0.50	NA
		125	11.00±0.30	NA	NA	NA	NA	NA	NA	NA	13.00±0.50	NA
		62.5	NA	NA	NA	NA	NA	NA	NA	NA	9.50±0.50	NA
5	L5	1000	NA	13.00±0.18	NA	NA	15.00±0.59	16.00±0.41	NA	NA	NA	10.00±0.50
		500	NA	12.00±0.43	NA	NA	14.00±0.64	14.00±0.81	NA	NA	NA	11.00±0.18
		250	NA	11.00±0.24	NA	NA	14.00±0.49	12.00±0.21	NA	NA	NA	12.00±0.18
		125	NA	13.00±0.69	NA	NA	12.00±0.81	12.00±0.80	NA	NA	NA	13.00±0.10
		62.5	NA	13.00±0.11	NA	NA	9.00±0.24	15.00±0.47	NA	NA	NA	10.00±0.47
6	L6	1000	NA	NA	NA	14.00±0.69	15.00±0.62	NA	15.00±0.80	14.00±0.63	11.00±0.50	NA
		500	NA	NA	NA	12.00±0.81	14.00±0.24	NA	15.00±0.81	13.00±0.94	12.00±0.50	NA
		250	NA	NA	NA	13.00±0.81	13.00±0.80	NA	12.00±0.81	13.00±0.63	10.00±0.00	NA
		125	NA	NA	NA	12.00±0.50	13.00±0.24	NA	13.00±0.47	12.00±0.81	13.00±0.10	NA
		62.5	NA	NA	NA	13.00±0.81	12.00±0.47	NA	12.00±0.81	11.00±0.24	11.00±0.50	NA
7	1	1000	18.00±0.24	12.00±0.40	NA	NA	18.00±0.50	15.00±0.30	NA	NA	NA	13.00±0.50
		500	17.00±0.50	12.50±0.70	NA	NA	17.00±0.50	13.50±0.40	NA	NA	NA	12.00±0.50

		250	14.00±0.50	10.00±0.20	NA	NA	14.00±0.50	11.50±0.40	NA	NA	NA	12.00±0.10
		125	12.00±0.50	NA	NA	NA	12.00±0.25	11.50±0.20	NA	NA	NA	11.00± 0.20
		62.5	11.00±0.81	9.00±0.70	NA	NA	11.00±0.20	9.50±0.40	NA	NA	NA	NA
8	2	1000	NA	20.00±0.40	NA	NA	25 ±0.40	11±0.10	NA	NA	24.00 ±0.20	NA
		500	NA	23.00±0.14	NA	NA	27 ±0.40	12 ±0.50	NA	NA	26.00 ±0.40	NA
		250	NA	18.00±0.50	NA	NA	25.00 ± 0.50	11.67±0.47	NA	NA	25.00±0.50	NA
		125	NA	17.00±0.50	NA	NA	22.00 ±0.30	10.67±0.40	NA	NA	22.00±0.50	NA
		62.5	NA	15.00±0.75	NA	NA	18.00 ±0.20	10.00±0.30	NA	NA	20.00±0.50	NA
9	3	1000	NA	NA	NA	21.00±0.11	NA	19.00±0.10	21.00±0.20	19.00±0.12	18.00±0.12	NA
		500	NA	NA	NA	19.00±0.21	NA	22.00±0.21	20.00±0.20	21.00±0.30	16.00±0.20	NA
		250	NA	NA	NA	19.00±0.30	NA	21.00±0.30	15.00±0.05	22.00±0.10	19.00±0.30	NA
		125	NA	NA	NA	18.00±0.15	NA	19.00±0.07	18.00±0.20	19.00±0.01	15.00±0.20	NA
		62.5	NA	NA	NA	16.00±0.94	NA	20.00±0.03	19.00±0.20	16.00±0.03	16.00±0.10	NA
10	4	1000	28.00 ±0.10	NA	NA	NA	NA	NA	NA	NA	21.00 ±0.20	NA
		500	21.00±0.10	NA	NA	NA	NA	NA	NA	NA	19.00±0.10	NA
		250	19.00±0.12	NA	NA	NA	NA	NA	NA	NA	18.00±0.20	NA
		125	20.00±0.21	NA	NA	NA	NA	NA	NA	NA	19.00±0.10	NA
		62.5	NA	NA	NA	NA	NA	NA	NA	NA	13.00±0.20	NA
11	5	1000	NA	19.00±0.20	NA	NA	25.00±0.21	21.00±0.11	NA	NA	NA	18.00±0.10
		500	NA	16.00±0.21	NA	NA	21.00±0.20	19.00±0.20	NA	NA	NA	16.00±0.20
		250	NA	14.00±0.24	NA	NA	19.00±0.12	17.00±0.10	NA	NA	NA	19.00±0.10
		125	NA	21.00±0.22	NA	NA	20.00±0.10	18.00±0.20	NA	NA	NA	16.00±0.10
		62.5	NA	20.00±0.10	NA	NA	15.00±0.20	17.00±0.17	NA	NA	NA	15.00±0.30
12	6	1000	NA	NA	NA	18.00±0.01	22.00±0.12	NA	20.00±0.10	17.00±0.13	18.00±0.30	NA
		500	NA	NA	NA	16.00±0.10	19.00±0.40	NA	19.00±0.20	16.00±0.04	17.00±0.20	NA
		250	NA	NA	NA	19.00±0.30	18.00±0.10	NA	18.00±0.40	17.00±0.10	17.00±0.01	NA
		125	NA	NA	NA	17.00±0.40	18.00±0.11	NA	21.00±0.10	19.00±0.20	16.00±0.10	NA
		62.5	NA	NA	NA	16.00±0.20	19.00±0.04	NA	18.00±0.30	15.00±0.24	19.00±0.10	NA
13	Gentamicin	1000	20.00±0.47	22.00±0.47	16.00±0.47	29.00±0.94	25.00±0.47	29.00±0.82	32.00±0.82	28.00±0.82	36.00±0.47	28.00±0.47
		500	26.00±0.47	27.00±0.94	15.00±0.82	28.00±0.94	21.00±0.47	21.00±0.82	30.00±0.94	26.00±0.82	33.00±0.47	27.00±0.47
		250	18.00±0.82	24.00±0.94	17.00±0.82	25.00±0.47	27.00±0.47	22.00±0.82	28.00±0.94	22.00±0.82	31.00±0.94	25.00±0.82
		125	18.00±0.82	21.00±0.47	16.00±0.82	23.00±0.47	24.00±0.47	24.00±0.47	25.00±0.47	20.00±0.47	29.00±0.94	20.00±0.82
		62.5	15.00±0.82	16.00±0.47	15.00±0.82	20.00±0.47	20.00±0.82	10.00±0.82	10.00±0.47	16.00±0.47	16.00±0.47	19.00±0.47
	DMSO	--	--	--	--	--	--	--	--	--	--	--

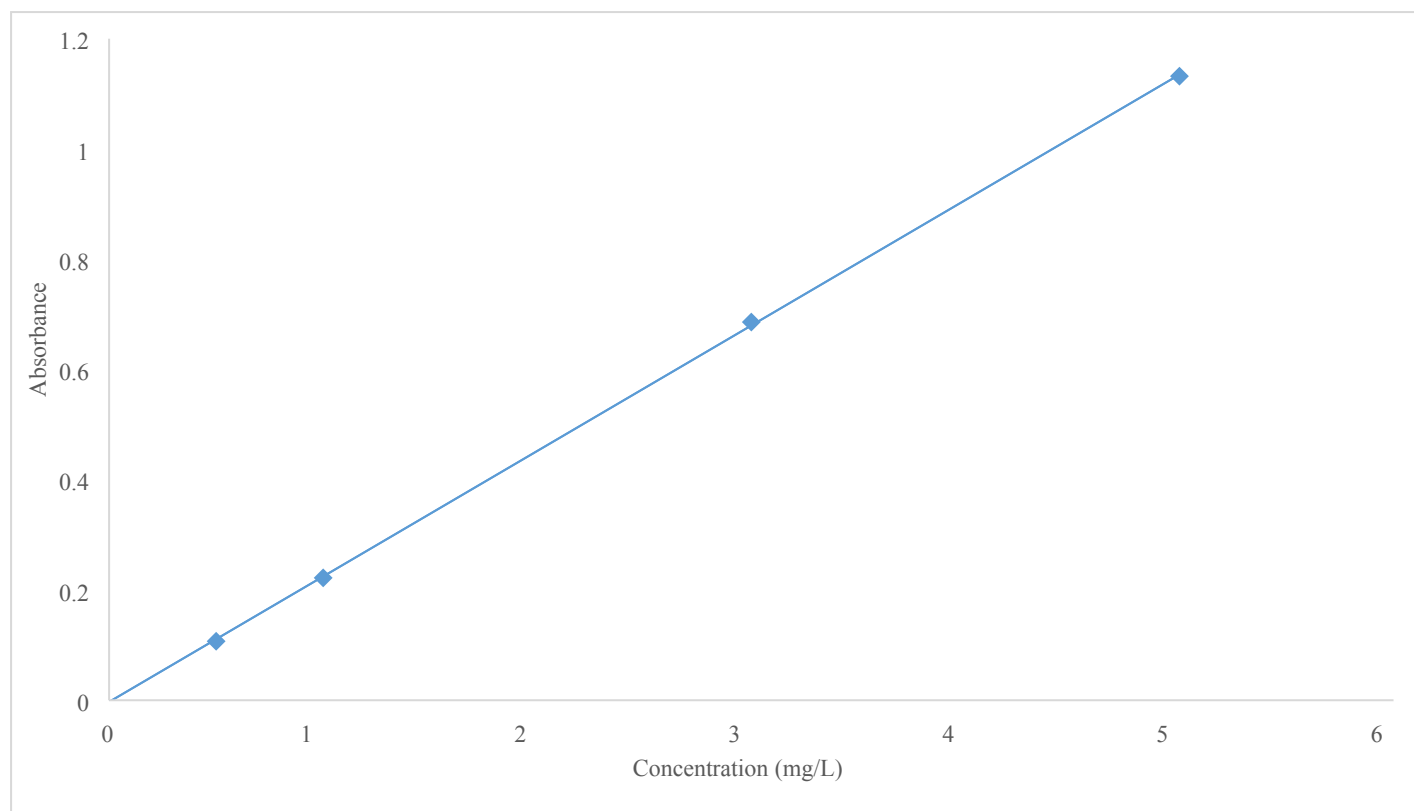


Figure S31: Calibration graph of **L1**

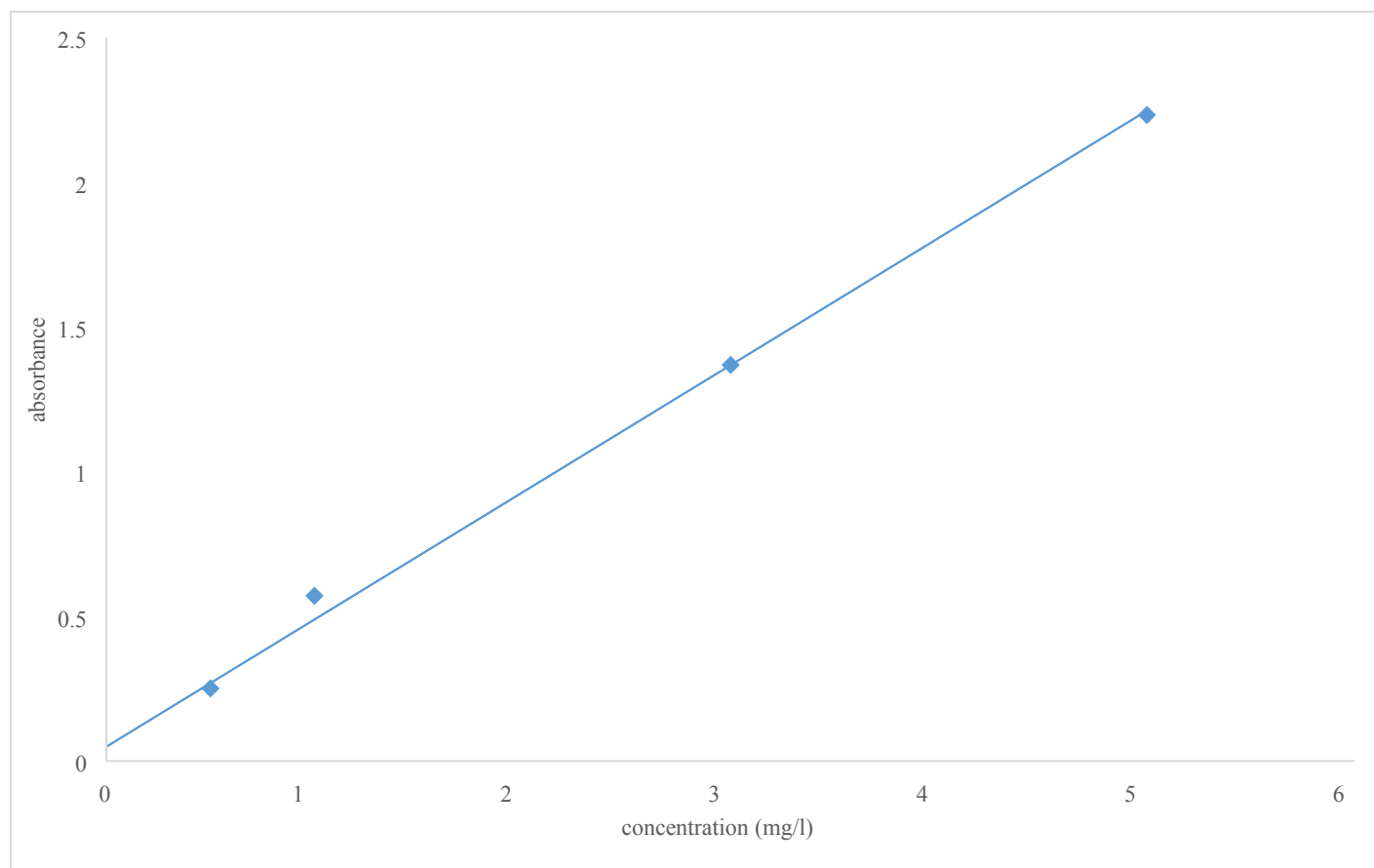


Figure S32: Calibration graph of **1**

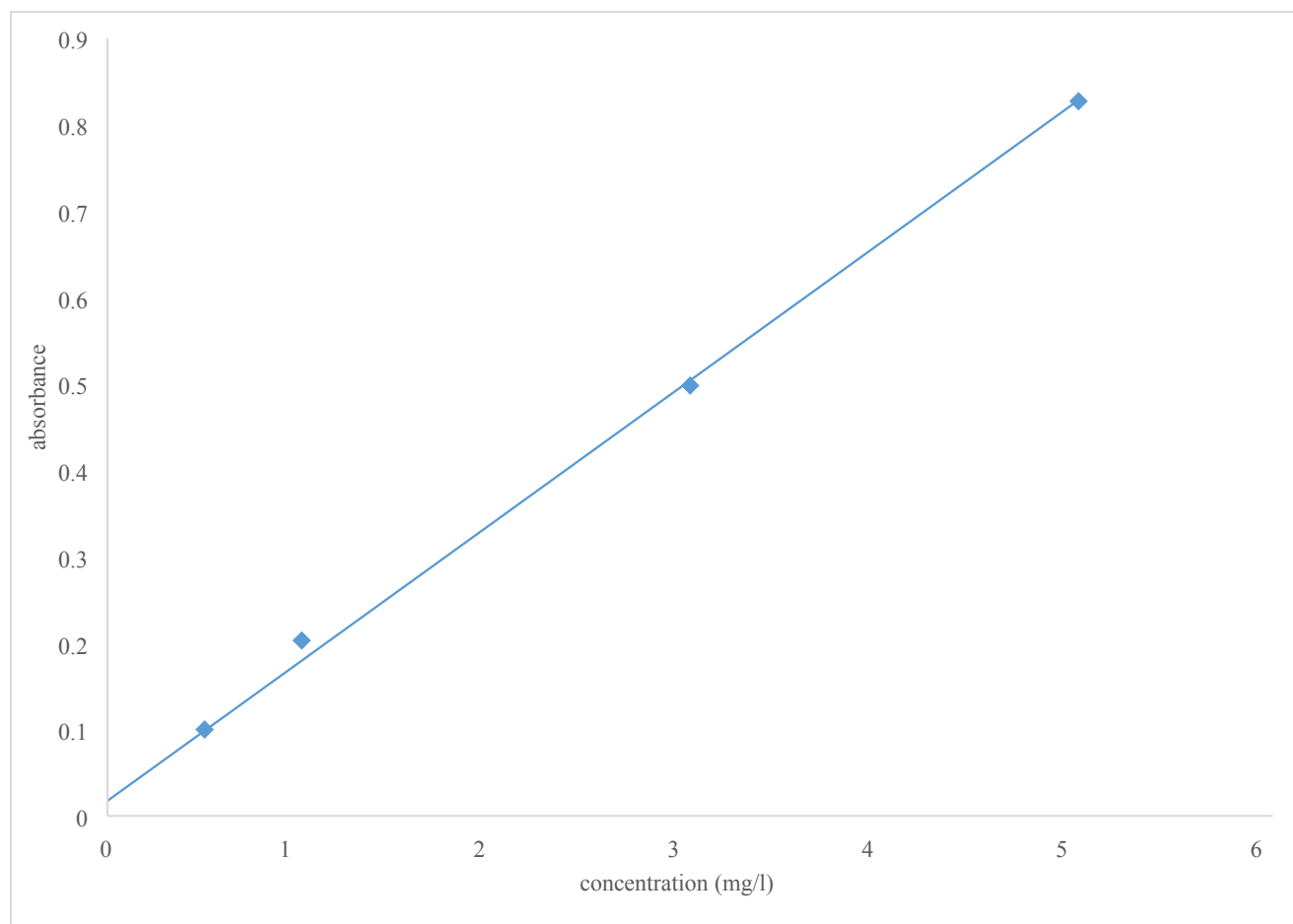


Figure S33: Calibration graph of **L2**

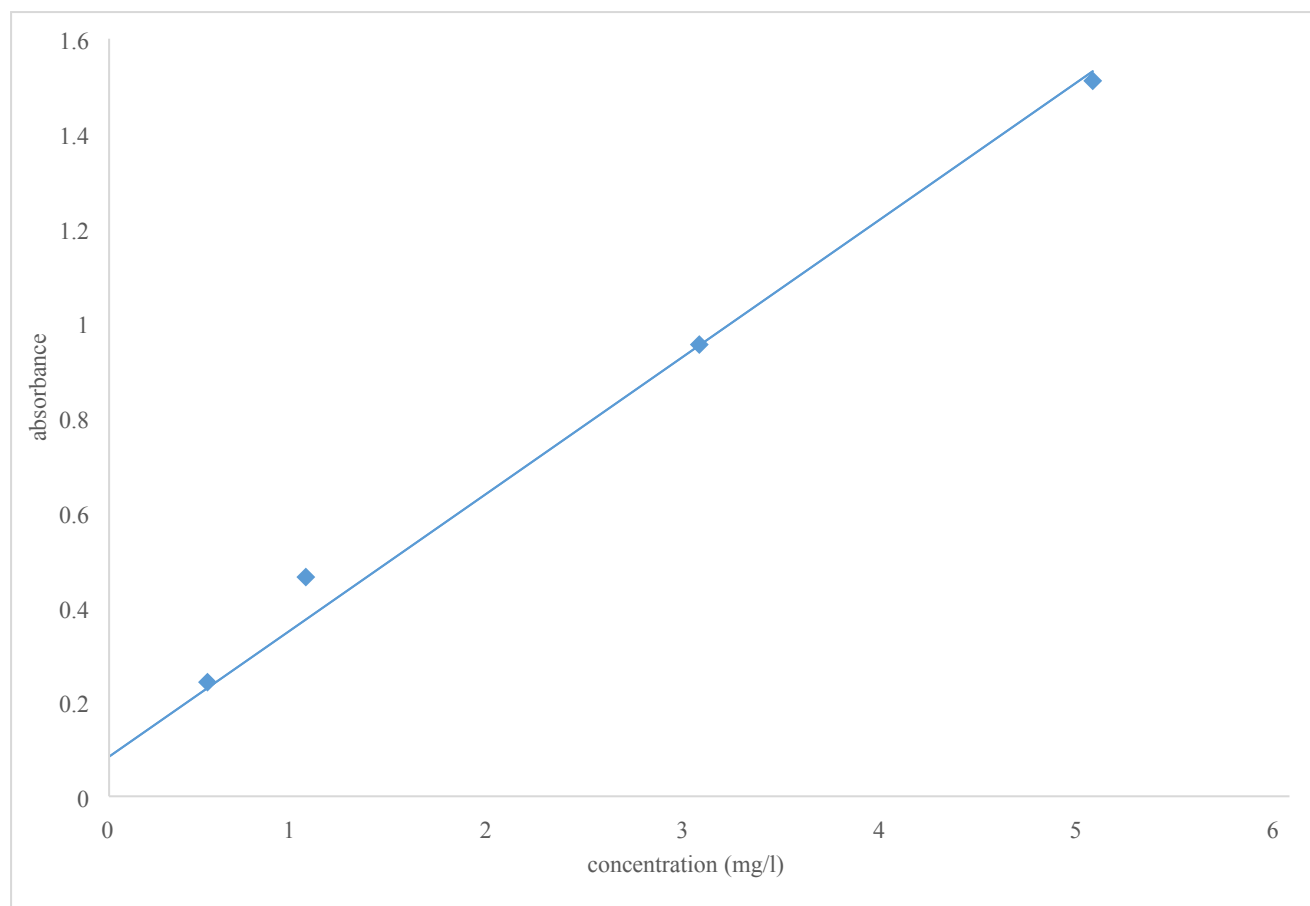


Figure S34: Calibration graph of **L3**

Compounds	Partition Coefficient	Log P
L1	10.17	1.01
L2	903.56	2.96
L3	0.15	-0.83

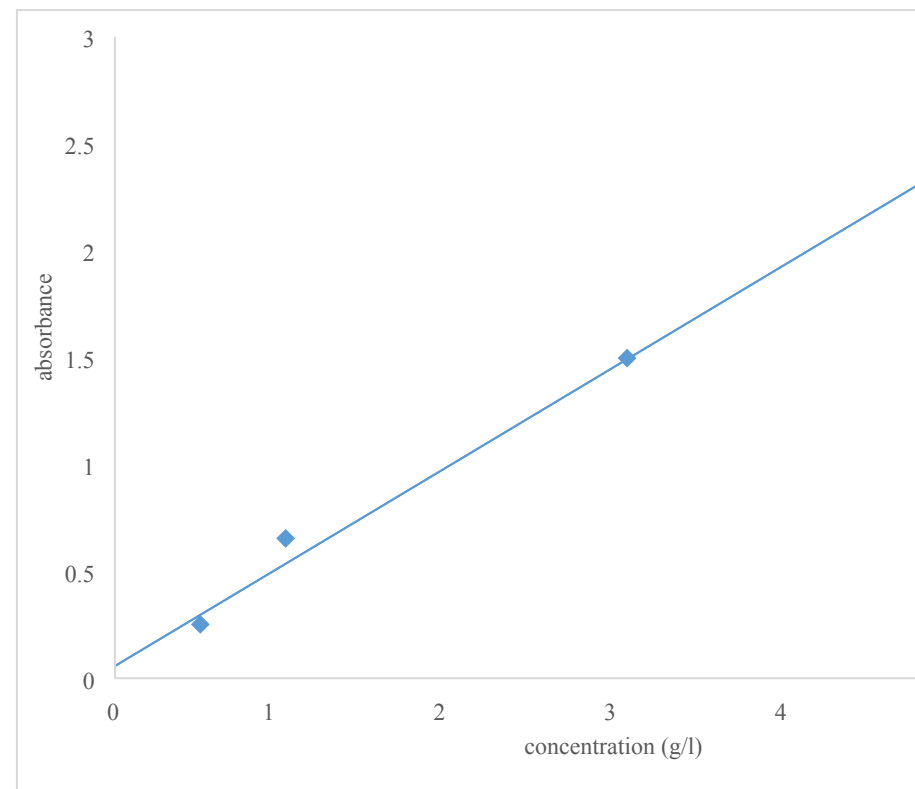


Figure S35: Calibration graph of **L6**

L4	0.3	-0.53
L5	8.71	0.94
L6	4.64	0.67
1	15.8	1.2
2	1698.24	3.23
3	0.11	-0.96
4	0.19	-0.72
5	12.59	1.1
6	8.13	0.91

Table S2: Partition Coefficient and Log P values of compounds in aqueous and octanol phases