

Synthesis, antibacterial and antibiofilm activity of new 1,2,3,5-tetrazine derivatives from coupling reactions of diazonium salt of 2-amino-6-nitrobenzothiazole with diverse substituted 2-aminobenzothiazole derivatives

Joseph Tsemeugne^{a*}, Yetiny Atuh Bah^a, Ulrich Joel Tsopmene^b, Armelle Tontsa Tsamo^a, Jérôme Ndefo Ndefongang^a, Pierre Mkounga^a, Emmanuel Fondjo Sopbué^{c*}, Jean Paul Dzoyem^b and Augustin Ephrem Nkengfack^a

^aLaboratory of Natural Products and Applied Organic Synthesis (LANAPOS), Department of Organic Chemistry, Faculty of Science, University of Yaounde I, P.O. Box 812 Yaounde, Republic of Cameroon;

Email: tsemeugne@yahoo.fr

^bLaboratory of Microbiology and Antimicrobial Substances, Department of Biochemistry, Faculty of Science, University of Dschang, PO Box 67 Dschang, Cameroon;

^cLaboratory of Applied Synthetic Organic Chemistry, Department of Chemistry, Faculty of Science, University of Dschang, P.O. Box 67 Dschang, Republic of Cameroon; Email: sopbue@yahoo.fr

Table of contents

Figures	Materials	Pages
Figure S1	UV spectrum of compound 4a in methanol as solvent.....	2
Figure S2	IR spectrum of compound 4a	2
Figure S3	¹ H-NMR (DMSO- <i>d</i> ₆ , 600 MHz) spectrum of compound 4a	3, 4
Figure S4	¹³ C(H)-NMR ¹ H (DMSO- <i>d</i> ₆ , 150 MHz) of compound 4a	4, 5
Figure S5	HSQC spectrum of compound 4a	6
Figure S6	COSY ¹ H- ¹ H spectrum of compound 4a	6
Figure S7	HMBC spectrum of compound 4a	7
Figure S8	HRMS ESI-Positive mode of compound 4a	7
Figure S9	UV spectrum of compound 4b in methanol as solvent.....	8
Figure S10	IR spectrum of compound 4b	8
Figure S11	¹ H-NMR (DMSO- <i>d</i> ₆ , 600 MHz) spectrum of compound 4b and expanded ¹ H-NMR spectrum	9,10
Figure S12	¹³ C(H)-NMR ¹ H (DMSO- <i>d</i> ₆ , 150 MHz) of compound 4b and expanded ¹³ C spectrum	10-12
Figure S13	HSQC spectrum of compound 4b	13
Figure S14	COSY ¹ H- ¹ H spectrum of compound 4b	13
Figure S15	HMBC spectrum of compound 4b	14
Figure S16	HRMS ESI-Positive mode of compound 4b	14, 15
Figure S17	UV spectrum of compound 4c in methanol as solvent.....	15
Figure S18	IR spectrum of compound 4c	16
Figure S19	¹ H-NMR (DMSO- <i>d</i> ₆ , 600 MHz) spectrum of compound 4c and expanded ¹ H-NMR spectrum	16, 17
Figure S20	¹³ C(H)-NMR ¹ H (DMSO- <i>d</i> ₆ , 150 MHz) of compound 4c and expanded ¹³ C spectrum	18, 19
Figure S21	HSQC spectrum of compound 4c	20
Figure S22	COSY ¹ H- ¹ H spectrum of compound 4c	20
Figure S23	HMBC spectrum of compound 4c	21
Figure S24	HRMS ESI-Positive mode of compound 4c	21
Figure S25	UV spectrum of compound 4d in methanol as solvent.....	22
Figure S26	IR spectrum of compound 4d	22
Figure S27	¹ H-NMR (DMSO- <i>d</i> ₆ , 600 MHz) spectrum of compound 4d and expanded ¹ H-NMR spectrum	23
Figure S28	¹³ C(H)-NMR ¹ H (DMSO- <i>d</i> ₆ , 150 MHz) of compound 4d and expanded ¹³ C spectrum ...	24
Figure S29	HSQC spectrum of compound 4d	25
Figure S30	COSY ¹ H- ¹ H spectrum of compound 4d	26
Figure S31	HMBC spectrum of compound 4d	26
Figure S32	HRMS ESI-Positive mode of compound 4d	27
Figure S33	Powder XRD patterns of compound 4a	28

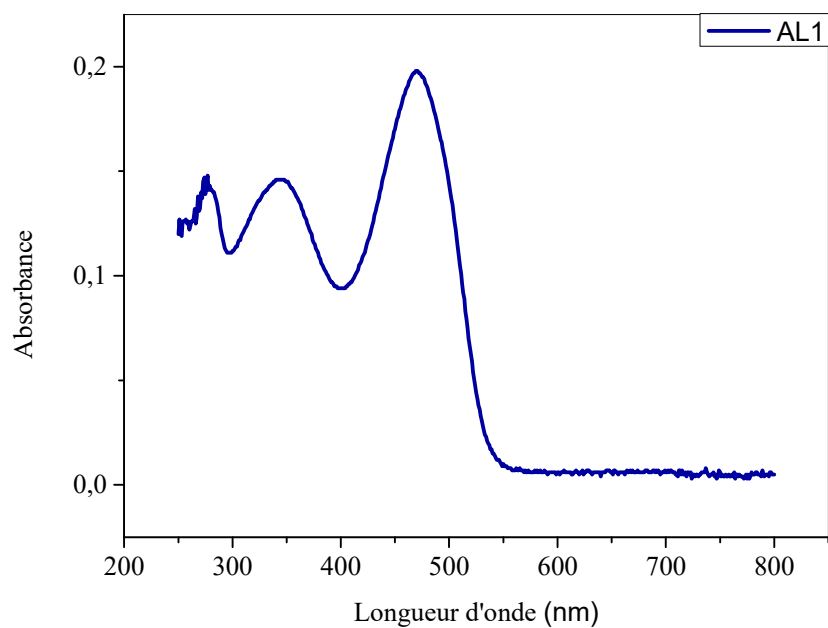


Figure S1: UV spectrum of compound **4a** in methanol as solvent

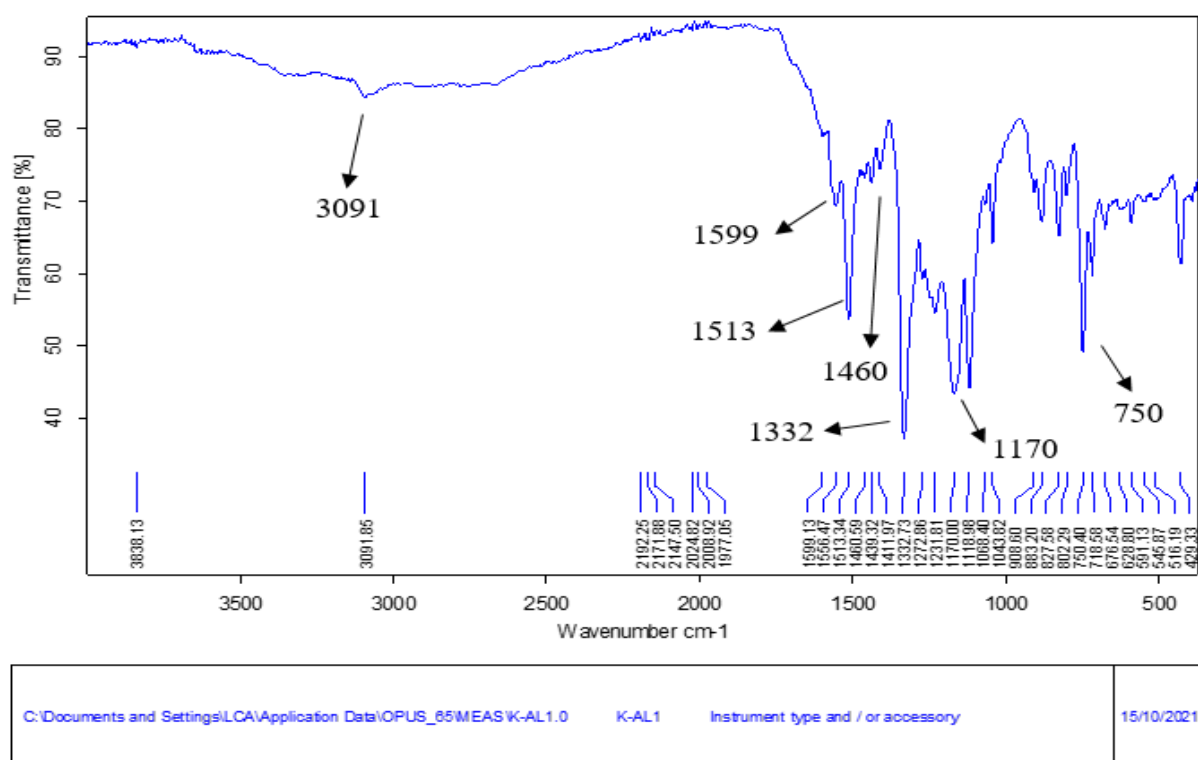


Figure S2: IR spectrum of compound **4a**

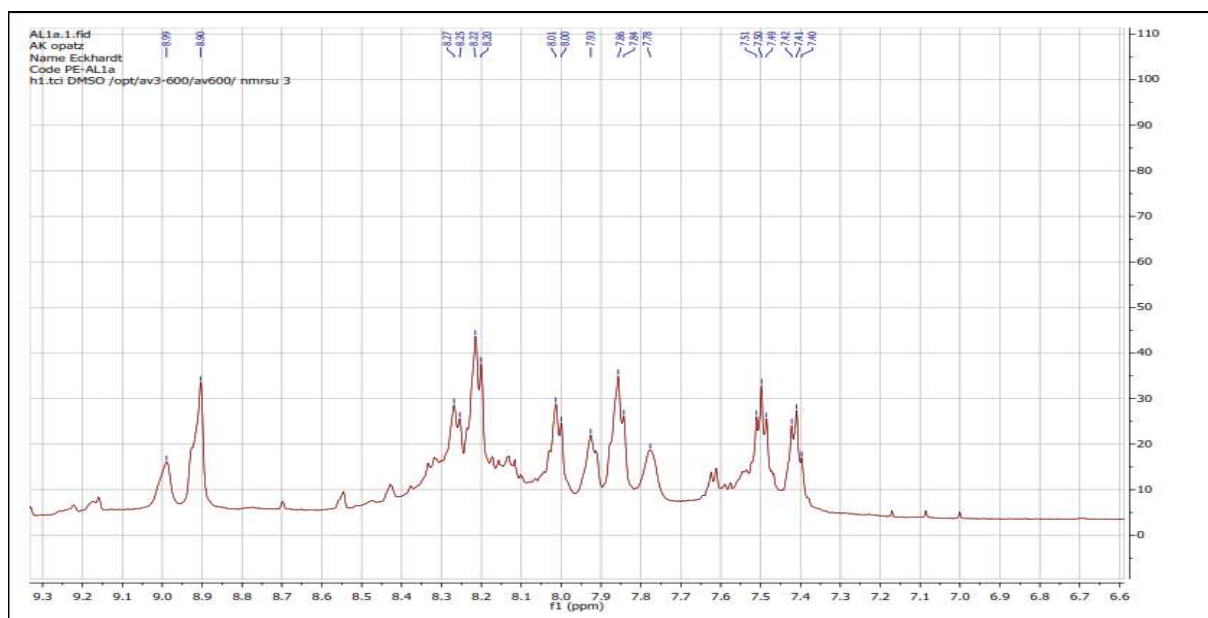
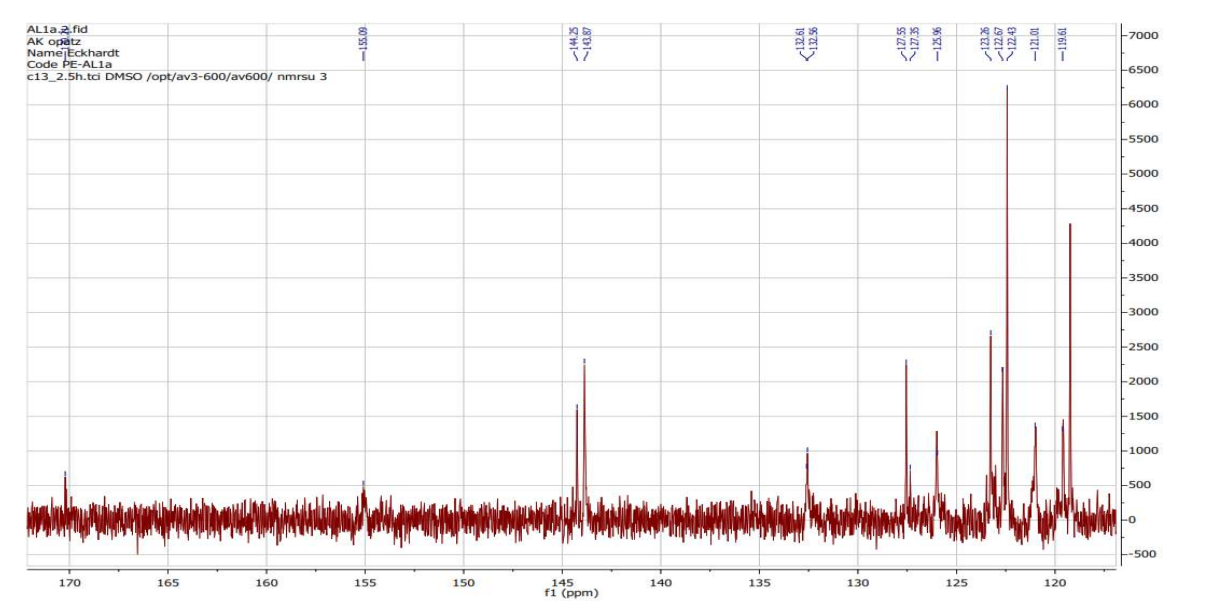


Figure S3: ^1H -NMR (DMSO- d_6 , 400 MHz) spectrum of compound **4a**



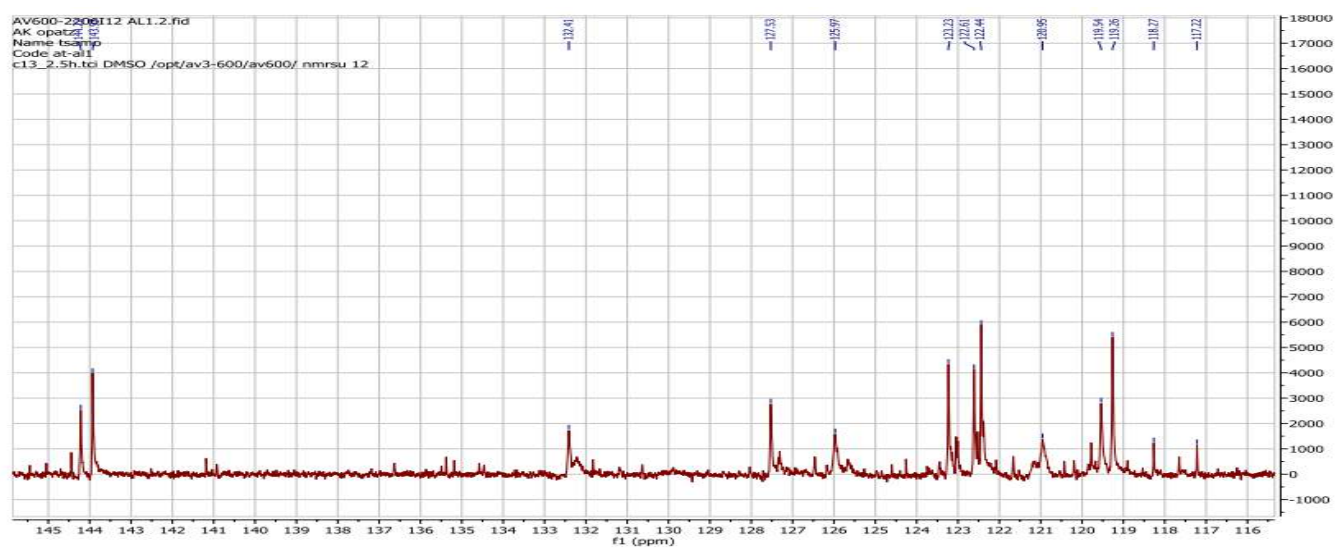
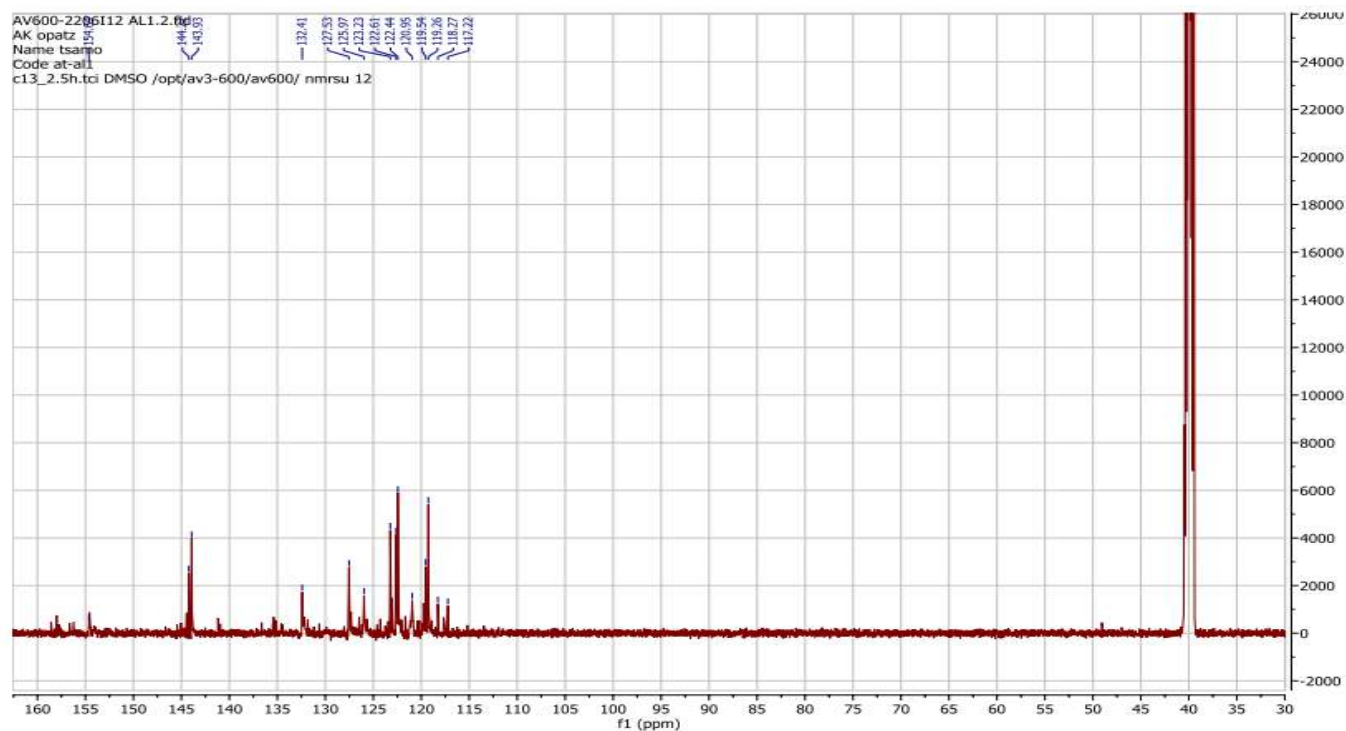


Figure S4: $^{13}\text{C}(\text{H})\text{-NMR } ^1\text{H}$ (DMSO- d_6 , 100 MHz) of compound **4a**

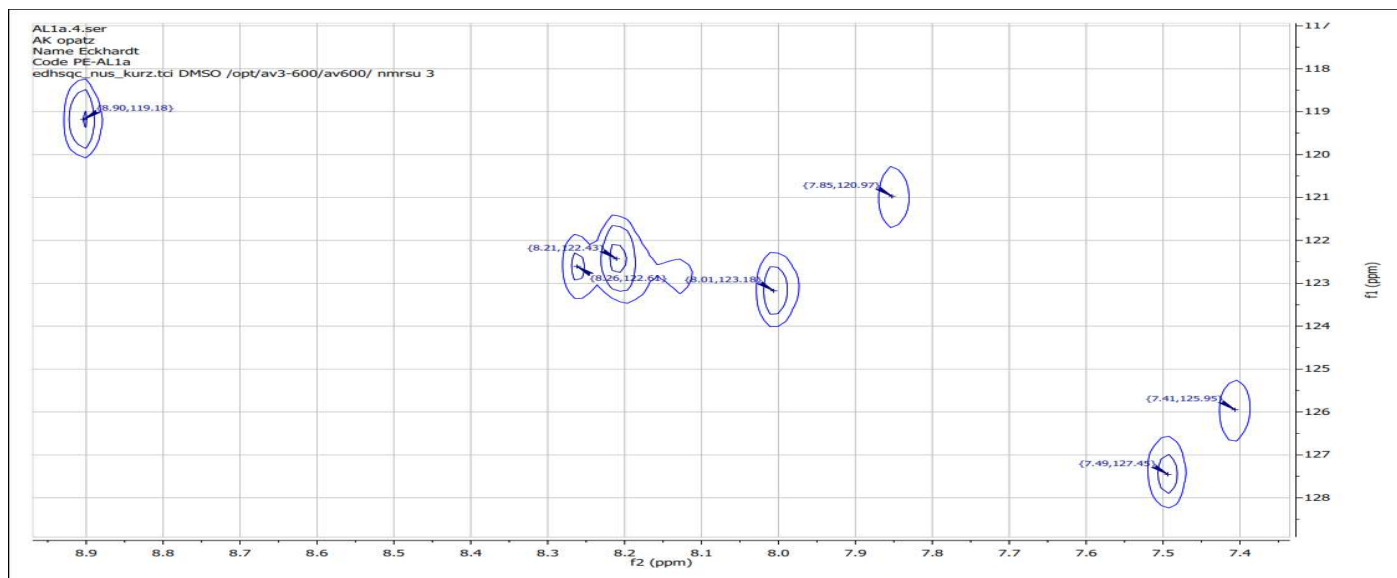


Figure S5: HSQC spectrum of compound **4a**

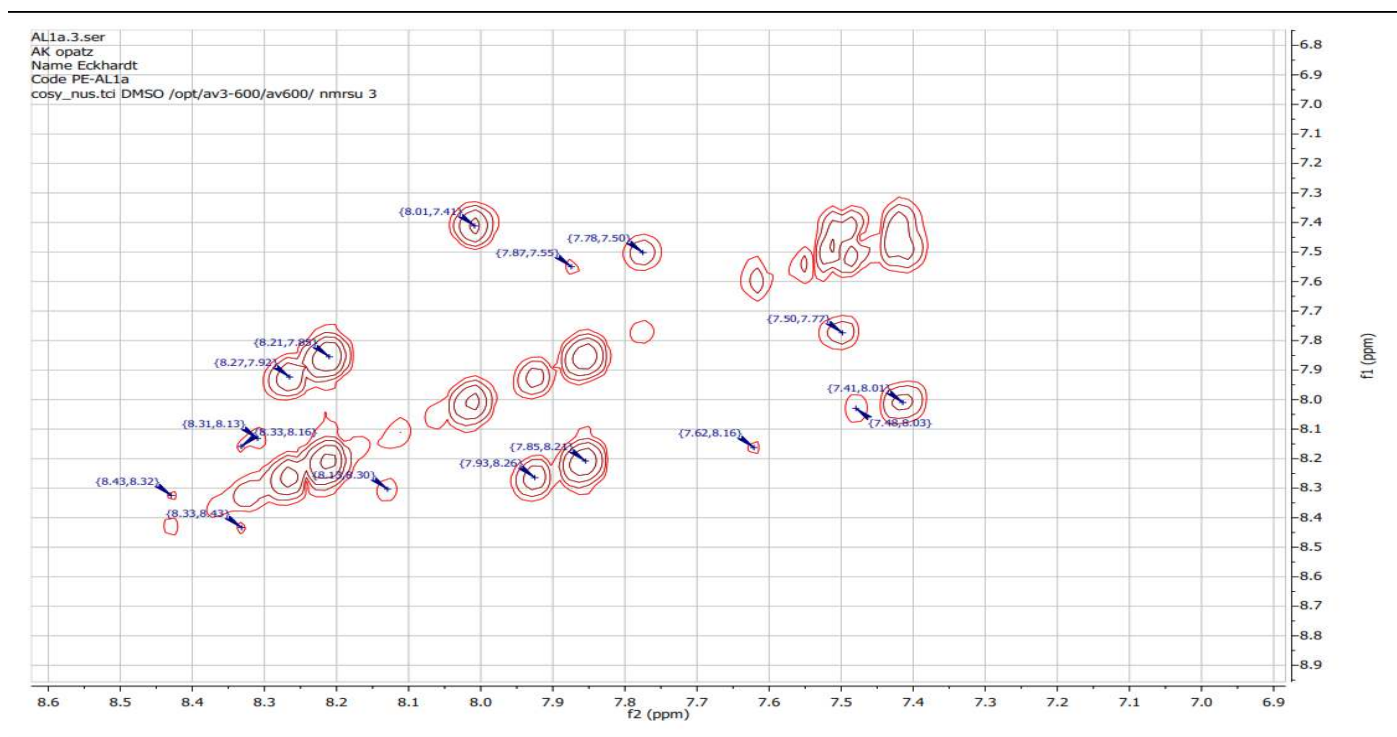


Figure S6: COSY ^1H - ^1H spectrum of compound **4a**

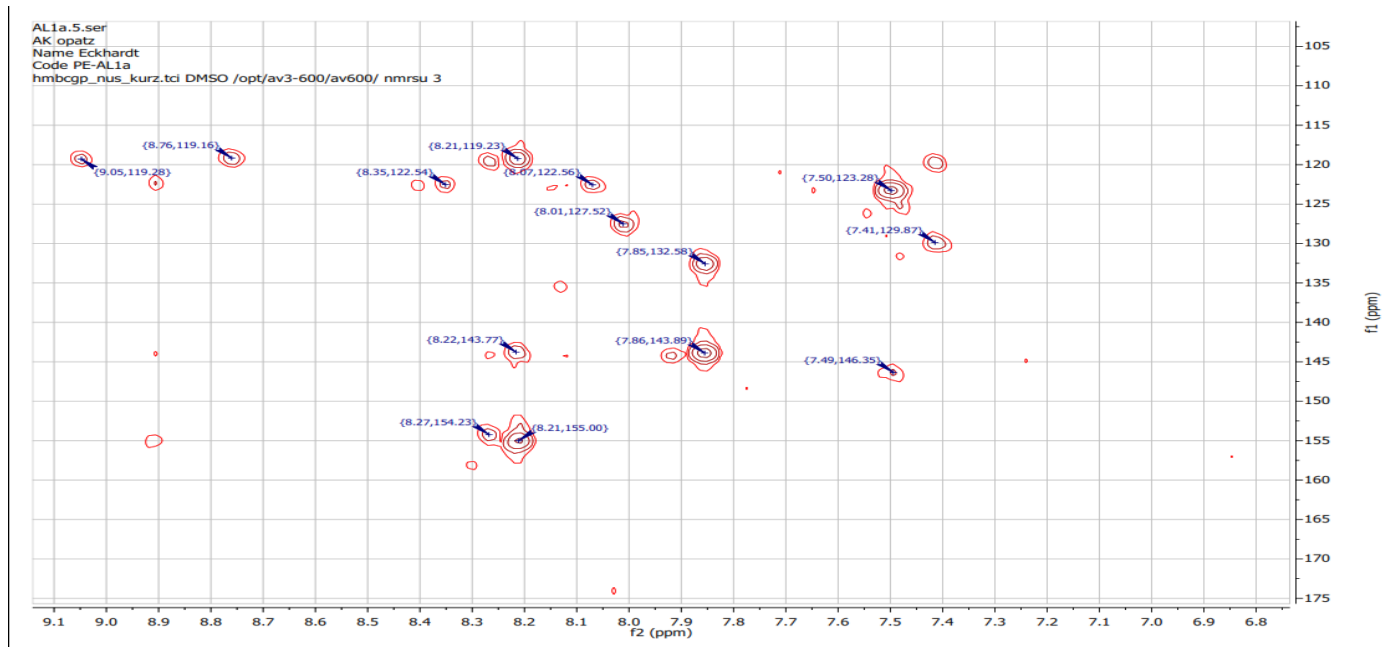


Figure S7: HMBC spectrum of compound **4a**

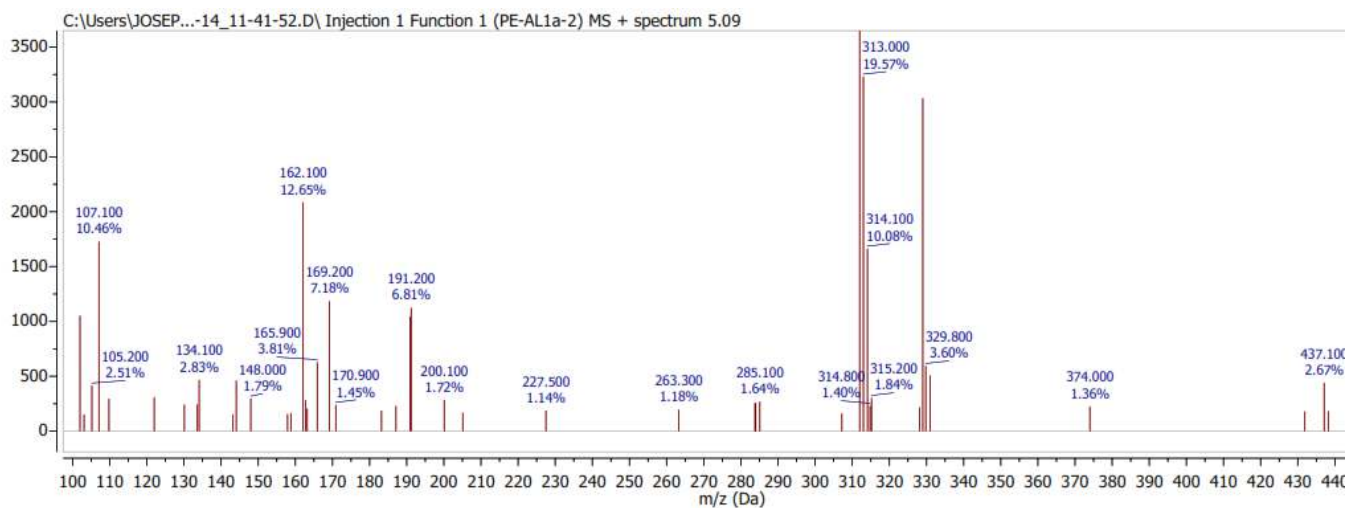


Figure S8: HRMS ESI-Positive mode of compound **4a**

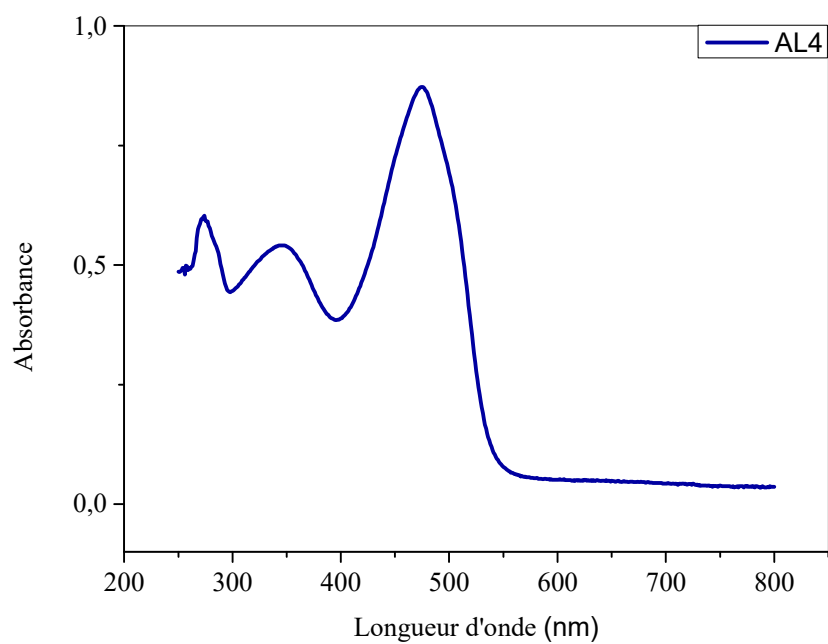
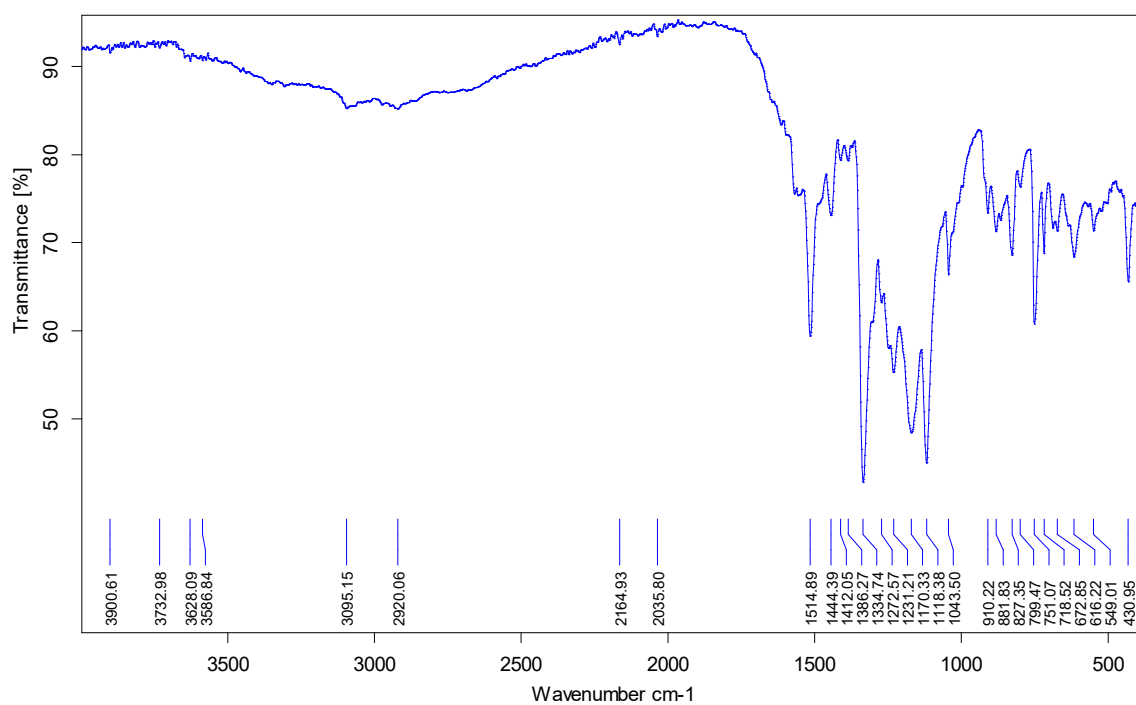


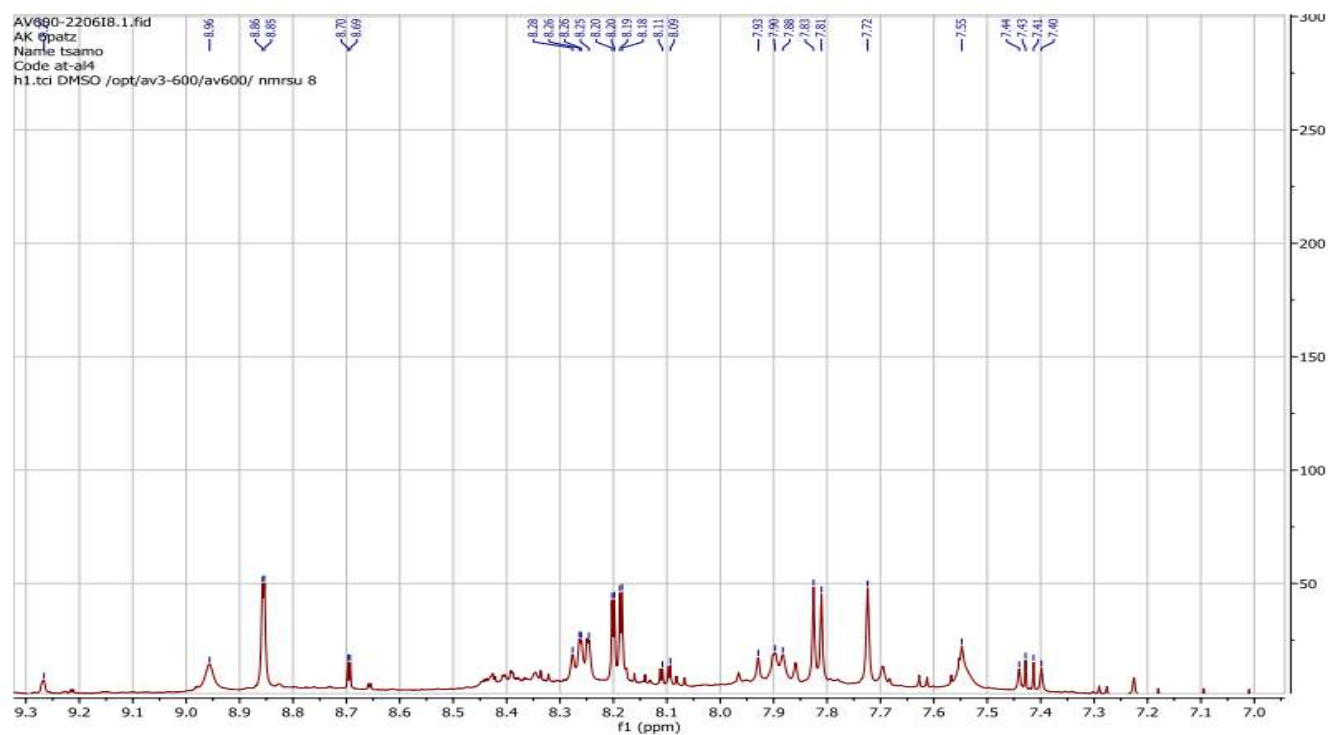
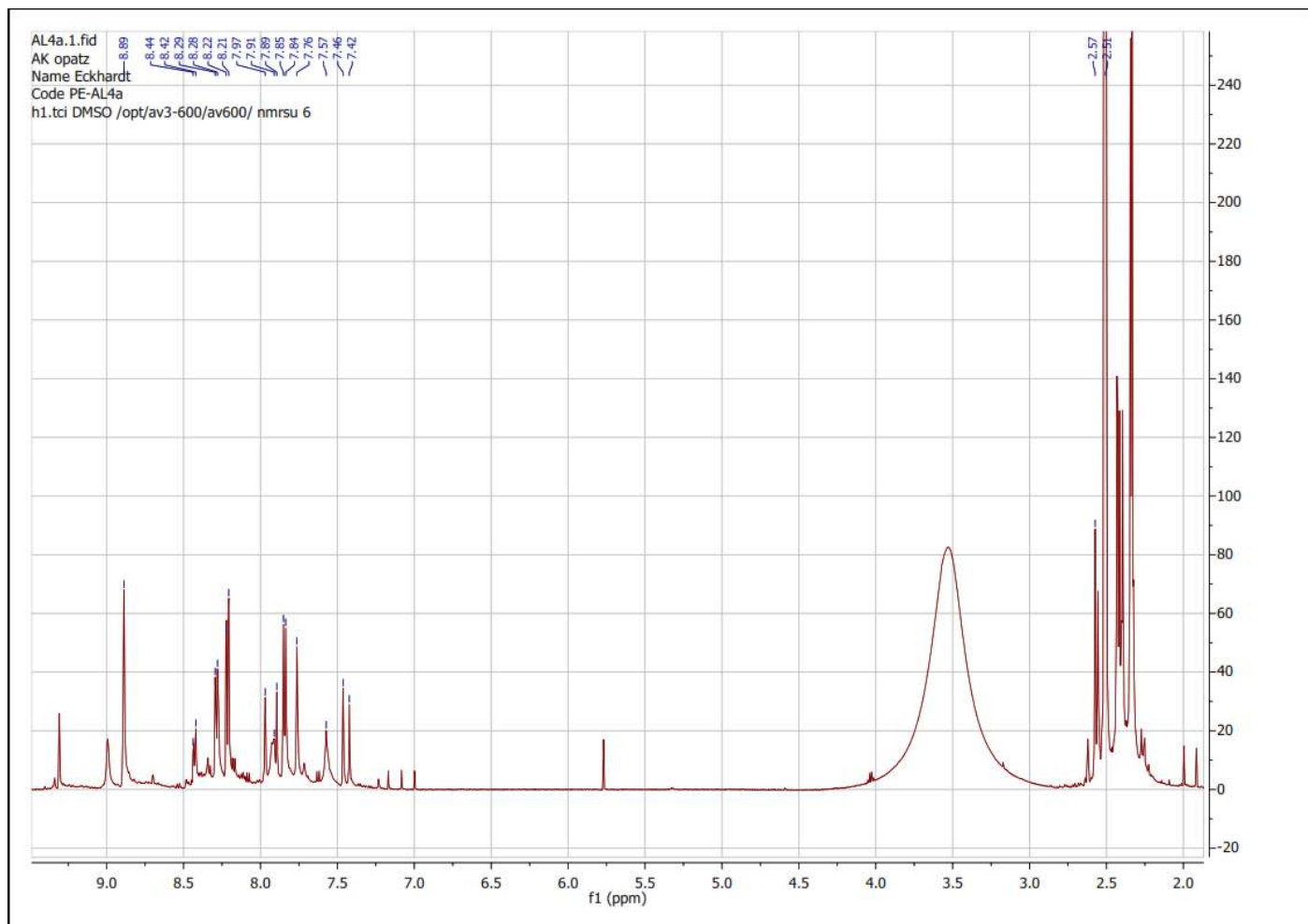
Figure S9: UV spectrum of compound **4b** in methanol as solvent



C:\Documents and Settings\LCA\Application Data\OPUS_65\MEAS\K-AL4.0	K-AL4	Instrument type and / or accessory	15/10/2021
---	-------	------------------------------------	------------

Seite 1 von 1

Figure S10: IR spectrum of compound **4b**



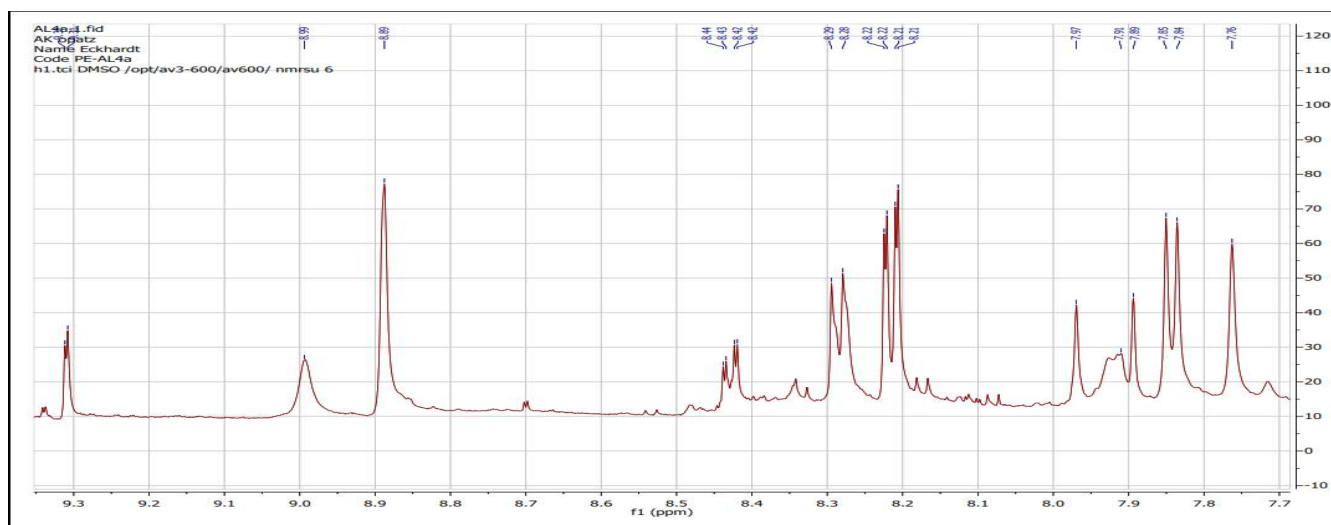
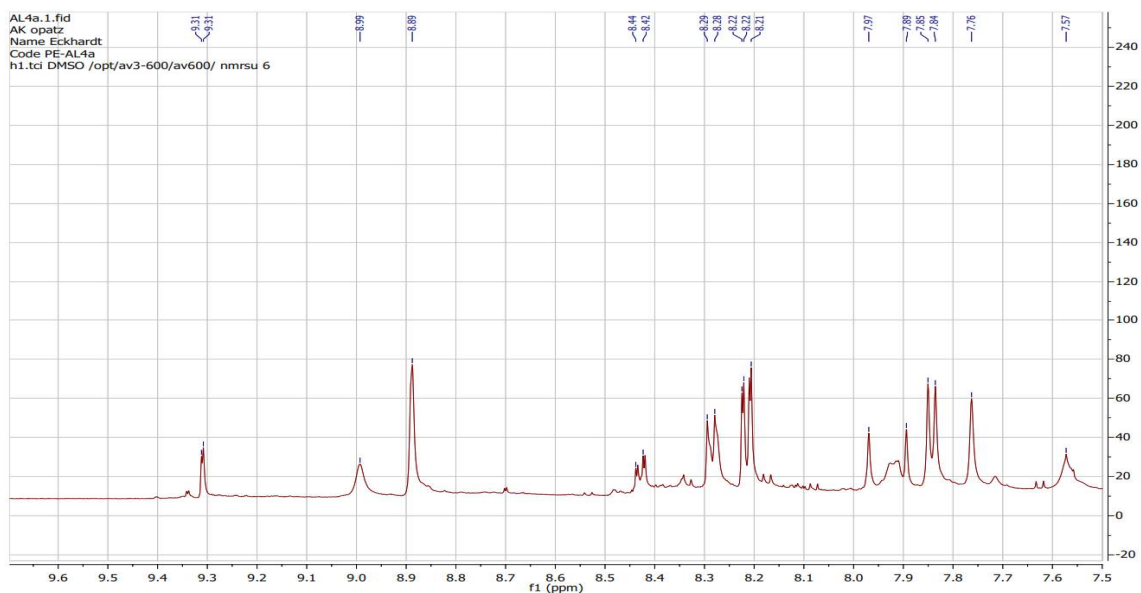
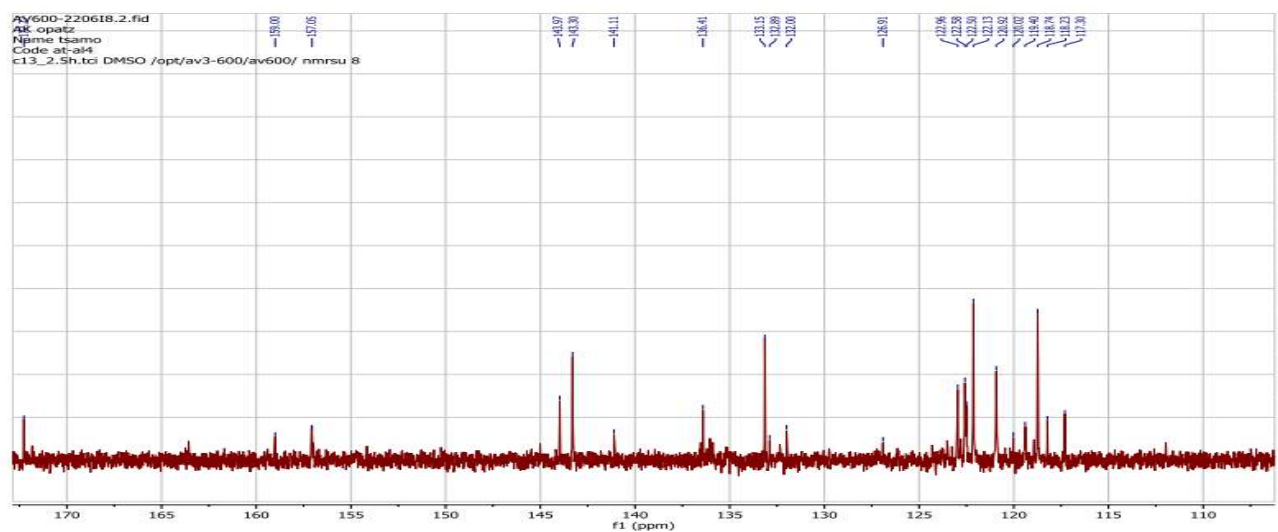
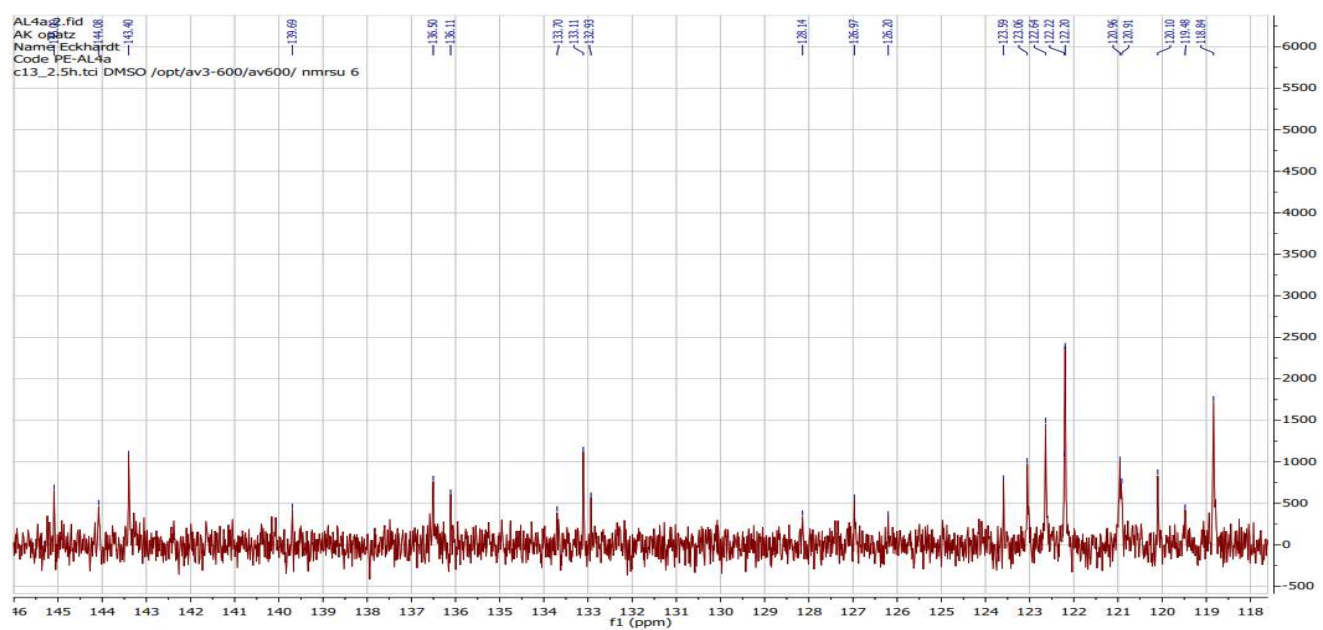
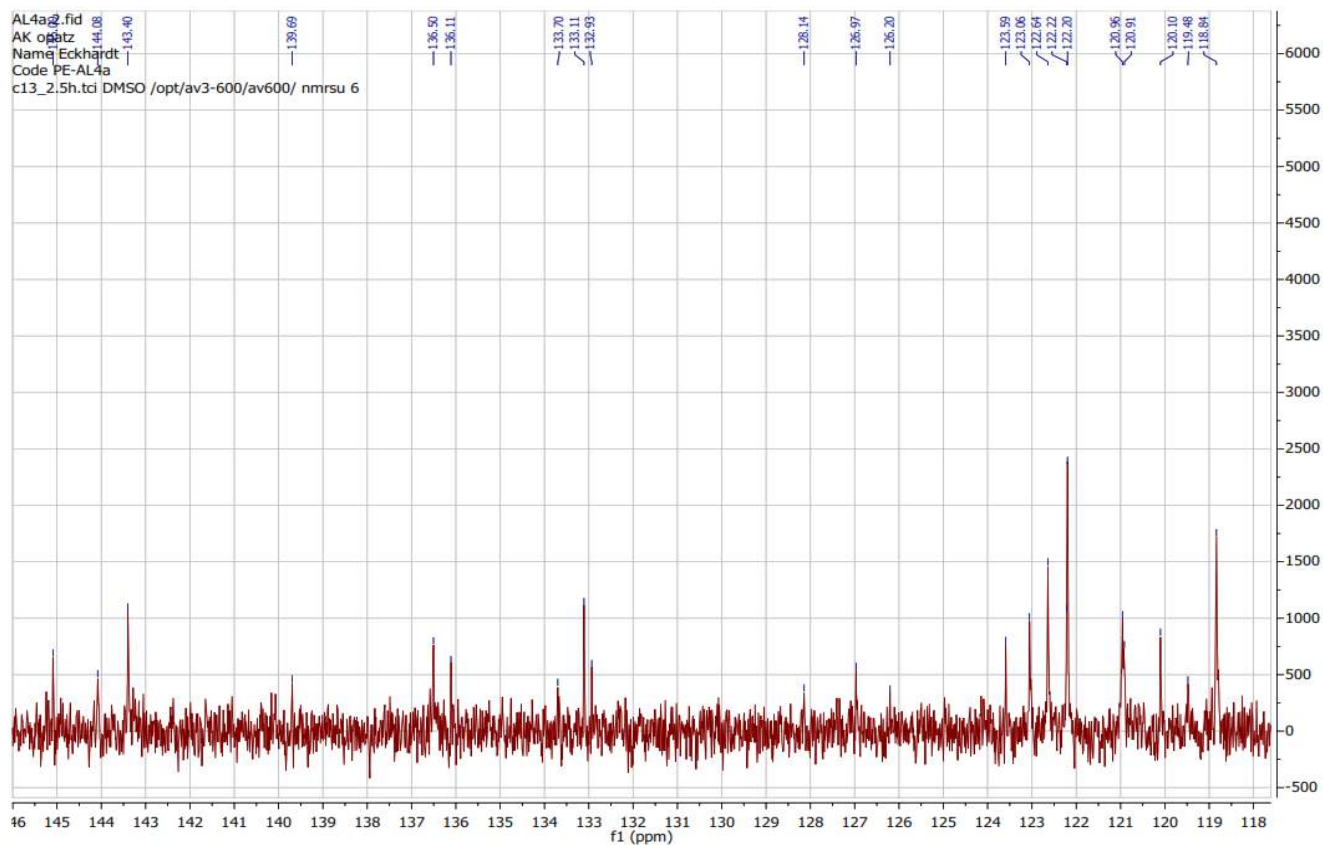


Figure S11: ^1H -NMR (DMSO- d_6 , 400 MHz) spectrum of compound **4b**





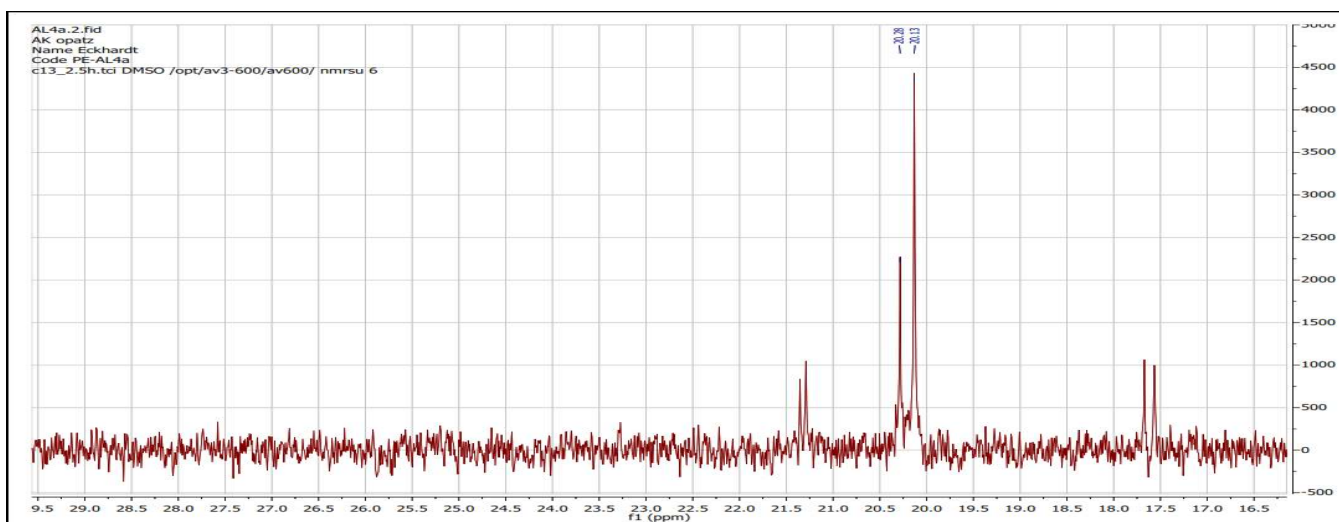
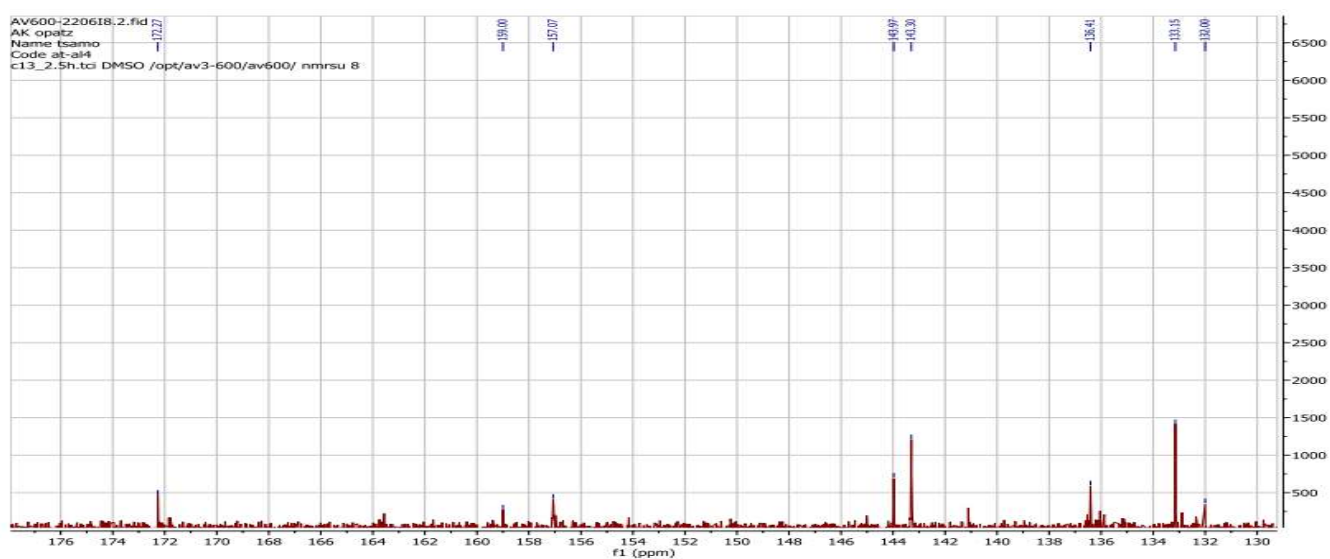
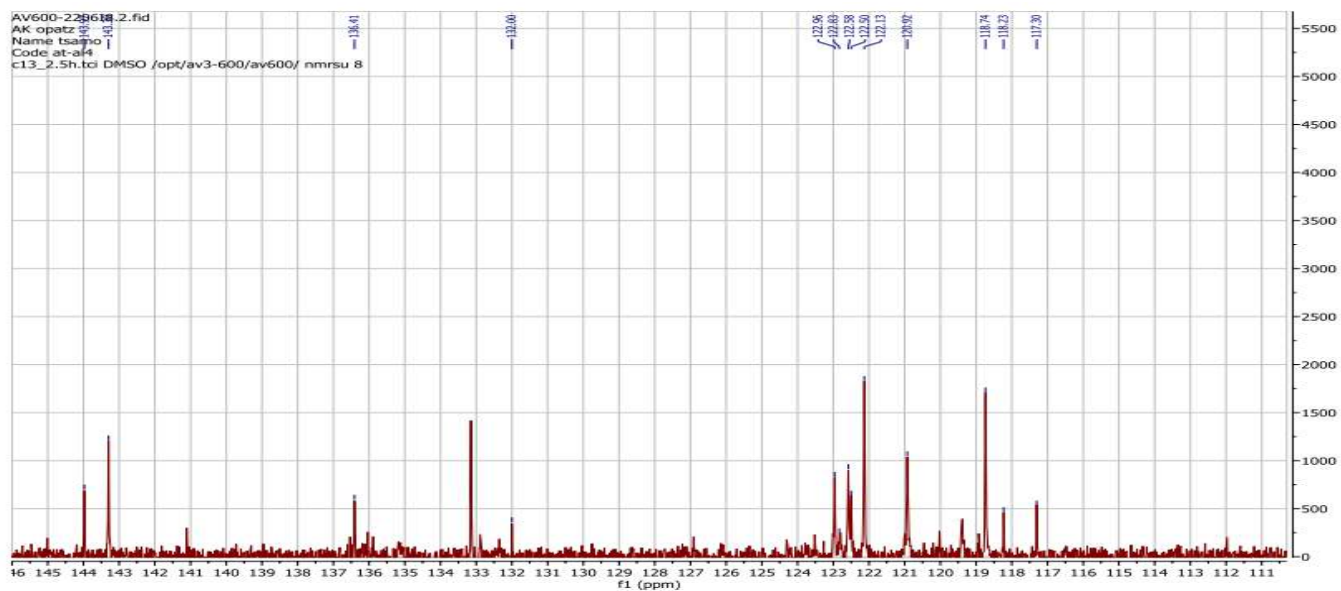


Figure S12: $^{13}\text{C}(\text{H})\text{-NMR } ^1\text{H}$ (DMSO- d_6 , 100 MHz) of compound **4b**

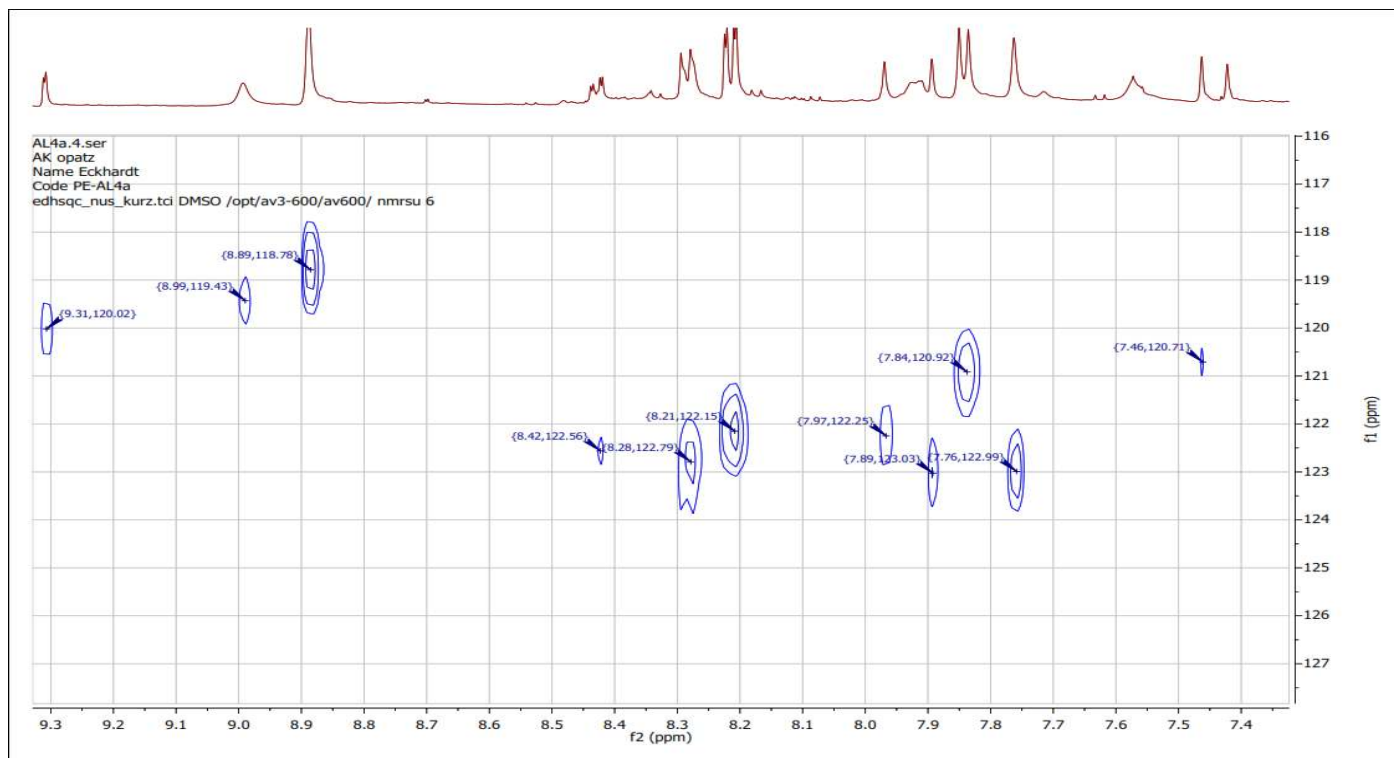


Figure S13: HSQC spectrum of compound **4b**

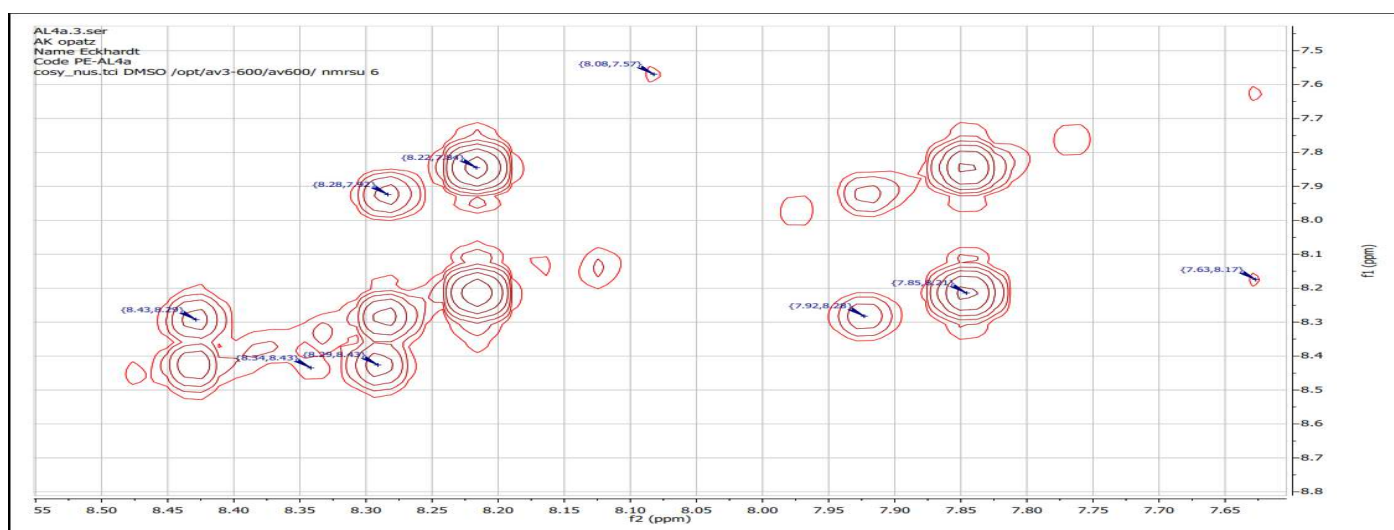


Figure S14: COSY ^1H - ^1H spectrum of compound **4b**

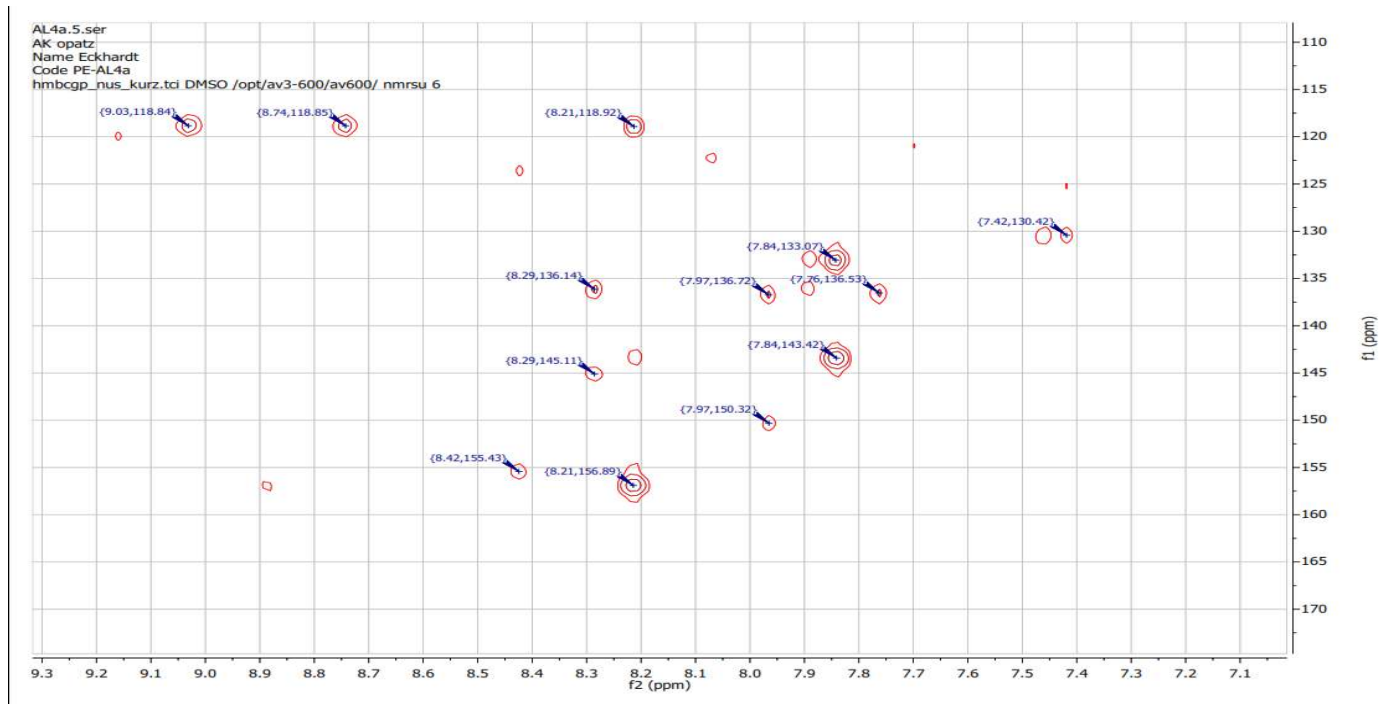
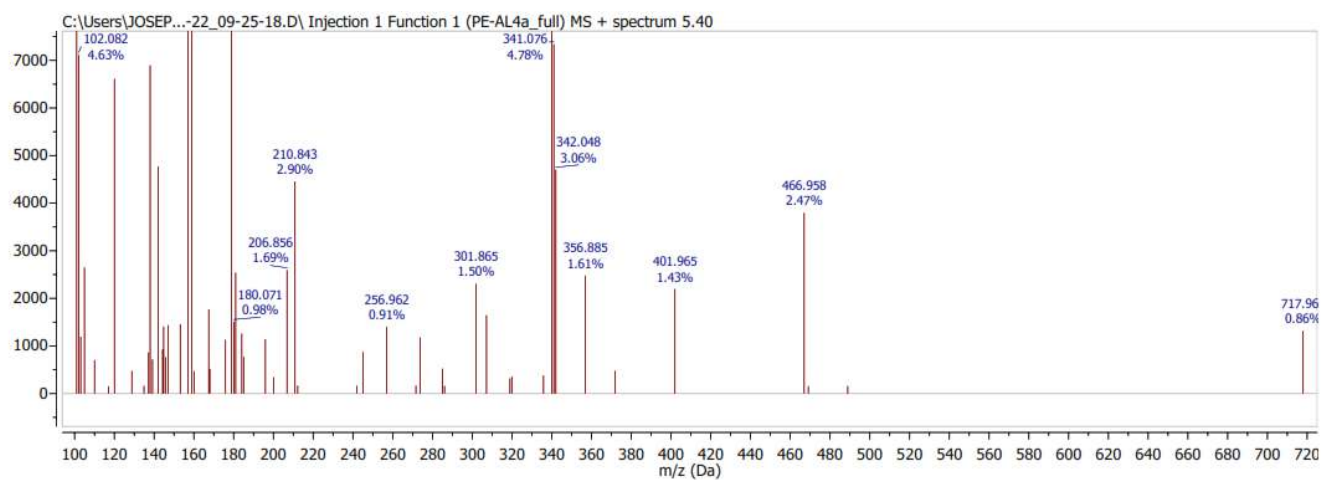


Figure S15: HMBC spectrum of compound **4b**



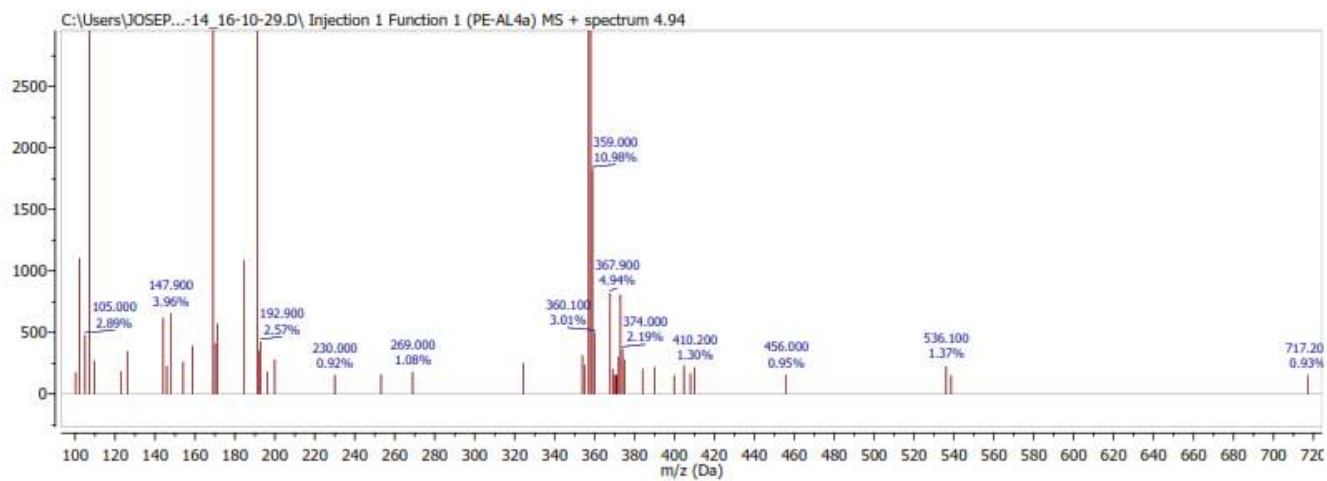


Figure S16: HRMS ESI-Positive mode of compound **4b**

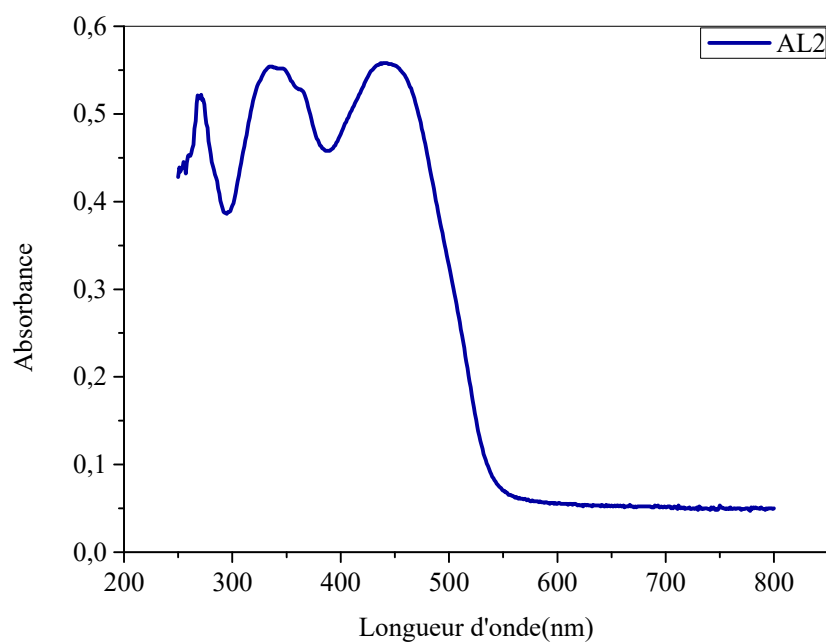
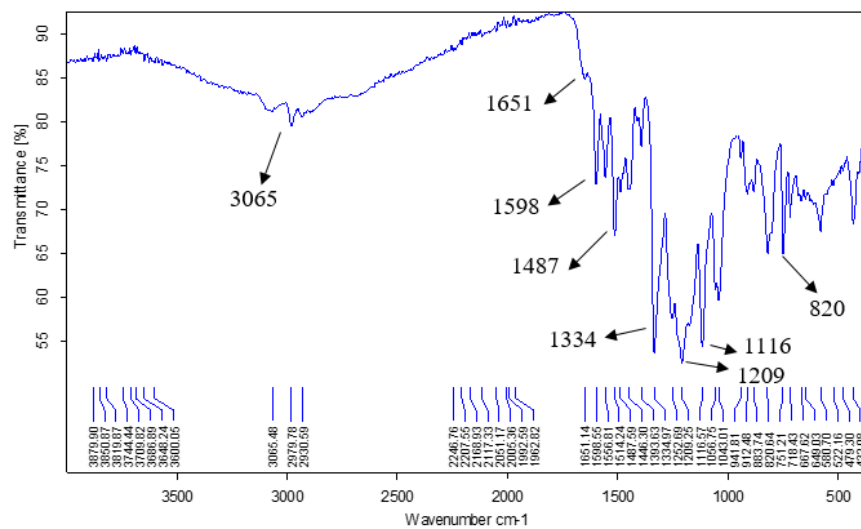
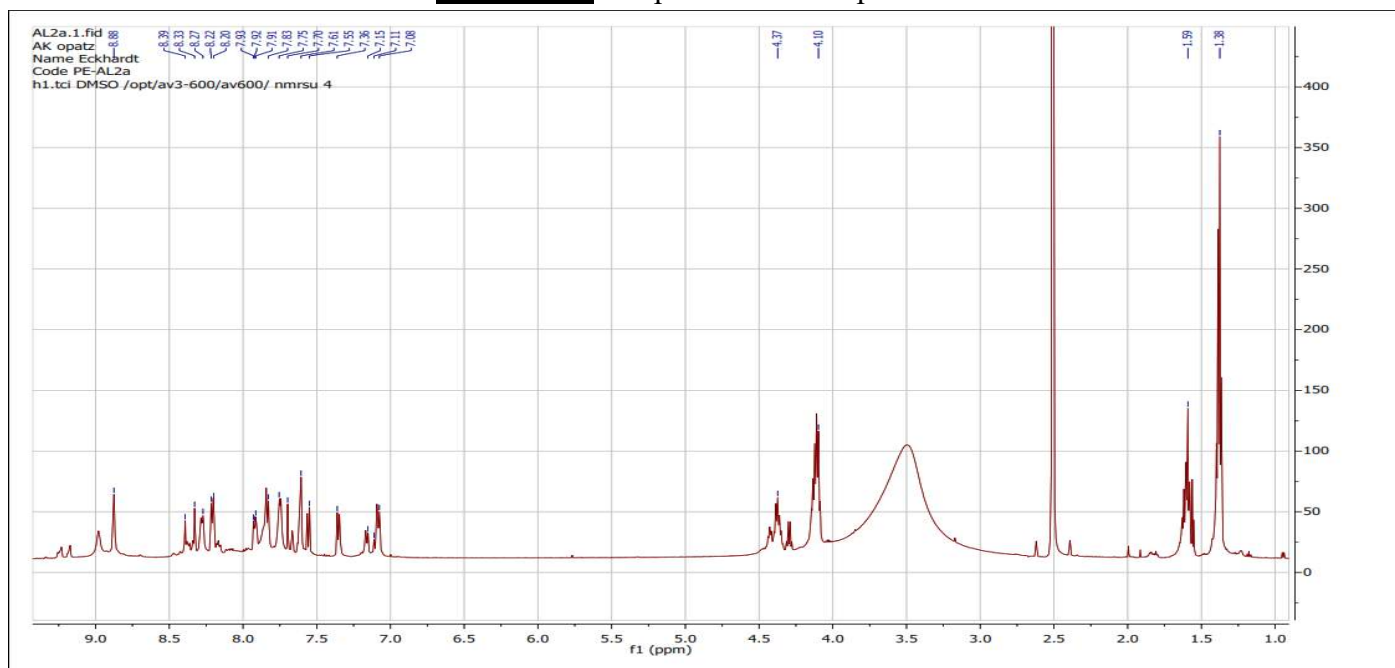


Figure S17: UV spectrum of compound **4c** in Methanol as solvent



C:\Documents and Settings\LCA\Application Data\OPUS_85\MEAS\K-AL2.0	K-AL2	Instrument type and / or accessory	15/10/2021
---	-------	------------------------------------	------------

Figure S18: IR spectrum of compound 4c



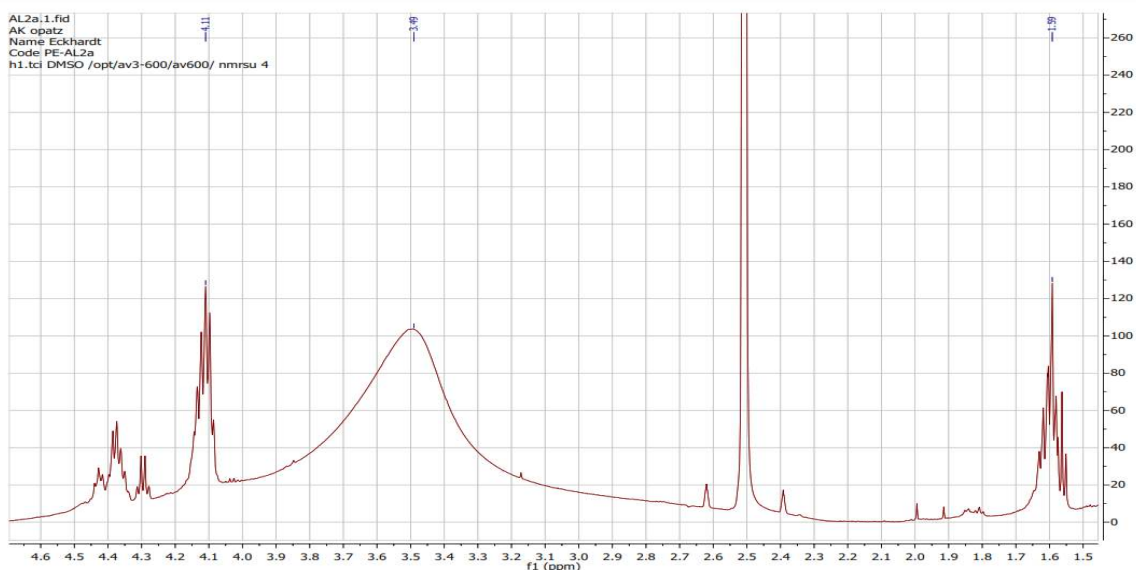
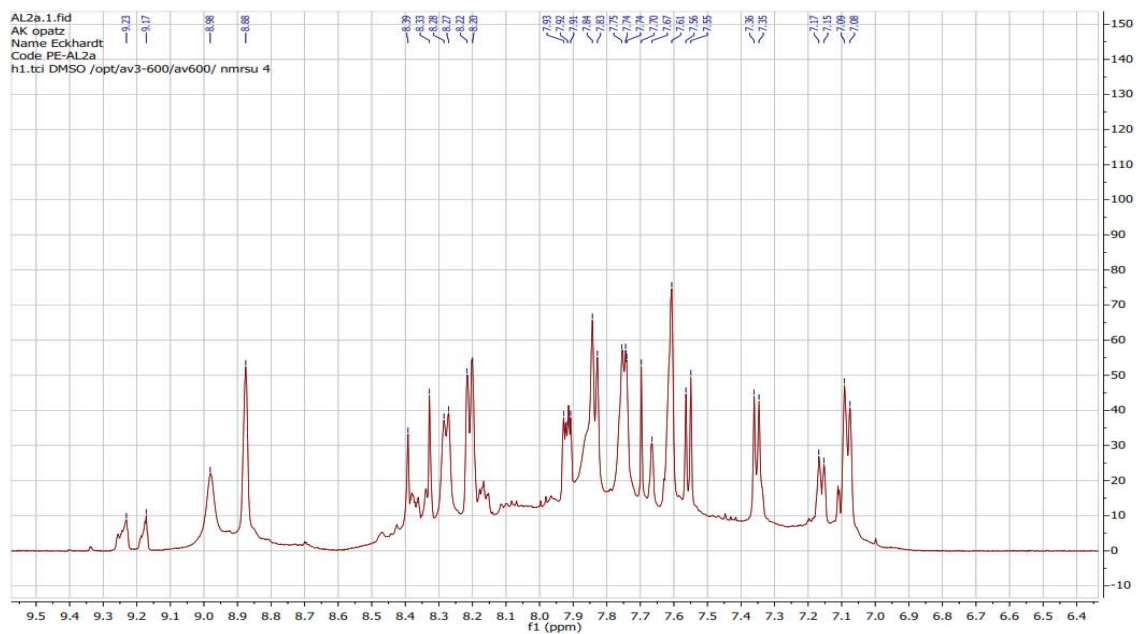
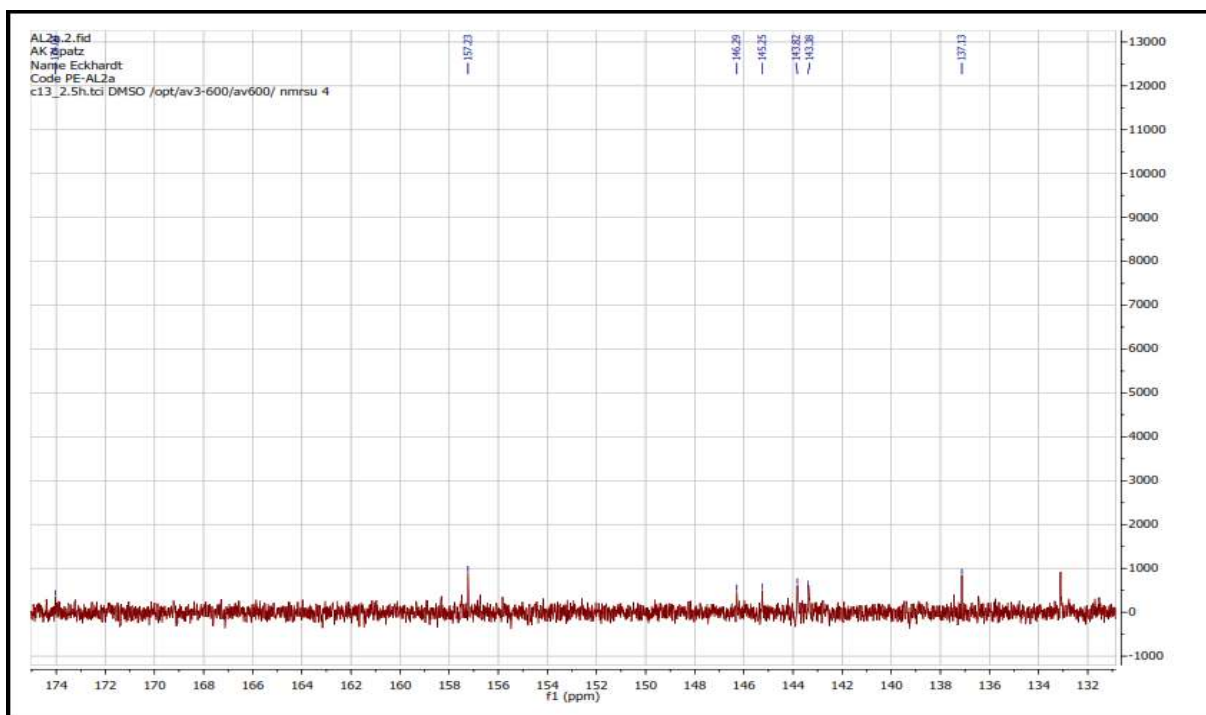
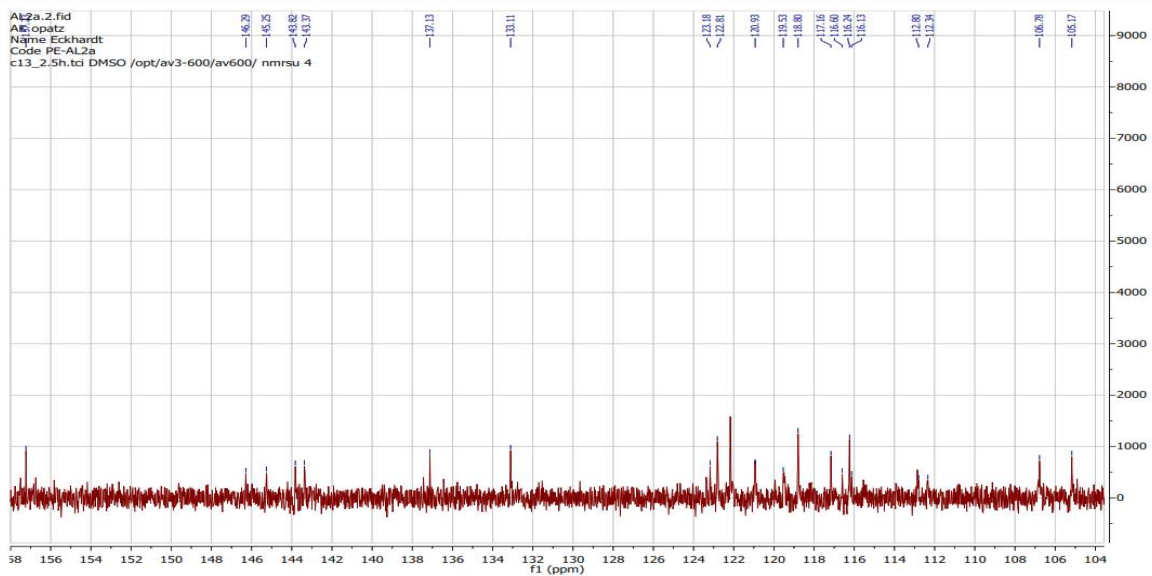


Figure S19: ^1H -NMR (DMSO- d_6 , 400 MHz) spectrum of compound **4c**



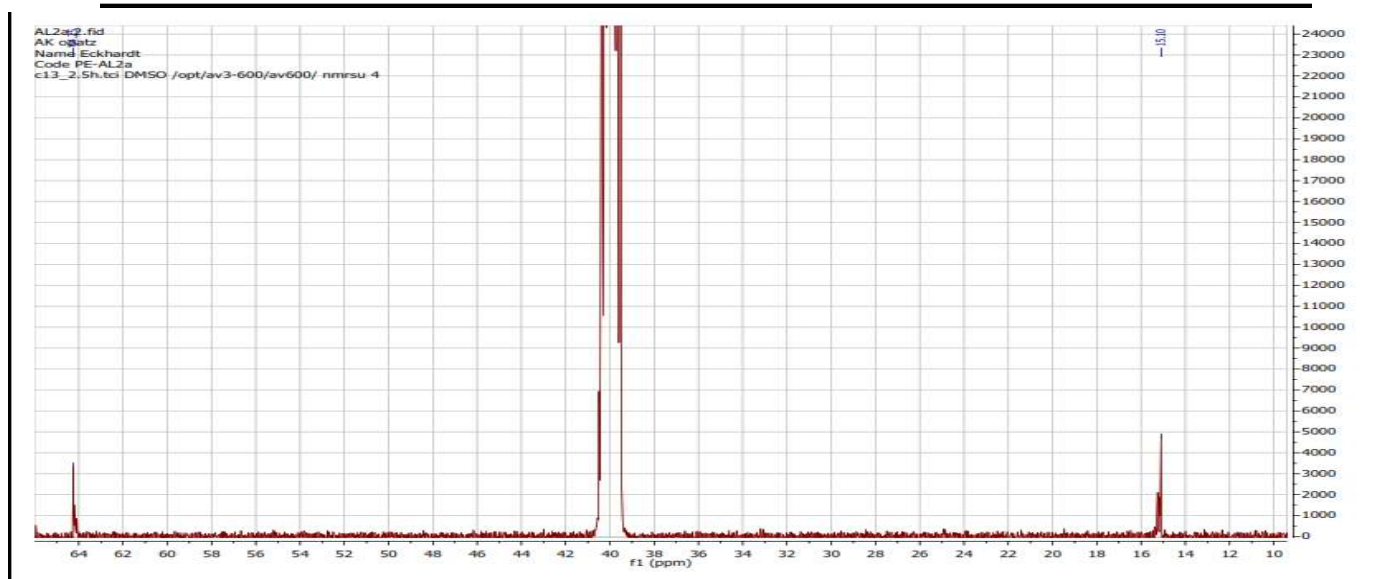
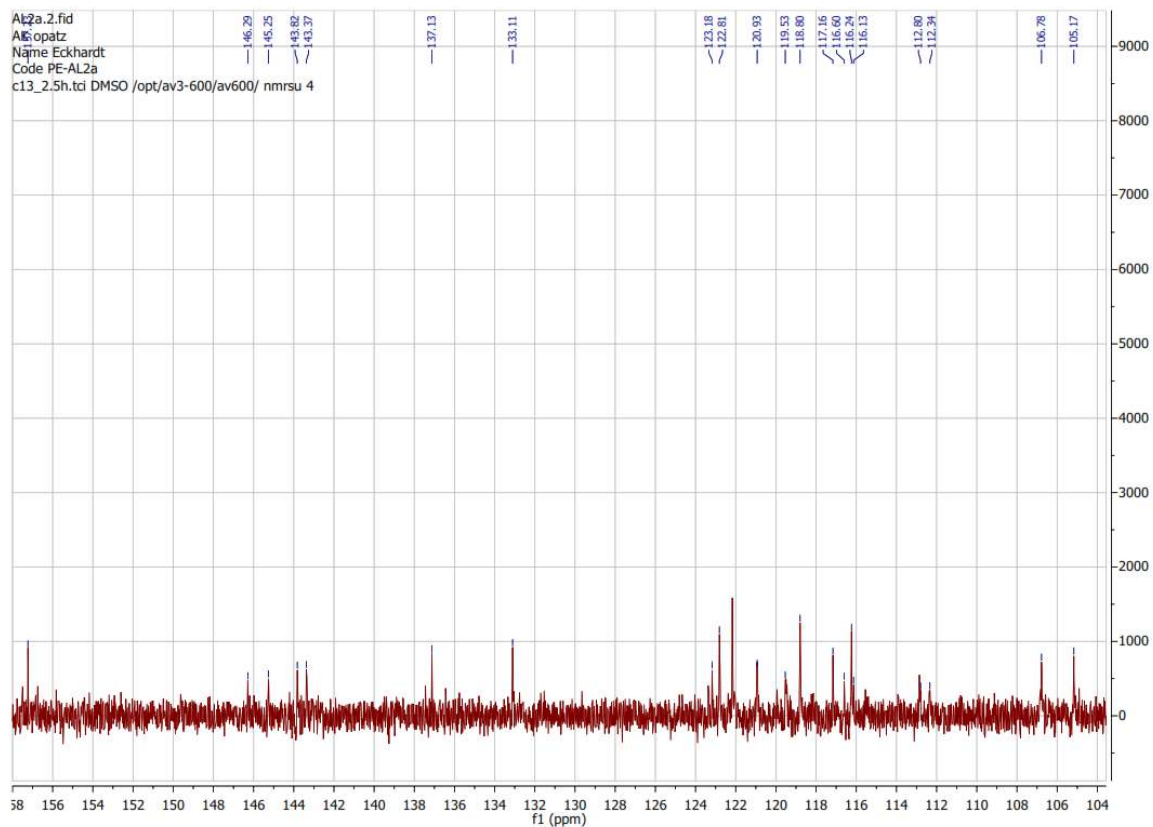


Figure S20: $^{13}\text{C}(^1\text{H})$ -NMR (DMSO- d_6 , 100 MHz) of compound **4c**

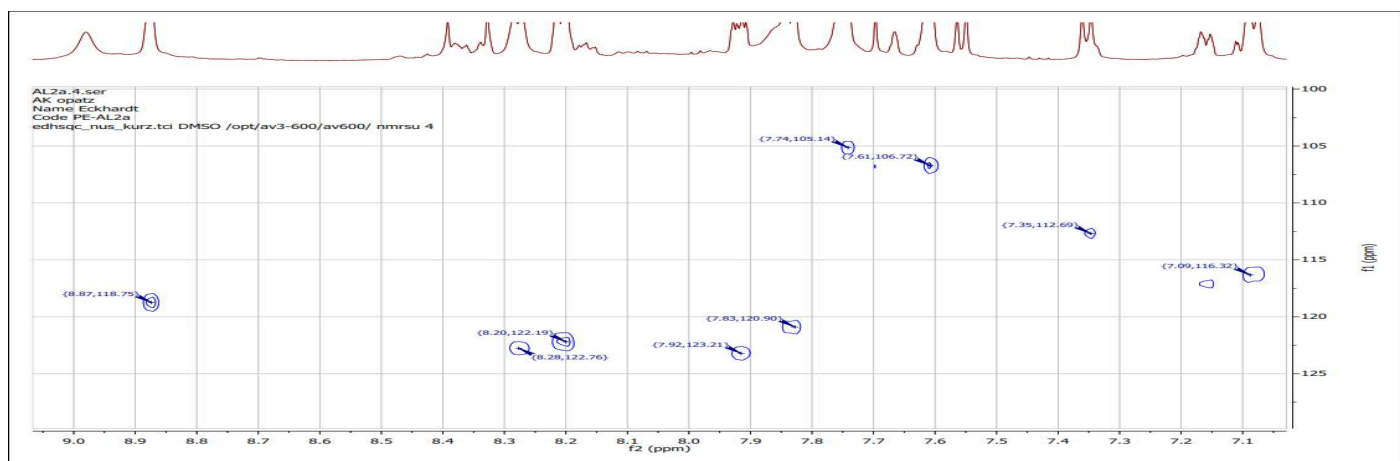


Figure S21: HSQC spectrum of compound **4c**

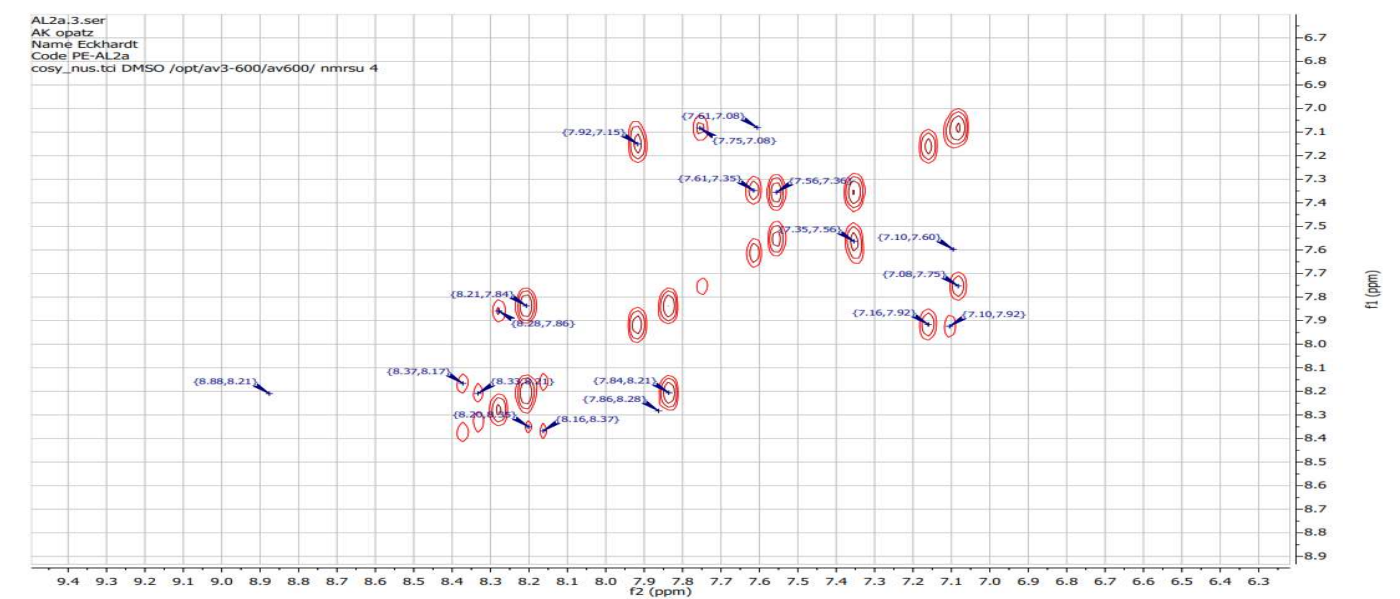
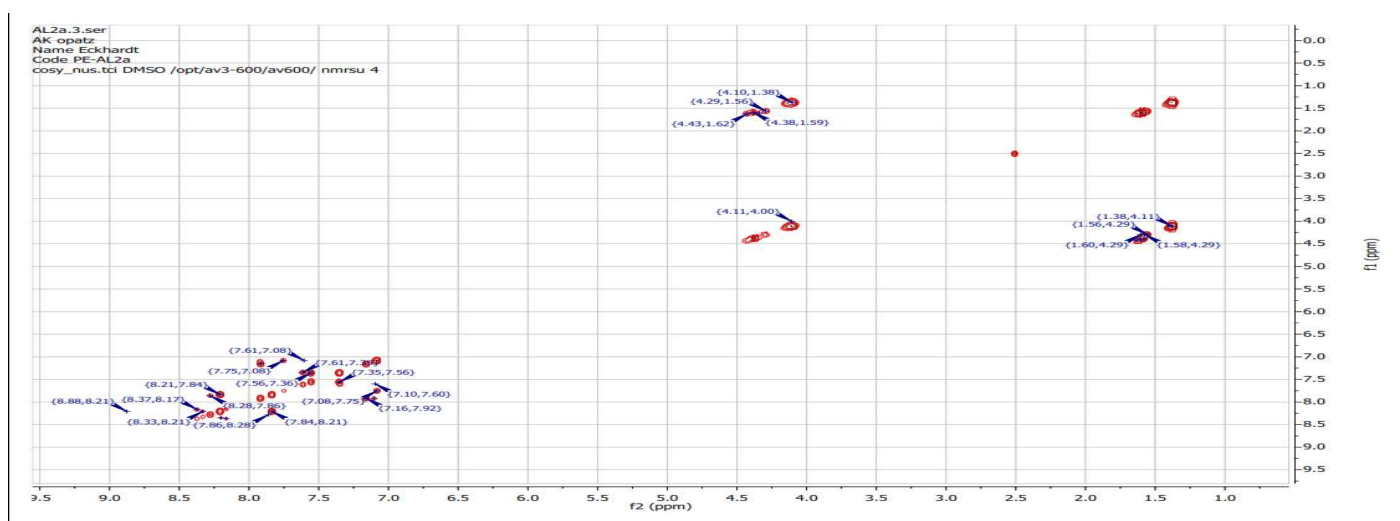


Figure S22: COSY 1H-1H spectrum of compound **4c**

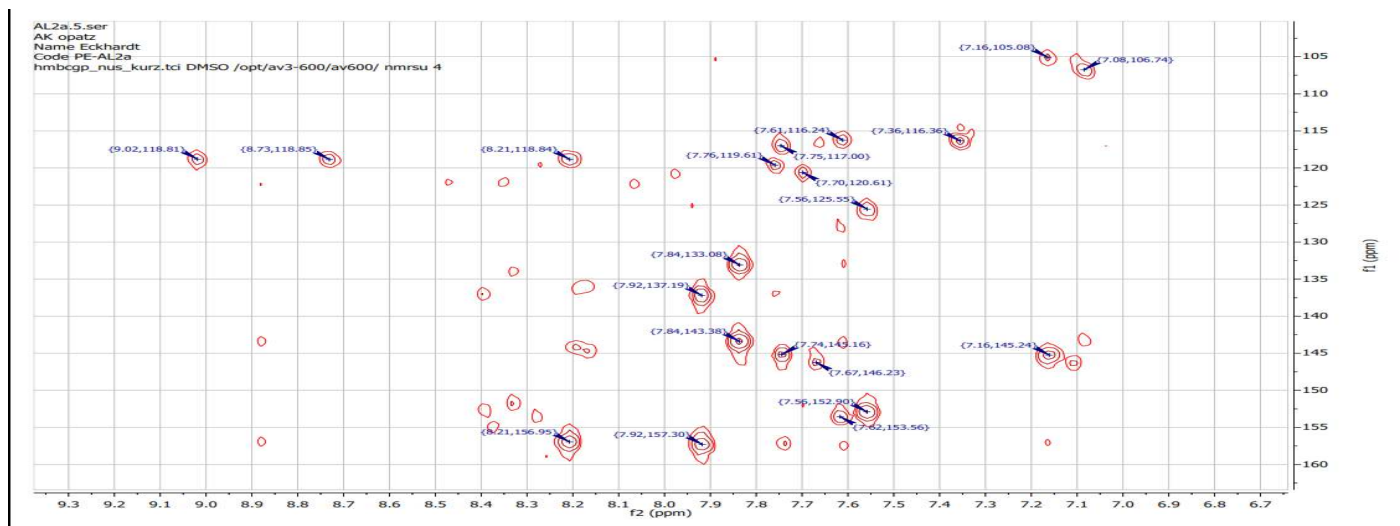


Figure S23: HMBC spectrum of compound **4c**

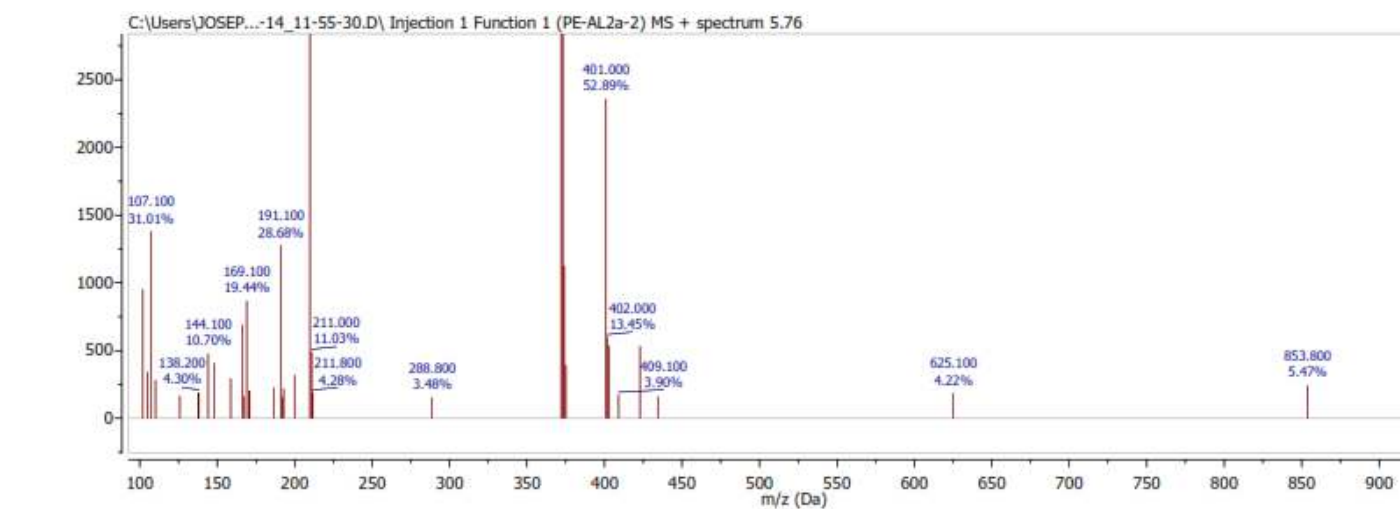
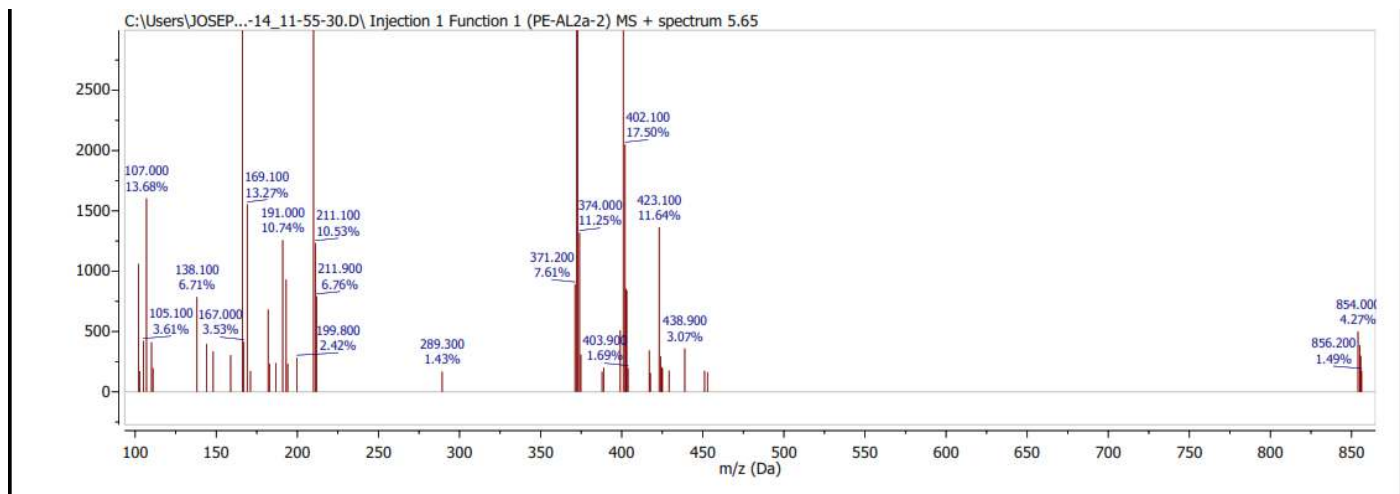


Figure S24: HRMS ESI-Positive mode of compound **4c**

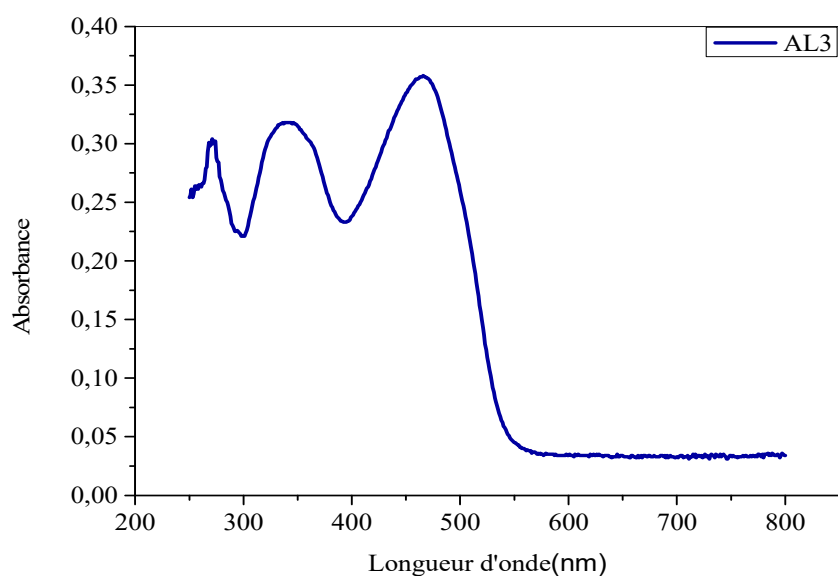
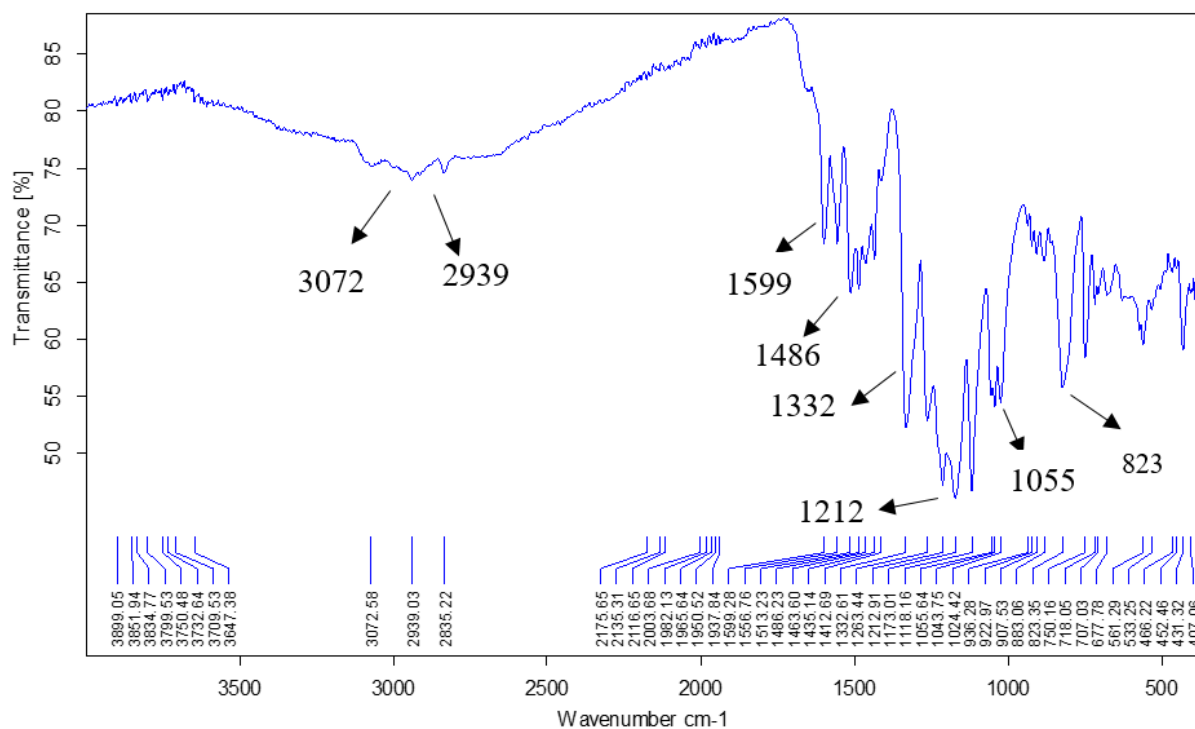


Figure S25: UV spectrum of compound **4d** in methanol as solvent



C:\Documents and Settings\LCA\Application Data\OPUS_65\MEAS\K-AL3.0

K-AL3

Instrument type and / or accessory

15/10/2021

Figure S26: IR spectrum of compound **4d**

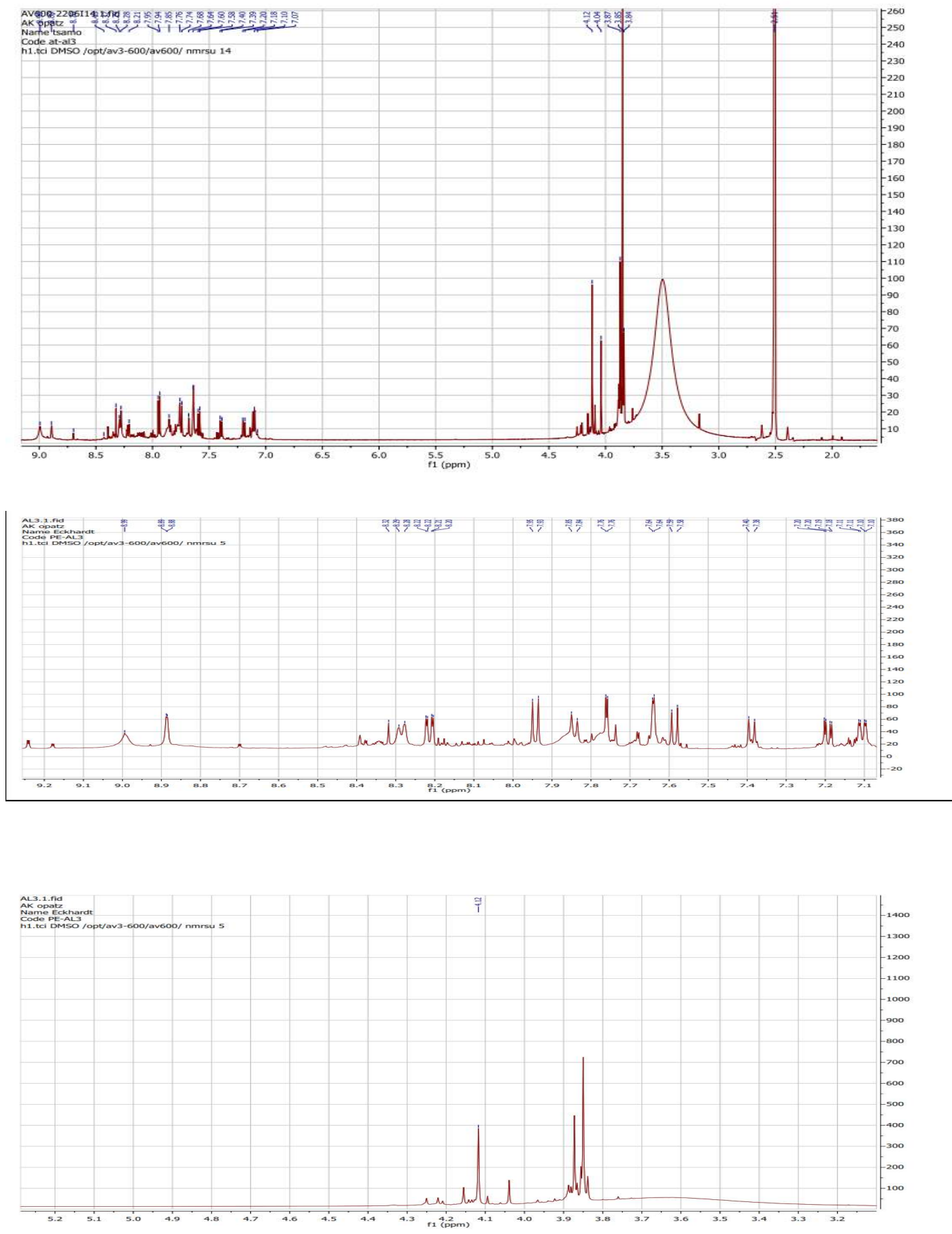


Figure S27: ^1H -NMR (DMSO- d_6 , 400 MHz) spectrum of compound **4d**

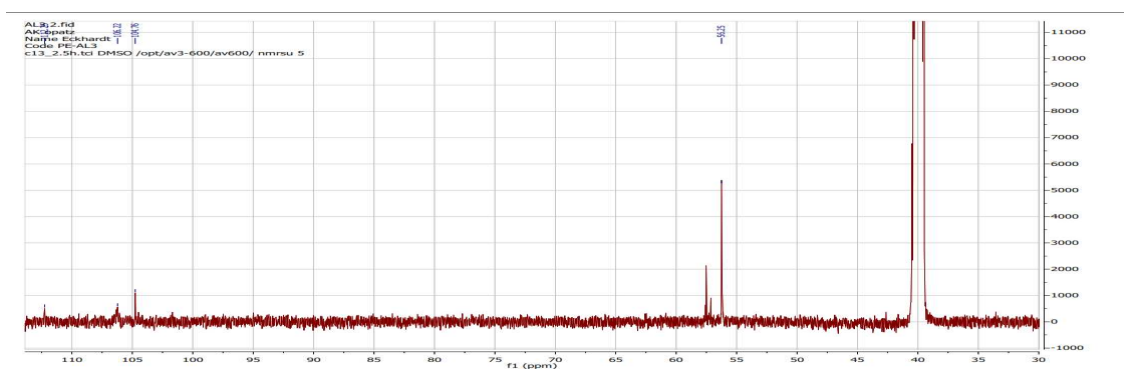
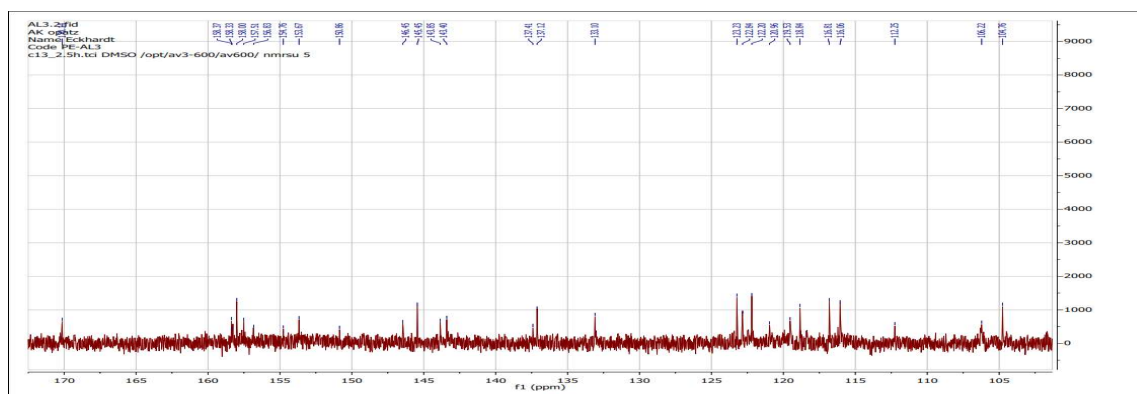
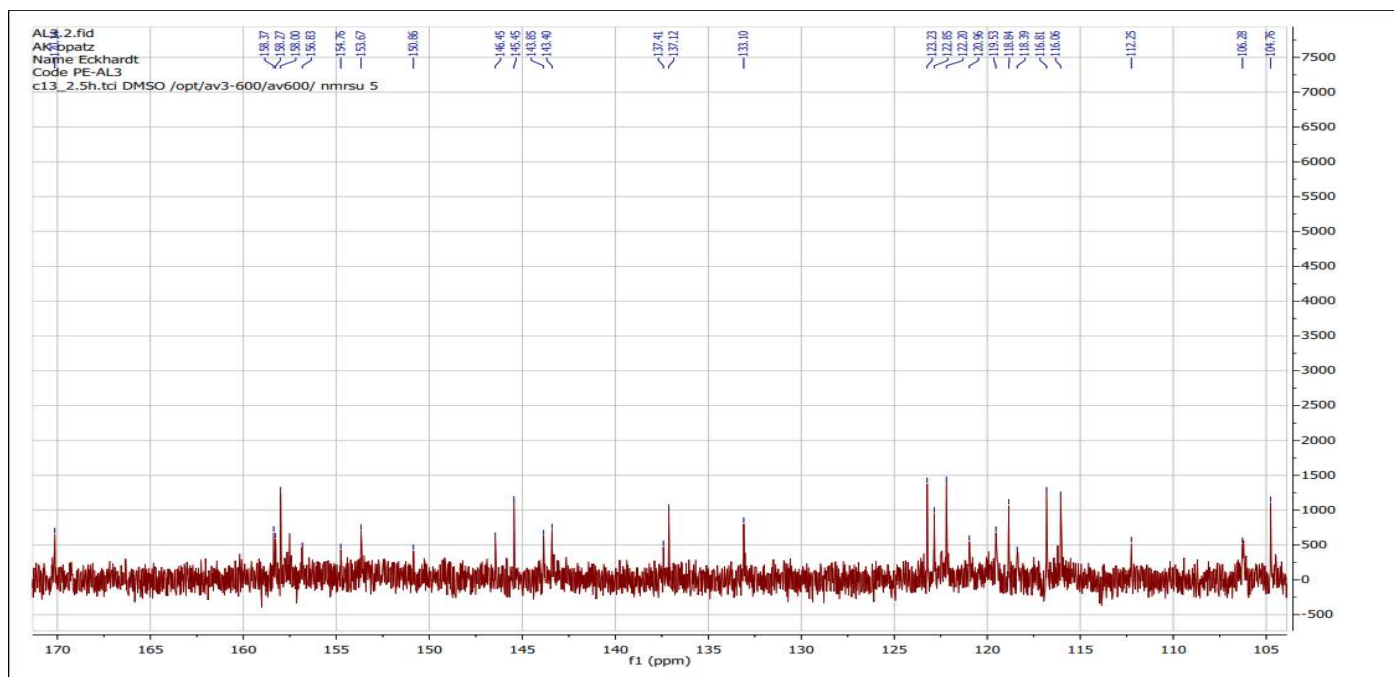


Figure S28: $^{13}\text{C}(\text{H})\text{-NMR } ^1\text{H}$ (DMSO- d_6 , 100 MHz) of compound **4d**

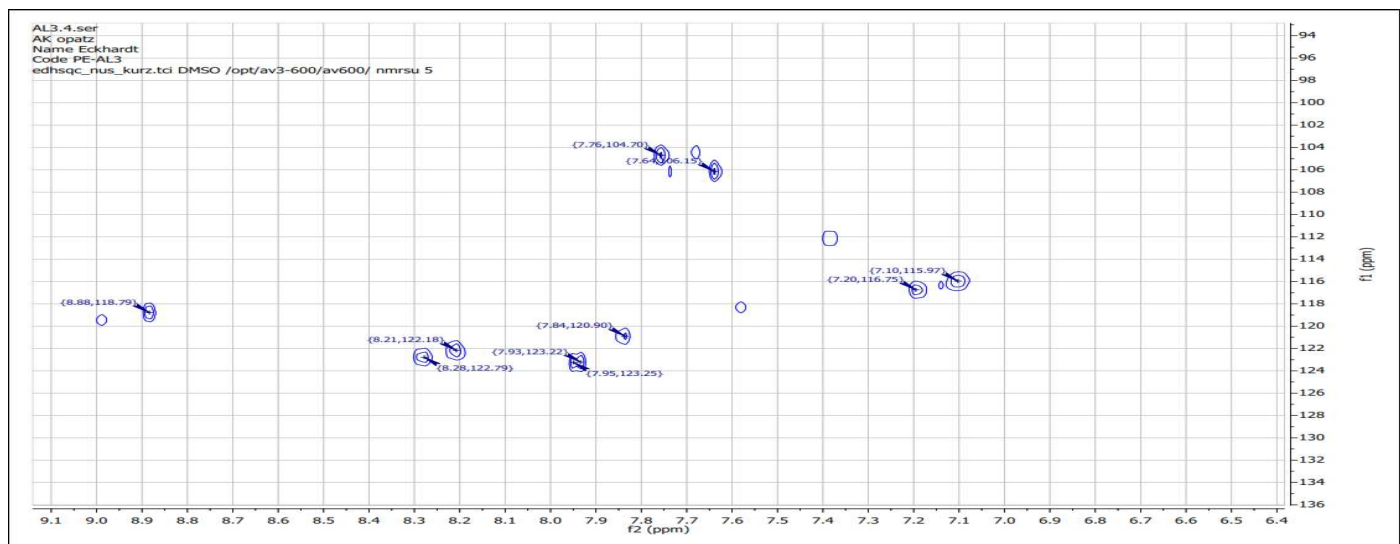
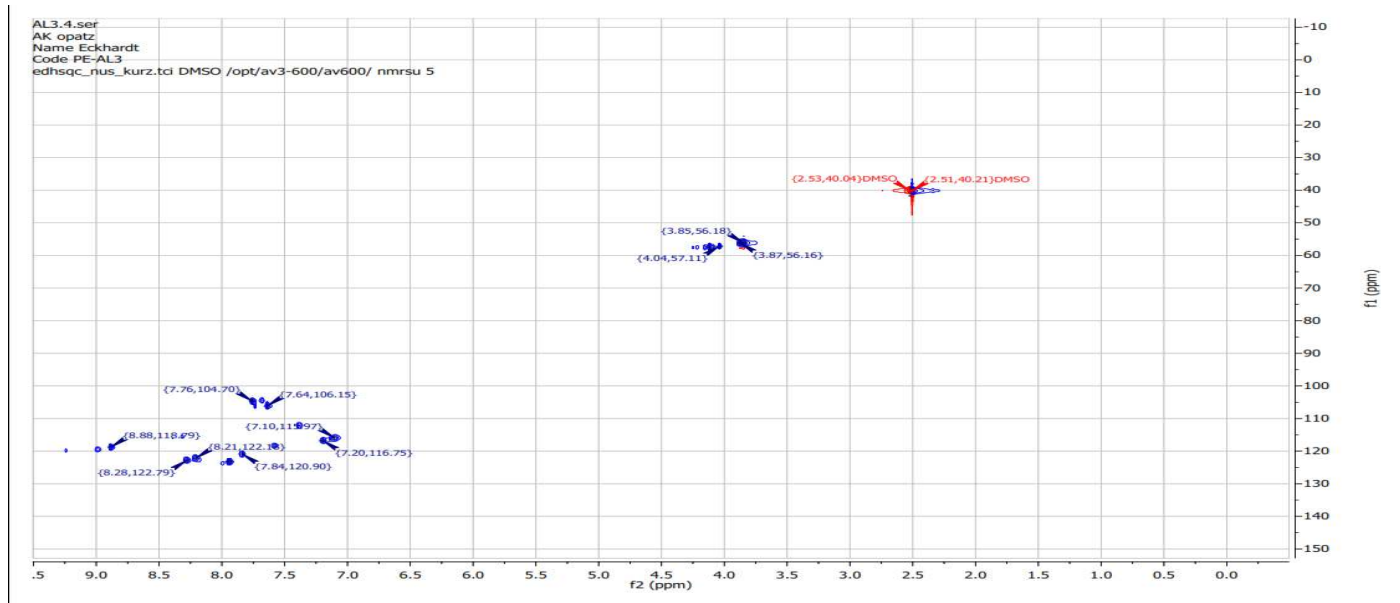


Figure S29: HSQC spectrum of compound **4d**

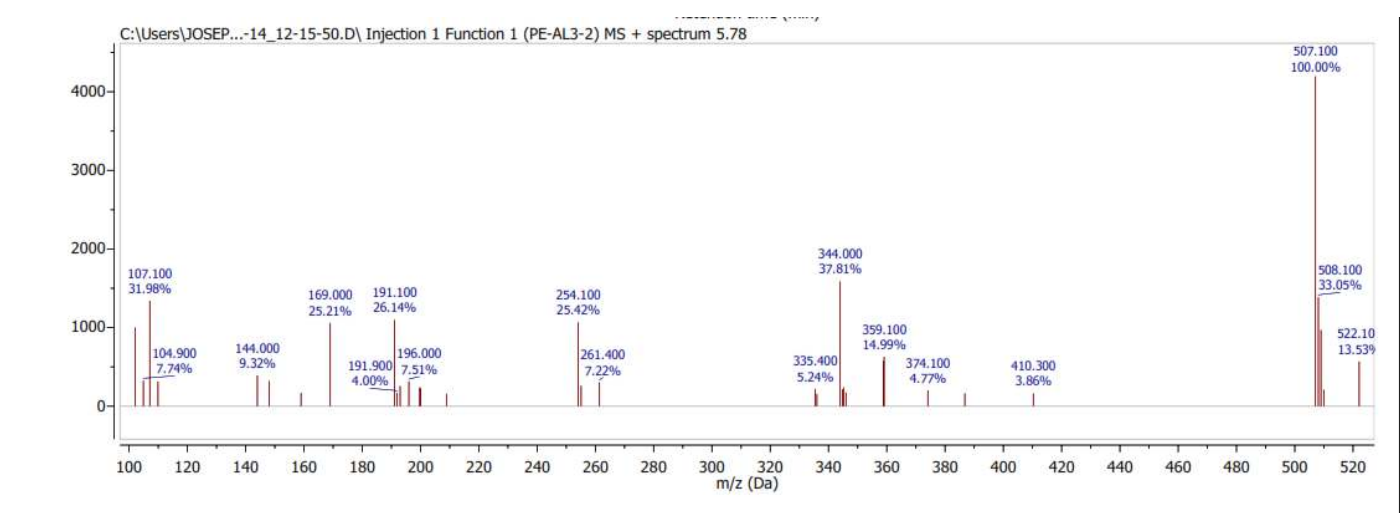
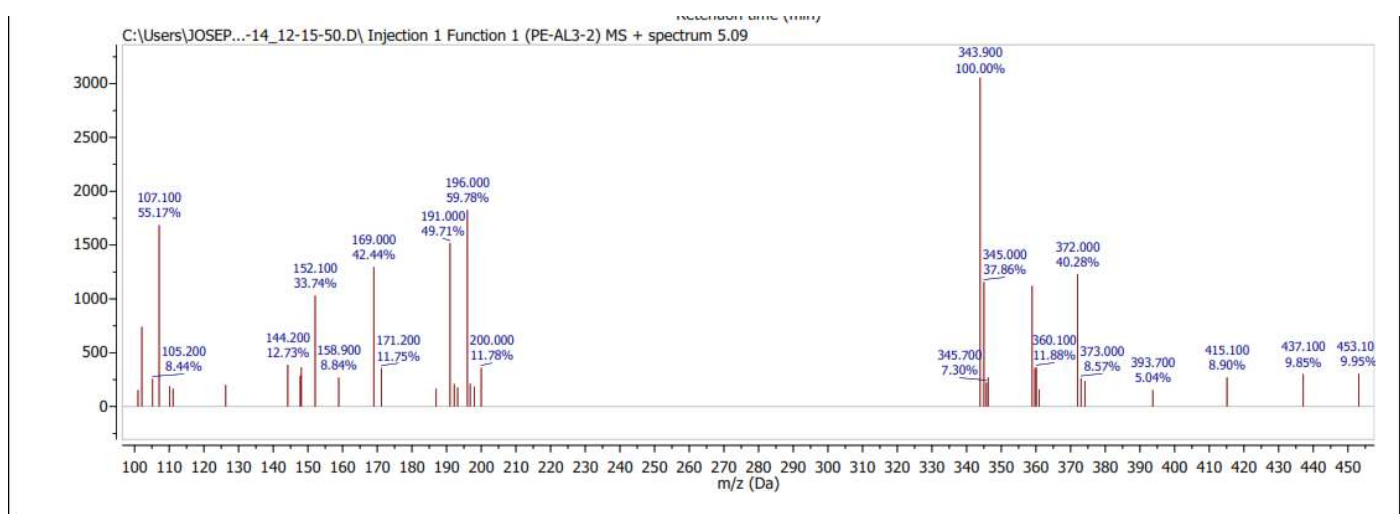
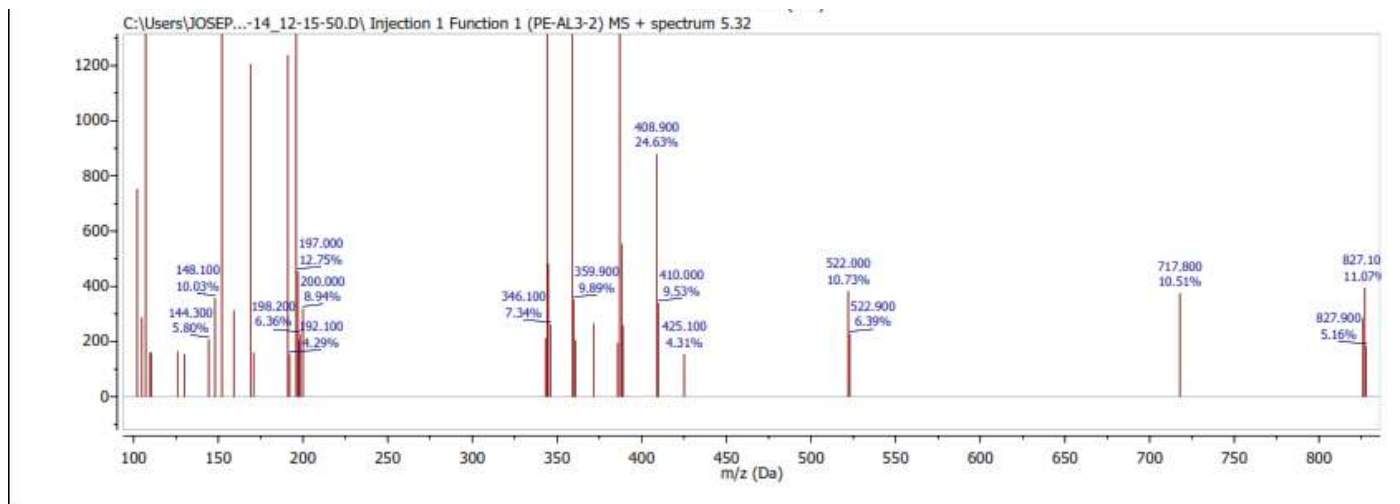


Figure S32: HRMS ESI-Positive mode of compound **4d**

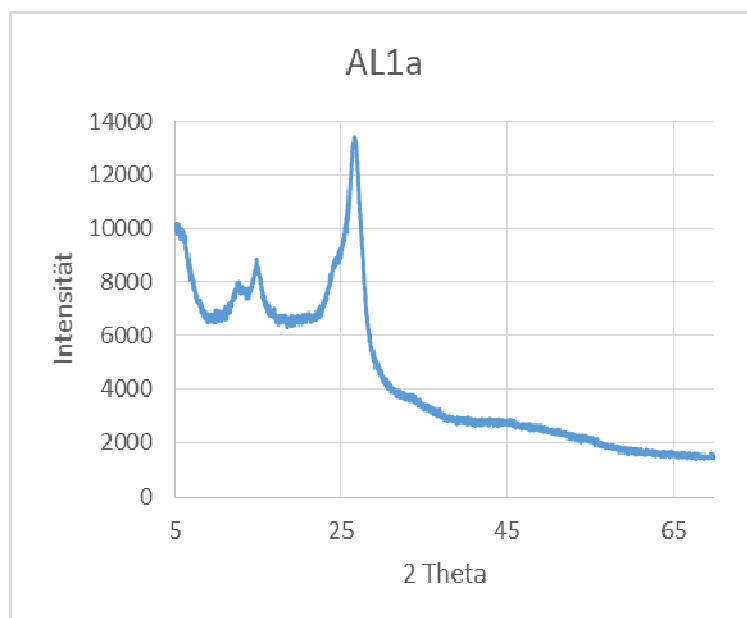


Figure S33: Powder XRD patterns of compound 4a