

# Discovery of New Boswellic Acid Hybrid 1*H*-1,2,3-Triazoles for Diabetic Management: In Vitro and In Silico Studies

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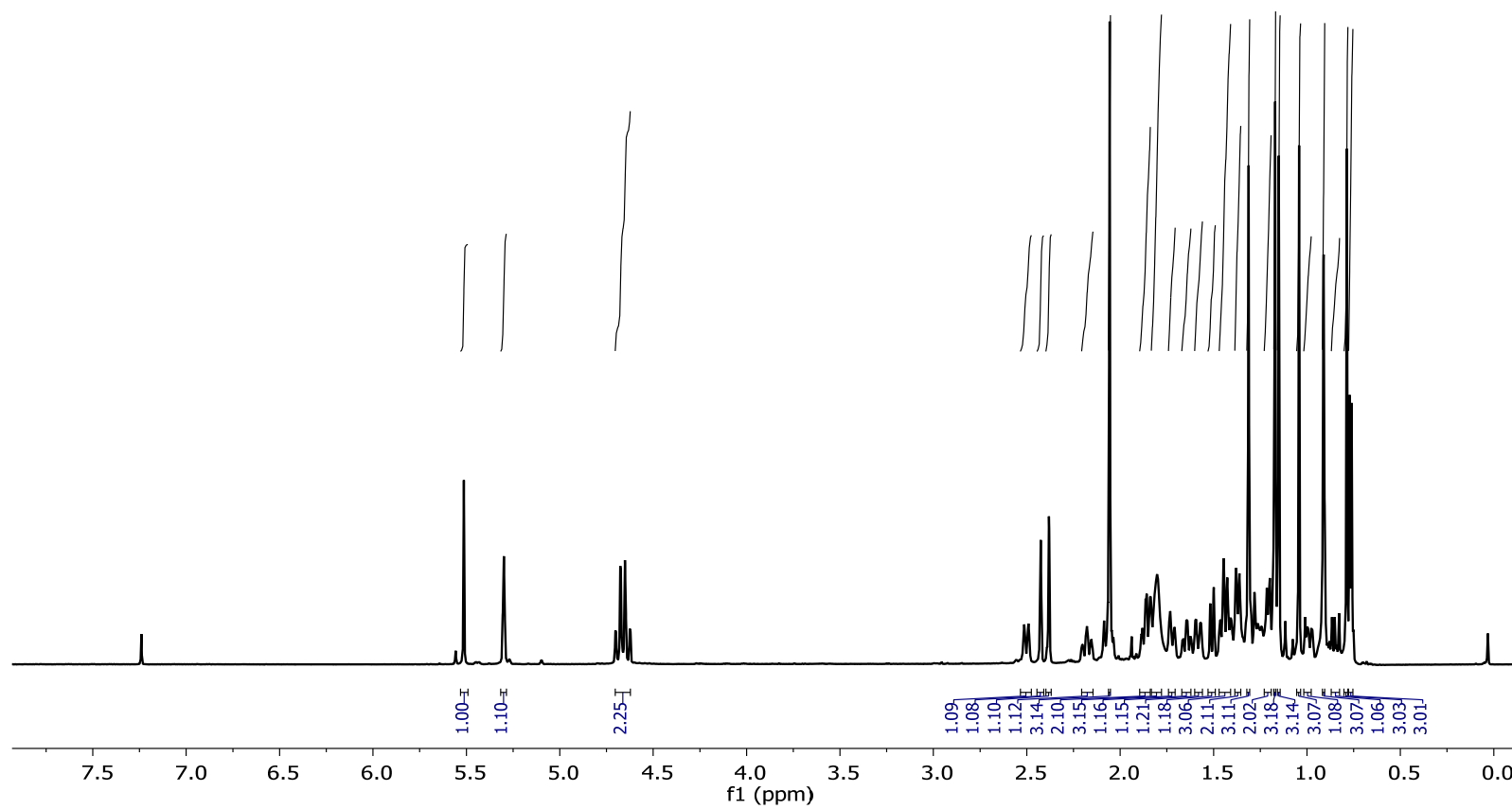
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03-Feb-2020.3.fid  
Dr. Kumar/SK-AKBA-Propargyl/CDCI3  
PROTON



**Figure S1:**  $^1\text{H}$ -NMR spectrum (600 MHz,  $\text{CDCl}_3$ ) of compound 3

03-Feb-2020.5.fid  
Dr. Kumar/SK-AKBA-Propargyl/CDCl<sub>3</sub>  
C13CPD

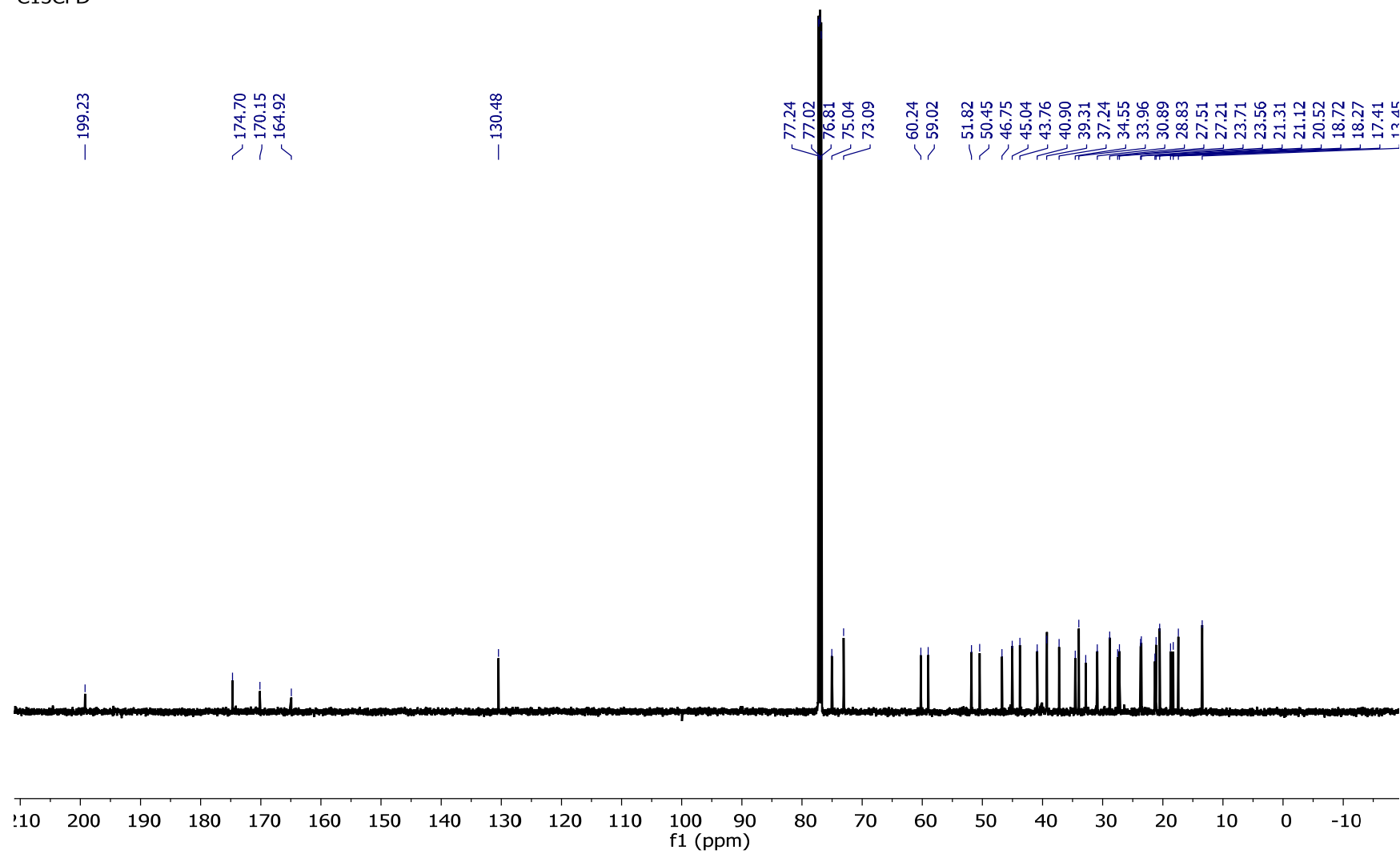
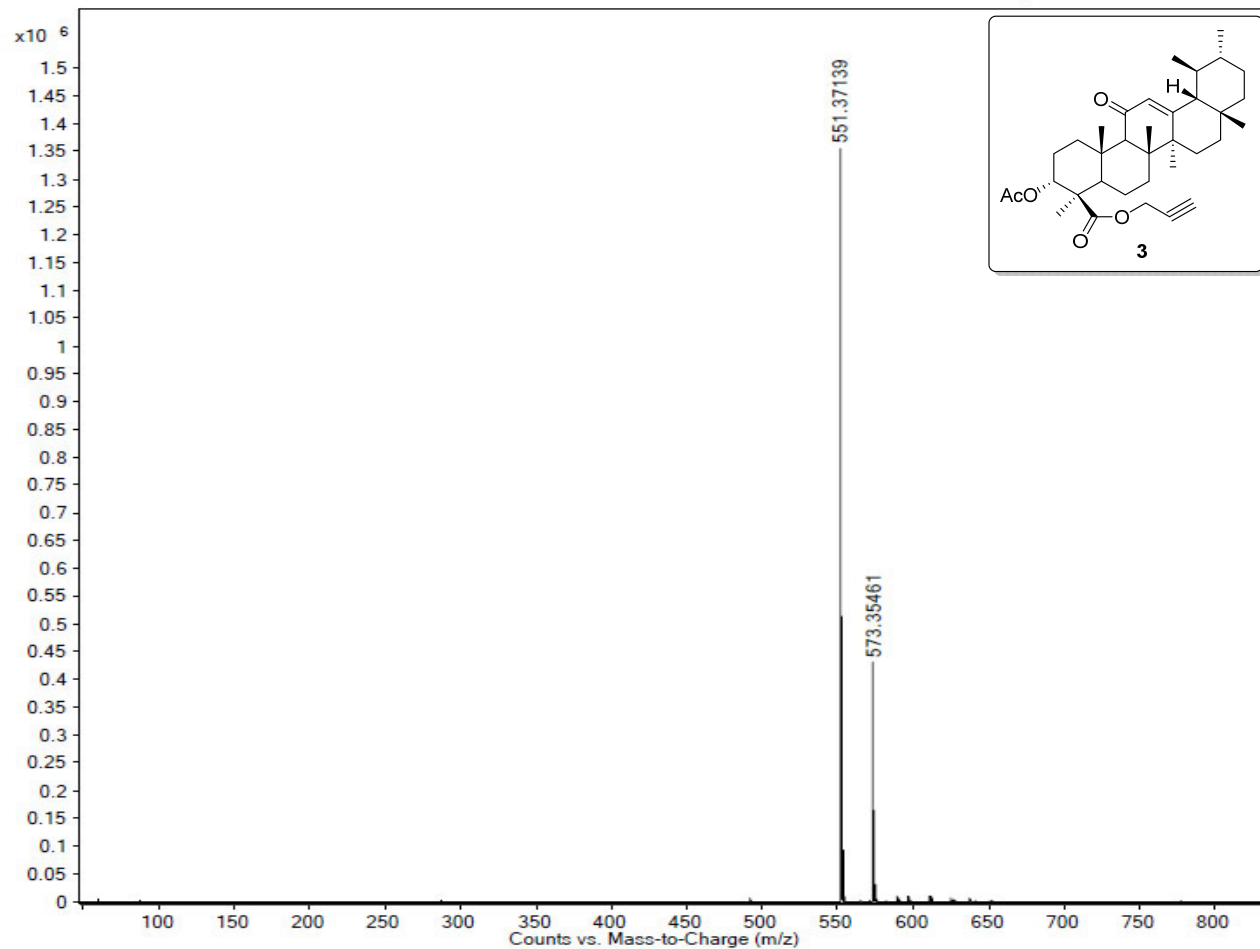


Figure S2: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound 3

<b>Sample Name</b>	SK-AKBA-PROP	<b>Position</b>	Vial 21	<b>Instrument Name</b>	Instrument 1
<b>User Name</b>		<b>Inj Vol</b>	2	<b>InjPosition</b>	
<b>Sample Type</b>	Sample	<b>IRM Calibration Status</b>	Success	<b>Data Filename</b>	SK-AKBA-PROP_POS_01.d
<b>ACQ Method</b>	POSITIVE ION METHOD MS.m	<b>Comment</b>	SK	<b>Acquired Time</b>	18-Oct-20 12:57:03 PM



**Figure S3:** HRMS spectrum of compound 3



21-Feb-2021.1.fid  
Dr. A. Satya Kumar / SK-KBA-Prop (4) / CDCl<sub>3</sub>  
PROTON

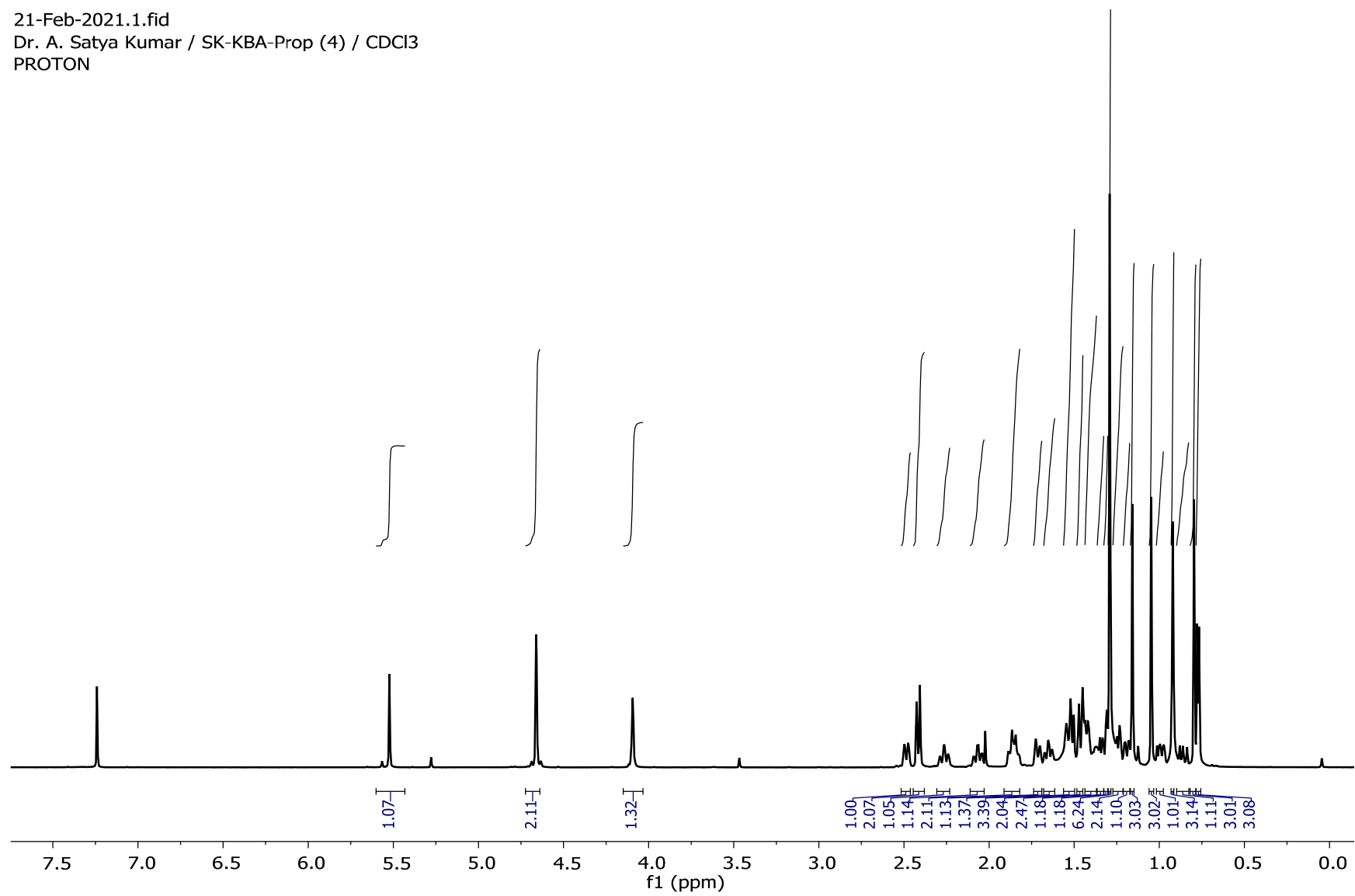


Figure S4: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 4

21-Feb-2021.2.fid  
Dr. A. Satya Kumar / SK-KBA-Prop (4) / CDCl<sub>3</sub>  
C13CPD

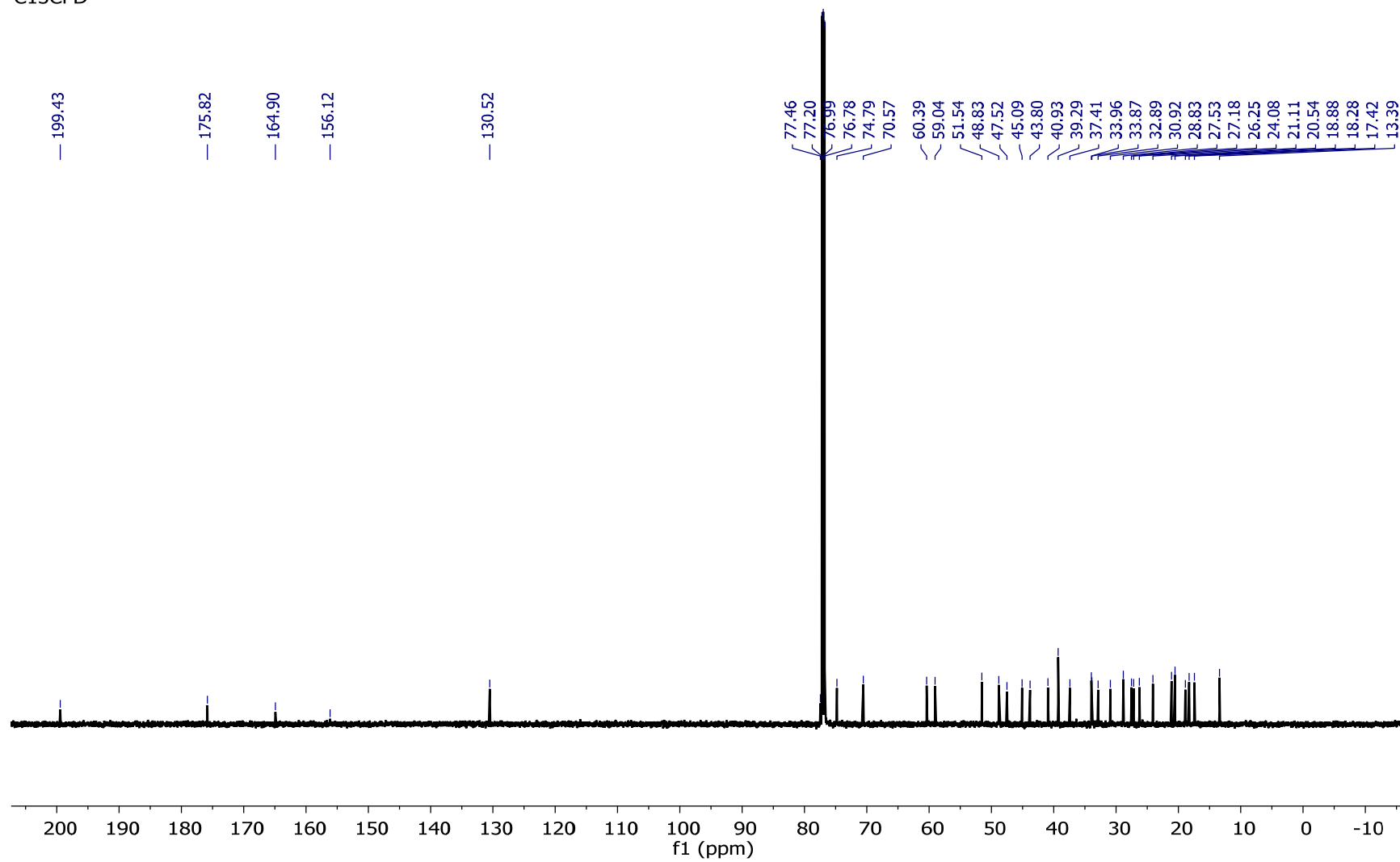


Figure S5: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound 4

Sample Name	KBA-PRO-A	Position	Vial 62	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	KBA-PRO-A_POS.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment		Acquired Time	24-Feb-21 12:20:31 PM

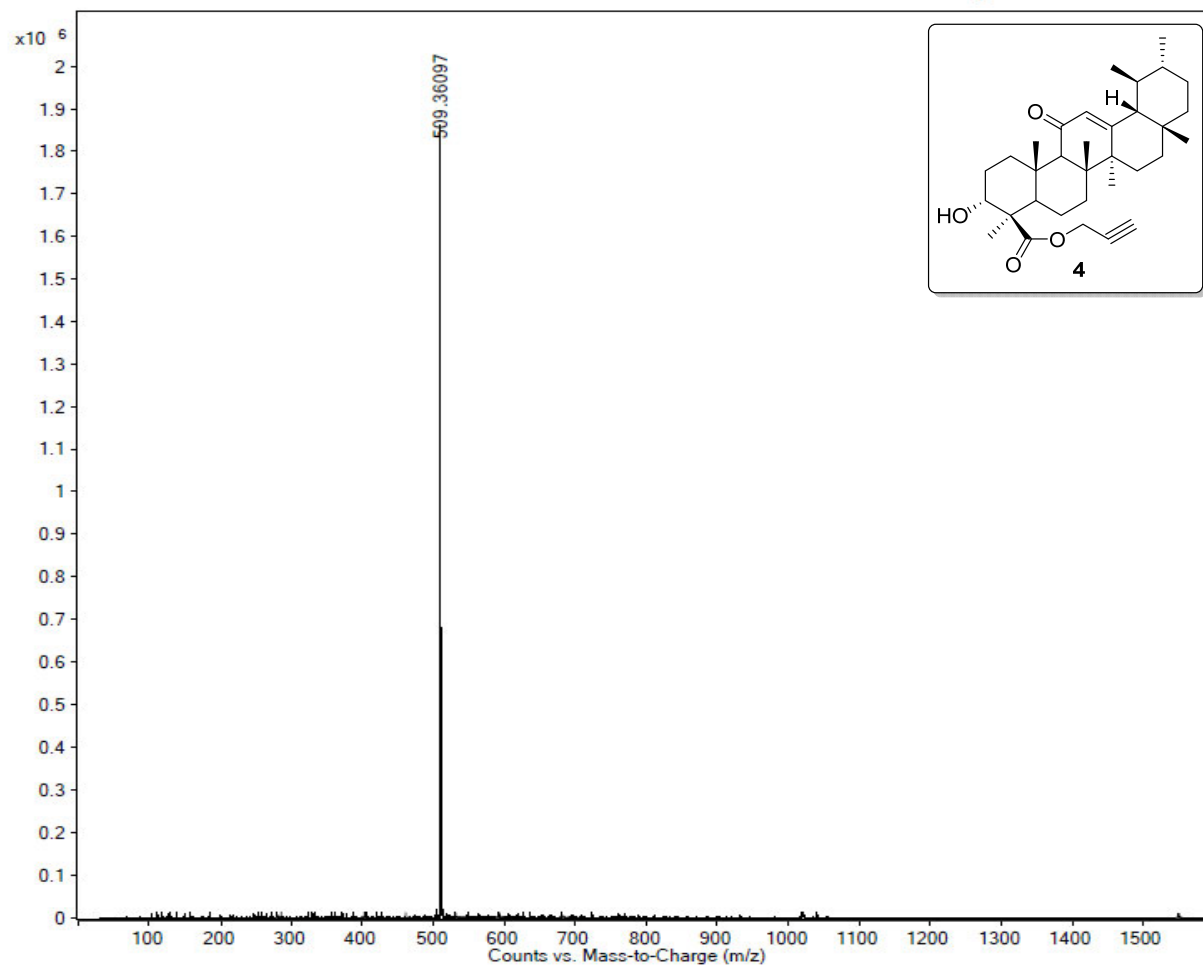


Figure S6: HRMS spectrum of compound 4

11-Nov-2020.6.fid  
Dr. Kumar/SK-AKBA-4a-(1)/CDCl<sub>3</sub>  
PROTON

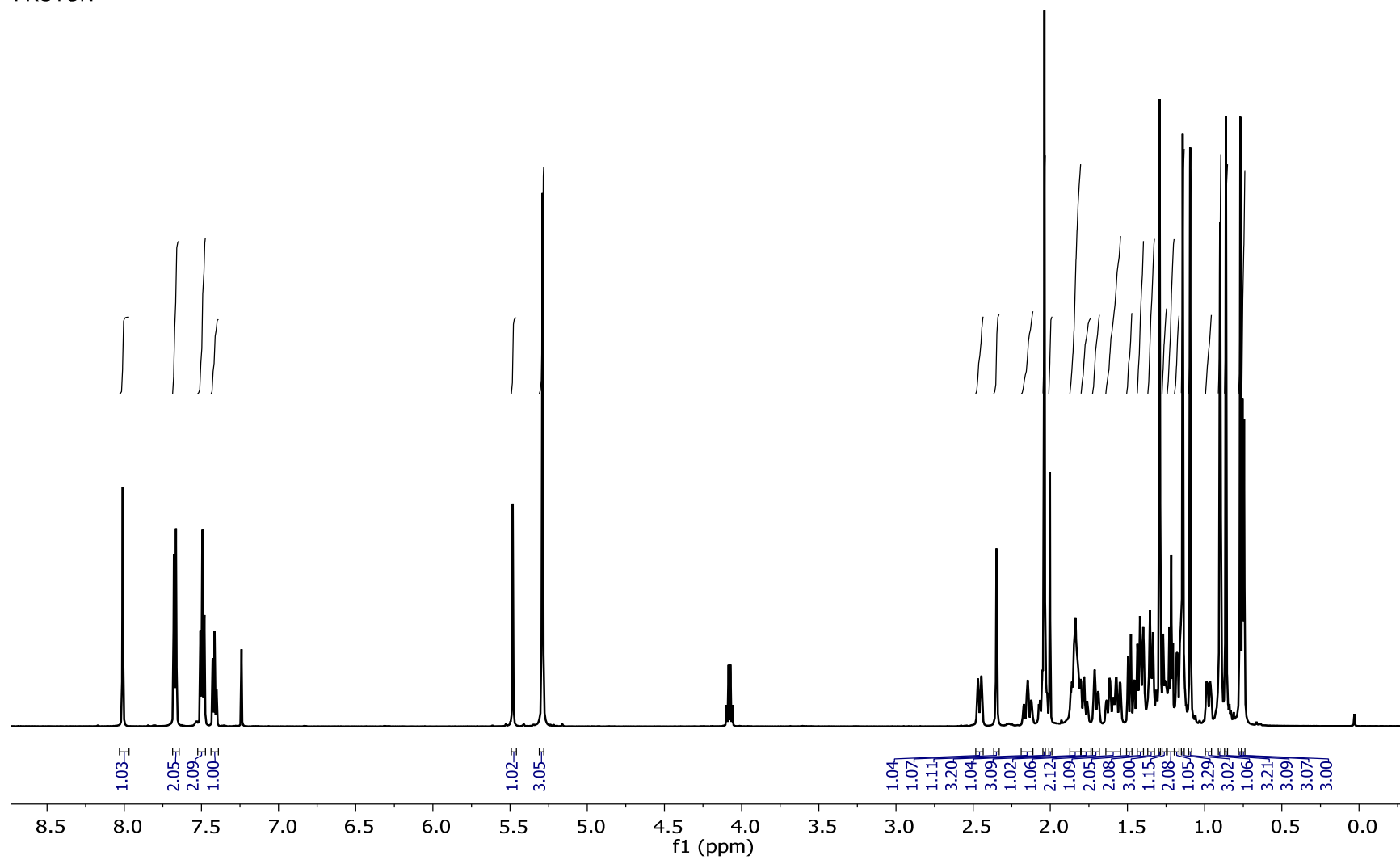


Figure S7: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 6a

11-Nov-2020.7.fid  
Dr. Kumar/SK-AKBA-4a-(1)/CDCl<sub>3</sub>  
C13CPD

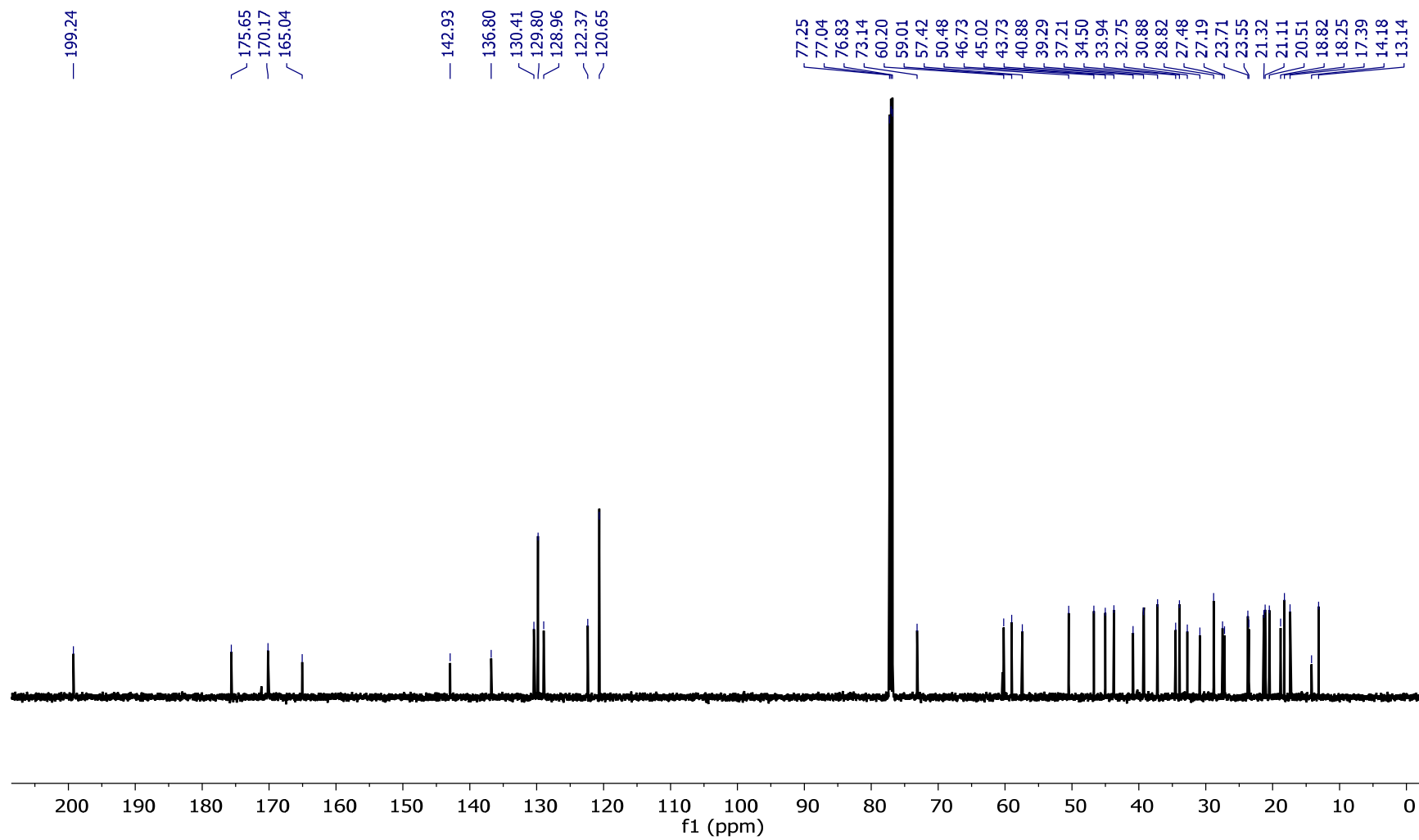


Figure S8: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound 6a

Sample Name	SK-AKBA-4A	Position	Vial 14	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SK-AKBA-4A_POS_01.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment	SK	Acquired Time	11-Nov-20 3:19:42 PM

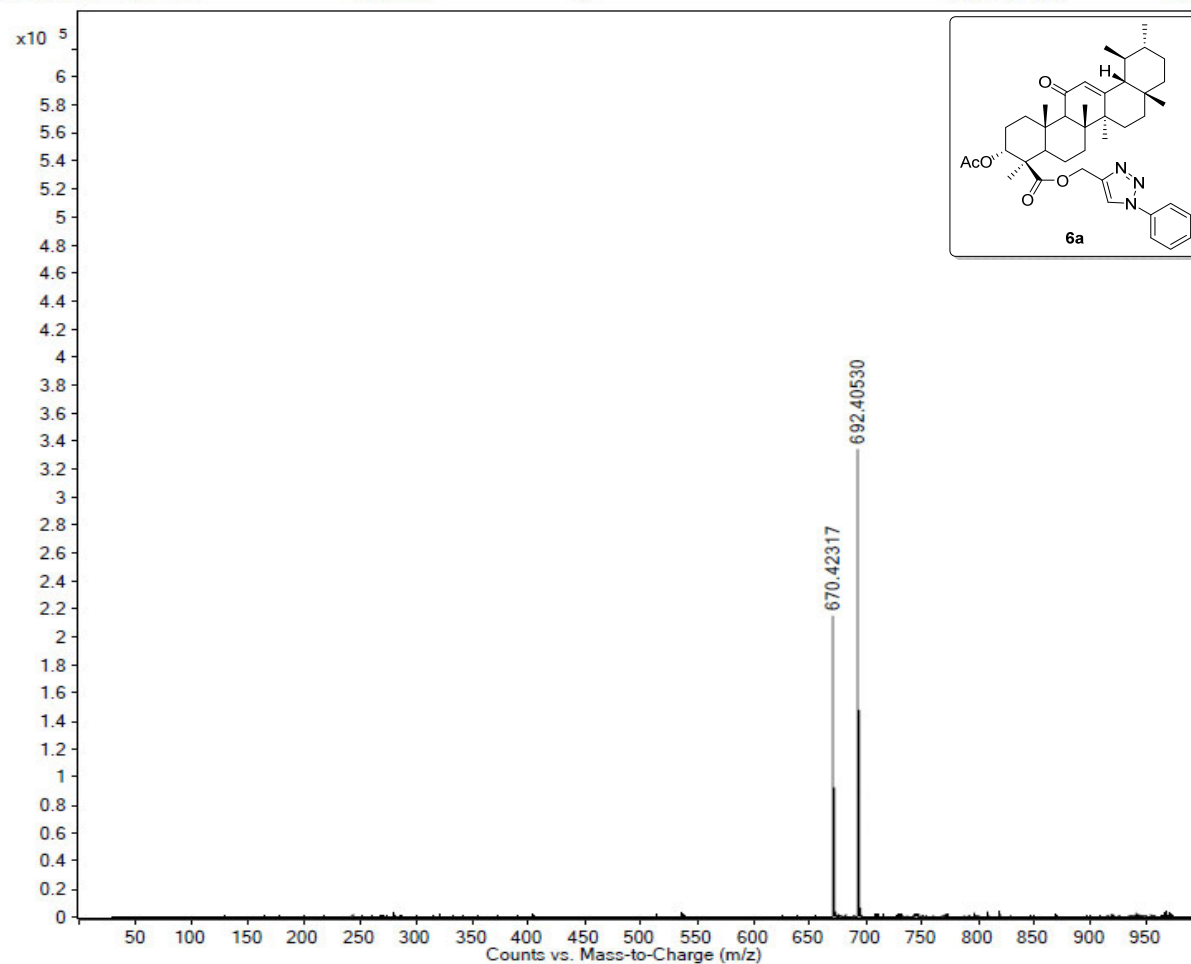


Figure S9: HRMS spectrum of compound 6a

15-Nov-2020.6.fid  
Dr. Kumar/SK-AKBA-4b(1)/CDCl<sub>3</sub>  
PROTON

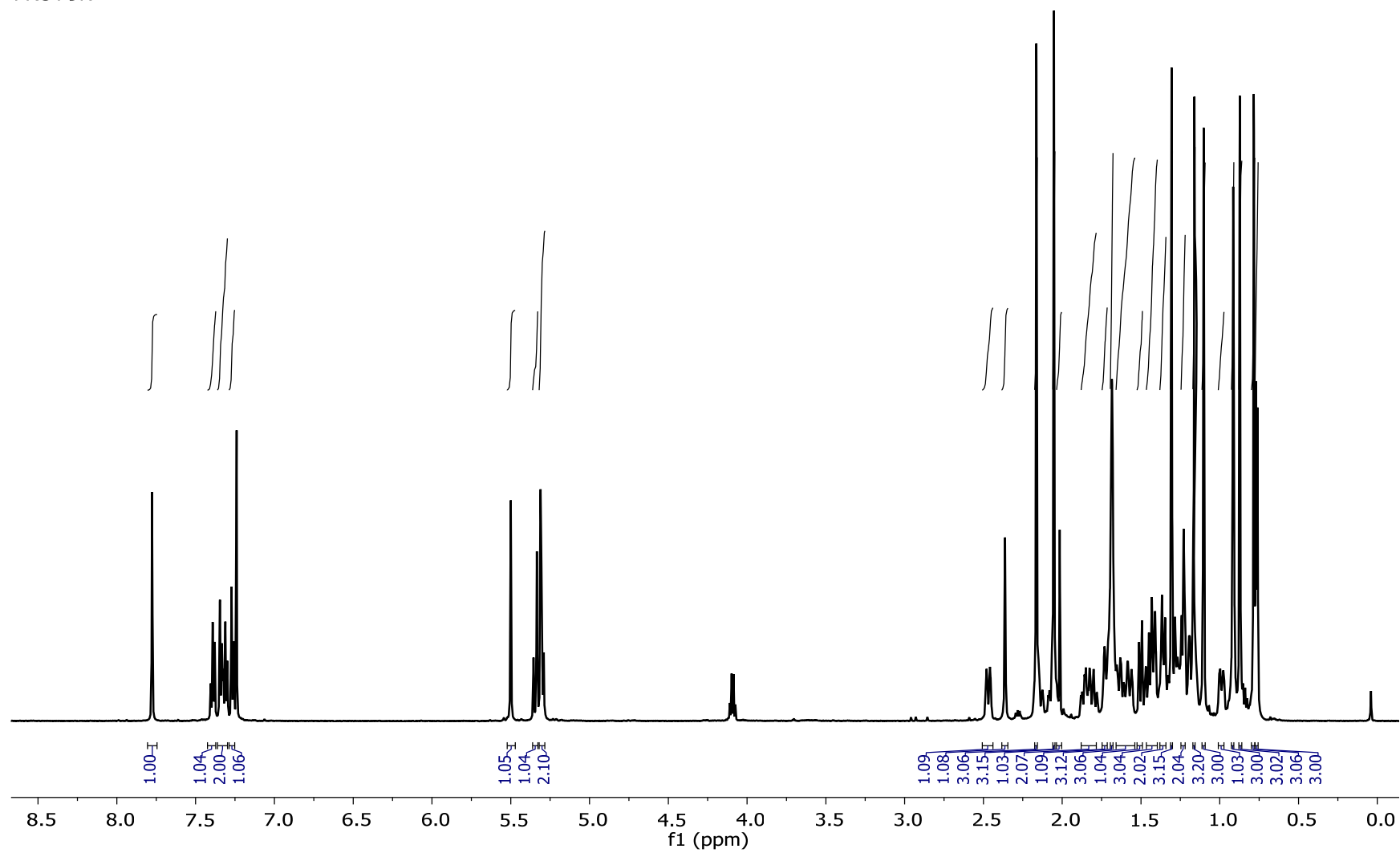


Figure S10: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound **6b**

15-Nov-2020.7.fid  
Dr. Kumar/SK-AKBA-4b(1)/CDCl<sub>3</sub>  
C13CPD

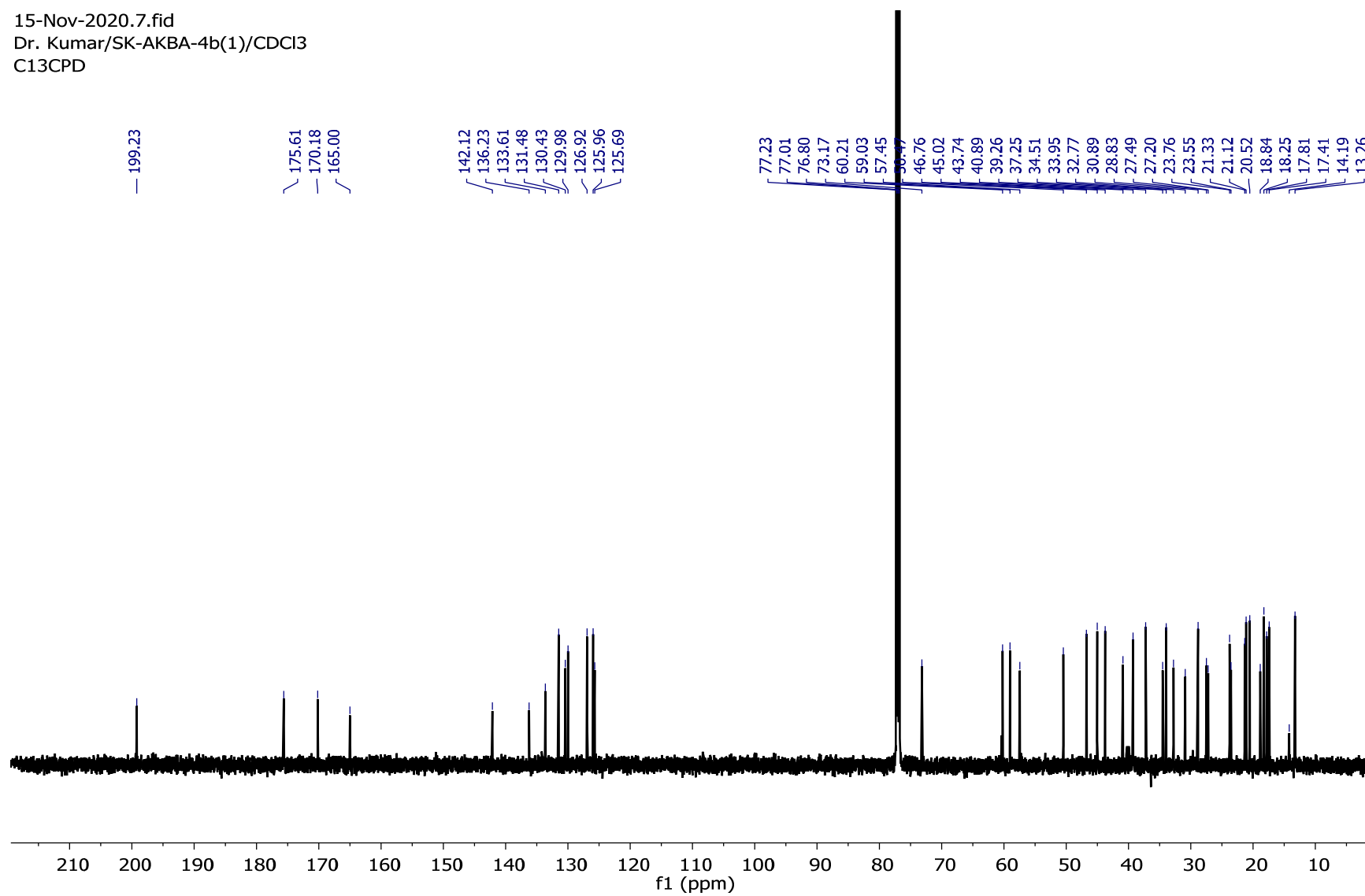


Figure S11: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound **6b**



Sample Name	SK-AKBA-4B	Position	Vial 15	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SK-AKBA-4B_POS_01.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment	SK	Acquired Time	11-Nov-20 3:25:23 PM

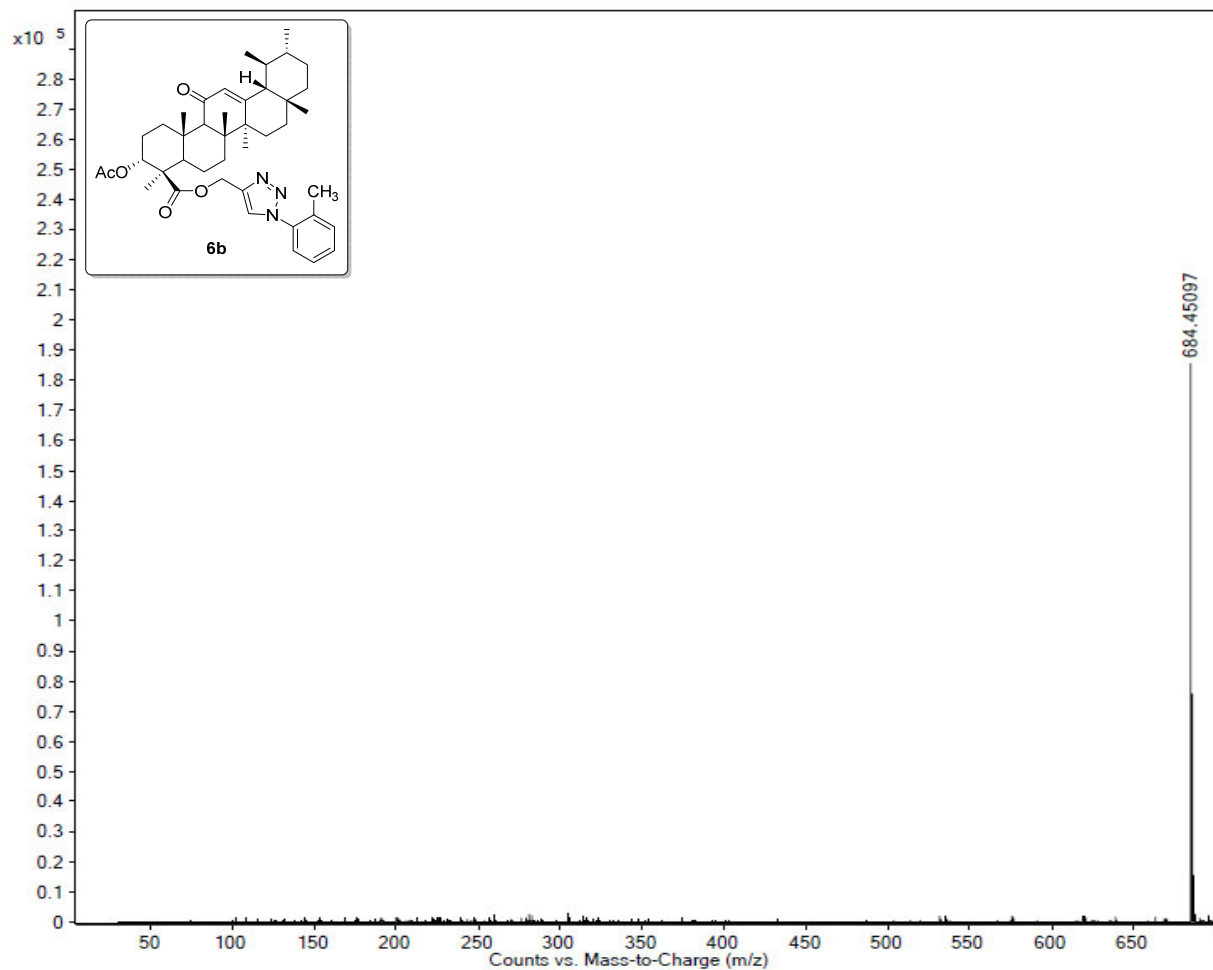


Figure S12: HRMS spectrum of compound **6b**

09-Dec-2020.1.fid  
Dr. Kumar/SK-AKBA-4C/CDCl<sub>3</sub>  
PROTON

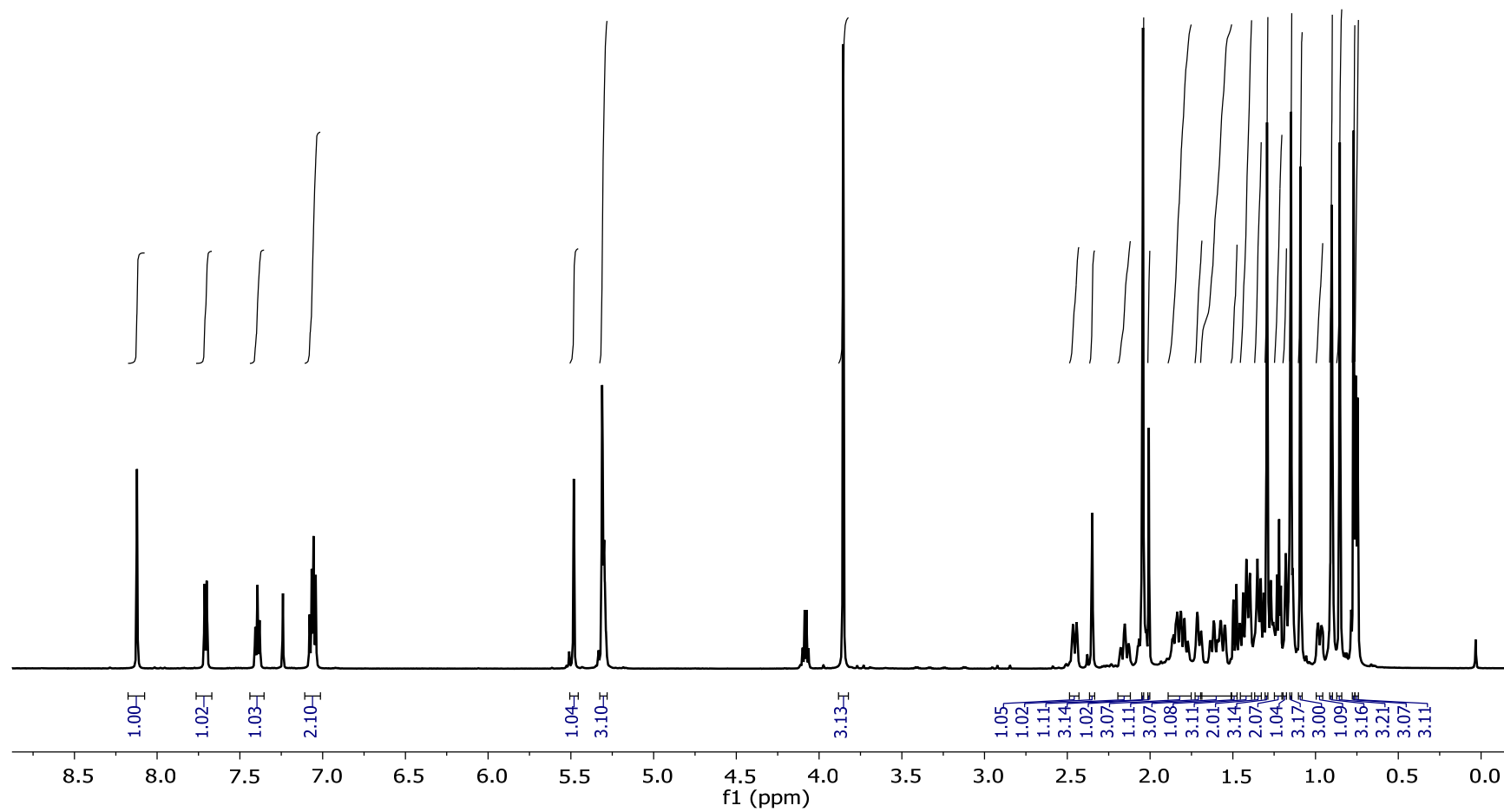


Figure S13: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 6c

09-Dec-2020.7.fid  
Dr. Kumar/SK-AKBA-4C/CDCl<sub>3</sub>  
C13CPD

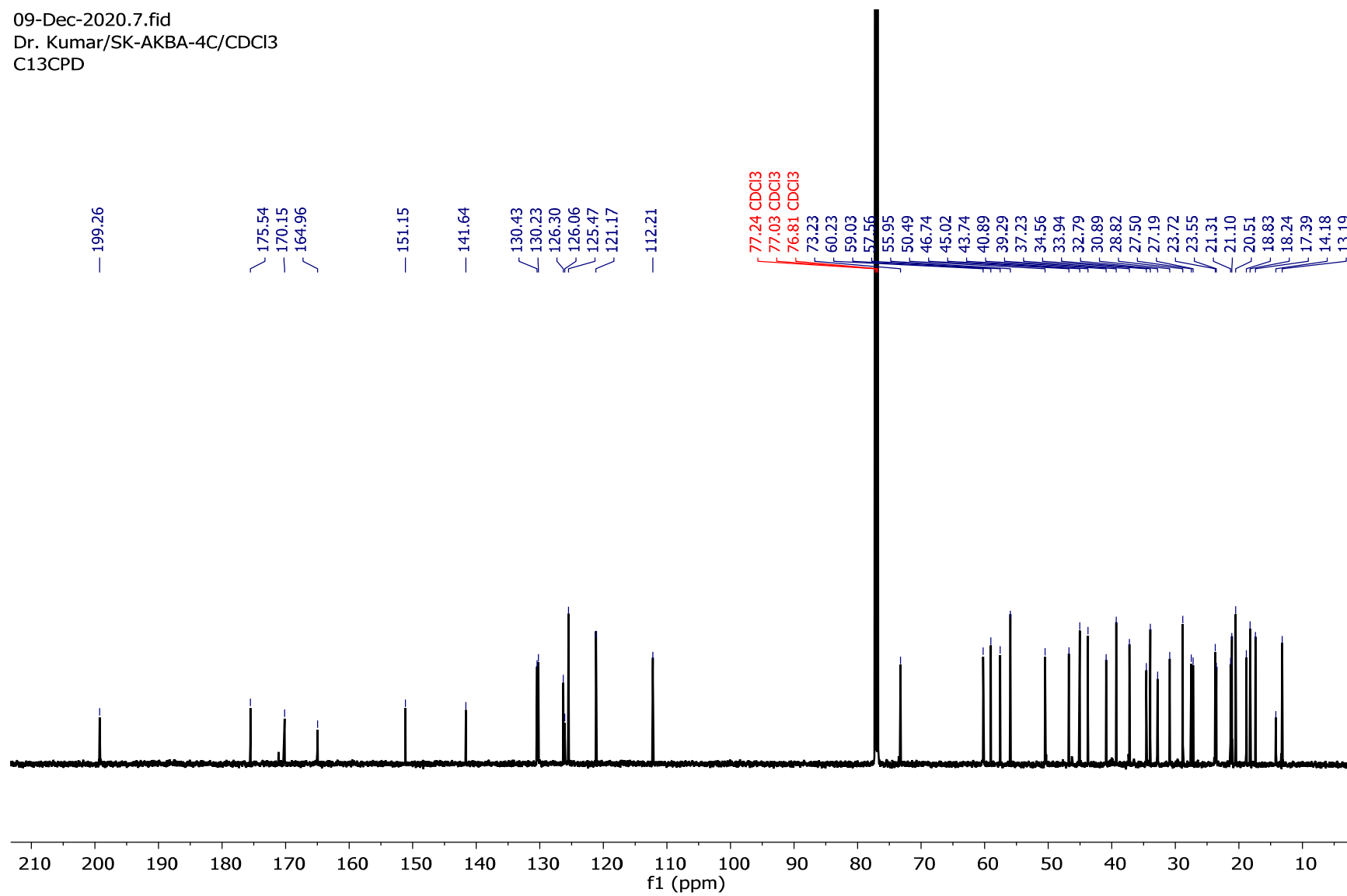


Figure S14: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound **6c**

<b>Sample Name</b>	SK-AKBA-4C	<b>Position</b>	Vial 41	<b>Instrument Name</b>	Instrument 1
<b>User Name</b>		<b>Inj Vol</b>	2	<b>InjPosition</b>	
<b>Sample Type</b>	Sample	<b>IRM Calibration Status</b>	Success	<b>Data Filename</b>	SK-AKBA-4C_POS_01.d
<b>ACQ Method</b>	POSITIVE ION METHOD MS.m	<b>Comment</b>	SK	<b>Acquired Time</b>	11-Nov-20 3:02:18 PM

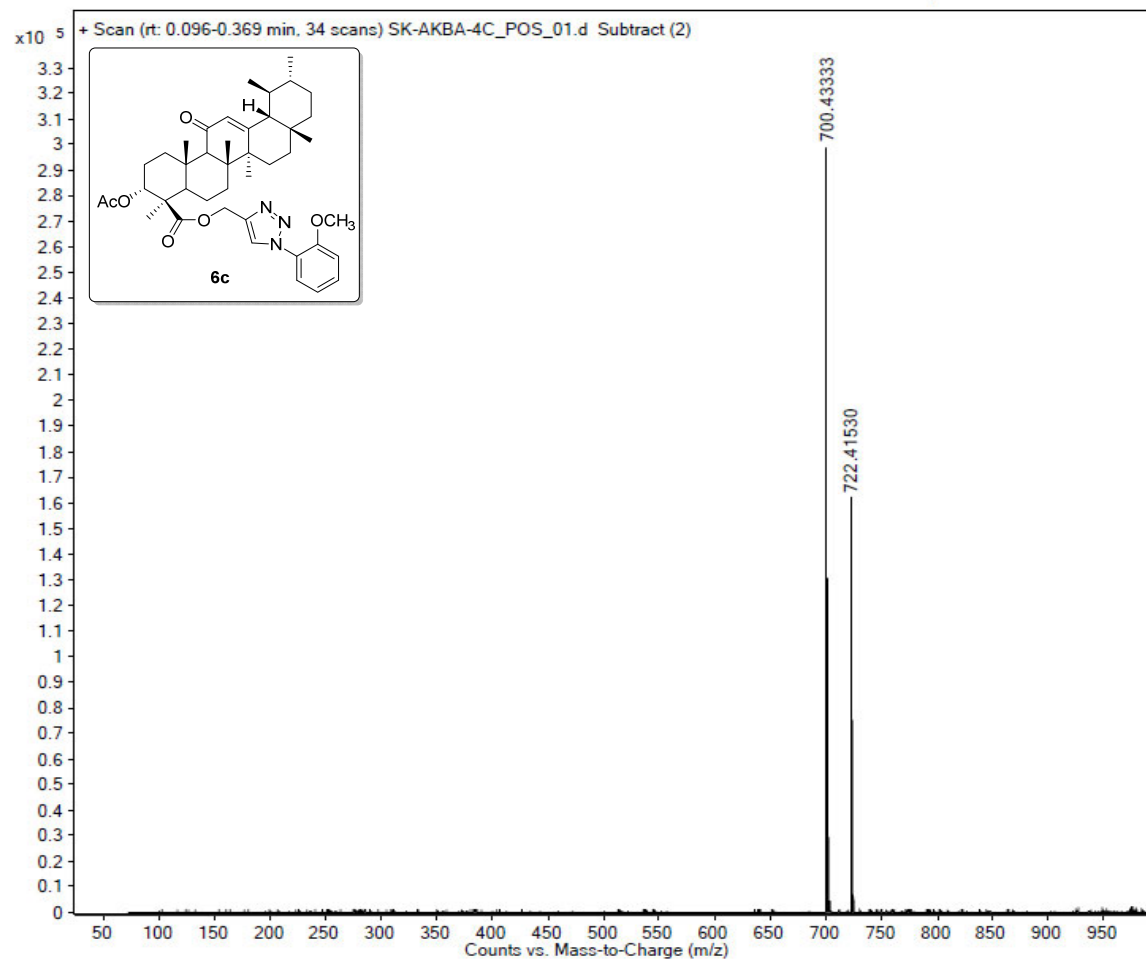


Figure S15: HRMS spectrum of compound 6c

15-Nov-2020 1 fid  
1H-NMR (600 MHz, CDCl<sub>3</sub>)  
Dr. Kumar/SK-AKBA-4D/CDCl<sub>3</sub>  
PROTON

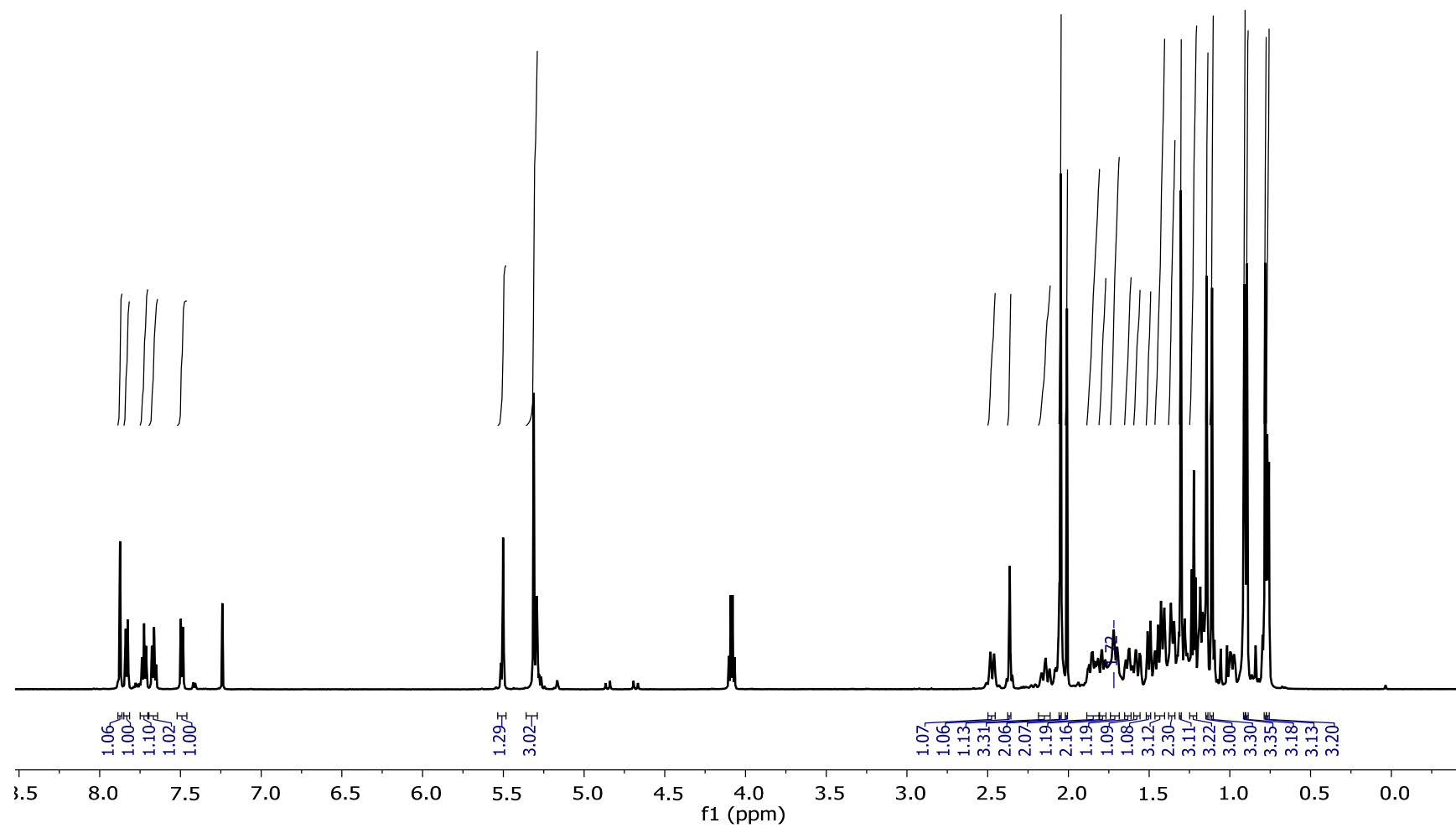


Figure S16: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 6d

15-Nov-2020.2.fid  
Dr. Kumar/SK-AKBA-4D/CDCl<sub>3</sub>  
C13CPD

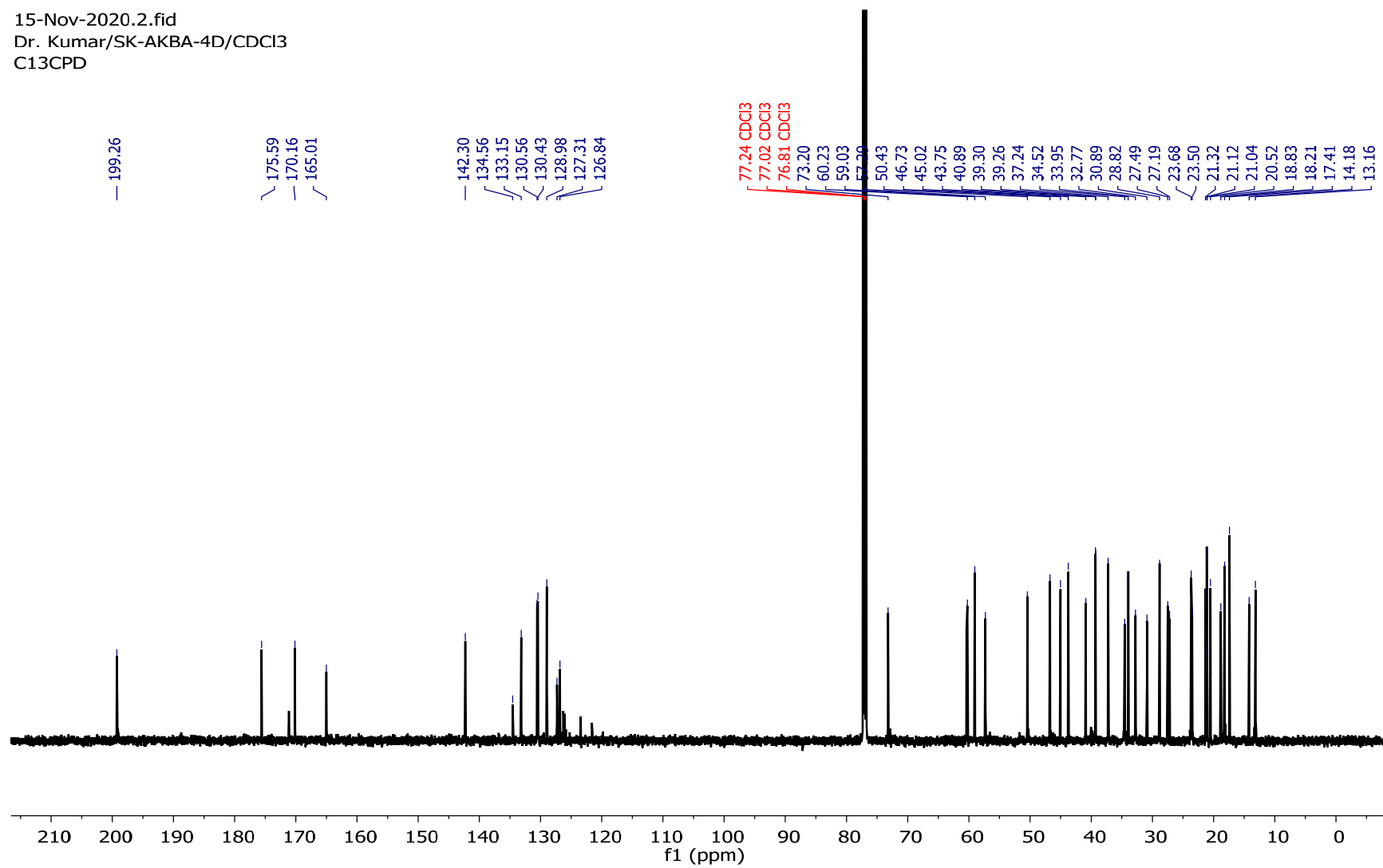
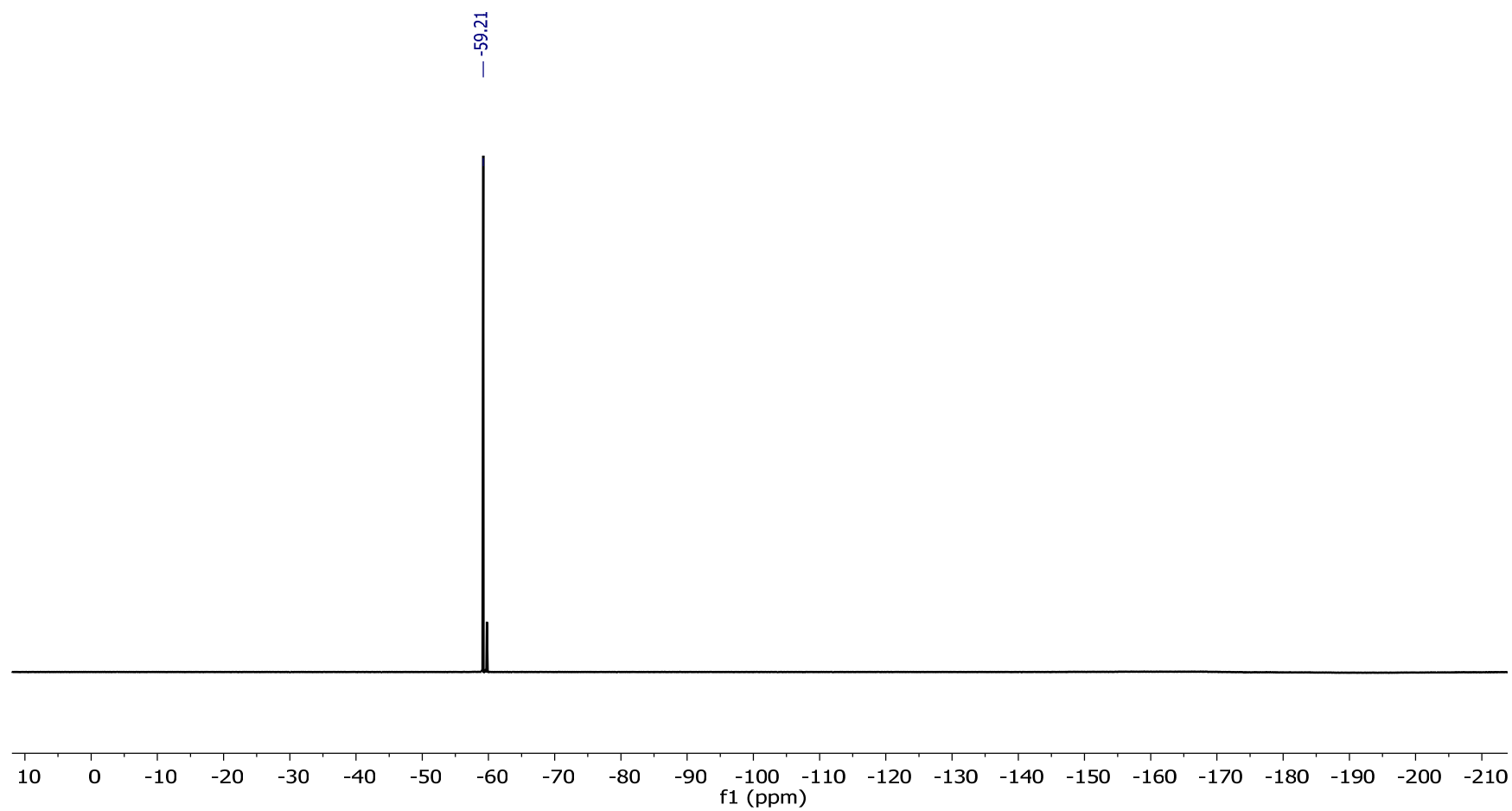


Figure S17: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound 6d

15-Nov-2020.5.fid  
Dr. Kumar/SK-AKBA-4D/CDCl<sub>3</sub>  
F19CPD



**Figure S18:** <sup>19</sup>F-NMR spectrum (564 MHz, CDCl<sub>3</sub>) of compound **6d**

Sample Name	SK-AKBA-4D	Position	Vial 42	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SK-AKBA-4D_POS_01.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment	SK	Acquired Time	11-Nov-20 3:07:56 PM

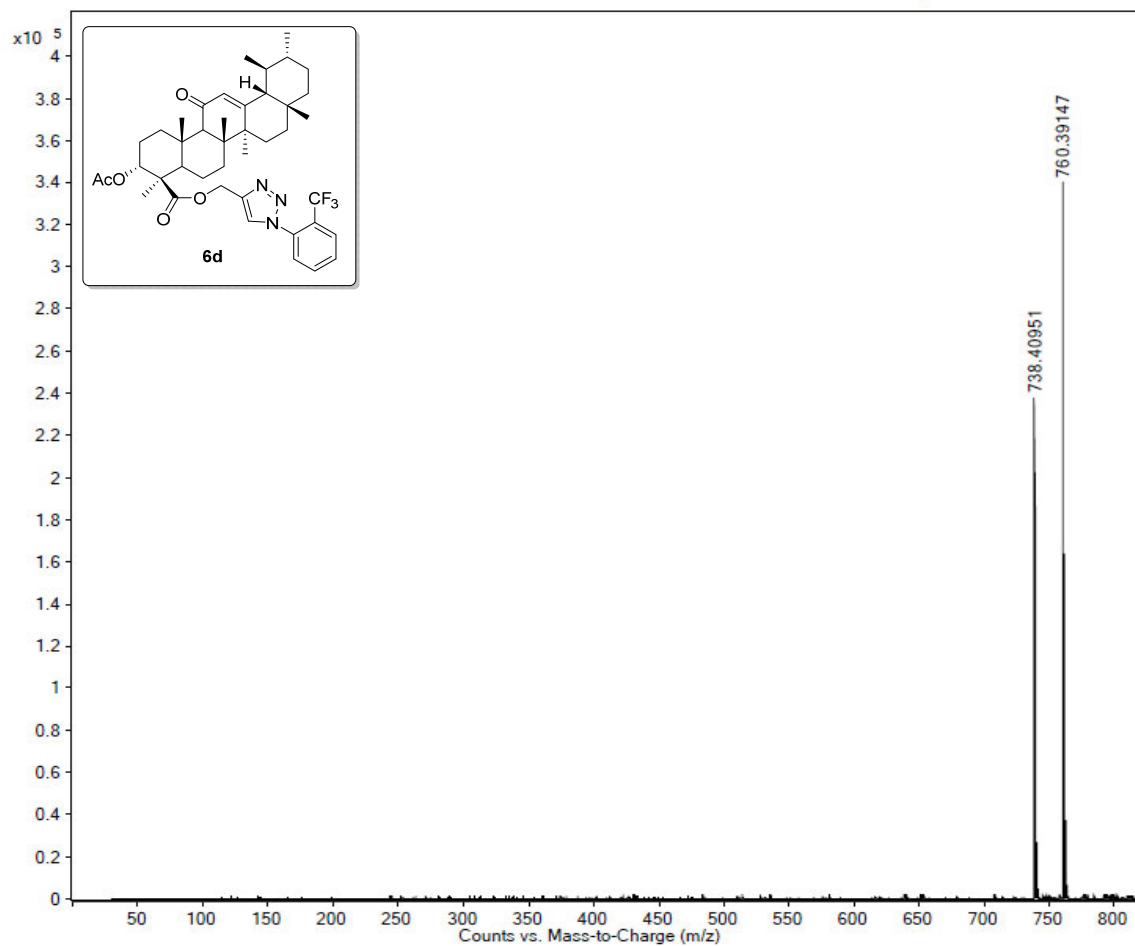


Figure S19: HRMS spectrum of compound **6d**



09-Dec-2020.2.fid  
Dr. Kumar/SK-AKBA-4E/CDCl<sub>3</sub>  
PROTON

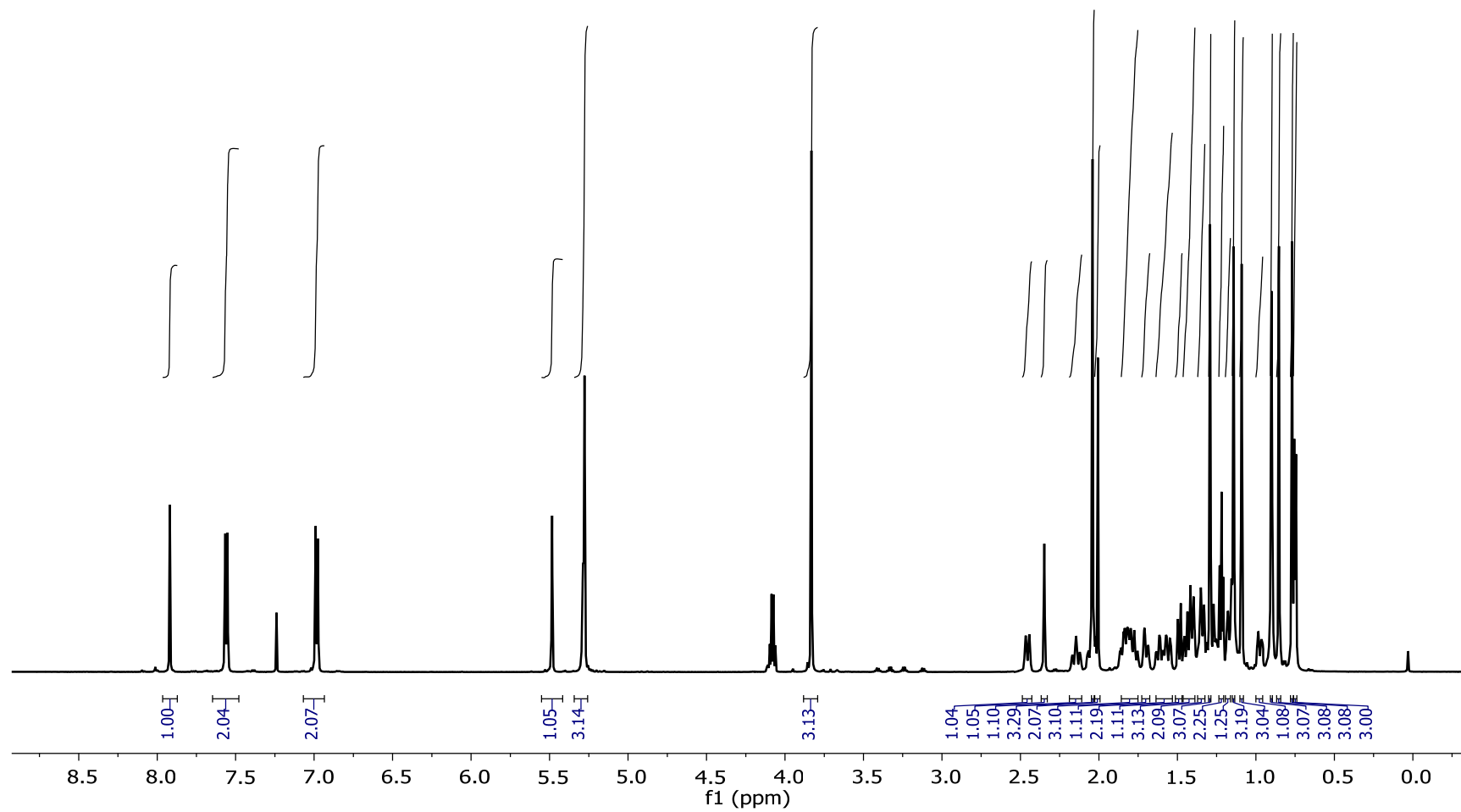


Figure S20: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 6e

09-Dec-2020.10.fid  
Dr. Kumar/SK-AKBA-4E/CDCl<sub>3</sub>  
C13CPD

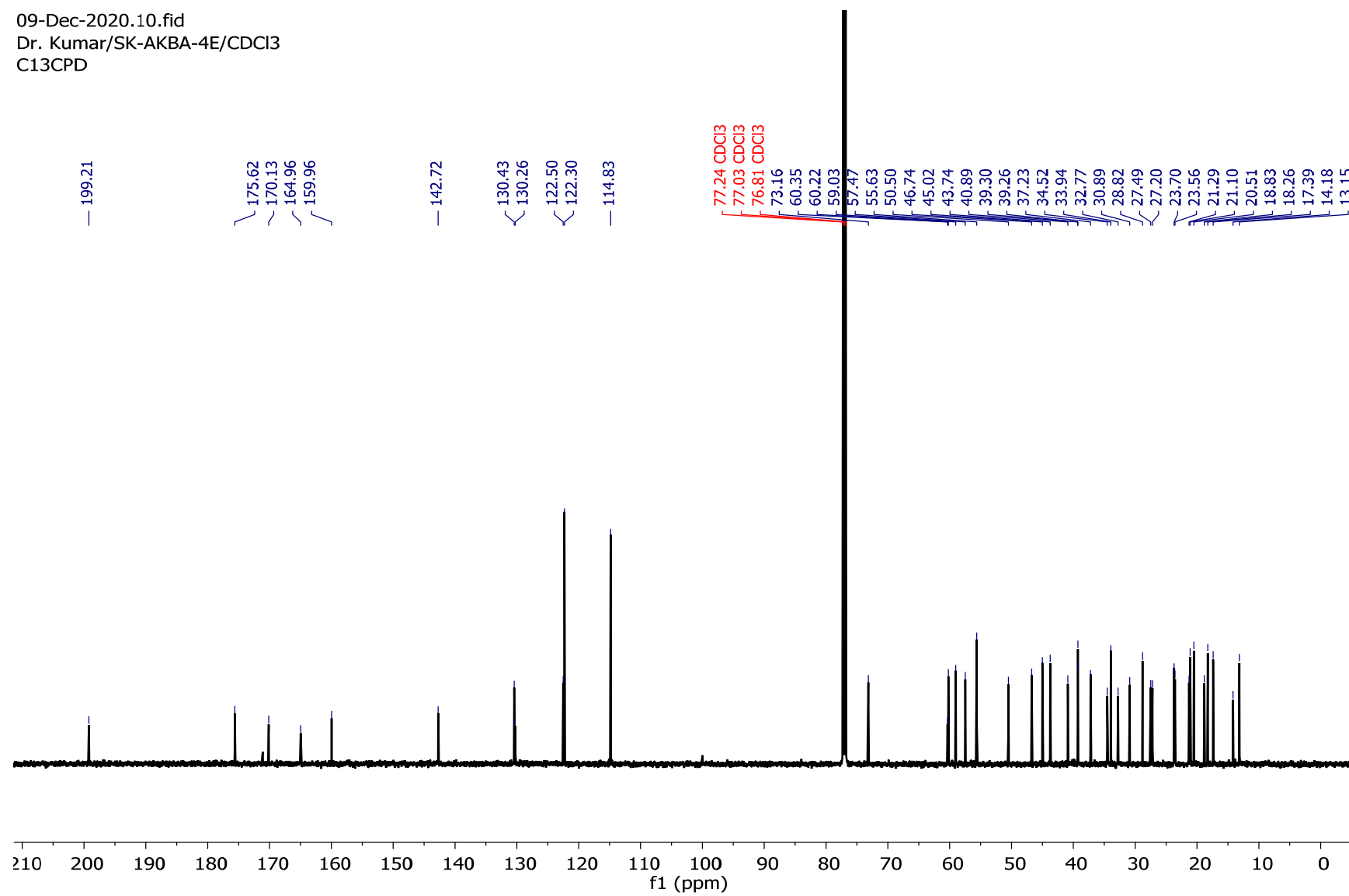


Figure S21: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound **6e**

Sample Name	4E	Position	Vial 44	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	4E_POS_01.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment	SK	Acquired Time	20-Nov-20 6:38:30 PM

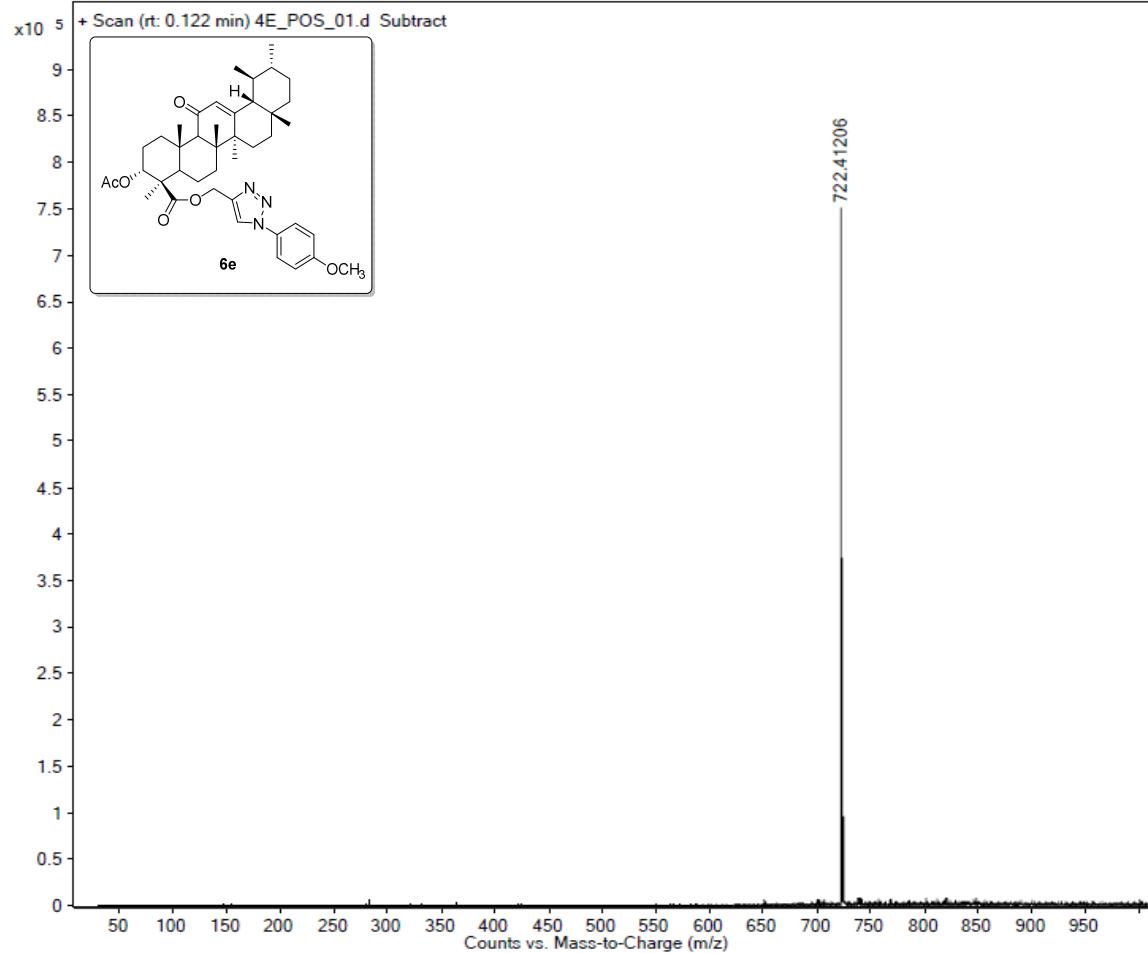


Figure S22: HRMS spectrum of compound **6e**

09-Dec-2020.3.fid  
Dr. Kumar/SK-AKBA-4F/CDCl<sub>3</sub>  
PROTON

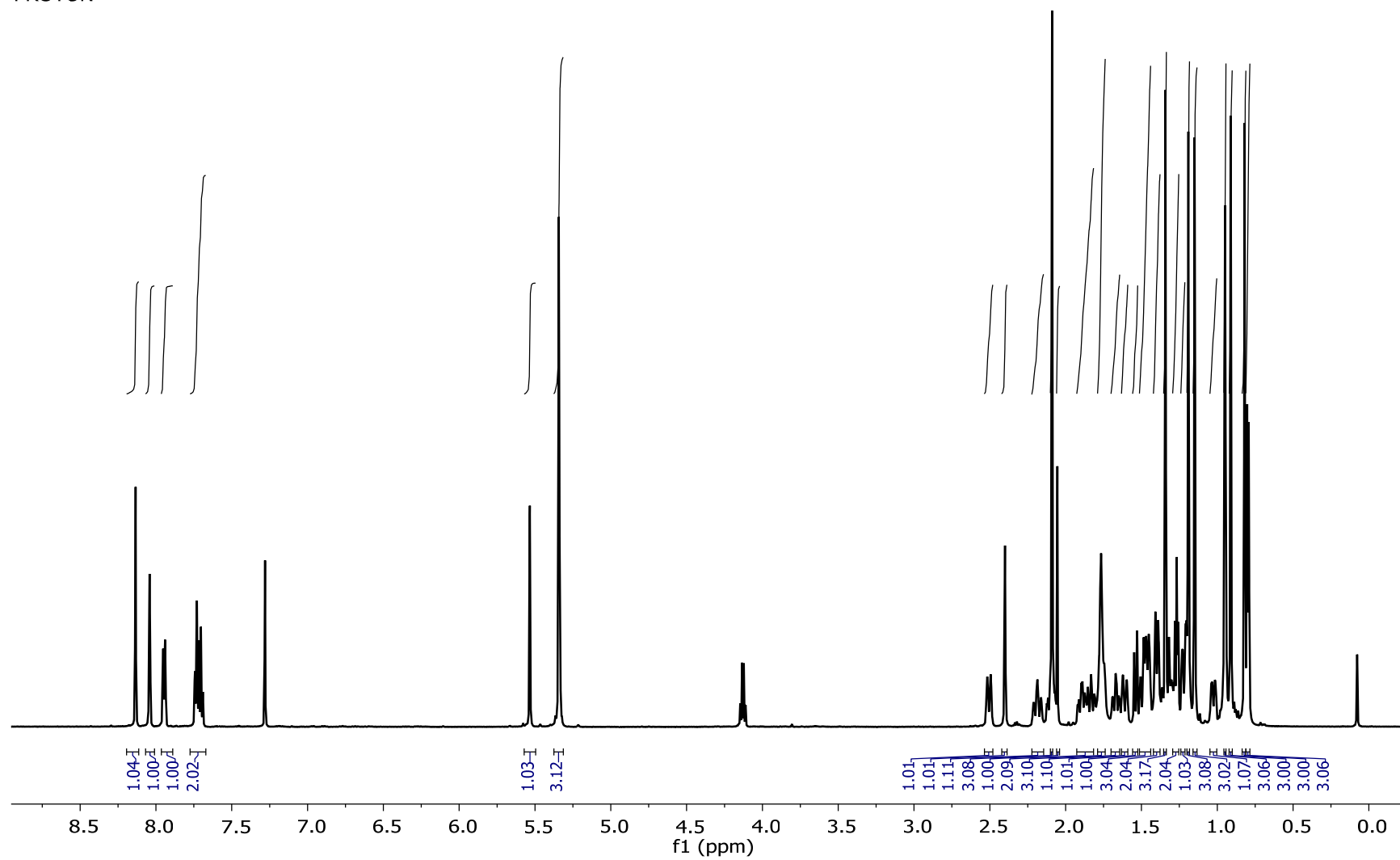


Figure S23: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 6f

09-Dec-2020.13.fid  
Dr. Kumar/SK-AKBA-4F/CDCl<sub>3</sub>  
C13CPD

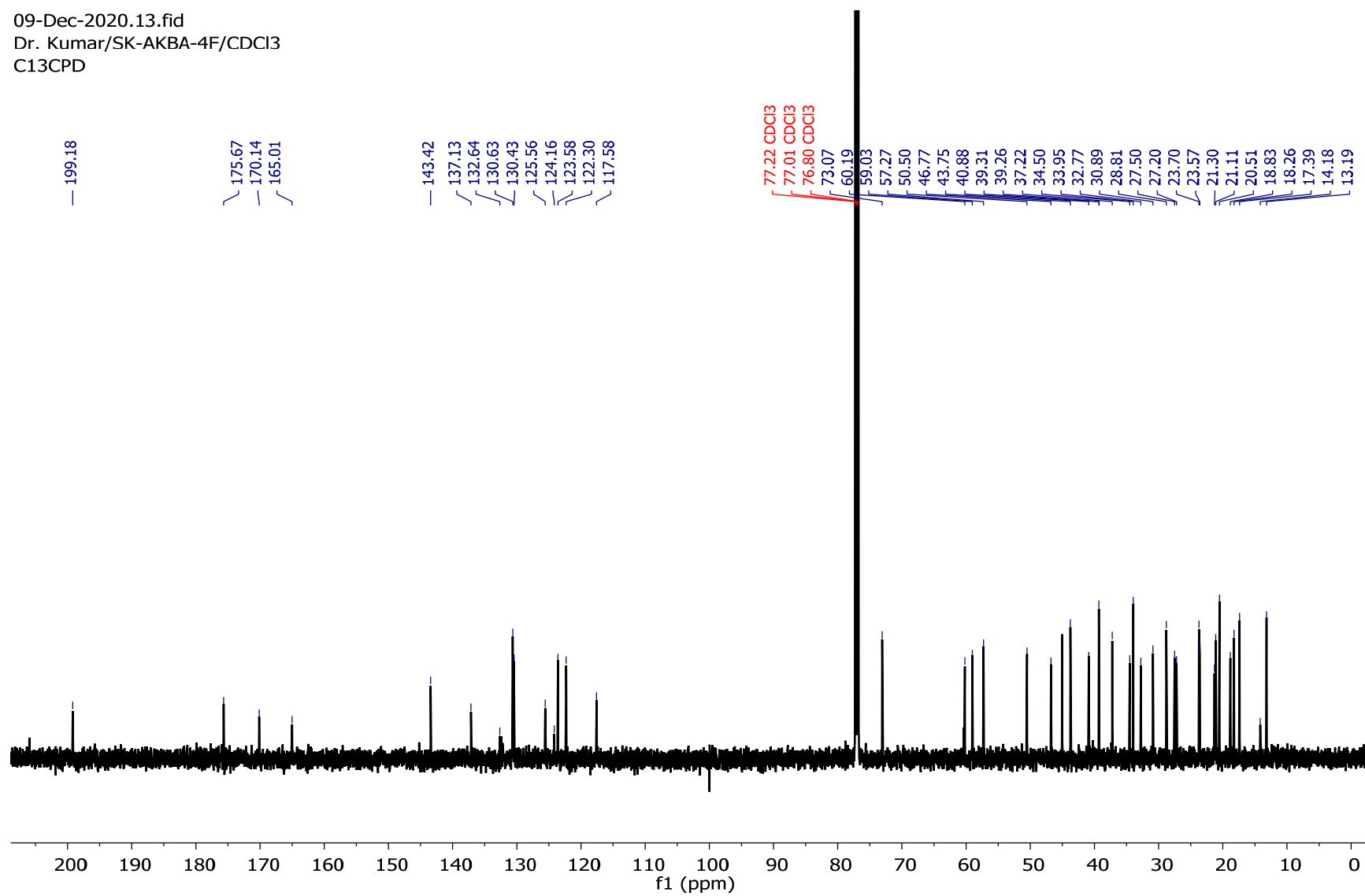


Figure S24: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound 6f

09-Dec-2020.25.fid  
Dr. Kumar/SK-AKBA-4F/CDCl<sub>3</sub>  
F19CPD

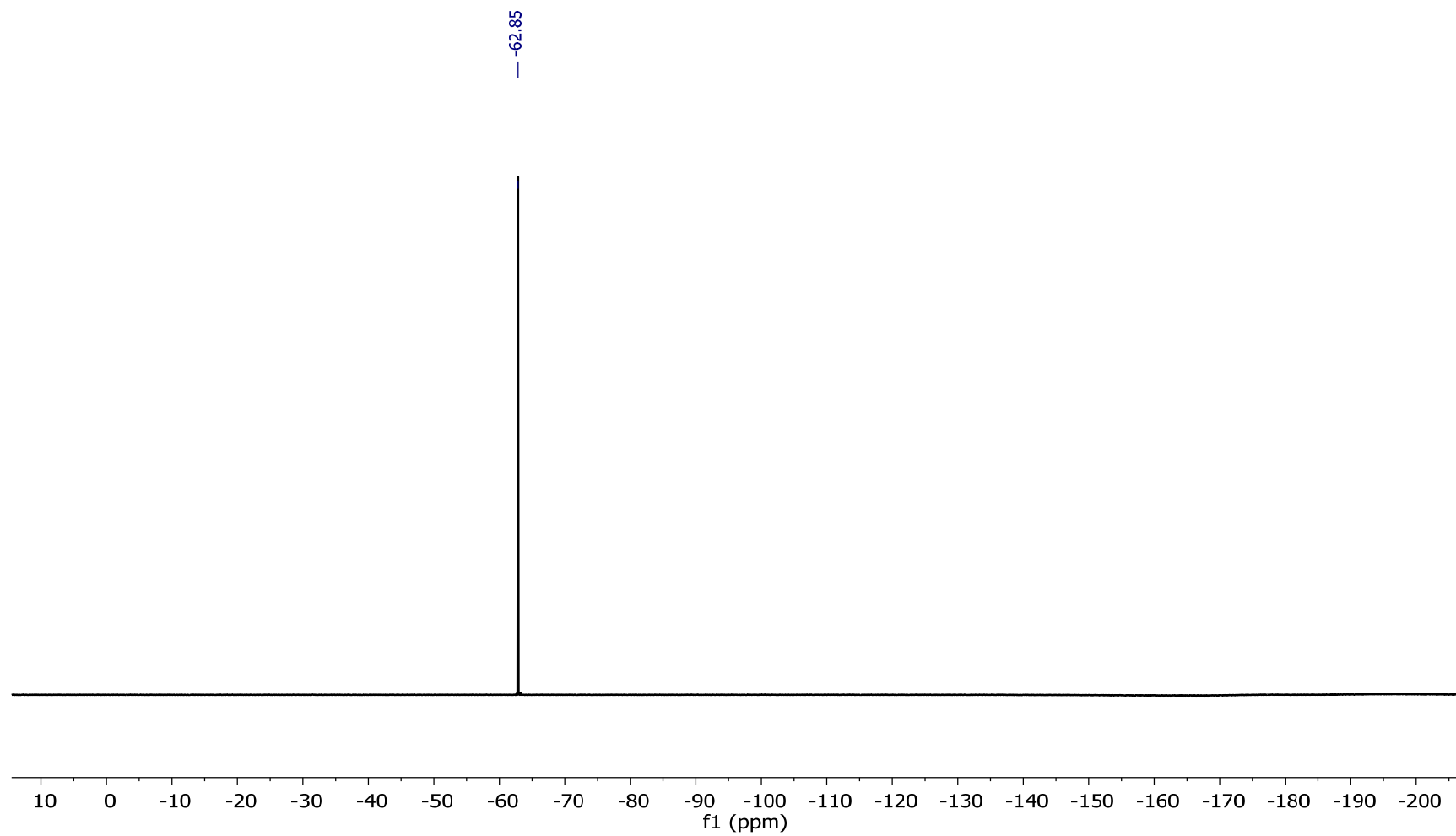


Figure S25: <sup>19</sup>F-NMR spectrum (564 MHz, CDCl<sub>3</sub>) of compound **6f**

Sample Name	4F	Position	Vial 45	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	4F_POS_01.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment	SK	Acquired Time	20-Nov-20 6:44:00 PM

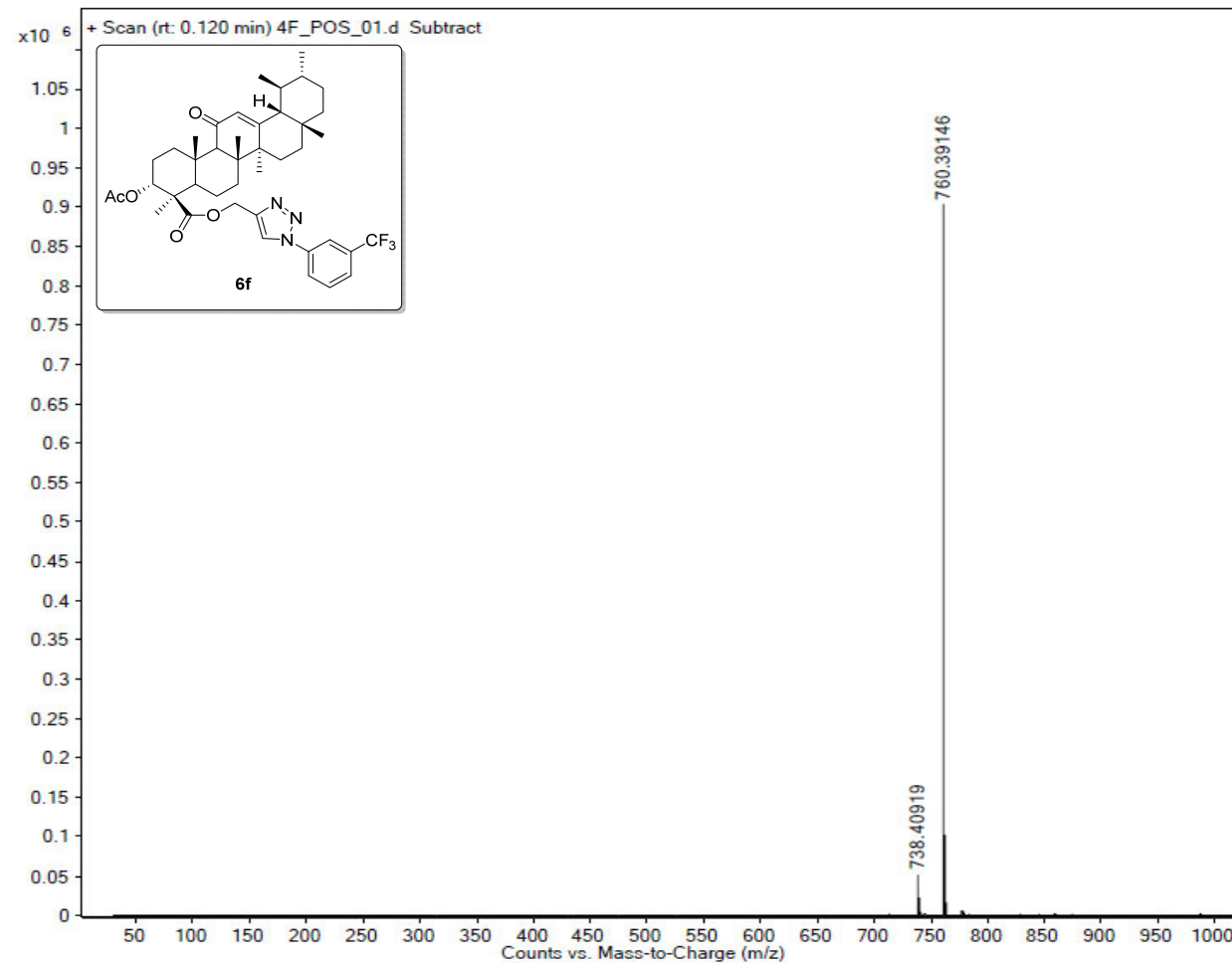


Figure S26: HRMS spectrum of compound **6f**

09-Dec-2020.4.fid  
Dr. Kumar/SK-AKBA-4G/CDCl<sub>3</sub>  
PROTON

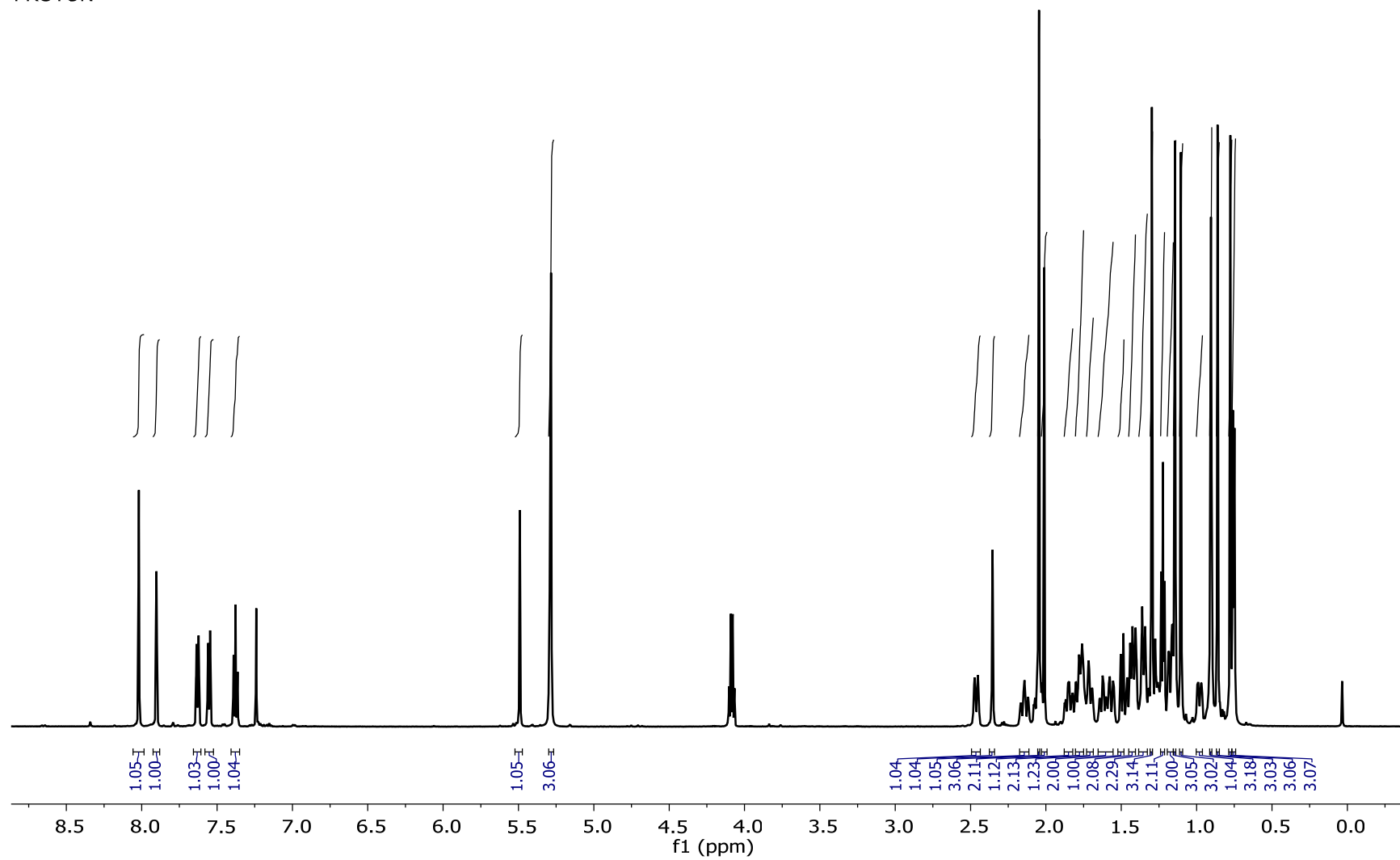


Figure S27: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 6g



09-Dec-2020.16.fid  
Dr. Kumar/SK-AKBA-4G/CDCl<sub>3</sub>  
C13CPD

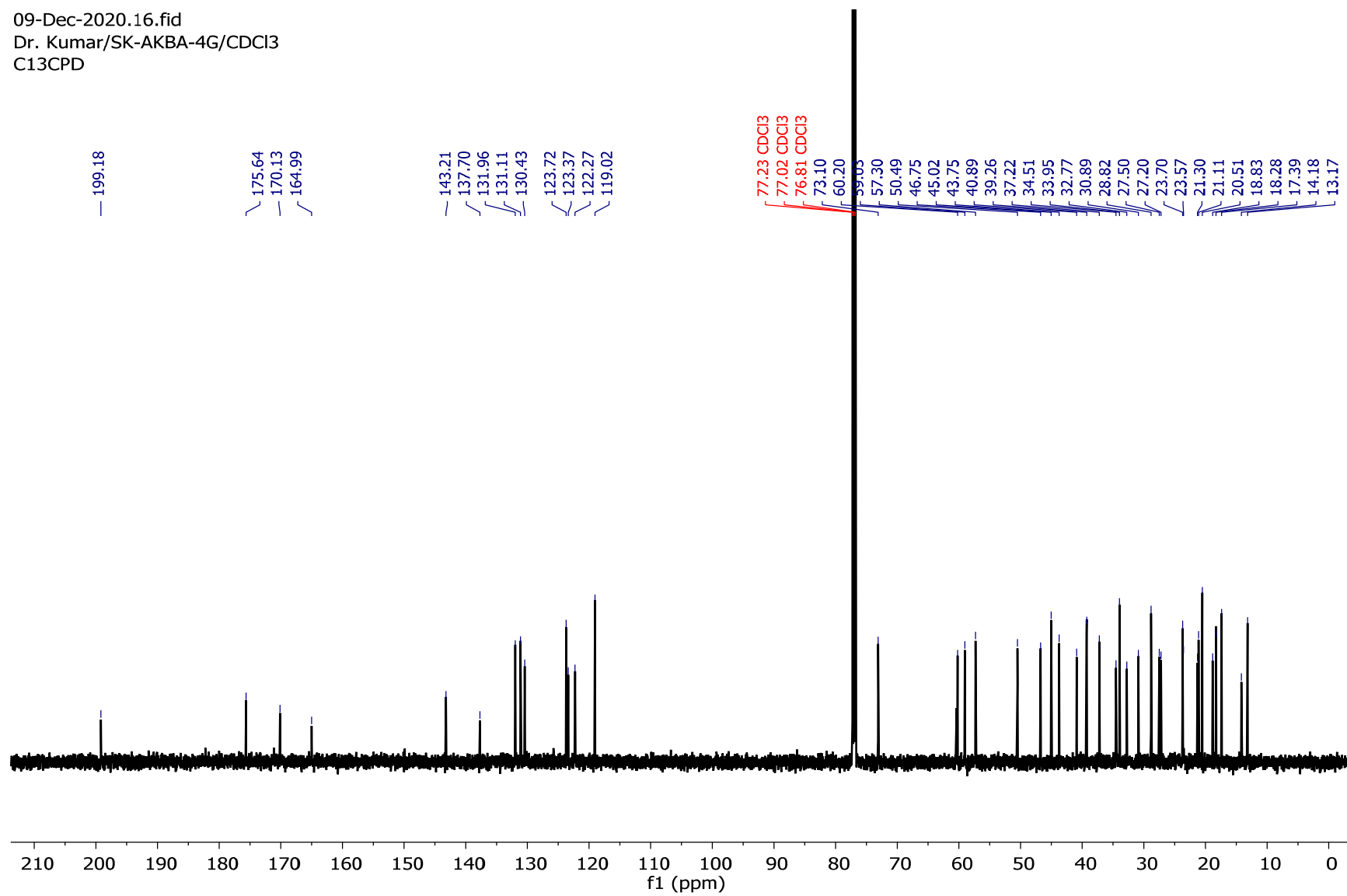


Figure S28: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound **6g**

Sample Name	4G	Position	Vial 46	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	4G_POS_01.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment	SK	Acquired Time	20-Nov-20 6:49:35 PM

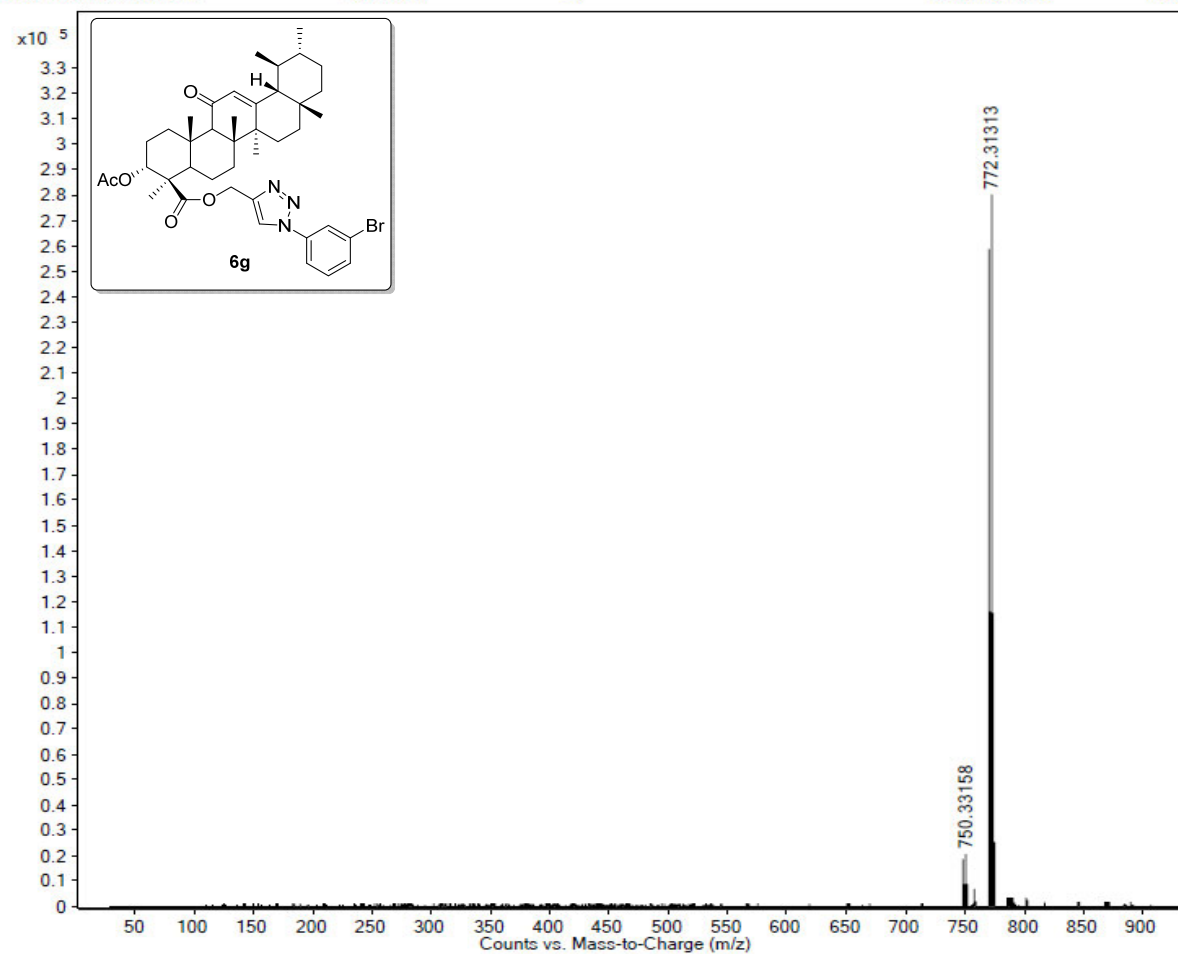


Figure S29: HRMS spectrum of compound 6g

09-Dec-2020.5.fid  
Dr. Kumar/SK-AKBA-4H/CDCl<sub>3</sub>  
PROTON

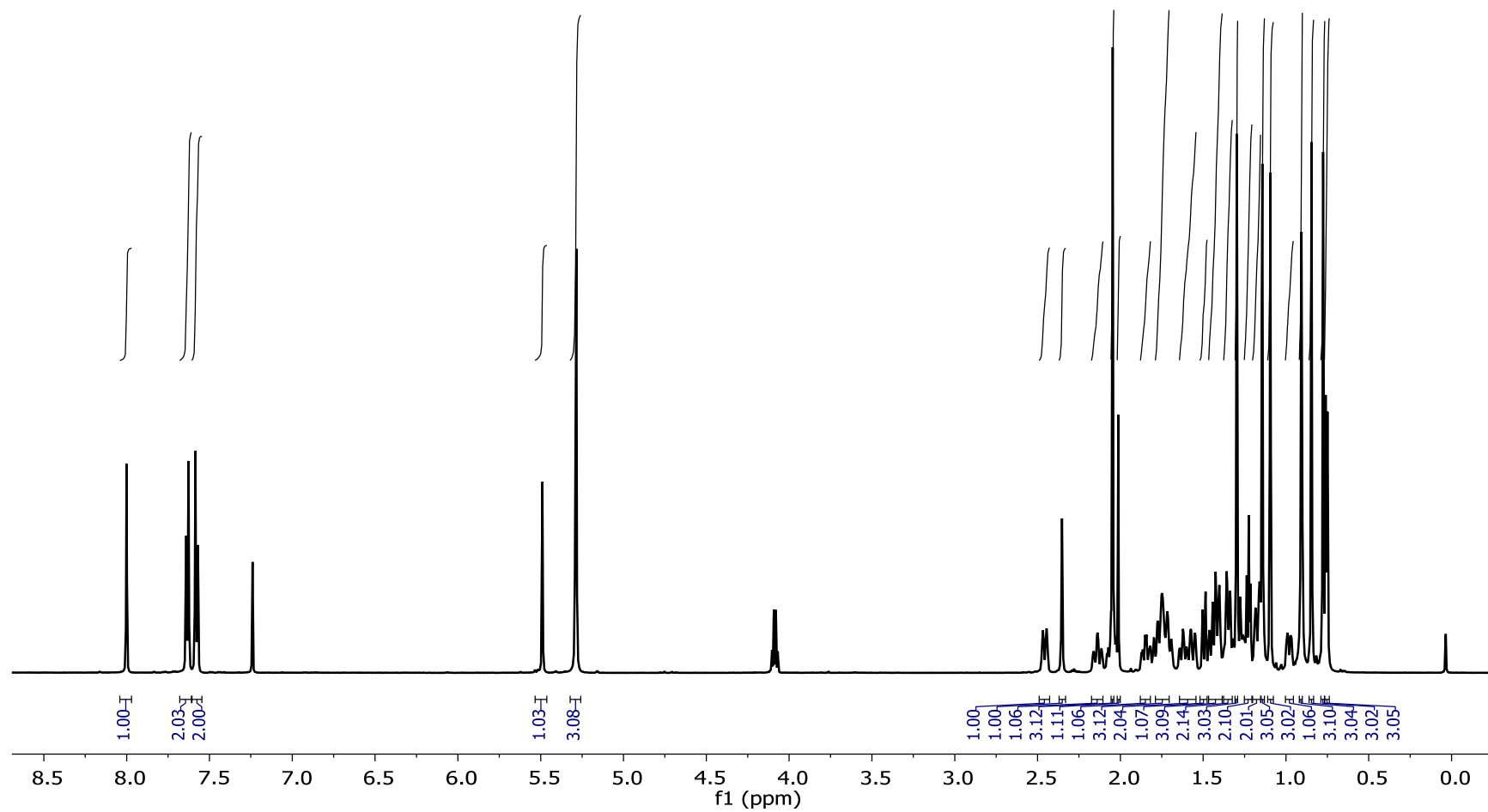


Figure S30: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 6h

09-Dec-2020.19.fid  
Dr. Kumar/SK-AKBA-4H/CDCl<sub>3</sub>  
C13CPD

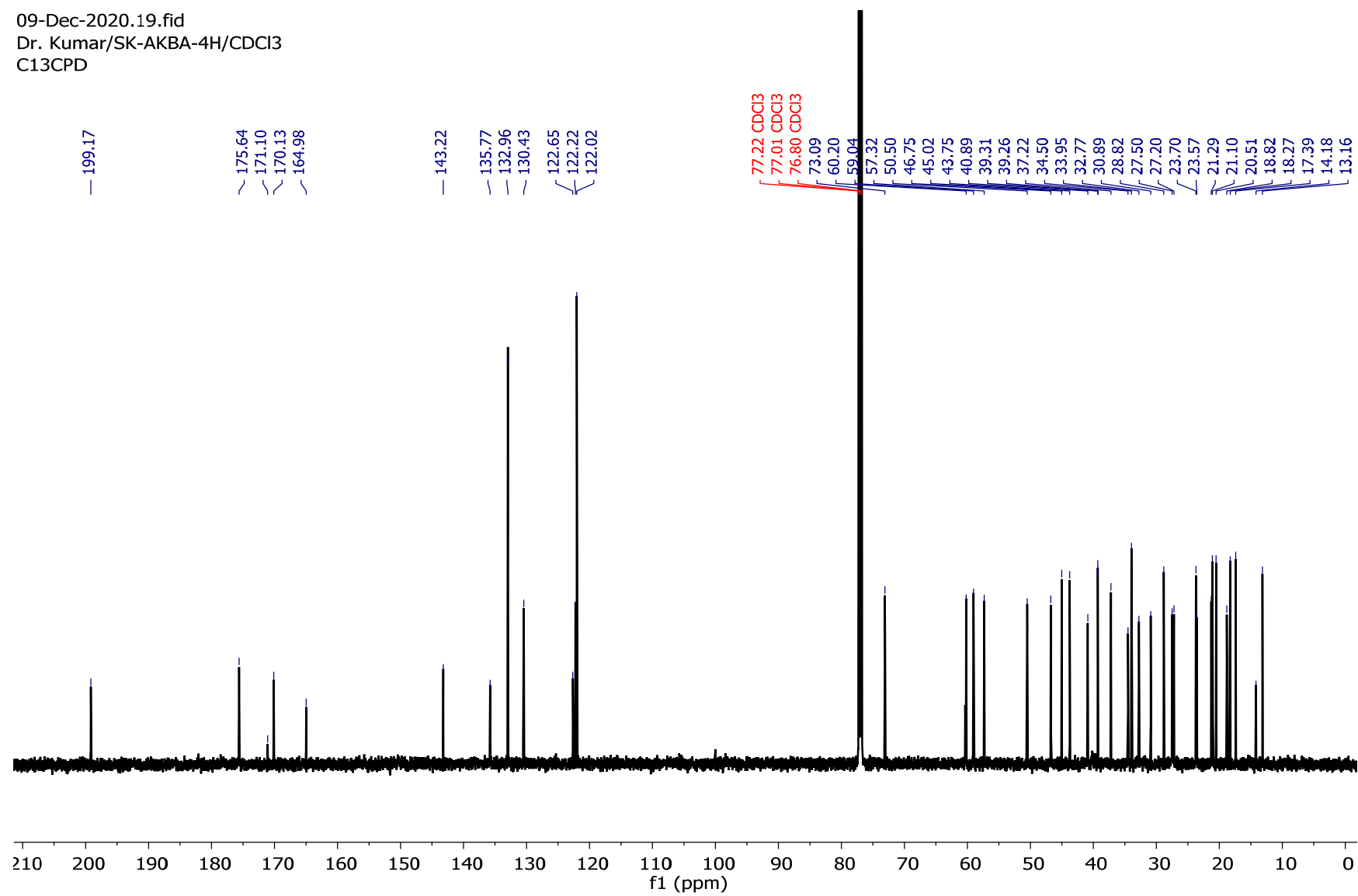


Figure S31: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound **6h**

Sample Name  
User Name  
Sample Type  
ACQ Method

4H  
Sample  
POSITIVE ION METHOD MS.m

Position  
Inj Vol  
IRM Calibration Status  
Comment

Vial 47  
2  
Success  
SK

Instrument Name  
InjPosition  
Data Filename  
Acquired Time

Instrument 1  
Instrument 1  
4H\_POS\_02.d  
20-Nov-20 6:55:10 PM

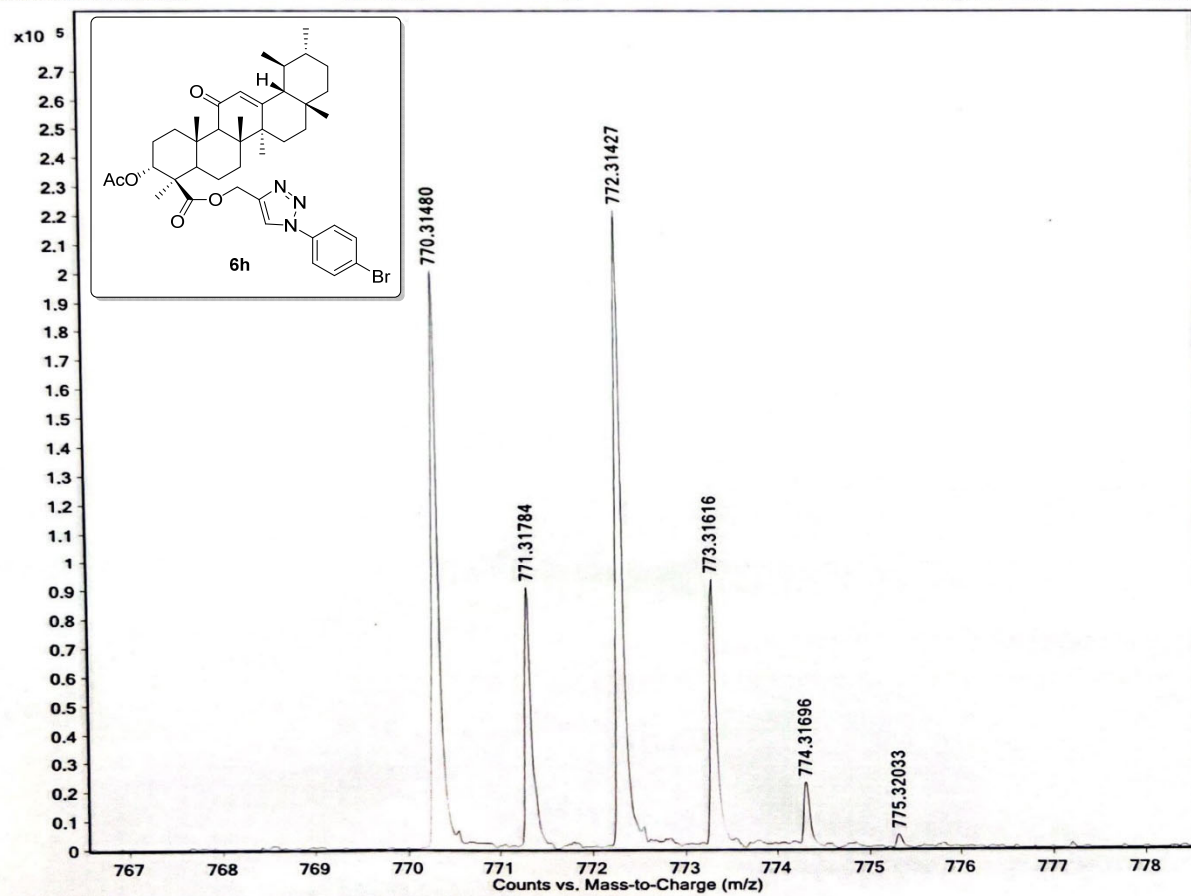


Figure S32: HRMS spectrum of compound 6h

28-Dec-2020.4.fid  
Dr. Kumar/SK-AKBA-4i/CDCl<sub>3</sub>  
PROTON

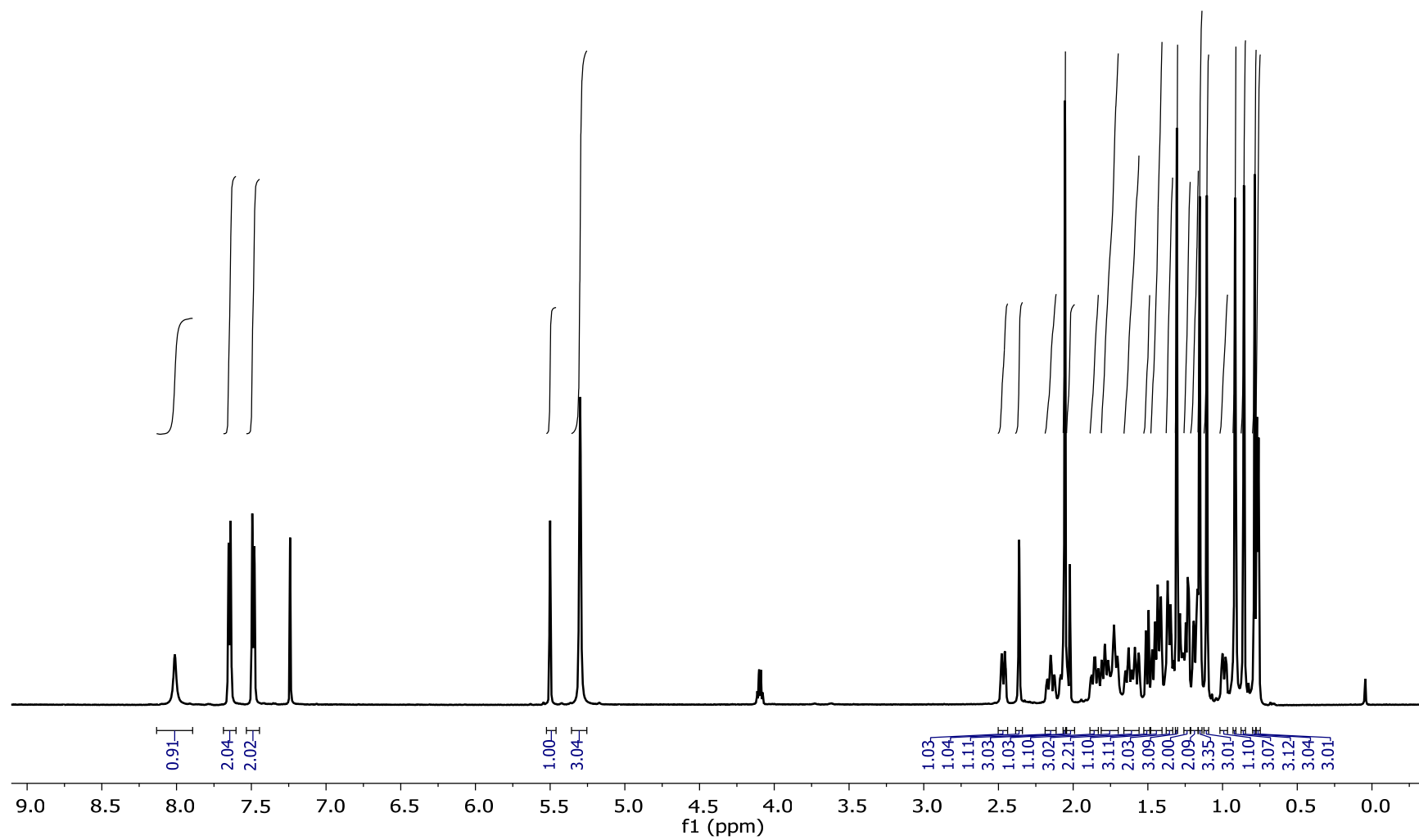


Figure S33: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 6i

28-Dec-2020.10.fid  
Dr. Kumar/SK-AKBA-4i/CDCl<sub>3</sub>  
C13CPD

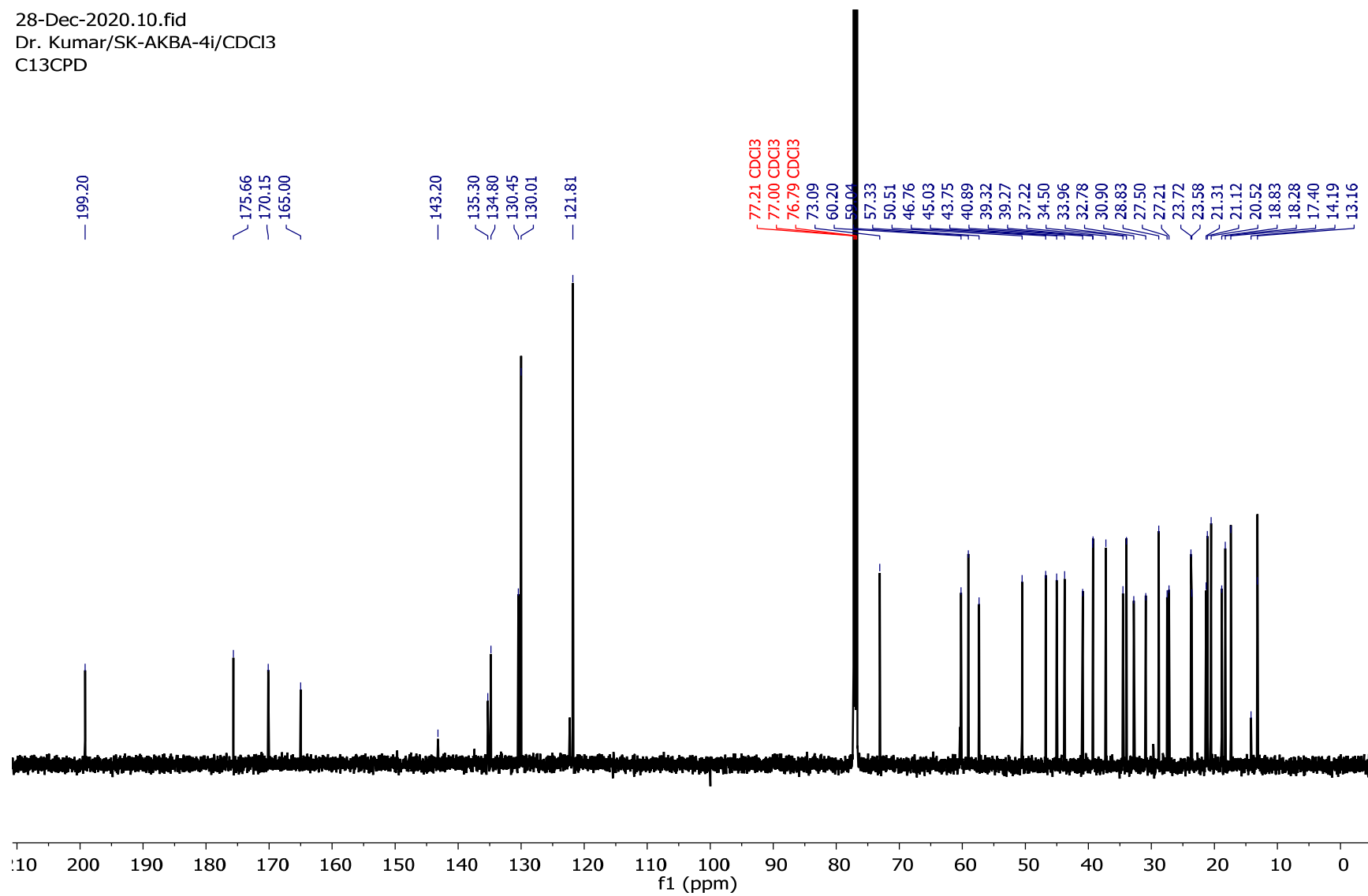


Figure S34: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound **6i**

Sample Name	SK-AKBA-4I	Position	Vial 1	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SK-AKBA-4I_POS_01.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment	SK	Acquired Time	28-Dec-20 2:32:25 PM

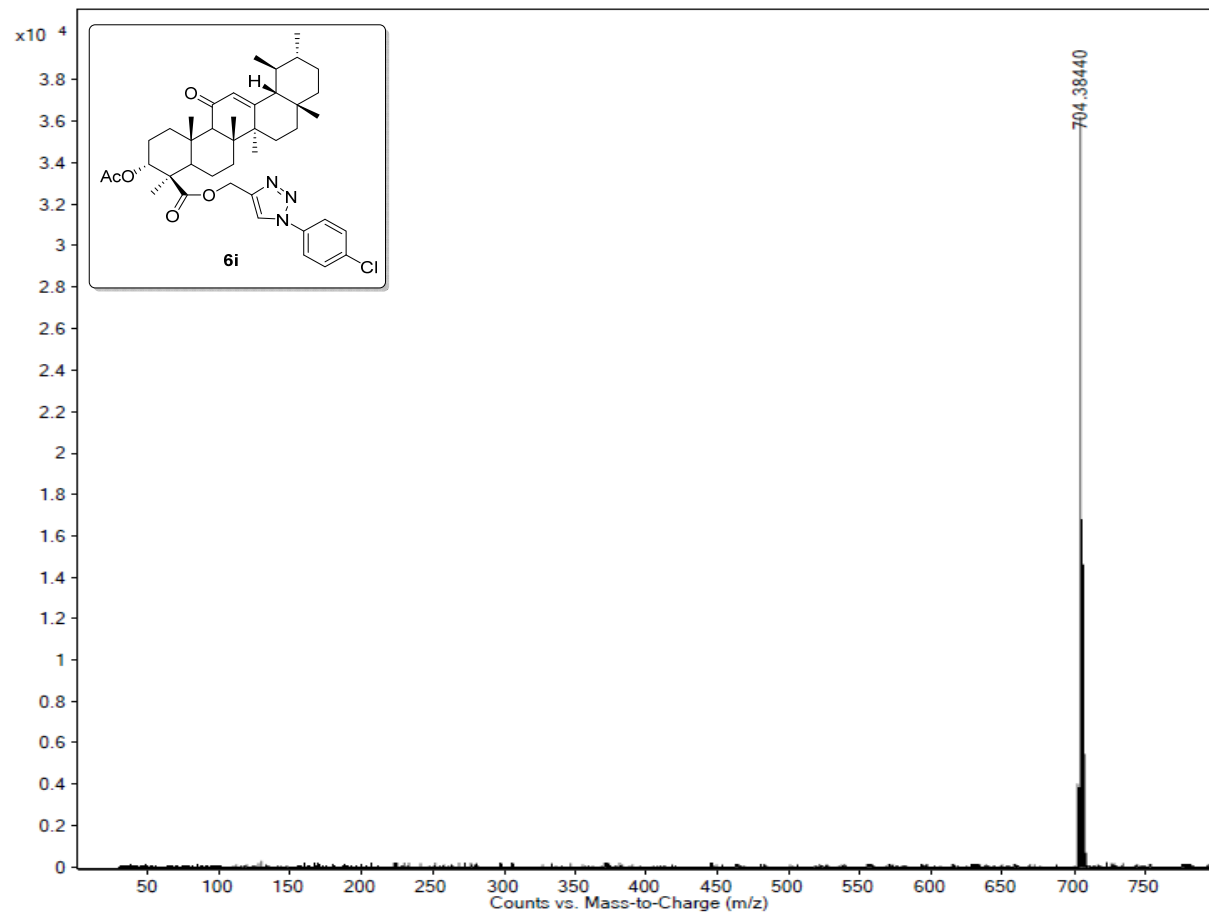


Figure S35: HRMS spectrum of compound **6i**



28-Dec-2020.6.fid  
Dr. Kumar/SK-AKBA-4j/CDCl<sub>3</sub>  
PROTON

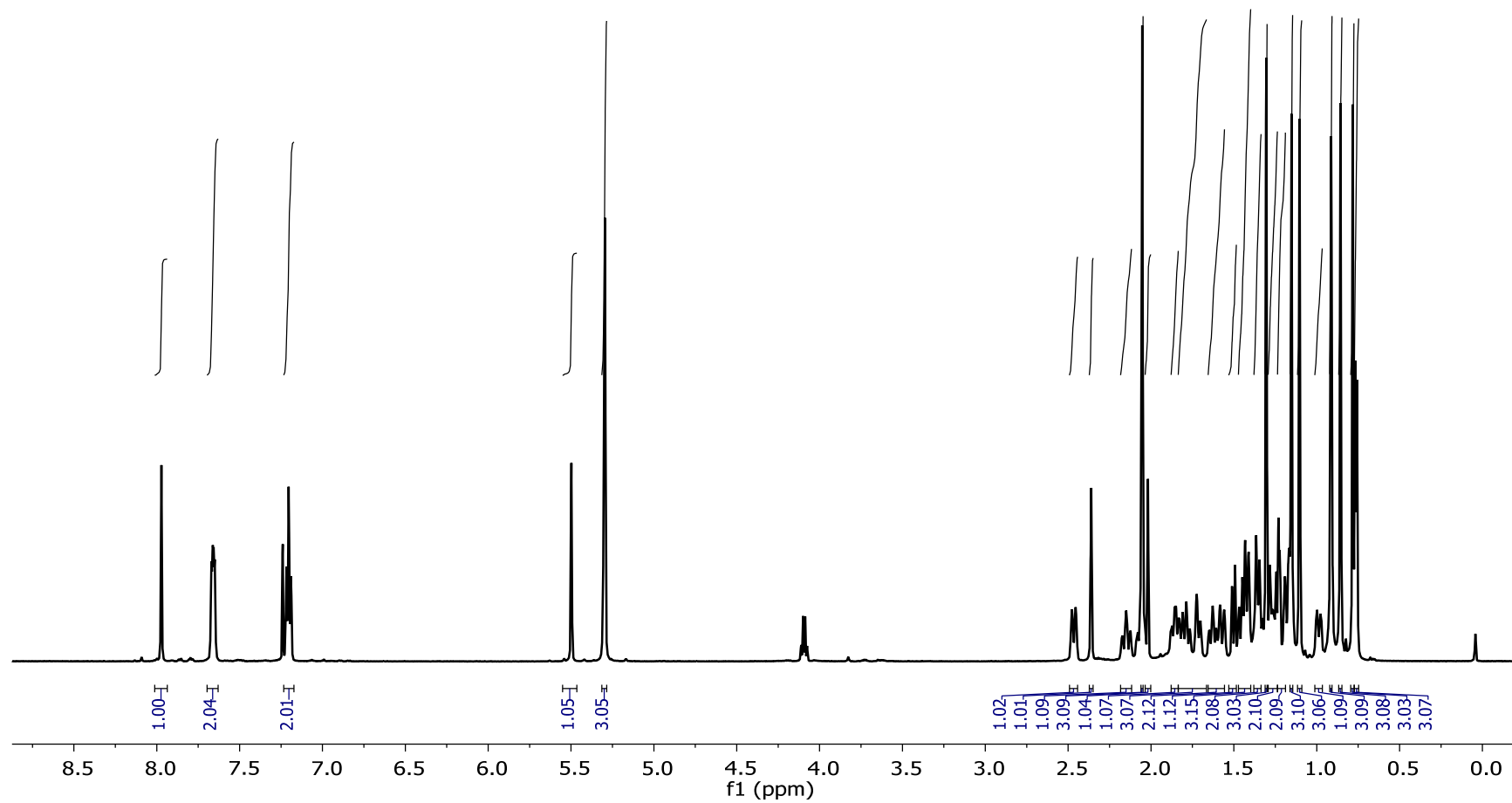


Figure S36: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 6j

28-Dec-2020.18.fid  
Dr. Kumar/SK-AKBA-4j/CDCl<sub>3</sub>  
C13CPD

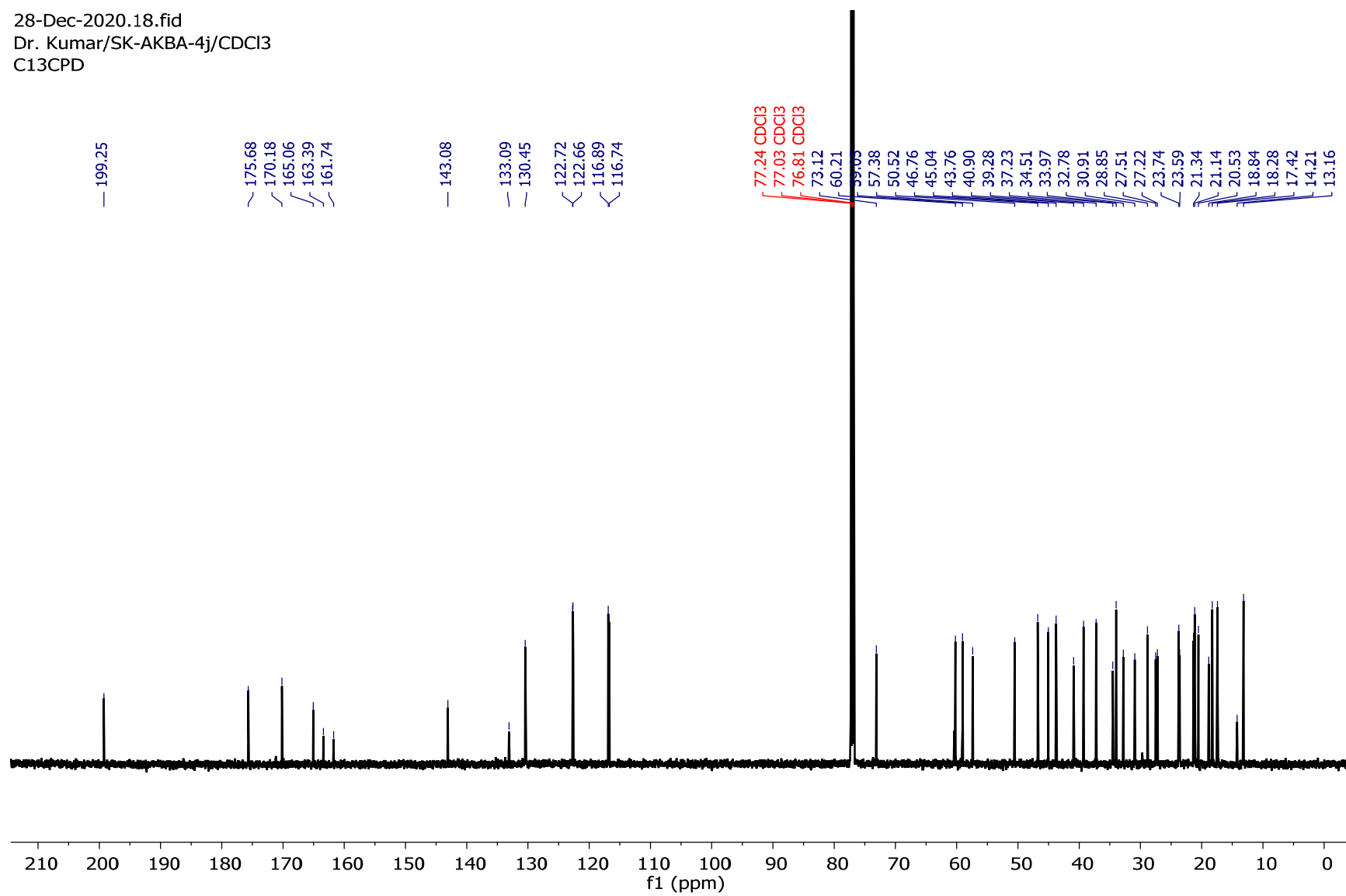


Figure S37: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound **6j**

28-Dec-2020.7.fid  
Dr. Kumar/SK-AKBA-4j/CDCl<sub>3</sub>  
F19CPD

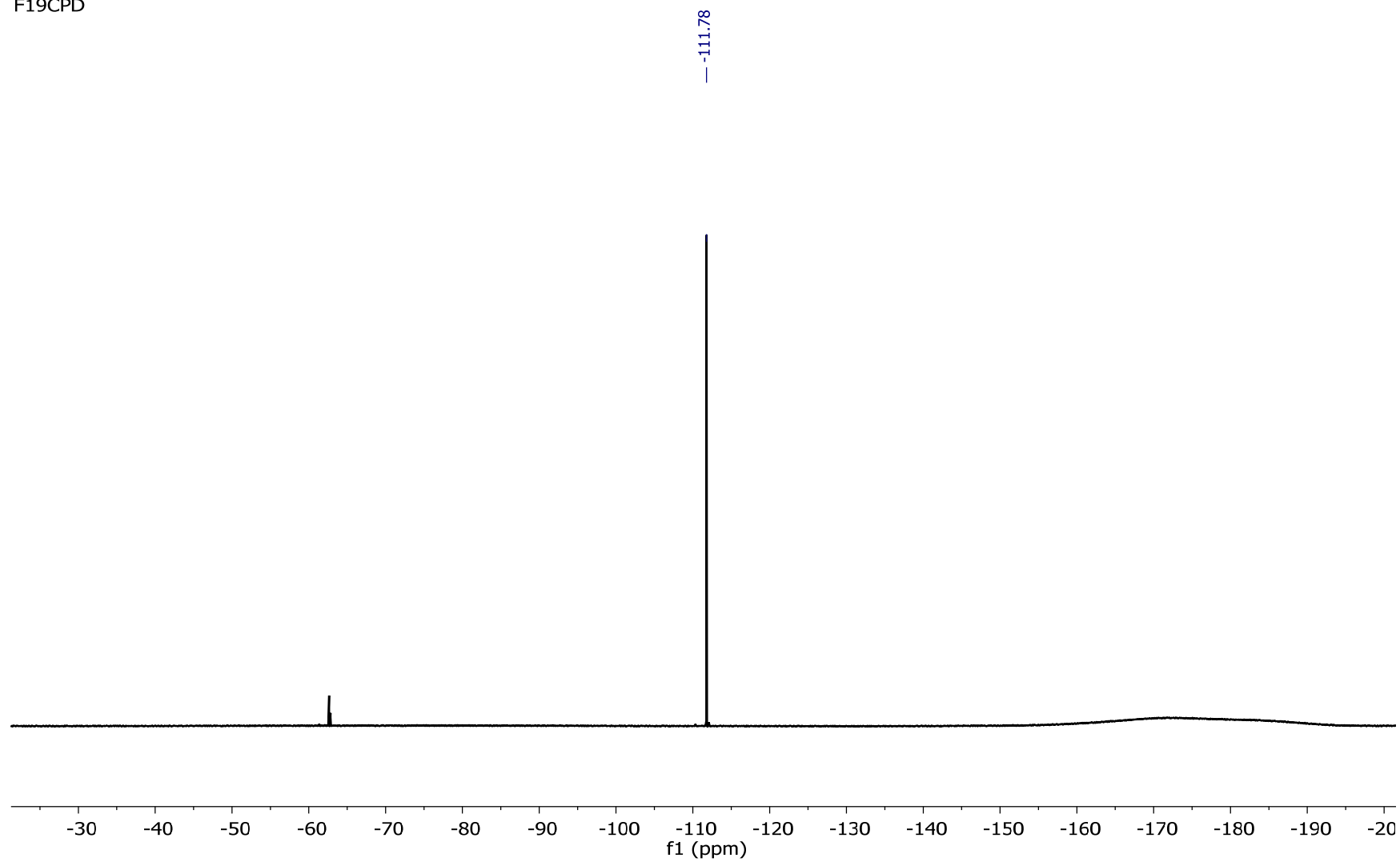


Figure S38: <sup>19</sup>F-NMR spectrum (564 MHz, CDCl<sub>3</sub>) of compound **6j**

Sample Name	SK-AKBA-4J	Position	Vial 2	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SK-AKBA-4J_POS_01.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment	SK	Acquired Time	28-Dec-20 2:38:01 PM

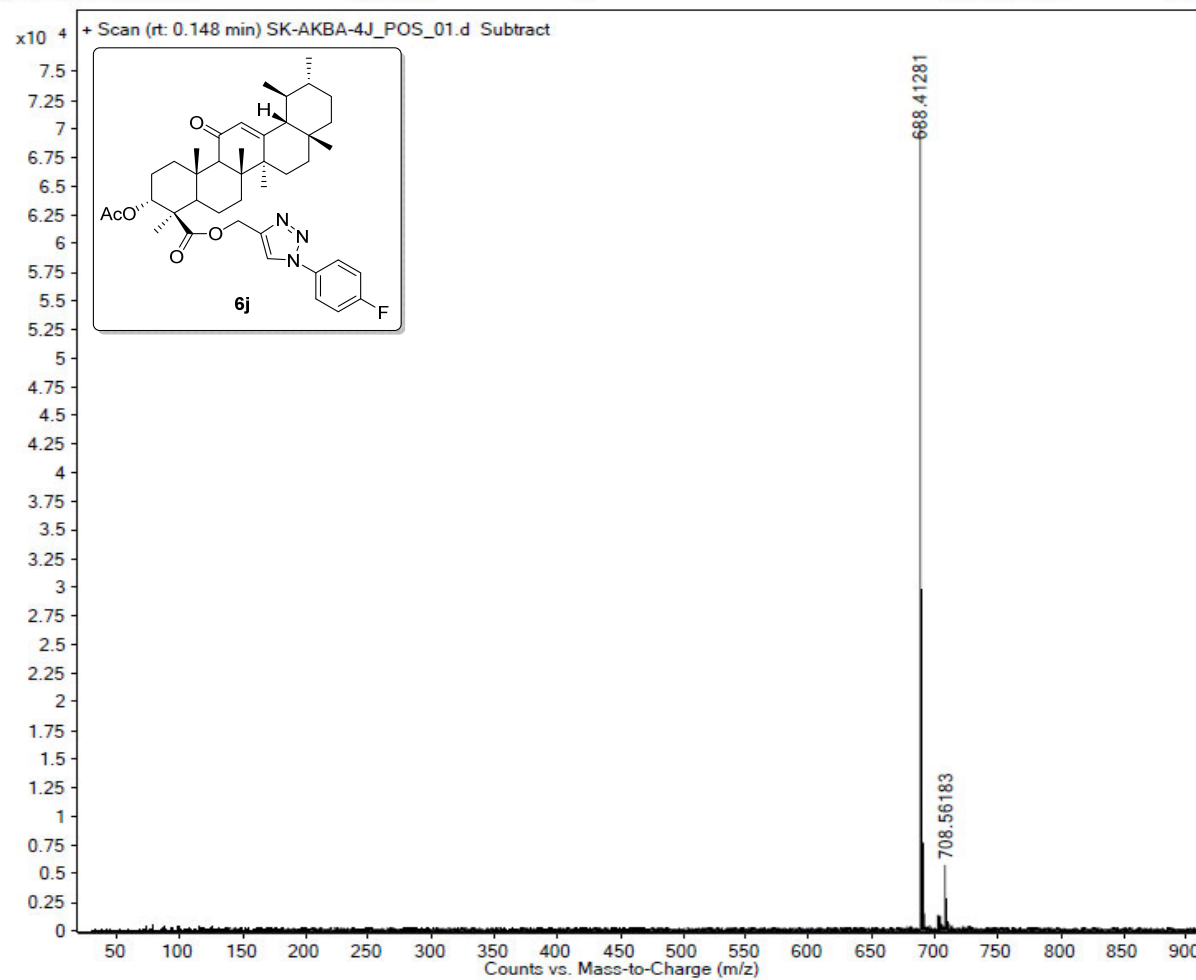


Figure S39: HRMS spectrum of compound **6j**

28-Dec-2020.8.fid  
Dr. Kumar/SK-AKBA-4k/CDCl<sub>3</sub>  
PROTON

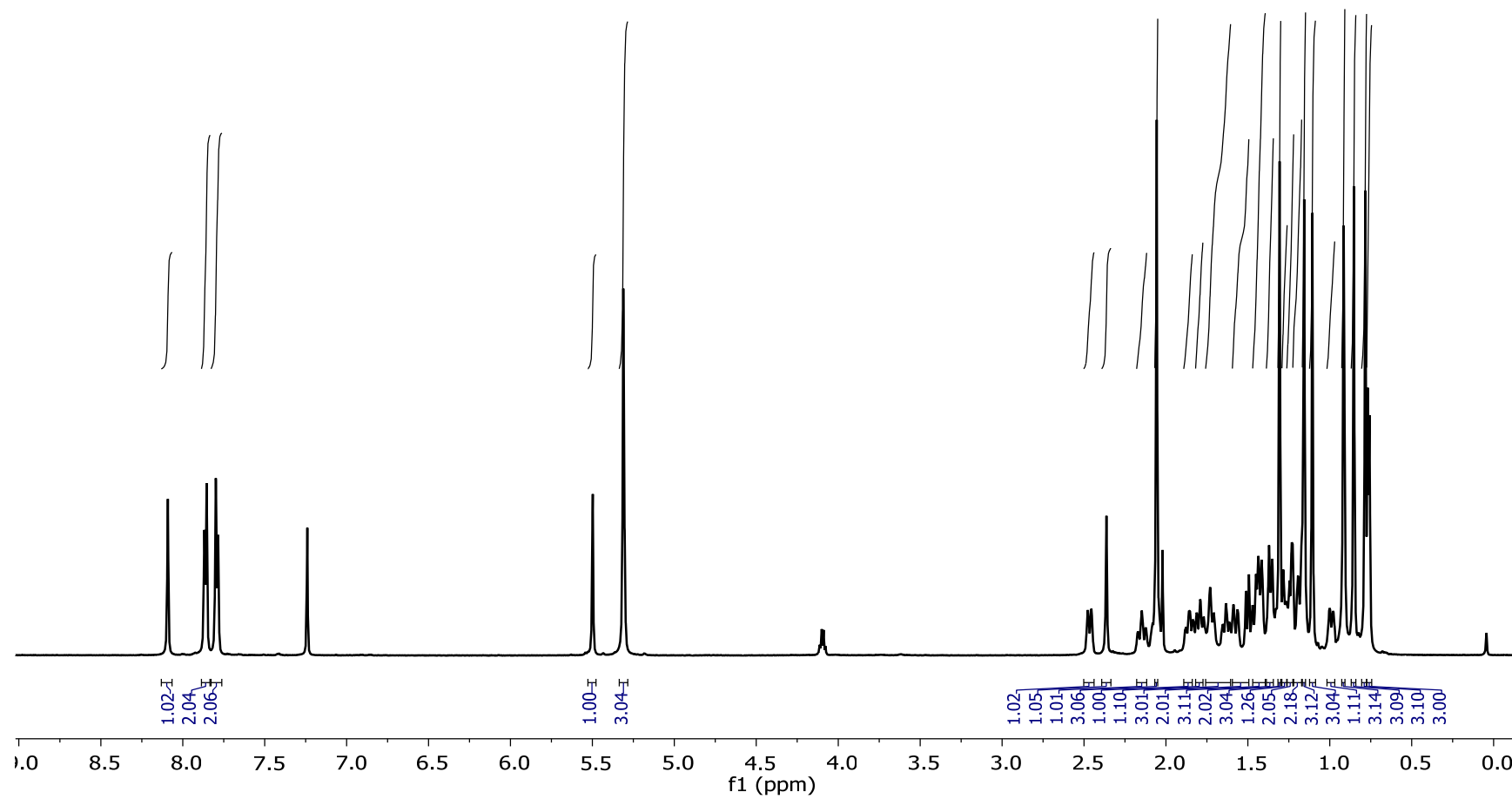


Figure S40: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound **6k**

28-Dec-2020.17.fid  
Dr. Kumar/SK-AKBA-4k/CDCl<sub>3</sub>  
C13CPD

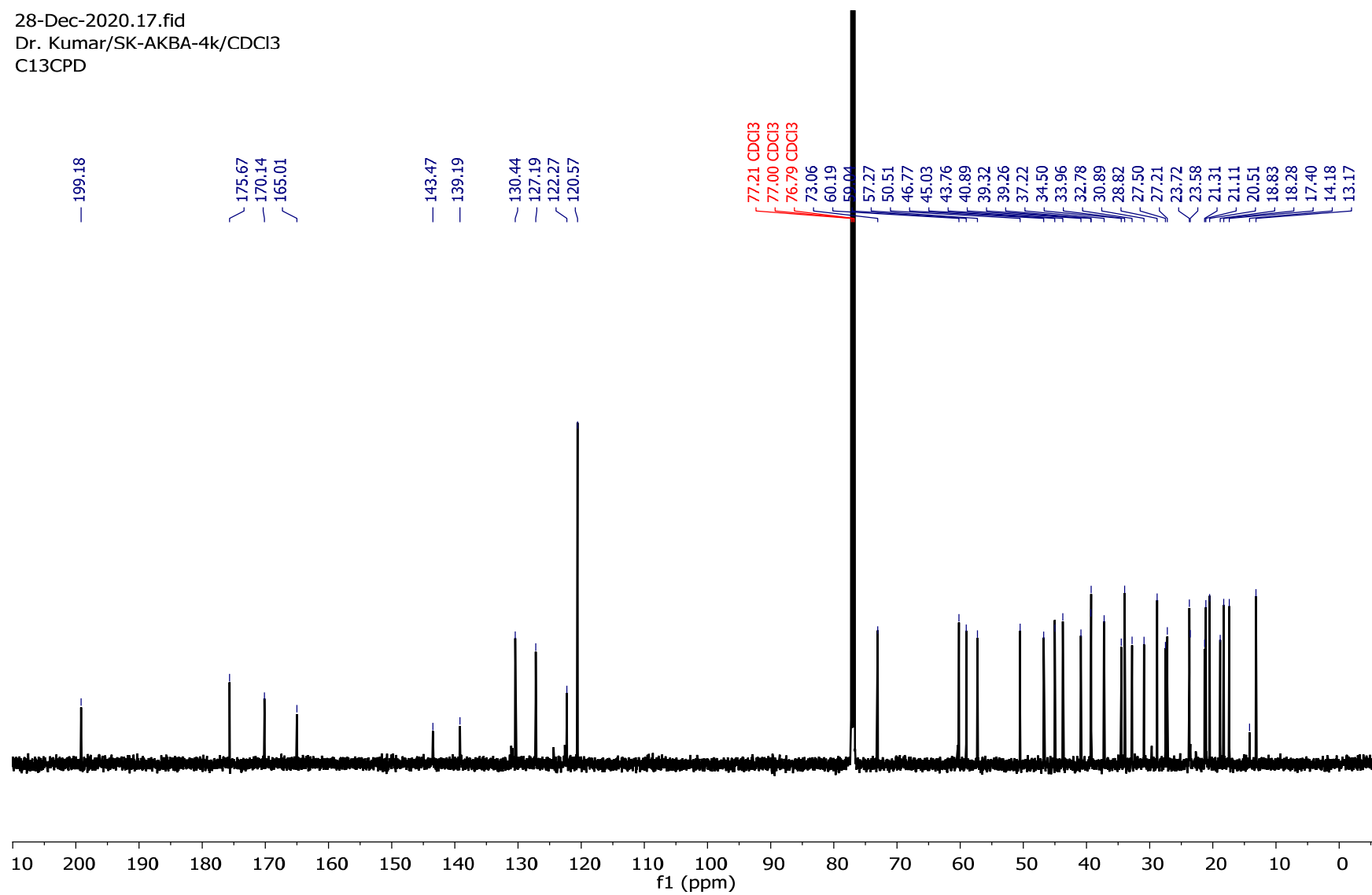
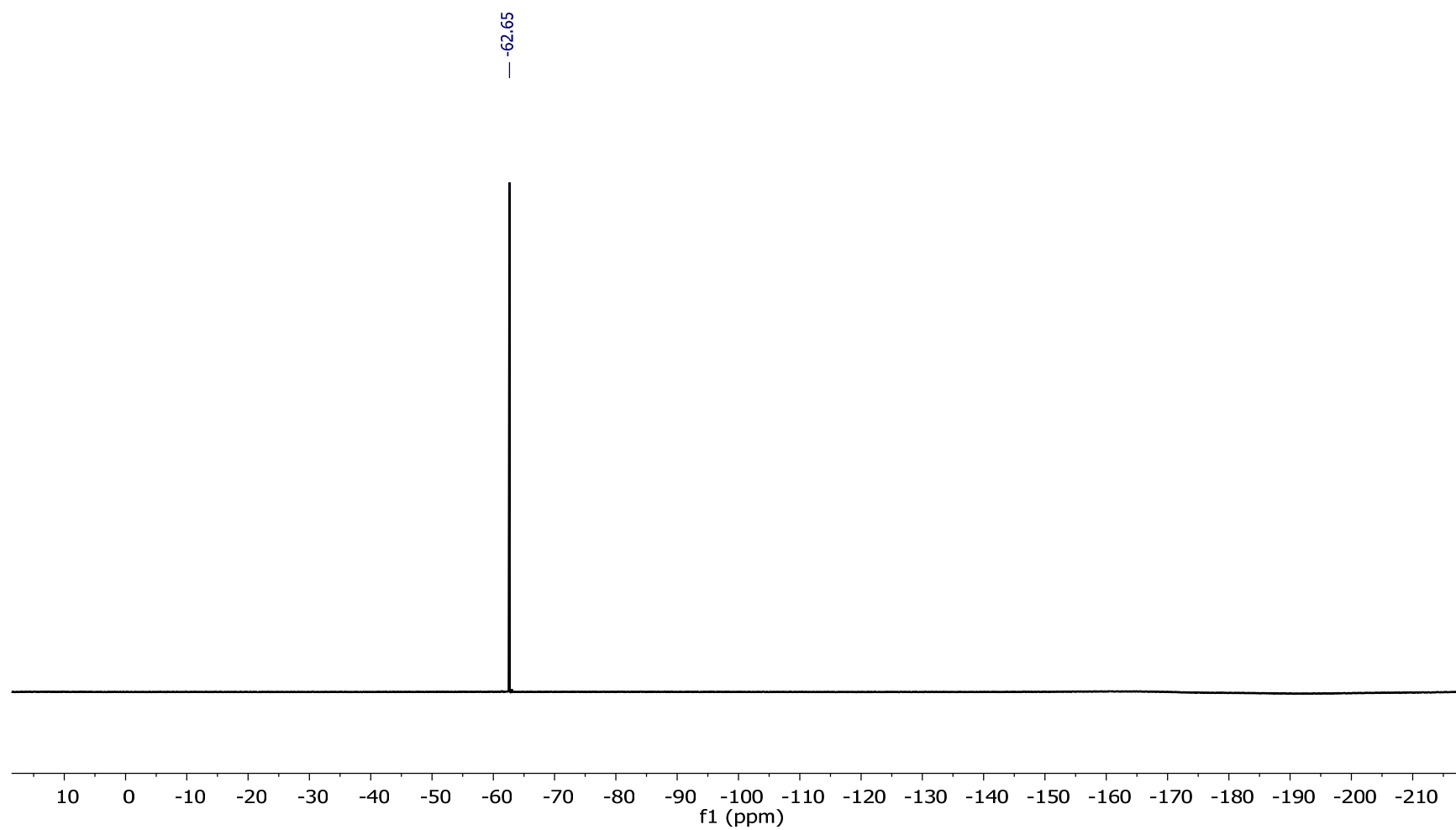


Figure S41: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound 6k

28-Dec-2020.9.fid  
Dr. Kumar/SK-AKBA-4k/CDCl<sub>3</sub>  
F19CPD



**Figure S42:** <sup>19</sup>F-NMR spectrum (564 MHz, CDCl<sub>3</sub>) of compound **6k**

Sample Name	SK-AKBA-4K	Position	Vial 3	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SK-AKBA-4K_POS_01.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment	SK	Acquired Time	28-Dec-20 2:43:36 PM

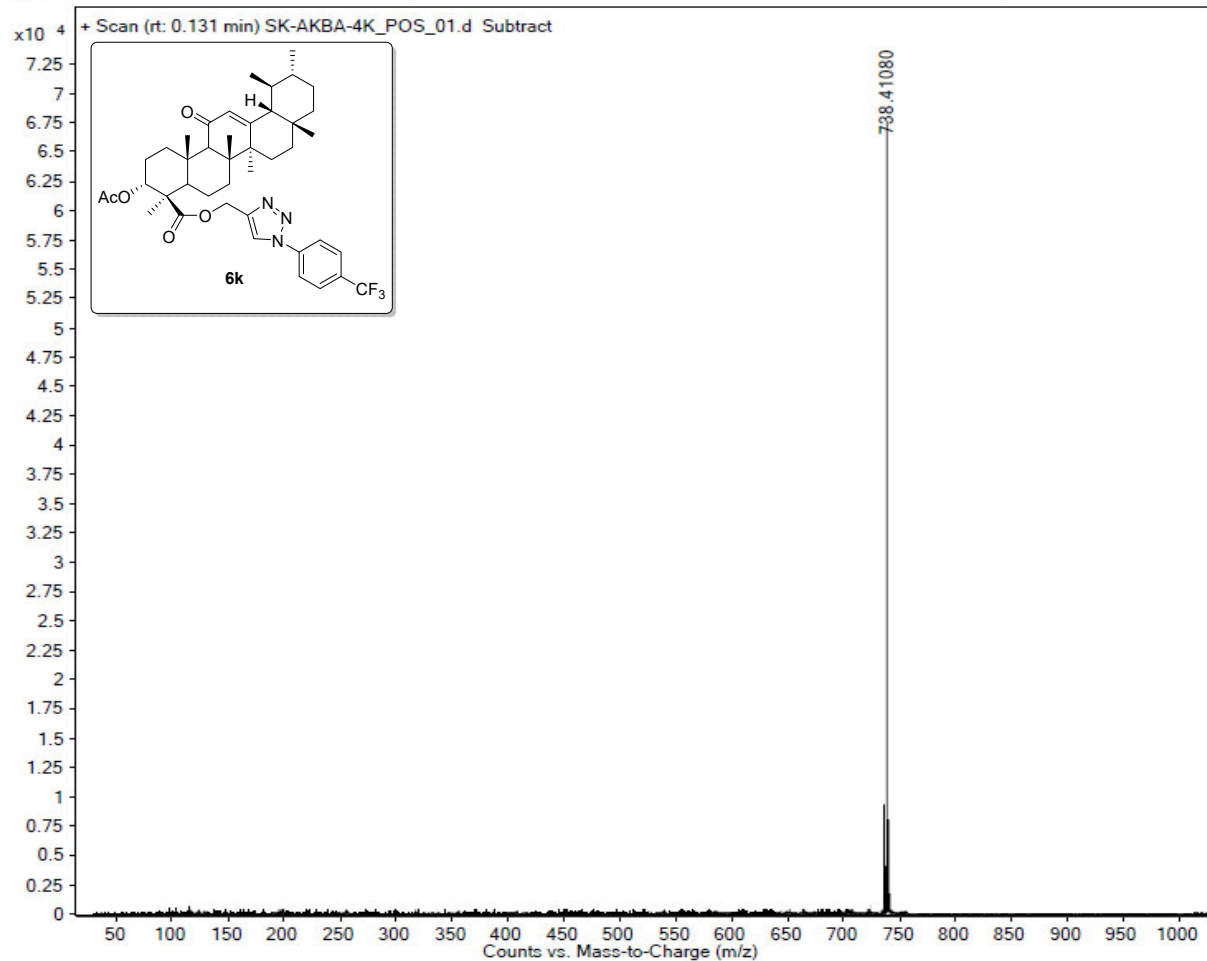


Figure S43: HRMS spectrum of compound 6k



07-Mar-2021.18.fid  
Dr. A. Satya Kumar / SK-KBA-7a / CDCl<sub>3</sub>  
PROTON

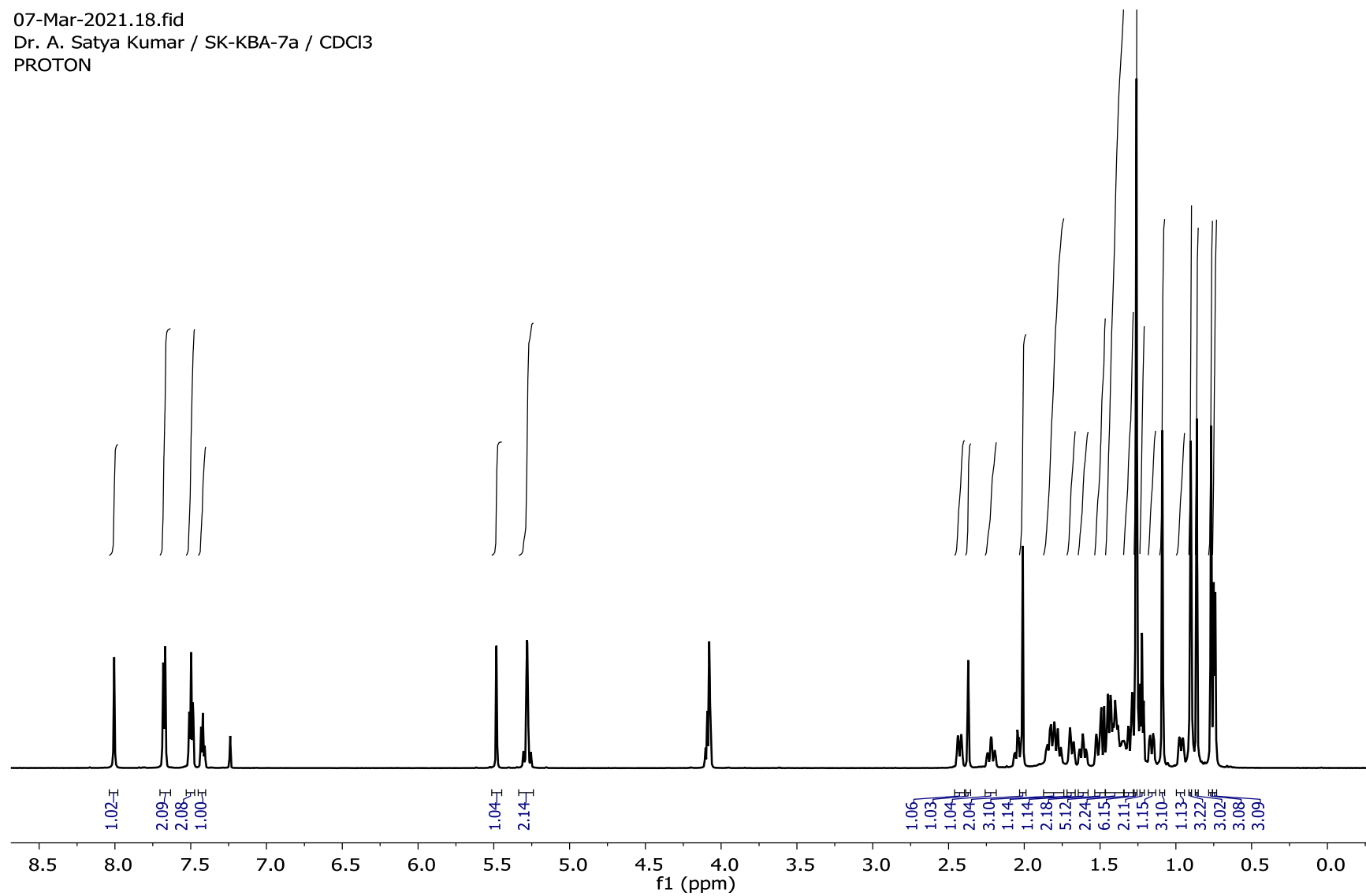


Figure S44: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 7a

07-Mar-2021.19.fid  
Dr. A. Satya Kumar / SK-KBA-7a / CDCl<sub>3</sub>  
C13CPD

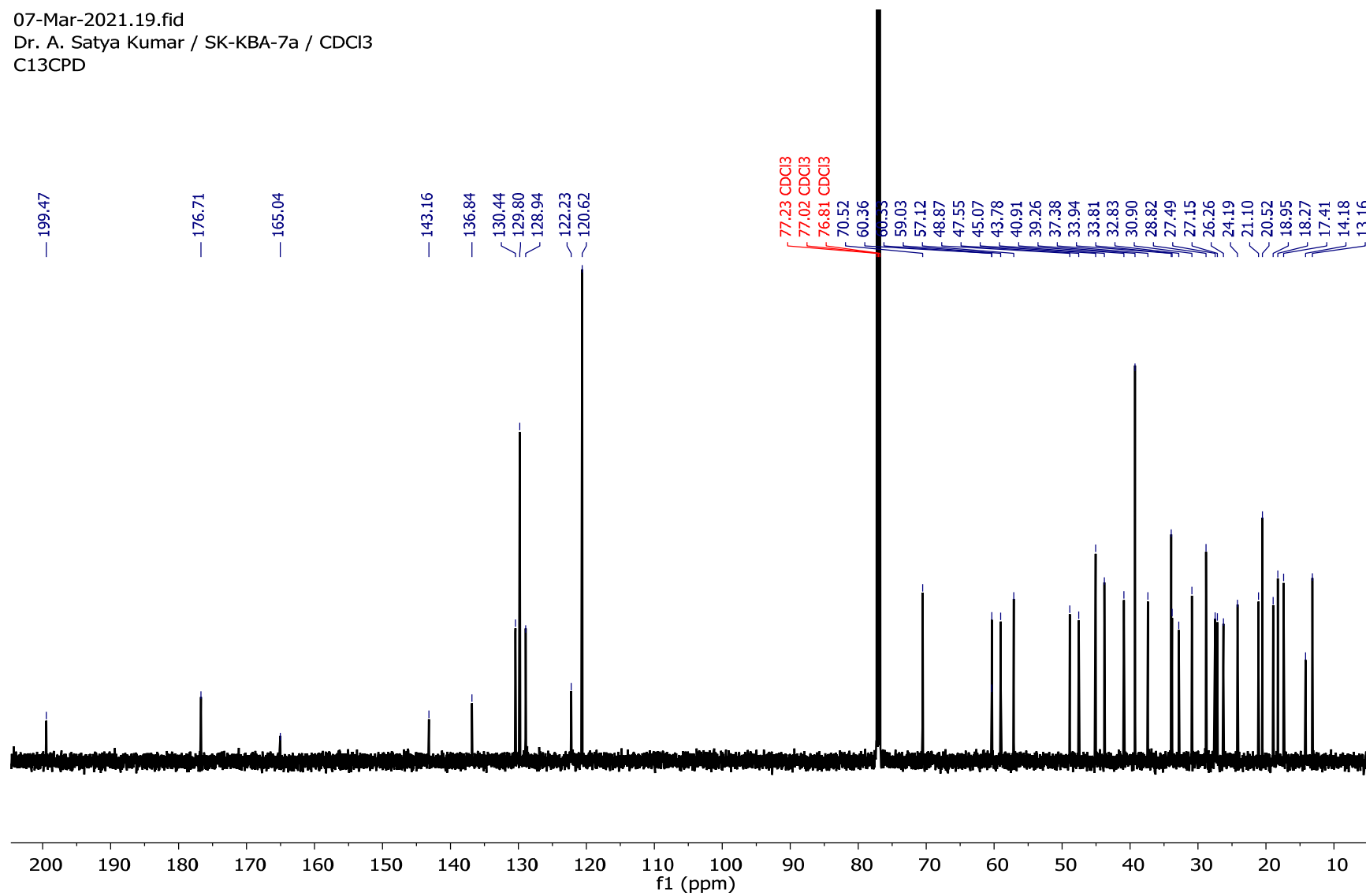


Figure S45: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound 7a

Sample Name	SK-KBA-7A	Position	Vial 41	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SK-KBA-7A.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment	PARTHA	Acquired Time	17-Mar-21 12:09:31 PM

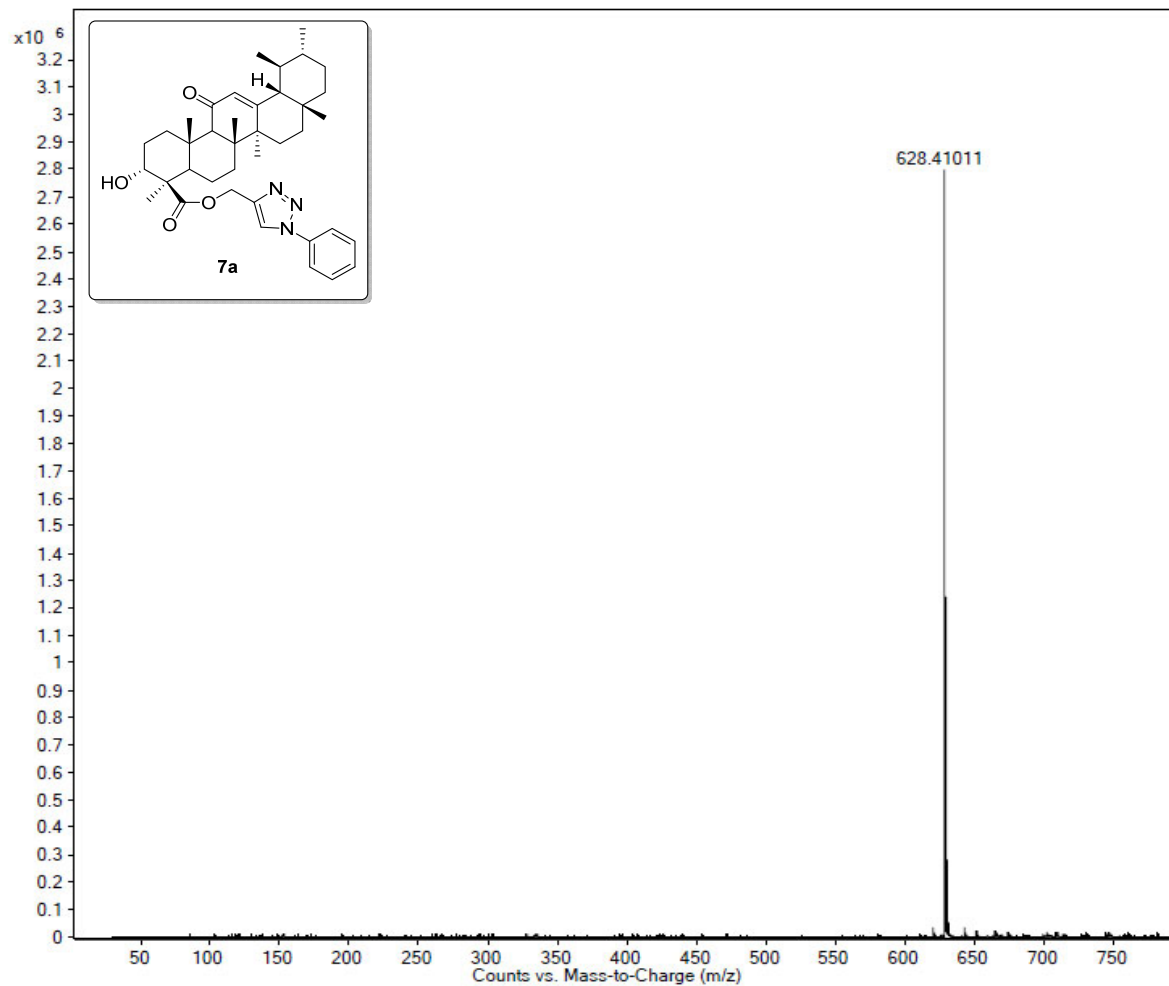


Figure S46: HRMS spectrum of compound 7a

07-Mar-2021.22.fid  
Dr. A. Satya Kumar / SK-KBA-7b / CDCl<sub>3</sub>  
PROTON

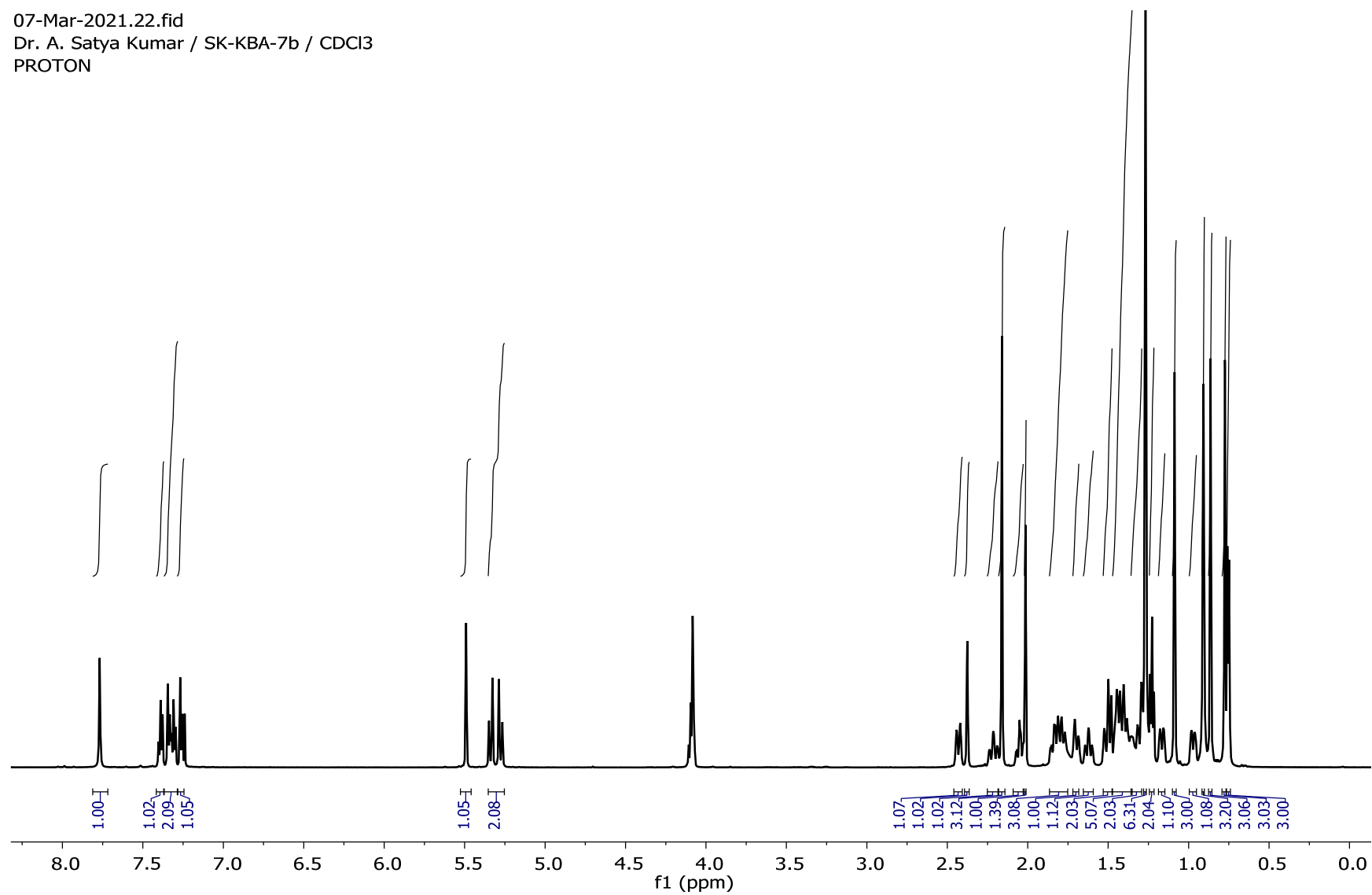


Figure S47: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound **7b**

07-Mar-2021.23.fid  
Dr. A. Satya Kumar / SK-KBA-7b / CDCl<sub>3</sub>  
C13CPD

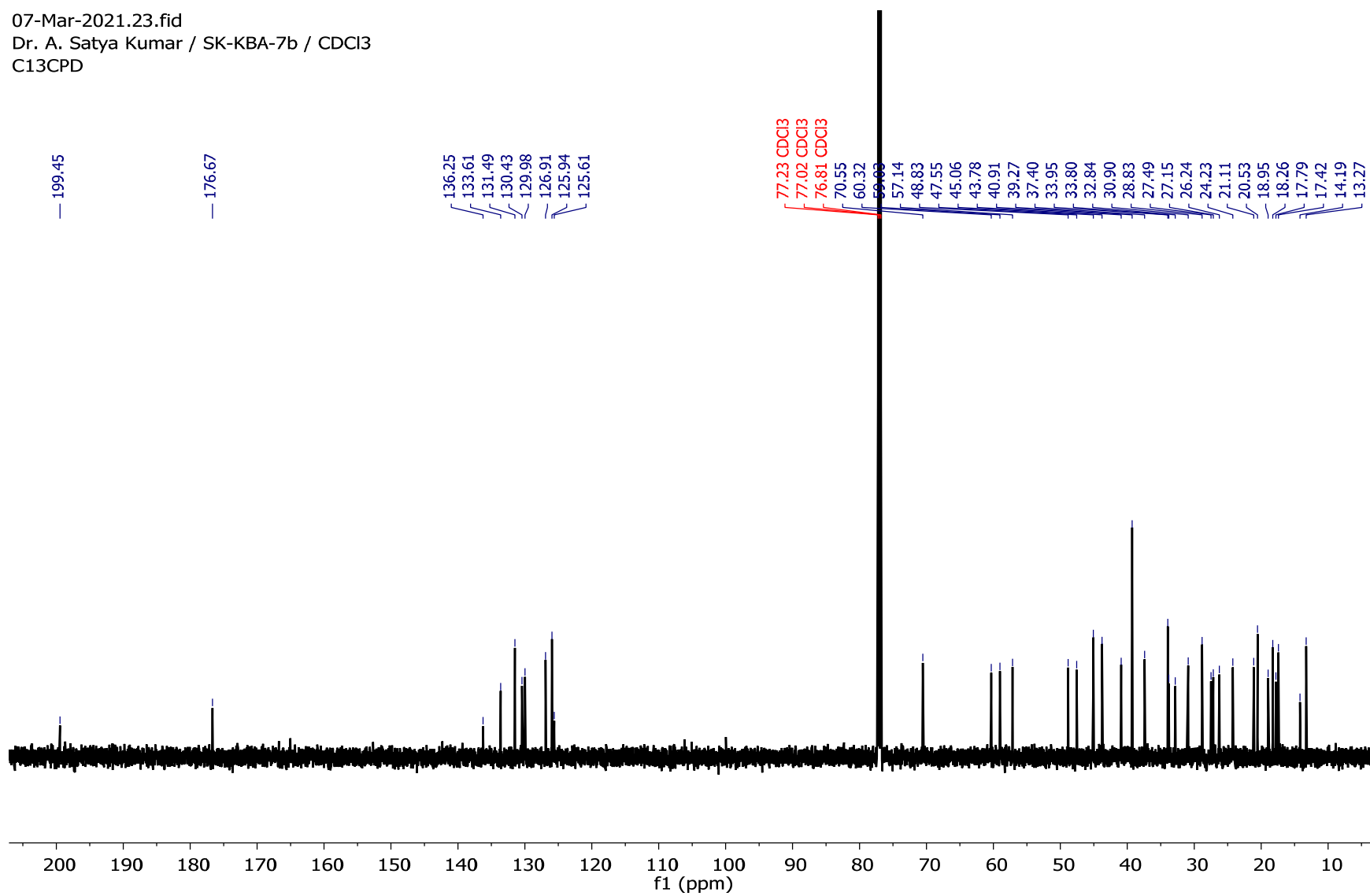


Figure S48: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound **7b**

Sample Name	SK-KBA-7B	Position	Vial 42	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SK-KBA-7B.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment	PARTHA	Acquired Time	17-Mar-21 12:18:56 PM

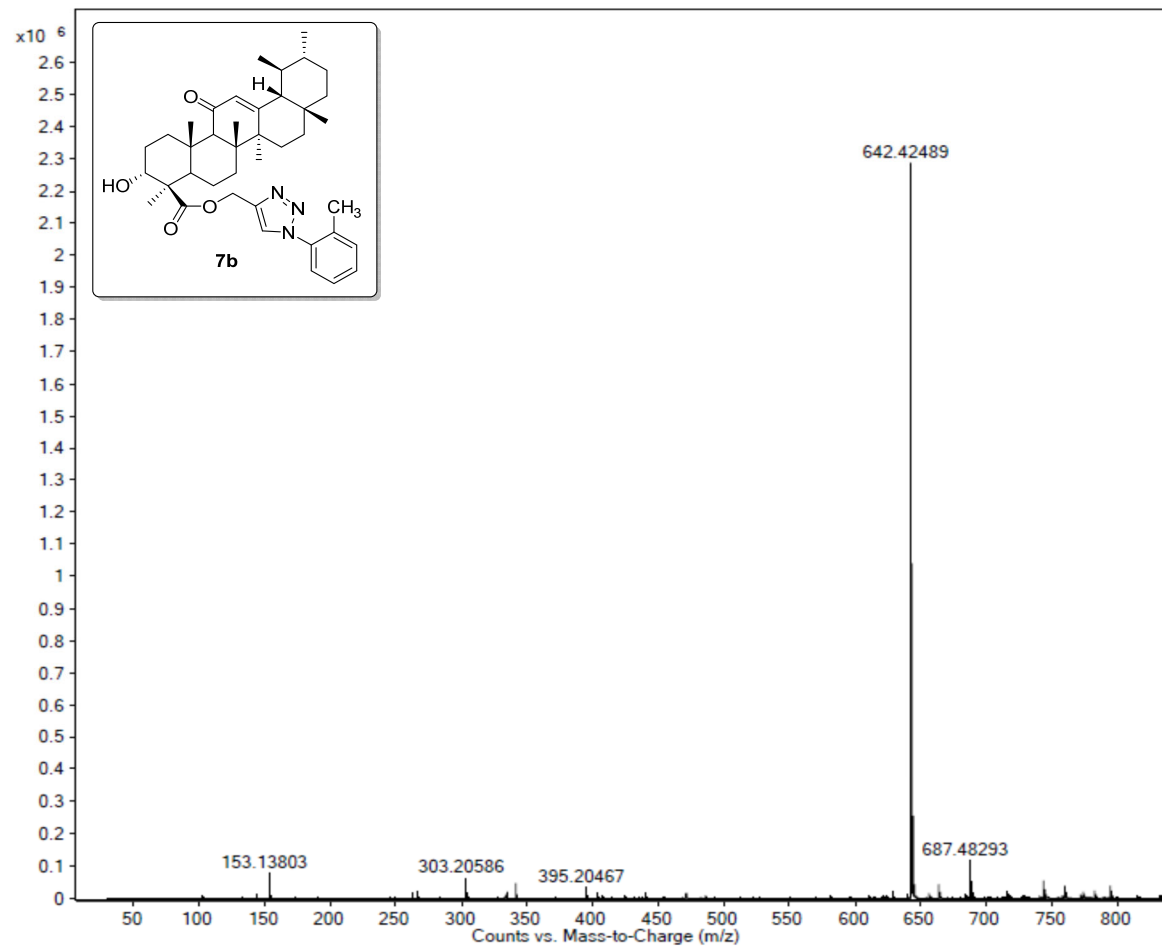


Figure S49: HRMS spectrum of compound **7b**

07-Mar-2021.26.fid  
Dr. A. Satya Kumar / SK-KBA-7c / CDCl<sub>3</sub>  
PROTON

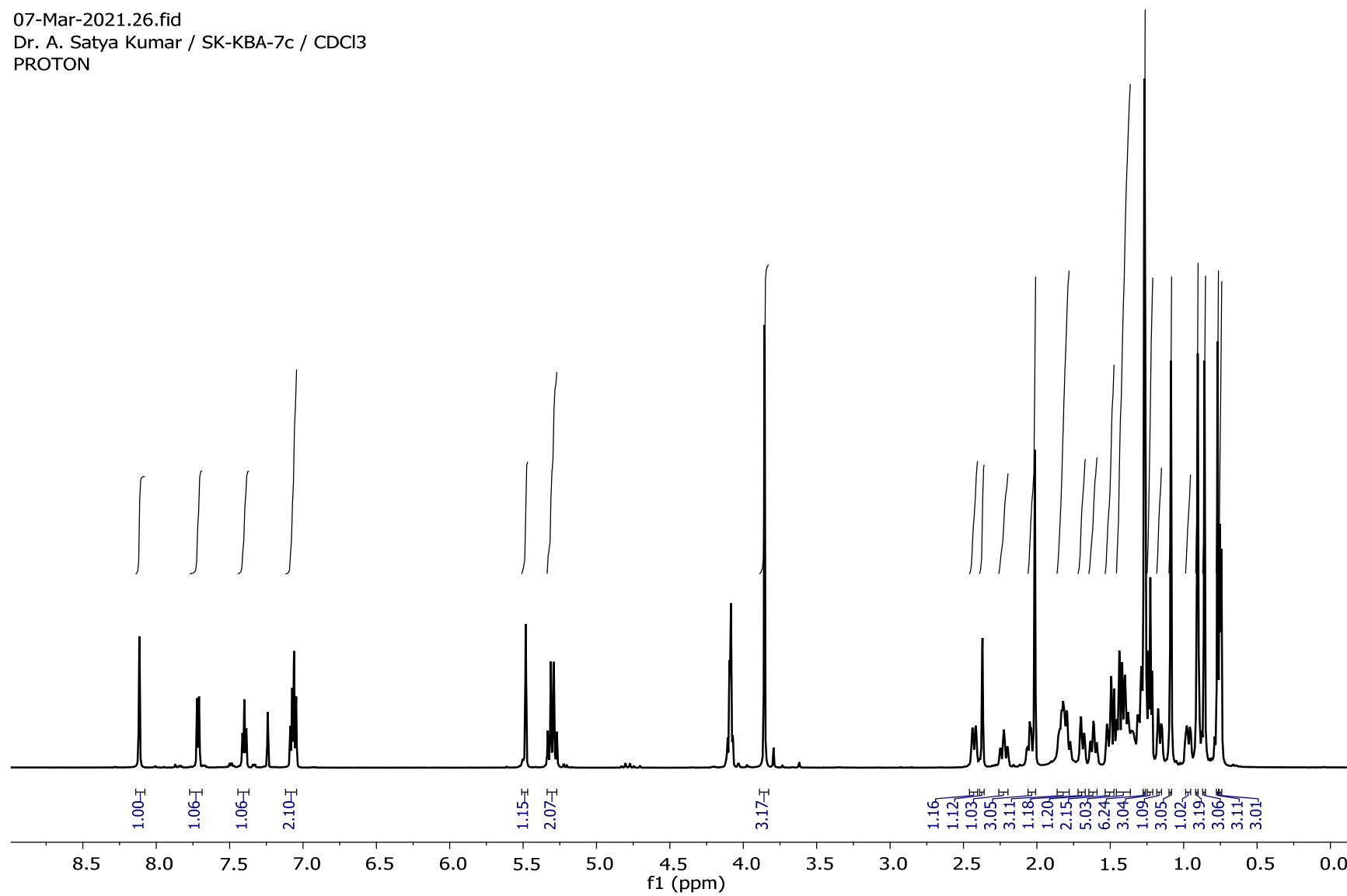


Figure S50: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 7c

07-Mar-2021.27.fid  
Dr. A. Satya Kumar / SK-KBA-7c / CDCl<sub>3</sub>  
C13CPD

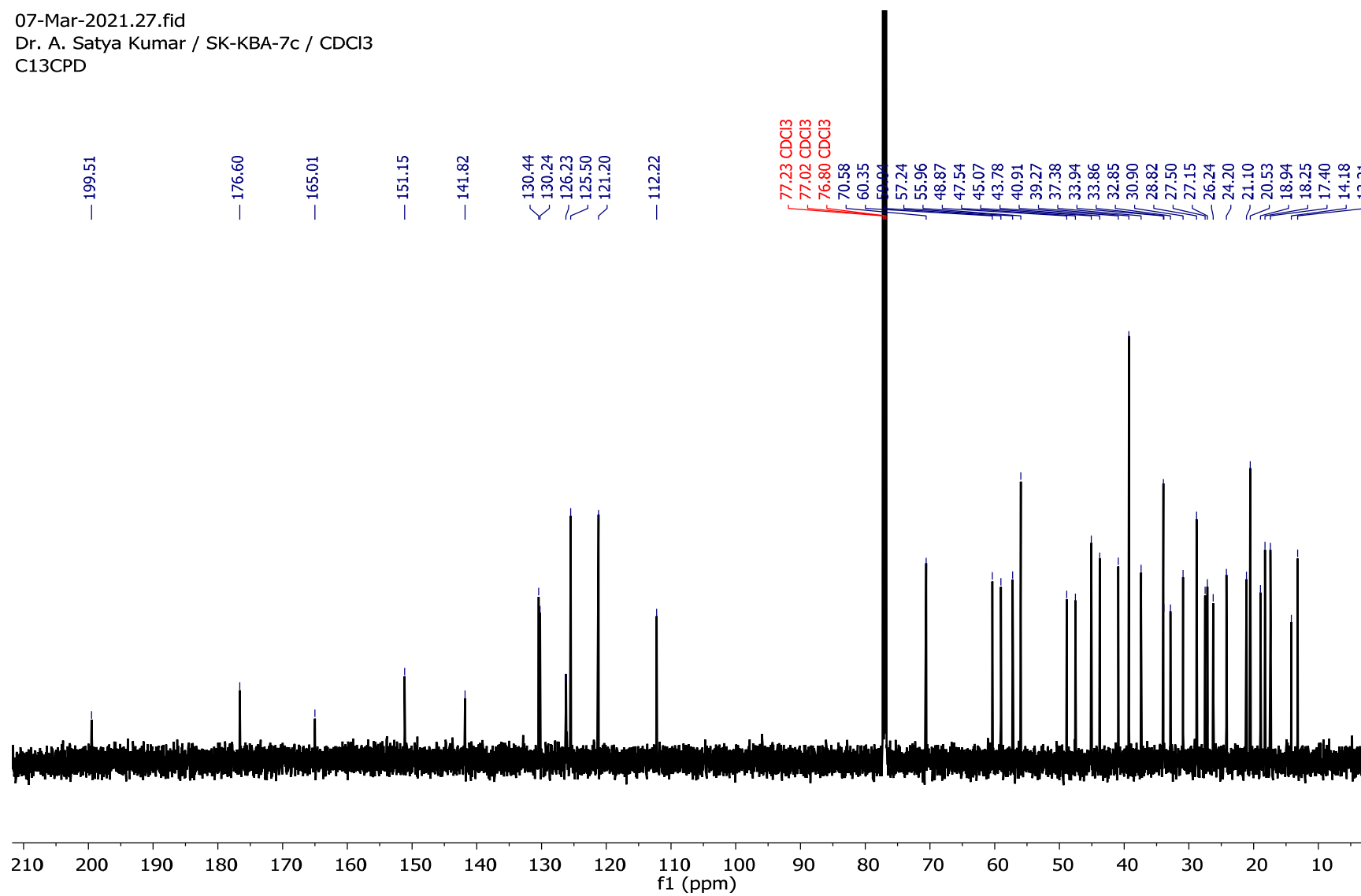


Figure S51: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound 7c



Sample Name	SK-KBA-7C	Position	Vial 43	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SK-KBA-7C.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment	PARTHA	Acquired Time	17-Mar-21 12:24:32 PM

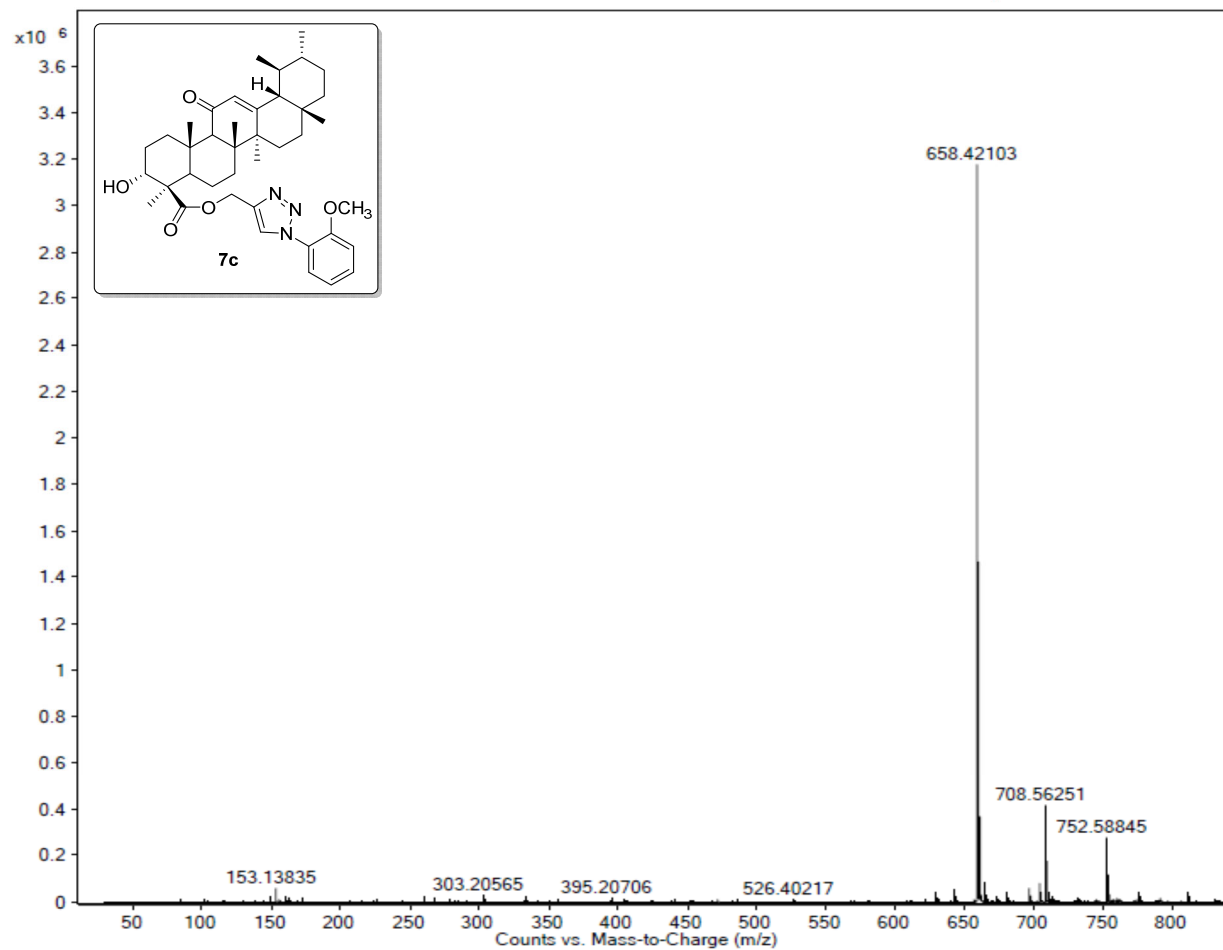


Figure S52: HRMS spectrum of compound 7c

08-Mar-2021.1.fid  
Dr. A. Satya Kumar / SK-KBA-7d / CDCl<sub>3</sub>  
PROTON

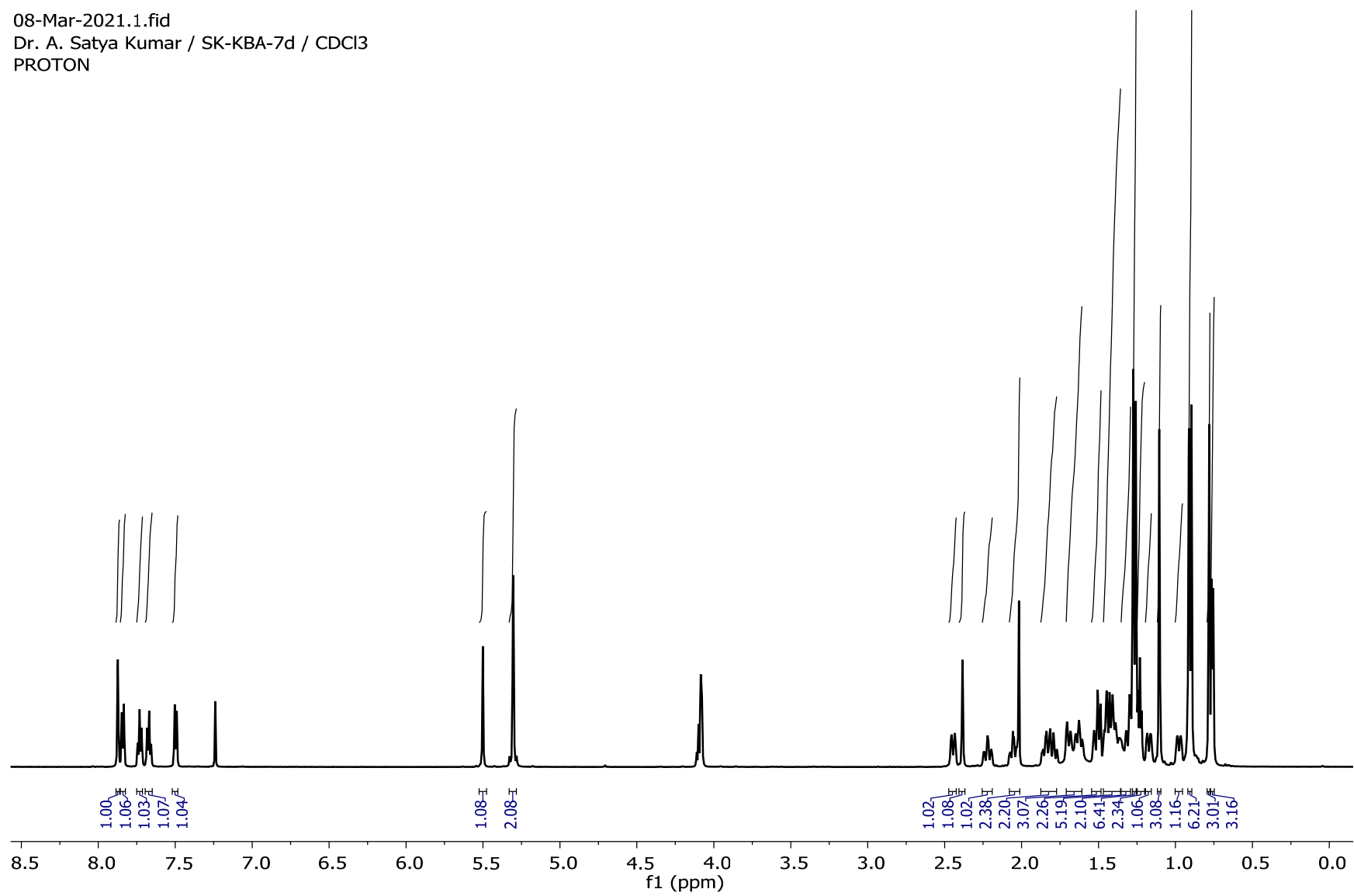


Figure S53: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 7d

08-Mar-2021.2.fid  
Dr. A. Satya Kumar / SK-KBA-7d / CDCl<sub>3</sub>  
C13CPD

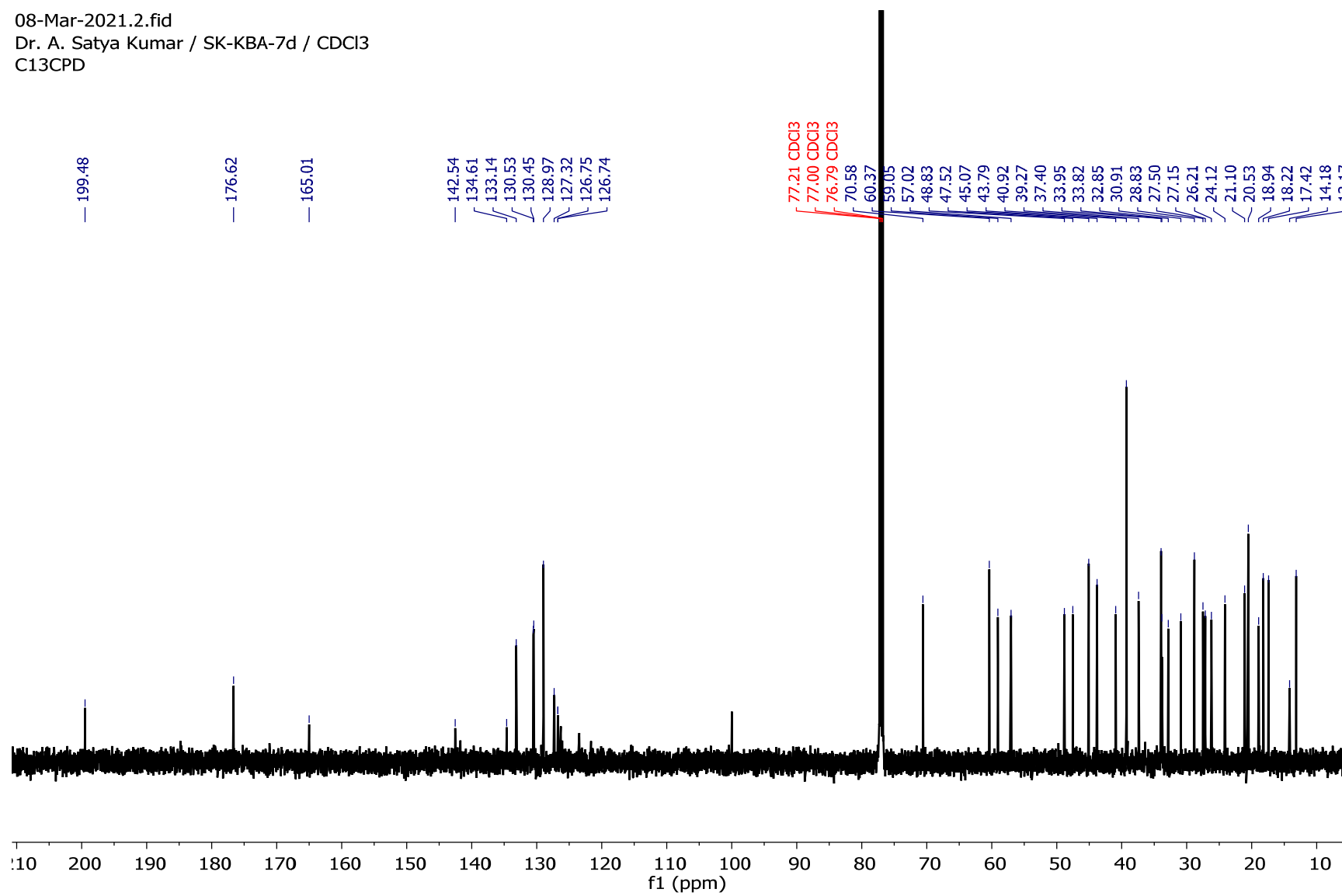


Figure S54: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound 7d

08-Mar-2021.5.fid  
Dr. A. Satya Kumar / SK-KBA-7d / CDCl<sub>3</sub>  
F19CPD

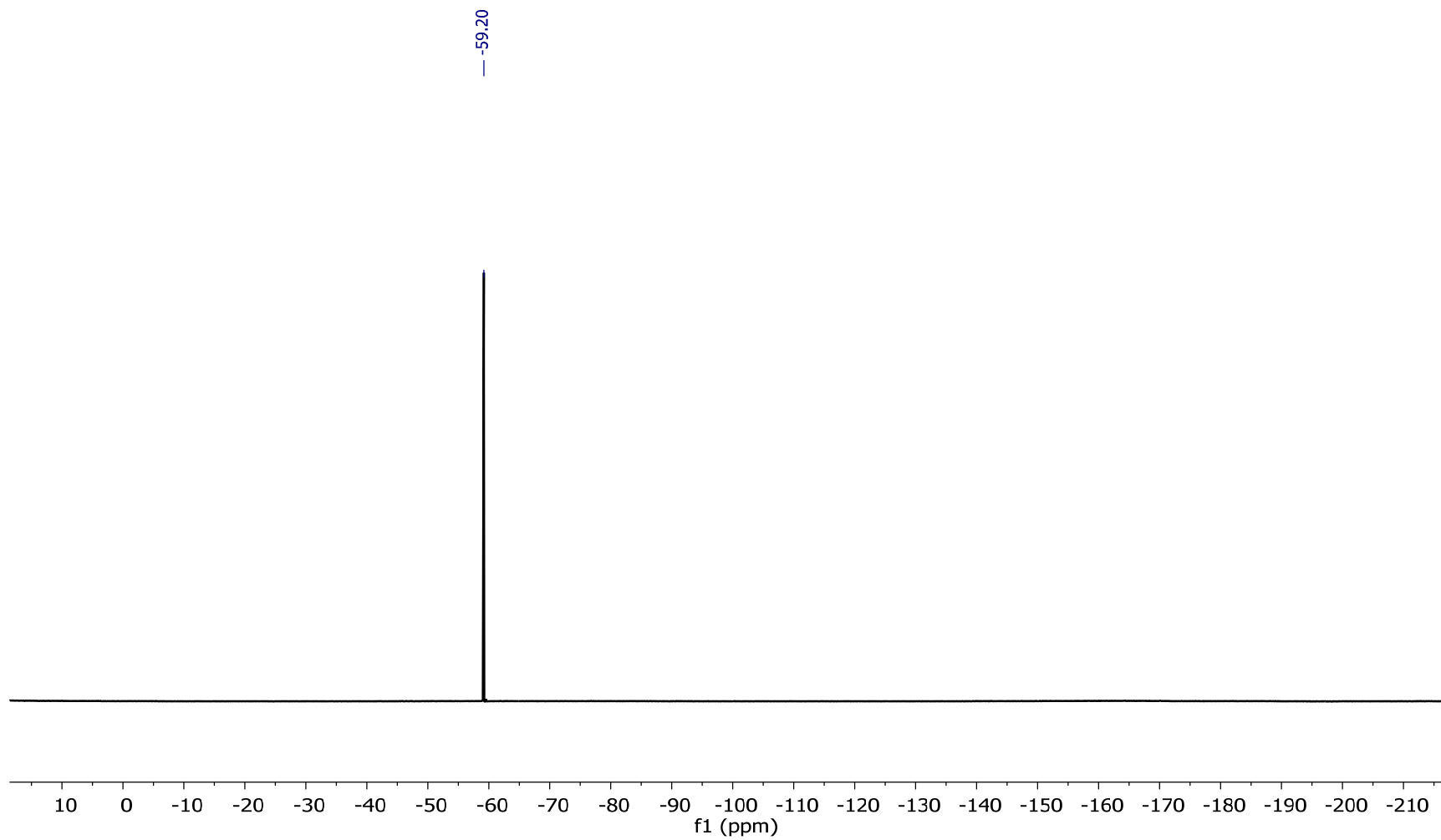


Figure S55: <sup>19</sup>F-NMR spectrum (564 MHz, CDCl<sub>3</sub>) of compound **7d**

Sample Name	SK-KBA-7D	Position	Vial 44	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SK-KBA-7D.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment	PARTHA	Acquired Time	17-Mar-21 12:30:19 PM

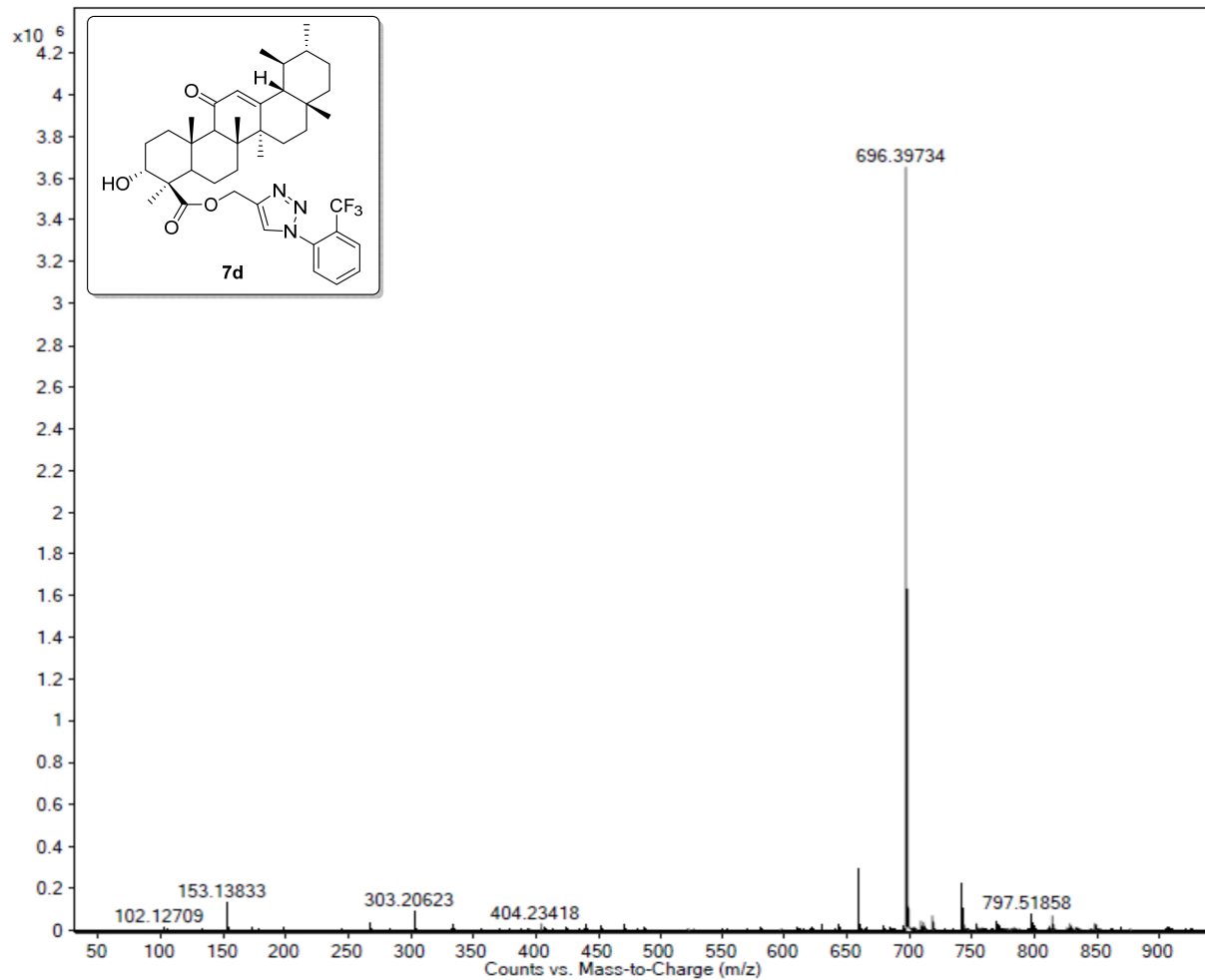


Figure S56: HRMS spectrum of compound 7d

08-Mar-2021.6.fid  
Dr. A. Satya Kumar / SK-KBA-7e / CDCl<sub>3</sub>  
PROTON

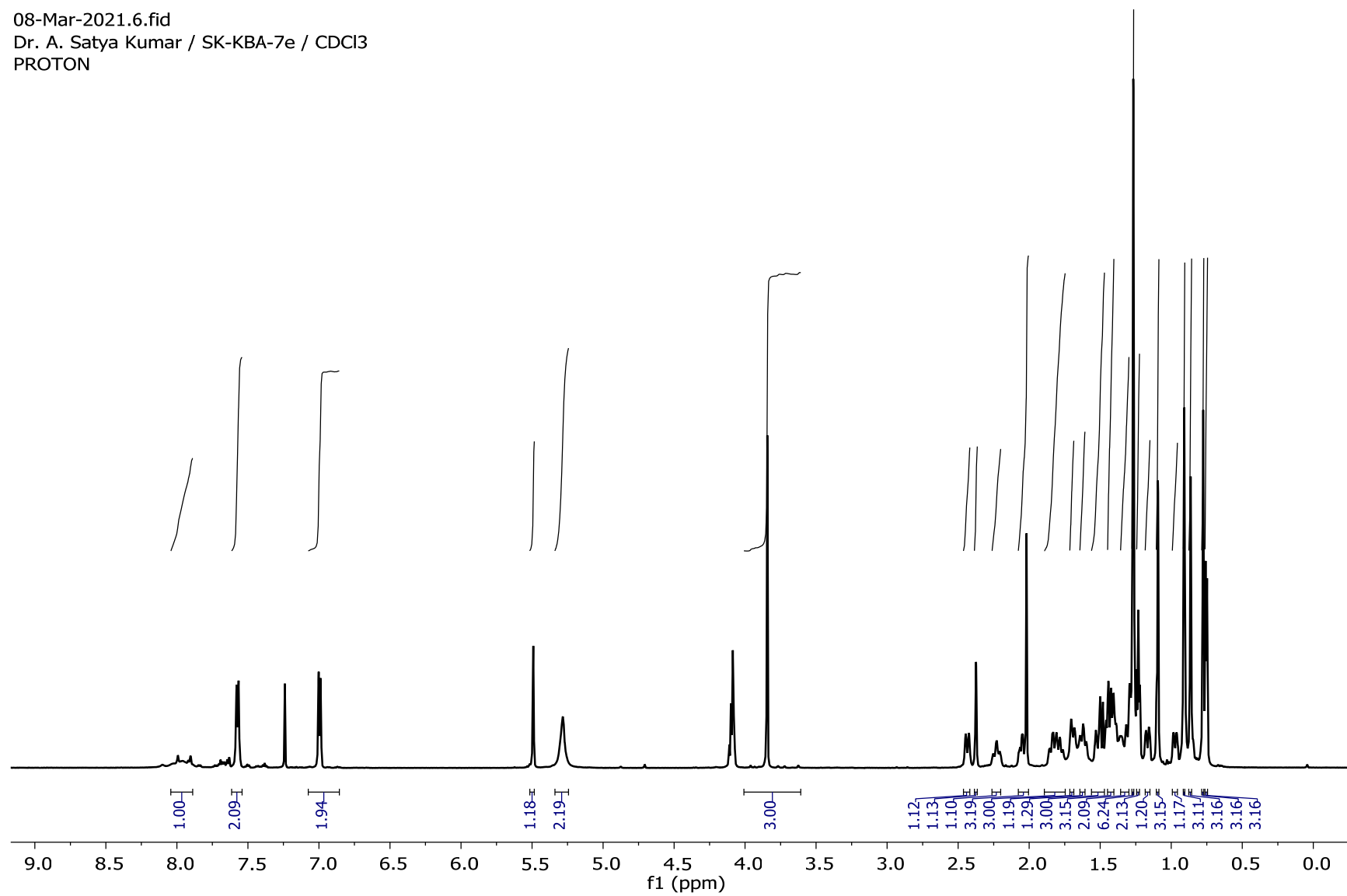


Figure S57: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 7e

08-Mar-2021.7.fid  
Dr. A. Satya Kumar / SK-KBA-7e / CDCl<sub>3</sub>  
C13CPD

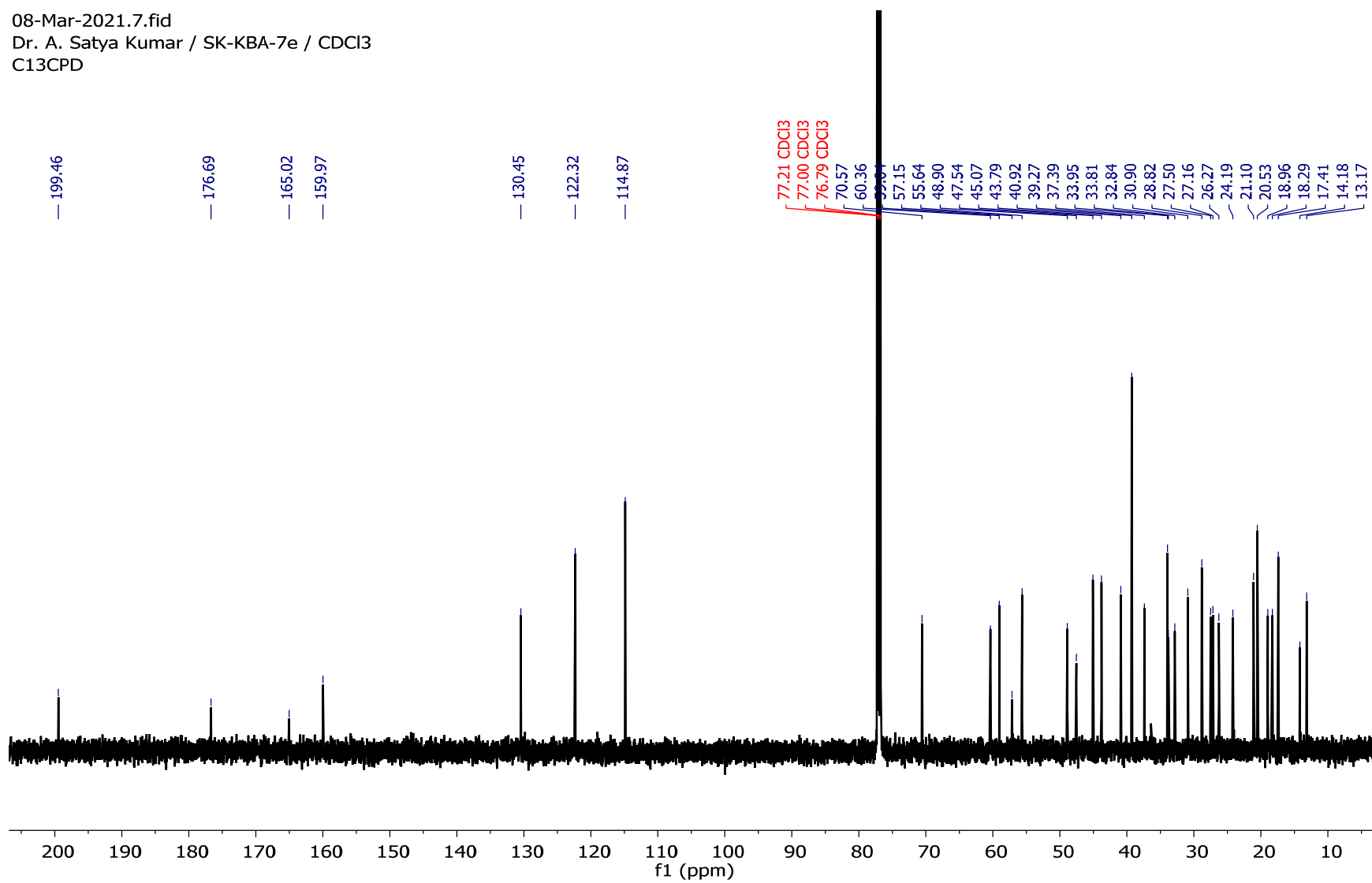


Figure S58: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound 7e

Sample Name	SK-KBA-7E	Position	Vial 45	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SK-KBA-7E.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment	PARTHA	Acquired Time	17-Mar-21 12:36:03 PM

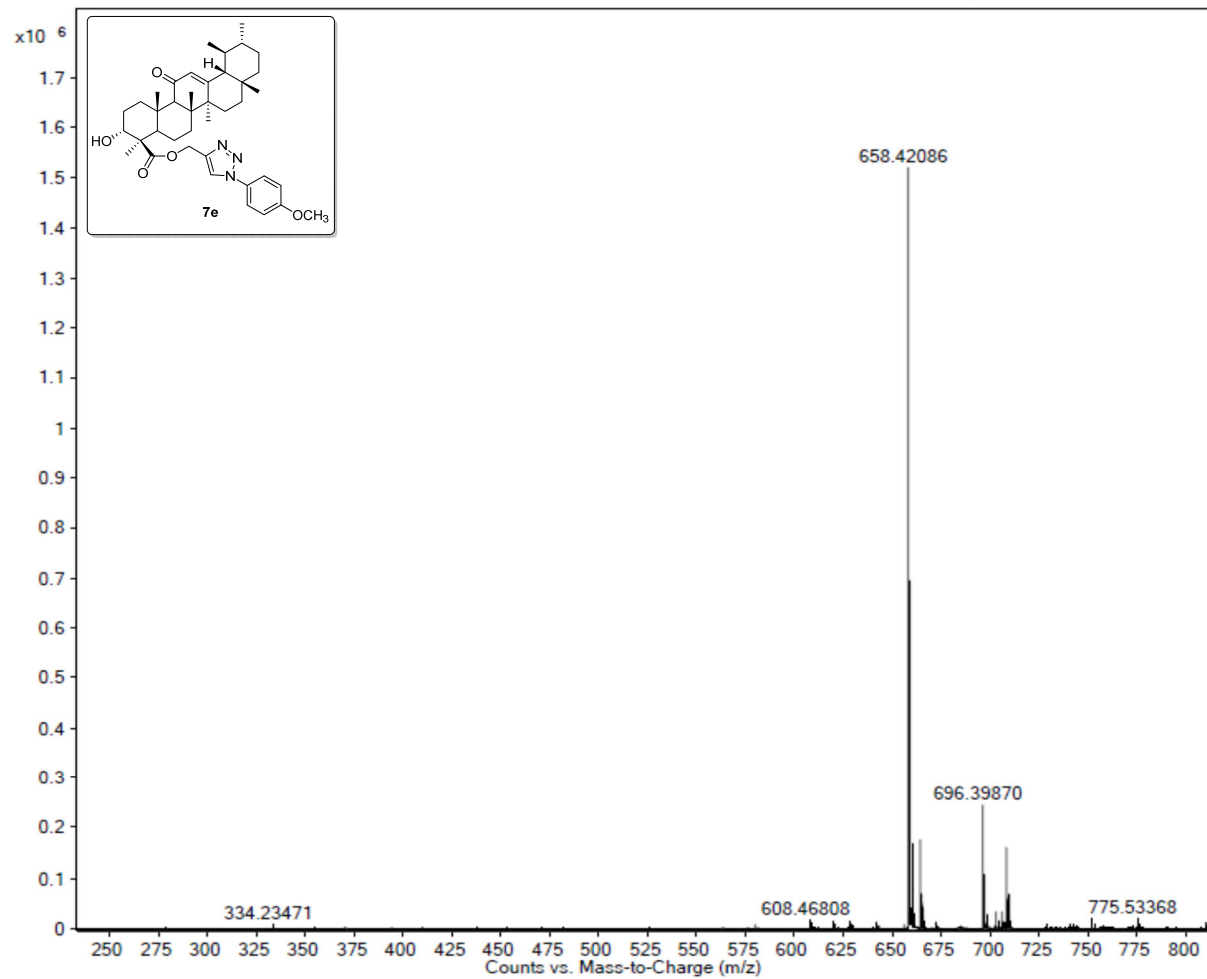


Figure S59: HRMS spectrum of compound **7e**



08-Mar-2021.10.fid  
Dr. A. Satya Kumar / SK-KBA-7f / CDCl<sub>3</sub>  
PROTON

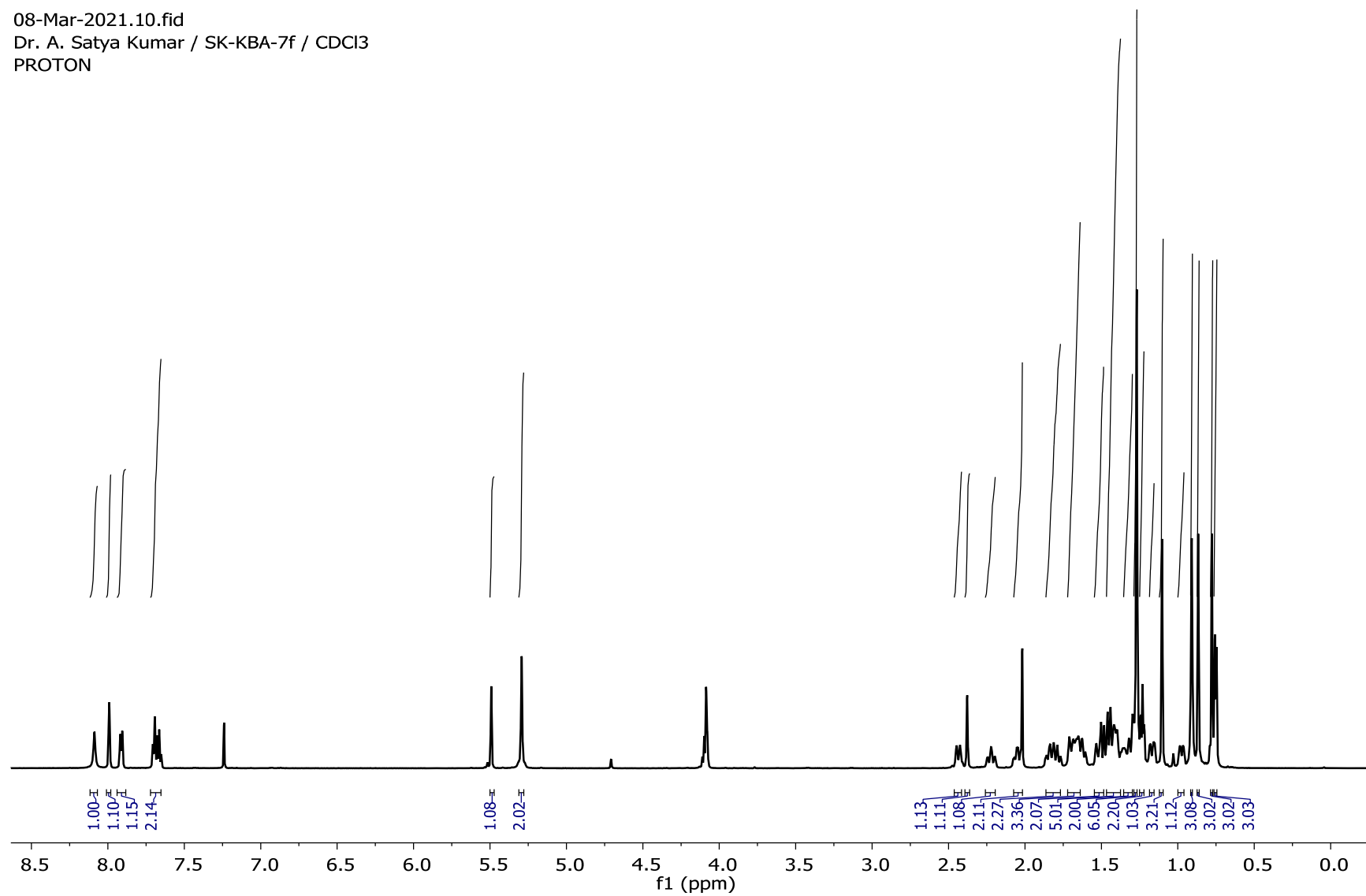


Figure S60: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 7f

08-Mar-2021.11.fid  
Dr. A. Satya Kumar / SK-KBA-7f / CDCl<sub>3</sub>  
C13CPD

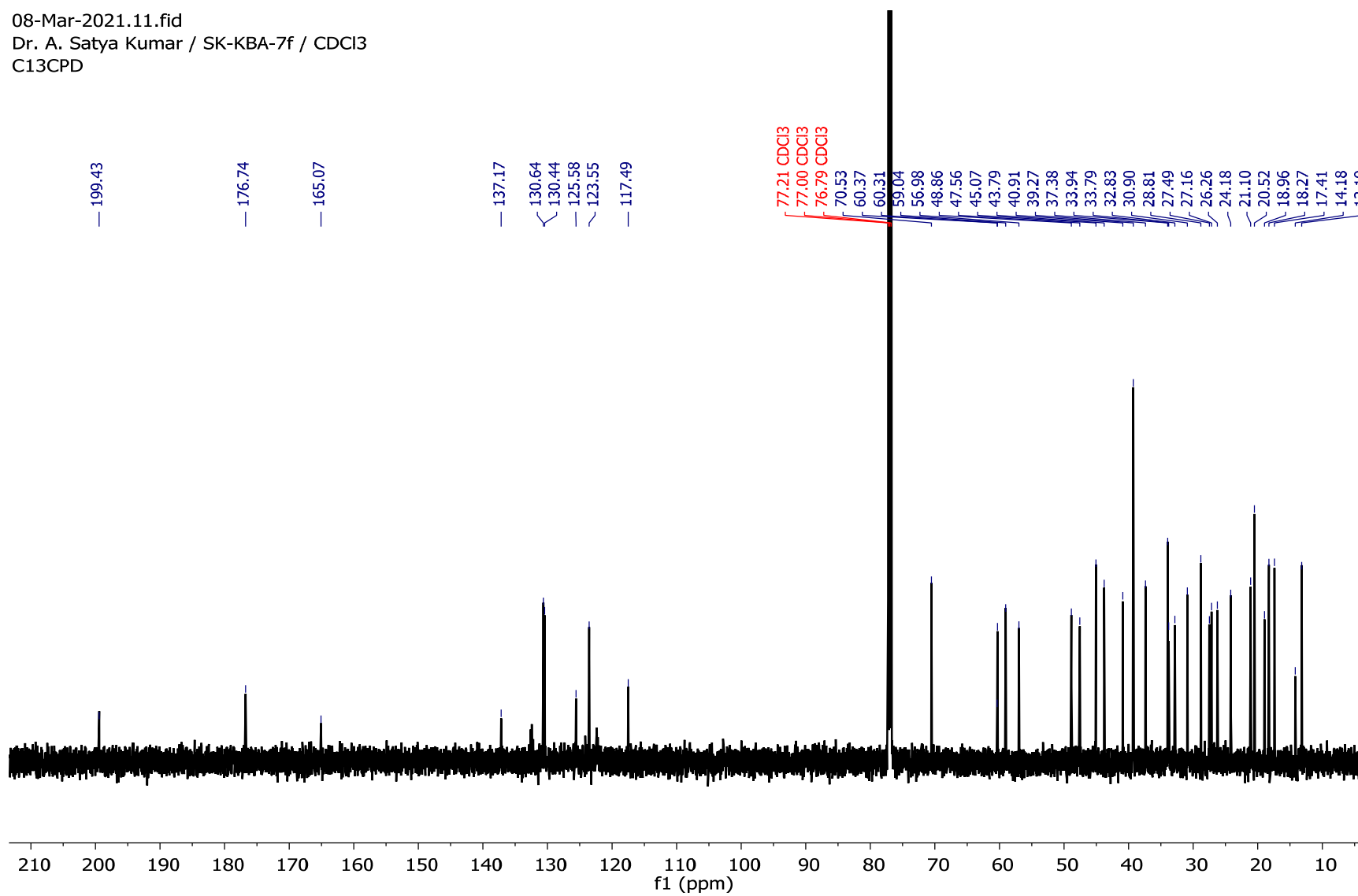
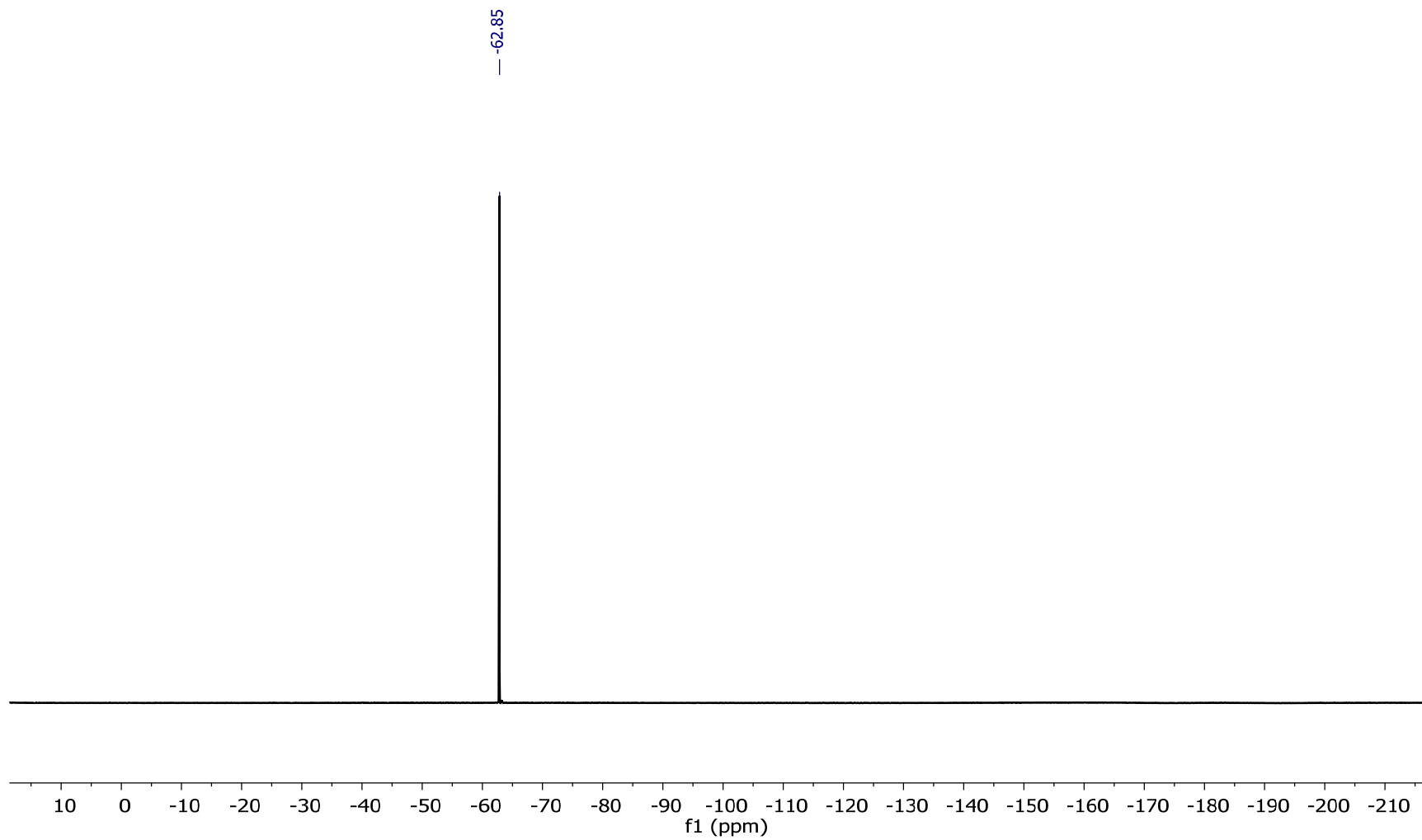


Figure S61: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound 7f

08-Mar-2021.14.fid  
Dr. A. Satya Kumar / SK-KBA-7f / CDCl<sub>3</sub>  
F19CPD



**Figure S62:** <sup>19</sup>F-NMR spectrum (564 MHz, CDCl<sub>3</sub>) of compound **7f**

Sample Name	SK-KBA-7F	Position	Vial 46	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SK-KBA-7F.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment	PARTHA	Acquired Time	17-Mar-21 12:41:31 PM

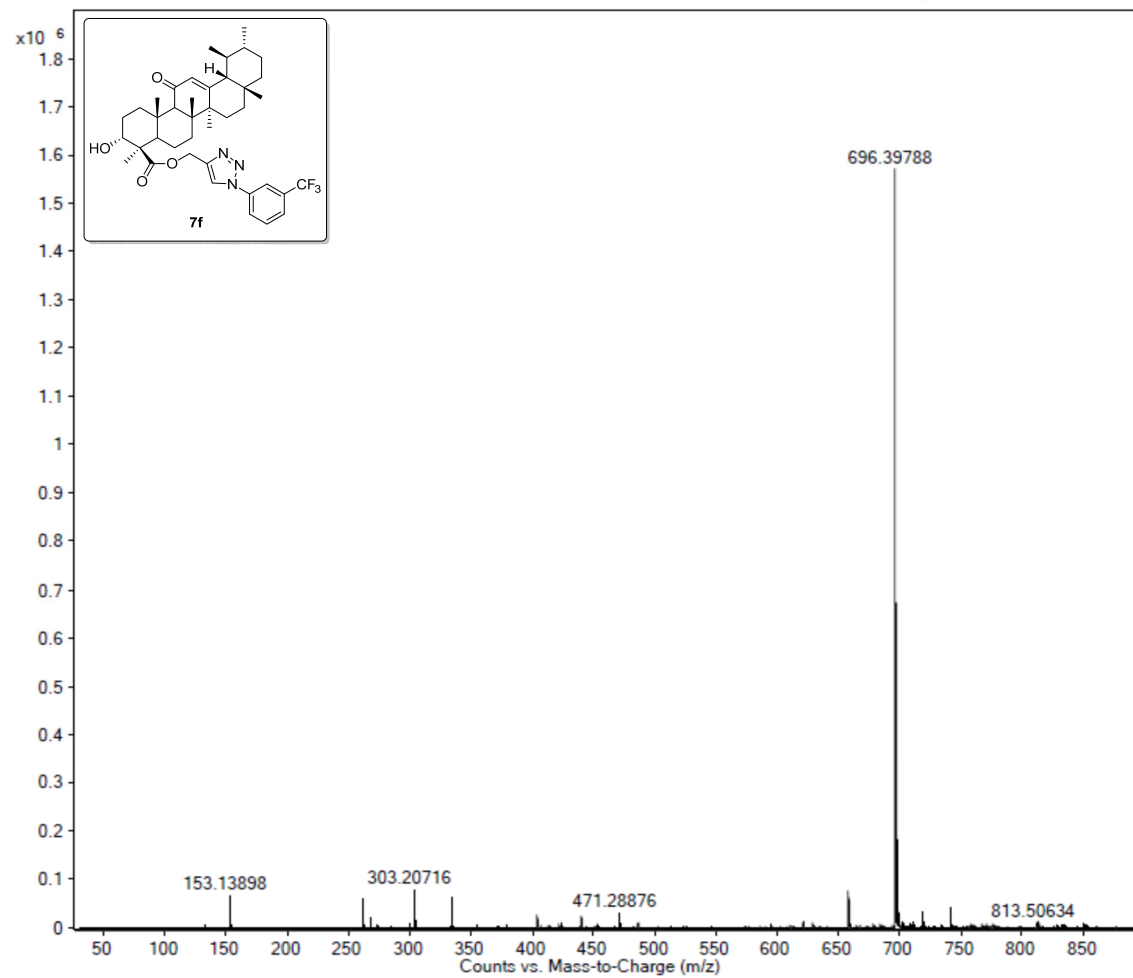


Figure S63: HRMS spectrum of compound **7f**

08-Mar-2021.15.fid  
Dr. A. Satya Kumar / SK-KBA-7g / CDCl<sub>3</sub>  
PROTON

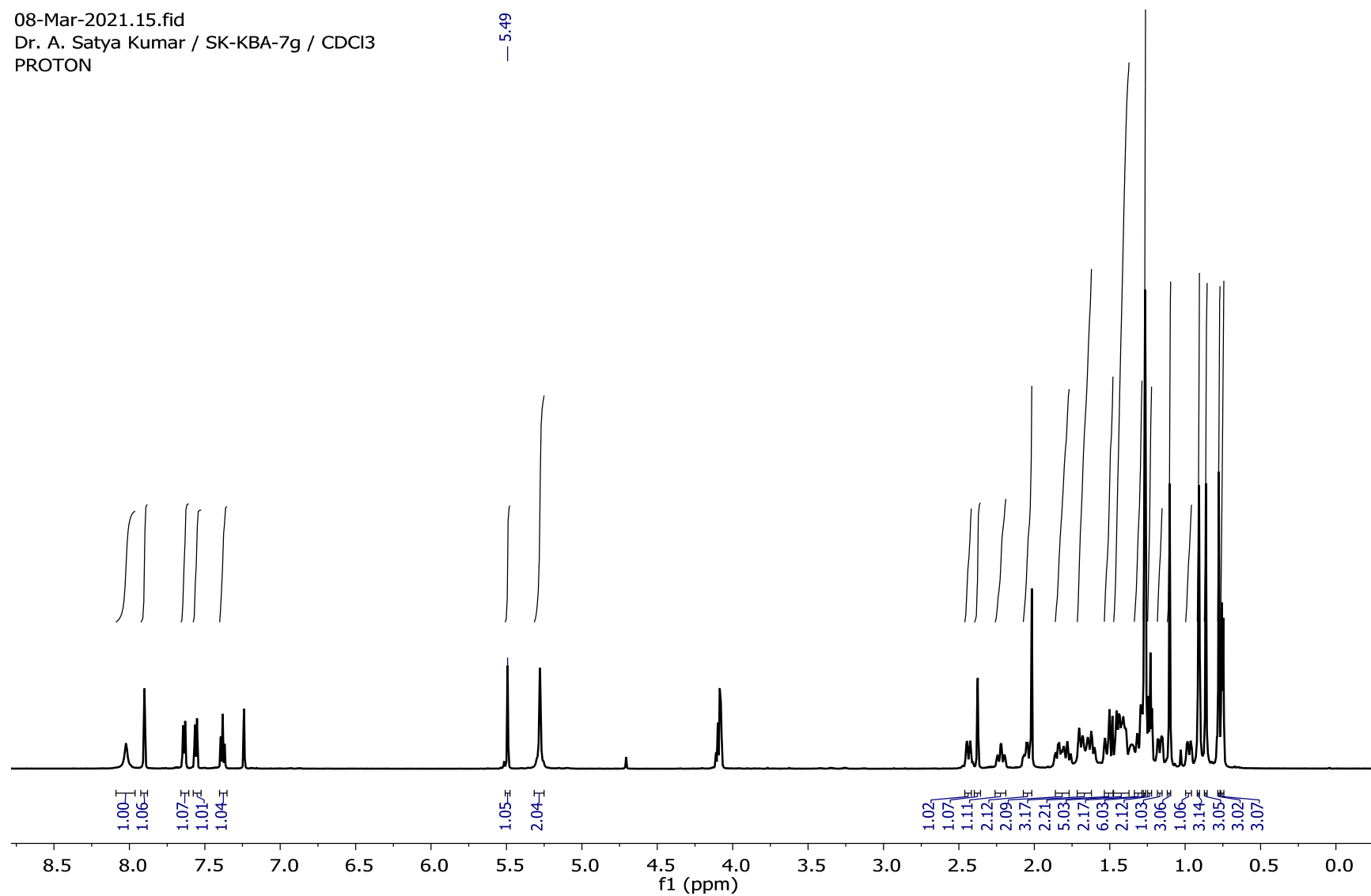


Figure S64: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 7g

08-Mar-2021.16.fid  
Dr. A. Satya Kumar / SK-KBA-7g / CDCl<sub>3</sub>  
C13CPD

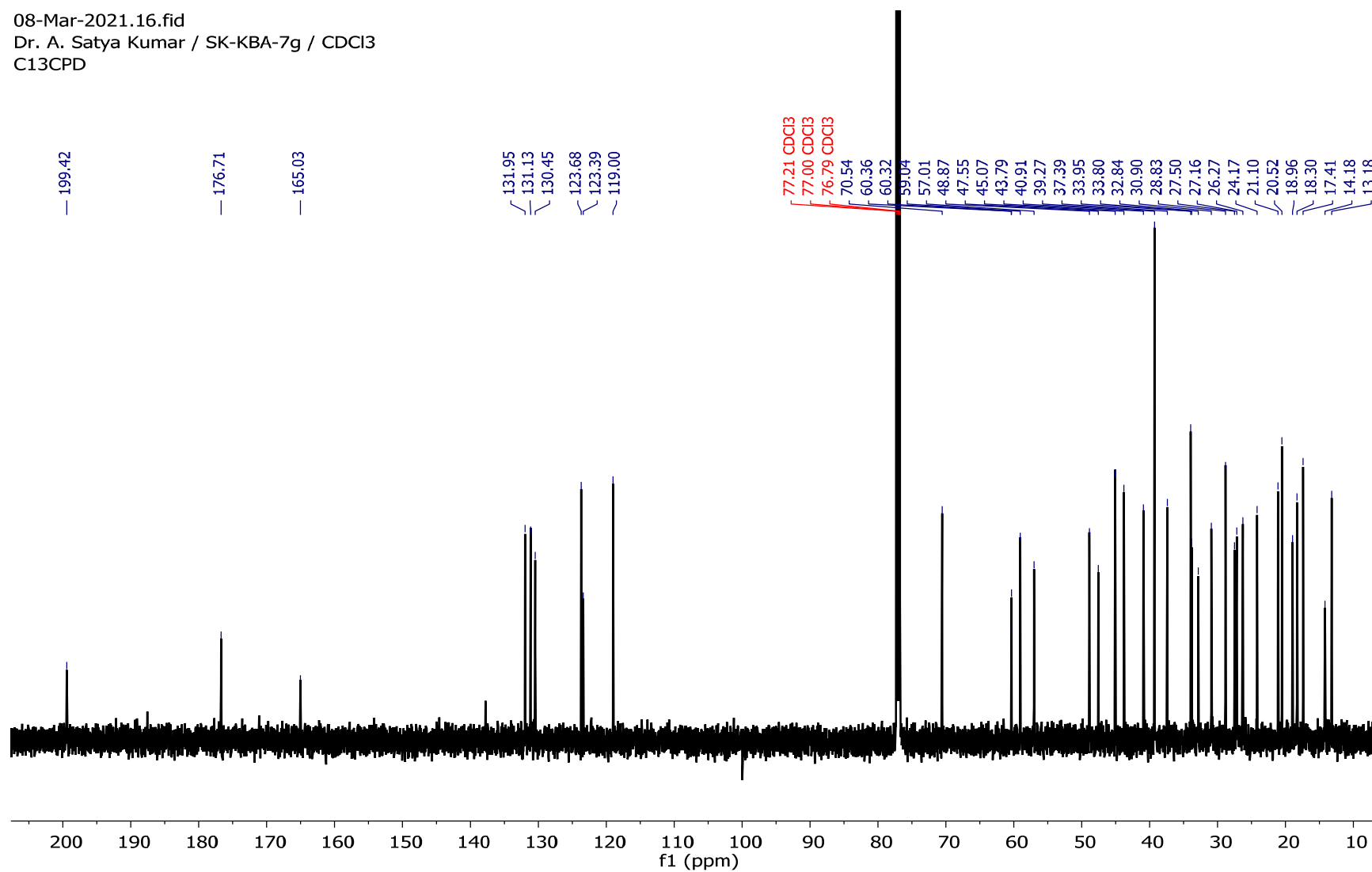


Figure S65: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound 7g

Sample Name  
User Name  
Sample Type  
ACQ Method

SK-KBA-7G  
Sample  
POSITIVE ION METHOD MS.m

Position  
Inj Vol  
IRM Calibration Status  
Comment

Vial 47  
2  
Success  
PARTHA

Instrument Name  
InjPosition  
Data Filename  
Acquired Time

Instrument 1  
  
SK-KBA-7G.d  
17-Mar-21 12:47:05 PM

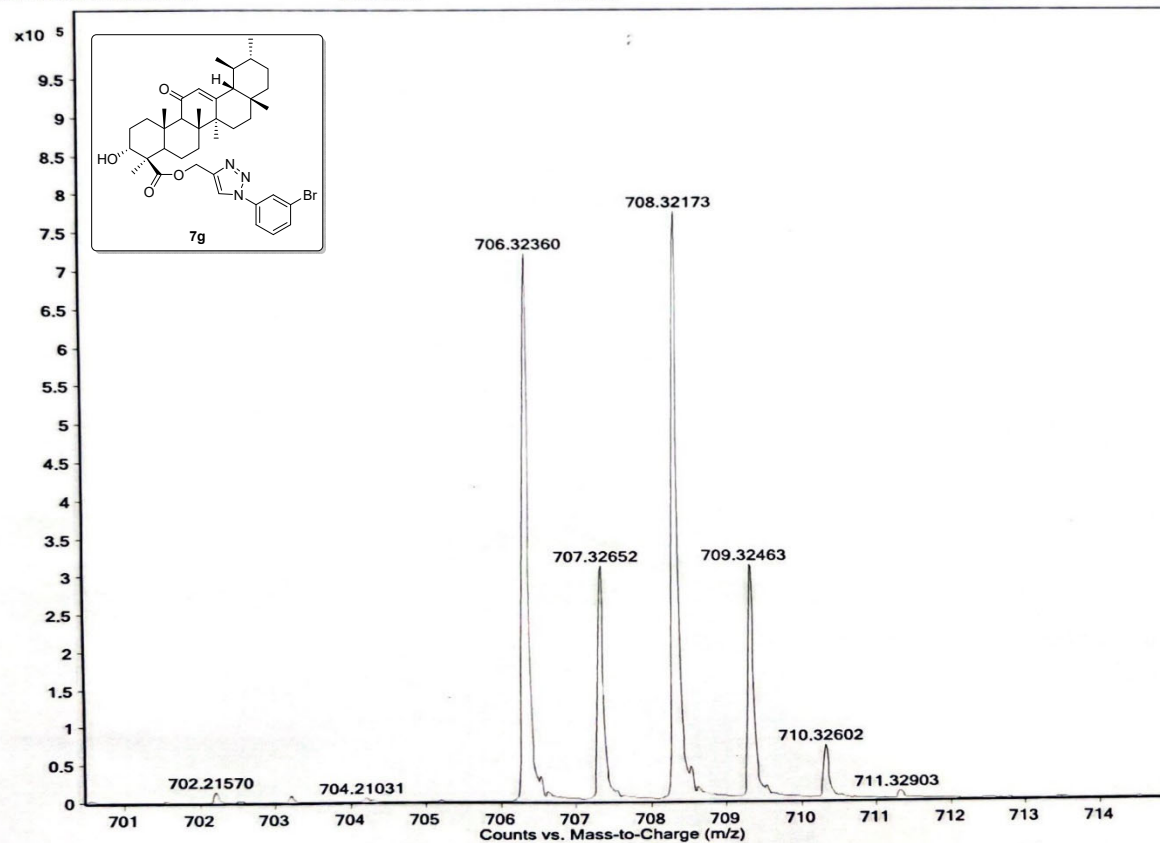


Figure S66: HRMS spectrum of compound 7g

08-Mar-2021.19.fid  
Dr. A. Satya Kumar / SK-KBA-7h / CDCl<sub>3</sub>  
PROTON

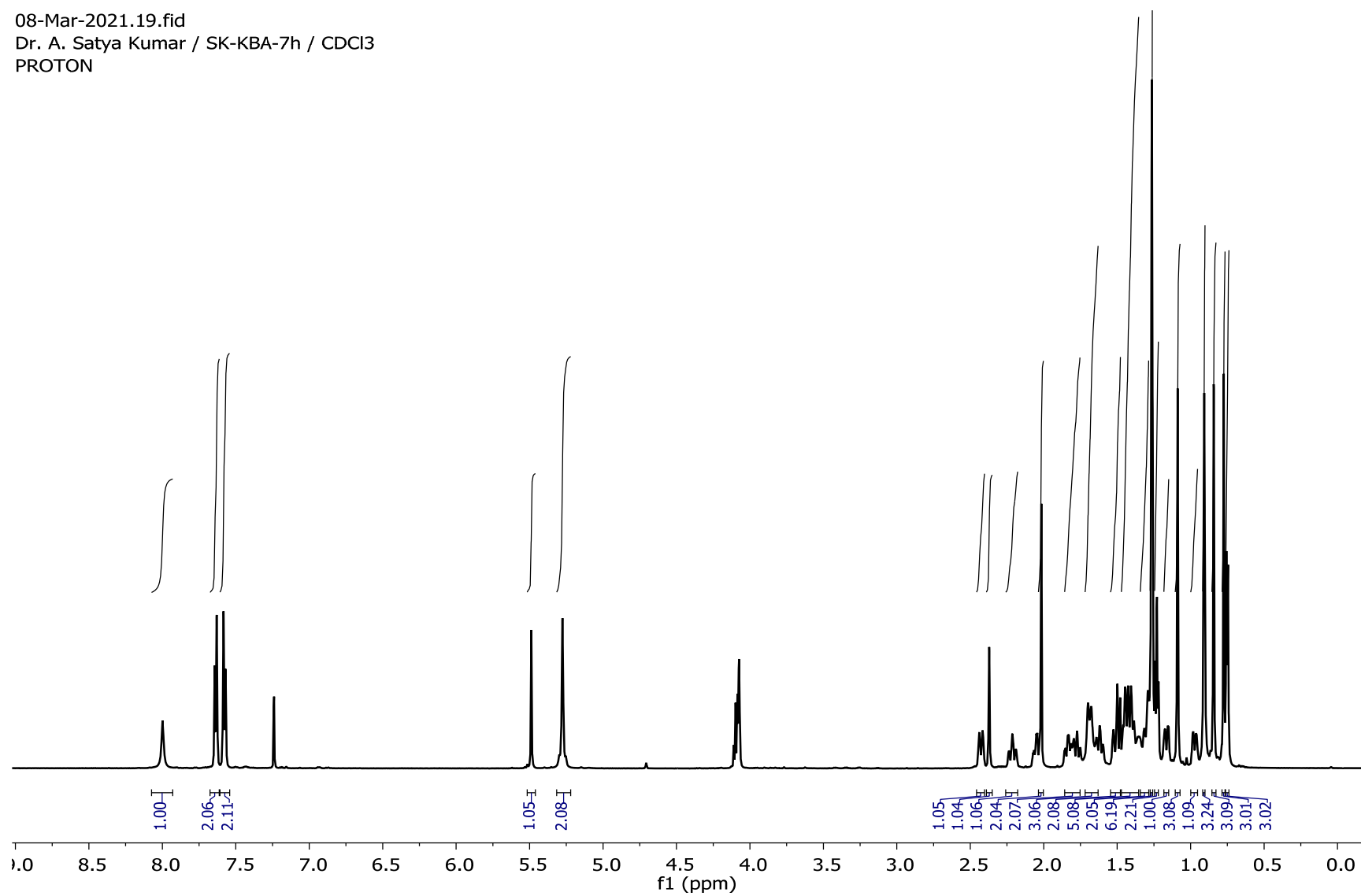


Figure S67: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 7h



08-Mar-2021.20.fid  
Dr. A. Satya Kumar / SK-KBA-7h / CDCl<sub>3</sub>  
C13CPD

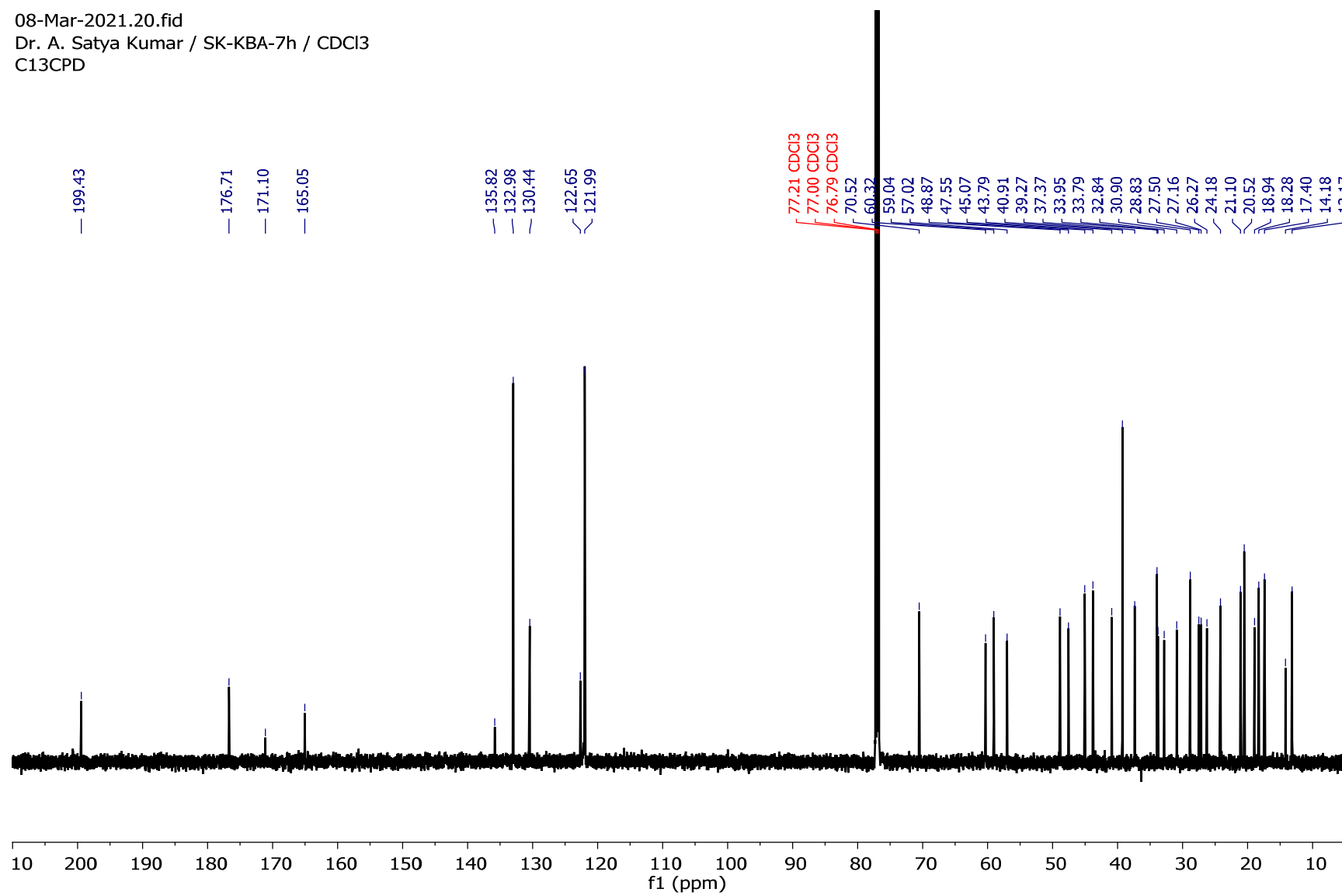


Figure S68: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound **7h**

Sample Name  
User Name  
Sample Type  
ACQ Method

SK-KBA-7H  
Sample  
POSITIVE ION METHOD MS.m

Position  
Inj Vol  
IRM Calibration Status  
Comment

Vial 48  
2  
Success  
PARTHA

Instrument Name  
InjPosition  
Data Filename  
Acquired Time

Instrument 1  
  
SK-KBA-7H.d  
17-Mar-21 12:52:46 PM

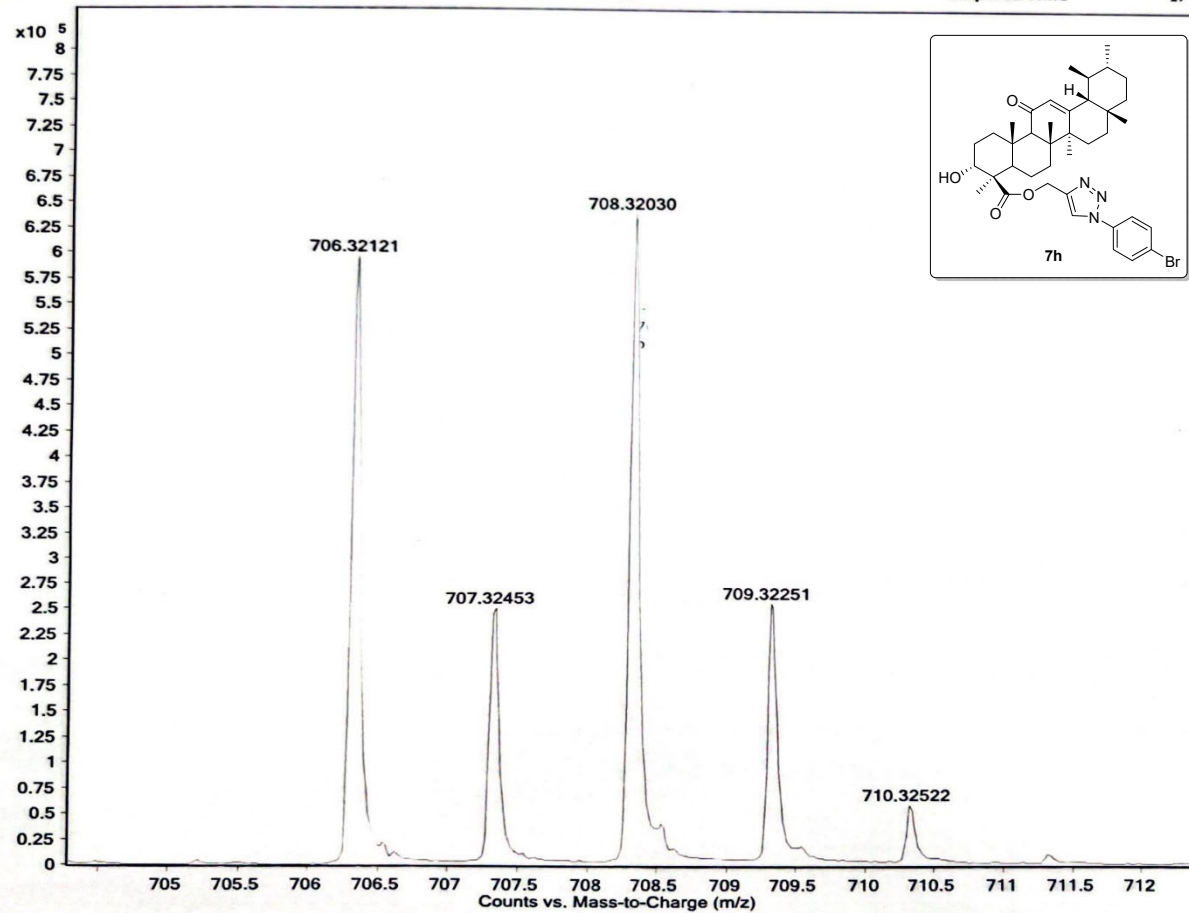


Figure S69: HRMS spectrum of compound 7h

21-Mar-2021.19.fid  
Dr. Kumar/SK-KBA-7I/ CDCl<sub>3</sub>  
PROTON

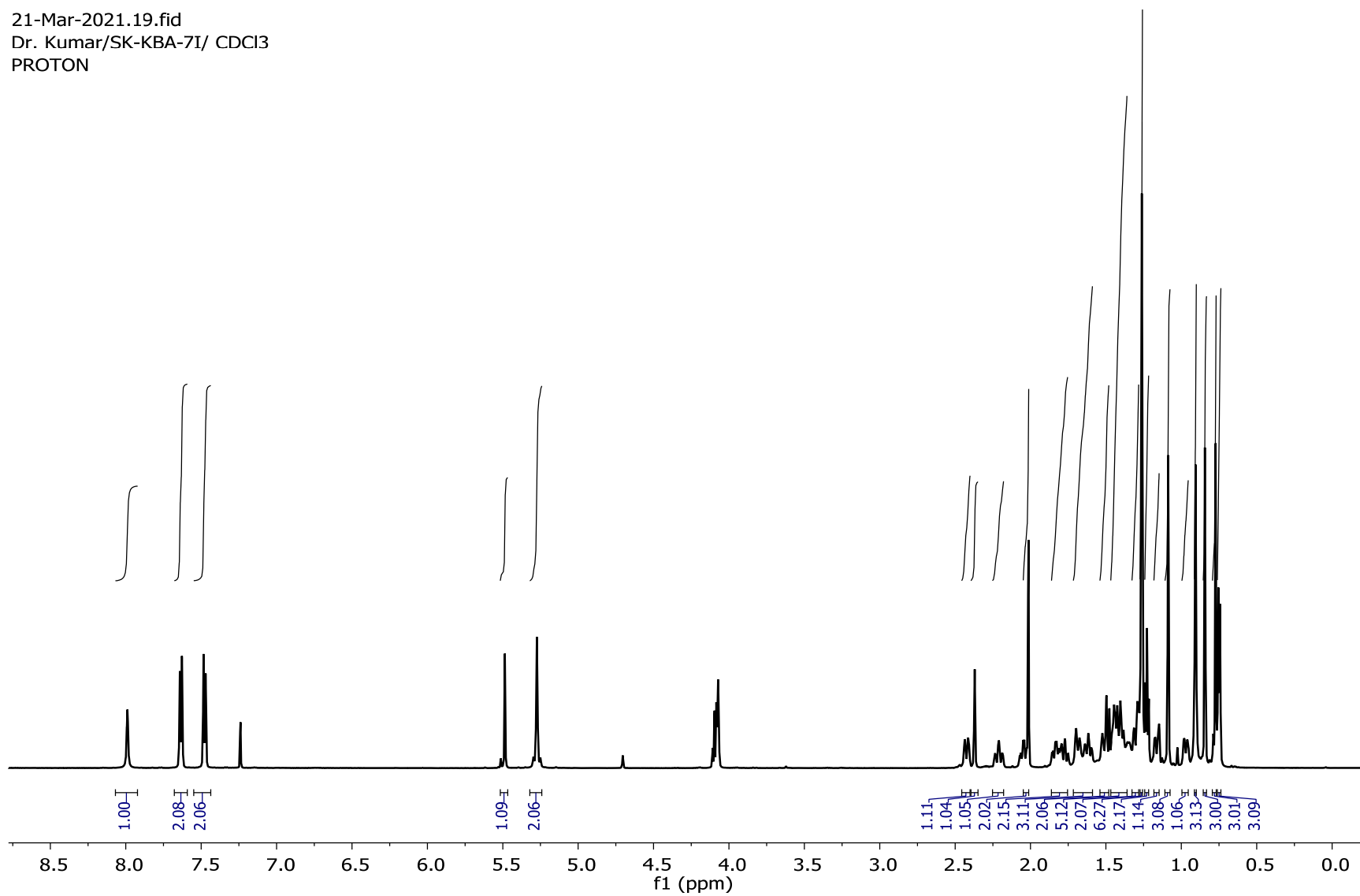


Figure S70: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 7i

21-Mar-2021.20.fid  
Dr. Kumar/SK-KBA-7I/ CDCl<sub>3</sub>  
C13CPD

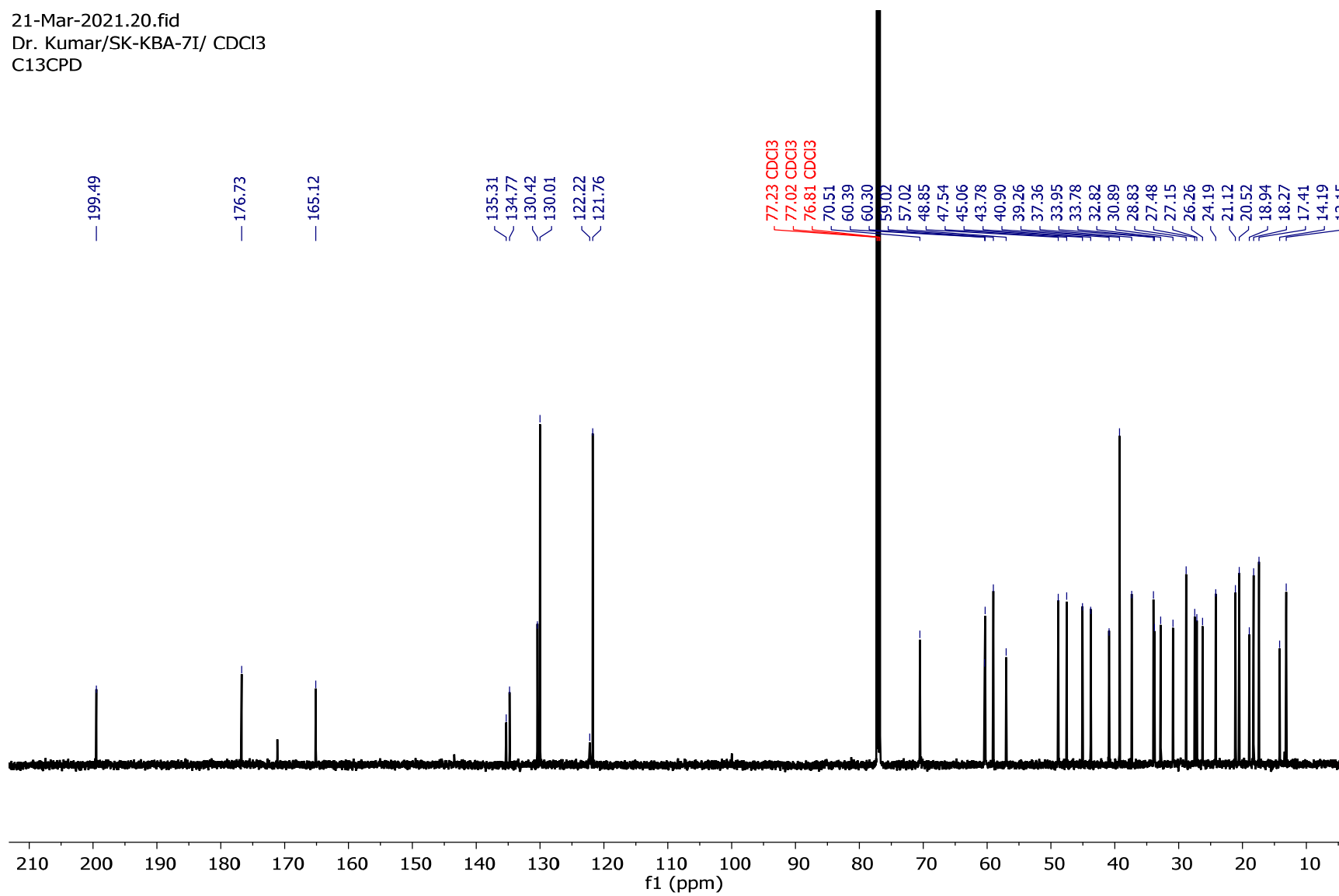


Figure S71: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound **7i**

Sample Name	SK-KBA-7I	Position	Vial 34	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SK-KBA-7I.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment		Acquired Time	22-Mar-21 2:56:25 PM

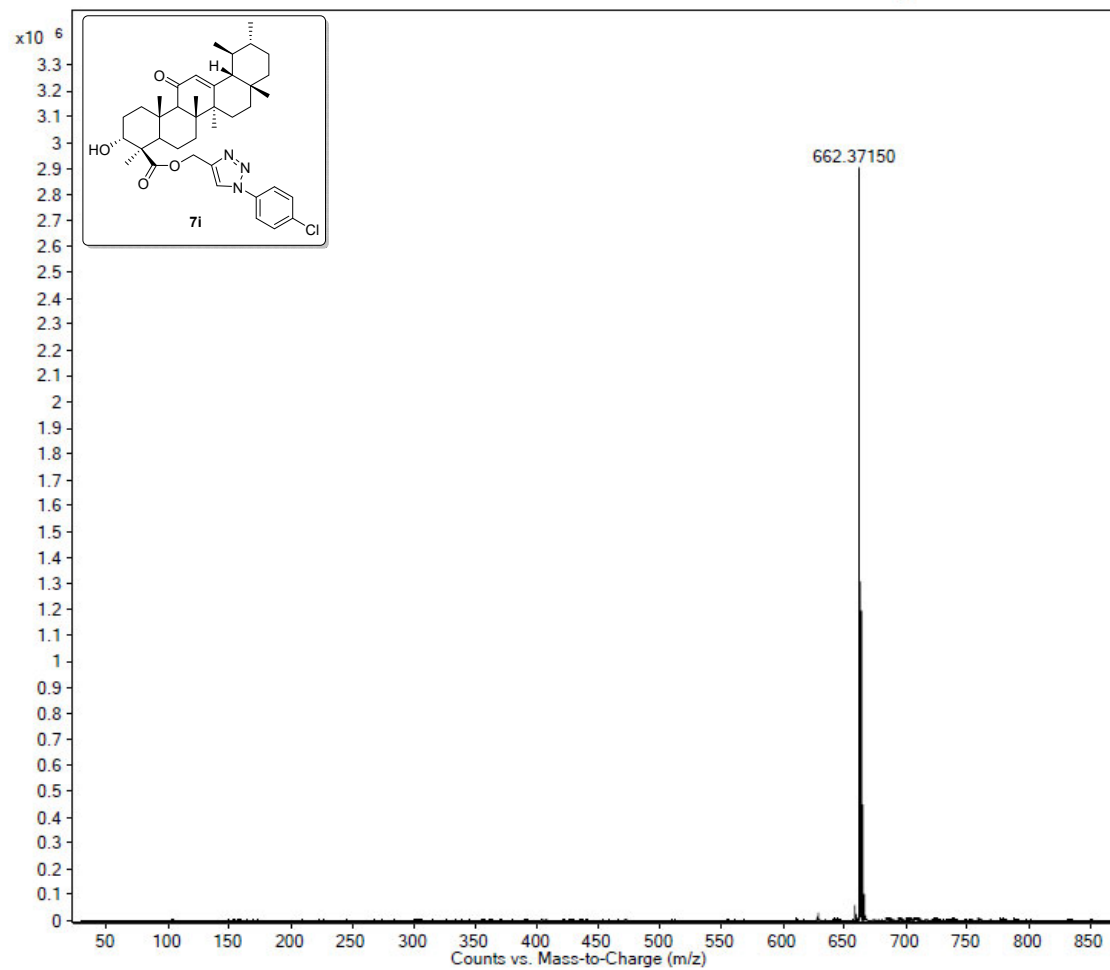


Figure S72: HRMS spectrum of compound **7i**

21-Mar-2021.24.fid  
Dr. Kumar/SK-KBA-7J/ CDCl<sub>3</sub>  
PROTON

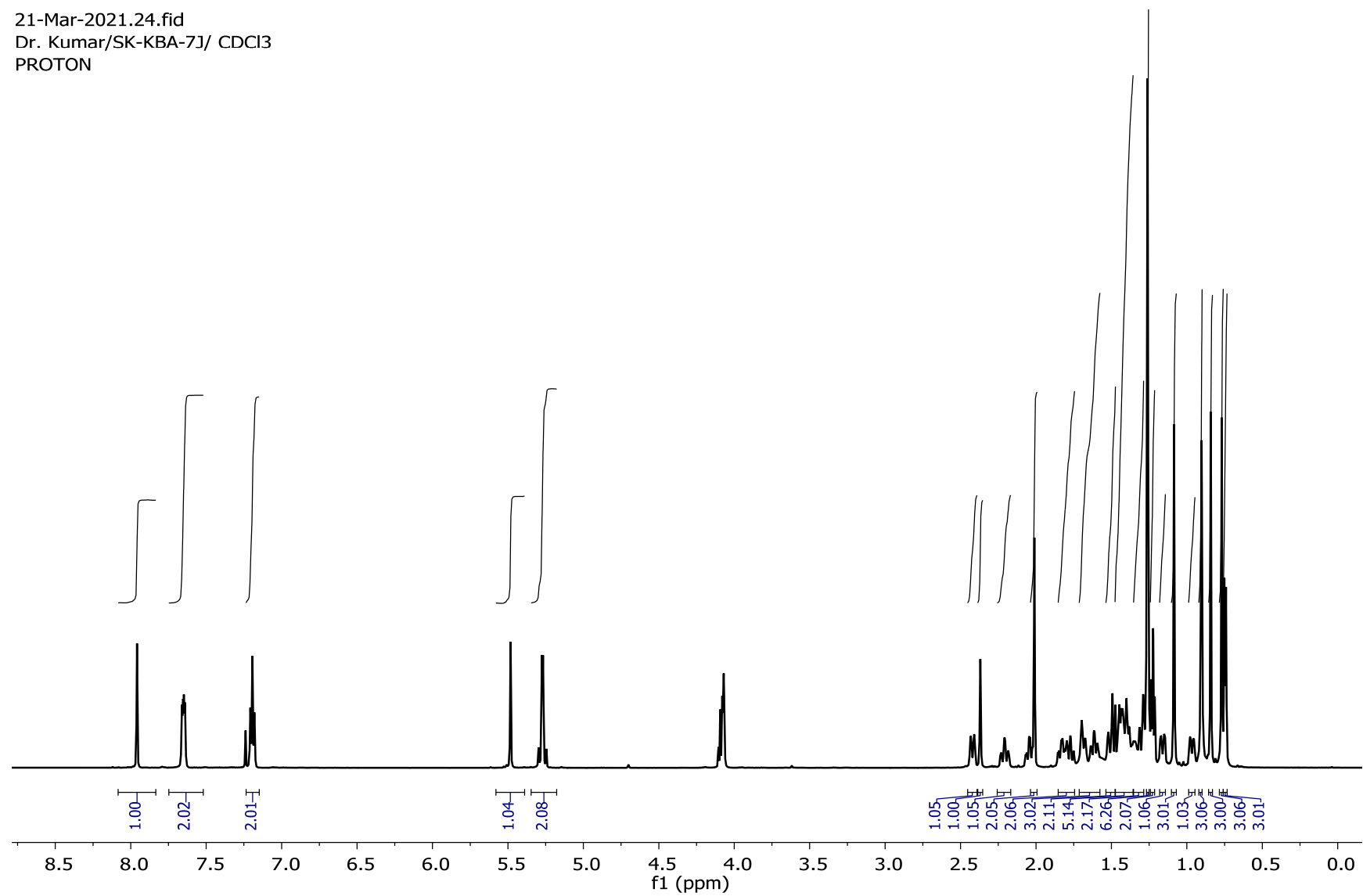


Figure S73: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 7j

21-Mar-2021.25.fid  
Dr. Kumar/SK-KBA-7J/ CDCl<sub>3</sub>  
C13CPD

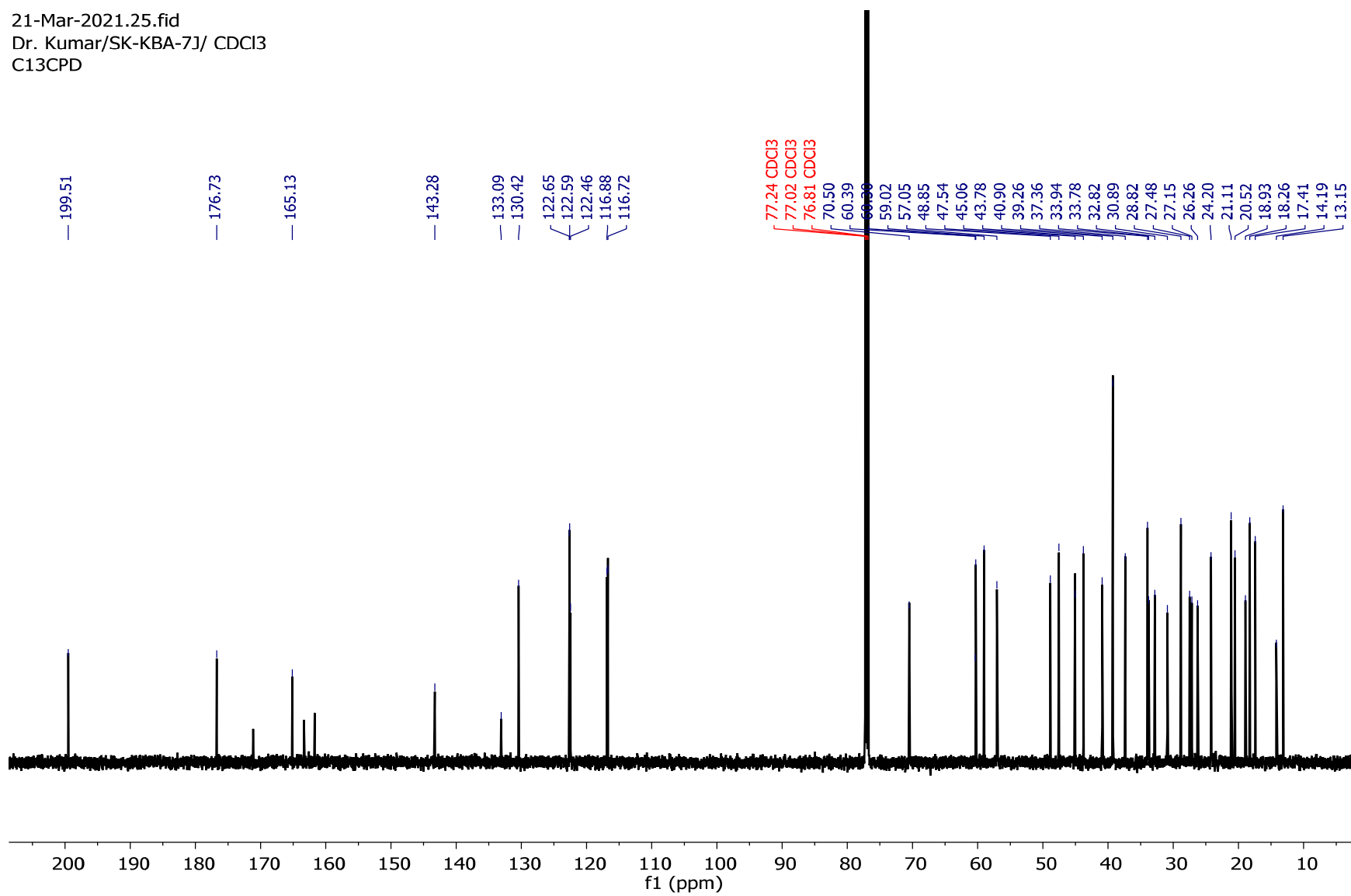
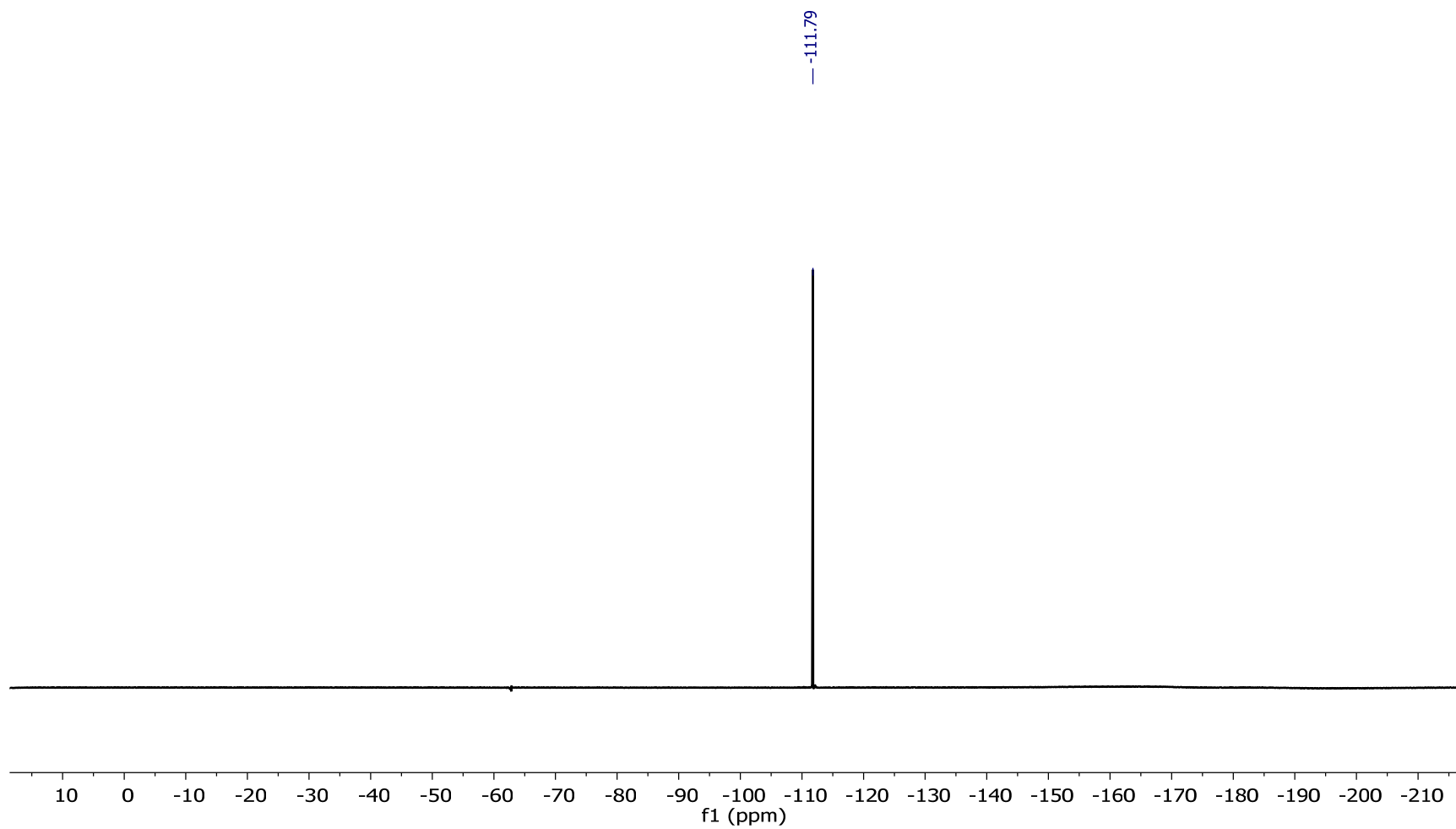


Figure S74: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound 7j

21-Mar-2021.28.fid  
Dr. Kumar/SK-KBA-7J/ CDCl<sub>3</sub>  
F19CPD



**Figure S75:** <sup>19</sup>F-NMR spectrum (564 MHz, CDCl<sub>3</sub>) of compound 7j



Sample Name	SK-KBA-7J	Position	Vial 35	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SK-KBA-7J.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment		Acquired Time	22-Mar-21 3:02:06 PM

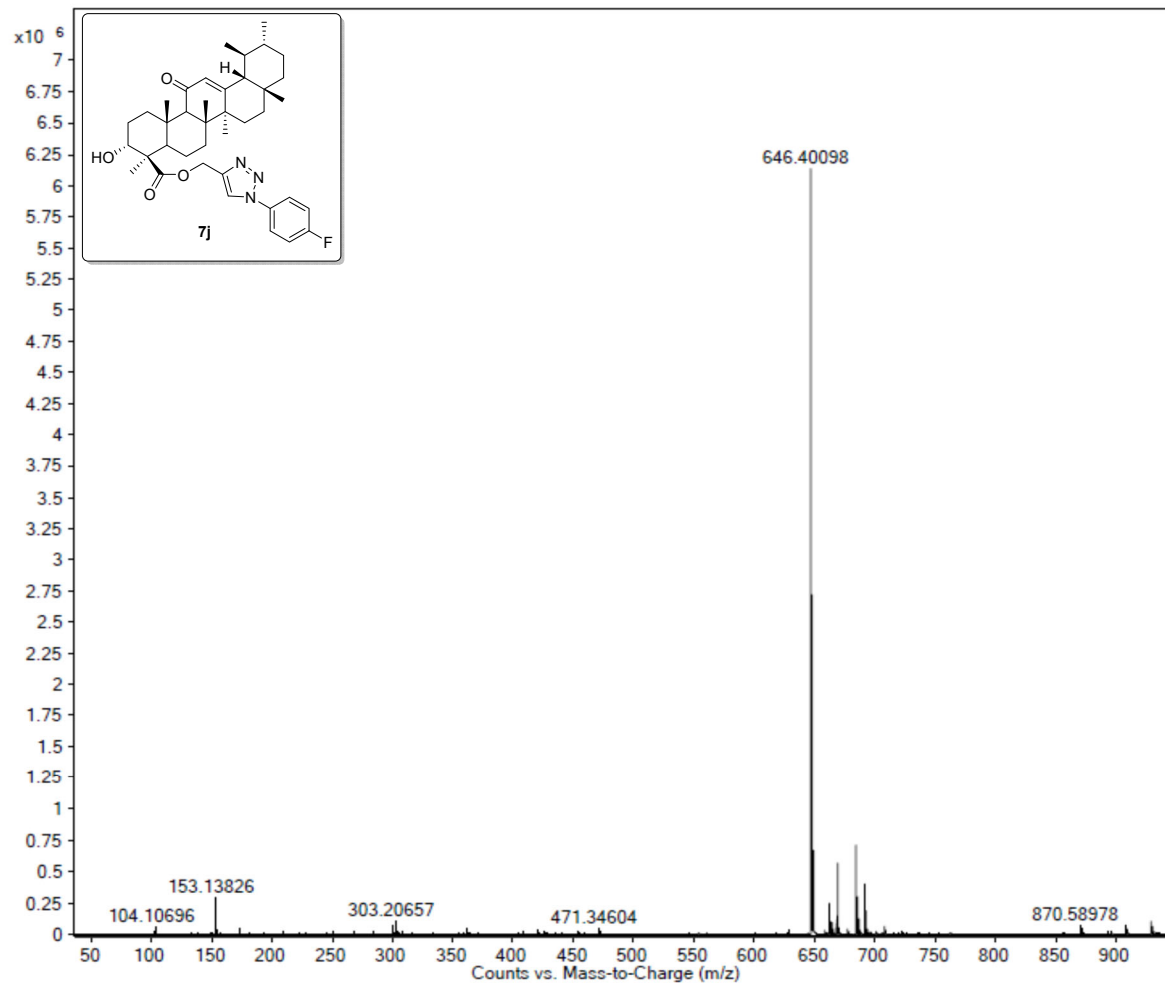


Figure S76: HRMS spectrum of compound 7j

21-Mar-2021.29.fid  
Dr. Kumar/SK-KBA-7K/ CDCl<sub>3</sub>  
PROTON

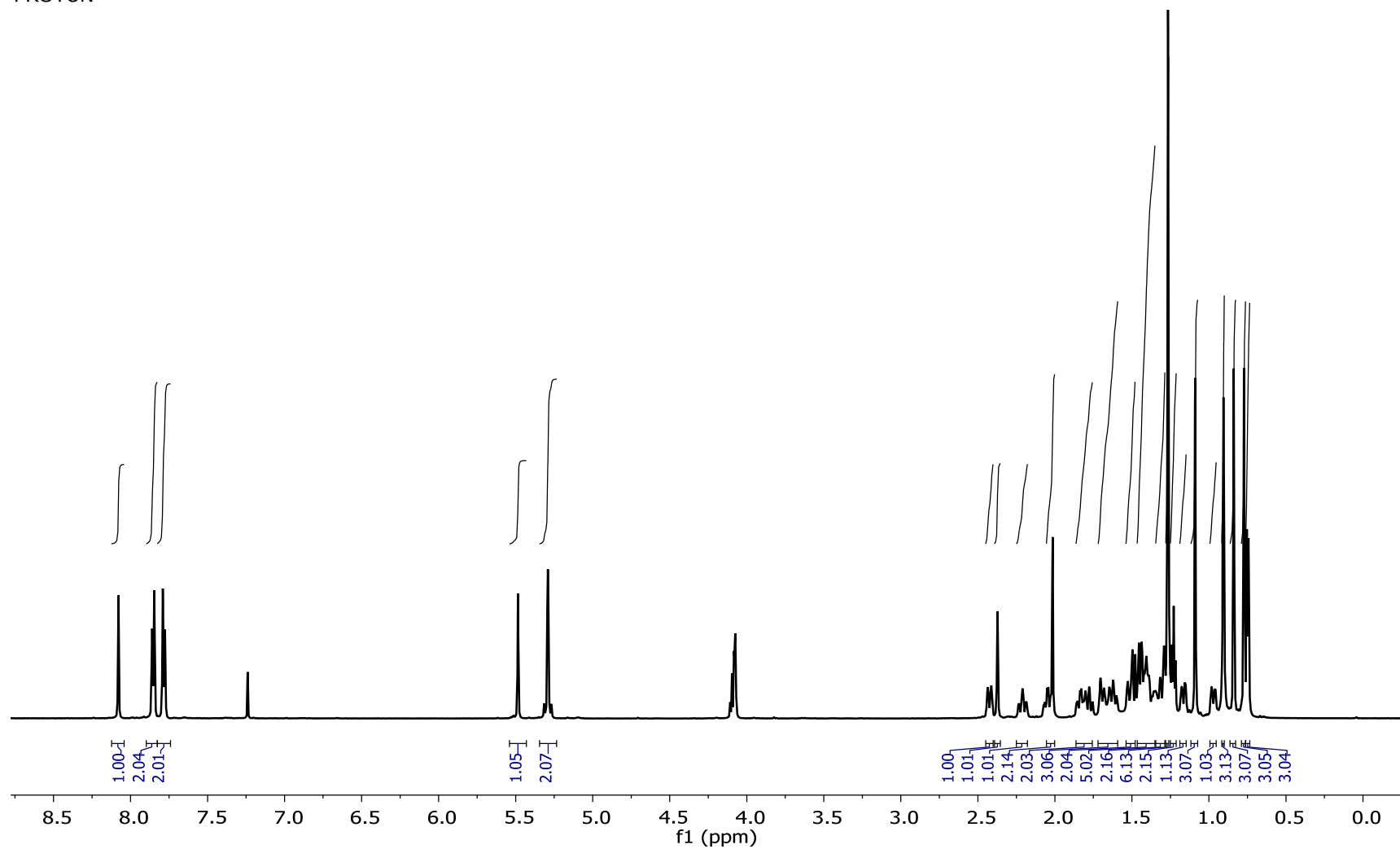


Figure S77: <sup>1</sup>H-NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 7k

21-Mar-2021.30.fid  
Dr. Kumar/SK-KBA-7K/ CDCl<sub>3</sub>  
C13CPD

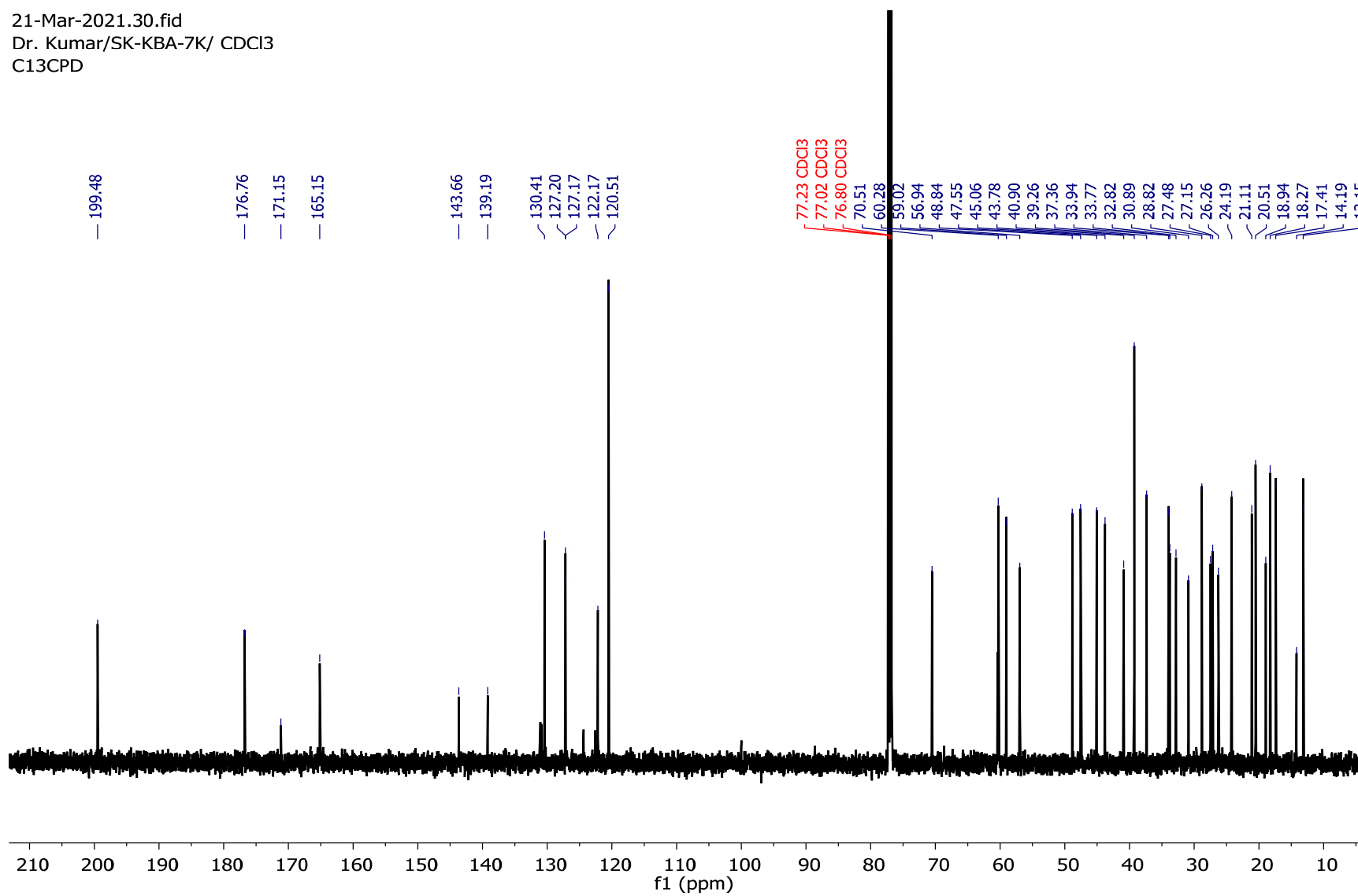


Figure S78: <sup>13</sup>C-NMR spectrum (150 MHz, CDCl<sub>3</sub>) of compound 7k

21-Mar-2021.33.fid  
Dr. Kumar/SK-KBA-7K/ CDCl<sub>3</sub>  
F19CPD

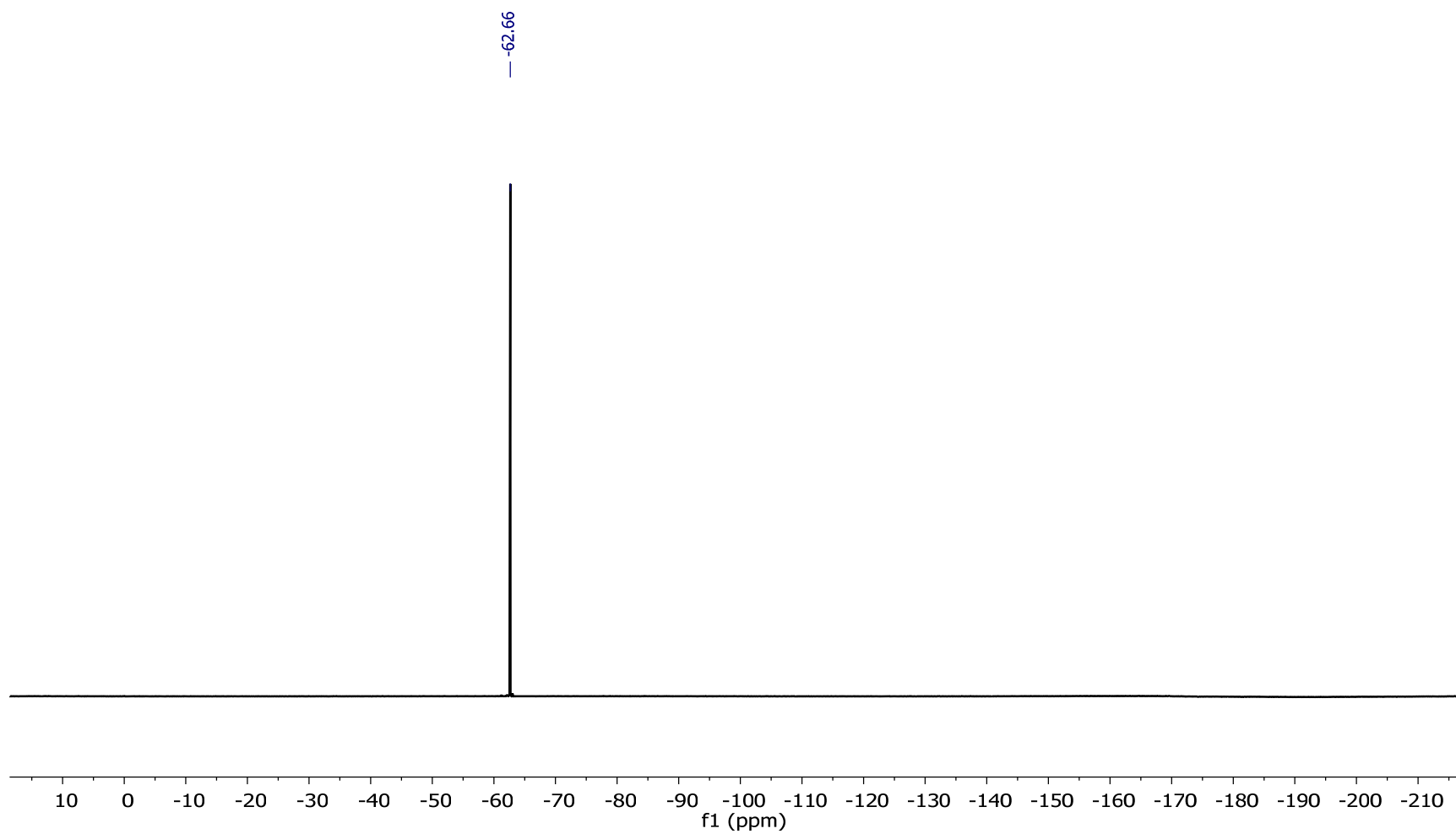


Figure S79: <sup>19</sup>F-NMR spectrum (564 MHz, CDCl<sub>3</sub>) of compound **7k**

Sample Name	SK-KBA-7K	Position	Vial 36	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SK-KBA-7K.d
ACQ Method	POSITIVE ION METHOD MS.m	Comment		Acquired Time	22-Mar-21 3:07:40 PM

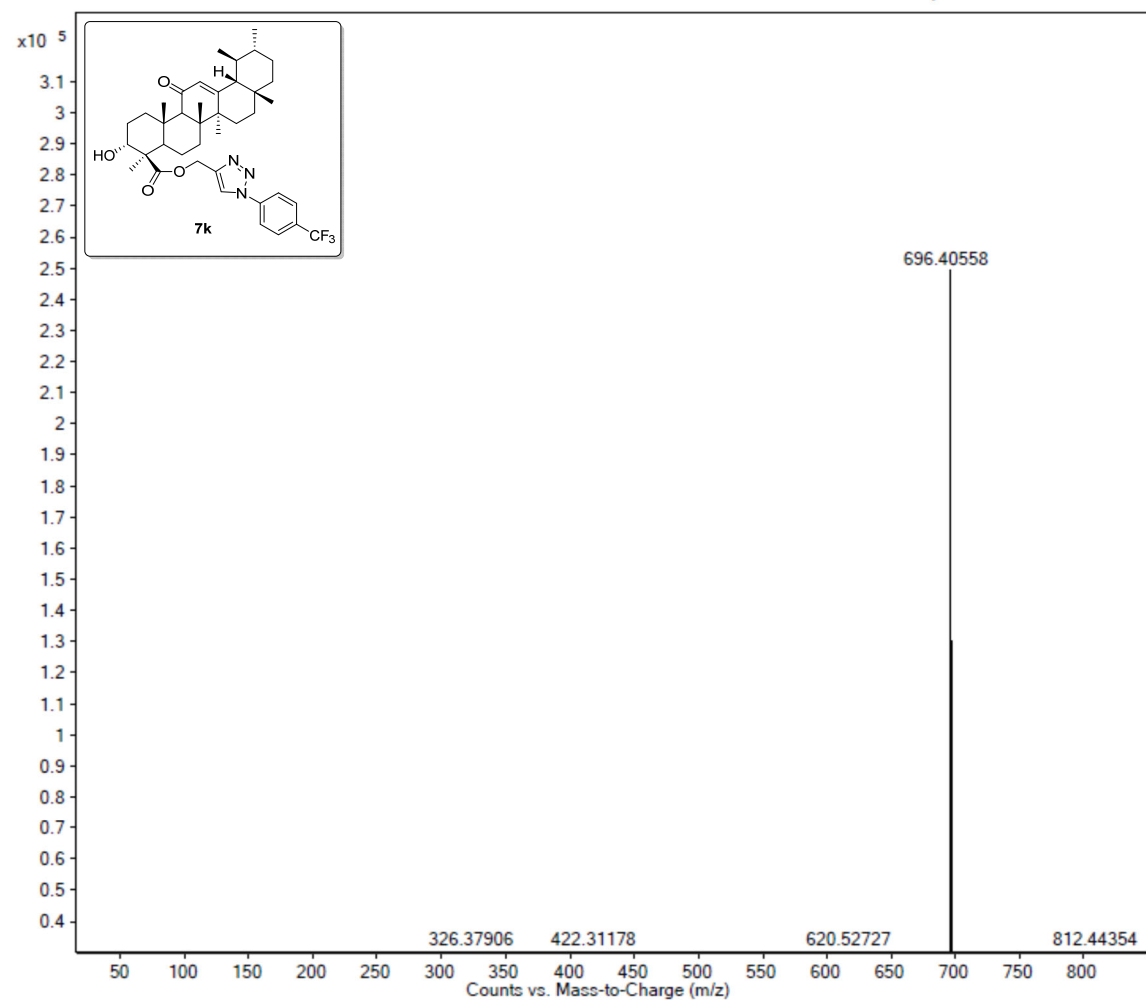
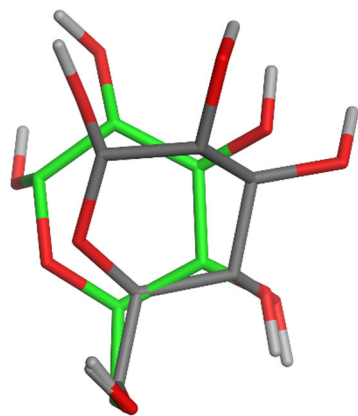


Figure S80: HRMS spectrum of compound **7k**



**Figure S81.** The re-docked conformation (green stick model) of maltose is superimposed on the X-ray conformation (grey stick model) present in the PDB code 3A4A

**Table S1.** The docking results of all the compounds.

Compounds	Score (Kcal/mol)	Ligand Atom	Receptor Atom	Interaction	Distance (Å)
<b>6f</b>	-9.18	O75	NE2-HIS280	HBA	2.00
		O97	N-ARG315	HBA	2.55
		O98	N-ARG315	HBA	2.44
		O86	OG-SER240	HBA	2.09
<b>7h</b>	-8.74	O58	O-SER157	HBD	2.59
		O77	N-ARG315	HBA	2.37
<b>6j</b>	-8.79	O86	OG-SER240	HBA	2.49
		O98	N-ARG315	HBA	2.26
		O99	N-ARG315	HBA	2.23
<b>6h</b>	-8.74	N84	NH1-ARG442	HBA	2.18
		O86	N-ARG315	HBA	1.83
<b>6g</b>	-8.67	O75	NE2-HIS280	HBA	1.95
		O86	OG-SER240	HBA	2.11
<b>6c</b>	-7.78	O76	NE2-HIS280	HBA	2.19
		O86	OG-SER240	HBA	2.48
		O104	NE2-GLN279	HBA	2.38
<b>6k</b>	-7.89	O75	NE2-HIS280	HBA	2.35
<b>7g</b>	-7.66	O58	OE2-GLU411	HBD	2.32

		O78	NE2-GLN279	HBA	2.07
<b>7k</b>	-7.04	O77	NE2-HIS280	HBA	2.13
		O78	NE2-HIS280	HBA	2.12
<b>6e</b>	-7.55	O75	NE2-HIS280	HBA	1.96
<b>6a</b>	-7.24	N84	NE2-HIS351	HBA	2.53
<b>7b</b>	-7.21	O58	NH1-ARG442	HBA	2.87
		6-ring	6-ring-TYR72	$\pi$ - $\pi$	3.85
<b>7c</b>	-7.35	O58	OD2-ASP242	HBD	1.67
<b>6b</b>	-7.02	O76	NE2-HIS280	HBA	2.08
		O86	OG-SER240	HBA	2.44
<b>7a</b>	-7.11	N87	NE2-HIS280	HBA	2.27
		5-ring	CD2-PHE303	$\pi$ -H	3.61
<b>6d</b>	-7.05	O75	NE2-GLN279	HBA	2.30
		F98	NE2-HIS351	HBA	1.86
<b>7e</b>	-7.45	O88	OG-SER240	HBA	2.13
<b>7f</b>	-7.53	N87	NE2-GLN279	HBA	3.09
		F102	NE2-HIS112	HBA	2.98
<b>7d</b>	-6.98	F100	NH2-ARG213	HBA	2.88
<b>7j</b>	-6.36	O58	OD1-ASP215	HBD	1.97
		O58	OD2-ASP215	HBD	2.37



		O88	NE2-GLN279	HBA	1.89
		O78	NE2-HIS351	HBA	2.20
		6-ring	6-ring- PHE301	$\pi$ - $\pi$	3.29
		O75	NH1-ARG442	HBA	2.21
		O99	ND2-ASN350	HBA	2.21
<b>6i</b>	-6.45	N85	NE2-HIS351	HBA	2.40
		O86	NH1-ARG315	HBA	2.83
		5-ring	NE2-HIS351	$\pi$ -H	3.48
		O58	O-TYR158	HBD	2.78
		C11	5-ring-HIS280	$\pi$ -H	4.09
<b>7i</b>	-6.59	C10	5-ring-HIS280	$\pi$ -H	3.93
		6-ring	6-ring- PHE303	$\pi$ - $\pi$	3.54
<b>3</b>	-6.15	O75	NH1-ARG442	HBA	2.01
<b>4</b>	-6.20	O58	NH1-ARG442	HBA	2.13
		O58	OD1-ASP215	HBD	2.73
<b>2 (KBA)</b>	-4.44	O78	NH1-ARG442	HBA	2.87
		O83	NH2-ARG213	HBA	1.69
<b>1 (AKBA)</b>	-3.23	O84	NE2-HIS351	HBA	1.98

HBA = Hydrogen bond acceptor, HBD = Hydrogen bond donor.

**Table S2.** Crystal data of the compound **4**.

<b>Compound</b>	<b>4</b>
Chemical formula	C <sub>33</sub> H <sub>47</sub> O <sub>4</sub>
Mr	507.70
Crystal system, space group	Orthorhombic, P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Temperature (K)	296
a (Å)	13.834(5)
b (Å)	23.617(8)
c (Å)	8.757(3)
$\alpha$ (°)	90
$\beta$ (°)	90
$\gamma$ (°)	90
V (Å <sup>3</sup> )	2861.0(17)
Z	4
$\mu$ (mm <sup>-1</sup> )	0.08
Absorption correction	Multi-scan, SADABS
T <sub>min</sub> , T <sub>max</sub>	0.6596, 0.7451
No. of measured, independent and observed [I > 2 $\sigma$ (I)] reflections	43500, 4914, 3977
R <sub>int</sub>	0.0770
(sin $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.591
R[F <sup>2</sup> > 2 $\sigma$ (F <sup>2</sup> )], wR(F <sup>2</sup> ), S	0.0418, 0.1056, 1.043
No. of reflections	4914
No. of parameters	344
No. of restraints	1
$\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ (eÅ <sup>-3</sup> )	0.164, -0.163