

## Supporting Information

*Org. Commun.* 19:1 (2026):e26013780

### DBUHI<sub>3</sub>-catalyzed efficient synthesis of 1,4-dihydropyridines

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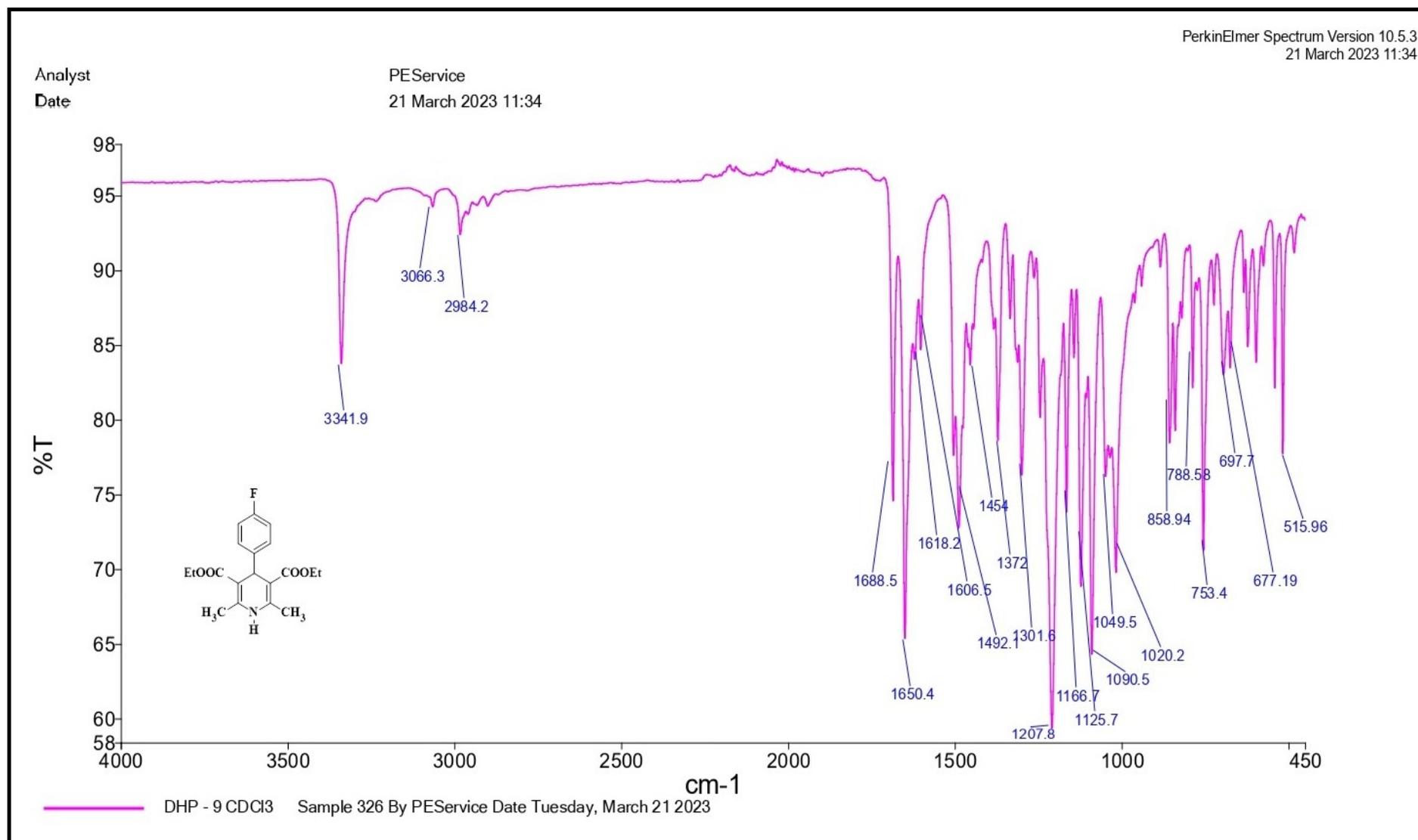
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**Figure S1:** IR spectrum of diethyl 4-(5-fluorophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**4c**)

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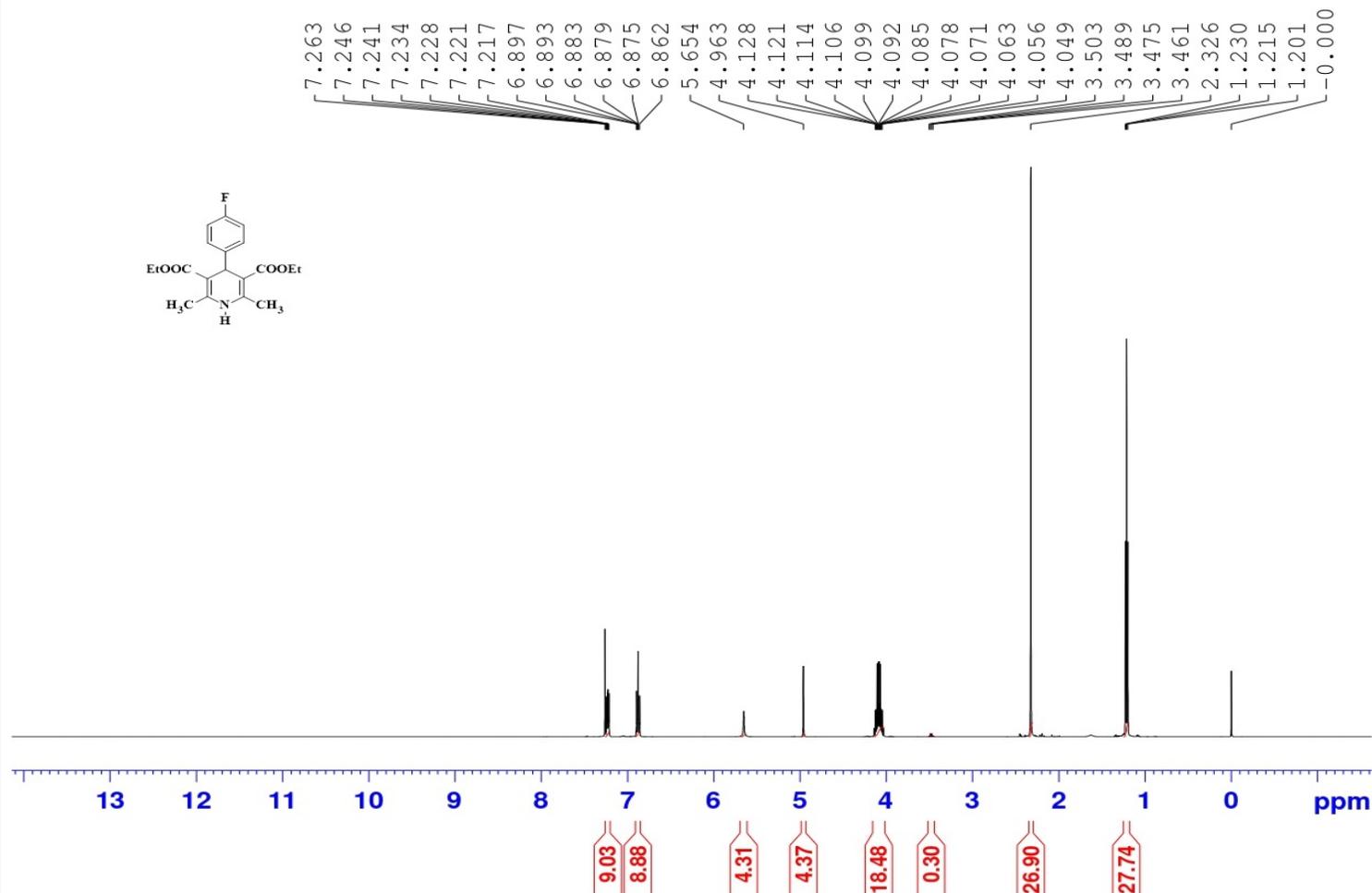


Figure S2: <sup>1</sup>H-NMR spectrum of diethyl 4-(5-fluorophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (4c)

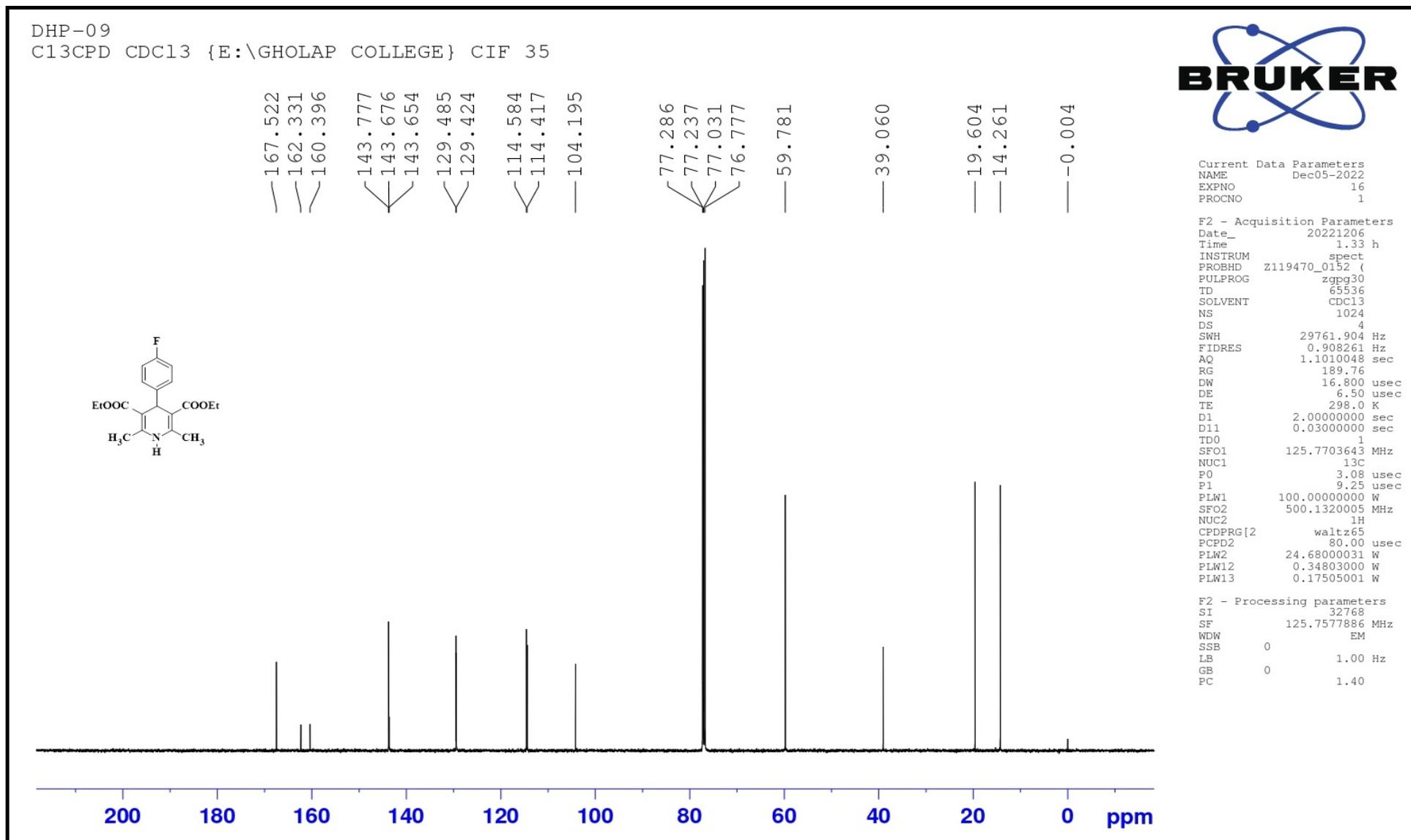
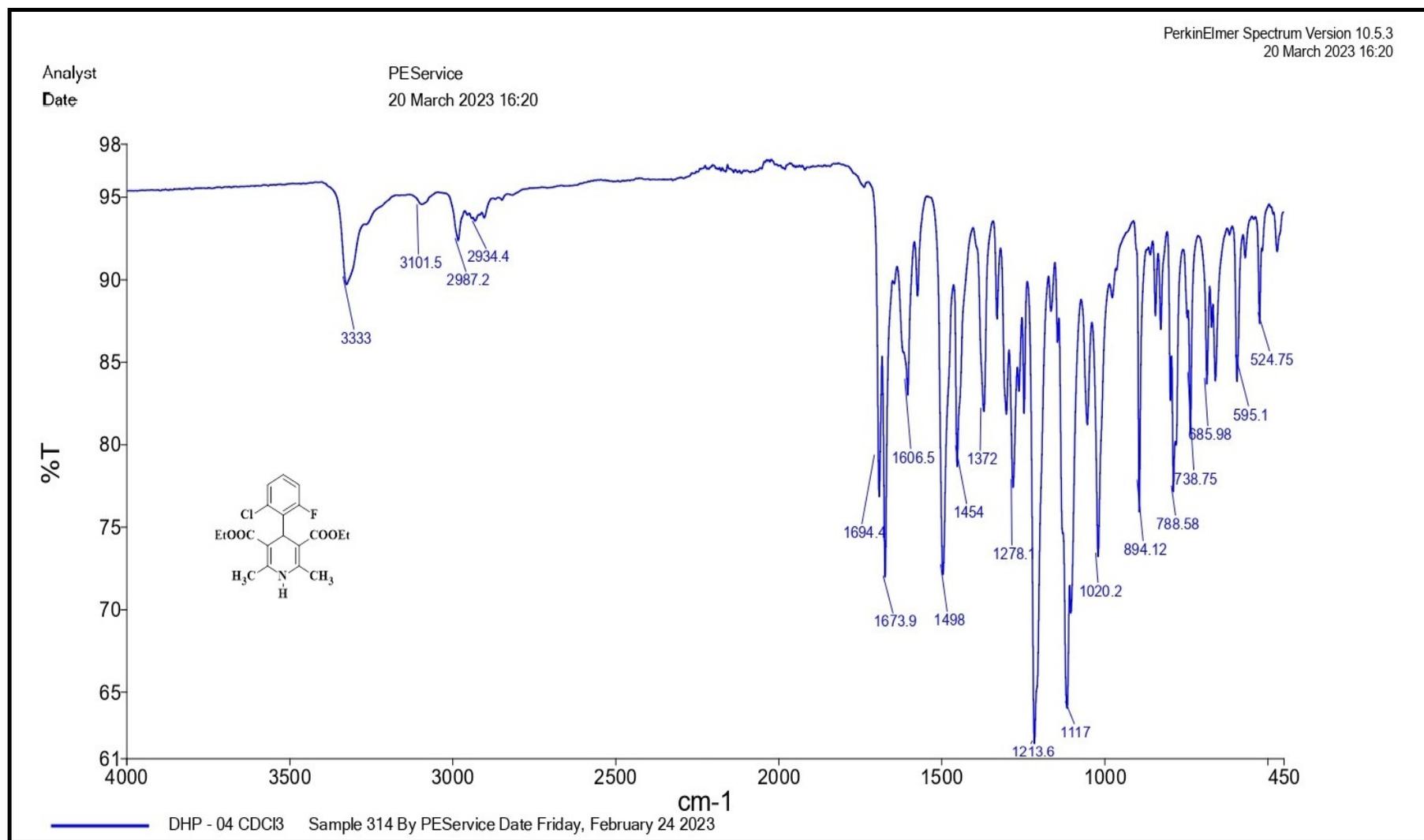


Figure S3:  $^{13}\text{C}$ -NMR spectrum of diethyl 4-(5-fluorophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**4c**)



**Figure S4:** IR spectrum of diethyl 4-(2-chloro-6-fluorophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**4d**)

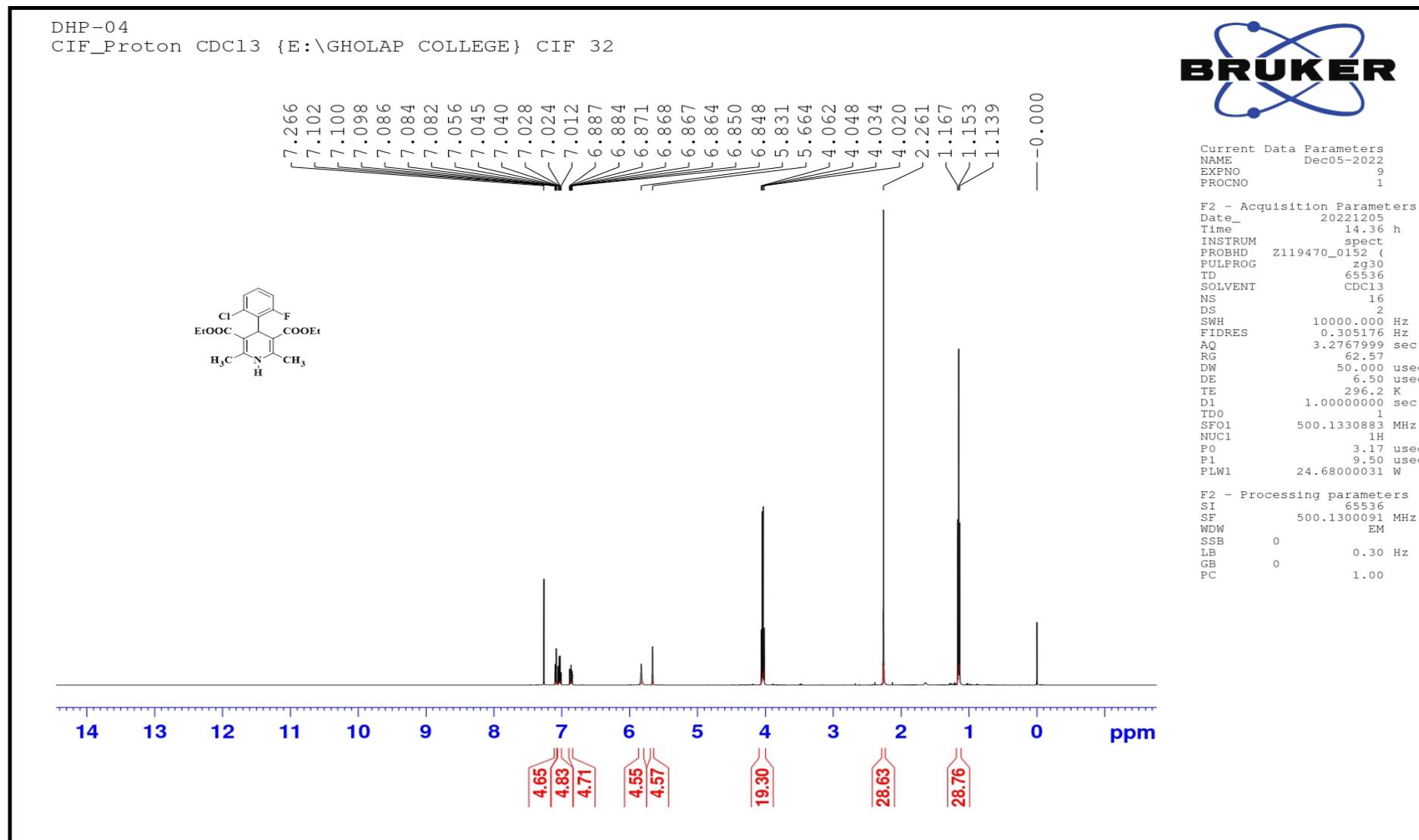


Figure S5: <sup>1</sup>H-NMR spectrum of diethyl 4-(2-chloro-6-fluorophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**4d**)

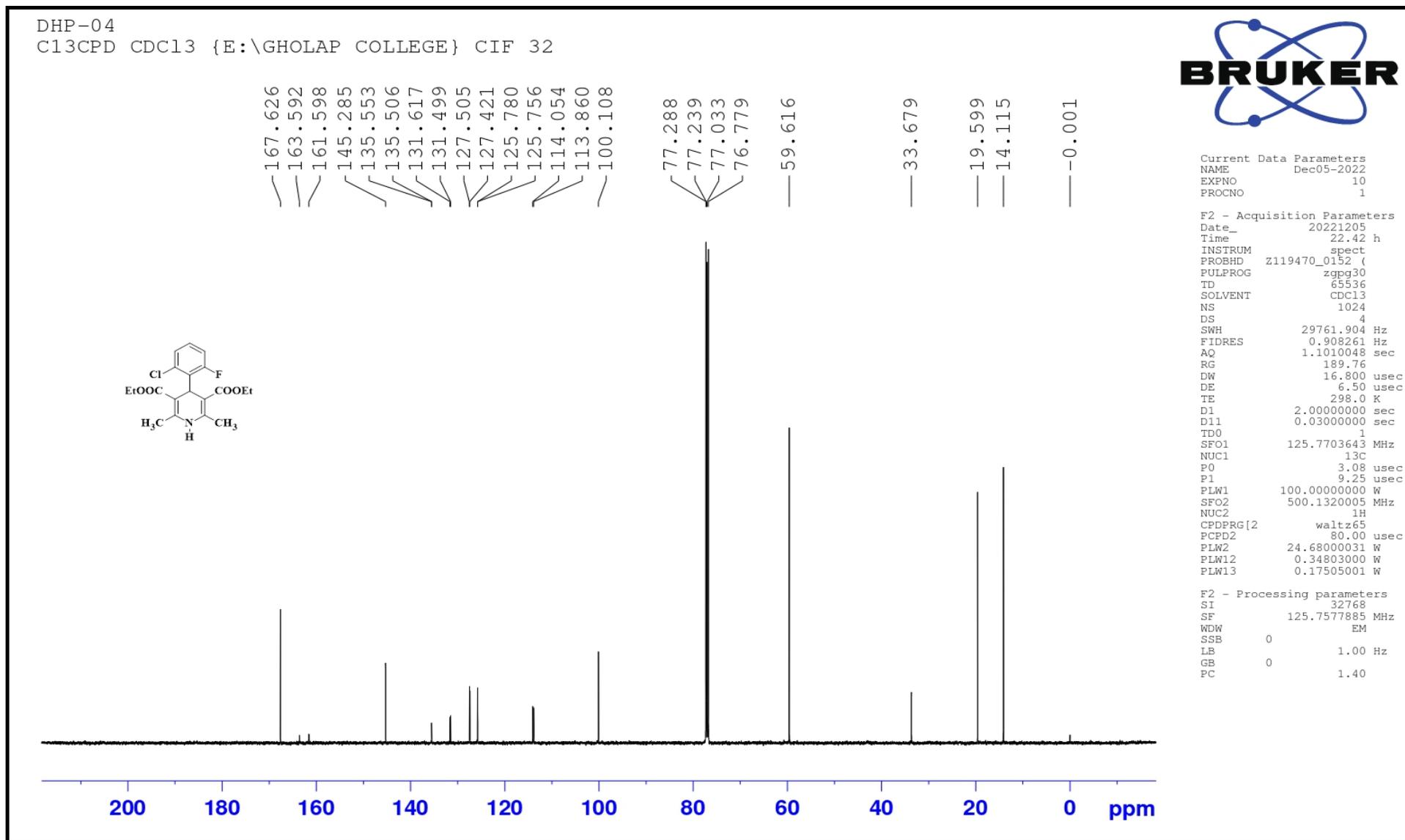


Figure S6:  $^{13}\text{C}$ -NMR spectrum of diethyl 4-(2-chloro-6-fluorophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**4d**)

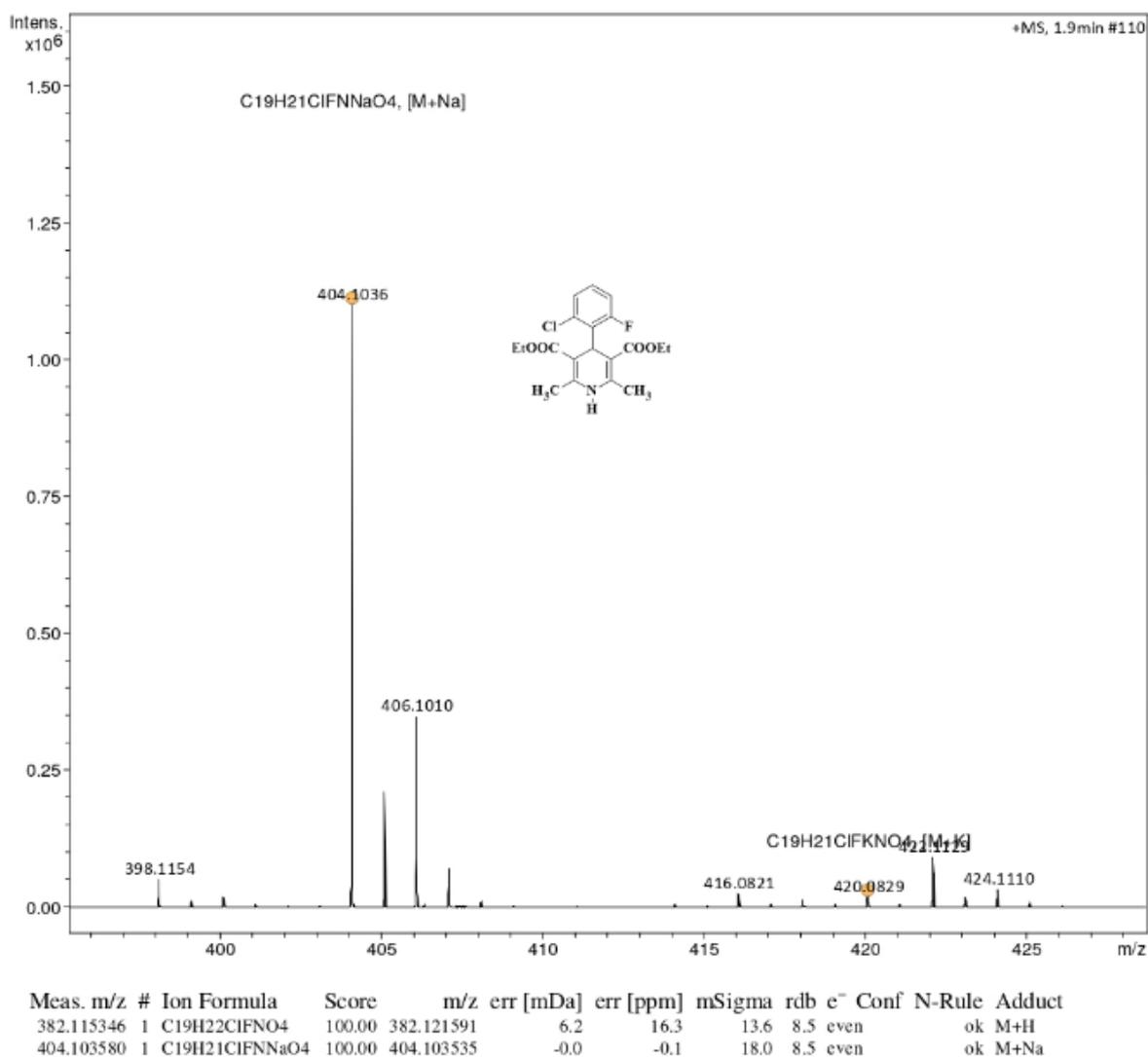
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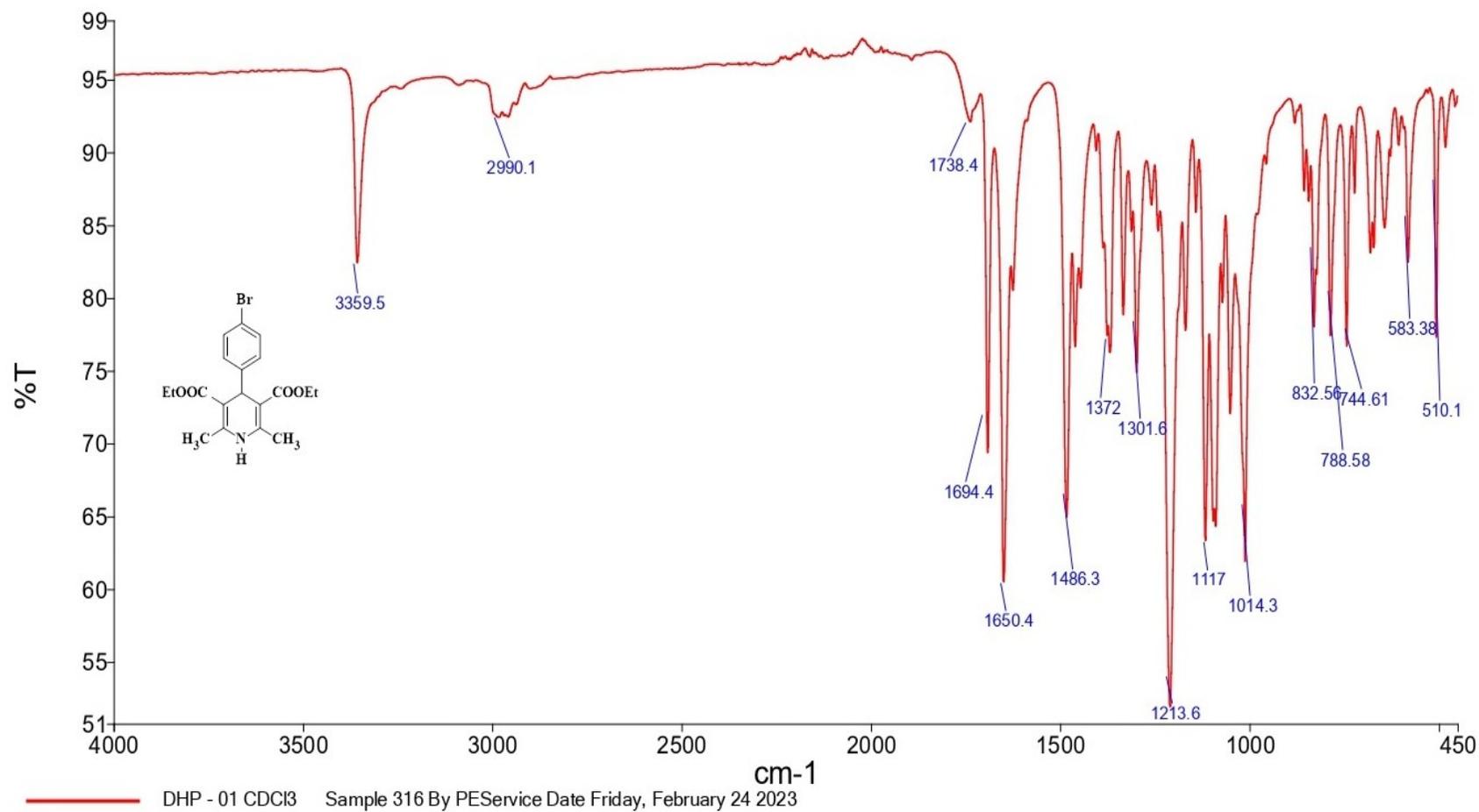
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**Figure S7:** HRMS spectrum of diethyl 4-(2-chloro-6-fluorophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**4d**)

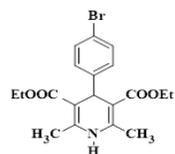
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**Figure S8:** IR spectrum of diethyl 4-(4-bromophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**4e**)

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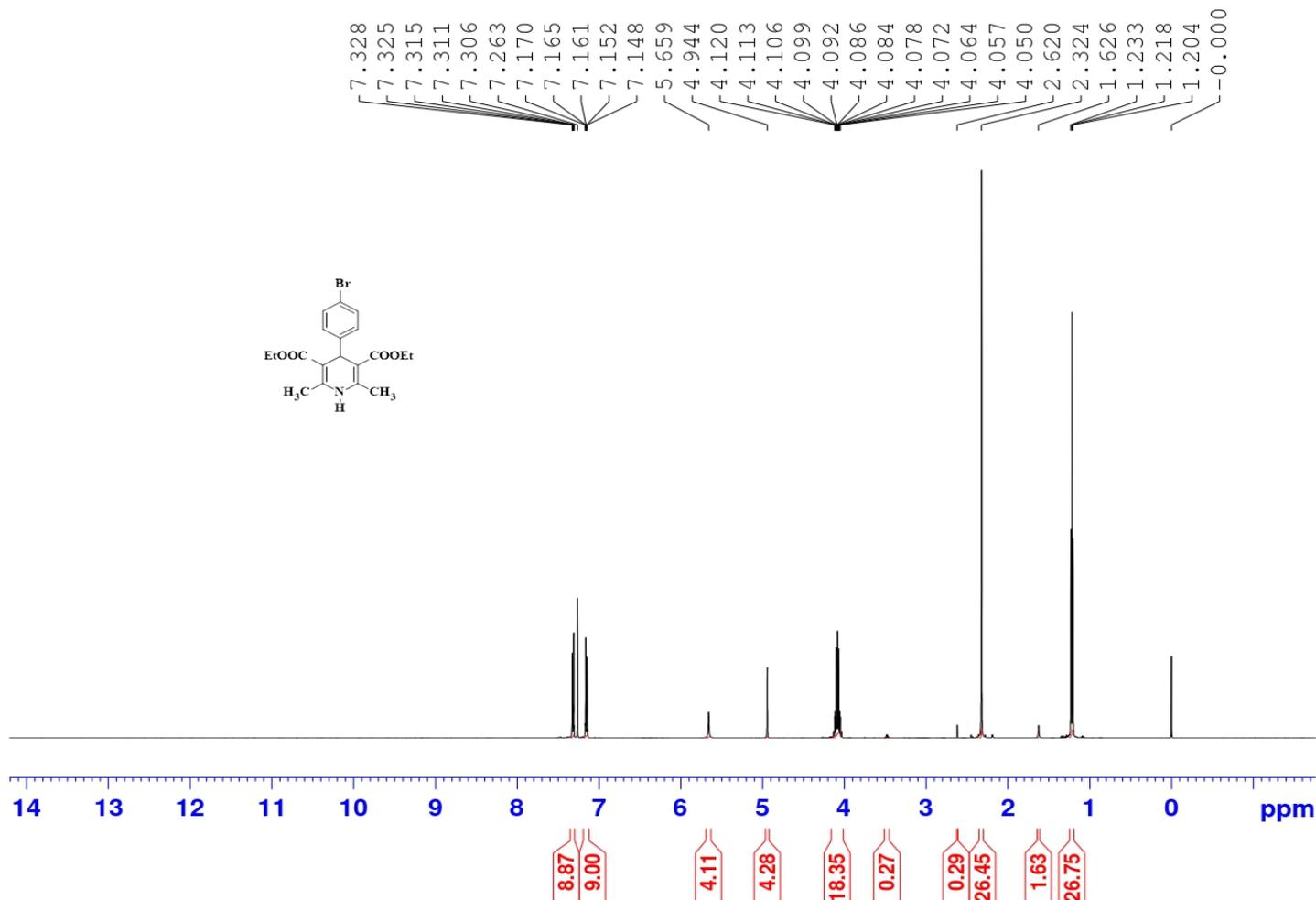


Figure S9: <sup>1</sup>H-NMR spectrum of diethyl 4-(5-bromophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (4e)

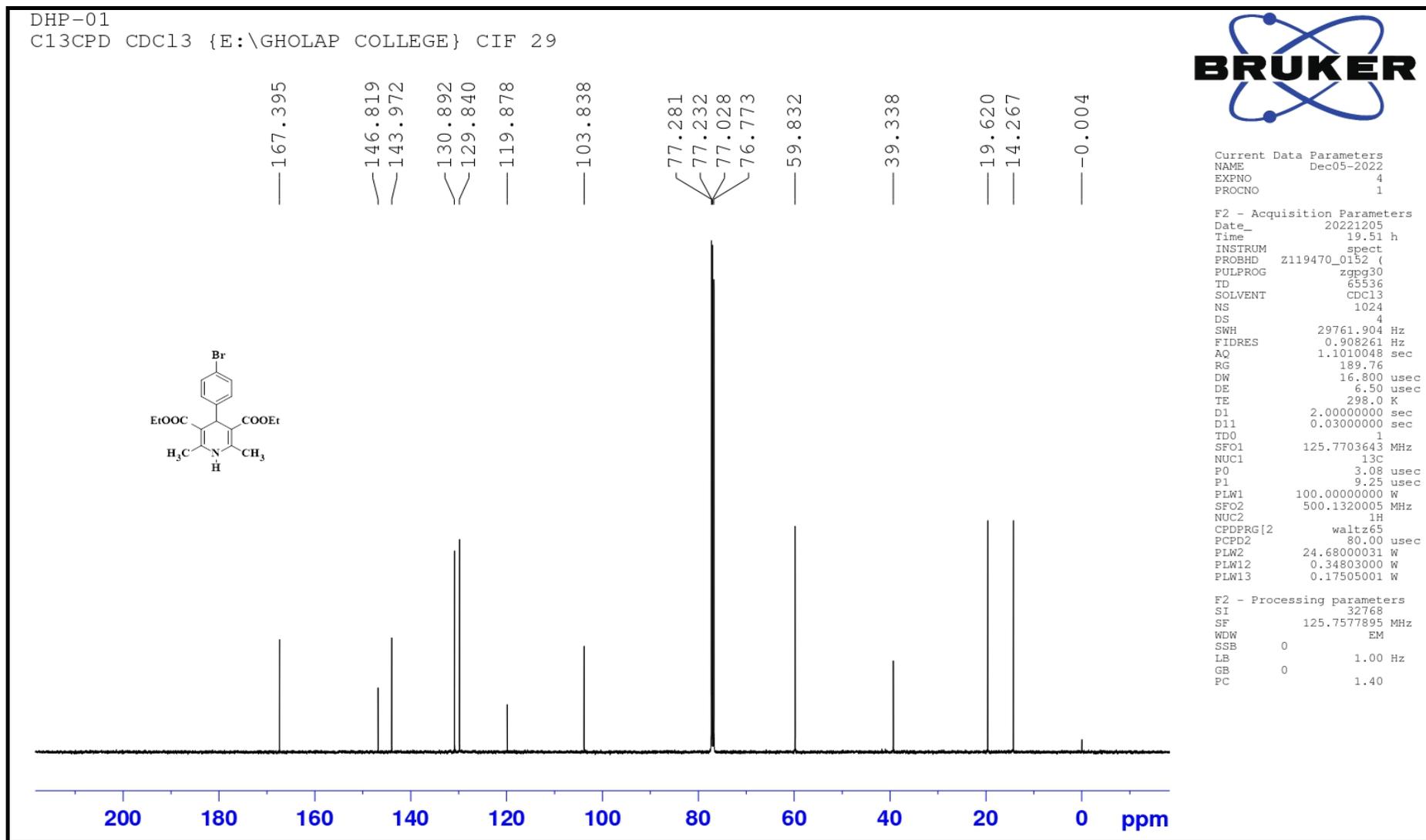


Figure S10:  $^{13}\text{C}$ -NMR spectrum of diethyl 4-(5-bromophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (4e)

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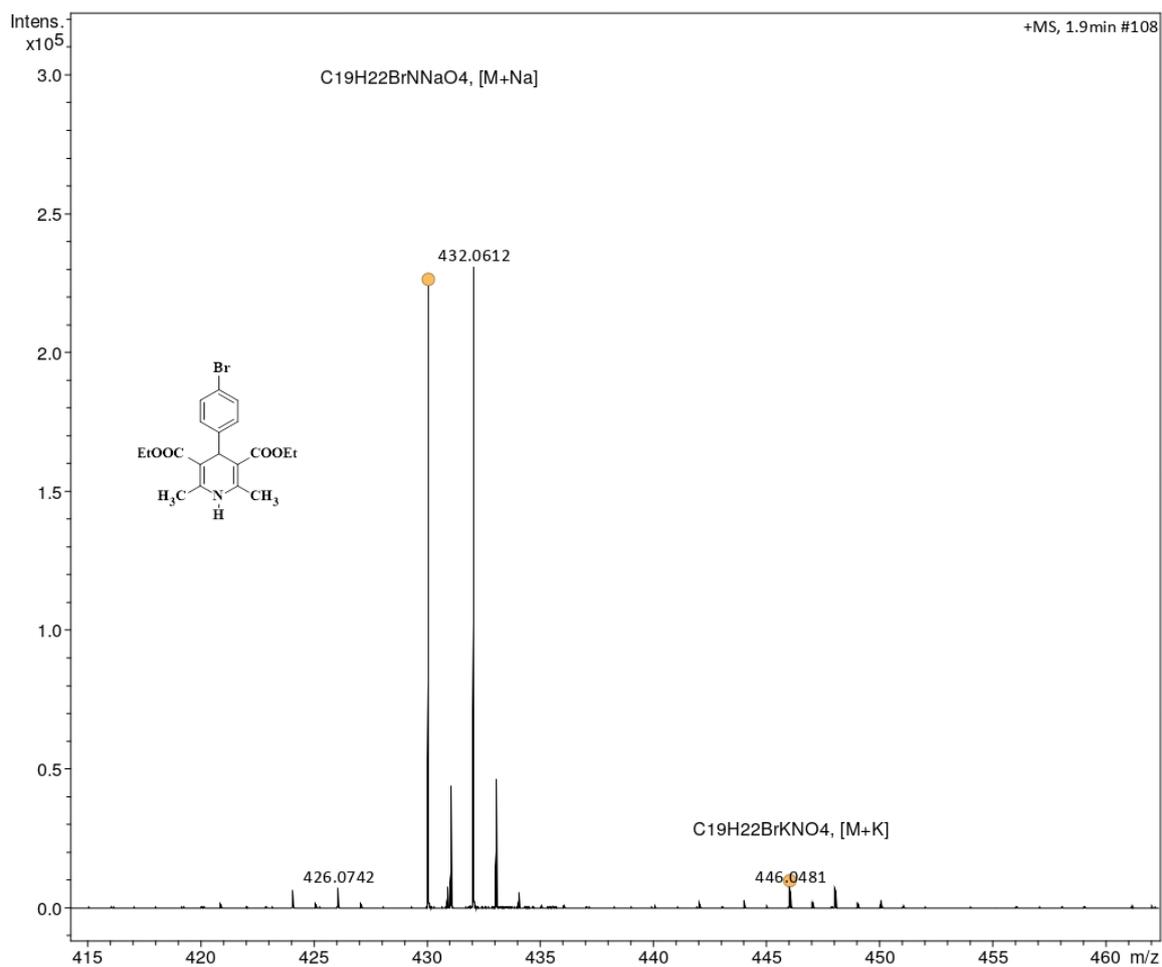
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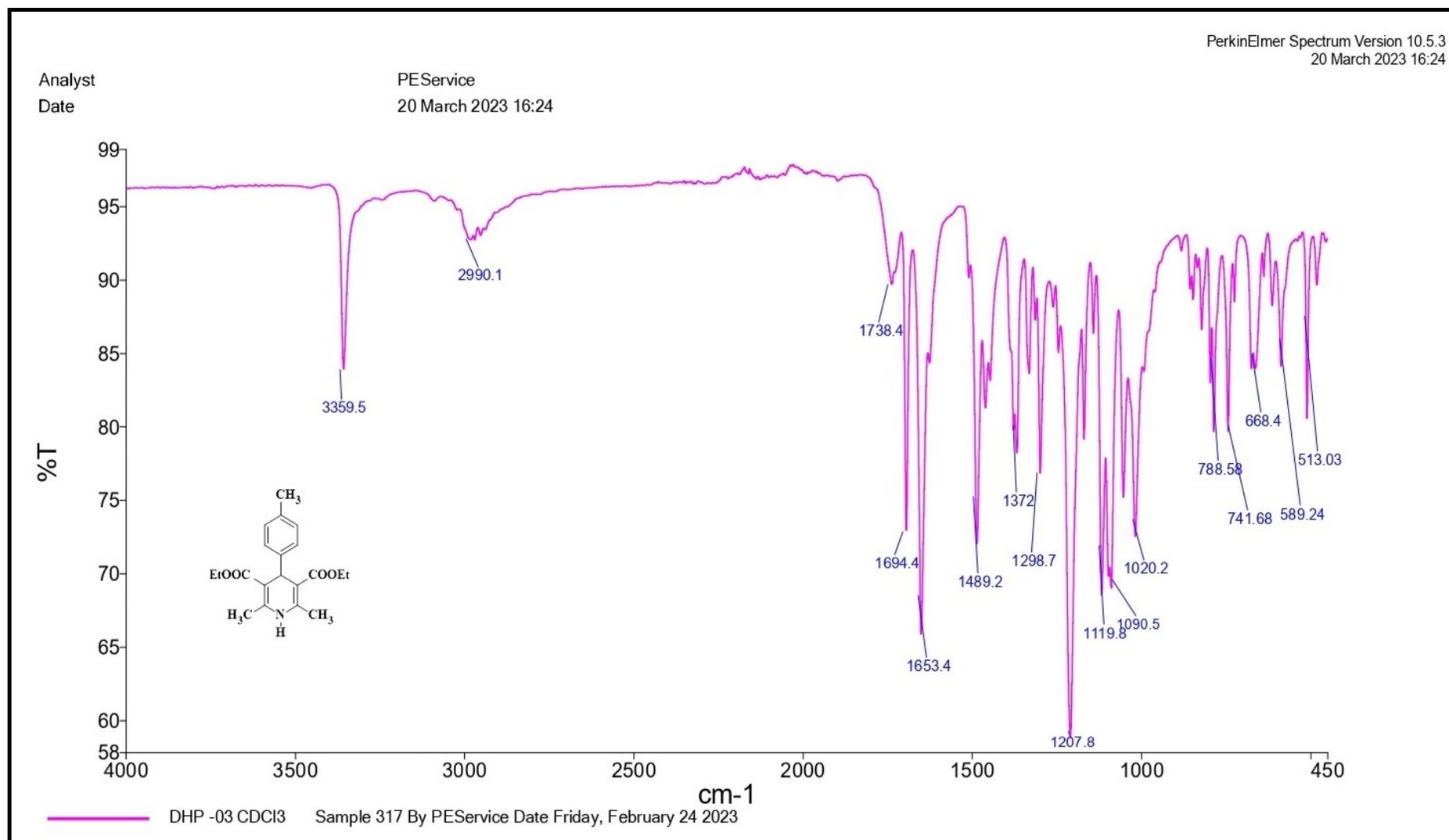
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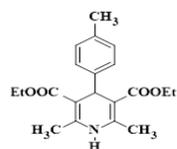
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**Figure S11:** HRMS spectrum of diethyl 4-(4-bromophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**4e**)



**Figure S12:** IR spectrum of diethyl 2,6-dimethyl-4-(*p*-tolyl)-1,4-dihydropyridine-3,5-dicarboxylate (**4g**)

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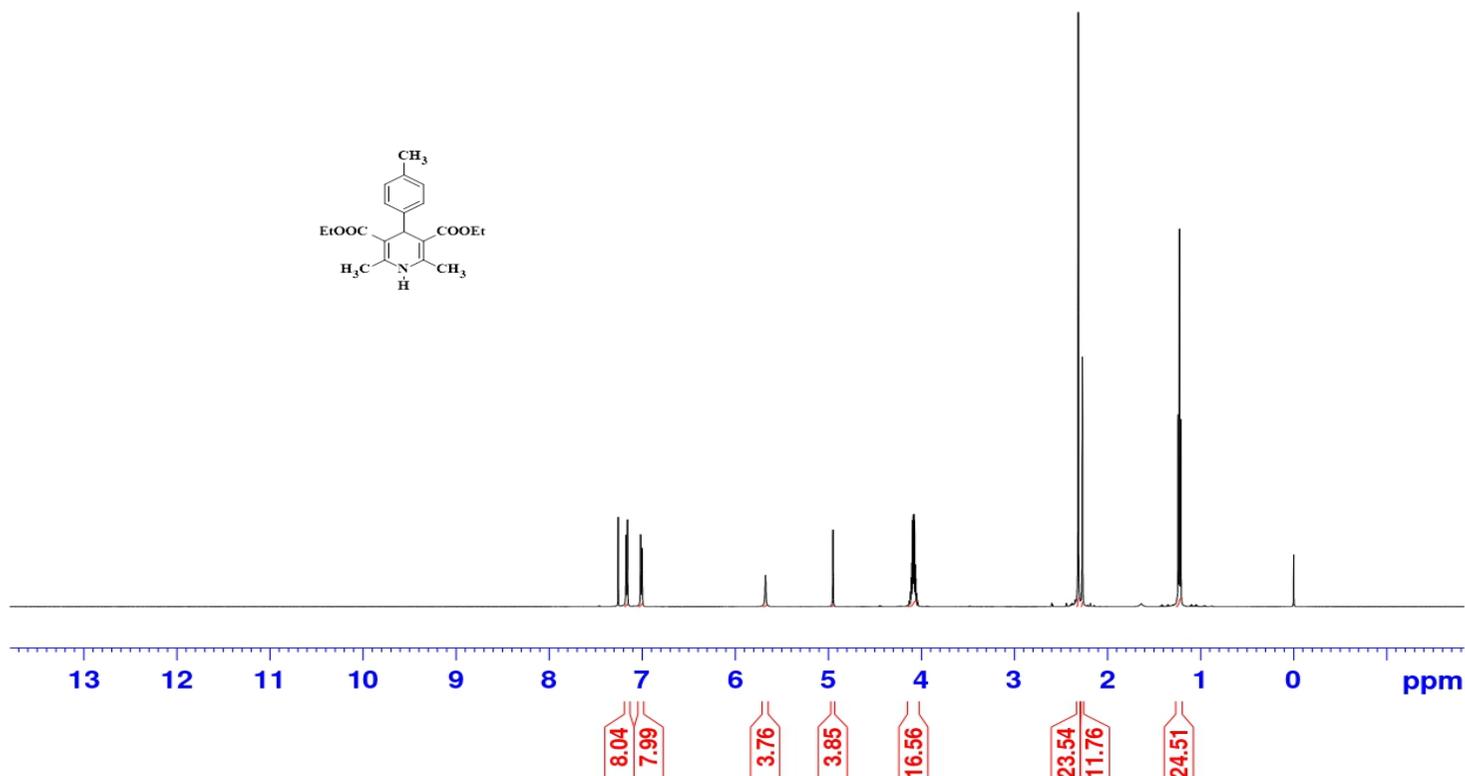


Figure S13: <sup>1</sup>H-NMR spectrum of diethyl 2,6-dimethyl-4-(*p*-tolyl)-1,4-dihydropyridine-3,5-dicarboxylate (**4g**)

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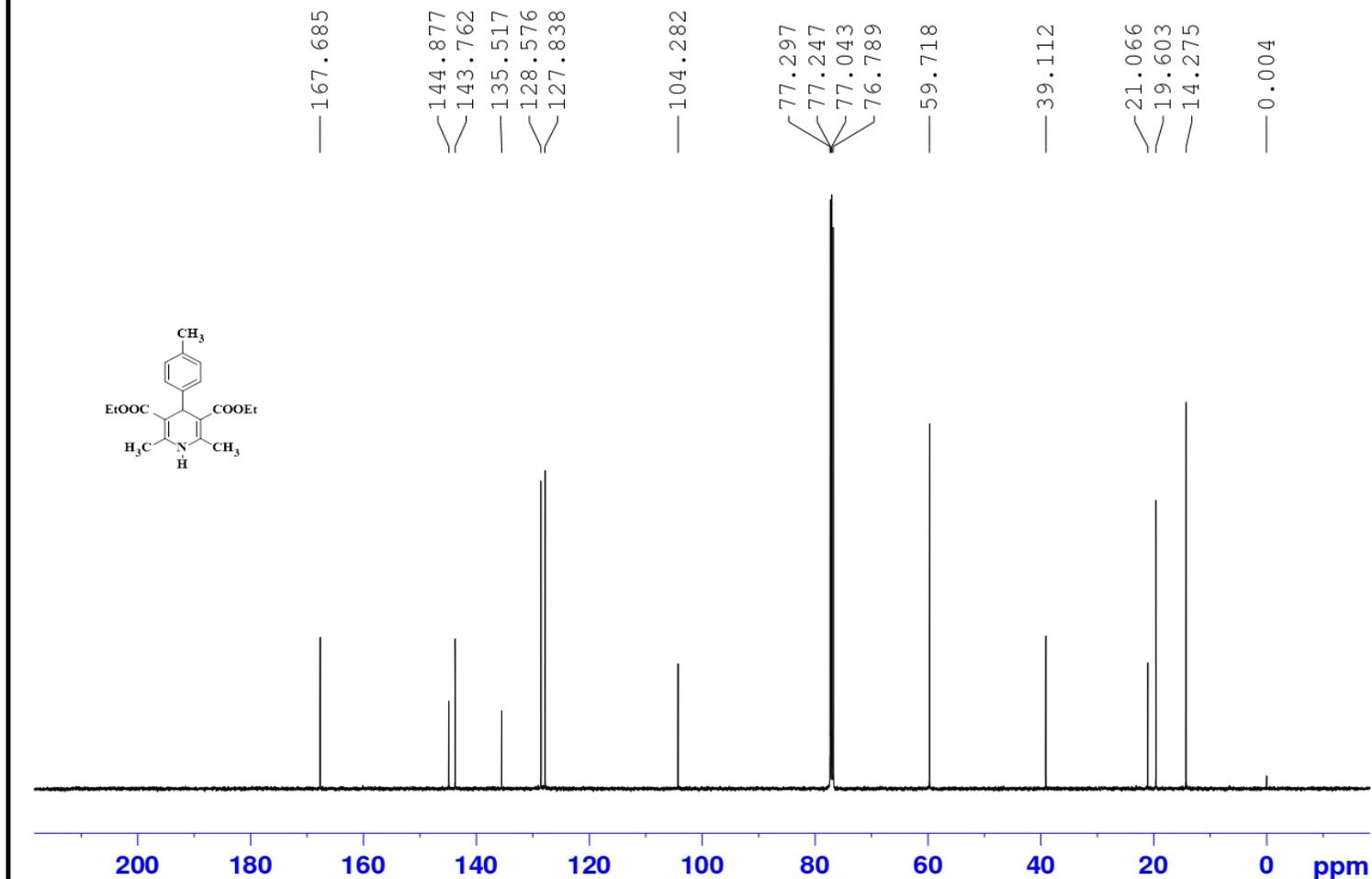
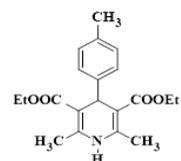


Figure S14:  $^{13}\text{C}$ -NMR spectrum of diethyl 2,6-dimethyl-4-(*p*-tolyl)-1,4-dihydropyridine-3,5-dicarboxylate (**4g**)

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Analysis Info

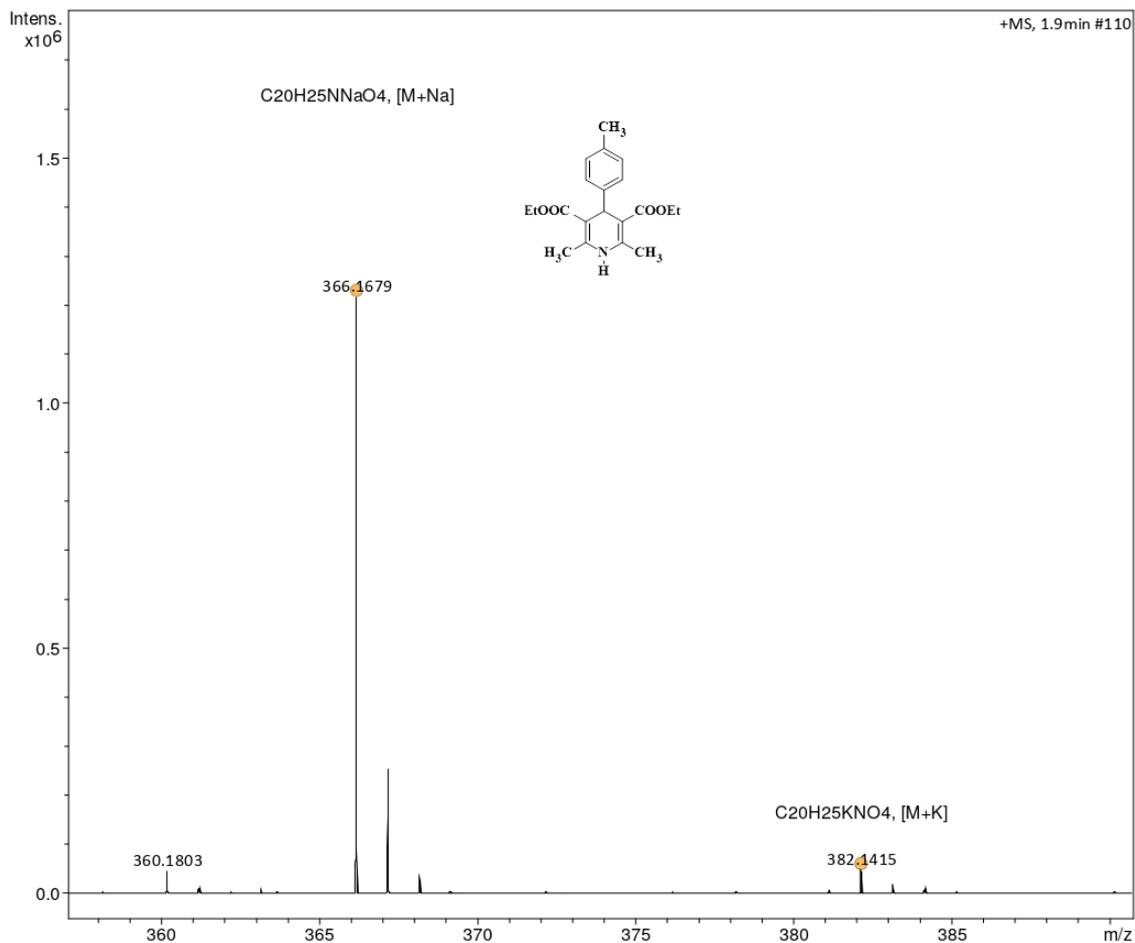
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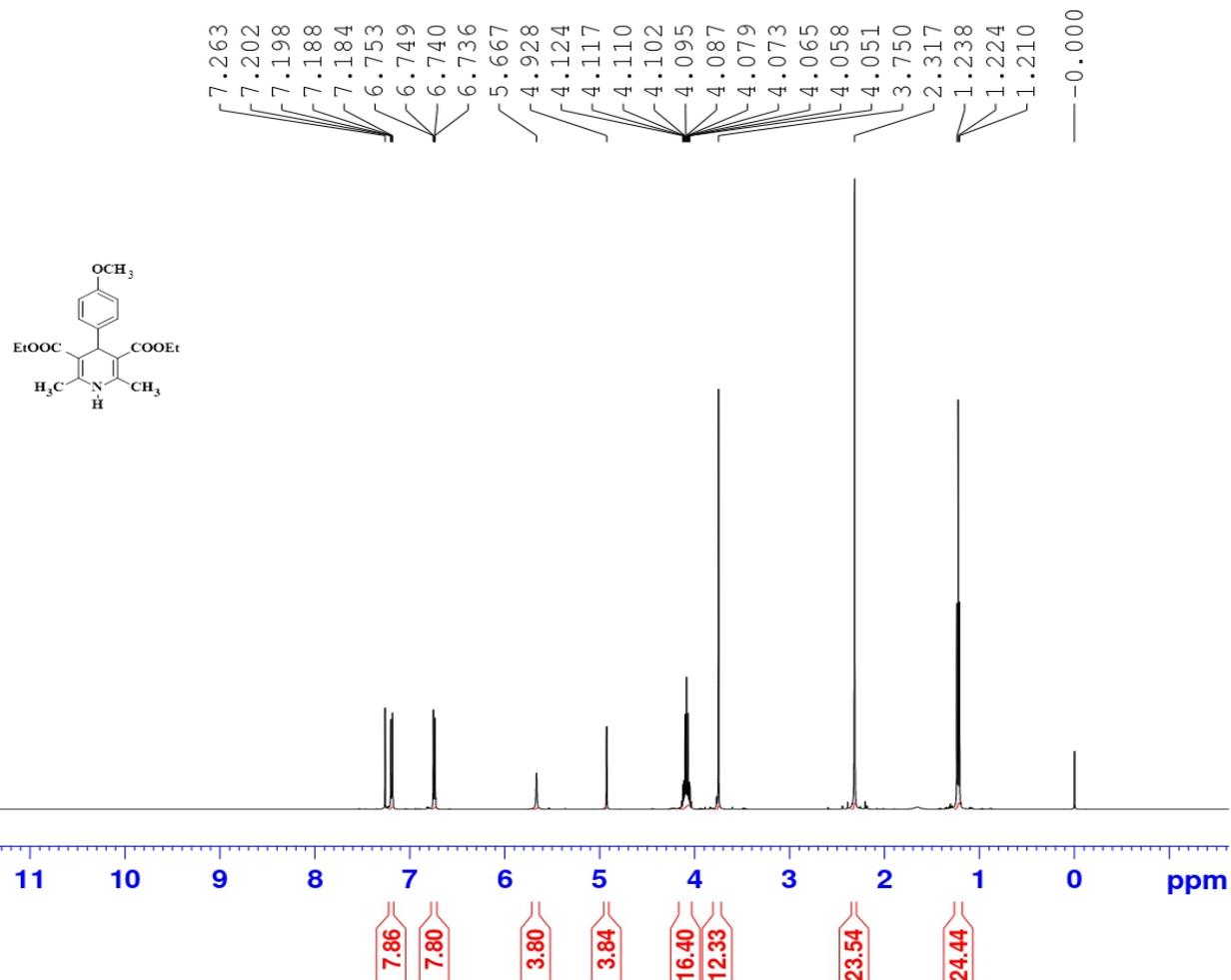
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366.167923	1	C20H25NNaO4	100.00	366.167579	-0.3	-0.9	9.6	8.5	even		ok	M+Na

Figure S15: HRMS spectrum diethyl 2,6-dimethyl-4-(*p*-tolyl)-1,4-dihydropyridine-3,5-dicarboxylate (4g)

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Figure S16: <sup>1</sup>H-NMR spectrum of diethyl 4-(4-methoxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (4h)

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NS 1024  
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FIDRES 0.908261 Hz  
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RG 189.76  
DW 16.800 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 125.7703643 MHz  
NUC1 13C  
P0 3.08 usec  
P1 9.25 usec  
PLW1 100.00000000 W  
SFO2 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 80.00 usec  
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PLW12 0.34803000 W  
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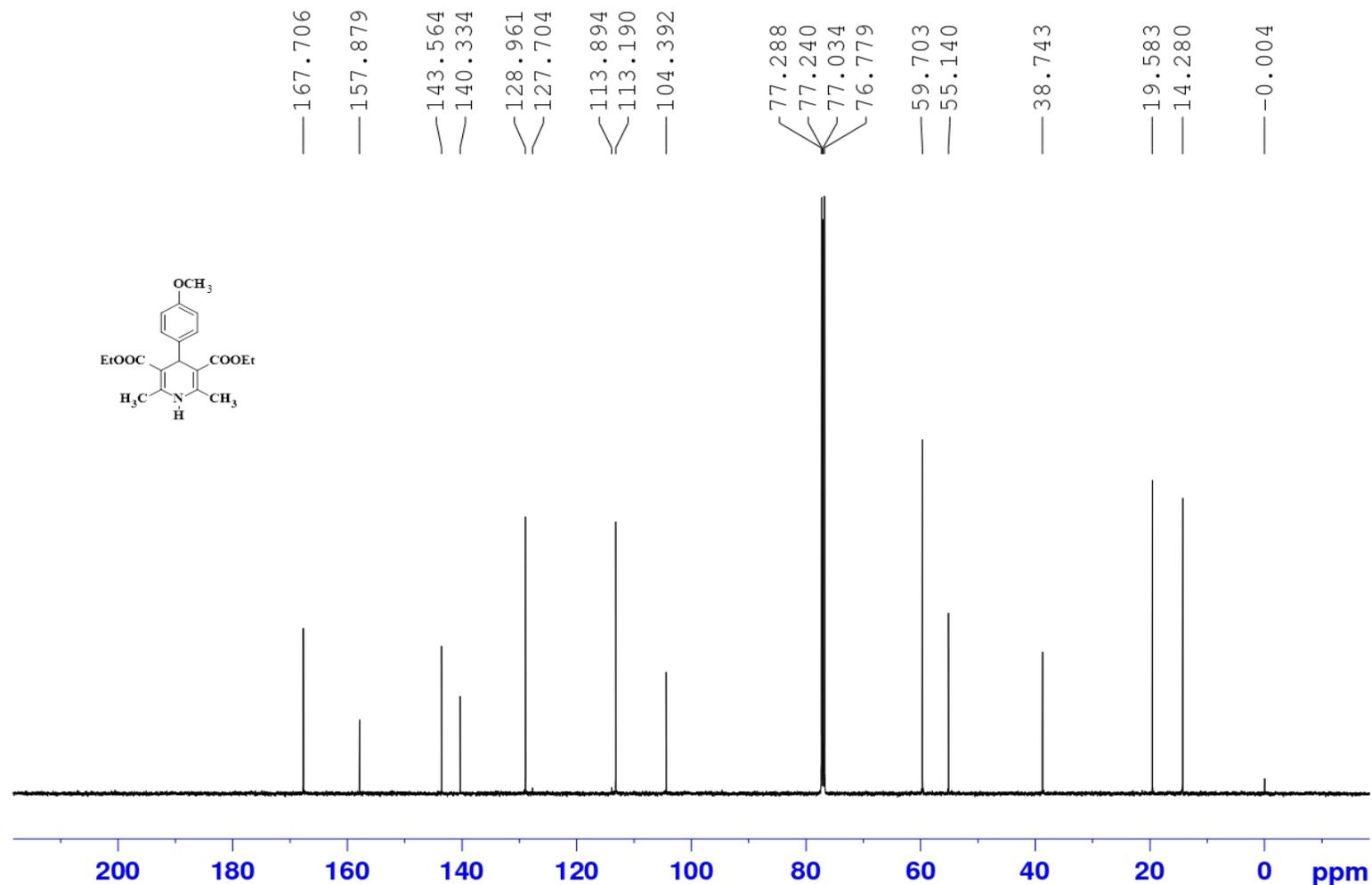
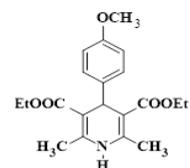


Figure S17:  $^{13}\text{C}$ -NMR spectrum of diethyl 4-(4-methoxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**4h**)

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Analysis Info

Analysis Name D:\Data\2022\DEC\SPPU COLLEGE\BABURAO GHOLAP COLLEGE\RAMESH  
 GAWADE\DHP-02\_GB4\_01\_4799.d  
 Method dlc\_ms50-1200mz\_10min\_0.120mlflow\_95b.m  
 Sample Name DHP-02  
 Comment

Acquisition Date 12/23/2022 1:36:57 PM

Operator CIF  
 Instrument impact HD 1819696.00184

Acquisition Parameter

Source Type ESI Ion Polarity Positive Set Nebulizer 1.7 Bar  
 Focus Active Set Capillary 4500 V Set Dry Heater 200 °C  
 Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 7.0 l/min  
 Scan End 1200 m/z Set Charging Voltage 2000 V Set Divert Valve Source  
 Set Corona 0 nA Set APCI Heater 0 °C

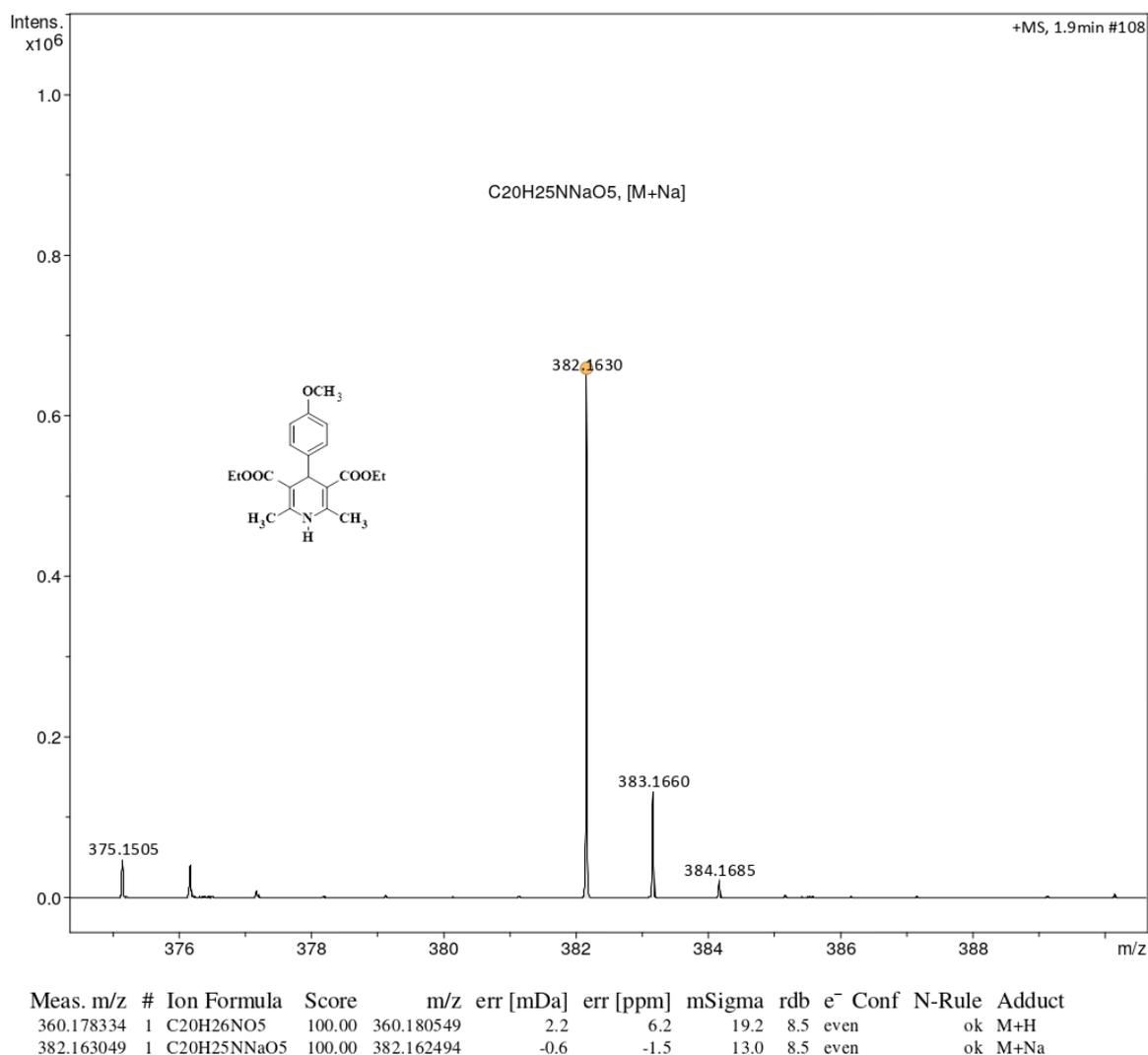
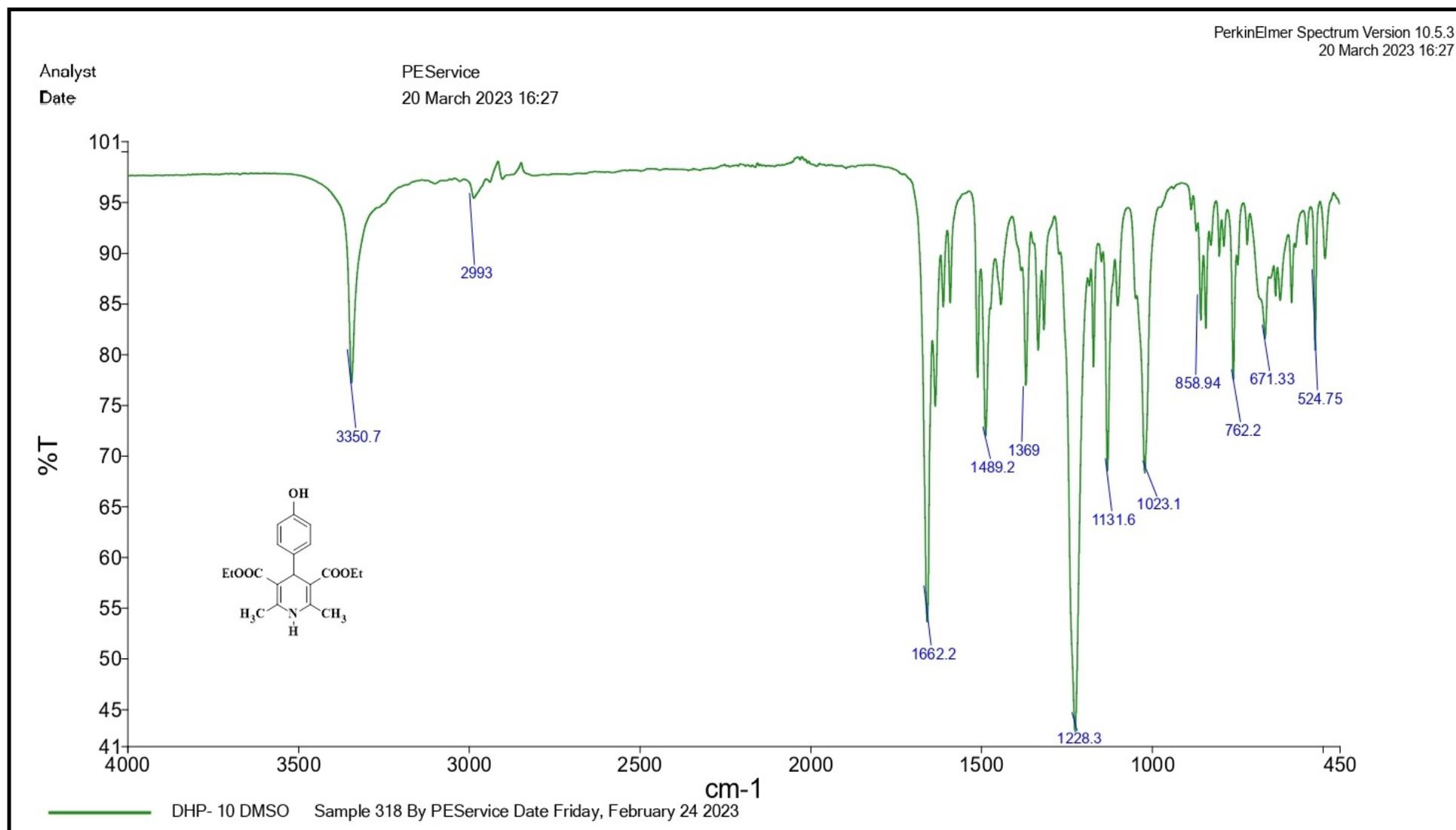


Figure S18: HRMS spectrum of diethyl 4-(4-methoxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (4h)



**Figure S19:** IR spectrum of diethyl 4-(4-hydroxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**4k**)

DHP-10  
CIF\_Proton DMSO {E:\GHOLAP COLLEGE} CIF 28



Current Data Parameters  
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EXPNO 1  
PROCNO 1

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PULPROG zg30  
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SOLVENT DMSO  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.2767999 sec  
RG 62.57  
DW 50.000 usec  
DE 6.50 usec  
TE 295.9 K  
D1 1.00000000 sec  
TDO 1  
SFO1 500.1330883 MHz  
NUC1 1H  
P0 3.17 usec  
P1 9.50 usec  
PLW1 24.68000031 W

F2 - Processing parameters  
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LB 0.30 Hz  
GB 0  
PC 1.00

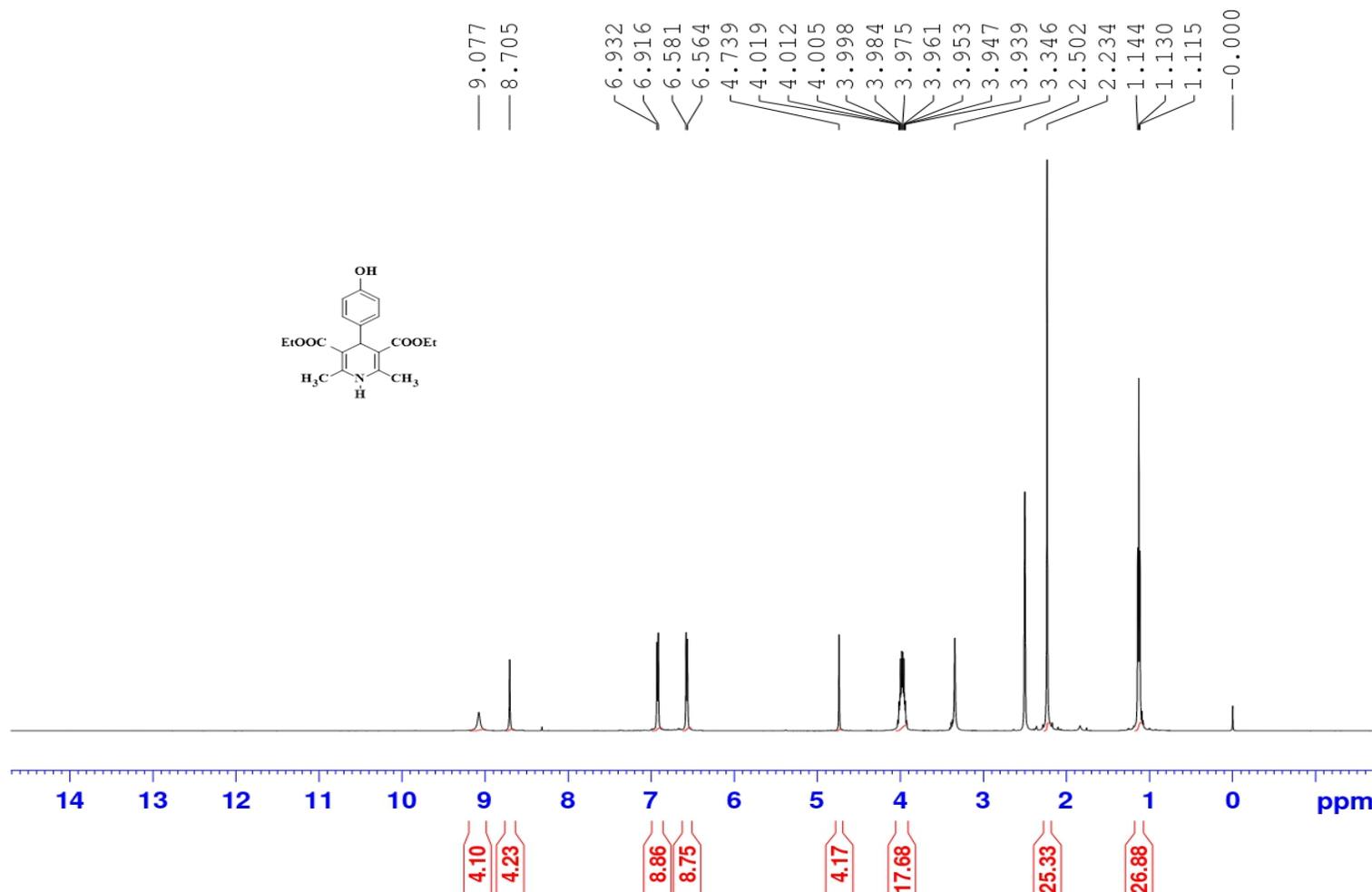
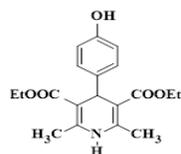


Figure S20: <sup>1</sup>H-NMR spectrum of diethyl 4-(4-hydroxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (4k)

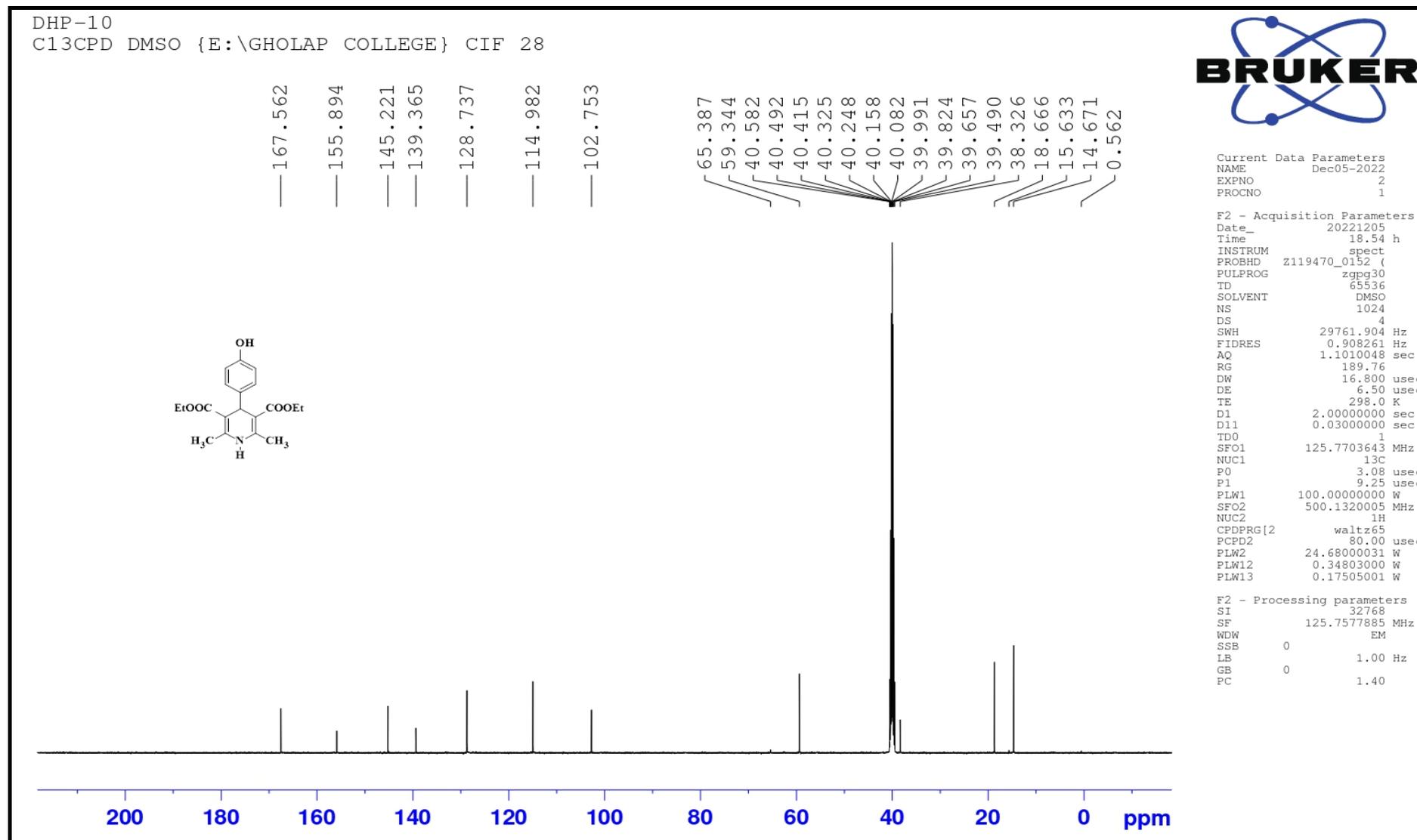


Figure S21: <sup>13</sup>C-NMR spectrum of diethyl 4-(4-hydroxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (**4k**)

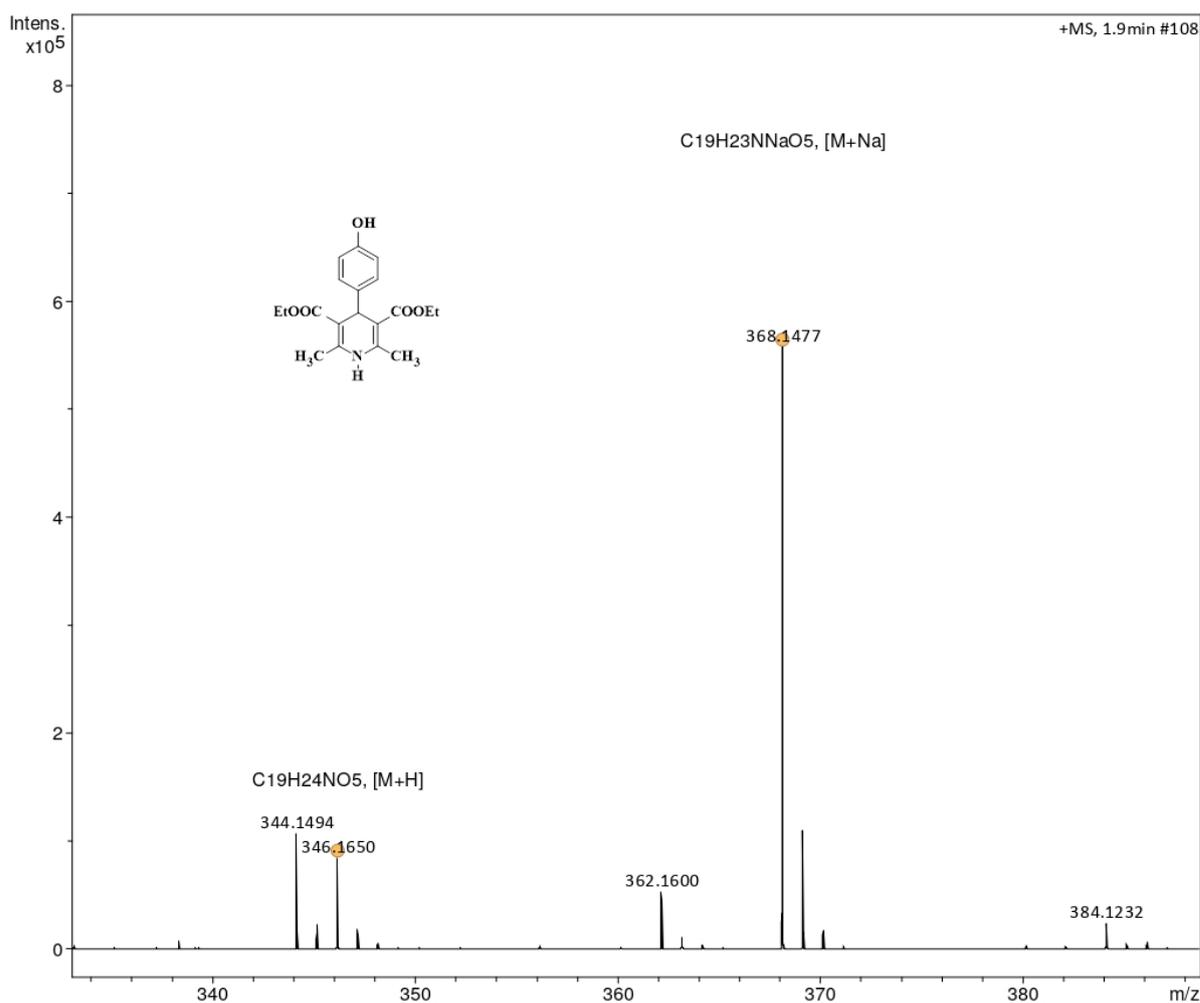
Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info

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 Method dlc\_ms50-1200mz\_10min\_0.120mlflow\_95b.m Operator CIF  
 Sample Name DHP-10 Instrument impact HD 1819696.00184  
 Comment

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e <sup>-</sup>	Conf	N-Rule	Adduct
346.165022	1	C19H24NO5	100.00	346.164899	-0.1	-0.4	19.2	8.5	even		ok	M+H
368.147700	1	C19H23NNaO5	100.00	368.146844	-0.9	-2.3	9.5	8.5	even		ok	M+Na

Figure S22: HRMS spectrum of diethyl 4-(4-hydroxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (4k)

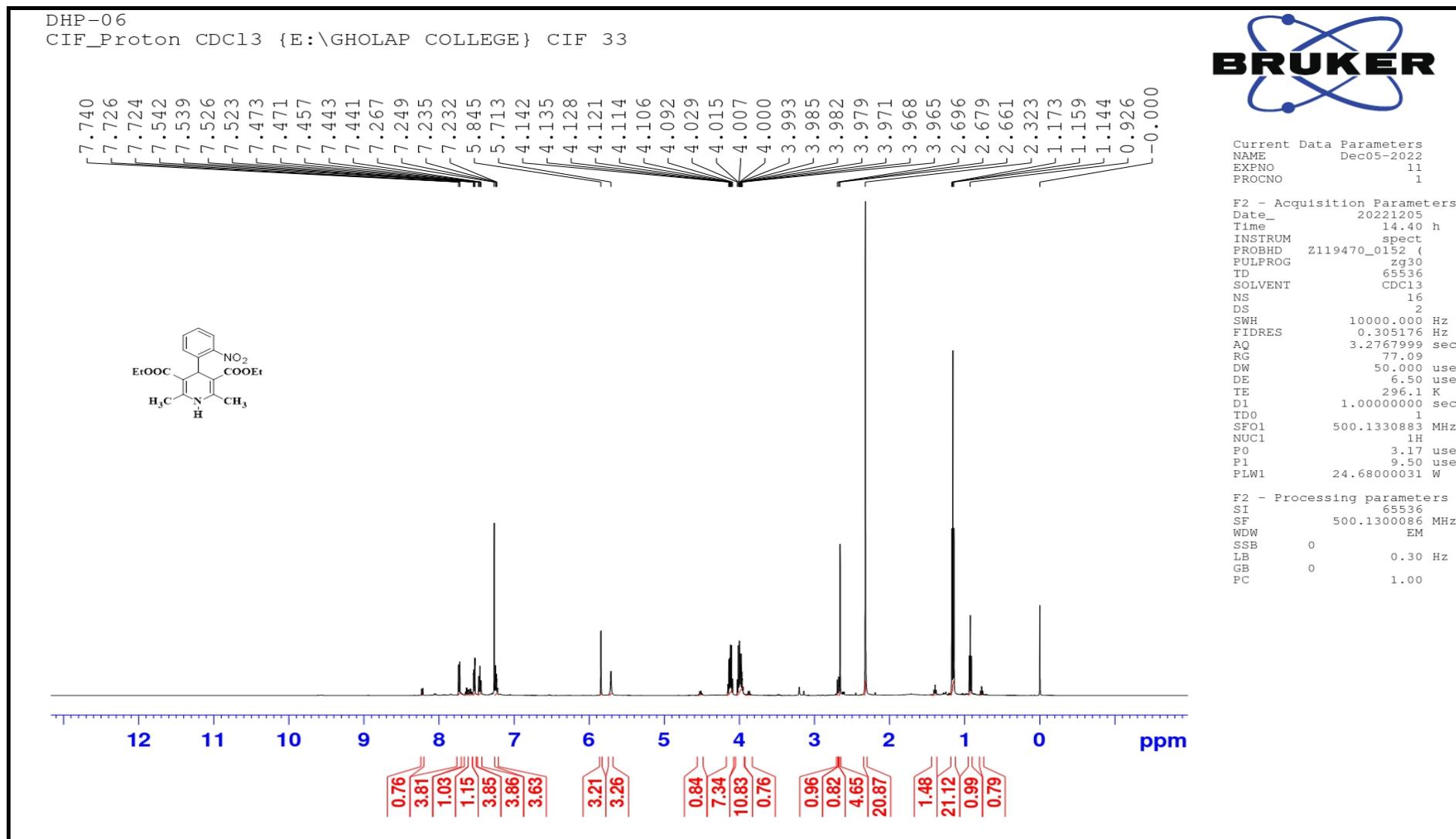
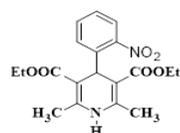


Figure S23:  $^{13}\text{C}$ -NMR spectrum of diethyl 2,6-dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate (**4m**)

DHP-06  
C13CPD CDC13 {E:\GHOLAP COLLEGE} CIF 33



167.241  
166.817  
156.960  
147.818  
147.700  
144.805  
144.449  
142.602  
132.984  
132.765  
132.367  
131.355  
130.886  
129.492  
126.937  
124.936  
124.345  
124.003  
104.018  
77.287  
77.238  
77.033  
76.778  
62.448  
61.422  
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34.686  
23.651  
23.143  
19.659  
14.144  
13.865  
13.588  
13.380  
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Current Data Parameters  
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EXPNO 12  
PROCNO 1

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PULPROG zgpg30  
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SOLVENT CDC13  
NS 1024  
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SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
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RG 189.76  
DW 16.800 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SF01 125.7703643 MHz  
NUC1 13C  
P0 3.08 usec  
P1 9.25 usec  
PLW1 100.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 80.00 usec  
PLM2 24.68000031 W  
PLM12 0.34803000 W  
PLM13 0.17505001 W

F2 - Processing parameters  
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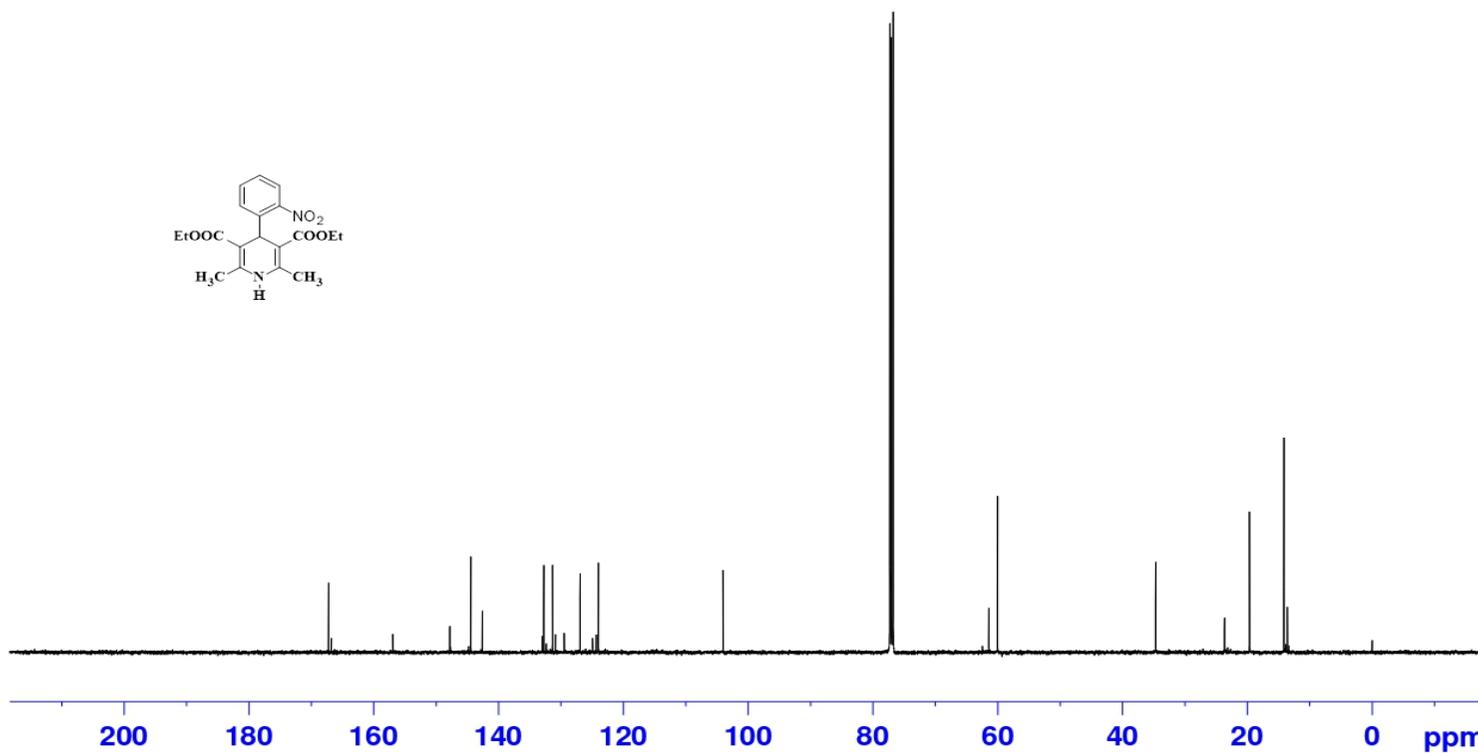


Figure S24: <sup>13</sup>C-NMR spectrum of diethyl 2,6-dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate (4m)

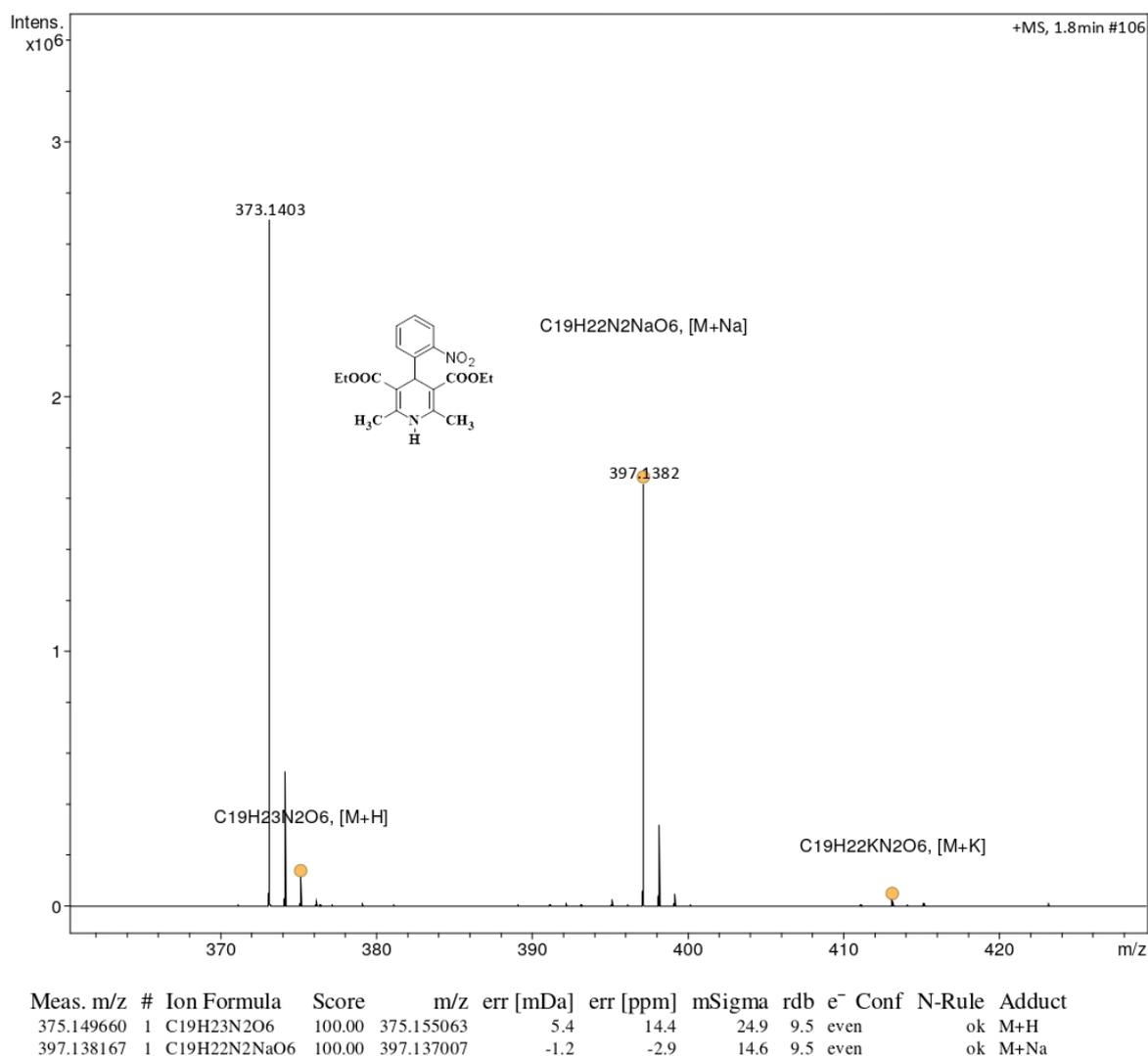
**Savitribai Phule Pune University - Central Instrumentation Facility**

**Analysis Info**

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 Sample Name: DHP-06  
 Operator: CIF  
 Instrument: impact HD  
 Comment: 1819696.00184

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
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Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



**Figure S25:** HRMS spectrum of diethyl 2,6-dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate (**4m**)

DHP-08  
CIF\_Proton CDC13 {E:\GHOLAP COLLEGE} CIF 34



Current Data Parameters  
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EXPNO 13  
PROCNO 1

F2 - Acquisition Parameters  
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SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.2767999 sec  
RG 88.03  
DW 50.000 usec  
DE 6.50 usec  
TE 296.2 K  
D1 1.00000000 sec  
TDO 1  
SFO1 500.1330883 MHz  
NUC1 1H  
P0 3.17 usec  
P1 9.50 usec  
PLW1 24.68000031 W

F2 - Processing parameters  
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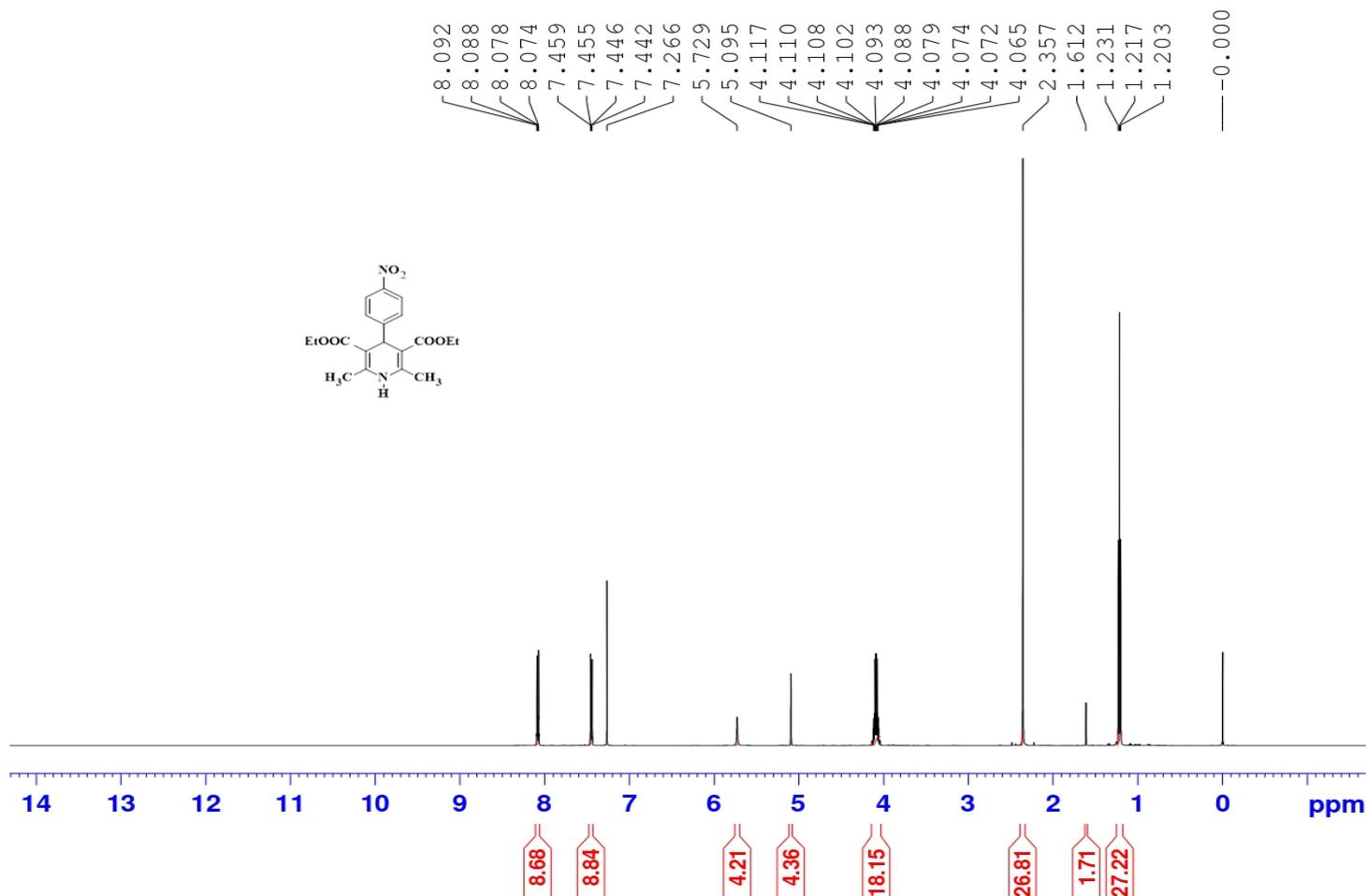
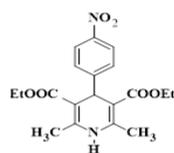


Figure S26: <sup>1</sup>H-NMR spectrum of diethyl 2,6-dimethyl-4-(4-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate (**4n**)

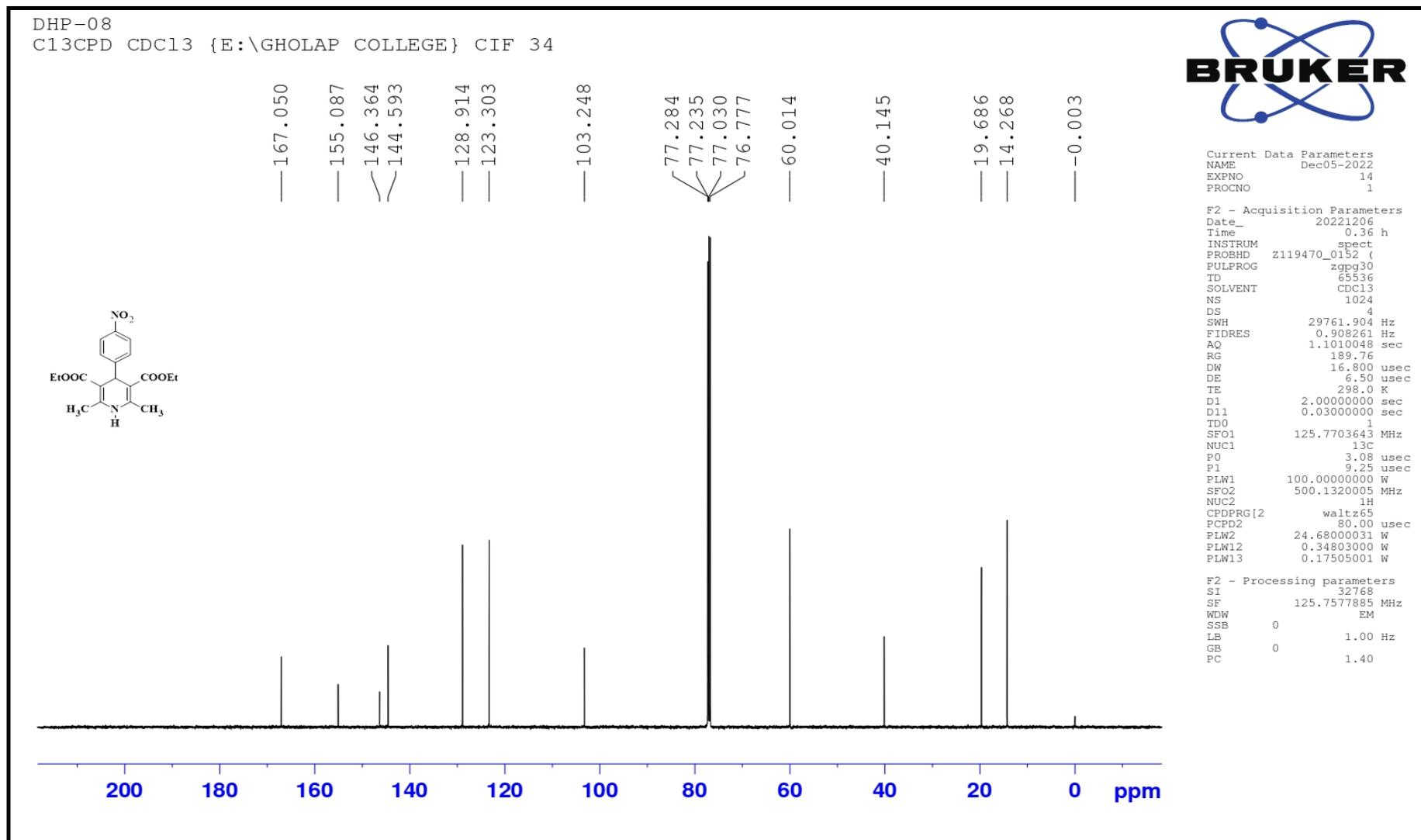


Figure S27: <sup>13</sup>C-NMR spectrum of diethyl 2,6-dimethyl-4-(4-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate (**4n**)

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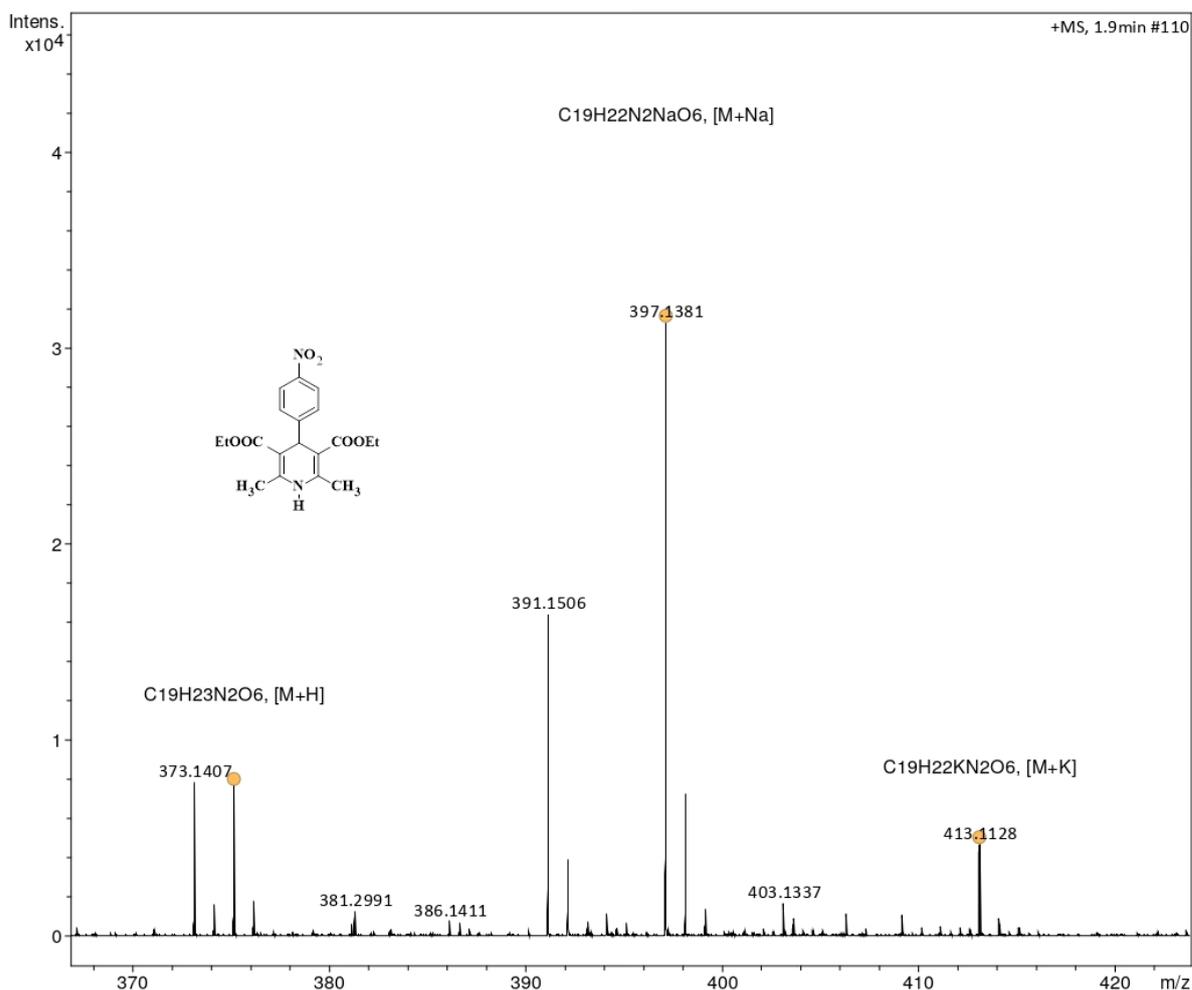
Analysis Info

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 Sample Name DHP-08  
 Comment

Acquisition Date 12/23/2022 5:19:11 PM  
 Operator CIF  
 Instrument impact HD 1819696.00184

Acquisition Parameter

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Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup>	Conf	N-Rule	Adduct
375.156001	1	C <sub>19</sub> H <sub>23</sub> N <sub>2</sub> O <sub>6</sub>	100.00	375.155063	-0.9	-2.5	12.2	9.5	even	ok	M+H
397.138103	1	C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> NaO <sub>6</sub>	100.00	397.137007	-1.1	-2.8	9.8	9.5	even	ok	M+Na

Figure S28: HRMS spectrum of diethyl 2,6-dimethyl-4-(4-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate (4n)

## Characterization of DBUHI<sub>3</sub>

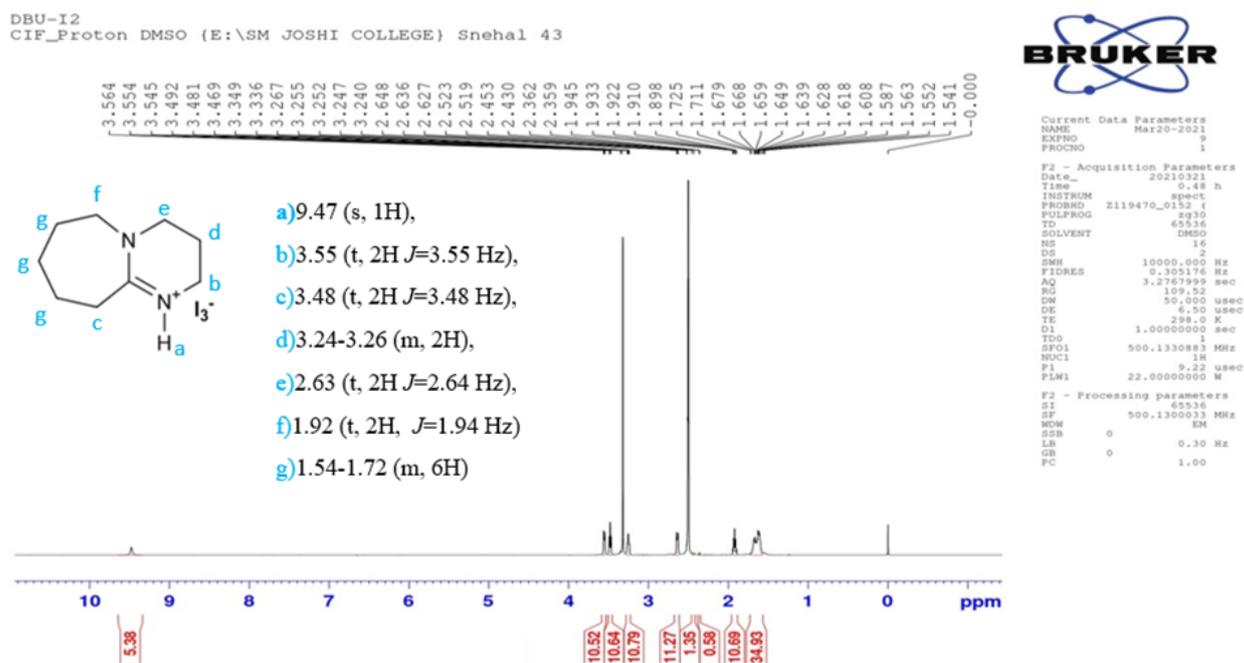


Figure S29: <sup>1</sup>H-NMR spectrum of DBUHI<sub>3</sub> complex

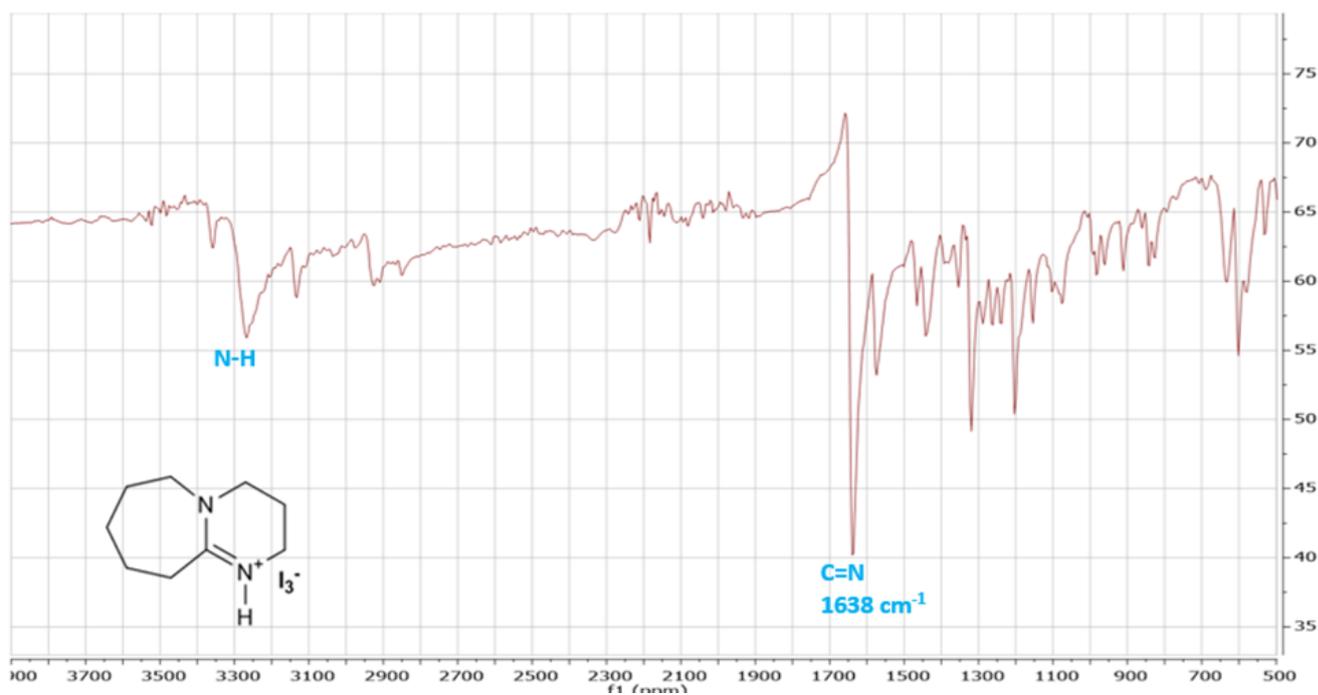


Figure S30: IR spectrum of DBUHI<sub>3</sub> complex

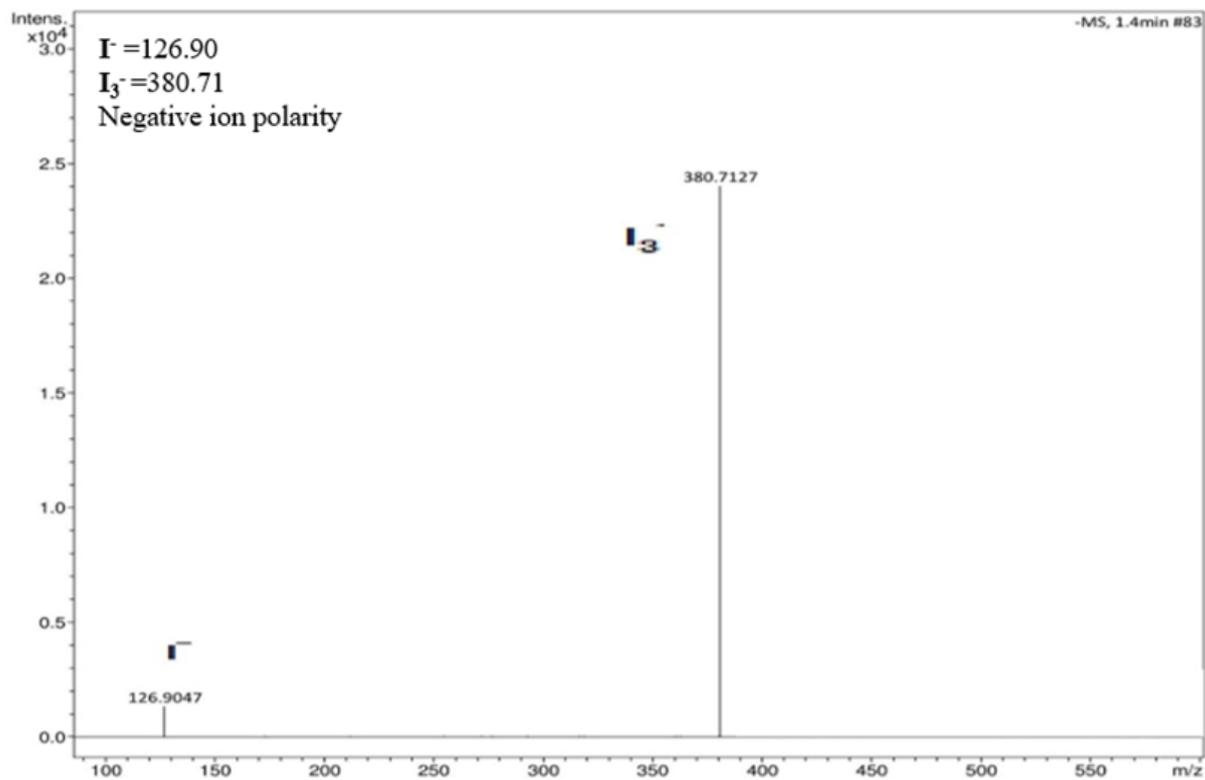
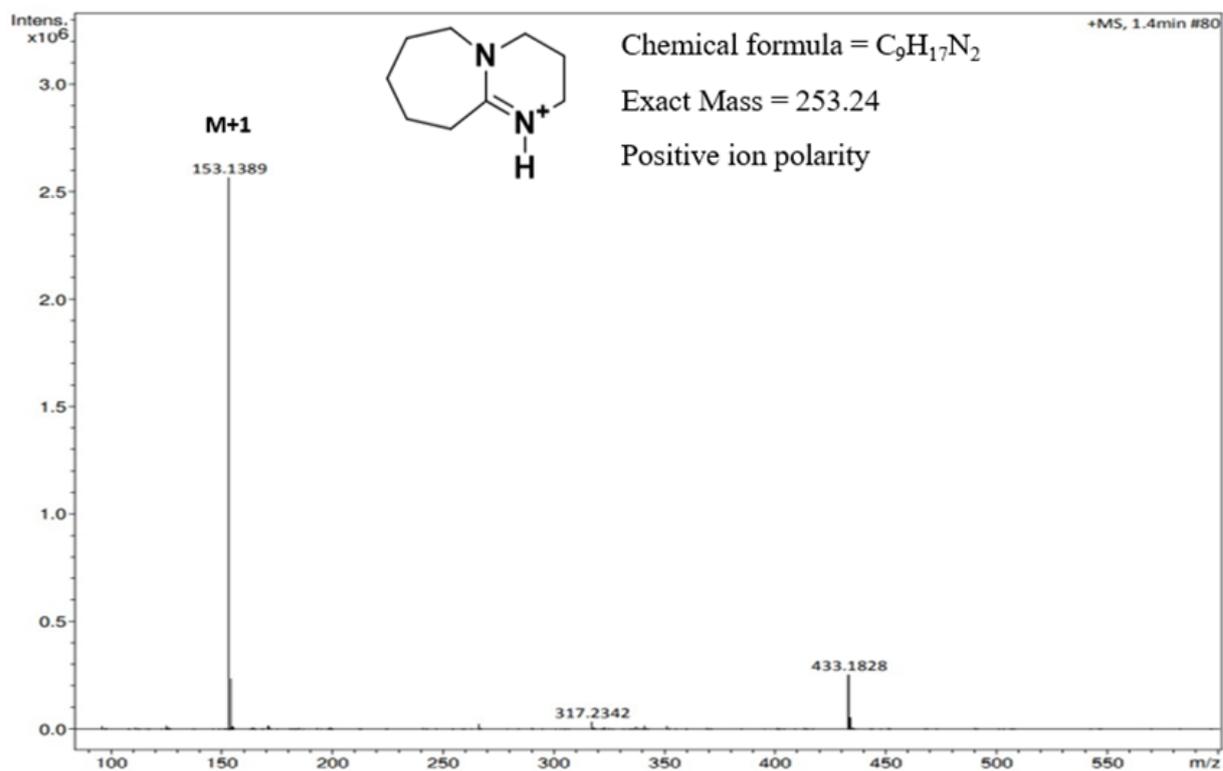
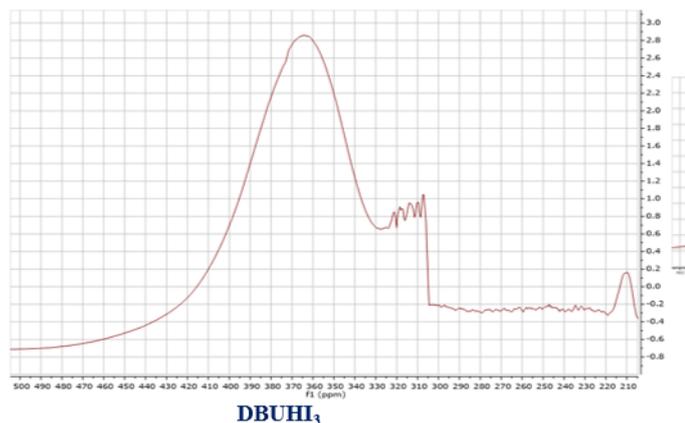


Figure S31: HRMS spectrum of DBUHI<sub>3</sub> complex

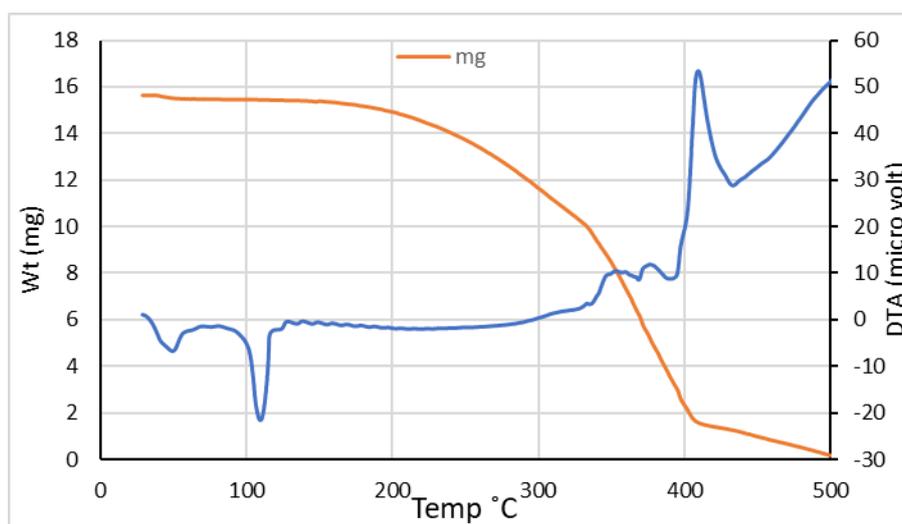


**Figure S32:** UV-Visible Spectrum of DBUHI<sub>3</sub> complex

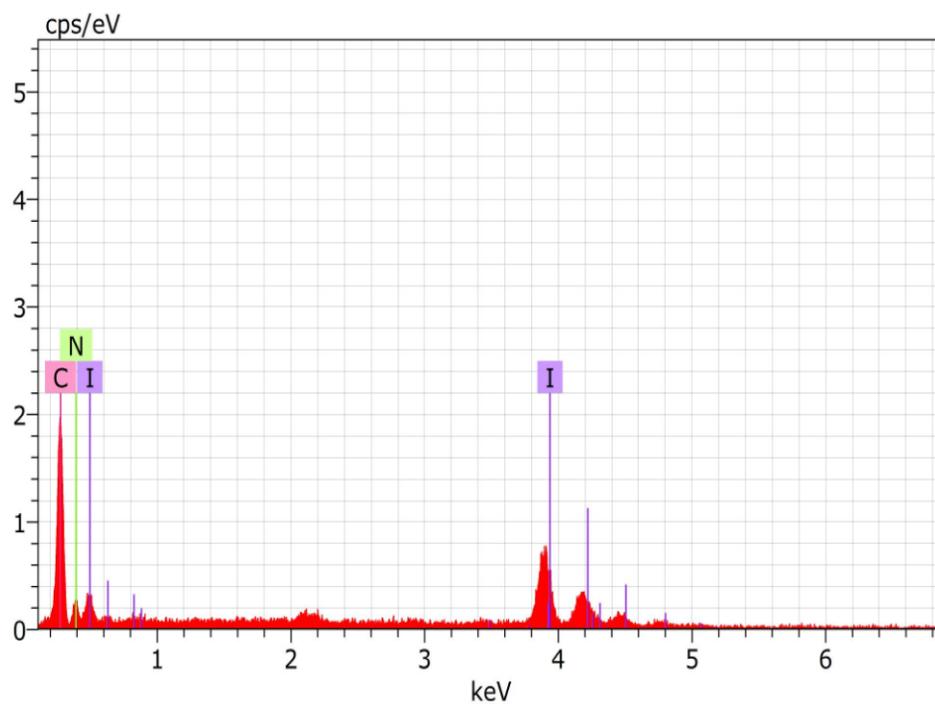
**Table S1:** Elemental analysis of DBUHI<sub>3</sub> complex (C, H, N, I, (O) Element Analysis of Amine-iodine complexes)

**1a. DBUH Iodine Complex**

Element	No. of At.	Mol wt.	% Theor.	%Pract.
C	9	12.01	20.24	20.31
H	17	1.0079	3.20	3.46
N	2	14.01	5.24	5.51
I	3	126.91	71.30	70.72



**Figure S33:** TGA-DTA Graph of DBUHI<sub>3</sub> complex



**Figure S34:** Field Emission Scanning Electron Microscopy Energy Dispersive X-ray Spectroscopy (FESEM - EDX)