

Supplementary data for the article:

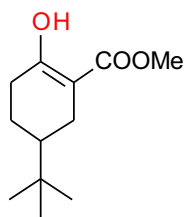
Popović-Djordjević, J.; Stepanović, S.; Došen-Mićović, L.; Ivanović, E.; Ivanović, M. D. High-Yielding Method for Preparation of Carbocyclic or N-Containing Heterocyclic β -Keto Esters Using in Situ Activated Sodium Hydride in Dimethyl Sulphoxide. *Green Chemistry Letters and Reviews* **2016**, *9* (1), 61–68. <https://doi.org/10.1080/17518253.2016.1145744>

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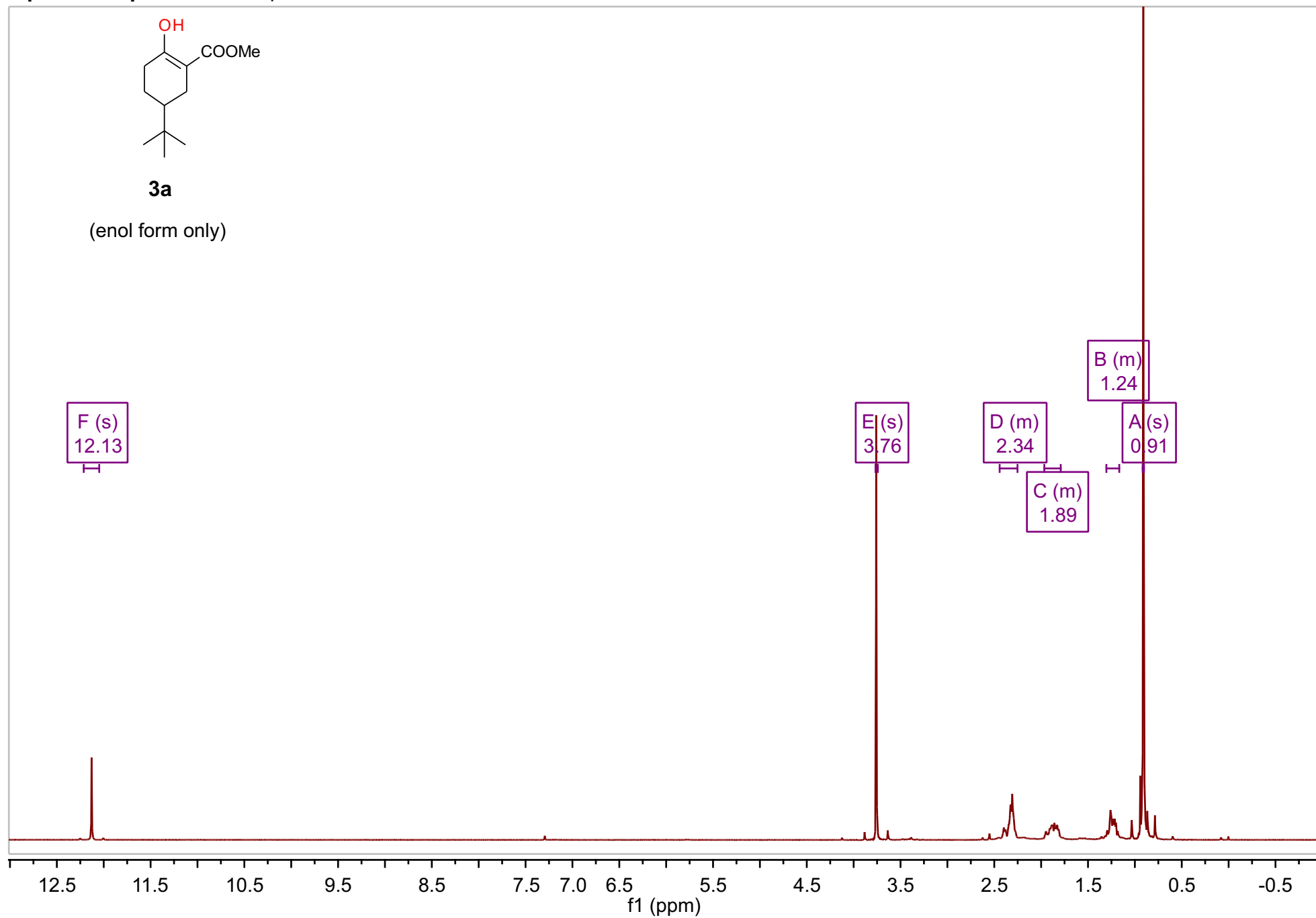
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Spectroscopic data. Compound 3a ¹H NMR

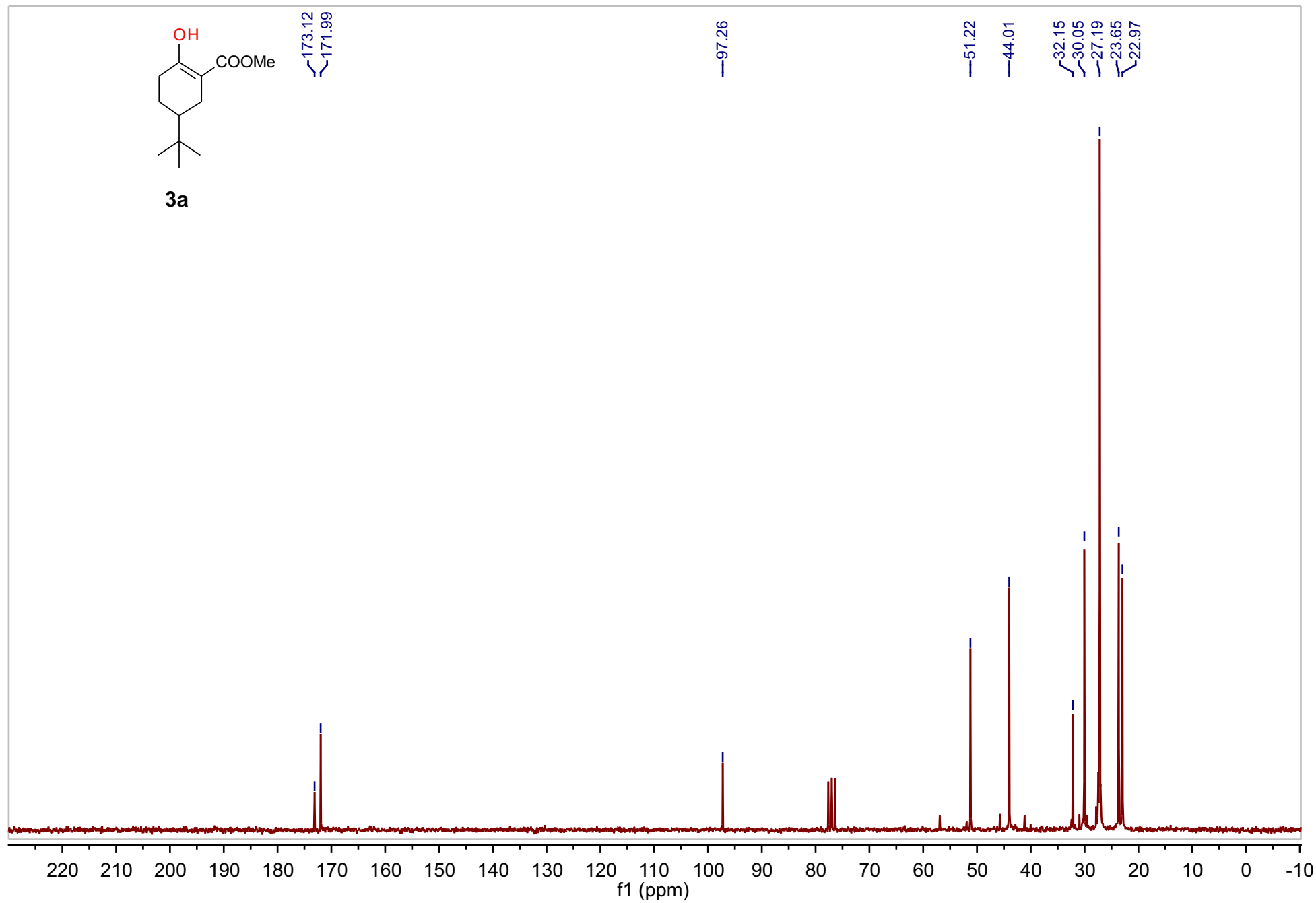


3a

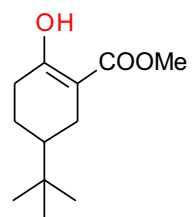
(enol form only)



Spectroscopic data. Compound **3a** ^{13}C NMR

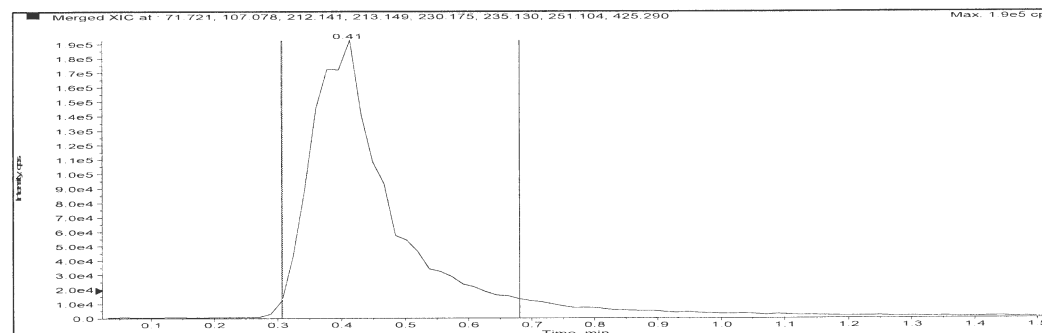


Spectroscopic data. Compound 3a HRMS

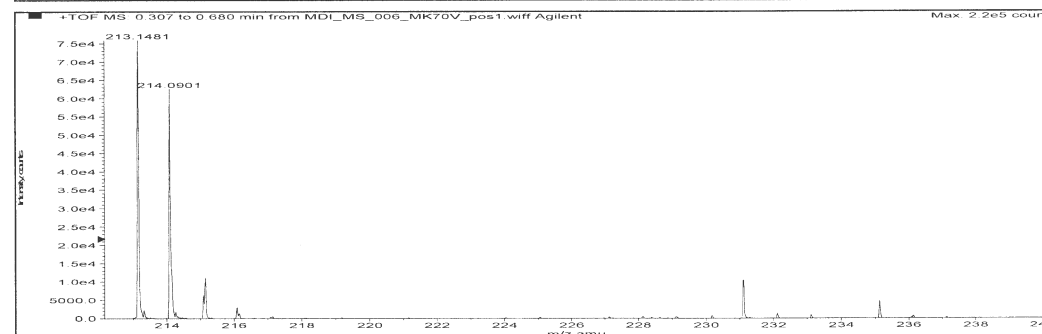
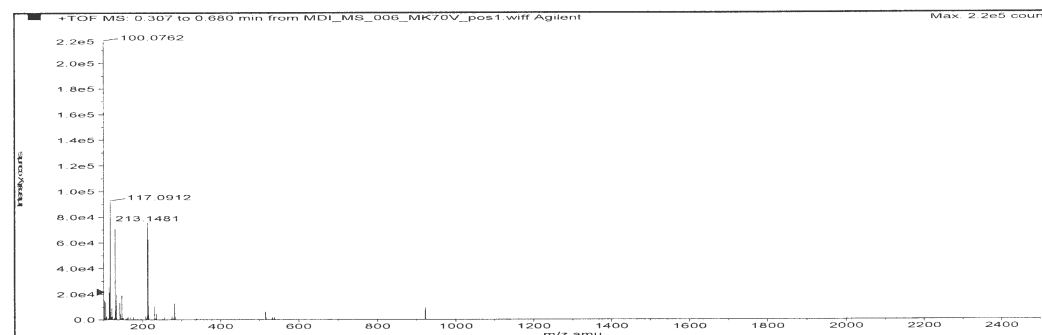


3a

Sample Name: MDI_MS_006 Sample Location: P1-E2 Sample Id: Operator: Milka
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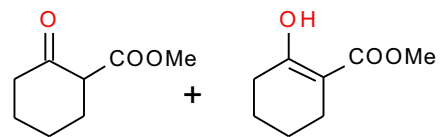
Merged XIC, Period# : 1 Experiment# : 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C12H20O3	--	212.14124	0.41	1.67179 E6	--

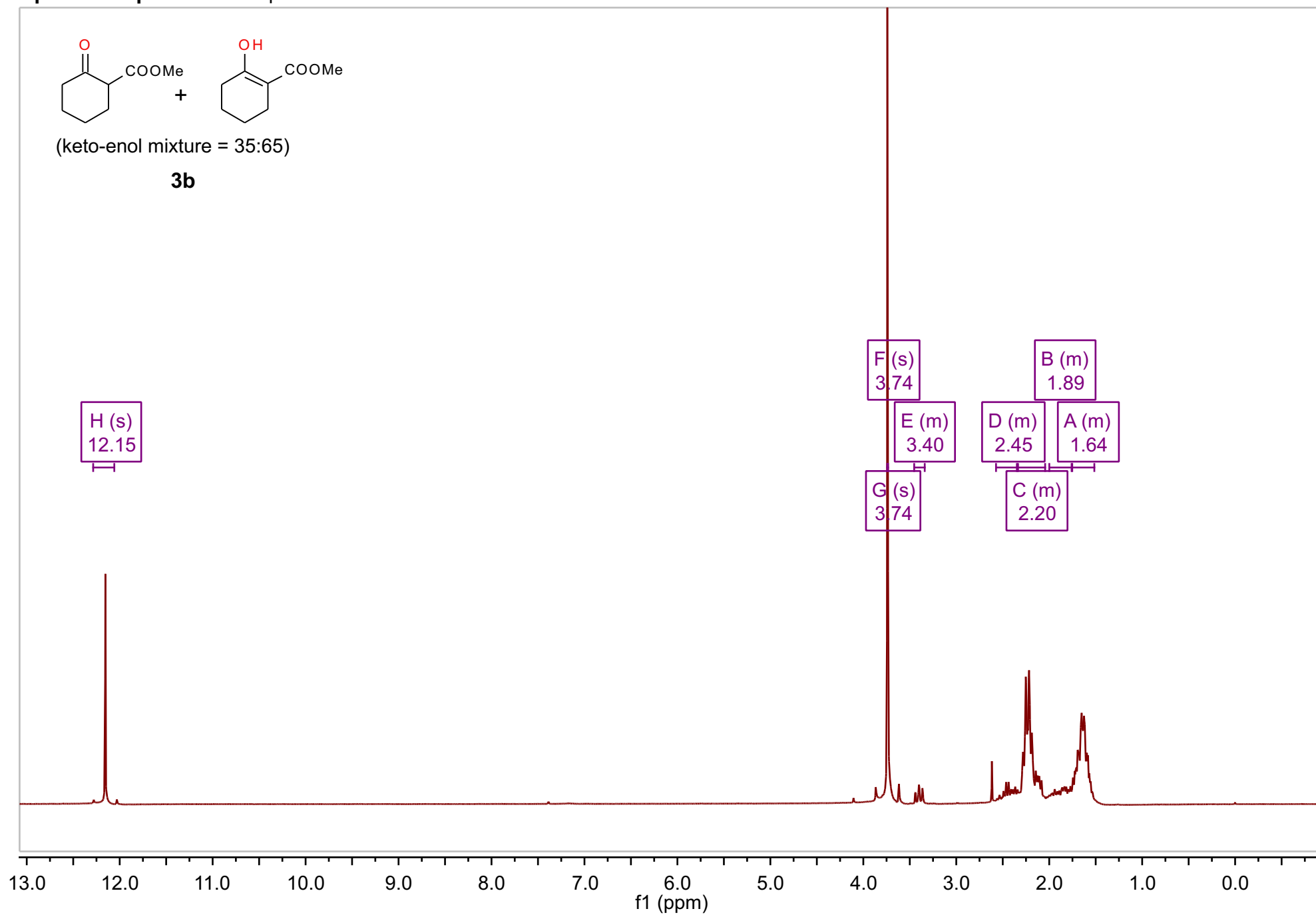
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	77555.37	213.14852	213.14814	-0.38593	-1.81	--
[M+Na] ⁺	4713.84	235.13047	235.13028	-0.18425	-0.78	--

Spectroscopic data. Compound **3b** ^1H NMR

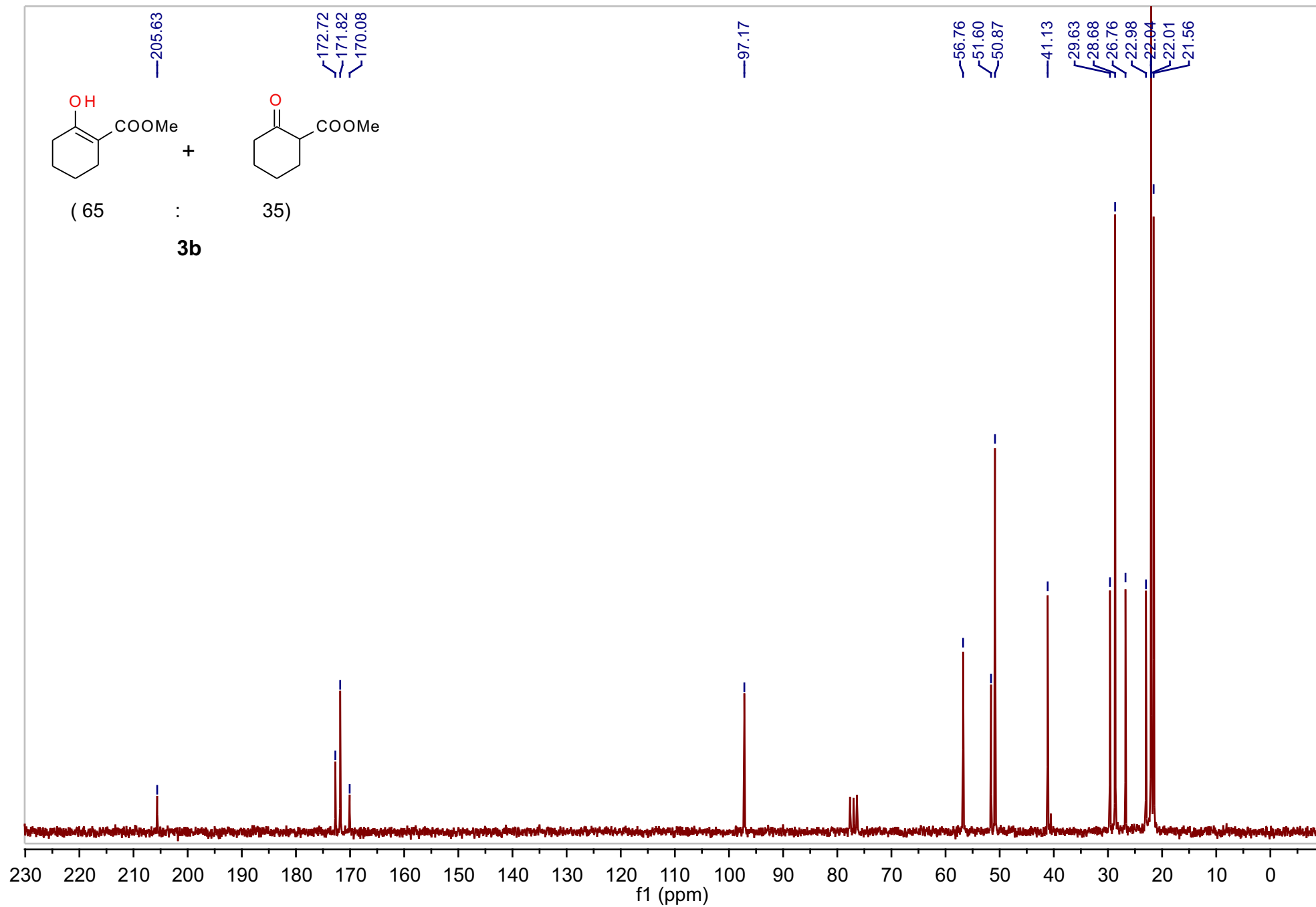


(keto-enol mixture = 35:65)

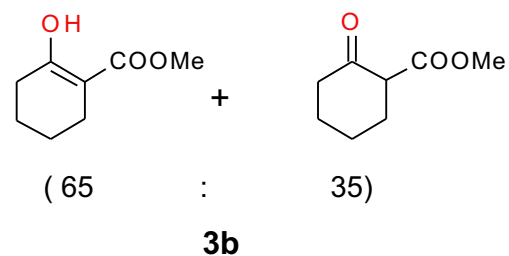
3b



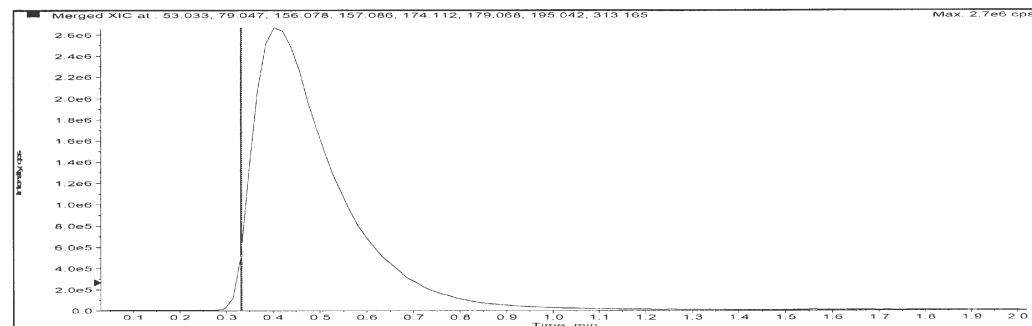
Spectroscopic data. Compound **3b** ¹³C NMR



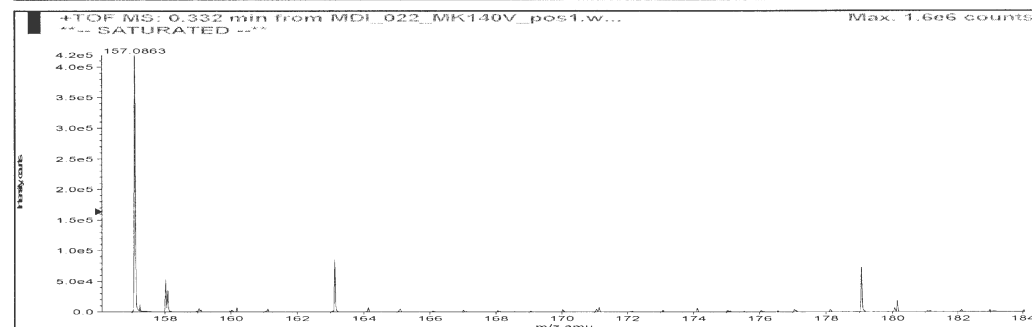
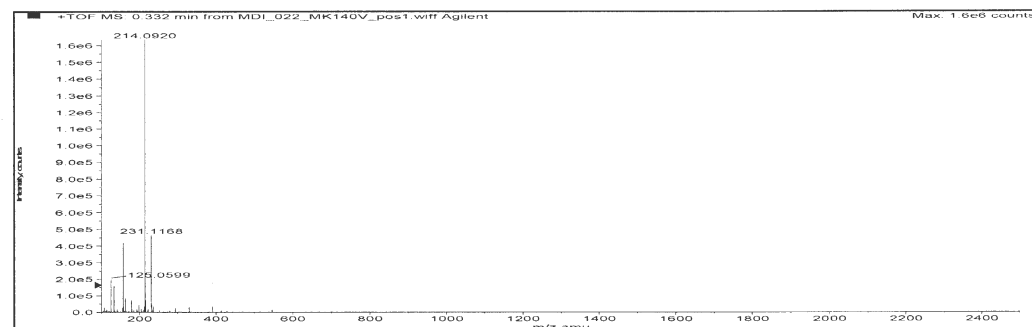
Spectroscopic data. Compound **3b** HRMS



Sample Name: MDI_022 Sample Location: P1-F2 Sample Id: Operator: Milka
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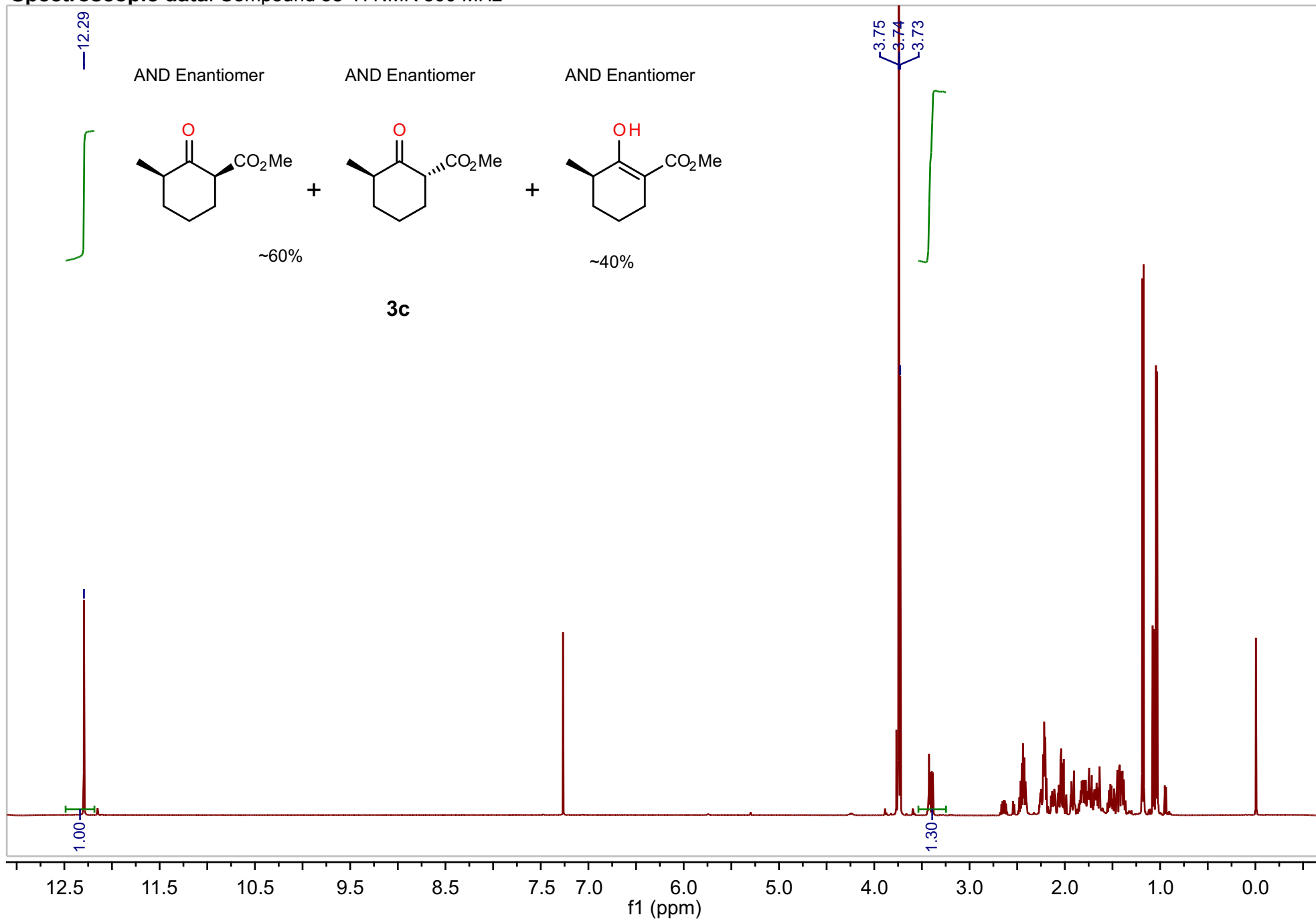
Merged XIC, Period# : 1 Experiment# : 1



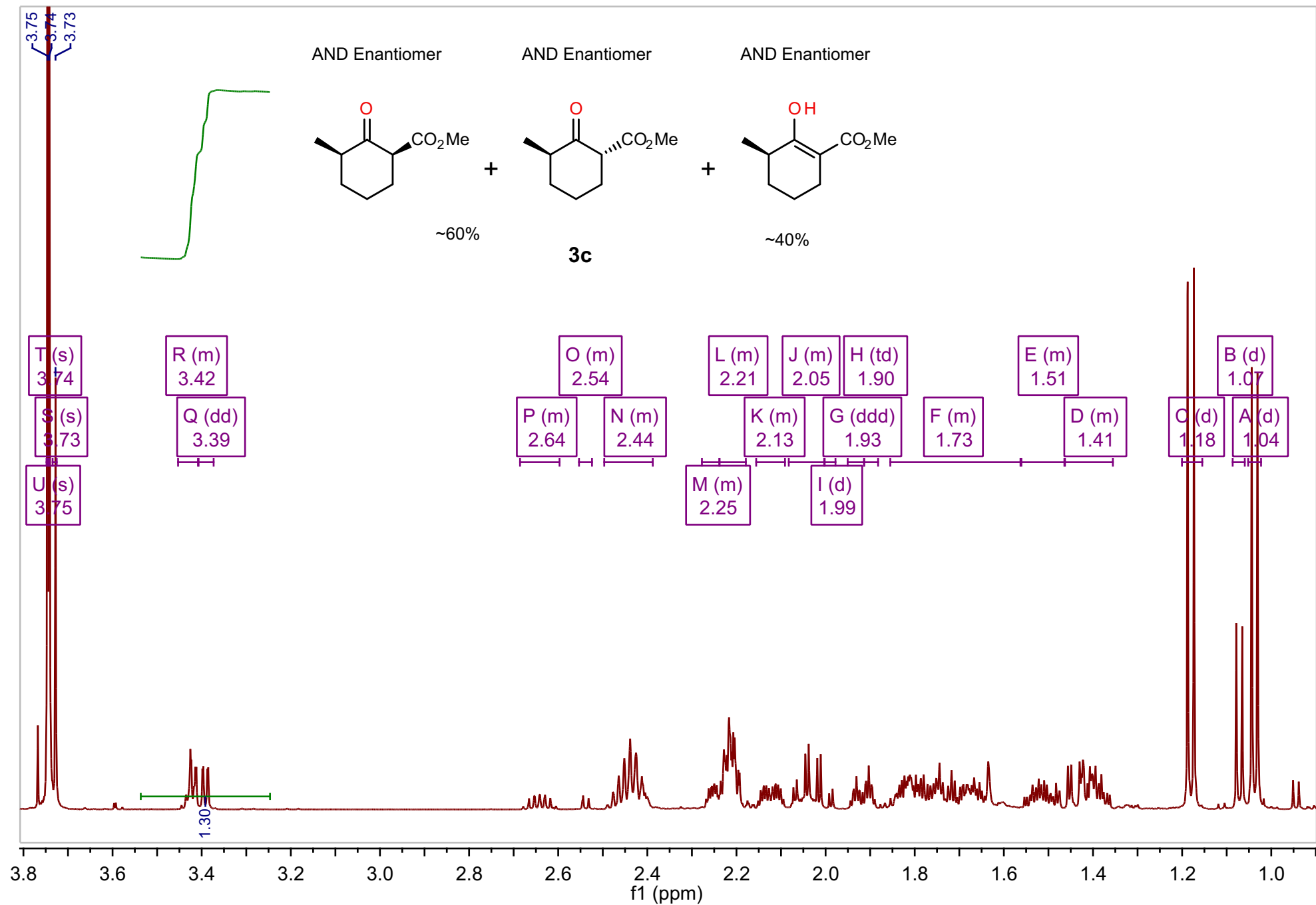
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C8H12O3	--	156.07864	0.41	3.19480 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	451040.43	157.08592	157.08626	0.34315	2.18	--
[M+Na] ⁺	75006.25	179.06787	179.06832	0.45637	2.55	--

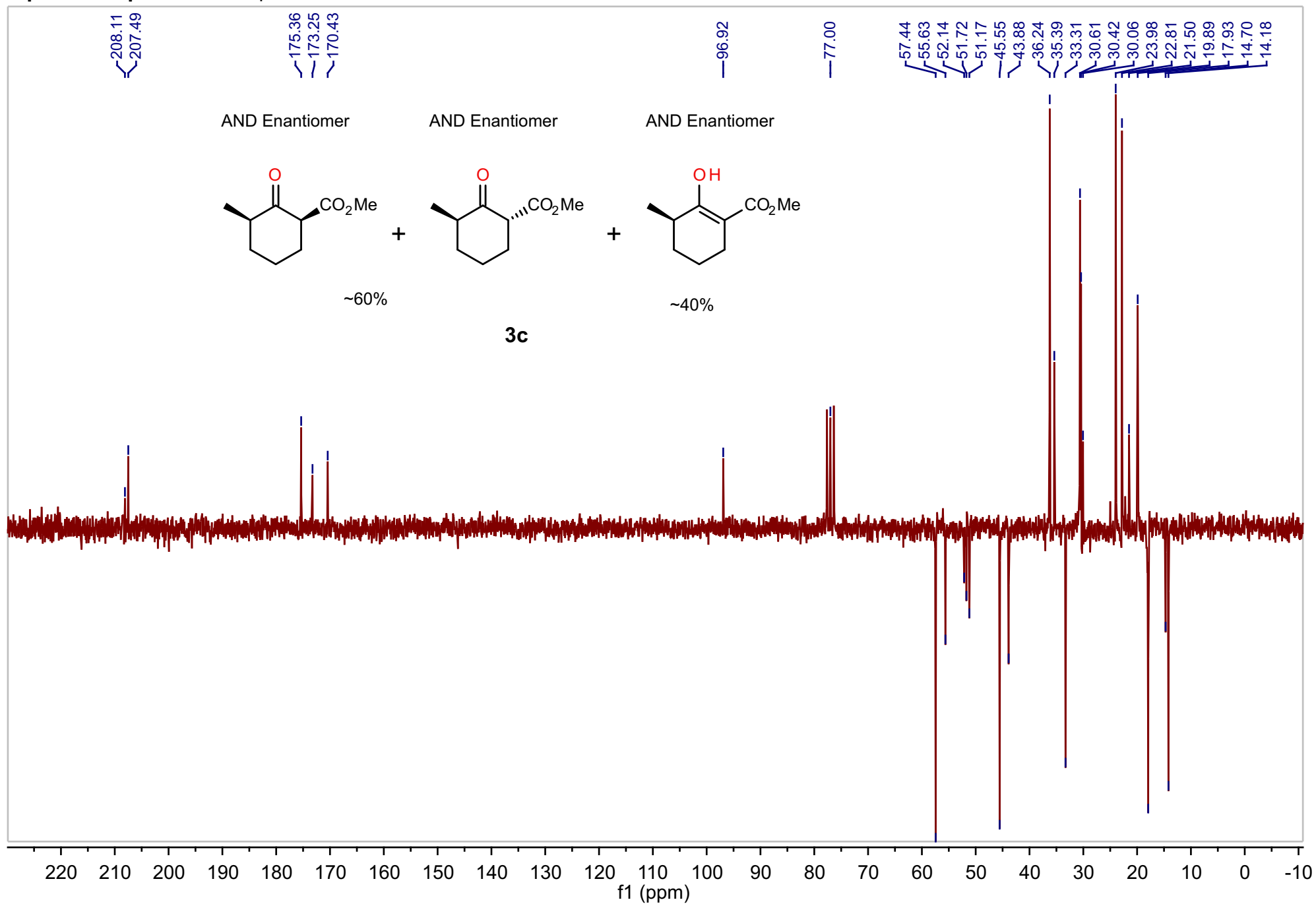
Spectroscopic data. Compound **3c** ^1H NMR 500 MHz



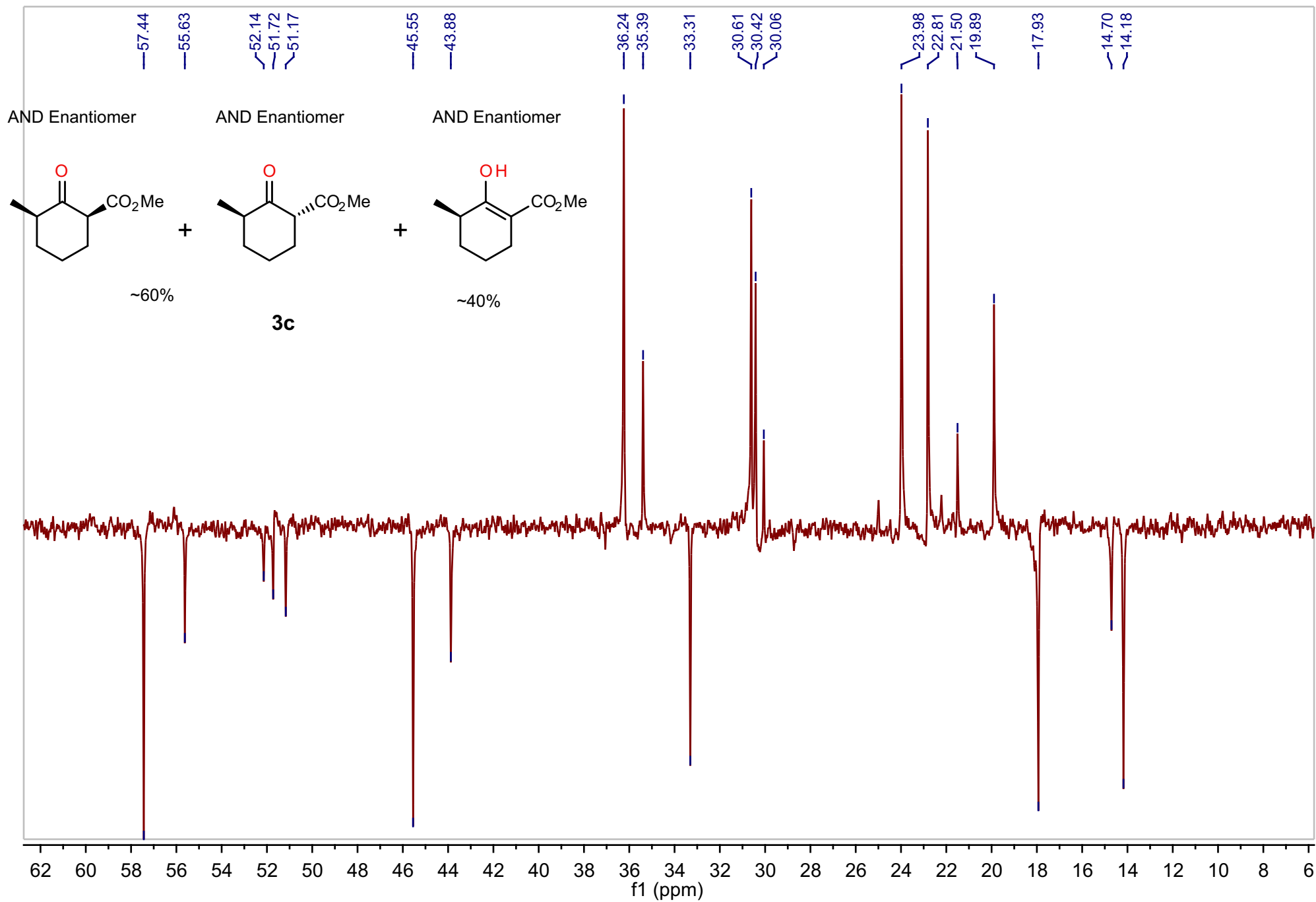
Spectroscopic data. Compound **3c** ¹H NMR 500 MHz, expanded



Spectroscopic data. Compound **3c** APT NMR

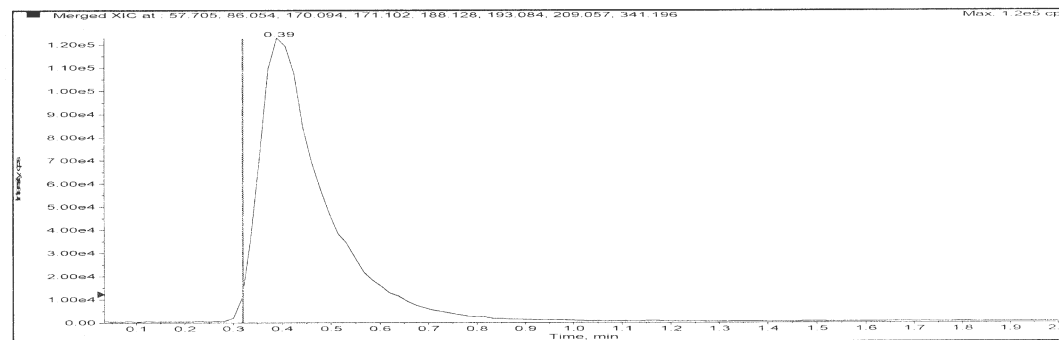
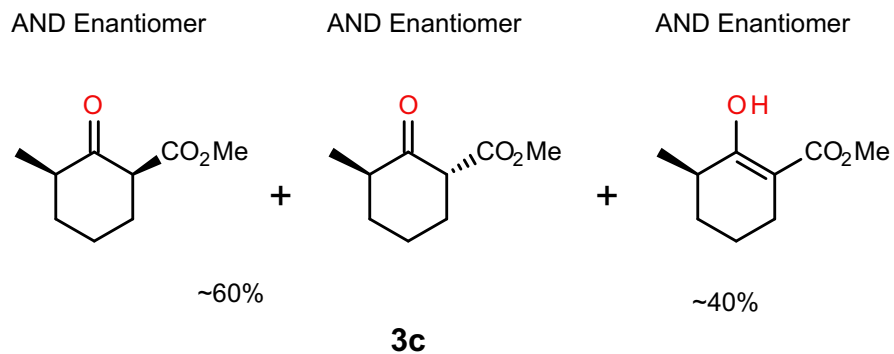


Spectroscopic data. Compound 3c APT NMR expanded

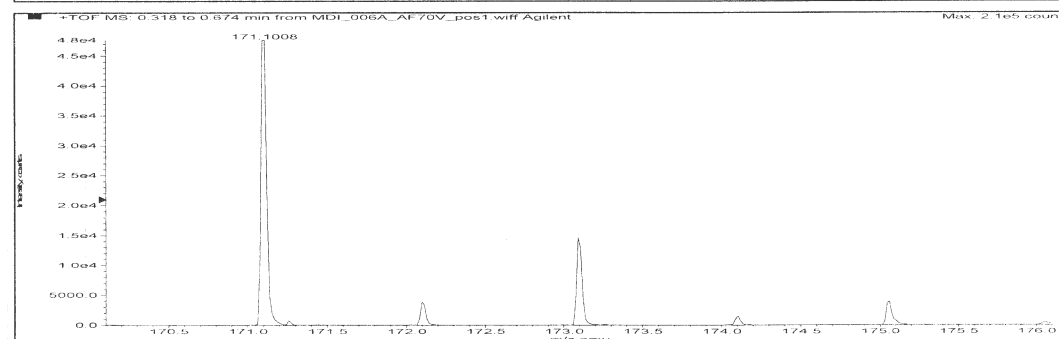
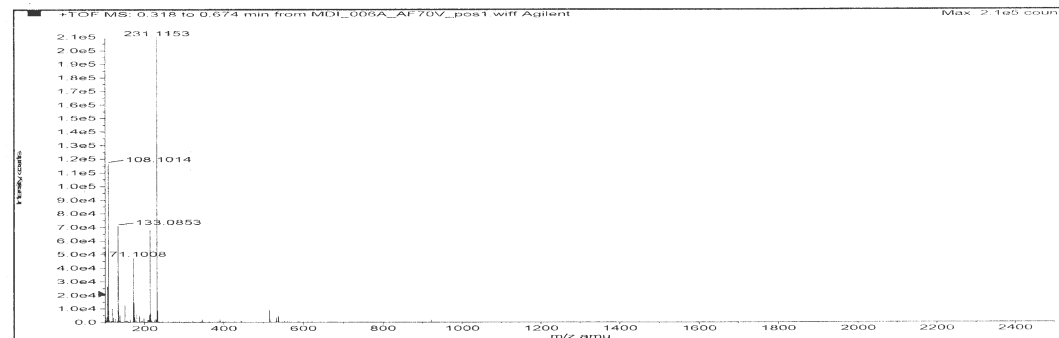


Spectroscopic data. Compound 3c HRMS

Sample Name: MDI_006A Sample Location: P1-C7 Sample Id: Operator: Milka
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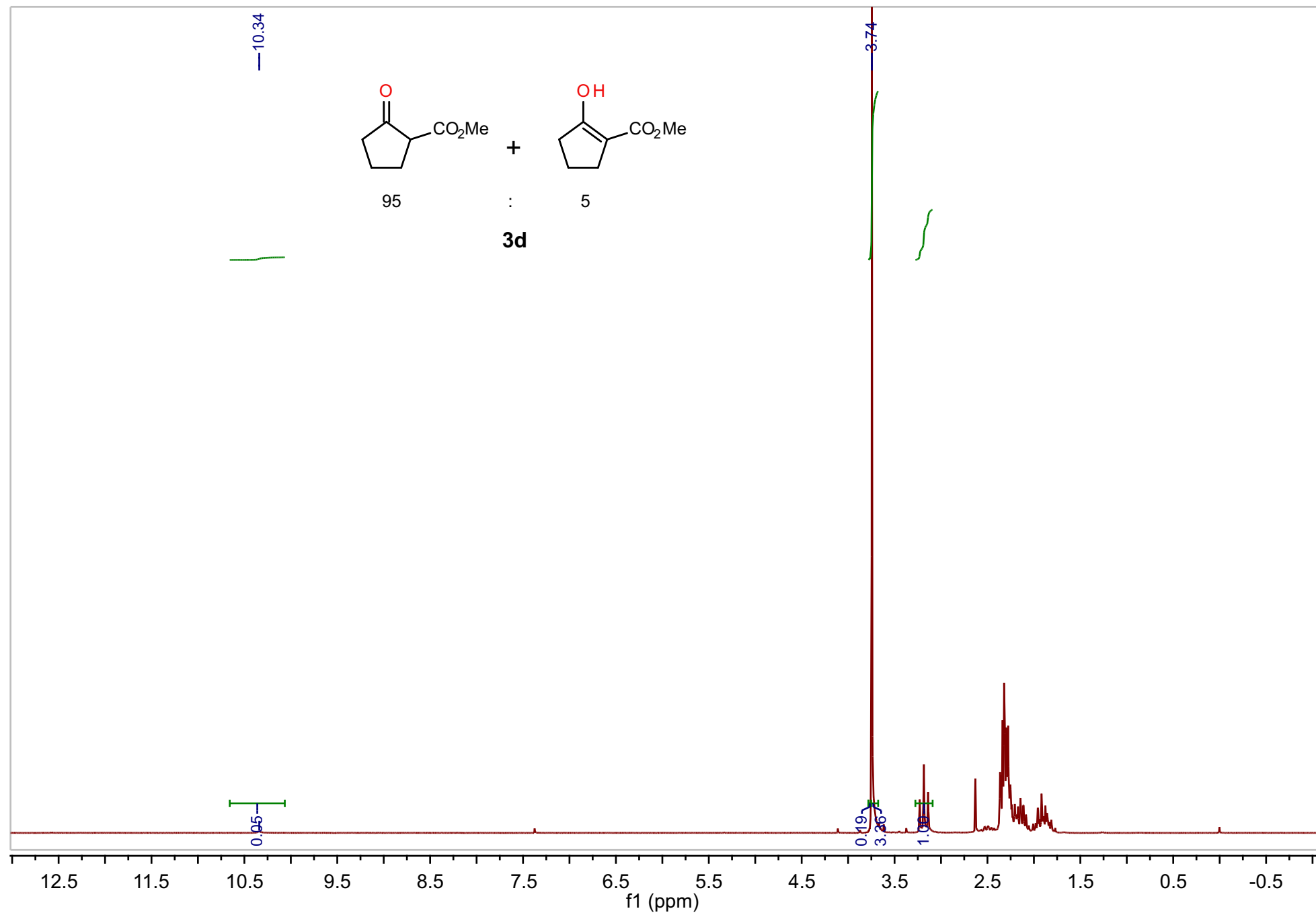
Merged XIC, Period# : 1 Experiment# : 1



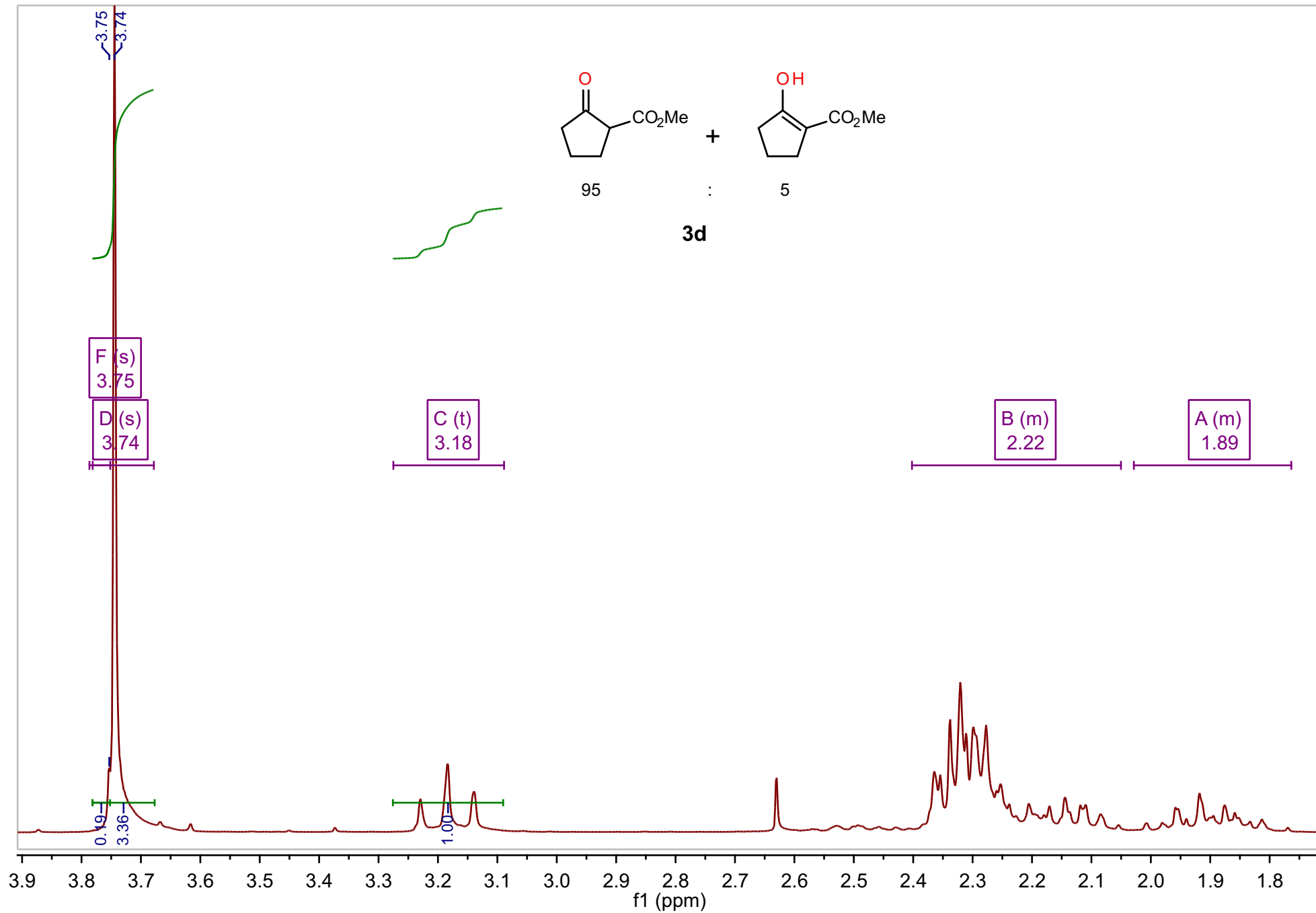
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C9H14O3	--	170.09429	0.39	1.11987 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	51122.82	171.10157	171.10077	-0.79577	-4.65	--

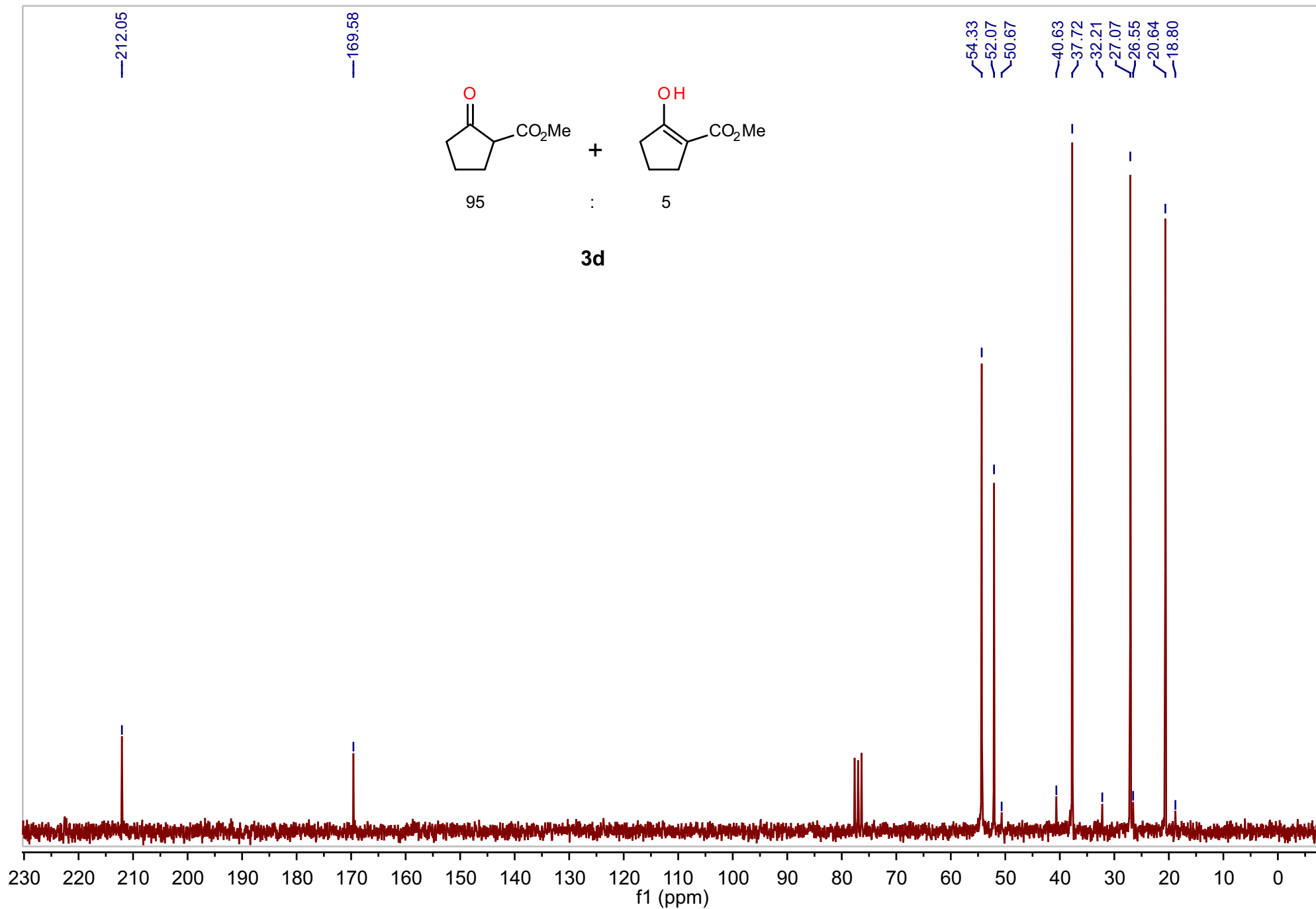
Spectroscopic data. Compound **3d** ^1H NMR



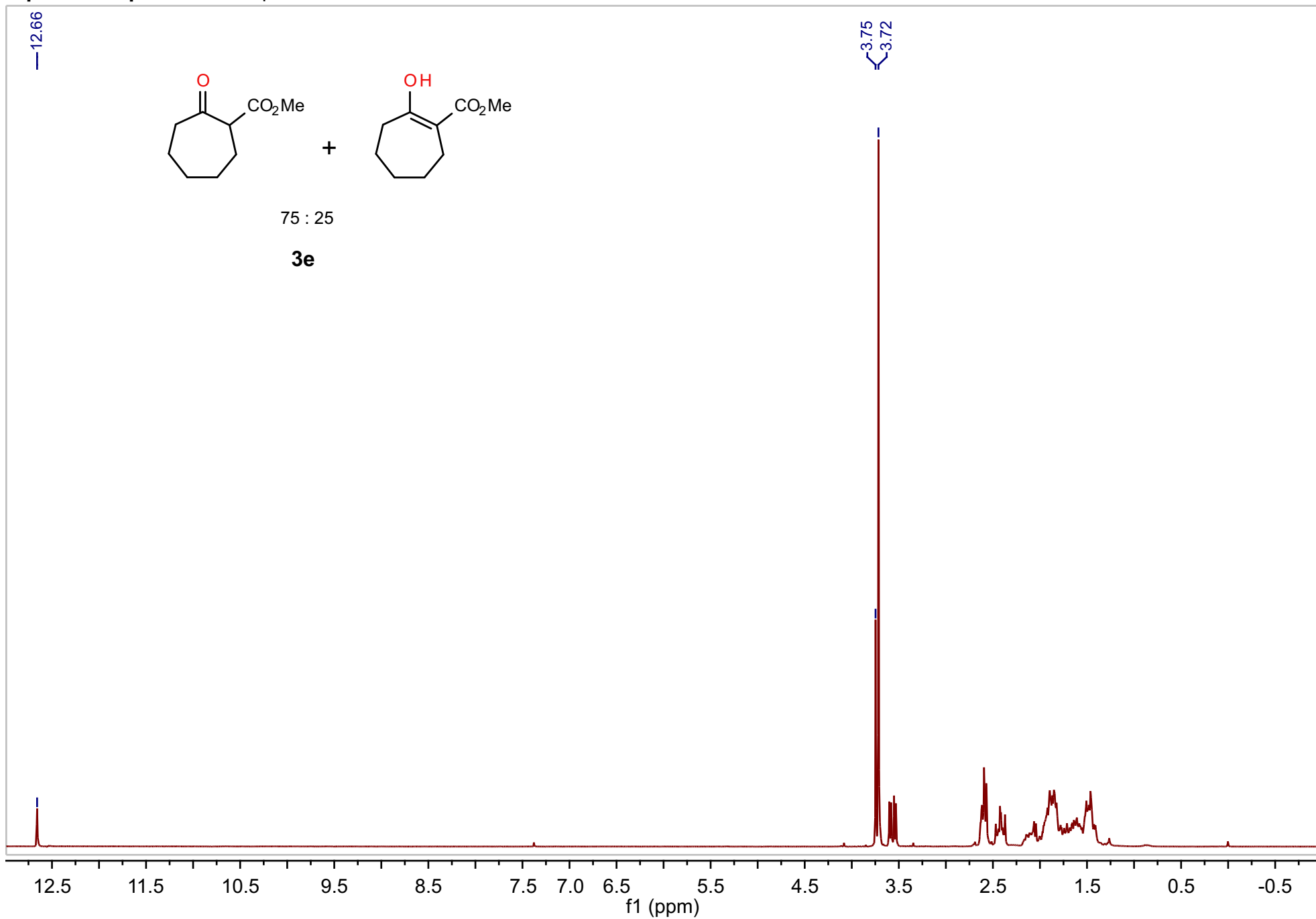
Spectroscopic data. Compound **3d** ^1H NMR expanded



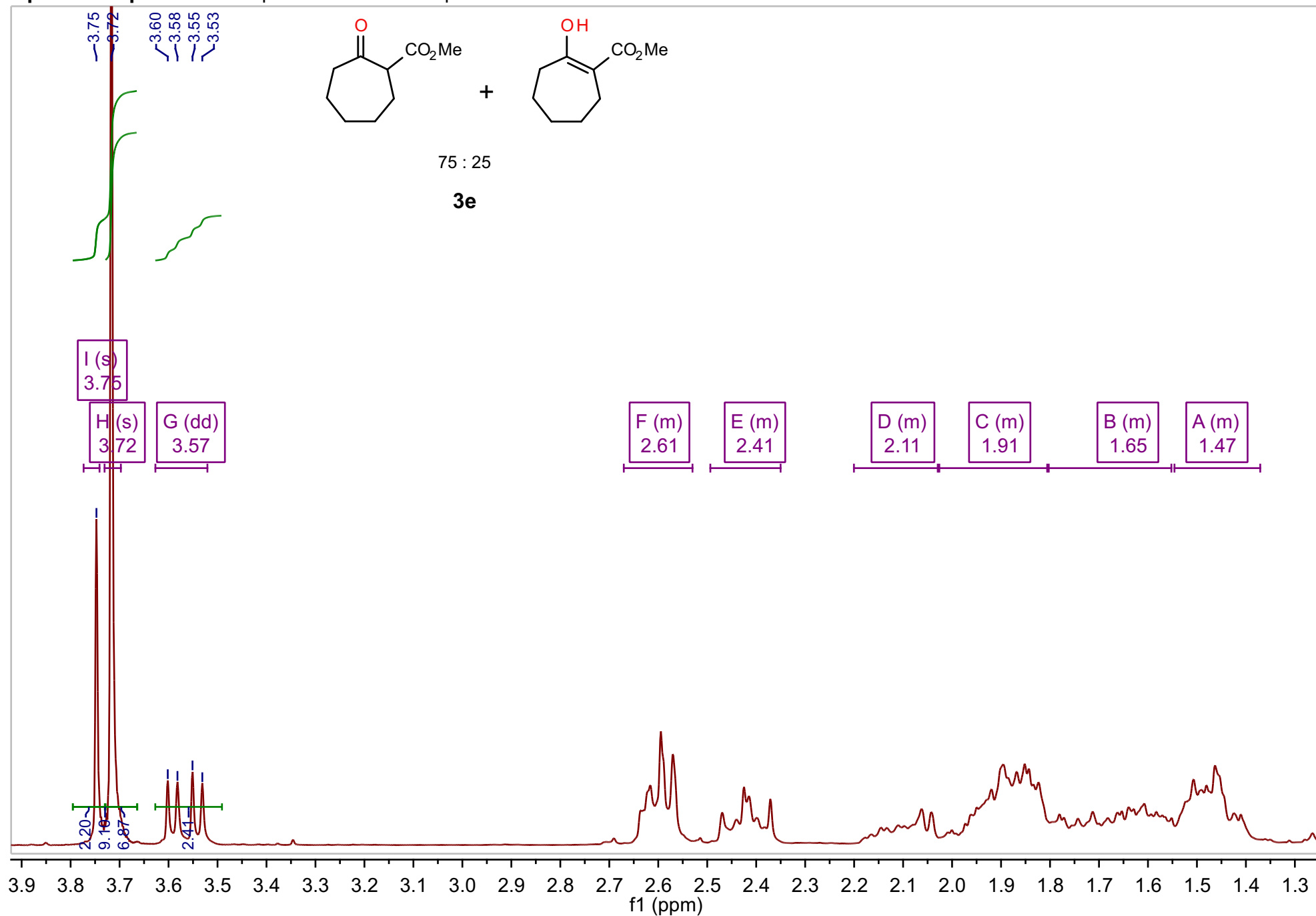
Spectroscopic data. Compound **3d** ^{13}C NMR



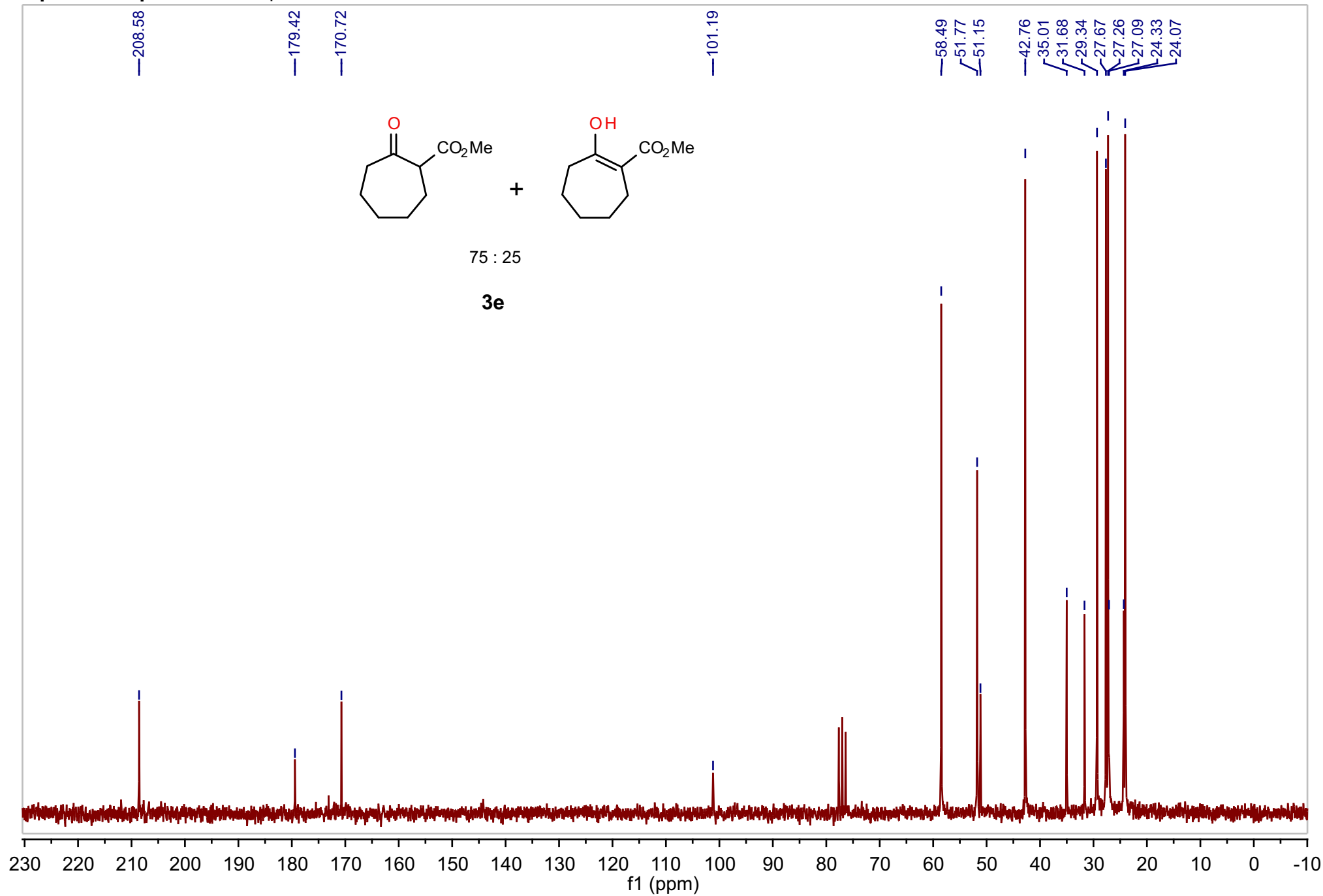
Spectroscopic data. Compound **3e** ^1H NMR



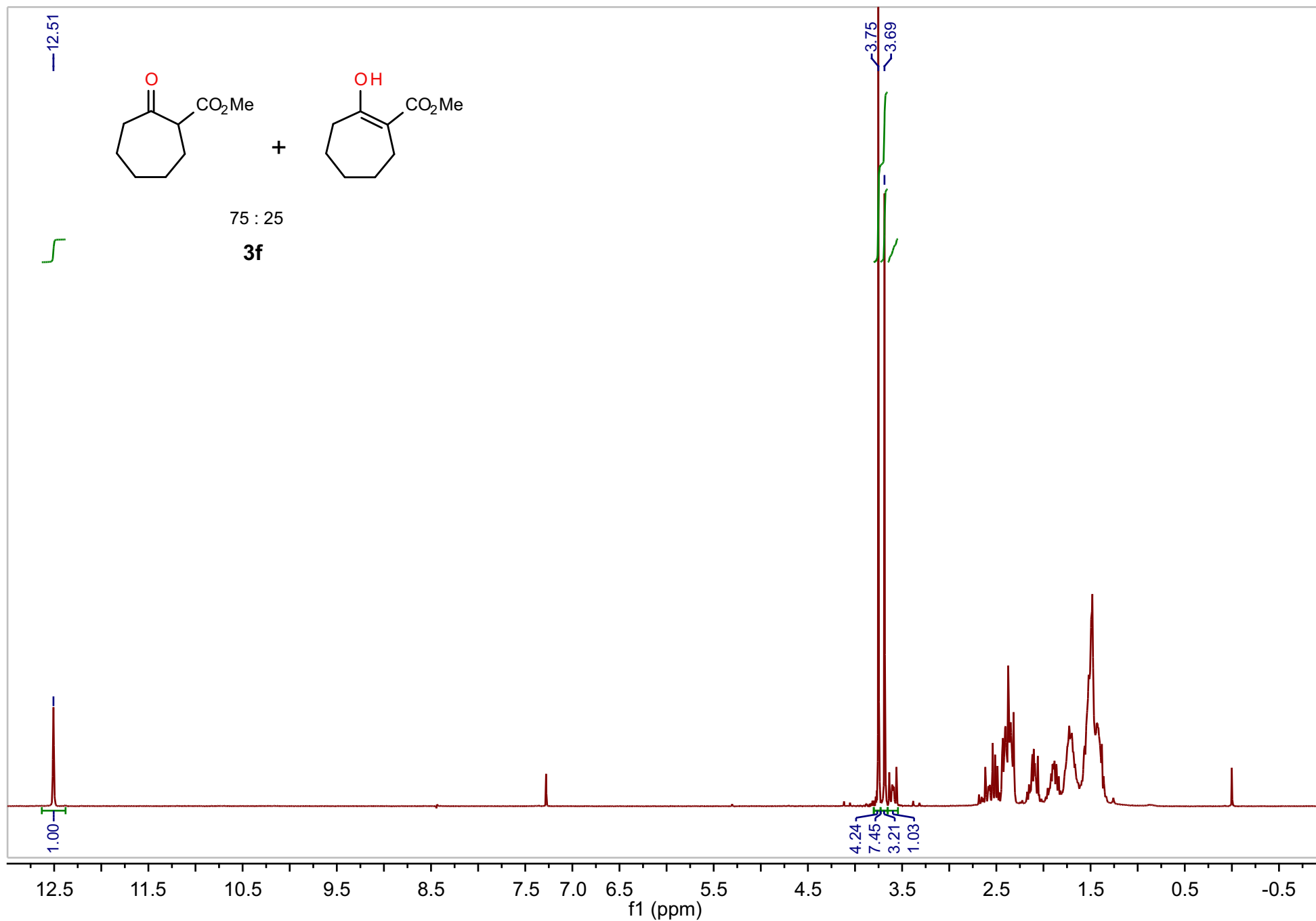
Spectroscopic data. Compound **3e** ¹H NMR expanded



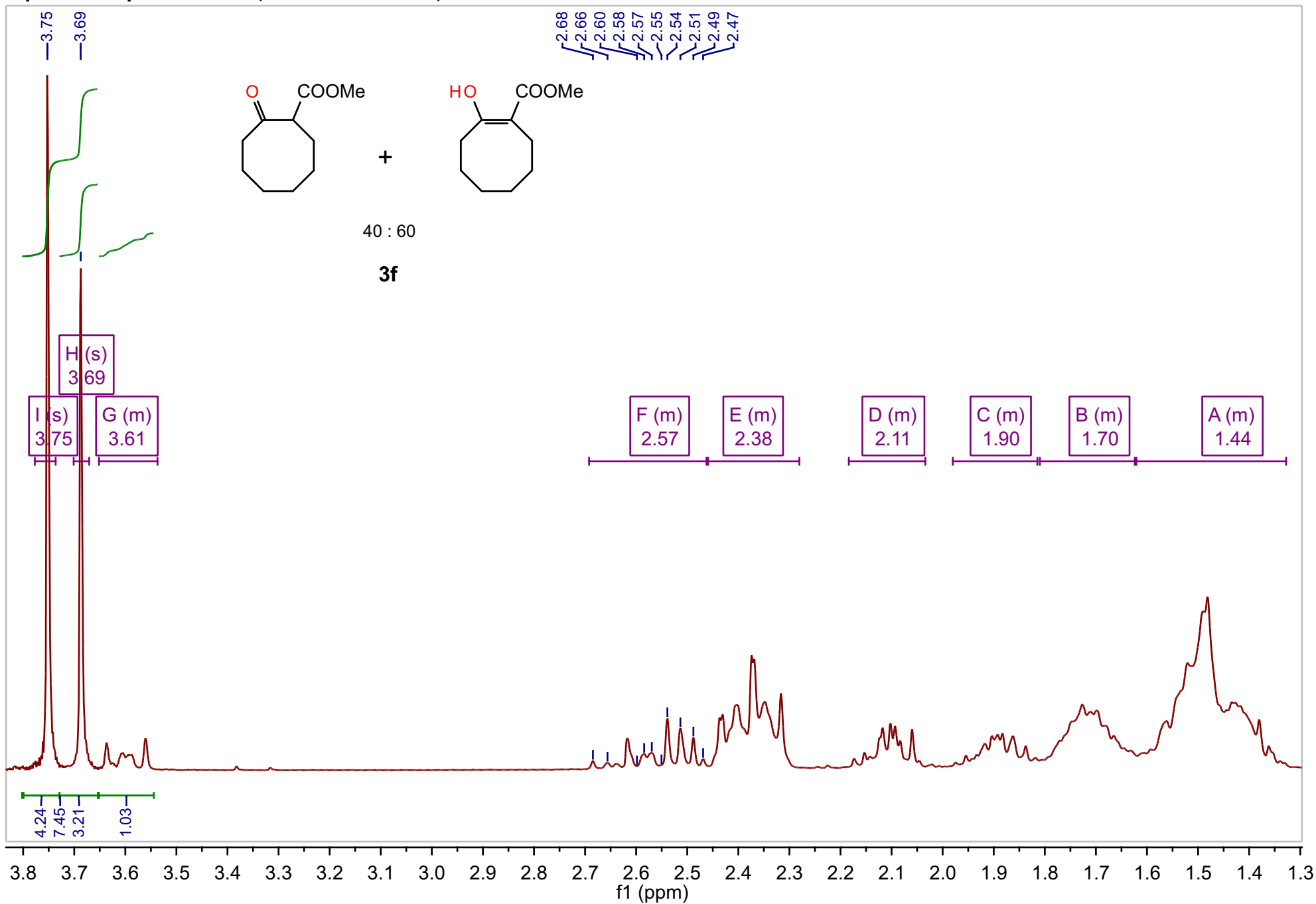
Spectroscopic data. Compound **3e** ¹³C NMR



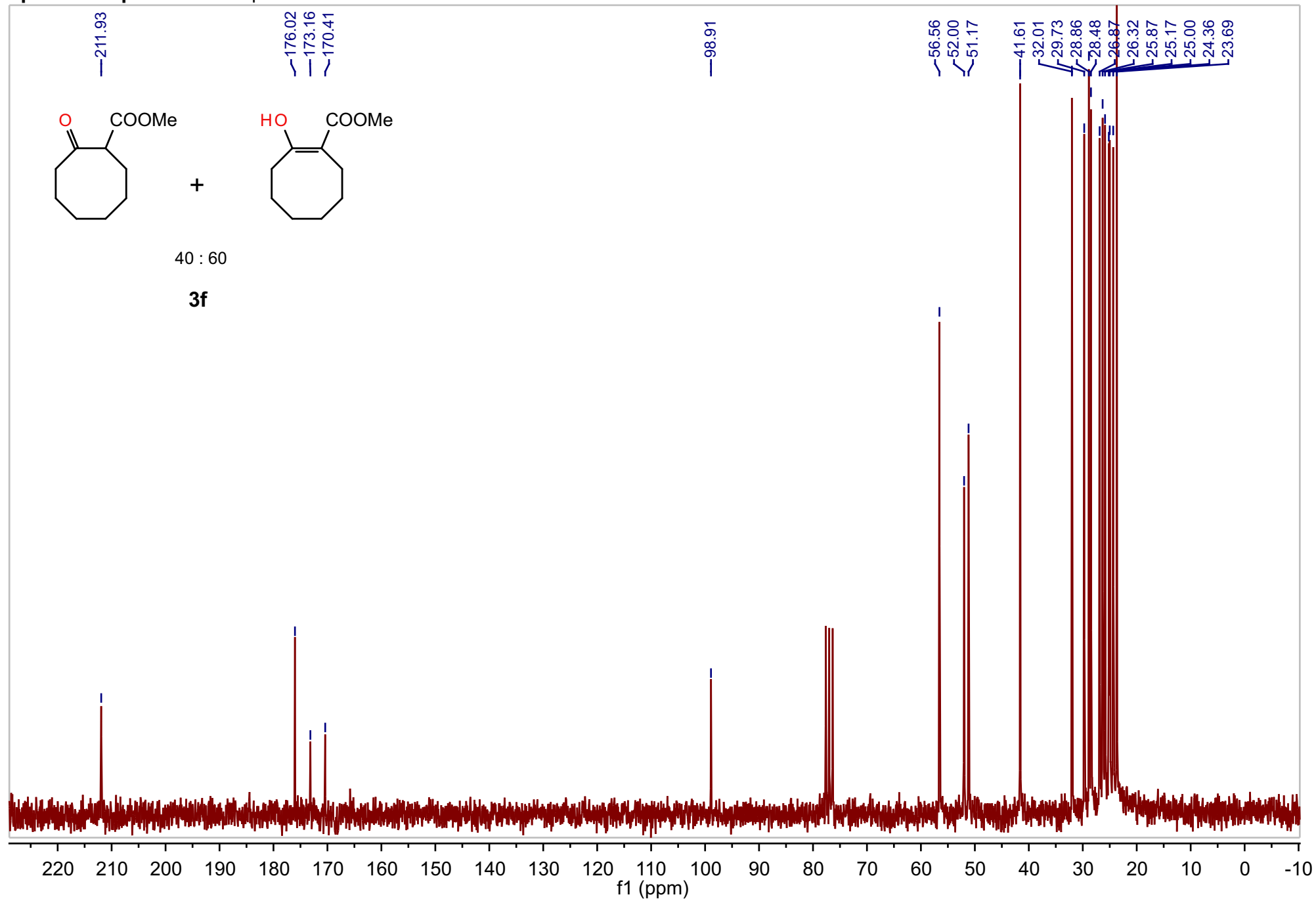
Spectroscopic data. Compound **3f** ^1H NMR



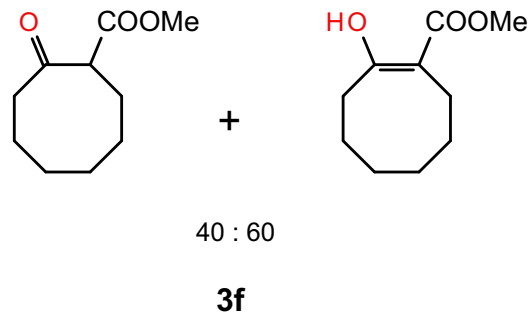
Spectroscopic data. Compound **3f** ¹H NMR expanded



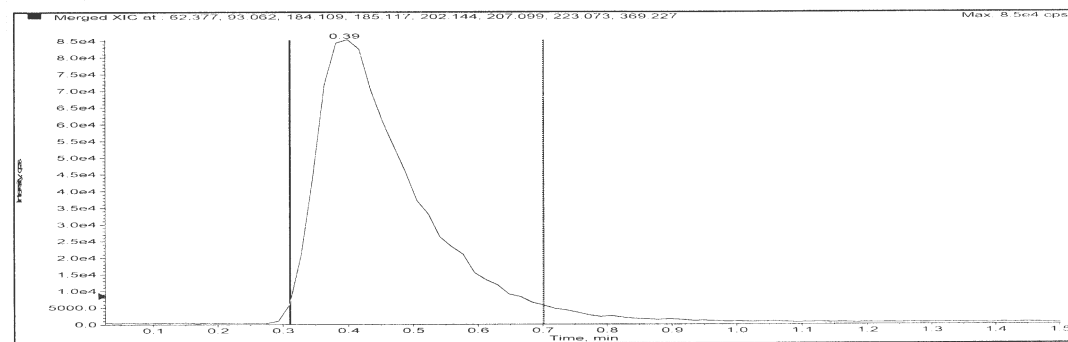
Spectroscopic data. Compound **3f** ¹³C NMR



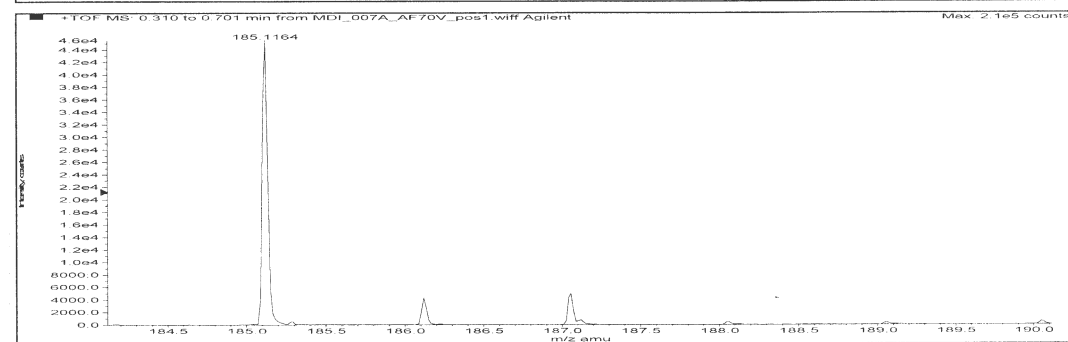
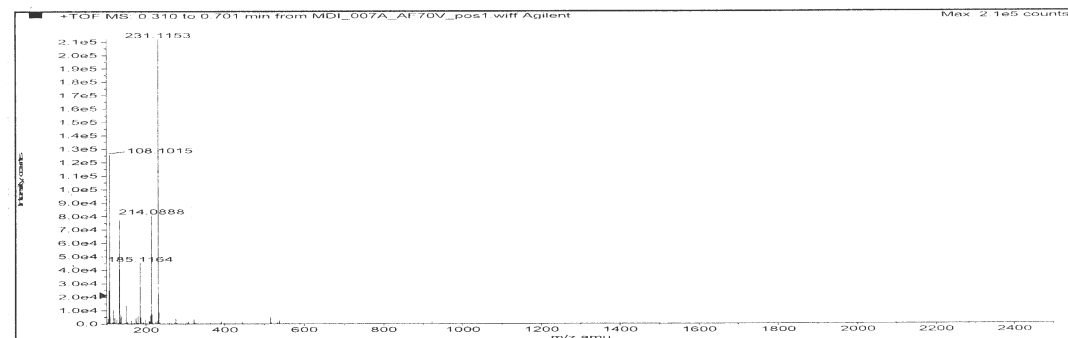
Spectroscopic data. Compound 3f HRMS



Sample Name: MDI_007A Sample Location: P1-C1 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Roglic\Data\MDI_007A_AF70V_pos1.wiff Acq Time: August 02 2012, 03:54:06 PM
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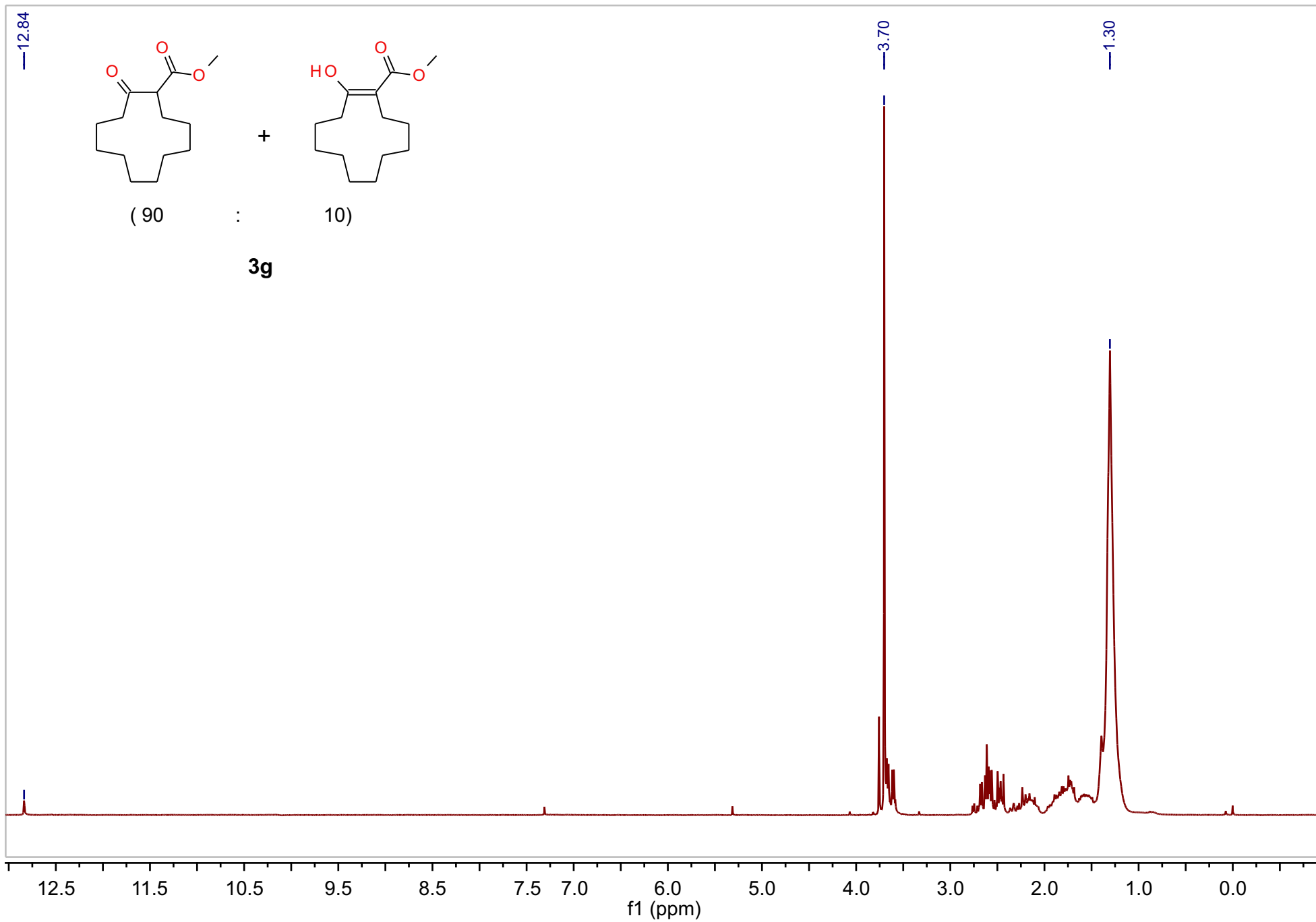
Merged XIC, Period# : 1 Experiment# : 1



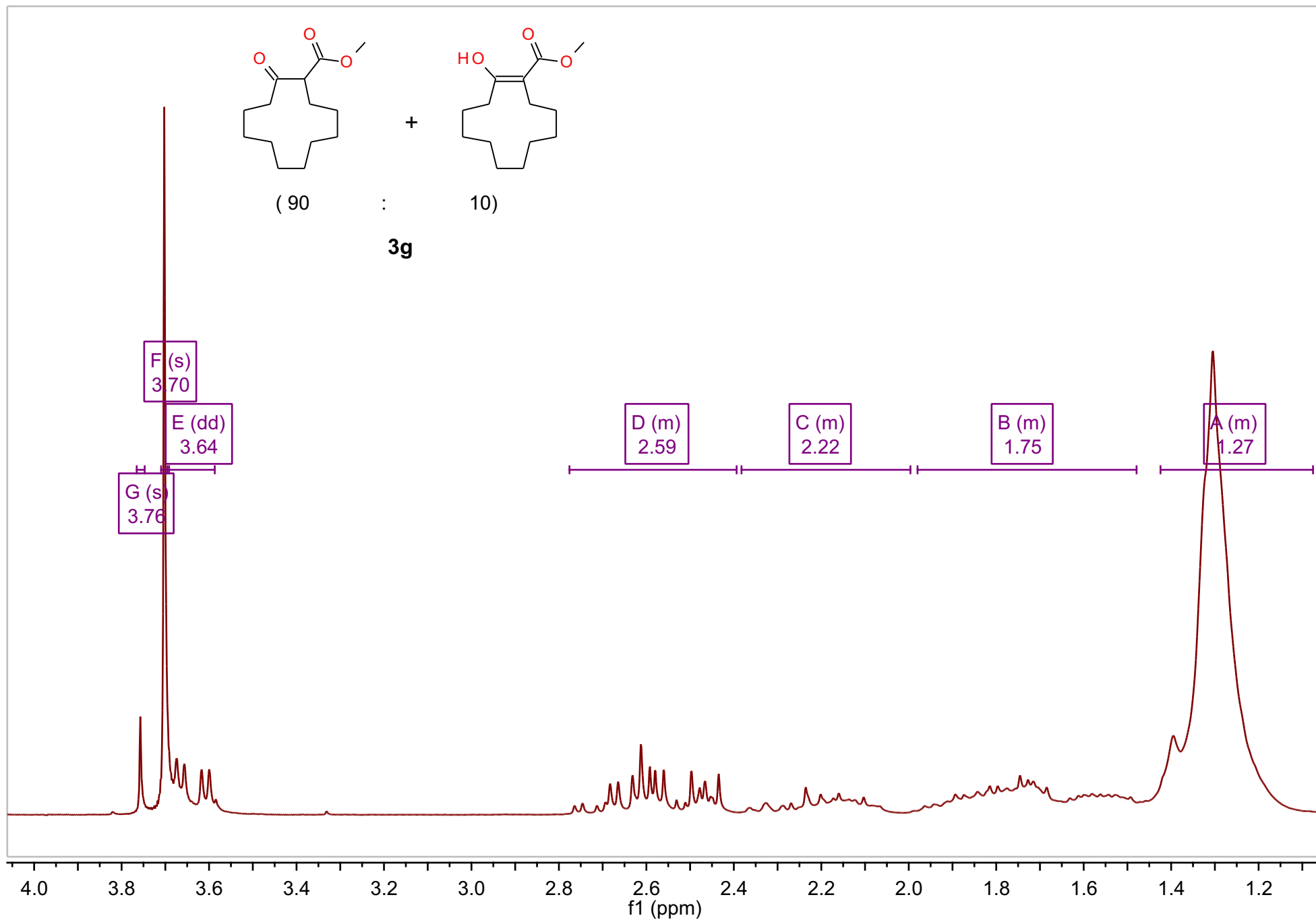
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C10H16O3	--	184.10994	0.39	8.99164 E5	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	45908.03	185.11722	185.11640	-0.82466	-4.45	--

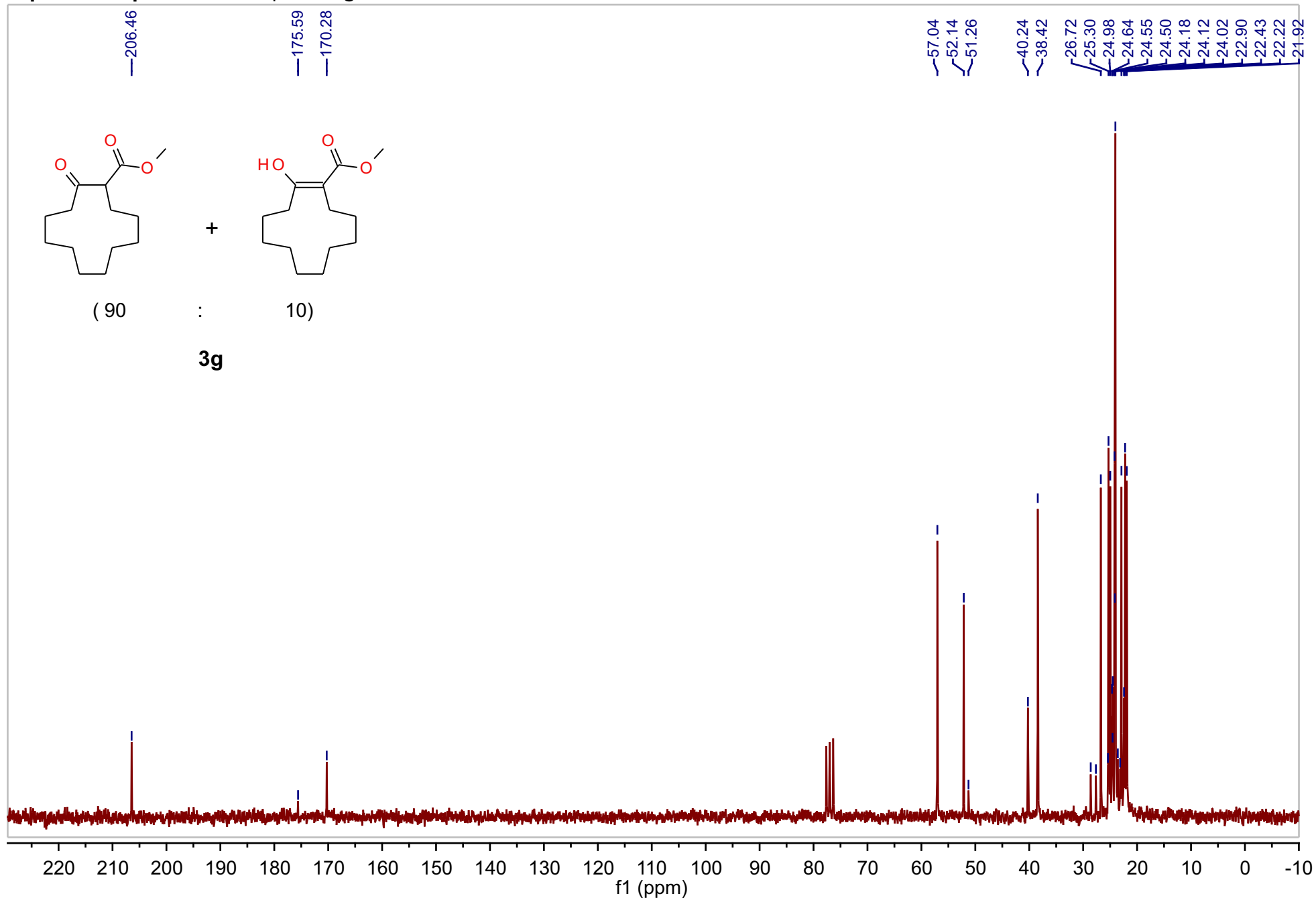
Spectroscopic data. Compound **3g** ^1H NMR



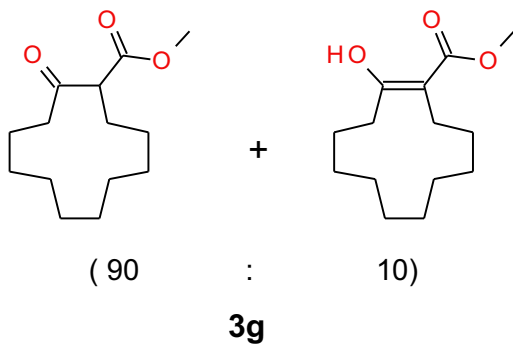
Spectroscopic data. Compound **3g** ^1H NMR expanded



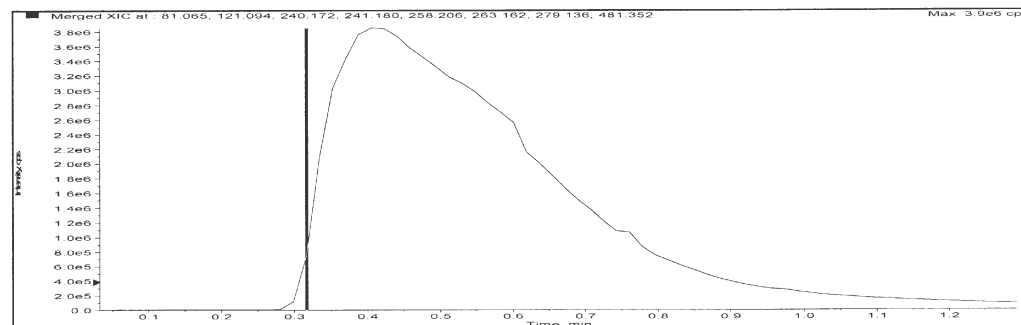
Spectroscopic data. Compound **3g** ¹³C NMR



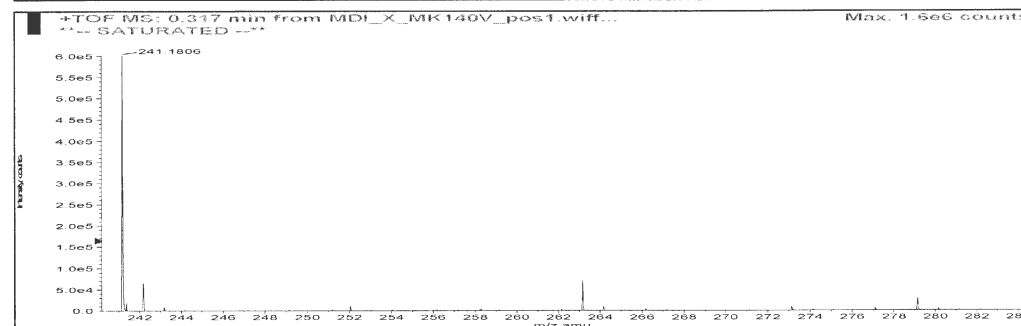
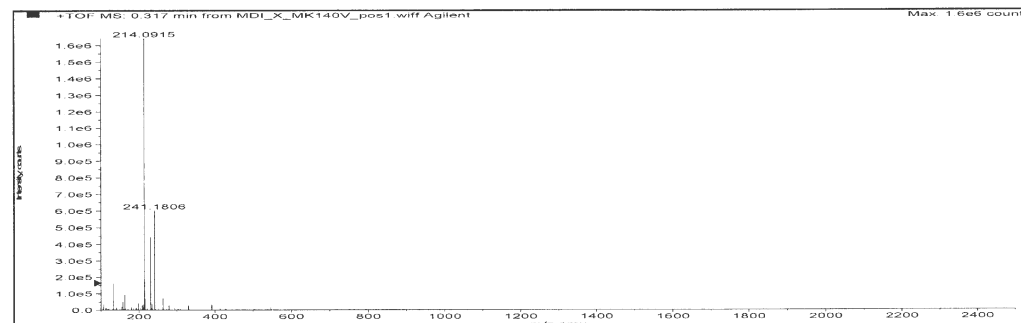
Spectroscopic data. Compound 3g HRMS



Sample Name: MDL_X Sample Location: P1-F3 Sample Id: Operator: Milka
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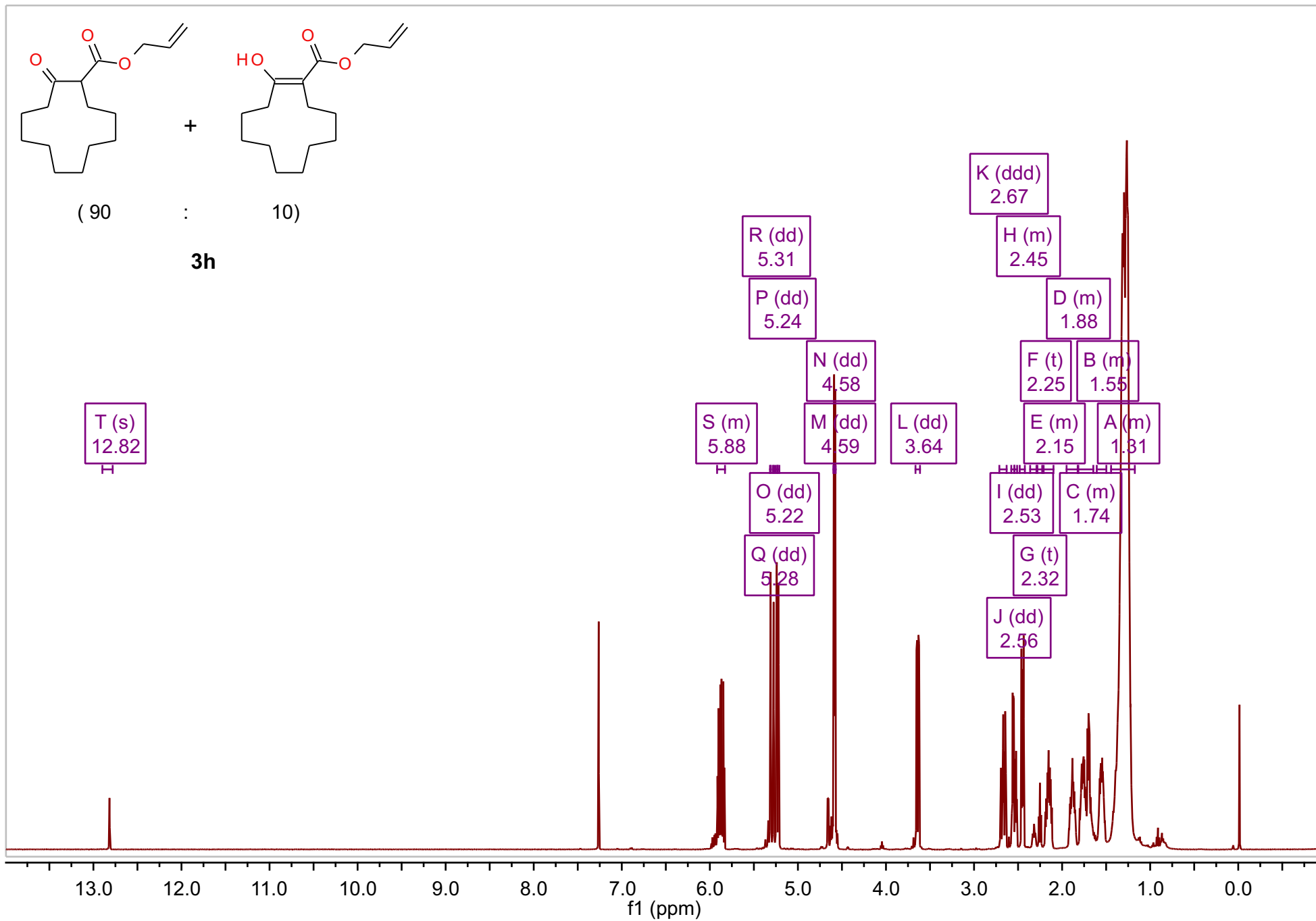
Merged XIC, Period#: 1 Experiment#: 1



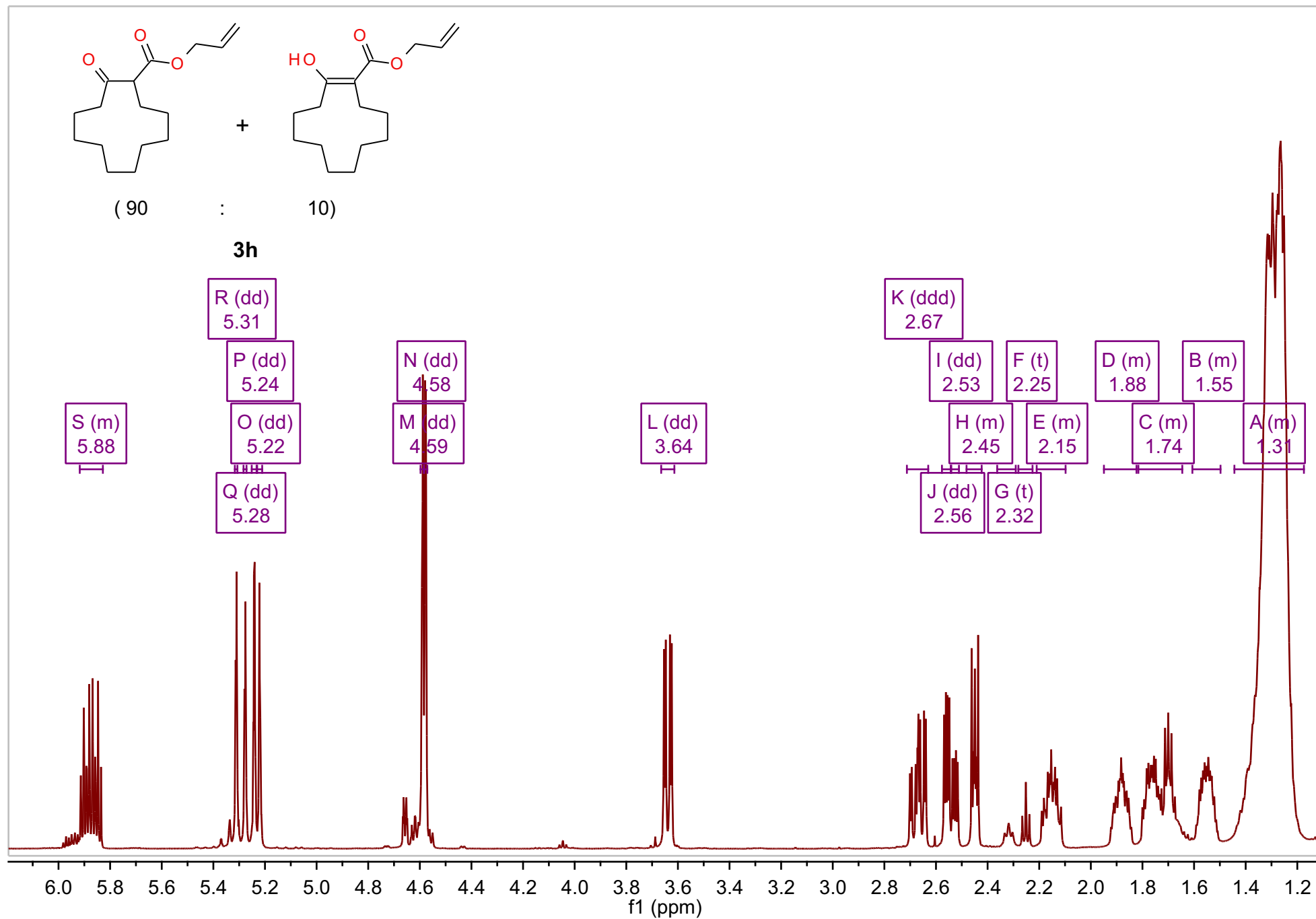
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C14H24O3	--	240.17254	0.41	7.50792 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	610309.26	241.17982	241.18055	0.72906	3.02	--
[M+Na] ⁺	70600.04	263.16177	263.16204	0.27390	1.04	--
[M+K] ⁺	29119.99	279.13570	279.14342	7.71870	27.65	--

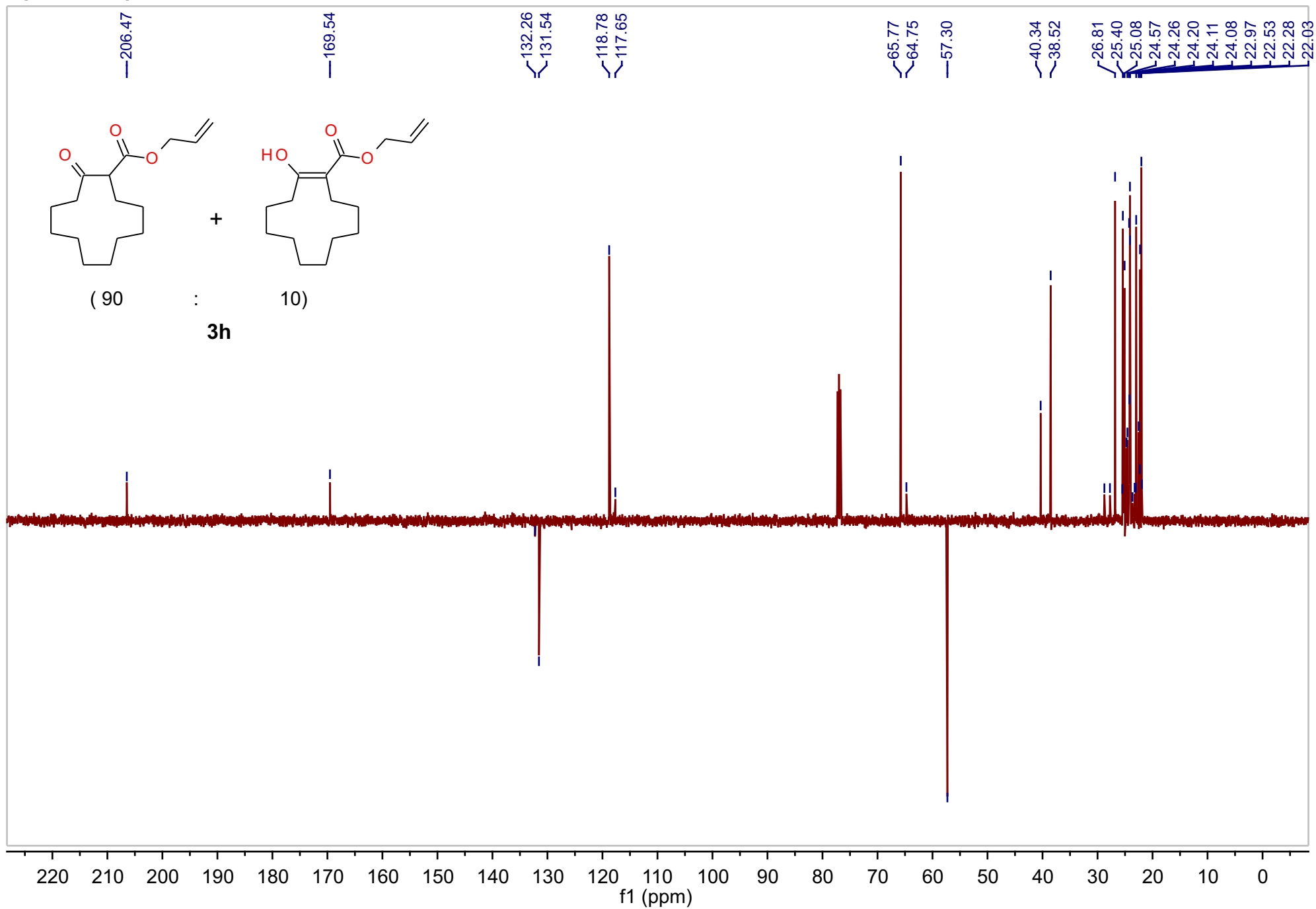
Spectroscopic data. Compound **3h** ¹H NMR 500 MHz



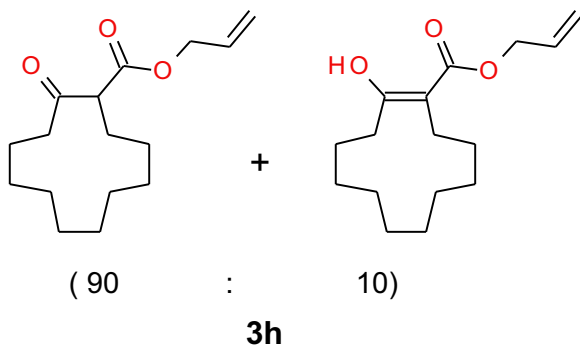
Spectroscopic data. Compound **3h** ¹H NMR 500 MHz expanded



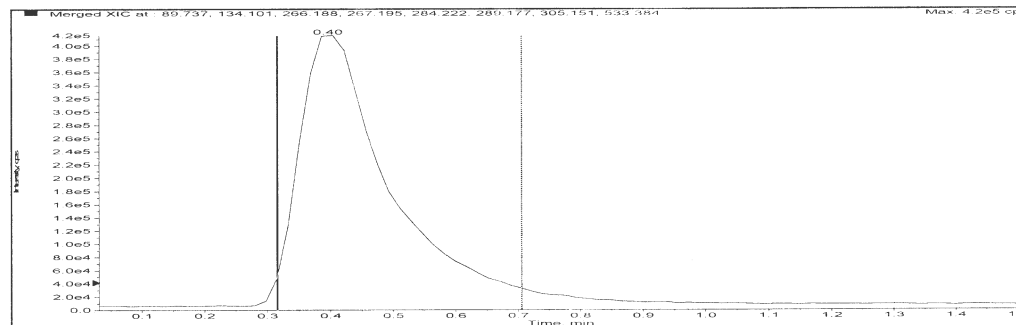
Spectroscopic data. Compound 3h APT 500 MHz



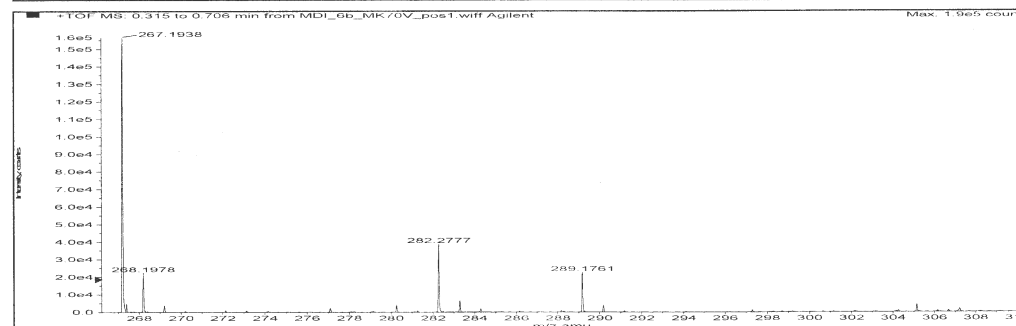
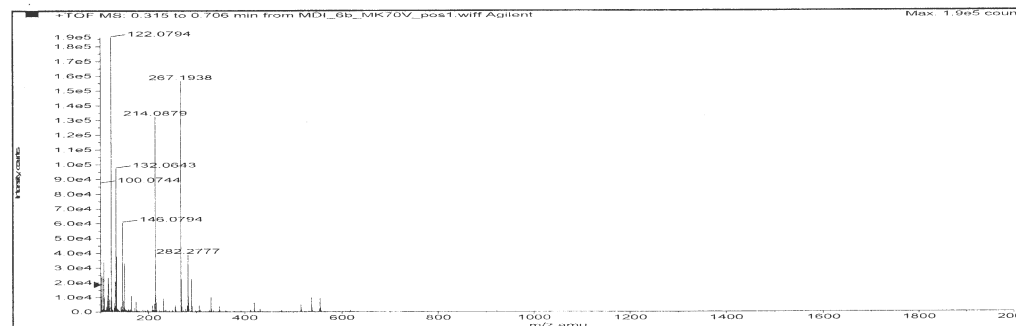
Spectroscopic data. Compound 3h HRMS



Sample Name: **6b** Sample Location: **P1-E6** Sample Id: Operator: **Milka**
 Data File Name: **D:\PE Sciex Data\Projects\Roglic\Data\MDI_6b_MK70V_pos1.wiff** Acq Time: **July 18 2012, 03:43:31 PM**
 Method: **d:\TOF Software\damethods\Night_Seq_Comp_ident1.anmlefc.xml**



Merged XIC, Period#: 1 Experiment#: 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C16H26O3	--	266.18819	0.40	4.14250 E6	--

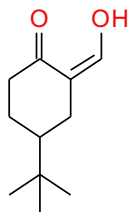
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	161613.71	267.19547	267.19375	-1.72015	-6.44	--
[M+Na] ⁺	23761.16	289.17742	289.17613	-1.28847	-4.46	--
[M+K] ⁺	4355.29	305.15135	305.15090	-0.45474	-1.49	--

Spectroscopic data. Compound **3i** ^1H NMR

14.35

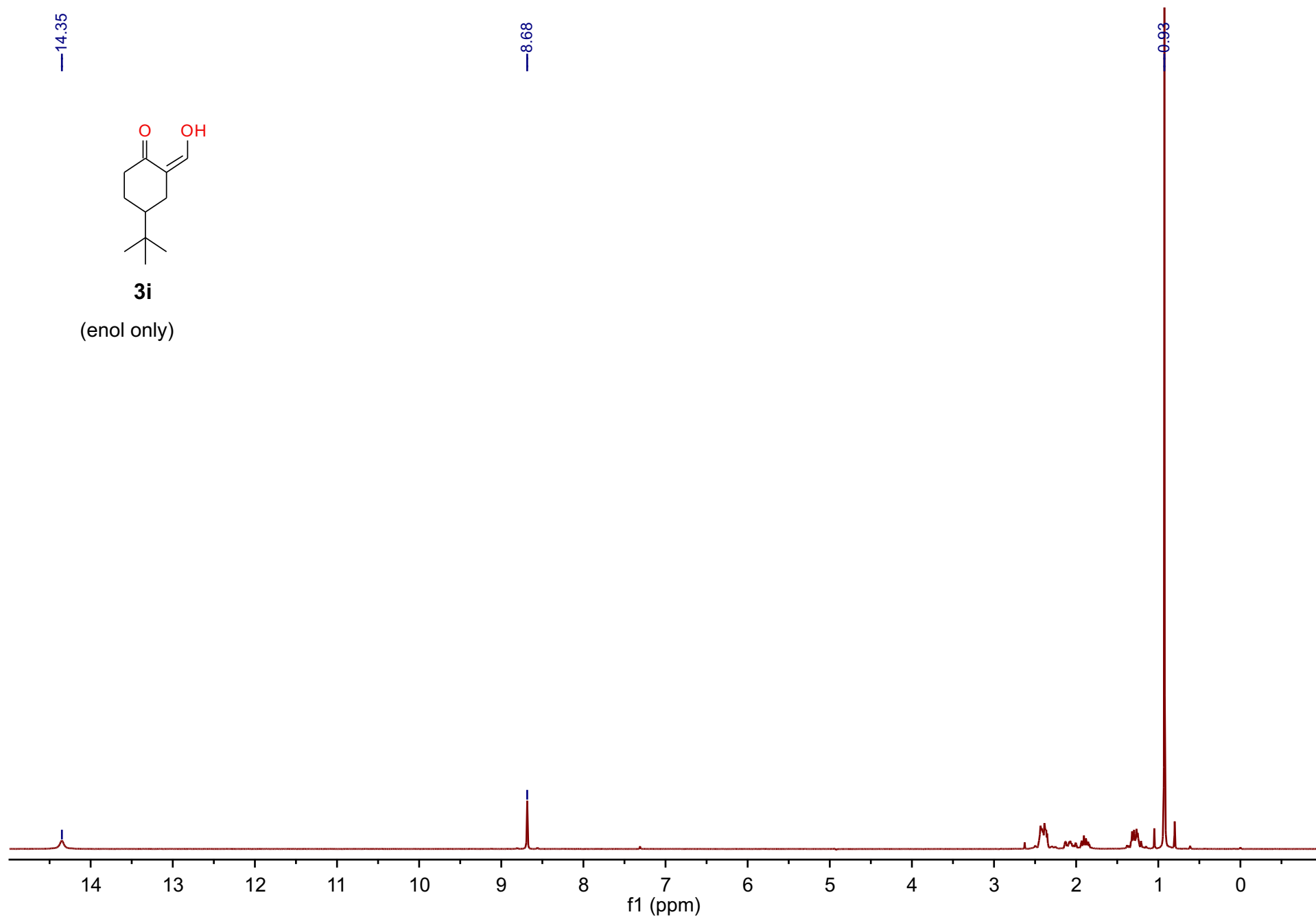
8.68

0.93

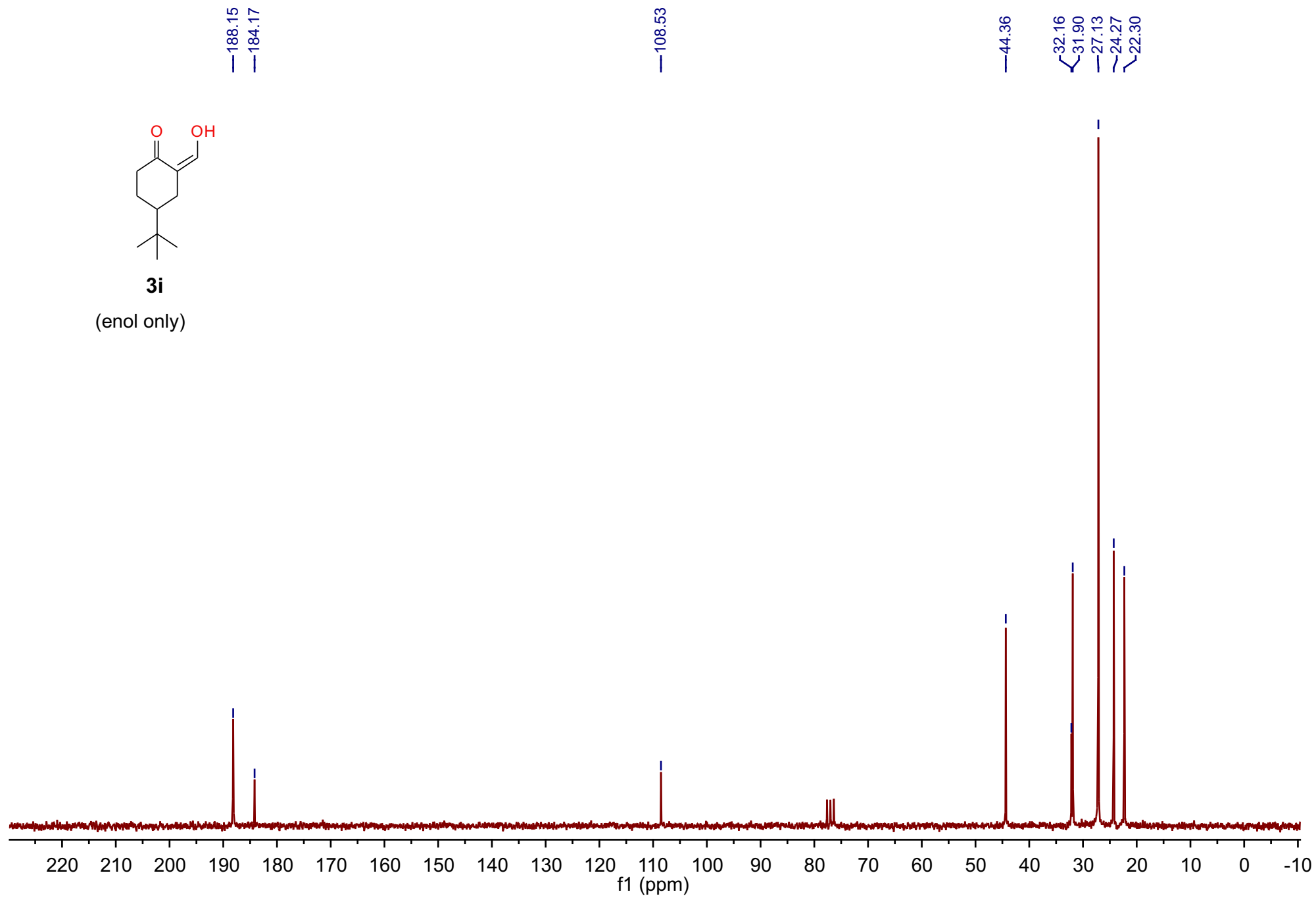
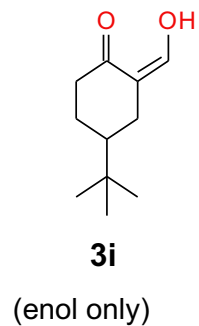


3i

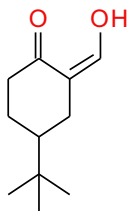
(enol only)



Spectroscopic data. COMPOUND 3i ¹³C NMR



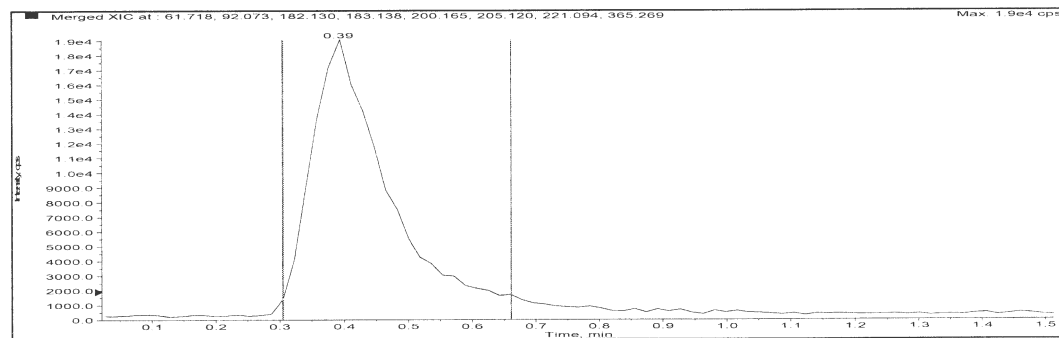
Spectroscopic data. Compound 3i HRMS



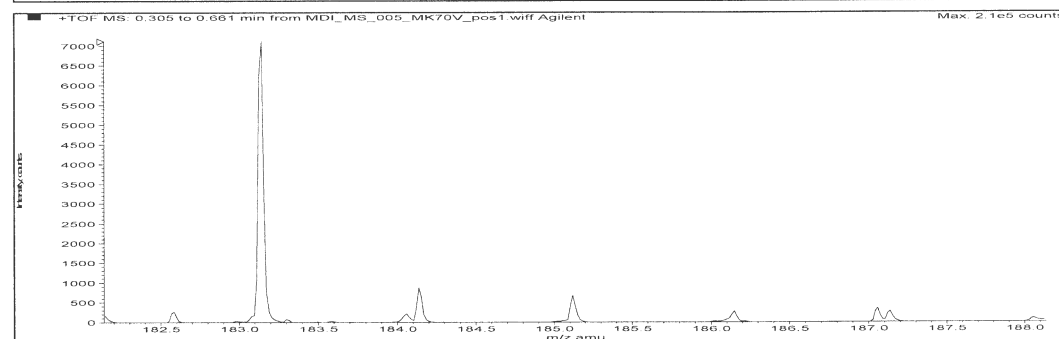
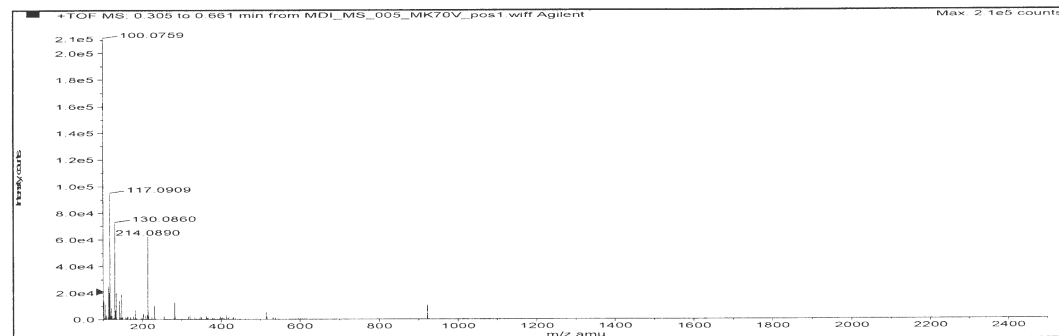
3i

(enol only)

Sample Name: MDI_MS_005 Sample Location: P1-E1 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Rogific\Data\MDI_MS_005_MK70V_pos1.wiff Acq Time: April 26 2012, 03:34:09 PM
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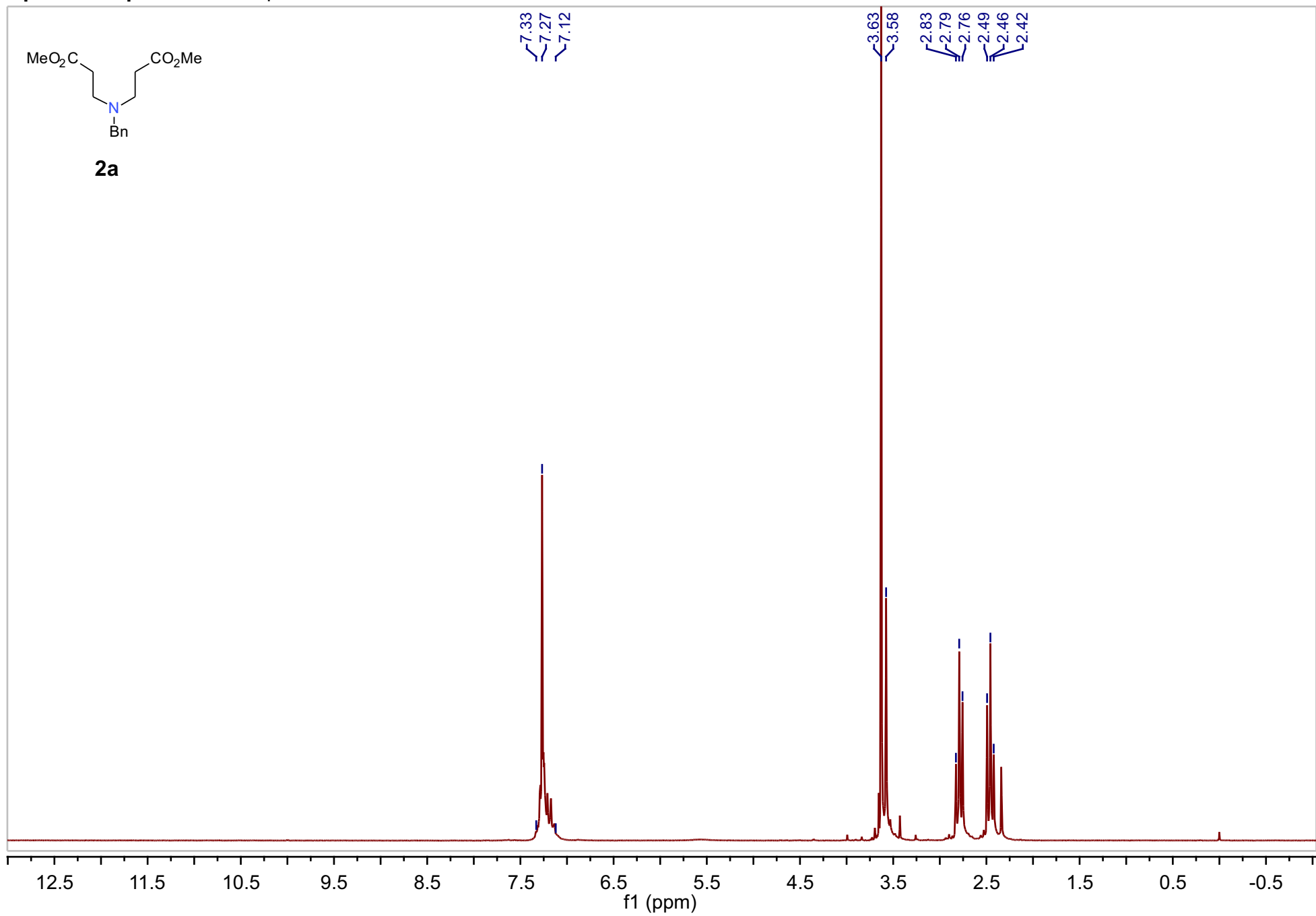
Merged XIC, Period# : 1 Experiment# : 1



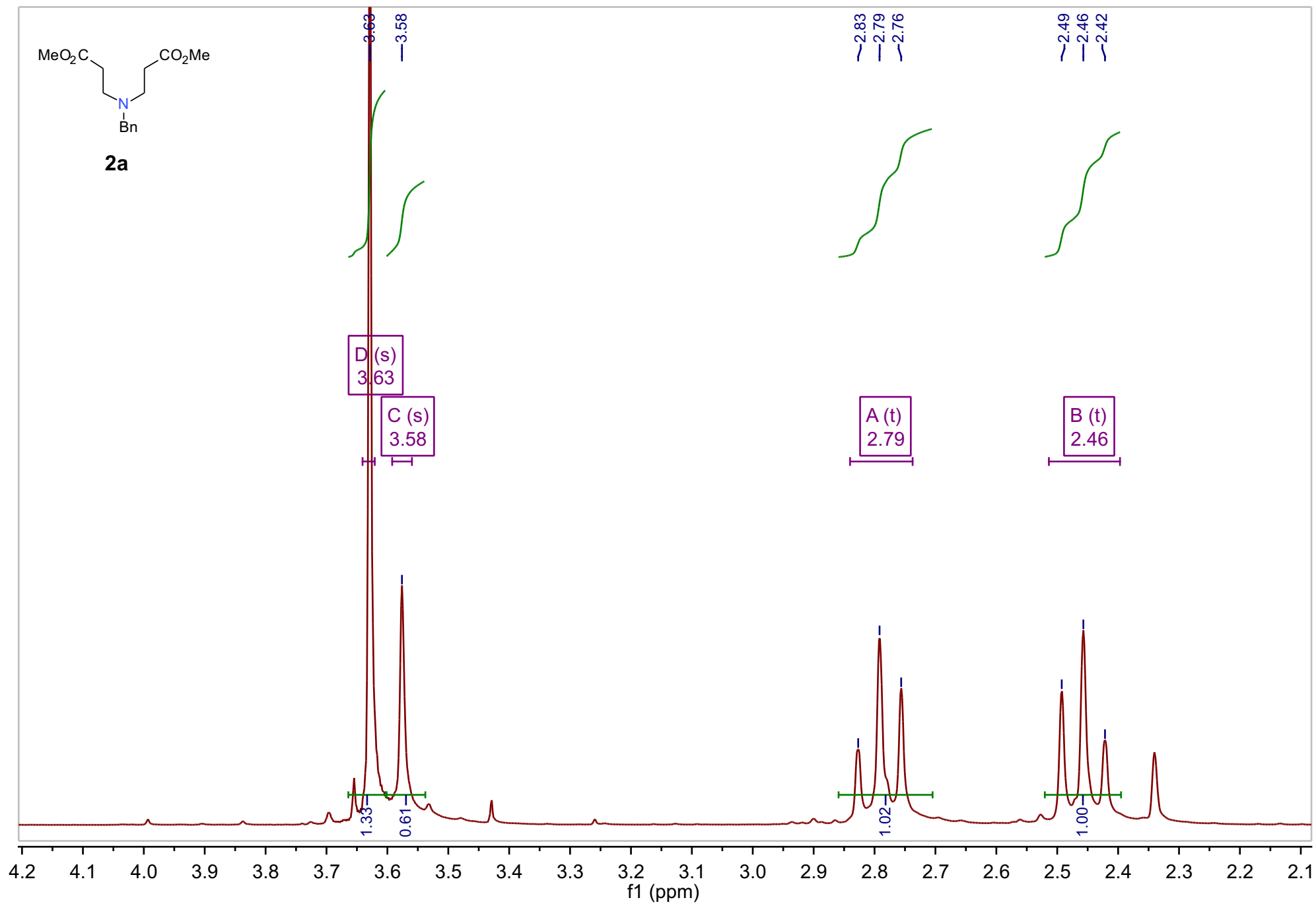
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C11H18O2	--	182.13068	0.39	1.59884 E5	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	7349.92	183.13796	183.13735	-0.60202	-3.29	--

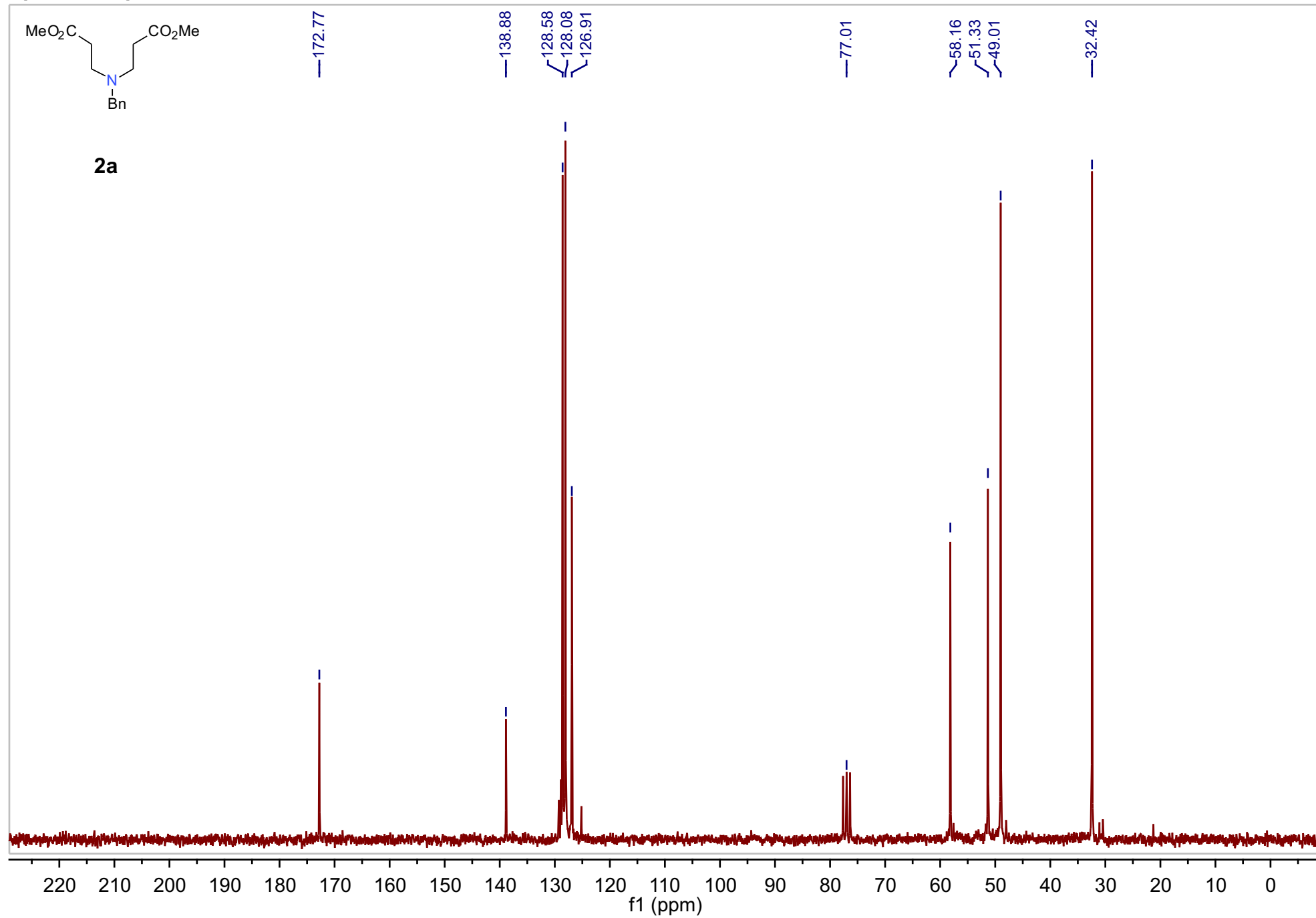
Spectroscopic data. Compound **2a** ^1H NMR



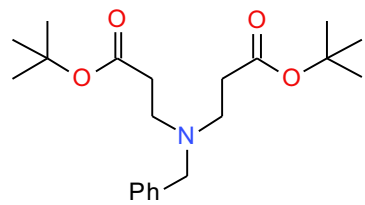
Spectroscopic data. Compound **2a** ¹H NMR expanded



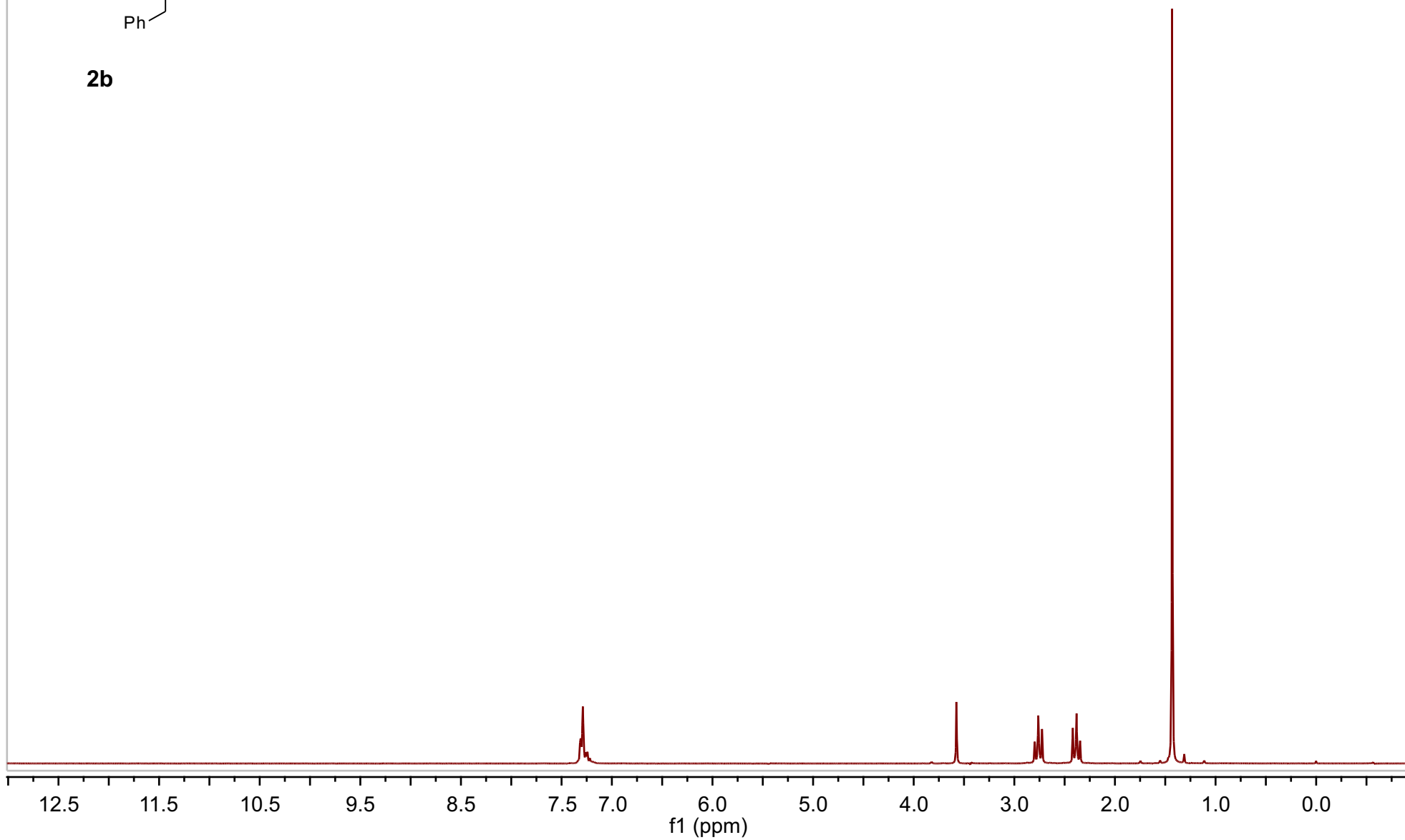
Spectroscopic data. Compound **2a** ^{13}C NMR



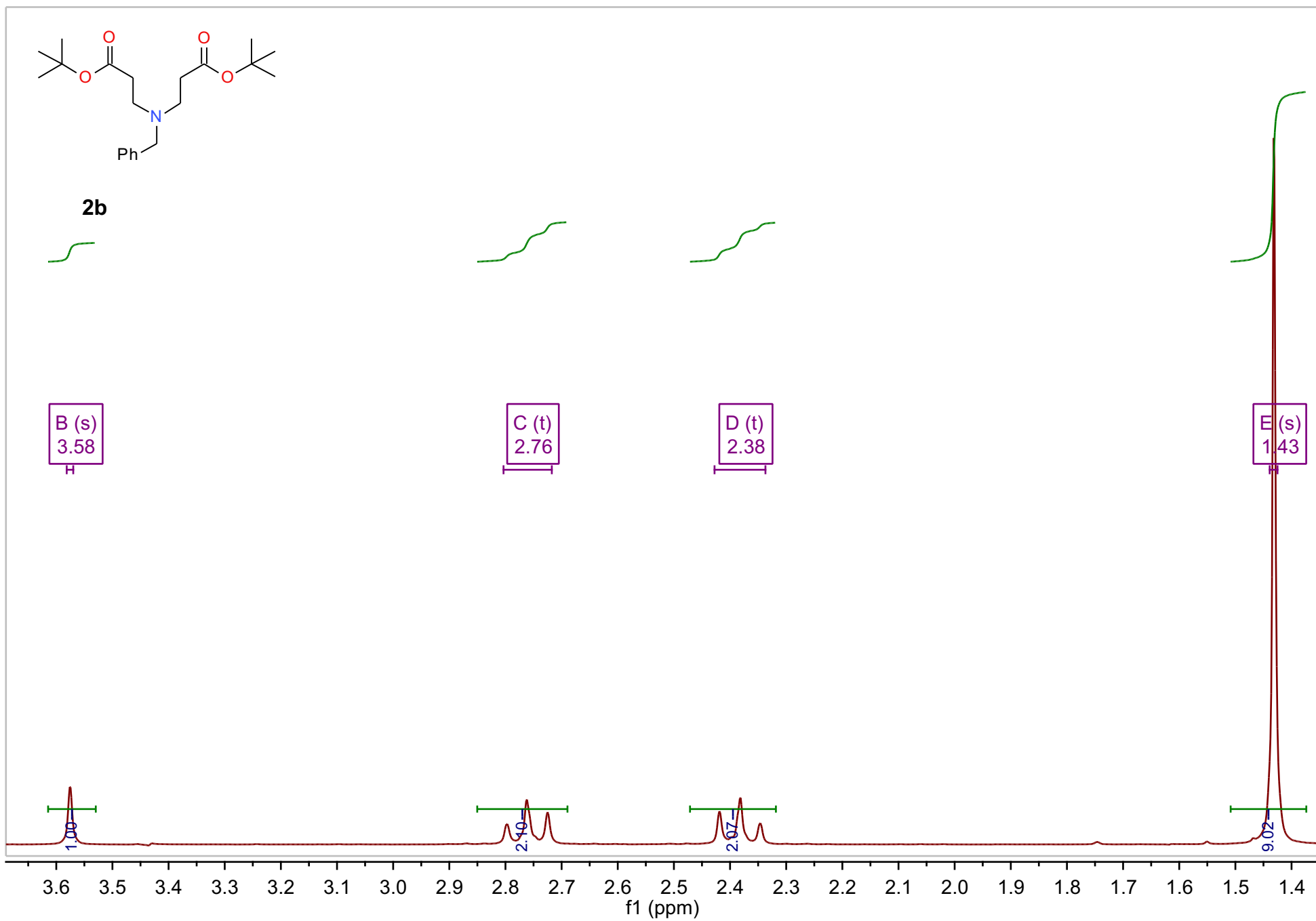
Spectroscopic data. Compound **2b** ^1H NMR



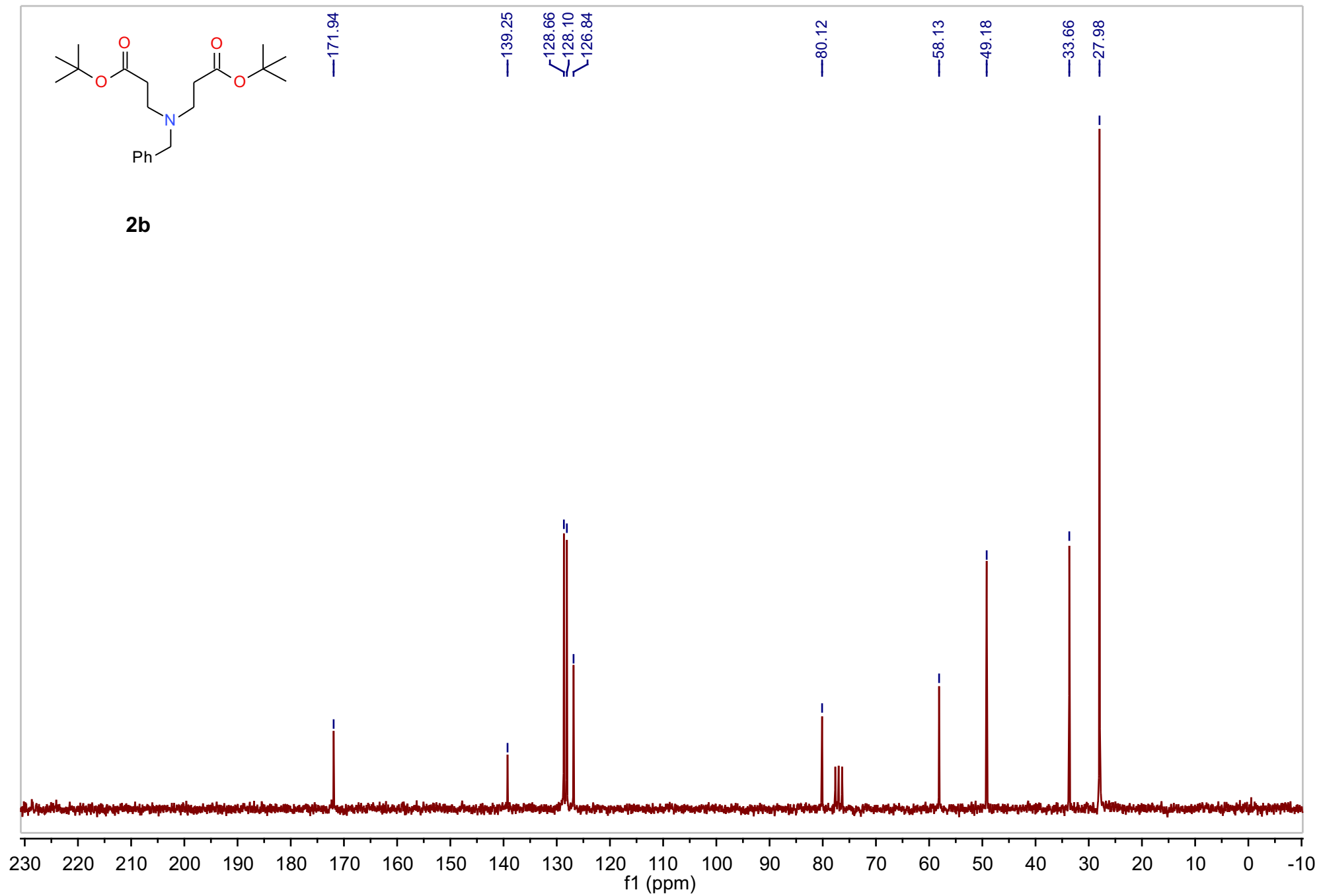
2b



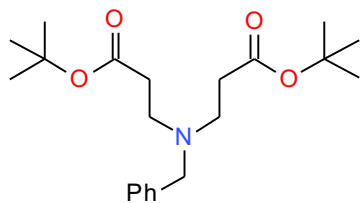
Spectroscopic data. Compound **2b** ¹H NMR expanded



Spectroscopic data. Compound **2b** ^{13}C NMR

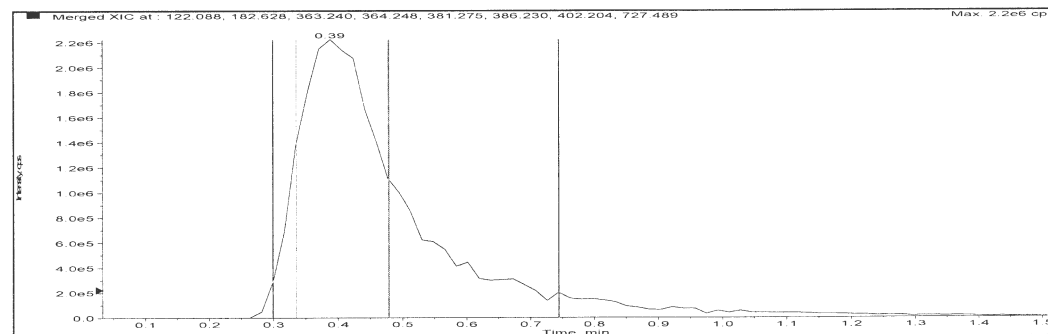


Spectroscopic data. Compound 2b HMRS

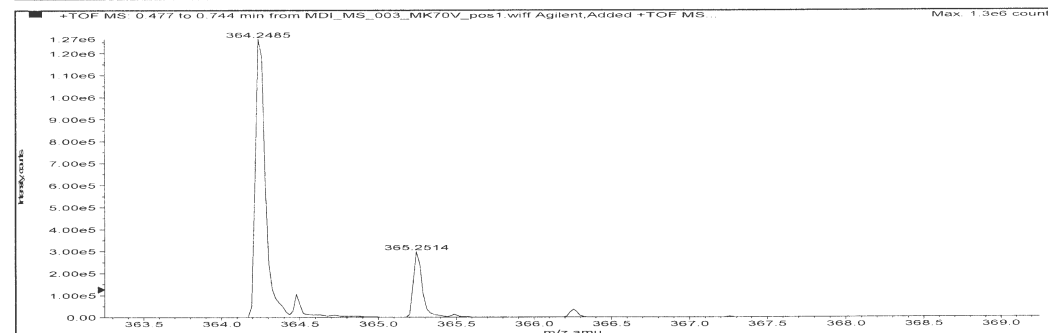
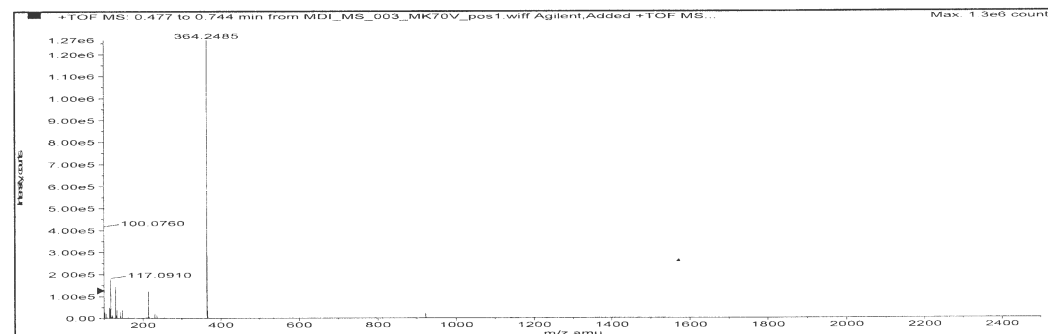


2b

Sample Name: MDI_MS_003 Sample Location: P1-D8 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Roglic\Data\MDI_MS_003_MK70V_pos1.wiff Acq Time: April 26 2012, 03:28:48 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.an\lefc.xml



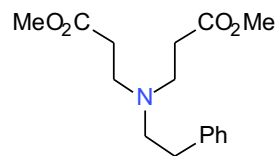
Merged XIC, Period# : 1 Experiment# : 1



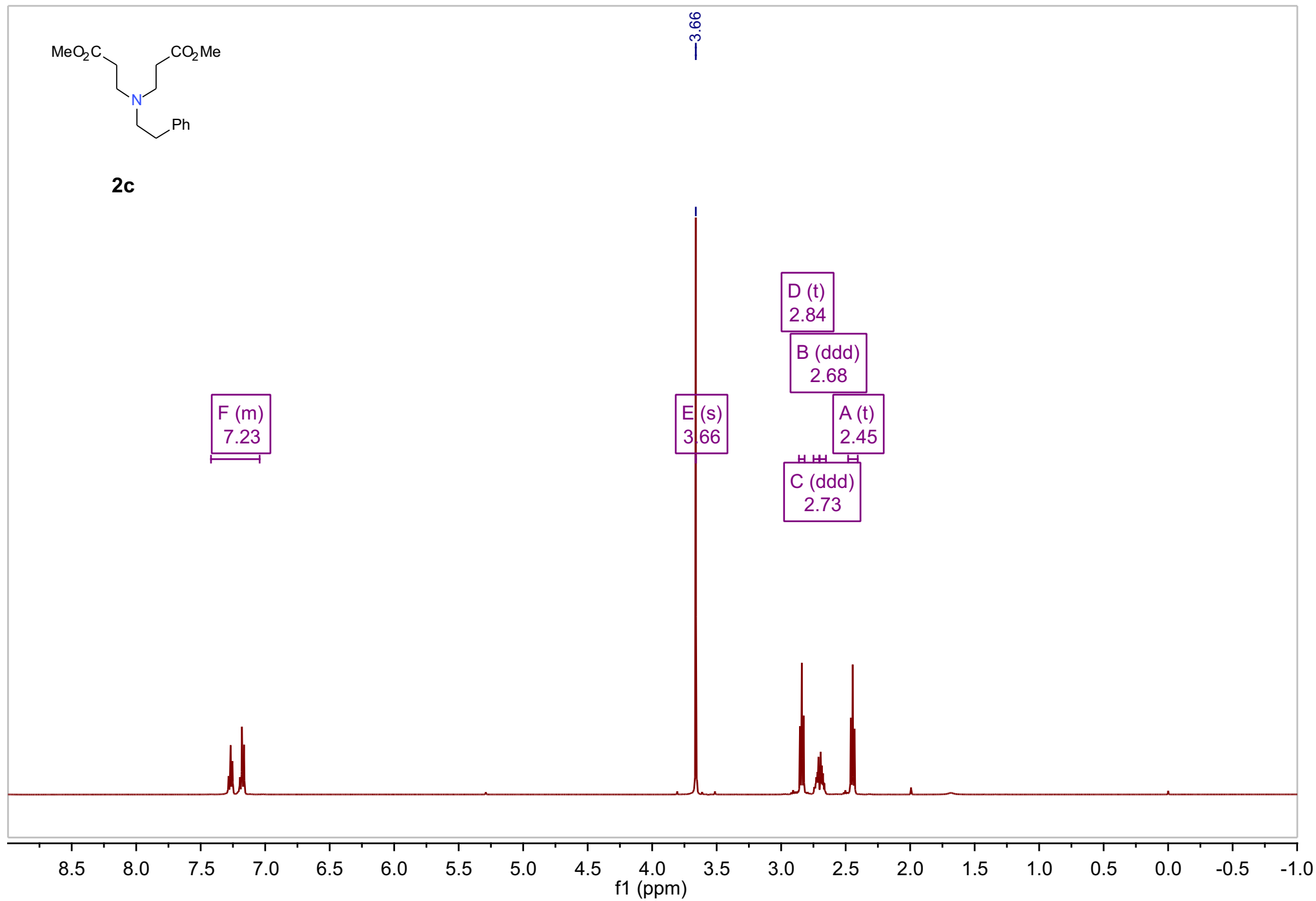
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C21H33NO4	--	363.24096	0.39	2.48771 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1323270.34	364.24824	364.24845	0.21657	0.59	--

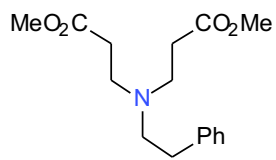
Spectroscopic data. Compound **2c** ^1H NMR



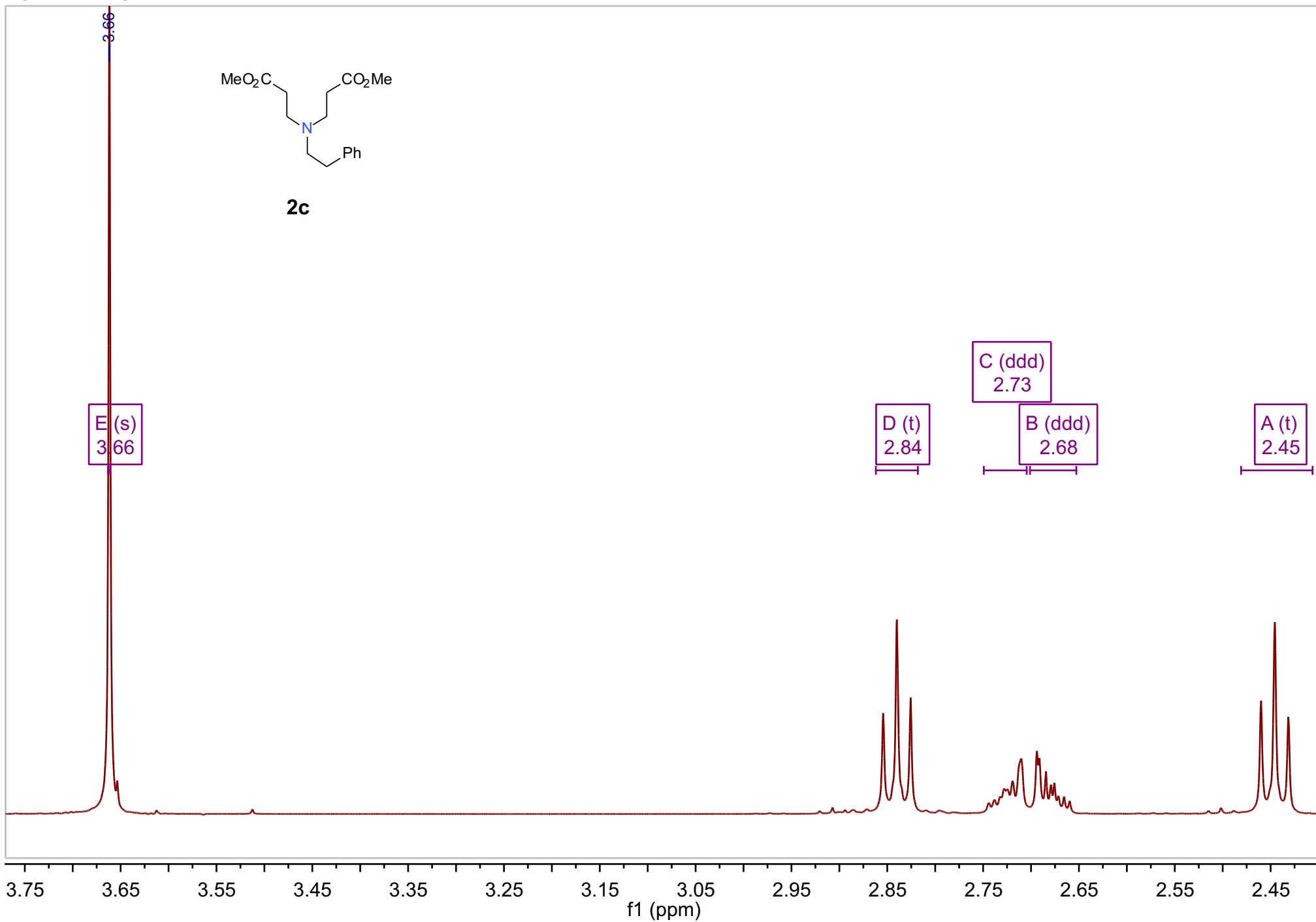
2c



Spectroscopic data. Compound **2c** ¹H NMR expanded

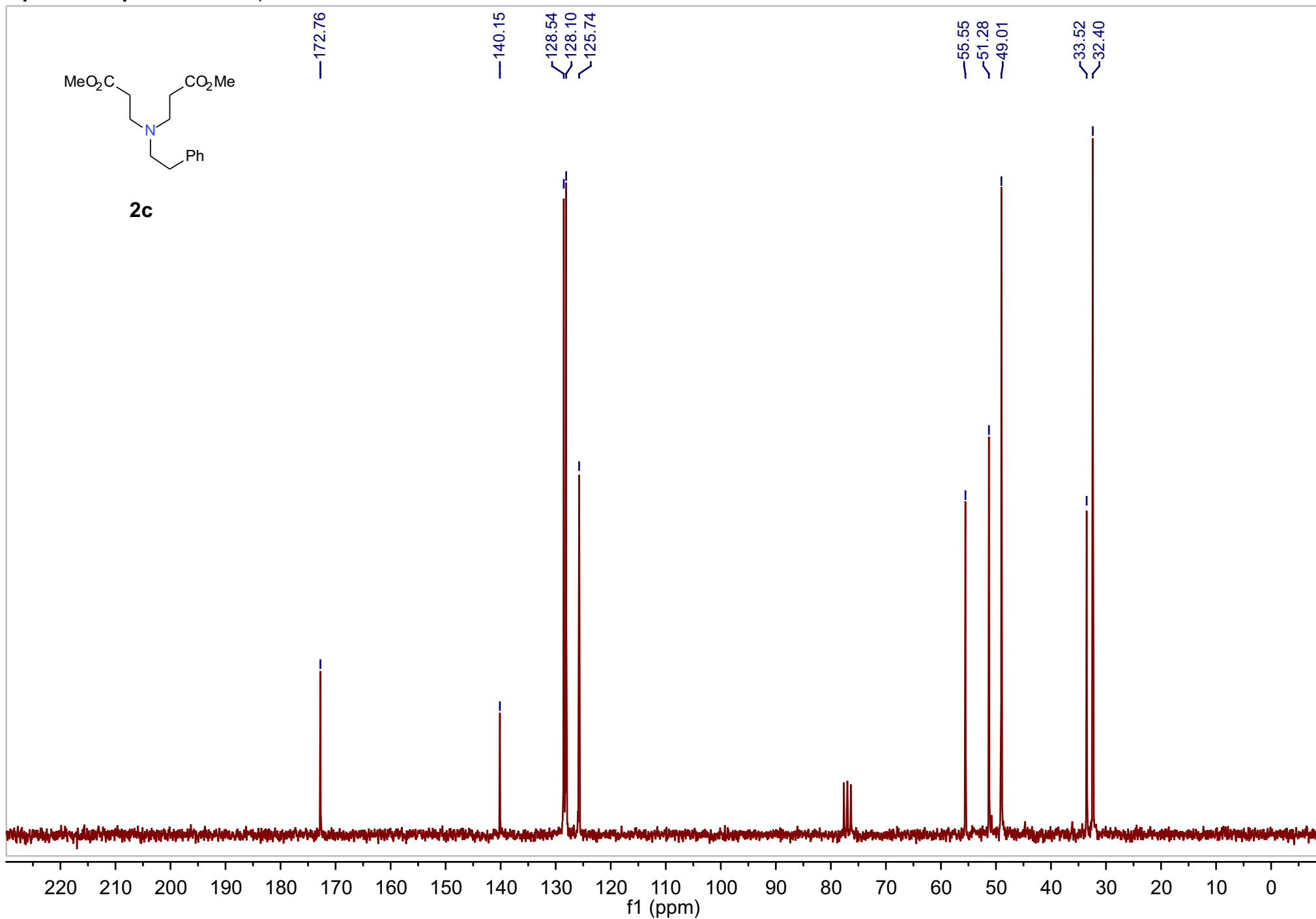


2c

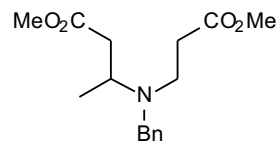


f1 (ppm)

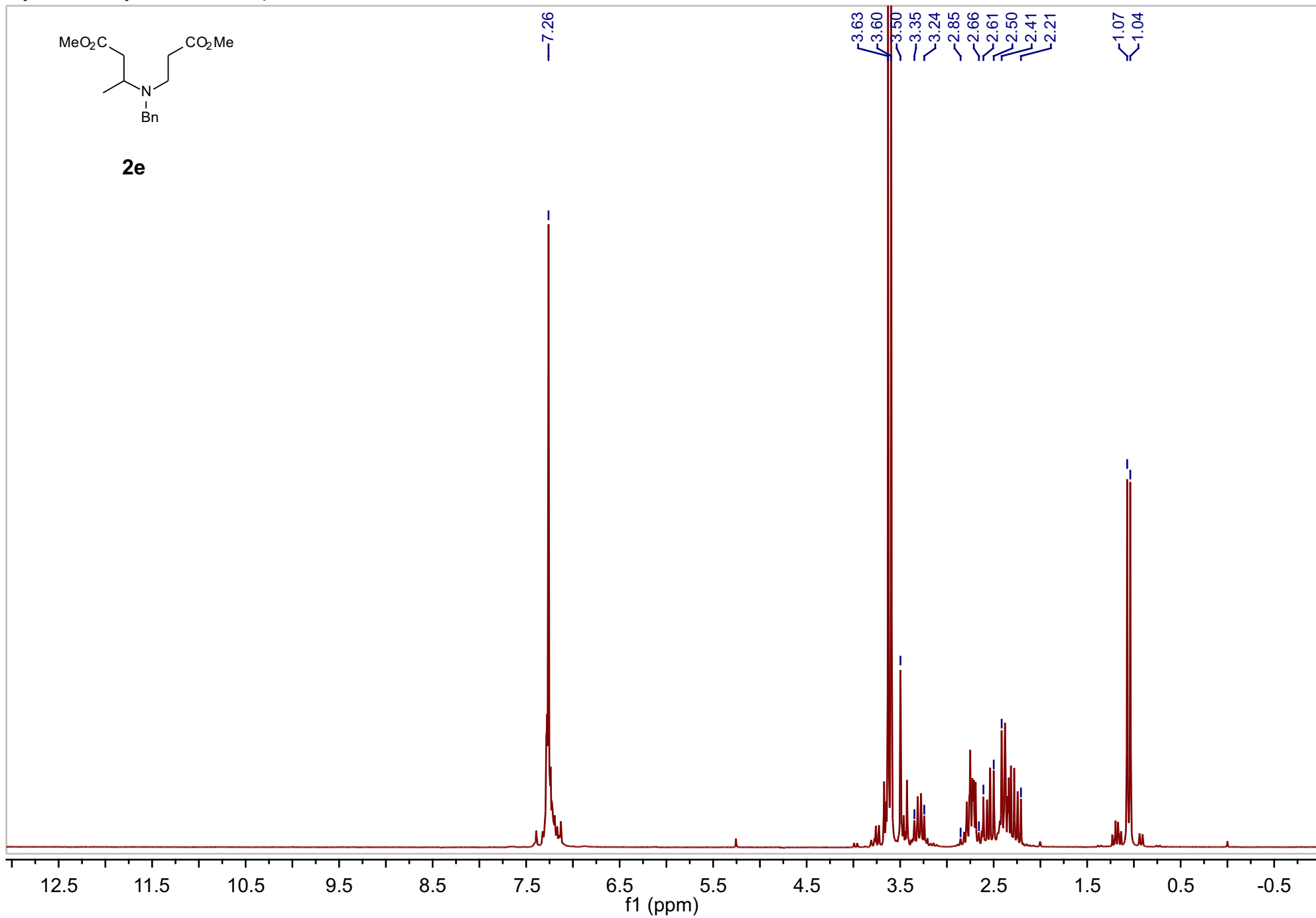
Spectroscopic data. Compound **2c** ^{13}C NMR



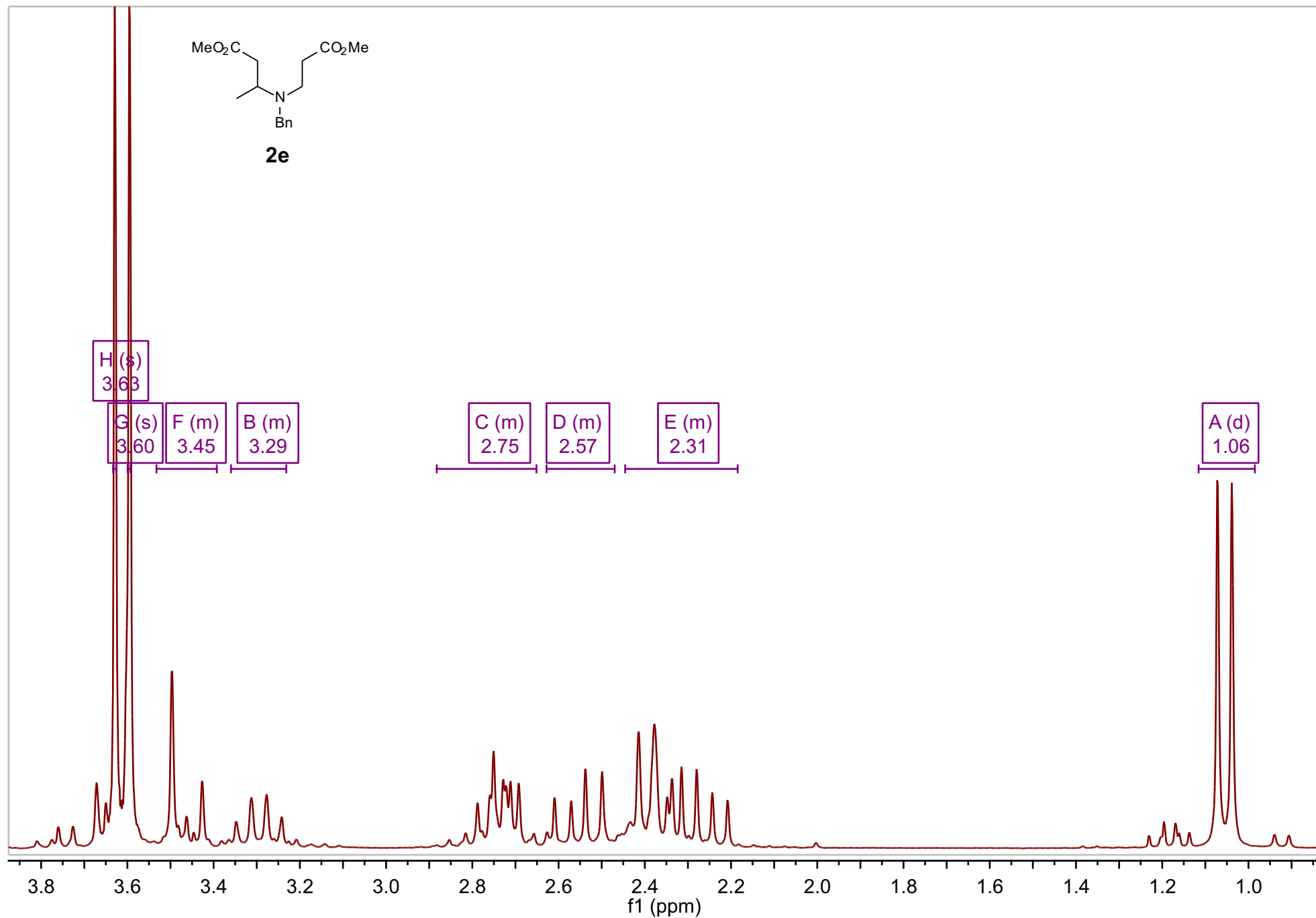
Spectroscopic data. Compound **2e** ¹H NMR



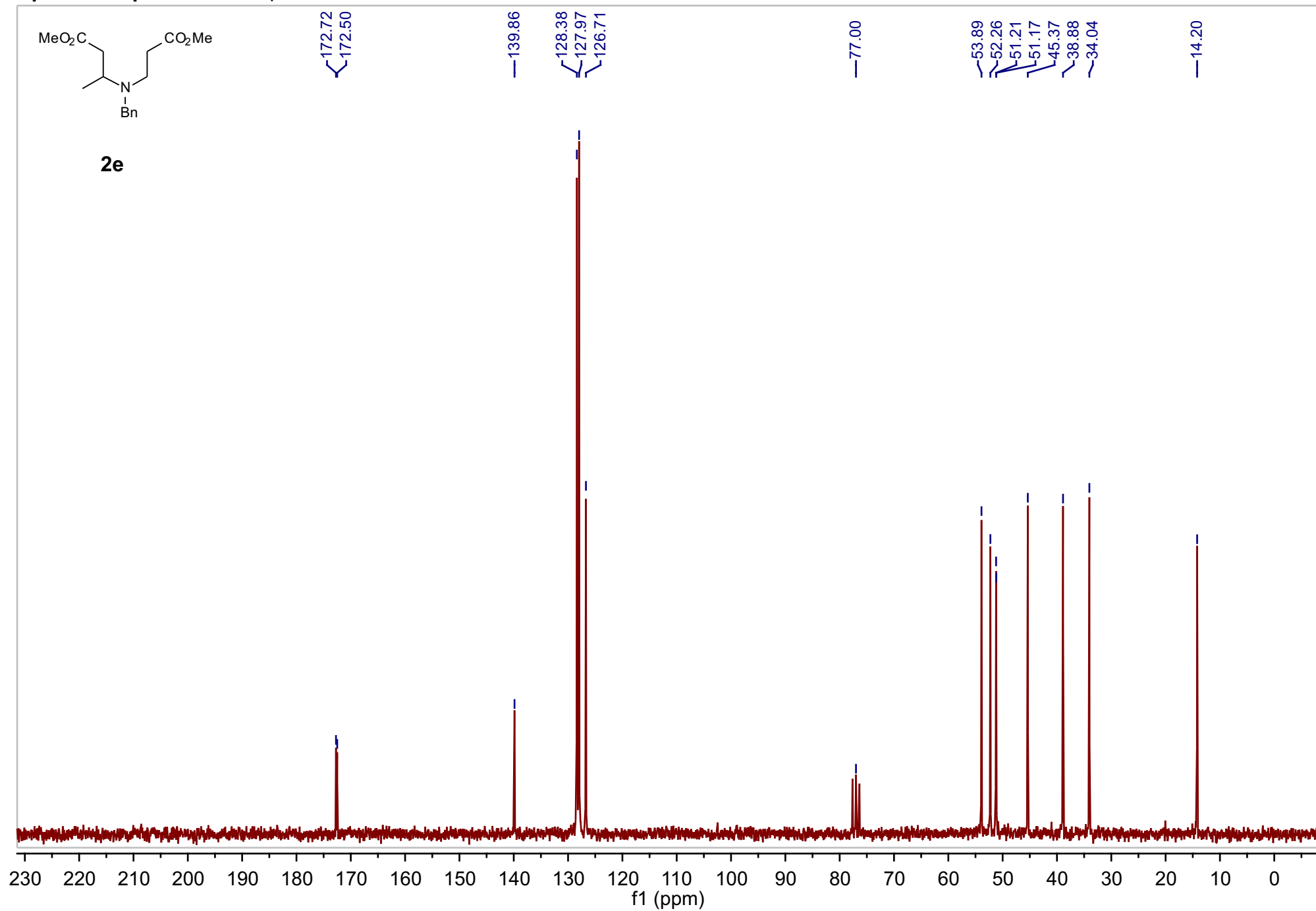
2e



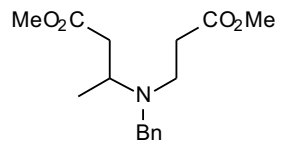
Spectroscopic data. Compound **2e** ¹H NMR expanded



Spectroscopic data. Compound **2e** ¹³C NMR

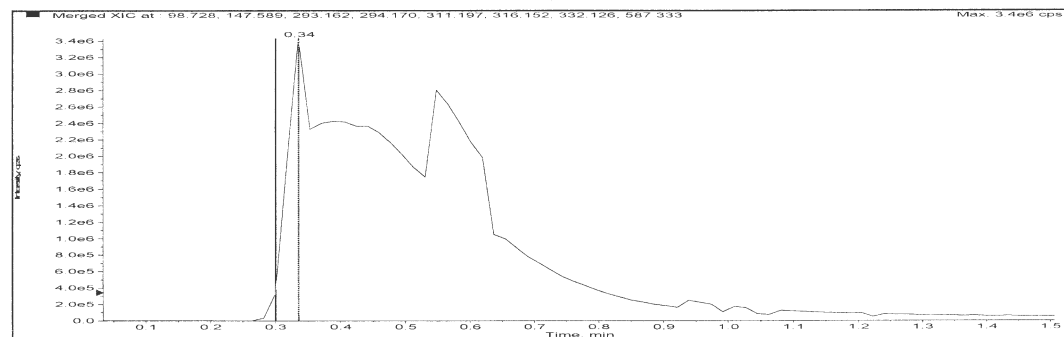


Spectroscopic data. Compound 2e HRMS

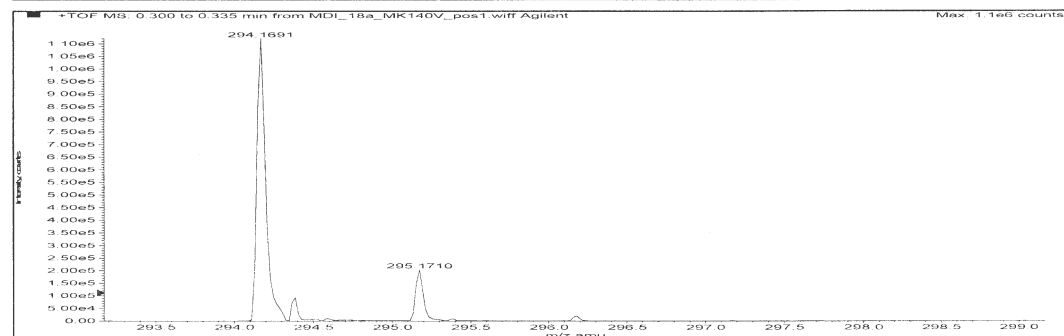
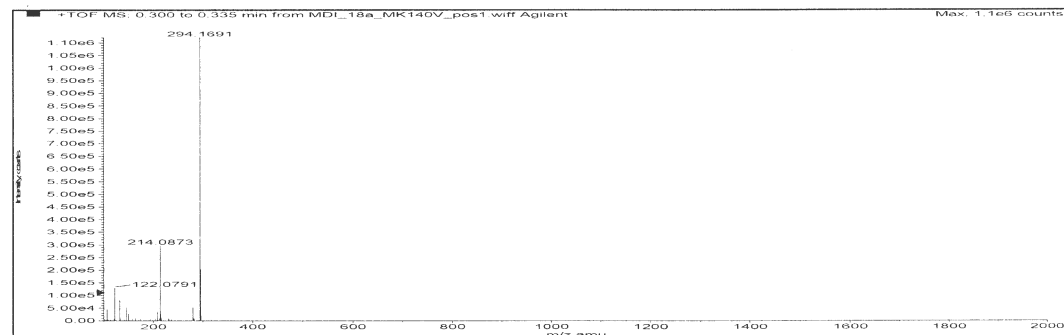


2e

Sample Name: 18a Sample Location: P1-F4 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Roglic\Data\MDL_18a_MK140V_pos1.wiff Acq Time: July 18 2012, 04:37:00 PM
 Method: d:\TOF Software\damethods\Night_Seq_Comp_ident1.anmlefc.xml



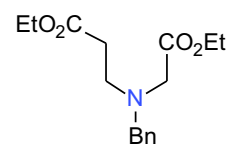
Merged XIC, Period# : 1 Experiment# : 1



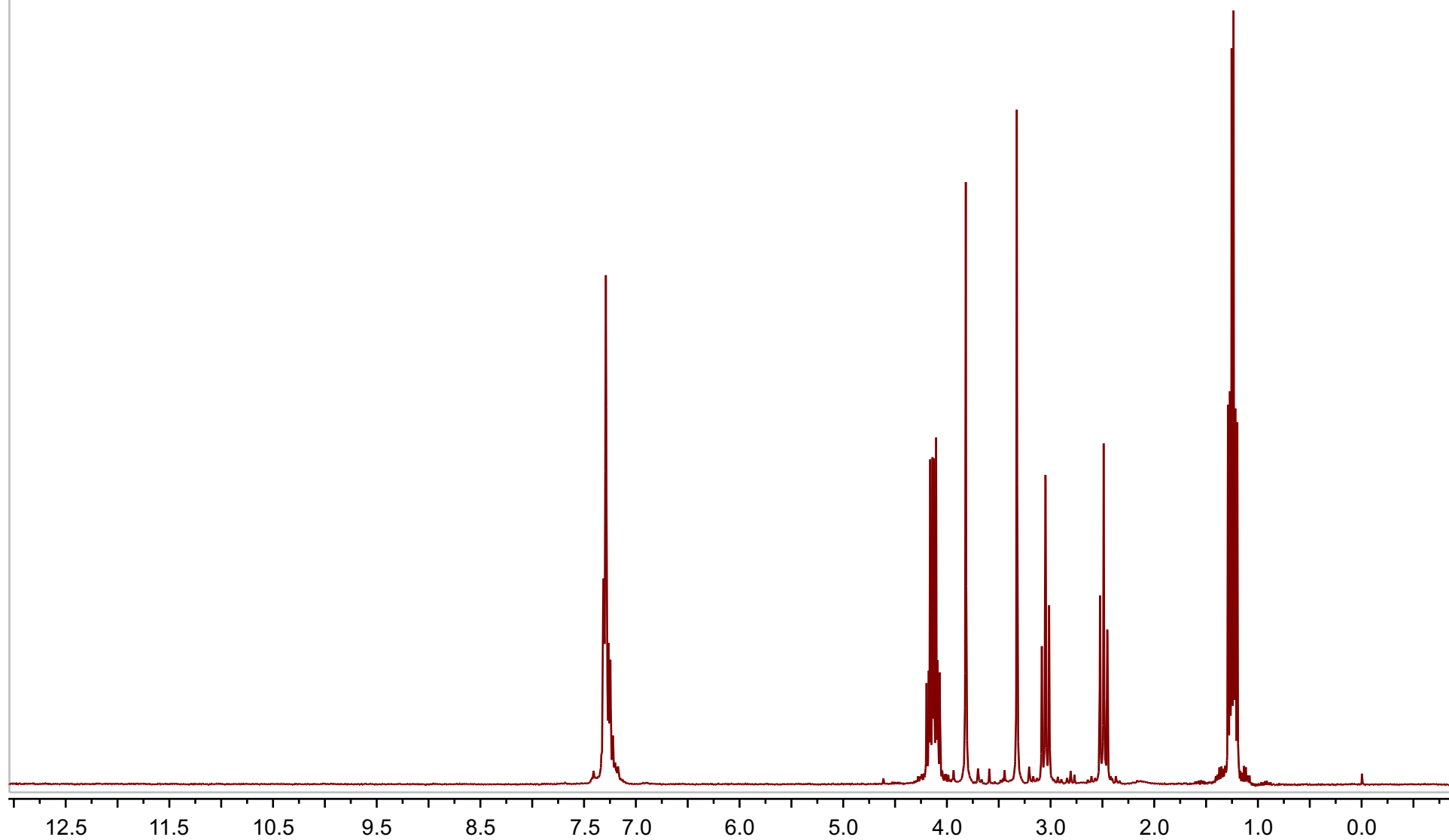
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C16H23NO4	--	293.16271	0.34	3.08524 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1121569.59	294.16998	294.16908	-0.90965	-3.09	--

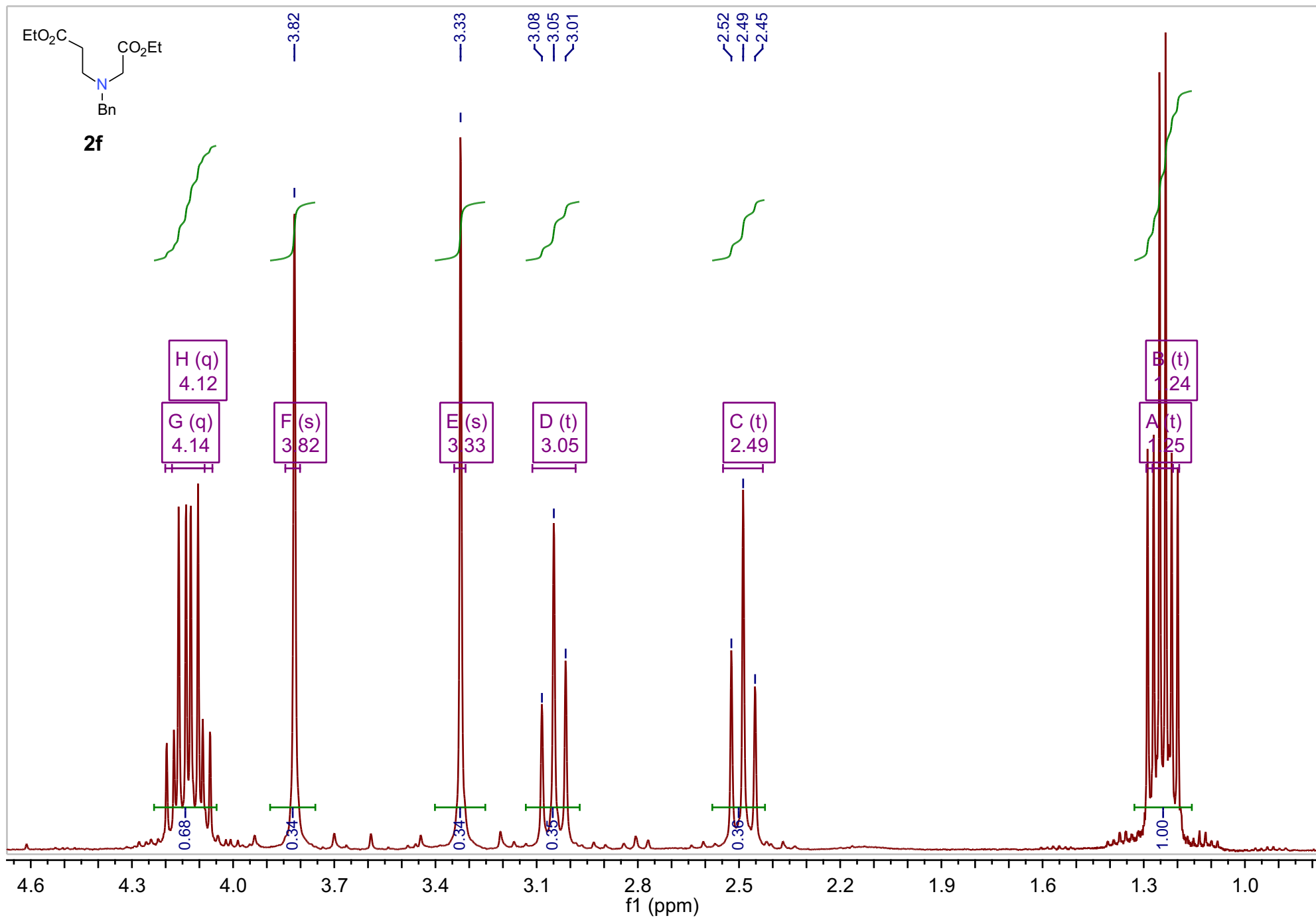
Spectroscopic data. Compound **2f** ^1H NMR



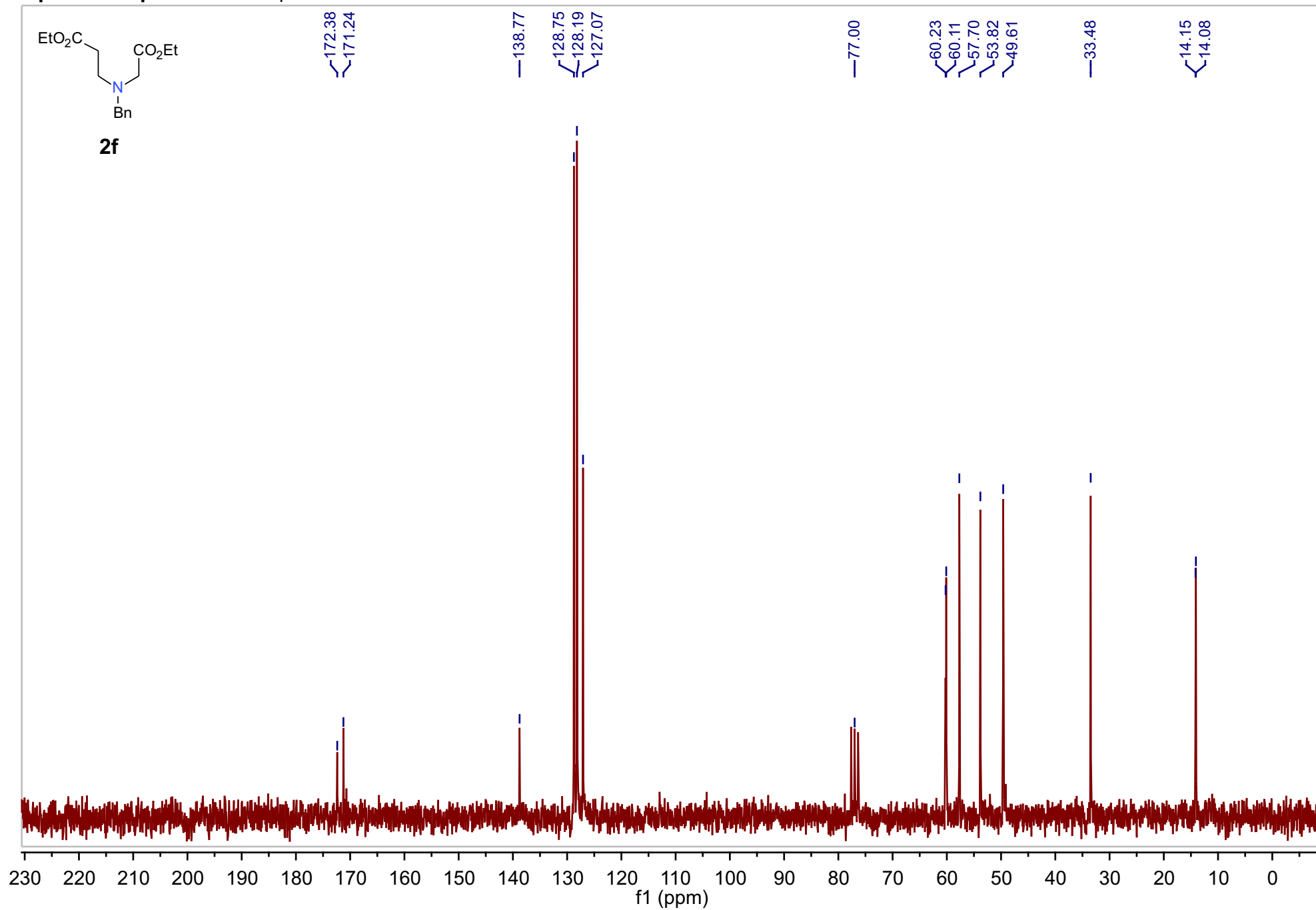
2f



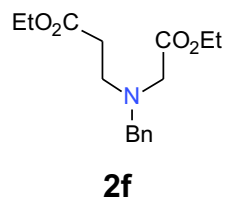
Spectroscopic data. Compound 2f ¹H NMR



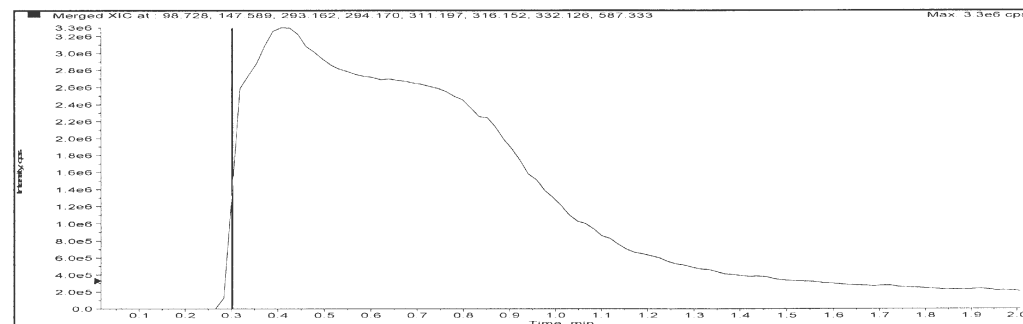
Spectroscopic data. Compound **2f** ^{13}C NMR



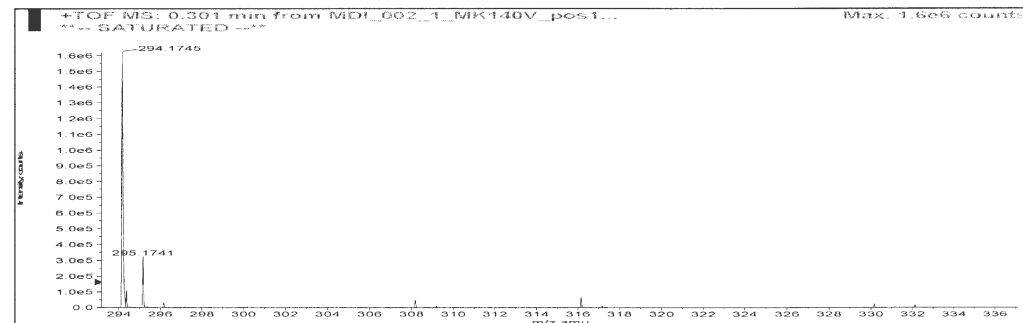
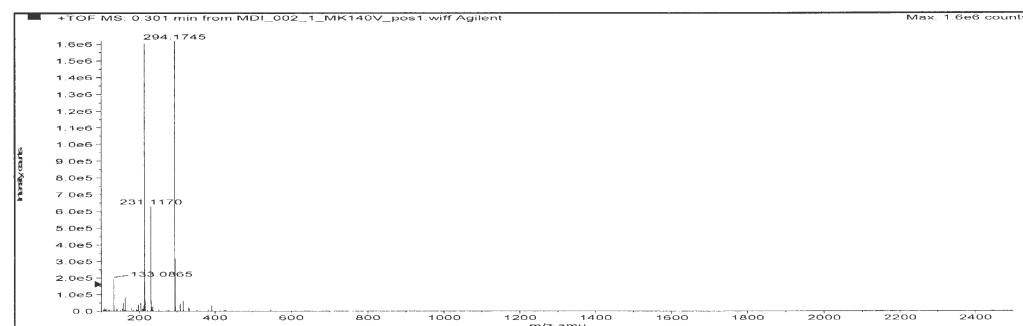
Spectroscopic data. Compound 2f HRMS



Sample Name: MDI_002_1 Sample Location: P1-E3 Sample Id: Operator: Milka
 Data File Name: D:\PE_Sciex_Data\Projects\Roglic\Data\MDI_002_1_MK140V_pos1.wiff Acq Time: August 26 2011, 12:08:52 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml



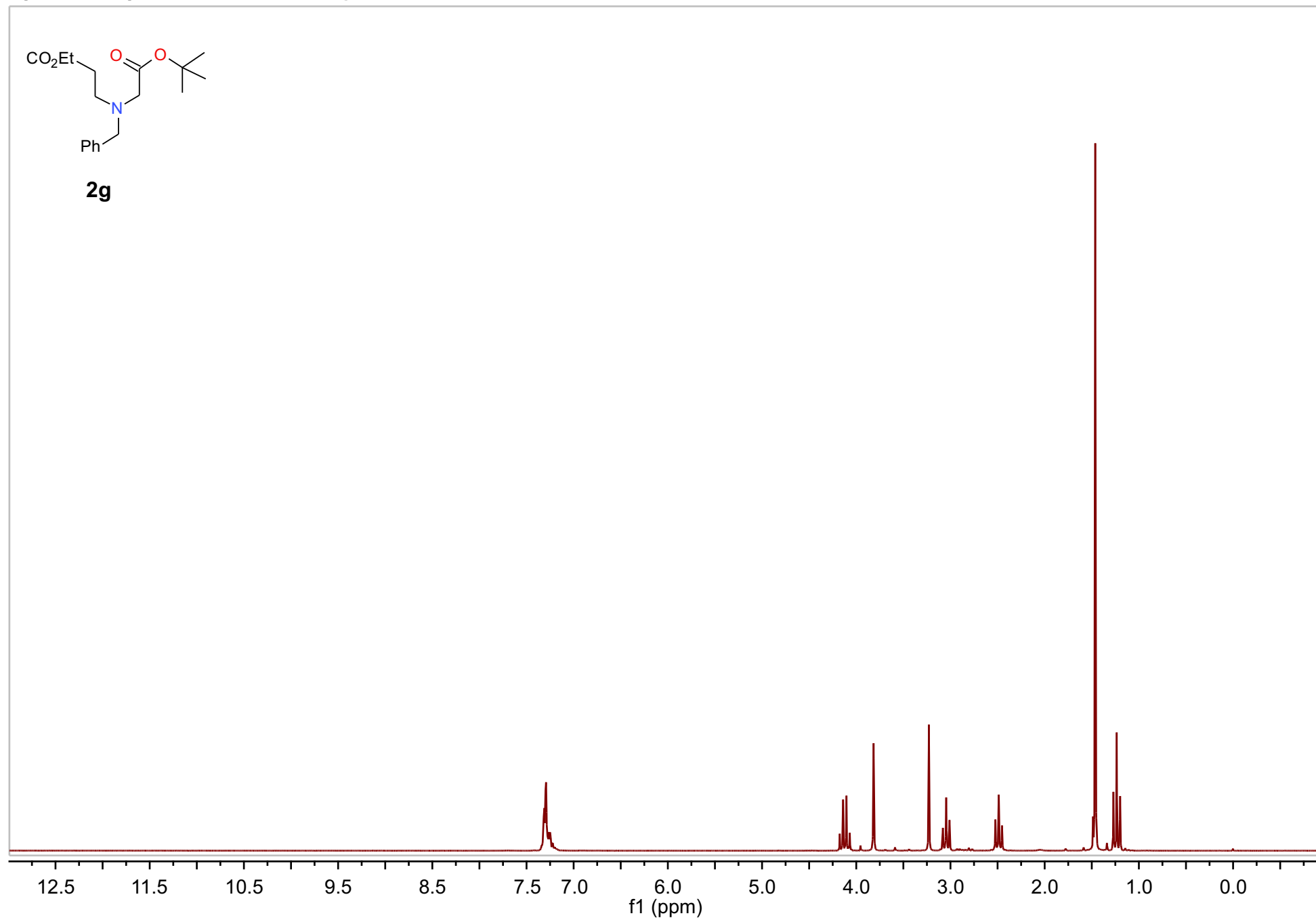
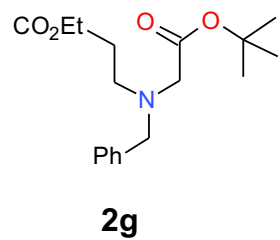
Merged XIC, Period# : 1 Experiment# : 1



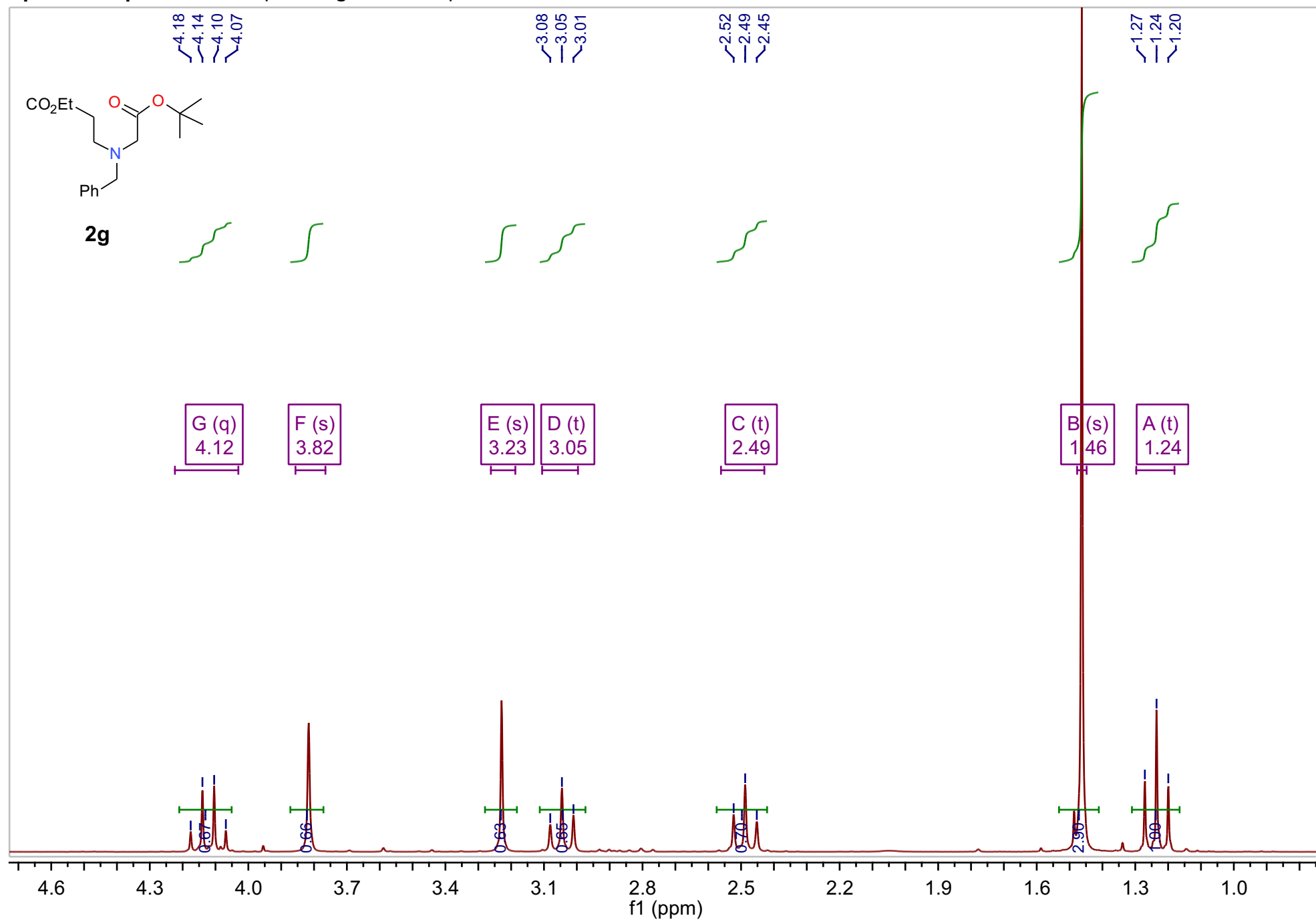
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C16H23NO4	--	293.16271	0.42	1.14600 E8	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1621508.70	294.16998	294.17447	4.48819	15.26	--
[M+Na] ⁺	65982.77	316.15193	316.15251	0.57856	1.83	--
[M+K] ⁺	17201.46	332.12587	332.12637	0.50015	1.51	--

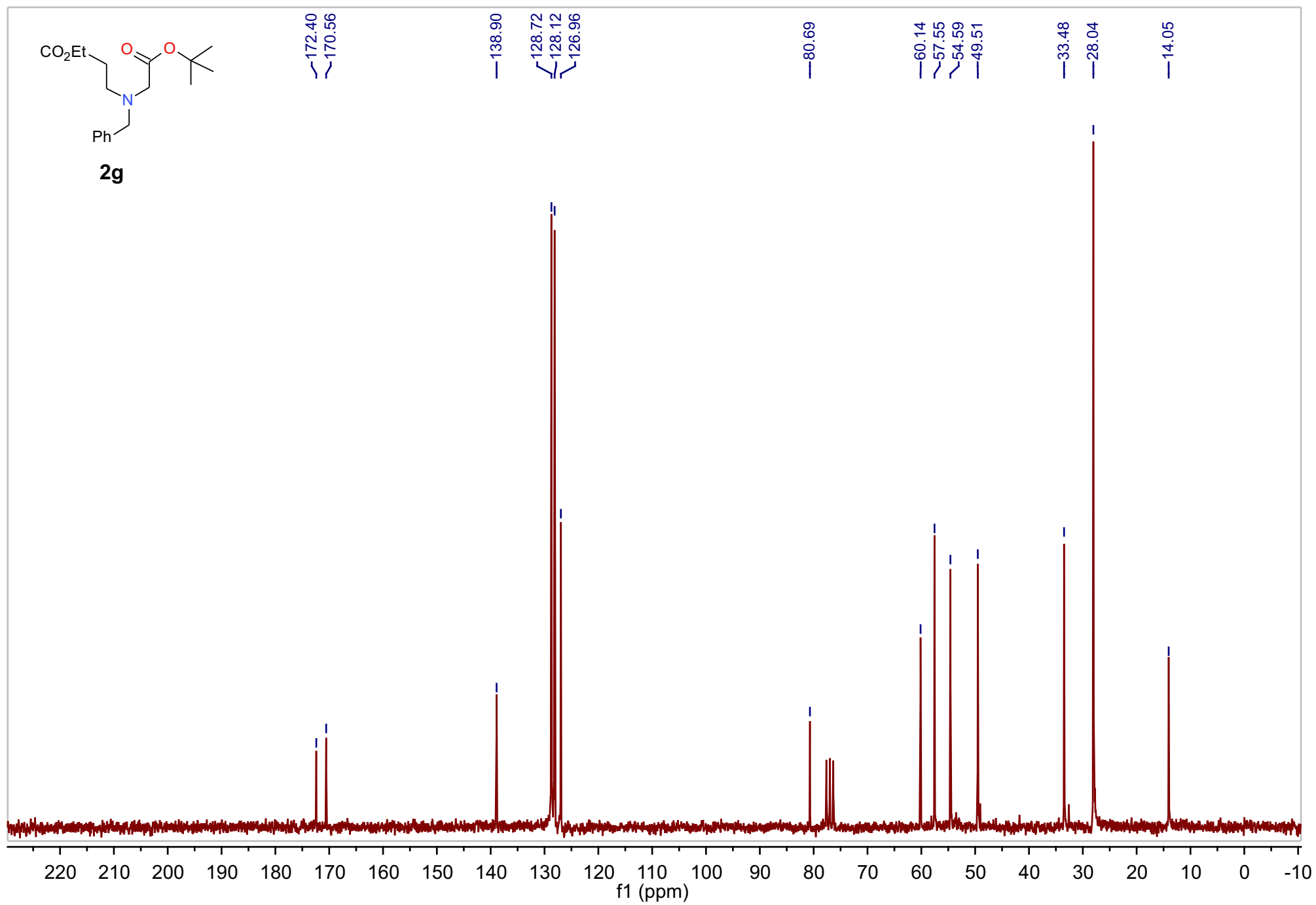
Spectroscopic data. Compound **2g** ^1H NMR



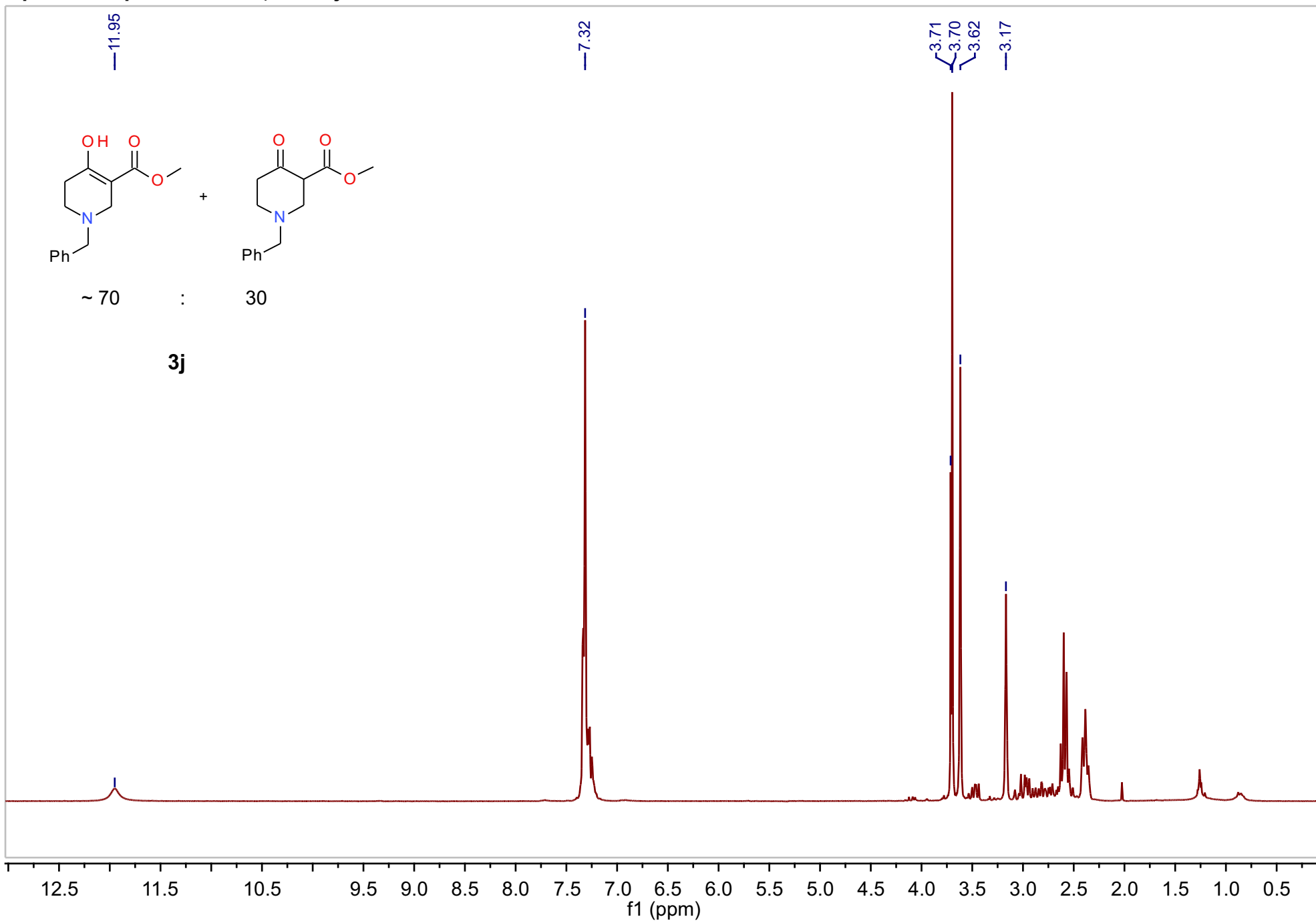
Spectroscopic data. Compound **2g** ¹H NMR expanded



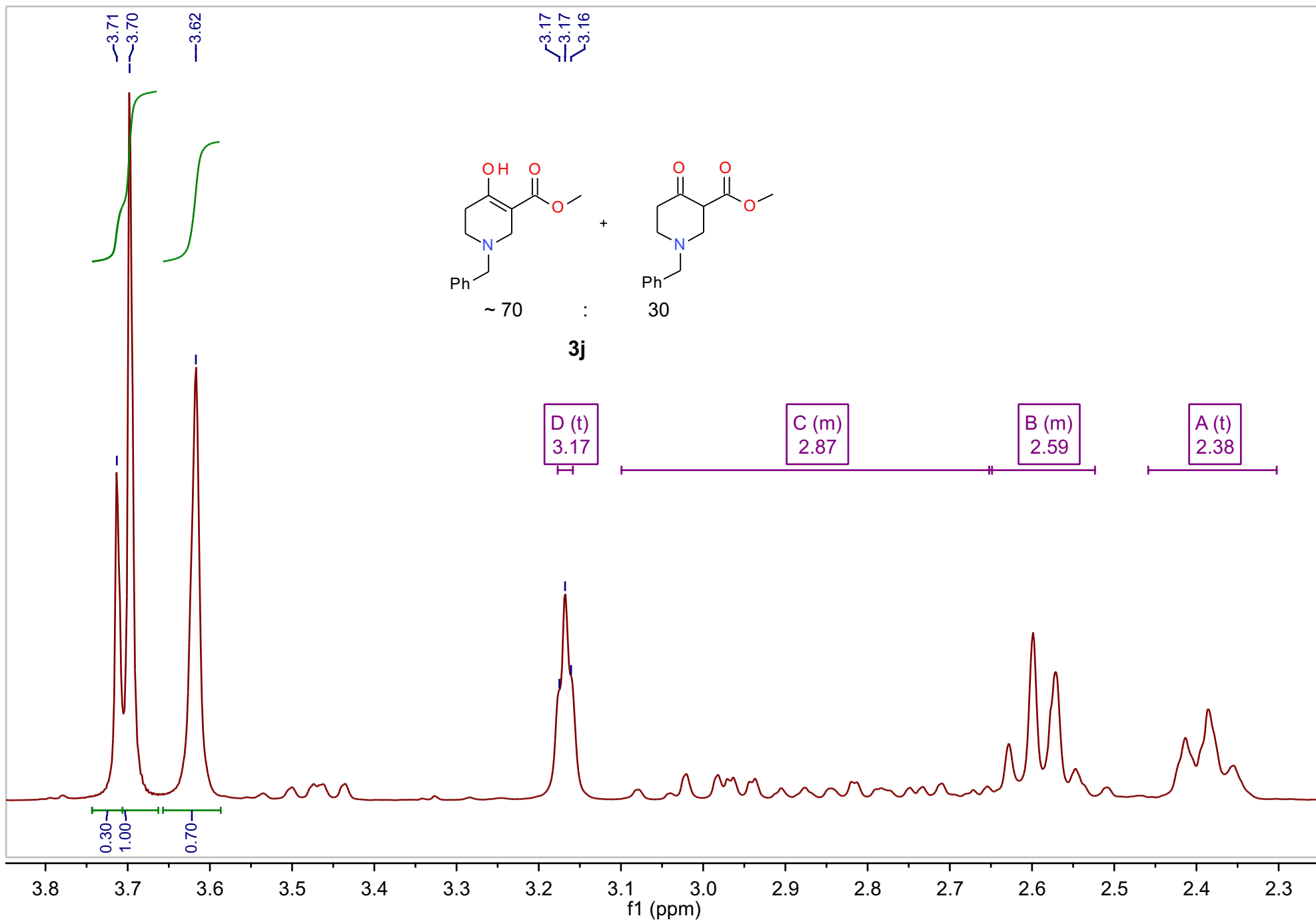
Spectroscopic data. Compound **2g** ^{13}C NMR



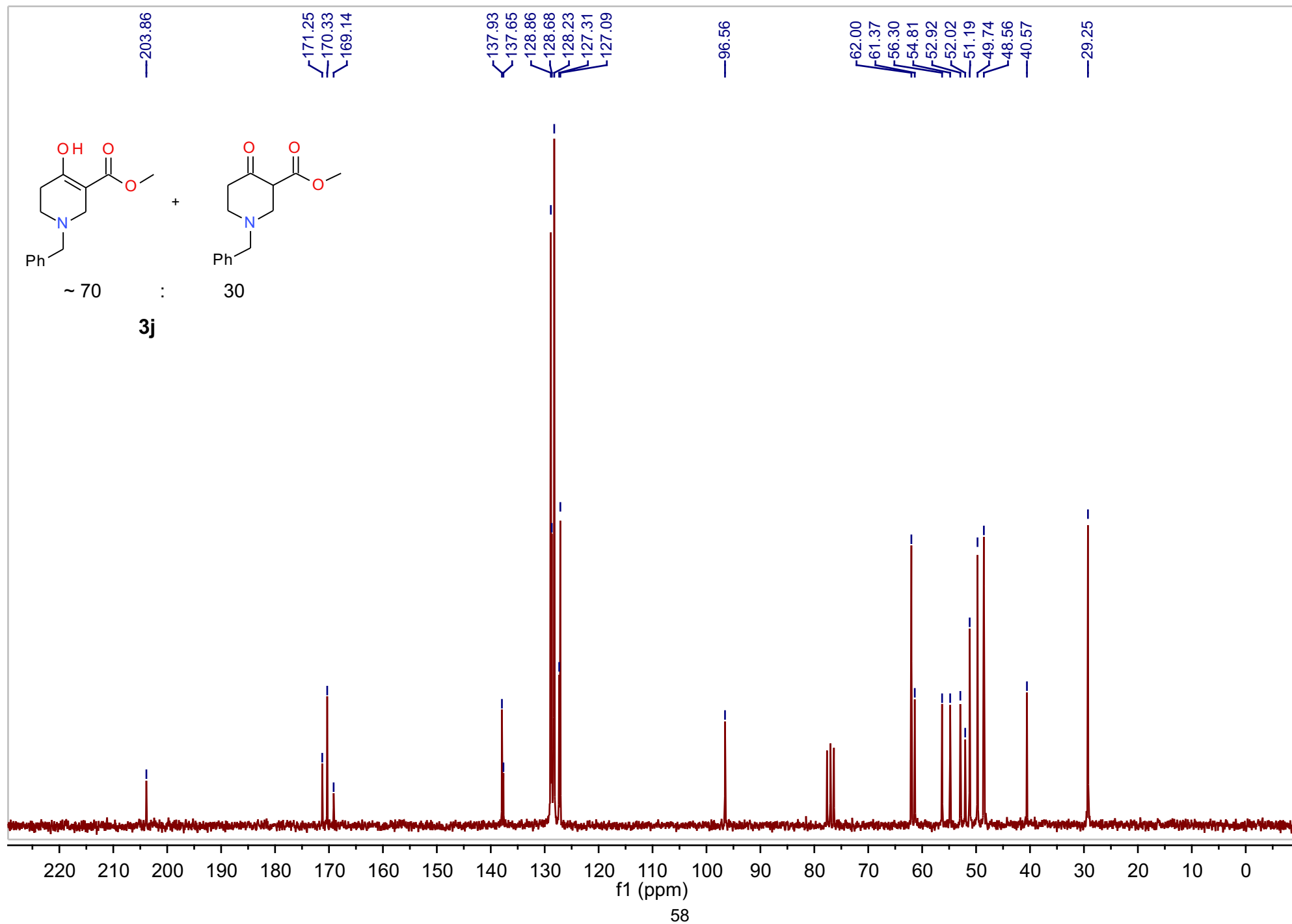
Spectroscopic data. Compound **3j** ¹H NMR



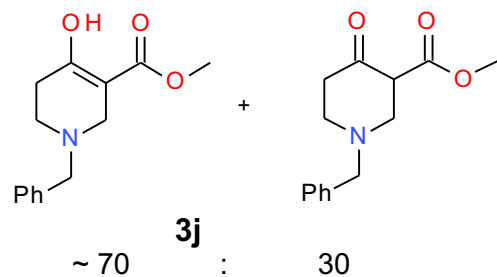
Spectroscopic data. Compound **3j** ¹H NMR expanded



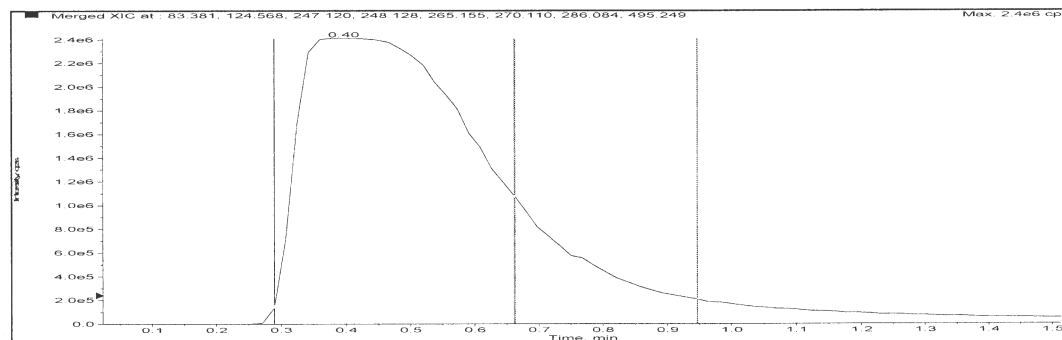
Spectroscopic data. Compound **3j** ^{13}C NMR



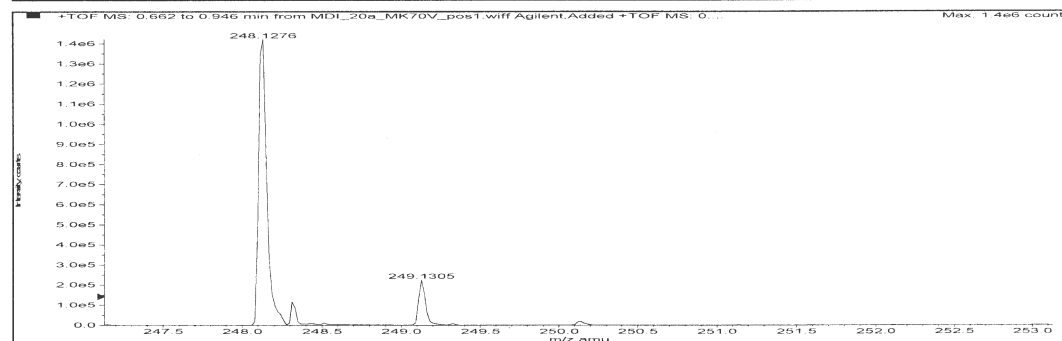
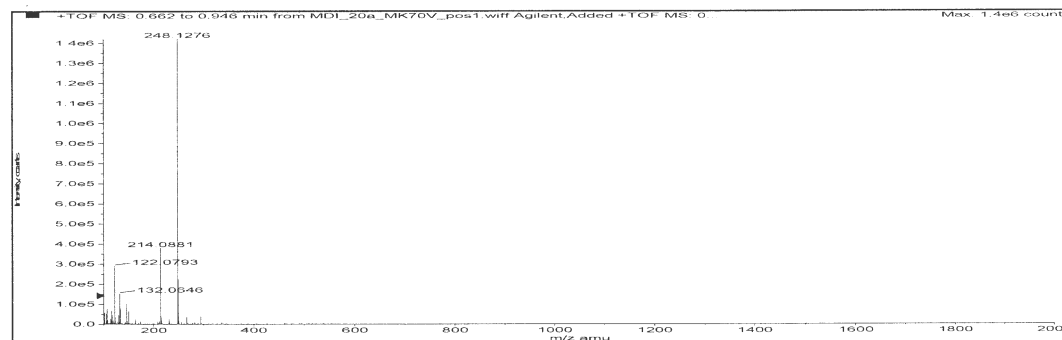
Spectroscopic data. Compound 3j HRMS



Sample Name: 20a Sample Location: P1-F5 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Roglic\Data\MDI_20a_MK70V_pos1.wiff Acq Time: July 18 2012, 04:14:57 PM
 Method: d:\TOF Software\damethods\Night_Seq_Comp_ident1.anml\efc.xml



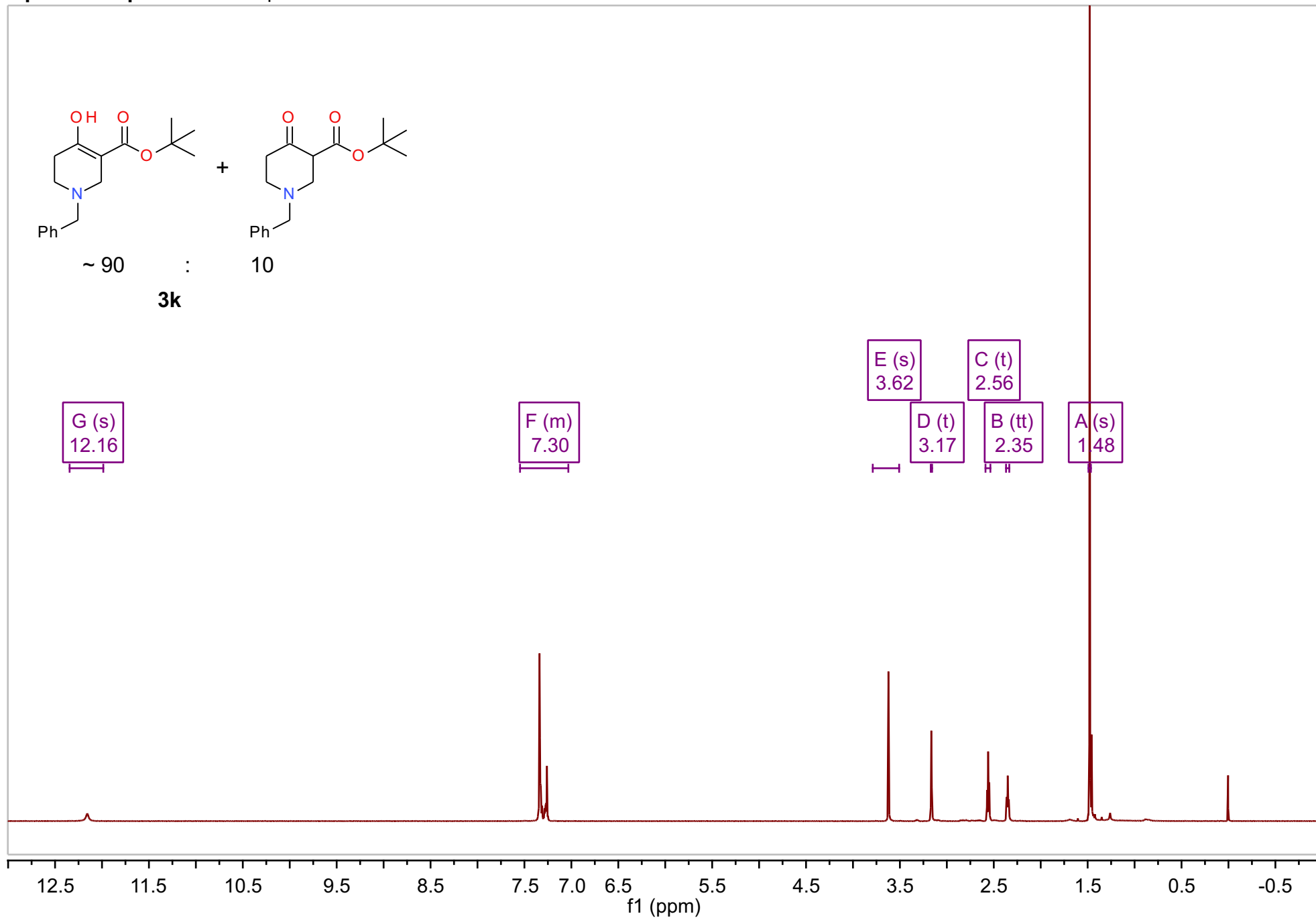
Merged XIC, Period# : 1 Experiment# : 1



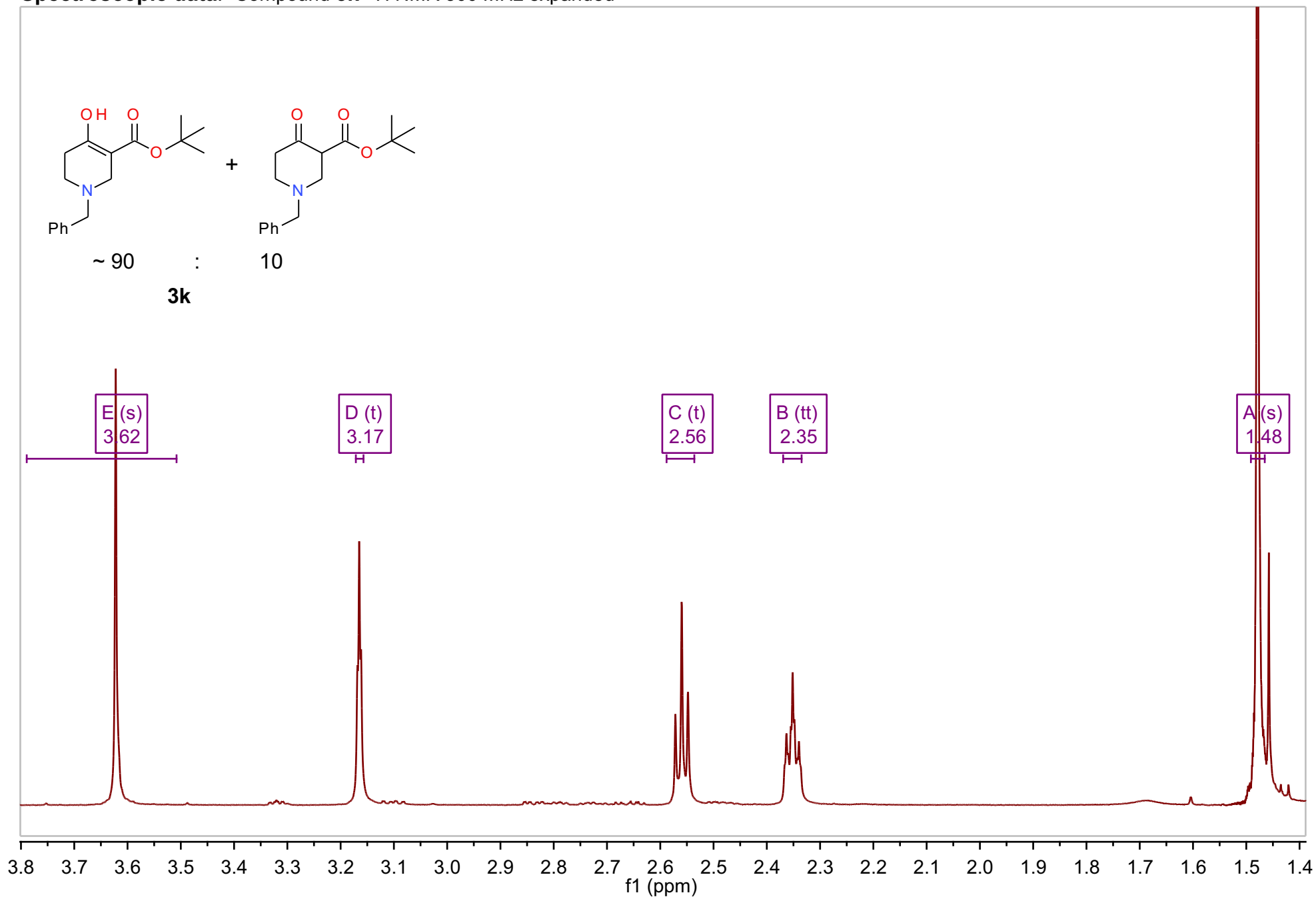
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C14H17NO3	--	247.12084	0.40	5.09171 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1472138.72	248.12812	248.12756	-0.55629	-2.24	--

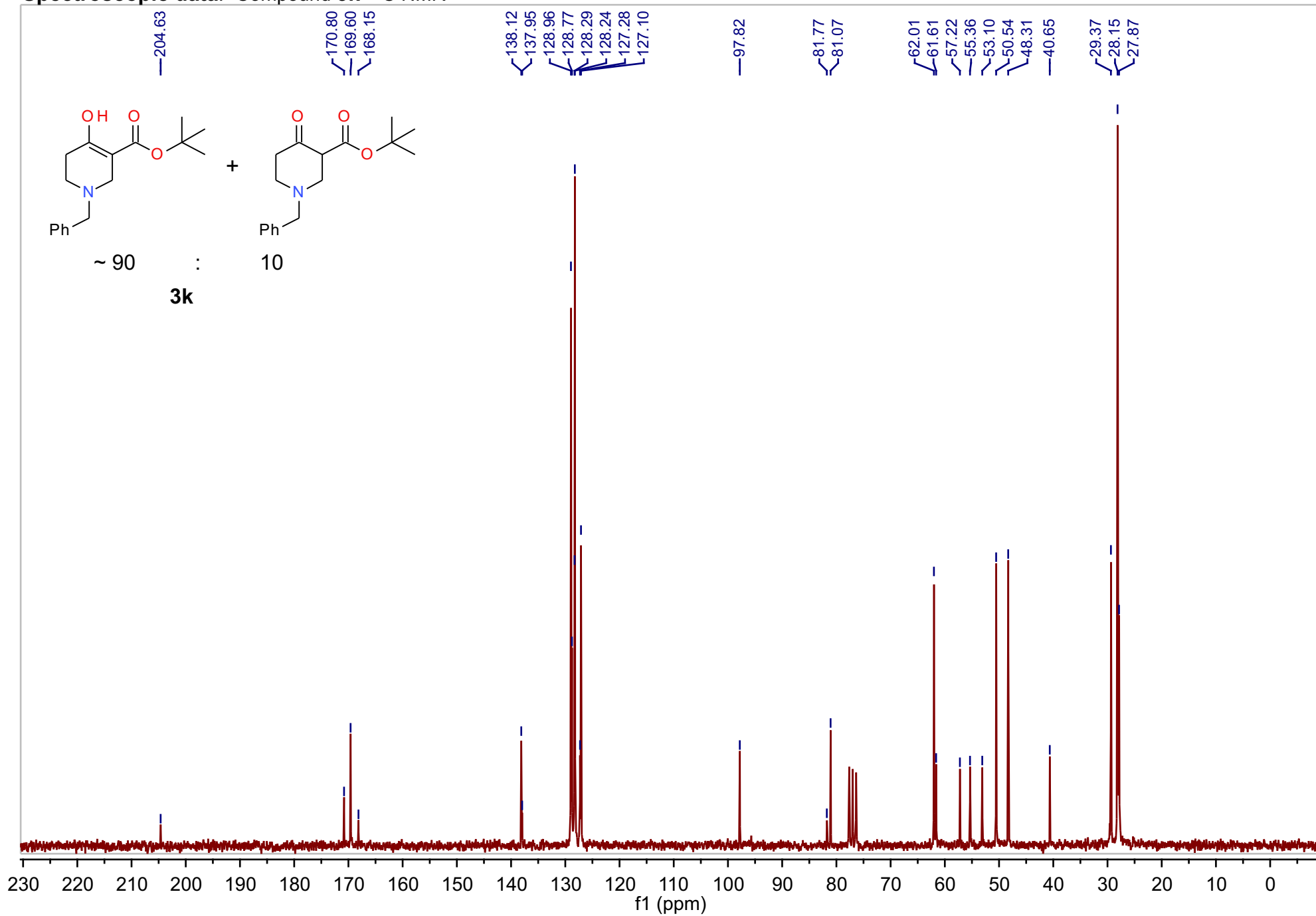
Spectroscopic data. Compound **3k** ¹H NMR 500 MHz



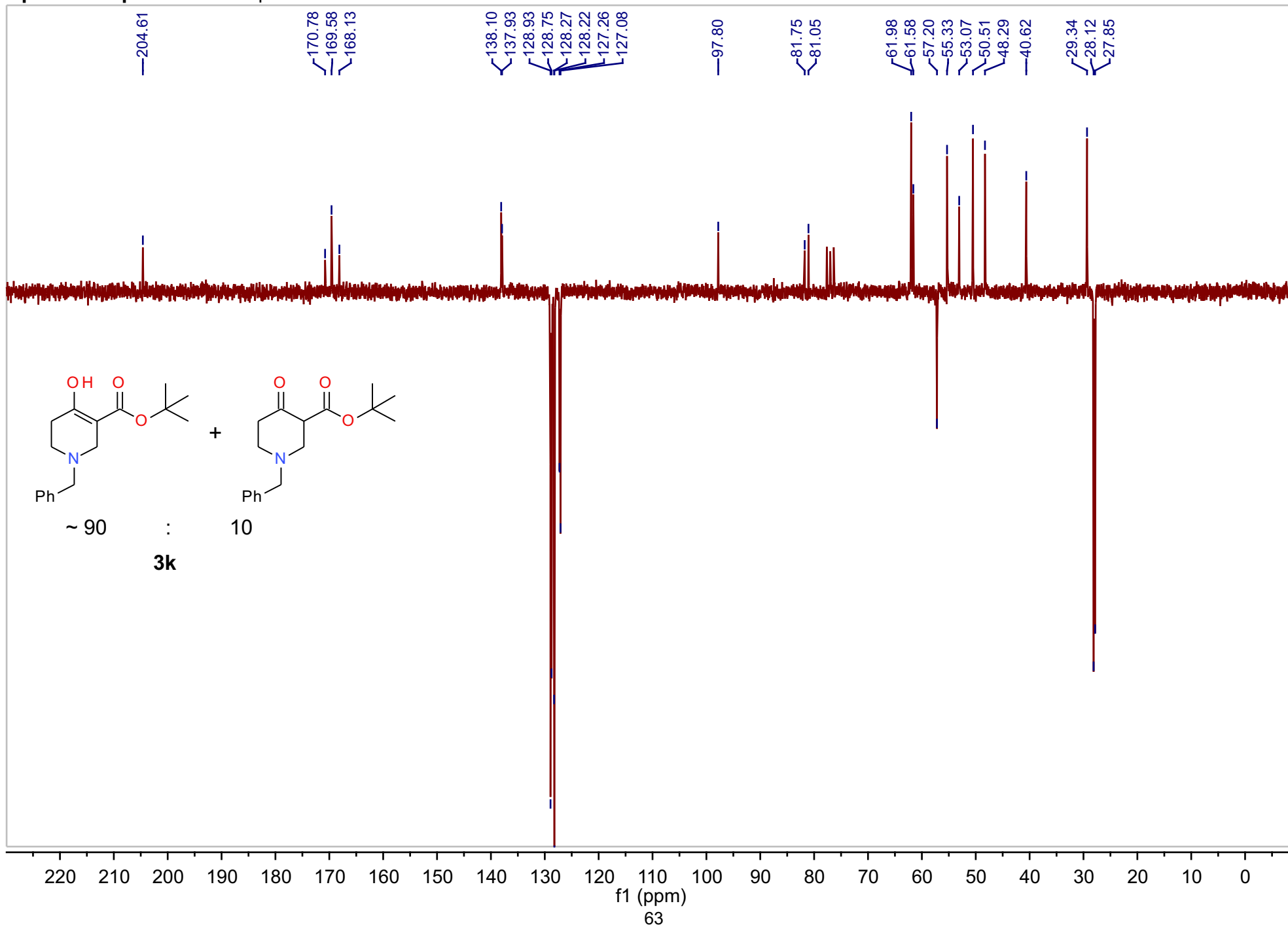
Spectroscopic data. Compound **3k** ^1H NMR 500 MHz expanded



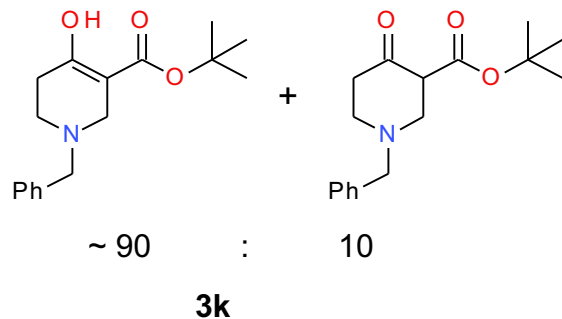
Spectroscopic data. Compound **3k** ¹³C NMR



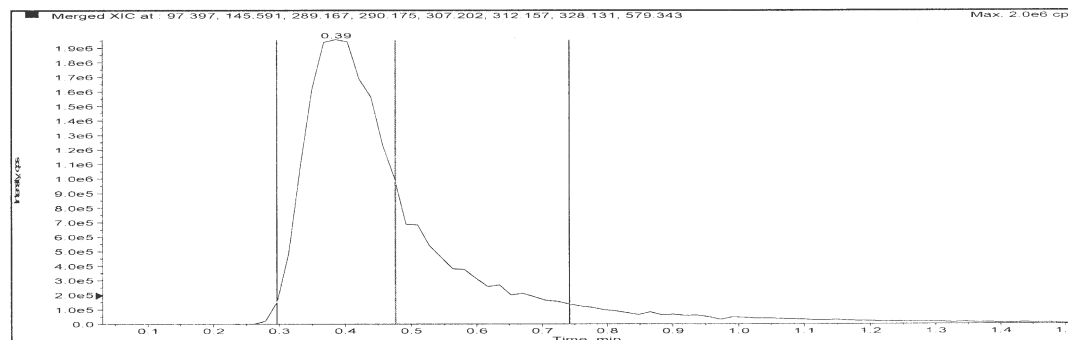
Spectroscopic data. Compound **3k** APT



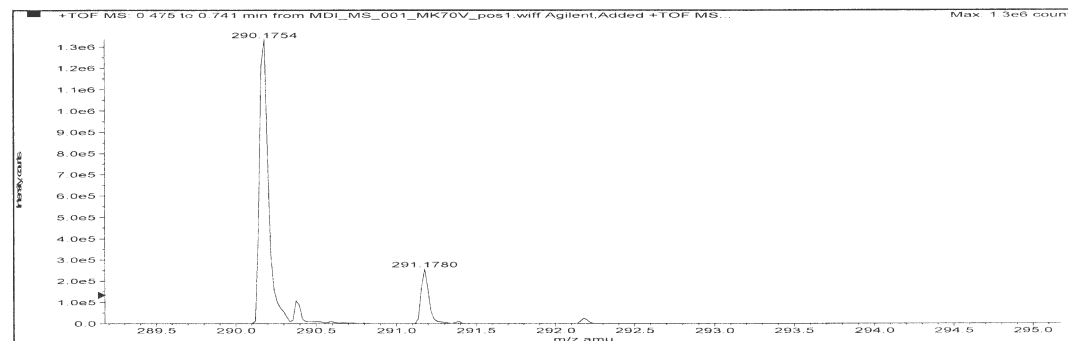
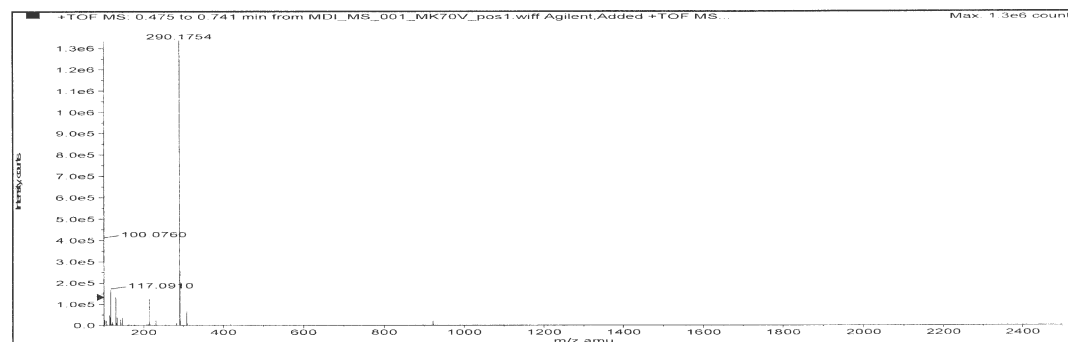
Spectroscopic data. Compound 3k HRMS



Sample Name: MDI_MS_001 Sample Location: P1-D6 Sample Id: Operator: Milka
Data File Name: D:\PE Sciex Data\Projects\Roglic\Data\MDI_MS_001_MK70V_pos1.wiff Acq Time: April 26 2012, 03:23:29 PM
Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anml\efc.xml



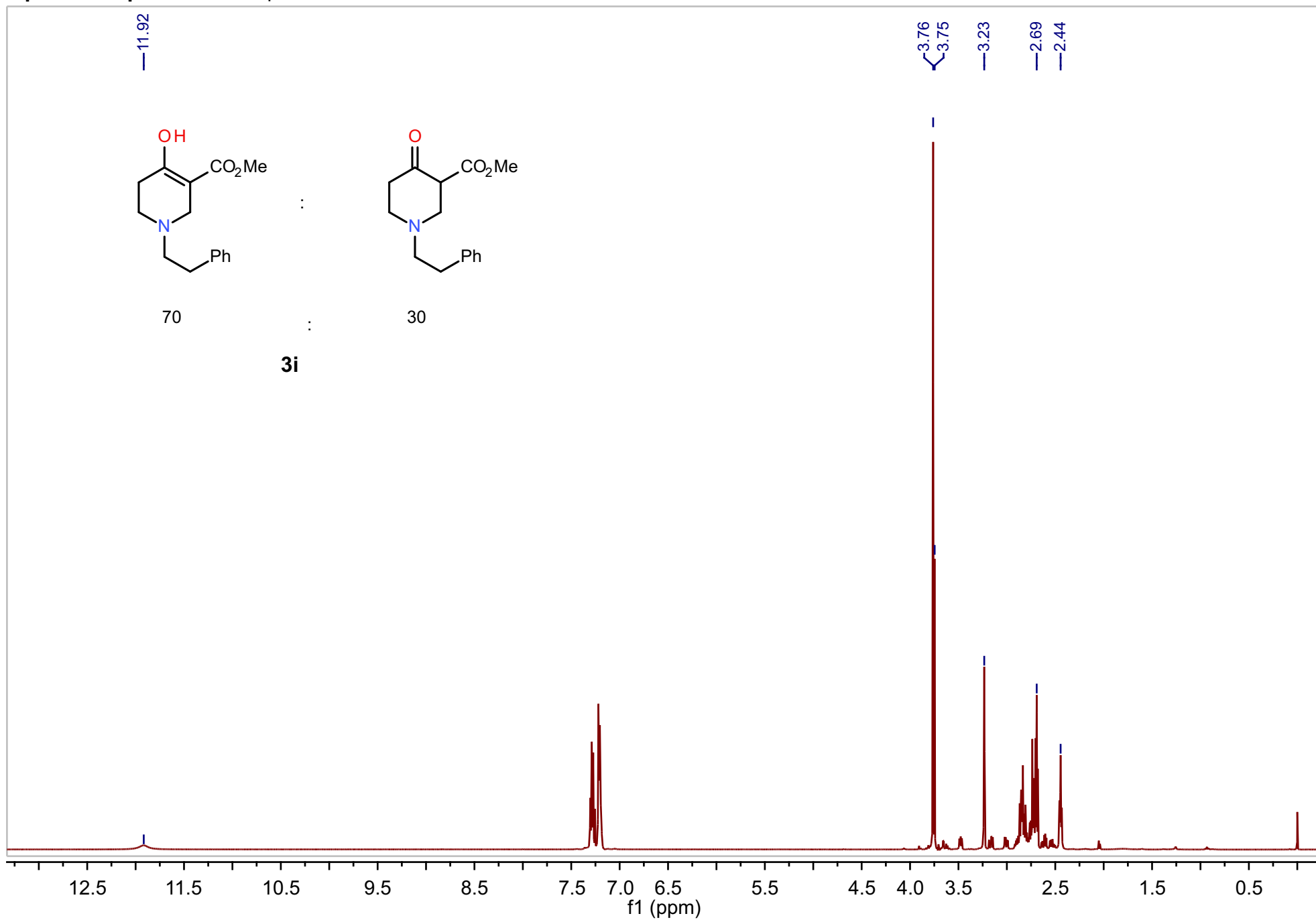
Merged XIC, Period# : 1 Experiment# : 1



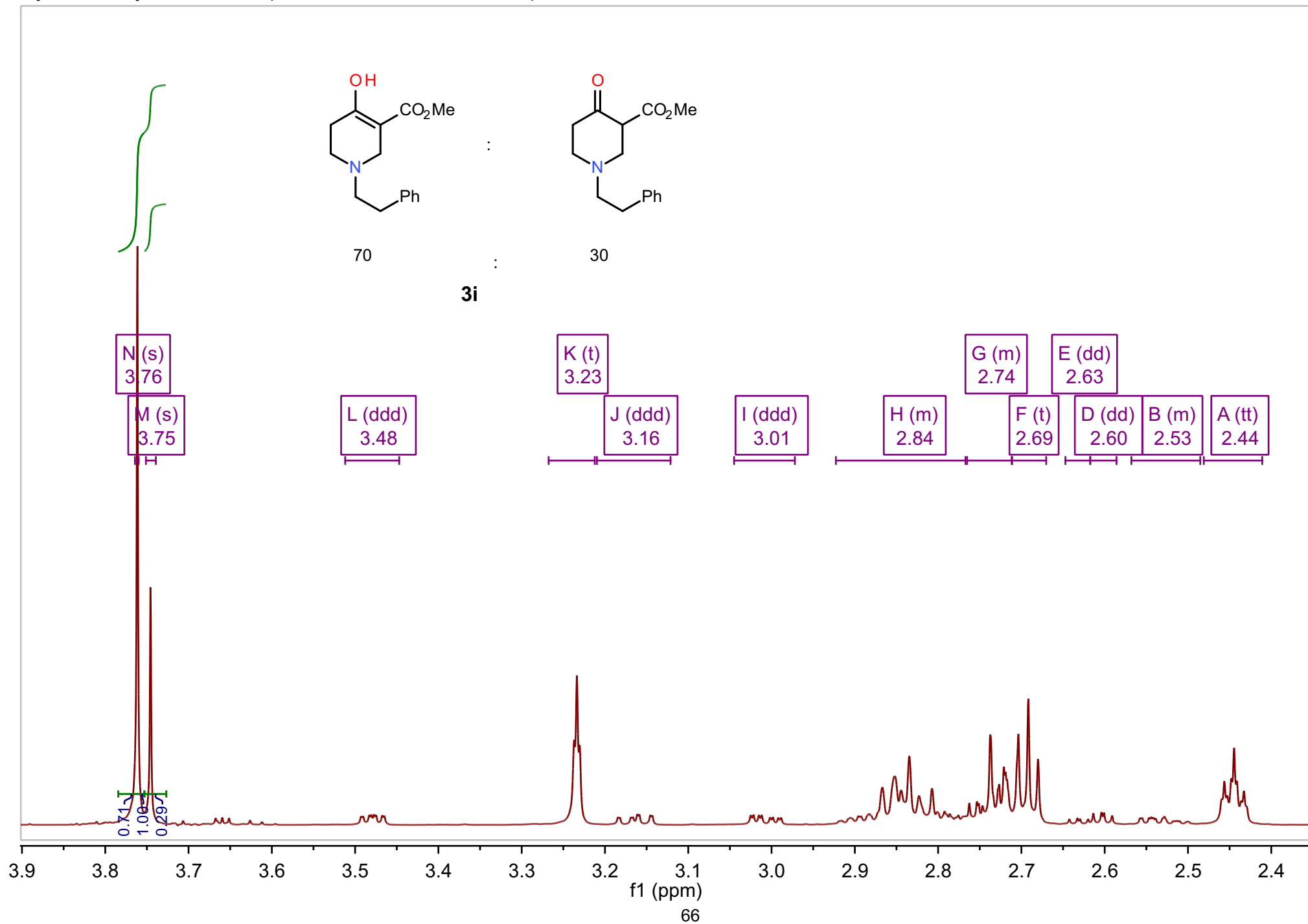
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C17H23NO3	--	289.16779	0.39	2.13424 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1370692.21	290.17507	290.17536	0.28999	1.00	--

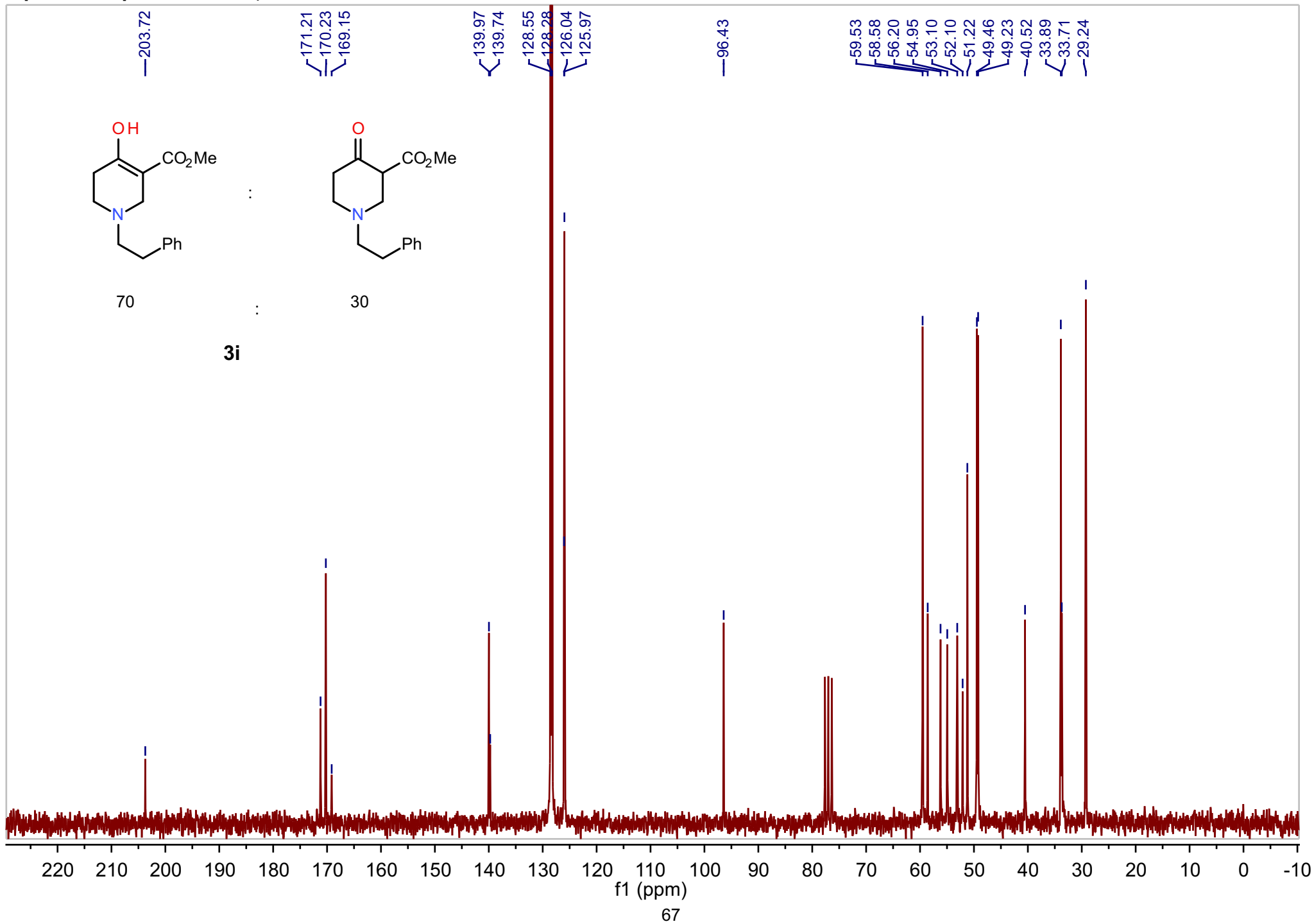
Spectroscopic data. Compound **3i** ¹H NMR 500 MHz



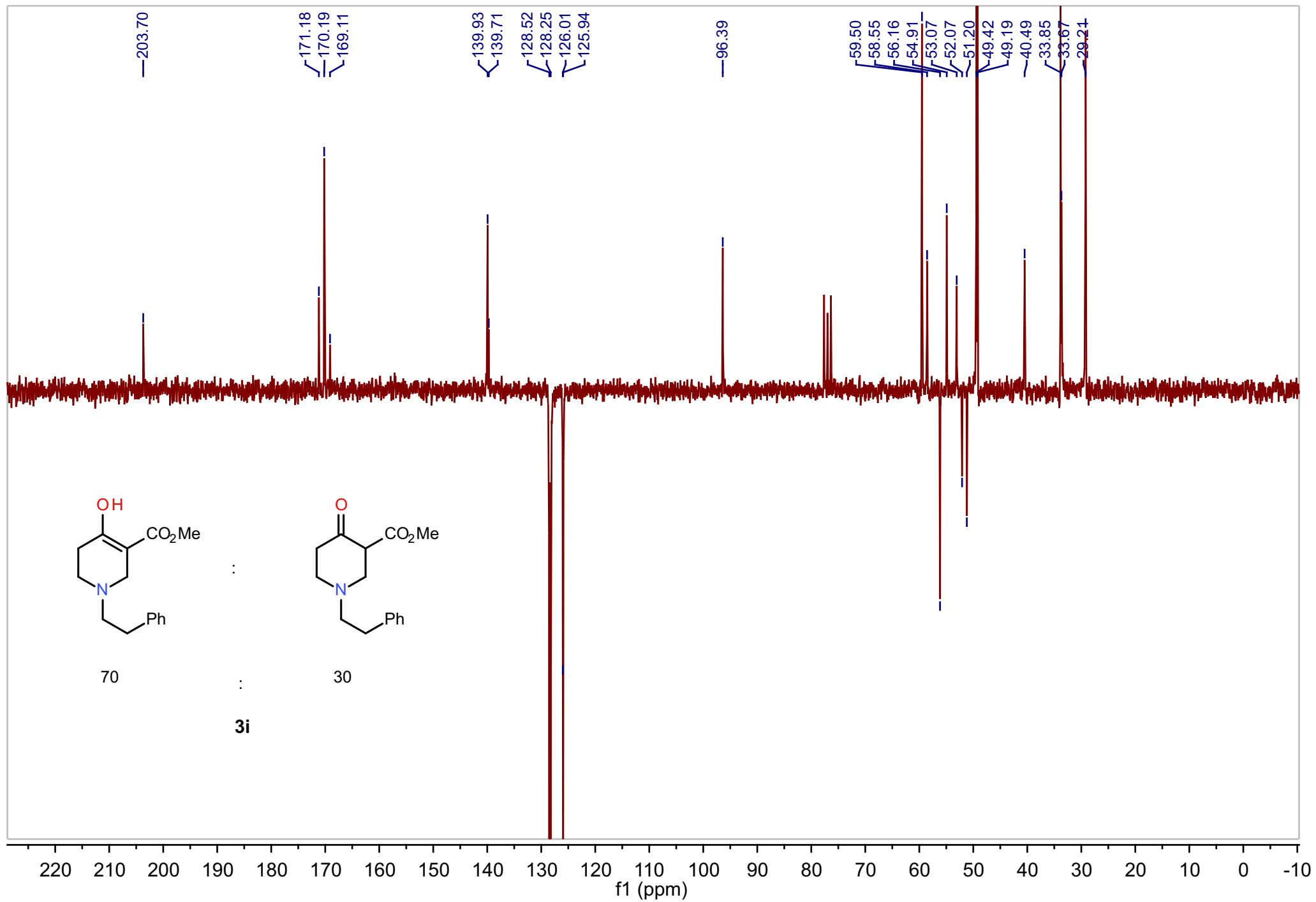
Spectroscopic data. Compound **3i** ¹H NMR 500 MHz expanded



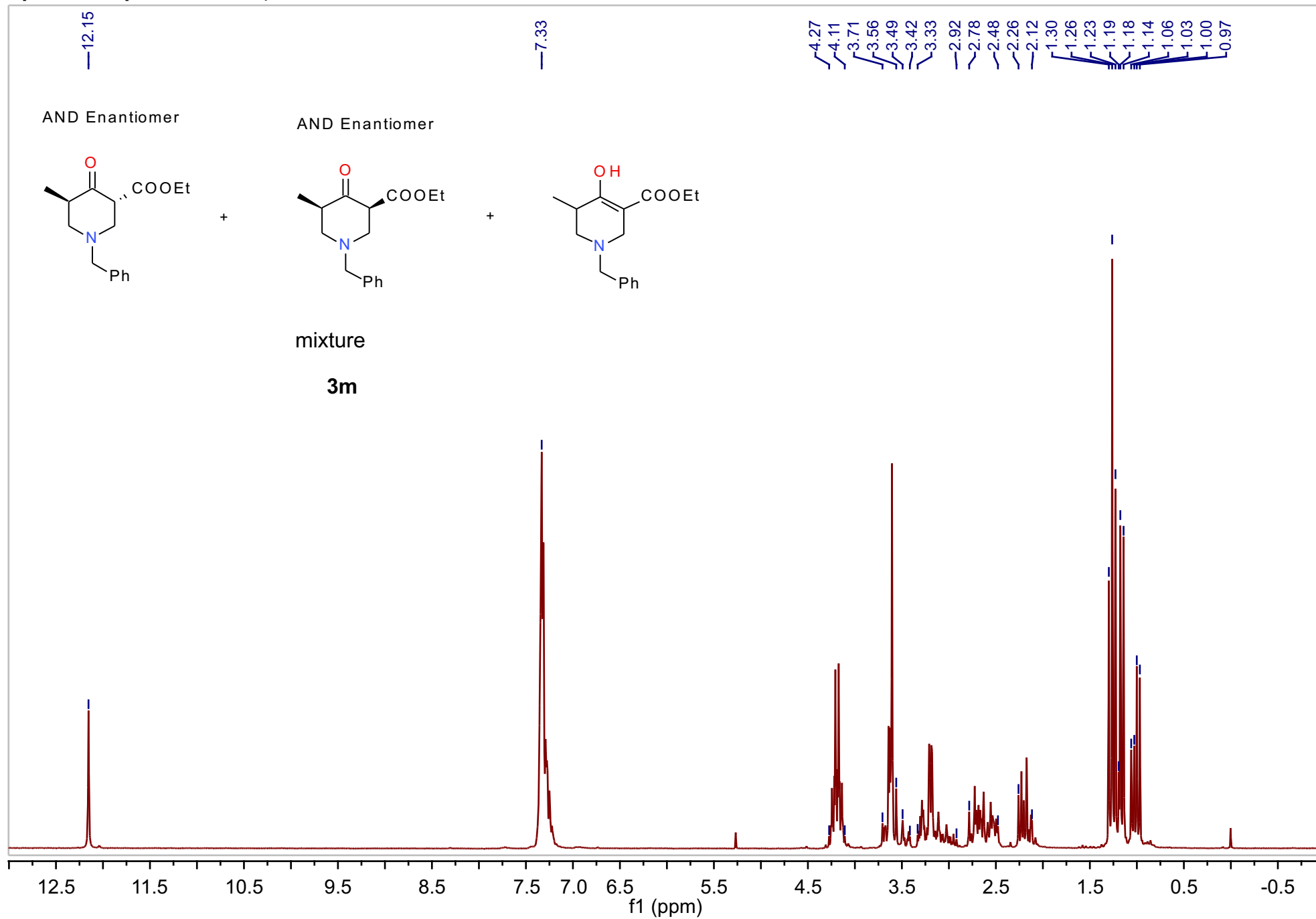
Spectroscopic data. Compound **3i** ¹³C NMR



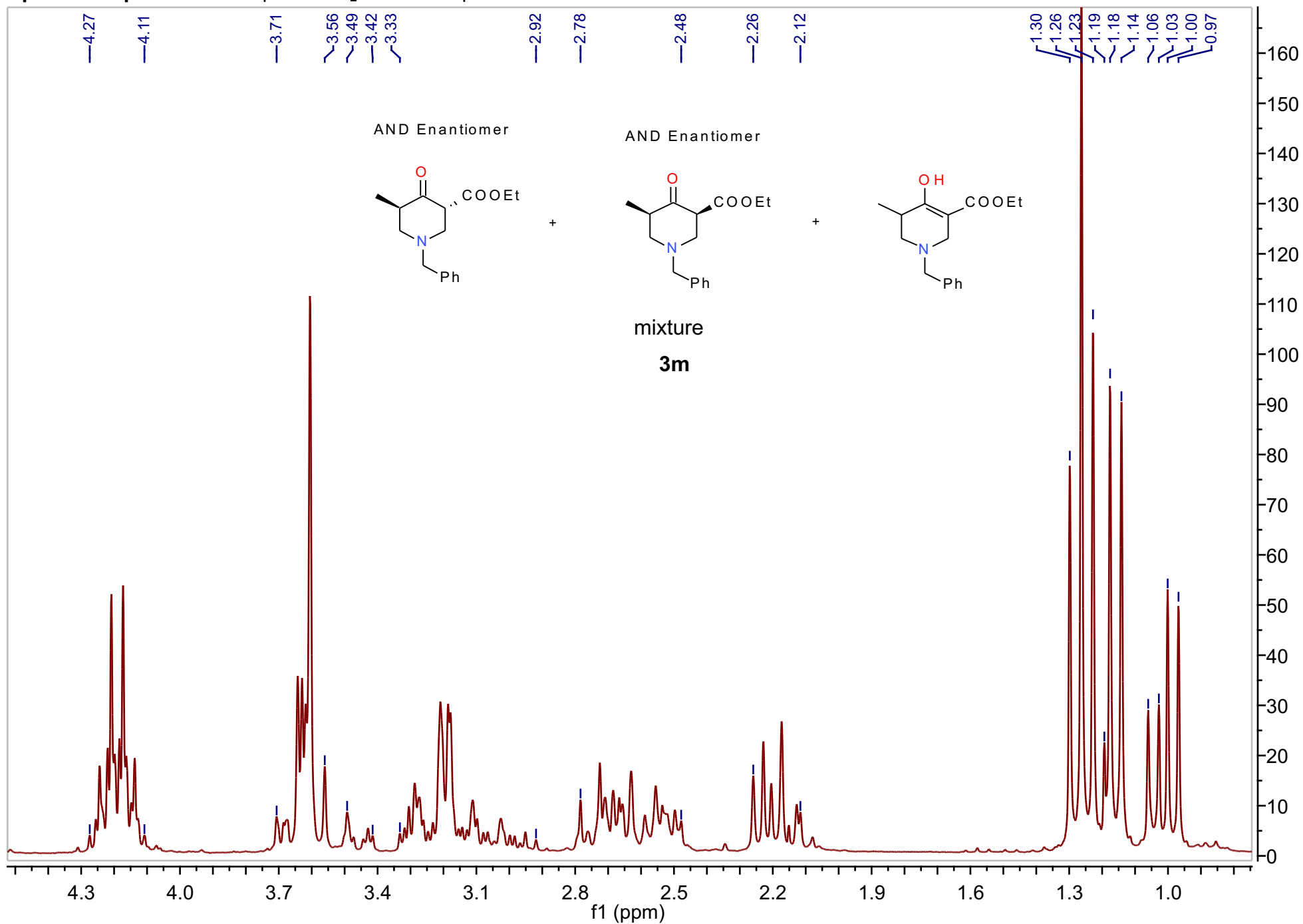
Spectroscopic data. Compound **3i** ¹C APT



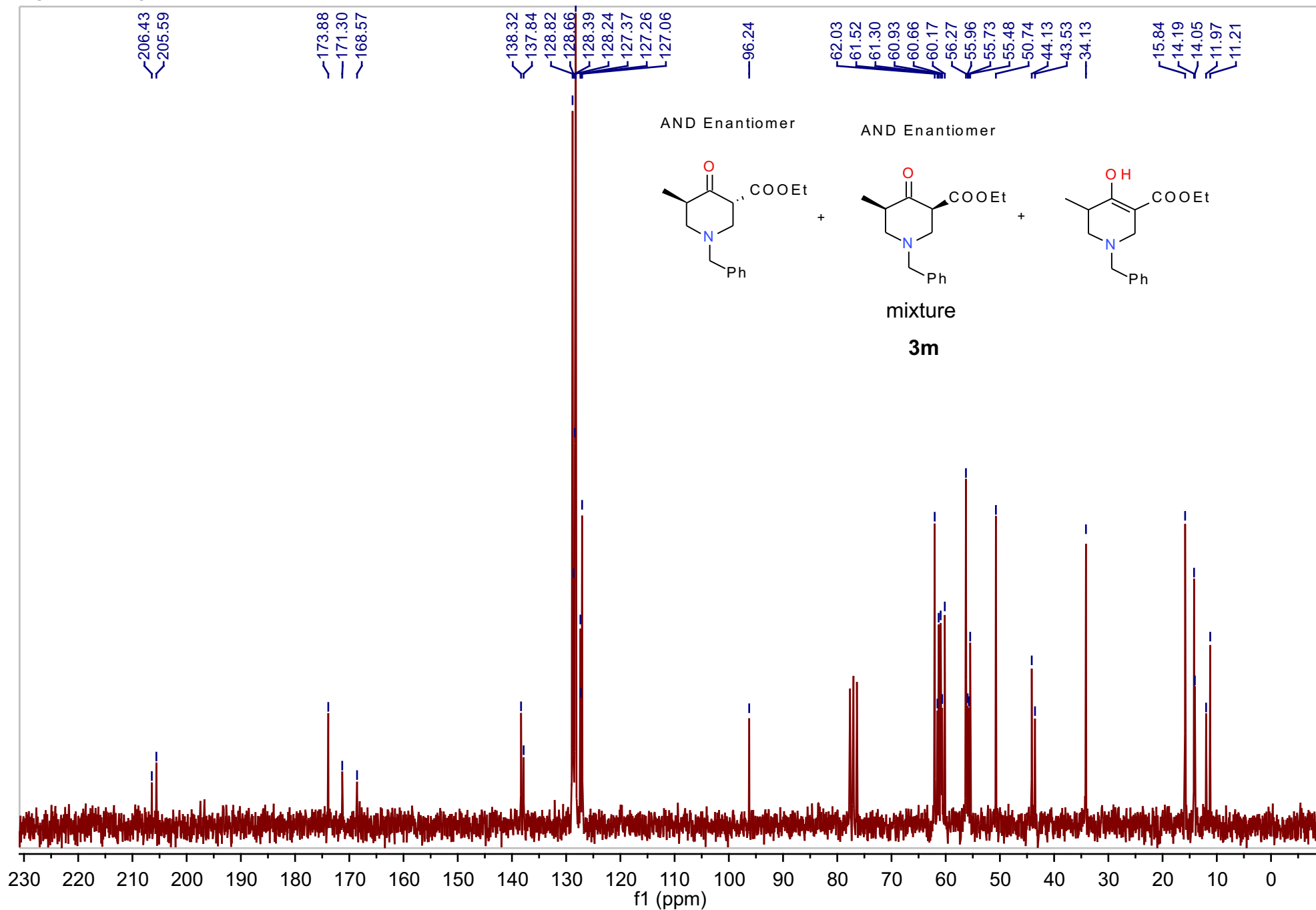
Spectroscopic data. Compound 3m_ ¹H NMR



Spectroscopic data. Compound 3m_ ¹H NMR expanded

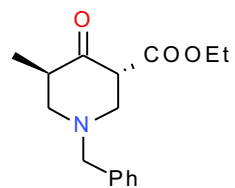


Spectroscopic data. Compound 3m_ ¹³C NMR

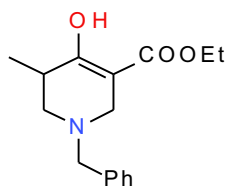
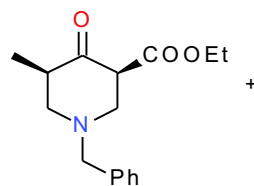


Spectroscopic data. Compound 3m_HRMS

AND Enantiomer

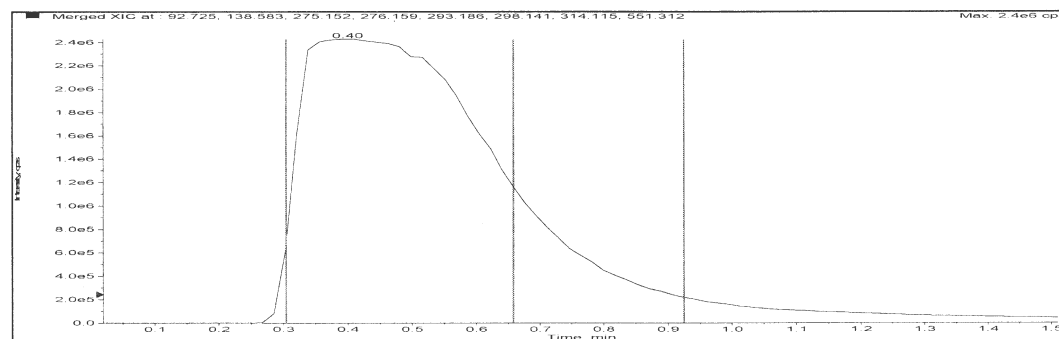


AND Enantiomer

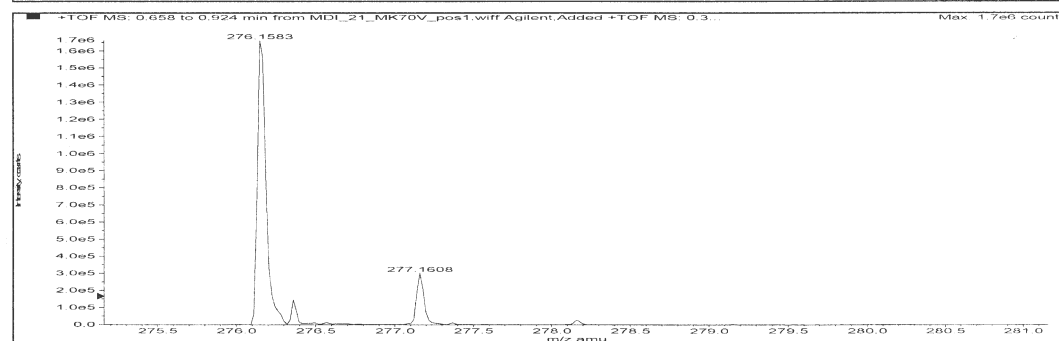
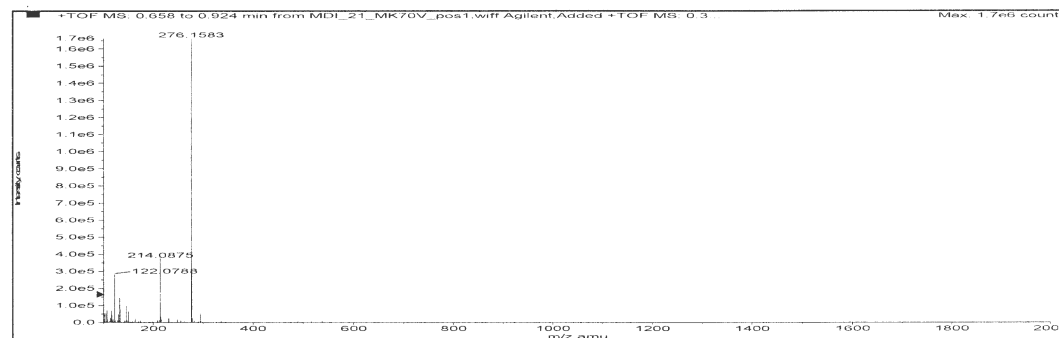


mixture
3m

Sample Name: 21 Sample Location: P1-F6 Sample Id: Operator: Milka
Data File Name: D:\PE Sciex Data\Projects\Roglic\Data\MDI_21_MK70V_pos1.wiff Acq Time: July 18 2012, 04:17:26 PM
Method: d:\TOF Software\damethods\Night_Seq_Comp_ident1.am\efc.xml



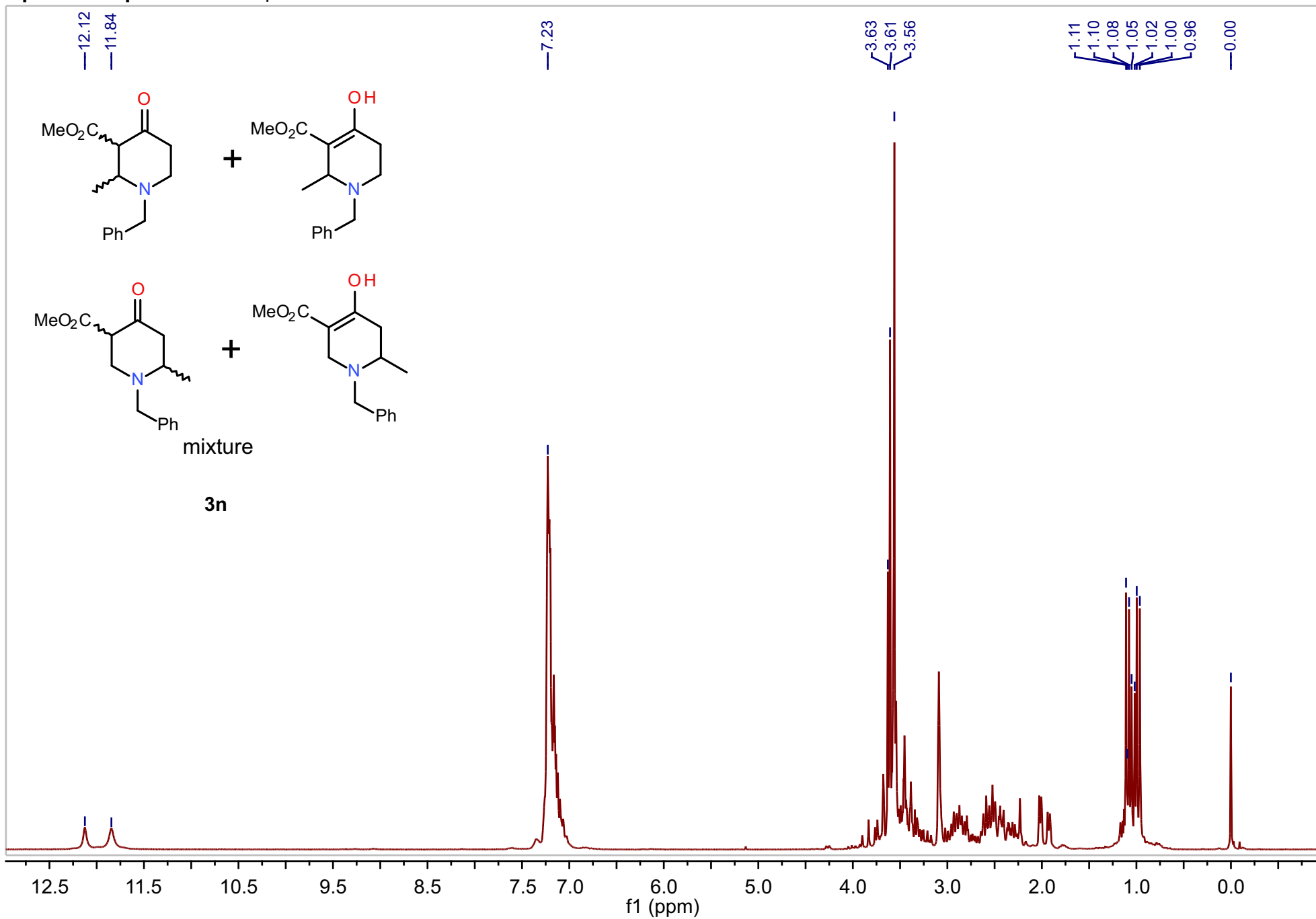
Merged XIC, Period# : 1 Experiment# : 1



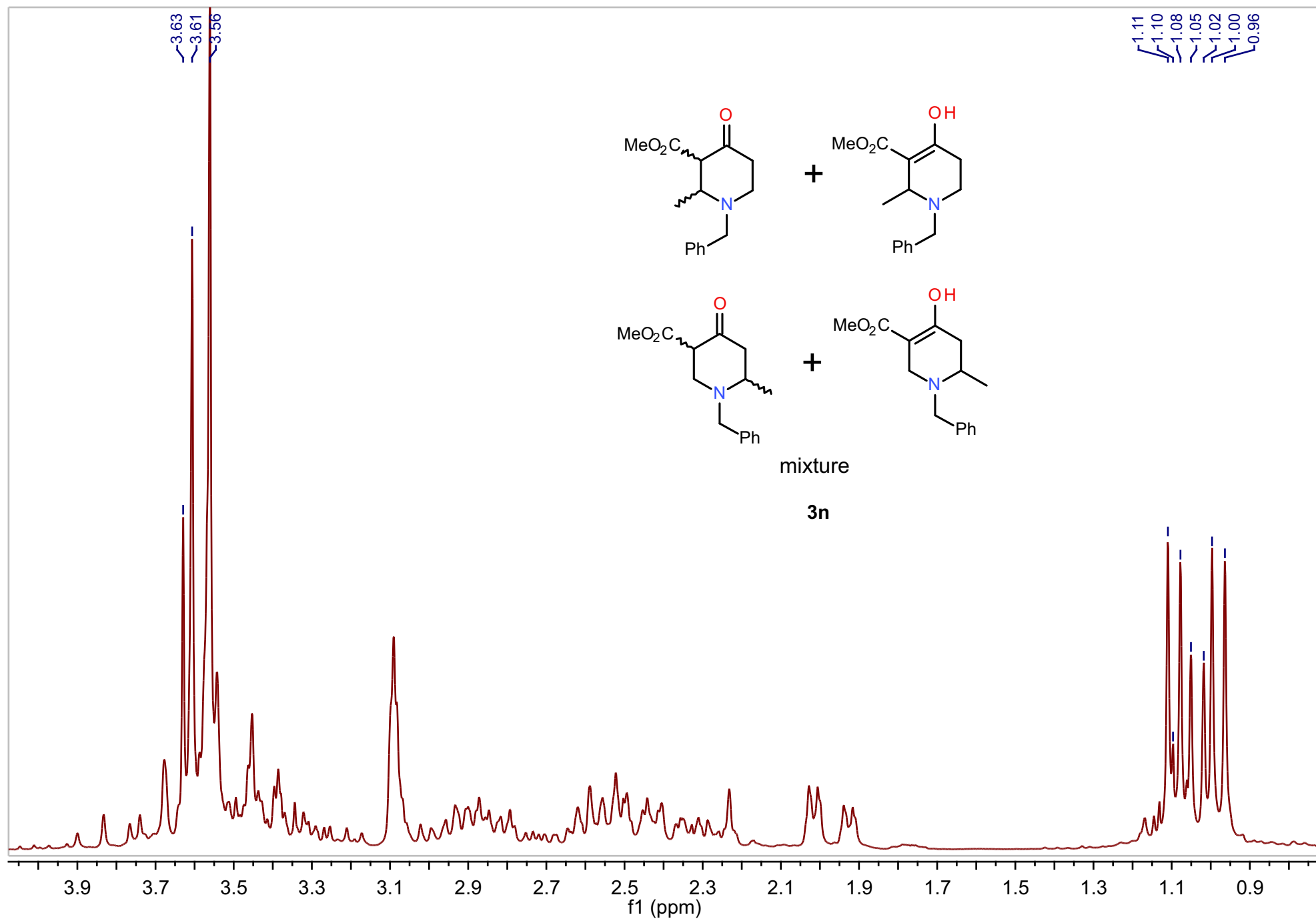
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C16H21NO3	--	275.15214	0.40	5.21218 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1742203.78	276.15942	276.15833	-1.09331	-3.96	--

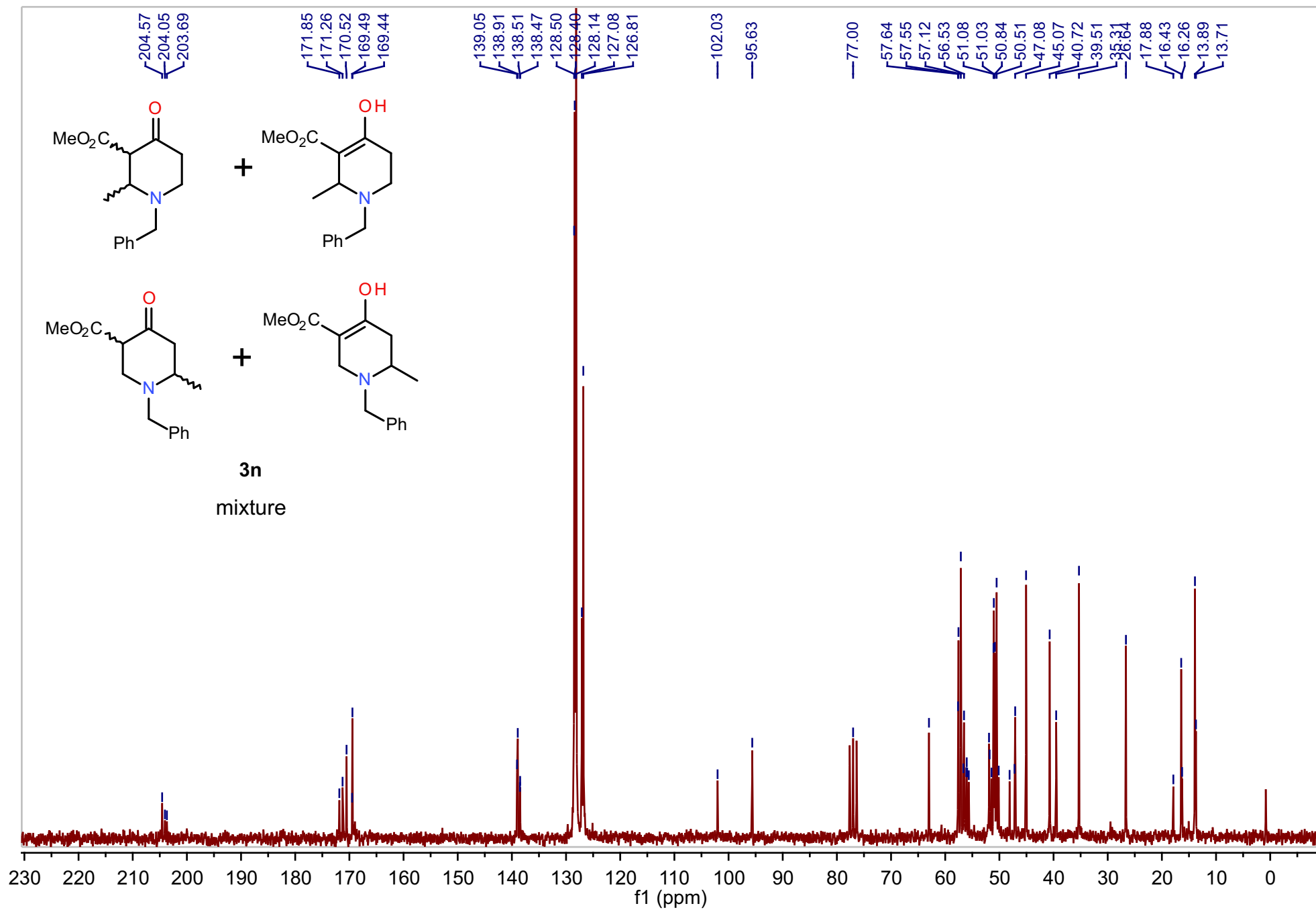
Spectroscopic data. Compound 3n ¹H NMR



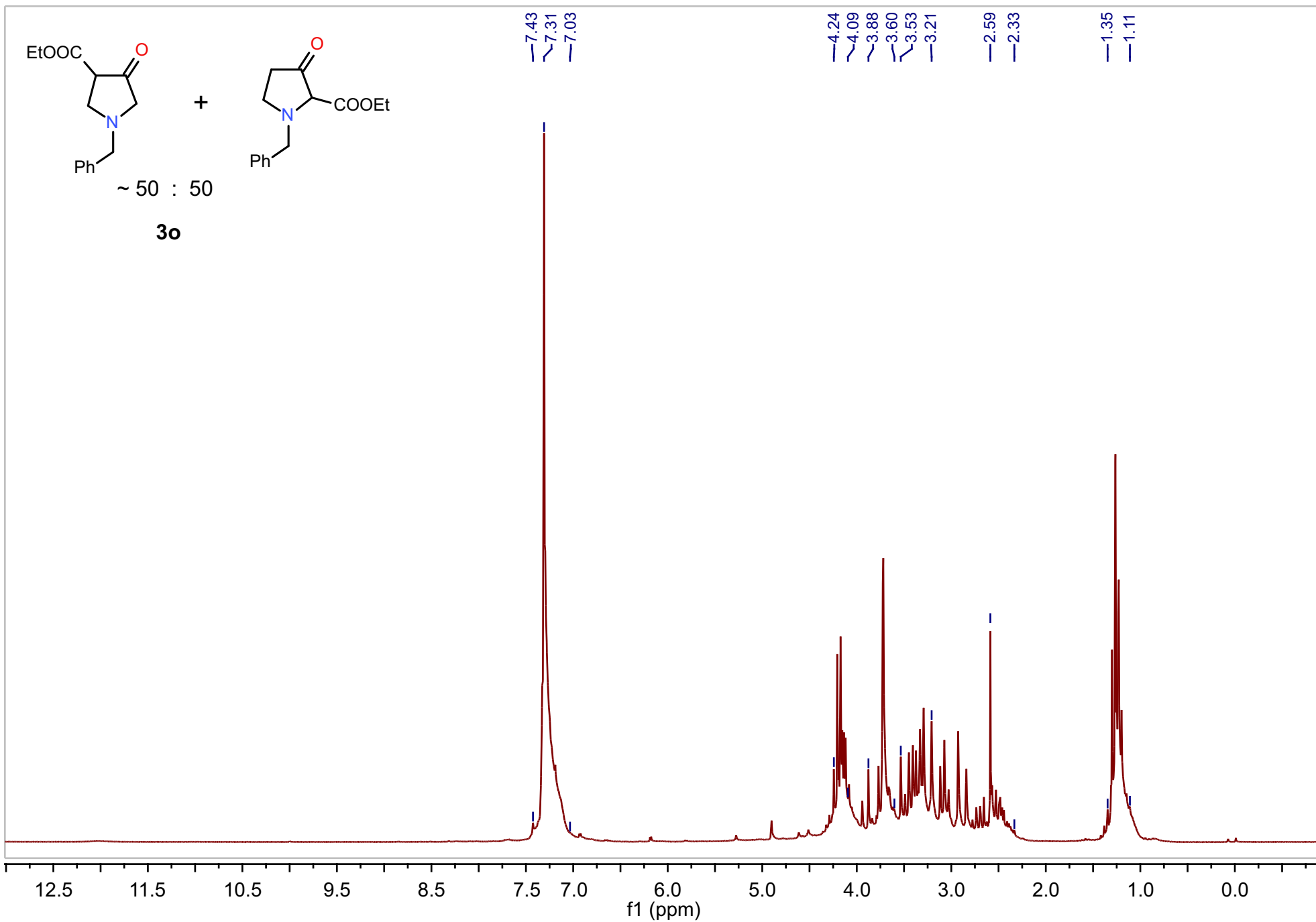
Spectroscopic data. Compound 3n ¹H NMR expanded



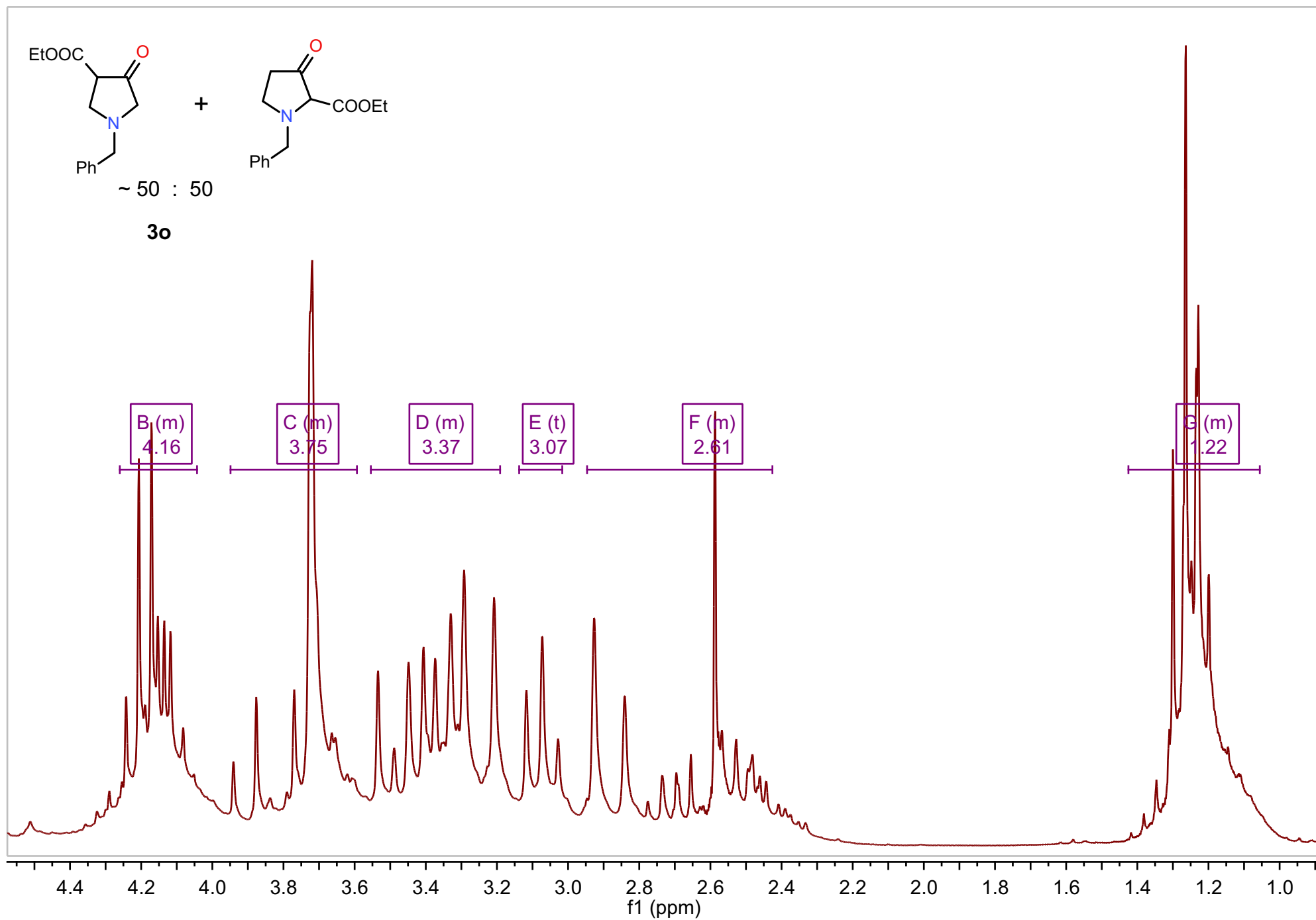
Spectroscopic data. Compound **3n** ^{13}C NMR



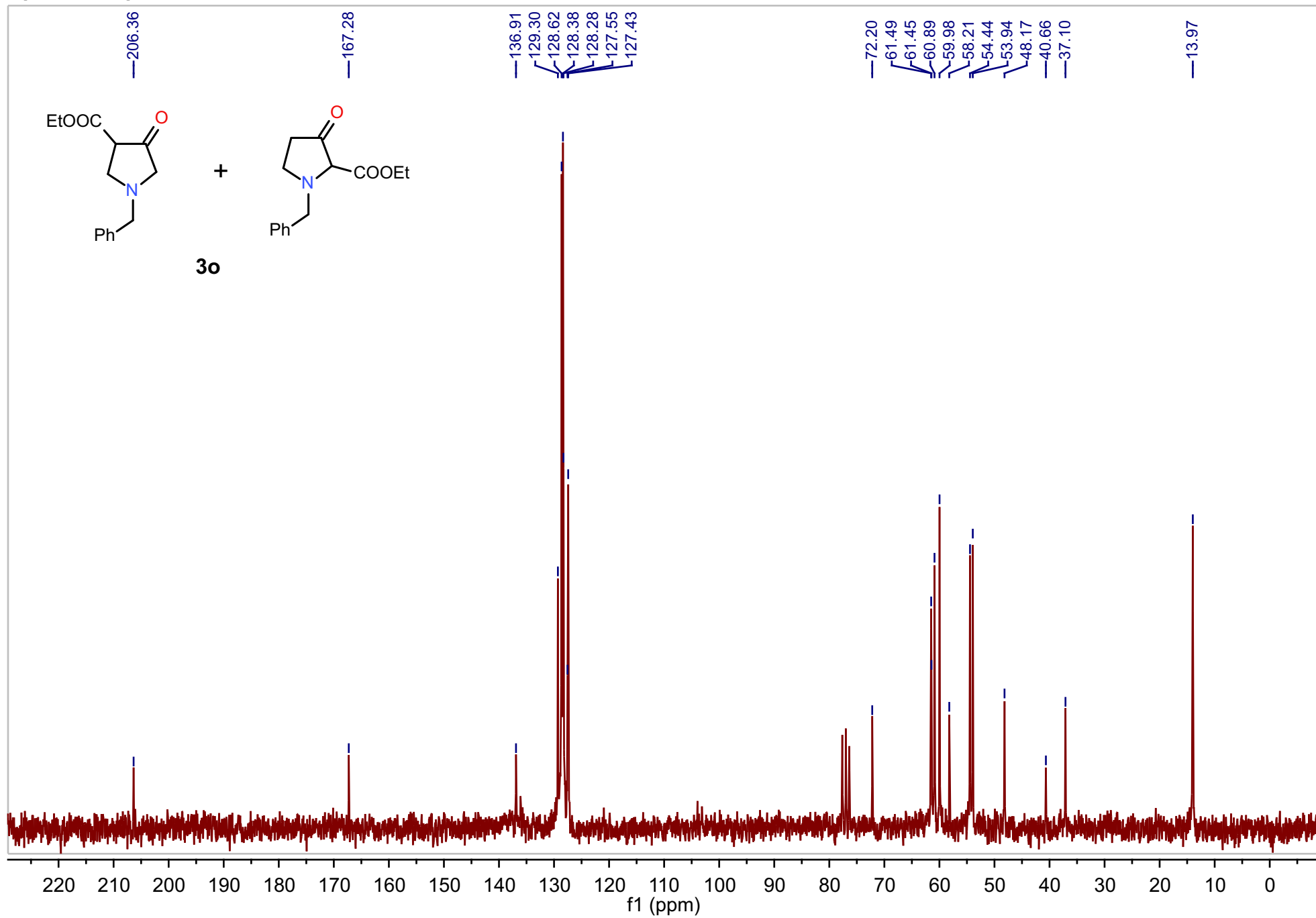
Spectroscopic data. Compound **3o** ¹H NMR



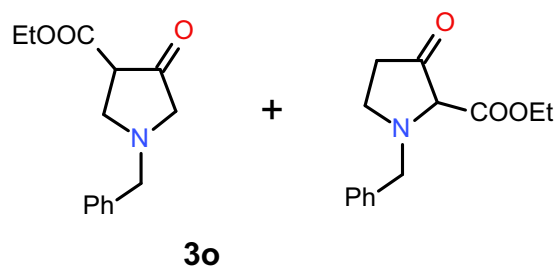
Spectroscopic data. Compound **3o** ^1H NMR expanded



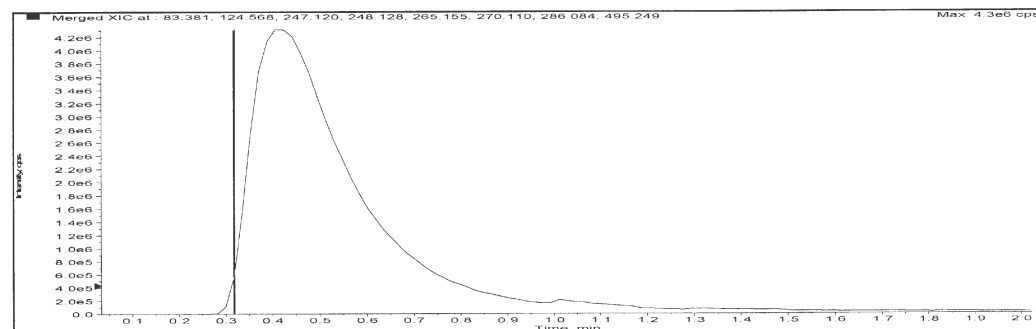
Spectroscopic data. Compound **3o** ¹³C NMR



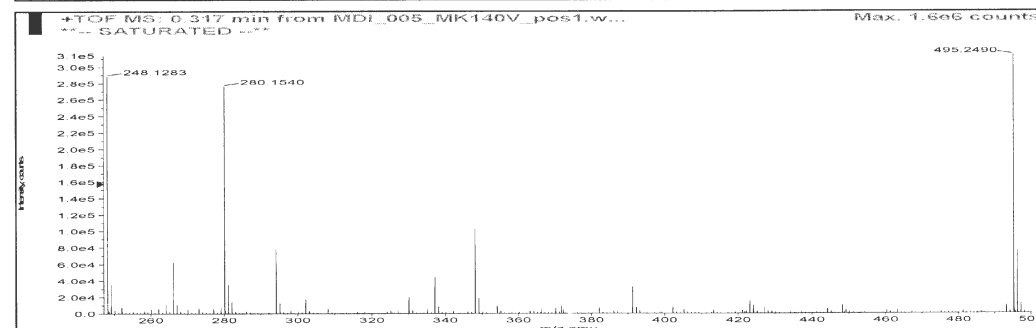
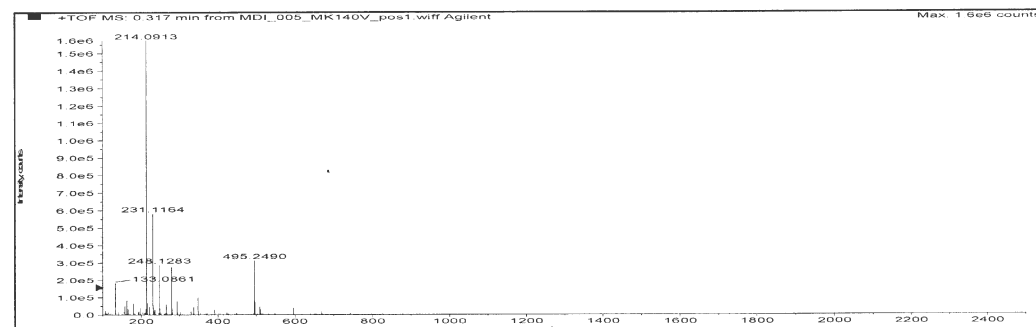
Spectroscopic data. Compound **3o** HRMS



Sample Name: MDI_005 Sample Location: P1-E5 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Roglic\Data\MDI_005_MK140V_pos1.wiff Acq Time: August 26 2011, 12:15:14 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anml\efc.xml



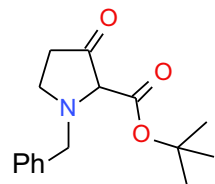
Merged XIC, Period# : 1 Experiment# : 1



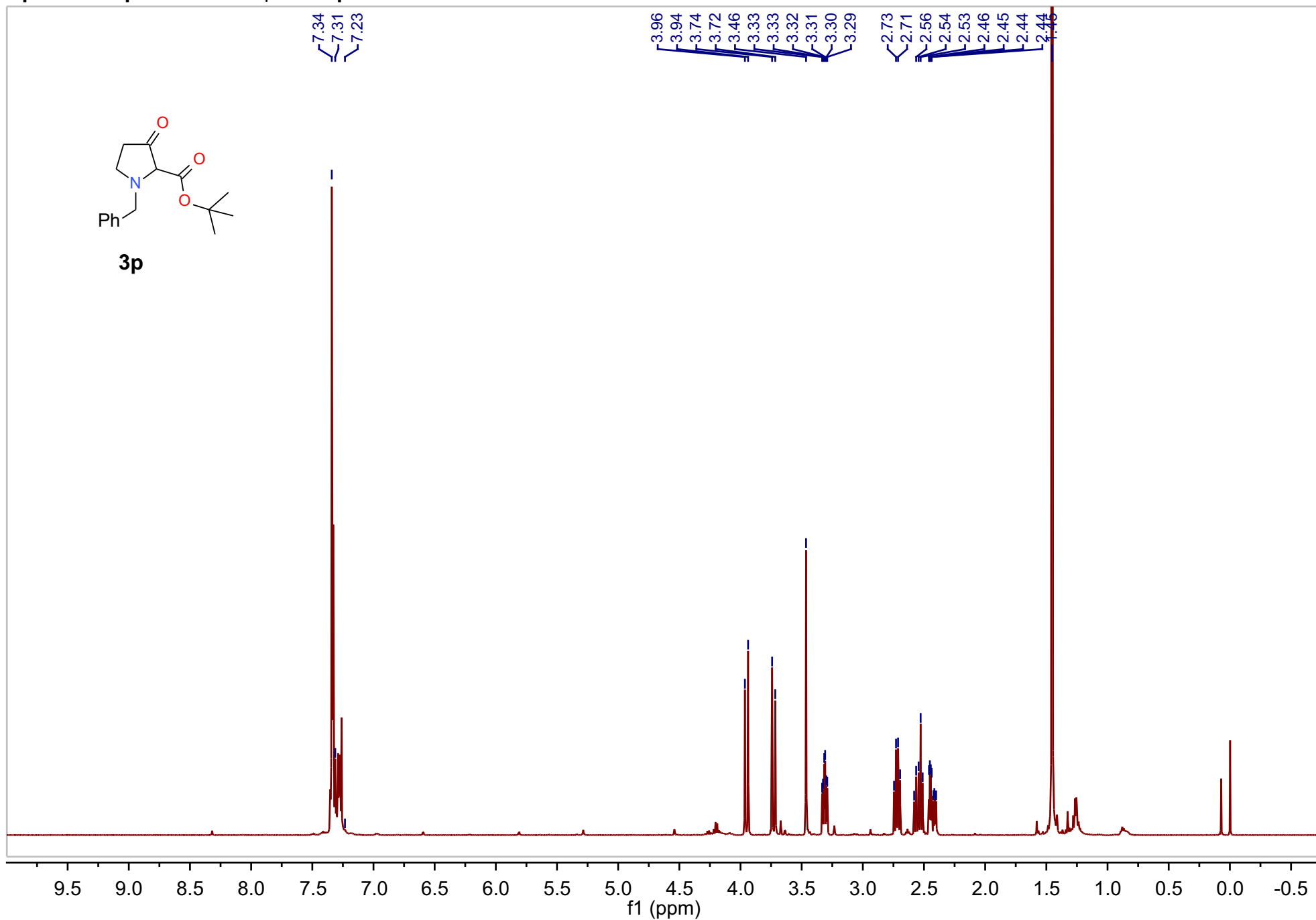
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C ₁₄ H ₁₇ NO ₃	--	247.12084	0.41	6.25140 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	297405.70	248.12812	248.12831	0.19052	0.77	--
[2M+H] ⁺	314289.51	495.24896	495.24897	0.00712	0.01	--

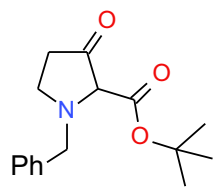
Spectroscopic data. Compound **3p** ¹H NMR 500 MHz



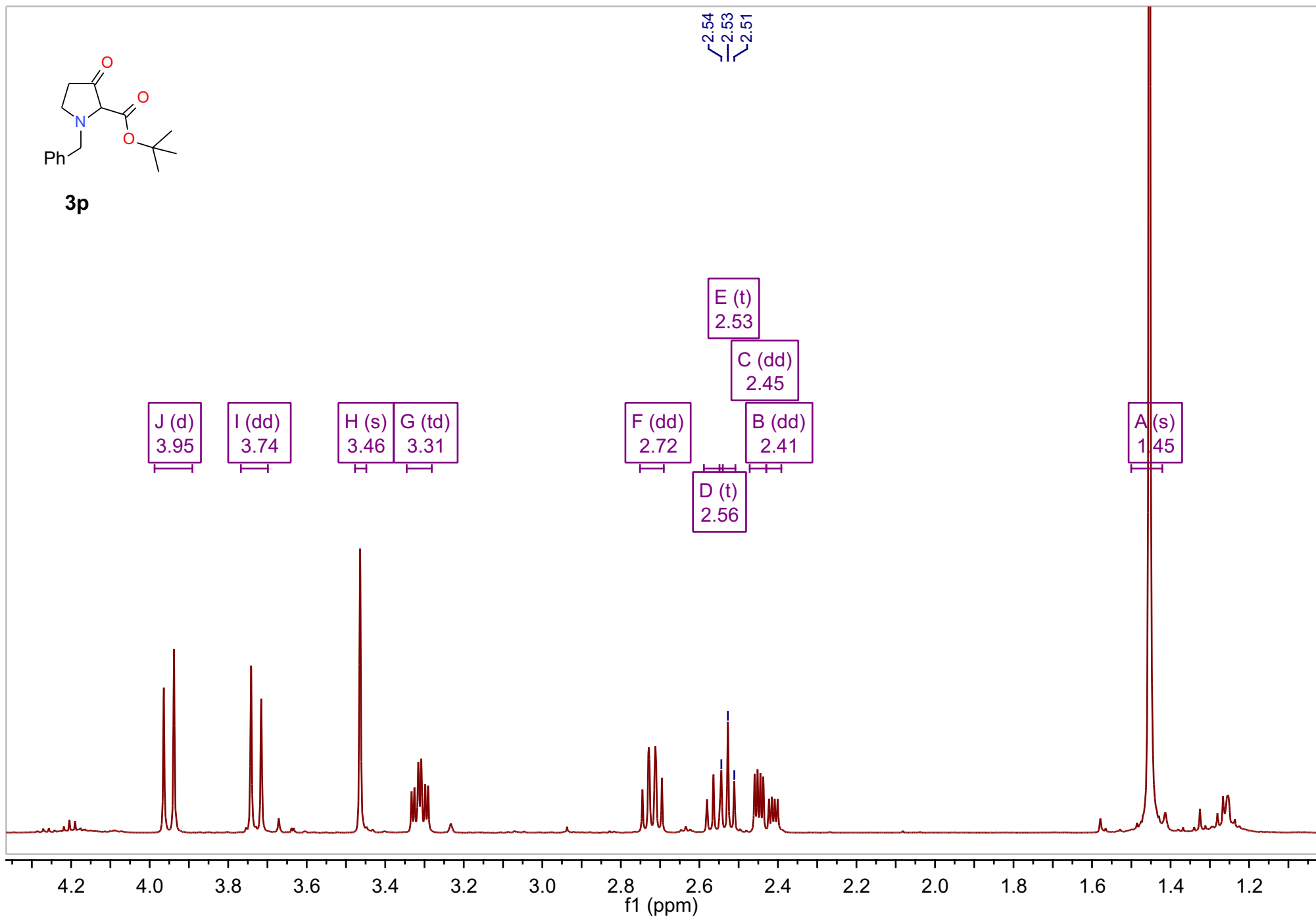
3p



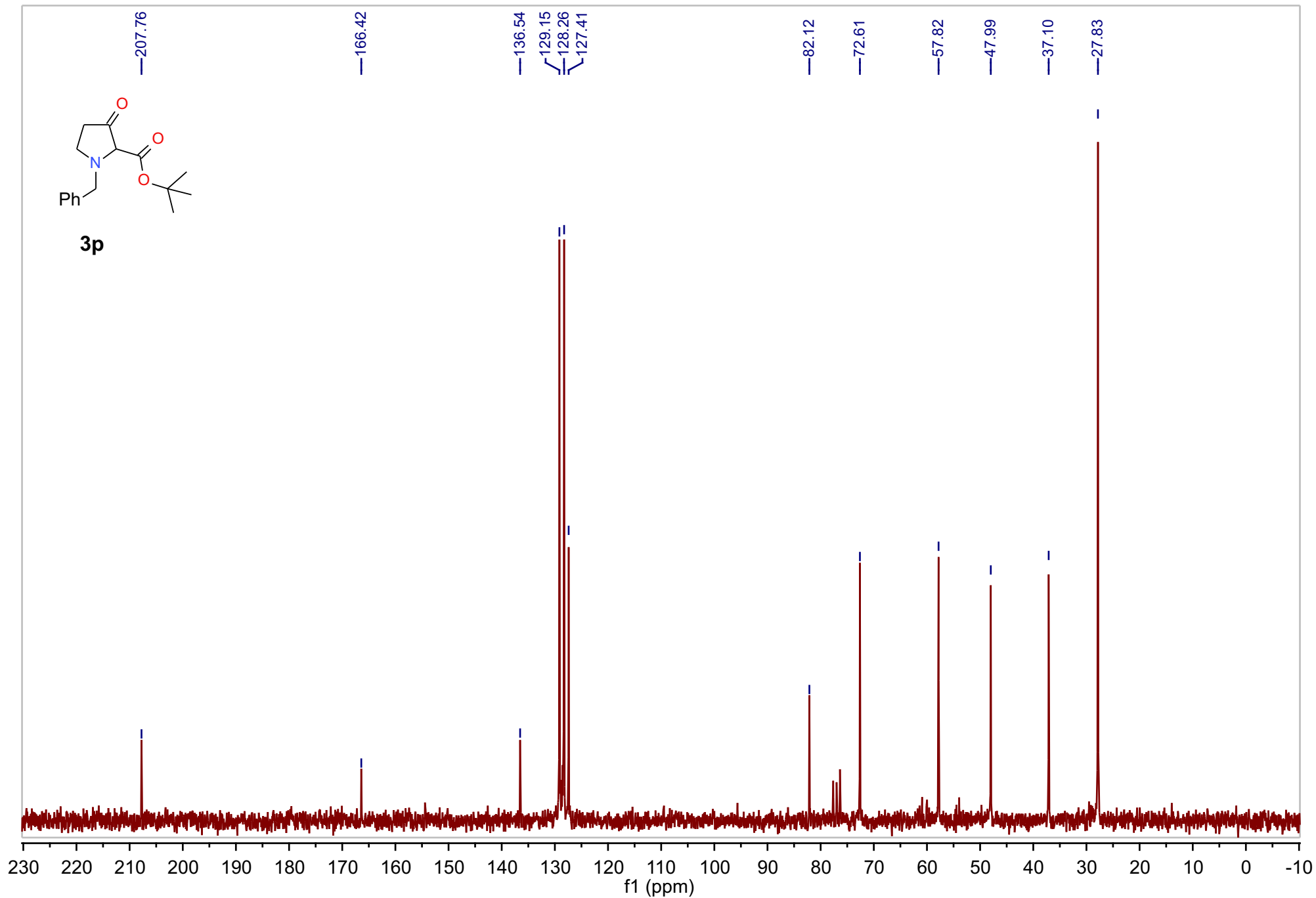
Spectroscopic data. Compound **3p** ^1H NMR 500 MHz expanded



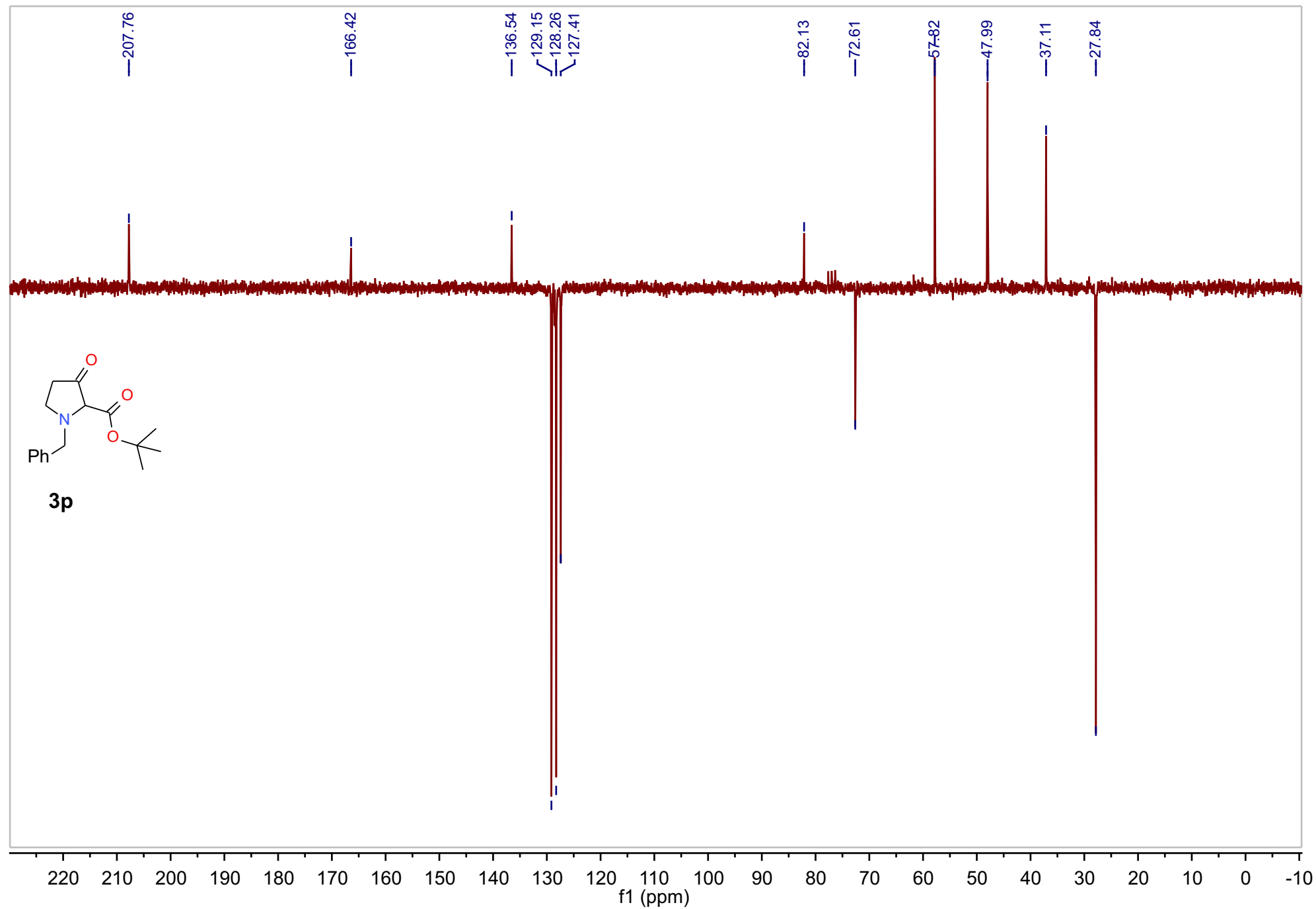
3p



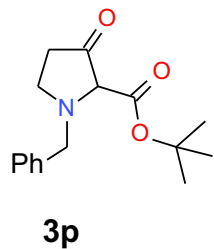
Spectroscopic data. Compound **3p** ^{13}C NMR



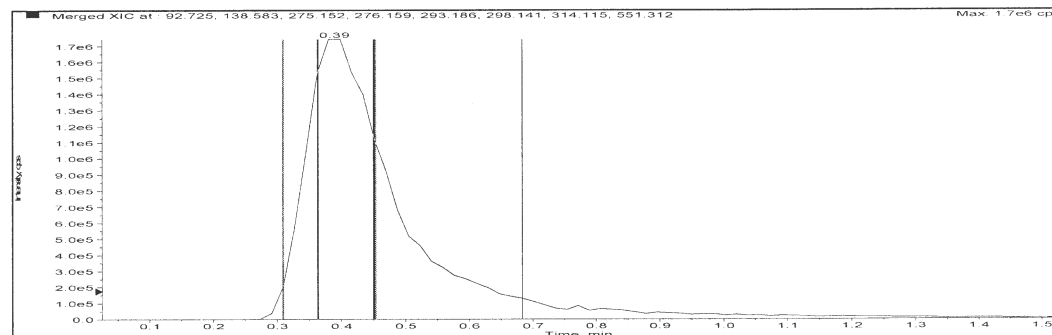
Spectroscopic data. Compound **3p** APT



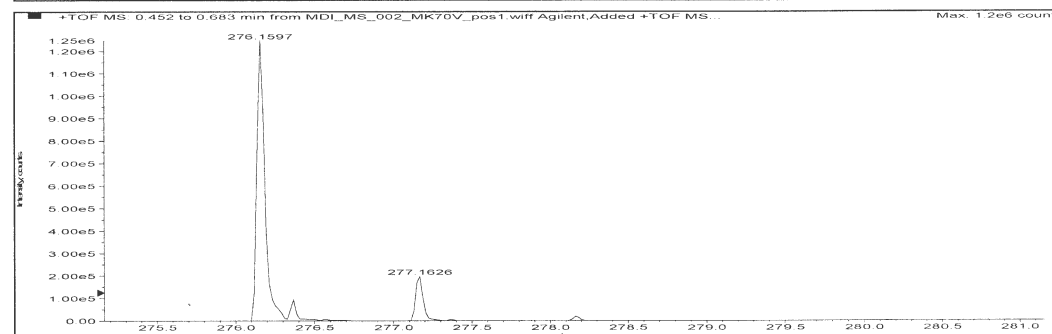
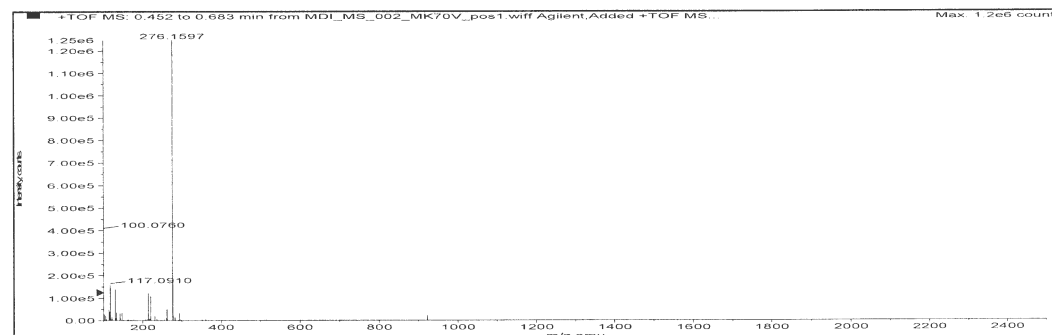
Spectroscopic data. Compound 3p HRMS



Sample Name: MDI_MS_002 Sample Location: P1-D7 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Roglic\Data\MDI_MS_002_MK70V_pos1.wiff Acq Time: April 26 2012, 03:26:08 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anml\efc.xml



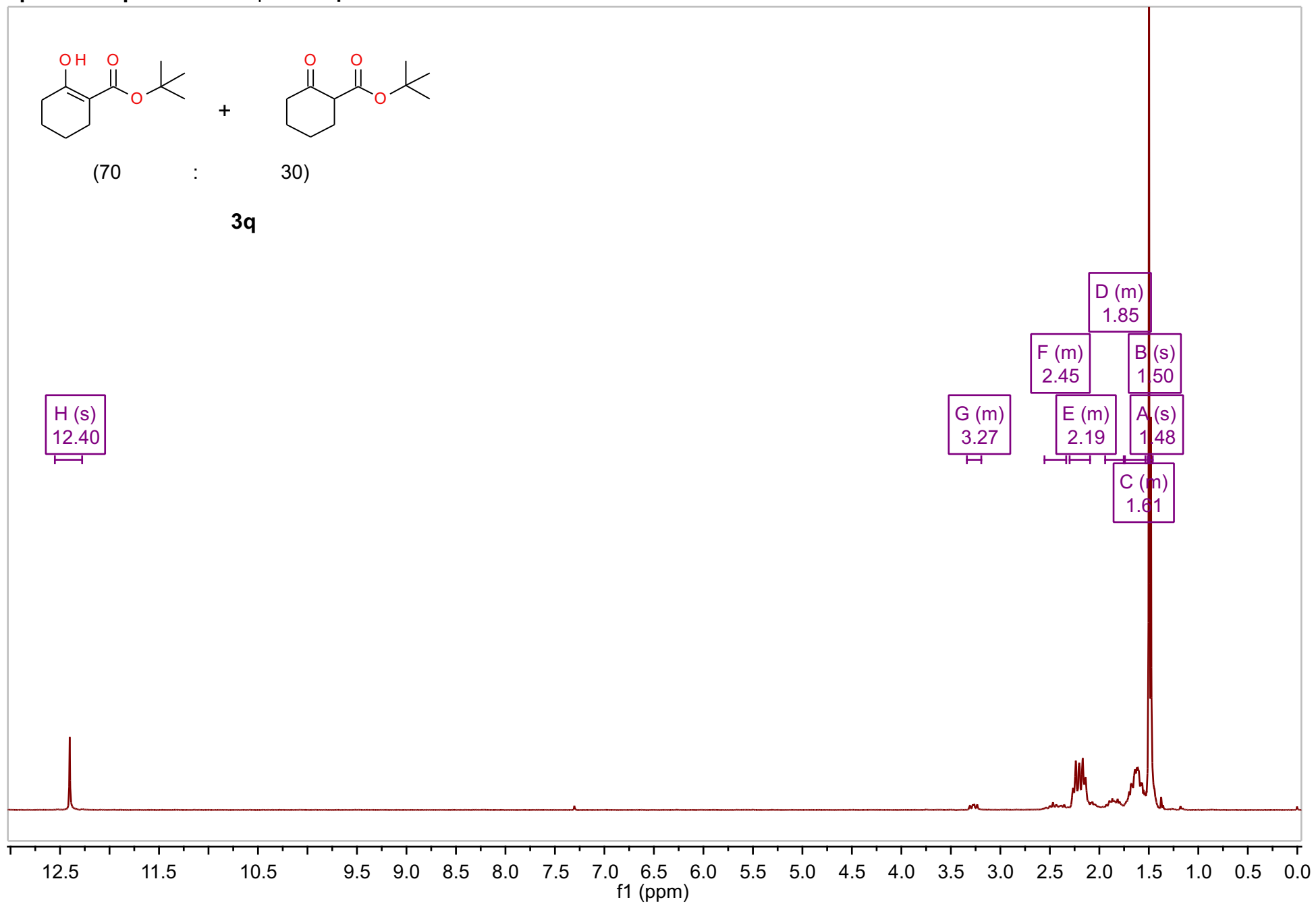
Merged XIC, Period# : 1 Experiment# : 1



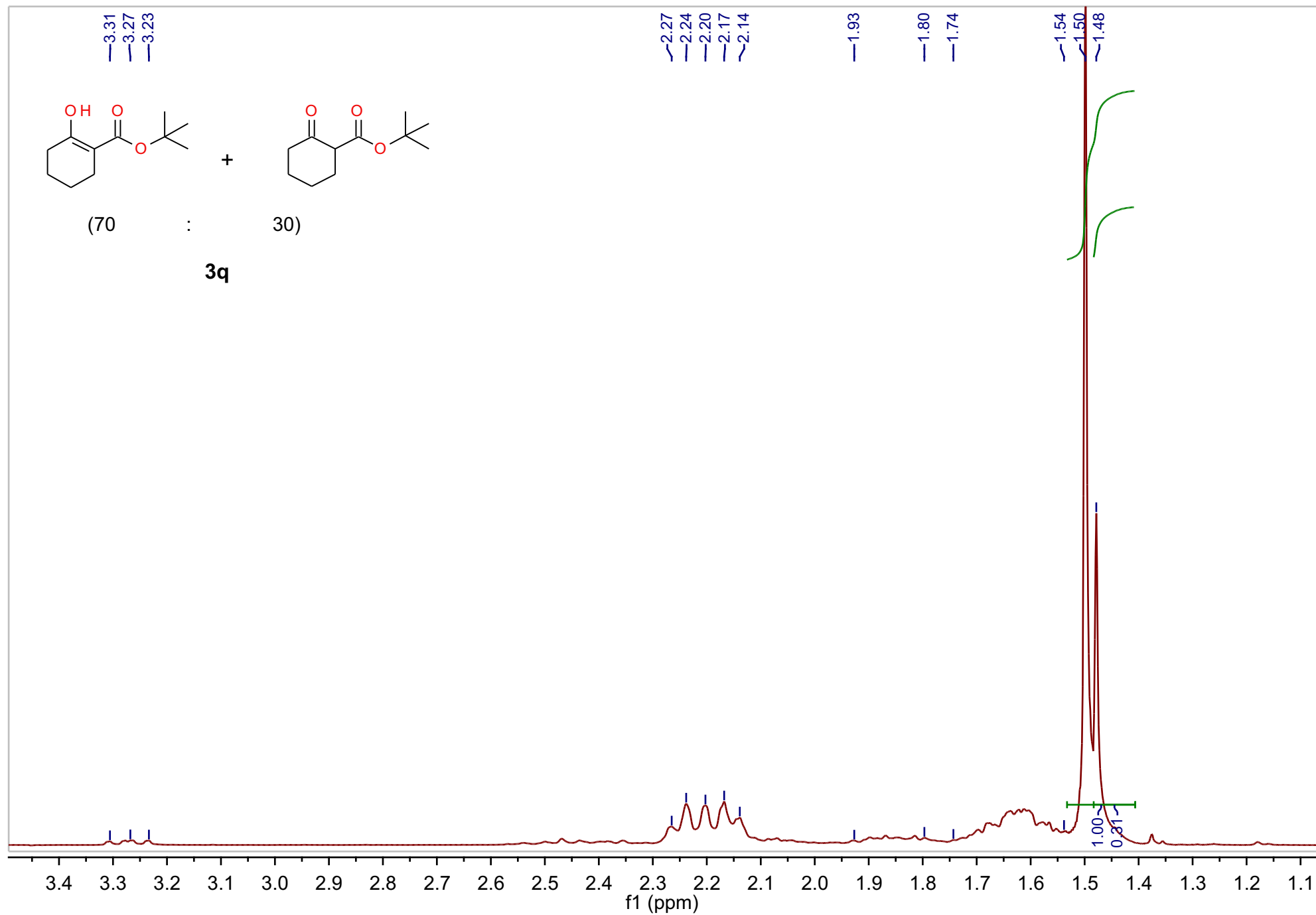
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C16H21NO3	--	275.15214	0.39	1.69105 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1249211.20	276.15942	276.15968	0.26228	0.95	--

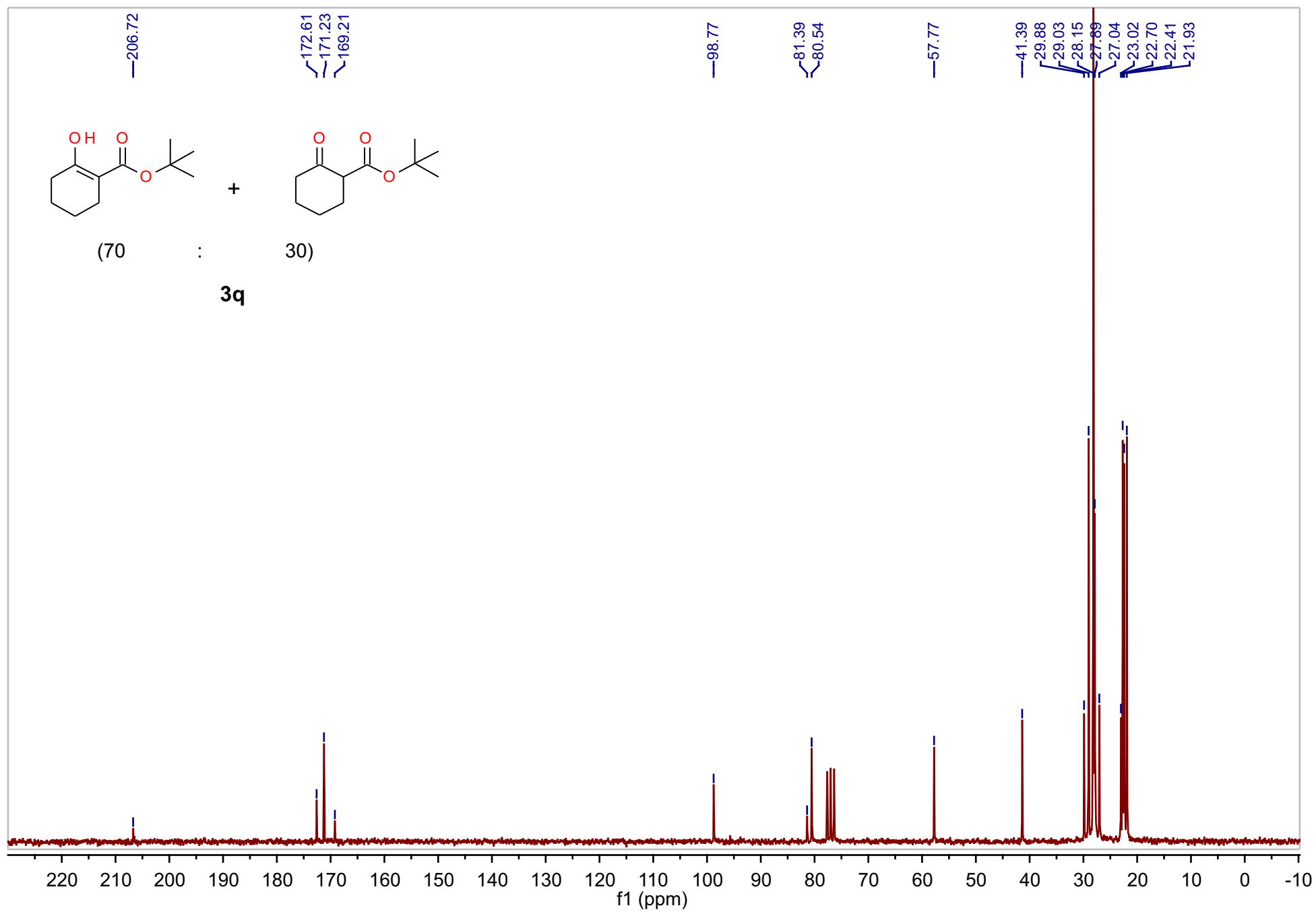
Spectroscopic data. Compound **3q** ¹H NMR



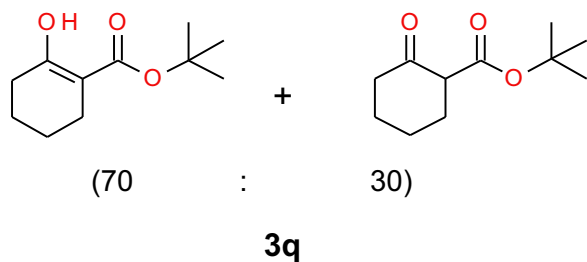
Spectroscopic data. Compound 3q ¹H NMR expanded



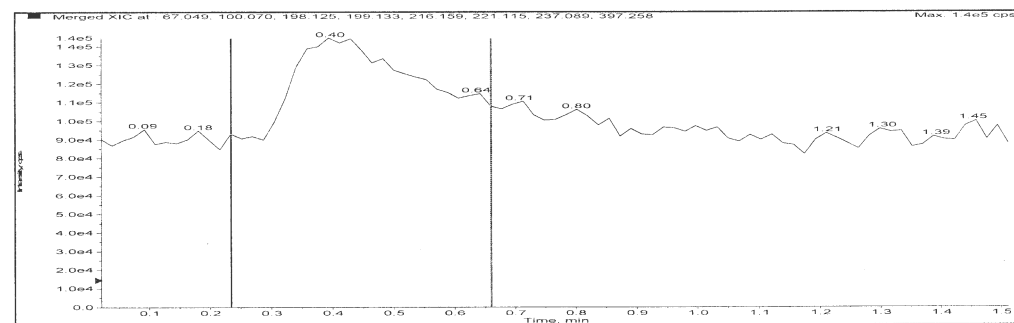
Spectroscopic data. Compound **3q** ^{13}C NMR



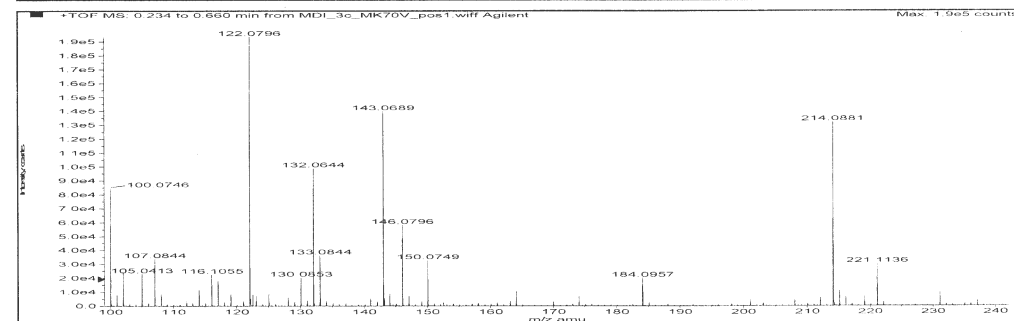
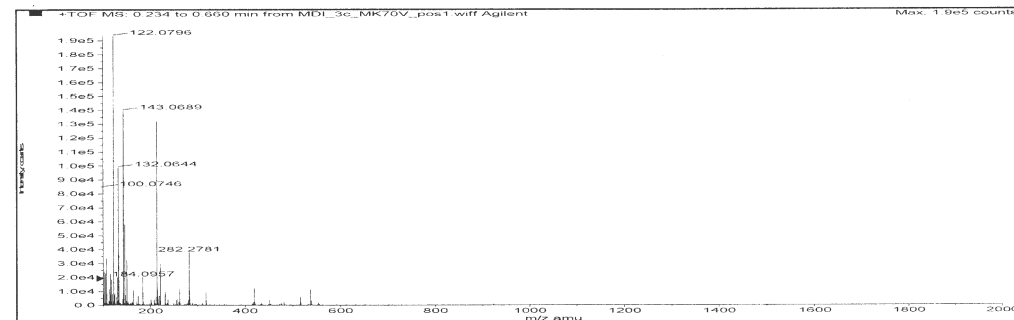
Spectroscopic data. Compound 3q HRMS



Sample Name: 3c Sample Location: P1-E5 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Roglic\Data\MDI_3c_MK70V_pos1.wiff Acq Time: July 18 2012, 03:41:01 PM
 Method: d:\TOF Software\damethods\Night_Seq_Comp_ident1.anm\efc.xml



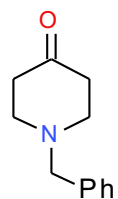
Merged XIC, Period# : 1 Experiment# : 1



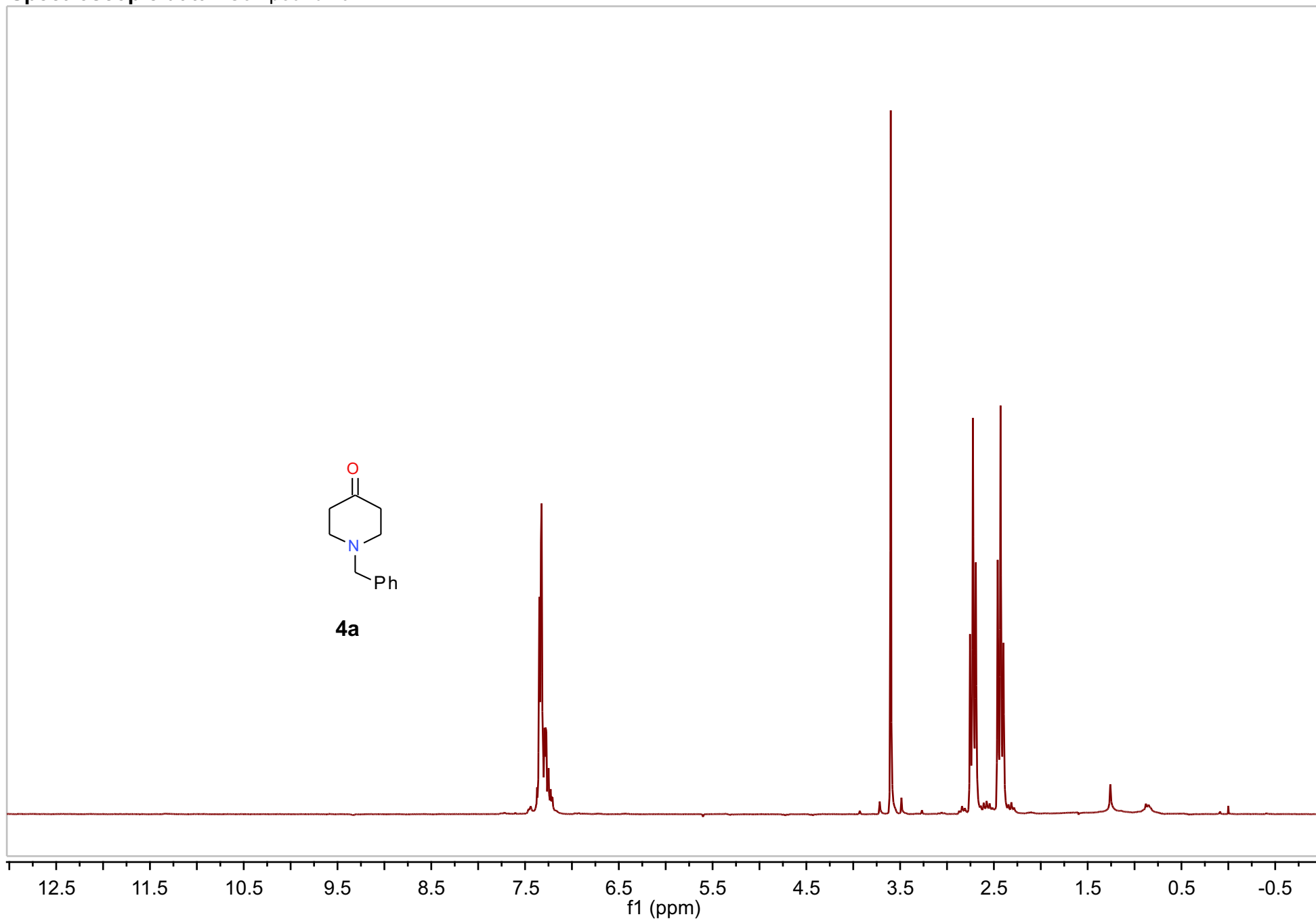
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C11H18O3	--	198.12559	0.40	6.49319 E5	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+2H] ²⁺	91940.14	100.07007	100.07459	4.51439	45.11	--
[M+Na] ⁺	30533.06	221.11482	221.11363	-1.18560	-5.36	--
[M+K] ⁺	4141.18	237.08875	237.08785	-0.90468	-3.82	--

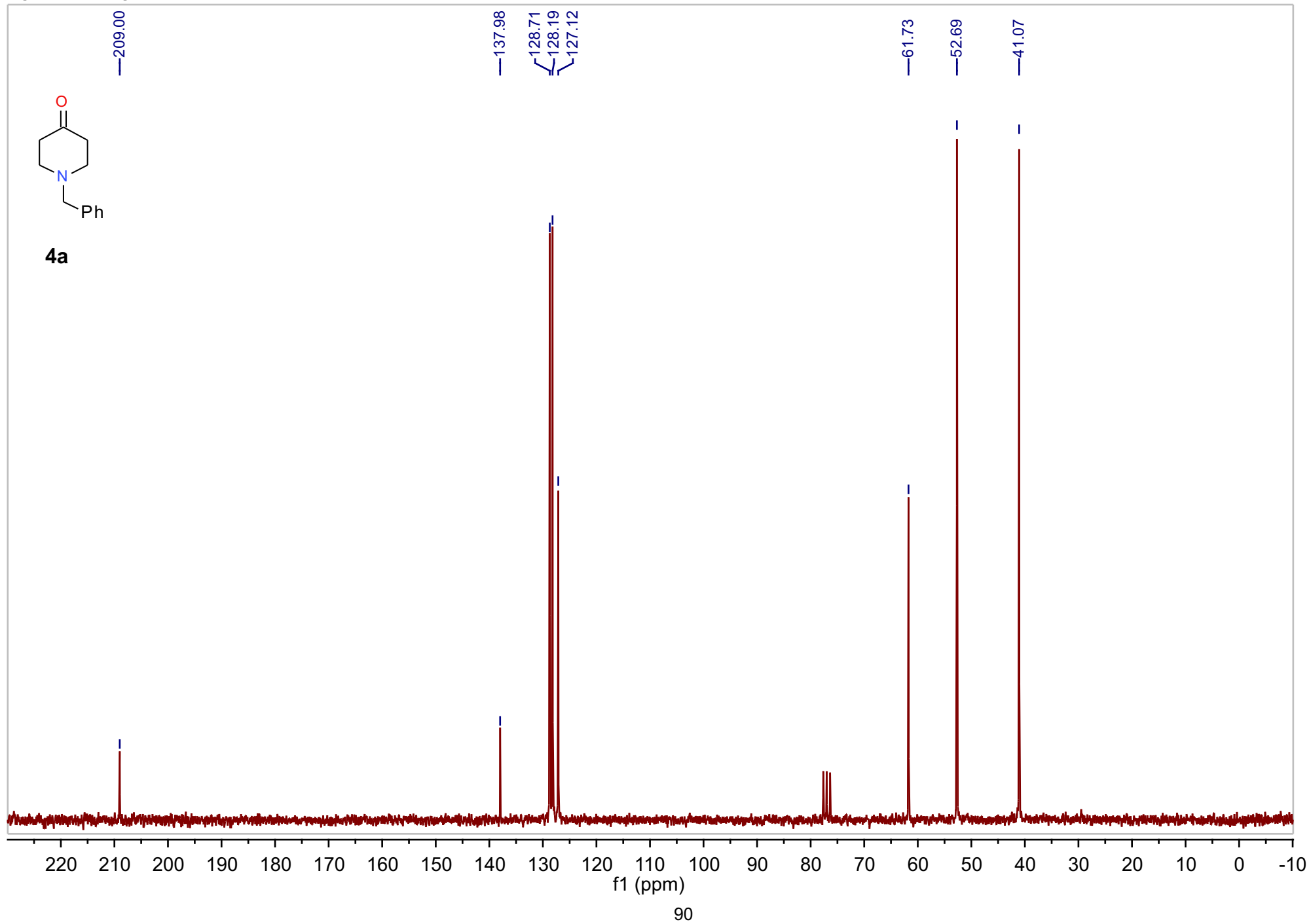
Spectroscopic data. Compound **4a** ^1H NMR



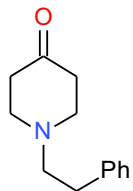
4a



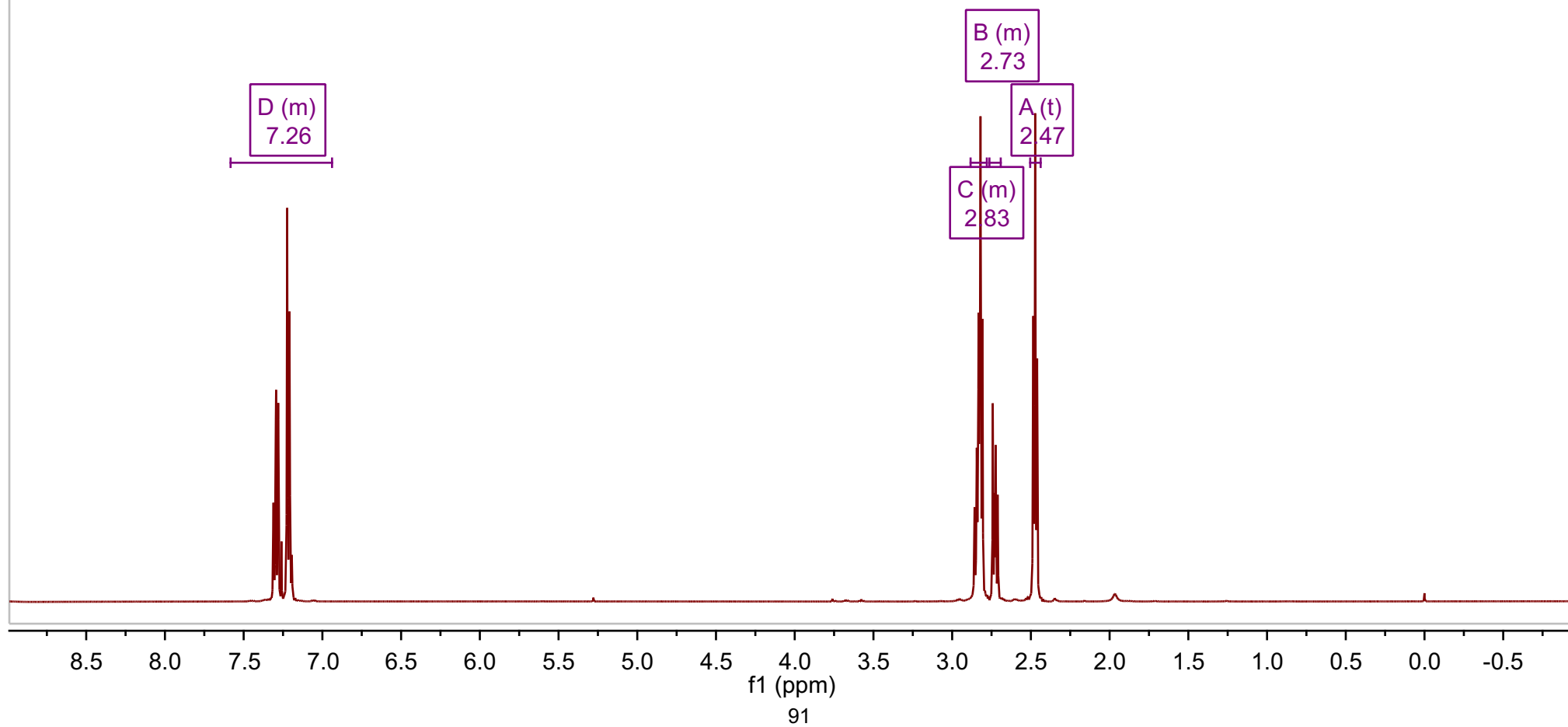
Spectroscopic data. Compound **4a** ^{13}C NMR



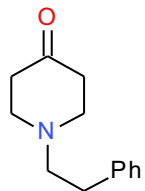
Spectroscopic data. Compound **4b** ¹H NMR



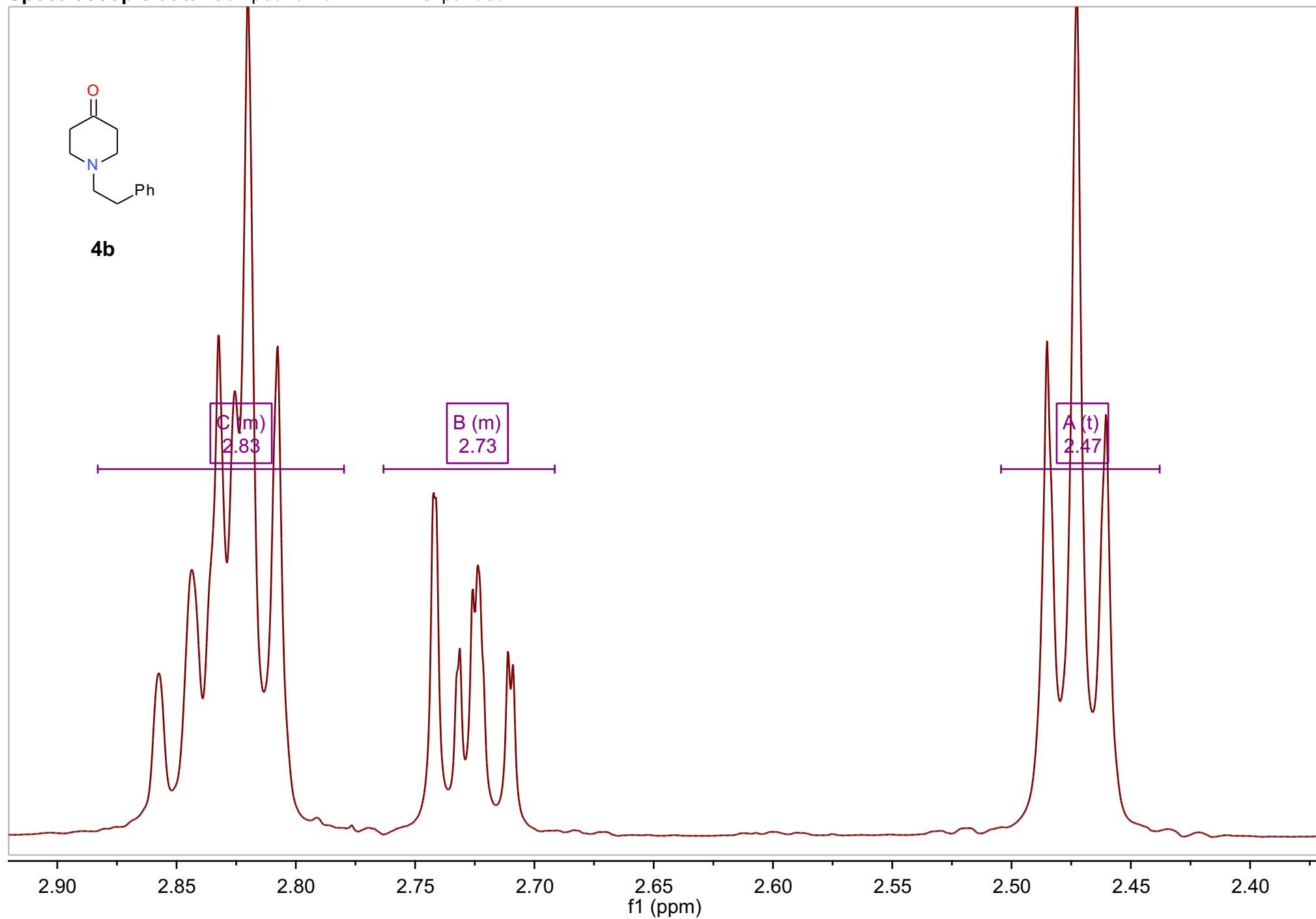
4b



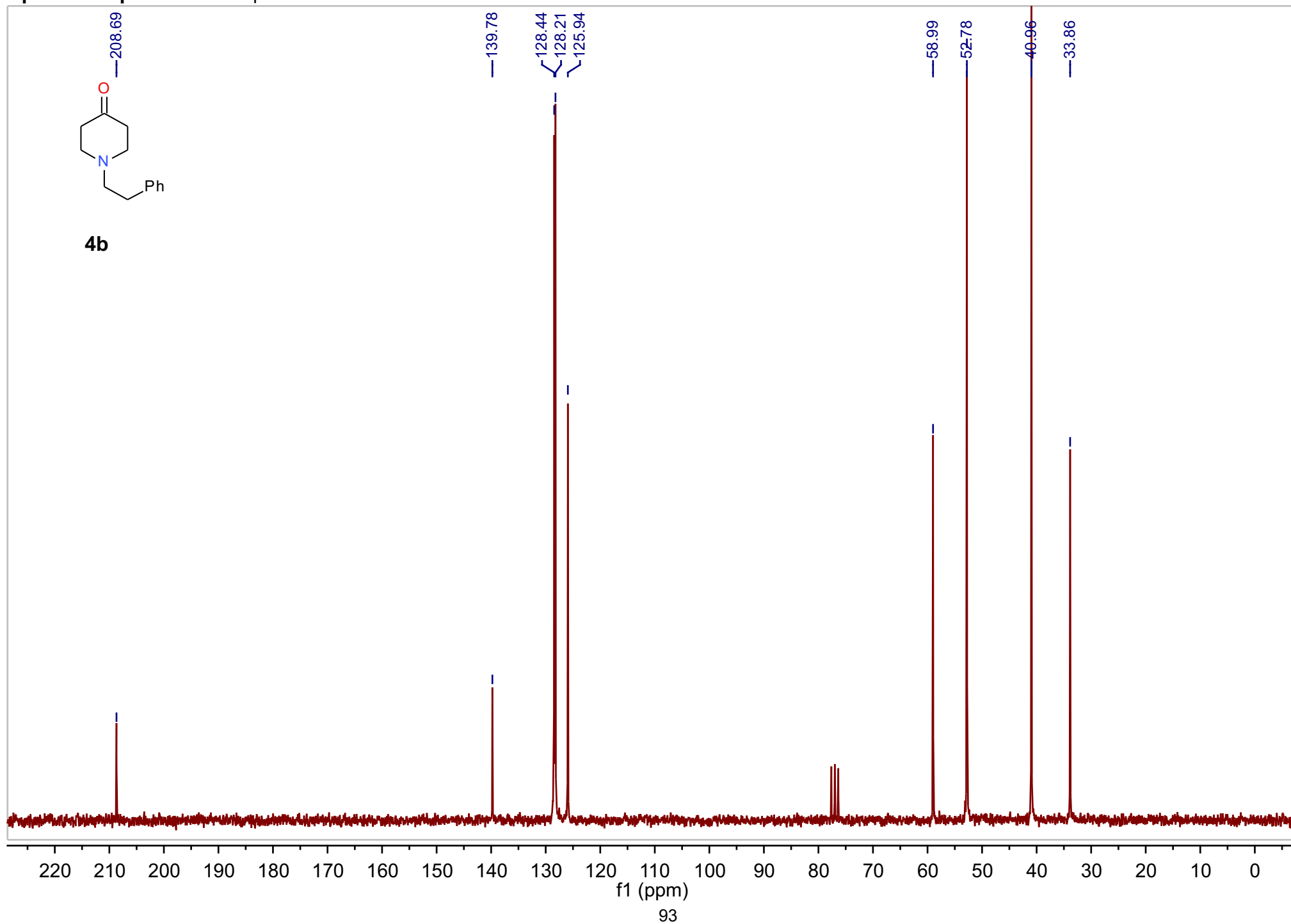
Spectroscopic data. Compound **4b** ¹H NMR expanded



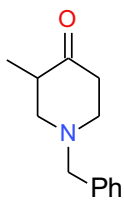
4b



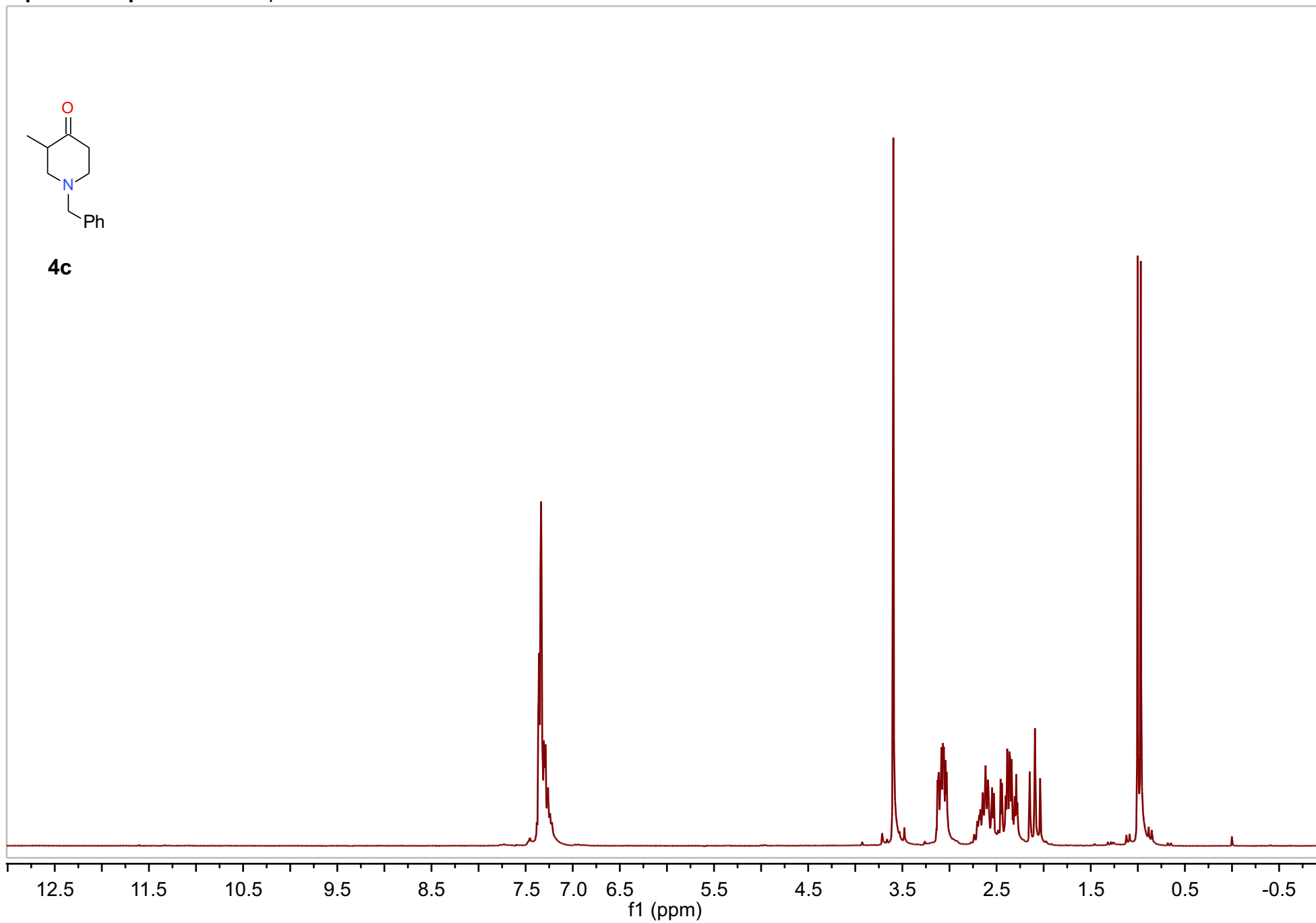
Spectroscopic data. Compound **4b** ^{13}C NMR



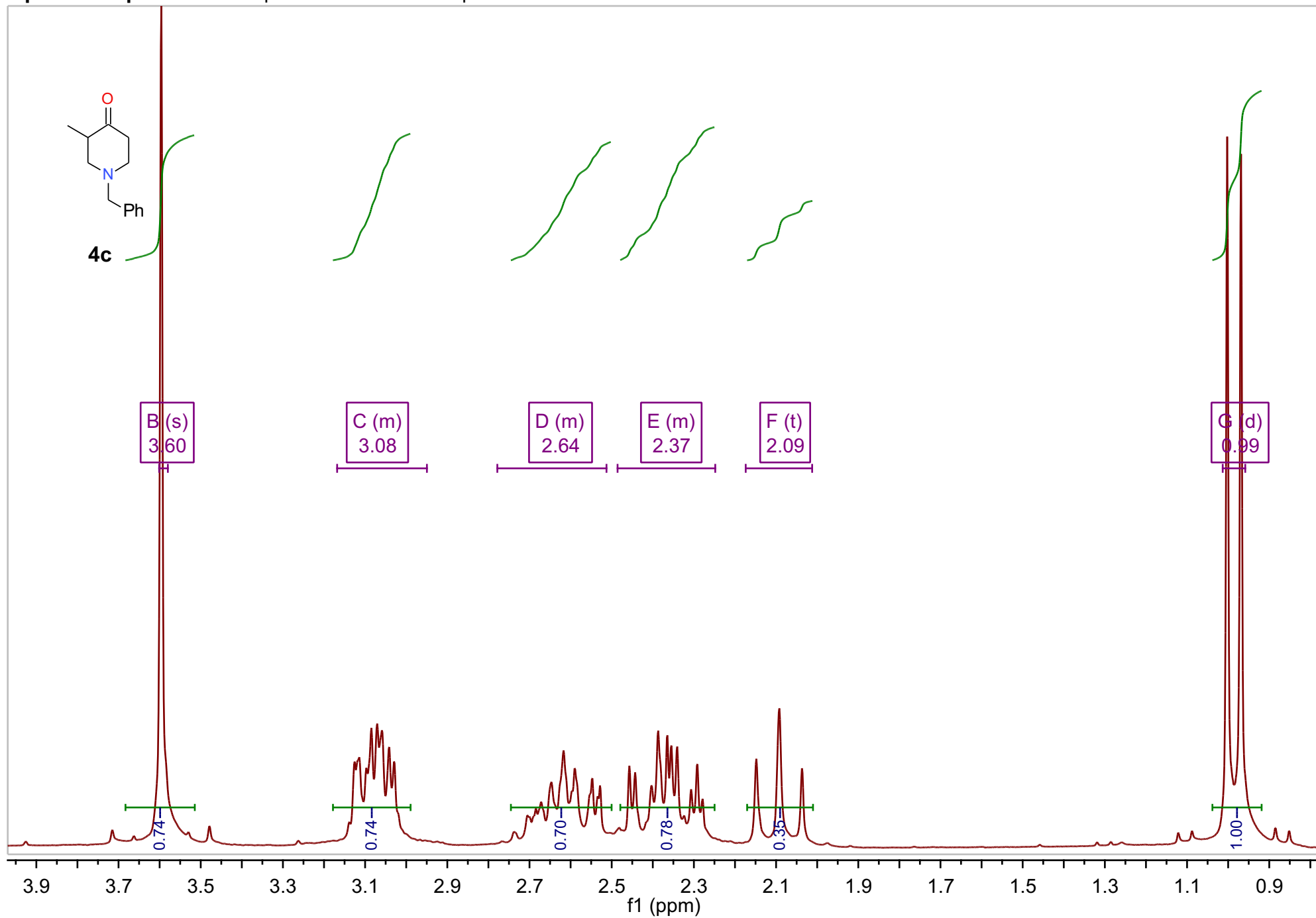
Spectroscopic data. Compound **4c** ^1H NMR



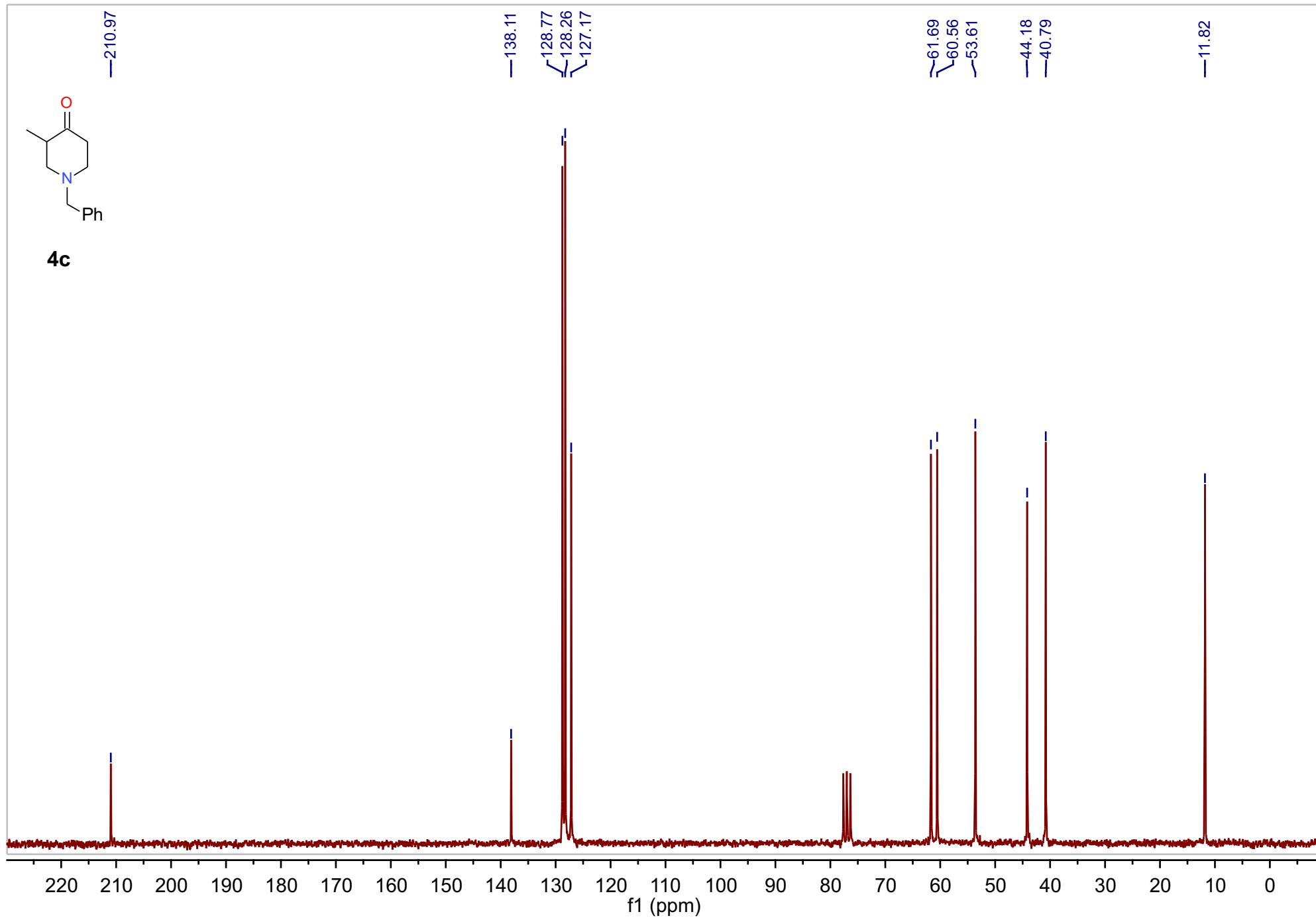
4c



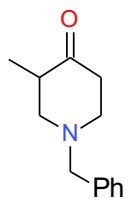
Spectroscopic data. Compound **4c** ¹H NMR expanded



Spectroscopic data. Compound **4c** ^{13}C NMR

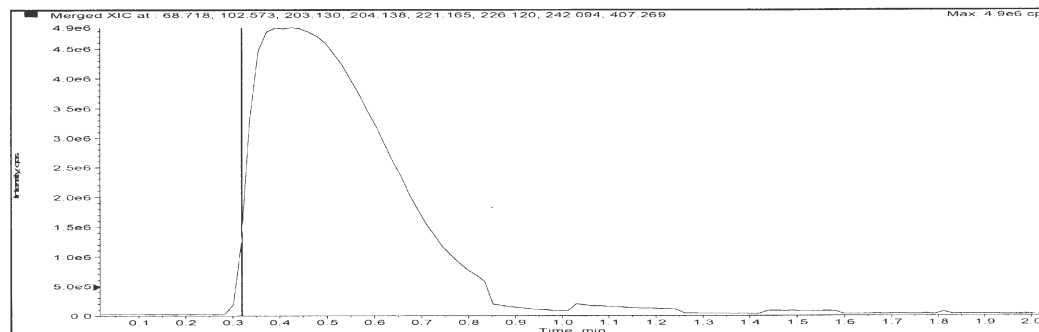


Spectroscopic data. Compound 4c HRMS

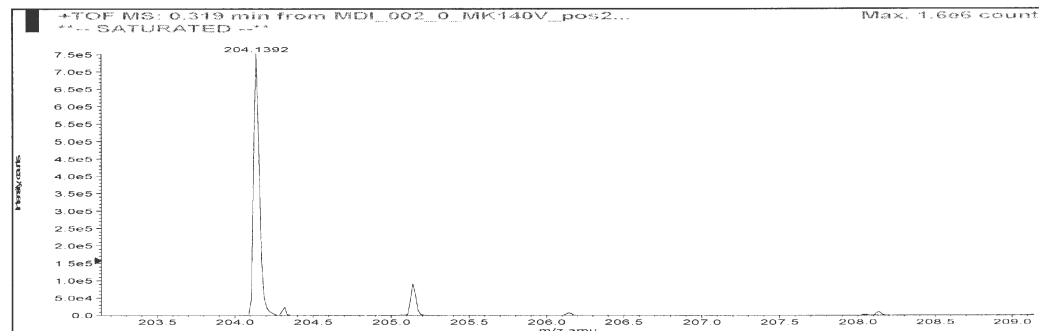
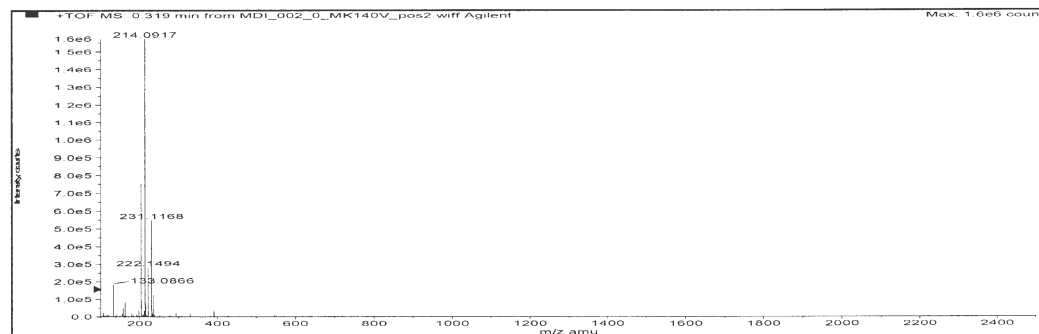


4c

Sample Name: MDI_002_0 Sample Location: P1-E2 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\RoglicData\MDI_002_0_MK140V_pos2.wiff Acq Time: August 26 2011, 12:20:06 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmefc.xml



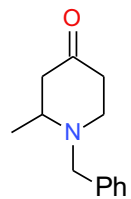
Merged XIC, Period# : 1 Experiment# : 1



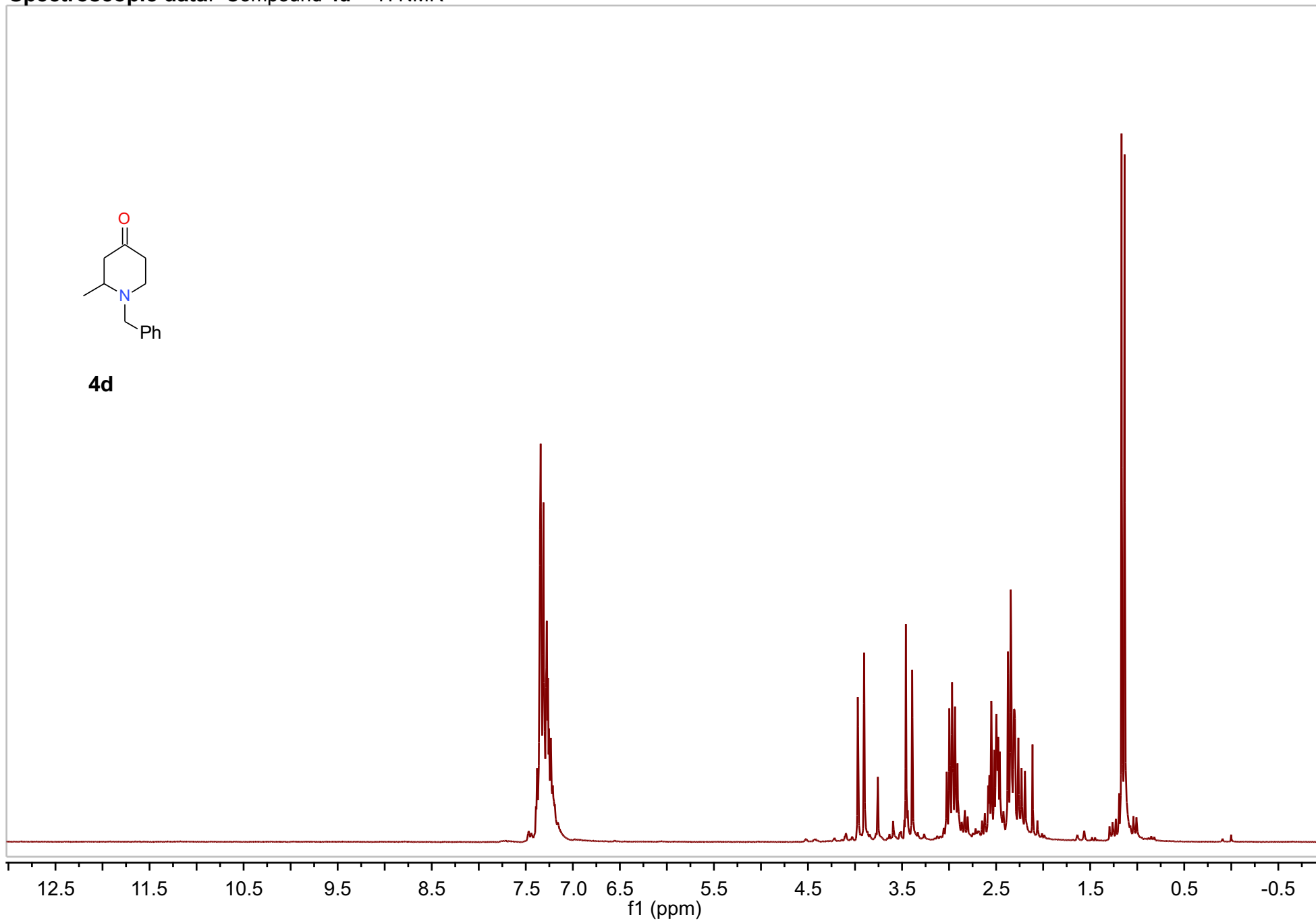
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C13H17NO	--	203.13101	0.43	9.51613 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	752877.10	204.13829	204.13921	0.91630	4.49	--

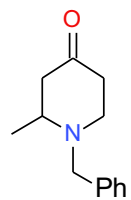
Spectroscopic data. Compound **4d** ^1H NMR



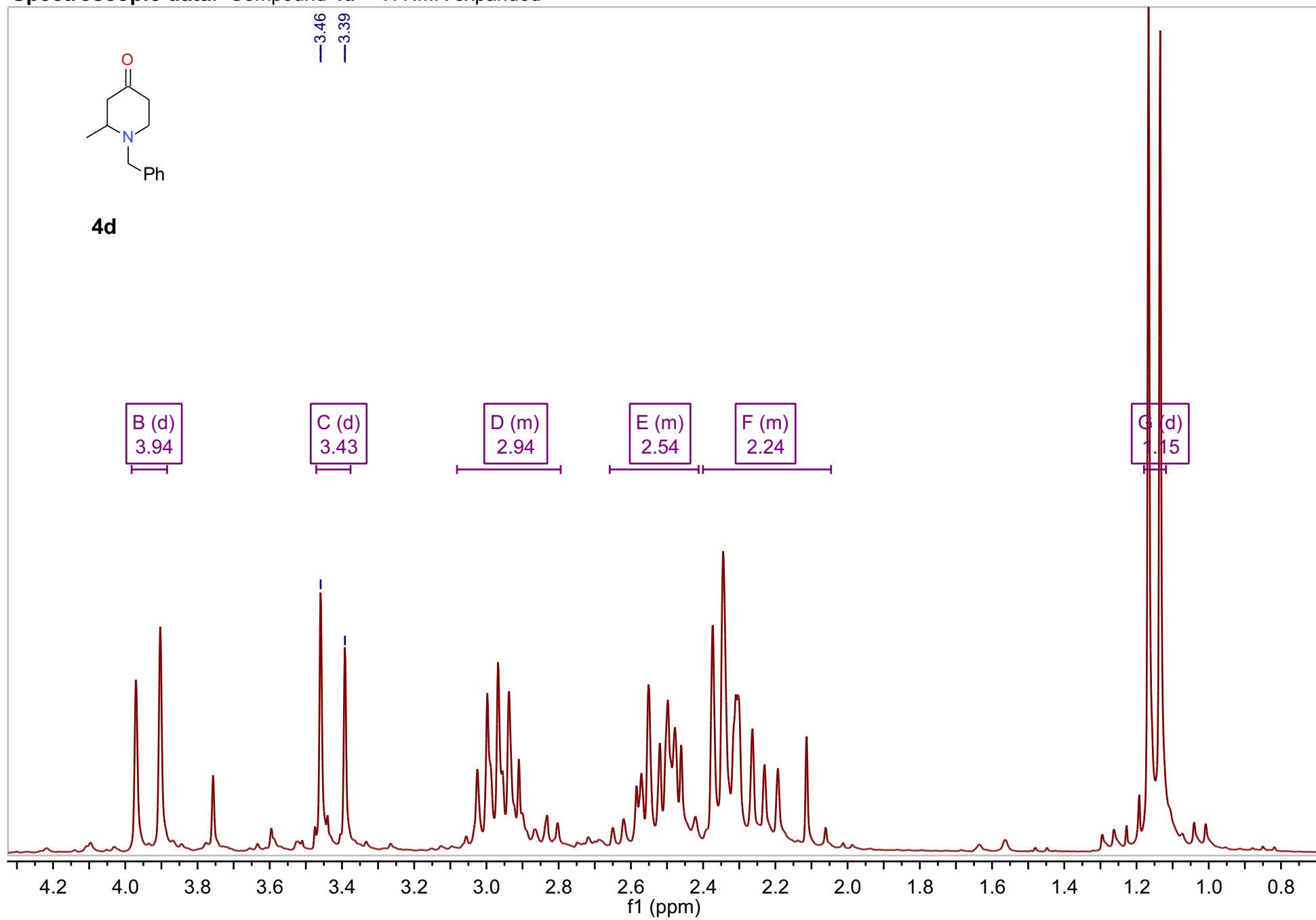
4d



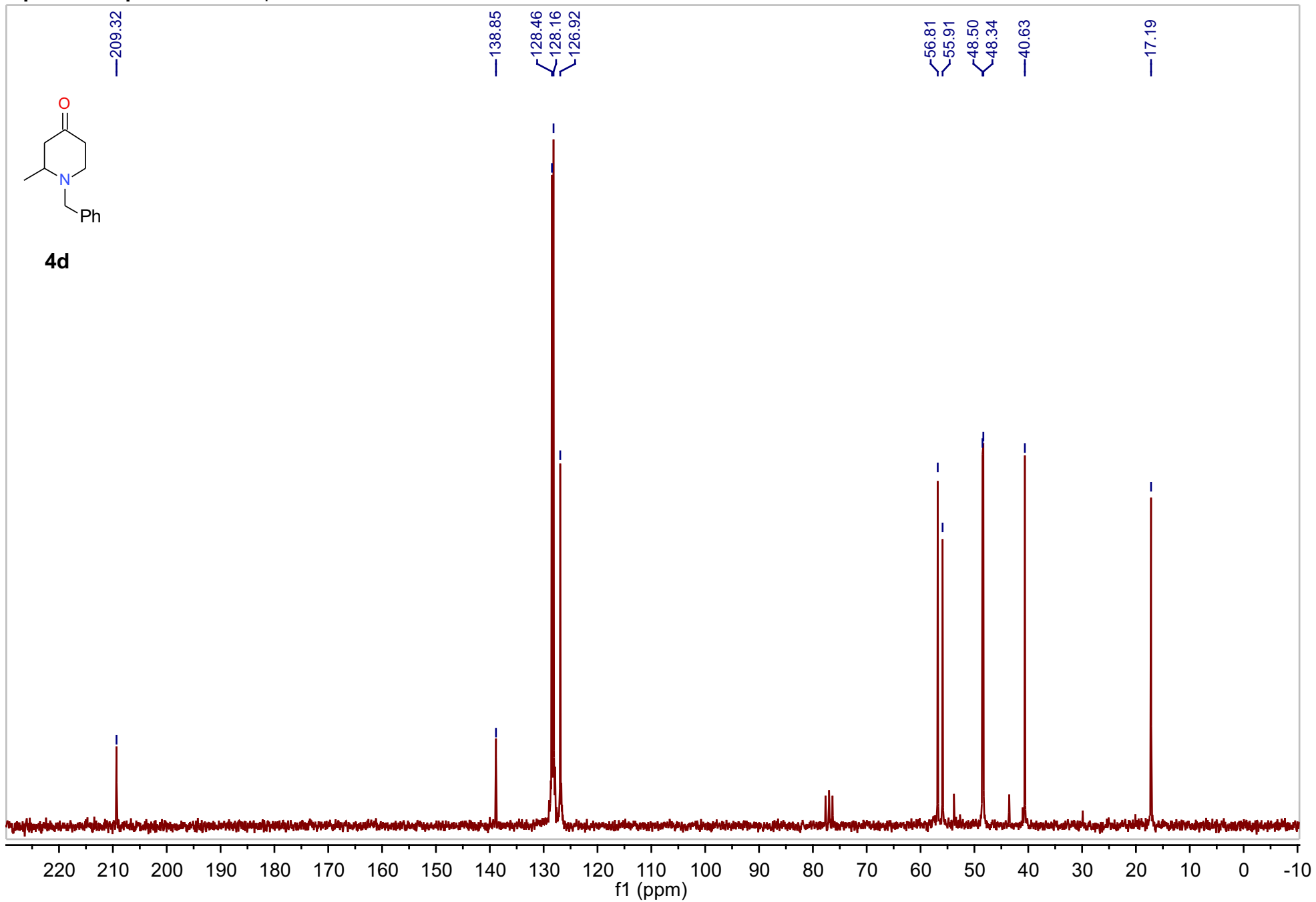
Spectroscopic data. Compound **4d** ¹H NMR expanded



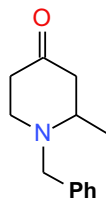
4d



Spectroscopic data. Compound **4d** ^{13}C NMR



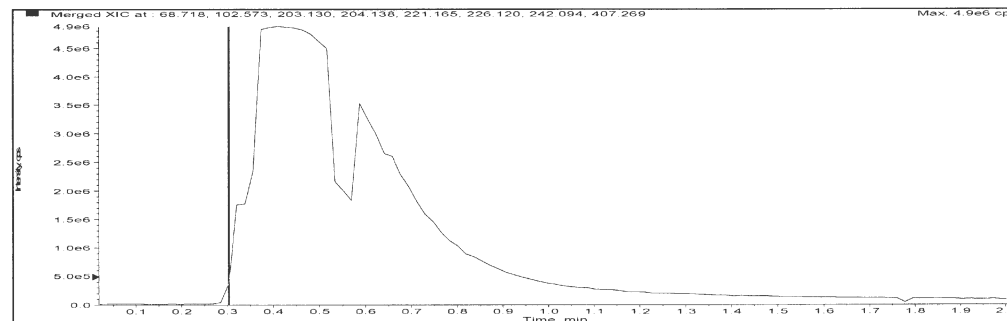
Spectroscopic data. Compound 4d HRMS



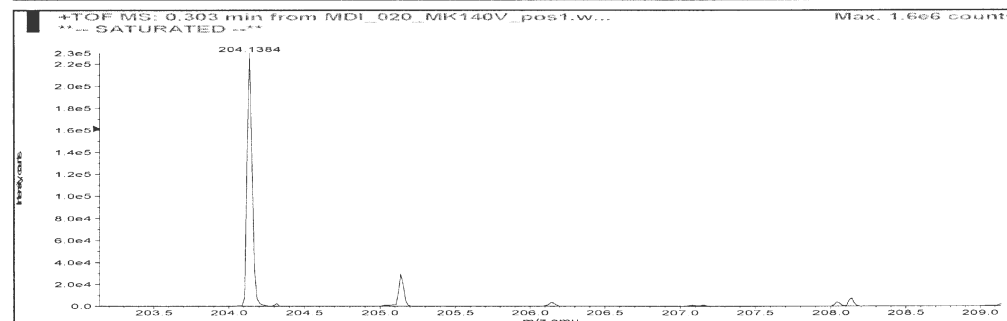
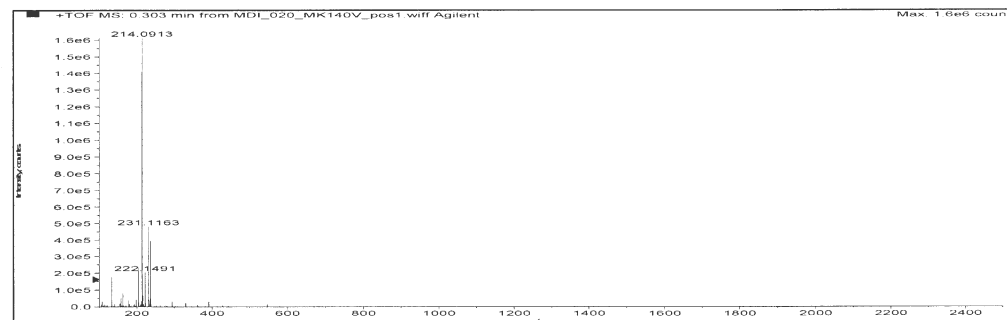
4d

Sample Name: MDI_020 Sample Location: P1-E9 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Roglic\Data\MDI_020_MK140V_pos1.wiff Acq Time: August 26 2011, 12:32:50 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml

One or more scans have failed IRM. Review the data file for details.



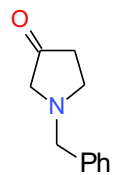
Merged XIC, Period# : 1 Experiment# : 1



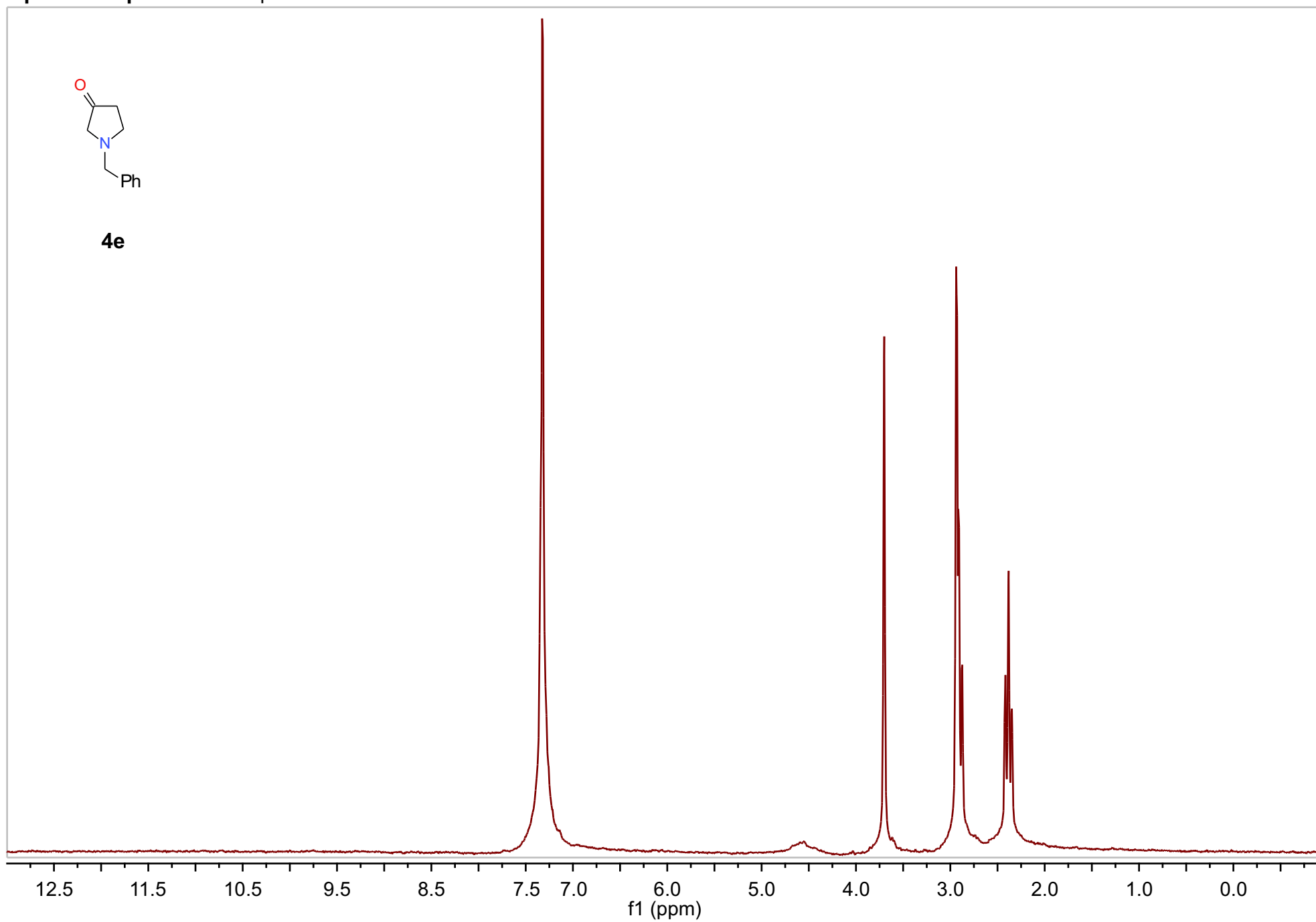
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C13H17NO	--	203.13101	0.41	4.18930 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	229864.52	204.13829	204.13845	0.15850	0.78	--

Spectroscopic data. Compound **4e** ^1H NMR



4e



Spectroscopic data. Compound **4e** ^{13}C NMR

