

Supporting Information

A New Method for Production of Chiral 2-Aryl-2-fluoropropanoic Acids Using an Effective Kinetic Resolution of Racemic 2-Aryl-2-fluoropropanoic Acids

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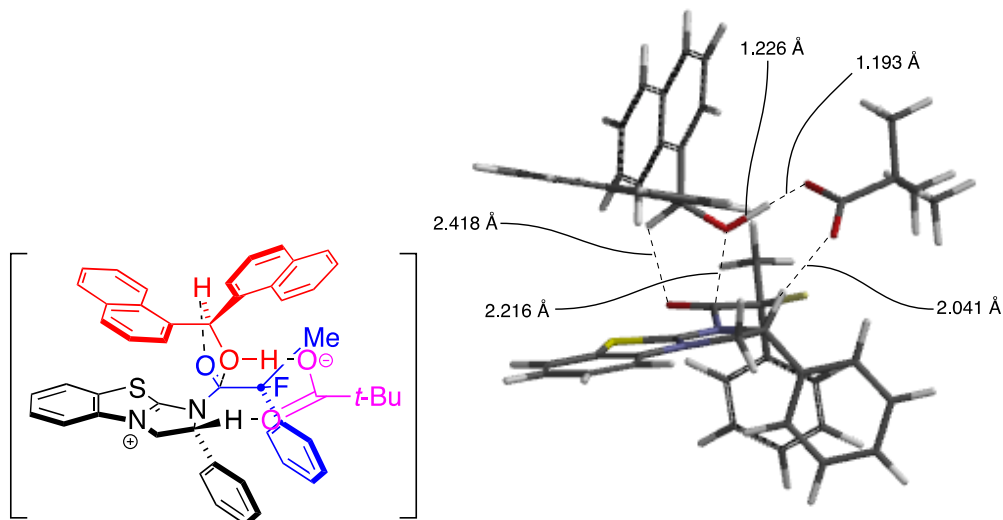
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Supplementary Material

S2-7 Cartesian Coordinates of (*S*)-**ts** and (*R*)-**ts**

S8-73 ¹H and ¹³C-NMR Spectroscopic Data of Compounds

All calculations were performed with the program package *Spartan '10* 1.1.0 of Wavefunction Inc. All structures were optimized and subjected to frequency analysis with the B3LYP/6-31G* method, followed by single point B3LYP/6-31G* calculation.



Transition Structure (*S*)-**ts**

E(B3LYP/6-31G*) = −2840.88644 au

$\nu_{TS} = 593i \text{ cm}^{-1}$

Cartesian Coordinates (Angstroms)

Atomic Number X Y Z

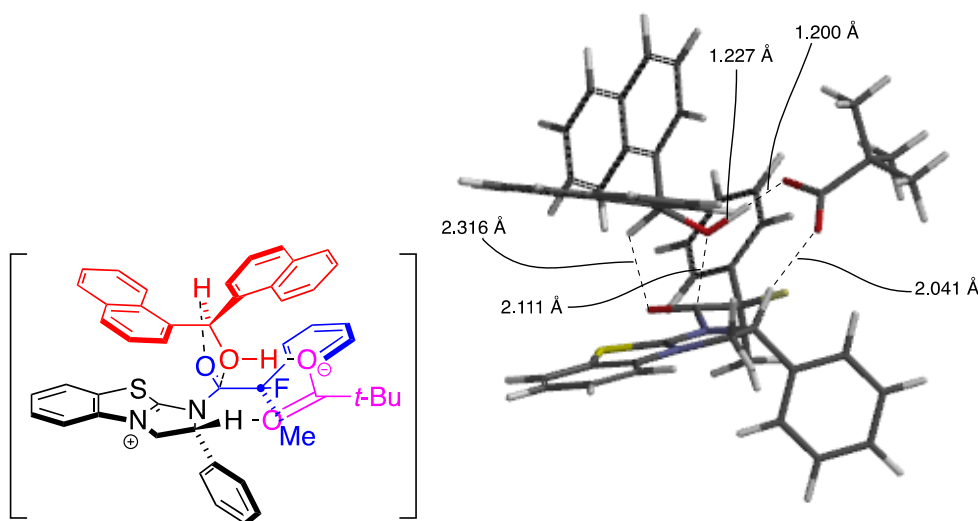
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6	-0.988443005	2.427409235	1.607086796
6	-1.726854186	1.215230178	0.941511935
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6	-3.995033255	0.706434573	1.866621776
6	-5.368827286	0.933756912	1.961478814
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1	3.816435072	-5.811671024	-2.803530077
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6	5.467197684	1.215201211	-0.907717294
1	5.971855826	1.058689544	-1.857674534
1	-2.306359717	-3.105319692	-1.881333244
9	-2.517325816	-1.248063568	-0.077379298

Requested basis set is 6-31G(d)

There are 323 shells and 964 basis functions



Transition Structure (*R*)-ts

E(B3LYP/6-31G*) = −2840.88100 au

 $\nu_{ts} = 702i \text{ cm}^{-1}$

Cartesian Coordinates (Angstroms)

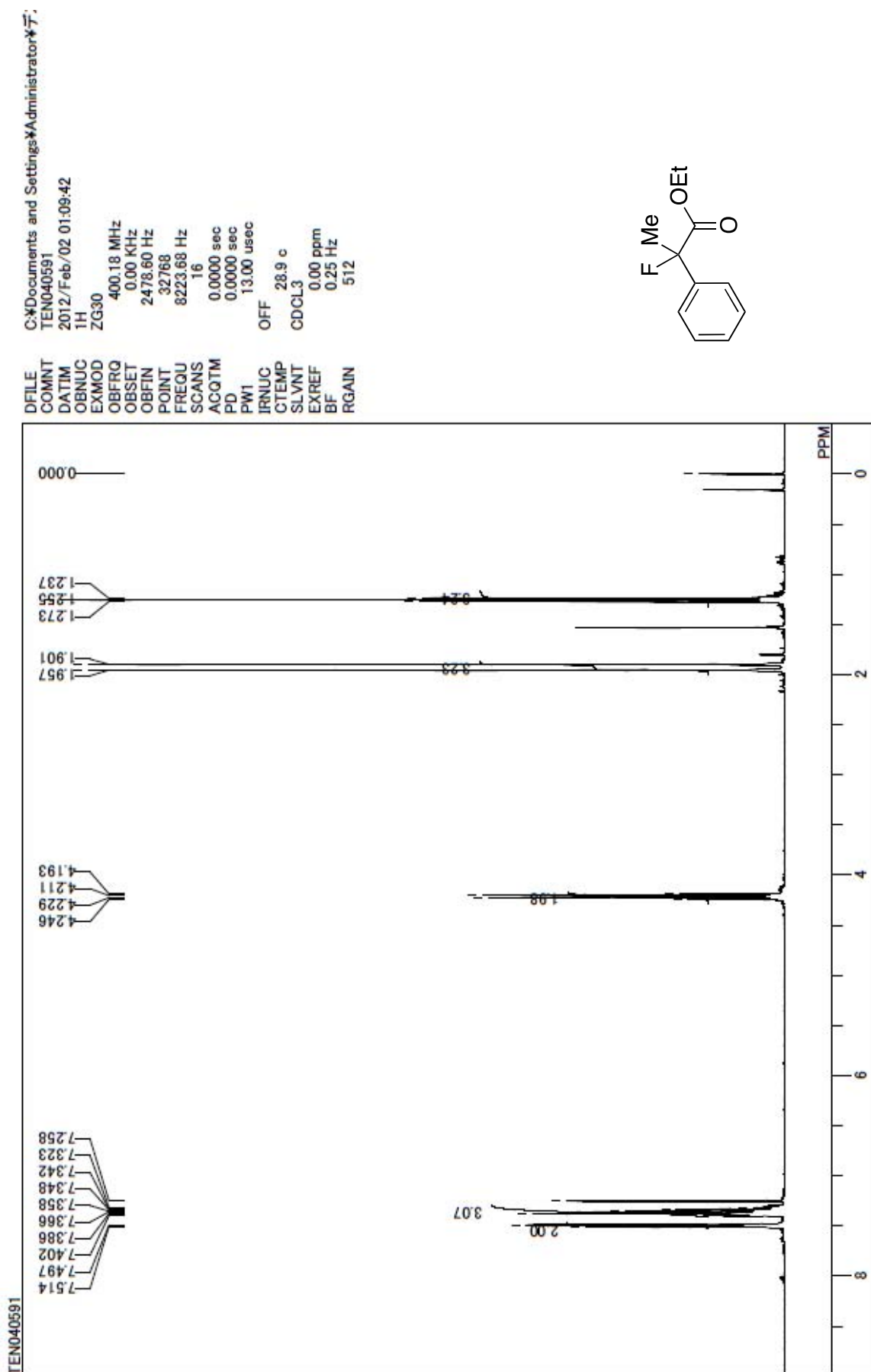
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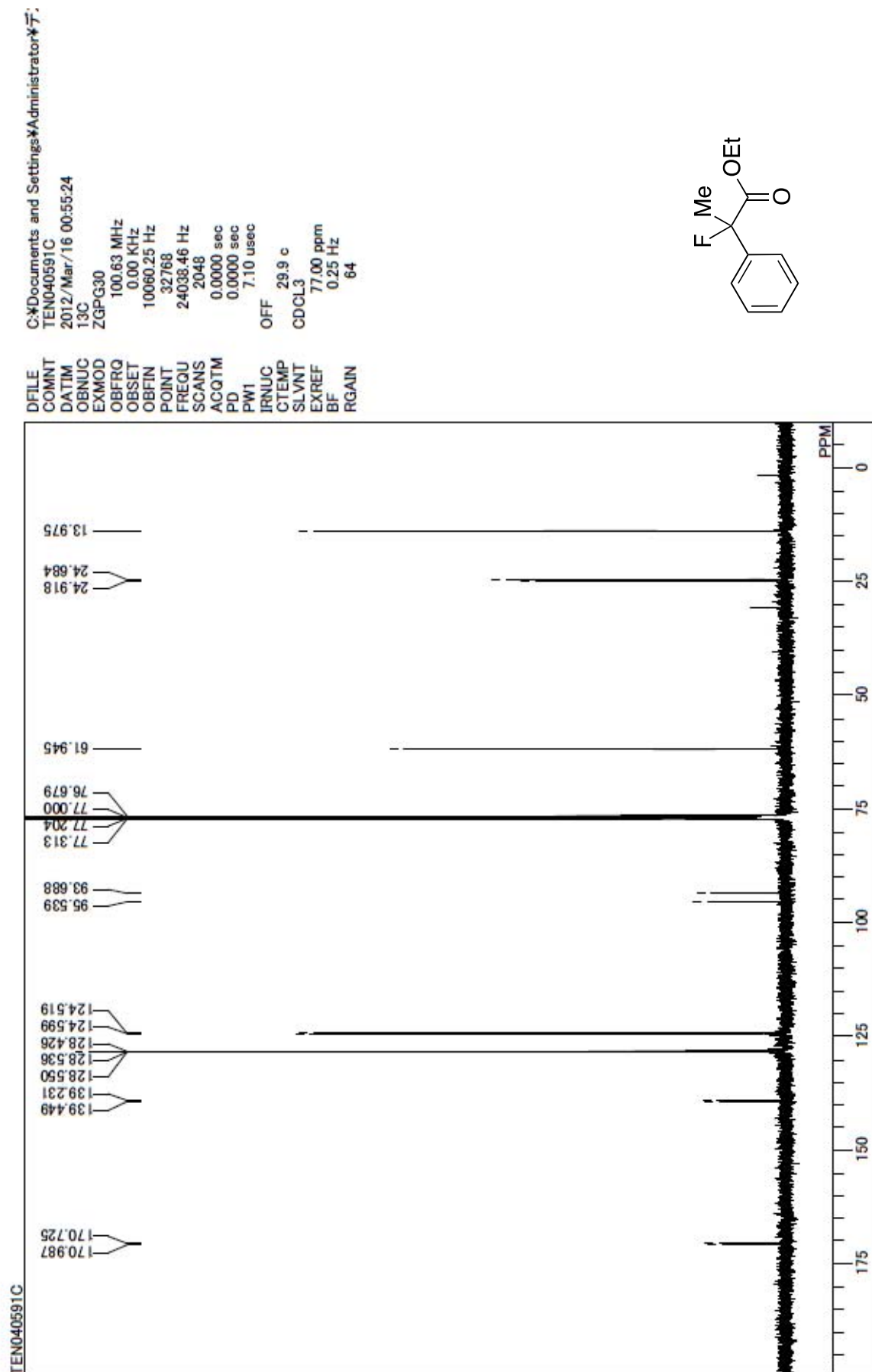
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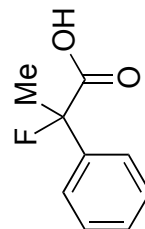
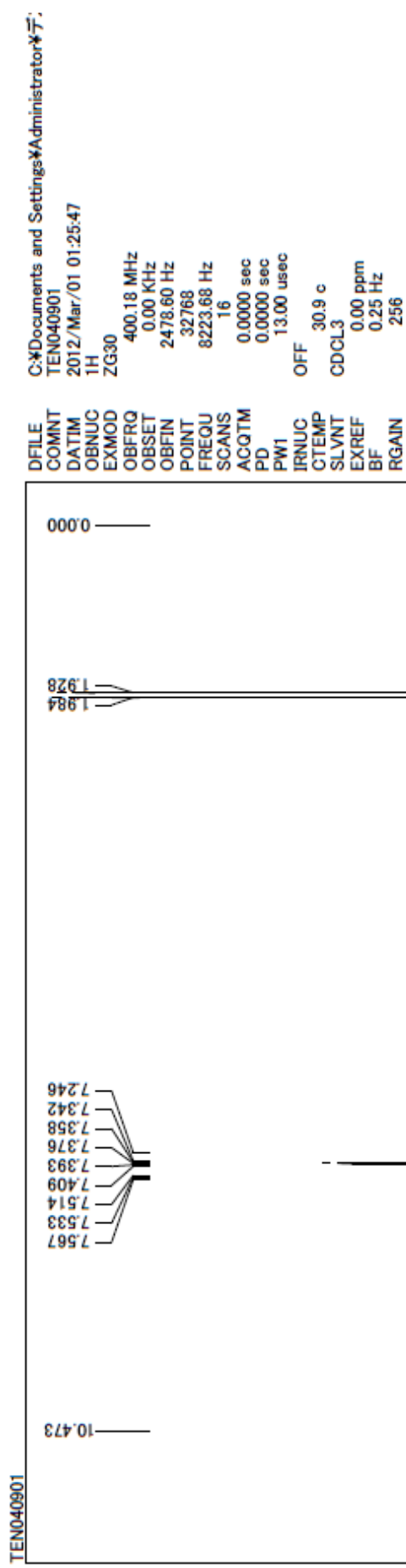
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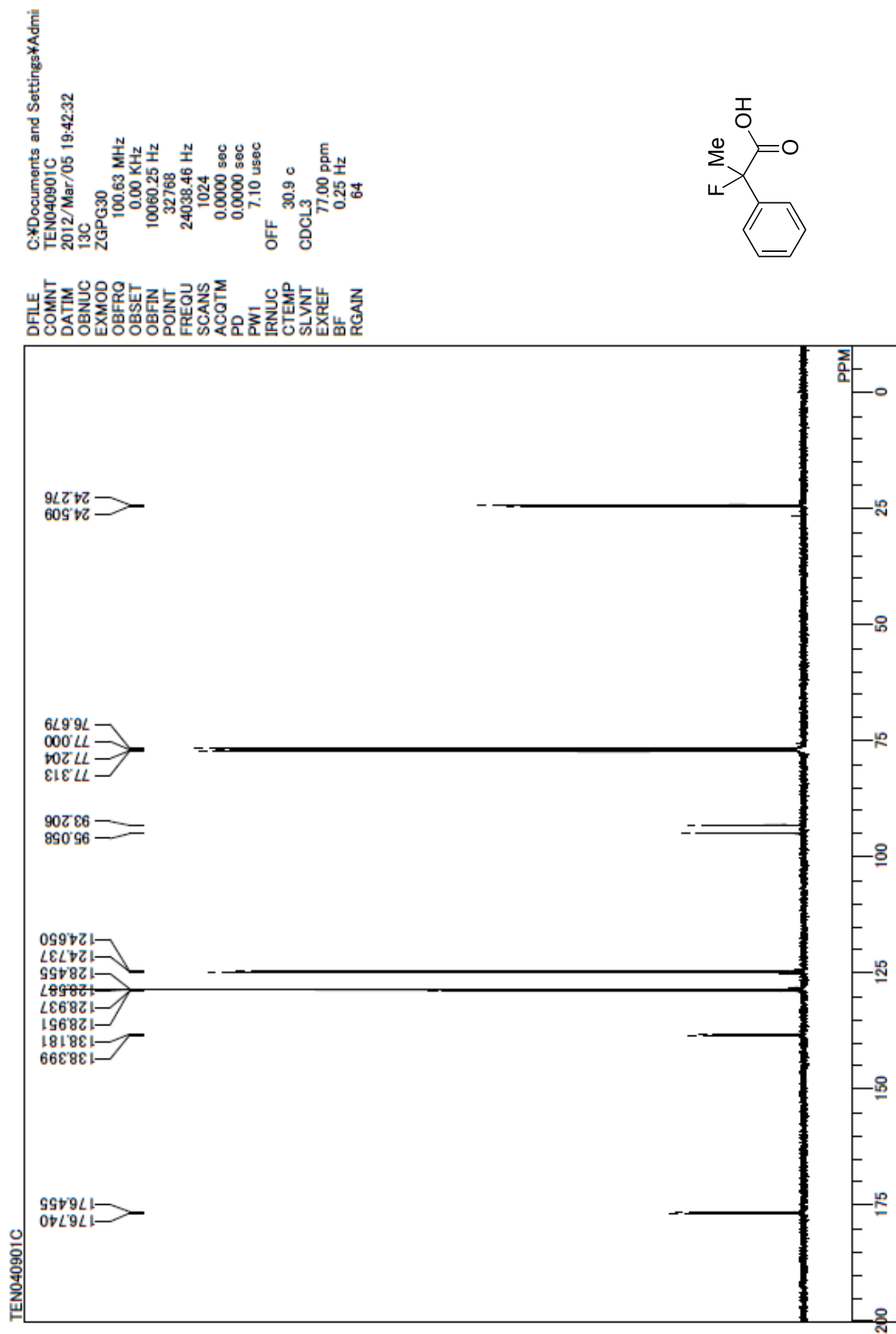
Requested basis set is 6-31G(d)

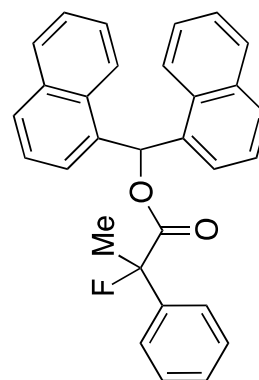
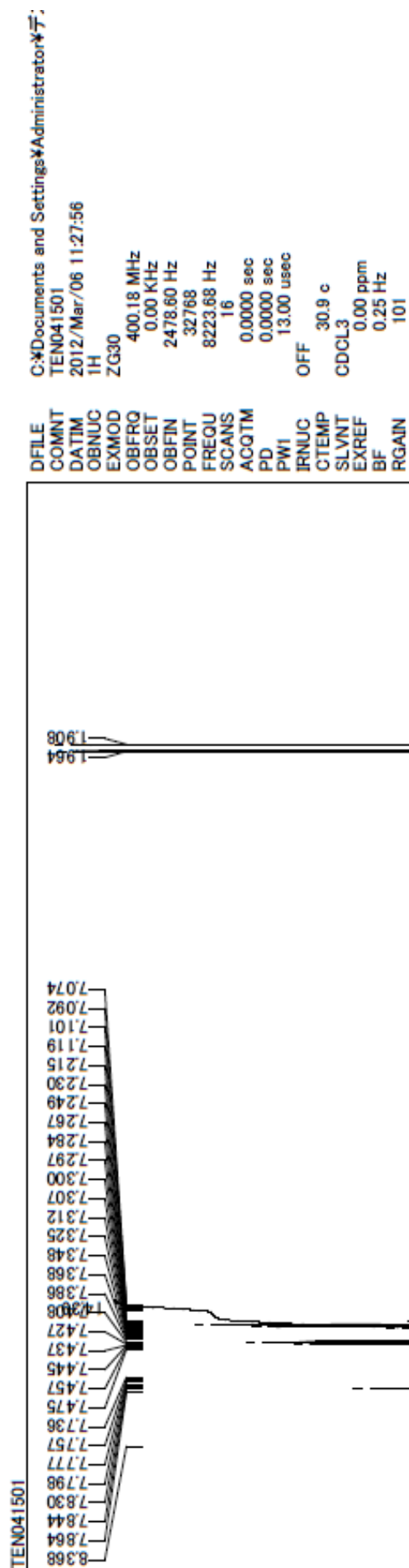
There are 323 shells and 964 basis functions

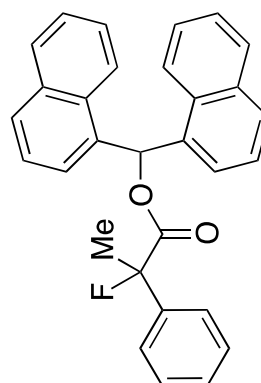
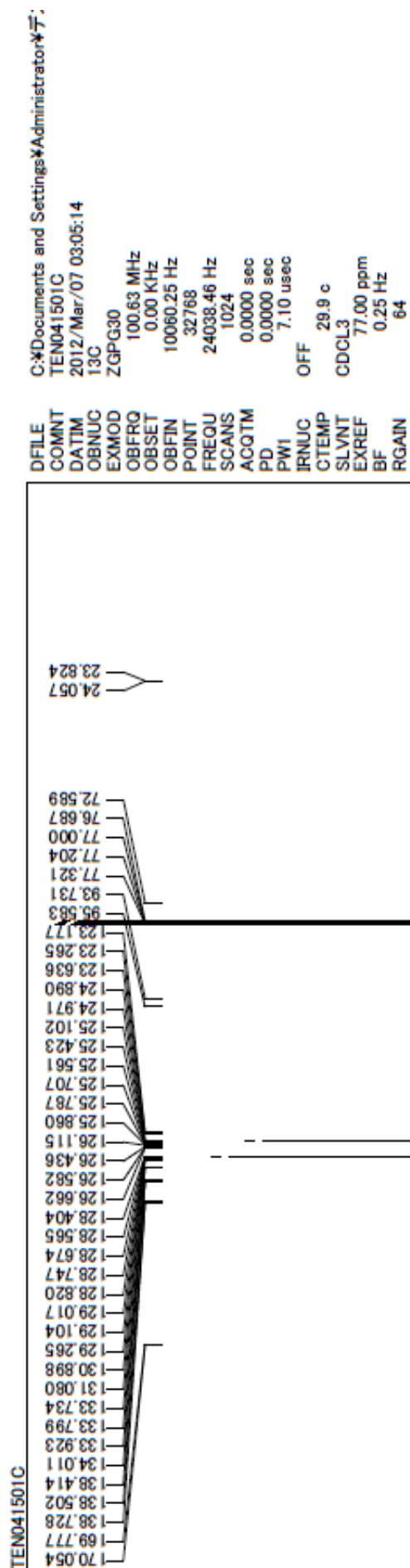


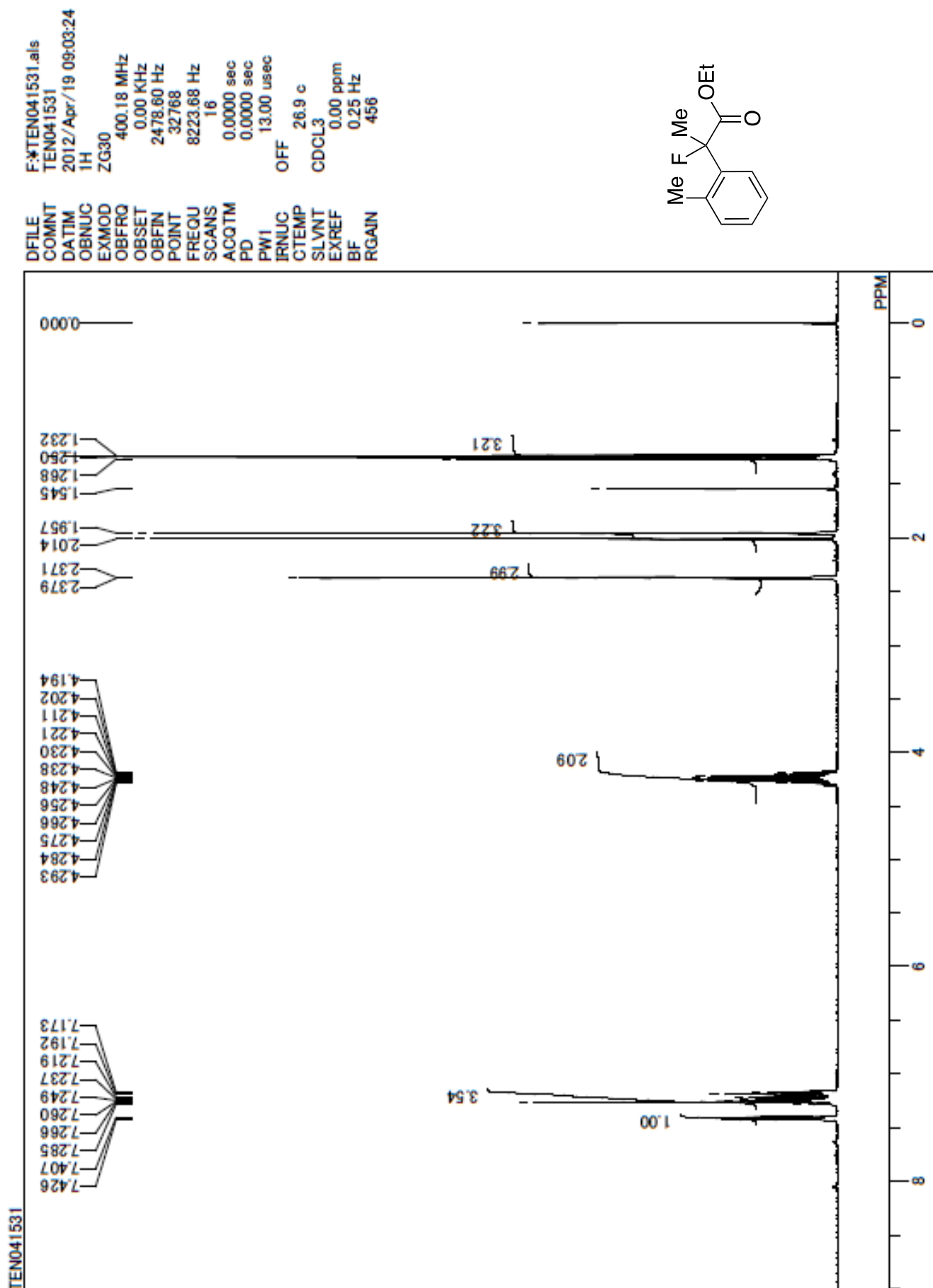


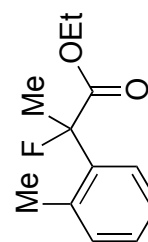
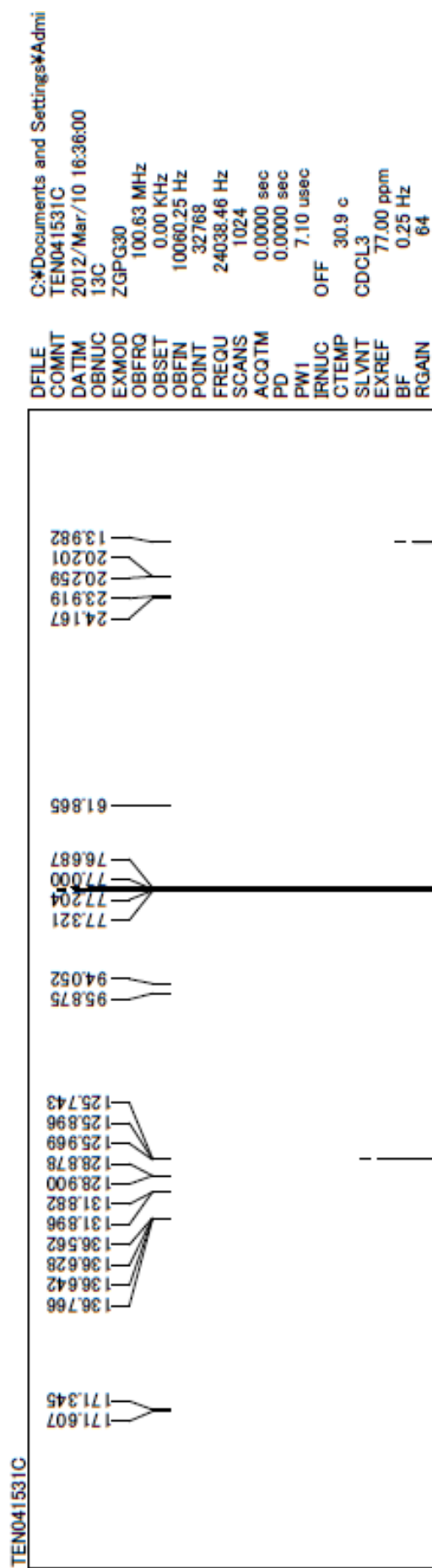


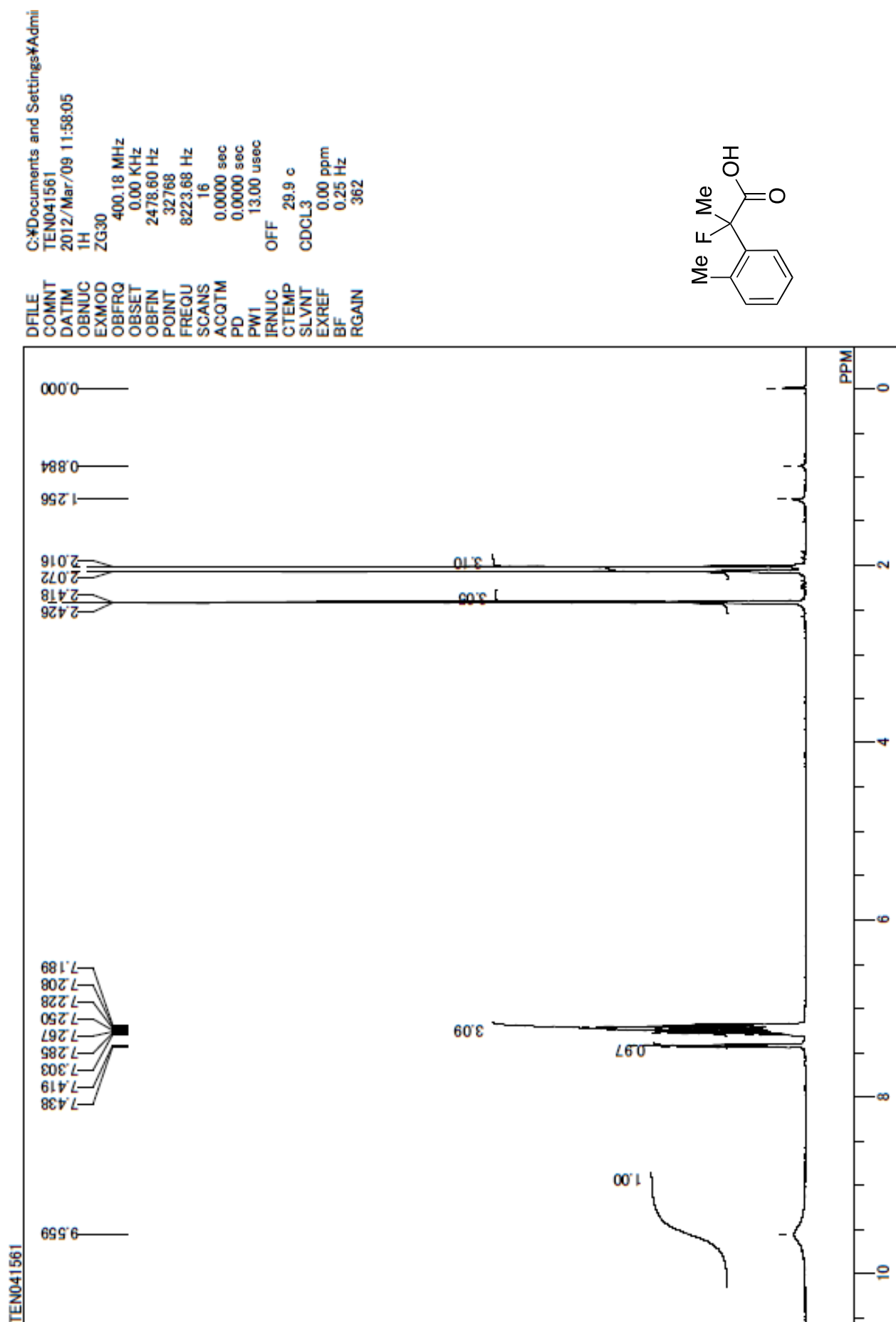


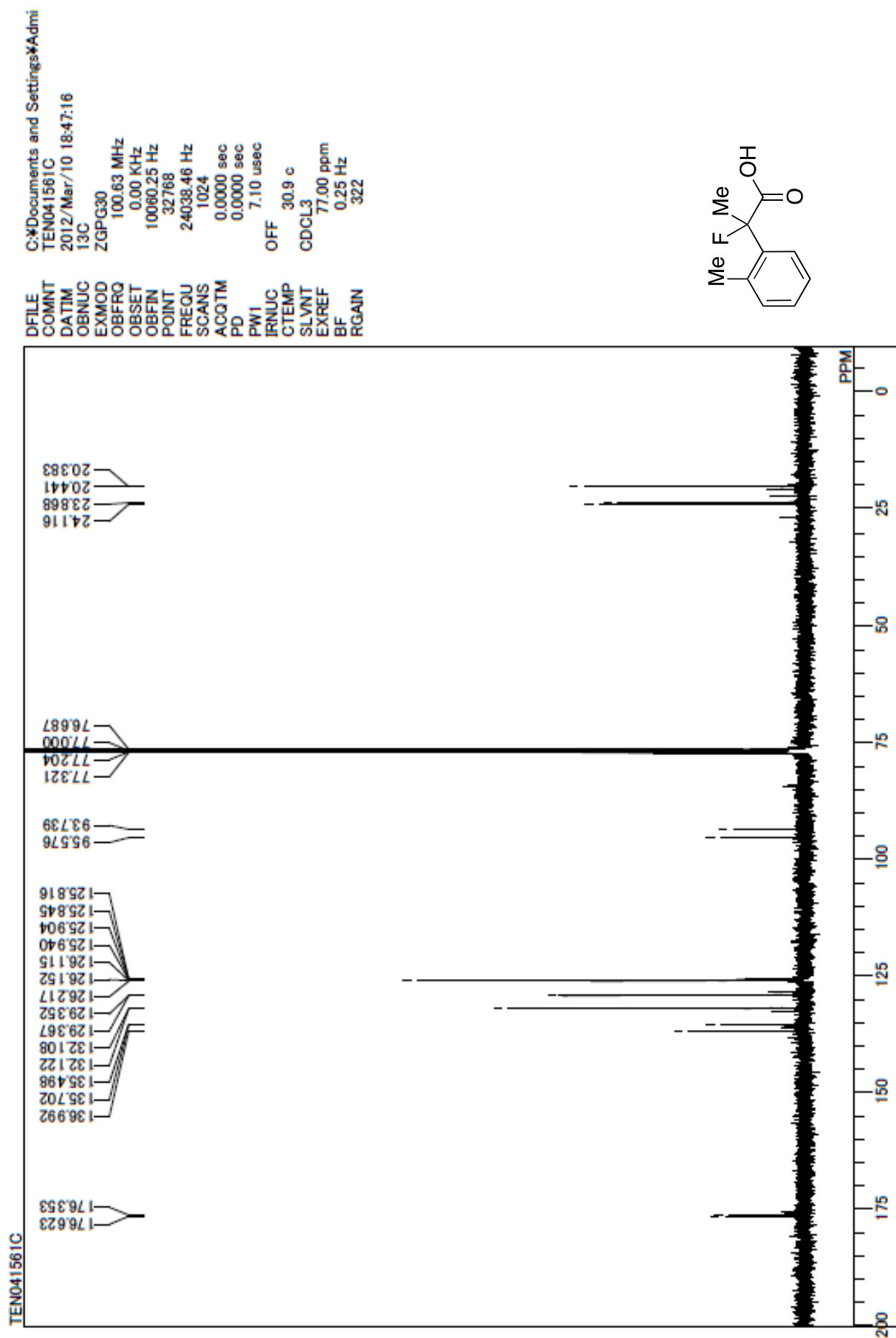


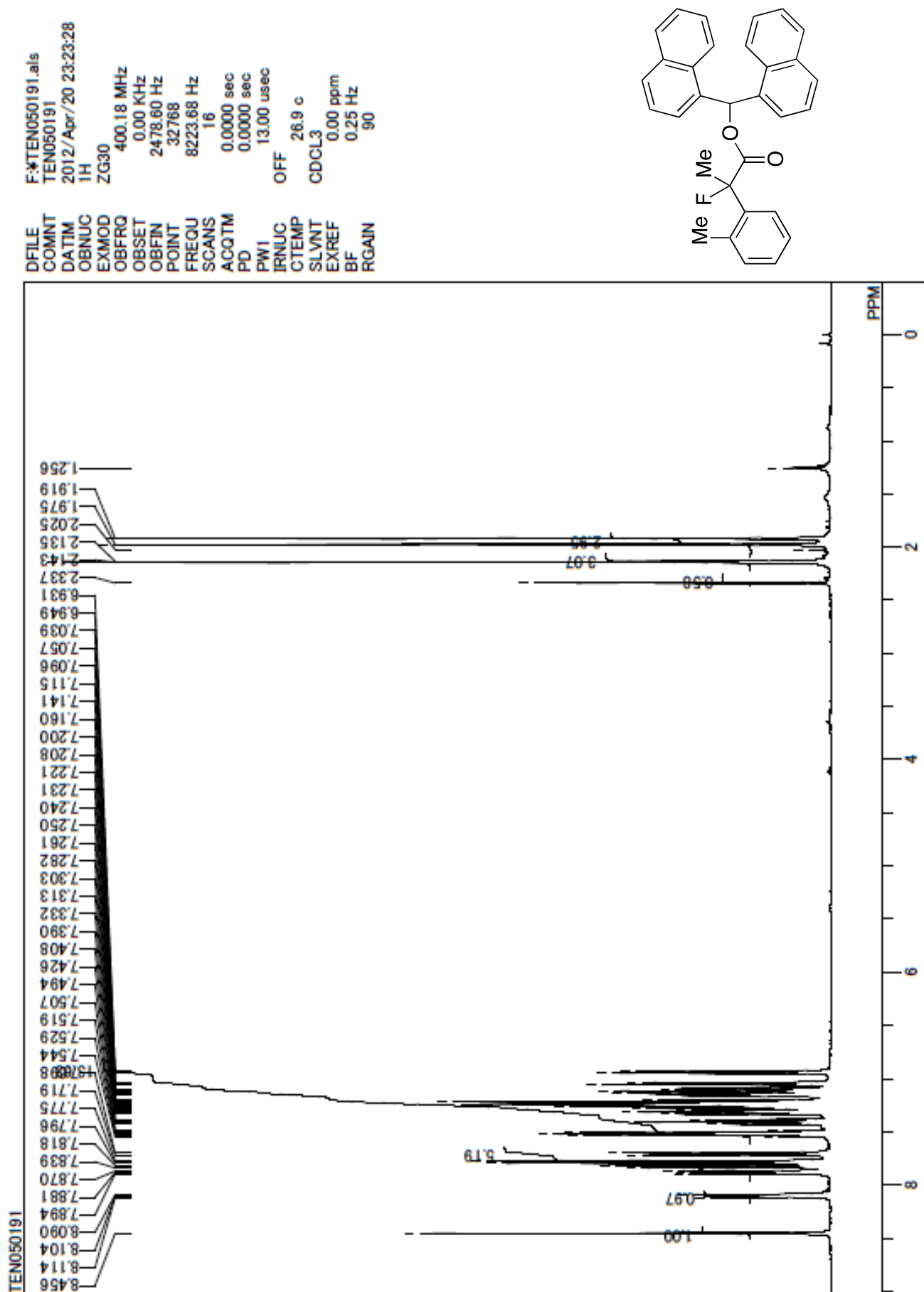


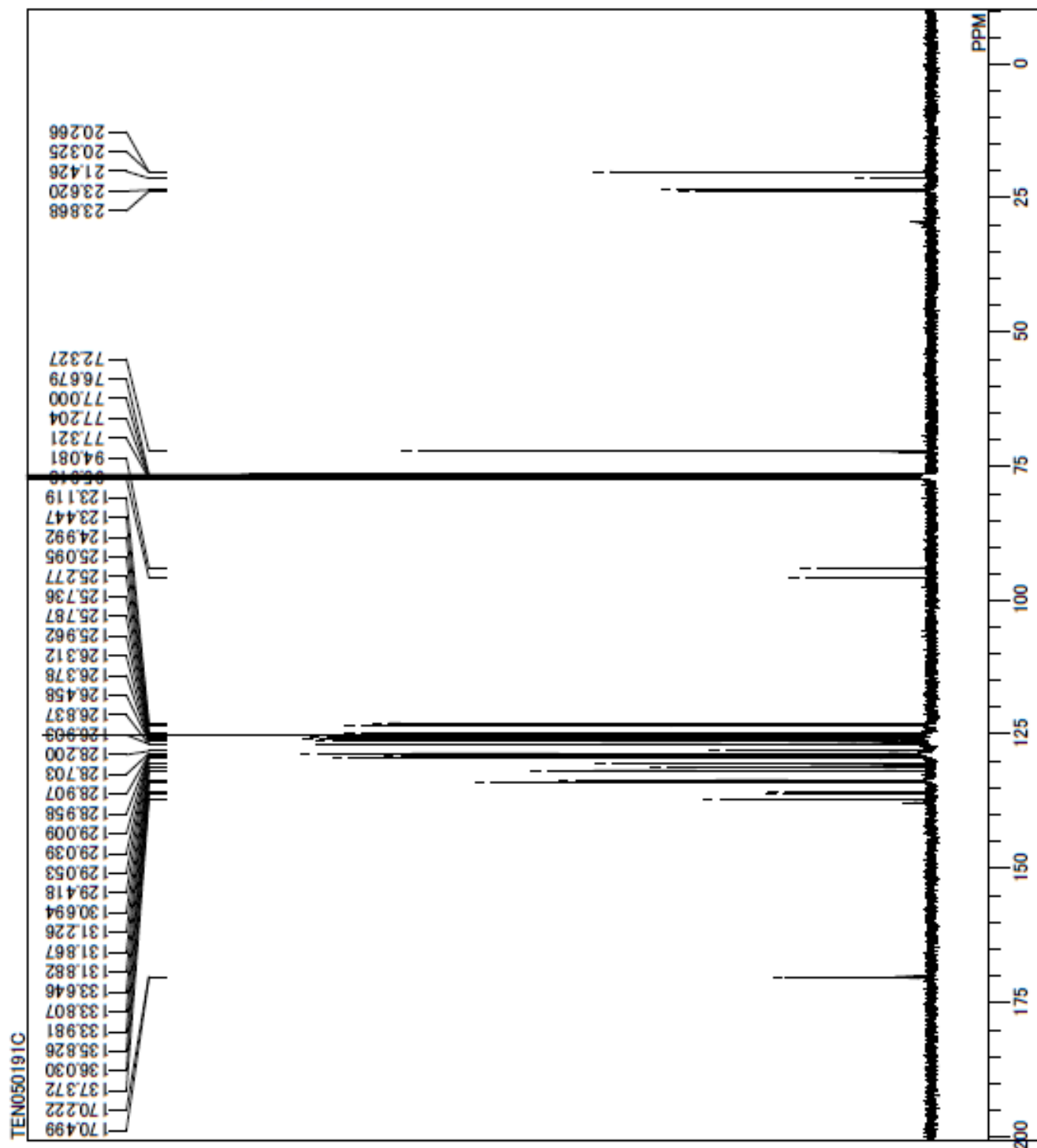




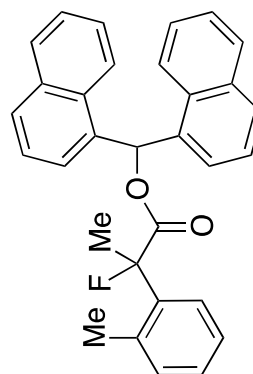


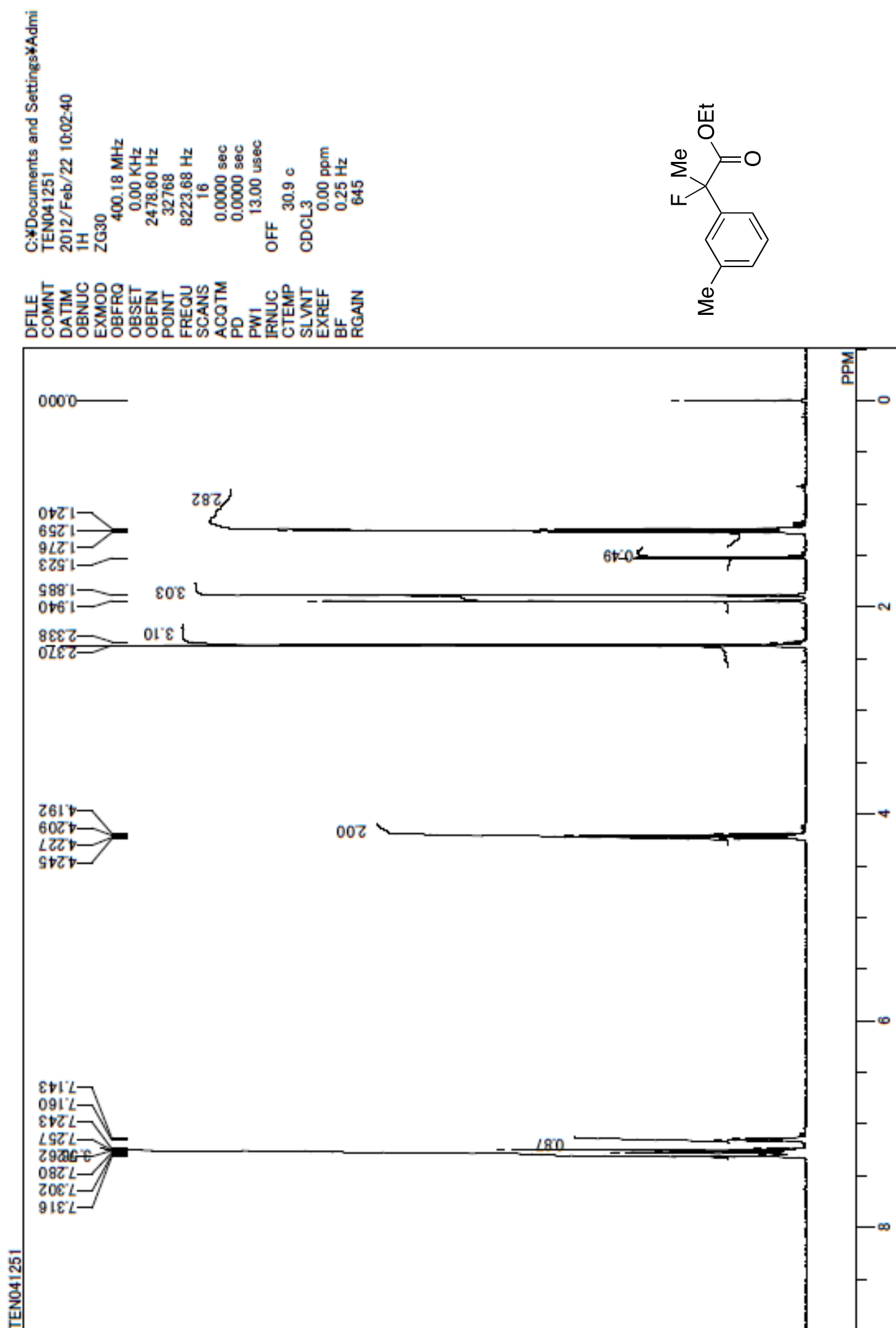


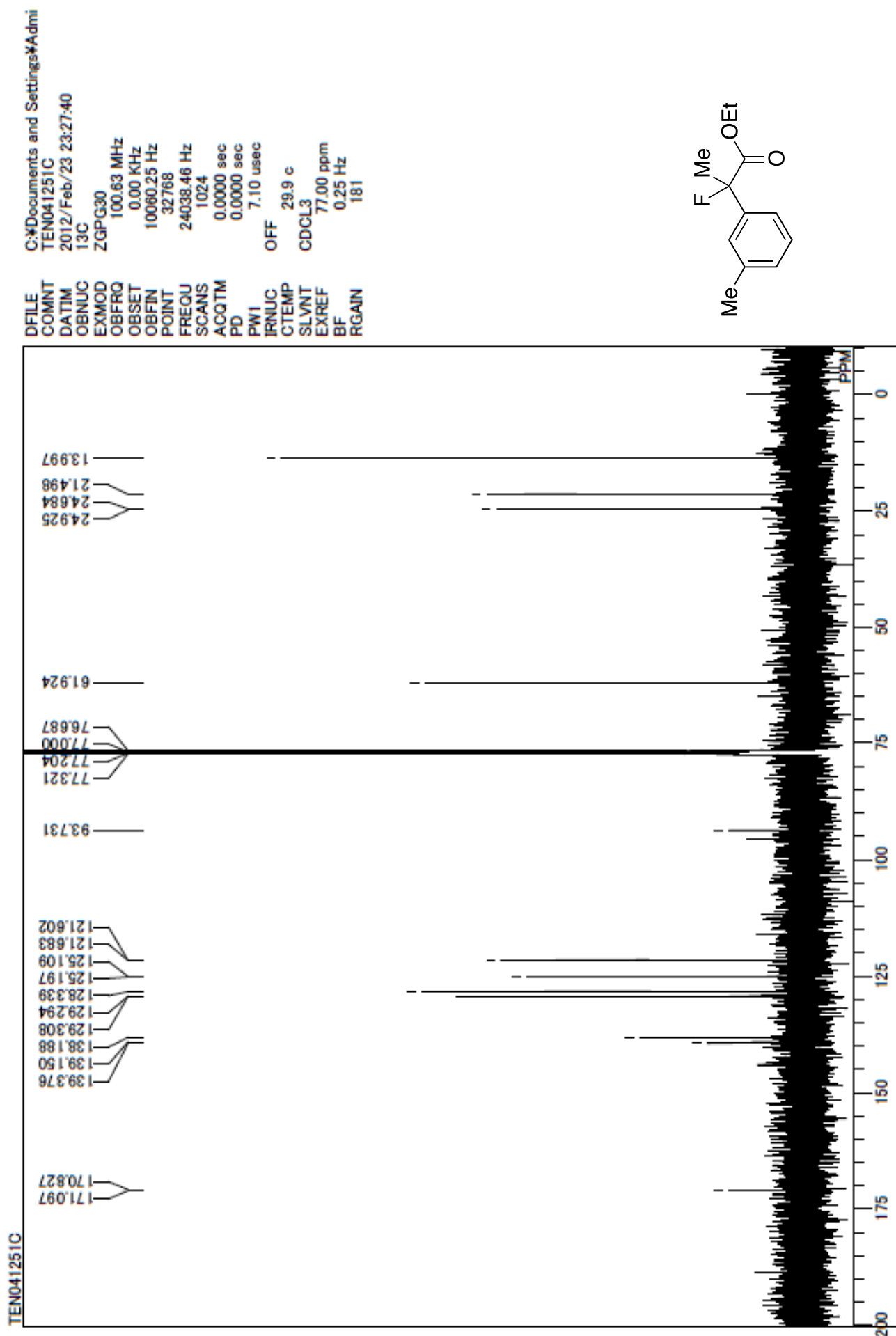


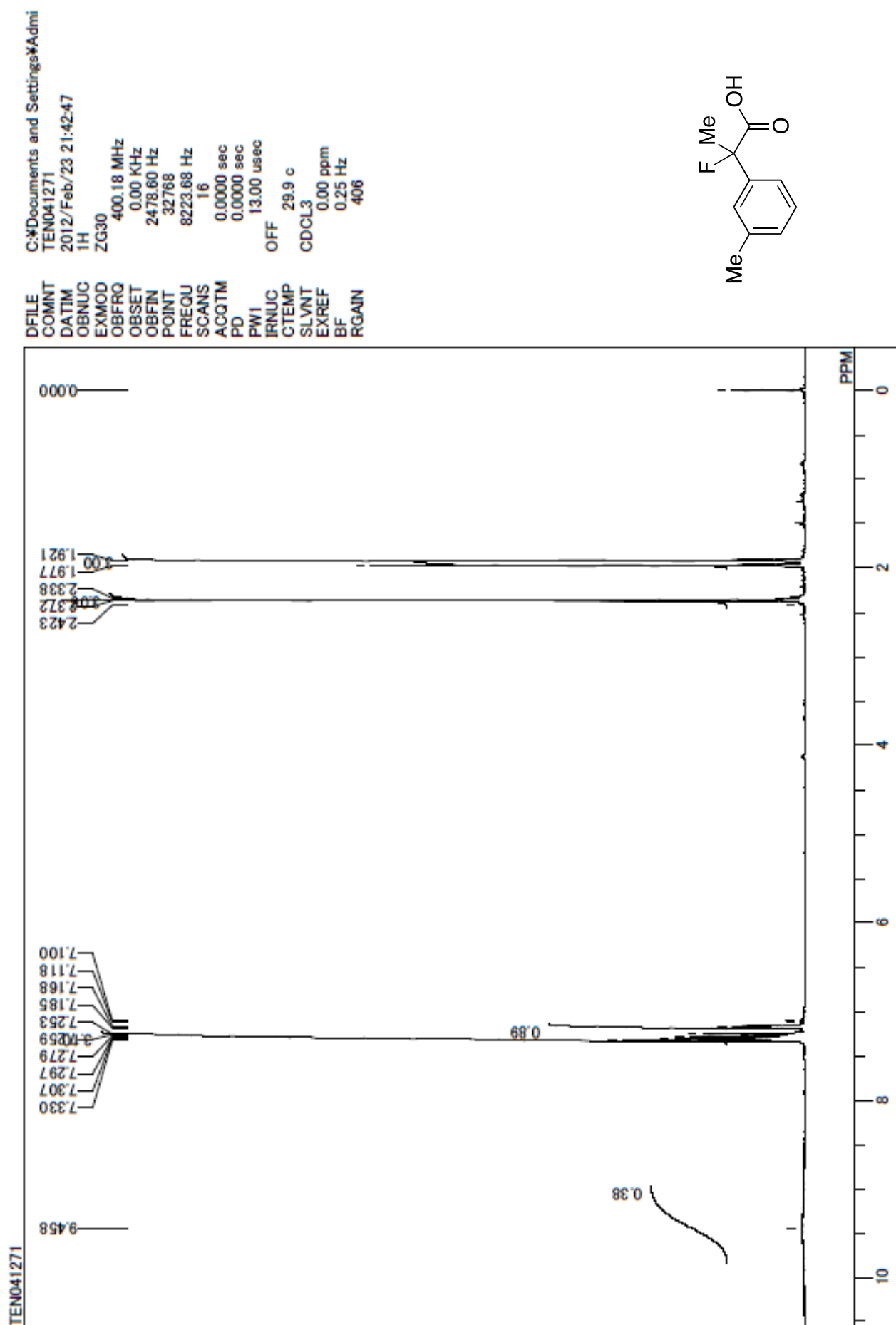


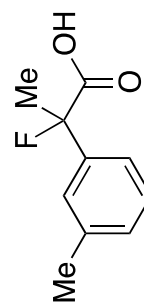
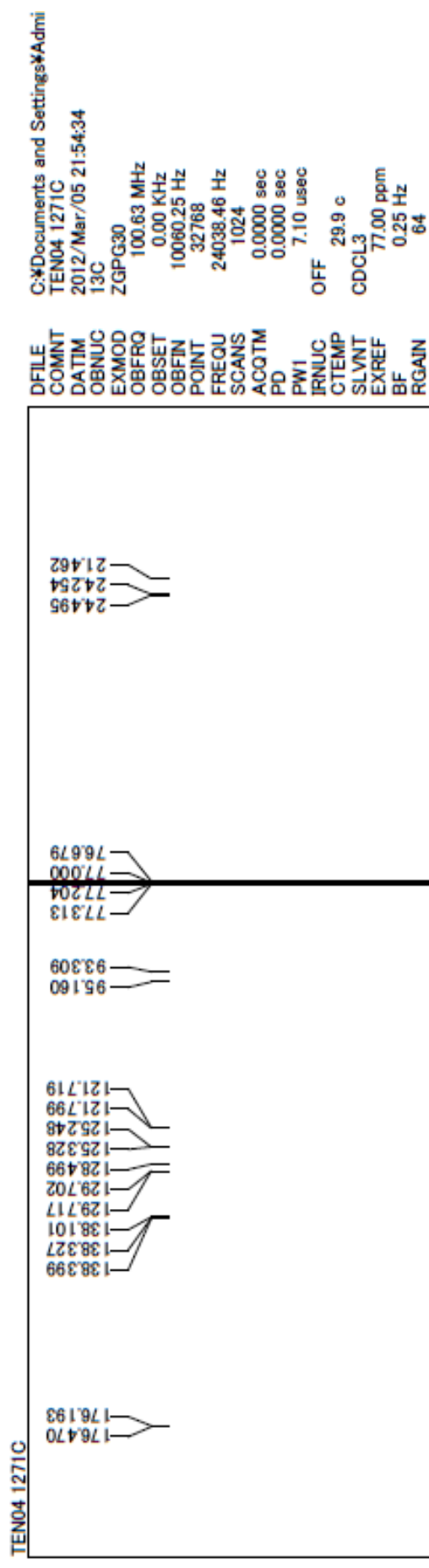
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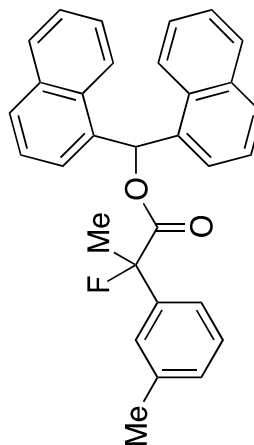
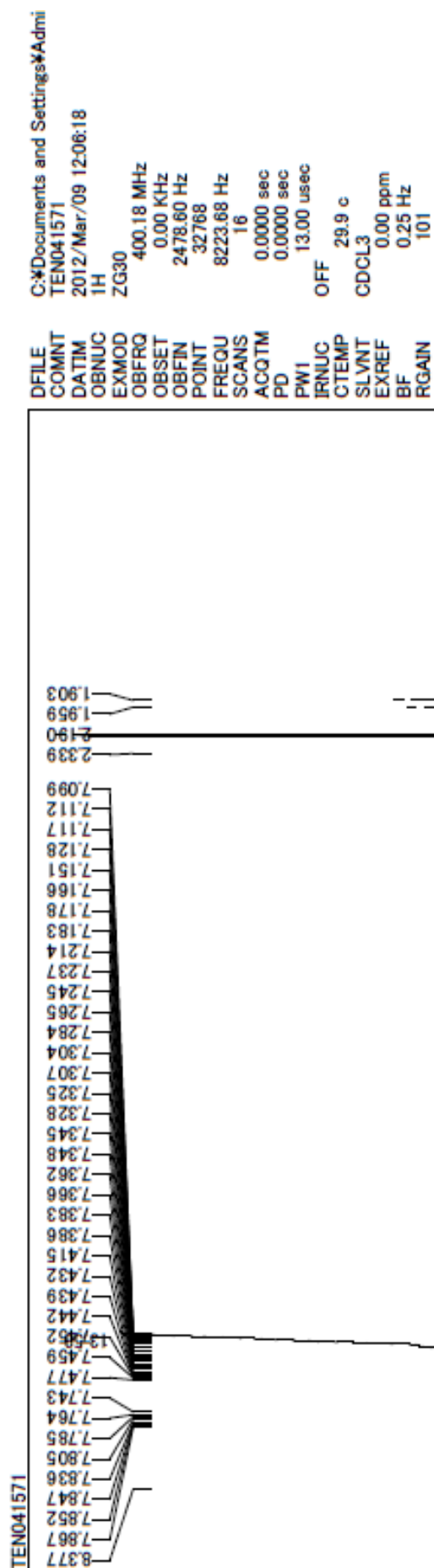


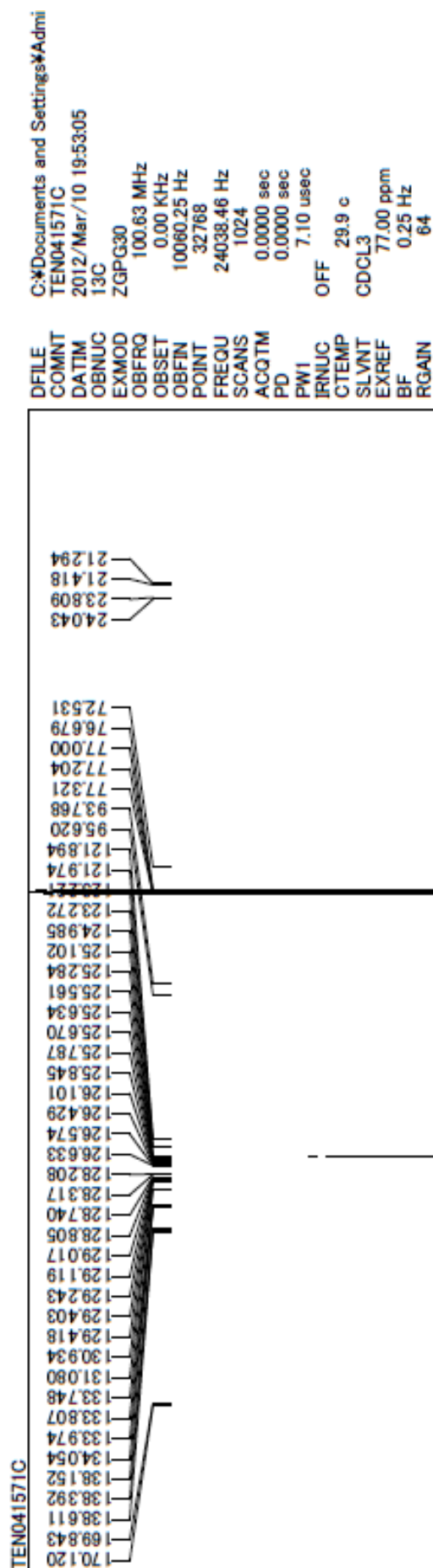


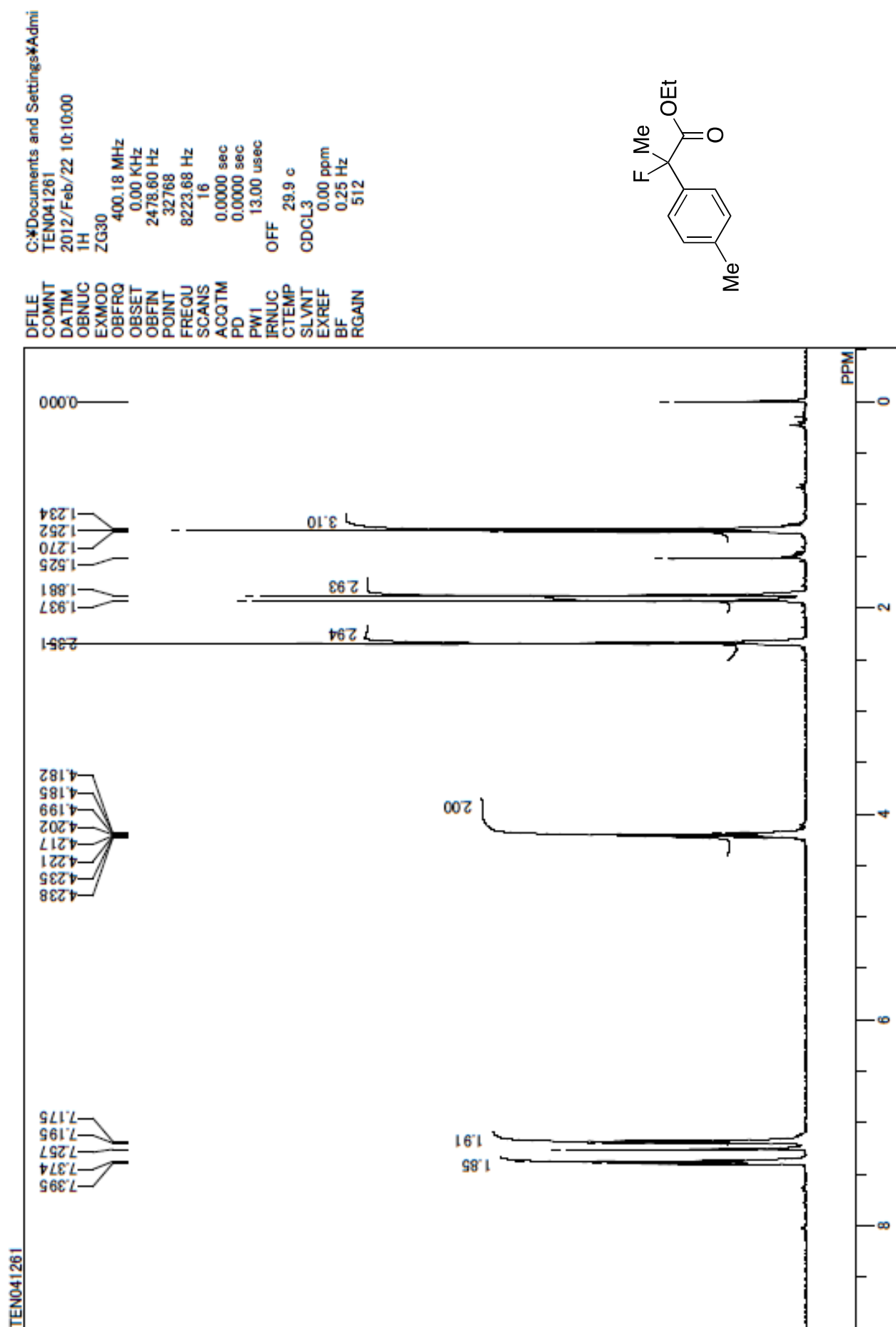


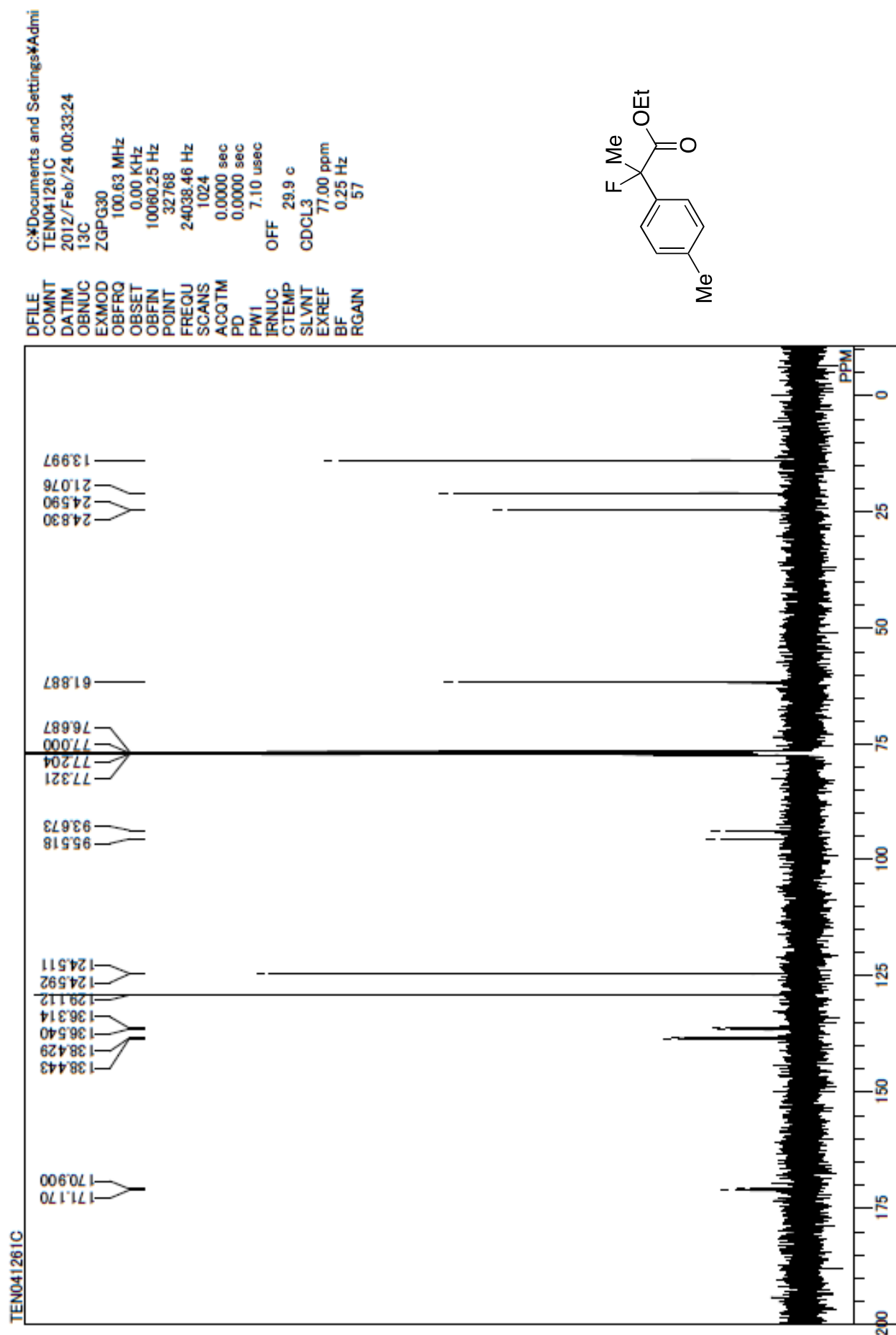


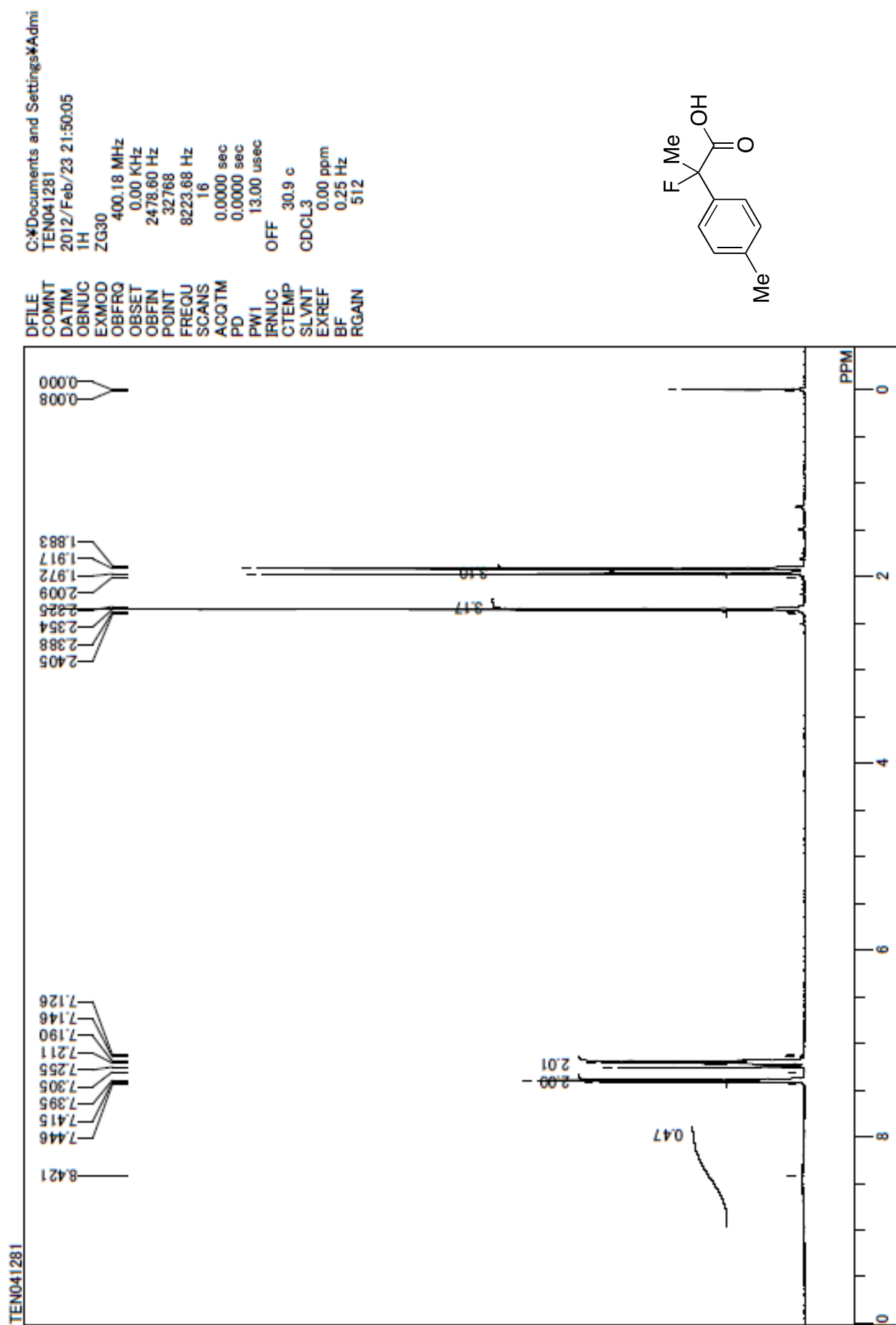


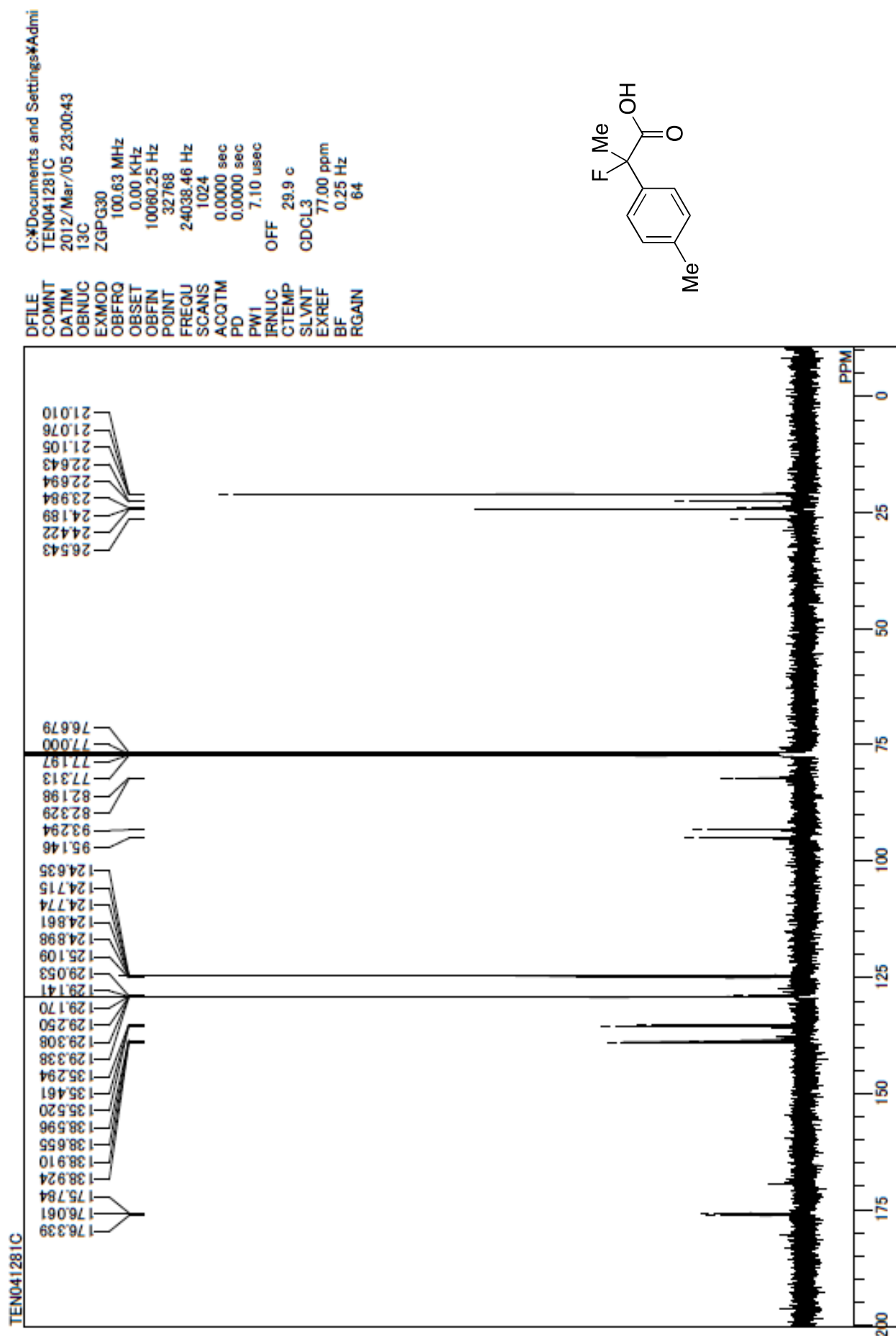


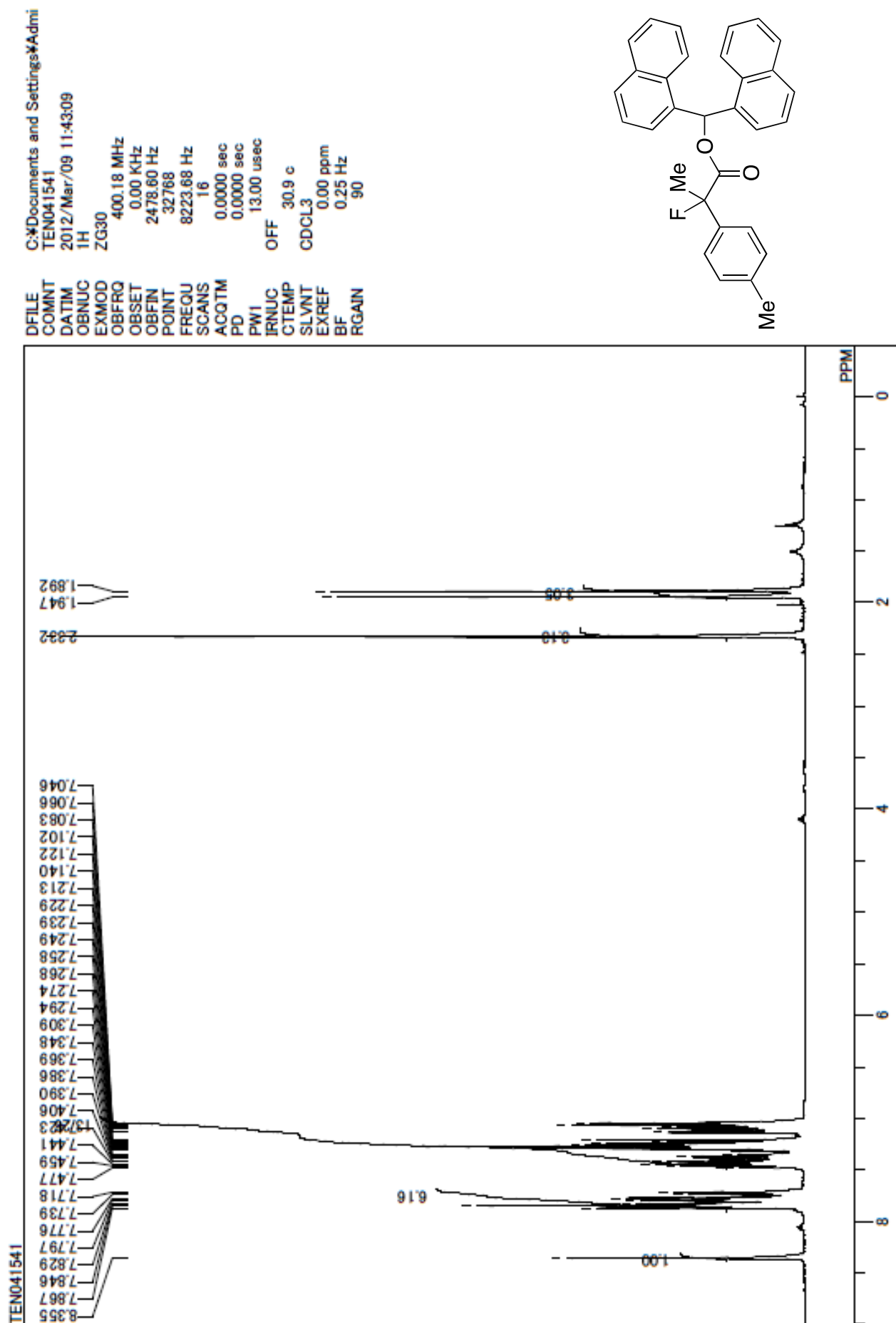


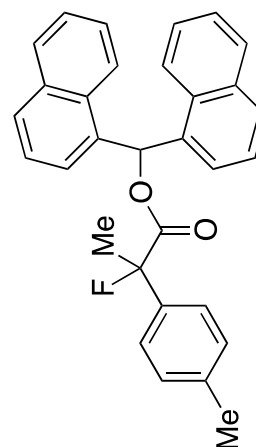
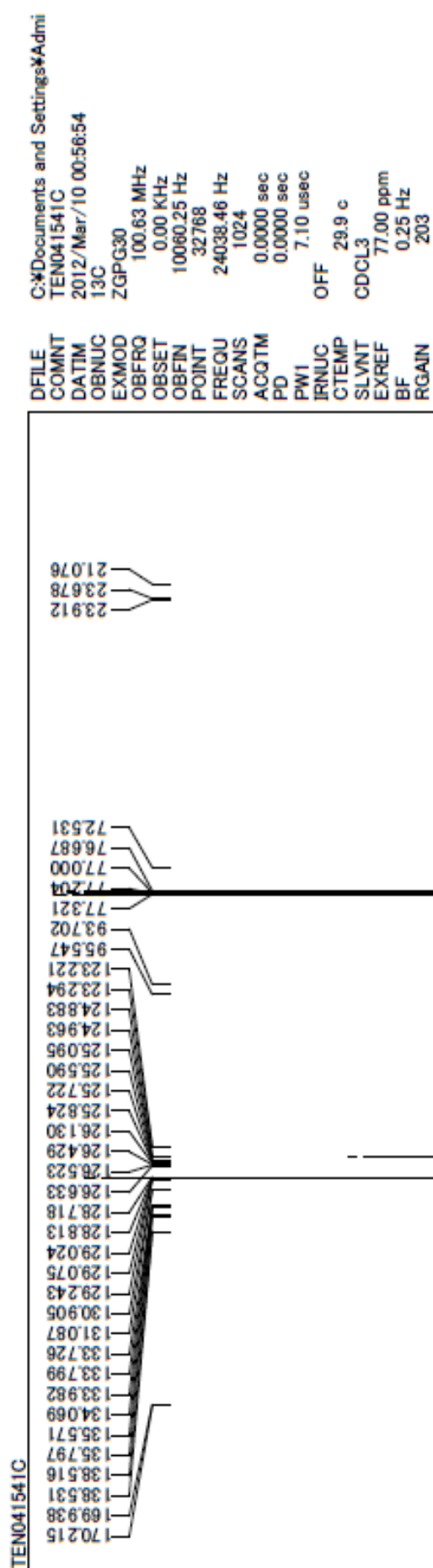


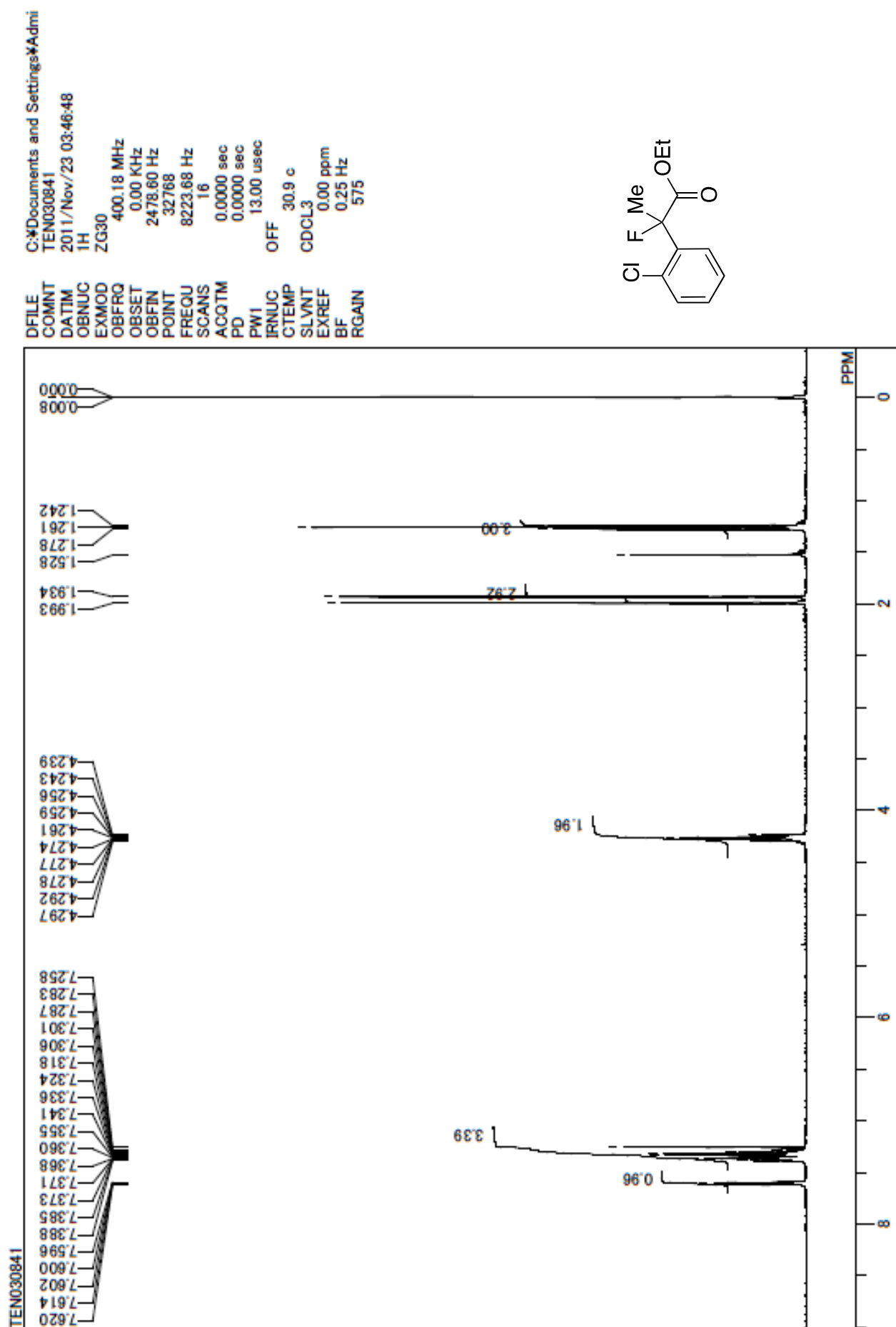


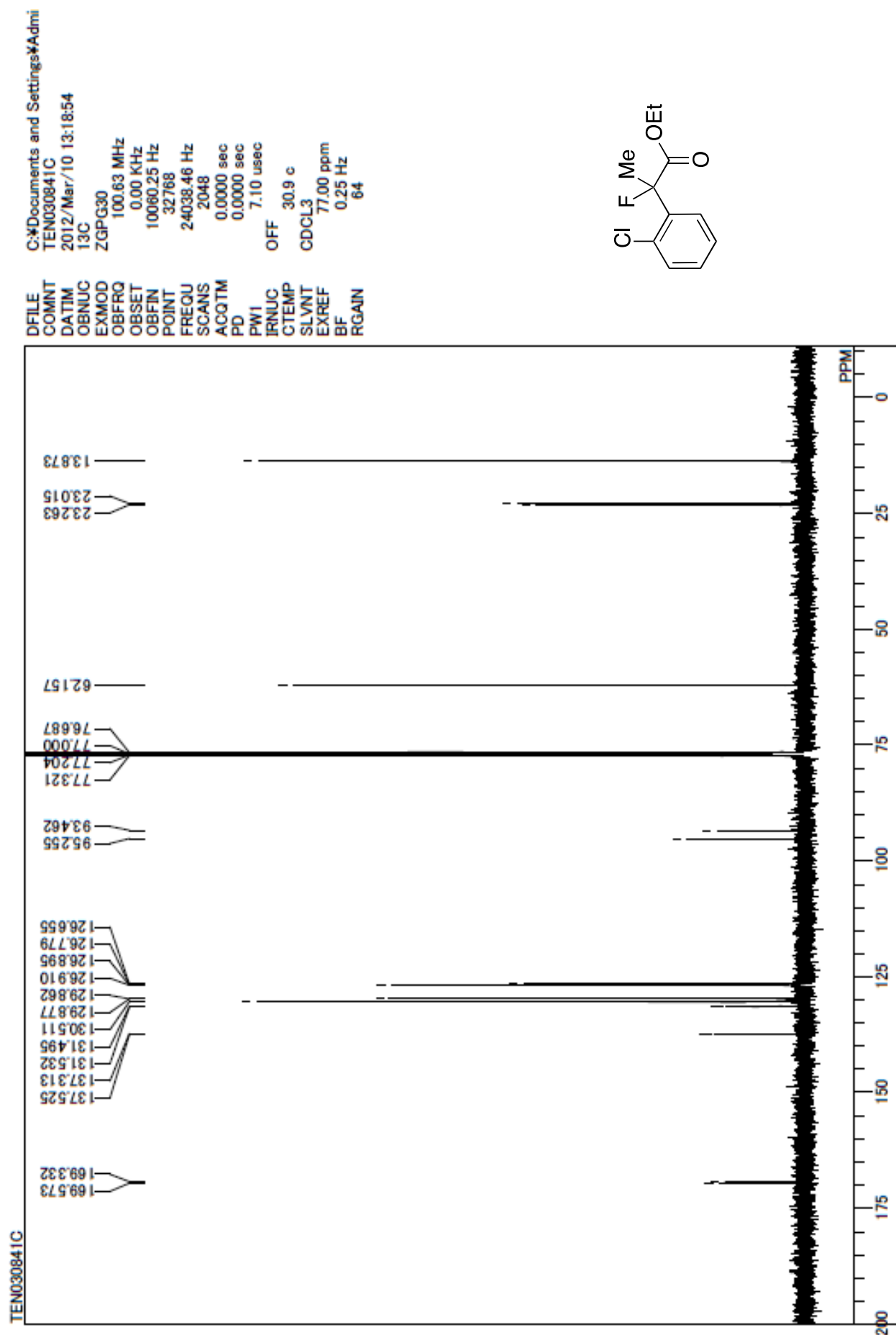


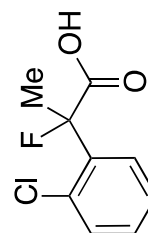
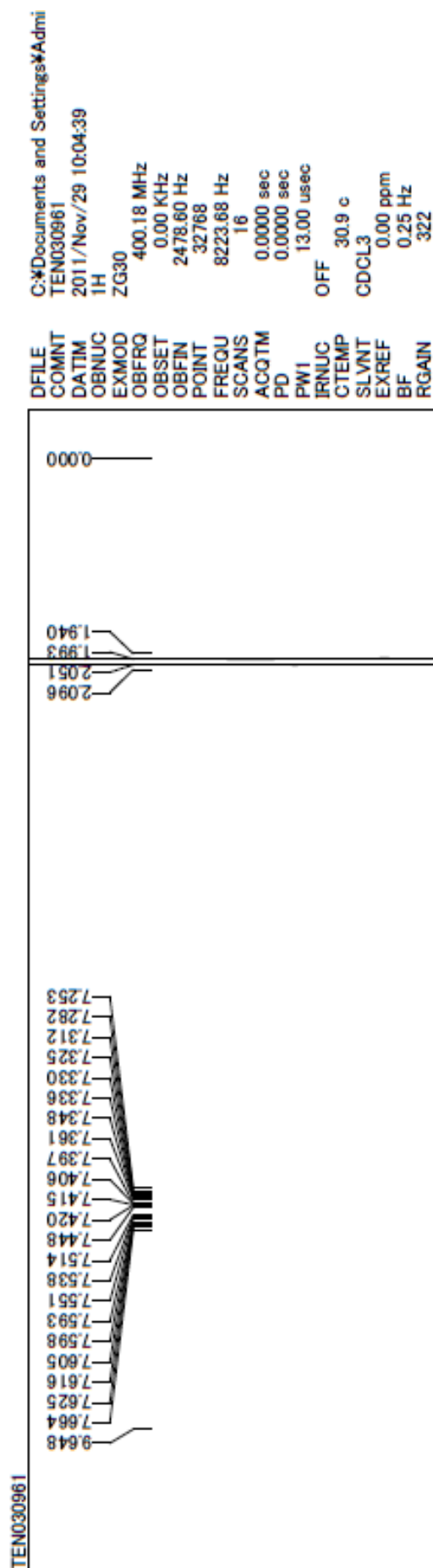


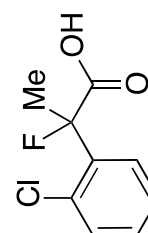
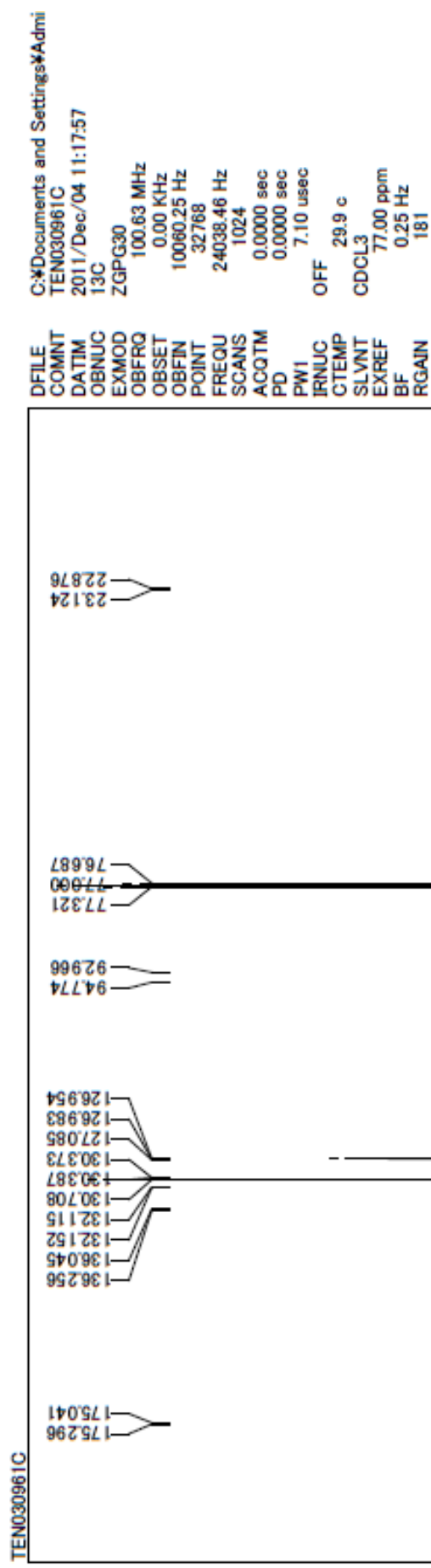


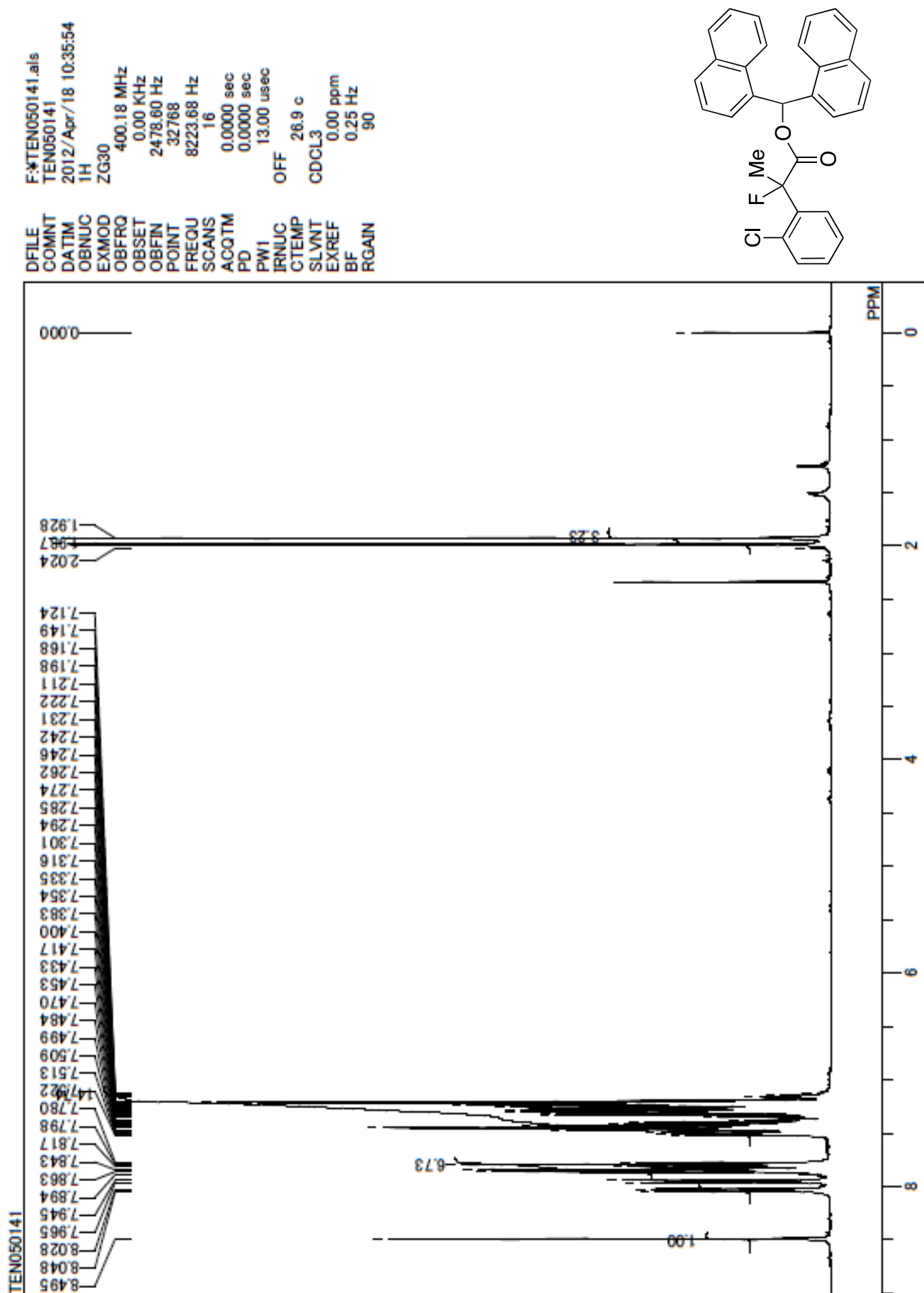


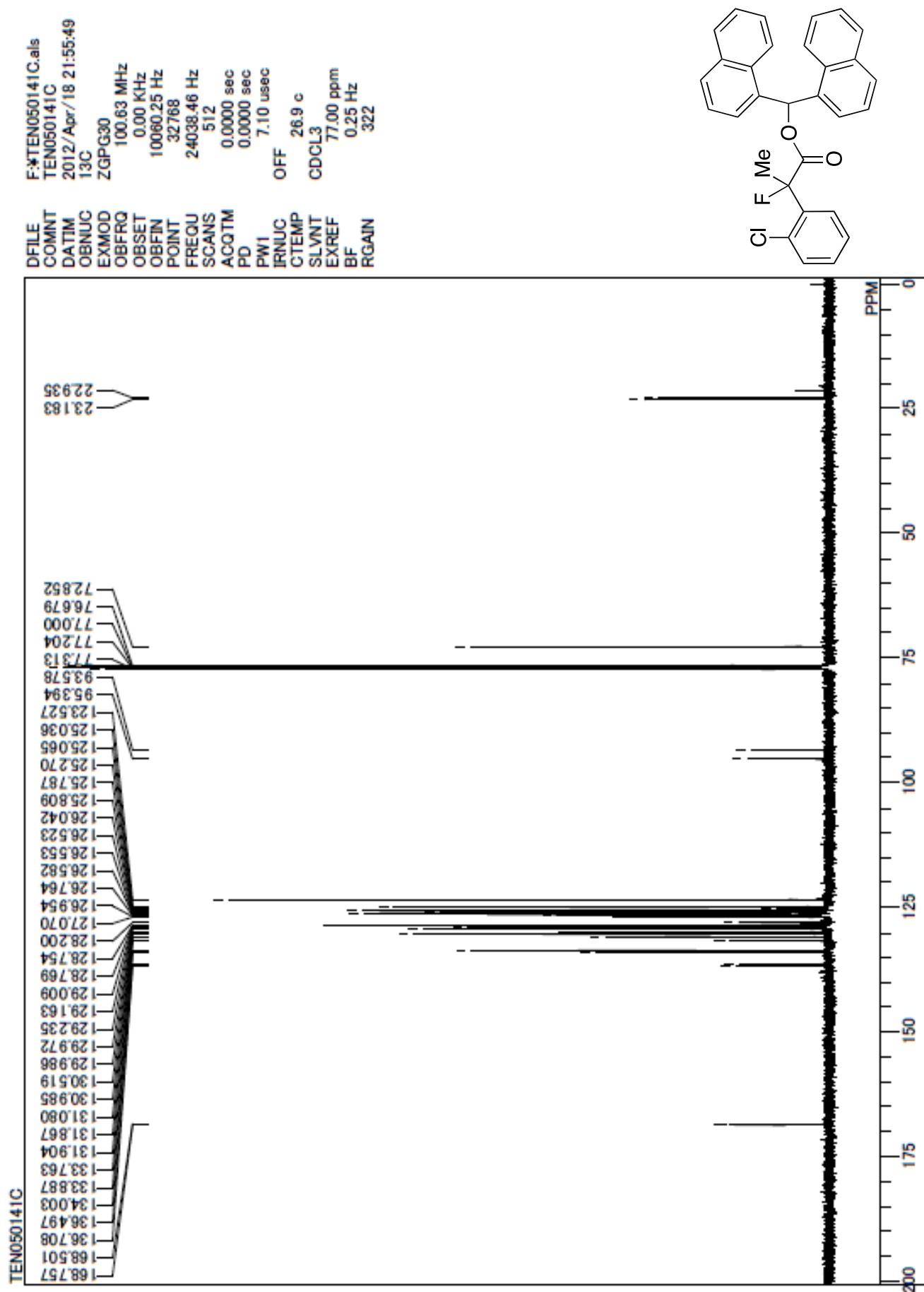


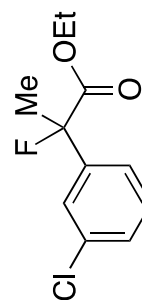
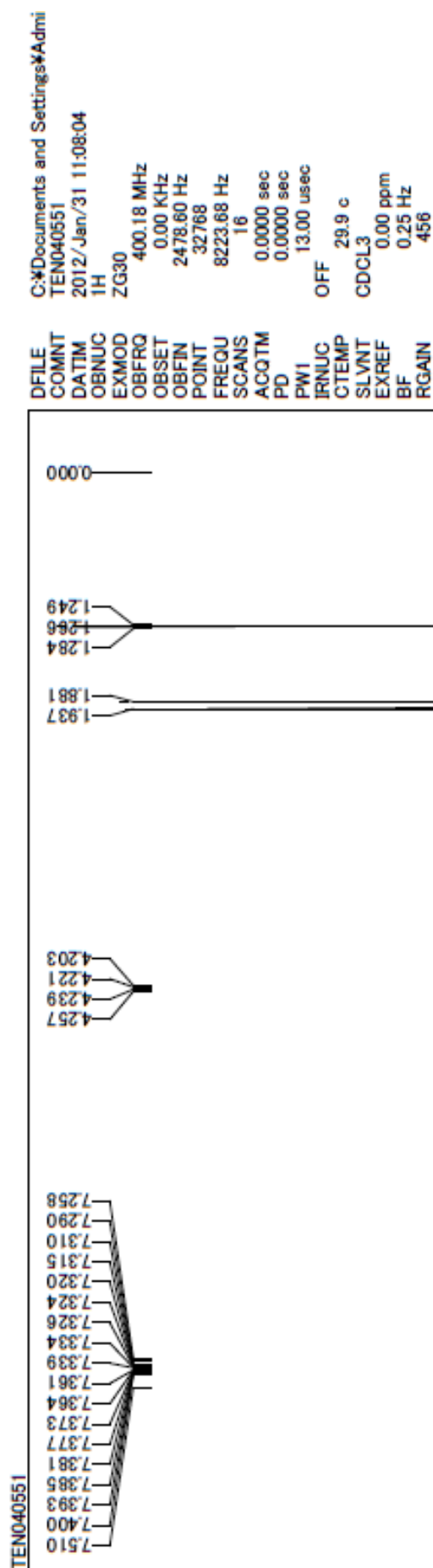


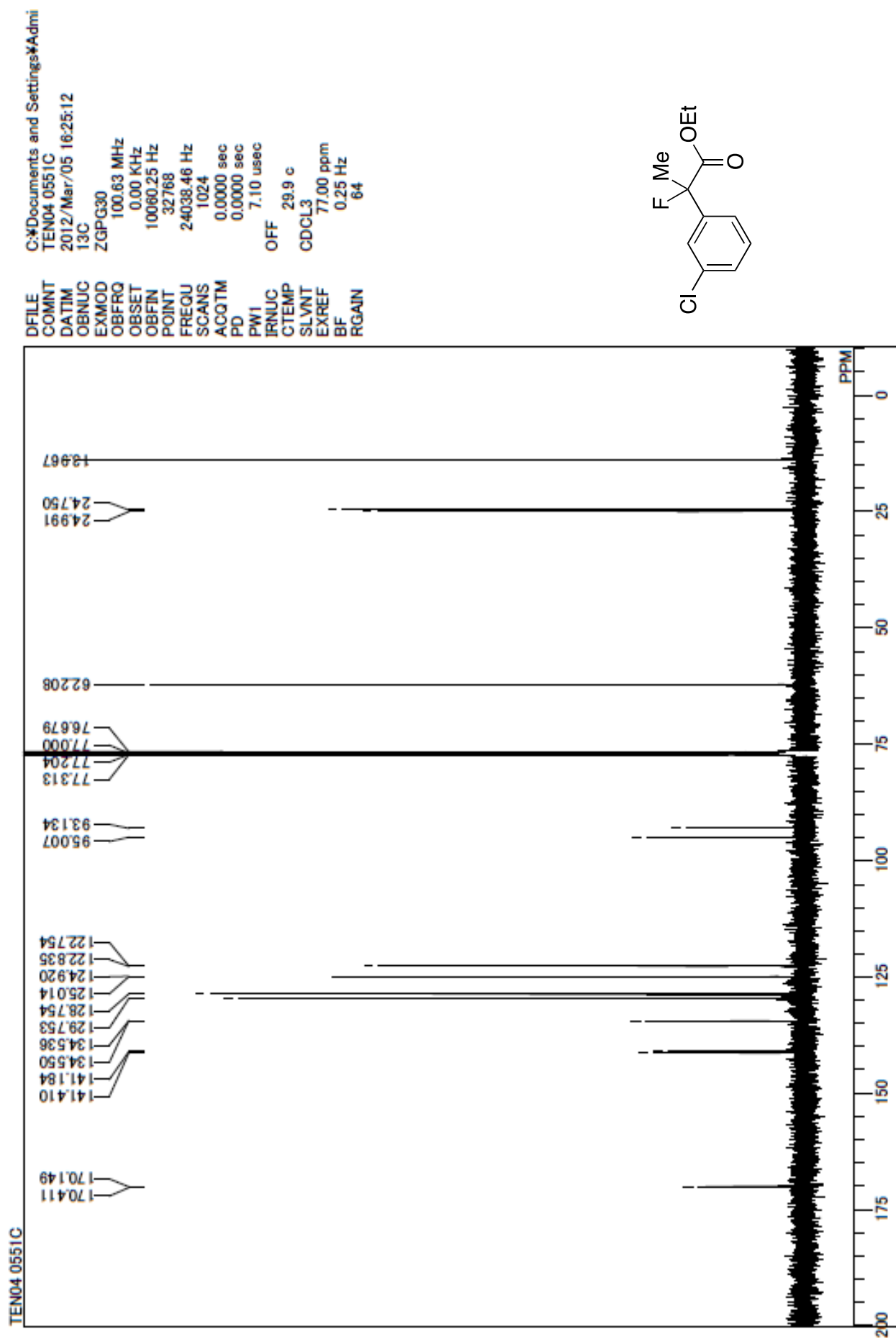


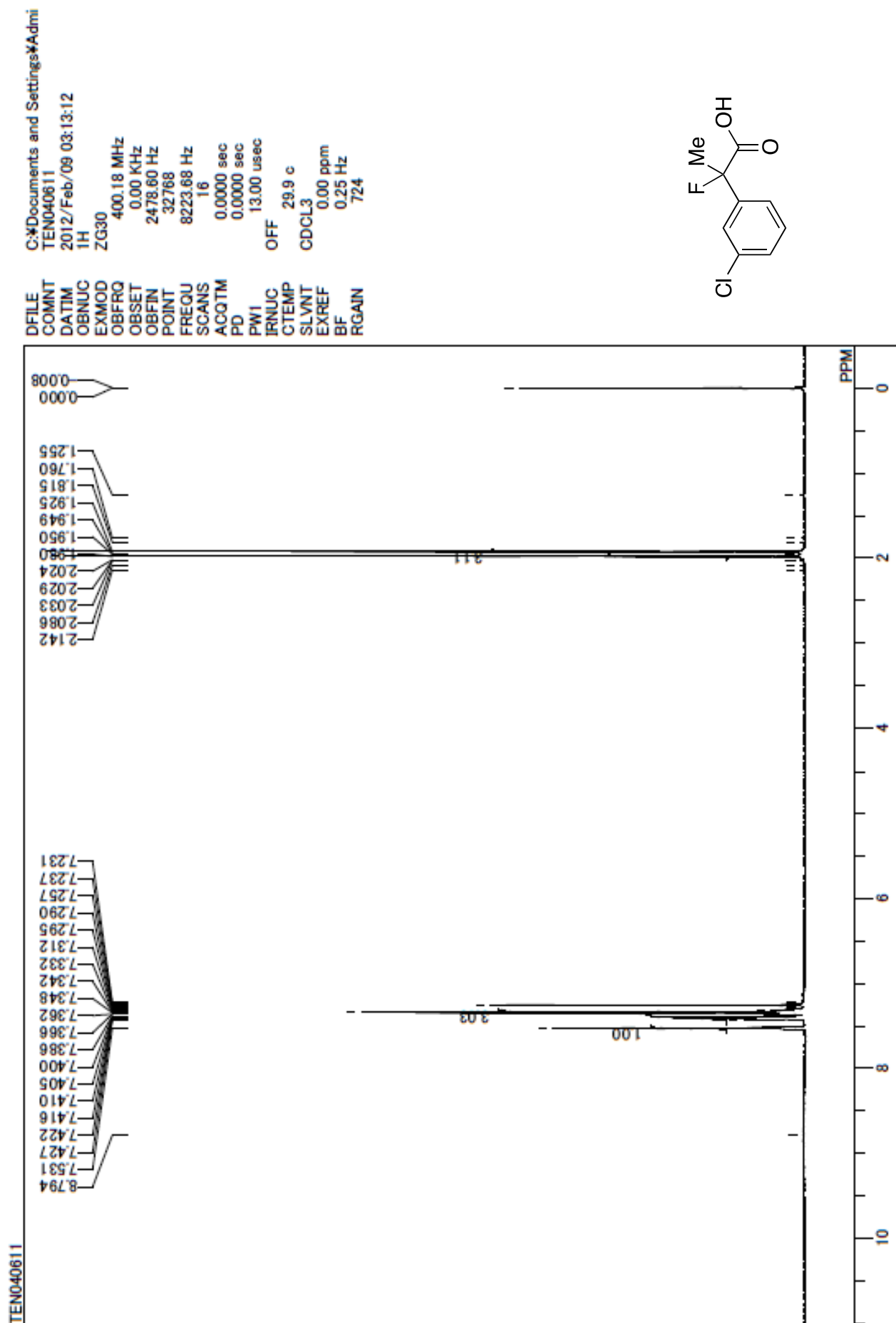


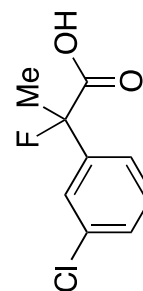
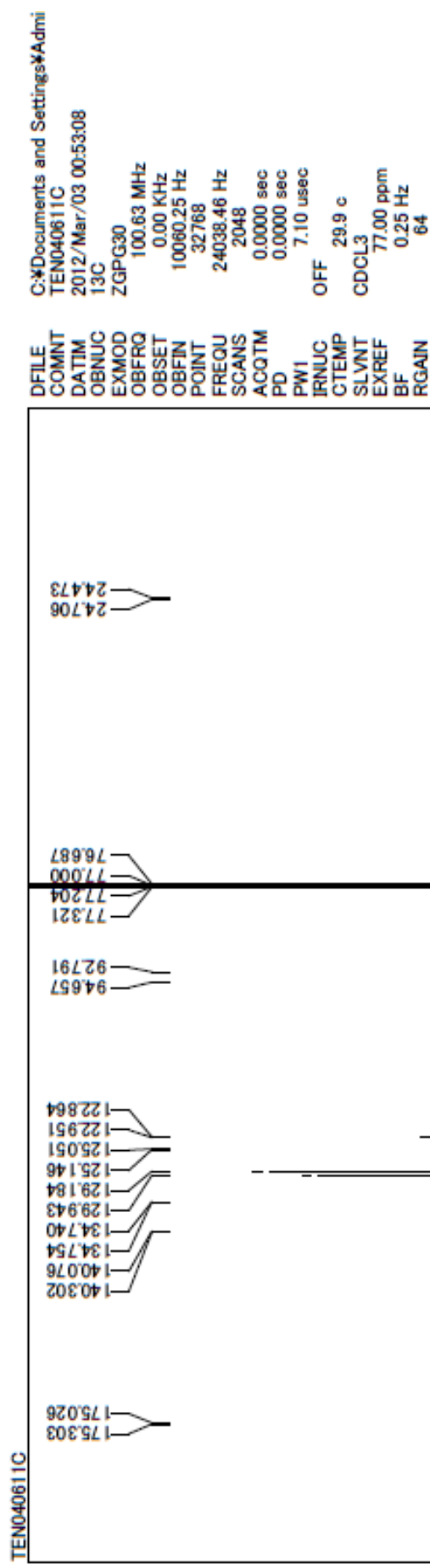


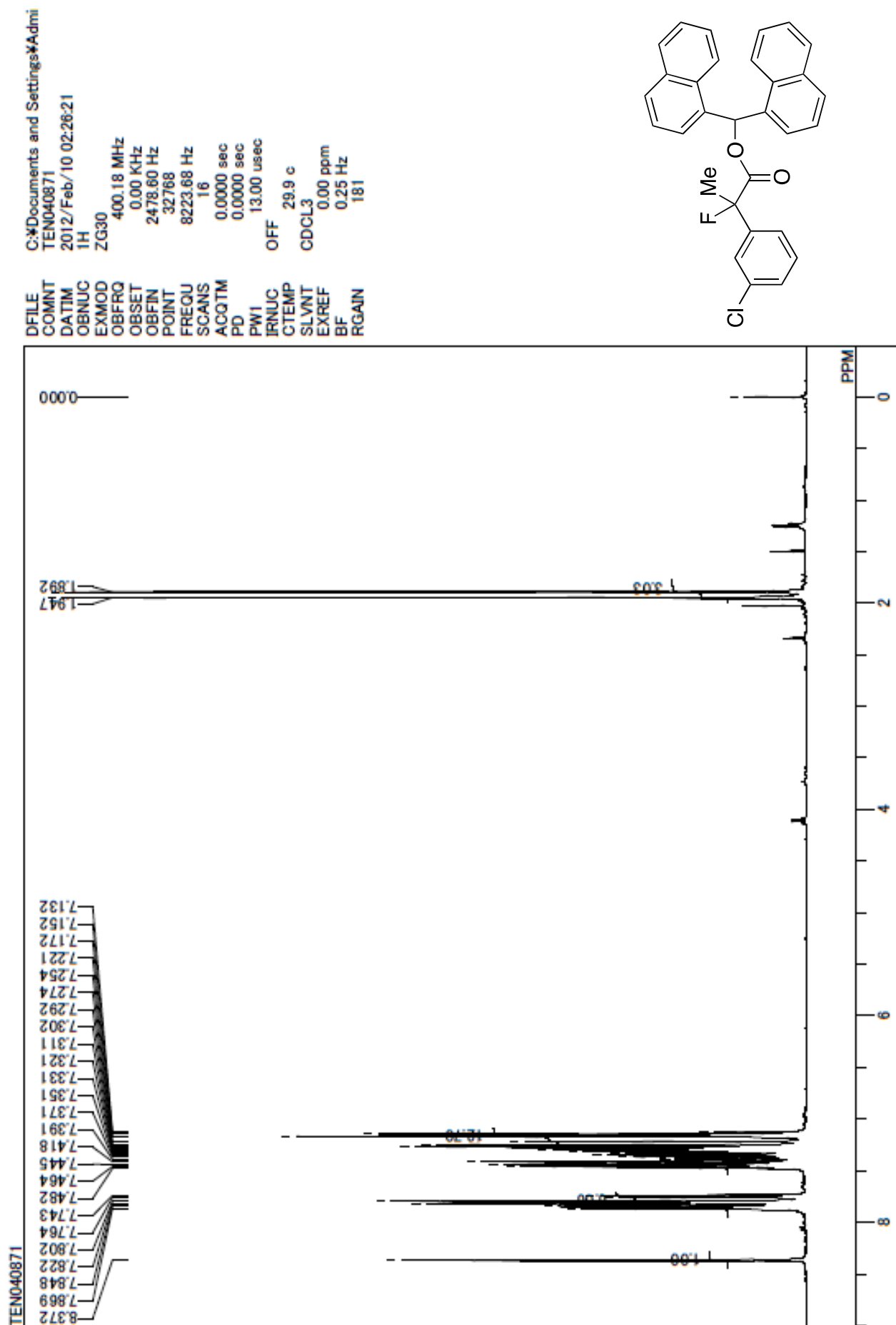


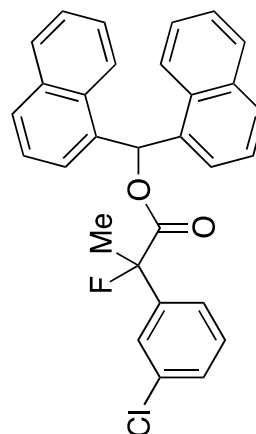
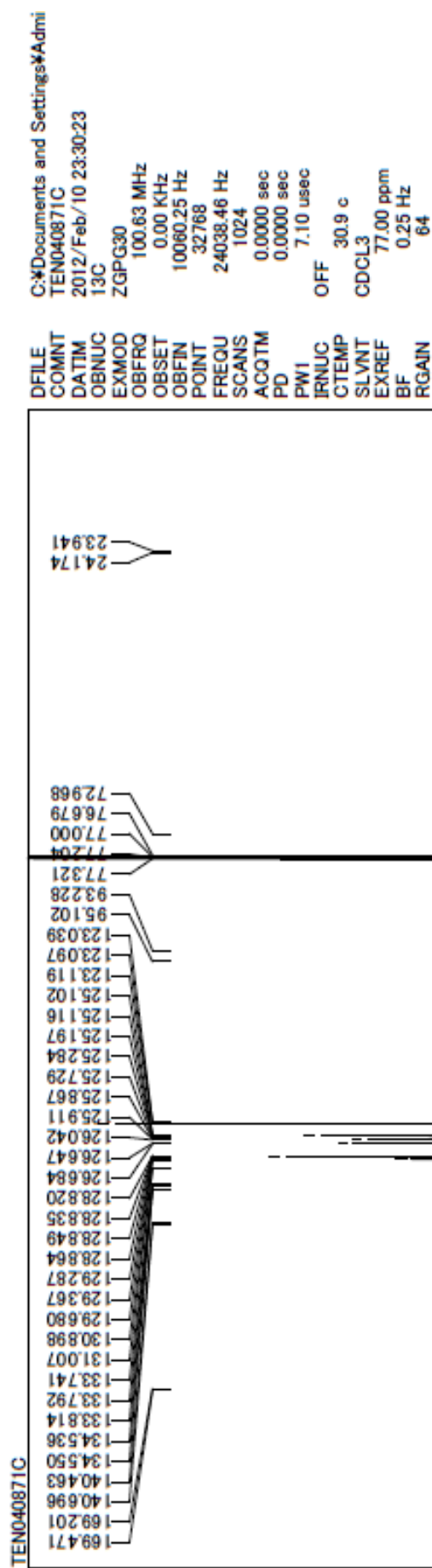


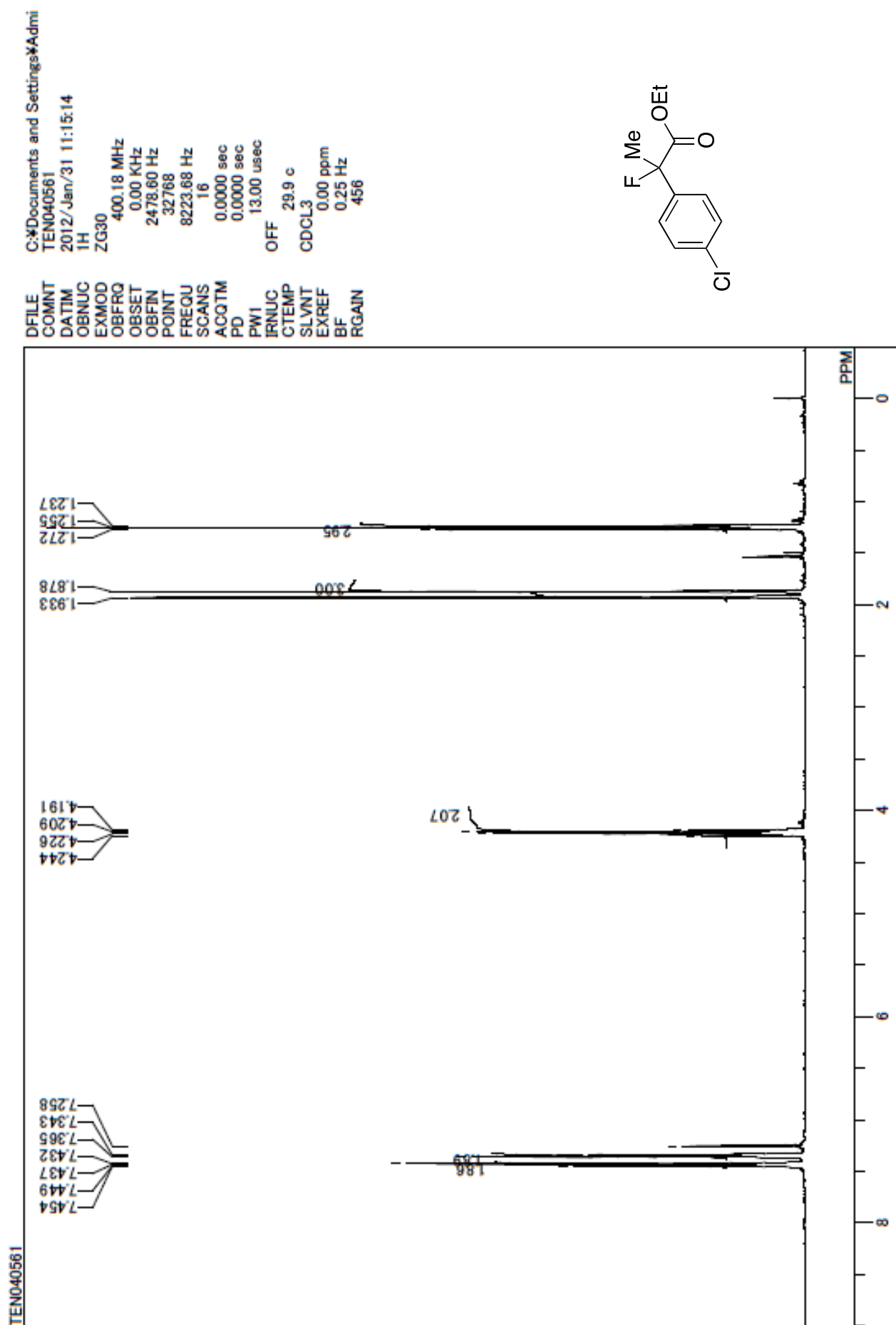


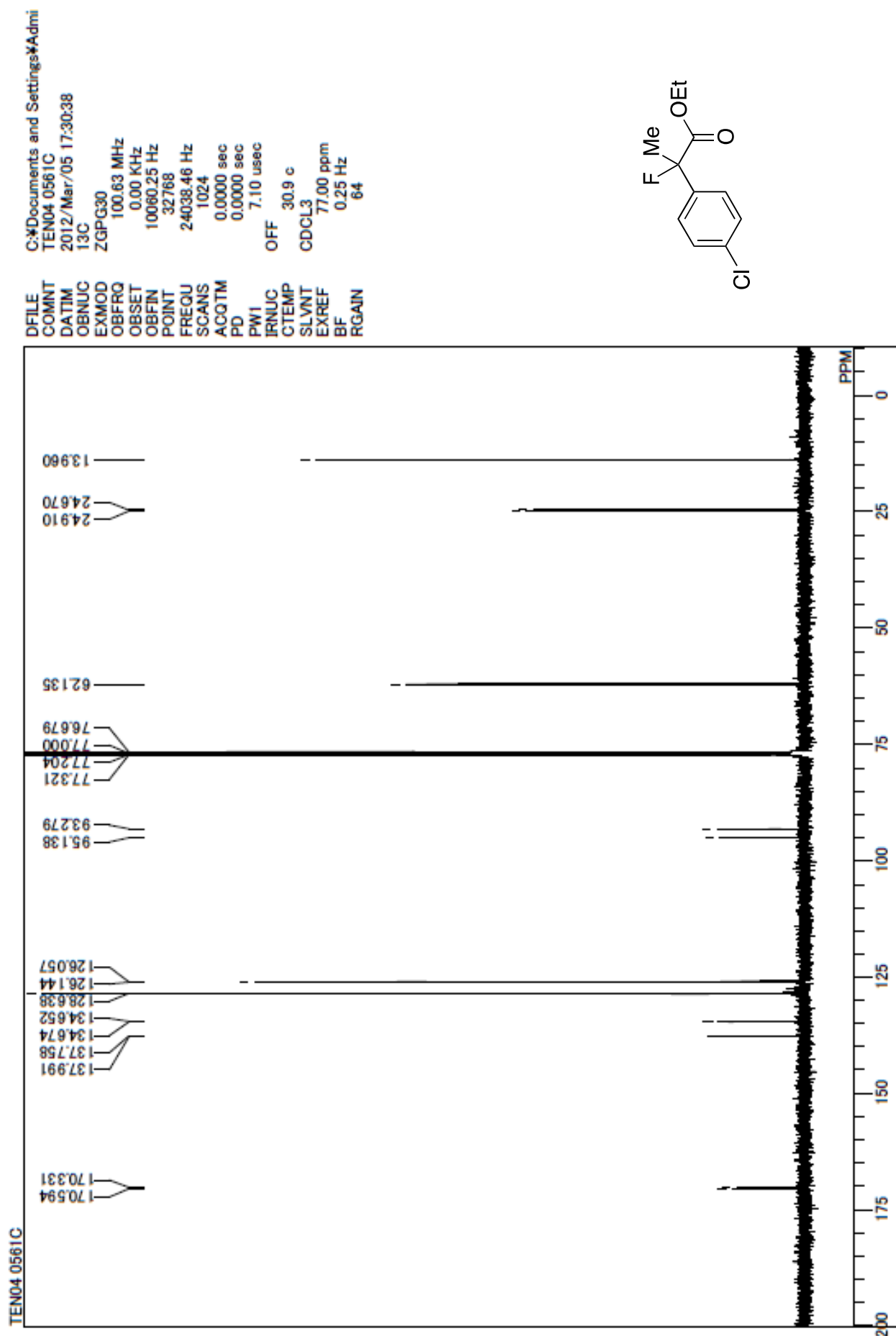


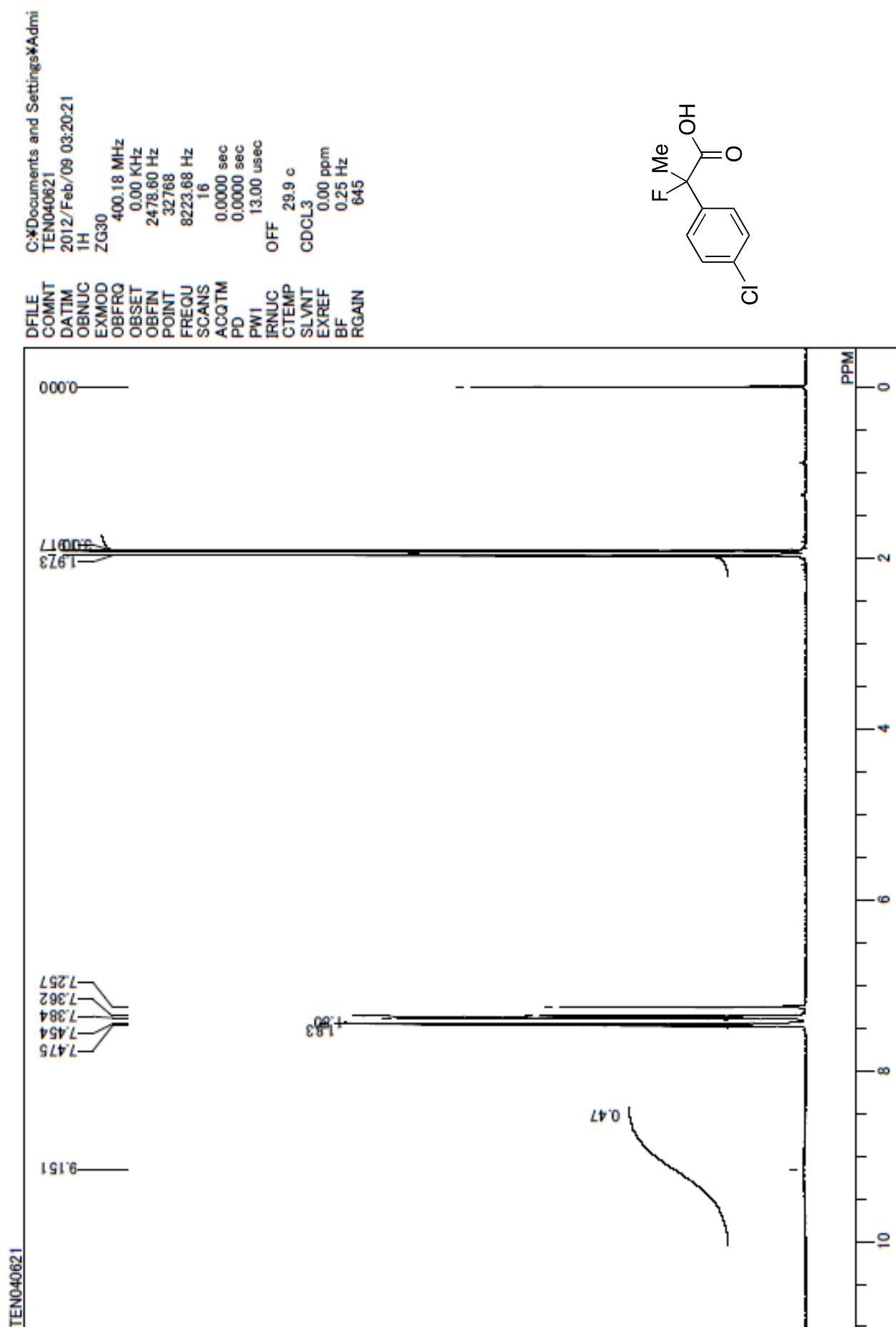


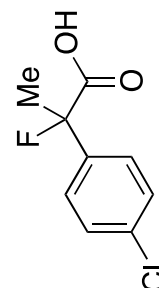
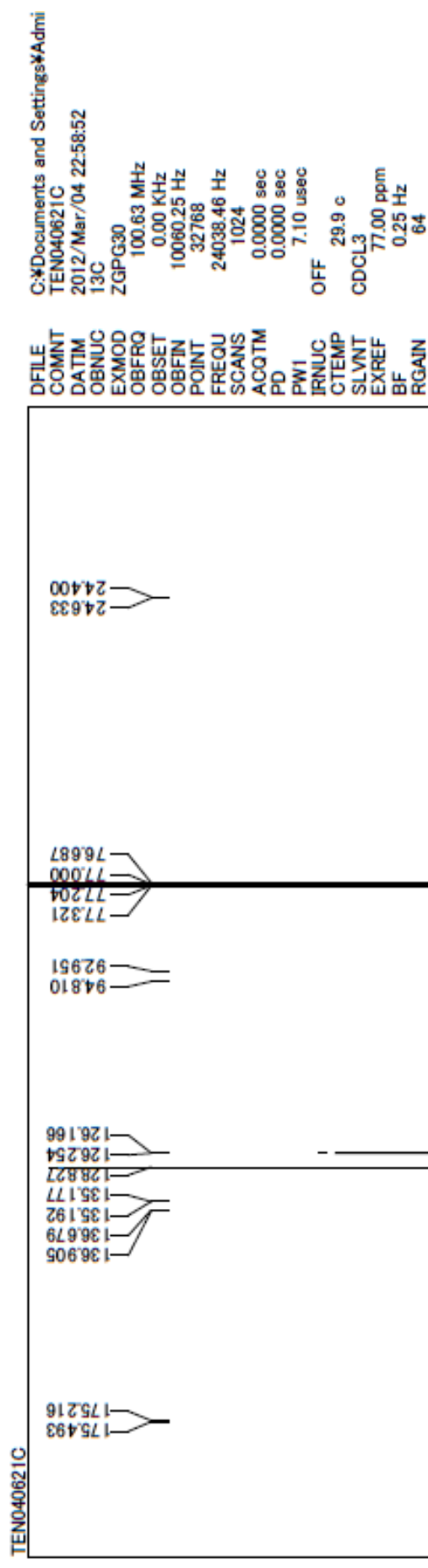


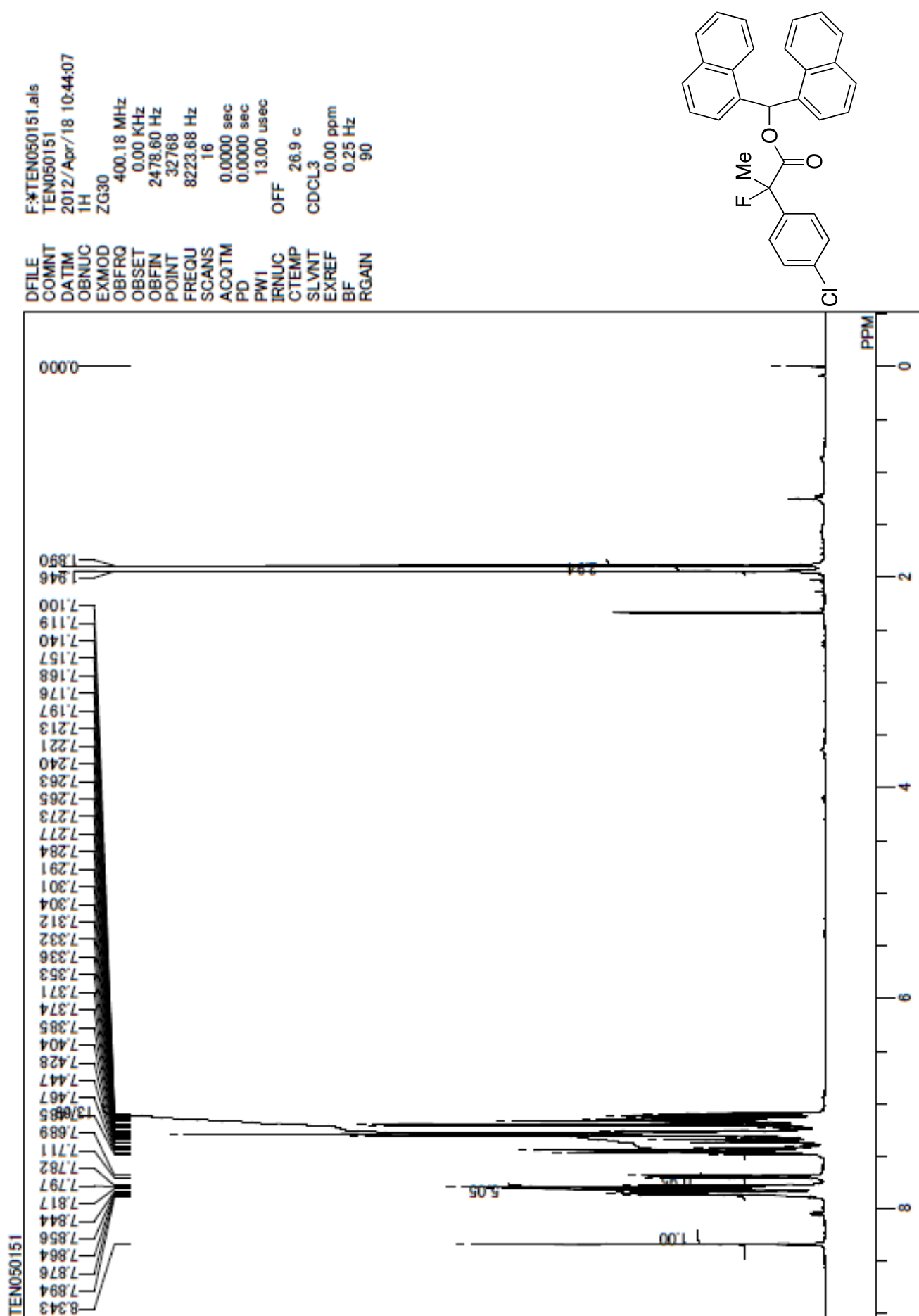


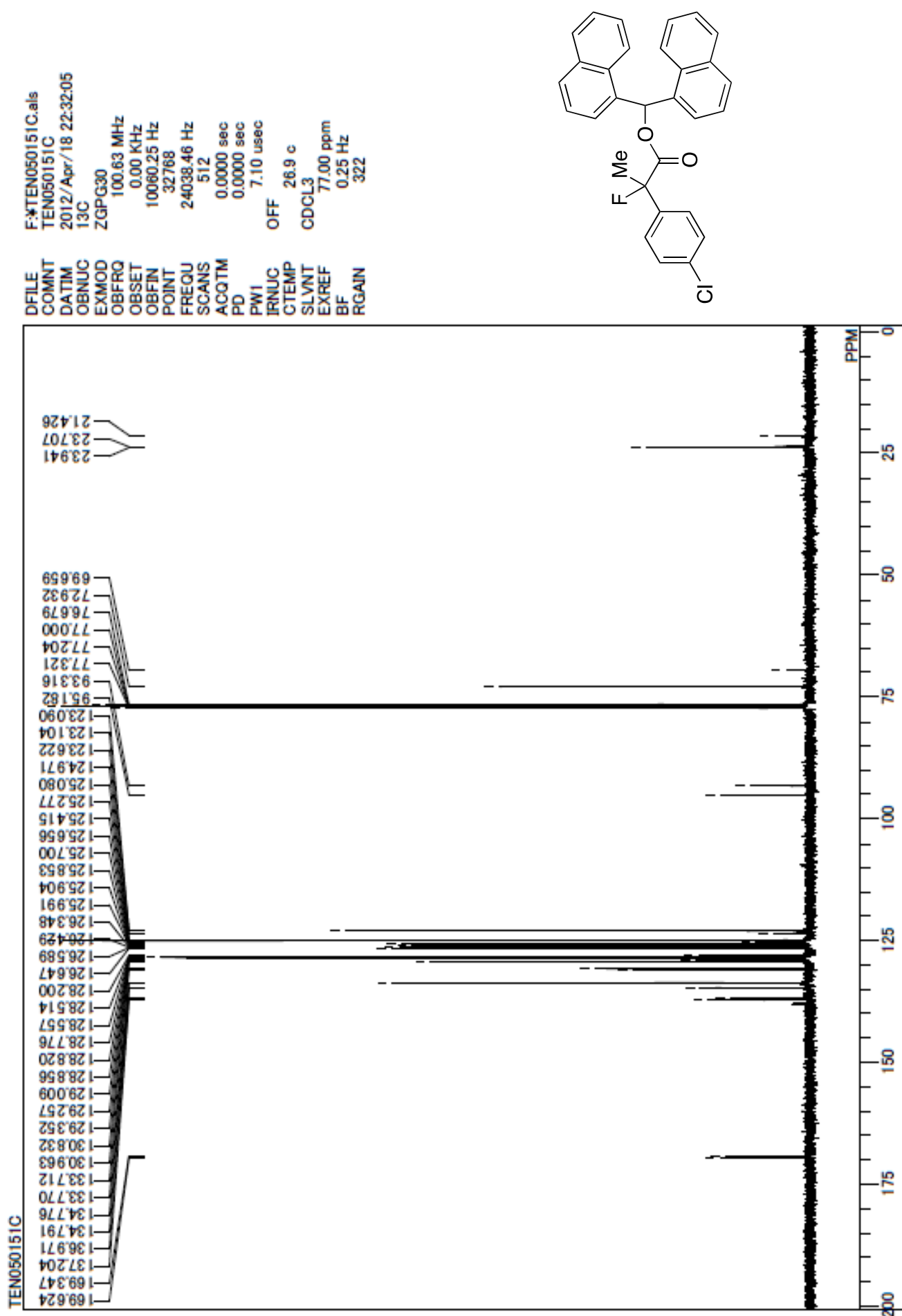


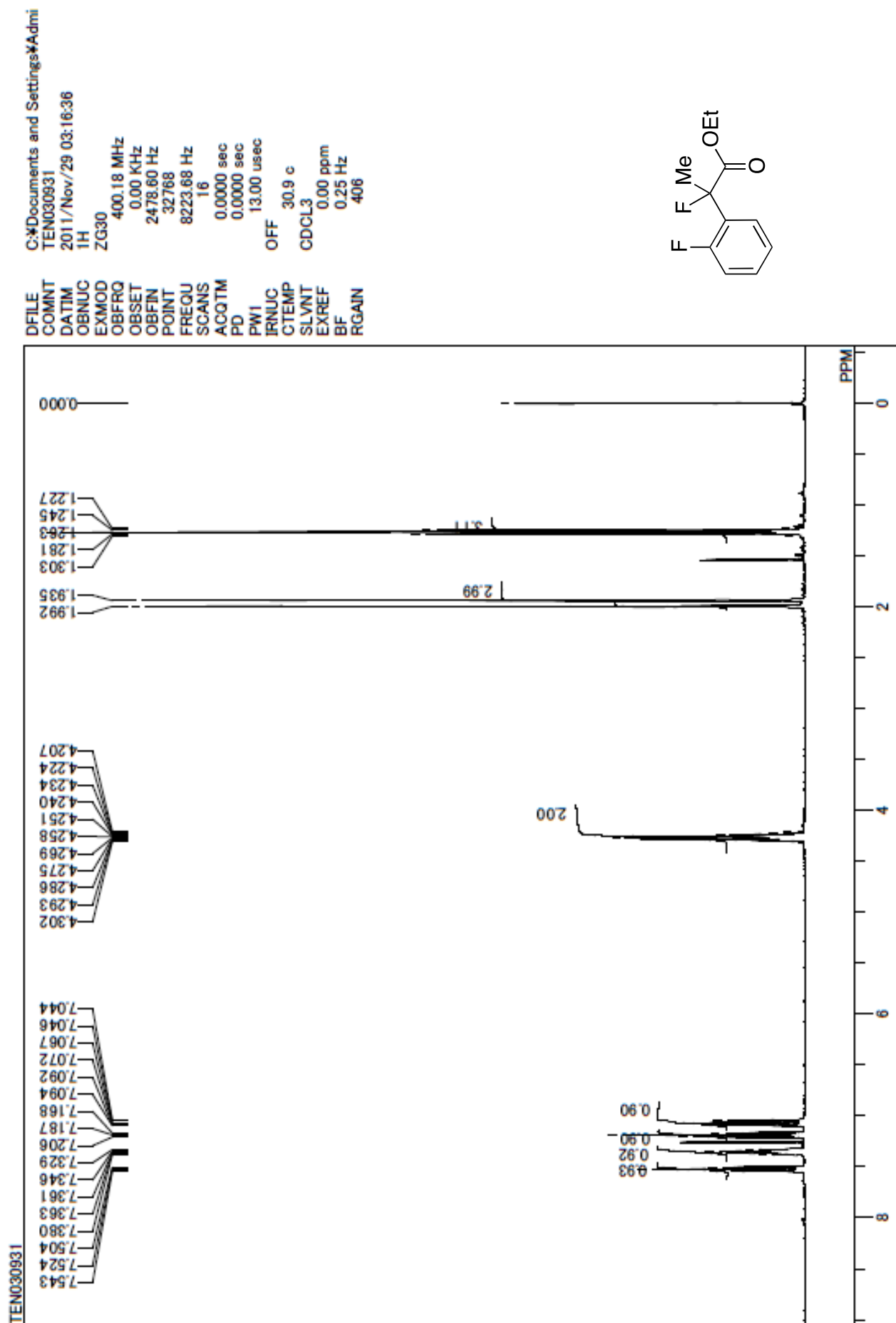


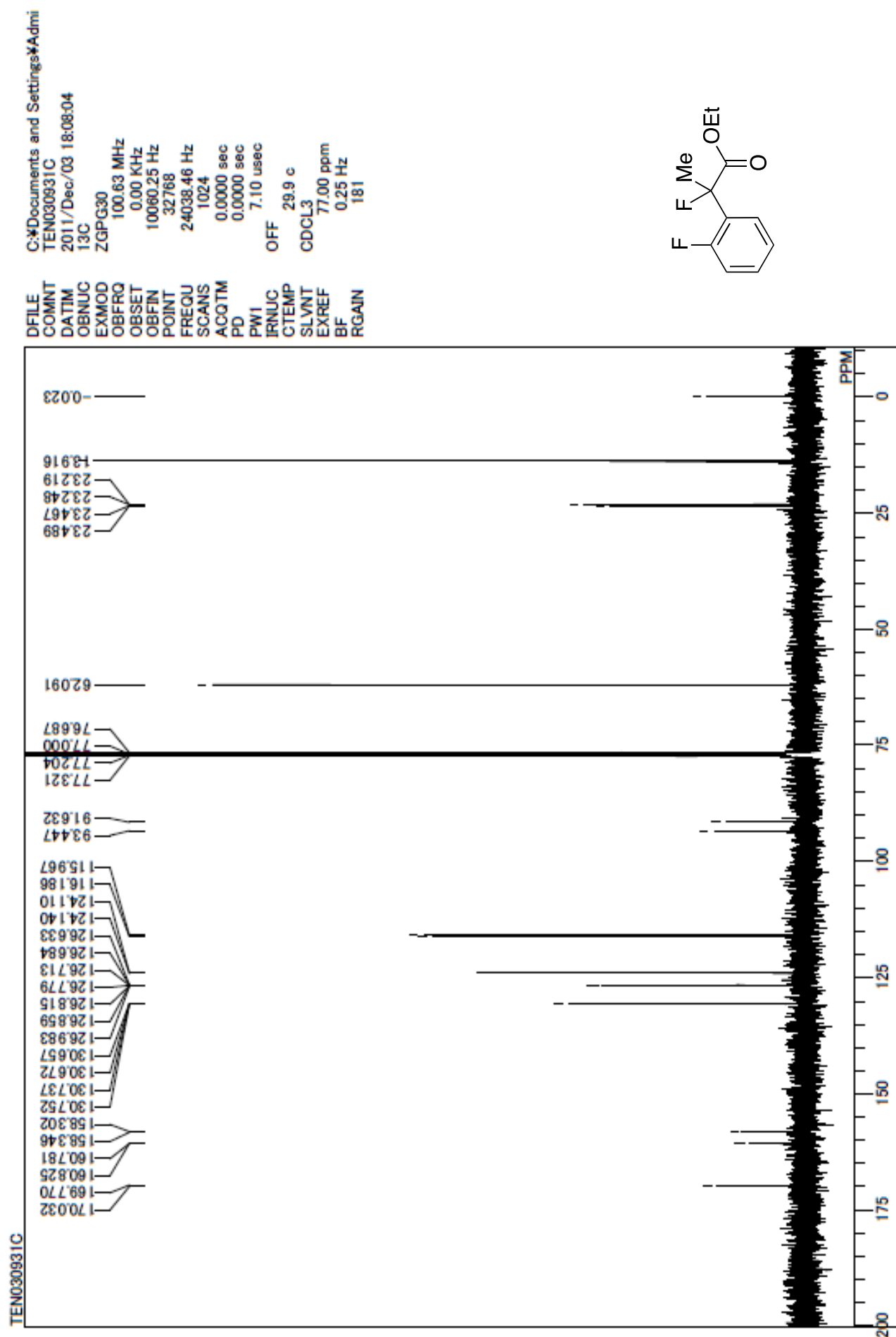


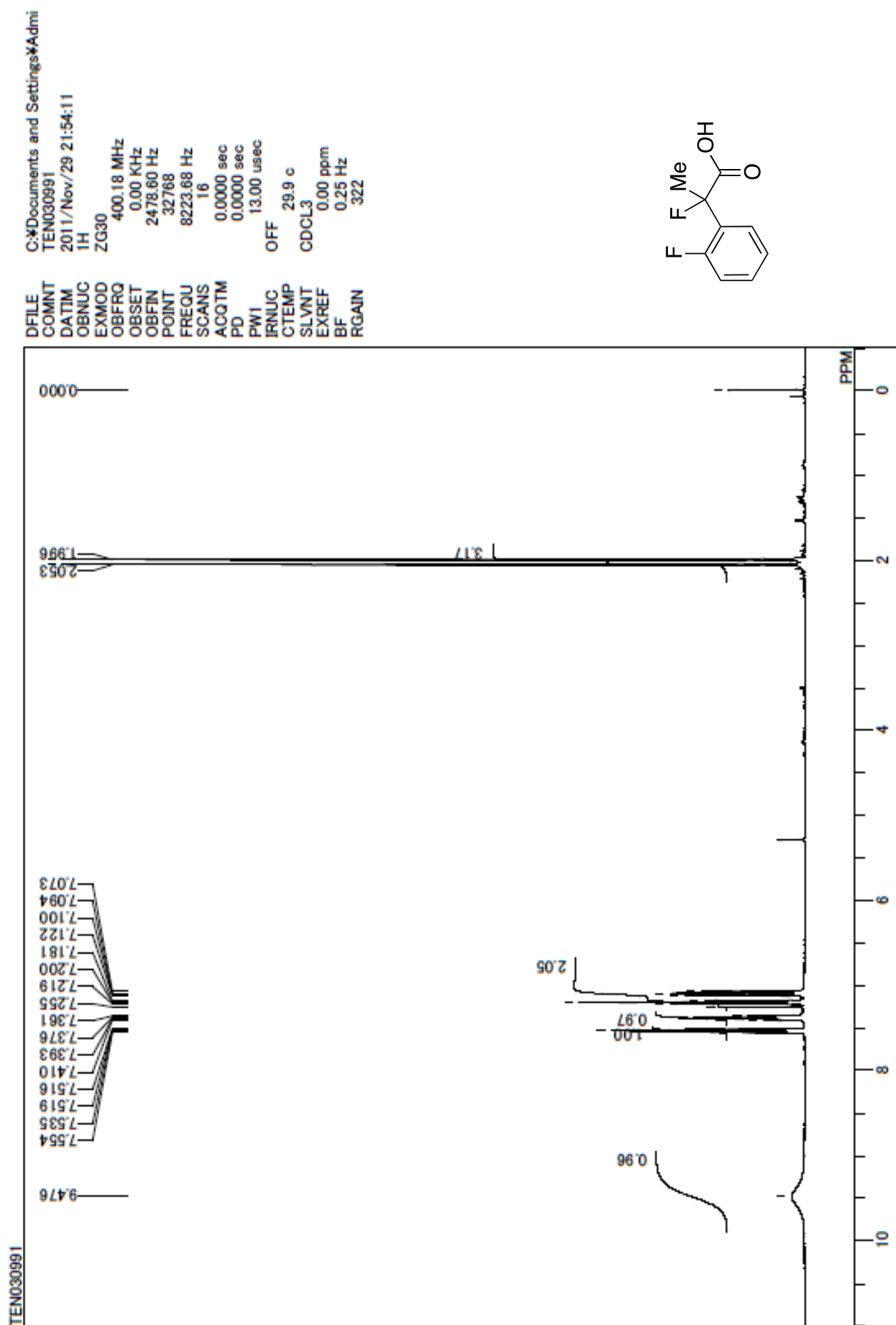


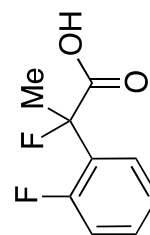
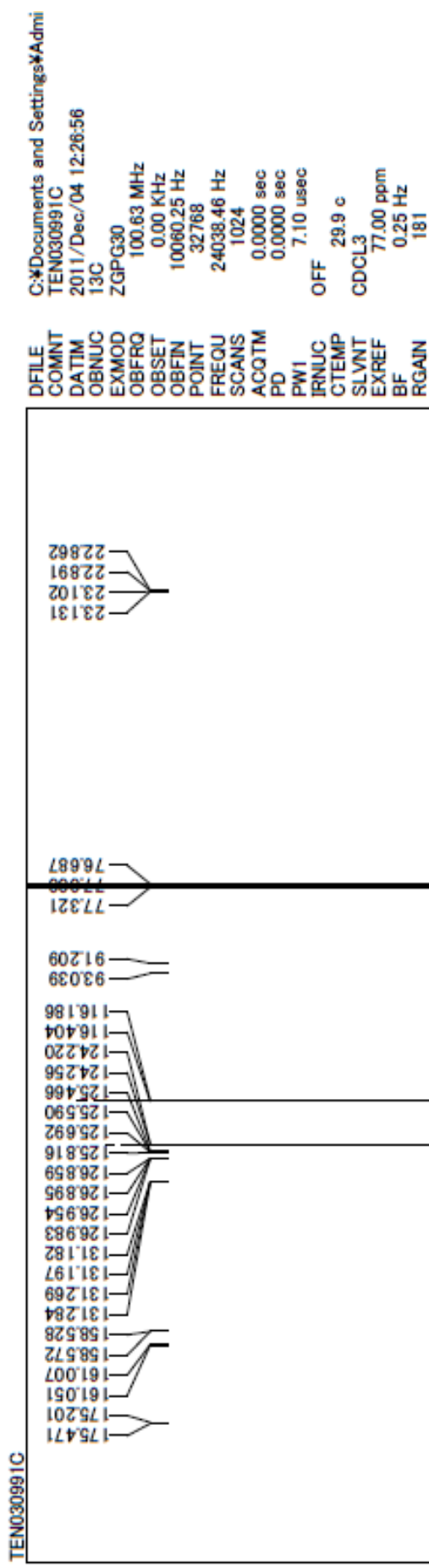


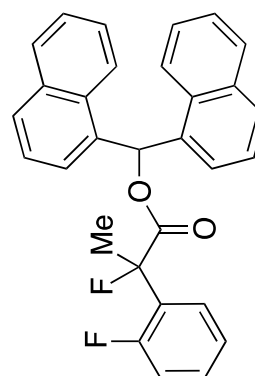
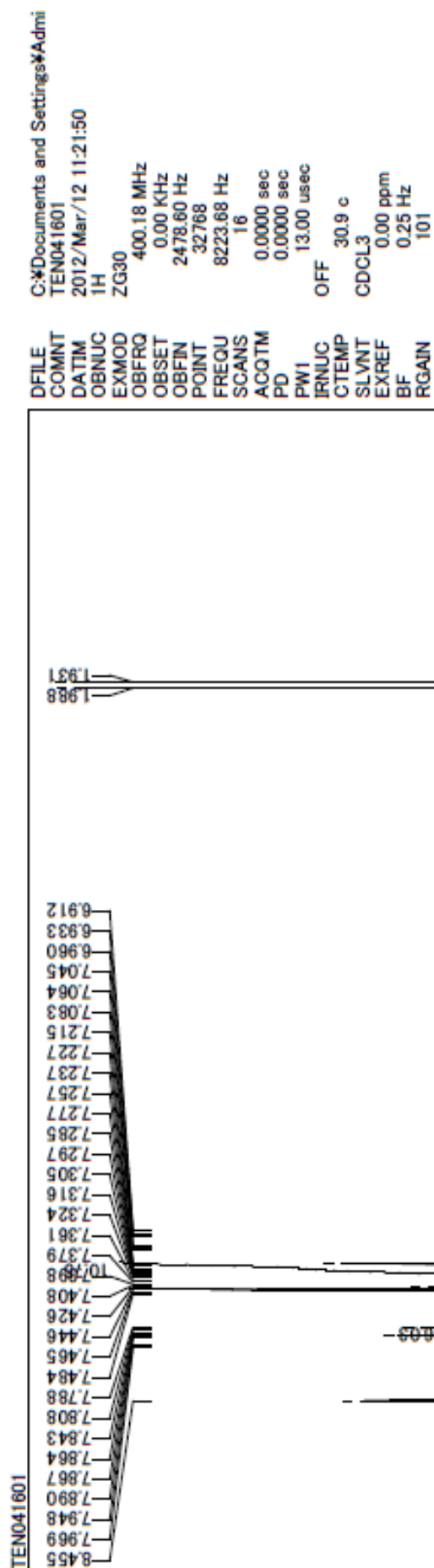


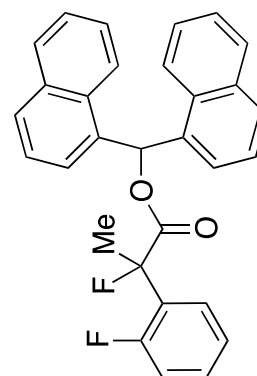
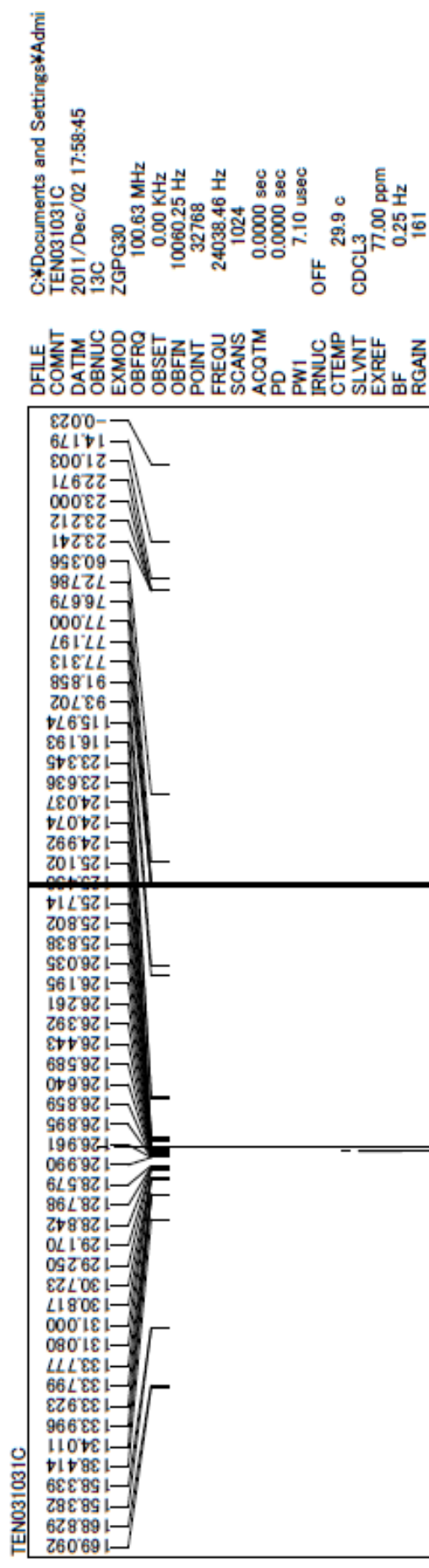


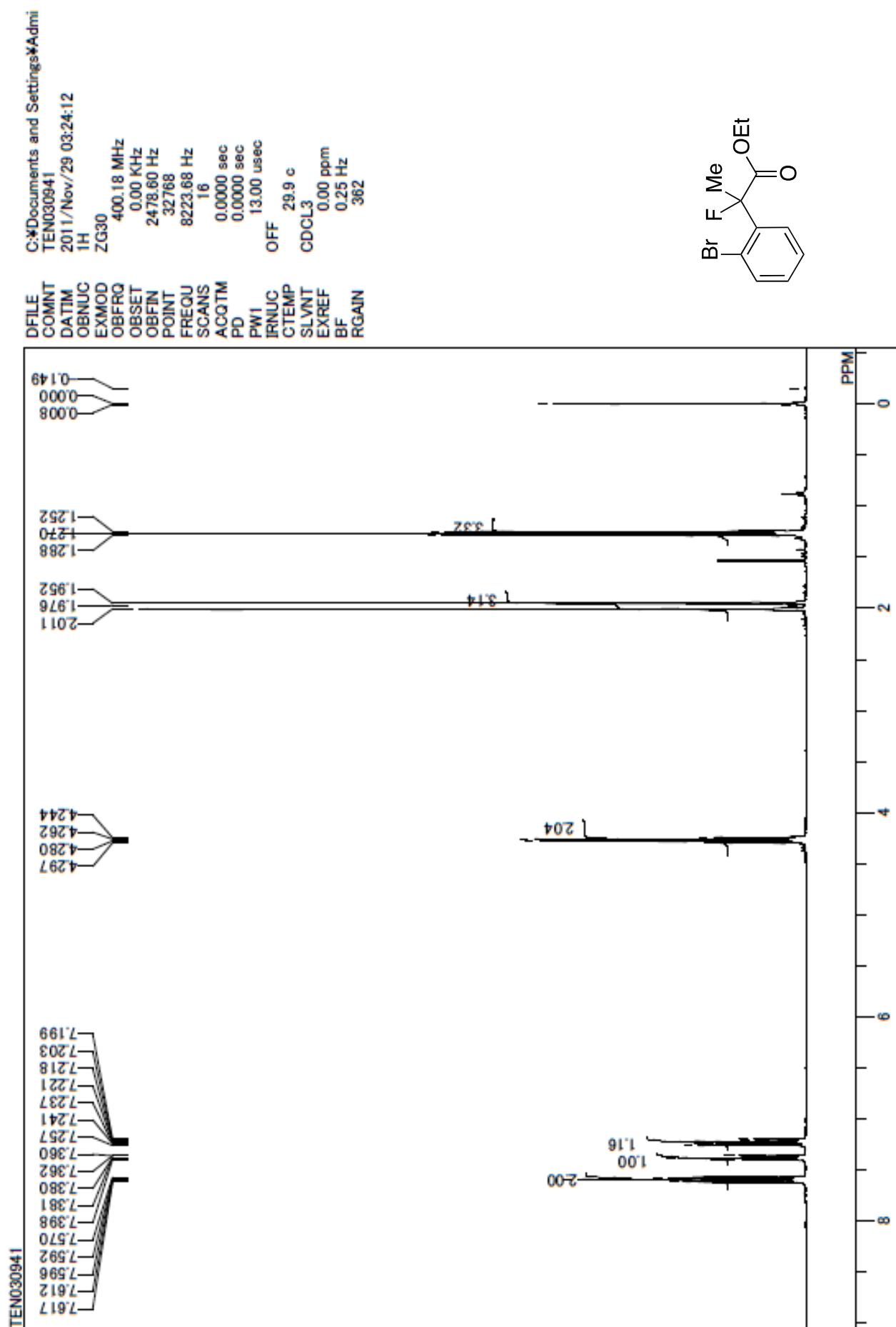


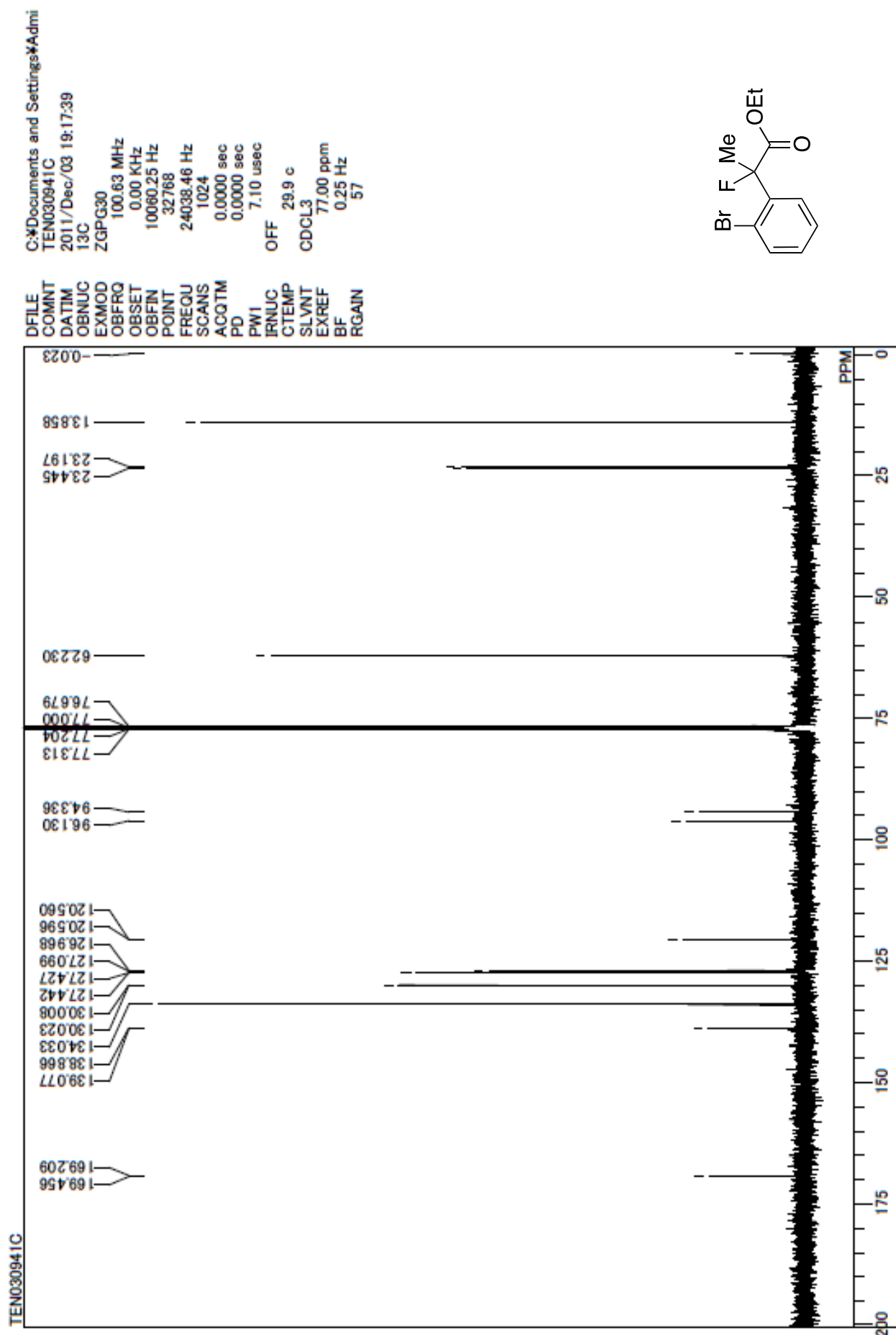


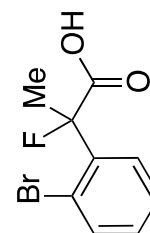
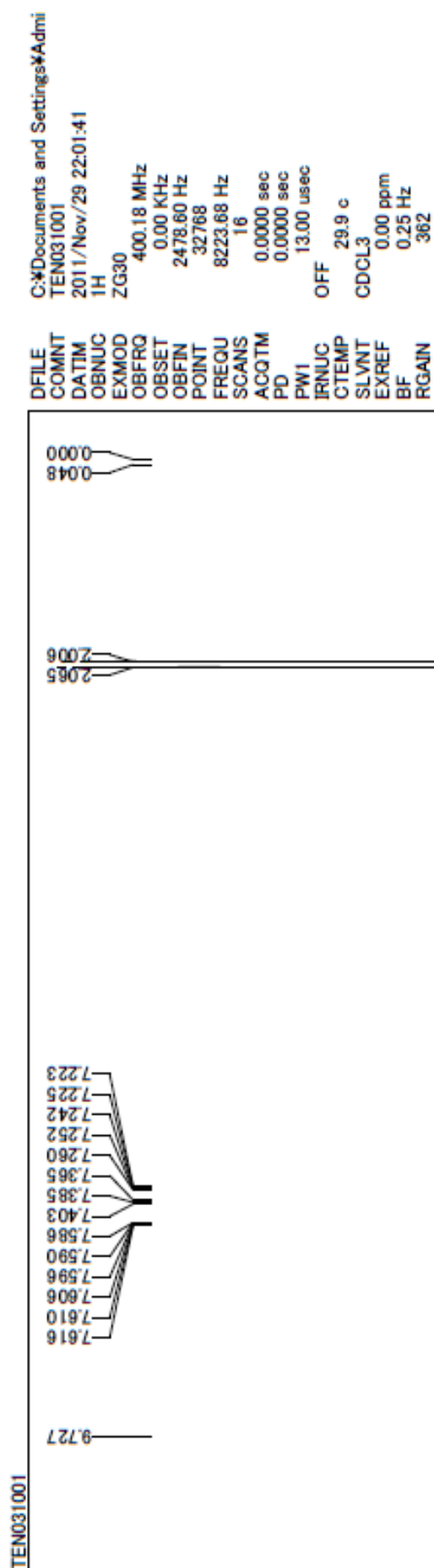


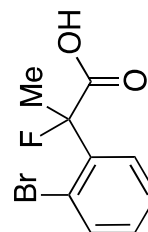
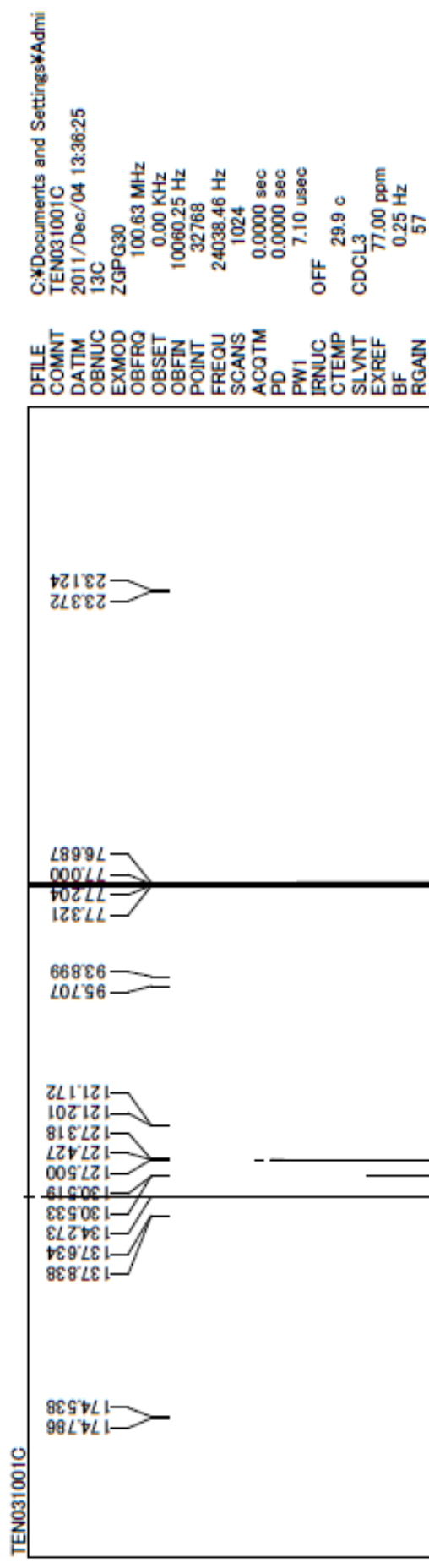


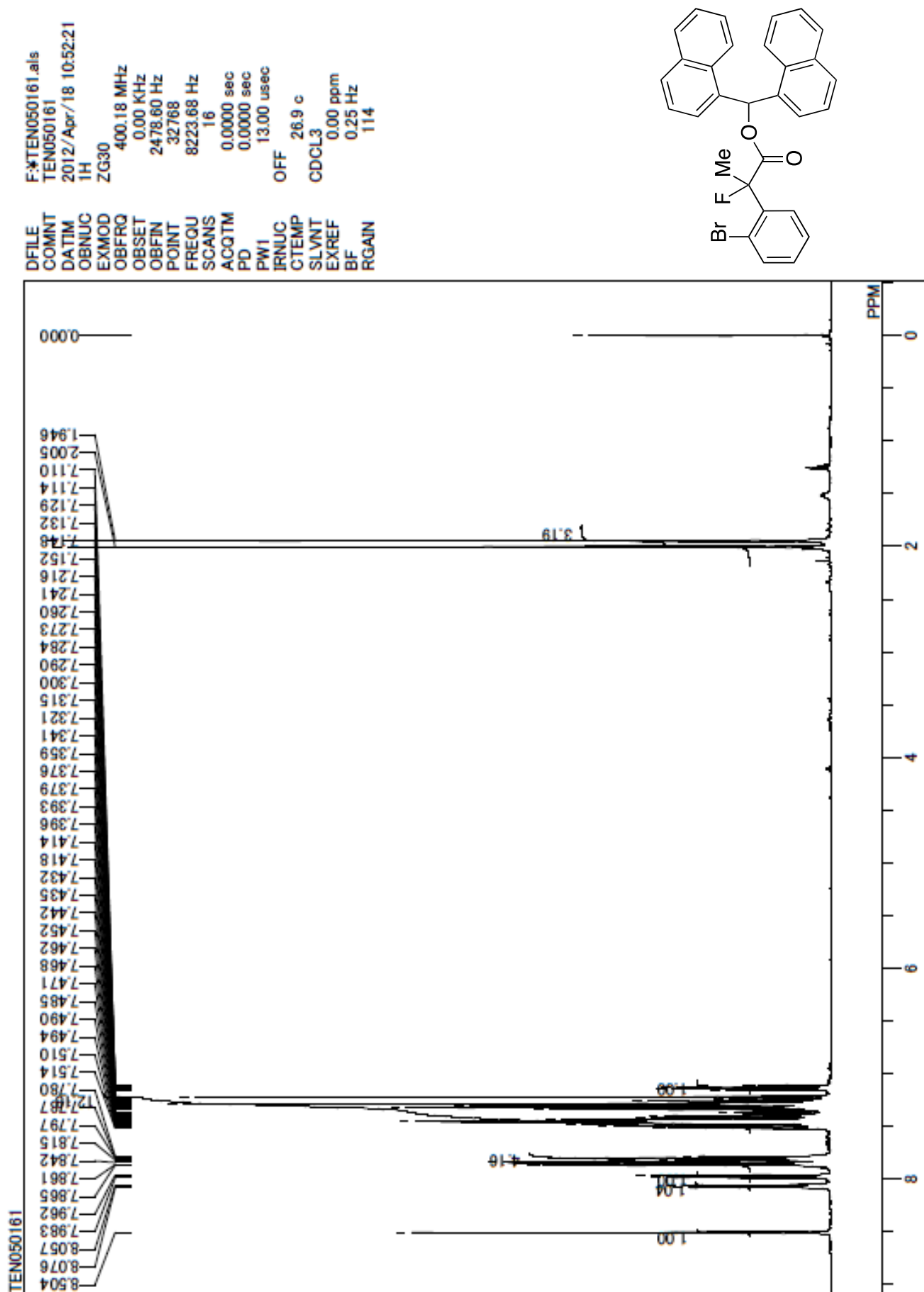


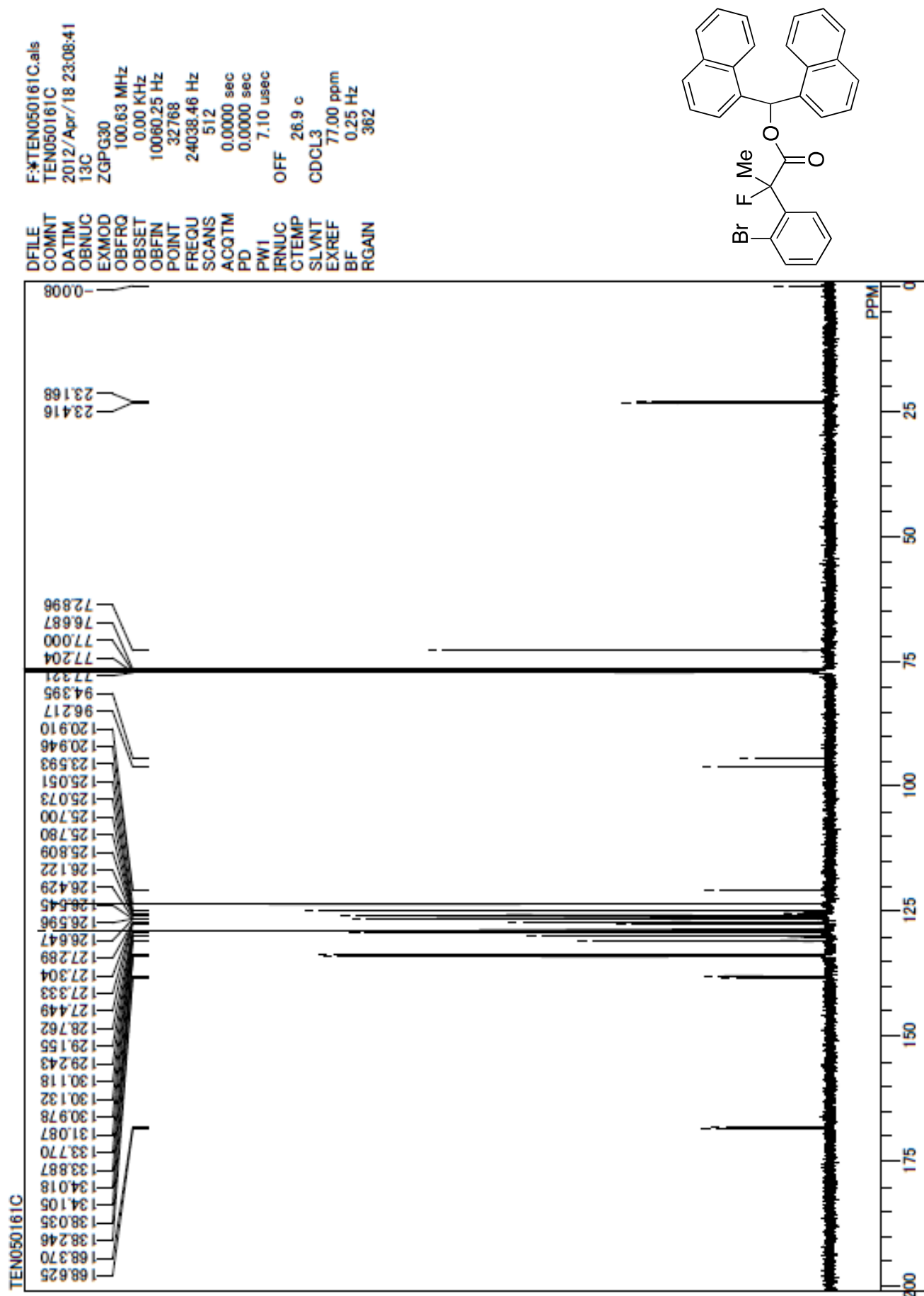


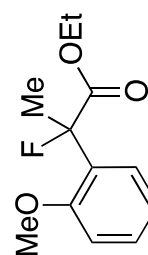
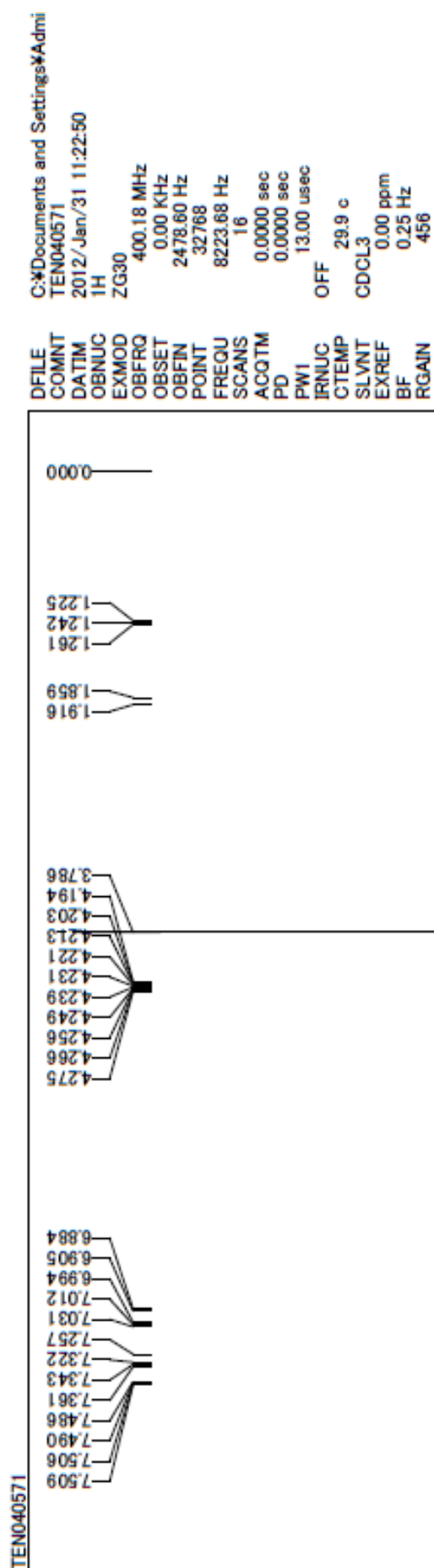


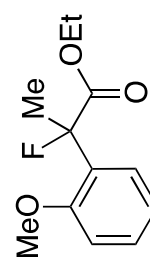
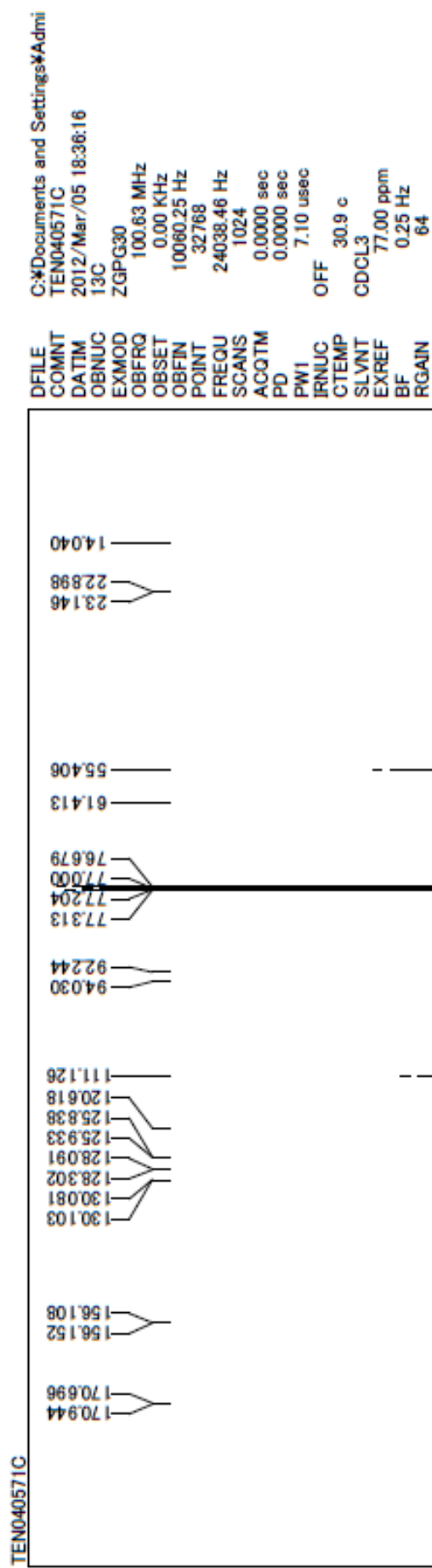


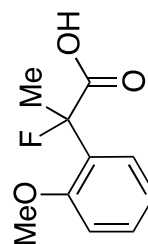
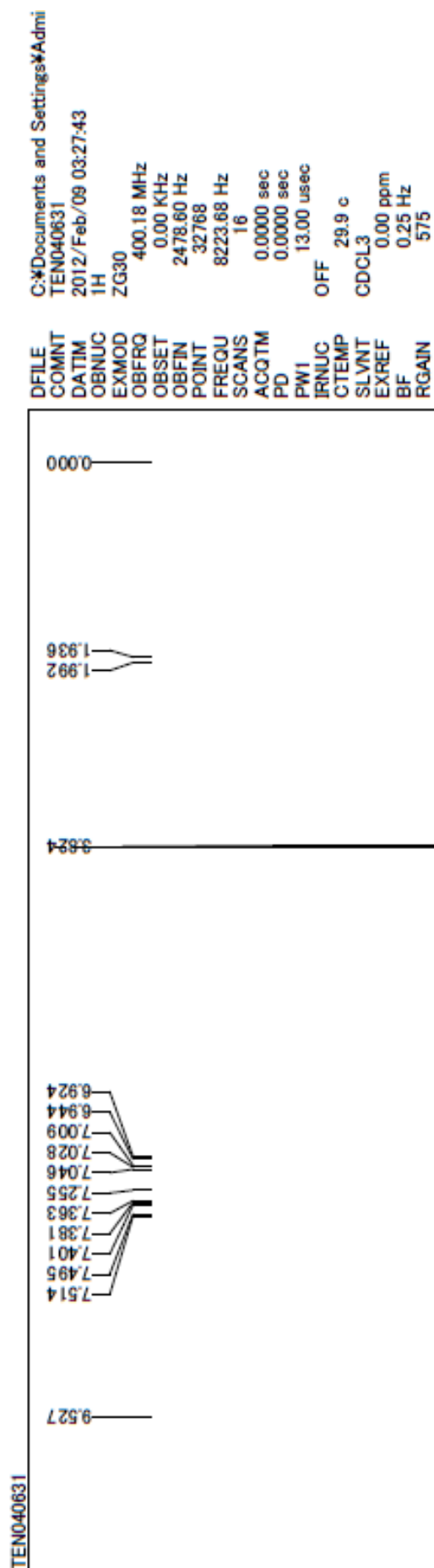


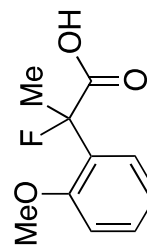
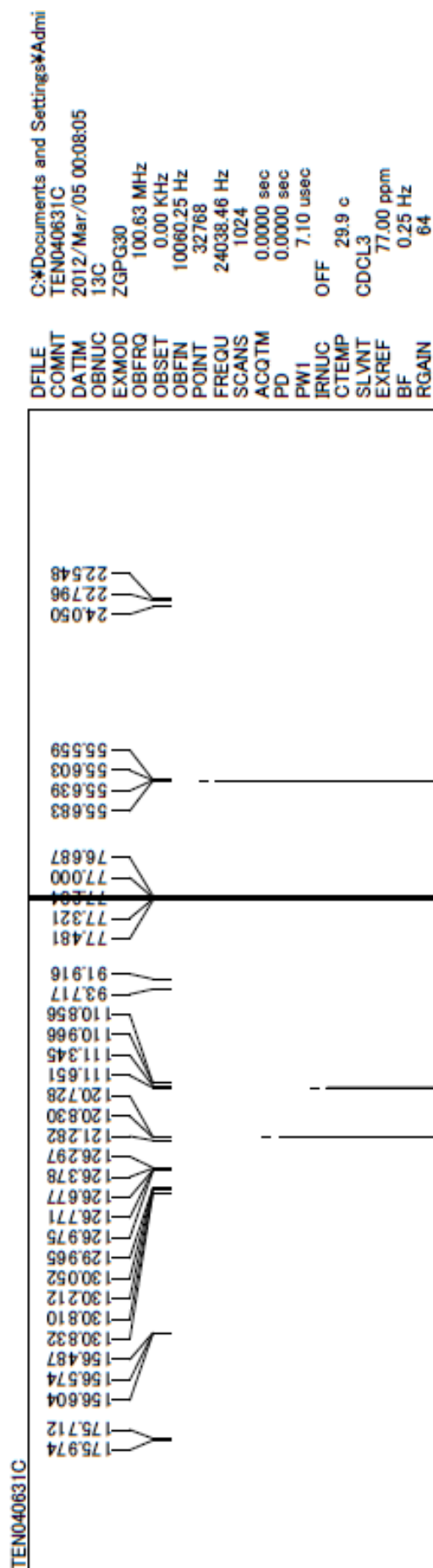




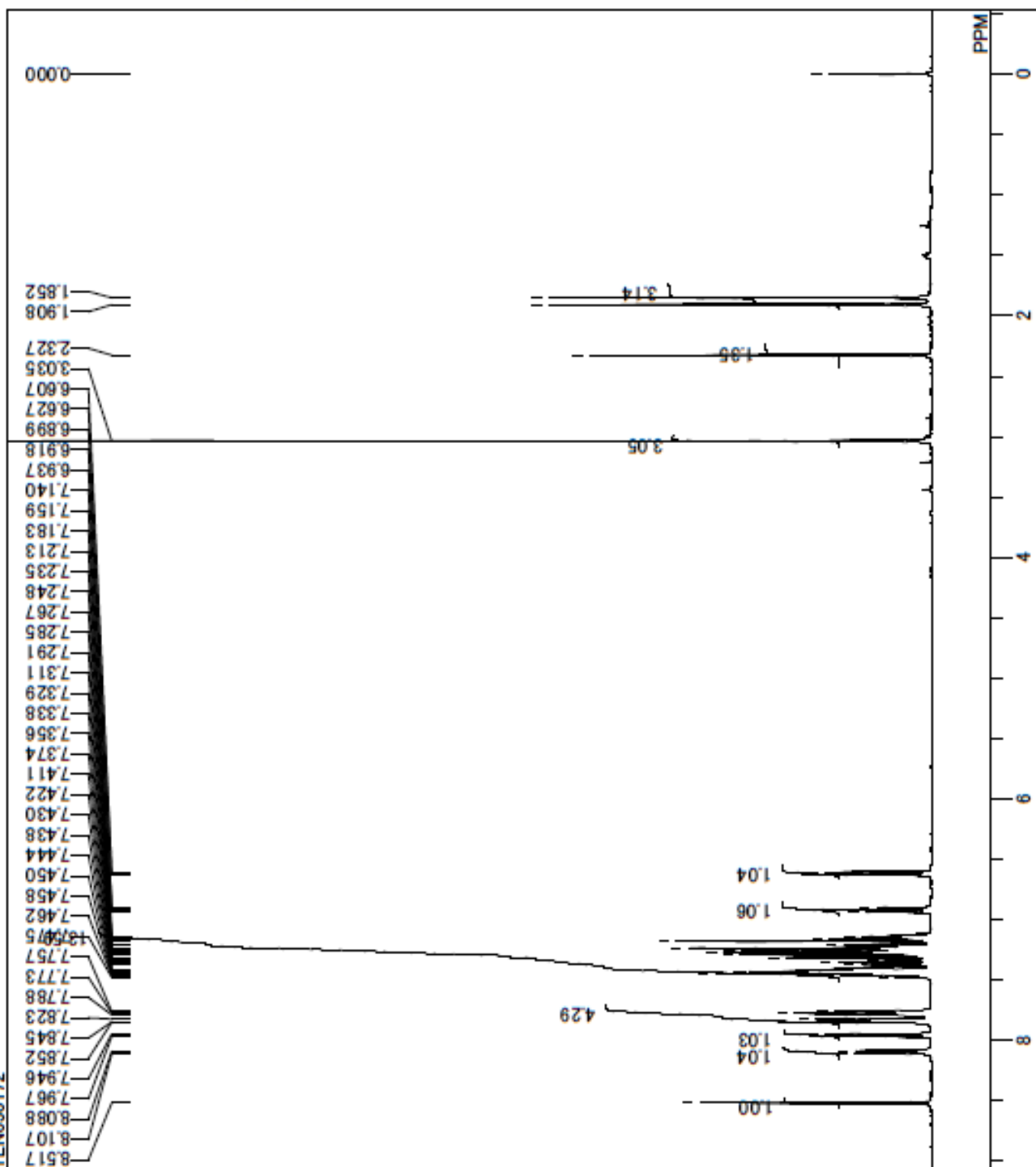








TEN050172



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 FREQU 8223.68 Hz
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 ACQTM 0.0000 sec
 PD 0.0000 sec
 PW1 13.00 usec
 IRNUC OFF
 CTEMP 26.9 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.25 Hz
 RGAIN 81

