Supporting Information

An Expedient Ruthenium(II) Catalyzed Multicomponent Access to Phthalazinones Bearing Trisubstituted Alkenes

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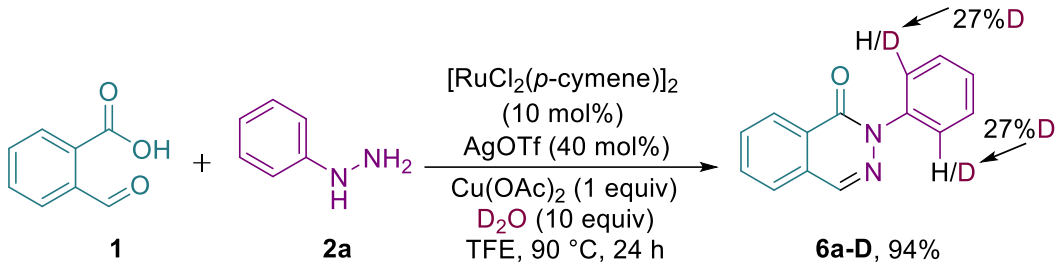
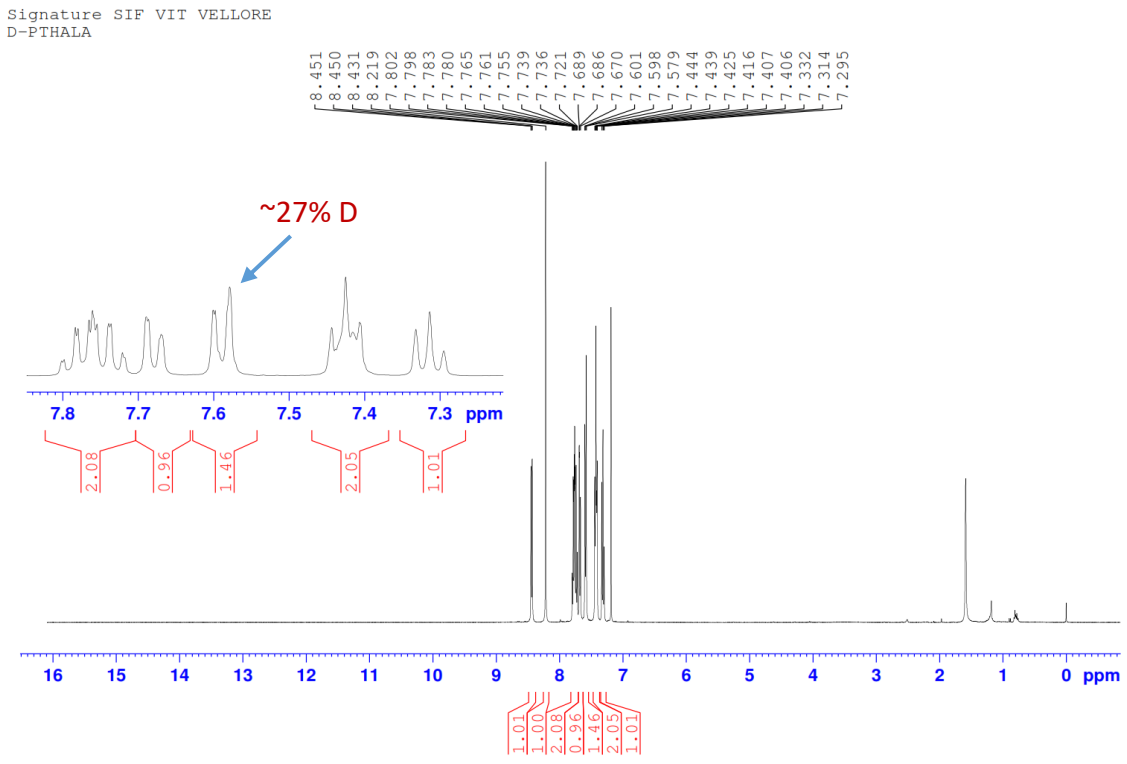
Table of Contents

1. Mechanistic studies

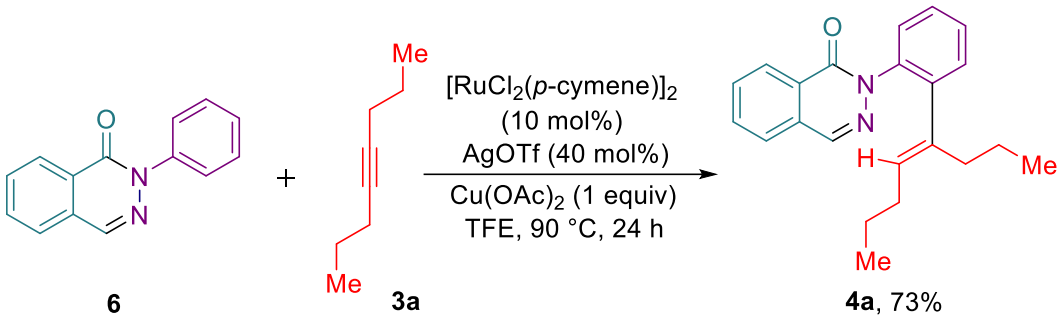
1. 1. H/D exchange experiment without 4-octyne:



An oven-dried Schlenk tube (15 mL) equipped with a stir bar was charged with 2-carboxy benzaldehyde **1** (0.33 mmol, 1 equiv), phenyl hydrazine derivative **2a** (0.36 mmol, 1.1 equiv), $[RuCl_2(p\text{-cymene})]_2$ (10 mol%), AgOTf (40 mol%), $Cu(OAc)_2$ (0.33 mmol, 1 equiv), D_2O (3.3 mmol, 10 equiv) and 1 mL of TFE was added. Then the tube was flushed with nitrogen and screw capped under nitrogen flow and placed in a preheated oil bath at 90 °C for 24 h. After the indicated time, the reaction mixture was cooled and concentrated. The crude material was purified by column chromatography on silica gel (100-200 mesh) using *n*-hexane – ethyl acetate as eluent, to yield **6a-D**.



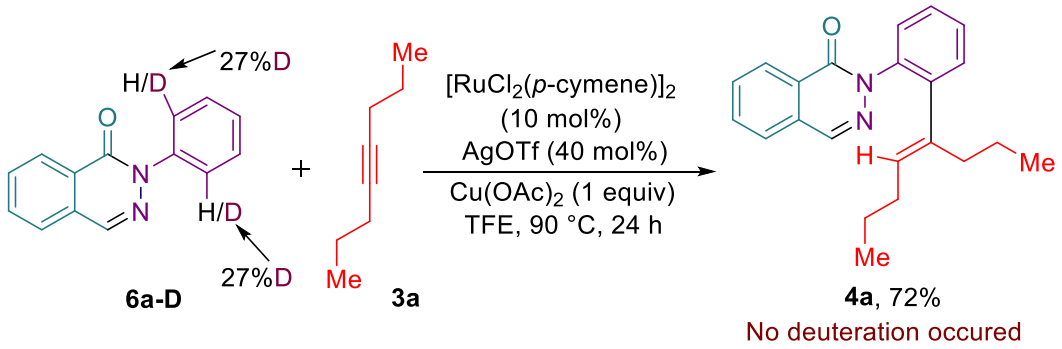
1. 2. Reaction between intermediate with 4-octyne:



6 **3a** **4a**, 73%

An oven-dried Schlenk tube (15 mL) equipped with a stir bar was charged with **6** (0.33 mmol, 1 equiv), $[RuCl_2(p\text{-cymene})]_2$ (10 mol%), AgOTf (40 mol%), $Cu(OAc)_2$ (0.33 mmol, 1 equiv), and 1 mL of TFE was added. Then to this solution alkyne derivative **3a** (0.66 mmol, 2 equiv) was added and the tube was flushed with nitrogen and screw capped under nitrogen flow and placed in a preheated oil bath at 90 °C for 24 h. After the indicated time, the reaction mixture was cooled and concentrated. The crude material was purified by column chromatography on silica gel (100-200 mesh) using *n*-hexane – ethyl acetate as eluent, to yield **4a**.

1. 3. H/D exchange experiment with 4-octyne:

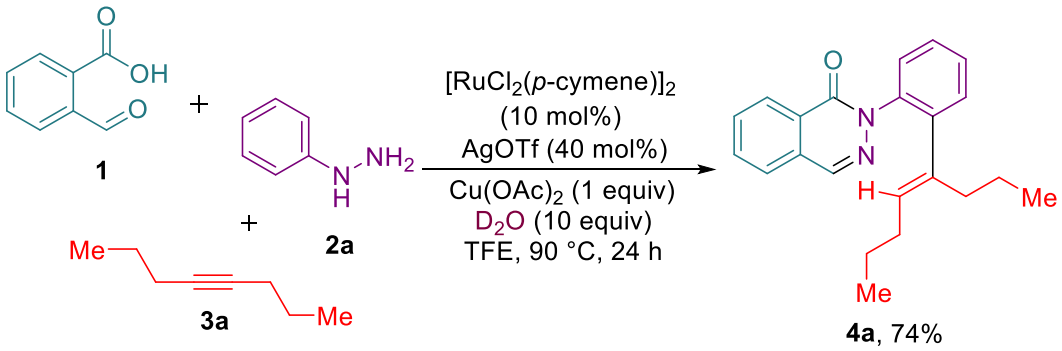


6a-D **3a** **4a**, 72%

No deuteration occured

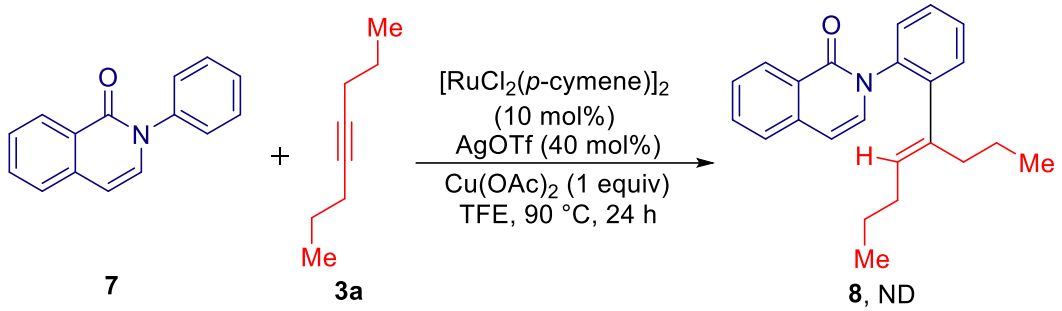
An oven-dried Schlenk tube (15 mL) equipped with a stir bar was charged with **6a-D** (0.33 mmol, 1 equiv), $[RuCl_2(p\text{-cymene})]_2$ (10 mol%), AgOTf (40 mol%), $Cu(OAc)_2$ (0.33 mmol, 1 equiv), and 1 mL of TFE was added. Then to this solution alkyne derivative **3a** (0.66 mmol, 2 equiv) was added and the tube was flushed with nitrogen and screw capped under nitrogen flow and placed in a preheated oil bath at 90 °C for 24 h. After the indicated time, the reaction mixture was cooled and concentrated. The crude material was purified by column chromatography on silica gel (100-200 mesh) using *n*-hexane – ethyl acetate as eluent, to yield **4a**.

1. 4. H/D exchange experiment with 4-octyne:



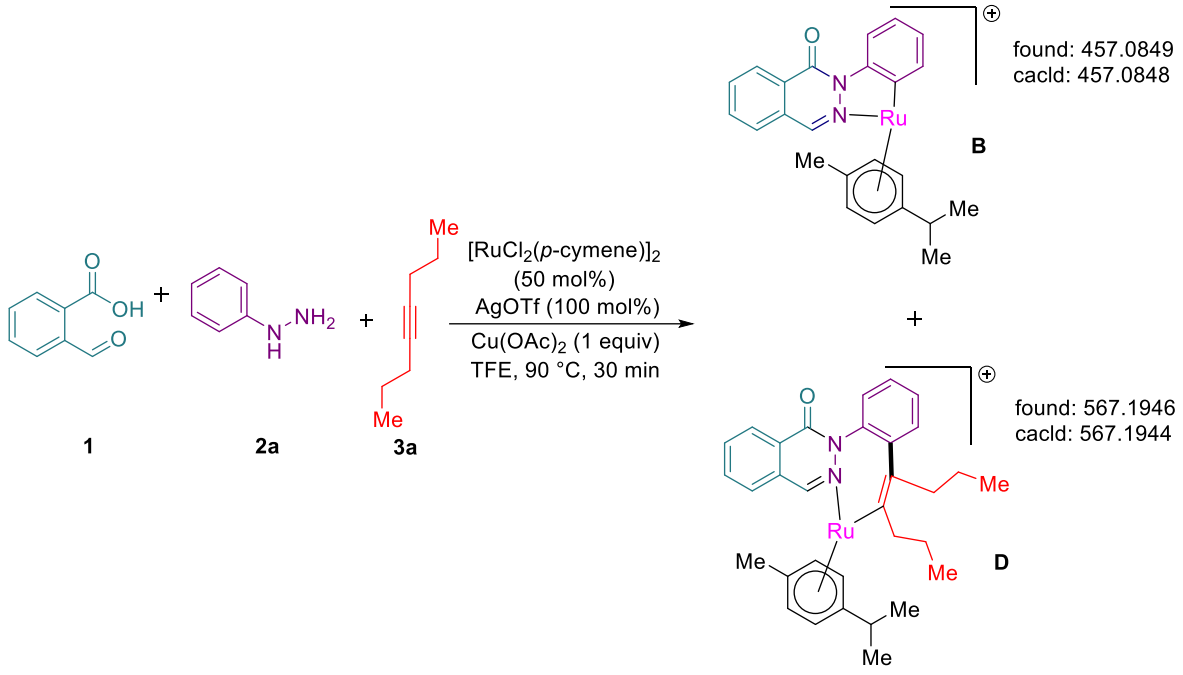
An oven-dried Schlenk tube (15 mL) equipped with a stir bar was charged with 2-carboxy benzaldehyde **1** (0.33 mmol, 1 equiv), phenyl hydrazine derivative **2a** (0.36 mmol, 1.1 equiv), $[RuCl_2(p\text{-cymene})]_2$ (10 mol%), AgOTf (40 mol%), $Cu(OAc)_2$ (0.33 mmol, 1 equiv), D_2O (3.3 mmol, 10 equiv) and 1 mL of TFE was added. Then to this solution alkyne derivative **3a** (0.66 mmol, 2 equiv) was added and the tube was flushed with nitrogen and screw capped under nitrogen flow and placed in a preheated oil bath at 90 °C for 24 h. After the indicated time, the reaction mixture was cooled and concentrated. The crude material was purified by column chromatography on silica gel (100-200 mesh) using *n*-hexane – ethyl acetate as eluent, to yield **4a**.

1. 5. Investigation of directing group:

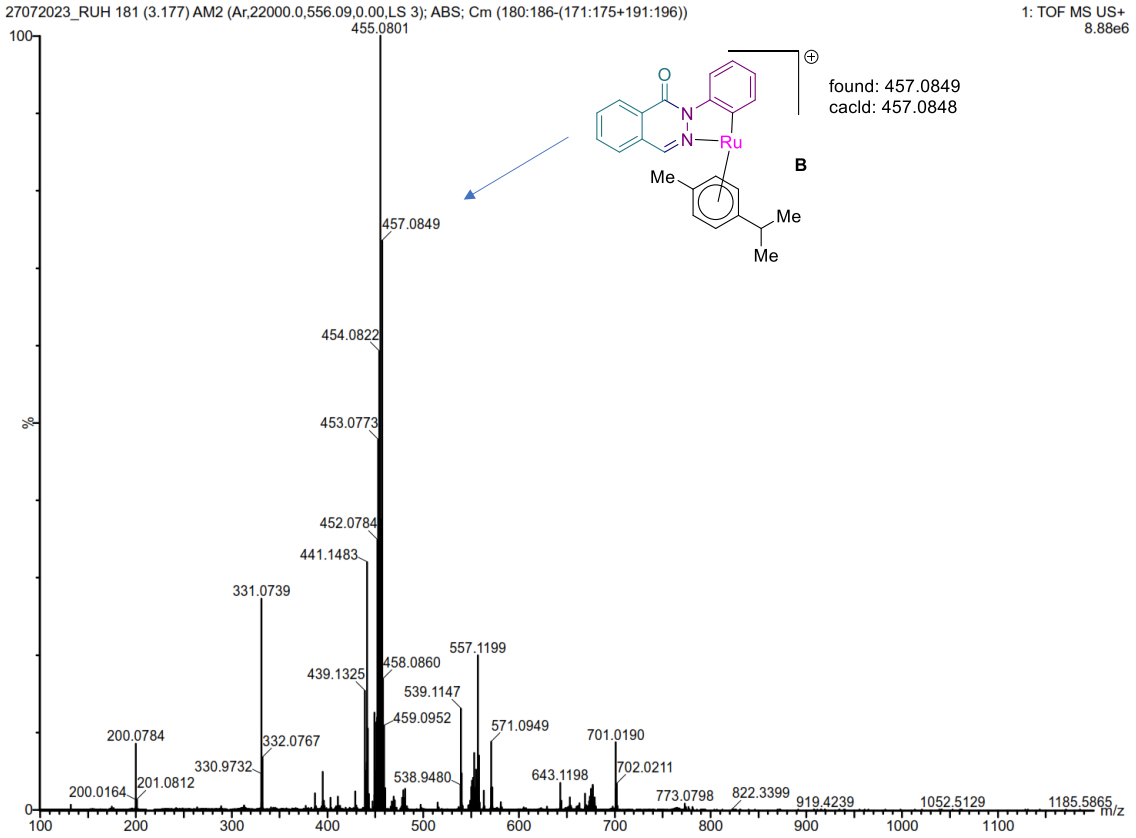


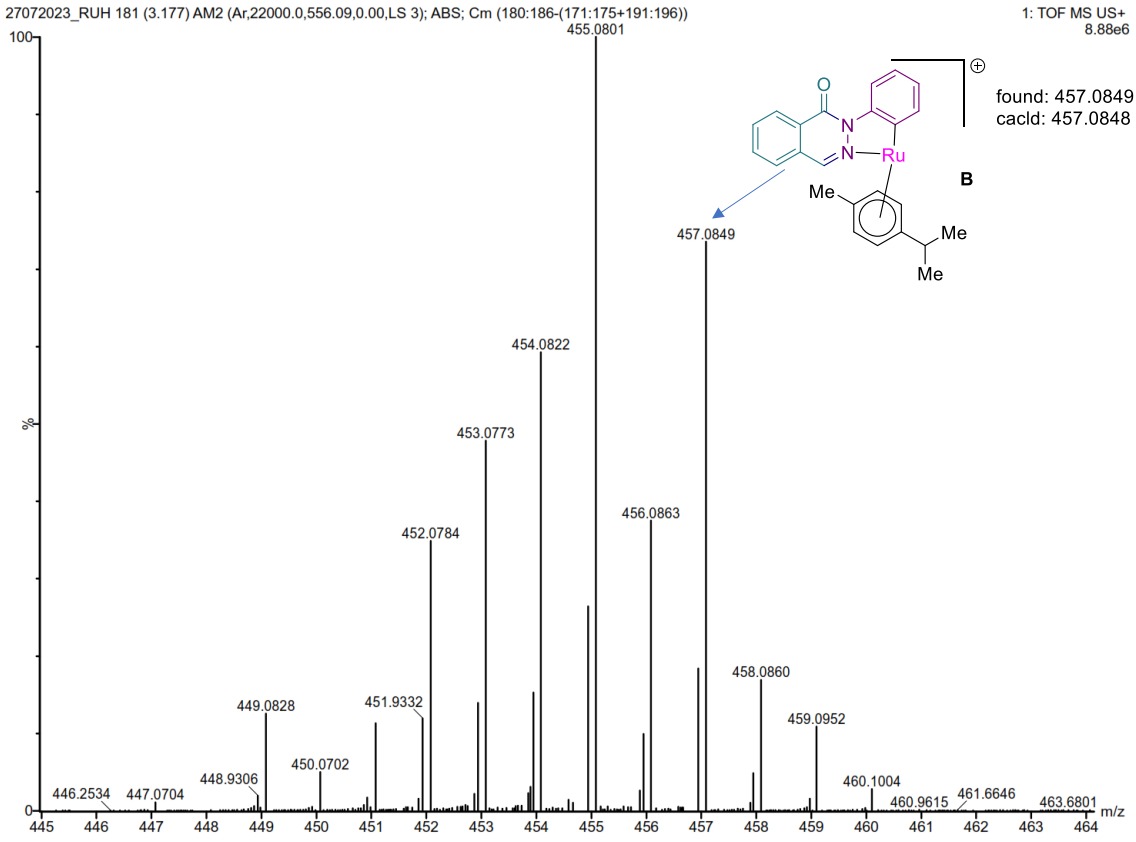
An oven-dried Schlenk tube (15 mL) equipped with a stir bar was charged with **7** (0.33 mmol, 1 equiv), $[RuCl_2(p\text{-cymene})]_2$ (10 mol%), AgOTf (40 mol%), $Cu(OAc)_2$ (0.33 mmol, 1 equiv), and 1 mL of TFE was added. Then to this solution alkyne derivative **3a** (0.66 mmol, 2 equiv) was added and the tube was flushed with nitrogen and screw capped under nitrogen flow and placed in a preheated oil bath at 90 °C for 24 h. No reaction occurred and the starting material recovered after the mentioned time.

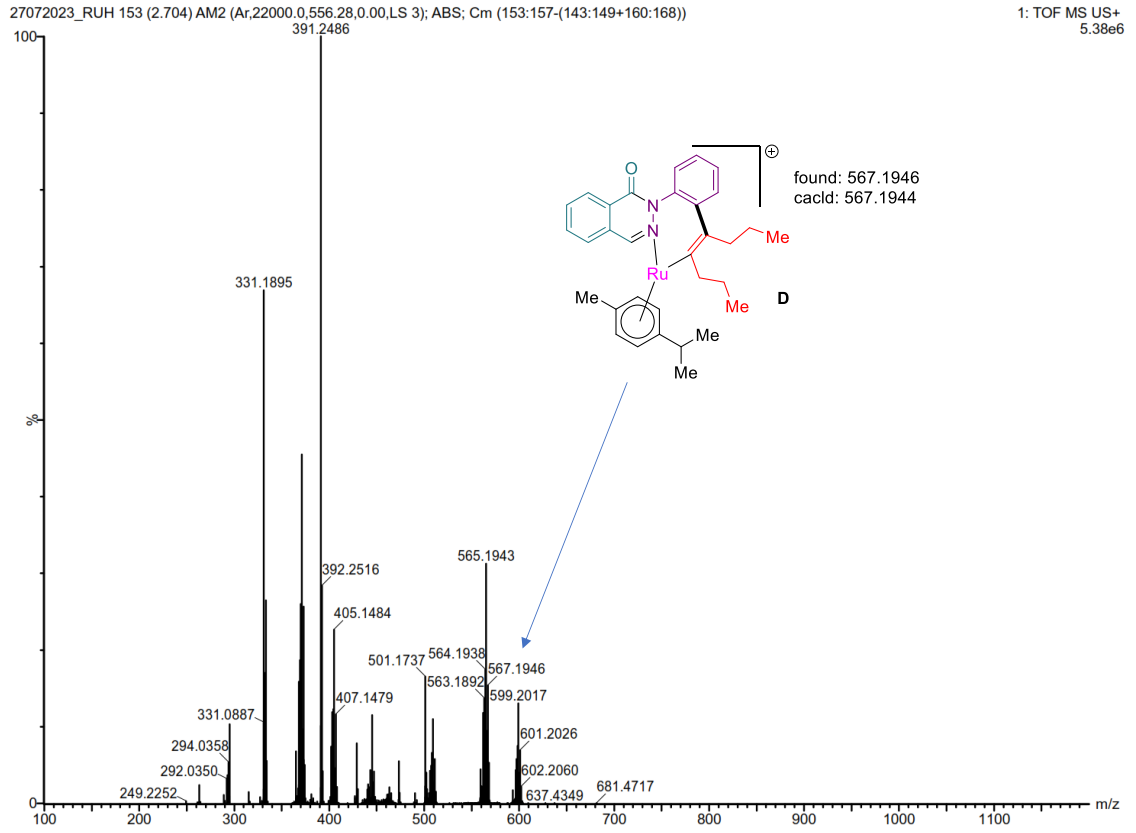
2. Mass spectrometry studies for determining intermediates

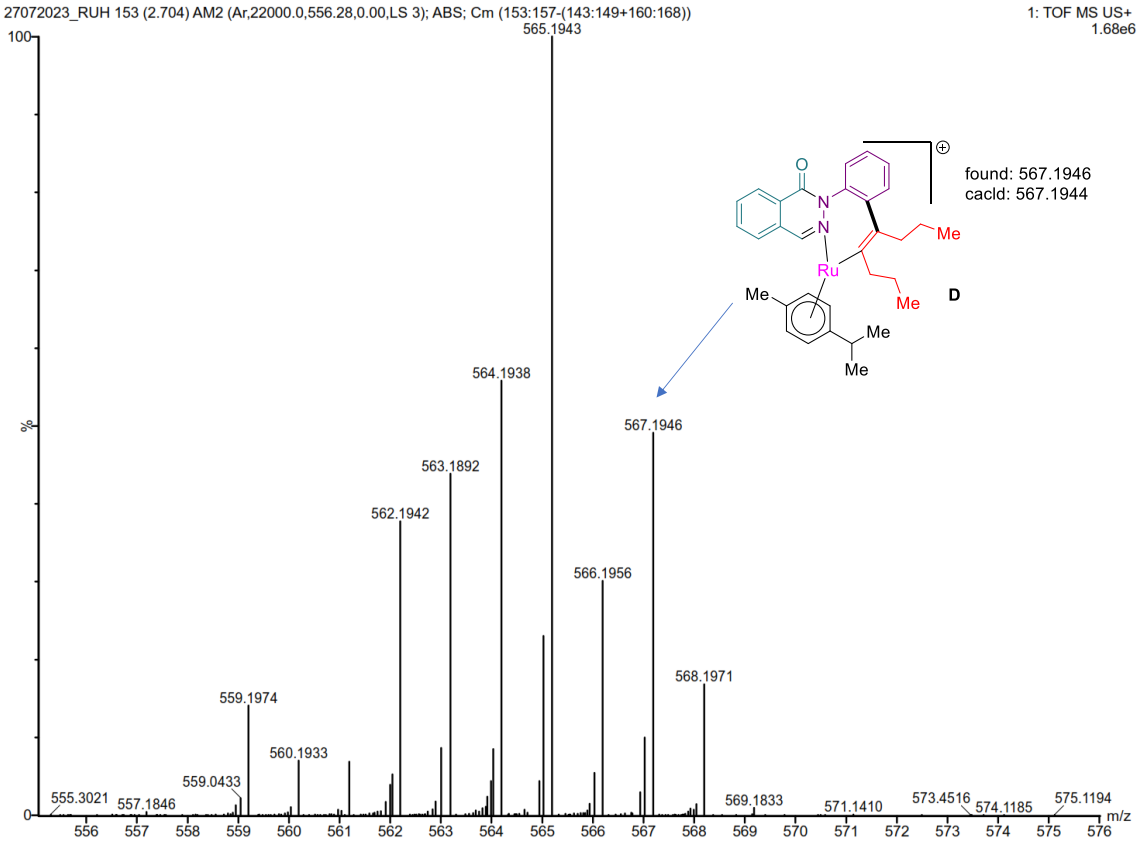


An oven-dried Schlenk tube (15 mL) equipped with a stir bar was charged with 2-carboxy benzaldehyde **1** (0.33 mmol, 1 equiv), phenyl hydrazine derivative **2a** (0.36 mmol, 1.1 equiv), $[RuCl_2(p\text{-cymene})]_2$ (50 mol%), AgOTf (100 mol%), $Cu(OAc)_2$ (0.33 mmol, 1 equiv), and 1 mL of TFE was added. Then to this solution alkyne derivative **3a** (0.66 mmol, 2 equiv) was added and the tube was flushed with nitrogen and screw capped under nitrogen flow and placed in a preheated oil bath at 90 °C for 30 min. This reaction mixture was subjected to mass spectrometry analysis (ESI-HRMS).


27072023_RUH 181 (3.177) AM2 (Ar,22000.0,556.09,0.00,LS 3); ABS; Cm (180:186-(171:175+191:196))
1: TOF MS US+
8.88e6
found: 457.0849
cacld: 457.0848
B
455.0801
457.0849
454.0822
453.0773
452.0784
441.1483
331.0739
557.1199
458.0860
439.1325
539.1147
459.0952
571.0949
701.0190
200.0784
332.0767
330.9732
702.0211
538.9480
643.1198
200.0164
201.0812
773.0798
822.3399
919.4239
1052.5129
1185.5865
%
m/z


27072023_RUH 181 (3.177) AM2 (Ar,22000.0,556.09,0.00,LS 3); ABS; Cm (180:186-(171:175+191:196))
1: TOF MS US+
8.88e6
found: 457.0849
cacld: 457.0848
B
455.0801
457.0849
454.0822
453.0773
456.0863
452.0784
458.0860
459.0952
449.0828
451.9332
450.0702
448.9306
460.1004
460.9615
461.6646
463.6801
446.2534
447.0704
%
m/z


27072023_RUH 153 (2.704) AM2 (Ar,22000.0,556.28,0.00,LS 3); ABS; Cm (153:157-(143:149+160:168))
1: TOF MS US+
5.38e6
found: 567.1946
cacld: 567.1944
D
391.2486
331.1895
565.1943
392.2516
405.1484
564.1938
501.1737
567.1946
563.1892
599.2017
407.1479
331.0887
601.2026
294.0358
602.2060
292.0350
637.4349
681.4717
249.2252
m/z


27072023_RUH 153 (2.704) AM2 (Ar,22000.0,556.28,0.00,LS 3); ABS; Cm (153:157-(143:149+160:168))
1: TOF MS US+
1.68e6
found: 567.1946
cacld: 567.1944
D
565.1943
564.1938
567.1946
563.1892
562.1942
566.1956
568.1971
559.1974
560.1933
559.0433
555.3021
557.1846
569.1833
571.1410
573.4516
574.1185
575.1194
m/z

3. Computational details

DFT calculations were carried out employing 6-31G* basis set[1] at B3LYP level of theory[2] and using the Gaussian 16 software[3]. Images of frontier Molecular orbitals were generated using the Gaussview[4] program.

4. Cartesian Coordinates and Z-matrices of the Structures

Cartesian coordinates for the optimized structures:

Table T1. Cartesian coordinates for **4a**

Symbolic Z-matrix

Charge = 0 Multiplicity = 1

C	1.58694800	0.63058000	-1.85221400
C	2.77489400	0.41701500	-1.06717900
C	2.69736000	-0.52351500	-0.01997900
C	1.43329500	-1.23598300	0.23152000
H	4.04866300	1.82051400	-2.10728500
H	1.59155000	1.34293400	-2.67376900
C	3.98713400	1.09494300	-1.30025400
C	3.81777300	-0.78271800	0.78295800
C	5.00621800	-0.10806800	0.54214600
C	5.08941800	0.83198100	-0.50100700
H	3.72418000	-1.51199800	1.58070100
H	5.87723600	-0.30442200	1.16087800
H	6.02451100	1.35520800	-0.68104500
O	1.26922600	-2.05898900	1.12631900
N	0.38990700	-0.89182400	-0.64337900
N	0.46176400	0.01466500	-1.66028700
C	-0.87963800	-1.57702300	-0.53593800
C	-1.96852100	-0.96855000	0.10895200
C	-0.99392900	-2.83722400	-1.12298100
C	-3.18013700	-1.67685500	0.13621600
C	-2.20575100	-3.52260100	-1.07961500

H	-0.12776600	-3.27054600	-1.61367600
C	-3.30390100	-2.93555600	-0.45036700
H	-4.03394300	-1.22223800	0.63127600
H	-2.29091700	-4.50397600	-1.53740000
H	-4.25630200	-3.45760400	-0.41281400
C	-1.86157400	0.35200500	0.81203400
C	-2.31552300	1.49155500	0.26760800
H	-2.23838000	2.39988200	0.86229700
C	-2.93412800	1.66507600	-1.09495400
H	-3.96601300	2.03252300	-0.97146100
H	-3.00501700	0.69691500	-1.60053400
C	-2.17847400	2.65148600	-2.01233400
H	-2.66339300	2.63736000	-2.99791900
H	-1.15934100	2.27538200	-2.16103000
C	-2.13496800	4.09535200	-1.49958100
H	-1.58430600	4.17740800	-0.55560400
H	-1.64199500	4.75467800	-2.22366000
H	-3.14583600	4.48800700	-1.32976800
C	-1.27849800	0.25422000	2.21481500
H	-1.94856400	-0.38446200	2.81326500
H	-0.33898700	-0.31345400	2.16819900
C	-1.04320600	1.57008500	2.96328300
H	-0.39029900	2.21998900	2.36498700
H	-1.99309600	2.10920600	3.07827800
C	-0.41888900	1.34784600	4.34533300
H	-1.06320700	0.72332600	4.97618700
H	0.55218000	0.84459200	4.26640100
H	-0.26188400	2.29848600	4.86782800

Z-matrix

1 2 1.5 6 1.0 16 2.0

2 3 1.5 7 1.5

3 4 1.0 8 1.5

4 14 2.0 15 1.0

5 7 1.0

6

7 10 1.5

8 9 1.5 11 1.0

9 10 1.5 12 1.0

10 13 1.0

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15 16 1.0 17 1.0

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17 18 1.5 19 1.5

18 20 1.5 27 1.0

19 21 1.5 22 1.0

20 23 1.5 24 1.0

21 23 1.5 25 1.0

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23 26 1.0

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27 28 2.0 40 1.0

28 29 1.0 30 1.0

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30 31 1.0 32 1.0 33 1.0

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33 34 1.0 35 1.0 36 1.0

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36 37 1.0 38 1.0 39 1.0

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40 41 1.0 42 1.0 43 1.0

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43 44 1.0 45 1.0 46 1.0

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46 47 1.0 48 1.0 49 1.0

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Table T2. Cartesian coordinates for **4b**

Symbolic Z-matrix

Charge = 0 Multiplicity = 1

C	-2.18600300	-1.80936600	1.14194900
C	-3.07509800	-1.18479600	0.19798100
C	-2.49087900	-0.58145000	-0.93417000
C	-1.02899800	-0.61298800	-1.11151000
H	-4.92582800	-1.62583000	1.22489700
H	-2.58040400	-2.30853200	2.02388900
C	-4.47482100	-1.16040100	0.35224700
C	-3.29841500	0.03362300	-1.90221800
C	-4.67592400	0.05377500	-1.73661100
C	-5.26381900	-0.54449700	-0.60727400

H	-2.81866600	0.48364100	-2.76484700
H	-5.30533700	0.53239700	-2.48149700
H	-6.34358300	-0.52455400	-0.48772600
O	-0.44877000	-0.16533700	-2.09460800
N	-0.32844100	-1.21664700	-0.05365700
N	-0.89395900	-1.82768100	1.02762500
C	1.10744200	-1.34920100	-0.11880900
C	1.95916900	-0.23735700	-0.02220200
C	1.62774600	-2.63987000	-0.24249900
C	3.34156300	-0.48111000	-0.08054500
C	3.00071000	-2.84714200	-0.28455100
H	0.94012600	-3.47759700	-0.30405400
C	3.88402600	-1.76196200	-0.20562500
H	4.01473300	0.36961900	-0.00493400
H	3.38918200	-3.85808200	-0.38327600
C	1.48409900	1.17930500	0.10737900
C	0.95759600	1.66347300	1.24368600
H	0.68048900	2.71583600	1.25650000
C	0.74288900	0.92973000	2.54222900
H	1.50383600	1.26356700	3.26749200
H	0.90153100	-0.14423300	2.40408800
C	-0.64663700	1.15972100	3.17411900
H	-0.75467600	0.46881100	4.02088600
H	-1.42318400	0.88151200	2.45006600
C	-0.89191900	2.59064400	3.66727900
H	-0.86522900	3.31825000	2.84811800
H	-1.87311600	2.67787300	4.14843000
H	-0.13379600	2.89057600	4.40186800
C	1.72227700	2.02311200	-1.13692700
H	2.80064200	2.00746200	-1.36297900
H	1.24199500	1.50918100	-1.97887900

C	1.24831700	3.47904000	-1.09309000
H	0.17159500	3.50641100	-0.87851100
H	1.74246800	4.01123300	-0.26877700
C	1.52350900	4.21511400	-2.40903900
H	2.59623700	4.23096500	-2.63857200
H	1.01342000	3.72803000	-3.24868200
H	1.17758000	5.25425900	-2.36411500
C	5.37909600	-1.97751400	-0.24073900
H	5.91989400	-1.02684400	-0.27823700
H	5.72490700	-2.52215900	0.64719900
H	5.67659100	-2.56809200	-1.11562400

Z-matrix

1 2 1.5 6 1.0 16 2.0

2 3 1.5 7 1.5

3 4 1.0 8 1.5

4 14 2.0 15 1.0

5 7 1.0

6

7 10 1.5

8 9 1.5 11 1.0

9 10 1.5 12 1.0

10 13 1.0

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15 16 1.0 17 1.0

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17 18 1.5 19 1.5

18 20 1.5 26 1.0

19 21 1.5 22 1.0

20 23 1.5 24 1.0

21 23 1.5 25 1.0

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26 27 2.0 39 1.0

27 28 1.0 29 1.0

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49 50 1.0 51 1.0 52 1.0

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Table T3. Cartesian coordinates for **4d**

Symbolic Z-matrix

Charge = 0 Multiplicity = 1

C	-2.15152500	-1.95406200	1.23064800
C	-3.11354100	-1.53413300	0.24605900
C	-2.61450300	-0.91492700	-0.91782000
C	-1.16323600	-0.72806400	-1.08579700
H	-4.88757300	-2.19905900	1.28797600
H	-2.47621300	-2.45403100	2.14014900
C	-4.50203400	-1.72130800	0.39092100
C	-3.49386200	-0.49378100	-1.92626300
C	-4.85974000	-0.68166900	-1.77006800
C	-5.36325100	-1.29637900	-0.60914600
H	-3.07753100	-0.02599500	-2.81206000
H	-5.54531800	-0.35402600	-2.54643200
H	-6.43444800	-1.43994300	-0.49703800
O	-0.64631500	-0.25164100	-2.09062400
N	-0.39095200	-1.15526900	0.00769600
N	-0.87059800	-1.77824000	1.12321300
C	1.04794200	-1.06789100	-0.04814400
C	1.72167700	0.16970500	0.00129200
C	1.76374400	-2.26058900	-0.11105200
C	3.11753400	0.14794200	-0.04255100
C	3.15716300	-2.27009300	-0.13951600
H	1.21701200	-3.19807400	-0.13493800
C	3.84011400	-1.04991600	-0.10907100
H	3.67643300	1.07780000	-0.00409300

H	3.68519300	-3.21498900	-0.18868400
C	1.02958100	1.49931100	0.06853300
C	0.43823200	1.94684300	1.18768700
H	-0.00277000	2.94122600	1.15617700
C	0.35040700	1.25029700	2.52116800
H	1.05178000	1.73567300	3.22039800
H	0.67890900	0.21028100	2.43080900
C	-1.05495900	1.28413500	3.15892200
H	-1.04801500	0.62278700	4.03569300
H	-1.77996700	0.85415200	2.45615100
C	-1.52293700	2.67799800	3.59364600
H	-1.61413700	3.36475900	2.74452600
H	-2.50441000	2.62939100	4.07973200
H	-0.82024500	3.12555800	4.30794700
C	1.12886500	2.30986600	-1.21568000
H	2.19588100	2.44634900	-1.45363500
H	0.72764600	1.69082900	-2.02786200
C	0.43933700	3.67742800	-1.22928600
H	-0.62797500	3.55093400	-1.00326500
H	0.85147300	4.31376600	-0.43430800
C	0.59215900	4.38769700	-2.57884400
H	1.64851500	4.55952900	-2.82016300
H	0.16101600	3.79009000	-3.39093900
H	0.08899900	5.36153900	-2.57572900
O	5.19812600	-0.91856500	-0.13212700
C	5.98450500	-2.09769300	-0.19448700
H	5.78108100	-2.67117100	-1.10854200
H	7.02378900	-1.76411400	-0.20249600
H	5.81720200	-2.74134600	0.67935900

Z-matrix

1 2 1.5 6 1.0 16 2.0

2 3 1.5 7 1.5

3 4 1.0 8 1.5

4 14 2.0 15 1.0

5 7 1.0

6

7 10 1.5

8 9 1.5 11 1.0

9 10 1.5 12 1.0

10 13 1.0

11

12

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15 16 1.0 17 1.0

16

17 18 1.5 19 1.5

18 20 1.5 26 1.0

19 21 1.5 22 1.0

20 23 1.5 24 1.0

21 23 1.5 25 1.0

22

23 49 1.0

24

25

26 27 2.0 39 1.0

27 28 1.0 29 1.0

28

29 30 1.0 31 1.0 32 1.0

30

31

32 33 1.0 34 1.0 35 1.0

33

34

35 36 1.0 37 1.0 38 1.0

36

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39 40 1.0 41 1.0 42 1.0

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42 43 1.0 44 1.0 45 1.0

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45 46 1.0 47 1.0 48 1.0

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48

49 50 1.0

50 51 1.0 52 1.0 53 1.0

51

52

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Table T4. Cartesian coordinates for **4e**

Symbolic Z-matrix

Charge = 0 Multiplicity = 1

C	-2.50253000	-2.02747000	1.03920200
C	-3.43701000	-1.44343900	0.11335900
C	-2.90068300	-0.72006300	-0.97109400
C	-1.44085200	-0.59490100	-1.12112500

H	-5.24800100	-2.12944700	1.07467300
H	-2.85654200	-2.61361500	1.88400800
C	-4.83401100	-1.57095900	0.23905500
C	-3.75237100	-0.13611700	-1.92039900
C	-5.12700500	-0.26584300	-1.78298700
C	-5.66745600	-0.98473300	-0.70128700
H	-3.30845400	0.40859500	-2.74684500
H	-5.79084300	0.18807200	-2.51331300
H	-6.74523600	-1.08190600	-0.60370200
O	-0.89574600	-0.04054800	-2.06924200
N	-0.69751800	-1.18064100	-0.08249200
N	-1.21396200	-1.90697500	0.95134100
C	0.74534200	-1.16857500	-0.12717400
C	1.48461800	0.01897200	0.02027100
C	1.39131400	-2.39535100	-0.27953200
C	2.88292200	-0.08600100	-0.01884900
C	2.78080600	-2.46429600	-0.30104100
H	0.79191700	-3.29499100	-0.37785000
C	3.55365800	-1.30499400	-0.17351400
H	3.46036800	0.82784100	0.09734700
H	3.26823900	-3.42880900	-0.42211300
C	0.87189000	1.37827000	0.18467900
C	0.27953500	1.77225200	1.32356300
H	-0.09871600	2.79189500	1.36297100
C	0.10958500	0.97894200	2.59316100
H	0.79413200	1.38386500	3.35723800
H	0.40754300	-0.06226700	2.43534800
C	-1.32113900	1.01446700	3.17233200
H	-1.37216500	0.29449500	4.00009300
H	-2.02672000	0.65756400	2.41127800
C	-1.76682900	2.38964900	3.68307600

H	-1.80347700	3.13439500	2.87997000
H	-2.76844300	2.33880900	4.12585400
H	-1.08185000	2.76607600	4.45346500
C	1.05240500	2.28296700	-1.02635400
H	2.13186800	2.38791200	-1.22121000
H	0.65004300	1.74984800	-1.89643600
C	0.42566300	3.67838700	-0.95152400
H	-0.65207200	3.58366500	-0.76305500
H	0.84218700	4.23337000	-0.09988300
C	0.64852200	4.48221600	-2.23743700
H	1.71803000	4.62111300	-2.43909400
H	0.21288500	3.97061500	-3.10401000
H	0.19112500	5.47611900	-2.17036200
C	5.66505000	-0.60408000	-1.39336600
H	5.44499900	0.46769600	-1.32263800
H	6.75512700	-0.71879200	-1.42618600
H	5.25395800	-0.96670200	-2.34167000
C	5.69466000	-0.90013100	1.12911400
H	5.47911800	0.15916800	1.31227600
H	5.30314100	-1.47188800	1.97750900
H	6.78455100	-1.01920300	1.11000500
C	5.07484400	-1.37617200	-0.19823200
H	5.34404800	-2.43376800	-0.32506100

Z-matrix

1 2 1.5 6 1.0 16 2.0

2 3 1.5 7 1.5

3 4 1.0 8 1.5

4 14 2.0 15 1.0

5 7 1.0

6

7 10 1.5

8 9 1.5 11 1.0

9 10 1.5 12 1.0

10 13 1.0

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15 16 1.0 17 1.0

16

17 18 1.5 19 1.5

18 20 1.5 26 1.0

19 21 1.5 22 1.0

20 23 1.5 24 1.0

21 23 1.5 25 1.0

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23 57 1.0

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26 27 2.0 39 1.0

27 28 1.0 29 1.0

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29 30 1.0 31 1.0 32 1.0

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32 33 1.0 34 1.0 35 1.0

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35 36 1.0 37 1.0 38 1.0

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39 40 1.0 41 1.0 42 1.0

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42 43 1.0 44 1.0 45 1.0

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45 46 1.0 47 1.0 48 1.0

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49 50 1.0 51 1.0 52 1.0 57 1.0

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53 54 1.0 55 1.0 56 1.0 57 1.0

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57 58 1.0

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Table T5. Cartesian coordinates for **4f**

Symbolic Z-matrix

Charge = 0 Multiplicity = 1

C	-2.58052300	-2.08345200	1.11213100
C	-3.54616400	-1.61238900	0.15446200
C	-3.05429400	-0.89784200	-0.95663000
C	-1.60654200	-0.66887200	-1.10087200
H	-5.31083900	-2.39186000	1.13073700
H	-2.89878700	-2.65725300	1.97931400

C	-4.93088500	-1.84006900	0.27473400
C	-3.93696200	-0.42183000	-1.93733700
C	-5.29928000	-0.64977600	-1.80520900
C	-5.79564800	-1.36023700	-0.69711300
H	-3.52600600	0.11889800	-2.78320200
H	-5.98749400	-0.27991600	-2.55995700
H	-6.86399300	-1.53499700	-0.60384400
O	-1.09435300	-0.11492800	-2.06744500
N	-0.83240300	-1.15328700	-0.03295700
N	-1.30366200	-1.87073600	1.02818100
C	0.60546500	-1.03342800	-0.06808300
C	1.25293800	0.21040700	0.03584400
C	1.34716000	-2.20832500	-0.16641900
C	2.65416300	0.20803600	0.00784300
C	2.73938900	-2.17472300	-0.17849200
H	0.82176800	-3.15606900	-0.23167300
C	3.42727200	-0.95781700	-0.09531700
H	3.15264000	1.16981800	0.09073200
H	3.27843800	-3.11164600	-0.25847400
C	0.54008000	1.52576400	0.14574300
C	-0.08631000	1.91711300	1.26722200
H	-0.53967900	2.90640500	1.26703600
C	-0.20426600	1.16145900	2.56545000
H	0.44869600	1.64064400	3.31408900
H	0.16531000	0.13814400	2.44668400
C	-1.63567100	1.11992000	3.14256700
H	-1.64047200	0.42700900	3.99460400
H	-2.31364500	0.69069500	2.39388800
C	-2.17407800	2.47893300	3.60547800
H	-2.25750000	3.19161000	2.77721300
H	-3.17160200	2.37644000	4.04855100

H	-1.51834300	2.92622800	4.36327800
C	0.65953600	2.39505800	-1.09815000
H	1.72965700	2.56445200	-1.29914000
H	0.29452900	1.80430800	-1.94732800
C	-0.05878500	3.74730800	-1.07359800
H	-1.12869500	3.58846000	-0.88331600
H	0.31700700	4.35810000	-0.24139900
C	0.11414500	4.51847300	-2.38693100
H	1.17240800	4.72302700	-2.59194700
H	-0.28220800	3.94801900	-3.23544700
H	-0.41027600	5.48054800	-2.35595200
C	5.63464600	-2.24221000	-0.23531700
H	5.35024200	-2.75039400	-1.16373700
H	6.72396500	-2.12341500	-0.24422700
H	5.38145900	-2.89762600	0.60585100
C	5.41392900	0.00440700	-1.31016400
H	5.08854900	-0.44027500	-2.25748000
H	5.00302400	1.01806400	-1.25915200
H	6.50746100	0.08798400	-1.33087100
C	4.96398300	-0.86118700	-0.10906600
C	5.45264300	-0.20742800	1.20547400
H	5.15440300	-0.80441600	2.07488900
H	6.54670900	-0.12733200	1.20710800
H	5.04489900	0.80017500	1.33667100

Z-matrix

1 2 1.5 6 1.0 16 2.0

2 3 1.5 7 1.5

3 4 1.0 8 1.5

4 14 2.0 15 1.0

5 7 1.0

6

7 10 1.5

8 9 1.5 11 1.0

9 10 1.5 12 1.0

10 13 1.0

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15 16 1.0 17 1.0

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17 18 1.5 19 1.5

18 20 1.5 26 1.0

19 21 1.5 22 1.0

20 23 1.5 24 1.0

21 23 1.5 25 1.0

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23 57 1.0

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26 27 2.0 39 1.0

27 28 1.0 29 1.0

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29 30 1.0 31 1.0 32 1.0

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32 33 1.0 34 1.0 35 1.0

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35 36 1.0 37 1.0 38 1.0

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39 40 1.0 41 1.0 42 1.0

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42 43 1.0 44 1.0 45 1.0

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45 46 1.0 47 1.0 48 1.0

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49 50 1.0 51 1.0 52 1.0 57 1.0

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53 54 1.0 55 1.0 56 1.0 57 1.0

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57 58 1.0

58 59 1.0 60 1.0 61 1.0

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Table T6. Cartesian coordinates for **4g**

Symbolic Z-matrix

Charge = 0 Multiplicity = 1

C	-2.18656100	-1.78778200	1.13963200
C	-3.06683900	-1.15065900	0.19543400

C	-2.47472500	-0.55359900	-0.93606500
C	-1.01352800	-0.60333500	-1.11240500
H	-4.92322400	-1.56902000	1.22150800
H	-2.58829300	-2.28301700	2.02043800
C	-4.46601600	-1.10855700	0.34949600
C	-3.27388400	0.07258600	-1.90383100
C	-4.65111700	0.11007600	-1.73832600
C	-5.24681000	-0.48160600	-0.60971000
H	-2.78853900	0.51738900	-2.76602100
H	-5.27418800	0.59735700	-2.48287200
H	-6.32621400	-0.44794500	-0.49038000
O	-0.42521300	-0.16205000	-2.09334500
N	-0.32150700	-1.21716600	-0.05420100
N	-0.89488200	-1.82268800	1.02706100
C	1.11123700	-1.36685600	-0.12059900
C	1.97482200	-0.25964100	-0.02306600
C	1.61285800	-2.66484800	-0.24485400
C	3.35445800	-0.50850600	-0.08359800
C	2.98305100	-2.90094900	-0.28871300
H	0.91372100	-3.49250300	-0.30424900
C	3.83249200	-1.80470700	-0.21010000
H	4.06368600	0.30929600	-0.01014000
H	3.39004300	-3.90154500	-0.38539300
C	1.51185900	1.16069900	0.10854600
C	0.98564300	1.64374100	1.24524000
H	0.71771600	2.69831000	1.26013100
C	0.76148600	0.90865300	2.54119500
H	1.52763600	1.23025200	3.26628000
H	0.90519700	-0.16714400	2.40080000
C	-0.62440500	1.15678700	3.17424700
H	-0.74215800	0.46369700	4.01778300

H	-1.40519400	0.89327300	2.44922000
C	-0.84776300	2.58899600	3.67399000
H	-0.81019100	3.32023400	2.85847700
H	-1.82753900	2.68859700	4.15545700
H	-0.08534400	2.87374400	4.41006200
C	1.76426600	2.00585300	-1.13207700
H	2.84409200	1.98532900	-1.35054600
H	1.28673000	1.49786200	-1.97911900
C	1.29821600	3.46426600	-1.08590600
H	0.22040700	3.49697000	-0.87765500
H	1.79081800	3.99077700	-0.25711500
C	1.58565600	4.20272600	-2.39787200
H	2.65973500	4.21321000	-2.62086000
H	1.07758900	3.72158400	-3.24210700
H	1.24545100	5.24358000	-2.35110400
F	5.16645800	-2.00499400	-0.24997800

Z-matrix

1 2 1.5 6 1.0 16 2.0

2 3 1.5 7 1.5

3 4 1.0 8 1.5

4 14 2.0 15 1.0

5 7 1.0

6

7 10 1.5

8 9 1.5 11 1.0

9 10 1.5 12 1.0

10 13 1.0

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15 16 1.0 17 1.0

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17 18 1.5 19 1.5

18 20 1.5 26 1.0

19 21 1.5 22 1.0

20 23 1.5 24 1.0

21 23 1.5 25 1.0

22

23 49 1.0

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26 27 2.0 39 1.0

27 28 1.0 29 1.0

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29 30 1.0 31 1.0 32 1.0

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32 33 1.0 34 1.0 35 1.0

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35 36 1.0 37 1.0 38 1.0

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39 40 1.0 41 1.0 42 1.0

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42 43 1.0 44 1.0 45 1.0

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45 46 1.0 47 1.0 48 1.0

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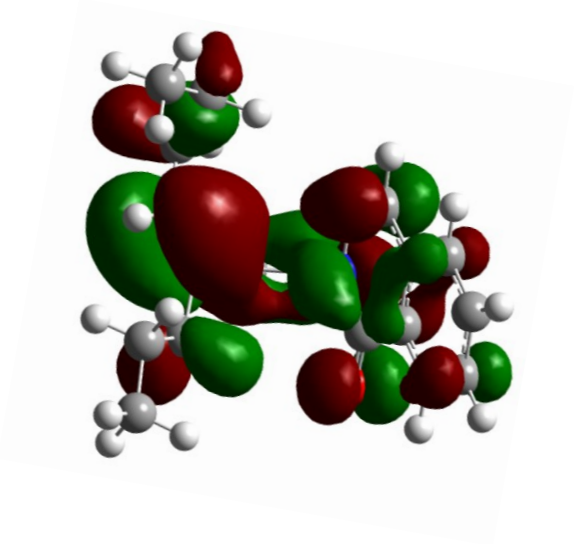
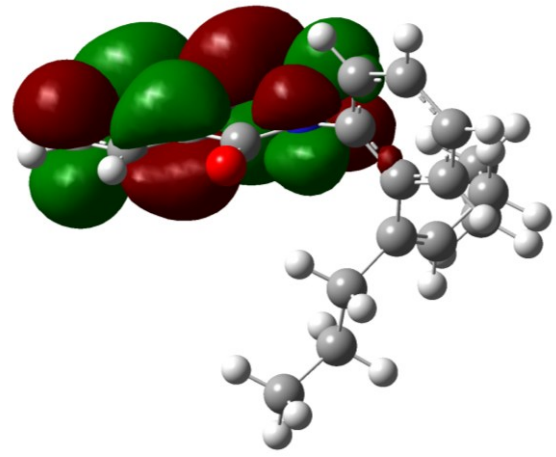
5. Frontier Molecular Orbital surfaces

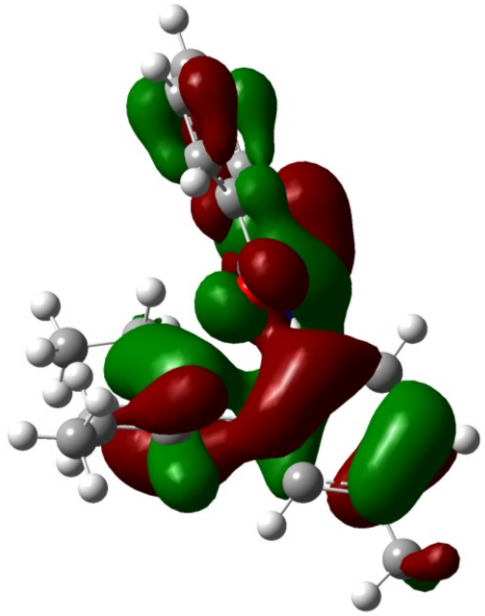
4a HOMO



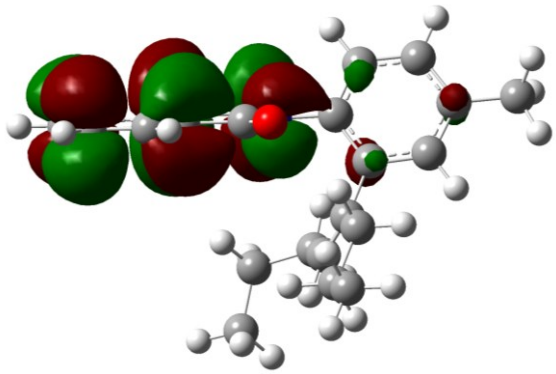
4a LUMO



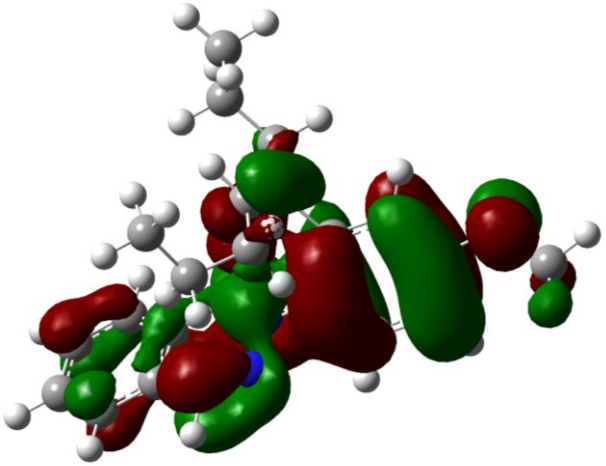
4b HOMO



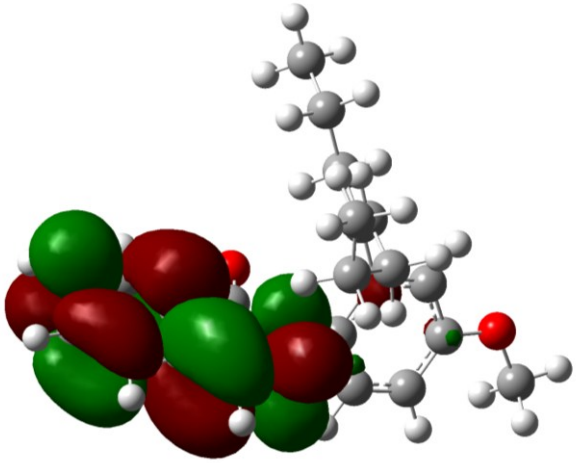
4b LUMO



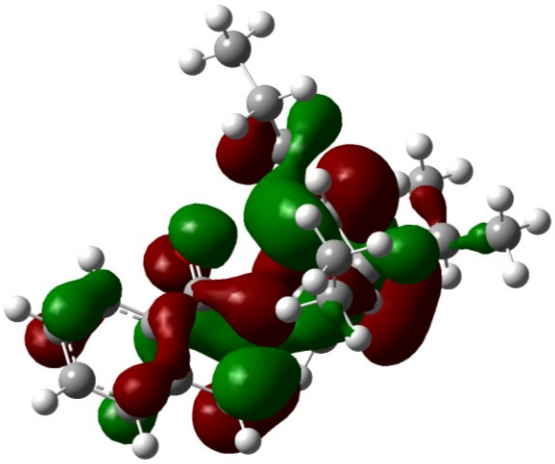
4d HOMO



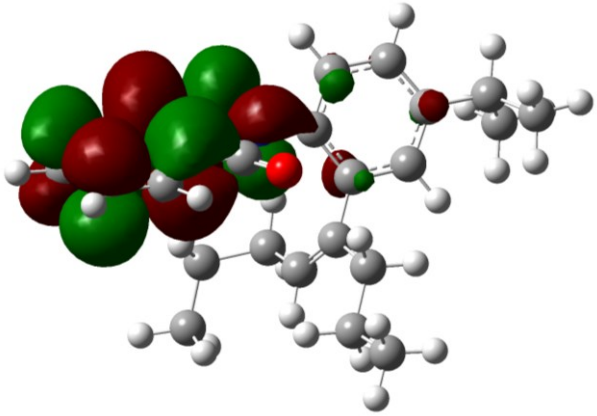
4d LUMO



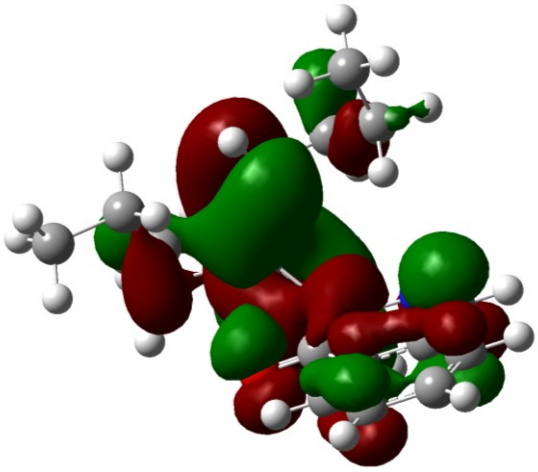
4e HOMO



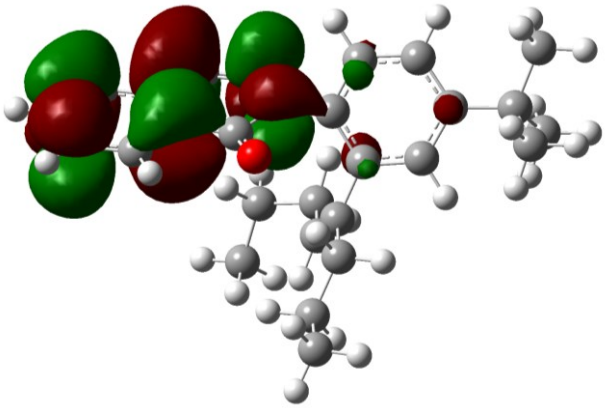
4e LUMO



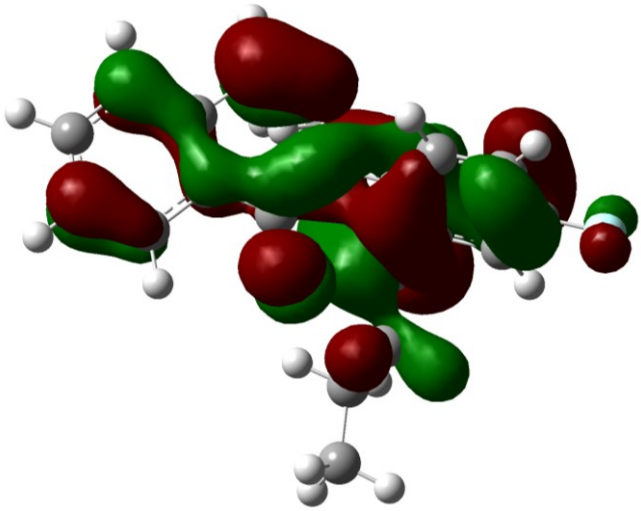
4f HOMO



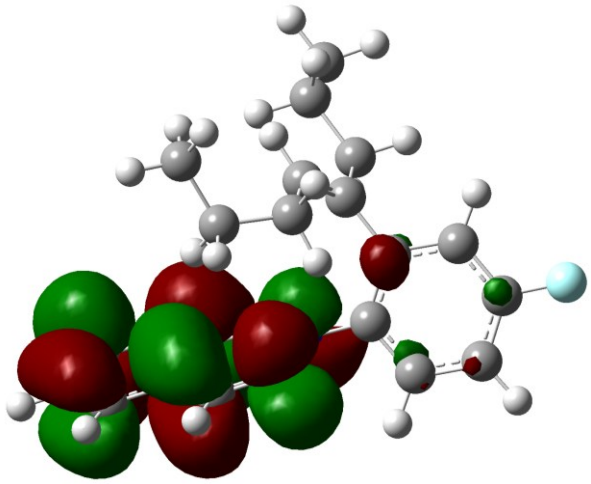
4f LUMO



4g HOMO

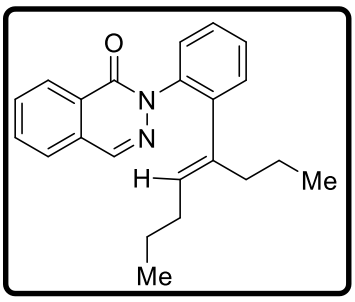


4g LUMO



6. Characterization Data:

2-(2-(oct-4-en-4-yl)phenyl)phthalazin-1(2H)-one (4a):



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 90/10)

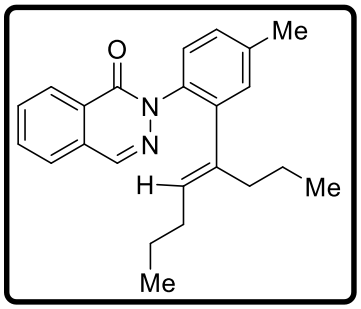
Yield: 82 mg, 74%; 1506 mg, 68%, pale-yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.39 (d, *J* = 7.76 Hz, 1H), 8.12 (s, 1H), 7.76 (t, *J* = 7.3 Hz, 1H), 7.70 (t, *J* = 7.52 Hz, 1H), 7.65 (d, *J* = 7.68 Hz, 1H), 7.32-7.25 (m, 4H), 5.33 (t, *J* = 7.4 Hz, 1H), 2.05 (t, *J* = 7.8 Hz, 2H), 1.85 (q, *J* = 7.29 Hz, 2H), 1.30-1.20 (m, 2H), 1.05-0.95 (m, 2H), 0.73 (t, *J* = 7.32 Hz, 3H), 0.58 (t, *J* = 7.36 Hz, 3H) ppm.

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 158.4, 141.6, 138.6, 136.26, 136.20, 132.2, 130.6, 130.4, 129.1, 128.7, 127.5, 127.4, 127.0, 126.2, 126.0, 124.9, 32.0, 29.1, 21.5, 20.6, 13.1, 12.5 ppm.

HR-MS: $[M+H]^+$ calculated for $C_{22}H_{25}N_2O$, 333.1961; found, 333.1960; mass error : 0.30 ppm.

2-(4-methyl-2-(oct-4-en-4-yl)phenyl)phthalazin-1(2H)-one (4b):



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 90/10)

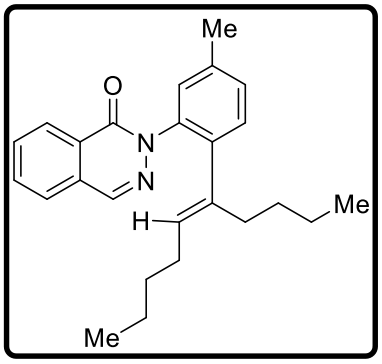
Yield: 86 mg, 74%; pale-yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.40 (d, *J* = 7.76 Hz, 1H), 8.11 (s, 1H), 7.76 (t, *J* = 7.38 Hz, 1H), 7.70 (t, *J* = 7.5 Hz, 1H), 7.66 (d, *J* = 7.68 Hz, 1H), 7.17 (d, *J* = 7.92 Hz, 1H), 7.11-7.07 (m, 2H), 5.32 (t, *J* = 7.42 Hz, 1H), 2.33 (s, 3H), 2.05 (t, *J* = 7.82 Hz, 2H), 1.85 (q, *J* = 7.29 Hz, 2H), 1.31-1.22 (m, 2H), 1.05-0.96 (m, 2H), 0.74 (t, *J* = 7.3 Hz, 3H), 0.59 (t, *J* = 7.34 Hz, 3H) ppm.

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 159.5, 142.3, 138.3, 137.3, 137.2, 133.1, 131.6, 131.2, 130.6, 129.7, 128.5, 128.0, 127.7, 127.1, 125.9, 33.1, 30.1, 22.5, 21.7, 21.2, 14.1, 13.5 ppm.

HR-MS: $[M+H]^+$ calculated for $C_{23}H_{27}N_2O$, 347.2118; found, 347.2120; mass error : 0.57 ppm.

2-(2-(dec-5-en-5-yl)-5-methylphenyl)phthalazin-1(2H)-one (4c):



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 90/10)

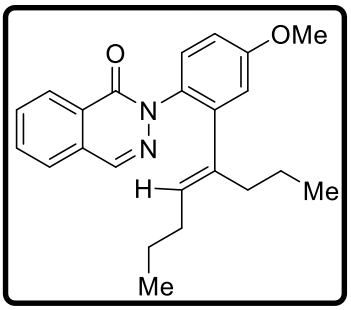
Yield: 83 mg, 66%; pale-yellow oil.

^{1}H NMR (400 MHz, CDCl3) δ: 8.40 (d, *J* = 7.76 Hz, 1H), 8.12 (s, 1H), 7.76 (td, *J* = 7.42 Hz, 1H), 7.71 (td, *J* = 6.96 Hz, 1H), 7.66 (d, *J* = 7.84 Hz, 1H), 7.16-7.11 (m, 2H), 7.10 (s, 1H), 5.26 (t, *J* = 7.46 Hz, 1H), 2.30 (s, 3H), 2.07 (t, *J* = 7.64 Hz, 2H), 1.85 (q, *J* = 7.08 Hz, 2H), 1.21-1.13 (m, 4H), 0.95-0.87 (m, 4H), 0.75-0.73 (m, 3H), 0.52 (t, *J* = 6.98 Hz, 3H) ppm.

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 159.4, 139.7, 139.4, 137.1, 136.9, 133.1, 131.6, 131.0, 129.84, 129.80, 129.4, 128.5, 128.4, 127.1, 125.9, 31.6, 30.8, 30.7, 27.7, 22.8, 22.0, 20.8, 13.9, 13.8 ppm.

HR-MS: $[M+H]^+$ calculated for $C_{25}H_{31}N_2O$, 375.2431, found, 375.2431; mass error : 0.00 ppm.

2-(4-methoxy-2-(oct-4-en-4-yl)phenyl)phthalazin-1(2H)-one (4d):



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 88/12)

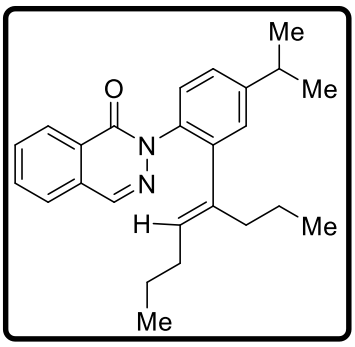
Yield: 94 mg, 78%; pale-yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.39 (d, *J* = 7.8 Hz, 1H), 8.10 (s, 1H), 7.75 (td, *J* = 7.4 Hz, 1H), 7.70 (td, *J* = 7.58 Hz, 1H), 7.65 (d, *J* = 7.88 Hz, 1H), 7.20-7.18 (m, 1H), 6.83 (dd, *J* = 8.56 Hz, 1H), 6.78 (d, *J* = 2.84 Hz, 1H), 5.33 (t, *J* = 7.42 Hz, 1H), 3.78 (s, 3H), 2.04 (t, *J* = 7.82 Hz, 2H), 1.84 (q, *J* = 7.30 Hz, 2H), 1.31-1.22 (m, 2H), 1.04-0.95 (m, 2H), 0.73 (t, *J* = 7.32 Hz, 3H), 0.57 (t, *J* = 7.36 Hz, 3H) ppm.

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 158.6, 158.3, 142.9, 136.2, 132.1, 131.8, 130.6, 130.3, 128.7, 127.9, 127.5, 126.1, 124.9, 114.5, 111.3, 54.4, 32.0, 29.0 28.6, 21.5, 20.6, 13.1, 12.5 ppm.

HR-MS: $[M+H]^+$ calculated for $C_{23}H_{27}N_2O_2$, 363.2067, found, 363.2068; mass error : 0.27 ppm.

2-(4-isopropyl-2-(oct-4-en-4-yl)phenyl)phthalazin-1(2H)-one (4e):



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 90/10)

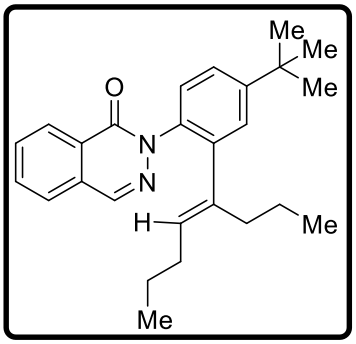
Yield: 90 mg, 72%; colourless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.39 (dd, *J* = 7.76 Hz, 1H), 8.10 (s, 1H), 7.75 (td, *J* = 7.4 Hz, 1H), 7.69 (td, *J* = 7.56 Hz, 1H), 7.64 (dd, *J* = 7.8 Hz, 1H), 7.20-7.18 (m, 1H), 7.15-7.13 (m, 1H), 7.09 (d, *J* = 1.96 Hz, 1H), 5.31 (t, *J* = 7.42 Hz, 1H), 2.93-2.82 (m, 1H), 2.05 (t, *J* = 7.82 Hz, 2H), 1.84 (q, *J* = 7.29 Hz, 2H), 1.30-1.23 (m, 2H), 1.21 (d, *J* = 6.92 Hz, 1H), 1.04-0.95 (m, 2H), 0.73 (t, *J* = 7.32 Hz, 3H), 0.58 (t, *J* = 7.36 Hz, 3H) ppm.

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 159.5, 149.1, 142.2, 137.5, 137.3, 137.1, 133.1, 131.6, 131.1, 129.7, 128.5, 128.2, 127.7, 127.1, 125.9, 125.3, 33.9, 33.1, 30.1, 23.9, 22.6, 21.7, 14.2, 13.6 ppm.

HR-MS: $[M+H]^+$ calculated for $C_{25}H_{31}N_2O$, 375.2431, found, 375.2432; mass error : 0.26 ppm.

2-(4-(tert-butyl)-2-(oct-4-en-4-yl)phenyl)phthalazin-1(2H)-one (4f):



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 89/11)

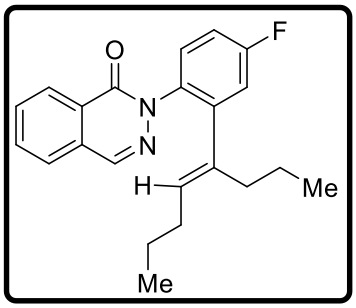
Yield: 89 mg, 69%; colourless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.40 (d, *J* = 7.8 Hz, 1H), 8.10 (s, 1H), 7.75 (t, *J* = 7.38 Hz, 1H), 7.70 (t, *J* = 7.46 Hz, 1H), 7.65 (d, *J* = 7.68 Hz, 1H), 7.31 (dd, *J* = 8.24 Hz, 1H), 7.24 (s, 1H), 7.20-7.18 (m, 1H), 5.32 (t, *J* = 7.4 Hz, 1H), 2.06 (t, *J* = 7.78 Hz, 2H), 1.85 (q, *J* = 7.28 Hz, 2H), 1.28 (s, 9H), 1.25-1.21 (m, 2H), 1.04-0.95 (m, 2H), 0.74 (t, *J* = 7.3 Hz, 3H), 0.58 (t, *J* = 7.34 Hz, 3H) ppm.

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 159.5, 151.3, 141.8, 137.6, 137.1, 133.1, 131.6, 131.0, 129.7, 128.5, 127.3, 127.1, 127.0, 125.9, 124.4, 34.6, 33.2, 31.3, 30.1, 22.6, 21.7, 14.1, 13.5 ppm.

HR-MS: $[M+H]^+$ calculated for $C_{26}H_{33}N_2O$, 389.2587, found, 389.2602; mass error : 3.85 ppm.

2-(4-fluoro-2-(oct-4-en-4-yl)phenyl)phthalazin-1(2H)-one (4g):



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 90/10)

Yield: 75 mg, 64%; pale-yellow oil.

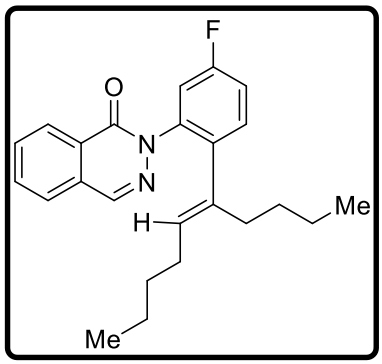
^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.38 (d, *J* = 7.8 Hz, 1H), 8.11 (s, 1H), 7.77 (td, *J* = 7.34 Hz, 1H), 7.71 (td, *J* = 7.48 Hz, 1H), 7.66 (d, *J* = 7.72 Hz, 1H), 7.27-7.23 (m, 1H), 7.00-6.95 (m, 2H), 5.34 (t, *J* = 7.42 Hz, 1H), 2.04 (t, *J* = 7.84 Hz, 2H), 1.84 (q, *J* = 7.29 Hz, 2H), 1.30-1.21 (m, 2H), 1.04-0.95 (m, 2H), 0.74 (t, *J* = 7.32 Hz, 3H), 0.57 (t, *J* = 7.36 Hz, 3H) ppm.

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ: 163.4 (d, *J* = 246.45 Hz), 159.5, 145.0 (d, *J* = 8.29 Hz), 137.5, 136.4, 135.7 (d, *J* = 2.96 Hz), 133.3, 132.1, 131.8, 129.8, 129.7, 128.4, 127.1, 126.0, 116.8 (d, *J* = 22.3 Hz), 114.2 (d, *J* = 22.65 Hz), 32.8, 30.1, 22.4, 21.6, 14.1, 13.5 ppm.

^{19}F NMR (376 MHz, $CDCl_3$) δ: -113.3 ppm

HR-MS: $[M+H]^+$ calculated for $C_{22}H_{24}FN_2O$, 351.1867, found, 351.1857; mass error : 2.84 ppm.

2-(2-(dec-5-en-5-yl)-5-fluorophenyl)phthalazin-1(2H)-one (4h):



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 90/10)

Yield: 76 mg, 60%; pale-yellow oil.

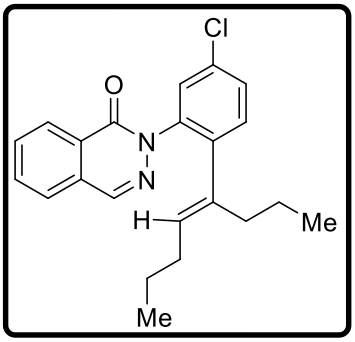
^{1}H NMR (400 MHz, CDCl3) δ: 8.39 (d, *J* = 7.76 Hz, 1H), 8.12 (s, 1H), 7.77 (td, *J* = 7.38 Hz, 1H), 7.72 (td, *J* = 7.56 Hz, 1H), 7.67 (d, *J* = 8.2 Hz, 1H), 7.23-7.19 (m, 1H), 7.06-7.01 (m, 2H), 5.27 (t, *J* = 7.44 Hz, 1H), 2.05 (t, *J* = 7.56 Hz, 2H), 1.85 (q, *J* = 7.05 Hz, 2H), 1.21-1.10 (m, 4H), 0.96-0.86 (m, 4H), 0.74 (t, *J* = 7.08 Hz, 3H), 0.53 (t, *J* = 6.96 Hz, 3H) ppm.

$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ: 161.3 (d, *J* = 245.42 Hz), 158.2, 139.5 (d, *J* = 9.54 Hz), 137.9 (d, *J* = 3.62 Hz), 136.5, 135.3, 132.4, 130.8, 130.7, 130.2 (d, *J* = 8.49 Hz), 128.7, 127.3, 126.1, 125.0, 114.7 (d, *J* = 20.51 Hz), 114.5 (d, *J* = 22.79 Hz), 30.5, 29.7, 28.6, 26.7, 21.7, 21.0, 12.8, 12.7 ppm.

^{19}F NMR (376 MHz, $CDCl_3$) δ: -115.1 ppm

HR-MS: $[M+H]^+$ calculated for $C_{24}H_{28}FN_2O$, 379.2180, found, 379.2180; mass error : 0.00 ppm.

2-(5-chloro-2-(oct-4-en-4-yl)phenyl)phthalazin-1(2H)-one (4i):



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 89/11)

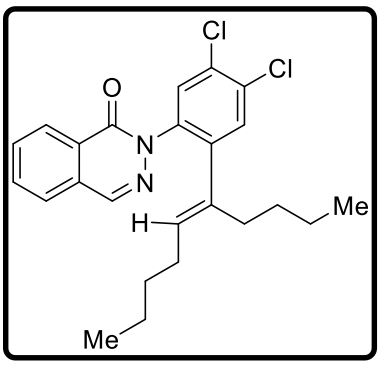
Yield: 64 mg, 52%; pale-yellow oil.

^{1}H NMR (400 MHz, CDCl3) δ: 8.38 (d, *J* = 7.8 Hz, 1H), 8.12 (s, 1H), 7.77 (td, *J* = 7.42 Hz, 1H), 7.72 (td, *J* = 7.58 Hz, 1H), 7.66 (d, *J* = 7.88 Hz, 1H), 7.30-7.27 (m, 2H), 7.20-7.18 (m, 1H), 5.32 (t, *J* = 7.44 Hz, 1H), 2.02 (t, *J* = 7.84 Hz, 2H), 1.84 (q, *J* = 7.30 Hz, 2H), 1.28-1.18 (m, 2H), 1.04-0.95 (m, 2H), 0.72 (t, *J* = 7.32 Hz, 3H), 0.58 (t, *J* = 7.36 Hz, 3H) ppm.

^{13}C{1H} NMR (100 MHz, CDCl3) δ: 159.2, 141.3, 140.4, 137.6, 136.3, 133.5, 132.3, 132.0, 131.9, 131.1, 129.7, 128.8, 128.4, 128.3, 127.1, 126.1, 32.9, 30.1, 22.5, 21.6, 14.1, 13.5 ppm.

HR-MS: $[M+H]^+$ calculated for $C_{22}H_{24}ClN_2O$, 367.1572, found, 367.1572; mass error : 0.00 ppm.

2-(4,5-dichloro-2-(dec-5-en-5-yl)phenyl)phthalazin-1(2H)-one (4j):



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 90/10)

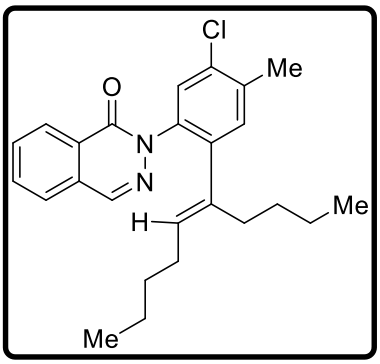
Yield: 66 mg, 46%; pale-yellow oil.

^{1}H NMR (400 MHz, CDCl$_3$) δ: 8.34 (d, *J* = 7.68 Hz, 1H), 8.09 (s, 1H), 7.73 (t, *J* = 7.16 Hz, 1H), 7.68 (t, *J* = 7.56 Hz, 1H), 7.63 (d, *J* = 7.6 Hz, 1H), 7.40-7.37 (m, 1H), 7.31 (s, 1H), 5.28 (t, *J* = 7.48 Hz, 1H), 2.02 (t, *J* = 7.58 Hz, 2H), 1.83 (q, *J* = 6.97 Hz, 2H), 1.19-1.10 (m, 4H), 0.94-0.89 (m, 4H), 0.72 (t, *J* = 7.02 Hz, 3H), 0.51 (t, *J* = 6.78 Hz, 3H) ppm.

^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) δ: 159.3, 142.9, 138.9, 137.9, 135.5, 133.6, 132.8, 132.5, 132.0, 131.3, 130.5, 130.2, 129.6, 128.2, 127.0, 126.2, 31.4, 30.6, 30.4, 27.7, 22.7, 22.0, 13.8, 13.7 ppm.

HR-MS: $[M+H]^+$ calculated for $C_{24}H_{27}Cl_2N_2O$, 429.1495, found, 429.1495; mass error : 0.00 ppm.

2-(5-chloro-2-(dec-5-en-5-yl)-4-methylphenyl)phthalazin-1(2H)-one (4k):



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 90/10)

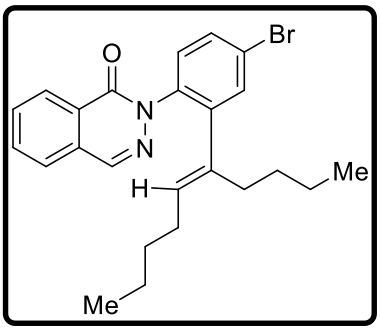
Yield: 76 mg, 56%; pale-yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.38 (d, *J* = 7.48 Hz, 1H), 8.11 (s, 1H), 7.76 (td, *J* = 7.38 Hz, 1H), 7.71 (td, *J* = 7.56 Hz, 1H), 7.66 (d, *J* = 7.8 Hz, 1H), 7.29 (s, 1H), 7.11 (s, 1H), 5.28 (t, *J* = 7.44 Hz, 1H), 2.34 (s, 3H), 2.06 (t, *J* = 7.58 Hz, 2H), 1.85 (q, *J* = 7.04 Hz, 2H), 1.24-1.09 (m, 4H), 0.97-0.90 (m, 4H), 0.75 (t, *J* = 7.08 Hz, 3H), 0.54 (t, *J* = 6.92 Hz, 3H) ppm.

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 158.3, 140.1, 137.1, 136.4, 135.4, 135.3, 132.3, 131.3, 130.9, 130.77, 130.74, 128.6, 127.5, 127.3, 126.0, 125.0, 30.5, 29.6, 28.6, 26.7, 21.7, 21.0, 18.8, 12.8, 12.7 ppm.

HR-MS: $[M+H]^+$ calculated for $C_{25}H_{30}ClN_2O$, 409.2041, found, 409.2046; mass error : 1.22 ppm.

2-(4-bromo-2-(dec-5-en-5-yl)phenyl)phthalazin-1(2H)-one (4l):



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 90/10)

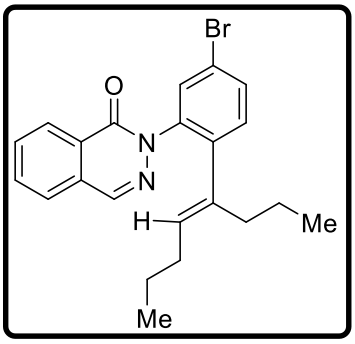
Yield: 101 mg, 69%; pale-yellow oil.

^{1}H NMR (400 MHz, CDCl3) δ: 8.38 (d, *J* = 7.76 Hz, 1H), 8.11 (s, 1H), 7.77 (td, *J* = 7.36 Hz, 1H), 7.71 (t, *J* = 7.52 Hz, 1H), 7.66 (d, *J* = 7.72 Hz, 1H), 7.42-7.40 (m, 2H), 7.18-7.14 (m, 1H), 5.30 (t, *J* = 7.46 Hz, 1H), 2.05 (t, *J* = 7.56 Hz, 2H), 1.86 (q, *J* = 7.00 Hz, 2H), 1.26-1.09 (m, 4H), 0.99-0.88 (m, 4H), 0.75 (t, *J* = 7.06 Hz, 3H), 0.54 (t, *J* = 6.86 Hz, 3H) ppm.

^{13}C{1H} NMR (100 MHz, CDCl3) δ: 159.3, 144.8, 138.7, 137.6, 136.2, 133.4, 132.9, 132.4, 131.8, 130.3, 129.77, 129.73, 128.3, 127.1, 126.1, 122.4, 31.5, 30.6, 30.5, 27.7, 22.7, 22.0, 13.87, 13.80 ppm.

HR-MS: $[M+H]^+$ calculated for $C_{24}H_{28}BrN_2O$, 439.1380, found, 439.1380; mass error : 0.00 ppm.

2-(5-bromo-2-(oct-4-en-4-yl)phenyl)phthalazin-1(2H)-one (4m):



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 90/10)

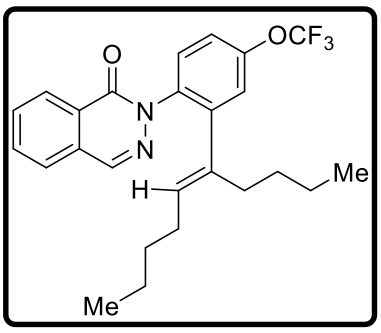
Yield: 75 mg, 55%; pale-yellow oil.

^{1}H NMR (400 MHz, CDCl3) δ: 8.36 (d, *J* = 7.72 Hz, 1H), 8.10 (s, 1H), 7.76 (td, *J* = 7.38 Hz, 1H), 7.70 (td, *J* = 7.5 Hz, 1H), 7.65 (d, *J* = 7.76 Hz, 1H), 7.43-7.40 (m, 2H), 7.13 (d, *J* = 8.36 Hz, 1H), 5.31 (t, *J* = 7.44 Hz, 1H), 2.01 (t, *J* = 7.82 Hz, 2H), 1.82 (q, *J* = 7.30 Hz, 2H), 1.26-1.17 (m, 2H), 1.03-0.94 (m, 2H), 0.71 (t, *J* = 7.32 Hz, 3H), 0.56 (t, *J* = 7.36 Hz, 3H) ppm.

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 159.2, 141.8, 140.7, 137.7, 136.3, 133.5, 132.0, 131.9, 131.7, 131.4, 131.2, 129.7, 128.3, 127.0, 126.1, 120.0, 32.8, 30.1, 22.5, 21.6, 14.1, 13.5 ppm.

HR-MS: $[M+H]^+$ calculated for $C_{22}H_{24}BrN_2O$, 411.1067, found, 411.1067; mass error : 0.00 ppm.

2-(2-(dec-5-en-5-yl)-4-(trifluoromethoxy)phenyl)phthalazin-1(2H)-one (4n):



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 88/12)

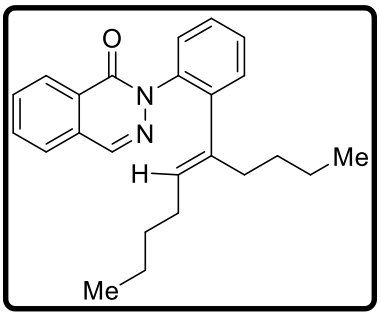
Yield: 101 mg, 68%; pale-yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.37 (d, *J* = 7.72 Hz, 1H), 8.12 (s, 1H), 7.76 (t, *J* = 7.42 Hz, 1H), 7.70 (t, *J* = 7.38 Hz, 1H), 7.66 (d, *J* = 7.52 Hz, 1H), 7.32 (d, *J* = 8.48 Hz, 1H), 7.13-7.10 (m, 2H), 5.31 (t, *J* = 7.44 Hz, 1H), 2.07 (t, *J* = 7.54 Hz, 2H), 1.86 (q, *J* = 6.96 Hz, 2H), 1.25-1.09 (m, 4H), 0.97-0.92 (m, 4H), 0.74 (t, *J* = 7.04 Hz, 3H), 0.52 (t, *J* = 6.82 Hz, 3H) ppm.

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 159.4, 148.8 (d, *J* = 1.4 Hz), 144.8, 138.1, 137.6, 136.2, 133.4, 132.4, 131.9, 129.7, 129.6, 128.3, 127.0, 126.1, 122.3, 121.7 (q, *J* = 255.99 Hz), 119.4, 31.4, 30.5, 30.4, 27.7, 22.6, 22.0, 13.78, 13.73 ppm.

^{19}F NMR (376 MHz, $CDCl_3$) δ: -57.7 ppm

HR-MS: $[M+H]^+$ calculated for $C_{25}H_{28}F_3N_2O_2$, 445.2097, found, 445.2097; mass error : 0.00 ppm.



2-(2-(dec-5-en-5-yl)phenyl)phthalazin-1(2H)-one (4o):

Purified by column chromatography on silica gel using (hexane/ethyl acetate = 90/10)

Yield: 100 mg, 83%; pale-yellow oil.

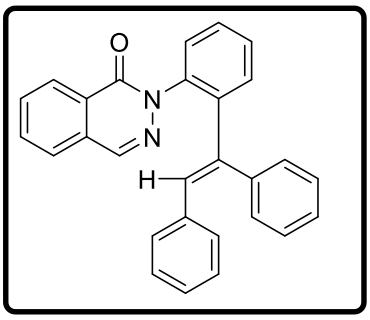
^{1}H NMR (400 MHz, CDCl3) δ: 8.39 (d, *J* = 7.72 Hz, 1H), 8.12 (s, 1H), 7.75 (t, *J* = 7.44 Hz, 1H), 7.70 (t, *J* = 6.94 Hz, 1H), 7.65 (d, *J* = 7.68 Hz, 1H), 7.33-7.25 (m, 4H), 5.29 (t, *J* = 7.42 Hz, 1H), 2.08 (t, *J* = 7.64 Hz, 2H), 1.86 (q, *J* = 7.02 Hz, 2H), 1.25-1.09 (m, 4H), 0.98-0.86 (m, 4H), 0.74 (t, *J* = 7.1 Hz, 3H), 0.52 (t, *J* = 6.9 Hz, 3H) ppm.

^{13}C{1H} NMR (100 MHz, CDCl3) δ: 159.4, 142.7, 139.7, 137.3, 137.1, 133.2, 131.7, 131.3, 130.0, 129.8, 128.6, 128.5, 128.1, 127.2, 127.0, 126.0, 31.6, 30.8, 30.7, 27.7, 22.8, 22.1, 13.9, 13.8 ppm.

HR-MS: $[M+H]^+$ calculated for $C_{24}H_{29}N_2O$, 361.2274, found, 361.2274; mass error : 0.00 ppm.

2-(2-(1,2-diphenylvinyl)phenyl)phthalazin-1(2H)-one (4p):

Purified by column chromatography on silica gel using (hexane/ethyl acetate = 88/12



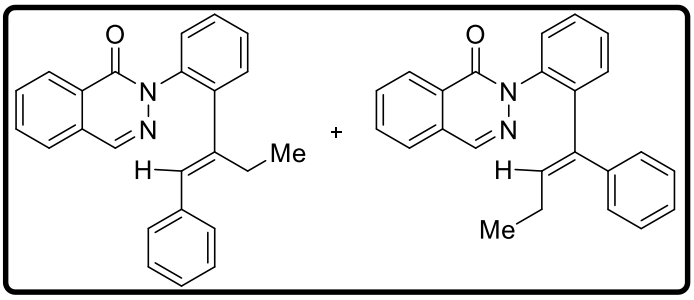
Yield: 51 mg, 38%; orange-coloured solid.

^{1}H NMR (400 MHz, CDCl$_3$) δ: 8.14 (d, *J* = 7.88 Hz, 1H), 7.90 (s, 1H), 7.63 (td, *J* = 7.46 Hz, 1H), 7.56 (td, *J* = 8.14 Hz, 1H), 7.50-7.47 (m, 1H), 7.46 (d, *J* = 7.52 Hz, 1H), 7.42-7.38 (m, 2H), 7.35-7.32 (m, 1H), 6.99-6.96 (m, 3H), 6.92-6.90 (m, 2H), 6.88-6.86 (m, 2H), 6.74-6.71 (m, 4H) ppm.

^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) δ: 158.6, 141.7, 140.2, 140.0, 138.9, 137.6, 137.2, 132.9, 131.4, 131.3, 131.0, 129.59, 129.51, 129.4, 128.8, 128.5, 128.1, 127.7, 127.6, 126.9, 126.8, 126.7, 125.5 ppm.

HR-MS: $[M+H]^+$ calculated for $C_{28}H_{21}N_2O$, 401.1648, found, 401.1654; mass error : 1.49 ppm.

2-(2-(1-phenylbut-1-en-2-yl)phenyl)phthalazin-1(2H)-one (4q):



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 88/12

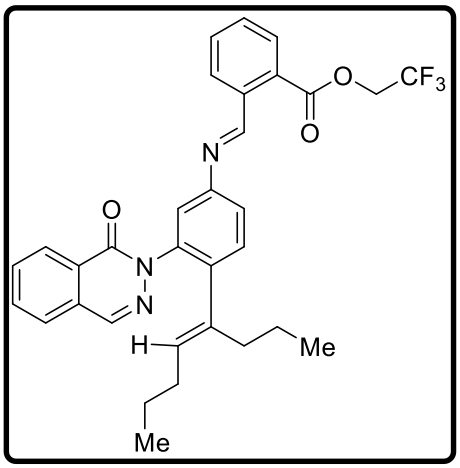
Yield: 69 mg, 59%; pale-yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.40 (d, *J* = 7.72 Hz, 1H), 8.22 (d, *J* = 7.84 Hz, 1H), 8.13 (s, 1H), 7.94 (s, 1H), 7.76-7.67 (m, 3H), 7.64-7.58 (m, 2H), 7.53 (d, *J* = 7.76 Hz, 1H), 7.38-7.37 (m, 4H), 7.33-7.28 (m, 4H), 7.14-7.11 (m, 2H), 7.05 (t, *J* = 7.22 Hz, 1H), 6.97 (d, *J* = 7.64 Hz, 2H), 6.93-6.82 (m, 5H), 6.38 (s, 1H), 5.74 (t, *J* = 7.4 Hz, 1H), 2.34 (q, *J* = 7.46 Hz, 2H), 2.04-1.96 (m, 2H), 0.91 (t, *J* = 7.5 Hz, 3H), 0.68 (t, *J* = 7.44 Hz, 3H) ppm.

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 159.5, 158.8, 141.7, 141.65, 141.63, 139.86, 139.83, 139.2, 138.0, 137.8, 137.49, 137.45, 135.2, 133.3, 133.0, 131.8, 131.3, 131.2, 130.1, 129.9, 129.7, 129.6, 129.1, 128.7, 128.6, 128.5, 128.4, 128.2, 128.0, 127.9, 127.8, 127.3, 127.1, 126.9, 126.5, 126.3, 126.1, 125.6, 24.7, 22.7, 14.1, 13.1 ppm.

HR-MS: $[M+H]^+$ calculated for $C_{24}H_{21}N_2O$, 353.1638, found, 353.1639; mass error : 0.28 ppm.

2,2,2-trifluoroethyl-2-(-((4-(-oct-4-en-4-yl)-3-(1-oxophthalazin-2(1H)-yl)phenyl)imino)methyl)benzoate (5):



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 70/30

Yield: 45 mg, 48%; orange coloured solid

^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.38 (d, *J* = 7.84 Hz, 1H), 8.20-8.16 (m, 3H), 7.85-7.79 (m, 2H), 7.75 (t, *J* = 7.52 Hz, 1H), 7.70-7.66 (m, 2H), 7.59-7.55 (m, 2H), 7.43 (d, *J* = 8.48 Hz, 1H), 6.38 (s, 1H), 5.41 (t, *J* = 7.42 Hz, 1H), 4.13-4.05 (m, 2H), 2.08 (t, *J* = 7.82 Hz, 2H), 1.88 (q, *J* = 7.26 Hz, 2H), 1.29-1.18 (m, 2H), 1.07-0.98 (m, 2H), 0.74 (t, *J* = 7.28 Hz, 3H), 0.60 (t, *J* = 7.32 Hz, 3H) ppm.

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ: 167.7, 159.3, 149.8, 146.6, 143.6, 140.3, 138.2, 136.2, 134.8, 133.8, 133.6, 132.2, 131.4, 130.9, 129.7, 128.1, 127.1, 126.8, 126.3, 125.7, 124.6 (q, *J* = 276.25 Hz), 124.2, 123.6, 123.4, 101.2, 66.0 (q, *J* = 35.24 Hz), 32.6, 30.2, 22.3, 21.7, 14.0, 13.5 ppm.

^{19}F NMR (376 MHz, $CDCl_3$) δ: -74.15 ppm

HR-MS: $[M+H]^+$ calculated for $C_{32}H_{31}F_3N_3O_3$, 562.2312, found, 562.2316; mass error : 0.71 ppm.

11. References

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2. Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **93**, 5648-5652 (1993).

3. Gaussian 16, Revision A.03, Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Scalmani, G., Barone, V., Petersson, G. A., Nakatsuji, H., Li, X., Caricato, M., Marenich, A. V., Bloino, J., Janesko, B. G., Gomperts, R., Mennucci, B., Hratchian, H. P., Ortiz, J. V., Izmaylov, A. F., Williams, J. L., Ding, F., Lipparini, F., Egidi, F., Goings, J., Peng, B., Petrone, A., Henderson, T., Ranasinghe, D., Zakrzewski, V. G., Gao, J., Rega, N., Zheng, G., Liang, W., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Throssell, K., Montgomery Jr. J. A., Peralta, J. E., Ogliaro, F., Bearpark, M. J., Heyd, J. J., Brothers, E. N., Kudin, K. N., Staroverov, V. N., Keith, T. A., Kobayashi, R., Normand, J., Ragavachari, K., Rendell, A. P., Burant, J. C., Iyengar, S. S., Tomasi, J., Cossi, M., Millam, J. M., Klene, M., Adamo, C., Cammi, R., Ochterski, J. W., Martin, R. L., Morokuma, K., Farkas, O., Foresman, J. B. & Fox, D. J. Gaussian, Inc., Wallingford CT (2016).

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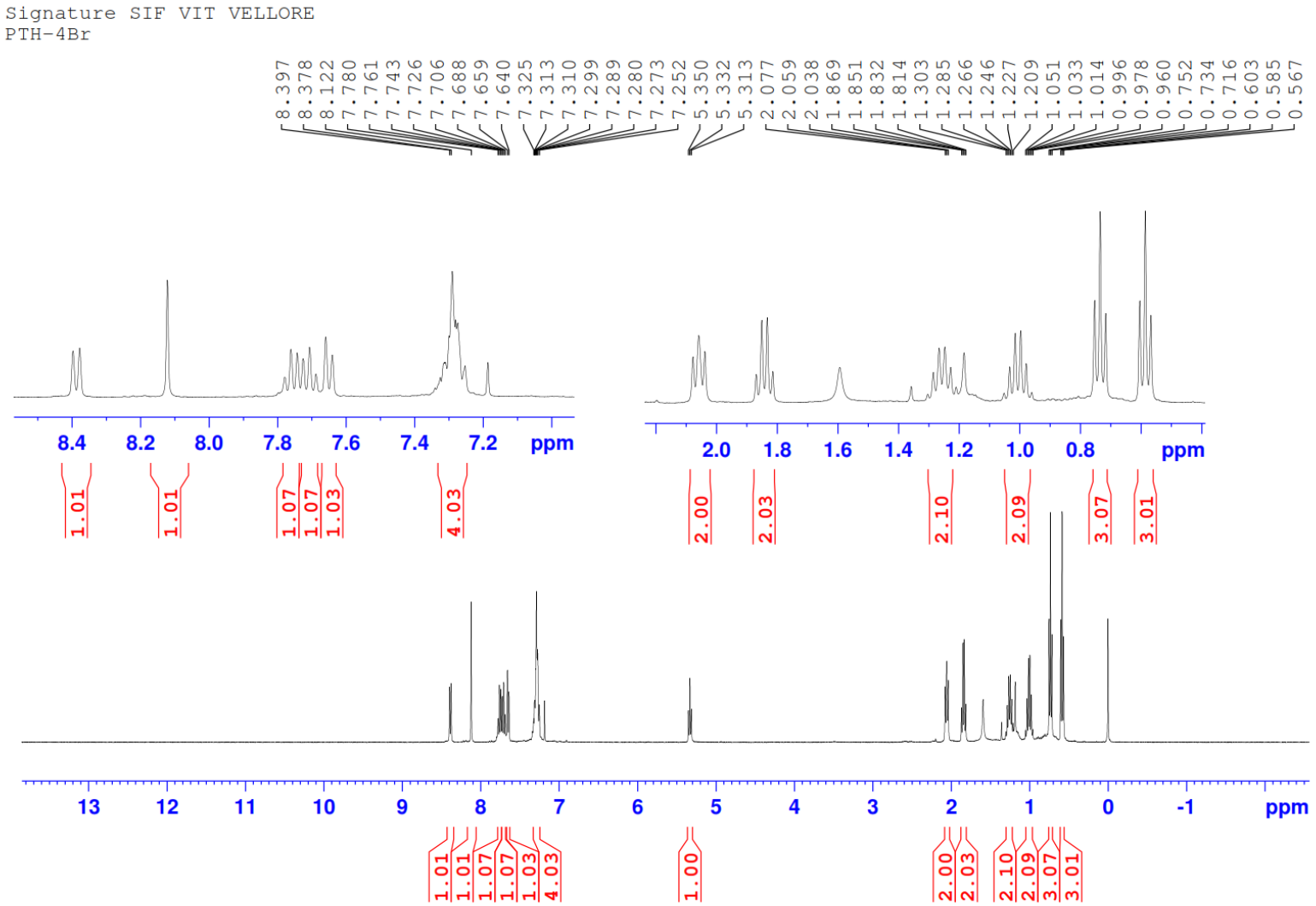
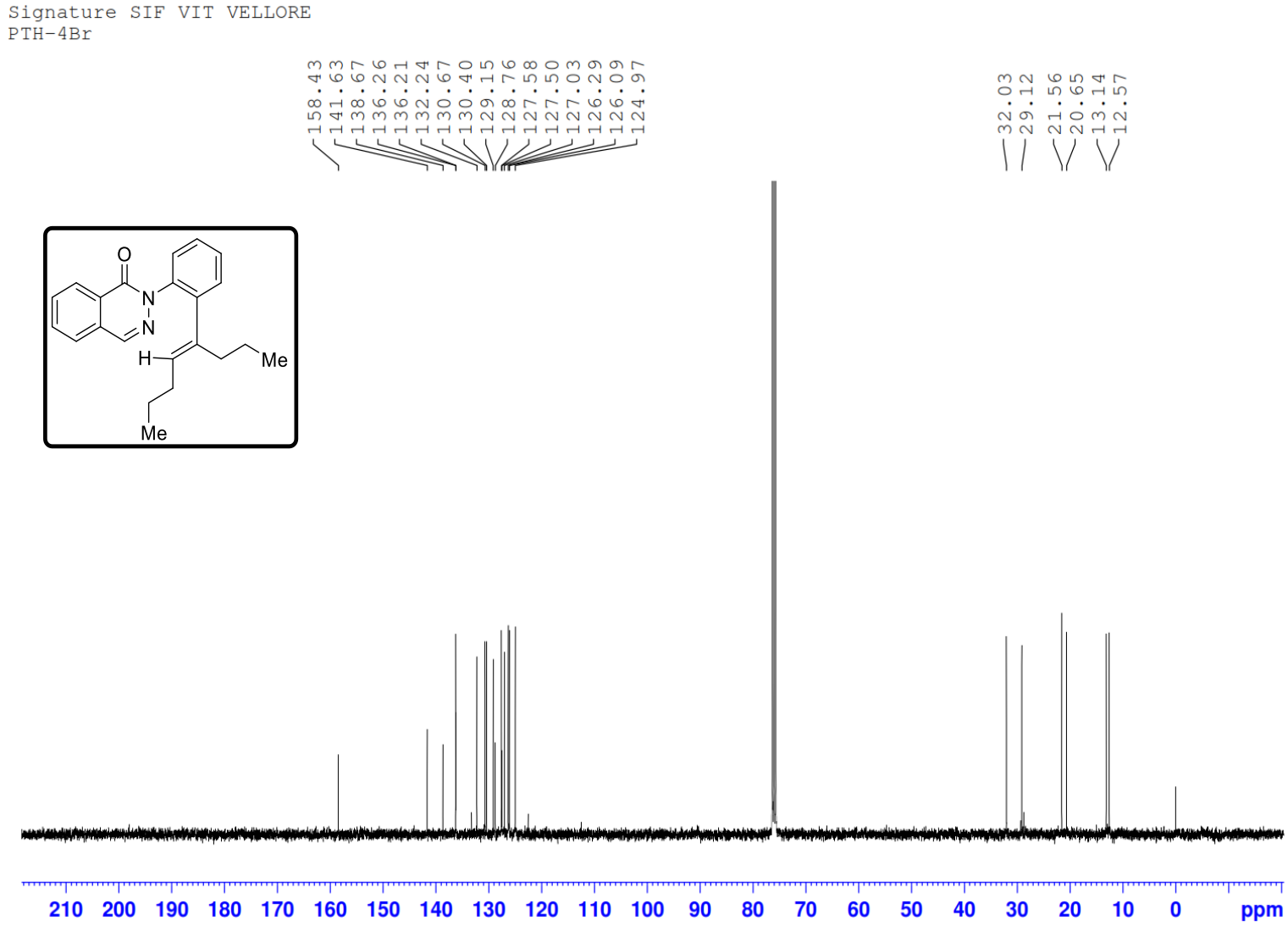
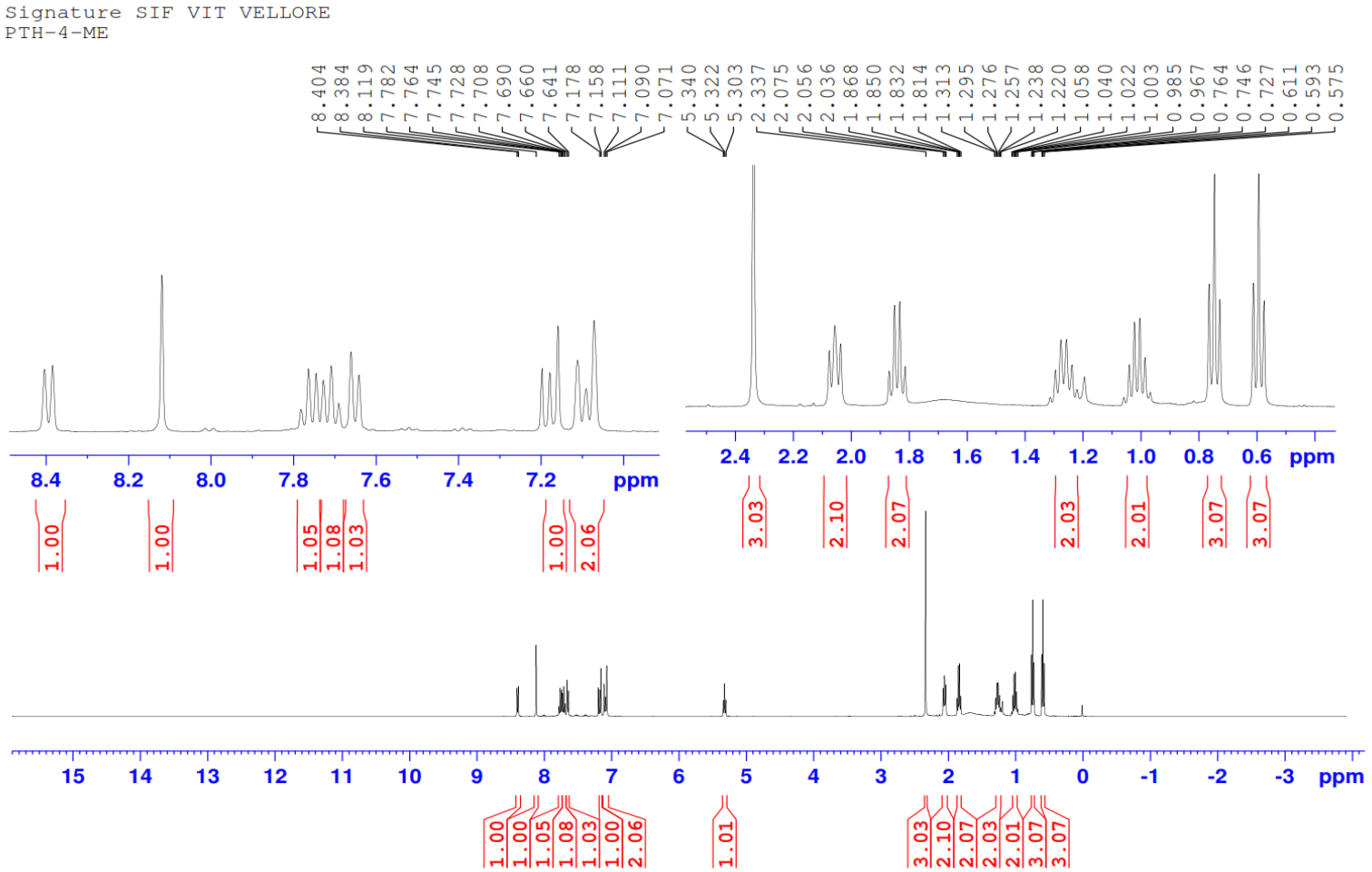
^{1}H NMR spectra of **4a**



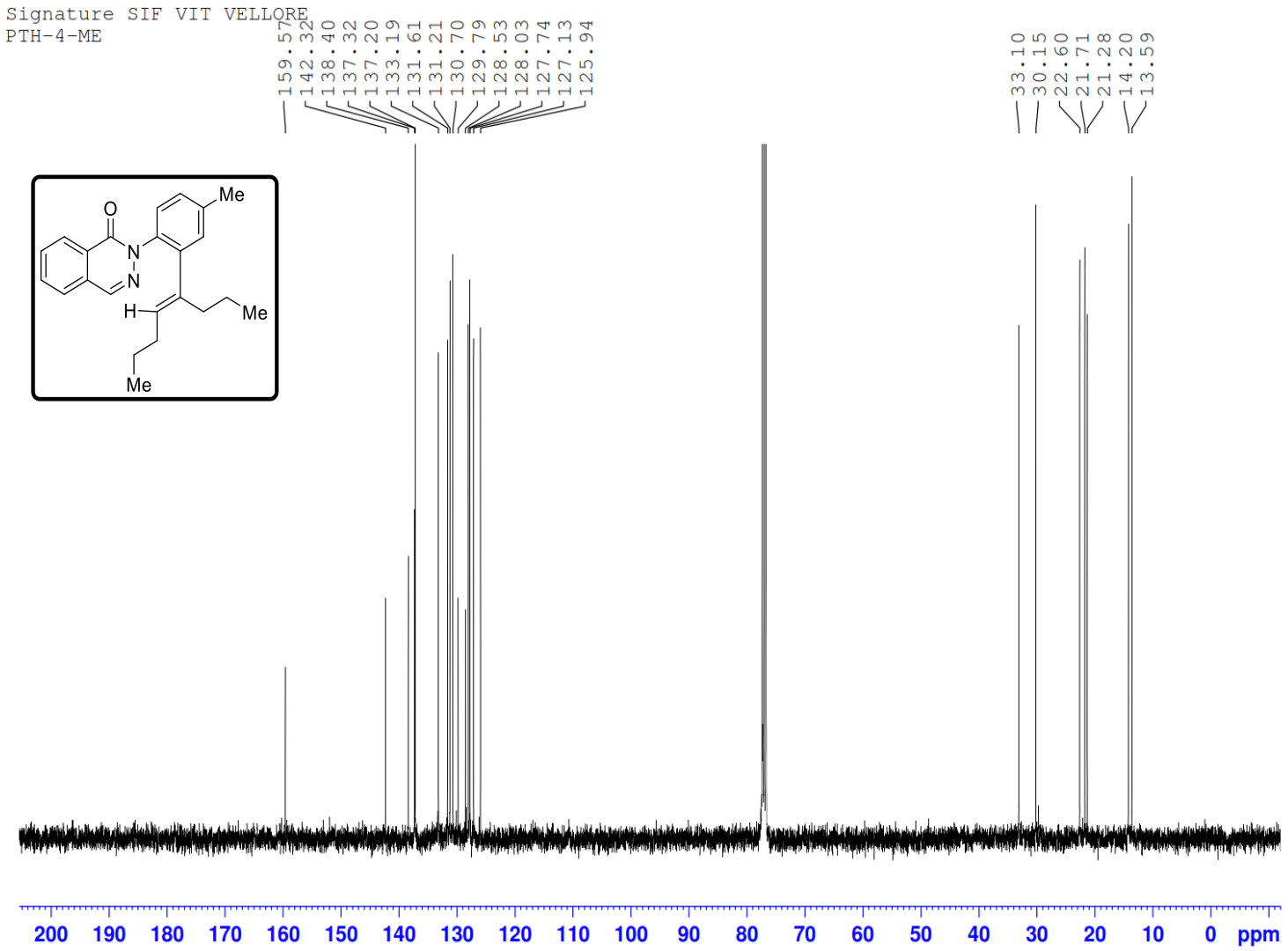
$^{13}C\{^{1}H\}$ NMR spectra of **4a**



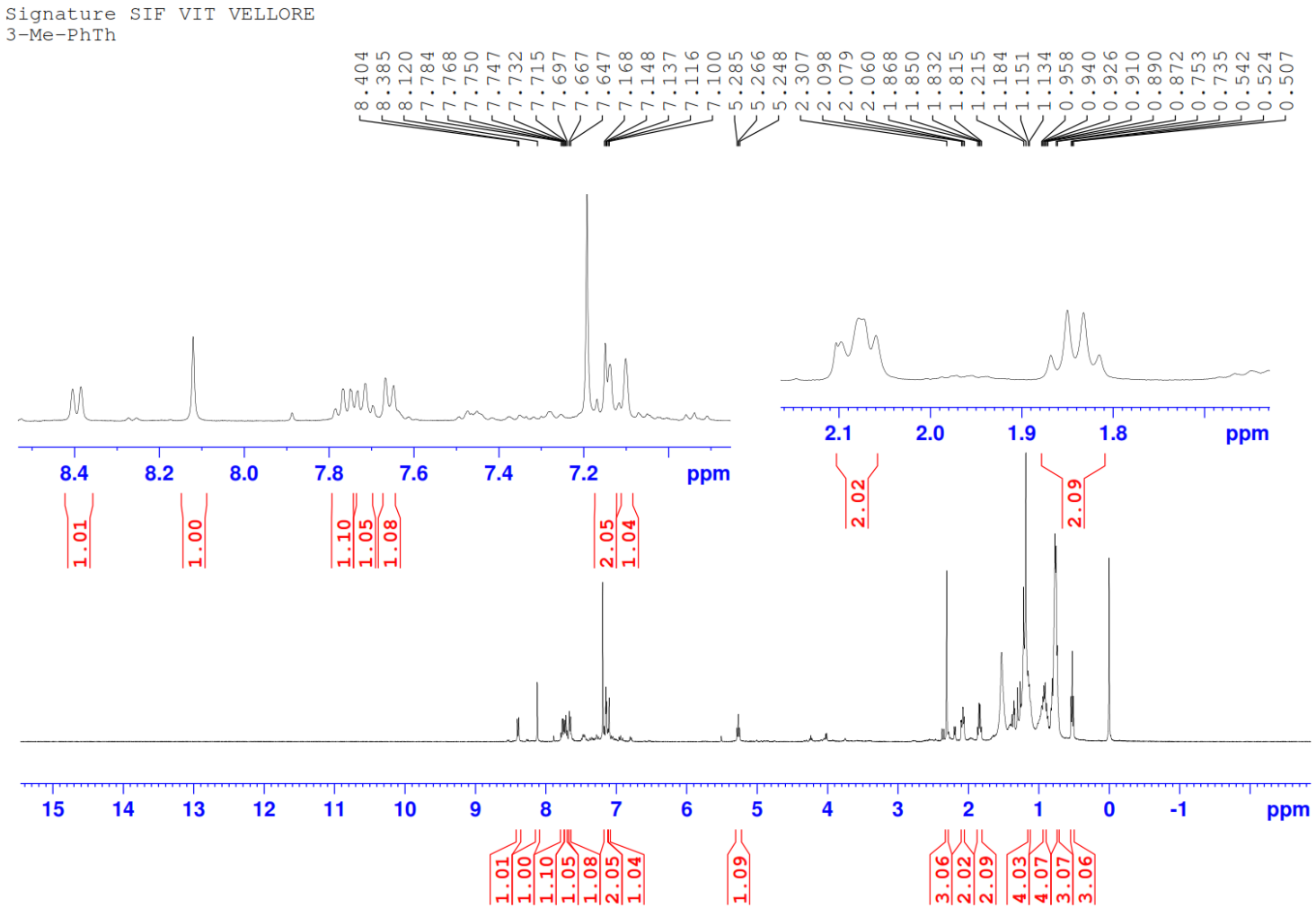
^{1}H NMR spectra of **4b**



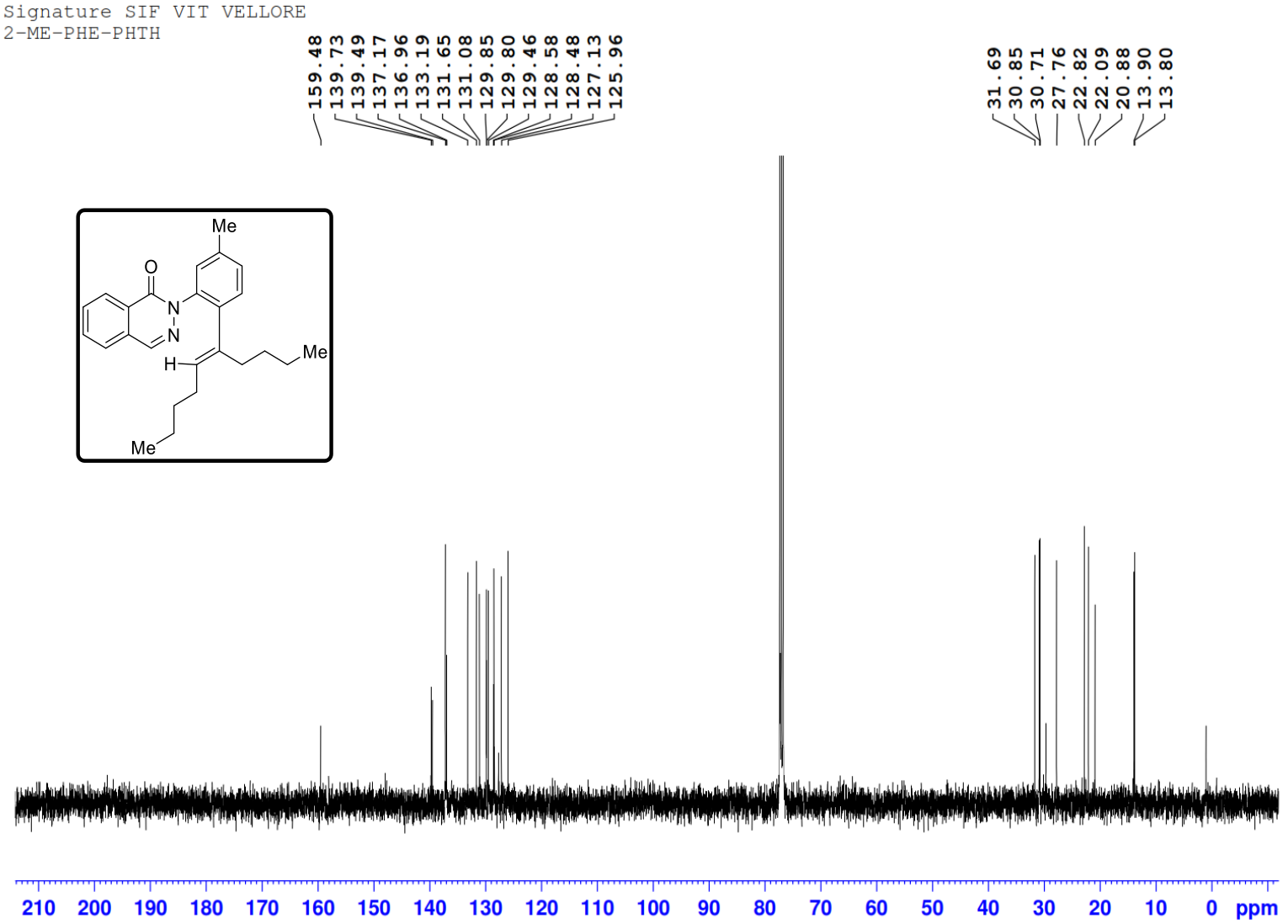
$^{13}C\{^{1}H\}$ NMR spectra of **4b**



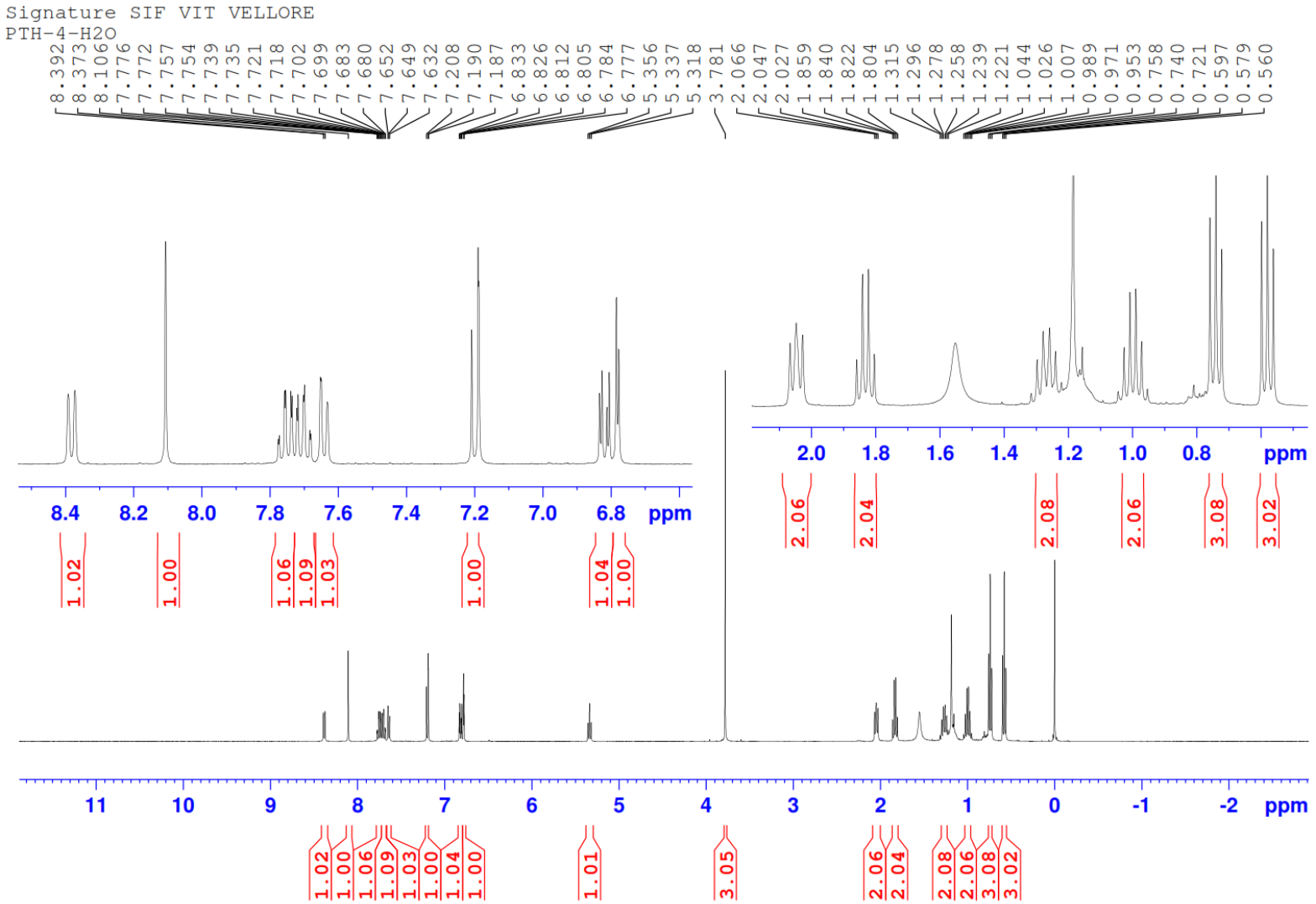
^{1}H NMR spectra of **4c**



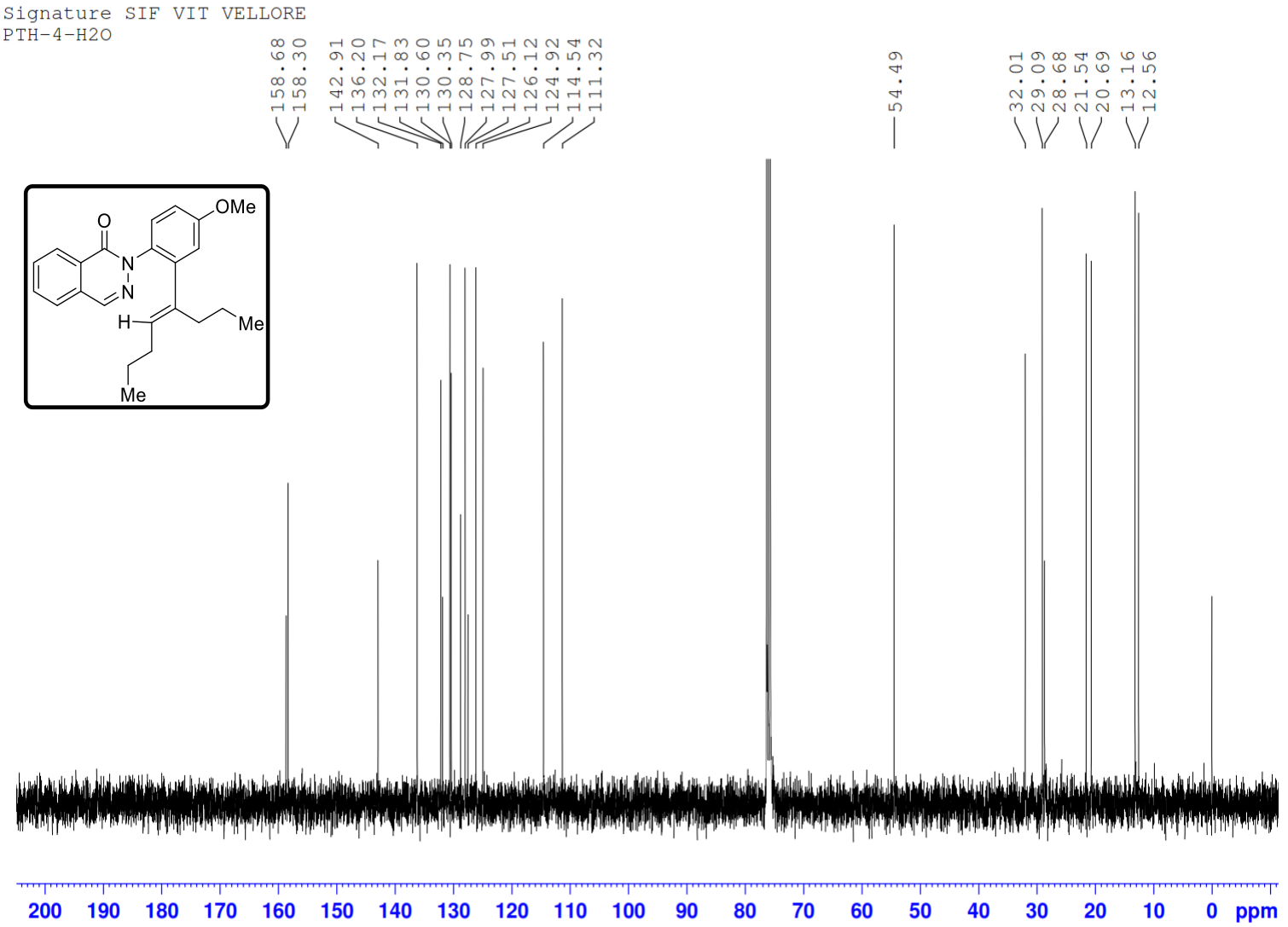
$^{13}C\{^{1}H\}$ NMR spectra of **4c**



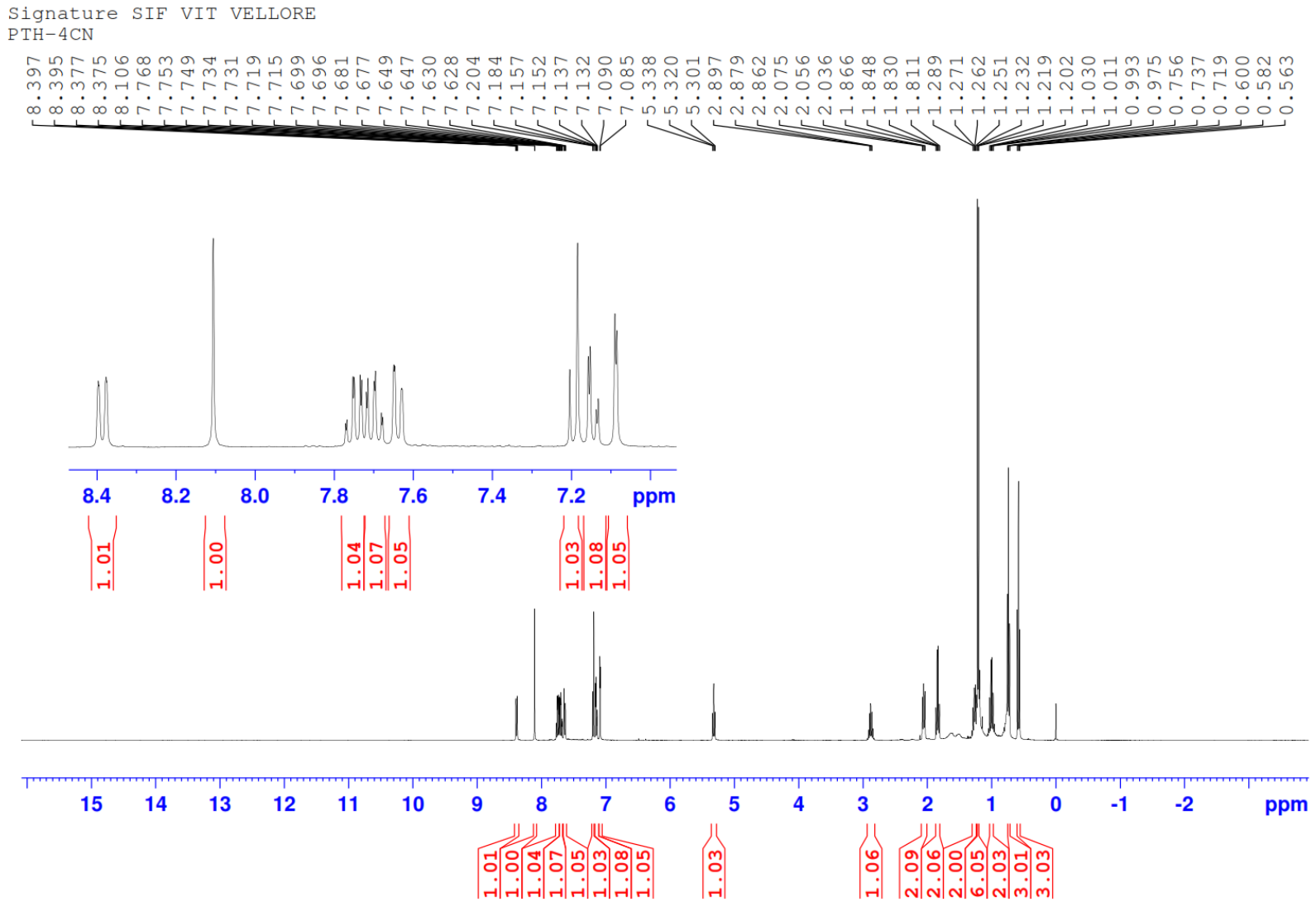
^{1}H NMR spectra of **4d**



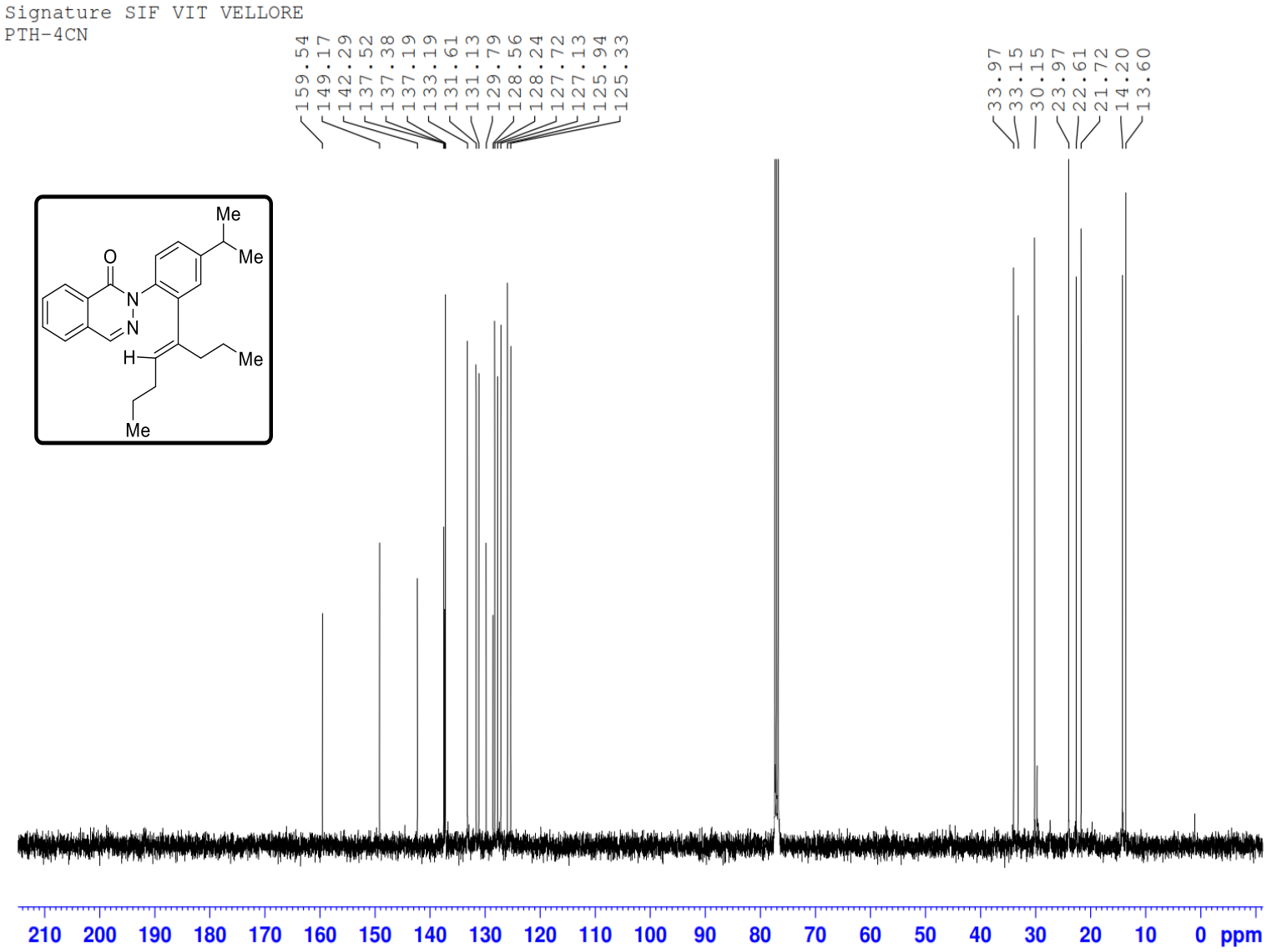
$^{13}C\{^{1}H\}$ NMR spectra of **4d**



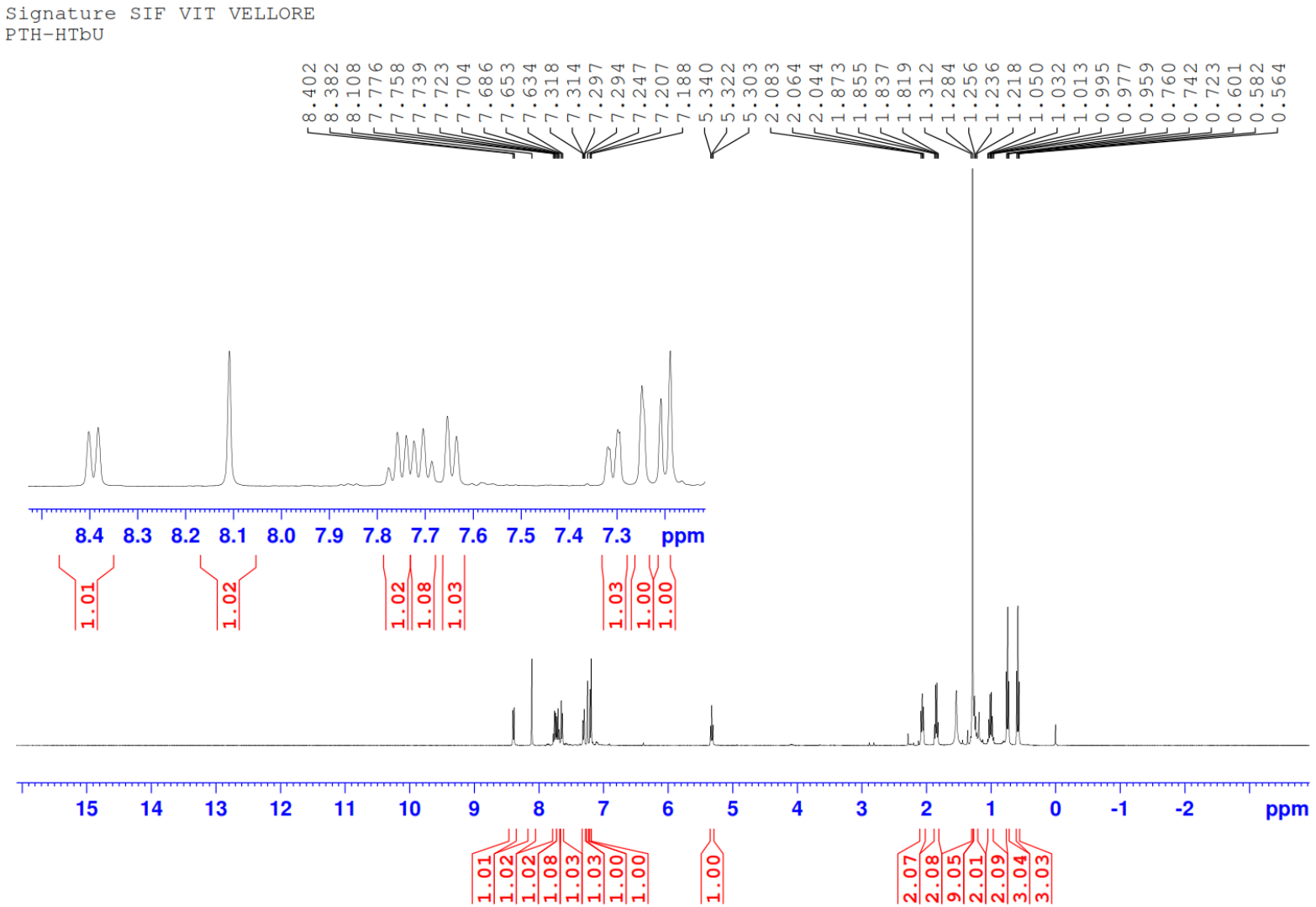
[1]H NMR spectra of **4e**



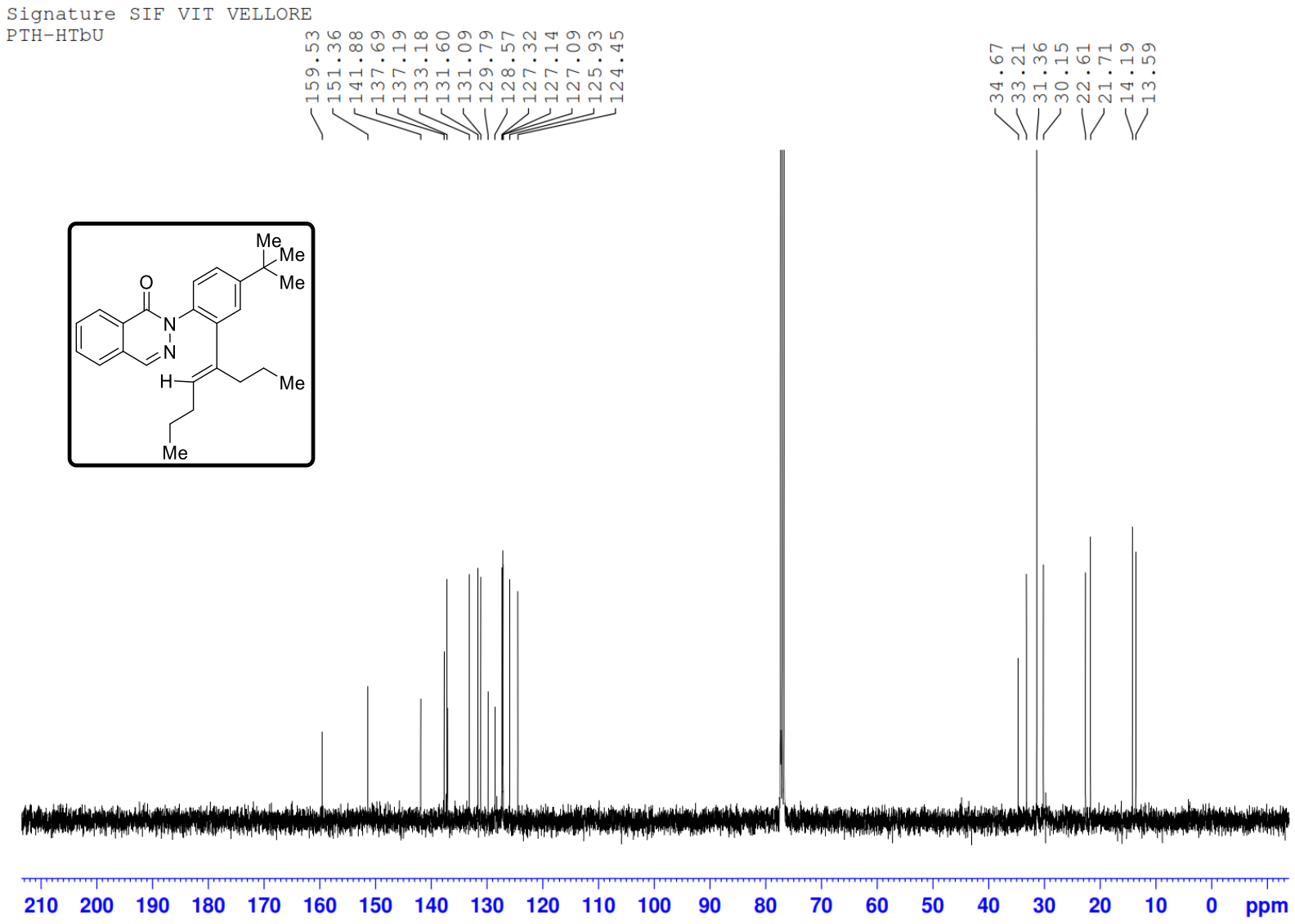
$^{13}C\{^{1}H\}$ NMR spectra of **4e**



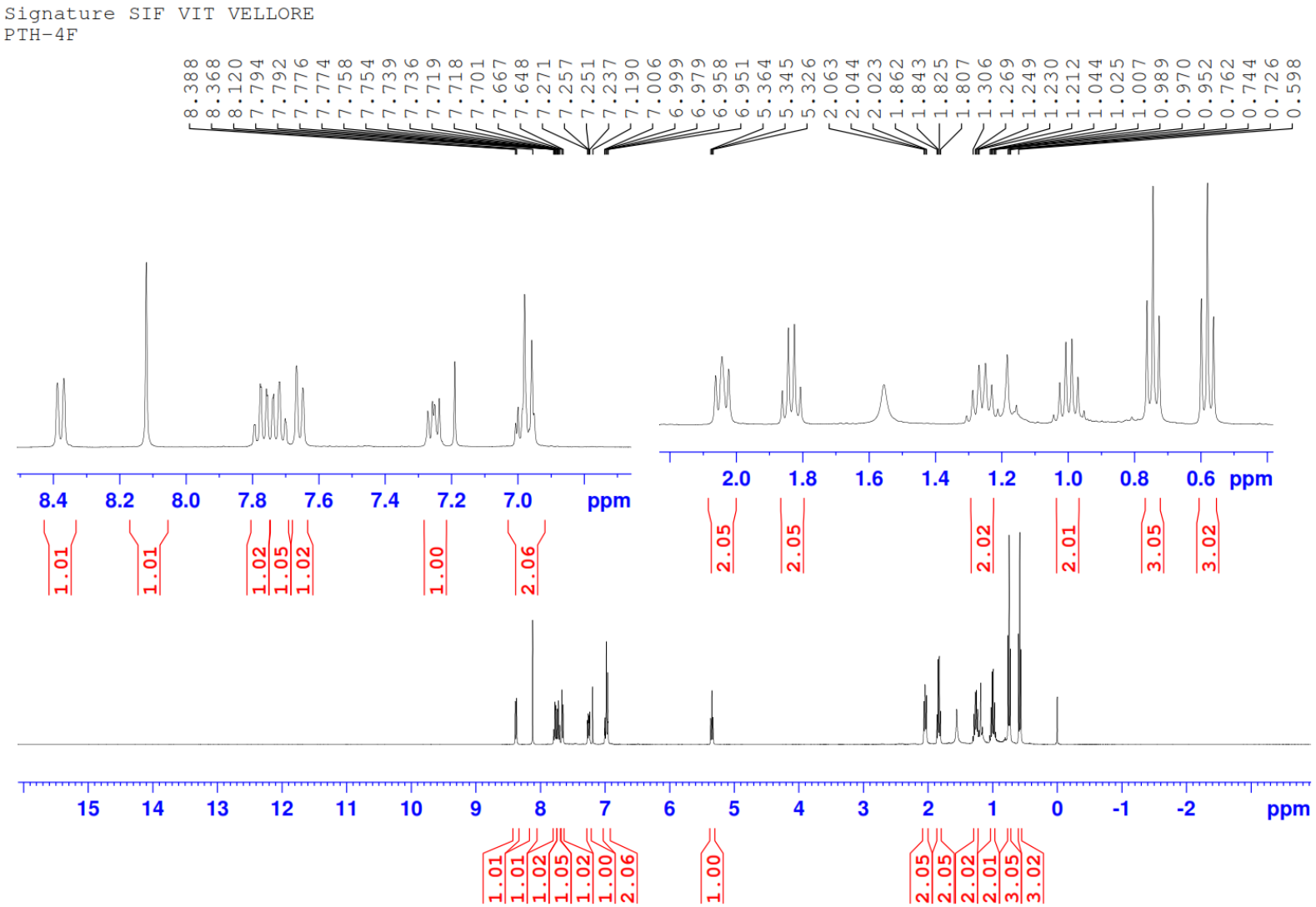
^{1}H NMR spectra of **4f**



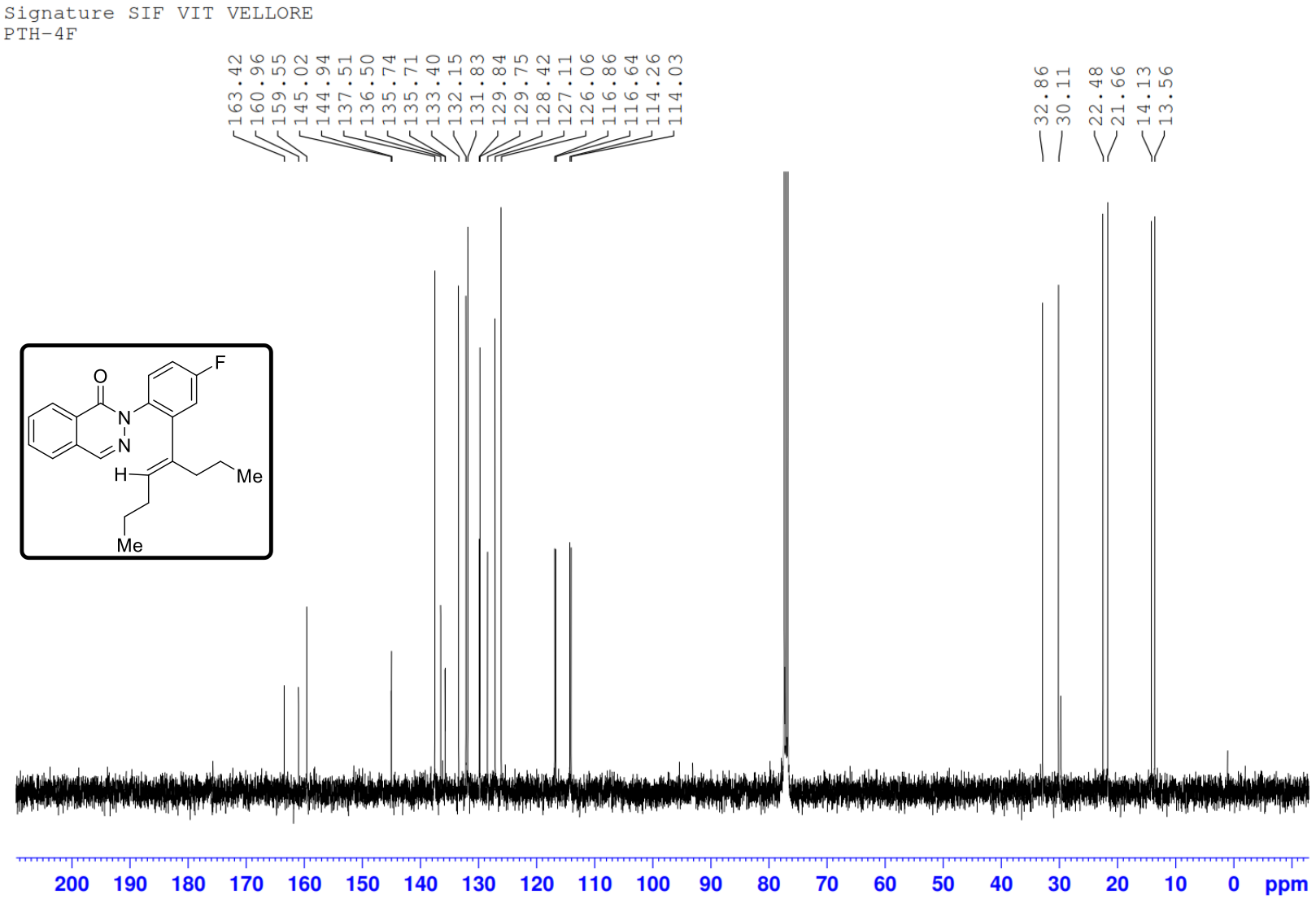
$^{13}C\{^{1}H\}$ NMR spectra of **4f**



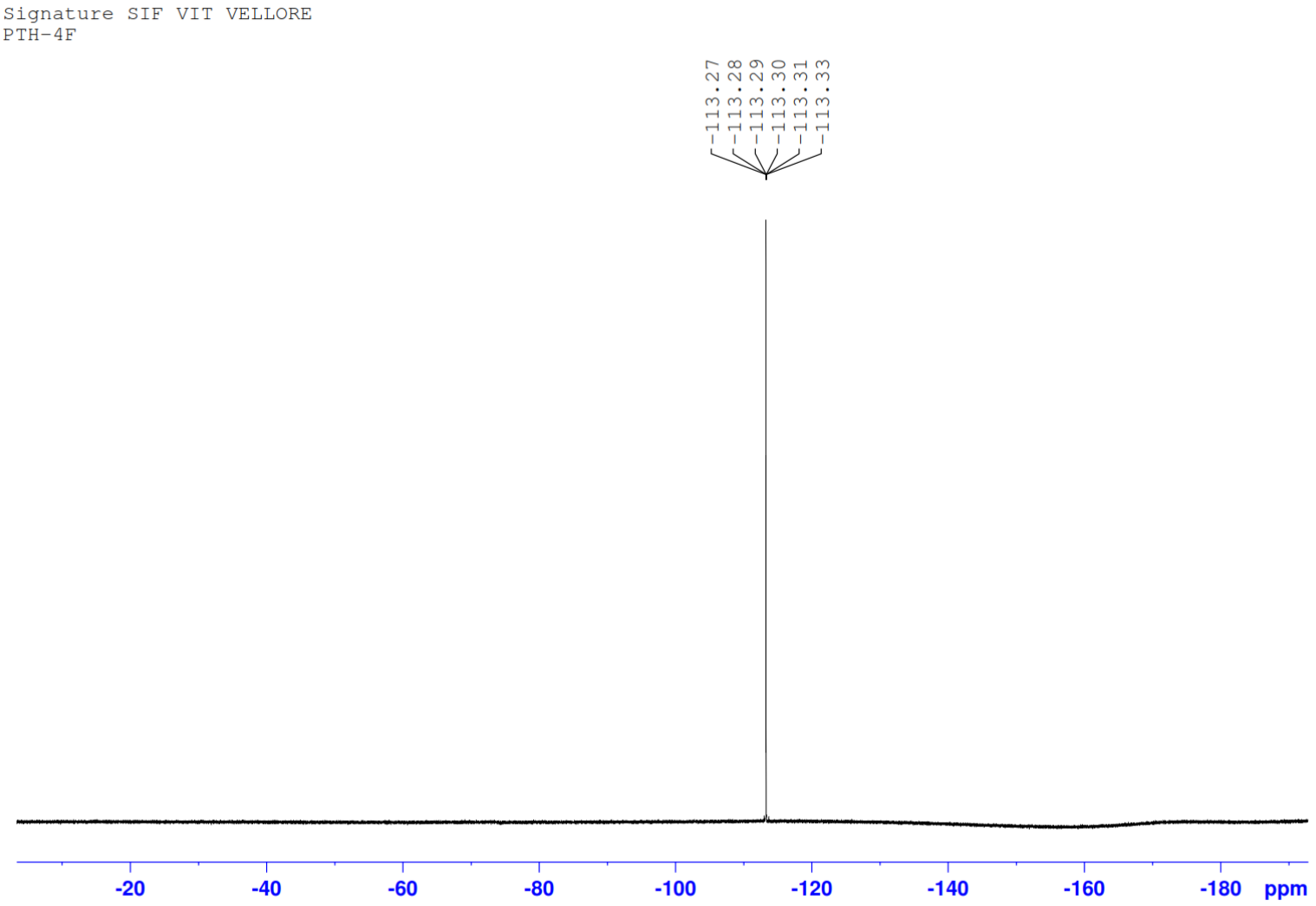
^{1}H NMR spectra of **4g**



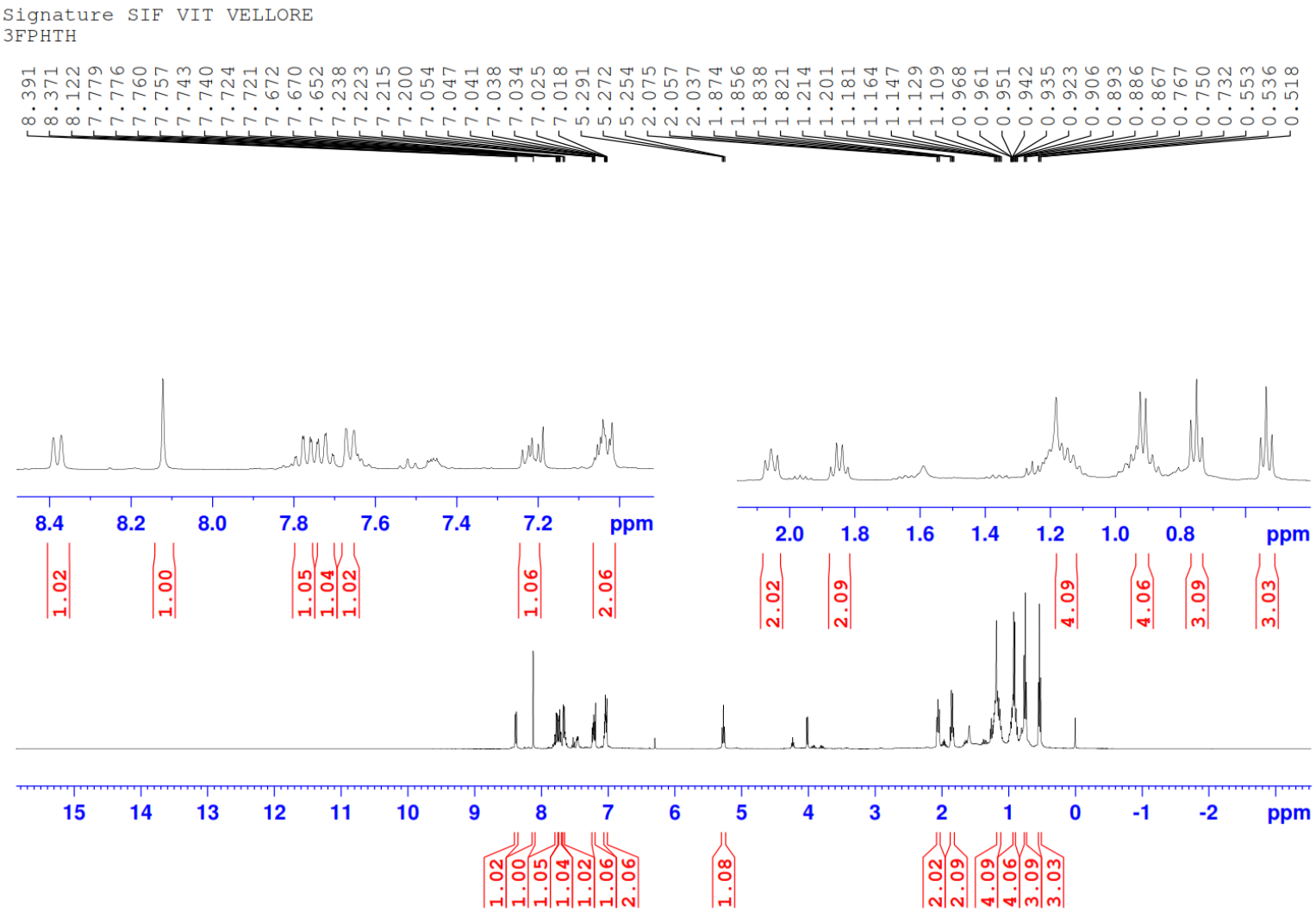
$^{13}C\{^{1}H\}$ NMR spectra of **4g**



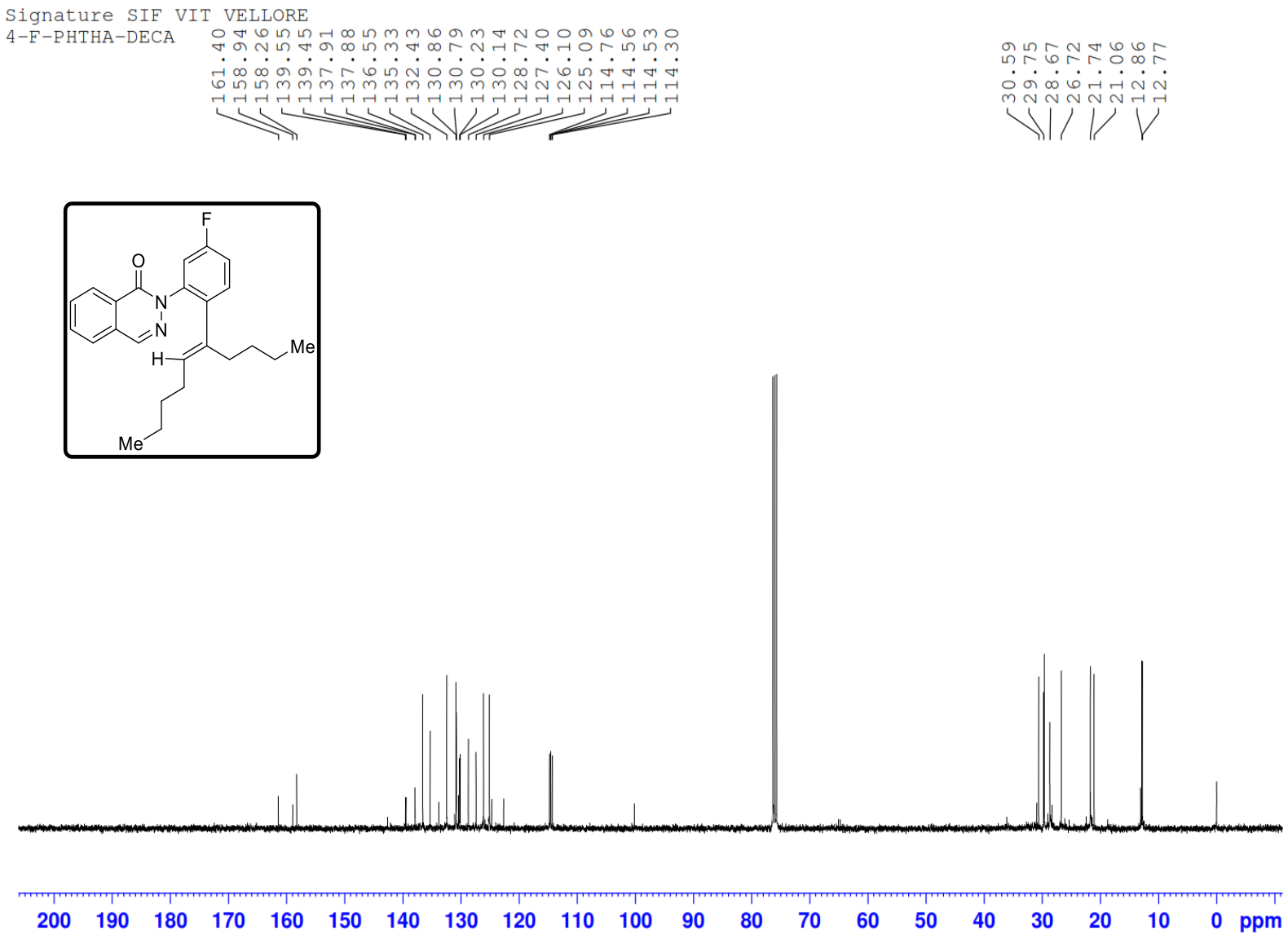
^{19}F NMR spectra of **4g**



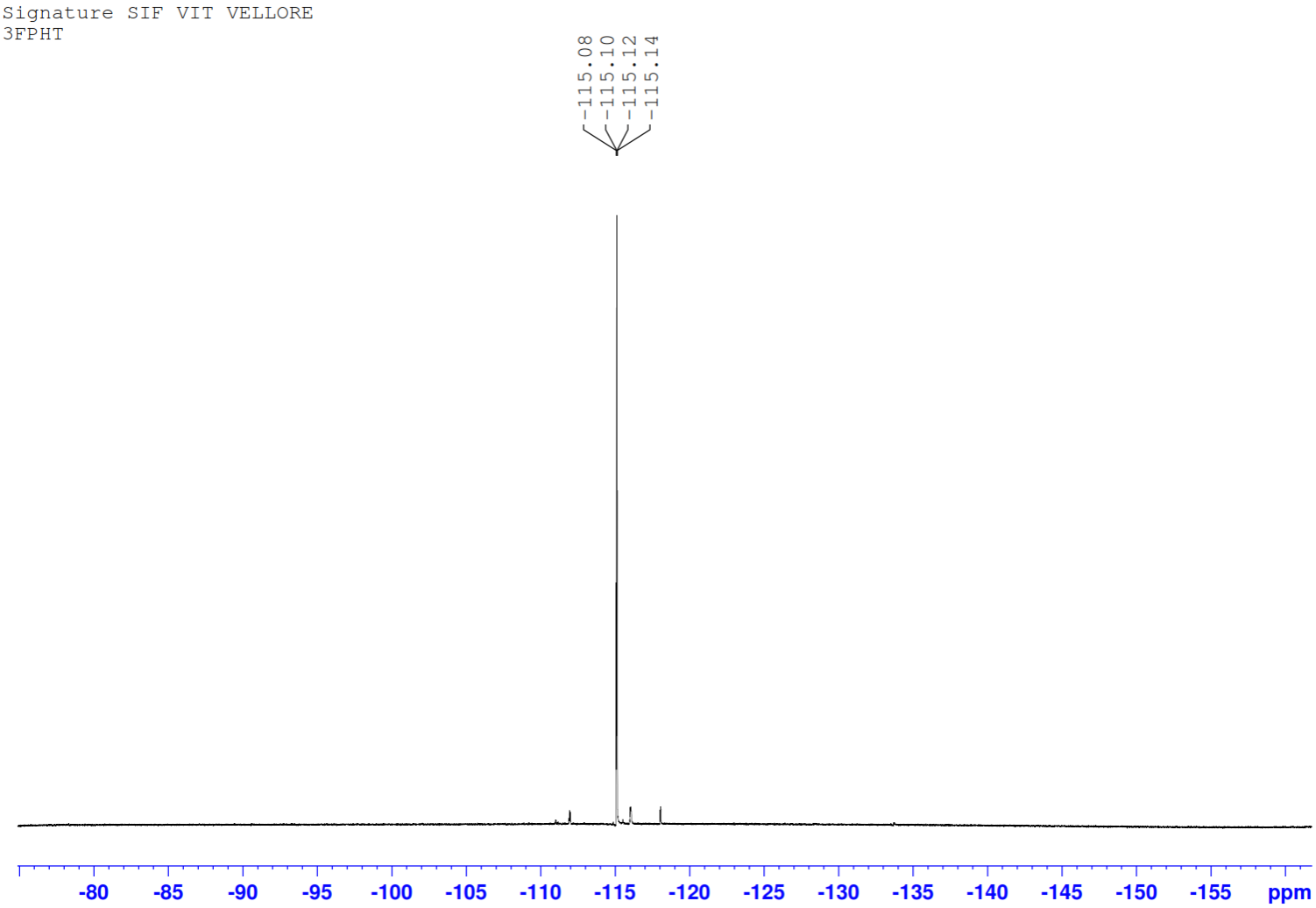
^{1}H NMR spectra of **4h**



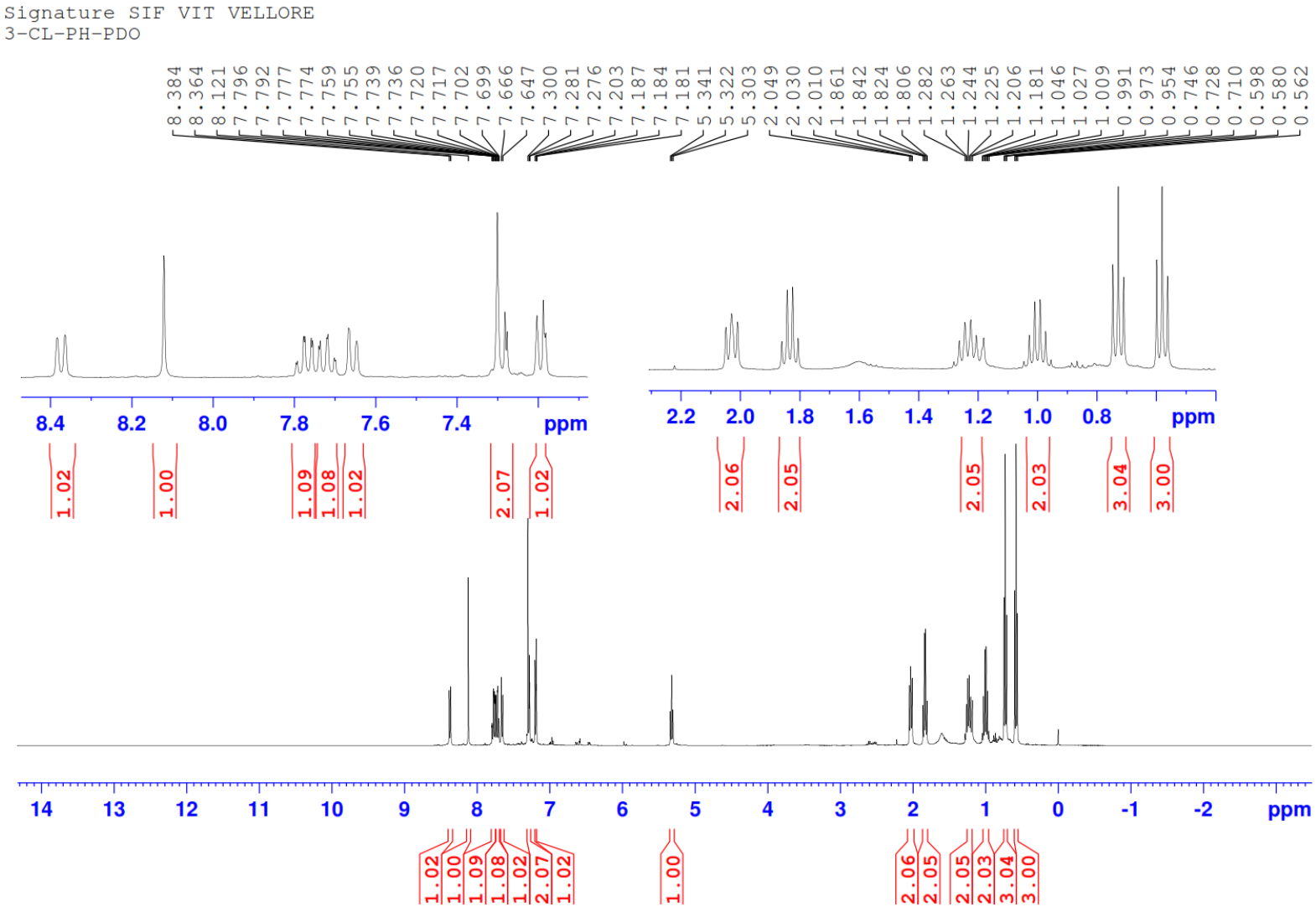
$^{13}C\{^{1}H\}$ NMR spectra of **4h**



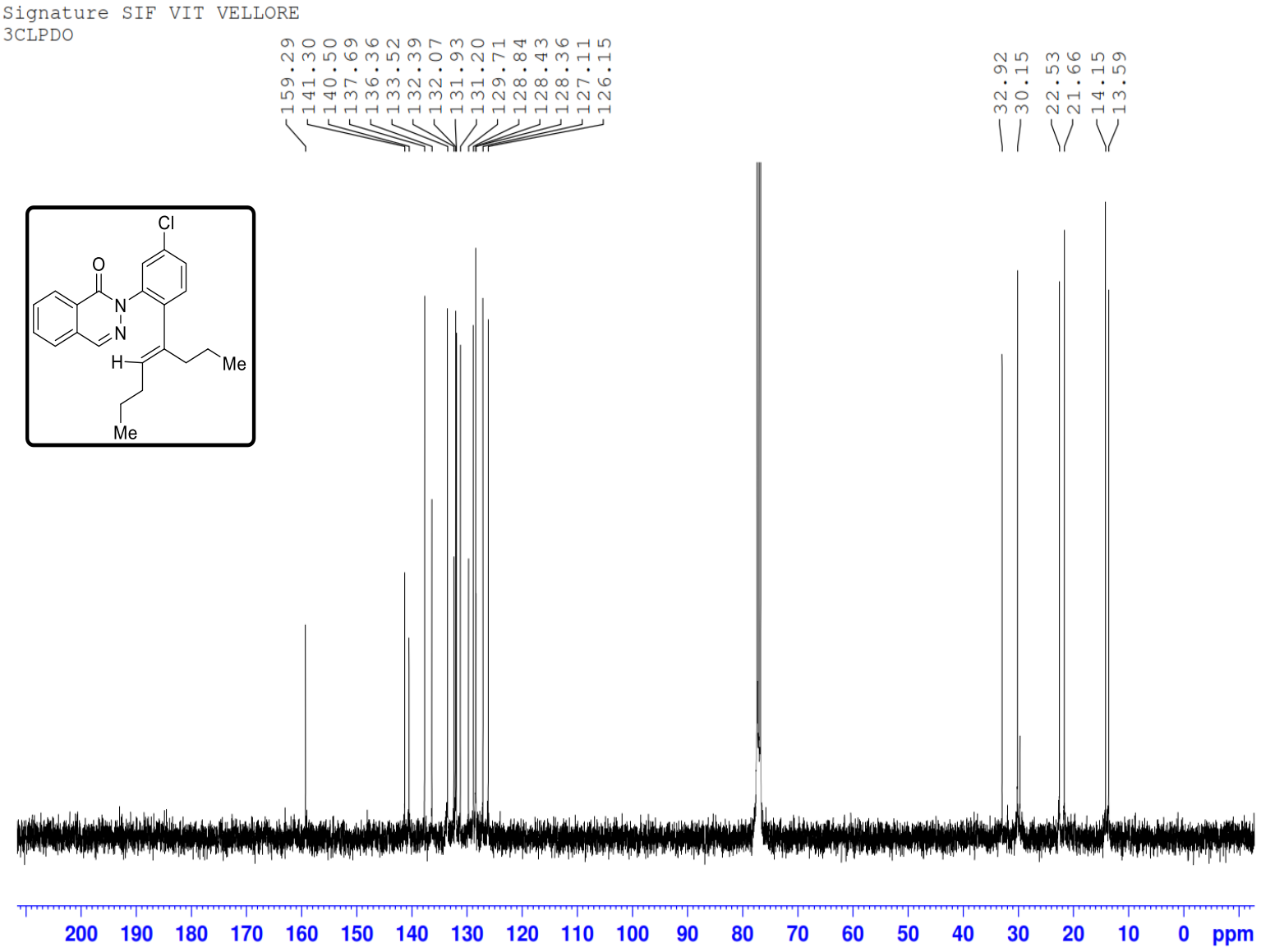
^{19}F NMR spectra of **4h**



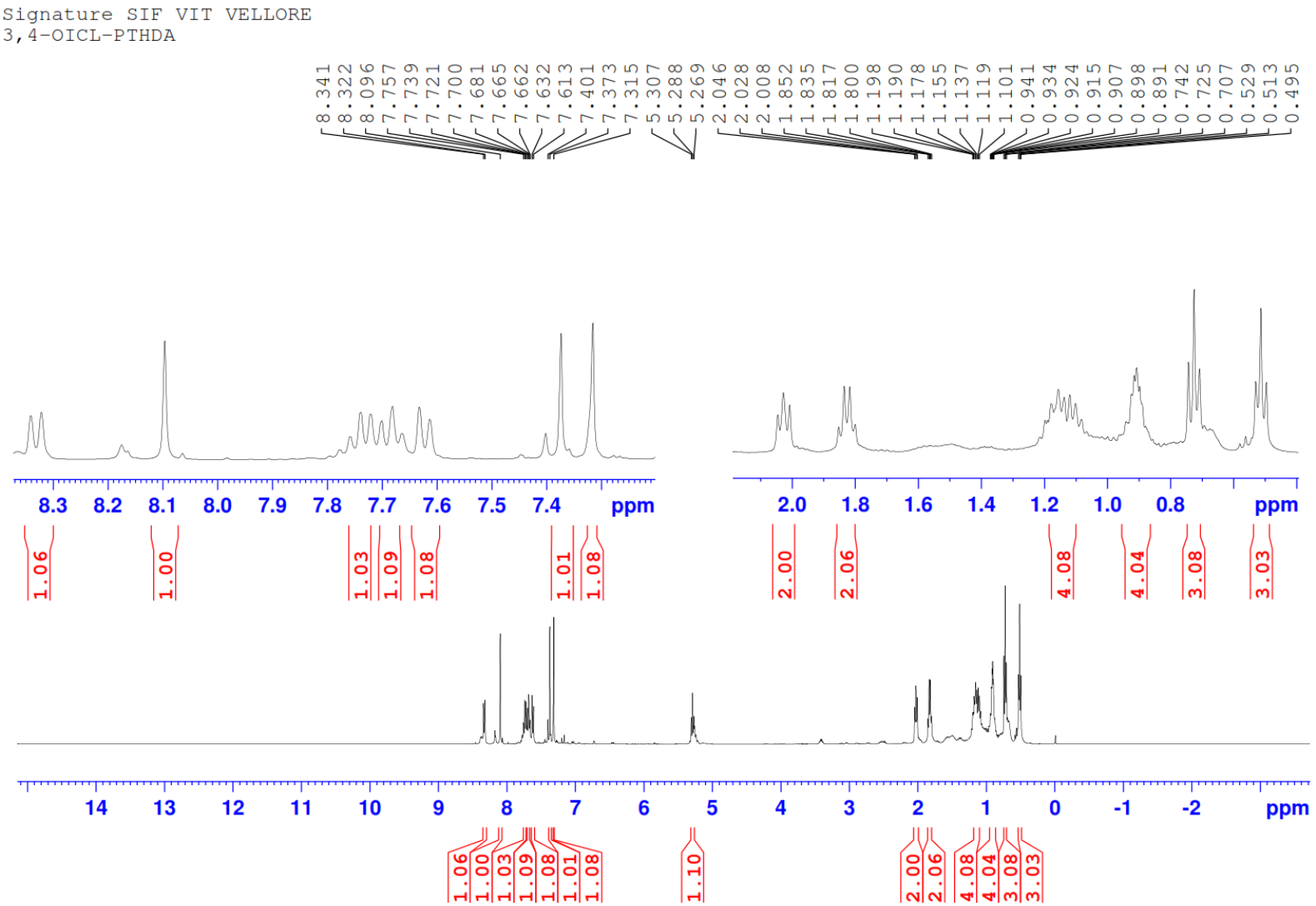
^{1}H NMR spectra of **4i**



$^{13}C\{^{1}H\}$ NMR spectra of **4i**



^{1}H NMR spectra of **4j**

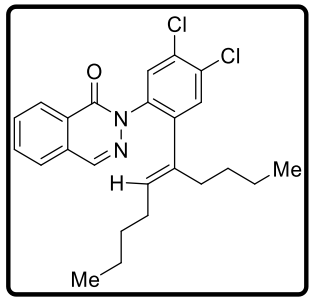


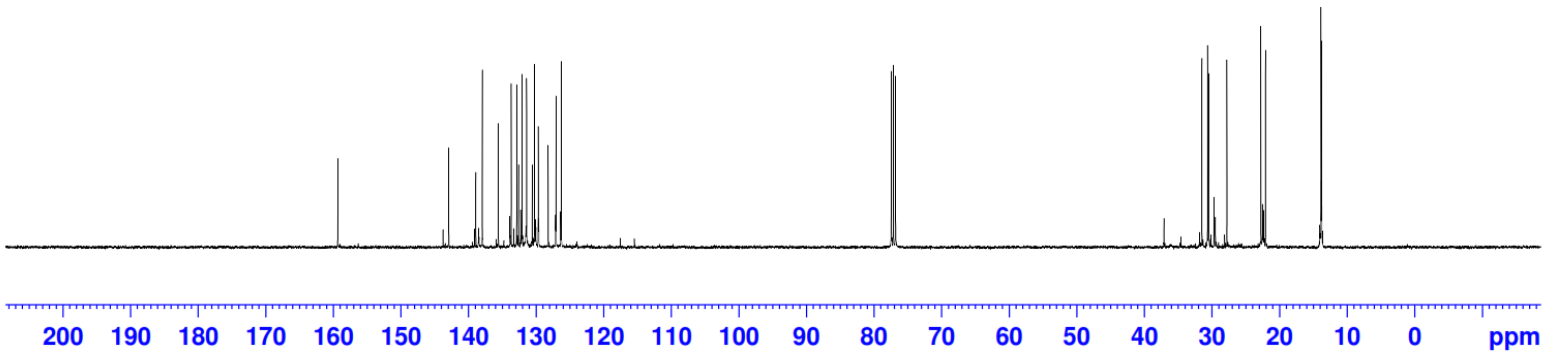
$^{13}C\{^{1}H\}$ NMR spectra of **4j**

Signature SIF VIT VELLORE
3,4-OICL-PTHDA

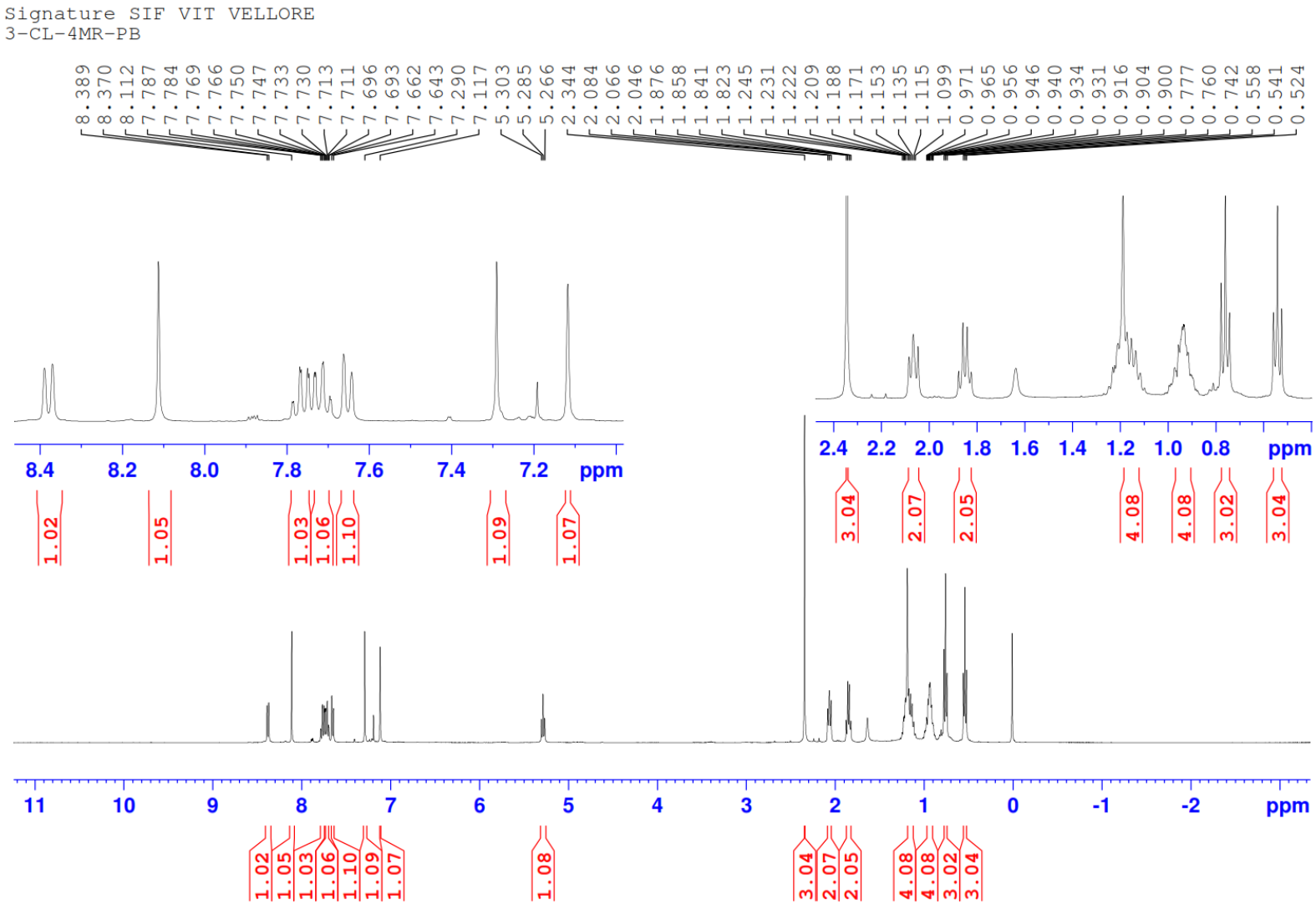
159.33
142.91
138.92
137.96
135.57
133.68
132.87
132.59
132.06
131.40
130.57
130.22
129.68
128.20
127.05
126.27

31.48
30.64
30.48
27.78
22.75
22.08
13.86
13.79

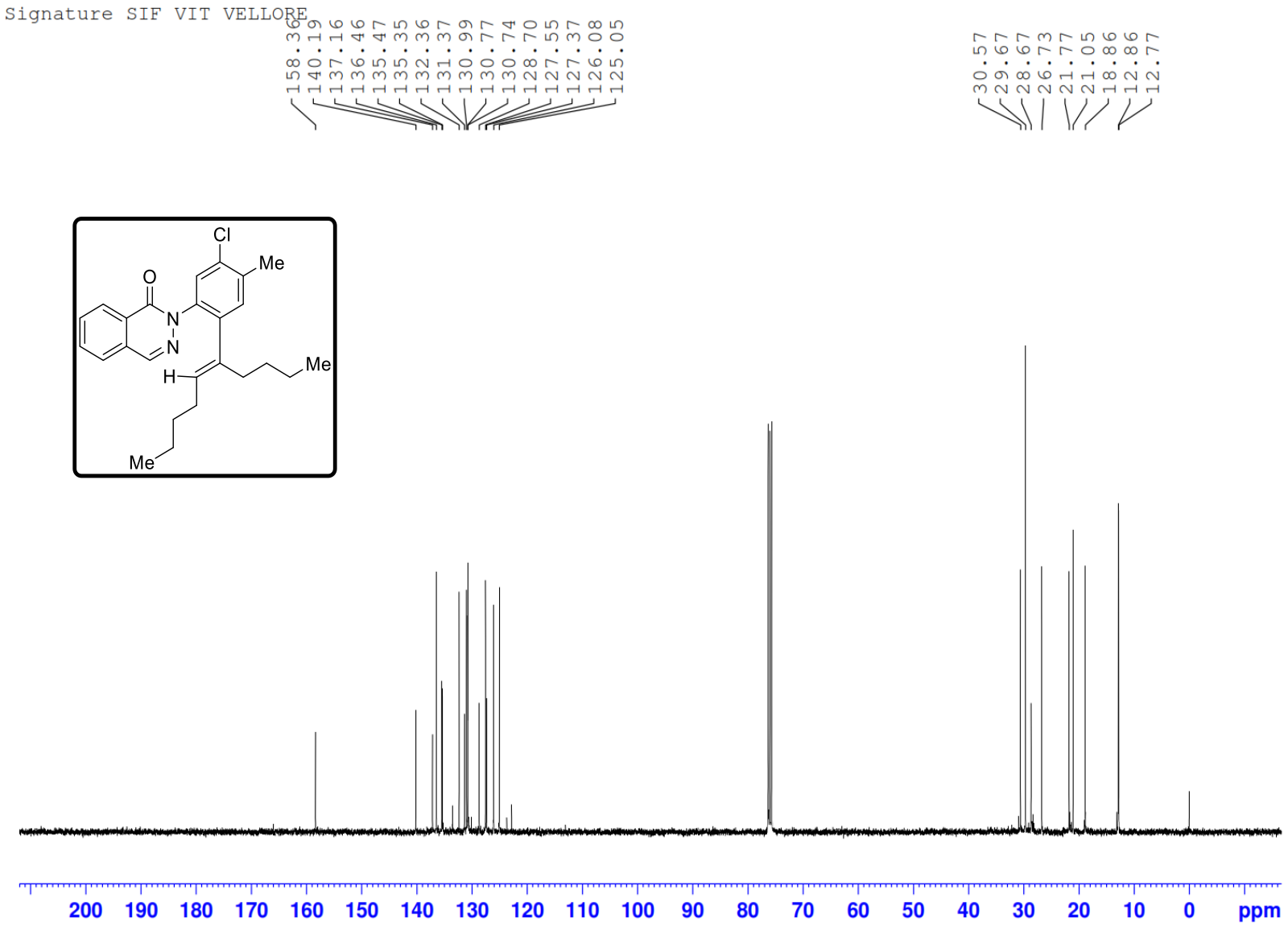




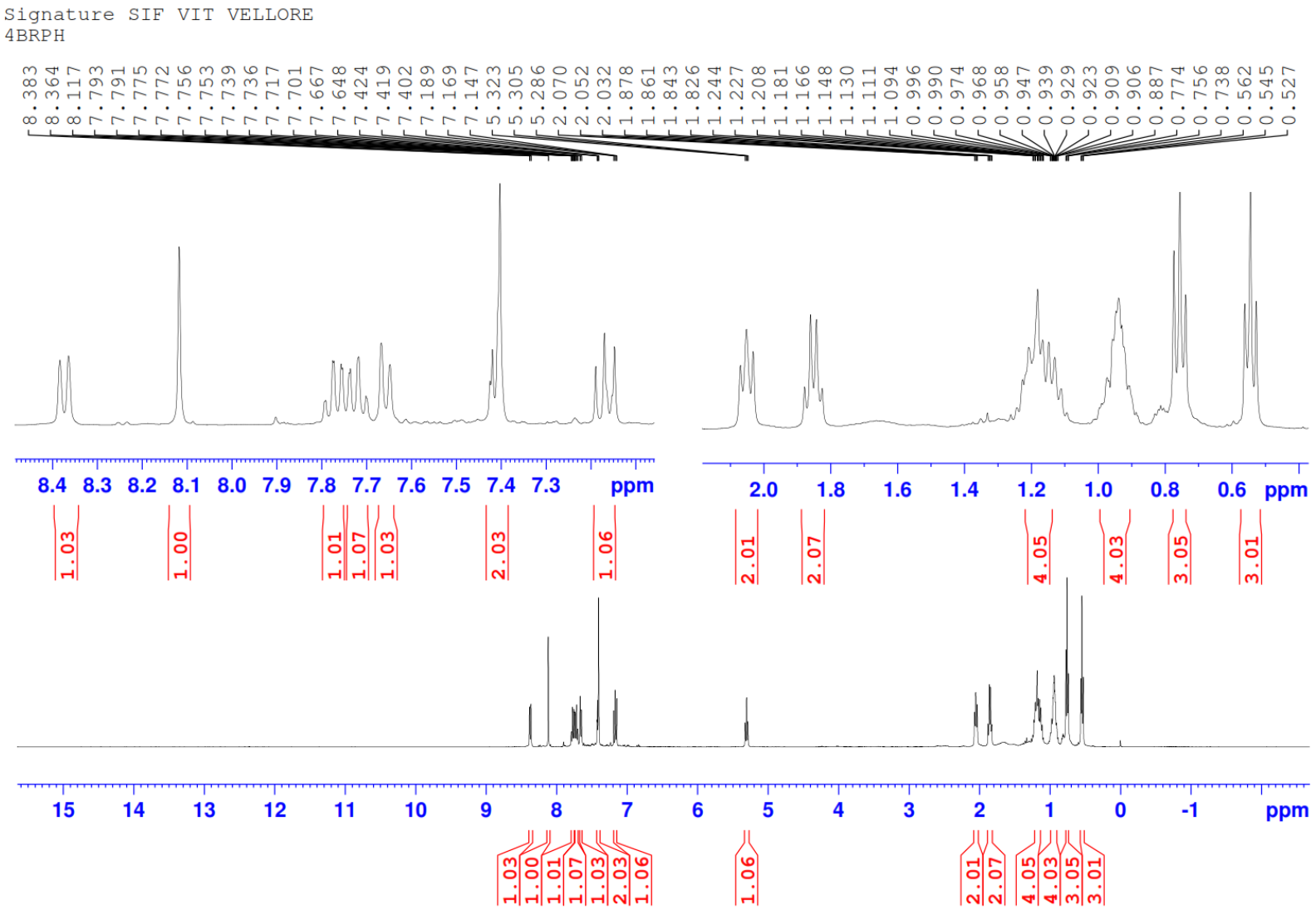
^{1}H NMR spectra of **4k**



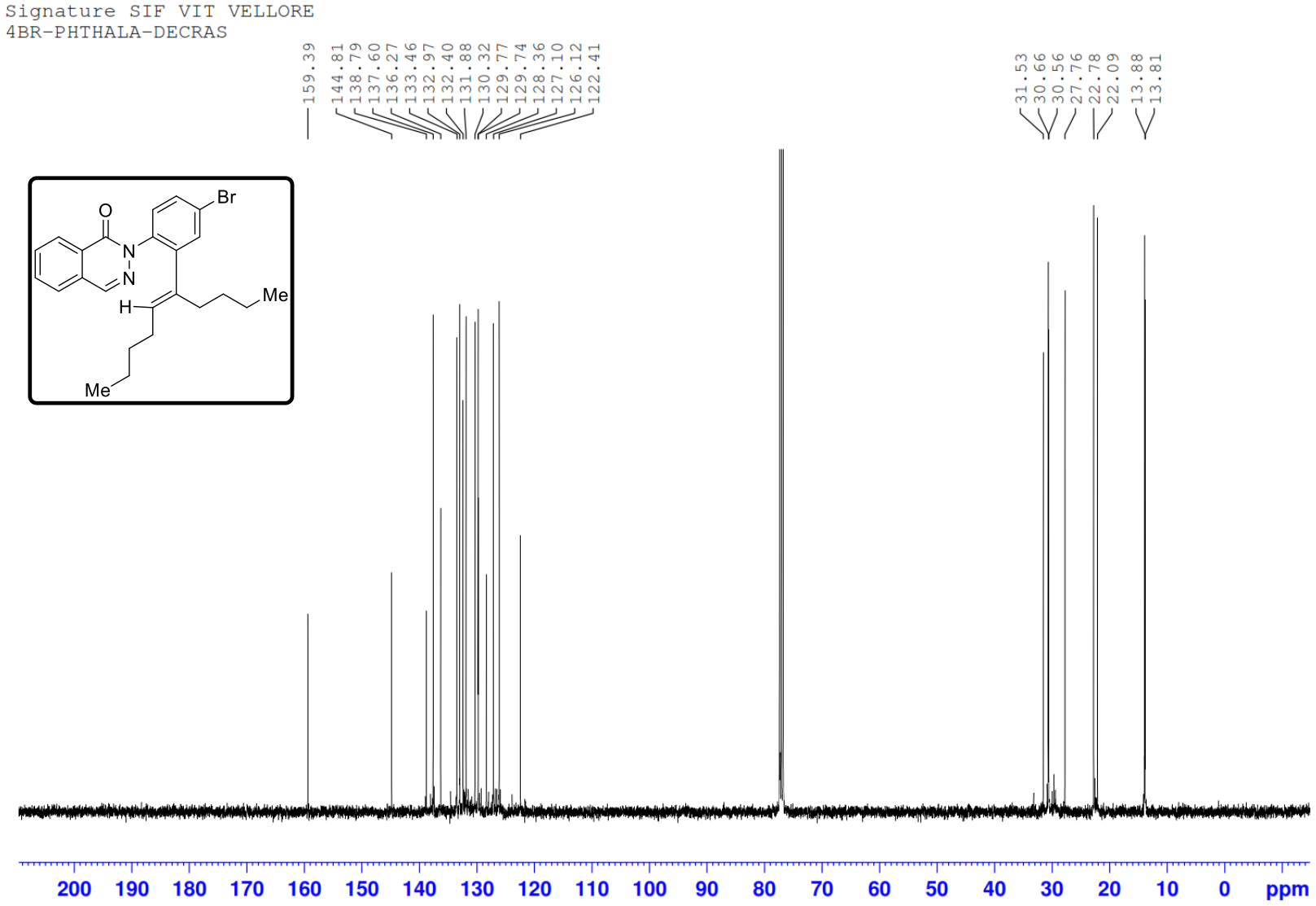
$^{13}C\{^{1}H\}$ NMR spectra of **4k**



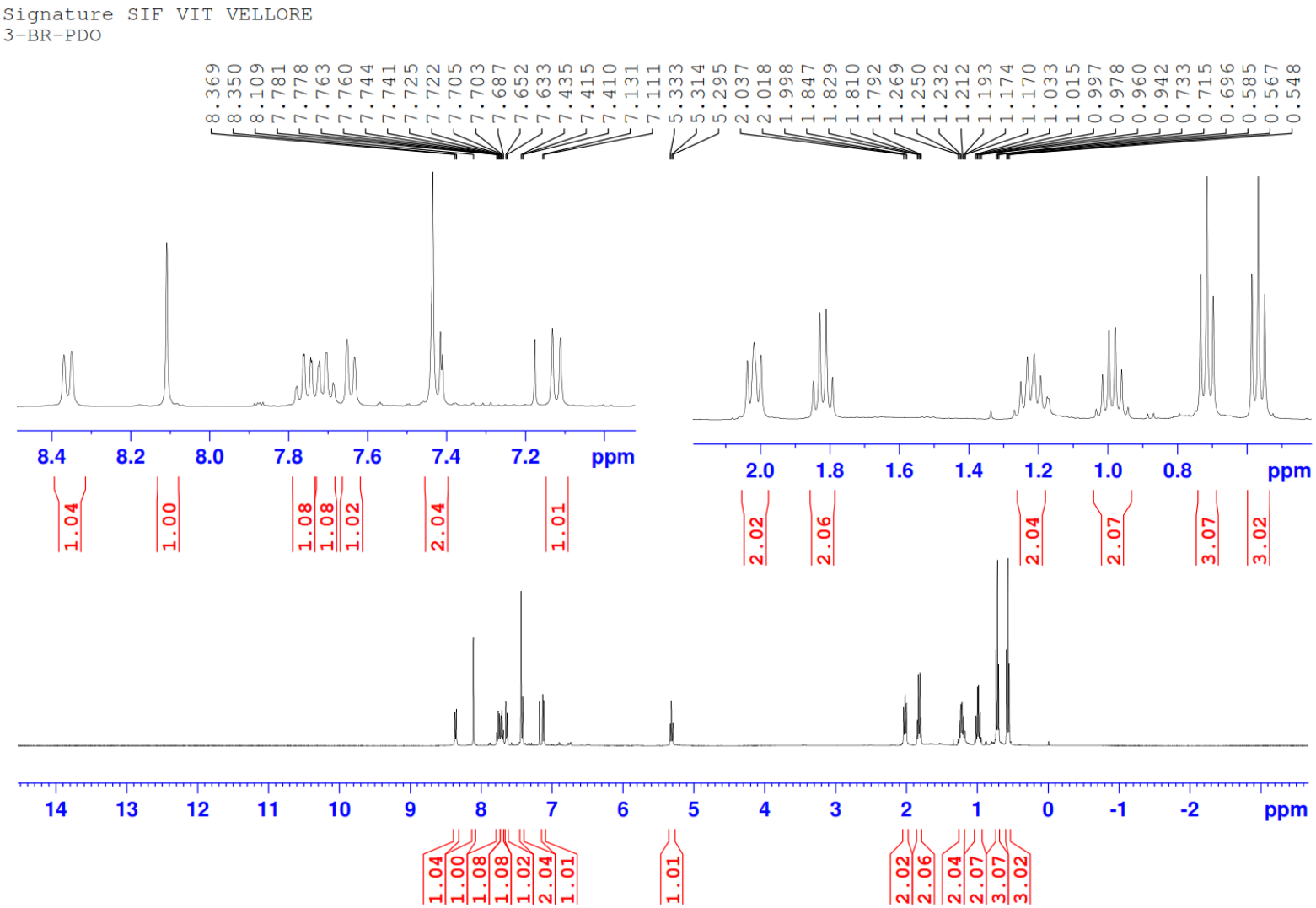
^{1}H NMR spectra of **4l**



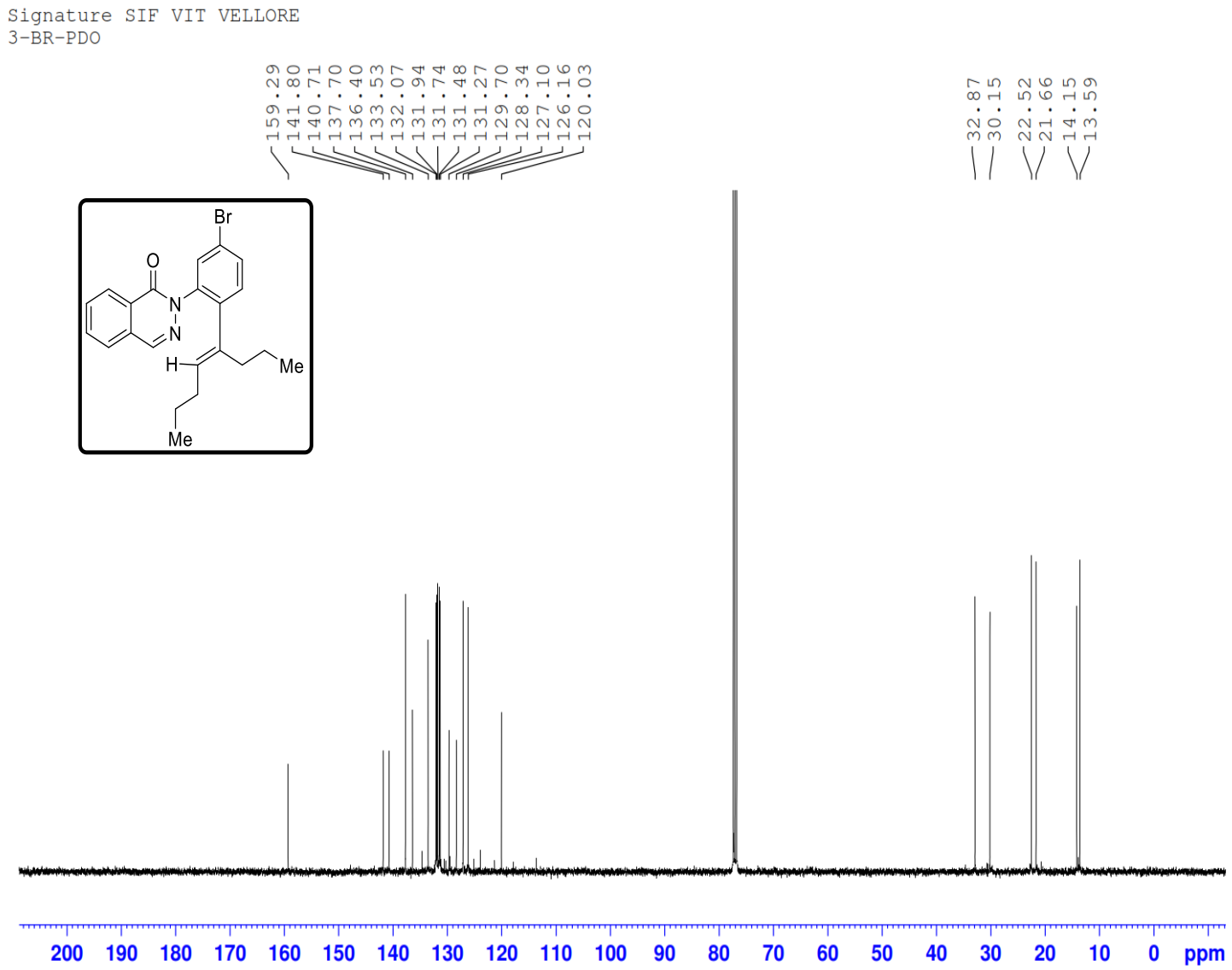
$^{13}C\{^{1}H\}$ NMR spectra of **4l**



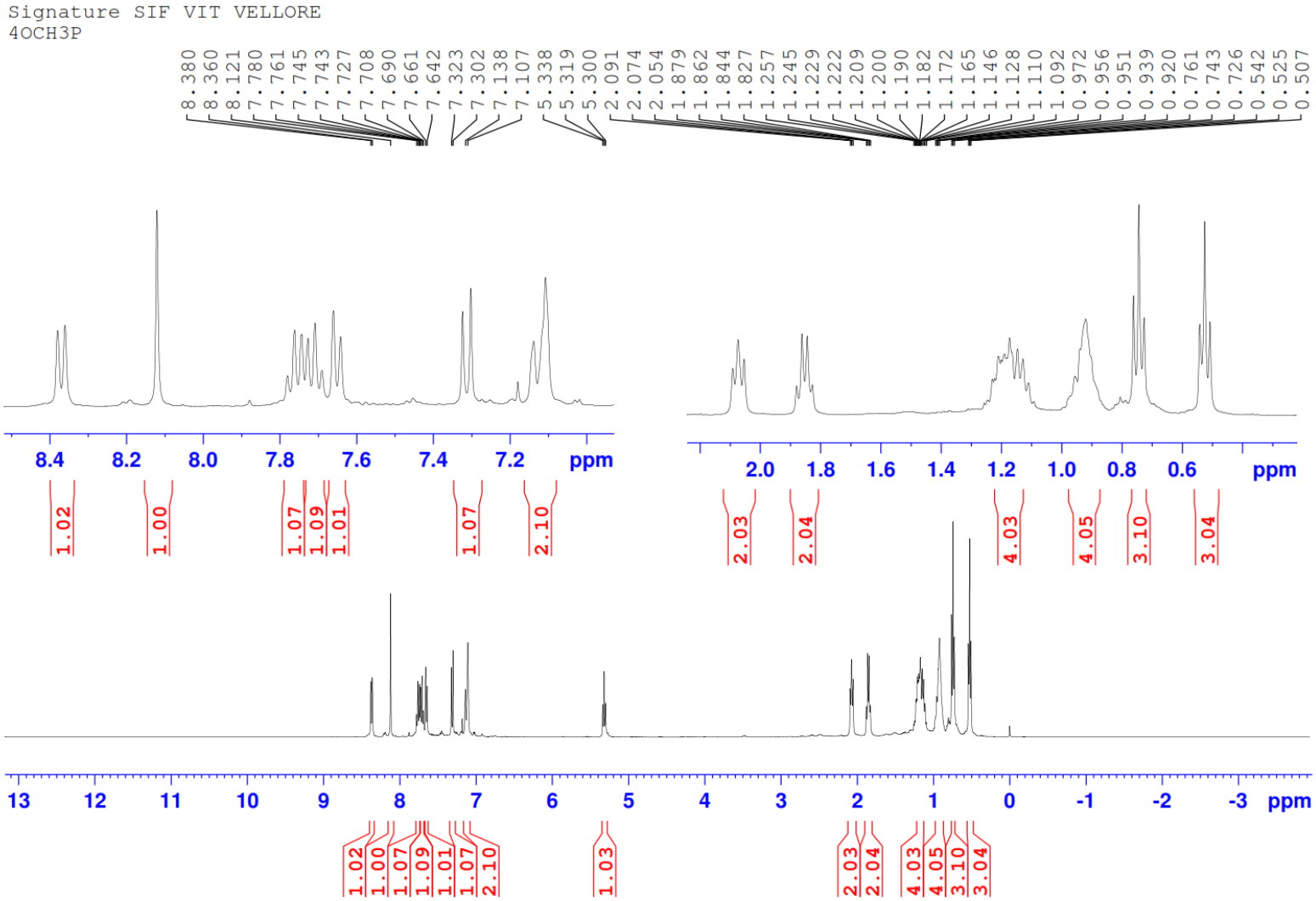
^{1}H NMR spectra of **4m**



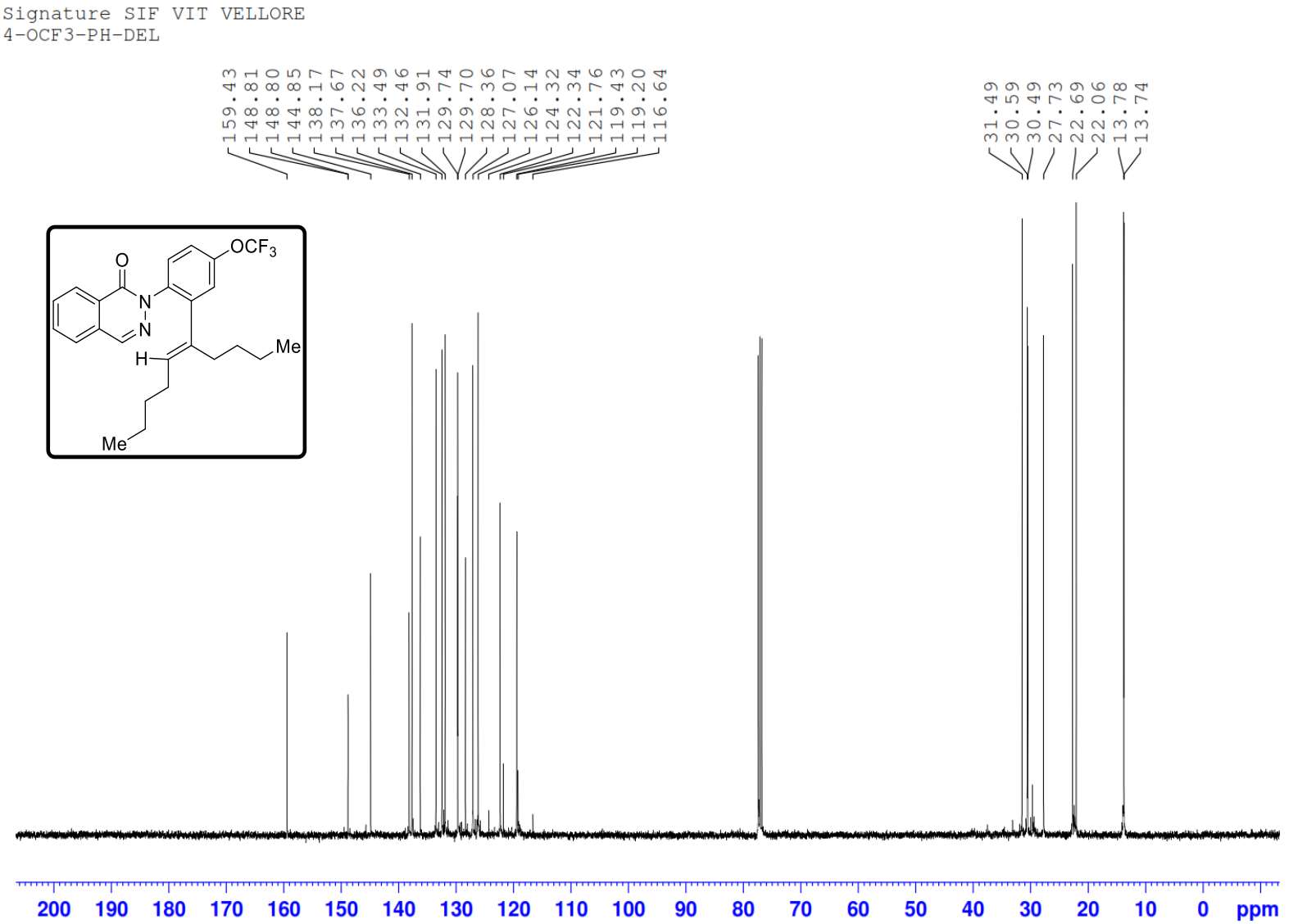
$^{13}C\{^{1}H\}$ NMR spectra of **4m**



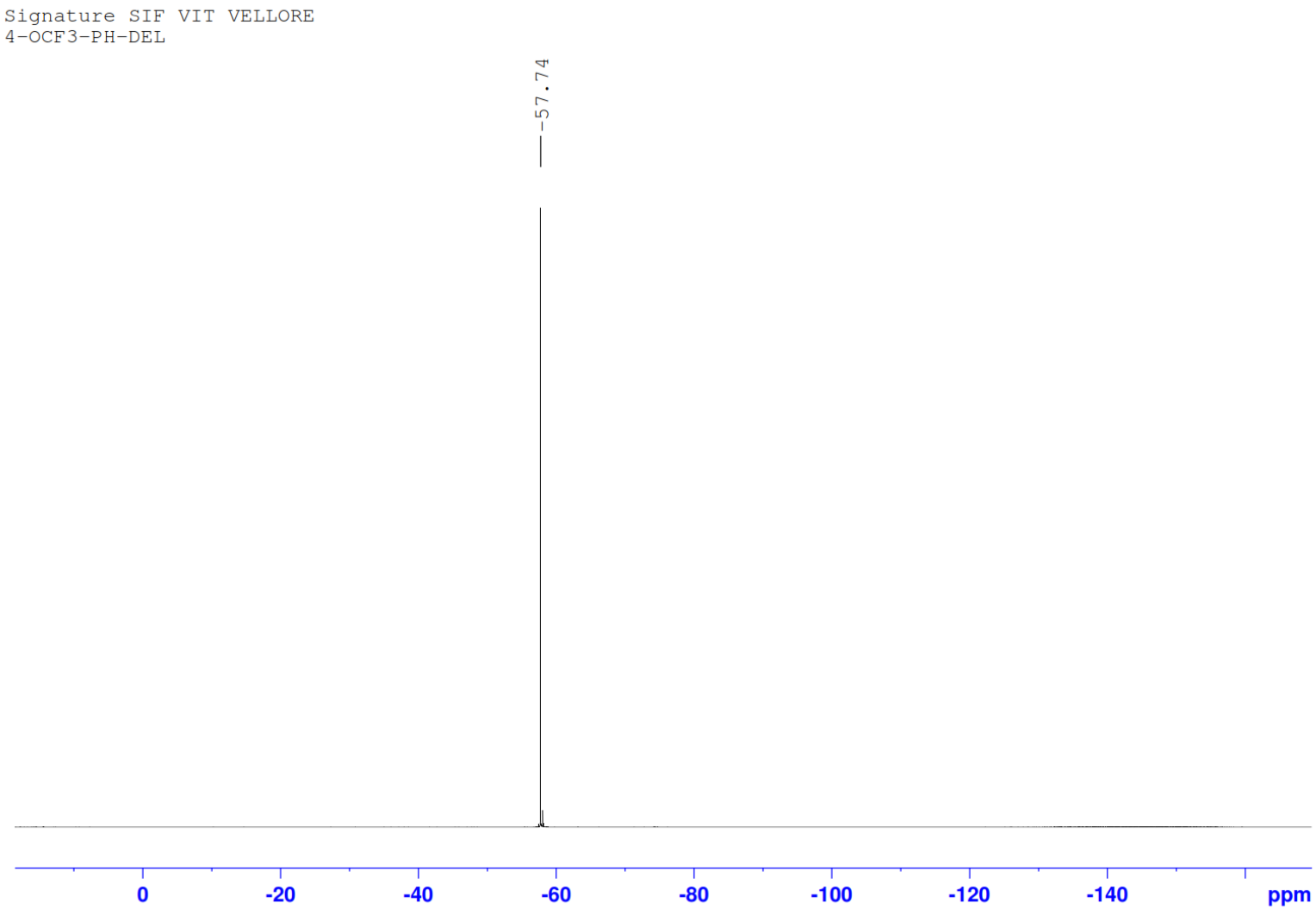
^{1}H NMR spectra of **4n**



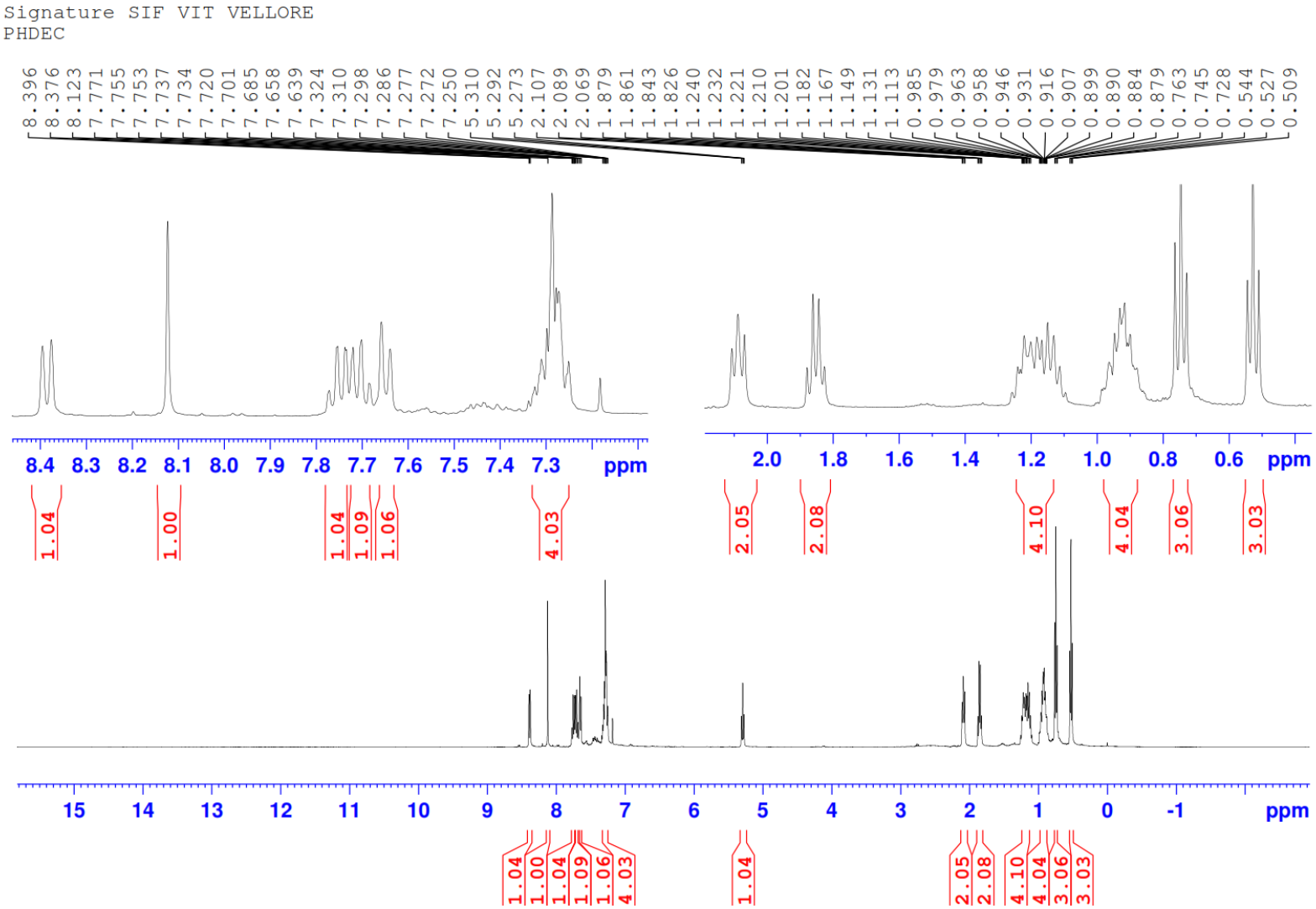
$^{13}C\{^{1}H\}$ NMR spectra of **4n**



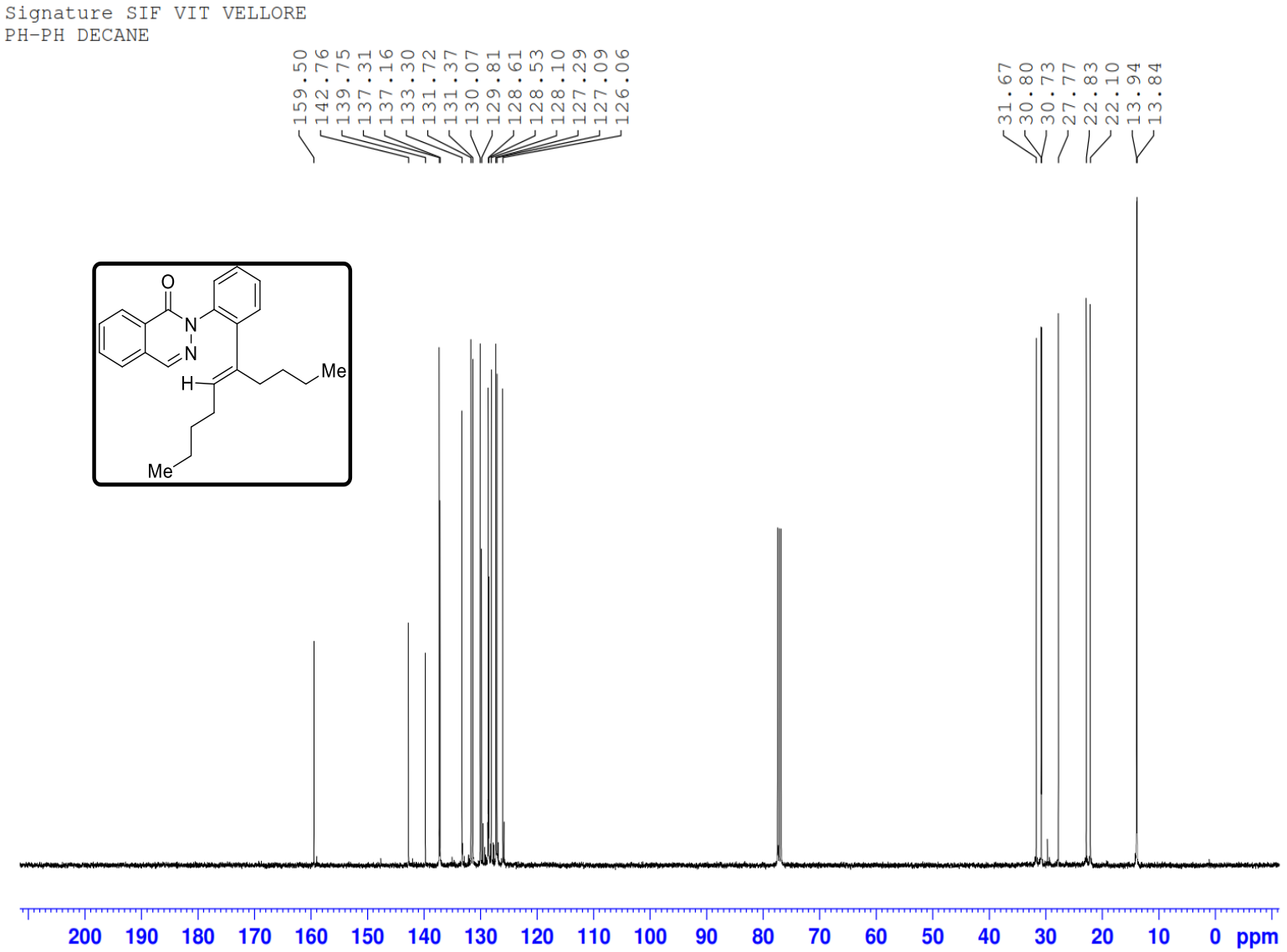
^{19}F NMR spectra of **4n**



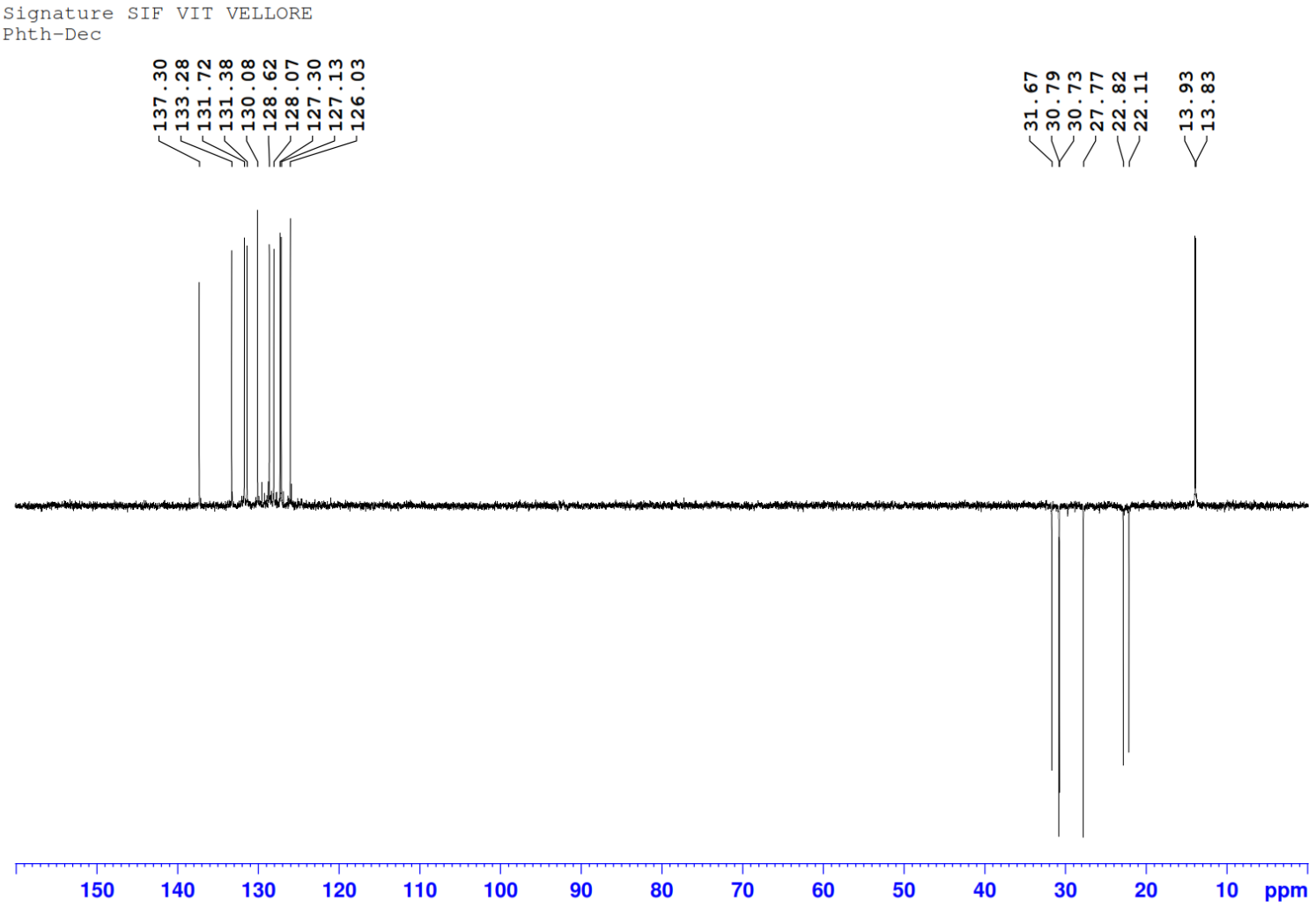
^{1}H NMR spectra of **4o**



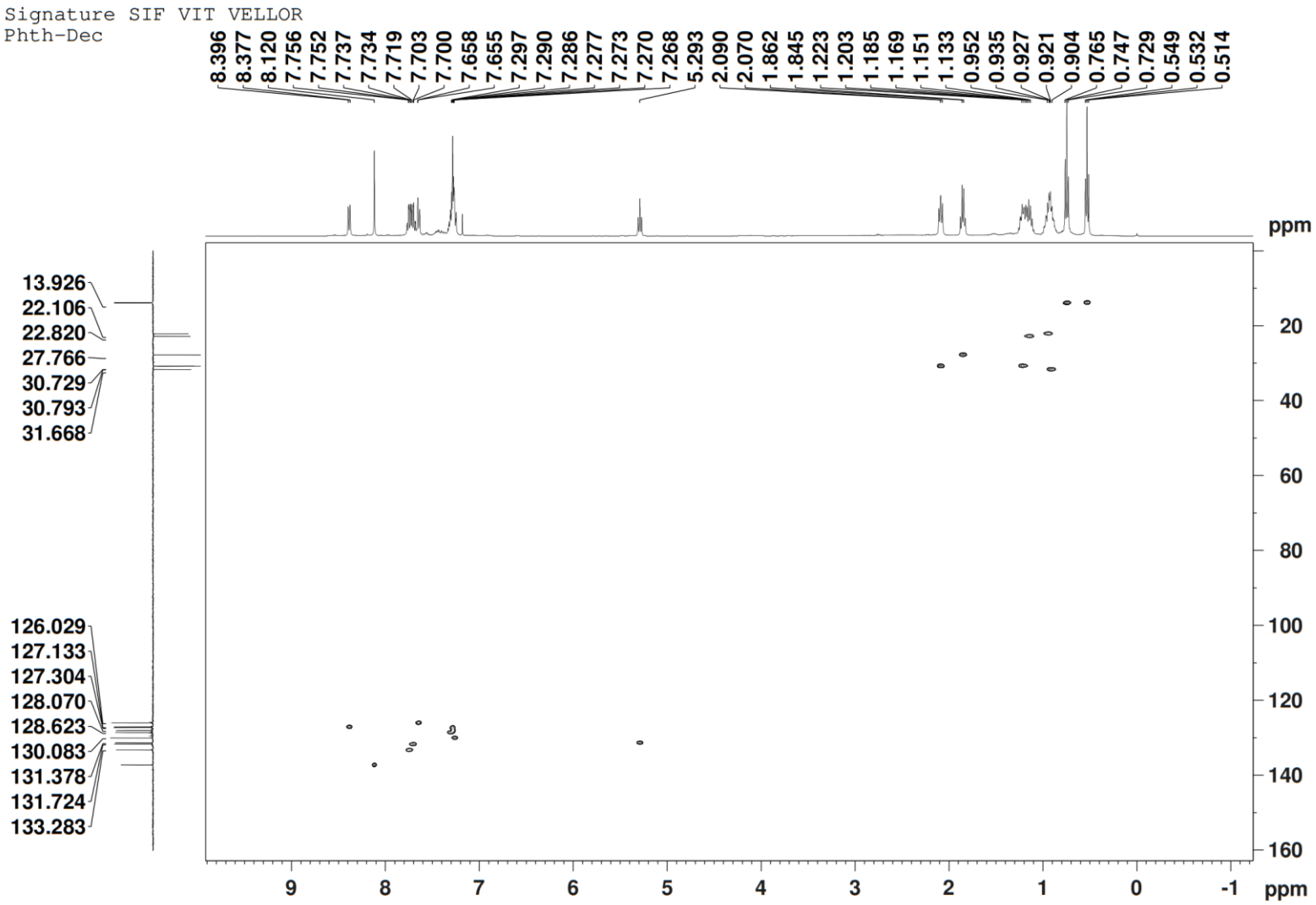
$^{13}C\{^{1}H\}$ NMR spectra of **4o**



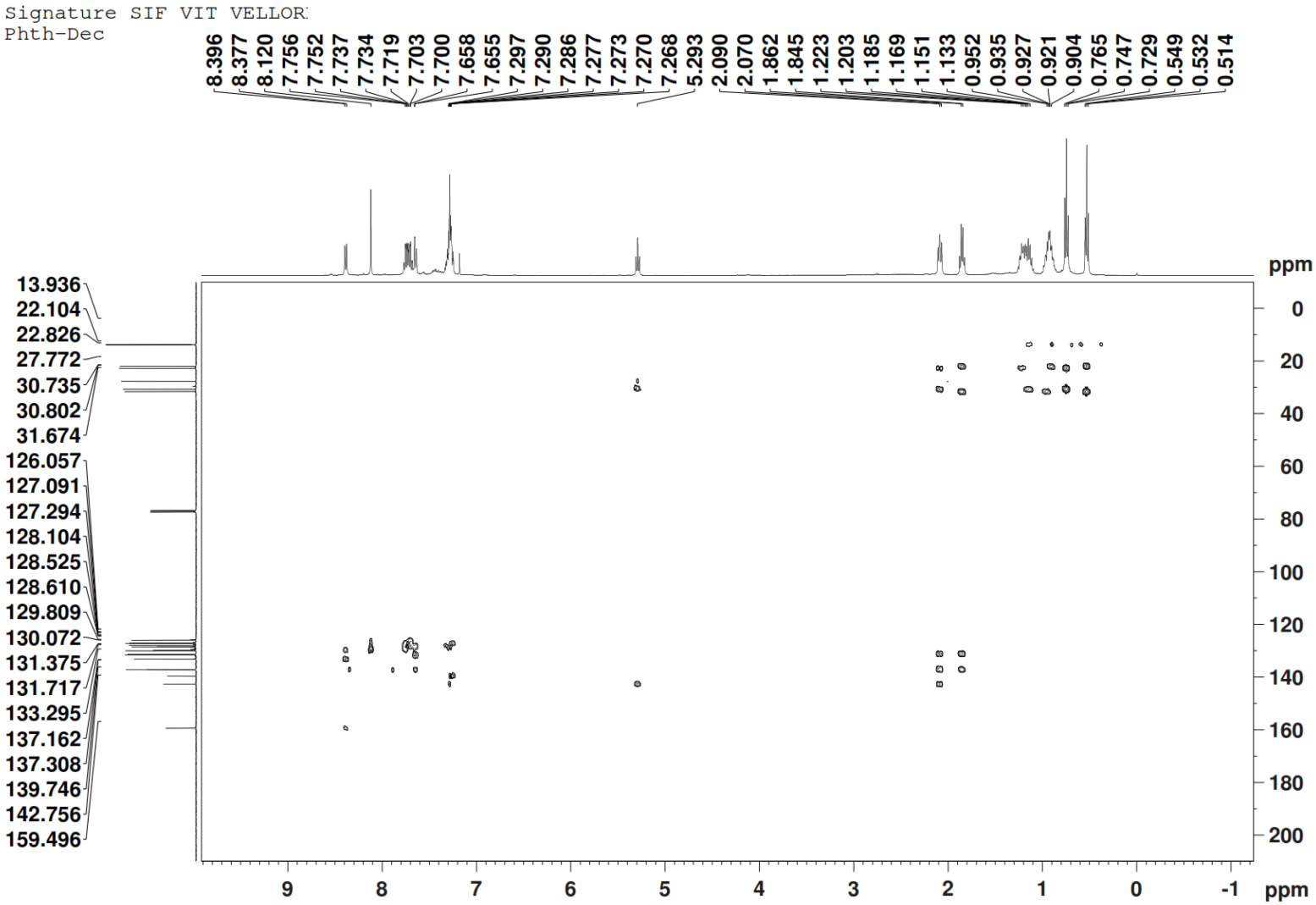
DEPT-135 NMR spectra of **4o**



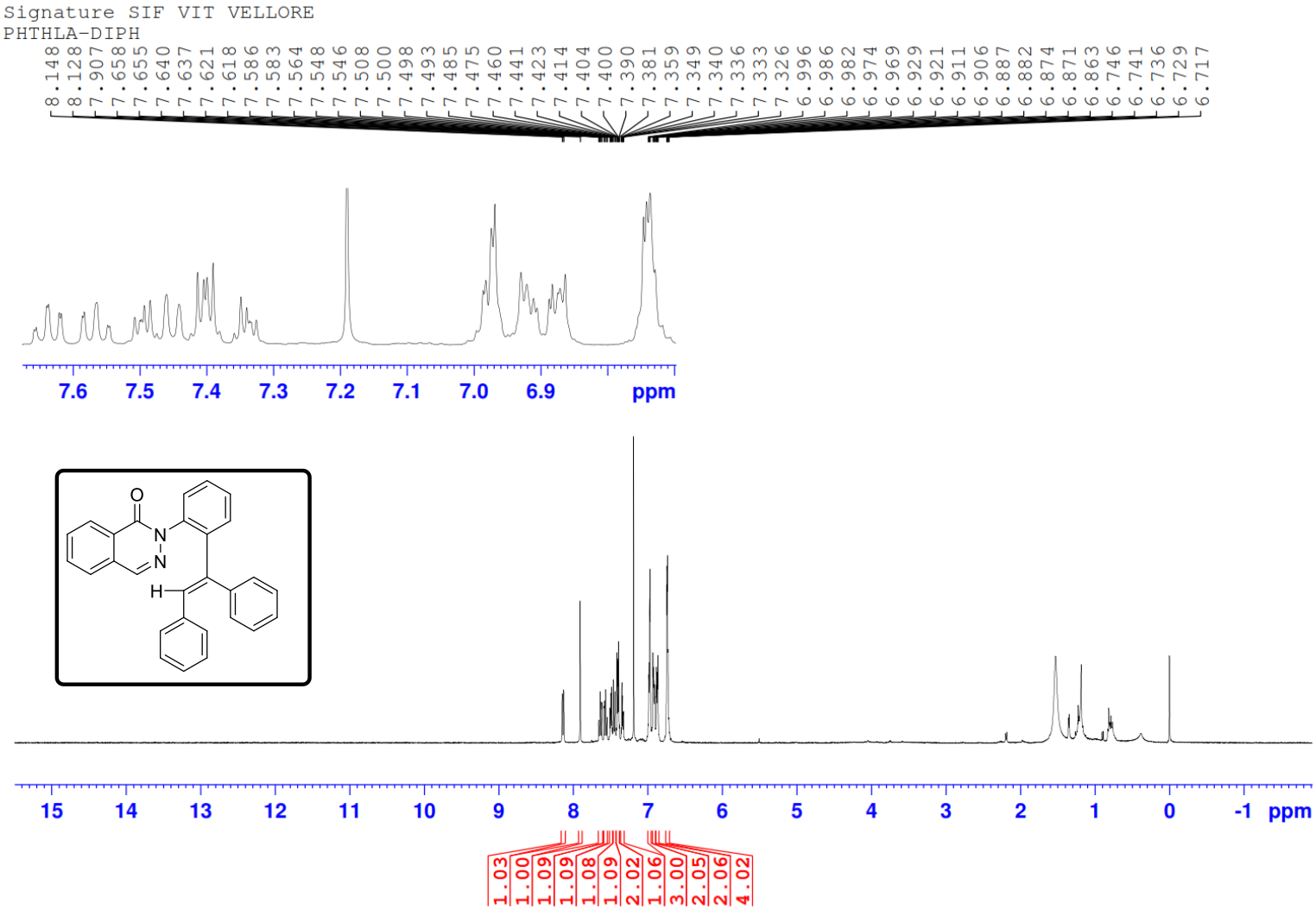
^{1}H-^{13}C (DEPT-135) HSQC NMR spectra of **4o**



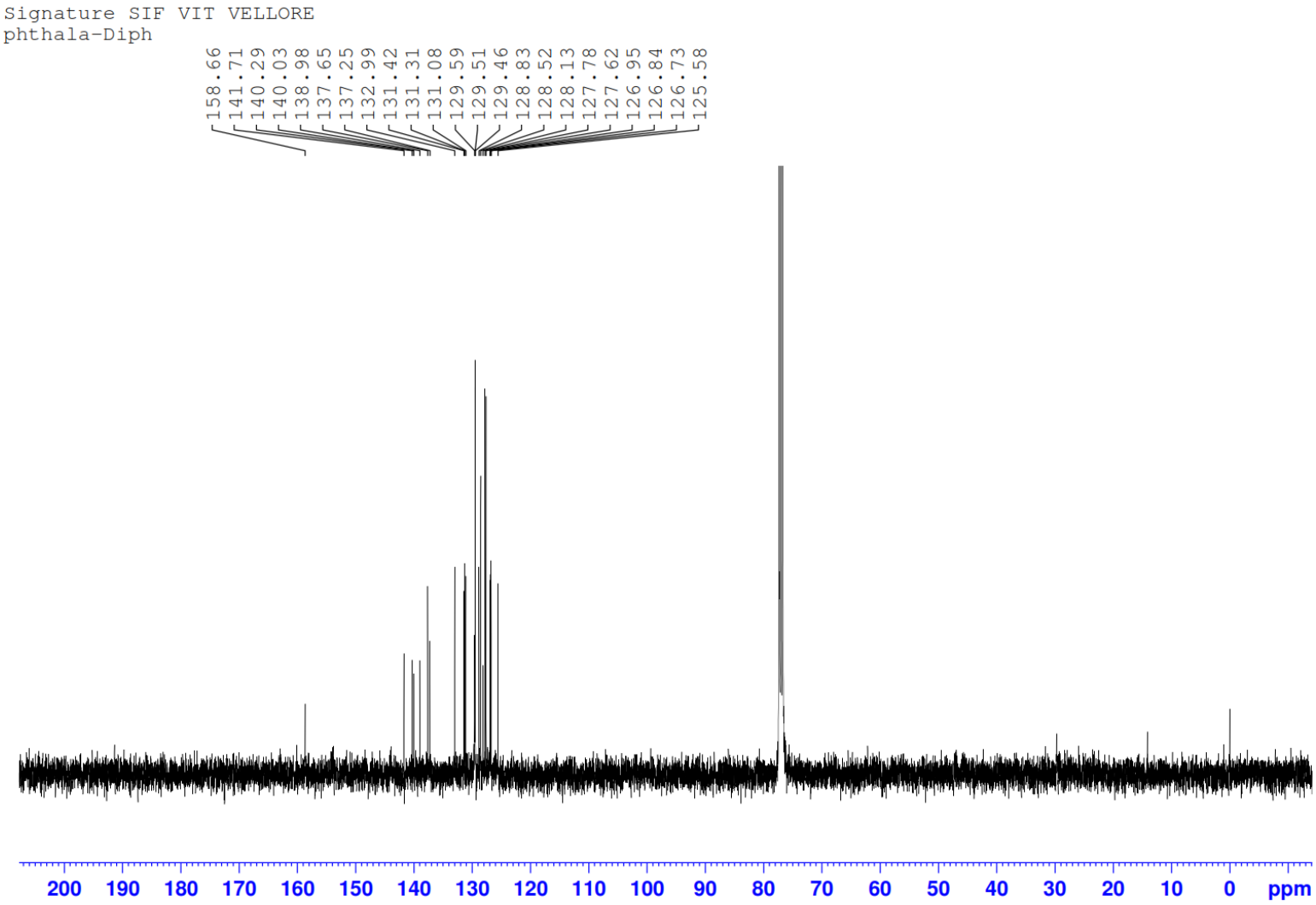
^{1}H-$^{13}C\{^{1}H\}$ HMBC NMR spectra of **4o**



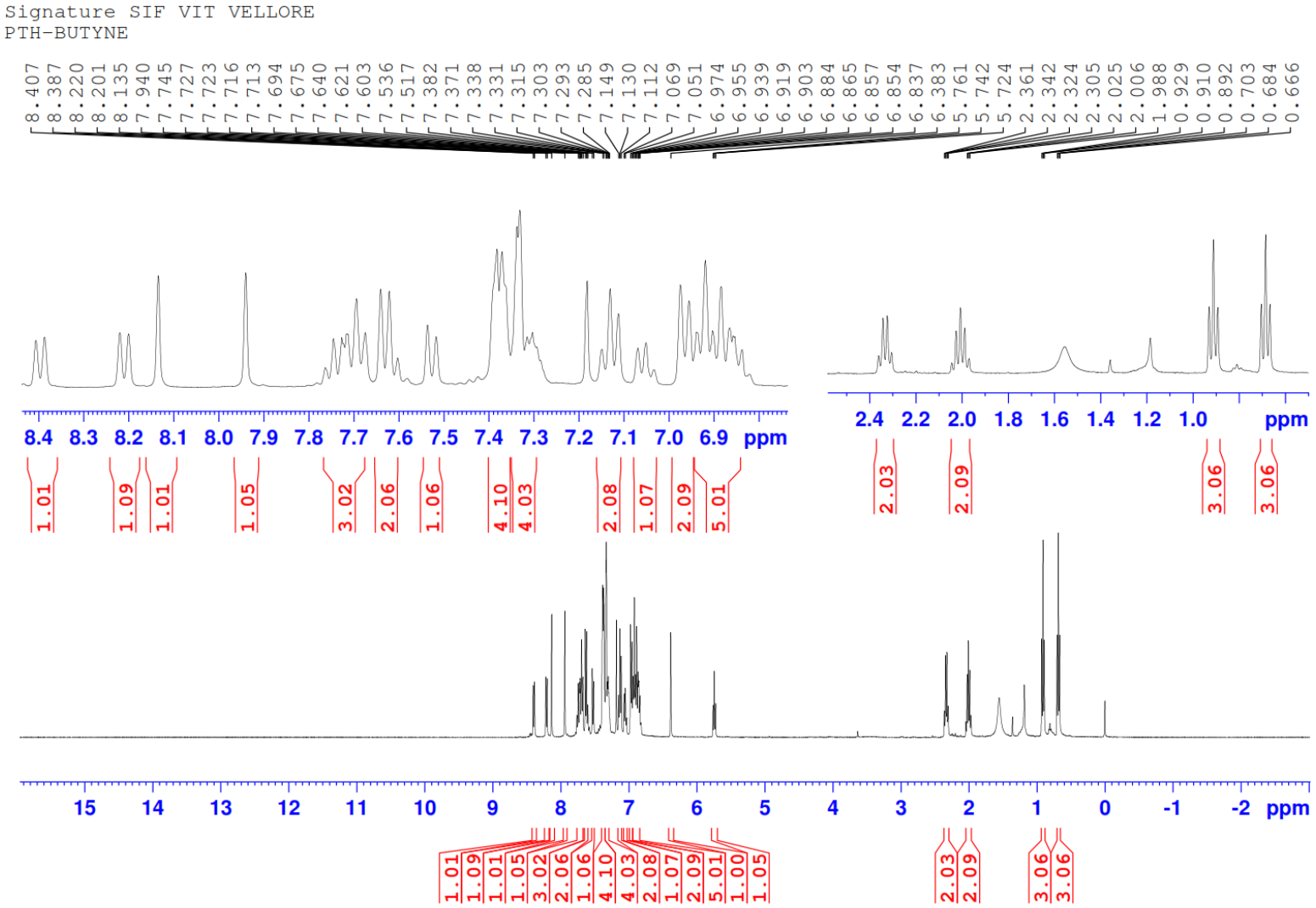
^{1}H NMR spectra of **4p**



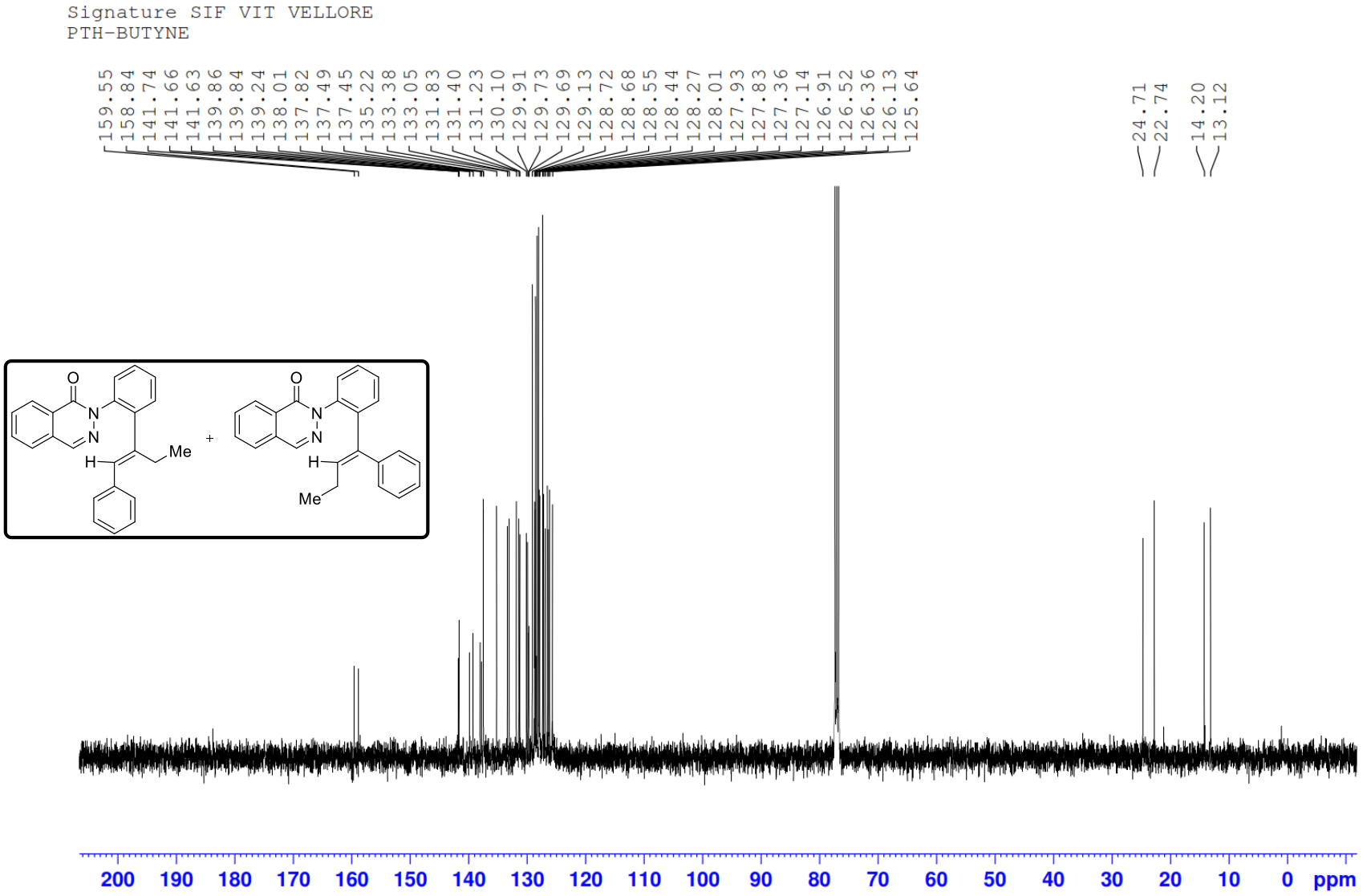
$^{13}C\{^{1}H\}$ NMR spectra of **4p**



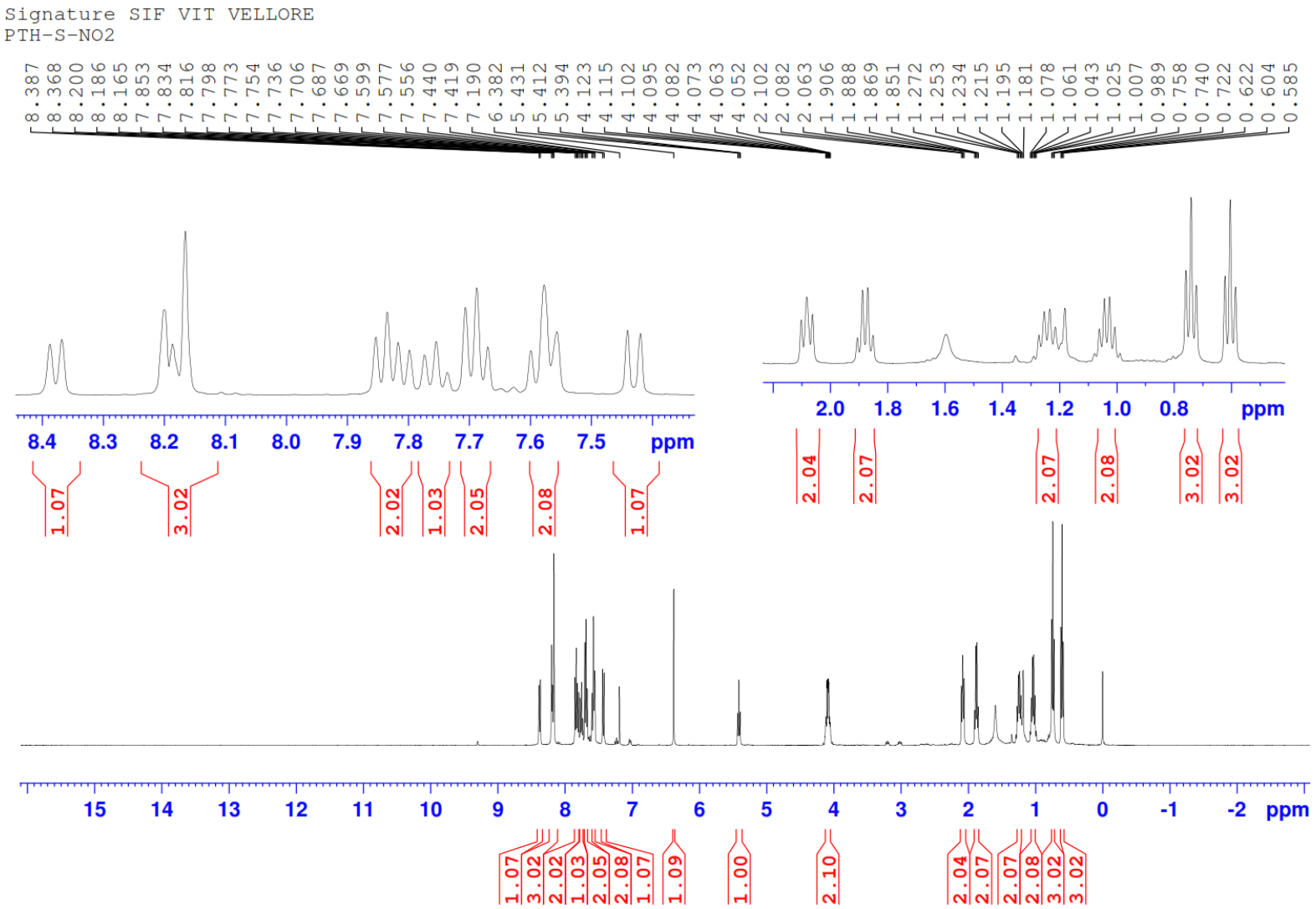
^{1}H NMR spectra of **4q**



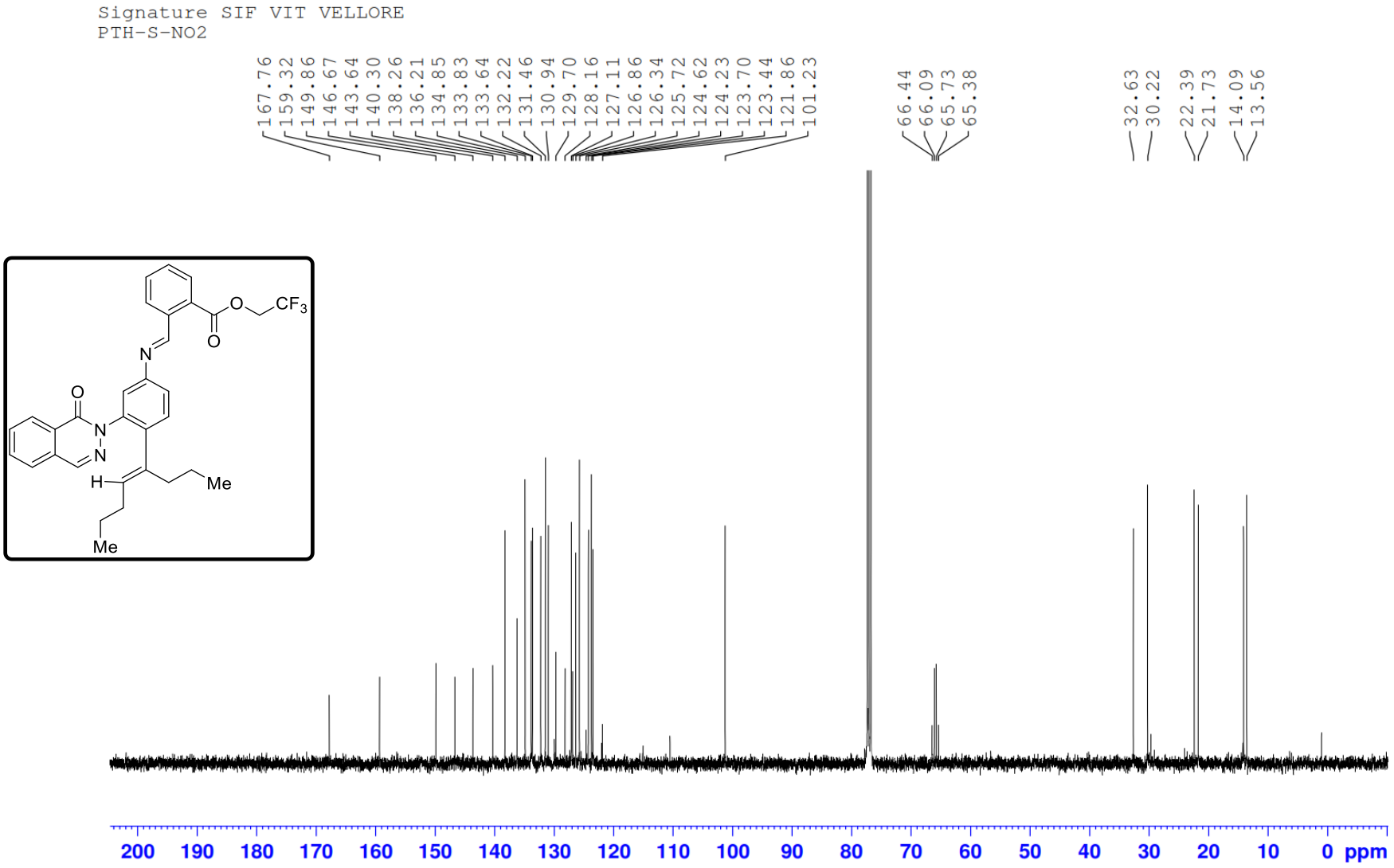
$^{13}C\{^{1}H\}$ NMR spectra of **4q**



^{1}H NMR spectra of **5**



$^{13}C\{^{1}H\}$ NMR spectra of **5**



^{19}F NMR spectra of **5**