## Supporting Information

# Diselenolodiselenole: selenium containing fused heterocycle for conjugated systems

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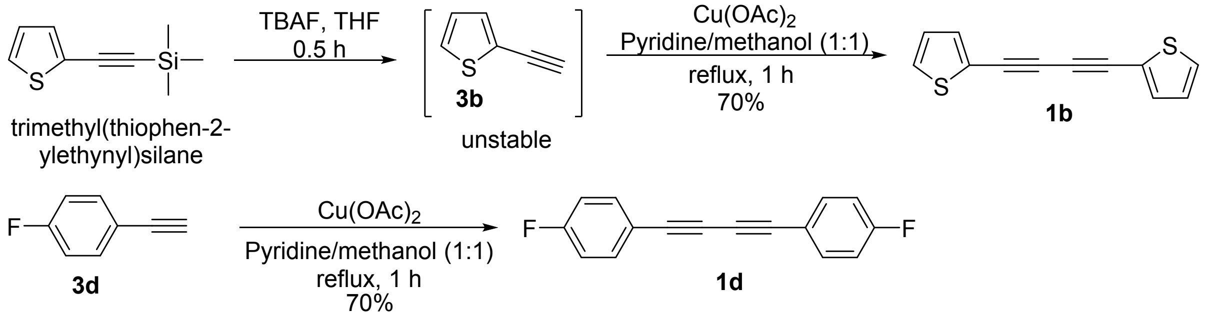
## Experimental section

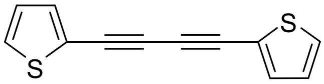
Phenyl acetylene and 4-fluorophenyl acetylene were obtained from Spectrochem (India). Selenium metal powder was purchased from SRL (India). $TBAPF_6$ and ethynyltrimethylsilane were purchased from Aldrich. Other reagents were commercially accessed and used as received. 1,2-DCE and *o*-DCB were dried by distilling over $P_2O_5$ before use. $^1H$ and $^{13}C$ NMR spectra were recorded on Jeol-ECS 400 MHz spectrometer as a solution in $CDCl_3$, DMSO-$d_6$ and $C_6D_6$ with tetramethylsilane (TMS) as the internal standard, chemical shifts ($\delta$) are reported in parts per million. Chemical shift in $^{77}Se$ NMR spectra were recorded using 1,2-diphenyldiselane as internal standard. Columns were prepared with silica gel (100-200 mesh, Merck, India). Ferrocene (Sigma–Aldrich) was used to as an electrochemical reference. Non-aqueous Ag/AgCl electrode was prepared by dipping silver wire into a solution of $FeCl_3$ and HCl. Electrochemical studies were carried out on a Princeton Applied Research 263A potentiostat using platinum (Pt) disk electrode as the working electrode, a platinum wire as counter electrode, and an AgCl coated Ag wire that was directly dipped in the electrolyte solution, as the reference electrode. Pt disk electrodes were polished with alumina, water, acetone and was dried with nitrogen before use to remove any incipient oxygen. The electrolyte used was 0.1 M $TBAPF_6$ in DCM. $E_{1/2}$ of the ferrocene/ferrocenium couple was calculated to be 0.36 V in $TBAPF_6$/DCM electrolyte/solvent system against Ag/AgCl reference electrode. UV-vis-NIR spectra were recorded in DCM on a Agilent Cary-60 UV-vis spectrophotometer.

Single crystals of **2a-2c** were obtained by slow evaporation from their solution in DCM. Suitable crystals were collected on a SuperNova, Dual, Cu/Mo at zero, Eos diffractometer. Using Olex2,[1] the structure was solved with the Superflip[2] structure solution programme using Charge Flipping and refined with the ShelXL[3] refinement package using Least Squares minimization.



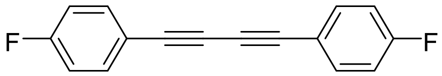
**Scheme S1** Synthesis of **1b** and **1d**.

**Synthesis of 1b**



Into a stirred solution of trimethyl(thiophen-2-ylethynyl)silane (720 mg, 4 mmol) in 15 ml THF was drop wise added tetrabutylammonium fluoride (5 mL, 1M in THF) and stirred for 0.5 h at rt. Then 20 mL of water was added to the reaction mixture and stirred for 5 min. and the aqueous layer was extracted with diethyl ether (3×20 mL). Organic phase was dried with anhydrous $Na_2SO_4$ and concentrated in rotovapor such that the desilylated product (**3b**) stays in small amount of solvent before using it directly for the next step. Compound **3b** in neat state decomposed upon standing. This was overcome by keeping small amount of solvent with **3b** during work up and this solution was injected directly to the reaction mixture of next Cu(II)-coupling reaction. Then in another three necked rb containing $Cu(OAc)_2$ (1.01g, 5.6 mmol) and 10 mL pyridine/methanol mixture (1:1 v/v) was added the previously kept solution of freshly prepared **3b** and refluxed for 2 h. After the consumption of **3b** (monitored from TLC) the reaction mixture was brought to rt followed by addition of 6 mL of 18*N* $H_2SO_4$ in ice-bath and stirred. Then resulting acidic aqueous solution was extracted with diethyl ether (3×20 mL). The ether layers were mixed, dried over anhydrous $Na_2SO_4$ and concentrated in rotovapor to result in a brown crude product. Column chromatography (alumina neutral activity I-II) of the crude using hexane as eluent gives faint yellow solid (300 mg, 70%) **1b**. $^1$H NMR (400 MHz, $\delta$, ppm, $CDCl_3$): 7.34 (m, 4H), 7.01 (m, 2H).

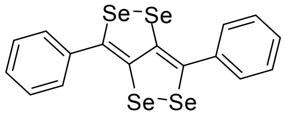
**Synthesis of 1d:**



To a saturated solution of 2.11 g (11.65 mmol) of finely powdered cupric acetate in 10 mL of a 1:1 by volume pyridine-methanol mixture, and contained in a 50-ml. round-bottomed flask fitted with a reflux condenser was added 1 g (8.33 mmol) of **3d**. The deep-blue suspension turned into green when heated under reflux. After 1 hour of heating, the solution was cooled and added dropwise to 10 ml. of 18*N* sulfuric acid, with stirring and external cooling in an ice-salt freezing mixture. The resulting white suspension is extracted with three 25-ml. portions of ether. The ether solution is then washed twice with water and dried over anhydrous magnesium sulfate. The ether layer was concentrated under reduced pressure to afford the colorless solid

(350 mg, yield = 70%) **1d**. The crude solid was directly used for the next step without further purification as it was found pure from NMR. $^1$H NMR (400 MHz, $\delta$, ppm, $CDCl_3$): 7.52 (m, 4H), 7.05 (m, 4H).

**Synthesis of 2a:**

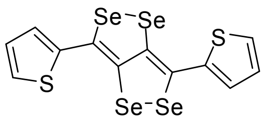


1,4-Diphenylbutadiyne **1a** (202 mg, 1 mmol) and neat selenium metal powder (316 mg, 4 mmol) were charged into a Schlenk flask, which was heated at 190 °C for 0.5 hours. The reaction was cooled and the resulting dark residue was purified by column chromatography on 100-200 mesh silica gel (1% $CH_2Cl_2$ in hexane) to result in the yellowish brown product **2a**. Yield: 119 mg, 23%. M. p.: 198 °C. $^1$H NMR (400 MHz, $\delta$, ppm, DMSO-$d_6$): 7.50 (m, 8H), 7.42 (m, 2H). $^{13}$C NMR (100 MHz, $\delta$, ppm, DMSO-$d_6$):137.1, 136.4, 129.6, 129.1, 125.8, 123.9. $^{77}$Se NMR ($\delta$, ppm, DMSO-$d_6$): 451.4, 311.8. HRMS (ESI+): calculated for $C_{16}H_{10}Se_4$, 521.7443; found 521.7468.

**With radical initiator:** 1,4-Diphenylbutadiyne **1a** (202 mg, 1 mmol), selenium metal powder (316 mg, 4 mmol) and 2,2′-azobis(2-methylpropionitrile) (AIBN) were charged into a pressure vessel containing 1,2-dichloroethane and heated at 190 °C for 0.5 hours. The reaction was monitored using TLC and stopped after two days due to its insignificant advancement. The resulting residue was purified by chromatography on 100-200 mesh silica gel (1% $CH_2Cl_2$ in hexane) to yield the product **2a** (10 mg, 2%). Lowering in reaction temperature did not improve the yield.

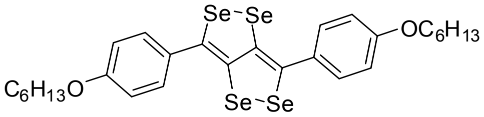
**With radical initiator in microwave:** 1,4-Diphenylbutadiyne **1a** (101 mg, 0.5 mmol), selenium metal powder (158 mg, 2 mmol) and 2,2,6,6-Tetramethylpiperidinyloxy (TEMPO) (7 mg, 10 mol%) were mixed in *o*-dichlorobenzene and charged into a microwave vial which was irradiated at 190 °C for 1 hour. The resulting reaction mixture was purified by column chromatography on 100-200 mesh silica gel (using 0-1% $CH_2Cl_2$ in hexane) to give the product (10 mg, 2%). At lower temperatures no better yield was received.

**Synthesis of 2b:**



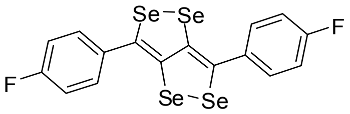
1,4-Di(thiophen-2-yl)buta-1,3-diyne **1b** (100 mg, 0.46 mmol) and neat selenium metal powder (193 mg, 1.84 mmol) were mixed well in a Schlenk flask and the resulting mixture was heated at 170 °C for 0.5 h. The reaction was cooled before charging the resulting residue for purification by chromatography on silica gel (2% $CH_2Cl_2$ in hexane) to afford the product **2b** (30 mg, 12%). M. p.: 130 °C. $^1$H NMR (400 MHz, $\delta$, ppm, DMSO-$d_6$): 7.76 (d, $J$ = 5.32 Hz, 2H), 7.26 (d, $J$ = 3.8 Hz, 2H), 7.18 (dd, $J$ = 4.6 Hz, $J$ = 3.8Hz, 2H). $^{13}$C NMR (100 MHz, $\delta$, ppm, DMSO-$d_6$): 137.7, 131.5, 128.64, 128.62, 127.4, 126.6. HRMS (ESI+): calculated for $C_{12}H_6S_2Se_4$ 533.6572; found 533.6531.

**Synthesis of 2c:**



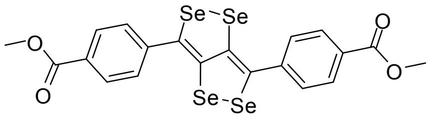
1,4-Bis(4-(hexyloxy)phenyl)buta-1,3-diyne **1c** (200 mg, 0.5 mmol) and neat selenium metal powder (157 mg, 2 mmol) were added into a Schlenk flask and mixed well before heating it at 205 °C for 0.5 h after which the reaction mixture became dark. The reaction was cooled and the resulting crude mixture was purified by chromatography on 100-200 mesh silica gel (using hexane as eluaet) to result in the product **2c** (118 mg, 30%). M. p.: 164 °C. $^1$H NMR (400 MHz, $\delta$, ppm, $C_6D_6$): 7.40 (d, $J$ = 8.4 Hz, 4H), 7.65 (d, $J$ = 6.23 Hz, 4H). $^{13}$C NMR (100 MHz, $\delta$, ppm, DMSO-$d_6$): 158.9, 146.3, 128.1, 127.3, 118.3, 115.3, 67.6, 31.1, 28.9, 25.1, 22.0, 13.9. HRMS (ESI+): calculated for $C_{28}C_{34}O_2Se_4$ 721.9220; found 721.9274.

**Synthesis of 2d:**



1,4-Bis(4-fluorophenyl)buta-1,3-diyne **1d** (200 mg, 0.5 mmol) and neat selenium metal powder (157 mg, 2 mmol) were charged into a Schlenk flask which was heated at 180 °C for 0.5 h. The reaction was cooled and the resulting residue was purified by chromatography on silica gel (using hexane as eluent) to afford the product **2d** (35 mg, 15%). M. p.; 184 °C. $^1$H NMR (400 MHz, $\delta$, ppm, DMSO-$d_6$): 7.56 (m, 4H), 7.34 (m, 4H). . $^{13}$C NMR (100 MHz, $\delta$, ppm, DMSO-$d_6$): 163.0 (d, $J$ = 251.7 Hz), 128.5 (d, $J$ = 34.3 Hz), 128.0, 127.7 (d, $J$ = 99.1 Hz), 124.9, 116.8 (d, $J$ = 87.7 Hz). HRMS (ESI+): calculated for 557.7255; found 556.7212.

**Synthesis of 2e:**



A Schlenk flask containing a mixture of dimethyl 4,4'-(buta-1,3-diyne-1,4-diyl)dibenzoate **1e** (100 mg, 0.31 mmol) and neat selenium metal powder (100 mg, 1.24 mmol) was heated at 205 °C for 0.5 h before taking it to rt. The resulting residue was purified by chromatography on 100-200 mesh silica gel (using hexane as eluent) to yield the product **2e** (20 mg, 10%). M. p.: 215°C. . $^{1}$H NMR (400 MHz, $\delta$, ppm, DMSO-$d_6$): 8.00 (d, $J$ = 6.8 Hz, 4H), 7.78 (d, $J$ = 6.8 Hz, 4H), 3.87 (s, 6H). $^{13}$C NMR (100 MHz, $\delta$, ppm, DMSO-$d_6$): 165.5, 132.6, 131.3, 130.4, 129.6, 128.6, 124.9, 67.4. HRMS (ESI+): calculated for $C_{20}H_{14}O_4Se_4$ 637.7553; found 637.7549.

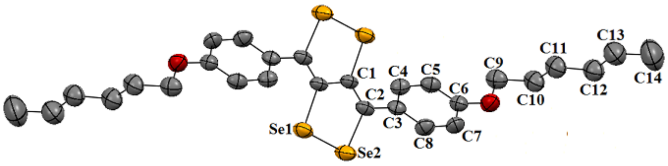
**Table S1.** Crystallographic data and refinement parameters for **2a-2c**.

| Parameters | **2a** | **2b** | **2c** |
|---|---|---|---|
| Empirical formula | $C_{16}$ $H_{10}$ $Se_4$ | $C_{12}$ $H_6$ $S_2$ $Se_4$ | $C_{28}$ $H_{34}$ $O_2$ $Se_4$ |
| Formula weight | 518.08 | 530.15 | 718.39 |
| Crystal system | Monoclinic | Monoclinic | Monoclinic |
| Space group | *P 21/c* | *C 2/c* | *P 21/c* |
| $T$ (K) | 109.16(10) | 293(2) | 140.82(10) |
| $a$ (Å) | 9.5965(5) | 24.5589(15) | 18.1478(13) |
| $b$ (C) | 13.4527(7) | 11.0932(5) | 5.4977(4) |
| $c$ (Å) | 5.8626(3) | 5.5670(3) | 14.5628(9) |
| $\alpha$ (°) | 90.00 | 90.00 | 90.00 |
| $\beta$ (°) | 91.639(5) | 92.535(4) | 92.282(7) |
| $\gamma$ (°) | 90.00 | 90.00 | 90.00 |
| $Z$ | 2 | 4 | 2 |
| $V$ (Å$^3$) | 756.54(7) | 1515.16(14) | 1451.79(18) |
| $D_x$ (g/cm$^3$) | 2.757 | 2.324 | 1.643 |
| Radiation | Cu Kα ($\lambda$ = 1.54184 Å) | Mo Kα ($\lambda$ = 0.71073 Å) | Mo Kα ($\lambda$ = 0.71073 Å) |
| μ(Mo Kα)/mm$^{-1}$ | 11.485 | 9.938 | 5.076 |
| $F$(0 0 0) | 584.0 | 984.0 | 708.0 |
| Crystal size/mm | 0.23 × 0.23 × 0.12 | 0.21 × 0.13 × 0.08 | 0.31 × 0.14 × 0.11 |
| $\theta$ range for data collection (°) | 3.31-65.92 | 2.01 -26.13 | 2.25-27.8290 |

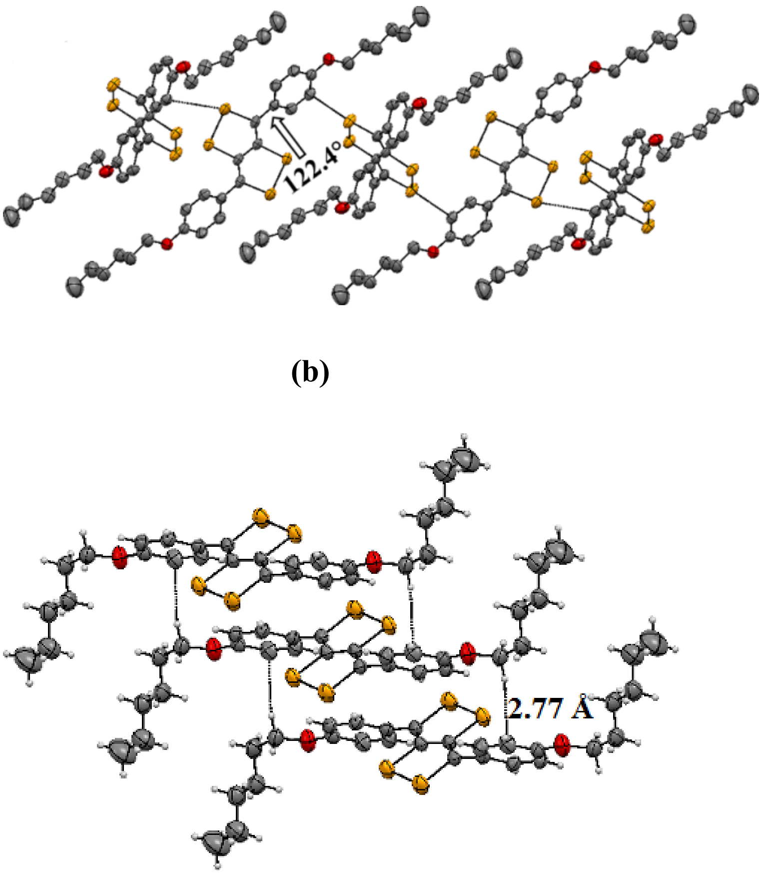
|  |  |  |  |
|---|---|---|---|
| Limiting indices | $-11 \leq h \leq 11, -15 \leq k \leq 15, -6 \leq l \leq 6$ | $-29 \leq h \leq 29, -13 \leq k \leq 13, -6 \leq l \leq 6$ | $-23 \leq h \leq 23, -7 \leq k \leq 7, -19 \leq l \leq 19$ |
| Reflections collected | 1229 | 1082 | 1882 |
| Data/restraints/parameters | 1316/0/91 | 1339/0/82 | 3152/0/155 |
| Unique reflections | 1316 | 1339 | 3152 |
| $R$ indices I > 2σ(I) | $R1$ = 0.0338, w$R2$ = 0.1063 | $R1$ = 0.0495, w$R2$ = 0.1302 | $R1$ = 0.0462, w$R2$ = 0.0870 |
| $R$ indices (all data) | $R1$ = 0.0358, w$R2$ = 0.1101 | $R1$ = 0.0578, w$R2$ = 0.1373 | $R1$ = 0.0889, w$R2$ = 0.1051 |
| $(\Delta/\sigma)_{max}$ | 0.001 | 0.001 | 0.001 |
| $(\Delta/\rho)_{max}$ (e Å$^{-3}$) | 0.712 | 0.787 | 0.647 |
| CCDC deposition number | 1011954 | 1011956 | 1011963 |

### Crystal structure of 2c

In **2c** the dihedral angle between the hexyloxy substituted phenyl ring and the central $C_4Se_4$ unit is 122.4° (C8-C3-C2-C1 = −122.4(5)). In crystal, **2c** exhibits π···Se interactions (Se2-C5 = 3.57 Å) between two anticofacially interacting molecules and also π···H-C (C7-H9B = 2.77 Å) interactions between two molecules from different layers (Fig. S13) to result in a 2D interpenetrating network in solid.



**(a)**

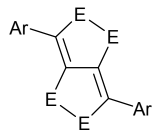


(b)

(c)

**Figure S1** (a) ORTEP diagram of **2c**, (b) packing through ab plane and torsional angle in **2c**, (c) π···H-C interaction in **2c**.

## DFT Calculation



**2a** E = Se, Ar = Ph
**2b** E = Se, Ar = Thiophene
**3a** E = S, Ar = Ph
**3a** E = S, Ar = Thiophene

DFT calculations **2a**, **2b**, **3a** and **3b** were carried out at B3LYP/6-31G(d) using Gaussian 09 program.[4] Optimized structures are shown in Figure S2. Optimized structure of **2a** showed less twisting (~47°) between the $C_4Se_4$ unit and phenyl capping than that was observed in the single crystal X-ray structure (~53°). The corresponding $C_4S_4$ derivative **3a** showed significantly larger value of dihedral angle (~39°) than the experimentally observed value (25°). As expected, optimized structures of $C_4S_4$ and $C_4Se_4$ derivatives with thiophene capping (**2b** and **3b**) showed planar structures.

TD-DFT calculated (at B3LYP/6-31G(d)) absorption spectra match with the experimentally observed two band structure, however, overestimate by ~20 nm (Figure S3).

Comparison between the experimental and calculated HOMO, LUMO energies and HOMO-LUMO gaps are given in Table 2.

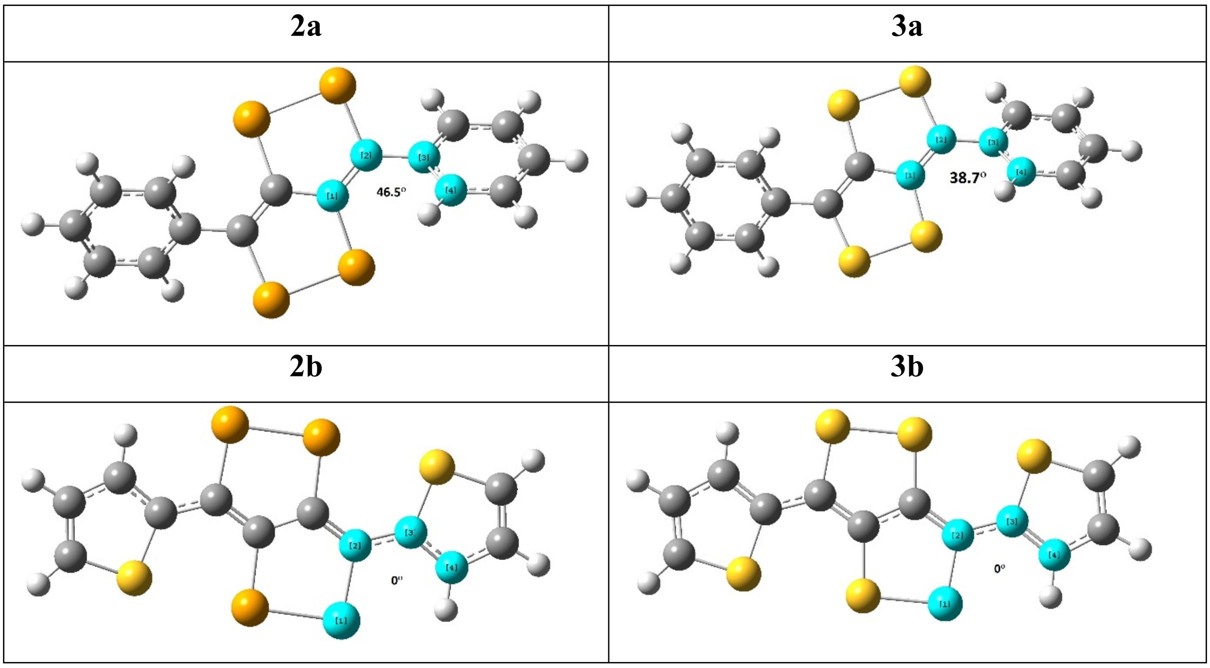


**Figure S2** Optimized structures of **2a**, **2b**, **3a** and **3b**.

**Table S2** Comparison between experimental and calculated properties.

| Comp-ound | $\lambda_{max}$ (nm) | | $E_g$ (eV)[a] | | HOMO (eV)[b] | | LUMO (eV)[c] | |
|---|---|---|---|---|---|---|---|---|
| | Expt[d] | Calc[e,f] | Expt[d] | Calc[e] | Expt[d] | Calc[e] | Expt[d] | Calc[e] |
| **2a** | 240,<br>440 | 274,<br>482 | 2.39 | 2.43 | −4.79 | −4.50 | −2.40 | −2.07 |
| **3a** | 260,<br>458 | 262,<br>460 | 2.38 | 2.62 | −4.86 | −4.64 | −2.48 | −2.01 |
| **2b** | 275,<br>484 | 296,<br>528 | 2.21 | 2.45 | −4.91 | −4.66 | −2.70 | −2.21 |
| **3b** | 270,<br>370 | 294,<br>494 | 2.88 | 2.54 | −5.59 | −4.73 | −2.71 | −2.18 |

[a] for expt: $E_g = E_g^{opt} = 1240/\lambda_{onset}$, for calc: $E_g$ = difference between HOMO and LUMO energies, [b] For Expt: $E_{HOMO} = -4.44 + E_{1/2}$, [c] $E_{LUMO} = E_{HOMO} + E_g^{opt}$, [d] Experimental values of thiophene analogues (ref 9 in the manuscript),[5] [e] calculations were carries of at B3LYP/6-31(d), [f] values are taken from TD-DFT calculated spectra.

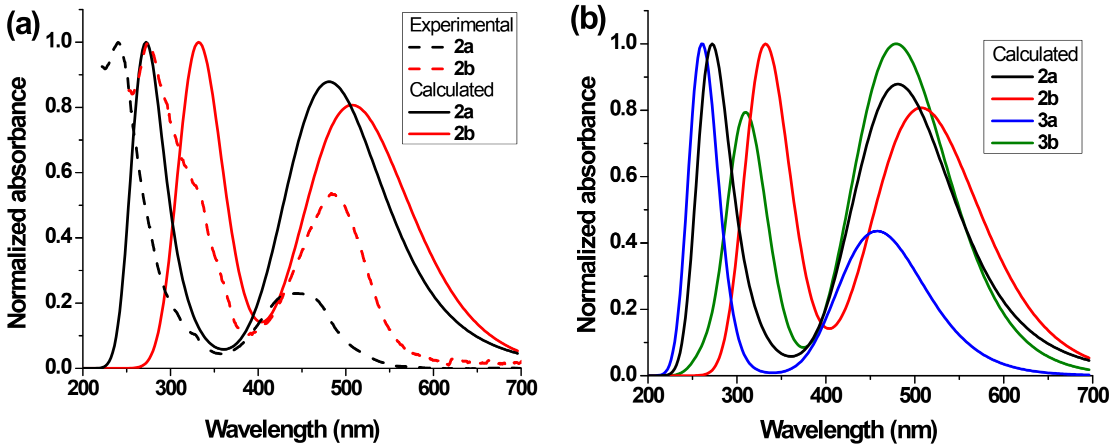


**Figure S3** (a) Experimental and calculated spectra of **2a** and **2b**. (b) Calculated spectra of sulfur analogues of **3a** and **3b**.

## References

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[2] *J. Appl. Cryst.*, 2007, **40**, 786-790.

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[4] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr. J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, Revision E.01*; Gaussian Inc.: Wallingford CT, 2009.

[5] D. J. Schipper, L. C. H. Moh, P. Müller and T. M. Swager, *Angew. Chem. Int. Ed.*, 2014, **53**, 5847.

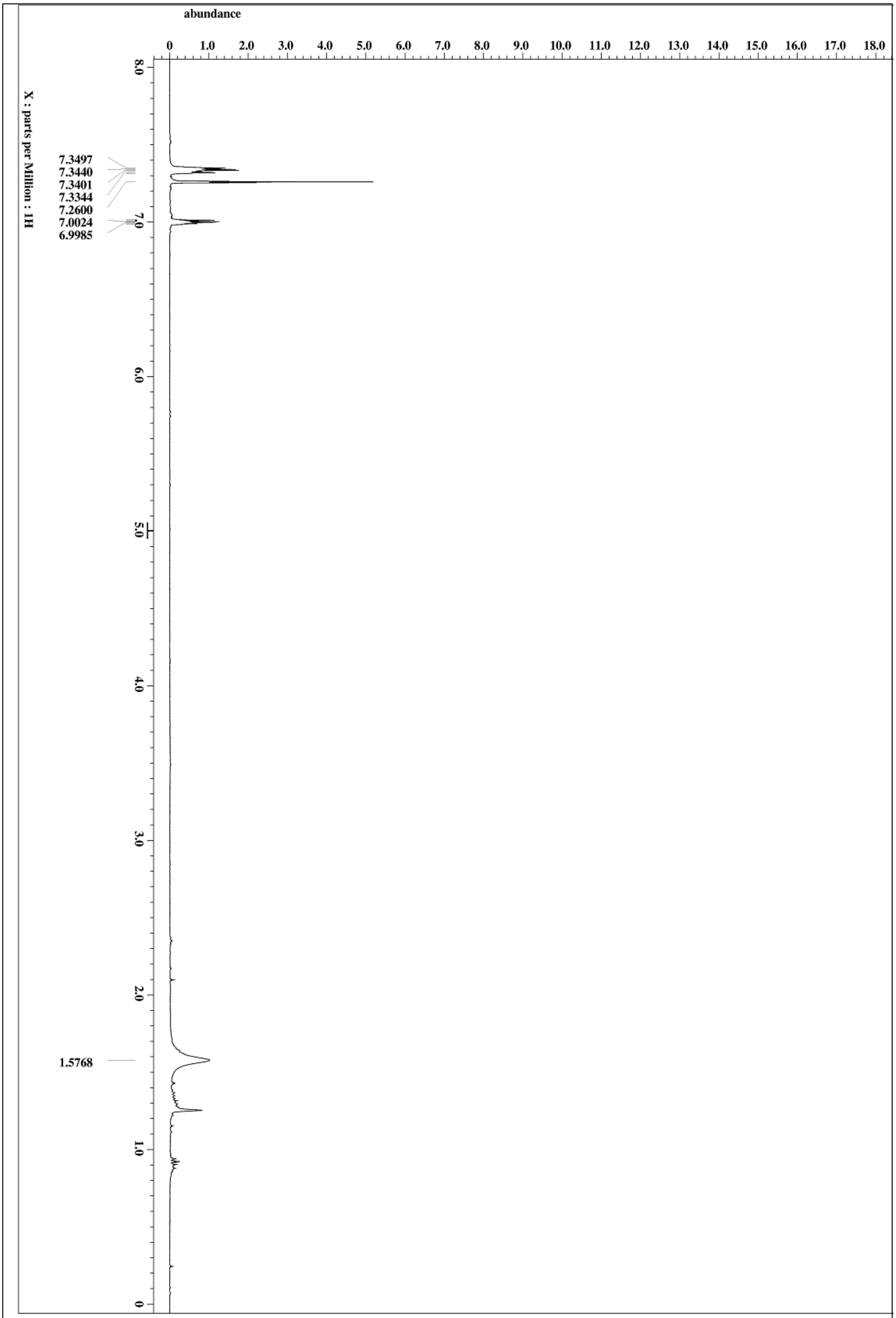

**Figure S4** $^1$H NMR of compound **1b**.

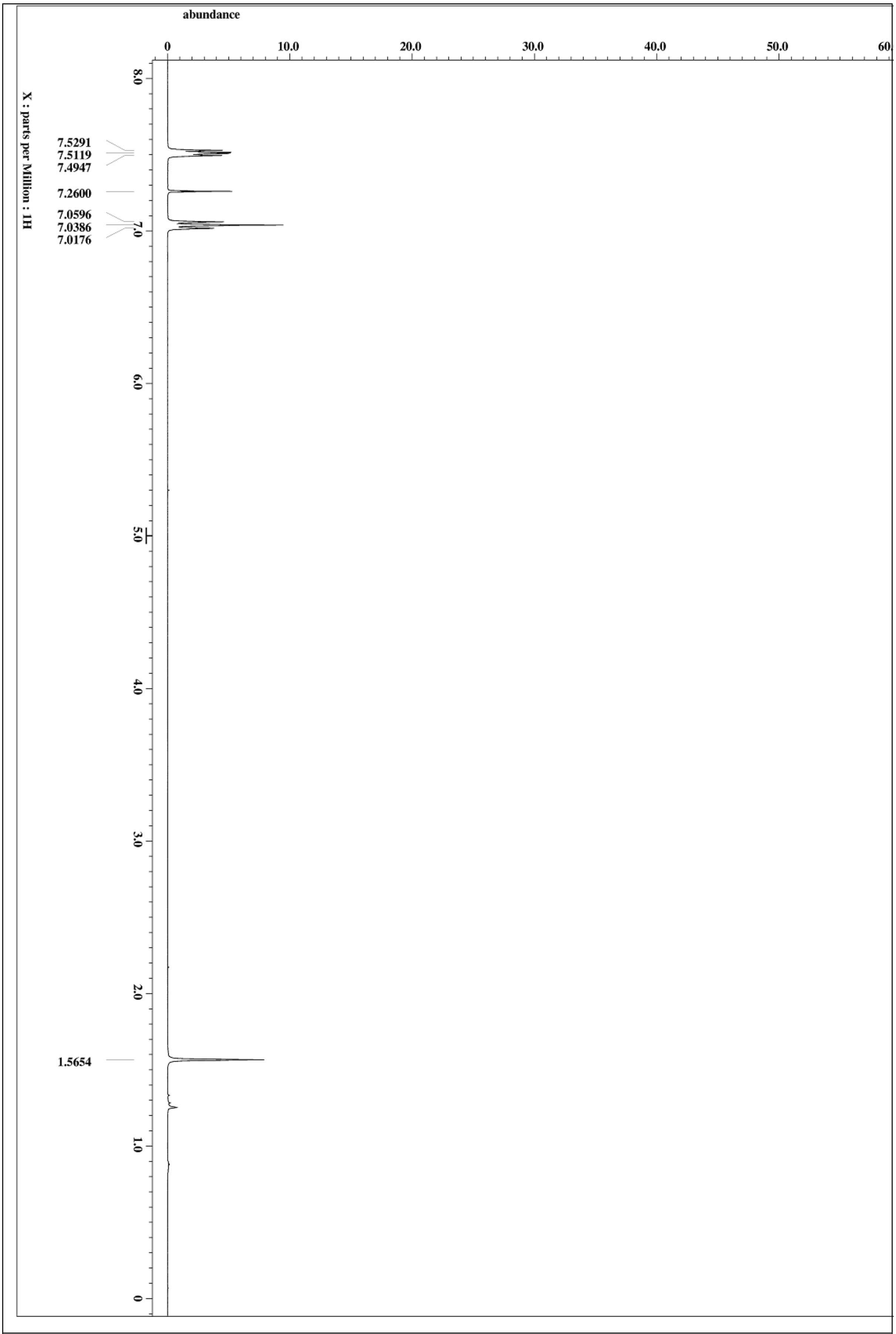

**Figure S5** $^1$H NMR of compound **1d**.

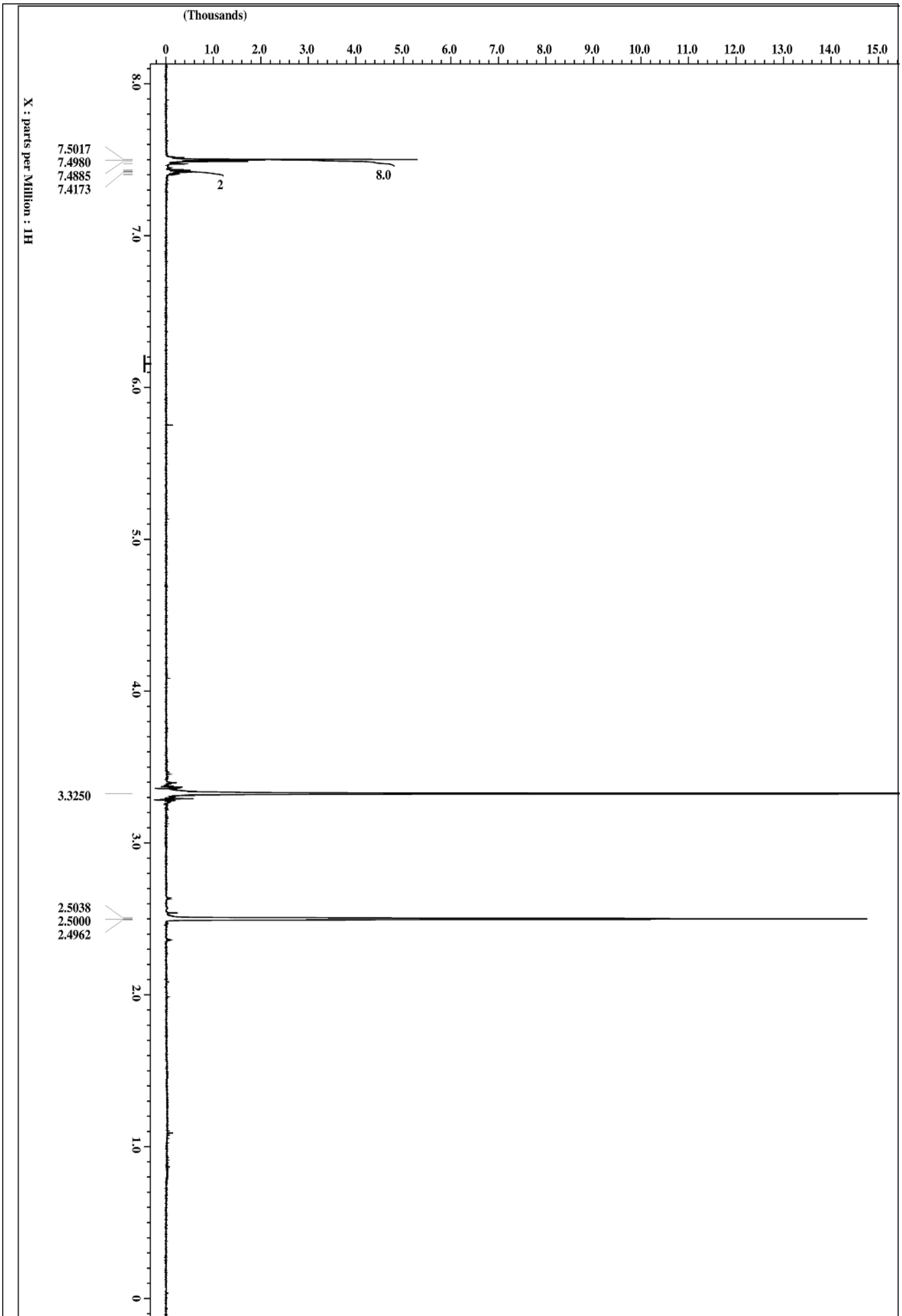

**Figure S6** $^1$H NMR of compound **2a**.

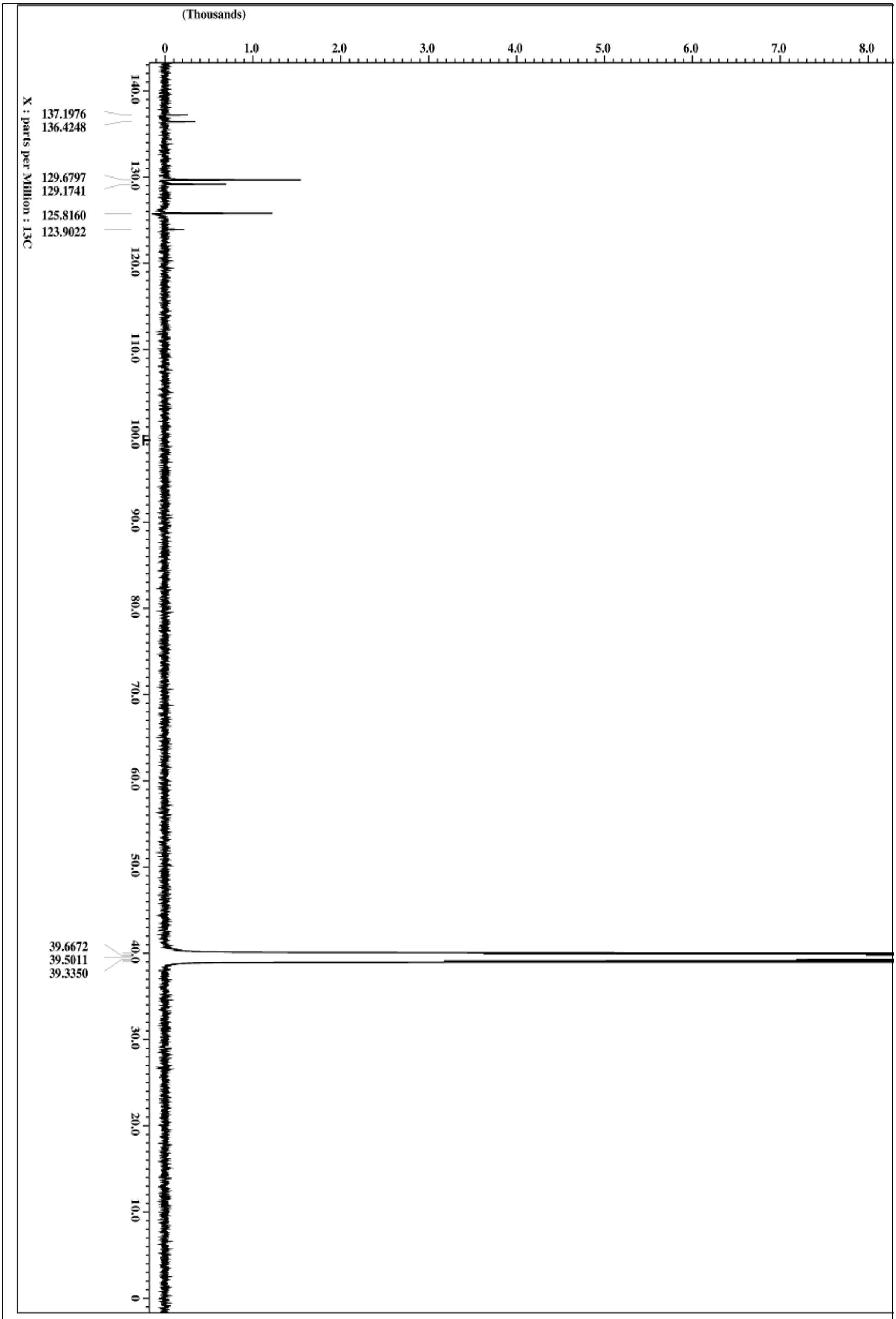

**Figure S7** $^{13}$C NMR of compound **2a**.

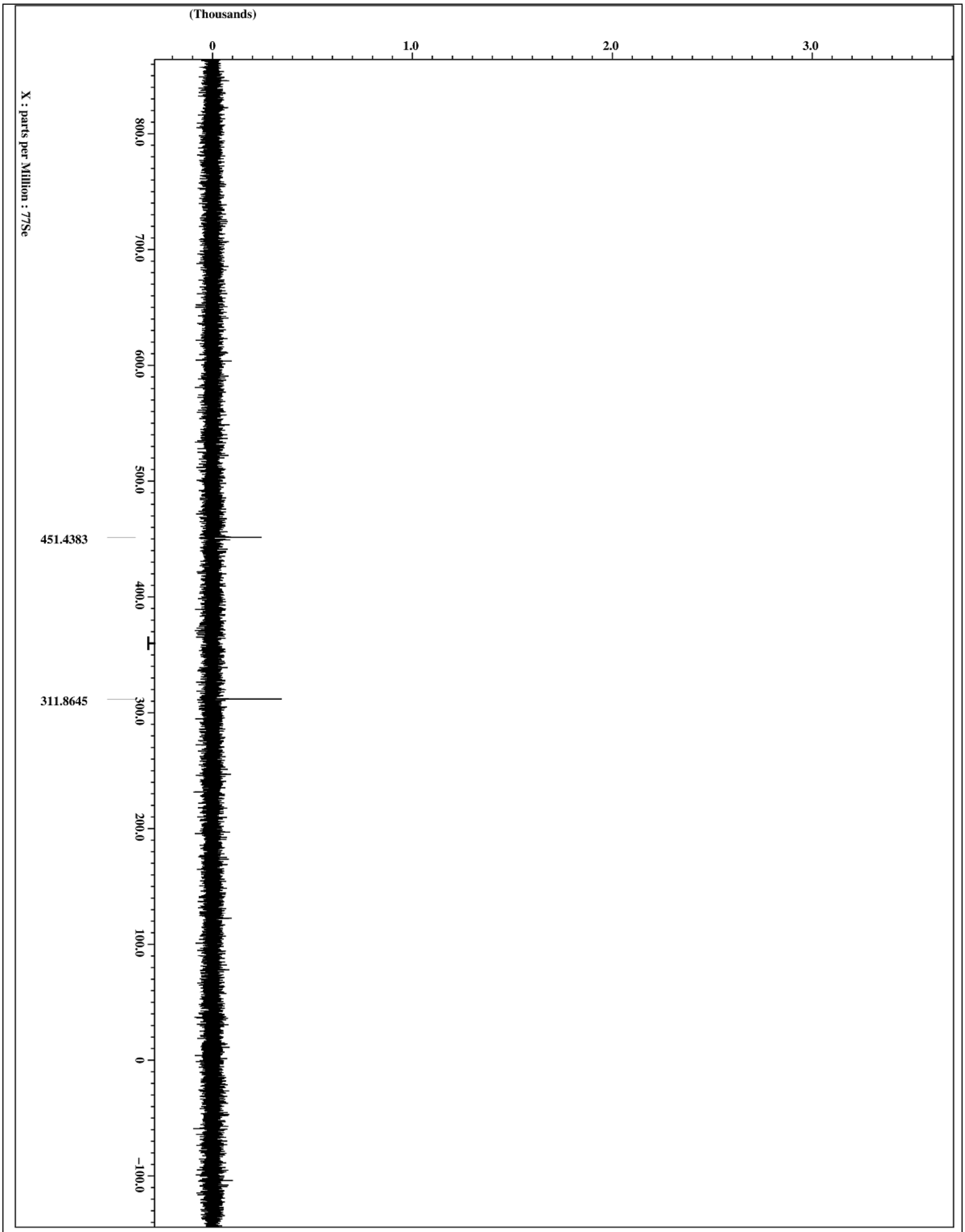

**Figure S8** $^{77}$Se NMR of compound **2a**.

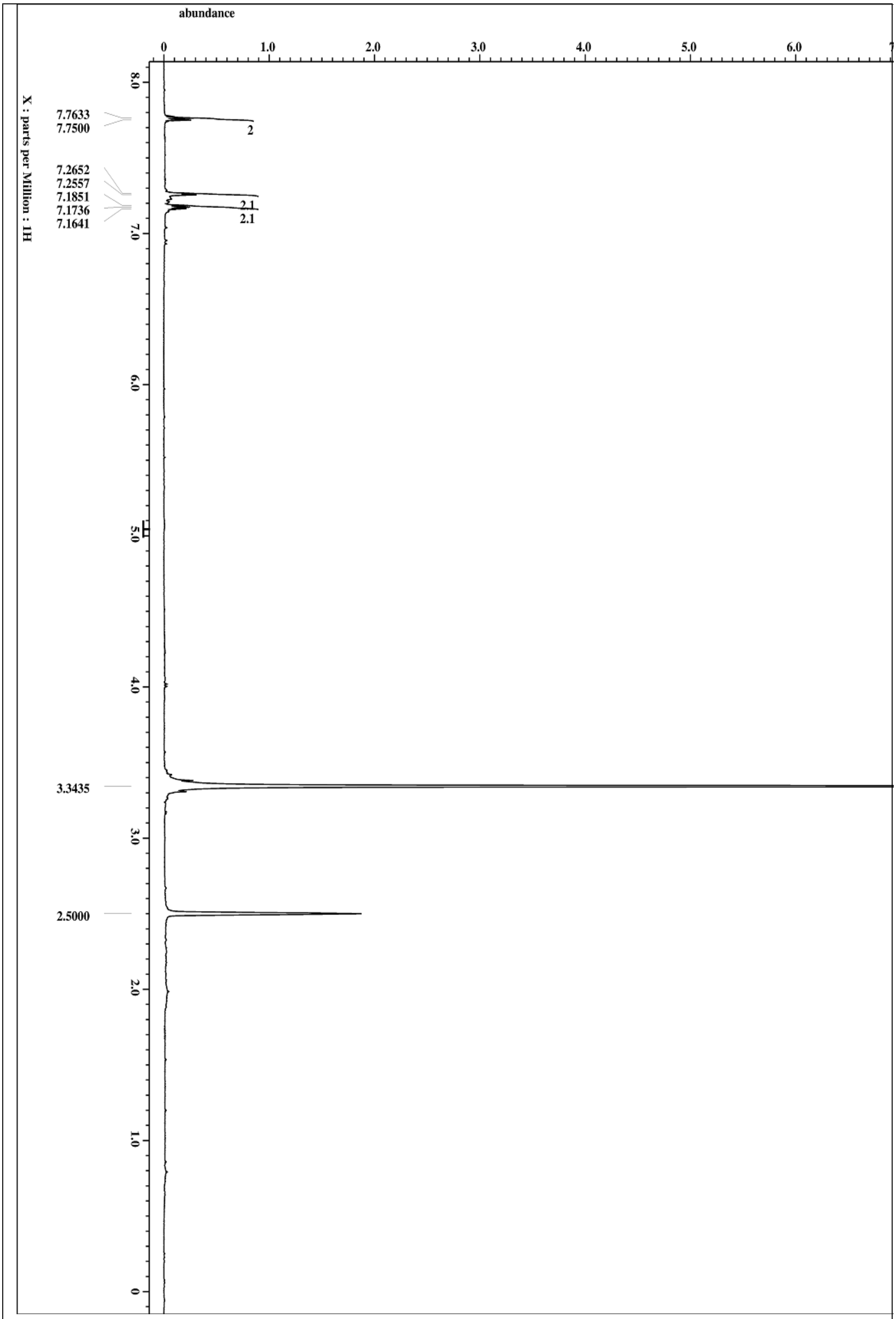

**Figure S9** $^1$H NMR of compound **2b**.

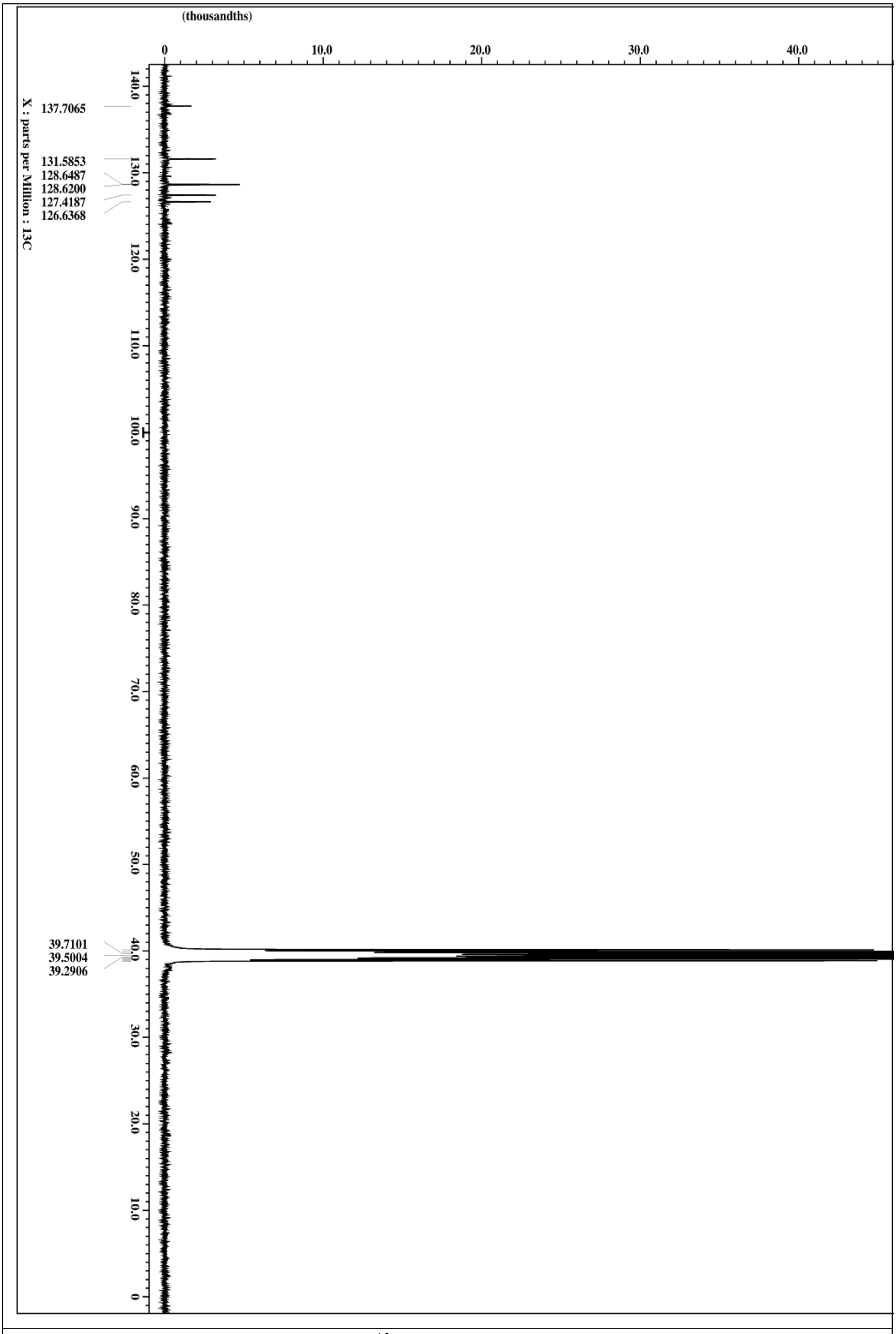

**Figure S10** $^{13}$C NMR of compound **2b**.

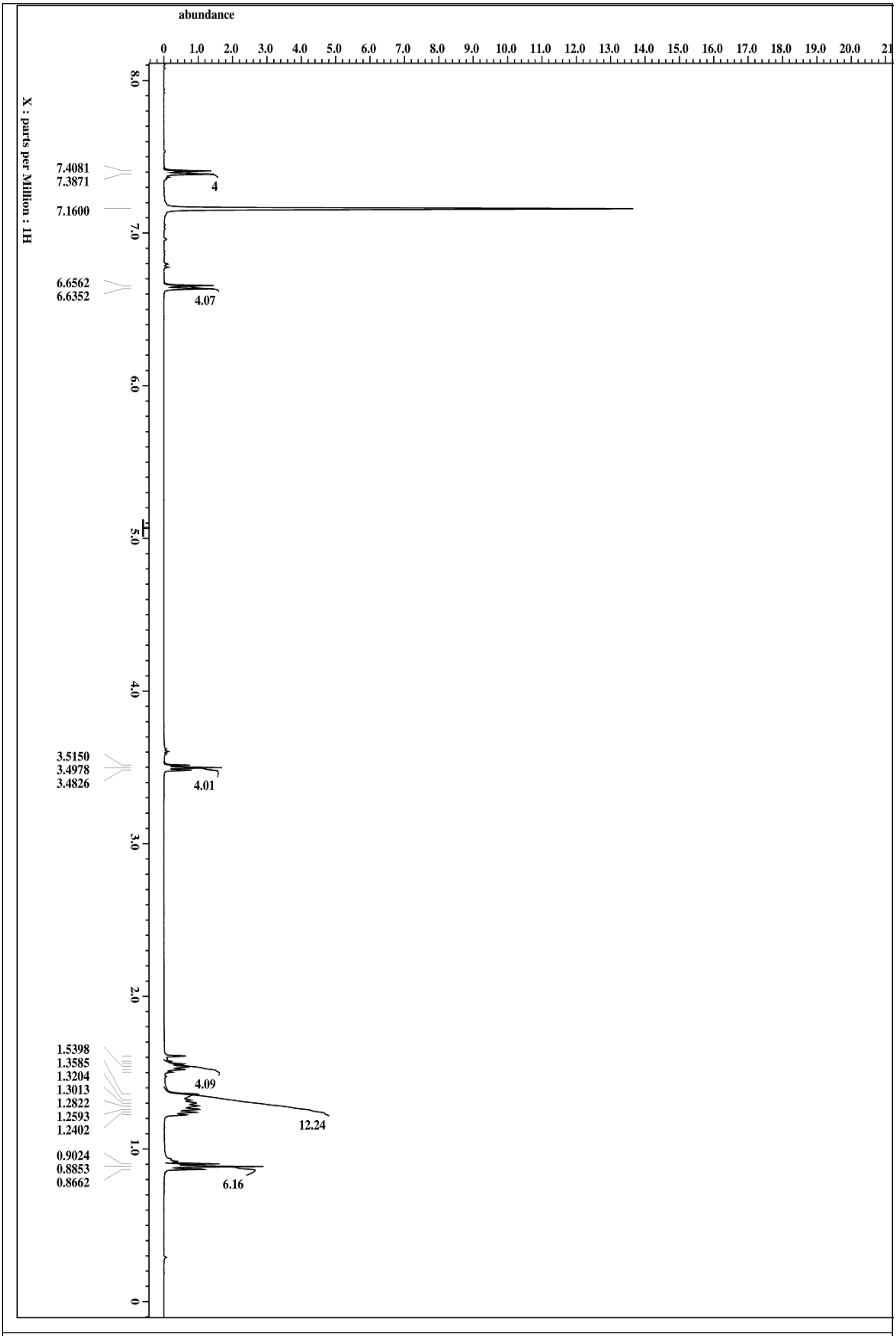

**Figure S11** $^1$H NMR of compound **2c**.

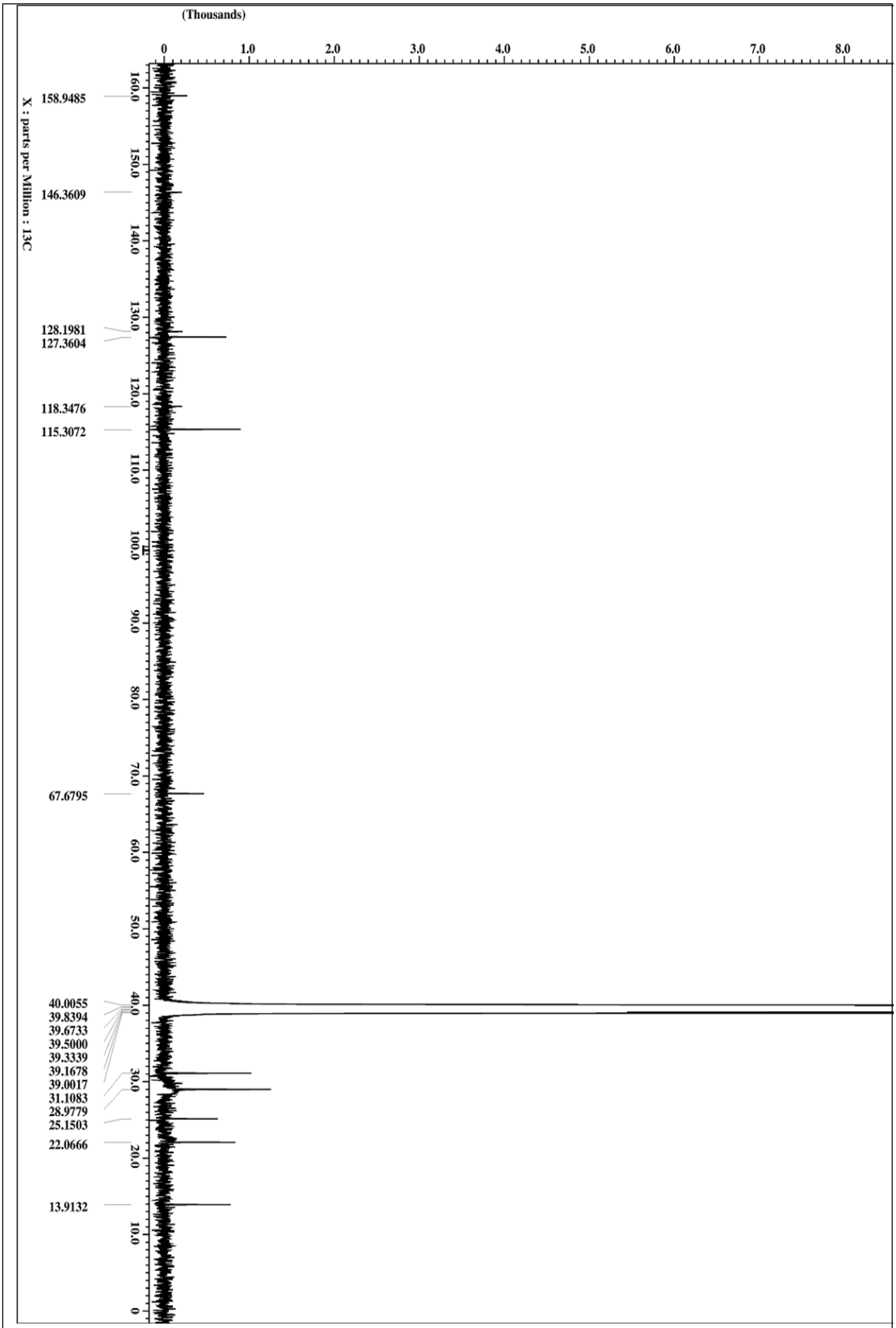

**Figure S12** $^{13}$C NMR of compound **2c**.

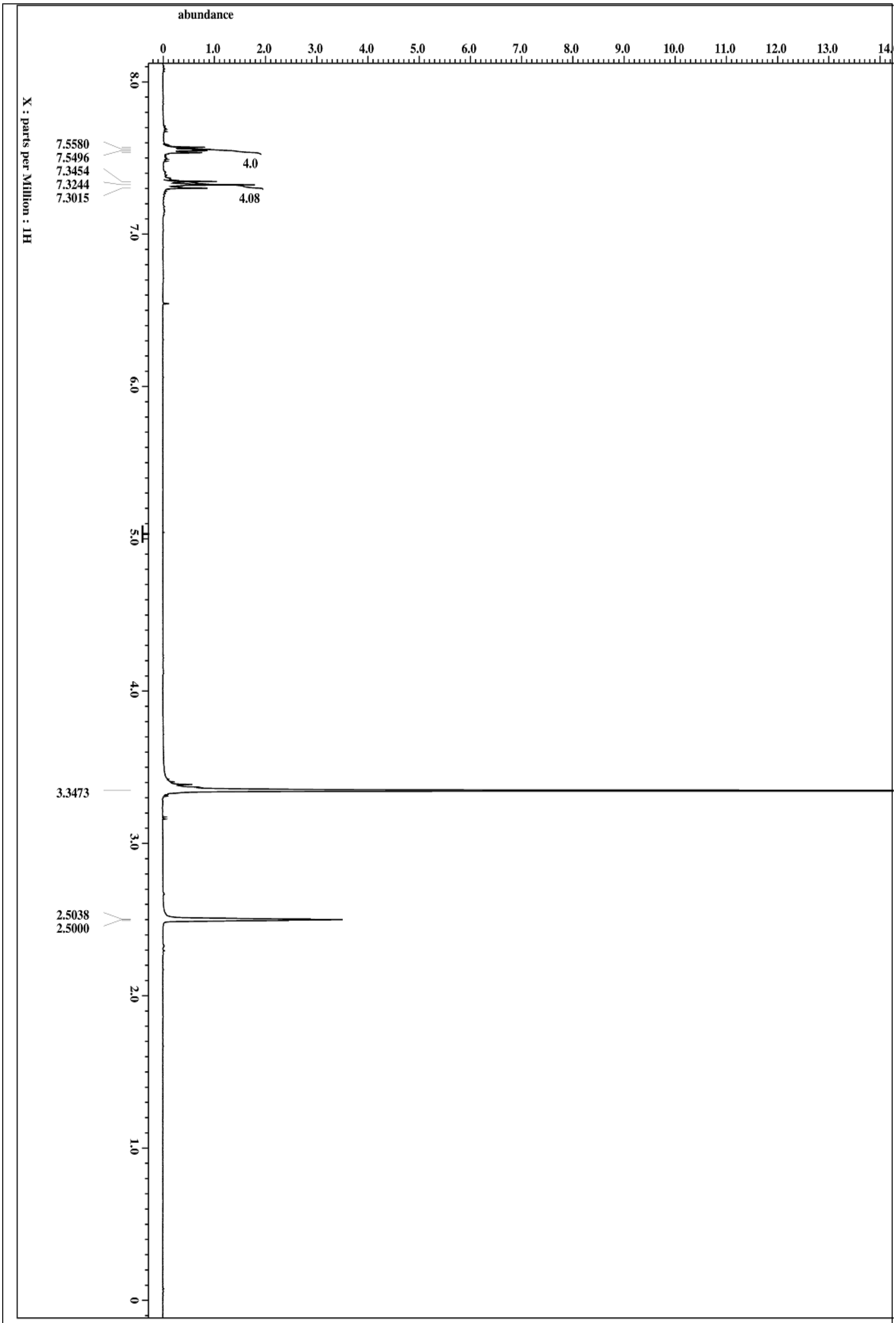

**Figure S13** $^1$H NMR of compound **2d**.

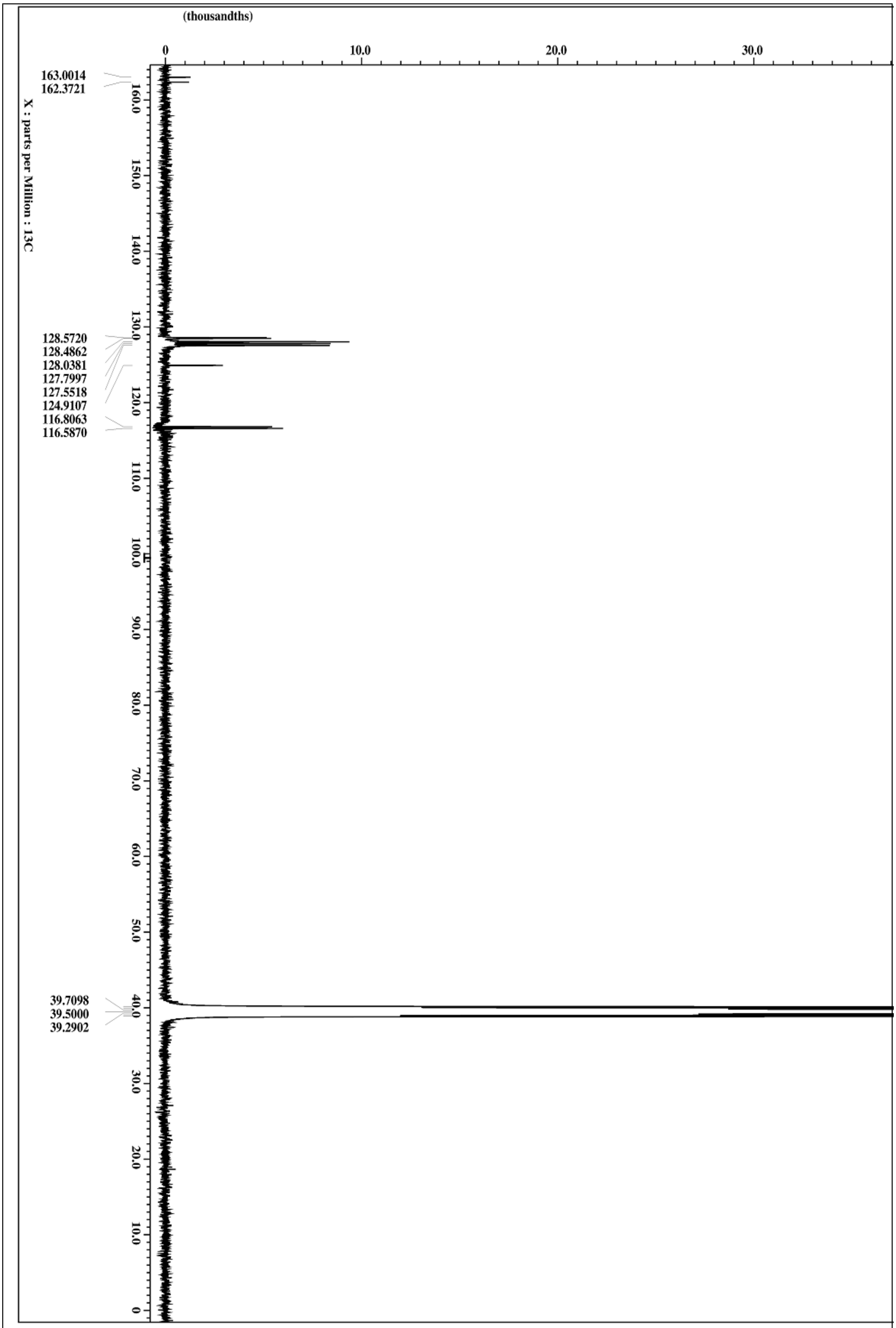

**Figure S14** $^{13}$C NMR of compound **2d**.

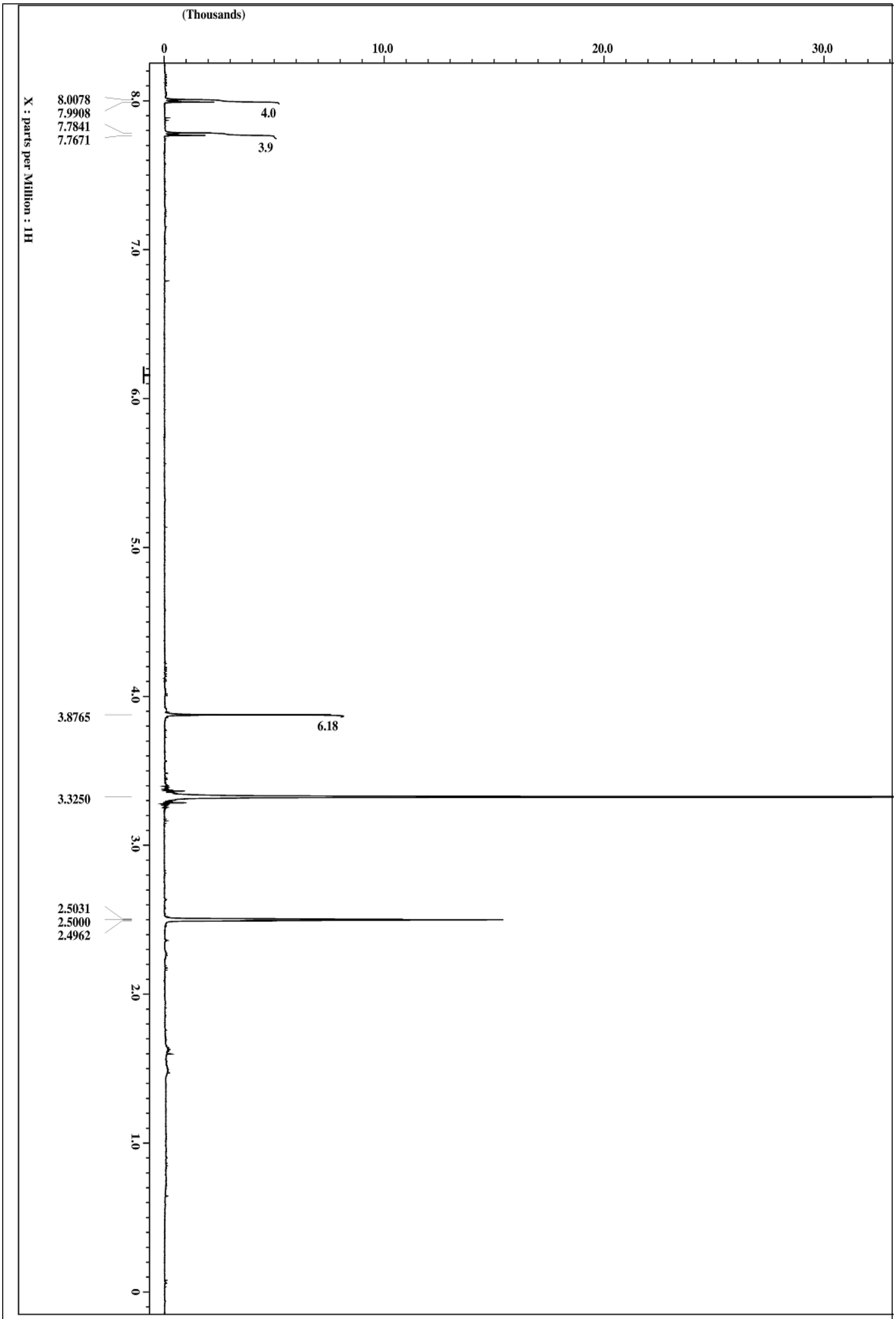

**Figure S15** $^1$H NMR of compound **2e**.

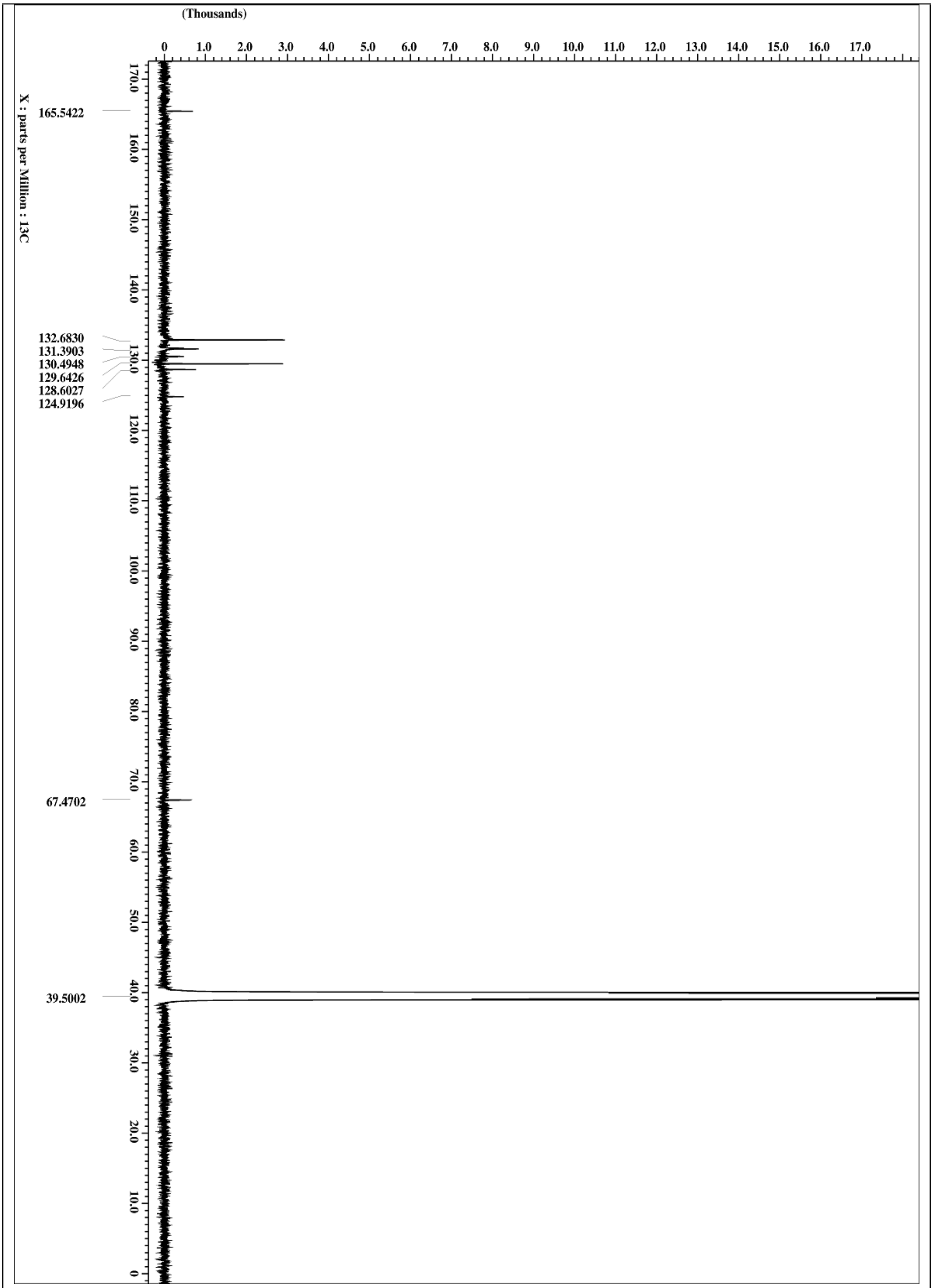

Figure S16 $^{13}$C NMR of compound **2e**.

## Coordinates of optimized structures of 2a, 2b, 3a and 3b.

**2a**

```
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.788246   -0.508754    0.015130
      2          6           0       -0.676372    0.262025   -0.035228
      3          6           0        0.676355   -0.262024   -0.035249
      4          6           0        1.788241    0.508740    0.015104
      5          6           0       -3.193764   -0.063309    0.061627
      6          6           0       -4.162302   -0.673054   -0.756216
      7          6           0       -3.599387    0.957530    0.941698
      8          6           0       -5.493947   -0.264821   -0.704465
      9          1           0       -3.856936   -1.459927   -1.440479
     10          6           0       -4.930936    1.364681    0.985565
     11          1           0       -2.863461    1.425245    1.588325
     12          6           0       -5.883272    0.755800    0.164643
     13          1           0       -6.227109   -0.742632   -1.348569
     14          1           0       -5.227597    2.151763    1.673525
     15          1           0       -6.921455    1.073734    0.203963
     16          6           0        3.193757    0.063274    0.061636
     17          6           0        4.162314    0.672942   -0.756240
     18          6           0        3.599365   -0.957465    0.941832
     19          6           0        5.493964    0.264731   -0.704403
     20          1           0        3.856966    1.459732   -1.440607
     21          6           0        4.930916   -1.364592    0.985786
     22          1           0        2.863416   -1.425132    1.588466
     23          6           0        5.883273   -0.755789    0.164828
     24          1           0        6.227140    0.742480   -1.348537
     25          1           0        5.227566   -2.151594    1.673842
     26          1           0        6.921459   -1.073703    0.204221
     27         34           0        0.785103   -2.181085   -0.235871
     28         34           0       -1.552256   -2.412331    0.097160
     29         34           0       -0.785150    2.181112   -0.235573
     30         34           0        1.552311    2.412321    0.096918
 ---------------------------------------------------------------------
```

**3a**

```
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.742525    0.579397   -0.091586
      2          6           0       -0.675964   -0.259125   -0.197996
      3          6           0        0.676073    0.259942   -0.197918
      4          6           0        1.742422   -0.578863   -0.091483
      5          6           0       -3.165632    0.227629    0.024542
      6          6           0       -4.024999    0.960653    0.865848
      7          6           0       -3.703879   -0.846544   -0.708342
      8          6           0       -5.369166    0.616793    0.982122
      9          1           0       -3.627865    1.786720    1.448735
     10          6           0       -5.048660   -1.191333   -0.582088
     11          1           0       -3.076523   -1.391052   -1.407683
     12          6           0       -5.887000   -0.463023    0.262905
     13          1           0       -6.012924    1.190248    1.643488
     14          1           0       -5.443081   -2.024039   -1.157969
     15          1           0       -6.935614   -0.730812    0.357321
     16          6           0        3.165644   -0.227763    0.024605
     17          6           0        4.024786   -0.961591    0.865476
     18          6           0        3.704314    0.846604   -0.707677
     19          6           0        5.369078   -0.618331    0.981897
     20          1           0        3.627332   -1.787802    1.447940
     21          6           0        5.049240    1.190798   -0.581271
     22          1           0        3.077252    1.391709   -1.406823
     23          6           0        5.887327    0.461696    0.263272
     24          1           0        6.012620   -1.192421    1.642922
     25          1           0        5.443938    2.023677   -1.156711
     26          1           0        6.936049    0.729019    0.357801
     27         16           0       -0.757571   -2.043101   -0.187874
     28         16           0        1.351658   -2.324107   -0.075982
     29         16           0       -1.352656    2.324795   -0.074880
```

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    30         16           0        0.758097    2.043859   -0.188943
 ---------------------------------------------------------------------
```

**2b**

```
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
      1         34           0       -1.514462   -2.454557    0.000037
      2         34           0        0.828445   -2.169230   -0.000158
      3         34           0        1.514472    2.454564    0.000117
      4         34           0       -0.828442    2.169240   -0.000301
      5          6           0        0.680897   -0.248109   -0.000047
      6          6           0       -0.680897    0.248118   -0.000059
      7          6           0       -3.199110   -0.191659    0.000008
      8          6           0       -4.278453   -1.063610   -0.000439
      9         16           0       -3.805182    1.466780    0.000654
     10          6           0       -5.543473   -0.426111   -0.000284
     11          1           0       -4.168686   -2.143075   -0.000938
     12          6           0       -5.453238    0.939832    0.000260
     13          1           0       -6.486092   -0.962247   -0.000587
     14          1           0       -6.248532    1.672773    0.000480
     15          6           0        3.199106    0.191654   -0.000009
     16          6           0        4.278456    1.063597   -0.000399
     17         16           0        3.805163   -1.466791    0.000534
     18          6           0        5.543470    0.426087   -0.000272
     19          1           0        4.168698    2.143063   -0.000838
     20          6           0        5.453223   -0.939855    0.000196
     21          1           0        6.486093    0.962215   -0.000541
     22          1           0        6.248511   -1.672803    0.000376
     23          6           0       -1.797422   -0.547142   -0.000025
     24          6           0        1.797421    0.547147   -0.000025
 ---------------------------------------------------------------------
```

**3b**

```
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        0.678246    0.246110    0.000340
      2          6           0       -0.678249   -0.246101    0.000333
      3          6           0       -3.157457    0.354221    0.000038
      4          6           0       -4.184874    1.283812    0.000638
      5         16           0       -3.832960   -1.272302   -0.001116
      6          6           0       -5.479891    0.705609    0.000341
      7          1           0       -4.014543    2.355160    0.001422
      8          6           0       -5.453759   -0.663228   -0.000434
      9          1           0       -6.396656    1.284846    0.000787
     10          1           0       -6.284788   -1.355386   -0.000738
     11          6           0        3.157456   -0.354221    0.000056
     12          6           0        4.184867   -1.283819    0.000627
     13         16           0        3.832973    1.272296   -0.001009
     14          6           0        5.479889   -0.705627    0.000341
     15          1           0        4.014527   -2.355167    0.001375
     16          6           0        5.453768    0.663211   -0.000399
     17          1           0        6.396649   -1.284872    0.000759
     18          1           0        6.284803    1.355362   -0.000692
     19          6           0       -1.738944    0.619844    0.000112
     20          6           0        1.738942   -0.619837    0.000110
     21         16           0       -0.800481   -2.022320    0.001057
     22         16           0        1.294988   -2.358254   -0.000522
     23         16           0        0.800476    2.022330    0.001032
     24         16           0       -1.294994    2.358262   -0.000413
 ---------------------------------------------------------------------
```