Electronic Supporting Information for

A Palladium complex of a macrocyclic selenium ligand: Catalyst for dehydroxymethylation of dihydroxy compounds

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EXPERIMENTAL SECTION

Crystallography: A DCM : EtOAC (4 mL, 2:2) solution of **C1** was slowly concentrated over a period of 10 days to afford suitable orange colored block like crystals. The crystals were carefully picked under a polarizing microscope and mounted on loop with the help of paraffin oil. The single-crystal X-ray data collection was carried out at Bruker D8 Quest PHOTON II diffractometer with monochromatic Mo Kα radiation (λ = 0.71073 Å) at 296(2) K operating at 50 kV voltage and 20 mA current by using ω and ϕ scan. The diffraction profiles were integrated with the SAINT program[s1] and the obtained data sets were reduced using the APEX3 software. Numerical absorption corrections (multi scan) were performed with SADABS program.[s2] The structure was solved and refined by the full matrix least-square method on F^2 using SHELXL-2016[s3] present in the WINGX package of programs (Version 2018-3).[s4] One can find B-level alerts are due to the significant disorder in the compounds **C1**, for which no further modelling was attempted. All the non-hydrogen atomic sites in the present structure were located successfully in different Fourier maps and finally refined with anisotropic displacement parameters. Hydrogen atoms were fixed geometrically in calculated positions and refined using the riding model. The details about the crystal structure solution and final refinement parameters for compound **C1** are listed in Table s1 along with data of **L1**. Selected bond distances and angles are given in Table s2. The crystallographic files can be obtained for the compounds **L1**, and **C1** (2192408 and 2192410), from the Cambridge Crystallographic Data Center (CCDC) via www.ccdc.cam.ac.uk/datarequest/cif. Selected bond lengths around the square planer geometry of palladium are shown in figure s1.

Table s1. Summary of crystallographic data.

	L1	**C1**
empirical formula	$C_{11}H_{13}OSe_{0.50}$	$C_{44}H_{52}Cl_2O_4PdSe_2$
formula weight	200.69	980.07
temperature [K]	293(2)	296(2)
Diffractometer	Rigaku Oxford 2018	Bruker D8 Quest PHOTON II
wavelength [Å]	1.54184	0.71073
crystal system	Orthorhombic	Monoclinic
space group	P n m a	P 21/c
unit cell dimensions:		
a[Å]	18.412(2)	24.3388(17)
b[Å]	23.1159(13)	10.2891(7)
c[Å]	4.7170(4)	18.3315(12)
α[°]	90.00	90
β[°]	90.00	109.150(2)
γ[°]	90.00	90
V[Å^3]	2007.6(3)	4336.6(5)
Z	8	4
ρ_{calc}[Mg/m^3]	1.328	1.501
μ[mm^{-1}]	2.611	2.269
F(000)	832	1984
crystal size [mm^3]	0.9 × 0.547 × 0.501	0.30 × 0.250 × 0.180
θ limit[°]	4.7990 to 64.6250	3.132 to 25.000
index range (h, k, l)	–16, 21, –20, 27, –4, 5	–28, 28,-12, 12, -21, 21
reflections collected	3480	75216
independent reflections	1802	7581
R(int)	0.0503	0.0284
max. and min. transmission	1.0000 and 0.18744	0.685 and 0.549
data/restraints/parameters	1802/0/ 115	7581/0/478
goodness-of-fit on F^2	1.056	1.034
R indices (final) [I> 2σ(I)]		
R_1	0.0999	0.0284
wR_1	0.1345	0.0665
R indices (all data)		
R_1	0.2731	0.0368
wR_2	0.3115	0.0692
largest diff. peak and hole [eÅ^{-3}]	2.254 and -1.060	0.635 and -0.575

Table s2. Key crystallographic distances [Å] and angles [°].

C1	
Bond	**Length (Å)**
Pd(1)—Se(1)	2.4320(3)
Pd(1)—Se(2)	2.4306(4)
Pd(1)—Cl(1)	2.2979(8)
Pd(1)—Cl(2)	2.2930(8)
Se(1)—Cl(1)	1.9770(3)
Se(2)—Cl(2)	1.9820(3)
C1	
Bond	**Angle (deg.)**
Se(2)—Pd(1)—Se(1)	169.20(1)
Cl(1)—Pd(1)—Se(2)	94.16(2)
Cl(2)—Pd(1)—Se(2)	86.12(2)
Cl(1)—Pd(1)—Se(1)	87.29(2)
Cl(2)—Pd(1)—Se(1)	93.22(2)
Cl(1)—Pd(1)—Cl(2)	175.75(4)

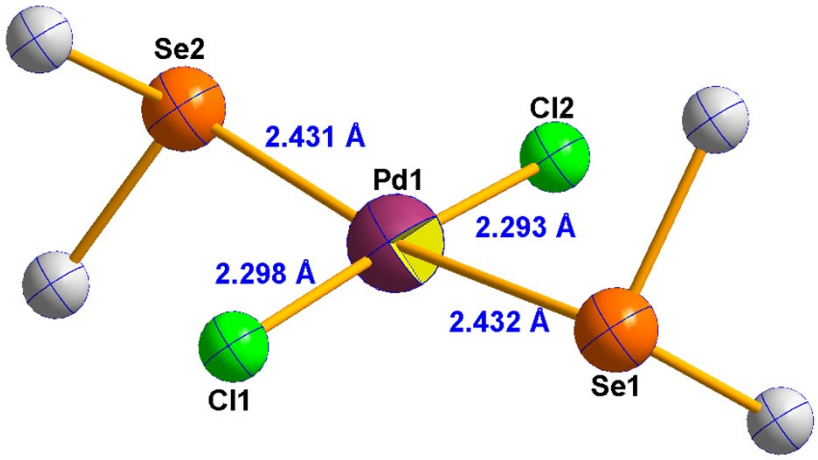


Figure s1. Selected bond lengths around the square planer geometry of palladium in **C1**.

Computational Studies of Selenium Inversion: To understand the selenium inversion process in the complex **C1**, we have calculated the energy barrier for the inversion process by employing the density functional method B3LYP.[s5-s8] We have employed a mixed basis set consisting of LANL2DZ[s8-s11] for heavy atoms (Pd, Se, Cl) to account for the relativistic effects and a 6-31G (D, P)[s12-s14] basis set for the lighter atoms (H, C, O). All the calculations are performed with Gaussian

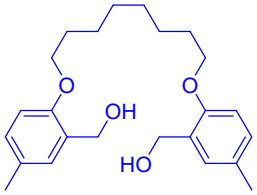
program package.[s15] To the end, we have optimized geometries **C1-R**, **TS** (pyramidal inversion) and **C1-P** (see Fig. 6). The **C1-R** and **C1-P** are local minima on the account of all positive frequencies and **TS** is a first order saddle point with one negative frequency of magnetude -118 cm^{-1}. The activation energy required for the pyramidal inversion is ~18.81 kcal/mol. This activation energy can easily be achieved at the elevated temperatures used in the variable temperature NMR (see main manuscript).

Table s3. Comparison on earlier reported dehydroxymethylation of mono-alcohols with current protocol.

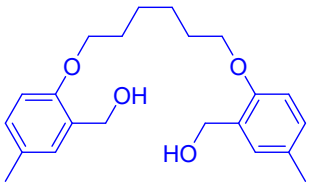
Catalyst	mol%	Time (h)	Temp. (˚C)	Yield (%)	Reference
$[To^{M}Rh(CO)_2]$	0.009	24	450 W Hg lamp.	>95	s16
$[Ir(coe)_2Cl]_2$, Ligand- rac-BINAP	2.5 and 5	8	164	61	s17
$Pd(OAc)_2$	8 - 16	24-48	130	93	s18
$[Ir(coe)_2Cl]_2$ Ligand- rac-BINAP, LiCl	2.5, 5, and 10	8	164	66-97	s19
$Ru(COD)Cl_2$ Ligand- $P(o\text{-}tolyl)_3$	5 and 12.5	16	177	90-93	s20
Pd/CeO_2.	3	5	180	>90	s21
Ni/CeO_2–NaNaph	10	24	150	67	s22
***Trans-*$PdCl_2(SeR_2)_2$**	***5***	***48 h***	***130***	***64-91***	***Current work***

Spectroscopic Data of Starting Materials:

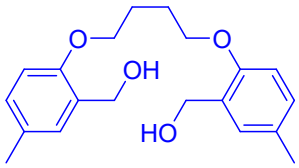
The starting materials (**3a-3t**) were synthesized by using an earlier reported procedure.[s23] The spectroscopic data of starting materials **3a-3l** are in agreement with the reported data.[s23]



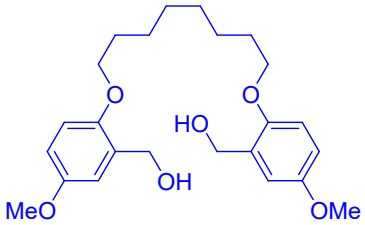
((Octane-1,8-diylbis(oxy))bis(5-methyl-2,1-phenylene))dimethanol) (3m): Appeared as off-white solid, (89%). ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm): 7.08 (s, 2H), 7.03 (d, J = 8 Hz, 2H), 6.76 (d, J = 8 Hz, 2H), 4.65 (s, 4H), 3.98 (t, J = 6 Hz, 4H, OCH_2), 2.94 (s, 1H), 2.88 (s, 1H), 2.28 (s, 6H), 1.79 – 1.81 (m, 4H), 1.40 – 1.48 (m, 8H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 154.7 (s), 129.6 (s), 129.3 (s), 128.9 (s), 128.8 (s), 111.0 (s), 68.0 (s), 62.0 (s), 29.2 (s), 29.2(s), 26.0 (s), 20.3 (s).



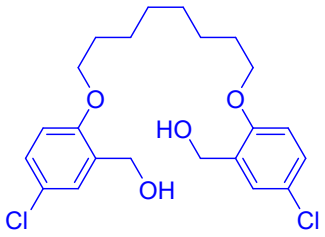
((Hexane-1,6-diylbis(oxy))bis(5-methyl-2,1-phenylene))dimethanol) (3n): Appeared as off-white solid, (92%). ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm): 7.08 (s, 2H), 7.03 (d, J = 8 Hz, 2H), 6.76 (d, J = 8.5 Hz, 2H), 4.63 (s, 4H), 4.00 (t, J = 6 Hz, 4H, OCH_2), 2.95 (s, 1H, OH), 2.88 (s, 1H, OH), 2.28 (s, 6H), 1.83 - 1.85 (m, 4H), 1.54 - 1.57 (m, 4H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 154.7 (s), 129.8 (s), 129.4 (s), 128.9 (s), 111.1 (s), 67.9 (s), 62.0 (s), 29.2 (s), 25.9 (s), 20.3 (s).



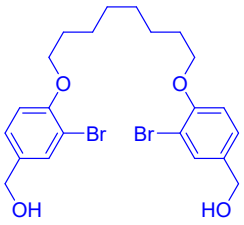
((Butane-1,4-diylbis(oxy))bis(5-methyl-2,1-phenylene))dimethanol) (3o): Appeared as off-white solid, (84%). ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm): 7.10 (s, 2H), 7.05 (d, J = 8 Hz, 2H), 6.77 (d, J = 5 Hz, 2H), 4.65 (s, 4H), 4.07 (t, J = 6 Hz, 4H, OCH_2), 2.95 (s, 1H, OH), 2.88 (s, 1H, OH), 2.50 (s, 2H), 2.29 (s, 6H), 2.00 (m, 4H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 154.5 (s), 129.8 (s), 129.5 (s), 129.0 (s), 128.9 (s), 111.1 (s), 67.5 (s), 61.9 (s), 26.2 (s), 20.3 (s).



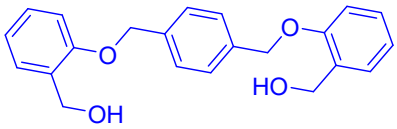
((Octane-1,8-diylbis(oxy))bis(5-methoxy-2,1-phenylene))dimethanol) (3p): Appeared as off-white solid, (83%). ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm): 6.83 (s, 6H), 3.91 (t, *J* = 6.5 Hz, 4H, OC*H*$_2$), 3.77 (s, 6H), 1.73 – 1.79 (m, 4H), 1.45 – 1.48 (m, 4H), 1.38 – 1.40 (s, 4H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 153.6 (s), 151.0 (s), 130.4 (s), 114.6 (s), 113.1 (s), 112.3 (s), 68.6 (s), 62.1 (s), 55.8 (s), 29.3 (s), 29.2(s), 26.1 (s).



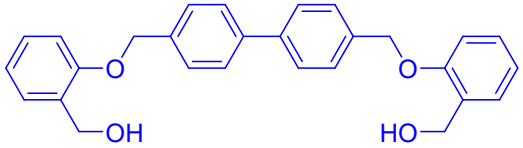
((Octane-1,8-diylbis(oxy))bis(5-chloro-2,1-phenylene))dimethanol) (3q): Appeared as white solid, (84%). ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm): 7.27 (d, *J* = 2.5 Hz, 2H), 7.18 (dd, *J* = 6.5 Hz, *J* = 2 Hz, 2H), 6.76 (d, *J* = 8.5 Hz, 2H), 4.64 (s, 4H), 3.97 (t, *J* = 6.5 Hz, 4H, OC*H*$_2$), 2.40 (s, 2H), 1.77 - 1.82 (m, 4H), 1.45 – 1.48 (m, 4H), 1.36 – 1.41 (m, 4H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 155.1 (s), 130.9 (s), 128.1 (s), 128.1 (s), 125.3 (s), 112.1 (s), 68.3 (s), 61.2 (s), 29.1 (s), 29.0 (s), 25.9 (s).



((Octane-1,8-diylbis(oxy)bis(3-bromo-4,1-phenylene))dimethanol) (3r) Appeared as off-white solid, (85%). ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm): 7.53 (d, *J* = 2.5 Hz, 2H), 7.21 (dd, *J* = 6.5 Hz, *J* = 2Hz, 2H), 6.85 (d, *J* = 8.5 Hz, 2H), 4.57 (s, 4H), 4.01 (t, *J* = 6.5 Hz, 4H, OC*H*$_2$), 1.91 (s, 2H), 1.81 – 1.84 (m, 4H), 1.50 – 1.53 (m, 4H), 1.40 – 1.42 (m, 4H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 154.9 (s), 134.3 (s), 132.1 (s), 127.1 (s), 113.1 (s), 112.2 (s), 69.2 (s), 64.2 (s), 29.1 (s), 28.9(s), 25.8 (s).

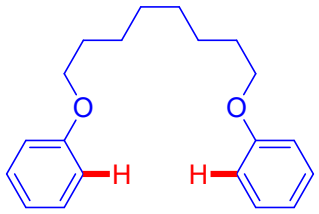


(((1,4-Phenylenebis(methylene))bis(oxy))bis(2,-1-phenylene))dimethanol) (3s): Appeared as off-white solid, (83%). ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm): 7.42 (s, 4H), 7.26 (dd, *J* = 22.5 Hz, *J* = 7 Hz, 4H), 6.92 - 6.97 (m, 4H), 5.11 (s, 4H), 4.72 (s, 4H), 1.23 (s, 2H, OH); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 156.4 (s), 136.7 (s), 129.5 (s), 128.9 (s), 128.8 (s),127.6 (s), 121.1 (s), 111.6 (s), 69.7 (s), 62.0 (s).

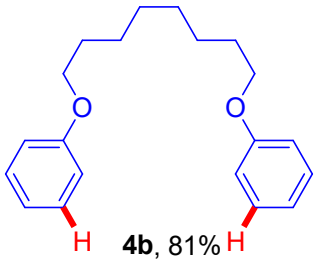


((([1,1'-Biphenyl]-4,4'-diylbis(methylene))bis(oxy))bis(2,-1-phenylene))dimethanol) (3t): Appeared as off-white solid, (89%). ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm): 7.63 (d, *J* = 8 Hz, 4H), 7.5a (d, *J* = 8 Hz, 4H), 7.33 (d, *J* = 8 Hz, 2H), 7.27 – 7.30 (m, 2H), 6.97-7.00 (m, 4H), 5.18 (s, 4H), 4.77 (s, 4H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 156.5 (s), 140.5 (s), 135.9 (s), 129.5 (s), 128.9 (s),128.8 (s), 127.8 (s), 127.4 (s), 121.1 (s), 111.7 (s), 69.8 (s), 62.1 (s).

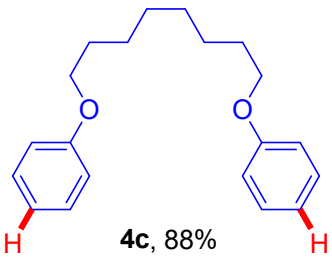
Spectroscopic Data of Dehydroxymethylated Product:



4a, 91%



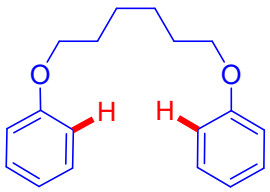
4b, 81%



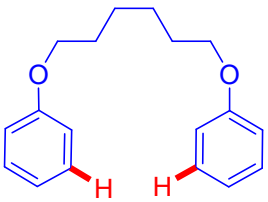
4c, 88%

1,8-Diphenoxyoctane (4a-4c): Appeared as white solid, ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm): 7.28 (t, *J* = 7.5 Hz, 4H), 6.93 (t, *J* = 7.5 Hz, 2H), 6.90 (d, *J* = 8 Hz, 4H), 3.95 (t, *J* = 6.5 Hz, 4H OC*H*$_2$), 1.76 – 1.82 (m, 4H), 1.46 – 1.49 (m, 4H), 1.39 – 1.41 (m, 4H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$)

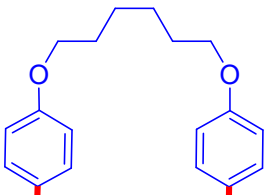
δ 159.1 (s), 129.3 (s), 120.4 (s), 114.5 (s), 67.8 (s, O*C*H_2), 29.7 (s), 29.2 (s), 26.0 (s).



4d, 86%

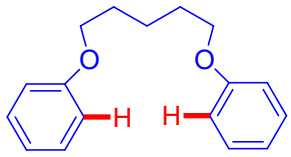


4e, 71%

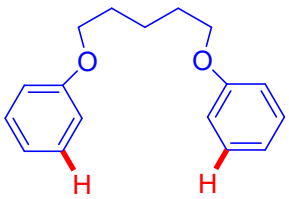


4f, 83%

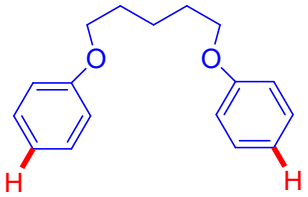
1,6-Diphenoxyhexane (4d-4f): Appeared as white solid, ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm): 7.29 (t, *J* = 7.5 Hz, 4H), 6.95 (t, *J* = 7.5 Hz, 2H), 6.91 (d, *J* = 8 Hz, 4H), 3.99 (t, *J* = 6 Hz, 4H, O*C*H_2), 1.81 – 1.85 (m, 4H), 1.55 – 1.58 (m, 4H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 159.0 (s), 129.4 (s), 120.4 (s), 114.5 (s), 67.6 (s, O*C*H_2), 29.2 (s), 25.8 (s).



4g, 81%

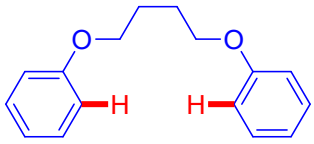


4h, 69%

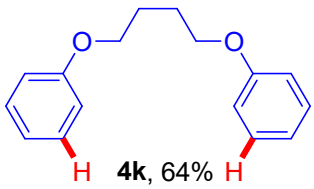


4i, 78%

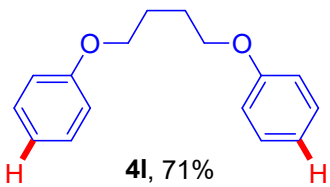
1,5-Diphenoxpentane (4g-4i): Appeared as off-white solid, **NMR** ($CDCl_3$, δ/ppm): **^{1}H** (500 MHz): 7.32 (t, *J* = 8.5 Hz, 4H), 6.98 (t, *J* = 7 Hz, 2H), 6.94 (d, *J* = 8 Hz, 4H), 4.02 (t, *J* = 6.5 Hz, 4H O*C*H_2), 1.88 – 1.93 (m, 4H), 1.68 – 1.73 (m, 2H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 159.0 (s), 129.3 (s), 120.5 (s), 114.4 (s), 67.5 (s, O*C*H_2), 29.0 (s), 22.7 (s).



4j, 75%



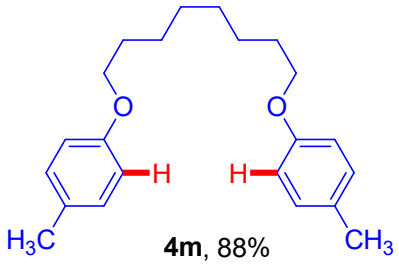
4k, 64%



4l, 71%

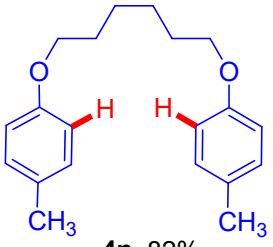
1,4-Diphenoxybutane (4j-4l): Appeared as White Solid, ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm):

7.28 (t, J = 7.5 Hz, 4H), 6.94 (t, J = 7.5 Hz, 2H), 6.90 (d, J = 8 Hz, 4H), 4.04 (t, J = 5.5 Hz, 4H, OCH_2), 1.98 – 2.00 (m, 4H),; $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$) δ 158.9 (s), 129.4 (s), 120.6 (s), 114.5 (s), 67.3 (s, OCH_2), 26.0 (s).



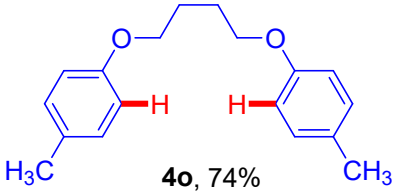
4m, 88%

1,8-Bis(p-tolyloxy)octane (4m) : Appeared as white solid, (88%). ^1H NMR (500 MHz $CDCl_3$, δ/ppm): 7.07 (d, J = 8 Hz, 4H), 6.80 (d, J = 8 Hz, 4H), 3.93 (t, J = 6.5 Hz, 4H, OCH_2), 2.29 (s, 6H), 1.74 - 1.80 (m, 4H), 1.45 - 1.48 (m, 4H), 1.38 – 1.40 (m, 4H); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$) δ 157.0 (s), 129.8 (s), 129.6 (s), 114.3 (s), 67.9 (s, OCH_2), 29.3 (s), 25.9 (s), 20.4 (s).



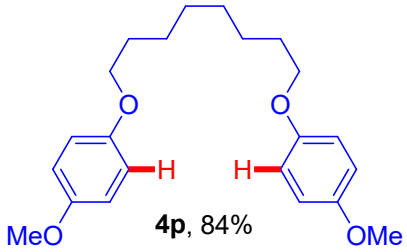
4n, 82%

1,6-Bis(p-tolyloxy)hexane (4n): Appeared as white solid, (82%). ^1H NMR (500 MHz $CDCl_3$, δ/ppm): 7.07 (d, J = 8.5 Hz, 4H), 6.80 (d, J = 8.5 Hz, 4H), 3.94 (t, J = 8.5 Hz, 4H, OCH_2), 2.28 (s, 6H), 1.79 - 1.81 (m, 4H), 1.50 – 1.55 (m, 4H); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$) δ 156.9 (s), 129.8 (s), 129.6 (s), 114.3 (s), 67.9 (s, OCH_2), 29.2 (s), 25.8 (s), 20.4 (s).



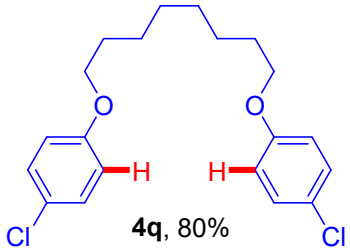
4o, 74%

1,4-Bis(p-tolyloxy)butane (4o): Appeared as white solid, (74%). ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm): 7.07 (d, *J* = 8.5 Hz, 4H), 6.80 (d, *J* = 8.5 Hz, 4H), 4.00 (t, *J* = 5 Hz, 4H, OCH_2), 2.29 (s, 6H), 1.94 - 1.97 (m, 4H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 156.8 (s), 129.8 (s), 129.7 (s), 114.3 (s), 67.5 (s, OCH_2), 29.0 (s), 20.4 (s).



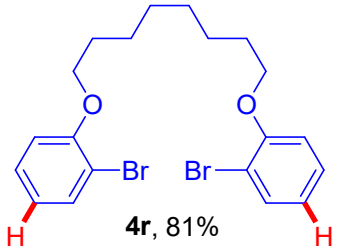
4p, 84%

1,8-Bis(4-methoxyphenoxy)octane (4p): Appeared as off-white solid. ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm): 6.83 (s, 8H), 3.91 (t, *J* = 6.5 Hz, 4H, OCH_2), 3.77 (s, 6H), 1.74 – 1.79 (m, 4H), 1.45 – 1.48 (m, 4H), 1.38 – 1.40 (m, 4H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 153.7 (s), 153.3 (s), 115.4 (s), 114.6 (s), 68.6 (s), 55.7 (s), 29.3 (s), 29.3 (s), 25.9 (s).



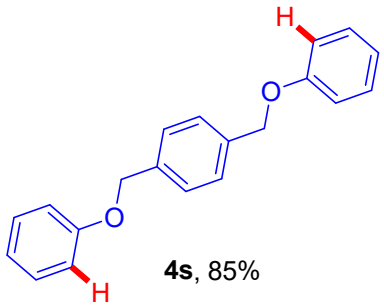
4q, 80%

1,8-bis(4-chlorophenoxy)octane (4q): Appeared as white solid. ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm: 7.29 (d, *J* = 6.5 Hz, 2H), 7.17 (t, *J* = 7.5 Hz, 2H), 6.87 (t, *J* = 7.5 Hz, 2H), 6.83 (d, *J* = 8 Hz, 2H), 4.03 (t, *J* = 5 Hz, 4H, OCH_2), 1.76 - 1.83 (m, 4H), 1.69 – 1.71 (m, 4H), 1.50 – 1.51 (m, 4H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 156.7 (s), 130.4 (s), 127.8 (s), 127.7 (s), 120.3 (s), 111.3 (s), 67.7 (s), 29.0 (s), 27.7 (s), 25.1 (s). 23.2 (s).



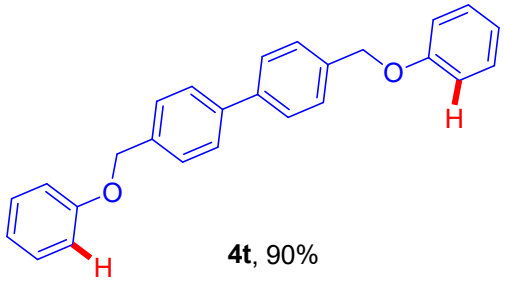
4r, 81%

1,8-bis(ortho-bromophenoxy)octane (4r): Appeared as white solid. ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm): 7.53 (dd, *J* = 12 Hz, *J* = 2 Hz, 2H), 7.22 – 7.26 (m, 2H), 6.88 (dd, *J* = 10.5 Hz, 1.5 Hz, 2H), 6.81 (td, *J* = 9 Hz, *J* = 2 Hz, 2H), 4.02 (t, *J* = 8 Hz, 4H, OC*H*$_2$), 1.81- 1.88 (m, 4H), 1.49 - 1.55 (m, 4H), 1.40 - 1.44 (m, 4H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 155.4 (s), 133.2 (s), 128.3 (s), 121.5 (s), 113.2 (s), 112.2 (s), 69.0 (s, OC*H*$_2$), 29.1 (s), 29.0 (s), 25.9 (s).



4s, 85%

1,4-bis(phenoxymethyl)benzene (4s): Appeared as white solid. ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm):7.46 (s, 4H), 7.28 - 7.31 (m, 5H), 6.96 – 6.99 (m, 5H), 5.08 (s, 4H, *OCH*$_2$); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 158.7 (s), 136.8 (s), 129.4 (s), 127.6 (s), 121.0 (s), 114.9 (s), 69.6 (s, OC*H*$_2$).



4t, 90%

4,4'-bis(phenoxymethyl)-1,1'-biphenyl (4t): Appeared as white solid. ^{1}H NMR (500 MHz $CDCl_3$, δ/ppm): 7.63 (d, *J* =8 Hz, 4H), 7.53 (d, *J* = 8 Hz, 4H), 7.33 (t, *J* = 7.5 Hz, 4H), 7.03 (d, *J* = 8Hz, 4H), 7.00 (t, *J* = 7.5 Hz, 2H), 5.13 (s, 4H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 158.7 (s), 140.4 (s), 136.2 (s), 129.4 (s), 127.9 (s),127.2(s), 120.9 (s), 114.8 (s), 69.6 (s).

Copies of spectral data

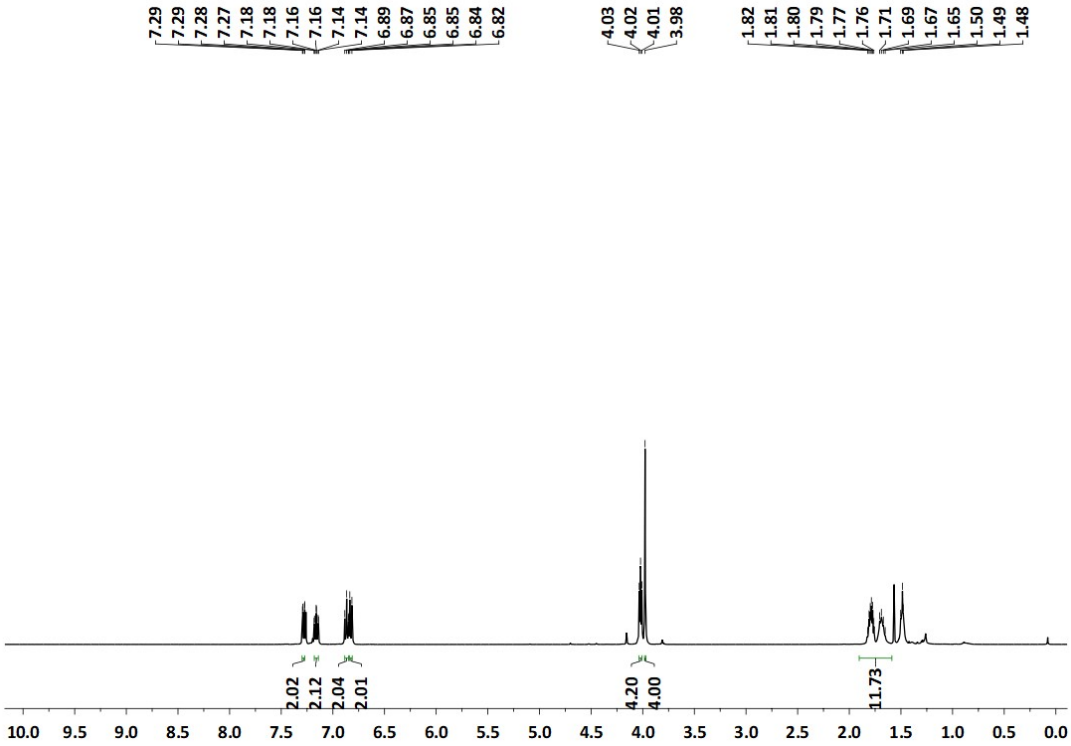


Figure s2. ^{1}H NMR spectrum of **L1**.

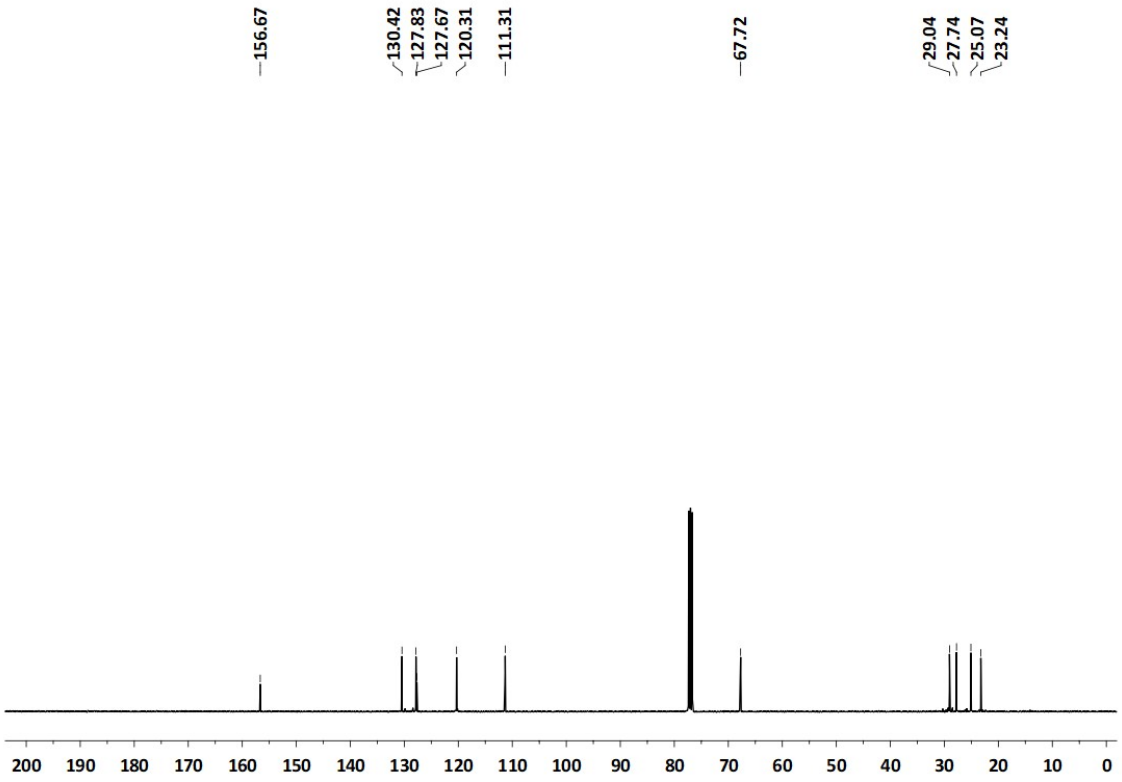


Figure s3. $^{13}C\{^{1}H\}$ NMR spectrum of **L1**.

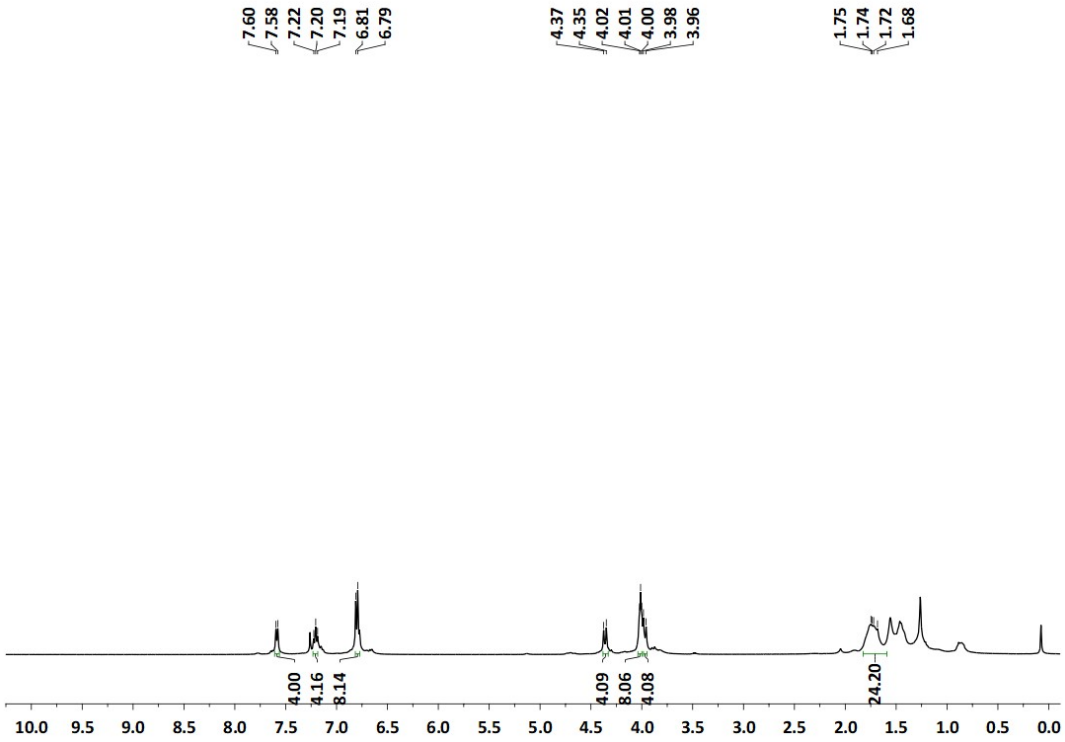


Figure s4. ^{1}H NMR spectrum of **C1**.

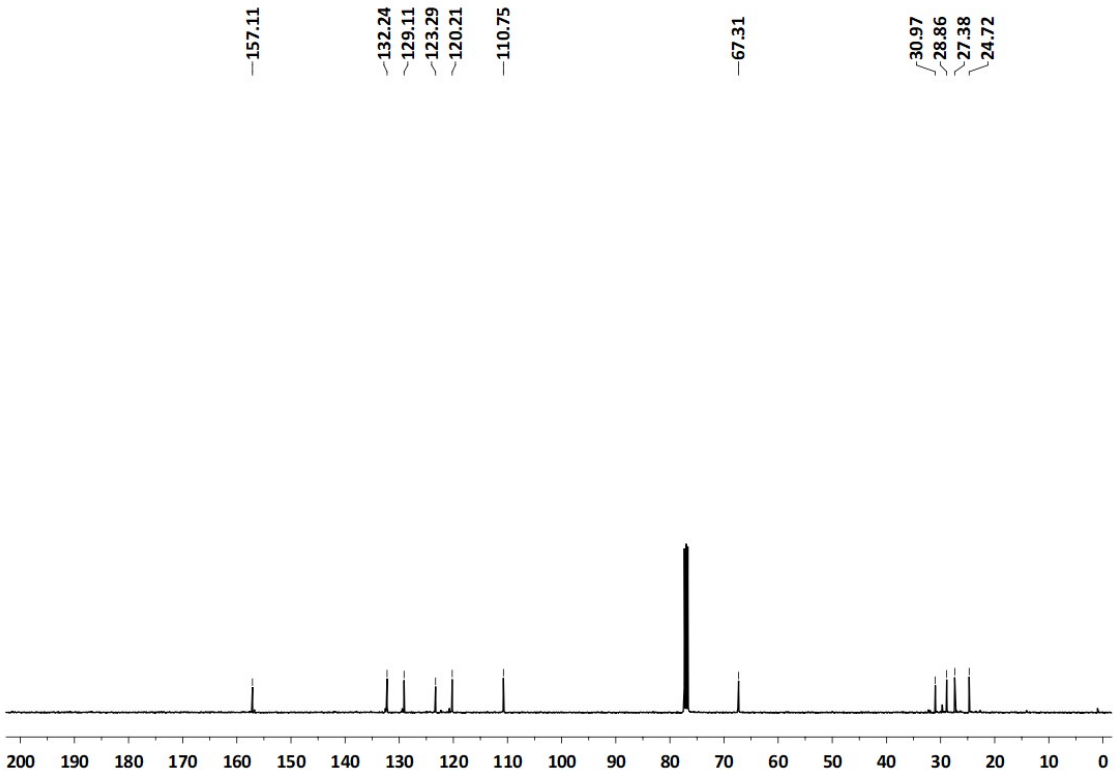


Figure s5. $^{13}C\{^{1}H\}$ NMR spectrum of **C1**.

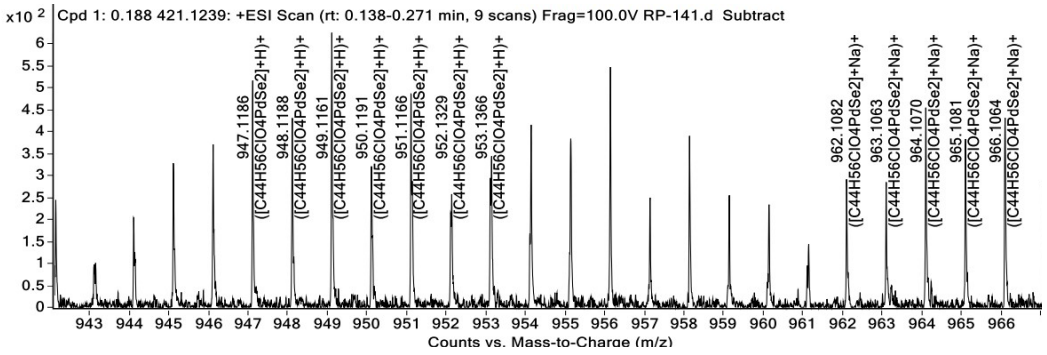


Figure s6. HRMS of **C1**.

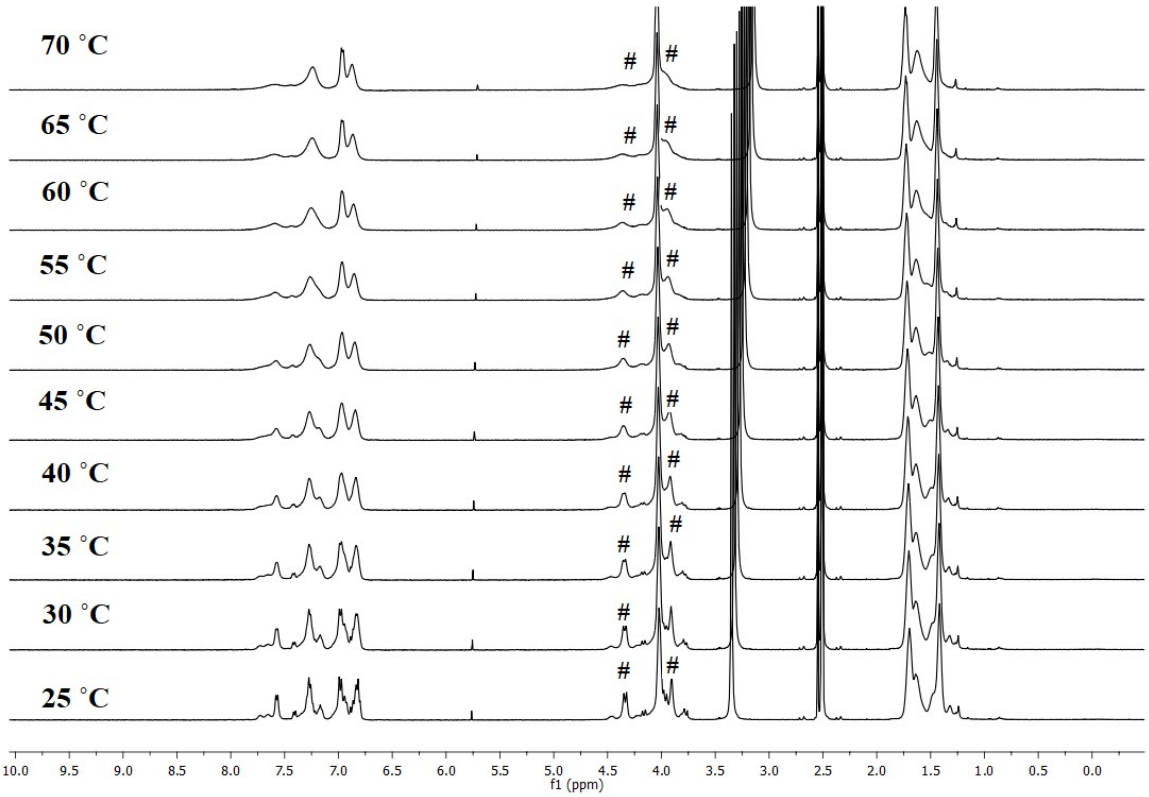


Figure s7. ^{1}H NMR spectrum of **C1** (DMSO-d_6) as a function of temperature. Coalescing signals are denoted with a #.

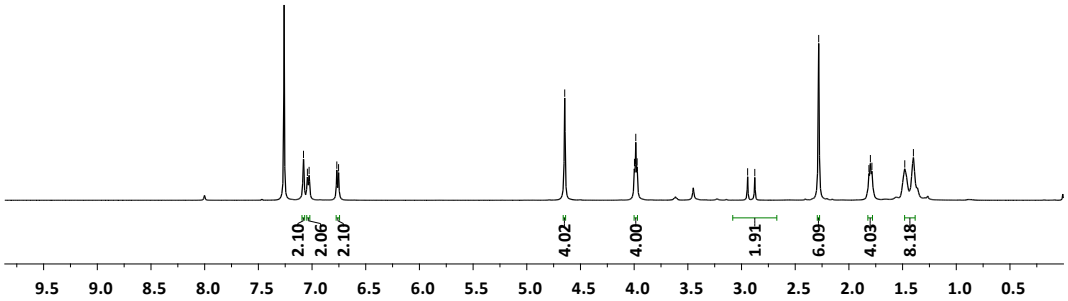


Figure s8. ^{1}H NMR spectrum of **3m.**

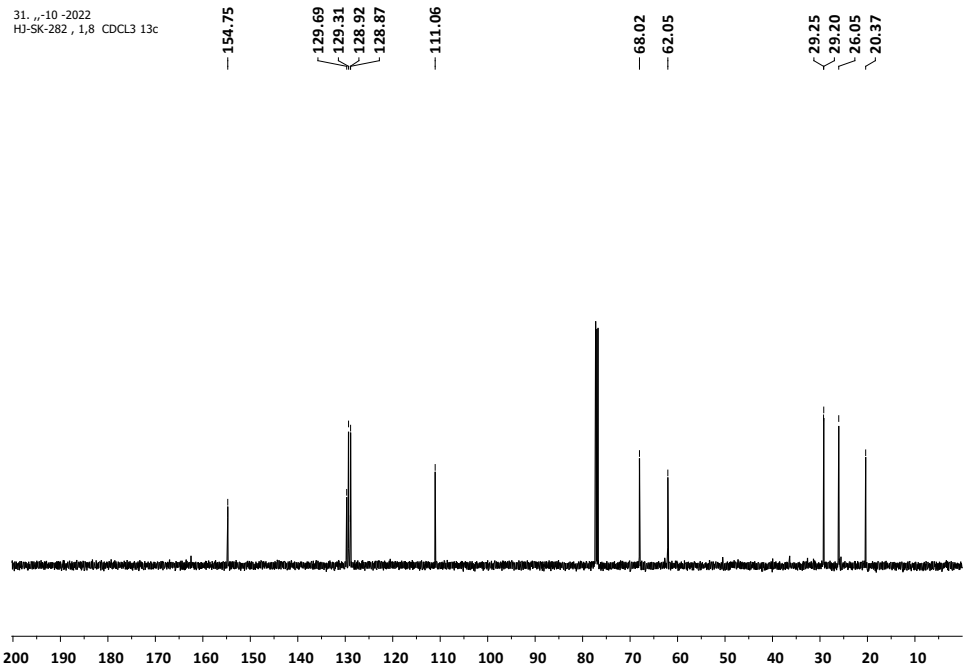


Figure s9. $^{13}C\{^{1}H\}$ NMR spectrum of **3m**.

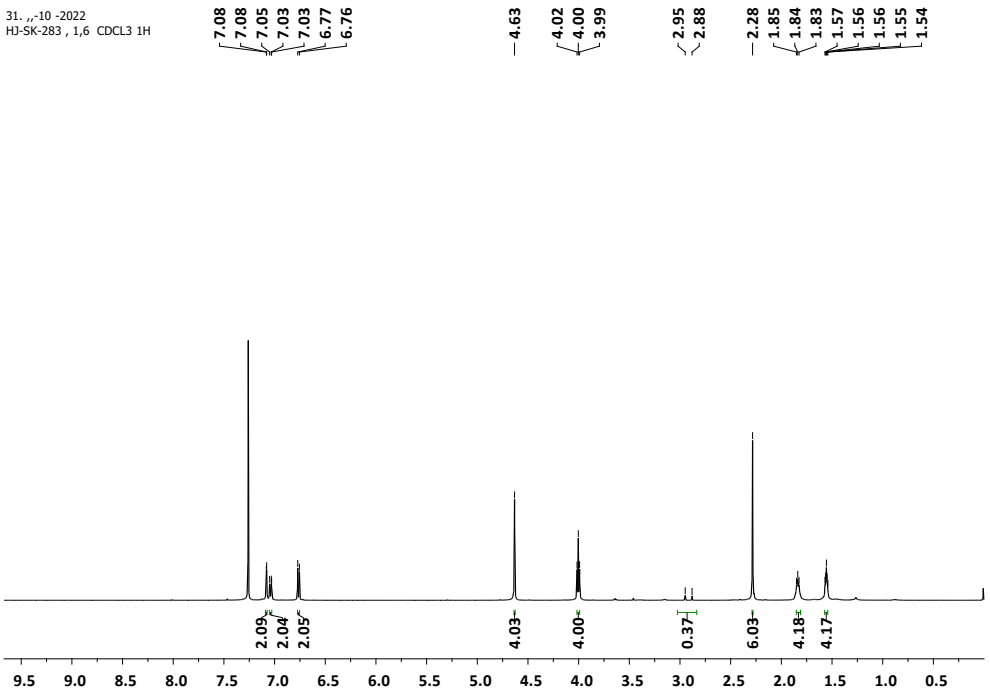


Figure s10. ^{1}H NMR spectrum of **3n.**

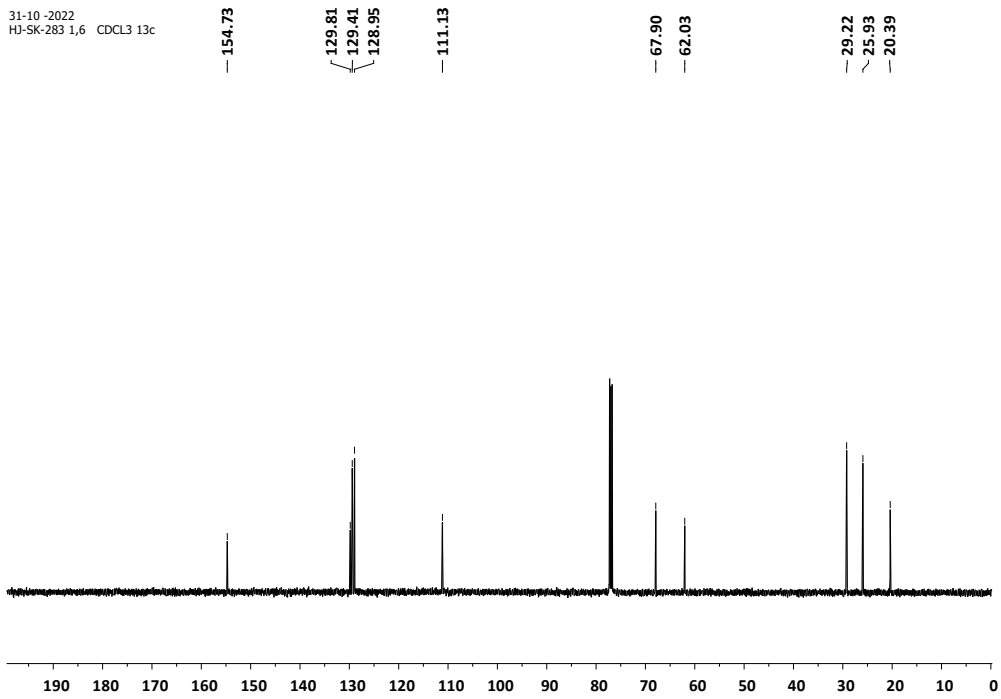


Figure s11. $^{13}C\{^{1}H\}$ NMR spectrum of **3n**.

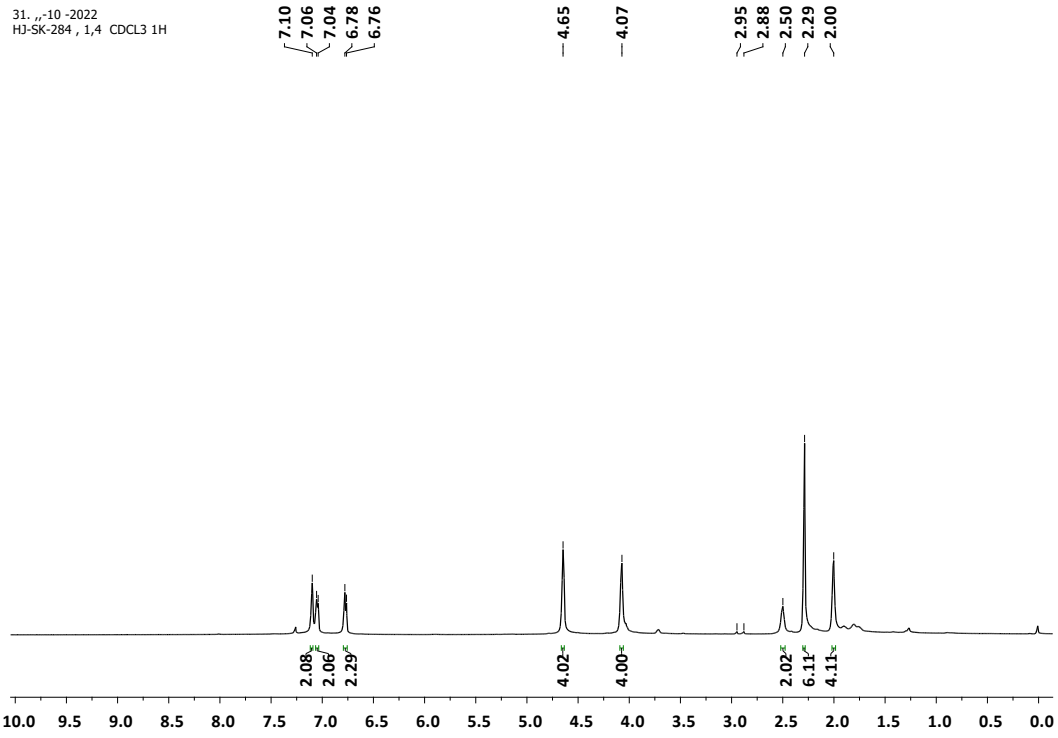


Figure s12. ^{1}H NMR spectrum of **3o.**

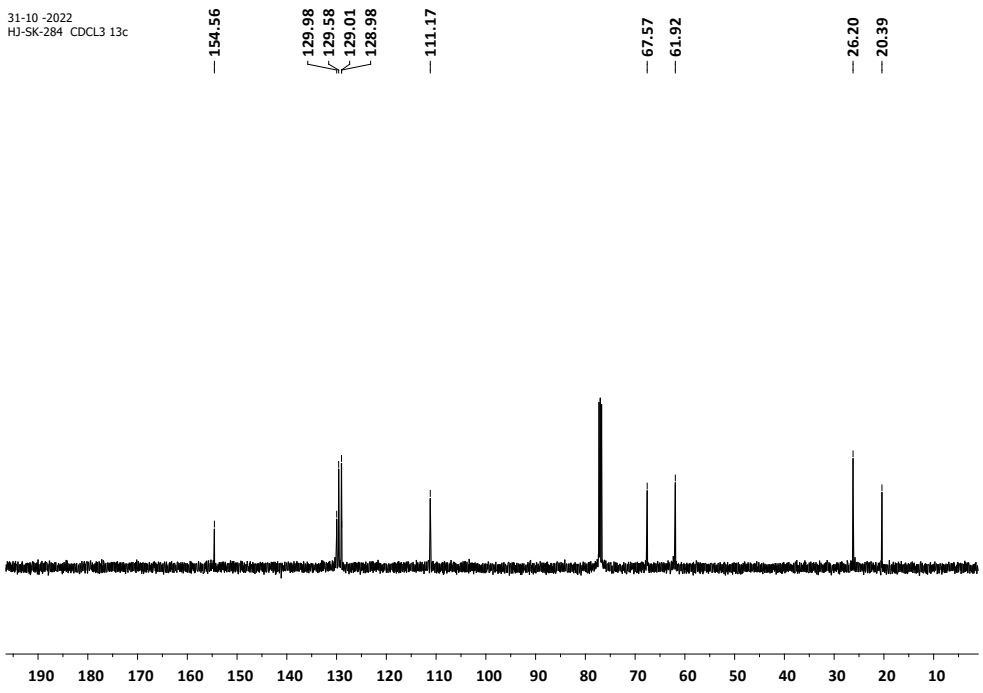


Figure s13. $^{13}C\{^{1}H\}$ NMR spectrum of **3o**.

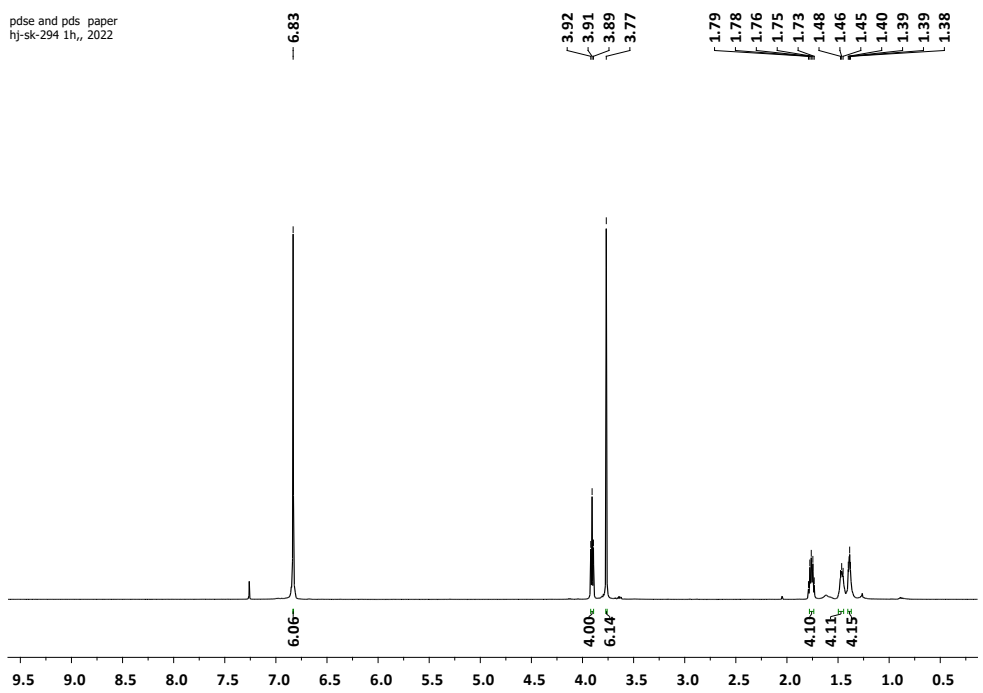


Figure s14. ^{1}H NMR spectrum of **3p.**

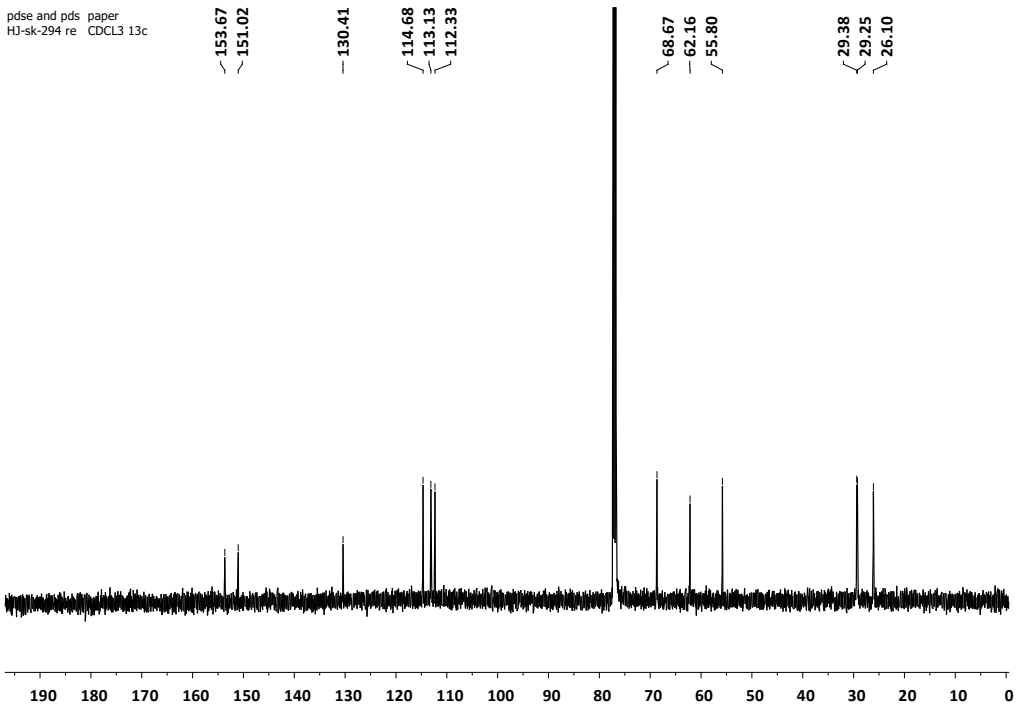


Figure s15. $^{13}C\{^{1}H\}$ NMR spectrum of **3p**.

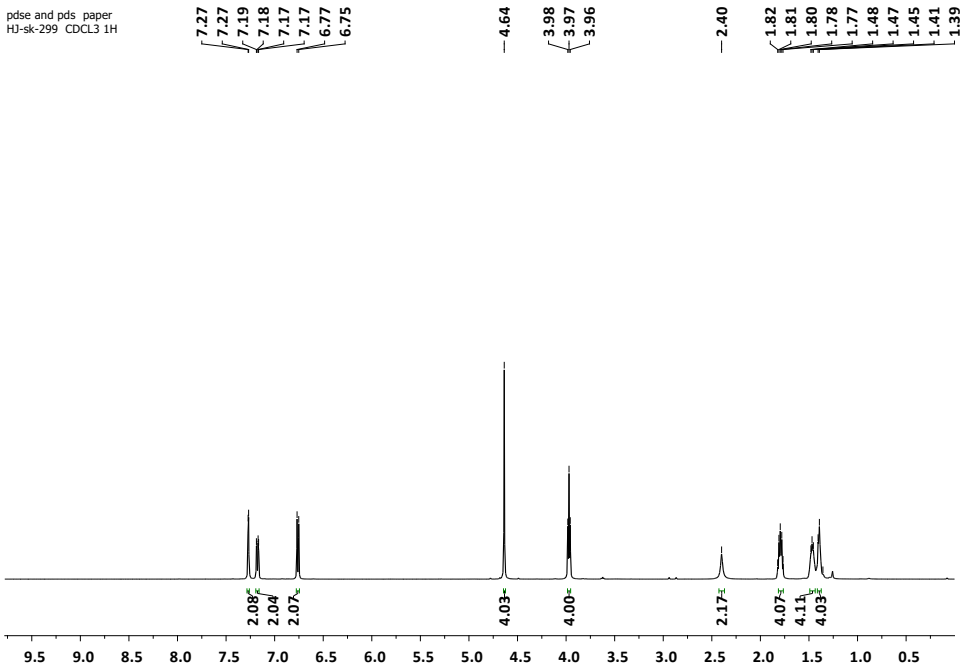


Figure s16. ^{1}H NMR spectrum of **3q.**

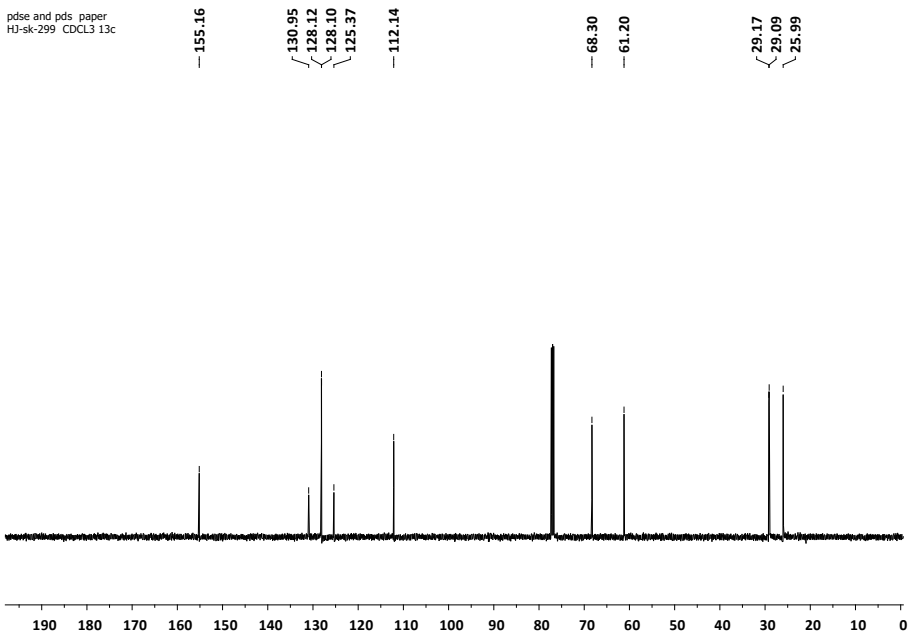


Figure s17. $^{13}C\{^{1}H\}$ NMR spectrum of **3q**.

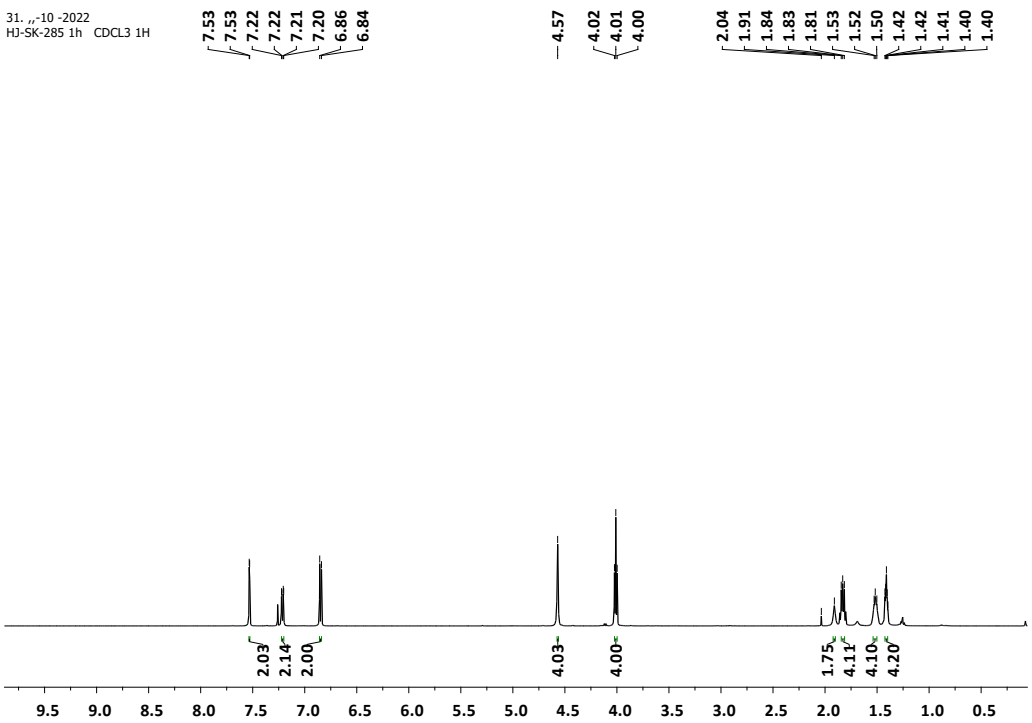


Figure s18. ^{1}H NMR spectrum of **3r.**

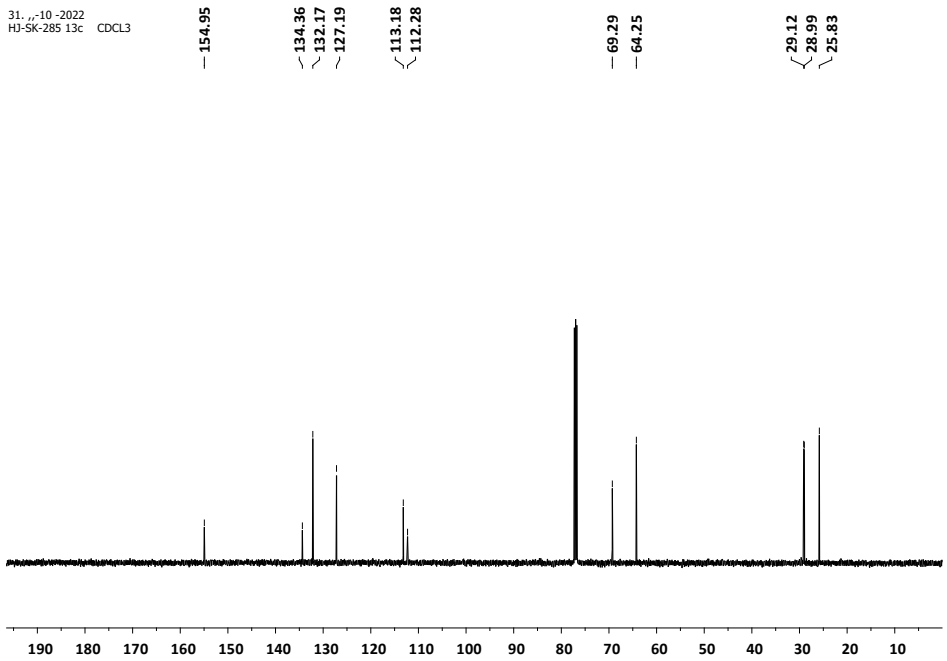


Figure s19. $^{13}C\{^{1}H\}$ NMR spectrum of **3r**.

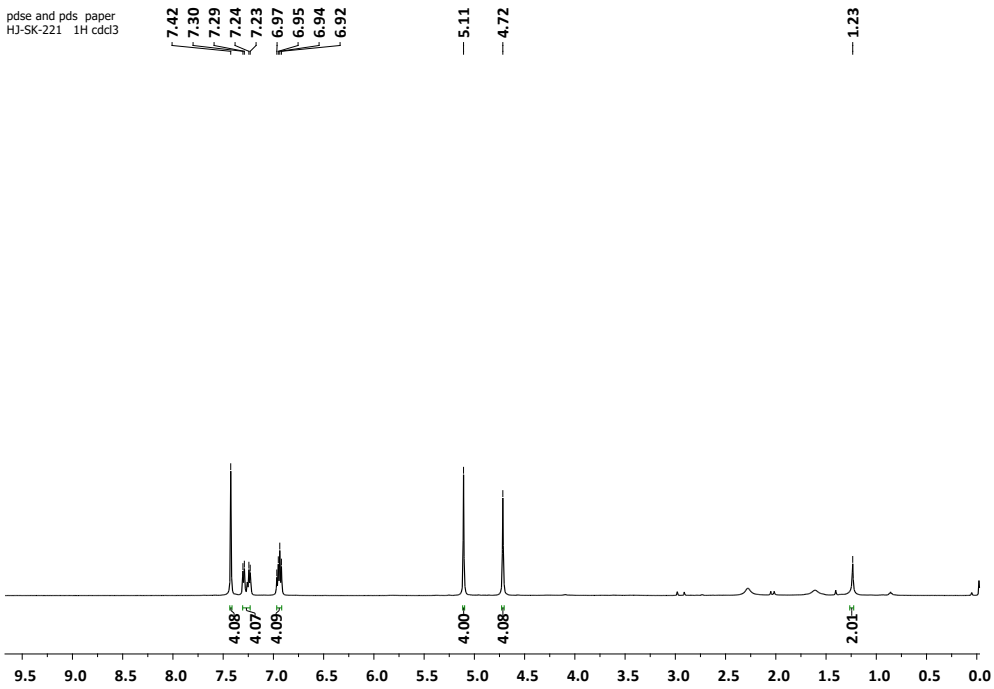


Figure s20. ^{1}H NMR spectrum of **3s.**

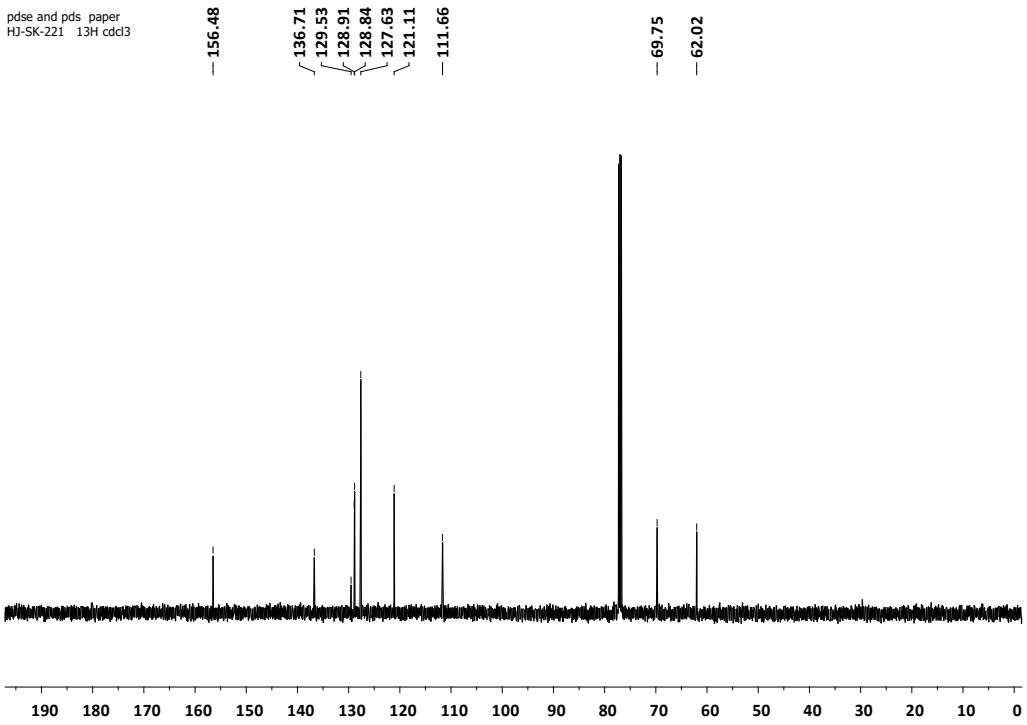


Figure s21. $^{13}C\{^{1}H\}$ NMR spectrum of **3s.**

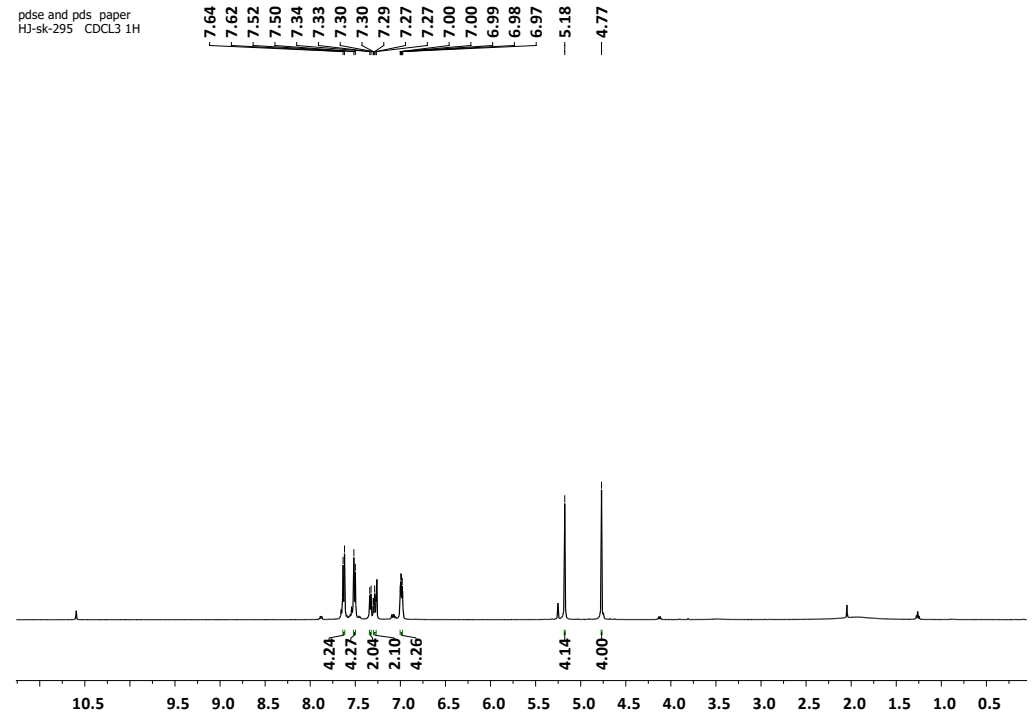


Figure s22. ^{1}H NMR spectrum of **3t.**

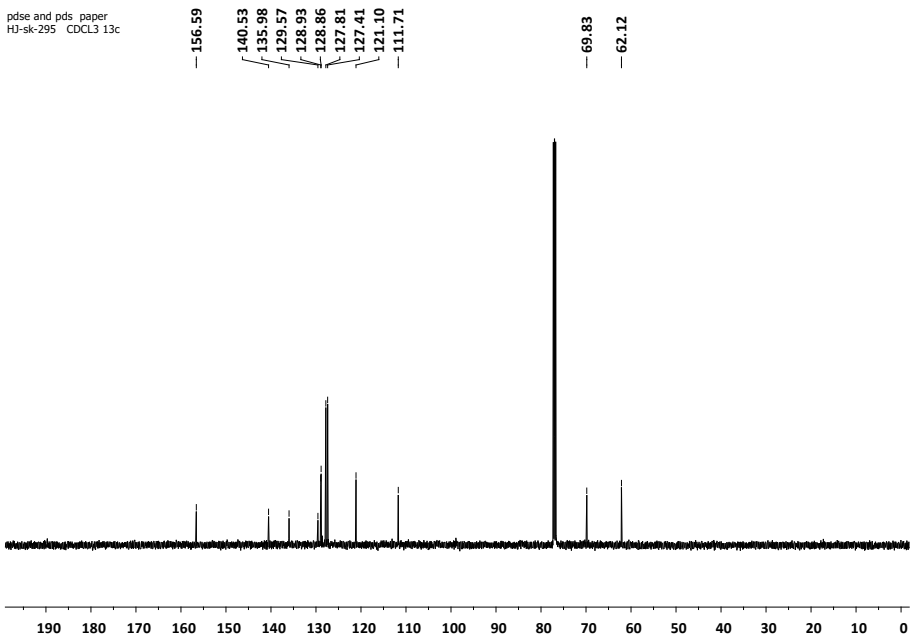


Figure s23. $^{13}C\{^{1}H\}$ NMR spectrum of **3t.**

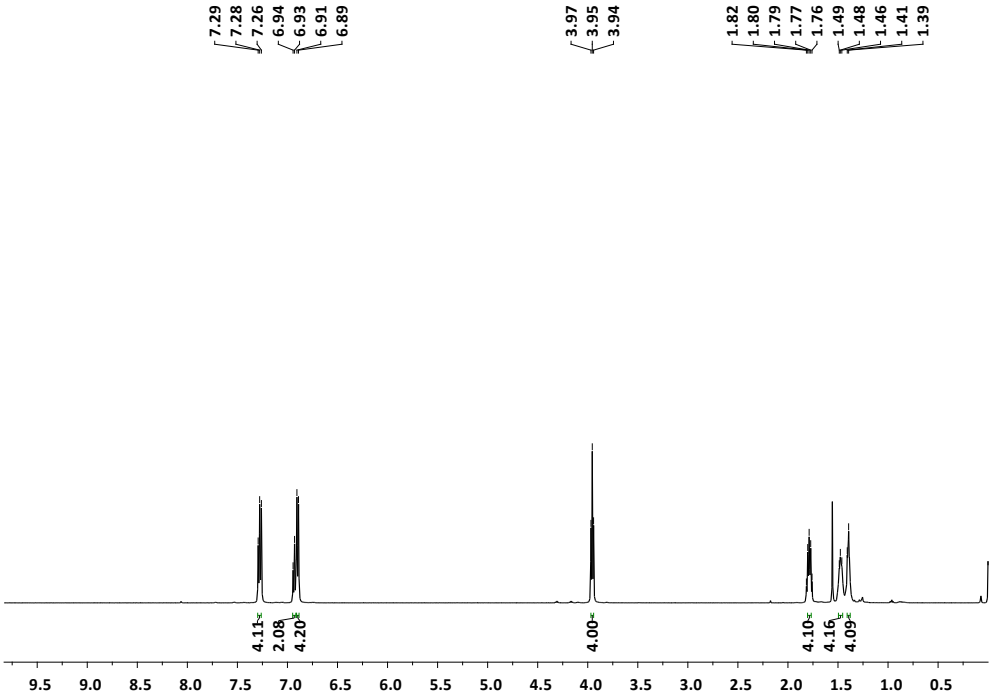


Figure s24. ^{1}H NMR spectrum of **4a, 4b, 4c.**

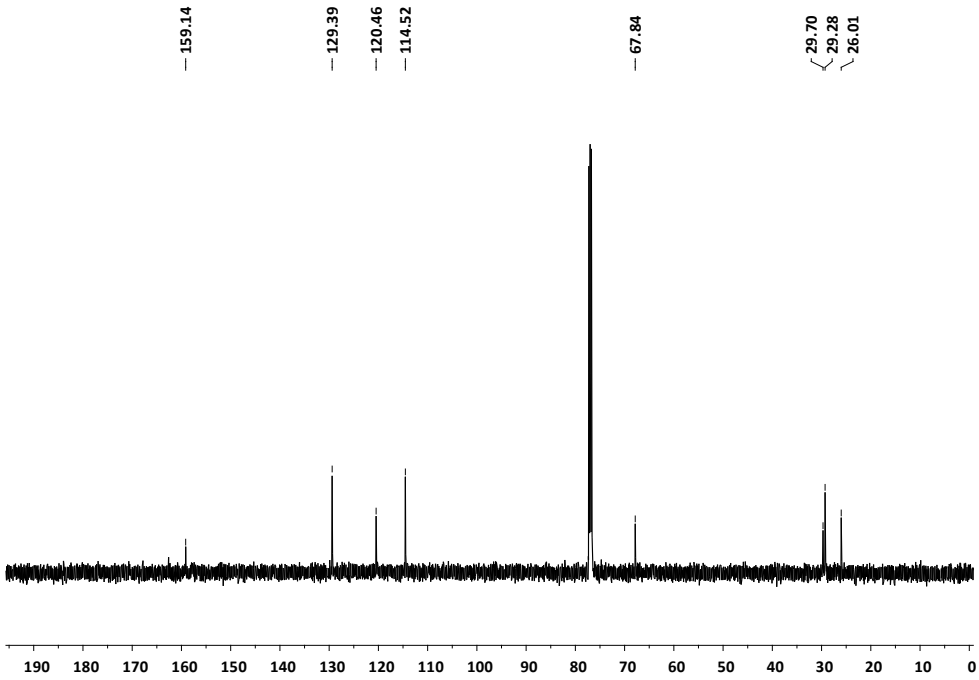


Figure s25. $^{13}C\{^{1}H\}$ NMR spectrum of **4a, 4b, 4c.**

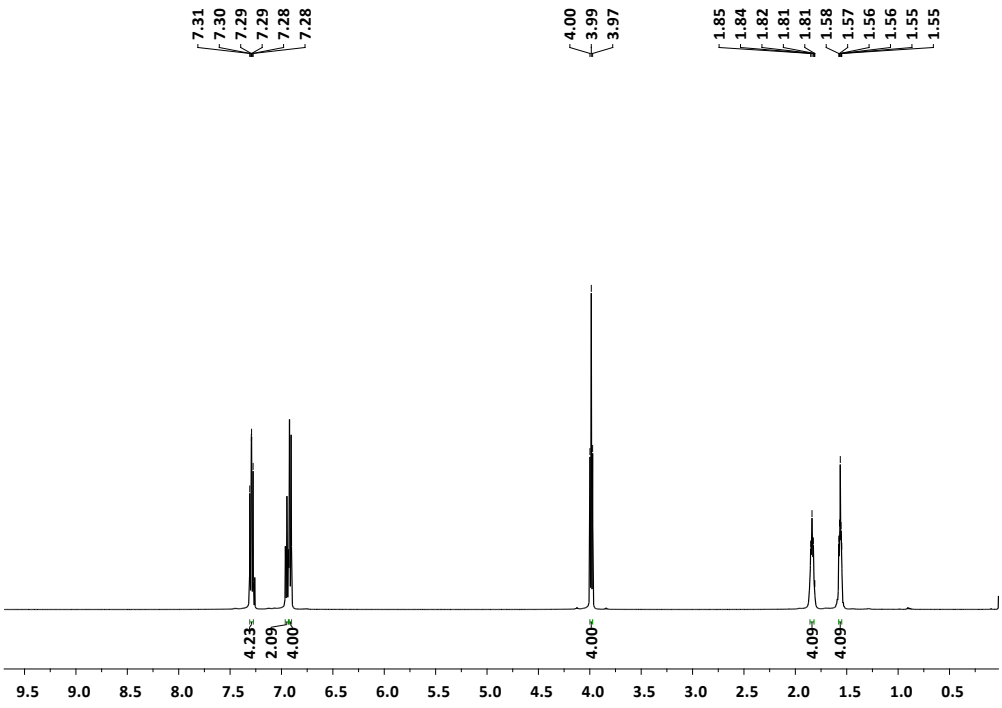


Figure s26. ^{1}H NMR spectrum of **4d, 4e, 4f.**

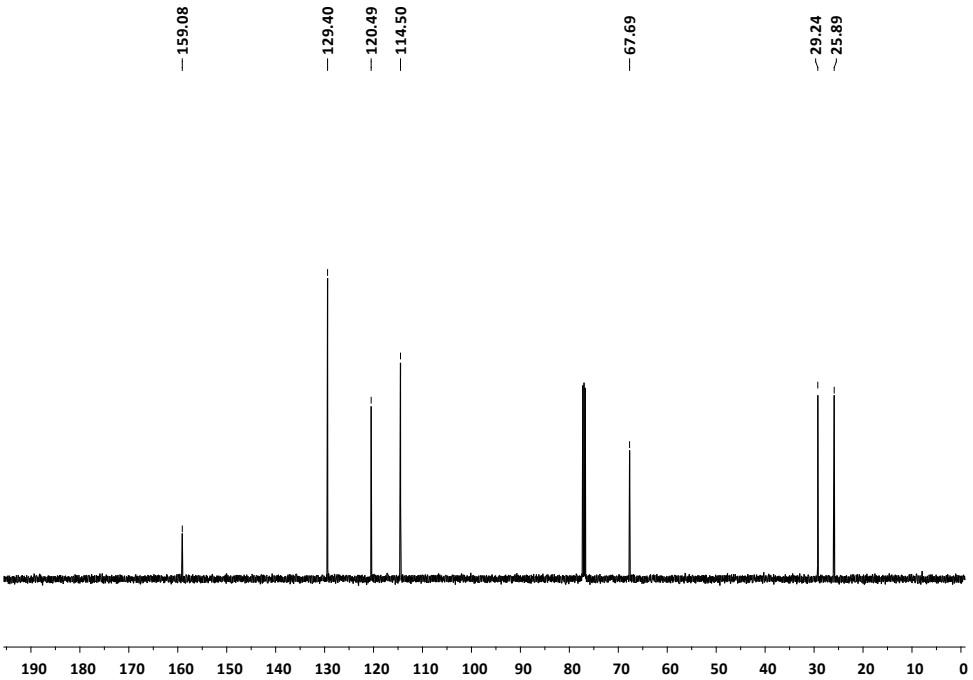


Figure s27. $^{13}C\{^{1}H\}$ NMR spectrum of **4d, 4e, 4f.**

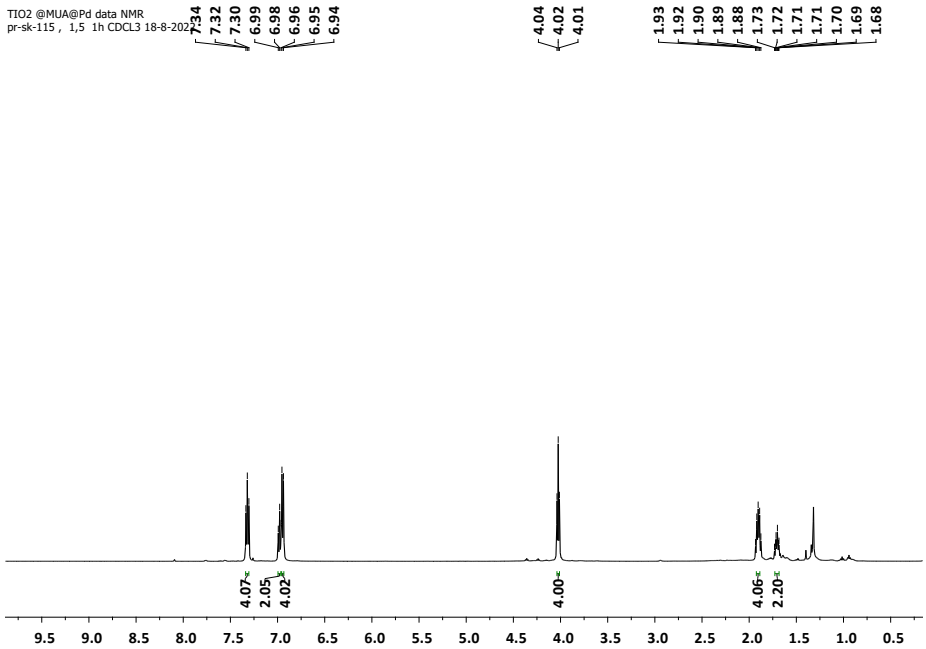


Figure s28. ^{1}H NMR spectrum of **4g, 4h, 4i.**

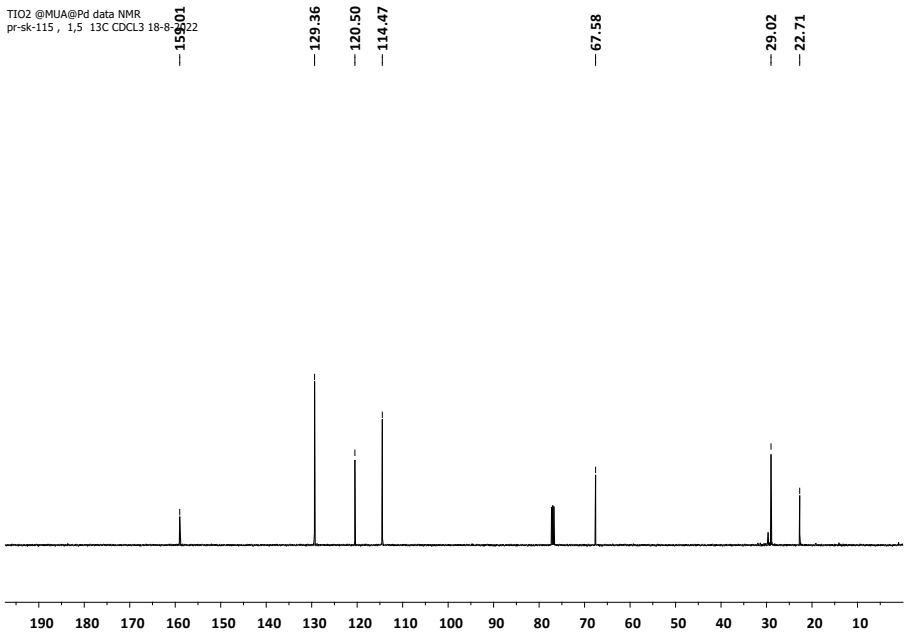


Figure s29. $^{13}C\{^{1}H\}$ NMR spectrum of **4g, 4h, 4i.**

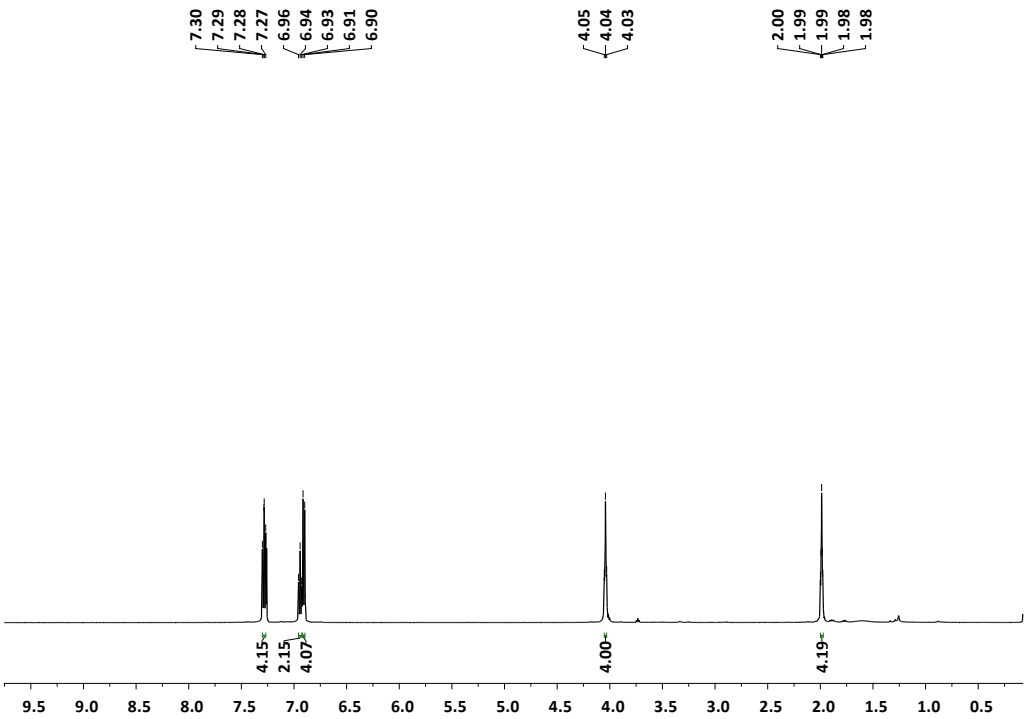


Figure s30. ^{1}H NMR spectrum of **4j, 4k, 4l.**

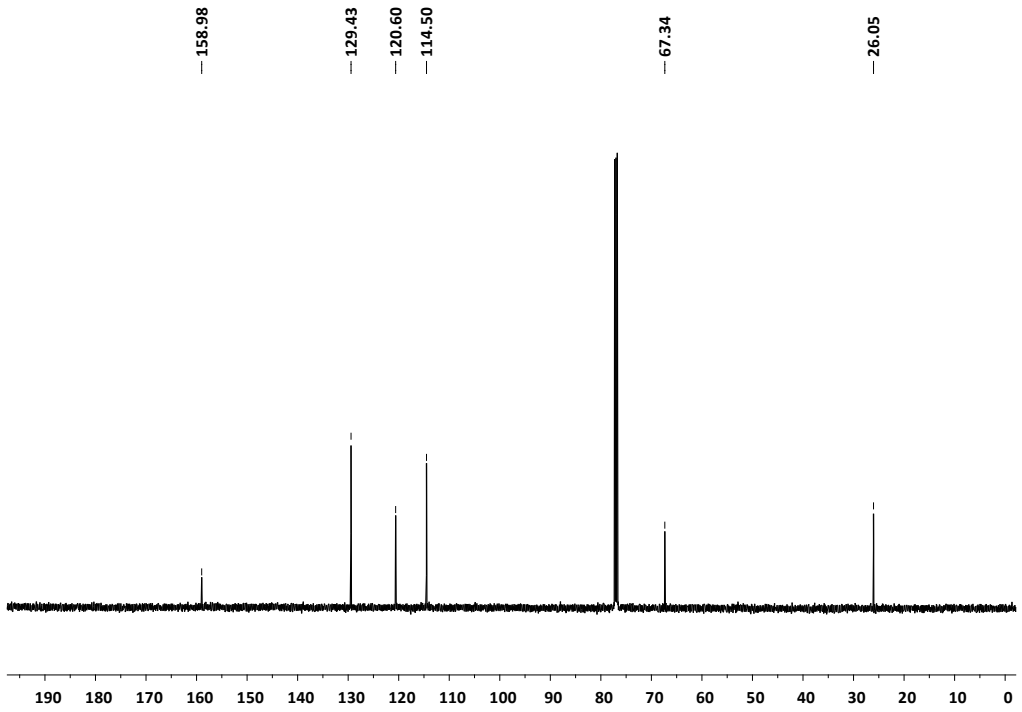


Figure s31. $^{13}C\{^{1}H\}$ NMR spectrum of **4j, 4k, 4l.**

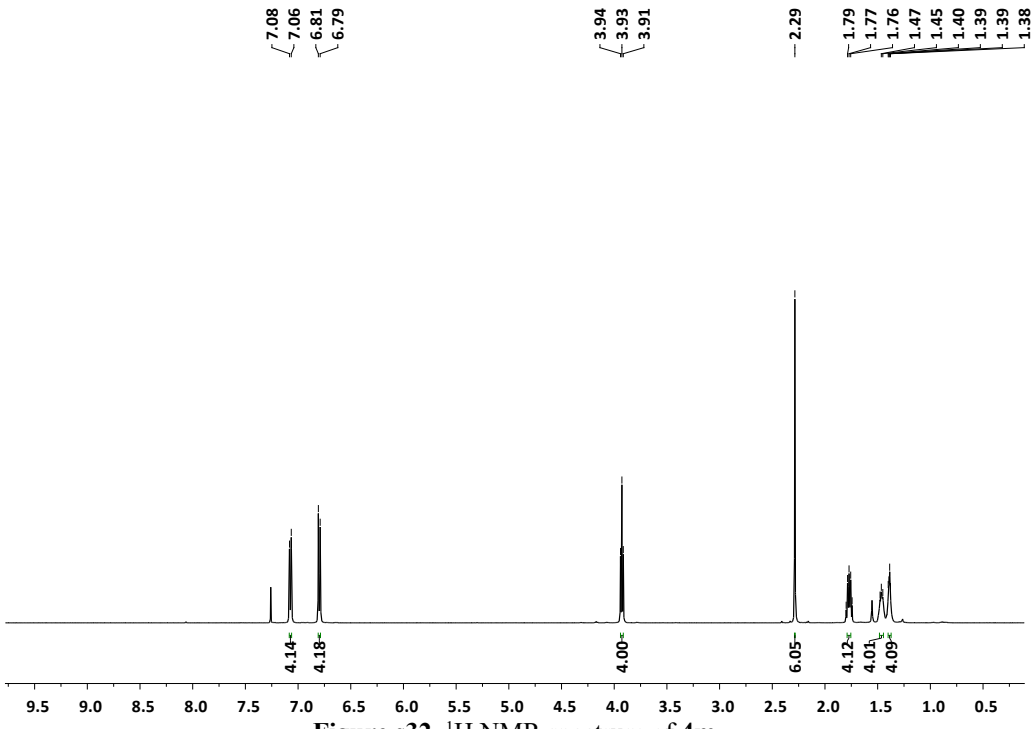


Figure s32. ^{1}H NMR spectrum of **4m.**

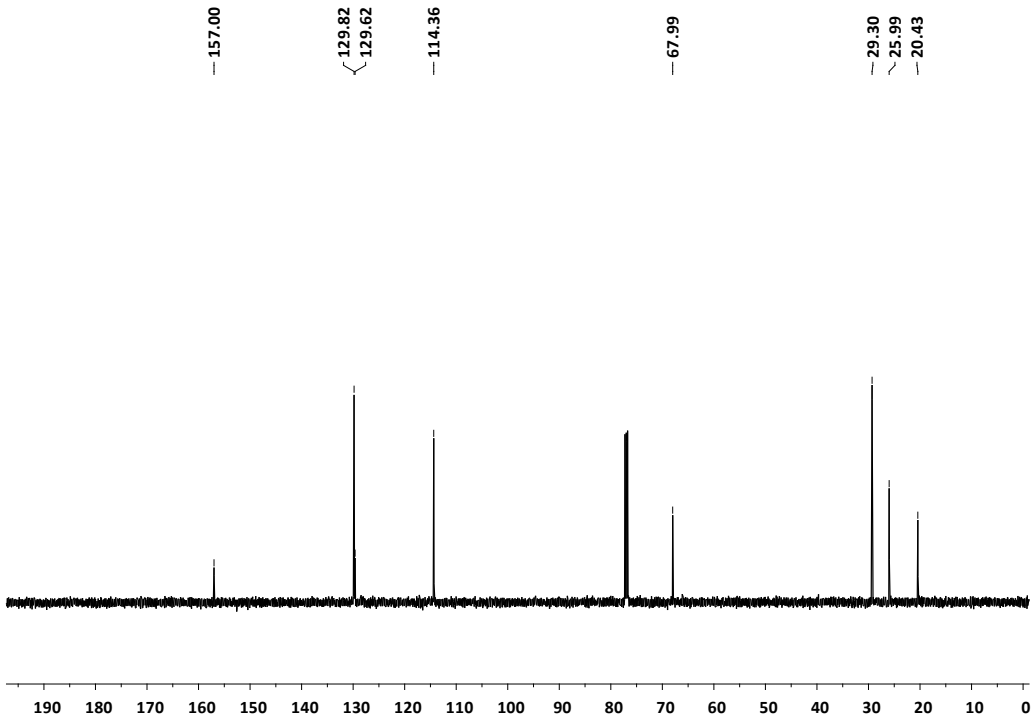


Figure s33. $^{13}C\{^{1}H\}$ NMR spectrum of **4m.**

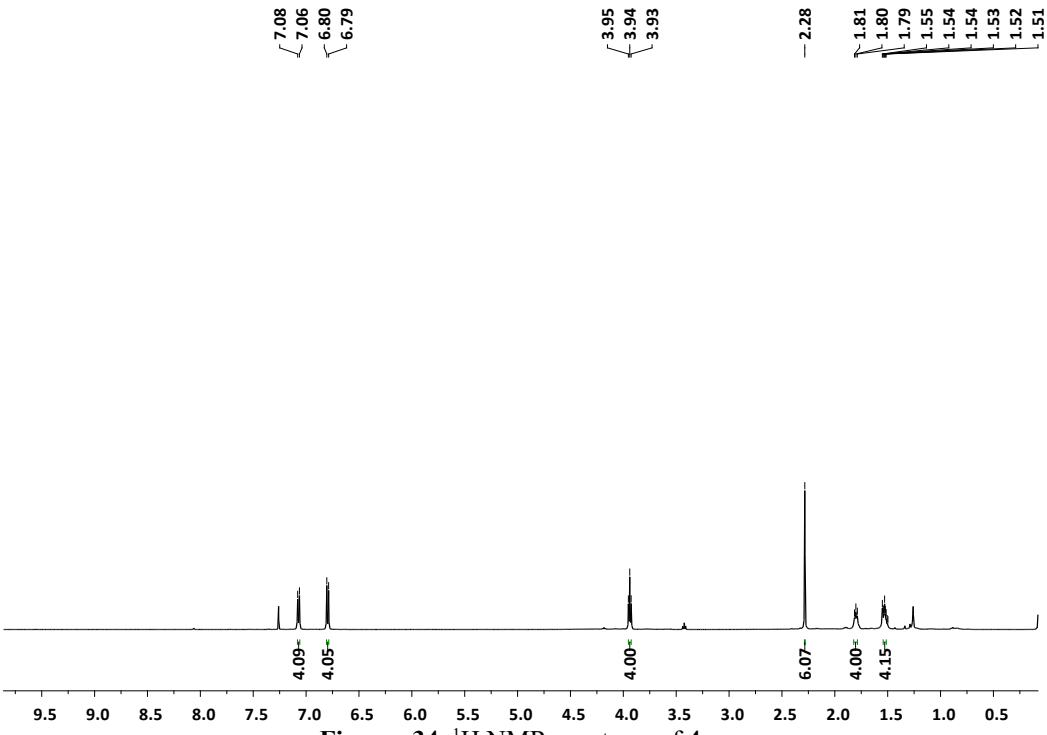


Figure s34. ^{1}H NMR spectrum of **4n.**

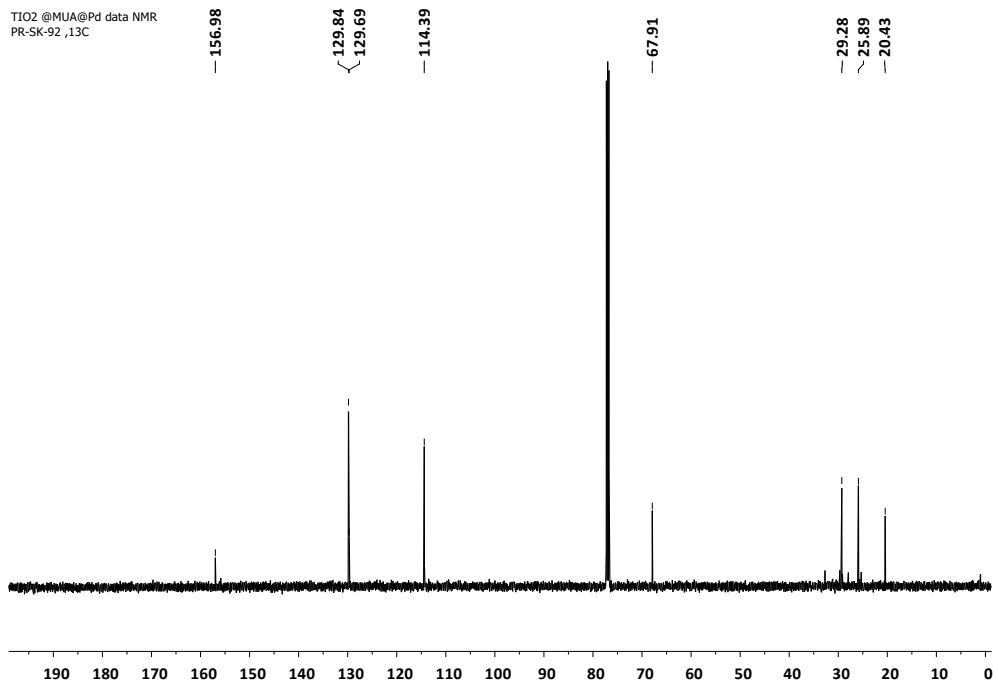


Figure s35. $^{13}C\{^{1}H\}$ NMR spectrum of **4n.**

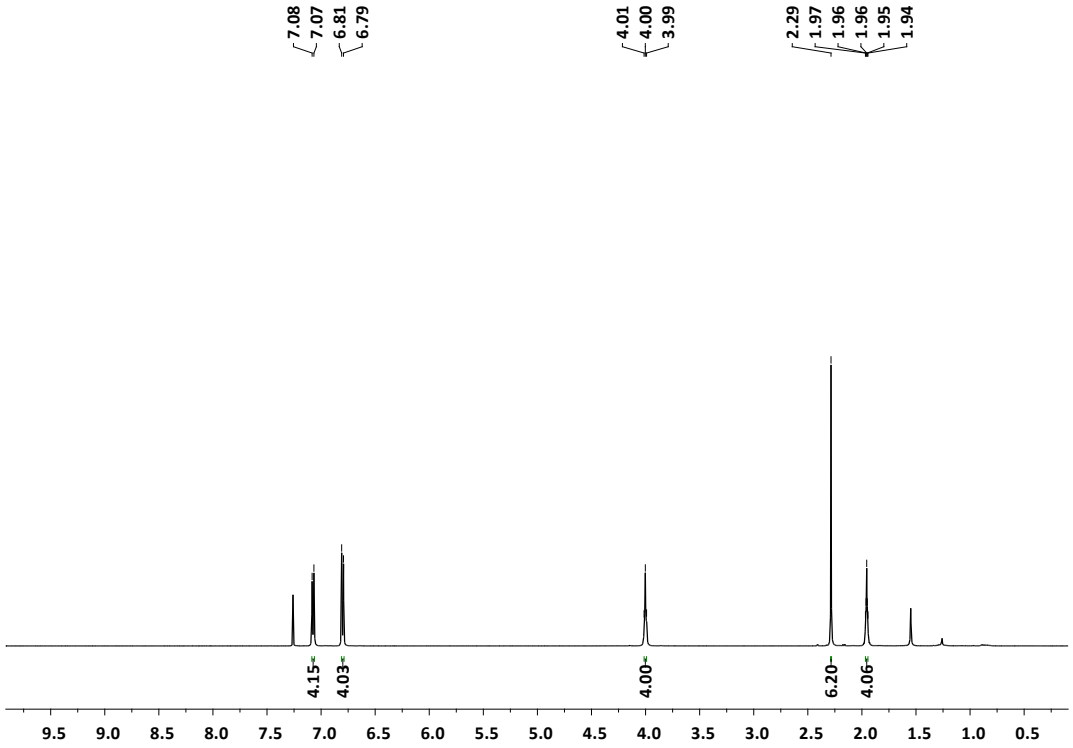


Figure s36. ^{1}H NMR spectrum of **4o.**

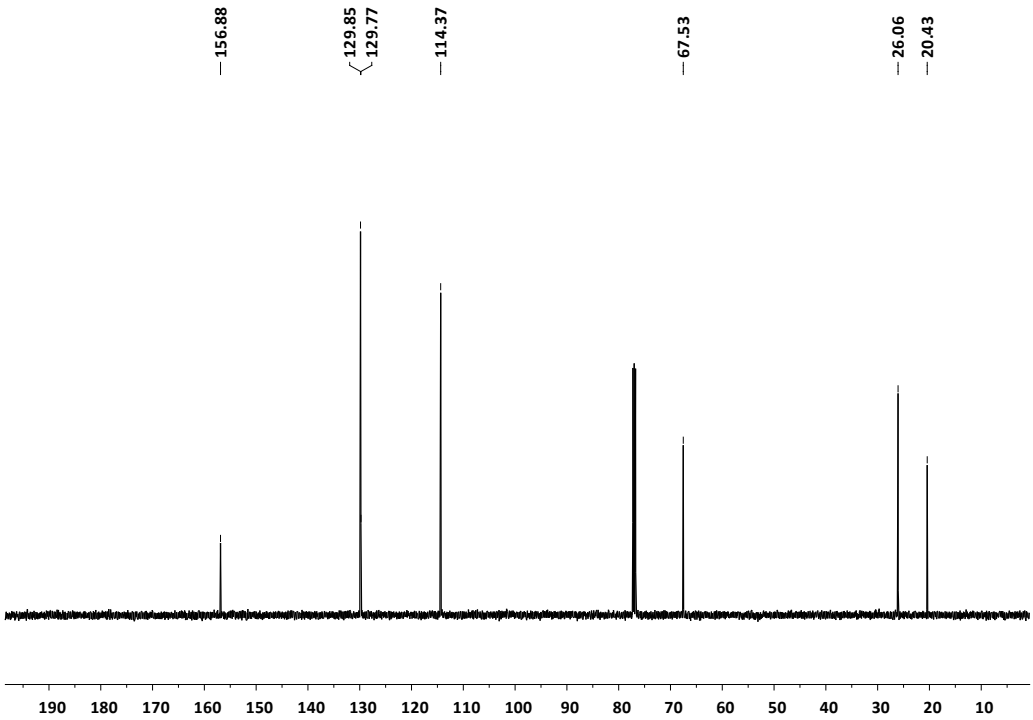


Figure s37. $^{13}C\{^{1}H\}$ NMR spectrum of **4o.**

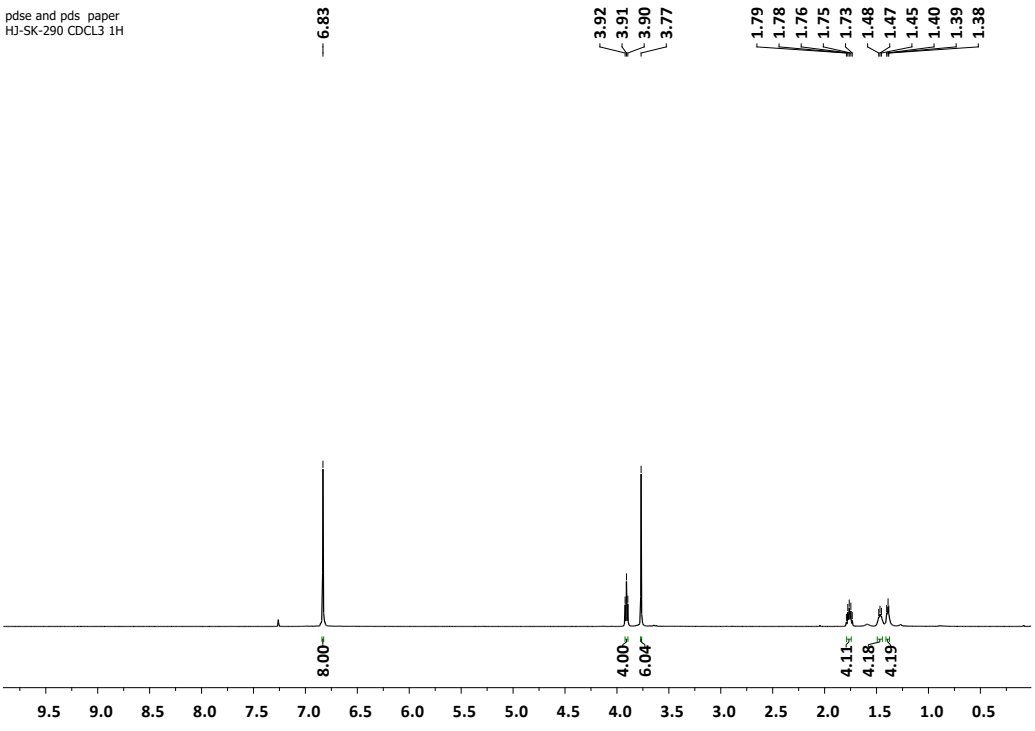


Figure s38. ^{1}H NMR spectrum of **4p.**

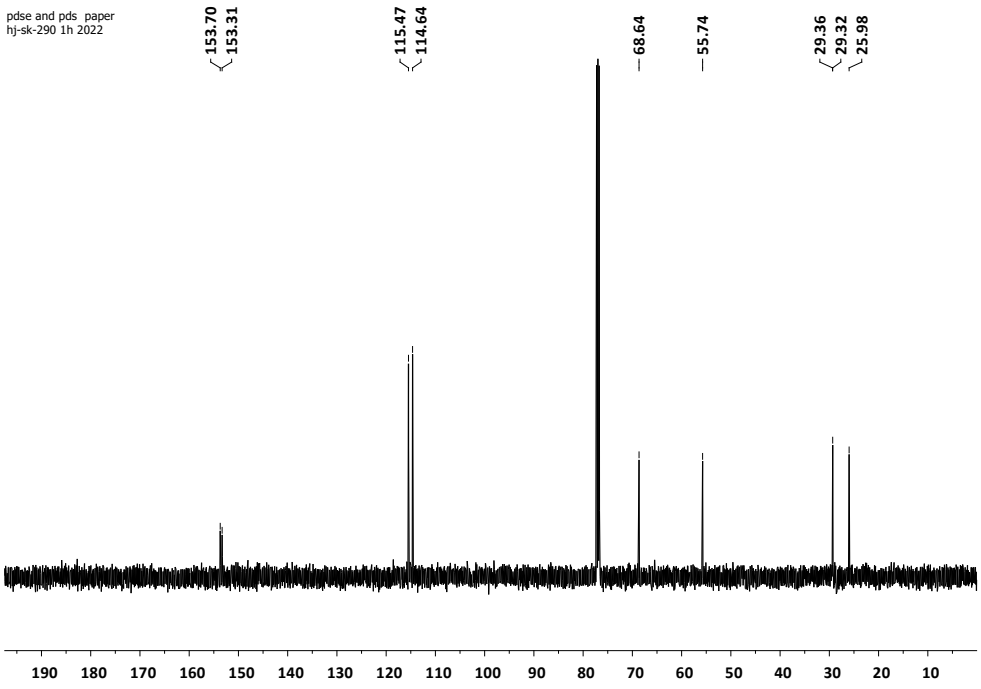


Figure s39. $^{13}C\{^{1}H\}$ NMR spectrum of **4p.**

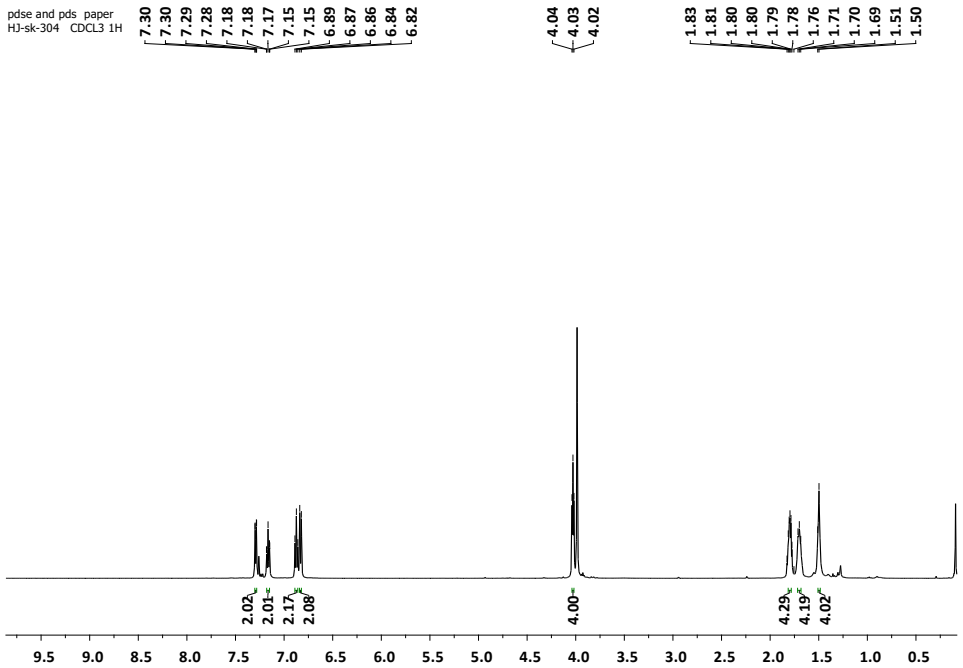


Figure s40. ^{1}H NMR spectrum of **4q.**

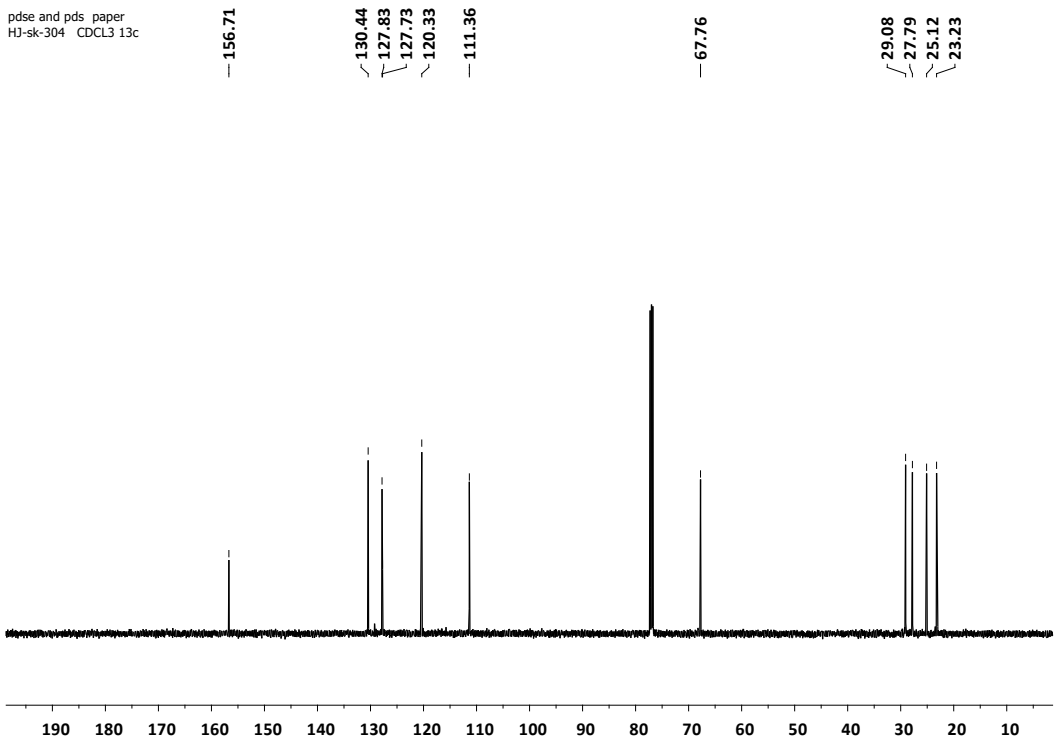


Figure s41. $^{13}C\{^{1}H\}$ NMR spectrum of **4q.**

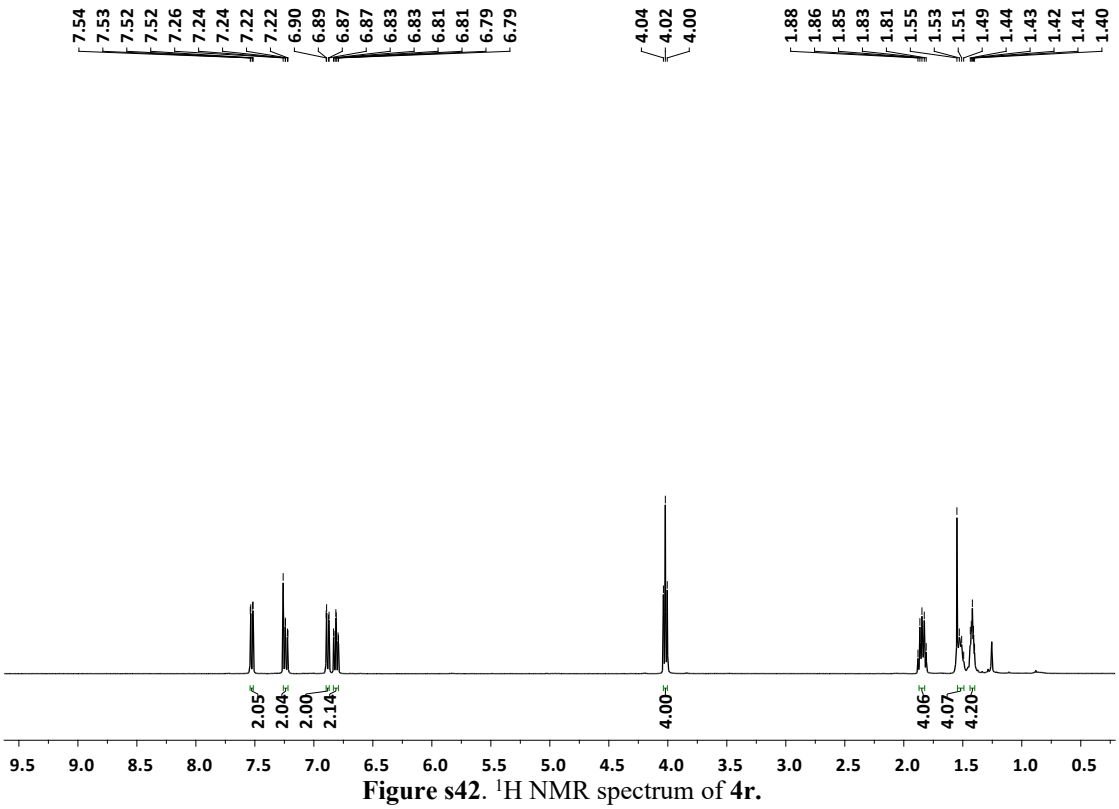


Figure s42. ^{1}H NMR spectrum of **4r.**

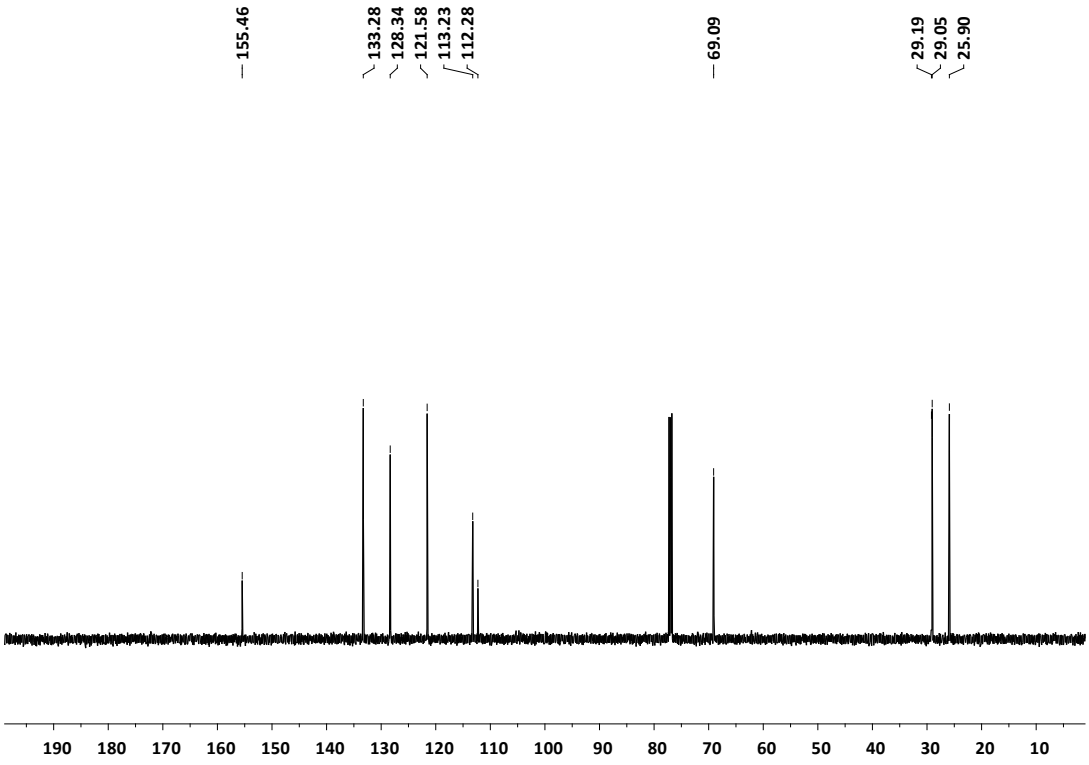


Figure s43. $^{13}C\{^{1}H\}$ NMR spectrum of **4r.**

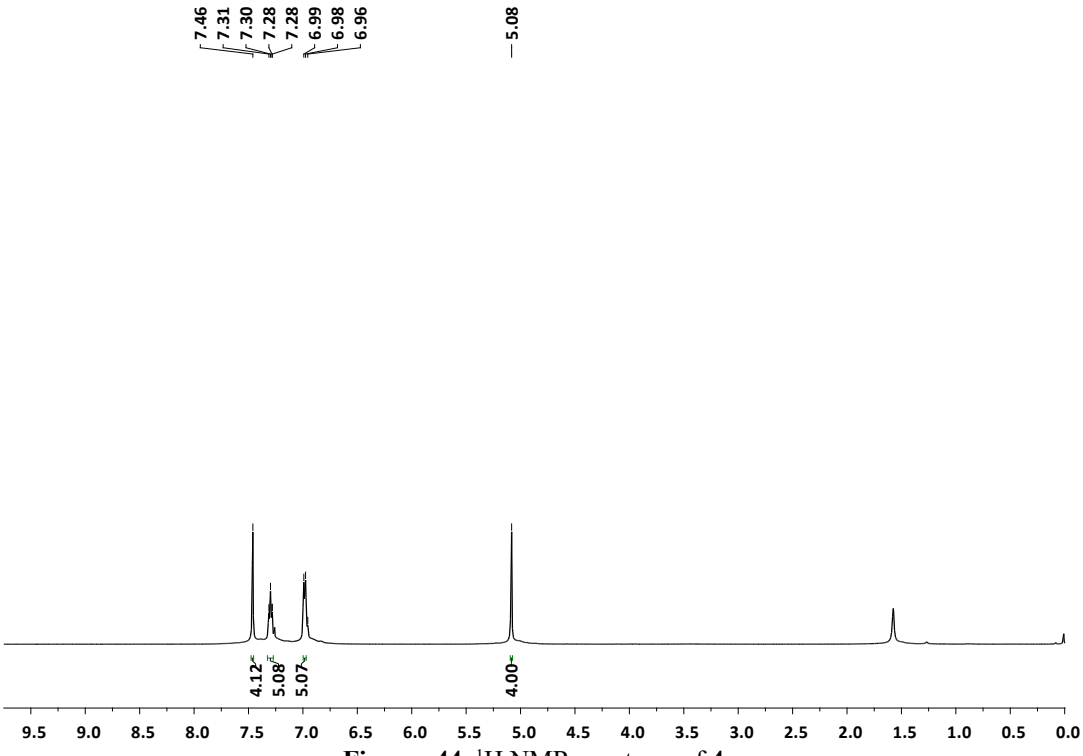


Figure s44. ^{1}H NMR spectrum of **4s.**

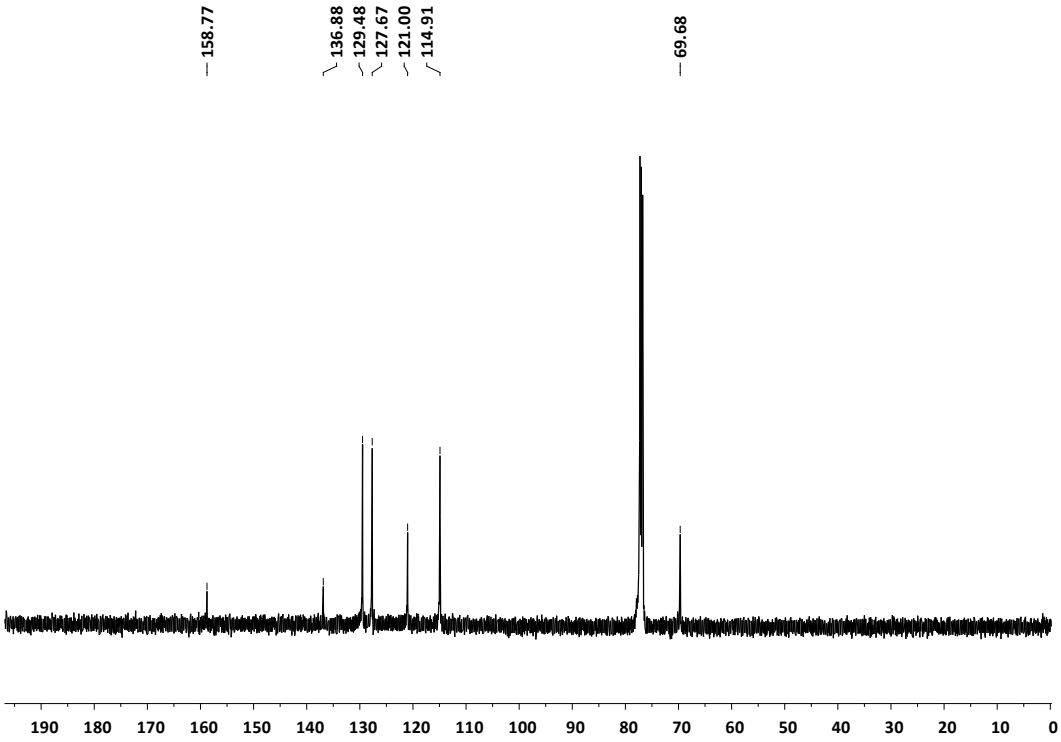


Figure s45. $^{13}C\{^{1}H\}$ NMR spectrum of **4s.**

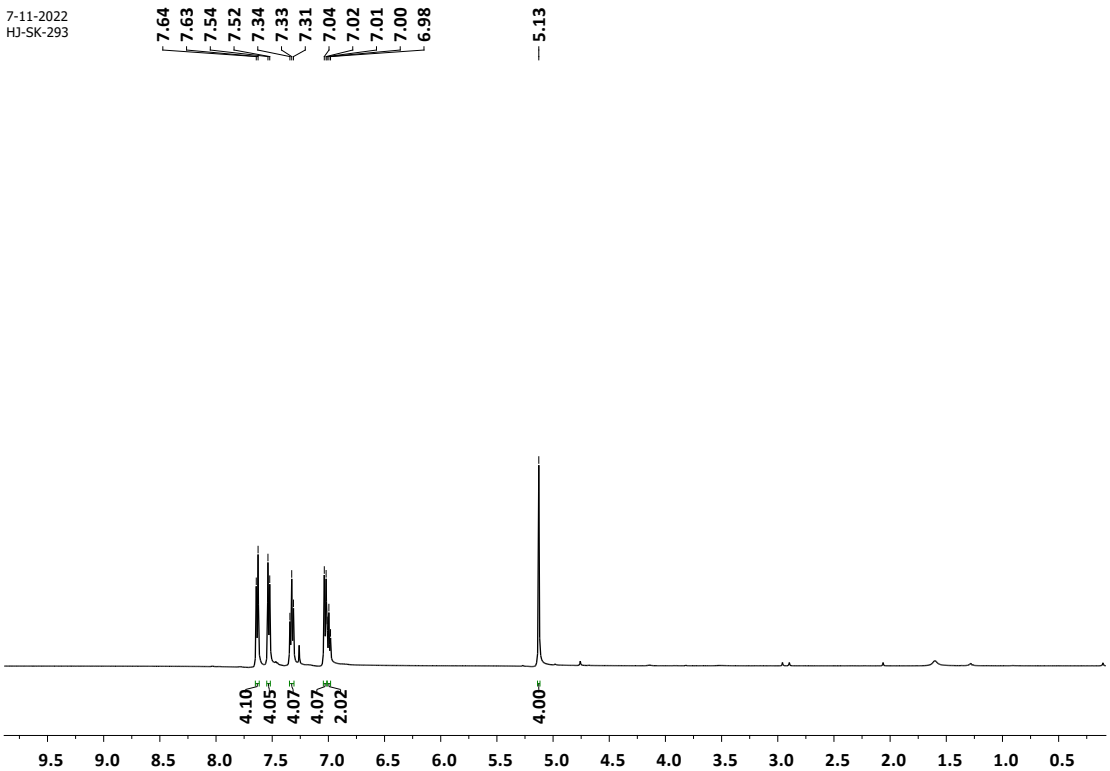


Figure s46. ^{1}H NMR spectrum of **4t.**

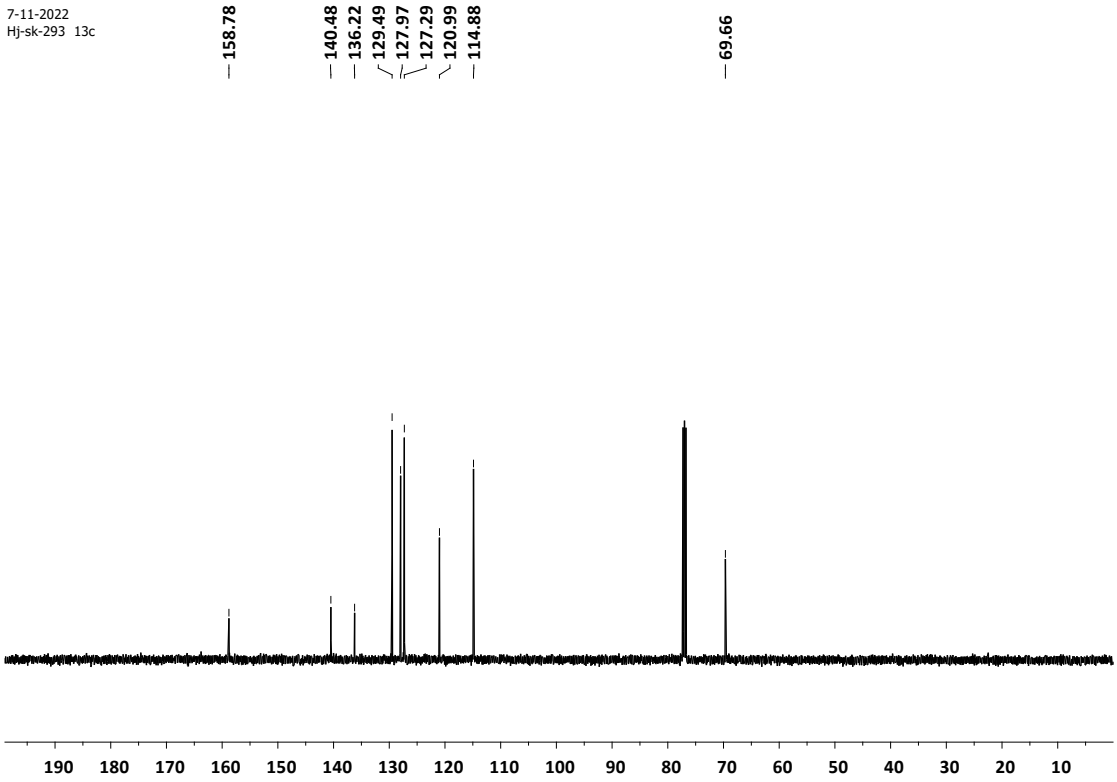


Figure s47. $^{13}C\{^{1}H\}$ NMR spectrum of **4t.**

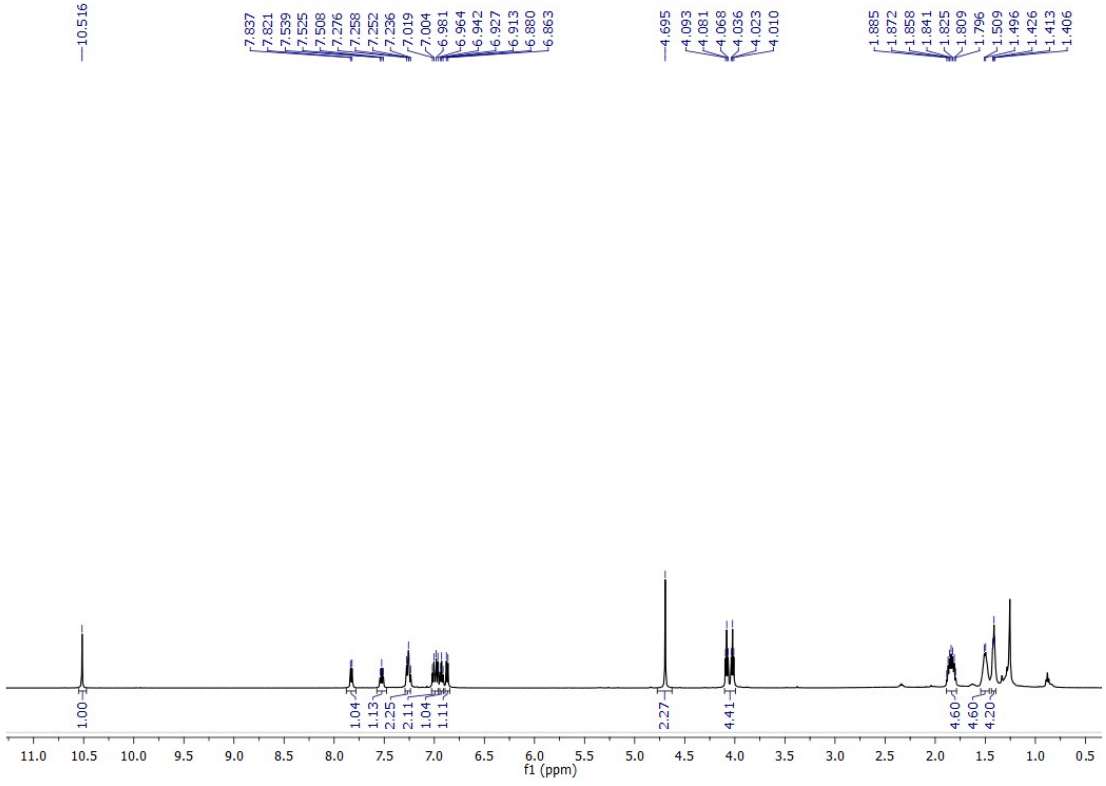


Figure s48. ^{1}H NMR spectrum of **5a.**

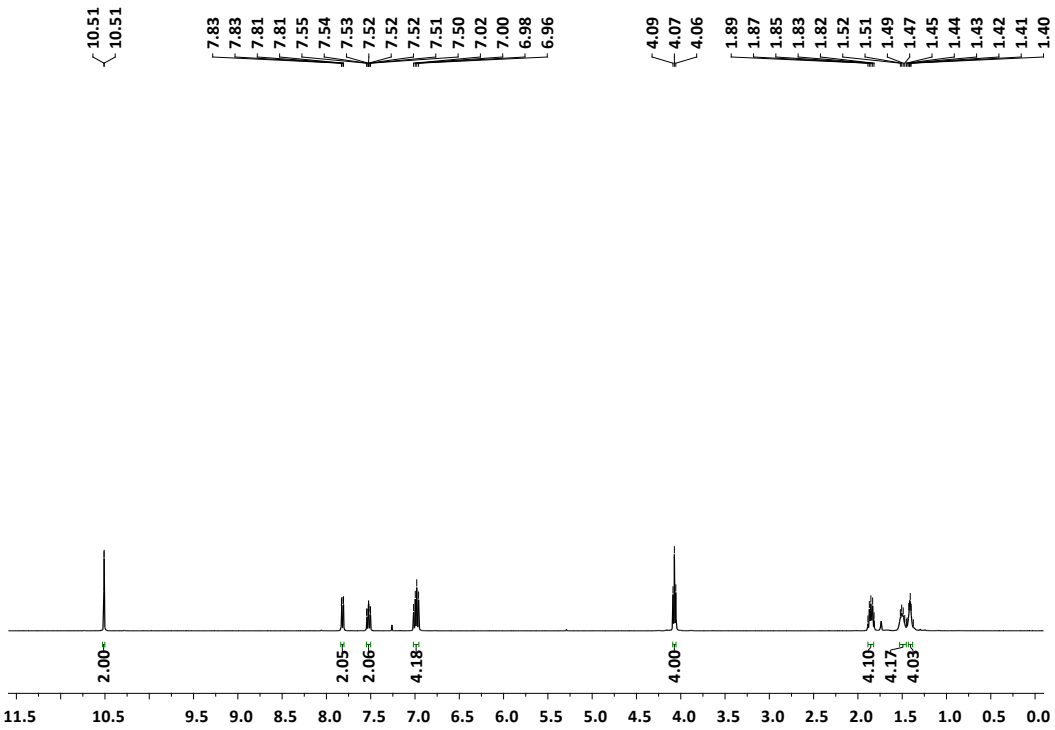


Figure s49. ^{1}H NMR spectrum of **6a**.

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Optimized cartesian coordinates (in angstrom units):

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C	-3.58508	-3.70881	-0.68859
H	-2.61568	-3.94834	-1.11868
C	-3.66025	-2.66115	0.23815
C	-2.42106	-1.93402	0.64795
H	-1.55264	-2.59381	0.66458
H	-2.50325	-1.42702	1.60739

TS (E=-2186.54032138 au)

Pd	-0.47553	0.14515	-0.05587
Se	2.08537	0.22060	0.17885
C	3.15575	-0.64193	1.70463
H	4.07416	-0.06162	1.76253
H	2.50045	-0.40449	2.54259
C	3.38939	-2.10901	1.57269
C	2.32633	-3.01033	1.71792
H	1.33068	-2.61070	1.89259
C	2.52550	-4.38738	1.63991

H	1.68551	-5.06527	1.75465
C	3.81005	-4.88133	1.41902
H	3.98338	-5.95211	1.35599
C	4.89073	-4.00864	1.28314
H	5.88211	-4.41197	1.11845
C	4.68784	-2.62452	1.35626
O	5.69848	-1.70993	1.24812
C	7.04546	-2.18267	1.20974
H	7.19714	-2.80491	0.31717
H	7.24340	-2.80403	2.09556
C	7.97533	-0.97811	1.17013
H	7.73766	-0.40469	0.26790
H	8.99966	-1.35600	1.04583
C	7.89398	-0.07946	2.41180
H	6.87728	0.31889	2.49320
H	8.04722	-0.69258	3.31019
C	8.92149	1.06950	2.42592
H	9.92619	0.64477	2.55637
H	8.73875	1.69159	3.31223
C	8.93431	1.95774	1.16947
H	9.74440	2.69314	1.26287
H	9.20364	1.33797	0.30530
C	7.61685	2.70019	0.88875
H	7.51129	3.52690	1.60207
H	6.76042	2.03958	1.05906
C	7.51267	3.24775	-0.54572
H	6.69459	3.97413	-0.61270
H	8.43304	3.78129	-0.81815
C	7.26772	2.16324	-1.59149
H	7.27795	2.58261	-2.60696
H	8.04775	1.39217	-1.54069
O	5.98676	1.58864	-1.32486
C	5.49460	0.61987	-2.15902
C	6.28838	-0.08764	-3.07070

H	7.34985	0.11588	-3.14825
C	5.71195	-1.06113	-3.88778
H	6.33946	-1.60552	-4.58798
C	4.34502	-1.32778	-3.81337
H	3.89475	-2.07954	-4.45389
C	3.55644	-0.61199	-2.91477
H	2.48746	-0.79684	-2.85547
C	4.10724	0.36339	-2.07571
C	3.24259	1.19486	-1.18338
H	2.43558	1.67864	-1.73975
H	3.80766	1.93950	-0.62983
Cl	-0.27582	1.03814	-2.29967
Cl	-0.66063	-0.76517	2.16371
Se	-2.96948	0.03476	-0.21608
C	-3.45887	1.84088	-1.04366
H	-2.80108	1.93285	-1.90716
H	-4.49964	1.71146	-1.34093
C	-3.26935	2.95513	-0.06971
C	-2.07948	3.69191	-0.06127
H	-1.30312	3.42507	-0.77275
C	-1.88499	4.74256	0.83588
H	-0.95537	5.30248	0.82561
C	-2.89333	5.06027	1.74283
H	-2.75684	5.87349	2.45013
C	-4.09148	4.34170	1.75771
H	-4.86109	4.60557	2.47241
C	-4.28330	3.28789	0.85693
O	-5.42038	2.53140	0.79683
C	-6.48135	2.82079	1.70923
H	-6.80247	3.86423	1.58440
H	-6.12193	2.70184	2.73987
C	-7.64899	1.88431	1.42304
H	-8.45481	2.16557	2.11475
H	-8.01961	2.08899	0.41144

C	-7.35191	0.38136	1.56213
H	-8.28673	-0.16008	1.36320
H	-6.64735	0.08514	0.77759
C	-6.80407	-0.03294	2.93544
H	-7.42145	0.42403	3.72243
H	-5.79390	0.37823	3.06023
C	-6.74394	-1.55029	3.19207
H	-6.35000	-1.69691	4.20467
H	-7.76474	-1.95901	3.20758
C	-5.88128	-2.35893	2.19635
H	-5.36545	-3.16553	2.73295
H	-5.09015	-1.72048	1.78640
C	-6.68098	-2.99166	1.04593
H	-7.37279	-3.74293	1.45206
H	-7.30332	-2.23957	0.55022
C	-5.80445	-3.68601	0.00334
H	-6.40265	-4.28105	-0.69734
H	-5.09551	-4.36222	0.49074
O	-4.97294	-2.76978	-0.72384
C	-5.48486	-2.05545	-1.76594
C	-6.79982	-2.15202	-2.23687
H	-7.51025	-2.81802	-1.76307
C	-7.20809	-1.38037	-3.32790
H	-8.23165	-1.46686	-3.68134
C	-6.32064	-0.51040	-3.95761
H	-6.63967	0.08502	-4.80697
C	-5.01112	-0.41578	-3.48457
H	-4.30373	0.24908	-3.97328
C	-4.57092	-1.17651	-2.39566
C	-3.16109	-1.08796	-1.91914
H	-2.49018	-0.61603	-2.63695
H	-2.75895	-2.05161	-1.60650