Electronic Supplementary Information

for

Chromium Catalysts for Selective Ethylene Oligomerization Featuring Binuclear PNP ligands

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CONTENTS

1. Crystallographic details

A suitable crystal was selected and carried out on a Bruker D8 VENTURE dual wavelength Mo/Cu diffractometer. The crystal was kept at 193.00 K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimization.

Table S1. Crystal data and structure refinement of ligand **2**.

Crystal and structure data	Ligand **2**
Empirical formula	$C_{54}H_{50}N_2P_4$
Formula weight	850.84
Temperature [K]	193.00
Crystal system	orthorhombic
Space group (number)	$Pbca$ (61)
a [Å]	9.0993(10)
b [Å]	19.8172(17)
c [Å]	54.043(7)
α [°]	90
β [°]	90
γ [°]	90
Volume [Å^3]	9745.2(18)
Z	8
ρ_{calc} [gcm^{-3}]	1.160
μ [mm^{-1}]	1.704
F(000)	3584
2θ Range(°)	9.51 to 137.19 (0.83 Å)
Index ranges	$-10 \leq h \leq 10$
	$-17 \leq k \leq 23$
	$-65 \leq l \leq 62$
Reflections collected	53974
Goodness-of-fit on F2	1.035

Final R indices [I>2sigma(I)]	R_1 = 0.0957
Largest diff. peak and hol	0.28/−0.30

2. Spectrum of Ligands

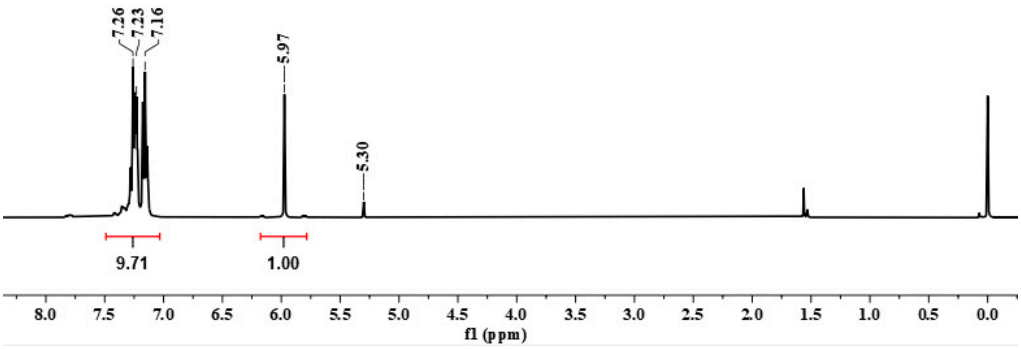

Figure S1. The ^{1}H NMR spectra of ligand **1**.

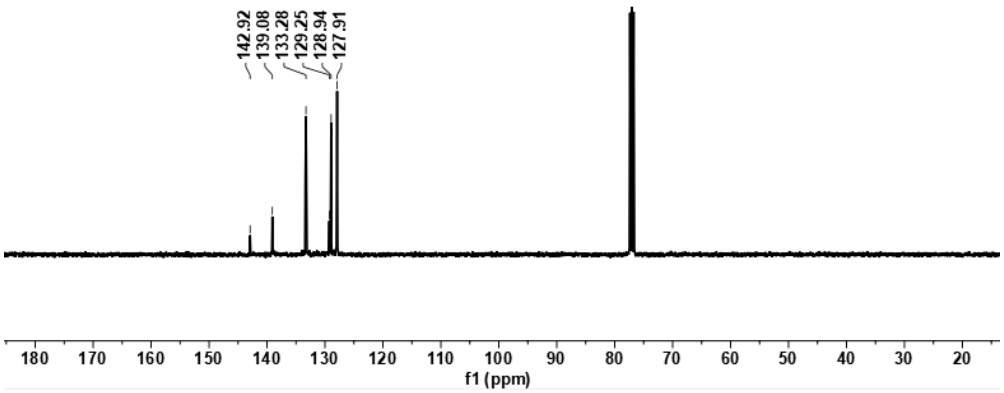

Figure S2. The ^{13}C NMR spectra of ligand **1**.

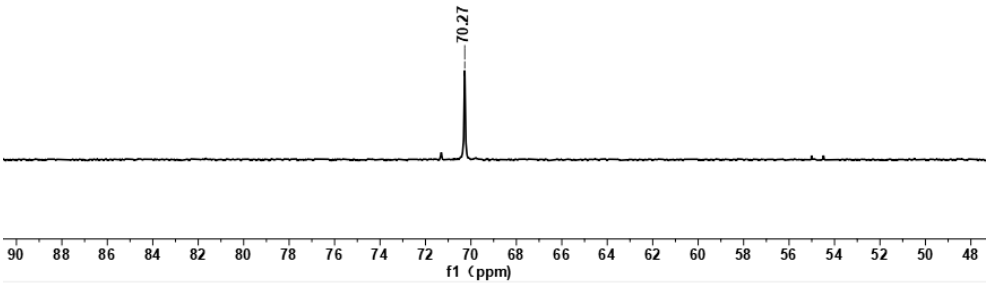

Figure S3. The ^{31}P NMR spectra of ligand **1**.

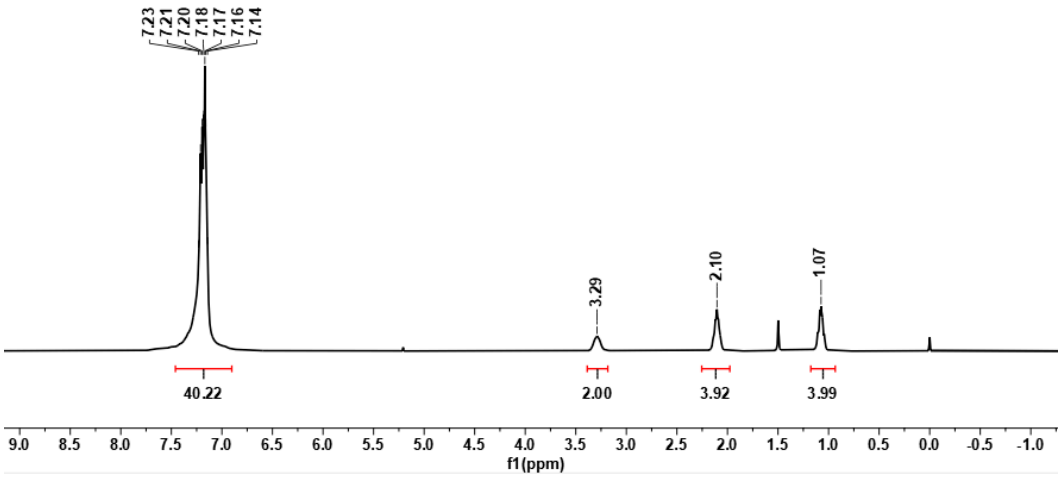

Figure S4. The ^{1}H NMR spectra of ligand **2**.

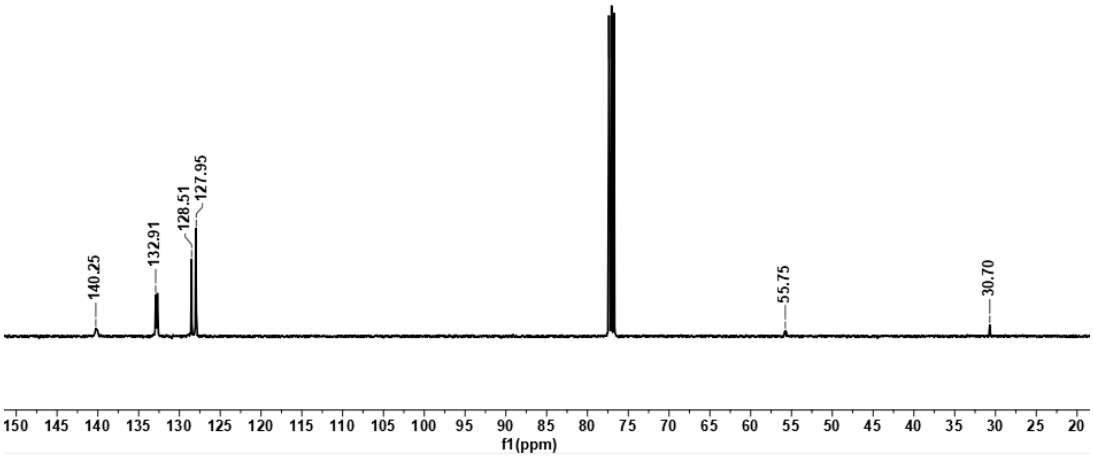

Figure S5. The ^{13}C NMR spectra of ligand **2**.

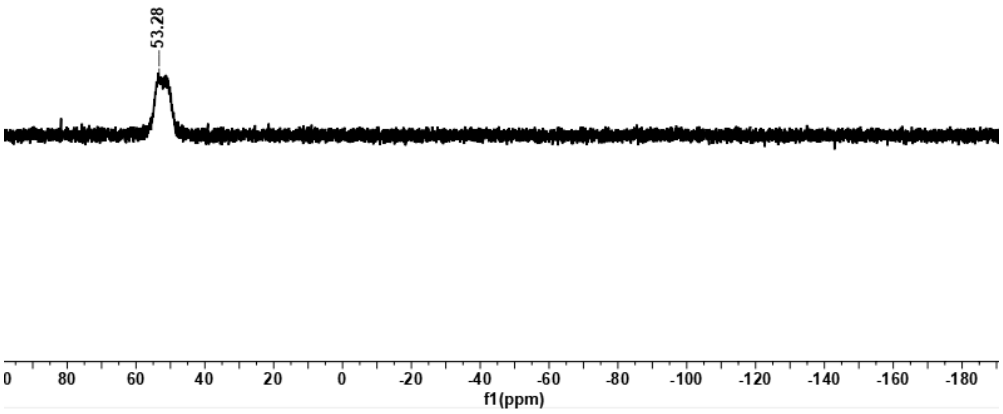

Figure S6. The ^{31}P NMR spectra of ligand **2**.

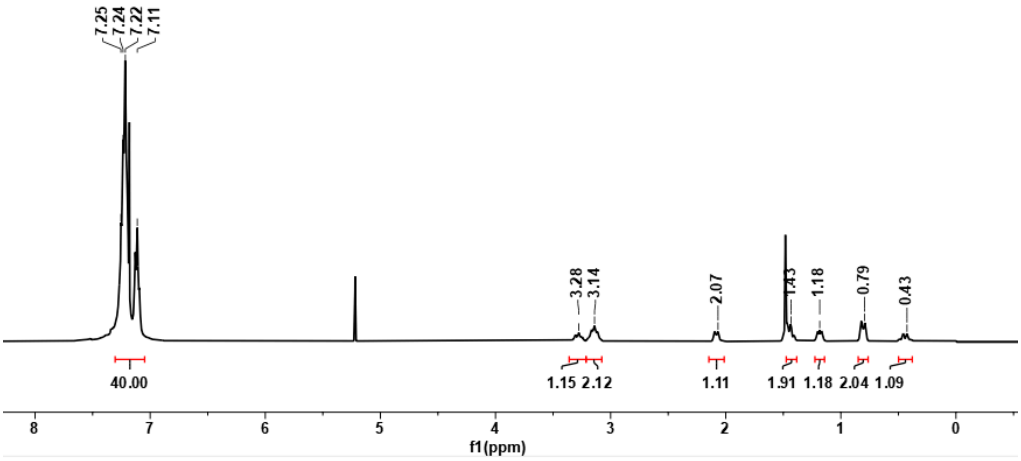

Figure S7. The ^{1}H NMR spectra of ligand **3**

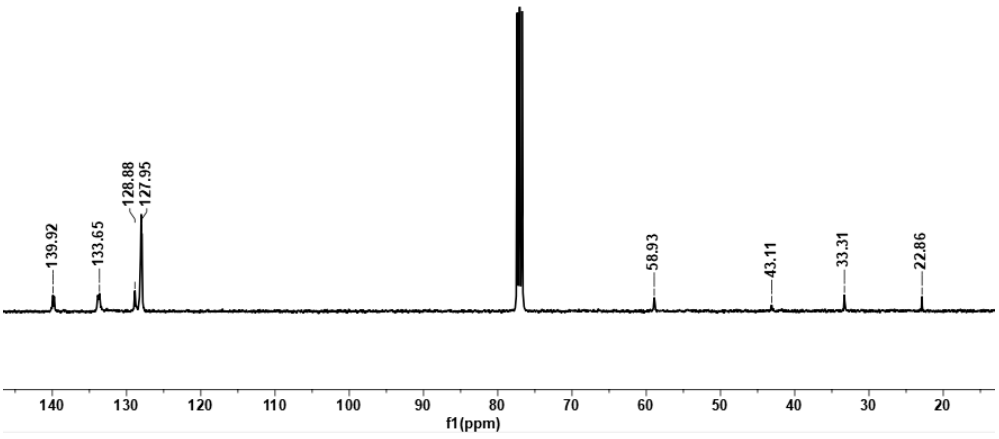

Figure S8. The ^{13}C NMR spectra of ligand **3**.

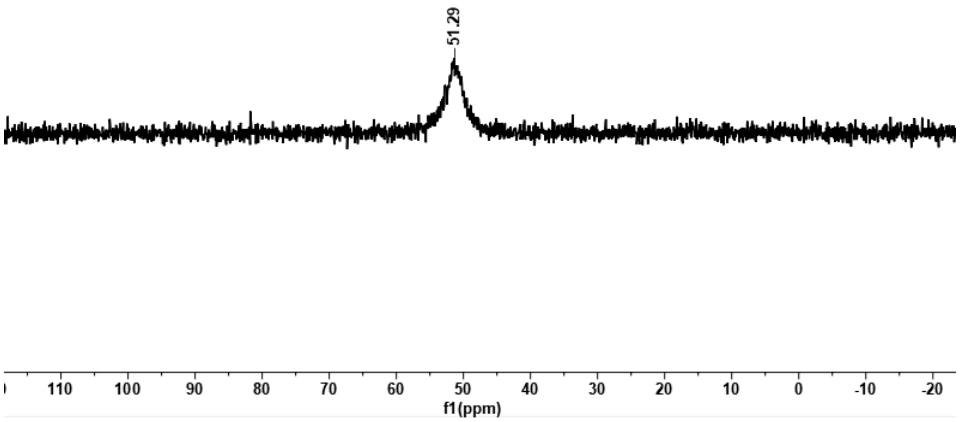

Figure S9. The ^{31}P NMR spectra of ligand **3**.

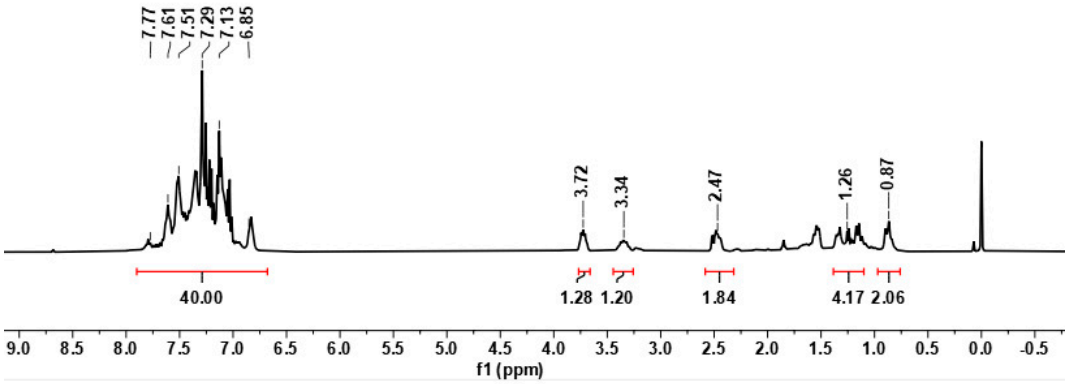

Figure S10. The ^{1}H NMR spectra of ligand **4**.

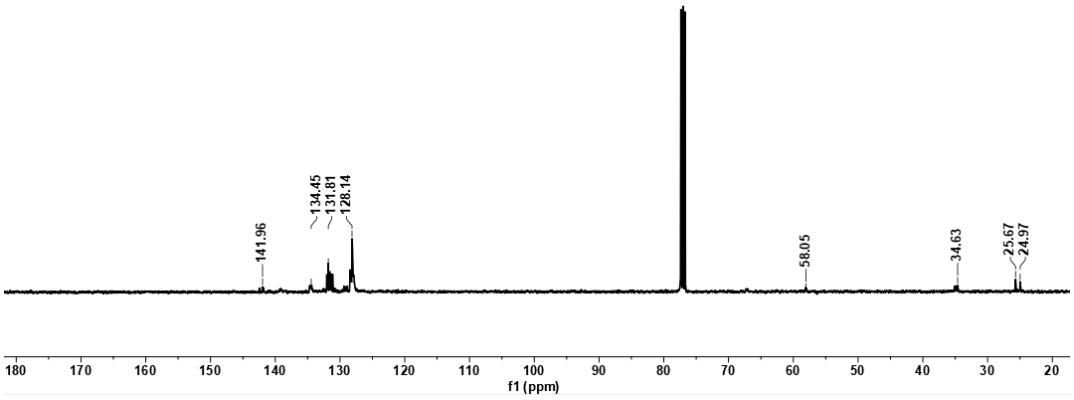

Figure S11. The ^{13}C NMR spectra of ligand **4**.

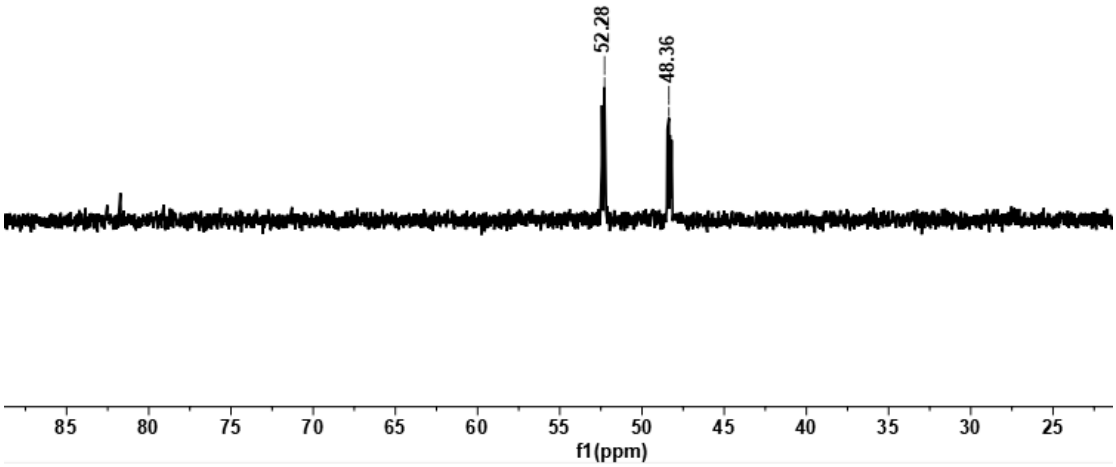

Figure S12. The ^{31}P NMR spectra of ligand **4**.

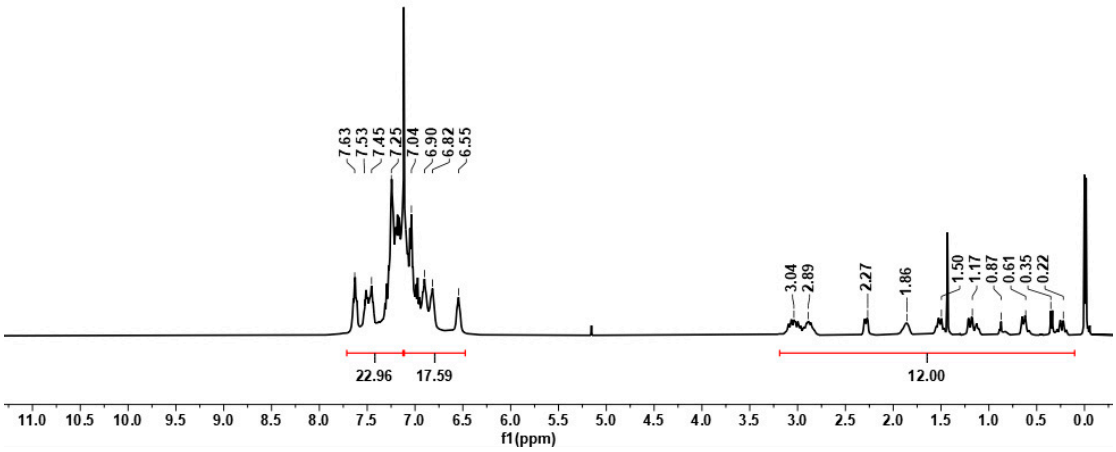

Figure S13. The ^{1}H NMR spectra of ligand **5**.

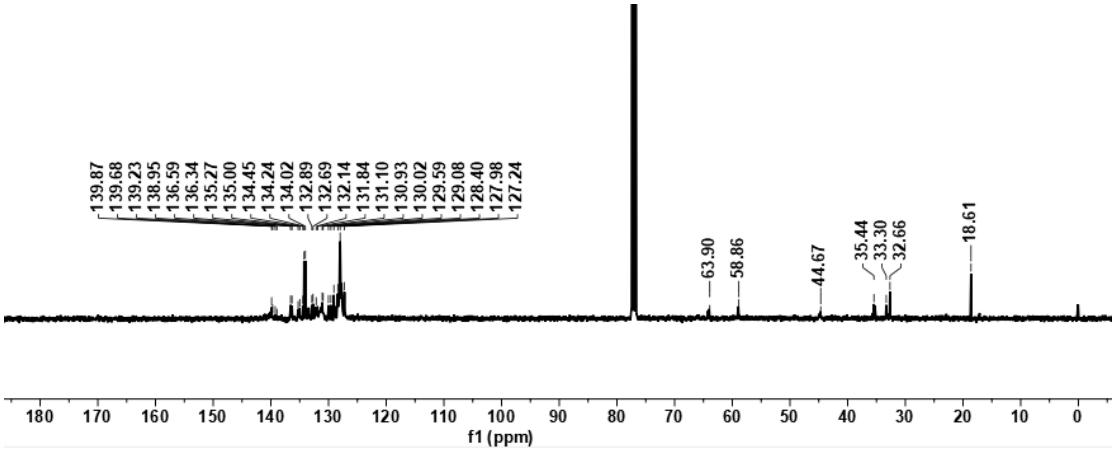

Figure S14. The ^{13}C NMR spectra of ligand **5**.

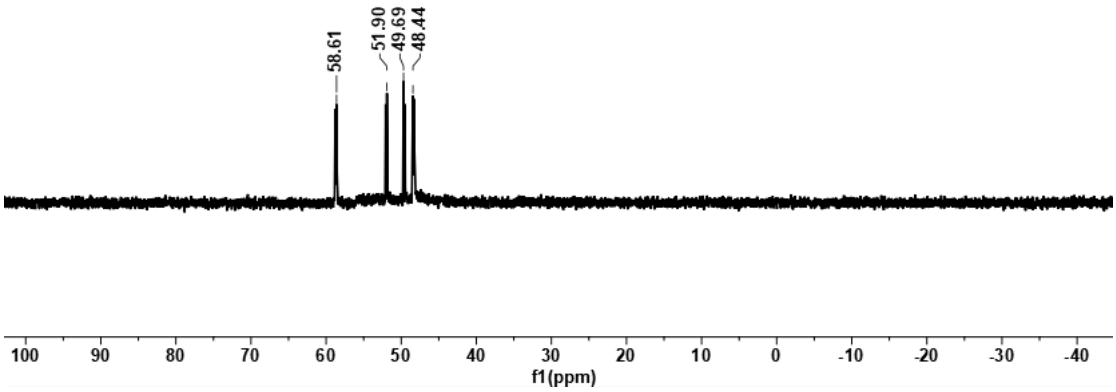

Figure S15. The ^{31}P NMR spectra of ligand **5**.

6. High Resolution Mass Spectrometry of Ligands

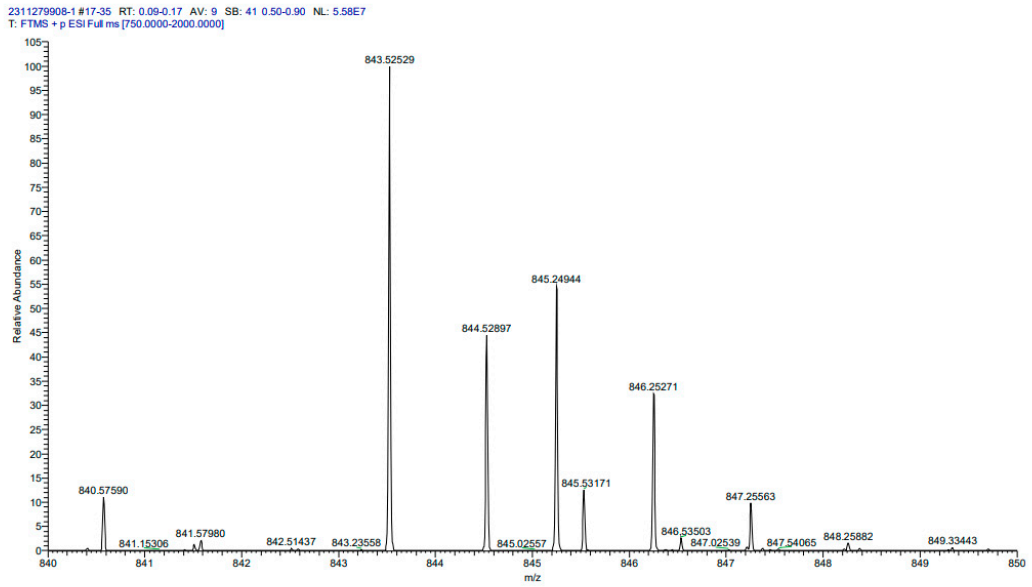

Figure S16. High Resolution Mass Spectrometry of **L1**

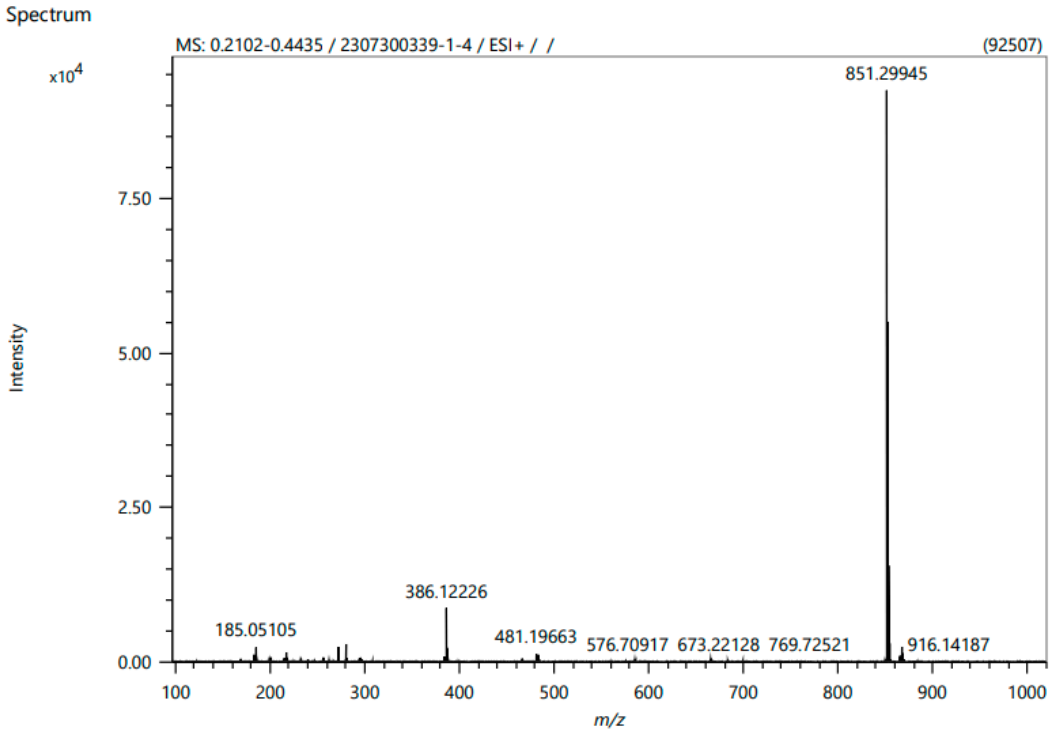

Figure S17. High Resolution Mass Spectrometry of **L2**

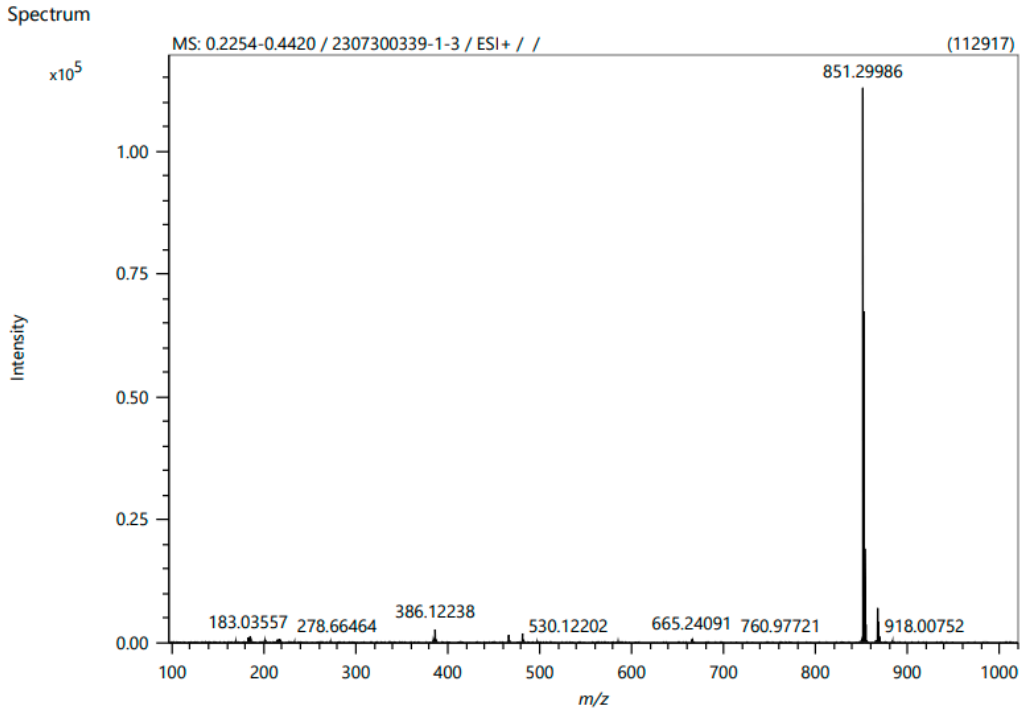

Figure S18. High Resolution Mass Spectrometry of **L3**

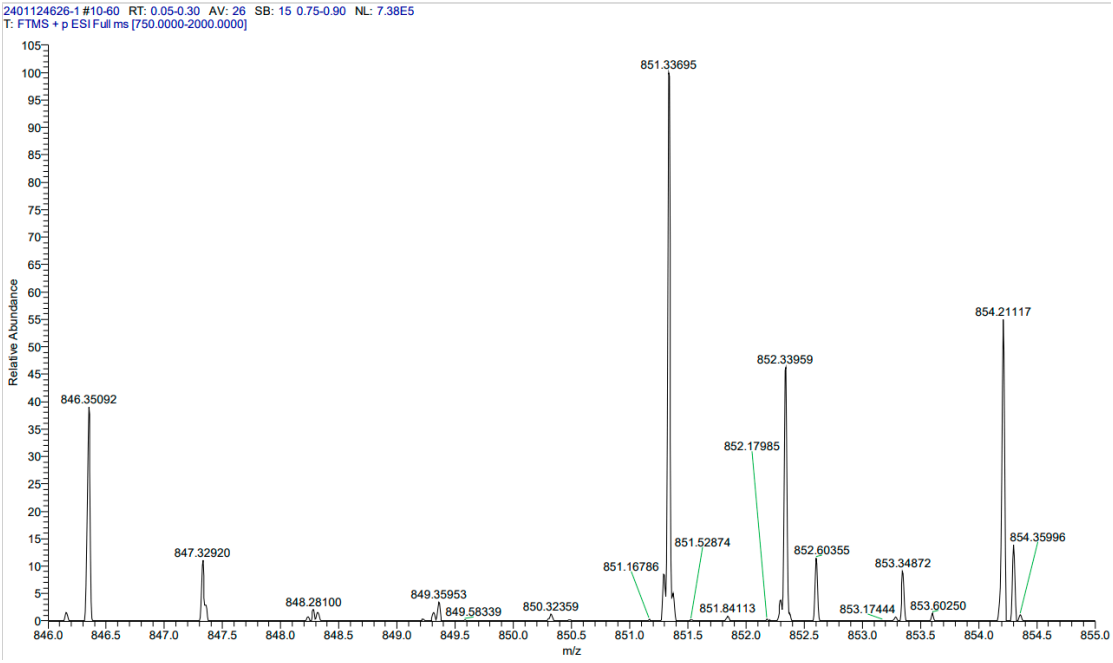

Figure S19. High Resolution Mass Spectrometry of **L4**

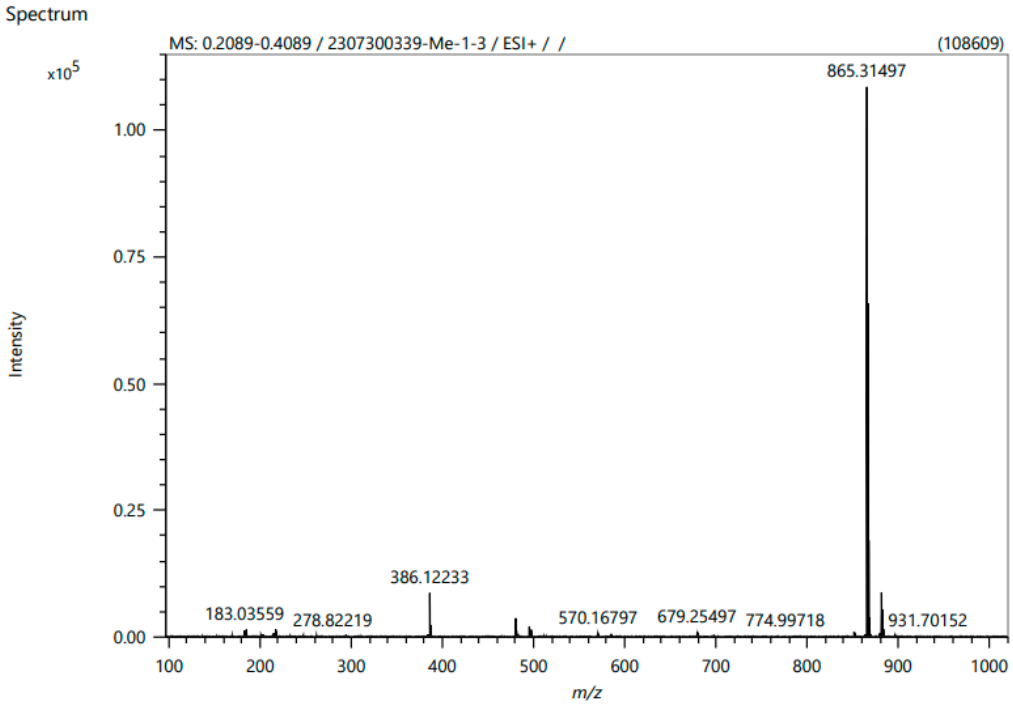

Figure S20. High Resolution Mass Spectrometry of **L5**

3. GC-MS spectrum of the typical oligomerization products

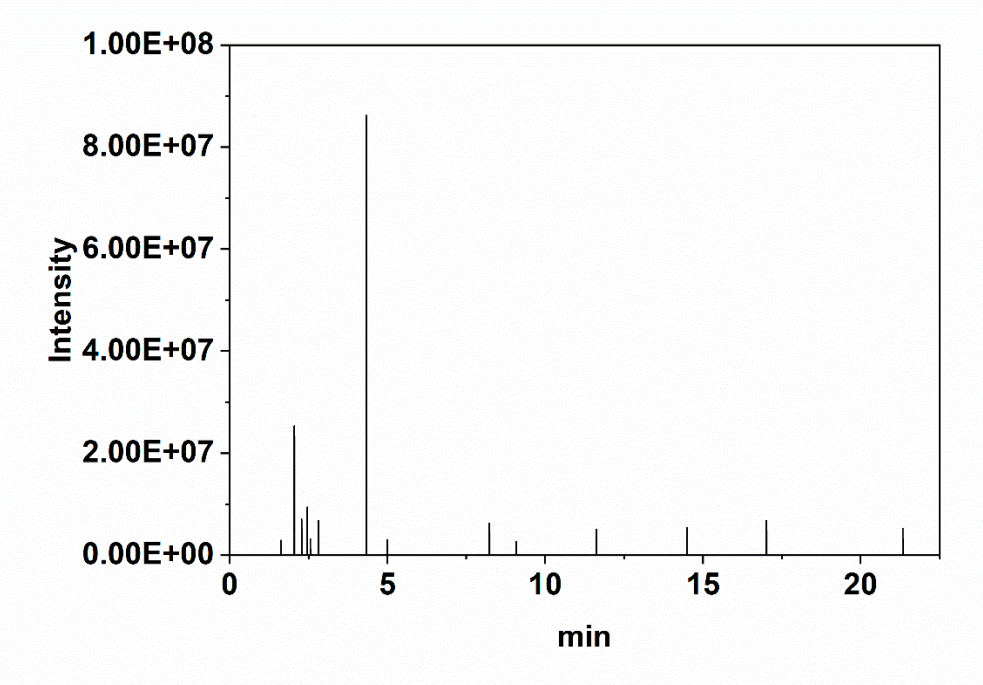

Figure S21. GC-MS spectrum of the oligomerization product obtained from entry 2 of Table 1.

Table S2. Corresponding residence time of chromatographic peak to the product.

Residence time	Oligomerization product
1.632	1-Butene
2.054	1-Hexene
2.287	Cyclopentane, methyl-
2.459	Cyclopentane, methylene-
2.562	Cyclohexane
2.822	Cyclopentane, 1,2-dimethy-
4.337	1-Octene
4.998	Cyclopentane, propyl-
8.241	1-Decene
9.086	Cyclopentane, pentyl-
11.626	1-Dodecene
14.496	1-Tetradecene
17.021	7-Hexadecene, (Z)-
21.333	1-Octadecene

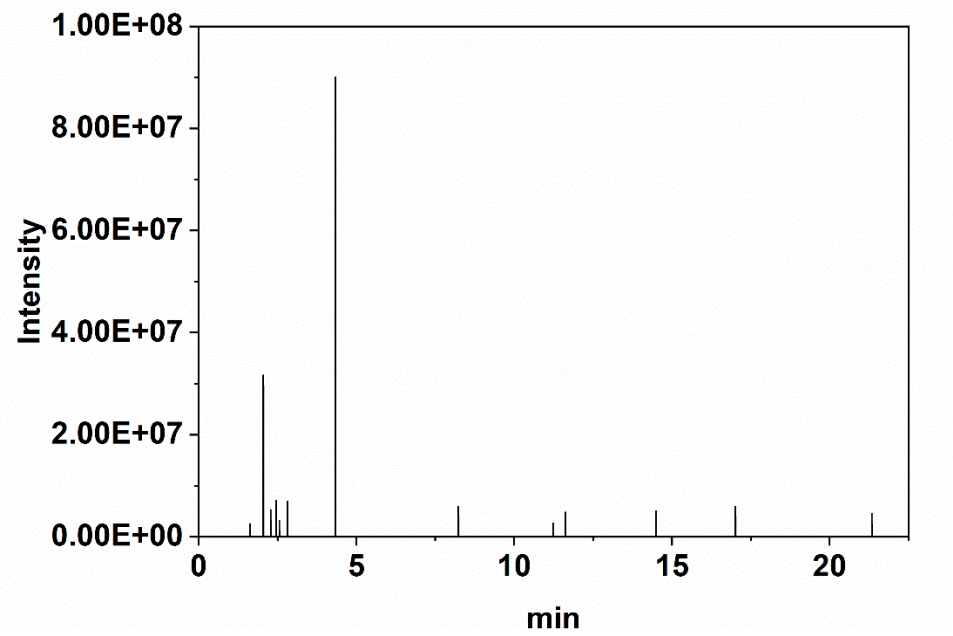

Figure S22. GC-MS spectrum of the oligomerization product obtained from entry 5 of Table 1.

Table S3. Corresponding residence time of chromatographic peak to the product.

Residence time	Liquid substance
1.632	1-Butene
2.054	1-Hexene
2.287	Cyclopentane, methyl-
2.459	Cyclopentane, methylene-
2.562	Cyclohexane
2.822	Cyclopentane, 1,2-dimethy-
4.337	1-Octene
4.998	Cyclopentane, propyl-
8.241	1-Decene
11.231	Decane, 5-methyl-6-methylene-1-
11.626	Dodecene
14.496	1-Tetradecene
17.021	7-Hexadecene, (Z)-
21.333	1-Octadecene

Computational methodology

All the density functional theory (DFT) calculations were performed by Gaussian 09 program [4] packages with M062X functional. Geometry optimizations were carried out in the gas phase with the 6-31G (d,p) basis set.

Optimized geometries from DFT calculations

L1

C	**0.58008**	**1.23631**	**-0.38497**
C	**-0.78153**	**1.18921**	**-0.07028**
C	**-1.38427**	**0.00851**	**0.40126**
C	**-0.53437**	**-1.10524**	**0.55055**
C	**0.80359**	**-1.06179**	**0.19658**
C	**1.41361**	**0.10672**	**-0.27646**
N	**2.80371**	**0.1548**	**-0.59401**
N	**-2.77732**	**-0.07698**	**0.69605**
P	**3.78463**	**-1.19751**	**-1.21556**
C	**4.23573**	**-2.34493**	**0.18315**
C	**5.38195**	**-3.11108**	**-0.11244**
C	**5.91249**	**-4.01589**	**0.81066**
C	**5.32811**	**-4.15198**	**2.0717**
C	**4.21504**	**-3.37442**	**2.3955**
C	**3.67244**	**-2.48333**	**1.46331**
C	**2.65081**	**-2.18842**	**-2.30811**
C	**2.64405**	**-1.76238**	**-3.65329**
C	**1.87097**	**-2.41164**	**-4.61633**
C	**1.10925**	**-3.52529**	**-4.25676**
C	**1.1346**	**-3.9877**	**-2.9345**
C	**1.89442**	**-3.32587**	**-1.96855**

P	**-4.0144**	**1.16592**	**0.53**
C	**-3.48448**	**2.6741**	**1.48185**
C	**-3.03471**	**3.88202**	**0.92852**
C	**-2.71015**	**4.96458**	**1.7481**
C	**-2.82324**	**4.85462**	**3.13579**
C	**-3.28469**	**3.66244**	**3.69931**
C	**-3.62519**	**2.58751**	**2.87829**
C	**-3.98447**	**1.70363**	**-1.23154**
C	**-4.88046**	**2.72732**	**-1.60086**
C	**-5.03977**	**3.08955**	**-2.93765**
C	**-4.32125**	**2.42422**	**-3.93526**
C	**-3.44089**	**1.39924**	**-3.58155**
C	**-3.27119**	**1.04168**	**-2.24202**
P	**-3.68986**	**-1.43796**	**1.45892**
C	**-4.08569**	**-2.52869**	**0.01451**
C	**-5.32629**	**-3.18514**	**0.0542**
C	**-5.72759**	**-4.02656**	**-0.98731**
C	**-4.89893**	**-4.21083**	**-2.09365**
C	**-3.66924**	**-3.54886**	**-2.15558**
C	**-3.26483**	**-2.71308**	**-1.11132**
C	**-2.99456**	**-1.92266**	**3.46172**
C	**-2.45149**	**-0.87085**	**4.20541**
C	**-1.27031**	**-1.03732**	**4.93867**
C	**-0.64133**	**-2.27745**	**4.95595**
C	**-1.19717**	**-3.34995**	**4.24402**
C	**-2.32659**	**-3.1614**	**3.45308**
P	**3.88541**	**1.54573**	**-0.48639**
C	**3.17557**	**2.90949**	**-1.53847**
C	**3.15428**	**2.69055**	**-2.92723**
C	**2.76479**	**3.70343**	**-3.80504**

C	**2.41431**	**4.96518**	**-3.31266**
C	**2.44679**	**5.19921**	**-1.93755**
C	**2.81891**	**4.17877**	**-1.05542**
C	**3.72921**	**2.19432**	**1.23788**
C	**2.83855**	**1.7294**	**2.22046**
C	**2.88857**	**2.23572**	**3.52148**
C	**3.82197**	**3.21481**	**3.86464**
C	**4.72322**	**3.67782**	**2.89923**
C	**4.68423**	**3.16326**	**1.60389**
H	**0.98102**	**2.1838**	**-0.72852**
H	**-1.352**	**2.10174**	**-0.19011**
H	**-0.94838**	**-2.01479**	**1.04901**
H	**1.38816**	**-1.95518**	**0.34798**
H	**5.86589**	**-2.98987**	**-1.07925**
H	**6.79184**	**-4.60054**	**0.55011**
H	**5.7475**	**-4.84427**	**2.79997**
H	**3.76268**	**-3.45608**	**3.38067**
H	**2.82308**	**-1.87938**	**1.75996**
H	**3.26019**	**-0.91363**	**-3.94682**
H	**1.87734**	**-2.05781**	**-5.64798**
H	**0.51257**	**-4.0416**	**-5.00396**
H	**0.56258**	**-4.87094**	**-2.65658**
H	**1.92851**	**-3.7275**	**-0.95456**
H	**-2.95417**	**3.98553**	**-0.15009**
H	**-2.36432**	**5.89268**	**1.30058**
H	**-2.56342**	**5.69599**	**3.77246**
H	**-3.39022**	**3.57379**	**4.77742**
H	**-4.00856**	**1.6726**	**3.32239**
H	**-5.4648**	**3.2402**	**-0.83894**
H	**-5.73409**	**3.88473**	**-3.20023**

H	-4.45142	2.69979	-4.97834
H	-2.87823	0.87392	-4.34946
H	-2.58544	0.24118	-1.98367
H	-5.98602	-3.02693	0.90375
H	-6.69169	-4.52716	-0.93925
H	-5.21211	-4.85892	-2.90919
H	-3.02276	-3.68162	-3.01887
H	-2.3108	-2.19819	-1.17644
H	-2.95149	0.09601	4.20515
H	-0.85899	-0.20184	5.49802
H	0.26383	-2.42542	5.53987
H	-0.73402	-4.33295	4.30559
H	-2.78552	-4.02016	2.97295
H	3.44699	1.71969	-3.32169
H	2.74626	3.5134	-4.87461
H	2.12458	5.76159	-3.99636
H	2.17774	6.17818	-1.54632
H	2.83443	4.374	0.01209
H	2.10427	0.96971	1.97852
H	2.18801	1.86246	4.26731
H	3.85407	3.60766	4.87669
H	5.46552	4.42982	3.15692
H	5.40881	3.51371	0.86907

L2

C	-0.41949	0.41795	-0.3509
C	1.03167	0.15542	-0.7564
C	2.01761	0.50164	0.36758
C	1.63155	-0.14104	1.70913
C	0.17832	0.19029	2.06504

C	**-0.73829**	**-0.32012**	**0.95218**
N	**-2.1794**	**-0.30943**	**1.33213**
N	**3.45054**	**0.29658**	**-0.01232**
P	**-2.33926**	**-1.05717**	**2.93066**
C	**-1.40557**	**-0.54292**	**4.42854**
C	**-2.15421**	**-0.25508**	**5.57214**
C	**-1.51996**	**0.1172**	**6.75495**
C	**-0.13301**	**0.21753**	**6.79644**
C	**0.62235**	**-0.08399**	**5.66333**
C	**-0.0104**	**-0.48203**	**4.49139**
C	**-1.32322**	**-2.59055**	**2.69169**
C	**-1.73753**	**-3.72473**	**3.40075**
C	**-1.04149**	**-4.92431**	**3.2945**
C	**0.07669**	**-5.01192**	**2.46563**
C	**0.48589**	**-3.89495**	**1.74408**
C	**-0.2147**	**-2.69472**	**1.85048**
P	**-3.25264**	**-0.43682**	**-0.02266**
C	**-3.04841**	**1.15987**	**-0.9227**
C	**-3.51639**	**2.29473**	**-0.24696**
C	**-3.45181**	**3.55245**	**-0.83662**
C	**-2.94652**	**3.68973**	**-2.12751**
C	**-2.49467**	**2.56533**	**-2.81252**
C	**-2.53516**	**1.30916**	**-2.21342**
C	**-2.48746**	**-1.67591**	**-1.14598**
C	**-3.05711**	**-1.87071**	**-2.41184**
C	**-2.60353**	**-2.88614**	**-3.24706**
C	**-1.59337**	**-3.74514**	**-2.81937**
C	**-1.05042**	**-3.58698**	**-1.54771**
C	**-1.50048**	**-2.56409**	**-0.71662**
P	**4.43296**	**0.9166**	**1.33199**

C	**4.13315**	**-0.22047**	**2.7506**
C	**3.23108**	**0.0137**	**3.79466**
C	**3.08501**	**-0.91343**	**4.81987**
C	**3.83145**	**-2.09047**	**4.81414**
C	**4.74087**	**-2.32884**	**3.78854**
C	**4.90245**	**-1.38997**	**2.77322**
C	**3.48999**	**2.42048**	**1.82274**
C	**2.52939**	**3.00428**	**0.99521**
C	**1.93405**	**4.21533**	**1.34298**
C	**2.29781**	**4.86171**	**2.51984**
C	**3.27082**	**4.2974**	**3.34336**
C	**3.87088**	**3.09394**	**2.99083**
P	**3.94521**	**0.7902**	**-1.66186**
C	**4.3618**	**-0.71438**	**-2.63582**
C	**5.48116**	**-0.63605**	**-3.46747**
C	**5.88387**	**-1.74039**	**-4.215**
C	**5.17847**	**-2.93709**	**-4.12531**
C	**4.06289**	**-3.02441**	**-3.29437**
C	**3.65588**	**-1.91797**	**-2.55563**
C	**2.90344**	**1.36134**	**-3.08349**
C	**2.97226**	**2.71879**	**-3.41986**
C	**2.14818**	**3.25607**	**-4.40677**
C	**1.27978**	**2.42115**	**-5.10534**
C	**1.24162**	**1.0579**	**-4.81871**
C	**2.04271**	**0.53249**	**-3.81024**
H	**-1.09783**	**0.08099**	**-1.14346**
H	**-0.58779**	**1.4934**	**-0.2002**
H	**1.13199**	**-0.90254**	**-1.02117**
H	**1.30038**	**0.73346**	**-1.64877**
H	**1.91613**	**1.58558**	**0.53603**

H	**1.72839**	**-1.22717**	**1.67651**
H	**2.31247**	**0.21894**	**2.48781**
H	**-0.09115**	**-0.27538**	**3.01996**
H	**0.04139**	**1.27292**	**2.18469**
H	**-0.47199**	**-1.3778**	**0.79847**
H	**-3.23942**	**-0.29397**	**5.52523**
H	**-2.11185**	**0.34811**	**7.6353**
H	**0.36295**	**0.52133**	**7.71337**
H	**1.70572**	**-0.02116**	**5.69635**
H	**0.58097**	**-0.75336**	**3.62365**
H	**-2.61167**	**-3.66456**	**4.04613**
H	**-1.37173**	**-5.79233**	**3.85666**
H	**0.62032**	**-5.94789**	**2.38142**
H	**1.3487**	**-3.95492**	**1.08734**
H	**0.09356**	**-1.83516**	**1.26363**
H	**-3.93051**	**2.19008**	**0.75385**
H	**-3.80875**	**4.42229**	**-0.29394**
H	**-2.90621**	**4.66786**	**-2.59665**
H	**-2.08177**	**2.66668**	**-3.81172**
H	**-2.12311**	**0.454**	**-2.73952**
H	**-3.8622**	**-1.2211**	**-2.74833**
H	**-3.04579**	**-3.01283**	**-4.23029**
H	**-1.24276**	**-4.54087**	**-3.46884**
H	**-0.27524**	**-4.26248**	**-1.19878**
H	**-1.08166**	**-2.4407**	**0.27669**
H	**2.61722**	**0.90853**	**3.79025**
H	**2.36902**	**-0.72613**	**5.61414**
H	**3.70695**	**-2.81728**	**5.61107**
H	**5.33237**	**-3.23882**	**3.78233**
H	**5.62354**	**-1.57088**	**1.97936**

H	2.24739	2.49359	0.07857
H	1.18469	4.65337	0.69067
H	1.83354	5.80446	2.79134
H	3.56521	4.79838	4.26032
H	4.63539	2.6657	3.63586
H	6.05727	0.28547	-3.50638
H	6.76003	-1.67123	-4.85241
H	5.49937	-3.80239	-4.69722
H	3.51426	-3.95812	-3.21217
H	2.80694	-1.98937	-1.88404
H	3.66647	3.36631	-2.88963
H	2.17419	4.32003	-4.62873
H	0.64103	2.83551	-5.8791
H	0.5784	0.40368	-5.37644
H	1.99189	-0.52706	-3.58231

L3

C	-0.8463	0.94181	-4.99823
C	0.52954	0.34186	-5.33731
C	1.48881	0.44133	-4.13818
C	0.87551	-0.27908	-2.92853
C	-0.50617	0.30219	-2.57646
C	-1.47374	0.25508	-3.77505
N	-2.85877	0.7321	-3.45218
N	1.93781	-0.73435	-1.32861
P	-4.18763	-0.36699	-3.10296
C	-3.8443	-1.11251	-1.43728
C	-3.21645	-0.36946	-0.42555
C	-3.13768	-0.85569	0.88041
C	-3.70012	-2.08982	1.20686

C	**-4.3501**	**-2.82945**	**0.21735**
C	**-4.42715**	**-2.3438**	**-1.08776**
C	**-3.89436**	**-1.80327**	**-4.24415**
C	**-4.62656**	**-1.79871**	**-5.44372**
C	**-4.49708**	**-2.8341**	**-6.37038**
C	**-3.6435**	**-3.90536**	**-6.10348**
C	**-2.91787**	**-3.93254**	**-4.91056**
C	**-3.03911**	**-2.88944**	**-3.99109**
P	**-3.47437**	**2.3729**	**-3.37388**
C	**-2.1274**	**3.4211**	**-2.63325**
C	**-2.16331**	**3.55347**	**-1.23378**
C	**-1.23428**	**4.34575**	**-0.55888**
C	**-0.26109**	**5.0442**	**-1.27628**
C	**-0.22589**	**4.94481**	**-2.66916**
C	**-1.15073**	**4.14217**	**-3.33963**
C	**-3.59187**	**2.99464**	**-5.11681**
C	**-3.6991**	**4.37583**	**-5.36019**
C	**-3.99399**	**4.85903**	**-6.63497**
C	**-4.20604**	**3.97298**	**-7.69249**
C	**-4.13074**	**2.5995**	**-7.45954**
C	**-3.83481**	**2.11628**	**-6.18433**
P	**2.24242**	**-2.28997**	**-0.57362**
C	**1.82962**	**-3.58888**	**-1.83756**
C	**0.57413**	**-4.18719**	**-2.03674**
C	**0.39779**	**-5.16942**	**-3.01104**
C	**1.47403**	**-5.57423**	**-3.80443**
C	**2.73007**	**-4.99946**	**-3.6109**
C	**2.90528**	**-4.02247**	**-2.62952**
C	**0.94607**	**-2.56051**	**0.7277**
C	**0.44292**	**-1.48616**	**1.47877**

C	**-0.36795**	**-1.70378**	**2.59303**
C	**-0.67957**	**-3.00266**	**2.99602**
C	**-0.16101**	**-4.08232**	**2.27991**
C	**0.64699**	**-3.8646**	**1.1638**
P	**3.15482**	**0.41617**	**-0.79646**
C	**3.73525**	**1.1944**	**-2.37597**
C	**4.102**	**2.54872**	**-2.45253**
C	**4.698**	**3.06584**	**-3.60461**
C	**4.94533**	**2.24018**	**-4.7017**
C	**4.60794**	**0.88716**	**-4.63131**
C	**4.02017**	**0.36942**	**-3.47789**
C	**2.20078**	**1.80101**	**0.00621**
C	**2.29768**	**1.86272**	**1.40704**
C	**1.60262**	**2.82838**	**2.13807**
C	**0.79862**	**3.75646**	**1.47675**
C	**0.70031**	**3.71861**	**0.08388**
C	**1.39767**	**2.75448**	**-0.64417**
H	**-1.50478**	**0.83874**	**-5.86374**
H	**-0.73593**	**2.01344**	**-4.81144**
H	**0.39926**	**-0.70042**	**-5.63273**
H	**0.95106**	**0.86596**	**-6.19918**
H	**1.6505**	**1.47084**	**-3.89555**
H	**0.78735**	**-1.35133**	**-3.14319**
H	**-0.92904**	**-0.25885**	**-1.73953**
H	**-0.38879**	**1.33773**	**-2.23883**
H	**-1.59053**	**-0.79943**	**-4.04716**
H	**-2.78155**	**0.59527**	**-0.66296**
H	**-2.63615**	**-0.26675**	**1.64345**
H	**-3.63901**	**-2.46884**	**2.22277**
H	**-4.79848**	**-3.78881**	**0.46042**

H	**-4.94383**	**-2.93216**	**-1.84044**
H	**-5.31393**	**-0.98058**	**-5.64293**
H	**-5.07358**	**-2.81196**	**-7.29069**
H	**-3.55283**	**-4.72081**	**-6.81551**
H	**-2.26008**	**-4.76936**	**-4.69187**
H	**-2.48**	**-2.93046**	**-3.06163**
H	**-2.93902**	**3.04034**	**-0.67116**
H	**-1.28286**	**4.43268**	**0.52284**
H	**0.45366**	**5.67582**	**-0.75635**
H	**0.52266**	**5.48966**	**-3.23754**
H	**-1.11909**	**4.09394**	**-4.4226**
H	**-3.55052**	**5.08347**	**-4.54956**
H	**-4.05915**	**5.93087**	**-6.80058**
H	**-4.43599**	**4.34936**	**-8.68494**
H	**-4.30373**	**1.89904**	**-8.27203**
H	**-3.79004**	**1.04555**	**-6.01611**
H	**-0.27257**	**-3.88004**	**-1.43127**
H	**-0.58472**	**-5.60732**	**-3.16161**
H	**1.33411**	**-6.33813**	**-4.5639**
H	**3.57512**	**-5.31744**	**-4.21488**
H	**3.89098**	**-3.59352**	**-2.46755**
H	**0.68887**	**-0.4692**	**1.19485**
H	**-0.75368**	**-0.85306**	**3.14814**
H	**-1.31065**	**-3.17208**	**3.86358**
H	**-0.38483**	**-5.09971**	**2.58906**
H	**1.04706**	**-4.72088**	**0.62954**
H	**3.9215**	**3.20777**	**-1.60958**
H	**4.96932**	**4.11743**	**-3.6421**
H	**5.40544**	**2.64396**	**-5.59885**
H	**4.80723**	**0.23156**	**-5.47444**

H	3.77994	-0.68797	-3.42769
H	2.92673	1.1445	1.92638
H	1.6943	2.85721	3.22009
H	0.25623	4.50958	2.04134
H	0.07828	4.43749	-0.44157
H	1.32232	2.76103	-1.72661
H	2.42262	-0.01644	-4.38984

L4

C	-0.12724	2.54547	1.02098
C	0.5321	1.6655	2.09085
C	0.97168	0.31352	1.51936
C	1.92043	0.53207	0.32626
C	1.17089	1.27865	-0.78791
C	0.77997	2.66056	-0.21303
N	2.25809	2.46246	3.19188
N	-0.46574	-1.5767	1.11295
P	3.50447	1.43305	3.89199
C	4.91436	1.48008	2.69499
C	5.0951	2.52335	1.77742
C	6.27104	2.61311	1.02852
C	7.28379	1.66644	1.18597
C	7.11408	0.62063	2.09782
C	5.94378	0.53404	2.84856
C	2.8067	-0.25847	3.57146
C	1.89796	-0.76286	4.51605
C	1.23056	-1.96828	4.29388
C	1.47847	-2.70151	3.13113
C	2.40322	-2.22786	2.19749
C	3.05893	-1.01544	2.41464

P	**2.25501**	**4.00381**	**4.00702**
C	**1.88282**	**5.2835**	**2.71718**
C	**2.95402**	**6.10857**	**2.34016**
C	**2.77519**	**7.13905**	**1.41282**
C	**1.52415**	**7.34674**	**0.83328**
C	**0.44532**	**6.5385**	**1.20253**
C	**0.6224**	**5.52881**	**2.14526**
C	**0.71474**	**4.03515**	**5.0391**
C	**0.00847**	**5.22213**	**5.29311**
C	**-1.04659**	**5.24498**	**6.20738**
C	**-1.40909**	**4.08666**	**6.89479**
C	**-0.69743**	**2.90561**	**6.6715**
C	**0.35769**	**2.88474**	**5.76188**
P	**-0.62299**	**-2.76116**	**-0.17225**
C	**0.97158**	**-3.71162**	**-0.05081**
C	**2.20248**	**-3.32146**	**-0.60452**
C	**3.35614**	**-4.07052**	**-0.37508**
C	**3.30053**	**-5.22445**	**0.40973**
C	**2.08165**	**-5.63346**	**0.95382**
C	**0.92711**	**-4.88558**	**0.71844**
C	**-0.32667**	**-1.74714**	**-1.69457**
C	**-0.69263**	**-0.39314**	**-1.7353**
C	**-0.58967**	**0.34279**	**-2.91661**
C	**-0.1189**	**-0.26346**	**-4.08205**
C	**0.23266**	**-1.61595**	**-4.06194**
C	**0.1235**	**-2.35196**	**-2.88163**
P	**-2.00061**	**-1.34344**	**1.89726**
C	**-1.63687**	**-1.17383**	**3.69838**
C	**-2.36126**	**-0.31281**	**4.53989**
C	**-2.20885**	**-0.37092**	**5.92681**

C	**-1.32825**	**-1.28524**	**6.50416**
C	**-0.62221**	**-2.16706**	**5.68102**
C	**-0.79047**	**-2.12387**	**4.29903**
C	**-2.65235**	**0.32757**	**1.39974**
C	**-3.63554**	**0.27354**	**0.39614**
C	**-4.26282**	**1.43091**	**-0.067**
C	**-3.92741**	**2.66688**	**0.48406**
C	**-2.9473**	**2.7399**	**1.47743**
C	**-2.3112**	**1.58389**	**1.92861**
H	**-0.31599**	**3.54397**	**1.42107**
H	**-1.10257**	**2.13003**	**0.7521**
H	**-0.15781**	**1.51607**	**2.92908**
H	**2.76267**	**1.1121**	**0.64106**
H	**1.81404**	**1.42306**	**-1.65641**
H	**0.29275**	**0.71425**	**-1.10579**
H	**1.6709**	**3.18639**	**0.0602**
H	**4.31982**	**3.27159**	**1.64832**
H	**6.38529**	**3.41928**	**0.31346**
H	**8.19633**	**1.7401**	**0.60158**
H	**7.89379**	**-0.12514**	**2.22532**
H	**5.82548**	**-0.28148**	**3.55789**
H	**1.70895**	**-0.20679**	**5.4307**
H	**0.52278**	**-2.33743**	**5.03055**
H	**0.96087**	**-3.64111**	**2.95913**
H	**2.61336**	**-2.78683**	**1.29023**
H	**3.74911**	**-0.65043**	**1.66414**
H	**3.93106**	**5.94755**	**2.78791**
H	**3.61287**	**7.77555**	**1.14273**
H	**1.38586**	**8.13288**	**0.09713**
H	**-0.52665**	**6.68555**	**0.74351**

H	**-0.22992**	**4.93112**	**2.44494**
H	**0.27417**	**6.1359**	**4.77125**
H	**-1.58752**	**6.17164**	**6.37836**
H	**-2.23256**	**4.10442**	**7.60267**
H	**-0.96378**	**1.99901**	**7.20787**
H	**0.90611**	**1.96324**	**5.59845**
H	**2.26926**	**-2.42409**	**-1.21097**
H	**4.30025**	**-3.74429**	**-0.80267**
H	**4.20084**	**-5.80436**	**0.59144**
H	**2.02904**	**-6.53553**	**1.55669**
H	**-0.02042**	**-5.20979**	**1.14181**
H	**-1.06098**	**0.09472**	**-0.84098**
H	**-0.86391**	**1.39156**	**-2.9172**
H	**-0.02795**	**0.3134**	**-4.99775**
H	**0.59281**	**-2.09976**	**-4.96588**
H	**0.40662**	**-3.40101**	**-2.88105**
H	**-3.05201**	**0.40827**	**4.11824**
H	**-2.77785**	**0.30903**	**6.55526**
H	**-1.20512**	**-1.32391**	**7.58254**
H	**0.05157**	**-2.89906**	**6.11742**
H	**-0.26138**	**-2.83606**	**3.67472**
H	**-3.91463**	**-0.69128**	**-0.01906**
H	**-5.01923**	**1.36363**	**-0.84338**
H	**-4.42488**	**3.57076**	**0.14298**
H	**-2.6717**	**3.69863**	**1.90291**
H	**-1.56217**	**1.66757**	**2.70614**
H	**1.46737**	**-0.28131**	**2.28981**
H	**0.26694**	**3.21741**	**-0.96908**
H	**2.25615**	**-0.41501**	**-0.04147**

L5

C	**-1.22819**	**0.94711**	**2.11411**
C	**-0.10511**	**0.3912**	**2.99918**
C	**0.44683**	**-0.9287**	**2.45063**
C	**0.9341**	**-0.73205**	**1.00313**
C	**-0.2552**	**-0.32944**	**0.11768**
C	**-0.76775**	**1.02913**	**0.65112**
N	**-1.71101**	**1.75633**	**-0.24106**
N	**1.8136**	**-1.83589**	**0.51418**
P	**-1.22704**	**3.23526**	**-1.06679**
C	**-0.34093**	**2.68163**	**-2.5936**
C	**-0.5339**	**1.41724**	**-3.16552**
C	**0.00806**	**1.11507**	**-4.41721**
C	**0.7469**	**2.06949**	**-5.11708**
C	**0.94671**	**3.33404**	**-4.55584**
C	**0.40181**	**3.63727**	**-3.31011**
C	**0.18845**	**3.8021**	**-0.00568**
C	**-0.13062**	**4.5706**	**1.12572**
C	**0.85464**	**4.93304**	**2.04535**
C	**2.18176**	**4.55084**	**1.83622**
C	**2.51919**	**3.81318**	**0.69904**
C	**1.53043**	**3.43961**	**-0.21194**
P	**-3.40635**	**1.46339**	**-0.52433**
C	**-3.60663**	**-0.37373**	**-0.68136**
C	**-3.87447**	**-0.85663**	**-1.97187**
C	**-4.09264**	**-2.21861**	**-2.19827**
C	**-4.02625**	**-3.1215**	**-1.13786**
C	**-3.7672**	**-2.65653**	**0.1545**
C	**-3.57489**	**-1.29563**	**0.37931**
C	**-4.26244**	**1.81001**	**1.08365**

C	**-5.41113**	**1.1093**	**1.48583**
C	**-6.13033**	**1.50335**	**2.61589**
C	**-5.72407**	**2.61157**	**3.35918**
C	**-4.5988**	**3.33357**	**2.9546**
C	**-3.88407**	**2.9419**	**1.82461**
P	**3.5498**	**-1.59437**	**0.596**
C	**3.78065**	**-0.84915**	**2.28482**
C	**3.60887**	**0.50609**	**2.6131**
C	**3.72308**	**0.93911**	**3.93375**
C	**4.01348**	**0.02635**	**4.95017**
C	**4.20233**	**-1.32105**	**4.63737**
C	**4.09316**	**-1.75156**	**3.31434**
C	**3.80361**	**-0.11573**	**-0.49153**
C	**2.96247**	**0.11781**	**-1.59009**
C	**3.22334**	**1.15586**	**-2.4857**
C	**4.33348**	**1.98068**	**-2.29953**
C	**5.19072**	**1.74962**	**-1.22019**
C	**4.93196**	**0.70767**	**-0.32903**
P	**1.45928**	**-3.33045**	**-0.30198**
C	**0.03986**	**-4.08627**	**0.60306**
C	**-0.97338**	**-4.81122**	**-0.04657**
C	**-1.90567**	**-5.55124**	**0.68374**
C	**-1.85055**	**-5.58101**	**2.07689**
C	**-0.83108**	**-4.88756**	**2.73526**
C	**0.11185**	**-4.16713**	**2.00593**
C	**0.76847**	**-2.919**	**-1.98068**
C	**1.70413**	**-3.04658**	**-3.02235**
C	**1.34495**	**-2.81752**	**-4.35127**
C	**0.03027**	**-2.47341**	**-4.66268**
C	**-0.91109**	**-2.33529**	**-3.63921**

C	**-0.54673**	**-2.55036**	**-2.31048**
H	**-2.1179**	**0.31827**	**2.20954**
H	**0.71049**	**1.12474**	**3.05433**
H	**-0.4701**	**0.25265**	**4.02315**
H	**-0.33984**	**-1.6899**	**2.46541**
H	**1.58898**	**0.14475**	**1.00607**
H	**0.05871**	**-0.20942**	**-0.91956**
H	**-1.03474**	**-1.09232**	**0.15038**
H	**0.12065**	**1.66023**	**0.67575**
H	**-1.11204**	**0.66619**	**-2.63707**
H	**-0.14014**	**0.12655**	**-4.83571**
H	**1.16646**	**1.83017**	**-6.08989**
H	**1.52447**	**4.08362**	**-5.0894**
H	**0.56032**	**4.62586**	**-2.88611**
H	**-1.15807**	**4.88512**	**1.28986**
H	**0.58741**	**5.51833**	**2.92053**
H	**2.94931**	**4.83497**	**2.55071**
H	**3.54658**	**3.51173**	**0.5165**
H	**1.8076**	**2.84149**	**-1.07117**
H	**-3.92413**	**-0.15587**	**-2.80103**
H	**-4.31116**	**-2.57229**	**-3.20173**
H	**-4.17467**	**-4.18283**	**-1.3128**
H	**-3.69913**	**-3.35621**	**0.98085**
H	**-3.40648**	**-0.9464**	**1.39082**
H	**-5.74692**	**0.24506**	**0.9217**
H	**-7.00855**	**0.93841**	**2.91608**
H	**-6.28171**	**2.91483**	**4.24041**
H	**-4.27778**	**4.20441**	**3.51953**
H	**-3.01373**	**3.51156**	**1.517**
H	**3.37519**	**1.23057**	**1.83976**

H	**3.57436**	**1.98974**	**4.16754**
H	**4.09755**	**0.3643**	**5.97905**
H	**4.43858**	**-2.03481**	**5.42139**
H	**4.24408**	**-2.80143**	**3.07523**
H	**2.09627**	**-0.51234**	**-1.75167**
H	**2.5488**	**1.32487**	**-3.3173**
H	**4.52873**	**2.79559**	**-2.99043**
H	**6.06241**	**2.38102**	**-1.07062**
H	**5.60473**	**0.54497**	**0.50857**
H	**-1.04049**	**-4.80518**	**-1.1284**
H	**-2.68207**	**-6.09994**	**0.15727**
H	**-2.58103**	**-6.1508**	**2.64372**
H	**-0.76253**	**-4.91847**	**3.81905**
H	**0.91691**	**-3.66095**	**2.52801**
H	**2.72409**	**-3.3366**	**-2.78418**
H	**2.08573**	**-2.92211**	**-5.13853**
H	**-0.26251**	**-2.31232**	**-5.69668**
H	**-1.93297**	**-2.05606**	**-3.8715**
H	**-1.29814**	**-2.44605**	**-1.53776**
H	**1.26614**	**-1.28747**	**3.07765**
C	**-1.63379**	**2.35262**	**2.59539**
H	**-1.94176**	**2.94167**	**1.7569**
H	**-2.44288**	**2.27176**	**3.29091**
H	**-0.79854**	**2.82098**	**3.07278**

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