

## Supporting Information For

### Electronic structural studies of newly synthesized sterically hindered analogue of *meta*-benziporphodimethene and its metal complexes

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Figure	Topic
S1.	<sup>1</sup> H-NMR of diol precursor (1)
S2.	<sup>1</sup> H-NMR of free base BPDM (2)
S3.	<sup>1</sup> H-NMR of Zn- <i>m</i> -BPDM (3)
S4.	<sup>1</sup> H-NMR of Cd- <i>m</i> -BPDM (4)
S5.	HRMS of free base BPDM (2) in APCI positive mode
S6a.	HRMS of Zn-BPDM (3) in APCI positive mode.
S6b.	MS of ZnCl-BPDM (3) in APCI positive mode.
S7a.	HRMS of Cd-BPDM (4) in APCI positive mode.
S7b.	MS of CdCl-BPDM (4) in APCI positive mode.
S8.	Fluorescence behavior of chlorozinc(II) 11,16-Bis(phenyl)-6,6,21,21-tetraphenyl- <i>meta</i> -benzi-6,21-porphoodimethene (3) in toluene solution upon excitation at 697 nm.
<b>Chart</b>	
S9	B3LYP/LANL2DZ optimized geometries for (a) Zinc syn conformer ; (b) Zinc anti conformer; (c) Cd syn conformer; (d) Cd anti conformer; when R"= H. at <i>sp</i> <sup>3</sup> meso carbons.
S10	B3LYP/LANL2DZ optimized geometries for (a) Zinc <i>syn</i> conformer; (b) Zinc <i>anti</i> conformer; (c) Cd <i>syn</i> conformer (d) Cd <i>anti</i> conformer; when R"= CH <sub>3</sub> , at <i>sp</i> <sup>3</sup> meso carbons.
S11	B3LYP/LANL2DZ optimized geometries for (a) Zinc syn conformer ; (b) Zinc anti conformer; (c) Cd syn conformer; (d) Cd anti conformer; when R"= Ph at <i>sp</i> <sup>3</sup> meso carbons.
S12	B3LYP/LANL2DZ optimized geometries for free base <i>m</i> -BPDM when (a) R"= H; (b) R"= methyl; (c) R" = Phenyl at <i>sp</i> <sup>3</sup> meso carbons.
S13	X-Ray geometries for (a') Zinc syn conformer; (c') Cd syn conformer ; when R"= CH <sub>3</sub> , at <i>sp</i> <sup>3</sup> meso carbons.
<b>Table</b>	

S14	Xyz-Coordinates of optimized geometry of compound 2 viz., free base m-BPDM, R"=Ph
S15	Xyz-Coordinates of optimized geometry of compound 3
S16	Xyz-Coordinates of optimized geometry of compound 4
S17	Xyz-Coordinates of optimized geometry of free base m-BPDM R"=H
S18	Xyz-Coordinates of optimized geometry of free base m-BPDM R"=CH <sub>3</sub>
S19	Xyz-Coordinates of optimized geometry of syn conformer of Zn(II) m-BPDM, R"=H
S20	Xyz-Coordinates of optimized geometry of anti-conformer of Zn(II) m-BPDM, R"=H
S21	Xyz-Coordinates of optimized geometry of syn conformer of Cd(II) m-BPDM, R"=H
S22	Xyz-Coordinates of optimized geometry of anti-conformer of Cd(II) m-BPDM, R"=H
S23	Xyz-Coordinates of optimized geometry of syn conformer of Zn(II) m-BPDM, R"=CH <sub>3</sub>
S24	Xyz-Coordinates of optimized geometry of anti-conformer of Zn(II) m-BPDM, R"=CH <sub>3</sub>
S25	Xyz-Coordinates of optimized geometry of syn conformer of Cd(II) m-BPDM, R"=CH <sub>3</sub>
S26	Xyz-Coordinates of optimized geometry of anti-conformer of Cd(II) m-BPDM, R"=CH <sub>3</sub>
S27	Xyz-Coordinates of optimized geometry of syn conformer of Zn(II) m-BPDM, R"=Ph
S28	Xyz-Coordinates of optimized geometry of anti-conformer of Zn(II) m-BPDM, R"=Ph
S29	Xyz-Coordinates of optimized geometry of syn conformer of Cd(II) m-BPDM, R"=Ph
S30	Xyz-Coordinates of optimized geometry of anti-conformer of Cd(II) m-BPDM, R"=Ph

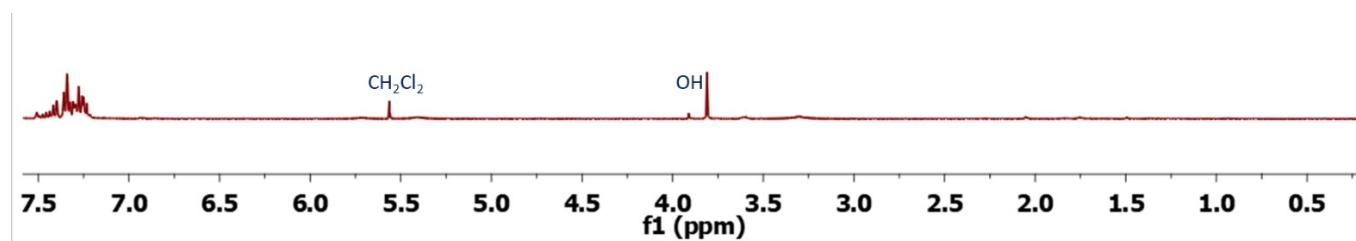


Figure S1. <sup>1</sup>H-NMR of 1,3-Bis(diphenylhydroxymethyl)benzene (1) precursor in CD<sub>3</sub>COCD<sub>3</sub>.

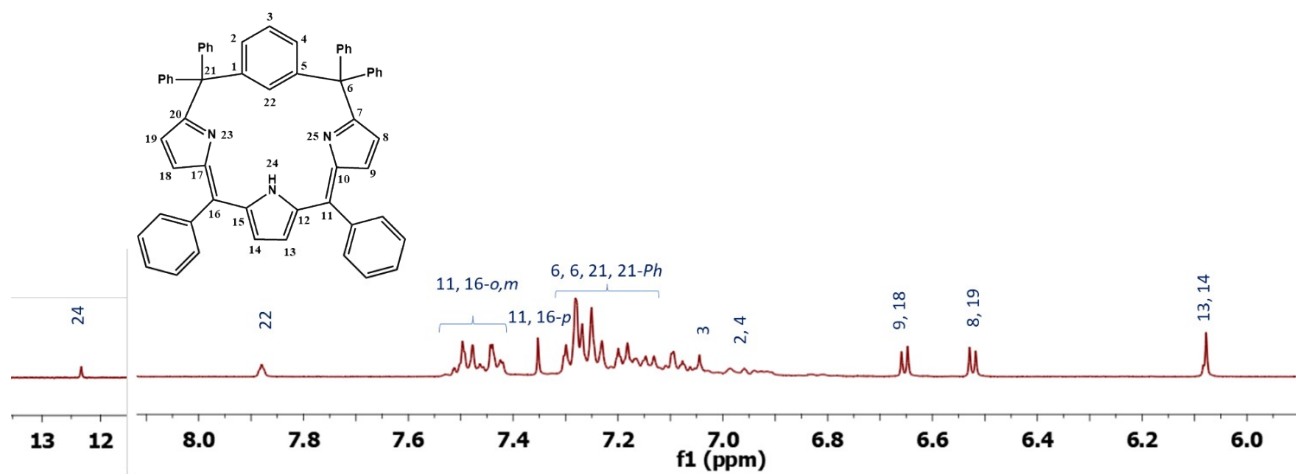
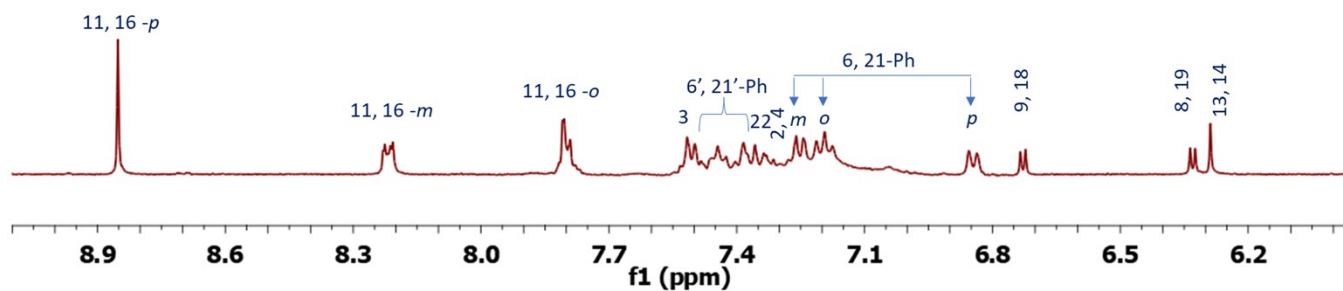
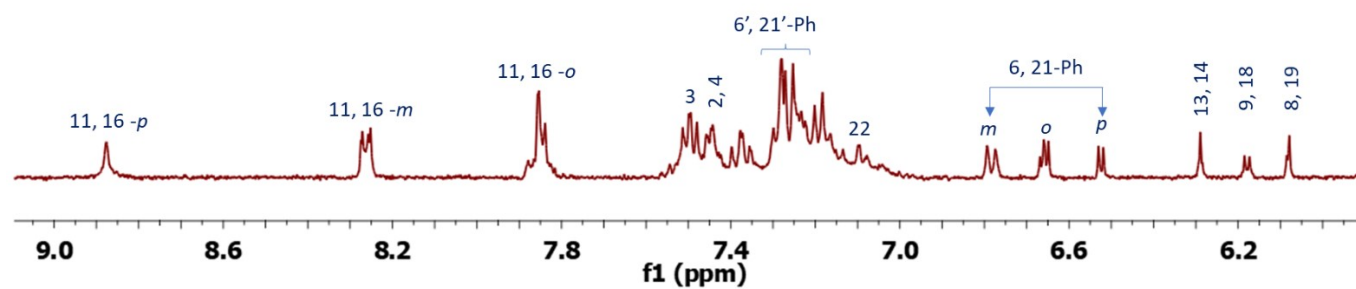


Figure S2. <sup>1</sup>H-NMR of 11,16-Bis(phenyl)-6,6,21,21-tetraphenyl-*meta*-benzi-6,21-porphoodimethene (2) in CD<sub>3</sub>COCD<sub>3</sub>.



**Figure S3.**  $^1\text{H}$ -NMR of chlorozinc(II) 11,16-Bis(phenyl)-6,6,21,21-tetraphenyl-*meta*-benzi-6,21-porphoodimethene (**3**) in  $\text{CD}_3\text{COCD}_3$ .



**Figure S4.**  $^1\text{H}$ -NMR of chlorocadmium(II) 11,16-Bis(phenyl)-6,6,21,21-tetraphenyl-*meta*-benzi-6,21-porphoodimethene (**4**) in  $\text{CD}_3\text{COCD}_3$ .

## Compound Spectrum SmartFormula Report

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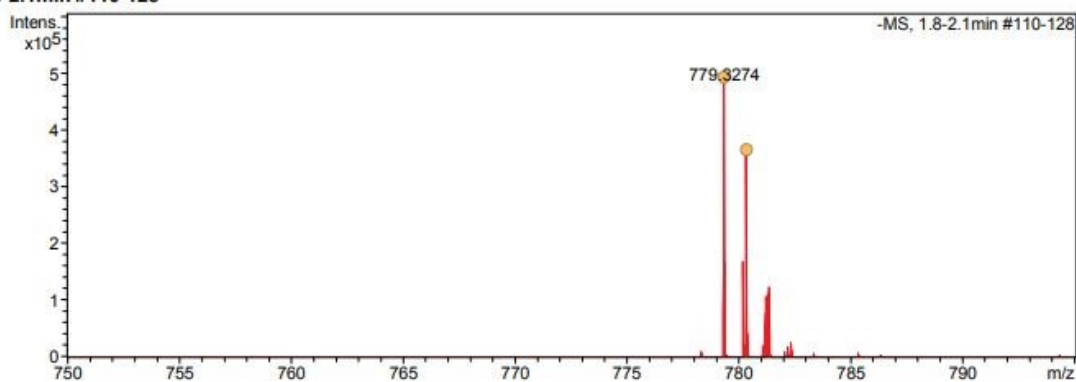
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Operator Larisa Panz  
 Instrument maXis impact 282001.00128

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Scan End	2000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	2000 nA	Set APCI Heater	200 °C

### -MS, 1.8-2.1min #110-128



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	err  [mDa]
779.3274	1	C58H42N3	780.3379	2580.6	818.5	1	-1.#J	39.5	even	ok	2013.8
	1	C58H41N3	779.3306	4.1	54.1	1	100.00	40.0	odd	ok	3.2
	1	C58H42N3	780.3379	1.5	818.5	1	100.00	39.5	even	ok	1.5
780.3320	1	C58H42N3	780.3384	8.2	160.9	1	100.00	39.5	even	ok	6.4
	1	C58H42N3	780.3384	8.2	160.9	1	100.00	39.5	even	ok	6.4

**Figure S5.** HRMS of **11,16-Bis(phenyl)-6,6,21,21-tetraphenyl-*meta*-benzi-6,21-porphoodimethene (2)** in APCI positive mode.

**Analysis Info**

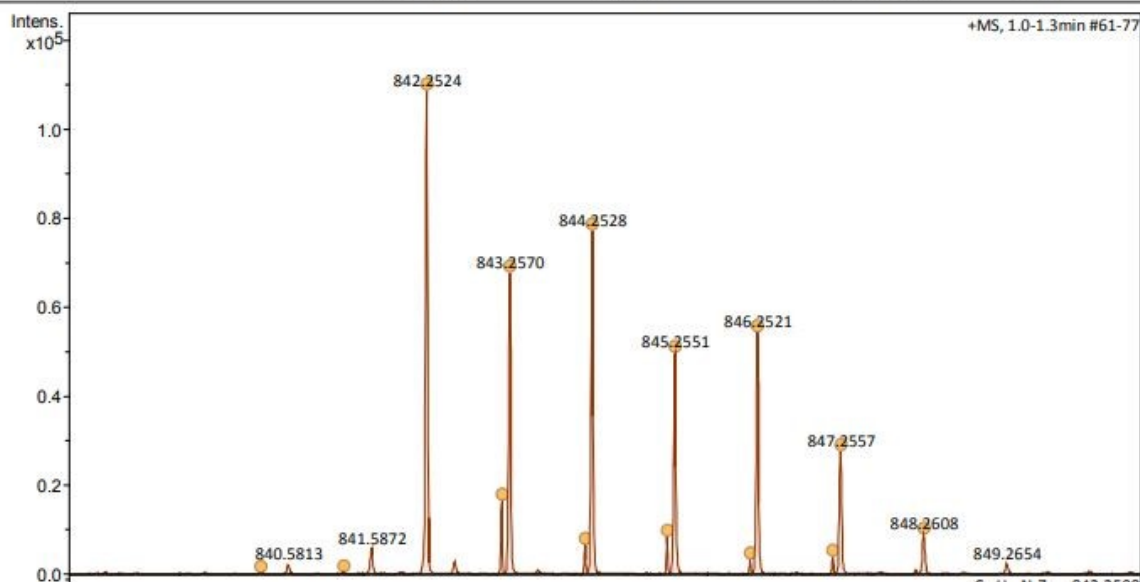
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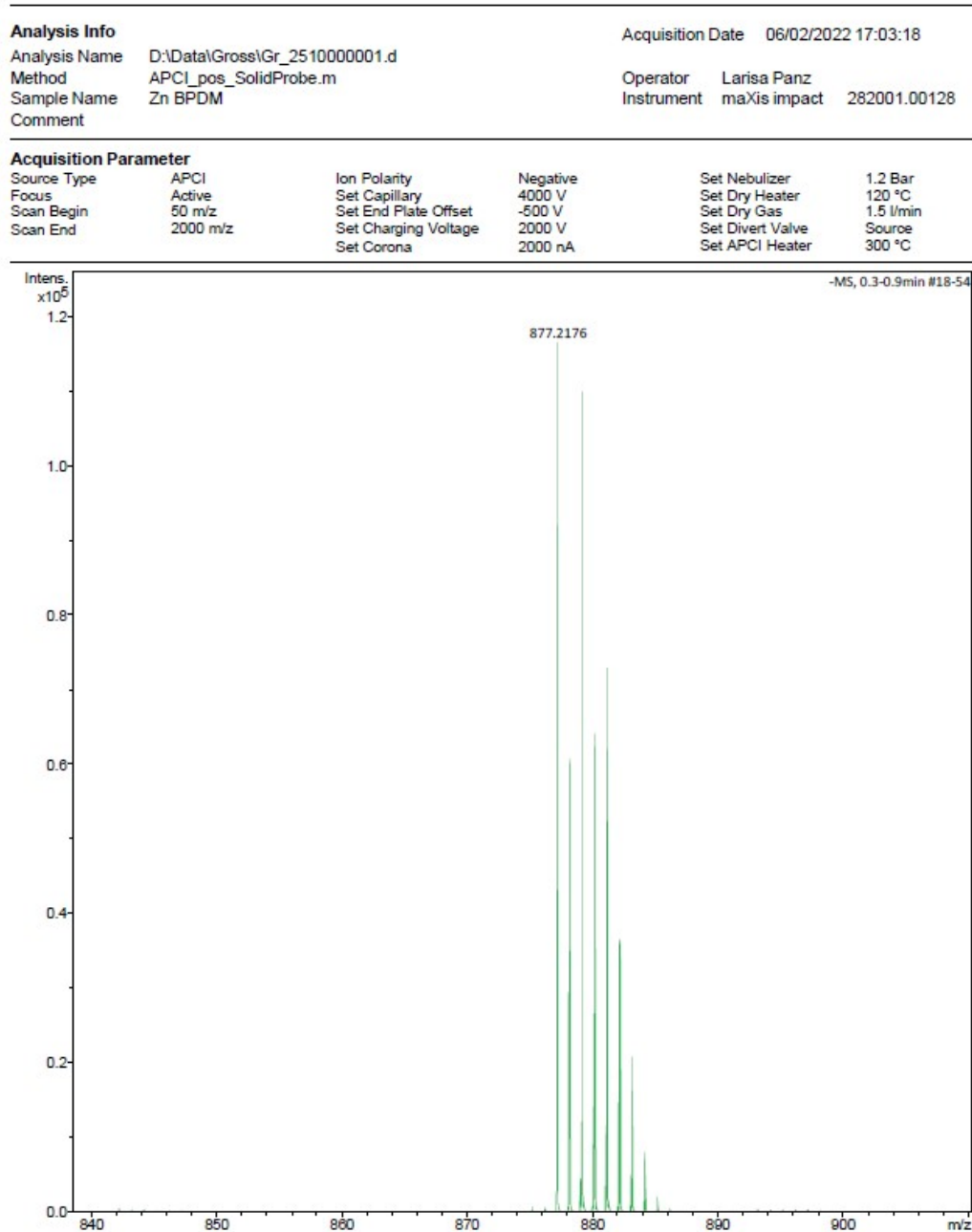
Operator Larisa Panz  
Instrument maXis impact 282001.00128

**Acquisition Parameter**

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Scan End	2000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	5000 nA	Set APCI Heater	200 °C



**Figure S6a.** HRMS of Zn(II) 11,16-Bis(phenyl)-6,6,21,21-tetraphenyl-*meta*-benzi-6,21-porphoodimethene (**3**) in APCI positive mode.



**Figure S6b.** MS of chlorozinc(II) 11,16-Bis(phenyl)-6,6,21,21-tetraphenyl-*meta*-benzi-6,21-porphoodimethene (3) in APCI positive mode.

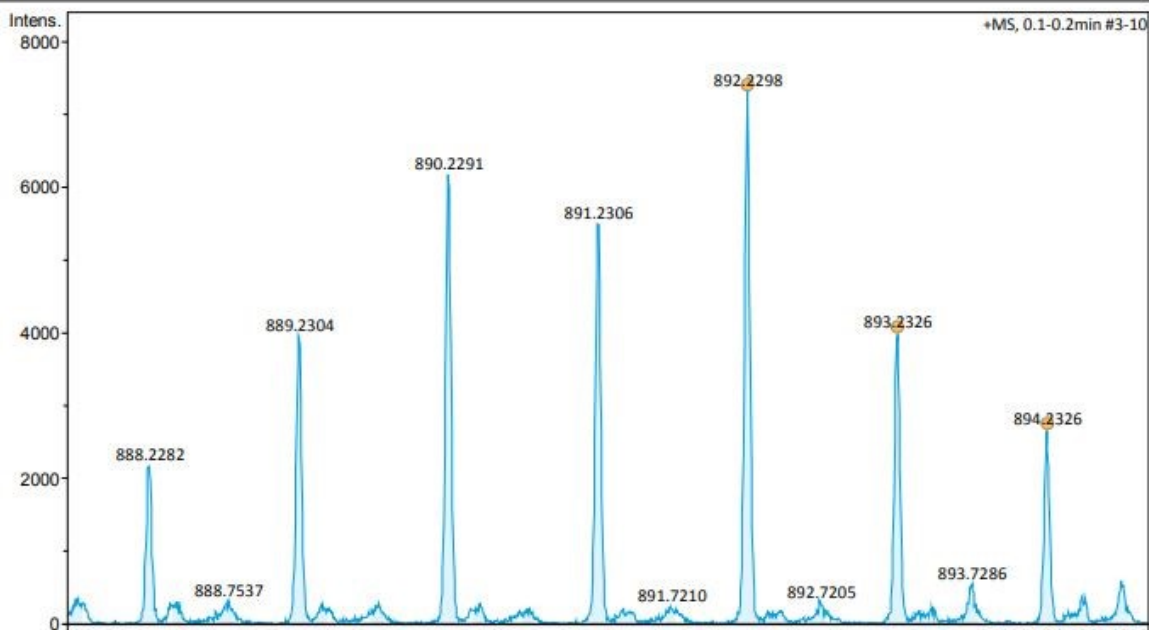
## Generic Display Report

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Method APCI\_pos\_SolidProbe.m  
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Comment

Acquisition Date 08/02/2022 10:53:50

Operator Larisa Panz  
Instrument maXis impact



**Figure S7a.** HRMS of cadmium(II) 11,16-Bis(phenyl)-6,6,21,21-tetraphenyl-*meta*-benzi-6,21-porphoodimethene (4) in APCI positive mode.

## Display Report

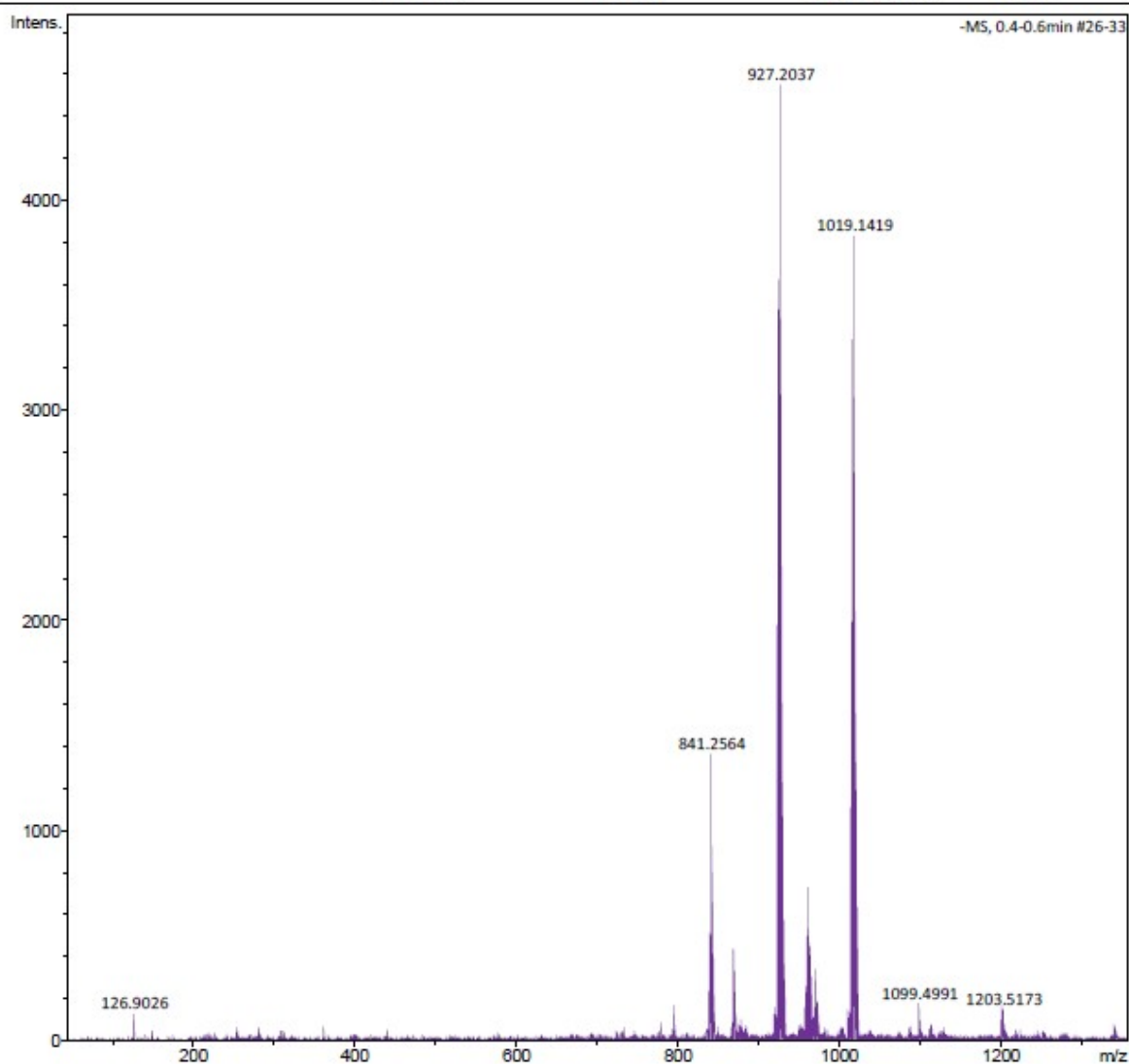
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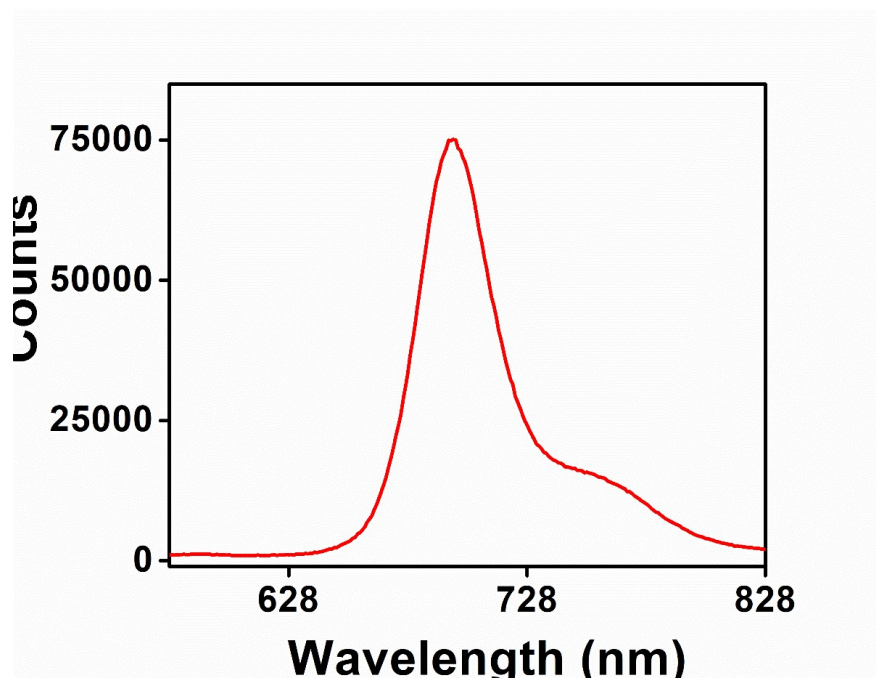
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Operator Larisa Panz  
Instrument maXis impact 282001.00128

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		Set Corona	2000 nA	Set APCI Heater	330 °C

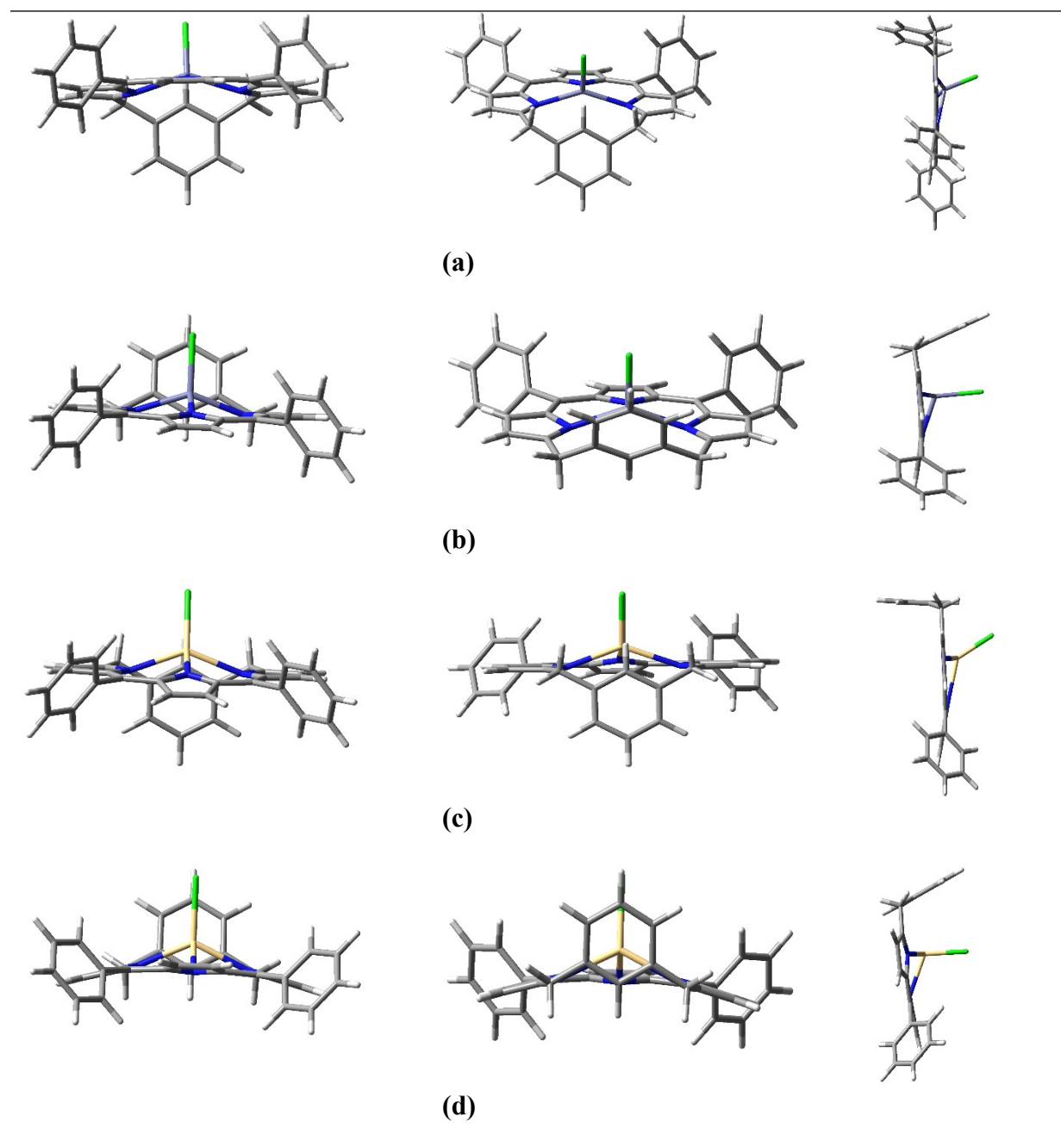


**Figure S7b.** MS of chlorocadmium(II) 11,16-Bis(phenyl)-6,6,21,21-tetraphenyl-meta-benzi-6,21-porphoodimethene (4) in APCI positive mode.

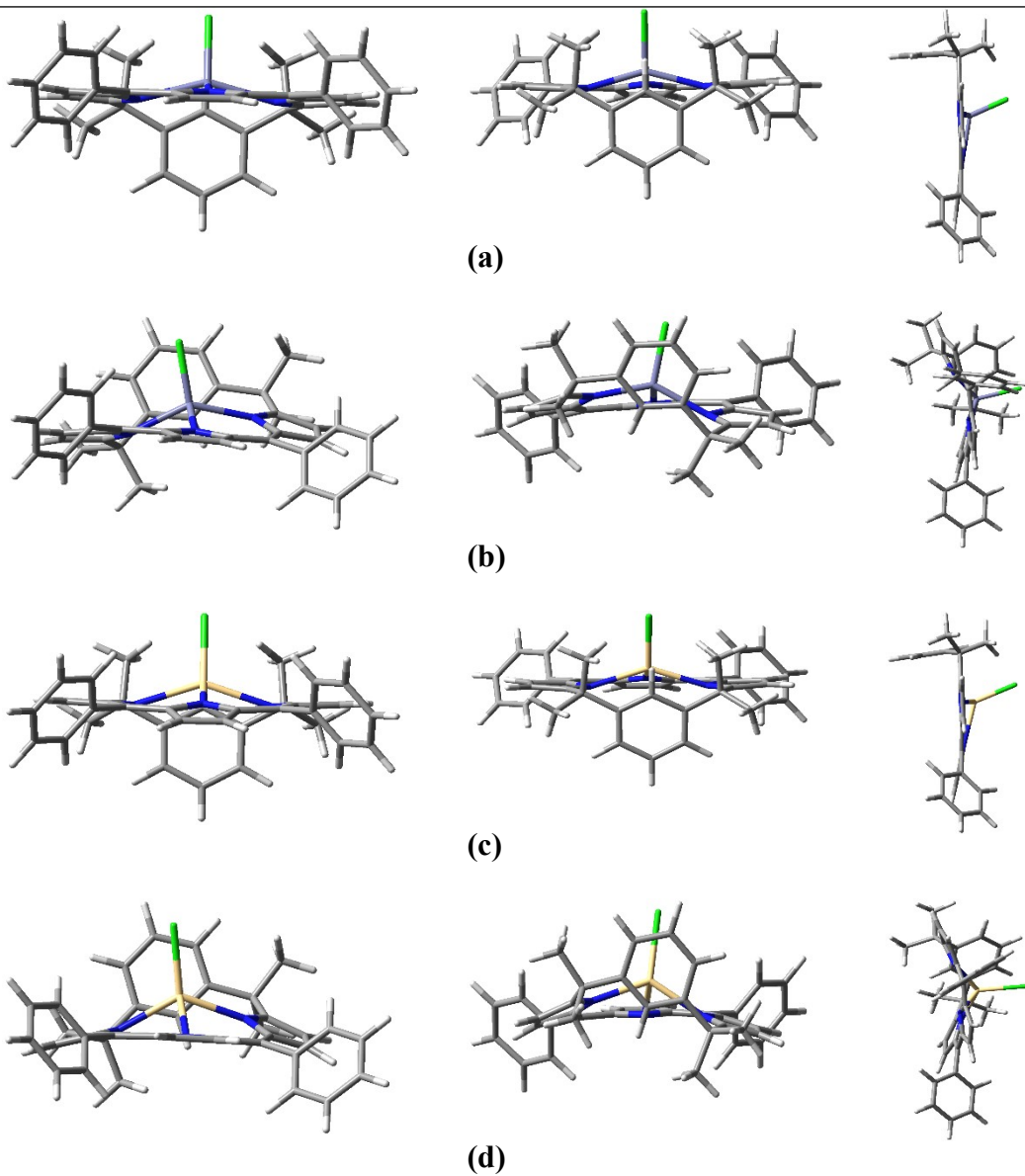


**Figure S8.** Fluorescence behavior of chlorozinc(II) 11,16-Bis(phenyl)-6,6,21,21-tetraphenyl-*meta*-benzi-6,21-porphoodimethene (3) in toluene solution upon excitation at 363 nm.

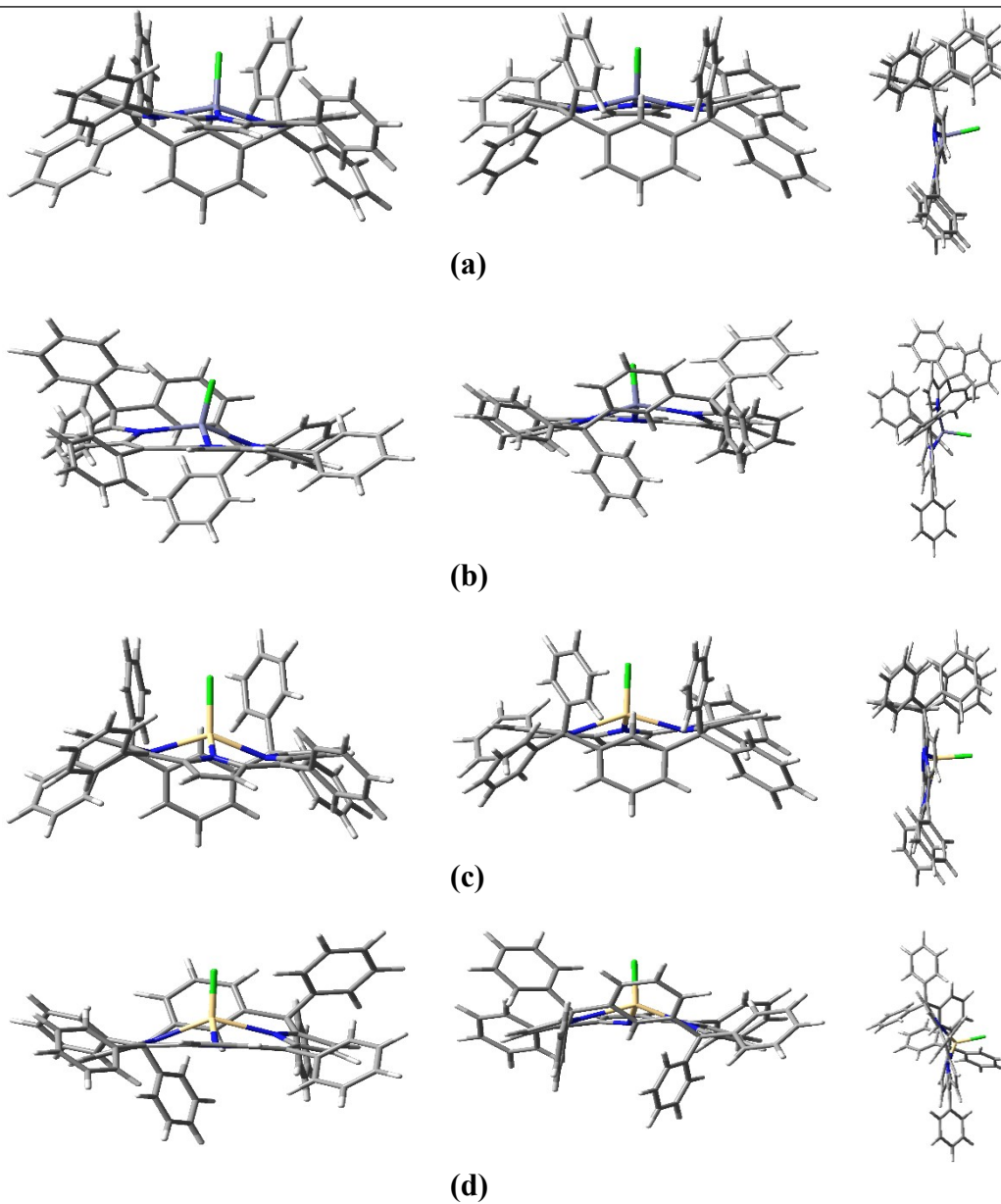
**Chart S9.** B3LYP/LANL2DZ optimized geometries for (a) Zinc syn conformer ; (b) Zinc anti conformer; (c) Cd syn conformer; (d) Cd anti conformer; when R''= H. at  $sp^3$  meso carbons.



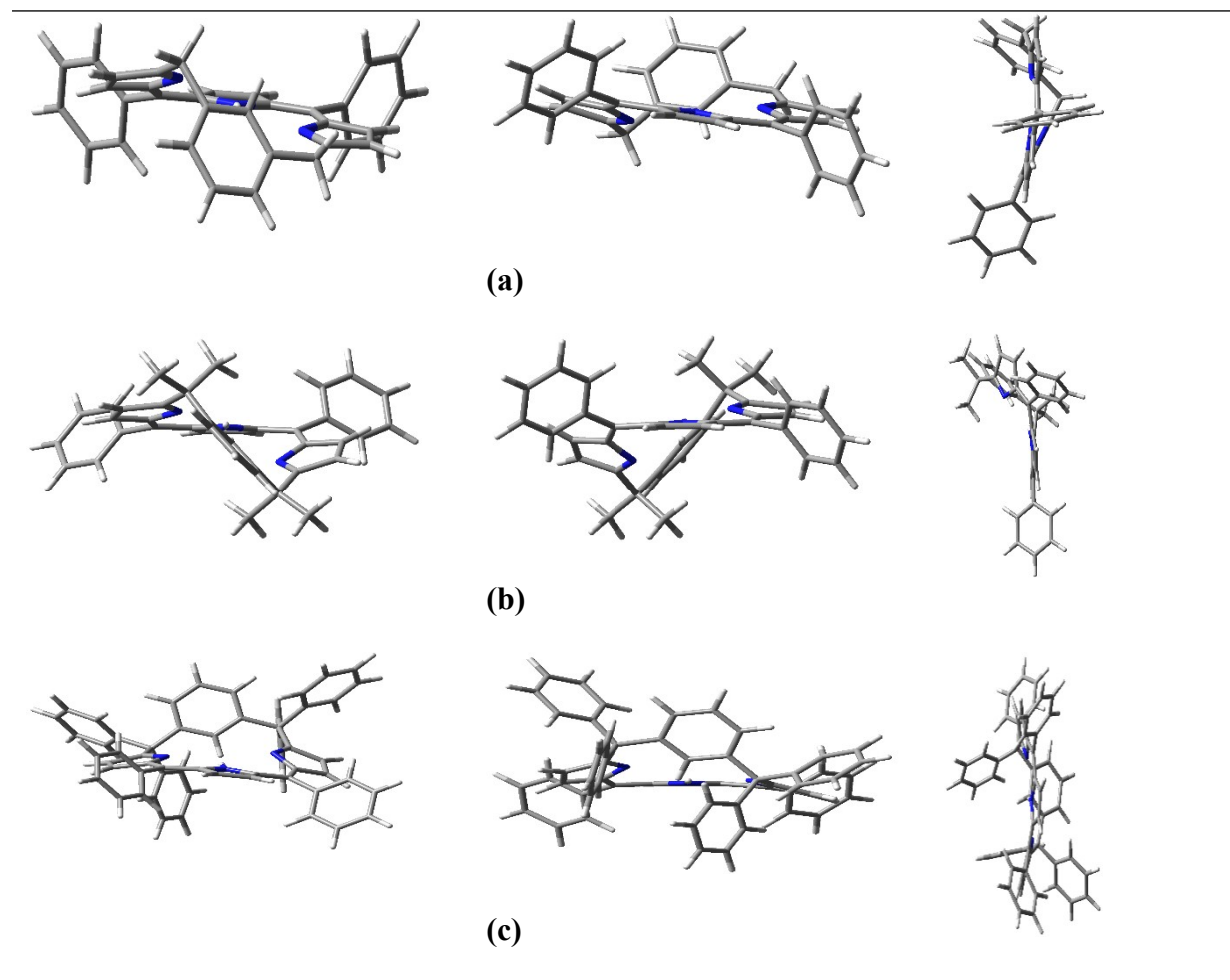
**Chart S10.** B3LYP/LANL2DZ optimized geometries for (a) Zinc *syn* conformer; (b) Zinc *anti* conformer; (c) Cd *syn* conformer (d) Cd *anti* conformer; when R''= CH<sub>3</sub>, at *sp*<sup>3</sup> meso carbons.



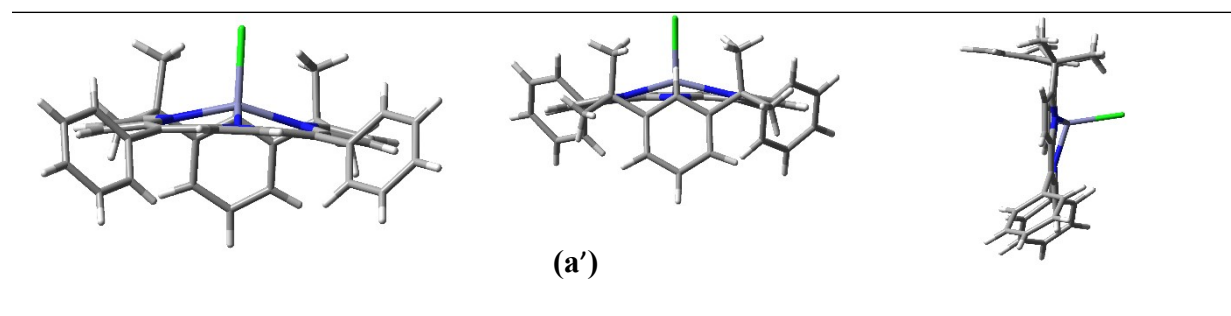
**Chart S11.** B3LYP/LANL2DZ optimized geometries for (a) Zinc syn conformer ; (b) Zinc anti conformer; (c) Cd syn conformer; (d) Cd anti conformer; when R''= Ph at  $sp^3$  meso carbons.

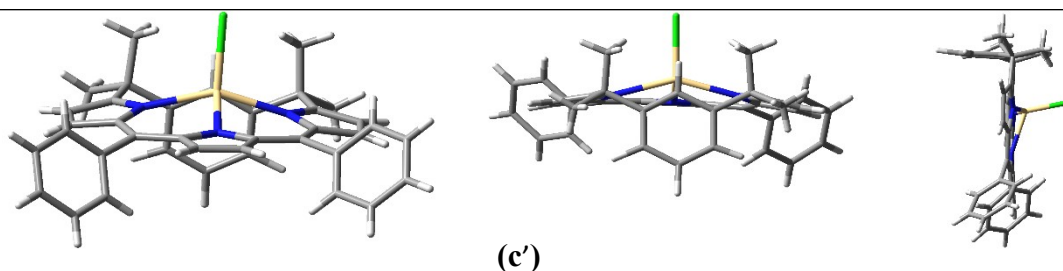


**Chart S12.** B3LYP/LANL2DZ optimized geometries for free base *m*-BPDM when (a) R''= H; (b) R''= methyl; (c) R'' = Phenyl at  $sp^3$  meso carbons.



**Chart S13.** X-Ray geometries for (a') Zinc *syn* conformer; (c') Cd *syn* conformer ; when R''= CH<sub>3</sub>, at  $sp^3$  meso carbons.





**Table S14.** Xyz-Coordinates of optimized geometry of compound 2 viz., free base m-BPDM, R''=Ph

N	2.088903000	-1.030720000	-0.130280000	C	8.141832000	0.435510000	2.123920000
N	2.047281000	1.626698000	0.102154000	H	0.349126000	8.478876000	-2.513584000
N	-1.001179000	1.467733000	0.322658000	H	9.152881000	0.458184000	2.473048000
C	-0.997398000	-3.552769000	1.342154000	C	-4.427926000	-0.087815000	-0.003473000
H	-0.459479000	-4.472646000	1.447267000	C	-5.636764000	-0.520293000	0.556245000
C	-2.043791000	-3.243855000	2.219181000	C	-4.328553000	0.114514000	-1.387263000
H	-2.308936000	-3.927406000	2.998193000	C	-6.747416000	-0.749588000	-0.266774000
C	-2.743672000	-2.036876000	2.075677000	H	-5.711845000	-0.675189000	1.612307000
H	-3.537008000	-1.797607000	2.752670000	C	-5.439436000	-0.114792000	-2.210352000
C	-2.409477000	-1.142650000	1.045918000	H	-3.404789000	0.444312000	-1.815512000
C	-1.369414000	-1.452104000	0.172883000	C	-6.649216000	-0.546336000	-1.650015000
H	-1.112127000	-0.775314000	-0.615178000	H	-7.670765000	-1.079696000	0.160916000
C	-0.657967000	-2.649307000	0.329251000	H	-5.363988000	0.039891000	-3.266379000
C	-3.208220000	0.166688000	0.900490000	H	-7.498146000	-0.720361000	-2.278332000
C	-2.358507000	1.299991000	0.266950000	C	-3.676213000	0.612584000	2.298270000
C	-3.008487000	2.444389000	-0.535593000	C	-4.880396000	1.315433000	2.440502000
H	-4.050577000	2.536828000	-0.760344000	C	-2.900476000	0.316253000	3.427468000
C	-2.053585000	3.304154000	-0.898005000	C	-5.308975000	1.721806000	3.711436000
H	-2.191520000	4.207245000	-1.454954000	H	-5.472503000	1.541551000	1.578265000
C	-0.728980000	2.761382000	-0.368213000	C	-3.329162000	0.723236000	4.698272000
C	0.498067000	3.443155000	-0.534995000	H	-1.980878000	-0.220760000	3.319774000
C	1.754690000	2.903334000	-0.208272000	C	-4.533623000	1.425420000	4.840355000
C	2.940200000	3.649202000	-0.158150000	H	-6.228171000	2.258262000	3.819835000
H	3.042583000	4.693527000	-0.366651000	H	-2.736843000	0.497762000	5.560188000
C	3.956263000	2.780851000	0.217026000	H	-4.861342000	1.735166000	5.810694000
H	4.986446000	3.028951000	0.367181000	C	0.207481000	-2.263043000	-1.983099000
C	3.373445000	1.521235000	0.355409000	C	-1.116053000	-2.114723000	-2.419134000
C	4.040667000	0.340150000	0.700804000	C	1.263674000	-1.801669000	-2.780530000
C	3.355658000	-0.865801000	0.567985000	C	-1.383685000	-1.501982000	-3.650598000
C	3.747521000	-2.235610000	1.086435000	H	-1.922188000	-2.469294000	-1.811446000
H	4.629287000	-2.489733000	1.637022000	C	0.995934000	-1.189437000	-4.012392000
C	2.751379000	-3.067966000	0.713722000	H	2.274585000	-1.916766000	-2.449316000
H	2.704496000	-4.114264000	0.933765000	C	-0.327892000	-1.037920000	-4.446446000
C	1.776809000	-2.338679000	-0.020549000	H	-2.394223000	-1.388553000	-3.982866000
C	0.500949000	-2.932938000	-0.627294000	H	1.802222000	-0.837559000	-4.621592000
C	0.456228000	4.873312000	-1.103894000	H	-0.532514000	-0.567795000	-5.385524000
C	1.647437000	5.587352000	-1.291351000	C	0.674896000	-4.449132000	-0.835150000
H	2.586271000	5.136459000	-1.043908000	C	1.943195000	-4.980599000	-1.106895000
C	-0.772534000	5.460756000	-1.433319000	C	-0.436616000	-5.297533000	-0.750163000
H	-1.681455000	4.913254000	-1.294373000	C	2.099417000	-6.361094000	-1.291327000
C	1.608664000	6.891975000	-1.802589000	H	2.792121000	-4.332913000	-1.173288000
H	2.517663000	7.437956000	-1.945495000	C	-0.280806000	-6.677634000	-0.933989000
C	-0.811248000	6.765182000	-1.943707000	H	-1.404428000	-4.891094000	-0.544252000
H	-1.749619000	7.214371000	-2.193785000	C	0.987327000	-7.209695000	-1.203442000
C	0.379013000	7.481566000	-2.126500000	H	3.067214000	-6.767383000	-1.499037000

C	5.493735000	0.373916000	1.208179000	H	-1.130203000	-7.325085000	-0.868386000
C	6.167086000	1.597580000	1.321840000	H	1.106774000	-8.263816000	-1.341866000
H	5.670210000	2.508090000	1.058969000	H	1.389214000	0.874127000	0.139443000
C	6.143390000	-0.818368000	1.554322000				
H	5.629052000	-1.752193000	1.468955000				
C	7.491959000	1.628592000	1.778486000				
H	8.007152000	2.562917000	1.863219000				
C	7.467440000	-0.787680000	2.011568000				
H	7.964015000	-1.698071000	2.274973000				

**Table S15.** Xyz-Coordinates of optimized geometry of ZnCl-m-BPDM (compound 3)

Zn	0.615804000	-0.150276000	-0.256954000	H	3.128582000	-7.775053000	3.387670000
Cl	1.013569000	-0.289136000	-3.399207000	H	8.803046000	2.476423000	-1.823499000
N	1.365430000	1.745882000	-0.103366000	C	-4.118622000	-1.075295000	0.108598000
N	2.384903000	-0.988834000	0.112051000	C	-5.237725000	-0.474360000	-0.516820000
N	-0.458280000	-1.841648000	0.164462000	C	-4.158340000	-1.256070000	1.505490000
C	-1.575856000	2.588438000	-1.995226000	C	-6.364291000	-0.087364000	0.224370000
H	-1.225294000	3.569691000	-2.299714000	H	-5.224308000	-0.299153000	-1.589527000
C	-2.121612000	1.717008000	-2.946614000	C	-5.286317000	-0.864708000	2.254549000
H	-2.220253000	2.041459000	-3.979441000	H	-3.312264000	-1.699004000	2.020239000
C	-2.516529000	0.412815000	-2.589769000	C	-6.396881000	-0.283441000	1.620247000
H	-2.920024000	-0.247973000	-3.348005000	H	-7.211458000	0.369172000	-0.282441000
C	-2.368752000	-0.030575000	-1.264142000	H	-5.290057000	-1.015722000	3.331687000
C	-1.859481000	0.877846000	-0.305292000	H	-7.267879000	0.016604000	2.198123000
H	-1.853089000	0.579384000	0.737768000	C	-3.197930000	-2.391301000	-1.928492000
C	-1.462734000	2.183437000	-0.645817000	C	-4.408707000	-3.110010000	-1.997895000
C	-2.863059000	-1.408335000	-0.759215000	C	-2.202391000	-2.666730000	-2.896299000
C	-1.791081000	-2.167609000	0.046273000	C	-4.630886000	-4.057939000	-3.016548000
C	-2.038960000	-3.451967000	0.617935000	H	-5.185124000	-2.943877000	-1.258821000
H	-2.992890000	-3.958870000	0.623167000	C	-2.422382000	-3.606481000	-3.914531000
C	-0.821894000	-3.941186000	1.078171000	H	-1.245452000	-2.155765000	-2.850955000
H	-0.639065000	-4.902034000	1.535264000	C	-3.642693000	-4.308628000	-3.983497000
C	0.184028000	-2.952065000	0.795563000	H	-5.573813000	-4.599446000	-3.046781000
C	1.579026000	-3.146991000	1.013302000	H	-1.640898000	-3.794155000	-4.646825000
C	2.615440000	-2.239648000	0.657476000	H	-3.813502000	-5.040461000	-4.769516000
C	4.047600000	-2.417608000	0.804241000	C	-0.946884000	2.602724000	1.850843000
H	4.533131000	-3.280119000	1.236681000	C	-2.264498000	2.560742000	2.366307000
C	4.656518000	-1.273448000	0.310913000	C	0.117794000	2.283163000	2.718079000
H	5.714222000	-1.054934000	0.283585000	C	-2.511179000	2.199949000	3.699261000
C	3.600046000	-0.367355000	-0.102114000	H	-3.102801000	2.819278000	1.724092000
C	3.751784000	0.993791000	-0.511881000	C	-0.126234000	1.928479000	4.060680000
C	2.712664000	1.975170000	-0.473703000	H	1.138986000	2.302889000	2.354066000
C	2.868016000	3.377919000	-0.728445000	C	-1.439361000	1.882577000	4.558313000
H	3.770826000	3.858504000	-1.073840000	H	-3.534052000	2.171838000	4.067414000
C	1.643179000	4.000064000	-0.446341000	H	0.712264000	1.688596000	4.710614000
H	1.418121000	5.051215000	-0.530545000	H	-1.626573000	1.608613000	5.593932000
C	0.743044000	2.978155000	-0.045221000	C	-1.232649000	4.563038000	0.379361000
C	-0.730793000	3.088407000	0.380521000	C	-0.527903000	5.526006000	1.140752000
C	2.000163000	-4.432377000	1.665686000	C	-2.444323000	4.961457000	-0.222964000
C	2.755641000	-5.391890000	0.953138000	C	-0.991731000	6.845051000	1.258547000
H	3.012070000	-5.202834000	-0.086160000	H	0.376828000	5.235931000	1.667088000
C	1.658897000	-4.702345000	0.011369000	C	-2.916412000	6.283492000	-0.104789000
H	1.086689000	-3.967667000	3.572365000	H	-3.038297000	4.246030000	-0.781429000
C	3.155826000	-6.592441000	1.568361000	C	-2.189895000	7.236269000	0.628797000
H	3.727423000	-7.323438000	1.001275000	H	-0.426674000	7.562204000	1.849536000
C	2.067605000	-5.897383000	3.630772000	H	-3.853796000	6.561049000	-0.581652000
H	1.804068000	-6.083400000	4.669370000	H	-2.553663000	8.256888000	0.720498000
C	2.816053000	-6.849071000	2.910788000				
C	5.138292000	1.428137000	-0.872543000				

C	5.821170000	0.792235000	-1.937352000
H	5.313335000	0.016185000	-2.503645000
C	5.812325000	2.442821000	-0.150681000
H	5.314512000	2.919268000	0.689430000
C	7.129936000	1.172508000	-2.283409000
H	7.630919000	0.681683000	-3.114410000
C	7.125857000	2.814404000	-0.487961000
H	7.630475000	3.587822000	0.086488000
C	7.789172000	2.185019000	-1.559483000

**Table S16.** Xyz-Coordinates of optimized geometry of CdCl-m-BPDM (compound 4)

Cl	-0.470190000	-1.860379000	-1.284123000	C	-4.406199000	-0.170953000	0.143284000
N	2.084622000	-0.990208000	-0.189130000	C	-5.581622000	-0.570590000	0.781086000
N	1.970733000	1.722280000	-0.039364000	C	-4.313348000	-0.192423000	-1.252986000
N	-1.062208000	1.548587000	0.222426000	C	-6.668019000	-1.018811000	0.019793000
C	-0.827362000	-3.246149000	1.849427000	H	-5.651121000	-0.533452000	1.847556000
H	-0.265720000	-4.132288000	2.047952000	C	-5.397334000	-0.644324000	-2.018202000
C	-1.806742000	-2.812126000	2.762628000	H	-3.414920000	0.136240000	-1.736359000
H	-1.978761000	-3.364770000	3.660763000	C	-6.572954000	-1.059883000	-1.380223000
C	-2.566017000	-1.658832000	2.496406000	H	-7.564195000	-1.330599000	0.507239000
H	-3.310283000	-1.332680000	3.193712000	H	-5.322912000	-0.673966000	-3.085883000
C	-2.345055000	-0.936745000	1.317561000	H	-7.400575000	-1.411936000	-1.960937000
C	-1.351406000	-1.336139000	0.441605000	C	-3.702949000	0.944878000	2.285509000
H	-1.165358000	-0.745281000	-0.434471000	C	-4.939798000	1.608269000	2.309584000
C	-0.589630000	-2.508101000	0.681815000	C	-2.921454000	0.881077000	3.448929000
C	-3.208392000	0.291850000	0.979284000	C	-5.399989000	2.190883000	3.496607000
C	-2.407378000	1.348906000	0.181441000	H	-5.533658000	1.671237000	1.416061000
C	-3.077114000	2.372522000	-0.755867000	C	-3.387565000	1.464137000	4.634336000
H	-4.106673000	2.387510000	-1.026343000	H	-1.970524000	0.388926000	3.430439000
C	-2.150871000	3.248265000	-1.154338000	C	-4.626653000	2.120166000	4.662403000
H	-2.302020000	4.096213000	-1.785075000	H	-6.343694000	2.692548000	3.510664000
C	-0.833494000	2.813297000	-0.523826000	H	-2.795359000	1.410391000	5.523395000
C	0.369516000	3.544049000	-0.614793000	H	-4.982574000	2.567256000	5.572867000
C	1.626419000	3.027416000	-0.200452000	C	0.042079000	-2.387373000	-1.748289000
C	2.752612000	3.810781000	0.097216000	C	-1.319731000	-2.293495000	-2.046116000
H	2.819407000	4.872806000	0.047336000	C	0.999389000	-1.996136000	-2.691864000
C	3.769535000	2.953654000	0.471449000	C	-1.732891000	-1.814092000	-3.292256000
H	4.752331000	3.239641000	0.778324000	H	-2.044970000	-2.591431000	-1.319771000
C	3.268210000	1.647861000	0.368628000	C	0.591653000	-1.512521000	-3.942679000
C	3.986456000	0.455628000	0.637358000	H	2.040559000	-2.063653000	-2.455663000
C	3.361959000	-0.769808000	0.463803000	C	-0.775633000	-1.423102000	-4.237214000
C	3.853696000	-2.120023000	0.938049000	H	-2.776765000	-1.746816000	-3.519786000
H	4.784063000	-2.337368000	1.412843000	H	1.322583000	-1.208752000	-4.669486000
C	2.865273000	-2.983824000	0.660171000	H	-1.089759000	-1.053794000	-5.185508000
H	2.868592000	-4.023747000	0.889803000	C	0.626391000	-4.450881000	-0.441957000
C	1.809651000	-2.294219000	0.020437000	C	1.856568000	-5.018980000	-0.791207000
C	0.478939000	-2.919621000	-0.373397000	C	-0.471370000	-5.273256000	-0.151367000
C	0.308349000	4.987902000	-1.160039000	C	1.990173000	-6.411494000	-0.862197000
C	1.482192000	5.751680000	-1.230143000	H	2.692841000	-4.387344000	-1.006384000
H	2.415155000	5.323757000	-0.931957000	C	-0.337913000	-6.667384000	-0.216949000
C	-0.911234000	5.556429000	-1.582664000	H	-1.411773000	-4.837845000	0.118875000
H	-1.811261000	4.981314000	-1.551171000	C	0.893517000	-7.235055000	-0.573693000
C	1.442107000	7.078411000	-1.691288000	H	2.930423000	-6.846418000	-1.136593000
H	2.341390000	7.652778000	-1.725676000	H	-1.172458000	-7.296101000	0.005293000
C	-0.946752000	6.883531000	-2.047051000	H	0.996750000	-8.298484000	-0.625350000
H	-1.879118000	7.317135000	-2.359999000	Cd	0.737140000	0.054845000	-0.470083000
C	0.230009000	7.643875000	-2.101956000				
C	5.441524000	0.501201000	1.142535000				
C	6.080090000	1.735242000	1.329266000				

H	5.566279000	2.642428000	1.095186000
C	6.134532000	-0.688862000	1.413434000
H	5.660938000	-1.631201000	1.246469000
C	7.393069000	1.781234000	1.815315000
H	7.870416000	2.727879000	1.967948000
C	7.450431000	-0.644167000	1.896429000
H	7.976676000	-1.555491000	2.109734000
C	8.077422000	0.589670000	2.097329000
H	0.202054000	8.653489000	-2.456018000
H	9.083135000	0.630473000	2.465915000

**Table S17.** Xyz-Coordinates of optimized geometry of free base m-BPDM R"<sup>=</sup>H

N	-0.091613000	-0.880787000	-0.053972000	H	-4.053793000	-0.933244000	2.224092000
H	-0.031041000	0.123183000	-0.196057000	H	-3.728158000	-2.803935000	-1.619293000
N	-1.733652000	1.261663000	-0.785320000	H	4.494527000	-2.161779000	1.535466000
N	1.941854000	0.889303000	0.911655000	H	2.373903000	-2.993218000	-2.097602000
C	-1.284948000	-1.544371000	0.048237000				
C	-0.980573000	-2.906402000	0.262048000				
H	-1.706293000	-3.690241000	0.403660000				
C	0.403836000	-3.035547000	0.251530000				
H	0.974047000	-3.938831000	0.394414000				
C	0.955540000	-1.748196000	0.072708000				
C	-2.771737000	0.401800000	-0.398800000				
C	-4.043344000	1.100549000	-0.505670000				
H	-5.013262000	0.684806000	-0.281377000				
C	-3.748394000	2.353053000	-0.941845000				
H	-4.434560000	3.162776000	-1.145845000				
C	-2.300951000	2.400991000	-1.112559000				
C	2.787348000	-0.100203000	0.392390000				
C	4.141637000	0.428851000	0.282947000				
H	4.996910000	-0.094921000	-0.114078000				
C	4.082786000	1.707901000	0.736749000				
H	4.888820000	2.425174000	0.801797000				
C	2.696858000	1.939674000	1.130868000				
C	-2.572913000	-0.914744000	-0.044387000				
C	-3.758708000	-1.773197000	0.268106000				
C	-4.414538000	-1.652544000	1.497936000				
C	-5.517940000	-2.450898000	1.791551000				
H	-6.016016000	-2.347153000	2.749009000				
C	-4.226674000	-2.709020000	-0.661326000				
C	-5.331730000	-3.504348000	-0.367175000				
H	-5.688497000	-4.219893000	-1.099566000				
C	-5.979184000	-3.378373000	0.860216000				
H	-6.838687000	-3.998427000	1.088486000				
C	2.349337000	-1.369201000	0.074642000				
C	3.328864000	-2.440619000	-0.249537000				
C	4.398794000	-2.721382000	0.613052000				
C	5.314086000	-3.724589000	0.306133000				
H	6.128936000	-3.935189000	0.989619000				
C	5.180024000	-4.459527000	-0.869541000				
H	5.894640000	-5.238705000	-1.109540000				
C	4.118756000	-4.192690000	-1.733424000				
H	4.009916000	-4.758731000	-2.651693000				
C	3.195780000	-3.199624000	-1.422416000				
C	2.159658000	3.203564000	1.748383000				
C	-1.543869000	3.568570000	-1.686365000				
C	1.332194000	4.064191000	0.800467000				
C	0.300123000	3.481377000	0.063529000				
H	0.119319000	2.421895000	0.163693000				

C	-0.491910000	4.230576000	-0.802729000
C	-0.253829000	5.604946000	-0.911245000
H	-0.862922000	6.208887000	-1.576659000
C	0.767971000	6.200794000	-0.177390000
H	0.946988000	7.266722000	-0.269152000
C	1.565225000	5.434143000	0.671519000
H	2.364454000	5.904678000	1.235369000
H	2.989395000	3.795213000	2.143337000
H	1.532096000	2.917620000	2.599641000
H	-1.040038000	3.213379000	-2.595039000
H	-2.262241000	4.325669000	-2.010851000

**Table S18.** Xyz-Coordinates of optimized geometry of free base m-BPDM R"=CH<sub>3</sub>

N	0.145528000	-1.326304000	0.070732000	H	1.767279000	4.711788000	3.227267000
H	0.094693000	-0.332945000	0.278288000	H	2.942336000	4.598755000	1.911950000
N	1.704011000	0.802130000	0.828666000	H	3.006971000	3.462645000	3.267715000
N	-1.883871000	0.402290000	-0.904709000	C	-1.276525000	3.606607000	-0.845129000
C	1.340146000	-1.960087000	-0.128436000	C	-0.337080000	3.024699000	0.009489000
C	1.043449000	-3.315689000	-0.392444000	H	-0.224357000	1.951479000	-0.004917000
H	1.769271000	-4.080231000	-0.616258000	C	0.461044000	3.771971000	0.878975000
C	-0.338308000	-3.467597000	-0.310942000	C	0.315047000	5.163255000	0.868576000
H	-0.903737000	-4.371709000	-0.468995000	H	0.910904000	5.791027000	1.517849000
C	-0.895236000	-2.198047000	-0.042904000	C	-0.615384000	5.763605000	0.024082000
C	2.758147000	0.029215000	0.321566000	H	-0.722581000	6.843271000	0.028901000
C	3.984356000	0.806532000	0.372764000	C	-1.412639000	4.998213000	-0.823002000
H	4.960971000	0.470046000	0.061076000	H	-2.127494000	5.498079000	-1.463693000
C	3.646239000	2.016695000	0.891235000	H	-2.095892000	-3.484822000	2.166397000
H	4.305576000	2.850041000	1.078035000	H	-4.620453000	-2.495031000	-1.156489000
C	2.214420000	1.961150000	1.180153000	H	3.838489000	-3.297858000	1.250197000
C	-2.711759000	-0.533321000	-0.270361000	H	4.041618000	-1.008257000	-2.368929000
C	-4.020484000	0.063485000	-0.040652000	H	-5.788730000	-5.588451000	1.579636000
H	-4.852775000	-0.403929000	0.462304000	H	6.928163000	-4.098123000	-1.621010000
C	-3.951730000	1.326966000	-0.535017000				
H	-4.733643000	2.071336000	-0.527966000				
C	-2.604169000	1.482725000	-1.087146000				
C	2.606246000	-1.280983000	-0.084083000				
C	3.805865000	-2.063701000	-0.511378000				
C	4.436205000	-1.790286000	-1.730602000				
C	5.554246000	-2.520518000	-2.127578000				
H	6.030410000	-2.299169000	-3.076186000				
C	4.315209000	-3.084443000	0.300310000				
C	5.435324000	-3.810539000	-0.096591000				
H	5.824247000	-4.592001000	0.546625000				
C	6.057112000	-3.531453000	-1.311970000				
C	-2.285118000	-1.808062000	0.045201000				
C	-3.252507000	-2.852942000	0.463715000				
C	-4.431686000	-3.078022000	-0.263525000				
C	-5.336485000	-4.057565000	0.135323000				
H	-6.237089000	-4.224452000	-0.444802000				
C	-5.082460000	-4.826938000	1.268611000				
C	-3.912342000	-4.617628000	1.997040000				
H	-3.709418000	-5.210748000	2.881634000				
C	-3.001371000	-3.647296000	1.594078000				
C	-2.060148000	2.702139000	-1.826350000				
C	1.388187000	3.039509000	1.879769000				
C	-1.079713000	2.233452000	-2.930873000				
H	-0.656949000	3.101849000	-3.442987000				
H	-1.600752000	1.611768000	-3.664538000				
H	-0.268390000	1.643521000	-2.507929000				

C	-3.226895000	3.451850000	-2.499804000
H	-2.852647000	4.248039000	-3.147025000
H	-3.907151000	3.901016000	-1.772614000
H	-3.801736000	2.763867000	-3.124300000
C	0.488659000	2.360370000	2.946580000
H	-0.116930000	3.115121000	3.455112000
H	1.101955000	1.843323000	3.690281000
H	-0.176703000	1.630500000	2.488216000
C	2.334616000	4.014922000	2.607044000

**Table S19.** Xyz-Coordinates of optimized geometry of syn conformer of Zn(II) m-BPDM, R"<sup>=</sup>H

Zn	-0.000029000	1.005914000	0.671233000	H	-3.340499000	4.333547000	-0.080976000
Cl	0.000102000	1.575729000	2.959972000	H	2.375785000	3.962654000	1.346971000
N	2.062658000	1.217187000	0.101061000	H	3.339742000	4.334088000	-0.080901000
N	0.000066000	-0.946021000	0.071006000				
N	-2.062768000	1.216940000	0.101204000				
C	1.221467000	4.416062000	-1.829628000				
H	2.162163000	4.534913000	-2.363668000				
C	-0.000357000	4.612652000	-2.501083000				
H	-0.000374000	4.902517000	-3.549413000				
C	-1.222168000	4.415991000	-1.829611000				
H	-2.162876000	4.534816000	-2.363636000				
C	-1.225976000	4.055320000	-0.467390000				
C	-0.000321000	3.913661000	0.206018000				
H	-0.000309000	3.689274000	1.271542000				
C	1.225310000	4.055413000	-0.467393000				
C	-2.501277000	3.726121000	0.279576000				
C	-2.906677000	2.273260000	0.168884000				
C	-4.289619000	1.847453000	0.162090000				
H	-5.143447000	2.508943000	0.218971000				
C	-4.284025000	0.471105000	0.085364000				
H	-5.136436000	-0.191341000	0.079053000				
C	-2.892992000	0.047950000	0.029067000				
C	-2.473995000	-1.280913000	-0.082329000				
C	-1.113946000	-1.743382000	-0.124075000				
C	-0.693827000	-3.085180000	-0.447036000				
H	-1.348595000	-3.912954000	-0.674141000				
C	0.694252000	-3.085088000	-0.447013000				
H	1.349135000	-3.912786000	-0.674058000				
C	1.114191000	-1.743226000	-0.124064000				
C	2.474208000	-1.280593000	-0.082445000				
C	2.893041000	0.048329000	0.028810000				
C	4.284018000	0.471700000	0.085064000				
H	5.136531000	-0.190611000	0.078725000				
C	4.289409000	1.848048000	0.161791000				
H	5.143146000	2.509662000	0.218584000				
C	2.906409000	2.273647000	0.168696000				
C	2.500675000	3.726387000	0.279551000				
C	-3.531516000	-2.341409000	-0.206064000				
C	-4.387325000	-2.383763000	-1.329934000				
H	-4.273048000	-1.642787000	-2.116946000				
C	-3.674259000	-3.323805000	0.800285000				
H	-3.023076000	-3.296600000	1.670173000				
C	-5.366228000	-3.387717000	-1.445628000				
H	-6.010216000	-3.413749000	-2.321314000				
C	-4.664338000	-4.316868000	0.692545000				
H	-4.772520000	-5.056329000	1.482177000				
C	-5.511592000	-4.354800000	-0.432429000				
C	3.531817000	-2.341007000	-0.206103000				

C	4.387549000	-2.383491000	-1.330025000
H	4.273144000	-1.642680000	-2.117172000
C	3.674696000	-3.323231000	0.800400000
H	3.023571000	-3.295925000	1.670326000
C	5.366519000	-3.387393000	-1.445615000
H	6.010442000	-3.413533000	-2.321345000
C	4.664849000	-4.316231000	0.692766000
H	4.773144000	-5.055548000	1.482517000
C	5.512031000	-4.354288000	-0.432259000
H	-6.272007000	-5.127257000	-0.518387000
H	6.272494000	-5.126704000	-0.518142000
H	-2.376468000	3.962575000	1.346963000

**Table S20.** Xyz-Coordinates of optimized geometry of anti-conformer of Zn(II) m-BPDM, R"<sup>=</sup>H

Zn	-0.151724000	1.020451000	0.229132000	H	2.450933000	4.407948000	0.951665000
Cl	-0.720873000	1.485312000	2.449219000	H	-2.053808000	2.904604000	-2.817486000
N	-2.013050000	0.759112000	-0.840040000	H	-3.510164000	3.544587000	-2.055313000
N	0.204256000	-0.973556000	-0.092422000				
N	1.898969000	1.472341000	-0.125891000				
C	-2.281145000	4.591268000	0.123407000				
H	-3.361789000	4.705928000	0.173194000				
C	-1.462014000	5.211615000	1.081048000				
H	-1.907619000	5.815854000	1.867032000				
C	-0.070527000	5.018766000	1.052490000				
H	0.552269000	5.462897000	1.825540000				
C	0.519985000	4.228246000	0.048290000				
C	-0.307566000	3.637095000	-0.926989000				
H	0.141091000	3.073514000	-1.744271000				
C	-1.706351000	3.791786000	-0.883607000				
C	2.020390000	4.039333000	0.008454000				
C	2.568170000	2.646552000	-0.203570000				
C	3.980750000	2.430328000	-0.434152000				
H	4.718636000	3.212841000	-0.551830000				
C	4.178660000	1.065913000	-0.461090000				
H	5.107867000	0.539279000	-0.619302000				
C	2.885646000	0.435664000	-0.252434000				
C	2.686629000	-0.949117000	-0.166435000				
C	1.423483000	-1.619382000	-0.049813000				
C	1.207244000	-3.041109000	0.099968000				
H	1.978182000	-3.793229000	0.175640000				
C	-0.166874000	-3.238265000	0.132129000				
H	-0.692830000	-4.177619000	0.217465000				
C	-0.779871000	-1.936520000	-0.002960000				
C	-2.185328000	-1.666095000	-0.143686000				
C	-2.735753000	-0.443222000	-0.544336000				
C	-4.143425000	-0.209332000	-0.827171000				
H	-4.938730000	-0.920401000	-0.661179000				
C	-4.250212000	1.069453000	-1.338753000				
H	-5.142804000	1.580092000	-1.673852000				
C	-2.917899000	1.632670000	-1.336285000				
C	-2.573671000	3.012147000	-1.853775000				
C	3.904223000	-1.829343000	-0.194916000				
C	4.857891000	-1.767091000	0.846675000				
H	4.700511000	-1.080213000	1.674144000				
C	4.107056000	-2.744050000	-1.253543000				
H	3.381585000	-2.797524000	-2.061199000				
C	5.989577000	-2.602661000	0.830483000				
H	6.707682000	-2.551660000	1.645224000				
C	5.247537000	-3.566876000	-1.278097000				

H	5.396909000	-4.255242000	-2.106390000
C	6.191282000	-3.501903000	-0.234194000
C	-3.107460000	-2.825133000	0.098227000
C	-3.192826000	-3.389655000	1.391841000
H	-2.603640000	-2.964086000	2.199992000
C	-3.881751000	-3.381700000	-0.944734000
H	-3.804579000	-2.968962000	-1.947337000
C	-4.051597000	-4.475199000	1.640191000
H	-4.119365000	-4.888134000	2.643603000
C	-4.727949000	-4.478574000	-0.698814000
H	-5.309945000	-4.903043000	-1.513353000
C	-4.819929000	-5.025760000	0.595468000
H	7.068830000	-4.143781000	-0.249583000
H	-5.478343000	-5.869678000	0.786937000
H	2.456200000	4.677809000	-0.777430000

**Table S21.** Xyz-Coordinates of optimized geometry of syn conformer of Cd(II) m-BPDM, R''=H

Cd	0.000026000	-1.114864000	0.770678000	H	3.337666000	-4.283322000	-0.321958000
Cl	0.000287000	-1.922903000	3.146761000	H	-2.402681000	-3.923509000	1.128800000
N	2.152703000	-1.153173000	0.008769000	H	-3.337589000	-4.283440000	-0.321350000
N	0.000013000	1.016558000	0.092392000				
N	-2.152713000	-1.153174000	0.008830000				
C	-1.221448000	-4.050964000	-2.086092000				
H	-2.160743000	-4.079240000	-2.634786000				
C	-0.000165000	-4.152334000	-2.777626000				
H	-0.000251000	-4.284904000	-3.857131000				
C	1.221223000	-4.050965000	-2.086281000				
H	2.160438000	-4.079247000	-2.635111000				
C	1.231812000	-3.893940000	-0.685334000				
C	2.531229000	-3.651281000	0.070209000				
C	2.994086000	-2.207030000	0.005260000				
C	4.374044000	-1.767541000	-0.028824000				
H	5.239159000	-2.416920000	-0.029188000				
C	4.351638000	-0.385133000	-0.044743000				
H	5.200393000	0.282357000	-0.050662000				
C	2.952660000	0.028386000	-0.039931000				
C	2.490164000	1.351635000	-0.099924000				
C	1.118051000	1.805250000	-0.117579000				
C	0.693718000	3.146979000	-0.455163000				
H	1.345989000	3.972656000	-0.697053000				
C	-0.693745000	3.146969000	-0.455139000				
H	-1.346022000	3.972642000	-0.697016000				
C	-1.118076000	1.805232000	-0.117563000				
C	-2.490178000	1.351617000	-0.099876000				
C	-2.952680000	0.028358000	-0.039860000				
C	-4.351643000	-0.385176000	-0.044704000				
H	-5.200417000	0.282290000	-0.050686000				
C	-4.374031000	-1.767594000	-0.028593000				
H	-5.239147000	-2.416972000	-0.028866000				
C	-2.994082000	-2.207062000	0.005495000				
C	-2.531135000	-3.651279000	0.070585000				
C	-1.231826000	-3.893942000	-0.685146000				
C	0.000047000	-3.867732000	0.005129000				
C	3.526991000	2.435694000	-0.206177000				
C	3.655012000	3.397679000	0.821933000				
H	3.005450000	3.340151000	1.691495000				
C	4.627597000	4.409792000	0.735704000				
H	4.724723000	5.132524000	1.542078000				
C	5.470977000	4.488897000	-0.390061000				

H	6.217503000	5.276392000	-0.459718000
C	5.339082000	3.543785000	-1.425572000
H	5.979308000	3.602242000	-2.302454000
C	4.378612000	2.519989000	-1.330977000
H	4.274505000	1.796527000	-2.135389000
C	-3.527034000	2.435649000	-0.206178000
C	-4.378536000	2.519981000	-1.331068000
H	-4.274289000	1.796591000	-2.135526000
C	-5.339045000	3.543733000	-1.425702000
H	-5.979165000	3.602227000	-2.302659000
C	-5.471118000	4.488759000	-0.390135000
H	-6.217678000	5.276218000	-0.459824000
C	-4.627875000	4.409608000	0.735729000
H	-4.725142000	5.132267000	1.542151000
C	-3.655241000	3.397545000	0.821995000
H	-3.005792000	3.339976000	1.691636000
H	0.000131000	-3.823868000	1.094630000
H	2.402988000	-3.923677000	1.128409000

**Table S22.** Xyz-Coordinates of optimized geometry of anti-conformer of Cd(II) m-BPDM, R''=H

Cd	-0.000012000	-1.147718000	0.336686000	H	-3.359557000	-4.161586000	-0.829770000
Cl	-0.000128000	-1.590452000	2.792912000	H	2.497364000	-3.663010000	-2.272686000
N	-2.131020000	-1.085634000	-0.543897000	H	3.359477000	-4.161687000	-0.829559000
N	0.000025000	1.054689000	-0.213345000				
N	2.131018000	-1.085704000	-0.543833000				
C	1.219387000	-4.741994000	0.618242000				
H	2.157876000	-5.025409000	1.088501000				
C	-0.000114000	-5.133495000	1.197280000				
H	-0.000149000	-5.719909000	2.111757000				
C	-1.219570000	-4.741949000	0.618177000				
H	-2.158094000	-5.025329000	1.088386000				
C	-1.232958000	-3.960336000	-0.555014000				
C	-2.542651000	-3.517983000	-1.181070000				
C	-2.953809000	-2.079529000	-0.934195000				
C	-4.301822000	-1.591507000	-1.143994000				
H	-5.141832000	-2.190415000	-1.469889000				
C	-4.284280000	-0.241222000	-0.852793000				
H	-5.108158000	0.454063000	-0.917164000				
C	-2.919071000	0.106445000	-0.480662000				
C	-2.477096000	1.408141000	-0.195166000				
C	-1.115569000	1.855558000	-0.044917000				
C	-0.693408000	3.203979000	0.273382000				
H	-1.345104000	4.037628000	0.487432000				
C	0.693515000	3.203964000	0.273368000				
H	1.345235000	4.037598000	0.487409000				
C	1.115641000	1.855527000	-0.044910000				
C	2.477155000	1.408071000	-0.195148000				
C	2.919097000	0.106360000	-0.480622000				
C	4.284300000	-0.241347000	-0.852735000				
H	5.108195000	0.453917000	-0.917117000				
C	4.301811000	-1.591638000	-1.143913000				
H	5.141808000	-2.190571000	-1.469793000				
C	2.953787000	-2.079626000	-0.934103000				
C	2.542610000	-3.518082000	-1.180939000				
C	1.232867000	-3.960381000	-0.554948000				
C	-0.000023000	-3.587401000	-1.137714000				
C	-3.538607000	2.464136000	-0.059662000				
C	-3.612481000	3.543753000	-0.969332000				
H	-2.896301000	3.606719000	-1.784511000				

C	-4.616919000	4.519497000	-0.839293000
H	-4.670020000	5.336266000	-1.555093000
C	-5.549688000	4.441145000	0.213752000
H	-6.320905000	5.200512000	0.318559000
C	-5.475791000	3.374871000	1.130474000
H	-6.186047000	3.309983000	1.951033000
C	-4.482830000	2.388152000	0.989647000
H	-4.423658000	1.569032000	1.701489000
C	3.538689000	2.464047000	-0.059667000
C	4.482938000	2.388042000	0.989618000
H	4.423773000	1.568920000	1.701456000
C	5.475916000	3.374745000	1.130423000
H	6.186193000	3.309842000	1.950962000
C	5.549804000	4.441023000	0.213705000
H	6.321036000	5.200378000	0.318496000
C	4.617008000	4.519397000	-0.839314000
H	4.670101000	5.336170000	-1.555110000
C	3.612552000	3.543668000	-0.969331000
H	2.896349000	3.606650000	-1.784490000
H	0.000011000	-3.026393000	-2.072135000
H	-2.497339000	-3.662864000	-2.272821000

**Table S23.** Xyz-Coordinates of optimized geometry of syn conformer of Zn(II) m-BPDM, R" $\text{=CH}_3$

Zn	-0.000033000	-0.638799000	0.498225000	C	4.735967000	4.527491000	-1.314012000
Cl	-0.000093000	-1.024938000	2.834736000	H	4.894535000	5.117491000	-2.213504000
N	-2.095498000	-0.834452000	-0.014977000	C	5.311808000	3.986055000	0.988802000
N	0.000133000	1.318215000	-0.105755000	H	5.909654000	4.162061000	1.879696000
N	2.095311000	-0.834777000	-0.014578000	C	5.522198000	4.760418000	-0.168453000
C	-1.219778000	-3.665203000	-2.103453000	C	-3.531848000	2.745997000	-0.145537000
H	-2.149236000	-3.685111000	-2.664414000	C	-3.740511000	3.533475000	-1.299621000
C	-0.000337000	-3.736279000	-2.796165000	H	-3.136002000	3.356492000	-2.185707000
H	-0.000330000	-3.825639000	-3.880173000	C	-4.327274000	2.980710000	0.998138000
C	1.219099000	-3.665385000	-2.103426000	H	-4.163435000	2.386238000	1.893313000
H	2.148563000	-3.685448000	-2.664370000	C	-4.734847000	4.528715000	-1.313949000
C	1.232148000	-3.549368000	-0.697043000	H	-4.893120000	5.118999000	-2.213306000
C	-0.000352000	-3.507952000	-0.016566000	C	-5.311280000	3.986704000	0.988579000
H	-0.000354000	-3.455331000	1.064249000	H	-5.909283000	4.162558000	1.879397000
C	-1.232846000	-3.549184000	-0.697070000	C	-5.521289000	4.761443000	-0.168495000
C	2.553425000	-3.353802000	0.067775000	H	6.286197000	5.534076000	-0.177588000
C	2.957545000	-1.883442000	-0.047294000	H	-6.285148000	5.535239000	-0.177567000
C	4.330065000	-1.427378000	-0.150913000				
H	5.201616000	-2.061502000	-0.209742000				
C	4.296154000	-0.051121000	-0.178296000				
H	5.132205000	0.626112000	-0.269252000				
C	2.901277000	0.349091000	-0.091774000				
C	2.471837000	1.678242000	-0.123225000				
C	1.113706000	2.140480000	-0.136627000				
C	0.694102000	3.520234000	-0.169480000				
H	1.348789000	4.378419000	-0.175313000				
C	-0.693365000	3.520376000	-0.169585000				
H	-1.347867000	4.378703000	-0.175475000				
C	-1.113258000	2.140704000	-0.136782000				
C	-2.471486000	1.678707000	-0.123499000				
C	-2.901179000	0.349613000	-0.092120000				
C	-4.296139000	-0.050300000	-0.178804000				
H	-5.132032000	0.627113000	-0.269865000				
C	-4.330386000	-1.426547000	-0.151173000				
H	-5.202086000	-2.060471000	-0.209934000				

C	-2.957974000	-1.882920000	-0.047577000
C	-2.554133000	-3.353339000	0.067673000
C	3.660798000	-4.273383000	-0.523434000
H	3.307856000	-5.311302000	-0.524744000
H	4.569041000	-4.230859000	0.088270000
H	3.935455000	-4.004492000	-1.549164000
C	2.436294000	-3.692862000	1.588899000
H	3.423550000	-3.602514000	2.058001000
H	2.090464000	-4.726980000	1.718440000
H	1.760626000	-3.017674000	2.122227000
C	-2.437185000	-3.692262000	1.588841000
H	-1.761621000	-3.017000000	2.122207000
H	-2.091335000	-4.726356000	1.718525000
H	-3.424505000	-3.601907000	2.057806000
C	-3.661601000	-4.272799000	-0.523536000
H	-4.569977000	-4.229871000	0.087942000
H	-3.308919000	-5.310804000	-0.524478000
H	-3.935933000	-4.004119000	-1.549409000
C	3.532406000	2.745341000	-0.145327000
C	3.741456000	3.532422000	-1.299608000
H	3.137092000	3.355283000	-2.185762000
C	4.327618000	2.980237000	0.998447000
H	4.163502000	2.386034000	1.893750000

**Table S24.** Xyz-Coordinates of optimized geometry of anti conformer of Zn(II) m-BPDM, R"=CH<sub>3</sub>.

Zn	-0.086463000	-0.634512000	0.426007000	C	-3.807120000	5.482383000	0.488365000
Cl	0.274262000	-1.100897000	2.694602000	H	-3.951231000	6.162762000	1.324135000
N	1.733925000	-1.074253000	-0.657521000	C	-4.195171000	4.877099000	-1.837512000
N	0.290973000	1.337489000	0.029359000	H	-4.632488000	5.092558000	-2.809491000
N	-2.163194000	-0.367818000	0.036121000	C	-4.384803000	5.768764000	-0.764101000
C	0.746007000	-4.563709000	0.451863000	C	4.038191000	1.895247000	0.225773000
H	1.735263000	-5.009785000	0.473221000	C	4.255567000	2.513335000	1.479586000
C	-0.132173000	-4.802138000	1.516780000	H	3.509612000	2.406783000	2.262880000
H	0.181625000	-5.435202000	2.342891000	C	5.015725000	2.037622000	-0.785476000
C	-1.395897000	-4.190808000	1.553438000	H	4.843835000	1.592701000	-1.762064000
H	-2.029568000	-4.353803000	2.416794000	C	5.436881000	3.235693000	1.723300000
C	-1.807988000	-3.348129000	0.504623000	H	5.597755000	3.690101000	2.697763000
C	-0.922438000	-3.141749000	-0.577263000	C	6.189573000	2.775122000	-0.546080000
H	-1.258855000	-2.533171000	-1.410325000	H	6.927008000	2.885470000	-1.337537000
C	0.360774000	-3.722817000	-0.615300000	C	6.407250000	3.371570000	0.710866000
C	-3.204358000	-2.709689000	0.468364000	H	-4.972824000	6.673022000	-0.901429000
C	-3.213136000	-1.226456000	0.080445000	H	7.317085000	3.936987000	0.897724000
C	-4.459709000	-0.520797000	-0.159624000				
H	-5.443236000	-0.967311000	-0.178899000				
C	-4.151508000	0.811230000	-0.317647000				
H	-4.837661000	1.628781000	-0.480684000				
C	-2.710398000	0.941343000	-0.193998000				
C	-2.032435000	2.167295000	-0.212794000				
C	-0.620363000	2.367834000	-0.073096000				
C	0.085321000	3.629833000	-0.099816000				
H	-0.367450000	4.605265000	-0.197972000				
C	1.439157000	3.335317000	-0.002511000				
H	2.264970000	4.031437000	-0.013397000				
C	1.550631000	1.894854000	0.055881000				
C	2.769509000	1.131487000	-0.006361000				
C	2.842627000	-0.224960000	-0.346077000				
C	4.065835000	-0.972999000	-0.586215000				
H	5.065794000	-0.612792000	-0.395833000				

C	3.700797000	-2.200730000	-1.105474000
H	4.357742000	-2.998526000	-1.418190000
C	2.252768000	-2.225521000	-1.146456000
C	1.375311000	-3.342933000	-1.715068000
C	-3.913598000	-2.794777000	1.856738000
H	-4.087129000	-3.840520000	2.137789000
H	-4.888727000	-2.298381000	1.819683000
H	-3.311527000	-2.312651000	2.634805000
C	-4.059735000	-3.511702000	-0.570964000
H	-5.096978000	-3.158829000	-0.596959000
H	-4.067246000	-4.572695000	-0.294362000
H	-3.642010000	-3.425741000	-1.580662000
C	0.687879000	-2.800351000	-3.004963000
H	0.149200000	-1.865023000	-2.824958000
H	-0.011429000	-3.544042000	-3.408329000
H	1.448467000	-2.594510000	-3.767760000
C	2.234889000	-4.565521000	-2.130544000
H	2.921915000	-4.294246000	-2.941378000
H	1.582940000	-5.369166000	-2.492436000
H	2.834372000	-4.963532000	-1.305695000
C	-2.855304000	3.412530000	-0.405339000
C	-3.040852000	4.315576000	0.664835000
H	-2.597900000	4.096268000	1.633029000
C	-3.439523000	3.703547000	-1.657723000
H	-3.290902000	3.019079000	-2.489228000

**Table S25.** Xyz-Coordinates of optimized geometry of syn conformer of Cd(II) m-BPDM, R"=CH<sub>3</sub>

Cd	-0.000114000	-0.760372000	0.650660000	H	6.262019000	5.619997000	-0.236755000
Cl	0.000234000	-1.268738000	3.120976000	C	4.639559000	4.659242000	-1.310621000
N	2.188162000	-0.793461000	-0.030659000	H	4.729596000	5.296675000	-2.186911000
N	0.000121000	1.361266000	-0.084318000	C	3.654009000	3.656270000	-1.277080000
N	-2.188344000	-0.793207000	-0.030531000	H	2.988197000	3.520505000	-2.125503000
C	-1.219197000	-3.358479000	-2.246409000	C	-3.532449000	2.807247000	-0.154238000
H	-2.148292000	-3.292208000	-2.804912000	C	-3.653495000	3.656614000	-1.277196000
C	-0.000439000	-3.347869000	-2.942689000	H	-2.987788000	3.520582000	-2.125658000
H	-0.000504000	-3.298696000	-4.029158000	C	-4.638852000	4.659778000	-1.310810000
C	1.218401000	-3.358627000	-2.246558000	H	-4.728844000	5.297080000	-2.187199000
H	2.147439000	-3.292513000	-2.805172000	C	-5.504482000	4.840351000	-0.213942000
C	1.237874000	-3.421964000	-0.836690000	H	-6.261018000	5.621031000	-0.236947000
C	2.584733000	-3.299659000	-0.082871000	C	-5.383138000	4.004273000	0.912580000
C	3.038385000	-1.835745000	-0.163398000	H	-6.042459000	4.139403000	1.766447000
C	4.397912000	-1.364465000	-0.352174000	C	-4.409123000	2.988917000	0.939074000
H	5.269370000	-1.985505000	-0.498552000	H	-4.314778000	2.346862000	1.810988000
C	4.350448000	0.016034000	-0.328185000	H	-0.000220000	-3.591091000	0.925520000
H	5.174553000	0.701086000	-0.462255000				
C	2.958629000	0.402278000	-0.130514000				
C	2.487824000	1.724287000	-0.115346000				
C	1.118220000	2.178819000	-0.082416000				
C	0.693721000	3.562259000	-0.051418000				
H	1.344221000	4.422979000	-0.016853000				
C	-0.693250000	3.562337000	-0.051355000				
H	-1.343656000	4.423128000	-0.016766000				
C	-1.117908000	2.178947000	-0.082373000				
C	-2.487563000	1.724607000	-0.115252000				
C	-2.958595000	0.402664000	-0.130391000				
C	-4.350451000	0.016658000	-0.328252000				
H	-5.174435000	0.701832000	-0.462425000				
C	-4.398179000	-1.363845000	-0.352041000				

H	-5.269744000	-1.984733000	-0.498441000
C	-3.038761000	-1.835353000	-0.163234000
C	-2.585269000	-3.299306000	-0.082574000
C	-1.238518000	-3.421835000	-0.836540000
C	-0.000280000	-3.484075000	-0.153704000
C	2.479593000	-3.692299000	1.423282000
H	1.816805000	-3.034307000	1.993691000
H	3.472359000	-3.631352000	1.885068000
H	2.123793000	-4.726726000	1.520476000
C	3.648496000	-4.232436000	-0.729467000
H	3.277104000	-5.263836000	-0.734213000
H	4.579356000	-4.213879000	-0.150661000
H	3.889416000	-3.952331000	-1.760529000
C	-2.480028000	-3.691731000	1.423644000
H	-1.817254000	-3.033615000	1.993922000
H	-2.124152000	-4.726119000	1.520969000
H	-3.472784000	-3.630788000	1.885446000
C	-3.649215000	-4.232054000	-0.728882000
H	-4.580006000	-4.213282000	-0.149972000
H	-3.277948000	-5.263500000	-0.733503000
H	-3.890215000	-3.952100000	-1.759966000
C	3.532893000	2.806743000	-0.154244000
C	4.409732000	2.988037000	0.938996000
H	4.315361000	2.345835000	1.810799000
C	5.383943000	4.003209000	0.912579000
H	6.043382000	4.138049000	1.766401000
C	5.505332000	4.839462000	-0.213805000

**Table S26.** Xyz-Coordinates of optimized geometry of anti conformer of Cd(II) m-BPDM, R"=CH<sub>3</sub>

Cd	0.099873000	-0.733347000	0.576690000	H	-7.371701000	4.008454000	0.635547000
Cl	-0.196936000	-1.012774000	3.040419000	C	-5.590035000	3.779017000	-0.581569000
N	-1.873570000	-1.095949000	-0.572353000	H	-5.848832000	4.586641000	-1.262129000
N	-0.290487000	1.381599000	-0.144697000	C	-4.393359000	3.065073000	-0.771029000
N	2.265696000	-0.322145000	-0.085201000	H	-3.735696000	3.318182000	-1.598533000
C	1.603713000	-3.989784000	1.432816000	C	2.873823000	3.474176000	-0.309184000
H	2.348541000	-4.105228000	2.210565000	C	2.613632000	4.436250000	-1.313083000
C	0.325467000	-4.539773000	1.634741000	H	1.823082000	4.253529000	-2.036026000
H	0.111049000	-5.068305000	2.559414000	C	3.382767000	5.610380000	-1.395351000
C	-0.685892000	-4.372128000	0.680695000	H	3.180541000	6.332567000	-2.182601000
H	-1.673240000	-4.774879000	0.881858000	C	4.409453000	5.852489000	-0.461284000
C	-0.434701000	-3.658133000	-0.514093000	H	4.997781000	6.765121000	-0.519487000
C	-1.574341000	-3.416544000	-1.531359000	C	4.666869000	4.906736000	0.549837000
C	-2.420305000	-2.219483000	-1.084634000	H	5.450365000	5.089130000	1.281202000
C	-3.849959000	-2.056232000	-1.270513000	C	3.911045000	3.722545000	0.619885000
H	-4.528521000	-2.795903000	-1.669683000	H	4.105748000	2.998173000	1.406175000
C	-4.162994000	-0.776124000	-0.849770000	H	1.086481000	-2.596986000	-1.626268000
H	-5.131768000	-0.298387000	-0.869382000				
C	-2.921053000	-0.141316000	-0.430510000				
C	-2.781761000	1.217406000	-0.100335000				
C	-1.543609000	1.945425000	0.020950000				
C	-1.398119000	3.363512000	0.278341000				
H	-2.200052000	4.056328000	0.484261000				
C	-0.040469000	3.646439000	0.226520000				
H	0.431958000	4.604503000	0.384498000				
C	0.640584000	2.396755000	-0.044530000				
C	2.059123000	2.215371000	-0.220719000				
C	2.756394000	0.999565000	-0.333610000				
C	4.145982000	0.884421000	-0.750578000				

H	4.779841000	1.709438000	-1.039998000
C	4.469620000	-0.456584000	-0.747955000
H	5.419160000	-0.897441000	-1.016337000
C	3.287722000	-1.178250000	-0.308671000
C	3.291226000	-2.687915000	-0.033761000
C	1.892752000	-3.269859000	0.257726000
C	0.859602000	-3.123714000	-0.704683000
C	-1.026673000	-3.071683000	-2.953207000
H	-0.473845000	-2.126726000	-2.961910000
H	-1.863012000	-2.965944000	-3.654090000
H	-0.371410000	-3.873602000	-3.317335000
C	-2.459486000	-4.686114000	-1.672564000
H	-1.834244000	-5.551460000	-1.921965000
H	-3.191101000	-4.556460000	-2.478559000
H	-3.013170000	-4.916687000	-0.756506000
C	3.876521000	-3.433450000	-1.279371000
H	3.266735000	-3.266361000	-2.174145000
H	3.905383000	-4.511783000	-1.081429000
H	4.897165000	-3.099100000	-1.497559000
C	4.270291000	-2.911918000	1.159780000
H	5.255262000	-2.496615000	0.922376000
H	4.399059000	-3.982979000	1.358961000
H	3.909329000	-2.422184000	2.071324000
C	-4.048666000	1.999993000	0.092413000
C	-4.922240000	1.669593000	1.153988000
H	-4.656473000	0.860848000	1.829614000
C	-6.110270000	2.396221000	1.353742000
H	-6.764453000	2.139390000	2.183238000
C	-6.450556000	3.450635000	0.484667000

**Table S27.** Xyz-Coordinates of optimized geometry of syn conformer of Zn(II) m-BPDM, R''=Ph.

Zn	-0.509937000	-0.476794000	0.460905000	C	2.514421000	4.353477000	-0.183432000
Cl	-0.562657000	0.033746000	2.761422000	C	0.926947000	3.906918000	1.593718000
N	0.677311000	-2.125197000	-0.135609000	C	3.390881000	4.947712000	0.737111000
N	-2.224145000	-1.438685000	-0.084114000	H	2.812294000	4.272258000	-1.226227000
N	-1.426225000	1.414153000	-0.112972000	C	1.806535000	4.499970000	2.521209000
C	2.727725000	-0.195292000	-2.362661000	H	-0.000596000	3.477463000	1.957127000
H	3.293668000	-1.043650000	-2.735562000	C	3.036459000	5.031258000	2.099508000
C	2.192477000	0.731605000	-3.261777000	H	4.347333000	5.337950000	0.396293000
H	2.366722000	0.612854000	-4.328571000	H	1.530033000	4.527436000	3.572240000
C	1.422756000	1.817340000	-2.800577000	H	3.713993000	5.488413000	2.816952000
H	1.035239000	2.529762000	-3.517870000	C	-0.128081000	4.148487000	-1.943740000
C	1.169733000	1.972539000	-1.426893000	C	0.233747000	5.510059000	-1.976780000
C	1.740071000	1.040341000	-0.527197000	C	-1.040752000	3.681994000	-2.922764000
H	1.615929000	1.197973000	0.541351000	C	-0.274541000	6.372000000	-2.970252000
C	2.531025000	-0.031747000	-0.971405000	H	0.901712000	5.915397000	-1.225844000
C	0.350069000	3.150736000	-0.833476000	C	-1.547039000	4.535202000	-3.914125000
C	-0.973120000	2.679102000	-0.206298000	H	-1.370545000	2.646044000	-2.896117000
C	-1.979968000	3.634824000	0.238311000	C	-1.161326000	5.890581000	-3.947579000
H	-1.853329000	4.707596000	0.242950000	H	0.021586000	7.418584000	-2.970654000
C	-3.095131000	2.913213000	0.581852000	H	-2.245345000	4.147290000	-4.652105000
H	-4.044969000	3.291380000	0.929570000	H	-1.553951000	6.556584000	-4.712265000
C	-2.788448000	1.508410000	0.352248000	C	3.050921000	-0.711817000	1.494779000
C	-3.710556000	0.472521000	0.469121000	C	3.738033000	0.468445000	1.860911000
C	-3.470982000	-0.916895000	0.172950000	C	2.558703000	-1.546038000	2.515651000
C	-4.456152000	-1.971320000	0.122408000	C	3.913750000	0.809912000	3.209545000
H	-5.513872000	-1.856117000	0.306189000	H	4.150272000	1.117944000	1.092431000
C	-3.776562000	-3.140932000	-0.192150000	C	2.744302000	-1.212363000	3.869341000
H	-4.193793000	-4.131303000	-0.296654000	H	2.007076000	-2.447235000	2.266876000

C	-2.377878000	-2.795470000	-0.313956000	C	3.422139000	-0.035077000	4.224093000
C	-1.291152000	-3.681994000	-0.588075000	H	4.433528000	1.729900000	3.466968000
C	0.077960000	-3.351158000	-0.559696000	H	2.335732000	-1.860008000	4.640669000
C	1.132046000	-4.233717000	-1.011062000	H	3.554714000	0.228248000	5.270891000
H	0.984982000	-5.218592000	-1.428224000	C	4.501654000	-1.572576000	-0.271448000
C	2.332339000	-3.566261000	-0.849395000	C	5.014014000	-2.723496000	0.373440000
H	3.315296000	-3.921797000	-1.112104000	C	5.407375000	-0.772410000	-0.999082000
C	2.025760000	-2.277301000	-0.283551000	C	6.364399000	-3.086262000	0.257418000
C	3.024339000	-1.138329000	-0.002160000	H	4.361274000	-3.326123000	0.998684000
C	-5.090929000	0.819116000	0.955935000	C	6.765209000	-1.128684000	-1.114533000
C	-6.187772000	0.868311000	0.068700000	H	5.068088000	0.141913000	-1.473720000
H	-6.032689000	0.669543000	-0.989114000	C	7.251954000	-2.292055000	-0.495252000
C	-5.299068000	1.085827000	2.327351000	H	6.726242000	-3.977105000	0.765721000
H	-4.457135000	1.037591000	3.013375000	H	7.438656000	-0.490320000	-1.682187000
C	-7.473390000	1.188564000	0.543556000	H	8.300330000	-2.567150000	-0.582702000
H	-8.309004000	1.233513000	-0.150917000				
C	-6.586961000	1.396387000	2.802239000				
H	-6.735958000	1.594381000	3.860898000				
C	-7.677353000	1.451077000	1.912425000				
C	-1.656125000	-5.094523000	-0.939404000				
C	-2.458809000	-5.369672000	-2.070945000				
H	-2.796488000	-4.549415000	-2.698917000				
C	-1.216643000	-6.172867000	-0.136947000				
H	-0.614631000	-5.970507000	0.744916000				
C	-2.800004000	-6.693278000	-2.401078000				
H	-3.404520000	-6.889241000	-3.283310000				
C	-1.574471000	-7.495016000	-0.456390000				
H	-1.239578000	-8.311400000	0.178753000				
C	-2.363107000	-7.760899000	-1.592469000				
H	-8.671346000	1.694862000	2.279881000				
H	-2.634390000	-8.783591000	-1.843113000				
C	1.260594000	3.839338000	0.226225000				

**Table S28.** Xyz-Coordinates of optimized geometry of anti conformer of Zn(II) m-BPDM, R''=Ph.

Zn	-0.582511000	0.345292000	-0.676091000	C	5.362849000	-0.445397000	-0.471363000
Cl	-0.732059000	0.484456000	-3.027733000	C	4.281223000	0.352880000	1.543680000
N	-1.696160000	-1.412192000	-0.144133000	C	6.394350000	-1.005863000	0.296989000
N	-2.122852000	1.428100000	0.094910000	H	5.383530000	-0.561781000	-1.551608000
N	0.851862000	1.687635000	0.109810000	C	5.313504000	-0.210895000	2.319189000
C	1.147348000	-2.955767000	-1.938949000	H	3.466075000	0.862134000	2.048615000
H	0.620657000	-3.854319000	-2.245656000	C	6.378145000	-0.888789000	1.701859000
C	1.939029000	-2.265116000	-2.865294000	H	7.205139000	-1.536831000	-0.196592000
H	2.036928000	-2.645604000	-3.878599000	H	5.278684000	-0.120066000	3.402484000
C	2.574322000	-1.061762000	-2.514323000	H	7.175769000	-1.323442000	2.299735000
H	3.158931000	-0.532013000	-3.257633000	C	3.603464000	1.662358000	-1.939340000
C	2.407173000	-0.526333000	-1.225858000	C	4.882532000	2.257585000	-1.963164000
C	1.645964000	-1.256861000	-0.286654000	C	2.683271000	2.003129000	-2.959826000
H	1.582782000	-0.893636000	0.733152000	C	5.247469000	3.144730000	-2.993627000
C	1.018259000	-2.470841000	-0.619214000	H	5.603381000	2.036341000	-1.182649000
C	3.119670000	0.763915000	-0.752735000	C	3.047713000	2.887530000	-3.987815000
C	2.203403000	1.727290000	0.022783000	H	1.677041000	1.589139000	-2.958121000
C	2.722452000	2.940724000	0.625613000	C	4.333798000	3.462353000	-4.014374000
H	3.765524000	3.218009000	0.661332000	H	6.241235000	3.587231000	-2.992583000
C	1.642893000	3.663756000	1.075389000	H	2.322221000	3.128836000	-4.760748000
H	1.656105000	4.633833000	1.548964000	H	4.614272000	4.148883000	-4.809948000
C	0.444085000	2.902705000	0.762073000	C	0.316122000	-2.697877000	1.854202000
C	-0.859915000	3.355972000	1.003027000	C	1.585108000	-2.974303000	2.417272000
C	-2.081155000	2.680826000	0.665000000	C	-0.657091000	-2.094271000	2.675427000
C	-3.432861000	3.145141000	0.890346000	C	1.873467000	-2.656764000	3.752561000

H	-3.712155000	4.082120000	1.348794000	H	2.352240000	-3.445228000	1.808199000
C	-4.283477000	2.150140000	0.422743000	C	-0.373636000	-1.781999000	4.020846000
H	-5.363540000	2.145831000	0.445541000	H	-1.632778000	-1.847255000	2.274114000
C	-3.445454000	1.073308000	-0.055922000	C	0.889975000	-2.060411000	4.567771000
C	-3.880588000	-0.222513000	-0.510153000	H	2.858418000	-2.879002000	4.156536000
C	-3.060519000	-1.359607000	-0.563541000	H	-1.143173000	-1.318085000	4.633908000
C	-3.472873000	-2.706796000	-0.911034000	H	1.106565000	-1.819463000	5.605960000
H	-4.432718000	-2.982273000	-1.321821000	C	0.186382000	-4.707184000	0.431632000
C	-2.414381000	-3.549790000	-0.620346000	C	-0.776852000	-5.457927000	1.147239000
H	-2.377997000	-4.619936000	-0.749368000	C	1.312150000	-5.392905000	-0.070098000
C	-1.342083000	-2.719828000	-0.113713000	C	-0.644104000	-6.844686000	1.316299000
C	0.048769000	-3.155795000	0.381821000	H	-1.624913000	-4.951307000	1.600078000
C	-1.014318000	4.687067000	1.686552000	C	1.452747000	-6.783991000	0.100102000
C	-1.525652000	5.798503000	0.980051000	H	2.093680000	-4.849221000	-0.589431000
H	-1.790704000	5.690184000	-0.068594000	C	0.472486000	-7.520787000	0.786028000
C	-0.664649000	4.840742000	3.046447000	H	-1.402138000	-7.393825000	1.870116000
H	-0.281125000	3.986787000	3.599202000	H	2.331454000	-7.285146000	-0.299577000
C	-1.673058000	7.043154000	1.619177000				
H	-2.055654000	7.893286000	1.059647000				
C	-0.825392000	6.082195000	3.689244000				
H	-0.559684000	6.183927000	4.738723000				
C	-1.326870000	7.188628000	2.976908000				
C	-5.326664000	-0.347890000	-0.874197000				
C	-5.858930000	0.475860000	-1.894858000				
H	-5.204391000	1.171695000	-2.412721000				
C	-6.185051000	-1.257325000	-0.213410000				
H	-5.794322000	-1.872625000	0.592604000				
C	-7.211932000	0.373536000	-2.261455000				
H	-7.601327000	0.999260000	-3.060625000				
C	-7.543119000	-1.345273000	-0.568470000				
H	-8.193414000	-2.040202000	-0.042701000				
C	-8.059960000	-0.535150000	-1.597925000				
H	-1.446182000	8.149430000	3.471858000				
H	-9.108386000	-0.608348000	-1.877012000				
C	4.294446000	0.254697000	0.137608000				

**Table S29.** Xyz-Coordinates of optimized geometry of syn conformer of Cd(II) m-BPDM, R"=Ph.

Cd	-0.184604000	0.524512000	0.499141000	C	3.064657000	-2.577541000	1.547753000
Cl	-0.305916000	0.284299000	2.989164000	C	3.565253000	-0.328706000	2.286260000
N	1.779491000	1.383830000	-0.250442000	C	3.170149000	-3.039576000	2.869178000
N	-1.099942000	2.430672000	-0.230536000	H	2.823073000	-3.287510000	0.761858000
N	-2.130735000	-0.449159000	-0.214985000	C	3.674200000	-0.787833000	3.610506000
C	-0.045696000	-2.544419000	-2.608072000	H	3.707770000	0.728911000	2.091188000
H	-0.809911000	-3.004675000	-3.218869000	C	3.479745000	-2.146183000	3.910951000
C	1.133496000	-2.100139000	-3.224468000	H	2.997076000	-4.091392000	3.082543000
H	1.247961000	-2.206414000	-4.300693000	H	3.890266000	-0.078376000	4.405253000
C	2.170383000	-1.535482000	-2.473664000	H	3.549500000	-2.499554000	4.936846000
H	3.071484000	-1.230469000	-2.986726000	C	4.604597000	-1.046933000	-0.930373000
C	2.061766000	-1.410162000	-1.071961000	C	5.457055000	-2.064185000	-0.448548000
C	3.222406000	-0.726850000	-0.251300000	C	5.029571000	-0.341026000	-2.084407000
C	2.999742000	0.804327000	-0.274931000	C	6.673119000	-2.368268000	-1.090296000
C	4.038240000	1.818069000	-0.270616000	H	5.194403000	-2.616777000	0.444663000
H	5.100508000	1.628555000	-0.270366000	C	6.241869000	-0.638651000	-2.727672000
C	3.406214000	3.045579000	-0.284250000	H	4.419743000	0.464805000	-2.482765000
H	3.871892000	4.019634000	-0.308172000	C	7.074745000	-1.660801000	-2.235729000
C	1.973806000	2.798494000	-0.275442000	H	7.305662000	-3.155103000	-0.685622000
C	0.988737000	3.798868000	-0.340041000	H	6.532932000	-0.071064000	-3.608675000
C	-0.439500000	3.638786000	-0.358166000	H	8.015493000	-1.893431000	-2.728963000
C	-1.416912000	4.706056000	-0.440366000	C	-1.100172000	-3.641812000	0.834204000
H	-1.196155000	5.758771000	-0.535342000	C	-0.136171000	-4.678397000	0.788197000
C	-2.669163000	4.115953000	-0.350756000	C	-1.651121000	-3.302262000	2.085083000
H	-3.628741000	4.611121000	-0.363967000	C	0.235833000	-5.376017000	1.947020000

C	-2.454148000	2.689417000	-0.218567000	H	0.329769000	-4.933233000	-0.160957000
C	-3.480565000	1.692170000	-0.038918000	C	-1.273882000	-3.994898000	3.252240000
C	-3.334334000	0.301283000	-0.008981000	H	-2.355139000	-2.482281000	2.172585000
C	-4.424744000	-0.649329000	0.167128000	C	-0.339972000	-5.041577000	3.189609000
H	-5.458493000	-0.386730000	0.337326000	H	0.971155000	-6.175297000	1.881834000
C	-3.890081000	-1.913485000	0.056419000	H	-1.699412000	-3.697287000	4.206925000
H	-4.409564000	-2.858704000	0.112570000	H	-0.051002000	-5.575735000	4.091777000
C	-2.465930000	-1.751839000	-0.203513000	C	-2.332389000	-3.896217000	-1.414165000
C	-1.507589000	-2.928816000	-0.488878000	C	-2.459567000	-5.280362000	-1.177605000
C	-0.206053000	-2.432971000	-1.214417000	C	-3.026521000	-3.357873000	-2.527882000
C	0.860810000	-1.862919000	-0.466341000	C	-3.227414000	-6.099622000	-2.030458000
C	1.479720000	5.222709000	-0.385155000	H	-1.981368000	-5.734111000	-0.318663000
C	2.006081000	5.831626000	0.775132000	C	-3.790801000	-4.168292000	-3.380687000
H	2.052969000	5.265464000	1.701962000	H	-2.985166000	-2.288823000	-2.720846000
C	2.451418000	7.166236000	0.739933000	C	-3.892816000	-5.552742000	-3.139738000
H	2.846884000	7.625277000	1.642775000	H	-3.307139000	-7.162996000	-1.816372000
C	2.385089000	7.904297000	-0.457629000	H	-4.309806000	-3.719450000	-4.224438000
H	2.732817000	8.934186000	-0.485377000	H	-4.486657000	-6.185056000	-3.795436000
C	1.864286000	7.300617000	-1.618861000				
H	1.812265000	7.861594000	-2.548925000				
C	1.407743000	5.969967000	-1.580988000				
H	1.006105000	5.506877000	-2.478918000				
C	-4.876517000	2.227735000	0.152606000				
C	-5.640710000	2.665698000	-0.950045000				
H	-5.221570000	2.604985000	-1.951552000				
C	-6.941883000	3.168140000	-0.759963000				
H	-7.523849000	3.495517000	-1.618263000				
C	-7.488436000	3.246265000	0.535856000				
H	-8.492481000	3.636921000	0.683146000				
C	-6.727086000	2.815328000	1.639644000				
H	-7.139780000	2.874357000	2.643850000				
C	-5.428817000	2.306002000	1.449479000				
H	-4.839878000	1.976959000	2.302045000				
H	0.792743000	-1.876674000	0.620014000				
C	3.255510000	-1.212417000	1.231304000				

**Table S30.** Xyz-Coordinates of optimized geometry of anti conformer of Cd(II) m-BPDM, R''=Ph.

Cd	0.407086000	0.440075000	-0.965765000	C	-0.993322000	-3.462135000	2.232529000
Cl	0.223856000	0.611505000	-3.454813000	C	1.273749000	-2.815926000	2.780036000
N	1.985924000	-1.036071000	-0.143598000	C	-1.328059000	-3.466960000	3.596788000
N	1.752426000	1.966188000	-0.008643000	H	-1.759726000	-3.708574000	1.503117000
N	-1.270653000	1.615747000	0.111786000	C	0.943690000	-2.821899000	4.148522000
C	-2.686386000	-1.654853000	-2.118611000	H	2.286602000	-2.557773000	2.489321000
H	-3.513999000	-1.296111000	-2.718120000	C	-0.358482000	-3.148067000	4.566554000
C	-1.936914000	-2.746814000	-2.569324000	H	-2.343496000	-3.715296000	3.895744000
H	-2.189995000	-3.218434000	-3.515160000	H	1.704824000	-2.568734000	4.883073000
C	-0.861568000	-3.240920000	-1.817706000	H	-0.614152000	-3.150118000	5.623561000
H	-0.324063000	-4.102228000	-2.188796000	C	0.976162000	-4.690014000	-0.120304000
C	-0.510596000	-2.649080000	-0.587316000	C	0.550306000	-5.784973000	0.660252000
C	0.675671000	-3.204462000	0.276985000	C	1.676199000	-4.974884000	-1.319423000
C	1.959240000	-2.374188000	0.044384000	C	0.809721000	-7.111370000	0.261301000
C	3.308634000	-2.903181000	0.126244000	H	0.026538000	-5.618646000	1.593809000
H	3.568434000	-3.938135000	0.285390000	C	1.937265000	-6.294166000	-1.721877000
C	4.171824000	-1.840609000	-0.047784000	H	2.030646000	-4.159000000	-1.943882000
H	5.250862000	-1.870920000	-0.059605000	C	1.502481000	-7.376197000	-0.931823000
C	3.360672000	-0.642145000	-0.176857000	H	0.471782000	-7.932392000	0.889539000
C	3.872449000	0.666343000	-0.198467000	H	2.477787000	-6.474090000	-2.648192000
C	3.130969000	1.888630000	-0.058928000	H	1.704215000	-8.399726000	-1.238598000
C	3.694756000	3.191580000	0.230307000	C	-4.112898000	-0.650889000	0.795706000
H	4.747686000	3.428346000	0.272217000	C	-5.011803000	-1.679909000	0.426888000
C	2.629166000	4.041142000	0.490369000	C	-3.921726000	-0.397209000	2.169047000
H	2.675591000	5.081828000	0.775084000	C	-5.712808000	-2.412847000	1.396523000

C	1.420025000	3.256580000	0.342756000	H	-5.157655000	-1.916711000	-0.623531000
C	0.083728000	3.702118000	0.642216000	C	-4.621605000	-1.132513000	3.146143000
C	-1.097591000	2.955325000	0.595416000	H	-3.223887000	0.369809000	2.490483000
C	-2.400279000	3.440764000	1.035661000	C	-5.524478000	-2.140131000	2.767049000
H	-2.594267000	4.424735000	1.435631000	H	-6.400419000	-3.196041000	1.085642000
C	-3.306292000	2.425832000	0.840299000	H	-4.455456000	-0.915628000	4.198849000
H	-4.368184000	2.439044000	1.036834000	H	-6.067967000	-2.705678000	3.520359000
C	-2.575631000	1.314213000	0.246783000	C	-4.200109000	0.723890000	-1.415084000
C	-3.293227000	0.076658000	-0.312692000	C	-5.585504000	0.919197000	-1.241493000
C	-2.363702000	-1.024342000	-0.900674000	C	-3.585410000	1.252211000	-2.576855000
C	-1.275279000	-1.534963000	-0.148871000	C	-6.345802000	1.599979000	-2.212367000
C	5.366901000	0.829970000	-0.280194000	H	-6.082891000	0.546495000	-0.351916000
C	6.206284000	0.502309000	0.806998000	C	-4.342694000	1.930155000	-3.544475000
H	5.768067000	0.121918000	1.726295000	H	-2.514810000	1.140022000	-2.735719000
C	7.598635000	0.684450000	0.713709000	C	-5.730170000	2.106613000	-3.370207000
H	8.232468000	0.435251000	1.561413000	H	-7.414047000	1.735239000	-2.058028000
C	8.169125000	1.188566000	-0.471080000	H	-3.846152000	2.321314000	-4.428900000
H	9.245369000	1.324871000	-0.545009000	H	-6.316276000	2.633780000	-4.119418000
C	7.336749000	1.518962000	-1.558327000				
H	7.767937000	1.908322000	-2.477313000				
C	5.943377000	1.349777000	-1.460603000				
H	5.302533000	1.608200000	-2.299830000				
C	-0.027990000	5.132961000	1.103055000				
C	0.058208000	6.184653000	0.164925000				
H	0.190540000	5.952707000	-0.888921000				
C	-0.038527000	7.524135000	0.585678000				
H	0.019908000	8.324186000	-0.148299000				
C	-0.209919000	7.828000000	1.950396000				
H	-0.280806000	8.863208000	2.275476000				
C	-0.287616000	6.783022000	2.891291000				
H	-0.415196000	7.008194000	3.947456000				
C	-0.200228000	5.442990000	2.469360000				
H	-0.255299000	4.637888000	3.198007000				
H	-1.079273000	-1.118206000	0.835536000				
C	0.311739000	-3.132570000	1.796860000				