Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Peptide cyclisation promoted by supramolecular complex formation

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General methods and materials

All reactions were performed under normal atmosphere, without precautions as N_2 or Ar atmosphere, unless stated otherwise. THF was distilled over sodium/benzophenone under N_2 atmosphere. Dichloromethane and methanol were distilled over CaH under N_2 atmosphere. Triethylamine was distilled over KOH pellets under N_2 atmosphere. All column chromatography was performed using SiO_2 (0.04 – 0.06 µm) unless otherwise specified. NMR spectra were recorded on a Bruker DRX 300, AMX 400 or DRX 500. ^{1}H NMR chemical shifts are given in ppm and referenced to the residual non-deuterated solvent: 7.26 ppm for $CDCl_3$, 5.32 ppm for CD_2Cl_2, 4.79 ppm for D_2O, and 2.50 ppm for DMSO.[17] ^{13}C NMR chemical shifts are referenced to the deuterated solvent: 77.10 ppm for $CDCl_3$, 53.84 ppm for CD_2Cl_2 and 39.52 for DMSO-d_6.[1]

LC-MS measurements were carried out on a Finnigan Surveyor LC and Finnigan LXQ equipped with Reprosil-Pur 120 C18-Q, 3µm, 50 x 4.6 mm column. Elution was performed using a gradient program from H_2O/0.1% HCO_2H to CH_3CN/0.1% HCO_2H over 5 or 10 minutes. MS (ESI+) spectra (positive ions) were recorded on a Finnigan LXQ in full scan mode (*m/z* = 100 – 2000).

HRMS (ESI+) spectra were recorded on an AccuTOF LC, JMS-T100LP Mass spectrometer (JEOL, Japan) using an ESI source with the following settings: needle voltage: 2000V, orifice 1 voltage: 90V, orifice 2 voltage: 9V, ring lens voltage 22V, orifice and desolvating temperature: 30 °C, spray temperature -40 °C. HRMS (FD+) spectra were recorded on an AccuTOF GC v 4g, JMS-T100GCV mass spectrometer (JEOL, Japan) with the following settings: GCMS (EI) filament ionizing voltage 70V, FD /FI probe equipped with FD Emitter, Carbotec (Germany) FD 13 µm, current rate 51.2mA/min over 1.2 min, counter electrode -10 kV, ion source 37V.

IR spectra were recorded on a Bruker Alpha FTIR. Microwave heating was carried out using a CEM discover (Model number: 908010).

ZnTPP[2], peptide **4**[3], Boc-Phe-β-Ala-OH[3], N_3-Phe-β-Ala-OH[4], and 2,6-bis(pyridin-4-ylethynyl)phenyl acetate **7**[5] were prepared according to literature procedures. Other compounds were obtained from commercially available sources (Sigma-Aldrich, Fluorochem) and used without further purification.

General cyclisation procedure

A general procedure for peptide cyclisation is as follows. Azide (0.042 mmol), PPh_3 (1.1 equiv, 0.046 mmol), porphyrin (3 equiv, 0.125 mmol) and 1,3,5-trimethoxy benzene (internal standard, 1 equiv, 0.042 mmol) were combined in a microwave vial and dissolved in 2.5 ml THF-d_8. The vial was heated in a microwave at 80 °C for 5 hours, after which 60 µl of water was added and the vessel heated for an additional hour at 80 °C in the microwave. Reaction yields were determined by ^{1}H NMR.

*Determination of association constants between ZnTPP and **7***

A host-guest NMR titration was performed by titrating a solution of host (ZnTPP in thf-d8) against a solution of host and guest (ZnTPP and 7 in thf-d8), keeping the host concentration constant. Peak shifts were fitted to a 2:1, non-cooperative binding using Bindfit v0.5. Found association constant: 236 ± 5% M^{-1} (28 °C).

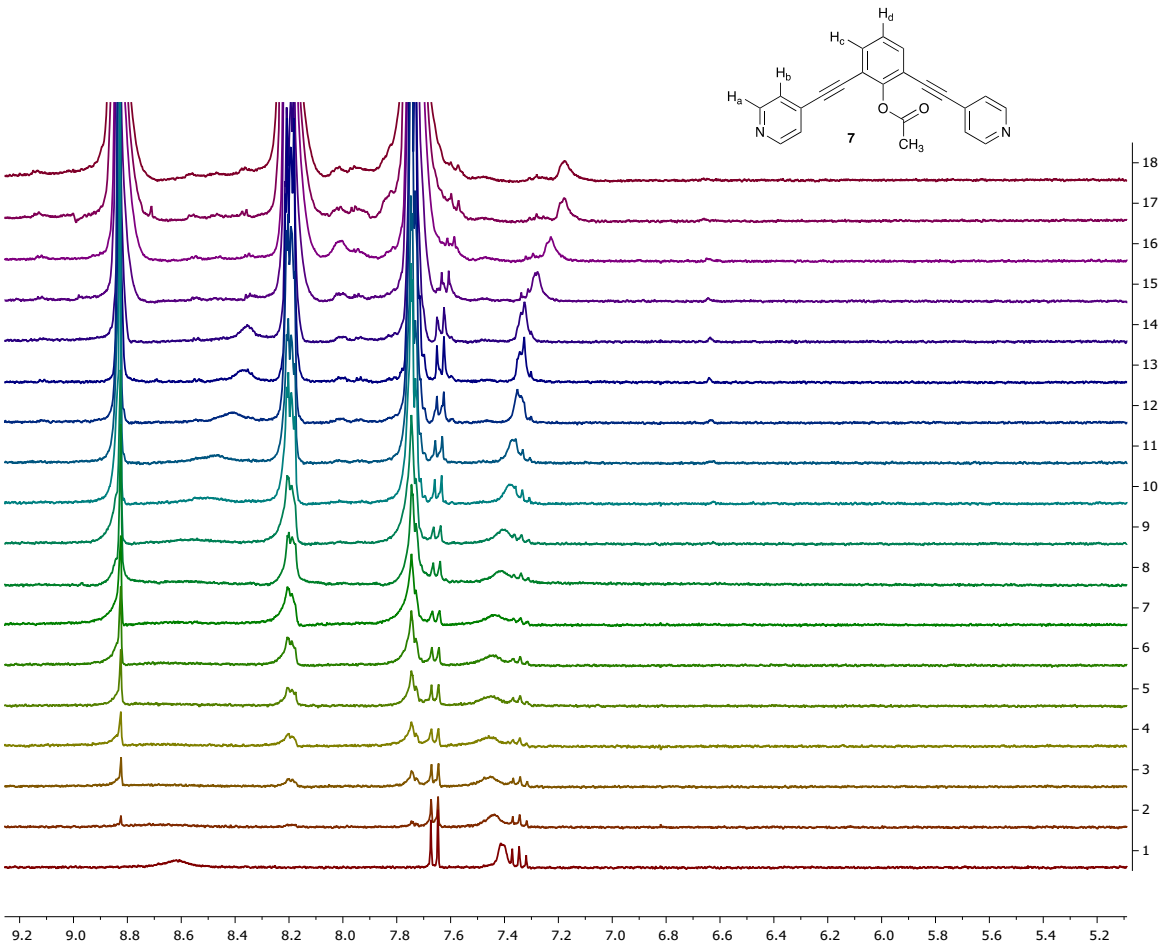


Figure S1: NMR spectra of 2,6-bis(pyridin-4-ylethynyl)phenyl acetate 7 and varying amounts of ZnTPP at 28 °C.

#	Host concentration / mM	Guest concentration / mM	Proton 1 shift	Proton 2 shift	Proton 3 shift	eq guest to host
1	1.1624	0.0000	7.65	7.4084	2.4133	0.00
2	1.1624	0.1992	7.65	7.4385	2.4113	0.17
3	1.1624	0.3968	7.64	7.454	2.4091	0.33
4	1.1624	0.5929	7.64	7.4504	2.4093	0.49
5	1.1624	0.7874	7.64	7.45	2.4092	0.66
6	1.1624	1.0763	7.64	7.4396	2.4074	0.90
7	1.1624	1.4563	7.64	7.4367	2.4049	1.21
8	1.1624	1.8304	7.64	7.4114	2.4032	1.53
9	1.1624	2.7410	7.64	7.3973	2.401	2.28
10	1.1624	3.6178	7.63	7.3776	2.3968	3.01
11	1.1624	4.4627	7.63	7.3696	2.3949	3.72
12	1.1624	5.2773	7.63	7.3521	2.3881	4.40
13	1.1624	6.8221	7.62	7.3437	2.3876	5.69
14	1.1624	7.6988	7.62	7.3375	2.3872	6.42
15	1.1624	10.9984	7.61	7.2775	2.3677	9.17
16	1.1624	13.8205	7.59	7.2284	2.345	11.52
17	1.1624	17.9898	7.57	7.1793	2.3279	14.99
18	1.1624	21.6232	7.57	7.1794	2.3293	18.02

Figure S2: Non-cooperative 1:2 fit of 7 and ZnTPP at room temperature

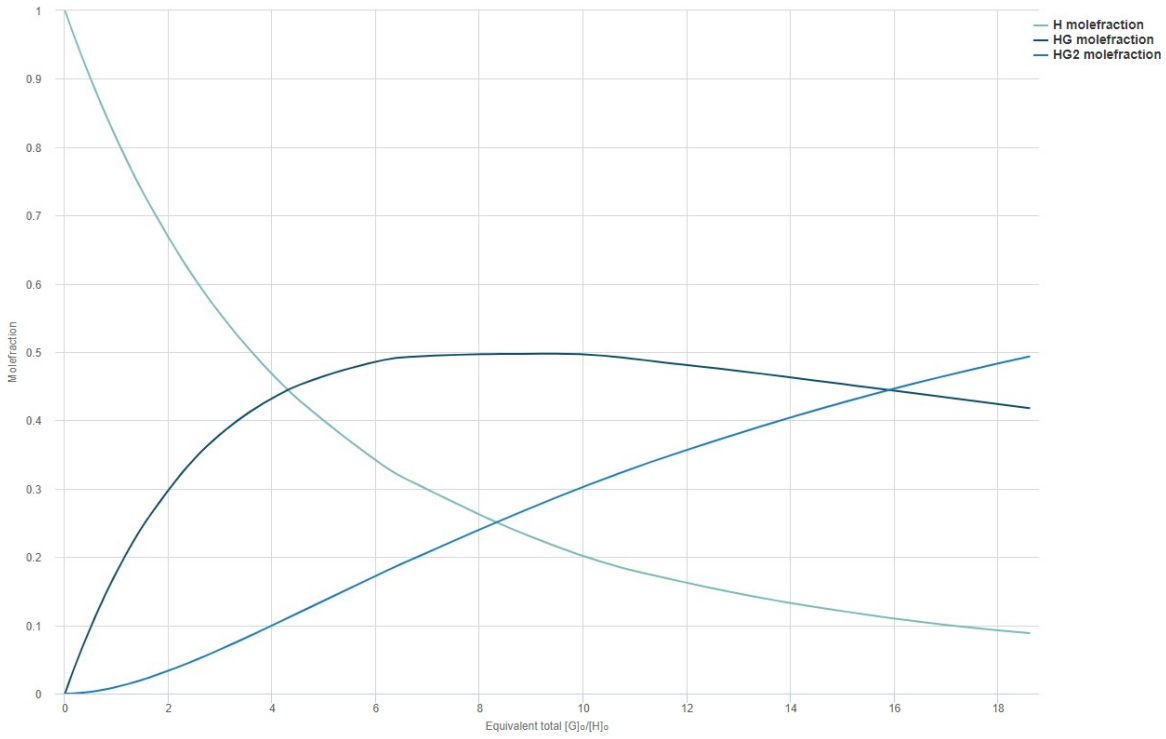


Figure S3: Calculated mole fractions of the non-cooperative 1:2 fit of 7 and ZnTPP at room temperature

Quality of fit

Fit	RMS	Covariance
Proton 1	3.6775e-3	2.2602e-2
Proton 2	1.3625e-2	2.3807e-2
Proton 3	4.1161e-3	2.3399e-2
Total	**8.4872e-3**	**2.2852e-2**

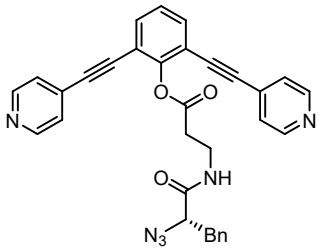
Coefficients

Fit	H	HG	HG2
Proton 1	7.6442	7.6506	7.4847
Proton 2	7.4421	7.4035	6.9155
Proton 3	2.4091	2.4156	2.2340

Figure S4: Details of the non-cooperative 1:2 fit of 7 and ZnTPP at room temperature

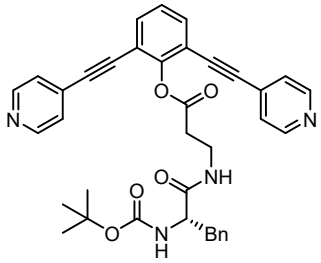
Syntheses of new compounds

Compound **1a**



Synthesised according to a modified literature procedure.[14] N_3-Phe-β-Ala-OH (0.5 mmol, 130 mg) and DCC (0.53 mmol, 110 mg) were dissolved in dry DCM (4 ml), placed under argon atmosphere, cooled to 0 °C and stirred for 30 minutes. **9** (0.5 mmol, 150 mg) was added and the mixture was stirred for two days at rt. The mixture was diluted with some ethyl acetate, filtered and immobilized on SiO_2. Purified twice using column chromatography (100% EtOAc), then DCM/acetone (3:1 → 2:1) to yield the compound as a dark oil (0.13 mmol, 67 mg, 25%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.67 – 8.61 (m, 4H), 8.62 – 8.59 (m, 2H), 7.63 (d, *J* = 8.1 Hz, 2H), 7.37 – 7.34 (m, 4H), 7.33 – 7.27 (m, 2H), 7.25 – 7.21 (m, 1H), 7.16 (d, *J* = 7.6 Hz, 2H), 3.93 (dd, *J* = 8.5, 4.1 Hz, 1H), 3.73 – 3.53 (m, 2H), 3.25 (dd, *J* = 14.1, 4.1 Hz, 1H), 3.00 – 2.82 (m, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 169.24, 168.74, 152.13, 150.49, 150.05, 149.88, 140.42, 135.95, 134.03, 130.39, 129.38, 128.65, 127.27, 126.48, 125.43, 125.39, 120.53, 117.44, 112.02, 99.99, 91.85, 87.61, 65.42, 38.61, 34.92, 33.72. **IR**: 2105, 1764, 1672, 1589 cm^{-1}. **MS** (ESI, $[M+H]^+$) *m/z* 541.2. **HRMS** (ESI, $[M+H]^+$) calc. for $C_{32}H_{24}N_6O_3$ 541.1983, found 541.2004.

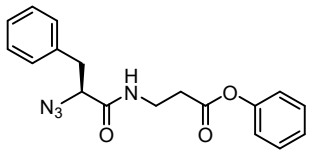
Compound **1b**



Similar procedure as **12**, with Boc-Phe-β-Ala-OH instead of N_3-Phe-β-Ala-OH. Yield: 157 mg, 0.27 mmol, 55%.

^{1}H NMR (400 MHz, THF-d_8) δ 8.61 (bs, 4H), 7.66 (d, *J* = 7.8 Hz, 2H), 7.44 (d, *J* = 5.0 Hz, 4H), 7.35 (t, *J* = 7.8 Hz, 1H), 7.24 – 7.09 (m, 5H), 6.36 (d, *J* = 8.7 Hz, 1H), 4.23 (q, *J* = 7.6 Hz, 1H),), 3.56 – 3.46 (m, 2H), 3.13 – 2.98 (m, 1H), 2.98 – 2.73 (m, 2H), 1.35 (s, 9H). **^{13}C NMR** (101 MHz, THF-d_8) δ 172.19, 168.87, 155.98, 153.64, 150.88, 138.72, 134.39, 130.65, 130.05, 128.68, 126.97, 126.87, 125.93, 118.43, 92.54, 87.95, 78.86, 56.65, 39.32, 35.79, 34.21, 30.45, 28.41. **IR**: 2926, 2219, 2082, 1768 cm^{-1}. **MS** (ESI, $[M+H]^+$) *m/z* 615.1. **HRMS** (FD+, $[M+H]^+$) calc. for $C_{37}H_{34}N_4O_5$ 615.2607, found 615.2602.

Compound **1c**



N_3-Phe-β-Ala-OH (163 mg, 0.62 mmol) and phenol (54 mg, 0.58 mmol) were combined in 10 ml DCM/THF (8:2 v/v). EDC·HCl (132 mg, 0.69 mmol) and DMAP (6 grains) were added and the mixture was stirred for 21 hours at rt, after which it was concentrated *in vacuo* and purified using column chromatography (PE/EtOAc 8:2) to obtain the compound as a colorless oil (24 mg, 0.07 mmol, 12%). (Low yield is due to solubility issues during the loading of the mixture on the column.) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.44 – 7.39 (m, 2H), 7.36 – 7.25 (m, 6H), 7.14 – 7.04 (m, 2H), 6.82 – 6.71 (bs, 1H), 4.32 – 4.14 (m, 1H), 3.72 – 3.53 (m, 2H), 3.35 (dd, *J* = 14.0, 4.5 Hz, 1H), 3.08 (dd, *J* = 14.0, 7.7 Hz, 1H), 2.82 – 2.66 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 170.76, 168.62, 135.99, 129.53, 128.63, 127.27, 126.06, 121.38, 65.45, 38.50, 34.71, 34.04. **IR**: 2920, 2111, 1754, 1662, 1529, 1493, 1195, 1165, 1148 cm^{-1}. **HRMS** (FD+, $[M]^+$) calc. for $C_{18}H_{18}N_4O_3$ 338.1379, found 338.1341.

Spectral data of new compounds

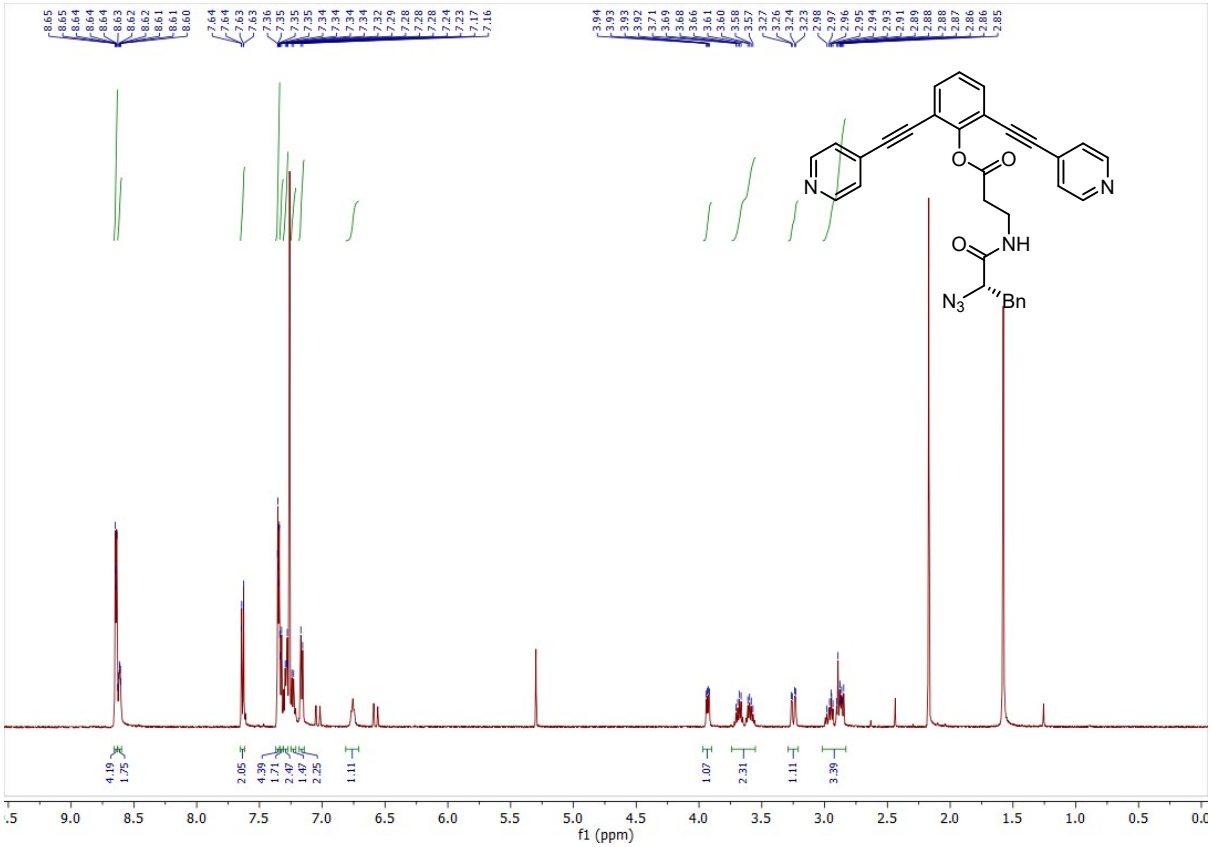


Figure S3: ^{1}H NMR of compound 1a.

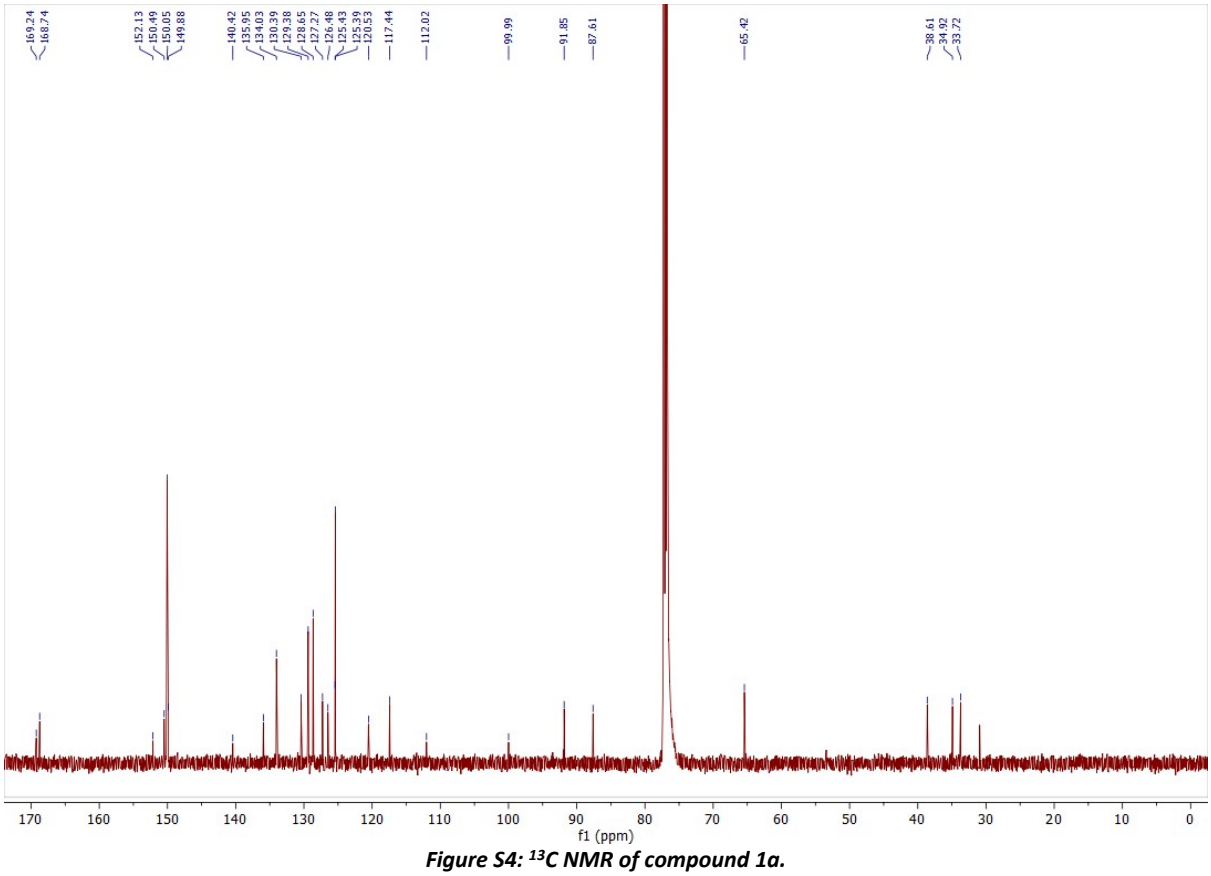


Figure S4: ^{13}C NMR of compound 1a.

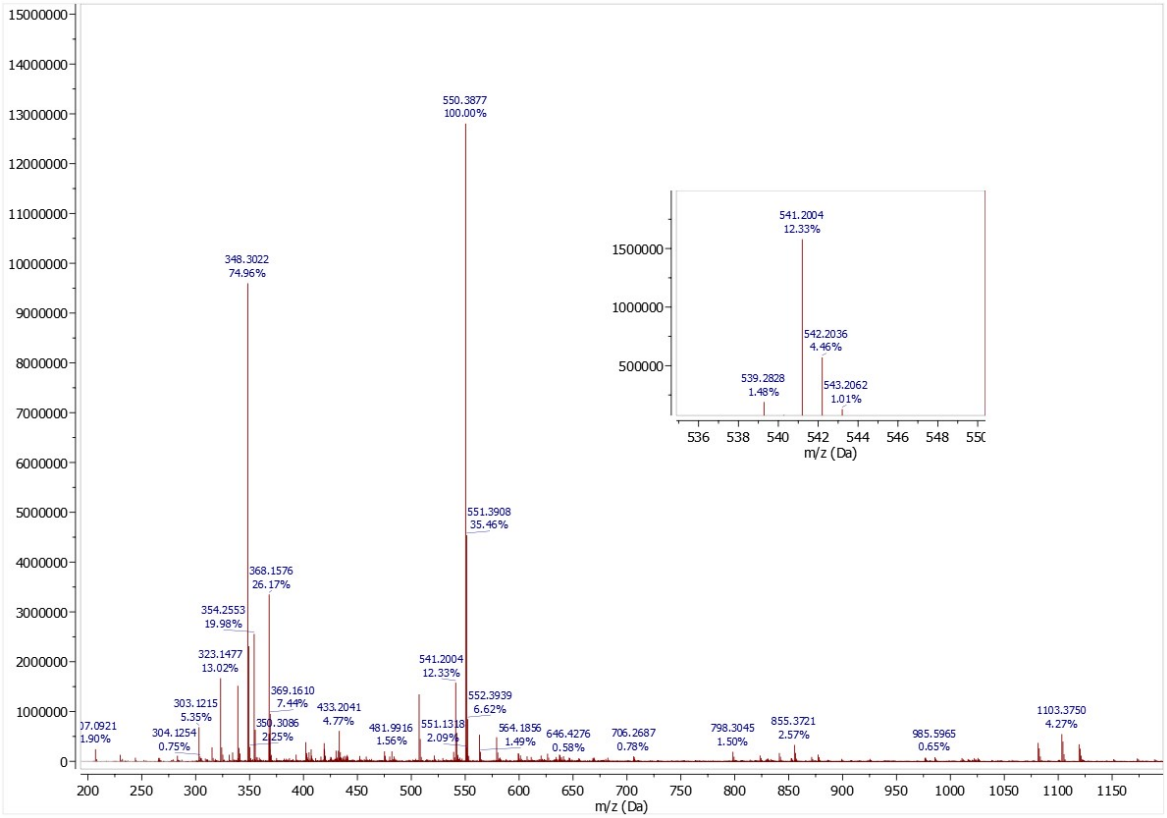


Figure S5: HRMS (ESI) spectrum of compound 1a. m/z 550.3877 originates from an impurity (see LC-MS results below).

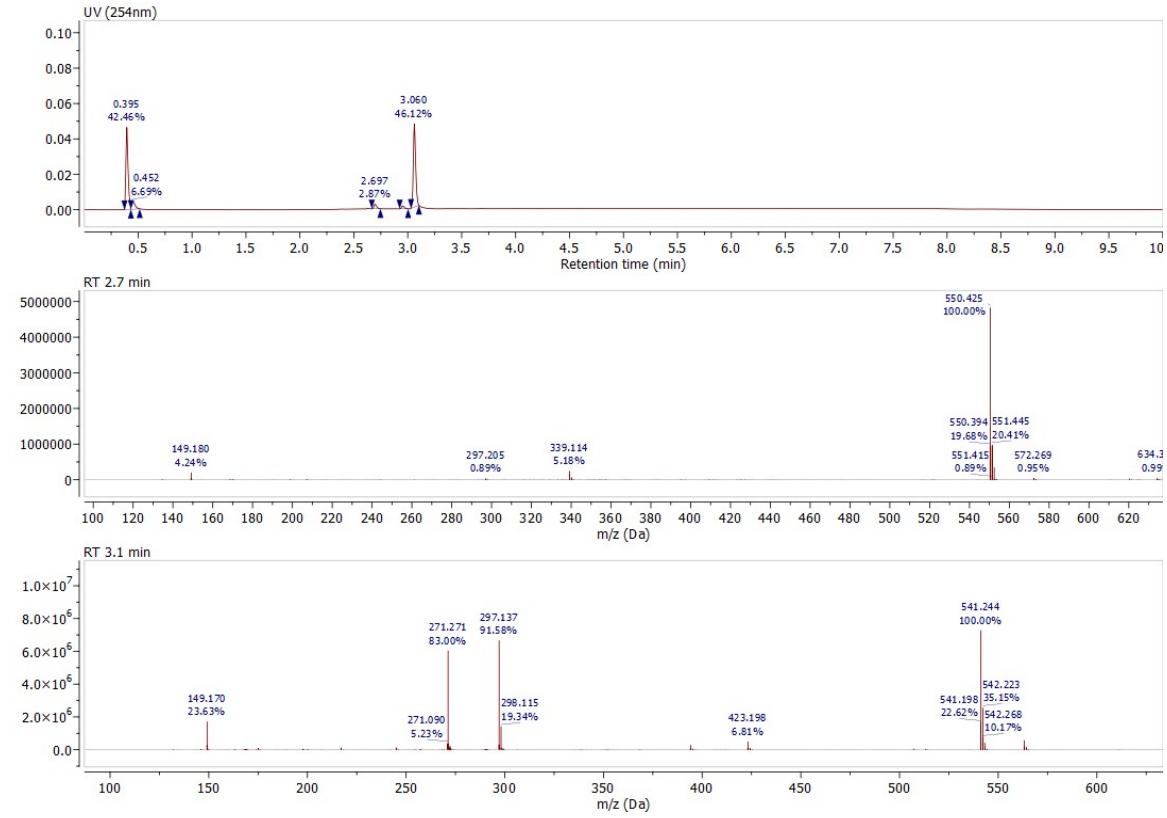


Figure S6: LC-MS traces (top: UV, 254 nm) and MS spectra of the peaks at RT 2.7 (middle: impurity, m/z 550.425) and RT 3.1 minutes (bottom: compound 1a, m/z 541.244).

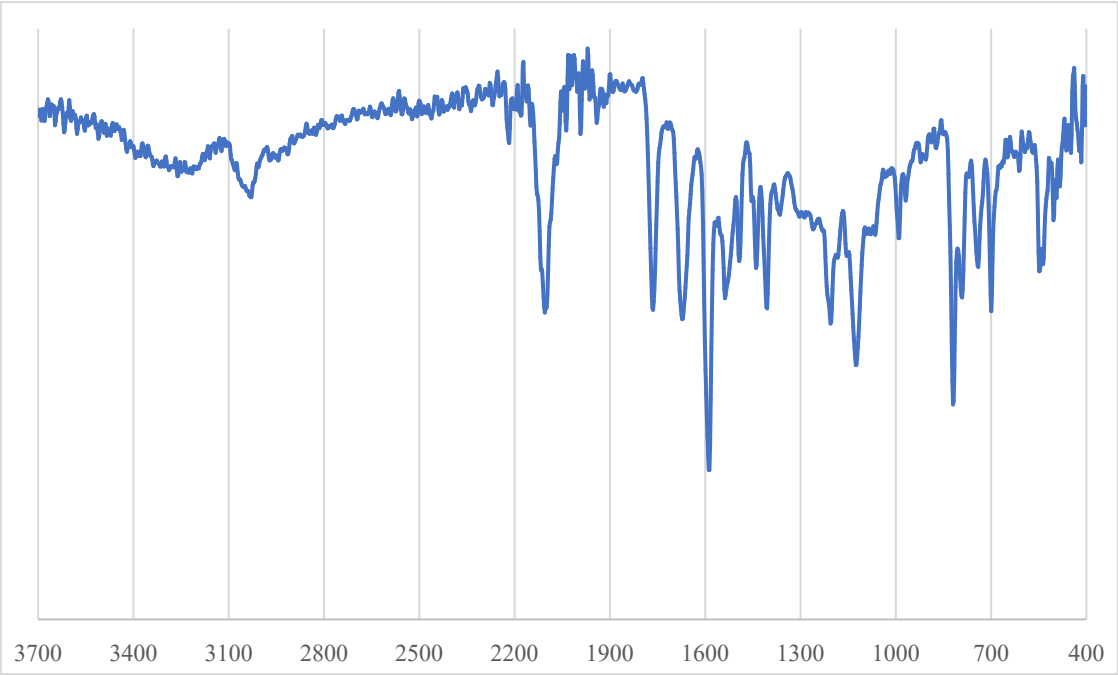


Figure S7: IR spectrum of compound 1a.

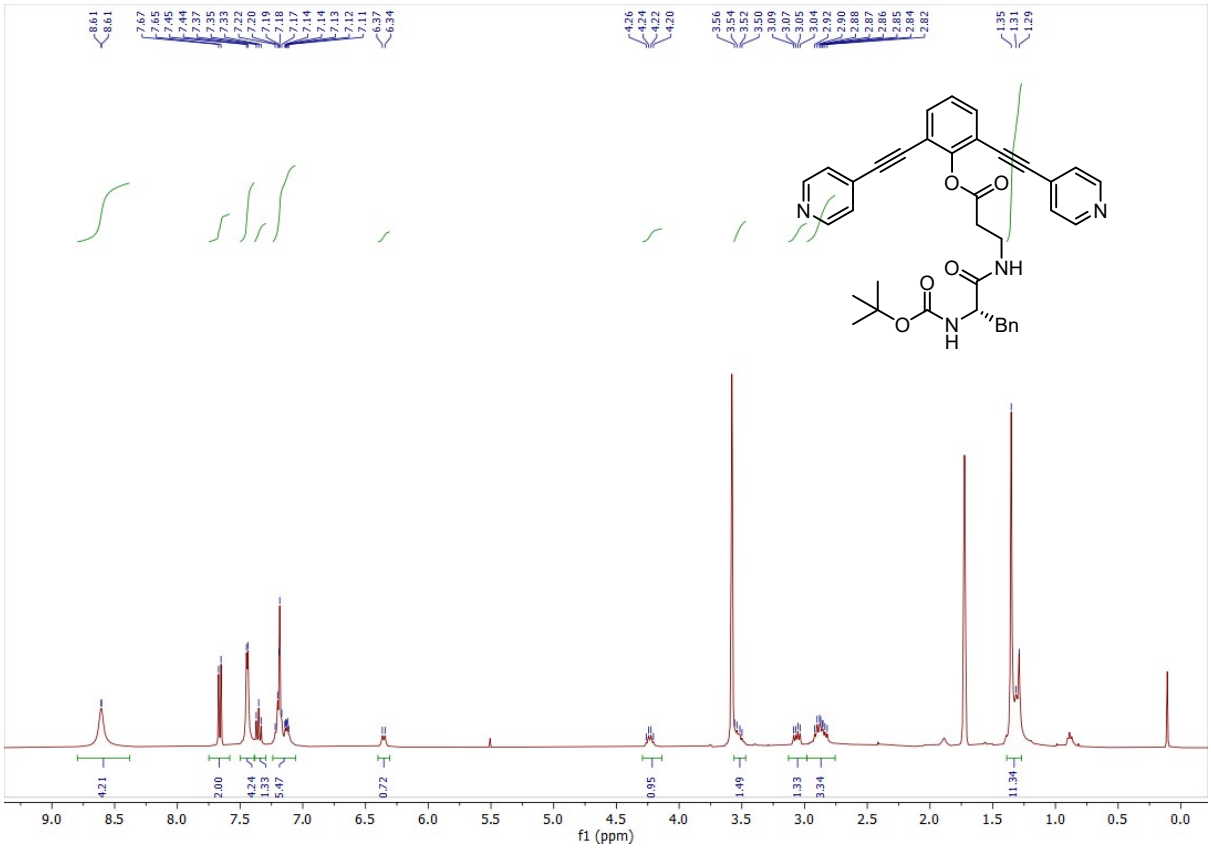


Figure S8: ^{1}H NMR of compound 1b.

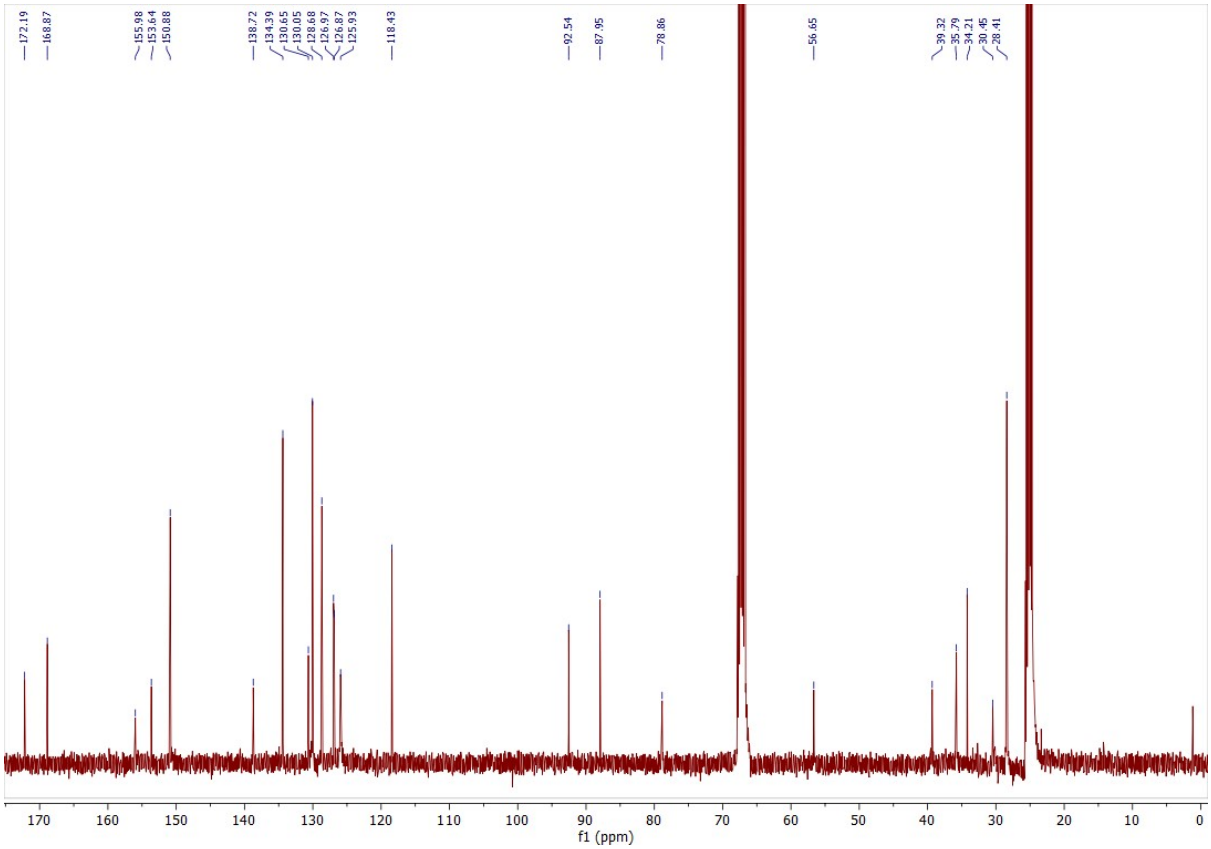


Figure S9: ^{13}C NMR of compound 1b.

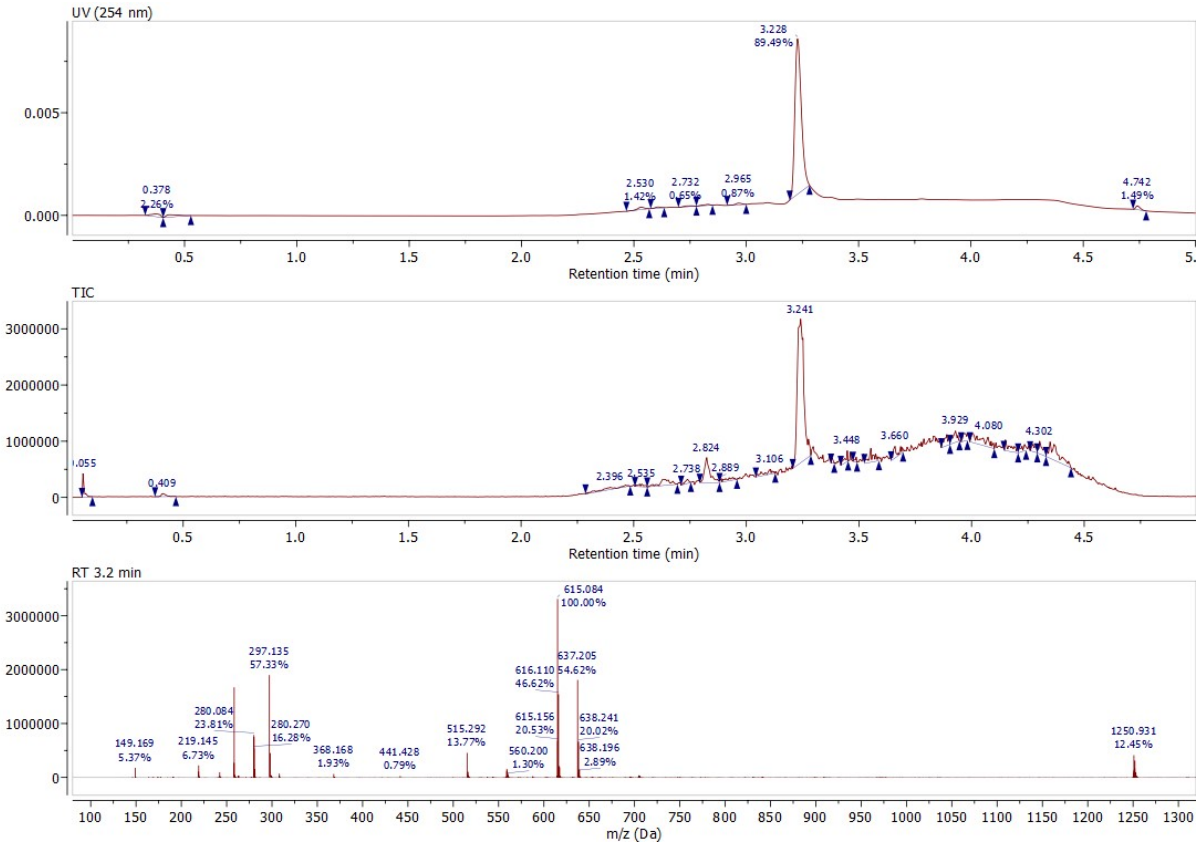


Figure S10: LC-MS traces of compound 1b (top: UV (254 nm), middle: TIC, bottom: ESI spectrum at RT 3.2 min).

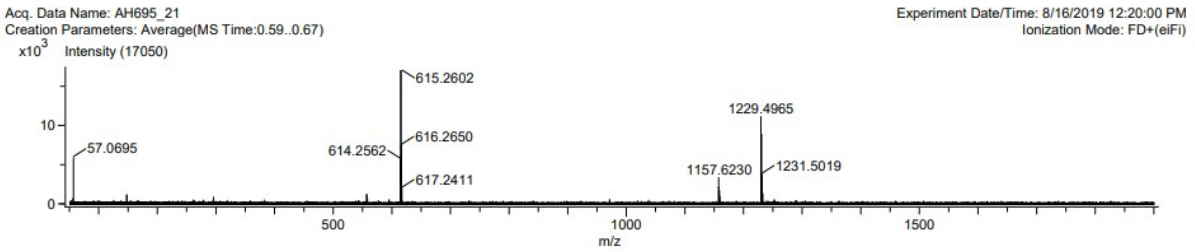


Figure S11: HRMS of compound 1b.

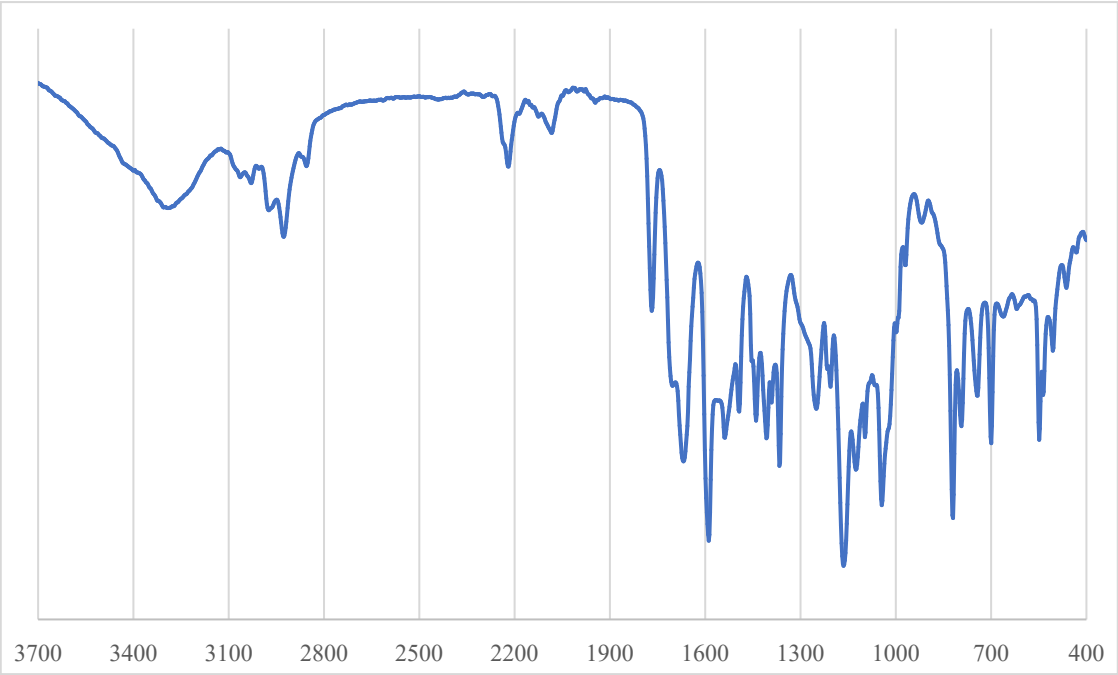


Figure S12: IR spectrum of compound 1b.

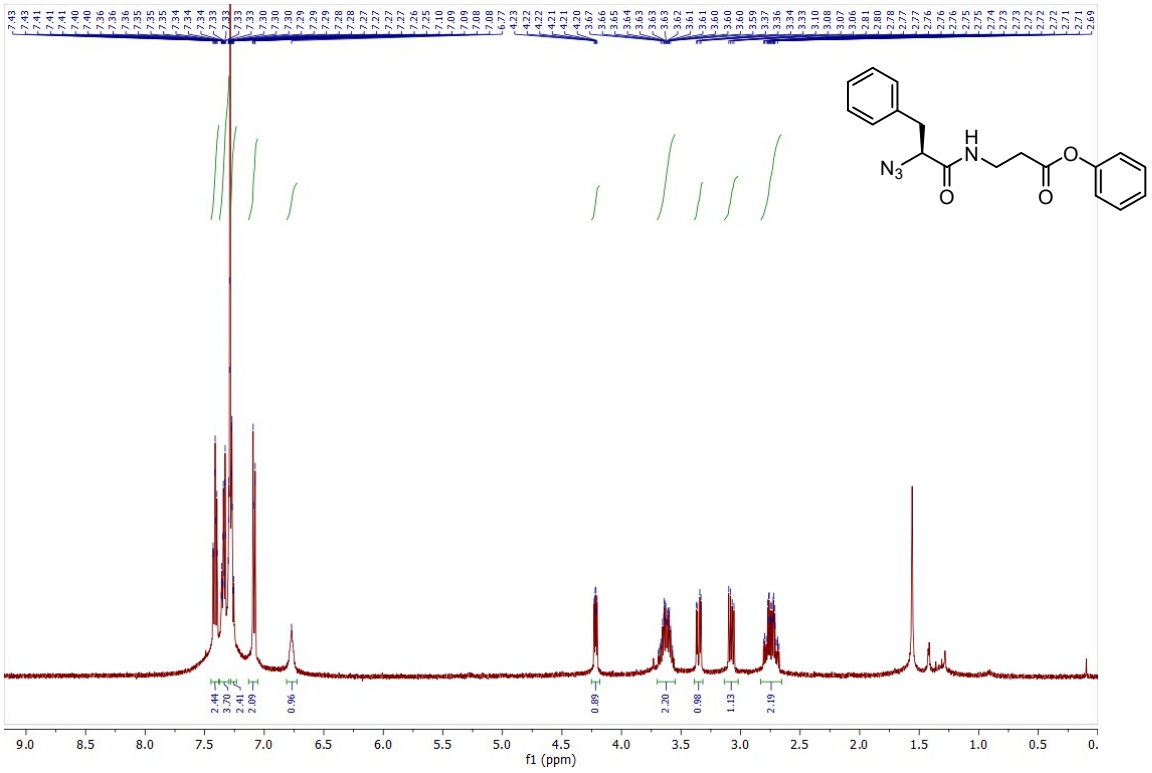


Figure S13: ^{1}H NMR of compound 1c.

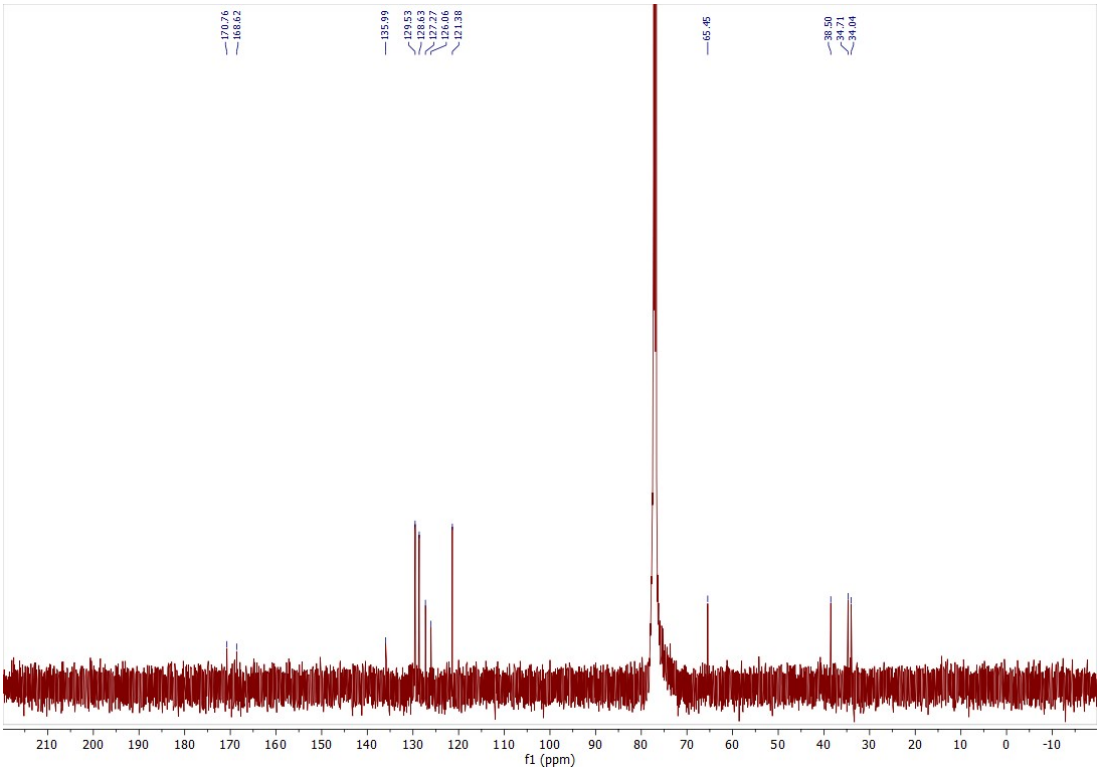


Figure S14: ^{13}C NMR of compound 1c.

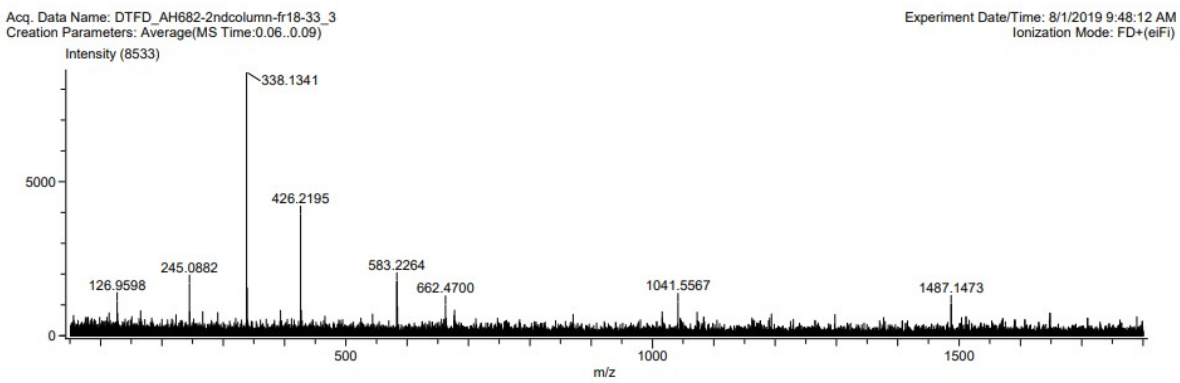


Figure S15: HRMS of compound 1c.

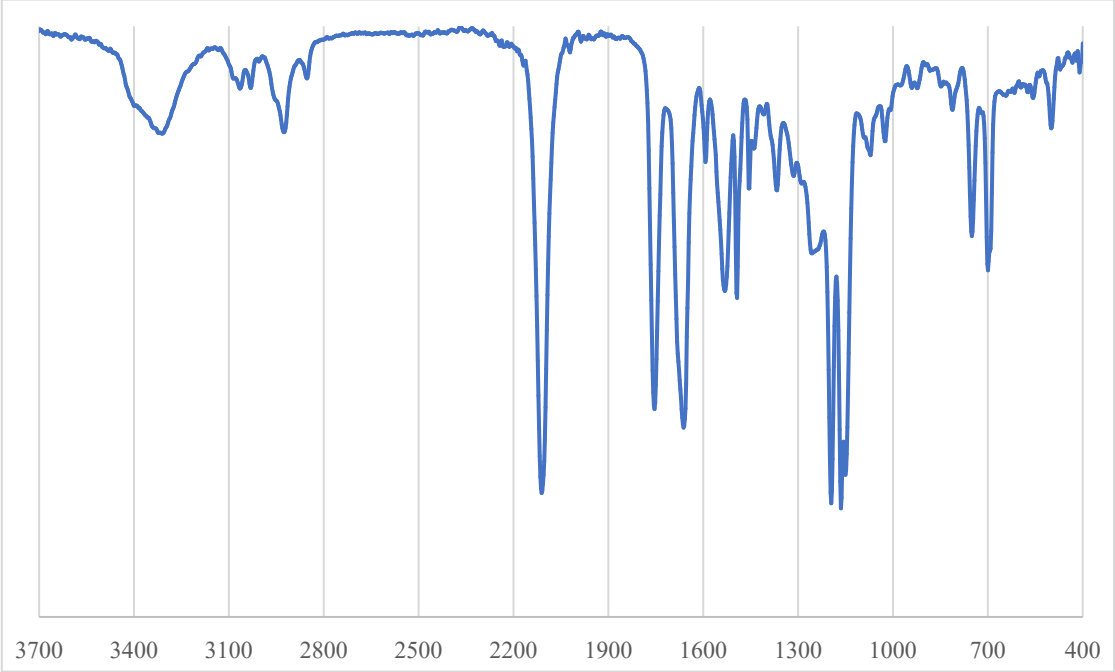


Figure S16: IR spectrum of compound 1c.

Computational details

DFT studies were performed on full atomic models using TURBOMOLE 7.3[6] coupled to the PQS Baker optimiser[7] via the BOpt package.[8] All geometries were fully optimised as minima at the BP86[9] / def2-TZVP[10] level of theory on an m4 integration grid, using Grimme's zero damping dispersion corrections.[11] All minima contained no imaginary vibrations in the frequency analysis of the Hessian matrix. Energy output was reported in Hartree and was converted to kcal mol^{-1} by multiplication with 627.5.

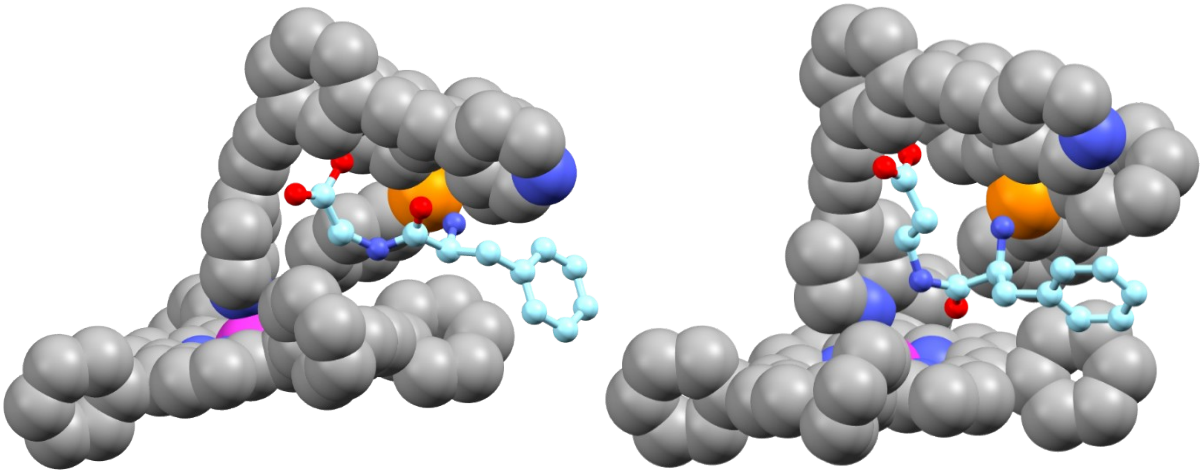


Figure S17: Calculated structures of transoid (A) and cisoid (B) isomers of iminophosphorane intermediate 3-ZnTPP (Turbomole, BP86, def2-TZVP).

Gibbs free energies of the calculated structures.

Amide rotation	Amide rotation	Energy (Eh)	N-C distance (Å)
3	Cisoid	-2715.26250	6.18
3	Transoid	-2715.25444	6.51
3-ZnTPP (**2**)	Cisoid	-6407.96363	4.07
3-ZnTPP (**2**)	Transoid	-6407.97517	6.38

3 cisoid xyz

-2715.26250 Eh

H	6.390000	-2.936000	-2.287000
C	5.438000	-2.451000	-2.071000
C	3.007000	-1.209000	-1.536000
C	4.414000	-3.178000	-1.465000
C	5.263000	-1.106000	-2.389000
C	4.037000	-0.455000	-2.123000
C	3.182000	-2.561000	-1.174000
H	4.558000	-4.222000	-1.190000
H	6.069000	-0.531000	-2.844000
C	2.151000	-3.203000	-0.447000
C	3.852000	0.924000	-2.389000
C	1.235000	-3.606000	0.253000
C	3.719000	2.121000	-2.589000
C	0.179000	-4.005000	1.109000
C	-0.546000	-3.043000	1.843000
C	-0.189000	-5.355000	1.276000
C	-1.236000	-5.662000	2.145000
C	-1.573000	-3.464000	2.684000
H	-0.294000	-1.987000	1.768000
H	0.335000	-6.140000	0.732000
H	-1.536000	-6.704000	2.286000
H	-2.133000	-2.727000	3.264000
C	3.603000	3.511000	-2.851000
C	2.726000	4.332000	-2.117000
C	4.377000	4.118000	-3.863000
C	4.234000	5.485000	-4.088000
C	2.670000	5.690000	-2.431000
H	2.102000	3.937000	-1.312000
H	5.069000	3.523000	-4.459000
H	4.823000	5.973000	-4.870000
H	1.995000	6.343000	-1.871000
N	-1.929000	-4.750000	2.847000
N	3.399000	6.278000	-3.395000
O	1.827000	-0.576000	-1.205000
C	0.659000	-0.992000	-1.850000
O	0.659000	-1.653000	-2.855000
C	-0.560000	-0.514000	-1.097000
H	-1.116000	-1.432000	-0.850000
H	-1.189000	0.052000	-1.800000
C	-0.294000	0.283000	0.178000
H	0.414000	-0.271000	0.815000
H	-1.235000	0.369000	0.733000
N	0.217000	1.617000	-0.102000
H	1.029000	1.656000	-0.720000
C	0.029000	2.771000	0.619000
C	-0.943000	2.724000	1.810000
H	-1.615000	1.853000	1.699000
O	0.657000	3.795000	0.339000
N	-0.178000	2.694000	3.037000
C	-1.869000	3.965000	1.807000
H	-2.326000	4.068000	0.810000
H	-1.248000	4.852000	1.988000
C	-2.924000	3.777000	2.863000
C	-4.752000	3.119000	4.909000
C	-2.706000	4.194000	4.184000
C	-4.087000	3.042000	2.583000
C	-4.996000	2.715000	3.593000
C	-3.607000	3.867000	5.199000
H	-1.808000	4.770000	4.409000
H	-4.274000	2.711000	1.558000
H	-5.894000	2.145000	3.353000
H	-3.412000	4.190000	6.223000
H	-5.454000	2.859000	5.702000
P	0.506000	1.489000	3.774000
C	1.349000	2.169000	5.234000
C	2.542000	3.206000	7.542000
C	2.463000	1.531000	5.797000
C	0.836000	3.331000	5.828000
C	1.435000	3.847000	6.977000
C	3.056000	2.049000	6.950000
H	2.884000	0.643000	5.322000
H	-0.020000	3.821000	5.366000
H	1.038000	4.756000	7.433000
H	3.928000	1.554000	7.381000
H	3.010000	3.613000	8.440000
C	-0.632000	0.220000	4.466000
C	-2.513000	-1.506000	5.639000
C	-2.005000	0.406000	4.243000
C	-0.213000	-0.825000	5.308000
C	-1.148000	-1.686000	5.884000
C	-2.939000	-0.455000	4.823000
H	-2.351000	1.258000	3.657000
H	0.844000	-0.947000	5.548000
H	-0.812000	-2.494000	6.535000
H	-4.002000	-0.285000	4.647000
H	-3.241000	-2.180000	6.091000
C	1.833000	0.612000	2.854000
C	3.965000	-0.475000	1.389000
C	2.650000	1.441000	2.063000
C	2.083000	-0.769000	2.884000
C	3.149000	-1.307000	2.158000
C	3.704000	0.898000	1.330000
H	2.436000	2.511000	2.012000
H	1.443000	-1.435000	3.462000
H	3.329000	-2.382000	2.181000
H	4.316000	1.545000	0.701000
H	4.791000	-0.899000	0.816000

3 transoid xyz

-2715.25444 Eh

C	6.991000	0.214000	-2.951000
H	8.021000	0.238000	-3.306000
C	4.351000	0.147000	-2.078000
C	6.447000	-0.986000	-2.495000
C	6.241000	1.390000	-2.933000
C	4.904000	1.378000	-2.483000
C	5.115000	-1.036000	-2.039000
H	7.044000	-1.898000	-2.478000
H	6.677000	2.334000	-3.257000
C	4.522000	-2.191000	-1.471000
C	4.104000	2.539000	-2.347000
C	3.908000	-3.070000	-0.889000
C	3.324000	3.438000	-2.078000
C	3.164000	-4.027000	-0.156000
C	1.756000	-4.070000	-0.241000
C	3.785000	-4.937000	0.724000
C	2.988000	-5.810000	1.462000
C	1.060000	-4.983000	0.549000
H	1.226000	-3.395000	-0.912000
H	4.869000	-4.944000	0.830000
H	3.453000	-6.518000	2.154000
H	-0.032000	-5.018000	0.508000
C	2.361000	4.393000	-1.667000
C	1.087000	3.958000	-1.248000
C	2.628000	5.775000	-1.609000
C	1.633000	6.628000	-1.131000
C	0.170000	4.901000	-0.789000
H	0.813000	2.904000	-1.261000
H	3.595000	6.167000	-1.923000
H	1.822000	7.704000	-1.072000
H	-0.816000	4.564000	-0.458000
N	1.646000	-5.847000	1.395000
N	0.421000	6.221000	-0.718000
O	3.055000	0.142000	-1.599000
C	2.065000	-0.443000	-2.394000
O	2.283000	-0.903000	-3.485000
C	0.734000	-0.373000	-1.693000
H	0.165000	-1.271000	-1.971000
H	0.186000	0.486000	-2.111000
C	0.829000	-0.209000	-0.174000
H	1.399000	0.704000	0.058000
H	1.376000	-1.057000	0.261000
N	-0.470000	-0.138000	0.479000
H	-0.609000	-0.679000	1.333000
C	-1.224000	0.994000	0.418000
C	-2.246000	1.140000	1.580000
H	-3.153000	0.592000	1.258000
O	-1.073000	1.855000	-0.457000
N	-1.784000	0.497000	2.773000
C	-2.654000	2.638000	1.698000
H	-3.278000	2.887000	0.827000
H	-1.759000	3.269000	1.611000
C	-3.365000	2.968000	2.982000
C	-4.664000	3.604000	5.401000
C	-2.727000	3.742000	3.961000
C	-4.664000	2.508000	3.240000
C	-5.310000	2.822000	4.437000
C	-3.368000	4.062000	5.160000
H	-1.709000	4.094000	3.781000
H	-5.175000	1.899000	2.491000
H	-6.322000	2.458000	4.620000
H	-2.846000	4.653000	5.914000
H	-5.165000	3.844000	6.339000
P	-0.631000	0.633000	3.819000
C	0.869000	1.649000	3.499000
C	3.216000	3.096000	2.943000
C	2.027000	1.464000	4.278000
C	0.912000	2.559000	2.433000
C	2.078000	3.278000	2.156000
C	3.188000	2.187000	4.006000
H	2.028000	0.728000	5.084000
H	0.045000	2.707000	1.793000
H	2.091000	3.970000	1.313000
H	4.078000	2.031000	4.617000
H	4.128000	3.652000	2.722000
C	-1.278000	1.130000	5.457000
C	-2.435000	1.776000	7.928000
C	-2.603000	0.758000	5.740000
C	-0.545000	1.844000	6.415000
C	-1.126000	2.172000	7.642000
C	-3.173000	1.072000	6.972000
H	-3.188000	0.263000	4.963000
H	0.472000	2.173000	6.200000
H	-0.554000	2.742000	8.376000
H	-4.206000	0.789000	7.176000
H	-2.887000	2.034000	8.887000
C	0.067000	-1.048000	4.042000
C	0.845000	-3.749000	4.009000
C	1.133000	-1.476000	3.229000
C	-0.584000	-1.984000	4.860000
C	-0.196000	-3.326000	4.841000
C	1.516000	-2.817000	3.212000
H	1.668000	-0.755000	2.610000
H	-1.402000	-1.664000	5.506000
H	-0.715000	-4.047000	5.474000
H	2.337000	-3.140000	2.569000
H	1.128000	-4.801000	3.967000

3 cisoid ZnTPP xyz

-6407.96363 Eh

H	7.588000	0.844000	-2.601000
C	6.552000	0.623000	-2.344000
C	3.906000	0.057000	-1.705000
C	6.166000	-0.700000	-2.124000
C	5.635000	1.667000	-2.221000
C	4.294000	1.402000	-1.883000
C	4.830000	-1.004000	-1.797000
H	6.890000	-1.511000	-2.197000
H	5.947000	2.701000	-2.364000
C	4.365000	-2.315000	-1.498000
C	3.332000	2.396000	-1.585000
C	3.822000	-3.359000	-1.172000
C	2.410000	3.070000	-1.155000
C	2.954000	-4.425000	-0.806000
C	2.253000	-5.154000	-1.789000
C	2.624000	-4.678000	0.541000
C	1.565000	-5.532000	0.833000
C	1.221000	-6.002000	-1.399000
H	2.478000	-5.013000	-2.845000
H	3.154000	-4.166000	1.342000
H	1.225000	-5.703000	1.855000
H	0.633000	-6.551000	-2.135000
C	1.341000	3.767000	-0.541000
C	0.368000	3.059000	0.200000
C	1.220000	5.170000	-0.596000
C	0.169000	5.782000	0.084000
C	-0.627000	3.780000	0.857000
H	0.402000	1.971000	0.284000
H	1.942000	5.762000	-1.158000
H	0.058000	6.869000	0.049000
H	-1.365000	3.249000	1.461000
N	0.851000	-6.162000	-0.115000
N	-0.746000	5.119000	0.812000
C	0.895000	-9.350000	1.889000
C	1.873000	-10.380000	1.595000
C	1.729000	-10.699000	0.274000
C	0.678000	-9.853000	-0.254000
N	0.186000	-9.052000	0.749000
C	0.719000	-8.737000	3.149000
C	0.310000	-9.801000	-1.616000
C	-0.580000	-8.872000	-2.196000
C	-0.816000	-8.728000	-3.618000
C	-1.622000	-7.634000	-3.782000
C	-1.928000	-7.132000	-2.458000
N	-1.284000	-7.903000	-1.517000
C	-2.737000	-6.009000	-2.174000
C	-3.091000	-5.569000	-0.879000
C	-4.053000	-4.520000	-0.608000
C	-4.126000	-4.389000	0.749000
C	-3.201000	-5.348000	1.319000
N	-2.604000	-6.063000	0.307000
C	-2.862000	-5.417000	2.686000
C	-1.865000	-6.251000	3.233000
C	-1.594000	-6.386000	4.647000
C	-0.582000	-7.296000	4.778000
C	-0.232000	-7.733000	3.443000
N	-1.023000	-7.079000	2.525000
H	2.588000	-10.791000	2.300000
H	2.299000	-11.424000	-0.298000
H	-0.411000	-9.371000	-4.392000
H	-1.979000	-7.213000	-4.716000
H	-4.610000	-3.968000	-1.358000
H	-4.738000	-3.691000	1.310000
H	-2.127000	-5.869000	5.438000
H	-0.139000	-7.670000	5.696000
C	-3.497000	-4.426000	3.600000
C	-4.628000	-2.470000	5.286000
C	-2.690000	-3.457000	4.223000
C	-4.881000	-4.399000	3.838000
C	-5.441000	-3.428000	4.672000
C	-3.249000	-2.489000	5.058000
H	-1.620000	-3.465000	4.022000
H	-5.515000	-5.150000	3.366000
H	-6.518000	-3.424000	4.848000
H	-2.602000	-1.738000	5.513000
C	-3.242000	-5.197000	-3.317000
C	-4.162000	-3.613000	-5.456000
C	-2.831000	-3.858000	-3.448000
C	-4.129000	-5.724000	-4.269000
C	-4.584000	-4.939000	-5.330000
C	-3.286000	-3.074000	-4.510000
H	-2.156000	-3.435000	-2.700000
H	-4.469000	-6.755000	-4.161000
H	-5.279000	-5.363000	-6.057000
H	-2.954000	-2.038000	-4.599000
C	0.972000	-10.781000	-2.529000
C	2.227000	-12.641000	-4.231000
C	0.643000	-12.144000	-2.467000
C	1.943000	-10.365000	-3.454000
C	2.565000	-11.286000	-4.299000
C	1.264000	-13.067000	-3.312000
H	-0.109000	-12.473000	-1.749000
H	2.210000	-9.308000	-3.500000
H	3.321000	-10.946000	-5.009000
H	0.992000	-14.122000	-3.253000
C	1.572000	-9.200000	4.280000
C	3.179000	-10.040000	6.439000
C	2.449000	-8.305000	4.916000
C	1.512000	-10.523000	4.748000
C	2.308000	-10.939000	5.817000
C	3.246000	-8.720000	5.985000
H	2.504000	-7.275000	4.559000
H	0.823000	-11.221000	4.270000
H	2.241000	-11.969000	6.171000

H	3.926000	-8.011000	6.461000
Zn	-0.963000	-7.331000	0.465000
H	3.800000	-10.366000	7.274000
H	-5.067000	-1.712000	5.935000
H	-4.519000	-3.000000	-6.285000
H	2.712000	-13.361000	-4.891000
O	2.623000	-0.246000	-1.319000
C	1.584000	-0.131000	-2.259000
O	1.744000	0.321000	-3.363000
C	0.342000	-0.719000	-1.655000
H	-0.458000	-0.696000	-2.404000
H	0.063000	-0.131000	-0.765000
C	0.671000	-2.144000	-1.188000
H	1.479000	-2.070000	-0.449000
H	1.062000	-2.710000	-2.045000
N	-0.430000	-2.950000	-0.646000
H	-0.308000	-3.938000	-0.880000
C	-0.809000	-2.883000	0.694000
C	-1.260000	-1.546000	1.294000
H	-1.662000	-1.837000	2.279000
O	-0.857000	-3.910000	1.368000
N	-0.155000	-0.599000	1.392000
C	-2.455000	-1.020000	0.454000
H	-3.083000	-1.892000	0.209000
H	-2.084000	-0.619000	-0.497000
C	-3.275000	0.007000	1.182000
C	-4.735000	1.923000	2.640000
C	-3.277000	1.353000	0.793000
C	-4.027000	-0.369000	2.307000
C	-4.746000	0.580000	3.034000
C	-4.002000	2.307000	1.515000
H	-2.691000	1.658000	-0.075000
H	-4.034000	-1.412000	2.629000
H	-5.314000	0.266000	3.911000
H	-3.982000	3.353000	1.203000
H	-5.298000	2.666000	3.207000
P	0.698000	-0.338000	2.702000
C	2.425000	0.014000	2.222000
C	5.038000	0.541000	1.334000
C	3.347000	-1.031000	2.053000
C	2.830000	1.327000	1.938000
C	4.130000	1.588000	1.501000
C	4.643000	-0.770000	1.611000
H	3.058000	-2.056000	2.279000
H	2.132000	2.155000	2.059000
H	4.423000	2.611000	1.269000
H	5.342000	-1.595000	1.469000
H	6.045000	0.743000	0.967000
C	0.201000	1.112000	3.705000
C	-0.685000	3.260000	5.270000
C	-1.127000	1.546000	3.620000
C	1.083000	1.752000	4.593000
C	0.641000	2.824000	5.367000
C	-1.569000	2.617000	4.401000
H	-1.812000	1.054000	2.931000
H	2.117000	1.412000	4.675000
H	1.333000	3.324000	6.047000
H	-2.604000	2.947000	4.313000
H	-1.026000	4.104000	5.871000
C	0.724000	-1.711000	3.922000
C	0.649000	-3.897000	5.691000
C	1.016000	-3.012000	3.472000
C	0.384000	-1.525000	5.272000
C	0.350000	-2.612000	6.149000
C	0.980000	-4.094000	4.349000
H	1.214000	-3.188000	2.418000
H	0.131000	-0.531000	5.639000
H	0.070000	-2.454000	7.191000
H	1.156000	-5.106000	3.982000
H	0.592000	-4.752000	6.365000

3 transoid ZnTPP xyz

-6407.97517 Eh

H	6.957000	1.383000	-2.899000
C	5.986000	0.945000	-2.669000
C	3.493000	-0.177000	-2.092000
C	5.913000	-0.364000	-2.194000
C	4.829000	1.702000	-2.837000
C	3.561000	1.159000	-2.539000
C	4.665000	-0.942000	-1.895000
H	6.816000	-0.954000	-2.041000
H	4.884000	2.733000	-3.183000
C	4.507000	-2.246000	-1.367000
C	2.377000	1.934000	-2.593000
C	4.121000	-3.314000	-0.922000
C	1.342000	2.576000	-2.532000
C	3.325000	-4.456000	-0.652000
C	2.556000	-4.973000	-1.716000
C	3.114000	-4.992000	0.634000
C	2.089000	-5.917000	0.808000
C	1.553000	-5.888000	-1.438000
H	2.692000	-4.586000	-2.725000
H	3.693000	-4.640000	1.487000
H	1.848000	-6.336000	1.786000
H	0.898000	-6.269000	-2.221000
C	0.132000	3.305000	-2.399000
C	-0.865000	2.873000	-1.501000
C	-0.113000	4.480000	-3.138000
C	-1.320000	5.151000	-2.947000
C	-2.031000	3.630000	-1.393000
H	-0.720000	1.971000	-0.902000
H	0.628000	4.854000	-3.845000
H	-1.531000	6.064000	-3.512000
H	-2.817000	3.316000	-0.700000
N	1.290000	-6.323000	-0.193000
N	-2.277000	4.751000	-2.094000
C	0.662000	-9.547000	1.801000
C	1.484000	-10.725000	1.604000
C	1.398000	-11.053000	0.281000
C	0.541000	-10.067000	-0.347000
N	0.115000	-9.165000	0.598000
C	0.444000	-8.899000	3.037000
C	0.259000	-10.017000	-1.732000
C	-0.416000	-8.968000	-2.394000
C	-0.645000	-8.894000	-3.824000
C	-1.213000	-7.676000	-4.077000
C	-1.366000	-7.010000	-2.801000
N	-0.896000	-7.826000	-1.797000
C	-1.886000	-5.713000	-2.625000
C	-2.158000	-5.099000	-1.385000
C	-2.808000	-3.815000	-1.231000
C	-2.966000	-3.609000	0.110000
C	-2.386000	-4.752000	0.791000
N	-1.892000	-5.633000	-0.145000
C	-2.308000	-4.914000	2.197000
C	-1.628000	-5.972000	2.847000
C	-1.654000	-6.219000	4.272000
C	-0.855000	-7.303000	4.508000
C	-0.357000	-7.748000	3.225000
N	-0.848000	-6.930000	2.233000
H	2.063000	-11.226000	2.373000
H	1.889000	-11.875000	-0.231000
H	-0.407000	-9.674000	-4.540000
H	-1.518000	-7.267000	-5.035000
H	-3.110000	-3.161000	-2.042000
H	-3.407000	-2.743000	0.593000
H	-2.223000	-5.650000	4.998000
H	-0.658000	-7.786000	5.459000
C	-2.971000	-3.888000	3.050000
C	-4.148000	-1.835000	4.589000
C	-2.239000	-3.208000	4.039000
C	-4.325000	-3.544000	2.876000
C	-4.902000	-2.526000	3.635000
C	-2.816000	-2.191000	4.798000
H	-1.193000	-3.465000	4.184000
H	-4.920000	-4.081000	2.135000
H	-5.946000	-2.257000	3.473000
H	-2.205000	-1.651000	5.520000
C	-2.151000	-4.906000	-3.855000
C	-2.604000	-3.321000	-6.133000
C	-1.080000	-4.298000	-4.527000
C	-3.452000	-4.715000	-4.343000
C	-3.677000	-3.929000	-5.476000
C	-1.304000	-3.506000	-5.656000
H	-0.064000	-4.434000	-4.153000
H	-4.287000	-5.187000	-3.822000
H	-4.694000	-3.791000	-5.845000
H	-0.459000	-3.029000	-6.155000
C	0.763000	-11.147000	-2.565000
C	1.715000	-13.291000	-4.124000
C	0.249000	-12.443000	-2.393000
C	1.764000	-10.944000	-3.529000
C	2.236000	-12.006000	-4.302000
C	0.719000	-13.505000	-3.166000
H	-0.530000	-12.607000	-1.647000
H	2.175000	-9.942000	-3.661000
H	3.019000	-11.831000	-5.042000
H	0.304000	-14.504000	-3.024000
C	1.066000	-9.479000	4.258000
C	2.243000	-10.527000	6.596000
C	1.951000	-8.705000	5.030000
C	0.778000	-10.787000	4.684000
C	1.362000	-11.306000	5.841000
C	2.536000	-9.223000	6.186000
H	2.181000	-7.688000	4.706000
H	0.078000	-11.389000	4.103000
H	1.119000	-12.321000	6.160000

H	3.227000	-8.608000	6.766000
Zn	-0.645000	-7.277000	0.192000
H	2.699000	-10.933000	7.500000
H	-4.593000	-1.006000	5.139000
H	-2.781000	-2.702000	-7.014000
H	2.083000	-14.121000	-4.728000
O	2.264000	-0.658000	-1.701000
C	1.668000	-1.727000	-2.362000
O	2.099000	-2.195000	-3.390000
C	0.428000	-2.147000	-1.615000
H	-0.009000	-3.011000	-2.127000
H	-0.271000	-1.302000	-1.688000
C	0.688000	-2.435000	-0.113000
H	1.627000	-1.946000	0.190000
H	0.798000	-3.514000	0.040000
N	-0.369000	-1.989000	0.779000
H	-0.859000	-2.680000	1.340000
C	-0.748000	-0.687000	0.867000
C	-1.676000	-0.355000	2.040000
H	-2.282000	-1.250000	2.287000
O	-0.291000	0.176000	0.107000
N	-0.908000	0.063000	3.188000
C	-2.642000	0.771000	1.597000
H	-3.129000	0.455000	0.661000
H	-2.023000	1.648000	1.359000
C	-3.683000	1.108000	2.629000
C	-5.617000	1.668000	4.605000
C	-3.352000	1.866000	3.764000
C	-5.002000	0.654000	2.496000
C	-5.965000	0.935000	3.469000
C	-4.305000	2.134000	4.748000
H	-2.333000	2.237000	3.866000
H	-5.276000	0.062000	1.620000
H	-6.987000	0.574000	3.342000
H	-4.027000	2.721000	5.625000
H	-6.365000	1.886000	5.370000
P	0.541000	-0.248000	3.707000
C	1.945000	0.136000	2.594000
C	4.015000	0.925000	0.874000
C	3.145000	-0.592000	2.548000
C	1.794000	1.262000	1.768000
C	2.824000	1.655000	0.916000
C	4.172000	-0.203000	1.683000
H	3.286000	-1.459000	3.194000
H	0.851000	1.809000	1.781000
H	2.686000	2.516000	0.262000
H	5.094000	-0.783000	1.640000
H	4.815000	1.225000	0.195000
C	0.757000	0.835000	5.154000
C	1.047000	2.433000	7.434000
C	-0.376000	1.248000	5.873000
C	2.033000	1.222000	5.584000
C	2.176000	2.022000	6.720000
C	-0.228000	2.044000	7.009000
H	-1.361000	0.942000	5.521000
H	2.916000	0.908000	5.023000
H	3.171000	2.330000	7.045000
H	-1.111000	2.364000	7.564000
H	1.160000	3.060000	8.320000
C	0.905000	-1.932000	4.368000
C	1.104000	-4.547000	5.400000
C	1.218000	-3.015000	3.525000
C	0.706000	-2.184000	5.736000
C	0.807000	-3.479000	6.248000
C	1.309000	-4.309000	4.039000
H	1.375000	-2.851000	2.459000
H	0.465000	-1.360000	6.408000
H	0.643000	-3.653000	7.313000
H	1.501000	-5.147000	3.371000
H	1.151000	-5.565000	5.786000

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