Supporting Information for

Insights on the Petasis Borono-Mannich Multicomponent Reaction Mechanism

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General

Chemicals and solvents were purchased from commercial sources and used without any further purification.

Petasis Borono-Mannich reactions

0.25 mmol of each reagent were dissolved in 2.5 mL of methanol (or toluene). The methanolic solutions were heated at 65 °C (90 °C for toluene) for four hours and aliquots taken from the solution to be analyzed by ESI(+)-MS(/MS) experiments. From the reaction mixture in methanol (using salicylaldehyde), some crystals formed. Some of them were suitable for single crystal X-ray analysis.

Mass Spectrometry experiments

ESI-MS analyses of the PBM reactions were performed using the 6550 iFunnel Q-TOF LC/MS system, constituted of an ESI source and a hybrid mass analyzer (quadrupole – time-of-flight). An aliquot of 10 μL of the reaction was diluted in 1 mL of methanol and the mass spectra was acquired in the positive ion mode in the *m/z* range of 100 to 1000. Source ionization conditions were: gas temp: 280 °C, drying gas: 11 L min^{-1}, nebulizer: 30 psi, sheath gas temp: 300 °C, sheath gas flow: 12 L min^{-1}, V_{cap}: 3000 V, nozzle: 0 V, fragmentor: 150 V. For MS/MS analyses, the ions of interest were selected in the quadrupole analyzer and transferred to the collision cell where the collision energy was adjusted from 10 to 40 V, depending on fragmentation of the ion of interest. Then, the ion products were analyzed by TOF analyzer in the *m/z* range of 50 until a value above that of the precursor ion. The software Agilent MassHunter (Agilent, Santa Clara, CA, USA) was used to acquire and process the data.

Theoretical calculations

All electronic structure calculation performed in this work were done within Kohn-Sham Density Functional Theory (DFT) formalism[1,2] using the PBE1PBE functional combined with the large cc-pVDZ basis set[3] for geometries optimizations. The transitions states were optimized using the Berny algorithm.[4] All structures were optimized and frequency calculations were performed to ensure the absence of any imaginary frequencies on local minima, and the presence of only one imaginary frequency on transition states; and were also used to compute zero-point vibrational energy (ZPVE). ZPVE were calculated at 298.15 K and 1 atm. Methanol has been considered as the reaction media (explicit treatment) for calculated structures. Both geometrical and electronic theoretical calculations were carried out using Gaussian 09 program suite.[5]

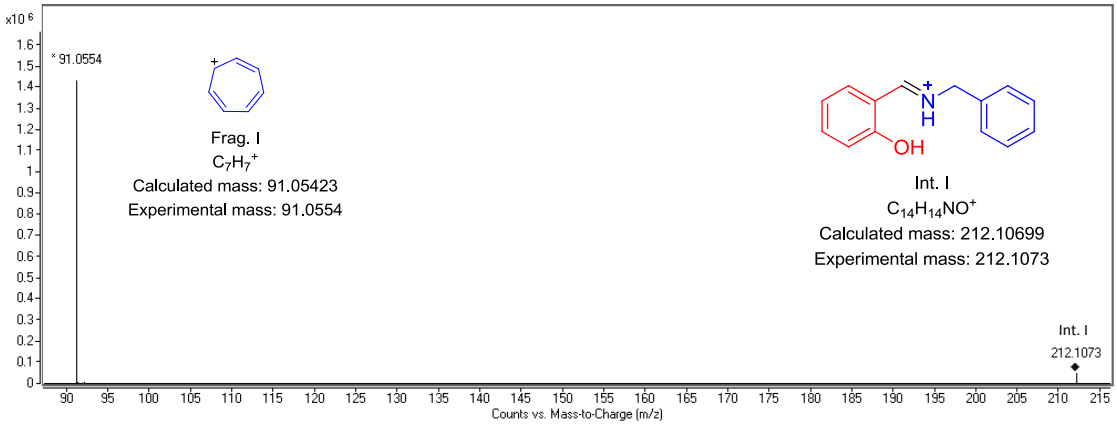

Figure S1. ESI(+)-MS/MS of the ion of *m/z* 212 observed during PBM reaction from benzylamine, phenylboronic acid and salicylaldehyde.

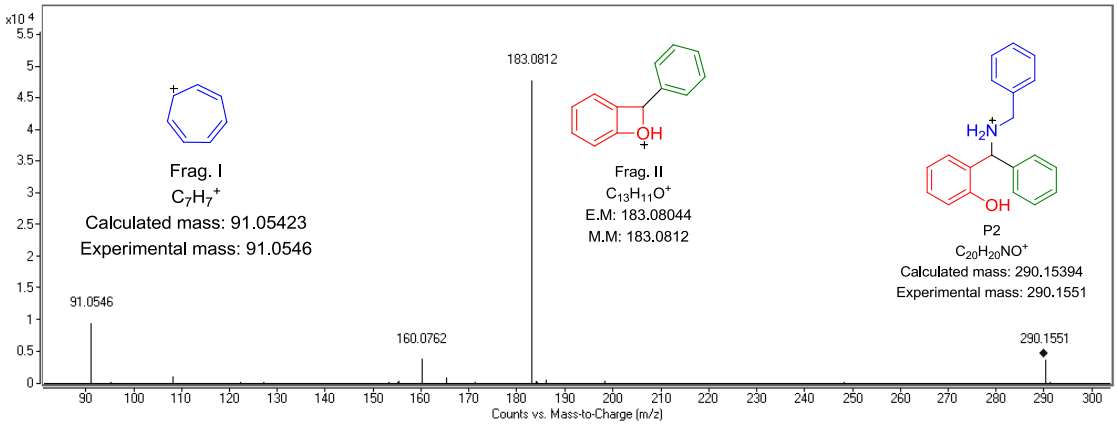

Figure S2. ESI(+)-MS/MS of the ion of *m/z* 290 observed during PBM reaction from benzylamine, phenylboronic acid and salicylaldehyde.

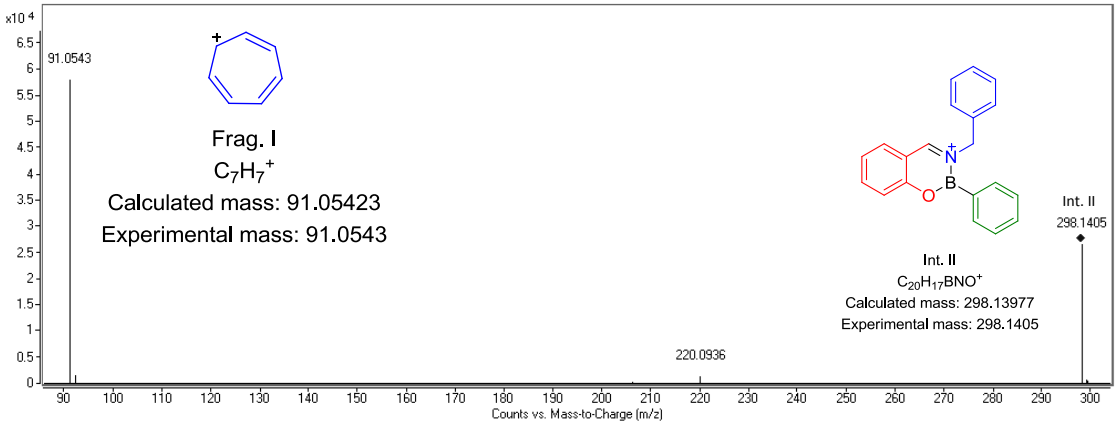

Figure S3. ESI(+)-MS/MS of the ion of *m/z* 298 observed during PBM reaction from benzylamine, phenylboronic acid and salicylaldehyde.

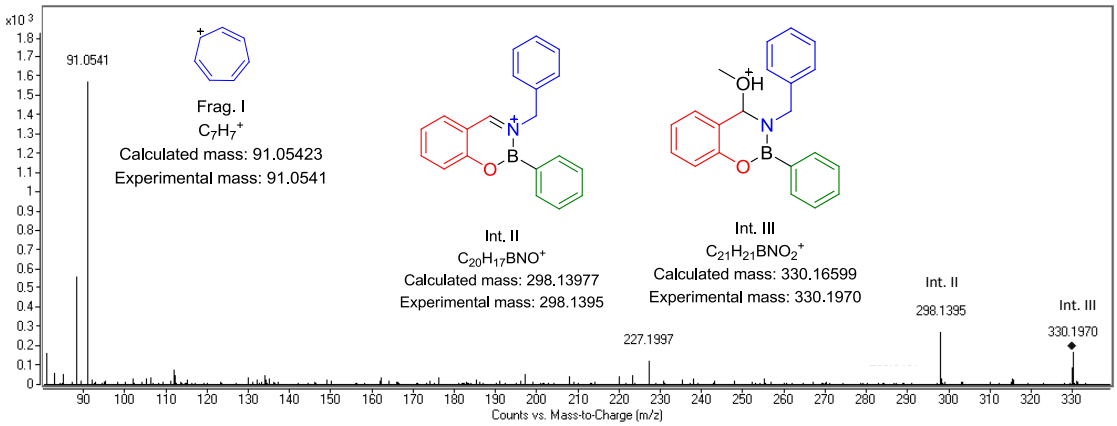

Figure S4. ESI(+)-MS/MS of the ion of *m/z* 330 observed during PBM reaction from benzylamine, phenylboronic acid and salicylaldehyde.

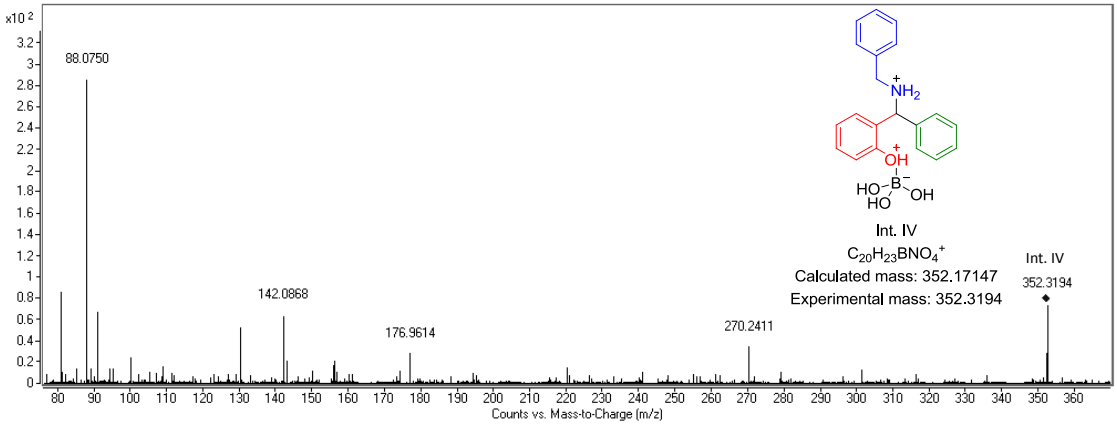

Figure S5. ESI(+)-MS/MS of the ion of *m/z* 352 observed during PBM reaction from benzylamine, phenylboronic acid and salicylaldehyde.

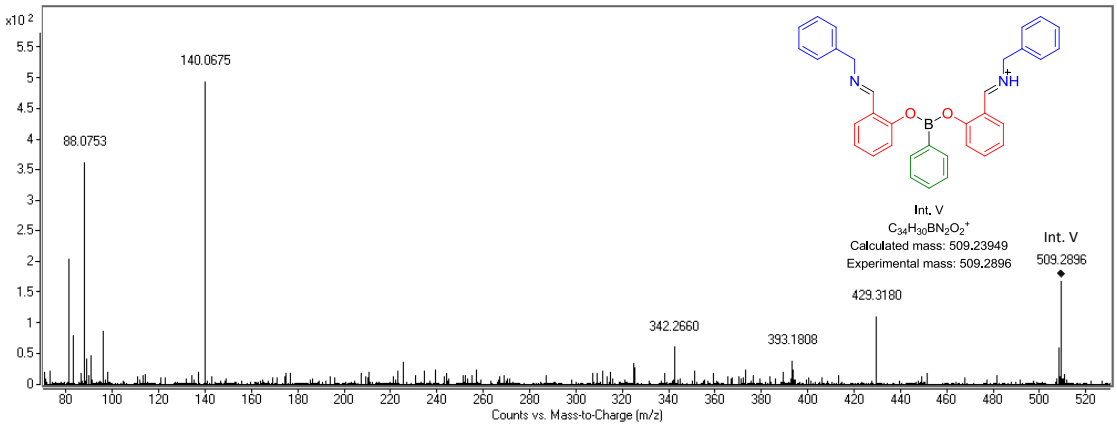

Figure S6. ESI(+)-MS/MS of the ion of *m/z* 509 observed during PBM reaction from benzylamine, phenylboronic acid and salicylaldehyde.

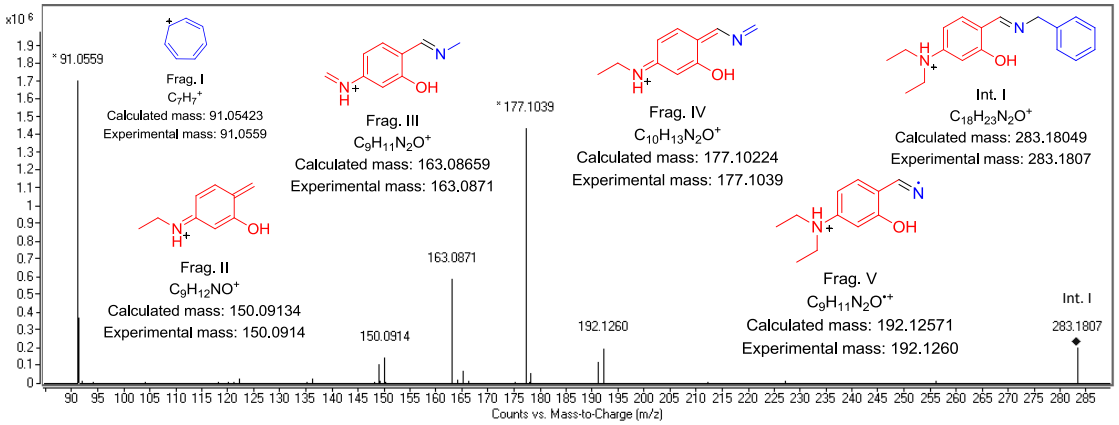

Figure S7. ESI(+)-MS/MS of the ion of *m/z* 283 observed during PBM reaction from benzylamine, phenylboronic acid and 4-diethyl-salicylaldehyde (charge-tagged aldehyde).

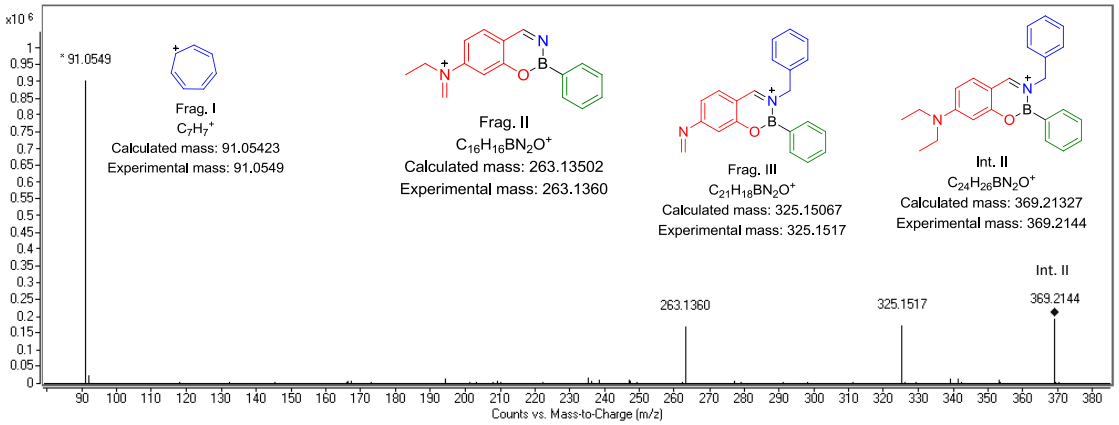

Figure S8. ESI(+)-MS/MS of the ion of *m/z* 369 observed during PBM reaction from benzylamine, phenylboronic acid and 4-diethyl-salicylaldehyde (charge-tagged aldehyde).

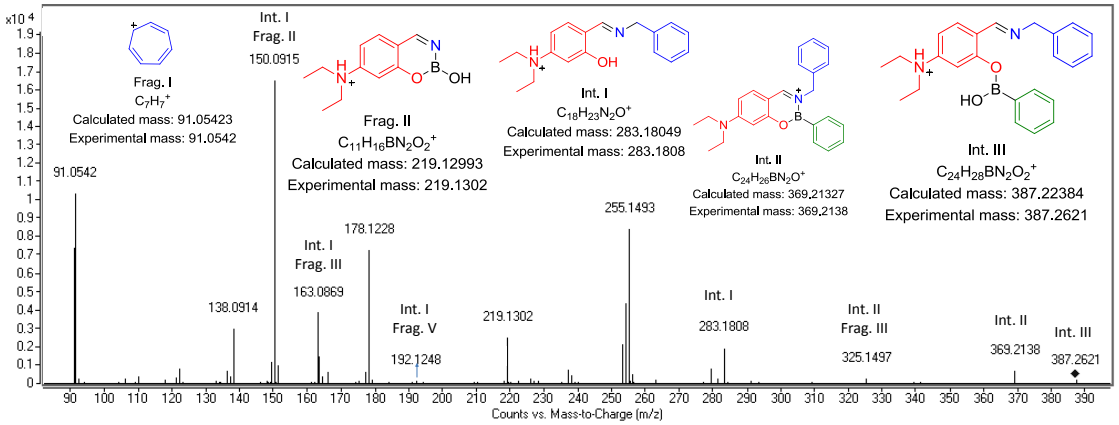

Figure S9. ESI(+)-MS/MS of the ion of *m/z* 387 observed during PBM reaction from benzylamine, phenylboronic acid and 4-diethyl-salicylaldehyde (charge-tagged aldehyde).

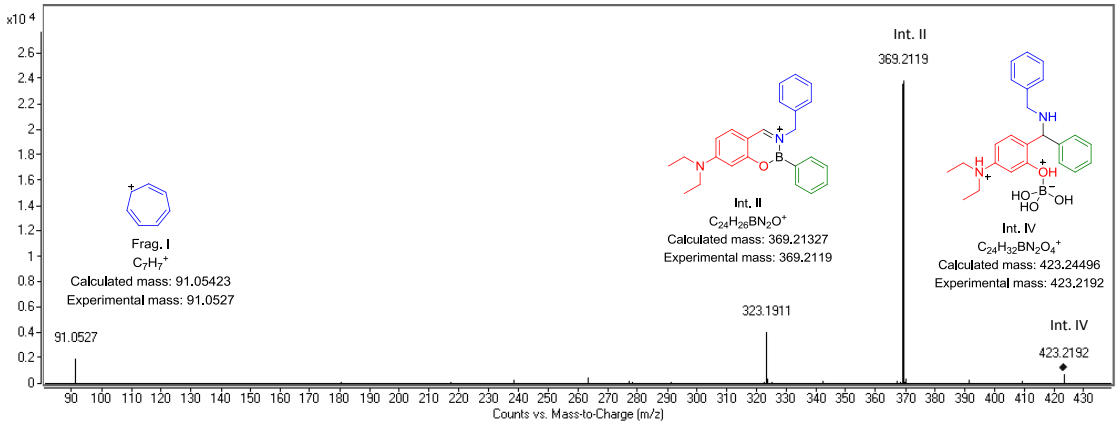

Figure S10. ESI(+)-MS/MS of the ion of *m/z* 423 observed during PBM reaction from benzylamine, phenylboronic acid and 4-diethyl-salicylaldehyde (charge-tagged aldehyde).

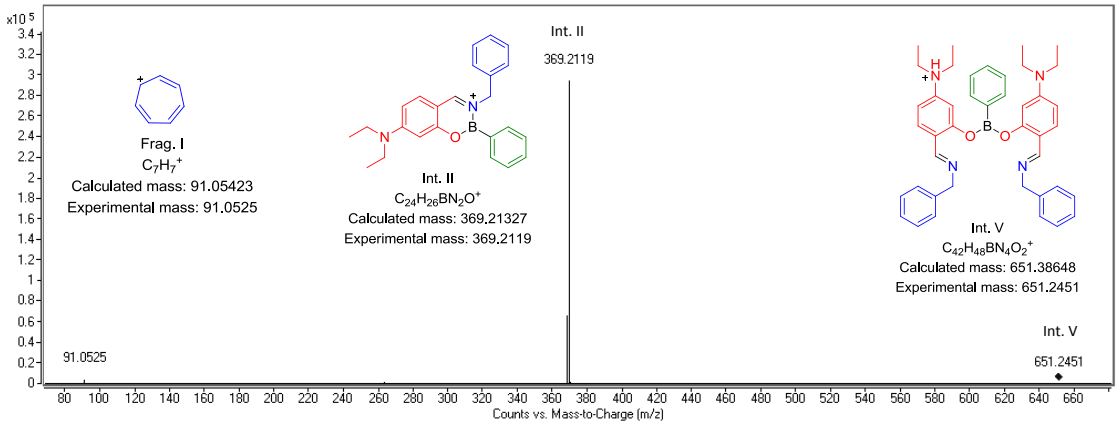

Figure S11. ESI(+)-MS/MS of the ion of *m/z* 651 observed during PBM reaction from benzylamine, phenylboronic acid and 4-diethyl-salicylaldehyde (charge-tagged aldehyde).

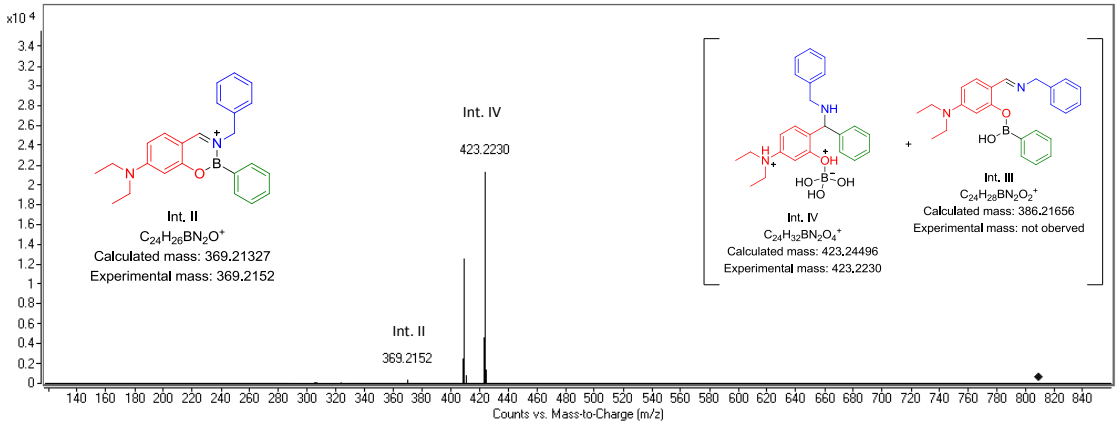

Figure S12. ESI(+)-MS/MS of the ion of *m/z* 809 observed during PBM reaction from benzylamine, phenylboronic acid and 4-diethyl-salicylaldehyde (charge-tagged aldehyde).

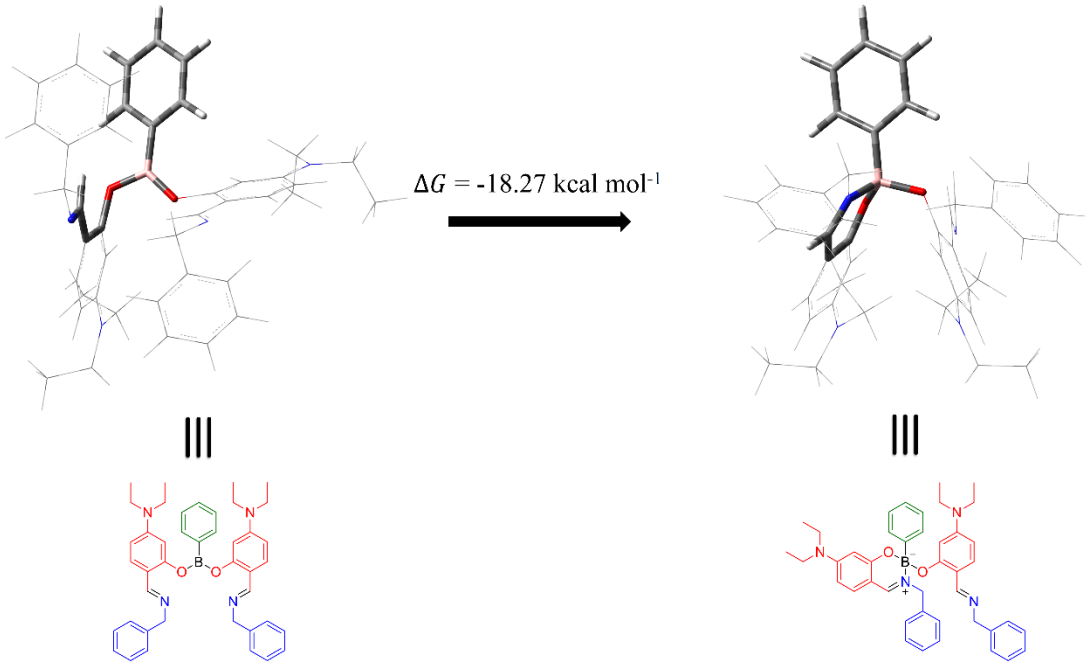

Figure S13. Formation of the cyclic intermediate in the PBM reaction. PBE1PBE/cc-pVDZ level of theory.

Table S1. X-ray diffraction data collection and refinement parameters.

Chemical formula	$C_{21}H_{20}NO_2B$
M (g mol^{-1})	329.19
Crystal system	Triclinic
Space group	*P-1*
Unit cell	
a (Å)	9.759(3)
b (Å)	10.000(3)
c (Å)	10.266(4)
α	107.921(2)
β	100.656(2)
γ	104.952(2)
V (Å^3)	882.11(5)
Z	2
Dc /g cm^{-3}	1.239
Index ranges	$-12 \le h \le 12$
	$-12 \le k \le 12$
	$-12 \le l \le 12$
Absorption coefficient /mm^{-1}	0.078
Absorption correction	multi-scan
Max/min transmission	0.9880 / 0.9773
Measured reflections	15422
Independent reflections / Rint	3675 / 0.0639
Refined parameters	232
R1 (F) / wR2 (F^2) (I > 2σ(I))	0.0536 / 0.1258
GooF	1.038
Largest diff. peak and hole (eÅ^{-3})	0.229 and -0.168
Deposit number CCDC	1060124

A

C	1.60554800	-2.60989000	0.00017900
C	1.47518500	-1.28531100	0.46656600
C	0.25518300	-0.61869200	0.50629700
C	-0.92426600	-1.26998300	0.06474300
C	-0.79350000	-2.60884400	-0.34015600
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H	2.33361000	-0.73641900	0.84720200
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H	0.43745600	-4.28991100	-0.77734000
C	-2.25662200	-0.68766900	0.00090200
O	0.20624700	0.60721200	1.06296100
C	2.99432100	-4.58655700	-0.47417800
H	2.06157500	-5.11570300	-0.24339500
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C	4.12713800	-5.33265600	0.21474500
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H	4.05524500	-1.64483700	1.93822900
H	5.08960700	-3.06230500	1.66789500
H	5.59948500	-1.45916700	1.07475900
N	2.84896300	-3.20920000	-0.04190000
B	0.54926000	1.81059600	0.31621100
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H	-1.26820200	1.66796300	-0.42988900
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C	3.15275200	2.05365700	0.66263800
C	2.32771600	1.94364000	-1.58606700
C	4.46111600	2.12502600	0.18639200
H	2.97277200	2.07896500	1.74118200
C	3.63347600	2.01264100	-2.07473100
H	1.48631600	1.87480500	-2.28067900
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H	-0.42045600	1.86877300	3.08368400
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H	1.59413300	4.88896600	-1.15364100
H	0.21896000	5.84177700	-1.80553300
H	1.01948400	6.35225200	-0.29574300

B

C	1.72054500	-2.48958200	0.04890100
C	1.53261400	-1.17268700	0.51703900
C	0.28608100	-0.55677800	0.54891300
C	-0.86243300	-1.25854800	0.10076600
C	-0.67533200	-2.59205900	-0.30095600
C	0.56432100	-3.20164100	-0.35147200
H	2.36613800	-0.58879000	0.90038600
H	-1.55039800	-3.16121400	-0.62764500
H	0.62738500	-4.21908900	-0.73173300
C	-2.21345000	-0.72743300	0.02980900
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H	2.28650000	-4.96931500	-0.22192600
H	3.36129000	-4.44251300	-1.52551200
C	4.34817500	-5.10261200	0.28272500
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O	-0.56311200	2.20340900	-0.59429600
H	-1.36593100	1.62952600	-0.35837700

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C	2.14956500	1.72685700	-1.64393200
C	4.38406700	2.27113700	-0.08297000
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C	3.41878200	1.73165300	-2.22429000
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C	-3.93721500	0.91387500	-0.08579900
H	-4.13728100	1.55375800	0.79135200
H	-4.03194000	1.57883900	-0.96148600
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C	-5.53549700	-0.71495000	1.00071700
C	-5.40082400	-0.67178100	-1.40024500
C	-6.48788500	-1.72980100	0.93183700
H	-5.21690800	-0.33361700	1.97467300
C	-6.35352200	-1.68600500	-1.47454100
H	-4.97616300	-0.25658700	-2.31828000
C	-6.89963100	-2.21786300	-0.30736500
H	-6.91384800	-2.13914800	1.85042200
H	-6.67449200	-2.06032000	-2.44908600
H	-7.64875800	-3.01040400	-0.36361500
O	0.43556700	3.00349400	1.49132400
H	0.00287600	3.94474500	0.83159600
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H	-0.00211900	1.95581100	3.21788000
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H	1.19829300	4.77086900	-1.13652900
H	-0.25027700	5.64303600	-1.73982700
H	0.58232400	6.21571800	-0.26770600

C

C	1.67908200	-2.53951600	-0.06627000
C	1.52903300	-1.22337300	0.41673000
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C	-0.87840500	-1.30371400	0.05599200
C	-0.73018500	-2.65932200	-0.32082200
C	0.49565200	-3.27226600	-0.38960200
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H	-1.62289800	-3.22625800	-0.59972400
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C	-2.17079900	-0.72580400	-0.02621200
O	0.14837200	0.58828900	1.05062000
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H	4.09376200	-4.59607600	-1.00179200
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H	3.81819900	-1.91580100	2.14727900
H	4.86464000	-3.31815300	1.81960800
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H	-1.67637900	1.27860800	-0.08089600
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C	4.45535500	1.97232800	-0.14317700
H	3.13772000	2.30372900	1.53565700
C	3.37338000	1.52237900	-2.24922200
H	1.21462400	1.49894100	-2.20938200
C	4.54320500	1.69221300	-1.50814000
H	5.36698000	2.12302900	0.44205000
H	3.43292900	1.31378300	-3.32103700
H	5.51945700	1.61814000	-1.99431500
C	-3.80537800	1.10160300	-0.10048300
H	-3.94305600	1.74777800	0.78191900
H	-3.83028200	1.76763700	-0.97808000
N	-2.46015000	0.54444500	-0.02114900
H	-3.01714600	-1.41412900	-0.13944500
C	-4.91574400	0.09179800	-0.17900800
C	-5.49418900	-0.42026000	0.98753300
C	-5.37821500	-0.36394800	-1.41816500
C	-6.51256100	-1.36834900	0.91788500
H	-5.14358300	-0.06798900	1.96115100
C	-6.39714000	-1.31163500	-1.49081000
H	-4.93668000	0.03250900	-2.33626200
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H	-6.95811100	-1.75543500	1.83648600
H	-6.75252000	-1.65365300	-2.46496100
H	-7.76659600	-2.55603600	-0.37802600
O	0.66083900	2.87573300	1.61365000
H	0.43906100	4.37385900	0.67047200
C	-0.37097000	2.83403900	2.56480100
H	-0.37912300	1.87333100	3.10815900

H	-0.21388600	3.64811600	3.29042200
H	-1.37016500	2.97378100	2.10658800
O	0.05786500	4.93880200	-0.04160100
H	-0.54667300	3.24091400	-0.56010700
C	1.11719000	5.54586100	-0.74430100
H	1.83868700	4.80957200	-1.14257400
H	0.68700400	6.10167200	-1.59175800
H	1.67147800	6.26861800	-0.11614500

D

C	3.53523600	0.52598700	0.18037300
C	2.80828700	-0.65589700	-0.03403300
C	1.40823500	-0.68625500	-0.06221500
C	0.68256600	0.50795800	0.11507900
C	1.40798800	1.67589600	0.37693700
C	2.79220200	1.70924100	0.40887400
H	3.30398800	-1.60951700	-0.20723800
H	0.85896700	2.60382100	0.56032000
H	3.28165100	2.65211800	0.64316000
C	-0.79376300	0.62705300	0.06693800
O	0.83304600	-1.87448500	-0.20228600
C	5.67544700	1.73398000	0.36703300
H	5.06994700	2.56579100	-0.01388000
H	5.84751200	1.93502700	1.44611800
C	7.00397000	1.75875700	-0.37424600
H	6.85268700	1.62160100	-1.45583200
H	7.49441300	2.73135700	-0.21545100
H	7.70060700	0.98236800	-0.02446000
C	5.61400300	-0.73567900	0.47435500
H	6.48874200	-0.49683100	1.10237700
H	4.96001600	-1.36253500	1.10268000
C	6.06279800	-1.52350300	-0.75040900
H	5.20834000	-1.78256000	-1.39291000
H	6.77363900	-0.94748200	-1.36062900
H	6.55565200	-2.45996500	-0.44384900
N	4.92241600	0.50933900	0.17745100
B	-0.61558000	-2.06162200	-0.31120900
O	-0.95572700	-3.43455700	0.08457600
C	-1.41491100	-1.10628700	0.89150500
C	-2.83217300	-1.17931800	0.81915900
C	-0.86441700	-1.05262300	2.20021400
C	-3.63489700	-1.17521200	1.95540700
H	-3.30338700	-1.32027600	-0.15656100
C	-1.65560300	-1.03429800	3.33789500
H	0.22244700	-1.00651100	2.30669500
C	-3.04797600	-1.08807300	3.21728700
H	-4.72018100	-1.25501100	1.86047800
H	-1.19530000	-0.98482700	4.32721200
H	-3.67471300	-1.07384300	4.11228400
C	-2.74837000	1.33453200	-1.17822900
H	-3.12105100	1.17725600	-2.20245100
H	-3.43089900	0.78228600	-0.50414800
N	-1.40969200	0.78932300	-1.12677700
H	-1.20617800	1.28980700	0.83778500
C	-2.80237400	2.80644000	-0.83763900
C	-1.83881100	3.69188800	-1.33414700
C	-3.83722800	3.31112900	-0.04693100
C	-1.91674600	5.05297700	-1.05153300
H	-1.01698300	3.30091700	-1.93824100
C	-3.91893600	4.67460700	0.23452900
H	-4.58763900	2.62650800	0.35755400
C	-2.95875700	5.54956900	-0.26785600
H	-1.15815200	5.73237700	-1.44643500
H	-4.73335700	5.05234600	0.85635200
H	-3.01819200	6.61694300	-0.04530500
O	-1.06478100	-1.75679900	-1.65471400
H	-1.19736900	0.01905100	-1.78137400
C	-0.11465700	-4.44633100	-0.42511300
H	-0.53547400	-5.42303000	-0.13680900
H	-0.03405100	-4.40692000	-1.52778900
H	0.90343700	-4.36703700	-0.00983700
H	-1.86277200	-2.28545300	-1.84335600
O	-3.22081200	-3.48943800	-1.35388600
H	-2.51943400	-3.65571300	-0.67678700
C	-3.53435600	-4.69557100	-2.00414800
H	-4.27274000	-4.47791600	-2.79072500
H	-2.65502300	-5.16405700	-2.48501400
H	-3.98466900	-5.43617400	-1.31664600

E

C	3.00193600	1.45330700	0.31394800
C	2.59513600	0.10796000	0.33649800
C	1.25253900	-0.25820800	0.38846000
C	0.22864300	0.69670300	0.43078900
C	0.64684500	2.03185900	0.40734500
C	1.97728400	2.42068600	0.35890500
H	3.31970800	-0.70378200	0.29201600
H	-0.12168100	2.80843200	0.44383000
H	2.20760400	3.48413600	0.39165500
C	-1.26653200	0.41691600	0.44542700
O	1.01183100	-1.60969700	0.46927700
C	4.74881100	3.17433000	0.16140100
H	3.96845100	3.71203500	-0.39286900
H	4.80155200	3.64217100	1.16817800
C	6.06409600	3.39081300	-0.57133200
H	6.01361400	2.98904100	-1.59477600
H	6.27517300	4.46915500	-0.63454500
H	6.91804700	2.92189800	-0.06007600

C	5.32295100	0.85627900	0.80966800
H	6.06902800	1.44172800	1.37371500
H	4.81736300	0.22380800	1.55784200
C	6.03095200	-0.02157900	-0.21517700
H	5.31194500	-0.62738500	-0.78677100
H	6.59958500	0.58259700	-0.93695800
H	6.73341100	-0.70673600	0.28598500
N	4.35066900	1.78253400	0.24827200
B	0.48215400	-2.38012200	-0.52969300
O	0.39794100	-3.74366300	-0.30620900
C	-3.20694700	0.61454500	-1.05426800
H	-3.47206700	0.30975600	-2.08126100
H	-3.81062100	-0.02734300	-0.38002600
N	-1.77751700	0.44110300	-0.91269700
H	-1.71763400	1.29452200	0.94318200
C	-3.64038600	2.05291900	-0.85875400
C	-2.84415300	3.10444300	-1.32596000
C	-4.85640100	2.35662200	-0.24153700
C	-3.26122500	4.42613200	-1.18827800
H	-1.88578800	2.86111900	-1.78968500
C	-5.27859700	3.67880900	-0.10480200
H	-5.48098400	1.54424800	0.14091900
C	-4.48183300	4.71886700	-0.57881300
H	-2.62907500	5.23615500	-1.56013900
H	-6.23169100	3.89716000	0.38234300
H	-4.80801600	5.75543500	-0.46916300
O	0.06119000	-1.87688600	-1.71855600
H	-1.39774600	-0.32628700	-1.46138700
C	0.76975000	-4.27780400	0.95578000
H	0.73326300	-5.37290800	0.87459000
H	1.78876700	-3.96741800	1.23173200
H	0.07236600	-3.94584300	1.73990400
H	-0.28692400	-2.60754900	-2.28300400
O	-0.71259000	-4.24776900	-2.74550500
H	-0.45190500	-4.45358500	-1.82753500
C	0.21549200	-4.87392100	-3.60824800
H	-0.03121900	-4.57440200	-4.63657400
H	1.25699100	-4.57061200	-3.39814500
H	0.15025500	-5.97481600	-3.54840700
C	-1.67219900	-0.77882800	1.30960300
C	-1.45233400	-0.72738900	2.69142500
C	-2.29340200	-1.91293200	0.78141400
C	-1.83226900	-1.77915000	3.51919400
H	-0.96879600	0.15419900	3.12117000
C	-2.67986300	-2.97001000	1.60749700
H	-2.47485600	-1.97610200	-0.29351700
C	-2.45189200	-2.90811900	2.97996000
H	-1.65017100	-1.71658000	4.59460700
H	-3.16613200	-3.84555900	1.17096200
H	-2.76005600	-3.73091800	3.62872500

Open form for the boron-containing intermediate (untagged)

C	-2.81512000	-1.59619400	-0.23430700
C	-2.31298200	-0.28305300	-0.11028100
C	-0.94941100	-0.02157400	-0.05744400
C	-0.00038500	-1.06697500	-0.09901000
C	-0.51868400	-2.36696600	-0.19844700
C	-1.87152800	-2.64835100	-0.26145500
H	-2.98419500	0.56851600	-0.06146800
H	0.19005200	-3.19919300	-0.22626000
H	-2.18861900	-3.68706900	-0.33138900
C	1.45455000	-0.93233700	-0.04348100
O	-0.48497100	1.24469400	0.09680400
C	-4.68434200	-3.18370000	-0.41254000
H	-5.68248400	-3.12515300	-0.87317900
H	-4.06645600	-3.76851000	-1.11455600
C	-4.78079700	-3.90985600	0.92541900
H	-5.46891800	-3.39395600	1.61149400
H	-5.15304900	-4.93612800	0.77827500
H	-3.79923800	-3.97069200	1.41861000
C	-5.12003200	-0.73628000	-0.31491900
H	-4.72475200	0.09505700	-0.92133200
H	-6.02603500	-1.08259600	-0.83628800
C	-5.49162700	-0.23600200	1.07731800
H	-5.97545100	-1.02578700	1.67129700
H	-4.60309700	0.10348400	1.63022900
H	-6.19218800	0.61095700	1.00492200
N	-4.16836000	-1.83066800	-0.34074700
B	-0.97611000	2.42961300	-0.38954100
O	-2.14605200	2.46012600	-1.09992800
H	-2.30430200	3.34022600	-1.45948200
C	-0.11488700	3.70121500	-0.09366400
C	1.22478200	3.55091400	0.30191800
C	-0.63066500	5.00045800	-0.21471600
C	2.01911700	4.66619400	0.55725200
H	1.62627600	2.53591900	0.38790100
C	0.15712100	6.11866700	0.04816100
H	-1.67745800	5.15439500	-0.50113800
C	1.48703500	5.95003600	0.43287800
H	3.06171700	4.53679400	0.85738300
H	-0.26435400	7.12216900	-0.04341700
H	2.10993300	6.82389100	0.63823500
C	3.57047900	0.10800900	0.07078600
H	3.92940900	0.72413500	-0.77243300
H	3.88122000	0.65310700	0.97954300
N	2.11569600	0.15703200	0.03236600
H	1.96904900	-1.91154600	-0.07932800
C	4.25560900	-1.23629300	0.03671100
C	4.60743400	-1.83166500	-1.17978400
C	4.52845400	-1.93095500	1.22053300

C	5.21947500	-3.08323300	-1.21459700
H	4.39965300	-1.30189100	-2.11354300
C	5.14015200	-3.18273000	1.19201000
H	4.25864100	-1.47964900	2.17931500
C	5.48770100	-3.76262000	-0.02723500
H	5.49229900	-3.52903700	-2.17376000
H	5.35056900	-3.70695400	2.12694200
H	5.97045000	-4.74191900	-0.05183800

Boron-containing cyclic intermediate (untagged)

C	3.52416800	-0.70310700	0.17246800
C	2.60523200	0.30709000	0.51314300
C	1.24388200	0.18243700	0.22860200
C	0.76920600	-0.98045600	-0.43858400
C	1.69555700	-1.97986600	-0.79680600
C	3.03250300	-1.86236500	-0.50685100
H	2.91177000	1.22774300	1.00450200
H	1.33521200	-2.87098700	-1.31765100
H	3.70861400	-2.66015000	-0.80525700
C	-0.60169000	-1.05777100	-0.76952200
O	0.42877900	1.16670500	0.52979400
C	5.81325600	-1.60843700	0.09591600
H	6.67475800	-1.51630100	0.77425600
H	5.38656300	-2.60501500	0.29261100
C	6.28804000	-1.51562500	-1.34991600
H	6.80712100	-0.56488500	-1.54127900
H	6.98831600	-2.33555800	-1.57430900
H	5.44465900	-1.58462900	-2.05301200
C	5.35989500	0.58847300	1.17045400
H	4.65152200	0.87124000	1.96526700
H	6.28629700	0.29147300	1.68516500
C	5.63536700	1.78294200	0.26406500
H	6.41223400	1.55163600	-0.47967300
H	4.72947700	2.09162000	-0.27811500
H	5.98296900	2.64015500	0.86157900
N	4.85292300	-0.59215900	0.49130400
B	-1.07323000	1.01998000	0.58804000
O	-1.51933700	0.53351100	1.87017800
H	-1.53890900	1.25977600	2.50308500
C	-1.71028800	2.43221000	0.12942400
C	-2.92098900	2.89600500	0.66797700
C	-1.08140600	3.25027200	-0.82184400
C	-3.48358400	4.11215200	0.27753900
H	-3.43445200	2.28675900	1.41942000
C	-1.63195900	4.46682300	-1.22106800
H	-0.12769600	2.92706000	-1.24796700
C	-2.83869800	4.90195100	-0.67225900
H	-4.42674200	4.44600200	0.71772500
H	-1.11671300	5.08402700	-1.96172900
H	-3.27261100	5.85575300	-0.98186200
C	-2.87031500	-0.32822200	-0.80185900
H	-3.41859400	0.52518600	-0.38233300
H	-2.95324100	-0.24499600	-1.89783400
N	-1.47103700	-0.15846900	-0.40876800
H	-0.95777500	-1.91269000	-1.35935200
C	-3.48542400	-1.62596300	-0.33506100
C	-3.38880000	-2.01176600	1.00857000
C	-4.18407400	-2.44042100	-1.22918700
C	-3.98705800	-3.19210100	1.43975000
H	-2.83392700	-1.37271400	1.70166400
C	-4.78744400	-3.62082200	-0.79349200
H	-4.26148900	-2.14661100	-2.27978100
C	-4.68935300	-3.99919800	0.54275600
H	-3.90717700	-3.48513900	2.48900400
H	-5.33140700	-4.24734200	-1.50373500
H	-5.15749600	-4.92407800	0.88659000

Open form for the intermediate from the double addition of the imine intermediate

C	3.49741700	-1.75382400	-1.71434200
C	2.83158900	-0.67414400	-1.09689200
C	1.51295600	-0.79366600	-0.67533400
C	0.76769800	-1.96456100	-0.88150300
C	1.43318100	-3.02824300	-1.50812000
C	2.75010700	-2.94251600	-1.91651200
H	3.32735300	0.27959000	-0.92808400
H	0.86465700	-3.94484100	-1.67437300
H	3.20130700	-3.80403600	-2.40556800
C	-0.64035200	-2.04511500	-0.49870800
O	0.88315800	0.28029700	-0.10991900
C	5.47082100	-2.74210300	-2.80185000
H	6.55497000	-2.61179100	-2.66404000
H	5.22271400	-3.70009200	-2.31496000
C	5.14884600	-2.81511300	-4.29083900
H	5.47646800	-1.90555200	-4.81588300
H	5.65911000	-3.67611700	-4.75074600
H	4.06797500	-2.92924300	-4.46127400
C	5.57683600	-0.44699000	-1.84792400
H	5.32101900	-0.05956800	-0.84815100
H	6.63898600	-0.73203000	-1.79273100
C	5.39602700	0.64616900	-2.89635600
H	5.74251800	0.31301400	-3.88607700
H	4.33986000	0.93920500	-2.99255000
H	5.97514100	1.54108100	-2.61871700
N	4.81972900	-1.66067700	-2.08660700
B	1.20970100	0.98991000	1.01676800
C	2.30789800	0.66453900	2.08144400
C	2.70974900	1.68464400	2.96099000

C	2.87929300	-0.60837000	2.24778000
C	3.65783300	1.45262600	3.95358800
H	2.26010600	2.67485800	2.86070800
C	3.81825000	-0.84915200	3.24852500
H	2.58276800	-1.42878700	1.59186600
C	4.21465800	0.18247900	4.09876100
H	3.95916900	2.26248500	4.62171300
H	4.24423100	-1.84825600	3.36456400
H	4.95613700	-0.00522900	4.87899200
N	-1.33478700	-3.10614100	-0.64650000
H	-1.07894000	-1.12157700	-0.08192300
C	-1.43604300	3.79677800	-1.42413400
C	-0.38978800	3.38805800	-0.57034100
C	-0.60864900	2.45586700	0.43295000
C	-1.87108900	1.89075900	0.66523800
C	-2.90598300	2.30162700	-0.18708400
C	-2.71310400	3.22416500	-1.19716800
H	0.61965100	3.78210000	-0.66877200
H	-3.89355200	1.86861100	-0.01845200
H	-3.56585300	3.51052700	-1.81020300
C	-2.09994700	0.94774700	1.75867200
O	0.45205100	2.11706600	1.24359400
C	-2.30071400	5.11513200	-3.31360100
H	-1.84544100	5.46040400	-4.25473700
H	-2.90627200	4.23422000	-3.58266000
C	-3.19691800	6.21188300	-2.74725300
H	-2.63097100	7.13764600	-2.56457200
H	-4.00889100	6.44503600	-3.45411400
H	-3.65252200	5.90358300	-1.79442300
C	0.08199800	5.31097700	-2.62904200
H	0.86286500	4.53773400	-2.53391300
H	0.13170600	5.65536300	-3.67333700
C	0.38475700	6.47581200	-1.69172500
H	-0.32340100	7.30419100	-1.84213600
H	0.32148100	6.16823600	-0.63732800
H	1.40079200	6.86004200	-1.87461800
N	-1.21786900	4.69618000	-2.44436200
C	-3.38844500	-0.60282200	2.99595700
H	-4.29760300	-0.25672900	3.51817800
H	-3.65391700	-1.58996500	2.57878200
N	-3.19110000	0.29082200	1.86411700
H	-1.27991800	0.85328300	2.49002300
C	-2.26101300	-0.75820100	3.98562400
C	-2.18215000	0.06135200	5.11643800
C	-1.24284100	-1.69381500	3.76761600
C	-1.11678900	-0.04969400	6.00816400
H	-2.96957500	0.79781600	5.29928600
C	-0.17361600	-1.80595400	4.65400700
H	-1.28855200	-2.34155600	2.88733200
C	-0.10777600	-0.98286300	5.77723500
H	-1.07380700	0.59657700	6.88774200
H	0.61465300	-2.53775400	4.46556900
H	0.73150000	-1.06800900	6.47051100
C	-2.72041700	-3.02751300	-0.24038200
H	-2.85300800	-3.71077800	0.62135800
H	-3.00553600	-2.01384300	0.10564200
C	-3.67208700	-3.47315600	-1.32768800
C	-4.94872700	-2.91032400	-1.41232800
C	-3.31354800	-4.46913900	-2.24108700
C	-5.85553000	-3.34231300	-2.37895800
H	-5.23287900	-2.11821700	-0.71387400
C	-4.21748400	-4.89936700	-3.20997000
H	-2.30994200	-4.89350900	-2.18657500
C	-5.49309900	-4.34050800	-3.28137000
H	-6.84854300	-2.88996700	-2.43163400
H	-3.92238300	-5.67732400	-3.91816100
H	-6.20044500	-4.67746500	-4.04230800

Cyclic intermediate from the double addition of the imine intermediate

C	1.03113400	-2.69307400	-1.74550500
C	1.34529700	-1.31939900	-1.72918900
C	0.37135800	-0.34060800	-1.52363100
C	-0.97988100	-0.70427600	-1.34027600
C	-1.28435800	-2.07182900	-1.34619700
C	-0.32613500	-3.04763100	-1.54663600
H	2.36162100	-0.96509200	-1.89154600
H	-2.32764100	-2.35728500	-1.19883700
H	-0.63834600	-4.09043800	-1.56216100
C	-2.01933800	0.30798700	-1.18897100
O	0.74308400	0.95982800	-1.53838900
C	1.66386800	-5.06045700	-2.00062800
H	2.57372500	-5.62942300	-1.75316000
H	0.93978800	-5.29756100	-1.20356000
C	1.12279800	-5.52381600	-3.34952500
H	1.86849500	-5.38850600	-4.14720500
H	0.85729700	-6.59230100	-3.31037000
H	0.22254800	-4.95838300	-3.63269300
C	3.38699500	-3.27819400	-2.14975500
H	3.65694400	-2.47653900	-1.44116800
H	4.00916700	-4.14287000	-1.87006600
C	3.72410600	-2.84811800	-3.57474100
H	3.56431400	-3.66956100	-4.28901700
H	3.10053400	-2.00015700	-3.89468800
H	4.78061600	-2.54200000	-3.64424300
N	2.00690000	-3.65412700	-1.92689700
B	0.93975400	1.72982300	-0.30018600
C	0.95466800	3.29862200	-0.64425300
C	0.93977300	4.25641000	0.38135800

C	0.98306400	3.76721000	-1.96494700
C	0.96059900	5.62281400	0.10497200
H	0.89729500	3.92212600	1.42262900
C	1.00296200	5.13219500	-2.25344900
H	0.97859200	3.03834200	-2.77928700
C	0.99468100	6.06498500	-1.21767200
H	0.94365300	6.34782500	0.92283300
H	1.02059100	5.47099200	-3.29253600
H	1.00887900	7.13480100	-1.43960300
N	-3.19565900	0.03896200	-0.76161100
H	-1.72961700	1.33581700	-1.46979700
C	-1.12710800	-1.04533200	3.14895700
C	-1.17182200	-0.00918500	2.19642600
C	-0.01305600	0.46912600	1.59803400
C	1.25176500	-0.05833700	1.96601400
C	1.29855000	-1.04171400	2.97453900
C	0.15515000	-1.52499400	3.56347600
H	-2.10897700	0.42629800	1.86105600
H	2.27007800	-1.43827000	3.28126800
H	0.23972600	-2.29497700	4.32715700
C	2.40812700	0.43032600	1.31475600
O	-0.10303700	1.44843700	0.71119500
C	-2.25218400	-2.57133200	4.71476000
H	-3.21745600	-3.09792800	4.69090600
H	-1.48925100	-3.33705700	4.49508600
C	-2.02314900	-1.98505300	6.10311100
H	-2.82174000	-1.27861400	6.37366200
H	-2.00563000	-2.78696100	6.85787800
H	-1.06587800	-1.44528600	6.15753200
C	-3.57634500	-1.20364900	3.10600300
H	-3.47588600	-1.04080800	2.02104100
H	-4.24507300	-2.07102600	3.21998400
C	-4.20174100	0.01541900	3.77325000
H	-4.39873600	-0.16441000	4.84111800
H	-3.54612100	0.89552500	3.69496100
H	-5.16017600	0.26009100	3.28930000
N	-2.27931700	-1.59319700	3.64159000
C	3.54750400	1.77956900	-0.35131900
H	3.42658900	1.54807400	-1.42099700
H	3.51870100	2.87709000	-0.27226700
N	2.34812200	1.27489100	0.32442100
H	3.39324500	0.08668000	1.65096900
C	4.85812400	1.25102600	0.15920900
C	5.46701000	0.14253900	-0.43841900
C	5.49588100	1.86162600	1.24556500
C	6.68062800	-0.34904100	0.03907300
H	4.98789300	-0.33343600	-1.29801500
C	6.70775800	1.37181400	1.72754400
H	5.03619800	2.73545300	1.71485700
C	7.30239200	0.26349200	1.12569100
H	7.14580200	-1.21096700	-0.44384800
H	7.19444300	1.86277000	2.57284200
H	8.25484600	-0.11811200	1.49917800
C	-4.11882100	1.14287200	-0.67479000
H	-4.30973700	1.34729300	0.39712300
H	-3.69622800	2.08018700	-1.09322100
C	-5.45625800	0.86789200	-1.32653000
C	-5.73419900	-0.34681900	-1.95535400
C	-6.44929100	1.85460000	-1.30312200
C	-6.97704200	-0.57023400	-2.54902100
H	-4.95998500	-1.11480000	-1.97210900
C	-7.68949400	1.63389000	-1.89457300
H	-6.24395100	2.81258700	-0.81614800
C	-7.95919700	0.41656800	-2.52146100
H	-7.17733700	-1.52598500	-3.03928700
H	-8.45076400	2.41704600	-1.86843600
H	-8.93116200	0.24147300	-2.98778700

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