Table S1: A brief description of the AHL synthase genes mentioned in Figure 2.

Genes	Organisms	Description	References
lasI	*Pseudomonas aeruginosa*	Required for the synthesis of PAI consisting of 3-oxo-N-(tetrahydro-2-oxo-3-furanyl)-dodecanamide also known as N-(3-oxododecanoyl) homoserine lactone, an autoinducer molecule which binds to LasR and thus acts in elastase biosynthesis regulation.	[25]
traI	*Agrobacterium fabrum*	Required for the synthesis of OHHL (N-(3-oxohexanoyl)-L-homoserine lactone), an autoinducer molecule which binds to TraR and thus acts in the control of conjugal transfer	[26]
expI	*Pectobacterium parmentieri*	Required for the synthesis of OHHL (N-(3-oxohexanoyl)-L-homoserine lactone), an autoinducer molecule which binds to ExpR and thus acts in virulence (soft rot disease) through the activation of genes for plant tissue macerating enzymes.	[27]
ainS	*Vibrio fischeri*	catalyzes the synthesis of N-octanoylhomoserine lactone.	[28]
esaI	*Pantoea stewartii* subsp. stewartii	Required for the synthesis of OHHL (N-(3-oxohexanoyl)-L-homoserine lactone), an autoinducer molecule which binds to EsaR.	[29]
luxI	*Aliivibrio fischeri*	Required for the synthesis of OHHL (N-(3-oxohexanoyl)-L-homoserine lactone) also known as VAI or N-(beta-ketocaproyl) homoserine lactone or 3-oxo-N-(tetrahydro-2-oxo-3-furanyl)-hexanamide, an autoinducer molecule which binds to LuxR and thus acts in bioluminescence regulation.	[30]
soll	*Ralstonia solanacearum*	Required for the synthesis of acyl-HSL autoinducers that bind to SolR.	[31]
bjaI	*Bradyrhizobium japonicum*	Catalyzes the synthesis of isovaleryl-HSL (IV-HSL)	[32, 33]
cepI	*Burkholderia cepacia*	Catalyzes the synthesis of synthesis of C8-HSL.	[34]
psyI	*Pseudomonas amygdali* pv. tabaci	Required for the synthesis of OHHL (N-(3-oxohexanoyl)-L-homoserine lactone)	[35]
rhll	*Pseudomonas aeruginosa*	Required for the synthesis of BHL (N-butanoyl-L-homoserine lactone), and HHL (N-hexanoyl-L-homoserine lactone) autoinducer molecules which bind to RhlR	[36]
anoI	*Acinetobacter nosocomialis*	Involved in the synthesis of the acyl-homoserine lactone (AHL) signal N-(3-hydroxydodecanoyl)-L-HSL (3-hydroxy-C12-HSL or OH-dDHL)	[37]
pagI	*P. agglomerans pv. gypsophilae*	Produces N-butanoyl-l-homoserine lactone (C4-HSL) as a major and N-hexanoyl-l-homoserine lactone (C6-HSL) as a minor QS signal.	[38]

luxM	*Vibrio harveyi*	Required for the synthesis of an autoinducer molecule beta-hydroxybutyryl homoserine lactone, which binds to LuxN and thus acts in bioluminescence regulation	[39]
yenI	*Yersinia enterocolitica*	Required for the synthesis of autoinducer molecules such as OHHL (N-(3-oxohexanoyl)-L-homoserine lactone), and HHL (N-hexanoyl-L-homoserine lactone).	[40]
RaiI	*Rhizobium etli*	Required for the synthesis of autoinducer molecules which bind to RaiR and that are involved in the restriction of nodule number.	[41]
bpsI	*Burkholderia pseudomallei*	BpsI–BpsR system produces N-octanoylhomoserine lactone (C8HL) and is positively auto-regulated by its AHL product	[42]
abaI	*Acinetobacter baumannii*	Involved in the synthesis of the acyl-homoserine lactone (AHL) signal N-(3-hydroxydodecanoyl)-L-HSL (3-hydroxy-C12-HSL or OH-dDHL). Required for normal biofilm development.	[43]
bpmI	*Burkholderia pseudomallei*	bpmIR system produce C10HSL, 3-hydroxy-C8HSL, 3-oxo-C10HSL, 3-hydroxy-C10HSL, and 3-oxo-C14HSL	[44]
vanM	*Vibrio anguillarum*	Required for the synthesis of N-(3-hydroxyhexanoyl) homoserine lactone (3-hydroxy-C6-HSL) and N-hexanoylhomoserine lactone (C6-HSL).	[45]
cinI	*Rhizobium leguminosarum*	Produces N-(3-hydroxy-7-cis-tetradecenoyl)-L-homoserine lactone	[46, 47]
bviL	*Burkholderia vietnamiensis* strain G4	Produces N-decahomoserine lactone	[48]
ypeI	*Yersinia pestis*	Produces N-3-oxooctanoyl-l-homoserine lactone and N-3-oxo-hexanoyl-l-homoserine lactone.	[49]
ypsI	*Yersinia pseudotuberculosis*	Produces 3-oxo-substituted C6, C7 and C8 AHLs and the unsubstituted C6 and C8 compounds	[50]

Table S2: Stereochemical analysis of acyl carrier protein (acpP) and AHL synthase

	Validation Parameters	AHL synthase	Goal
Protein geometry	Poor rotamers	3 (1.95%)	<0.3%
	Favored rotamers	144 (93.51%)	>98%
	Ramachandran outliers	0 (0.00%)	<0.05%
	Ramachandran favored	174 (97.21%)	>98%
	Rama distribution Z-score	0.58±0.62	Abs(Z score) < 2
	Cβ deviations >0.25Å	0 (0.00%)	0%
	Bad bonds	0/1502 (0.00%)	0%
	Bad angles	28/2045 (1.37%)	<0.1%
Peptide omegas	Cis Prolines	1/15 (6.67%)	≤1 per chain
	CaBLAM outliers	6 (3.4%)	<1.0%

Low-resolution criteria	CA Geometry outliers	4 (2.26%)	<0.5%
Additional	Chiral volume outliers	0/215	0

Note: Parameters highlighted in green were optimized to the required goal.

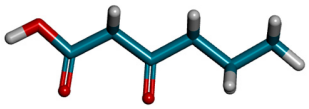
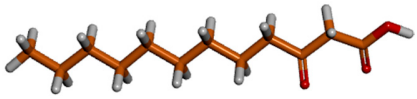
Table S3: The statistical t-test between the predictive AlphaFold- and modeler- based structure of probable AHL synthase.

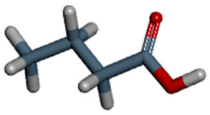
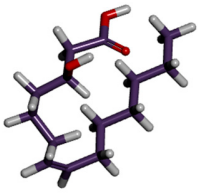
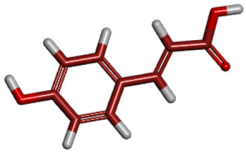
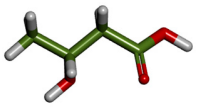
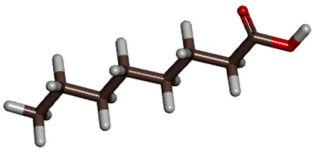
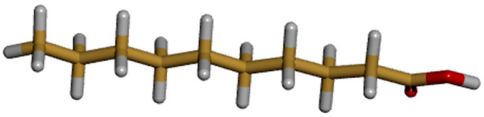
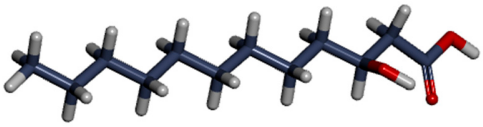
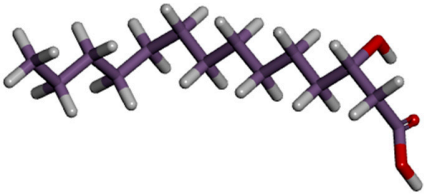
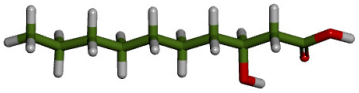
	Variable *1*	**Variable** *2*
Mean	-0.04155	-0.04092
Variance	2.13E-05	2.11E-05
Observations	181	181
Hypothesized Mean Difference	0	
df	360	
t Stat	-1.30117	
P(T<=t) one-tail	0.097016	
t Critical one-tail	1.649097	
P(T<=t) two-tail	0.194031	
t Critical two-tail	1.966575	

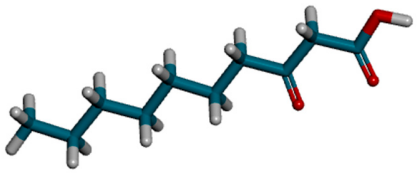
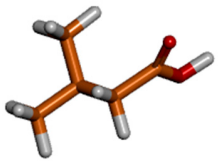
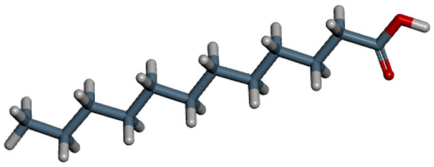
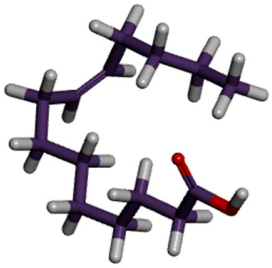
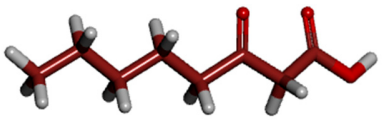
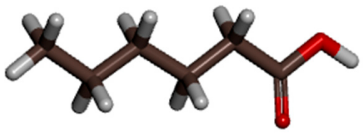
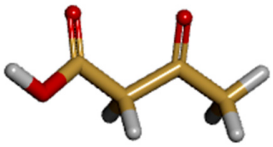
Table S4: The detailed interactions between the modeled AHL synthase and the AHL substrates (Available as an excel file).

Table S5: Details of fatty acyl molecules and their respective AHL products in different organisms reported in literature (Available as an excel file).

Table S6: Candidate fatty acyl molecules and their respective three-dimensional chemical structures used in this study

Precursor molecule name	**Precursor molecule CID**	**Chemical Structures**
3-Oxohexanoic acid	439658	
3-Oxododecanoic acid	439717	

Butyric acid	264	
(Z)-3-Hydroxy-7-tetradecenoic acid	44610299	
p-coumaric acid	637542	
3-hydroxybutanoic acid	441	
octanoic acid	379	
Decanoic acid	2969	
3-Hydroxydodecanoic acid	94216	
3-Hydroxytetradecanoic acid	16064	
3-Hydroxydecanoic acid	26612	

3-oxodecanoic acid	5282982	
Isovaleric acid	10430	
Dodecanoic acid	3893	
Myristoleic acid	5281119	
3-Oxooctanoic acid	128859	
Hexanoic acid	8892	
3-oxobutanoic acid	96	

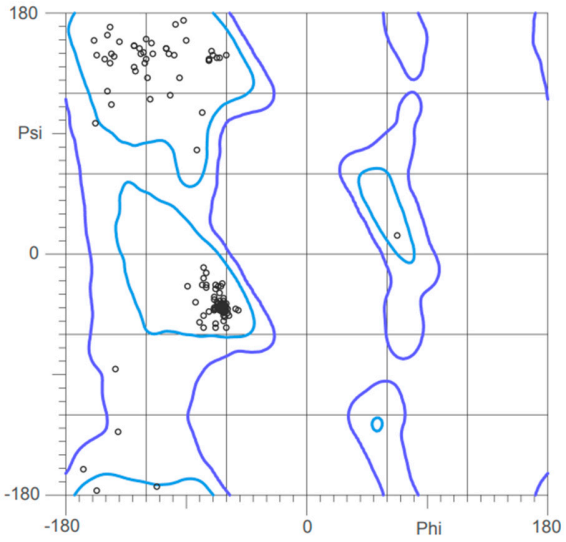


Figure S1: Ramachandran plot depicting measurement of backbone dihedral angles (ϕ, phi and ψ, psi) in acyl homoserine lactone (AHL) synthase.

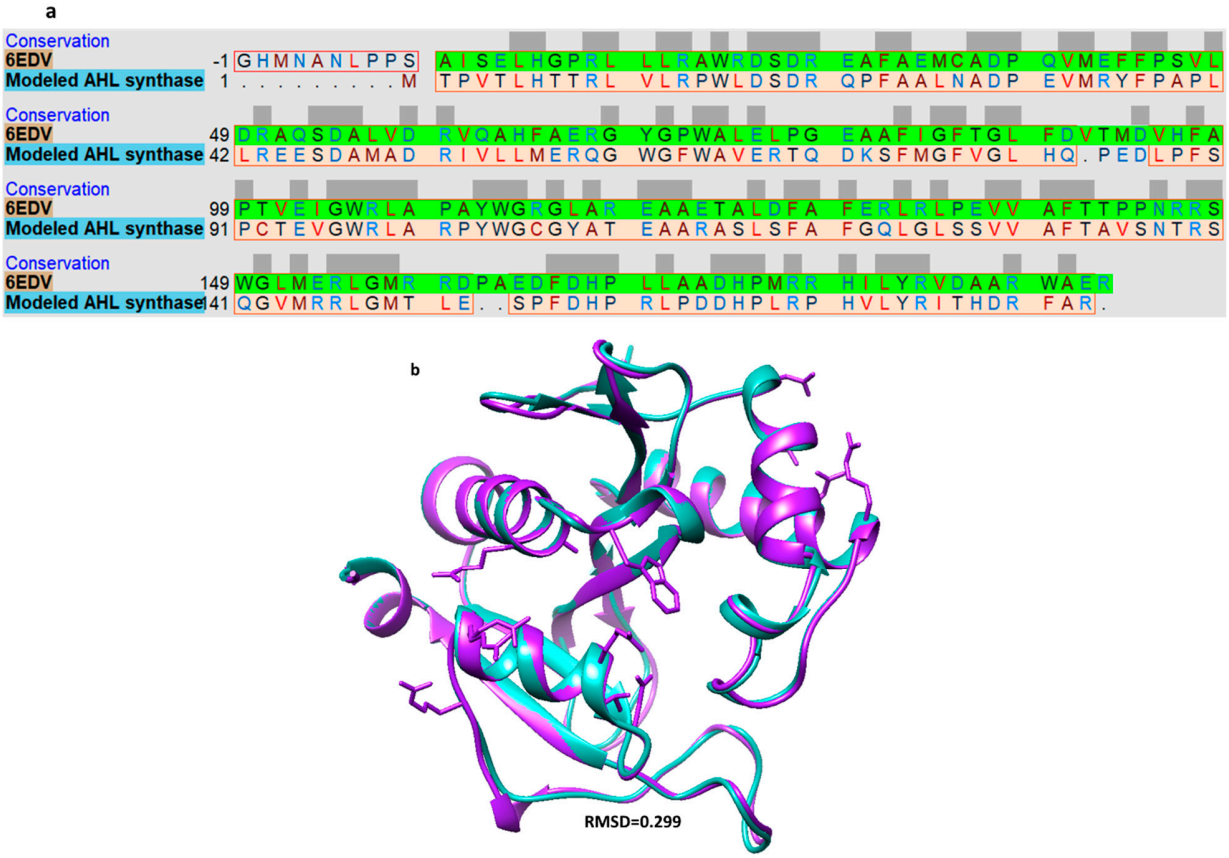


Figure S2: (a) The alignment of amino acids, and (b) superimposition, between the modeled AHL synthase and the template (#6EDV)

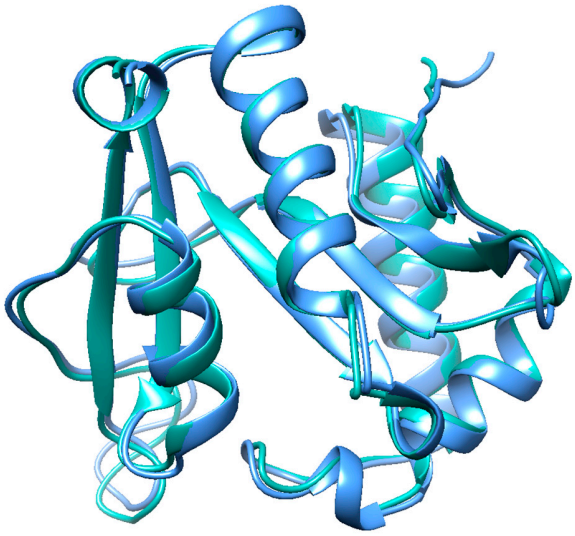


Figure S3: Superimposition between the predictive AlphaFold- (green) and modeler- based (blue) structure of probable AHL synthase.

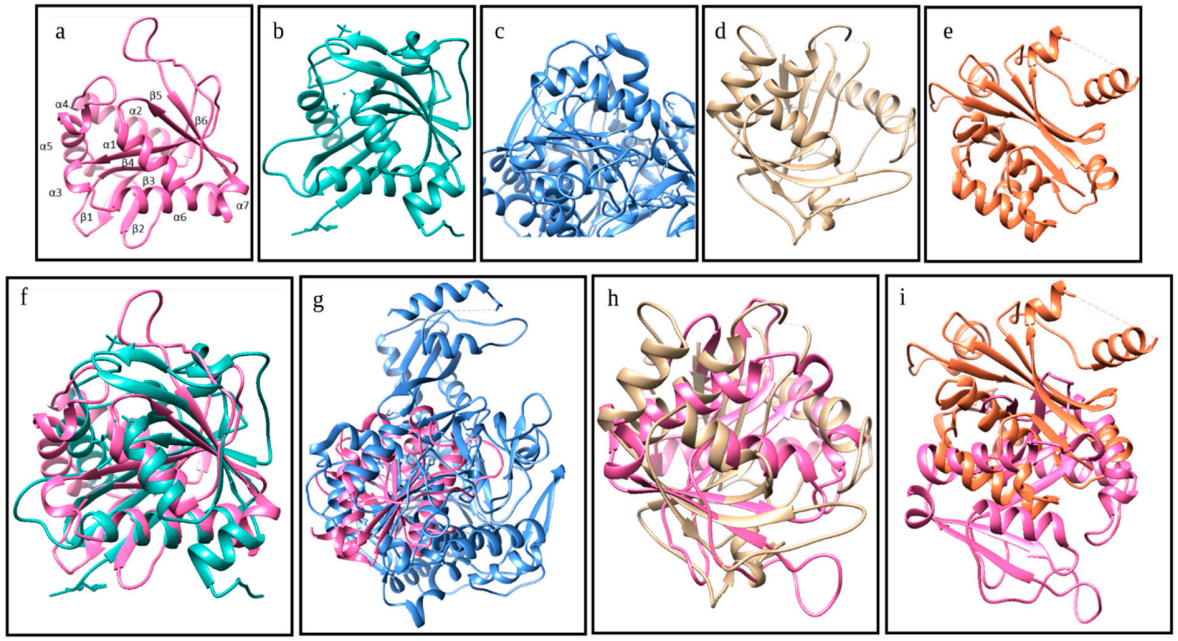


Figure S4: The individual structures of (a) modeled AHL synthase, (b) PDB# 1RO5, (c) PDB# 2P2F, (d) PDB# 6WNS, and (e) PDB# 1KZF. The superimposition between the modeled AHL synthase and (f) PDB# 1RO5, (g) PDB# 2P2F, (h) PDB# 6WNS, and (i) PDB# 1KZF.

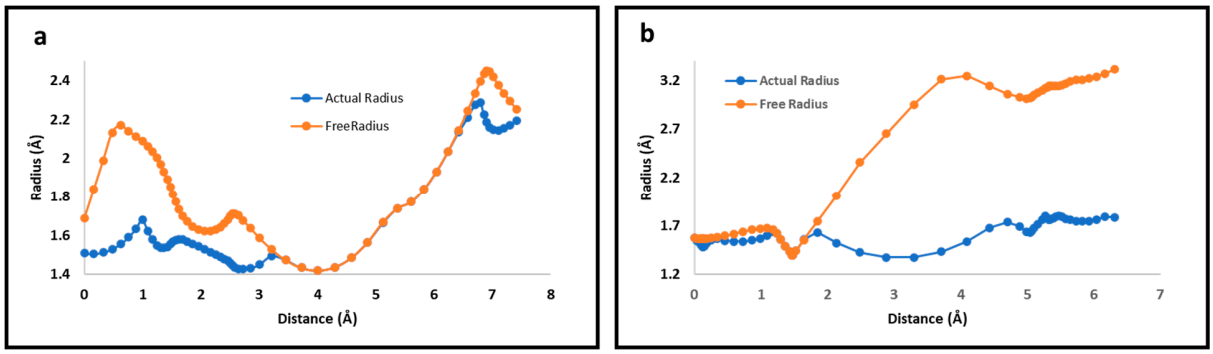


Figure S5: The actual and free radius variation with tunnel distances in (a) PS 2, and (b) PS 3.