

Supporting Information

Discovering Novel *Alternaria solani* Succinate Dehydrogenase Inhibitors by *In Silico* Modeling and Virtual Screening Strategies to Combat Early Blight

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Supplementary Data

Sequences of *A. solani* SDH subunits.

A. solani SDH subunit A

PVIDHEYDAIVVGAGGAGLRAAFGLAEAGFNTACISKLPTRSHTVAAQGGINAALGSM
HEDDWRWHMYDTVKGSDWLGQDAIHMTREAPQS VIELENYGCPFSRTDDGKMYQ
RAFGGQSQKYGKGGQAYRCCAAADRTGHALLHTLYGQSLRHNTKYFIEFFATDLIMED
GVCKGVVAYNQEDGTIHRFIAKNTVLATGGYGRAYFSC TSAHTCTGDGMAMVARAGL
PNQDLEFVQFHPTGIYGAGCLITEGSRGEGGYLLNSEGERFMERYAPTAKDLASRDVVS
RSMTLEIREGRGVGPEKDH IYLQLSHLPAEVLHERLPGISETAAIFAGVDVTKQPIPVLP
VHYNMGGIPTKYTGEVITQDAQGNDQVVPGLFACGEAASVSVHGANRLGANSLLDLIV
FGRAVSHTIRDNFSPGQKADPVSADAGADSI VLDQIRTS DGPKSTAEIRLQMOKVMQT
DVAVFRTQESLDEGVKKIHDVDADFANVGIKDRSMIWNSDLVETLELRNLLTCAVQTA
ESAANRKESRG AHAREDFPDRDDEQWMKHTLSWQKKPHGETQLGYRKVVGTTLDEAE
CKAVPPFKRTY

A. solani SDH subunits B (GenBank: AGS56260.1)

MASIRAFTRLATS DLVPVRPAVFSRGFASVNDVHAREPISKIAEKIAPDASRSPVPEKTS
TVPEPEPSKDAKTKTFHIYRWNPDEPTSKPKMQSYTLDLNKTGPMMLDALIRIKNEVDP
TLTFRRSCREGICGSCAMNIDGVNTLACLRIPTDTTKESRIYPLPHMYVVKDLVPDML
FYKQYRSVKPYLQRSTAAPDGREFRQSKEDRKKLDGLYECILCACCSTSCPSYWWNQE
EYLGPAVLLQSYRWIADSRDEKKAERQDALNNSMSLYRCRTILNCSRTCPKGLNPALAI
AEIKKSMAFT

***A. solani* SDH subunits C (AGS56262.1)**

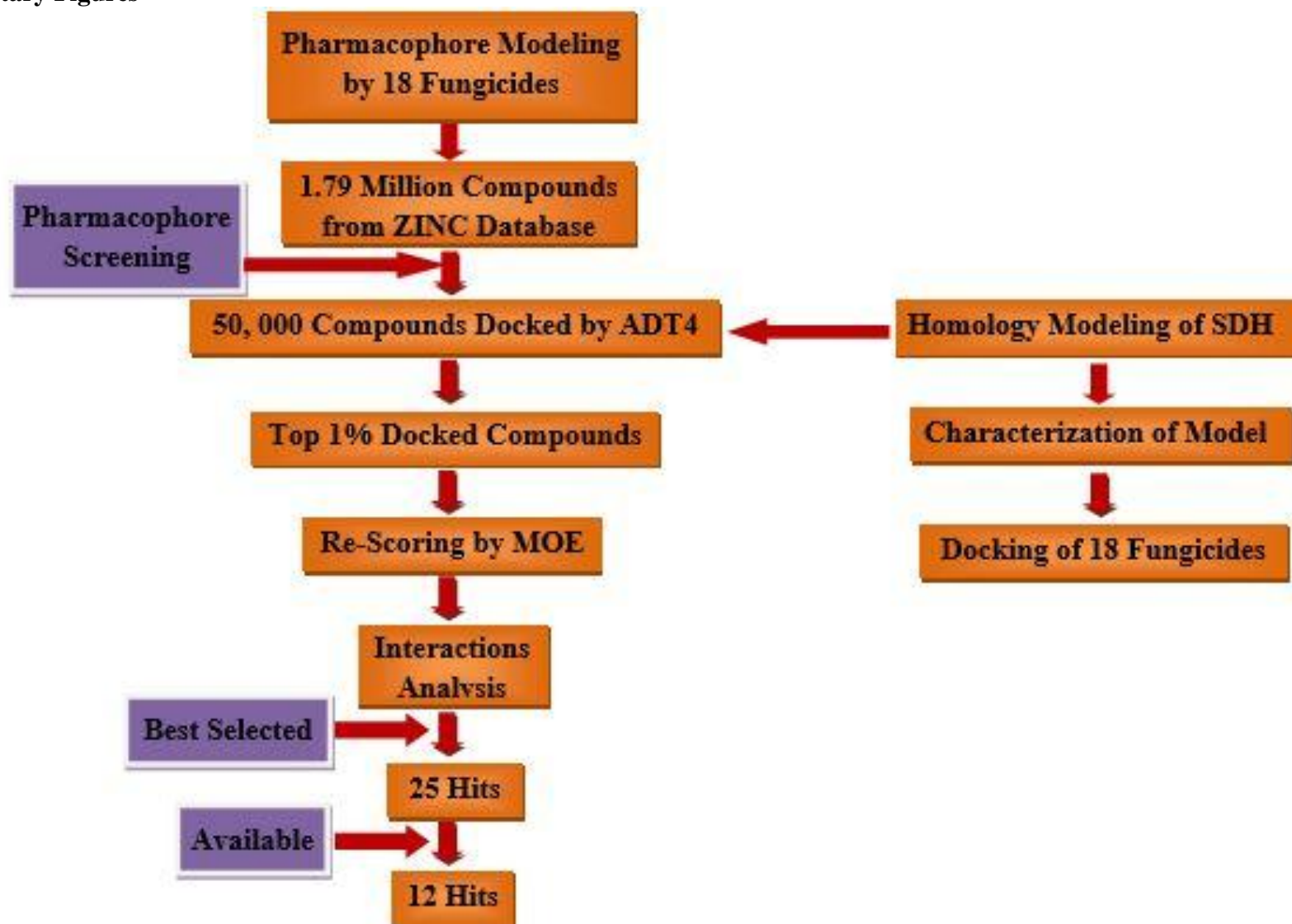
MASQRVFQLGLRRAAPGLRVQPVGRMVQRRLAA TEHASQSEAAEILAKQRINRPVSP
HLAIYRPQITWYASSLNRTGITLSGSLYLFGIAYLIAPYTGWHMETQSMVATVAAWPAA
AKAGLKAFYAFPPFFHSFNGLRHLSWDVGIGFKNQQVIRLGW

***A. solani* SDH subunits D (GenBank: AGS56264.1)**

MASVMRPGLLRQACPPAHASQRMLSTATATTSRPLAQQLRPAFQRSAVPKATRIAAFH
ATQRTQILPPLPQKIIGTTNDPVPVDPDYAHGSYHWSFERIVSAGLIPLTIAPFAAGSLNP
LTDSILCALLVVHSHIGFESCIIDYFPAKRVPKTRKAAMWALRAGTLTLGLALYSFETND
VGITE

Supplementary Figures and Tables

Supplementary Figures



Supplementary Figure S1. Schematic presentation of Computational Work Flow

```

SDHA          -----PVIDHEYDAIWWGAGGAGLRAAFGLAEAGFNTACISKLPTRSHVA
1YQ3A        -STKVSDSISTQYPVVDHEFDVVVWAGGAGLRAAFGLSEAGFNTACVTCLFPTRSHVA
1ZOYA        SSAKVSDAISTQYPVVDHEFDVVVWAGGAGLRAAFGLSEAGFNTACVTCLFPTRSHVA
              **:***:***:*****:*****:*****:*****

SDHA          AQQGINAALGSMHEDDWRWHMYDTVKGSDWLGQDQAIHYMTREAPQSVIELENYGCPFSR
1YQ3A        AQQGINAALGNMEDDNRWHFYDTVKGSDWLGQDQAIHYMTEQAPAAVIELENYGMPFSR
1ZOYA        AQQGINAALGNMEEDNNRWHFYDTVKGSDWLGQDQAIHYMTEQAPASVVELENYGMPFSR
              *****_*_*:***:*****:*****:*****_*_*:***** ****

SDHA          TDDGKMYQRAFGGQSQKYGKGGQAYRCCAAADRTGHALLHTLYGQSLRHNTKYFIEFFAT
1YQ3A        TEEGKIYQRAFGGQSLQFGKGGQAHRCVADRTGHSLHTLYGRSLRYDTSYFVEYFAL
1ZOYA        TEDGKIYQRAFGGQSLKFGKGGQAHRCVADRTGHSLHTLYGRSLRYDTSYFVEYFAL
              *_*:***:*****_*_*:*****:***_*_*:*****:*****:***_*_*:***

SDHA          DLIMEDGVCKGVVAYNQEDGTIHRFIAKNTVLATGGYGRAYFSCTS AHTCTGDGMAMVAR
1YQ3A        DLLMENGECRGIALCIEDGTIHRFRAKNTVIATGGYGRYFSCTS AHTSTGDGTAMVTR
1ZOYA        DLLMENGECRGIALCIEDGSIHRIRARNTVVATGGYGRYFSCTS AHTSTGDGTAMVTR
              **:*_*:***_*_*:***:***:***:*****:*****_*_*:*** **:*_*

SDHA          AGLPNQDLEFVQFHPTGIYAGCLITEGSRGEGYLLNSEGERFMERYAPTAKDLASRDV
1YQ3A        AGLPCQDLEFVQFHPTGIYAGCLITEGCRGEGGILINSQGERFMERYAPVAKDLASRDV
1ZOYA        AGLPCQDLEFVQFHPTGIYAGCLITEGCRGEGGILINSQGERFMERYAPVAKDLASRDV
              *****_*****:*****_*_*:*****_*_*:*****_*_*:*****

SDHA          VRSMTLEIREGRGVPEKDHVYLLQSHLPAEVLHERLPGISETAAIFAGVDVTKEPIPV
1YQ3A        VRSMTIEIREGRGCGPEKDHVYLLQSHLPPQQLATRLPGISETAMIFAGVDVTKEPIPV
1ZOYA        VRSMTLEIREGRGCGPEKDHVYLLQSHLPEQLAVRLPGISETAMIFAGVDVTKEPIPV
              *****:*****_*****:*** **_*_*:*****_*****:***

SDHA          LPTVHYNMGGIPTKYTGEVITQDAQGNDQVVPGLFACGEAASVSVHGANRLGANSLLDLI
1YQ3A        LPTVHYNMGGIPTNYKGVITH-VNGEDKVVVPGLYACGEAASASVHGANRLGANSLLDLV
1ZOYA        LPTVHYNMGGIPTNYKGVLRH-VNGQDQVVPGLYACGEAACASVHGANRLGANSLLDLV
              *****:***_*_*:***_*_*:***_*_*:*****:*****_*_*:*****:*****

SDHA          VFGRAVSHIRDNFSPGQKADPVSAADAGADSI SVLDQIRTS DGPKSTAEIRLQMOKVMQT
1YQ3A        VFGRAVSHIRDNFSPGQKADPVSAADAGADSI SVLDQIRTS DGPKSTAEIRLQMOKVMQT
1ZOYA        VFGRAVSHIRDNFSPGQKADPVSAADAGADSI SVLDQIRTS DGPKSTAEIRLQMOKVMQT
              *****_*_*:***_*_*:***_*_*:***_*_*:***_*_*:***_*_*:***_*_*:***_*_*:***_*_*

SDHA          DVAVFRTQESLDEGVKKIHDVDADFANVGIKDRSMIWNNDLVETLELRNLLTCAVQTAE
1YQ3A        HAAVFRTGSILQEGCEKLSQIYRDLAHLKTFDRGIWNNDLVETLELRNLLTCAVQTAE
1ZOYA        HAAVFRVGSVLQEGCEKILRLYDGLQHLKTFDRGMWNNDLVETLELRNLLTCAVQTAE
              ..****. *_**_*_*:***_*_*:***_*_*:***_*_*:***_*_*:***_*_*:***_*_*

SDHA          AANRKE SRGAHAREDFPDRDD-----EQW MKHTLSWQKKPHGETQLGY
1YQ3A        AEARKESRGAHAREDYKLRIDEFDYSKPLQGQQKRPFEHWRKHTLSYVDVKSGKVTLKY
1ZOYA        AEARKESRGAHAREDFKERVDEYDYSKPIQGGQQKPFQEHWRKHTLSYVDVKTGKVSLEY
              * *****_*_*:***_*_*:*****_*_*:*****_*_*:*****_*_*

SDHA          RKWVGTTLDEAECKAVPPFKRTY
1YQ3A        RPVIDRTLNEEDCSSVPPAIRSY
1ZOYA        RPVIDKTLNEADCATVPPAIRSY
              *_*_*:***_*_*:***_*_*:***_*_*

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Supplementary Figure S2 (A). Multiple sequence alignment of SDHA.

```

SDHB      MASIRAFTRLATSDLVPRPAVFSRGFASVNDVHAREPIISKIAEKIAPDASRSPVPESKT
1YQ3B     -----
1ZOYB     -----

SDHB      STVPEPEPSKDAKTKTFHIYRWNPDPTSKPKMQSYTLDLNKTGPMMLDALIRIKNEVDP
1YQ3B     ---AQTAAAATSRIKKFSIYRWDPDKPGDKPRMQTYEVDLNKCGPMVLDALIKIKNELDS
1ZOYB     ---AQTAAATAPRIKKFAIYRWDPDKTGDKPHMQTYEIDLNNCGPMVLDALIKIKNEIDS
          :   :   : *.* *****:**. .**:**:* :***: ***:*****:***:*

SDHB      TLTFRRSREGICGSCAMNIDGVNTLACLRIPTDTTKESRIYPLPHMYVVKDLVPMTL
1YQ3B     TLTFRRSREGICGSCAMNIAGGNTLACTKKIDPDLKTTKIYPLPHMYVVKDLVPLSN
1ZOYB     TLTFRRSREGICGSCAMNINGGNTLACTRRIDTNLDKVKIYPLPHMYVIKDLVPLSN
          *****:***:***: * ***** :* : * ::*****:*****:;;

SDHB      FYKQYRSVKPYLQRSTAAPDGR-EFRQSKEDRKKLDGLYECILCACCSTSCPSYWNQEE
1YQ3B     FYAQYKSIIEPYLKKKDESKQKQYLQSIEDRQKLDGLYECILCACCSTSCPSYWNGDK
1ZOYB     FYAQYKSIIEPYLKKKDESQEGKQYLQSIEREKLDGLYECILCACCSTSCPSYWNGDK
          ** *:*:***:.. : :*: :: ** *:*:*****:*****:*****:;;

SDHB      YLGPAVLLQSYRWIADSRDEKKAERQDALNNSMSLYRCRTILNCSRTCCKGLNPALIAIE
1YQ3B     YLGPAVLMQAYRWMIDSRDDYTEERLAQLQDPFSLYRCHTIMNCTRTCCKGLNPGKAIIE
1ZOYB     YLGPAVLMQAYRWMIDSRDDFTEERLAKLQDPFSLYRCHTIMNCTGTCPKGLNPGKAIIE
          *****:***:***: *****: . ** *:: :*****:***:**: ***** . ****

SDHB      IKKSMAFT-----
1YQ3B     IKKMMATYKEKAAAA
1ZOYB     IKKMMATYKEKKASV
          *** **

```

Supplementary Figure S2 (B). Multiple sequence alignment of SDHB.

```

SDHC      MASQRVFLGLRRAAAPGLRVQPVGRMVQRRLAATEHASQSEAAEILAKQRINRPVSPHL
1YQ3C     -----MATTAKEEMARFWEKNTKS-----SRPLSPHI
1ZOYC     -----LGT TAKEEMERFWKNLGS-----NRPLSPHI
          :   ... * :  : * .***:***:

SDHC      AIYRPQITWYASSLNIRITGITLSGSLYLFGIAYLIAPYTGWHMETQSMVATVAAWPAAAK
1YQ3C     SIYKWSLPMAMSIHRGTGVALSLGVSLFSLAALLLPEQ---FPHYVAVVKSLSLSPALI
1ZOYC     TIYRWSLPMAMSIHRGTGIALSAGVSLFGLSALLLPGN---FESHLELVKSLCLGPTLI
          :**: .: * :* **:**. : **.: * : * :   : .. . :

SDHC      AGLKAFYAFPPFFHSFNGLRHLSWVDVIGFKNQQVIRLW-----
1YQ3C     YSAKFALVFPLSYHTWNGIRHLVWDMGKGFKLSQVEQSGVVVILITLLSSAGIAAIS
1ZOYC     YTAKFGIVFPLMYHTWNGIRHLIWDLGKGLTIPQLTQSGVVVILITLVSSVGLAAM-
          * .**: :*:**:*** **:* *.. * : : *

```

Supplementary Figure S2 (C). Multiple sequence alignment of SDHC.

```

SDHD      MASVMRPGLLRQACPPAHASQRMLSTATATTSRPLAQQLRPAFQRSVAVPKATRIAAFHAT
1ZOYD     -----
1YQ3D     -----

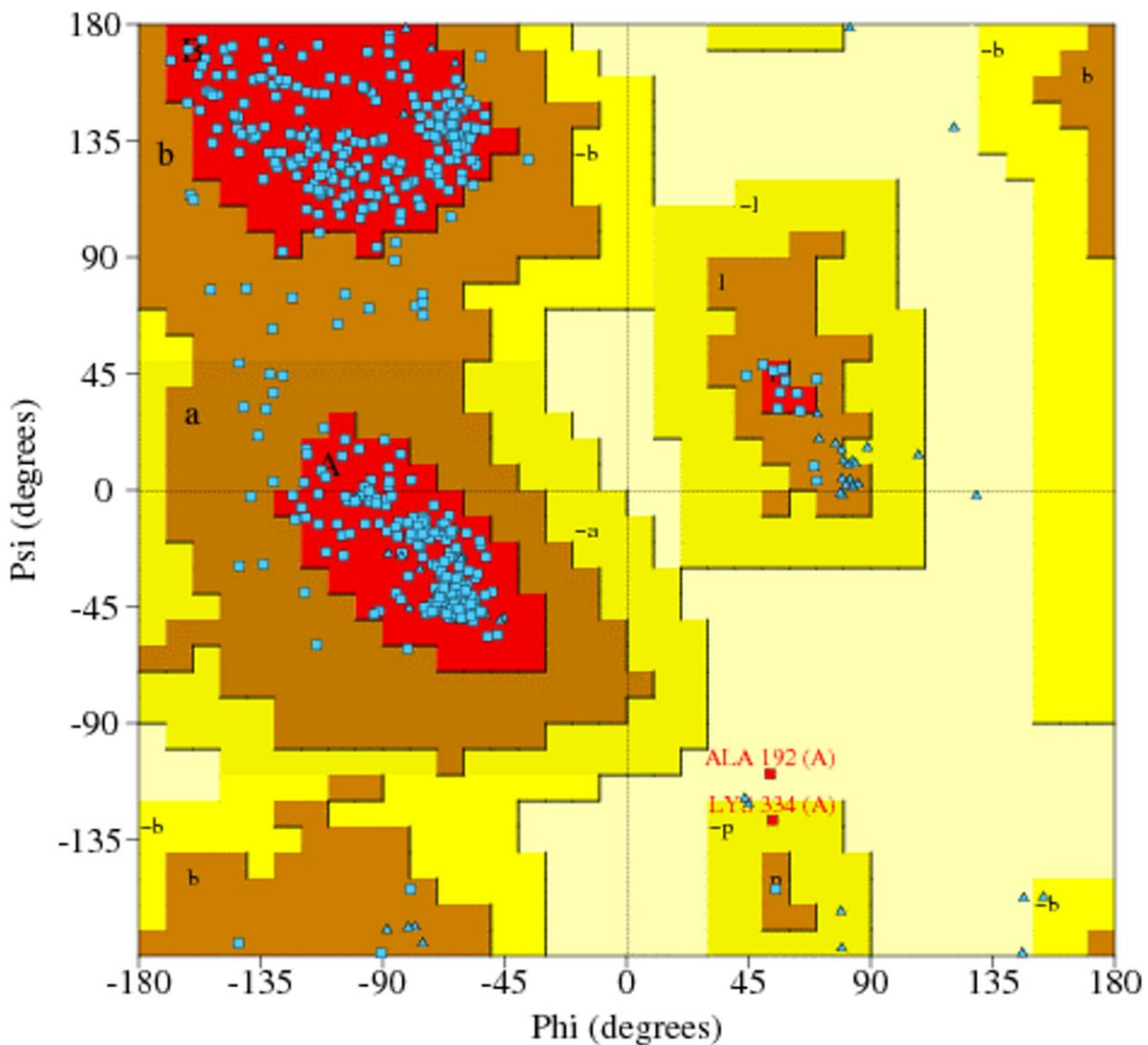
SDHD      QRTQILPPLPQKIIIGTTNDPVPVDPDYAHGSYHWSFERIVSAGLIPLTIAPFAAGSLNP
1ZOYD     -----ASSKAASLHWGTGERVSVLLLGLLPAAYLN--PCS
1YQ3D     -----GSSKAASLHWTSERAVSALLLGLLPAAYLY--PGP
              . . * ** : ** ** . * : * * :

SDHD      LTDSILCALLVHSHIGFESCIIDYFPAKRVPKTRKAAMWALRAGTLTLGLALYSFETND
1ZOYD     AMDYSLAAALTLHGHWGIGQVVDYVRGDALQKAAKAGLLALSFTFAG---LCYFNYHD
1YQ3D     AVDYSLAAALTLHGHWGLGQVITDYVHGDTPIKVANTGLYVLSAITFTG---LCYFNYYD
              * * . * * . : * . * * : . : ** . . . * . : : : . * * * : : * * : *

SDHD      VGITE-----
1ZOYD     VGICKAVAMLWKL
1YQ3D     VGICKAVAMLWSI
              *** ;

```

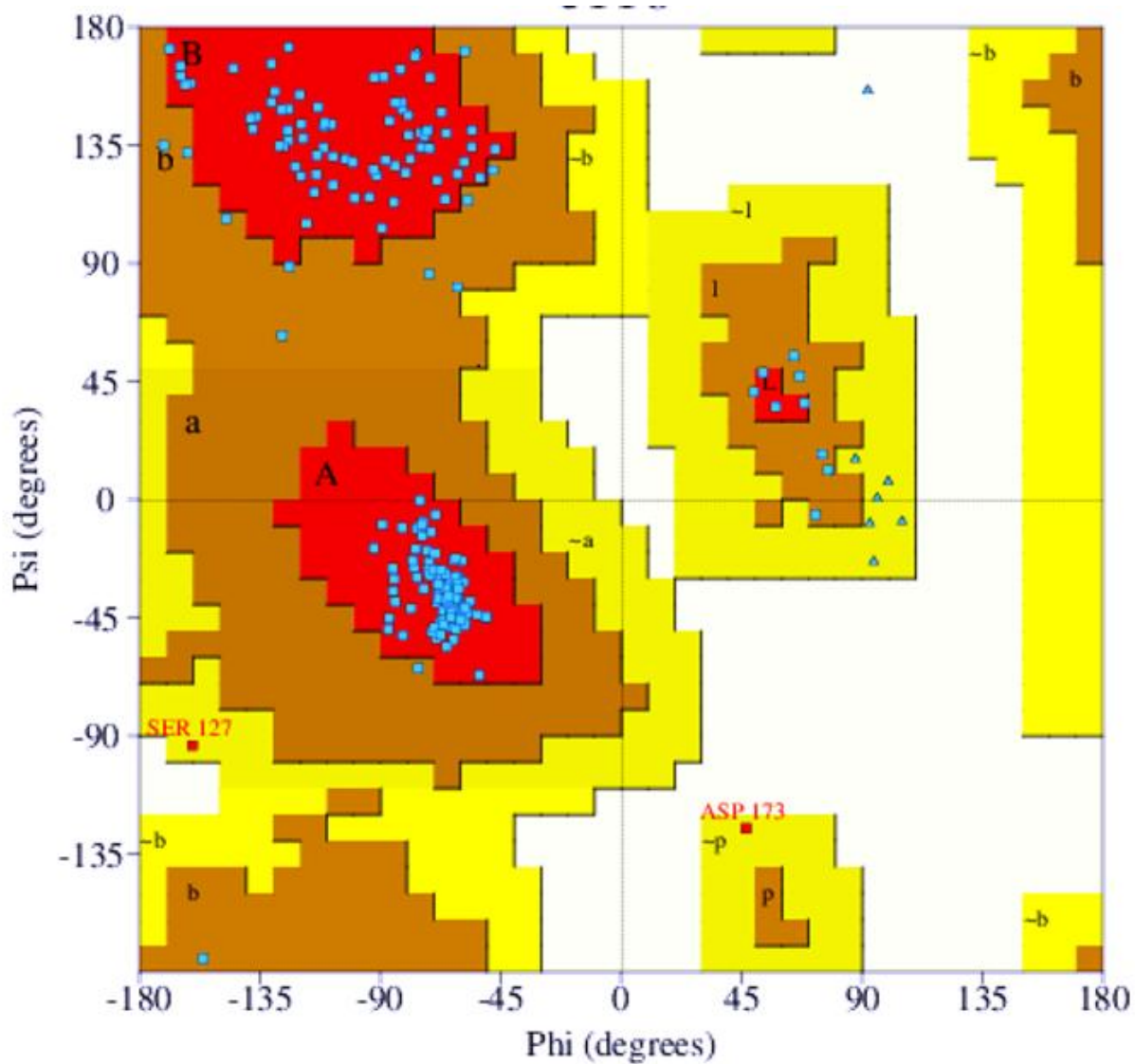
Supplementary Figure S2 (D). Multiple sequence alignment of SDHD.



Ramachandran Plot statistics

	No. of residues	%-tage
Most favored regions [A, B, L]	471	91.3%
Additional allowed regions [a,b,l,p]	43	8.3%
Generously allowed regions [~a,~b,~l,~p]	1	0.2%
Disallowed regions [XX]	1	0.2%*
Non-glycine and non-proline residues	516	100.0%
End-residues (excl. Gly and Pro)	1	
Glycine residues	61	
Proline residues	22	
Total number of residues	600	

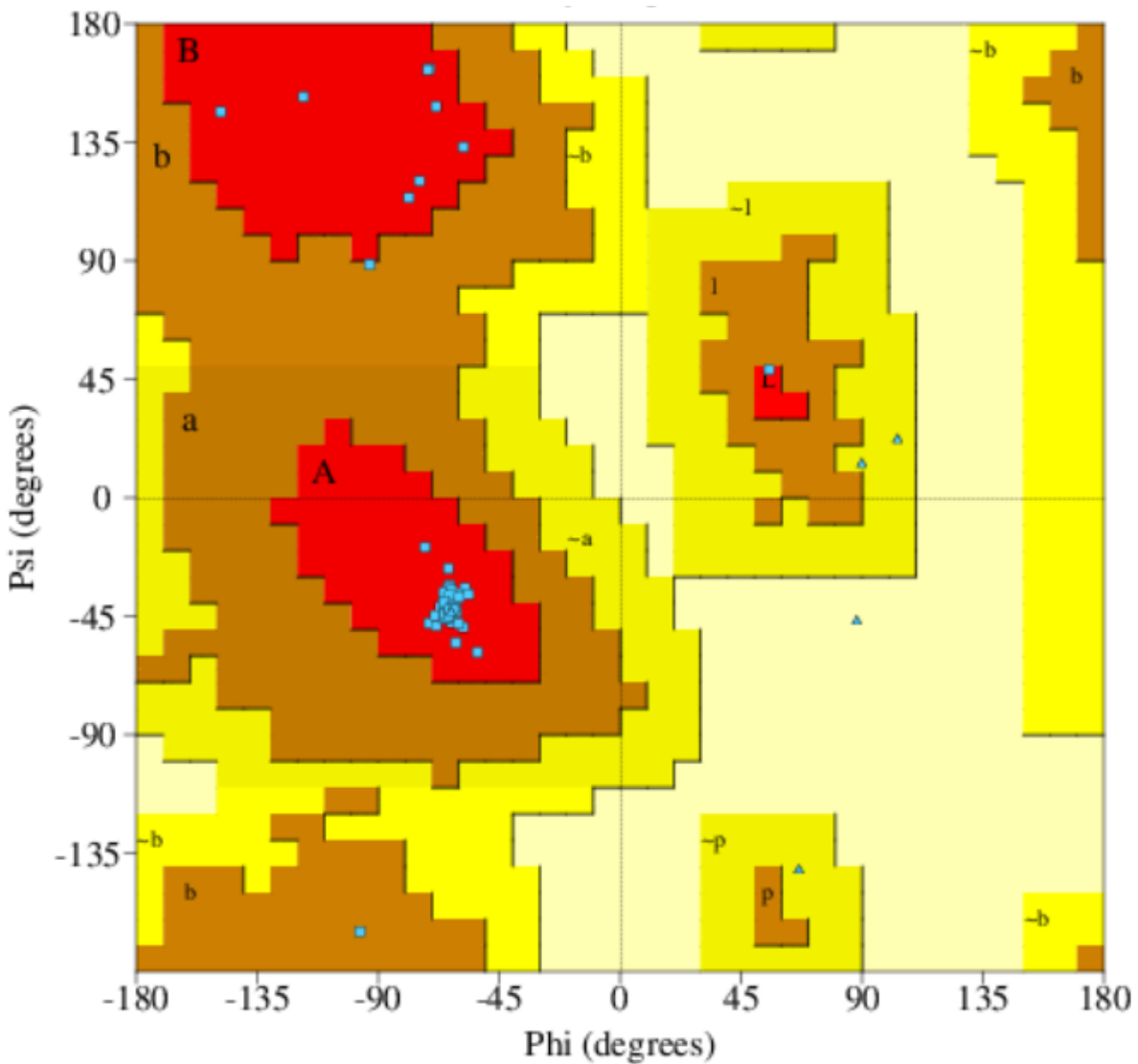
Supplementary Figure S3 (A). Ramachandran plot of Subunit A



Ramachandran Plot statistics

	No. of residues	%-tage
Most favored regions [A,B,L]	191	91.0%
Additional allowed regions [a,b,l,p]	17	8.1%
Generously allowed regions [~a,~b,~l,~p]	2	1.0%
Disallowed regions [XX]	0	0.0%
Non-glycine and non-proline residues	210	100.0%
End-residues (excl. Gly and Pro)	2	
Glycine residues	8	
Proline residues	15	
Total number of residues	235	

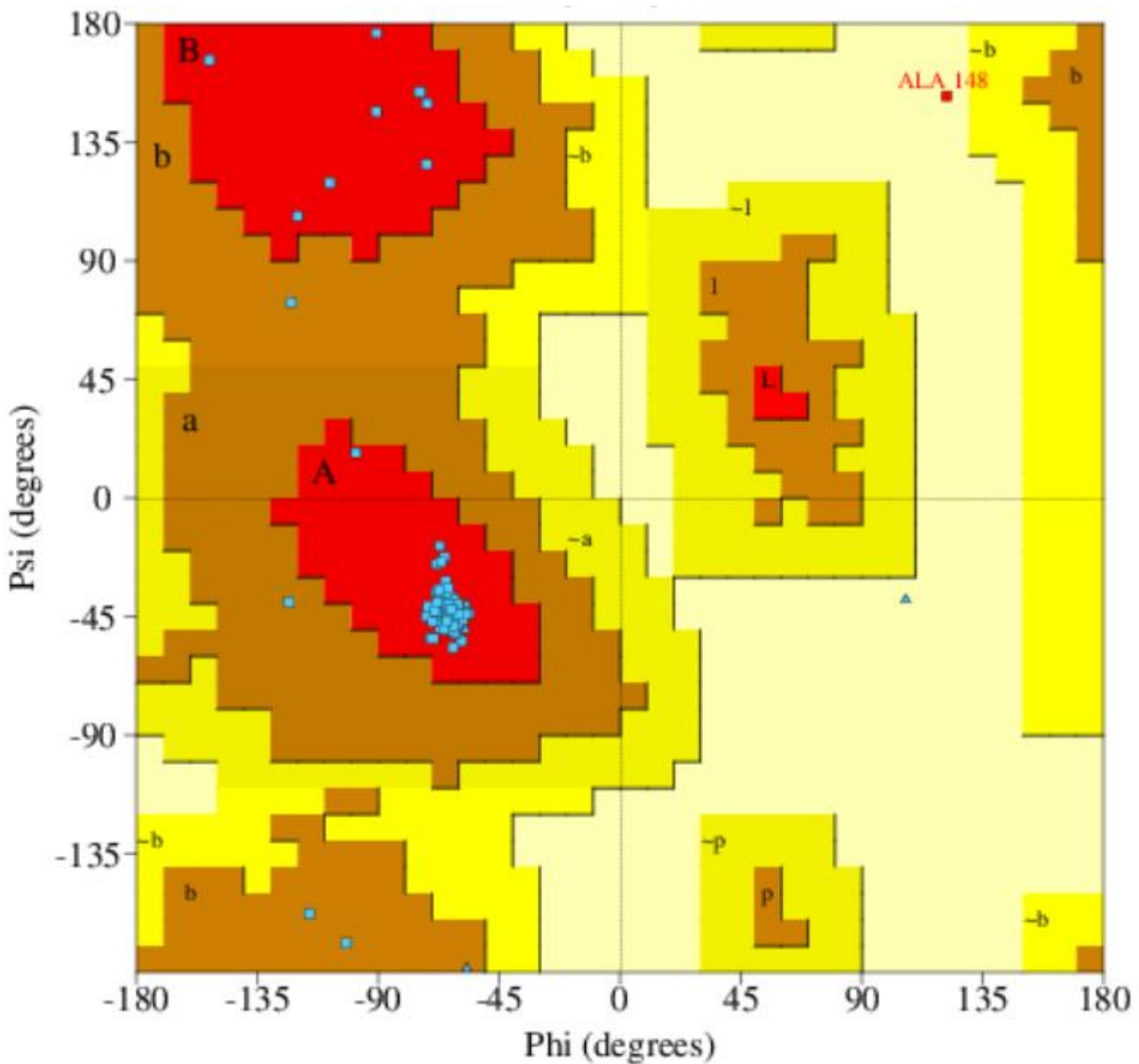
Supplementary Figure S3 (B). Ramachandran plot of Subunit B



Ramachandran Plot statistics

	No. of residues	%-tage
Most favored regions [A,B,L]	78	97.5%
Additional allowed regions [a,b,l,p]	2	2.5%
Generously allowed regions [~a,~b,~l,~p]	0	0.0%
Disallowed regions [XX]	0	0.0%
Non-glycine and non-proline residues	80	100.0%
End-residues (excl. Gly and Pro)	2	
Glycine residues	9	
Proline residues	3	
Total number of residues	94	

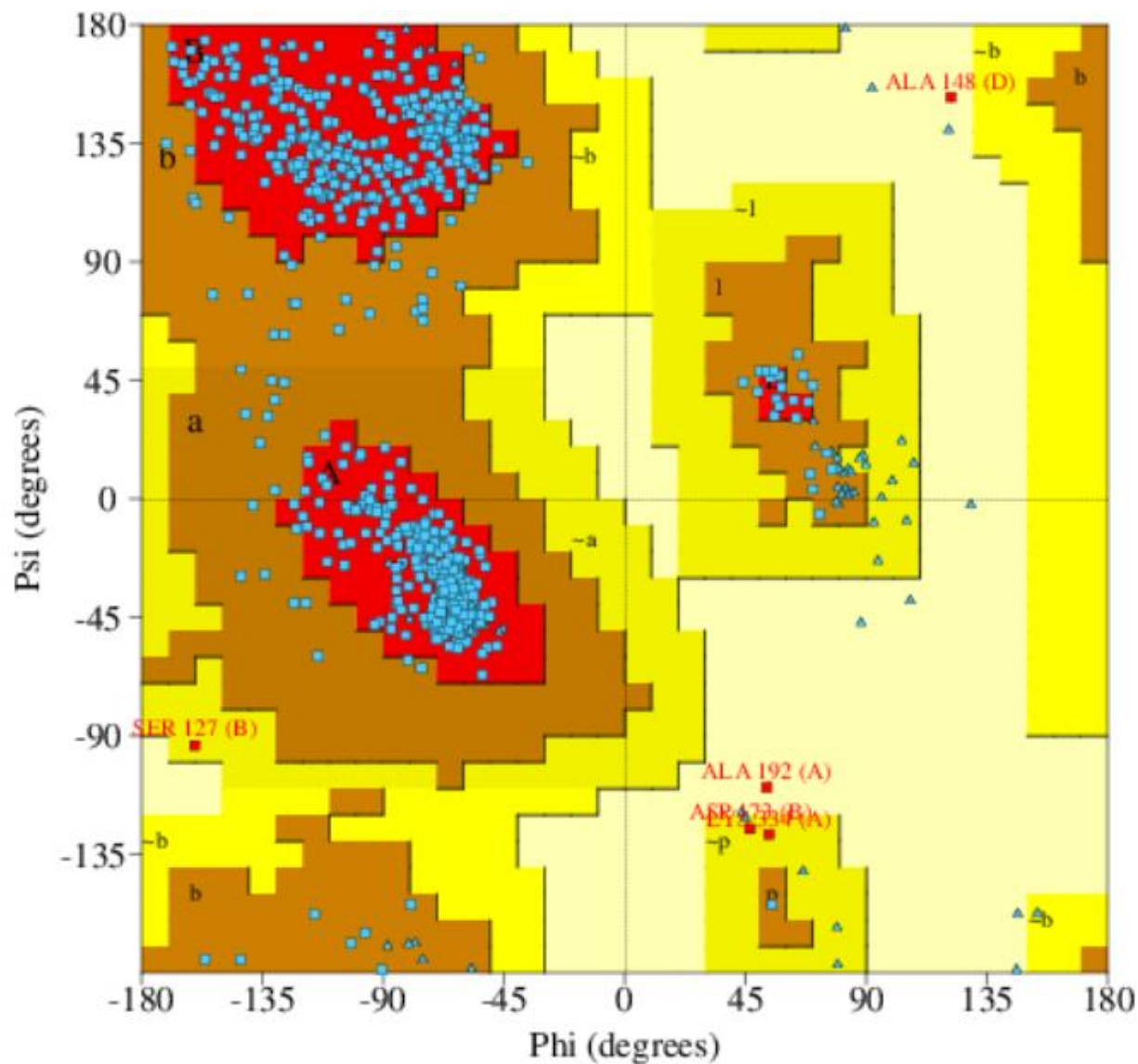
Supplementary Figure S3 (C). Ramachandran plot of Subunit C



Ramachandran Plot statistics

	No. of residues	%-tage
Most favoured regions [A,B,L]	81	94.2%
Additional allowed regions [a,b,l,p]	4	4.7%
Generously allowed regions [~a,~b,~l,~p]	0	0.0%
Disallowed regions [XX]	1	1.2%*
Non-glycine and non-proline residues	86	100.0%
End-residues (excl. Gly and Pro)	2	
Glycine residues	7	
Proline residues	6	
Total number of residues	101	

Supplementary Figure S3 (D). Ramachandran plot of Subunit D

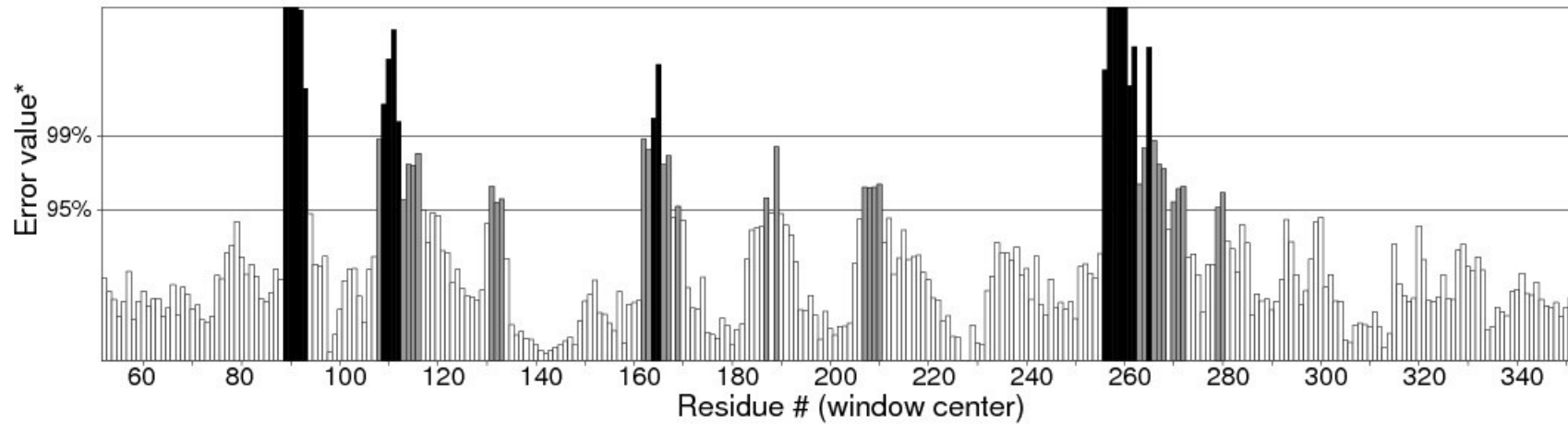


Ramachandran Plot statistics

	No. of residues	%-tage
Most favoured regions [A,B,L]	821	92.0%
Additional allowed regions [a,b,l,p]	66	7.4%
Generously allowed regions [~a,~b,~l,~p]	3	0.3%
Disallowed regions [XX]	2	0.2%*
Non-glycine and non-proline residues	892	100.0%
End-residues (excl. Gly and Pro)	7	
Glycine residues	85	
Proline residues	46	
Total number of residues	1030	

Supplementary Figure S3 (E). Ramachandran plot of complete model of SDH

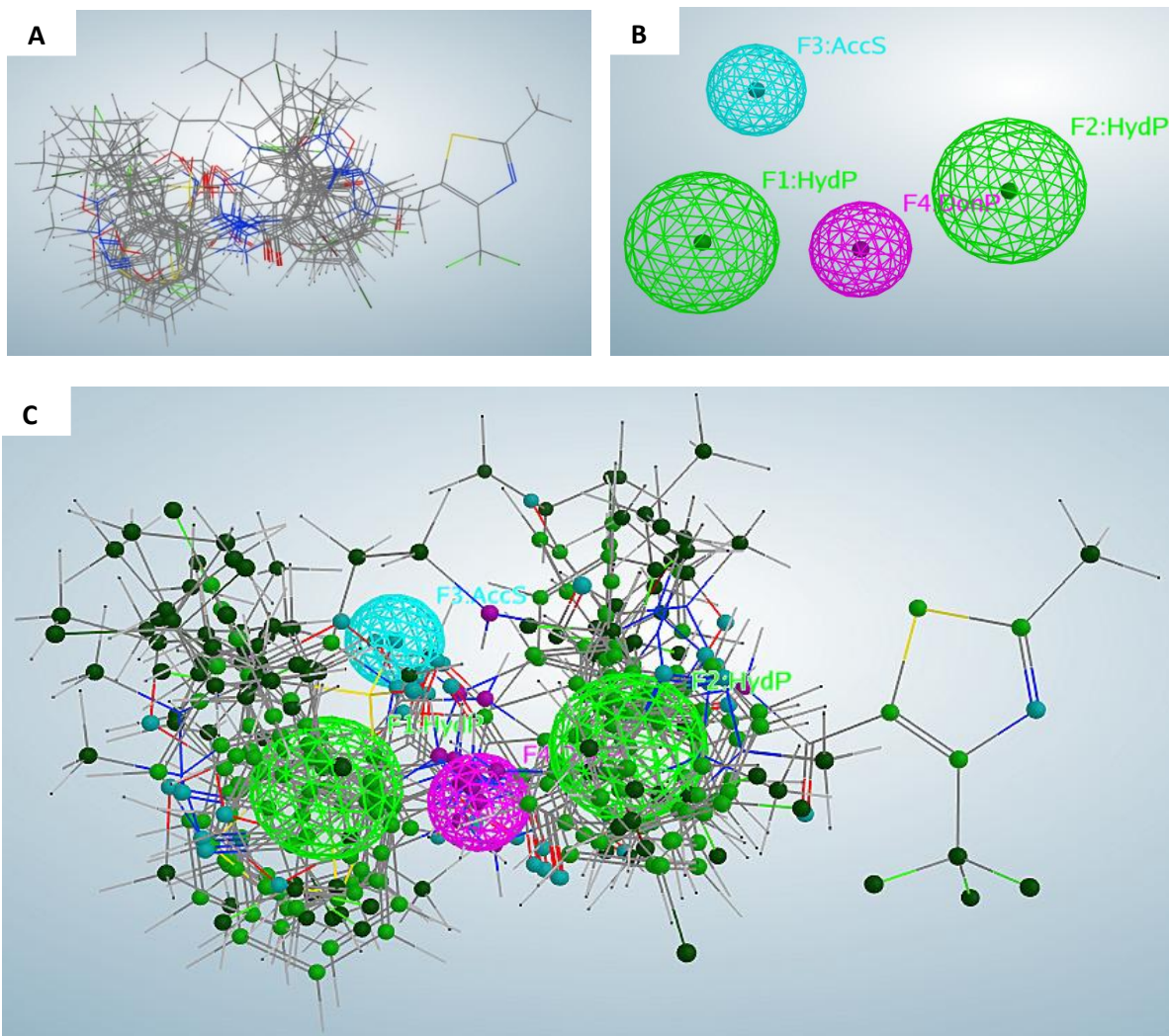
Program: ERRAT2
File: /var/www/SAVES/Jobs/2076096//errrat.pdb
Chain#:1
Overall quality factor**: 82.010



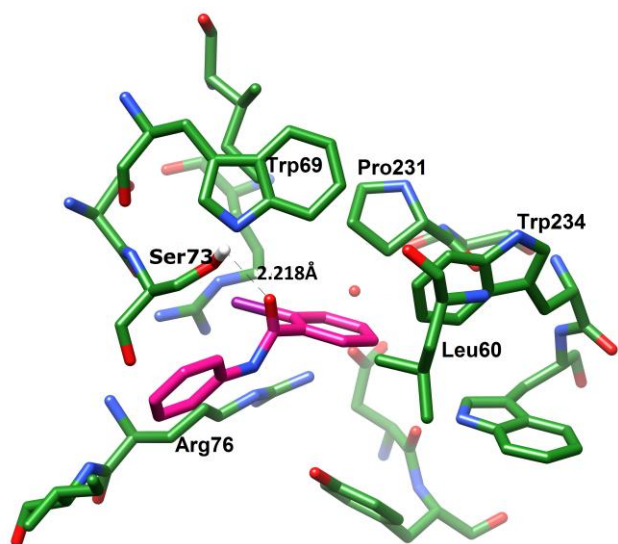
*On the error axis, two lines are drawn to indicate the confidence with which it is possible to reject regions that exceed that error value.

**Expressed as the percentage of the protein for which the calculated error value falls below the 95% rejection limit. Good high resolution structures generally produce values around 95% or higher. For lower resolutions (2.5 to 3Å) the average overall quality factor is around 91%.

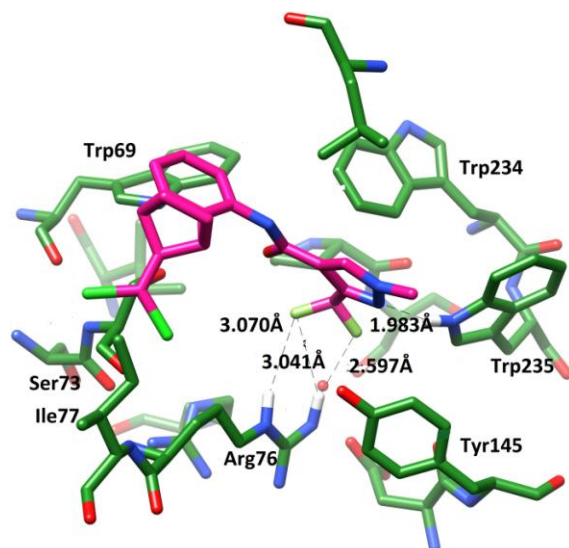
Supplementary Figure S4. ERRAT scores for the *A. solani* SDH model



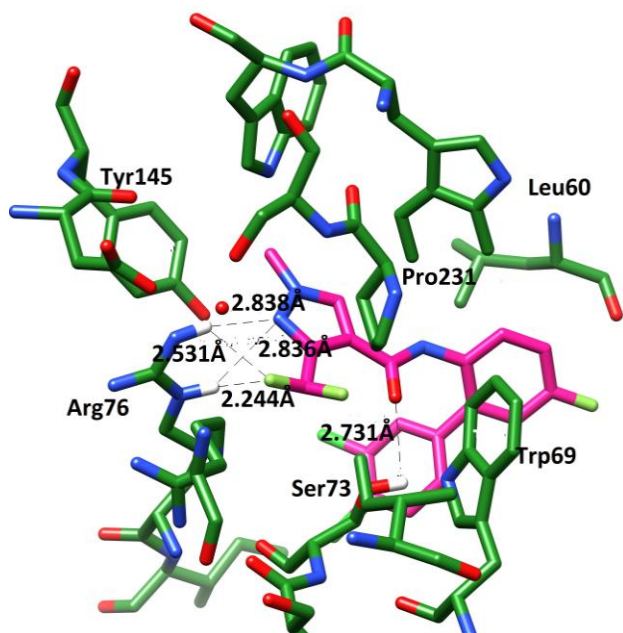
Supplementary Figure S5. (A) Superimposed view of 18 Fungicides (SDH inhibitors). The pharmacophoric features H-bond acceptor, H-bond donor, and Hydrophobic features are depicted in light blue, pink, and Green spheres, respectively (C) Superimposed view of 18 fungicides on the pharmacophore model.



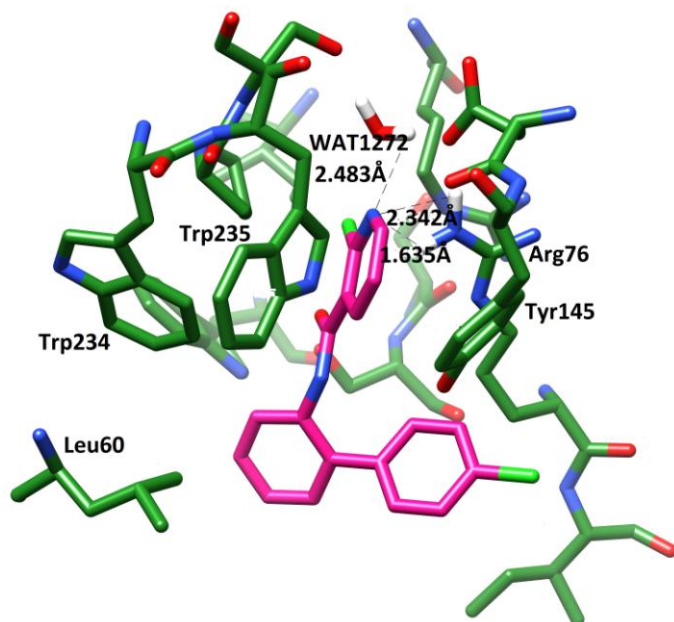
Benodanil



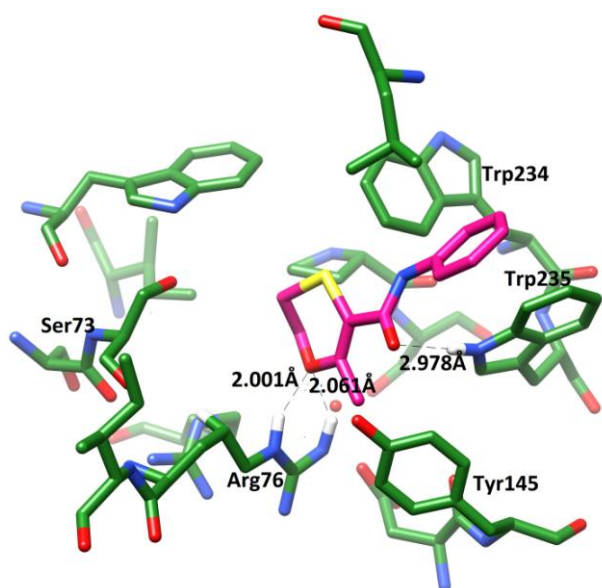
Benzovindiflupyr



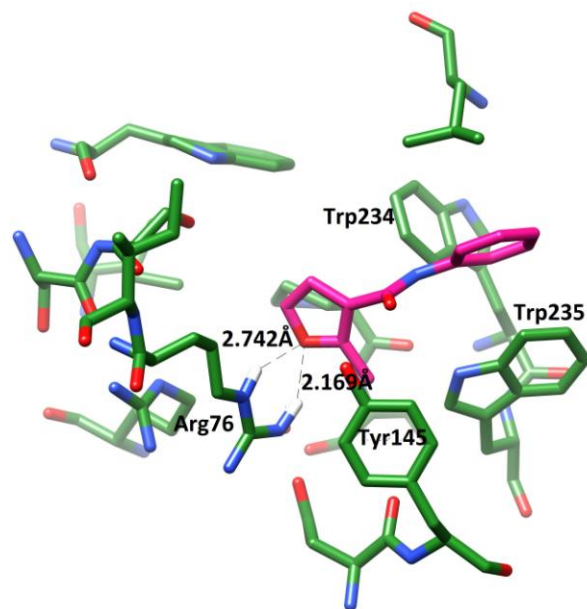
Bixafen



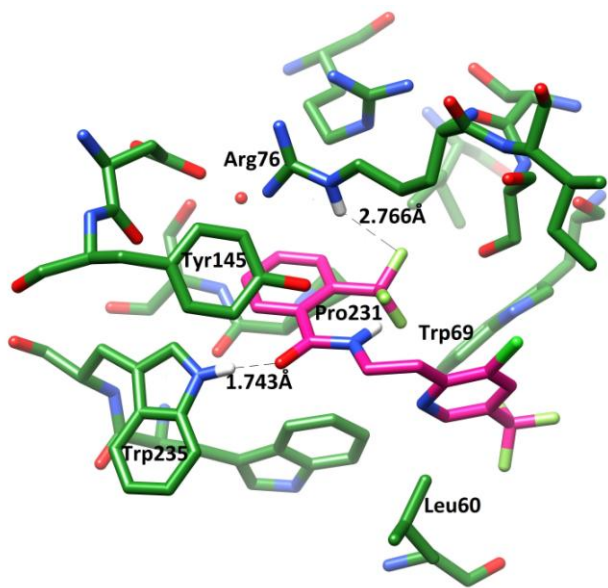
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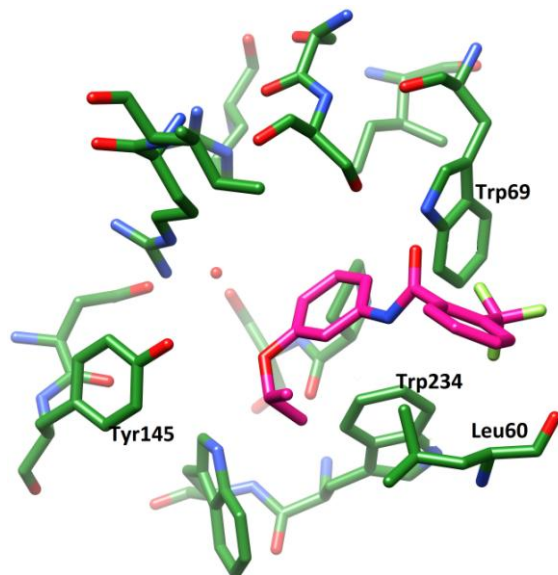
Carboxin



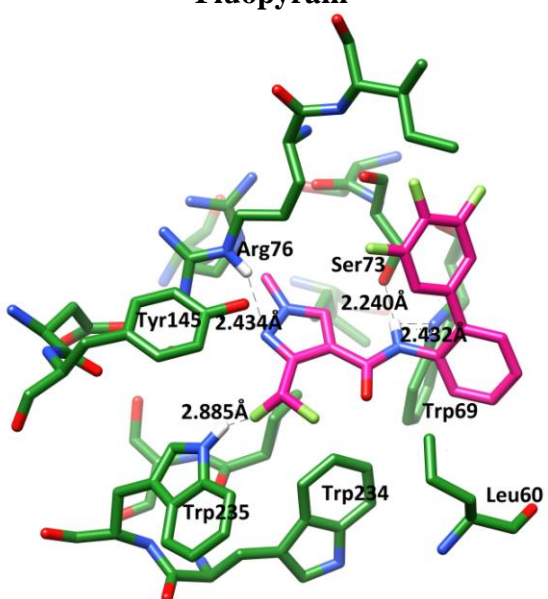
Fenfuram



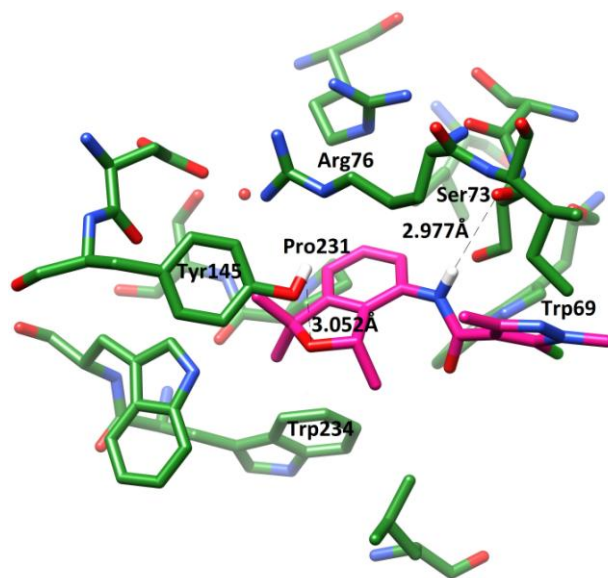
Fluopyram



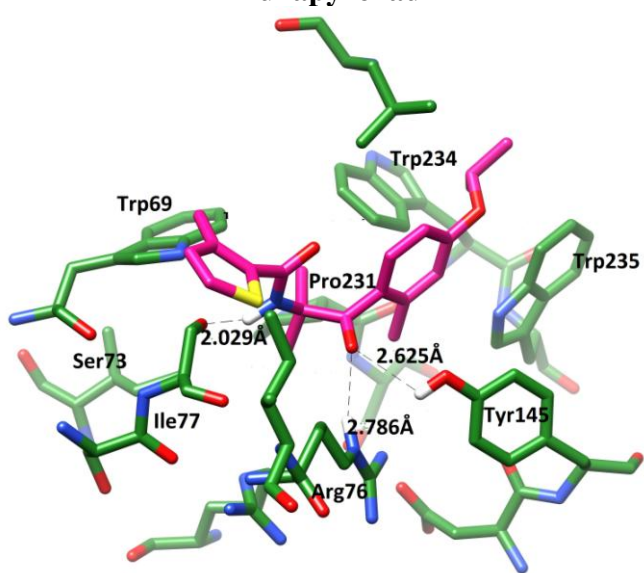
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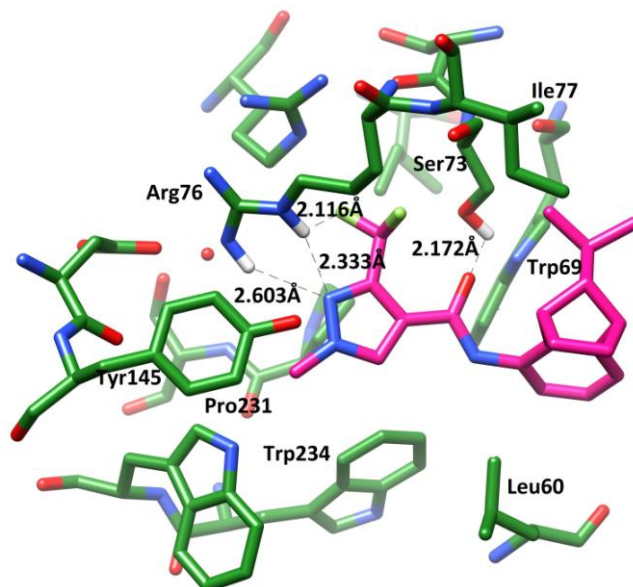
Fluxapyroxad



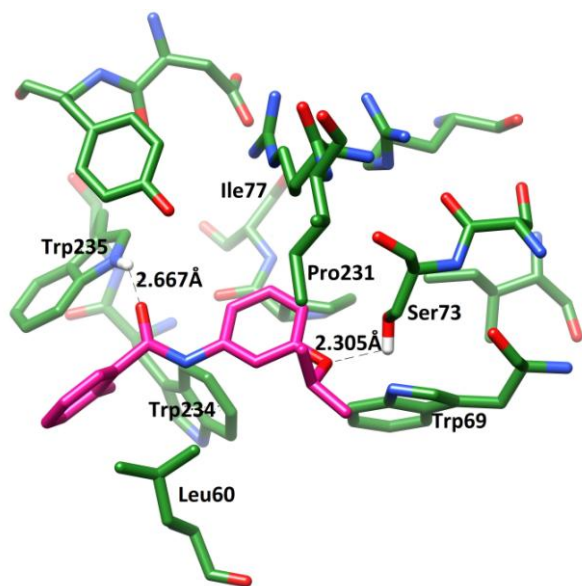
Furametpyr



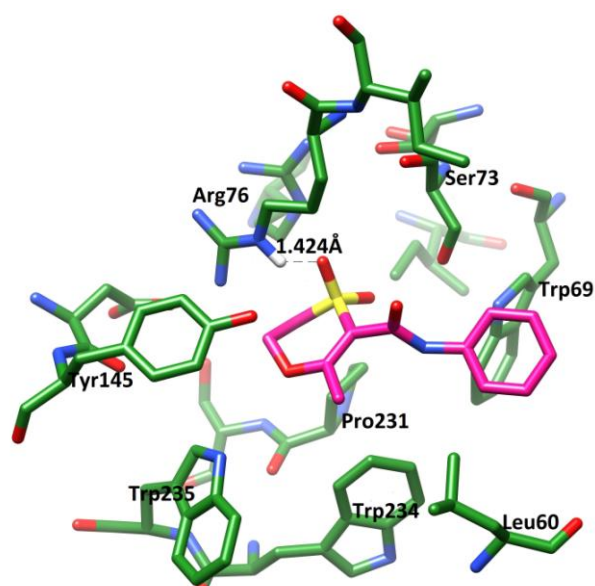
Isofetamid



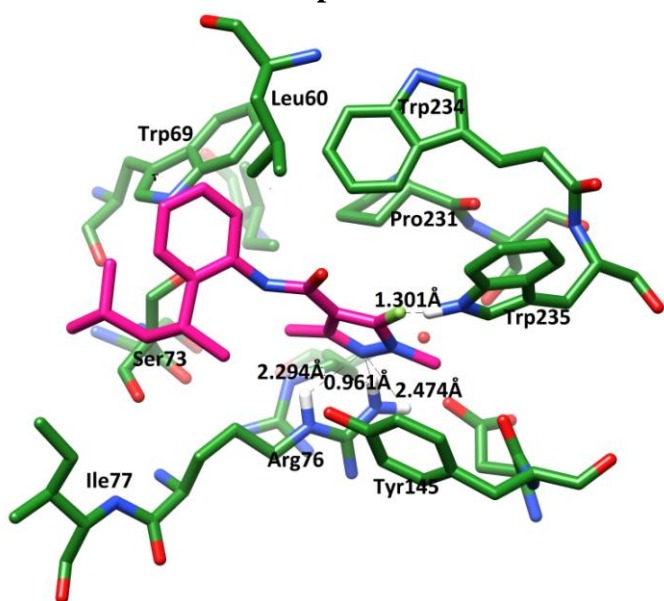
Isopyrazam



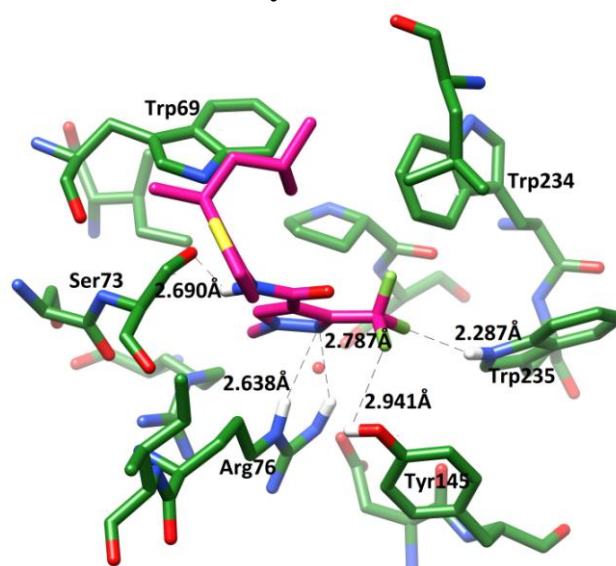
Mepronil



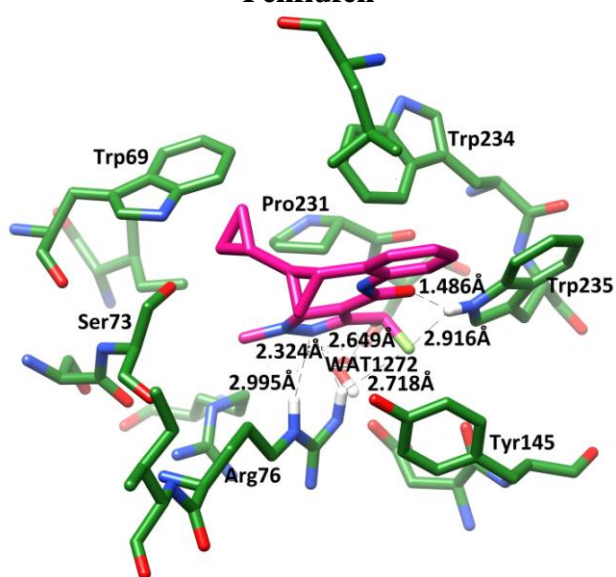
Oxycarboxin



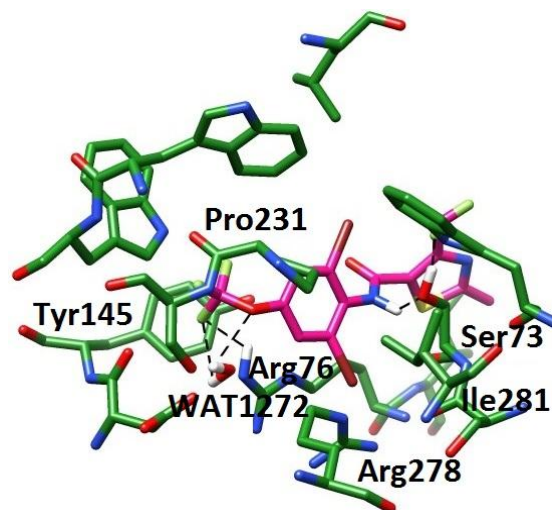
Penflufen



Penthiopyrad



Sedaxane



Thifluzamide

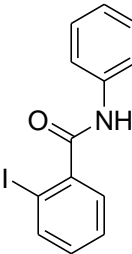
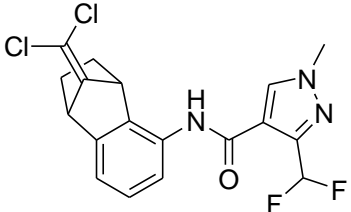
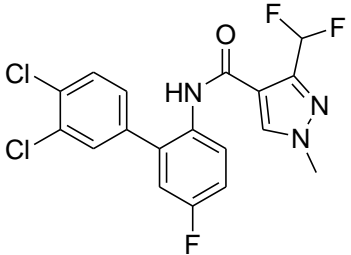
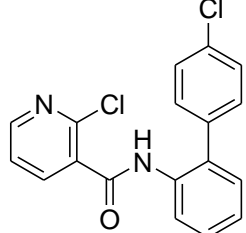
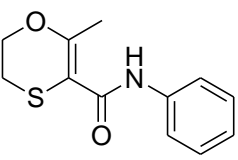
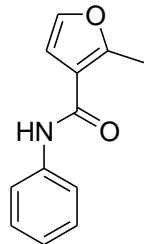
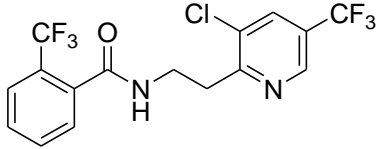
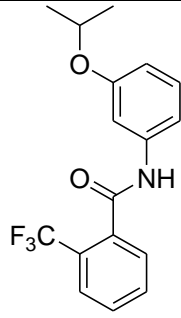
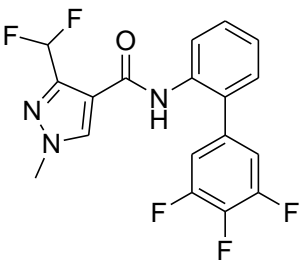
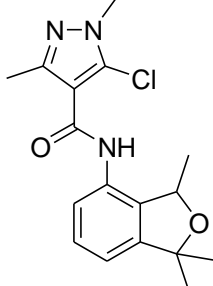
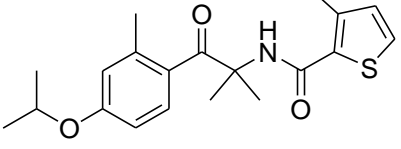
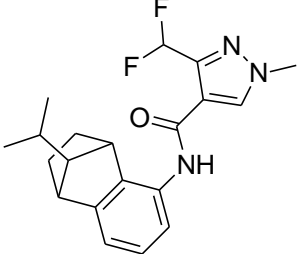
Supplementary Figure S6. The binding modes of 18 known SDHIs. The interacting residues are depicted in green stick and compounds in pink color. H-bonds are displayed in black dash lines.

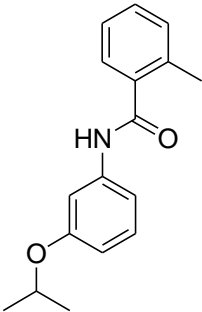
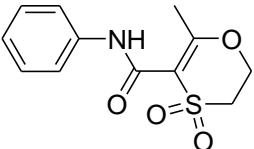
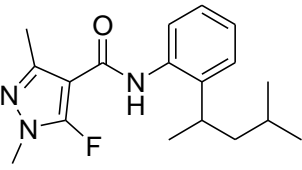
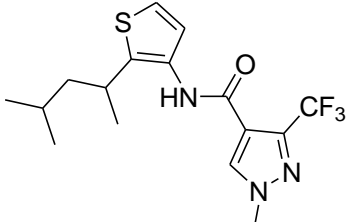
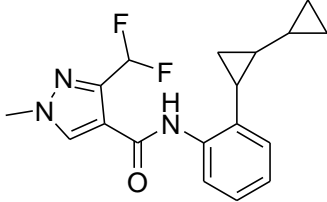
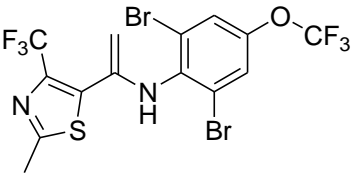
1.1 Supplementary Tables

Supplementary Table S1. Percent identities between *A. solani* SDHs and template sequences

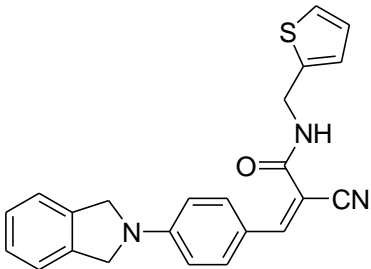
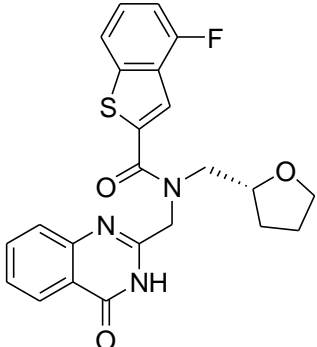
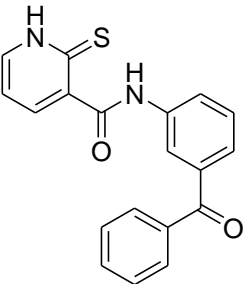
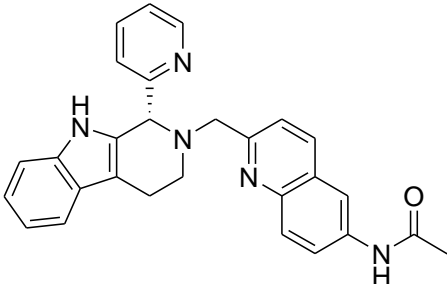
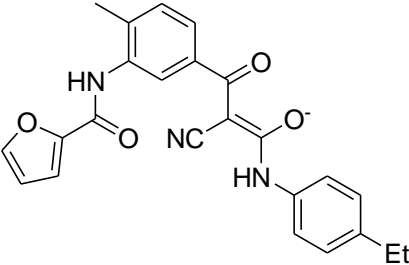
Subunit	Identity	PDB code	Organism	Protein name
SDH A	69%	1YQ3	<i>Gallus gallus</i>	Succinate dehydrogenase
	69%	1ZOY	<i>Sus scrofa</i>	Succinate:ubiquinoneoxidoreductase
	69%	4YTP	<i>Sus scrofa</i>	Succinate dehydrogenase
	62%	3VR8	<i>Ascarissuum</i>	Mitochondrial quinol-fumarate reductase
	62%	4YSX	<i>Ascaris suum</i>	Succinate dehydrogenase
	55%	1NEK	<i>Escherichia coli</i>	Succinate dehydrogenase
SDH B	69%	1YQ3	<i>Gallus gallus</i>	Succinate dehydrogenase
	67%	3ABV	<i>Sus scrofa</i>	Succinate dehydrogenase
	67%	1ZOY	<i>Sus scrofa</i>	Succinate:ubiquinoneoxidoreductase
	66%	3VR8	<i>Ascarissuum</i>	Quinol-fumarate reductase
	53%	1NEK	<i>Escherichia coli</i>	Succinate dehydrogenase
SDH C	37%	1ZOY	<i>Susscrofa</i>	Succinate:ubiquinoneoxidoreductase
	37%	2H88	<i>Gallus gallus</i>	Succinate dehydrogenase
	37%	1YQ3	<i>Gallus gallus</i>	Succinate dehydrogenase
	37%	2FLQ	<i>Geobacillusstearothermophilus</i>	Nitric Oxide Synthase
	36%	2FBW	<i>Gallus gallus</i>	Succinate dehydrogenase
	34%	1MJT	<i>Staphylococcus aureus</i>	Nitric-oxide synthase
	33%	2Y5B	<i>Homo sapiens</i>	Ubiquitin carboxyl-terminal hydrolase
	33%	3I3T	<i>Homo sapiens</i>	Ubiquitin carboxyl-terminal hydrolase
	33%	3MTN	<i>Homo sapiens</i>	Ubiquitin carboxyl-terminal hydrolase
	31%	3VR8	<i>Ascarissuum</i>	Quinol-fumarate reductase
SDH D	42%	2EOB	<i>Rattusnorvegicus</i>	1-phosphatidylinositol-4,5-bisphosphate phosphodiesterase
	36%	1ZOY	<i>Susscrofa</i>	Succinate:ubiquinoneoxidoreductase
	35%	1YQ3	<i>Gallus gallus</i>	Succinate dehydrogenase
	33%	1NP7	<i>Synechocystissp</i>	DNA photolyase
	31%	2JFK	<i>Homo sapiens</i>	Fatty acid synthase
	31%	2JFD	<i>Homo sapiens</i>	Fatty acid synthase
	31%	3HHD	<i>Homo sapiens</i>	Fatty acid synthase

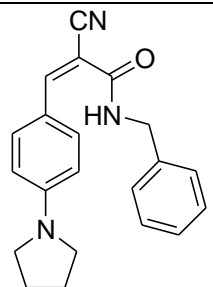
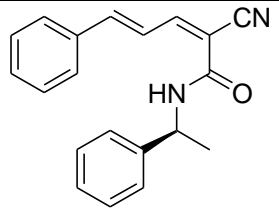
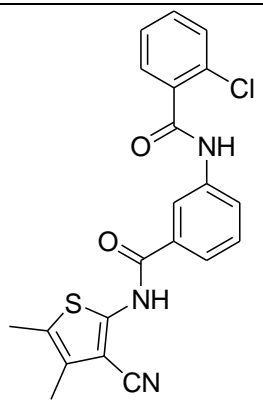
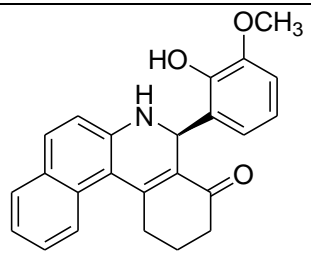
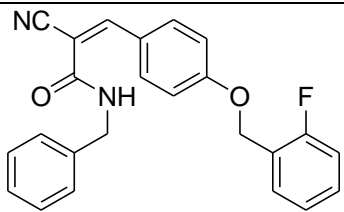
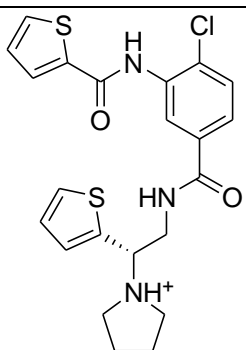
Supplementary Table S2. Chemical structure and Docking Scores of 18 known SDHIs (fungicides).

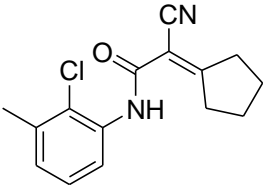
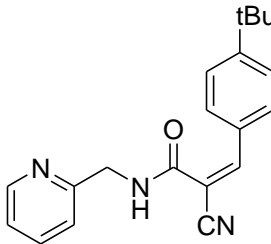
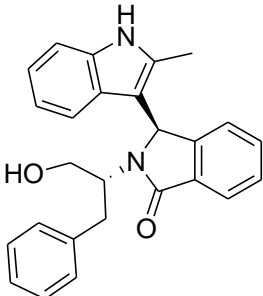
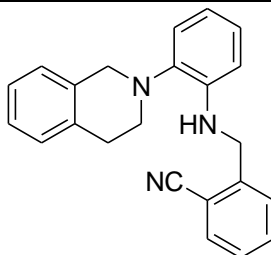
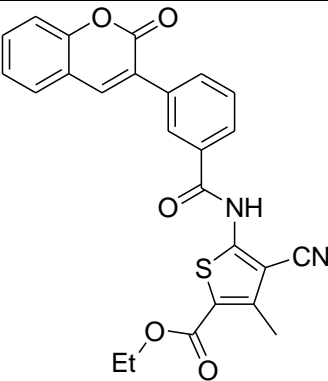
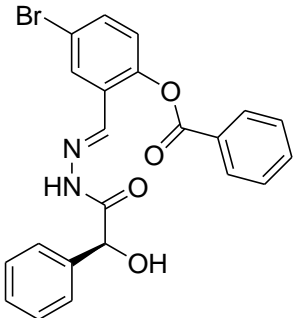
Sr.	Name	Chemical structure	Docking Scores	Sr.	Name	Chemical structure	Docking Scores
1	Benodanil		-9.45	2	Benzovindiflupyr		-9.69
3	Bixafen		-9.87	4	Boscalid		-10.47
5	Carboxin		-10.24	6	Fenfuram		-9.02
7	Fluopyram		-10.02	8	Flutolanil		-9.74
9	Fluxapyroxad		-9.96	10	Furametpyr		-10.63
11	Isofetamid		-10.46	12	Isopyrazam		-9.57

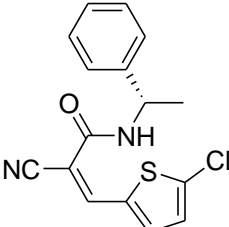
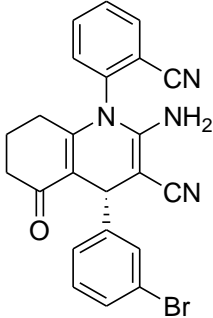
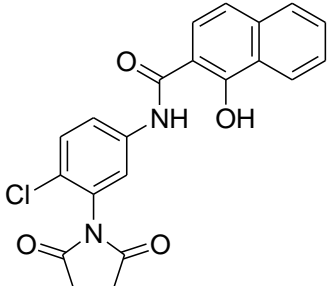
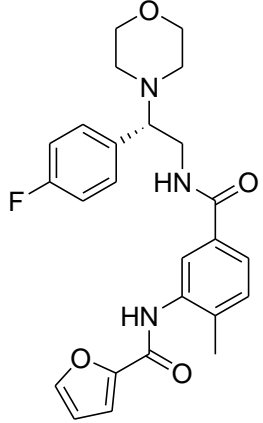
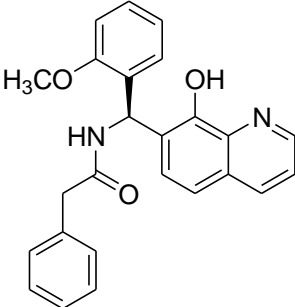
13	Mepronil		-10.51	14	Oxycarboxin		-11.07
15	Penflufen		-9.56	16	Penthiopyrad		-9.46
17	Sedaxane		-10.13	18	Thifluzamide		-11.67

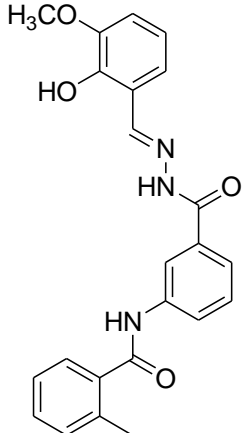
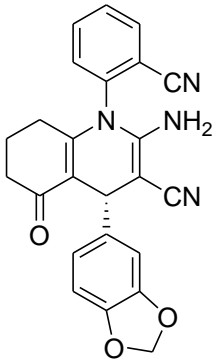
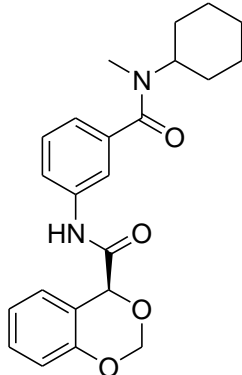
Supplementary Table S3. Chemical Structures and Docking Score of 25 compounds selected from ZINC database after docking, rescoring and interaction analysis

No.	ZINC ID	Compound Code	Structure	ADT Score	MOE Score
1	ZINC00781454	C1		-8.74	-5.2243
2	ZINC13037761	---		-8.25	-5.7331
3	ZINC78502784	---		-8.23	-5.2939
4	ZINC19837471	---		-8.22	-5.2954
5	ZINC50812116	---		-8.20	-4.4908

6	ZINC04498541	C2		-8.20	-5.2388
7	ZINC34378628	C12		-8.18	-5.1025
8	ZINC27260697	C3		-8.10	-4.1538
9	ZINC00795936	---		-8.00	-5.2242
10	ZINC32180696	C11		-8.00	-4.6726
11	ZINC36624363	---		-8.00	-4.6285

12	ZINC17007371	C10		-7.98	-4.4015
13	ZINC06512448	C9		-7.93	-4.8394
14	ZINC04731427	---		-7.87	-5.0271
15	ZINC32803988	---		-7.85	-4.3761
16	ZINC02409017	C4		-7.74	-4.5404
17	ZINC03102709	C6		-7.74	-4.95920

18	ZINC06183077	C8		-7.69	-3.4910
19	ZINC00689200	C5		-7.68	-3.7313
20	ZINC01436920	---		-7.68	-4.9843
21	ZINC18046772	---		-7.66	-4.4454
22	ZINC04903387	---		-7.63	-5.2351

23	ZINC05176439	C7		-7.61	-4.3706
24	ZINC00707182	---		-7.6	-3.5623
25	ZINC12196415	---		-7.60	-4.3058