Supplementary Data

Bioactive potential of secondary metabolites of rhizospheric fungus *Penicillium citrinum isolate-ABRF3*

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Supplementary Tables:

Table S1. *NMR spectra representing chemical shift range and type of compound.*

Sample	Chemical shift range, ppm	Type of compound	Type of proton
Ethyl oleate as standard	0.8	1° aliphatic	R-CH_3
	1.3	2° aliphatic	R_2-CH_2
	1.6	3° aliphatic	R_3-CH
	2.0	Carbonyl compounds	HC-C=O
	2.2	A To carbonyl (C is next to C=O)	R-CO-CH_3
EAF Column fraction of ABRF3	0.8	1° aliphatic	R-CH_3
	1.3	2° aliphatic	R_2-CH_2
	1.6	3° aliphatic	R_3-CH
	2.0	Carbonyl compounds	HC-C=O
	2.3	A To carbonyl (C is next to C=O)	R-CO-CH_3
	2.6	Alkynyl	RC≡C-H
	3.3	Ethers	HC-OR
	4.1	Esters	RCOO-CH
	5.3	Vinylic (H is attached to alkane C)	R_2C=HC-R

Table S2. *The zone of inhibition of column fractionation of ethanolic extract and antibiotic streptomycin tested against bacterial pathogen.*

Bacterial pathogen	**Zone of inhibition** [ƨ]						
	Column fraction of Ethanolic extract of *T. purpureogenus*					**Positive**[≠] **control Streptomycin**	**Negative**[≠] **control Ethanol**
	TOLUENE	**CHOLORORM**	**E. ACETATE**	**METHANOL**	**ACETONITRYLE**		
B.circulans (gram +ve)	Nd	11 ± 1.3	15.4 ± 1.25	Nd	16.16 ± 1.1	24.28 ±1.25	Nd
B.subtilis (gram +ve)	Nd	Nd	14.7 ± 1.15	Nd	15.81± 1.8	24.21 ± 0.93	Nd
S. aureus (gram +ve)	Nd	Nd	17.18 ± 1.3	Nd	17.16 ± 0.21	24.62 ± 1.05	Nd
R. eutrophae (gram –ve)	Nd	Nd	Nd	Nd	15.95 ± 1.03	25.33 ± 1.7	Nd

Nd-not detected

The superscript letters are significantly different ($p < 0.05$).

[ƨ]Inhibition zone excluding disc

[≠]6 mm disc as standard

Table S3. *Retention time of secondary metabolites and their respective retention time obtained by HPLC.*

No. of Peak	RT[min]	Area[mV*sec]	Area%	Height[mV]	Height%
1	2.1667	11.1491	0.76	0.8842	0.81
2	2.6	273.4511	18.76	21.8215	20.02
3	2.8667	522.3185	35.83	40.9223	37.55
4	3.0833	252.5314	17.32	19.6706	18.05
5	3.4333	82.9483	5.69	7.0892	6.51
6	3.95	94.3202	6.47	5.7981	5.32
7	4.55	88.2145	6.05	4.6661	4.28
8	4.6667	62.5403	4.29	4.2863	3.93
9	5	53.2769	3.65	3.2063	2.94
10	9.3167	17.1003	1.17	0.6333	0.58
		1457.851		108.9779	

Table S4. *Retention time of secondary metabolites and their respective retention time obtained by GCMS.*

No. of Peak	R. Time	I. Time	F. Time	Area	Area %	Height	Height %	A/H	Name
1	1.595	1.570	1.720	30367	0.08	7232	0.06	4.20	Carbon dioxide
2	1.783	1.720	1.865	35122557	93.61	10292604	89.58	3.41	Ethanol
3	2.050	2.035	2.080	10881	0.03	6861	0.06	1.59	2-propen-1-ol
4	2.100	2.080	2.140	195625	0.52	166660	1.45	1.17	Allyl fluoride
5	2.455	2.425	2.505	96682	0.26	68392	0.60	1.41	Ethyl acetate
6	2.545	2.515	2.575	46258	0.12	34265	0.30	1.35	Trichloromethane
7	2.597	2.575	2.660	286785	0.76	199316	1.73	1.44	1-propanol, 2-methyl
8	4.226	4.200	4.290	73414	0.20	38225	0.33	1.92	Ethane, 11-diethoxy
9	4.406	4.385	4.495	273613	0.73	118635	1.03	2.31	1-Butanol, 3-methyl-
10	4.522	4.495	4.605	103331	0.28	37515	0.33	2.75	1-Butanol, 2-methyl
11	5.261	5.220	5.305	68181	0.18	31318	0.27	2.18	Toluene
12	8.543	8.480	8.575	119969	0.32	37169	0.32	3.23	L-lactic acid
13	22.146	22.105	22.190	98328	0.26	48689	0.42	2.02	2-Propenoic Acid
14	25.358	25.330	25.420	26695	0.07	14009	0.12	1.91	Cyclopropanecaroxylic acid, undec-2 en
15	25.493	25.730	25.535	91693	0.24	42179	0.37	2.17	Hexadecanoic acid, ethyl ester
16	25.771	25.450	25.815	50250	0.13	20492	0.18	2.45	Trans-3,6-Dimethoxy-2-ethoxy-beta-meth
17	27.315	27.255	27.350	526046	1.40	208612	1.82	2.52	Linolenic acid ethyl ester
18	27.382	27.350	27.450	299783	0.80	117939	1.03	2.54	(E)-9-Octadecenoic acid ethyl ester
				37520458	100.00	11490112	100.00		

Table S5. *The wavenumber ranges for common functional groups obtained by FTIR.*

S. No.	Wavenumber (cm^{-1})	Functional group identified/Peak description
Obtained peak from ethyl acetate fraction of isolate ABRF3		
1	1011.71	CH_2 rocking
2	1077.29	C-O stretching
3	1188.2	C-OH rocking C-C stretching due to carboxylic acid, ether alcohol and esters
4	1376.27	C-H scissoring and bending vibrations
5	1458.25	COO- symmetric stretching
6	1519.97	C-N symmetric stretching
7	1703.22	C=O stretching
8	2010.88	C=C conjugated and C ≡C
9	2158.44	C≡C stretchdue to alkyne
10	2312.75	O-H bond
11	2929.03	CH_2 Asymmetric stretching
12	3134.46	OH stretch due to phenol and alcohol
13	3189.43	OH stretch due to phenol and alcohol
Obtained peak from acetonitrile fraction of isolate ABRF3		
1	1034.85	CH_2 rocking
2	1082.11	C-N symmetric stretching
3	1412.92	COO- symmetric stretching
4	1601.95	Carbonyl group
5	2138.18	Carbonyl group
6	2350.36	O-H bond
7	2945.43	OH stretch due to carboxylic acid
8	3260.8	OH stretch due to carboxylic acid

Table S6. *Fungal extract and their respective diameters of spots generated during Spot Assay along with control systems using S. cerevisiae BY4742.*

S. cerevisiae	**spots generated during Spot Assay** [a]				
	C	**C + E3**	**Positive[≠] control**		**Negative[≠] control**
			C + Ac	**C+ Ra**	**C+ Ny**
BY4742 strain	09 ± 0.62	13± 1.2	15± 1.07	17 ± 0.96	Nd

C- BY4742 yeast culture, C+E2- BY4742 yeast culture and ABRF2 extract, C+Ac- BY4742 yeast culture and Acarbose, C+ Ra- BY4742 yeast culture and Rapamycin, C+Ny- BY4742 yeast culture and fluconazole (Nystatin), Nd-not detected
The superscript letters are significantly different ($p < 0.05$).

Table S7. *Comparison between binding energy score (KCal/mol) from molecular docking for the compound (E)-9-Octadecenoic acid ethyl ester in antiaging and anticancer targets active site and to identify the probable mechanism of action.*

Molecule	**Targets used for molecular docking**						
	Binding energy (KCal/mol) of different targets for Antiaging molecular docking			**Binding energy (KCal/mol) of different targets for Anticancer molecular docking**			
	2L7E (SITE 1)	**2KM1 (SITE 8)**	**1AH8 (SITE 2)**	**6AU4 (SITE 4)**	**1MP8 (SITE 2)**	**3SSU (SITE 1)**	**1ELK (SITE 7)**
Doxorubicin	-10.9025	-12.0442	-22.4970	-20.4928	-26.9348	-10.5860	-23.8014
Metformin	-8.5177	-8.1610	-9.0651	-11.1820	-10.3616	-6.2210	-9.8247
Noscapine	-10.2413	-10.5427	-15.8712	-13.3896	-18.8507	-8.6372	-18.6032
Sirolimus	-8.7966	-6.2886	-19.4638	-10.1449	-9.0860	-8.9583	-12.9013
(E)-9-Octadecenoic acid ethyl ester	-10.4237	-11.1234	-10.0245	-10.7816	-11.2795	-8.1199	-11.8709

Table S8. *Comparison between binding energy score (KCal/mol) from molecular docking for the compound (E)-9-Octadecenoic acid ethyl ester with antiaging active sites to identify the probable mechanism of action in humans.*

Molecule	**Targets used for molecular docking in humans**		
	Binding energy (KCal/mol) of different targets for Antiaging molecular docking		
	1US7 Site	**4ZZH Site**	**5UGW Site 11**
Epigallocatechin galate	-30.0440	-15.0544	-18.5853
Metformin	-10.2450	-7.1900	-7.6913
Sirolimus	-17.0859	-9.4645	-10.7863
(E)-9-Octadecenoic acid ethyl ester	-10.6175	-10.9107	-10.3405

Supplementary Figures Legends

Figure SF1

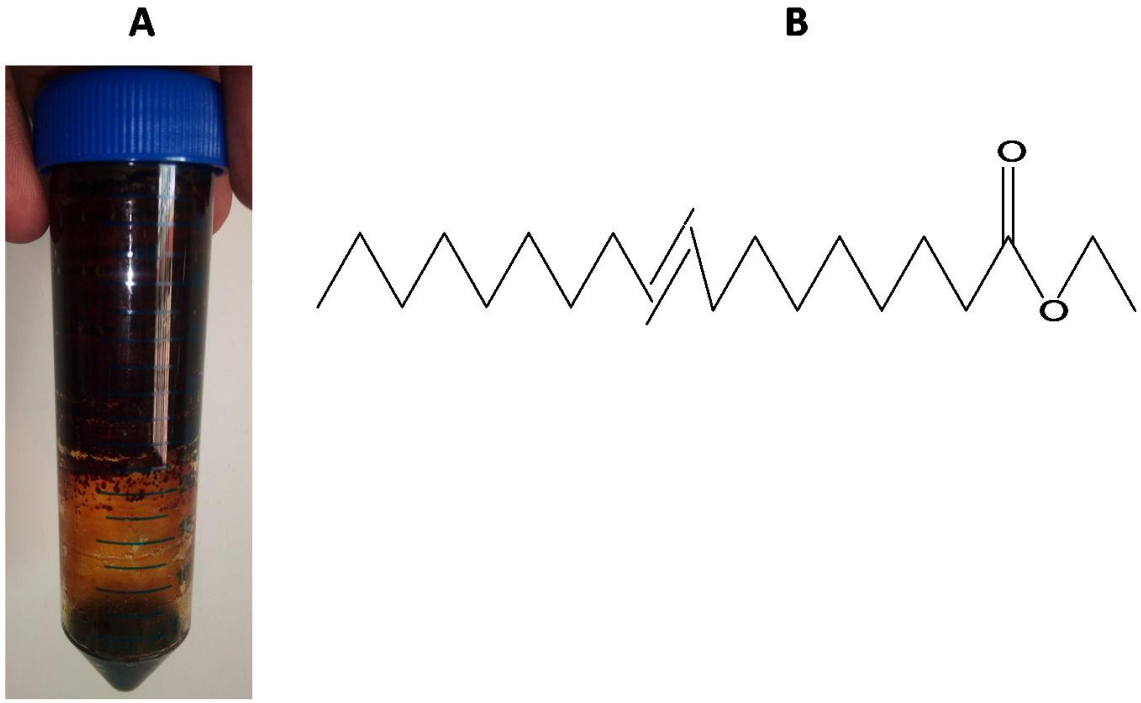

Figure SF1. *Fungal secondary metabolites isolated from Penecillium citrinum-ABRF3.* (A) Isolated brown sticky crude extract obtained from the *Penecillium citrinum-ABRF3* fungal strain. (B) Structure of the molecule (E)-9-Octadecenoic acid ethyl ester obtained by NMR spectrometry.

Figure SF2

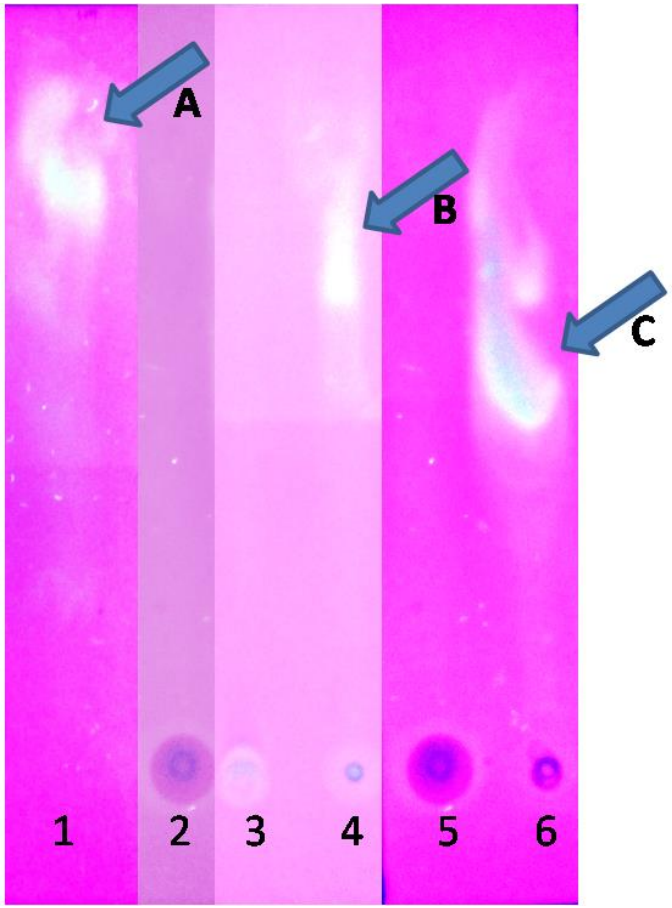

Figure SF2. *Chromatographic TLC analysis and visualization of spots undertaken in UV chamber.* (1) Crude ethanolic extract (100%), (2) Toluene soluble Column fraction, (3) Chloroform soluble Column fraction, (4) Ethyl Acetate soluble Column fraction, (5) Methanol soluble Column fraction, and (6) Acetonitrile soluble Column fraction.

Figure SF3

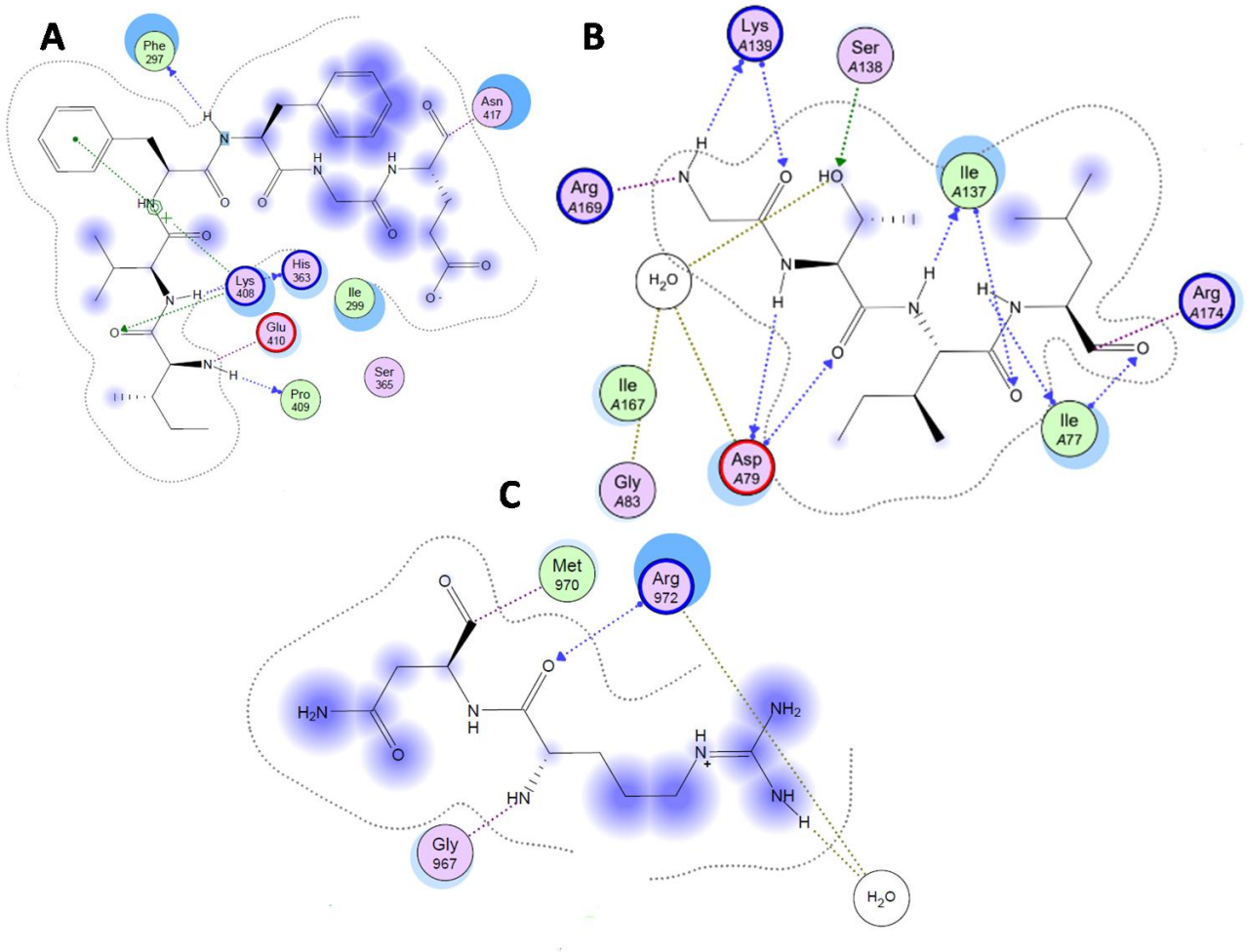

Figure SF3. *Molecular docking and 2D interaction*. Diagram showing (E)-9-Octadecenoic acid ethyl ester compound docking pose interaction with the key amino acids in the different Human antiaging targets active site. (**A)** (E)-9-Octadecenoic acid ethyl ester with

4ZZH: SIRT1/Activator Complex. Human SIRT1 construct (mini-hSIRT1) containing the minimal structural elements required for lysine deacetylation and catalytic activation by small-molecule sirtuin-activating compounds (STACs). **(B)** (E)-9-Octadecenoic acid ethyl ester with 1US7: Complex of Hsp90 and P50. The Mechanism of Hsp90 Regulation by the Protein Kinase-Specific Cochaperone p50(Cdc37). **(C)** (E)-9-Octadecenoic acid ethyl ester with 5UGW: Transferase. Interaction with crystal structure of the major quadruplex formed in the human telomerase thumb domain. (Distance in Å).