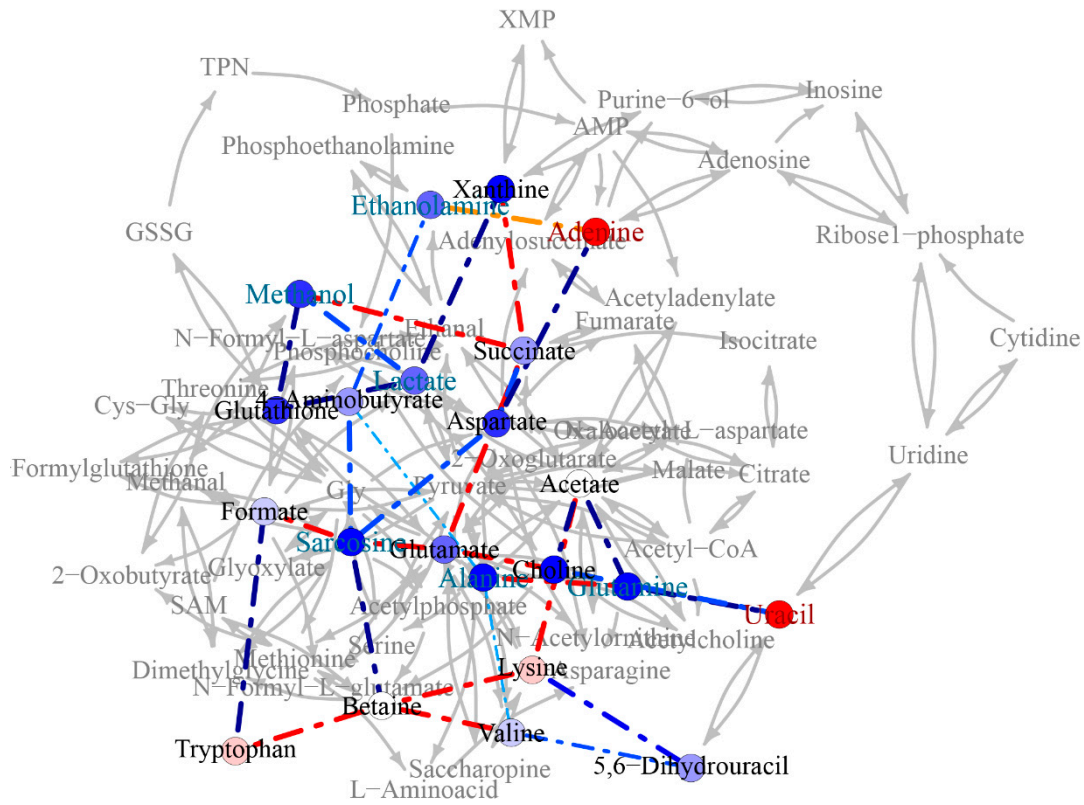


# The Antifungal Potential of Carvacrol against *Penicillium Digitatum* through <sup>1</sup>H-NMR Based Metabolomics Approach

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Table S1. Chemical shifts assignment of metabolites.

No	Metabolites	Chemical Shifts (ppm)
1	Isoleucine	0.92–0.945, 1.005–1.025, 1.215–1.305, 3.66–3.685
2	Leucine	0.96–0.975, 0.945–0.955, 1.65–1.70
3	Valine	0.98–1.005, 1.03–1.06, 2.245–2.28, 3.62–3.64
4	Lactate	1.325–1.355
5	Alanine	1.47–1.5, 3.775–3.805
6	Lysine	1.70–1.765, 1.90–1.94, 2.995–3.035
7	Putrescine	1.765–1.795, 3.035–3.055
8	4-Aminobutyrate	1.87–1.90, 2.28–2.325, 2.975–3.005
9	Acetate	1.94–1.95
10	Glutamate	2.025–2.105, 2.325–2.375
11	Acetaminophen	2.13–2.145, 6.88–6.925, 7.175–7.21
12	Succinate	2.395–2.415
13	Glutamine	2.45–2.485, 2.15–2.175
14	Glutathione	2.49–2.525, 2.545–2.58
15	5-6-Dihydrouracil	2.625–2.675, 3.39–3.425
16	Aspartate	2.675–2.725, 2.79–2.85, 3.875–3.895
17	Sarcosine	2.755–2.77, 3.63–3.64
18	Phenylalanine	3.11–3.13, 3.25–3.31
19	Ethanolamine	3.13–3.16
20	Choline	3.20–3.215
21	Betaine	3.24–3.25, 3.875–3.885
22	Arginine	3.25–3.275, 1.95–1.96
23	Methanol	3.355–3.365
24	Glycine	3.56–3.575
25	$\pi$ -Methylhistidine	3.745–3.75
26	Uracil	4.22–4.245, 4.34–4.375, 5.89–5.93
27	Tryptophan	7.25–7.29, 7.525–7.55, 7.72–7.745
28	Xanthine	7.91–7.93
29	Adenine	8.195–8.25
30	Formate	8.455–8.47



**Figure S1.** Correlation network analysis of D group at 12 h. The correlation of NMR was connected by dotted lines, colored according to Pearson correlation coefficient, and assisted with biochemical reaction by grey solid lines. Red and blue metabolites increased or decreased significantly. According to the corresponding folding changes, the circle is filled with color.