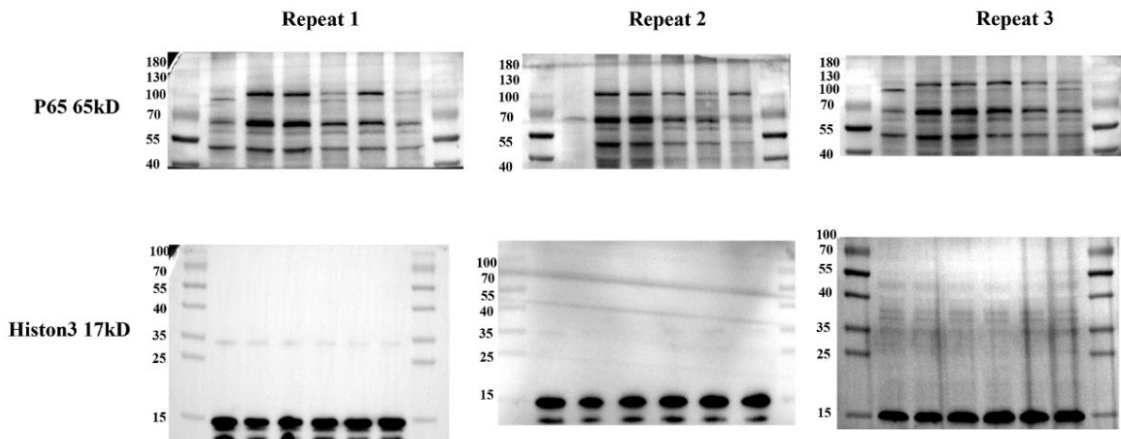
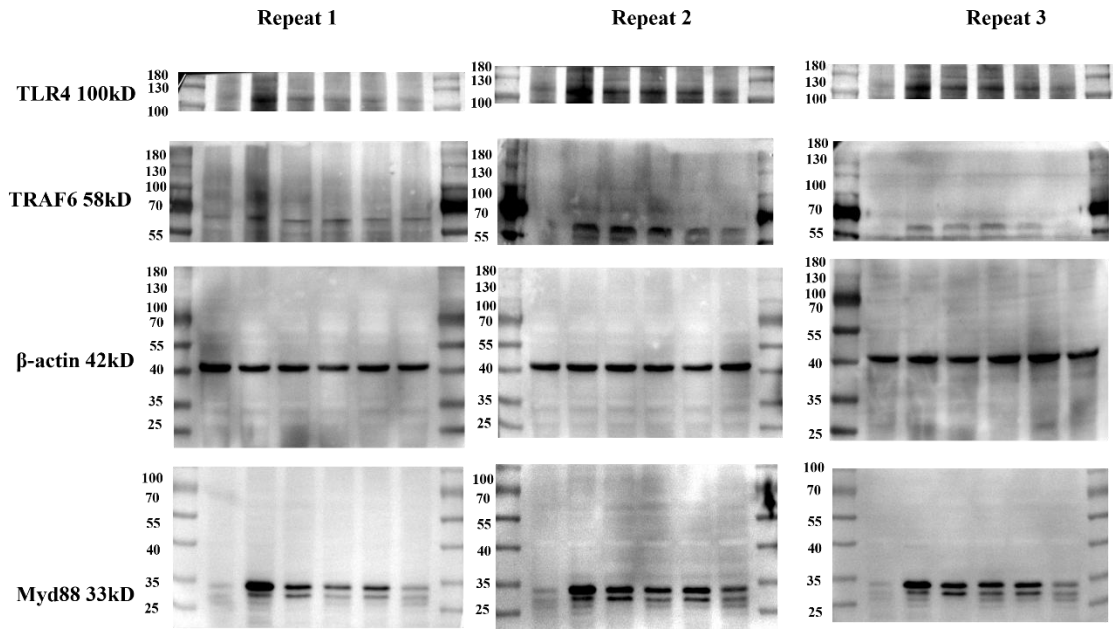


**Supplementary Figure 1 Molecular Docking.** A-D: Modified PD compound ligands dock to LPS (A), TLR4 (B), MyD88 (C), TRAF6 (D) and NF- $\kappa$ B (D).



Supplementary Figure 2 Example of original western blot for three repeats.

**Supplementary Table 1 Characterization of chemical constituents in Modified PD by liquid chromatography-mass spectrometry**

RT (min)	Formula	[M±H] <sup>±</sup> (m/z)			Reference ion	Identification
		Theoretical	Measured	Error (ppm)		
1.06	C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>	155.0696	156.0768	1.00727	[M+H] <sup>+</sup>	L-Histidine
1.29	C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>	147.0531	295.1134	148.0603	[2M+H] <sup>+</sup>	L-Glutamic Acid
1.39	C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub>	115.0636	116.0709	1.00728	[M+H] <sup>+</sup>	D-Proline
1.39	C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O <sub>5</sub>	243.0855	244.0927	1.00727	[M+H] <sup>+</sup>	Cytarabine
2.66	C <sub>5</sub> H <sub>7</sub> NO <sub>3</sub>	129.0429	130.0502	1.00728	[M+H] <sup>+</sup>	D-Pyroglutamic Acid
2.89	C <sub>9</sub> H <sub>11</sub> N O <sub>3</sub>	164.0475	182.0814	18.03385	[M+NH <sub>4</sub> ] <sup>+</sup>	L-Tyrosine
4.48	C <sub>10</sub> H <sub>13</sub> N O <sub>4</sub>	267.0968	268.1041	1.00728	[M+H] <sup>+</sup>	Adenosine
5.49	C <sub>11</sub> H <sub>20</sub> N O <sub>3</sub>	228.1477	229.1557	1.00727	[M+H] <sup>+</sup>	Prolylleucine
5.90	C <sub>9</sub> H <sub>11</sub> N O <sub>2</sub>	165.0778	164.0706	-1.00727	[M-H] <sup>-</sup>	L- Phenylalanine
7.18	C <sub>11</sub> H <sub>12</sub> N O <sub>2</sub>	204.0891	203.0818	-1.00728	[M-H] <sup>-</sup>	D-Tryptophan
9.86	C <sub>9</sub> H <sub>6</sub> O <sub>4</sub>	178.0267	179.0348	1.00728	[M+H] <sup>+</sup>	Esculetin

10.7	C <sub>20</sub> H <sub>17</sub> N	303.0886	336.122	33.033	[M+H+MeO	Berberine
55	O <sub>4</sub>			49	H] <sup>+1</sup>	
11.1	C <sub>10</sub> H <sub>8</sub> O <sub>5</sub>	208.0364	207.029	-	[M-H] <sup>-1</sup>	Fraxetin
57			1	1.0072		
11.9	C <sub>15</sub> H <sub>16</sub> O	340.0792	339.071	-	[M-H] <sup>-1</sup>	Esculin
8	9		9	1.0072		
14.8	C <sub>15</sub> H <sub>12</sub> O	256.0734	257.080	1.0072	[M+H] <sup>+1</sup>	Iso- liquiritigenin
7	4		7	8		
15.1	C <sub>26</sub> H <sub>30</sub> O	470.1938	471.201	1.0076	[M+H] <sup>+1</sup>	Limonin
38	8		5	2		
15.8	C <sub>26</sub> H <sub>30</sub> O	454.1988	455.206	1.0072	[M+H] <sup>+1</sup>	Obacunone
56	7			2		
16.2	C <sub>59</sub> H <sub>96</sub> O	1220.617	1265.61	44.998	[M+FA-H] <sup>-1</sup>	Anemoside B4
86	26		5	11		
19.7	C <sub>42</sub> H <sub>64</sub> O	841.4466	842.453	1.0072	[M+H] <sup>+1</sup>	Glycyrrhizic Acid
25	16		9	8		
21.5	C <sub>16</sub> H <sub>30</sub> O	254.2243	253.217	-	[M-H] <sup>-1</sup>	Palmitoleic Acid
65	2			1.0073		
21.7	C <sub>30</sub> H <sub>48</sub> O	456.36	455.352	-	[M-H] <sup>-1</sup>	Oleanolic Acid
55	3		7	1.0072		
21.9	C <sub>18</sub> H <sub>32</sub> O	280.24	279.232	-	[M-H] <sup>-1</sup>	Linoleic Acid
78	2		7	1.0073		
22.4	C <sub>16</sub> H <sub>32</sub> O	256.2399	255.232	-	[M-H] <sup>-1</sup>	Palmitic Acid
91	2		6	1.0073		
22.7	C <sub>18</sub> H <sub>34</sub> O	282.2556	281.248	-	[M-H] <sup>-1</sup>	Oleic Acid

2	2		3	1.0072		
				8		
23.7	C <sub>18</sub> H <sub>36</sub> O		283.264	-		
5	2	284.2714	1	1.0072	[M-H] <sup>-1</sup>	Stearic Acid
				6		

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**Table S2. Molecular docking results of core active components of Modified PD against LPS, TLR4, MyD88, TRAF6 and NF- $\kappa$ B (kcal/mol)**

Drugs	Compound	LPS	TLR4	MyD88	TRAF6	NF- $\kappa$ B
Positive medicine	Loperamide	-9.4	-9	-5.8	-6.4	-8.3
	Esculetin	-6.9	-6.6	-5.2	-5.7	-6.2
	Fraxetin	-7	-7.3	-5.4	-5.3	-6.7
Modified PD	Esculin	-8.1	-7.6	-6.4	-6.1	-8.2
	Anemoside B4	-8.7	-9	-6.7	-6.5	-7.8
	Oleanolic acid	-9.3	-9.9	-7.2	-6.4	-7.5
	Berberine	-8.8	-8.6	-6.2	-5.8	-8.8
	Limonin	-9.8	-9.4	-7.6	-7.3	-8.3
	Obacunone	-10.4	-9.7	-6.8	-6.6	-8
	Glycyrrhizic Acid	-11.2	-10.1	-8.2	-7.4	-8.2
	Iso-liquiritigenin	-7.7	-8.3	-5.6	-5.9	-7.9
	L-Phenylalanine	-5.5	-4.8	-4.7	-4.6	-5.7
	Prolylleucine	-7.6	-7.2	-6.3	-5.9	-8.1
	D-Proline	-8.8	-4.6	-3.9	-3.2	-4.2
	L-Histidine	-4.5	-4.5	-4.8	-3.9	-4.4
	L-Glutamic acid	-4.6	-4.9	-4.2	-4.1	-4.3
	L-Tyrosine	-6	-5.2	-4.7	-4.5	-5.8
	D-Pyroglutamic Acid	-5.7	-4.6	-4.5	-4.9	-4.6
	D-Tryptophan	-6	-5.3	-5.6	-4.6	-6.5
	Adenosine	-7.8	-6.8	-5.9	-5	-6.5
	Cytarabine	-7.5	-6.2	-5.7	-4.7	-5.8
	Oleic acid	-4.9	-5.2	-4.1	-3.5	-5.8
	Stearic acid	-4.8	-4.9	-3	-3.2	-5.3

Palmitic acid	-5.7	-4.9	-3	-3.1	-5.7
Palmitoleic acid	-5.5	-4.4	-3.3	-3.3	-5.4
Linoleic acid	-5.5	-5	-3.9	-4	-6

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