

Table S1 : List of bioactive compounds identified in LC-MS/MS data along with their implicated bioactivities. Literature search was undertaken to highlight compounds having immunomodulatory, redox modulatory activities or impacting immune signalling pathways.

S.No	Match	Compound class	Biological effect(s)	Activities/Mechanisms	Reference
1	<b>1,2,3-Trihydroxybenzene (Pyrogallol)</b>	Benzenoids (Phenolics)	Enhancement of therapeutic effect of human umbilical cord mesenchymal stem cells against LPS-mediated inflammation and lung injury	Activates Nrf2/HO-1 signalling	1
			Anti-inflammatory effect in bronchial epithelial cells	Regulates expression of pro-inflammatory genes	2
2	<b>10-Nitrolinoleic Acid</b>	Nitrated Fatty acids	Inhibition of proliferation of vascular smooth muscle cells	Activation of Keap1-Nrf2 pathway	3
			Anti-inflammatory effect	Inhibition of 5-lipoxygenase	4
3	<b>4-Hydroxybenzaldehyde</b>	Benzenoids (Phenolics)	Protective effect on blood-brain barrier	Enhances antioxidant capacity by activating the Nrf2/ARE pathway	5
			Antiepileptic and anticonvulsive activity	Anti-oxidative effect and GABAergic neuromodulation of the rat brain	6
4	<b>4-Hydroxycinnamic Acid (p-coumaric acid)</b>	Cinnamic acid (Phenolic)	Anti-Inflammatory effects in rat arthritis model	Decreases arthritis index, infiltration of inflammatory cells and levels of pro-inflammatory cytokines	7
			Attenuates alcohol exposed hepatic injury in experimental models	Inhibits MAPKs and apoptosis signalling by enhancing Nrf2 signalling	8
5	<b>4-Hydroxymethylcatechol</b>	Catechol (Phenolic)	Attenuation of rheumatoid arthritis	Inhibits PI3K/Akt/NF-κB signalling	9
6	<b>4-Hydroxyproline</b>	Amino acid	Attenuates DSS-induced colitis in mice	Inhibits NF-κB/IL-6 signalling and restores redox homeostasis.	10
7	<b>Adenosine</b>	Nucleoside	Modulation of microglial ROS production to regulate brain inflammation	Induces HO-1 expression through the activation of PI3K and Nrf2	11
8	<b>Alpha-Linolenic Acid</b>	Fatty acid	Anti-inflammatory effect in RAW 264.7	Downregulates inflammatory iNOS, COX-2, and TNF- by blocking activation of NF-κB and MAPKs	12
			Impediment of Cadmium-induced oxidative stress, neuroinflammation, and neurodegeneration in mouse brain	Reduces ROS production and NOS2 and enhanced the expression Nrf-2 and HO-1	13
9		Fatty acid	Modulation of inflammatory response in normal human keratinocytes	Reduced nuclear translocation of NF-κB p65 subunit and phosphorylation of the p38 MAPK and activated PPARγ	14

10	<b>Dodecanoic Acid (Lauric acid)</b>	Fatty acid	Anti-inflammatory properties against <i>Propionibacterium</i> acnes	Inhibits NF- $\kappa$ B activation and phosphorylation of MAP kinases	15
			Amelioration of LPS-induced liver inflammation in Sprague Dawley rats	Downregulates the expression of TLR4/NF- $\kappa$ B mediating proteins	16
11	<b>Erythritol</b>	Sugar alcohol (Polyol)	Improvement in non-alcoholic fatty liver disease condition	Enhances Nrf2/HO-1/NQO1 antioxidant Capacity	17
12		Dipeptide	Anti-inflammatory effects in sepsis models	Increases glutathione levels	18
			Alleviation of ethanol-induced hepatotoxicity	Suppresses oxidative stress, apoptosis, and inflammation	19
13	<b>Indoleacetic Acid</b>	Indole derivative	Anti-inflammatory and anti-oxidative activity in RAW264.7 cells	Downregulates NF- $\kappa$ B and upregulating HO-1	20
			Protective effect on H <sub>2</sub> O <sub>2</sub> -damaged human dental pulp stem cells	Increases the expression of Nrf2 and HO-1 through Akt pathway	21
14	<b>Isoquinoline</b>	Alkaloid	Activation of Nrf2-dependent transcription and hepatocellular protection	Disrupts Keap1-Nrf2 protein complex	22
			Anti-inflammatory activity against established adjuvant arthritis in rats	Reduces chronic inflammation	23
15	<b>L-Acetylcarnitine</b>	Fatty acyls	Neuroprotection during hypoxia in Sprague-Dawley rats	ERK1/2-Nrf2-regulated mitochondrial biosynthesis	24
			Protection against oxidative stress in rat astrocytes	Induction of HO-1 mediated by upregulation of Nrf2	25
16	<b>L-Arginine</b>	Amino acid	Stimulation of GSH synthesis and up-regulation of ARE-driven antioxidant expressions	Activation of Nrf2 pathway	26
			Amelioration of cardiac left ventricular oxidative stress in alloxan-induced hyperglycemic rats	Upregulation of eNOS, Akt and Nrf2, downregulation of Nf- $\kappa$ B	27
			Inhibition of LPS-induced inflammatory response and oxidative stress in IPEC-J2 cells	Reduction in the abundance of TLR4, MyD88, NF- $\kappa$ Bp65 and increase in the activity of Arg-1	28
17	<b>L-Isoleucine</b>	Amino acid	Improvement of intestinal immune function, antioxidant capacity and microbial population	Upregulation of Nrf2 and p38 MAPK and downregulation of Keap1 and ERK1	29
18	<b>L-Lysine</b>	Amino acid	Neuroprotection after mouse intracerebral hemorrhage injury	Suppresses pro-inflammatory response	30

19	<b>L-Serine</b>	Amino acid	Antioxidant and cytoprotective effects in human endothelial cells	Induction of Nrf2 activity and HO-1 expression	31
			Reduces oxidative stress and inflammation during aging in mice	Modulating the Sirt1/NFkB pathway	32
20	<b>L-Tryptophan</b>	Amino acid	Reduction in inflammation and enhancement of rate of recovery in DSS-induced colitis	Reduction of pro-inflammatory cytokines and ICAM-1	33
			Anti-inflammatory in Intestinal Epithelial Cells	Inhibition of JNK or IκBα phosphorylation	34
			Protection of hepatocytes against reactive oxygen species-dependent cell death via multiple pathways	Nrf2-dependent gene induction	35
			Modulation of intestinal immune response, barrier function, antioxidant status	Up-regulation of Nrf2 and downregulation of Keap1 gene expression	36
21	<b>L-Valine</b>	Amino acid	Anti-inflammatory activity in lipopolysaccharide (LPS) stimulated RAW 264.7 macrophages	Suppression of iNOS, COX-2, IL-6 expression	37
22	<b>1-Palmitoyl-sn-glycero-3-phosphocholine</b>	Phospholipid	Anti-inflammatory activity in LPS-stimulated human monocyte THP-1 cells	Reduces pro-inflammatory markers	38
23	<b>Monoolein</b>	Lipid	Inhibits lipopolysaccharide-induced inflammatory response	Attenuates the activation of MAPK and NF-κB pathways	39
24	<b>Nicotinic Acid</b>	Vitamin	Protection of liver against acetaminophen-induced hepatotoxicity in mice	Upregulation of Sirt1/Nrf2 antioxidative pathway	40
			Anti-inflammatory effects of nicotinic acid in human monocytes	Suppression of NF-κB signalling	41
25	<b>Palmitoylethanolamide</b>	Lipid	Regulation of NF-κB/Nrf2 pathways in benign prostatic hyperplasia	Inhibition of NF-κB and upregulation of Nrf-2	42
			Reduces inflammation and tissue injury associated with spinal cord injury	Reduction in NF-κB activation, and activation of peroxisome proliferator-activated receptor (PPAR)-α	43
26	<b>Phytosphingosine</b>	Sphingoid base	Inhibits TPA-Induced inflammatory epidermal hyperplasia in hairless mouse skin	Reduces edema, infiltration of inflammatory cells and generation of prostaglandin E2	44
27	<b>Pyridoxamine</b>	Vitamin	Protective function of pyridoxamine on retinal photoreceptor cells in diabetic mice	Activation of the p-Erk1/2/Nrf2/Trx/ASK1 signalling pathway	45
28	<b>Ricinoleic Acid</b>	Fatty acid	Acute and subchronic experimental models of inflammation	Reduces the edema induced by carrageenan and by complete Freund's adjuvant injection	46

29	<b>Sinapic Acid</b>	Cinnamic acid (Phenolic)	Amelioration of cardiac dysfunction and cardiomyopathy in streptozocin induced diabetic rats	Decreases NF- $\kappa$ B p65 DNA binding and enhanced Nrf2-ARE DNA-binding activity	47
			Amelioration of D-galactosamine/lipopolysaccharide-induced fulminant hepatitis in rats	Increases the activity of Nrf2/HO-1 signaling pathway	48
30	<b>trans-Ferulic Acid</b>	Cinnamic acid (Phenolic)	Cytoprotection against high glucose-induced oxidative stress in cardiomyocytes and hepatocytes	Keap1-Nrf2-ARE signaling pathway modulation	49
			Prevention of oxidative stress, inflammation, and liver injury in methotrexate-induced rats	Upregulation of Nrf2/HO-1 signaling	50
31	<b>Trigonelline</b>	Alkaloid	Mitigation of lipopolysaccharide-induced learning and memory impairment in rat	Suppression of hippocampal oxidative stress and inflammation by lowering NF- $\kappa$ B/TLR4 and AChE activity	51
			Improvement in the responsiveness of NSCLC cells to Cisplatin and Etoposide	Blocking activation and nuclear translocation of Nrf2 via inhibition of EGFR signalling pathway	52
32	<b>Vanillin</b>	Benzenoids (Phenolics)	Protection against cisplatin-induced nephrotoxicity in rats	Inhibition of NOX-4 and stimulation of Nrf2/HO-1 signalling pathway	53
			Gastroprotective effect against ulcer formation	Inflammatory response modulation involving downregulation of NF- $\kappa$ B	53
33	<b>D-Pantothenic acid</b>	Vitamin	Protection against kainic acid-induced status epilepticus and associated neurodegeneration in mice	Anti-inflammatory	54
			Inhibition of RANKL induced osteoclastogenesis and ovariectomy induced osteoporosis	Upregulation of FoxO1, FoxO2 and Nrf2	55
34	<b>2,3,4,5-Tetrahydroxypentanal (Pectin)</b>	Heteropolysaccharide	Alleviation of high fat diet-induced nonalcoholic fatty liver disease in mice	-	56
			Anti-inflammatory action in diabetic rats	Decreased volume of edema, release of myeloperoxidase, neutrophil infiltration and levels of TNF- and iNOS	57
35	<b>Eleostearic acid (Punicic acid)</b>	Conjugated fatty acid	Amelioration of experimental inflammatory bowel disease in mice	PPAR $\gamma$ -dependent and -independent mechanisms	58
			Inhibition of TNF $\alpha$ -induced neutrophil hyperactivation and protection from experimental colon inflammation in rats	Targeting p38MAPKinase/Ser345-p47phox-axis and MPO release	59

36	<b>12-Oxo phytodienoic acid</b>	Lipid	Attenuation of inflammation and modulation of macrophage polarization	Inhibition of mPGES-1, NF- $\kappa$ B pathway and activation of Nrf2/HO-1 pathway.	60
			Attenuation of lipopolysaccharide-induced inflammation in microglia	Inhibiting NF- $\kappa$ B and p38 MAPK and inducing SOCS-1	61
37	<b>N-(p-Coumaroyl) serotonin</b>	Polyphenolics	Suppression of proinflammatory cytokine production from monocytes	Inhibiting NF- $\kappa$ B activation	62
			Improvement of vascular distensibility and inhibition of aortic hyperplasia	Inhibition of phosphorylation of PDGF receptor $\beta$ and ERK1/2, and Ca(2+) release	63
38	<b>(6E,8Z,11Z,14Z)-5-Oxo-6,8,11,14-icosatetraenoic acid (5-oxo-EETE)</b>	Fatty acids	Nrf2 Activation in Human Umbilical Vascular Endothelial Cells	Increasing nuclear translocation of Nrf2	64
39	<b>L-Glutathione</b>	Tripeptides	Attenuation of IL-13-induced asthma in mice	Buffering inflammation-associated reactive oxygen species	65
40	<b>Hymecromone (4-methylumbelliferone)</b>	Coumarins (Phenolics)	Suppression of Fc $\epsilon$ RI-mediated mast cell activation and allergic inflammation	Inhibited phosphorylation of SYK, NF- $\kappa$ B p65, ERK1/2, p38, and JNK	66
41	<b>Tricin 5-O-<math>\beta</math>-D-glucoside</b>	Flavones (Phenolics)	Anti-inflammatory effects in LPS induced hPBMCs and carrageenan induced rats	Blocking TLR4/NF- $\kappa$ B/STAT signalling cascade	67
			Attenuation of cerebral ischemia/reperfusion injury through inhibiting nerve cell autophagy, apoptosis and inflammation	Activating the PI3K/Akt signalling pathway	68

## Abbreviations

AChE: Acetylcholinesterase  
 Akt: Protein kinase B (PKB)  
 ARE : Antioxidant responsive element  
 Arg-1: Arginase-1  
 ASK 1: Apoptosis signal-regulating kinase 1  
 COX2: Cyclooxygenase-2  
 DSS: Dextran sodium sulphate  
 EGFR: Epidermal growth factor receptor  
 eNOS: Endothelial Nitric oxide synthase  
 ERK1/2: Extracellular signal-regulated kinases 1/2  
 FoxO1: forkhead box O2  
 HO-1: Hemeoxygenase-1  
 hPBMCs: Human peripheral blood mononuclear cells  
 ICAM1: Intercellular Adhesion Molecule 1  
 iNOS: inducible Nitric oxide synthase  
 IL: Interleukin  
 JNK: c-Jun N-Terminal Kinase  
 Keap1: Kelch-like ECH-associated protein 1  
 LPS: Lipopolysaccharides  
 MAPKs : Mitogen activated protein kinases  
 mPGES-1: Microsomal prostaglandin E synthase-1  
 MPO: Myeloperoxidase  
 MyD88: Myeloid differentiation primary response 88

NF- $\kappa$ B: Nuclear factor kappa light chain enhancer of activated B cells  
 NOS2- Nitric oxide synthase 2  
 NOX: NADPH oxidase  
 NQO1: NAD(P)H quinone dehydrogenase 1  
 Nrf-2: Nuclear factor erythroid 2-related factor 2  
 NSCLC: Non-small cell lung cancer  
 PDGF: Platelet-derived growth factor  
 PI3K: Phosphoinositide 3-kinase  
 PPAR: peroxisome proliferator-activated receptor  
 RANKL: Receptor activator of nuclear factor kappa-B ligand  
 SIRT 1: Sirtuin (silent mating type information regulation 2 homolog) 1  
 SOCS-1: Suppressor of cytokine signalling 1  
 STAT: signal transducer and activator of transcription  
 SYK: Spleen tyrosine kinase  
 TLR 4 :Toll like receptor 4  
 TNF: Tumour necrosis factor  
 TPA: 12-O-tetradecanoylphorbol-13-acetate  
 TrX: Thioredoxin

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