Supplementary Data

Exploring natural colorants from plants to insects: Chemistry, functions, and modern uses

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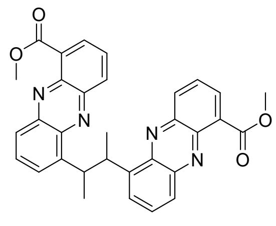
Supplementary Figures



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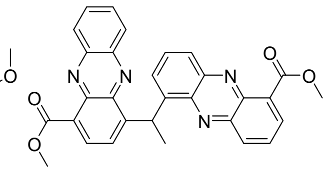

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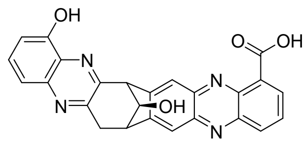

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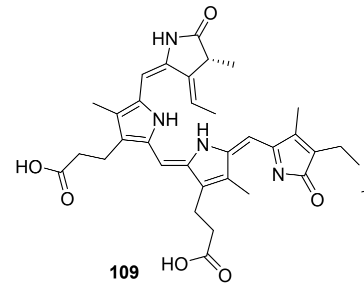

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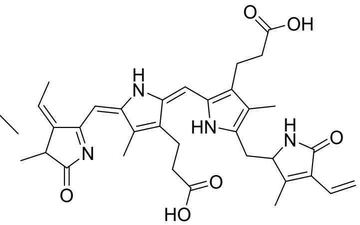

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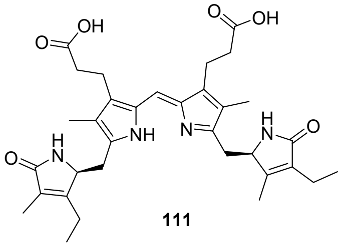

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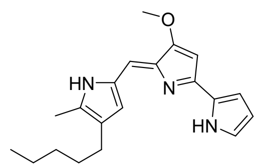

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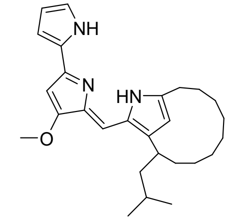

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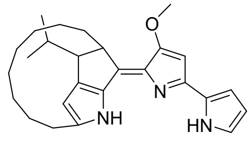

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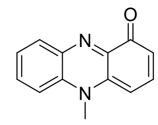

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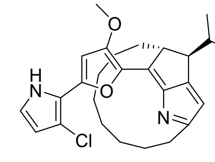

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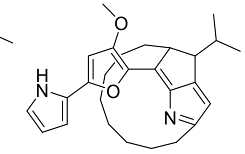

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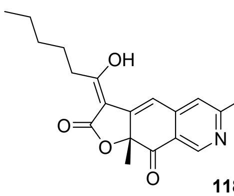

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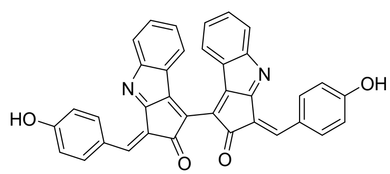

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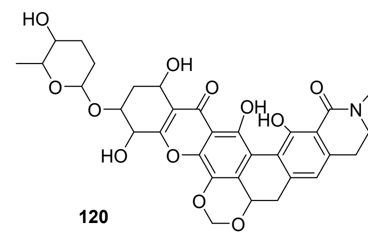

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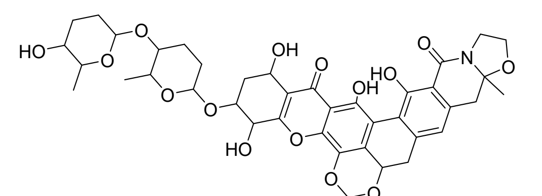

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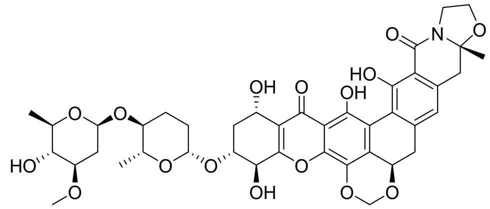

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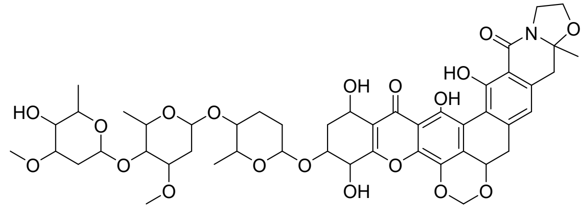

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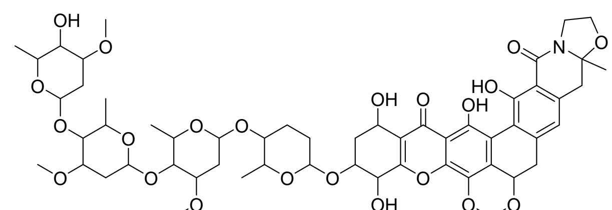

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Figure S1. Structurally identified alkaloids and alkaloid-related pigments (**106-124**). Chirality is indicated where known; otherwise, the configuration is left unspecified

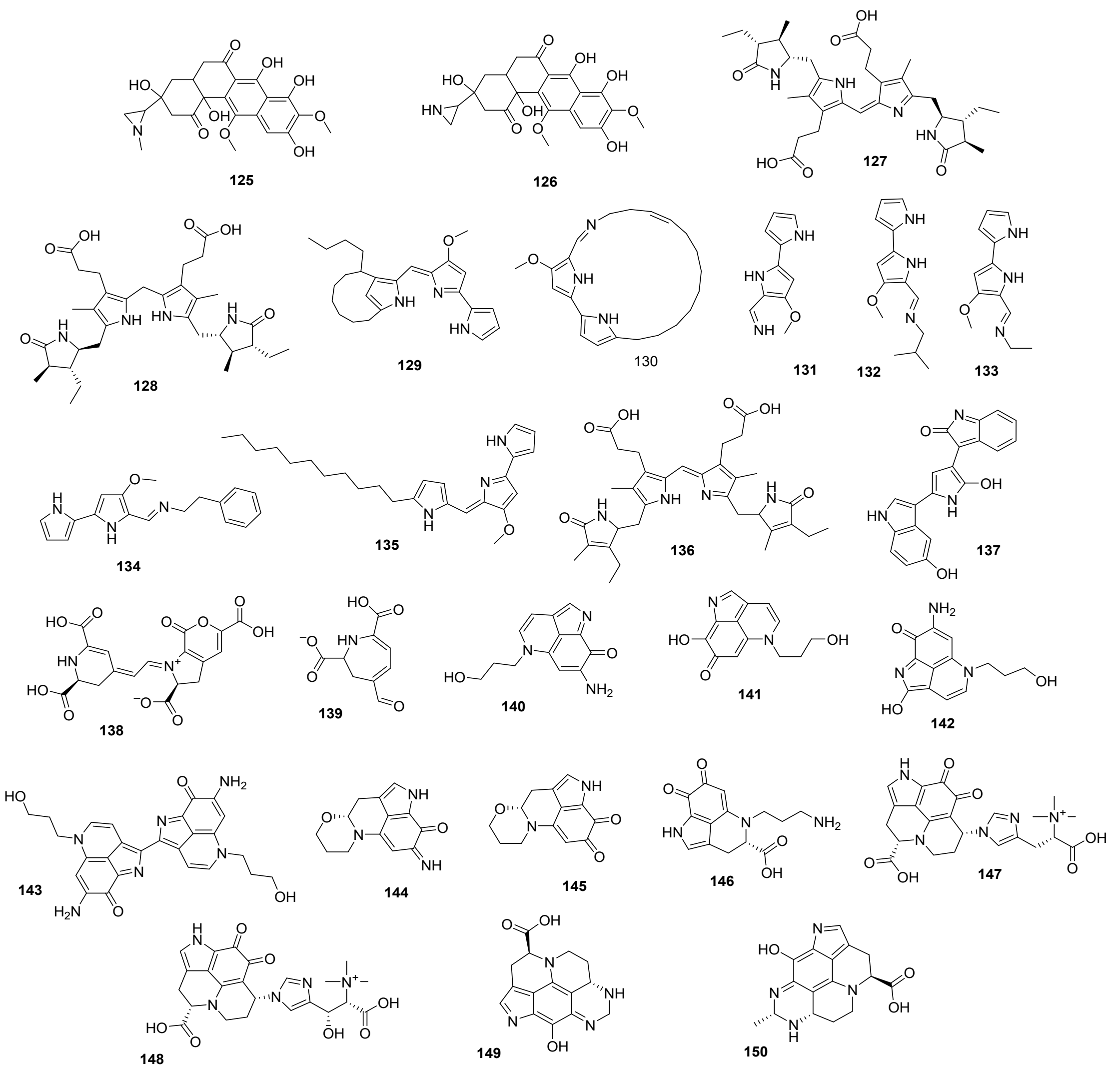

Figure S2. Structurally identified alkaloids and alkaloids-related pigments (**125-150**). Chirality is indicated where known; otherwise, the configuration is left unspecified

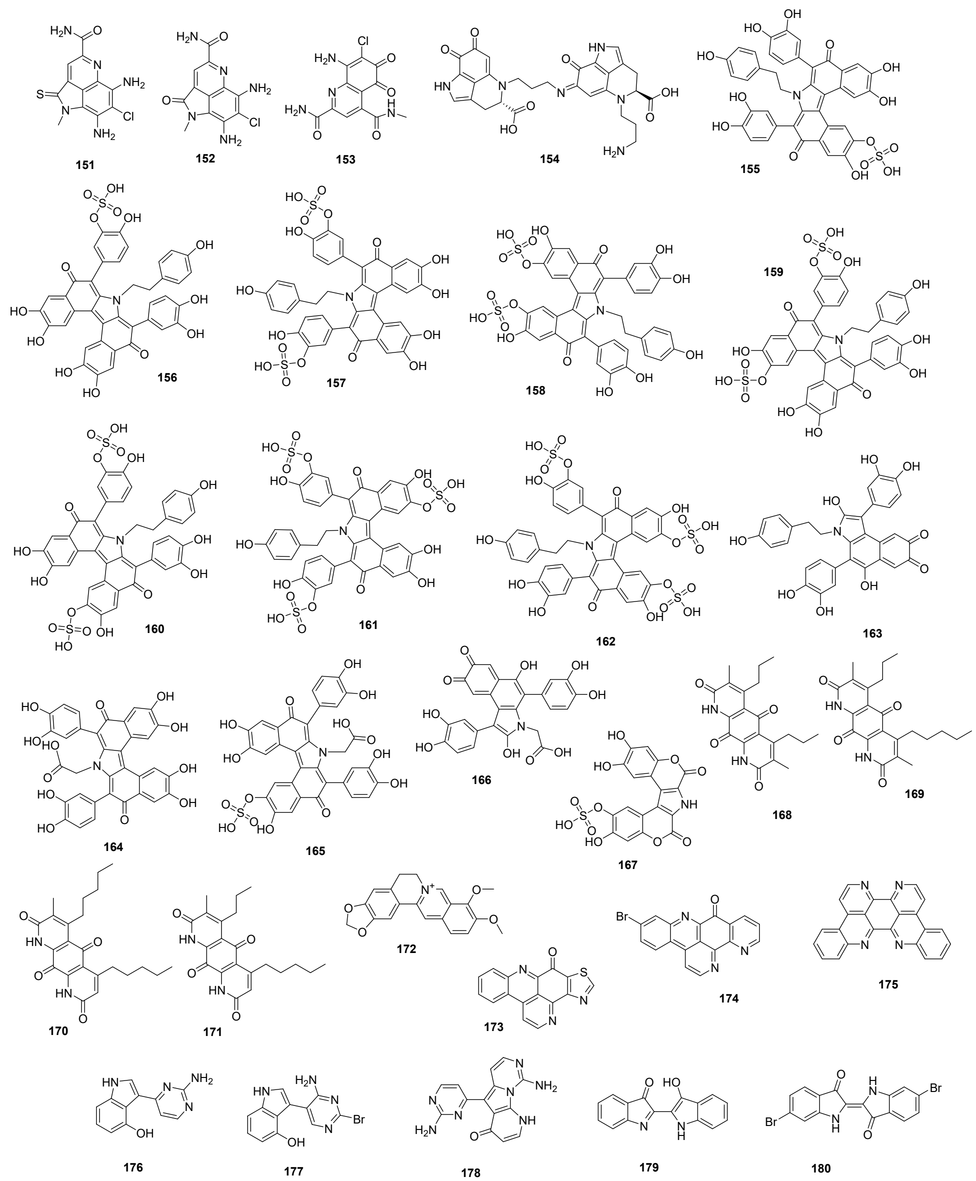

Figure S3. Structurally identified alkaloids and alkaloids-related pigments (**151-180**). Chirality is indicated where known; otherwise, the configuration is left unspecified

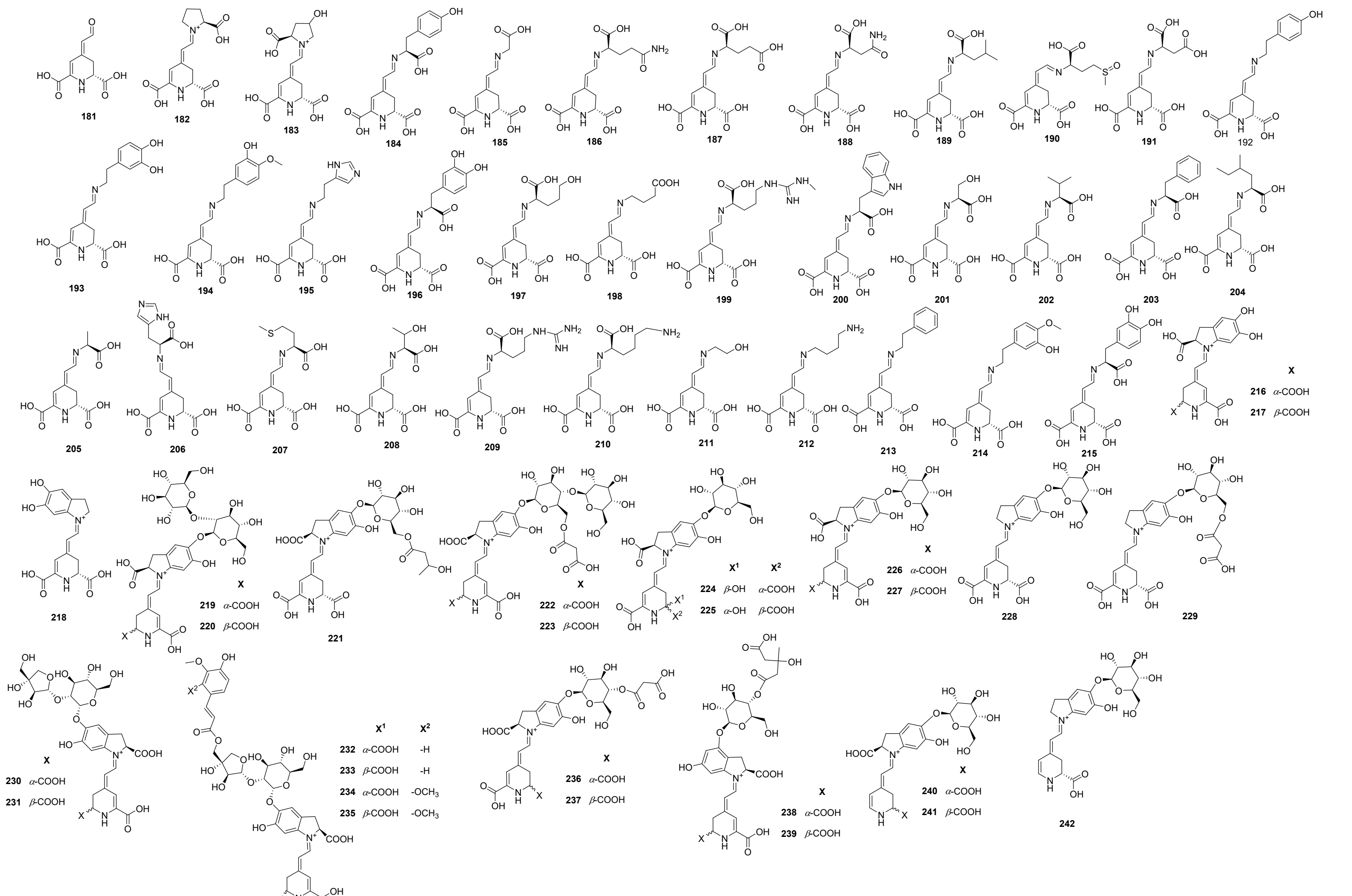

Figure S4. Structurally identified betalain pigments (**181-242**). Chirality is indicated where known; otherwise, the configuration is left unspecified

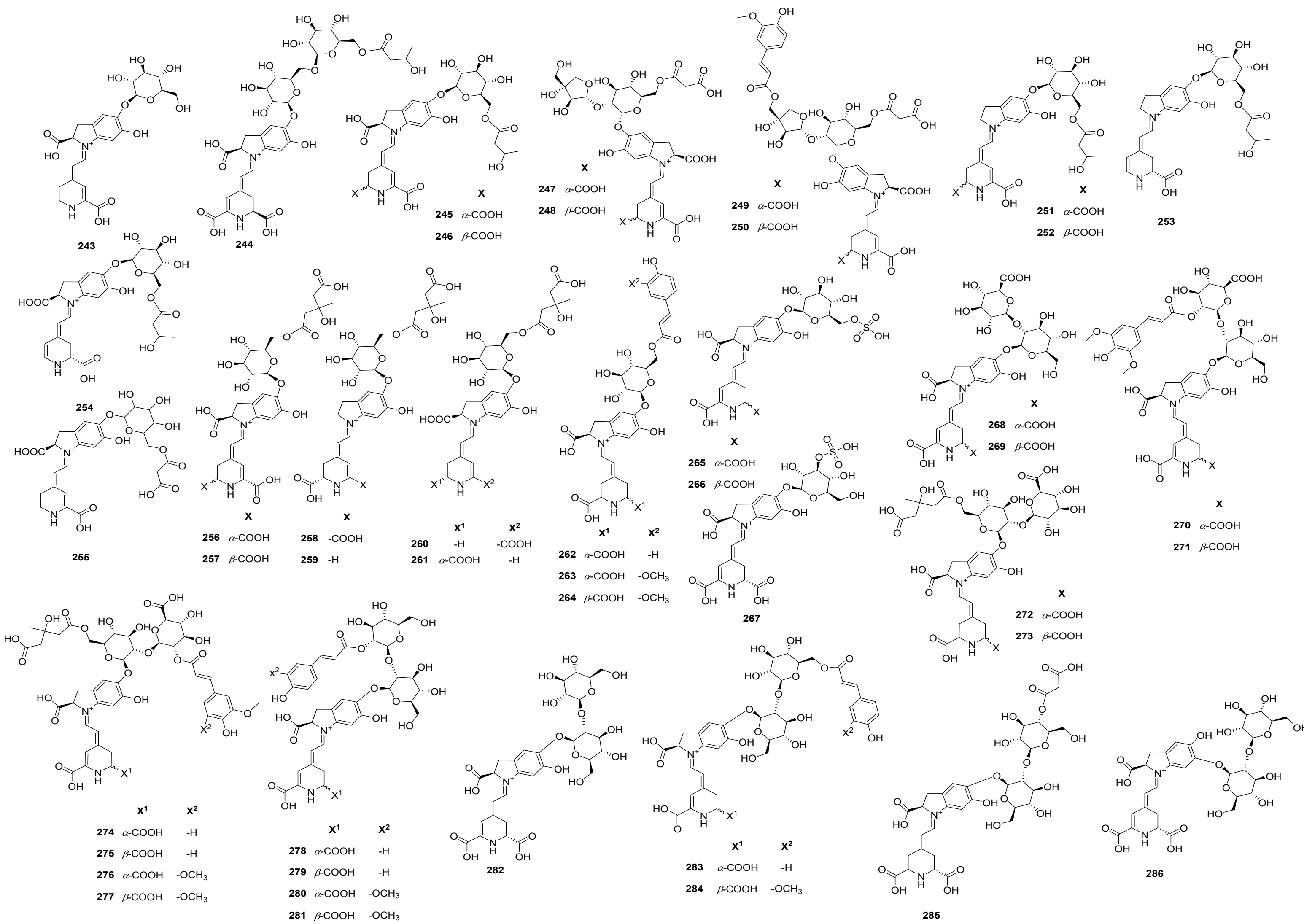

Figure S5. Structurally identified betalain pigments (**243-286**). Chirality is indicated where known; otherwise, the configuration is left unspecified

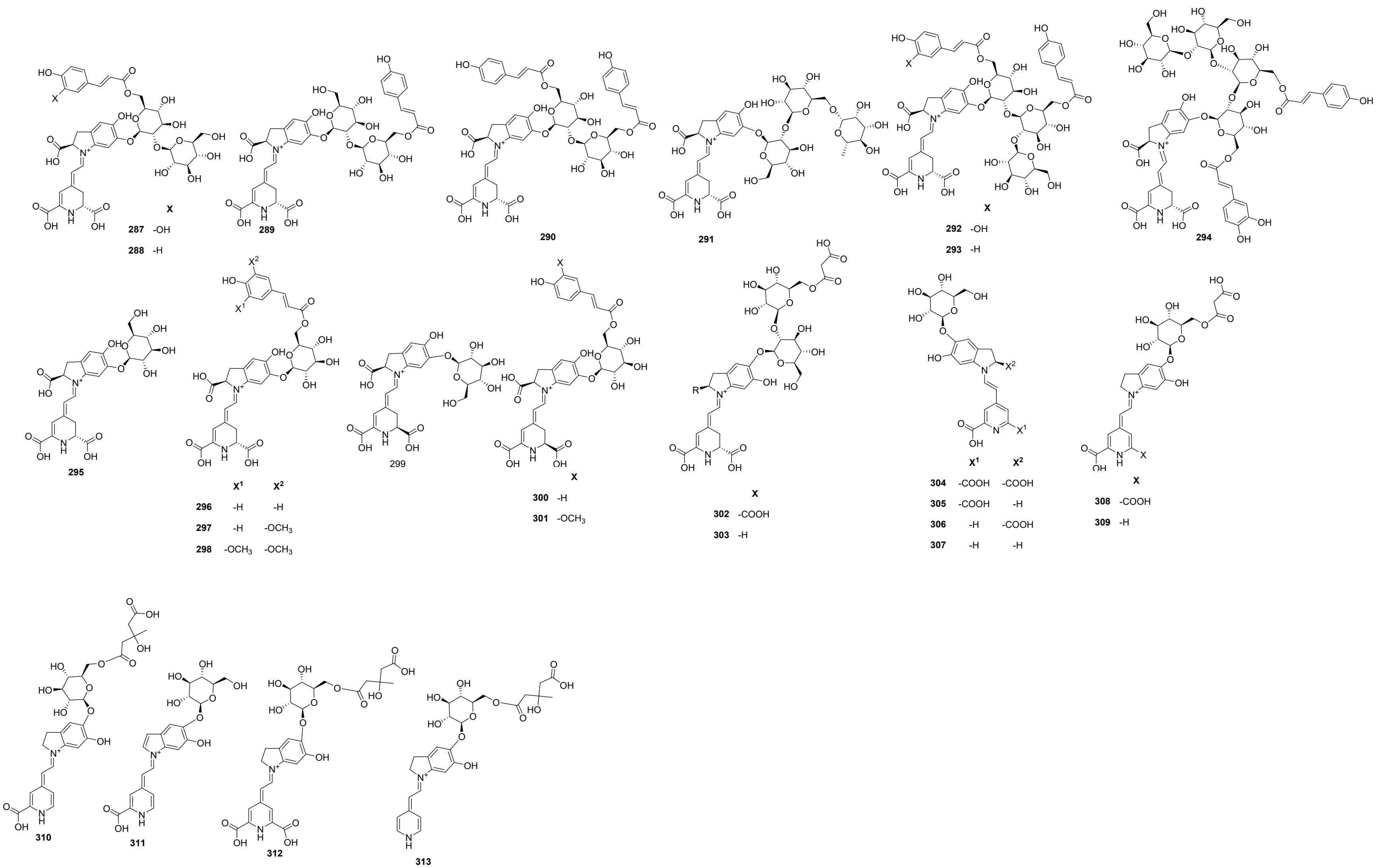

Figure S6. Structurally identified betalain pigments (**287-313**). Chirality is indicated where known; otherwise, the configuration is left unspecified

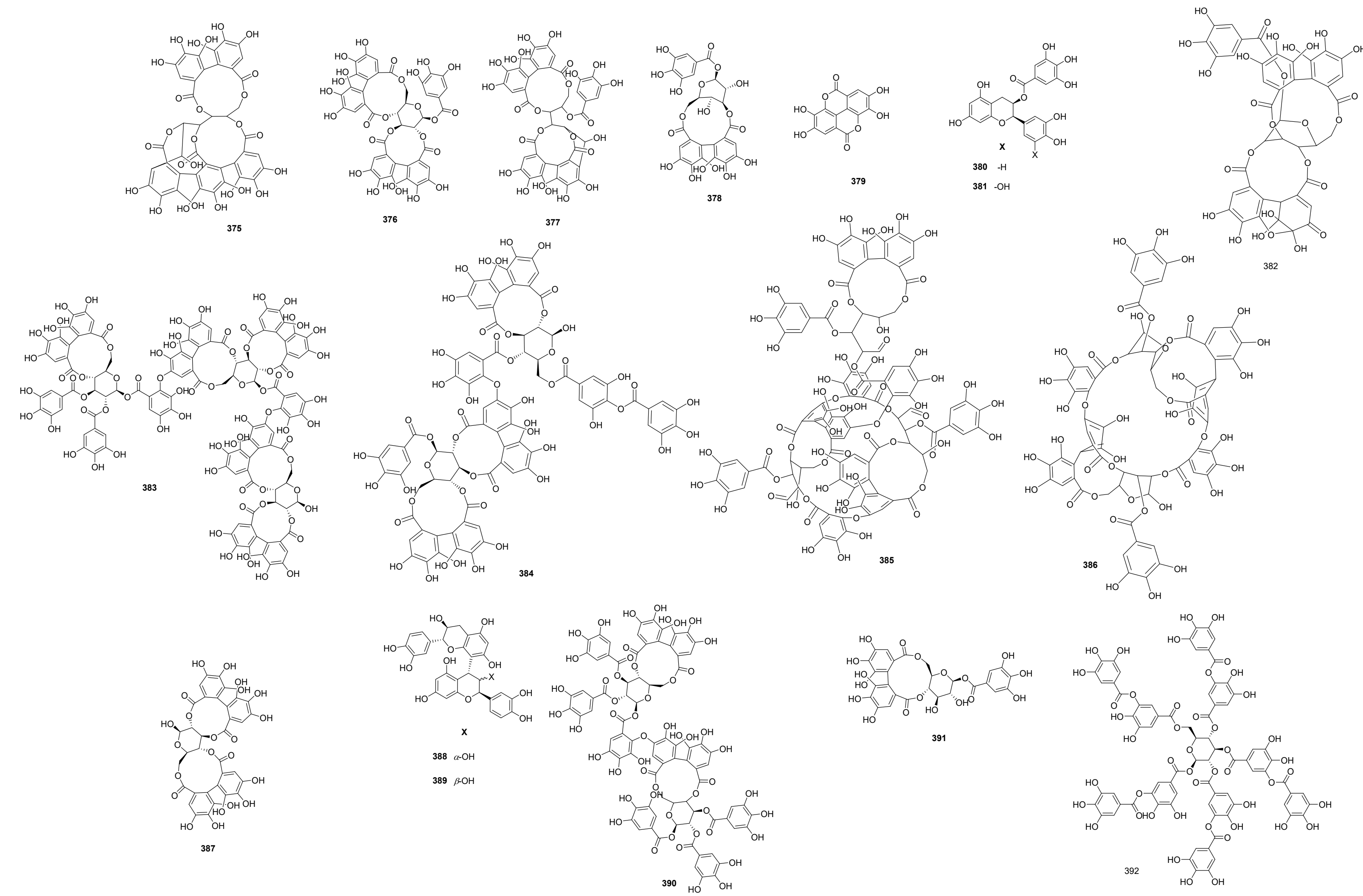

Figure S7. Selected identified tannins isolated from plants (**375-382**). Chirality is indicated where known; otherwise, the configuration is left unspecified

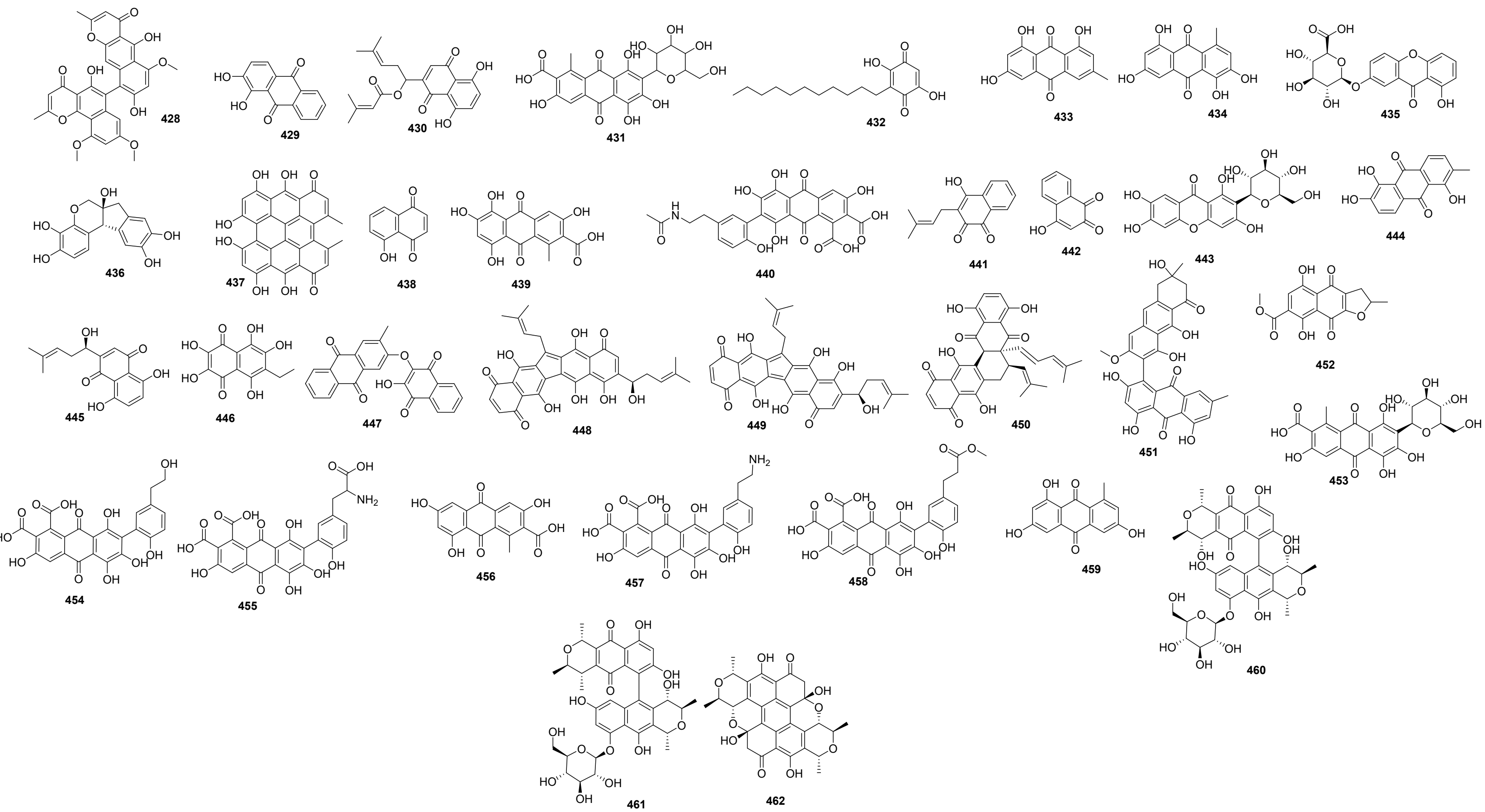

Figure S8. Selected identified quinonoid and pyranonaphthoquinone compounds (**428-462**). Chirality is indicated where known; otherwise, the configuration is left unspecified

Supplementary Tables

Table S1. Selected identified carotenoids isolated from different natural sources.

Compound Number	Chemical Class	Compound Name	Natural Sources	Biological Activity	References
1.	Xanthophylls	Lutein	• **Plants:** *Daucus carota, Carica papaya, Cucurbita pepo, Citrullus lanatus, Ipomoea batatas, Dioscorea spp., Solanum lycopersicum, Capsicum annuum, Capsicum annuum, Brassica oleracea* var. *sabellica, Mangifera indica, Actinidia deliciosa, Spinacia oleracea, Brassica oleracea var. italica, Cucumis melo* var., *Persea americana, and Citrus sinensis, Sorghum spp.*, *Oryza sativa, Triticum monococcum* • **Algae:** *Dunaliella* spp., *Chlorella spp., Haematococcus* spp., *Muriellopsis* spp., *Chlamydomonas spp., Spirulina spp., Cladophora fascicularis, Cladophora glomerata, Acanthophora delilei, Ceramium tenuicorne, Champia compressa* • **Fungi/Yeasts:** *Phytomyces blakesleanus, Blakeslea trispora, Neurospora crassa* • **Bacteria**: *Halophilic spp., Myco/myxobacterium spp., Paracoccus spp.*, and *Streptomyces* spp. • **Insects:** *Alcimocoris japonensis, Plautia stali, Nezara antennata, Sastragala esakii, Acanthocoris sordidus* • **Others:** yellow egg yolks, and human milk, Abalone, *Haliotis discus discus, turban shell, Turbo cornutus,* dolphin, and yellow warbler birds	Antioxidant • ↑ mRNA • ↓ Oxidative stress (OS) • ↓ ROS • ↓ NIK/IKK • ↓ PI3K/PTEN/Akt. Hepatoprotection • ↑ mRNA • ↑ Protein expressions of Nrf-2 (NQO1, HO-1 and GST) Treatment for osteoarthritis • ↓ NF-κB and COX-2 • ↓ IL-6, TNF-α and IL-1β • ↓ Cleavage of caspase-3 Neuroprotection • ↑ Endogenous oxidative system • ↓ TNF-α, IL-1β and NO formation • ↑ Phosphorylation of ERK1/2 • ↓ p3, JNK- and Akt-stimulated NF-κB activation • ↓ ROS Anti-inflammatory • ↓ TNF-α and IL-1β • ↓ iNOS and COX-2 Cardioprotection • ↓ CK-MB • ↓ cTn T • ↓ IL-1β, IL-6, TNF-α • ↓ NF-κB p65 • ↓ Caspase-3 and -9 • Regulates Nrf-2/HO-1 Diabetic retinopathy • ↑ SIRT1 mRNA Anticancer • Regulates 3-kinase (PI3K)/Akt phosphoinositide	[1-11]

Compound Number	Chemical Class	Compound Name	Natural Sources	Biological Activity	References
				Bone remodeling • ↓ mRNA RANKL Treatment for burn-induced multiple organ injury • ↓ TNF-α and caspase-3 • ↓ ROS Treatment for optic nerve injury • ↓ MDA, IL-1β and TNF-α Treatment for severe traumatic brain injury • ↓ IL-1β, IL-6 and MCP-1 • Regulates NF-κB p65/ICAM-1/Nrf-2	
2.		Fucoxanthin	• **Algae:** *Chorda filum, Padina gymnospora, Phaeodactylum tricornutum, Odontella aurita, Chaetoceros calcitrans, Nitzchia laevis, Isochrysis galbana, Odontella sinensis, Skeletonema costatum, Kjellmaniella crassifolia, Saccharina japonica, Cystoseira hakodatensis, Phaeodactylum tricornutum* • **Others:** Abalone, *Haliotis discus discus,* turban shell, *Turbo cornutus,* oysters, clams, mice	- Anti-mutagenic, anti-diabetic, anti-obesity, anti-inflammatory and anti-neoplastic actions. -Fucoxanthin induces uncoupling protein 1 (UCP1) in abdominal white adipose tissue (WAT) mitochondria, leading to the oxidation of fatty acids and heat production in WAT. -Fucoxanthin improves insulin resistance and decreases blood glucose levels through the regulation of cytokine secretions from WAT. - Fucoxanthin exhibited antibacterial activity against *Streptococcus agalactiae* (mean ZOI 12.2 mm), *S. epidermidis* (mean ZOI 11.2 mm), and *S. aureus* (mean ZOI 11.0 mm), and in the microdilution test towards *S. agalactiae* with the minimal inhibitory concentration (MIC) of 62.5 µg/mL. On the other hand, fucoxanthin was not active against strict anaerobic bacteria.	[5, 8, 12, 13]
3.		Fucoxanthinol	• **Algae:** *Chorda filum, Padina gymnospora* • **Others:** Sea squirt *Halocynthia roretzi,* mice	- Anti-diabetic, anti-obesity, anti-inflammatory and anti-neoplastic actions. -Anti-proliferative and cancer preventing influences is mediated through different signaling pathways, including the caspases, Bcl-2 proteins, MAPK, PI3K/Akt, JAK/STAT, AP-1, GADD45, and several other molecules that are involved in cell cycle arrest, apoptosis, anti-angiogenesis or inhibition of metastasis.	[5, 8, 14]
4.		Halocynthiaxanthin	• **Algae:** *Chorda filum, Padina gymnospora*		[5, 8]

Compound Number	Chemical Class	Compound Name	Natural Sources	Biological Activity	References
			• **Others:** Sea squirt *Halocynthia roretzi*		
5.		Zeaxanthin	• **Plants:** *Daucus carota, Carica papaya, Cucurbita pepo, Citrullus lanatus, Ipomoea batatas, Dioscorea spp., Solanum lycopersicum, Capsicum annuum, Capsicum annuum, Brassica oleracea* var. *sabellica, Mangifera indica, Actinidia deliciosa, Spinacia oleracea, Brassica oleracea var. italica, Cucumis melo var., Persea americana, and Citrus sinensis, Sorghum* spp. • **Algae:** *Dunaliella spp., Chlorella spp., Haematococcus spp., Muriellopsis spp., Chlamydomonas spp., Spirulina* spp., *Codium carolinianum, Pterocladia capillacea* • **Fungi/Yeasts:** *Phytomyces blakesleanus, Blakeslea trispora, Neurospora crassa* • **Bacteria:** *Halophilic spp., Myco/myxobacterium spp., Paracoccus* spp., *and Streptomyces spp.* • **Insects:** *Parastrachia japonensis, Poecilocoris lewisi, Halyomorpha halys, Alcimocoris japonensis, Plautia stali, Nezara antennata, Sastragala esakii, Acanthocoris sordidus* • **Others:** Yellow egg yolks, human milk, Abalone, *Haliotis discus discus, turban shell, Turbo cornutus, and Cyprinidae* fish	-Zeaxanthin is effective against AMD, cataract, and LDL oxidation, thus emphasizing its use in nutraceutical formulations.	[1-7, 15]
6.		Violaxanthin	• **Algae:** *Cystoseira compressa, Cystoseira humilis, Fucus vesiculosus, Lobophora variegata, Codium isthmocladum*	- Violaxanthin possessed potent lipid peroxidation inhibitory and very weak $^1O_2$ quenching activities. -Violaxanthin strongly scavenging of ABTS+ radicals, with EC_{50} of 15.25 µg/mL.	[3, 8, 16, 17]
7.		Antheraxanthin	• **Algae:** *Codium taylori* • **Insects:** *Parastrachia japonensis, Poecilocoris lewisi, Nezara antennata*	Antioxidant • ↑ mRNA • ↓ Oxidative stress (OS) • ↓ ROS • ↓ NIK/IKK • ↓ PI3K/PTEN/Akt.	[1, 8, 18]

Compound Number	Chemical Class	Compound Name	Natural Sources	Biological Activity	References
8.		Neoxanthin	• **Algae:** *Ulva clathrata*	Photoprotective, anti-cancer, antioxidant and chemo-preventive activity	[3, 19, 20]
9.	Carotenes	α-Carotene	• **Plants:** *Daucus carota, Carica papaya, Cucurbita pepo, Citrullus lanatus, Ipomoea batatas, Dioscorea spp., Solanum lycopersicum, Capsicum annuum, Capsicum annuum, Brassica oleracea var. sabellica, Mangifera indica, Actinidia deliciosa, Spinacia oleracea, Brassica oleracea var. italica, Cucumis melo* var.*, Persea americana, and Citrus sinensis, Sorghum spp.* • **Algae:** *Dunaliella spp., Chlorella spp., Haematococcus spp., Muriellopsis spp., Chlamydomonas spp., Spirulina spp., Chondrus crispus, Digenea simplex, Furcellaria lumbricalis, Galaxaura obtusata, Gelidiella acerosa, Gelidium micropterum* • **Fungi/Yeasts:** *Phytomyces blakesleanus, Blakeslea trispora, Neurospora crassa* • **Bacteria:** *Halophilic spp., Myco/myxobacterium spp., Paracoccus spp., and Streptomyces spp.* • **Insects:** *Shivaphis celti, Aphis gossypii, A. nerii, A. spiraecola, Semiaphis heraclei, Toxoptera citricida, Acyrthosiphon pisum, Ectatosoma tiaratum* • **Others:** *Abalone, Haliotis discus discus, and turban shell, Turbo cornutus*	Anti-cancer, antioxidant activity	[1-7, 21]
10.		β-Carotene	• **Plants:** *Daucus carota, Carica papaya, Cucurbita pepo, Citrullus lanatus, Ipomoea batatas, Dioscorea spp., Solanum lycopersicum, Capsicum annuum, Capsicum annuum, Brassica oleracea var. sabellica, Mangifera indica, Actinidia deliciosa, Spinacia oleracea, Brassica oleracea* var. *italica, Cucumis melo* var.*, Persea americana, and*	Immuno-enhancement anti-cancer, antioxidant activity	[1-9, 22-24]

Compound Number	Chemical Class	Compound Name	Natural Sources	Biological Activity	References
			Citrus sinensis, Sorghum spp. • **Algae*:*** *Dunaliella spp., Chlorella spp., Haematococcus spp., Muriellopsis spp., Chlamydomonas spp., Spirulina spp., Dictyopteris hoytii, Dictyota bartayresiana, Dictyota cervicornis, Dictyosiphon foeniculaceus, Valoniopsis pachynema, Gracilaria birdiae, Gracilaria cornea, Gracilaria crassa, Gracilaria tenuistipitata* • **Fungi/Yeasts:** *Phytomyces blakesleanus, Blakeslea trispora, Neurospora crassa, Phaffia rhodozyma, Blakeslea trispora* • **Bacteria:** *Halophilic spp., Myco/myxobacterium spp., Paracoccus spp., and Streptomyces spp., Archaebacteria spp.,* • **Insects:** *Shivaphis celti, Aphis gossypii, A. nerii, A. spiraecola, Semiaphis heraclei, Toxoptera citricida, Acyrthosiphon pisum, Brevicoryne brassicae, Uroleucon formosanum, U. kikioensis, Macrosiphum euphorbiae, Megoura crassicauda, Ceratovacuna nekoashi, Schlechtendalia chinensis, Hecalus prasinus, Nephotettix cincticeps, Graptopsaltria nigrofuscata, Tanna japonensis, Cryptotympana facialis, Poecilocoris lewisi, Halyomorpha halys, Alcimocoris japonensis, Nezara antennata, Sastragala esakii, Haematoloecha nigrorufa, Isyndus obscurus, Sirthenea flavipes, Corythucha marmorata, Orius sauteri, Aquarius elongatus, Gerris latiabdominis, Metrocoris histrio, Ranatra chinensis, Appasus majo, Notonecta triguttata, Acyrthosiphon pisum, Ectatosoma tiaratum* • **Others: Y**ellow egg yolks, Abalone, *Haliotis discus discus,* and turban shell, *Turbo cornutus, dolphin, flamingo feathers birds*		
11.	Xanthophylls	Loroxanthin	• **Algae:** *Chlamydomonas nivalis*	Antioxidant	[3, 25]

Compound Number	Chemical Class	Compound Name	Natural Sources	Biological Activity	References
12.		Canthaxanthin	• **Algae:** *Chlamydomonas nivalis* • **Fungi/Yeasts:** mushroom *Cantharellus cinnabarinus* • **Bacteria:** (G+) *Paracoccus* spp. • **Others:** yellow egg yolks, spindle shell *Fushinus perplexus,* flamingo feathers birds	Immuno-enhancement anti-cancer, antioxidant activity	3, 5, 26
13.		Astaxanthin	• **Plants:** *Daucus carota, Carica papaya, Cucurbita pepo, Citrullus lanatus, Ipomoea batatas, Dioscorea spp., Solanum lycopersicum, Capsicum annuum, Capsicum annuum, Brassica oleracea* var. *sabellica, Mangifera indica, Actinidia deliciosa, Spinacia oleracea, Brassica oleracea* var. *italica, Cucumis melo* var., *Persea americana,* and *Citrus sinensis.* • **Algae:** *Dunaliella* spp.*, Chlorella zofingiensis, Haematococcus pluvialis, Muriellopsis spp., Chlamydomonas spp., Spirulina spp., Neochloris wimmeri* • **Fungi/Yeasts:** *Phytomyces blakesleanus, Blakeslea trispora, Neurospora crassa, Phaffia rhodozyma* • **Bacteria:** *Halophilic spp., Myco/myxobacterium spp., Paracoccus* spp., *and Streptomyces spp., (G+)Paracoccus* spp. • **Others:** shrimp, salmon fish, jelly fish, *Cyprinidae fish, starfish, whelk Buccinum bayani, spindle shell Fushinus perplexus, Whales, and flamingo feathers birds*	Anti-cancer, antioxidant activity	1-7, 9, 27
14.		Fritschiellaxanthin	• **Algae:** *Chlamydomonas nivalis*		3
15.		*β*-cryptoxanthin	• **Plants:** *Daucus carota, Carica papaya, Cucurbita pepo, Citrullus lanatus, Ipomoea batatas, Dioscorea spp., Solanum lycopersicum, Capsicum annuum, Capsicum annuum, Brassica oleracea var. sabellica, Mangifera indica, Actinidia deliciosa, Spinacia*	-Provitamin A, anti-obesity effects, antioxidant activities, anti-inflammatory and anti-cancer activity. -Stimulatory effects on osteoblastic bone formation and inhibitory effects on osteoclastic	1-8, 28, 29

Compound Number	Chemical Class	Compound Name	Natural Sources	Biological Activity	References
			oleracea, Brassica oleracea var. italica, Cucumis melo var.*, Persea americana, and Citrus sinensis.* • **Algae:** *Dunaliella spp., Chlorella spp., Haematococcus spp., Muriellopsis spp., Chlamydomonas spp., Spirulina spp.,* • **Fungi/Yeasts:** *Phytomyces blakesleanus, Blakeslea trispora, Neurospora crassa* • **Bacteria:** *Halophilic spp., Myco/myxobacterium spp., Paracoccus spp., and Streptomyces spp.* • **Insects:** *Hecalus prasinus, Nephotettix cincticeps, Parastrachia japonensis, Plautia stali, Sastragala esakii, Isyndus obscurus, Sirthenea flavipes, Orius sauteri, Aquarius elongatus, A. paludum, Gerris latiabdominis, Metrocoris histrio, Nepidae Ranatra, Belostomatidae Appasus, Notonecta triguttata*	bone resorption *in vitro*, thereby increasing bone mass. *β*-Cryptoxanthin has an effect on the gene expression of various proteins that are related osteoblastic bone formation and osteoclastic bone resororption *in vitro*	
16.	Carotenes	Lycopene	• **Plants:** *Daucus carota, Carica papaya, Cucurbita pepo, Citrullus lanatus, Ipomoea batatas, Dioscorea spp., Solanum lycopersicum, Capsicum annuum, Capsicum annuum, Brassica oleracea var. sabellica, Mangifera indica, Actinidia deliciosa, Spinacia oleracea, Brassica oleracea var. italica, Cucumis melo* var.*, Persea americana, and Citrus sinensis.* • **Algae:** *Dunaliella spp., Chlorella spp., Haematococcus spp., Muriellopsis spp., Chlamydomonas spp., Spirulina spp.,* • **Fungi/Yeasts:** *Phytomyces blakesleanus, Blakeslea trispora, Neurospora crassa* • **Bacteria:** *Halophilic spp., Myco/myxobacterium spp., Paracoccus spp., and Streptomyces spp.*	Antioxidant • ↑ mRNA • ↓ Oxidative stress (OS) • ↓ ROS • ↓ NIK/IKK • ↓ PI3K/PTEN/Akt. Anti-inflammatory • ↓ TNF-α and IL-1β • ↓ iNOS and COX-2 Cardioprotection • ↓ CK-MB • ↓ cTn T • ↓ IL-1β, IL-6, TNF-α • ↓ NF-κB p65 • ↓ Caspase-3 and -9 • Regulates Nrf-2/HO-1 Anticancer • Regulates 3-kinase (PI3K)/Akt phosphoinositide	1-8, 30
17.	Xanthophylls	Retinol	• **Plants***: Sorghum spp.*	An important physiological regulator of normal	31, 32

Compound Number	Chemical Class	Compound Name	Natural Sources	Biological Activity	References
				growth, vision, reproduction, and cellular differentiation and proliferation.	
18.		Capsanthin	• **Plants**: *Capsicum annuum*	-Strong antioxidative effect, preventive effect of obesity-related diseases, upregulate endurance performance of athletes by reducing oxygen consumption (VO_2) and the heart rate. -Chemopreventive, antitumor, skin photo-protective, anti-inflammatory, and antidiabetic activities	[31, 33, 34]
19.		Capsorubin	• **Plants**: *Capsicum annuum*		
20.	Carotenes	Prolycopene	• **Plants:** *Solanum lycopersicum 'Jen's Tangerine'*		[31]
21.	Xanthophylls	Persicaxanthin	• **Plants:** *Citrus spp.*	Antioxidant	[31, 35]
22.		Peridinin	• **Others**: Sea snail, dinoflagellates, bivalves	Antioxidant	[5]
23.	Carotenes	Isorenieratene	• **Others**: Marine sponge, *Reniera japonica*	Antioxidant	[5]
24.		Renieratene	• **Others**: Marine sponge, *Reniera japonica*	Antioxidant	[5]
25.		Renierapurpurin	• **Others**: Marine sponge, *Reniera japonica*	Antioxidant	[5]
26.	Xanthophylls	Bixin	• **Plants:** *Bixa orellana* L.	Antioxidant	[36]
27.		Deinoxanthin	• **Bacteria:** *Deinococcus radiodurans*	Antioxidant	[37]
28.		Siphonaxanthin	• **Algae:** *Codium cylindricum*	Antioxidant	[38]
29.		Myxol	• **Bacteria:** *Flavobacterium spp.*	Antioxidant	[39]
30.		Crocin	• **Plants:** *Crocus sativus* L.	Antioxidant	[40]
31.		Actinioerythrin	• **Others:** Sea anemones *Actinia equina and Tealia felina*	Antioxidant	[5]
32.		Β-apocarotenal	• **Others:** Sea hare *Aplysia kurodai*	Antioxidant	[5]
33.		Diatoxanthin	• **Others:** Scallops and ark shells	Photochemoprevention through lowering MMP-9 levels and IL-1β	[5, 41-44]
34.		Alloxanthin		Antioxidant • ↑ mRNA • ↓ Oxidative stress (OS) • ↓ ROS • ↓ NIK/IKK • ↓ PI3K/PTEN/Akt. Anti-inflammatory	

Compound Number	Chemical Class	Compound Name	Natural Sources	Biological Activity	References
				• ↓ TNF-α and IL-1*β*	
35.		Pectenol			
36.		Pectenolone			
37.		4-Hydroxyalloxanthin		Antioxidant	
38.		Corbiculaxanthin	• **Others:** Brackish clam: *Corbicula japonica,* freshwater clam: *Corbicula sandai*		5
39.		Corbiculaxanthin 3′-acetate			
40.		2,3′-dihydroxycanthaxanthin	• **Others:** Hermit crab: *Paralithodes brevipes*		5
41.		4-keto-4′-hydroxydiatoxanthin	• **Others:** Starfish: *Acanthaster planci*		5
42.		3′-epigobiusxanthin			
43.		Cucumariaxanthin A	• **Others:** Sea cucumber *Cucumaria japonica*		5, 45
44.		Amarouciaxanthin A	• **Others:** Tunicate *Amaroucium pliciferum,* mice	Amarouciaxanthin A significantly decreased glycerol-3-phosphate dehydrogenase (GPDH) activity, the mRNA expressions of adipocyte fatty acid binding protein (aP2), lipoprotein lipase (LPL), and glucose-transporter 4 (Glut4) in 3T3-L1 cells, and the expression levels of peroxisome proliferator-activated receptor γ (PPARγ) and CCAAT-enhancer-binding protein α (C/EBPα), which are the key adipogenic transcriptional factors, were also decreased. Consequently, amarouciaxanthin A, suppressed 3T3-L1 adipocyte differentiation.	5, 46
45.		Amarouciaxanthin B			
46.		Tunaxanthin	• **Others:** Fish belonging to *Perciformes*		5, 47
47.		7,8-Dehydro-*β*-micropteroxanth	• **Others:** Black bass *Micropterus salmoides*		5

Compound Number	Chemical Class	Compound Name	Natural Sources	Biological Activity	References
		in			
48.		*β*-Micropteroxanthin			
49.		Salmoxanthin	• **Others:** Salmon *Oncorhynchus keta*		48
50.		Deepoxysalmoxanthin			
51.		Gobiusxanthin	• **Others:** Freshwater goby *Rhinogobius brunneus*		49
52.	Carotenes	Torulene	• **Insects:** *Aphis spiraecola, Brevicoryne brassicae, Acyrthosiphon pisum*		1, 50
53.	Xanthophylls	Echinenone	• **Insects:** *Graptopsaltria nigrofuscata, Tanna japonensis, Isyndus obscurus, Aquarius elongatus, A. paludum, Gerris latiabdominis, Metrocoris histrio, Notonecta triguttata*		1, 50
54.		Rhodoxanthin	• **Plants:** *Taxus baccata and Lonicera morrowii* • **Others:** *Phoenicircus nigricollis, Ptilinopus jambu, Ptilinopus pulchellus, Ptilinopus magnificus, Ptilinopus solomonensis.*		

Table S2. Selected identified carotenoproteins which are isolated from invertebrates.

Species	Organ	Carotenoids (Compound number)	Protein	References

Species	Organ	Carotenoids (Compound number)	Protein	References
Pecten maximus	Ovary	Xanthophylls	Glycolipoprotein	[51]
Tettigonia viridissima	Skin	Lutein **(1)** + bile pigment	Albumin	[51]
Tettigonia cantens	Skin	Lutein **(1)** + bile pigment	Albumin	[51]
Sphinx ligustri	Skin	Lutein **(1)** + bile pigment	Globulin	[51]
Meconium varium	Skin	Lutein **(1)** + bile pigment	Albumin	[51]
Dixippus morosus	Blood	*β*-carotene **(10)** +bile pigment	Globulin	[51]
Idothea montereyensis	Exoskeleton, eggs, blood	Canthaxanthin **(12)**	Lipoprotein	[51]
Idothea granulosa	Exoskeleton, epidermis, blood, eggs	Canthaxanthin **(12)**	Lipoprotein	[51]
Palinurus vulgaris	Carapace, ovary, eggs, hypodermis	Astaxanthin **(13)** and others	Lipoprotein	[51]
Astacus astacus	Carapace	Astaxanthin **(13)**	Albumin	[51]
Cancer pagurus	Ovary	Astaxanthin **(13)** + other xanthophylls	Glycolipoprotein	[51]
Lepas anatifera	Eggs	Astaxanthin **(13)**	Euglobulin	[51]
Pomacea canaliculata	Albumen gland, eggs	Astaxanthin **(13)**	Glycoprotein	[51]

Table S3. Selected chlorophylls and bacteriochlorophyllides, identified structures.

Compound Number	Chemical class	Compound name	Natural source	Biological Activity	References
55.	Chlorophylls	Chlorin	• **Algae:** *Sargassum wightii*	Antioxidant, Antimutagenic/Antigenotoxic activity, Photosensitizer-	[8, 52]

Compound Number	Chemical class	Compound name	Natural source	Biological Activity	References
				photodynamic therapy	
56.		Phytol	• **Algae:** *Sargassum wightii, Zonaria tournefortii*	Antioxidant, Antimutagenic/Antigenotoxic activity, Photosensitizer-photodynamic therapy	8, 52
57.		Chlorophyll A	• **Algae:** *Sargassum wightii, Zonaria tournefortii, Caulerpa cylindracea, Caulerpa lentillifera, Halymenia agardhi, Hypnea musciformis, Palisada tenerrina, Porphyra necnamessis*	Antioxidant, Antimutagenic/Antigenotoxic activity, Photosensitizer-photodynamic therapy	8, 52
58.		Chlorophyll B	• **Algae:** *Caulerpa racemosa, Caulerpa sertularioides*	Antioxidant, Antimutagenic/Antigenotoxic activity, Photosensitizer-photodynamic therapy	8, 52
59.		Chlorophyll C	• **Algae:** *Sargassum filipendula, Sargassum ilicifolium, Sargassum muticum, Sargassum polycustum*	Antioxidant, Antimutagenic/Antigenotoxic activity, Photosensitizer-photodynamic therapy	8, 52
60.		Chlorophyll D	• **Algae:** *Liagora erecta*	Antioxidant, Antimutagenic/Antigenotoxic activity, Photosensitizer-photodynamic therapy	8, 52
61.	Bacteriochlorophyllides	Bacteriochlorophyll a	• **Bacteria:** *Gemmatimonas phototrophica*	Perspectives for cancer therapy, skin anti-aging activities	53-55
62.		Bacteriochlorophyllide b	• **Bacteria:** *Gemmatimonas phototrophica*	Perspectives for cancer therapy	53
63.		Bacteriochlorophyllide d	• **Bacteria:** *Gemmatimonas phototrophica*	Perspectives for cancer therapy	53
64.		Bacteriochlorophyllide g	• **Bacteria:** *Gemmatimonas phototrophica*	Perspectives for cancer therapy	53

Table S4. Selected identified alkaloids and alkaloids-related pigments.

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	References

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	References
75.	Prodigiosin	2-(*p*-Hydroxybenzyl) prodigiosin	• **Bacteria:** *Pseudo alteromonas rubra*	Suppress the reactivation of herpes simplex virus type 1 (HSV-1). Cytotoxic against SKOV-3 (human ovarian adenocarcinoma) cell line.	[56]
76.		2,2'-[3-Methoxy-1'amyl-5'-methyl-4-(1-pyrryl)] dipyrryl-methene	• **Bacteria:** *Micrococcus* sp., *Serratia marcescens* Bizio	Potent cytotoxic activity towards cancer cells. Inhibits proliferation of both human T, B and murine T cells (Selective T cell immunosuppressive).	[57]
77.	Polyenoyltetramic acid	Physarorubinic acid	• **Mold:** *Physarum polycephalum* Schwein.		[58]
78.	Diketopiperazines	Brevianamide A	• **Fungus:** *Penicillium brevicompactum*	Cytotoxic activity, Antifeedant activity against *Spodoptera frugiperda*, *Heliothis virescens* larvae.	[59]
79.		(-)-Brevianamide C	• **Fungus:** *Penicillium brevicompactum* DFFSCS025	Cytotoxic against HCT116 (human colon cancer) cell line with IC_{50} = 15.6 μM.	[60]
80.		Brevianamide K	• **Fungus:** *Aspergillus versicolor* (Vuillemin) *Tiraboschi* strain pt20	Antibacterial activities against *Escherichia coli, Staphylococcus aureus* with inhibition zones 7, 7 mm at 30 μg/disk	[61]
81.		Brevianamide O	• **Fungus:** *Aspergillus versicolor* (Vuillemin) Tiraboschi		[62]
82.		Brevianamide P			
83.		Brevianamide S		Significant antibacterial activity against *Bacille Calmette-Guerin* (Pasteur 1173P2) (BCG) (MIC = 6.25, 50, 100, 25 μg/mL, respectively).	[63]
84.		Brevianamide T			
85.		Brevianamide V			
86.		Brevianamide U			
87.		Brevianamide X	• **Fungus:** *Penicillium brevicompactum* DFFSCS025		[60]
88.		Brevianamide Y			
89.		Gartryprostatin C	• **Fungus:** *Aspergillus* sp. GZWMJZ-258	Strong cytotoxic effect on MV4-11 (acute myeloid leukemia) with IC_{50} = 0.22 μM. moderate effect for K562 (chronic myeloid leukemia), HL-60 (human caucasian pro-myelocytic leukemia), A549 (human lung adenocarcinoma) with IC_{50} >10 μM	[64]
90.	Indoloquinazoline	Candidine	• **Yeast:** *Yarrowia*	Effective and safe treatment in patients	[65]

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	References
			lipolytica	with recalcitrant warts with 0.1 cc in three times per day, for four weeks	
91.	Prodigiosin	Cycloprodigiosin	• **Bacteria:** *Pseudoalteromonas Denitrificans, Beneckea gazogenes*	Selective inhibitor of T cell proliferation. Antitumor potential with Ras-PI3K-Akt Pathway activation. Induced Apoptosis in PC12 Cells	[66]
92.	Tripyrrole	Heptyl prodigiosin	• **Bacteria:** *Alphaproteobacteria*	Antimalarial against the chloroquine-sensitive strain *Plasmodium falciparum* 3D7. 5 and 20 mg/kg subcutaneous extended survival of *P. berghei* ANKA strain-infected mice	[67]
93.	Diazadiphenoquinones	Indigoidine	• **Bacteria:** *Phaeobacter daeponensis* Y4I, *Leisingera* sp. JC1	Antioxidant and antimicrobial activities	[68]
94.	Tripyrrole	Metacycloprodigiosin	• **Bacteria:** *Streptomyces spectabilis* BCC 4785 *Streptomyces longisporusruber* Waksman, *Saccharopolyspora* sp. nov.	Cytotoxic activities against P388 (mouse lymphoma), HL60 (human peripheral blood promyeloblast), A-549 (human lung carcinoma), BEL-7402 (human hepatic carcinoma), SPCA4 (human lung carcinoma), KB (human epidermoid carcinoma), BC-1 (human breast cancer), and Vero (African green monkey kidney fibroblasts) cell lines with IC_{50} = 0.007, 0.022, 0.11, 0.028, 7.52 µM, 0.36±0.02, 0.27±0.01, and 1.35±0.28 µg/mL respectively. Antimalarial activity against *Plasmodium falciparum* K1, with IC_{50} = 0.0050±0.0010 µg/mL. Suppress T-cell proliferation on murine skin and heart transplants	[69]
95.	Pyrazinone	Neoaspergillic acid	• **Fungi:** *Aspergillus sclerotiorum* G.A. Huber	Antibacterial activity against *S. aureus, S. epidermidis, B. subtilis, B. dysenteriae, B. proteus, E. coli* with MIC = 0.98, 0.49, 1.95, 7.8, 7.8, 15.62	[70]

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	References
				μg/mL, respectively. Anticancer potential: against SPC A-1 (lung cancer), BEL-7402 (hepatocellular carcinoma), SGC-7901 (gastric carcinoma) and K562 (erythromyeloblastoid leukemia) cell lines with IC_{50} ranges of 7.99–24.90 μg/mL.	
96.	Phenazine	Baraphenazine E	• **Bacteria:** *Streptomyces* sp. PU-10 A	Cytotoxic activity against A549 (human non-small-cell lung), PC3 (human prostate) with IC_{50} = 2.4, 4.7 μM. Antibacterial activity against *M. aurum, S. aureus, M. luteus, B. subtilis* with MIC = 30, 4, 7.5, and 7.5 μM, respectively.	[71]
97. 98. 99.		Izumiphenazine A Izumiphenazine B Izumiphenazine C	• **Bacteria:** *Streptomyces* sp. IFM 11204	Synergistic activity in TRAIL-resistant AGS cells with 30, 20 μM, respectively.	[72]
100.		Saphenamycin	• **Bacteria:** *Streptomyces antibioticus* Tü 2706., *Streptomyces canarius* MG314-hF8	Strong anti-bacterial activity against *Bacillus subtilis* PC1219., *B. subtilis* NRRL B-558 with MIC <0.05 μg/mL	[73]
101. 102.		Strepoxazine A Phencomycin	• **Bacteria:** *Streptomyces* sp. SBT345	Cytotoxic activity against HL-60 (human promyelocytic leukaemia) cells with IC_{50} = 8±2.33, >50 μg/mL, respectively.	[74]
103.		Tubermycin B	• **Bacteria:** *Streptomyces anulatus* 9663, *Streptomyces misakiensis* Nakamura	Notable anti-bacterial activity against *Mycobacterium tuberculosis* BCG, *M. tuberculosis* H31 R v (streptomycin resistant with MIC = 12.5, 10 μg/mL, respectively. Cytotoxic activity against HL-60 (human promyelocytic leukemia) cells with IC_{50} >50 μg/mL.	[75]
104.		Endophenazine B	• **Bacteria:** *Streptomyces anulatus* 9663		[75]
105.		Phenazostatin A	• **Bacteria:**	Neuro-protective activity: protect N18-	[76]

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	References
106. 107.		Phenazostatin B Phenazostatin C	*Streptomyces* sp. 833	RE-105 cells (neuroblastoma-retinal hybrid line) with EC_{50} = 0.34, 0.33, 0.37 μM, respectively.	
108.		Diastaphenazine	• **Bacteria:** *Streptomyces diastaticus subsp. ardesiacus*	Antibacterial activity against *S. aureus* with MIC = 64μg/mL.	77
109.	Tetrapyrrole	Phycocyanobilin	• ***Cyanobacteria*** *Spirulina platensis Gomont and* algae *Aphanizomenon flos-aquae (Linnaeus)* Ralfs ex Bornet & Flahault	Antioxidant activity, Nephroprotection against diabetic outcome by inhibiting oxidative stress	78
110.		Phycoerythrobilin	Cyanobacteria and red algae	Antioxidant activity, Anti-inflammatory activities through the suppression of mast cells degranulation	79
111.		Phycourobilin	• **Cyanobacteria:** *Oscillatoria* sp. and red algae		80
112.	Prodiginines	Prodigiosin	• **Bacteria*: Serratia marcescens* *Bizio, Vibrio psychroerythrus*	Anticancer activity against various cancer cell lines. Antimalarial activity, antifungal, antibacterial and immunosuppressant	81
113. 114.	Tripyrrole	Prodigiosin R1 Prodigiosin R2	• **Bacteria:** *Streptomyces griseoviridis* 2464-S5	Cytotoxic activity against HeLa and HT1080 (human fibrosarcoma) cells with IC_{50} = 1.7 and 3.3 & 0.41 and 0.82 μM, respectively.	82
115.	Phenazinone	Pyocyanin	• **Bacteria:** *Pseudomonas aeruginosa* Migula	Antibacterial activity against Micrococcus luteus with MIC = 2 μg/mL. Antifungal activity against C albicans and A fumigatus were MIC >64 μg/mL	83
116.	Dipyrrole	Roseophilin	• **Bacteria:** *Streptomyces griseoviridis* 2464-S5	Cytotoxic activity against KS62 (human erythroid leukemia) and KB (human epidermoid carcinoma), HT-1080 (human fibrosarcoma), C6 (rat glioma), MCF7 (human breast cancer), T-47D (human breast cancer) cells with IC_{50} = 0.34,	84

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	References
				0.88, 1.0, 0.72, 2.1, and 1.9 µM, respectively	
117.		Dechlororoseophilin		Cytotoxic activity against HT-1080 (human fibrosarcoma), C6 (rat glioma), MCF7 (human breast cancer), T-47D (human breast cancer) cells with IC_{50} = 2.6, 2.1, 2.7, 2.0 µM, respectively	[85]
118.	Azaphilones	Rubropunctamine	Mold *Monascus purpureus* Went	Antibacterial activity against *Bacillus megaterium* MCM B-357, *B. mycoides* MCM B-358, and *B. subtilis* MCM B-310	[86]
119.	Indole-benzylidene	Scytonemin	• **Blue-green alga:** *Nostoc punctiforme* ATCC 29133, *Scytonema sp. R77DM, Calothrix* spp	Photoprotection activity against short wavelength, Antiproliferative potential. Anti-inflammatory activity	[87]
120. 121. 122. 123. 124.	Xantheno-benzodioxino-isoquinoline	Kigamicin A Kigamicin B Kigamicin C Kigamicin D Kigamicin E	• **Bacteria:** *Amycolatopsis* sp. ML630-mF1	The best antimicrobial activity observed against various strains of *Bacillus subtilis, Bacillus cereus, Corynebacterium bovis, and Staphylococcus aureus* with 0.025<MIC <0.39 µg/mL& 0.025<MIC <0.20 µg/mL& 0.05<MIC<0.2 µg/mL& 0.025<MIC<0.39 µg/mL& 0.025<MIC<0.78 µg/mL, respectively.	[88]
125.	Tetrahydrobenzo[α]anthracene	Azicemicin A	Bacteria: *Amycolatopsis* sp. MJ126-NF4	The antimicrobial activity observed against Micrococcus luteus IFO3333 with MIC = 12.5 µg/mL. Corynebacterium bovis 1510 with MIC = 25 µg/mL	[89]
126.		Azicemicin B			
127.	Tetrapyrrol	Stercobilin	*Fecal, produced by bacteria in the gut*		[90]
128.		Stercobilinogen			[91]
129.	Prodiginine	Streptorubin B	• **Bacteria:** *Streptomyces coelicolor A3, Saccharopolyspora sp., actinomycete* strain	A slight antimicrobial activity against methicillin-resistant *Staphylococcus aureus* subsp. aureus N315 with MIC ≤32 µg/mL, Inhibition of bacterial	[92]

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	References
			B4358 and *Streptomyces abikoensis*	biofilm formation of methicillin-resistant *Staphylococcus aureus* subsp. aureus N315 with IC_{50} = 0.22 μg/mL	
130.	Tambjamine	Tambjamine MYP1	• **Marine bacterium:** *Pseudoalteromonas citrea*		93
131.		Tambjamine A	• **Marine ascidian:** *Atapozoa sp*		94
132.		Tambjamine C		Cytotoxic effect against HL-60, MDAMB435, HCT-8, SF-295 cancer cell lines with IC_{50} = 0.70, 3.42, 1.41, 1.64 μg/mL, respectively& with IC_{50} >25 μg/mL & with IC_{50} = 0.80, 2.27, 1.04, 1.08 μg/mL,respectively.	
133.		Tambjamine E			
134.		Tambjamine F			
135.	Tripyrrole	Undecylprodigiosin	• **Bacteria:** *Streptomyces* spp. *Serratia marcescens* SS-1	Anticancer effect on human breast carcinoma cell lines [BT-20 (IC_{50} = 8.57 μM), MCF-7 (IC_{50} = 3.25 μM), MDA-MB-231 (IC_{50} = 7.53 μM) and T47D (IC_{50} = 3.61 μM)] and nonmalignant human breast epithelial [MCF-10 A (IC_{50} = 4.76 μM)] cell line	95
136.	Tetrapyrrole	Urobilin	*Mammalian urine*		96
137.	Bis-indole	Violacein	• **Marine bacteria:** *Chromobacterium violaceum, Massilia* sp. strain NR 4–1	Cytotoxic potential. Antibacterial activity against *Staphylococcus aureus* and other gram-positive pathogens, antiviral potentia	97
138.	Betacyanins	Muscapurpurin	• **Mushroom:** *Amanita muscaria* (L.) Hook		98
139.	Azepine	Muscaflavin			
140.	Pyrroloquinone	Mycenaflavin A	• **Mushroom:** *Mycena haematopus* (Pers.: Fr.) P. Kumm.	Antibacterial activity against *Azovibrio restrictus, Azoarcus tolulyticus* with inhibition zones 0.8, 1.0 cm/ 1 μmol, respectively	99
141.		Mycenaflavin B		Antibacterial activity against *Azovibrio restrictus* with inhibition zone 1.0 cm/ 1 μmol	
142.		Mycenaflavin C			
143.		Mycenaflavin D			
144.	Pyrroloquinone	Haematopodin B		Antibacterial activity *Azovibrio restrictus, Azoarcus tolulyticus*. with	

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	References
				inhibition zones 1.0, 3.3 cm/1µmol, respectively	
145.		Haematopodin			
146.		Mycenarubin A			
147.		Pelianthinarubin A			100
148.		Pelianthinarubin B			
149.		Sanguinone A	• **Mushroom:** *Mycena sanguinolenta* (Alb. & Schwein.) P.Kumm.		101
150.		Sanguinone B			
151.		Ammosamide A	• **Marine bacteria:** *Streptomyces* strain CNR-698	Cytotoxic against HCT-116 colon carcinoma cells, with IC_{50} = 320 nM	102
152.		Ammosamide B			
153.		Ammosamide D		Cytotoxic against the MIA PaCa-2 (pancreatic cancer) cell line with IC_{50} = 3.2 µM	103
154.	Pyrrole	Mycenarubin B	• **Mushroom:** *Mycena rosea* (Schumach.) Gramberg		104
155.		Baculiferin A	• **Marine sponge:** *Iotrochota baculifera* Ridley	Anti-human immunodeficiency virus type 1 IIIB (HIV-1 IIIB) activities on MT-4 (human T-cell) and MAGI (HeLa-CD4-LTR-β-gal) cells with IC_{50} >25µg/mL& IC_{50} = 7.6, 3.7 µg/mL & IC_{50} = 2.2, 1.3 µg/mL& IC_{50} = 8.4, 1.2 µg/mL& IC_{50} = 4.6, 2.7 µg/mL& IC_{50} = 4.6, 2.7 µg/mL & IC_{50} = 3.2, 4.4 µg/mL & IC_{50} = 1.4, 1.3 µg/mL & IC_{50} = 5.5, <0.4 µg/mL & IC_{50} = 7.0, 4.1 µg/mL & IC_{50} = 5.0, 0.2 µg/mL & IC_{50} = 4.4, <0.1 µg/mL	105
156.		Baculiferin B			
157.		Baculiferin C			
158.		Baculiferin D			
159.		Baculiferin E			
160.		Baculiferin F			
161.		Baculiferin G			
162.		Baculiferin H			
163.		Baculiferin K			
164.		Baculiferin L			
165.		Baculiferin M			
166.		Baculiferin N			
167.		Baculiferin O		Anticancer activities against the HCT-8, Bel-7402, BGC-823, A549, and A2780 tumor cell lines with IC_{50} = 33.1 µM	
168.	Diaza-Anthracene	Diazaquinomycin A	• **Bacteria:** *Streptomyces* sp. OM-704	Antifolate antibiotic inhibits thymidylate synthase. cytotoxic against Vero (monkey kidney epithetical) and Raji (human lymphoblastoid) cells, and the OVCAR5 (ovarian cancer) cell	106

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	References
				with LC_{50} = 8.8 μM. Also showed cytotoxicity against a panel of human cancerous [MDA-MB-435 (0.09 μM), MDA-MB-231 (3.6 μM), HT-29 (5.7 μM), OVCAR3 (0.48 μM), OVACR4 (4.3 μM), Kuramochi (9.4 μM)]. Antibacterial activities against Micrococcus luteus ATCC 9341, Streptococcus faecium IFO 3181 with MIC = 6.25, 3.13 μg/mL, respectively	
169.		Diazaquinomycin C			
170.		Diazaquinomycin E		Anti-cancer activity cytotoxicity against the OVCAR5 (ovarian cancer) cell with LC_{50} = 9.0 μM	
171.		Diazaquinomycin F			
172.	Isoquinoline	Berberine	• **Plants:** *Berberis aristata, Rhizoma coptidis, Phellodendron amurense and Berberis vulgaris*	Dyes	[107]
173.	Kuanoniamines	Kuanoniamine A	Genus *Cystodytes* (tunicates)		[108-110]
174.		2-Bromoleptoclinidinone			
175.		Eilatin			
176.	Indoles	Meridianin A	• **Green deep-sea tunicate***: Aplidium meridianum*		
177.		Psammopemmin A			
178.		Variolin B			
179.		Indigo	• **Plants***: Perisicaria tinctoria, Isatis tinctoria, and Indigofera tinctoria*		[111-113]
180.		Tyrian	*Levantine* Sea snails		

Table S5. List of betalains pigments mainly isolated from plants.

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	Reference
181.	Betaxanthins	Betalamic acid	*Beta vulgaris* L.		[114]

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	Reference
182.		Indicaxanthin	*Opuntia ficus-indica* L.	Antioxidant ↑ Resistance to oxidative hemolysis ↓ ROS production, glutathione depletion, PGE2 release, and Ca^{2+} entry Perferryl-Hb reduction ↑ Resistance to oxidative hemolysis ↓ Vit E and GSH depletion ↓ Lipid and hemoglobin oxidation Anti-inflammatory ↓ ROS formation ↓ NF-κB transcriptional activity ↓expression of adhesion molecules (ICAM-1; VCAM-1; ELAM-1) Preserved activity of cholesterol efflux system ABC-A1 ↓ expression of ICAM-1 ↓ NF-κB activation ↑ lipid hydroperoxides ↑ HNE formation Modulation of prostaglandin biosynthetic pathway: ↓ mPGES-1 expression ↑ COX2 and MPGDS expression ↑ Synthesis of proresolvin cyclopentenone ↓ active NOX-1 assembly ↓ ROS generation ↓ NF-κB activation ↓ COX2 and NOS expression ↑ release of IL6, IL8, PGE2, NO ↓ expression of inflammatory IL6, IL8, COX2, NOS, NOX-1 ↑ expression of glutamate-cysteine ligase catalytic subunit (GCLC) and glutathione peroxidase-1 (GPX-1) Anti-apoptotic ↓ NOX-4 basal activity ↓ NOX-4 over-expression ↓ NF-κB activation ↓ intracellular Ca2+ ↓ mitochondrial apoptotic pathway ↓ O2•− and ROS production ↓ transglutaminase 2 expression	[115, 116]

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	Reference
				↓ caspase 3 expression ↑ nestin and cyclin-D1	
183.		Portulacaxanthin I	*Portulaca grandiflora* (Hook.)		117, 118
184.		Portulacaxanthin II	*Portulaca grandiflora/Beta vulgaris* L.		119
185.		Portulacaxanthin III	*Portulaca grandiflora/Beta vulgaris* L.		119
186.		Vulgaxanthin I	*Beta vulgaris* L.	lowering inflammatory markers and mitigating oxidative stress, implying the potential to ameliorate inflammatory intestinal disease	120, 121
187.		Vulgaxanthin II			120
188.		Vulgaxanthin III			120
189.		Vulgaxanthin IV	*Beta vylgaris var. lutea/Beta vulgaris L. ssp. cicla* [L.]		122
190.		Miraxanthin I	*Mirabilis jalapa* L.		117
191.		Miraxanthin II			117
192.		Miraxanthin III			117
193.		3-Methoxy tyramine-Bx			117
194.		Miraxanthin V		Hepcidin antagonist *in silico* for iron deficiency anemia	117, 123
195.		Histamine-Bx			117
196.		Dopaxanthin	*Glottiphyllum longum*		124
197.		Humilixanthin	*Rivina humilis* L.		125
198.		ɣ-Aminobutyric acid-Bx	*Beta vulgaris* L.		126
199.		Methylated arginine	*Amaranthus tricolor* L.		127
200.		Tryptophan-Bx	*Celosia argentea var. cristata*		128
201.		Serine-Bx	*Beta vulgaris* L.		126
202.		Valine-Bx			126
203.		Phenylalanine-Bx			126
204.		Isoleucine-Bx			126
205.		Alanine-Bx			126
206.		Muscaaurin VII	*Beta vulgaris L. ssp. cicla* [L.] Alef.		126
207.		Methionine-Bx	*Opuntia sp.*		129

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	Reference
208.		Threonine-Bx	*Beta vulgaris L. ssp. cicla* [L.] Alef.		130
209.		Arginine-Bx	*Gomphrena globosa*		131
210.		Lysine-Bx	*Gomphrena globosa*		131
211.		Ethanolamine-Bx	*Beta vulgaris L. ssp. cicla* [L.] Alef.		130
212.		Putrescine-Bx	*Bougainvillea sp.*		130
213.		Phenethylamine-Bx	*Opuntia spp.*		118
214.		3-Methoxytyramine betaxanthin	*Celosia cristata*		132
215.		Dopaxanthin	*Lampranthus productus*		133
216.	Betacyanins	Betanidin	*Beta vulgaris* L.		134
217.		Isobetanidin	*Hylocereus polyrhizus*		135
218.		2-Descarboxy-betanidin	*Carpobrotus acinaciformis* L.		136
219.		Betanidin 5-*O*-*β*-sophoroside	*Hylocereus polyrhizus*		135
220.		Isobetanidin 5-*O*-*β*-sophoroside			135
221.		Betanidin-5-*O*-(6’-*O*-3-hydroxy-butyryl)-β-glucoside			137
222.		Betanidin-6’-*O*-malonyl-5-*O*-*β*-sophoroside	*Hylocereus polyrhizus, H. ocamponis, H. undatus*		135
223.		Isobetanidin-6’-*O*-malonyl-5-*O*-*β*-sophoroside	*Hylocereus polyrhizus, H. ocamponis, H. undatus*		135
224.		15-Hydroxybetanidin-5-*O*-*β*-glucoside	*Hylocereus polyrhizus*		135
225.		15-Hydroxyisobetanidin-5-*O*-*β*-glucoside	*Hylocereus polyrhizus*		135
226.		Betanin	*Beta vulgaris* L		134
227.		Isobetanin	*Hylocereus polyrhizus*		135
228.		2-Descarboxy-betanin	*Beta vulgaris* L.		138
229.		6’-*O*-Malonyl-2-descarboxy-betanin	*Beta vulgaris* L		138

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	Reference
230.		2’-*O*-Apiosyl-betanin	*Hylocereus ocamponis*		135
231.		2’-*O*-Apiosyl-isobetanin	*Hylocereus polyrhizus*		135
232.		2’-*O*-[5’’-*O*-(E)-feruloyl]-Apiosyl-betanin	*Phytolacca americana* L		139
233.		2’-*O*-[5’’-*O*-(*E*)-feruloyl]-Apiosyl-isobetanin	*Hylocereus polyrhizus, H. ocamponis, H. undatus*		135
234.		2’-*O*[5’’-*O*-(*E*)-sinapoyl]-Apiosyl-betanin	*Hylocereus ocamponis*		135
235.		2’-*O*-[5’’-*O*-(*E*)-sinapoyl]-Apiosyl-isobetanin	*Hylocereus polyrhizus, H. ocamponis, H. undatus*		135
236.		4’-*O*-Malonyl-betanin	*Hylocereus ocamponis*		135
237.		4’-Malonyl-isobetanin	*Hylocereus polyrhizus*		135
238.		4’-*O*-(3’’-hydroxy-3’’-methyl-glutaryl)-Betanin	*Hylocereus polyrhizus, H. ocamponis, H. undatus*		135
239.		4’-*O*-(3’’-hydroxy-3’’-methyl-glutaryl)-Isobetanin	*Hylocereus polyrhizus, H. ocamponis, H. undatus*		135
240.		17-Decarboxy-betanin	*Hylocereus polyrhizus*		135
241.		17-Decarboxy-isobetanin			135
242.		2,17-Bidecarboxy-betanin			135
243.		15-Decarboxy-betanin			135
244.		Isobutyrylbetanin			135
245.		Phyllocactin	*Phyllocactus hybridus*		140
246.		Isophyllocactin	*Hylocereus polyrhizus*		135
247.		2’-*O*-Apiosyl-phyllocactin	*Schlumbergera buckleyi*		141
248.		2’-*O*-Apiosyl-isophyllocactin	*Hylocereus polyrhizus*		135
249.		2’-*O*-[5’’-*O*-(*E*)-feruloyl]-Apiosyl-phyllocactin	*Schlumbergera buckleyi*		141

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	Reference
250.		2’-*O*-[5’’-*O*-(*E*)-feruloyl]-Apiosyl-isophyllocactin	*Hylocereus polyrhizus, H. ocamponis, H. undatus*		135
251.		2-Decarboxy-phyllocactin	*Hylocereus polyrhizus*		135
252.		2-Decarboxy-isophyllocactin			135
253.		2,17-Bidecarboxyphyllocactin			135
254.		17-Decarboxy-phyllocactin			135
255.		15-Decarboxy-phyllocactin			135
256.		Hylocerenin			142
257.		Isohylocerenin			135
258.		2-Decarboxy-hylocerenin			135
259.		2,17-Bidecarboxy-hylocerenin			135
260.		15-Decarboxy-hylocerenin			135
261.		17-Decarboxy-hylocerenin			135
262.		Lampranthin I	*Lampranthus sp.*		143
263.		Lampranthin II			143
264.		Isolampranthin II			143
265.		Prebetanin	*Beta vulgaris*		144
266.		Isoprebetanin			144
267.		Rivinianin	*Rivina humilis* L.		125
268.		Amaranthin	*Celosia cristata* L.		145
269.		Isoamaranthin	*Amaranthus cruentus*		132
270.		Sinapoyl-amaranthin	*Gomphrena globosa* L.		131
271.		(2’’-*O*-*E*-Sinapoyl)-isoamaranthine	*Iresine herbstii* Hook. f.		146
272.		Iresinin I			146
273.		Isoiresinin I	*Amaranthus cruentus*		132
274.		(2’’’-*O*-*E*-Feruloyl)-iresinin I	*Iresine herbstii* Hook. f.		146
275.		(2’’’-*O*-*E*-Feruloyl)-isoiresinin I			146
276.		(2’’’-*O*-*E*-Sinapoyl)-iresinin I			146
277.		(2’’’-*O*-*E*-Sinapoyl)-isoiresinin I			146
278.		Celosianin I	*Celosia cristata* var. cristata		145
279.		Isocelosianin I	*Amaranthus cruentus*		132

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	Reference
280.		Celosianin II	*Celosia cristata* var. *cristata*		145
281.		Isocelosianin II	*Amaranthus cruentus*		132
282.		Bougainvillein-r I	*Bougainvillea* ‘‘Mrs. Butt’’		136
283.		Bougainvillein-r III			136
284.		Feruloyl-bougainvillein-r I	*Ullucus tuberosus Caldas*		147
285.		4’-*O*-Malonyl-bougainvillein-r I	*Mammillaria spp*		148
286.		Bougainvillein-v	*Bougainvillea glabra* var. *sanderiana*		136
287.		6’-*O*-(*E*)-Caffeoyl bougainvillein-v	*Bougainvillea glabra Choisy*		149
288.		6’-*O*-(*E*)-*p*-Coumaroyl-bougainvillein-v			149
289.		6’’-*O*-(*E*)-*p*-Coumaroyl-bougainvillein-v			149
290.		6’,6’’-di-*O*-(*E*)-*p*-Coumaroyl-bougainvillein-v			149
291.		6’’-*O*-Rhamnosyl-bougainvillein-v	*Bougainvillea glabra* var. *sanderiana*		149
292.		2’’-*O*-[6’-*O*-(*E*)-caffeoyl]-[6’’-*O*-(*E*)-*p*-coumaroyl]-Glucosyl-bougainvillein-v	*Bougainvillea glabra Choisy*		149
293.		2’’-*O*-[6’,6’’-di-*O*-(*E*)-*p*-coumaroyl]-Glucosyl-bougainvillein-v			149
294.		2’’-*O*-[6’-*O*-(*E*)-caffeoyl]-[6’’-*O*-(*E*)-*p*-coumaroyl]-Sophorosyl-bougainvillein-v			149
295.		Gomphrenin I	*Gomphrena globosa* L.		150
296.		Gomphrenin II			150
297.		Gomphrenin III			150
298.		Gomphrenin IV			150
299.		Isogomphrenin I	*Hylocereus polyrhizus*		135
300.		Isogomphrenin II	*Gomphrena globosa*		132
301.		Isogomphrenin III			132
302.		Mammillarinin	*Mammillaria spp*		148

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	Reference
303.		2-Descarboxy-mammillarinin			148
304.		Neobetanin	*Beta vulgaris*		151
305.		2-Decarboxy-neobetanin	*Hylocereus polyrhizus*		135
306.		17-Decarboxy-neobetanin			135
307.		2,17-Bidecarboxyneobetanin			135
308.		2-Decarboxy-neobetanidin 5-*O*-(6'-*O*-malonyl)-*β*-glucoside			135
309.		2,17-Bidecarboxyneobetanidin 5-*O*-(6'-*O*-malonyl)-*β*-glucoside			135
310.		2,17-Bidecarboxyneobetanidin 5-*O*-(6'-*O*-3-hydoxy-3-methyl-glutryl)-*β*-glucoside			135
311.		Neobetanidin 5-*O*-*β*-glucoside, bidecarboxylated, dehydrogenated			135
312.		2-Decarboxy-neobetanidin 5-*O*-(6'-*O*-3-hydoxy-3-methyl-glutryl)-*β*-glucoside			135
313.		2,15,17-Tridecarboxy-neobetanidin-5-*O*-(6'-*O*-3-hydoxy-3-methyl-glutryl)-*β*-glucoside			135

Table S6. Selected identified pteridine isolated from insects.

Compound Number	Chemical Class	Compound Name	Natural Source	Biological Activity	References

314.	Pterin	Leucopterin	• **Insects:** Pieris brassicae	Dye	152
315.	Pterin	Xanthopterin	• **Insects:** Gonepteryx rhamni	Dye	152

Table S7. Different classes of anthocyanins which are the predominant pigments in flowering plants, ferns, mosses and liverworts.

Compound Num.	Chemical Class	Compound Name	Natural Source	References

Compound Num.	Chemical Class	Compound Name	Natural Source	References
316.	Anthocyanidins	Pelargonidin (Pg)		[153]
317.		Cyanidin (Cy)		
318.		Peonidin (Pn)		
319.		7 Methyl peonidin		
320.		Delphinidin (Dp)		
321.		5 Methyl delphinidin		
322.		Petunidin (Pt)		
323.		5 Methyl petunidin	*Alstroemeria* spp.	
324.		Malvidin (Mv)		
325.		5 Methyl malvidin		
326.		7 Methyl malvidin		
327.		5 Methyl cyanidin		
328.		7 Methyl cyanidin		
329.		6 Hydroxy pelargonidin		
330.		6 Hydroxy cyanidin		[153]
331.		6 Hydroxy delphinidin		
332.	3-Deoxyanthocyanins	Apigeninidin (Ap)		
333.		7 Methyl apigeninidin		
334.		Luteolinidin (Lt)	*Eustoma grandiflorum*	
335.		5 Methyl luteolinidin		
336.		Tricetinidin (Tr)		
337.		Carajurone		
338.		Carajurin		
339.		5 Methyl 6 hydroxy luteolinidin		[153]
340.		5,4’ Dimethyl 6 hydroxy luteolinidin		
341.	Spagnorubins	Sphagnorubin A	*Hyacinthus orientalis*	
342.		Sphagnorubin B		
343.		Sphagnorubin C		
344.	Rosacyanins	Rosacyanin B		[154]
345.		Rosacyanin A1		
346.		Rosacyanin A2	*Rosa hybrida* cv.	
347.		Degalloyl rosacyanins A1		
348.		Ellago rosacyanin A1		
349.	Auronidins	Riccionidin A	*Ricciocarpos natans*	[155]
350.		Auronidin-2’-neohesperidoside		
351.	Pyranoanthocyanidins	5 Carboxypyranopelargonidin (CPg)	*Hyacinthus orientalis*	[153]
352.		5 Carboxypyranocyanidin (CCy)		
353.	Proanthocyanidins	catechin (4α~8) pelargonidin 3 glucoside	*Fragaria ananassa*	[156]

Compound Num.	Chemical Class	Compound Name	Natural Source	References
354.		afzelechin(4α~8) pelargonidin 3 glucoside		
355.	Wine pigment	Mv3gl-8-propyl-8-catchin		157
356.		4-vinylcatechin -7-malvidin-3-glucoside		
357.		Pinotin A	wine pigment	
358.		Portisin A		
359.		Pyranoanthocyanin dimers		
360.	Acylated anthocyanidins	Ternatin A1	*Clitoria ternatea*	158

154 **Table S8.** Identified anthocyanins in selected fruit, vegetables, and grains.

Number	Identified Compounds Names	Natural Source	References
1.	Cy, Dp, 6 hydroxyCy, 6 hydroxyDp 3(6rut), Cy 3(malonylglu), Dp 3(malonylglu)	*Alstroemeria spp.*	[153]
2.	Cy, Dp, Pn 3(6rut), Pn 3glu, Pn 3,5diglu	*Antirrhinum spp.*	[153]
3.	Cy 3(6malonyl2glucuronosylglu)	*Bellis perennis*	[153]
4.	Bisdeacylplatyconin, Violdelphin, Campanin, Monodeacylcampanin, Rubrocampanin	*Campanula spp.*	[153]
5.	Mv , Pt 37di(6malonylglu), Dp 3glu7(6malonylglu), Dp , Pt 3,7diglu, Pt 3(6rut), Pt 3,5diglu	*Crocus spp.*	[153]
6.	Cy , Pg 3(6malylglu), Pg 3,5(6,6cyclic malyldiglu)	*Dianthus caryophyllus*	[153]
7.	Cy 3(2sop), Cy 3glu, Cy 3,5diglu, Pg 3(2sop), Pg 3glu, Pg 3,5diglu	*Erythrina spp.*	[153]
8.	Dp, Cy, Pg 3(6rhamnosylgal)5(6acylglu)	*Eustoma grandiflorum*	[153]
9.	Gentiodelphins, Gentiocyanins, Albireodelphins, Cy 3glu	*Gentiana spp.*	[153]
10.	Mv 3glu5(6acetylglu), Dp 3glu, Cy 3,5diglu	*Geranium spp.*	[153]
11.	Cy 3(2sop), Cy 3(2sam), Dp 3(2sam), Cy, Mv, Dp 3(6malonylglu), Pt 3(6malonylglu)	*Hibiscus spp.*	[153]
12.	Acylated Cy, Pg, Dp 3,5diglu, Pt 3,5diglu	*Hyacinthus orientalis*	[153]
13.	Dp, Mv, Pt, Pn 3(coumaryl6rut)5glu, Cy 3(coumaryl6rut)5glu	*Iris ensata*	[153]
14.	Acylated Cy 3(6rut)5,3’diglu, Dp 3(6rut)5,3’diglu, Dp 3(6rut)5,3’,5’triglu	*Lobelia erinus*	[153]
15.	Mv 3(6malonylglu)5glu, Mv 3,5diglu	*Malva sylvestris*	[153]
16.	Cy 3(malonyl2sam)7glu	*Meconopsis spp.*	[153]
17.	Cy, Pn, Mv, Dp , Pt 3glu, Cy 3,5diglu, Mv 3,5diglu	*Metrosideros spp.*	[153]
18.	Dp 3(2galloyl6acetylgal), Cy 3(2galloyl6acetylgal), Dp 3(6acetylgal), Dp 3’(2galloyl6acetylgal)	*Nymphaea spp.*	[153]
19.	Pn, Cy, Pg 3glu, Pg 3,5diglu	*Paeonia spp.*	[153]
20.	Pg, Cy, Pn, Dp, Pt , Mv 3glu5(6acetylglu), Mv 3,5diglu	*Pelargonium spp.*	[153]
21.	Acylated Mv, Pt 3(6rut)5glu, Pn 3(6rut)5glu, Mv, Pt, Cy , Pn 3glu, Pn 3,5diglu, Pn 3(6rut)5glu, Pn 3(6rut)	*Petunia spp.*	[153]
22.	Cy 3glu, Pn 3glu	*Picea abies*	[153]
23.	Cy, Pg , Pn 3,5diglu, Pn 3glu	*Rosa spp.*	[153]
24.	Pt , Mv 3(6rut)5glu	*Saintpaulia ionantha*	[153]
25.	Pg, Cy , Dp 3(6rut), Pg , Cy 3(6(2acetylrhamnosyl)glu)	*Tulipa spp.*	[153]
26.	Acylated Pg, Cy , Dp 3,5diglu, Dp 3glu	*Verbena spp.*	[153]
27.	Cy 3gal, Cy 3ara, Cy 3glu	*Aronia melanocarpa*	[153]
28.	Cy 3glu	*Citrus paradisis*	[153]
29.	Cy , Dp 3glu, Cy 3(4acetylglu)	*Citrus sinensis*	[153]
30.	Dp, Cy , Pg 3(6rut)	*Cyphomandra betacea*	[153]
31.	Cy 3(6rut), Cy 3glu	*Euterpe sp.*	[153]
32.	Pg , Cy 3glu, Pg3(6rut)	*Fragaria ananassa*	[153]
33.	Cy 3(6rut), 3glu, Mv 3(acetylglu)	*Litchi chinensis*	[153]
34.	Cy 3gal, Cy 3ara, Cy 3glu	*Malus pumila*	[153]
35.	Pn 3gal, 7 MethylCy 3gal	*Mangifera indica*	[153]
36.	Cy & Dp 3glu, Cy 3(6malonylglu)	*Passiflora edulis*	[153]

Number	Identified Compounds Names	Natural Source	References
37.	Cy 3(6rut), Cy 3glu	*Prunus avium*	[153]
38.	Cy 3(2glu6rut), Cy 3(6rut), Cy 3glu, Cy 3(2sop)	*Prunus cerasus*	[153]
39.	Cy, Pn 3glu, Pn 3(6rut)	*Prunus domestica*	[153]
40.	Cy 3glu	*Prunus persica var. nectarina*	[153]
41.	Cy 3glu	*Prunus persica*	[153]
42.	Cy 3gal, Cy 3 glu, Cy 3 ara, Cy 3 rut, Pg 3 rut, Pg 3 gal, Pn 3 glu, Cy 3 succinylglu, Cy malylrhamnoside	*Pyrus communis cv.*	[153, 159]
43.	Cy , Dp 3glu, Dp 3(6rut)	*Ribes nigrum*	[153]
44.	Cy 3(2xylosyl6rut), Cy 3(2sam), Cy 3(6rut), Cy 3(2glu6rut), Cy 3glu	*Ribes rubrum*	[153]
45.	Cy 3xyloside, Cy 3(6rut), Cy 3(6coumarylglu), Cy 3(6caffeoylglu), Pn 3glu	*Ribes uva crispa*	[153]
46.	Cy 3(2sop), Cy 3glu, Cy 3(6rut), Cy 3(2glu6rut)	*Rubus idaeus*	[153]
47.	Cy 3glu, Cy 3(6rut)	*Rubus spp.*	[153]
48.	Cy 3(2sam), Cy 3glu, Cy 3(2sam)5glu	*Sambucus nigra*	[153]
49.	Dp, Cy, Pt, Mv, Pn 3glu, Pn 3gal, Pn 3ara	*Vaccinium corumbosum*	[153]
50.	Cy , Pn 3gal, Pn 3ara, Pn 3glu	*Vaccinium macrocarpon*	[153]
51.	Dp, Cy, Pt, Mv, Pn 3glu, Pn 3gal, Pn 3ara	*Vaccinium myrtillus*	[153]
52.	Cy 3gal, Cy 3ara	*Vaccinium vites idaea*	[153]
53.	Mv, Pt, Pn , Cy 3glu, Cy 3,5diglu, Cy 3(6coumarylglu), Cy 3(acetylglu), Cy 3(6coumarylglu)5glu	*Vitis spp.*	[153]
54.	Cy 3 glu, Cy 3 rut, Dp 3 gal, Dp 3 glu, Dp 3 rut, Pn 3 glu	*Euterpe oleracea Martius*	[160]
55.	Cy 3,5 dihex, Cy 3 gal, Cy 3 glu, Cy 3 lat, Cy 3 rut, Dp 3 glu, Mv 3,5 dihex, Pg 3,5 diglu, Pg 3 pentoxilhex, Pg 3 rut, Pg hex, Pn 3 rut	*Berberis lycium Royle*	[161]
56.	Cy 3 ara, Cy 3 gal, Cy 3 glu, Dp 3 ara, Dp 3 glu, Dp 3 gal, Mv 3 ara, Mv 3 gal, Mv 3 glu, Pn 3 ara, Pn 3 gal, Pn 3 glu, Pt 3 ara, Pt 3 gal, Pt 3 glu	*Vaccinium myrtillus L.*	[162]
57.	Cy 3 glu, Cy 3 rutl Dp, Mv, Pg, Pg 3 glu, Pn	*Rubus fruticosus L.*	[163]
58.	Cy 3 glu, Cy 3 rut, Dp 3 glu, Dp 3 rut	*Ribes nigrum L.*	[164]
59.	Cy 3 ara, Cy 3 gal, Cy 3 glu, Dp 3 ara, Dp 3 gal, Dp 3 glu, Mv 3 ara, Mv 3 gal, Mv 3 glu, Pn 3 gal, Pn 3 glu, Pt 3 ara, Pt 3 gal, Pt 3 glu	*V. corymbosum L.*	[162]
60.	Cy 3 ara, Cy 3 gal, Pn 3 ara, Pn 3 gal	*V. oxycoccos L.*	[162]
61.	Cy 3 glu, Cy 3 gal, Cy 3 ara, Cy 3 sop, Cy 3 rut, Dp 3 glu, Dp 3 gal, Mv 3,5 diglu	*Canarium odonthophyllum Miq.*	[165]
62.	Cy 3 glu, Cy 3 sam, Cy diglu, Cy sam glu, Dp 3 glu, Dp 3,5 diglu, Dp 3 sam, Dp 3 sam 5 glu	*Aristotelia chilensis (Mol.) Stuntz*	[166]
63.	Cy 3 (caffeoyl) diglu, Cy 3 (cis p coumaroyl) diglu, Cy 3 (trans p coumaroyl) diglu, Cy 3 diglu, Dp 3 (p coumaroyl) hexose, Dp 3 (caffeoyl) diglu, Pg 3 (p coumaroyl) diglu, Pg 3 diglu	*Nitraria tangutorun Bobr.*	[167]
64.	Cy 3 glu, Cy 3 rut, Dp 3 glu, Dp 3 rut, Mv 3 glu, Pg 3 glu, Pn 3 glu	*Mahonia aquifolium (Pursh) Nutt*	[168]
65.	Cy 3,5 diglu, Cy 3 glu, Cy pen, Dp 3,5 di glu, Dp 3 glu, Pg 3,5 di glu, Pg 3 glu	*Punica granatum cv.*	[169]

Number	Identified Compounds Names	Natural Source	References
66.	Cy 3 glu, Cy 3 rut, Cy 3 sop	*Mollar de Elche* *Rubus idaeus L.*	170
67.	Cy 3 glu, Dp 3 glu, Mv 3 acetylglu, Mv 3 glu, Mv 3 p coumarylglu, Pn 3 acetylglu, Pn 3 glu, Pn 3 p coumarylglu, Pt 3 glu	*Vitis vinifera L.*	171
68.	Cy 3 xylosyl glu gal, Cy 3 xylosyl gal, Cy 3 xylosyl glu gal coumaric acid, Cy 3 xylosyl glu gal ferulic acid, Cy 3 xylosyl glu galsinapic acid	*Daucus carota ssp. sativus var. atrorubens Alef.*	172
69.	Cy 3 gal, Cy 3 glu, Dp 3 glu, Pn 3 glu	*Glycine max (L.)*	173
70.	Cy 3 (6″ malonylglu), Cy 3,5 diglu, Cy 3 dimalonylglu, Cy 3 glu, Cy 3 malonylglu, Cy 3 malonylglu, Cy 3 succinylglu, Pg 3 (6″ maolonylglu), Pg 3 dimalonylglu, Pg 3 glu, Pn 3 (6″ malonylglu), Pn 3 dimalonylglu, Pn 3 glu	*Zea mays L.*	174
71.	Cy 3 (caffeoyl sop) 5 glu, Cy 3 (caffeoyl feruloyl sop) 5 glu, Cy 3 (caffeoyl p hydroxybenzoylsop) 5 glu, Cy 3 (dicaffeoylsop) 5 glu, Cy 3 (feruloyl sop) 5 glu, Cy 3 (p hydroxybenzoylsop) 5 glu, Cy 3 sop 5 glu, Pg 3 (caffeoyl feruloyl sop) 5 glu, Pn 3 (caffeoyl sop) 5 glu, Pn 3 (caffeoyl feruloyl sop) 5 glu, Pn 3 (caffeoyl p coumaroyl sop) 5 glu, Pn 3 (caffeoyl p hydroxybenzoylsop) 5 glu, Pn 3 (dicaffeoylsop) 5 glu, Pn 3 (feruloyl sop) 5 glu, Pn 3 (feruloyl p coumaroyl sop) 5 glu, Pn 3 (feruloyl p hydroxybenzoylsop) 5 glu, Pn 3 (p hydroxybenzoylsop) 5 glu, Pn 3 sop 5 glu	*Ipomoea batatas L*	175
72.	Cy 3 glu, Cy 3 rut, Dp 3 glu, Dp 3 rut, Cy 3 diglu 5 glu, Cy 3 (caffeoyl)(p coumaroyl) diglu 5 glu, Cy 3 (sinapoyl) diglu 5 glu, Cy 3 (caffeoyl sinapoyl) diglu 5 glu, Cy 3 (p coumaroyl)(sinapoyl) triglu 5 glu, Cy 3 (feruloyl)(sinapoyl) triglu 5 glu, Cy 3 (p coumaroyl) diglu 5 glu, Cy 3 (sinapoyl) diglu 5 glu, Cy 3 (p coumaroyl)(sinapoyl) diglu 5 glu, Cy 3 (feruloyl)(sinapoyl) diglu 5 glu, Cy 3 (sinapoyl)(sinapoyl) diglu 5 glu, Cy 3 (sinapoyl) diglu 5 (sinapoyl) glu	*Brassica oleracea L. var. capitata L.*	176
73.	Cy, Cy 3 glu, Pn 3 glu	*Oryza sativa L. cv. Heugjinju*	177
74.	Dp 3 (caffeoyl) rut 5 glu, Dp 3 (feruloyl) rut 5 glu, Dp 3 (trans coumaroyl) rut 5 glu, Mv 3 (feruloyl) rut 5 glu, Mv 3 (p coumaroyl) rut 5 glu, Pt 3 (feruloyl) rut 5 glu, Pt 3 (trans coumaroyl) rut 5 glu	*Solanum lycopersicum L. cv. Del/Ros1*	178
75.	Dp 3 (6’’ p coumaroyl) rut, Cy 3 (6’’ p coumaroyl) rut, Dp 3 (p coumaroyl) glu, Cy 3 (p coumaroyl glu) , Dp 3 pyranoside.	*Clitoria ternatea L.*	179
76.	Cy 3 (6’’ cinnamoyl)glu, Afzelechin(4α 8)Pg3,5 diglu, Catechin(4α 8)Pg 3 glu, Afzelechin(4α 8)Pg 3 sop, Afzelechin(4α 8)Pg 3 glu, Pg 3 glu	*Rubus chingii Hu*	180
77.	Catechin-(4α-8)-cy-3,5-diglu	*Zea mays L.*	181

ara: arabinoside, Cy: cyanidin, Dp: delphinidin, Mv: malvidin, Pg: pelargonidin, pen: pentoside, Pn: peonidin, Pt: petunidin, gal: galatoside, glu: glucoside, hex: hexoside, lat: lathyroside, rut: rutinoside, sam: sambubioside, sop: sophoroside.

Table S9. Selected identified tannins isolated from plants

Compound Number	Chemical class	Compounds Names	Natural Source	Biological activity	References
361.	Ellagitannins	Gemin D	Tamarix nilotica		182
362.		Hippomanin A			182
363.		Hirtellin A			182
364.		Hirtellin B			182
365.		Hirtellin C			183
366.		Hirtellin D			183
367.		Isohirtellin C			183
368.		Remurin A			184
369.		Remurin B			184
370.		Tamarixinin A			185
371.		Tamarixinin B			185
372.		Tellimagrandin I			183
373.		Tellimagrandin II			183
374.		Agrimoniin	*Agrimonia pilosa*	Active *in vitro* against *Helicobacter pylori*-MIC (25 µg/mL)	186
375.		Castalagin	*Quercus suber*	Active *in vivo* against ethanol-induced peptic ulcers/Intragastric/50.0 mg/kg	187, 188
376.		Casuarictin	*Casuarina stricta*	Active *in vitro* against *Helicobacter pylori*-MIC (12.5 µg/mL)	186, 189
377.		Casuarinin	*Casuarina stricta*	Active *in vitro* against *Helicobacter pylori*-MIC (12.5 µg/mL)	186, 190
378.		Corilagin	*Geranium thunbergii*	Active *in vitro* against *Helicobacter pylori*-MIC (6.25 µg/mL)	186, 191
379.		Elagic acid	*Elaeagnus umbellata*	Active *in vivo* against stress-induced peptic ulcers(water immersion)/intraperitoneal/5, 10 and 25 mg/kg	192, 193
380.	Complex tannins	Epicatechin gallate	*Vitis vinifera*	Minimal active *in vitro* against *Helicobacter pylori*-MIC (50 µg/mL)	194
381.		Epigallocatechin gallate	*Vitis vinifera*	Active *in vitro* against *Helicobacter pylori*-MIC (25 µg/mL)	194
382.	Ellagitannins	Geraniin	*Geranium thunbergii*	Active *in vitro* against *Helicobacter pylori*-MIC (12.5 µg/mL)	186
383.		Heterophylliin G	*Corylus heterophylla*	Active *in vitro* against *Helicobacter pylori*-MIC (12.5 µg/mL)	195
384.		Nobotanin B	*Melastoma candidum*	Active *in vitro* against *Helicobacter pylori*-MIC (12.5 µg/mL)	186, 189

Compound Number	Chemical class	Compounds Names	Natural Source	Biological activity	References
385.		Oenothein A	*Oenothera stricta*	Active *in vitro* against *Helicobacter pylori*-MIC (12.5 µg/mL)	186
386.		Oenothein B	*Oenothera stricta*	Active *in vitro* against *Helicobacter pylori*-MIC (12.5 µg/mL)	196
387.		Pedunculagin	*Quercus suber*	Active *in vivo* against ethanol-induced peptic ulcers/Intragastric/50.0 mg/kg	187, 197
388.	Complex tannins	Procyanidin B1	*Vitis vinifera*		186, 198
389.		Procyanidin B3	*Vitis vinifera*	Minimal active *in vitro* against *Helicobacter pylori*-MIC (50 µg/mL)	186, 198
390.	Ellagitannins	Rugosin D	*Rosa rugosa*	Active *in vitro* against *Helicobacter pylori*-MIC (25 µg/mL)	186
391.		Strictinin	*Elaeagnus umbellata*	Active *in vitro* against *Helicobacter pylori*-MIC (6.25 µg/mL)	186, 199
392.	Gallotannins	Tannic acid	*Rosa rugosa*	Active *in vivo* against Shay ulcer/oral/50.0 mg/kg	186, 200, 201

Table S10. Selected identified quinonoids, and pyranonaphthoquinones compounds.

Compound Number	Chemical Class	Compounds Name	Source	Biological Activity	References
393.	Anthraquinones	Catenarin	• **Fungus:** *Pyrenophora triticirepentis* (Died.) Drechsler. *Drechslera spp., Bipolaris sorokiniana* (Sacc.) Shoemaker	Antibacterial against Gram-positive bacteria Aureobacterium liquefaciens, Arthrobacter globiformis, Bacillus brevis, B. circulans, B. subtilis and Curtobacterium plantarum.	202, 203
394.	Quinones	Fumigatin	• **Fungus***:* *Penicittium spinulosum* Thorn *and Aspergillus fumigatus Fresenius.*	Antibacterial potential	204
395.	Anthraquinones	Helminthosporin	• **Fungus:** *Rumex abyssinicus* Jacq, • **Bacteria:** *Drechslera holmii* (Luttr.) Subram. & B.L. Jain *and Drechslera ravenelii* (M.A. Curtis) Subramanian & Jain	acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) inhibition with IC_{50} = 2.7 and 11.4 µg/mL against respectively	205
396.	Naphthoquinone C-glycosides	Anhydroexfoliamycin	• **Bacteria:** *Streptomyces exfoliatus*	Neuroprotective activity: ameliorates hallmarks of Alzheimer's disease *in vitro* and *in vivo* models	206
397.	Anthraquinones	Himalomycin A	• **Bacteria:** *Streptomyces* sp. B6921	Antibacterial activity against *Escherichia coli*, *Staphylococcus aureus*, *Streptomyces viridochromogenes*, *Bacillus subtilis*	207
398.		Himalomycin B			

Compound Number	Chemical Class	Compounds Name	Source	Biological Activity	References
399.		Fridamycin D			
400.		Islandicin	• **Fungus:** *Talaromyces islandicus* WF-38-12	Mutagenic activity in bacteria	208
401.	Benzoisochromens	Purpurogenone	*Penicillium purpurogenum* Stoll (fungi)		209
402.	Naphthopyrones	Rubrofusarin	• **Fungus:** *Fusarium graminearum* Schwabe., *Cassia obtusifolia* L seeds.	Inhibit tyrosine phosphatase 1B (PTP1B) and human monoamine oxidase A (hMAO A) with IC_{50} = 16.95±0.49, and 5.90±0.99 μM, respectively	210
403.	Perylenequinones	Shiraiachromes A	Parasitic fungus	Anti-angiogenic effects	211
404.	Perylenequinones	Hypocrellin A	*Shiraia bambusicola*		212
405.		Hypocrellin B	P. Henn		
406.		Hypocrellin D		Cytotoxic activities against tumor cell lines, Bel-7721, A-549 and Anip-973, with IC_{50} = 1.8, 8.8, 38.4 mg/mL, respectively.	
407.	Perylenequinones	Calphostin A	Fungus	Cytotoxic activity against HeLa S3 (human cervix carcinoma) and MCF-7 cells with IC_{50} = 0.38, 0.28 μM & IC_{50} = 2.56, 1.61 μM & IC_{50} = 0.23, 0.18 μM & IC_{50} = 8.45, 2.69 μM & IC_{50} = 0.24, 0.16	213
408.		Calphostin B	*Cladosporium*		
409.		Calphostin C	*cladosporioides*		
410.		Calphostin D	FERMBP-1285		
411.		Calphostin I			
412.	Naphthoquinones	Xylindein	fung*i Chlorociboria aeruginosa* (Oeder) Seaver strain UAMH 11657		214
413.	Pyranonaphthoquinones	Astropaquinone A	fungus *Astrosphaeriella papuana* YMF1.01181	Antagonistic activity against nine fungi and four bacterial strains	215
414.		Astropaquinone B			
415.		Astropaquinone C			
416.	Naphthoquinones	Dihydrolindbladione	*Myxomycete Lindbladia tubulina* Fr.	Cytotoxic active against P388/S (mouse leukemia), P388/VCR (+) (vincristine-resistant P388 cell), and P388/VCR (+) (vincristine-sensitive P388 cell) lines with 11<IC_{50} <14 μg/mL.	216
417.	Naphthoquinones	Fusarubinoic acid	*Nectria haematococca*		217

Compound Number	Chemical Class	Compounds Name	Source	Biological Activity	References
			(Berk. and Br.) Wr		
418.	Naphthalenediones	Spinochrome A	Sea urchins *Echinothrix genus* Sea urchins, *Echinometra spp.*, *Psammechinus spp*, *Mesocentrotus spp.*, *Echinothrix spp.*, *Strongylocentrotus spp.*	Antibacterial activity against *E. coli*, *B. subtilis*, *Cobetia marina*, *Shewanella oneidensis* Cytotoxic activity against HeLa cells with EC_{50} = 341.7 µM. Antioxidant activity in DPPH assay EC_{50} = 22.17 µM. Relatively strong activity against *Shewanella oneidensis* (EC_{50} <250 µM)	218
419.		Spinochrome B		Antibacterial activity against *E. coli*, *B. subtilis*, *Vibrio aestuarianus*, *Cobetia marina*, *Shewanella oneidensis* cytotoxic activity against HeLa cells with EC_{50} >500 µM. Antioxidant activity in DPPH assay EC_{50} = 29.38 µM. High antibacterial activity against Escherichia coli (EC_{50}<30 µM	218
420.	Naphthoquinones	Fumaquinone	*Streptomyces fumanus* (LL F42248).	Antimicrobial activity against selected Gram-positive bacteria with MIC of about 64 µg/mL	219
421.	Xanthones	Bikaverin	*Gibberella fujikuroi* (Sawada) Wollenw., and *Fusarium oxysporum* Schlecht. emend. Snyder & Hansen	Effective against *Leishmania brasiliensis*. Neuroprotective effects in H_2O_2-induced oxidative stress mediated neuronal damage in SH-SY5Y cell line with 100–500 µg/mL	220
422.	Xanthones	Griseoxanthone C	*Ulocladium, Penicillium* sp. NH-7-1, and *Fusarium* spp	Antimicrobial potential against *Bacillus megaterium*, *B. subtilis* (IC_{50} = 1.29±0.45 µM), and *Candida albicans* (IC_{50} = 149±2.75 µM). Antiviral activity on Hepatitis C Virus (HCV) NS3-NS4 A protease with IC_{50} = 19.88±1.35 µM	221
423.	Xanthones	Fallacinol	Marine Sponge-Associated Fungus *Talaromyces stipitatus* KUFA 0207		222
424.	Ansabenzoquinones	Rhizopogone	*Rhizopogon pumilionus* (Ade) Bataille mushroom		223
425.	Benzoisochromanequinones	Actinorhodin	*Streptomyces coelicolor* A3	Antibacterial potential against *B. subtilis* 168, *Micrococcus luteus*, *Listeria monocytogenes* EGD,	224

Compound Number	Chemical Class	Compounds Name	Source	Biological Activity	References
				Staphylococcus aureus ATCC 29213 with MIC=6.4 μM. Also, against *S. aureus* ATCC BAA-44, *S. epidermidis* ATCC 14990 with MIC = 12.8 μM.	
426.	Quinone	Albatrellin	*Albatrellus flettii* Morse ex Pouzar Mushroom		225
427.		Grifolinone B			
428.	Naphtho-γ-pyrones	Rubasperone D	Endophytic Fungus *Aspergillus tubingensis* (GX1-5E)	Mild cytotoxicity against MCF-7 (breast cancer), MDA-MB-435 (Melanoma), Hep3B (human hepatoma), Huh7 (human liver cancer), SNB19 (human astrocytoma), and U87MG (human primary glioblastoma) cells with 80< IC_{50} <110 μM	226
429.	Anthraquinones	Alizarin	Roots of *Rubia tinctorum* L.	Antioxidant activity in various assesses. Inhibition tyrosinase, *α*-amylase, and *α*-glycosidase. Inhibit cell proliferation of the osteosarcoma Saos-2, MG-63, and U-2 OS cells (IC_{50} = 27.5, 29.0, and 69.9 μg/mL, respectively) and breast carcinoma (IC_{50} = MDA-MB-231 cells, 62.1 μg/mL)	227
430.	Naphthoquinone	Alkanin	roots of *Alkanna tinctoria* (L.) Tausch	Antioxidant activity, antimicrobial effect against *Staphylococcus aureus* and *S. epidermidis*. wound healing potential, antitumor activity, and antithrombotic properties	228
431.	Anthraquinones	Carmine	Dried bodies of female cochineal insects *(Porphyrophora* spp.	IgE-mediated allergen	229
432.	Benzoquinones	Embelin	Aerial parts of *Datisca cannabina* L.	Showed following potential: antioxidant, antitumor, anti-inflammatory, analgesic, anthelmintic, antifertility and antimicrobial antidiabetic	230
433.	Anthraquinones	Emodin	Roots of *Polygonum spp., Rheum spp, and Reynoutria japonica* Houtt	Showed following potential: laxative, antibacterial and anti-inflammatory. Antiviral blocks the SARS coronavirus spike protein and angiotensin-converting enzyme 2 interaction.	231
434.	Tetrahydroxy anthraquinone	Erythrolaccin	Secretion of insect, *Kerria lacca Kerr*		232

Compound Number	Chemical Class	Compounds Name	Source	Biological Activity	References
435.	Xanthonoid glycoside	Euxanthic acid	Secretion to animal urine fed on leaves of *Mangifera indica* L		[233]
436.	Napthodianthrones	Hypericin	Leaves and petals *Hypericum* spp.	Showed a light-enhanced direct antiviral effect (virucidal effect) against murine cytomegalovirus (MCMV), Sindbis virus, and human immunodeficiency virus type 1 (HIV I). Showed antibacterial activity, combination with light irradiation could induce significant killing of S. aureus methicillin-sensitive and -resistant. Showed anti-inflammatory effect at concentrations of <0.4 µM with leukotriene B4 release inhibition	[234]
437.	Quinones	Juglone	Various parts of *Juglans nigra* Linnaeus	Cytotoxic effect by induction of oxidative stress, cell membrane damage, and clastogenic action against cultured melanoma tumor cells	[235]
438.	Tetrahydroxy anthraquinones	Kermesic acid	Insects, *Porphyrophora polonica* L., P. *hameli* BRANDT.		[236]
439.	Tetrahydroxy anthraquinones	Laccaic acid A	Insects, *Laccifer lacca* Kerr.	Showed synergistic efficacy with phenethyl isothiocyanate combination in colorectal cancer with inhibition of DNA methyltransferase-1 and Histone deacetylase-1. Showed anticancer potential *via* DNA methyltransferase 1 inhibition	[237]
440.	Naphthoquinones	Lapachol	Bark of Tabebuia *avellanedae* Lorentz ex Griseb. and other *Bignoniaceae* plants	Showed anticancer, antibacterial and antifungal activity	[238]
441.	Naphthoquinones	Lawsone	leaves of *Lawsonia inermis* L.	Protective effect on L-Arginine induced acute pancreatitis in rats with 100– 200 mg/kg. Wound and skin tissue regeneration potential	[239]
442.	Xanthonoids	Mangiferin	Fruit and aerial parts of *Mangifera indica* L.	Antitumor, antiviral, and immunomodulatory effects antidiabetic potential, antihyperlipidemic and antiatherogenic	[240]
443.	Anthraquinones	Morindone	*Morinda* spp.	Interact with DNA structure	[241]

Compound Number	Chemical Class	Compounds Name	Source	Biological Activity	References
444.	Naphthoquinones	Shikonin	Roots of *Alkanna tinctoria* (L.) Tausch, *Lithospermum erythrorhizon* Sieb. et Zucc	Anticancer potential with induced apoptosis Caspase-3 activity in T24 (human bladder cancer cell), induce apoptosis and decrease cell migration in the SKOV 3 (human ovarian cells) IC_{50} = 10.38 µmol, and 16 µM. Anti-inflammation activity with reduce lipopolysaccharides (LPS)-mediated TNF-α release in rat primary macrophage at 4 µM. Inhibit lipid peroxidation at concentrations range 45–100 µM	242
445.	Naphthoquinones	Echinochrome A	Sea urchins*, Echinus esculentus* Linnaeus	DPPH free-radical scavenger with EC_{50} = 3.6±0.2 µM., used for preventing reperfusion damage during myocardial infarction	243
446.	Anthraquinone - naphthoquinone	Newbouldiaquinone A	Roots of *Newbouldia laevis* (P. Beauv.) Seem. Ex Bureau.	Active against Gram-negative bacteria with the minimal inhibition concentration, MIC = 0.75–23.8 µM. Also showed antimalarial activity (Plasmodium falciparum)	244
447.	Dimeric naphthoquinones	Shikometabolin A	Roots of *Lithospermum erythrorhizon* Siebold & Zucc.	Cytotoxic against PC-3 (human prostate cancer) and ACHN (human renal adenocarcinoma), A459 (adenocarcinomic human alveolar basal epithelial),	245
448.		Shikometabolin B		SW620 (human colon carcinoma), K562 (human	
449.		Shikometabolin C		myelogenous leukemia), and Du145 (human prostate cancer) cells with IC_{50} = 5.21, 5.33, 5.46, 5.26, 6.48, and >10 µg/mL respectively & IC_{50} = 5.80, 6.74, >10, 8.09, 8.24, and >10 µg/mL respectively & IC_{50} >10 µg/mL	
450.	Anthraquinones	Diaporthemins B	Endophytic fungus: *Diaporthe melonis* Beraha & M.J. O'Brien		246
451.	Naphthoquinones	Haemoventosin	Lichen: *Ophioparma ventosa* (L.) Norman	Cytotoxic against B16 (murine melanoma) and HaCaT (human epidermal keratinocyte) cells with IC_{50} = 2.40±0.4 and 14.20±1.0 µM, respectively. Also showed antioxidant potential in nitroblue tetrazolium (NBT) assay with = 1.90±0.4 µM	247
452.	Naphthoquinones	Ruberythric acid	Roots of *Rubia cordifolia* L	ABTS*+ radical scavenging as total equivalent trolox equivalent (TEAC = 0.219±0.007 mM)	248

Compound Number	Chemical Class	Compounds Name	Source	Biological Activity	References
453.	Anthraquinones	Cochineal	• **Insects:** *Dactylopius coccus*		152, 249
454.		Laccaic acid B	• **Insects:** *Kerria lacca*		250
455.		Laccaic acid C	• **Insects:** *Kerria lacca*		
456.		Laccaic acid D	• **Insects:** *Kerria lacca*		
457.		Laccaic acid E	• **Insects:** *Kerria lacca*		
458.		Laccaic acid F	• **Insects:** *Kerria lacca*		
459.		Desoxyerythrolaccin	• **Insects:** *Kerria lacca*		251
460.	Pyranonaphthoquinones	Protoaphin-fb	• **Insects:** *Aphis fabae*		252
461.		Protoaphin-sl	• **Insects:** *Tuberolachnus salignus*		253
462.		Xanthoaphin	• **Insects:** *Gonepteryx rhamni*		254

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