Supplementary Table 1. Results of LC/MS analysis of non- nitrogenous compounds identified through positive and negative ionization mode of ethanol extract of "Magahi pan"

Non –nitrogenous compounds	Chemical formula	MW	RT	Positive /negative ionization mode ($[M+H]^+$/$[M+H]^-$)	MS/MS
Styrene	C_8H_8	104.6	2.31	$[M+H]^+$	107.07, 106.07, 105.07
1,1-(Tetrahydro-6a-hydroxy -2-3a,5trimethylfuro(2,3-d)1,3dioxole-2,5diyl)bisethanone	$C_{12}H_{18}O_6$	258.11	2.389	$[M+H]^+$	278.13,277.14, 276.14
Hydroxycoumarin	$C_9H_6O_3$	162.03	6.007	$[M+H]^+$	164.04,163.04
Sedanonic acid	$C_{12}H_{18}O_3$	210.12	6.582	$[M+H]^+$	212.13,211.13
Benzyl beta Primeveroside	$C_{18}H_{26}O_{10}$	402.15	6.71	$[M+H]^+$	422.19,421.19,420.18
Eremopetasinorone –A	$C_{13}H_{18}O_2$	206.13	7.37	$[M+H]^+$	208.14,207.13
2,6 Dimethoxy-4-propylphenol	$C_{11}H_{16}O_3$	196.10	10.19	$[M+H]^+$	199.11,198.12,197.11
Chenodeoxycholic acid sulphate	$C_{24}H_{40}O_7S$	472.25	7.65	$[M+H]^+$	492.28,491.28,490.28
3' Glucosyl-2,4,6-trihydroxyacetophenone	$C_{14}H_{18}O_9$	330.09	7.65	$[M+H]^+$	333.11,332.10,331.10
3-Hydroxymandelic acid	$C_8H_8O_4$	168.04	8.62	$[M+H]^+$	170.05,169.04
Eremopetasinorol	$C_{13}H_{20}O_2$	208.14	10.14	$[M+H]^+$	210.15,209.15
2,6 Dimethoxy-4-propylphenol	$C_{11}H_{16}O_3$	196.10	10.19	$[M+H]^+$	199.12,198.12,197.11
p-Mentha-1,3,,5,8-tetreene	$C_{10}H_{12}$	132.09	10.25	$[M+H]^+$	134.10,133.10
2,3,6 –Trimethyl phenol	$C_9H_{12}O$	136.08	10.26	$[M+H]^+$	135.45,134.45
5,6,7,3,4 Pentahydroxyisoflavone	$C_{15}H_{10}O_7$	302.04	10.08	$[M+H]^+$	301.09,300.9
Monotropein	$C_{16}H_{22}O_{11}$	390.11	11.05	$[M+H]^+$	410.15,409.15,409.14
Corchorifatty acid	$C_{18}H_{32}O_5$	328.22	11.34	$[M+H]^+$	348.26,347.26,346.25
7,8,3,4 –Tetrahydroxyisoflavone	$C_{15}H_{10}O_6$	286.04	11.52	$[M+H]^+$	289.06,288.05, 287.05
2,2,7,7- Tetramethyl -1,6-dioxaspiro[4,4] nnona-3,8diene	$C_{11}H16O_2$	180.11	11.81	$[M+H]^+$	182.12, 181.12
10-Hydroxy-2,8 -decadiene-4,6diynoic acid	$C_{10}H_8O_3$	176.04	13.25	$[M+H]^+$	178.05,177.05
Monoisobutyl phthalic acid	$C_{12}H_{14}O_4$	222.08	13.25	$[M+H]^+$	224.09,223.09
Sucrose -octaacetate	$C_{28}H_{38}O_{19}$	678.200	13.36	$[M+H]^+$	698.24,697.23,696.23
Cyclotetradecane	$C_{14}H_{28}$	196.21	14.10	$[M+H]^+$	216.25, 215.25, 214.25
2,2,7,7-Tetramethyl -1,6doxaspiro[4,4]nona-3,8diene	$C_{11}H_{16}O_2$	180.11	14.36	$[M+H]^+$	182.12, 181.12
Diglycolic acid	$C_4H_6O_5$	134.02	13.17	$[M+H]^+$	134.01,133.01
Dihydrocaffeic acid 3-O-glucoride	$C_{15}H_{18}O_{10}$	358.09	8.047	$[M+H]^+$	358.09,
4,7-Dihydroxy-2H-1 benzopyran-2-one	$C_9H_6O_4$	178.02	8.25	$[M+H]^+$	178.02,177.01
Cis –p coumaric acid	$C_9H_8O_3$	164.04	9.391	$[M+H]^+$	165.04l,164.04, 163.02
2-Methoxy-1,4-benzoquinone	$C_7H_6O_3$	164.04	9.89	$[M+H]^+$	139.03,138.03,137.02
3-Methoxy-4,5 methylenedioxybenzoic acid	$C_9H_8O_5$	196.03	10.14	$[M+H]^+$	197.03,196.03,195.03
Luteolin- 6 C glucoside 8 C arabinoside	$C_{27}H_{30}O_{16}$	610.15	10.36	$[M+H]^+$	645.12,610.12
4-Methylphenyl acetic acid	$C_9H_{10}O_2$	150.06	12.33	$[M+H]^+$	150.0,149.0
Myricanene B 5[arabinosyl] (1,6) glucoside	$C_{32}H_{42}O_{13}$	634.26	10.53	$[M+H]^+$	695.28,694.27,693.24
Coniferyl Alcohol	$C_{10}H_{12}O_3$	180.07	10.99	$[M+H]^+$	180.07,179.07
Methyl N-9(methylbutyl)glycine	$C_9H_{16}O_4$	188.10	11.20	$[M+H]^+$	188.10,187.09
Rutin	$C_{27}H_{30}O_{16}$	610.10	12.26	$[M-H]^-$	610.0
5,6,7,3',4', Pentahydroxyisoflavone	$C_{15}H_{10}O_7$	302.04	12.577	$[M-H]^-$	302.10,309.10

MW: molecular weight; RT: retention time; [M+H]+: positive ionization mode; [M+H]: negative ionization mode; MS/MS- A: tandem mass spectrometry

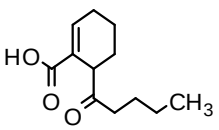
Supplementary Table 2. Results of LC/MS analysis of nitrogenous compounds identified through positive and negative ionization mode of ethanolic extract of "Magahi Pan"

Name of nitrogenous compounds	Chemical formula	MW	RT	Positive /negative ionization mode ($[M+H]^+$/$[M+H]^-$)	MS/MS
Choline chloride	$C_5H_{13}NO$	103.09	1.134	$[M+H]^+$	106.11,105.11 104.10
Prothoate	$C_9H_{20}NO_3PS_2$	285.06	1.144	$[M+H]^+$	288.07,287.07,286.06
R-95913	$C_{18}H_{18}FNO_2S$	331.10	1.195	$[M+H]^+$	334.11,333.11,332.11
Aminocaproic acid	$C_6H_{13}NO_2$	131.09	1.207	$[M+H]^+$	133.10,132.10
N-(10Deoxy-1fructosyl) isoleucine	$C_{12}H_{23}NO_7$	293.14	1.213	$[M+H]^+$	296.16,295.15,294.15
1-Nitroheptane	$C_7H_{15}NO_2$	145.11	1.568	$[M+H]^+$	147.12,146.11
3-Pyridylacetic acid	$C_7H_7NO_2$	137.04	1.944	$[M+H]^+$	139.05,138.05
1Aminocyclohexanecar boxylic acid	$C_7H_{13}NO_2$	143.09	1.952	$[M+H]^+$	1167.08,166.08,145.10,144.
2-0-Acetylpseudolycorine	$C_{18}H_{21}NO_5$	331.14	2.114	$[M+H]^+$	334.15,333.15,332.15
Picollinic acid	$C_6H_5NO_2$	123.03	2.119	$[M+H]^+$	125.04,124.03
3-(Dimethylamino)propyl benzoate	$C_{12}H_{17}NO_2$	207.12	2.196	$[M+H]^+$	210.14,209.13,208.13
Aminocaproic acid	$C_6H_{13}NO_2$	131.09	2.283	$[M+H]^+$	131.09
2,5-Dihydro2,4,5-trimethyloxozole	$C_6H_{11}NO$	113.08	2.998	$[M+H]^+$	115.09,114.09
N-Benzoyl-4-methoxyanthranilate	$C_{15}H_{13}NO_4$	271.08	3.501	$[M+H]^+$	274.10,273.09,272.09
Carbendazin	$C_9H_9N_3O_2$	191.07		$[M+H]^+$	194.08,193.08,192.07
Metominostrobin	$C_{16}H_{16}N_2O_3$	284.11	5.207	$[M+H]^+$	287.12,286.12,285.12
6-Methylquinoline	$C_{10}H_9N$	143.07	5.762	$[M+H]^+$	142.08,
Miraxanthin –III	$C_{17}H_{18}N_2O_5$	330.12	6.025	$[M+H]^+$	33.13,332.13,331.12
Istamycin	$C_{19}H_{37}N_5O_6$	431.27	7.288	$[M+H]^+$	434.28,433.28,432.22
Netilmicin	$C_{21}H_{41}N_5O_7$	475.27	7.558	$[M+H]^+$	478.30,477.31,476.30
2-(Acetylamino)-1,5-anhydro -2-deoxy-3—b-D galactopyranosyl -D-arabino-Hex-1-enitol	$C_{14}H_{23}NO_{10}$	365.13	8.628	$[M+H]^+$	368.14,367.14,366.13
Benzotropine	$C_{21}H_{25}NO$	307.19	10.63	$[M+H]^+$	306.19
Tymazoline	$C_{14}H_{20}N_2O$	232.15	10.64	$[M+H]^+$	235.16,234.16,233.16
2-(Acetylamino)-1,5anhydro -2-deoxy-3-o-b-D galactopyranosyl -Darabino-hex-1-enitol	$C_{14}H_{23}NO_{11}$	365.13	11.14	$[M+H]^+$	368.14,367.14,366.13
Ticarcillin	$C_{15}H_{16}N_2O_6S_2$	384.04	13.65	$[M+H]^+$	431.03,430.04, 429.04

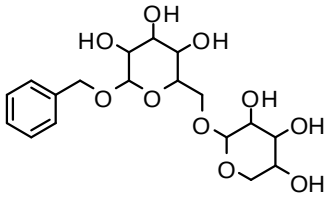
MW: molecular weight; RT: retention time; [M+H]+: positive ionization mode; [M+H]-: negative ionization mode; MS/MS: a tandem mass spectrometry

Supplementary Table 3. Amino acids present at binding site and type of interaction between receptor and ligand

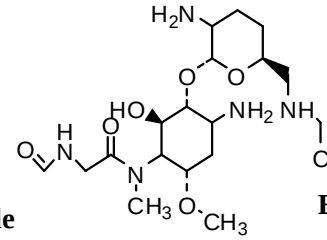
Name of Ligands	Type of Interaction and Physicochemical properties of ligands	Details of amino acid present at the binding site of H^+/K^+-ATPase enzyme
R-95913	Hydrogen bond acceptor=4	AGLN176;APRO175;AGLN177
	Hydrogen bond donor=1	AGLN188;ATHR179;AMET202
	Hydrogen bond donor=1	AGLU201;AVAL200;AALA178
	Vander wall Interaction=1	APRO209;AASP206;AMET257
	Pi-Anion Interaction=1	AARG207;AAGLY205
	Aromatic heavy atoms=11	
	Fraction Csp3 saturation =0.39	
	Molar Refractivity=92.34	
	Topographical surface area=68.78A^2	
	Skin permeability= (-5.84cm/sec)	
2-O-Acetylpseudolycorine	Hydrogen bond acceptor=6	AARG701;AMET677;AGLY627
	Hydrogen bond donor=2	ATHR702;APRO704;ASER703
	Vander wall interaction=6	ATHR228;AGLU247;ALEU246
	Pi-anion Interaction =2	APHE253;AASN224;AARG236
	Pi-alkyl interaction=1	AARG249;AGLN234;AGLU230
	Aromatic heavy atoms=24	AHIS629
	Fraction Csp3 saturation=0.50	
	Molar refractivity=90.44	
	Topographical surface area=79.23A^2	
	Skin permeability= (-8.02cm/sec)	
Netilmicin	Hydrogen bond acceptor=12	AGLY727;ASER225;AASN393
	Hydrogen bond donor=8	AASP223;ASER226;AMET257
	Vander wall Interaction =14	AARG207;APHE254;ALEU89
	Pi anion Interaction=0	AILE276;AASP749;AALA750
	Pi alkyl Interaction=0	ASER255;AVAL728;ASER748
	Aromatic heavy atoms=0	ALYS171;AASN172;AILE745
	Fraction Csp3 saturation=0.90	AGLY747;AASP726;AALA746
	Molar refractivity=1117.83	
	Topographical surface area=199.73A^2	
	Skin permeability=(-12.0cm/sec)	
5,6,7,3',4' Pentahydroxyisoflavone	Hydrogen bond acceptor=7	ALEU471;ATHR472;AGLN422
	Hydrogen bond donor=5	APHE420;ATHR419;AASP410
	Vander wall Interaction=10	AALA409;APHE468;AVAL397
	Pi-alkyl=3	ATHR396;ALEU465;AALA565
	Aromatic heavy atoms=12	ATHR463;AMET395;AARG394
	Fraction Csp3 saturations=0.0	APRO452;ALYS467;ATHR411
	Molar refractivity=78.0	AGLN415
	Topographical surface area=131.36A^2	
	Skin permeability= (-6.84cm/sec)	
Benztropine	Hydrogen bond acceptor=2	AARG394;ALYS467;AASP223
	Hydrogen bond donor =0	AALA464;APRO233;ASER231
	Vander wall interaction = 9	AALA460;ALEU259;AMET395
	Pi alkyl Interaction=5	AASP459;AASP459;AGLY458
	Aromatic heavy atoms= 12	AILE457;AGLY205;ACYS258
	Fraction Csp3 saturation=0.45	AMET257;AVAL456;ATHR463
	Molar refractivity=102.83	
	Topographical polar surface area=12.47A^2	
	Skin permeability=(-4.84cm/sec)	
Luteolin	Hydrogen bond acceptor=6	ALEU89;AALA750;AVAL728
	Hydrogen bond donor=4	AALA88;APHE254;AILE276
	Vander wall Interaction=11	ASER255;ASER226;APRO175
	Pi-alkyl interaction=0	ASAN190;ASAP192;AGLN176
	Aromatic heavy atoms=16	ALAN191;AASN87;AARG207
	Fraction Csp3 saturation = 0.24	ALEU173;AASN172;APHE170
	Molar Refractivity=85.32	AASP749;ALYS171;ALYS752
	Topographical surface area=107.22	AGLY 747:ASER7



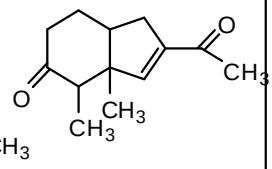
Sedanonic acid



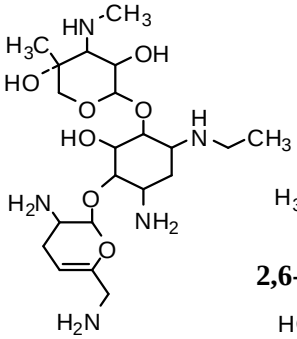
Benzyl beta-primeveroside



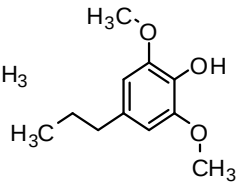
Istamycin C1



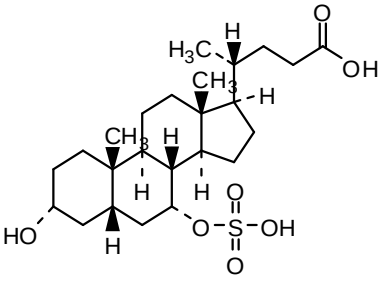
Eremopetasinorone A



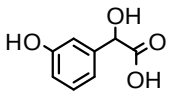
Netilmicin



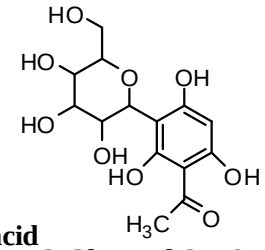
2,6-Dimethoxy-4-propylphenol



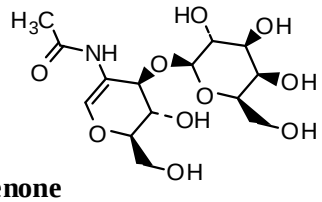
Chenodeoxycholic *cis* Sulphte



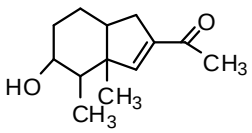
3-Hydroxymadelic acid



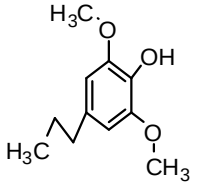
3-Glucosyl-2,4-6 trihydroxyacetophenone



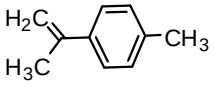
2-(acetylmino)-1,5-anhydro-2-deoxy-3-O-b-galactopyranosyl-D-arabino-Hex-1-enitol



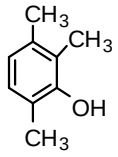
Eremopetasinorol



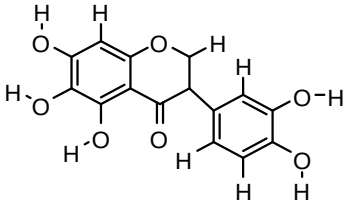
2,6-Dimethoxy-4-propylphenol



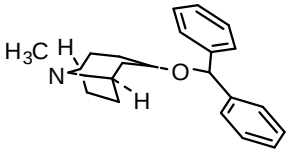
p-Mentha-1,3,5,8-tetraene



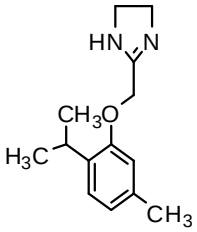
2,3,6-Trimethylphenol



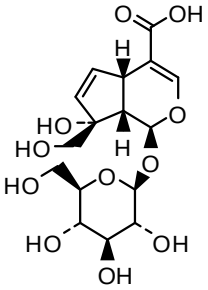
5,6,7,3',4'-Pentahydroxyisoflvone



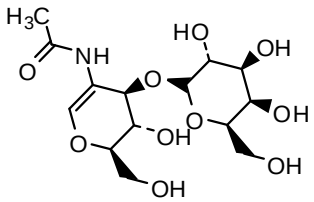
Benztropine

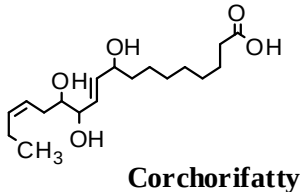


Tymazoline



Monotropein





Corchorifatty acid F

2-(acetylamino)-1,5-anhydro-2-deoxy-3-O-b-D-galactopyranosyl-D-arabino-Hex-1-enitol

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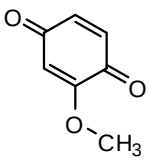
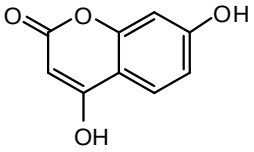
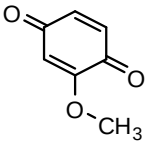


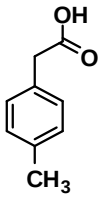
2-Methoxy-1,4-benzoquinone



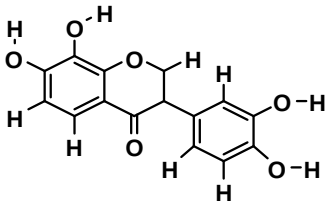
4,7-Dihydroxy-2H-1benzopyrn-2-one



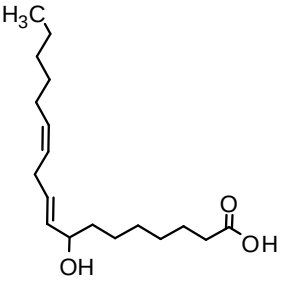
2-Methoxy-1,4-benzoquinone



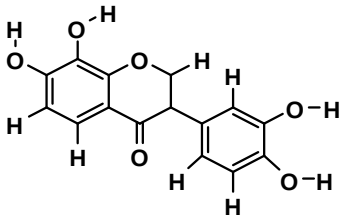
4-Methylphenyl cetic acid



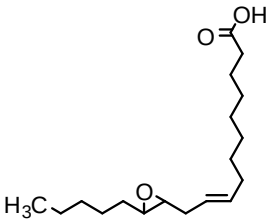
5,6,7,3',4'-Pentahydroxyisoflavone



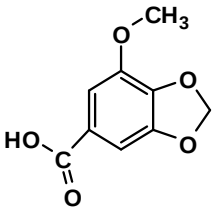
8S-HODE



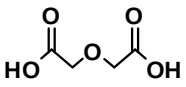
7,8,3',4'- Tetrahydroxyisoflvone



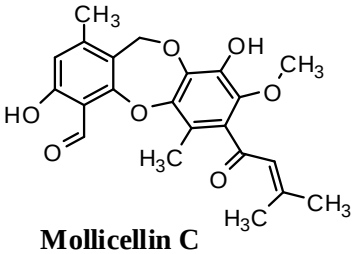
12,13EpODE



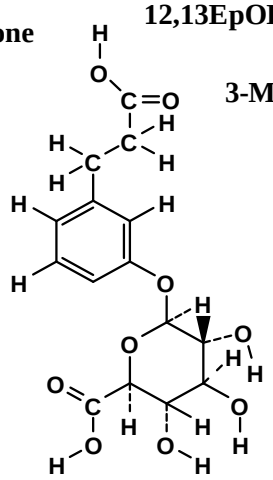
3-Methoxy-4,5-methylenedioxybenzoic acid



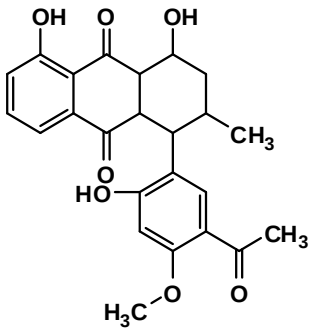
Diglycolic cid



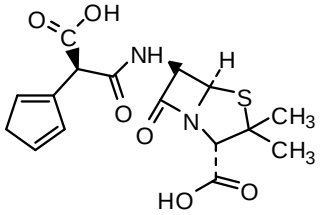
Mollicellin C



Dihydrocaffeic acid 3-O-glucuronide

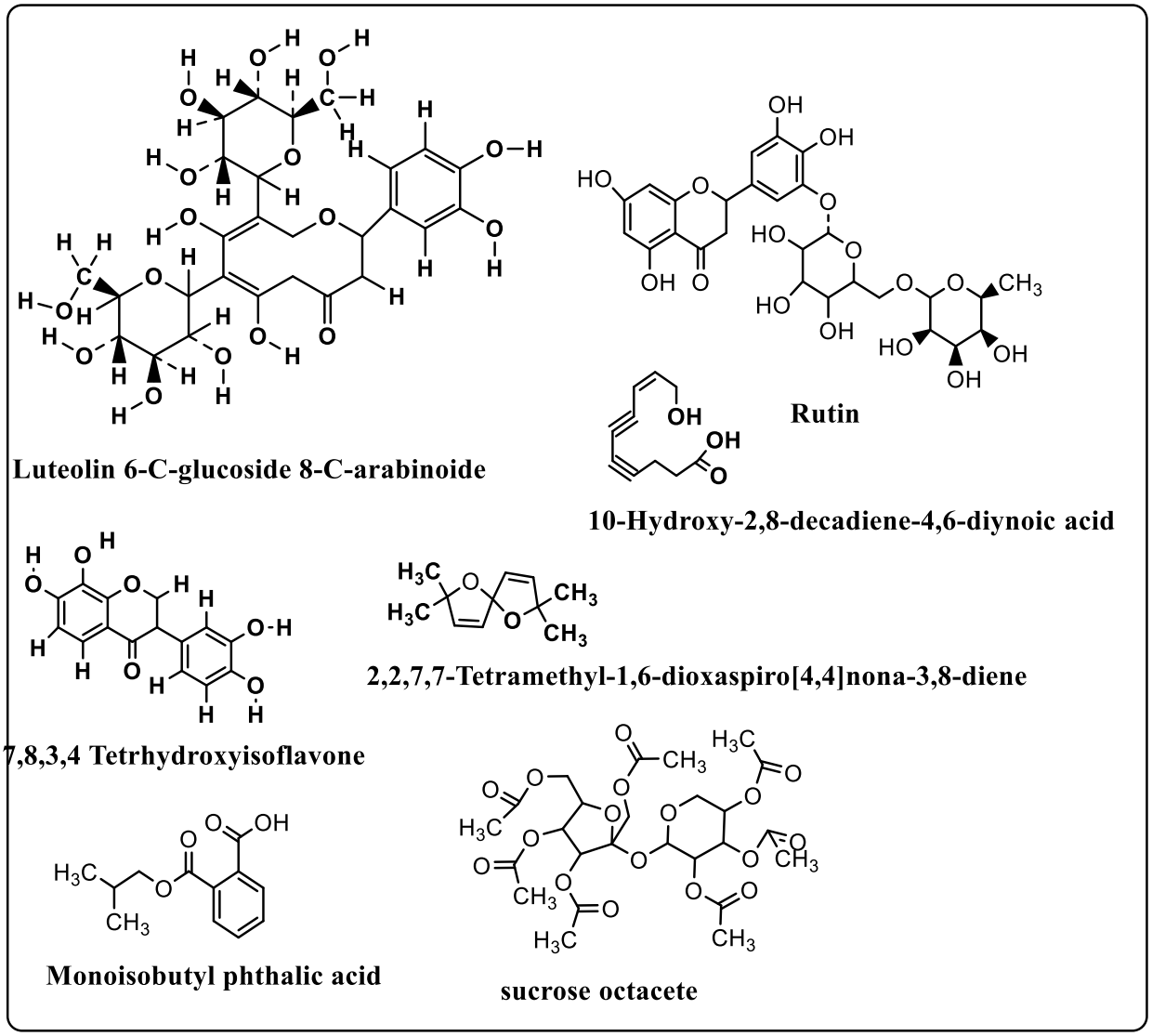


Knipholone



Ticarcillin

Continued .....



Supplementary Figure 1. Name and chemical structure of compounds identified in ethanol extract of "Magahi Pan" through negative and positive ionization mode