Table S1: Central composite design (CCD) for the independent variables and corresponding response value in RSM and ANN (predicted)

Run	Independent variables			Responses (predicted)							
	(X_1)	(X_2)	(X_3)	(Y_1)		(Y_2)		(Y_3)		(Y_4)	
				RSM	ANN	RSM	ANN	RSM	ANN	RSM	ANN
1	75	4	70	4.30	4.41	3.16	3.19	10.81	10.77	1.38	1.24
2	25	2	50	3.81	3.59	2.55	2.65	10.25	10.24	1.47	1.42
3	75	2	50	3.90	4.11	2.55	2.58	9.75	9.72	1.16	0.98
4	100	3	60	4.30	4.27	3.44	3.11	10.11	10.73	1.12	0.96
5	75	2	70	3.50	3.49	2.56	2.49	9.95	9.95	1.17	1.45
6	50	3	60	4.53	4.34	3.10	2.97	10.45	10.36	1.40	1.37
7	0	3	60	3.00	3.09	2.52	2.96	9.57	9.79	0.91	0.96
8	75	4	50	4.31	3.08	2.95	3.32	9.88	9.9	0.88	0.88
9	50	3	60	4.30	4.34	3.15	2.97	10.40	10.36	1.46	1.37
10	50	3	60	4.51	4.34	3.09	2.97	10.42	10.36	1.43	1.37
11	50	3	80	3.78	3.78	2.26	2.40	9.50	9.59	1.10	1.09
12	50	3	60	4.46	4.34	3.01	2.97	10.48	10.36	1.45	1.37
13	50	3	60	4.48	4.34	3.12	2.97	10.41	10.36	1.43	1.37
14	25	4	70	3.15	3.15	2.16	2.19	9.60	9.62	1.00	1.10
15	50	3	60	4.51	4.34	2.95	2.97	10.2	10.36	1.45	1.37
16	50	3	40	3.85	3.83	2.48	2.45	9.60	9.89	0.92	0.93
17	25	2	70	3.25	3.21	2.15	2.16	9.36	9.4	1.12	1.29
18	50	1	60	2.87	3.14	2.03	2.13	9.80	9.64	1.32	1.36
19	50	5	60	2.90	2.98	2.50	2.49	9.90	9.8	0.86	0.85
20	25	4	50	2.96	2.95	2.38	2.17	9.53	9.6	0.75	0.74

X_1: Ethanol concentration (%); X_2: time (h); X_3: temperature (^{0}C); (Y_1): total phenolic content (mgGAE/g) (TPC); (Y_2): total flavonoid content (mgCAE/g) (TFC); (Y_3): DPPH-radical scavenging activity (% inhibition); (Y_4): cupric reducing antioxidant capacity (µM ascorbic acid equivalent) (CUPRAC).

Table S2: Independent process variables with experimental ranges and levels for heat reflux extraction of ripe Ajwa dates pulp (RADP).

| Input variables	Variable range and levels (coded)						
	unit	Code	$-\alpha$	-1	0	+1	$+\alpha$
Ethanol concentration (EtOH)	%	X_1	0	25	50	75	100
Time	h	X_2	1	2	3	4	5
Temperature	^{0}C	X_3	40	50	60	70	80
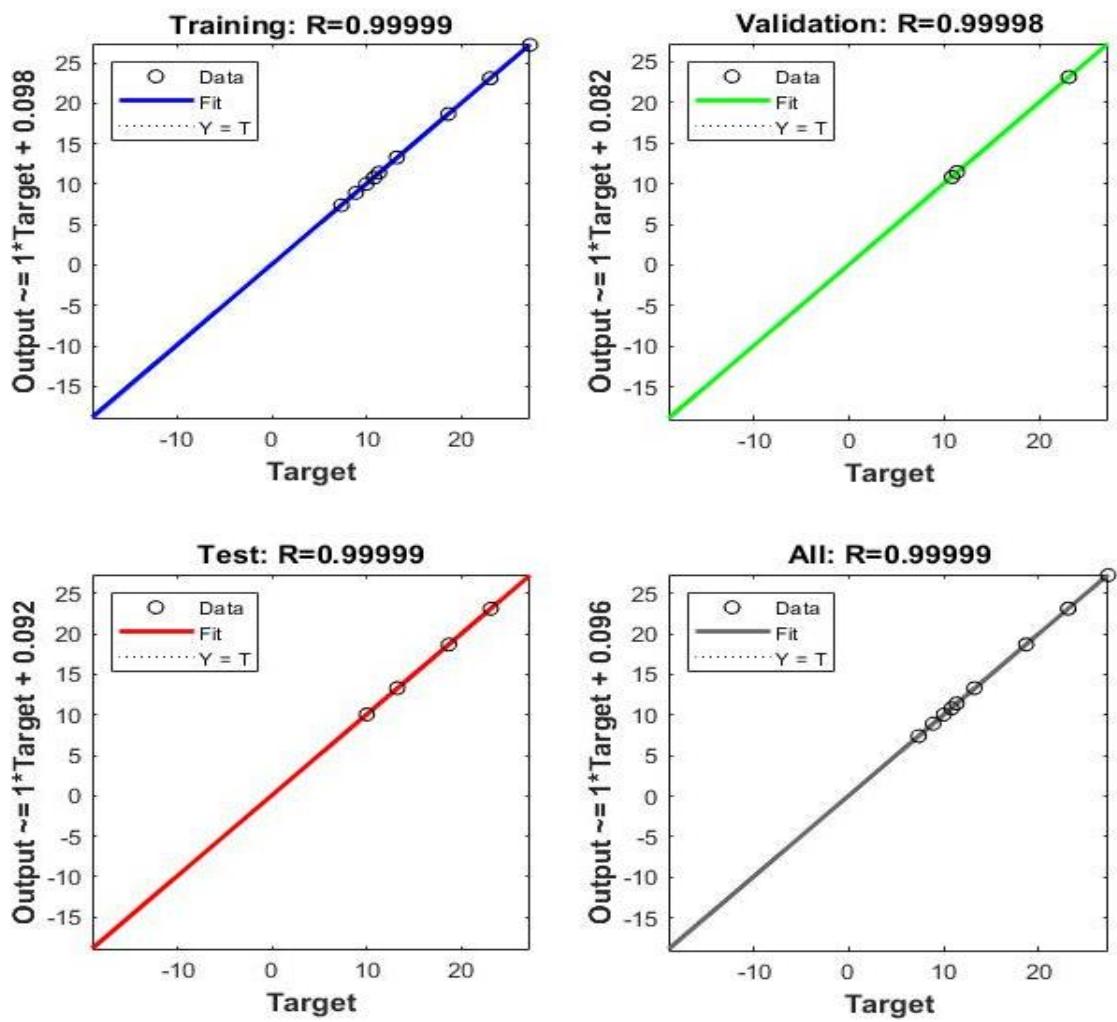
Figure S1: The R² value of training, validation, test and overall for TPC during ANN.
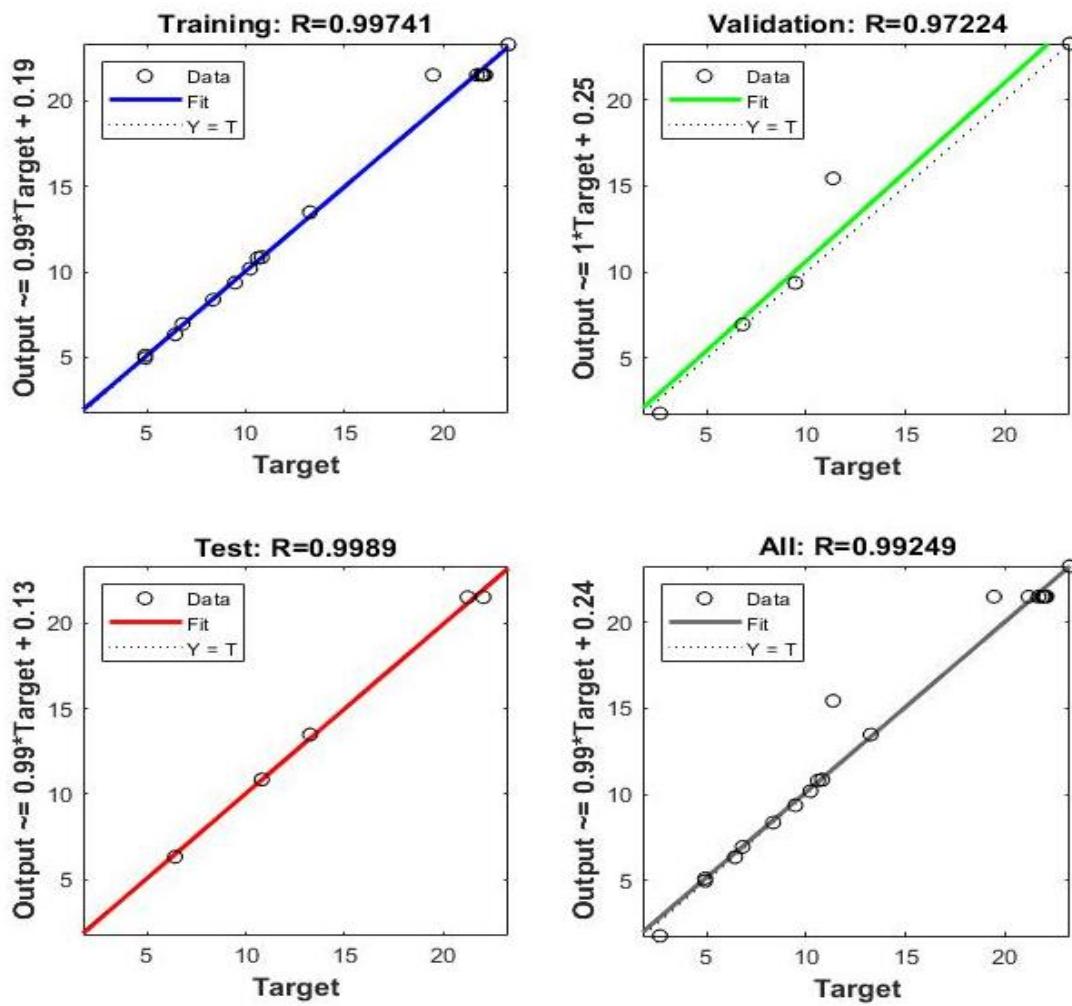
Figure S2: The R² value of training, validation, test and overall for TFC during ANN.
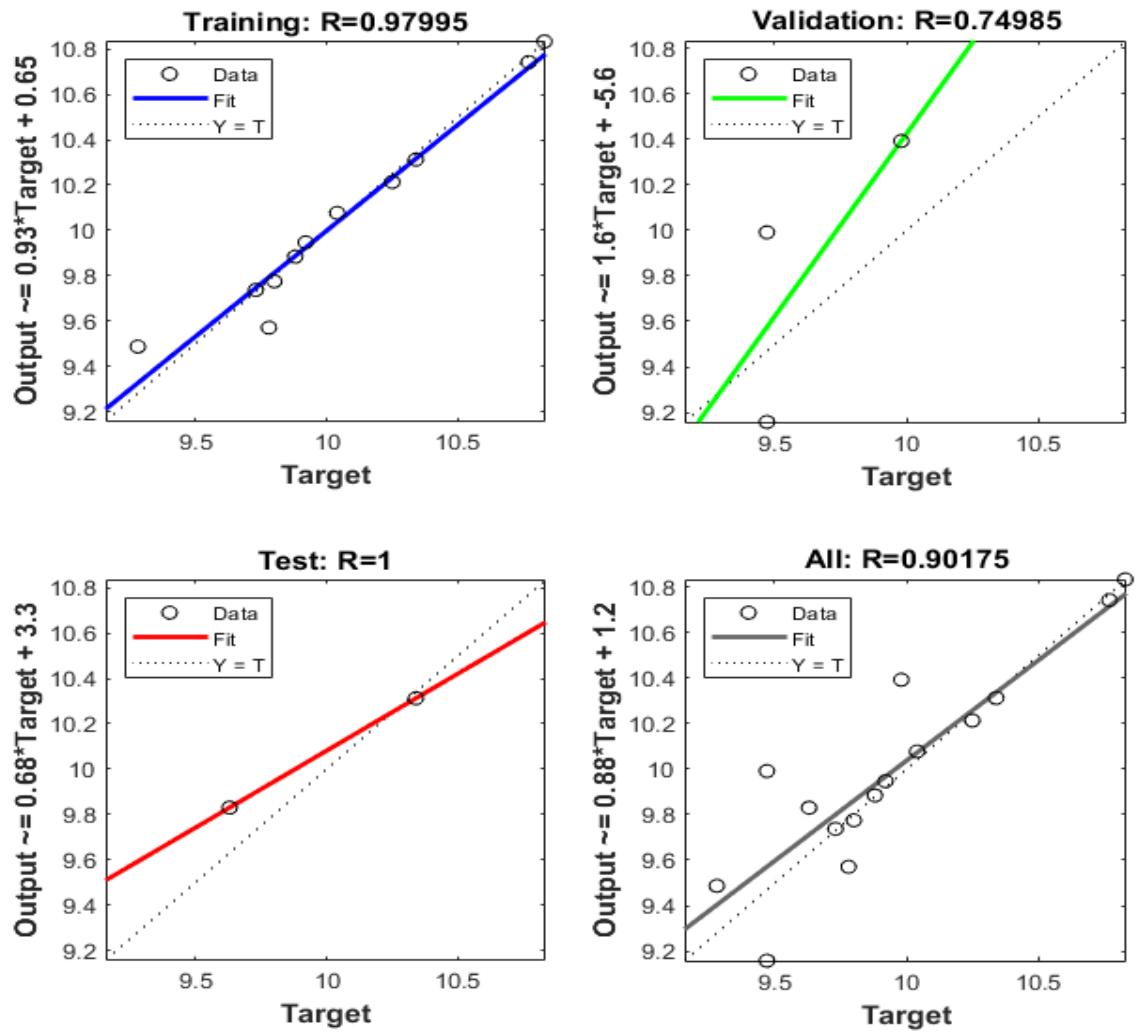
Figure S3: The R² value of training, validation, test and overall for DPPH during ANN.
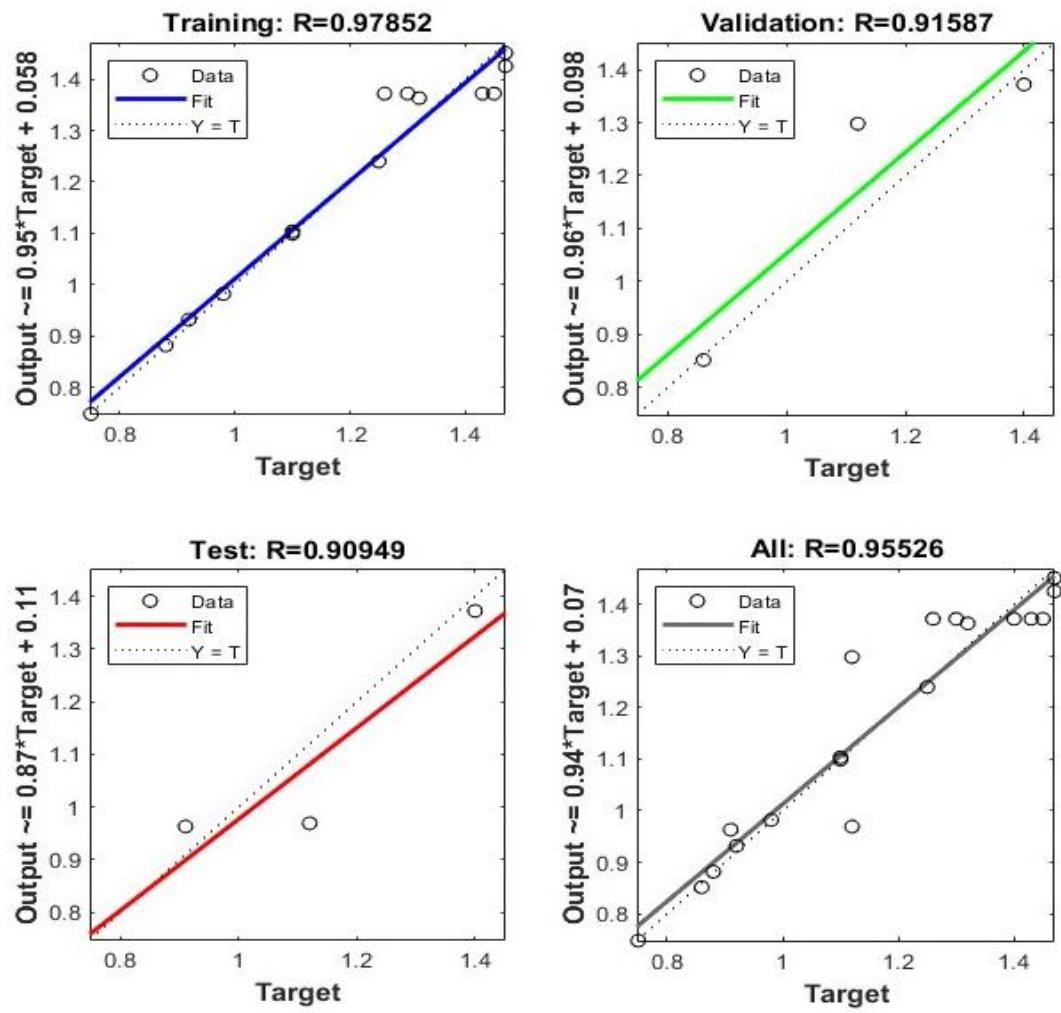
Figure S4: The R² value of training, validation, test and overall for CUPRAC during ANN.

(A)

Formula: $C_5H_3O_3^-$
Mass: 111.0088

−CO

Chemical Formula: $C_6H_4O_4$
Exact Mass: 140.0110
Calculated Mass[M-H]−:139.0031
Observed Mass[M-H]−: 139.0037
Coumalic acid

−COO

Formula: $C_5H_3O_2^-$
Mass: 95.0139

(B)

Formula: $C_{33}H_{39}O_{13}^-$
Mass: 643.2396

−2XCH₃

Formula: $C_7H_3O_4^-$
Mass: 151.0037

Formula: $C_9H_9O_4^-$
Mass: 181.0506

−Hexosyl
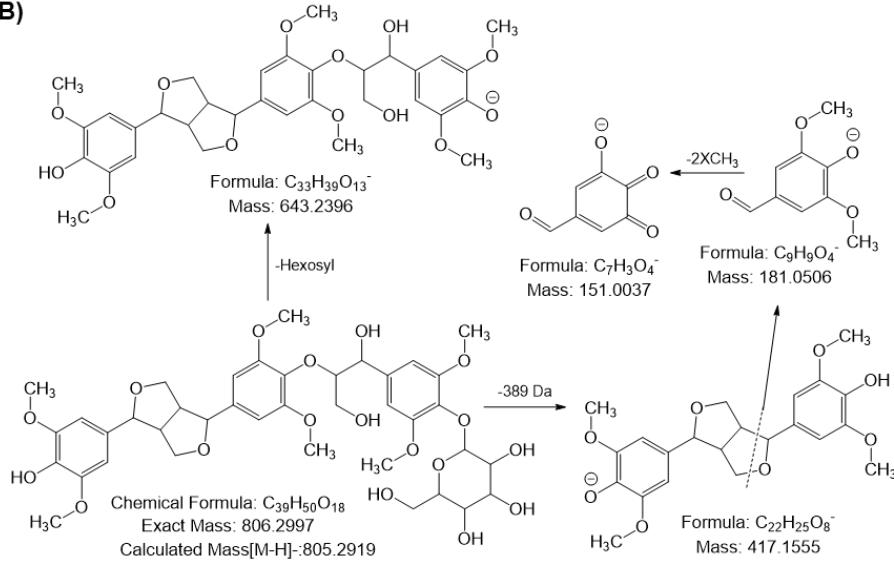
Chemical Formula: $C_{39}H_{50}O_{18}$
Exact Mass: 806.2997
Calculated Mass[M-H]−:805.2919
Observed Mass[M-H]−: 805.2926
**Erythro-1-(4''-O-hexoside-3.5-dimethoxyphenyl)-
2-syringaresinoxyl-propane-1.3-diol**

−389 Da

Formula: $C_{22}H_{25}O_8^-$
Mass: 417.1555

(C)

Formula: $C_6H_{10}NO_2^-$
Mass: 128.0717

−COO-CO

Formula: $C_8H_{10}NO_5^-$
Mass: 200.0564

−91 Da

Formula: $C_{11}H_{16}NO_8^-$
Mass: 290.0881

−H₂O
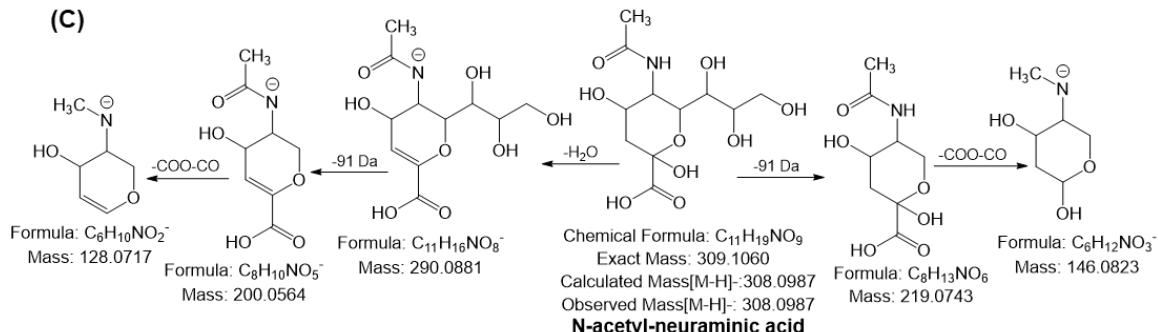
Chemical Formula: $C_{11}H_{19}NO_9$
Exact Mass: 309.1060
Calculated Mass[M-H]−:308.0987
Observed Mass[M-H]−: 308.0987
N-acetyl-neuraminic acid

−91 Da

Formula: $C_8H_{13}NO_6$
Mass: 219.0743

−COO-CO

Formula: $C_6H_{12}NO_3^-$
Mass: 146.0823

(D)

Formula: $C_6H_{10}NO_2^-$
Mass: 128.0717

−COO-CO

Formula: $C_8H_{10}NO_5^-$
Mass: 200.0564

−91 Da

Formula: $C_{11}H_{16}NO_8^-$
Mass: 290.0881

−lactose
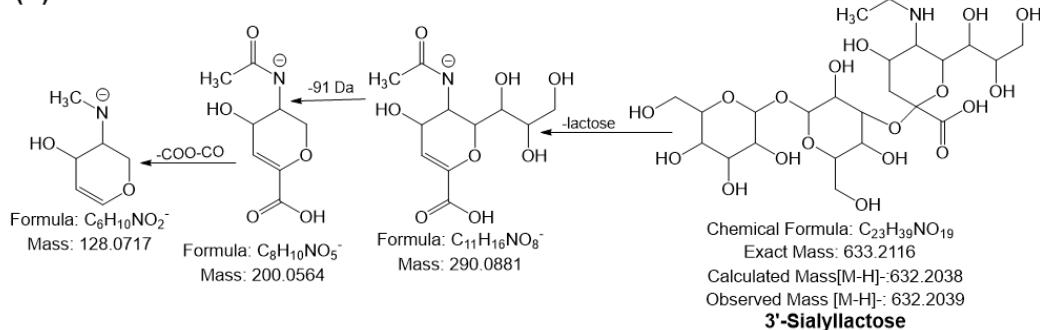
Chemical Formula: $C_{23}H_{39}NO_{19}$
Exact Mass: 633.2116
Calculated Mass[M-H]−:632.2038
Observed Mass [M-H]−: 632.2039
**3'-Sialyllactose**

Figure S5: Possible mass fragmentation behaviour of identified compounds in RADP. (A) coumalic acid, (B) Erythro-1-(4''-O-β-D-glucopyranoside-3,5-dimethyoxyphenyl)-2-syringaresinoxyl-propane-1,3-diol, (C) N-acetyl-α-neuraminic acid, and (D) 6'-sialyllactose.
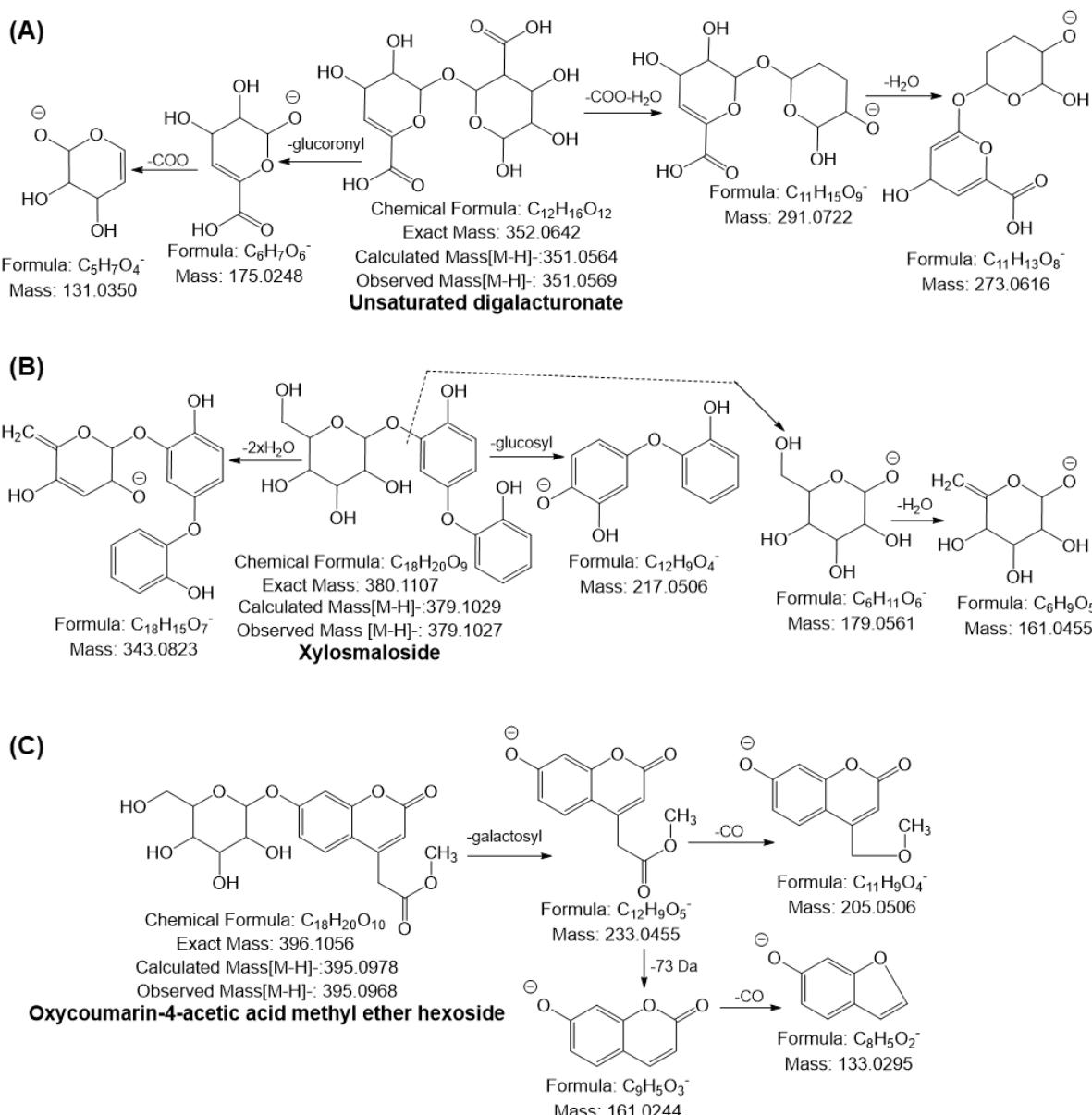
Figure S6: Possible mass fragmentation behaviour of identified compounds in RADP. (A) Unsaturated digalacturonate, (B) Xylosmaloside and (C) Oxycoumarin-4-acetic acid methyl ester hexoside.