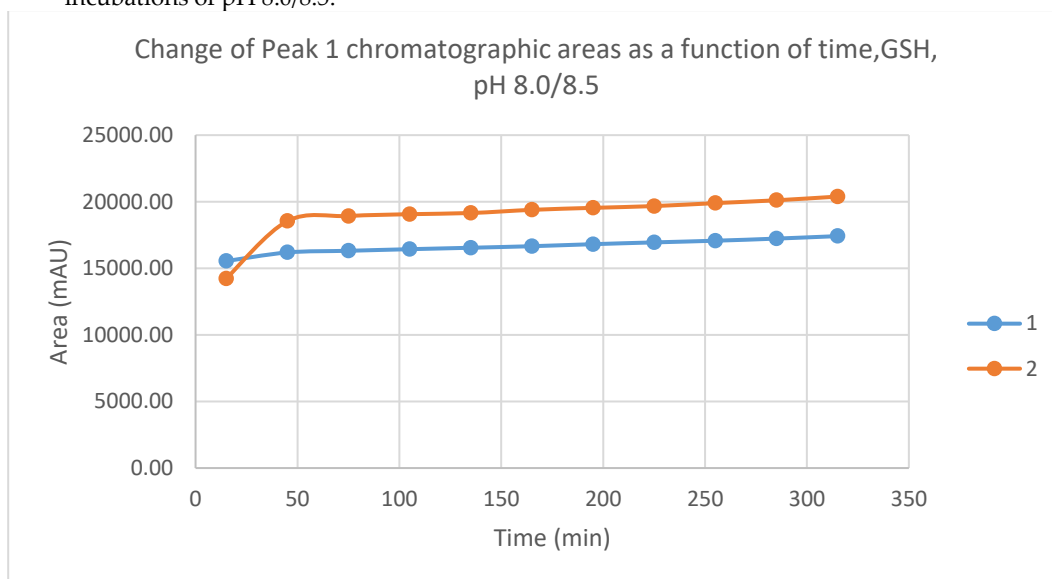
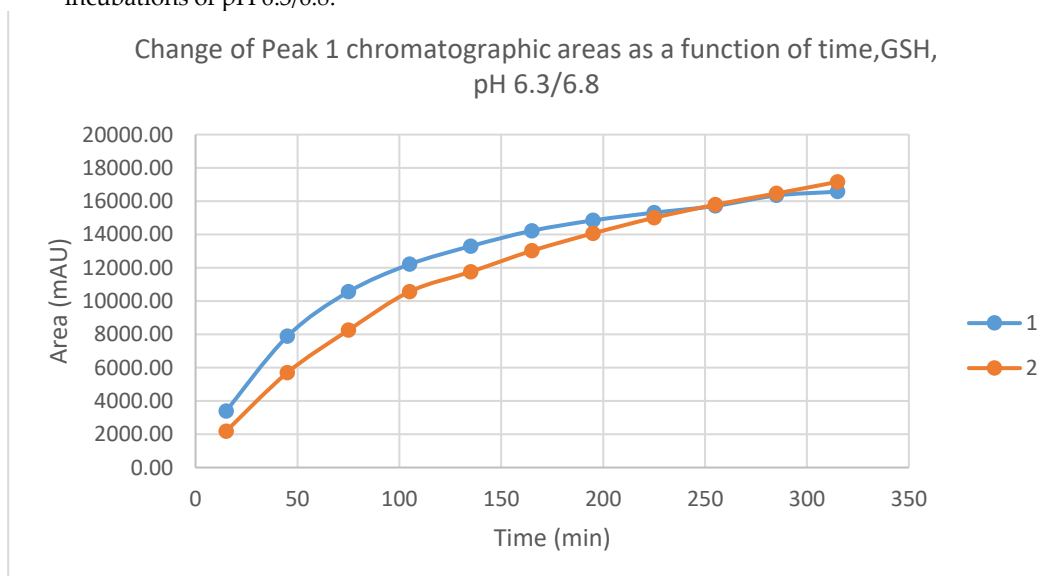


## Supplementary materials

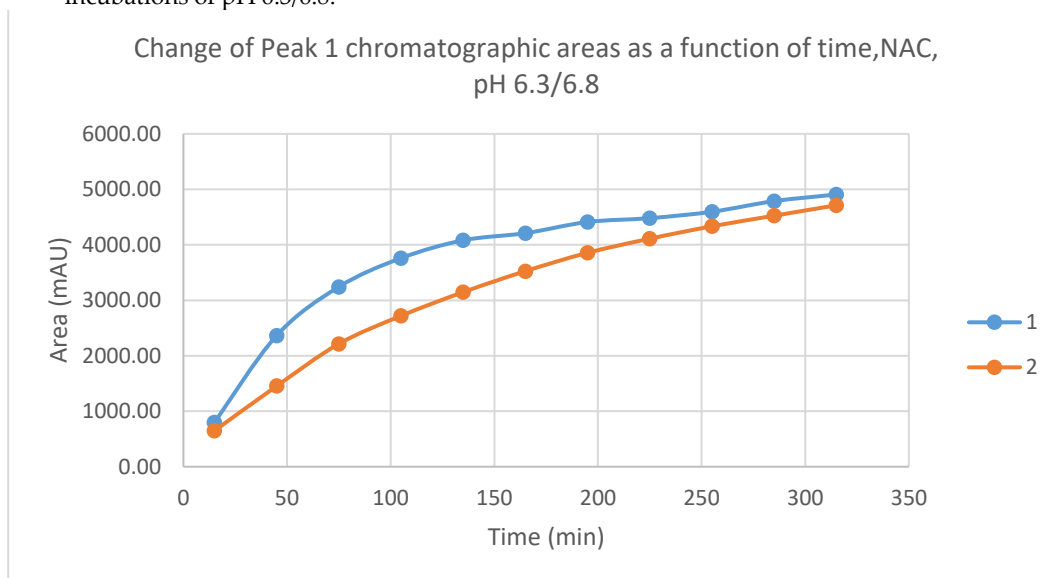
**Figure S1.** Change in the chromatographic peak area of Adduct-1 of chalcones **1** and **2** in the chalcone-GSH incubations of pH 8.0/8.5.



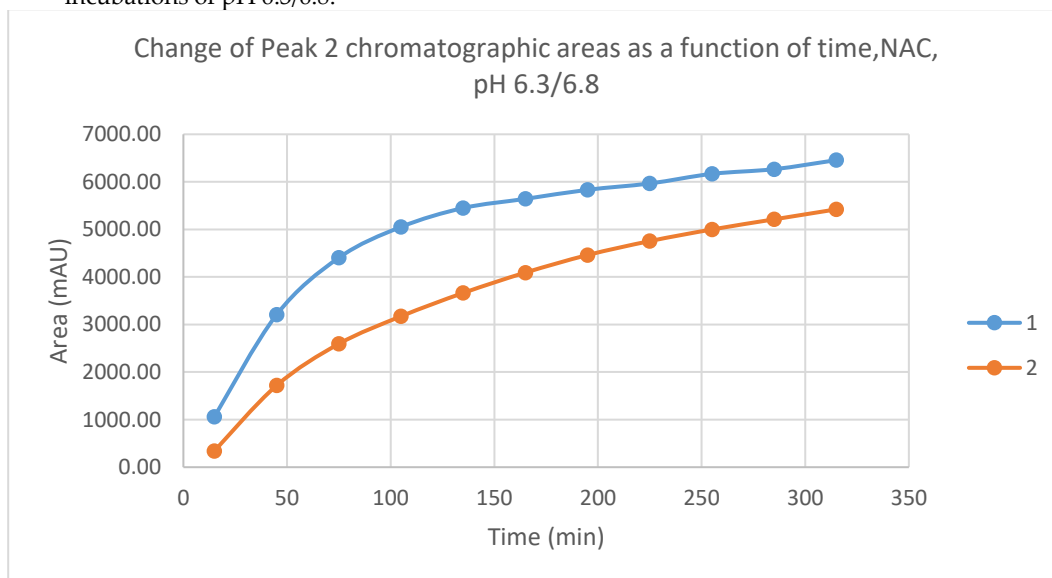
**Figure S2.** Change in the chromatographic peak area of Adduct-1 of chalcones **1** and **2** in the chalcone-GSH incubations of pH 6.3/6.8.



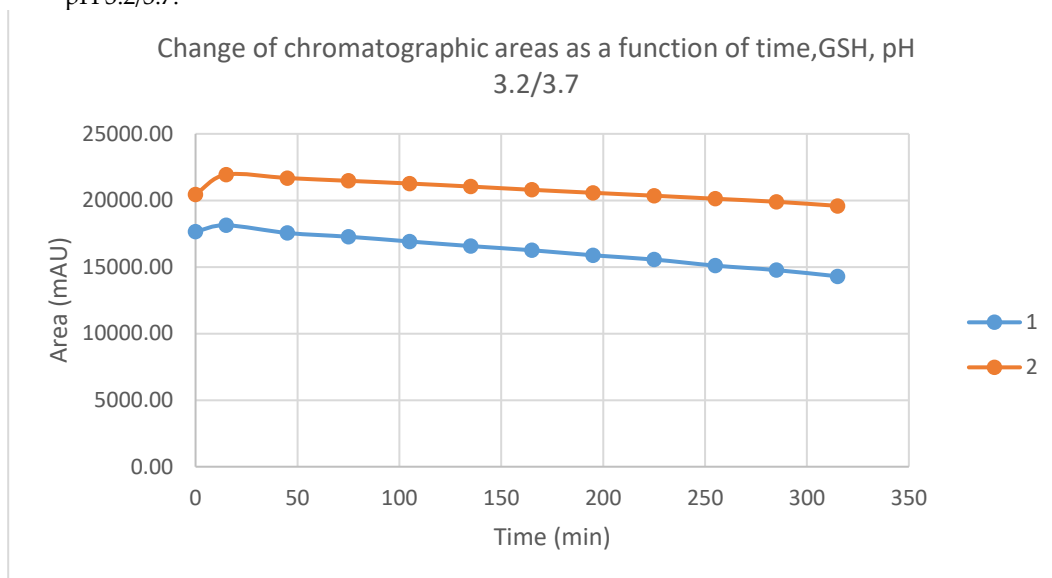
**Figure S3.** Change in the chromatographic peak area of Adduct-1 of chalcones **1** and **2** in the chalcone-NAC incubations of pH 6.3/6.8.



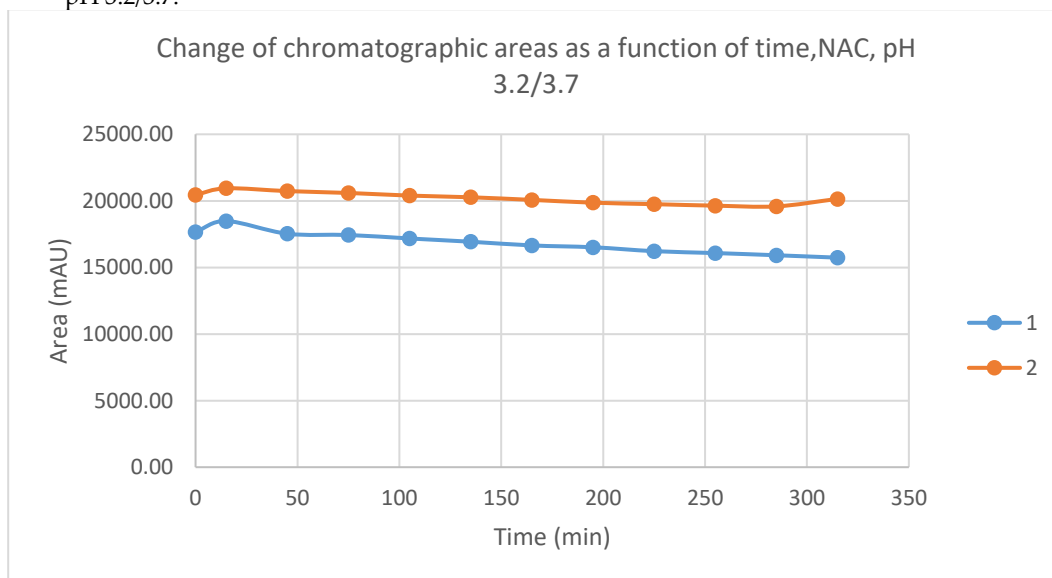
**Figure S4.** Change in the chromatographic peak area of Adduct-2 of chalcones **1** and **2** in the chalcone-NAC incubations of pH 6.3/6.8.



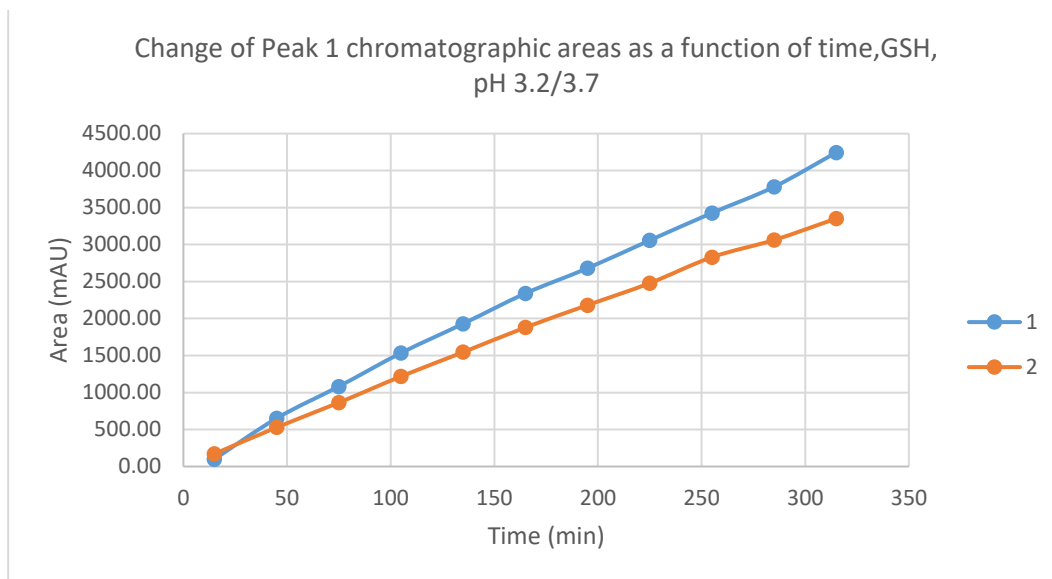
**Figure S5.** Change in the chromatographic peak area of chalcones **1** and **2** in the chalcone-GSH incubations of pH 3.2/3.7.



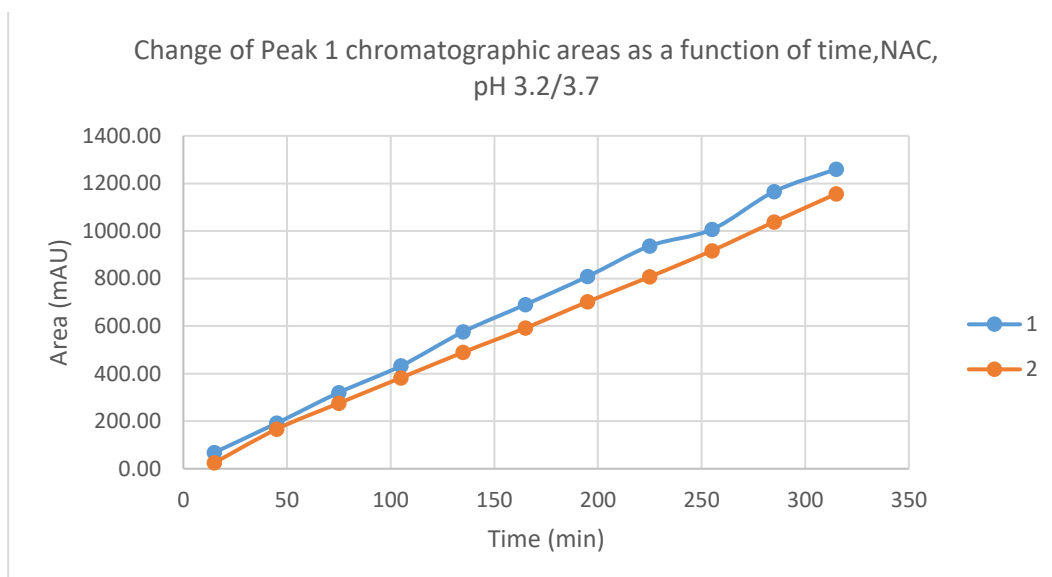
**Figure S6.** Change in the chromatographic peak area of chalcones **1** and **2** in the chalcone-NAC incubations of pH 3.2/3.7.



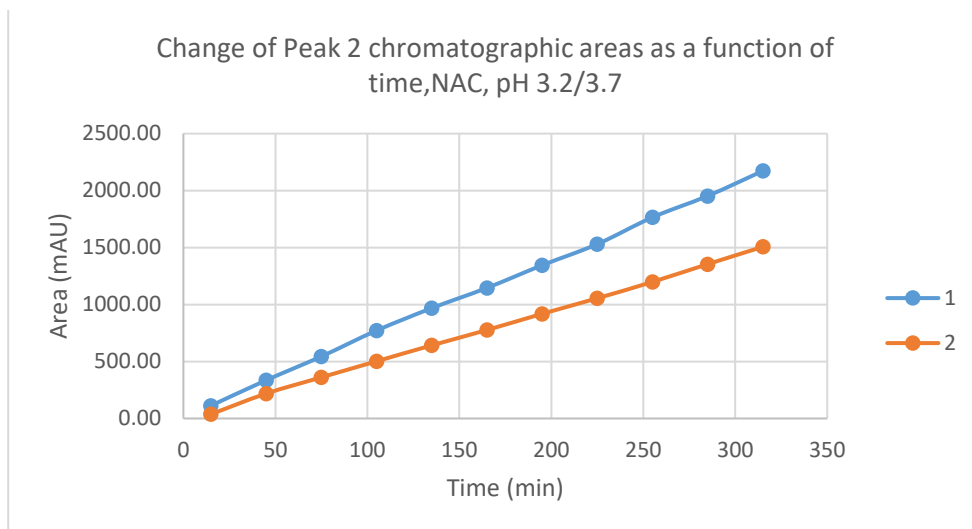
**Figure S7.** Change in the chromatographic peak area of Adduct-1 of chalcones **1** and **2** in the chalcone-GSH incubations of pH 3.2/3.7.



**Figure S8.** Change in the chromatographic peak area of Adduct-1 of chalcones **1** and **2** in the chalcone-NAC incubations of pH 3.2/3.7.



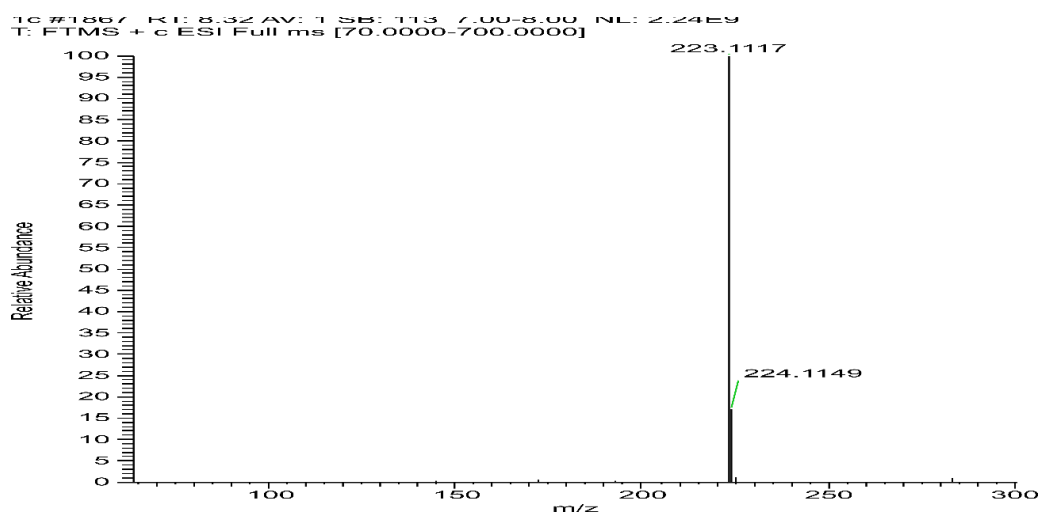
**Figure S9.** Change in the chromatographic peak area of Adduct-2 of chalcones **1** and **2** in the chalcone-NAC incubations of pH 3.2/3.



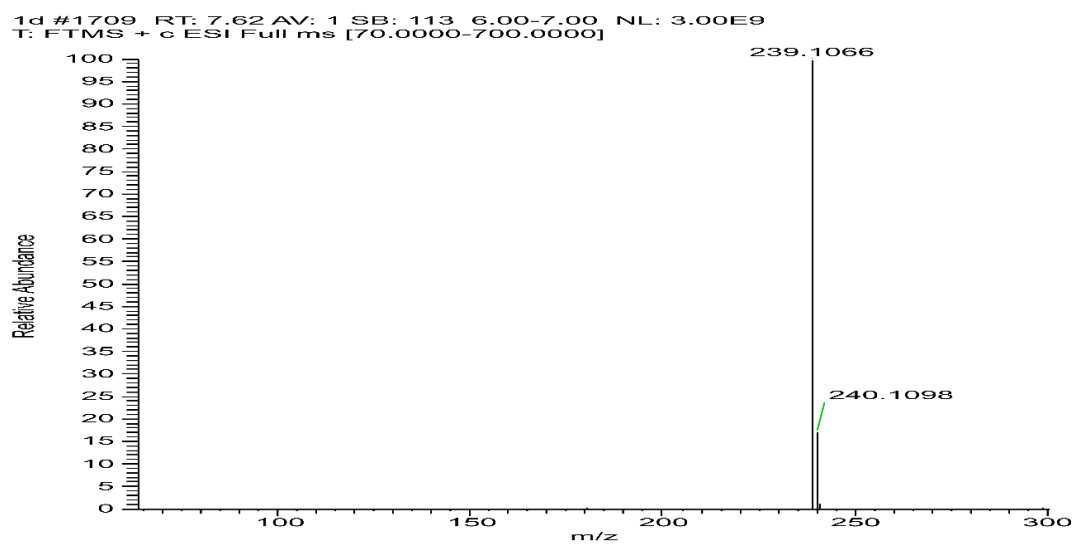
**Table S1.** Mass spectrometry data

Type	Value	1	2
Chalcone	Formula	C <sub>16</sub> H <sub>14</sub> O	C <sub>16</sub> H <sub>14</sub> O <sub>2</sub>
	[M+H] <sup>+</sup> <sub>th</sub>	223.1123	239.1072
	[M+H] <sup>+</sup> <sub>m</sub>	223.1117	239.1066
	ΔM	-2.69	-2.51
Chalcone-GSH adduct	Formula	C <sub>26</sub> H <sub>31</sub> N <sub>3</sub> O <sub>7</sub> S	C <sub>26</sub> H <sub>31</sub> N <sub>3</sub> O <sub>8</sub> S
	[M+H] <sup>+</sup> <sub>th</sub>	530.1961	546.1910
	[M+H] <sup>+</sup> <sub>m</sub>	530.1946	546.1892
	ΔM	-2.83	-3.30
	Number of isomers	1	1
Chalcone-NAC adduct	Formula	C <sub>21</sub> H <sub>23</sub> NO <sub>4</sub> S	C <sub>21</sub> H <sub>23</sub> NO <sub>5</sub> S
	[M-H] <sup>-</sup> <sub>th</sub>	384.1270	400.1219
	[M-H] <sup>-</sup> <sub>m</sub>	384.1246	400.1191
	ΔM	-6.25	-7.00
	Number of isomers	2	2

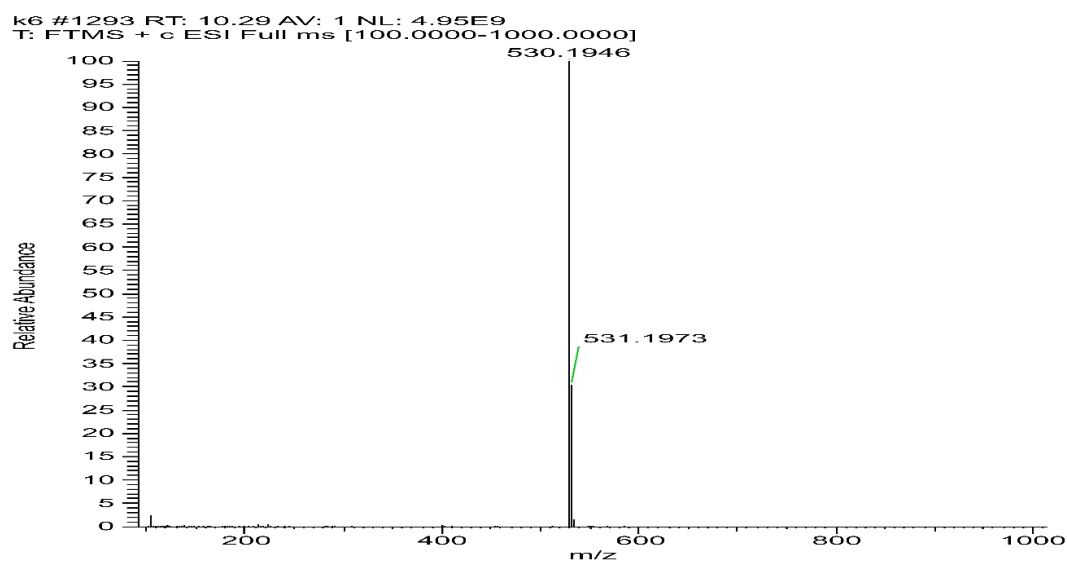
**Figure S10.** High resolution, positive mode HESI MS spectrum of chalcone 1.



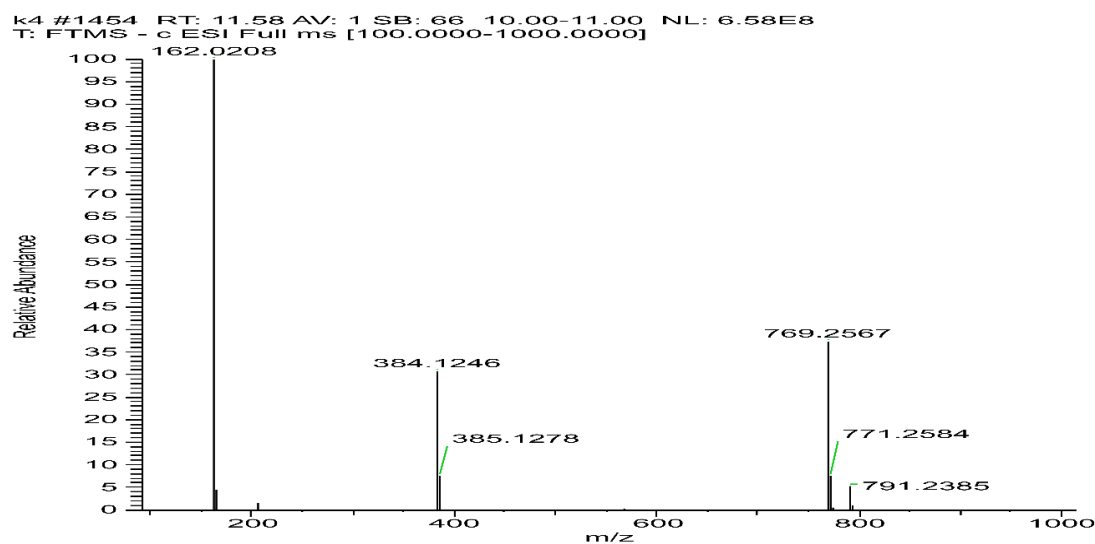
**Figure S11.** High resolution, positive mode HESI MS spectrum of chalcone 2.



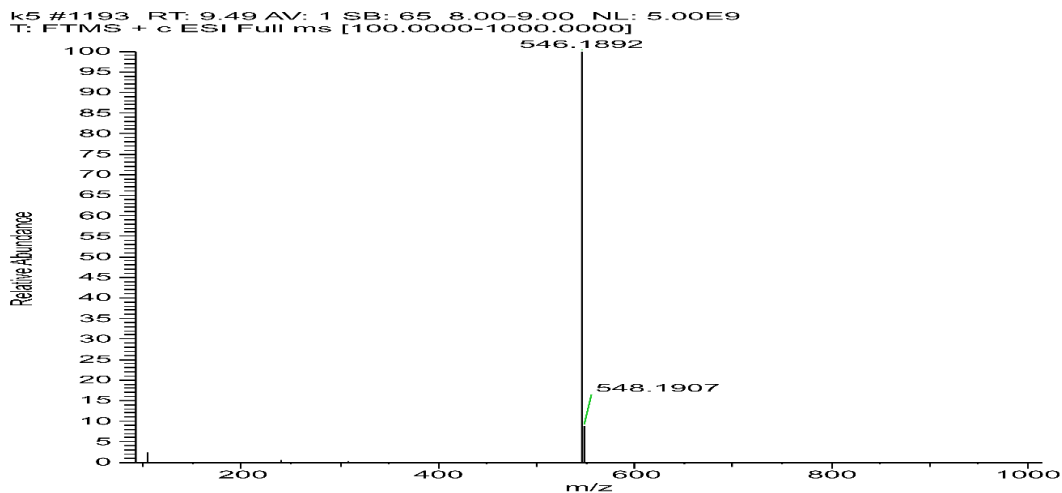
**Figure S12.** High resolution, positive mode HESI MS spectrum of chalcone 1-GSH conjugate.



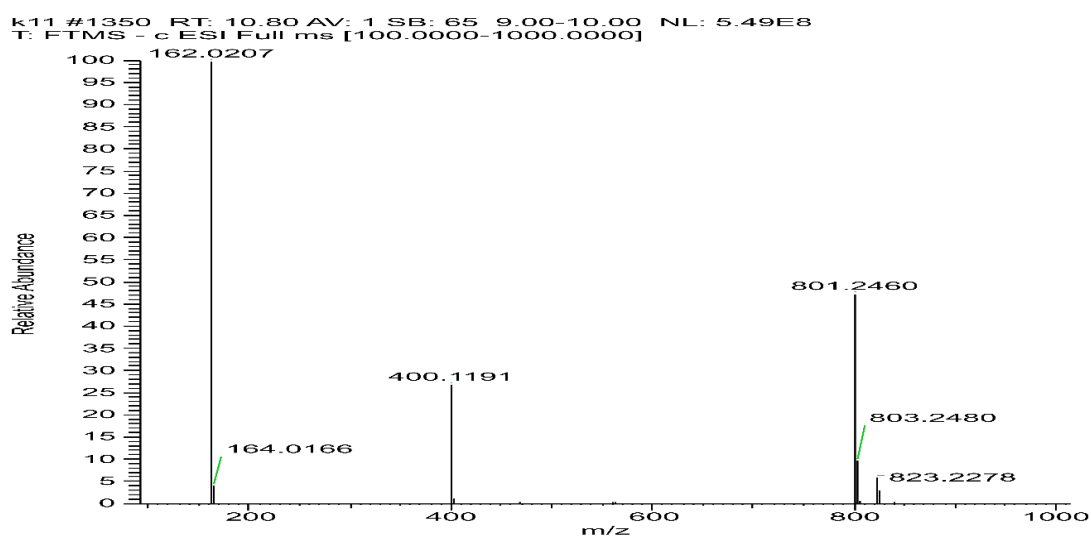
**Figure S13.** High resolution, negative mode HESI MS spectrum of chalcone 1-NAC conjugate.



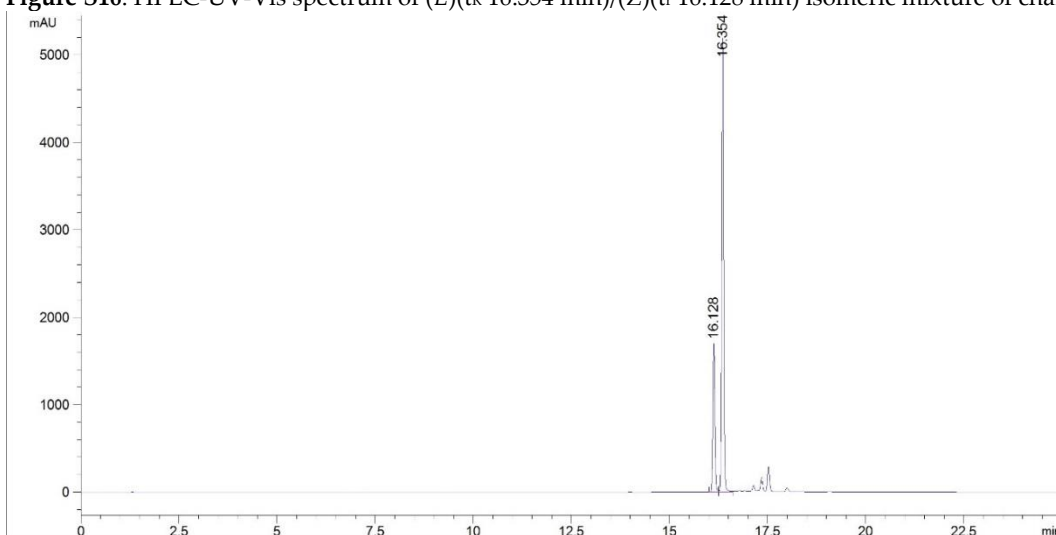
**Figure S14.** High resolution, positive mode HESI MS spectrum of chalcone 2-GSH conjugate.



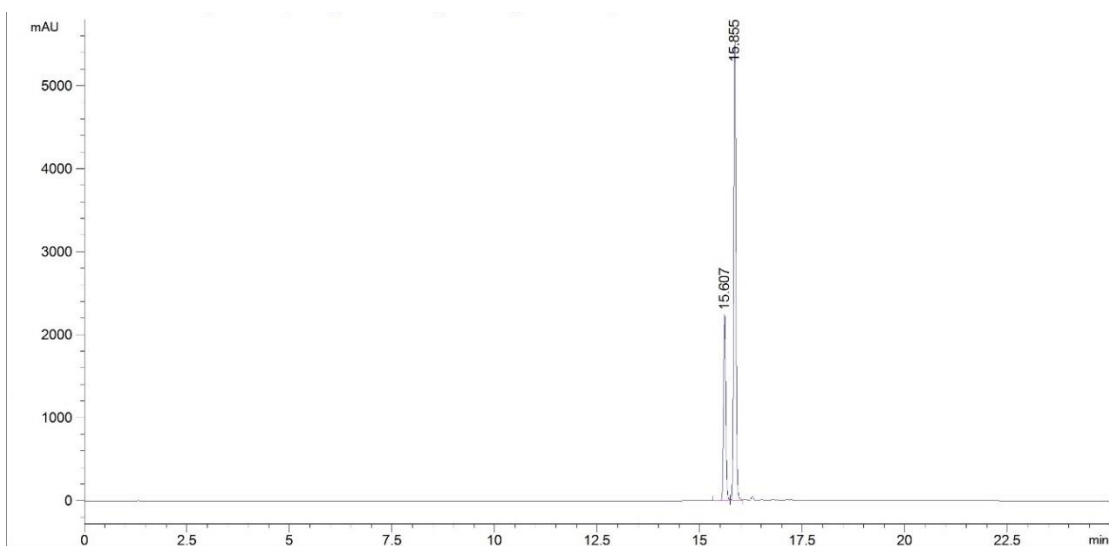
**Figure S15.** High resolution, negative mode HESI MS spectrum of chalcone 2-NAC conjugate.



**Figure S16.** HPLC-UV-Vis spectrum of (*E*)( $t_r$  16.354 min)/(*Z*)( $t_r$  16.128 min) isomeric mixture of chalcone 1.

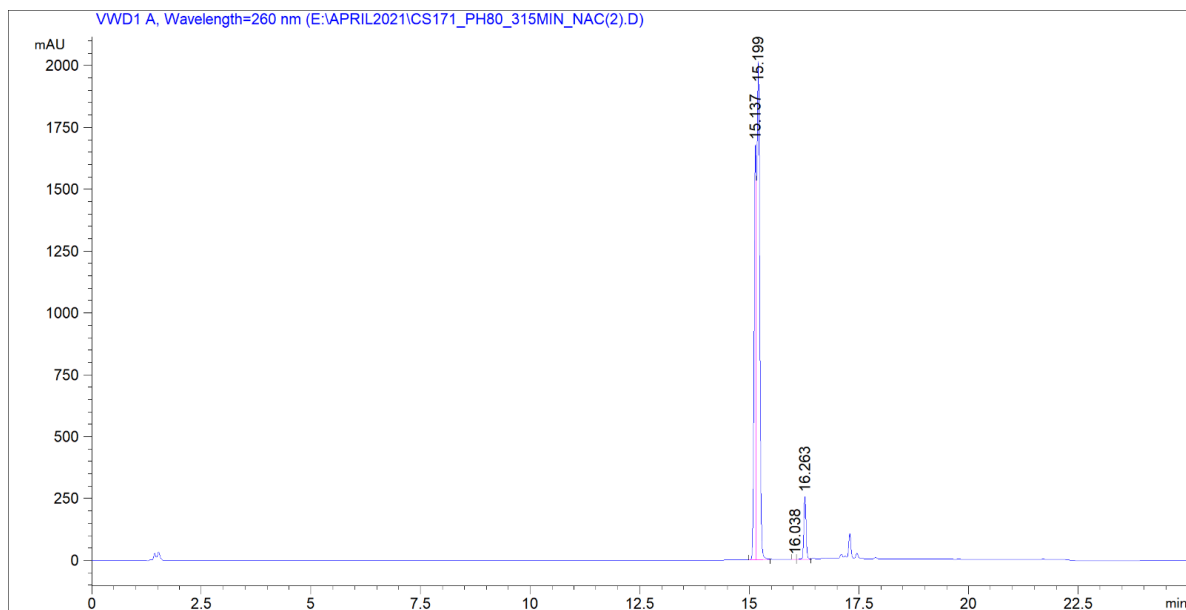


**Figure S17.** HPLC-UV-Vis spectrum of (*E*)( $t_r$  15.607 min)/(*Z*)( $t_r$  15.855 min) isomeric mixture of chalcone 2.

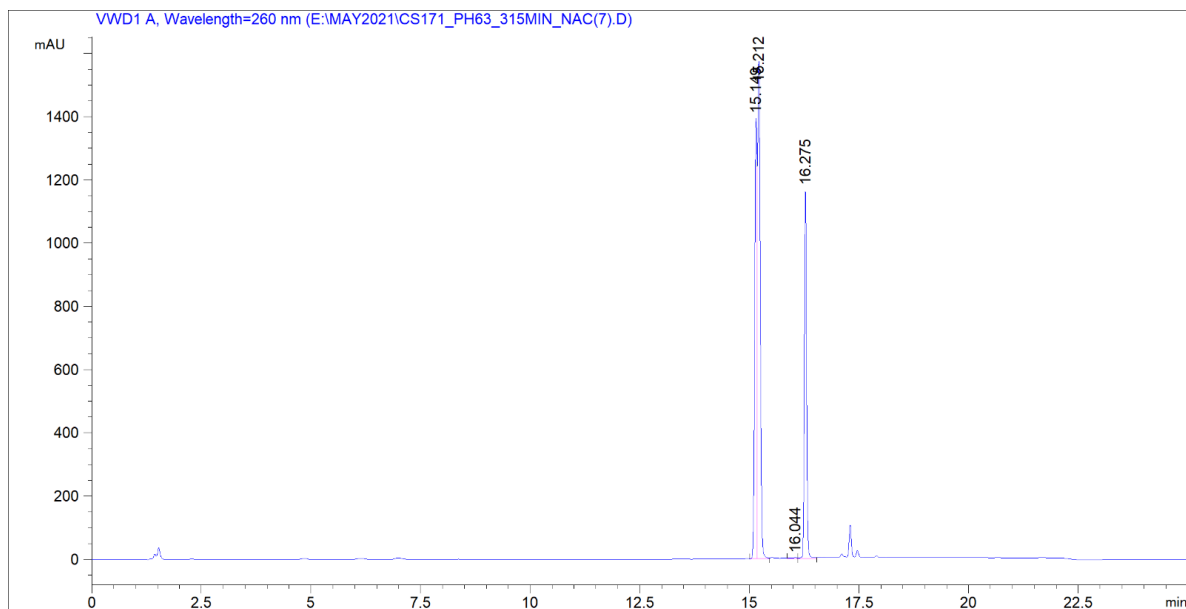




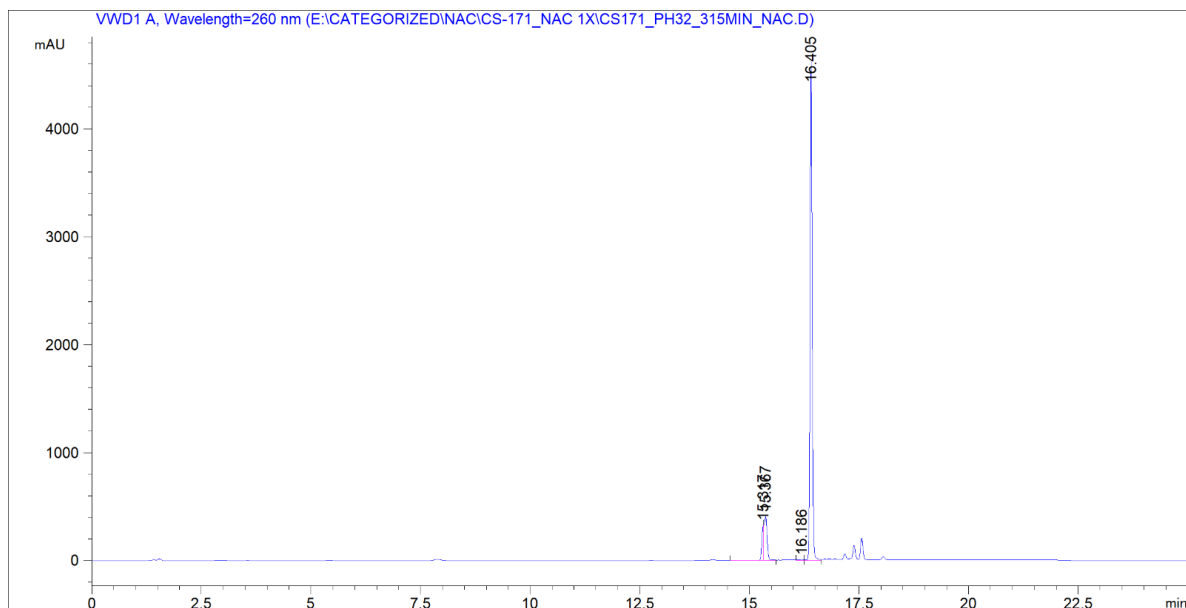
**Figure S18.** HPLC-UV-Vis chromatogram of pH 8.0/8.5 incubation (315-minute timepoint) of chalcone **1** and NAC.



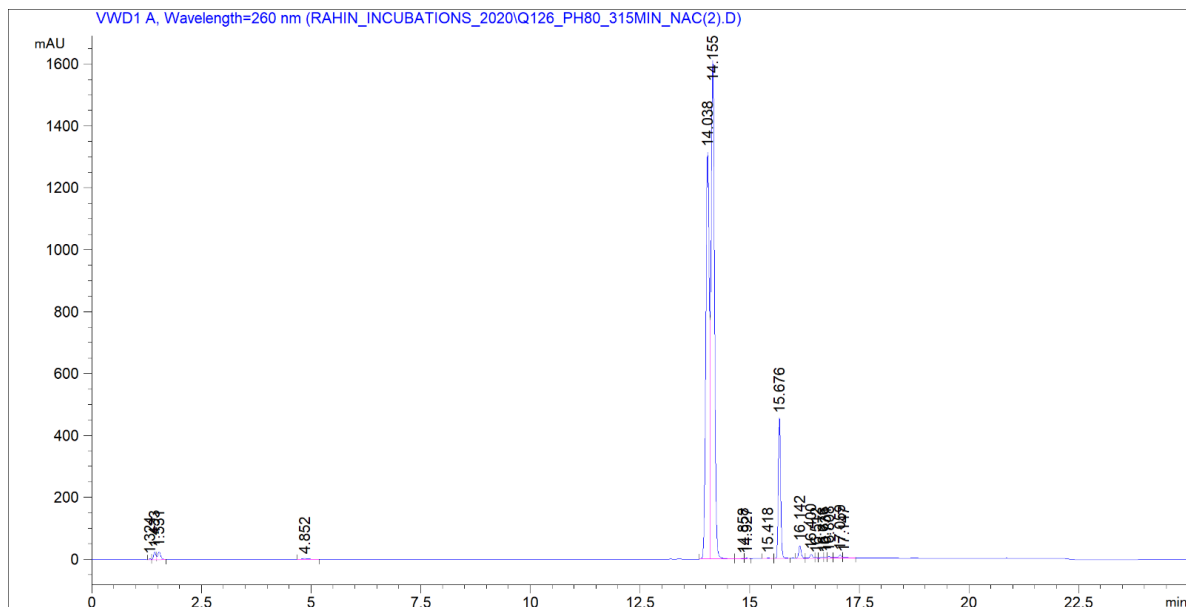
**Figure S19.** HPLC-UV-Vis chromatogram of pH 6.3/6.8 incubation (315-minute timepoint) of chalcone **1** and NAC.



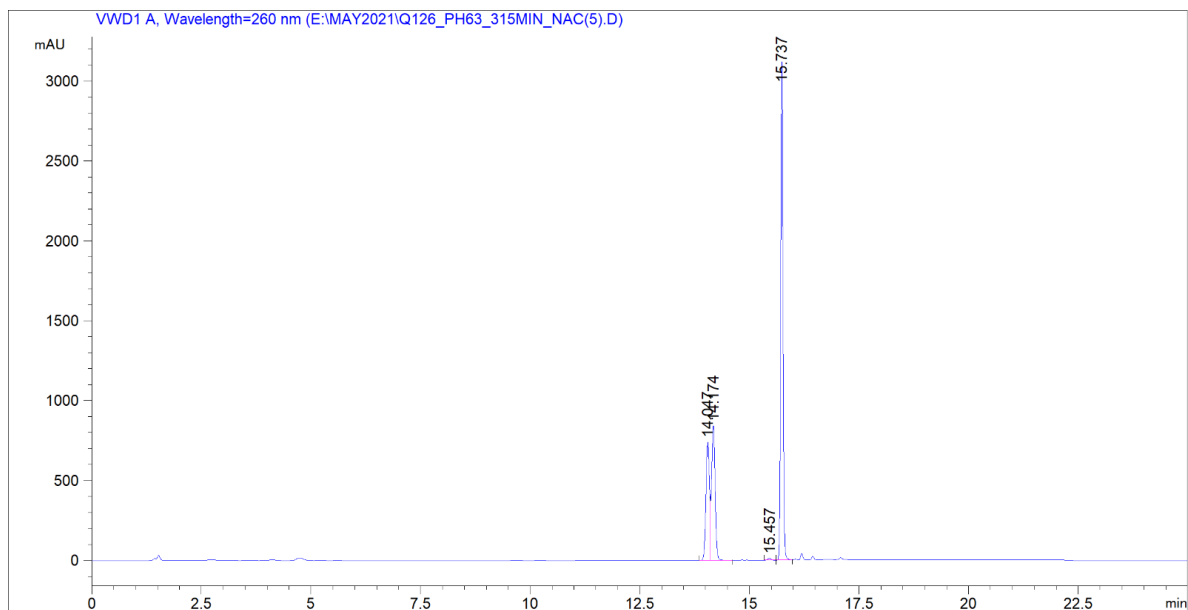
**Figure S20.** HPLC-UV-Vis chromatogram of pH 3.2/3.7 incubation (315-minute timepoint) of chalcone **1** and NAC.



**Figure S21.** HPLC-UV-Vis chromatogram of pH 8.0/8.5 incubation (315-minute timepoint) of chalcone **2** and NAC.



**Figure S22.** HPLC-UV-Vis chromatogram of pH 6.3/6.8 incubation (315-minute timepoint) of chalcone **2** and NAC.



**Figure S23.** HPLC-UV-Vis chromatogram of pH 3.2/3.7 incubation (315-minute timepoint) of chalcone **2** and NAC..

