

4c #2095 RT: 9.34 AV: 1 SB: 113 7.00-8.00 NL: 4.35E9
T: FTMS + c ESI Full ms [70.0000-700.0000]

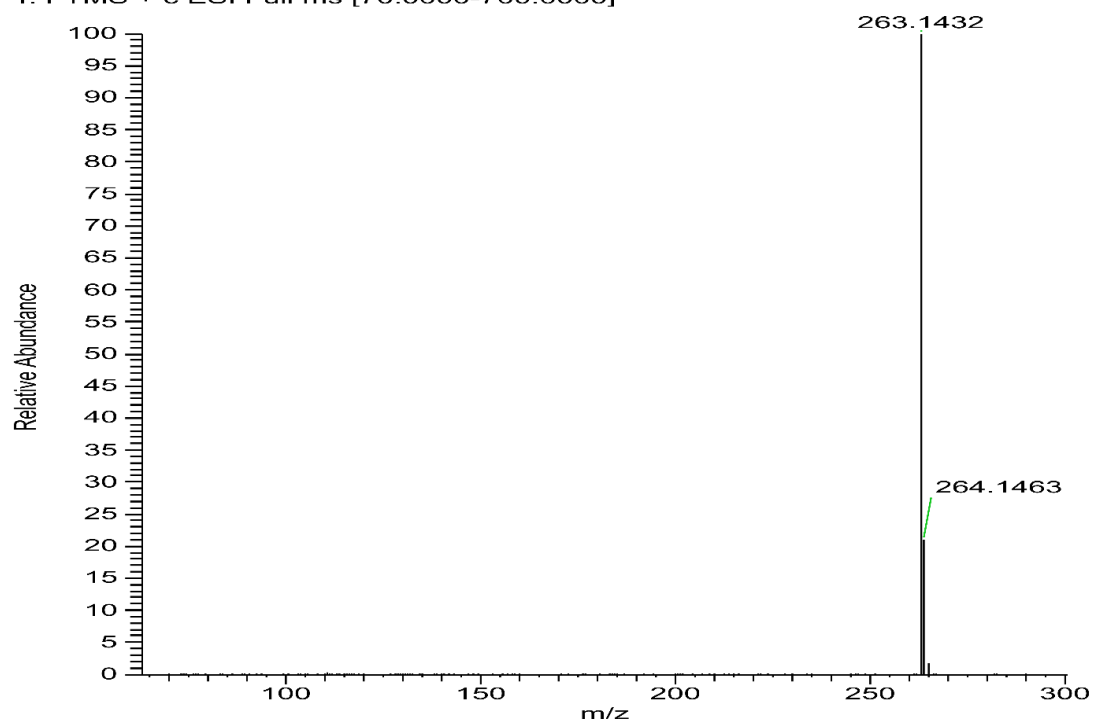


Figure S1. High-resolution, positive-mode HESI MS spectrum of **IIb**.

4d #1929 RT: 8.60 AV: 1 SB: 113 7.00-8.00 NL: 2.31E9
T: FTMS + c ESI Full ms [70.0000-700.0000]

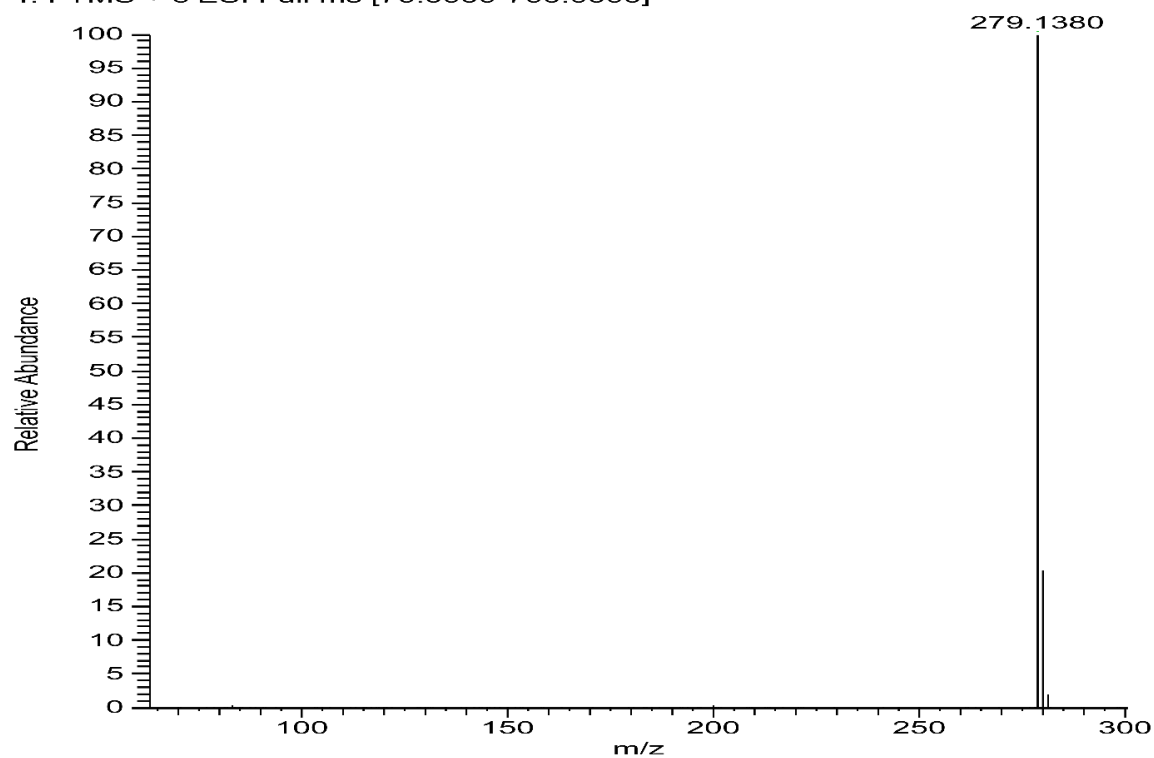


Figure S2. High-resolution, positive-mode HESI MS spectrum of **IIc**.

k5 #1467 RT: 11.14 AV: 1 SB: 67 9.00-10.00 NL: 7.86E7
T: FTMS + c ESI Full ms [70.0000-1000.0000]

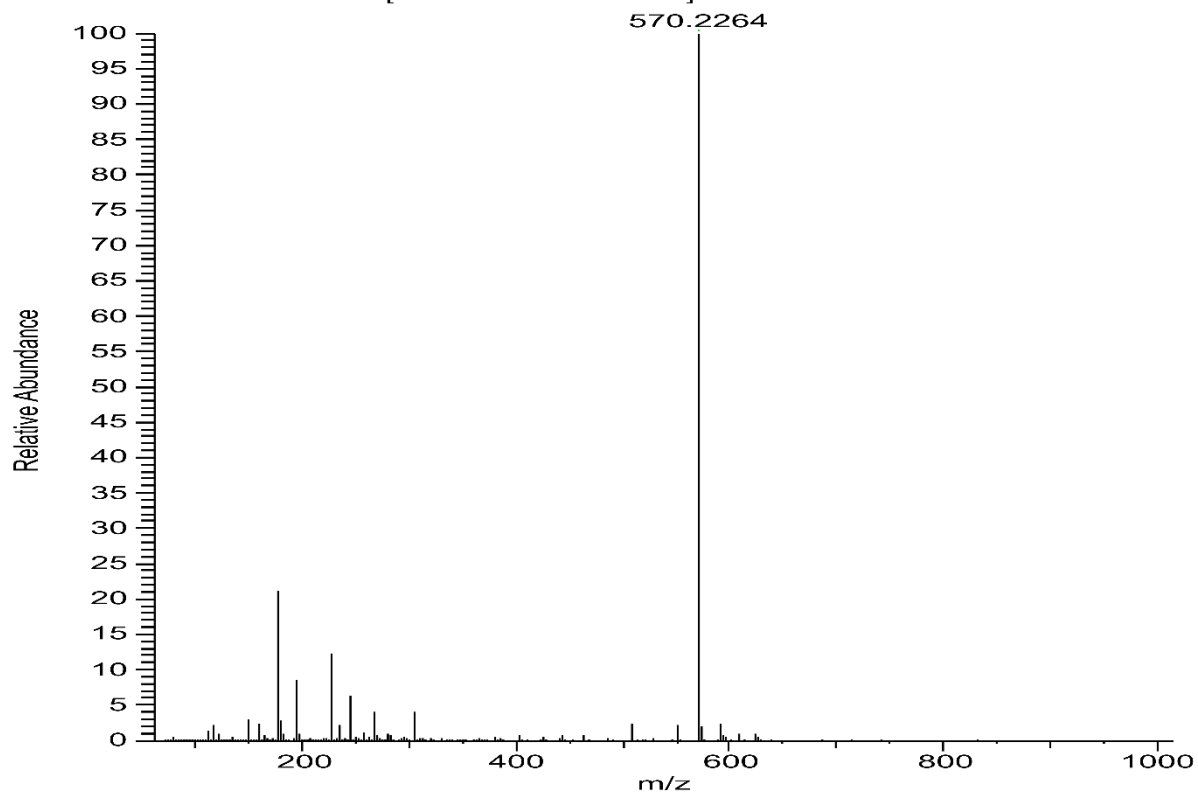


Figure S3. High-resolution, positive-mode HESI MS spectrum of **IIb-GSH** conjugate.

i4 #1562 RT: 12.44 AV: 1 SB: 66 11.00-12.00 NL: 1.13E8
T: FTMS - c ESI Full ms [100.0000-1000.0000]

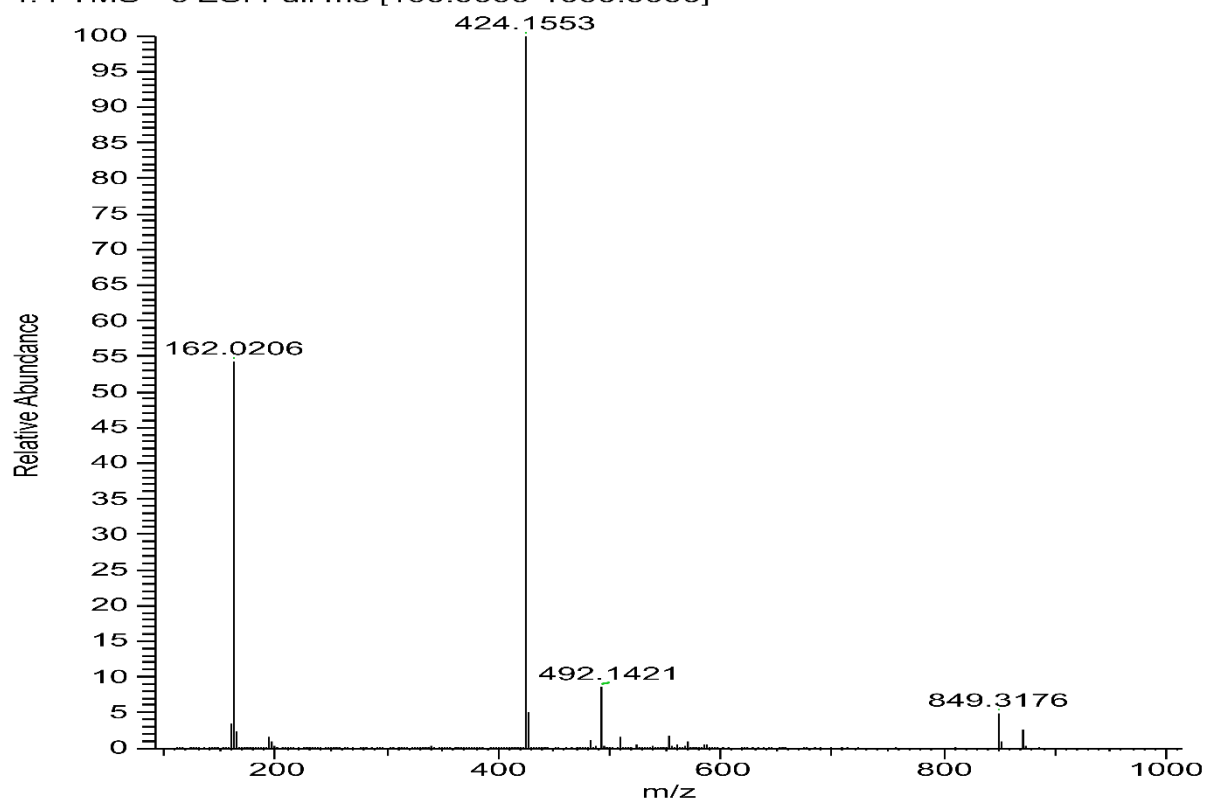


Figure S4. High-resolution, negative-mode HESI MS spectrum of **IIb**-NAC conjugate.

k4 #1435 RT: 10.89 AV: 1 SB: 66 9.00-10.00 NL: 5.23E7
T: FTMS + c ESI Full ms [70.0000-1000.0000]

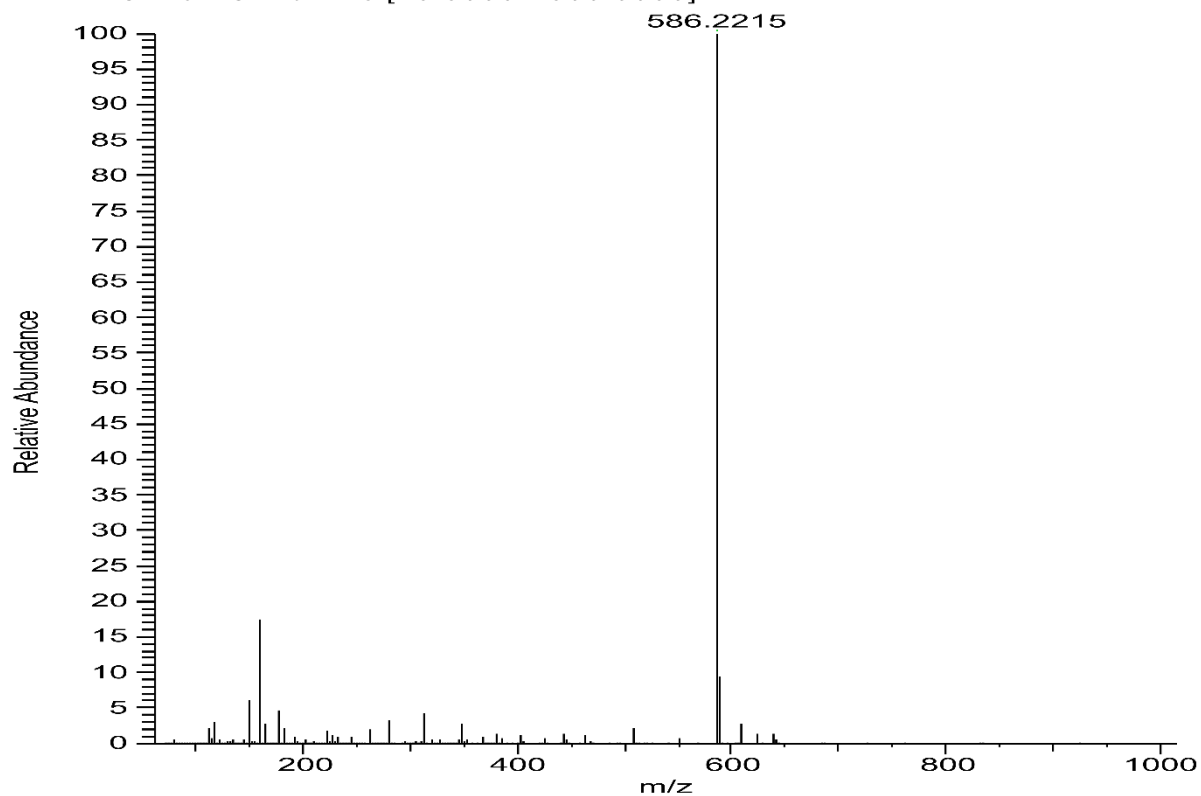


Figure S5. High-resolution, positive-mode HESI MS spectrum of **IIc**-GSH conjugate.

i7 #1472 RT: 11.75 AV: 1 SB: 66 10.00-11.00 NL: 1.33E8
T: FTMS - c ESI Full ms [100.0000-1000.0000]

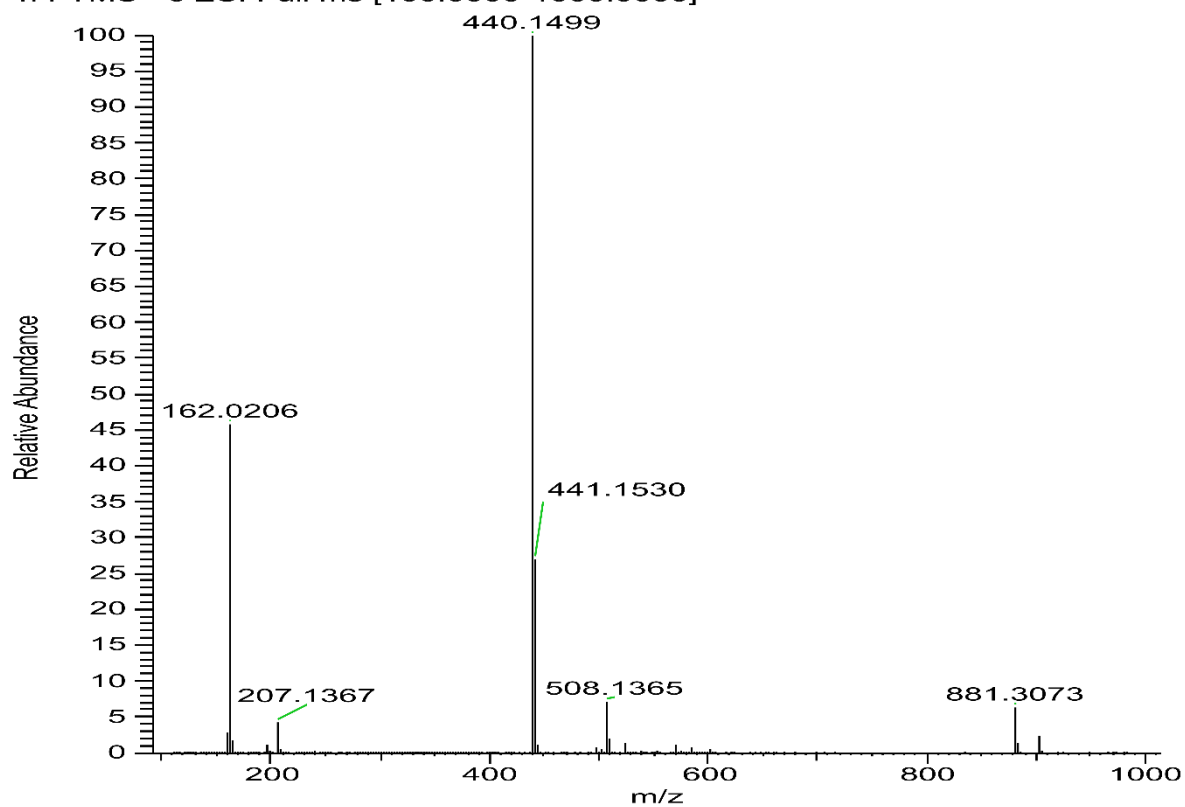


Figure S6. High-resolution, negative-mode HESI MS spectrum of **IIc**-NAC conjugate.

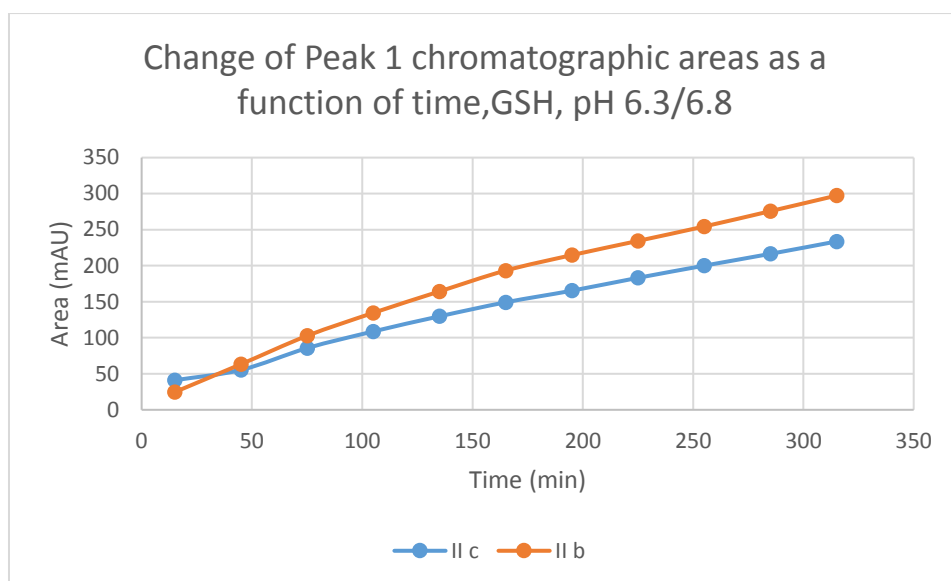


Figure S7. Change in the chromatographic peak area of adduct 1 of **II b** and **II c** in the chalcone–GSH incubations at pH 6.3/6.8.

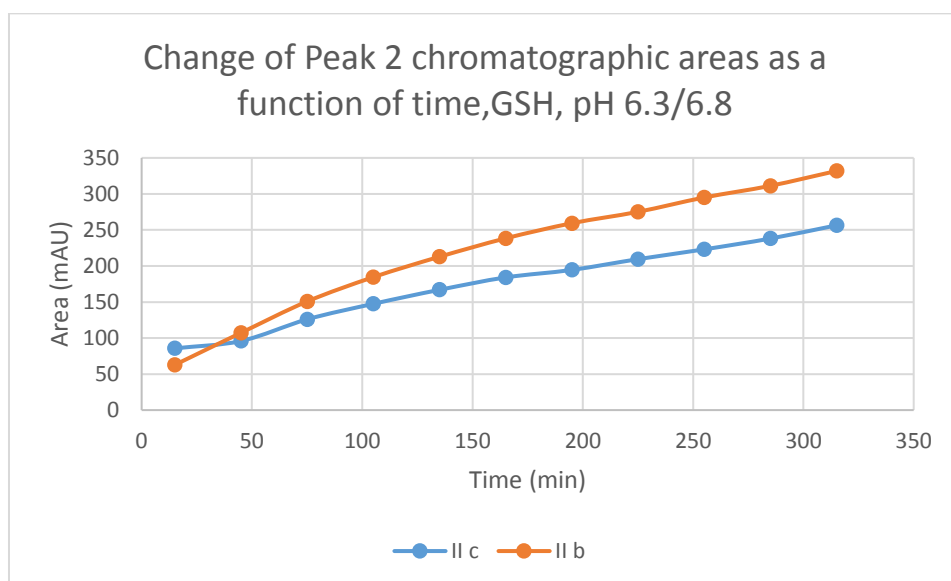


Figure S8. Change in the chromatographic peak area of adduct 2 of **IIb** and **IIc** in the chalcone–GSH incubations at pH 6.3/6.8.

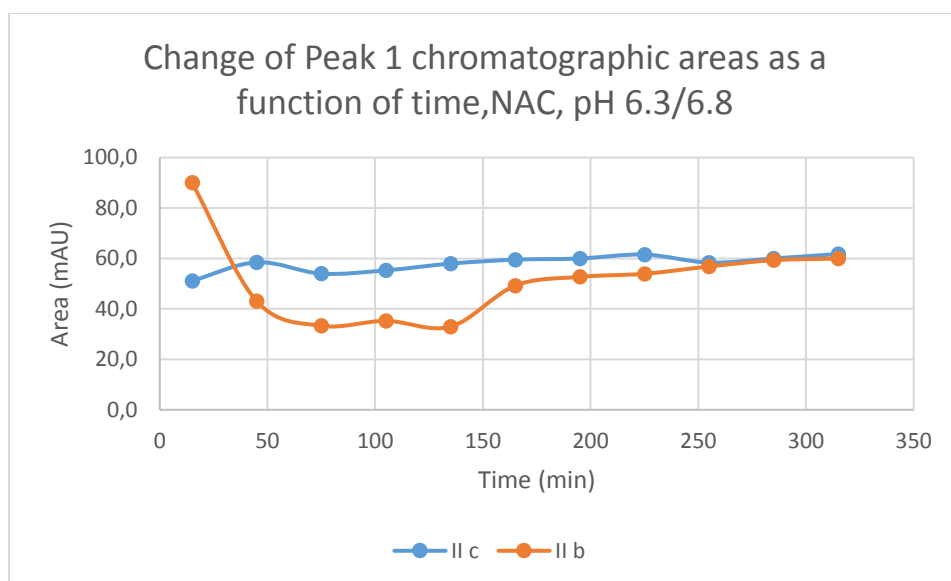


Figure S9. Change in the chromatographic peak area of adduct 1 of **IIb** and **IIc** in the chalcone–NAC incubations at pH 6.3/6.8.

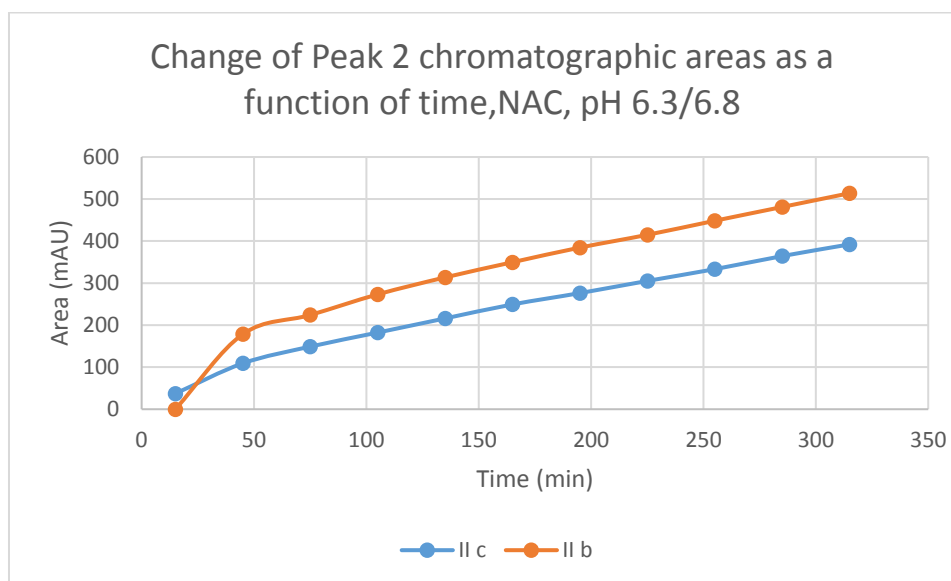


Figure S10. Change in the chromatographic peak area of adduct 2 of **IIb** and **IIc** in the chalcone–NAC incubations at pH 6.3/6.8.

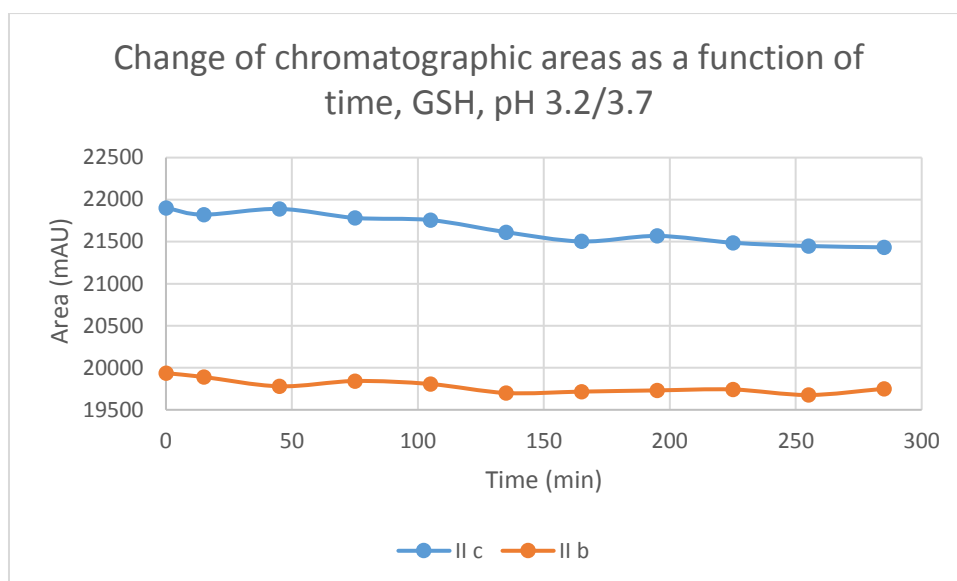


Figure S11. Change in the chromatographic peak area of **IIb** and **IIc** in the chalcone–GSH incubations at pH 3.2/3.7.

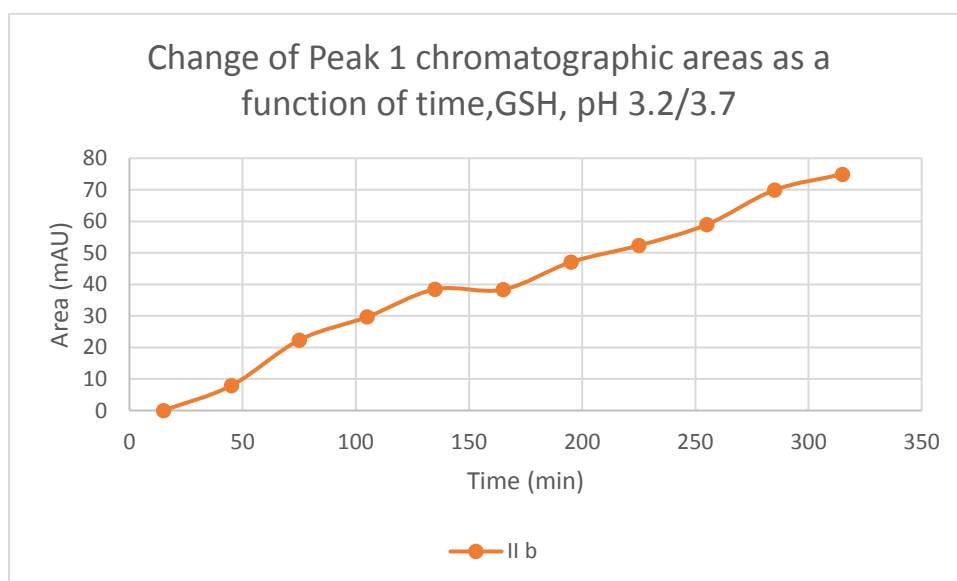


Figure S12. Change in the chromatographic peak area of adduct 1 of **IIb** in the chalcone–GSH incubations at pH 3.2/3.7.

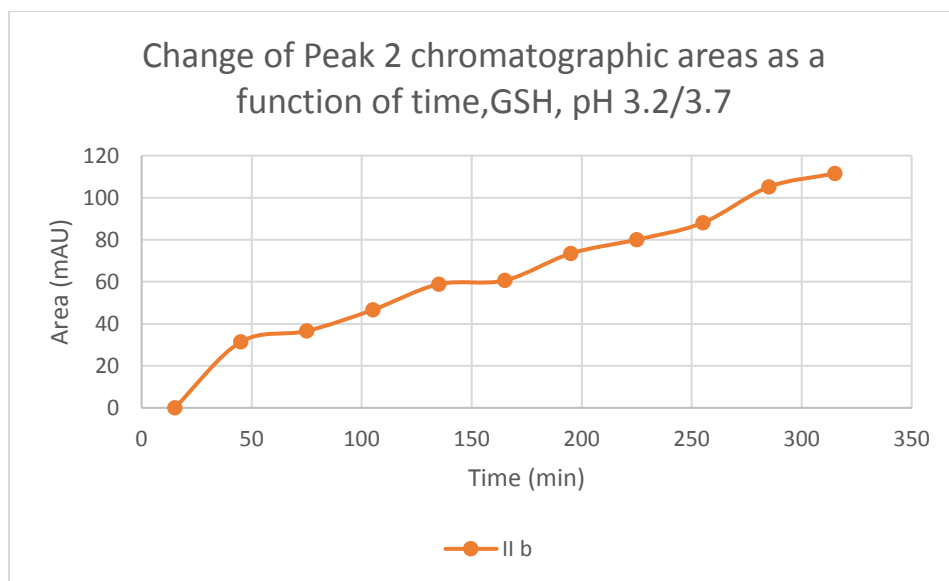


Figure S13. Change in the chromatographic peak area of adduct 2 of **IIb** in the chalcone–GSH incubations at pH 3.2/3.7.

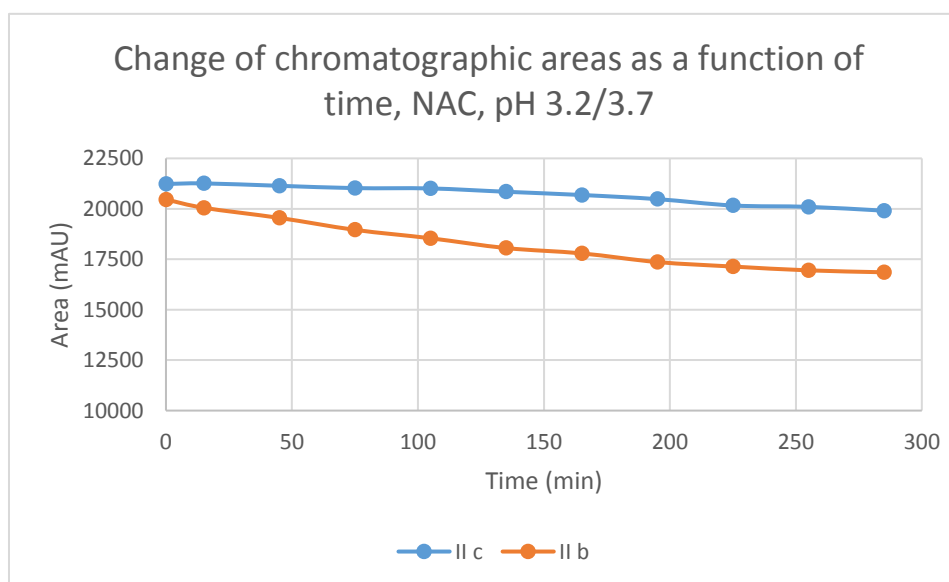


Figure S14. Change in the chromatographic peak area of **IIb** and **IIc** in the chalcone–NAC incubations at pH 3.2/3.7.

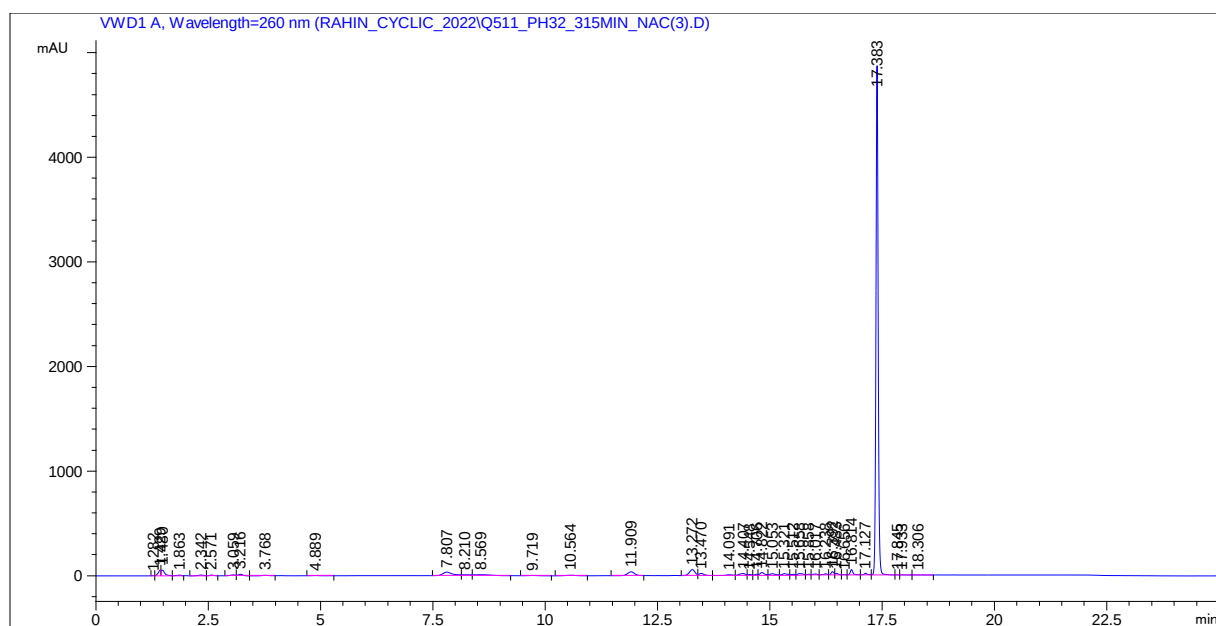


Figure S15. HPLC-UV chromatogram of pH 3.2/3.7 incubation (315 min time point) of **IIb** and NAC.

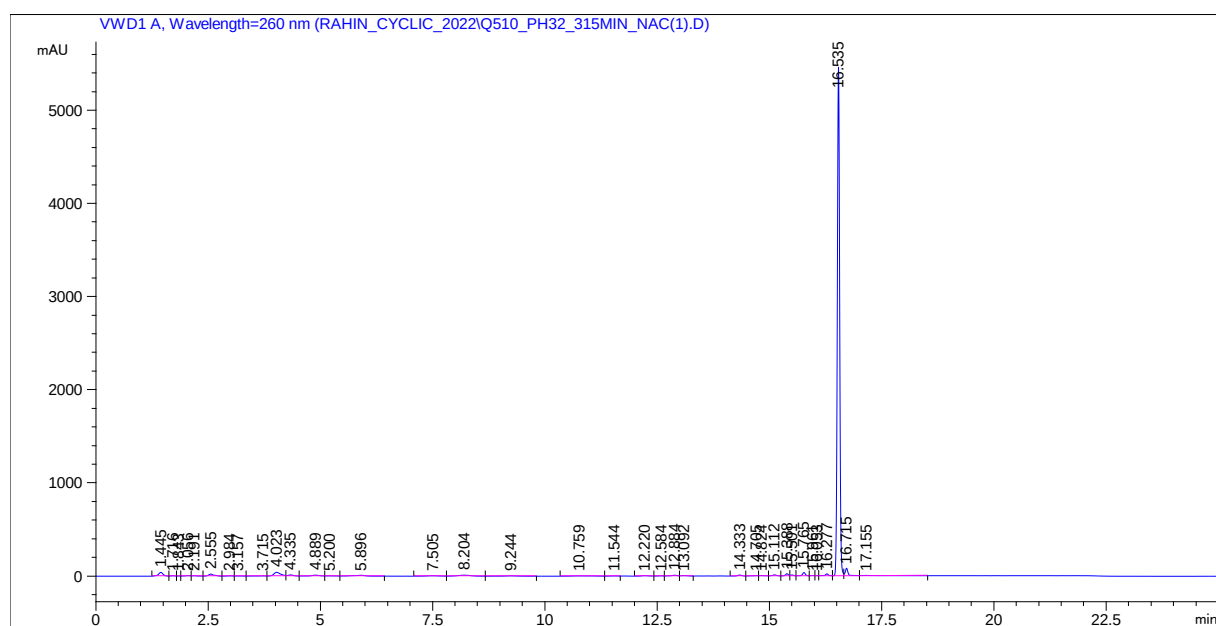


Figure S16. HPLC-UV chromatogram of pH 3.2/3.7 incubation (315 min time point) of **IIc** and NAC.

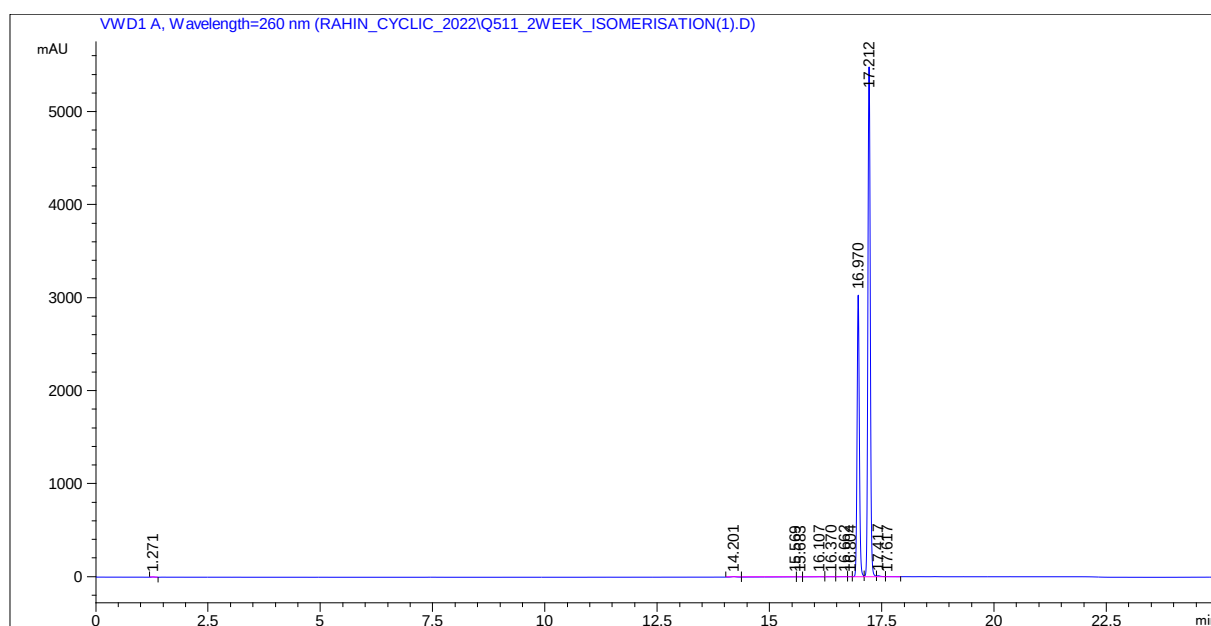


Figure S17. HPLC-UV spectrum of (*E*)(t_R 17.21 min)/(*Z*)(t_R 16.97 min) isomeric mixture of **I**ib****.

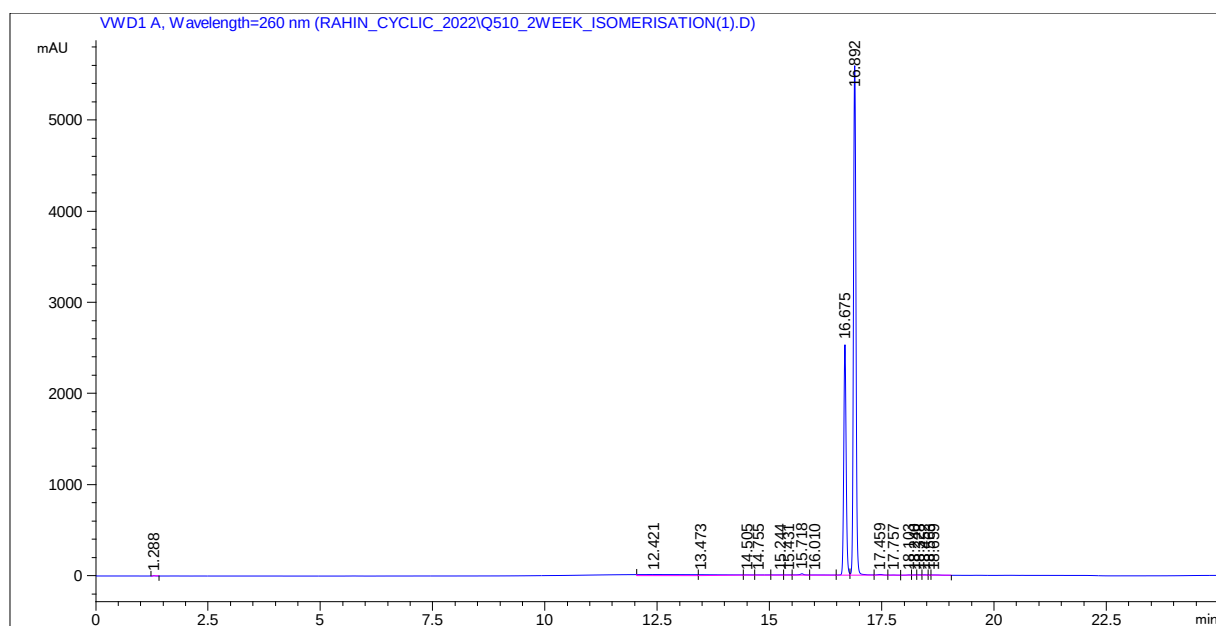


Figure S18. HPLC-UV-VIS spectrum of (*E*)(t_R 16.89 min)/(*Z*)(t_R 16.675 min) isomeric mixture of **IIc**.