**Supplementary Material for:**

# Synthesis and Inhibition Activity Study of Triazinyl-Substituted Amino(alkyl)-Benzenesulfonamide Conjugates with Polar and Hydrophobic Amino Acids as Inhibitors of Human Carbonic Anhydrases I, II, IV, IX, and XII

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**S1.** 2,2′-[(6-({4-sulfamoylbenzyl}amino)-1,3,5-triazine-2,4-diyl)diimino]dipropanoic acid **11** and its IR (a), $^{1}H$ (b), $^{13}C$ (c) NMR and LC-DAD/MS (d) spectra

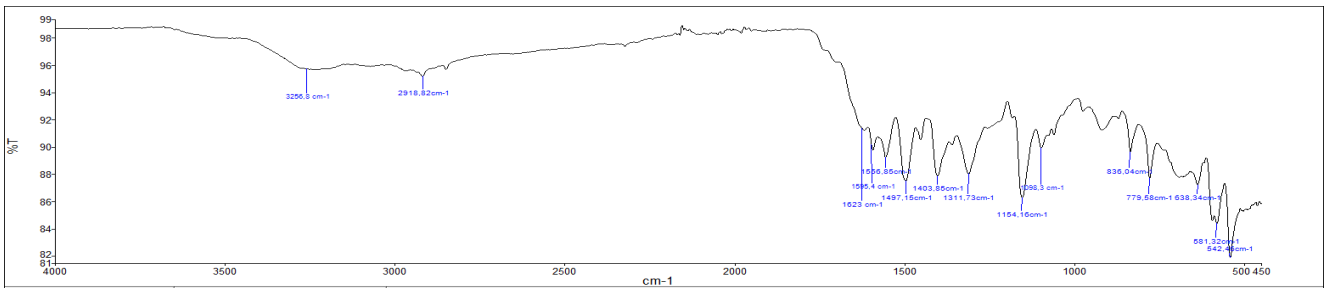


**Figure S1a**. IR spectra of product **11.**

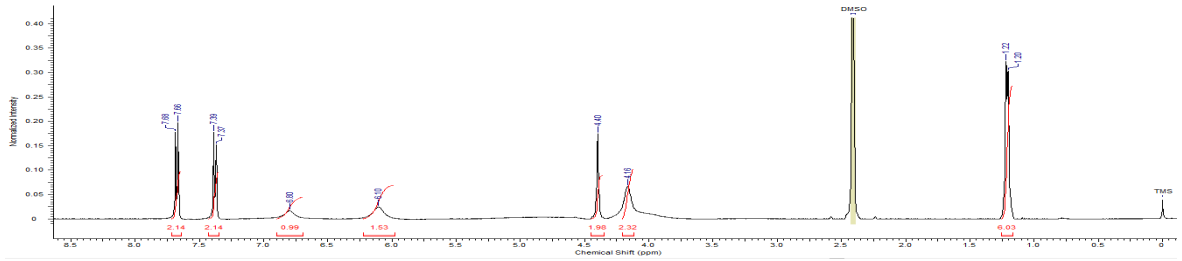


**Figure S1b**. $^{1}H$ NMR spectra of product **11.**

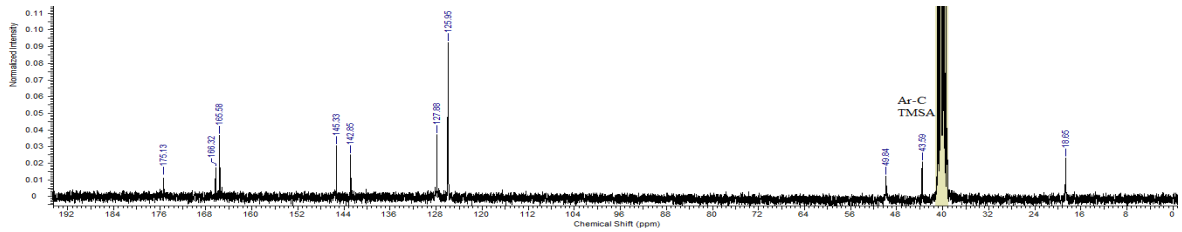


**Figure S1c.** $^{13}C$ NMR spectra of product **11.**

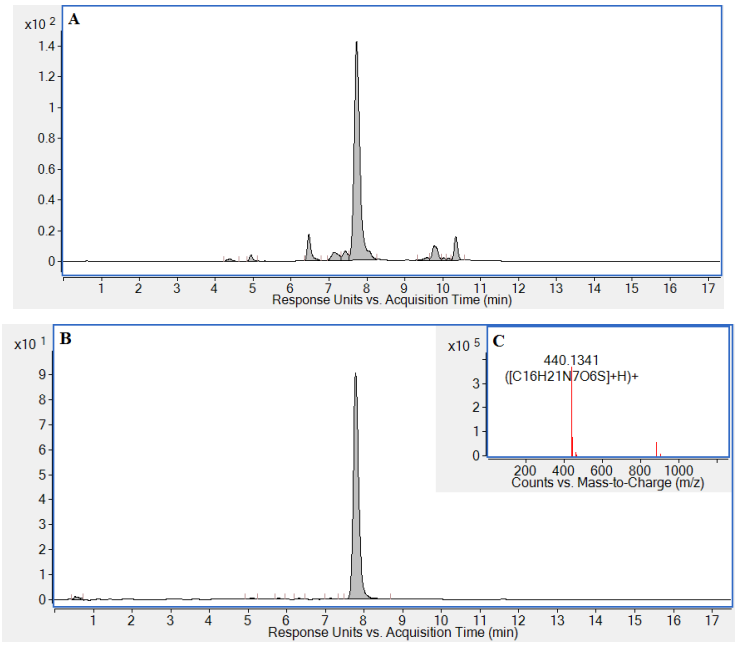


**Figure S1d**. HILIC-DAD-QTOF analysis of product **11**. Purity profile (HILIC-DAD - 254 nm) before (panel A) and after (panel B) semi-preparative chromatography. Panel C – MS spectrum of the desired compound (the major peak from UV chromatogram).

**S2.** 2,2′-[(6-({4-sulfamoylbenzyl}amino)-1,3,5-triazine-2,4-diyl)diimino]bis(3-(4-hydroxyphenyl)propanoic acid) **12** and its IR (a), $^{1}H$ (b), $^{13}C$ (c) NMR and DAD/MS (d) spectra

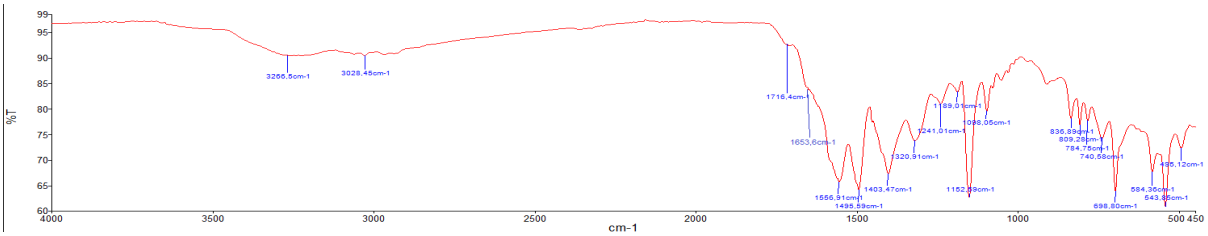


**Figure S2a.** IR spectra of product **12.**

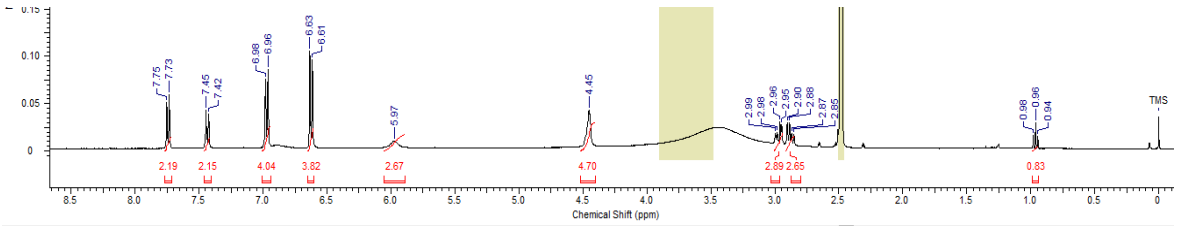


**Figure S2b**. $^{1}H$ NMR spectra of product **12.**

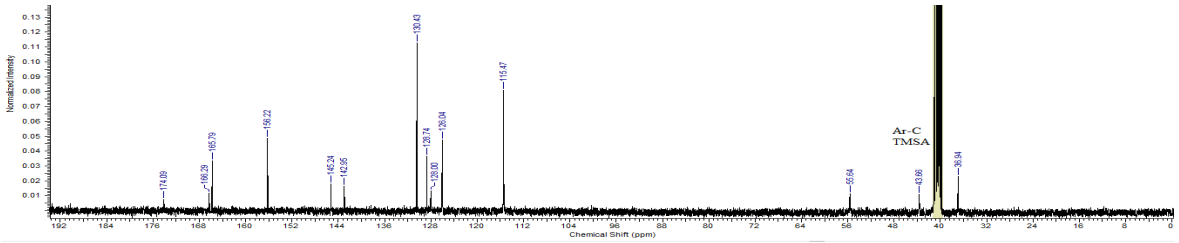


**Figure S2c**. $^{13}C$ NMR spectra of product **12.**

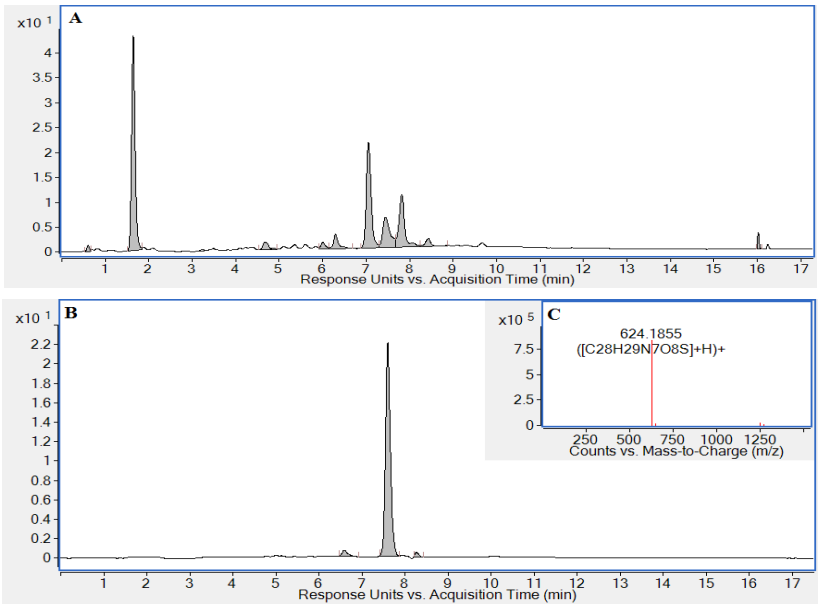


**Figure S2d**. HILIC-DAD-QTOF analysis of product **12**. Purity profile (HILIC-DAD - 254 nm) before (panel A) and after (panel B) semi-preparative chromatography. Panel C – MS spectrum of the desired compound (the major peak from UV chromatogram).

**S3.** 2,2′-[(6-({4-sulfamoylbenzyl}amino)-1,3,5-triazine-2,4-diyl)diimino]bis(3-(*1H*-indol-3-yl)propanoic acid) **13** and its IR (a), $^{1}H$ (b), $^{13}C$ (c) NMR and DAD/MS (d) spectra

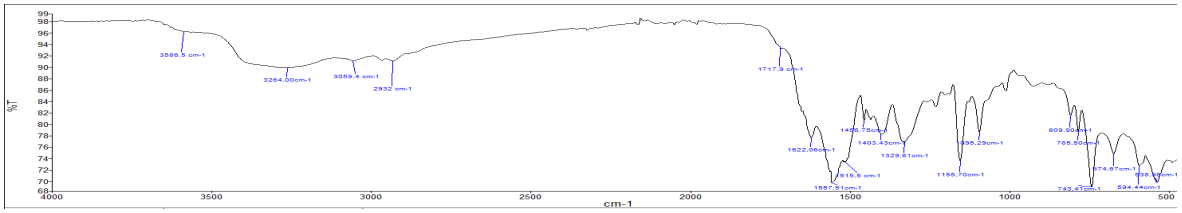


**Figure S3a**. IR spectra of product **13.**

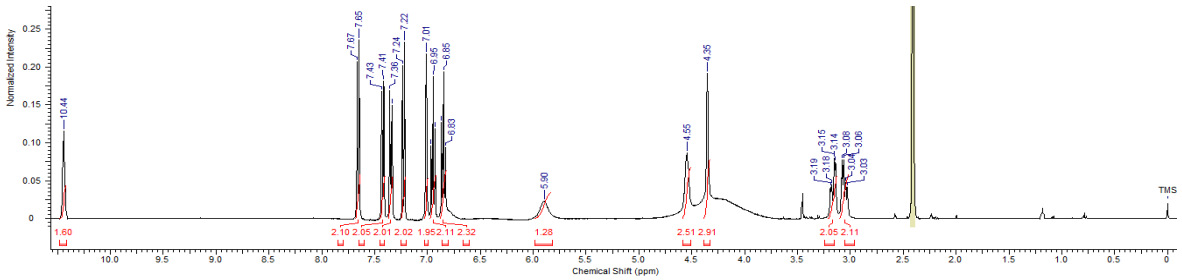


**Figure S3b**. $^{1}H$ NMR spectra of product **13.**

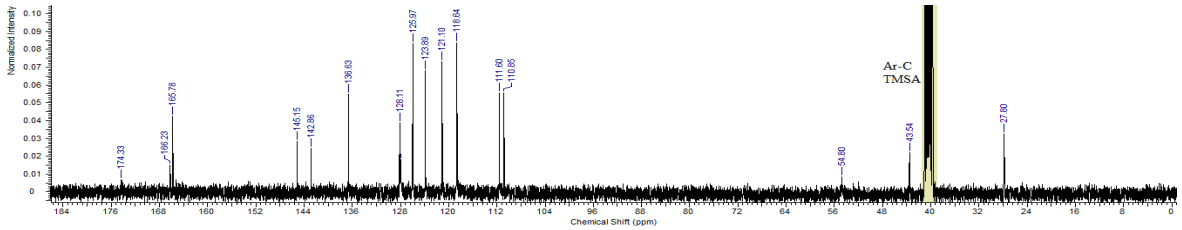


**Figure S3c**. $^{13}C$ NMR spectra of product **13.**

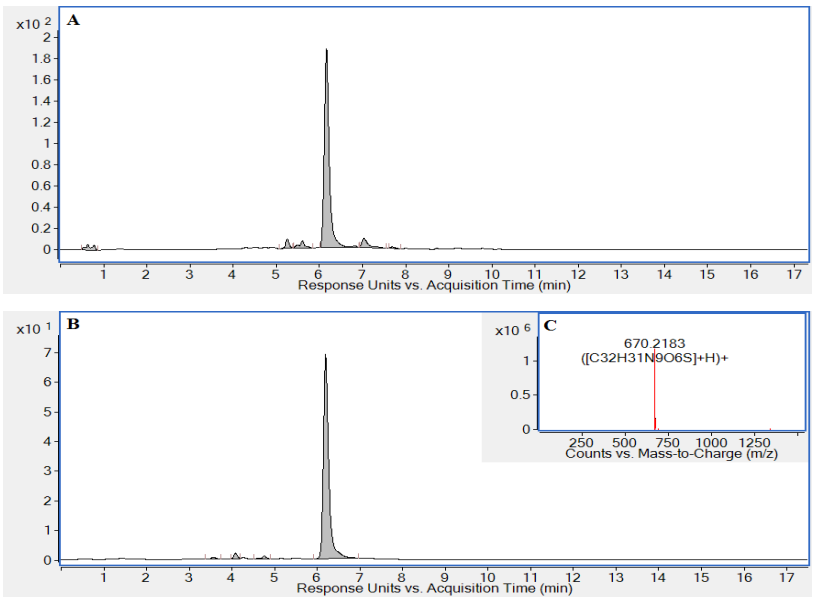


**Figure S3d**. HILIC-DAD-QTOF analysis of product **13**. Purity profile (HILIC-DAD - 254 nm) before (panel A) and after (panel B) semi-preparative chromatography. Panel C – MS spectrum of the desired compound (the major peak from UV chromatogram).

**S4**. 2,2′-[(6-({4-sulfamoylbenzyl}amino)-1,3,5-triazine-2,4-diyl)diimino]bis(3-hydroxypropanoic acid) **14** and its IR (a), $^{1}H$ (b), $^{13}C$ (c) NMR and DAD/MS (d) spectra

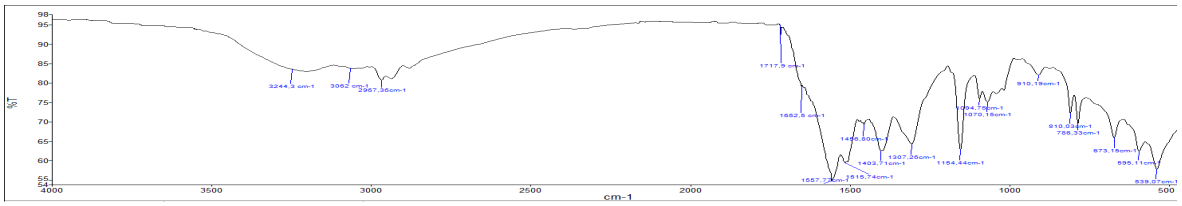


**Figure S4a.** IR spectra of product **14.**

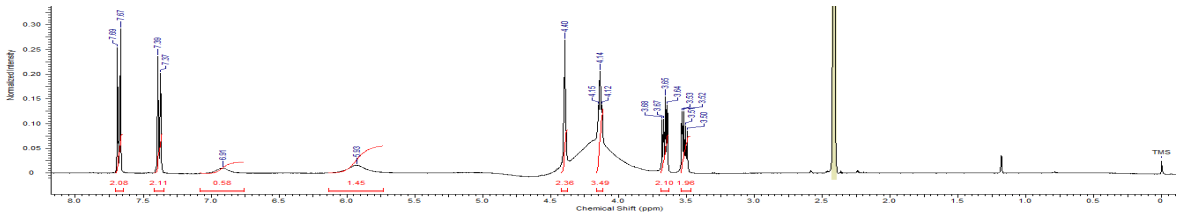


**Figure S4b**. $^{1}H$ NMR spectra of product **14.**

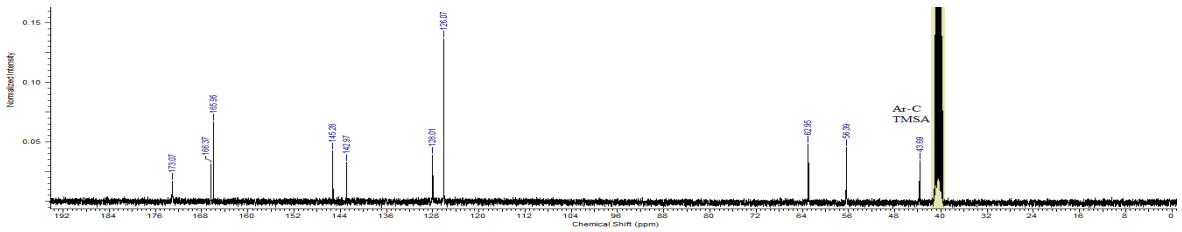


**Figure S4c**. $^{13}C$ NMR spectra of product **14.**

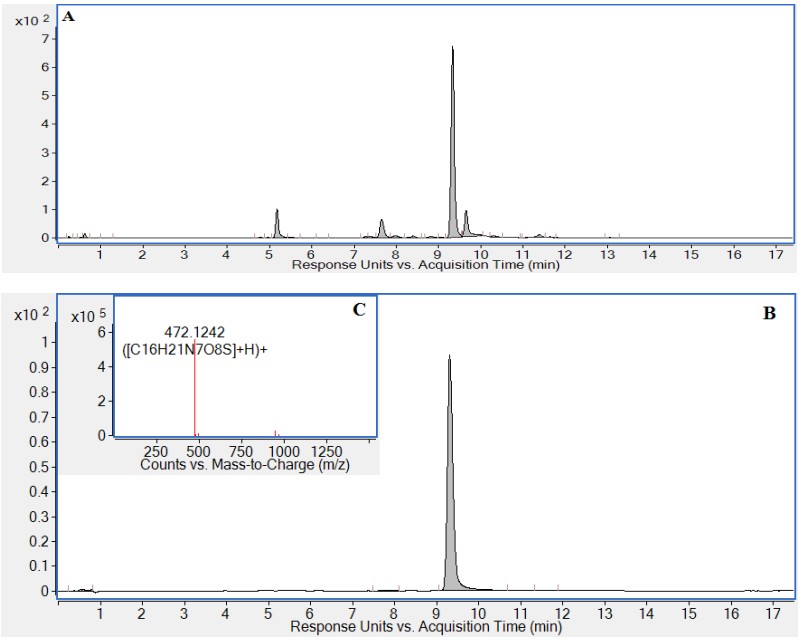


**Figure S4d**. HILIC-DAD-QTOF analysis of product **14**. Purity profile (HILIC-DAD - 254 nm) before (panel A) and after (panel B) semi-preparative chromatography. Panel C – MS spectrum of the desired compound (the major peak from UV chromatogram).

**S5.** 2,2′-[(6-({4-sulfamoylbenzyl}amino)-1,3,5-triazine-2,4-diyl)diimino]bis(3-hydroxybutanoic acid) **15** and its IR (a), $^{1}H$ (b), $^{13}C$ (c) NMR and DAD/MS (d) spectra.

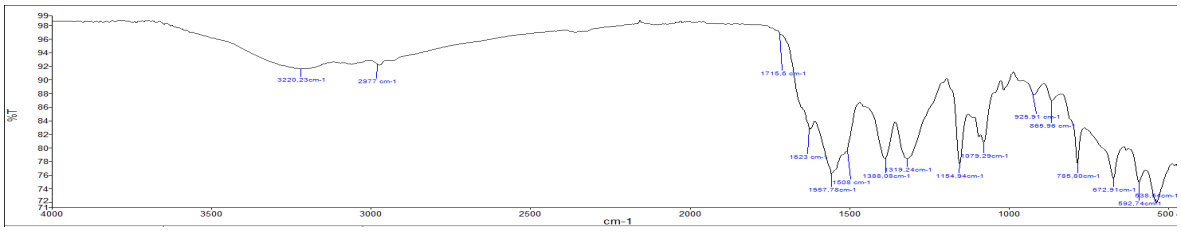


**Figure S5a**. IR spectra of product **15.**

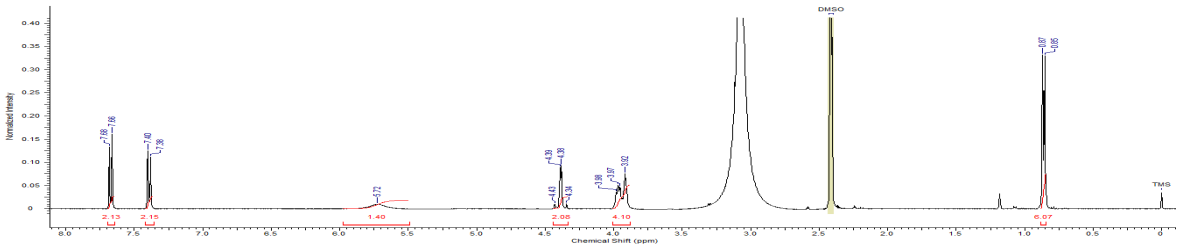


**Figure S5b**. $^{1}H$ NMR spectra of product **15.**

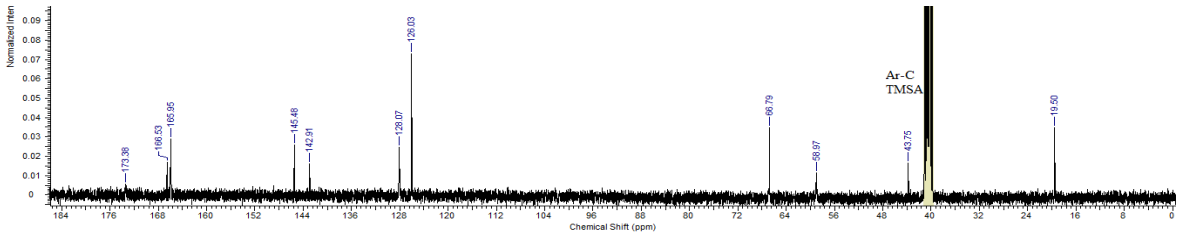


**Figure S5c**. $^{13}C$ NMR spectra of product **15.**

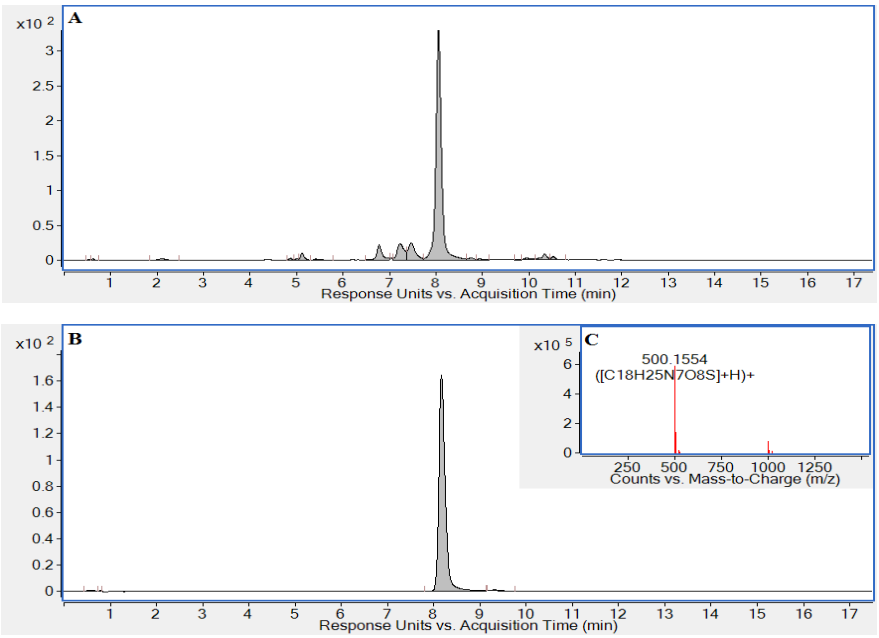


**Figure S5d**. HILIC-DAD-QTOF analysis of product **15**. Purity profile (HILIC-DAD - 254 nm) before (panel A) and after (panel B) semi-preparative chromatography. Panel C – MS spectrum of the desired compound (the major peak from UV chromatogram).

**S6.** 2,2´-[(6-({4-sulfamoylbenzyl}amino)-1,3,5-triazine-2,4-diyl)diimino]bis(3-carbamoylpropanoic acid) **16** and its IR (a), $^{1}H$ (b), $^{13}C$ (c) NMR and DAD/MS (d) spectra.

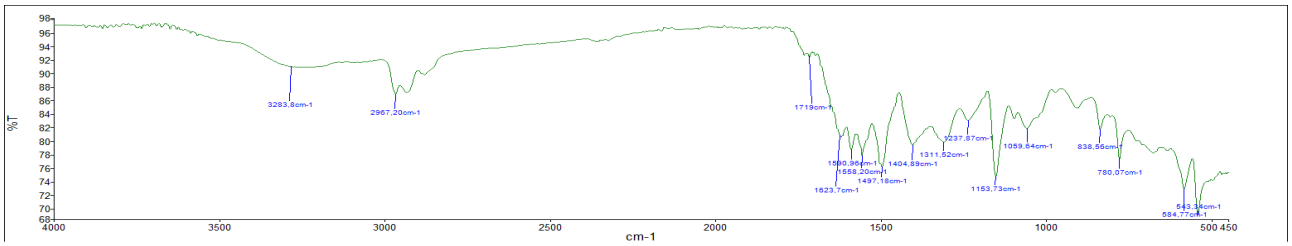


**Figure S6a.** IR spectra of product **16.**

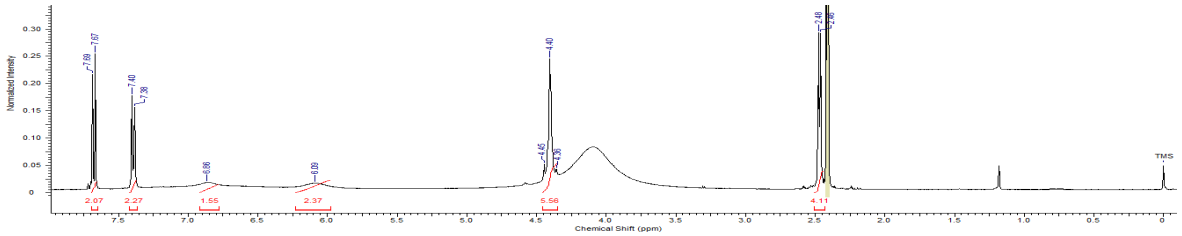


**Figure S6b.** $^{1}H$ NMR spectra of product **16.**

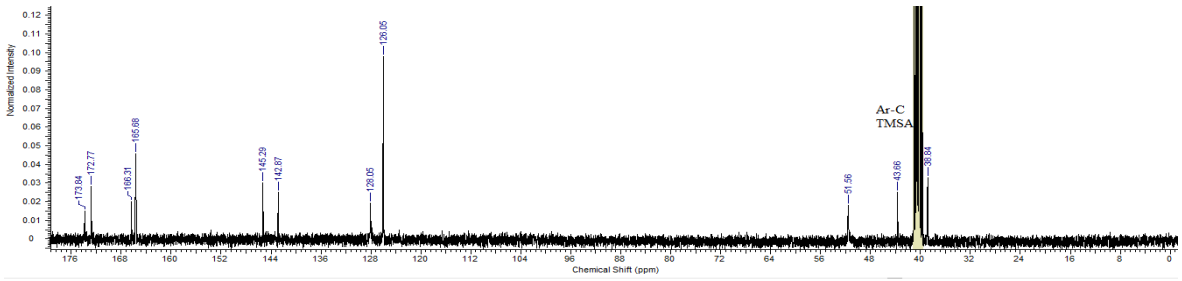


**Figure S6c**. $^{13}C$ NMR spectra of product **16.**

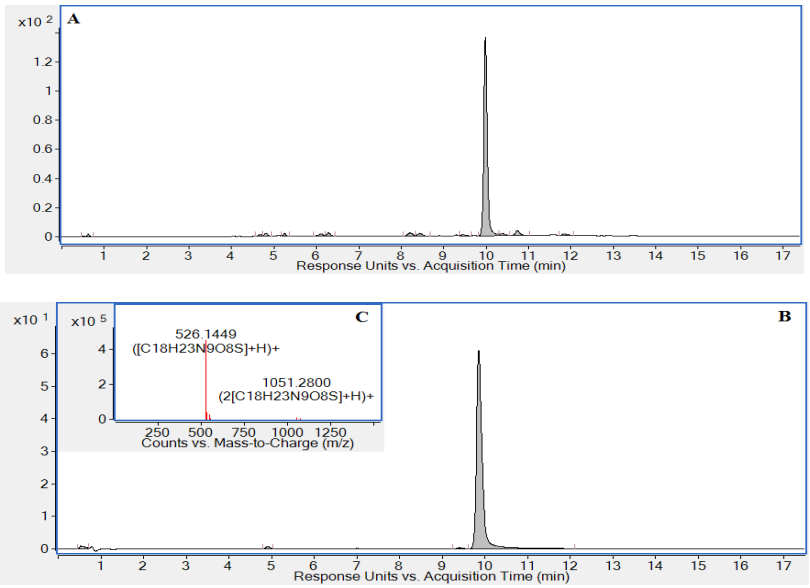


**Figure S6d**. HILIC-DAD-QTOF analysis of product **16**. Purity profile (HILIC-DAD - 254 nm) before (panel A) and after (panel B) semi-preparative chromatography. Panel C – MS spectrum of the desired compound (the major peak from UV chromatogram).

S7. 2,2′-[(6-({4-sulfamoylbenzyl}amino)-1,3,5-triazine-2,4-diyl)diimino]bis(4-carbamoylbutanoic acid) **17** and its IR (a), $^{1}H$ (b), $^{13}C$ (c) NMR and DAD/MS (d) spectra

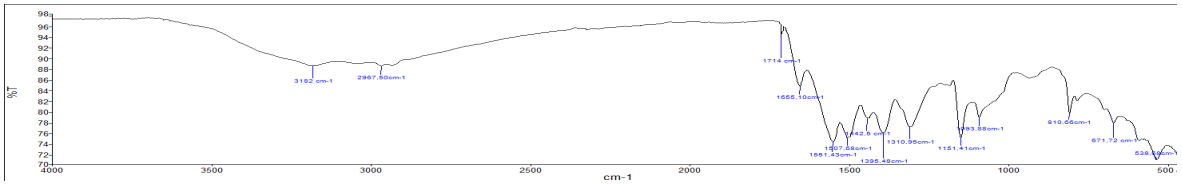


**Figure S7a**. IR spectra of product **17.**

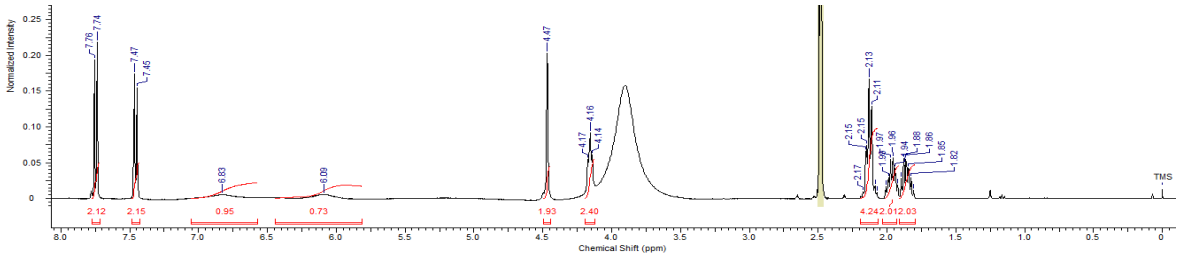


**Figure S7b**. $^{1}H$ NMR spectra of product **17.**

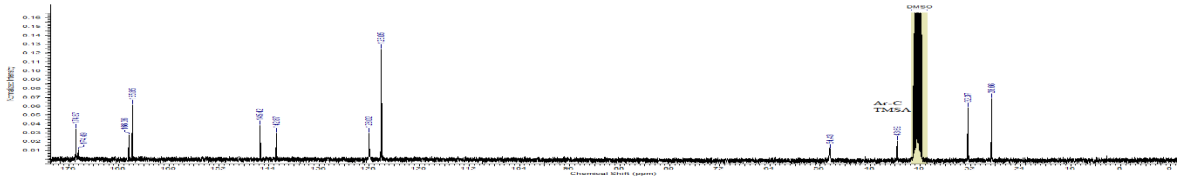


**Figure S7c**. $^{13}C$ NMR spectra of product **17.**

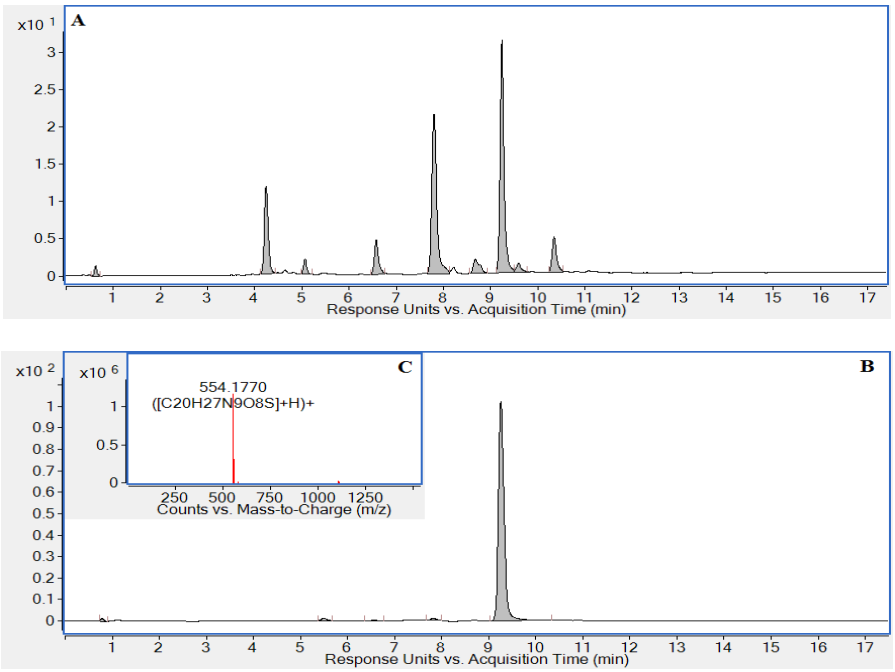


**Figure S7d**. HILIC-DAD-QTOF analysis of product **17**. Purity profile (HILIC-DAD - 254 nm) before (panel A) and after (panel B) semi-preparative chromatography. Panel C – MS spectrum of the desired compound (the major peak from UV chromatogram).

**S8**. 2,2′-[(6-({2-(4-sulfamoylphenyl)ethyl}amino)-1,3,5-triazine-2,4-diyl)diimino]dipropanoic acid **18** and its IR (a), $^{1}H$ (b), $^{13}C$ (c) NMR and DAD/MS (d) spectra

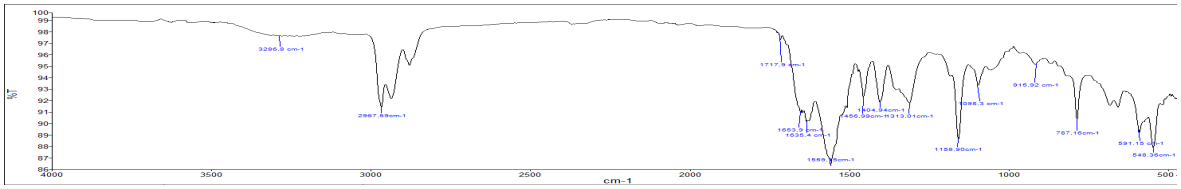

**Figure S8a**. IR spectra of product **18.**

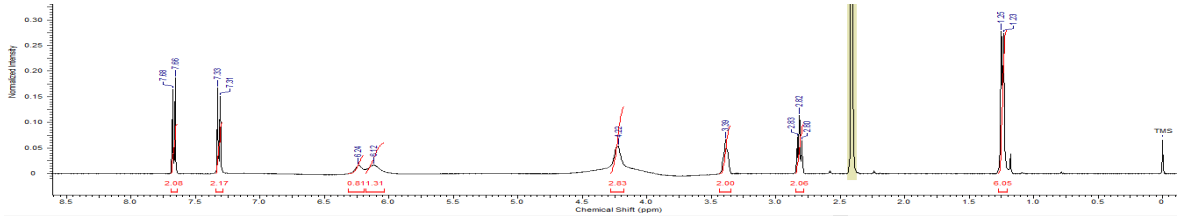

**Figure S8b**. $^{1}H$ NMR spectra of product **18.**

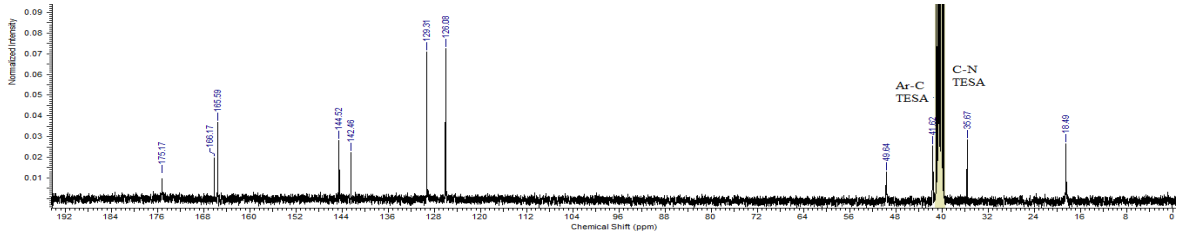


**Figure S8c**. $^{13}C$ NMR spectra of product **18.**

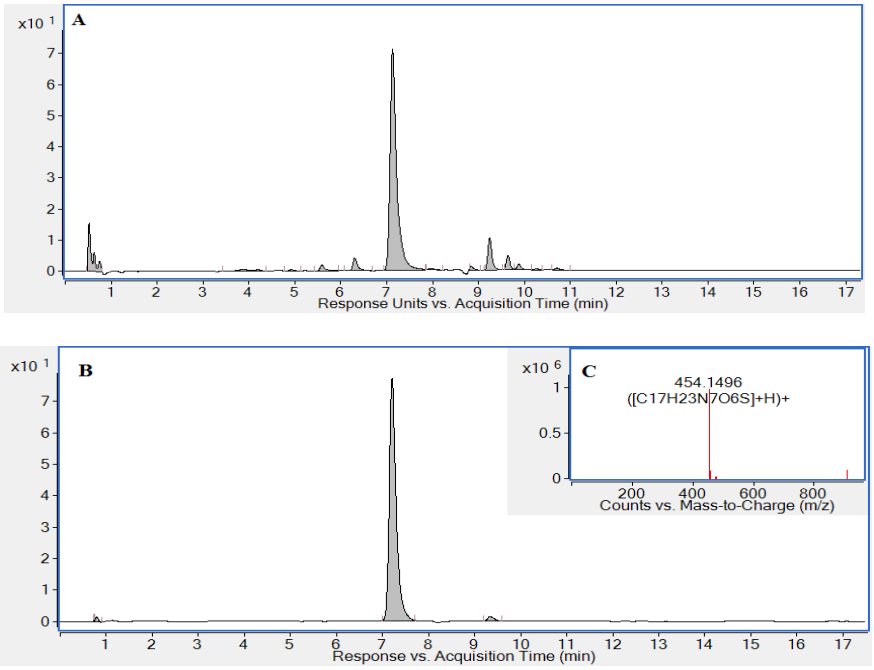


**Figure S8d**. HILIC-DAD-QTOF analysis of product **18**. Purity profile (HILIC-DAD - 254 nm) before (panel A) and after (panel B) semi-preparative chromatography. Panel C – MS spectrum of the desired compound (the major peak from UV chromatogram).

**S9**. 2,2′-[(6-({2-(4-sulfamoylphenyl)ethyl}amino)-1,3,5-triazine-2,4-diyl)diimino]bis(3-(4-hydroxyphenyl)propanoic acid) **19** and its IR (a), $^{1}H$ (b), $^{13}C$ (c) NMR and DAD/MS (d) spectra.

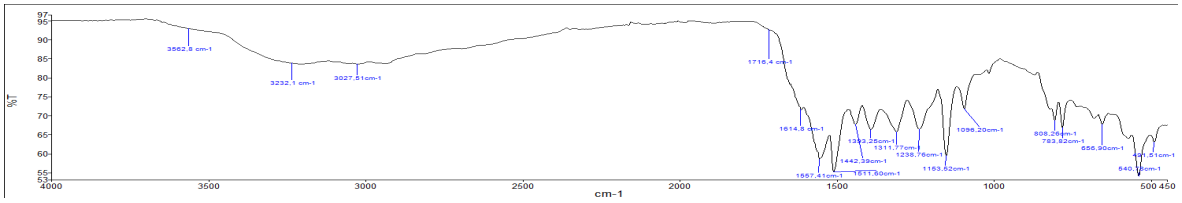


**Figure S9a.** IR spectra of product **19.**

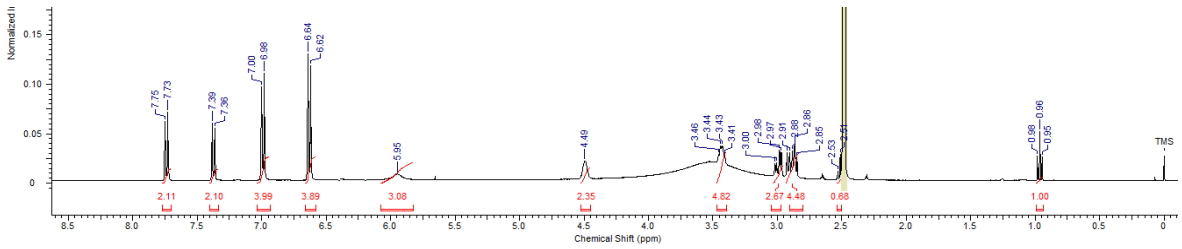


**Figure S9b**. $^{1}H$ NMR spectra of product **19.**

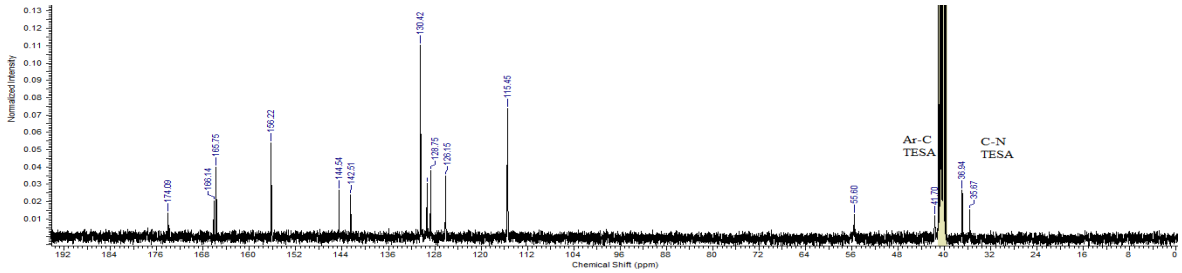


**Figure S9c**. $^{13}C$ NMR spectra of product **19.**

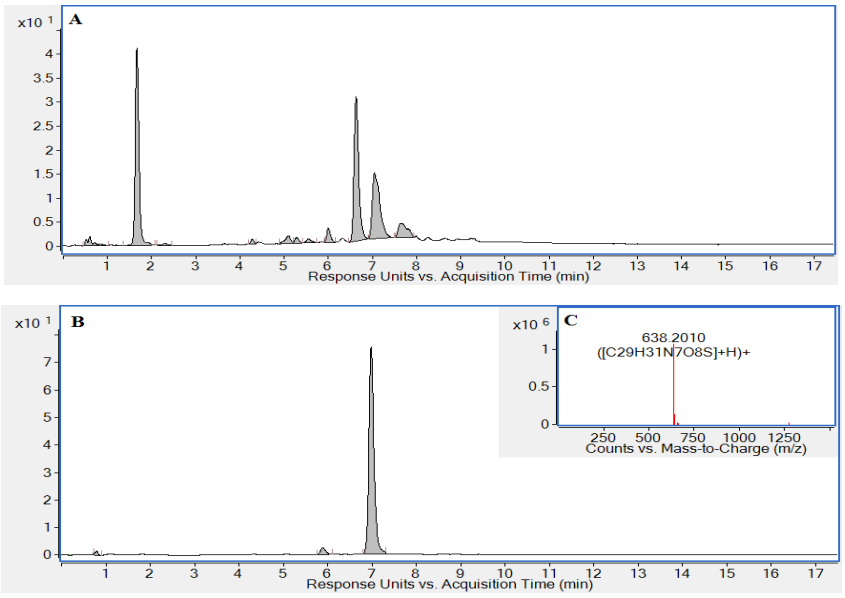


**Figure S9d**. HILIC-DAD-QTOF analysis of product **19**. Purity profile (HILIC-DAD - 254 nm) before (panel A) and after (panel B) semi-preparative chromatography. Panel C – MS spectrum of the desired compound (the major peak from UV chromatogram).

**S10.** 2,2′-[(6-({2-(4-sulfamoylphenyl)ethyl}amino)-1,3,5-triazine-2,4-diyl)diimino]bis(3-(*1H*-indol-3-yl)propanoic acid) **20** and its IR (a), $^{1}$H (b), $^{13}$C (c) NMR and DAD/MS (d) spectra

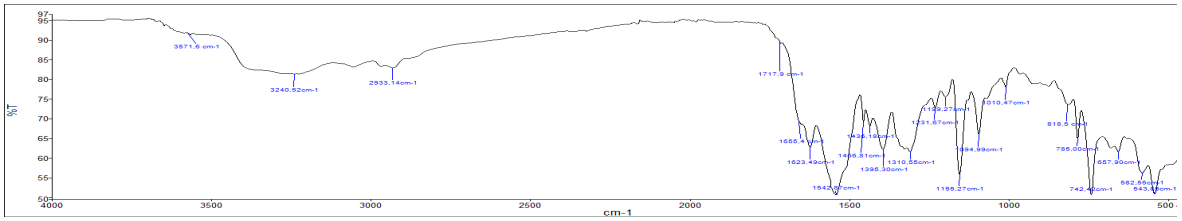


**Figure S10a**. IR spectra of product **20.**

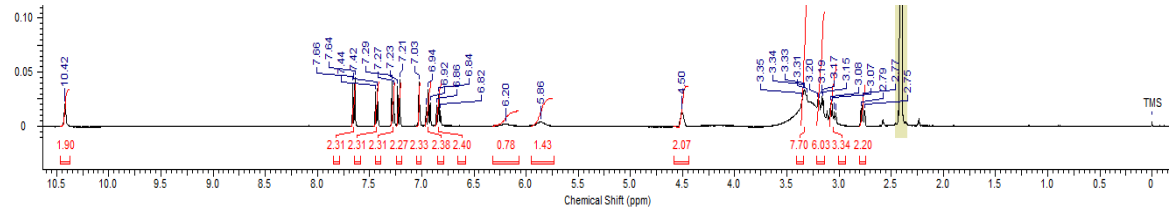


**Figure S10b**. $^{1}$H NMR spectra of product **20.**

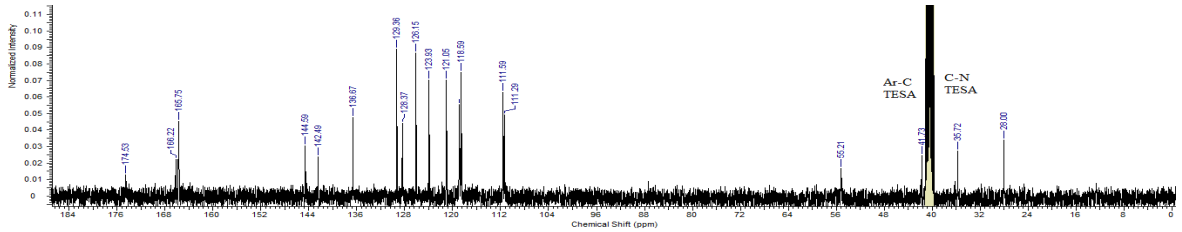


**Figure S10c**. $^{13}$C NMR spectra of product **20.**

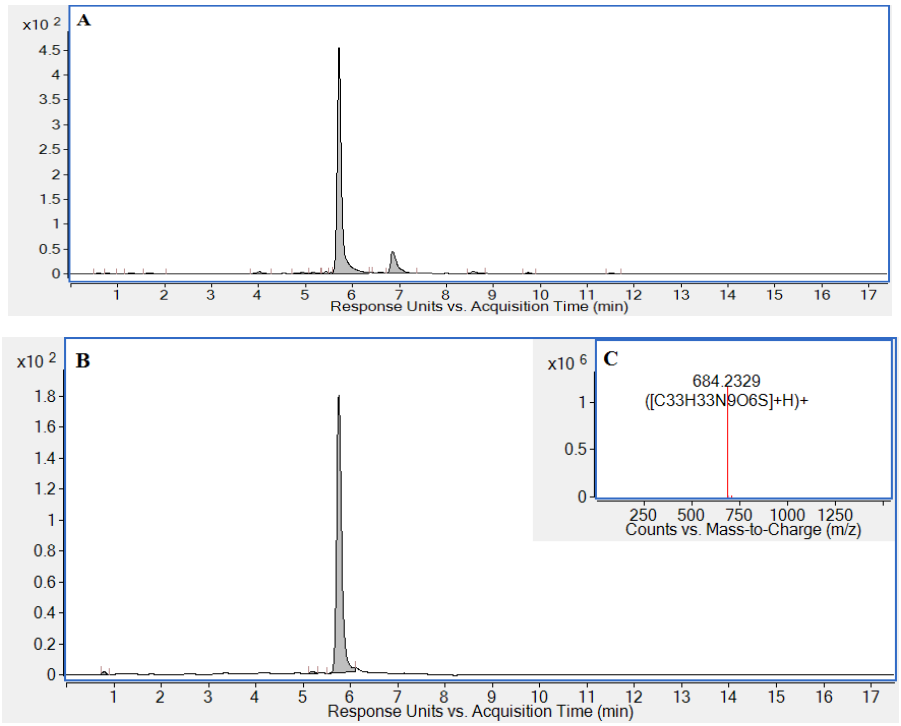


**Figure S10d**. HILIC-DAD-QTOF analysis of product **20**. Purity profile (HILIC-DAD - 254 nm) before (panel A) and after (panel B) semi-preparative chromatography. Panel C – MS spectrum of the desired compound (the major peak from UV chromatogram).

**S11**. 2,2′-[(6-({2-(4-sulfamoylphenyl)ethyl}amino)-1,3,5-triazine-2,4-diyl)diimino]bis(3-hydroxypropanoic acid) **21** and its IR (a), $^{1}H$ (b), $^{13}C$ (c) NMR and DAD/MS (d) spectra

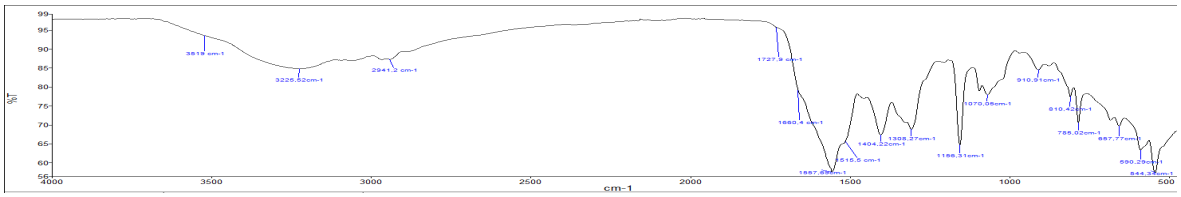


**Figure S11a**. IR spectra of product **21.**

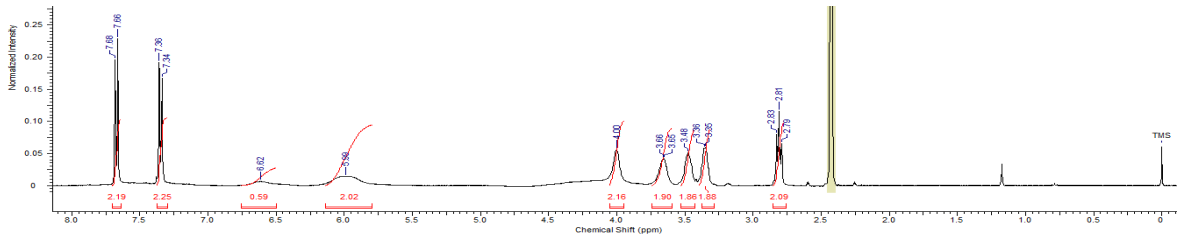


**Figure S11b**. $^{1}H$ NMR spectra of product **21.**

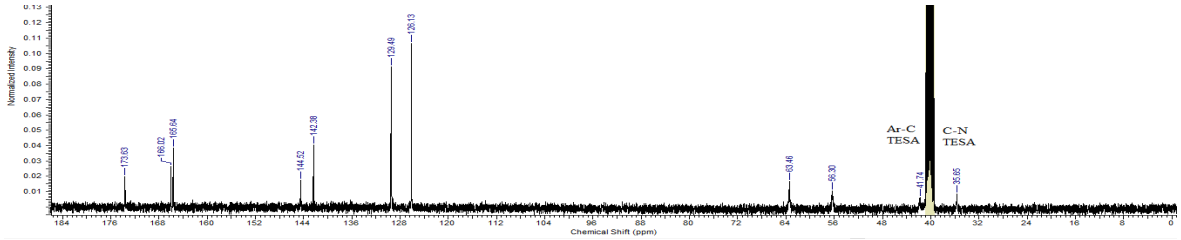


**Figure S11c**. $^{13}C$ NMR spectra of product **21.**

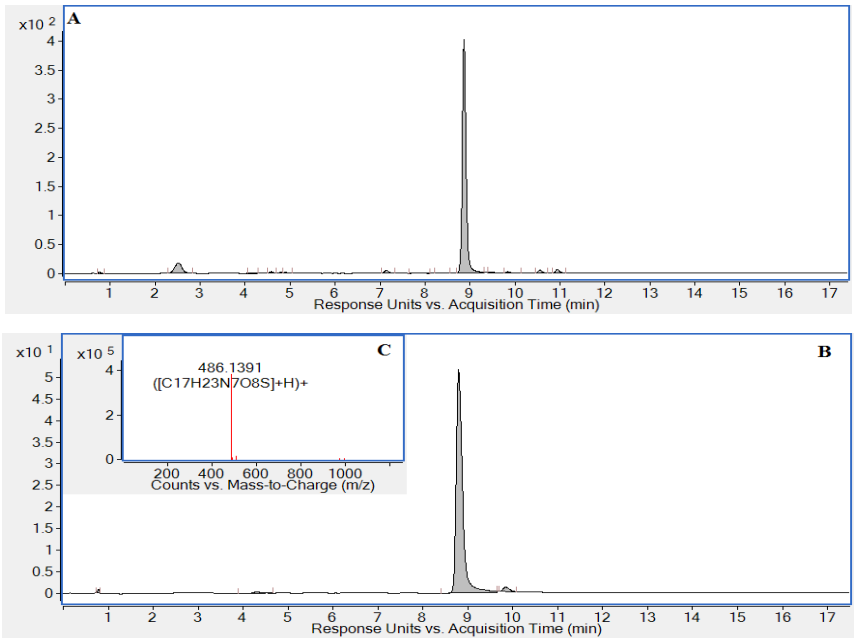


**Figure S11d**. HILIC-DAD-QTOF analysis of product **21**. Purity profile (HILIC-DAD - 254 nm) before (panel A) and after (panel B) semi-preparative chromatography. Panel C – MS spectrum of the desired compound (the major peak from UV chromatogram).

**S12**. 2,2′-[(6-({2-(4-sulfamoylphenyl)ethyl}amino)-1,3,5-triazine-2,4-diyl)diimino]bis(3-hydroxybutanoic acid) **22** and its IR (a), $^{1}H$ (b), $^{13}C$ (c) NMR and DAD/MS (d) spectra

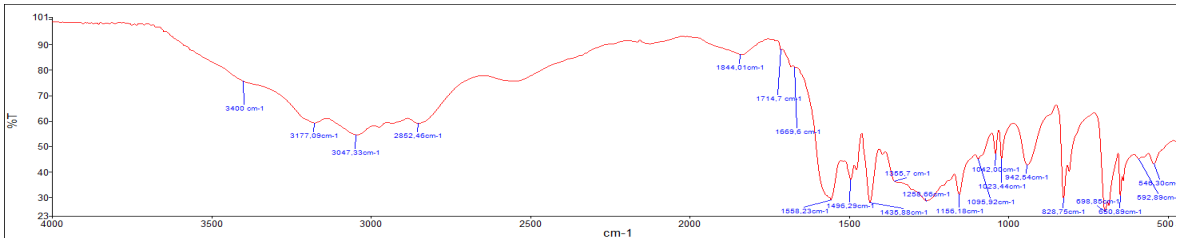


**Figure S12a**. IR spectra of product **22.**

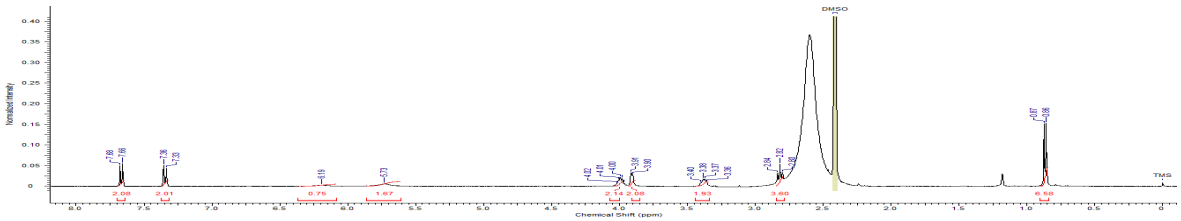


**Figure S12b**. $^{1}H$ NMR spectra of product **22.**

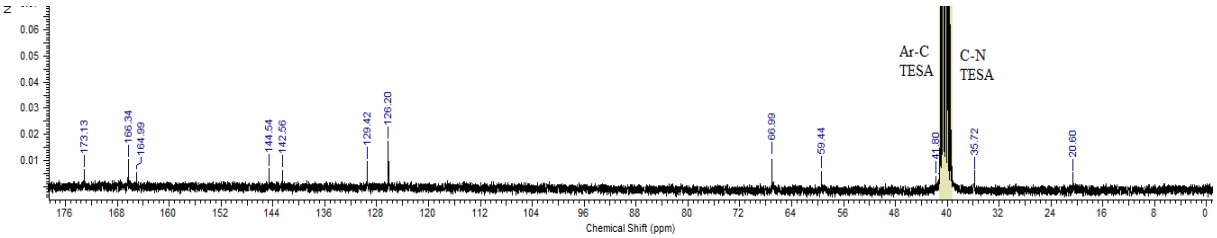


**Figure S12c**. $^{13}C$ NMR spectra of product **22.**

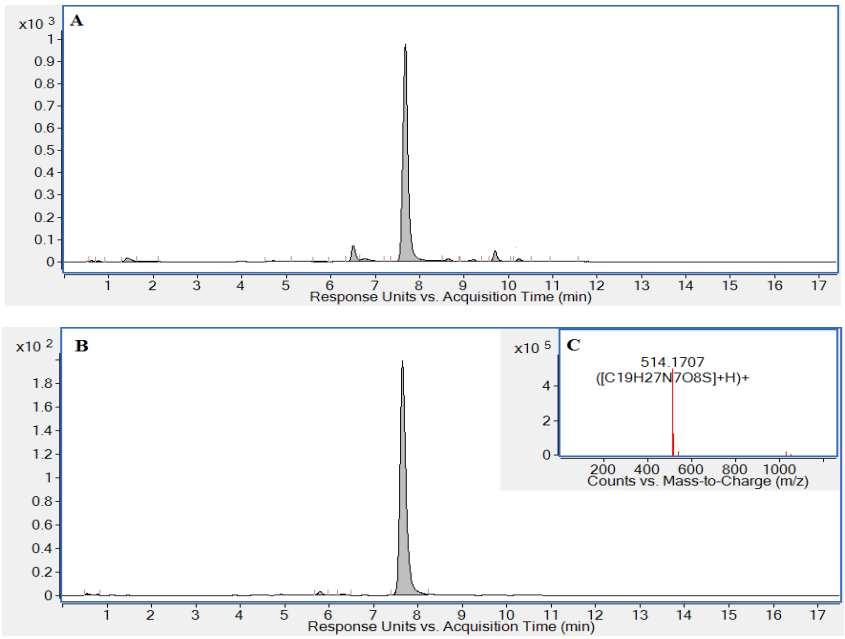


**Figure S12d**. HILIC-DAD-QTOF analysis of product **22**. Purity profile (HILIC-DAD - 254 nm) before (panel A) and after (panel B) semi-preparative chromatography. Panel C – MS spectrum of the desired compound (the major peak from UV chromatogram).

**S13**. 2,2′-[(6-({2-(4-sulfamoylphenyl)ethyl}amino)-1,3,5-triazine-2,4-diyl)diimino]bis(3-carbamoylpropanoic acid) **23** and its IR (a), $^{1}H$ (b), $^{13}C$ (c) NMR and DAD/MS (d) spectra

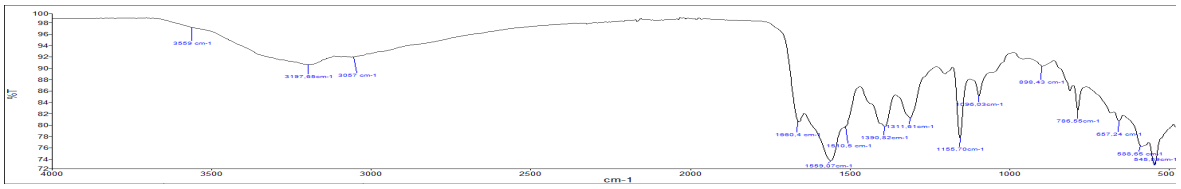

**Figure S13a**. IR spectra of product **23.**

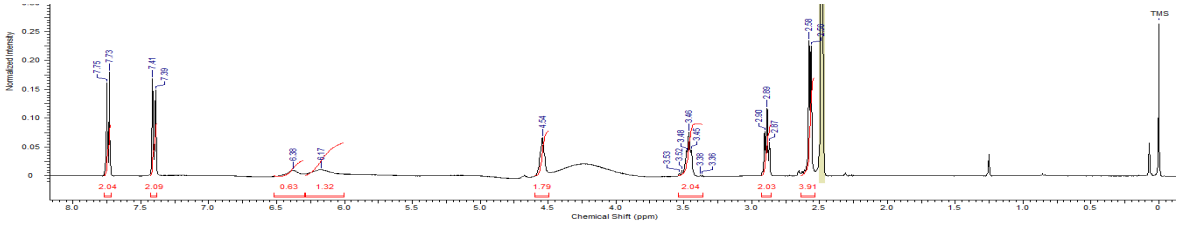

**Figure S13b**. $^{1}H$ NMR spectra of product **23.**

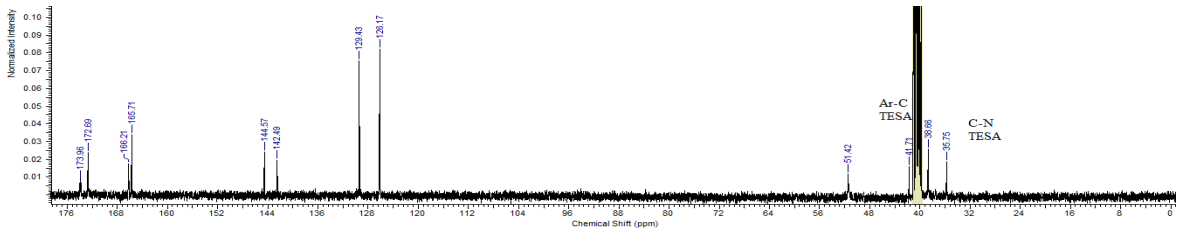


**Figure S13c**. $^{13}C$ NMR spectra of product **23.**

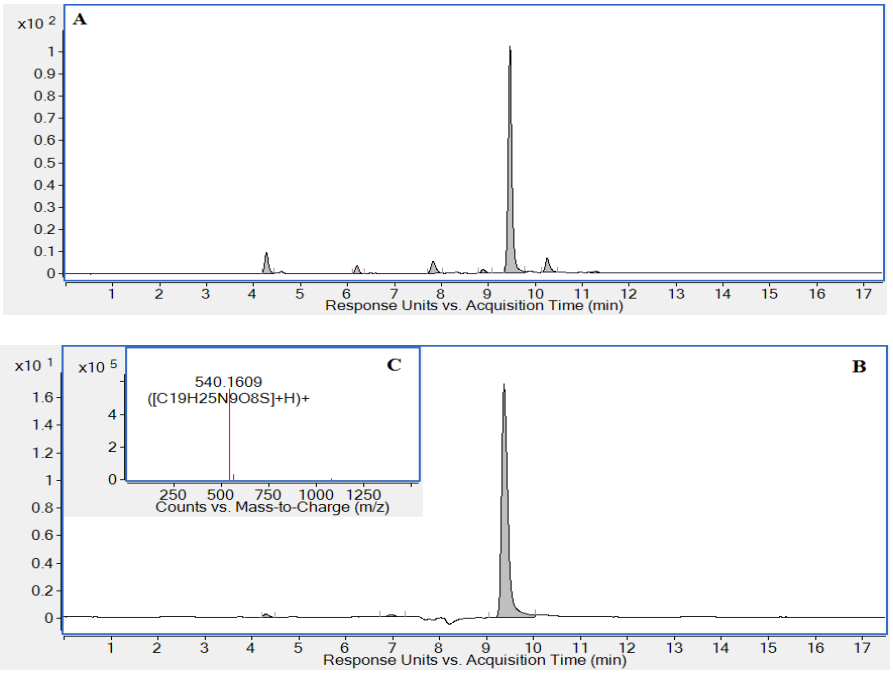


**Figure S13d**. HILIC-DAD-QTOF analysis of product **23**. Purity profile (HILIC-DAD - 254 nm) before (panel A) and after (panel B) semi-preparative chromatography. Panel C – MS spectrum of the desired compound (the major peak from UV chromatogram).

**S14**. 2,2′-[(6-({2-(4-sulfamoylphenyl)ethyl}amino)-1,3,5-triazine-2,4-diyl)diimino]bis(4-carbamoylbutanoic acid) **24** and its IR (a), $^{1}H$ (b), $^{13}C$ (c) NMR and DAD/MS (d) spectra

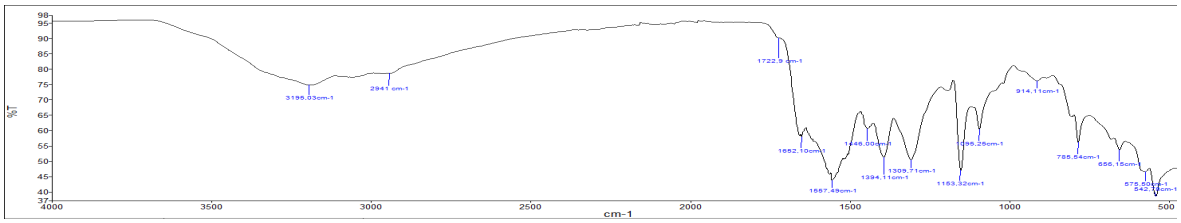


**Figure S14a**. IR spectra of product **24.**

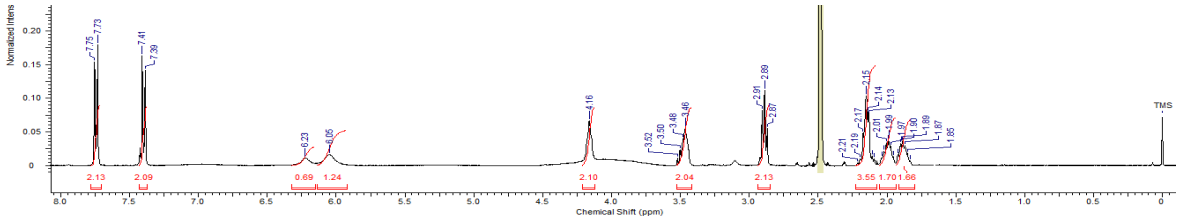


**Figure S14b**. $^{1}H$ NMR spectra of product **24.**

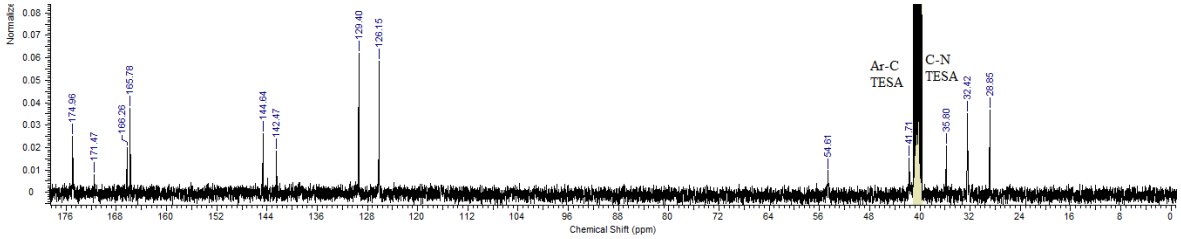


**Figure S14c**. $^{13}C$ NMR spectra of product **24.**

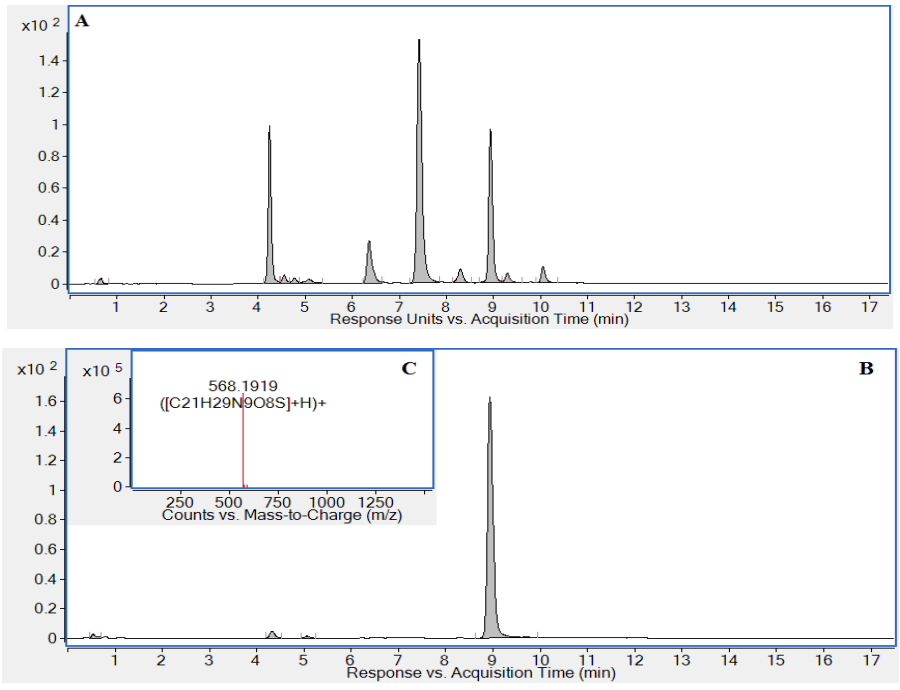


**Figure S14d**. HILIC-DAD-QTOF analysis of product **24**. Purity profile (HILIC-DAD - 254 nm) before (panel A) and after (panel B) semi-preparative chromatography. Panel C – MS spectrum of the desired compound (the major peak from UV chromatogram).