

Supporting information for

Optimization and Comparison of Synthetic Procedures for Group of Triazinyl-substituted Benzene-sulfonamide Conjugates with Amino Acids

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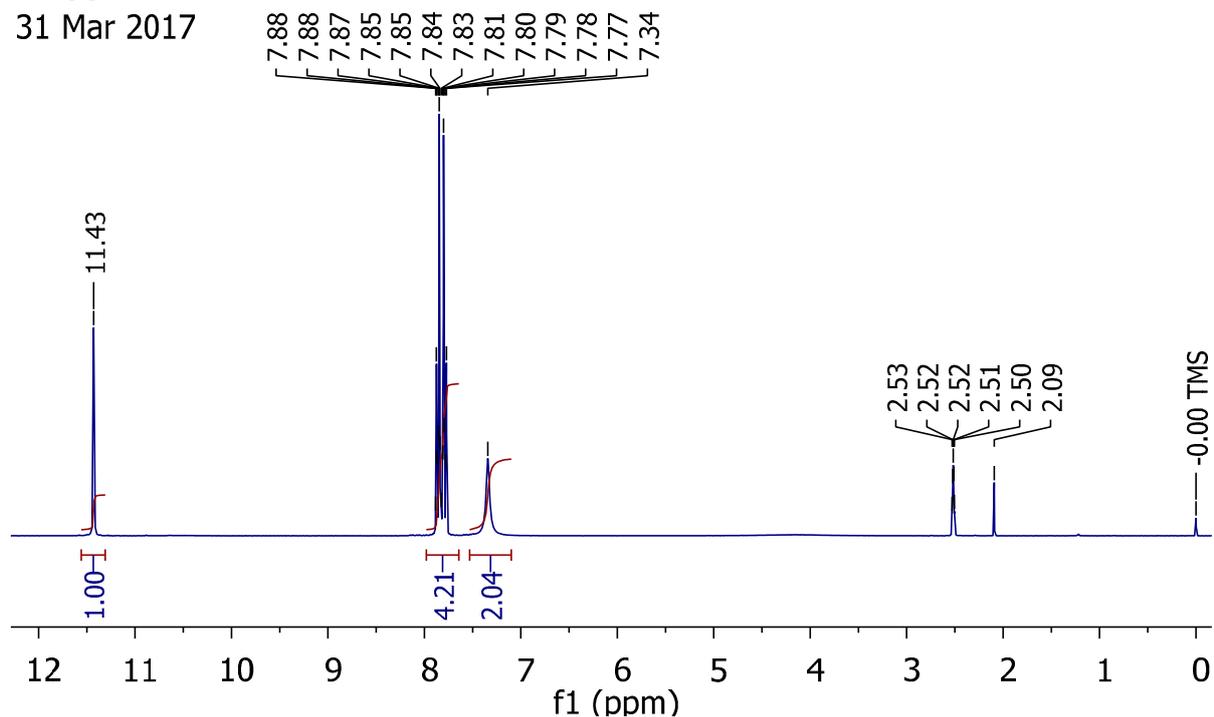
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¹H NMR, 300 MHz
DK032
DMSO
31 Mar 2017



¹³C NMR, 75 MHz
DK032
DMSO
31 Mar 2017

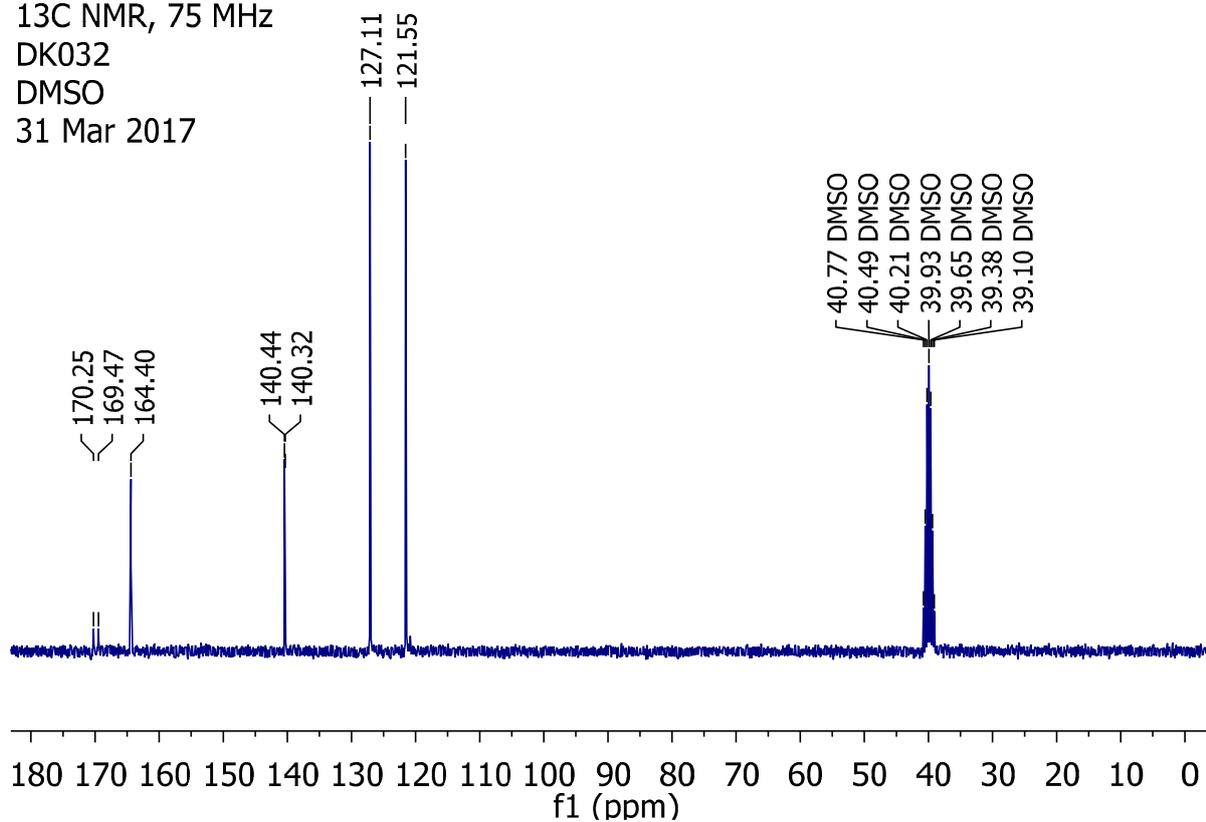
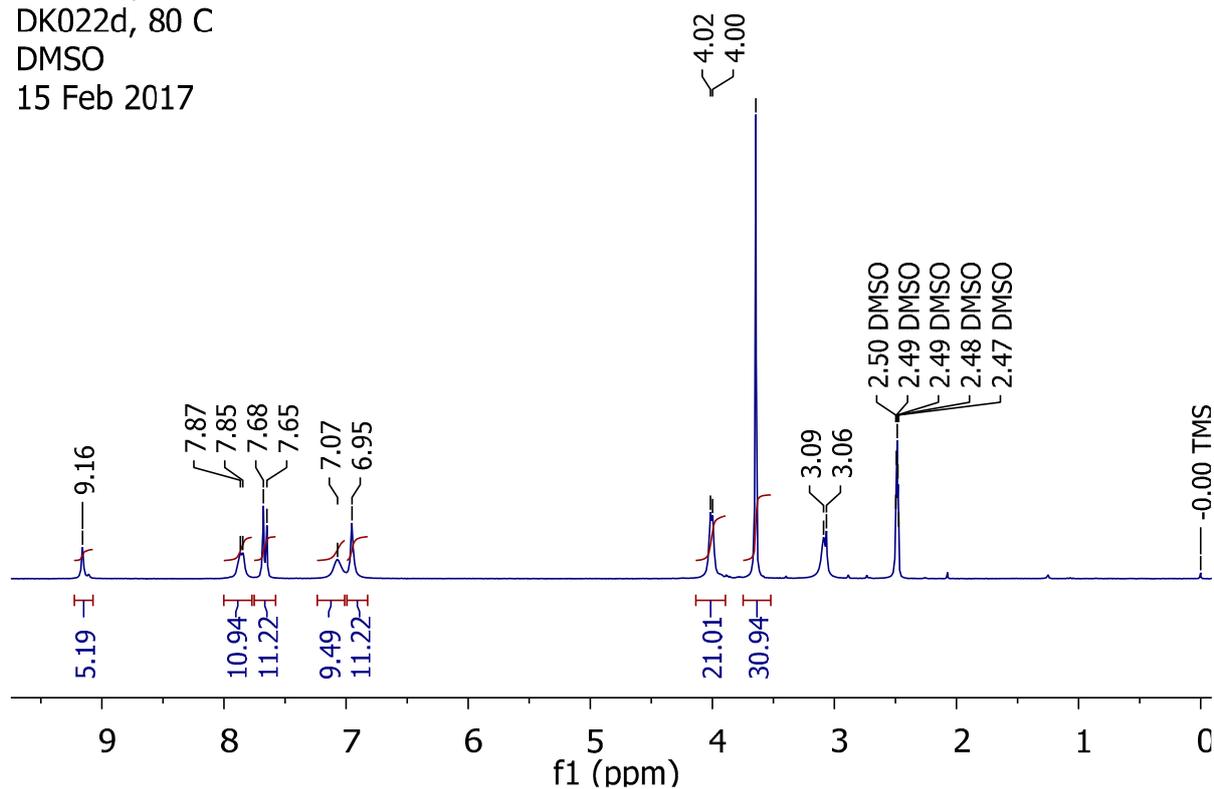


Figure S1: ¹H and ¹³C NMR spectra of 4-(4',6'-dichloro-1',3',5'-triazin-2'-ylamino)benzenesulfonamide **1**

¹H NMR, 300 MHz
DK022d, 80 C
DMSO
15 Feb 2017



¹³C NMR, 75 MHz
DK022d, 80 C
DMSO
15 Feb 2017

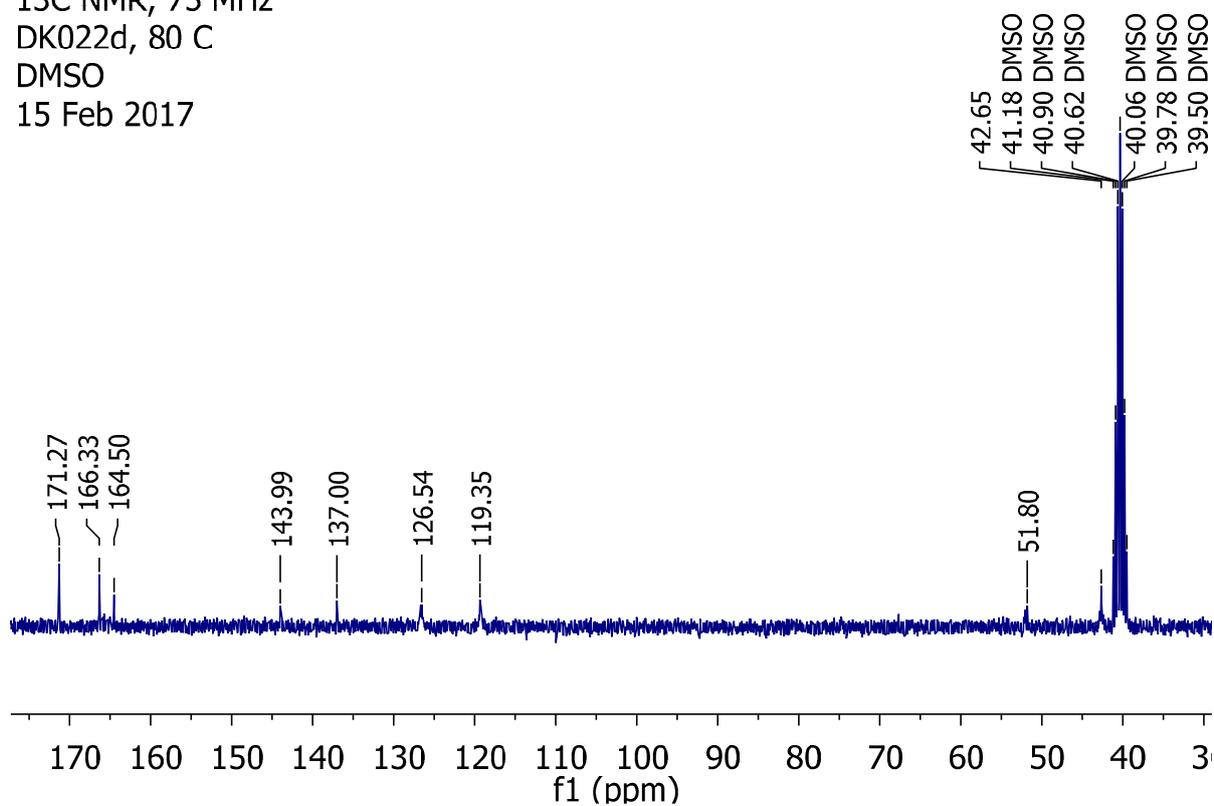
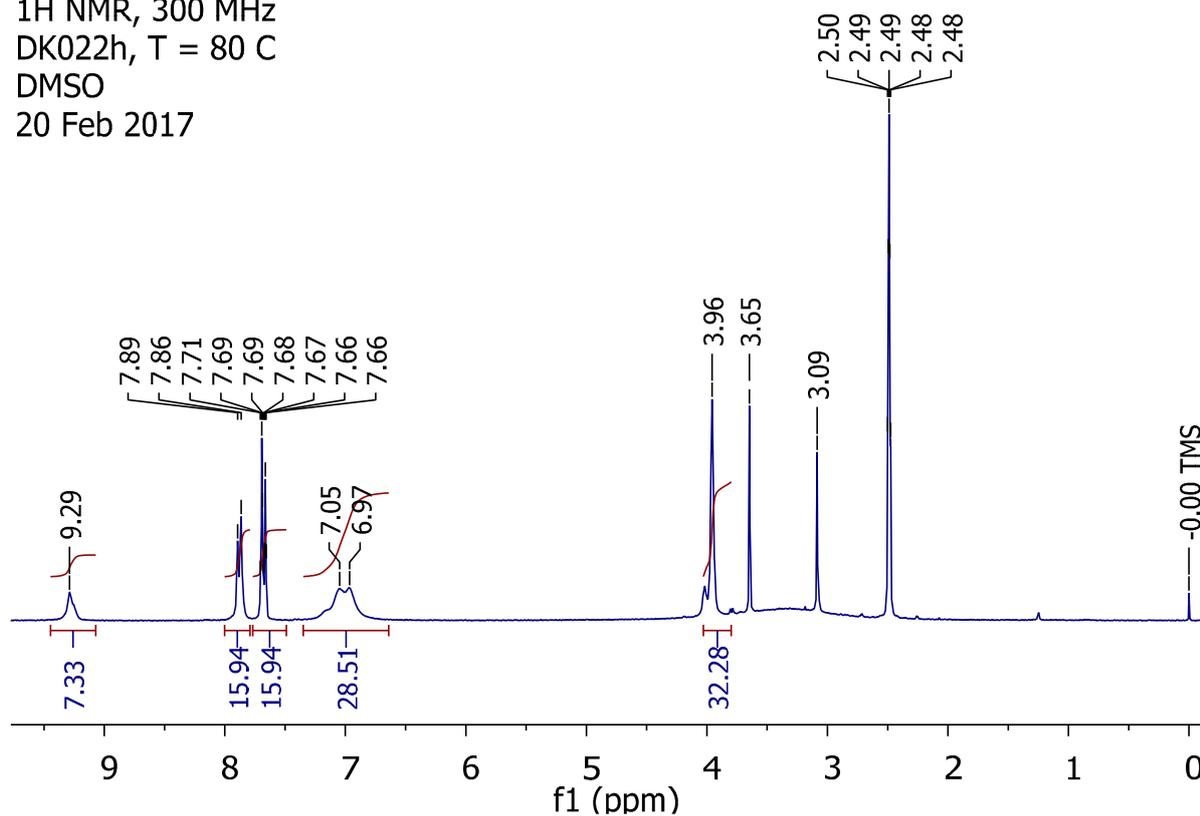


Figure S2: ¹H and ¹³C NMR spectra of dimethyl 2',2''-[6'-(4-sulfamoylphenylamino)-1',3',5'-triazine-2',4'-diyl]-bis(azanediy)diacetate 2

¹H NMR, 300 MHz
DK022h, T = 80 C
DMSO
20 Feb 2017



¹³C NMR, 75 MHz
DK022h, T = 80 C
DMSO
20 Feb 2017

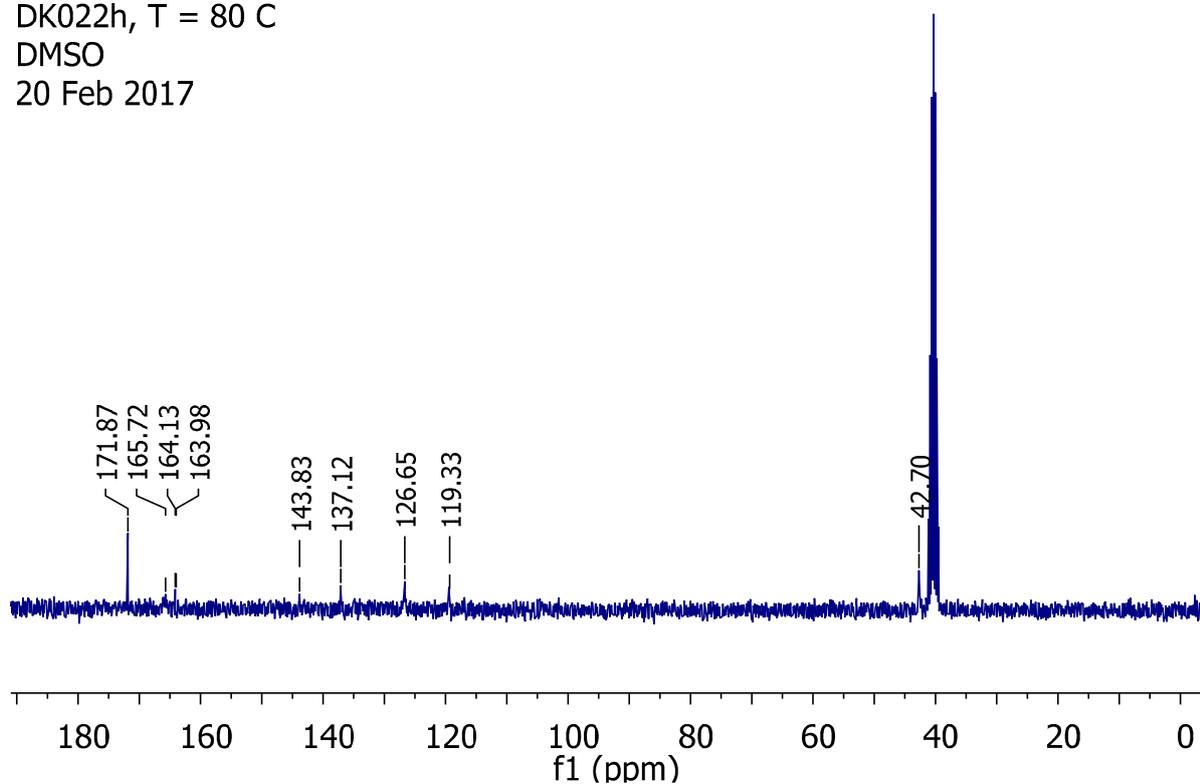
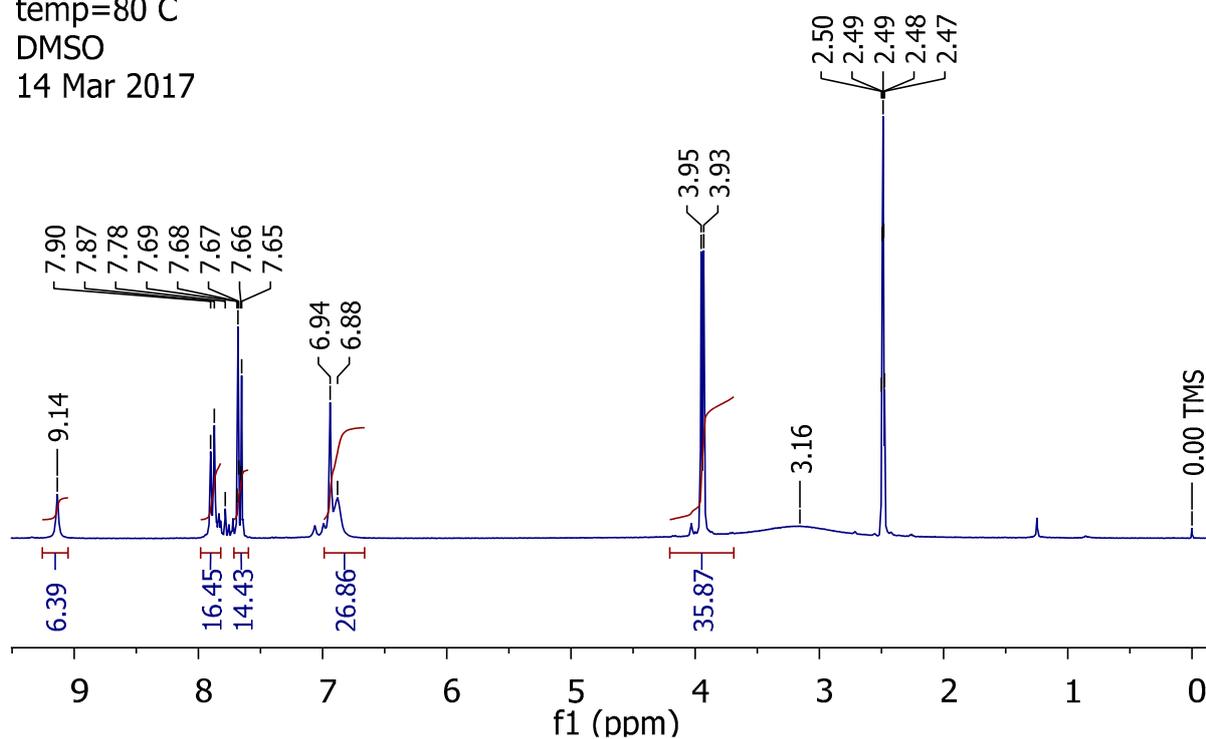


Figure S3: ¹H and ¹³C NMR spectra of 2'',2'''-[6'-(4-sulfamoylphenylamino)-1',3',5'-triazine-2',4'-diyl]-bis(azanediy)diacetic acid **3** prepared according to the *Scheme 3*

¹H NMR, 300 MHz
DK009
temp=80 C
DMSO
14 Mar 2017



¹³C NMR, 75 MHz
DK009
temp=80 C
DMSO
14 Mar 2017

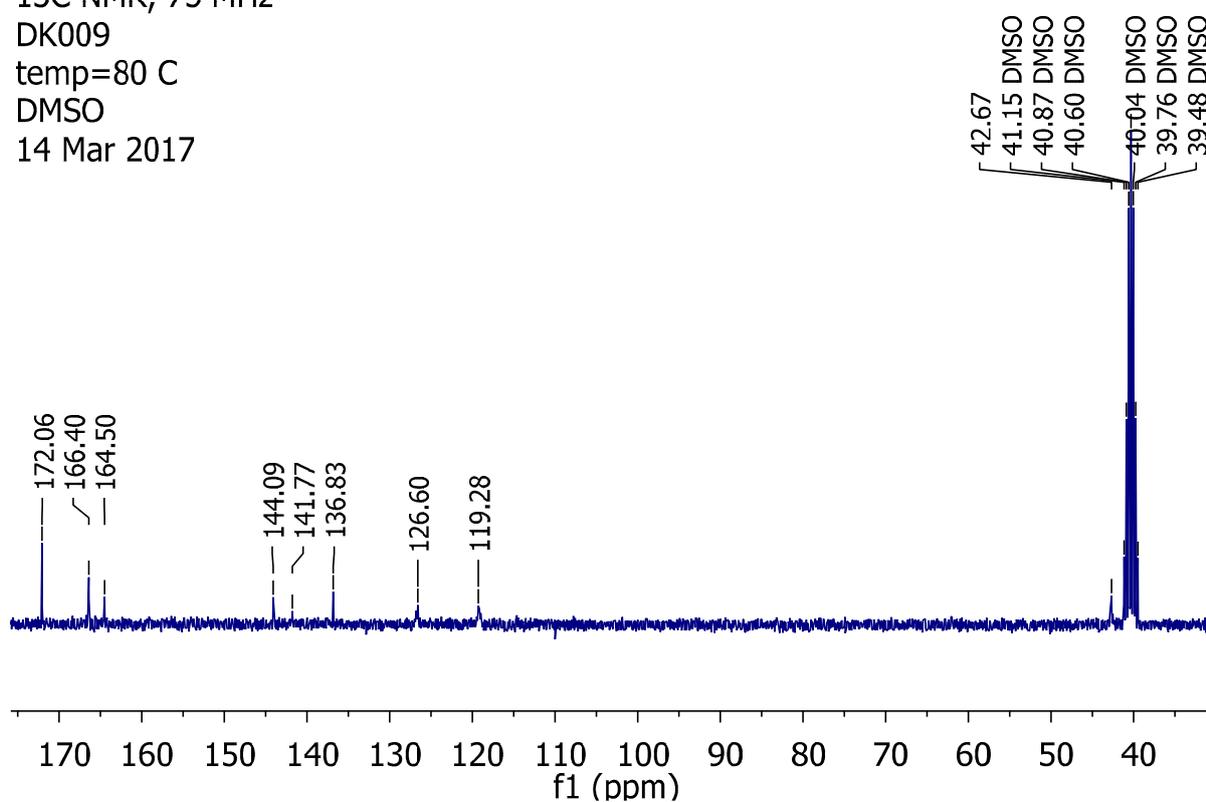
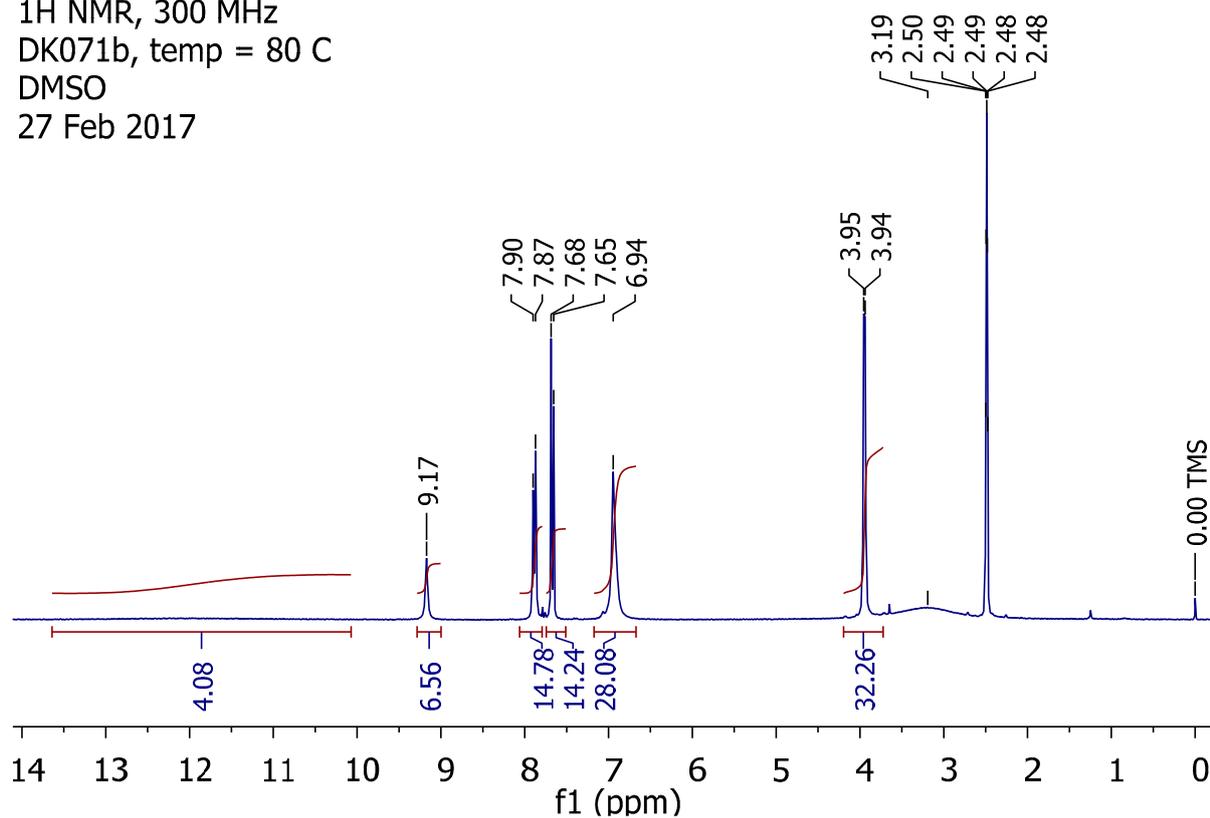


Figure S4: ¹H and ¹³C NMR spectra of 2'',2'''-[6'-(4-sulfamoylphenylamino)-1',3',5'-triazine-2',4'-diyl]-bis(azanediy)diacetic acid **3** prepared according to the *Scheme 4*

¹H NMR, 300 MHz
DK071b, temp = 80 C
DMSO
27 Feb 2017



¹³C NMR, 75 MHz
DK071b, temp = 80 C
DMSO
27 Feb 2017

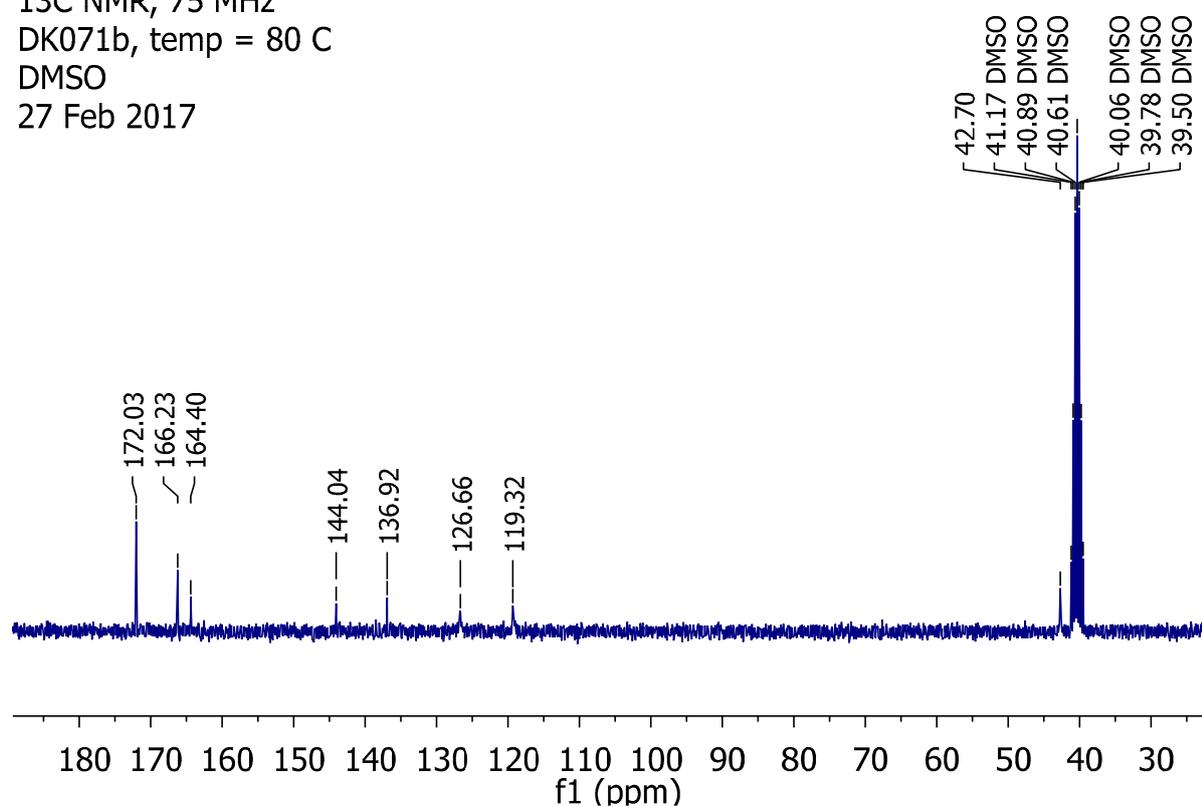
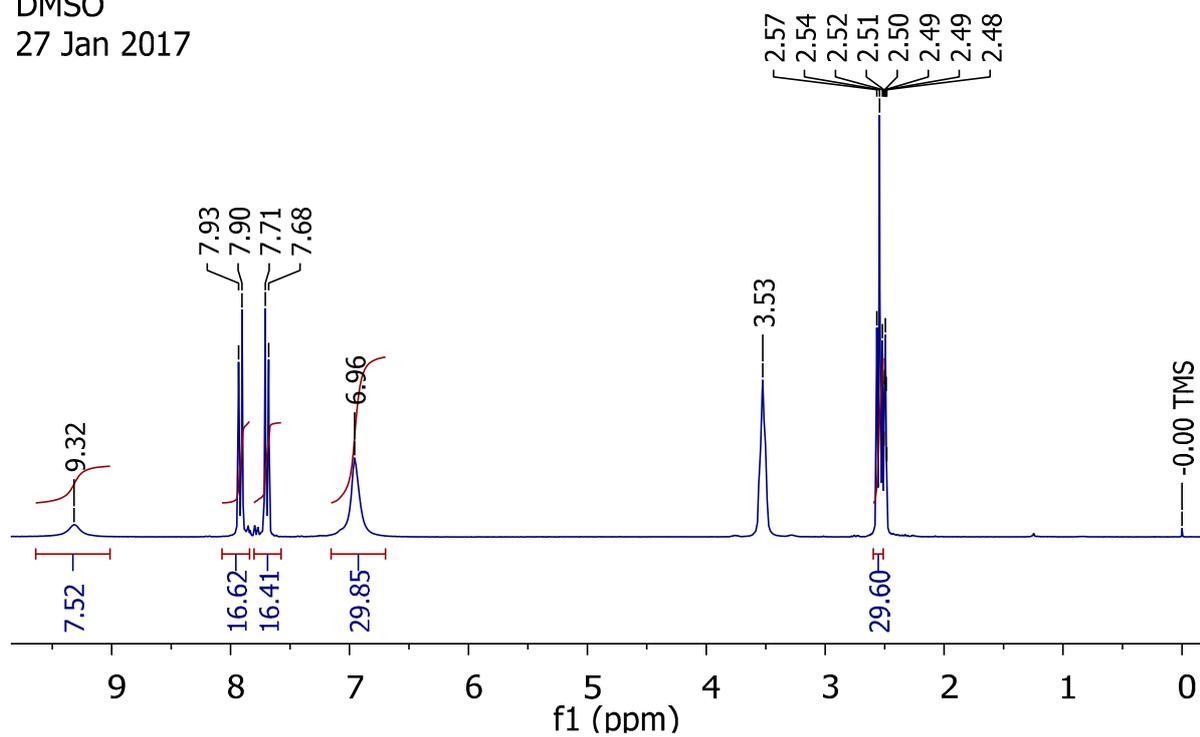


Figure S5: ¹H and ¹³C NMR spectra of 2'',2''-[6'-(4-sulfamoylphenylamino)-1',3',5'-triazine-2',4'-diyl]-bis(azanediy)diacetic acid **3** prepared according to the *Scheme 5*

¹H NMR, 300 MHz
DK072a
DMSO
27 Jan 2017



¹³C NMR, 75 MHz
DK072a
DMSO
27 Jan 2017

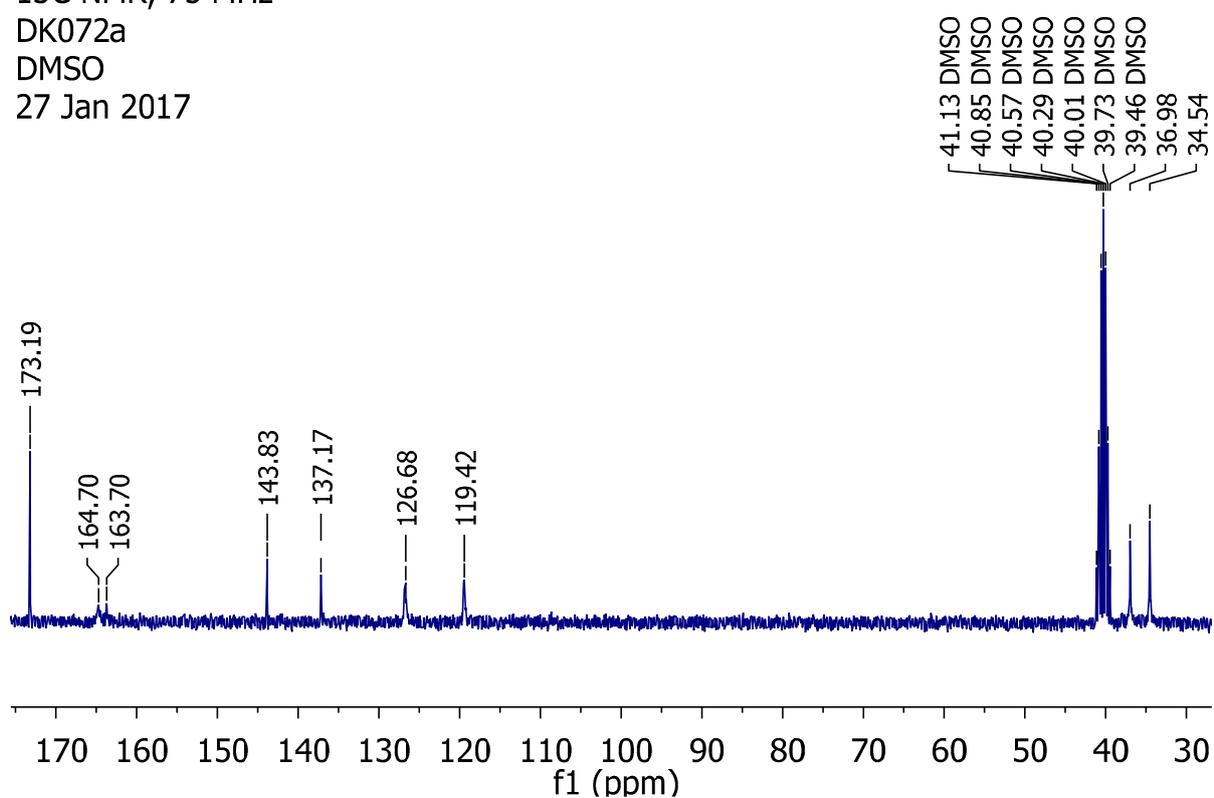


Figure S6: ¹H and ¹³C NMR spectra of 3'',3'''-[6'-(4-sulfamoylphenylamino)-1',3',5'-triazine-2',4'-diyl]-bis(azanediy) dipropanoic acid **4**

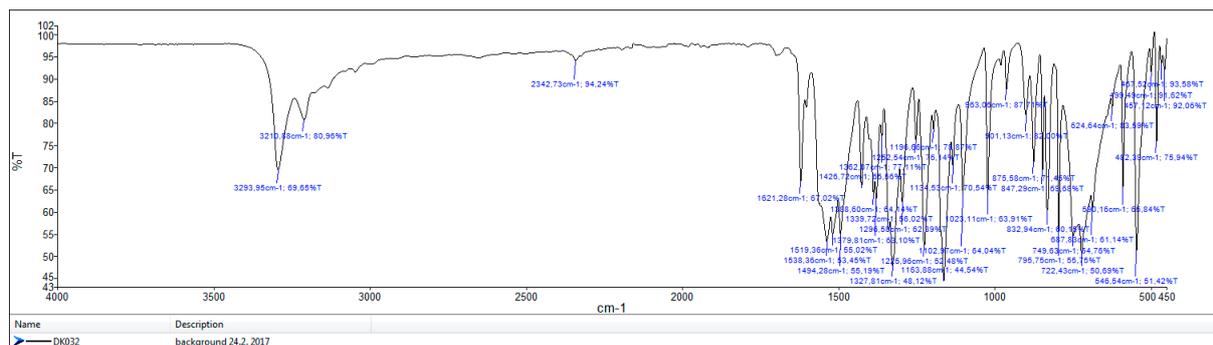


Figure S7: IR spectrum of 4-(4',6'-dichloro-1',3',5'-triazin-2'-ylamino)-benzenesulfonamide **1**

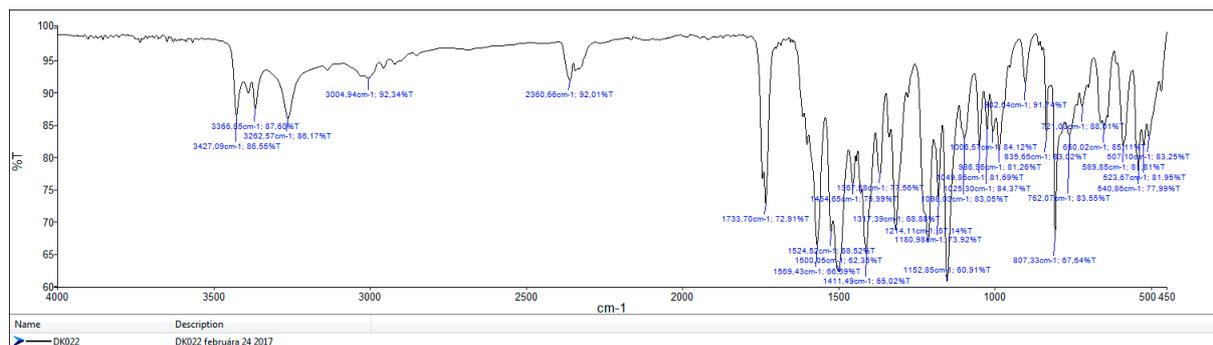


Figure S8: IR spectrum of dimethyl 2'',2'''-[6'-(4-sulfamoylphenylamino)-1',3',5'-triazine-2',4'-diyl]-bis(azanediy1) diacetate **2**

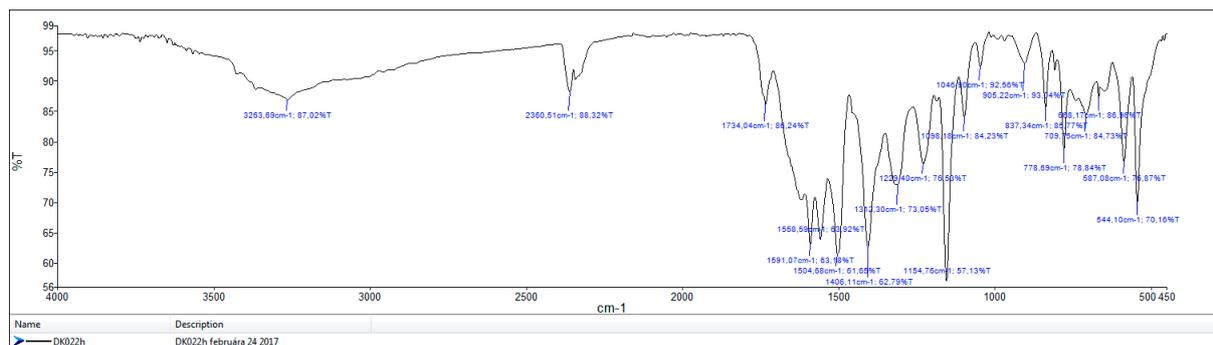


Figure S9: IR spectrum of 2'',2'''-[6'-(4-sulfamoylphenylamino)-1',3',5'-triazine-2',4'-diyl]-bis(azanediy)diacetic acid **3** prepared according to the *Scheme 3*

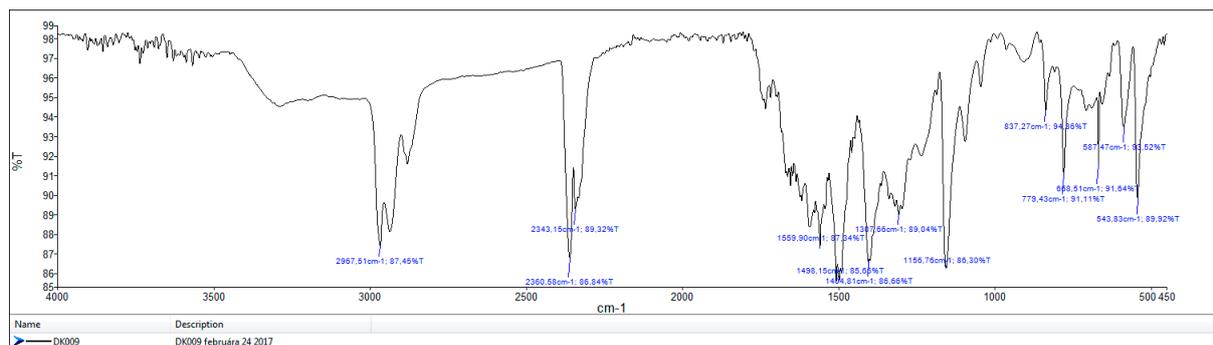


Figure S10: IR spectrum of 2'',2'''-[6'-(4-sulfamoylphenylamino)-1',3',5'-triazine-2',4'-diyl]-bis(azanediyl)diacetic acid **3** prepared according to the *Scheme 4*

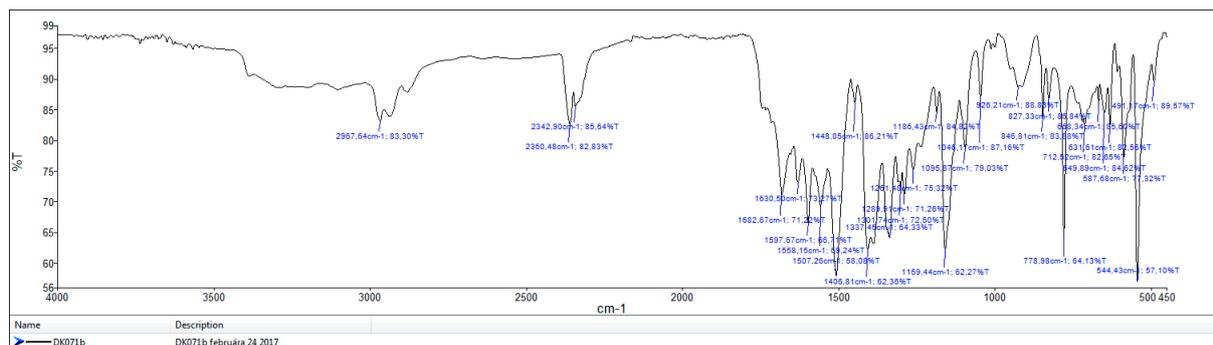


Figure S11: IR spectrum of 2'',2'''-[6'-(4-sulfamoylphenylamino)-1',3',5'-triazine-2',4'-diyl]-bis(azanediy)diacetic acid **3** prepared according to the *Scheme 5*

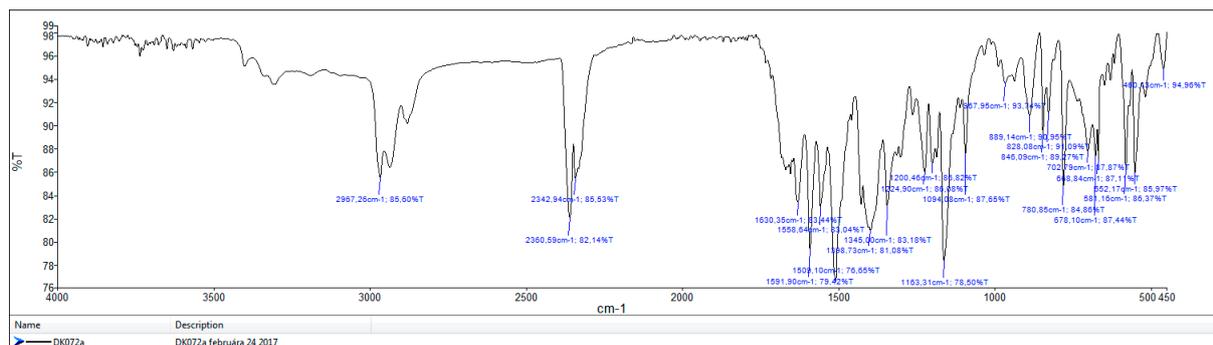


Figure S12: IR spectrum of 3'',3'''-[6'-(4-sulfamoylphenylamino)-1',3',5'-triazine-2',4'-diyl]bis(azanediy) dipropanoic acid **4**

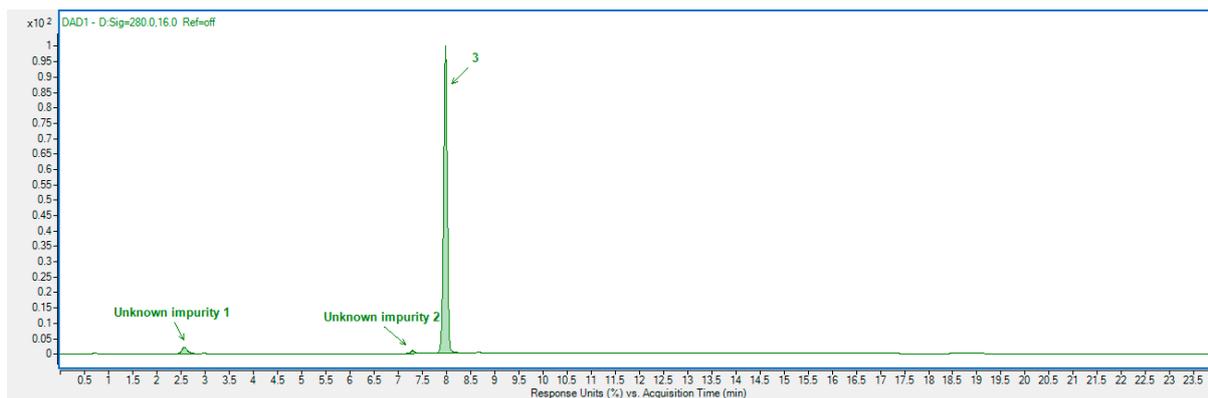


Figure S13: HPLC-UV (280 nm) profile of 2'',2'''-[6'-(4-sulfamoylphenylamino)-1',3',5'-triazine-2',4'-diyl]-bis(azanediy1)diacetic acid **3**. Calculated purity of the compound **3** (based on peak areas acquired by HPLC-UV) was 95.51%. Two unknown impurities (3.45% and 1.04%) were detected in the chromatogram. For the analytical conditions see section 3.1.

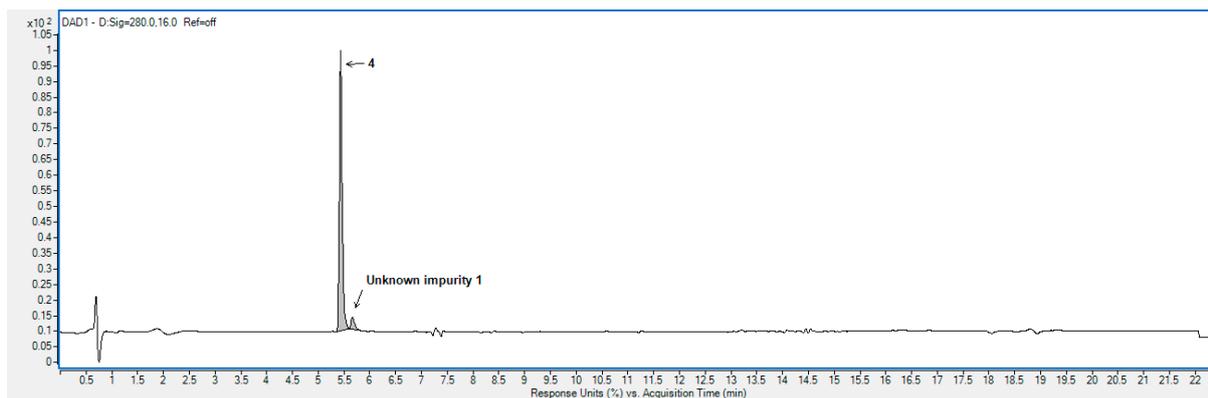


Figure S14: HPLC-UV (280 nm) profile of 3'',3'''-[6'-(4-sulfamoylphenylamino)-1',3',5'-triazine-2',4'-diyl]-bis (azanediyldipropanoic acid **4**). Calculated purity of the compound **4** (based on peak areas acquired by HPLC-UV) was 94.98%. One unknown impurity (5.02%) was detected in the chromatogram. For the analytical conditions see section 3.1.