Supplemental data

I. New cocrystals

I-1. Caffeine (CAF)-Salicylic acid (SAA)

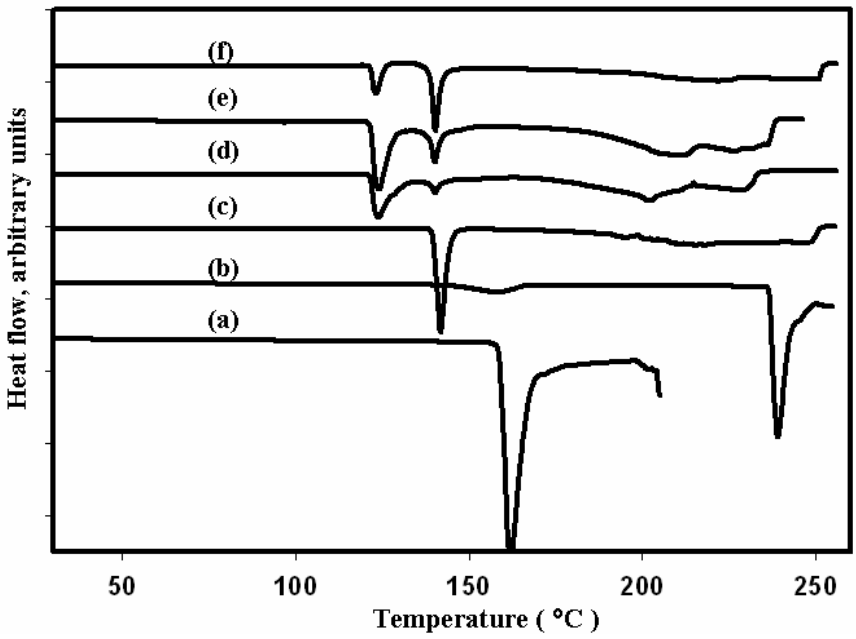

Fig. I-1a. DSC heating curves of (a) salicylic acid (SAA), (b) caffeine (CAF) and (c) CAF-SAA cocrystal prepared by the slurry method. The curves (d) (e) and (f) are physical mixtures of CAF: SAA at 1:2, 1:1 and 2:1 molar ratios, respectively.

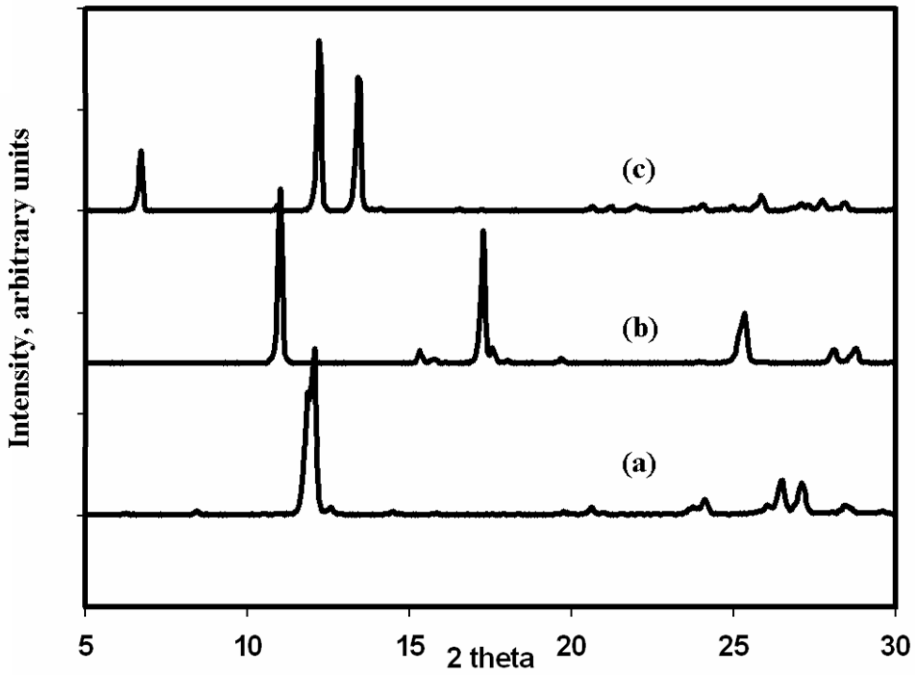

Fig. I-1b. XRD patterns of (a) caffeine (CAF), (b) salicylic acid (SAA) and (c) CAF-SAA cocrystal prepared by the slurry method.

I-2. Caffeine (CAF)- Saccharin (SAC)

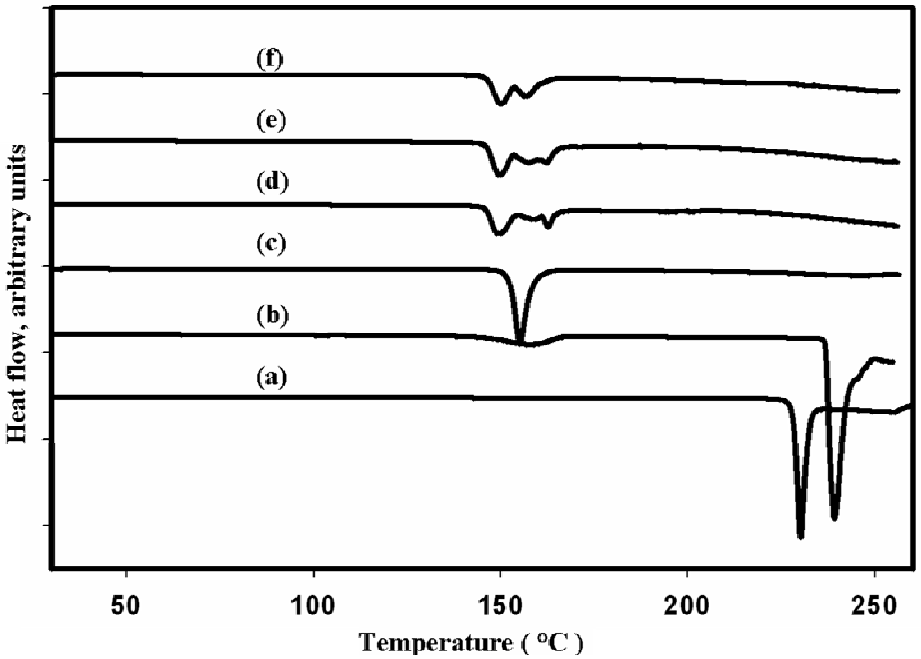

Fig. I-2a. DSC heating curves of (a) saccharin (SAC), (b) caffeine (CAF) and (c) CAF-SAC cocrystal prepared from eutectic melt. The curves (d) (e) and (f) are physical mixtures of CAF: SAC at 1:2, 1:1 and 2:1 molar ratios, respectively.

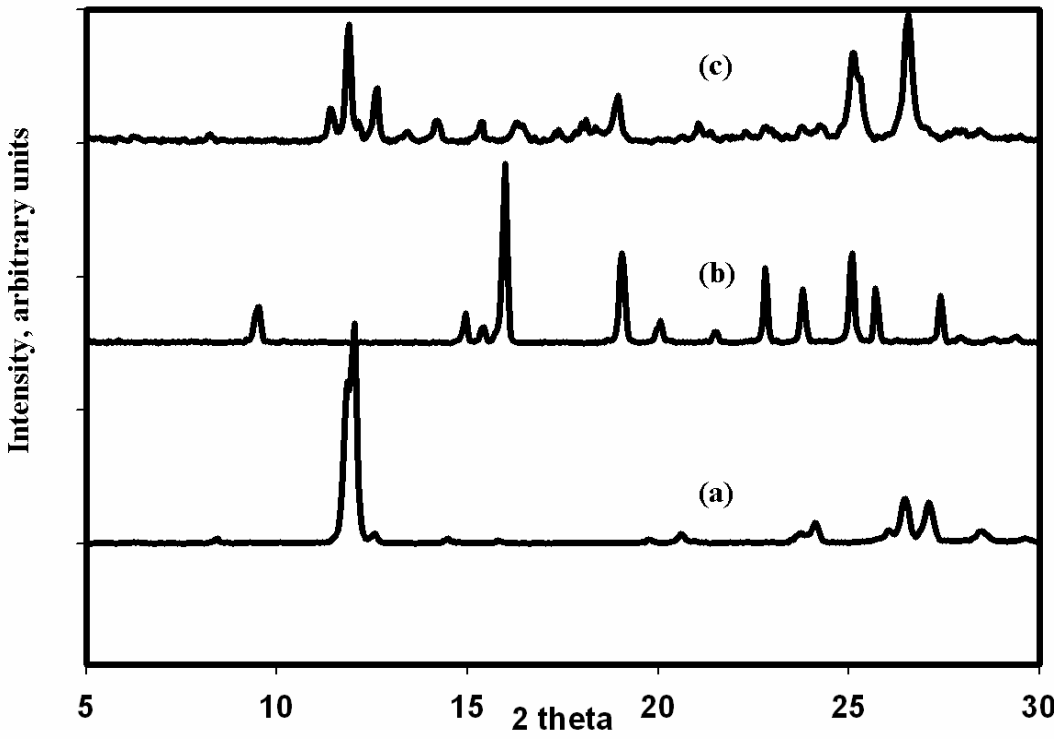

Fig. I-2b. XRD patterns of (a) caffeine (CAF), (b) saccharin (SAC) and (c) CAF-SAC cocrystal prepared from eutectic melt.

I-3. Carbamazepine (CBZ)-Glutaric acid (GLA)

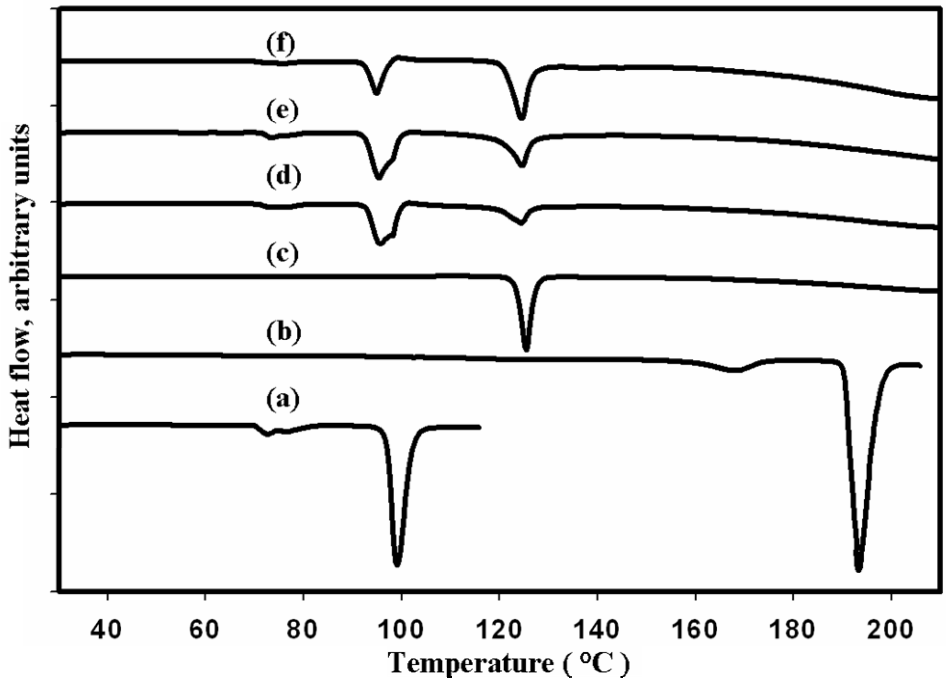

Fig. I-3a. DSC heating curves of (a) glutaric acid (GLA), (b) carbamazepine (CBZ) and (c) CBZ-GLA cocrystal prepared by the slurry method. The curves (d) (e) and (f) are physical mixtures of CBZ: GLA at 1:2, 1:1 and 2:1 molar ratios, respectively.

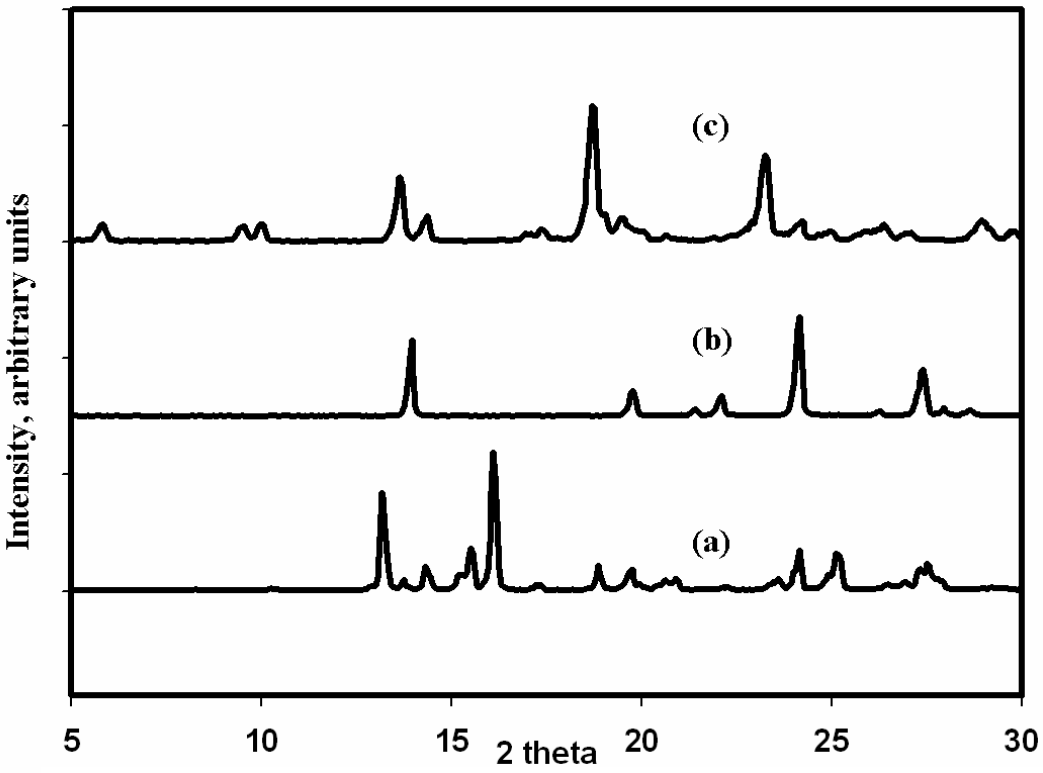

Fig. I-3b. XRD patterns of (a) carbamazepine (CBZ), (b) glutaric acid (GLA) and (c) CBZ-GLA cocrystal prepared by the slurry method.

I-4. Carbamazepine (CBZ)- Salicylic acid (SAA)

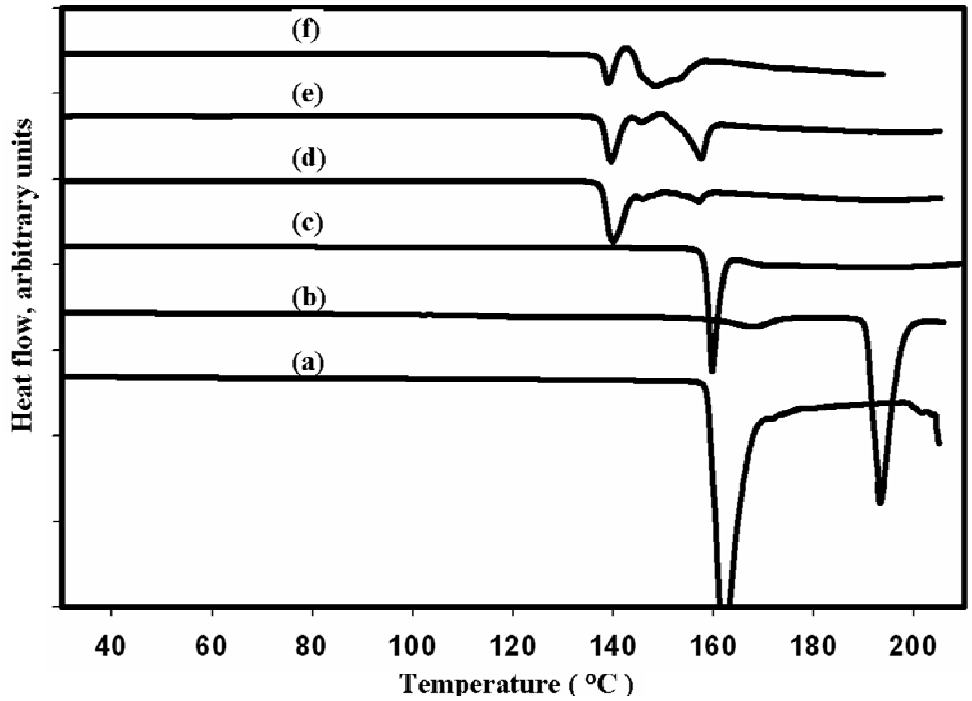

Fig. I-4a. DSC heating curves of (a) salicylic acid (SAA), (b) carbamazepine (CBZ) and (c) CBZ-SAA cocrystal prepared by the slurry method. The curves (d) (e) and (f) are physical mixtures of CBZ: SAA at 1:2, 1:1 and 2:1 molar ratios, respectively.

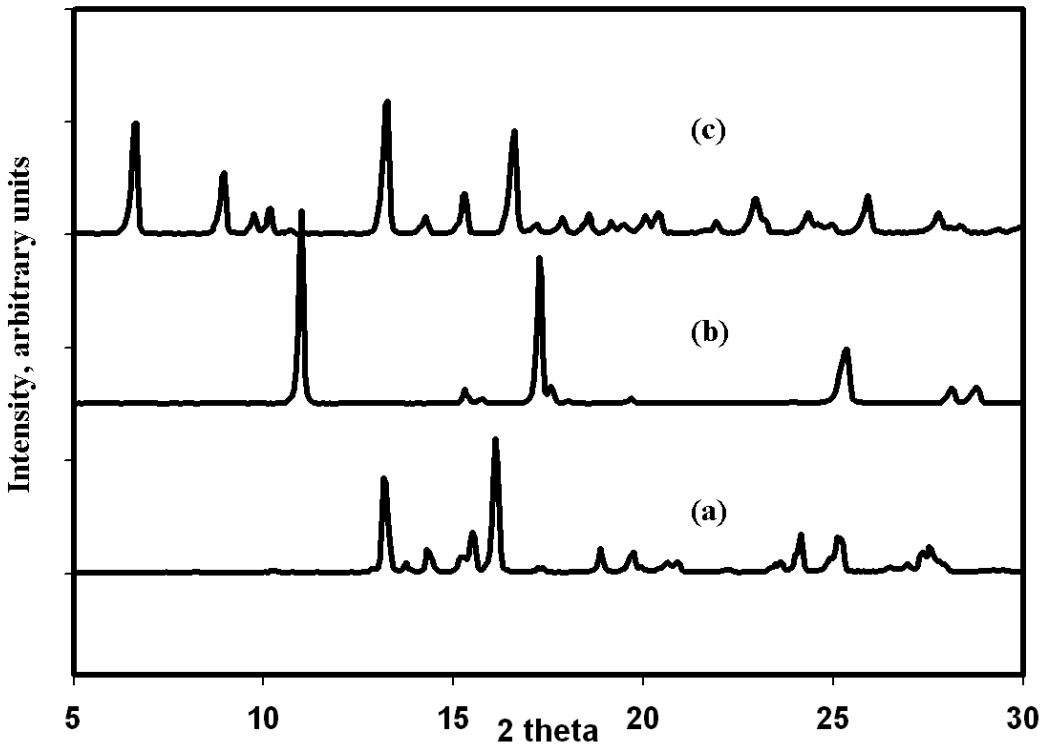

Fig. I-4b. XRD patterns of (a) carbamazepine (CBZ), (b) salicylic acid (SAA) and (c) CBZ-SAA cocrystal prepared by the slurry method.

I-5. Carbamazepine (CBZ)- Urea (URE)

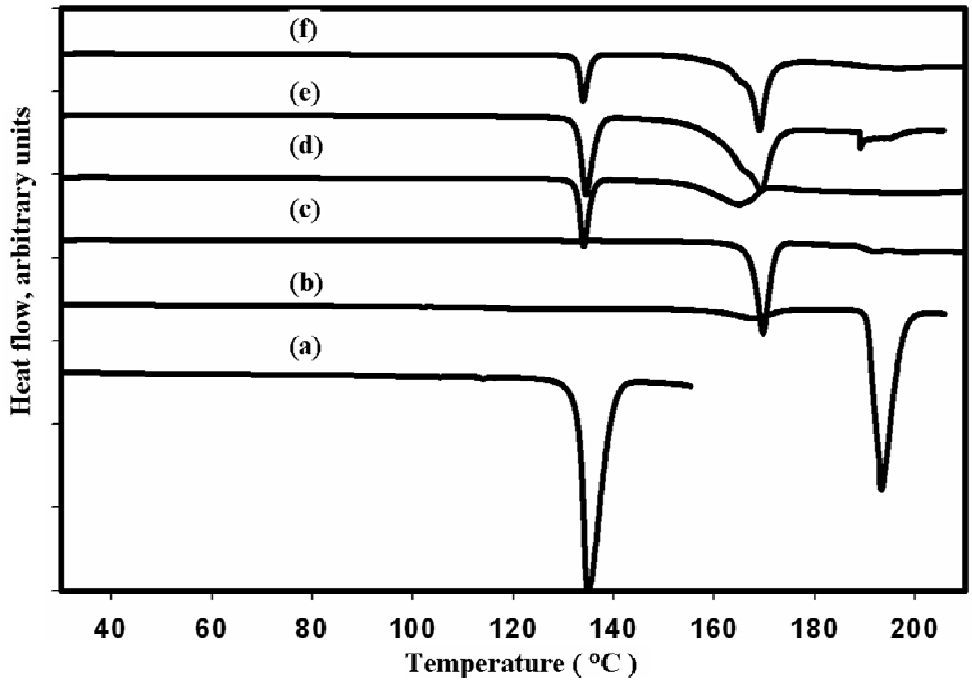

Fig. I-5a. DSC heating curves of (a) urea (URE), (b) carbamazepine (CBZ) and (c) CBZ-URE cocrystal prepared by the slurry method. The curves (d) (e) and (f) are physical mixtures of CBZ: URE at 1:2, 1:1 and 2:1 molar ratios, respectively.

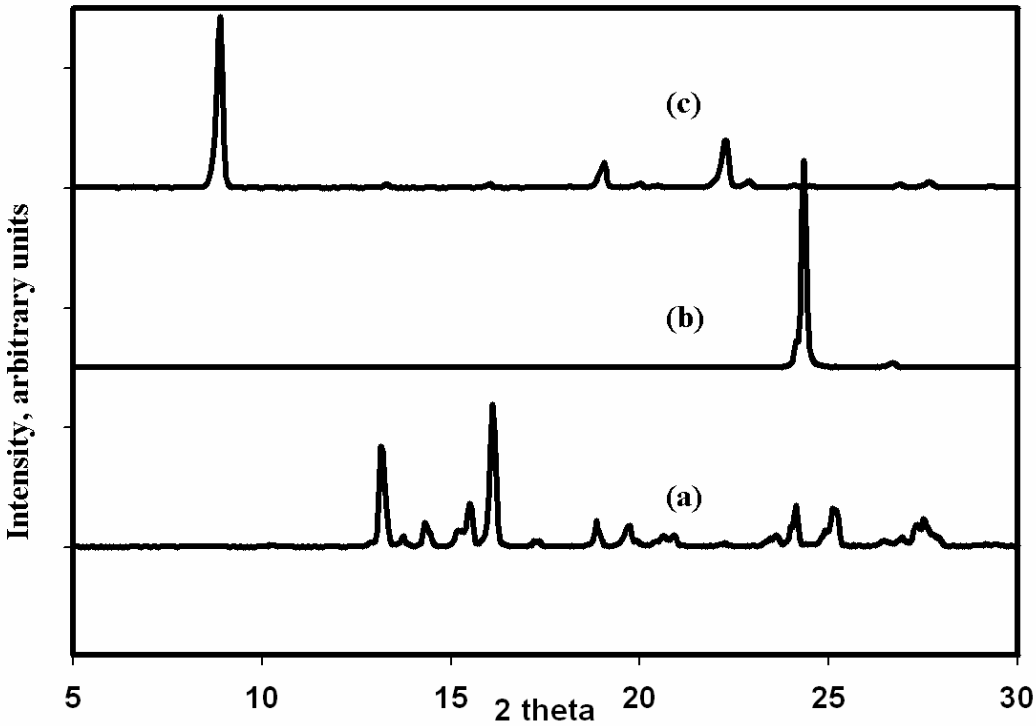

Fig. I-5b. XRD patterns of (a) carbamazepine (CBZ), (b) urea (URE) and (c) CBZ-URE cocrystal prepared by the slurry method.

I-6. Sulfamethazine(SFZ)- Nicotinamide(NCT)

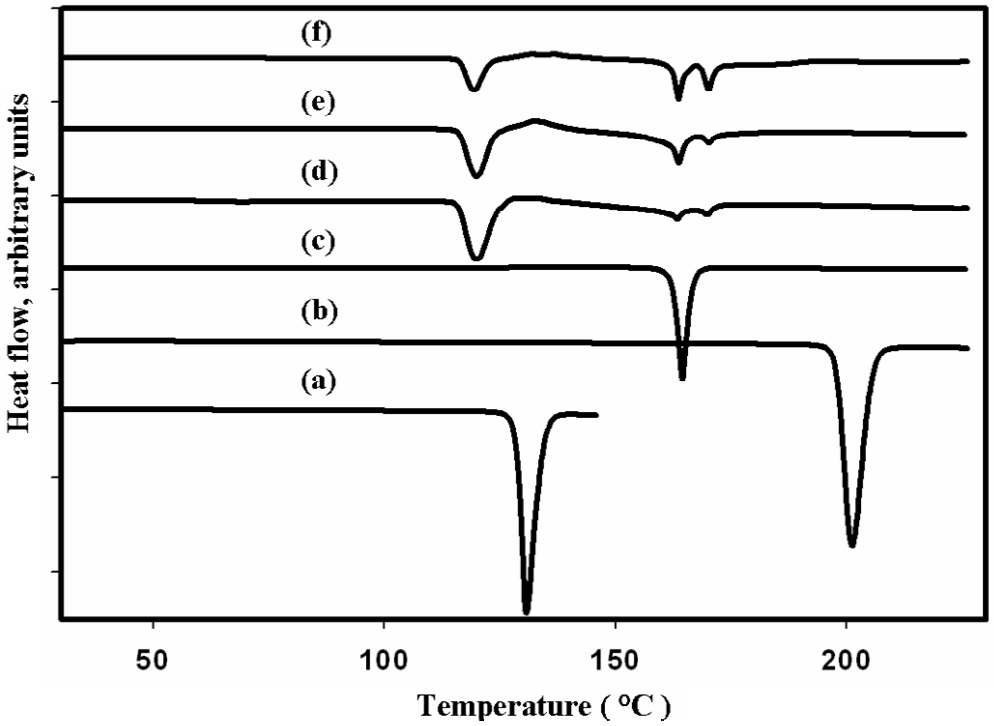

Fig. I-6a. DSC heating curves of (a) nicotinamide (NCT), (b) sulfamethazine (SFZ), (c) SFZ-NCT cocrystal prepared by the slurry method. The curves (d) (e) and (f) are physical mixtures of SFZ: NCT at 1:2, 1:1 and 2:1 molar ratios, respectively.

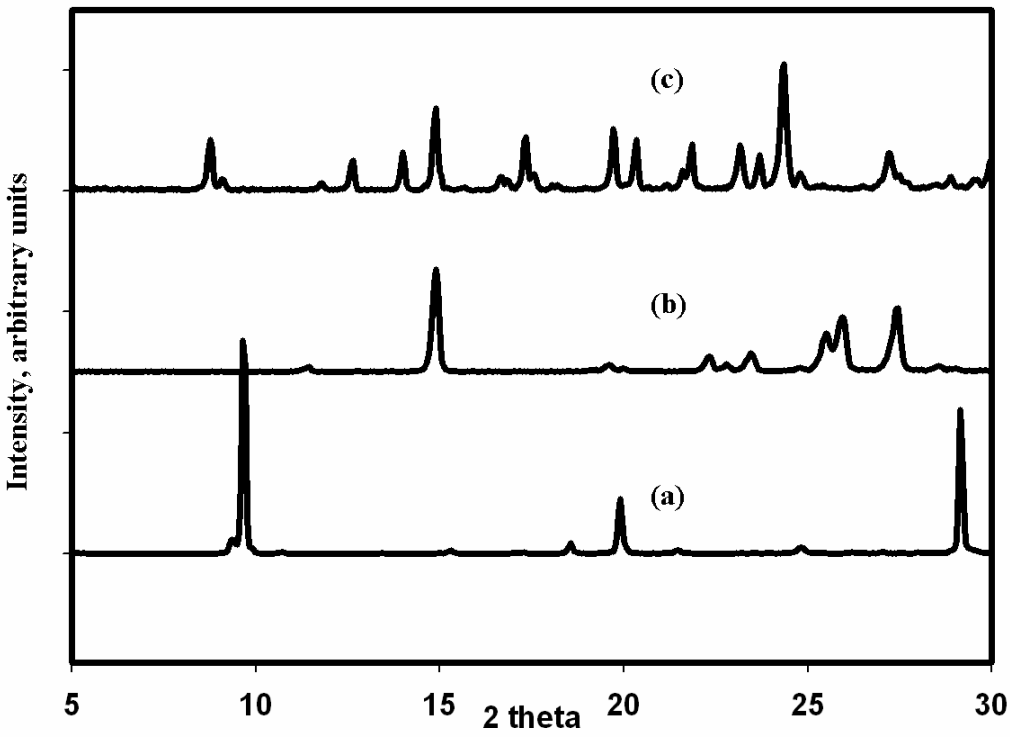

Fig. I-6b. XRD patterns of (a) sulfamethazine (SFZ), (b) nicotinamide (NCT), (c) SFZ-NCT cocrystal prepared by the slurry method.

I-7. Sulfamethazine (SFZ)- Saccharin(SAC)

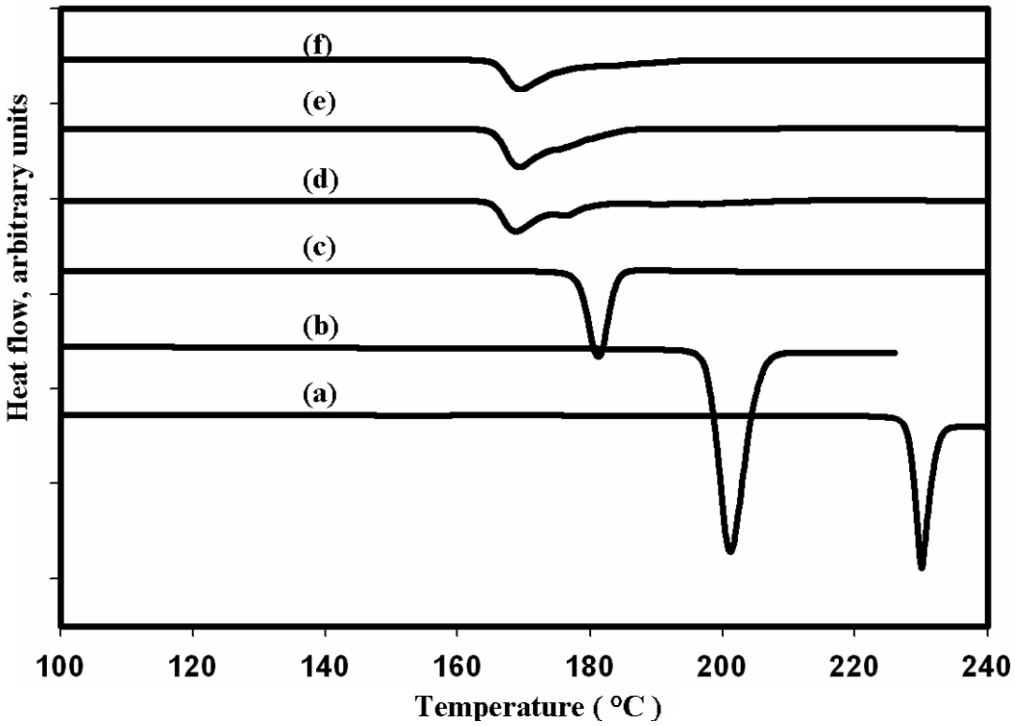

Fig. I-7a. DSC heating curves of (a) saccharin (SAC), (b) sulfamethazine (SFZ) and (c) SFZ-SAC cocrystal prepared by the slurry method. The curves (d) (e) and (f) are physical mixtures of SFZ: SAC at 1:2, 1:1 and 2:1 molar ratios, respectively.

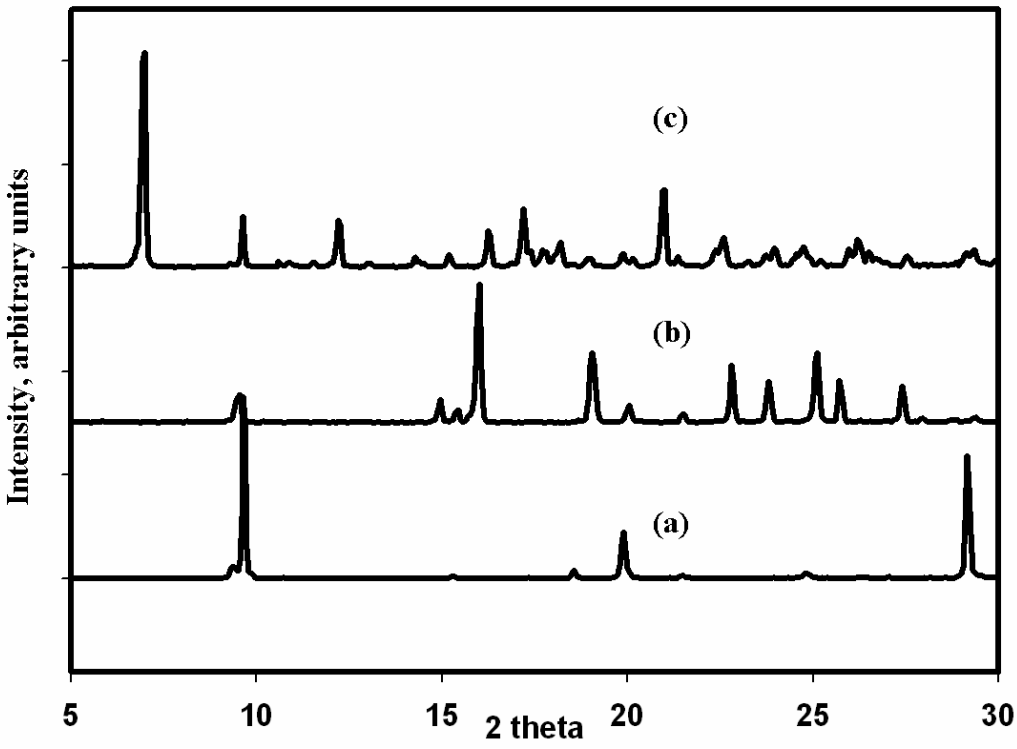

Fig. I-7b. XRD patterns of (a) sulfamethazine (SFZ), (b) saccharin (SAC) and (c) SFZ-SAC cocrystal prepared by the slurry method.

I-8. Theophylline (TPL)- Saccharin(SAC)

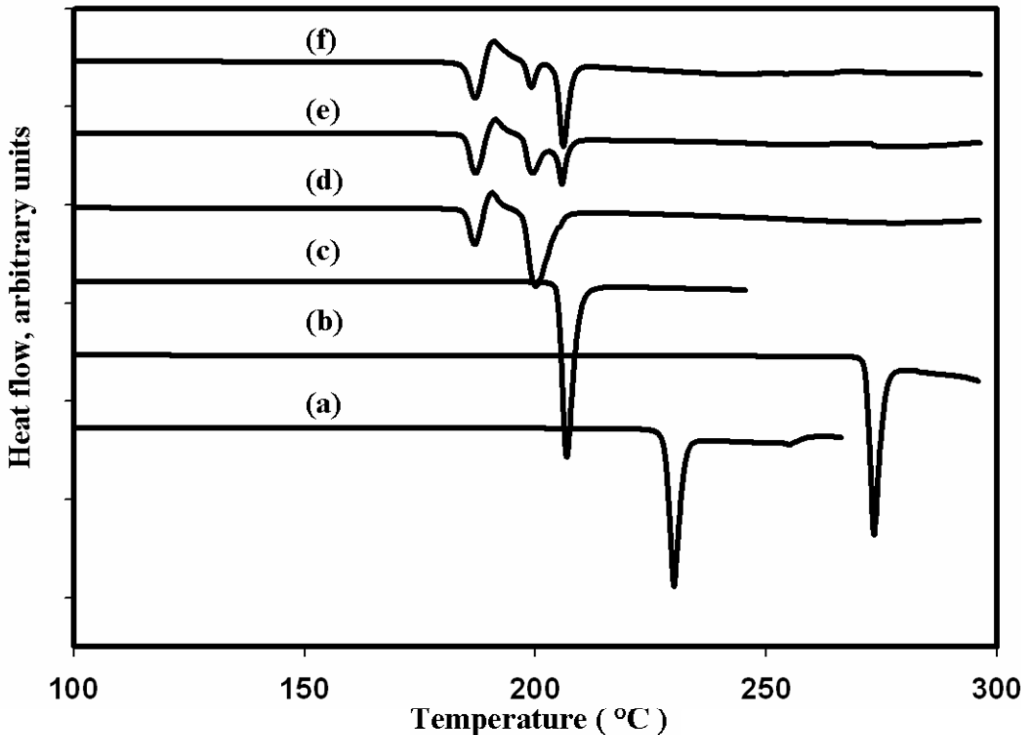

Fig. I-8a. DSC heating curves of (a) saccharin (SAC), (b) theophylline (TPL) and (c) TPL-SAC cocrystal prepared by the slurry method. The curves (d) (e) and (f) are physical mixtures of TPL: SAC at 1:2, 1:1 and 2:1 molar ratios, respectively.

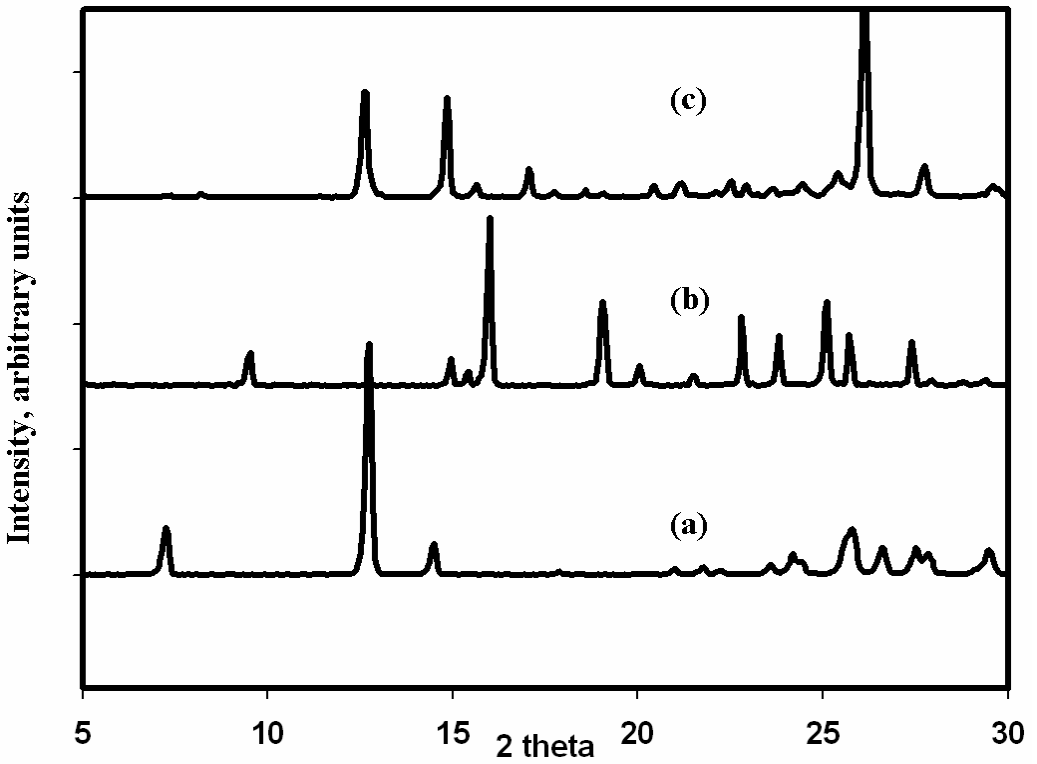

Fig. I-8b. XRD patterns of (a) theophylline (TPL), (b) saccharin (SAC) and (c) TPL-SAC cocrystal prepared by the slurry method.

II. Reported cocrystal

II-1. Caffeine (CAF)-Glutaric acid (GLA)

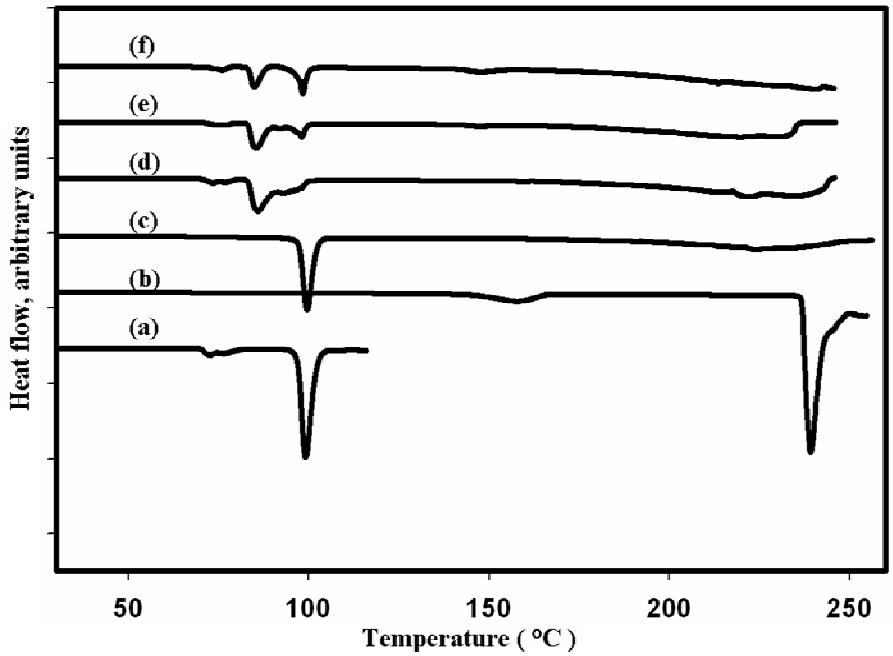

Fig. II-1. DSC heating curves of (a) glutaric acid (GLA),(b) caffeine (CAF) and (c) CAF-GLA cocrystal prepared by solid state grinding. The curves (d) (e) and (f) are physical mixtures of CAF: GLA at 1:2, 1:1 and 2:1 molar ratios, respectively.

II-2. Carbamazepine(CBZ)- Nicotinamide(NCT)

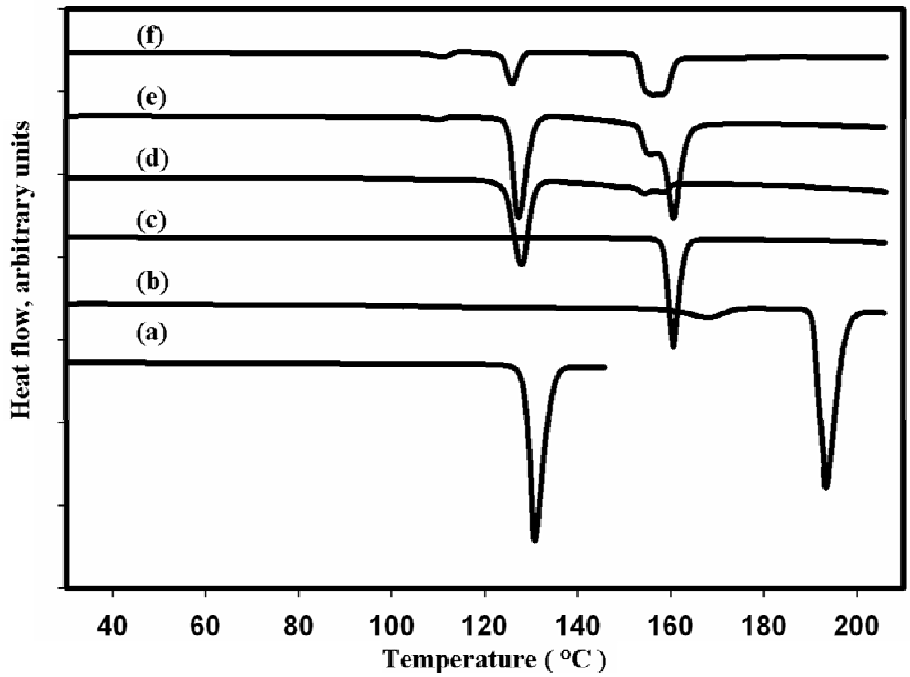

Fig. II-2. DSC heating curves of (a) nicotinamide (NCT), (b) carbamazepine(CBZ) and (c) CBZ-NCT cocrystal prepared by the slurry method. The curves (d) (e) and (f) are physical mixtures of CBZ: NCT at 1:2, 1:1 and 2:1 molar ratios, respectively.

II-3. Carbamazepine(CBZ)- Saccharin (SAC)

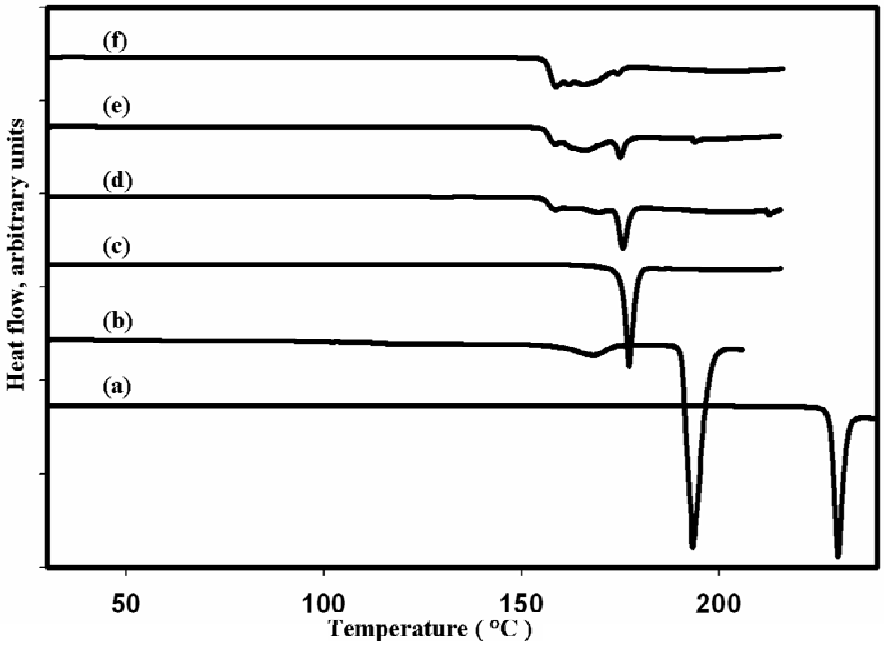

Fig. II-3. DSC heating curves of (a) saccharin (SAC), (b) carbamazepine(CBZ) and (c) CBZ-SAC cocrystal prepared by the slurry method. The curves (d) (e) and (f) are physical mixtures of CBZ: SAC at 1:2, 1:1 and 2:1 molar ratios, respectively.

II-4. Sulfamethazine(SFZ)- Salicylic acid (SAA)

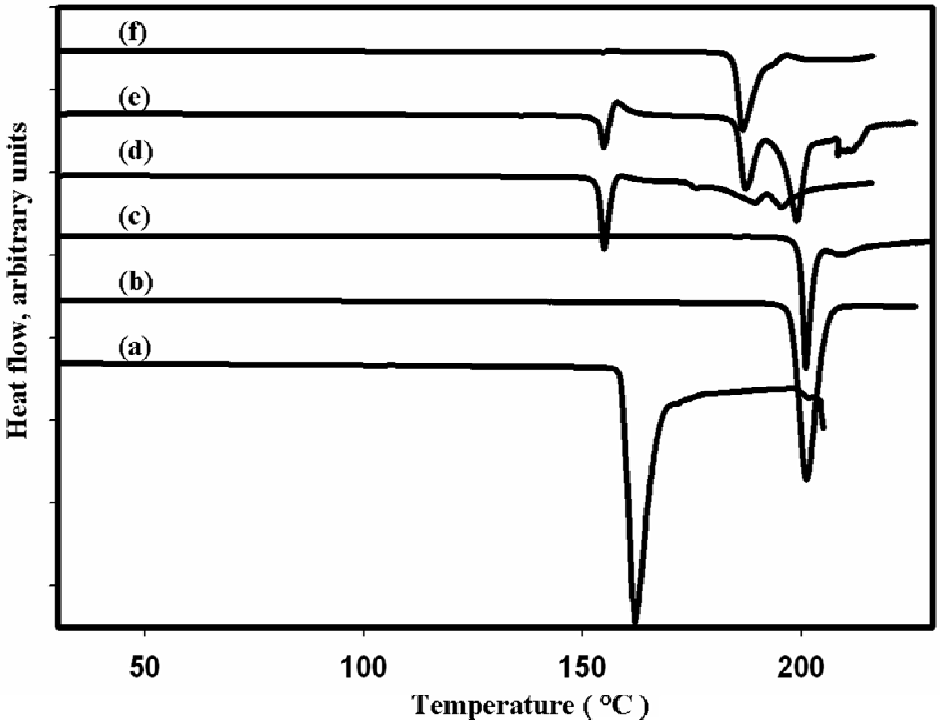

Fig. II-4. DSC heating curves of (a) salicylic acid (SAA), (b) sulfamethazine(SFZ) and (c) SFZ-SAA cocrystal prepared by the slurry method. The curves (d) (e) and (f) are physical mixtures of SFZ: SAA at 1:2, 1:1 and 2:1 molar ratios, respectively.

II-5. Theophylline(TPL)- Glutaric acid (GLA)

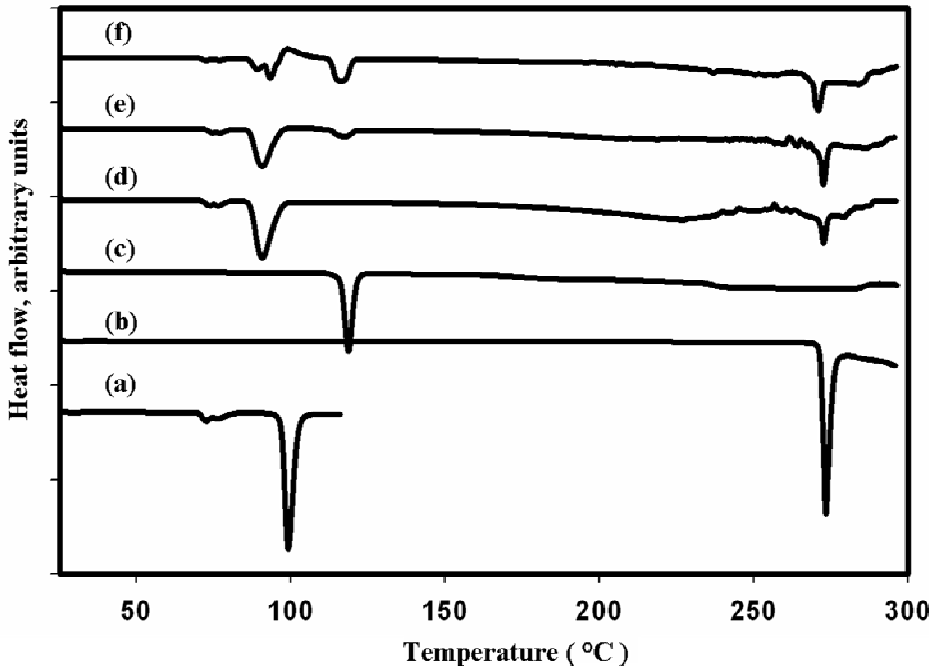

Fig. II-5. DSC heating curves of (a) glutaric acid (GLA), (b) theophylline (TPL) and (c) TPL-GLA cocrystal prepared by the slurry method. The curves (d) (e) and (f) are physical mixtures of TPL: GLA at 1:2, 1:1 and 2:1 molar ratios, respectively.

I-6. Theophylline (TPL)-Nicotinamide(NCT)

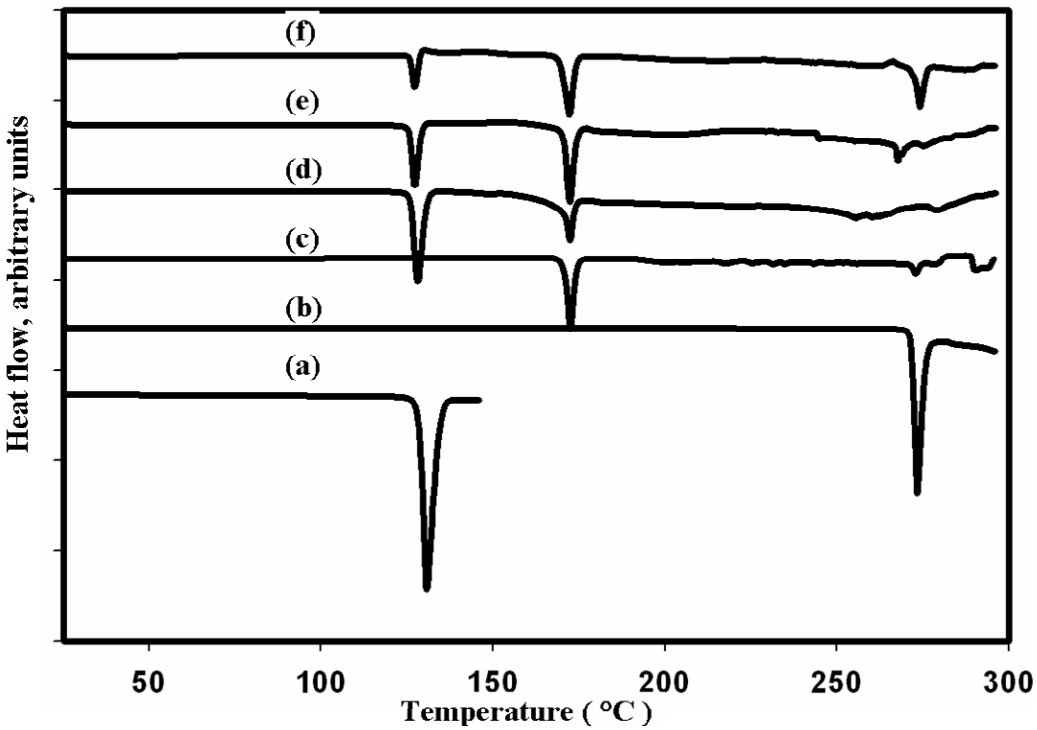

Fig. I-6. DSC heating curves of (a) nicotinamide (NCT), (b) theophylline (TPL) and (c) TPL-NCT cocrystal prepared by the slurry method. The curves (d) (e) and (f) are physical mixtures of TPL: NCT at 1:2, 1:1 and 2:1 molar ratios, respectively.

II-7. Theophylline (TPL)- Salicylic acid (SAA)

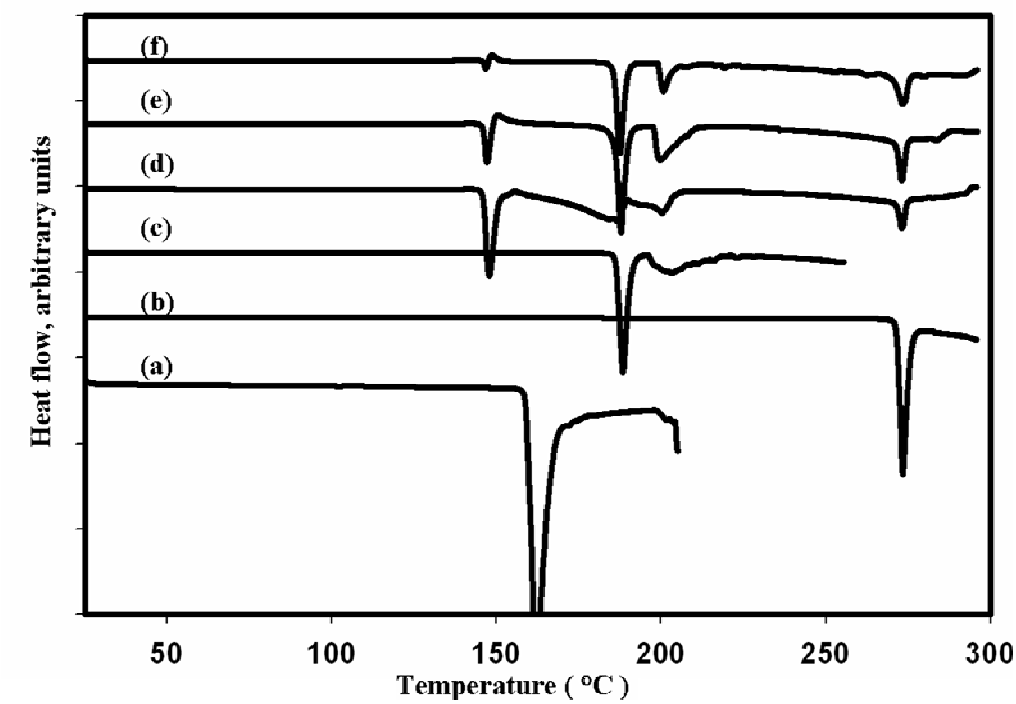

Fig. II-7. DSC heating curves of (a) salicylic acid (SAA), (b) theophylline (TPL) and (c) TPL-SAA cocrystal prepared by the slurry method. The curves (d) (e) and (f) are physical mixtures of TPL: SAA at 1:2, 1:1 and 2:1 molar ratios, respectively.

II-8. Theophylline (TPL)-Urea (URE)

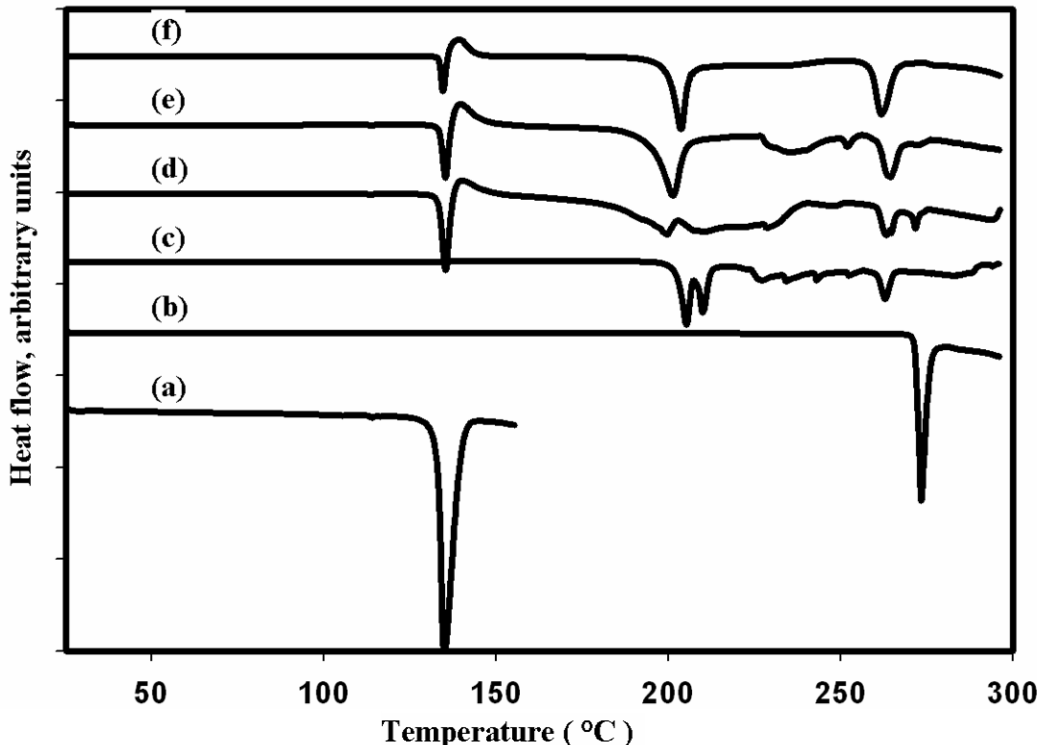

Fig. II-8. DSC heating curves of (a) urea (URE), (b) theophylline (TPL) and (c) TPL-URE cocrystal prepared by the slurry method. The curves (d) (e) and (f) are physical mixtures of TPL: URE at 1:2, 1:1 and 2:1 molar ratios, respectively.

III. No cocrystal formation

III-1. Caffeine (CAF)- Nicotinamide (NCT)

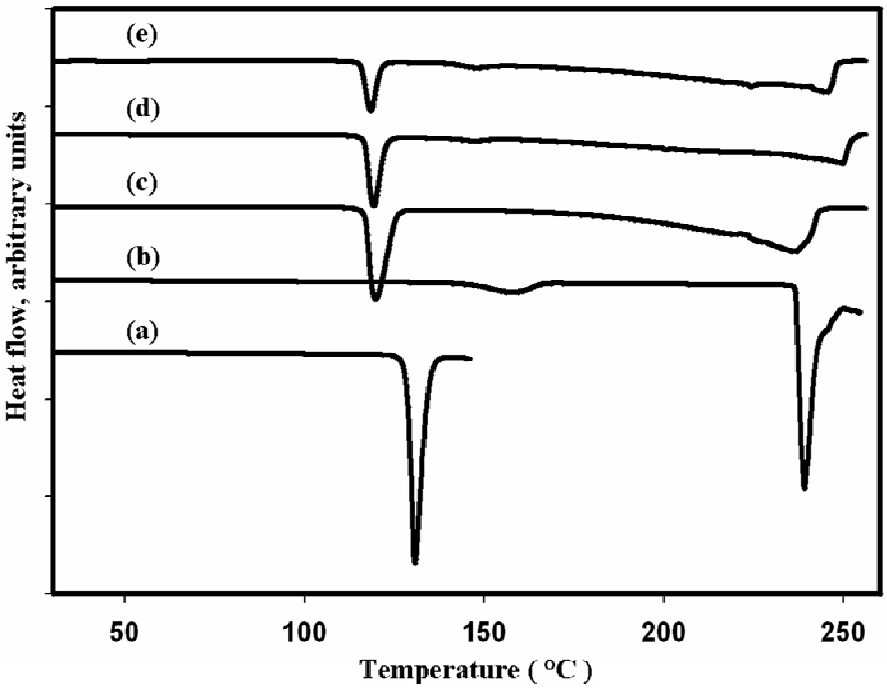

Fig. III-1. DSC heating curves of (a) nicotinamide (NCT), (b) caffeine (CAF), (c) (d) and (e) CAF: NCT physical mixtures at 1:2, 1:1 and 2:1 molar ratios, respectively.

III-2. Caffeine (CAF)- Urea (URE)

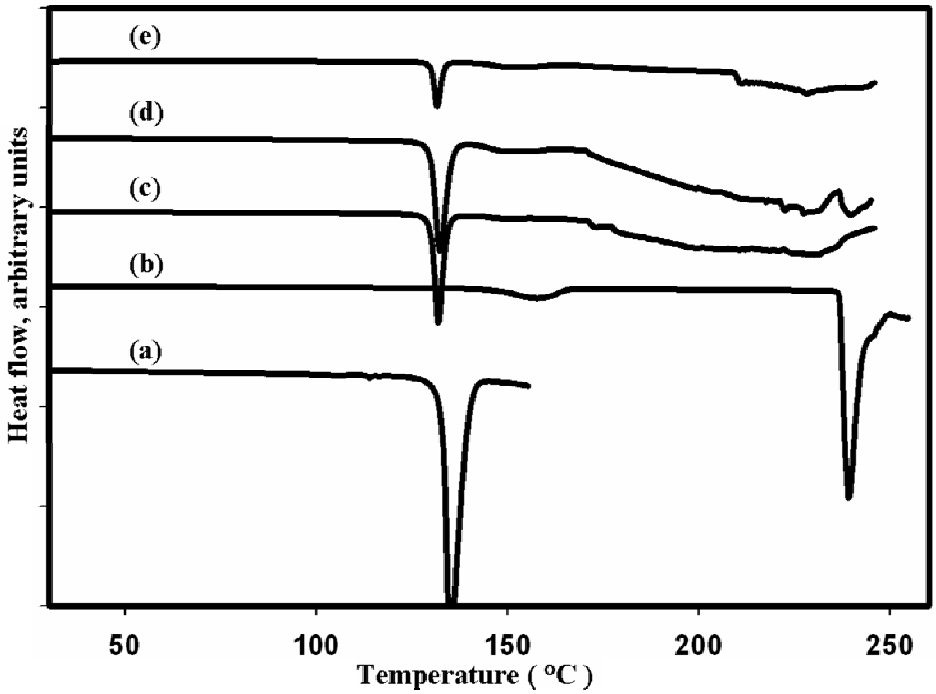

Fig. III-2. DSC heating curves of (a) urea (URE), (b) caffeine (CAF), (c) (d) and (e) CAF: URE physical mixtures at 1:2, 1:1 and 2:1 molar ratios, respectively.

III-3. Sulfamethazine(SFZ)- Glutaric acid (GLA)

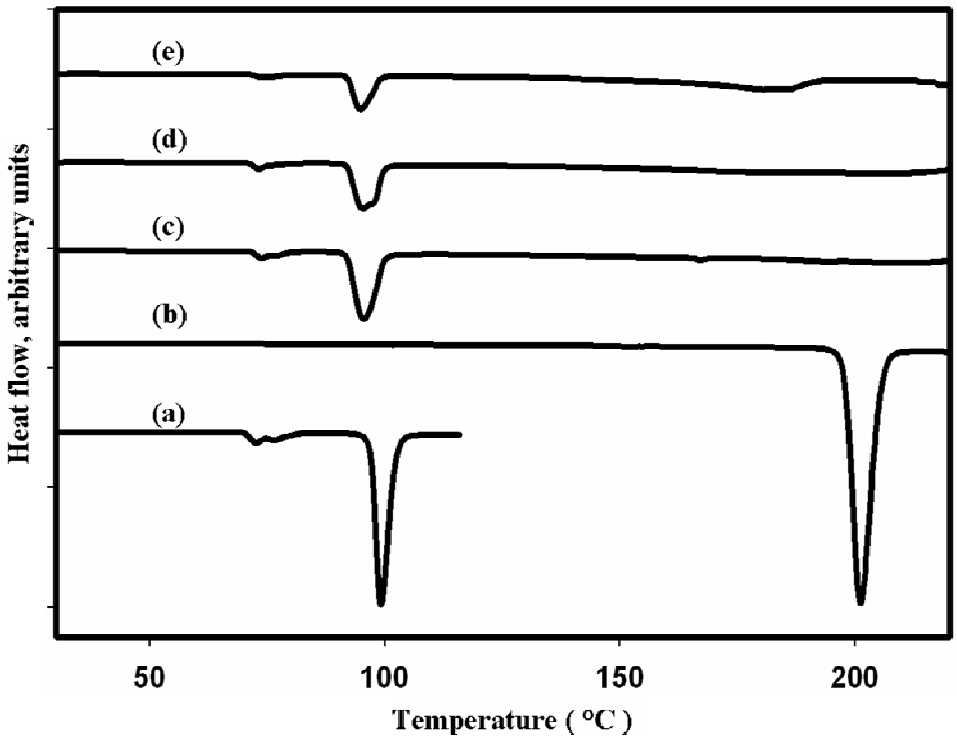

Fig. III-3. DSC heating curves of (a) glutaric acid (GLA), (b) sulfamethazine(SFZ), (c) (d) and (e) SFZ: GLA physical mixtures at 1:2, 1:1 and 2:1 molar ratios, respectively.

III-4. Sulfamethazine(SFZ)- Urea (UR)

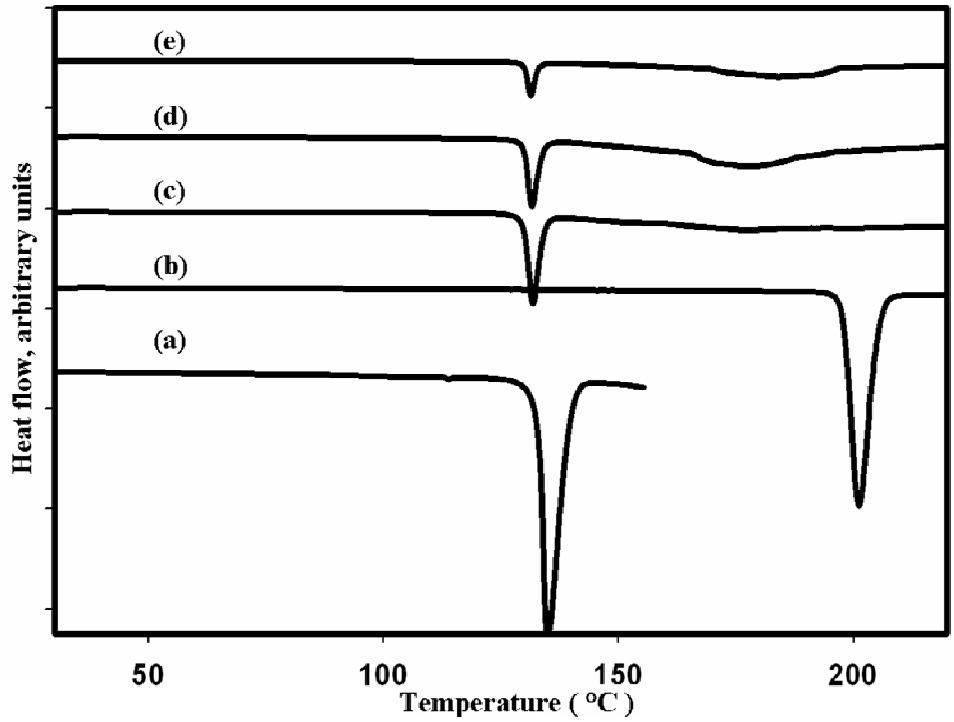

Fig. III-4. DSC heating curves of (a) urea (URE), (b) sulfamethazine(SFZ), (c) (d) and (e) SFZ: URE physical mixtures at 1:2, 1:1 and 2:1 molar ratios, respectively.