

**Evaluating the Use of Differential Scanning Calorimetry for the Analysis of Illicit
Substances and Their Adulterants**

Supplementary Files

Supplementary Table 1: Overview of mixtures prepared with sugars.

Mixture Components	Composition (weight %)				
	10:90	30:70	50:50	70:30	90:10
Caffeine/D-Glucose	✓	✓	✓	✓	✓
D-Glucose/D-Fructose			✓		
D-Fructose/Caffeine			✓	✓	
Sucrose/Caffeine			✓		

Supplementary Table 2: Overview of two-component mixtures prepared with ephedrine HCl.

Mixture Components	Composition (weight %)				
	10:90	30:70	50:50	70:30	90:10
Ephedrine/Caffeine	✓	✓	✓	✓	✓
Ephedrine/Paracetamol	✓	✓	✓	✓	✓
Ephedrine/4-Methoxyphenol	✓	✓	✓	✓	✓

Supplementary Table 3: Overview of three-component mixtures prepared with ephedrine HCl.

Mixture Components	Composition (weight %)					
	35:60:5	40:50:10	40:40:20	40:30:30	40:20:40	40:10:50
Ephedrine/Caffeine/ Paracetamol	✓	✓		✓		✓
Ephedrine/Caffeine/ Sorbitol		✓	✓	✓	✓	✓

Supplementary Table 4: Overview of the mixtures prepared with common adulterants.

Mixture Components	Composition (weight %)					
	30:70	50:50	70:30	90:10	33:33:33	60:20:20
Caffeine/Paracetamol/Dimethyl Sulfone					✓	✓
Caffeine/Paracetamol/Magnesium Stearate					✓	
Caffeine/Aminophenazone		✓				
Caffeine/Aspirin		✓				
Caffeine/Benzocaine		✓				
Caffeine/Citric Acid		✓				
Caffeine/Cellulose		✓				
Caffeine/Creatinine		✓				
Caffeine/Dimethyl Sulfone		✓				
Caffeine/Ibuprofen		✓				
Caffeine/Inositol		✓				
Caffeine/Lidocaine		✓				
Caffeine/Magnesium Stearate		✓				
Caffeine/Maltose		✓				
Caffeine/Paracetamol		✓	✓	✓		
Caffeine/Phenacetin		✓				
Caffeine/Phenobarbital		✓				
Caffeine/Phenolphthalein		✓				
Caffeine/Quinine		✓				
Caffeine/Salicylamide		✓				
Caffeine/Sorbitol		✓				
Caffeine/Starch		✓				
Caffeine/Tetramisole HCl		✓				
Caffeine/Thiamine		✓				
Paracetamol/Aminophenazone		✓				
Paracetamol/Aspirin		✓				
Paracetamol/Benzocaine		✓				
Paracetamol/Citric Acid		✓				
Paracetamol/Cellulose		✓				
Paracetamol/Creatinine		✓				
Paracetamol/Dimethyl Sulfone		✓				

Paracetamol/Ibuprofen		✓			
Paracetamol/Inositol		✓			
Paracetamol/Lidocaine		✓			
Paracetamol/Magnesium Stearate	✓	✓			
Paracetamol/Maltose		✓			
Paracetamol/Phenacetin		✓			
Paracetamol/Phenobarbital		✓			
Paracetamol/ Phenolphthalein		✓			
Paracetamol/Quinine		✓			
Paracetamol/Salicylamide		✓			
Paracetamol/Sorbitol		✓			
Paracetamol/Starch		✓			
Paracetamol/Thiamine		✓			
Tetramisole HCl/ Aminophenazone		✓			
Tetramisole HCl/Benzocaine		✓			
Tetramisole HCl/Citric Acid		✓			
Tetramisole HCl/Creatinine		✓			
Tetramisole HCl/Ibuprofen		✓			
Tetramisole HCl/Inositol		✓			
Tetramisole HCl/Lidocaine		✓			
Tetramisole HCl/Maltose		✓			
Tetramisole HCl/Paracetamol		✓			
Tetramisole HCl/Phenacetin		✓			
Tetramisole HCl/ Phenobarbital		✓			
Tetramisole HCl/ Phenolphthalein		✓			
Tetramisole HCl/Quinine		✓			
Tetramisole HCl/Salicylamide		✓			
Tetramisole HCl/Sorbitol		✓			
Tetramisole HCl/Starch		✓			
Tetramisole HCl/Thiamine		✓			

Supplementary Table 5: Peaks present in the thermograms of the mixtures containing sugars.

Sample ID	Peak 1		Peak 2		Peak 3		Peak 4	
	°C	W/g	°C	W/g	°C	W/g	°C	W/g
Caffeine/D-Glucose 10:90	73.58	-0.506	152.32	-1.564				
Caffeine/D-Glucose 30:70	73.98	-0.310	155.56	-1.320				
Caffeine/D-Glucose 50:50	75.26	-0.496	155.04	-1.315	200.33	-0.952	223.34	-1.695
Caffeine/D-Glucose 70:30	77.98	-0.345	156.48	-0.854	201.73	-0.888	232.40	-1.077
Caffeine/D-Glucose 90:10	158.04	-0.845	215.25	-1.014	242.39	-1.068		
D-Glucose/D-Fructose 50:50	117.87	-1.194	154.58	-1.031				
D-Fructose/Caffeine 50:50	121.41	-1.372	193.51	-1.699				
D-Fructose/Caffeine 70:30	119.70	-1.802	190.82	-2.903				
Sucrose/Caffeine 50:50	158.28	-0.667	189.17	-2.125	209.50	-0.870	228.63	-2.052

Supplementary Table 6: Peaks present in the thermograms of the three component mixtures with ephedrine HCl.

Sample ID	Peak 1		Peak 2		Peak 3	
	°C	W/g	°C	W/g	°C	W/g
Ephedrine/Caffeine/ Paracetamol 35:60:5	128.67	-0.022	154.23	0.000	191.38	-0.248
Ephedrine/Caffeine/ Paracetamol 40:50:10	128.42	-0.151	184.1	-0.197		
Ephedrine/Caffeine/ Paracetamol 40:30:30	131.21	-0.551	248.43	-0.144		
Ephedrine/Caffeine/ Paracetamol 40:10:50	134.22	-0.980				
Ephedrine/Caffeine/ Sorbitol 40:50:10	96.47	-0.230	186.28	-0.141		
Ephedrine/Caffeine/ Sorbitol 40:40:20	96.70	-2.400	183.95	-2.676		
Ephedrine/Caffeine/ Sorbitol 40:30:30	97.25	-3.116				
Ephedrine/Caffeine/ Sorbitol 40:20:40	96.87	-3.245				
Ephedrine/Caffeine/ Sorbitol 40:10:50	97.61	-2.282				

Supplementary Table 7: Peaks present in the thermograms of the mixtures with ephedrine HCl and caffeine.

Sample ID	Peak 1		Peak 2		Peak 3	
	°C	W/g	°C	W/g	°C	W/g
Ephedrine/Caffeine 10:90	159.16	-0.338	199.19	-0.766	230.83	-1.586
Ephedrine/Caffeine 30:70	159.00	-0.388	199.73	-1.898	225.28	-0.788
Ephedrine/Caffeine 50:50	159.82	-0.272	200.25	-3.732		
Ephedrine/Caffeine 70:30	200.60	-4.215				
Ephedrine/Caffeine 90:10	200.95	-1.989	211.58	-2.362		

Supplementary Table 8: Peaks present in the thermograms of the mixtures with ephedrine HCl and paracetamol.

Sample ID	Peak 1		Peak 2	
	°C	W/g	°C	W/g
Ephedrine/Paracetamol 10:90	136.63	-1.436	164.02	-2.017
Ephedrine/Paracetamol 30:70	138.51	-3.299		
Ephedrine/Paracetamol 50:50	138.77	-2.869		
Ephedrine/Paracetamol 70:30	137.98	-1.966	194.95	-0.717
Ephedrine/Paracetamol 90:10	137.23	-1.462	205.70	-1.125

Supplementary Table 9: Peaks present in the thermograms of the mixtures with ephedrine HCl and MEHQ.

Sample ID	Peak 1		Peak 2	
	°C	W/g	°C	W/g
Ephedrine/4-Methoxyphenol 10:90	57.32	-2.354		
Ephedrine/4-Methoxyphenol 30:70	51.84	-2.790	245.54	-1.730
Ephedrine/4-Methoxyphenol 50:50	53.46	-1.350	245.71	-0.742
Ephedrine/4-Methoxyphenol 70:30	53.09	-1.627	176.49	-0.699
Ephedrine/4-Methoxyphenol 90:10	52.03	-0.701	206.53	-0.981

Supplementary Table 10: Peaks present in the thermograms of the caffeine mixtures.

Sample ID	Peak 1		Peak 2		Peak 3		Peak 4		Peak 5	
	°C	W/g	°C	W/g	°C	W/g	°C	W/g	°C	W/g
Caffeine/Aminophenazone	106.35	-1.363	151.06	-0.144	161.65	-0.129	233.17	0.414		
Caffeine/Aspirin	114.81	-2.485	208.81	0.044						
Caffeine/ Benzocaine	83.10	-3.293								
Caffeine/Citric Acid	67.54	-1.234	130.53	-0.581						
Caffeine/Cellulose	159.65	-0.019	237.20	-2.949						
Caffeine/ Creatinine	159.83	0.140	232.70	-1.500						
Caffeine/Dimethyl Sulfone	107.46	-2.444	147.09	-0.163	179.77	-0.179				
Caffeine/ Ibuprofen	75.04	-2.474	147.90	0.050						
Caffeine/Inositol	158.40	0.025	226.47	-6.643						
Caffeine/ Lidocaine	67.91	-2.164	148.54	-0.061	186.23	-0.045				
Caffeine/ Magnesium Stearate	94.29	-0.176	123.13	-1.159	160.38	-0.176	237.57	-2.910		
Caffeine/Maltose	130.76	-1.760	159.48	-0.168	211.99	-0.454				
Caffeine/ Paracetamol 50:50	144.33	-3.557								
Caffeine/ Paracetamol 70:30	144.14	-2.916	257.96	-1.814						
Caffeine/ Paracetamol 90:10	142.98	-0.882	157.41	-0.456	227.27	-1.199				
Caffeine/ Phenacetin	128.93	-3.061	149.89	-0.099	192.55	-0.121				
Caffeine/ Phenobarbital	161.45	-0.060	172.32	-0.069	214.10	-0.347	230.20	-1.079	243.09	-0.319
Caffeine/ Phenolphthalein	159.45	0.004	181.25	-1.952						
Caffeine/Quinine	161.44	-2.095								
Caffeine/Salicylamide	126.67	-2.666	149.28	-3.686						
Caffeine/Sorbitol	100.28	-2.579	161.59	-0.177	202.86	-0.457				
Caffeine/Starch	155.31	0.048	237.15	-3.361						
Caffeine/ Tetramisole HCl	160.01	0.199	212.85	-2.544						
Caffeine/Thiamine	160.00	0.202	216.64	0.169	233.26	-1.918				

Supplementary Table 11: Peaks present in the thermograms of the three component mixtures of common cutting agents.

Sample ID	Peak 1		Peak 2		Peak 3		Peak 4	
	°C	W/g	°C	W/g	°C	W/g	°C	W/g
Caffeine/ Paracetamol/ Dimethyl Sulfone 33:33:33	99.18	-2.543	177.33	-0.647	266.18	-0.809		
Caffeine/ Paracetamol/ Dimethyl Sulfone 60:20:20	99.75	-1.682	148.72	-0.495				
Caffeine/ Paracetamol/ Magnesium Stearate 33:33:33	94.66	-0.294	123.55	-1.014	150.36	-1.102	228.76	-0.465

Supplementary Table 12: Peaks present in the thermograms of the paracetamol mixtures.

Sample ID	Peak 1		Peak 2		Peak 3		Peak 4	
	°C	W/g	°C	W/g	°C	W/g	°C	W/g
Paracetamol/ Aminophenazone	86.81	-0.901	229.38	0.823				
Paracetamol/ Aspirin	122.05	-3.049	195.23	0.117				
Paracetamol/ Benzocaine	88.46	-3.659	137.66	-0.201				
Paracetamol/Citric Acid	62.83	-0.958	79.89	-0.112	133.40	-1.538		
Paracetamol/ Cellulose	170.89	-2.520						
Paracetamol/ Creatinine	158.68	-3.016						
Paracetamol/ Dimethyl Sulfone	98.84	-4.185						
Paracetamol/ Ibuprofen	77.78	-1.887	147.70	-0.470				
Paracetamol/ Inositol	170.13	-3.658	223.66	-4.548				
Paracetamol/ Lidocaine	61.54	-0.604	132.07	-0.115				
Paracetamol/ Magnesium Stearate 50:50	120.15	-1.126	170.00	-3.514				
Paracetamol/ Magnesium Stearate 30:70	94.70	-0.756	123.76	-2.744	169.72	-3.475		
Paracetamol/ Maltose	131.71	-1.816	164.83	-1.553				
Paracetamol/ Phenacetin	118.65	-4.558						
Paracetamol/ Phenobarbital	153.60	-1.560						
Paracetamol/ Phenolphthalein	164.67	-4.757						
Paracetamol/ Quinine	140.21	-1.209						
Paracetamol/ Salicylamide	122.54	-5.775						
Paracetamol/ Sorbitol	99.76	-3.731	158.27	-1.044				
Paracetamol/ Starch	91.34	-0.111	170.74	-5.342				
Paracetamol/ Thiamine	82.63	0.028	148.78	-1.294	209.37	-0.020	236.86	-0.128

Supplementary Table 13: Peaks present in the thermograms of the tetramisole HCl mixtures.

Sample ID	Peak 1		Peak 2		Peak 3		Peak 4		Peak 5	
	°C	W/g	°C	W/g	°C	W/g	°C	W/g	°C	W/g
Tetramisole HCl/Aminophenazone	107.51	-0.934	231.31	0.240						
Tetramisole HCl/Benzocaine	86.66	-1.290								
Tetramisole HCl/Citric Acid	67.98	-0.947	112.02	-0.475						
Tetramisole HCl/Creatinine	191.89	-1.216	237.03	-0.111						
Tetramisole HCl/Ibuprofen	78.09	-2.147	107.79	-0.196	203.28	-0.268				
Tetramisole HCl/Inositol	182.51	-1.687	211.01	-0.253						
Tetramisole HCl/Lidocaine	68.75	-1.794	222.51	0.520						
Tetramisole HCl/Maltose	130.79	-1.475								
Tetramisole HCl/Paracetamol	120.95	-0.625	146.31	-0.330	169.42	-0.293				
Tetramisole HCl/Phenacetin	120.61	-2.582								
Tetramisole HCl/Phenobarbital	134.58	-0.069	174.26	-0.135	188.83	-0.184	213.60	0.228	229.96	0.192
Tetramisole HCl/Phenolphthalein	157.62	-0.346	210.02	-0.330	228.79	-0.405				
Tetramisole HCl/Quinine	133.74	-0.194	165.73	-0.226	224.35	0.663				
Tetramisole HCl/Salicylamide	102.48	-1.457								
Tetramisole HCl/Sorbitol	99.66	-2.017	229.23	-0.193						
Tetramisole HCl/ Starch	209.36	-1.690								
Tetramisole HCl/Thiamine	82.18	0.205	220.28	-1.497						

Supplementary Table 14: Peaks present in the crude and purified NPS.

Sample ID	Peak 1		Peak 2		Peak 3	
	°C	W/g	°C	W/g	°C	W/g
Methylone Crude	234.39	-2.742	239.73	4.427		
Methylone Pure	235.88	-3.061	241.08	4.685		
MMC Crude	185.65	-0.578	221.01	-1.437	241.17	-3.187
MMC Pure	207.00	-1.158	234.10	-0.819	252.20	-2.030

Supplementary Table 15: Peaks present in the thermograms of the cocaine HCl mixtures.

Sample ID	Peak 1		Peak 2		Peak 3		Peak 4		Peak 5	
	°C	W/g	°C	W/g	°C	W/g	°C	W/g	°C	W/g
Cocaine/ Aminophenazone	109.36	-2.350	219.63	0.282						
Cocaine/Benzocaine	90.54	-3.171	180.86	-0.446	235.22	-1.041				
Cocaine/Caffeine	160.41	-0.290	195.94	-4.312	230.00	-0.795				
Cocaine/Creatinine	190.54	-1.001	223.74	-0.095						
Cocaine/Ibuprofen	77.29	-3.533	177.83	-0.476	224.90	-0.587				
Cocaine/Inositol	191.78	-1.603	221.05	-1.529	222.88	-1.524	237.77	-0.060		
Cocaine/Lidocaine	70.07	-2.470	182.24	-0.435	230.89	-0.693				
Cocaine/Maltose	132.29	-2.346	161.16	-0.440						
Cocaine/Paracetamol	133.02	-0.742	153.80	-0.664	163.12	-0.677	185.30	-0.540	238.85	-1.156
Cocaine/Phenacetin	123.76	-4.215	238.69	-0.873						
Cocaine/Salicylamide	107.65	-1.207	172.04	-0.302	239.10	-0.951				
Cocaine/Starch	204.41	-4.148	228.49	-0.250						
Cocaine/Tetramisole HCl	197.54	-2.121								

Supplementary Table 16: Peaks present in the thermograms of the heroin HCl mixtures.

Sample ID	Peak 1		Peak 2		Peak 3		Peak 4		Peak 5	
	°C	W/g	°C	W/g	°C	W/g	°C	W/g	°C	W/g
Heroin/Citric Acid	64.74	-1.396	108.20	-0.361	151.06	-1.710	191.57	-3.503		
Heroin/Caffeine	96.88	-0.236	117.34	-0.237	161.78	-0.411	200.92	-0.540	230.73	-1.451
Heroin/Inositol	227.22	-6.672								
Heroin/Lidocaine	69.44	-2.599								
Heroin/Paracetamol	142.07	0.058	168.37	-2.303						
Heroin/Phenacetin	107.74	-0.170	123.43	-2.717						
Heroin/Phenobarbital	55.79	0.067	79.31	0.098	103.59	0.167	155.62	0.218	178.57	0.193
	198.12	0.152	207.99	0.138	239.66	0.459				
Heroin/Phenolphthalein	101.12	0.022	120.91	0.039	188.97	-0.077				
Heroin/Quinine	55.05	0.287	101.75	0.507	149.37	0.389	172.92	-0.633		
Heroin/Sorbitol	98.55	-4.431								
Heroin/Tetramisole HCl	107.32	-0.252	126.28	-0.231	166.44	-0.096	218.92	-0.849		
Heroin/Thiamine	91.31	-0.360	106.31	-0.318	219.45	-0.301				

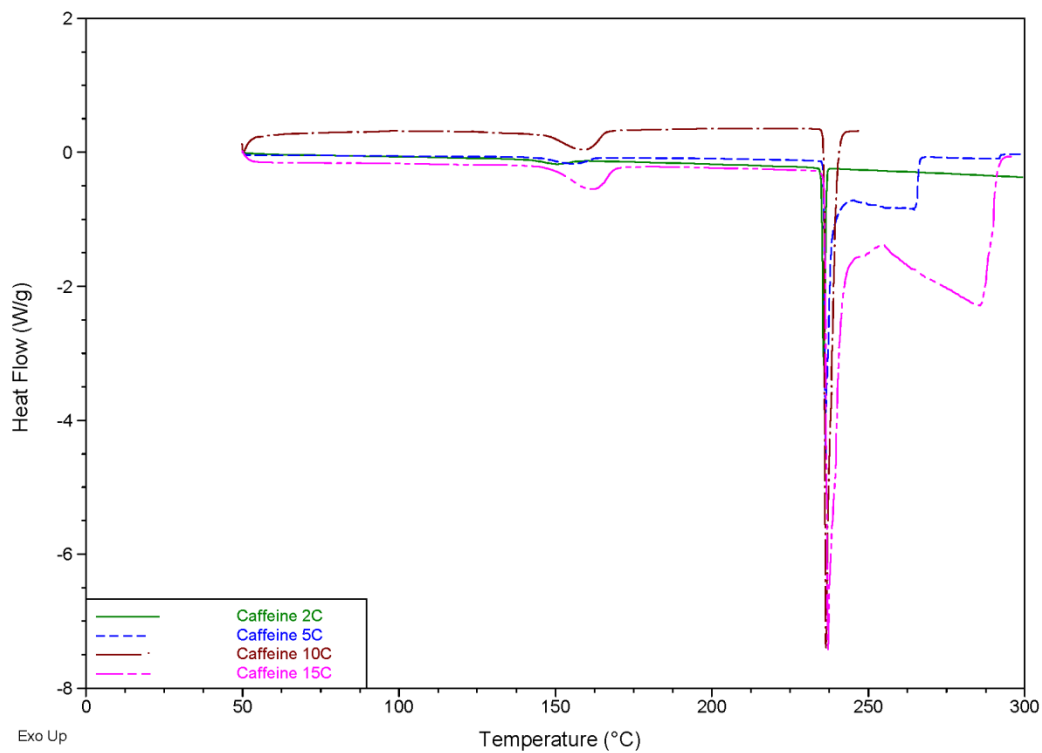
Supplementary Table 17: Peaks present in the thermograms of the MA HCl mixtures.

Sample ID	Peak 1		Peak 2		Peak 3	
	°C	W/g	°C	W/g	°C	W/g
MA/Aspirin	103.01	-1.436	182.75	-0.389		
MA/Caffeine	135.65	-2.584	161.07	-0.288	212.10	-0.354
MA/Dimethyl Sulfone	101.77	-1.148				
MA/Lidocaine	69.31	-2.821	114.06	-0.481		
MA/Paracetamol	103.97	-1.234				

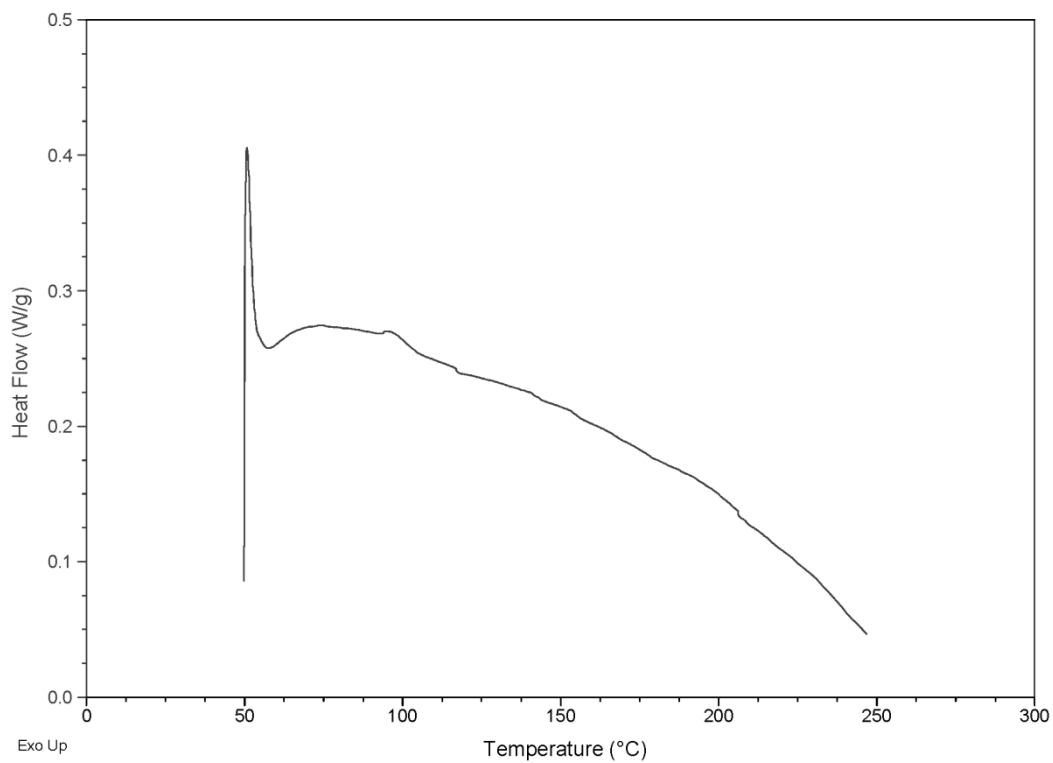
Supplementary Table 18: Peaks present in the thermograms of the MDMA HCl mixtures.

Sample ID	Peak 1		Peak 2		Peak 3		Peak 4	
	°C	W/g	°C	W/g	°C	W/g	°C	W/g
MDMA/Caffeine	63.89	-0.495	103.55	-0.286	147.97	-0.708	212.53	-0.475
MDMA/Cellulose	63.89	-0.678	153.18	-1.481				
MDMA/Dimethyl Sulfone	63.86	-0.305	102.89	-1.877				
MDMA/Magnesium Stearate	65.04	-1.109	91.50	-0.288	119.92	-1.225	152.52	-1.657
MDMA/ Paracetamol	63.83	-0.748	111.20	-0.397				

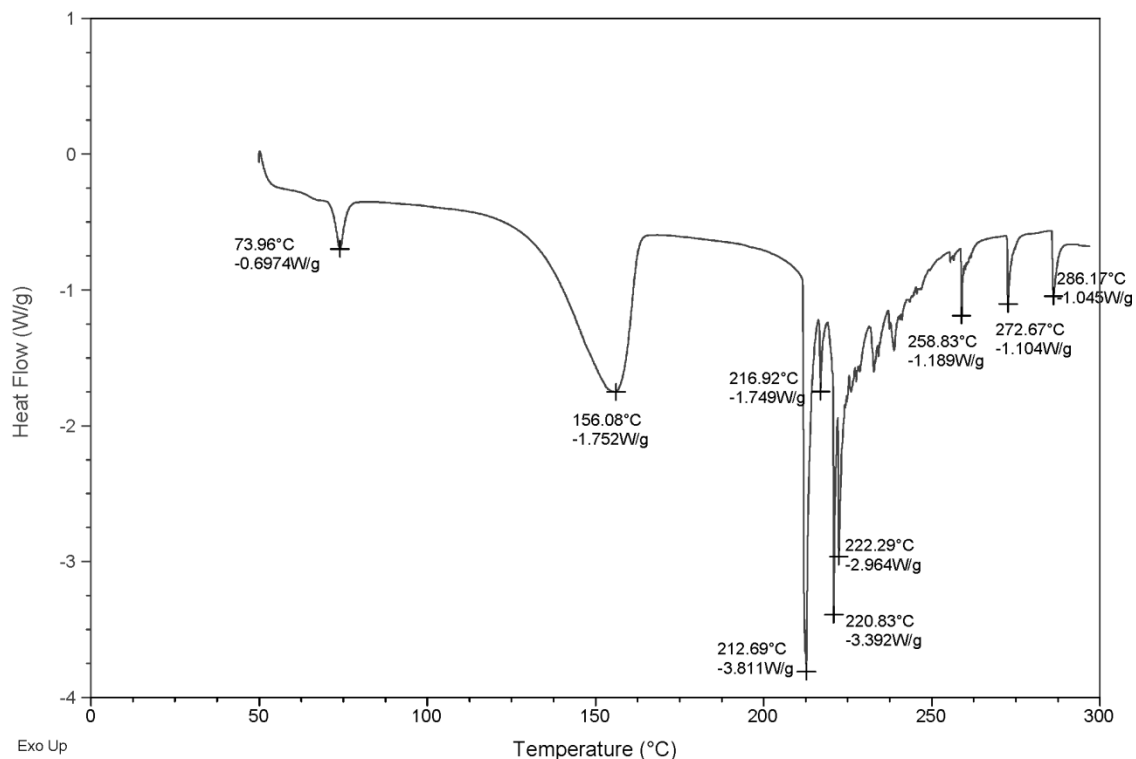
Supplementary Figure 1: Overlaid thermograms of pure caffeine standards run at heating rates of $15\text{ }^{\circ}\text{Cmin}^{-1}$, $10\text{ }^{\circ}\text{Cmin}^{-1}$, $5\text{ }^{\circ}\text{Cmin}^{-1}$ and $2\text{ }^{\circ}\text{Cmin}^{-1}$ (Temperature range: $50\text{-}300\text{ }^{\circ}\text{C}$).



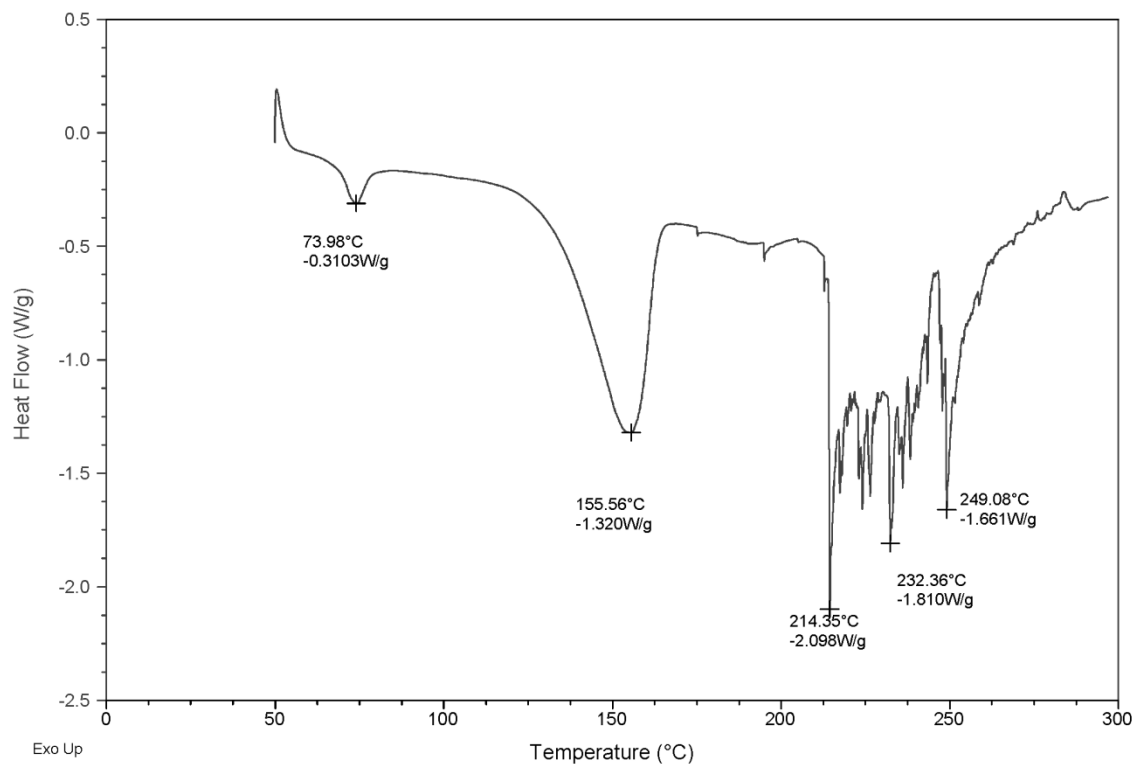
Supplementary Figure 2: Thermogram of the pure sample of phenolphthalein.



Supplementary Figure 3: Thermogram of the pure sample of D-glucose (Temperature range: 50-300 °C).



Supplementary Figure 4: Thermogram for the 30:70 w/w mixture of caffeine and D-glucose (Temperature range: 50-300 °C).



Supplementary Figure 5: Overlaid DSC thermograms of the crude and purified methylene HCl samples (Temperature range: 50-300 °C).

