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**Supporting information for article:**

**New polymorphs of an old drug. Conformational and synthon  
polymorphism of 5-nitrofurazone**

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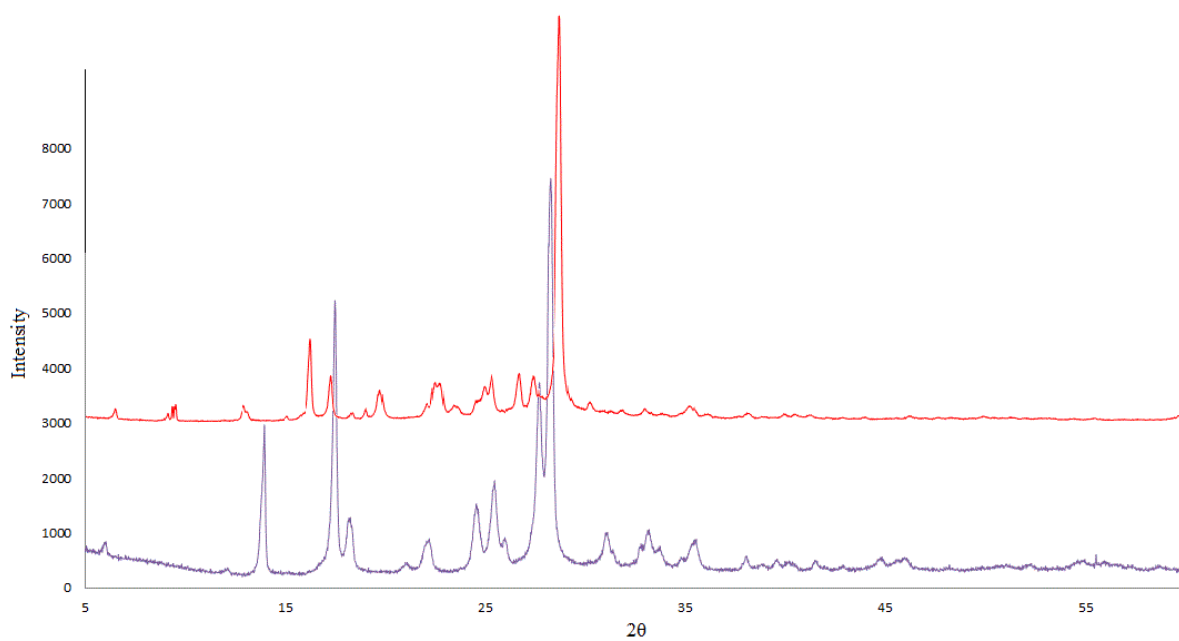
**S1. Power X-Ray Diffraction****S2. Raman Spectroscopy coupled with microscopy****S3. Thermogravimetric Analysis (TGA-DTA)****S4. Differential Scanning Calorimetry (DSC)****Figure S1** X-ray power diffraction patterns of form  $\beta$  (purple) and form  $\gamma$  (red).

Table S1

Structure	RMSD	O4-C6-N3-N2 ( $\tau_1$ )	C3-C4-C5-N2 ( $\tau_2$ )	C5-N2-N3-H1 ( $\tau_3$ )	O4-C6-N3-H1 ( $\tau_4$ )	C3-C4-C5-H5 ( $\tau_5$ )
NFZ01 (Form $\beta$ )	0	-176.40	174.79	-2	4	174
NFZ02 (Form $\gamma$ )	0.041	-174.79	-179.58	-4	5	177
WERVEU (Form $\alpha$ )	1.512	-4.5814	178.283	-12.9536	-175.586	-2.75831
EDELUV	0.082	175.844	-1.89071	-11.9615	9.47162	178.111
TUBQOW	0.086	-178.236	-8.25971	1.72625	2.2552	171.214
EVERED02	0.093	-179.037	0.858448	12.6635	-7.81408	-179.093
BZALSC01	0.106	-178.662	3.50346	-6.45782	1.46918	-175.454
TUBRIR	0.116	-179.35	4.63619	-5.68894	-0.141134	-176.22
IJOXAH	0.117	-177.761	-8.73823	3.25221	-10.4962	171.293
MUKXEV	0.118	178.019	-6.48667	-11.5732	19.0226	173.323
TUBRAJ	0.119	177	18.5598	-2.59624	1.03849	-163.247
LATFIV	0.136	178.019	8.30683	11.1873	-2.65418	-170.174
EVERED	0.14	179.137	-5.07741	7.26989	-14.4621	174.938
LATFER	0.154	179.87	-6.54916	-4.26091	-0.0715084	172.694
TUBQUC	0.155	179.02	-1.51075	-14.4372	-0.839717	178.169
YOYNOP	0.215	-174.251	12.2424	-5.90378	13.3625	-167.953
FUNDUN	0.533	178.435	175.374	-2.65564	10.0818	-0.171567
GAQDOT	0.561	179.447	-178.683	1.05388	-2.56612	1.38813
TAKREC01	0.571	-173.001	-175.336	-16.8244	23.7748	2.40787
YAVVAU	0.574	169.046	179.178	-9.99604	2.75475	-0.887864
KUHGEA	0.575	174.787	178.6	-3.05544	4.37587	-0.269426
KEZKIK	0.615	179.886	0.329944	-7.94651	-0.154906	-179.692
FUDQIE	0.615	179.966	14.6645	-0.393809	-0.0773696	-165.889
EVERED01	0.616	-177.839	1.82849	4.11368	2.20501	-178.212
MOPBUP	0.622	-179.498	-4.07769	2.67764	-11.6731	175.959
YIFTOX	0.622	178.808	-5.26595	-2.56539	10.3577	174.711
DUMZAN	0.624	-174.972	19.0963	1.85811	-0.407912	-161.039
YIFVUF	0.624	179.36	-1.66696	-1.37375	8.54234	178.319
YOYNOP01	0.625	-173.9	11.4121	1.13197	6.15417	-168.574
MOPCAW	0.625	175.327	4.48073	-15.759	14.7786	-175.603
BZALSC10	0.629	-178.737	3.56509	6.13212	-11.2866	-176.561
YAGFIX	0.632	178.175	8.70904	-3.47441	11.1705	-171.318
ETIXOU	0.639	178.209	9.16094	-0.399243	9.85924	-167.888
TUBREN	0.64	-177.998	-18.7017	-0.659326	2.24959	161.321
YEFGOH	0.644	-176.869	3.54182	6.88225	-12.3085	-179.965
PAVZAP	0.656	177.068	-31.6699	-17.8542	-2.92513	148.354
TIVGOU	0.84	178.55	-176.812	-2.48099	2.63207	0.60944
WIGPAF	0.839	-169.806	-176.207	-1.3112	11.5047	3.76197
YEFGIB	0.843	176.124	-164.441	11.4023	-3.84952	15.6505

TAKREC	0.853	173.05	175.282	1.13991	-10.9449	-4.17186
ZAMZUI	0.869	-172.024	178.286	-2.34573	2.23501	-1.21534

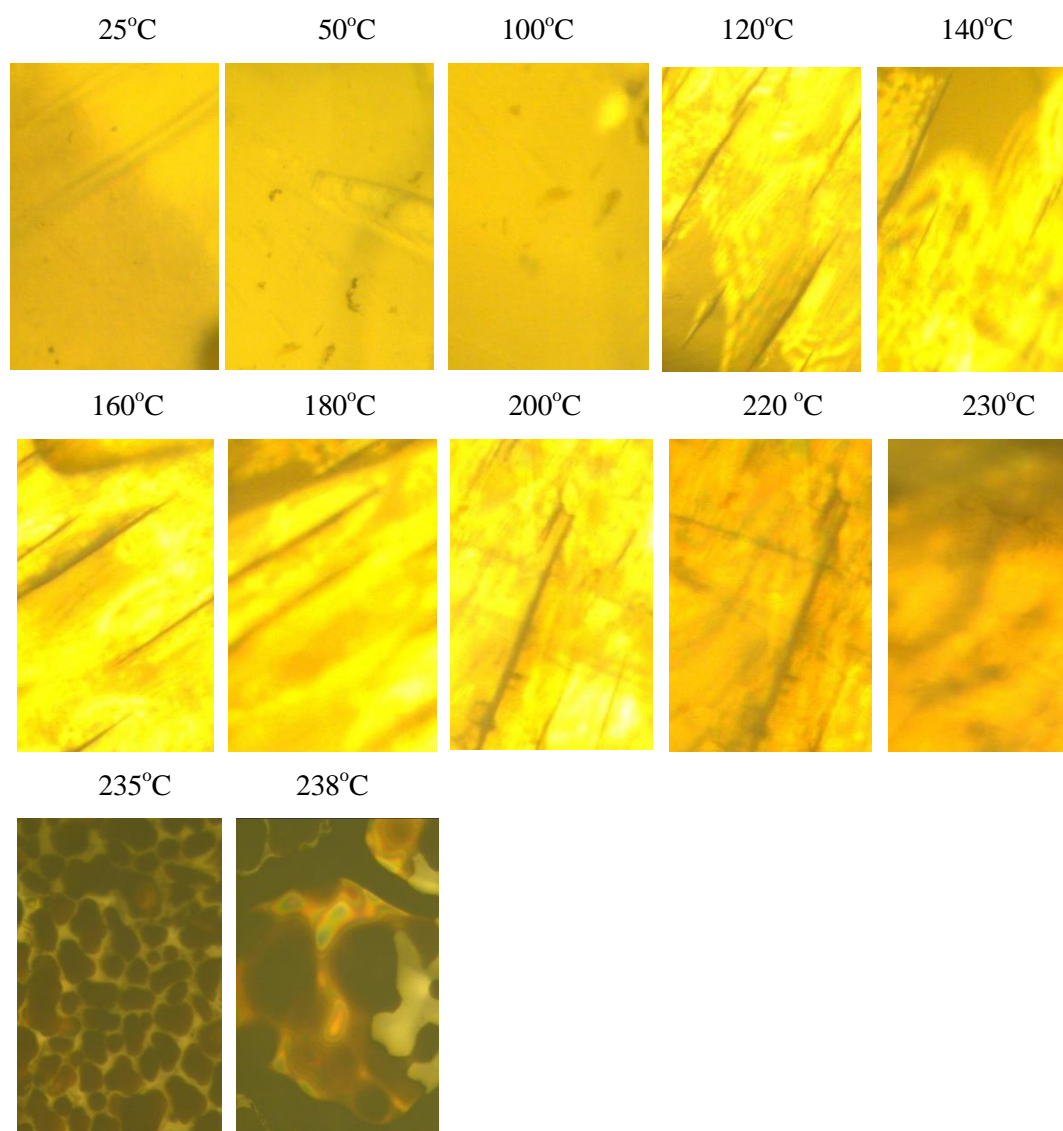
**Table S2** Band position and assignment of the vibrational modes, observed in ATR FT-IR and Raman spectra of two polymorphs.

Assignment	$\beta$ -polymorph		$\gamma$ -polymorph	
	IR	R	IR	R
$\nu_{as}$ NH <sub>2</sub> $\nu$ N-H $\nu_s$ NH <sub>2</sub>	3457 m 3357 m 3287 m 3233 m		3508 m 3429 m 3386 m	
$\nu$ C-H	3154 m 3235 m 3121 m 3014 m		3134 m 3116 m	
	2917 m 2885 m 2850 m			
$\nu_{arom}$ C-H	1817vw 1809vw 1753vw		1818 vw	
$\nu$ C=O	1702 m		1707 s	
$\nu$ C=N Furan ring $\nu$ C=C	1677 m 1646 sh 1629sh	1677 vw	1660 sh 1627 vw	1647v w
$\delta$ NH <sub>2</sub> in plane bend $\delta$ N-H in plane bend	1595sh 1580 s 1566sh	1597 s  1568 w	1595 s 1579 s 1565 s	1598 s 1575 w
Furan ring		1521 w		1530vw 1512 vw 1502 vw
$\nu$ C-C	1535m		1534 m	
$\nu_{as}$ NO <sub>2</sub>	1499 s	1471 vs	1498 s	1473 vs 1448 m
$\nu$ N-C-N			1468 s	
$\nu$ C-N-N	1430 s b		1419 s	
$\nu_s$ NO <sub>2</sub>	1389 s	1392 w	1387 s	1388 w
$\gamma$ NH <sub>2</sub> oop bend	1349 vs 1326 s 1314s 1281 sh	1359 sh 1349 m 1328 s 1313 m 1279 vw	1349 s 1331 vs 1314 s 1288 sh	1338 vs 1317 w
$\nu$ C-N	1250 s	1254 m	1255 s	1258 m
$\nu$ N-N	1198s	1200 m-s 1184 m	1198s	1204 sh 1200 m 1193 m

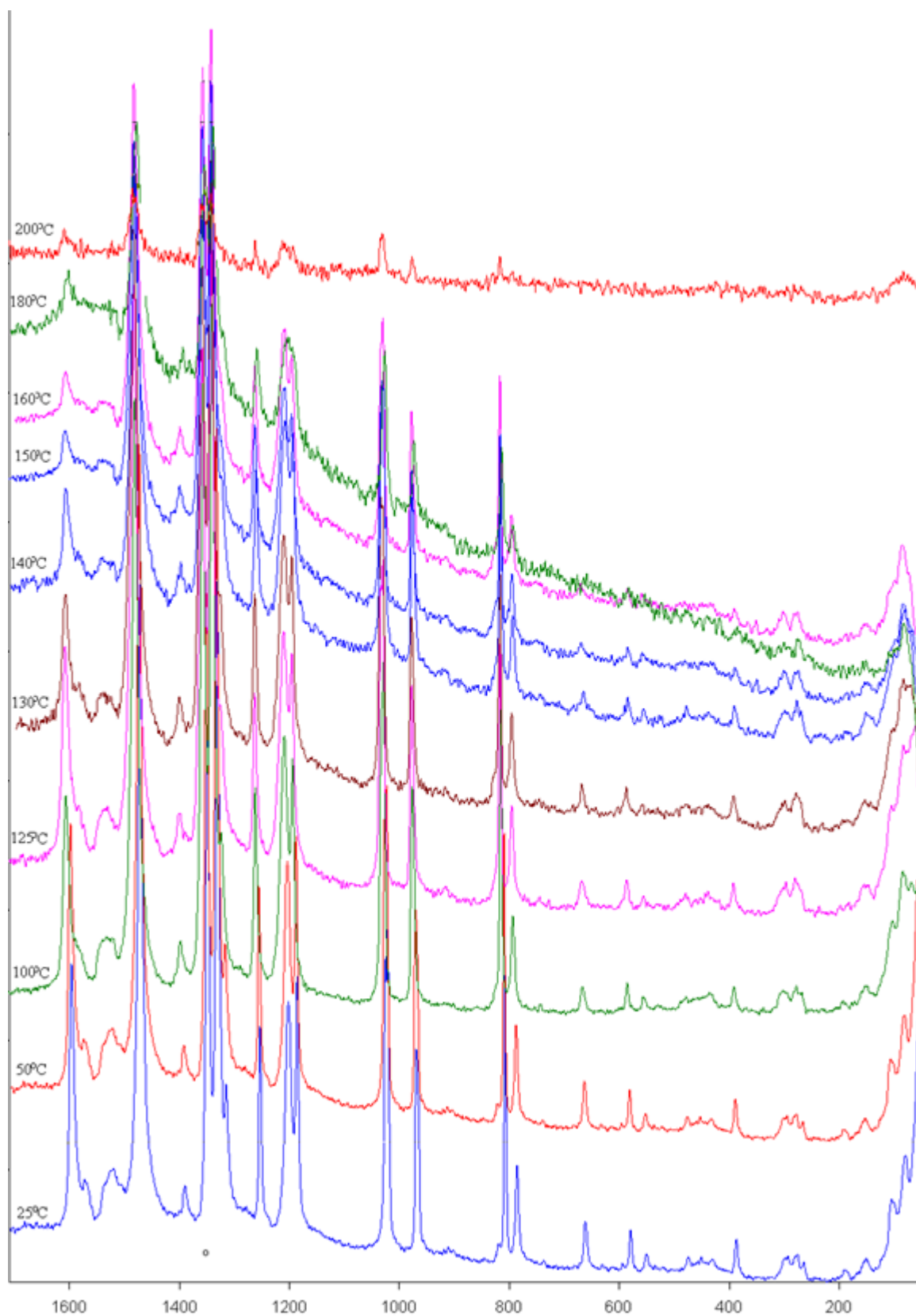
$\delta$ C-H	1148 s		1148 s	1150 vw
	1090sh		1080 s	
$\delta$ N-H	1018 s n	1020 m-s	1023 s 1013 s	1037 m 1026 m-s
	968 m-s, n	967 m	970 m	972 m
		913 vw 902 vw	919 s d 912 s d	924 vw 910 vw
	901 vs, n		866 b m	
$\delta$ NO <sub>2</sub> scissoring	818 vs, n 806 s	818 vw 807 m	826 s 810ms	832 vw 813 w
$\gamma$ NH <sub>2</sub> oop bend	784 m-s	786 w	784 m	786 w
$\gamma$ N-H oop bend	759 s n		758 m	
$\delta$ (C-H)arom )	734 vs	734 vw	733 s	736 vw
$\delta$ C-H	720 sh		712 m	
$\omega$ NO <sub>2</sub> wagging	663w 647 w-m	662 vw	675 w 650 w	663 vw
$\rho$ NO <sub>2</sub> rocking	592 m 580 sh	580 vw	562 s 547 s	578 vw 554 vw
	549 m	550 vw		
	454s	472 vw	474 s	
	427 vs	430 vw		427 vw

Abbreviants: vs- very strong, s- strong, m – medium, w –weak, vw- very weak,

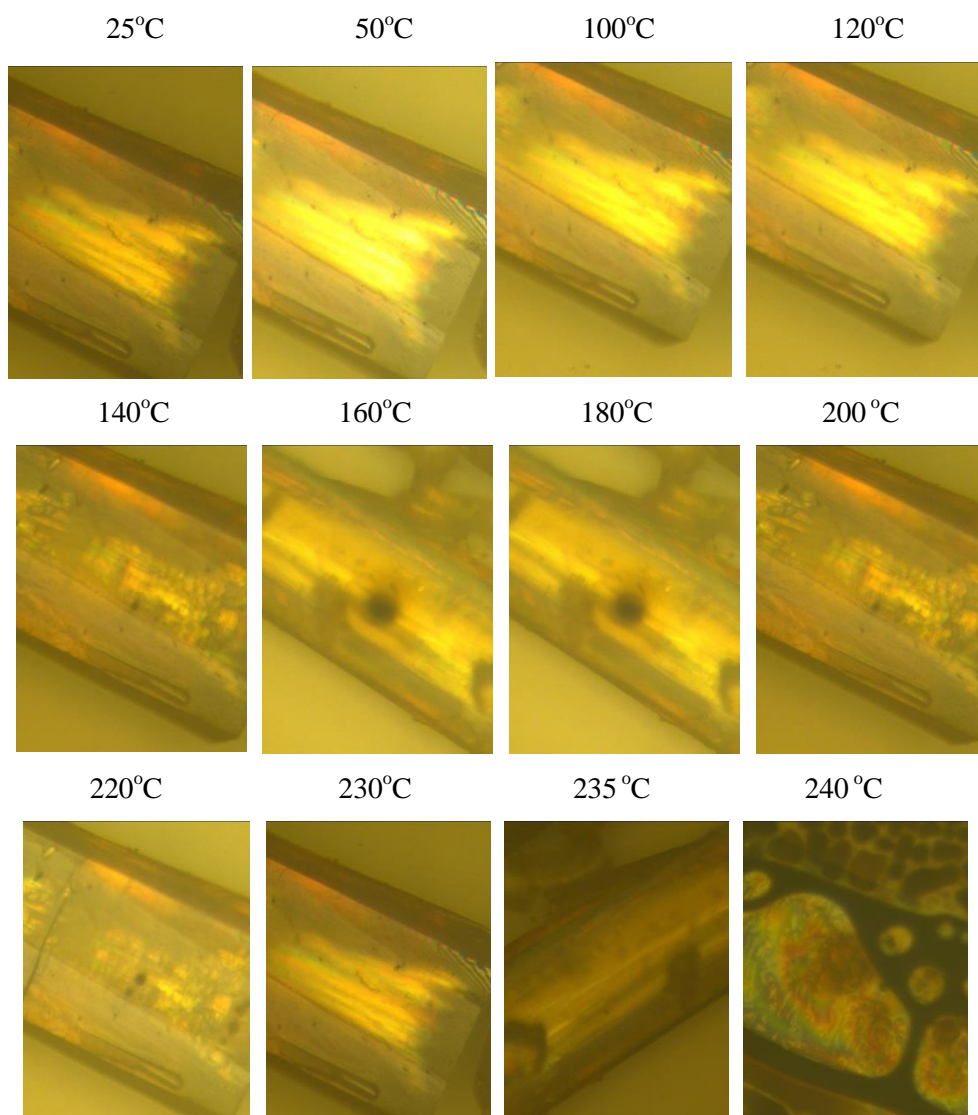
$\nu$ - stretching,  $\delta$ - in plane deformation vibration,  $\gamma$  – out-of-plane deformation vibration



**Figure S2** Raman microscopy snapshots of  $\beta$ -polymorph showing the morphological changes at rising temperatures up to the decomposition of the crystal.

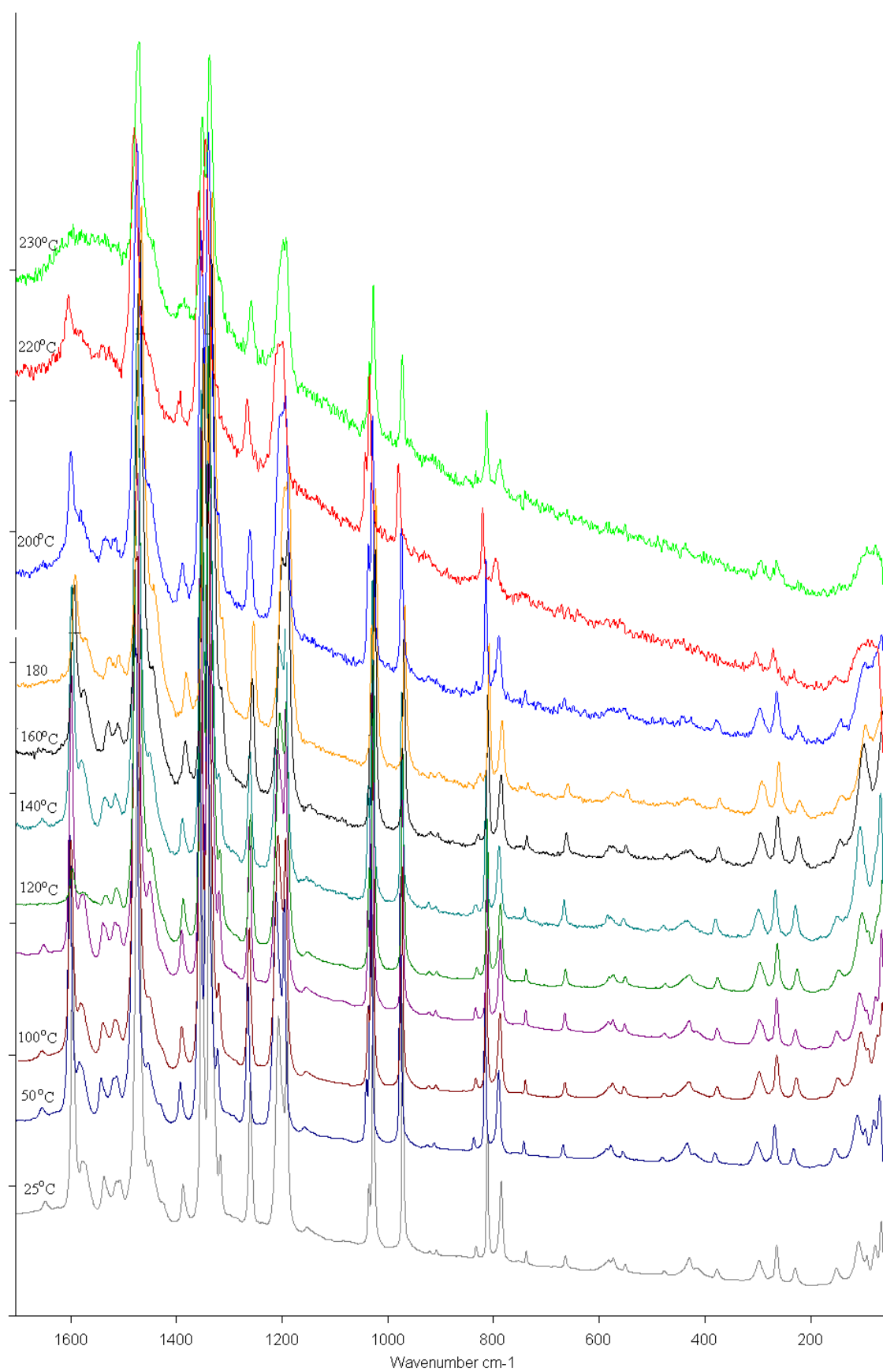


**Figure S3** FT-Raman spectra of  $\beta$ -form measured as function of the temperature.



**Figure S4** Raman microscopy snapshots of  $\gamma$ -polymorph taken at rising temperatures up to the decomposition of the crystal.





**Figure S5** FT-Raman spectra of  $\gamma$ -form measured as function of the temperature.

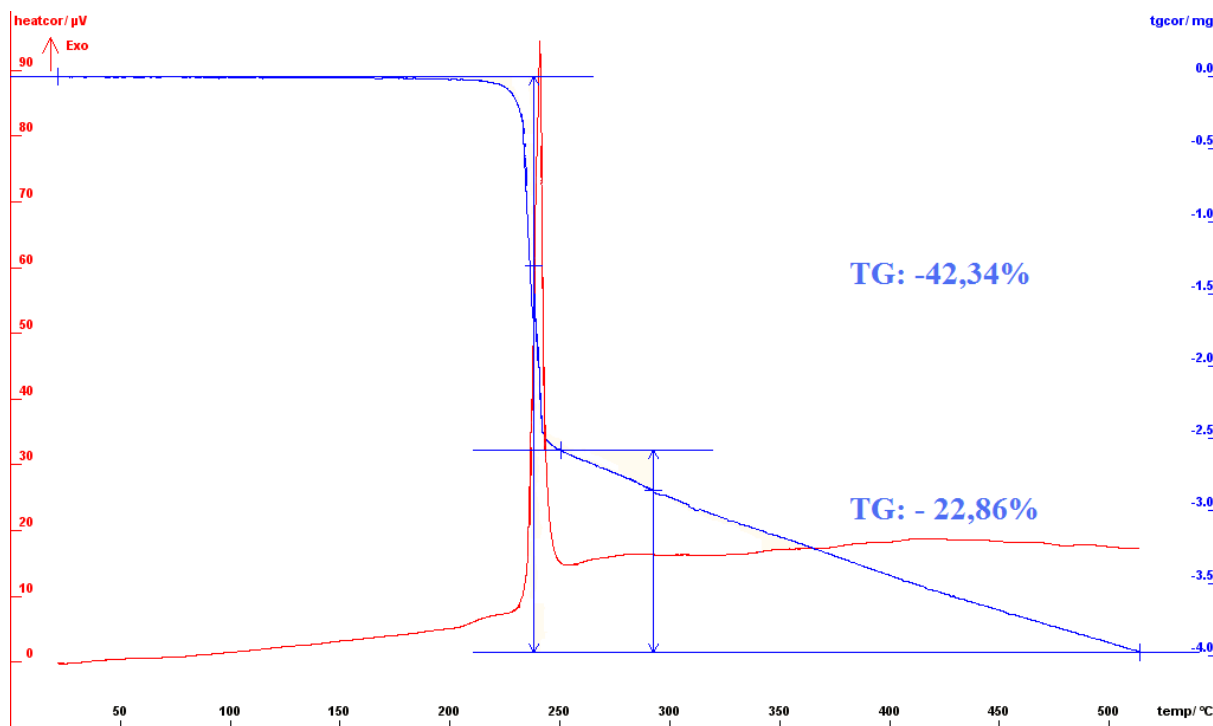


Figure S6 TG-DTA curves of form  $\beta$  NFZ.

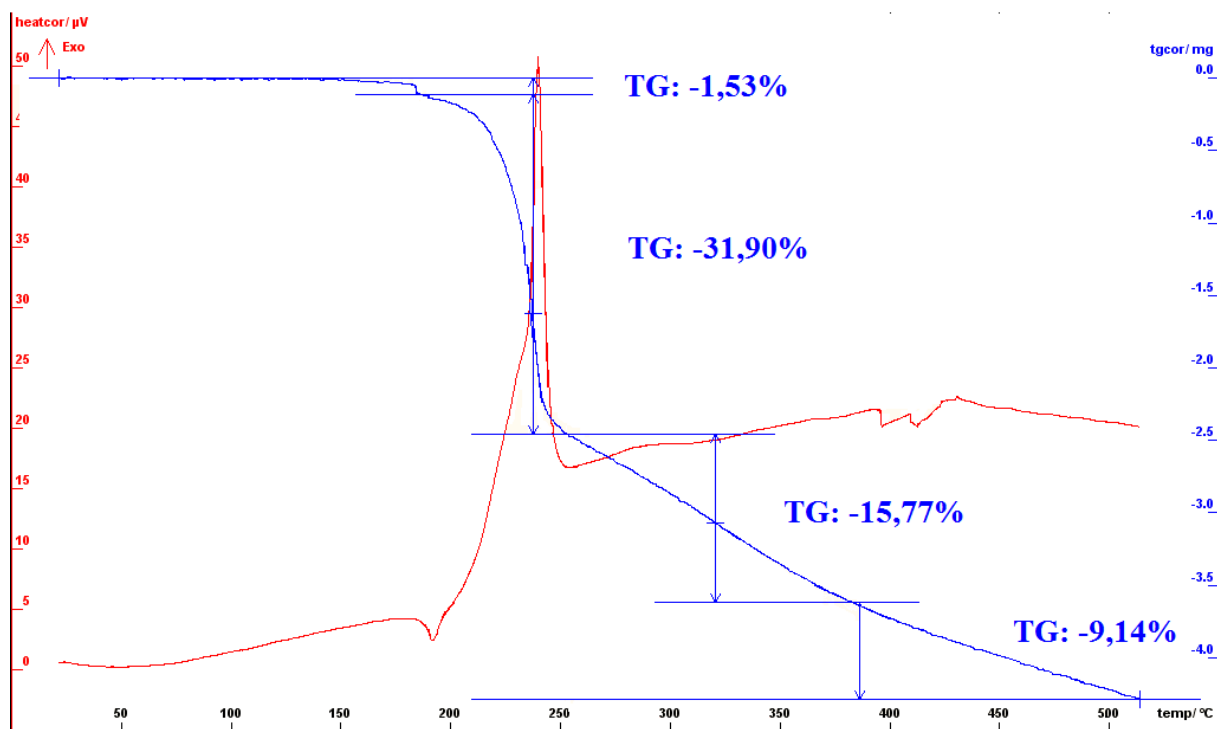
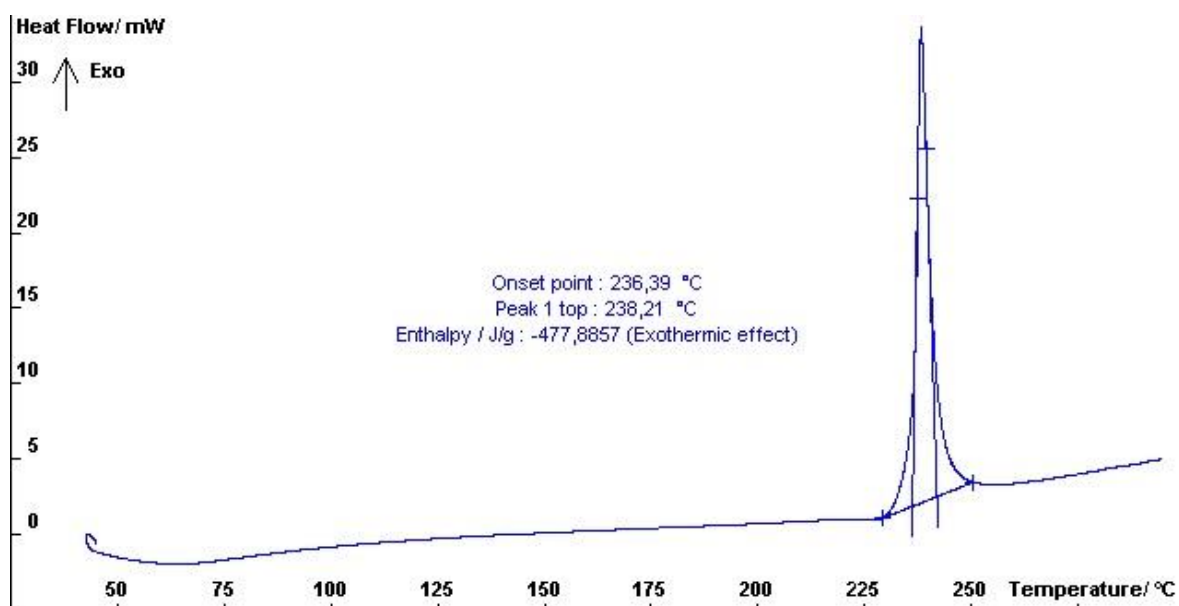
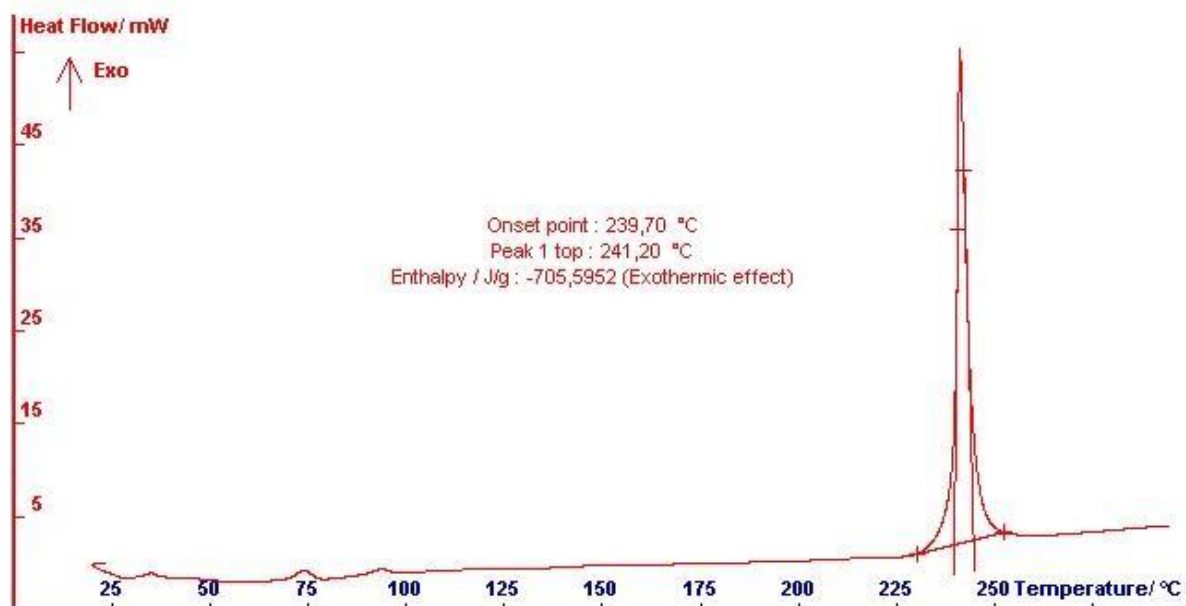


Figure S7 TG-DTA curves of form  $\gamma$  NFZ.



**Figure S8** DSC heating curve of  $\beta$ -form NFZ recorded at speed rate 5°C/min.



**Figure S9** DSC heating curve of  $\gamma$ -form NFZ recorded at speed rate 5°C/min.

