

forward (FW) and reverse (RV) primers	target gene	sequence	amplicon size (bp)
<i>hPTPRG FW</i>	<i>human</i>	5'-GTTCAAGCTAATACCACTCG-3'	
<i>hPTPRG RV</i>	<i>PTPRG</i>	5'-TGGAAACAAATGAGAATGGG-3'	155
<i>hBACT FW</i>	<i>human</i>	5'-TGACCCAGATCATGTTGAG-3'	
<i>hBACT RV</i>	β -actin	5'-CTTCTCCTTAATGTCACGCAC-3'	290
<i>BCR/ABL FW</i>	<i>Bcr/Abl</i>	5'-GATGCTGACCAACTCGTGTG-3'	
<i>BCR/ABL RV</i>	<i>Bcr/Abl</i>	5'-AGCAGATACTCAGCGGCATT-3'	411-486
<i>BCR/ABL FW</i>	<i>Bcr/Abl</i>	5'-GTT CCT GAT CCT CTG ACT ATG AGCGTG-3'	
<i>BCR/ABL RV</i>	<i>Bcr/Abl</i>	5'-TGTGATTATAGCCTAAGACCCGGAG-3'	411-486
(external round nested PCR)			
<i>mPTPRGex FW</i>	<i>mouse</i>	5'-ATCCTATTATCCACGGGCTG-3'	
<i>mPTPRGex RV</i>	<i>Ptpg</i>	5'-TGTAAATGTCCTCTCTCGTC-3'	483
(internal round nested PCR)			
<i>mPTPRGin FW</i>	<i>mouse</i>	5'-GTACCTGAGAAATAACTCCGAC-3'	
<i>mPTPRGin RV</i>	<i>PTPRG</i>	5'-AGAGCTGCAAACCTTAGAGG-3'	144
<i>mβACT FW</i>	<i>mouse</i>	5'-GTACCTGAGAAATAACTCCGAC-3'	
<i>mβACT RV</i>	β -actin	5'-GAGCAATGATCTGATCTTCATGG-3'	145

Table 1. Forward (FW) and reverse (RV) primers used for RT-PCR of *BCR/ABL*, human (*h*) and mouse (*m*) *PTPRG* and human and mouse beta actin (β ACT) genes.

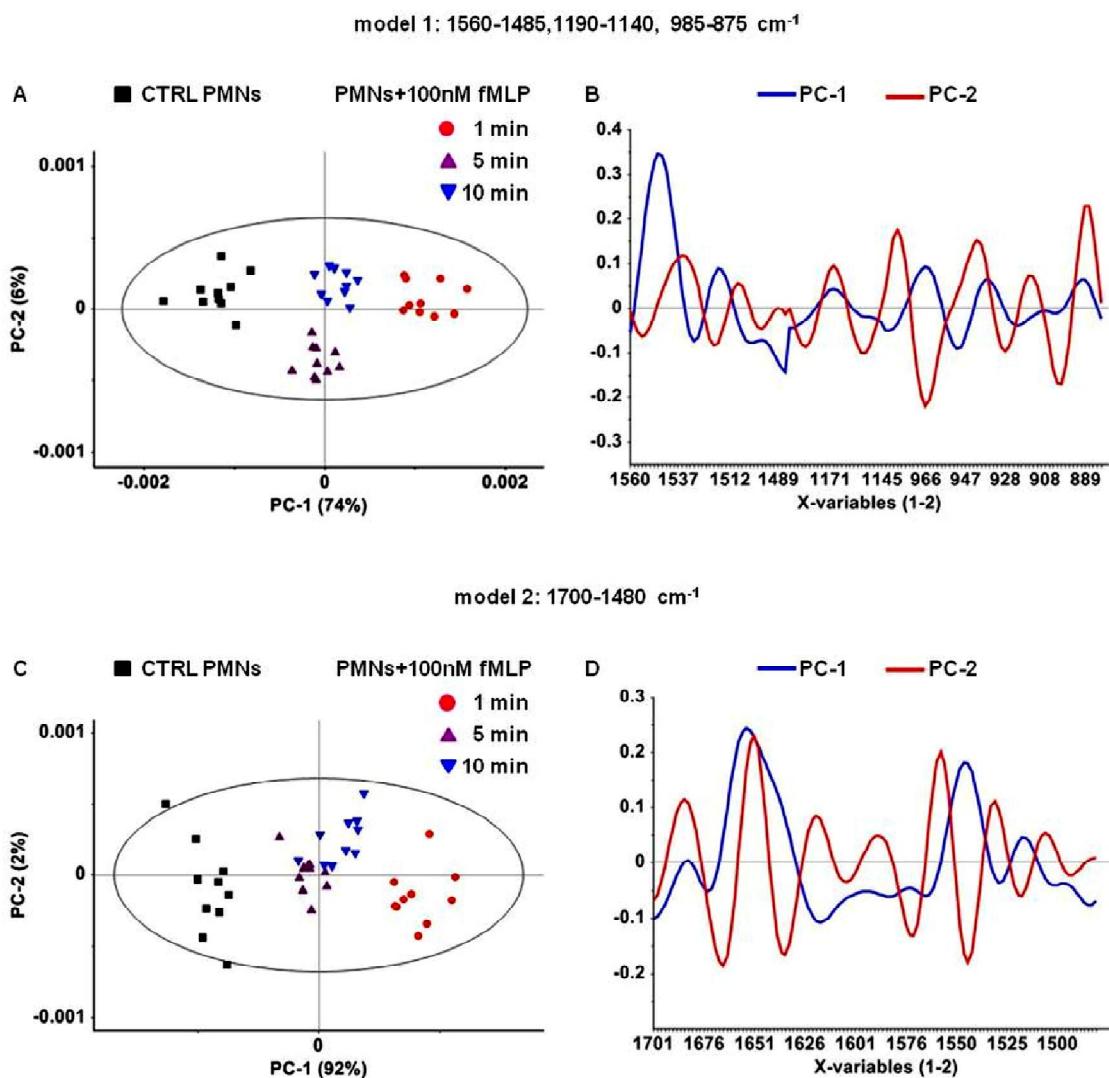


Figure S1. MicroFTIR performed with the conventional IR source (globar) and principal component analysis (PCA) with models 1 (A-B) and 2 (C-D), respectively. The dataset comprises the spectra of PMNs exposed to 100 nM fMLP for 1 min (red dot), 5 min (violet triangle) and 10 min (blue inverted triangle), and the spectra of non stimulated CTRL PMNs (black box). Each symbol represents the average spectrum mediating IR signals from 10-12 cells spread over an area of 30x30 μm^2 in sizes. Grey ellipse delimits 95% confidence interval. Statistics are available in supplementary material S5.

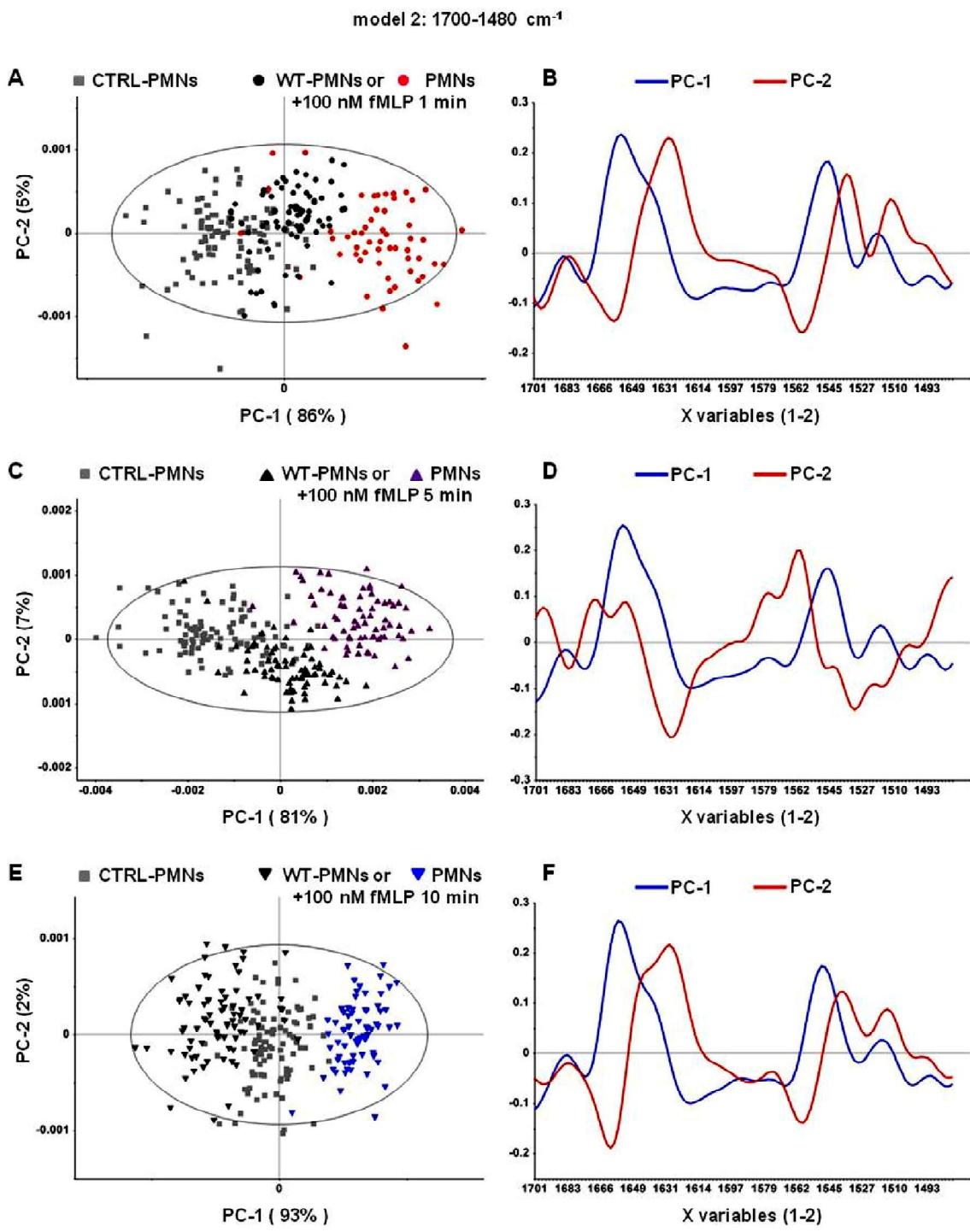


Figure S2. SR microFTIR and principal component analysis (PCA) with the model 2 (1700-1480 cm⁻¹). The dataset composes of spectra of neutrophil leukocytes pre-incubated with 100 nM wortmannin (WT-PMNs) the specific and irreversible inhibitor of phosphoinositol 3 phosphate kinase (PI3K) activity and stimulated with 100 nM fMLP (black symbols), the spectra of PMNs stimulated with fMLP without the inhibition of PI3K (red, violet, and blue symbols) and the spectra of non stimulated CTRL PMNs (grey box). fMLP stimulation for 1, 5, and 10 min is indicated by dot, triangle and inverted triangles, respectively. Grey ellipse delimits 95% confidence interval. Statistics are available in supplementary material S5.

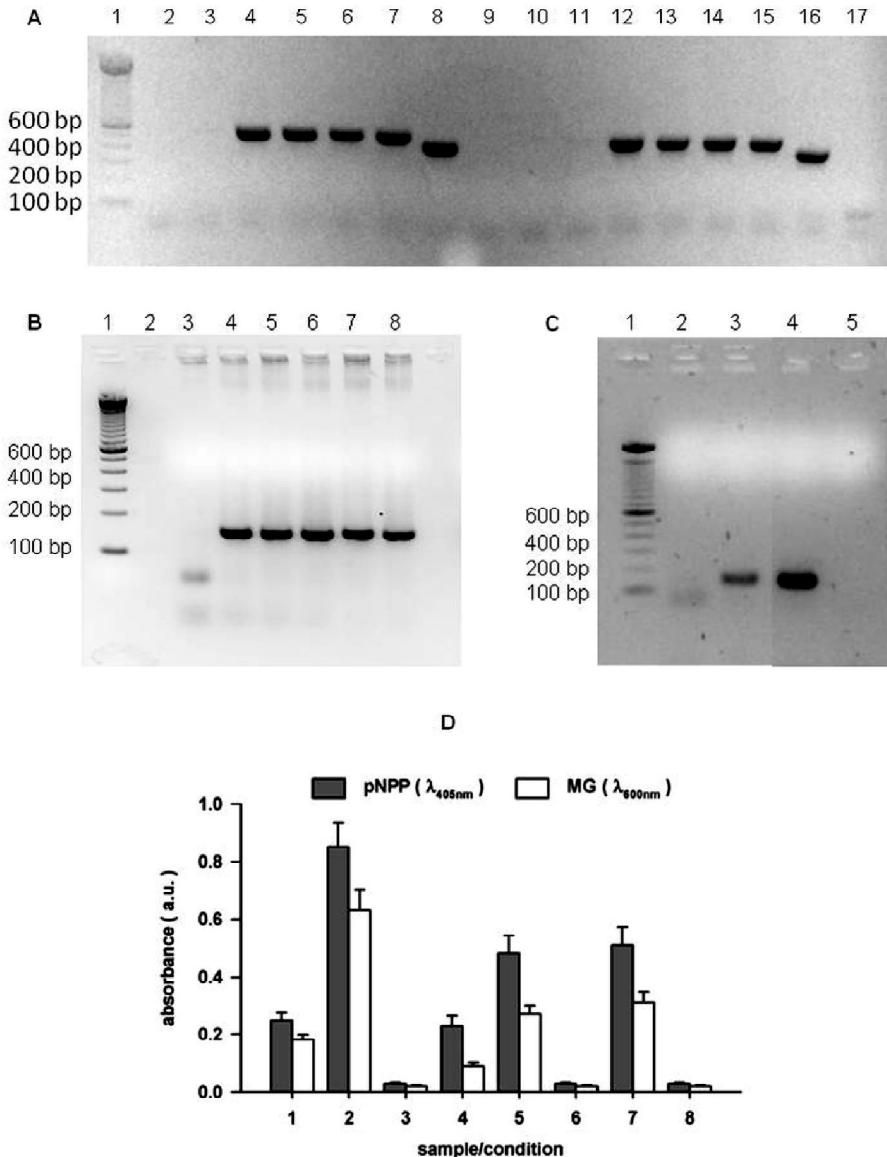
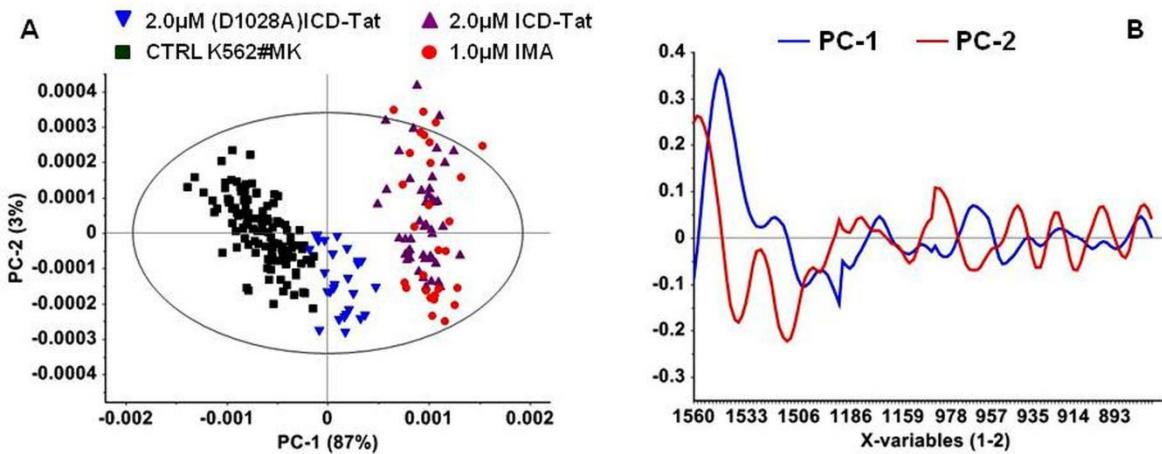


Figure S3. The presence of p210^{BCR/ABL} (A) and of mouse (B) or human (C) *PTPRG* cDNAs checked in Ba/F3 and in K562 cells sub-clones by polymerase chain reaction (RT-PCR). A (p210^{BCR/ABL}) lanes: base pair (100bp) ladder (1); Ba/F3#PAR (2,3, 10, and 11); Ba/F3 transfected with p210^{BCR/ABL} cDNA (Ba/F3#WT, 4 and 12); K562#MK (5,13), K562#G1 (6,14), K562#DA (7,15); BCR/ABL positive CTRL MEG-01 leukemia cell line (8 and 16); H₂O (9 and 17), respectively. B (m*PTPRG*) lanes: bp ladder (1); H₂O (2); H₂O PCR ms nest483 F/R (3); Ba/F3#PAR (4 and 5); Ba/F3#WT (6 and 7); CTRL mouse F317L cells (8). C (h*PTPRG*) lanes: bp ladder (1); K562#MK (2); K562#DA (3); K562#G1 (4); H₂O (5), respectively. D: protein phosphatase activity (mean \pm SD of 2 independent experiments) determined by p-Nitrophenyl Phosphate (pNPP, grey bars) and malachite green (MG) assays, respectively. Sample/condition: K562#MK (1), K562#G1 (2), K562#G1 + 0.2 mM Na₃VO₄ (3); K562#DA (4), Ba/F3#PAR (5), Ba/F3#PAR + 0.2 mM Na₃VO₄ (6); Ba/F3#WT (7), and Ba/F3#WT + 0.2 mM Na₃VO₄ cell lysates (50 μ L sample adjusted to 1 mg total protein/mL cell lysate + 150 μ L 50 mM Tris buffer pH 7.4, containing 1 mM EDTA and 1 mM DTT), respectively. In the MG assay 150 μ M ENDpYINASL phosphopeptide was used as a substrate for PTP activity.

model 1: 1560-1485,1190-1140, 985-875 cm^{-1}



model 2: 1700-1480 cm^{-1}

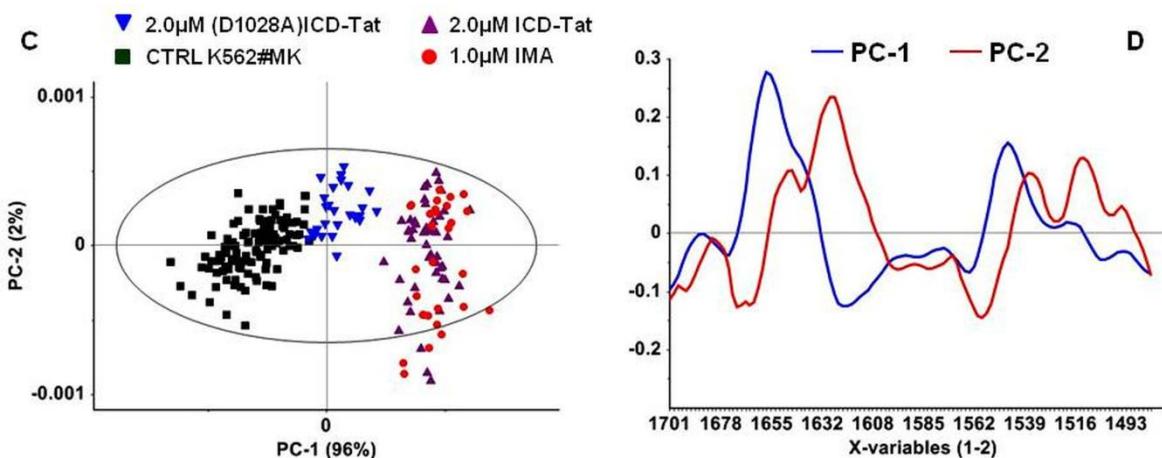


Figure S4. MicroFTIR performed with the conventional IR source (globar) and PCA with models 1 (A-B) and 2 (C-D) applied to explore K562#MK cells exposed to different experimental conditions. Each symbol average IR signals from 10-12 cells spread within 30x30 μm^2 spot areas. CTRL K562#MK (black box), and K562#MK samples exposed for 24 hours to 2.0 μM ICD-Tat (violet triangle) or to 2.0 μM (D1028A)ICD-Tat (blue inverted triangle) recombinant proteins, or to 1.0 μM imatinib mesylate (IMA) (red dot) are shown. Grey ellipse delimits 95% confidence interval. Statistics are available in supplementary material S5.

S5. Statistics performed on PCA data.

Figure 1 AB, model 1800-875 cm⁻¹

variables	type of test	result	comparison	significance level P<0.05
PC-1	Kruskal-Wallis One Way ANOVA on Ranks All Pairwise Multiple Comparison (Dunn's Method)	H = 171.568, (P=<0.001)	1 min fMLP vs. CTRL 5 min fMLP vs CTRL 10 min fMLP vs CTRL 1 min fMLP vs. 5 min fMLP 1 min fMLP vs. 10 min fMLP 5 min fMLP vs. 10 min fMLP	YES YES YES NO ^(a) NO ^(b) NO
PC-2	Kruskal-Wallis One Way ANOVA on Ranks All Pairwise Multiple Comparison (Dunn's Method)	H = 221.591, (P=<0.001)	1 min fMLP vs CTRL 5 min fMLP vs CTRL 10 min fMLP vs CTRL 1 min fMLP vs. 5 min fMLP 1 min fMLP vs. 10 min fMLP 5 min fMLP vs. 10 min fMLP	NO YES YES YES YES YES

Figure 1 CD, model 1 (1560-1485, 1190-1140, 985-875 cm⁻¹)

Kruskal-Wallis One Way ANOVA on Ranks	H = 182.147, (P=<0.001)	P=<0.001	
PC-1	All Pairwise Multiple Comparison (Dunn's Method)	1 min fMLP vs. CTRL 5 min fMLP vs CTRL 10 min fMLP vs CTRL 1 min fMLP vs. 5 min fMLP 1 min fMLP vs. 10 min fMLP 5 min fMLP vs. 10 min fMLP	YES YES YES YES NO ^(c) YES
PC-2	Kruskal-Wallis One Way ANOVA on Ranks All Pairwise Multiple Comparison (Dunn's Method)	H = 234.088, (P=<0.001)	P=<0.001

Figure 1 EF, model 2 (1700-1480 cm⁻¹)

Kruskal-Wallis One Way ANOVA on Ranks	H = 200.912, (P=<0.001)		
PC-1	All Pairwise Multiple Comparison (Dunn's Method)	1 min fMLP vs. CTRL 5 min fMLP vs CTRL 10 min fMLP vs CTRL 1 min fMLP vs. 5 min fMLP 1 min fMLP vs. 10 min fMLP 5 min fMLP vs. 10 min fMLP	YES YES YES YES YES NO ^(d)
PC-3	Kruskal-Wallis One Way ANOVA on Ranks All Pairwise Multiple Comparison (Dunn's Method)	H = 151.194, (P=<0.001)	

^(a) Mann-Whitney Rank Sum Test: T = 4853, P = 0.009^(b) Mann-Whitney Rank Sum Test: T = 4537, P = 0.042^(c) Mann-Whitney Rank Sum Test: T = 4471, P = 0.042^(d) t-test: t = 2.019, P = 0.045**Figure S5. Statistics performed on PCA data**

Figure S1 AB, model 1 (1560-1485, 1190-1140, 985-874 cm⁻¹)

variables	Type of test	result	comparison	significance level P<0.05
PC-1	Kruskal-Wallis One Way ANOVA	F = 206.842, (P<0.001)	1 min fMLP vs. CTRL 5 min fMLP vs CTRL 10 min fMLP vs CTRL 1 min fMLP vs. 5 min fMLP 1 min fMLP vs. 10 min fMLP 5 min fMLP vs. 10 min fMLP	YES YES YES YES YES YES
	All Pairwise Multiple Comparison (Holm-Sidak method)			
PC-2	Kruskal-Wallis One Way ANOVA	F = 46.756, (P<0.001)	1 min fMLP vs. CTRL 5 min fMLP vs CTRL 10 min fMLP vs CTRL 1 min fMLP vs. 5 min fMLP 1 min fMLP vs. 10 min fMLP 5 min fMLP vs. 10 min fMLP	NO YES NO YES NO YES
	All Pairwise Multiple Comparison (Holm-Sidak method)			

Figure S1 CD, model 2 (1700-1480 cm⁻¹)

	Kruskal-Wallis One Way ANOVA	P=<0.001
PC-1		
	1 min fMLP vs. CTRL	P<0.05
	5 min fMLP vs CTRL	P<0.05
	10 min fMLP vs CTRL	P=0.970
	1 min fMLP vs. 5 min fMLP	P<0.05
	1 min fMLP vs. 10 min fMLP	P<0.05
	5 min fMLP vs. 10 min fMLP	P<0.05
PC-2	Kruskal-Wallis One Way ANOVA on Ranks	P=0.243
	1 min fMLP vs. CTRL	P = 0.710
	5 min fMLP vs CTRL	P = 0.352
	10 min fMLP vs CTRL	P=0.980
	1 min fMLP vs. 5 min fMLP	P=0.059
	1 min fMLP vs. 10 min fMLP	P=0.710
	5 min fMLP vs. 10 min fMLP	P=0.352

Figure S5. Statistics performed on PCA data

Figure 2 AB (1 min fMLP stimulation), model 1 (1560-1485, 1190-1140, 985-875 cm⁻¹)

variables	Type of test	Comparison	significance level
PC-1	Kruskal-Wallis One Way ANOVA on Ranks	PMNs +100 nM fMLP 1 min vs. CTRL PMNs	P=<0.001
		WT-PMNs +100 nM fMLP 1 min vs. CTRL PMNs	P<0.05
	All Pairwise Multiple Comparison (Dunn's Method)	PMNs +100 nM fMLP 1 min vs. WT-PMNs +100 nM fMLP 1 min	P<0.05
		WT-PMNs +100 nM fMLP 1 min	
PC-2	Kruskal-Wallis One Way ANOVA	PMNs +100 nM fMLP 1 min vs. CTRL PMNs	P=<0.001
		WT-PMNs +100 nM fMLP 1 min vs. CTRL PMNs	P<0.05
	All Pairwise Multiple Comparison Procedures (Holm-Sidak method)	PMNs +100 nM fMLP 1 min vs. WT-PMNs +100 nM fMLP 1 min	P<0.05
		WT-PMNs +100 nM fMLP 1 min	

Figure 2 CD (5 min fMLP stimulation), model 1 (1560-1485, 1190-1140, 985-875 cm⁻¹)

PC-1	Kruskal-Wallis One Way ANOVA	PMNs +100 nM fMLP 5 min vs. CTRL PMNs	P=<0.001
		WT-PMNs +100 nM fMLP 5 min vs. CTRL PMNs	P<0.05
	All Pairwise Multiple Comparison Procedures (Holm-Sidak method)	PMNs +100 nM fMLP 5 min vs. WT-PMNs +100 nM fMLP 5 min	P<0.05
		WT-PMNs +100 nM fMLP 5 min	
PC-2	Kruskal-Wallis One Way ANOVA on Ranks	PMNs +100 nM fMLP 5 min vs. CTRL PMNs	P=<0.001
		WT-PMNs +100 nM fMLP 5 min vs. CTRL PMNs	P<0.05
	All Pairwise Multiple Comparison (Dunn's Method)	PMNs +100 nM fMLP 1 min vs. WT-PMNs +100 nM fMLP 5 min	P=0.498
		WT-PMNs +100 nM fMLP 5 min	P<0.05

Figure 2 EF (10 min fMLP stimulation), model 1 (1560-1485, 1190-1140, 985-875 cm⁻¹)

PC-1	Kruskal-Wallis One Way ANOVA on Ranks	PMNs +100 nM fMLP 10 min vs. CTRL PMNs	P=<0.001
		WT-PMNs +100 nM fMLP 10 min vs. CTRL PMNs	P<0.05
	All Pairwise Multiple Comparison (Dunn's Method)	PMNs +100 nM fMLP 10 min vs. WT-PMNs +100 nM fMLP 10 min	P<0.05
		WT-PMNs +100 nM fMLP 10 min	
PC-2	Kruskal-Wallis One Way ANOVA	PMNs +100 nM fMLP 10 min vs. CTRL PMNs	P=<0.001
		WT-PMNs +100 nM fMLP 10 min vs. CTRL PMNs	P<0.05
	All Pairwise Multiple Comparison Procedures (Holm-Sidak method)	PMNs +100 nM fMLP 10 min vs. WT-PMNs +100 nM fMLP 10 min	P<0.05
		WT-PMNs +100 nM fMLP 10 min	

Figure S5. Statistics performed on PCA data

Figure S2 AB (1 min fMLP stimulation), model 2 (1700-1480 cm⁻¹)

variables	Type of test	comparison	significance level
PC-1	Kruskal-Wallis One Way ANOVA on Ranks		P=<0.001
		PMNs +100 nM fMLP 1 min vs. CTRL PMNs	P<0.05
	All Pairwise Multiple Comparison (Dunn's Method)	WT-PMNs +100 nM fMLP 1 min vs. CTRL PMNs	P<0.05
		PMNs +100 nM fMLP 1 min vs. WT-PMNs +100 nM fMLP 1 min	P<0.05
	Kruskal-Wallis One Way ANOVA on Ranks		P=<0.001
		PMNs +100 nM fMLP 1 min vs. CTRL PMNs	P=0.860
PC-2	All Pairwise Multiple Comparison (Dunn's Method)	WT-PMNs +100 nM fMLP 1 min vs. CTRL PMNs	P<0.05
		PMNs +100 nM fMLP 1 min vs. WT-PMNs +100 nM fMLP 1 min	P<0.05

Figure S2 CD (5 min fMLP stimulation), model 2 (1700-1480 cm⁻¹)

	Kruskal-Wallis One Way ANOVA on Ranks		P=<0.001
PC-1		PMNs +100 nM fMLP 5 min vs. CTRL PMNs	P<0.05
	All Pairwise Multiple Comparison (Dunn's Method)	WT-PMNs +100 nM fMLP 5 min vs. CTRL PMNs	P<0.05
		PMNs +100 nM fMLP 5 min vs. WT-PMNs +100 nM fMLP 5 min	P<0.05
	Kruskal-Wallis One Way ANOVA on Ranks		P=<0.001
		PMNs +100 nM fMLP 5 min vs. CTRL PMNs	P<0.05
	All Pairwise Multiple Comparison (Dunn's Method)	WT-PMNs +100 nM fMLP 5 min vs. CTRL PMNs	P=0.498
PC-2		PMNs +100 nM fMLP 1 min vs. WT-PMNs +100 nM fMLP 5 min	P<0.05

Figure S2 EF (10 min fMLP stimulation), model 2 (1700-1480 cm⁻¹)

	Kruskal-Wallis One Way ANOVA		P=<0.001
PC-1		PMNs +100 nM fMLP 10 min vs. CTRL PMNs	P<0.05
	All Pairwise Multiple Comparison (Dunn's Method)	WT-PMNs +100 nM fMLP 10 min vs. CTRL PMNs	P<0.05
		PMNs +100 nM fMLP 10 min vs. WT-PMNs +100 nM fMLP 10 min	P<0.05
	Kruskal-Wallis One Way ANOVA		P=<0.001
		PMNs +100 nM fMLP 10 min vs. CTRL PMNs	P<0.05
	All Pairwise Multiple Comparison Procedures (Holm-Sidak method)	WT-PMNs +100 nM fMLP 10 min vs. CTRL PMNs	P<0.05
PC-2		PMNs +100 nM fMLP 10 min vs. WT-PMNs +100 nM fMLP 10 min	P<0.05

Figure S5. Statistics performed on PCA data

Figure 4 AB, model 1 (1560-1485, 1190-1140, 985-874 cm⁻¹)

variables	Type of test	comparison	significance level: P<0.05
PC-1	t-test on tne means	Ba/F3 PAR vs. Ba/F3WT	P=<0.001
PC-2	Mann-Whitney Rank Sum Test		P=0.124

Figure 4 CD, model 2 (1560-1485, 1190-1140, 985-874 cm⁻¹)

Kruskal-Wallis One Way ANOVA on Ranks		
PC-1	K562#MK vs. K562#DA	P<0.05
All Pairwise Multiple Comparison (Dunn's Method)	K562#MK vs. K562#G1	P<0.05
	K562#G1 vs. K562#DA	P<0.05
Kruskal-Wallis One Way ANOVA on Ranks		
PC-2	K562#MK vs. K562#DA	P=0.538
Mann-Whitney Rank Sum Test	K562#MK vs. K562#G1	P=0.054
	K562#G1 vs. K562#DA	P=0.706

Figure 4 EF, model 1 (1700-1480 cm⁻¹)

PC-1	t-test on tne means	P=<0.001
PC-2	Mann-Whitney Rank Sum Test	P=0.329

Figure 4 GH, model 2 (1700-1480 cm⁻¹)

Kruskal-Wallis One Way ANOVA on Ranks		
PC-1	K562#MK vs. K562#DA	P<0.05
All Pairwise Multiple Comparison (Dunn's Method)	K562#MK vs. K562#G1	P<0.05
	K562#G1 vs. K562#DA	P<0.05
Kruskal-Wallis One Way ANOVA		
PC-2	K562#MK vs. K562#DA	P=0.724
All Pairwise Multiple Comparison (Holm-Sidak method)	K562#MK vs. K562#G1	P<0.05
	K562#G1 vs. K562#DA	P<0.05

Figure S5. Statistics performed on PCA data

Figure 5 AB, model 1 (1560-1485, 1190-1140, 985-874 cm⁻¹)

variables	Type of test	comparison	significance level P<0.05
	Kruskal-Wallis One Way ANOVA on Ranks		P=<0.001
		CTRL K562#MK vs. 1.0 µM IMA	YES
		CTRL K562#MK vs. 2.0 µM ICD-Tat	YES
PC-1	All Pairwise Multiple Comparison (Dunn's Method)	CTRL K562#MK vs. 2.0 µM (D1028A)ICD-Tat	YES
		1.0 µM IMA vs. 2.0 µM (D1028A)ICD-Tat	YES
		1.0 µM IMA vs. 2.0 µM ICD-Tat	NO
		2.0 µM ICD-Tat vs. 2.0 µM (D1028A)ICD-Tat	YES
	Kruskal-Wallis One Way ANOVA on Ranks		P=<0.001
		CTRL K562#MK vs. 1.0 µM IMA	NO
		CTRL K562#MK vs. 2.0 µM ICD-Tat	NO
PC-2	All Pairwise Multiple Comparison (Dunn's Method)	CTRL K562#MK vs. 2.0 µM (D1028A)ICD-Tat	YES
		1.0 µM IMA vs. 2.0 µM (D1028A)ICD-Tat	YES
		1.0 µM IMA vs. 2.0 µM ICD-Tat	NO
		2.0 µM ICD-Tat vs. 2.0 µM (D1028A)ICD-Tat	YES

Figure 5 CD, model 2 (1700-1480 cm⁻¹)

	Kruskal-Wallis One Way ANOVA on Ranks		P=<0.001
		CTRL K562#MK vs. 1.0 µM IMA	YES
		CTRL K562#MK vs. 2.0 µM ICD-Tat	YES
PC-1	All Pairwise Multiple Comparison (Dunn's Method)	CTRL K562#MK vs. 2.0 µM (D1028A)ICD-Tat	YES
		1.0 µM IMA vs. 2.0 µM (D1028A)ICD-Tat	YES
		1.0 µM IMA vs. 2.0 µM ICD-Tat	NO
		2.0 µM ICD-Tat vs. 2.0 µM (D1028A)ICD-Tat	YES
	Kruskal-Wallis One Way ANOVA on Ranks		P=0.243
		CTRL K562#MK vs. 1.0 µM IMA	NO
		CTRL K562#MK vs. 2.0 µM ICD-Tat	NO
PC-2	All Pairwise Multiple Comparison (Dunn's Method)	CTRL K562#MK vs. 2.0 µM (D1028A)ICD-Tat	YES
		1.0 µM IMA vs. 2.0 µM (D1028A)ICD-Tat	YES
		1.0 µM IMA vs. 2.0 µM ICD-Tat	NO
		2.0 µM ICD-Tat vs. 2.0 µM (D1028A)ICD-Tat	YES

Figure S5. Statistics performed on PCA data

Figure 6 AB, model 1 (1560-1485, 1190-1140, 985-874 cm⁻¹)

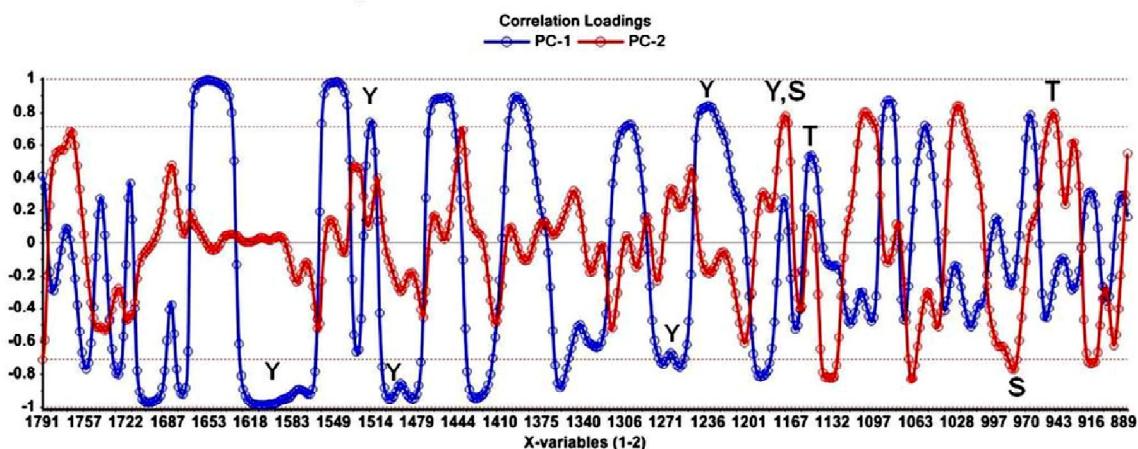
variables	Type of test	comparison	significance level P<0.05
PC-1	Kruskal-Wallis One Way ANOVA		P=<0.001
		CTRL K562#G1 vs. CTRL K562#MK	YES
	All Pairwise Multiple Comparison (Holm-Sidak Method)	CTRL K562#G1 vs. 0.5 µM IMA #G1	YES
		CTRL K562#G1 vs. 0.5 µM IMA #MK	YES
		CTRL K562#MK vs. 0.5 IMA µM #G1	YES
		CTRL K562#MK vs. 0.5 IMA µM #MK	YES
		0.5 µM IMA #G1 vs. 0.5 µM IMA #MK	YES
PC-2	Kruskal-Wallis One Way ANOVA on Ranks		P=<0.001
		CTRL K562#G1 vs. CTRL K562#MK	YES
	All Pairwise Multiple Comparison (Dunn's Method)	CTRL K562#G1 vs. 0.5 µM IMA #G1	YES
		CTRL K562#G1 vs. 0.5 µM IMA #MK	YES
		CTRL K562#MK vs. 0.5 IMA µM #G1	YES
		CTRL K562#MK vs. 0.5 IMA µM #MK	YES
		0.5 µM IMA #G1 vs. 0.5 µM IMA #MK	YES

Figure 6 CD, model 2 (1700-1480 cm⁻¹)

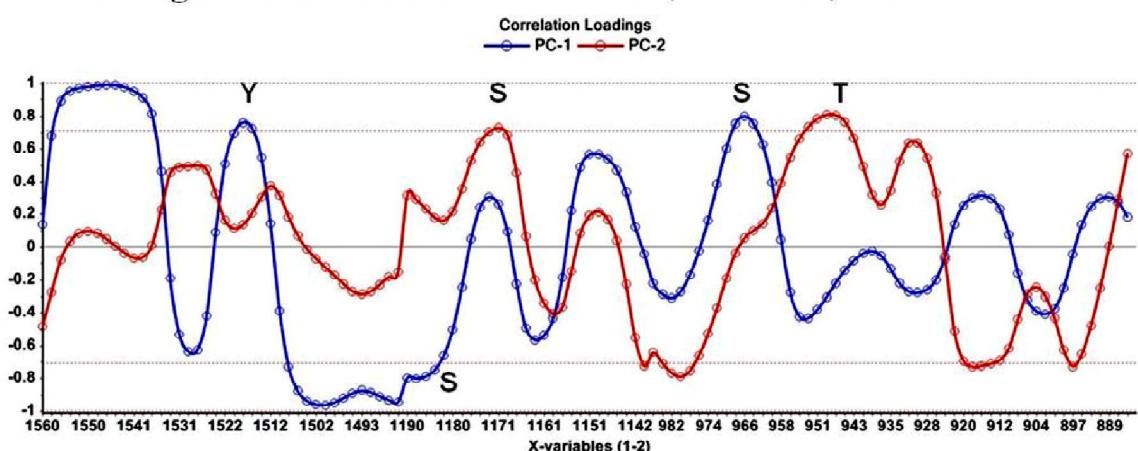
	Kruskal-Wallis One Way ANOVA		P=<0.001
PC-1		CTRL K562#G1 vs. CTRL K562#MK	YES
		CTRL K562#G1 vs. 0.5 µM IMA #G1	YES
	All Pairwise Multiple Comparison (Holm-Sidak Method)	CTRL K562#G1 vs. 0.5 µM IMA #MK	YES
		CTRL K562#MK vs. 0.5 IMA µM #G1	YES
		CTRL K562#MK vs. 0.5 IMA µM #MK	YES
		0.5 µM IMA #G1 vs. 0.5 µM IMA #MK	YES
	Kruskal-Wallis One Way ANOVA on Ranks		P=0.243
PC-2		CTRL K562#G1 vs. CTRL K562#MK	YES
		CTRL K562#G1 vs. 0.5 µM IMA #G1	YES
	All Pairwise Multiple Comparison (Dunn's Method)	CTRL K562#G1 vs. 0.5 µM IMA #MK	YES
		CTRL K562#MK vs. 0.5 IMA µM #G1	YES
		CTRL K562#MK vs. 0.5 IMA µM #MK	YES
		0.5 µM IMA #G1 vs. 0.5 µM IMA #MK	YES

Figure S5. Statistics performed on PCA data

S6 Figure 1 AB: model 1800-875 cm⁻¹



S6 Figure 1 CD: model 1: 1560-1485, 1190-140, 985-875 cm⁻¹



S6 Figure 1 EF: model 2: 1700-1480 cm⁻¹

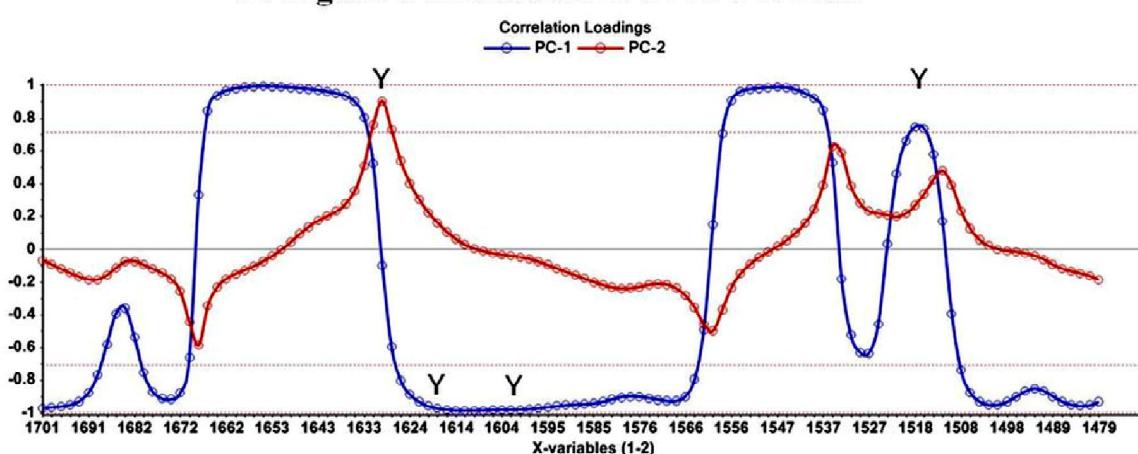


Figure S6. Correlation loadings of PCA in Figure 1 AB. The unsupervised identification of variables giving major contributions to the models. Values that lie within the upper and lower bounds of the plot are modelled by PCs. Those that lie between the two lower bounds are not. An attempt has been made to assign tyrosine (Y), serine (S), and threonine (T) according to the data available in the literature (Refs 43-48).