Supporting information for: "1064 nm Dispersive Raman Micro-Spectroscopy and Optical Trapping of Pharmaceutical Aerosols"

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Signal processing

Figure S1 shows the raw data for optically-trapped salmeterol xinafoate from a Serevent pMDI, along with two forms of post-acquisition processing.

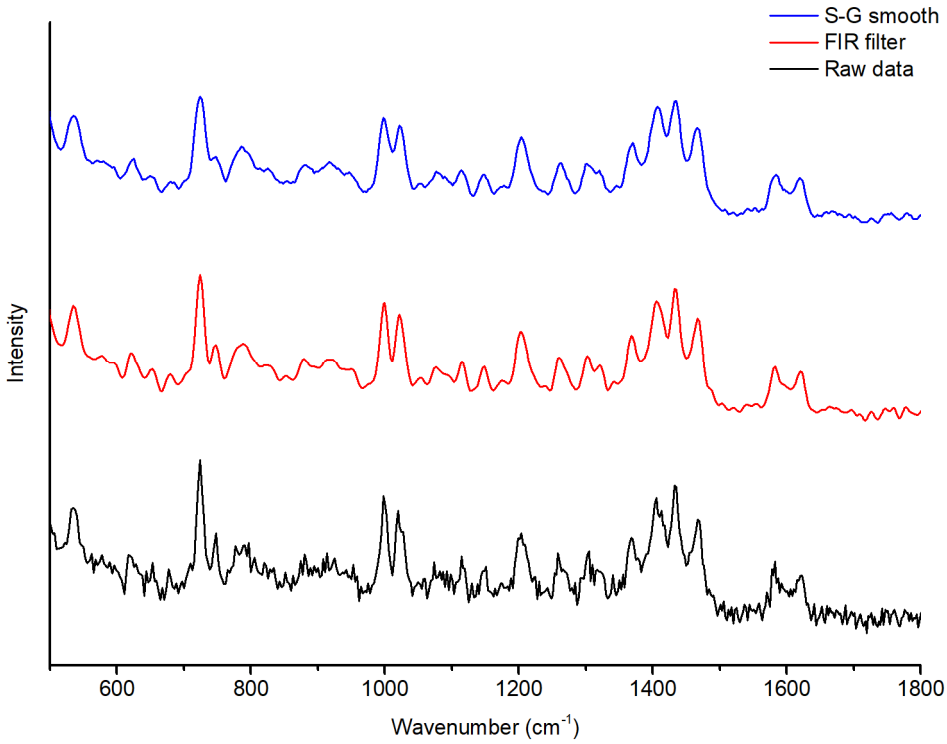

Figure S1: 1064 nm dispersive Raman spectra for optically trapped salbutamol sulfate. Black – raw data; red – following frequency impulse response (FIR) filtering; blue – following Savitzky-Golay (S-G) smoothing.

Both methods make identifying the main spectral features from background noise more straightforward, with loss of some resolution. FIR (low-pass) filtering retains slightly better spectral resolution, especially for closely co-located peaks (e.g. 748 cm^{-1} close to 724 cm^{-1}).

Particle coverslip morphology

An optical image of a salbutamol sulfate particle deposited on a coverslip is shown in Figure S2. A pool of water surrounds the particle as the ambient relative humidity is increased, which is an artefact related to contact between the particle and the surface.

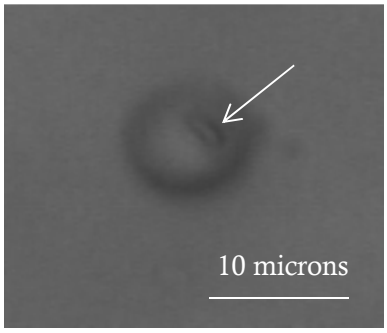

Figure S2: Particle of salbutamol sulfate residing on a coverslip at RH 94%. The particle is surrounded by pool of water, an unrealistic morphology which deviates from its airborne behaviour.

Assignment of spectral features

Tables S1-S3 give a full assignment of the three pMDI Raman spectra from Figure 3.

Table S1: Assignment of Raman spectral features for salmeterol xinafoate from a Serevent pMDI. A – Ali et al.[1]; D – Davidson et al.[2]; s – strong, m – medium, w – weak, vw – very weak, b – broad, sh – shoulder; * – unique to polymorph I.

Wavenumber (cm^{-1})	Feature	Refs (cm^{-1})
413		
444	In-plane skeletal deformation	A 445w
488	In-plane $\delta(CC)_{chain}$	A 494mw
535	Out-of-plane δ(COC)	A 538m; D 554
578	In-plane δ(CCN)	A 578w
601	In-plane δ(CCC)	A 605vw
623	Ring deformation	A 621mw
653	Out-of-plane $\delta(CC)_{ring}$	A 648w
680		
724	$r(CH_2)$	A 726s; D 730
748	Ring vibration	A 749mw*
788	Out-of-plane $\delta(CH)_{ring}$ (benzoic acid)	A 779mw; D 788
823	Skeletal stretch	A 822w
852	Out-of-plane $\delta(CH)_{chain}$	A 855vw
881	v(CNC)	A 880w
920		
951	$r(CH_2)$	A 955vw
1000	Symmetric ring stretch	A 1000s; D 1000-1028
1022		A 1021s; D 1000-1028
1029		A 1029m,sh*; D 1000-1028
1052	Ring vibration	A 1054vw*
1077	In-plane δ(CC)	A 1074vw
1114		
1149	v_{as}(C-NH)	A 1149m*; D 1145
1175	$\delta(CH)_{ring}$	A 1178w
1204	v(CN)	A 1203s; D 1204
1261	δ(CH)	A 1260m; D 1257
1302	In-plane δ(CH)	A 1304m
1320	Ring vibration	A 1323m
1346	δ(CH)	A 1350w*
1369	$\delta(OCH_2)$	A 1369ms
1405	Ring stretch	A 1405s*; D 1400-1420
1432	δ(CH)	A 1434s
1467	δ(CH)	A 1466s
1582	Ring stretch	A 1581m; D 1580-1616
1597		A 1594m*; D 1580-1616
1620	Ring stretch (benzoic acid)	A 1621m; D 1627
2863	$v(CH_2)$	A 2862m
2904	$v(CH)_{ring}$	A 2905m
2933	$v_{as}(CH_2)$	A 2937m
3060	v(CH)	A 3060m

Table S2: Assignment of Raman spectral features for salbutamol sulfate from a Salamol pMDI. A – Ali et al.[3]; D – Davidson et al.[2]; s – strong, m – medium, w – weak, vw – very weak, b – broad, sh – shoulder.

Wavenumber (cm^{-1})	**Feature**	**Refs (cm^{-1})**
448		
464	$\delta(CC)_{chain}$	A 465vw
485		A 487vw
584	Out-of-plane $\delta(CCC)_{ring}$	A 589w
653	CH wagging	A 648w; D 656
709		
751	Ring vibration	A 747m; D 752
777	v(C-C-O)	A 780ms; D 784
880	$\delta(CH)_{ring}$	A 881w
934	Out-of-plane δ(CH)	A 937mw
975	v_{as}(C-OH)	A 978s; D 977
997		
1058	Complex mode involving H-bonded phenolic OH	A 1062w; D 1059
1077		A 1080w; D 1074
1117		
1151	v(S=O)	A 1156vw; D 1154
1206	v(C-OH) (Complex, H-bonded mode)	A 1205w
1240		
1261	δ(CH)	A 1255m; D 1257
1297		
1358	Mixed modes	A 1360w; D 1360
1445	Ring stretch	D 1450
1465	$\delta(CH_2\text{-}N)$	A 1468m; D 1463
1542		
1613	Complex mode	A 1616ms; D 1615
1662		
2817		A 2821vw
2850		A 2854w
2888	$v(CH_3)$	A 2880m
2896	$v(CH_2)$ (attached to OH)	A 2899m
2930	v(CH) (attached to OH)	A 2927m,br
2972	$v_{as}(CH_3)$	A 2973m,sh
2989	$v_{as}(CH_3)$	A 2990ms
3063	$v(CH_2)$ and $v(CH_3)$	A 3062m

Table S3: Assignment of Raman spectral features for ciclesonide from a Alvesco pMDI. F – Feth et al.[4]; D – Davidson et al.[2]; s – strong, m – medium, w – weak, sh – shoulder.

Wavenumber (cm^{-1})	**Feature**	**Refs (cm^{-1})**
532		
647		
698	$r(CH_2)$	F 698w
785	$r(CH_2)$	F 784w
826	δ(C=C-C=O)	F 823w; D 800-900 (multiple)
925		
967	ν(C-C)	D 963
1030	ν(C-O) (secondary alcohols and ethers)	F 1032-1199wm (multiple); D 1029
1074		
1109		D 1112
1133		
1154		
1194		
1238	ν(C-O) (ester)	F 1239w; D 1242
1327	δ(CH) (isopropyl)	D 1330 (multiple peaks)
1347	$\delta(CH_2)$ and $\delta(CH_3)$	F 1346-1468wm (multiple); D 1443
1385		
1442		
1467		
1604	ν(C=C)	F 1604m; D 1601
1620		F 1612m
1657	ν(C=O) (α,β-unsaturated)	F 1655s; D 1654
1729	ν(C=O) (ketones, esters)	F 1733w
1744		F 1747w
2860	$\nu(CH_2)/\nu(CH_3)$	F 2849-2968s
2941		

References

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