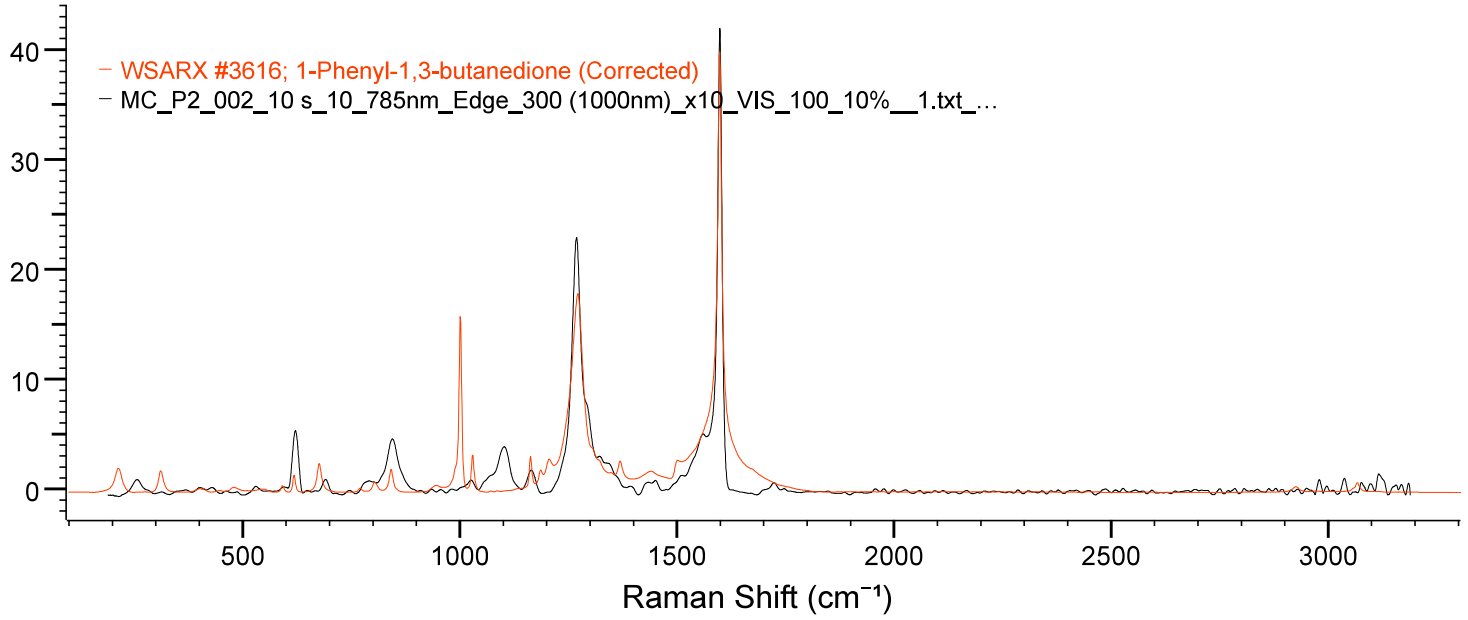

Manual Corrections: None
Ranges: Full
Search Algorithm: Correlation
Query Path: E:\1. Análises SNOM\#MPs PEIXE MOCAMBIQUE\MC MZ MPT\MC P2 002 10 ...

Name	Value
Resulting HQI	72.29
Database Abbreviation	WSARX
Database Title	Raman - Sigma-Aldrich Library of Raman Spectra - Wiley
Record ID	3616
Name	1-Phenyl-1,3-butanedione
Brand	ALDRICH
CAS Registry Number	93-91-4
Catalog Number	B11907
Exact Mass	162.068079564 u
Formula	$C_{10}H_{10}O_2$
Formula (reported)	C10H10O2
InChI	InChI=1S/C10H10O2/c1-8(11)7-10(12)9-5-3-2-4-6-9/h2-6H,7H2,1H3
InChIKey	CVBUKMMMRLOKQR-UHFFFAOYSA-N
Molecular Weight	162.1852 g/mol
Purity	99%
Synonyms	Benzoylacetone
Wiley ID	SIAL_RAMAN_003672

