Yasuda-Shedlovsky Result

Sample name:	**CS000189**	Experiment start time:	**07/09/2011 21:54:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07027**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07027_CS000189_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	4.67	±0.04	22.89	-1286.2045	0.9888	0.200 M	26.4°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11I-07027 Points 99 to 147	20.08 %	Up	UV-metric pKa	77.1	45.0 M	0.206 M	26.3°C	☑	4.56
11I-07027 Points 50 to 98	27.06 %	Up	UV-metric pKa	76.8	41.4 M	0.201 M	26.1°C	☑	4.50
11I-07027 Points 3 to 49	35.94 %	Up	UV-metric pKa	75.8	36.6 M	0.193 M	26.9°C	☑	4.37

Graphs

Sample name:	**CS000189**	Experiment start time:	**07/09/2011 21:54:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07027**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07027_CS000189_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11I-07027 Points 3 to 49

Graphs

Sample name:	**CS000189**	Experiment start time:	**07/09/2011 21:54:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07027**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07027_CS000189_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11I-07027 Points 50 to 98

Graphs

Sample name:	**CS000189**	Experiment start time:	**07/09/2011 21:54:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07027**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07027_CS000189_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11I-07027 Points 99 to 147

Graphs

Sample name:	**CS000189**	Experiment start time:	**07/09/2011 21:54:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07027**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07027_CS000189_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000189		
Sample by	Volume	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Molecular weight	295.30		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
pKa 1	4.00	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
logp (XH +)	-10.00	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
logP (neutral X)	-10.00	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r