Yasuda-Shedlovsky Result

Sample name:	**CS000055**	Experiment start time:	**12/08/2011 16:30:32**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-12011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-12011_CS000055_UV-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	7.23	±0.01	-2.94	929.5288	0.9986	0.182 M	26.6°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-12011 Points 89 to 132	26.90 %	Up	UV-metric pKa	76.5	41.4 M	0.188 M	26.7°C	☑	7.59
11H-12011 Points 46 to 87	35.44 %	Up	UV-metric pKa	75.9	36.9 M	0.184 M	26.8°C	☑	7.73
11H-12011 Points 4 to 44	46.64 %	Up	UV-metric pKa	74.8	30.8 M	0.172 M	26.1°C	☑	7.99

Graphs

Sample name:	**CS000055**	Experiment start time:	**12/08/2011 16:30:32**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-12011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-12011_CS000055_UV-metric psKa.t3r**		

UV-metric psKa Titration 1 of 3 11H-12011 Points 4 to 44 Quality: Good

Graphs

Sample name:	**CS000055**	Experiment start time:	**12/08/2011 16:30:32**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-12011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-12011_CS000055_UV-metric psKa.t3r**		

UV-metric psKa Titration 2 of 3 11H-12011 Points 46 to 87 Quality: Good

Graphs

Sample name:	**CS000055**	Experiment start time:	**12/08/2011 16:30:32**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-12011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-12011_CS000055_UV-metric psKa.t3r**		

UV-metric psKa Titration 3 of 3 11H-12011 Points 89 to 132 Quality: Good

Graphs

Sample name:	**CS000055**	Experiment start time:	**12/08/2011 16:30:32**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-12011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-12011_CS000055_UV-metric psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000055		
Sample by	Volume		
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	12/08/2011 10:00:58	E:\T3 DATA\1108\11H-01007_CS00077_pH-metric psKa.t3r
Molecular weight	303.30		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	12/08/2011 10:00:58	E:\T3 DATA\1108\11H-01007_CS00077_pH-metric psKa.t3r
pKa 1	5.00		
logp (XH +)	-10.00	12/08/2011 10:00:58	E:\T3 DATA\1108\11H-01007_CS00077_pH-metric psKa.t3r
logP (neutral X)	-10.00		