Yasuda-Shedlovsky Result

Sample name:	**CS000165**	Experiment start time:	**09/09/2011 14:37:02**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-09013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-09013_CS000165_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	6.20	±0.00	6.26	131.5152	0.9970	0.207 M	26.3°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11I-09013 Points 106 to 158	23.46 %	Up	UV-metric pKa	76.9	43.3 M	0.212 M	26.3°C	☑	6.34
11I-09013 Points 54 to 105	31.35 %	Up	UV-metric pKa	76.5	39.1 M	0.209 M	26.1°C	☑	6.39
11I-09013 Points 3 to 53	42.49 %	Up	UV-metric pKa	75.3	33.1 M	0.201 M	26.4°C	☑	6.49

Graphs

Sample name:	**CS000165**	Experiment start time:	**09/09/2011 14:37:02**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-09013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-09013_CS000165_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11I-09013 Points 3 to 53

Graphs

Sample name:	**CS000165**	Experiment start time:	**09/09/2011 14:37:02**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-09013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-09013_CS000165_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11I-09013 Points 54 to 105

Graphs

Sample name:	**CS000165**	Experiment start time:	**09/09/2011 14:37:02**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-09013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-09013_CS000165_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11I-09013 Points 106 to 158

Graphs

Sample name:	**CS000165**	Experiment start time:	**09/09/2011 14:37:02**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-09013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-09013_CS000165_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000165		
Sample by	Volume		
Sample volume	0.0150 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	448.30		
Individual pKa ionic environments	No		
Number of pKas	1	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample is a	Base	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r