Yasuda-Shedlovsky Result

Sample name:	**CS000150**	Experiment start time:	**01/09/2011 13:07:21**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01014_CS000150_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	7.64	±0.01	5.61	293.4327	0.9801	0.204 M	26.9°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11I-01014 Points 112 to 164	19.89 %	Up	UV-metric pKa	76.8	45.1 M	0.208 M	27.0°C	☑	7.77
11I-01014 Points 57 to 111	26.48 %	Up	UV-metric pKa	76.7	41.7 M	0.207 M	26.4°C	☑	7.82
11I-01014 Points 3 to 56	35.14 %	Up	UV-metric pKa	75.8	37.0 M	0.195 M	27.2°C	☑	7.92

Graphs

Sample name:	**CS000150**	Experiment start time:	**01/09/2011 13:07:21**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01014_CS000150_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11I-01014 Points 3 to 56

Graphs

Sample name:	**CS000150**	Experiment start time:	**01/09/2011 13:07:21**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01014_CS000150_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11I-01014 Points 57 to 111

Graphs

Sample name:	**CS000150**	Experiment start time:	**01/09/2011 13:07:21**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01014_CS000150_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11I-01014 Points 112 to 164

Graphs

Sample name:	**CS000150**	Experiment start time:	**01/09/2011 13:07:21**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01014_CS000150_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000150		
Sample by	Volume		
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	385.40		
Individual pKa ionic environments	No		
Number of pKas	1	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample is a	Base	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r