Yasuda-Shedlovsky Result

Sample name:	**CS000031**	Experiment start time:	**01/09/2011 11:06:21**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01009_CS000031_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	4.71	±0.01	11.49	-393.1407	0.9953	0.202 M	26.3°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11I-01009 Points 107 to 151	19.77 %	Up	UV-metric pKa	77.1	45.2 M	0.207 M	26.3°C	✓	4.74
11I-01009 Points 54 to 106	26.31 %	Up	UV-metric pKa	76.9	41.8 M	0.203 M	26.0°C	✓	4.75
11I-01009 Points 3 to 53	35.16 %	Up	UV-metric pKa	76.0	37.0 M	0.196 M	26.7°C	✓	4.75

Graphs

Sample name:	**CS000031**	Experiment start time:	**01/09/2011 11:06:21**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01009_CS000031_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11I-01009 Points 3 to 53

Graphs

Sample name:	**CS000031**	Experiment start time:	**01/09/2011 11:06:21**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01009_CS000031_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11I-01009 Points 54 to 106

Graphs

Sample name:	**CS000031**	Experiment start time:	**01/09/2011 11:06:21**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01009_CS000031_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11I-01009 Points 107 to 151

Graphs

Sample name:	**CS000031**	Experiment start time:	**01/09/2011 11:06:21**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11I-01009_CS000031_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000031		
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	406.46		
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