Yasuda-Shedlovsky Result

Sample name:	**CS000100**	Experiment start time:	**12/08/2011 18:53:48**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-12014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-12014_CS000100_UV-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	4.76	±0.09	36.01	-2308.7081	0.9883	0.186 M	25.9°C
Yasuda-Shedlovsky	6.85	±0.04	-8.73	1355.8652	0.9938	0.186 M	25.9°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1	
11H-12014 Points 96 to 146	25.33 %	Up	UV-metric pKa	76.7	42.3 M	0.192 M	26.4°C	☑	4.32	☑
11H-12014 Points 48 to 94	32.75 %	Up	UV-metric pKa	76.4	38.3 M	0.189 M	26.1°C	☑	4.17	☑
11H-12014 Points 4 to 46	43.56 %	Up	UV-metric pKa	75.6	32.5 M	0.178 M	25.1°C	☑	3.97	☑

Graphs

Sample name:	**CS000100**	Experiment start time:	**12/08/2011 18:53:48**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-12014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-12014_CS000100_UV-metric psKa.t3r**		

UV-metric psKa Titration 1 of 3 11H-12014 Points 4 to 46

Graphs

Sample name:	**CS000100**	Experiment start time:	**12/08/2011 18:53:48**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-12014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-12014_CS000100_UV-metric psKa.t3r**		

UV-metric psKa Titration 2 of 3 11H-12014 Points 48 to 94

Graphs

Sample name:	**CS000100**	Experiment start time:	**12/08/2011 18:53:48**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-12014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-12014_CS000100_UV-metric psKa.t3r**		

UV-metric psKa Titration 3 of 3 11H-12014 Points 96 to 146

Graphs

Sample name:	**CS000100**	Experiment start time:	**12/08/2011 18:53:48**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-12014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-12014_CS000100_UV-metric psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000100	12/08/2011 18:52:54	E:\T3 DATA\1107\11G-31007_CS000100_pH-metric psKa.t3r
Sample by	Volume		
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	12/08/2011 18:52:54	E:\T3 DATA\1107\11G-31007_CS000100_pH-metric psKa.t3r
Molecular weight	473.30		
Individual pKa ionic environments	No		
Number of pKas	2	12/08/2011 18:52:54	E:\T3 DATA\1107\11G-31007_CS000100_pH-metric psKa.t3r
Sample is a	Base	12/08/2011 18:52:54	E:\T3 DATA\1107\11G-31007_CS000100_pH-metric psKa.t3r
pKa 1	4.00	12/08/2011 18:52:54	E:\T3 DATA\1107\11G-31007_CS000100_pH-metric psKa.t3r
pKa 2	8.00	12/08/2011 18:52:54	E:\T3 DATA\1107\11G-31007_CS000100_pH-metric psKa.t3r
logP (XH2 2+)	-10.00	12/08/2011 18:52:54	E:\T3 DATA\1107\11G-31007_CS000100_pH-metric psKa.t3r
logp (XH +)	-10.00	12/08/2011 18:52:54	E:\T3 DATA\1107\11G-31007_CS000100_pH-metric psKa.t3r
logP (neutral X)	-10.00	12/08/2011 18:52:54	E:\T3 DATA\1107\11G-31007_CS000100_pH-metric psKa.t3r