Yasuda-Shedlovsky Result

Sample name:	**CS000112**	Experiment start time:	**26/08/2011 16:31:03**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26012_CS000112_UV-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	2.45	±0.10	25.84	-1688.3629	0.9696	0.188 M	26.6°C
Yasuda-Shedlovsky	8.98	±0.01	12.48	-137.6728	0.9199	0.188 M	26.6°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1	
11H-26012 Points 91 to 136	24.93 %	Up	UV-metric pKa	76.6	42.5 M	0.193 M	26.9°C	☑	2.16	☑
11H-26012 Points 47 to 89	32.07 %	Up	UV-metric pKa	76.1	38.7 M	0.191 M	27.1°C	☑	2.10	☑
11H-26012 Points 4 to 45	42.01 %	Up	UV-metric pKa	75.6	33.4 M	0.181 M	25.8°C	☑	1.96	☑

Graphs

Sample name:	**CS000112**	Experiment start time:	**26/08/2011 16:31:03**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26012_CS000112_UV-metric psKa.t3r**		

UV-metric psKa Titration 1 of 3 11H-26012 Points 4 to 45

Graphs

Sample name:	**CS000112**	Experiment start time:	**26/08/2011 16:31:03**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26012_CS000112_UV-metric psKa.t3r**		

UV-metric psKa Titration 2 of 3 11H-26012 Points 47 to 89

Graphs

Sample name:	**CS000112**	Experiment start time:	**26/08/2011 16:31:03**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26012_CS000112_UV-metric psKa.t3r**		

UV-metric psKa Titration 3 of 3 11H-26012 Points 91 to 136

Graphs

Sample name:	**CS000112**	Experiment start time:	**26/08/2011 16:31:03**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26012_CS000112_UV-metric psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000112		
Sample by	Volume		
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	26/08/2011 14:14:04	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	375.39		
Individual pKa ionic environments	No		
Number of pKas	2		
Sample is a	Base	26/08/2011 14:14:04	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	26/08/2011 14:14:04	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 2	9.00		
logP (XH2 2+)	-10.00	26/08/2011 14:14:04	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	26/08/2011 14:14:04	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00		