Yasuda-Shedlovsky Result

Sample name:	**CS000104**	Experiment start time:	**25/08/2011 17:05:04**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25017_CS000104_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.55	±0.09	30.92	-2002.1958	0.9718	0.206 M	26.1°C
Yasuda-Shedlovsky	9.51	±0.01	7.88	263.7863	0.9831	0.206 M	26.1°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-25017 Points 104 to 155	20.88 %	Up	UV-metric pKa	77.1	44.6 M	0.211 M	26.2°C	☑	3.32
11H-25017 Points 53 to 103	27.35 %	Up	UV-metric pKa	76.8	41.2 M	0.207 M	25.8°C	☑	3.20
11H-25017 Points 3 to 52	37.59 %	Up	UV-metric pKa	75.8	35.7 M	0.199 M	26.4°C	☑	2.97

Graphs

Sample name:	**CS000104**	Experiment start time:	**25/08/2011 17:05:04**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25017_CS000104_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11H-25017 Points 3 to 52

Graphs

Sample name:	**CS000104**	Experiment start time:	**25/08/2011 17:05:04**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25017_CS000104_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11H-25017 Points 53 to 103

Graphs

Sample name:	**CS000104**	Experiment start time:	**25/08/2011 17:05:04**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25017_CS000104_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11H-25017 Points 104 to 155

Graphs

Sample name:	**CS000104**	Experiment start time:	**25/08/2011 17:05:04**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25017**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25017_CS000104_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000104		
Sample by	Volume		
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	25/08/2011 14:45:10	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	351.64		
Individual pKa ionic environments	No		
Number of pKas	2		
Sample is a	Base	25/08/2011 14:45:10	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	25/08/2011 14:45:10	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 2	9.20		
logP (XH2 2+)	-10.00	25/08/2011 14:45:10	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	25/08/2011 14:45:10	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00		