Yasuda-Shedlovsky Result

Sample name:	**CS000140**	Experiment start time:	**29/08/2011 13:09:34**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29012_CS000140_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.58	±0.16	32.18	-2081.1568	0.9518	0.206 M	28.0°C
Yasuda-Shedlovsky	10.40	±0.01	14.66	-195.4470	0.9701	0.206 M	28.0°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-29012 Points 107 to 160	23.42 %	Up	UV-metric pKa	76.1	43.2 M	0.210 M	28.5°C	☑	3.26
11H-29012 Points 54 to 106	32.55 %	Up	UV-metric pKa	75.9	38.4 M	0.209 M	27.6°C	☑	3.09
11H-29012 Points 3 to 53	43.67 %	Up	UV-metric pKa	74.7	32.4 M	0.198 M	27.8°C	☑	2.81

Graphs

Sample name:	**CS000140**	Experiment start time:	**29/08/2011 13:09:34**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29012_CS000140_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11H-29012 Points 3 to 53

Graphs

Sample name:	**CS000140**	Experiment start time:	**29/08/2011 13:09:34**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29012_CS000140_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11H-29012 Points 54 to 106

Graphs

Sample name:	**CS000140**	Experiment start time:	**29/08/2011 13:09:34**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29012_CS000140_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11H-29012 Points 107 to 160

Graphs

Sample name:	**CS000140**	Experiment start time:	**29/08/2011 13:09:34**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29012_CS000140_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000140		
Sample by	Volume		
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	376.46		
Individual pKa ionic environments	No		
Number of pKas	2		
Sample is a	Base	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 2	9.30		
logP (XH2 2+)	-10.00	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00		