Yasuda-Shedlovsky Result

Sample name:	**CS000116**	Experiment start time:	**25/08/2011 15:10:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25012_CS000116_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.58	±0.13	32.50	-2131.6693	0.9494	0.199 M	25.3°C
Yasuda-Shedlovsky	9.48	±0.16	2.63	673.4990	0.5784	0.199 M	25.3°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-25012 Points 103 to 154	20.51 %	Up	UV-metric pKa	77.3	44.8 M	0.205 M	25.5°C	☑	3.34
11H-25012 Points 52 to 102	27.42 %	Up	UV-metric pKa	77.1	41.2 M	0.202 M	25.0°C	☑	3.19
11H-25012 Points 3 to 51	37.08 %	Up	UV-metric pKa	76.2	36.0 M	0.191 M	25.5°C	☑	2.98

Graphs

Sample name:	**CS000116**	Experiment start time:	**25/08/2011 15:10:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25012_CS000116_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11H-25012 Points 3 to 51 Quality: Good

Graphs

Sample name:	**CS000116**	Experiment start time:	**25/08/2011 15:10:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25012_CS000116_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11H-25012 Points 52 to 102 Quality: Good

Graphs

Sample name:	**CS000116**	Experiment start time:	**25/08/2011 15:10:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25012_CS000116_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11H-25012 Points 103 to 154 Quality: Good

Graphs

Sample name:	**CS000116**	Experiment start time:	**25/08/2011 15:10:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25012_CS000116_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000116		
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		