Yasuda-Shedlovsky Result

Sample name:	**CS000166**	Experiment start time:	**08/09/2011 10:35:44**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-08006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-08006_CS000166_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.79	±0.04	-7.32	1000.1874	0.9776	0.203 M	27.1°C
Yasuda-Shedlovsky	8.78	±0.09	-10.40	1628.4890	0.9609	0.203 M	27.1°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1	
11I-08006 Points 106 to 157	20.32 %	Up	UV-metric pKa	76.7	44.9 M	0.207 M	27.2°C	☑	4.04	☑
11I-08006 Points 54 to 105	27.53 %	Up	UV-metric pKa	76.6	41.1 M	0.206 M	26.6°C	☑	4.15	☑
11I-08006 Points 3 to 53	38.27 %	Up	UV-metric pKa	75.4	35.4 M	0.198 M	27.4°C	☑	4.38	☑

Graphs

Sample name:	**CS000166**	Experiment start time:	**08/09/2011 10:35:44**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-08006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-08006_CS000166_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11I-08006 Points 3 to 53

Graphs

Sample name:	**CS000166**	Experiment start time:	**08/09/2011 10:35:44**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-08006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-08006_CS000166_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11I-08006 Points 54 to 105

Graphs

Sample name:	**CS000166**	Experiment start time:	**08/09/2011 10:35:44**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-08006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-08006_CS000166_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11I-08006 Points 106 to 157

Graphs

Sample name:	**CS000166**	Experiment start time:	**08/09/2011 10:35:44**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-08006**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-08006_CS000166_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000166		
Sample by	Volume		
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown		
Molecular weight	446.49		
Individual pKa ionic environments	No		
Number of pKas	2		
Sample is a	Base		
pKa 1	4.00		
pKa 2	9.50		
logP (XH2 2+)	-10.00		
logp (XH +)	-10.00		
logP (neutral X)	-10.00		