Yasuda-Shedlovsky Result

Sample name:	**CS000085**	Experiment start time:	**25/08/2011 15:33:31**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25013_CS000085_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	2.99	±0.02	21.80	-1337.5653	0.9967	0.198 M	25.5°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-25013 Points 102 to 152	20.32 %	Up	UV-metric pKa	77.3	44.9 M	0.205 M	25.5°C	☑	2.86
11H-25013 Points 51 to 101	27.24 %	Up	UV-metric pKa	77.1	41.3 M	0.201 M	25.0°C	☑	2.83
11H-25013 Points 3 to 50	37.01 %	Up	UV-metric pKa	76.0	36.1 M	0.189 M	26.0°C	☑	2.65

Graphs

Sample name:	**CS000085**	Experiment start time:	**25/08/2011 15:33:31**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25013_CS000085_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11H-25013 Points 3 to 50 Quality: Good

Graphs

Sample name:	**CS000085**	Experiment start time:	**25/08/2011 15:33:31**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25013_CS000085_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11H-25013 Points 51 to 101 Quality: Good

Graphs

Sample name:	**CS000085**	Experiment start time:	**25/08/2011 15:33:31**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25013_CS000085_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11H-25013 Points 102 to 152 Quality: Good

Graphs

Sample name:	**CS000085**	Experiment start time:	**25/08/2011 15:33:31**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25013_CS000085_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000085		
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	337.34		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	25/08/2011 14:45:10	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	3.00		
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		