Yasuda-Shedlovsky Result

Sample name:	**CS000029**	Experiment start time:	**25/08/2011 20:20:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25025**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25025_CS000029_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.05	±0.08	27.78	-1783.7993	0.9783	0.202 M	27.7°C
Yasuda-Shedlovsky	3.84	±0.07	-7.84	1041.5070	0.9504	0.202 M	27.7°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-25025 Points 104 to 155	21.02 %	Up	UV-metric pKa	76.5	44.5 M	0.208 M	27.7°C	☑	2.85
11H-25025 Points 53 to 103	27.58 %	Up	UV-metric pKa	76.3	41.1 M	0.204 M	27.3°C	☑	2.76
11H-25025 Points 3 to 52	38.00 %	Up	UV-metric pKa	75.2	35.5 M	0.194 M	28.1°C	☑	2.52

Graphs

Sample name:	**CS000029**	Experiment start time:	**25/08/2011 20:20:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25025**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25025_CS000029_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11H-25025 Points 3 to 52

Graphs

Sample name:	**CS000029**	Experiment start time:	**25/08/2011 20:20:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25025**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25025_CS000029_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11H-25025 Points 53 to 103

Graphs

Sample name:	**CS000029**	Experiment start time:	**25/08/2011 20:20:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25025**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25025_CS000029_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11H-25025 Points 104 to 155

Graphs

Sample name:	**CS000029**	Experiment start time:	**25/08/2011 20:20:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25025**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25025_CS000029_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000029		
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	313.34		
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	4.50		
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		