Yasuda-Shedlovsky Result

Sample name:	**CS000112**	Experiment start time:	**25/08/2011 19:07:14**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25022**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25022_CS000112_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	2.34	±0.07	22.33	-1419.2200	0.9723	0.206 M	27.1°C
Yasuda-Shedlovsky	8.94	±0.02	12.15	-114.4720	0.7985	0.206 M	27.1°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-25022 Points 104 to 155	20.93 %	Up	UV-metric pKa	76.7	44.6 M	0.211 M	27.2°C	☑	2.21
11H-25022 Points 53 to 103	27.38 %	Up	UV-metric pKa	76.5	41.2 M	0.207 M	26.8°C	☑	2.13
11H-25022 Points 3 to 52	37.71 %	Up	UV-metric pKa	75.5	35.6 M	0.199 M	27.5°C	☑	1.97

Graphs

Sample name:	**CS000112**	Experiment start time:	**25/08/2011 19:07:14**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25022**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25022_CS000112_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11H-25022 Points 3 to 52

Graphs

Sample name:	**CS000112**	Experiment start time:	**25/08/2011 19:07:14**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25022**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25022_CS000112_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11H-25022 Points 53 to 103

Graphs

Sample name:	**CS000112**	Experiment start time:	**25/08/2011 19:07:14**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25022**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25022_CS000112_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11H-25022 Points 104 to 155

Graphs

Sample name:	**CS000112**	Experiment start time:	**25/08/2011 19:07:14**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-25022**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-25022_CS000112_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000112		
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	375.39		
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		