Yasuda-Shedlovsky Result

Sample name:	**CS000196**	Experiment start time:	**07/09/2011 22:16:04**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07028**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07028_CS000196_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	6.45	±0.03	19.10	-852.5638	0.9848	0.204 M	26.2°C
Yasuda-Shedlovsky	8.66	±0.00	13.21	-219.7815	0.9941	0.204 M	26.2°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1	
11I-07028 Points 105 to 156	19.75 %	Up	UV-metric pKa	77.1	45.2 M	0.209 M	26.1°C	☑	6.40	☑
11I-07028 Points 53 to 104	26.61 %	Up	UV-metric pKa	76.9	41.6 M	0.207 M	25.8°C	☑	6.38	☑
11I-07028 Points 3 to 52	35.56 %	Up	UV-metric pKa	76.0	36.8 M	0.198 M	26.6°C	☑	6.32	☑

Graphs

Sample name:	**CS000196**	Experiment start time:	**07/09/2011 22:16:04**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07028**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07028_CS000196_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11I-07028 Points 3 to 52

Graphs

Sample name:	**CS000196**	Experiment start time:	**07/09/2011 22:16:04**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07028**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07028_CS000196_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11I-07028 Points 53 to 104

Graphs

Sample name:	**CS000196**	Experiment start time:	**07/09/2011 22:16:04**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07028**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07028_CS000196_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11I-07028 Points 105 to 156

Graphs

Sample name:	**CS000196**	Experiment start time:	**07/09/2011 22:16:04**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07028**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07028_CS000196_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000196		
Sample by	Volume	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Molecular weight	458.52		
Individual pKa ionic environments	No		
Number of pKas	2		
Sample is a	Base	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
pKa 1	6.00		
pKa 2	8.90		
logP (XH2 2+)	-10.00	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
logp (XH +)	-10.00		
logP (neutral X)	-10.00		