Yasuda-Shedlovsky Result

Sample name:	**CS000173**	Experiment start time:	**07/09/2011 19:46:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07022**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07022_CS000173_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	6.75	±0.03	23.48	-1173.4286	0.9888	0.204 M	25.7°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11I-07022 Points 105 to 156	19.86 %	Up	UV-metric pKa	77.4	45.2 M	0.208 M	25.5°C	☑	6.67
11I-07022 Points 53 to 104	26.86 %	Up	UV-metric pKa	77.0	41.5 M	0.206 M	25.3°C	☑	6.62
11I-07022 Points 3 to 52	36.14 %	Up	UV-metric pKa	76.1	36.5 M	0.197 M	26.2°C	☑	6.49

Graphs

Sample name:	**CS000173**	Experiment start time:	**07/09/2011 19:46:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07022**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07022_CS000173_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11I-07022 Points 3 to 52

Graphs

Sample name:	**CS000173**	Experiment start time:	**07/09/2011 19:46:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07022**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07022_CS000173_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11I-07022 Points 53 to 104

Graphs

Sample name:	**CS000173**	Experiment start time:	**07/09/2011 19:46:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07022**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07022_CS000173_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11I-07022 Points 105 to 156

Graphs

Sample name:	**CS000173**	Experiment start time:	**07/09/2011 19:46:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07022**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07022_CS000173_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000173		
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	361.47		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
pKa 1	6.20		
logp (XH +)	-10.00	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
logP (neutral X)	-10.00		