Yasuda-Shedlovsky Result

Sample name:	**CS000029**	Experiment start time:	**01/09/2011 10:41:09**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01008**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01008_CS000029_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	2.99	±0.02	22.10	-1350.7457	0.9956	0.198 M	27.2°C
Yasuda-Shedlovsky	3.95	±0.04	-3.91	747.3252	0.9705	0.198 M	27.2°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1	
11I-01008 Points 108 to 147	19.97 %	Up	UV-metric pKa	77.0	45.1 M	0.205 M	26.5°C	☑	2.92	☑
11I-01008 Points 55 to 107	26.43 %	Up	UV-metric pKa	76.6	41.7 M	0.201 M	26.7°C	☑	2.83	☑
11I-01008 Points 3 to 54	35.29 %	Up	UV-metric pKa	75.4	36.9 M	0.190 M	28.4°C	☑	2.62	☑

Graphs

Sample name:	**CS000029**	Experiment start time:	**01/09/2011 10:41:09**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01008**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01008_CS000029_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11I-01008 Points 3 to 54

Graphs

Sample name:	**CS000029**	Experiment start time:	**01/09/2011 10:41:09**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01008**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01008_CS000029_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11I-01008 Points 55 to 107

Graphs

Sample name:	**CS000029**	Experiment start time:	**01/09/2011 10:41:09**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01008**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01008_CS000029_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11I-01008 Points 108 to 147

Graphs

Sample name:	**CS000029**	Experiment start time:	**01/09/2011 10:41:09**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01008**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01008_CS000029_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000029		
Sample by	Volume		
Sample volume	0.0120 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	01/09/2011 10:40:23	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	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 2	4.50		
logP (XH2 2+)	-10.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00		