Yasuda-Shedlovsky Result

Sample name:	**CS000034**	Experiment start time:	**26/08/2011 20:18:22**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-26015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26015_CS000034_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.73	±0.01	-2.59	627.7570	0.9996	0.173 M	26.7°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-26015 Points 79 to 121	29.85 %	Down	pH-metric	76.2	39.9 M	0.190 M	27.3°C	☑	4.06
11H-26015 Points 40 to 78	41.32 %	Down	pH-metric	75.4	33.7 M	0.180 M	26.4°C	☑	4.20
11H-26015 Points 3 to 39	61.85 %	Down	pH-metric	71.6	22.3 M	0.151 M	26.5°C	☑	4.83

Graphs

Sample name:	**CS000034**	Experiment start time:	**26/08/2011 20:18:22**
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Assay ID:	**11H-26015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26015_CS000034_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-26015 Points 3 to 39

Sample

- CS000034 concentration factor 1.000
- Base pKa 1 4.83

Sample graphs

Other graphs

Sample name:	**CS000034**	Experiment start time:	**26/08/2011 20:18:22**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-26015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26015_CS000034_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-26015 Points 40 to 78

Sample

- CS000034 concentration factor 1.000
- Base pKa 1 4.20

Sample graphs

Other graphs

Sample name:	**CS000034**	Experiment start time:	**26/08/2011 20:18:22**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-26015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26015_CS000034_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-26015 Points 79 to 121

Sample

CS000034 concentration factor 1.000
Base pKa 1 4.06

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000034		
Sample by	Weight		
Sample weight	0.001010 g		
Formula weight	436.92 g/mol		
Solubility	Unknown	26/08/2011 19:04:28	E:\T3 DATA\1108\11H-25023_CS000115_Fast UV psKa.t3r
Molecular weight	436.92		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	26/08/2011 19:04:28	E:\T3 DATA\1108\11H-25023_CS000115_Fast UV psKa.t3r
pKa 1	5.00		
logp (XH +)	-10.00	26/08/2011 19:04:28	E:\T3 DATA\1108\11H-25023_CS000115_Fast UV psKa.t3r
logP (neutral X)	-10.00	26/08/2011 19:04:28	E:\T3 DATA\1108\11H-25023_CS000115_Fast UV psKa.t3r