

## Sheet1

BRBRANCHNAME,(	STESTEPNAME,C,2	OPOPNAME,C,16	AMOLUNI'	NAME,C,30
3 Activated ester	-4			Triazole-Ester
1 Main	-9	1 Reaction	1 g	Final Product
2 Wittig Salt	-4			Wittig-salt
1 Main	4 Oxidation	1 Reaction	911 g	Diphenylmethyl-ester
1 Main	4 Oxidation	1 Reaction	8.85 l	Dichloromethane (purum)
1 Main	4 Oxidation	1 Reaction	26.7 g	Potassium bromide
1 Main	4 Oxidation	1 Reaction	70.2 ml	HCl 37%
1 Main	4 Oxidation	1 Reaction	6.55 l	Water
1 Main	4 Oxidation	1 Reaction	19.8 g	TEMPO
1 Main	4 Oxidation	1 Reaction	108 ml	Dichloromethane (purum)
1 Main	4 Oxidation	2 Filter&Rinse	360 g	Dicalite
1 Main	4 Oxidation	2 Filter&Rinse	2 l	Dichloromethane (purum)
1 Main	4 Oxidation	2 Filter&Rinse	2 l	Water
1 Main	4 Oxidation	3 Extraction	12 l	Dichloromethane (purum)
1 Main	4 Oxidation	4 Extraction	1.55 kg	Sodium chloride
1 Main	4 Oxidation	4 Extraction	9.0 l	Water
1 Main	4 Oxidation	5 Evaporation		***** Operation Only *****
1 Main	4 Oxidation	6 Drying		***** Operation Only *****
1 Main	8 Deprotection	1 Reaction	450 g	Triazol-ester
1 Main	8 Deprotection	1 Reaction	1.98 l	Trifluoroacetic acid
1 Main	8 Deprotection	1 Reaction	120 ml	Triethylsilane
1 Main	8 Deprotection	1 Reaction	7.3 l	TBME(purum)
1 Main	8 Deprotection	2 Filter&Rinse	3 l	TBME(purum)
1 Main	8 Deprotection	3 Crystallization	50 ml	TBME(purum)
2 Wittig Salt	2 Lactamization	1 Reaction	100 g	2-Bromo-4-chloro-buty.
2 Wittig Salt	2 Lactamization	1 Reaction	54.4 g	NaOH pearls
2 Wittig Salt	2 Lactamization	1 Reaction	500 ml	Dichloromethane (purum)
2 Wittig Salt	2 Lactamization	1 Reaction	9.26 g	TBAF-hydrogensulfate
2 Wittig Salt	2 Lactamization	1 Reaction	35.6 g	Cyclopropylmethylamin
2 Wittig Salt	2 Lactamization	1 Reaction	100 ml	Dichloromethane (purum)
2 Wittig Salt	2 Lactamization	2 Extraction	50 g	Water
2 Wittig Salt	2 Lactamization	2 Extraction	250 ml	Water
2 Wittig Salt	2 Lactamization	2 Extraction	60 g	Ammoniumchloride
2 Wittig Salt	2 Lactamization	2 Extraction	300 ml	Water
2 Wittig Salt	2 Lactamization	2 Extraction	300 ml	Water
2 Wittig Salt	2 Lactamization	3 Evaporation		***** Operation Only *****
2 Wittig Salt	3 Wittig-salt	1 Reaction	90.0 g	Cyclopropylmethyl-lactam
2 Wittig Salt	3 Wittig-salt	1 Reaction	180 ml	Acetone (purum)
2 Wittig Salt	3 Wittig-salt	1 Reaction	180 ml	THF (purum)
2 Wittig Salt	3 Wittig-salt	1 Reaction	154 g	Triphenylphosphine
2 Wittig Salt	3 Wittig-salt	2 Filter&Rinse	90 ml	Acetone (purum)
2 Wittig Salt	3 Wittig-salt	2 Filter&Rinse	360 ml	Ethylacetate (purum)
2 Wittig Salt	3 Wittig-salt	3 Drying		***** Operation Only *****
2 Wittig Salt	3 Wittig-salt	4 Evaporation		***** Operation Only *****
2 Wittig Salt	3 Wittig-salt	5 Suspension	90 ml	Acetone (purum)
2 Wittig Salt	3 Wittig-salt	5 Suspension	90 ml	THF (purum)
2 Wittig Salt	3 Wittig-salt	6 Filter&Rinse	20 ml	THF (purum)
2 Wittig Salt	3 Wittig-salt	6 Filter&Rinse	20 ml	Acetone (purum)

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2 Wittig Salt	3 Wittig-salt	7 Drying			***** Operation Only *****
3 Activated ester	3 Esterification	1 Reaction	1.06	kg	Free acid
3 Activated ester	3 Esterification	1 Reaction	36.0	l	THF (purum)
3 Activated ester	3 Esterification	1 Reaction	405	g	1-Hydroxybenzotriazole
3 Activated ester	3 Esterification	1 Reaction	550	g	Dicyclohexylcarbodiimide
3 Activated ester	3 Esterification	2 Filter&Rinse	2	l	THF (purum)
3 Activated ester	3 Esterification	3 Evaporation			***** Operation Only *****
3 Activated ester	3 Esterification	4 Suspension	8.0	l	Isopropylether
3 Activated ester	3 Esterification	5 Filter&Rinse	1.0	l	Isopropylether
3 Activated ester	3 Esterification	6 Drying			***** Operation Only *****
1 Main	3 Esterification	1 Reaction	633	g	N-BOC-derivative
1 Main	3 Esterification	1 Reaction	3.64	l	THF (purum)
1 Main	3 Esterification	1 Reaction	1.55	l	Diphenyldiazomethans-solr
1 Main	3 Esterification	2 Filter&Rinse	2.4	l	Hexane (purum)
1 Main	3 Esterification	3 Drying			***** Operation Only *****
1 Main	3 Esterification	4 Evaporation			***** Operation Only *****
1 Main	3 Esterification	5 Suspension	1.0	l	Hexane (purum)
1 Main	3 Esterification	6 Filter&Rinse	150	ml	Hexane (purum)
1 Main	3 Esterification	6 Filter&Rinse	50	ml	THF (purum)
1 Main	3 Esterification	6 Filter&Rinse	750	ml	Hexane (purum)
1 Main	3 Esterification	7 Crystallization	1.5	l	Hexane (purum)
2 Wittig Salt	1 Bromination	1 Reaction	280	g	4-Chlorobutyr. chloride
2 Wittig Salt	1 Bromination	1 Reaction	546	g	NBS
2 Wittig Salt	1 Bromination	1 Reaction	560	ml	Dichloromethane (purum)
2 Wittig Salt	1 Bromination	1 Reaction	12	g	Thionylchloride
2 Wittig Salt	1 Bromination	1 Reaction	3.60	ml	HBr(48%)
2 Wittig Salt	1 Bromination	2 Evaporation			***** Operation Only *****
2 Wittig Salt	1 Bromination	3 Suspension	1.40	l	Hexane (purum)
2 Wittig Salt	1 Bromination	4 Filter&Rinse	350	ml	Hexane (purum)
2 Wittig Salt	1 Bromination	4 Filter&Rinse	350	ml	Hexane (purum)
2 Wittig Salt	1 Bromination	4 Filter&Rinse	350	ml	Hexane (purum)
2 Wittig Salt	1 Bromination	4 Filter&Rinse	350	ml	Hexane (purum)
2 Wittig Salt	1 Bromination	4 Filter&Rinse	350	ml	Hexane (purum)
2 Wittig Salt	1 Bromination	4 Filter&Rinse	350	ml	Hexane (purum)
2 Wittig Salt	1 Bromination	5 Evaporation			***** Operation Only *****
1 Main	1 Saponification	1 Reaction	983	g	Ethylester
1 Main	1 Saponification	1 Reaction	8	l	Water
1 Main	1 Saponification	1 Reaction	7	l	Methanol (purum)
1 Main	1 Saponification	1 Reaction	280	g	Sodium hydroxide
1 Main	1 Saponification	1 Reaction	820	ml	Water
1 Main	1 Saponification	1 Reaction	580	ml	HCl 37%
1 Main	1 Saponification	1 Reaction	580	ml	Water
1 Main	1 Saponification	2 Filter&Rinse	7	l	Water
1 Main	1 Saponification	2 Filter&Rinse	7	l	Acetone (purum)
1 Main	1 Saponification	3 Distillation			***** Operation Only *****
3 Activated ester	2 Saponification	1 Reaction	1.28	kg	Trityl-derivative
3 Activated ester	2 Saponification	1 Reaction	336	g	Sodium hydroxide
3 Activated ester	2 Saponification	1 Reaction	4.7	l	Water
3 Activated ester	2 Saponification	1 Reaction	4.7	kg	Sodium hydroxide

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3 Activated ester	2 Saponification	1 Reaction	8.0	l	Ethylacetate (purum)
3 Activated ester	2 Saponification	1 Reaction	700	ml	HCl 37%
3 Activated ester	2 Saponification	2 Extraction	30	l	Water
3 Activated ester	2 Saponification	3 Filter&Rinse	4	l	Water
3 Activated ester	2 Saponification	3 Filter&Rinse	4	l	Ethylacetate (purum)
3 Activated ester	2 Saponification	4 Drying			***** Operation Only *****
1 Main	2 BOC-protection	1 Reaction	624	g	Carboxylic acid
1 Main	2 BOC-protection	1 Reaction	4.0	l	Water
1 Main	2 BOC-protection	1 Reaction	1.17	kg	BOC-anhydride
1 Main	2 BOC-protection	1 Reaction	5.40	l	Dioxane (purum)
1 Main	2 BOC-protection	1 Reaction	2.06	l	NaOH(4N)
1 Main	2 BOC-protection	1 Reaction	9.0	ml	HCl 37%
1 Main	2 BOC-protection	1 Reaction	96	ml	Water
1 Main	2 BOC-protection	2 Filter&Rinse	2.6	l	Water
1 Main	2 BOC-protection	2 Filter&Rinse	2	l	Dioxane (purum)
1 Main	2 BOC-protection	3 Extraction	10.6	l	Ethylacetate (purum)
1 Main	2 BOC-protection	4 Suspension	482	ml	HCl 37%
1 Main	2 BOC-protection	4 Suspension	5.3	l	Water
1 Main	2 BOC-protection	5 Filter&Rinse	5.3	l	Water
1 Main	2 BOC-protection	6 Drying			***** Operation Only *****
1 Main	6 Deprotection	1 Reaction	356	g	Coupling product
1 Main	6 Deprotection	1 Reaction	500	ml	Acetic acid
1 Main	6 Deprotection	1 Reaction	260	ml	Acetic acid
1 Main	6 Deprotection	1 Reaction	500	ml	HCl 37%
1 Main	6 Deprotection	1 Reaction	1.14	l	Water
1 Main	6 Deprotection	1 Reaction	570	ml	TBME(purum)
1 Main	6 Deprotection	2 Extraction	620	ml	TBME(purum)
1 Main	6 Deprotection	2 Extraction	620	ml	TBME(purum)
1 Main	6 Deprotection	2 Extraction	290	ml	Water
1 Main	6 Deprotection	3 Suspension	290	ml	Methanol (purum)
1 Main	6 Deprotection	3 Suspension	600	ml	NaOH(4N)
1 Main	6 Deprotection	4 Filter&Rinse	1.54	l	Water
1 Main	6 Deprotection	4 Filter&Rinse	310	ml	Methanol (purum)
1 Main	6 Deprotection	5 Drying			***** Operation Only *****
3 Activated ester	1 Protection	1 Reaction	450	g	Heterocycle
3 Activated ester	1 Protection	1 Reaction	7.0	l	Ethylacetate (purum)
3 Activated ester	1 Protection	1 Reaction	92.0	g	Sodium hydride (60%)
3 Activated ester	1 Protection	1 Reaction	640	g	Triphenylchloromethane
3 Activated ester	1 Protection	1 Reaction	3.7	l	Ethylacetate (purum)
3 Activated ester	1 Protection	2 Evaporation			***** Operation Only *****
3 Activated ester	1 Protection	3 Suspension	4.0	l	Ice water
3 Activated ester	1 Protection	4 Filter&Rinse	2.0	l	Ice water
3 Activated ester	1 Protection	4 Filter&Rinse	2.0	l	Ice water
3 Activated ester	1 Protection	5 Drying			***** Operation Only *****
1 Main	7 Esterification	1 Reaction	210	g	Aminoacid
1 Main	7 Esterification	1 Reaction	600	ml	DMF (purum)
1 Main	7 Esterification	1 Reaction	130	ml	Triethylamin
1 Main	7 Esterification	1 Reaction	360	g	Aktivester
1 Main	7 Esterification	1 Reaction	840	ml	DMF (purum)

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1 Main	7 Esterification	1 Reaction	60	ml	DMF (purum)
1 Main	7 Esterification	2 Reaction	8.7	l	Water
1 Main	7 Esterification	2 Reaction	80	ml	HCl 37%
1 Main	7 Esterification	2 Reaction	900	ml	Water
1 Main	7 Esterification	2 Reaction	4.2	l	Dichloromethane (purum)
1 Main	7 Esterification	3 Extraction	600	ml	Water
1 Main	7 Esterification	3 Extraction	60	g	Sodium bicarbonate
1 Main	7 Esterification	3 Extraction	1.8	l	Water
1 Main	7 Esterification	4 Suspension	400	g	Sodium sulfate
1 Main	7 Esterification	5 Filter&Rinse	500	ml	Dichloromethane (purum)
1 Main	7 Esterification	5 Filter&Rinse	250	ml	DMF (purum)
1 Main	7 Esterification	6 Evaporation			***** Operation Only *****
1 Main	7 Esterification	7 Drying			***** Operation Only *****
1 Main	5 Wittig-reaction	1 Reaction	814	g	Aldehyde
1 Main	5 Wittig-reaction	1 Reaction	935	g	Wittig-Salt
1 Main	5 Wittig-reaction	1 Reaction	2.13	l	Toluene (purum)
1 Main	5 Wittig-reaction	1 Reaction	209	g	KOtBu
1 Main	5 Wittig-reaction	1 Reaction	1.06	l	THF (purum)
1 Main	5 Wittig-reaction	1 Reaction	1.28	l	THF (purum)
1 Main	5 Wittig-reaction	2 Extraction	157	ml	HCl 37%
1 Main	5 Wittig-reaction	2 Extraction	4.26	l	Water
1 Main	5 Wittig-reaction	2 Extraction	4.26	l	Toluene
1 Main	5 Wittig-reaction	2 Extraction	6.0	l	Toluene
1 Main	5 Wittig-reaction	2 Extraction	187	g	Sodium bicarbonate
1 Main	5 Wittig-reaction	2 Extraction	3.7	l	Water
1 Main	5 Wittig-reaction	2 Extraction	3.2	l	Water
1 Main	5 Wittig-reaction	3 Suspension	1.0	kg	Sodium sulfate
1 Main	5 Wittig-reaction	4 Filter&Rinse	3.2	l	Toluene (purum)
1 Main	5 Wittig-reaction	5 Suspension	9.6	l	Methanol (purum)
1 Main	5 Wittig-reaction	6 Filter&Rinse	1.60	l	Hexane (purum)
1 Main	5 Wittig-reaction	7 Drying			***** Operation Only *****

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QUALITY,C,25	PRICE,N,ADIMIOPTIM	OPCC	UNITAMOUN	MOLWEI	YIELD,PRCC	CALCAMOU	ICAL
	0.00	0				546.610	1.3171441
	0.00	0 0	1.00	0.00	0.0010000	632.600 11.00	1 1.0000000 kg
	0.00	0				480.390	2.3790394
GC: 98.1% by weight	0.00	0 0	3.00	0.00	0.9110000	496.600 81.00	1 2.5673318 kg
Fluka 66750	23.10	0 0	3.00	0.00	8.8500000	0.000 81.00	1 24.9406002 l
Fluka 60095	2.90	0 0	3.00	0.00	0.0267000	0.000 81.00	1 0.0752445 kg
Fluka 84426	16.10	0 0	3.00	0.00	0.0702000	0.000 81.00	1 0.1978339 l
B-1003	0.11	0 0	3.00	0.00	6.5500000	0.000 81.00	1 18.4588623 l
Aldrich 2564-83-2	1000.00	0 0	3.00	0.00	0.0198000	0.000 81.00	1 0.0557993 kg
Fluka 66750	23.10	0 0	3.00	0.00	0.1080000	0.000 81.00	1 0.3043599 l
B-1010	1.10	0 0	0.50	0.00	0.3600000	0.000 81.00	5 1.0145329 kg
Fluka 66750	23.10	0 0	0.50	0.00	2.0000000	0.000 81.00	5 5.6362938 l
B-1003	0.11	0 0	0.50	0.00	2.0000000	0.000 81.00	5 5.6362938 l
Fluka 66750	23.10	0 0	0.50	0.00	12.0000000	0.000 81.00	2 33.8177630 l
B-22000	8.06	0 0	0.50	0.00	1.5500000	0.000 81.00	2 4.3681277 kg
B-1003	0.11	0 0	0.50	0.00	9.0000000	0.000 81.00	2 25.3633222 l
	0.00	0 0	0.50	0.00	0.0000000	0.000 81.00	51 0.0000000
	0.00	0 0	1.00	0.00	0.0000000	0.000 81.00	53 0.0000000
	0.00	0 0	5.00	0.00	0.4500000	632.600 79.00	1 1.2658228 kg
Fluka 91700	70.00	0 0	5.00	0.00	1.9800000	0.000 79.00	1 5.5696203 l
Fluka 90550	280.00	0 0	5.00	0.00	0.1200000	0.000 79.00	1 0.3375527 l
Fluka 20252	18.50	0 0	5.00	0.00	7.3000000	0.000 79.00	1 20.5344585 l
Fluka 20252	18.50	0 0	0.50	0.00	3.0000000	0.000 79.00	5 8.4388186 l
Fluka 20252	18.50	0 0	6.00	0.00	0.0500000	0.000 79.00	3 0.1406470 l
	0.00	0 0	1.50	0.00	0.1000000	219.900 88.00	1 1.9336161 kg
Fluka 71691	4.00	0 0	1.50	0.00	0.0544000	0.000 88.00	1 1.0518872 kg
Fluka 66750	23.10	0 0	1.50	0.00	0.5000000	0.000 88.00	1 9.6680806 l
Fluka 86875	80.00	0 0	1.50	0.00	0.0092600	0.000 88.00	1 0.1790529 kg
Fluka xyz	116.00	0 0	1.50	0.00	0.0356000	0.000 88.00	1 0.6883673 kg
Fluka 66750	23.10	0 0	1.50	0.00	0.1000000	0.000 88.00	1 1.9336161 l
B-1003	0.11	1 0	0.30	0.00	0.0500000	0.000 88.00	2 0.9668081 kg
B-1003	0.11	1 0	0.30	0.00	0.2500000	0.000 88.00	2 4.8340403 l
Merck 2435	2.12	1 0	0.30	0.00	0.0600000	0.000 88.00	2 1.1601697 kg
B-1003	0.11	1 0	0.30	0.00	0.3000000	0.000 88.00	2 5.8008484 l
B-1003	0.11	1 0	0.30	0.00	0.3000000	0.000 88.00	2 5.8008484 l
	0.00	0 0	0.50	0.00	0.0000000	0.000 88.00	51 0.0000000
GC: 89% by weight	0.00	0 0	8.00	0.00	0.0900000	218.090 64.00	1 1.6875764 kg
Fluka 00585	20.00	2 0	8.00	0.00	0.1800000	0.000 64.00	1 3.3751529 l
Fluka 87370	34.00	0 0	8.00	0.00	0.1800000	0.000 64.00	1 3.3751529 l
Aldrich 0123	20.08	0 0	8.00	0.00	0.1540000	0.000 64.00	1 2.8876308 kg
Fluka 00585	20.00	1 0	0.50	0.00	0.0900000	0.000 64.00	5 1.6875764 l
Fluka 45770	21.20	2 0	0.50	0.00	0.3600000	0.000 64.00	5 6.7503058 l
	0.00	0 0	1.00	0.00	0.0000000	0.000 64.00	53 0.0000000
	0.00	0 0	1.00	0.00	0.0000000	0.000 64.00	51 0.0000000
Fluka 00585	20.00	0 0	4.50	0.00	0.0900000	0.000 64.00	6 1.6875764 l
Fluka 87370	34.00	0 0	4.50	0.00	0.0900000	0.000 64.00	6 1.6875764 l
Fluka 87370	34.00	0 0	1.00	0.00	0.0200000	0.000 64.00	5 0.3750170 l
Fluka 00585	20.00	0 0	1.00	0.00	0.0200000	0.000 64.00	5 0.3750170 l

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	0.00	0	0	5.00	0.00	0.0000000	0.000	64.00	53	0.0000000
	0.00	0	0	2.00	0.00	1.0600000	429.500	90.00	1	1.1499432 kg
Fluka 87370	34.00	2	0	2.00	0.00	36.0000000	0.000	90.00	1	39.0546736 l
Fluka 54802	200.00	0	0	2.00	0.00	0.4050000	0.000	90.00	1	0.4393651 kg
Fluka 36650	30.00	0	0	2.00	0.00	0.5500000	0.000	90.00	1	0.5966686 kg
Fluka 87370	34.00	2	0	0.20	0.00	2.0000000	0.000	90.00	5	2.1697041 l
	0.00	0	0	1.00	0.00	0.0000000	0.000	90.00	51	0.0000000
Fluka abcd	20.00	2	0	1.00	0.00	8.0000000	0.000	90.00	6	8.6788164 l
Fluka abcd	20.00	0	0	0.20	0.00	1.0000000	0.000	90.00	5	1.0848520 l
	0.00	0	0	10.00	0.00	0.0000000	0.000	90.00	53	0.0000000
GC: 96% by weight	0.00	0	0	24.00	0.00	0.6330000	330.360	82.00	1	2.0828064 kg
Fluka 87370	34.00	0	0	24.00	0.00	3.6400000	0.000	82.00	1	11.9769592 l
B-1005	20.00	0	0	24.00	0.00	1.5500000	0.000	82.00	1	5.1000788 l
Fluka 52770	59.20	0	0	0.15	0.00	2.4000000	0.000	82.00	5	7.8968962 l
	0.00	0	0	0.50	0.00	0.0000000	0.000	82.00	53	0.0000000
	0.00	0	0	0.50	0.00	0.0000000	0.000	82.00	51	0.0000000
Fluka 52770	59.20	0	0	0.50	0.00	1.0000000	0.000	82.00	6	3.2903734 l
Fluka 52770	59.20	0	0	0.50	0.00	0.1500000	0.000	82.00	5	0.4935560 l
Fluka 87370	34.00	0	0	0.50	0.00	0.0500000	0.000	82.00	5	0.1645187 l
Fluka 52770	59.20	0	0	0.50	0.00	0.7500000	0.000	82.00	5	2.4677801 l
Fluka 52770	59.20	0	0	0.00	0.00	1.5000000	0.000	82.00	3	4.9355601 l
Fluka 24030	15.00	0	0	1.50	0.00	0.2800000	141.080	95.00	1	1.3058307 kg
Fluka 18350	20.00	0	0	1.50	0.00	0.5460000	0.000	95.00	1	2.5463699 kg
Fluka 66750	23.10	2	0	1.50	0.00	0.5600000	0.000	95.00	1	2.6116614 l
B-2030	15.00	0	0	1.50	0.00	0.0120000	0.000	95.00	1	0.0559642 kg
B-5050	12.80	0	0	1.50	0.00	0.0036000	0.000	95.00	1	0.0167893 l
	0.00	0	0	1.00	0.00	0.0000000	141.080	95.00	51	0.0000000
Fluka 52770	59.20	3	0	0.05	0.00	1.4000000	0.000	95.00	6	6.5291535 l
Fluka 52770	59.20	0	0	0.50	0.00	0.3500000	0.000	95.00	5	1.6322884 l
Fluka 52770	59.20	0	0	0.50	0.00	0.3500000	0.000	95.00	5	1.6322884 l
Fluka 52770	59.20	0	0	0.50	0.00	0.3500000	0.000	95.00	5	1.6322884 l
Fluka 52770	59.20	0	0	0.50	0.00	0.3500000	0.000	95.00	5	1.6322884 l
Fluka 52770	59.20	0	0	0.50	0.00	0.3500000	0.000	95.00	5	1.6322884 l
Fluka 52770	59.20	0	0	0.50	0.00	0.3500000	0.000	95.00	5	1.6322884 l
	0.00	0	0	1.50	0.00	0.0000000	0.000	95.00	51	0.0000000
Aldrich 007	270.00	0	0	1.50	0.00	0.9830000	272.280	70.00	1	3.0654141 kg
B-1003	0.11	0	0	1.50	0.00	8.0000000	0.000	70.00	1	24.9474191 l
Fluka 65550	7.40	2	0	1.50	0.00	7.0000000	0.000	70.00	1	21.8289917 l
Fluka 71693	19.90	0	0	1.50	0.00	0.2800000	0.000	70.00	1	0.8731597 kg
B-1003	0.11	0	0	1.50	0.00	0.8200000	0.000	70.00	1	2.5571105 l
Fluka 84426	16.10	0	0	1.50	0.00	0.5800000	0.000	70.00	1	1.8086879 l
B-1003	0.11	0	0	1.50	0.00	0.5800000	0.000	70.00	1	1.8086879 l
B-1003	0.11	0	0	0.50	0.00	7.0000000	0.000	70.00	5	21.8289917 l
Fluka 00585	20.00	0	0	0.50	0.00	7.0000000	0.000	70.00	5	21.8289917 l
	0.00	0	0	24.00	0.00	0.0000000	0.000	70.00	52	0.0000000
GC: 92% by weight	0.00	0	0	24.00	0.00	1.2800000	457.560	88.00	1	1.3921261 kg
Fluka 71693	19.90	0	0	24.00	0.00	0.3360000	0.000	88.00	1	0.3654331 kg
B-2020	0.11	0	0	24.00	0.00	4.7000000	0.000	88.00	1	5.1117132 l
Fluka 71693	19.90	0	0	24.00	0.00	4.7000000	0.000	88.00	1	5.1117132 kg

Sheet1

Fluka 45770	21.20	2	0	24.00	0.00	8.0000000	0.000	88.00	1	8.7007884 l
Fluka 84426	16.10	0	0	24.00	0.00	0.7000000	0.000	88.00	1	0.7613190 l
B-1003	0.11	0	0	1.00	0.00	30.0000000	0.000	88.00	2	32.6279564 l
B-1003	0.11	1	0	0.50	0.00	4.0000000	0.000	88.00	5	4.3503942 l
Fluka 45770	21.20	1	0	0.50	0.00	4.0000000	0.000	88.00	5	4.3503942 l
	0.00	0	0	6.00	0.00	0.0000000	0.000	88.00	53	0.0000000
GC: 99.2% by weight	0.00	0	0	72.00	0.00	0.6240000	230.250	80.00	1	1.8145590 kg
B-1003	0.11	0	0	72.00	0.00	4.0000000	0.000	80.00	1	11.6317884 l
Fluka 34660	140.00	0	0	72.00	0.00	1.1700000	0.000	80.00	1	3.4022981 kg
Fluka 42530	46.30	0	0	72.00	0.00	5.4000000	0.000	80.00	1	15.7029143 l
B-1004	0.13	0	0	72.00	0.00	2.0600000	0.000	80.00	1	5.9903710 l
Fluka 84426	16.10	0	0	72.00	0.00	0.0090000	0.000	80.00	1	0.0261715 l
B-1003	0.11	0	0	72.00	0.00	0.0960000	0.000	80.00	1	0.2791629 l
B-1003	0.11	0	0	0.50	0.00	2.6000000	0.000	80.00	5	7.5606625 l
Fluka 42530	46.30	0	0	0.50	0.00	2.0000000	0.000	80.00	5	5.8158942 l
Fluka 45770	21.20	0	0	0.50	0.00	10.6000000	0.000	80.00	2	30.8242392 l
Fluka 84426	16.10	0	0	0.15	0.00	0.4820000	0.000	80.00	6	1.4016305 l
B-1003	0.11	0	0	0.15	0.00	5.3000000	0.000	80.00	6	15.4121196 l
B-1003	0.11	0	0	0.15	0.00	5.3000000	0.000	80.00	5	15.4121196 l
	0.00	0	0	6.00	0.00	0.0000000	0.000	80.00	53	0.0000000
	0.00	0	0	2.50	0.00	0.3560000	615.700	89.00	1	1.5211830 kg
Fluka 45740	23.50	0	0	2.50	0.00	0.5000000	0.000	89.00	1	2.1364930 l
Fluka 45740	23.50	0	0	2.50	0.00	0.2600000	0.000	89.00	1	1.1109764 l
Fluka 84426	16.10	0	0	2.50	0.00	0.5000000	0.000	89.00	1	2.1364930 l
B-1003	0.11	0	0	2.50	0.00	1.1400000	0.000	89.00	1	4.8712041 l
Fluka 20252	18.50	0	0	2.50	0.00	0.5700000	0.000	89.00	1	2.4356021 l
Fluka 20252	18.50	0	0	0.50	0.00	0.6200000	0.000	89.00	2	2.6492514 l
Fluka 20252	18.50	0	0	0.50	0.00	0.6200000	0.000	89.00	2	2.6492514 l
B-1003	0.11	0	0	0.50	0.00	0.2900000	0.000	89.00	2	1.2391660 l
Fluka 65550	7.40	0	0	2.00	0.00	0.2900000	0.000	89.00	6	1.2391660 l
B-1004	0.13	0	0	2.00	0.00	0.6000000	0.000	89.00	6	2.5637916 l
B-1003	0.11	0	0	0.15	0.00	1.5400000	0.000	89.00	5	6.5803986 l
Fluka 65550	7.40	0	0	0.15	0.00	0.3100000	0.000	89.00	5	1.3246257 l
	0.00	0	0	2.00	0.00	0.0000000	0.000	89.00	53	0.0000000
Merck xyz	105.00	0	0	4.00	0.00	0.4500000	215.230	61.00	1	1.0735036 kg
Fluka 45770	21.20	3	0	4.00	0.00	7.0000000	0.000	61.00	1	16.6989450 l
B-4390-5	23.76	0	0	4.00	0.00	0.0920000	0.000	61.00	1	0.2194718 kg
Fluka 93000	30.00	0	0	4.00	0.00	0.6400000	0.000	61.00	1	1.5267607 kg
Fluka 45770	21.20	0	0	4.00	0.00	3.7000000	0.000	61.00	1	8.8265852 l
	0.00	0	0	1.00	0.00	0.0000000	215.230	61.00	51	0.0000000
B-0008	0.20	0	0	0.50	0.00	4.0000000	0.000	61.00	6	9.5422543 l
B-0008	0.20	1	0	0.20	0.00	2.0000000	0.000	61.00	5	4.7711271 l
B-0008	0.20	1	0	0.20	0.00	2.0000000	0.000	61.00	5	4.7711271 l
	0.00	0	0	6.00	0.00	0.0000000	0.000	61.00	53	0.0000000
	0.00	0	0	24.00	0.00	0.2100000	349.420	91.00	1	0.7683341 kg
Fluka 40255	26.00	0	0	24.00	0.00	0.6000000	0.000	91.00	1	2.1952402 l
Fluka 90342	21.80	0	0	24.00	0.00	0.1300000	0.000	91.00	1	0.4756354 l
<= Activated ester	0.00	0	3	24.00	0.00	0.3600000	0.000	91.00	1	1.3171441 kg
Fluka 40255	26.00	0	0	24.00	0.00	0.8400000	0.000	91.00	1	3.0733363 l

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Fluka 40255	26.00	0	0	24.00	0.00	0.0600000	0.000	91.00	1	0.2195240 l
B-1003	0.11	0	0	1.50	0.00	8.7000000	0.000	91.00	1	31.8309827 l
Fluka 84426	16.10	0	0	1.50	0.00	0.0800000	0.000	91.00	1	0.2926987 l
B-1003	0.11	0	0	1.50	0.00	0.9000000	0.000	91.00	1	3.2928603 l
Fluka 66750	23.10	0	0	1.50	0.00	4.2000000	0.000	91.00	1	15.3666813 l
B-1003	0.11	0	0	0.50	0.00	0.6000000	0.000	91.00	2	2.1952402 l
Fluka 71630	16.20	0	0	0.50	0.00	0.0600000	0.000	91.00	2	0.2195240 kg
B-1003	0.11	0	0	0.50	0.00	1.8000000	0.000	91.00	2	6.5857206 l
Fluka 71970	20.50	0	0	0.15	0.00	0.4000000	0.000	91.00	6	1.4634935 kg
Fluka 66750	23.10	0	0	0.15	0.00	0.5000000	0.000	91.00	5	1.8293668 l
Fluka 40255	26.00	0	0	0.15	0.00	0.2500000	0.000	91.00	5	0.9146834 l
	0.00	0	0	0.50	0.00	0.0000000	0.000	91.00	51	0.0000000
	0.00	0	0	6.00	0.00	0.0000000	0.000	91.00	53	0.0000000
GC: 98.4 area%	0.00	0	0	2.50	0.00	0.8140000	494.600	59.00	1	2.0711637 kg
<= Wittig Salt	0.00	0	2	2.50	0.00	0.9350000	0.000	59.00	1	2.3790394 kg
Fluka 89682	20.40	0	0	2.50	0.00	2.1300000	0.000	59.00	1	5.4196298 l
Fluka 60100	190.00	0	0	2.50	0.00	0.2090000	0.000	59.00	1	0.5317853 kg
Fluka 87370	34.00	0	0	2.50	0.00	1.0600000	0.000	59.00	1	2.6970928 l
Fluka 87370	34.00	0	0	2.50	0.00	1.2800000	0.000	59.00	1	3.2568667 l
Fluka 84426	16.10	0	0	1.00	0.00	0.1570000	0.000	59.00	2	0.3994751 l
B-1003	0.11	0	0	1.00	0.00	4.2600000	0.000	59.00	2	10.8392596 l
Fluka 2222	7.35	0	0	1.00	0.00	4.2600000	0.000	59.00	2	10.8392596 l
Fluka 2222	7.35	0	0	1.00	0.00	6.0000000	0.000	59.00	2	15.2665628 l
Merck 9876	0.60	0	0	1.00	0.00	0.1870000	0.000	59.00	2	0.4758079 kg
B-1003	0.11	0	0	1.00	0.00	3.7000000	0.000	59.00	2	9.4143804 l
B-1003	0.11	0	0	1.00	0.00	3.2000000	0.000	59.00	2	8.1421668 l
Fluka 71970	20.50	0	0	0.15	0.00	1.0000000	0.000	59.00	6	2.5444271 kg
Fluka 89682	20.40	0	0	0.15	0.00	3.2000000	0.000	59.00	5	8.1421668 l
Fluka 65550	7.40	0	0	1.50	0.00	9.6000000	0.000	59.00	6	0.0000000 l
Fluka 52770	59.20	0	0	0.15	0.00	1.6000000	0.000	59.00	5	4.0710834 l
	0.00	0	0	18.00	0.00	0.0000000	0.000	59.00	53	0.0000000



.CUNIT,C,2