Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

SUPPLEMENTARY INFORMATION:

A Review of Organic Small Molecules Based Hole-Transporting Material for Meso-Structured Organic-Inorganic Perovskite Solar Cells

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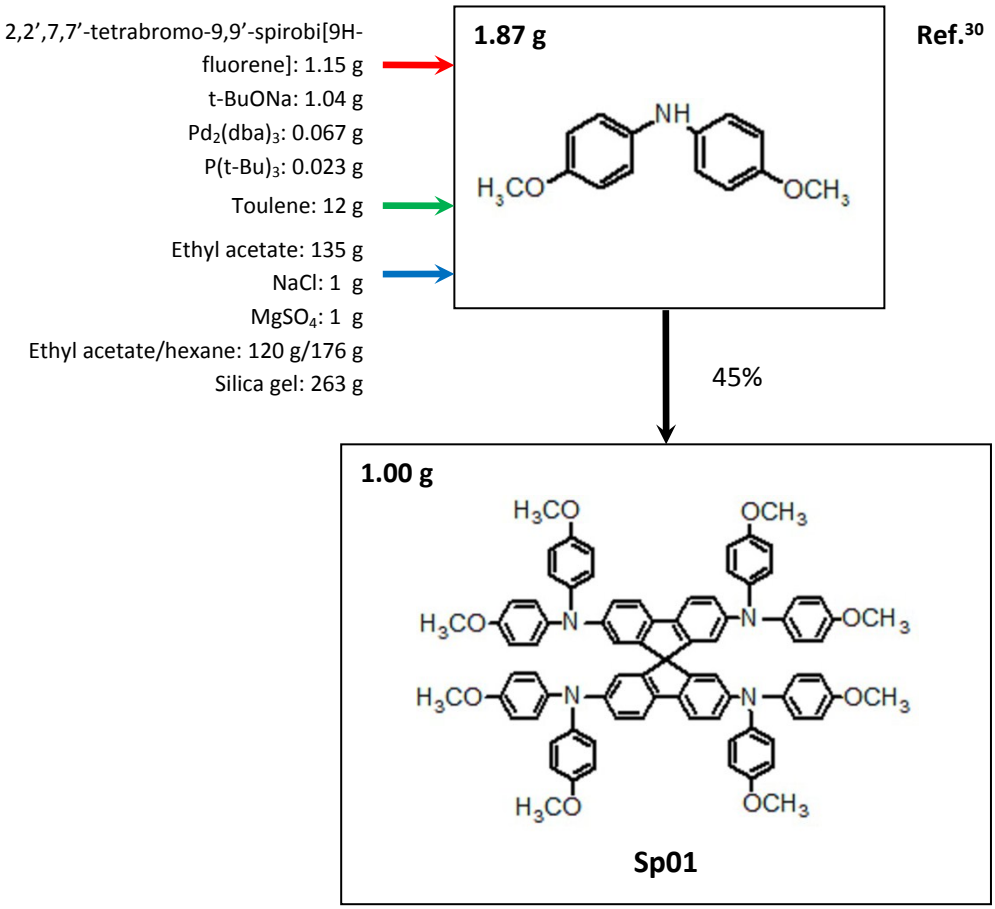


Fig. S01 Flowchart describing the synthesis of 1 gram of HTM **Sp01**[30]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

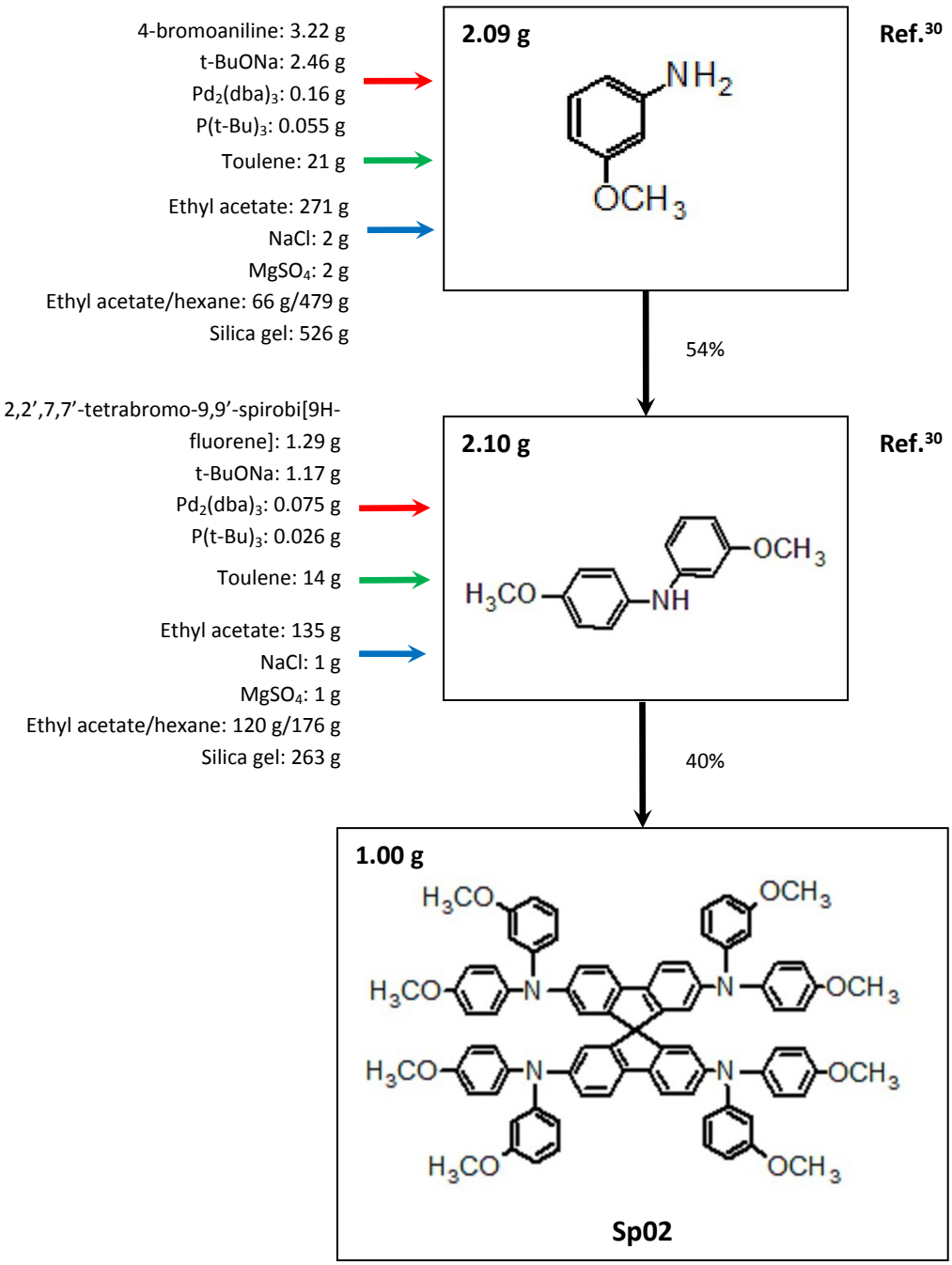


Fig. S02 Flowchart describing the synthesis of 1 gram of HTM **Sp02**[30]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

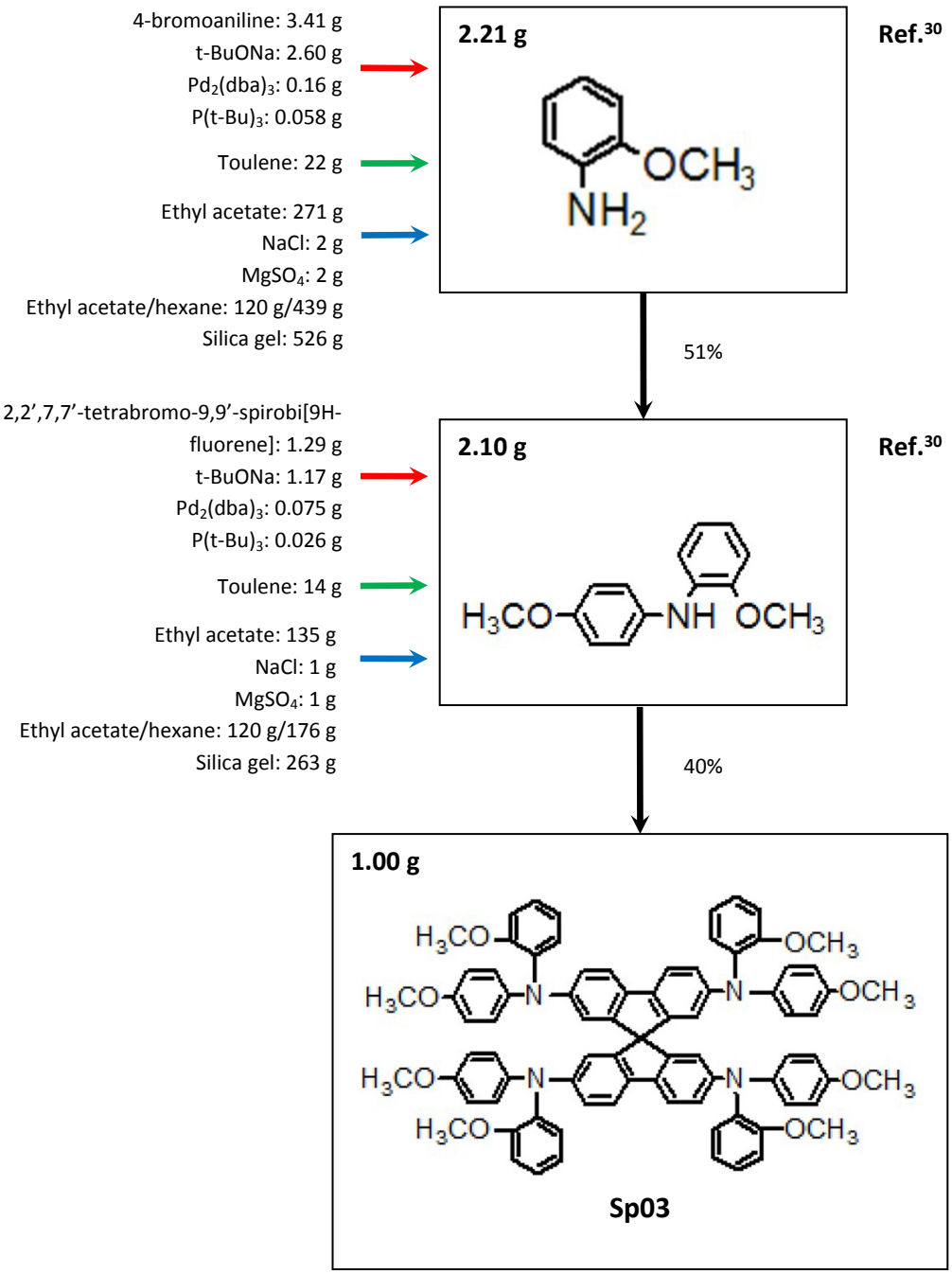


Fig. S03 Flowchart describing the synthesis of 1 gram of HTM **Sp03**[30]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

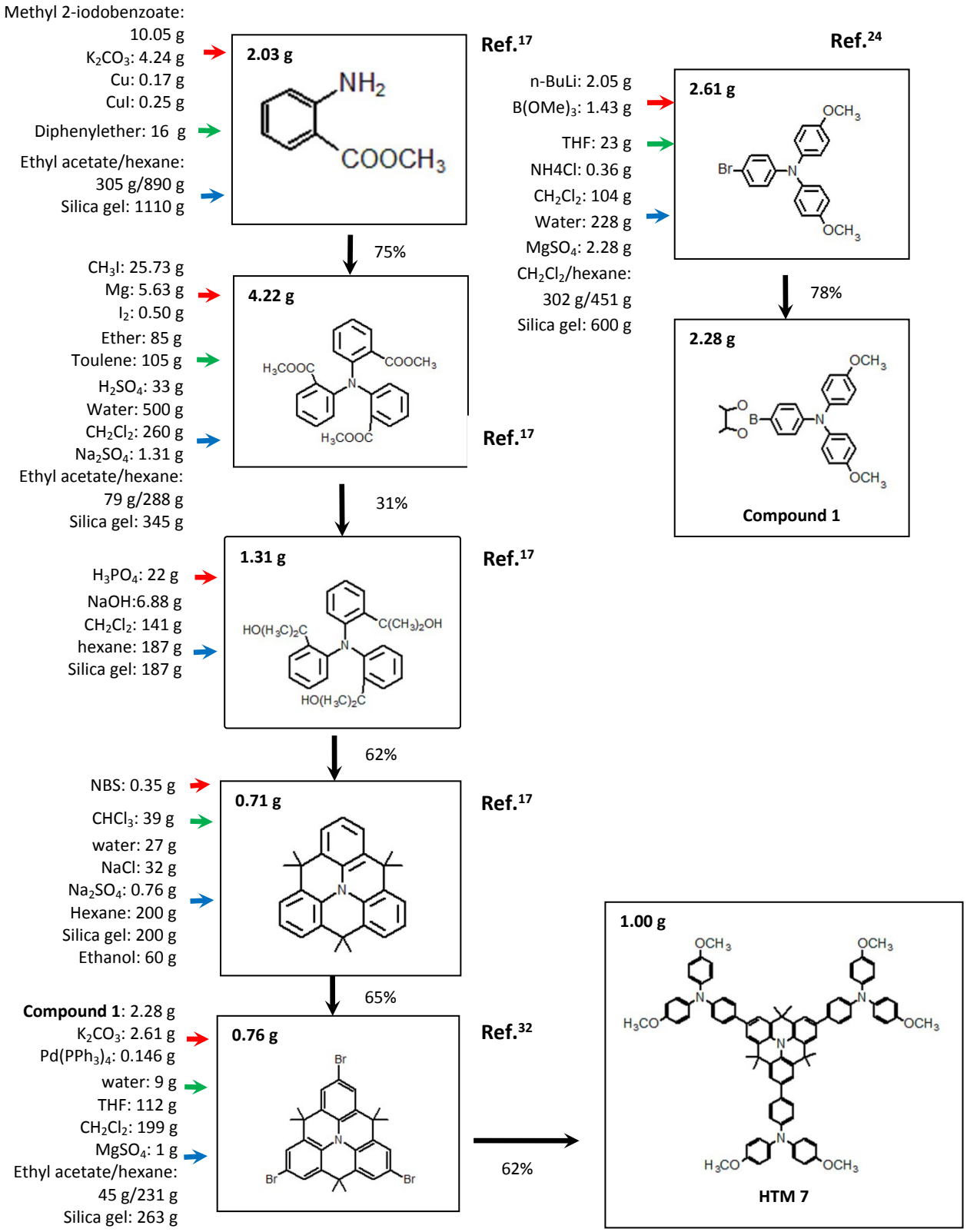


Fig. S04 Flowchart describing the synthesis of 1 gram of HTM **7**[17, 24, 32]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

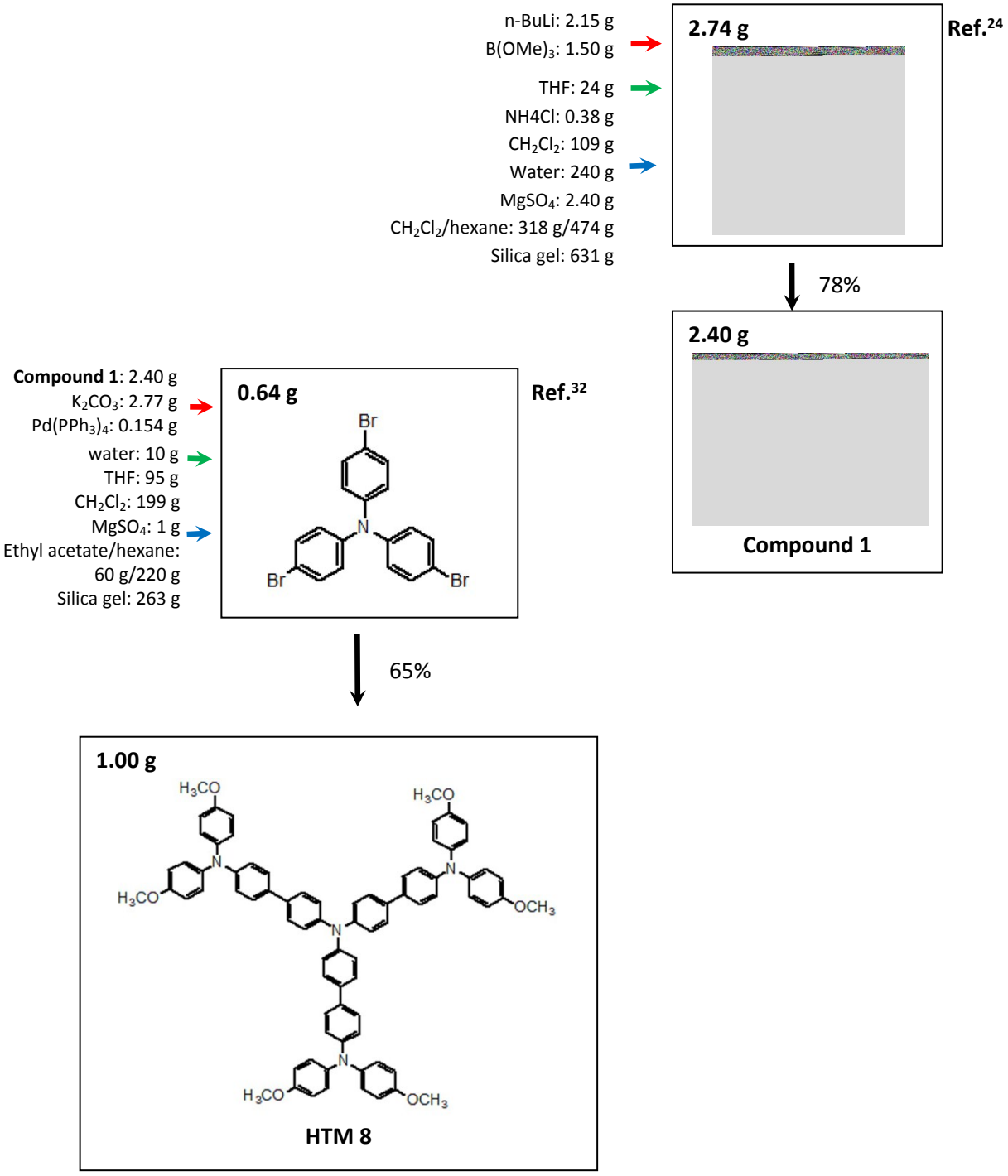


Fig. S05 Flowchart describing the synthesis of 1 gram of HTM **8** [24, 32]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

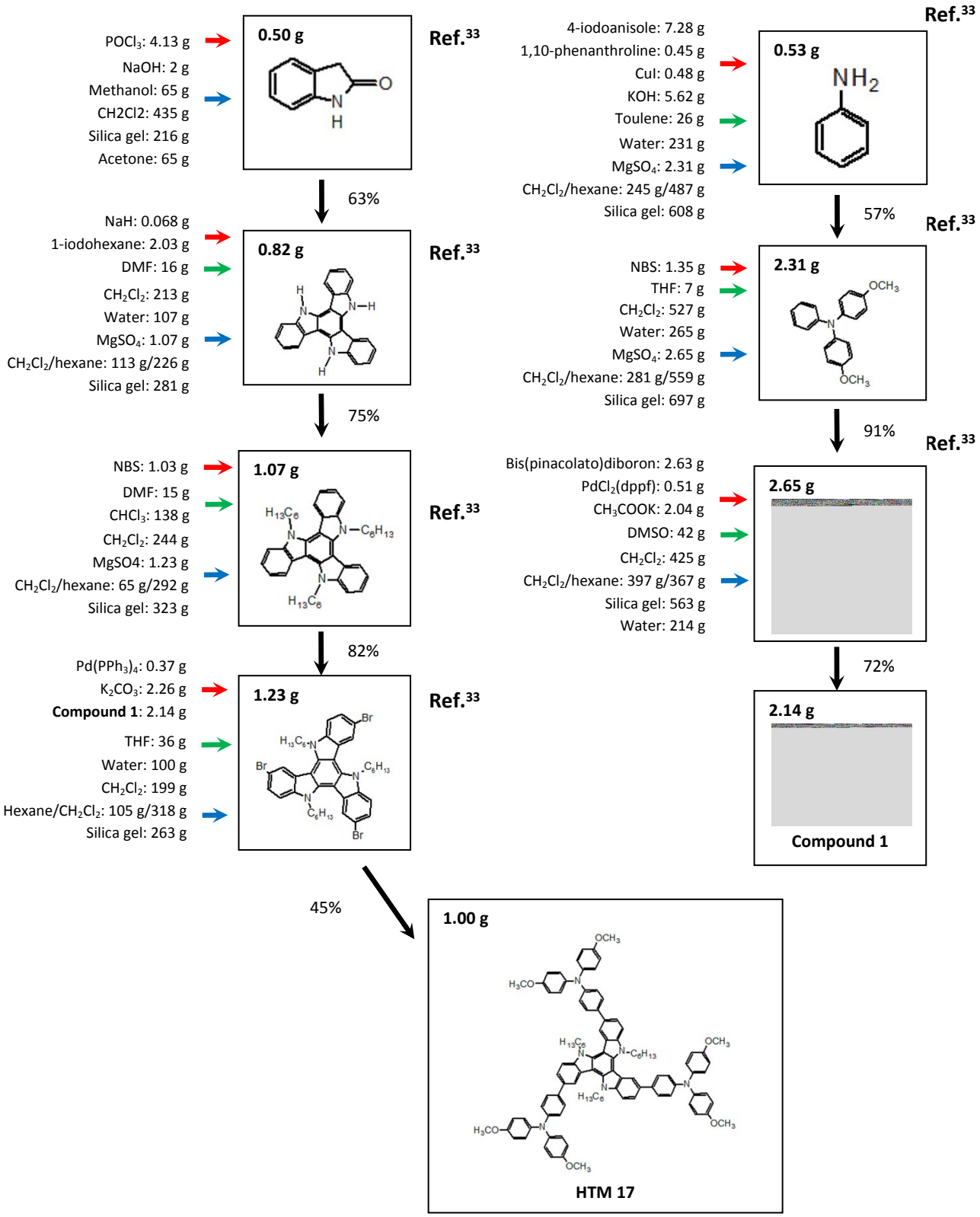


Fig. S06 Flowchart describing the synthesis of 1 gram of HTM **17**[33]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

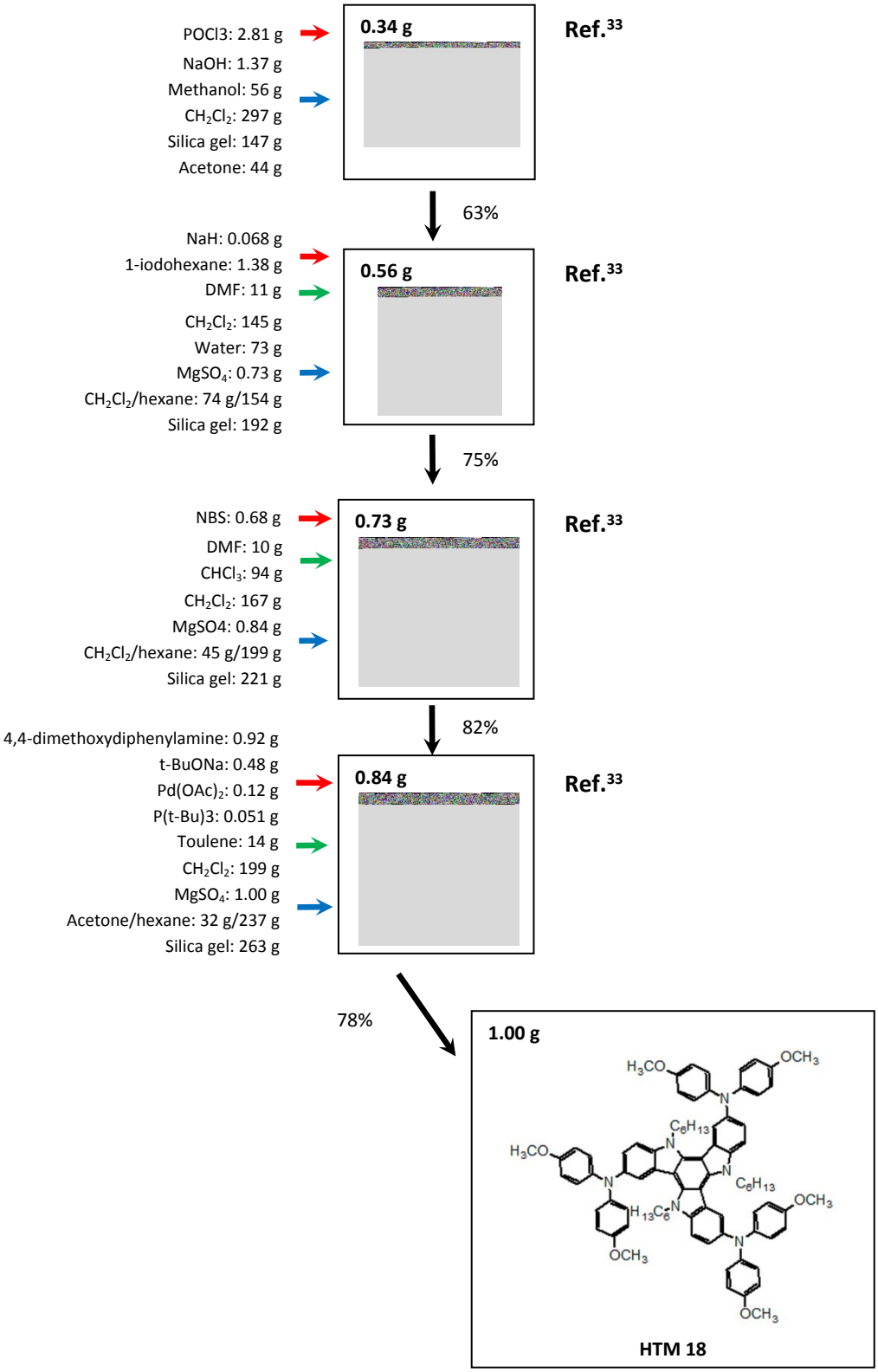


Fig. S07 Flowchart describing the synthesis of 1 gram of HTM **18**[33]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

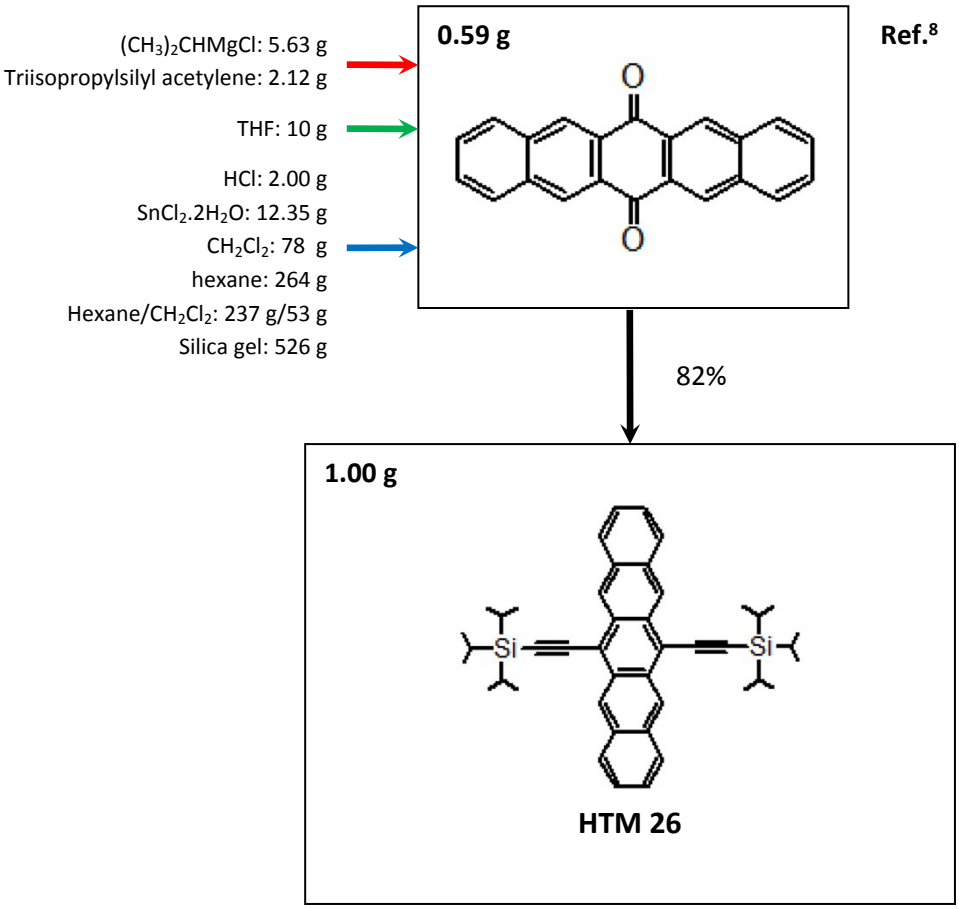


Fig. S08 Flowchart describing the synthesis of 1 gram of HTM **26**[8]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

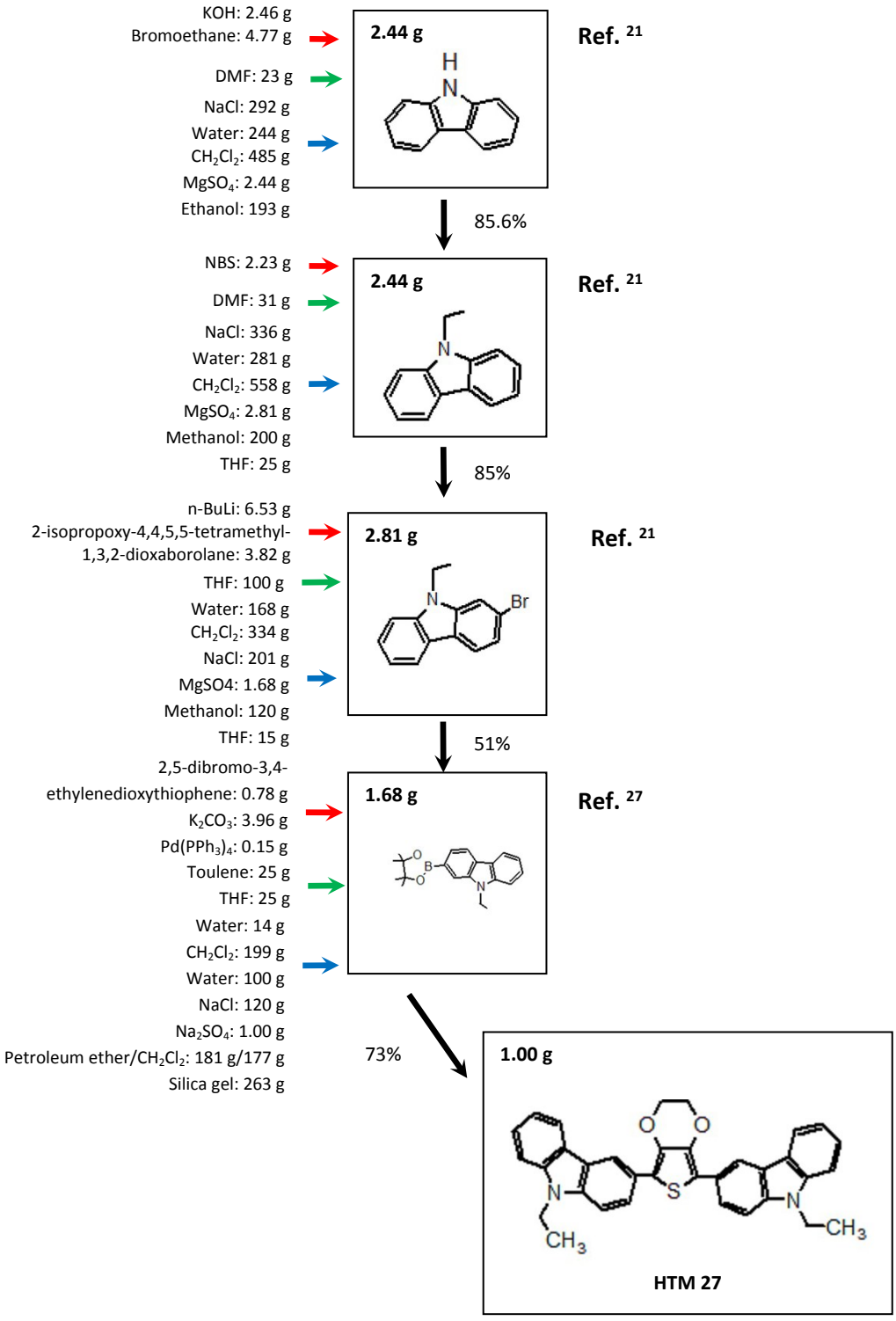


Fig. S09 Flowchart describing the synthesis of 1 gram of HTM **27**[21, 27]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

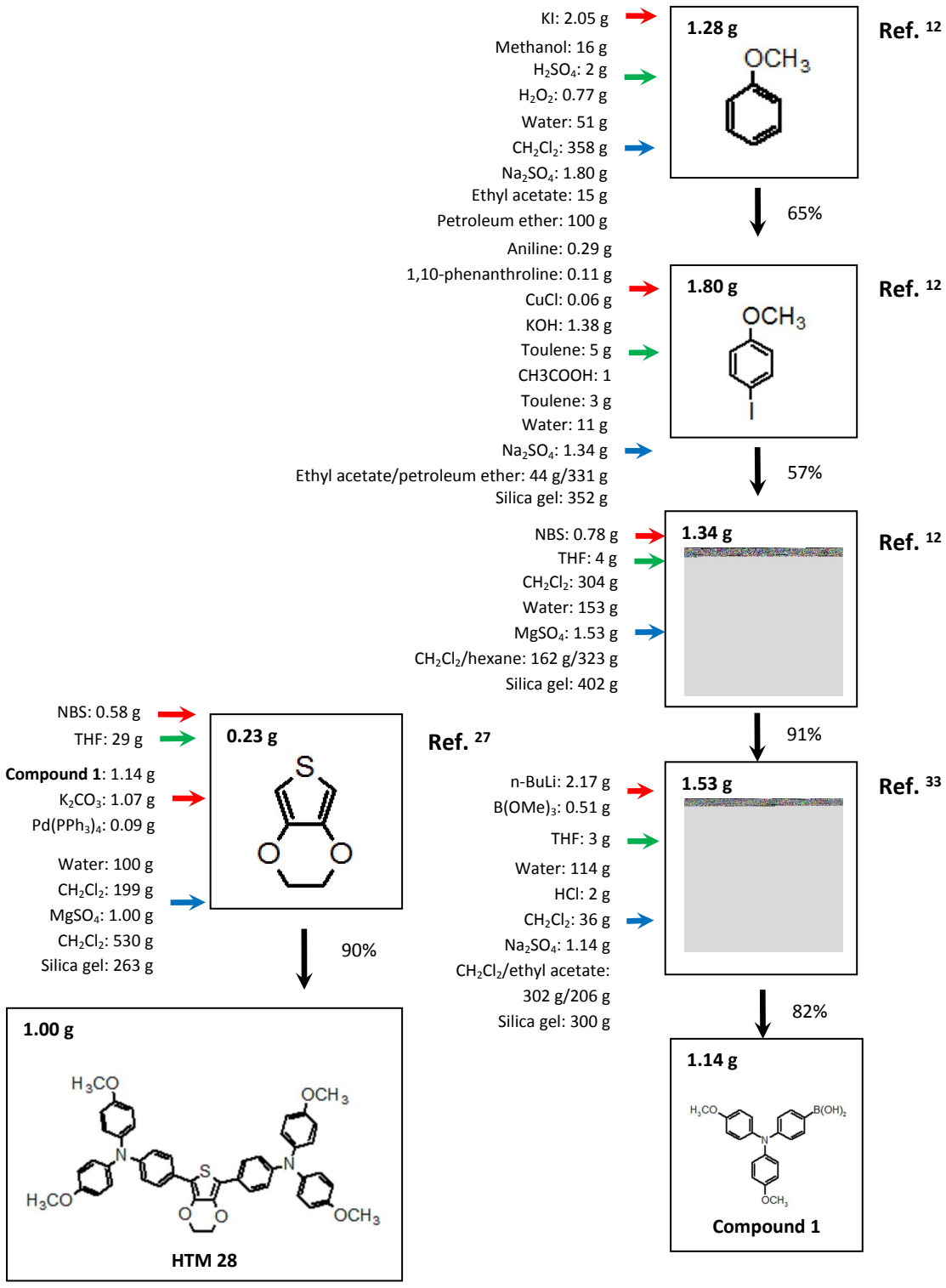


Fig. S10 Flowchart describing the synthesis of 1 gram of HTM **28**[12, 27]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

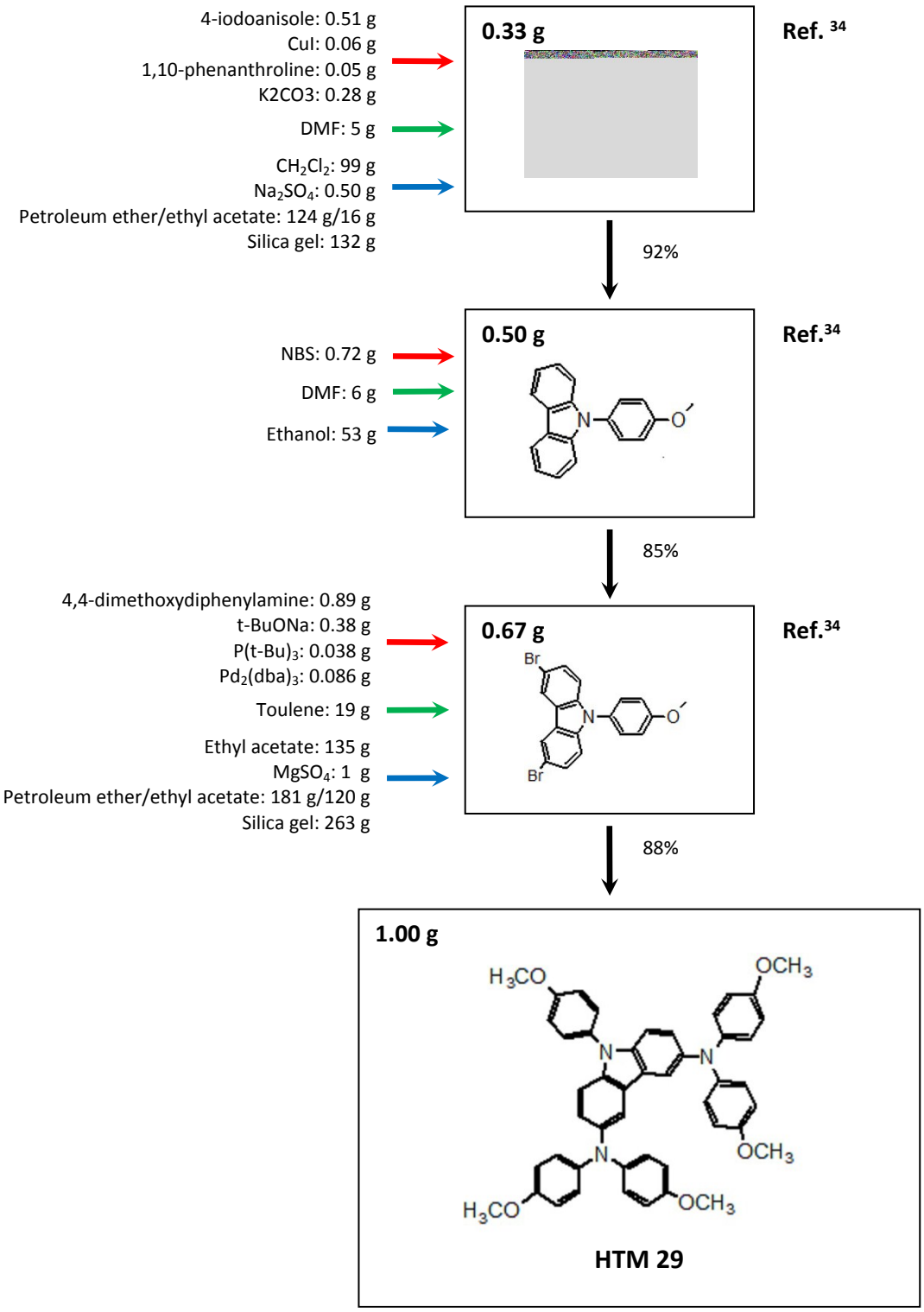


Fig. S11 Flowchart describing the synthesis of 1 gram of HTM **29**[34]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

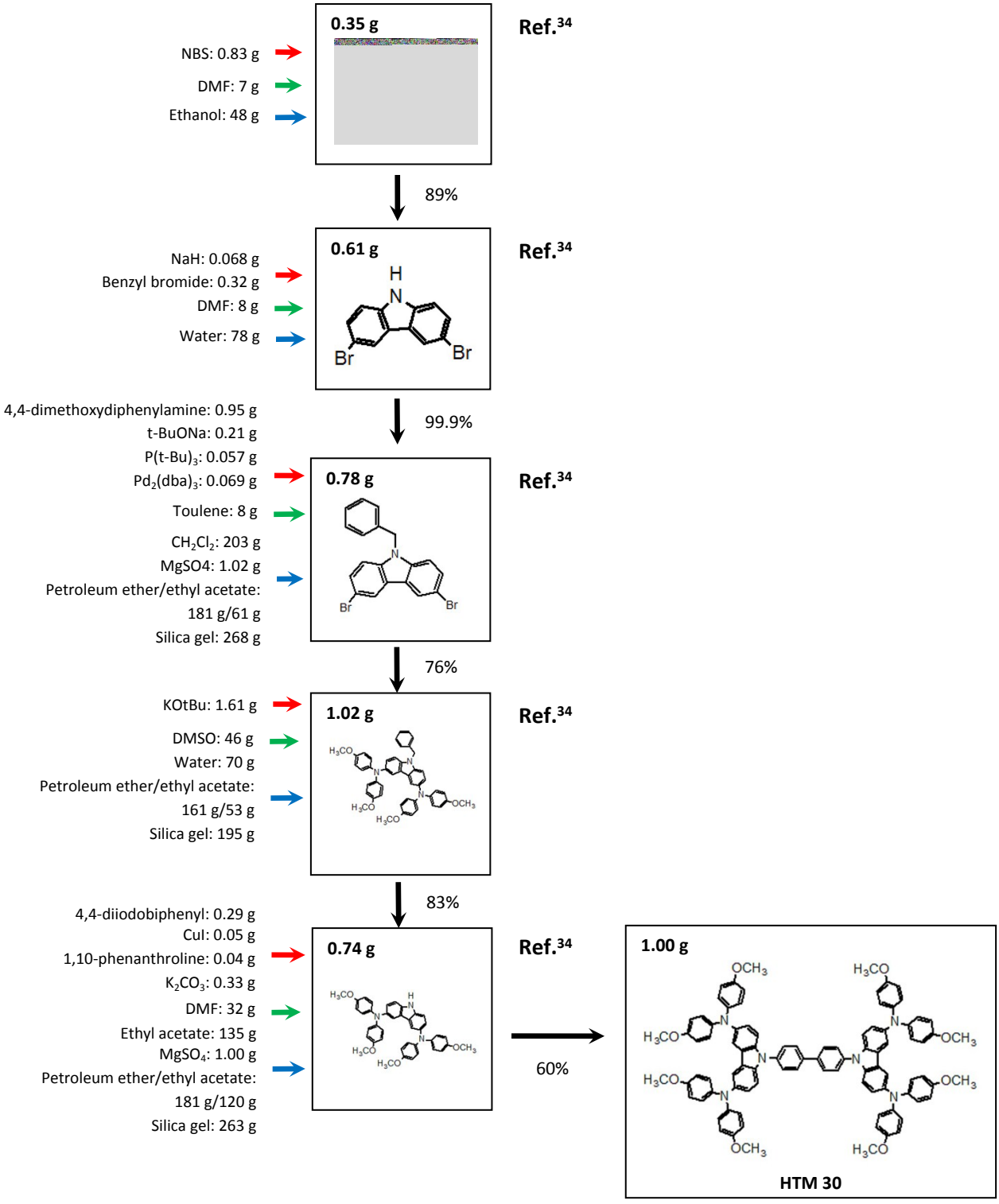


Fig. S12 Flowchart describing the synthesis of 1 gram of HTM **30**[34]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

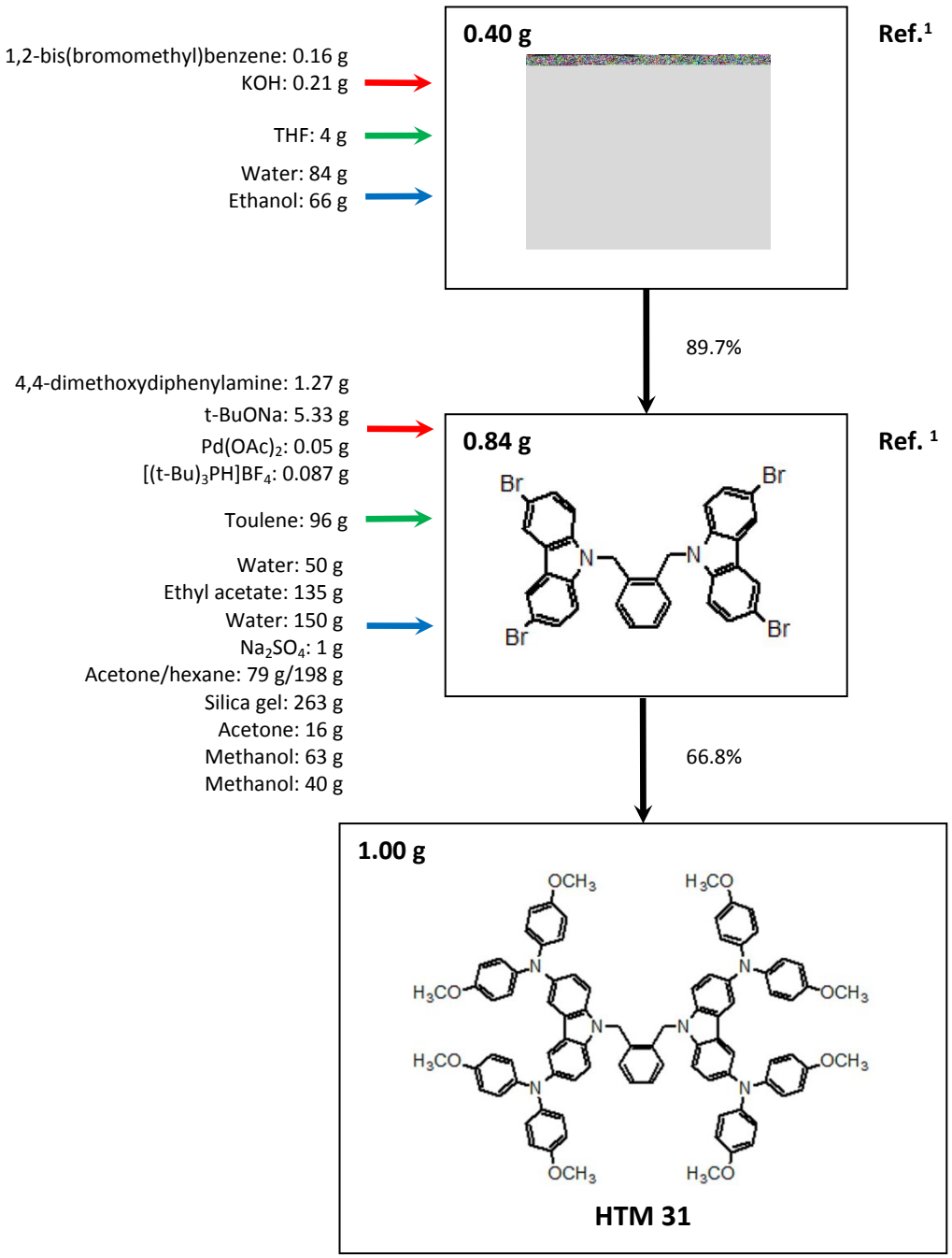


Fig. S13 Flowchart describing the synthesis of 1 gram of HTM **31**[1]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

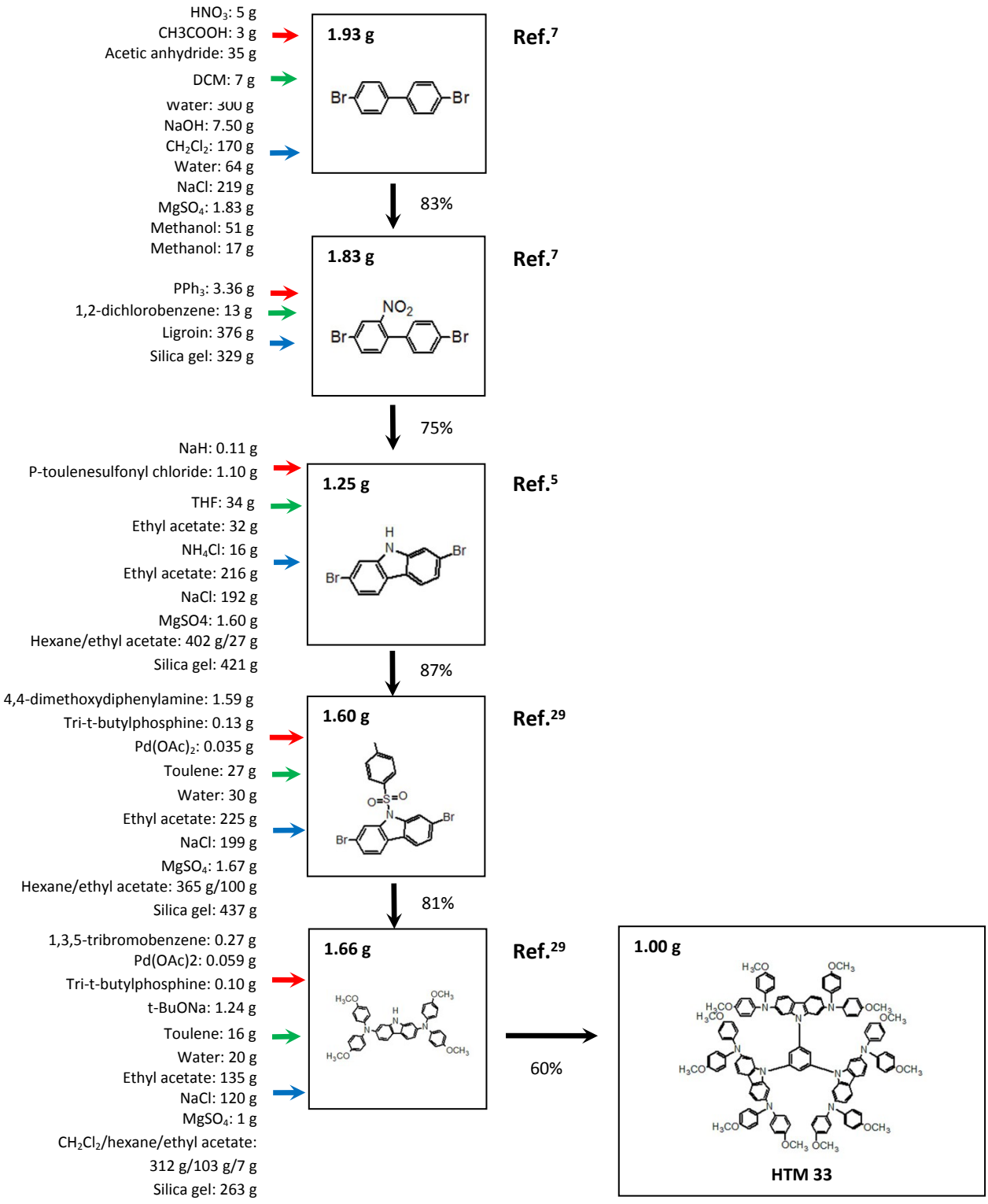


Fig. S14 Flowchart describing the synthesis of 1 gram of HTM **33**[5, 7, 29]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

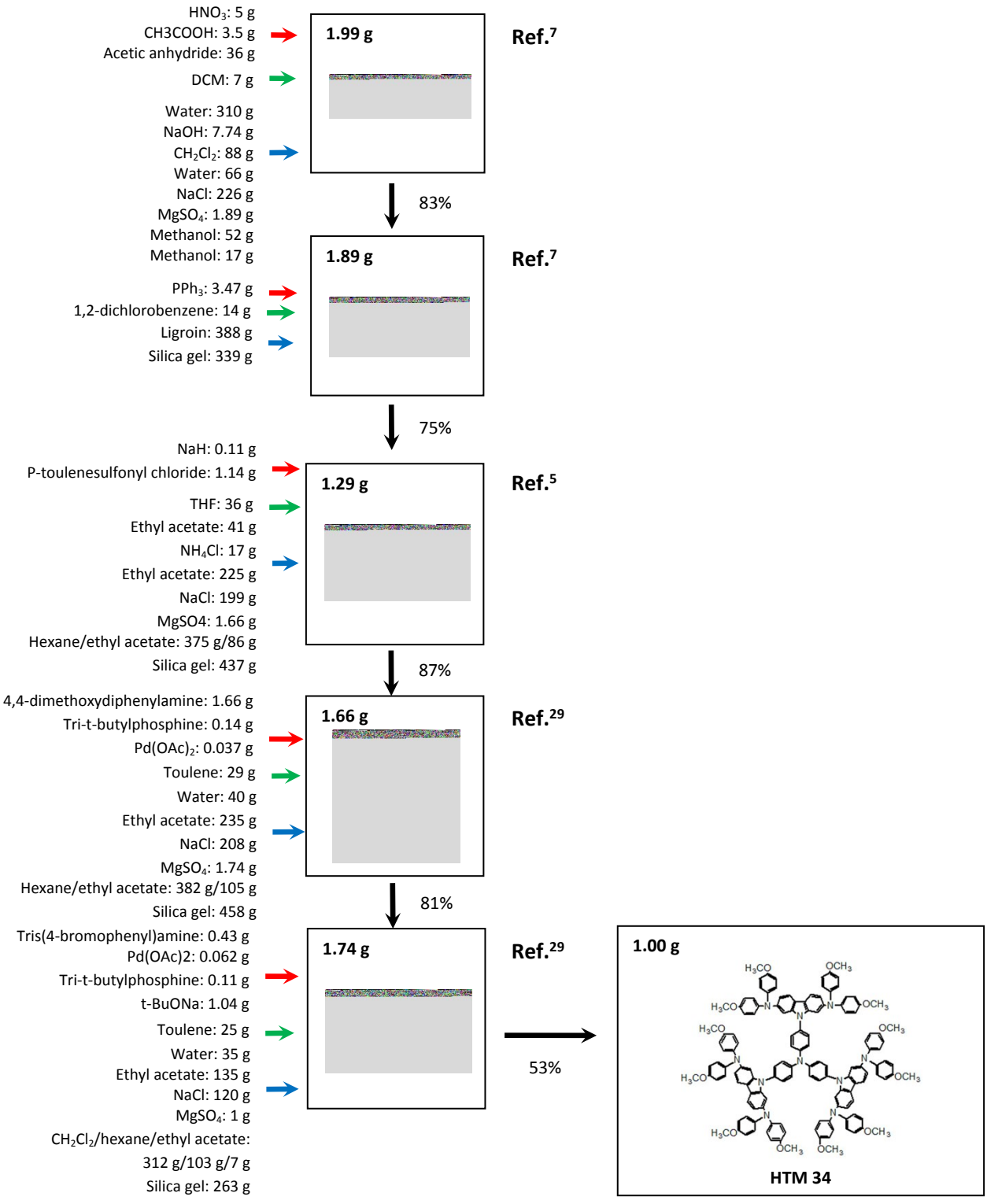


Fig. S15 Flowchart describing the synthesis of 1 gram of HTM **34**[5, 7, 29]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

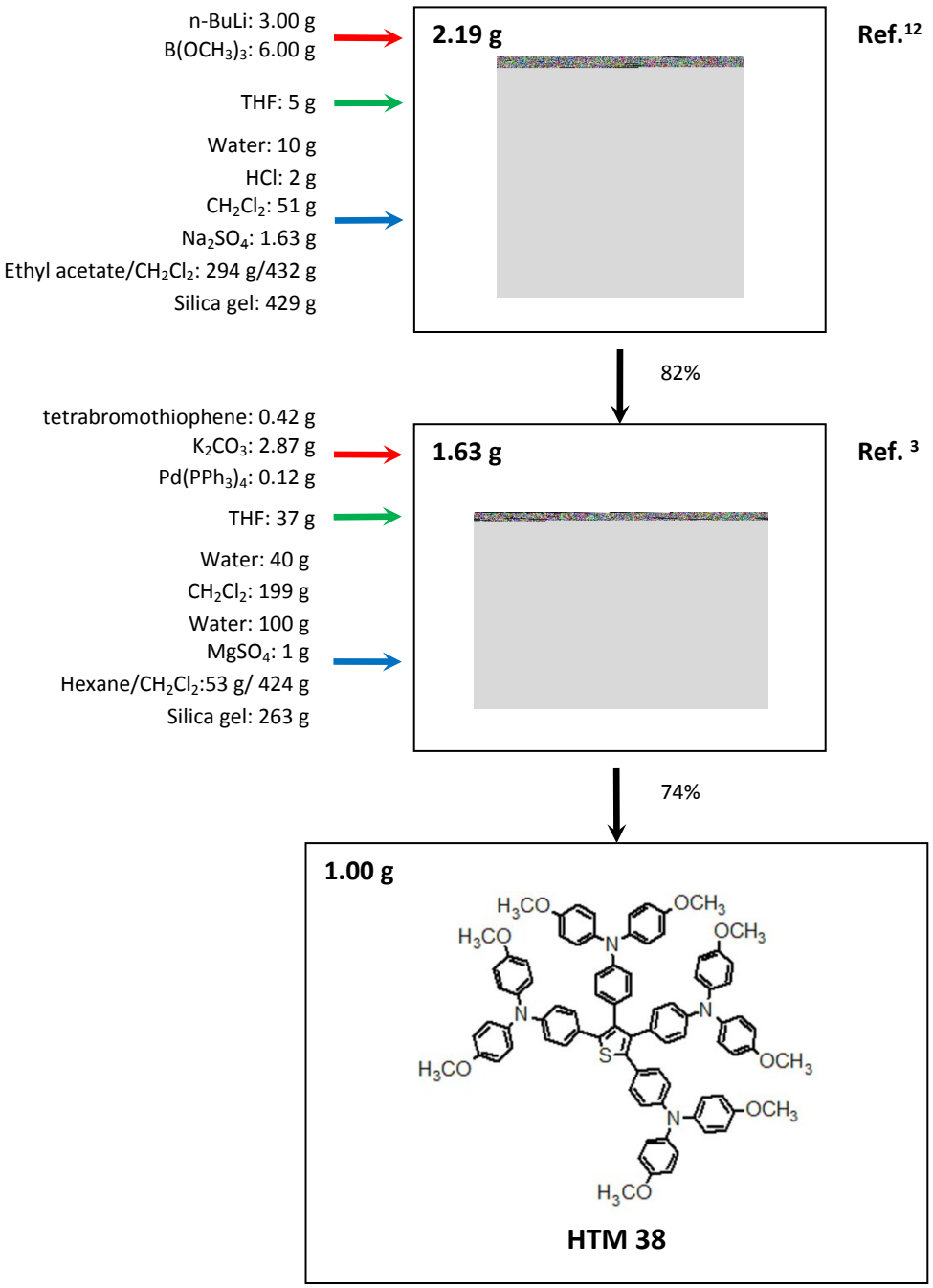


Fig. S16 Flowchart describing the synthesis of 1 gram of HTM **38**[3, 12]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

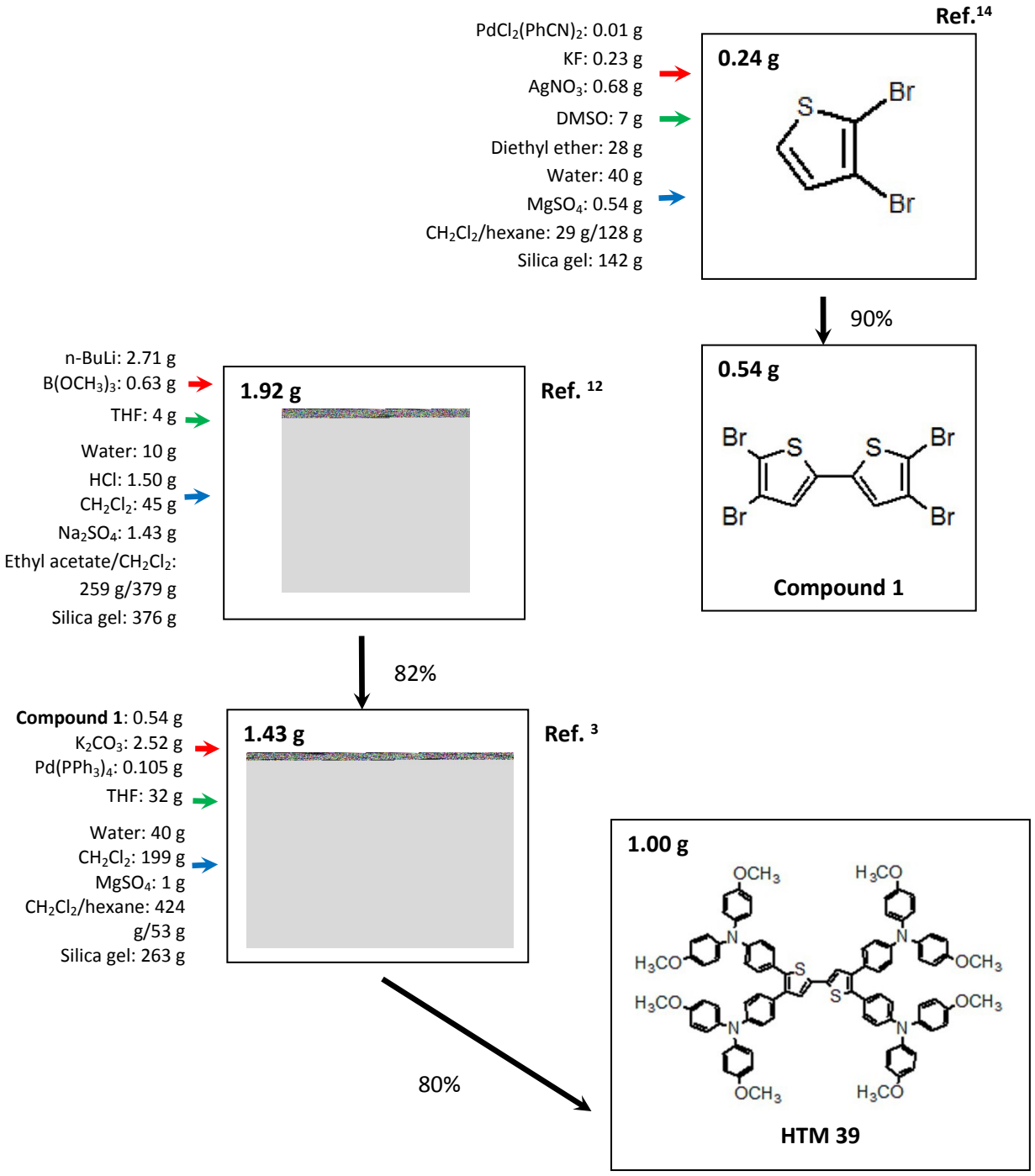


Fig. S17 Flowchart describing the synthesis of 1 gram of HTM **39**[3, 12, 14]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

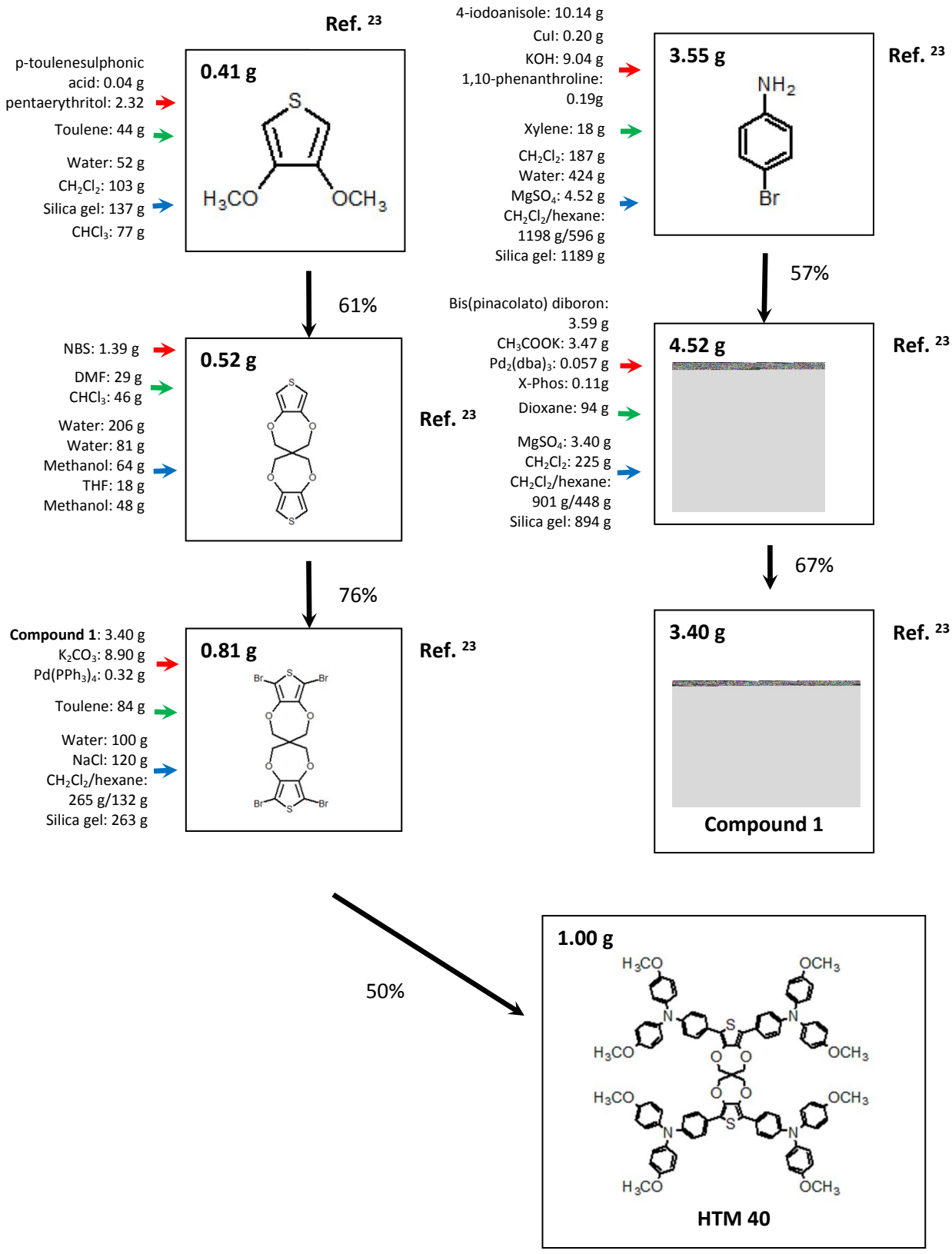
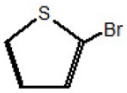


Fig. S18 Flowchart describing the synthesis of 1 gram of HTM **40**[23]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

Mg: 0.14 g
$PdCl_2(dppf).DCM$: 0.02 g
2,3-dibromothiophene: 0.80 g
Diethyl ether: 5 g
Methanol: 1 g
Na_2SO_4/silica gel: 0.74 g/ 74 g
Diethyl ether: 52 g
Silica gel: 195 g
Petroleum ether: 201 g

0.56 g

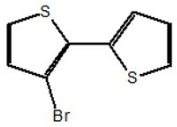


Ref.[18]

88%

NBS: 1.09 g
$CHCl_3$: 10 g
CH_3COOH: 5 g
CH_2Cl_2: 98 g
Water: 15 g
$NaHCO_3$: 0.37 g
Water: 7 g
NaCl: 9 g
Na_2SO_4: 0.74 g
Petroleum ether: 201 g
Silica gel: 195 g

0.74 g

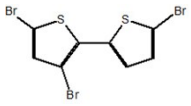


Ref.[18]

61%

n-BuLi: 1.48 g
$(CH_3)_3SiCl$: 0.38 g
Diethyl ether: 11 g
Water: 64 g
Diethyl ether: 36 g
Water: 34 g
NaCl: 41 g
MgSO4: 0.64 g
Petroleum ether: 174 g
Silica gel: 168 g

0.74 g

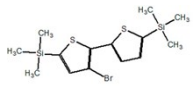


Ref.[18]

89%

Compound 1: 0.56 g
n-BuLi: 0.65 g
Diethyl ether: 17 g
Water: 21 g
NaCl: 13 g
$MgSO_4$: 0.97 g
Petroleum ether/ CH_2Cl_2:
147 g/ 228 g
Silica gel: 255 g

0.64 g

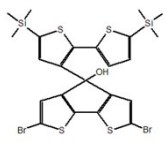


Ref.[18]

91%

NBS: 0.59 g
CH_2Cl_2: 26 g
$Na_2S_2O_3$: 11.70 g
CH_2Cl_2: 147 g
Water: 20 g
NaCl: 11.73 g
$MgSO_4$: 0.74 g
Petroleum ether/CH_2Cl_2:
101 g/196 g
Silica gel: 195 g

0.97 g

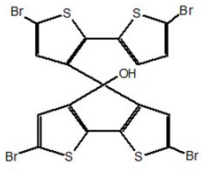


Ref.[18]

75%

$BF_3.Et_2O$: 2.06 g
CH_2Cl_2: 742 g
Ethanol: 29 g
Water: 187 g
CH_2Cl_2: 91 g
Water: 344 g
$MgSO_4$: 0.46 g
Petroleum ether/CH_2Cl_2:
94 g/61 g
Silica gel: 121 g

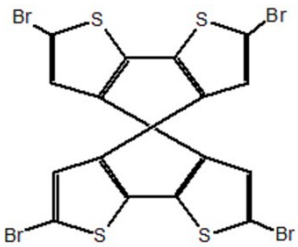
0.74 g



Ref.[18]

64%

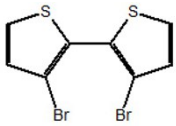
0.46 g



Compound 2

DIPA: 0.69 g
n-BuLi: 2.74 g
$(CH_3)_3SiCl$: 0.91 g
THF: 36 g
Water: 111 g
Diethyl ether: 17 g
NaCl: 133 g
$MgSO_4$: 1.11 g

0.94 g

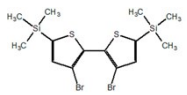


Ref.[18]

82%

n-BuLi: 1.99 g
$(CH_3)_2NCOCl$: 0.25 g
THF: 10 g
NH_4Cl: 0.5 g
Petroleum ether: 28 g
$MgSO_4$: 0.66 g
CH_2Cl_2/petroleum ether:
87g/135 g
Silica gel: 174 g

1.11 g

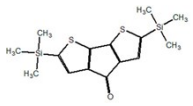


Ref.[18]

83%

NBS: 0.61 g
THF: 12 g
CH_2Cl_2: 74 g
Water: 31 g
NaCl: 18 g
$MgSO_4$: 0.56 g
Methanol: 71 g

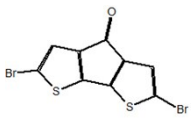
0.66 g



Ref.[18]

81%

0.56 g



Compound 1

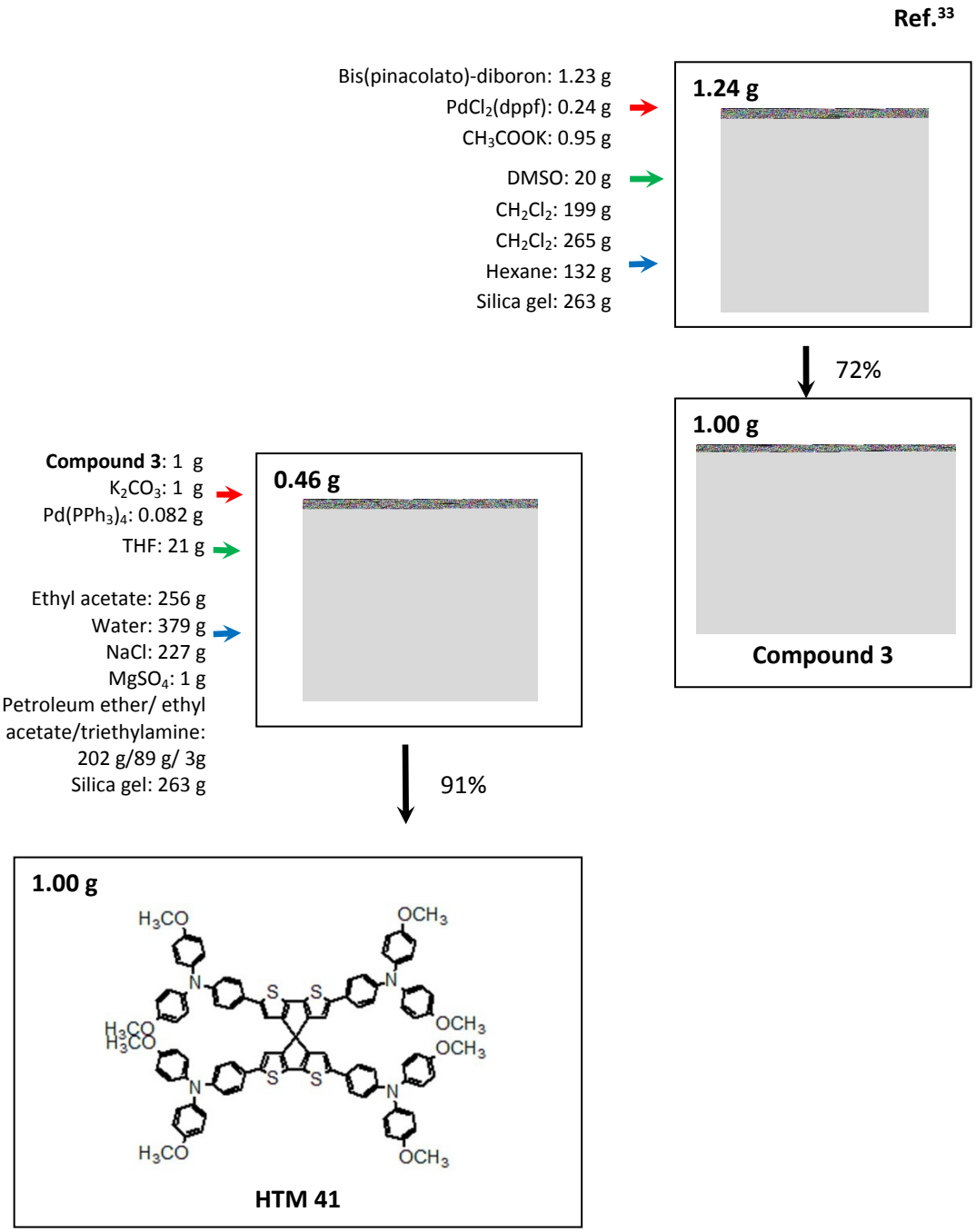


Fig. S19 Flowchart describing the synthesis of 1 gram of HTM **41**[18]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

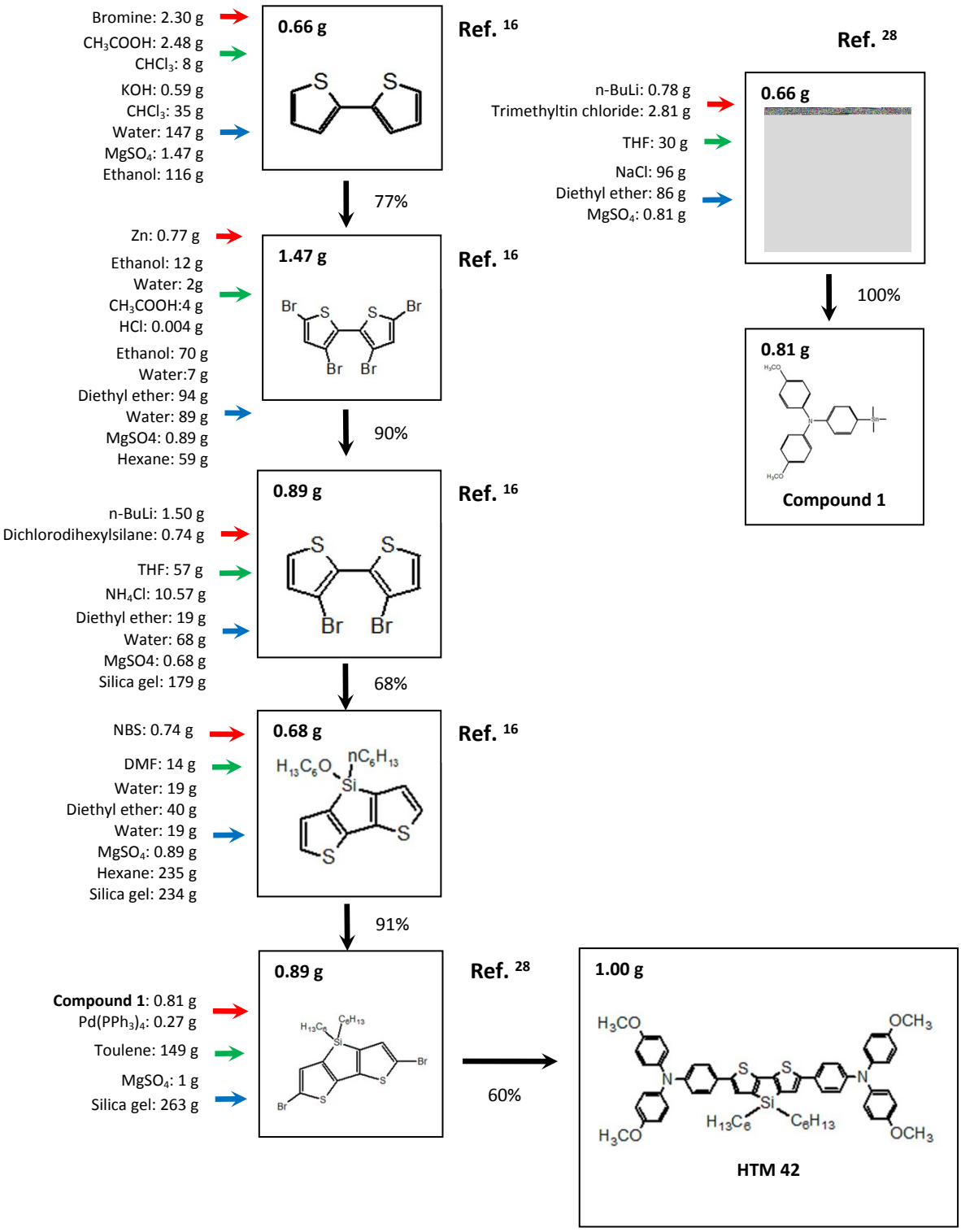


Fig. S20 Flowchart describing the synthesis of 1 gram of HTM **42**[16, 28]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

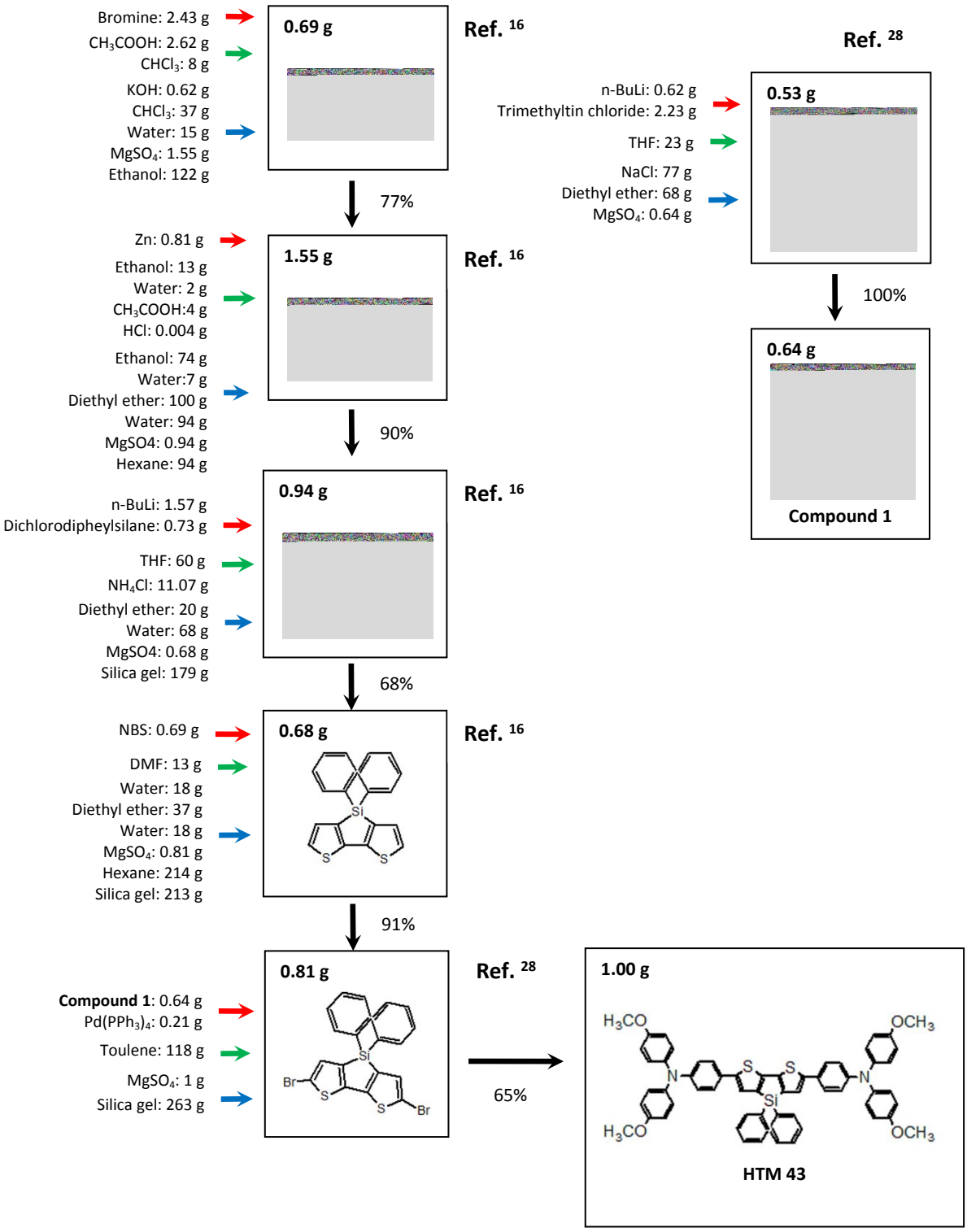


Fig. S21 Flowchart describing the synthesis of 1 gram of HTM **43**[16, 28]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

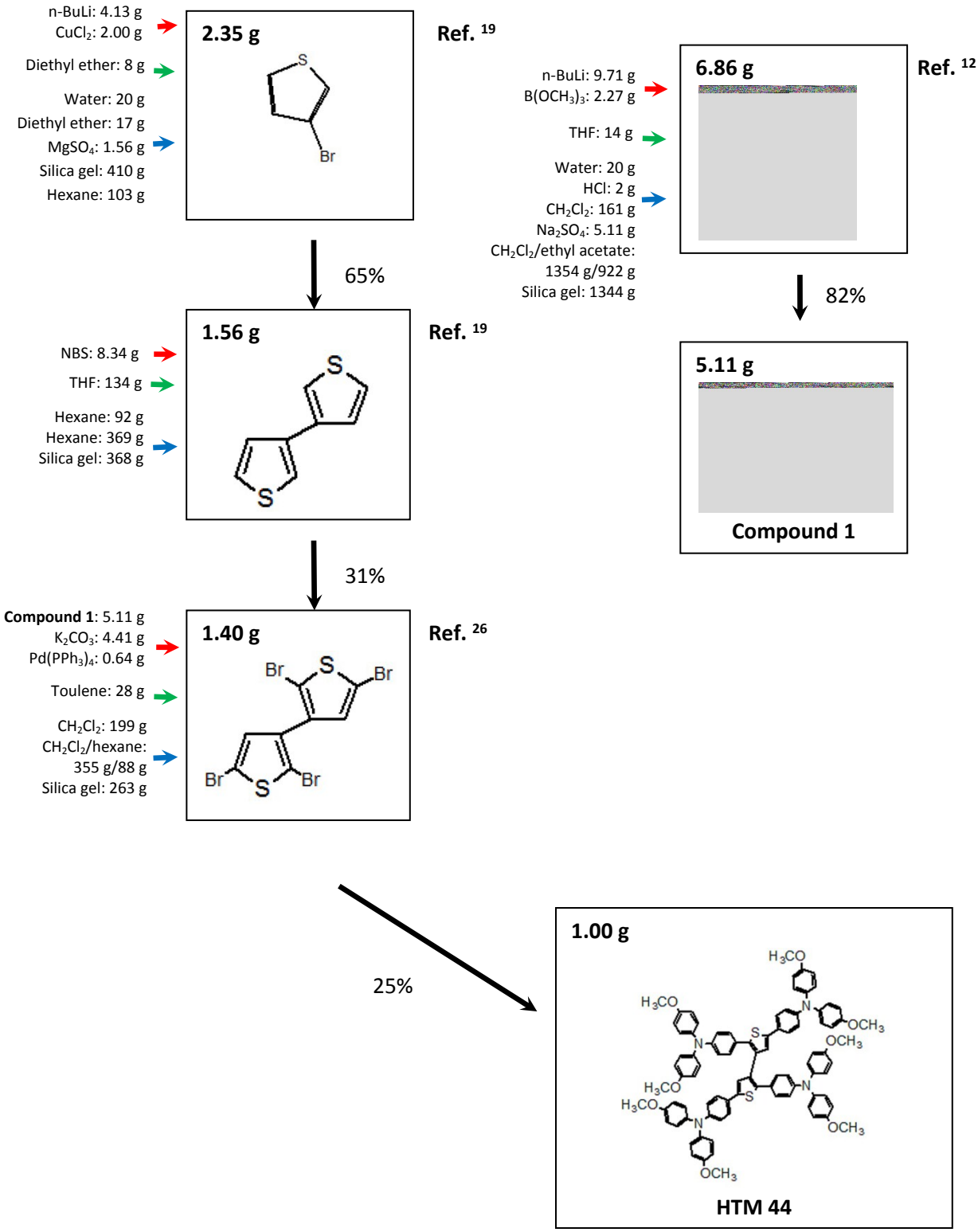


Fig. S22 Flowchart describing the synthesis of 1 gram of HTM **44**[12, 19, 26]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

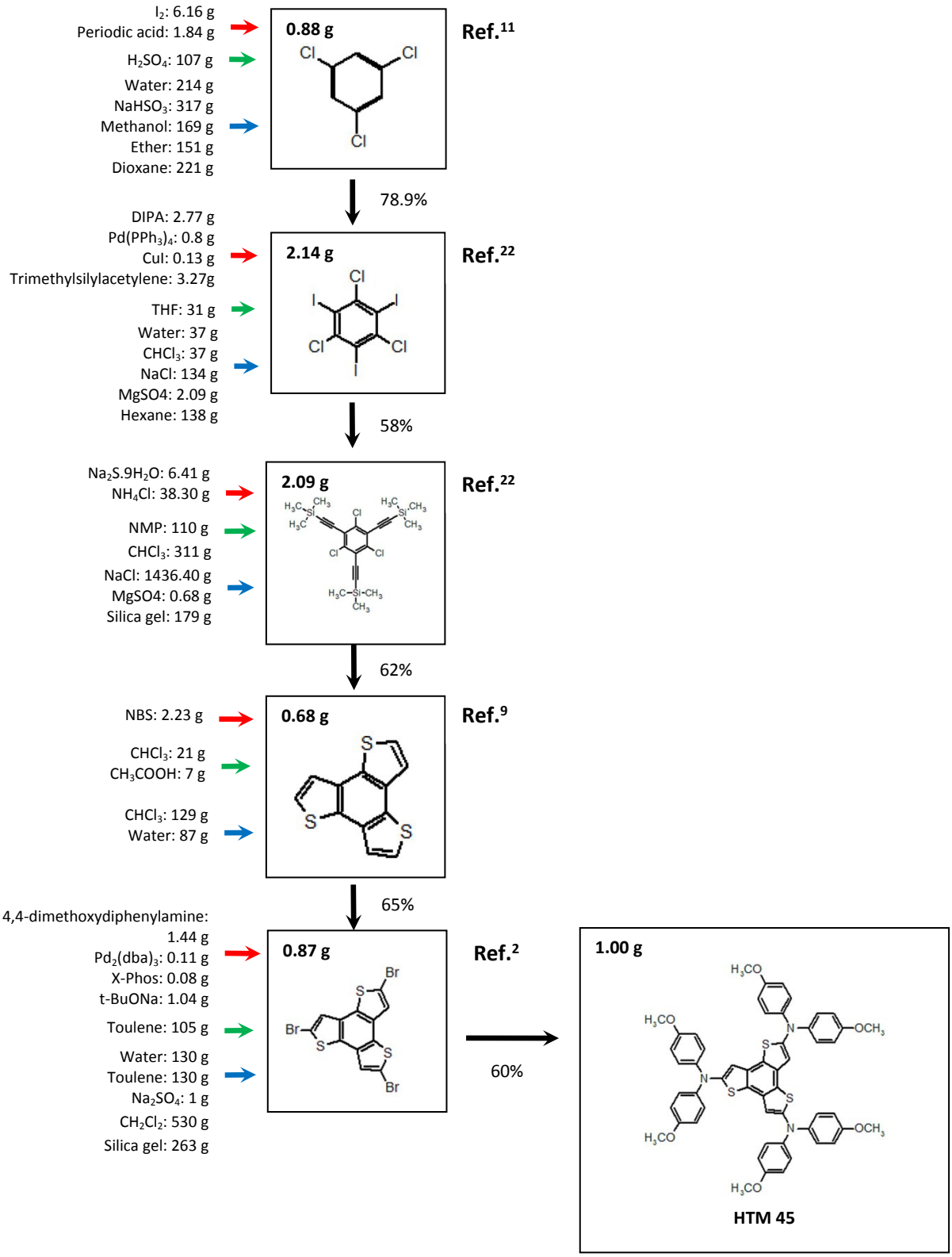


Fig. S23 Flowchart describing the synthesis of 1 gram of HTM **45**[2, 9, 11, 22]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

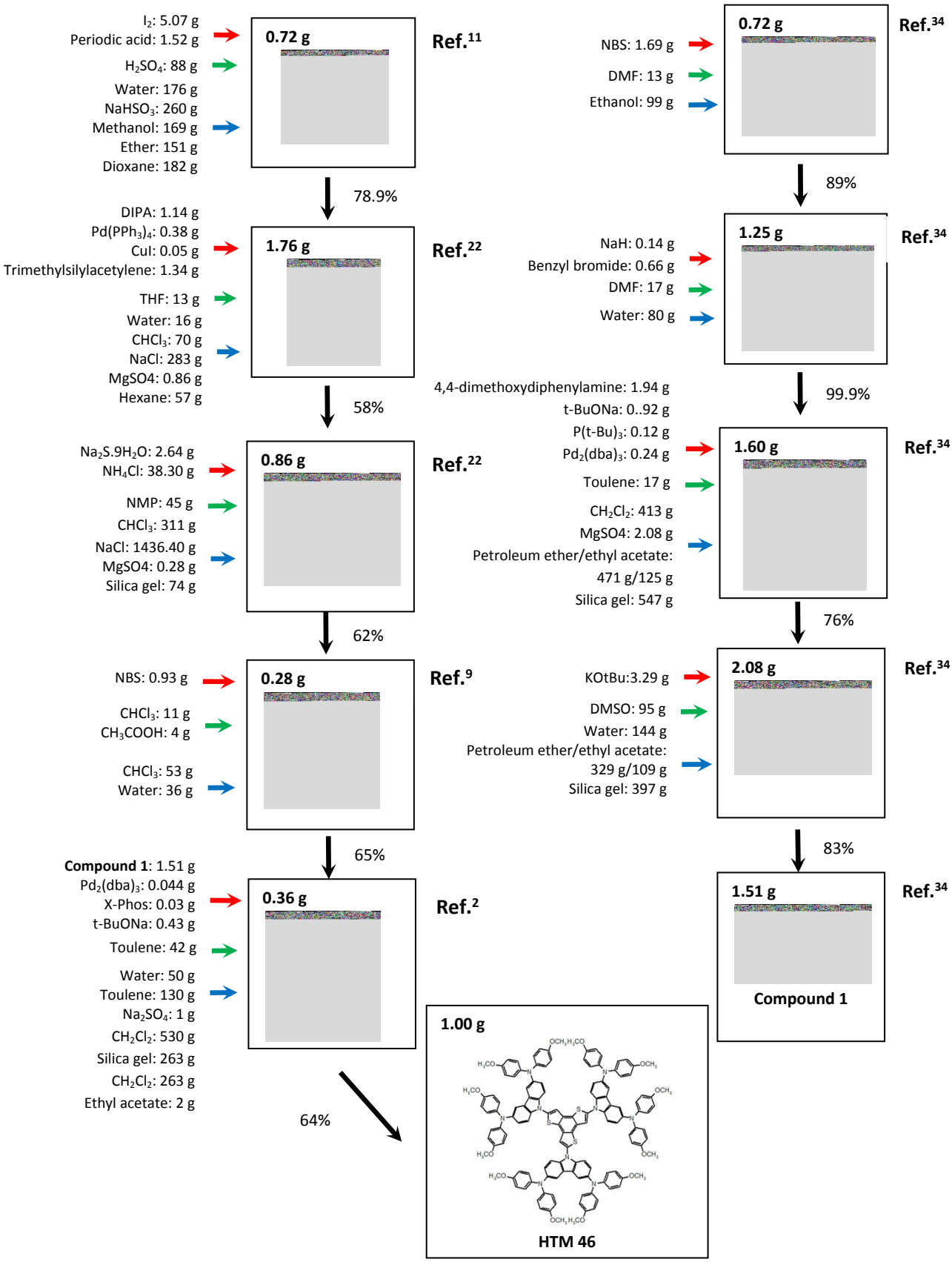


Fig. S24 Flowchart describing the synthesis of 1 gram of HTM **46**[2, 9, 11, 22, 34]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

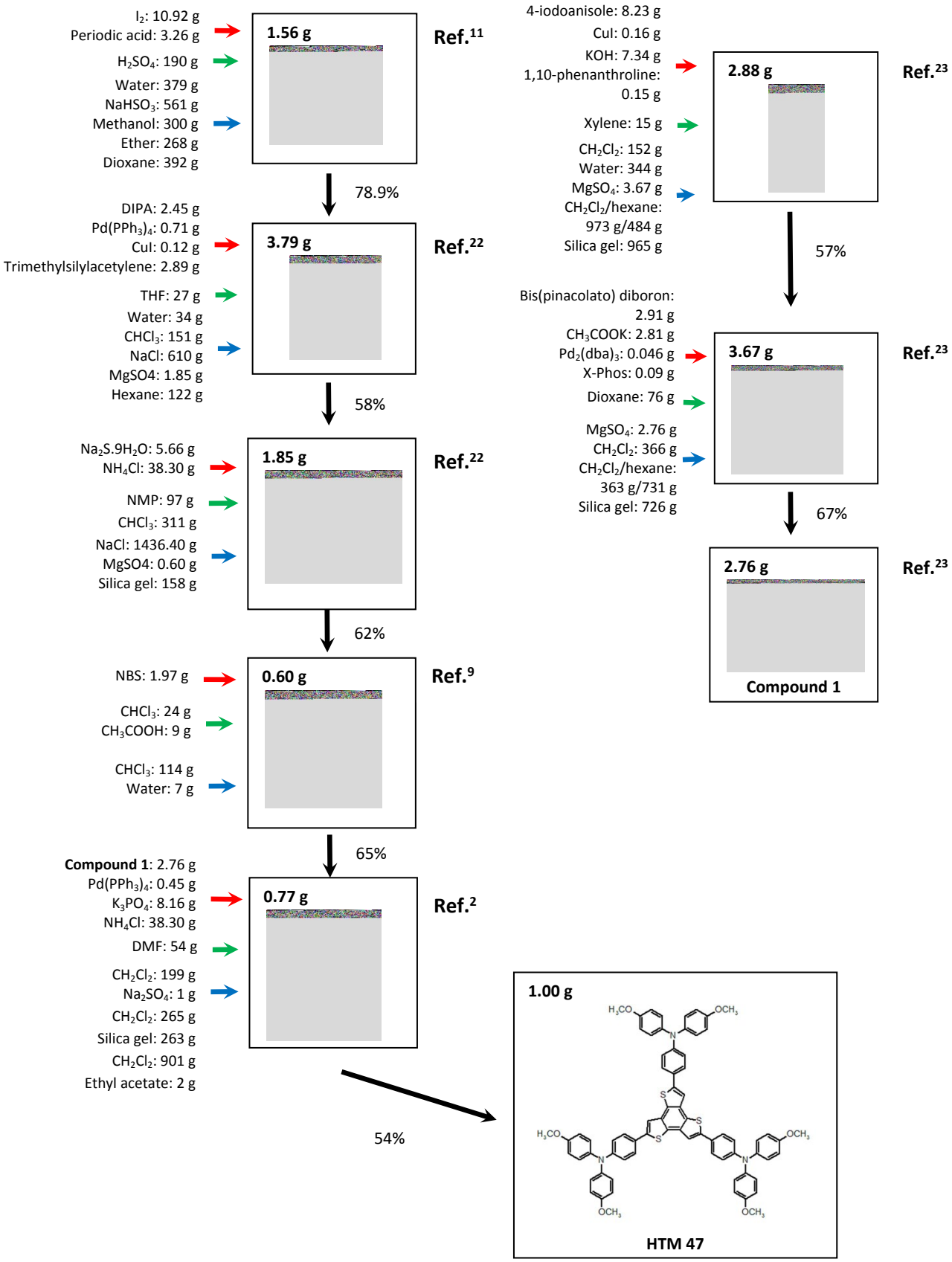


Fig. S25 Flowchart describing the synthesis of 1 gram of HTM **47**[2, 9, 11, 22, 23] . The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

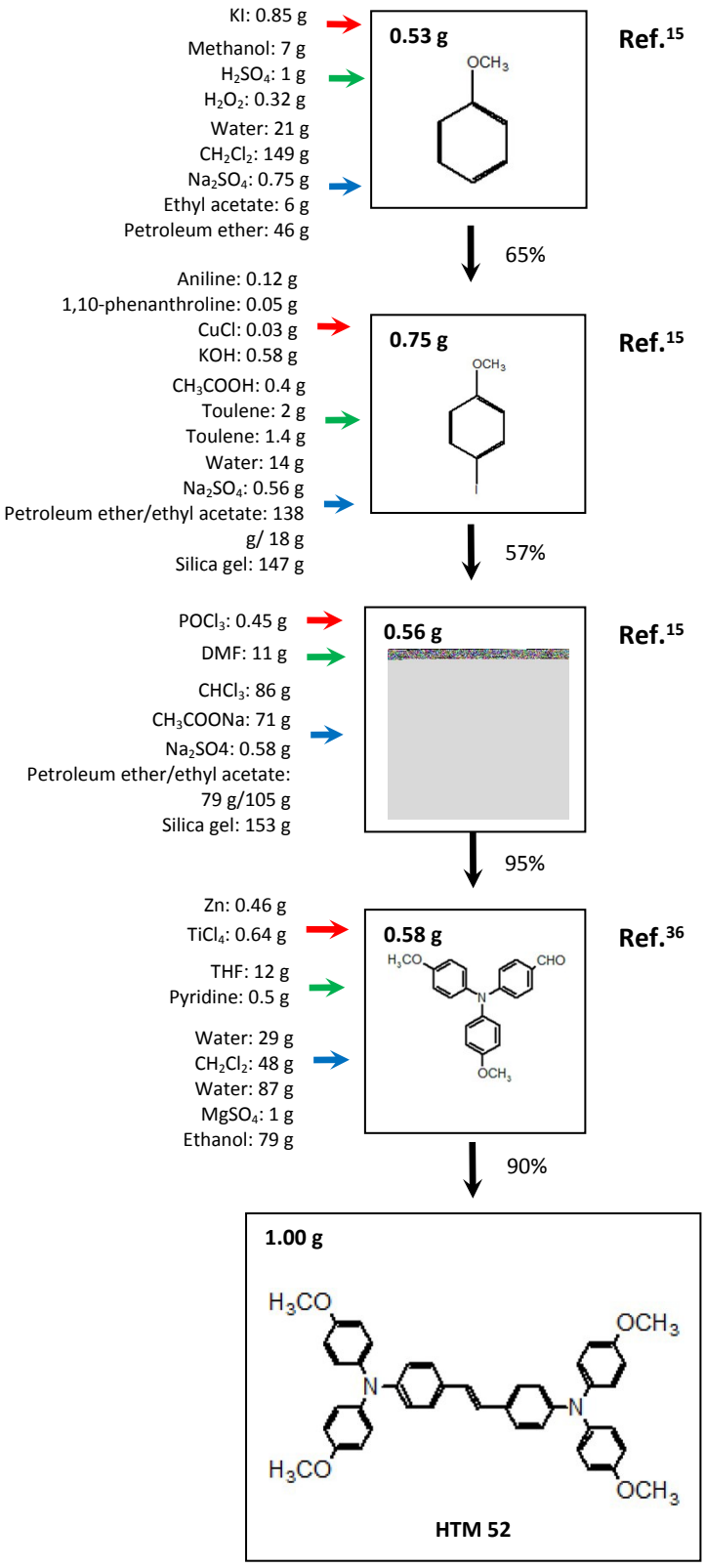


Fig. S26 Flowchart describing the synthesis of 1 gram of HTM **52**[15, 36]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

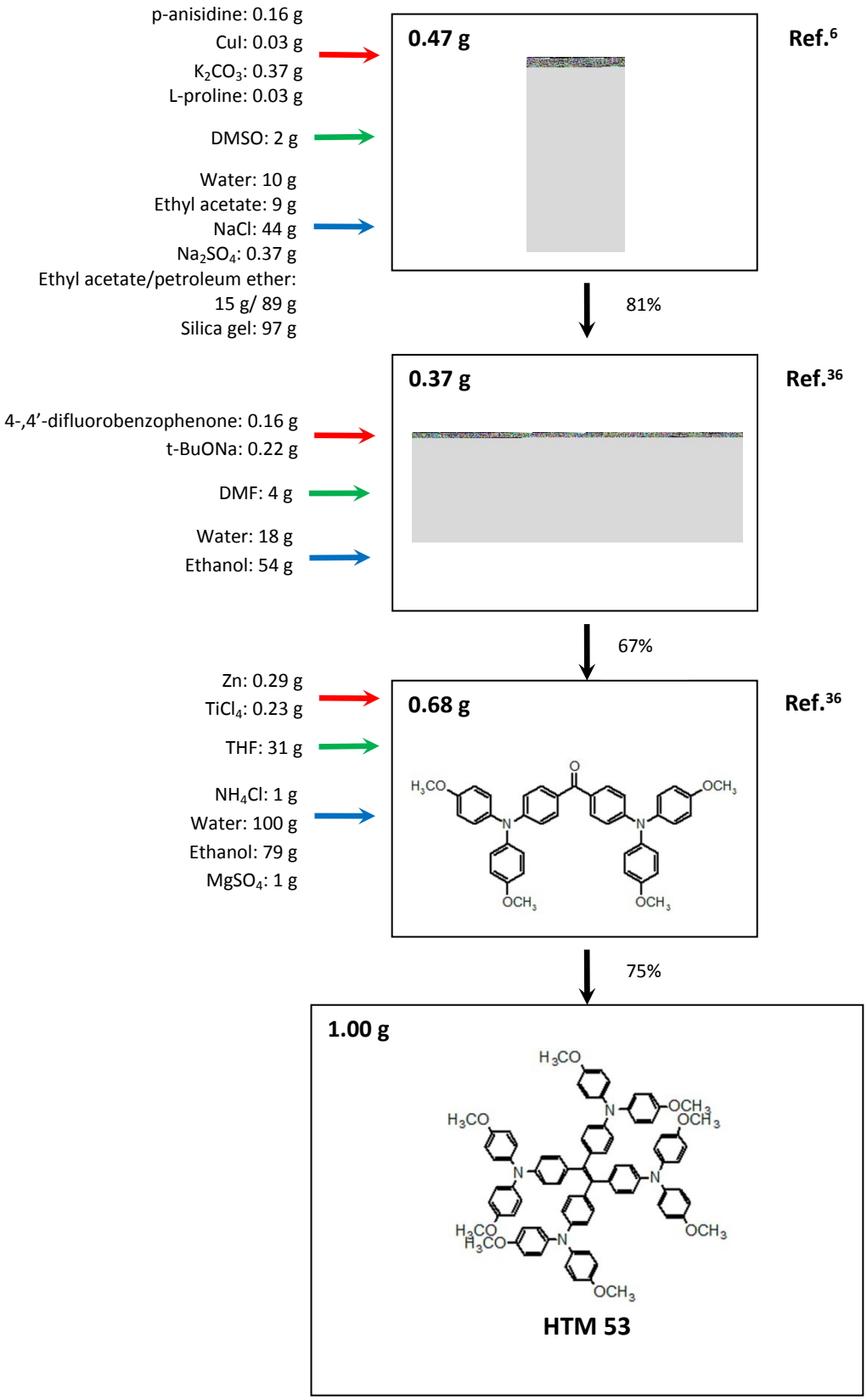


Fig. S27 Flowchart describing the synthesis of 1 gram of HTM **53**[6, 36]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

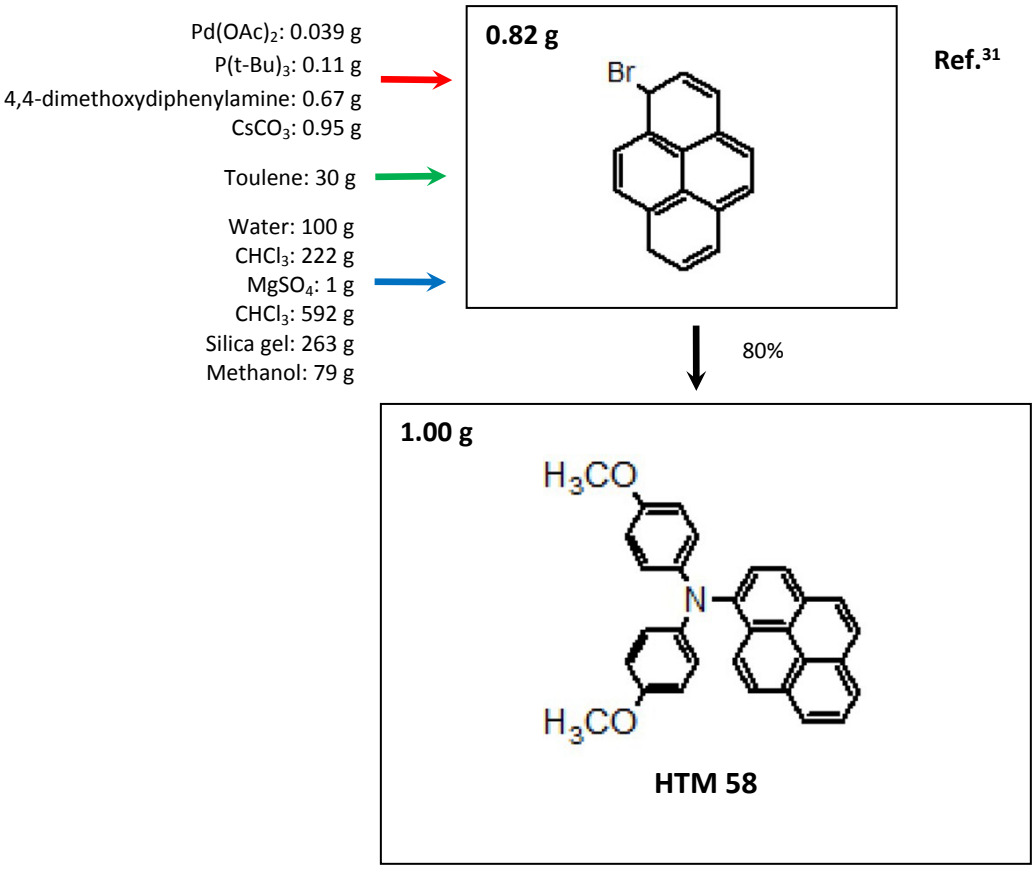


Fig. S28 Flowchart describing the synthesis of 1 gram of HTM **58**[31]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

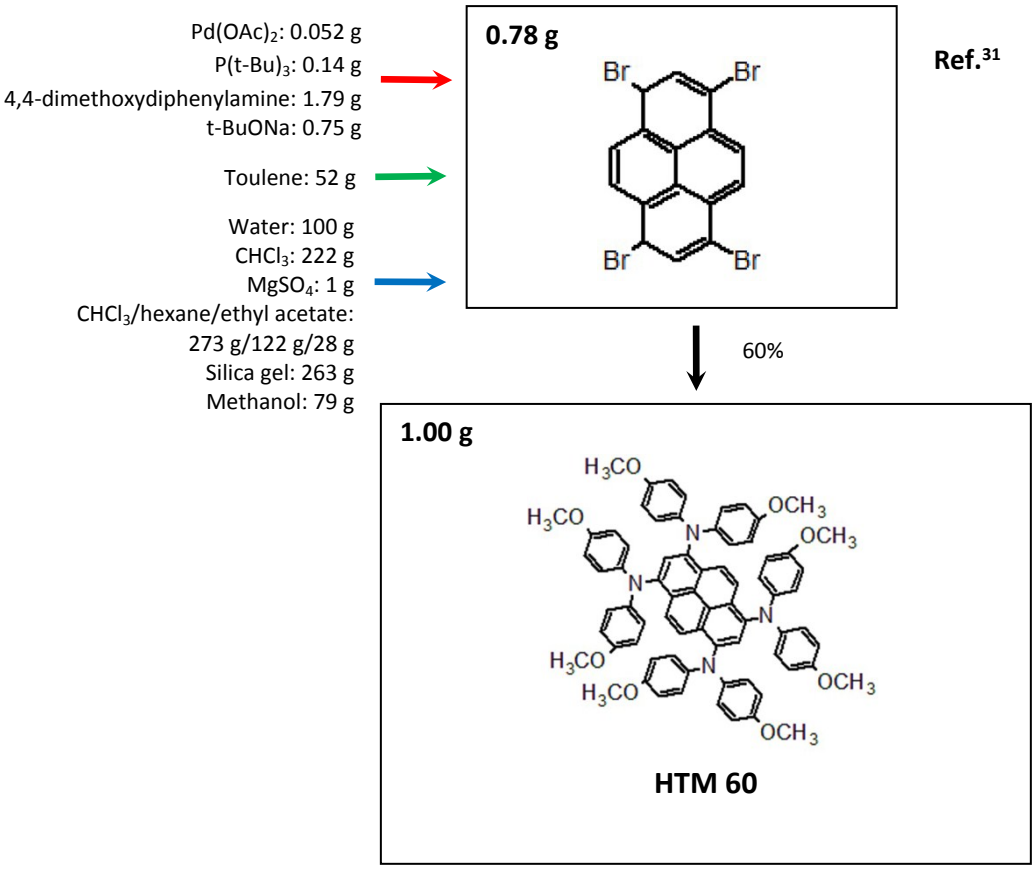


Fig. S29 Flowchart describing the synthesis of 1 gram of HTM **60**[31]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

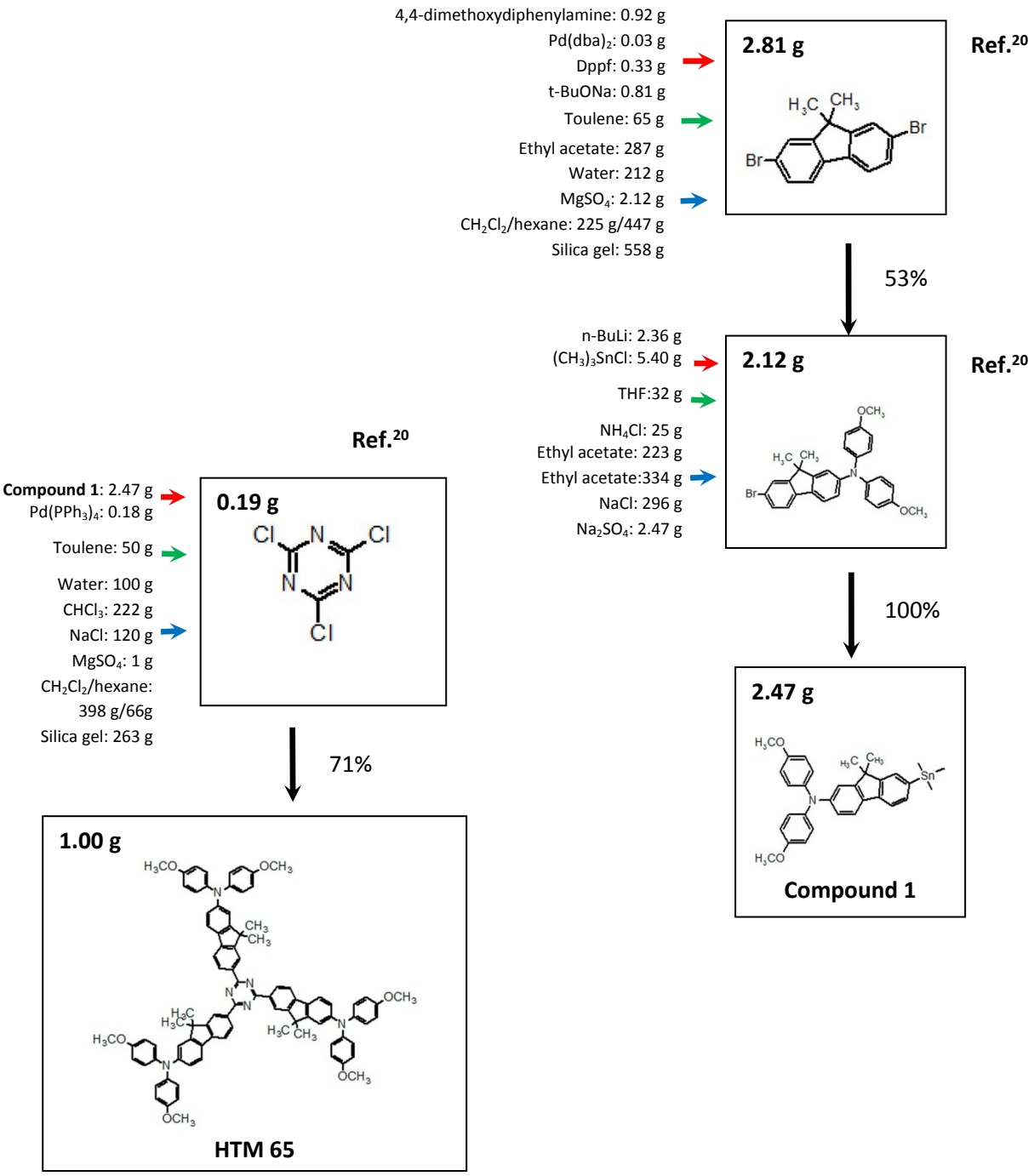


Fig. S30 Flowchart describing the synthesis of 1 gram of HTM **65**[20]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

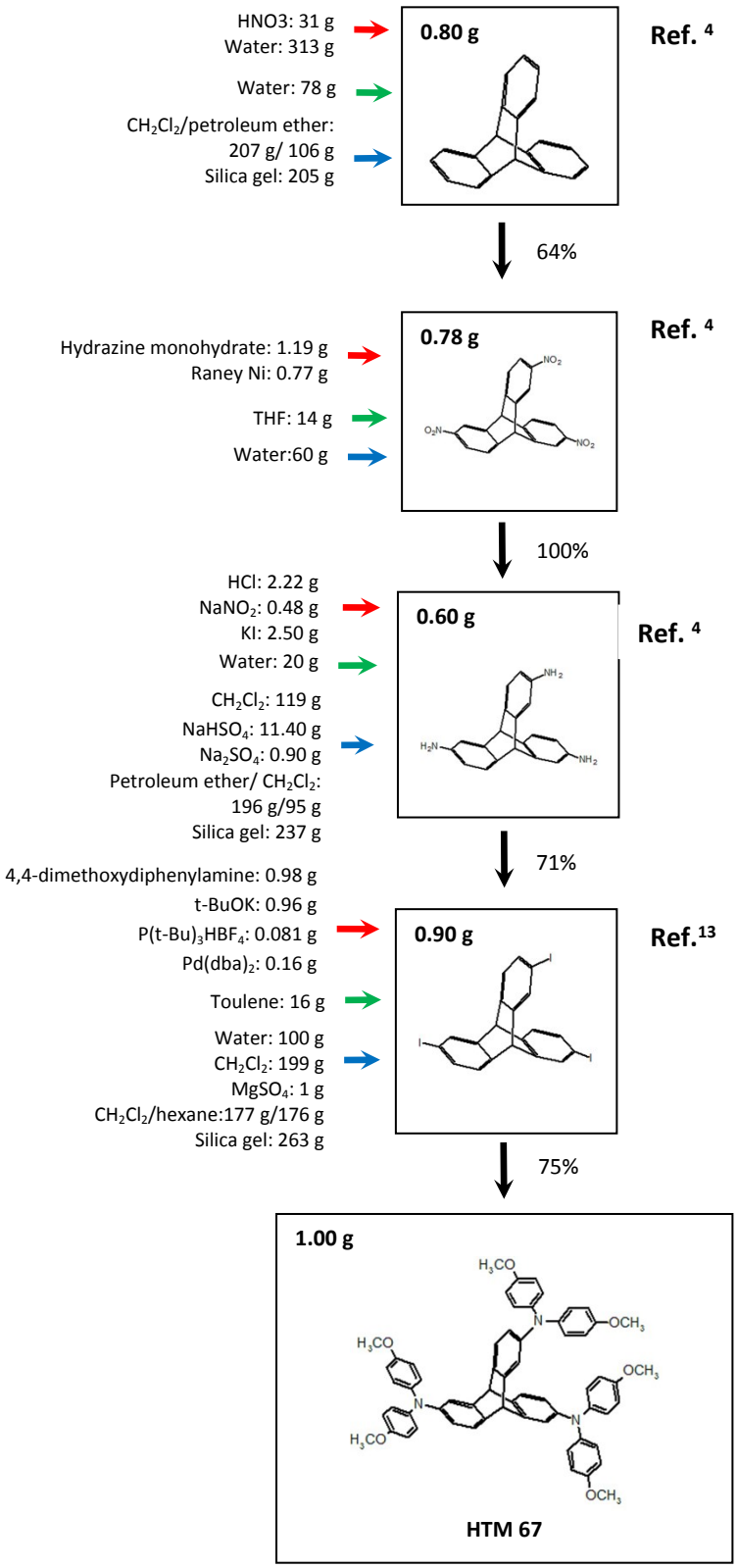


Fig. S31 Flowchart describing the synthesis of 1 gram of HTM **67**[4, 13]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

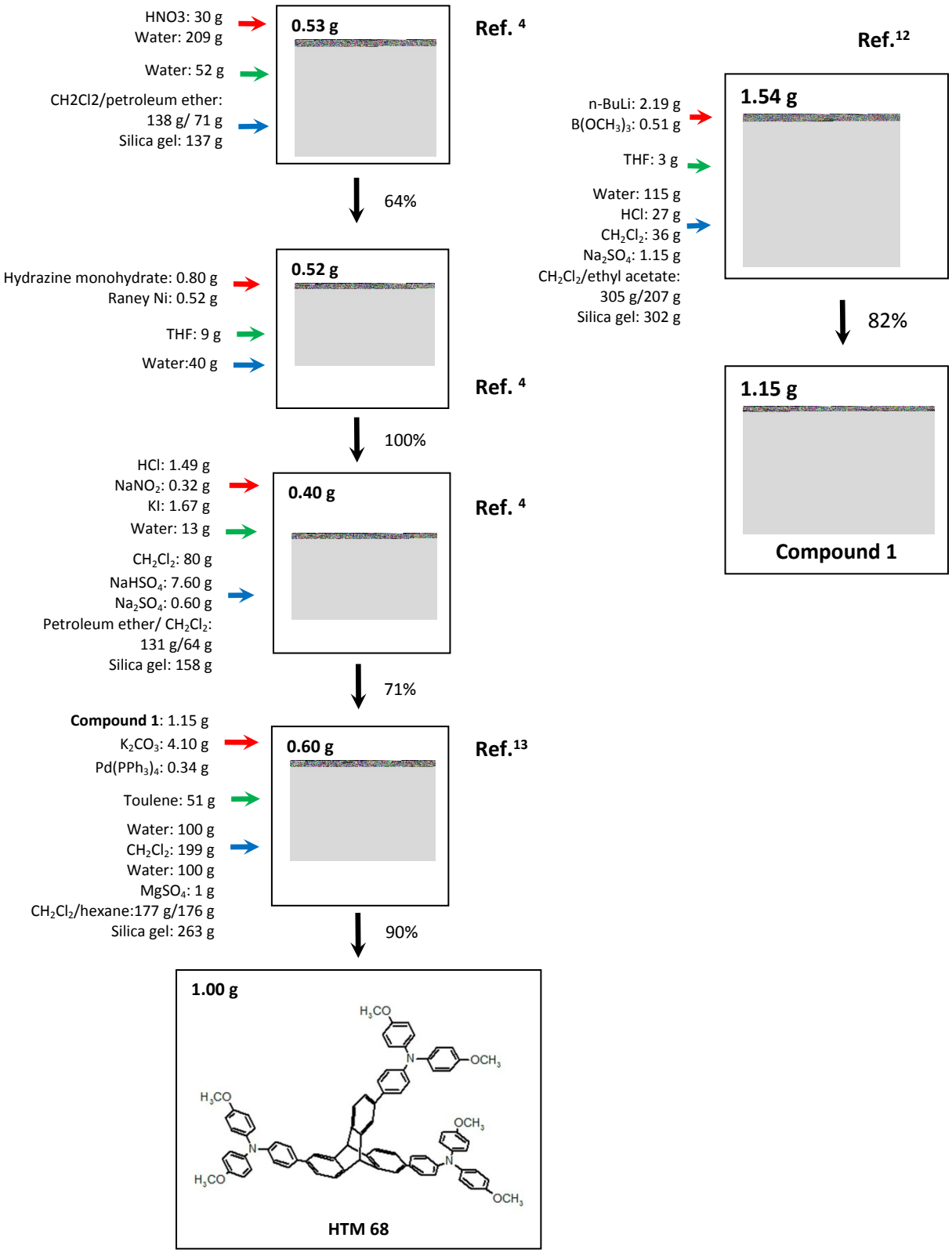


Fig. S32 Flowchart describing the synthesis of 1 gram of HTM **68**[4, 12, 13]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

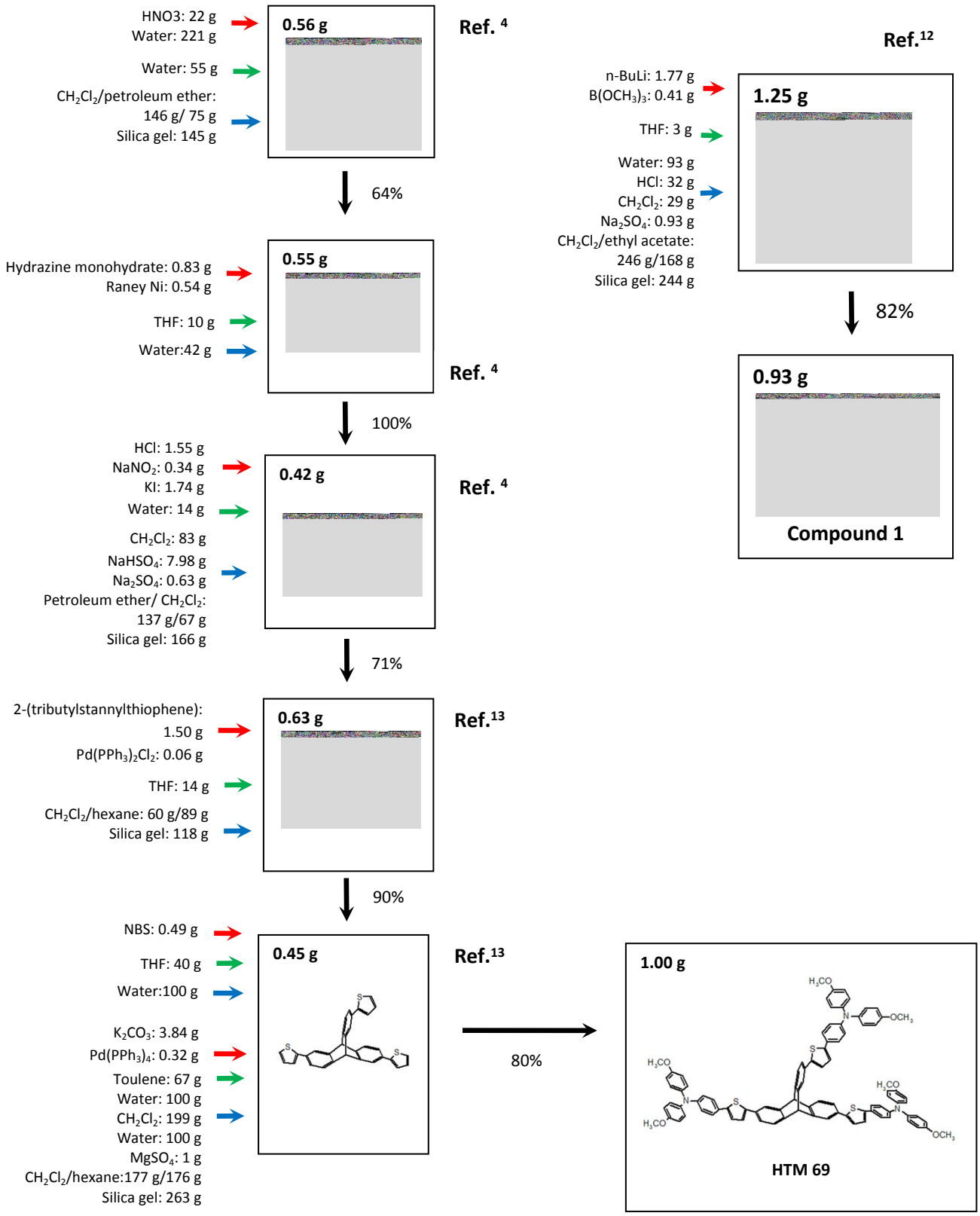


Fig. S33 Flowchart describing the synthesis of 1 gram of HTM **69**[4, 12, 13]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

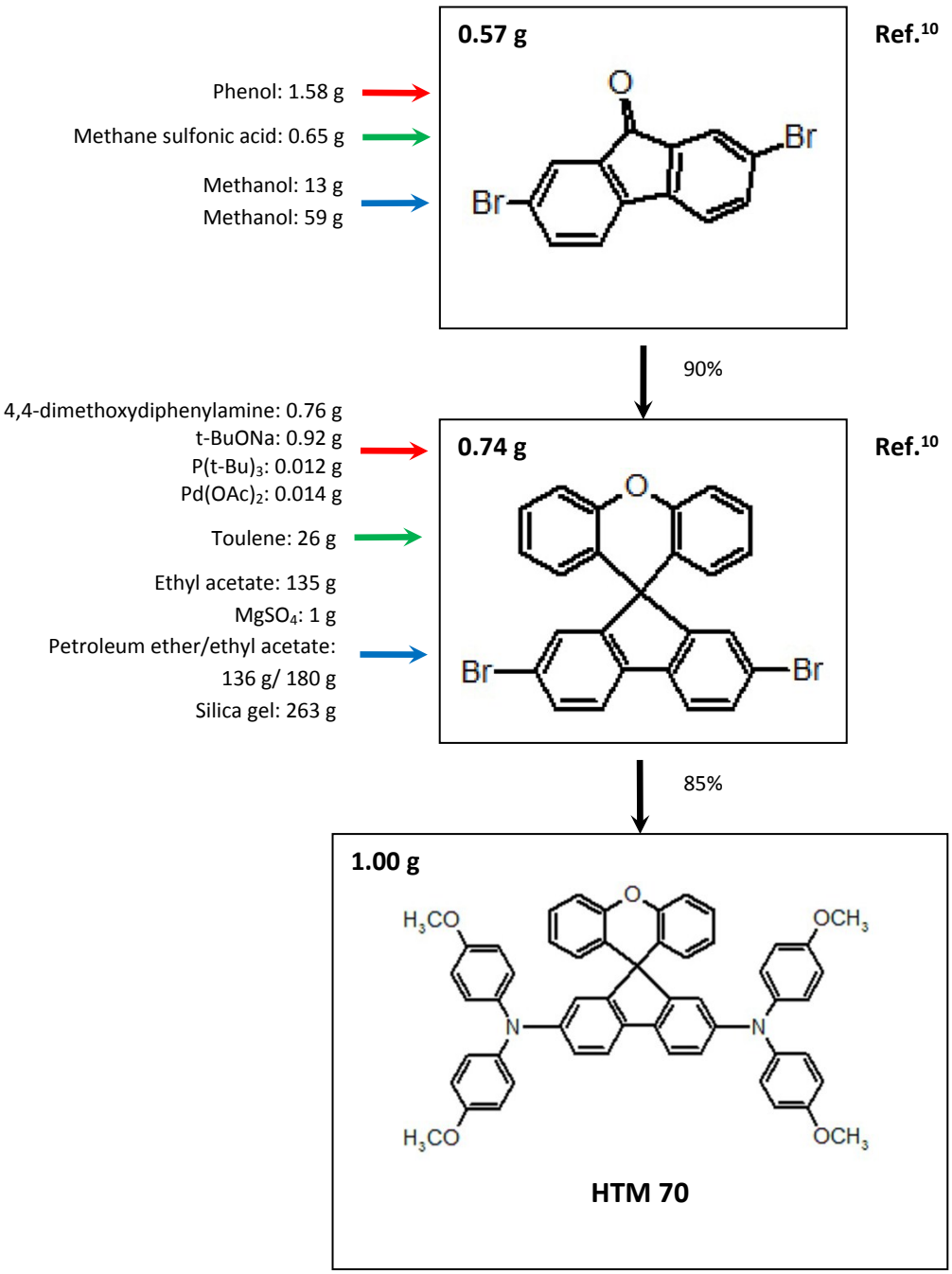


Fig. S34 Flowchart describing the synthesis of 1 gram of HTM **70**[10]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

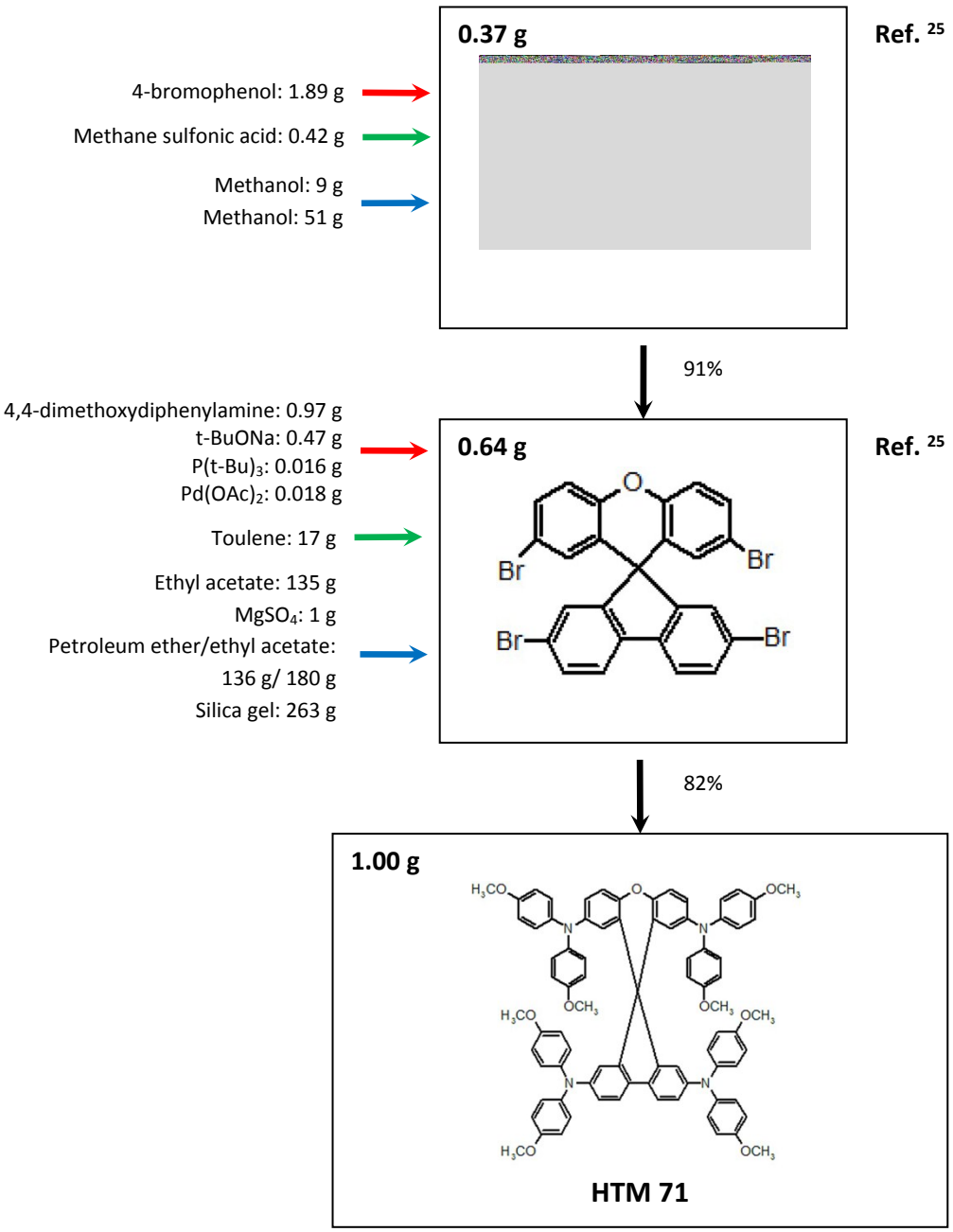


Fig. S35 Flowchart describing the synthesis of 1 gram of HTM **71**[25]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

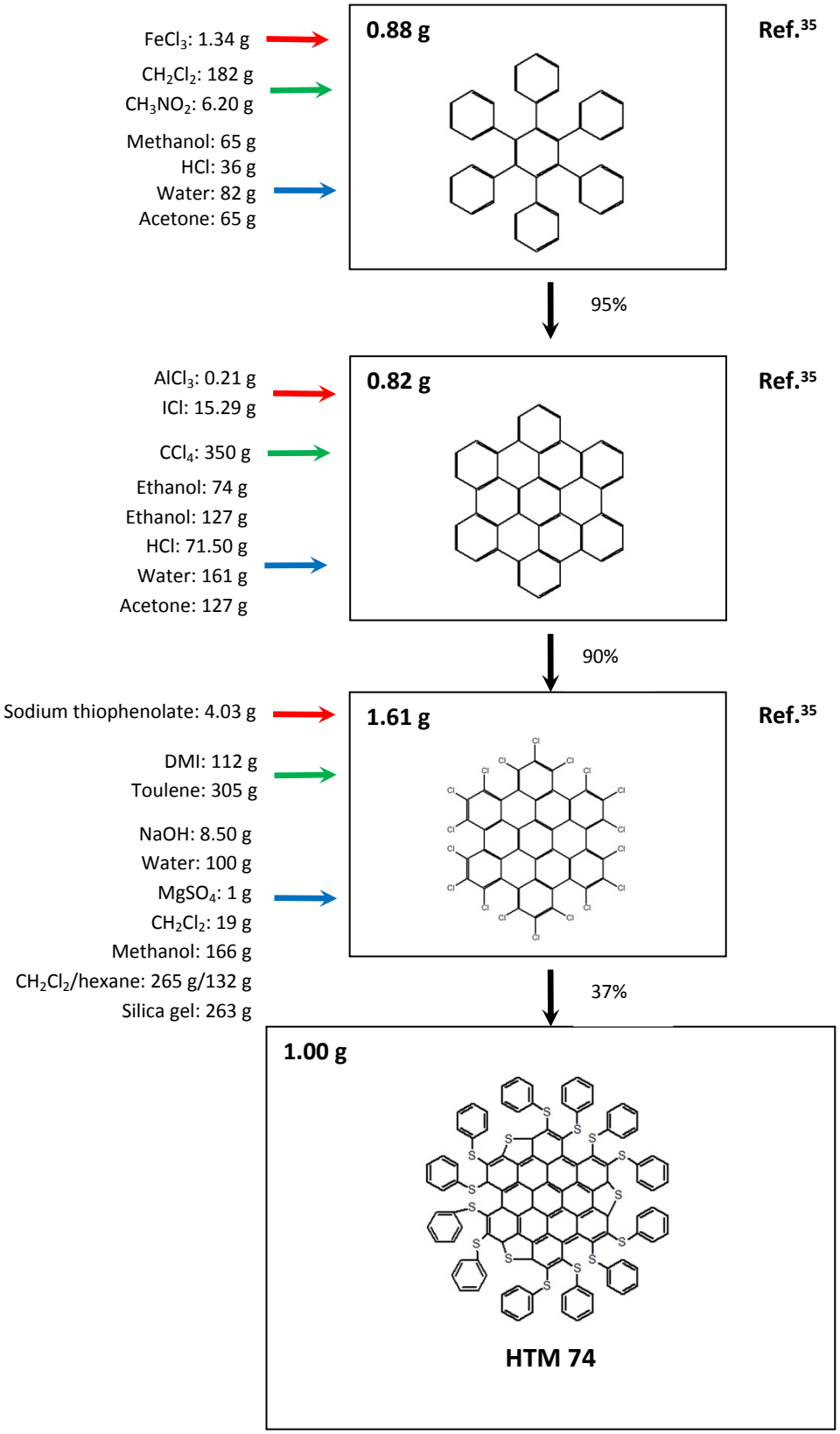


Fig. S36 Flowchart describing the synthesis of 1 gram of HTM **74**[35]. The required quantities of reagents (red arrow), solvents (green arrow) and work up materials (blue arrow) are listed for each step.

Table S01 Materials quatities and cost for the synthesis of 1 g of HTM **Sp01**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
2,2',7,7'-tetrabromo-9,9'-spirobi[9H-fluorene]	1.15			95900.00	110.29	273.62
4,4'-dimethoxydiphenylamine	1.87			54900.00	102.66	
t-BuONa	1.04			307.00	0.32	
$Pd_2(dba)_3$	0.067			14900.00	1.00	
$P(t\text{-}Bu)_3$	0.023			34500.00	0.78	
Toulene		12		69.48	0.83	
Ethyl acetate			135	80.16	10.82	
NaCl (brine)			1	50.70	0.05	
$MgSO_4$			1	144.20	0.14	
Ethyl acetate			120	80.16	9.62	
Hexane			176	117.91	20.75	
Silica gel 60			263	62.20	16.36	
Total						**273.62**

Table S02 Materials quatities and cost for the synthesis of 1 g of HTM **Sp02**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
m-anisidine	2.09			374.00	0.78	125.27
4-bromoaniline	3.22			455.00	1.47	
t-BuONa	2.46			307.00	0.75	
$Pd_2(dba)_3$	0.16			14900.00	2.31	
$P(tBu)_3$	0.055			34500.00	1.90	
Toulene		21		69.48	1.46	
Ethyl acetate			271	80.16	21.72	
NaCl (brine)			2	50.70	0.10	
$MgSO_4$			2	144.20	0.29	
Ethyl acetate			66	80.16	5.29	
Hexane			479	117.91	56.48	
Silica gel 60			526	62.20	32.72	
2,2',7,7'-tetrabromo-9,9'-spirobi[9H-fluorene]	1.29			95900.00	123.71	184.79
t-BuONa	1.17			307.00	0.36	
$Pd_2(dba)_3$	0.075			14900.00	1.12	
$P(t\text{-}Bu)_3$	0.026			34500.00	0.88	
Toulene		14		69.48	0.97	
Ethyl acetate			135	80.16	10.82	
NaCl (brine)			1	50.70	0.05	
$MgSO_4$			1	144.20	0.14	
Ethyl acetate			120	80.16	9.62	
Hexane			176	117.91	20.75	
Silica gel 60			263	62.20	16.36	
Total						**310.06**

Table S03 Materials quatities and cost for the synthesis of 1 g of HTM **Sp03**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
m-anisidine	2.21			148.40	0.33	124.86
4-bromoaniline	3.41			455.00	1.55	
t-BuONa	2.60			307.00	0.80	
$Pd_2(dba)_3$	0.16			14900.00	2.44	
$P(tBu)_3$	0.058			34500.00	2.00	
Toulene		22		69.48	1.53	
Ethyl acetate			271	80.16	21.72	
NaCl (brine)			2	50.70	0.10	
$MgSO_4$			2	144.20	0.29	
Ethyl acetate			120	80.16	9.62	
Hexane			439	117.91	51.76	
Silica gel 60			526	62.20	32.72	
2,2',7,7'-tetrabromo-9,9'-spirobi[9H-fluorene]	1.29			95900.00	123.71	184.80
t-BuONa	1.17			307.00	0.36	
$Pd_2(dba)_3$	0.075			14900.00	1.12	
$P(tBu)_3$	0.026			34500.00	0.89	
Toulene		14		69.48	0.97	
Ethyl acetate			135	80.16	10.82	
NaCl (brine)			1	50.70	0.05	
$MgSO_4$			1	144.20	0.14	
Ethyl acetate			120	80.16	9.62	
Hexane			176	117.91	20.75	
Silica gel 60			263	62.20	16.36	
Total						**309.66**

Table S04 Materials quatities and cost for the synthesis of 1 g of HTM **7**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
4-bromo-4,4-dimethoxytriphenylamine	2.61			79800.00	208.18	325.38
n-butyllithium (2.5M)	2.05			110.63	0.23	
2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane	1.43			1276.32	1.83	
THF		23		109.79	2.53	
NH_4Cl			0.36	79.50	0.03	
Dichloromethane			104	53.58	5.57	
Water			228	0	0	
$MgSO_4$			2.28	144.20	0.33	
Dichloromethane			302	53.58	16.18	
Hexane			451	117.91	53.18	
Silica gel 60			600	62.20	37.32	
Methyl anthranilate	2.03			1520.00	3.09	242.89
Methyl 2-iodobenzoate	10.05			2736.00	27.50	
K_2CO_3	4.24			142.00	0.60	
Copper powder	0.17			15840.00	2.69	
Copper(I) iodide	0.25			285.00	0.07	
Diphenylether		16		657.03	10.51	
Ethyl acetate			305	80.16	24.45	
Hexane			890	117.91	104.94	
Silica gel			1110	62.20	69.04	
Iodomethane	25.73			327.19	8.42	104.74
Magnesium turning	5.63			116.00	0.65	
Iodine	0.50			456.00	0.23	
Ether		85		129.89	11.04	
Toulene		105		69.48	7.30	
H_2SO_4			33	38.59	1.27	
Dichloromethane			260	53.58	13.93	
Water			500	0	0	
Na_2SO_4			1.31	115.80	0.15	
Ethyl acetate			79	80.16	6.33	
Hexane			288	117.91	33.96	
Silica gel 60			345	62.20	21.46	
H_3PO_4	22			84.27	1.85	43.67
NaOH			6.88	84.50	0.58	
Dichloromethane			141	53.58	7.55	
Hexane			187	117.91	22.05	
Silica gel 60			187	62.20	11.63	
Chloroform		39		49.66	1.94	
NaCl			32	29.24	0.94	
Water			27	0	0	
Na_2SO_4			0.76	115.80	0.09	
Hexane			200	117.91	23.58	
Silica gel 60			200	62.20	12.44	
Ethanol			60	218.63	13.12	

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K_2CO_3	2.61			142.00	0.37	73.27
$Pd(PPh_3)_4$	0.146			17750.00	2.59	
THF		112		109.79	12.30	
Water		9		0	0	
CH_2Cl_2			199	53.58	10.66	
$MgSO_4$			1	144.20	0.14	
Ethyl acetate			45	80.16	3.61	
Hexane			231	117.91	27.24	
Silica gel 60			263	62.20	16.36	
Total						**842.08**

Table S05 Materials quatities and cost for the synthesis of 1 g of HTM **8**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
4-bromo-4,4-dimethoxytriphenylamine	2.74			79800.00	218.65	341.84
n-butyllithium (2.5M)	2.15			110.63	0.24	
2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane	1.50			1276.32	1.91	
THF		24		109.79	2.63	
NH_4Cl			0.38	79.50	0.03	
Dichloromethane			109	53.58	5.84	
Water			240	0	0	
$MgSO_4$			2.40	144.20	0.35	
Dichloromethane			318	53.58	17.04	
Hexane			474	117.91	55.89	
Silica gel 60			631	62.20	39.25	
Tris(4-bromophenyl)amine	0.64			10800.00	6.91	78.38
K_2CO_3	2.77			142.00	0.39	
$Pd(PPh_3)_4$	0.154			17750.00	2.73	
THF		95		109.79	10.43	
Water		10		0	0	
Dichloromethane			199	53.58	10.66	
$MgSO_4$			1	144.20	0.14	
Ethyl acetate			60	80.16	4.81	
Hexane			220	117.91	25.94	
Silica gel 60			263	62.20	16.36	
Total						**420.22**

Table S06 Materials quatities and cost for the synthesis of 1 g of HTM **17**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
4-iodoanisole	7.28			804.00	5.85	118.20
Aniline	0.53			160.47	0.09	
1,10-phenanthroline	0.45			2995.00	1.35	
Copper iodide	0.48			285.00	0.14	
KOH	5.62			47.60	0.27	
Toulene		26		69.48	1.81	
Water			231	0	0	
$MgSO_4$			2.31	144.20	0.33	
Dichloromethane			245	53.58	13.13	
Hexane			487	117.91	57.42	
Silica gel 60			608	62.20	37.82	
N-bromosuccinimide	2.31			117.50	0.16	153.87
THF		7		109.79	0.77	
Dichloromethane		527		53.58	28.24	
Water			265	0	0	
$MgSO_4$			2.65	144.20	0.38	
Dichloromethane			281	53.58	15.06	
Hexane			559	117.91	65.91	
Silica gel 60			697	62.20	43.35	
Bis(pinacolato)-diboron	2.63			8100.00	21.30	162.52
$Pd(dppf)Cl_2$	0.51			28640.00	14.61	
CH_3COOK	2.04			63.00	0.13	
DMSO		42		98.64	4.14	
Water		214		0	0	
Dichloromethane			425	53.58	22.77	
Dichloromethane			397	53.58	21.27	
Hexane			367	117.91	43.27	
Silica gel 60			563	62.20	35.02	
2-Indolinone	0.50			6160.00	3.08	49.08
$POCl_3$	4.13			56.41	0.23	
NaOH			2	53.20	0.11	
Methanol			65	60.18	3.91	
Dichloromethane			435	53.58	23.31	
Silica gel 60			216	62.20	13.44	
Acetone			65	76.99	5.00	
Sodium hydride	0.068			2200.00	0.15	64.90
1-iodohexane	2.03			526.00	1.07	
DMF		16		120.76	1.93	
Water		107		0	0	
Dichloromethane			213	53.58	11.41	
$MgSO_4$			1.07	144.20	0.15	
Dichloromethane			113	53.58	6.05	
Hexane			226	117.91	26.65	
Silica gel 60			281	62.20	17.48	

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N-bromosuccinimide	1.03			117.50	0.12	80.04
DMF		15		120.76	1.81	
Chloroform		138		49.66	6.85	
Dichloromethane			244	53.58	13.07	
$MgSO_4$			1.23	144.20	0.18	
Dichloromethane			65	53.58	3.48	
Hexane			292	117.91	34.43	
Silica gel 60			323	62.20	20.09	
$Pd(PPh_3)_4$	0.37			17750.00	6.57	67.28
K_2CO_3	2.26			142.00	0.32	
THF		36		109.79	3.95	
Water		100		0	0	
Dichloromethane			199	53.58	10.66	
Dichloromethane			318	53.58	17.04	
Hexane			105	117.91	12.38	
Silica gel 60			263	62.20	16.36	
Total						**695.87**

Table S07 Materials quatities and cost for the synthesis of 1 g of HTM **18**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
2-Indolinone	0.34			6160.00	2.09	34.14
$POCl_3$	2.81			56.41	0.16	
NaOH			1.37	53.20	0.07	
Methanol			56	60.18	3.37	
Dichloromethane			297	53.58	15.91	
Silica gel 60			147	62.20	9.14	
Acetone			44	76.99	3.39	
Sodium hydride	0.068			2200.00	0.15	44.30
1-iodohexane	1.38			526.00	0.73	
DMF		11		120.76	1.33	
Water		73		0	0	
Dichloromethane			145	53.58	7.77	
$MgSO_4$			0.73	144.20	0.11	
Dichloromethane			77	53.58	4.13	
Hexane			154	117.91	18.16	
Silica gel 60			192	62.20	11.94	
N-bromosuccinimide	0.68			117.50	0.08	54.65
DMF		10		120.76	1.21	
Chloroform		94		49.66	4.67	
Dichloromethane			167	53.58	8.95	
$MgSO_4$			0.84	144.20	0.12	
Dichloromethane			45	53.58	2.41	
Hexane			199	117.91	23.46	
Silica gel 60			221	62.20	13.75	
4,4-Dimethoxydiphenylamine	0.92			54900.00	50.51	112.75
t-BuONa	0.48			315.00	0.15	
$Pd(OAc)_2$	0.12			25550.00	3.07	
$(t\text{-}Bu)_3P$	0.051			9372.82	0.48	
Toulene		14		69.48	0.97	
Dichloromethane			199	53.58	10.66	
$MgSO_4$			1	144.20	0.14	
Acetone			32	76.99	2.46	
Hexane			237	117.91	27.94	
Silica gel 60			263	62.20	16.36	
Total						**245.84**

Table S08 Materials quatities and cost for the synthesis of 1 g of HTM **26**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
Isopropyl magnesium chloride solution	5.63			164.10	0.92	202.48
6,13-pentacenequinone	0.59			124000.00	73.16	
Triisopropylsilyl acetylene	2.12			10800.00	22.90	
THF		10.00		109.79	1.10	
HCl			2	210.81	0.42	
$SnCl_2.2H_2O$			12.35	419.00	5.17	
Dichloromethane			78	53.58	4.18	
hexane			264	117.91	31.13	
hexane			237	117.91	27.94	
Dichloromethane			53	53.58	2.84	
Silica gel 60			526	62.20	32.72	
Total						**202.48**

Table S09 Materials quatities and cost for the synthesis of 1 g of HTM **27**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
Carbazole	2.44			327.60	0.80	80.37
Potassium hydroxide	2.46			47.60	0.12	
Bromoethane	4.77			66.20	0.32	
DMF		23		90.04	2.07	
NaCl			292	29.24	8.54	
Water			244	0.00	0.00	
Dichloromethane			485	53.58	25.99	
$MgSO_4$			2.44	144.20	0.35	
Ethanol			193	218.63	42.20	
N-Bromosuccinimide	2.23			117.50	0.26	57.96
DMF		31		90.04	2.79	
NaCl			336	29.24	9.82	
Water			281	0.00	0.00	
Dichloromethane			558	53.58	29.90	
$MgSO_4$			2.81	144.20	0.41	
Methanol			200.00	60.18	12.04	
THF			25.00	109.79	2.74	
n-butyllithium (1.6M)	6.53			238.97	1.56	50.30
2-isopropoxy-4,4,5,5-tetramethyl -1,3,2-dioxaborolane	3.82			1276.32	4.88	
THF		100		109.79	10.98	
Water			168	0.00	0.00	
Dichloromethane			334	53.58	17.90	
NaCl			201	29.24	5.88	
$MgSO_4$			1.68	144.20	0.24	
Methanol			120	60.18	7.22	
THF			15	109.79	1.65	
K_2CO_3	3.96			142	0.56	65.96
2,5-dibromo-3,4-ethylenedioxythiophene	0.78			237	0.18	
$Pd(PPh_3)_4$	0.15			17750	2.66	
Toulene		25		69.48	1.74	
THF		25		109.79	2.74	
Water			14	0.00	0.00	
Dichloromethane			199	53.58	10.66	
Water			100	0.00	0.00	
NaCl			120	29.24	3.51	
Na_2SO_4			1	115.80	0.12	
Petroleum ether			181	99.12	17.94	
Dichloromethane			177	53.58	9.48	
Silica gel 60			263	62.20	16.36	
Total						**254.60**

Table S10 Materials quatities and cost for the synthesis of 1 g of HTM **28**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
Methoxybenzene/anisole	1.28			125.63	0.16	32.67
KI, potassium iodide	2.05			274.00	0.56	
Methanol		16		60.18	0.96	
H_2SO_4		2		38.59	0.08	
H_2O_2		0.77		526.67	0.41	
Water			51	0.00	0	
DCM			358	53.58	19.18	
Na_2SO_4			1.80	115.80	0.21	
Ethyl acetate			15	80.16	1.20	
Petroleum ether			100	99.12	9.91	
Aniline	0.29			160.47	0.05	59.45
1,10-phenanthroline	0.11			2995.00	0.33	
CuCl	0.06			125.40	0.01	
KOH	1.38			47.60	0.07	
Toulene		5		69.48	0.35	
Acetic acid		1		55.10	0.06	
Toulene		3		69.48	0.21	
Water			11	0.00	0.00	
Na_2SO_4			1.34	115.80	0.16	
Ethyl acetate			44	80.16	3.53	
Petroleum ether			331	99.12	32.81	
silica gel 60			352	62.20	21.89	
N-bromosuccinimide	0.78			117.50	0.09	88.81
THF		4		109.79	0.44	
Dichloromethane			304	53.58	16.29	
Water			153	0.00	0.00	
$MgSO_4$			1.53	144.20	0.22	
Dichloromethane			162	53.58	8.68	
Hexane			323	117.91	38.08	
Silica gel 60			402	62.20	25.00	
n-butyllithium (1.6M)	2.17			238.97	0.52	54.47
Trimethyl borate, $B(OCH_3)_3$	0.51			93.56	0.05	
THF		3		109.79	0.33	
Water			114	0.00	0	
HCl			2	80.65	0.16	
Dichloromethane			36	53.58	1.93	
Na_2SO_4			1.14	115.80	0.13	
Ethyl acetate			206	80.16	16.51	
Dichloromethane			302	53.58	16.18	
Silica gel 60			300.00	62.20	18.66	
3,4-ethylenedioxythiophene	0.23			7110.00	1.64	62.18
N-bromosuccinimide	0.58			117.50	0.07	
THF		29		109.79	3.18	
K_2CO_3	1.07			142.00	0.15	
$Pd(PPh_3)_4$	0.09			17750.00	1.58	
Water			100	0.00	0.00	
Dichloromethane			199	53.58	10.66	
$MgSO_4$			1	144.20	0.14	
Dichloromethane			530	53.58	28.40	
Silica gel 60			263	62.20	16.36	
Total						**297.58**

Table S11 Materials quatities and cost for the synthesis of 1 g of HTM **29**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
4-iodoanisole	0.51			804.00	0.41	28.49
Carbazole	0.33			327.60	0.11	
CuI	0.06			285.00	0.02	
1,10-phenanthroline	0.05			2995.00	0.16	
K_2CO_3	0.28			142.00	0.04	
DMF		5		120.76	0.60	
Dichloromethane			99	53.58	5.30	
Na_2SO_4			0.50	115.80	0.06	
Petroleum ether			124	99.12	12.29	
Ethyl acetate			16	80.16	1.28	
silica gel 60			132	62.20	8.21	
N-bromosuccinimide	0.72			117.50	0.08	12.31
DMF		6		120.76	0.72	
Ethanol			53	218.63	11.59	
4,4-dimethoxydiphenylamine	0.89			54900.00	48.86	107.77
t-BuONa, sodium tert-butoxide	0.38			307.00	0.12	
Toulene		19		69.48	1.32	
$(t\text{-}Bu)_3P$, tri tert butylphosphine	0.038			34500.00	1.31	
tris(dibenzylideneacetone)dipalladium(0), $Pd_2(dBa)_3$	0.086			14900.00	1.28	
Ethyl acetate			135	80.16	10.82	
$MgSO_4$			1	144.20	0.14	
Petroleum ether			181	99.12	17.94	
Ethyl acetate			120	80.16	9.62	
Silica gel 60			263	62.20	16.36	
Total						**148.57**

Table S12 Materials quatities and cost for the synthesis of 1 g of HTM **30**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
Carbazole	0.35			327.60	0.11	11.55
N-bromosuccinimide	0.83			117.50	0.10	
DMF		7		120.76	0.85	
Ethanol			48	218.63	10.49	
NaH	0.068			2200	0.15	1.24
Benzyl bromide	0.32			377	0.12	
DMF		8		120.76	0.97	
Water			78	0.00	0.00	
4,4-dimethoxydiphenylamine	0.95			54900.00	52.16	106.29
t-BuONa, sodium tert-butoxide	0.21			307.00	0.06	
Tri tert butylphosphine,$(t\text{-}Bu)_3P$,	0.057			34500.00	1.97	
tris(dibenzylideneacetone)dipalladium(0), $Pd_2(dBa)_3$	0.069			14900.00	1.03	
Toulene		8.00		69.48	0.56	
Dichloromethane			203	53.58	10.88	
$MgSO_4$			1.02	144.20	0.15	
Petroleum ether			181	99.12	17.94	
Ethyl acetate			61	80.16	4.89	
Silica gel 60			268	62.20	16.67	
KOtBu, potssium tert-butoxide	1.61			508.87	0.82	37.69
DMSO		46		98.64	4.54	
Water			70	0.00	0.00	
Petroleum ether			161	99.12	15.96	
Ethyl acetate			53	80.16	4.25	
Silica gel 60			195	62.20	12.13	
4,4'-diiodobiphenyl	0.29			2572	0.75	59.68
CuI	0.05			285.00	0.01	
1,10-phenanthroline	0.04			2995.00	0.13	
K_2CO_3	0.33			142.00	0.05	
DMF		32		120.76	3.86	
Ethyl acetate			135	80.16	10.82	
$MgSO_4$			1	144.20	0.14	
Petroleum ether			181	99.12	17.94	
Ethyl acetate			120	80.16	9.62	
Silica gel 60			263	62.20	16.36	
Total						**216.46**

Table S13 Materials quatities and cost for the synthesis of 1 g of HTM **31**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
3,6-dibromocarbazole	0.40			19100.00	7.64	22.83
1,2-bis(bromomethyl)benzene	0.16			1920.00	0.31	
KOH	0.21			47.60	0.01	
THF		4		109.79	0.44	
Water			84	0.00	0.00	
Ethanol			66	218.63	14.43	
4,4-dimethoxydiphenylamine	1.27			54900.00	69.72	145.59
$Pd(OAc)_2$, palladium(ii) acetate	0.05			25550.00	1.28	
t-BuONa, sodium tert-butoxide	5.33			307.00	1.64	
tri-tert-butylphosphonium tetrafluoroborate	0.087			24500.00	2.13	
Toulene		96		69.48	6.67	
Water			50	0.00	0.00	
Ethyl acetate			135	80.16	10.82	
Water			150	0.00	0.00	
Na_2SO_4			1	115.80	0.12	
Acetone			79	76.99	6.08	
Hexane			198	117.91	23.35	
Silica gel 60			263	62.20	16.36	
Acetone			16	76.99	1.23	
Methanol			63	60.18	3.79	
Methanol			40	60.18	2.41	
Total						**168.42**

Table S14 Materials quatities and cost for the synthesis of 1 g of HTM **33**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
HNO_3	5			211.49	1.06	25.78
Acetic acid glacial	3			55.1	0.17	
4,4-dibromobiphenyl	1.93			696	1.34	
Dichloromethane		7		53.58	0.38	
Acetic anhydride	35			73.52	2.57	
Water			300	0.00	0.00	
NaOH			7	53.20	0.40	
Dichloromethane			170	53.58	9.11	
Water			64	0.00	0.00	
NaCl			219	29.24	6.40	
$MgSO_4$			1.83	144.20	0.26	
Methanol			51	60.18	3.07	
Methanol			17	60.18	1.02	
PPH_3,triphenylphosphine	3.36			200	0.67	37.42
1,2-dichlorobenzene		13		70.14	0.91	
P950 ligroin,petroleum spirits			376	40.89	15.37	
silica gel 60			329	62.20	20.46	
NaH	0.11			2200	0.24	106.81
p-toulenesulfonyl chloride	1.10			81.6	0.09	
THF		34		109.79	3.73	
Ethyl acetate			32	80.16	2.57	
NH_4CL			16	79.5	1.27	
Ethyl acetate			216	80.16	17.31	
NaCl			192	29.24	5.61	
$MgSO_4$			1.60	144.20	0.23	
Hexane			402	117.91	47.40	
Ethyl acetate			27	80.16	2.16	
Silica gel 60			421	62.20	26.19	
4,4-dimethoxydiphenylamine	1.59			54900.00	87.29	196.88
$Pd(OAc)_2$, palladium(ii) acetate	0.035			25550.00	0.89	
Tri-t-butylphosphine	0.13			34500.00	4.49	
Toulene		27		69.48	1.88	
Water			30	0.00	0.00	
Ethyl acetate			225	80.16	18.04	
NaCl			199	29.24	5.82	
$MgSO_4$			1.67	144.20	0.24	
Hexane			365	117.91	43.04	
Ethyl acetate			100	80.16	8.02	
Silica gel 60			437	62.20	27.18	

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1,3,5-tribromobenzene	0.27			1950.00	0.53	67.23
$Pd(OAc)_2$, palladium(ii) acetate	0.059			25550.00	1.51	
Tri-tert-butylphosphine	0.1			34500.00	3.45	
t-BuONa, sodium tert-butoxide	1.24			307.00	0.38	
Toulene		16		69.48	1.11	
Water			20	0.00	0.00	
Ethyl acetate			135	80.16	10.82	
NaCl			120	29.24	3.51	
$MgSO_4$			1	144.20	0.14	
Dichloromethane			312	53.58	16.72	
Hexane			103	117.91	12.14	
Ethyl acetate			7	80.16	0.56	
Silica gel 60			263	62.20	16.36	
Total						**434.12**

Table S15 Materials quatities and cost for the synthesis of 1 g of HTM **34**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
HNO_3	5			211.49	1.06	21.82
Acetic acid glacial	3.5			55.1	0.19	
4,4-dibromobiphenyl	1.99			696	1.39	
Dichloromethane		7		53.58	0.38	
Acetic anhydride	36			73.52	2.65	
Water			310	0.00	0.00	
NaOH			7.74	53.20	0.41	
Dichloromethane			880	53.58	4.72	
Water			66	0.00	0.00	
NaCl			226	29.24	6.61	
$MgSO_4$			1.89	144.20	0.27	
Methanol			52	60.18	3.13	
Methanol			17	60.18	1.02	
PPH_3,triphenylphosphine	3.47			200	0.69	38.63
1,2-dichlorobenzene		14		70.14	0.98	
P950 ligroin,petroleum spirits			388	40.89	15.87	
silica gel 60			339	62.20	21.09	
NaH	0.11			2200	0.24	111.31
p-toulenesulfonyl chloride	1.14			81.6	0.09	
THF		36		109.79	3.95	
Ethyl acetate			41	80.16	3.29	
NH_4CL			17	79.5	1.35	
Ethyl acetate			225	80.16	18.04	
NaCl			199	29.24	5.82	
$MgSO_4$			1.66	144.20	0.24	
Hexane			375	117.91	44.22	
Ethyl acetate			86	80.16	6.89	
Silica gel 60			437	62.20	27.18	
4,4-dimethoxydiphenylamine	1.66			54900.00	91.13	206.04
$Pd(OAc)_2$, palladium(ii) acetate	0.037			25550.00	0.95	
Tri-t-butylphosphine	0.14			34500.00	4.83	
Toulene		29		69.48	2.01	
Water			40	0.00	0.00	
Ethyl acetate			235	80.16	18.84	
NaCl			208	29.24	6.08	
$MgSO_4$			1.74	144.20	0.25	
Hexane			382	117.91	45.04	
Ethyl acetate			105	80.16	8.42	
Silica gel 60			458	62.20	28.49	

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Tris(4-bromophenyl)amine	0.43			10800.00	4.64	72.34
$Pd(OAc)_2$, palladium(ii) acetate	0.062			25550.00	1.58	
Tri-tert-butylphosphine	0.11			34500.00	3.80	
t-BuONa, sodium tert-butoxide	1.04			307.00	0.32	
Toulene		25		69.48	1.74	
Water			35	0.00	0.00	
Ethyl acetate			135	80.16	10.82	
NaCl			120.00	29.24	3.51	
$MgSO_4$			1.00	144.20	0.14	
Dichloromethane			312.00	53.58	16.72	
Hexane			103.000	117.91	12.14	
Ethyl acetate			7.000	80.16	0.56	
Silica gel 60			263.000	62.20	16.36	
Total						**450.13**

Table S16 Materials quatities and cost for the synthesis of 1 g of HTM **38**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
4-bromo-4,4-dimethoxytriphenylamine	2.19			79800.00	174.76	253.07
n-butyllithium (1.6M)	3			238.97	0.72	
Trimethyl borate, $B(OCH_3)_3$	6			93.56	0.56	
THF		5		109.79	0.55	
Water			10	0.00	0.00	
HCl			2	80.65	0.16	
Dichloromethane			51	53.58	2.73	
Na_2SO_4			1.63	115.80	0.19	
Ethyl acetate			294	80.16	23.57	
Dichloromethane			432	53.58	23.15	
Silica gel 60			429	62.20	26.68	
Tetrabromothiophene	0.42			12920.00	5.43	68.16
K_2CO_3	2.87			142.00	0.41	
$Pd(PPh_3)_4$	0.12			17750.00	2.13	
THF		37		109.79	4.06	
Water			40	0.00	0.00	
Dichloromethane			199	53.58	10.66	
Water			100	0.00	0.00	
$MgSO_4$			1	144.20	0.14	
Dichloromethane			424	53.58	22.72	
Hexane			53	117.91	6.25	
Silica gel 60			263	62.20	16.36	
Total						**321.23**

Table S17 Materials quatities and cost for the synthesis of 1 g of HTM **39**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
4-bromo-4,4-dimethoxytriphenylamine	1.92			79800.00	153.22	221.51
n-butyllithium (1.6M)	2.71			238.97	0.65	
Trimethyl borate, $B(OCH_3)_3$	0.63			93.56	0.06	
THF		4		109.79	0.44	
Water			10	0.00	0.00	
HCl			1.50	80.65	0.12	
DCM			45	53.58	2.41	
Na_2SO_4			1.43	115.80	0.17	
Ethyl acetate			259	80.16	20.76	
Dichloromethane			379	53.58	20.31	
Silica gel 60			376	62.20	23.39	
2,3-dibromothiophene	0.24			15660.00	3.76	35.23
Bis(benzonitrile)palladium(II)chloride, $PdCl_2(PhCN)_2$	0.01			40850.00	0.47	
Potassium fluoride	0.23			392.00	0.09	
$AgNO_3$	0.68			2240.00	1.52	
DMSO		7		98.64	0.69	
Diethyl ether			28	112.18	3.14	
Water			40	0.00	0.00	
$MgSO_4$			0.54	144.20	0.08	
Dichloromethane			29	53.58	1.55	
Hexane			128	117.91	15.09	
Silica gel 60			142	62.20	8.83	
K_2CO_3	2.52			142.00	0.36	61.87
$Pd(PPh_3)_4$	0.105			17750.00	1.86	
THF		32		109.79	3.51	
Water			40	0.00	0.00	
Dichloromethane			199	53.58	10.66	
Water			100	0.00	0.00	
$MgSO_4$			1	144.20	0.14	
Dichloromethane			424	53.58	22.72	
Hexane			53	117.91	6.25	
Silica gel 60			263	62.20	16.36	
Total						318.61

Table S18 Materials quatities and cost for the synthesis of 1 g of HTM **40**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
3,4-dimethoxythiophene	0.41			37600.00	15.42	61.86
p-Toulenesulphonic acid	0.04			118.40	0.00	
Pentaerythritol	2.32			1100.00	25.52	
Toulene		44		69.48	3.06	
Water			52	0.00	0.00	
Dichloromethane			103	53.58	5.52	
Silica gel 60			137	62.20	8.52	
Chloroform			77	49.66	3.82	
N-bromosuccinimide	1.39			117.50	0.16	13.78
DMF		29		90.04	2.61	
Chloroform		46		49.66	2.28	
Water			206	0.00	0.00	
Water			81	0.00	0.00	
Methanol			64	60.18	3.85	
THF			18	109.79	1.98	
Methanol			48	60.18	2.89	
4-bromoaniline	3.55			455.00	1.62	231.60
4-iodoanisole	10.14			804.00	8.15	
CuI	0.20			285.00	0.06	
KOH	9.04			47.60	0.43	
1,10-phenanthroline	0.19			2995.00	0.57	
Xylene		18		79.53	1.69	
Dichloromethane			187	53.58	10.02	
Water			424	0.00	0.00	
$MgSO_4$			4.52	144.20	0.65	
Dichloromethane			1198	53.58	64.19	
Hexane			596	117.91	70.27	
Silica gel 60			1189	62.20	73.96	
Bis(pinacolato)-diboron	3.59			8100.00	29.08	209.51
Potassium acetate	3.47			63.00	0.22	
Tris(dibenzylideneacetone)dipalladium(0), $Pd_2(dBa)_3$	0.057			14900.00	0.85	
2-Dicyclohexylphosphino-2',4',6'-Triisopropylbiphenyl, X-Phos	0.11			7980.00	0.88	
Dioxane		94		102.03	9.23	
$MgSO_4$			3.4	144.20	0.49	
Dichloromethane			225	53.58	12.06	
Hexane			448	117.91	52.82	
Dichloromethane			901	53.58	48.28	
Silica gel 60			894	62.20	55.61	
K_2CO_3	8.90			142.00	1.26	62.41
$Pd(PPh_3)_4$	0.32			17750.00	5.68	
Toulene		84		69.48	5.84	
Water			100	0.00	0.00	
NaCl			120	29.24	3.51	
Hexane			132	117.91	15.56	
Dichloromethane			265	53.58	14.20	
Silica gel 60			263	62.20	16.36	
Total						**579.16**

Table S19 Materials quatities and cost for the synthesis of 1 g of HTM **41**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
3,3'-dibromo-2,2'-bithiophene	0.94			42000.00	39.48	50.24
Diisopropylamine,DIPA	0.69			123.55	0.09	
n-butyllithium (1.6M)	2.74			238.97	0.65	
Trimethylsilyl chloride	0.91			126.75	0.12	
THF		36		109.79	3.95	
Water			111	0.00	0.00	
Diethyl ether			17	112.18	1.91	
NaCl			133	29.24	3.89	
$MgSO_4$			1.11	144.20	0.16	
n-butyllithium (1.6M)	1.99			238.97	0.48	33.40
N,N-dimethylcarbamyl chloride	0.25			203.00	0.05	
NH_4CL			0.5	79.5	0.04	
THF		10		109.79	1.10	
Petroleum ether			28	99.12	2.78	
$MgSO_4$			0.66	144.20	0.10	
Dichloromethane			87	53.58	4.66	
Petroleum ether			135	99.12	13.38	
silica gel 60			174	62.20	10.82	
N-bromosuccinimide	0.61			117.50	0.07	10.23
THF		12		109.79	1.32	
Dichloromethane			74	53.58	3.96	
Water			31	0.00	0.00	
NaCl			18	29.24	0.53	
$MgSO_4$			0.56	144.20	0.08	
Methanol			71	60.18	4.27	
2-bromothiophene	0.56			526.00	0.29	56.48
Mg	0.14			158.50	0.02	
$PdCl_2(dppf).CH_2Cl_2$ complex	0.02			21000.00	0.44	
2,3-dibromothiophene	0.80			15660.00	12.53	
diethyl ether		5		112.18	0.56	
Methanol			1	60.18	0.06	
Na_2SO_4			0.74	115.80	0.09	
Silica gel 60			74	62.20	4.60	
Diethyl ether			52	112.18	5.83	
Silica gel 60			195	62.20	12.13	
Petroleum ether			201	99.12	19.92	
N-bromosuccinimide	1.09			117.50	0.13	38.57
Chloroform		10		49.66	0.50	
Acetic acid glacial		5		55.1	0.28	
Dichloromethane			98	53.58	5.25	
Water			15	0.00	0.00	
$NaHCO_3$			0.37	52.70	0.02	
Water			7	0.00	0.00	
NaCl			9	29.24	0.26	
Na_2SO_4			0.74	115.80	0.09	
Petroleum ether			201	99.12	19.92	
silica gel 60			195	62.20	12.13	

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n-butyllithium (1.6M)	1.48			238.97	0.35	34.66
Trimethylsilyl chloride	0.38			126.75	0.05	
Diethyl ether		11		112.18	1.23	
Water			64	0.00	0.00	
Diethyl ether			36	112.18	4.04	
Water			34	0.00	0.00	
NaCl			41	29.24	1.20	
$MgSO_4$			0.64	144.20	0.09	
Petroleum ether			174	99.12	17.25	
Silica gel 60			168	62.20	10.45	
n-butyllithium (1.6M)	0.65			238.97	0.16	45.64
NH_4CL			5.19	167.64	93.88	
Diethyl ether		17		79.5	0.41	
Water			21	112.18	1.91	
NaCl			13	0.00	0.00	
$MgSO_4$			0.97	29.24	0.38	
Petroleum ether			147	144.20	0.14	
Dichloromethane			228	99.12	14.57	
Silica gel 60			255	53.58	12.22	
N-bromosuccinimide	0.59			117.50	0.07	43.73
Dichloromethane		26		53.58	1.39	
$Na_2S_2O_3$			11.70	111.00	1.30	
Dichloromethane			147	53.58	7.88	
Water			20	0.00	0.00	
NaCl			11.73	29.24	0.34	
$MgSO_4$			0.74	144.20	0.11	
Petroleum ether			101	99.12	10.01	
Dichloromethane			196	53.58	10.50	
Silica gel 60			195	62.20	12.13	
Boron trifluoride diethyl ether, $BF_3.Et_2O$	2.06			86.00	0.18	71.33
Dichloromethane		742		53.58	39.76	
Ethanol		29		218.63	6.34	
Water		187		0.00	0.00	
Dichloromethane			91	53.58	4.88	
Water			344	0.00	0.00	
$MgSO_4$			0.46	144.20	0.07	
Petroleum ether			94	99.12	9.32	
Dichloromethane			61	53.58	3.27	
Silica gel 60			121	62.20	7.53	
4-bromo-4,4-dimethoxytriphenylamine	1.24			79800.00	98.95	174.61
Bis(pinacolato)-diboron	1.23			8100.00	9.96	
$PdCl_2$(dppf), [1,1'-Bis(diphenylphosphino) ferrocene] dichloropalladium(II) (1:1)	0.24			28640.00	6.87	
Potassium acetate	0.95			63.00	0.06	
DMSO		20		98.64	1.97	
DCM			199	53.58	10.66	
DCM			265	53.58	14.20	
Hexane			132	117.91	15.56	
Silica gel 60			263	62.20	16.36	

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$Pd(PPh_3)_4$	0.082			17750.00	1.46	74.98
K_2CO_3	1			142.00	0.14	
THF		21		109.79	2.31	
Ethyl acetate			256	80.16	20.52	
Water			379	0.00	0.00	
NaCl			227	29.24	6.64	
$MgSO_4$			1	144.20	0.14	
Petroleum ether			202	99.12	20.02	
Ethyl acetate			89	80.16	7.13	
Triethylamine			3	86.78	0.26	
Silica gel 60			263	62.20	16.36	
Total						**633.88**

Table S20 Materials quatities and cost for the synthesis of 1 g of HTM **42**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
Bromine	2.30			88.65	0.20	39.26
2,2-bithiophene	0.66			16950.00	11.19	
Acetic acid glacial		2.48		55.1	0.14	
Chloroform		8		49.66	0.40	
KOH			0.59	47.60	0.03	
Chloroform			35	49.66	1.74	
Water			147	0.00	0.00	
$MgSO_4$			1.47	144.20	0.21	
Ethanol			116	218.63	25.36	
Zn dust	0.77			10460.00	8.05	43.83
Ethanol		12		218.63	2.62	
Water		2		0.00	0.00	
Acetic acid glacial		4		55.1	0.22	
HCl		0.004		80.65	0.00	
Ethanol			70	218.63	15.30	
Water			7	0.00	0.00	
Diethyl ether			94	112.18	10.54	
Water			89	0.00	0.00	
$MgSO_4$			0.89	144.20	0.13	
Hexane			59	117.91	6.96	
n-butyllithium (1.6M)	1.50			238.97	0.36	31.36
Dichlorodihexylsilane	0.74			14240.00	10.54	
THF		57		109.79	6.26	
NH_4CL			10.57	79.5	0.84	
Diethyl ether			19	112.18	2.13	
Water			68	0.00	0.00	
$MgSO_4$			0.68	144.20	0.10	
Silica gel 60			179	62.20	11.13	
N-bromosuccinimide	0.74			117.50	0.09	48.23
DMF		14		90.04	1.26	
Water			19	0.00	0.00	
Diethyl ether			40	112.18	4.49	
Water			19	0.00	0.00	
$MgSO_4$			0.89	144.20	0.13	
Hexane			235	117.91	27.71	
Silica gel 60			234	62.20	14.55	
4-bromo-4,4-dimethoxytriphenylamine	0.66			79800.00	52.67	72.43
n-butyllithium (2.5M)	0.78			110.63	0.09	
Trimethyltin chloride	2.81			1356.28	3.81	
THF		30		109.79	3.29	
NaCl			96	29.24	2.81	
Diethyl ether			86	112.18	9.65	
$MgSO_4$			0.81	144.20	0.12	
$Pd(PPh_3)_4$	0.27			17750.00	4.79	31.65
Toulene		149		69.48	10.35	
$MgSO_4$			1	144.20	0.14	
Silica gel 60			263	62.20	16.36	
Total						266.76

Table S21 Materials quatities and cost for the synthesis of 1 g of HTM **43**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
Bromine	2.43			88.65	0.22	41.22
2,2-bithiophene	0.69			16950.00	11.70	
Acetic acid glacial		2.62		55.1	0.14	
Chloroform		8		49.66	0.40	
KOH			0.62	47.60	0.03	
Chloroform			37	49.66	1.84	
Water			155	0.00	0.00	
$MgSO_4$			1.55	144.20	0.22	
Ethanol			122	218.63	26.67	
Zn dust	0.81			10460.00	8.47	46.38
Ethanol		13		218.63	2.84	
Water		2		0.00	0.00	
Acetic acid glacial		4		55.1	0.22	
HCl		0.0035		80.65	0.00	
Ethanol			74	218.63	16.18	
Water			7	0.00	0.00	
Diethyl ether			100	112.18	11.22	
Water			94	0.00	0.00	
$MgSO_4$			0.94	144.20	0.14	
Hexane			62	117.91	7.31	
n-butyllithium (1.6M)	1.57			238.97	0.38	21.50
Dichlorodiphenylsilane	0.73			256.00	0.19	
THF		60		109.79	6.59	
NH_4CL			11.07	79.5	0.88	
Diethyl ether			20	112.18	2.24	
Water			68	0.00	0.00	
$MgSO_4$			0.68	144.20	0.10	
Silica gel 60			179	62.20	11.13	
N-bromosuccinimide	0.69			117.50	0.08	44.00
DMF		13		90.04	1.17	
Water			18	0.00	0.00	
Diethyl ether			37	112.18	4.15	
Water			18	0.00	0.00	
$MgSO_4$			0.81	144.20	0.12	
Hexane			214	117.91	25.23	
Silica gel 60			213	62.20	13.25	
4-bromo-4,4-dimethoxytriphenylamine	0.53			79800.00	42.29	57.88
n-butyllithium (2.5M)	0.62			110.63	0.07	
Trimethyltin chloride	2.23			1356.28	3.02	
THF		23		109.79	2.53	
NaCl			77	29.24	2.25	
Diethyl ether			68	112.18	7.63	
$MgSO_4$			0.64	144.20	0.09	
$Pd(PPh_3)_4$	0.21			17750.00	3.73	28.43
Toulene		118		69.48	8.20	
$MgSO_4$			1	144.20	0.14	
Silica gel 60			263	62.20	16.36	
Total						239.41

Table S22 Materials quatities and cost for the synthesis of 1 g of HTM **44**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
3-bromothiophene	2.35			2735.00	6.43	47.90
n-butyllithium solution	4.13			110.63	0.46	
$CuCl_2$	2			171.50	0.34	
Diethyl ether		8		112.18	0.90	
Water			20	0.00	0.00	
Diethyl ether			17	112.18	1.91	
$MgSO_4$			1.56	144.20	0.22	
Silica gel 60			410	62.20	25.50	
Hexane			103	117.91	12.14	
N-bromosuccinimide	8.34			117.50	0.98	92.94
THF		134		109.79	14.71	
Hexane			92	117.91	10.85	
Hexane			369	117.91	43.51	
Silica gel 60			368	62.20	22.89	
4-bromo-4,4-dimethoxytriphenylamine	6.86			79800.00	547.43	790.93
n-butyllithium (1.6M)	9.71			238.97	2.32	
Trimethyl borate, $B(OCH_3)_3$	2.27			93.56	0.21	
THF		14		109.79	1.54	
Water			20	0.00	0.00	
HCl			2	80.65	0.16	
Dichloromethane			161	53.58	8.63	
Na_2SO_4			5.11	115.80	0.59	
Ethyl acetate			922	80.16	73.91	
Dichloromethane			1354	53.58	72.55	
Silica gel 60			1344	62.20	83.60	
$Pd(PPh_3)_4$	0.64			17750.00	11.36	70.24
K_2CO_3	4.41			142.00	0.63	
Toulene		28		69.48	1.95	
Dichloromethane			199	53.58	10.66	
Dichloromethane			353	53.58	18.91	
Hexane			88	117.91	10.38	
Silica gel 60			263	62.20	16.36	
Total						1002.01

Table S23 Materials quatities and cost for the synthesis of 1 g of HTM **45**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
Trichlorobenzene	0.88			673.00	0.59	96.90
Iodine chips	6.16			456.00	2.81	
Periodic acid	1.84			2470.00	4.54	
Sulfuric acid		107		38.59	4.13	
Water			214	0.00	0.00	
Sodium bisulfite			317	102.50	32.49	
Methanol			169	60.18	10.17	
Ether			151	129.89	19.61	
Dioxane			221	102.03	22.55	
Diisopropylamine,DIPA	2.77			123.55	0.47	44.56
THF		31		109.79	3.40	
$Pd(PPh_3)_4$	0.80			17750.00	14.20	
CuI	0.13			285.00	0.04	
Trimethylsilylacetylene	3.27			1260.00	4.12	
Water			37	0.00	0.00	
Chloroform			37	49.66	1.84	
NaCl			134	29.24	3.92	
$MgSO_4$			2.09	144.20	0.30	
Hexane			138	117.91	16.27	
Sodium sulfide nonahydrate	6.41			201.00	1.29	83.87
N-methyl pyrrolidone		110		101.65	10.86	
NH_4Cl	38.30			79.50	3.04	
Chloroform			311	49.66	15.44	
NaCl			1436.40	29.24	42.00	
$MgSO_4$			0.68	144.20	0.10	
Silica gel 60			179	62.20	11.13	
N-bromosuccinimide	2.23			117.50	0.26	8.10
Chloroform		21		49.66	1.04	
Acetic acid glacial		7		55.1	0.39	
Chloroform			129	49.66	6.41	
Water			87	0.00	0.00	
4,4-dimethoxydiphenylamine	1.44			54900.00	79.06	142.88
Tris(dibenzylideneacetone)dipalladium(0), $Pd_2(dBa)_3$	0.11			14900.00	1.64	
2-Dicyclohexylphosphino-2',4',6'-Triisopropylbiphenyl, X-Phos	0.08			7980.00	0.66	
Toulene		105		69.48	7.30	
t-BuONa, sodium tert-butoxide	1.04			307.00	0.32	
Water			130	0.00	0.00	
Toulene			130	69.48	9.03	
Na_2SO_4			1	115.80	0.12	
Dichloromethane			530	53.58	28.40	
Silica gel 60			263	62.20	16.36	
Total						**376.30**

Table S24 Materials quatities and cost for the synthesis of 1 g of HTM **46**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
Trichlorobenzene	0.72			673.00	0.48	84.95
Iodine chips	5.07			456.00	2.31	
Periodic acid	1.52			2470.00	3.75	
Sulfuric acid		88		38.59	3.40	
Water			176	0.00	0.00	
Sodium bisulfite			260	102.50	26.65	
Methanol			169	60.18	10.17	
Ether			151	129.89	19.61	
Dioxane			182	102.03	18.57	
Diisopropylamine,DIPA	1.14			123.55	0.20	28.67
THF		13		109.79	1.43	
$Pd(PPh_3)_4$	0.38			17750.00	6.75	
CuI	0.05			285.00	0.02	
Trimethylsilylacetylene	1.34			1260.00	1.69	
Water			16	0.00	0.00	
Chloroform			70	49.66	3.48	
NaCl			283	29.24	8.27	
$MgSO_4$			0.86	144.20	0.12	
Hexane			57	117.91	6.72	
Sodium sulfide nonahydrate	0.86			132.11	113.62	70.13
N-methyl pyrrolidone		2.64		201.00	0.53	
NH_4Cl	45			101.65	4.46	
Chloroform			38.30	79.50	3.04	
NaCl			311	49.66	15.44	
$MgSO_4$			1436.40	29.24	42.00	
Silica gel 60			0.28	144.20	0.04	
N-bromosuccinimide	0.93			117.50	0.11	3.51
Chloroform		11		49.66	0.55	
Acetic acid glacial		4		55.1	0.22	
Chloroform			53	49.66	2.63	
Water			36	0.00	0.00	
Carbazole	0.72			327.60	0.24	23.65
N-bromosuccinimide	1.69			117.50	0.20	
DMF		13		120.76	1.57	
Ethanol			99	218.63	21.64	
NaH	0.14			2200	0.31	2.61
Benzyl bromide	0.66			377	0.25	
DMF		17		120.76	2.05	
Water			80	0.00	0.00	
4,4-dimethoxydiphenylamine	1.94			54900.00	106.51	228.84
t-BuONa, sodium tert-butoxide	0.92			307.00	0.28	
Tri tert butylphosphine,$(t\text{-}Bu)_3P$	0.12			34500.00	4.14	
Tris(dibenzylideneacetone)dipalladium(0), $Pd_2(dBa)_3$	0.24			14900.00	3.58	
Toulene		17		69.48	1.18	
Dichloromethane			413	53.58	22.13	
$MgSO_4$			2.08	144.20	0.30	
Petroleum ether			471	99.12	46.69	
Ethyl acetate			125	80.16	10.02	
Silica gel 60			547	62.20	34.02	

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KOtBu, potssium tert-butoxide	3.29			508.87	1.67	77.09
DMSO		95		98.64	9.37	
Water			144	0.00	0.00	
Petroleum ether			329	99.12	32.61	
Ethyl acetate			109	80.16	8.74	
Silica gel 60			397	62.20	24.69	
Tris(dibenzylideneacetone)dipalladium(0), $Pd_2(dBa)_3$	0.044			14900.00	0.66	72.13
2-Dicyclohexylphosphino-2',4',6'-Triisopropylbiphenyl, X-Phos	0.03			7980.00	0.27	
Toulene		42		69.48	2.92	
t-BuONa, sodium tert-butoxide	0.43			307.00	0.13	
Water			50	0.00	0.00	
Toulene			130	69.48	9.03	
Na_2SO_4			1	115.80	0.12	
Dichloromethane			530	53.58	28.40	
Silica gel 60			263	62.20	16.36	
Dichloromethane			263	53.58	14.09	
Ethyl acetate			2	80.16	0.16	
Total						**591.57**

Table S25 Materials quatities and cost for the synthesis of 1 g of HTM **47**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
Trichlorobenzene	1.56			673.00	1.05	171.78
Iodine chips	10.92			456.00	4.98	
Periodic acid	3.26			2470.00	8.05	
Sulfuric acid		190		38.59	7.33	
Water			379	0.00	0.00	
Sodium bisulfite			561	102.50	57.50	
Methanol			300	60.18	18.05	
Ether			268	129.89	34.81	
Dioxane			392	102.03	40.00	
Diisopropylamine,DIPA	2.45			123.55	0.42	59.65
THF		27		109.79	2.96	
$Pd(PPh_3)_4$	0.71			17750.00	12.60	
CuI	0.12			285.00	0.03	
Trimethylsilylacetylene	2.89			1260.00	3.64	
Water			34	0.00	0.00	
Chloroform			151	49.66	7.50	
NaCl			610	29.24	17.84	
$MgSO_4$			1.85	144.20	0.27	
Hexane			122	117.91	14.39	
Sodium sulfide nonahydrate	5.66			201.00	1.14	81.13
N-methyl pyrrolidone		97		101.65	9.59	
NH_4Cl	38.30			79.50	3.04	
Chloroform			311	49.66	15.44	
NaCl			1436.40	29.24	42.00	
$MgSO_4$			0.60	144.20	0.09	
Silica gel 60			158	62.20	9.83	
N-bromosuccinimide	1.97			117.50	0.23	7.58
Chloroform		24		49.66	1.19	
Acetic acid glacial		9		55.1	0.50	
Chloroform			114	49.66	5.66	
Water			77	0.00	0.00	
4-bromoaniline	2.88			455.00	1.31	188.04
4-iodoanisole	8.23			804.00	6.62	
CuI	0.16			285.00	0.05	
KOH	7.34			47.60	0.35	
1,10-phenanthroline	0.15			2995.00	0.45	
Xylene		15		79.53	1.37	
Dichloromethane			152	53.58	8.14	
Water			344	0.00	0.00	
$MgSO_4$			3.67	144.20	0.53	
Dichloromethane			973	53.58	52.13	
Hexane			484	117.91	57.07	
Silica gel 60			965	62.20	60.02	

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Bis(pinacolato)-diboron	2.91			8100.00	23.57	179.80
Potassium acetate	2.81			63.00	0.18	
Tris(dibenzylideneacetone)dipalladium(0), $Pd_2(dBa)3$	0.046			14900.00	0.69	
2-Dicyclohexylphosphino-2',4',6'-Triisopropylbiphenyl, X-Phos	0.09			7980.00	0.73	
Dioxane		76		102.03	7.50	
$MgSO_4$			2.76	144.20	0.40	
Dichloromethane			366	53.58	19.61	
Hexane			363	117.91	42.80	
Dichloromethane			731	53.58	39.17	
Silica gel 60			726	62.20	45.16	
K_3PO_4, tripotassium phosphate	8.16			636.00	5.19	112.51
$Pd(PPh_3)_4$	0.45			17750.00	7.99	
DMF		54		120.76	6.52	
NH_4Cl	38.30			79.50	3.04	
Dichloromethane			199	53.58	10.66	
Na_2SO_4			1	115.80	0.12	
Dichloromethane			265	53.58	14.20	
Silica gel 60			263	62.20	16.36	
Dichloromethane			901	53.58	48.28	
Ethyl acetate			2	80.16	0.16	
Total						**800.49**

Table S26 Materials quatities and cost for the synthesis of 1 g of HTM **52**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
Methoxybenzene, anisole	0.53			125.63	0.07	14.13
KI	0.85			386.00	0.33	
Methanol		7		60.18	0.42	
Sulfuric acid		1		38.59	0.04	
H_2O_2		0.32		526.67	0.17	
Water			21	0.00	0.00	
Dichloromethane			149	53.58	7.98	
Na_2SO_4			0.75	115.80	0.09	
Ethyl acetate			6	80.16	0.48	
Petroleum ether			46	99.12	4.56	
Aniline	0.12			160.47	0.02	24.78
1,10-phenanthroline	0.05			2995.00	0.14	
CuCl	0.03			125.40	0.00	
KOH	0.58			47.60	0.03	
Acetic acid glacial		0.4		55.1	0.02	
Toulene		2		69.48	0.14	
Toulene		1.4		69.48	0.10	
Water			14	0.00	0.00	
Na_2SO_4			0.56	115.80	0.06	
Ethyl acetate			18	80.16	1.44	
Petroleum ether			138	99.12	13.68	
Silica gel 60			147	62.20	9.14	
$POCl_3$	0.45			56.41	0.03	40.81
DMF		11		90.04	0.99	
Chloroform			86	49.66	4.27	
CH_3COONa			71	136.5	9.69	
Na_2SO_4			0.58	115.80	0.07	
Ethyl acetate			105	80.16	8.42	
Petroleum ether			79	99.12	7.83	
Silica gel 60			153	62.20	9.52	
Zn dust	0.46			87.60	0.04	21.63
Titanium tetrachloride	0.64			292.40	0.19	
THF		12		109.79	1.32	
Pyridine		0.5		185.58	0.09	
Water			29	0.00	0.00	
Dichloromethane			48	53.58	2.57	
Water			87	0.00	0.00	
$MgSO_4$			1	144.20	0.14	
Ethanol			79	218.63	17.27	
Total						**101.34**

Table S27 Materials quatities and cost for the synthesis of 1 g of HTM **53**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
4-iodoanisole	0.47			804.00	0.38	18.78
p-anisidine	0.16			123.50	0.02	
CuI	0.03			285.00	0.01	
K_2CO_3	0.37			142.00	0.05	
L-proline	0.03			511.00	0.02	
DMSO		2		98.64	0.20	
Water			10	0.00	0.00	
Ethyl acetate			9	80.16	0.72	
NaCl			44	29.24	1.29	
Na_2SO_4			0.37	115.80	0.04	
Ethyl acetate			15	80.16	1.20	
Petroleum ether			89	99.12	8.82	
Silica gel 60			97	62.20	6.03	
4,4'-difluorobenzophenone	0.16			2905.00	0.46	12.82
t-BuONa, sodium tert-butoxide	0.22			307.00	0.07	
DMF		4		120.76	0.48	
Water			18	0.00	0.00	
Ethanol			54	218.63	11.81	
Zn dust	0.29			87.60	0.03	20.99
Titanium tetrachloride	0.23			292.40	0.07	
THF		31		109.79	3.40	
NH_4Cl			1	79.50	0.08	
Water			100	0.00	0.00	
$MgSO_4$			1	144.20	0.14	
Ethanol			79	218.63	17.27	
Total						**52.59**

Table S28 Materials quatities and cost for the synthesis of 1 g of HTM **58**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
$Pd(OAc)_2$, palladium(ii) acetate	0.039			25550.00	1.00	153.70
Tri-t-butylphosphine	0.11			34500.00	3.80	
1-bromopyrene	0.82			58200.00	47.72	
4,4-dimethoxydiphenylamine	0.67			54900.00	36.78	
$CsCO_3$	0.95			674.00	0.64	
Toulene		30		69.48	2.08	
Chloroform			222	49.66	11.02	
Water			100	0.00	0.00	
$MgSO_4$			1	144.20	0.14	
Chloroform			592	49.66	29.40	
Silica gel 60			263	62.20	16.36	
Methanol			79	60.18	4.75	
Total						**153.70**

Table S29 Materials quatities and cost for the synthesis of 1 g of HTM **60**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
$Pd(OAc)_2$, palladium(ii) acetate	0.052			25550.00	1.33	191.88
Tri-t-butylphosphine	0.14			34500.00	4.83	
1,3,6,8-tetrabromopyrene	0.78			27100.00	21.14	
4,4-dimethoxydiphenylamine	1.79			54900.00	98.27	
t-BuONa, sodium tert-butoxide	0.75			307.00	0.23	
Toulene		52		69.48	3.61	
Chloroform			222	49.66	11.02	
Water			100	0.00	0.00	
$MgSO_4$			1	144.20	0.14	
Chloroform			273	49.66	13.56	
Hexane			122	117.91	14.39	
Ethyl acetate			28	80.16	2.24	
Silica gel 60			263	62.20	16.36	
Methanol			79	60.18	4.75	
Total						**191.88**

Table S30 Materials quatities and cost for the synthesis of 1 g of HTM **65**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
4,4-dimethoxydiphenylamine	0.92			54900.00	50.51	262.80
2,7-dibromo-9,9-dimethyl-9H-fluorene	2.81			29000.00	81.49	
Palladium(0) bis(dibenzylideneacetone), $Pd(dba)_2$	0.03			33900.00	1.15	
1,1'-Ferrocenediyl-bis(diphenylphosphine), dppf	0.33			6380.00	2.11	
t-BuONa, sodium tert-butoxide	0.81			307.00	0.25	
Toulene		65		69.48	4.52	
Water			212	0.00	0.00	
Ethyl acetate			287	80.16	23.01	
$MgSO_4$			2.12	144.20	0.31	
Dichloromethane			225	53.58	12.06	
Hexane			447	117.91	52.71	
Silica gel 60	558.00		558	62.20	34.71	
n-butyllithium (1.6M)	2.36			238.97	0.56	67.07
Trimethyltin chloride solution	5.40			1356.28	7.42	
THF		32		109.79	3.51	
NH_4CL			25	79.5	1.99	
Ethyl acetate			223	80.16	17.88	
Ethyl acetate			334	80.16	26.77	
NaCl			296	29.24	8.66	
Na_2SO_4			2.47	115.80	0.29	
Cyanuric chloride	0.19			51.90	0.01	66.86
$Pd(PPh_3)_4$	0.18			17750.00	3.23	
Toulene		50		69.48	3.47	
Water			100	0.00	0.00	
Chloroform			222	49.66	11.02	
NaCl			120	29.24	3.51	
$MgSO_4$			1	144.20	0.14	
Dichloromethane			398	53.58	21.32	
Hexane			66	117.91	7.78	
Silica gel 60			263	62.20	16.36	
Total						**396.73**

Table S31 Materials quatities and cost for the synthesis of 1 g of HTM **67**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
Triptycene	0.80			18550.00	14.84	52.29
HNO_3	31			99.08	3.10	
Water	313			0.00	0.00	
Water		78		0.00	0.00	
DCM			207	53.58	11.09	
Petroleum ether			106	99.12	10.51	
Silica gel 60			205	62.20	12.75	
Hydrazine monohydrate	1.19			292.00	0.35	2.38
THF		14		109.79	1.54	
Raney Ni	0.77			641.00	0.49	
Water			60	0.00	0.00	
HCl	2.22			80.65	0.18	47.52
Sodium nitrite,$NaNO_2$	0.48			135.20	0.06	
Potassium iodide	2.50			417.00	1.04	
Water		20		0.00	0.00	
Dichloromethane			119	53.58	6.38	
Sodium bisulfate,$NaHSO_4$			11.40	43.20	0.49	
Na_2SO_4			0.90	115.80	0.10	
Dichloromethane			95	53.58	5.09	
Petroleum ether			196	99.12	19.43	
Silica gel 60			237	62.20	14.74	
4,4-dimethoxydiphenylamine	0.98			54900.00	53.80	119.94
Potassium tert-butoxide, t-BuOK	0.96			224.00	0.22	
Tri-tert-butylphosphonium tetrafluoroborate, $P(t\text{-}Bu)_3HBF_4$	0.081			24500.00	1.98	
Palladium(0) bis(dibenzylideneacetone), $Pd(dba)_2$	0.16			33900.00	5.42	
Toulene		16		69.48	1.11	
Dichloromethane			199	53.58	10.66	
Water			100	0.00	0.00	
$MgSO_4$			1	144.20	0.14	
Dichloromethane			177	53.58	9.48	
Hexane			176	117.91	20.75	
Silica gel 60			263	62.20	16.36	
Total						**222.12**

Table S32 Materials quatities and cost for the synthesis of 1 g of HTM **68**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
Triptycene	0.53			18550.00	9.83	34.86
HNO_3	29.66			99.08	2.07	
Water	209			0.00	0.00	
Water		52		0.00	0.00	
DCM		138		53.58	7.39	
Petroleum ether			71	99.12	7.04	
Silica gel 60			137	62.20	8.52	
Hydrazine monohydrate	0.80			292.00	0.23	1.56
THF		9		109.79	0.99	
Raney Ni	0.52			641.00	0.33	
Water			40	0.00	0.00	
HCl	1.49			80.65	0.12	31.79
Sodium nitrite,$NaNO_2$	0.32			135.20	0.04	
Potassium iodide	1.67			417.00	0.70	
Water		13		0.00	0.00	
Dichloromethane			80	53.58	4.29	
Sodium bisulfate,$NaHSO_4$			7.60	43.20	0.33	
Na_2SO_4			0.60	115.80	0.07	
Dichloromethane			64	53.58	3.43	
Petroleum ether			131	99.12	12.98	
Silica gel 60			158	62.20	9.83	
4-bromo-4,4-dimethoxytriphenylamine	1.54			79800.00	122.89	179.75
n-butyllithium (1.6M)	2.19			238.97	0.52	
Trimethyl borate, $B(OCH_3)_3$	0.51			93.56	0.05	
THF		3		109.79	0.33	
Water			115	0.00	0.00	
HCl			27	80.65	2.18	
Dichloromethane			36	53.58	1.93	
Na_2SO_4			1.15	115.80	0.13	
Ethyl acetate			207	80.16	16.59	
Dichloromethane			305	53.58	16.34	
Silica gel 60			302	62.20	18.78	
K_2CO_3	4.10			142.00	0.58	67.56
$Pd(PPh_3)_4$	0.34			17750.00	6.04	
Toulene		51		69.48	3.54	
Water			100	0.00	0.00	
Dichloromethane			199	53.58	10.66	
Water			100	0.00	0.00	
$MgSO_4$			1	144.20	0.14	
Dichloromethane			177	53.58	9.48	
Hexane			176	117.91	20.75	
Silica gel 60			263	62.20	16.36	
Total						**315.51**

Table S33 Materials quatities and cost for the synthesis of 1 g of HTM **69**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
Triptycene	0.56			18550.00	10.39	36.85
HNO_3	21.95			99.08	2.19	
Water	221			0.00	0.00	
Water		55		0.00	0.00	
Dichloromethane		146		53.58	7.82	
Petroleum ether			75	99.12	7.43	
Silica gel 60			145	62.20	9.02	
Hydrazine monohydrate	0.83			292.00	0.24	1.69
THF		10		109.79	1.10	
Raney Ni	0.54			641.00	0.35	
Water			42	0.00	0.00	
HCl	1.55			80.65	0.13	33.26
Sodium nitrite,$NaNO_2$	0.34			135.20	0.05	
Potassium iodide	1.74			417.00	0.73	
Water		14		0.00	0.00	
Dichloromethane			83	53.58	4.45	
Sodium bisulfate,$NaHSO_4$			7.98	43.20	0.34	
Na_2SO_4			0.63	115.80	0.07	
Dichloromethane			67	53.58	3.59	
Petroleum ether			137	99.12	13.58	
Silica gel 60			166	62.20	10.33	
2-(tributylstannyl)thiophene	1.50			1920.00	2.88	26.27
Palladium(II)bis(triphenylphosphine) dichloride,$Pd(PPh_3)_2Cl_2$	0.06			13800.00	0.80	
THF		14		109.79	1.54	
Dichloromethane			60	53.58	3.21	
Hexane			89	117.91	10.49	
Silica gel 60			118	62.20	7.34	
4-bromo-4,4-dimethoxytriphenylamine	1.25			79800.00	99.75	146.61
n-butyllithium (1.6M)	1.77			238.97	0.42	
Trimethyl borate, $B(OCH_3)_3$	0.41			93.56	0.04	
THF		3		109.79	0.33	
Water			93	0.00	0.00	
HCl			32	80.65	2.58	
Dichloromethane			29	53.58	1.55	
Na_2SO_4			0.93	115.80	0.11	
Ethyl acetate			168	80.16	13.47	
Dichloromethane			246	53.58	13.18	
Silica gel 60			244	62.20	15.18	
N-bromosuccinimide	0.49			117.50	0.06	4.45
THF		40		109.79	4.39	
K_2CO_3	3.84			142.00	0.55	68.28
$Pd(PPh_3)_4$	0.32			17750.00	5.68	
Toulene		67		69.48	4.66	
Water			100	0.00	0.00	
Dichloromethane			199	53.58	10.66	
Water			100	0.00	0.00	
$MgSO_4$			1	144.20	0.14	
Dichloromethane			177	53.58	9.48	
Hexane			176	117.91	20.75	
Silica gel 60			263	62.20	16.36	
Total						**317.40**

Table S34 Materials quatities and cost for the synthesis of 1 g of HTM **70**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
Phenol	1.58			69.09	0.11	12.41
2,7-dibromo-9-fluorenone	0.57			13820.00	7.88	
methane sulfonic acid		0.65		145.85	0.09	
Methanol			13	60.18	0.78	
Methanol			59	60.18	3.55	
4,4-dimethoxydiphenylamine	0.76			54900.00	41.72	99.82
t-BuONa, sodium tert-butoxide	0.92			307.00	0.28	
Toulene		26		69.48	1.81	
Tri tert butylphosphine, $(t\text{-}Bu)_3P$	0.012			34500.00	0.41	
$Pd(OAc)_2$, palladium(ii) acetate	0.014			25550.00	0.36	
Ethyl acetate			135	80.16	10.82	
$MgSO_4$			1	144.20	0.14	
Petroleum ether			136	99.12	13.48	
Ethyl acetate			180	80.16	14.43	
Silica gel 60			263	62.20	16.36	
Total						**112.23**

Table S35 Materials quatities and cost for the synthesis of 1 g of HTM **71**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
4-bromophenol	1.89			457	0.86	9.65
2,7-dibromo-9-fluorenone	0.37			13820	5.11	
methane sulfonic acid		0.42		145.85	0.06	
Methanol			9	60.18	0.54	
Methanol			51	60.18	3.07	
4,4-dimethoxydiphenylamine	0.97			54900.00	53.25	110.82
t-BuONa, sodium tert-butoxide	0.47			307.00	0.14	
Toulene		17		69.48	1.18	
$(t\text{-}Bu)_3P$, tri tert butylphosphine	0.016			34500.00	0.55	
$Pd(OAc)_2$, palladium(ii) acetate	0.018			25550.00	0.46	
Ethyl acetate			135	80.16	10.82	
$MgSO_4$			1	144.20	0.14	
Petroleum ether			136	99.12	13.48	
Ethyl acetate			180	80.16	14.43	
Silica gel 60			263	62.20	16.36	
Total						**120.47**

Table S36 Materials quatities and cost for the synthesis of 1 g of HTM **74**

Chemical name	Weight reagent (g/g)	Weight solvent (g/g)	Weight workup (g/g)	Price of chemical ($/kg)	Material cost ($/g product)	Cost per step ($/step)
Hexaphenylbenzene	0.88			73900	65.03	87.49
$FeCl_3$, ferric chloride	1.34			51.8	0.07	
Dichloromethane		182		53.58	9.75	
CH_3NO_2, nitromethane		6.20		132.21	0.82	
Methanol			65	60.18	3.91	
HCl			36	80.65	2.90	
Water			82	0.00	0.00	
Acetone			65	76.99	5.00	
$AlCl_3$	0.21			205	0.04	151.44
Icl, chloroiodide	15.29			906	13.85	
CCl_4		350		223.02	78.06	
Ethanol			74	218.63	16.18	
Ethanol			127	218.63	27.77	
HCl			71.50	80.65	5.77	
Water			161	0.00	0.00	
Acetone			127	76.99	9.78	
Sodium thiophenolate	4.03			3690	14.87	128.62
1,3-dimethyl-1-imidazolidinone, DMI		112		311	34.83	
NaOH			8.50	53.20	0.45	
Toulene		305		69.48	21.19	
Water			100	0.00	0.00	
$MgSO_4$			1	144.20	0.14	
Dichloromethane			19	53.58	1.02	
Methanol			166	60.18	9.99	
Dichloromethane			265	53.58	14.20	
Hexane			132	117.91	15.56	
Silica gel 60			263	62.20	16.36	
Total						**367.55**

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