



Supplementary Information

Supplementary Table 1. Original dataset containing 1002 patients with esophageal cancer that underwent surgical therapy. 110 patient characteristics are listed with amount and percentage if not otherwise depicted. Missing variables are not listed individually, but represent the remainder if the sum of the individual variables does not add up to 100 percent.

	No.	%
Total patients (<i>n</i>)	1002	
CLINICAL CHARACTERISTICS		
Age at surgical treatment, mean \pm SD (y)	62.2 \pm 10.1	
Sex assigned at birth		
<i>Female</i>	157	15.7
<i>Male</i>	845	84.3
BMI, mean \pm SD (kg/m ²)	25.9 \pm 4.6	
Height, mean \pm SD (cm)	176 \pm 9.5	
Weight at primary staging (kg)	83.3 \pm 18.3	
Weight loss		
<i>yes/no</i>	100/114	9.98/11.3
<i>kg, mean \pm SD</i>	4.9 \pm 7.5	
<i>months, mean \pm SD</i>	2.7 \pm 3.6	
Ogilvie Dysphagia Scale		
0	53	5.3
1	58	5.8
2	44	4.4
3	23	2.3
4	6	0.6
Duration dysphagia, mean \pm SD (y)	2.3 \pm 2.4	
Preoperative WBC count ($\times 10^9/L$)		
< 4.4	33	3.3
> 4.4	668	66.7
Preoperative platelet count ($\times 10^9/L$)		
< 150	18	1.8
> 150	683	68.2
ASA-Score		
1	31	3.1
2	394	39.3
3	271	27.05
4	5	0.5
MEDICAL HISTORY		
ECOG-Score		
0	195	19.5

1	207	20.7
2	62	61.9
3	9	0.9
Arterial hypertension, yes/no	309/ 204	30.8/ 20.4
Antiplatelet agents		
<i>none</i>	453	45.2
<i>any</i>	15	1.5
<i>ASA</i>	93	9.3
AT-II receptor antagonist, yes/no	84/ 429	8.4/ 42.8
ACE-inhibitor, yes/no	113/ 399	11.3/ 39.8
Statins, yes/no	97/ 417	9.7/ 41.6
Diuretics, yes/no	116/ 398	11.6/ 39.7
Beta-blocker, yes/no	164/ 349	16.4/ 34.8
Calcium channel blocker, yes/no	66/ 448	6.6/ 44.7
Smoking history		
<i>Non-smoker</i>	279	27.8
<i>Smoker</i>	153	15.3
<i>Ex-smoker</i>	177	17.7
Alcohol consumption		
<i>No alcohol</i>	326	32.5
<i>1-3 times/week</i>	41	4.1
<i>4-5 times/week</i>	8	0.8
<i>daily</i>	35	3.5
MEDICAL TREATMENT		
Neoadjuvant therapy, yes/no	692/ 263	69.1/ 26.2
Type of neoadjuvant therapy		
<i>CROSS protocol [1]</i>	401	40.02
<i>FLOT protocol [2]</i>	109	10.9
<i>other</i>	204	20.4
One-/Two-stage procedure		
<i>One-stage</i>	667	66.6
<i>Two-stage</i>	34	3.4
Surgical procedure (Ivor-Lewis- Esophagectomy)		
<i>Open</i>	80	7.9
<i>Hybrid</i>	587	58.6
<i>Totally minimally invasive</i>	15	1.5
<i>Robot-Assisted</i>	18	1.8
<i>Minimally Invasive</i>		

COMPLICATIONS			
Clavien-Dindo-classification			
<i>none</i>	274	27.3	
<i>1</i>	30	2.9	
<i>2</i>	59	5.9	
<i>3a</i>	230	22.9	
<i>3b</i>	31	3.1	
<i>4a</i>	61	6.1	
<i>4b</i>	14	1.4	
<i>5</i>	1	0.1	
Postoperative pneumonia, yes/no	72/ 629	7.2/ 62.8	
Postoperative pylorospasm, yes/no	139/ 513	13.9/ 51.2	
Anastomosis leak, yes/no	50/ 651	4.9/ 64.9	
Secondary chest drainage, yes/no	57/ 545	5.7/ 54.4	
Re-intubation, yes/no	64/ 636	6.4/ 63.5	
Tracheostomy, yes/no	43/ 656	4.3/ 65.5	
Re-admission intensive-care unit, yes/no	50/ 650	4.9/ 64.9	
TUMOR ASSOCIATED FACTORS			
Histology			
<i>ACC</i>	842	84.03	
<i>SCC</i>	147	14.7	
<i>other</i>	12	1.2	
Adenocarcinoma of esophagogastric junction			
<i>Siewert I</i>	284	28.3	
<i>Siewert II</i>	174	17.4	
<i>Siewert III</i>	12	1.2	
Tumor distance to the incisors, mean \pm SD (cm)			
<i>Proximal margin</i>	33.2 \pm 5.2		
<i>Distal margin</i>	39.1 \pm 4.4		
Tumor stenosis at primary staging (endoscopically), yes/no	135/ 53	13.5/ 5.3	
CLINICAL TNM-STAGING AT PRIMARY STAGING			
cT			
<i>1</i>	31	3.1	
<i>2</i>	49	4.9	
<i>3</i>	269	26.8	
<i>4</i>	3	2.9	
cN			
<i>0</i>	25	24.9	
<i>1</i>	168	16.8	

	2	13	1.3
	3	3	0.3
	<i>x</i>	111	11.1
cM			
	0	241	24.1
	1	27	2.7
	<i>x</i>	24	2.4
PATHOLOGICAL TNM CLASSIFICATION			
pT			
	0	135	13.5
	1a/1b	248	24.8
	2	157	15.7
	3	440	43.9
	4a/b	17	1.7
	<i>Tis</i>	1	0.1
pN			
	0	513	511.9
	1	250	24.9
	2	135	13.5
	3	100	9.9
pL			
	0	600	59.9
	1	226	22.6
pV			
	0	762	76.04
	1	59	5.9
R			
	0	885	88.3
	1	40	3.9
	2	3	0.3
Positive lymph nodes, mean ± SD (n)		2.3 ± 4.7	
Total resected lymph nodes, mean ± SD (n)		30.8 ± 11.3	
Positive lymph node quotient, mean ± SD (n)		0.07 ± 0.14	
Pathological tumor margin distance, mean ± SD (mm)			
	<i>Proximal margin</i>	36.7 ± 18.1	
	<i>Distal margin</i>	45.2 ± 23.4	
Tumor regression grade			
	1: > 50% rest vital tumor cells (RVT)	127	12.7
	2: 10 - 50% RVT	146	14.6
	3: < 10 % RVT	130	12.9
	4: no RVT	118	11.8
BIOMARKER			

Insulin-like growth factor II mRNA-binding protein 3 (IMP-3) [3]		
0: no expression	59	58.9
1: weak expression	61	6.1
2: moderate expression	125	12.5
E-Cadherin		
0: no expression	8	0.8
1: weak expression	60	5.9
2: moderate expression	175	17.5
Carbonic anhydrase IX (CAIX)		
0: no expression	128	12.8
1: weak expression	62	6.2
2: moderate expression	43	4.3
Class III β -tubulin (TUBB3) [4]		
0: no expression	55	5.5
1: weak expression	66	6.6
2: moderate expression	55	5.5
3: strong expression	52	5.2
TP-53 mutation [5]		
0: mutant = no expression	97	9.7
1: wild-type protein	111	11.07
2: mutant = overexpression	282	28.1
Ki-67 (expression, %)		
1: 1% – 9%	97	9.7
2: 10% – 19%	42	4.2
3: 20% – 39%	84	8.4
4: $\geq 40\%$	66	6.6
Murine double minute-2 (MDM-2), IHC		
0: negative	267	26.6
1: weak/moderate, few cells	16	15.9
2: weak/moderate, many cells	16	15.9
3: strong expression	6	0.6
MDM2, FISH [5]		
0: negative amplification	288	28.7
1: positive amplification	16	1.6
Lymphocyte activation gene-3 (LAG-3)		
0: negative	200	19.9
1: 1-2%	59	5.9
2: 3-5%	15	1.5

High mobility group box 1 (HMGB-1)		
0: no expression	84	8.4
1: weak expression	59	5.9
2: moderate expression	65	6.5
3: strong expression	137	13.7
MutL homolog 1 (MLH-1)		
0: Microsatellite instability	15	1.5
1: Microsatellite stable	493	49.3
CD-3		
1: low expression	198	19.8
2: high expression	72	7.2
CD3, expression tumor center [6]		
0: peritumoral	248	24.8
2: intratumoral	22	2.2
X-linked inhibitor of apoptosis protein (XIAP) [7]		
0: no expression	25	2.5
1: weak expression	118	11.8
2: moderate expression	84	8.4
3: strong expression	38	3.8
Mesothelin (Novocastra antibody) [8]		
0: no expression	208	20.8
1: low/moderate	74	7.4
2: high	42	4.2
Mesothelin (Ventana antibody) [8]		
0: no expression	155	15.4
1: low/moderate	92	9.2
2: high	73	7.3
Claudin (expression, %)		
0: no expression	267	26.6
1: $\geq 5\%$ - 49%	38	3.8
2: $\geq 50\%$	26	2.6
AT-rich interactive domain 1A (ARID1A) [9]		
0: mutated/deleted gene	43	4.3
1: intact gene	464	46.3
SMARCA4 (BRG-1) [9]		
0: mutated/deleted gene	11	1.1
1: intact gene	432	43.1
SMARCA2 (BRM) [9]		
0: mutated/deleted gene	39	3.9
1: intact gene	414	41.3

Indoleamine 2,3-dioxygenase (IDO) expressed on tumor infiltrating lymphocytes [10]		
0: negative expression	168	16.8
1: low inflammation	123	12.3
2: high inflammation	52	5.2
Indoleamine 2,3-dioxygenase (IDO) expressed on tumor cells		
0: no expression	300	29.9
1: weak expression	30	2.9
2: high expression	14	1.4
T-cell immunoglobulin and mucin-domain containing-3 (TIM-3)		
0: negative expression	158	15.8
1: low inflammation	109	10.9
2: high inflammation	67	6.7
Aldo-keto reductase family 1 (AKR1)		
0: negative	35	3.5
1: low level	120	11.9
2: intermediate level	86	8.6
3: high level	52	5.2
Gremlin1 (GREM1)		
0: negative	22	2.2
1: low level	142	14.2
2: high level	64	6.4
c-MYC		
0: no amplification	294	29.3
1: low amplification	22	2.2
2: high amplification	41	4.1
KRAS		
0: negative amplification	296	29.5
1: positive amplification	70	6.9
GATA-binding factor (GATA6) [11]		
0: negative amplification	311	31.03
1: positive amplification	33	3.3
Her2/neu, IHC [12]		
0: negative staining	438	43.7
1: very weak	1	0.1
2: weak/moderate	15	1.5
3: strong	29	2.9
Her2/neu, FISH [12]		
0: negative amplification	326	32.5
1: positive amplification	31	3.1

Loss of Y-chromosome (LoY), long arm [13]			
0: negative	170	16.9	
1: positive	125	12.5	
LoY, short arm [13]			
0: negative	164	16.4	
1: positive	131	13.1	
Phosphatase and tensin homolog deleted on chromosome 10 (PTEN)			
0: negative	32	3.2	
1: weak signal	74	7.4	
2: normal signal	296	29.5	
Fructose-1,6-bisphosphatase 1 (FBP1) [14]			
0: no expression	65	6.4	
1: weak	94	9.4	
2: moderate	133	13.3	
3: strong	78	7.8	
Ubiquilin-4 (UBQLN4, dots/tumorcells)			
0: 0 or < 1	71	7.1	
1: 1-3	125	12.5	
2: 4-9	105	10.5	
3: ≥ 10	18	1.8	
Trimethylation of lysine 27 on histone H3 (H3K27me3)			
0: negative	42	4.2	
1: partly positive	67	6.7	
2: completely positive	185	18.5	
p16, IHC			
0: negative	276	27.5	
1: partly positive	44	4.4	
2: completely positive	63	6.3	
p16, FISH			
0: no deletion	202	20.2	
1: hemizygous deletion	35	3.5	
2: homozygous deletion	78	7.8	
Trophoblast Cell Surface Antigen 2 (TROP2) [15], (H-Score expression level)			
0: no expression	43	4.3	
1: weak expression	85	8.5	
2: moderate expression	183	18.3	
3: strong expression	76	7.6	
AKR			
0: no expression	28	2.8	
1: weak expression	88	8.8	

2: moderate expression	120	11.9
3: strong expression	104	10.4
F-box and WD repeat domain containing 7 (FBXW7)		
0: negative	28	2.8
1: weak signal	59	5.9
2: normal signal	294	29.3
Cyclin D1, IHC		
0: no expression	161	16.1
1: weak expression	166	16.6
2: moderate expression	59	5.9
3: strong expression	4	0.4
Cyclin D1, FISH		
0: no amplification	274	27.3
1: polyribosome	12	1.2
2: amplification	13	1.3
Cyclin Dependent Kinase 6 (CDK6), FISH		
0: no amplification	169	16.9
2: amplification	13	1.3
Periostin		
0: negative	93	9.3
1: >5% - 30%	178	17.8
2: >30%	226	22.6
Matrix metalloproteinase-2 (MMP-2)		
0: no expression	99	9.9
1: weak expression	226	22.6
2: moderate expression	159	15.9
Homeobox protein NANOG		
0: no expression	130	12.9
1: weak expression	127	12.7
2: moderate expression	235	23.5
Cytokeratin 6 (CK6)		
0: negative	369	36.8
1: weak positive	74	7.4
2: strong positive	46	4.6
N-myc down-regulated gene 1 (NDRG1)		
0: no expression	46	4.6
1: weak expression	109	10.9
2: moderate expression	92	9.2
3: strong expression	134	13.4
Thymidine phosphorylase (TYMP)		
0: no expression	152	15.2
1: weak expression	160	15.9

	2: moderate expression	120	11.9
	3: strong expression	57	5.7
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Growth differentiation factor 15 (GDF-15), tumor cells			
	0: negative	80	7.9
	1: low	96	9.6
	2: medium	76	7.6
	3: strong	6	0.6
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GDF15, stroma			
	0: negative	54	5.4
	1: low	111	11.1
	2: medium	87	8.7
	3: strong	6	0.6
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Mast cells			
	0: negative	171	17.1
	1: weak positive	278	27.8
	2: strong positive	102	10.2
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Natural killer cells (NK cells)			
	0: negative	329	32.8
	1: weak positive	217	21.7
	2: strong positive	8	0.8
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Tumor-infiltrating plasma cells (TIP)			
	0: negative	285	28.4
	1: weak positive	196	19.6
	2: strong positive	72	7.2
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Supplementary Table 2. Hyperparameters for each model after optimization. Randomized and Grid Search Cross Validation was used for Random Forest (RF), XG-Boost (XG) and Logistic Regression (LR). Best hyperparameters for Artificial Neural Network (ANN) and TabNet (TN) were selected using *Optuna*, an open-source optimization framework.

	Baseline Dataset	Primary Staging Dataset (PS)	PS Dataset including tumor biomarker
RF	n_estimators= 62, max_depth = 19, min_samples_split = 2, min_samples_leaf = 3, bootstrap=True, max_features='auto'	n_estimators= 65, max_depth = 15, min_samples_split = 2, min_samples_leaf = 3, bootstrap=False, max_features='auto'	n_estimators= 45, max_depth = 13, min_samples_split = 3, min_samples_leaf = 2, bootstrap=False, max_features='auto'
	<i>AI-driven Reduced Datasets</i>	n_estimators= 45, max_depth = 17, min_samples_split = 4, min_samples_leaf = 3, bootstrap=True, max_features='auto'	n_estimators= 36, max_depth = 22, min_samples_split = 2, min_samples_leaf = 3, bootstrap=True, max_features='auto'
XG	n_estimators = 79, max_depth = 12, subsample = 0.7, colsample_bytree = 0.6, learning_rate = 0.05, reg_lambda = 0.7, gamma = 0.1	n_estimators = 68, max_depth = 8, subsample = 0.8, colsample_bytree = 0.7, learning_rate = 0.05, reg_lambda = 1, gamma = 0.1	n_estimators = 75, max_depth = 5, subsample = 0.8, colsample_bytree = 0.5, learning_rate = 0.05, gamma = 0.4, reg_lambda = 0.5
	<i>AI-driven Reduced Datasets</i>	n_estimators = 29, max_depth = 9, subsample = 0.5, colsample_bytree = 0.6, learning_rate = 0.05, reg_lambda = 0.5, gamma = 0.1,	n_estimators = 63, max_depth = 3, subsample = 0.6, colsample_bytree = 0.5, learning_rate = 0.1, reg_lambda = 0.1, gamma = 0.0
ANN	embed_p=0.35, ps=0.5, layers=[120], n_epochs = 8, lr_max=0.00898	embed_p=0.2, ps=0.3, layers=[25, 140], n_epochs = 15, lr_max=0.003804471	embed_p=0.6, ps=0.45, layers=[100, 75], n_epochs = 8, lr_max=0.00500528
	<i>AI-driven Reduced Datasets</i>	embed_p=0.25, ps=0.55, layers=[140, 140], n_epochs = 16, lr_max=0.006370	embed_p=0.8, ps=0.7, layers=[75], n_epochs = 17, lr_max=0.0044824595
TN	mask_type = entmax, cat_emb_dim = 5, optimizer_fn=torch.optim.Adam, n_a = 16, n_d = 60, n_shared = 4,	mask_type = entmax, cat_emb_dim = 4, optimizer_fn=torch.optim.Adam, n_a = 60, n_d = 16, n_shared = 1,	mask_type = entmax, cat_emb_dim = 2, optimizer_fn=torch.optim.Adam, n_a = 40, n_d = 36, n_shared = 5,

	n_steps = 3, n_independent = 1, optimizer_params=dict(lr=2e-2), scheduler_params=step_size:12, gamma:1.0, scheduler_fn=torch.optim.lr_scheduler.StepLR,	n_steps = 1, n_independent = 1, optimizer_params=dict(lr=2e-2), scheduler_params=step_size:12, gamma":1.4, scheduler_fn=torch.optim.lr_scheduler.StepLR	n_steps = 5, n_independent = 1, optimizer_params=dict(lr=2e-2), scheduler_params=step_size:20, gamma:1.4, scheduler_fn=torch.optim.lr_scheduler.StepLR
<i>AI-driven Reduced Datasets</i>	mask_type = 'entmax', cat_emb_dim = 4, optimizer_fn=torch.optim.Adam, n_a = 12, n_d = 48, n_shared = 1, n_steps = 5, n_independent = 3, optimizer_params=dict(lr=2e-2), scheduler_params=step_size:10, gamma:1.4, scheduler_fn=torch.optim.lr_scheduler.StepLR,		mask_type = 'entmax', cat_emb_dim = 1, optimizer_fn=torch.optim.Adam, n_a = 52, n_d = 28, n_shared = 3, n_steps = 9, n_independent = 2, optimizer_params=dict(lr=2e-2), scheduler_params=step_size:6, gamma:1.2, scheduler_fn=torch.optim.lr_scheduler.StepLR
LR	penalty = none, max_iter = 2000, solver = saga	penalty = none, max_iter = 3000, solver = sag	penalty = none, max_iter = 5000, solver = saga

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Supplementary References

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