

Table S1. Full MWCNTs dataset table

Index	Code ¹	Group ¹	Type ¹	Length ave. ¹ (nm)	Diameter ave. ¹ (nm)	Diameter std ¹ (nm)	BET ¹ (m ² /g)	%Fe ¹	%Co ¹	%Ni ¹
0	NRCWE-040	Group I	PRISTINE	518.9	22.1	7.8	150	0.2	0.001	518.9
1	NRCWE-041	Group I	OH	1005	26.9	10.1	152	0.13	0.001	1005
2	NRCWE-042	Group I	COOH	723.2	30.2	14.2	141	0.08	0	723.2
3	NRCWE-043	Group II	PRISTINE	771.3	55.6	18.1	82	0.008	0.001	771.3
4	NRCWE-044	Group II	OH	1330	32.7	13.6	74	0.004	0.002	1330
5	NRCWE-045	Group II	COOH	1553	30.2	15.6	119	1.17	0.25	1553
6	NRCWE-046	Group III	PRISTINE	717.2	29.1	16.1	223	0.008	0.25	717.2
7	NRCWE-047	Group III	OH	532.5	22.6	10.1	216	0.007	0.25	532.5
8	NRCWE-048	Group III	COOH	1604	17.9	17.9	185	0.007	0.24	1604
9	NRCWE-049	Group III	NH2	731.1	14.9	5.6	199	0.004	0.25	731.1
10	NM-400	Standard materials	PRISTINE	847	11	3.0	254	0.2607	0.1063	847
11	NM-401	Standard materials	PRISTINE	4048	67	24.0	18	0.05	-	4048
12	NM-402	Standard materials	PRISTINE	1372	11	3.0	226	1.31	-	1372
13	NM-403	Standard materials	PRISTINE	1373	13	3.0	227	2.31	-	1373
14	NRCWE-006	Standard materials	PRISTINE	5700	65	25.0	26	0.680	-	5700
Index	%Mg ¹	%Mn ¹	Purity ² (%)	Z ave. ³ (nm) (batch)	PdI ³ (batch)	Z ave. ³ (nm) (12.5 µg/ml)	PdI ³ (12.5 µg/ml)	Z ave. ³ (nm) (200 µg/ml)	PdI ³ (200 µg/ml)	ROS ³
0	0.01	0.002	98.60	195.6	0.358	159	0.398	262	0.408	1.7
1	0.02	0.001	99.20	218.7	0.501	236	0.484	235	0.496	3.0

2	0.03	0.001	99.20	195.2	0.382	155	0.314	190	0.425	0.8
3	0.01	-	98.50	177.0	0.237	145	0.254	154	0.306	2.3
4	0.02	-	98.60	202.2	0.236	437	0.478	605	0.580	1.7
5	0.02	0.002	96.30	192.4	0.227	336	0.477	295	0.391	1.5
6	0.22	0.3	98.70	182.9	0.434	598	0.504	1159	0.497	6.6
7	0.22	0.3	98.70	200.1	0.402	244	0.446	307	0.484	2.1
8	0.19	0.28	98.80	182.2	0.397	152	0.465	128	0.372	2.1
9	0.19	0.29	98.80	212.5	0.602	197	0.867	217	0.639	3.4
10	-	-	90.00	168.1	0.385	274	0.582	270	0.592	5.1
11	0.015	-	99.19	923.8	0.323	570	0.463	652	0.502	0.0
12	0.001	0.001	92.97	171.3	0.407	456	0.482	213	0.465	7.7
13	1.001	1.001	90.00	200.2	0.407	587	0.514	291	0.506	1.9
14	-	-	99.00	633.3	0.256	832	0.459	2102	0.448	0.3
Index	Peak³ (µg/ml)	0 µg/ml viability³ (%)	12.5 µg/ml viability³ (%)	25 µg/ml viability³ (%)	50 µg/ml viability³ (%)	100 µg/ml viability³ (%)	200 µg/ml viability³ (%)	0 µg/ml proliferation³ (%)	12.5 µg/ml proliferation³ (%)	25 µg/ml proliferation³ (%)
0	12.50	94	95	96	97	97	99	100	95	85
1	12.50	93	94	96	96	96	98	100	79	62
2	12.50	94	95	96	97	98	99	100	89	96
3	12.50	96	96	98	98	99	99	100	105	115
4	12.50	96	96	97	98	98	99	100	99	96
5	12.50	94	97	96	98	98	98	100	95	100

6	6.25	96	98	98	98	99	99	100	93	88
7	6.25	97	99	99	99	99	99	100	99	105
8	6.25	97	97	98	98	99	100	100	95	97
9	12.50	96	97	97	99	99	98	100	95	80
10	5.60	97	97	98	99	99	98	100	105	105
11	11.25	96	96	94	94	95	95	100	77	64
12	12.50	97	97	98	98	99	96	100	113	100
13	12.50	96	97	98	98	99	98	100	83	94
14	11.25	95	94	93	93	91	94	100	75	73
Index	50 µg/ml prolife- ration³ (%)	100 µg/ml prolife- ration³ (%)	200 µg/ml prolife- ration³ (%)	CEA: C.H.N.O³ (wt%)	OH³ (mmol/g)	COOH³ (mmol/g)	Endo- toxins³ (EU/ml)	Geno- toxicity²		
0	60	67	62	96.00	0.35	0.18	0.18	0		
1	50	54	59	97.00	1.69	0.84	0.44	0		
2	72	79	56	96.00	4.09	2.04	0.26	0		
3	114	111	101	96.00	0.18	0.09	0.25	0		
4	95	91	77	97.00	0.23	0.11	0.27	1		
5	104	79	29	93.00	0.63	0.31	0.34	1		
6	112	97	10	96.00	0.63	0.32	0.19	0		
7	90	79	19	97.00	0.26	0.13	0.01	0		
8	84	81	42	96.00	0.58	0.29	0.03	0		
9	83	79	20	97.00	0.33	0.16	0.05	0		

10	121	102	115	88.00	0.79	0.40	0.24	1
11	52	50	47	98.00	0.03	0.02	0.31	0
12	99	104	47	92.00	0.28	0.14	0.01	1
13	77	78	14	97.00	0.19	0.09	0.01	1
14	55	55	55	98.00	0.08	0.04	0.51	1

Table S2. Scaled dataset

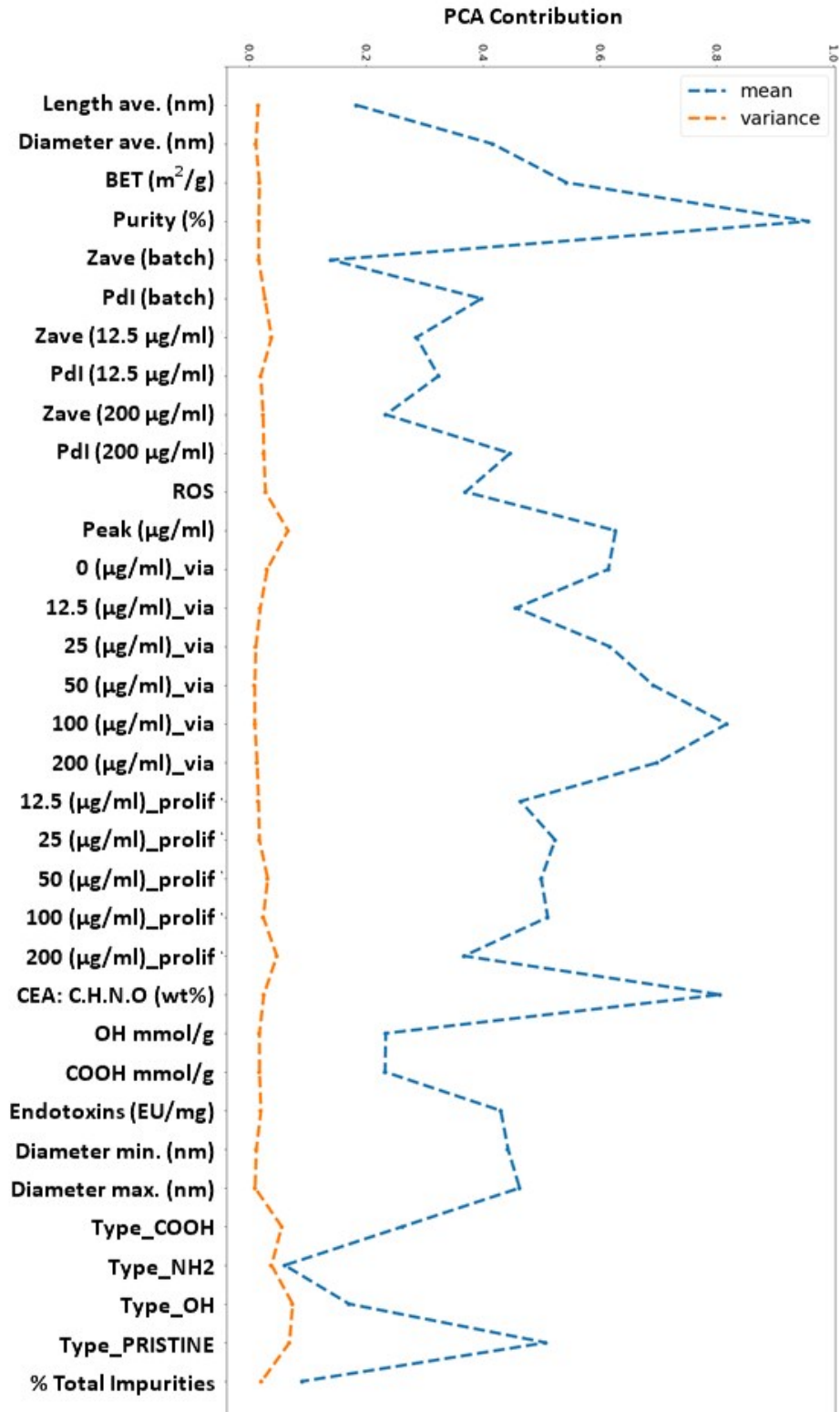
A/A	Length ave.	Diameter ave.	Diameter max	Diameter r min	BET	Total Impurities	Purity	Zave batch	PdI batch	Zave (12.5 µg/ml)
0	0.0000	0.1982	0.2065	0.3326	0.559	0.1349	0.9348	0.0364	0.3493	0.0204
1	0.0938	0.2839	0.2987	0.3907	0.5678	0.0757	1.0000	0.0670	0.7307	0.1325
2	0.0394	0.3429	0.3948	0.3721	0.5212	0.0498	1.0000	0.0359	0.4133	0.0146
3	0.0487	0.7964	0.7753	0.8721	0.2712	0.2199	0.9239	0.0118	0.0267	0.0000
4	0.1565	0.3875	0.4195	0.4442	0.2373	0.1907	0.9348	0.0451	0.0240	0.4250
5	0.1996	0.3429	0.4130	0.3395	0.4280	0.5177	0.6848	0.0322	0.0000	0.2780
6	0.0383	0.3232	0.4052	0.3023	0.8686	0.1368	0.9456	0.0196	0.5520	0.6594
7	0.0026	0.2071	0.2429	0.2907	0.8390	0.1364	0.9456	0.0423	0.4667	0.1441
8	0.2094	0.1232	0.2831	0.0000	0.7076	0.1250	0.9565	0.0187	0.4533	0.0102
9	0.0410	0.0696	0.0844	0.2163	0.7669	0.1282	0.9565	0.0587	1.0000	0.0757
10	0.0633	0.0000	0.0000	0.1861	1.0000	0.0577	0.0000	0.0000	0.4213	0.1878
11	0.6811	1.0000	1.0000	1.0000	0.0000	0.0000	0.9989	1.0000	0.2560	0.6187
12	0.1647	0.0000	0.0000	0.1861	0.8814	0.2378	0.3228	0.0042	0.4800	0.4527
13	0.1649	0.0357	0.0260	0.2326	0.8856	1.0000	0.0000	0.0425	0.4800	0.6434
14	1.0000	0.9643	0.9870	0.9302	0.0339	0.1172	0.9783	0.6156	0.0773	1.0000
A/A	PdI (12.5 µg/ml)	Zave (200 µg/ml)	PdI (200 µg/ml)	ROS	Peak	0 µg/ml viability	12.5 µg/ml viability	25 µg/ml viability	50 µg/ml viability	100 µg/ml viability
0	0.2349	0.0679	0.3063	0.2208	1.0000	0.2500	0.2000	0.5000	0.6667	0.7500
1	0.3752	0.0542	0.5706	0.3896	1.0000	0.0000	0.0000	0.5000	0.5000	0.6250
2	0.0979	0.0314	0.3574	0.1039	1.0000	0.2500	0.2000	0.5000	0.6667	0.8750
3	0.0000	0.0132	0.0000	0.2987	1.0000	0.7500	0.4000	0.8333	0.8333	1.0000
4	0.3654	0.2416	0.8228	0.2208	1.0000	0.7500	0.4000	0.6667	0.8333	0.8750
5	0.3638	0.0846	0.2553	0.1948	1.0000	0.2500	0.6000	0.5000	0.8333	0.8750
6	0.4078	0.5223	0.5736	0.8571	0.0942	0.7500	0.8000	0.8333	0.8333	1.0000
7	0.3132	0.0907	0.5345	0.2727	0.0942	1.0000	1.0000	1.0000	1.0000	1.0000
8	0.3442	0.0000	0.1982	0.2727	0.0942	1.0000	0.6000	0.8333	0.8333	1.0000
9	1.0000	0.0451	1.0000	0.4416	1.0000	0.7500	0.6000	0.6667	1.0000	1.0000
10	0.5351	0.0719	0.8589	0.6623	0.0000	1.0000	0.6000	0.8333	1.0000	1.0000
11	0.3409	0.2654	0.5886	0.0000	0.8188	0.7500	0.4000	0.1667	0.1667	0.5000
12	0.3719	0.043	0.4775	1.0000	1.0000	1.0000	0.6000	0.8333	0.8333	1.0000
13	0.4241	0.0826	0.6006	0.2467	1.0000	0.7500	0.6000	0.8333	0.8333	1.0000
14	0.3344	1.0000	0.4264	0.0390	0.8188	0.5000	0.0000	0.0000	0.0000	0.0000
A/A	200 µg/ml viability	12.5 µg/ml prolife-	25 µg/ml prolife-	50 µg/ml prolife-	100 µg/ml prolife-	200 µg/ml prolife-	CEA: C,H,O,N	OH	COOH	Endo- toxins

	ration	ration	ration	ration	ration	ration	ration	ration	ration	ration
0	0.8333	0.5263	0.4340	0.1408	0.2787	0.4952	0.8000	0.0788	0.0792	0.3400
1	0.6667	0.1053	0.0000	0.0000	0.0656	0.4667	0.9000	0.4089	0.4059	0.3400
2	0.8333	0.3684	0.6415	0.3099	0.4754	0.4381	0.8000	1.0000	1.0000	0.5000
3	0.8333	0.7895	1.0000	0.9014	1.0000	0.8667	0.8000	0.0369	0.0346	0.4800
4	0.8333	0.6316	0.6415	0.6338	0.6721	0.6381	0.9000	0.0493	0.0445	0.5200
5	0.6667	0.5263	0.7170	0.7606	0.4754	0.1809	0.5000	0.1478	0.1436	0.6600
6	0.8333	0.4737	0.4906	0.8732	0.7705	0.0000	0.8000	0.1478	0.1485	0.3600
7	0.8333	0.6316	0.8113	0.563	0.4754	0.0857	0.9000	0.0566	0.0545	0.0000
8	1.0000	0.5263	0.6604	0.4789	0.5082	0.3048	0.8000	0.1355	0.1337	0.0400
9	0.6667	0.5263	0.3396	0.4648	0.4754	0.0952	0.9000	0.0739	0.0693	0.0800
10	0.6667	0.7895	0.8113	1.0000	0.8525	1.0000	0.0000	0.1872	0.1881	0.4600
11	0.1667	0.0526	0.0377	0.0282	0.0000	0.3524	1.0000	0.0000	0.0000	0.8200
12	0.3333	1.0000	0.7170	0.6901	0.8852	0.3524	0.4000	0.0616	0.0594	0.0000
13	0.6667	0.2105	0.6038	0.3803	0.4590	0.0381	0.9000	0.0394	0.0346	0.0000
14	0.0000	0.0000	0.2075	0.0704	0.0820	0.4286	1.0000	0.0123	0.0099	1.0000
A/A	Type COOH	Type NH2	Type OH	Type PRISTI NE	Geno-toxicity					
0	0.0000	0.0000	0.0000	1.0000	0					
1	0.0000	0.0000	1.0000	0.0000	0					
2	1.0000	0.0000	0.0000	0.0000	0					
3	0.0000	0.0000	0.0000	1.0000	0					
4	0.0000	0.0000	1.0000	0.0000	1					
5	1.0000	0.0000	0.0000	0.0000	1					
6	0.0000	0.0000	0.0000	1.0000	0					
7	0.0000	0.0000	1.0000	0.0000	0					
8	1.0000	0.0000	0.0000	0.0000	0					
9	0.0000	1.0000	0.0000	0.0000	0					
10	0.0000	0.0000	0.0000	1.0000	1					
11	0.0000	0.0000	0.0000	1.0000	0					
12	0.0000	0.0000	0.0000	1.0000	1					
13	0.0000	0.0000	0.0000	1.0000	1					
14	0.0000	0.0000	0.0000	1.0000	1					

Table S3. PCA dataset

A/A	PC 1	PC 2	PC 3	PC 4	PC 5	PC 6	PC 7	PC 8	PC 9	Genotoxicity
0	0.2187	0.0456	0.0425	-0.4852	-0.4652	0.1204	0.1000	0.5607	-0.2241	0
1	0.5249	1.1784	-0.6954	-0.1097	-0.6085	0.5401	-0.3300	0.1612	0.0525	0
2	0.1061	1.3023	0.7826	-0.6204	0.1976	0.3805	0.0527	0.0528	0.2026	0
3	0.0572	-0.5460	1.2166	0.3645	-0.7096	-0.3147	0.4530	0.3280	-0.0164	0
4	0.0367	0.3926	0.0256	0.7897	-0.6642	-0.2099	-0.2244	-0.5362	0.1277	1
5	-0.0509	0.5487	0.7410	-0.3366	0.3305	-0.5234	-0.2004	-0.5444	0.1450	1
6	-0.5025	-0.7042	-0.2013	0.3150	0.5228	0.2102	0.0785	0.4440	0.7402	0
7	-0.9193	0.3723	-0.3978	1.0885	0.1443	-0.1407	-0.3306	0.2361	-0.1325	0
8	-0.7851	0.6034	0.3461	0.2191	0.9078	-0.0598	0.0154	0.2250	-0.4000	0
9	-0.6650	0.4813	-1.0894	-0.2062	0.0315	-0.2615	0.9981	-0.3187	0.0155	0
10	-1.2646	-1.0787	0.2122	-0.0467	0.0366	0.9070	-0.0900	-0.4971	-0.3159	1
11	2.1077	-0.4449	-0.2175	0.1864	0.2671	-0.0380	0.2368	0.0530	-0.4026	0
12	-0.9519	-0.9321	-0.0955	-0.4278	-0.2666	-0.0227	0.0228	-0.1122	0.1385	1
13	-0.4856	-0.6157	-0.5491	-0.7773	-0.0428	-0.6935	-0.6374	0.1789	-0.1151	1
14	2.5738	-0.6031	-0.1206	0.0466	0.3185	0.1060	-0.1443	-0.2312	0.1846	1

Fig S1. Mean and variance of features in the PCA dataset



Eq. S1. Confusion Matrix ⁴

		<u>Real</u>	
		Class 0	Class 1
<u>Predicted</u>	Class 0	TN	FP
	Class 1	FN	TP

TN (True-Negative): Number of observations that belong in “Class 0” and the model predicted “Class 0”.

TP (True-Positive): Number of observations that belong in “Class 1” and the model predicted “Class 1”.

FN (False-Negative): Number of observations that belong in “Class 1” and the model predicted “Class 0”.

FP (False-Positives): Number of observations that belong in “Class 0” and the model predicted “Class 1”.

Eq. S2. Precision formula ⁴

$$Precision = \frac{TP}{TP + FP}$$

Where TP represent the “true-positive” and FP the “false-positive” observations.

Eq. S3. Sensitivity formula ⁴

$$Sensitivity = \frac{TP}{TP + FN}$$

Where TP represent the “true-positive” and FN the “false-negative” observations.

Eq. S4. Specificity formula ⁴

$$Specificity = \frac{TN}{TN + FP}$$

Where TN represent the “true-negative” and FP the “false-positive” observations.

Eq. S5. F1-Score formula ⁴

$$F1 - Score = 2 \times \frac{Precision \times Recall}{Precision + Recall}$$

Where Precision and recall as defined above.

Eq. S6. Accuracy formula ⁴

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

Where TP represent the “true-positive”, TN the “true-negative”, FP the “false-positive” and FN the “false-negative” observations.

Eq. S7. MCC formula ⁴

$$MCC = \frac{TP \times TN - FP \times FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}}$$

Where TP represent the “true-positive”, TN the “true-negative”, FP the “false-positive” and FN the “false-negative” observations.

References

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³ P. Jackson, K. Kling, K. Jensen, P. Clausen, A. Madsen, H. Wallin and U. Vogel, *Environ Mol Mutagen.*, 2015, **56**(2), 183-203.

⁴ https://scikit-learn.org/stable/modules/model_evaluation.html