
**SUPPLEMENTARY MATERIALS
TO
On Structure Sensitivity and Chemical
Applicability of Some Novel Degree-based
Topological Indices**

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Table 4. Structure sensitivity (*SS*) and abruptness (*Abr*) of different topological indices of trees from $n = 4$ to 10 vertices.

Topological Indices		$n = 4$	$n = 5$	$n = 6$	$n = 7$	$n = 8$	$n = 9$	$n = 10$
M_1	<i>SS</i>	0.1833	0.1768	0.1381	0.1151	0.0964	0.0835	0.0726
	<i>Abr</i>	0.1833	0.19762	0.2090	0.1934	0.1815	0.1708	0.1623
M_2	<i>SS</i>	0.1181	0.1448	0.1403	0.1296	0.1209	0.1111	0.1032
	<i>Abr</i>	0.1181	0.1448	0.2054	0.2308	0.2546	0.2642	0.2706
$R_{-1/2}$	<i>SS</i>	0.1002	0.0953	0.0744	0.0599	0.0484	0.0404	0.0339
	<i>Abr</i>	0.1002	0.1046	0.1053	0.0919	0.0855	0.0779	0.0709
SCI	<i>SS</i>	0.0983	0.0942	0.0734	0.0594	0.0482	0.0404	0.0341
	<i>Abr</i>	0.0983	0.1028	0.1039	0.0915	0.0849	0.0776	0.0714
H	<i>SS</i>	0.2020	0.1945	0.1519	0.1214	0.0972	0.0803	0.0669
	<i>Abr</i>	0.2020	0.2106	0.2101	0.1829	0.1691	0.1524	0.1381
AZI	<i>SS</i>	0.9742	0.7278	0.4616	0.3029	0.2017	0.1515	0.1182
	<i>Abr</i>	0.9742	0.7572	0.5960	0.4378	0.3384	0.2878	0.2506
ABC	<i>SS</i>	0.1443	0.1007	0.0691	0.0501	0.0382	0.0309	0.0255
	<i>Abr</i>	0.1443	0.1115	0.1000	0.08274	0.0704	0.0634	0.0569
GA	<i>SS</i>	0.1052	0.0984	0.0746	0.0596	0.0474	0.0393	0.0326
	<i>Abr</i>	0.1052	0.1086	0.1051	0.0908	0.0823	0.0743	0.0671

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Algorithm 1 A pseudocode, implemented in MATLAB R2019a, to compute the structure sensitivity (SS) and abruptness (Abr) of topological indices (TIs) for a data set of trees of given vertex.

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Require:  $\Omega = \{\text{Set of all trees with given number of vertices}\}$ 
1:  $A = \text{Zeroes}(|\Omega|, 23)$ 
2:  $B = \text{Zeroes}(|\Omega|, 23)$ 
3:  $C = \text{Zeroes}(1, 23)$ 
4:  $D = \text{Zeroes}(1, 23)$ 
5: for  $i = 1 : |\Omega|$  (for a tree  $T_i$  in  $n$ -vertex trees data set  $\Omega$ ) do
6:    $S = \{\text{Trees with } GED = 2 \text{ from tree } T_i\}$      $\triangleright$  use Python networkx package to
      compute  $GED$ 
7:    $E = [23 \text{ TIs of tree } T_i]_{1 \times 23}$             $\triangleright$  calculate TIs of tree  $T_i$ 
8:    $F = [23 \text{ TIs of the trees in set } S]_{23 \times |S|}$      $\triangleright$  compute topological indices
9:    $G = \text{Zeroes}(23, |S|)$ 
10:   $H = \text{Zeroes}(1, 23)$ 
11:   $I = \text{Zeroes}(1, 23)$ 
12:  for  $j = 1 : 23$  do                                 $\triangleright$  Implementation of Step-3
13:     $p = 0$ 
14:    for  $k = 1 : |S|$  do
15:       $q = \left| \frac{F(j,k) - E(j)}{E(j)} \right|$ 
16:       $p = q + p$ 
17:       $G(j, k) = q$ 
18:    end for
19:     $SS(T_i, TIs) = \frac{p}{|S|}$ 
20:     $Abr(T_i, TIs) = \max(G(j); :)$ 
21:     $H(j) = SS(T_i, TIs)$          $\triangleright$  Give all 23  $SS$ -values of each TIs for a tree  $T_i$ 
22:     $I(j) = Abr(T_i, TIs)$         $\triangleright$  Give all 23  $Abr$ -values of each TIs for a tree  $T_i$ 
23:  end for
24:   $disp(H)$ 
25:   $disp(I)$ 
26:   $A(i, :) = H(1, :)$ 
27:   $B(i, :) = I(1, :)$ 
28: end for
29:  $disp(A)$ 
30:  $disp(B)$ 
31: for  $l = 1 : 23$  do                                 $\triangleright$  Implementation of Step-4
32:    $r = 0$ 
33:    $t = 0$ 
34:   for  $m = 1 : |\Omega|$  do
35:      $r = A(l, m) + r$ 
36:      $t = B(l, m) + t$ 
37:   end for            $\triangleright$  To obtain the average of  $SS$  and  $Abr$  values of all the  $T_i$ 
38:    $SS(\Omega, TIs) = \frac{r}{|\Omega|}$ 
39:    $Abr(\Omega, TIs) = \frac{t}{|\Omega|}$ 
40:    $C(l) = SS(\Omega, TIs)$ 
41:    $D(l) = Abr(\Omega, TIs)$ 
42: end for
43:  $disp(C)$             $\triangleright$  Give all 23  $SS$ -values of each TIs for data set  $\Omega$ 
44:  $disp(D)$             $\triangleright$  Give all 23  $Abr$ -values of each TIs for data set  $\Omega$ 

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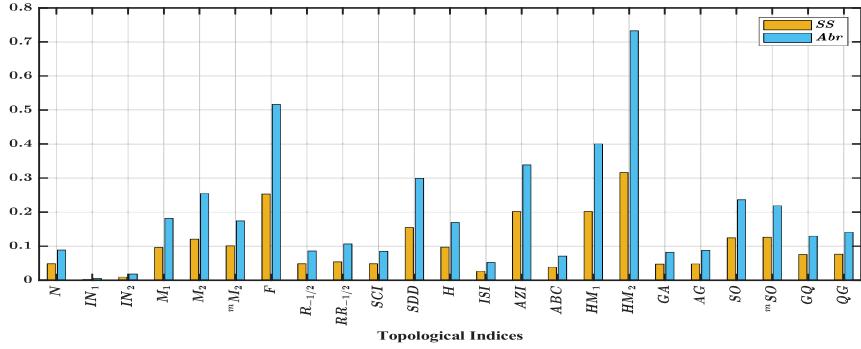


Figure 7. Comparison of *SS* and *Abr* of different topological indices for the data set of 23 trees with 8 vertices.

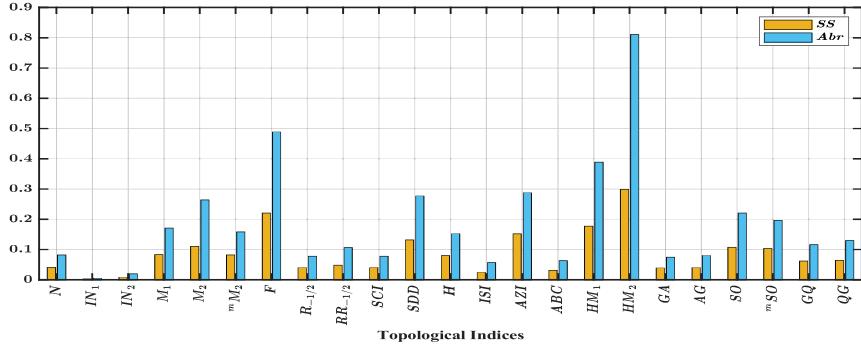


Figure 8. Comparison of *SS* and *Abr* of different topological indices for the data set of 47 trees with 9 vertices.

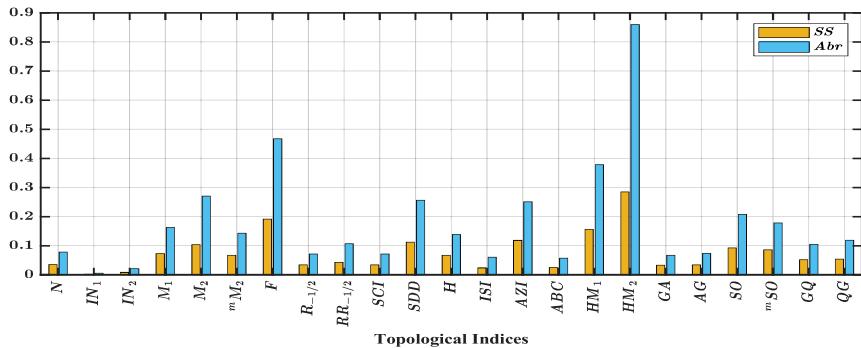


Figure 9. Comparison of *SS* and *Abr* of different topological indices for the data set of 106 trees with 10 vertices.

Table 5. Correlation coefficient among the different degree-based topological indices of decane isomers.

	N	IN_1	IN_2	M_1	M_2	mM_2	F	$R_{-1/2}$	$RR_{-1/2}$	SCI	SDD	H	ISI	AZI	ABC	HM ₁	HM ₂	GA	AG	SO	mSO	GQ	QG
N	1																						
IN_1	0.1457	1																					
IN_2	-0.099	-0.9789	1																				
M_1	0.9977	0.1515	-0.0228	1																			
M_2	0.9527	-0.1162	0.2847	0.9497	1																		
mM_2	-0.9423	-0.2888	0.1256	-0.9221	-0.5601	1																	
F	0.9709	0.2359	0.1223	0.9814	0.8905	-0.8765	1																
$R_{-1/2}$	-0.9834	-0.1843	0.6369	-0.9644	0.9217	0.9855	-0.9222	1															
$RR_{-1/2}$	0.9806	0.073	0.1842	0.9764	0.9627	0.8974	0.9310	0.9576	1														
SCI	-0.9889	-0.1479	0.0020	-0.0747	-0.9385	0.9577	-0.9292	0.9886	-0.9704	1													
SDD	0.9902	0.2688	-0.1378	0.9917	0.9660	-0.9429	0.9840	-0.9726	0.9154	-0.9738	1												
H	-0.9739	-0.1567	0.0001	-0.0547	-0.9397	0.9866	-0.9601	0.9983	-0.9512	0.9967	-0.9577	1											
ISI	0.0591	-0.9517	0.9943	0.0429	0.3469	0.0414	-0.0644	-0.0468	0.2566	-0.0776	-0.0691	-0.0786	1										
AZI	-0.8453	-0.4496	0.3163	-0.8223	-0.6895	0.9476	-0.7822	0.0663	-0.7639	0.8897	-0.8650	0.9087	0.2466	1									
ABC	0.9346	0.2954	-0.1323	0.932	0.8393	-0.9996	0.8589	-0.9818	0.8883	-0.9711	0.93541	-0.9838	-0.0482	-0.0511	1								
HM ₁	0.9814	0.1733	0.0578	0.9921	0.9285	0.8792	0.9974	0.9349	0.9541	0.9436	0.9849	0.9158	0.0921	0.7779	0.8685	1							
HM ₂	0.8652	-0.2012	0.4128	0.8583	0.9655	-0.7708	0.7904	-0.8412	0.8339	-0.8501	0.8927	-0.8444	0.41855	-0.5592	0.7588	0.8301	1						
GA	-0.9916	-0.1941	0.0485	-0.9815	-0.9284	0.9745	-0.9413	0.9969	-0.9641	0.9981	-0.9824	0.9925	-0.0258	0.8974	-0.9697	-0.9523	-0.8409	1					
AG	0.9945	0.2451	-0.1068	0.9920	0.9173	-0.9379	0.9728	-0.9850	0.9555	-0.9801	0.9978	-0.9737	-0.0371	-0.8796	0.9513	0.9772	0.8195	-0.9925	1				
SO	0.9968	0.1839	-0.0562	0.9994	0.9390	-0.9255	0.9864	-0.9606	0.93691	-0.9757	0.9949	-0.9559	0.0065	-0.8331	0.1969	0.9924	0.8428	-0.9823	0.9944	1			
mSO	-0.9619	-0.1228	-0.0356	-0.9415	-0.9161	0.9831	-0.8761	0.9981	-0.9490	0.9916	-0.9397	-0.1144	0.0975	-0.8983	-0.8533	-0.8948	-0.8456	-0.0591	-0.9398	1			
GQ	-0.9821	-0.1515	0.0029	0.3678	-0.9301	0.9739	-0.9149	0.9905	-0.9637	0.9979	-0.9646	0.9967	-0.0719	0.9015	0.41724	-0.9301	-0.8482	0.9967	0.7576	-0.9673	0.9935	1	
QG	0.9952	0.2326	-0.0936	0.9900	0.9213	-0.9631	0.9067	-0.9892	0.9589	-0.9904	0.9955	-0.9795	-0.0217	-0.8851	0.9569	0.9727	0.8285	-0.9957	0.9996	0.9929	-0.9605	-0.9851	1

Table 6. Statistical parameters of linear QSPR model for boiling point (BP) of octane isomers.

Linear Models	R	R ²	Adjusted-R ²	RMSE	SSE
$BP = -8.0910 \times N + 231.6000$	-0.7506	0.5633	0.5342	4.112	253.6000
$BP = -61.7500 \times IN_1 + 572.5000$	-0.1958	0.0384	-0.0258	6.1020	558.4000
$BP = 12.7500 \times IN_2 + 28.4200$	0.1246	0.0155	-0.0501	6.1740	571.7000
$BP = -1.7880 \times M_1 + 168.6000$	-0.7124	0.5076	0.4748	4.3660	286.0000
$BP = -0.7725 \times M_2 + 137.4000$	-0.4234	0.1793	0.1246	5.6370	476.6000
$BP = 34.3600 \times {}^mM_2 + 44.6300$	0.8824	0.7786	0.7639	2.9270	128.5000
$BP = -0.2487 \times F + 133.8000$	-0.6965	0.4851	0.4507	4.465	299.0000
$BP = 36.9200 \times R_{-1/2} - 21.3300$	0.84063	0.7067	0.6871	3.3700	170.3000
$BP = -5.2110 \times RR_{-1/2} + 187.7000$	-0.5622	0.3160	0.2704	5.1460	397.2000
$BP = 38.8200 \times SCI - 18.6100$	0.8151	0.6643	0.6419	3.6050	194.9000
$BP = -1.9840 \times SDD + 152.2000$	-0.8409	0.7071	0.6875	3.3680	170.1000
$BP = 20.5100 \times H + 44.7500$	0.8387	0.7034	0.6837	3.3880	172.2000
$BP = 3.4400 \times ISI + 91.5100$	0.0924	0.0085	-0.0576	6.1950	575.7000
$BP = 0.7829 \times AZI + 78.5600$	0.9176	0.8421	0.8315	2.4730	91.7100
$BP = -27.0200 \times ABC + 255.8000$	-0.8859	0.7849	0.7706	2.8860	124.9000
$BP = -0.1653 \times HM_1 + 137.2000$	-0.6318	0.3992	0.3591	4.8230	348.9000
$BP = -0.0319 \times HM_2 + 119.3000$	-0.2559	0.0655	0.0032	6.0150	542.7000
$BP = 22.2800 \times GA - 30.2700$	0.8408	0.7069	0.6874	3.3680	170.2000
$BP = -17.8600 \times AG + 249.9000$	-0.8414	0.7080	0.6885	3.3620	169.6000
$BP = -1.899 \times SO + 157.7000$	-0.7509	0.5638	0.5347	4.1090	253.3000
$BP = 23.1800 \times {}^mSO + 61.9600$	0.8347	0.6968	0.6766	3.4260	176.1000
$BP = 14.1400 \times GQ + 27.5400$	0.8376	0.7016	0.6817	3.3990	173.3000
$BP = -9.75405 \times QG + 193.4000$	-0.8414	0.7079	0.6884	3.3630	169.6000

Table 7. Statistical parameters of linear QSPR model for critical temperature (CT) of octane isomers.

Linear Models	R	R ²	Adjusted-R ²	RMSE	SSE
$CT = -1.9560 \times N + 319.2000$	-0.1244	0.0155	-0.0502	9.004	1216.0000
$CT = -339.3000 \times IN_1 + 2809.0000$	-0.7378	0.5443	0.5140	6.1260	562.8000
$CT = 106.6000 \times IN_2 - 425.6000$	0.7141	0.5100	0.4773	6.3520	605.3000
$CT = -0.2464 \times M_1 + 298.3000$	-0.0673	0.0045	-0.0618	9.0540	1230.0000
$CT = 0.7936 \times M_2 + 266.8000$	0.2982	0.0889	0.0282	8.6620	1125.0000
$CT = 26.7800 \times {}^mM_2 + 236.6000$	0.4717	0.2225	0.1706	8.0020	960.4000
$CT = -0.0321 \times F + 293.3000$	-0.0617	0.0038	-0.0626	9.0570	1231.0000
$CT = 19.2000 \times R_{-1/2} + 220.3000$	0.2997	0.0898	0.0292	8.6570	1124.0000
$CT = 1.9200 \times RR_{-1/2} + 263.7000$	0.1420	0.02016	-0.0452	8.9830	1210.0000
$CT = 16.5900 \times SCI + 234.1000$	0.2388	0.0570	-0.0058	8.8120	1165.0000
$CT = -1.0660 \times SDD + 311.2000$	-0.3098	0.0959	0.0357	8.6280	1117.0000
$CT = 10.4500 \times H + 255.4000$	0.2931	0.0859	0.0249	8.6760	1129.0000
$CT = 38.0300 \times ISI + 40.6700$	0.7007	0.4909	0.4570	6.4750	628.8000
$CT = 0.7581 \times AZI + 256.3000$	0.6092	0.3712	0.3292	7.1960	776.8000
$CT = -21.5100 \times ABC + 403.5000$	-0.4836	0.2338	0.1828	7.9430	946.4000
$CT = 0.0154 \times HM_1 + 288.6000$	0.0403	0.0016	-0.0649	9.0670	1233.0000
$CT = 0.0836 \times HM_2 + 277.1000$	0.4604	0.2119	0.1594	8.0560	973.4000
$CT = 11.3600 \times GA + 217.1000$	0.2940	0.0864	0.0255	8.6740	1128.0000
$CT = -9.4420 \times AG + 362.5000$	-0.3051	0.0931	0.0326	8.6420	1120.0000
$CT = -0.4847 \times SO + 301.9000$	-0.1314	0.0173	-0.0483	8.9960	1214.0000
$CT = 11.3700 \times {}^mSO + 265.2000$	0.2809	0.0789	0.0175	8.7090	1138.0000
$CT = 6.8810 \times GQ + 248.6000$	0.2794	0.0781	0.0166	8.7130	1139.0000
$CT = -5.0920 \times QG + 332.2000$	-0.3011	0.0907	0.0301	8.6530	1123.0000

Table 8. Statistical parameters of linear QSPR model for critical pressure (CP) of octane isomers.

Linear Models	R	R ²	Adjusted-R ²	RMSE	SSE
$CP = 1.5340 \times N + 4.2380$	0.6127	0.3754	0.3338	1.1420	19.5700
$CP = -66.5700 \times IN_1 + 520.6000$	-0.9089	0.8261	0.8145	0.6026	5.4480
$CP = 22.4100 \times IN_2 - 124.1000$	0.9427	0.8886	0.8812	0.4823	3.4900
$CP = 0.3830 \times M_1 + 14.8400$	0.6571	0.4318	0.3939	1.0890	17.8000
$CP = 0.3792 \times M_2 + 15.0600$	0.8950	0.8010	0.7877	0.6447	6.2340
$CP = -2.0480 \times {}^mM_2 + 30.6500$	-0.2265	0.0513	-0.0119	1.4080	29.7200
$CP = -0.0536 \times F + 22.2700$	0.6465	0.4180	0.3792	1.1030	18.2300
$CP = -4.5330 \times R_{-1/2} + 43.1400$	-0.4443	0.1974	0.1439	1.2950	25.1400
$CP = 1.7490 \times RR_{-1/2} + 1.8210$	0.8121	0.6595	0.6369	0.8432	10.6700
$CP = -5.6400 \times SCI + 45.7900$	-0.5098	0.2599	0.2106	1.2430	23.1800
$CP = 0.2346 \times SDD + 22.0000$	0.4281	0.1832	0.1288	1.3060	25.5900
$CP = -2.5740 \times H + 35.2100$	-0.4531	0.2053	0.1523	1.2880	24.8900
$CP = 8.2400 \times ISI - 27.6800$	0.9532	0.9086	0.9025	0.4368	2.8620
$CP = -0.0134 \times AZT + 27.1100$	-0.0674	0.0045	-0.0618	1.4420	31.1800
$CP = 1.5100 \times ABC + 18.5900$	0.2132	0.0455	-0.0182	1.4120	29.9000
$CP = 0.0444 \times HM_1 + 20.3200$	0.7305	0.5336	0.5025	0.9869	14.6100
$CP = 0.0274 \times HM_2 + 22.0100$	0.9480	0.8987	0.8920	0.4599	3.1730
$CP = -2.7970 \times GA + 44.6300$	-0.4545	0.2065	0.1536	1.287	24.8600
$CP = 2.1520 \times AG + 10.1500$	0.4366	0.1907	0.1367	1.3000	25.3500
$CP = 0.3537 \times SO + 18.3900$	0.6020	0.3625	0.3200	1.1540	19.9700
$CP = -3.0240 \times {}^mSO + 33.3100$	-0.4689	0.2199	0.1678	1.2760	24.4400
$CP = -1.8630 \times GQ + 37.9100$	-0.4752	0.2258	0.1742	1.272	24.25
$CP = 1.1930 \times QG + 16.8100$	0.4431	0.1964	0.1428	1.2960	25.1800

Table 9. Statistical parameters of linear QSPR model for heats of vaporization (HV) of octane isomers.

Linear Models	R	R ²	Adjusted-R ²	RMSE	SSE
$HV = -2.4330 \times N + 73.6600$	-0.9387	0.8811	0.8732	0.5157	3.9900
$HV = 12.8600 \times IN_1 - 57.1100$	0.1697	0.0288	-0.0359	32.5900	1.4740
$HV = -6.1490 \times IN_2 + 79.6800$	-0.2499	0.0625	-3.359e-05	1.448	31.4600
$HV = -0.5558 \times M_1 + 55.2900$	-0.9215	0.8492	0.8391	0.5809	5.0610
$HV = -0.3275 \times M_2 + 48.2400$	-0.7467	0.5576	0.5281	0.9948	14.8500
$HV = 8.4990 \times {}^mM_2 + 21.1700$	0.9081	0.8246	0.8130	0.6263	5.8840
$HV = -0.0777 \times F + 44.4900$	-0.9048	0.8187	0.8067	0.6368	6.082
$HV = 10.0800 \times R_{-1/2} + 1.3860$	0.9545	0.9110	0.9051	0.4462	2.9860
$HV = -1.8750 \times RR_{-1/2} + 64.8300$	-0.8417	0.7084	0.6889	0.8077	9.7850
$HV = 10.9600 \times SCI + 0.8975$	0.9569	0.9157	0.9101	0.4343	2.83
$HV = -0.5386 \times SDD + 48.700$	-0.9497	0.9020	0.8954	0.4683	3.2900
$HV = 5.6210 \times H + 19.3500$	0.9562	0.9143	0.9086	0.4378	2.8760
$HV = -2.5450 \times ISI + 55.0900$	-0.2844	0.0809	0.0196	1.4340	30.8400
$HV = 0.1806 \times AZT + 30.1600$	0.8804	0.7752	0.7602	0.7092	7.5440
$HV = -6.6460 \times ABC + 73.1900$	-0.9064	0.8215	0.8096	0.6319	5.9900
$HV = -0.0559 \times HM_1 + 46.0500$	-0.8772	0.7696	0.7542	0.7180	7.7320
$HV = -0.0184 \times HM_2 + 41.3700$	-0.6147	0.3779	0.3364	1.1800	20.8800
$HV = 6.1180 \times GA - 1.2970$	0.9606	0.9228	0.9176	0.4157	2.5920
$HV = -4.8660 \times AG + 75.3400$	-0.9538	0.9097	0.9037	0.4493	3.0280
$HV = -0.5691 \times SO + 51.4100$	-0.9361	0.8762	0.8680	0.5262	4.1530
$HV = 6.3990 \times {}^mSO + 23.9600$	0.9588	0.9192	0.9138	0.4251	2.7110
$HV = 3.9210 \times GQ + 14.3500$	0.9661	0.9334	0.9290	0.3859	2.2340
$HV = -2.6650 \times QG + 60.0300$	-0.9564	0.9147	0.9091	0.4367	2.8610

Table 10. Statistical parameters of linear QSPR model for molar refraction (MR) of octane isomers.

Linear Models	R	R ²	Adjusted-R ²	RMSE	SSE
$MR = -0.0909 \times N + 40.3400$	-0.2763	0.0763	0.0147	0.1827	0.5006
$MR = 9.4650 \times IN_1 - 31.2200$	0.9824	0.9652	0.9628	0.0355	0.0189
$MR = -3.0520 \times IN_2 + 59.5300$	-0.9762	0.9530	0.9498	0.0412	0.0255
$MR = -0.0255 \times M_1 + 39.7900$	-0.3284	0.1078	0.0484	0.1795	0.4835
$MR = -0.0375 \times M_2 + 40.1500$	-0.6723	0.4520	0.4155	0.1407	0.2970
$MR = -0.1629 \times {}^mM_2 + 39.3500$	-0.1369	0.0188	-0.0467	0.1883	0.5318
$MR = -0.0034 \times F + 39.2900$	-0.3083	0.0951	0.0347	0.1808	0.4904
$MR = 0.1207 \times R_{-1/2} + 38.5800$	0.0899	0.0081	-0.0580	0.1893	0.5376
$MR = -0.1548 \times RR_{-1/2} + 41.2100$	-0.5465	0.2987	0.2519	0.1592	0.3801
$MR = 0.2357 \times SCI + 38.2200$	0.1620	0.0263	-0.0387	0.1876	0.5277
$MR = -0.0042 \times SDD + 39.1000$	-0.0579	0.0033	-0.0631	0.1898	0.5402
$MR = 0.0765 \times H + 38.7600$	0.1024	0.0105	-0.0555	0.1891	0.5363
$MR = -1.1000 \times ISI + 46.2600$	-0.9676	0.9362	0.9320	0.0480	0.0346
$MR = -0.0073 \times AZI + 39.3500$	-0.2802	0.0785	0.0171	0.1825	0.4994
$MR = 0.1382 \times ABC + 38.3000$	0.1483	0.0219	-0.0432	0.1880	0.5301
$MR = -0.0033 \times HM_1 + 39.4900$	-0.4188	0.1754	0.1204	0.1726	0.4469
$MR = -0.0029 \times HM_2 + 39.5000$	-0.7667	0.5878	0.5604	0.1220	0.2234
$MR = 0.0747 \times GA + 38.5400$	0.0923	0.0085	-0.0576	0.1893	0.5374
$MR = -0.0447 \times AG + 39.3600$	-0.0689	0.0048	-0.0616	0.1896	0.5394
$MR = -0.0199 \times SO + 39.4800$	-0.2584	0.06677	0.0046	0.1836	0.5058
$MR = 0.1053 \times {}^mSO + 38.7800$	0.1241	0.0154	-0.0502	0.1886	0.5336
$MR = 0.0616 \times GQ + 38.6400$	0.1194	0.0143	-0.0515	0.1887	0.5342
$MR = -0.0273 \times QG + 39.2400$	-0.0772	0.0059	-0.0603	0.1895	0.5387

Table 11. Statistical parameters of linear QSPR model for molar volume (MV) of octane isomers.

Linear Models	R	R ²	Adjusted-R ²	RMSE	SSE
$MV = -0.9130 \times N + 174.4000$	-0.1993	0.0397	-0.0243	2.591	100.7000
$MV = 127.4000 \times IN_1 - 784.1000$	0.9503	0.9031	0.8967	0.8230	10.1600
$MV = -41.0400 \times IN_2 + 437.0000$	-0.9437	0.8906	0.8833	0.8746	11.4700
$MV = -0.2705 \times M_1 + 169.4000$	-0.2537	0.0644	0.0019	2.5580	98.1200
$MV = -0.4737 \times M_2 + 175.4000$	-0.6110	0.3733	0.3315	2.0930	65.7200
$MV = -3.4160 \times {}^mM_2 + 168.0000$	-0.2064	0.0426	-0.0212	2.5870	100.4000
$MV = -0.0363 \times F + 164.0000$	-0.2389	0.0571	-0.0058	2.5680	98.8900
$MV = 0.2273 \times R_{-1/2} + 160.3000$	0.0122	0.0001	-0.0665	2.6440	104.9000
$MV = -1.8700 \times RR_{-1/2} + 187.5000$	-0.4746	0.2253	0.1736	2.3270	81.2500
$MV = 1.6710 \times SCI + 155.4000$	0.0825	0.0068	-0.0594	2.6350	104.2000
$MV = 0.0152 \times SDD + 160.8000$	0.0151	0.0002	-0.0664	2.6440	104.9000
$MV = 0.2384 \times H + 160.3000$	0.0229	0.0005	-0.0661	2.6430	104.8000
$MV = -14.8000 \times ISI + 258.4000$	-0.9357	0.8756	0.8673	0.9327	13.0500
$MV = -0.1307 \times AZI + 167.1000$	-0.3604	0.1299	0.0719	2.4670	91.2500
$MV = 2.8380 \times ABC + 146.2000$	0.2190	0.0479	-0.0155	2.5800	99.8500
$MV = -0.0389 \times HM_1 + 166.5000$	-0.3504	0.1228	0.0643	2.4770	92.0000
$MV = -0.0385 \times HM_2 + 167.4000$	-0.7269	0.5284	0.4970	1.8160	49.4600
$MV = 0.1521 \times GA + 160.1000$	0.0135	0.0002	-0.0665	2.6440	104.9000
$MV = 0.0542 \times AG + 160.7000$	0.0060	3.614e-05	-0.0666	2.6440	104.9000
$MV = -0.1967 \times SO + 165.6000$	-0.1831	0.0335	-0.0309	2.5990	101.4000
$MV = 0.4938 \times {}^mSO + 160.0000$	0.0418	0.0018	-0.0648	2.6420	104.7000
$MV = 0.2628 \times GQ + 159.5000$	0.0366	0.0013	-0.0652	2.6420	104.7000
$MV = -0.0044 \times QG + 161.2000$	-0.0009	8.07e-07	-0.0667	2.6440	104.9000

Table 12. Statistical parameters of linear QSPR model for surface tension (ST) of octane isomers.

Linear Models	R	R ²	Adjusted-R ²	RMSE	SSE
$ST = -0.6265 \times N + 29.9400$	-0.3994	0.1595	0.1035	0.8300	10.3300
$ST = -28.8200 \times IN_1 + 234.8000$	-0.6281	0.3945	0.3542	0.7045	7.4440
$ST = 8.5520 \times IN_2 - 36.6300$	0.5743	0.3298	0.2851	0.7412	8.2400
$ST = -0.1260 \times M_1 + 24.6800$	-0.3452	0.1191	0.0604	0.8497	10.8300
$ST = 0.0087 \times M_2 + 20.5800$	0.0328	0.0011	-0.0655	0.9049	12.2800
$ST = 3.9850 \times {}^mM_2 + 12.7800$	0.7034	0.4948	0.4612	0.6435	6.2110
$ST = -0.0177 \times F + 22.2400$	-0.3414	0.1165	0.0576	0.8510	10.8600
$ST = 3.5730 \times R_{-1/2} + 7.7320$	0.5592	0.3127	0.2668	0.7506	8.4510
$ST = -0.1754 \times RR_{-1/2} + 23.3200$	-0.1300	0.0169	-0.0486	0.8977	12.0900
$ST = 3.4970 \times SCI + 8.8850$	0.5046	0.2546	0.2049	0.7816	9.1640
$ST = -0.1964 \times SDD + 24.6100$	-0.5720	0.3272	0.2823	0.7426	8.2720
$ST = 1.9650 \times H + 14.1900$	0.5524	0.3051	0.2588	0.7547	8.5430
$ST = 2.9630 \times ISI + 1.3560$	0.5472	0.2994	0.2527	0.7578	8.6130
$ST = 0.1001 \times AZI + 16.3000$	0.8064	0.6503	0.6270	0.5354	4.2990
$ST = -3.1620 \times ABC + 37.4200$	-0.7125	0.5076	0.4748	0.6353	6.0540
$ST = -0.0092 \times HM_1 + 22.1200$	-0.2407	0.0579	-0.0049	0.8787	11.5800
$ST = 0.0037 \times HM_2 + 20.2400$	0.2015	0.0406	-0.0233	0.8868	11.8000
$ST = 2.1480 \times GA + 6.9170$	0.5573	0.3106	0.2646	0.7517	8.4760
$ST = -1.7530 \times AG + 34.1700$	-0.5677	0.3223	0.2772	0.7453	8.3320
$ST = -0.1500 \times SO + 24.2800$	-0.4075	0.1661	0.1105	0.8268	10.2500
$ST = 2.1810 \times {}^mSO + 15.9300$	0.5398	0.2914	0.2442	0.7621	8.7120
$ST = 1.3340 \times GQ + 12.6800$	0.5429	0.2948	0.2478	0.7603	8.6700
$ST = -0.9516 \times QG + 28.5800$	-0.5641	0.3182	0.2728	0.7475	8.3820

Table 13. Statistical parameters of linear QSPR model for melting point (MP) of octane isomers.

Linear Models	R	R ²	Adjusted-R ²	RMSE	SSE
$MP = -9.6450 \times N + 307.5000$	-0.3204	0.1027	0.0211	18.3	3684
$MP = 157.3000 \times IN_1 - 1001.0000$	0.1773	0.0314	-0.0566	19.0100	3977.0000
$MP = -51.5100 \times IN_2 + 512.8000$	-0.1810	0.03276	-0.0552	19.0000	3971.0000
$MP = -2.2010 \times M_1 + 234.6000$	-0.3154	0.0995	0.0176	18.3300	3697.0000
$MP = -1.3440 \times M_2 + 207.7000$	-0.2711	0.0735	-0.0108	18.6000	3804.0000
$MP = 30.9800 \times {}^mM_2 + 104.9000$	0.2719	0.0739	-0.0103	18.5900	3802.0000
$MP = -0.3014 \times F + 191.4000$	-0.3017	0.0910	0.0084	18.4200	3732.0000
$MP = 39.2700 \times R_{-1/2} + 23.4900$	0.3142	0.0987	0.0168	18.3400	3700.0000
$MP = -7.7220 \times RR_{-1/2} + 276.3000$	-0.3052	0.0932	0.0107	18.4000	3723.0000
$MP = 43.1100 \times SCI + 20.1600$	0.3206	0.1028	0.0212	18.3000	3684.0000
$MP = -2.0950 \times SDD + 207.9000$	-0.3108	0.0966	0.0145	18.3600	3709.0000
$MP = 21.9100 \times H + 93.4300$	0.3153	0.0994	0.0176	18.3300	3697.0000
$MP = -18.5900 \times ISI + 288.9000$	-0.1805	0.0326	-0.0554	19.0000	3972.0000
$MP = 0.6401 \times AZI + 138.4000$	0.2531	0.0640	-0.0210	18.6900	3843.0000
$MP = -24.1100 \times ABC + 293.9000$	-0.2697	0.0728	-0.0115	18.6000	3807.0000
$MP = -0.2158 \times HM_1 + 197.5000$	-0.2979	0.0888	0.0059	18.4400	3741.0000
$MP = -0.0685 \times HM_2 + 178.3000$	-0.2021	0.0408	-0.0464	18.9200	3938.0000
$MP = 23.6800 \times GA + 14.1200$	0.3139	0.0986	0.0166	18.3400	3701.0000
$MP = -18.8900 \times AG + 311.2000$	-0.3118	0.0972	0.0152	18.3600	3706.0000
$MP = -2.2330 \times SO + 218.8000$	-0.3152	0.0994	0.0175	18.3300	3698.0000
$MP = 25.0200 \times {}^mSO + 111.2000$	0.3179	0.1011	0.0194	18.3200	3691.0000
$MP = 15.1900 \times GQ + 74.5800$	0.3171	0.1006	0.0188	18.3200	3693.0000
$MP = -10.3400 \times QG + 251.7000$	-0.3128	0.0978	0.0158	18.3500	3704.0000

Table 14. Statistical parameters of linear QSPR model for standard enthalpy of formation (DHF_{FORM}) of octane isomers.

Linear Models	R	R ²	Adjusted-R ²	RMSE	SSE
DHF _{FORM} = 0.0249 × N + 3.4150	0.0168	0.0003	-0.0664	0.8585	11.0600
DHF _{FORM} = -33.2600 × IN ₁ + 250.6000	0.7642	0.5842	0.5564	0.5537	4.599
DHF _{FORM} = 10.6604 × IN ₂ - 67.8800	0.7549	0.5699	0.5412	0.5631	4.7570
DHF _{FORM} = 0.0209 × M ₁ + 3.1420	0.0602	0.0036	-0.0628	0.8571	11.0200
DHF _{FORM} = 0.0972 × M ₂ 0.8439	0.3861	0.1491	0.09233	0.7920	9.4100
DHF _{FORM} = 1.5530 × ^m M ₂ 0.6357	0.2890	0.0835	0.0224	0.8220	10.1300
DHF _{FORM} = 0.0019 × F + 3.6220	0.0399	0.0016	-0.0649	0.8579	11.0400
DHF _{FORM} = 0.7610 × R _{-1/2} + 0.9849	0.1256	0.0158	-0.0499	0.8518	10.8800
DHF _{FORM} = 0.3326 × RR _{-1/2} - 0.9179	0.2599	0.0676	0.0054	0.8291	10.3100
DHF _{FORM} = 0.4802 × SCI + 2.1350	0.0731	0.0053	-0.0609	0.8563	11.0000
DHF _{FORM} = -0.0514 × SDD + 4.7630	-0.1578	0.0249	-0.0401	0.8479	104.0000
DHF _{FORM} = 0.3952 × H + 2.4400	0.1171	0.0137	-0.0520	0.8527	10.9100
DHF _{FORM} = 3.8350 × ISI + -21.4400	0.7468	0.5577	0.5282	0.5711	4.8920
DHF _{FORM} = 0.0498 × AZI + 1.5140	0.4231	0.1790	0.1243	0.778	9.0790
DHF _{FORM} = -1.2600 × ABC + 10.3800	-0.2994	0.0897	0.0289	0.8192	10.0700
DHF _{FORM} = 0.0051 × HM ₁ + 3.0730	0.1399	0.0196	-0.0458	0.8502	10.8400
DHF _{FORM} = 0.0087 × HM ₂ + 2.3570	0.5047	0.2547	0.2050	0.7413	8.2420
DHF _{FORM} = 0.5037 × GA + 0.5123	0.1378	0.0189	-0.0464	0.8504	10.8500
DHF _{FORM} = -0.4433 × AG + 7.1460	-0.1514	0.0229	-0.0422	0.8487	10.8100
DHF _{FORM} = -0.0009 × SO + 3.7980	-0.0026	6.783e - 06	-0.0667	0.8586	11.0600
DHF _{FORM} = 0.3944 × ^m SO + 2.8900	0.1029	0.0106	-0.0554	0.8541	10.9400
DHF _{FORM} = 0.2851 × GQ + 2.0320	0.1224	0.0149	-0.0507	0.8522	10.8900
DHF _{FORM} = -0.2347 × QG + 5.6850	-0.1467	0.0215	-0.0437	0.8493	10.8200

Table 15. Statistical parameters of linear QSPR model for density (DENS) of octane isomers.

Linear Models	R	R ²	Adjusted-R ²	RMSE	SSE
DENS = 0.042 × N + 0.6486	0.2068	0.0428	-0.0210	0.0114	0.0019
DENS = -0.5612 × IN ₁ - 779.8000	0.9512	0.9047	0.8984	0.0036	0.0002
DENS = 0.1810 × IN ₂ - 0.5070	0.9451	0.8933	0.8861	0.0038	0.0002
DENS = 0.0012 × M ₁ + 0.6718	0.2612	0.0682	0.0061	0.0112	0.0019
DENS = 0.0021 × M ₂ + 0.6456	0.6170	0.3807	0.3394	0.0092	0.0013
DENS = 0.0145 × ^m M ₂ + 0.6798	0.1995	0.0398	-0.0242	0.0114	0.0019
DENS = 0.0002 × F + 0.6962	0.2465	0.0608	-0.0018	0.0113	0.0019
DENS = -0.0016 × R _{-1/2} + 0.7151	-0.0196	0.0004	-0.0663	0.0116	0.0020
DENS = 0.0083 × RR _{-1/2} + 0.5913	0.4813	0.2316	0.1804	0.0102	0.0016
DENS = -0.0080 × SCI + 0.7366	-0.0900	0.0081	-0.0580	0.0116	0.0020
DENS = -3.354e - 05 × SDD + 0.7098	-0.0076	5.775e - 05	-0.0665	0.0116	0.0020
DENS = -0.0014 × H + 0.7139	-0.0304	0.0009	-0.0657	0.0116	0.0020
DENS = 0.0653 × ISI + 0.2800	0.9374	0.8786	0.8705	0.0041	0.0002
DENS = 0.0006 × AZI + 0.6836	0.3532	0.1247	0.0664	0.0109	0.0018
DENS = -0.0121 × ABC + 0.7726	-0.2120	0.0449	-0.0187	0.01138	0.0019
DENS = 0.0002 × HM ₁ + 0.6848	0.3577	0.1279	0.0698	0.0109	0.0018
DENS = 0.0002 × HM ₂ + 0.6812	0.7319	0.5356	0.5047	0.0079	0.0009
DENS = -0.0011 × GA + 0.7160	-0.0212	0.0005	-0.0662	0.01164	0.0020
DENS = 6.293e - 05 × AG + 0.7087	0.0016	2.512e - 06	-0.0667	0.0116	0.0020
DENS = 0.0009 × SO + 0.6885	0.1907	0.0342	-0.0302	2.5580	100.5000
DENS = -0.0026 × ^m SO + 0.7149	-0.0493	0.0024	-0.0641	0.0116	0.0020
DENS = -0.0014 × GQ + 0.7178	-0.0445	0.0019	-0.0646	0.0116	0.0020
DENS = 0.0002 × QG + 0.7077	0.0085	7.297e - 05	-0.0666	0.0116	0.0020

Table 16. Statistical parameters of linear QSPR model for total surface area (TSA) of octane isomers.

Linear Models	R	R ²	Adjusted-R ²	RMSE	SSE
TSA = -12.7700 × N + 572.5000	-0.4875	0.2376	0.1868	13.2100	2616.0000
TSA = 709.0000 × IN ₁ - 4875.0000	0.9249	0.8554	0.8458	5.7510	5.7510
TSA = -233.1000 × IN ₂ + 1954.0000	-0.9369	0.8778	0.8696	5.2880	419.4000
TSA = -3.1620 × M ₁ + 483.4000	-0.5183	0.2687	0.2199	12.9300	2510.0000
TSA = -3.4050 × M ₂ + 489.9000	-0.7679	0.5896	0.5623	9.6890	1408.0000
TSA = 14.4300 × ^m M ₂ + 357.9000	0.1525	0.0233	-0.0419	14.9500	3352.0000
TSA = -0.4099 × F + 419.5000	-0.4721	0.2229	0.1711	13.3300	2667.0000
TSA = 37.8000 × R _{-1/2} + 248.4000	0.3541	0.1254	0.0671	14.1500	3001.0000
TSA = -15.6900 × RR _{-1/2} + 608.6000	-0.6962	0.4848	0.4504	10.8600	1768.0000
TSA = 47.7600 × SCI + 223.8000	0.4124	0.1701	0.1148	13.7800	2848.0000
TSA = 1.7160 × SDD + 420.0000	-0.2992	0.0895	0.0288	14.4300	3124.0000
TSA = 21.9700 × H + 312.8000	0.3696	0.1366	0.0791	14.0500	2963.0000
TSA = -84.6500 × ISI + 943.8000	-0.9357	0.8755	0.8672	5.3370	427.3000
TSA = 0.0992 × AZI + 382.6000	0.0478	0.0023	-0.0642	15.1100	3424.0000
TSA = -10.8300 × ABC + 443.9000	-0.1460	0.0213	-0.0439	14.9600	3358.0000
TSA = -0.3602 × HM ₁ + 437.3000	-0.5663	0.3206	0.2754	12.4700	2331.0000
TSA = -0.2400 × HM ₂ + 426.4000	-0.7929	0.6288	0.6040	9.2150	1274.0000
TSA = 22.1300 × GA + 243.7000	0.3436	0.1180	0.0592	14.2000	3027.0000
TSA = -16.1900 × AG + 510.2000	-0.3139	0.0985	0.0384	14.3600	3094.0000
TSA = -2.8260 × SO + 451.9000	-0.4596	0.2112	0.1587	13.4300	2707.0000
TSA = 26.6700 × ^m SO + 327.1000	0.3951	0.1561	0.0998	13.8900	2896.0000
TSA = 15.4100 × GQ + 292.8000	0.3754	0.1409	0.0836	14.0200	2948.0000
TSA = -9.1370 × QG + 461.4000	-0.3242	0.1051	0.0455	14.3100	3071.0000