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

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

Require: Ω={Set of all trees with given number of vertices}

$A = Zeroes(|\Omega|, 23)$
$B = Zeroes(|\Omega|, 23)$
$C = Zeroes(1, 23)$
$D = Zeroes(1, 23)$
for $i = 1 : |\Omega|$ (for a tree T_i in n-vertex trees data set Ω) **do**
    $S = \{$Trees with $GED = 2$ from tree $T_i\}$ ▷ use Python networkx package to compute GED
    $E = [23\ TIs$ of tree $T_i]_{1\times 23}$ ▷ calculate TIs of tree T_i
    $F = [23\ TIs$ of the trees in set $S]_{23\times|S|}$ ▷ compute topological indices
    $G = Zeroes(23, |S|)$
    $H = Zeroes(1, 23)$
    $I = Zeroes(1, 23)$
    for $j = 1 : 23$ **do** ▷ Implementation of Step-3
        $p = 0$
        for $k = 1 : |S|$ **do**
            $q = \left|\frac{F(j,k)-E(j)}{E(j)}\right|$
            $p = q + p$
            $G(j, k) = q$
        end for
        $SS(T_i, TIs) = \frac{p}{|S|}$
        $Abr(T_i, TIs) = \max(G(j); :)$
        $H(j) = SS(T_i, TIs)$ ▷ Give all 23 SS-values of each TIs for a tree T_i
        $I(j) = Abr(T_i, TIs)$ ▷ Give all 23 Abr-values of each TIs for a tree T_i
    end for
    $disp(H)$
    $disp(I)$
    $A(i, :) = H(1, :)$
    $B(i, :) = I(1, :)$
end for
$disp(A)$
$disp(B)$
for $l = 1 : 23$ **do** ▷ Implementation of Step-4
    $r = 0$
    $t = 0$
    for $m = 1 : |\Omega|$ **do**
        $r = A(l, m) + r$
        $t = B(l, m) + t$
    end for ▷ To obtain the average of SS and Abr values of all the T_i
    $SS(\Omega, TIs) = \frac{r}{|\Omega|}$
    $Abr(\Omega, TIs) = \frac{t}{|\Omega|}$
    $C(l) = SS(\Omega, TIs)$
    $D(l) = Abr(\Omega, TIs)$
end for
$disp(C)$ ▷ Give all 23 SS-values of each TIs for data set Ω
$disp(D)$ ▷ Give all 23 Abr-values of each TIs for data set Ω

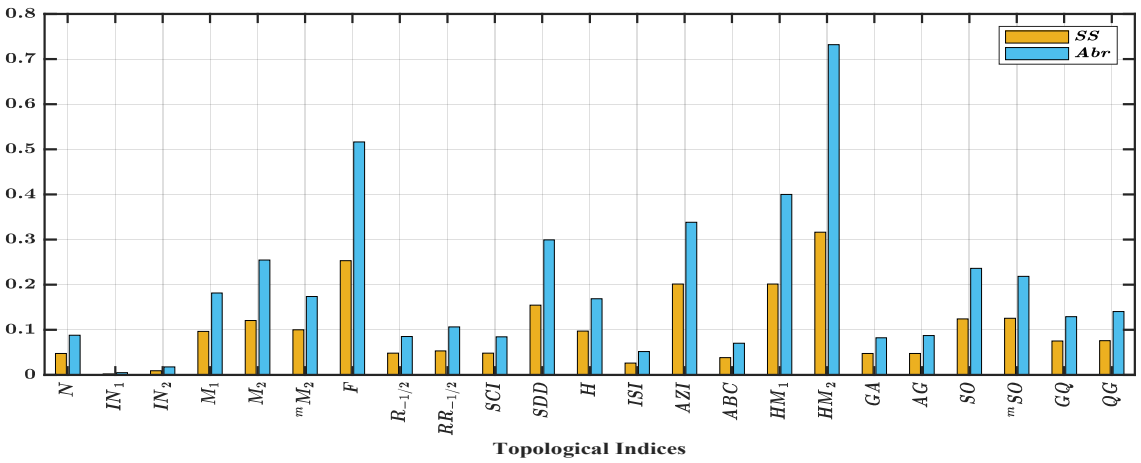

Figure 7. Comparison of SS and Abr of different topological indices for the data set of 23 trees with 8 vertices.

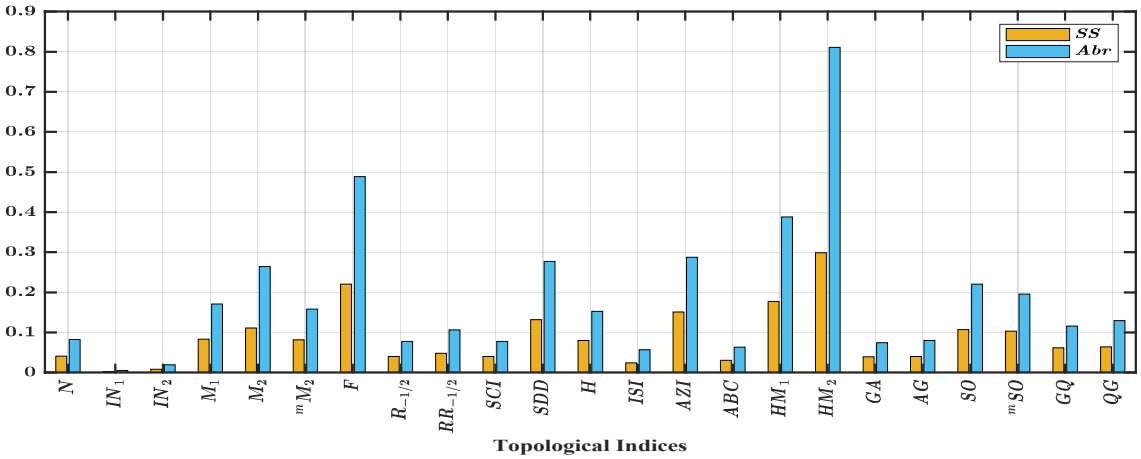

Figure 8. Comparison of SS and Abr of different topological indices for the data set of 47 trees with 9 vertices.

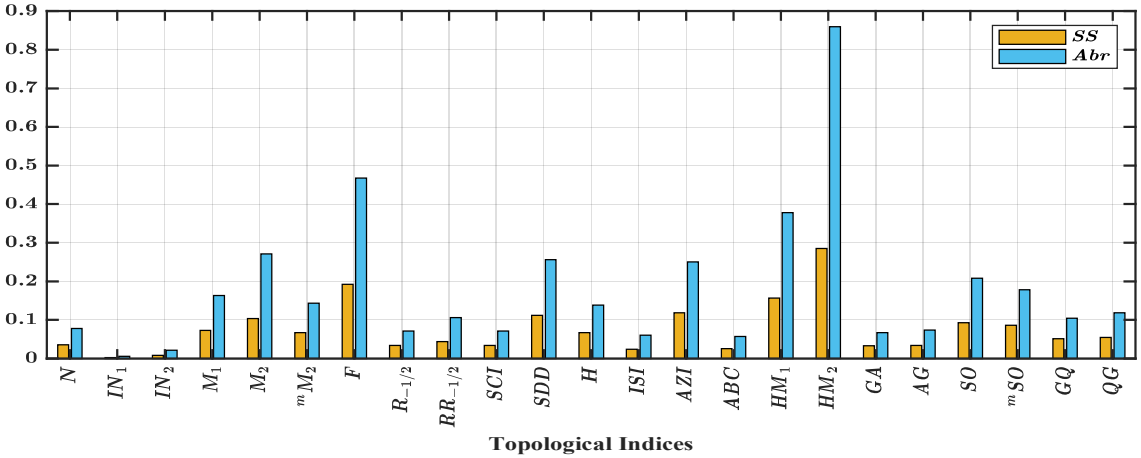

Figure 9. Comparison of SS and Abr of different topological indices for the data set of 106 trees with 10 vertices.

Table 3. 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	−0.0099	−0.9789	1																				
M_1	**0.9977**	0.1515	−0.0228	1																			
M_2	0.9527	−0.1452	0.2817	0.9497	1																		
${}^mM_2$	−0.9423	−0.2888	0.1256	−0.9221	−0.8501	1																	
F	0.9709	0.2319	−0.1223	0.9841	0.8995	−0.8705	1																
$R_{-1/2}$	−0.9831	−0.1843	0.0309	−0.9694	−0.9217	0.9855	−0.9222	1															
$RR_{-1/2}$	0.9806	−0.0473	0.1842	0.9764	**0.9927**	−0.8974	0.9310	−0.9576	1														
SCI	−0.9889	−0.1479	−0.0020	−0.9767	−0.9385	0.9757	−0.9292	**0.9986**	−0.9704	1													
SDD	**0.9902**	0.2688	−0.1378	**0.9917**	0.9060	−0.9429	0.9840	−0.9726	0.9454	−0.9738	1												
H	−0.9739	−0.1567	0.0001	−0.9567	−0.9197	0.9866	−0.9001	**0.9983**	−0.9542	**0.9967**	−0.9577	1											
ISI	0.0591	−0.9517	**0.9943**	0.0429	0.3469	0.0414	−0.0644	−0.0468	0.2506	−0.0776	−0.0691	−0.0786	1										
AZI	−0.8453	−0.4496	0.3163	−0.8223	−0.6895	0.9476	−0.7822	0.9063	−0.7639	0.8897	−0.8650	0.9087	0.2466	1									
ABC	0.9346	0.2954	−0.1323	0.9132	0.8393	**-0.9996**	0.8599	−0.9818	0.8883	−0.9711	0.93541	−0.9838	−0.0482	−0.9541	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	0.0021	−0.7779	0.8685	1							
HM_2	0.8652	−0.2612	0.4128	0.8583	0.9655	−0.7708	0.7904	−0.8412	0.9339	−0.8591	0.8027	−0.8444	0.4855	−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	−0.1083	**0.9920**	0.9173	−0.9579	0.9728	−0.9850	0.9555	−0.9861	**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	−0.9696	0.9691	−0.9757	**0.9949**	−0.9559	0.0095	−0.8331	0.9169	**0.9924**	0.8428	−0.9823	**0.9944**	1			
${}^mSO$	−0.9619	−0.1228	−0.0356	−0.9415	−0.9161	0.9831	−0.8761	**0.9931**	−0.9490	**0.9916**	−0.9397	**0.9982**	−0.1144	0.9075	−0.9813	−0.8948	−0.8453	0.9846	−0.9591	−0.9398	1		
GQ	−0.9824	−0.1515	0.0029	−0.9678	−0.9301	0.9759	−0.9149	**0.9965**	−0.9637	**0.9979**	−0.9646	**0.9967**	−0.0719	0.9015	−0.9724	−0.9301	−0.8482	**0.9967**	−0.9796	−0.9673	**0.9935**	1	
QG	**0.9952**	0.2326	−0.0936	**0.9909**	0.9213	−0.9631	0.9667	−0.9892	0.9589	**-0.9904**	**0.9955**	−0.9795	−0.0217	−0.8851	0.9569	0.9727	0.8258	**-0.9957**	**0.9996**	**0.9929**	−0.9665	−0.9851	1

Table 4. Physical properties of octane isomers

Physical properties → / Octane isomers ↓	BP	CT	CP	HV	MR	MV	ST	MP	DHFORM	DENS	TSA
n-Octane	125.6650	296.2000	24.6400	41.4800	39.1922	162.6050	21.7600	216.3000	4.1400	0.7025	415.3000
2-Methyl heptane	117.6470	288.0000	24.8000	39.6800	39.2316	163.6530	20.6000	164.1600	3.0600	0.6980	407.8500
3-Methyl heptane	118.9250	292.0000	25.6000	39.8300	39.1001	161.8450	21.1700	152.6000	3.2900	0.7058	397.3400
4-Methyl heptane	117.7090	290.0000	25.6000	39.6700	39.1174	162.1200	21.0000	152.0000	4.0000	0.7046	396.0400
3-Ethyl hexane	118.5340	292.0000	25.7400	39.4000	38.9400	160.0760	21.5100	–	3.5900	0.7136	379.0400
2,2-Dimethyl hexane	106.8400	279.0000	25.6000	37.2900	39.2500	164.2890	19.6000	151.9700	2.5600	0.6953	405.1100
2,3-Dimethyl hexane	115.6070	293.0000	26.6000	38.7900	38.9800	160.4130	20.9900	–	4.2300	0.7121	384.9300
2,4-Dimethyl hexane	109.4290	282.0000	25.8000	37.7600	39.1300	163.0930	20.0500	–	2.8000	0.7004	388.1100
2,5-Dimethyl hexane	109.1030	279.0000	25.0000	37.8600	39.2500	164.7150	19.7300	182.0000	2.5000	0.6935	395.0800
3,3-Dimethyl hexane	111.9690	290.8400	27.2000	37.9300	39.0000	160.8870	20.6300	147.0000	3.1700	0.7100	389.7900
3,4-Dimethyl hexane	117.7250	298.0000	27.4000	39.0200	38.8400	158.6530	21.6400	–	4.9700	0.7200	376.9100
3-Ethyl-2-methyl pentane	115.4500	295.0000	27.4000	38.5200	38.8300	158.8070	21.5200	158.2000	5.0800	0.7193	368.1000
3-Ethyl-3-methyl pentane	118.2590	305.0000	28.9000	37.9900	38.7100	157.0390	21.9900	182.2000	4.7600	0.7274	366.9900
2,2,3-Trimethyl pentane	109.841	294.0000	28.2000	36.9100	38.9200	159.51700	20.6700	160.8900	4.0900	0.7161	371.7500
2,2,4-Trimethyl pentane	99.2380	271.1500	25.5000	35.1300	39.2600	165.0960	18.7700	165.8000	3.1300	0.6919	392.1900
2,3,3-Trimethyl pentane	114.7600	303.0000	29.0000	37.2200	38.7600	157.2980	21.5600	172.2200	4.5200	0.7262	377.4000
2,3,4-Trimethyl pentane	113.467	295.0000	27.6000	37.6100	38.8600	158.8510	21.1400	163.9000	4.3200	0.7191	368.9300

Table 5. Topological indices of octane isomers

Topological indices → / Octane isomers ↓	N	IN_1	IN_2	${}^mM_2$	SDD	ISI	HM_1	HM_2	AG	SO	${}^mSO$	GQ	QG
Octane	13.4641	7.4495	6.6329	2.2500	15.0000	6.3333	98.0000	88.0000	7.1213	18.6143	2.6622	6.7889	7.2361
2-Methyl heptane	13.9681	7.4470	6.6439	2.0833	17.3333	6.3667	114.0000	106.0000	7.3907	20.6515	2.4177	6.4044	7.7409
3-Methyl heptane	13.9362	7.4299	6.6899	2.16667	16.6667	6.4833	116.0000	121.0000	7.3173	20.5024	2.4725	6.4850	7.6087
4-Methyl heptane	13.9362	7.4299	6.6899	2.1667	16.6667	6.4833	116.0000	121.0000	7.3173	20.5024	2.4725	6.4850	7.6087
3-Ethyl hexane	13.9043	7.4128	6.7358	2.2500	16.0000	6.6000	118.0000	136.0000	7.2438	20.3533	2.5272	6.5656	7.4766
2,2-Dimethyl hexane	14.8897	7.4448	6.6545	1.8750	21.7500	6.4000	152.0000	148.0000	7.8713	24.7344	2.1055	5.8468	8.6093
2,3-Dimethyl hexane	14.4176	7.4182	6.7347	2.0278	18.6667	6.6167	134.0000	164.0000	7.5454	22.3995	2.2625	6.1789	8.0319
2,4-Dimethyl hexane	14.4402	7.4274	6.7009	2.0000	19.0000	6.5167	132.0000	139.0000	7.5866	22.5395	2.2279	6.1005	8.1135
2,5-Dimethyl hexane	14.4721	7.4445	6.6550	1.9167	19.6667	6.4000	130.0000	124.0000	7.6600	22.6886	2.1732	6.0199	8.2456
3,3-Dimethyl hexane	14.8352	7.4176	6.7312	2.0000	20.5000	6.6000	156.0000	184.0000	7.7426	24.4914	2.1803	5.9497	8.3876
3,4-Dimethyl hexane	14.3857	7.4011	6.7806	2.1111	18.0000	6.7333	136.0000	179.0000	7.4719	22.2504	2.3173	6.2596	7.8997
3-Ethyl-2-methyl pentane	14.3857	7.4011	6.7806	2.1111	18.0000	6.7333	136.0000	179.0000	7.4719	22.2504	2.3173	6.2596	7.8997
3-Ethyl-3-methyl pentane	14.7807	7.3903	6.8080	2.1250	19.2500	6.8000	160.0000	220.0000	7.6139	24.2477	2.2550	6.0526	8.1659
2,2,3-Trimethyl pentane	15.3221	7.4102	6.7705	1.8333	22.8333	6.7309	174.0000	241.0000	7.9963	26.3732	1.9684	5.6676	8.8437
2,2,4-Trimethyl pentane	15.3937	7.4424	6.6655	1.7083	24.0833	6.4333	168.0000	166.0000	8.1407	26.7716	1.8610	5.4624	9.1141
2,3,3-Trimethyl pentane	15.2994	7.4000	6.8014	1.8750	22.2500	6.8143	176.0000	262.0000	7.9411	26.2789	1.9883	5.6898	8.7541
2,3,4-Trimethyl pentane	14.8989	7.4065	6.7796	1.8889	20.6667	6.7500	152.0000	207.0000	7.7735	24.2967	2.0525	5.8730	8.4550

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	1139.000
$CT = -5.0920 \times QG + 332.2000$	-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
$CP = -0.0134 \times AZI + 27.1100$	-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
$HV = 8.4990 \times {}^{m}M_2 + 21.1700$	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
$HV = 0.1806 \times AZI + 30.1600$	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
$HV = -0.0552 \times HM_1 + 46.0500$	-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
$HV = 6.3990 \times {}^{m}SO + 23.9600$	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
$MR = -0.0252 \times M_1 + 39.7900$	-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
$MR = -0.1629 \times {}^{m}M_2 + 39.3500$	-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
$MR = 0.1053 \times {}^{m}SO + 38.7800$	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
$MP = 30.9800 \times {}^m M_2 + 104.9000$	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
$MP = 25.0200 \times {}^m SO + 111.2000$	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 (DHFORM) of octane isomers.

Linear Models	R	R^2	**Adjusted**$-R^2$	$RMSE$	SSE
$DHFORM = 0.0249 \times N + 3.4150$	0.0168	0.0003	-0.0664	0.8585	11.0600
$DHFORM = -33.2600 \times IN_1 + 250.6000$	**0.7642**	**0.5842**	0.5564	0.5537	4.599
$DHFORM = 10.6600 \times IN_2 - 67.8800$	0.7549	0.5699	0.5412	0.5631	4.7570
$DHFORM = 0.0209 \times M_1 + 3.1420$	0.0602	0.0036	-0.0628	0.8571	11.0200
$DHFORM = 0.0972 \times M_2 0.8439$	0.3861	0.1491	0.09233	0.7920	9.4100
$DHFORM = 1.5530 \times {}^m M_2 0.6357$	0.2890	0.0835	0.0224	0.8220	10.1300
$DHFORM = 0.0019 \times F + 3.6220$	0.0399	0.0016	-0.0649	0.8579	11.0400
$DHFORM = 0.7610 \times R_{-1/2} + 0.9849$	0.1256	0.0158	-0.0499	0.8518	10.8800
$DHFORM = 0.3326 \times RR_{-1/2} - 0.9179$	0.2599	0.0676	0.0054	0.8291	10.3100
$DHFORM = 0.4802 \times SCI + 2.1350$	0.0731	0.0053	-0.0609	0.8563	11.0000
$DHFORM = -0.0514 \times SDD + 4.7630$	-0.1578	0.0249	-0.0401	0.8479	104.0000
$DHFORM = 0.3952 \times H + 2.4400$	0.1171	0.0137	-0.0520	0.8527	10.9100
$DHFORM = 3.8350 \times ISI + -21.4400$	0.7468	0.5577	0.5282	0.5711	4.8920
$DHFORM = 0.0498 \times AZI + 1.5140$	0.4231	0.1790	0.1243	0.778	9.0790
$DHFORM = -1.2600 \times ABC + 10.3800$	-0.2994	0.0897	0.0289	0.8192	10.0700
$DHFORM = 0.0051 \times HM_1 + 3.0730$	0.1399	0.0196	-0.0458	0.8502	10.8400
$DHFORM = 0.0087 \times HM_2 + 2.3570$	0.5047	0.2547	0.2050	0.7413	8.2420
$DHFORM = 0.5037 \times GA + 0.5123$	0.1378	0.0189	-0.0464	0.8504	10.8500
$DHFORM = -0.4433 \times AG + 7.1460$	-0.1514	0.0229	-0.0422	0.8487	10.8100
$DHFORM = -0.0009 \times SO + 3.7980$	-0.0026	$6.783e-06$	-0.0667	0.8586	11.0600
$DHFORM = 0.3944 \times {}^m SO + 2.8900$	0.1029	0.0106	-0.0554	0.8541	10.9400
$DHFORM = 0.2851 \times GQ + 2.0320$	0.1224	0.0149	-0.0507	0.8522	10.8900
$DHFORM = -0.2347 \times QG + 5.6850$	-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
$DENS = 0.0042 \times N + 0.6486$	0.2068	0.0428	-0.0210	0.0114	0.0019
$DENS = -0.5612 \times IN_1 - 779.8000$	$\mathbf{-0.9512}$	**0.9047**	0.8984	0.0036	0.0002
$DENS = 0.1810 \times IN_2 - 0.5070$	0.9451	0.8933	0.8861	0.0038	0.0002
$DENS = 0.0012 \times M_1 + 0.6718$	0.2612	0.0682	0.0061	0.0112	0.0019
$DENS = 0.0021 \times M_2 + 0.6456$	0.6170	0.3807	0.3394	0.0092	0.0013
$DENS = 0.0145 \times {}^mM_2 + 0.6798$	0.1995	0.0398	-0.0242	0.0114	0.0019
$DENS = 0.0002 \times F + 0.6962$	0.2465	0.0608	-0.0018	0.0113	0.0019
$DENS = -0.0016 \times R_{-1/2} + 0.7151$	-0.0196	0.0004	-0.0663	0.0116	0.0020
$DENS = 0.0083 \times RR_{-1/2} + 0.5913$	0.4813	0.2316	0.1804	0.0102	0.0016
$DENS = -0.0080 \times SCI + 0.7366$	-0.0900	0.0081	-0.0580	0.0116	0.0020
$DENS = -3.354e-05 \times SDD + 0.7098$	-0.0076	$5.775e-05$	-0.0665	0.0116	0.0020
$DENS = -0.0014 \times H + 0.7139$	-0.0304	0.0009	-0.0657	0.0116	0.0020
$DENS = 0.0653 \times ISI + 0.2800$	0.9374	0.8786	0.8705	0.0041	0.0002
$DENS = 0.0006 \times AZI + 0.6836$	0.3532	0.1247	0.0664	0.0109	0.0018
$DENS = -0.0121 \times ABC + 0.7726$	-0.2120	0.0449	-0.0187	0.01138	0.0019
$DENS = 0.0002 \times HM_1 + 0.6848$	0.3577	0.1279	0.0698	0.0109	0.0018
$DENS = 0.0002 \times HM_2 + 0.6812$	0.7319	0.5356	0.5047	0.0079	0.0009
$DENS = -0.0011 \times GA + 0.7160$	-0.0212	0.0005	-0.0662	0.01164	0.0020
$DENS = 6.293e-05 \times AG + 0.7087$	0.0016	$2.512e-06$	-0.0667	0.0116	0.0020
$DENS = 0.0009 \times SO + 0.6885$	0.1907	0.0342	-0.0302	2.5880	100.5000
$DENS = -0.0026 \times {}^mSO + 0.7149$	-0.0493	0.0024	-0.0641	0.0116	0.0020
$DENS = -0.0014 \times GQ + 0.7178$	-0.0445	0.0019	-0.0646	0.0116	0.0020
$DENS = 0.0002 \times QG + 0.7077$	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
$TSA = -12.7700 \times N + 572.5000$	-0.4875	0.2376	0.1868	13.2100	2616.0000
$TSA = 709.0000 \times IN_1 - 4875.0000$	0.9249	0.8554	0.8458	5.7510	5.7510
$TSA = -233.1000 \times IN_2 + 1954.0000$	$\mathbf{-0.9369}$	**0.8778**	0.8696	5.2880	419.4000
$TSA = -3.1620 \times M_1 + 483.4000$	-0.5183	0.2687	0.2199	12.9300	2510.0000
$TSA = -3.4050 \times M_2 + 489.9000$	-0.7679	0.5896	0.5623	9.6890	1408.0000
$TSA = 14.4300 \times {}^mM_2 + 357.9000$	0.1525	0.0233	-0.0419	14.9500	3352.0000
$TSA = -0.4099 \times F + 419.5000$	-0.4721	0.2229	0.1711	13.3300	2667.0000
$TSA = 37.8000 \times R_{-1/2} + 248.4000$	0.3541	0.1254	0.0671	14.1500	3001.0000
$TSA = -15.6900 \times RR_{-1/2} + 608.6000$	-0.6962	0.4848	0.4504	10.8600	1768.0000
$TSA = 47.7600 \times SCI + 223.8000$	0.4124	0.1701	0.1148	13.7800	2848.0000
$TSA = 1.7160 \times SDD + 420.0000$	-0.2992	0.0895	0.0288	14.4300	3124.0000
$TSA = 21.9700 \times H + 312.8000$	0.3696	0.1366	0.0791	14.0500	2963.0000
$TSA = -84.6500 \times ISI + 943.8000$	-0.9357	0.8755	0.8672	5.3370	427.3000
$TSA = 0.0992 \times AZI + 382.6000$	0.0478	0.0023	-0.0642	15.1100	3424.0000
$TSA = -10.8300 \times ABC + 443.9000$	-0.1460	0.0213	-0.0439	14.9600	3358.0000
$TSA = -0.3602 \times HM_1 + 437.3000$	-0.5663	0.3206	0.2754	12.4700	2331.0000
$TSA = -0.2400 \times HM_2 + 426.4000$	-0.7929	0.6288	0.6040	9.2150	1274.0000
$TSA = 22.1300 \times GA + 243.7000$	0.3436	0.1180	0.0592	14.2000	3027.0000
$TSA = -16.1900 \times AG + 510.2000$	-0.3139	0.0985	0.0384	14.3600	3094.0000
$TSA = -2.8260 \times SO + 451.9000$	-0.4596	0.2112	0.1587	13.4300	2707.0000
$TSA = 26.6700 \times {}^mSO + 327.1000$	0.3951	0.1561	0.0998	13.8900	2896.0000
$TSA = 15.4100 \times GQ + 292.8000$	0.3754	0.1409	0.0836	14.0200	2948.0000
$TSA = -9.1370 \times QG + 461.4000$	-0.3242	0.1051	0.0455	14.3100	3071.0000