

Screening Rules for Leads of Fungicides, Herbicides, and Insecticides[†]

Bin Liu,[§] Fucheng Zhu,[§] Ying Huang,[§] Yuhui Wang,[§] Fei Yu,[§] Botao Fan,[#] and Jianhua Yao^{*,§}

⁸Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Road, Shanghai, China, and [#]ITODYS, University of Paris 7, Bâtiment Lavoisier 15, rue Jean Antoine de Baïf, 75205 Paris Cedex 13, France

To increase efficiency of finding leads in pesticide design, reasonable screening rules for leads of fungicide, herbicide, and insecticide, respectively, are desired. Previous works showed that "Rule 5" of Lipinski is not a suitable screening rule for leads of pesticide and proposed rules for leads of fungicide, insecticide, and herbicide, which were combined by logarithmic ratio of octanol-water partition coefficient (log *P*), number of hydrogen bond donors, molecular weight, number of hydrogen bond acceptors, polar surface area, carcinogenic toxicity, and mutagenic toxicity. Herein, three sets of screening rules for leads of fungicide, insecticide, and herbicide, respectively, are presented. Each set of screening rules involves seven descriptors, which were selected by Kolmogorov–Smirnov test, ANOVA, Kruskal–Wallis test, and Pearson product-moment correlation, from more than 450 descriptors calculated by Codessa. Their accuracies are about 82, 83, and 89%, respectively.

KEYWORDS: Screening rules; fungicide; insecticide; herbicide; descriptors

INTRODUCTION

Pesticides are applied in farming more seriously because the protection of the environment and human health is paid more attention. At present, the standards for evaluating satisfactory pesticides are maximum effects, minimum toxicity, and environmental friendliness. Drawbacks of traditional approaches used in pesticide design in cost and pollution had appeared. Now, an in silico approach is widely applied in pesticide design because of its advantages. Screening rule is the key of in silico screening. Reasonable screening rules are necessary and important to estimate the potential of compounds to become leads of pesticides.

There were a few published works about screening rules for leads of pesticides. Tice confirmed that Lipinski's "rule of 5" is not fit to determine whether a compound is a possible lead of agrochemicals and proposed screening rules for insecticides and pre-emergence and postemergence herbicides, respectively, which included the molecular properties molecular mass, log P, hydrogen bond donor, hydrogen bond acceptor, polar surface area (PSA), and rotatable bonds (1, 2). Our previous work proposed a set of screening rules combining the molecular properties log P, molecular weight (MW), number of hydrogen bond acceptors (NHA), number of hydrogen bond donors (NHD), PSA, mutagenic toxicity, and carcinogenic toxicity for leads of herbicides, fungicides, and insecticides, respectively (3). Unfortunately, their accuracies are not satisfactory in estimating leads of herbicides, fungicides, or insecticides. Therefore, to find more accurate screening rules, more molecular properties or descriptors should be calculated and analyzed.

In this work, more than 1000 compounds that had one of three bioactivities, fungicide, herbicide, or insecticide, were investigated. More than 450 descriptors of every compound were calculated by Codessa (Comprehensive Descriptors for Structural and Statistical Analysis, v2.63) (4). The descriptors are classified into six types: constitutional, that is, relative number of single bonds, gravitation index, etc.; topological, that is, average bonding information content (order 1), Kier and Hall index (order 2), Randic index (order 0), etc.; geometrical, that is, XY shadow, ZX shadow, etc.; electrostatic, that is, atomic charge weighted PPSA, atomic charge weighted PNSA, etc.; quantum-chemical, that is, total charge weighted PPSA, fractional PPSA (PPSA-2/TMSA), etc.; thermodynamics, that is, final heat of formation, internal entropy (300 K), and so on (5). The distributions of the descriptors were analyzed by using the Kolmogorov-Smirnov test (6), ANOVA (7, 8), and the Kruskal-Wallis test (9, 10). Their correlation is calculated by Pearson product-moment correlation (11, 12).

Herein, we will propose three sets of screening rules for leads of fungicides, herbicides, and insecticides, respectively, which combined seven irredundant descriptors except for the properties mentioned in previous works. They are a complement of the previous screening rules (1-3).

MATERIALS AND METHODS

Data. In this work, 1285 agrochemicals were selected from various reference sources including the *e-Pesticide Manual (13)*, a book,

[†]Part of the ECUST-Qian Pesticide Cluster.

^{*}Corresponding author (telephone +86-21-54925266; fax +86-21-54925264; e-mail yaojh@mail.sioc.ac.cn).

	I able I.	TUU CUMPUUNUS		erungicide	ITallilly	Sei
--	-----------	---------------	--	------------	-----------	-----

training	9	training	g
set ID	compound	set ID	compound
2	etaconazole	113	bupirimate
3	tecoram	114	thiophanate
5	zarilamid	117	cvpendazole
6	trichlamide	119	kasugamycin
9	2,4-dinitro-6-(1-	124	ofurace
	propylpentyl)phenyl		
	metnyl carbonate	405	loss and the second second
10	tenpropimorpn	125	kresoxim-metnyi
12	Lebucoriazole	120	capialol
13	1 <i>H</i> -imidazole-1-ethanol	120	mecarbinziu
15	quintozene	130	oxycarboxin
17	thioquinox	131	cymoxanil
18	penconazole	136	fludioxonil
20	azaconazole	138	cyproconazole
22	cyprodinil	139	famoxadone
23	milneb	142	iminoctadine
24	anilazine	143	falimorph
25	drazoxolon	144	tridemorph (mixture)
28	thiochlorfenphim	154	spiroxamine
30	mucochloric anhydride	155	thiram
34	fluazinam	159	thiabendazole
36	debacarb	165	ethaboxam
39	natamycin	170	nuarimol
40	ethoxyquin	171	pefurazoate
42	furalaxyl	172	iprovalicarb
43	furametpyr	180	rabenzazole
44	thicyofen	182	tioxymid
45	cyprofuram	183	buthiobate
52	fuberidazole	185	fenaminosulf
57	captan	186	2-(1-ethylhexyl)-4,6-dinitrophenyl methyl carbonate
58	benalaxyl	188	sultropen
66	dichlofluanid	190	2-butanamine
68	azithiram	191	diclobutrazol
69	dichlone	192	isovaledione
70	2,3-dihydro-5-phenyl-1,4- dithi-ine	194	bismerthiazol
	1,1,4,4-tetraoxide		
74	furcarbanil	199	penthiopyrad
78	2-acetyl-5-methyl-3-	200	boscalid
	oxopent-4-en-5-olide		
82	nitrothal-isopropyl	202	mandipropamid
83	salicylanilide	204	2,3-dichloro-
84	benodanil	207	4-(propylsulfonyl)pyridine 2-((hydroxymethyl)amino)-2-
			methylpropanol
89	ferimzone	209	irgarol
90	oxadixyl	211	tetrachloro- 4-(methylsulfonyl)pyridine
97	triazbutil	214	4.6-dichloro-2-phenvlphenol
100	carbamorph	217	benzisothizaolin-3-one
101	iprodione	218	dehvdroabietvlamine
103	halacrinate	219	bis(propylsulfonyl)ethylene
104	imibenconazole	223	2-naphthol
105	hymexazol	227	2.4-dimethyphenol
106	iprobenfos	229	4-nitrophenol
109	phosdiphen	233	4.5-dibromosalicvlanilide
111	dodine	234	potassium N-hydroxymethyl-
112	tetraconazole	235	N-methyldithiocarbamate
			,

Pesticides, An International Guide to 1800 Pest Control Chemicals (14), published works (15, 16), U.S. EPA (17), and SciFinder (a Chemical Abstracts Service database) (18), in which 301 compounds showed fungicide activity, 426 showed insecticide activity, and 558 showed herbicide activity.

Each type of chemical was divided randomly into two sets: training and test. The ratio of training to test was about 5:1. Actually, 253, 355, and 465 compounds were in the fungicide, insecticide, and herbicide training sets, respectively. Some of them, 100 compounds, in each training set are listed in **Tables 1**, **2**, and **3**, respectively, and 48, 71, and 93 compounds in the fungicide, insecticide, and herbicide test sets are listed in **Tables 4**, **5**, and **6**, respectively.

Method. All related descriptors in this paper were calculated by using a package of chemical descriptors, Codessa, which can calculate six types of descriptors: constitutional, topological, geometrical, electrostatic, quantum-chemical, and thermodynamics. Constitutional descriptors are simple descriptors that reflect only the molecular composition of the compound, that is, number of atoms, absolute and relative numbers of C, H, O, S, N, F, Cl, Br, I, and P atoms, number of bonds, number of rings, etc. Topological descriptors (also called topological indices), that is, Wiener index (19), information content index, and its derivatives (orders 0-2) (20), etc., describe the atomic connectivity in the molecule (21, 22). Geometrical descriptors are concerned with the size, shape, relative position, and properties of space of molecules, that is, shadow indices (23), molecular surface area (24), and so on. Electrostatic descriptors reflect characteristics of the charge distribution of the molecule, that is, topological electronic index (25), charged partial surface area (26), etc. Quantum-chemical descriptors are calculated from quantum chemical data (27). There are five types of quantum-chemical descriptors: charge distribution-related, valency-related, quantum mechanical energy-related, quantum mechanical molecular rotational-vibrational, and molecular salvation (5, 28). Thermodynamic descriptors relate to molecular interrelation of energy with chemical reactions or with a physical change of state and involve descriptors as follows: thermodynamic heat of formation of the molecule at 300 K, vibrational enthalpy of the molecule (at T = 300 K), translational enthalpy of the molecule (at T = 300 K), vibrational entropy of the molecule (at T =300 K), rotational entropy of the molecule (at T = 300 K), etc. (5).

Three sets of descriptors to become the screening rules for leads of fungicides, insecticides, and herbicides, respectively, would be proposed when the analysis work was finished. Herein, four data analysis methods, the K-S test (6), ANOVA (7, 8), K-W test (9, 10), and Pearson correlation coefficient (11, 12), were used in the flowchart shown in **Figure 1**.

The Kolmogorov–Smirnov statistic for a given cumulative distribution function F(x) is shown in eq 1

$$D_n = \sup[|F_n(x) - F_0(x)|]$$
(1)

where $F_n(x)$ is the empirical distribution function of a sample, $F_0(x)$ is a hypothetical distribution function, Sup[] is the supremum of set *S*, *n* is the sum of samples in the set, and D_n is the Kolmogorov–Smirnov statistic.

ANOVA is a collection of statistical models, and their associated procedures, in which the observed variance is partitioned into components due to different explanatory variables. In principle, there are three models: fixed-effects models, random-effects models, and mixed-effect models. In this work, the fixed-effects models were used.

The K-W test is a nonparametric method for testing the equality of population medians among three or more groups of sample data. It was used in this process if the descriptor was not in normal distribution. The static H is calculated by eq 2

$$H = \frac{12}{N(N+1)} \left(\frac{R_1^2}{n_1} + \frac{R_2^2}{n_2} + \dots \frac{R_k^2}{n_k} \right) - 3(N+1)$$
(2)

where *N* is the total of samples, k is the total of groups of samples, R_i is the sum of orders of samples in the *i*th group, and n_i is the sum of samples in the *i*th group.

The Pearson product-moment correlation coefficient is a measure of the correlation (linear dependence) between two variables X and Y. It is widely used in the sciences as a measure of the strength of linear dependence between two variables. The coefficient (r) between two descriptors in a candidate set was calculated by eq 3. If r was >0.9 between the two descriptors, the two were correlated, and one of them was removed from the candidate set.

$$r = l_{xy} / \sqrt{l_{xx} l_{yy}} \tag{3}$$

Table 2. 100 Compounds in the Insecticide Training Set

training set ID	compound	training set ID	compound
4	butathiofos	138	azothoate
5	chlorthiophos	144	dimefox
7	dieldrin	146	bufencarb
8	cycloprothrin	148	carbon disulfide
9	biopermethrin; biopermethrine	149	carbophenothion
12	diethyl 5-methylpyrazol-3-yl phosphate	152	chlormephos
17	2-isovalervlindan-1.3-dione	154	chlorprazophos
18	2-methyl(prop-2-ynyl)aminophenyl methylcarbamate	155	butocarboxim
24	azadirachtin	156	cvanthoate
25	amitraz	163	dialifos: dialiphos: dialifor
26	azamethiphos	165	cartap
27	azinphos-methyl	174	carbofuran
29	azinphos-ethyl	183	aldicarb
33	cvfluthrin	185	chlorthiophos
34	allyxycarb (BSI, F-ISO); allyxycarbe; APC	196	cevadine
37	hunrofezin	199	chloropicrin
38	4-methyl(nron-2-vnyl)amino-3 5-yylyl methylcarbamate	222	cyromazine
44	dichloryos	224	chlorfluazuron
46	HHDN	227	chlorfenanyr
53	decarbofuran	228	chromafenozide
55	anahasina	220	cvanonhos
57	diazinon	234	chlorovrifos
64	dicbloroethyl ether	236	
65	bioresmethrin	200	chlorovrifoe-methyl
68	acenhate	243	bendiocarb
71	aberhiavelen: ablerhiavelene	244	
71	carbosulfan	240	alanyoarh
72	diflubonzuron	201	aldovucarb; aldovucarbo
75	butoxycarbovim	200	aluoxycalb, aluoxycalbe
75	diafonthiuron	270	2 (2 butovuothovu) otbul thiopuonoto
20	1 brome 2 ablereathana	270	
0U 91	hutopato	200	actyonne Bover 22/100
01	Dulonale	202	Dayer 22/190
02		290	(2) - u u u u u - 0 - 0 - 0 - 0 - 0 - 0 - 0
00	diaratanhaa	300	(3)-ineliophene
00	diovelopil	302	dimethonomid D
07	UICYCIAIIII	305	(117127) hovedeedienel
00	2-(4,5-uimetriyi-1,5-uioxolan-2-yi)phenyi metriyicarbamate	310	(TTZ, T3Z)-THEXAUECAULETIAL
90	2-(4-chiloro-3,5-xylyloxy)ethanol	014	(Z,Z)-3, IS-OCIAUECAUIEII-1-01 ACEIAIE
93	Dayer 22408	314	2,6-umitro-4-octyphenyi crotonate
94 05	Dromienvinios	315	3-nydroxy-1-octene
95	Dioalietnin	316	3-methyl-2-cyclonexenone
97	2-chlorovinyl dietnyl phosphate	319	1,2,4-trimetnoxybenzene
99		320	DEET
100	amiaitnion; amiaipnos	321	carboturan pnenol
	chiomenvinpnos	324	r , it i-nexadecadien-i-oi, acetate, $(r \angle 1E)$ -
115	3-promo-1-cnioroprop-1-ene	326	(E)-IV-((4-nyaroxy-3-methoxypnenyl)-methyl)-8-methyl-6-nonenamide
118	3-metnyi-1-phenyipyrazoi-5-yi dimethyicarbamate	329	DOMYI
121	5,5-aimethyl-3-oxocyclohex-1-enyl dimethylcarbamate	335	allantoin
130	2-(4-chloro-3,5-xylyloxy)ethanol	349	chiorphoxim
132	DAEP	352	bistrifluoron

 l_{xx} is calculated by eq 4, and l_{yy} is calculated by eq 5.

$$l_{xx} = \sum_{i=1}^{n} (x_i - \overline{x})^2 / (n-1)$$
(4)

$$l_{xy} = \sum_{i=1}^{n} (x_i - \overline{x})(y_i - \overline{y})/(n-1)$$
 (5)

The corresponding four modules in SPSS version 13.0(29) were used to do the K–S test, ANOVA, K–W test, and Pearson correlation. In the analysis processing, CISOC-LSS (30) was used to get scatter plots and bar charts of analysis objects.

RESULTS AND DISCUSSION

Six types of descriptors, constitutional, topological, geometrical, electrostatic, quantum-chemical, and thermodynamic, including 485 descriptors, were calculated for each compound in the three training sets by Codessa. Among these descriptors, 155 descriptors were element-dependent, 189 were element-independent and in continuous distribution, and 34 were elementindependent and in discrete distribution; 107 descriptors were element-independent and equal to zero. The 189 descriptors listed in **Table 7**, selected from the 485 descriptors, were analyzed further by K–S test, ANOVA, K–W test, and scatter plots.

The K-S test was used to analyze the 189 descriptors. The corresponding result showed that 17 descriptors (listed in **Table 8**) were in normal population and 172 were not in normal population. ANOVA was used to calculate differences among the 17 descriptors (listed in **Table 8**). Except for the geometrical descriptor, XY shadow/XY rectangle, which could not be a candidate for screening rules because it had no significant difference among the three types of compounds in the training sets, the

Table 3. 100 Compounds in the Herbicide Training Set

training set		training set		
ID	compound	ID	compound	
4	240	100	bromobonil	
4	2,4-D	132		
9	pentanochior	134	dinosam	
10	ethorumesate	143	cliodinate	
12	2,4,5-1	145	simetryn	
15	dichlormate	148	thitensulturon	
16	carfentrazone-ethyl	159	chloroxynil	
17	trifop	160	benzipram	
18	trifop-methyl (unsaturated stereochemistry)	162	trimeturon	
19	sulfentrazone	165	fluothiuron	
20	chlorimuron-ethyl	189	amiprofos-methyl	
22	tri-allate	210	EXD	
23	trietazine	211	dimexano	
24	UBI-S734	244	chloroacetic acid	
27	dimethametryn	245	chlorimuron	
28	daimuron	246	fluoroxypyr-meptyl	
29	tricamba	247	fluoroxypyr-2-butoxy-1-	
33	karbutilate	248	flampron-M	
34	azafenidin	249	flamprop-M-methyl	
36	azimsulfuron	273	imazanyr	
37	prometryn	282	isovabon	
20	amitrolo	202	ablerflurenel methyl	
20		200	oulfooulfuron	
39	2,4,0-1D	299		
45	difiutenican	300	2,4-D-DUIOTYI	
40		301	tepraloxydim	
48	Isopropalin	302	monolinuron	
49	butachlor	303	cinmethylin	
52	aclonifen	304	anilofos	
53	dicamba	305	molinate	
54	halosafen	306	asulam	
55	isocil	307	atrazine	
58	amidosulfuron	309	benazolin	
67	fluoroxypyr	310	2,4-D-butyl	
68	MCPA	311	imazamethabenz	
69	metazachlor	314	benazolin-ethyl	
70	bromoxynil	320	ethalfluralin	
72	propyzamide	337	metolachlor	
73	propaguizafop	362	procyazine	
75	metamitron	363	nitrofluorfen	
76	flamprop-M-isopropyl	364	prvnachlor	
79	2.4-D-isoctvl	371	methoxyphenone	
83	bentazone	372	diethatyl-ethyl	
84	fluchloralin	389	di-allate	
86	isonolinato	302	cvprazole	
01	morfamquat dichlorida	102	amibuzin	
91		402	honzovilnen	
94	propanone	412		
96	perfluidone	413	2,4,5-T-isoctyl	
99	tetrafluoron	423	pyrithiobac	
100	methiuron	433	isoxachlortole	
124	pyriclor	436	2,4-DB, butoxyethyl ester	
131	terbucarb	439	2-(M-chlorophenoxy)- propionamide	

others became candidates. The K–W test was used to handle the 172 descriptors not in normal population. The result showed that 34 descriptors (in **Table 9**) were not candidates because they had no significant difference (significance ≥ 0.05) among the three types of compounds. Therefore, after the K–S test, ANOVA, and K–W test, we got a set of candidates including 154 descriptors. When scatter plots and bar charts of the 154 descriptors were analyzed, 35 descriptors (listed in **Table 10**) showed characters of screening rules for leads of fungicides, insecticides, and herbicides, respectively. Corresponding data ranges are shown in **Table 11**.

Table 4. 48 Compounds in the Fund	gicide Test Se	ŧ
-----------------------------------	----------------	---

test set		test se	test set		
ID	compound	ID	compound		
1	fenapanil	25	etridiazole		
2	4-(1-ethylhexyl)-2,6-dinitrophenyl methyl carbonate	26	tolylfluanid		
3	binapacryl	27	imazalil		
4	ICIA 0858	28	fenamidone		
5	azoxystrobin	29	flusulfamide		
6	etem	30	chlorothalonil		
7	(<i>RS</i>)- <i>N</i> -(3,5-dichlorophenyl)- 2-(methoxymethyl)succinimide	31	dinobuton		
8	SSF109 (shionogi)	32	ethirimol		
9	benzamorf	33	flutolanil		
10	chloroneb	34	metazoxolon		
11	prochloraz	35	mebenil		
12	2-pyridinethiol 1-oxide	36	ditalimfos		
13	methfuroxam	37	polyoxin D		
14	thifluzamide	38	BR enantiomer		
15	biphenyl	39	proquinazid		
16	hexachlorobenzene	40	chloro-2- cyclopentylphenol		
17	dichlozoline	41	5-chlorosalicylanilide		
18	diphenylamine	42	(1,1'-biphenyl)-2-ol, 5-chloro-		
19	dicloran	43	glutaraldehyde		
20	bromuconazole	44	4-tert-butylphenol,		
21	hexaconazole	45	aureonuclemycin		
22	sec-butylamine	46	metominostrobin		
23	prothiocarb	47	myclozolin		
24	hexylthiofos	48	piperalin		

Sixteen groups of descriptors listed in **Table 12** were generated when the 35 descriptors were clustered according to their definition. If one descriptor was selected from each group, then 41472 combinations of candidate sets were generated. Also, Pearson correlation coefficients among the 35 for the three types of compounds, respectively, were calculated and are given in the Supporting Information (STable 1). Three sets with higher sensitivity and low coefficients for leads of fungicides, insecticides, and herbicides, respectively, are shown in **Tables 13**, **14**, and **15** when they were tested by compounds in the three test sets listed in **Tables 4**, **5**, and **6**, respectively.

All descriptors listed in **Tables 13**, **14**, and **15** were clustered again by Pearson correlation coefficients listed in the Supporting Information (STable 1) and were tested by the three test sets.

Fungicide. The descriptors in Table 13 were grouped into (1), (4, 13, 15, 20, 26, 34), (9), (12), (16, 18), (29), (10, 33), (24), and (25) by Pearson's coefficients. They were tested by the three sets, and the results in Table 16 show that the two electrostatic descriptors, 24 (PPSA-3 atomic charge weighted PPSA [Zefirov's PC]) and 25 (RPCG relative positive charge (OMPOS/OTPLUS) [Zefirov's PC]), were not able to differentiate the three types of compounds because they did not present the characters of fungicides among the three types of compounds. The two descriptors were removed from candidate sets. The screening rules for leads of fungicides involved seven descriptors, average bonding information content (order 1), FNSA-2 fractional PNSA (PNSA-2/TMSA) [Zefirov's PC], final heat of formation/number of atoms, internal enthalpy (300 K)/number of atoms, Randic index (order 0), total molecular one-center E-N attraction/number of atoms, and WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [quantum-chemical PC], and their data ranges are listed in Table 17. They were tested by three test sets, and the best result is listed in Table 18.

Table 5. 71 Compounds in the Insecticide Test Set

test set ID) compound	test set ID	compound
1	γ -benzene hexachloride	37	profenofos
2	acrinathrin	38	demeton-S
3	β -cypermethrin	39	trimedlure-A
4	2,2,2-trichloro-1-(3,4-	40	hydrogen cyanide
	dichlorophenyl)ethyl acetate		, , ,
5	thiocarboxime	41	clothianidin
6	transpermethrin	42	coumaphos
7	aminocarb	43	avermectin B1b
8	sulfoxide (ESA)	44	bifenthrin
9	benfuracarb	45	chlordane
10	methocrotophos	46	cyphenothrin [(1R)
			-trans- isomers]
11	fenobucarb	47	thiofanox
12	1.1-dichloro-2.2-bis(4-	48	monocrotophos
	ethylphenyl)ethane		· · · · · · · · · · · ·
13	transfluthrin	49	phenthoate
14	chlordecone	50	mecarbam
15	ethion	51	sulfluramid
16	fosmethilan	52	emamectin
17	2-(1.3-dithiolan-2-vl)phenvl	53	ethohexadiol
	dimethylcarbamate		
18	fosthietan	54	methacrifos
19	hydroprene	55	1.1-dichloro-1-nitroethane
20	ethoate-methyl	56	nitrilacarb
21	2-thiocvanatoethyl laurate	57	phenkapton
22	heptachlor	58	pirimiphos-ethyl
23	coumithoate	59	fenazox
24	DSP	60	nicotine
25	leptophos	61	ethiprole
26	hvdramethvlnon	62	tetradecanal
27	IPSP	63	oxvpurinol
28	methoxychlor	64	trans-phosphamidon
29	bromophos-ethyl	65	(E)-6-dodecen-1-vl acetate
30	isopropyl <i>O</i> -(methoxyamino-	66	5-pentvl
	thiophosphoryl)salicylate		dihvdrofuranone
31	cvanofenphos	67	benzocaine
32	demeton-Q	68	1 <i>H</i> -pyrazole-3-
			carbonitrile
33	dicapthon	69	novaluron
34	morphothion	70	methothrin
35	fenitrothion	71	fluovrazofos
36	B-1492		
~~			

Information in **Table 18** shows that the accuracy of the set of screening rules for leads of fungicides was 82%; those for leads of insecticides and herbicides were 56 and 70%, respectively. It was more suitable for fungicide leads than the others because it only made 18% error for this type of lead, but 44 and 30% errors for the other two types of leads, respectively.

Insecticide. The descriptors in **Table 14** were grouped into (2), (4, 15, 17, 20, 23, 26, 30, 35), (5), (7), (8), (10, 23), (11), (29), and (15, 23, 24, 30) by Pearson's coefficients. They were tested by the three sets, and the results in **Table 19** show that two descriptors, 2 (average information content (order 1), a topological descriptor) and 7 (ESP-RPCG relative positive charge (QMPOS/QTPLUS) [quantum-chemical PC], a quantum-chemical descriptor), were not able to differentiate the three types of compounds because they could not present the characters of insecticides among the three types of compounds. They were removed from candidate sets. The screening rules for leads of insecticides involved seven descriptors, ESP-DPSA-3 difference in CPSAs (PPSA-2/TMSA) [quantum-chemical PC], FPSA-2 fractional PPSA (PPSA-2/TMSA) [quantum-chemical PC], final

Table 6. 93 Compounds in the Herbicide Test Set

test set	· ·	test set	
ID	compound	ID	compound
	oompound	10	compound
1	propachlor	48	pretilachlor
2	chlorfenac	49	diquat dibromide
3	cyanatryn	50	halosulfuron
4	clomazone	51	2,4-DB-butyl
5	dinofenate	52	flucarbazone
6	isoxaben	53	clodinafop
7	phenmedipham-ethyl	54	metribuzin
8	SMY 1500	55	flazasulfuron
9	iodobonil	56	flumioxazin
10	fluometuron	57	fluridone
11	EL 177	58	ethametsulfuron-methyl
12	chlorthiamid	59	haloxyfop
13	FMC 19873	60	simazine
14	pyridate	61	terbutryn
15	trifopsime	62	2,4-D-isopropyl
16	dichlobenil	63	chlorbromuron
17	rimsulfuron	64	cvclosulfamuron
18	sulcotrione	65	dimethenamid
19	ACD 10614	66	dimepiperate
20	bensulfuron-methyl	67	acetochlor
21	fluoronitrofen	68	EPTC
22	buthiuron	69	fosamine-ammonium
23	bensulfuron	70	tribenuron-methyl
24	benzofenap	71	fluthiacet-methyl
25	diclofon	72	tridiphane
26	tralkoxydim	73	dinoseb acetate
27	chlorotoluron	74	dipropetryn
28	sulalycanin	75	L \$830556
20	nronham	76	phenobenzuron
30	dimethinin	77	flumezin
31	MCPA	78	chlorfennron (racemate)
30	credazine	70	diethamquat dichloride
33	chlorovuron	80	thidiazimin
34	henzofluor	81	2 4-DEP
35	brompyrazon	82	eqlinazine-ethyl
36	fluoromidine	83	proglinazine
37	flumeteulem	8/	clodinaton-proparavl
38	diuron	85	pyriminobac-methyl
20	fonovanron P othyl	96	pyrininobac-metriyi
39 40	chlorazifon proparavl	00 97	4.5 diablara 2. N actul 2(24)
40	(P) icomor	07	4,5-010111010-2-19-000191-3(217)-
41	(n)-isolitiei	00	MCRA isopropul astor
40	imazanio	00 90	nicolinaton
42 42	othiolato	00	
40	ennolate	90	AINI I-/ UOO
44	piuxali	91	quizal0l0p-etityi
40	carbetamide	92	
40 47	mefluidide	93	паркајат

heat of formation, PPSA-3 atomic charge weighted PPSA [Zefirov's PC], total molecular one-center E-N attraction/number of atoms, and ZX shadow, and their data ranges are listed in **Table 20**. They were tested by three test sets, and the best result is listed in **Table 21**.

Information in **Table 21** shows that the accuracy of the set of screening rules for leads of insecticides was 83%. Those for leads of fungicides and herbicides were 60 and 74%, respectively. It was more suitable for insecticide leads than the others because it only made 17% error for this type of lead compounds, but 40 and 26% errors for the other two types of leads, respectively.

Herbicide. The descriptors in **Table 15** were grouped into (1), (7), (13, 14, 15, 23, 24, 26, 28), (9, 22), (10, 23), (16, 29), (16, 32), and (20, 14, 28) by Pearson's coefficients. They were tested by the three sets, and the results in **Table 22** show that a





no.	descriptor	type
1	$(1/2) \times$ BETA polarizability (DIP)	electrostatic
2	$(1/6) \times$ GAMMA polarizability (DIP)	electrostatic
3	$1 \times BETA$ polarizability (DIP)	electrostatic
4	1× GAMMA polarizability (DIP)	electrostatic
5	ALFA polarizability (DIP)	electrostatic
6	average bonding information content (order 0)	topological
7	average bonding information content (order 1)	topological
8	average bonding information content (order 2)	topological
9	average complementary information content (order 0)	topological
10	average complementary information content (order 1)	topological
11	average complementary information content (order 2)	topological
12	average information content (order 0)	topological
13	average information content (order 1)	topological
14	average information content (order 2)	topological
15	average structural information content (order 0)	topological
16	average structural information content (order 1)	topological
17	average structural information content (order 2)	topological
18	Balaban index	topological
19	bonding information content (order 0)	topological
20	bonding information content (order 1)	topological
21	bonding information content (order 2)	topological
22	complementary information content (order 0)	topological
23	complementary information content (order 1)	topological
24	complementary information content (order 2)	topological
25	DPSA-1 difference in CPSAs (PPSA1-PNSA1) [quantum-chemical PC]	guantum-chemical
26	DPSA-1 difference in CPSAs (PPSA1-PNSA1) [Zefirov's PC]	electrostatic
27	DPSA-2 difference in CPSAs (PPSA2-PNSA2) [quantum-chemical PC]	quantum-chemical
28	DPSA-2 difference in CPSAs (PPSA2-PNSA2) [Zefirov's PC]	electrostatic
29	DPSA-3 difference in CPSAs (PPSA3-PNSA3) [Zefirov's PC]	electrostatic
30	ESP-DPSA-1 difference in CPSAs (PPSA1-PNSA1) [quantum-chemical PC]	quantum-chemical
31	ESP-DPSA-2 difference in CPSAs (PPSA2-PNSA2) [quantum-chemical PC]	quantum-chemical
32	ESP-DPSA-3 difference in CPSAs (PPSA3-PNSA3) [quantum-chemical PC]	quantum-chemical
33	ESP-FNSA-1 fractional PNSA (PNSA-1/TMSA) [quantum-chemical PC]	quantum-chemical
34	ESP-FNSA-2 fractional PNSA (PNSA-2/TMSA) [quantum-chemical PC]	quantum-chemical
35	ESP-FNSA-3 fractional PNSA (PNSA-3/TMSA) [quantum-chemical PC]	quantum-chemical
36	ESP-FPSA-1 fractional PPSA (PPSA-1/TMSA) [quantum-chemical PC]	quantum-chemical
37	ESP-FPSA-2 fractional PPSA (PPSA-2/TMSA) [quantum-chemical PC]	quantum-chemical
38	ESP-FPSA-3 fractional PPSA (PPSA-3/TMSA) [quantum-chemical PC]	quantum-chemical
39	ESP-Min net atomic charge	quantum-chemical
40	ESP-PNSA-1 partial negative surface area [quantum-chemical PC]	quantum-chemical
41	ESP-PNSA-2 total charge weighted PNSA [quantum-chemical PC]	quantum-chemical
42	ESP-PNSA-3 atomic charge weighted PNSA [quantum-chemical PC]	quantum-chemical
43	ESP-PPSA-1 partial positive surface area [quantum-chemical PC]	quantum-chemical
44	ESP-PPSA-2 total charge weighted PPSA [quantum-chemical PC]	quantum-chemical
45	ESP-PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]	quantum-chemical

Table 7. Continued

The second sec	no	descrintor	type
66 ESP-NROC restine registre drage (GMR/SQCTPLINS) (partimit-herman PC) quartimit-herman 77 ESP-NROC restine partie drage (GMR/SQCTPLINS) (partimit-herman PC) quartimit-herman 78 ESP-NROC restine partie drage (GMR/SQCTPLINS) (partimit-herman PC) quartimit-herman 78 ESP-NROC value hermalities and (partimit-herman PC) quartimit-herman 78 ESP-NROC Value hermalities and (partimit-herman PC) quartimit-herman 78 ESP-NROC Value hermalities and (partimit-herman PC) quartimit-herman 78 ESP-NROC Value hermalities (PSN-NROCNO) (partimit-mellinal PC) quartimit-herman 79 ESP-NROC Value hermalities (PSN-NROCNO) (partimit-mellinal PC) quartimit-herman 79 fml hes of formation thermolytamic quartimit-herman 79 fml hes of formation thermolytamic quartimit-herman 70 fml hes of formation thermolytamic quartimit-herman 71 fml hes of formation thermolytamic quartimit-herman 72 fml hes of formation thermolytamic quartimit-herman 73 fml hes of formation thermolytamic quartimit-herman 74 FMSA-1 faction FMSA-1178A) (quartimit-herman QUartimit-herman 75 fml hes of formation thermolytamic Quartimit-h	10.		турс
77 ESP PNCS relative peaks or upped A (AMMES*MCG) [quantum-chemical PC] quantum-chemical 88 ESP-PNCS Multing points charge (AMMCS*MCS) [quantum-chemical PC] quantum-chemical 89 ESP-PNCS Multing points charge (AMMCS*MCS*MCG) [quantum-chemical PC] quantum-chemical 81 ESP-WNS-X verginate PNSA (PNSA*MSX*MOG) [quantum-chemical PC] quantum-chemical 82 ESP-WNS-X verginate PNSA (PNSA*MSX*MOG) [quantum-chemical PC] quantum-chemical 83 ESP-WNSA Verginate PNSA (PNSA*MSX*MOG) [quantum-chemical PC] quantum-chemical 84 ESP-WNSA Verginate PNSA (PNSA*MSX*MOG) [quantum-chemical PC] quantum-chemical 85 ESP-WNSA Verginate PNSA (PNSA*MSX*MOG) [quantum-chemical PC] quantum-chemical 86 ESP-WNSA verginate PNSA (PNSA*MSX*MOG) [quantum-chemical PC] quantum-chemical 87 fmail head of formation*Los (PNSA*MSX*MOG) [quantum-chemical PC] quantum-chemical 88 FNSA+ functional PNSA (PNSA*MSA*MSA) [quantum-chemical PC] quantum-chemical 89 FNSA+ functional PNSA (PNSA*MSA) [quantum-chemical PC] quantum-chemical 80 FNSA+ functional PNSA (PNSA*MSA) [quantum-chemical PC] quantum-chemical 81 FNSA+ functional PNSA (PNSA*MSA) [quantum chemical PC] quantum-chemical <td>46</td> <td>ESP-RNCG relative negative charge (QMNEG/QTMINUS) [quantum-chemical PC]</td> <td>quantum-chemical</td>	46	ESP-RNCG relative negative charge (QMNEG/QTMINUS) [quantum-chemical PC]	quantum-chemical
48 ESP-HPCS reduce positiv change (MM-SSITULS) (pustimu-chemical PC) quantum-chemical 50 ESP-NDA Nati mode positiv change SA (SAM-OSC) (quantum-chemical PC) quantum-chemical 51 ESP-NDA Nati mode positiv change SA (SAM-OSC) (quantum-chemical PC) quantum-chemical 52 ESP-NDA Nati mode positiv change SA (SAM-OSC) (quantum-chemical PC) quantum-chemical 53 ESP-NDA SA weighted PNA (PNAST TMSA/1000) (quantum-chemical PC) quantum-chemical 54 ESP-NDA SA weighted PNA (PNAST TMSA/1000) (quantum-chemical PC) quantum-chemical 55 ESP-NDA SA weighted PNA (PNAST TMSA/1000) (quantum-chemical PC) quantum-chemical 66 Final hara of formation thermodynamic 67 Final hara of formation thermodynamic 68 FINSA - final inter of formation thermodynamic 69 FINSA - final inter of formation thermodynamic 60 FINSA - final inter of formation thermodynamic 61 FINSA - final inter of formation thermodynamic 62 FINSA - final inter of formation thermodynamic 63 FINSA - final inter of formation thermodynamic 64 FINSA - final inter of formation thermodynamic 65 FINSA - final inter of formation thermodynamic 66 FINSA - fin	47	ESP-RNCS relative negative charged SA (SAMNEG*RNCG) [quantum-chemical PC]	quantum-chemical
94 ESP-RNA:S Haske provide analy quartum-formical PC] quartum-formical PC] 95 ESP-RNA:S A segue PNR SAL (PNRS-TISA-1000) (quartum-formical PC] quartum-formical PC] 95 ESP-RNA:S A segue PNR SAL (PNRS-TISA-1000) (quartum-formical PC] quartum-formical PC] 96 ESP-RNA:S A segue PNR SAL (PNRS-TISA-1000) (quartum-formical PC] quartum-formical PC] 96 ESP-RNA:A variety PNRS-TISA-1000 (quartum-formical PC] quartum-formical PC] 96 ESP-RNA:A variety PNRS-TISA-1000 (quartum-formical PC] quartum-formical PC] 96 ESP-RNA:A variety PNRS-TISA-1000 (quartum-formical PC] quartum-formical PC] 96 FINSA-1 training PNRS-RNA:TISA-1000 (quartum-formical PC] quartum-formical PC] 97 FINSA-1 training PNRS-RNA:TISA-1000 (quartum-formical PC] quartum-formical PC] 98 FINSA-1 training PNRS-	48	ESP-RPCG relative positive charge (QMPOS/QTPLUS) [quantum-chemical PC]	quantum-chemical
 Bern Machan Bern Machan Bern (PESA - THISBURDOR TILL TO - Chemical PC) BER MARKA Vergüller PRA (PRACT THISBURDOR TILL TO - Chemical PC) BER MARKA Vergüller PRA (PRACT THISBURDOR TILL TO - Chemical PC) BER MARKA Vergüller PRA (PRACT THISBURDOR TILL TO - Chemical PC) BER MARKA Vergüller PRA (PRACT THISBURDOR TILL TO - Chemical PC) BER MARKA Vergüller PRA (PRACT THISBURDOR TILL TO - Chemical PC) BER MARKA Vergüller PRA (PRACT THISBURDOR TILL TO - Chemical PC) BER MARKA VERSA VERSA THISBURDOR TILL TO - Chemical PC) BER MARKA VERSA THISBURDOR TILL TO - Chemical PC) BER MARKA VERSA VERSA THISBURDOR TILL TO - Chemical PC) BER MARKA VERSA VERSA THISBURDOR TILL TO - Chemical PC) BER MARKA VERSA VERSA THISBURDOR TO - Chemical PC) BER MARKA VERSA VERSA THISBURDOR TO - Chemical PC) BER MARKA VERSA VERSA THISBURDOR TO - Chemical PC) BER MARKA VERSA VERSA THISBURDOR TO - Chemical PC) BER MARKA VERSA VERSA VERSA THISBURDOR TO - Chemical PC) BER MARKA VERSA VERSA VERSA VERSA THISBURDOR TO - Chemical PC) BER MARKA VERSA VERSA VERSA VERSA THISBURDOR TO - Chemical PC) BER MARKA VERSA VER	49	ESP-RPUS relative positive charged SA (SAMPUS'RPUG) [quantum-chemical PC]	quantum-chemical
 a) c) c) mixed a magnetic mask (Prescriptings) motor) (paralum-thema inc) c) c) mixed a magnetic mask (Prescriptings) (paralum-thema PC) c) c) c	50	ESP-IMSA total molecular surface area [quantum-chemical PC]	quantum-chemical
 ESP-MINSA a registral PRA (PEAR TINSA 1000) [partime-shemical PC] ESP-MINSA 2000 [PCA (PEAR TINSA 1000) [partime-shemical PC] gantime-shemical ESP-MINSA 2000 [PCA (PEAR TINSA 1000) [partime-shemical PC] gantime-shemical ESP-MINSA 2000 [PCA (PEAR TINSA 1000) [partime-shemical PC] gantime-shemical Final heat of tomation thermodynamic final heat of tomation, ol atoms thermodynamic PINSA fractional PINSA (PINSA 1715A) (2010v 5 PC] electrostalic PINSA fractional PINSA (PINSA 2715A) (2010v 5 PC] electrostalic PINSA fractional PINSA (PINSA 2715A) (2010v 5 PC] electrostalic PINSA fractional PINSA (PINSA 2715A) (2010v 5 PC] electrostalic PINSA fractional PINSA (PINSA 2715A) (2010v 5 PC] electrostalic PINSA fractional PINSA (PINSA 2715A) (2010v 5 PC] electrostalic PINSA fractional PINSA (PINSA 2715A) (2010v 5 PC] electrostalic PINSA fractional PINSA (PINSA 2715A) (2010v 5 PC] electrostalic PINSA fractional PINSA (PINSA 2715A) (2010v 5 PC] electrostalic PINSA fractional PINSA (PINSA) (2010v 5 PC] electrostalic PINSA fractional PINSA (PIN	50	ESF-WINSA-T Weighted DNSA (FINSAT TIMSA/1000) [quantum chemical PC]	quantum chemical
24 CSP-MPSA.1 registrice IPSA (PPSA TTMSA/1000) (parathm-chemical PC) quantum-chemical 25 CSP-MPSA.3 registrice IPSA (PPSA TTMSA/1000) (parathm-chemical PC) quantum-chemical 26 CSP-MPSA.3 registrice IPSA (PPSA TTMSA/1000) (quantum-chemical PC) quantum-chemical 26 PNSA.1 fractional PNSA (PNSA-1/MSA) (zetrocy PC) quantum-chemical 26 PNSA.1 fractional PNSA (PNSA-1/MSA) (zetrocy PC) quantum-chemical 26 PNSA.2 fractional PNSA (PNSA-2/MSA) (zetrocy PC) quantum-chemical 26 PNSA.2 fractional PNSA (PNSA-2/MSA) (zetrocy PC) quantum-chemical 26 PNSA.2 fractional PNSA (PNSA-2/MSA) (zetrocy PC) quantum-chemical 26 PNSA.3 fractional PPSA (PSA-1/MSA) (zetrocy PC) quantum-chemical 26 PPSA.1 fractical PPSA (PSA-1/MSA) (zetrocy PC) quantum-chemical 27 gravitation index (al boxis) Zetrocks 2/MSA (zetrocy PC) quantum-chemical 27 gravitation index (al boxis) Zetrocks 2/MSA (zetrocy PC) quantum-chemical 27 gravitation index (al pans) Zetrocks 2/MSA (zetrocy PC) quantum-chemical 27 gravitation index (al pans) Zetrocks 2/MSA (zetrocy PC	52	ESF-WINSA-2 weighted PNSA (PNSA2 TWSA/1000) [quantum-chemical PC]	quantum-chemical
55 ESP.MPSA2 avgidted PPSA (PSAS TUSA1100) [guantum-chemical PC] quantum-chemical 56 ESP.MPSA2 avgidted PPSA (PSAS TUSA1100) [guantum-chemical PC] quantum-chemical 57 Inclusial of formation/on atoms thermodynamic 58 FIASA-1 fractional PISA (PSAS-1TMSA) [guantum-chemical PC] quantum-chemical 59 FNSA-1 fractional PISA (PSAS-1TMSA) [guantum-chemical PC] quantum-chemical 51 FNSA-2 fractional PISA (PSAS-1TMSA) [guantum-chemical PC] quantum-chemical 52 FNSA-2 fractional PISA (PSAS-1TMSA) [guantum-chemical PC] quantum-chemical 53 FNSA-5 fractional PISA (PSAS-1TMSA) [guantum-chemical PC] quantum-chemical 64 FNSA-5 fractional PISA (PSAS-1TMSA) [guantum-chemical PC] quantum-chemical 65 FPSA-1 fractional PPSA (PSAS-1TMSA) [guantum-chemical PC] quantum-chemical 66 FPSA-1 fractional PPSA (PSAS-1TMSA) [guantum-chemical PC] quantum-chemical 71 Grantum-chemical PSAS-1 fractional PPSA (PSAS-1TMSA) [guantum-chemical PC] quantum-chemical 72 FPSA-2 fractional PPSA (PSAS-1TMSA) [guantum-chemical PC] quantum-chemical 73 theodocal PPSA (PSAS-1TMSA) [guantum-chemical PC] quantum-chemical 74 FPSAS-1 fractional PPSA (PSAS-1TMSA) [guantum-chemical PC] quantum-chemical 75 TPSAS-1 fractional PSAS (PSAS-	54	ESI-WINGA-5 weighted PPSA (PPSA1*TMSA/1000) [quantum-chemical PC]	quantum-chemical
59 ESP-WF2A-9 segnine (PPSA, PPSA, TMSA/1000) [quantum-chemical PC] quantum-chemical 57 final hoat of formation: thermodynamic 58 final hoat of formation: thermodynamic 59 PKSA-1 fractional PNSA (PKSA-117KSA) [Zelivo's PC] electrostatic 60 PKSA-2 fractional PNSA (PKSA-117KSA) [Zelivo's PC] electrostatic 61 PKSA-2 fractional PNSA (PKSA-177KSA) [Zelivo's PC] electrostatic 62 PKSA-3 fractional PNSA (PKSA-177KSA) [Zelivo's PC] electrostatic 63 PKSA-3 fractional PNSA (PKSA-177KSA) [Zelivo's PC] electrostatic 64 PKSA-3 fractional PNSA (PKSA-177KSA) [Zelivo's PC] electrostatic 65 PFSA-1 fractional PSA (PKSA-177KSA) [Zelivo's PC] electrostatic 66 PFSA-2 fractional PSA (PKSA-177KSA) [Zelivo's PC] electrostatic 71 gavalutori index (al pairs) constitutornal PC] 72 gavalutori index (al pairs) constitutornal PC] 73 HOMO - LMUC energy quantum-chemical PC] electrostatic 74 HOMO energy quantum-chemical PC] electrostatic 75 HOMO - lawage electrostatic electrostatic 76 ornage of the Orsager-Kikwood solvation energy quantum-chemical PC] 77	55	ESP-WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [quantum-chemical PC]	quantum-chemical
57 final head of formation: thermodynamic 58 final head of formation: thermodynamic 59 FNSA-1 fractional PNSA (PISA-1/MSA) (pantum-chemical PC) quantum-chemical 60 FNSA-2 fractional PNSA (PISA-1/MSA) (pantum-chemical PC) quantum-chemical 61 FNSA-2 fractional PNSA (PISA-2/MSA) (pantum-chemical PC) quantum-chemical 62 FNSA-3 fractional PNSA (PISA-2/MSA) (pantum-chemical PC) quantum-chemical 64 FNSA-3 fractional PNSA (PISA-2/MSA) (pantum-chemical PC) quantum-chemical 65 FPSA-1 fractical PPSA (PISA-1/MSA) (pantum-chemical PC) quantum-chemical 66 FPSA-1 fractical PPSA (PPSA-1/MSA) (pantum-chemical PC) quantum-chemical 67 FPSA-2 fractical PPSA (PPSA-1/MSA) (pantum-chemical PC) quantum-chemical 70 FPSA-3 fractical PPSA (PPSA-3/MSA) (pantum-chemical PC) quantum-chemical 71 gravitation index (al bords) constitutional 72 gravitation index (al bords) constitutional 73 HOMO - LUMO energy qap quantum-chemical PC 74 HOMO - LUMO energy (qap quantum-chemical 75 HOMO-1 energy quantum-chemical 76 oraga du Ho Onsager-Kinkood solvation energy quantum-chemical 77 information conteff (coder 1)	56	ESP-WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [quantum-chemical PC]	quantum-chemical
39 tinal heat of ormations thermodynamic 39 FINSA I Inacional PINSA (PINSA I/TXMSA) [Zativo's PC] electrostatic 60 FINSA I Inacional PINSA (PINSA - ITXMSA) [Zativo's PC] electrostatic 61 FINSA 2 Inacional PINSA (PINSA - ITXMSA) [Zativo's PC] electrostatic 62 FINSA 2 Inacional PINSA (PINSA - TIXMSA) [Zativo's PC] electrostatic 63 FINSA 3 Inacional PINSA (PINSA - TIXMSA) [Zativo's PC] electrostatic 64 FINSA 3 Inacional PINSA (PISA - TIXMSA) [Zativo's PC] electrostatic 65 FIPSA 1 Inacional PINSA (PISA - TIXMSA) [Zativo's PC] electrostatic 66 FIPSA 2 Inacional PISA (PISA - TIXMSA) [Zativo's PC] electrostatic 71 gravitation index (al Daris) gravitation index (al Daris) gravitation index (al Daris) 72 gravitation index (al Daris) gravitation organic gravitation index (al Daris) 73 HOMO - energy quantum-chemical gravitation organic 74 HOMO - energy quantum-chemical gravitation index (al Daris) 75 HOMO - energy quantum-chemical gravitation organic 76 oragge of the Dasager - Kitewood shutton energy quantum-chemical 77 information cornerin (code 1) topological 78 HOMO - energy <td>57</td> <td>final heat of formation</td> <td>thermodynamic</td>	57	final heat of formation	thermodynamic
59 FNSA-1 fractional PNSA (PNSA-1/TMSA) (partum-shemical PC) quantum-shemical 60 FNSA-2 fractional PNSA (PNSA-1/TMSA) (partum-shemical PC) quantum-shemical 61 FNSA-2 fractional PNSA (PNSA-2/TMSA) (partum-shemical PC) quantum-shemical 62 FNSA-3 fractional PNSA (PNSA-2/TMSA) (partum-shemical PC) quantum-shemical 63 FNSA-3 fractional PNSA (PNSA-2/TMSA) (partum-shemical PC) quantum-shemical 66 FPSA-1 fractional PPSA (PPSA-1/TMSA) (partum-shemical PC) quantum-shemical 67 FPSA-2 fractional PPSA (PPSA-1/TMSA) (partum-shemical PC) quantum-shemical 68 FPSA-2 fractional PPSA (PPSA-1/TMSA) (partum-shemical PC) quantum-shemical 70 FPSA-3 fractional PPSA (PPSA-1/TMSA) (partum-shemical PC) quantum-shemical 71 gravitation index (all paris) constitutional 72 gravitation index (all paris) constitutional 73 HOMO - LUMO energy quantum-shemical PC) quantum-shemical 74 HOMO - LUMO energy quantum-shemical PC topological 75 HOMO - LUMO energy quantum-shemical PC topological 76 omage - Kinocod solvation energy quantum-shemical 77 information conterf (coder 0) topological 78 information conterf (coder 1) topological 78	58	final heat of formation/no. of atoms	thermodynamic
60 FNSA-1 fractional PNSA (PNSA /TMSA) (Zelrov PC) electrostatic 61 FNSA-2 fractional PNSA (PNSA Z/TMSA) (Zelrov PC) electrostatic 62 FNSA-3 fractional PNSA (PNSA Z/TMSA) (Zelrov PC) electrostatic 63 FNSA-4 fractional PNSA (PNSA Z/TMSA) (Zelrov PC) electrostatic 64 FNSA-3 fractional PNSA (PNSA Z/TMSA) (Zelrov PC) electrostatic 65 FPSA-1 fractional PPSA (PPSA Z/TMSA) (Zelrov PC) electrostatic 66 FPSA-2 fractional PPSA (PPSA Z/TMSA) (Zelrov PC) electrostatic 67 FPSA-2 fractional PPSA (PPSA Z/TMSA) (Zelrov PC) electrostatic 68 FPSA-2 fractional PPSA (PPSA Z/TMSA) (Zelrov PC) electrostatic 71 gravitation index (all pairs) constitutional 72 gravitation index (all pairs) constitutional 73 HOMO energy quantum-chemical 74 HOMO energy quantum-chemical 75 HOMO energy quantum-chemical 76 omage of the Onsager-Krkwood solvation energy quantum-chemical 77 information content (coder 0) topological 78 HOMO energy qquantum-chemical <t< td=""><td>59</td><td>FNSA-1 fractional PNSA (PNSA-1/TMSA) [quantum-chemical PC]</td><td>guantum-chemical</td></t<>	59	FNSA-1 fractional PNSA (PNSA-1/TMSA) [quantum-chemical PC]	guantum-chemical
61 FNSA-2 factorian PNSA (PNSA-2/TMSA) (pantum-chemical PC) quantum-chemical 62 FNSA-4 factorian PNSA (PNSA-2/TMSA) (pantum-chemical PC) quantum-chemical 63 FNSA-6 factorian PNSA (PNSA-2/TMSA) (pantum-chemical PC) quantum-chemical 64 FNSA-1 factorian PPSA (PSA-1/TMSA) (pantum-chemical PC) quantum-chemical 65 FPSA-1 factorian PPSA (PSA-1/TMSA) (pantum-chemical PC) quantum-chemical 66 FPSA-2 factorian PPSA (PSA-2/TMSA) (pantum-chemical PC) quantum-chemical 67 FPSA-2 factorian PPSA (PSA-2/TMSA) (pantum-chemical PC) quantum-chemical 68 FPSA-3 factorian PPSA (PSA-2/TMSA) (pantum-chemical PC) quantum-chemical 71 gravitation index (ql bords) gravitation index (ql bords) quantum-chemical 72 gravitation index (ql bords) gravitation index (ql bords) quantum-chemical 73 HOMO – LUMO energy gap quantum-chemical quantum-chemical 74 HOMO – LUMO energy Gap quantum-chemical quantum-chemical 75 HOMO-1 (order 0) tpological tpological 76 onage of the OrsagerKokwood solvation energy quantum-chemical quantum-chemical 77 information content (order 0) tpological tpological 78 information content (order 1) t	60	FNSA-1 fractional PNSA (PNSA-1/TMSA) [Zefirov's PC]	electrostatic
82 FNSA-2 factorian PNSA (PNSA-2/TMSA) [Zelitov's PC] electostatic 83 FNSA-5 factorian PNSA (PNSA-3/TMSA) [Zelitov's PC] electostatic 84 FNSA-5 factorian PNSA (PNSA-3/TMSA) [Zelitov's PC] electostatic 85 FPSA-1 fractorian PPSA (PPSA-1/TMSA) [Zelitov's PC] electostatic 86 FPSA-4 fractorian PPSA (PPSA-1/TMSA) [Zelitov's PC] electostatic 87 FPSA-5 fractorian PPSA (PPSA-7/TMSA) [Zelitov's PC] electostatic 88 FPSA-5 fractorian PPSA (PPSA-7/TMSA) [Zelitov's PC] electostatic 89 FPSA-5 fractorian PPSA (PPSA-3/TMSA) [Zelitov's PC] electostatic 80 FPSA-5 fractorian PPSA (PPSA-3/TMSA) [Zelitov's PC] electostatic 81 FPSA-5 fractorian PPSA (PPSA-3/TMSA) [Zelitov's PC] electostatic 82 gravitation index (al bords) constitutorial 72 gravitation index (al bords) constitutorial 73 HOMO-1 energy quantum-chemical 74 HOMO-1 energy quantum-chemical 75 HOMO-1 energy quantum-chemical 76 omage of the Onsage-Kitwood solvation energy quantum-chemical 77 information content (order 1) topological 78 information content (order 2) topological 79 information c	61	FNSA-2 fractional PNSA (PNSA-2/TMSA) [guantum-chemical PC]	guantum-chemical
63 FN8A-5 factorian PNSA (PNSA-7MSA) (pantum-chemical PC) quantum-chemical 64 FN8A-5 factorian PNSA (PNSA-7MSA) (pantum-chemical PC) quantum-chemical 65 FPSA-1 fractorian PPSA (PPSA-7MSA) (pantum-chemical PC) quantum-chemical 66 FPSA-2 fractorian PPSA (PPSA-7MSA) (pantum-chemical PC) quantum-chemical 67 FPSA-2 fractorian PPSA (PPSA-7MSA) (pantum-chemical PC) quantum-chemical 68 FPSA-3 fractorian PPSA (PPSA-7MSA) (pantum-chemical PC) quantum-chemical 71 gravitation index (ql bords) quantum-chemical 72 gravitation index (ql bords) quantum-chemical 73 HOMO – LUMO energy quantum-chemical 74 HOMO – transgr quantum-chemical 75 HOMO – transgr quantum-chemical 76 ondage of the Drasger-Krikenod solvation energy quantum-chemical 77 information content (order 0) ttpological 78 information content (order 1) ttpological 79 information content (order 0) ttpological 80 internal enthalpy (30 K)n. of atoms ttprodynamic 81 internal enthalpy (30 K)n. of atoms ttprodynamic 82 internal heat (30 K) in of atoms ttprodynamic 83 internal heat (30 K) in	62	FNSA-2 fractional PNSA (PNSA-2/TMSA) [Zefirov's PC]	electrostatic
64 FNSA-3 fractional PNSA (FNSA-TNLSA) [Zentrov PC] electrostatic 65 FPSA-1 fractional PPSA (PSA-TNLSA) [Qentrov-Anemical PC] epathem-chemical 66 FPSA-4 fractional PPSA (PSA-2TNLSA) [Qentrov-Anemical PC] epathem-chemical 67 FPSA-2 fractional PPSA (PSA-2TNLSA) [Qentrov-Anemical PC] epathem-chemical 68 FPSA-3 fractional PPSA (PSA-3TNLSA) [Qentrov-FPC] epathem-chemical 70 FPSA-3 fractional PPSA (PSA-3TNLSA) [Qentrov-FPC] epathem-chemical 71 gravitation index (all bords) constitutional 72 gravitation index (all bords) constitutional 73 HOMO - LUMO energy gap quantum-chemical 74 HOMO- Chemicage quantum-chemical 75 HOMO-1 (order 1) topological 76 information content (order 1) topological 77 information content (order 2) topological 80 internal entrapy (300 K)/no. of atoms thermodynamic 81 internal entrapy (300 K)/no. of atoms thermodynamic 82 internal heat (300 K)/no. of atoms topological 83 internal heat (300 K)/no. of atoms topological 84 internal heat (300 K)/no. of atoms topological 85 internal heat (300 K)/no. of atoms <	63	FNSA-3 fractional PNSA (PNSA-3/TMSA) [quantum-chemical PC]	quantum-chemical
66 FPSA-1 fractional PPSA (PSA-17MSA) [Quantum-chemical PC] electrostatic 67 FPSA-2 fractional PPSA (PSA-17MSA) [Quantum-chemical PC] electrostatic 68 FPSA-2 fractional PPSA (PSA-27MSA) [Quantum-chemical PC] electrostatic 70 FPSA-3 fractional PPSA (PSA-37MSA) [Quantum-chemical PC] electrostatic 71 gravitation index (al bords) constitutional 72 gravitation index (al bords) constitutional 73 HOMO - LUMO energy gap quantum-chemical 74 HOMO energy quantum-chemical 75 HOMO-1 energy quantum-chemical 76 onage of the OnsagerKirkwood solvation energy quantum-chemical 77 information content (order 1) topological 78 information content (order 1) topological 79 information content (order 1) topological 70 information content (order 1) topological 71 information content (order 1) topological 72 information content (order 1) topological 73 information content (order 1) topological 74 information content (order 1) topological 75 information content (order 1) topological 76 stopological <td>64</td> <td>FNSA-3 fractional PNSA (PNSA-3/TMSA) [Zefirov's PC]</td> <td>electrostatic</td>	64	FNSA-3 fractional PNSA (PNSA-3/TMSA) [Zefirov's PC]	electrostatic
66 FPSA:1 fractional PPSA (PPSA:1TMSA) [Canturo: Archimical PC] quanturo-themical 67 FPSA:2 fractional PPSA (PPSA:2MSA) [Qanturo:Ahemical PC] quanturo-themical 68 FPSA:2 fractional PPSA (PPSA:2MSA) [Qanturo:Ahemical PC] quanturo:Ahemical 70 FPSA:3 fractional PPSA (PPSA:3MSA) [Qanturo:Ahemical PC] quanturo:Ahemical 71 gravitation index (al bonds) constitutional 72 gravitation index (al bonds) constitutional 73 HOMO - LUMO energy gap quanturo:Ahemical 74 HOMO - Interry quanturo:Ahemical 75 HOMO-1 (order 1) topological 76 onage of the Cinsager-Kitkwood solvation energy quanturo:Ahemical 77 information content (order 1) topological 78 information content (order 2) topological 80 internal entalpy (300 K) thermodynamic 81 internal entalpy (300 K) topological 83 internal ental (000 K)/ino. of atoms thermodynamic 84 internal ental (000 K)/ino. of atoms thermodynamic 85 Kier shape index (order 1) topological 86 Kier shape index (order 3) topological 87 Kier shape index (order 3) topological 88 <td>65</td> <td>FPSA-1 fractional PPSA (PPSA-1/TMSA) [quantum-chemical PC]</td> <td>quantum-chemical</td>	65	FPSA-1 fractional PPSA (PPSA-1/TMSA) [quantum-chemical PC]	quantum-chemical
67 PFSA:2 fractional PFSA (PFSA:2TMSA) (partum-chemical PC) ejectostatic 68 PFSA:2 fractional PFSA (PFSA:2TMSA) (partum-chemical PC) ejectostatic 70 PFSA:3 fractional PFSA (PFSA:2TMSA) (partum-chemical PC) ejectostatic 71 gravitation index (all bonds) constitutional 72 gravitation index (all bonds) constitutional 73 HOMO - LUMO energy gap quantum-chemical 74 HOMO - Energy quantum-chemical 75 HOMO-1 energy quantum-chemical 76 onage of the OnsageKinkwood solvation energy quantum-chemical 77 information content (order 1) topological 78 information content (order 2) topological 79 information content (order 2) topological 80 internal enthalpy (300 K/ho. of atoms thermodynamic 82 internal enthalpy (300 K/ho. of atoms thermodynamic 84 internal heat (300 K/ho. of atoms thermodynamic 85 internal heat (300 K/ho. of atoms thermodynamic 86 Kier shape index (order 3) topological 87 Kier shape index (order 3) topological 88 Kier shape index (order 3) topological 89 Molex shape index (or	66	FPSA-1 fractional PPSA (PPSA-1/TMSA) [Zefirov's PC]	electrostatic
68 FPSA 2 fractional PPSA (PPSA-2TINSA) [Zentrov's PC] electrostatic 70 FPSA 3 fractional PPSA (PPSA-3TINSA) [Zentrov's PC] electrostatic 71 gravitation index (all paris) constitutional 72 gravitation index (all paris) constitutional 73 HOMO - LUMO energy gap quantum-chemical 74 HOMO energy quantum-chemical 75 HOMO - Insergy quantum-chemical 76 omage of the Onsager – Kirkwood solvation energy quantum-chemical 77 information content (order 0) tapological 78 information content (order 2) tapological 80 internal enthaly (300 K) thermodynamic 81 internal enthaly (300 K) thermodynamic 82 internal enthaly (300 K) thermodynamic 84 internal enthaly (300 K) thermodynamic 85 internal ental (300 K) tapological 86 Ker fasbap index (order 1) tapological 87 Ker shape index (order 1) tapological 88 Ker shape index (order 1) tapological 89 Ker shape index (order 2) tapological 91 Ker shape index (order 1) tapological 92 molecular volume/K	67	FPSA-2 fractional PPSA (PPSA-2/TMSA) [quantum-chemical PC]	quantum-chemical
69 FFSA:5 factional PFSA (PFSA:3TMSA) (guantum-chemical PC) quantum-chemical 70 FFSA:5 factional PFSA (PFSA:3TMSA) (Zefiro's PC) electrostatic 71 gravitation index (all bands) constitutional 72 gravitation index (all bands) constitutional 73 HOMO – LUMO energy gap quantum-chemical 74 HOMO 1 energy quantum-chemical 75 HOMO-1 tenergy quantum-chemical 76 omage of the Onsager – Krikwood solvation energy quantum-chemical 77 information content (order 1) tepological 78 information content (order 1) tepological 79 information content (order 2) tepological 80 internal entralay (300 K) thermodynamic 81 internal entralay (300 K) thermodynamic 82 internal entralay (300 K) thermodynamic 83 internal entralay (300 K) thermodynamic 84 internal heat (300 K) factoms thermodynamic 85 internal heat (300 K) factoms tpological 86 Ker shape index (order 1) topological topological 89 Ker shape index (order 3) topological 80 Ker shape index (order	68	FPSA-2 fractional PPSA (PPSA-2/TMSA) [Zefirov's PC]	electrostatic
70 FPSA.3 factional PPSA (PPSA.37IMSA) [2efirov's PC] electrostatic 71 gravitation index (all pairs) constitutional 72 gravitation index (all pairs) quantum-chemical 73 HOMO – LUMO energy og quantum-chemical 74 HOMO – Starger – Kirkwood solvation energy quantum-chemical 75 HOMO-1 energy quantum-chemical 76 cmage of the Onsager – Kirkwood solvation energy quantum-chemical 77 information content (order 0) topological 78 information content (order 2) topological 79 information content (order 2) topological 80 internal entropy (300 K)n. thermodynamic 81 internal entropy (300 K)n. thermodynamic 82 internal heat (300 K) thermodynamic 83 internal heat (300 K) topological 84 internal heat (300 K) topological 85 internal heat (300 K) topological 86 Kier shape index (order 1) topological 87 Kier shape index (order 2) topological 89 Kier shape index (order 2) topological 91 Kier and Hall index (order 2) topological 92 molecular wolme	69	FPSA-3 fractional PPSA (PPSA-3/TMSA) [quantum-chemical PC]	quantum-chemical
71 gravitation index (all pairs) constitutional 72 gravitation index (all pairs) constitutional 73 HOMO energy gap quantum-chemical 74 HOMO energy quantum-chemical 75 HOMO-1 energy quantum-chemical 76 nonage of the Onsager-Kirkwod solvation energy quantum-chemical 77 information content (order 0) topological 78 information content (order 1) topological 79 information content (order 2) topological 80 internal enthalpy (300 K) thermodynamic 81 internal enthalpy (300 K) thermodynamic 82 internal entropy (300 K) thermodynamic 83 internal entropy (300 K) thermodynamic 84 internal entropy (300 K) thermodynamic 85 internal heat (300 K) thermodynamic 86 Kier fachtling index topological 87 Kier shape index (order 1) topological 88 Kier shape index (order 3) topological 90 Kier ant Hall index (order 1) topological 91 Kier ant Hall index (order 2) topological 92 molecular surdiac (order 3) topological	70	FPSA-3 fractional PPSA (PPSA-3/TMSA) [Zefirov's PC]	electrostatic
72 gravitation index (all pairs) constitutional 73 HOMO - LUMO energy gap quantum-chemical 74 HOMO energy quantum-chemical 75 HOMO-1 energy quantum-chemical 76 onage of the Onsager-Kirkwood solvation energy quantum-chemical 77 information content (order 0) topological 78 information content (order 2) topological 80 infernal enthalpy (300 K) thermodynamic 81 infernal enthalpy (300 K) thermodynamic 82 internal enthopy (300 K) thermodynamic 83 internal enthopy (300 K) thermodynamic 84 internal enthopy (300 K) thermodynamic 85 internal heat (300 K) thermodynamic 86 Kier fascillity index topological 87 Kier shape index (order 1) topological 88 Kier shape index (order 2) topological 89 Kier shape index (order 3) topological 91 Kier and Hall index (order 1) topological 92 Kier and Hall index (order 3) topological 93 Kier and Hall index (order 3) topological 94 lowesh romalin more diversition quantum-chemical <	71	gravitation index (all bonds)	constitutional
73 HOMO energy gap quantum-chemical 74 HOMO energy quantum-chemical 75 HOMO-1 energy quantum-chemical 76 onage of the Onsager-Krikwood solvation energy quantum-chemical 77 information content (order 0) topological 78 information content (order 1) topological 79 information content (order 2) topological 80 internal enthalpy (300 K) thermodynamic 81 internal enthalpy (300 K) thermodynamic 82 internal entropy (300 K) thermodynamic 83 internal heat (300 K) thermodynamic 84 internal heat (300 K) thermodynamic 85 internal heat (300 K) thermodynamic 86 Kier fakebility Index topological 87 Kier shape index (order 1) topological 88 Kier shape index (order 2) topological 99 Kier and Hall index (order 0) topological 91 Kier and Hall index (order 1) topological 92 Kier and Hall index (order 2) topological 93 Kier and Hall index (order 2) topological 94 lowest normal mode vibrational frequency quantum-chemical	72	gravitation index (all pairs)	constitutional
44 HOM energy quantum-chemical 75 HOMO-1 energy quantum-chemical 76 onage of the Onsager-Kirkwood solvation energy quantum-chemical 77 information content (order 1) topological 78 information content (order 2) topological 79 information content (order 2) topological 80 internal enthalpy (300 K)/no. of atoms thermodynamic 81 internal enthalpy (300 K)/no. of atoms thermodynamic 82 internal entropy (300 K)/no. of atoms thermodynamic 84 internal heat (300 K)/no. of atoms thermodynamic 85 internal heat (300 K)/no. of atoms thermodynamic 86 Kier shape index (order 1) topological 87 Kier shape index (order 2) topological 89 Kier shape index (order 3) topological 90 Kier and Hall index (order 3) topological 91 Kier and Hall index (order 3) topological 92 Kier and Hall index (order 3) topological 93 Kier and Hall index (order 3) topological 94 lowest normal mode vibrational frequency quantum-chemical 95 molecular subjet constitutinal 96	73	HOMO – LUMO energy gap	quantum-chemical
15 HOMO-1 energy quantum-chemical 76 ornage of the Ossager-Kirkwood solvation energy quantum-chemical 77 information content (order 0) topological 78 information content (order 1) topological 79 information content (order 2) topological 80 internal enthalpy (300 K) thermodynamic 81 internal enthalpy (300 K) thermodynamic 82 internal entropy (300 K) thermodynamic 83 internal entropy (300 K) thermodynamic 84 internal entropy (300 K) thermodynamic 85 internal heat (300 K) thermodynamic 86 Kier flexibility index topological 87 Kier shape index (order 1) topological 88 Kier shape index (order 1) topological 99 Kier shape index (order 2) topological 91 Kier and Hall index (order 1) topological 92 Kier and Hall index (order 1) topological 93 Kier and Hall index (order 2) topological 94 lowest normal mode vibrational frequency quantum-chemical 93 Kier and Hall index (order 2) topological 94 lowest normal to inertia A	74	HOMO energy	quantum-chemical
16 Ontage of the Unsage – MixWood Solvation energy qualitum-chemical 77 information content (order 1) topological 78 information content (order 2) topological 80 internal enthalpy (300 K) thermodynamic 81 internal enthalpy (300 K) thermodynamic 82 internal entropy (300 K) thermodynamic 83 internal entropy (300 K) thermodynamic 84 internal entropy (300 K) thermodynamic 85 internal entropy (300 K) thermodynamic 86 Kier theability index topological 87 Kier shape index (order 1) topological 88 Kier shape index (order 2) topological 89 Kier shape index (order 1) topological 90 Kier and Hall index (order 0) topological 91 Kier and Hall index (order 0) topological 92 Kier and Hall index (order 2) topological 93 Kier and Hall index (order 2) topological 94 lowest normal mode vibrational frequency quantum-chemical 95 molecular volume geometrical 96 molecular volume/XYZ box geometrical 97 molecular volume/XYZ box geomet	75	HOMO-1 energy	quantum-chemical
1/ Information content (order 1) topological 78 information content (order 1) topological 79 information content (order 2) topological 80 internal enthalpy (300 K) thermodynamic 81 internal enthalpy (300 K) thermodynamic 82 internal entropy (300 K) thermodynamic 83 internal heat (300 K) thermodynamic 84 internal heat (300 K). otoms 85 internal heat (300 K). thermodynamic 86 Kier flexibility index topological 87 Kier shape index (order 1) topological 88 Kier shape index (order 2) topological 90 Kier and Hall index (order 2) topological 91 Kier and Hall index (order 0) topological 92 Kier and Hall index (order 3) topological 93 Kier and Hall index (order 3) topological 94 lowest normal mode wibrational frequency geometrical 95 molecular volume geometrical 96 molecular volume geometrical 97 molecular volume geometrical 98 molecular volume geometrical 99 moment of inertia A	76	omage of the Unsager-Kirkwood solvation energy	quantum-cnemical
73 Information content (order 2) topological 74 information content (order 2) topological 80 internal enthalpy (300 K) thermodynamic 81 internal entropy (300 K) thermodynamic 82 internal entropy (300 K) thermodynamic 83 internal entropy (300 K) thermodynamic 84 internal entropy (300 K) thermodynamic 85 internal heat (300 K) thermodynamic 86 Kier flexibility index topological 87 Kier shape index (order 1) topological 88 Kier shape index (order 2) topological 90 Kier anape index (order 2) topological 91 Kier and Hall index (order 0) topological 92 Kier and Hall index (order 2) topological 93 Kier and Hall index (order 2) topological 94 lowest normal mode vibrational frequency quantum-chemical 95 molecular volume geometrical 96 molecular volume geometrical 97 molecular volume geometrical 98 molecular volume/XZ box geometrical 99 moment of ineria A geometrical 100 moment of	70	information content (order 0)	topological
3 Internal initiality (300 K)/n. of atoms thermodynamic 80 internal enthalpy (300 K)/n. of atoms thermodynamic 81 internal enthalpy (300 K)/n. of atoms thermodynamic 82 internal entropy (300 K)/n. of atoms thermodynamic 83 internal entropy (300 K)/n. of atoms thermodynamic 84 internal heat (300 K)/n. of atoms thermodynamic 85 internal heat (300 K)/n. of atoms thermodynamic 86 Kier shape index (order 1) topological 87 Kier shape index (order 2) topological 88 Kier shape index (order 2) topological 90 Kier and Hall index (order 2) topological 91 Kier and Hall index (order 1) topological 92 Kier and Hall index (order 2) topological 93 Kier and Hall index (order 2) topological 94 lowest normal mode vibrational frequency quantur-chemical 95 molecular volume/XYZ box geometrical 96 molecular volume/XYZ box geometrical 101 moment of inertia A geometrical 102<	70	information content (order 2)	topological
00 Internal entraly (300 K)/no. of atoms thermodynamic 81 Internal entropy (300 K)/no. of atoms thermodynamic 82 Internal entropy (300 K)/no. of atoms thermodynamic 84 internal heat (300 K)/no. of atoms thermodynamic 85 internal heat (300 K)/no. of atoms thermodynamic 86 Kier fisibility index topological 87 Kier shape index (order 1) topological 88 Kier shape index (order 2) topological 90 Kier and Hall index (order 0) topological 91 Kier and Hall index (order 1) topological 92 Kier and Hall index (order 1) topological 93 Kier and Hall index (order 2) topological 94 lowest normal mode vibrational frequency quantum-chemical 95 molecular volumeX geometrical 96 molecular volumeX quantum-chemical 97 molecular volumeX geometrical 98 molecular volumeX quantum-chemical 101 moment of inertia A geometrical 102 no. of occcupied electronic levels/	80	internal enthalpy (300 K)	thermodynamic
22 internal entropy (300 K) thermodynamic 33 internal entropy (300 K) thermodynamic 34 internal entropy (300 K) thermodynamic 35 internal heat (300 K) thermodynamic 36 Kier shape index (00rder 1) thermodynamic 37 Kier shape index (order 1) topological 38 Kier shape index (order 2) topological 39 Kier shape index (order 0) topological 30 Kier and Hall index (order 0) topological 31 Kier and Hall index (order 3) topological 32 Kier and Hall index (order 3) topological 33 Kier and Hall index (order 3) topological 34 lowest normal mode vibrational frequency quantum-chemical 35 molecular volume X/X box geometrical 36 molecular volume X/X box geometrical 37 molecular volume X/X box geometrical 38 moment of inertia B geometrical 39 molecular volume X/X box geometrical 30 no-of occupied electronic levels. quantum-chemical 310 moment of inertia B geometrical 32 no-of occupied electronic levels. quantum-chemical	81	internal enthalpy (300 K)/no_of atoms	thermodynamic
Base internal heat (300 K)/no. of atoms thermodynamic Base internal heat (300 K) thermodynamic Base internal heat (300 K)/no. of atoms thermodynamic Base internal heat (300 K)/no. of atoms thermodynamic Base internal heat (300 K)/no. of atoms topological Base Kier shape index (order 1) topological Base Kier shape index (order 2) topological Base Kier shape index (order 3) topological Base Kier and Hall index (order 2) topological Base Kier and Hall index (order 3) topological Base molecular surface area geometrical Base molecular surface area geometrical Base molecular surface area geometrical Base molecular volume geometrical Base molecular volume geometrical Base molecular volume geometrical Base molecular volume/XYZ box ge	82	internal entropy (300 K)	thermodynamic
44 internal heat (300 K) thermodynamic 85 internal heat (300 K)/no. of atoms thermodynamic 86 Kier shape index (order 1) topological 87 Kier shape index (order 2) topological 88 Kier shape index (order 3) topological 90 Kier and Hall index (order 0) topological 91 Kier and Hall index (order 1) topological 92 Kier and Hall index (order 2) topological 93 Kier and Hall index (order 2) topological 94 lowest normal mode vibrational frequency quantum-chemical 95 molecular volume geometrical 96 molecular volume/YYZ box geometrical 97 molecular volume/YYZ box geometrical 98 molecular volume/YYZ box geometrical 99 moment of inertia A geometrical 100 moment of inertia B geometrical 101 moment of inertia B geometrical 102 no. of occupied electronic levels/no. of atoms quantum-chemical 103 no. of occupied vipted PNSA [Cefrov's PC] el	83	internal entropy (300 K)/no. of atoms	thermodynamic
B5 internal heat (300 K)/no. of atoms thermodynamic B6 Kier flexibility index topological B7 Kier shape index (order 1) topological B8 Kier shape index (order 2) topological B9 Kier and Hall index (order 0) topological 90 Kier and Hall index (order 1) topological 91 Kier and Hall index (order 1) topological 92 Kier and Hall index (order 1) topological 93 Kier and Hall index (order 2) topological 94 lowest romal mode vibrational frequency quantum-chemical 95 molecular volume geometrical 96 molecular volume/XZ box geometrical 97 molecular volume/XZ box geometrical 98 molecular volume/XZ box geometrical 99 moment of inertia B geometrical 100 moment of inertia B geometrical 101 moment of inertia C quantum-chemical 102 no. of occupied electronic levels quantum-chemical 103 no. of occupied electronic levels quantum-chemical 104 PNSA-1 partial negative surface area [Zefirov's PC] electrostatic 105 PNSA-2 total charge weighted PNS	84	internal heat (300 K)	thermodynamic
86Kier flexibility indextopological87Kier shape index (order 1)topological88Kier shape index (order 2)topological89Kier shape index (order 3)topological90Kier and Hall index (order 0)topological91Kier and Hall index (order 1)topological92Kier and Hall index (order 2)topological93Kier and Hall index (order 2)topological94lowest normal mode vibrational frequencyquantum-chemical95molecular volumegeometrical96molecular volume/XVZ boxgeometrical97molecular volumegeometrical98molecular volumegeometrical99moment of inertia Ageometrical100moment of inertia Bgeometrical101moment of inertia Bgeometrical102no. of occupied electronic levelsquantum-chemical PC]103no. of occupied electronic levels (Quantum-chemical PC]quantum-chemical104PNSA-1 parial negative surface area [Quantum-chemical PC]quantum-chemical105PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-1 parial positive surface area [Zefirov's PC]electrostatic101PPSA-2 total charge weighted PNSA [Quantum-chemical PC]quantum-chemical102PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic103PPSA-2 total ch	85	internal heat (300 K)/no. of atoms	thermodynamic
87Kier shape index (order 1)topological88Kier shape index (order 2)topological89Kier shape index (order 3)topological90Kier and Hall index (order 0)topological91Kier and Hall index (order 1)topological92Kier and Hall index (order 2)topological93Kier and Hall index (order 3)topological94lowest normal mode vibrational frequencyquantum-chemical95molecular sufface areageometrical96molecular volume/XYZ boxgeometrical97molecular volume/XYZ boxgeometrical98molecular volume/XYZ boxgeometrical99moment of inertia Ageometrical100moment of inertia Bgeometrical101moment of inertia Ageometrical102no. of occupied electronic levelsquantum-chemical103no. of occupied velectoric levels/no. of atomsquantum-chemical104PNSA-1 partial negative surface area [Zefirov's PC]electrostatic105PNSA-1 partial negative surface area [Zefirov's PC]electrostatic108PNSA-2 total charge weighted PNSA [Quantum-chemical PC]quantum-chemical109PPSA-1 partial positive surface area [Zefirov's PC]electrostatic109PPSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic101PPSA-2 total charge weighted PPSA [Quantum-chemical PC]quantum-chemical <td>86</td> <td>Kier flexibility index</td> <td>topological</td>	86	Kier flexibility index	topological
88Kier shape index (order 2)topological89Kier shape index (order 3)topological90Kier and Hall index (order 0)topological91Kier and Hall index (order 1)topological92Kier and Hall index (order 2)topological93Kier and Hall index (order 3)topological94lowest normal mode vibrational frequencyquantum-chemical95molecular surface areageometrical96molecular volume/XYZ boxgeometrical98molecular veightconstitutional99moment of inertia Ageometrical90moment of inertia Cgeometrical101moment of inertia Cgeometrical102no. of occupied electronic levelsquantum-chemical103no. of occupied electronic levels/no. of atomsquantum-chemical104PNSA-1 partial negative surface area [Zefirov's PC]electrostatic105PNSA-1 partial negative surface area [Zefirov's PC]electrostatic106PNSA-2 total charge weighted PNSA [Quantum-chemical PC]quantum-chemical107PNSA-2 total charge weighted PNSA [Quantum-chemical PC]electrostatic108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-4 total charge weighted PNSA [Quantum-chemical PC]quantum-chemical101PPSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic102PPSA-4 total charge weighted PNSA [Zefirov's PC]electrostatic103PPSA-4 total charge we	87	Kier shape index (order 1)	topological
89Kier shape index (order 3)topological90Kier and Hall index (order 0)topological91Kier and Hall index (order 1)topological92Kier and Hall index (order 2)topological93Kier and Hall index (order 3)topological94lowest normal mode vibrational frequencyquantum-chemical95molecular surface areageometrical96molecular volumegeometrical97molecular volume/XYZ boxgeometrical98molecular volume/XYZ boxgeometrical99moment of inertia Ageometrical100moment of inertia Bgeometrical101moment of inertia Cgeometrical102no. of occupied electronic levelsquantum-chemical PC]103no. of occupied electronic levels/no. of atomsquantum-chemical104PNSA-1 partial negative surface area [Zefirov's PC]electrostatic105PNSA-2 total charge weighted PNSA [Quantum-chemical PC]quantum-chemical106PNSA-2 total charge weighted PNSA [Quantum-chemical PC]quantum-chemical107PNSA-2 total charge weighted PNSA [Quantum-chemical PC]electrostatic108PNSA-2 total charge weighted PNSA [Quantum-chemical PC]quantum-chemical109PPSA-1 partial positive surface area [Zefirov's PC]electrostatic109PPSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic101PPSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic102PPSA-1 partia	88	Kier shape index (order 2)	topological
90Kier and Hall index (order 0)topological91Kier and Hall index (order 1)topological92Kier and Hall index (order 2)topological93Kier and Hall index (order 3)topological94lowest normal mode vibrational frequencyquantum-chemical95molecular sufface areageometrical96molecular volume/XYZ boxgeometrical97molecular wolume/XYZ boxgeometrical98molecular weightconstitutional99moment of inertia Ageometrical100moment of inertia Bgeometrical101moment of inertia Cgeometrical102no. of occupied electronic levels/no. of atomsquantum-chemical103no. of occupied electronic levels/no. of atomsquantum-chemical104PNSA-1 partial negative surface area [Zefirov's PC]electrostatic105PNSA-1 partial negative surface area [Zefirov's PC]electrostatic108PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic109PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic101PPSA-2 total charge weighted PPSA [Quantum-chemical PC]quantum-chemical102PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic103PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic104PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic105PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic108PNS	89	Kier shape index (order 3)	topological
91Kier and Hall index (order 1)topological92Kier and Hall index (order 2)topological93Kier and Hall index (order 3)topological94lowest normal mode vibrational frequencyquantum-chemical95molecular surface areageometrical96molecular volumegeometrical97molecular volume/XYZ boxgeometrical98molecular volume/XYZ boxgeometrical99moment of inertia Ageometrical100moment of inertia Bgeometrical101moment of inertia Cgeometrical102no. of occupied electronic levelsquantum-chemical103no. of occupied electronic levels/no. of atomsquantum-chemical104PNSA-1 partial negative surface area [quantum-chemical PC]quantum-chemical105PNSA-1 partial negative surface area [quantum-chemical PC]quantum-chemical106PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic107PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]quantum-chemical109PPSA-1 partial positive surface area [Quantum-chemical PC]quantum-chemical101PPSA-2 total charge weighted PPSA [Quantum-chemical PC]quantum-chemical102PPSA-1 partial positive surface area [Quantum-chemical PC]electrostatic103PPSA-1 partial positive surface area [Quantum-chemical PC]electrostatic104PNSA-2 total charge weighted PPSA [Zefir	90	Kier and Hall index (order 0)	topological
92Kier and Hall index (order 2)topological93Kier and Hall index (order 3)topological94lowest normal mode vibrational frequencyquantum-chemical95molecular surface areageometrical96molecular volume/XYZ boxgeometrical97molecular weightconstitutional98monent of inertia Ageometrical100moment of inertia Bgeometrical101moment of inertia Cgeometrical102no. of occupied electronic levelsquantum-chemical103no. of occupied electronic levelsquantum-chemical104PNSA-1 partial negative surface area [quantum-chemical PC]quantum-chemical105PNSA-1 partial negative surface area [Zefirov's PC]electrostatic106PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic107PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [Zefirov's PC]electrostatic110PPSA-2 total charge weighted PPSA [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [Zefirov's PC]electrostatic112PPSA-2 total charge weighted PPSA [Zefirov's PC]electrostatic113PPSA-3 atomic charge weighted PPSA [Zefirov's PC]electrostatic	91	Kier and Hall index (order 1)	topological
93Kier and Hall index (order 3)topological94lowest normal mode vibrational frequencyquantum-chemical95molecular surface areageometrical96molecular volumegeometrical97molecular volume/XYZ boxgeometrical98molecular weightconstitutional99moment of inertia Ageometrical100moment of inertia Bgeometrical101moment of inertia Cgeometrical102no. of occupied electronic levelsquantum-chemical103no. of occupied electronic levels/no. of atomsquantum-chemical104PNSA-1 partial negative surface area [Zefirov's PC]electrostatic105PNSA-1 partial negative surface area [Zefirov's PC]electrostatic106PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic107PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [Zefirov's PC]electrostatic110PPSA-1 partial positive surface area [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [Quantum-chemical PC]electrostatic112PPSA-2 total charge weighted PPSA [Quantum-chemical PC]electrostatic113PPSA-3 atomic charge weighted PPSA [Quantum-chemical PC]electrostatic	92	Kier and Hall index (order 2)	topological
94lowest normal mode vibrational frequencyquantum-chemical95molecular surface areageometrical96molecular volumegeometrical97molecular volume/XYZ boxgeometrical98molecular veightconstitutional99moment of inertia Ageometrical100moment of inertia Bgeometrical101moment of inertia Cgeometrical102no. of occupied electronic levelsquantum-chemical103no. of occupied electronic levels/no. of atomsquantum-chemical104PNSA-1 partial negative surface area [quantum-chemical PC]quantum-chemical105PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic109PSA-1 partial positive surface area [quantum-chemical PC]quantum-chemical110PPSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [quantum-chemical PC]quantum-chemical110PPSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [Quantum-chemical PC]quantum-chemical113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]quantum-chemical113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]quantum-chemical	93	Kier and Hall index (order 3)	topological
95molecular surface areageometrical96molecular volumegeometrical97molecular volume/XYZ boxgeometrical98molecular weightconstitutional99moment of inertia Ageometrical100moment of inertia Bgeometrical101moment of inertia Cgeometrical102no. of occupied electronic levelsquantum-chemical103no. of occupied electronic levelsquantum-chemical104PNSA-1 partial negative surface area [quantum-chemical PC]quantum-chemical105PNSA-1 partial negative surface area [Zefirov's PC]electrostatic108PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [Zefirov's PC]electrostatic110PPSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [Quantum-chemical PC]quantum-chemical113PPSA-3 atomic charge weighted PPSA [Zefirov's PC]electrostatic	94	lowest normal mode vibrational frequency	quantum-chemical
96molecular volumegeometrical97molecular volume/XYZ boxgeometrical98molecular weightconstitutional99moment of inertia Ageometrical100moment of inertia Bgeometrical101moment of inertia Cgeometrical102no. of occupied electronic levelsquantum-chemical103no. of occupied electronic levels/no. of atomsquantum-chemical104PNSA-1 partial negative surface area [quantum-chemical PC]quantum-chemical105PNSA-1 partial negative surface area [Zefirov's PC]electrostatic106PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic107PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [quantum-chemical PC]quantum-chemical110PPSA-1 partial positive surface area [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]quantum-chemical	95	molecular surface area	geometrical
97molecular volume/XYZ boxgeometrical98molecular weightconstitutional99moment of inertia Ageometrical100moment of inertia Bgeometrical101moment of inertia Cgeometrical102no. of occupied electronic levelsquantum-chemical103no. of occupied electronic levels/no. of atomsquantum-chemical104PNSA-1 partial negative surface area [quantum-chemical PC]quantum-chemical105PNSA-1 partial negative surface area [Zefirov's PC]electrostatic106PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic107PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [quantum-chemical PC]quantum-chemical110PPSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [quantum-chemical PC]electrostatic113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]electrostatic	96	molecular volume	geometrical
98molecular weightconstitutional99moment of inertia Ageometrical100moment of inertia Bgeometrical101moment of inertia Cgeometrical102no. of occupied electronic levelsquantum-chemical103no. of occupied electronic levels/no. of atomsquantum-chemical104PNSA-1 partial negative surface area [quantum-chemical PC]electrostatic105PNSA-1 partial negative surface area [Zefirov's PC]electrostatic106PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic107PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [Zefirov's PC]electrostatic110PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [quantum-chemical PC]electrostatic113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]quantum-chemical	97	molecular volume/XYZ box	geometrical
99moment of inertia Ageometrical100moment of inertia Bgeometrical101moment of inertia Cgeometrical102no. of occupied electronic levelsquantum-chemical103no. of occupied electronic levels/no. of atomsquantum-chemical104PNSA-1 partial negative surface area [quantum-chemical PC]quantum-chemical105PNSA-1 partial negative surface area [Zefirov's PC]electrostatic106PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic107PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [Zefirov's PC]electrostatic110PPSA-1 partial positive surface area [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [quantum-chemical PC]electrostatic113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]quantum-chemical	98	molecular weight	constitutional
100moment of inertia Bgeometrical101moment of inertia Cgeometrical102no. of occupied electronic levelsquantum-chemical103no. of occupied electronic levels/no. of atomsquantum-chemical104PNSA-1 partial negative surface area [quantum-chemical PC]quantum-chemical105PNSA-1 partial negative surface area [Zefirov's PC]electrostatic106PNSA-2 total charge weighted PNSA [Quantum-chemical PC]quantum-chemical107PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [Zefirov's PC]quantum-chemical110PPSA-1 partial positive surface area [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [Quantum-chemical PC]electrostatic113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]quantum-chemical	99	moment of inertia A	geometrical
101moment of inertia Cgeometrical102no. of occupied electronic levelsquantum-chemical103no. of occupied electronic levels/no. of atomsquantum-chemical104PNSA-1 partial negative surface area [quantum-chemical PC]quantum-chemical105PNSA-1 partial negative surface area [Zefirov's PC]electrostatic106PNSA-2 total charge weighted PNSA [quantum-chemical PC]quantum-chemical107PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [Zefirov's PC]electrostatic110PPSA-1 partial positive surface area [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [Quantum-chemical PC]electrostatic113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]quantum-chemical	100	moment of inertia B	geometrical
102no. of occupied electronic levelsquantum-chemical103no. of occupied electronic levels/no. of atomsquantum-chemical104PNSA-1 partial negative surface area [quantum-chemical PC]quantum-chemical105PNSA-1 partial negative surface area [Zefirov's PC]electrostatic106PNSA-2 total charge weighted PNSA [quantum-chemical PC]quantum-chemical107PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [Zefirov's PC]electrostatic110PPSA-1 partial positive surface area [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [Zefirov's PC]electrostatic113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]quantum-chemical	101	moment of inertia C	geometrical
103100. 0f occupied electronic levels/to of alonisquantum-chemical104PNSA-1 partial negative surface area [quantum-chemical PC]quantum-chemical105PNSA-1 partial negative surface area [Zefirov's PC]electrostatic106PNSA-2 total charge weighted PNSA [quantum-chemical PC]quantum-chemical107PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [Quantum-chemical PC]quantum-chemical110PPSA-1 partial positive surface area [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [Zefirov's PC]electrostatic113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]quantum-chemical	102	no. of occupied electronic levels	quantum-chemical
104PNSA-1 partial negative surface area [quantum-chemical PC]quantum-chemical105PNSA-1 partial negative surface area [Zefirov's PC]electrostatic106PNSA-2 total charge weighted PNSA [quantum-chemical PC]quantum-chemical107PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic108PNSA-1 partial positive surface area [quantum-chemical PC]quantum-chemical109PPSA-1 partial positive surface area [Zefirov's PC]electrostatic110PPSA-1 partial positive surface area [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [Zefirov's PC]electrostatic113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]quantum-chemical	103	no. or occupied electronic levels/no. or atoms DNSA 1 partial pagative surface area [quantum chamical DC]	
105PNOACH partial negative surface area [26000 S PC]electrostatic106PNSA-2 total charge weighted PNSA [quantum-chemical PC]quantum-chemical107PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [quantum-chemical PC]quantum-chemical110PPSA-1 partial positive surface area [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [Zefirov's PC]electrostatic113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]quantum-chemical	104	FINGA-1 partial negative surface area [Quantum-chemical PC]	quantum-cnemical
1007PNSA-2 total charge weighted PNSA [Zefirov's PC]electrostatic108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [quantum-chemical PC]quantum-chemical110PPSA-1 partial positive surface area [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [Zefirov's PC]electrostatic113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]quantum-chemical	106	I NOAT I Parliar regarive surface area [Zerilov 5 FO] PNSA-2 total charge weighted DNSA [guantum-chamical DC]	duantum chomical
108PNSA-3 atomic charge weighted PNSA [Zefirov's PC]electrostatic109PPSA-1 partial positive surface area [quantum-chemical PC]quantum-chemical110PPSA-1 partial positive surface area [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [Zefirov's PC]electrostatic113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]quantum-chemical	107	FINGA-2 total charge weighted PNGA [Yudhuh-Chemical PG] PNSA-2 total charge weighted PNSA [Zafirov's PC]	quantum-chemical
109PPSA-1 partial positive surface area [quantum-chemical PC]quantum-chemical110PPSA-1 partial positive surface area [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [Zefirov's PC]electrostatic113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]quantum-chemical	108	PNSA-3 atomic charge weighted PNSA [Zelliov 5 FO]	electrostatio
110PPSA-1 partial positive surface area [Zefirov's PC]electrostatic111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [Zefirov's PC]electrostatic113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]quantum-chemical	109	PPSA-1 nartial positive surface area [duantum-chemical PC]	auantum-chemical
111PPSA-2 total charge weighted PPSA [quantum-chemical PC]quantum-chemical112PPSA-2 total charge weighted PPSA [Zefirov's PC]electrostatic113PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]quantum-chemical	110	PPSA-1 partial positive surface area [γ uantum onemican ro]	electrostatio
112 PPSA-2 total charge weighted PPSA [Zefirov's PC] electrostatic 113 PPSA-3 atomic charge weighted PPSA [quantum-chemical PC] quantum-chemical	111	PPSA-2 total charge weighted PPSA [guantum-chemical PC]	quantum-chemical
113 PPSA-3 atomic charge weighted PPSA [quantum-chemical PC] quantum-chemical	112	PPSA-2 total charge weighted PPSA [Zefirov's PC]	electrostatic
	113	PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]	quantum-chemical

Table 7. Continued

114 PPSA-3 atomic drops weighted PPSA (Editor's PC) electrosition 115 principal moment of ineria A no. of atoms Hermodynamic 116 principal moment of ineria B no. of atoms Hermodynamic 117 principal moment of ineria B no. of atoms Hermodynamic 118 principal moment of ineria B no. of atoms Hermodynamic 119 principal moment of ineria B no. of atoms Hermodynamic 120 principal moment of ineria B no. of atoms Hermodynamic 121 Principal moment of ineria B no. of atoms Hermodynamic 122 Principal moment of ineria B no. of atoms Hormodynamic 123 Principal moment of ineria B no. of atoms Hormodynamic 124 Pradic index (oder 2) Hormodynamic Hormodynamic 125 relative molecular wagits constitutional Hormodynamic 126 relative molecular wagits constitutional Hormodynamic 127 PrACC relative molecular wagits constitutional Hermodynamic 128 relative molecular wagits constitutional Hermodynamic 129 PrACC relative proteinal endropy (300 K) no. of atoms Hermodynamic 130 relative proteinal endropy (300 K) no. of atoms Hermodynamic 131 relati	no.	descriptor	type
115 princpair normer of ineria A thermodynamic 116 princpair normer of ineria A thermodynamic 117 princpair normer of ineria B thermodynamic 118 princpair normer of ineria B thermodynamic 119 princpair normer of ineria B thermodynamic 111 princpair normer of ineria A thermodynamic 112 Rande index (order 2) topological 113 relative no. of argin bords constitutional 114 RNCG selute regative charge (DMMEGOTINMUS) [Zatirov FC] electroalac 119 relative regative charge (SM CNC) constitutional 111 relative regative charge (SM CNC) constitutional 112 relative regative charge (SM CNC) constitutional 113 relative regative charge (SM CNC) constitutional 114 PROS relative pastive charge (SM CNC) constitutional 115 relative regative charge (SM CNC)	114	PPSA-3 atomic charge weighted PPSA [Zefirov's PC]	electrostatic
116 principal moment of ineria Arx. of atoms Hermodynamic 117 principal moment of ineria Brx. of atoms Hermodynamic 118 principal moment of ineria Crx. Hermodynamic 120 principal moment of ineria Crx. Hermodynamic 121 Paradic finde (order 0) Hermodynamic 122 Paradic finde (order 0) Hermodynamic 123 Paradic finde (order 0) Hermodynamic 124 Faradic finde (order 0) Hermodynamic 125 realitive molecular veight constitutional 126 realitive molecular veight constitutional 127 PRIOS finders molecular veight constitutional 128 realitive molecular veight constitutional 129 PRIOS finders molecular veight constitutional 120 realitive molecular veight constitutional 121 realitive molecular veight constitutional 123 PRIOS finders molecular veight constitutional 124 PRIOS finders molecular veight constitutional 125 realitive molecular veight constitutional 126 realitive molecular veight constitutional 127 PRIOS finders molecular veight contoticeular veight	115	principal moment of inertia A	thermodynamic
117 principal moment of nerits B hemodynamic 118 principal moment of nerits C hemodynamic 120 principal moment of nerits CNo. of atoms hemodynamic 121 Randic index (ode 0) topological 122 Randic index (ode 7) topological 123 Randic index (ode 2) topological 124 Randic index (ode 2) topological 125 Randic index (ode 2) topological 126 Paradic index (ode 2) topological 127 RNGC relative negative charge (OMNEGOTNINUS) [cantum-chemical PC] quartan-chemical 128 RNGC relative negative charge (OMNEGOTNINUS) [cantum-chemical PC] quartan-chemical 129 RNGC relative negative charge (OMNEGOTNINUS) [cantum-chemical PC] quartan-chemical 130 rotational entropy (300 K)/n. of atoms hemodynamic 131 rotational entropy (300 K)/n. of atoms hemodynamic 132 rotational entropy (300 K)/n. of atoms hemodynamic 133 rotational entropy (300 K)/n. of atoms hemodynamic 134 RPCG relative positive charge (AMNEGOTNUS) [Cantum chemical PC] quartan-chemical 135 RPCG relative positive charge (AMNCGOTPLUS) [Cantum chemical PC] quartan-chemical 136 RPCG relative posi	116	principal moment of inertia A/no. of atoms	thermodynamic
118 principal moment of ineria Cinc. of atoms thermodynamic 120 principal moment of ineria Cinc. of atoms thermodynamic 121 Rando index (order 1) topological 122 Rando index (order 2) topological 123 Rando index (order 2) topological 124 Rando index (order 2) topological 125 Rando index (order 2) topological 126 relative molecular (order 2) constitutional 127 RNCS orabiv ongalve onage (OMREGOTINIUS) [calmur -temical PC] quantum -temical 128 RNCS relative negalve onage (OMREGOTINIUS) [calmur -temical PC] quantum -temical 129 relational interpression (QMR Cinc Talmus) [calmur -temical PC] quantum -temical 120 relational interpression (QMR Cinc Talmus) [calmur > PC] quantum -temical 121 relational interpression (QM Kino di atoms thermodynamic 122 relational interpression (QM Kino di atoms thermodynamic 123 relational interpression (QM Kino di atoms thermodynamic 124 relational interpression (QM Kino di atoms thermodynamic 125 RPCS relative possible charge SA (SMMCPS/PDC) [calmur > PC] quantum -temical 126 relative possible charge SA (SMMCPS/PDC) [calmur > PC] quantum -tem	117	principal moment of inertia B	thermodynamic
119 principal moment of ineria C Inernodynamic 120 principal moment of ineria C (no. d atoms toppogoal 121 Randic index (oder 0) toppogoal 122 Randic index (oder 2) toppogoal 123 Randic index (oder 2) toppogoal 124 Randic index (oder 2) toppogoal 125 relative molecular weights constitutional 126 RNCS entative mogetive draps (CMMESOTINIUS) [Quantum-chemical PC] extensative 127 RNCS entative mogetive draps (CMMESOTINIUS) [Quantum-chemical PC] extensative 128 RNCS entative mogetive draps (CMMESOTINIUS) [Quantum-chemical PC] extensative 129 relative mogetive draps (CMMESOTINIUS) [Quantum-chemical PC] extensative 120 relative mogetive draps (CMMESOTINIUS) [Quantum-chemical PC] extensative 121 relative mogetive draps (CMMESOTINIUS) [Quantum-chemical PC] quantum-chemical 123 relative mogetive draps (CMMESOTINIUS) [Quantum-chemical PC] quantum-chemical 124 RPCS relative positive draps (CMMESOTINIUS) [Quantum-chemical PC] quantum-chemical 125 relative positive draps (CMMESOTINIUS) [Quantum-chemical PC] quantum-chemical 126 relative positive draps (CMMESOTINIUS) [Quantum-chemical PC] quantum-chemical 127	118	principal moment of inertia B/no. of atoms	thermodynamic
120 principal moment of inetia Cino, of atoms thermodynamic 121 Rando index (order 1) topologial 122 Rando index (order 2) topologial 123 Rando index (order 3) topologial 124 Rando index (order 3) constitutional 125 native no. of angle bonds constitutional 126 native no. of angle bonds constitutional 127 RACC retains regative chage SALKSCOTININUS) (zantum-chemical PC) constitutional 128 maticative no. of angle bonds constitutional 129 maticative no. of angle SALKSCOTININUS) (zantum-chemical PC) constitutional 120 maticative no. of angle SALKMOSCOTININUS (zantum-chemical PC) constitutional 121 maticative no. of angle SALKMOSCOTINUS (zafursy PC) quartum-chemical 122 naticative no.of angle SALKMOSCOTINUS (zafursy PC) quartum-chemical 123 maticative no.of angle SALKMOSCOTINUS (zafursy PC) quartum-chemical 124 RPCS relative positive national of angle SALKMOSCOTINUS (zafursy PC) quartum-chemical 125 maticative positive national of angle SALKMOSCOTINUS (Zafursy PC) quartum-chemical 126 atsoctatil information content (order 1) topological 127 statoctatil information content (order 2)	119	principal moment of inertia C	thermodynamic
121 Radic index (order 0) topological 122 Radic index (order 2) topological 123 Radic index (order 2) topological 124 Radic index (order 3) constitutional 125 naladva molecular weight constitutional 126 naladva molecular weight constitutional 127 PNCG atabite negative charge (CMNEGCDTINUS) (2afrav PC) electrostatic 128 NCG statiste negative charge (CMNEGCDTINUS) (2afrav PC) electrostatic 129 NNCS statiste negative charge (CMNEGCDTINUS) (2afrav PC) electrostatic 130 cotacional entropy (2001 () electrostatic 131 cotacional entropy (2001 () cataritacional entropy (2001 () 132 cotacional entropy (2001 () cataritacional entropy (2001 () 133 cotacional entropy (2001 () cataritacional entropy (2001 () 134 RPCC relative positive charge (CMNEGC) (CMNUS) (2afrav PC) cataritacional entropy (2001 () 135 RPCC relative positive charge (SAMEGCPNECO) (2afravi PC) cataritacional entropy (2001 () 136 RPCC relative positive charge (SAMEGCPNECO) (2afravi PC) cataritacional entropy (2001 () 137 statutacian information contern (coder 1) topological 138 statutacinal information contern (coder 1)	120	principal moment of inertia C/no. of atoms	thermodynamic
122 Randb index (roler 1) topologial 123 Randb index (roler 2) topologial 124 Randb index (roler 3) topologial 125 relative no. of single bonds constitutional 126 relative no. of single bonds constitutional 127 RNCG relative negative charge (CMNEGOTINNUS) [Quantum-chemical PC] quantum-chemical 128 RNCG relative negative charge (CMNEGOTINNUS) [Zelativs PC] electrostatic 129 RNCG relative negative charge (CMNEGOTINNUS) [Zelativs PC] electrostatic 130 relational entitipy (SOX K)in. o d famas thermodynamic 131 relational entitipy (SOX K)in. o d famas thermodynamic 132 relational entitipy (SOX K)in. o d famas thermodynamic 134 RPCG relative positive charge (CMPCGOTPHCG) [Quantum-chemical PC] quantum-chemical 136 RPCG relative positive charge (CMPCGOTPHCG) [Quantum-chemical PC] quantum-chemical 137 stancharal information content (roler 1) topologial 138 stancharal information content (roler 2) topologial 139 stancharal information content (roler 2) quantum-chemical 139 stancharal information content (roler 2) quantum-chemical 140 tobal probabilis stance anaga (SIAN'SFPCG) [Quantum-chemic	121	Randic index (order 0)	topological
123 Rardic index (order 2) topologial 124 Rardic index (order 3) topologial 125 relative molecular weight constitutional 126 relative molecular weight constitutional 127 RNCG stative negative charge (CMNEGOTMINUS) [Qathurs-chemical PC] electrostatic 128 RNCG stative negative charge (CMNEGOTMINUS) [Zathurs PC] electrostatic 129 RNCS stative negative charge (CMNEGOTMINUS) [Zathurs PC] electrostatic 130 crotational entropy (200 K) thermodynamic 131 crotational entropy (200 K) thermodynamic 132 rotational entropy (200 K) thermodynamic 133 crotational entropy (200 K) thermodynamic 134 RPCG relative pashe charge (MPCG) (201 K) USI (Zathurs PC] eathurs-chemical 135 RPCG relative pashe charge (MPCG) (201 K) USI (Zathurs PC] eathurs-chemical 136 structural information content (order 1) topologial 137 structural information content (order 1) topologial 138 structural information content (order 1) topologial 140 TMSA total indexitar strafts are a [Qanturm-chemical PC] edertostatic 141 TMSA total indexitar strafts are a [Qanturm-chemical ederostatic 142	122	Randic index (order 1)	topological
124 Randic index (order 5) topological 125 relative no. of angle brods constitutional 126 relative no. of angle brods constitutional 127 RNCG relative negative change (CMNRSQ/TMINUS) [claritry's PC] electrostric 128 RNCS relative negative change (CMNRSQ/TMINUS) [claritry's PC] electrostric 130 relative negative change (CMRSQ/TMINUS) [Claritry's PC] electrostric 131 relative negative change (CMRSQ/TMISQ) [Claritry's PC] quantum-chemical 132 relative negative change (CMRSQ/TMISQ) [Claritry's PC] quantum-chemical 133 relative positive change (CMRSQ/TMISQ) [Claritry's PC] quantum-chemical 134 RPCS relative positive change (CMRSQ/TMRSQ) [Claritry's PC] quantum-chemical 135 relative positive change (CMRSQ/TMRSQ) [Claritry's PC] electrostric 136 structural information content (corder 2) topological 137 structural information content (corder 2) topological 140 TMSA hald molecular surface seria (Laritry's PC] electrostric 141 topological quantum-chemical 142 topographic electronic index (al boxid) (Laritry's PC] electrostric 143 topological quantum-chemical 144 total inforgi (300 K)	123	Randic index (order 2)	topological
125 relative motion on of angle bonds constitutional 126 relative nogatio charge (ANR-GOTMINUS) [quantum-themical PC] quantum-themical 127 RNCG relative negatio charge (ANR-GOTMINUS) [quantum-themical PC] quantum-themical 128 RNCG relative negatio charge (ANR-GOTMINUS) [quantum-themical PC] quantum-themical 129 RNCS weltive negation charge (AS, (ASM-GF PRCG) [Zalinov's PC] quantum-themical 131 robational entropy (300 K/no. of atoms thermodynamic 132 robational entropy (300 K/no. of atoms thermodynamic 133 robational entropy (300 K/no. of atoms thermodynamic 134 RPCG relative positive charged SA (SAM-PGS PRCG) [Quantum-charnical PC] quantum-chemical 135 RPCS relative positive charged SA (SAM-PGS PRCG) [Quantum-chemical PC] topological 136 structural information content (coter 1) topological 137 structural information content (coter 2) topological 141 TMSA total molecular surface anne (quantum-chemical PC) quantum-chemical 142 topographic electromic indica (al bonds) 2/elfov's PC] electrostalic 143 topological topological topological	124	Randic index (order 3)	topological
126 relative no.d ragie bruts constitutional 127 RNCG relative negative drage (CMNEGGTMINUS) [quantum-chemical PC] electrostatic 128 RNCS relative negative drage (CMNEGGTMINUS) [claritor's PC] electrostatic 129 RNCS relative negative drage (CMNEGGTMINUS) [claritor's PC] electrostatic 131 rotational entropy (300 K) ho. of atoms thermodynamic 132 rotational entropy (300 K) ho. of atoms thermodynamic 133 rotational entropy (300 K) ho. of atoms thermodynamic 134 RPCS relative positive draged SA (SAMPOS RPCG) [Zelirov's PC] electrostatic 137 structural information contert (order 1) topological 138 structural information contert (order 1) topological 140 TMSA bata imolecular surface area [Zelirov's PC] electrostatic 141 TMSA bata imolecular surface area [Zelirov's PC] electrostatic 142 topographic electronic index (al pans) [Zelirov's PC] electrostatic 143 topological quantum-chemical 144 total entropy (300 K). datoms quantum-chemical 145 total entropy (300 K). datoms quantum-chemical 146 total molecular surface area [Zelirov's PC] electrostatic 147 total molecu	125	relative molecular weight	constitutional
12/ HNCL relative negative drage (contres) (Clinicus) (plantum-hermical PC) quantum-hermical 128 RNCS relative negative charge SA (SAMHEG'PNCG) (Zelirov's PC) electrostitic 130 robbional enthipty (300 K) no. d atoms thermodyramic 131 robbional enthipty (300 K) no. d atoms thermodyramic 132 robbional enthipty (300 K) no. d atoms thermodyramic 133 robbional entropy (300 K) atoms thermodyramic 134 RPCS relative positive charged SA (SAMPCS PRCG) (Quantum-charnical PC) quantum-charnical 135 RPCS relative positive charged SA (SAMPCS PRCG) (Quantum-charnical PC) quantum-charnical 136 RPCS relative positive charged SA (SAMPCS PRCG) (Quantum-charnical PC) quantum-charnical 137 structural information content (coter 1) topological 138 structural information content (coter 2) topological 140 TMSA total molecular surface ana (Quantum-charnical PC) quantum-charnical 141 TMSA total molecular surface ana (Quantum charnical PC) quantum-charnical 142 topological topological topological 143 topological topological topological 144 topological topological topological 145 topological topological	126	relative no. of single bonds	constitutional
129 FRCS relative negative Charge M (AMM/CSU (MM/CSU (2010) SPC) electrostatic 130 rotational entropy (300 K)ho. of atoms thermodynamic 131 rotational entropy (300 K)ho. of atoms thermodynamic 132 rotational entropy (300 K)ho. of atoms thermodynamic 133 rotational heat capacity (300 K)ho. of atoms thermodynamic 134 FRCS relative positive charge (ALM/POSC/TPLUS) [Zelirov's PC] quantum-chemical 135 Fredse positive charged (ALM/POSC/TPLUS) [Zelirov's PC] quantum-chemical 136 FRCS relative positive charged (ALM/POSC/TPLUS) [Zelirov's PC] quantum-chemical 137 structural information content (coder 1) toppolgical 138 structural information content (coder 2) quantum-chemical 140 TRASA total inforcation content (coder 2) electrostatic 141 TRASA total inforcation content (coder 2) electrostatic 142 topgoraphic electronic index (al paris) [Zelirov's PC] electrostatic 143 topagraphic electronic index (al paris) [Zelirov's PC] electrostatic 144 total entropy (300 K)ho. of atoms quantum-chemical 145 total inforcatic and atoms quantum-chemical 146 total entropy (300 K)ho. of atoms thermodynamic 147 <	127	RNCG relative negative charge (QMNEG/QTMINUS) [quantum-chemical PC]	quantum-chemical
129 rhttest leginer entingener entingener entitiette 130 rotational entinger (300 K)/no. of atoms thermodynamic 131 rotational entinger (300 K)/no. of atoms thermodynamic 132 rotational entinger (300 K)/no. of atoms thermodynamic 133 rotational heat capacity (300 K)/no. of atoms thermodynamic 134 RPGC relative positive charged SA (SAMPOS RPC0) (guantum-chenical PC) quantum-chenical 135 RPCS relative positive charged SA (SAMPOS RPC0) (guantum-chenical PC) quantum-chenical 136 structural information content (order 0) topological 137 structural information content (order 1) topological 138 structural information content (order 2) electrostatic 140 TMSA total molecular surface area [ZeliroVs PC] electrostatic 141 TMSA total molecular surface area [ZeliroVs PC] electrostatic 142 topographic electronic ndex (all ponts) [ZeliroVs PC] electrostatic 143 topographic electronic ndex (all ponts) [ZeliroVs PC] electrostatic 144 total entinety (300 K)/no. of atoms quantum-chenical 145 total entinety (300 K)/no. of atoms quantum-chenical 146 total entinety (300 K)/no. of atoms quantum-chenical 147 <t< td=""><td>128</td><td>RINGG relative negative charge (QMINEG/QIMINUS) [Zetirov's PG]</td><td>electrostatic</td></t<>	128	RINGG relative negative charge (QMINEG/QIMINUS) [Zetirov's PG]	electrostatic
130 rotativa emically (300 K) for anite internodynamic 131 rotativa emically (300 K) for a forms internodynamic 132 rotativa emically (300 K) for a forms internodynamic 133 rotativa emically (300 K) for a forms internodynamic 134 RPCS relative positive charged (AGMMOS PPCG) (quantum-chenical PC) quantum-chenical 135 RPCS relative positive charged (AGMMOS PPCG) (quantum-chenical PC) quantum-chenical 136 Shoutural information content (order 0) topological 137 shoutural information content (order 1) topological 138 shoutural information content (order 2) topological 139 shoutural information content (order 2) topological 140 TRASA total inforcation content (order 2) topological 141 TRASA total inforcation context (abords 7/2 electrostatic 142 topographic electronic infox (al paris) (Zefino's PC) electrostatic 143 total enhalpy (300 K) no. of atoms quantum-chenical 144 total enhalpy (300 K) no. of atoms quantum-chenical 145 total enhalpy (300 K) no. of atoms quantum-chenical 146 total enhalpy (300 K) no. of atoms quantum-chenical 151 total enhalped (300 K) No. of atoms qua	129	RINUS relative negative charge SA (SAMINEG RINUG) [Zenrov's PU]	electrostatic
131 Industria finitop/1000 (N) Itemodynamic 132 Industria finitop/1000 (N) Itemodynamic 133 Industria finitop/1000 (N) Itemodynamic 134 HPCG relative positive charged SA (SAMPOS HPCG) (guantum-chemical PC) quantum-chemical 135 HPCS relative positive charged SA (SAMPOS HPCG) (guantum-chemical PC) quantum-chemical 136 HPCS relative positive charged SA (SAMPOS HPCG) (guantum-chemical PC) quantum-chemical 137 structural information content (order 0) topological 138 structural information content (order 1) topological 140 TMSA total molecular surface area [Zelitov's PC] electrostatic 141 TMSA total molecular surface area [Zelitov's PC] electrostatic 142 topographic electronic ndex (al londs) [Zelitov's PC] electrostatic 143 topographic electronic ndex (al londs) [Zelitov's PC] electrostatic 144 total entropy (300 K) nd anis) [Zelitov's PC] electrostatic 145 total entropy (300 K) nd anis) quantum-chemical 146 total entropy (300 K) nd anise quantum-chemical 151 total entropy (300 K) nd anise quantum-chemical 152 total inflocular one-center E-E repulsion/no. of atoms quantum-che	130	rotational entropy (200 K)/no. of atoms	thermodynamic
12 Instance mixed (200 K) No. 0 atoms Instance mixed (200 K) 133 crotation heat capachy (200 K) atoms the modynamic 134 RPCS relative positive charge (QMPCS) (2FILUS) [Zelirov's PC] quantum-chemical 135 RPCS relative positive charged SA (SAMPCS) RPCG) [Zelirov's PC] teptobigical 136 RPCS relative positive charged SA (SAMPCS) RPCG) [Zelirov's PC] teptobigical 137 structural information content (order 1) topological 138 structural information content (order 2) topological 140 TMSA total molecular surface area [Quantum-chemical PC] electrostatic 141 TMSA total molecular surface area [Quantum-chemical PC] electrostatic 142 topographic electronic index (al pine) [Zelirov's PC] electrostatic 143 topid enhalpy (300 K) quantum-chemical 144 total enhalpy (300 K) quantum-chemical 145 total enhalpy (300 K) datas 146 total entropy (300 K) datas 151 total molecular one-centre E + attacation quantum-chemical 152 total molecular one-centre	100	rotational entropy (300 K)	thermodynamic
Internet of the stage (OMPCASTIPLUS) (Zetrov's PC) Canadian chemical 135 RPCG relative positive charges (GMPCASTIPLUS) (Zetrov's PC) quantum-chemical 136 RPCG relative positive charges (GMPCASTIPLUS) (Zetrov's PC) electrostatic 137 structural information content (order 1) topological 138 structural information content (order 1) topological 140 TMSA total molecular surface area [Quantum-chemical PC] quantum-chemical 141 TMSA total molecular surface area [Quantum-chemical PC] electrostatic 142 toporganice electronic index (al paris) [Zetrov's PC] electrostatic 143 toporganice electronic index (al paris) [Zetrov's PC] electrostatic 144 total enhalpy (30 K)/is. of elons quantum-chemical 145 total enhalpy (30 K)/is. of elons quantum-chemical 146 total enhalpy (30 K)/is. of atoms thermodynamic 151 total molecular once enter F-E repulsion quantum-chemical 152 total molecular once enter F-E repulsion quantum-chemical 153 total molecular once enter F-E repulsion quantum-chemical 154 </td <td>132</td> <td>rotational heat capacity (300 K)/no. of atoms</td> <td>thermodynamic</td>	132	rotational heat capacity (300 K)/no. of atoms	thermodynamic
BPCS relative positive charged SA (SAMPOS*PRCG) [quantum-chemical PC] quantum-chemical 136 RPCS relative positive charged SA (SAMPOS*PRCG) [Zelfov's PC] electrostatic 137 structural information content (order 1) topological 138 structural information content (order 2) topological 139 structural information content (order 2) electrostatic 140 TMSA total molecular surface area [Quantum-chemical PC] electrostatic 142 topographic electroni index (all bonds) [Zelfor/s PC] electrostatic 143 topographic electroni index (all bonds) [Zelfor/s PC] electrostatic 144 total dipole of the molecule quantum-chemical 145 total entrapy (300 K)no. of atoms quantum-chemical 146 total entrapy (300 K)no. of atoms quantum-chemical 150 total heat capach (300 K) atoms quantum-chemical 151 total heat capach (300 K) atoms quantum-chemical 152 total molecular one-center E-E repulsion quantum-chemical 153 total and capach (300 K) atoms quantum-chemical 1	134	BPCG relative positive charge (OMPOS/OTPLUS) [Zefirov's PC]	quantum-chemical
196 RPCS relative positive draged SA (SMPOS'RPCG) [Zatirov's PC] description 197 structural information content (order 1) topological 198 structural information content (order 2) topological 199 structural information content (order 2) topological 140 TMSA total molecular surface are [ZetIrov's PC] electrostatic 141 TMSA total molecular surface are [ZetIrov's PC] electrostatic 142 topographic electronic index (all bonds) [ZetIrov's PC] electrostatic 143 topographic electronic index (all bonds) [ZetIrov's PC] electrostatic 144 total enthalpy (300 K) quantum-chemical 145 total enthalpy (300 K) quantum-chemical 146 total enthalpy (300 K) quantum-chemical 150 total heat capacity (300 K) of atoms quantum-chemical 151 total heat capacity (300 K) of atoms quantum-chemical 152 total molecular one-centre E-E repuision quantum-chemical 153 total heat capacity (300 K) of atoms quantum-chemical 154 total	135	BPCS relative positive charged SA (SAMPOS*BPCG) [quantum-chemical PC]	quantum-chemical
37 structural information content (order i) topological 38 structural information content (order i) topological 39 structural information content (order 2) topological 140 TMSA total molecular surface are [Guantum-chemical PC] electrostatic 141 TMSA total molecular surface are [Guantum-chemical PC] electrostatic 142 topographic electronic index (all bords) [Zefirov's PC] electrostatic 143 topological guantum-chemical 144 total entrapy (300 K) quantum-chemical 145 total entrapy (300 K) quantum-chemical 146 total entrapy (300 K) quantum-chemical 147 total entrapy (300 K) ftermedynamic 150 total heat capachy (300 K) quantum-chemical 151 total heat capachy (300 K) quantum-chemical 152 total molecular one-center E-E Erepuision quantum-chemical 153 total molecular one-center E-E Erepuision quantum-chemical 154 total molecular one-center E-E and and one quantum-chemical 155 total molecular one-center E-E and and one quantum-chemical <t< td=""><td>136</td><td>RPCS relative positive charged SA (SAMPOS*RPCG) [Zefirov's PC]</td><td>electrostatic</td></t<>	136	RPCS relative positive charged SA (SAMPOS*RPCG) [Zefirov's PC]	electrostatic
139 structural information content (order 1) topological 139 structural information content (order 2) topological 140 TMSA total molecular surface area [Quantum-chemical PC] quantum-chemical 141 TMSA total molecular surface area [Quantum-chemical PC] electrostatic 142 topographic electronic index (all boxis) [Zefirov's PC] electrostatic 143 topographic electronic index (all boxis) [Zefirov's PC] quantum-chemical 144 total enthapy (300 K) quantum-chemical 145 total enthapy (300 K) quantum-chemical 146 total enthapy (300 K) quantum-chemical 147 total entropy (300 K) quantum-chemical 148 total entropy (300 K) quantum-chemical 150 total heat capacity (300 K) thermodynamic 151 total heat capacity (300 K) quantum-chemical 152 total molecular one-center E-E repuision quantum-chemical 153 total molecular one-center E-E repuision quantum-chemical 154 total molecular one-center E-E repuision quantum-chemical 155 total molecular one-center E-E repuision quantum-chemical 156 total molecular one-center E-E repuision quantum-chemical 157 tota	137	structural information content (order 0)	topological
199structural information content (order 2)topological140TMSA total molecular surface area (glanutum-chemical PC)quantum-chemical141TMSA total molecular surface area (glanutum-chemical PC)electrostatic142topographic electronic index (all bonts) (Zefiror's PC)electrostatic143topographic electronic index (all bonts) (Zefiror's PC)electrostatic144total dipole of the moleculequantum-chemical145total enthalpy (300 K)quantum-chemical146total enthalpy (300 K)for atomsquantum-chemical147total entropy (300 K)of atomsquantum-chemical148total entropy (300 K)of atomsthermodynamic150total heat capacity (300 K)of atomsquantum-chemical151total indecical one center E-E repulsionquantum-chemical152total indecical one center E-E repulsionquantum-chemical153total molecular one-center E-E repulsionquantum-chemical154total indecical one-center E-E repulsionquantum-chemical155total molecular one-center E-N attractionquantum-chemical156total molecular one-center E-N attractionquantum-chemical157total molecular one-center E-N attractionquantum-chemical158total indicical row-center resonance energyquantum-chemical159transitional entropy (300 K)atomsthermodynamic161transitional entropy (300 K)of atomsthermodynamic <trr>162</trr>	138	structural information content (order 1)	topological
140TMSA total molecular surface area [Quantum-chemical PC]electrostatic141TMSA total molecular surface area [Zelino's PC]electrostatic142topographic electronic index (all bords) [Zelino's PC]electrostatic143topographic electronic index (all bords) [Zelino's PC]electrostatic144total dipole of the moleculequantum-chemical145total enthalpy (300 K)quantum-chemical146total enthalpy (300 K)quantum-chemical147total enthalpy (300 K)quantum-chemical148total entropy (300 K)quantum-chemical149total entropy (300 K)/no. of atomsthermodynamic150total heat capacity (300 K)/no. of atomsquantum-chemical151total heat capacity (300 K)/no. of atomsquantum-chemical152total molecular one-center FE- repulsionquantum-chemical153total molecular one-center FE- repulsionquantum-chemical154total molecular one-center FE- repulsionquantum-chemical155total molecular one-center FE- repulsionquantum-chemical156total molecular one-center FE- repulsionquantum-chemical157total molecular con-center FE- repulsionquantum-chemical158total molecular con-center FE- repulsionquantum-chemical159tanalational entraly (300 K)/no. of atomsthermodynamic151total molecular con-center FE- repulsionquantum-chemical152total molecular con-center FE- repulsionquantum-chemical <t< td=""><td>139</td><td>structural information content (order 2)</td><td>topological</td></t<>	139	structural information content (order 2)	topological
141 TMSA total molecular surface area [Żelfirov's PC] electrostatic 142 topographic electronic index (all bonds) [Żelfirov's PC] electrostatic 143 topographic electronic index (all paris) [Żelfirov's PC] electrostatic 144 total enthalpy (300 K) quantum-chemical 145 total enthalpy (300 K). quantum-chemical 146 total entropy (300 K). quantum-chemical 147 total entropy (300 K). thermodynamic 148 total entropy (300 K). of atoms 150 total hat capacity (300 K). of atoms 151 total hote (aptic (300 K)). of atoms 152 total molecular one-center E-Ferpulsion. quantum-chemical 153 total molecular one-center E-Ferpulsion. quantum-chemical 154 total molecular one-center E-Ferpulsion. quantum-chemical 155 total molecular one-center E-Ferpulsion. quantum-chemical 156 total molecular one-center E-Ferpulsion. ot atoms quantum-chemical 157 total molecular one-center E-N attraction. quantum-chemical thermodynamic 158 total molecular one-center E-Repuls	140	TMSA total molecular surface area [guantum-chemical PC]	quantum-chemical
142topographic electronic index (all bonds) [Zefirov's PC]electrostatic143topographic electronic index (all pairs) [Zefirov's PC]electrostatic144total dipole of the moleculequantum-chemical145total enthalpy (300 K)n.quantum-chemical146total enthalpy (300 K)n.of atomsquantum-chemical147total enthalpy (300 K)n.of atomsquantum-chemical148total entropy (300 K)n.of atomsthermodynamic149total heat capacity (300 K)n.of atomsthermodynamic150total heat capacity (300 K)n.of atomsthermodynamic151total heat capacity (300 K)n.of atomsquantum-chemical152total molecular one-center E-E repulsionquantum-chemical153total molecular one-center E-E repulsionquantum-chemical154total molecular one-center E-N attractionquantum-chemical155total molecular two-center resonance energyquantum-chemical158total molecular two-center resonance energyquantum-chemical159total policit-tarage comp of the molecular dipolequantum-chemical151total policit-tarage comp of the molecular dipolequantum-chemical152total policit-tarage comp of the molecular dipolequantum-chemical153total molecular two-center resonance energyquantum-chemical154total molecular two-center resonance energyquantum-chemical155total molecular two-center resonance energyquantum-chemical <td>141</td> <td>TMSA total molecular surface area [Zefirov's PC]</td> <td>electrostatic</td>	141	TMSA total molecular surface area [Zefirov's PC]	electrostatic
143topographic electronic index (all pairs) [Żefirov's PC]electrostatic144total dipole of the moleculequantum-chemical145total enthalpy (300 K).quantum-chemical146total enthalpy (300 K).quantum-chemical147total entropy (300 K).quantum-chemical148total entropy (300 K).of atoms149total entropy (300 K).of atoms150total heat capacity (300 K)of atoms151total heat capacity (300 K).of atoms152total heat capacity (300 K).of atoms153total molecular one-center E-F repulsionquantum-chemical154total molecular one-center E-F repulsion.quantum-chemical155total molecular one-center E-F attraction.quantum-chemical156total molecular one-center E-N attraction.quantum-chemical157total molecular two-center resonance energy.quantum-chemical158total molecular two-center resonance energy.quantum-chemical159translational entopy (300 K).of atomsthermodynamic161translational entopy (300 K).of atomsthermodynamic162translational entopy (300 K).of atomsthermodynamic163vibrational entopy (300 K).of atomsthermodynamic164translational entopy (300 K).of atomsthermodynamic165vibrational entopy (300 K).of atomsthermodynamic166vibrational entopy (300 K).of atomsthermodynamic	142	topographic electronic index (all bonds) [Zefirov's PC]	electrostatic
144total dipole of the moleculequantum-chemical145total enthalpy (300 K)/no. of atomsquantum-chemical146total enthalpy (300 K)/no. of atomsquantum-chemical147total entropy (300 K)quantum-chemical148total entropy (300 K)/no. of atomsthermodynamic149total heat capacity (300 K)/no. of atomsthermodynamic150total heat capacity (300 K)/no. of atomsthermodynamic151total hybridization comp of the molecular dipolequantum-chemical152total molecular one-center E-E repulsion/no. of atomsquantum-chemical153total molecular one-center E-E repulsion/no. of atomsquantum-chemical154total molecular one-center E-E repulsion/no. of atomsquantum-chemical155total molecular two-center resonance energyquantum-chemical156total molecular two-center resonance energyquantum-chemical157total molecular two-center resonance energy/no. of atomsquantum-chemical158total anolecular two-center resonance energy/no. of atomsthermodynamic159translational enthaly (300 K)/no. of atomsthermodynamic161translational enthaly (300 K)/no. of atomsthermodynamic152total molecular two-center resonance energythermodynamic153total molecular two-center resonance energythermodynamic154total molecular two-center resonance energythermodynamic155total molecular two-center resonance energythermodynamic156 <t< td=""><td>143</td><td>topographic electronic index (all pairs) [Zefirov's PC]</td><td>electrostatic</td></t<>	143	topographic electronic index (all pairs) [Zefirov's PC]	electrostatic
145total enthalpy (300 K)no. of atomsquantum-chemical146total enthalpy (300 K)no. of atomsquantum-chemical147total entropy (300 K)no. of atomsthermodynamic148total entropy (300 K)no. of atomsthermodynamic149total heat capacity (300 K)no. of atomsthermodynamic150total heat capacity (300 K)no. of atomsquantum-chemical151total hybridization comp of the molecular dipolequantum-chemical152total molecular one-center E-E repulsionquantum-chemical153total molecular one-center E-E repulsionquantum-chemical154total molecular one-center E-A attractionquantum-chemical155total molecular one-center E-A attractionquantum-chemical156total molecular wo-center resonance energyquantum-chemical157total molecular wo-center resonance energyquantum-chemical158total point-charge comp of the molecular dipolequantum-chemical159translational entropy (300 K)no. of atomsthermodynamic161translational entropy (300 K)no. of atomsthermodynamic162translational entropy (300 K)no. of atomsthermodynamic163vibrational entropy (300 K)no. of atomsthermodynamic164vibrational entropy (300 K)no. of atomsthermodynamic165vibrational entropy (300 K)no. of atomsthermodynamic166vibrational entropy (300 K)no. of atomsthermodynamic167vibrational entropy (300 K)no. of atomsthermodynamic	144	total dipole of the molecule	quantum-chemical
146total entropy (300 K)/no. of atomsquantum-chemical147total entropy (300 K)/no. of atomsthermodynamic148total entropy (300 K)/no. of atomsthermodynamic149total heat capacity (300 K)/no. of atomsthermodynamic150total heat capacity (300 K)/no. of atomsquantum-chemical151total hotecuarone-center E-E repulsion/no. of atomsquantum-chemical152total molecular one-center E-E repulsion/no. of atomsquantum-chemical153total molecular one-center E-A attraction/no. of atomsquantum-chemical154total molecular one-center E-A attraction/no. of atomsquantum-chemical155total molecular noe-center E-A attraction/no. of atomsquantum-chemical156total molecular wo-center resonance energy/no. of atomsquantum-chemical157total molecular wo-center resonance energy/no. of atomsquantum-chemical158total polin-charge comp of the molecular dipolequantum-chemical159translational entropy (300 K)/no. of atomsthermodynamic161translational entropy (300 K)/no. of atomsthermodynamic162translational entropy (300 K)/no. of atomsthermodynamic163vibrational entropy (300 K)/no. of atomsthermodynamic164vibrational entropy (300 K)/no. of atomsthermodynamic165vibrational entropy (300 K)/no. of atomsthermodynamic166vibrational entropy (300 K)/no. of atomsthermodynamic167vibrational entropy (300 K)/no. of atomsthermody	145	total enthalpy (300 K)	quantum-chemical
147total entropy (300 K)quantum-chemical148total entropy (300 K)thermodynamic149total entropy (300 K)thermodynamic150total heat capacity (300 K)thermodynamic151total hybridization comp of the molecular dipolequantum-chemical152total molecular one-center E-E repulsion/no. of atomsquantum-chemical153total molecular one-center E-N attractionquantum-chemical154total molecular one-center E-N attractionquantum-chemical155total molecular one-center E-N attractionquantum-chemical156total molecular two-center resonance energyquantum-chemical157total molecular two-center resonance energyquantum-chemical158total point-charge comp of the molecular dipolequantum-chemical159translational entrapy (300 K)/no. of atomsthermodynamic161translational entrapy (300 K)/no. of atomsthermodynamic162translational entrapy (300 K)/no. of atomsthermodynamic163vibrational entrapy (300 K)/no. of atomsthermodynamic164vibrational entropy (300 K)/no. of atomsthermodynamic165vibrational entropy (300 K)/no. of atomsthermodynamic166vibrational entropy (300 K)/no. of atomsthermodynamic167vibrational entropy (300 K)/no. of atomsthermodynamic168vibrational entropy (300 K)/no. of atomsthermodynamic170WINSA-1 weighted PNSA (PNSA:TIMSA/1000) [quantum-chemical PC]quantum-chemical	146	total enthalpy (300 K)/no. of atoms	quantum-chemical
148 total heat capacity (300 K)/n.o. f atoms thermodynamic 150 total heat capacity (300 K)/n.o. f atoms thermodynamic 151 total hybridization comp of the molecular dipole quantum-chemical 152 total molecular one-center E-E repulsion/n.o. of atoms quantum-chemical 153 total molecular one-center E-N attraction quantum-chemical 154 total molecular one-center E-N attraction quantum-chemical 155 total molecular one-center E-N attraction quantum-chemical 156 total molecular one-center E-N attraction quantum-chemical 157 total molecular two-center resonance energy quantum-chemical 158 total molecular two-center resonance energy quantum-chemical 159 translational entropy (300 K)/no. of atoms thermodynamic 161 translational entropy (300 K)/no. of atoms thermodynamic 162 translational entropy (300 K)/no. of atoms thermodynamic 163 vibrational entropy (300 K)/no. of atoms thermodynamic 164 vibrational entropy (300 K)/no. of atoms thermodynamic 165 vibrational entropy (300 K)/no. of atoms thermodynamic	147	total entropy (300 K)	quantum-chemical
149total heat capacity (300 K)/no. of atomsthermodynamic150total heat capacity (300 K)/no. of atomsquantum-chemical151total hybridization comp of the molecular dipolequantum-chemical152total molecular one-center E-E repulsionquantum-chemical153total molecular one-center E-E repulsionquantum-chemical154total molecular noe-center E-N attraction/no. of atomsquantum-chemical155total molecular two-center resonance energyquantum-chemical156total molecular two-center resonance energyquantum-chemical157total molecular two-center resonance energyquantum-chemical158total point-charge comp of the molecular dipolequantum-chemical159translational enthaly (300 K)/no. of atomsthermodynamic160translational enthaly (300 K)/no. of atomsthermodynamic161translational enthaly (300 K)/no. of atomsthermodynamic162translational enthaly (300 K)/no. of atomsthermodynamic163vibrational enthaly (300 K)/no. of atomsthermodynamic164vibrational enthaly (300 K)/no. of atomsthermodynamic165vibrational entropy (300 K)/no. of atomsthermodynamic166vibrational entropy (300 K)/no. of atomsthermodynamic167vibrational heat capacity (300 K)/no. of atomsthermodynamic168vibrational heat capacity (300 K)/no. of atomsthermodynamic170WNSA-1 weighted PNSA (PNSA1*TMSA1000) [Zeifrov's PC]electrostatic1	148	total entropy (300 K)/no. of atoms	thermodynamic
150 total heat capacity (300 K)no. of atoms thermodynamic 151 total molecular one-center E-E repulsion quantum-chemical 152 total molecular one-center E-E repulsion/no. of atoms quantum-chemical 153 total molecular one-center E-N attraction/no. of atoms quantum-chemical 155 total molecular voe-center E-N attraction/no. of atoms quantum-chemical 156 total molecular woe-center resonance energy quantum-chemical 157 total anoicular two-center resonance energy/no. of atoms quantum-chemical 158 total point-charge comp of the molecular dipole quantum-chemical 159 translational entropy (300 K)/no. of atoms thermodynamic 161 translational entropy (300 K)/no. of atoms thermodynamic 162 translational entropy (300 K)/no. of atoms thermodynamic 163 vibrational entropy (300 K)/no. of atoms thermodynamic 164 vibrational entropy (300 K) thermodynamic 165 vibrational entropy (300 K)/no. of atoms thermodynamic 166 vibrational entropy (300 K)/no. of atoms thermodynamic 167 vibrational entropy (300 K)/no. of atoms thermodynamic 168 vibrational entropy (300 K)/no. of atoms thermodynamic 169 vibrational	149	total heat capacity (300 K)	thermodynamic
151 total hybridization comp of the molecular dipole qualitum-chemical 152 total molecular one-center F-E repulsion/no. of atoms quantum-chemical 153 total molecular one-center F-N attraction quantum-chemical 154 total molecular one-center F-N attraction/no. of atoms quantum-chemical 155 total molecular two-center resonance energy quantum-chemical 156 total molecular two-center resonance energy/no. of atoms quantum-chemical 157 total molecular two-center resonance energy/no. of atoms quantum-chemical 158 total point-charge comp of the molecular dipole quantum-chemical 159 translational entropy (300 K/no. of atoms thermodynamic 161 translational entropy (300 K/no. of atoms thermodynamic 162 translational entropy (300 K/no. of atoms thermodynamic 164 vibrational entropy (300 K) thermodynamic 165 vibrational entropy (300 K) thermodynamic 166 vibrational entropy (300 K) thermodynamic 167 vibrational entropy (300 K) thermodynamic 168 vibrational entropy (300 K) thermodynamic 169 Wiener index tpological 170 WNSA-1 weighted PNSA (PNSA*TMSA/1000) [quantum-chemical PC] quantum-	150	total heat capacity (300 K)/no. of atoms	thermodynamic
132 total molecular one-center E-F. repulsion/no. of atoms quantum-chemical 153 total molecular one-center E-N attraction/no. of atoms quantum-chemical 154 total molecular one-center E-N attraction/no. of atoms quantum-chemical 155 total molecular two-center resonance energy quantum-chemical 156 total molecular two-center resonance energy quantum-chemical 157 total molecular two-center resonance energy quantum-chemical 158 total point-charge comp of the molecular dipole quantum-chemical 159 translational enthopy (300 K/no. of atoms thermodynamic 161 translational entropy (300 K/no. of atoms thermodynamic 162 translational entropy (300 K/no. of atoms thermodynamic 163 vibrational entropy (300 K/no. of atoms thermodynamic 164 vibrational entropy (300 K/no. of atoms thermodynamic 165 vibrational entropy (300 K/no. of atoms thermodynamic 166 vibrational entropy (300 K/no. of atoms thermodynamic 167 vibrational heat capacity (300 K/no. of atoms thermodynamic 168 vibrational heat capacity (300 K/no. of atoms thermodynamic 170 WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC] quantum-chemical <	151	total hybridization comp of the molecular dipole	quantum-chemical
135Ibida Indecdation Directer Ide 2: Explosition to additiseQualitum-chemical1364total molecular one-center E-N attractionquantum-chemical1355total molecular two-center E-N attraction / of atomsquantum-chemical1366total molecular two-center resonance energyquantum-chemical1377total molecular two-center resonance energyquantum-chemical138total point-charge comp of the molecular dipolequantum-chemical139translational entropy (300 K)/no. of atomsthermodynamic160translational entropy (300 K)/no. of atomsthermodynamic161translational entropy (300 K)/no. of atomsthermodynamic162translational entropy (300 K)/no. of atomsthermodynamic163vibrational entropy (300 K)/no. of atomsthermodynamic164vibrational entropy (300 K)/no. of atomsthermodynamic165vibrational entropy (300 K)/no. of atomsthermodynamic166vibrational entropy (300 K)/no. of atomsthermodynamic167vibrational entropy (300 K)/no. of atomsthermodynamic168vibrational entropy (300 K)/no. of atomsthermodynamic170WISA-1 weighted PNSA (PNSA1*TMSA/1000) [Quantum-chemical PC]quantum-chemical171WISA-1 weighted PNSA (PNSA1*TMSA/1000) [Quantum-chemical PC]quantum-chemical173WISA-2 weighted PNSA (PNSA2*TMSA/1000) [Quantum-chemical PC]quantum-chemical174WISA-3 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic175WISA-3 weighted PNSA (152	total molecular one-center E-E repulsion	quantum-chemical
104Total indicular one-center E-N attractionquantum-chemical155total molecular two-center resonance energyquantum-chemical166total molecular two-center resonance energy/no. of atomsquantum-chemical157total molecular two-center resonance energy/no. of atomsquantum-chemical158total point-charge coenter E-N attraction/no. of atomsquantum-chemical159translational entropy (300 K/)no. of atomsthermodynamic160translational entropy (300 K/)no. of atomsthermodynamic161translational entropy (300 K/)no. of atomsthermodynamic162translational entropy (300 K/)no. of atomsthermodynamic163vibrational enthalpy (300 K/)no. of atomsthermodynamic164vibrational enthalpy (300 K/)no. of atomsthermodynamic165vibrational entropy (300 K/)no. of atomsthermodynamic166vibrational entropy (300 K/)no. of atomsthermodynamic167vibrational entropy (300 K/)no. of atomsthermodynamic168vibrational heat capacity (300 K/)no. of atomsthermodynamic170WINSA-1 weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical171WINSA-1 weighted PNSA (PNSA1*TMSA/1000) [Zefirov's PC]electrostatic172WINSA-2 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic173WINSA-2 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic174WINSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic175WINSA-3 weighted	153	total molecular one-center E-E repulsion/no. or atoms	quantum chemical
135total molecular two-center resonance energyquantum-chemical136total molecular two-center resonance energy/no. of atomsquantum-chemical137total molecular two-center resonance energy/no. of atomsquantum-chemical138total point-charge comp of the molecular dipolequantum-chemical139translational entropy (300 K)/no. of atomsthermodynamic160translational entropy (300 K)/no. of atomsthermodynamic161translational entropy (300 K)/no. of atomsthermodynamic162translational entropy (300 K)/no. of atomsthermodynamic163vibrational entropy (300 K)thermodynamic164vibrational entropy (300 K)thermodynamic165vibrational entropy (300 K)thermodynamic166vibrational entropy (300 K)/no. of atomsthermodynamic167vibrational entropy (300 K)/no. of atomsthermodynamic168vibrational heat capacity (300 K)/no. of atomsthermodynamic169Wiener indextopological170WISA-1 weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical171WISA-1 weighted PNSA (PNSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical173WISA-2 weighted PNSA (PNSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical174WISA-3 weighted PNSA (PNSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical175WISA-3 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic176WPSA-1 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostati	154	total molecular one-center E-N attraction/no. of atoms	quantum-chemical
100Idea inforcement resonance energy/no. of atomsquantum-chemical157total molecular two-center resonance energy/no. of atomsquantum-chemical158total point-charge comp of the molecular dipolequantum-chemical159translational entropy (300 K)/no. of atomsthermodynamic160translational entropy (300 K)/no. of atomsthermodynamic161translational entropy (300 K)/no. of atomsthermodynamic162translational entropy (300 K)/no. of atomsthermodynamic163vibrational enthalpy (300 K)/no. of atomsthermodynamic164vibrational enthalpy (300 K)/no. of atomsthermodynamic165vibrational entropy (300 K)/no. of atomsthermodynamic166vibrational entropy (300 K)/no. of atomsthermodynamic167vibrational entropy (300 K)/no. of atomsthermodynamic168vibrational heat capacity (300 K)/no. of atomsthermodynamic169Wiener indextopological170WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical171WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic172WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical173WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical174WNSA-3 weighted PNSA (PNSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical175WNSA-3 weighted PPSA (PPSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical176WPSA-1 weighted PPSA (PPSA	155	total molecular two-center reconance energy	quantum-chemical
153Iotal point-charge comp of the molecular dipolequantum-chemical153translational entropy (300 K)/no. of atomsthermodynamic160translational entropy (300 K)/no. of atomsthermodynamic161translational entropy (300 K)/no. of atomsthermodynamic162translational entropy (300 K)/no. of atomsthermodynamic163vibrational entropy (300 K)thermodynamic164vibrational entropy (300 K)thermodynamic165vibrational entropy (300 K)thermodynamic166vibrational entropy (300 K)thermodynamic167vibrational entropy (300 K)thermodynamic168vibrational entropy (300 K)/no. of atomsthermodynamic169Wieneri ndextopological170WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical171WNSA-1 weighted PNSA (PNSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical172WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic173WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic174WNSA-3 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic175WNSA-3 weighted PNSA (PSA3*TMSA/1000) [Zefirov's PC]electrostatic176WPSA-1 weighted PPSA (PSA2*TMSA/1000) [Zefirov's PC]electrostatic177WPSA-1 weighted PPSA (PSA2*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PSA2*TMSA/1000) [Zefirov's PC]electrostatic179WPSA-2 weighted PPSA (PSA2*TMS	157	total molecular two-center resonance energy	quantum-chemical
159translational enthalpy (300 K)/no. of atomsthermodynamic160translational entropy (300 K)thermodynamic161translational entropy (300 K)/no. of atomsthermodynamic162translational heat capacity (300 K)/no. of atomsthermodynamic163uibrational enthalpy (300 K)thermodynamic164vibrational enthalpy (300 K)/no. of atomsthermodynamic165vibrational entropy (300 K)thermodynamic166vibrational entropy (300 K)/no. of atomsthermodynamic167vibrational entropy (300 K)/no. of atomsthermodynamic168vibrational heat capacity (300 K)thermodynamic169Wiener indextopological170WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [Quantum-chemical PC]quantum-chemical171WNSA-2 weighted PNSA (PNSA1*TMSA/1000) [Quantum-chemical PC]quantum-chemical173WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic174WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic175WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]quantum-chemical176WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic177WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic179<	158	total noint-charge comp of the molecular dipole	quantum-chemical
160translational entropy (300 K)thermodynamic161translational entropy (300 K)/no. of atomsthermodynamic162translational heat capacity (300 K)/no. of atomsthermodynamic163vibrational enthalpy (300 K)thermodynamic164vibrational enthalpy (300 K)thermodynamic165vibrational entropy (300 K)thermodynamic166vibrational entropy (300 K)thermodynamic167vibrational entropy (300 K)thermodynamic168vibrational heat capacity (300 K)thermodynamic169Wiener indextopological170WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical171WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic173WNSA-2 weighted PNSA (PNSA3*TMSA/1000) [quantum-chemical PC]quantum-chemical175WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic176WPSA-1 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic176WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Quantum-chemical PC]quantum-chemical177WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Quantum-chemical PC]quantum-chemical179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic179WPSA	159	translational enthalov (300 K)/no. of atoms	thermodynamic
161translational entropy (300 K)/no. of atomsthermodynamic162translational heat capacity (300 K)/no. of atomsthermodynamic163vibrational enthalpy (300 K)thermodynamic164vibrational entropy (300 K)/no. of atomsthermodynamic165vibrational entropy (300 K)thermodynamic166vibrational entropy (300 K)thermodynamic167vibrational entropy (300 K)/no. of atomsthermodynamic168vibrational heat capacity (300 K)thermodynamic169Wiener indextopological170WISA-1 weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical171WISA-2 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic172WISA-2 weighted PNSA (PNSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical173WISA-2 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic174WISA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic175WISA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic176WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic177WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic179WPSA-2 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic179WPSA-2 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	160	translational entropy (300 K)	thermodynamic
162translational heat capacity (300 K)/no. of atomsthermodynamic163vibrational enthalpy (300 K)thermodynamic164vibrational enthalpy (300 K)/no. of atomsthermodynamic165vibrational entropy (300 K)thermodynamic166vibrational entropy (300 K)/no. of atomsthermodynamic167vibrational heat capacity (300 K)/no. of atomsthermodynamic168vibrational heat capacity (300 K)/no. of atomsthermodynamic169Wiener indextopological170WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [Quantum-chemical PC]quantum-chemical171WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [Quantum-chemical PC]electrostatic173WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic174WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic175WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic176WPSA-1 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic177WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000)	161	translational entropy (300 K)/no. of atoms	thermodynamic
163vibrational enthalpy (300 K)thermodynamic164vibrational enthalpy (300 K)/no. of atomsthermodynamic165vibrational entropy (300 K)thermodynamic166vibrational entropy (300 K)/no. of atomsthermodynamic167vibrational heat capacity (300 K)thermodynamic168vibrational heat capacity (300 K)/no. of atomsthermodynamic169Wiener indextopological170WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical171WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [quantum-chemical PC]electrostatic172WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic174WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Quantum-chemical PC]quantum-chemical175WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Quantum-chemical PC]quantum-chemical176WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Quantum-chemical PC]electrostatic177WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Quantum-chemical PC]quantum-chemical178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Quantum-chemical PC]quantum-chemical179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Quantum-chemical PC]quantum-chemical178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Quantum-chemical PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Quantum-chemical PC]electrostatic179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Quantum-chemical PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Quantum-chemical PC]elect	162	translational heat capacity (300 K)/no. of atoms	thermodynamic
164vibrational enthalpy (300 K)/no. of atomsthermodynamic165vibrational entropy (300 K)thermodynamic166vibrational entropy (300 K)/no. of atomsthermodynamic167vibrational heat capacity (300 K)thermodynamic168vibrational heat capacity (300 K)/no. of atomsthermodynamic169Wiener indextopological170WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical171WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical172WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical173WNSA-2 weighted PNSA (PNSA3*TMSA/1000) [quantum-chemical PC]quantum-chemical174WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [quantum-chemical PC]quantum-chemical175WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic176WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]quantum-chemical177WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic181WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	163	vibrational enthalpy (300 K)	thermodynamic
165vibrational entropy (300 K)thermodynamic166vibrational entropy (300 K)/no. of atomsthermodynamic167vibrational heat capacity (300 K)thermodynamic168vibrational heat capacity (300 K)/no. of atomsthermodynamic169Wiener indextopological170WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical171WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [Zefirov's PC]electrostatic172WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic173WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic174WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic175WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic176WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic177WPSA-1 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic181WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	164	vibrational enthalpy (300 K)/no. of atoms	thermodynamic
166vibrational entropy (300 K)/no. of atomsthermodynamic167vibrational heat capacity (300 K)thermodynamic168vibrational heat capacity (300 K)/no. of atomsthermodynamic169Wiener indextopological170WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical171WNSA-2 weighted PNSA (PNSA1*TMSA/1000) [Zefirov's PC]electrostatic172WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic173WNSA-2 weighted PNSA (PNSA3*TMSA/1000) [quantum-chemical PC]quantum-chemical174WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [quantum-chemical PC]electrostatic175WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic176WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic177WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic179WPSA-2 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic181WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	165	vibrational entropy (300 K)	thermodynamic
167vibrational heat capacity (300 K)thermodynamic168vibrational heat capacity (300 K)/no. of atomsthermodynamic169Wiener indextopological170WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical171WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [Zefirov's PC]electrostatic172WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic173WNSA-2 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic174WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Quantum-chemical PC]quantum-chemical175WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic176WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic177WPSA-1 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical179WPSA-2 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic180WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	166	vibrational entropy (300 K)/no. of atoms	thermodynamic
168vibrational heat capacity (300 K)/no. of atomsthermodynamic169Wiener indextopological170WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical171WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [Zefirov's PC]electrostatic172WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical173WNSA-2 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic174WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic175WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic176WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic177WPSA-1 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic180WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic181WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	167	vibrational heat capacity (300 K)	thermodynamic
169Wiener Indextopological170WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical171WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [Zefirov's PC]electrostatic172WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical173WNSA-2 weighted PNSA (PNSA3*TMSA/1000) [Quantum-chemical PC]electrostatic174WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [quantum-chemical PC]electrostatic175WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic176WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic177WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic179WPSA-2 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic180WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic181WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	168	vibrational heat capacity (300 K)/no. of atoms	thermodynamic
170WNSA-1 Weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical171WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [Zefirov's PC]electrostatic172WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical173WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic174WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [quantum-chemical PC]quantum-chemical175WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic176WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Quantum-chemical PC]quantum-chemical177WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Quantum-chemical PC]quantum-chemical179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic180WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]quantum-chemical181WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	169	Wiener index	topological
171WNSA-1 Weighted PNSA (PNSA1*TMSA/1000) [2/Enrov's PC]electrostatic172WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical173WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic174WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [quantum-chemical PC]quantum-chemical175WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic176WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Quantum-chemical PC]quantum-chemical177WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic180WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]quantum-chemical181WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	170	WNSA-1 weighted PNSA (PNSA1*TMSA/1000) [quantum-chemical PC]	quantum-cnemical
172WINSA-2 weighted FNSA (FNSA2 TMSA/1000) [quantum-chemical PC]quantum-chemical173WNSA-2 weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]electrostatic174WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [quantum-chemical PC]quantum-chemical175WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic176WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Quantum-chemical PC]quantum-chemical177WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Quantum-chemical PC]quantum-chemical179WPSA-2 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic180WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Quantum-chemical PC]quantum-chemical181WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	179	WINDA-I WEIGHIEU FINDA (FINDAI I MIDA/1000) [ZEIIFOV S MU] WINDA-2 Waighted PNISA (PNISA/1000) [guantum abamical PC]	
173WINSA-2 weighted FNSA (FNSA2 TMSA/1000) [25000 S FC]Electrostatic174WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [quantum-chemical PC]quantum-chemical175WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic176WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical177WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic180WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [quantum-chemical PC]quantum-chemical181WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	172	WINGA-2 Weighted FINGA (FINGA/ TWOA/ TWO/) [Yudhiluin-Chennical FO] WINGA-2 Weighted FINGA (FINGA/1000) [Zafiravia FO]	quantum-chemical
175WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]electrostatic176WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical177WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic180WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Quantum-chemical PC]quantum-chemical181WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	174	WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [cullantum-chemical PC]	quantum-chamical
176WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [quantum-chemical PC]quantum-chemical177WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic180WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [quantum-chemical PC]quantum-chemical181WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	175	WNSA-3 weighted PNSA (PNSA3*TMSA/1000) [Zefirov's PC]	electrostatic
177WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]electrostatic178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic180WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [quantum-chemical PC]quantum-chemical181WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	176	WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [guantum-chemical PC]	quantum-chemical
178WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [quantum-chemical PC]quantum-chemical179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic180WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [quantum-chemical PC]quantum-chemical181WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	177	WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [Zefirov's PC]	electrostatic
179WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]electrostatic180WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [quantum-chemical PC]quantum-chemical181WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	178	WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [guantum-chemical PC]	guantum-chemical
180WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [quantum-chemical PC]quantum-chemical181WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]electrostatic	179	WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [Zefirov's PC]	electrostatic
181 WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC] electrostatic	180	WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [quantum-chemical PC]	quantum-chemical
	181	WPSA-3 weighted PPSA (PPSA3*TMSA/1000) [Zefirov's PC]	electrostatic

Α	rtic	le
1	i u c	20

Table 7. Continued

no.	descriptor	type
182	XY shadow	geometrical
183	XY shadow/XY rectangle	geometrical
184	YZ shadow	geometrical
185	YZ shadow/YZ rectangle	geometrical
186	zero-point vibrational energy	thermodynamic
187	zero-point vibrational energy/no. of atoms	thermodynamic
188	ZX shadow	geometrical
189	ZX shadow/ZX rectangle	geometrical

Table 8. 17 Descriptors in Normal Population

no.	descriptor	no.	descriptor
1	bonding information content (order 0)	10	total entropy (300 K)
2	DPSA-1 difference in CPSAs (PPSA1-PNSA1) [quantum-chemical PC]	11	total molecular two-center resonance energy/no. of atoms
3	DPSA-1 difference in CPSAs (PPSA1-PNSA1) [Zefirov's PC]	12	vibrational enthalpy (300 K)/no. of atoms
4	ESP-DPSA-1 difference in CPSAs (PPSA1-PNSA1) [quantum-chemical PC]	13	vibrational entropy (300 K)
5	ESP-PPSA-1 partial positive surface area [quantum-chemical PC]	14	XY shadow/XY rectangle
6	internal entropy (300 K)	15	YZ shadow
7	molecular surface area	16	YZ shadow/YZ rectangle
8	PPSA-1 partial positive surface area [Zefirov's PC]	17	ZX shadow/ZX rectangle
9	structural information content (order 0)		

Table 9. 34 Descriptors Removed from the Candidate Set by K-W Test

no.	descriptor	significance
1	$(1/6) \times$ GAMMA polarizability (DIP)	0.427
2	1× GAMMA polarizability (DIP)	0.427
3	ALFA polarizability (DIP)	0.415
4	average complementary information content (order 0)	0.209
5	complementary information content (order 0)	0.294
6	ESP-FNSA-1 fractional PNSA (PNSA-1/TMSA) [quantum-chemical PC]	0.247
7	ESP-FNSA-3 fractional PNSA (PNSA-3/TMSA) [guantum-chemical PC]	0.442
8	ESP-FPSA-1 fractional PPSA (PPSA-1/TMSA) [guantum-chemical PC]	0.247
9	ESP-FPSA-2 fractional PPSA (PPSA-2/TMSA) [guantum-chemical PC]	0.098
10	ESP-PPSA-2 total charge weighted PPSA	0.107
11	ESP-RNCG relative negative charge	0.121
12	ESP-RNCS relative negative charged SA (SAMNEG*RNCG) [quantum-chemical PC]	0.439
13	ESP-RPCS relative positive charged SA (SAMPOS*BPCG) [quantum-chemical PC]	0.085
14	ESP-WPSA-1 weighted PPSA (PPSA1*TMSA/1000) [guantum-chemical PC]	0.056
15	ESP-WPSA-2 weighted PPSA (PPSA2*TMSA/1000) [guantum-chemical PC]	0.085
16	FPSA-3 fractional PPSA (PPSA-3/TMSA) [Zefirov's PC]	0.093
17	image of the Onsager-Kirkwood solvation energy	0.773
18	molecular volume	0.083
19	PPSA-3 atomic charge weighted PPSA [quantum-chemical PC]	0.096
20	principal moment of inertia A	0.056
21	RPCS relative positive charged SA (SAMPOS*RPCG) [quantum-chemical PC]	0.276
22	rotational enthalpy (300 K)/no. of atoms	0.065
23	rotational entropy (300 K)/no. of atoms	0.092
24	rotational heat capacity (300 K)/no. of atoms	0.065
25	total dipole of the molecule	0.466
26	total entropy (300 K)/no. of atoms	0.105
27	total hybridization comp of the molecular dipole	0.369
28	total point-charge comp of the molecular dipole	0.067

Table 9. Continued

no.	descriptor	significance
29	translational enthalov (300 K)/no. of atoms	0.065
30	translational entropy (300 K)/no. of atoms	0.074
31	translational heat capacity (300 K)/no. of atoms	0.065
32	WPSA-3 weighted PPSA (PPSA3*TMSA/1000)	0.345
	[quantum-chemical PC]	
33	XY shadow	0.136
34	zero-point vibrational energy	0.148

quantum-chemical descriptor, 7 (ESP-RPCG relative positive charge (QMPOS/QTPLUS) [quantum-chemical PC]), was not significant for herbicides because it was not able to make a difference between fungicide and herbicide. It was removed from candidate sets. The screening rules for herbicides involves seven descriptors: average bonding information content (order 1), internal enthalpy (300 K)/number of atoms, Kier and Hall index (order 2), PNSA-3 atomic charge weighted PNSA [Zefirov's PC], PPSA-2 total charge weighted PPSA [quantum-chemical PC], total heat capacity (300 K), and vibrational entropy (300 K)/number of atoms, and their data ranges are listed in **Table 23**. They were tested by three test sets, and the best result is listed in **Table 24**.

Information listed in **Table 22** shows that the accuracy of the set of screening rules for leads of herbicides was 89%. Those for leads of fungicides and insecticides were 74 and 63%, respectively. It was more significant for herbicide leads than the others because it only made 11% error for this type of lead compounds, but 26 and 37% errors for the other two types of leads, respectively.

Three test results listed in **Tables 18, 21**, and **24**, respectively, show that the accuracies of the three sets of screening rules were > 80% for their objects, respectively, but unsatisfactory performance was seen for screening out the others. The possible reasons could be proposed as follows. (1) All compounds used in this work had only one of the three confirmed and published activities. However, it is possible for them to have more than one kind of activity. (2) The analysis methods used in this work would not be perfect. (3) The descriptors calculated by

Table 10.	35 Descri	ptors in the	Candidate	Set of th	e Screening	Rules

no.	descriptor	type
1	average bonding information content (order 1)	topological
2	average information content (order 1)	topological
3	average structural information content (order 1)	topological
4	bonding information content (order 0)	topological
5	ESP-DPSA-3 difference in CPSAs (PPSA3-PNSA3) [quantum-chemical PC]	quantum-chemical
6	ESP-PNSA-3 atomic charge weighted PNSA	quantum-chemical
7	ESP-RPCG relative positive charge	quantum-chemical
8	FNSA-2 fractional PNSA (PNSA-2/TMSA)	quantum-chemical
9	FNSA-2 fractional PNSA (PNSA-2/TMSA)	electrostatic
10	FPSA-2 fractional PPSA (PPSA-2/TMSA)	quantum-chemical
44	[qualitum-chemical FO]	thormodynamia
10	final heat of formation/no. of atoms	thermodynamic
12	aravitation index (all pairs)	constitutional
14	information content (order 0)	topological
15	information content (order 0)	topological
16	internal onthalow (200 K)/no. of atoms	thormodynamia
17	internal entropy (300 K)/10. Of atoms	thermodynamic
10	internal entropy (300 K)/pa, of stoms	thormodynamic
10	internal best (300 K)	thermodynamic
20	Kier and Hall index (order 2)	topological
20	Kier and Hall index (order 2)	topological
20	PNSA-3 atomic charge weighted PNSA	electrostatic
22	[Zefirov's PC]	electrostatic
23	PPSA-2 total charge weighted PPSA [quantum-chemical PC]	quantum-chemical
24	PPSA-3 atomic charge weighted PPSA [Zefirov's PC]	electrostatic
25	RPCG relative positive charge (QMPOS/QTPLUS) [Zefirov's PC]	electrostatic
26	Randic index (order 0)	topological
27	structural information content (order 0)	topological
28	total heat capacity (300 K)	thermodynamic
29	total molecular one-center	guantum-chemical
	E-N attraction/no. of atoms	
30	vibrational enthalpy (300 K)	thermodynamic
31	vibrational enthalpy (300 K)/no. of atoms	thermodynamic
32	vibrational entropy (300 K)/no. of atoms	thermodynamic
33	WNSA-3 weighted PNSA (PNSA3*TMSA/1000)	quantum-chemical
	[quantum-chemical PC]	
34	WPSA-2 weighted PPSA (PPSA2*TMSA/1000)	quantum-chemical
35	ZX shadow	geometrical

Codessa would not be sufficient for finding perfect screening rules. Other software will be applied in our future works.

In principle, satisfactory screening rules should be sensitive for a specific type of compounds and dormant for others. Herein, we proposed three sets of screening rules, which include seven descriptors listed in **Tables 18**, **21**, and **24**, for leads of fungicides, insecticides, and herbicides, respectively. Their accuracies were 82, 83, and 89%, respectively. In principle, the three screening rules only could be used to satisfactorily estimate fungicide leads, insecticide leads, and herbicide leads, respectively. They were necessary conditions for a compound to become a fungicide lead, insecticide lead, or herbicide lead and a complement of screening rules proposed previously by us and Tice.

In any case, these rules can be used to aid researchers in virtual screening and provide references in pesticide design.

Table 11. Data Range of Candidate Screening Rules for Leads of Fungicides, Insecticides, and Herbicides

	data range				
no. ^a	fungicide	insecticide	herbicide		
1	[0.5, 0.785)	[0.455, 0.725)	[0.5, 0.8)		
2	[2.68, 3.82)	[2.74, 3.64)	[2.68, 4.06)		
3	[0.53, 0.782)	[0.47, 0.722)	[0.494, 0.794)		
4	[6.5, 18)	[9, 18.5)	[9.5, 20.5)		
5	[48, 132)	[56, 140)	[60, 168)		
6	[-65, -15)	[-77.5, -17.5)	[-92.5, -15)		
7	[0.062, 0.271)	[0.062, 0.304)	[0.073, 0.282)		
8	[-1.11, -0.2)	[-1.46, -0.2)	[-1.46, -0.13)		
9	[-0.345, -0.06)	[-0.375, -0.06)	[-0.465, -0.09)		
10	[0.6, 2.1)	[0.8, 2.9)	[0.6, 2.8)		
11	[-155, 85)	[-245, 25)	[-215, 40)		
12	[-5, 2.6)	[-7.4, 1)	[-7.4, 0.6)		
13	[2200, 6200)	[2000, 6800)	[2200, 7400)		
14	[39, 102)	[39, 105)	[42, 117)		
15	[48, 192)	[60, 216)	[66, 210)		
16	[248, 368)	[284, 422)	[272, 410)		
17	[49, 141)	[81, 173)	[73, 161)		
18	[2.49, 3.96)	[2.63, 4.17)	[2.56, 3.89)		
19	[36, 96)	[48, 108)	[39, 105)		
20	[3, 7.8)	[2.7, 9.3)	[3, 7.8)		
21	[1.75, 5.25)	[1.25, 6.25)	[1.5, 5.25)		
22	[-21, -2)	[-22, -3)	[-28, -4)		
23	[140, 1330)	[280, 1610)	[140, 1540)		
24	[4.8, 11.1)	[5.5, 12.5)	[5.5, 12.5)		
25	[0.045, 0.198)	[0.09, 0.27)	[0.063, 0.216)		
26	[8.5, 19)	[8.5, 20.5)	[9.5, 21)		
27	[8, 18)	[9.5, 19)	[9.5, 20)		
28	[40, 100)	[52, 112)	[46, 109)		
29	[-190, -90)	[-180, -90)	[-210, -90)		
30	[4500, 15500)	[7000, 17000)	[6000, 17500)		
31	[223, 356)	[258, 391)	[258, 391)		
32	[1.4, 2.65)	[1.75, 3)	[1.7, 2.75)		
33	[-29, -3]	[-43, -3)	[-35, -3)		
34	[0, 650)	[0, 1000)	[0, 900)		
35	[27, 81)	[39, 93)	[39, 90)		

^a Corresponding to that in **Table 10**.

Table 12. 16 Groups of Descriptors Clustered by Their Definition

no.	descriptor no. ^a	definition
1	5, 6, 22, 33	relating to atomic charge
2	11, 12, 19, 28	relating to heat
3	1, 2, 3	relating to information of order 1
4	4, 14, 27	relating to information of order 0
5	16, 30, 31	relating to enthalpy
6	17, 18, 32	relating to entropy
7	7, 25	relating to relative positive charge
8	8, 9	relating to fractional partial negatively charged surface area
9	13, 35	relating to molecular shape
10	20, 21	relating to Kier and Hall index
11	23, 34	relating to weighted PPSA
12	10	fractional PPSA
13	15	information content (order 2)
14	24	atomic charge weighted PPSA
15	26	Randic index (order 0)
16	29	total molecular one-center E-N attraction/no. of atoms

^a Corresponding to that in **Table 10**.

ABBREVIATIONS USED

Log *P*, logarithmic ratio of octanol—water partition coefficient (*P*); NHD, number of hydrogen bond donors; NHA, number of

 Table 13. Most Suitable Test Result of Screening Rules for Leads of Fungicides among 41472 Combinations

screening rule ^a	fungicide ^b	insecticide ^b	herbicide ^t
1, 4, 9, 10, 12, 13, 15, 16, 18, 20, 24, 25, 26, 29, 33, 34	80%	54%	74%

^a Screening rule represented by the number of a descriptor corresponding to that in **Table 10**. ^b If a compound has five descriptors in this screening rule that are not in the data ranges, the compound will not be a lead of fungicide.

 Table 14. Most Suitable Test Result of Screening Rules for Leads of Insecticides among 41472 Combinations

screening rule ^a	fungicide ^b	insecticide ^b	herbicide ^b
2, 4, 5, 7, 8, 10, 11, 15, 17, 20, 23, 24, 26, 29, 30, 35	70%	80%	76%

^a Screening rule represented by the number of a descriptor corresponding to that in **Table 10**. ^b If a compound has five descriptors in this screening rule that are not in the data ranges, the compound will not be a lead of insecticide.

 Table 15. Most Suitable Test Result of Screening Rules for Leads of

 Herbicides among 41472 Combinations

screening rule ^a	fungicide ^b	insecticide ^b	herbicide ^b
1, 7, 9, 10, 13, 14, 15, 16, 20, 22, 23, 24, 26, 28, 29, 32	68%	72%	91%

^a Screening rule represented by the number of a descriptor corresponding to that in **Table 10**. ^b If a compound has five descriptors in this screening rule which are not in the data ranges, the compound will not be a lead of herbicide.

Table 16. Test Results of the Two Electrostatic Descriptors, 24 and 25

descriptor no. ^a	fungicide	insecticide	herbicide
24	76%	82%	72%
25	72%	66%	87%

^a Corresponding to that in **Table 10**.

Table 17. Screening Rules for Leads of Fungicides

descriptor no. ^a	data range	descriptor no. ^a	data range
1	[0.5, 0.785)	26	[8.5, 19)
9	[-0.345, -0.06)	29	[-190, -90)
12	[-5, 2.6)	33	[-29, -3)
16	[248, 368)		

^a Corresponding to that in **Table 10**.

Table 18. Test Result of Screening Rules for Leads of Fungicides

screening rule ^a	fungicide ^b	insecticide ^b	herbicide ^b	
1, 9, 12, 16, 26, 29, 33	82%	56%	70%	

^a Screening rule represented by the number of a descriptor corresponding to that in **Table 10**. ^b If a compound has two descriptors in this screening rule that are not in the data ranges, the compound will not be a lead of fungicide.

Table 19. Test Results of the Two Descriptors, 2 and 7

descriptor no. ^a	fungicide	insecticide	herbicide
2 7	60%	62%	62%
	82%	77%	82%

^a Corresponding to that in **Table 10**.

Table 20. Screening Rules for Leads of Insecticide

no. of descriptor ^a	data range	no. of descriptor ^a	data range
5	[56, 140)	24	[5.5, 12.5)
8	[-1.46, -0.2)	29	[-180, -90)
10	[0.8, 2.9)	35	[39, 93)
11	[-245, 25)		

^a Corresponding to that in **Table 10**.

 Table 21. Test Result of Screening Rules for Leads of Insecticide

screening rule ^a	fungicide ^b	insecticide ^b	herbicide ^b
5, 8, 10, 11, 24, 29, 35	60%	83%	74%

^a Screening rule represented by the number of a descriptor corresponding to that in **Table 10**. ^b If a compound has two descriptors in this screening rule which are not in the data ranges, the compound will not be a lead of insecticide.

Table 22. Test Result of Descriptor 7

descriptor no. ^a	fungicide	insecticide	herbicide
7	80%	63%	80%

^a Corresponding to that in **Table 10**.

 Table 23.
 Screening Rules for Leads of Herbicides

descriptor no. ^a	data range	descriptor no. ^a	data range
1	[0.5, 0.8)	23	[140, 1540)
16	[272, 410)	28	[46, 109)
20	[3, 7.8)	32	[1.7, 2.75)
22	[-28, -4)		- ,

^a Corresponding to that in **Table 10**.

Table 24. Test Result of Screening	Rules	for Leads	of	Herbicides
------------------------------------	-------	-----------	----	------------

screening rule ^a	fungicide ^b	insecticide ^b	herbicide ^t
1, 16, 20, 22, 23, 28, 32	74%	63%	89%

^a Screening rule represented by the number of a descriptor corresponding to that in **Table 10**. ^b If a compound has two descriptors in this screening rule that are not in the data ranges, the compound will not be a lead of insecticide.

hydrogen bond acceptors; MW, molecular weight; PSA, polar surface area; K–S test, Kolmogorov–Smirnov test; ANOVA, analysis of variance; K–W test, Kruskal–Wallis test; PNSA, partial negatively charged surface area; PPSA, partial positively charged surface area.

Supporting Information Available: Pearson correlation coefficients amont 35 descriptors. This material is available free of charge via the Internet at http://pubs.acs.org.

LITERATURE CITED

- (1) Tice, C. M. Selecting the right compounds for screening: does Lipinski's rule of 5 for pharmaceuticals apply to agrochemicals? *Pest Manag. Sci.* 2001, *57*, 3–16.
- (2) Tice, C. M. Selecting the right compounds for screening: use of surface-area parameters. *Pest Manag. Sci.* 2002, 58, 219–233.
- (3) Liu, B.; Yu, F.; Yao, J. H.; Liao, Q.; Fan, B. T. Screening rules of lead compounds of herbicide, fungicide and insecticide. *Chin. J. Pest. Sci.* 2007, 9, 220–228.
- (4) Semichem, Inc. http://www.semichem.com/codessa/default.php.
- (5) CODESSA Reference Manual.
- (6) http://en.wikipedia.org/wiki/K-S_test.
- (7) Fisher, R. A. In *Statistical Methods for Research Workers*; Oliver and Boyd: Edinburgh, Scotland, 1925.
- (8) http://en.wikipedia.org/wiki/Analysis_of_variance.
- (9) http://en.wikipedia.org/wiki/Wallis statistic.
- (10) Kruskal, W. H.; Wallis, W. A. Use of ranks in one-criterion variance analysis. J. Am. Statis. Assoc. 1952, 47, 583–621.

- (11) http://en.wikipedia.org/wiki/Pearson_product-moment_correlation_ coefficient.
- (12) Cann, A. J. In *Maths from Scratch for Biologists*; Wiley: West Sussex, U.K., 2003; pp 135–146.
- (13) Tomlin, C. D. S. In *The e-Pesticide Manual*, 12th ed.; British Crop Protection Council: Surrey, U.K., 2000.
- (14) In Pesticides, An International Guide to 1800 Pest Control Chemicals, 2md ed.; Milne, G. W. A., Ed.; Ashgate Publishing: Surrey, U.K., 2004.
 (15) Patent PCT/CN03/00343.
- (16) Okazawa, A.; Akamatsu, M.; Nishiwaki, H.; Nakagawa, Y.; Miyagawa, H.; Nishimura, K.; Ueno, T. Three-dimensional quantitative structure-activity relationship analysis of acyclic and cyclic chloronicotinyl insecticides. *Pest Manage. Sci.* 2000, *56*, 509–515.
- (17) http://www.epa.gov/.
- (18) http://www.cas.org/SCIFINDER/SCHOLAR.
- (19) Wiener, H. Structural determination of paraffin boiling points. J. Am. Chem. Soc. 1947, 69, 17–20.
- (20) Kier, L. B. Use of molecular negentropy to encode structure governing biological activity. J. Pharm. Sci. 1980, 69, 807–810.
- (21) Stankevich, I. V.; Stankevich, M. I.; Zefirov, N. S. Topological indices in organic chemistry. *Russ. Chem. Rev.* 1988, 57, 191–208.
- (22) El-Basil, S.; Randic, M. Equivalence of mathematical objects of interest in chemistry and physics. *Adv. Quantum Chem.* **1992**, *24*, 239–290.
- (23) Rohrbaugh, R. H.; Jurs, P. C. Descriptions of molecular shape applied in studies of structure/activity and structure/property relationships. *Anal. Chim. Acta* **1987**, *199*, 99–109.

- (24) Karelson, M. In *Molecular Descriptors in QSAR/QSPR*; Wiley: New York, 2000.
- (25) Osmialowski, K.; Halkiewicz, J.; Kaliszan, R. Quantum chemical parameters in correlation analysis of gas-liquid chromatographic retention indices of amines. J. Chromatogr., A 1986, 361, 63–69.
- (26) Stanton, D. T.; Jurs, P. C. Development and use of charged partial surface area structural descriptors in computer-assisted quantitative structure-property relationship studies. *Anal. Chem.* **1990**, *62*, 2323–2329.
- (27) Bodor, N.; Gabanyi, Z.; Wong, C.-K. A new method for the estimation of partition coefficient. J. Am. Chem. Soc. 1989, 111, 3783–3786.
- (28) Sannigrahi, A. B. AB initio molecular orbital calculations of bond index and valency. *Adv. Quantum Chem.* **1992**, *23*, 301–351.
- (29) SPSS Inc. http://www.spss.com/.
- (30) Lead Compound Screening System (CISOC-LSS), Registration Number (China): 096088.

Received for review July 29, 2009. Revised manuscript received November 15, 2009. Accepted November 19, 2009. This work received financial support from the Ministry of Science and Technology of China (Grants 2003CB114400 and 2006AA02Z339), the National Natural Science Foundation of China (Grant 20572081), and the Ministry of Environmental Protection of China (Grant 200709046).