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Prediction of calorific value of biomass based on elemental analysis

***Ayşe Özyuğuran* [a,*], *Serdar Yaman* [a], *Sadriye Küçükbayrak* [a]**

[a]*ITU, Chemical&Metallurgical Engineering Faculty, Chemical Engineering Department, Istanbul-34469, Turkey*

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ABSTRACT

Thirty nine different biomass samples ranging from various herbaceous/woody materials to juice pulps were used to develop linear as well as non-linear empirical equations that predict the lower heating value (LHV) and the higher heating value (HHV) based on the elemental analysis (C, H, N, O, and S) results of the biomass species. These equations were interpreted with respect to their prediction performance considering the predicted values and the experimental data. Several criteria such as mean absolute error (MAE), average absolute error (AAE), average bias error (ABE), and root mean square deviation (RMSD) were regarded. For the linear equations, it was found that the lowest values of MAE were 0.3119 MJ/kg and 0.2906 MJ/kg for HHV and LHV, respectively, and AAE(%) changed in the ranges of (1.6659-4.5917) for HHV and (1.8216-5.5039) for LHV. Besides, it was determined that ABE(%) varies in the intervals of (0.0549-0.2976) for HHV and (0.0519-0.4177) for LHV when linear equations were tested. The best results of RMSD (0.4230 and 0.3607 for HHV and LHV, respectively) were obtained for Equation#1 where all of the linear terms were considered. Also, the addition of the non-linear terms to the linear equations was also studied to check whether any further improvement can be achieved in predictions. However, the improvements created by non-linear equations were negligible and it was concluded that the linear empirical equations provide satisfactory prediction performance and they may be tried to estimate the calorific value of very wide range of biomasses.

1. Introduction

There is a growing consensus that the fossil energy sources should be gradually withdrawn from the power technology since they lead complicated global concerns such as greenhouse gases, political instability, dependence on other countries, etc. Besides, environmental pollution that takes place during exploitation, drilling, transportation, and usage of fossil fuels cannot be ignored. On the contrary, biomass is a CO_2-neutral fuel that does not influence the concentration of atmospheric CO_2 negatively. In addition, biomass can be easily found almost everywhere, and therefore it is cheap, abundant, and very easy to access [1]. Actually, biomass energy has been used in energy and power technologies with increasing shares day by day.

Biomass that is defined as any type of carbonaceous material except fossil fuels takes a significant part in green energy technologies since it is easy to find, renewable, and sustainable energy source [1]. According to this description woody/herbaceous crops and residues, agricultural leftovers, industrial and domestic wastes, municipal solid wastes (MSW), aquatic materials, forest by-products and residues are regarded as biomass energy resources. Despite this considerable variety in nature and properties of samples, they are mainly comprised of C, H, and O accompanied by some presence of N and S. Conversely, several different macromolecular ingredients including cellulose, hemicellulose, and lignin form the large portion of the molecular structure. Meanwhile, the amount of inorganics that form ash upon burning of biomass changes depending on type of the sample. That is, woody samples are poor in inorganics, while very large contents of inorganics may exist in waste materials. These varying characteristics of biomass also affect the "calorific value" in other words the "heating value" that is really the most important parameter to evaluate its fuel quality. That is why the calorific value of biomass cannot be forecasted

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* Corresponding author. Tel.: *0 (212) 285 30 30*
E-mail address: *kmayse@itu.edu.tr*

in most cases without measuring this property experimentally. Particularly in case of waste materials and herbaceous samples, the complexity of biomass makes it highly difficult to estimate the calorific value. The calorific value (heating value) is usually specified through burning of a specimen in calorimeter under well-controlled conditions, and in this way, higher heating value (HHV) is determined. Besides, lower heating value (LHV) is calculated via elimination of condensation heat of the forming water during combustion of H and moisture contents.

Calorific value estimation based on analysis results of biomass may be alternatively used provided that the analysis results have high accuracy and precision. The satisfactory prediction of HHV or LHV based on the elemental composition of biomass is a promising way since this approach does not deal with the type and distribution of the above mentioned macromolecules, and instead it only considers extents of the main elemental constituents of biomass. Actually, this approach has long been used to estimate the HHV or LHV of various coal samples globally. However, this approach was not so commonly applied yet for biomass. In this context, Channiwala and Parikh [2] complied the results of many investigations where HHV calculations were implemented considering both elemental analysis and proximate analysis results. In contrast to this, the literature that directly focus on the estimation of the HHV or LHV from the analysis results of biomass is scarce, and there have been only a few studies in this topic. Also, the existing literature on the assessment of HHV or LHV of biomass through such calculation-based approach was rather related to woody biomass types [2-9]. Motghare et al. [10] estimated the biomass calorific value upon the results of elemental analysis particularly for some waste species, and found that this approach is beneficial and gives highly reliable results.

This study attempts to apply the calculation-based method to predict HHV/LHV for miscellaneous waste biomasses, taking linear equations that contain elemental analysis results into consideration. Particularly, the most of the renewable fuel materials used in this study have not so far been chosen in investigations that target to describe the HHV/LHV prediction. For instance, some unusual samples including stems, fruit juice pulps, stalks, distinct agricultural leftovers, etc. have not been used in previous papers yet because they often show serious handling problems and tend to be easily decomposed.

2. Materials and Methods

2.1 Biomass Characterization

All of the biomasses used in the present paper are Turkish origin and provided from food/beverage industries and agricultural/forestry sector. They were kept in open container in laboratory to obtain air-dried (ad) specimens, and chopping and grinding operations were applied to reduce the particle size smaller than 250 µm. The proximate analysis was done according to ASTM standards, while Leco TruSpec® CHN model equipment with Leco TruSpec® S module was used to determine the elemental results. Determination of HHV was performed by adiabatic bomb calorimeter test using IKA C2000 model calorimeter operated under oxygen pressure of 30 atm. For this, 0.5 g of powdered (< 250 µm) biomass was placed into the sample holder and ignited by electricity current. This equipment is calibrated using benzoic acid and the measured results don’t deviate more than 1-2% from the mean values. Calculation of LHV based on HHV was implemented by simplified equation given as follows:

$$LHV = HHV - \left[\left(\frac{18.015*H}{2}\right) + \%moisture\right] * 5.85 \quad (1)$$

where, H is the hydrogen content of the sample.

Experiments were checked three times to assure the reproducibility and accuracy of the results, and they were used in predictions as long as they differ within ±0.5%.

2.2 Error Analyses for Prediction Performance

Four different forms of prediction error such as MAE (mean absolute error), AAE (average absolute error), ABE (average bias error), and RMSD (root mean square deviation) were established using following equations, and from which prediction performances could be evaluated.

$$\text{MAE} = \frac{1}{n}\sum_{i=1}^{n}\left|HHV_{(p)_i} - HHV_{(e)_i}\right| \quad (2)$$

$$\text{AAE} = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{HHV_{(p)_i} - HHV_{(e)_i}}{HHV_{(e)_i}}\right| \times 100 \quad (3)$$

$$\text{ABE} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{HHV_{(p)_i} - HHV_{(e)_i}}{HHV_{(e)_i}}\right) \times 100 \quad (4)$$

$$\text{RMSD} = \sqrt{\frac{\left(HHV_{(e)_i} - HHV_{(p)_i}\right)^2}{n}} \quad (5)$$

where, the indices of e and p represent the experimental and the predicted values of higher heating value. Likewise, the total number of the biomasses and any of the distinct biomass were represented by n and i, respectively. Of which, MAE shows the intimacy of the predicted HHV and the experimental HHV. From this point of view, low values of MAE indicate high prediction accuracy. Besides, the average absolute error (%) is estimated by AAE. Positive ABE means over-estimation whereas negative ABE means under-estimation

3. Results and Discussion

3.1 Sample Characterization

Results of the characterization tests are given in Table 1, and it is clear from this table that the samples differ seriously in terms of properties and the fuel characteristics. Although woody species have promising fuel properties such as low ash content and high calorific value, waste biomasses have relatively poor fuel characteristics.

Table 1. Analysis results of samples (on dry basis) [11]

	C	H	N	S	O	VM	FC	Ash	HHV	LHV
Samples	(%)					(%)			(MJ/kg)	
Elaeagnus	44.26	6.19	1.37	0.41	46.86	76.43	22.67	0.90	19.80	16.46
Tea caffeine	48.59	6.43	2.59	0.46	34.78	76.32	16.52	7.16	20.83	18.02
Ash tree wood	46.72	5.95	0.00	0.32	45.32	87.84	10.46	1.70	19.02	16.24
Green bean stem and husk	41.26	5.62	0.78	0.39	42.35	77.88	12.52	9.60	16.86	13.97
Red lentil hull	43.90	6.31	1.54	0.37	42.63	74.73	20.03	5.24	18.27	15.15
Chickpea husk	43.80	5.81	0.38	0.35	45.67	79.70	16.32	3.98	18.26	15.62
Tea waste	45.04	6.07	3.48	0.50	40.21	73.36	21.93	4.71	19.87	16.96
Cornstalk	42.02	5.58	1.24	0.43	43.53	76.79	16.02	7.19	16.55	14.19
Tobacco waste	37.02	5.01	2.20	0.45	39.95	72.85	11.78	15.36	14.51	12.26
Broad bean husk	40.11	5.52	1.35	0.33	44.98	74.97	17.33	7.70	16.24	13.50
Apricot stone	48.07	5.99	0.05	0.39	43.89	82.03	16.26	1.61	19.79	17.33
Apricot pulp	44.37	5.87	0.95	0.32	47.42	78.80	20.12	1.08	18.52	15.72
Peach pulp	43.84	6.51	1.04	0.37	42.80	71.21	23.34	5.44	18.23	15.11
Damson plum stone	50.81	6.36	1.07	0.36	40.39	82.33	16.67	1.00	21.23	18.81
Coconut shell	50.34	6.26	0.00	0.31	42.08	83.01	15.97	1.02	20.24	17.54
Cornelian cherry stone	49.03	5.86	0.05	0.34	42.67	79.27	18.67	2.06	19.84	17.44
Cacao husk	43.00	5.69	2.10	0.41	44.38	75.03	20.56	4.41	17.85	15.07
Peanut husk	46.89	5.90	0.61	0.37	46.07	79.32	20.53	0.15	19.16	16.53
Broad bean husk	41.33	5.90	0.39	0.34	46.32	74.88	19.40	5.73	16.80	13.90
Sunflower stem and stalk	37.94	5.19	0.31	0.35	46.15	77.37	12.58	10.05	15.08	12.55
Almond shell	47.70	5.88	0.05	0.31	42.58	81.70	14.82	3.48	19.53	16.81
Robinia pseudoacacia wood	46.30	6.08	0.05	0.35	46.20	86.19	12.80	1.01	18.31	15.59
Daphne	49.03	6.40	0.94	0.42	35.90	77.76	14.93	7.31	20.44	17.87
Thyme	44.53	6.01	0.81	0.36	39.34	75.04	16.00	8.96	18.16	15.27
Walnut shell	48.23	6.00	0.12	0.34	44.42	82.98	16.12	0.90	20.03	17.17
Locust bean	44.31	5.70	0.92	0.42	43.10	70.29	24.16	5.54	18.04	15.29
Flos lavandulae romanae	45.28	5.89	0.94	0.42	36.42	74.13	14.82	11.06	18.84	16.01
Apple pulp	47.05	6.70	0.86	0.35	42.73	82.56	15.13	2.31	19.85	17.15
Artichoke husk and waste	42.08	5.92	0.83	0.36	45.88	79.66	15.43	4.91	16.38	13.61
Sunflower stem	39.90	5.38	0.42	0.40	42.80	75.09	13.81	11.10	16.18	13.65
Sour cherry stem	44.78	5.75	0.50	0.40	43.22	77.48	17.16	5.36	18.27	15.62
Soybean residue	42.96	6.21	8.02	0.57	35.80	80.01	13.54	6.45	19.26	16.35
Black sesame residue	45.93	6.79	6.32	0.66	32.01	78.78	12.94	8.28	21.04	18.22
Cotton residue	45.24	6.46	6.37	0.65	33.41	74.97	17.16	7.87	19.90	17.02
Pea stem	38.97	5.45	1.79	0.42	40.31	74.67	12.27	13.06	16.31	13.57
Grape seed	50.47	6.20	2.42	0.47	35.83	74.26	21.12	4.62	21.70	18.73
Pine cone	48.28	5.73	0.10	0.40	43.89	80.92	17.48	1.60	20.07	16.96
Peach stone	51.98	6.13	0.02	0.48	40.41	86.42	12.61	0.97	20.31	17.85
Sour cherry stone	53.30	6.69	1.58	0.39	37.33	81.66	17.62	0.72	21.95	19.45

VM: volatile matter FC: fixed carbon

3.2 Calorific Value Prediction

Table 2 presents the linear equations used to calculate HHV and LHV, r^2 values, and the results of performance criteria. Equation#1 considers five parameters, while the other equations consider less parameters. For instance, the number of the parameters in the Equations #2-6 is four. Equation#1 that includes all of the parameters of elemental analysis gave the best prediction with respect to the coefficients of determination (r^2) as expected.

Table 2. Linear Equations and the prediction performances [11]

Eq. No	Linear Equations	r^2	SD	MAE	AAE (%)	ABE (%)	RMSD
1	$HHV = -4{,}914\,0 + 0{,}2611\,N + 0{,}4114\,C + 0{,}6114\,H + 0{,}3888\,S + 0{,}02097\,O$	0.9441	1.7379	0.3178	1.6978	0.0549	0.4230
	$LHV = -5{,}5232 + 0{,}2373\,N + 0{,}4334\,C + 0{,}2360H + 0{,}3732\,S + 0{,}000838\,O$	0.9582	1.7272	0.2915	1.8304	0.0654	0.3607
2	$HHV = -3{,}4643 + 0{,}2492\,N + 0{,}4045\,C + 0{,}6072\,H - 0{,}1618\,S$	0.9434	1.7373	0.3119	1.6659	0.0571	0.4256
	$LHV = -5{,}4653 + 0{,}2368N + 0{,}4331C + 0{,}2358H + 0{,}3511S$	0.9582	1.7271	0.2915	1.8304	0.0562	0.3607
3	$HHV = -4{,}6246 + 0{,}2732\,N + 0{,}4120\,C + 0{,}5992\,H + 0{,}01841\,O$	0.9440	1.7379	0.3186	1.7020	0.0562	0.4232
	$LHV = -5.2454 + 0.2489N + 0.4340C + 0.2243H - 0.00162O$	0.9581	1.7270	0.2925	1.8367	0.0519	0.3610
4	$HHV = -3.17334 + 0.3474\,N + 0.4593\,C - 0.4021\,S + 0.01972\,O$	0.9378	1.7321	0.3387	1.8134	0.0645	0.4461
	$LHV = -4.8513 + 0.2706\,N + 0.4519\,C + 0.06784\,S + 0.000356\,O$	0.9572	1.7264	0.2906	1.8216	0.0663	0.3649
5	$HHV = 1.5348 - 0.3434\,N + 3.4740\,H + 2.9958\,S - 0.1028\,O$	0.6916	1.4875	0.8524	4.5917	0.2976	0.9933
	$LHV = 1.2705 - 0.3996\,N + 3.2517\,H + 3.1196\,S - 0.1296\,O$	0.6702	1.4444	0.8698	5.5039	0.4177	1.0132
6	$HHV = -5.6318 + 0.3630\,C + 1.0237\,H + 4.1453\,S + 0.00389\,O$	0.9313	1.7261	0.3470	1.8483	0.0691	0.4689
	$LHV = -6.1755 + 0.3894\,C + 0.6107\,H + 3.7869\,S - 0.01468\,O$	0.9473	1.7173	0.3174	1.9923	0.0673	0.4049

Equations (#2- #6) ignore only one parameter compared to Equation#1. Among these equations, the best performance in HHV prediction belongs to Equation#3 that neglects effect of the content of S. Namely, Equation#3 yielded acceptable predictions for HHVs (r^2=0.9440). Moreover, LHV prediction performance of Equation#2 (r^2=0.9582) is exactly the same with those of Equation#1 that reveals the fact that oxygen content can be safely removed from the equation. Besides, the lowest r^2 was found if C content is removed from Equation#5. On the contrary, Setyawati et al. [12] correlated HHV of tropical peat based on its elemental analysis that ignores the C content and uses H, N, S, O, and ash contents.

The standard deviations (SD) of linear empirical equations varied within (1.4875-1.7379) for HHV and (1.4444-1.7272) for LHV. Concerning the error functions, MAE values indicate that the estimations of HHV and LHV can be made with a minimum mean absolute errors of 0.3119 MJ/kg and 0.2906 MJ/kg, respectively. Besides, AAE(%) values varied in the intervals of (1.6659-4.5917) for HHV and (1.8216-5.5039) for LHV. Although the upper limits of AAE(%) results may be thought as a bit high, these values are roughly consistent with the values reported in literature for this criterion. In their paper, Nhuchen and Abdul Salam [13] compiled the results of various studies about HHV prediction for lignocellulosic residues and wastes, chars, and coals that makes it possible to compare the error analysis and prediction performances for different types of fuels. They concluded that the maximum values of AAE(%) values are calculated in the case of the lignocellulosic residues as well as the other biomasses. On the other hand, coal samples showed generally better results. Chen et al. [6] also estimated the higher heating value of the torrefied (mildly pyrolyzed) biomass using its ultimate analysis, and revealed that the relative errors of raw biomasses reached 9.03%. Alternatively, Choi at al. [14] reported 8.57% of AAE value for prediction of HHV of the mixture of animal wastes for the equation where C, N, S, and O are incorporated. Similarly, Bousdira et al. [15] highlighted the importance of having low ash yield on prediction performance of calorific value prediction based on elementary composition. Unfortunately, the biomass species we used in this paper are very rich in inorganics, and accordingly they produce high yields of ash. Therefore, this is a significant concern originating from any unforeseen effects of the complicated nature of the inorganics. Also, the ABE(%) values altered within (0.0549-0.2976) for HHV and (0.0519-0.4177) for LHV, which can comparable with the results reported in literature [16]. The most promising values of RMSD (0.4230 and 0.3607 for HHV and LHV, respectively) were calculated if all parameters were involved (Equation#1).

Furthermore, in order to investigate the effects of non-linear terms in the form of squares of the parameters, new equations (#7-#11) were established. That is, Equation#7 excludes oxygen contents and the squares of the other ingredients (N^2, C^2, H^2, S^2) were added to their linear parameters. Likewise, Equations#8, 9, 10, and 11 exclude sulphur, hydrogen, carbon, and nitrogen contents, respectively. In this way, the new equations include squares of the related four, three, and two parameters. Table 3 presents these equations and the calculated r^2, SD, MAE, AAE, ABE, and RMSD results. These results revealed that the combination of non-linear terms did not improve so significantly the r^2 values calculated for the linear equations. The best r^2 values determined in the case of Equation#1 increased from 0.9441 to 0.9566 for HHV and from 0.9582 to 0.9668 for LHV when the sulphur content was ignored and the squares of the other four parameters were considered (Equation#8). Besides, a bit improvement took place in the prediction performance indicators. All in all, it can be concluded that the addition of the non-linear terms can not be recommended as a reliable approach to increase the prediction performance of the linear equations investigated in this paper.

4. Conclusions

This study revealed that the calorific values of the highly different biomass species can be safely predicted from their elemental analysis results. The thirty-nine different biomass species used in this study represent highly dissimilar structures in terms of the elemental analysis. Comparison of the experimental calorific values with the predicted calorific values, and the error analyses via MAE, AAE, ABE, and RMSD calculations showed that quite simple linear equations can be safely used to get the calorific value. Among the equations used, the equation that contains all of the parameters of elemental analysis provided the greatest prediction performance. Elimination of any parameter from this equation resulted in decrease in the prediction performance. However, addition of non-linear (squared) terms of the elemental analysis results did not provide improvement in performance of the linear equations. Thus, the use of linear equations of ultimate analysis results are recommended.

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Table 3. Non-linear Equations used and the prediction performances

Eq. No	Non-linear Equations	r^2	SD	MAE	AAE (%)	ABE (%)	RMSD
7	$HHV = -15.8566 + 0.4951\,N + 1.7601\,C + 5.4604\,H + 1.4769\,S - 0.02812\,N^2 - 0.01447\,C^2 + 0.4671\,H^2 - 2.6691\,S^2$	0.9556	1.7500	0.2885	1.5870	0.0942	0.3771
	$HHV = -16.1264 + 0.5064\,N + 1.7144\,C - 4.8484\,H - 0.8586\,S - 0.03065\,N^2 - 0.01398\,C^2 + 0.4153\,H^2$	0.9555	1.7475	0.2862	1.5735	0.0085	0.3774
	$HHV = -23.9224 + 0.5028\,N + 1.3785\,C + 0.2528\,H - 0.5169\,S - 0.03158\,N^2 - 0.01045\,C^2$	0.9546	1.7698	0.3832	2.0927	1.5776	0.4781
7	$LHV = 2.4879 + 0.4271\,N + 1.6322\,C - 11.4438\,H + 1.0062\,S - 0.0200\,N^2 - 0.01267\,C^2 + 0.9370\,H^2 - 1.9815\,S^2$	0.9662	1.7326	0.2617	1.6875	-0.0304	0.3245
	$LHV = 2.2876 + 0.4355\,N + 1.5983\,C - 10.9894\,H - 0.7277\,S - 0.02188\,N^2 - 0.0123\,C^2 + 0.8985\,H^2$	0.9662	1.7327	0.2514	1.6848	-0.0256	0.3248
	$LHV = 5.4060 + 0.2624\,N + 1.5159\,C - 11.4293\,H - 0.3867\,S - 0.01148\,C^2 + 0.9420\,H^2$	0.9639	1.7338	0.2696	1.7157	0.1103	0.3354
8	$HHV = -9.5129 + 0.4900\,N + 1.5545\,C - 3.9058\,H - 0.3211\,O - 0.03242\,N^2 - 0.01219\,C^2 + 0.3372\,H^2 + 0.00409\,O^2$	0.9566	1.7502	0.2839	1.5573	0.0449	0.3729
	$HHV = -14.7175 + 0.4883\,N + 1.2926\,C + 0.2188\,H - 0.3729\,O - 0.03307\,N^2 - 0.00945\,C^2 + 0.00467\,O^2$	0.9560	1.7481	0.2831	1.5468	0.0287	0.3753
	$HHV = -23.8290 + 0.5064\,N + 1.3355\,C + 0.2735\,H + 0.01165\,O - 0.03248\,N^2 - 0.00995\,C^2$	0.9547	1.7465	0.2895	1.5852	0.0018	0.3808
8	$LHV = 7.3723 + 0.4130\,N + 1.4676\,C - 10.0585\,H - 0.2655\,O - 0.02286\,N^2 - 0.01086\,C^2 + 0.8217\,H^2 + 0.00335\,O^2$	0.9668	1.7339	0.2605	1.6717	0.0229	0.3217
	$LHV = 2.0693 + 0.4259\,N + 1.5481\,C - 10.8196\,H + 0.0109\,O - 0.02233\,N^2 - 0.01173\,C^2 + 0.8870\,H^2$	0.9661	1.7358	0.2651	1.7083	0.1068	0.3251
	$LHV = 4.8380 + 0.2490\,N + 1.4924\,C - 11.1362\,H + 0.00164\,O - 0.01125\,C^2 + 0.9193\,H^2$	0.9638	1.7315	0.2680	1.7030	0.0025	0.3356
9	$HHV = -11.9276 + 0.5322\,N + 1.4068\,C + 3.4329\,S - 0.6077\,O - 0.03177\,N^2 - 0.01054\,C^2 - 5.2651\,S^2 + 0.00742\,O^2$	0.9561	1.7479	0.2862	1.5662	0.0035	0.3747
	$HHV = -13.4885 + 0.5504\,N + 1.3978\,C - 1.0829\,S - 0.4764\,O - 0.03589\,N^2 - 0.01044\,C^2 + 0.00584\,O^2$	0.9558	1.7485	0.2887	1.5803	0.0493	0.3762
	$HHV = -25.6364 + 0.5722\,N + 1.4851\,C - 0.6605\,S + 0.00709\,O - 0.03587\,N^2 - 0.01137\,C^2$	0.9538	1.7481	0.2921	1.6049	0.0792	0.3847

Table 3. Continue…

Eq. No	Non-linear Equations	r^2	SD	MAE	AAE (%)	ABE (%)	RMSD
9	$LHV = -4.1399 + 0.4129\,N + 0.8277\,C + 1.0241\,S - 0.4525\,O - 0.02311\,N^2 - 0.00416\,C^2 - 1.6864\,S^2 + 0.00545\,O^2$	0.9634	1.7322	0.2696	1.7130	0.0476	0.3376
	$LHV = -4.6399 + 0.4188\,N + 0.8248\,C - 0.4223\,S - 0.4104\,O - 0.02443\,N^2 - 0.00413\,C^2 + 0.00494\,O^2$	0.9634	1.7317	0.2684	1.7070	0.0464	0.3378
	$LHV = 4.7003 + 0.4250\,N + 0.4557\,C - 0.4251\,S - 0.4776\,O - 0.02321\,N^2 + 0.00587\,O^2$	0.9619	1.7303	0.2755	1.7390	0.0457	0.3444
10	$HHV = -63.3676 - 0.4996\,N + 27.2370\,H + 7.9872\,S - 0.3397\,O + 0.02661\,N^2 - 2.0138\,H^2 - 5.7886\,S^2 + 0.00232\,O^2$	0.7516	1.5506	0.7267	3.8914	0.2360	0.8914
	$HHV = -67.4014 - 0.4871\,N + 27.3544\,H + 6.2519\,S - 0.1473\,O + 0.02497\,N^2 - 2.0225\,H^2 - 3.5968\,S^2$	0.7514	1.5505	0.7304	3.9115	0.2178	0.8918
	$HHV = -67.7552 - 0.4730\,N + 27.7527\,H + 3.0500\,S - 0.1489\,O + 0.02160\,N^2 - 2.0581\,H^2$	0.7512	1.5500	0.7283	3.9011	0.2249	0.8922
10	$LHV = -52.6526 - 0.6553\,N + 22.2289\,H + 7.1848\,S - 0.2097\,O + 0.03954\,N^2 - 1.6085\,H^2 - 4.5180\,S^2 + 0.00048\,O^2$	0.7185	1.4955	0.7520	4.7456	0.3248	0.9362
	$LHV = -53.4812 - 0.6527\,N + 22.2530\,H + 6.8283\,S - 0.1701\,O + 0.0392\,N^2 - 1.6103\,H^2 - 4.0677\,S^2$	0.7185	1.4953	0.7527	4.7502	0.3273	0.9362
	$LHV = -53.8812 - 0.6368\,N + 22.7035\,H + 3.2072\,S - 0.1720\,O + 0.03539\,N^2 - 1.6505\,H^2$	0.7182	1.4953	0.7511	4.7418	0.3313	0.9367
11	$HHV = -5.6668 + 1.3547\,C - 1.4834\,H + 8.3792\,S - 0.6870\,O - 0.01075\,C^2 + 0.1770\,H^2 - 6.3435\,S^2 + 0.00806\,O^2$	0.9413	1.7351	0.3207	1.7197	0.0613	0.4334
	$HHV = -8.6907 + 1.2124\,C + 0.6759\,H + 7.8601\,S - 0.6898\,O - 0.00925\,C^2 - 5.7498\,S^2 + 0.00808\,O^2$	0.9411	1.7341	0.3236	1.7317	-0.0016	0.4341
	$HHV = -10.1398 + 1.1979\,C + 0.6475\,H + 2.7380\,S - 0.5422\,O - 0.00907\,C^2 + 0.00629\,O^2$	0.9406	1.7349	0.3181	1.7024	0.0566	0.4360
11	$LHV = 8.7097 + 1.2497\,C - 7.0316\,H + 5.1349\,S - 0.5485\,O - 0.00916\,C^2 + 0.6075\,H^2 - 2.7369\,S^2 + 0.00635\,O^2$	0.9531	1.7233	0.3004	1.8920	0.0691	0.3823
	$LHV = 7.5243 + 1.2185\,C - 6.6722\,H + 2.6985\,S - 0.4813\,O - 0.00882\,C^2 + 0.5770\,H^2 + 0.00553\,O^2$	0.9529	1.7232	0.2982	1.8783	0.0971	0.3828
	$LHV = -1.8445 + 0.7597\,C + 0.3757\,H + 2.7304\,S - 0.5398\,O - 0.00398\,C^2 + 0.00619\,O^2$	0.9512	1.7224	0.3034	1.9039	0.1061	0.3899