Tony O'Lenick – Siltech LLC, US
Kevin O'Lenick – SurfaTech Corporation, US

Green rating for compounds and formulations

Today's consumer and formulator have become increasingly aware of the consumption of resources that are not renewable. Products derived from fossil fuels are non-renewable. This includes products like gasoline, coal, natural gas, diesel, and other commodities. Green resources are defined as renewable resources, replenished by natural processes. Green products are renewable resources that include oxygen, fresh water, timber, and biomass. Green products also include commodities such as wood, paper, and leather. Furthermore, alcohol, oils from plants and seeds are considered green products.

These green raw materials are the most environmentally friendly and their use are the most conservative in minimising negative impact on the planet.

However, these basic green products cannot be combined in a way that provides consumer products that meet the demands of the consumer. For example, soap can be a green detergent, but it does not possess all the desirable properties that give the consumer a laundry detergent. In order to make high performance formulations, some materials that are not strictly speaking green are required.

While the concept of green products is straightforward, the ability of the formulator and the consumer to quantify the greenness of a given shampoo or other consumer product is elusive. Given a proper understanding, the consumer and formulator can make better informed, better educated decisions as to making products with the best combination of green properties and formulation attributes. In other words, the need of the consumer and the need of the environment can be intelligently determined.

All too often, the determination of the greenness of a raw material or formulation was more an emotional rather than a scientific decision and required an all-or-nothing approach to environmental stewardship. Simply put, materials are green or they are not. Unfortunately, the formulation of consumer products that are commercially acceptable require a trade-off in optimising the performance and greenness. Consumers demand many formulation benefits that cannot be achieved with all green ingredients. Some "non-green" products are required. The consumer then needs a systematic approach to develop a measurable metric for the level of greenness in a formulation and trade off some greenness for performance. This quest has resulted in the development of "Green Star Rating"[1] system or simply "GSR".

GSR

The Green Star Rating provides a process by which a formulator can easily ascertain the "greenness" of a raw material and, as importantly, a consumer can determine and compare the "greenness" of a formulation to similar types of products. This process allows the formulation chemist a way to break a molecule down into a green portion and a non-renewable resource portion. The evaluation of this data allows for the generation of a Green Star Value, which is the percentage of the molecule that is based upon green chemistry divided by 10.

Once this number is known, the effect of replacing one ingredient in a formulation with a "greener" compound can be ascertained. Specifically, if a raw material used in a formulation at 20% by weight has a Green Star Rating of 1 is replaced with a product with a Green Star Rating of 7, the impact on the formulation is (7-1) times 0.20 or 1.2. This means that much more renewable resources are being used in the formulation and its consumption will impact less negatively on the environment.

This approach allows the formulator to make greener products and the consumer to choose greener products. By greener products is meant products based upon a greater percentage of renewable resources. Greener products are those with a higher Green Star Rating.

The Green Star Rating is determined using the following steps:

1 Determining the empirical formula for chemical compounds used to make formulated products.
2 Determining which portions of the molecule are green.
3 Determining the percentage by weight of the green portion of the molecule.
4 Determining the green star value.
And optionally:
5 Optimising the formulation by selecting components with the greatest Green Star value.

Raw materials

Example 1: sodium coco alcohol derived from natural alcohol

Step one: determining the empirical formula for chemical compounds used to make formulated product.

Example: Sodium coco sulfate
$C_{12}H_{23}SO_4Na$

Step two: determining which portions of the molecule are green.

Example: Sodium coco sulfate
Renewable material natural alcohol
$C_{12}H_{23}$
Non-renewable synthetic sulfation
SO_4Na

Step three: determining the percentage by weight of the green portion of the molecule. This is done by multiplying the weight of each atom by the number of atoms in each portion.

Renewable natural alcohol
$C_{12}H_{23}$

Carbon has a molecular weight of 12, there are 12 present in the renewable portion, so the molecular weight contribution of the carbon is 12 times 12 or 144.

Hydrogen has a molecular weight of 1, there are 23 hydrogen atoms present in the renewable portion, so the molecular weight contribution of the hydrogen is 1 times 23 or 23.

The sum of all the elements in the renewable portion is 144+23 or 167.

The non-renewable portion is SO_4Na.

Sulfur has a molecular weight of 32, there is 1 sulfur atom present in the non-renewable portion so the molecular weight contribution of the sulfur is 1 times 32 or 32.

Oxygen has a molecular weight of 16, there are 4 oxygen atoms present in the non-renewable portion, so the molecular weight contribution of the hydrogen is 4 times 16 or 64.

Sodium has a molecular weight of 23, there is 1 sodium atom present in the non-renewable portion, so the molecular weight contribution of the sulfur is 1 times 23 or 23.

The sum of all the elements in the non-renewable portion is 32+64+23= 119

Total Molecular Weight =
Renewable portion +
Non-renewable portion

Total Molecular Weight =
167+ 119 = 289

Renewable portion/Total =
167/289 = 57.7%

Step 4: determining the Green Star Value
Green Star Value (GSV) =
% Renewable rounded to unit = 58

Example 2: Sodium laureth 3 sulfate

$C_{12}H_{23}O(CH_2CH_2O)_3SO_3Na$
Empirical formula: $C_{18}H_{35}O_7SNa$
Renewable natural alcohol
$C_{12}H_{23}$
Synthetic EO-Sulfate
$–(CH_2CH_2O)_3SO_4Na$

Calculations

Renewable portion

	C	H	N	O	P	S	Na	K
Number	12	23	0	0	0	0	0	0
MW	144	23	0	0	0	0	0	0
Total	167							

Non-renewable

	C	H	N	O	P	S	Na	K
Number	6	12	0	7	0	0	1	0
MW	72	12	0	112	0	0	23	0
Total	219							

Total	386
% Renewable	43
Green Star Rating	43

Formulation 1: Conditioning shampoo.

This product is based on sodium lauryl sulfate (synthetic alcohol).

	% Weight	% Solids	Example	GRS	Contribution
Water	55.0	–	–	–	–
Sodium lauryl sulfate	34.0	9.5	Example 3	0	0 (.095 x 0)
Cocamidopropyl betaine	8.0	2.8	Example 4	56	1.6 (.028 x 56)
Cocamid MEA	3.0	3.0	Example 6	71	2.1 (.03 x71)
Total					3.7

Formulation 2: Conditioning shampoo (version 1).

This product is based on sodium lauryl sulfate (synthetic alcohol) and SLES-3.

	% Weight	% Solids	Example	GRS	Contribution
Water	55.0	–	–	–	–
Sodium lauryl sulfate	17.0	4.5	Example 3	0	0 (.045 x 0)
Sodium laureth 3 sulfate	17.0	4.5	Example 2	43	2.0 (.045 x 43)
Cocamidopropyl betaine	8.0	2.8	Example 4	56	1.6 (.028 x 56)
Cocamid DEA	3.0	3.0	Example 5	63	1.9 (.03 x 63)
Total					5.5

Formulation 3: Conditioning shampoo.

This product is based on sodium coco sulfate (renewable alcohol).

	% Weight	% Solids	Example	GRS	Contribution
Water	55.0	–	–	–	–
Sodium coco sulfate	17.0	4.5	Example 1	58	2.6 (.045 x 58)
Sodium laureth 3 sulfate	17.0	4.5	Example 2	43	1.9 (.045 x 43)
Cocamidopropyl betaine	8.0	2.8	Example 4	56	1.6 (.028 x 56)
Cocamid DEA	3.0	3.0	Example 5	63	1.9 (.03 x 63)
Total					8.0

Formulation 4: Conditioning shampoo.

This product is based on sodium coco sulfate (renewable alcohol).

	% Weight	% Solids	Example	GRS	Contribution
Water	55.0	–	–	–	–
Sodium coco sulfate	17.0	4.5	Example 1	58	2.6 (.045 x 58)
Sodium laureth 3 sulfate	17.0	4.5	Example 2	43	1.9 (.045 x 43)
Cocamidopropyl betaine	8.0	2.8	Example 4	56	1.6 (.028 x 56)
Cocamid MEA	3.0	3.0	Example 6	71	2.1 (.03 x 71)
Total					8.2

Example 3: Sodium lauryl sulfate (ziegler alcohol derived)

Example: sodium lauryl sulfate
$C_{12}H_{23}SO_4Na$

Step 2: determine which parts of the molecule are natural (derived from green natural raw materials) and which synthetic.

Example: sodium lauryl sulfate
Synthetic $C_{12}H_{23}$ SO_4Na

Step 3:

Renewable portion

	C	H	N	O	P	S	Na
Number	0	0	0	0	0	0	0
MW	0	0	0	0	0	0	0
Total	0						

Non-renewable portion

	C	H	N	O	P	S	Na
Number	12	23	0	4	0	1	1
MW	144	23	0	64	0	31	23
Total	285						

Total	285
% renewable	0
Green Star Rating	0

Example 4: Cocamidopropyl betaine

Structure:

$$\begin{array}{c} CH_3 \\ | \\ C_{11}H_{23}C(O)\text{-}N(H)\text{-}(CH_2)_3\text{-}N^{+}\text{-}CH_2C(O)\text{-}O^{-} \\ | \\ CH_3 \end{array}$$

Formula: $C_{18}H_{38}O_3N_2$

Step 2: determine which parts of the molecule are natural (derived from green natural raw materials) and which synthetic.
Renewable
$C_{12}H_{23}O$
Non-renewable
$C_6H_{14}O_2N_2$

Step 3:
Renewable portion

	C	H	N	O	P	S	Na	K
Number	12	23	0	1	0	0	0	0
MW	144	23	0	16	0	0	0	0
Total	183							

Non-renewable

	C	H	N	O	P	S	Na	K
Number	6	14	2	2	0	0	0	0
MW	72	14	28	32	0	0	0	0
Total	146							

Total	329
% renewable	55.6
Green Star Rating	56

Example 5: Cocamid DEA
Structure:
$C_{11}H_{23}$-C(O)-N-$(CH_2CH_2OH)_2$
|
$C_{16}H_{30}O_3N$

Step 2: determine which parts of the molecule are natural (derived from green natural raw materials) and which synthetic.
$C_{11}H_{23}$-C(O)-N-$(CH_2CH_2OH)_2$
Renewable
$C_{12}H_{23}O$
Non-renewable
$C_4H_{10}O_2N$

Step 3:

	C	H	N	O	P	S	Na	K
Number	12	23	0	1	0	0	0	0
MW	144	23	0	16	0	0	0	0
Total	183							

Synthetic

	C	H	N	O	P	S	Na	K
Number	4	10	1	2	0	0	0	0
MW	48	10	14	32	0	0	0	0
Total	104							

Total	287
% renewable	63
Green Star Rating	63

Example 6: cocamid MEA
Structure:
$C_{11}H_{23}$-C(O)-NH-CH_2CH_2OH
|
$C_{14}H_{29}O_2N$

Step 2: determine which parts of the molecule are natural (derived from green natural raw materials) and which synthetic.
$C_{11}H_{23}$-C(O)-NH-CH_2CH_2OH
Renewable
$C_{12}H_{23}O$
Non-renewable
$C_2H_{60}N$

Step 3:
Renewable portion

	C	H	N	O	P	S	Na	K
Number	12	23	0	1	0	0	0	0
MW	144	23	0	16	0	0	0	0
Total	183							

Non-renewable

	C	H	N	O	P	S	Na	K
Number	2	6	1	2	0	0	0	0
MW	24	6	14	32	0	0	0	0
Total	76							

Total	259
% renewable	70.6
Green Star Rating	71

Formulations

The Green Star Process can also be used on any formulation.

Conditioning Shampoo

	% weight
Water	55.0
Sodium lauryl sulfate	18.0
Sodium laureth 3 sulfate	16.0
Cocamidopropyl betaine	8.0
Cocamid DEA	3.0

The simple formulations 1-4, opposite, show the power of the new system. Minor changes in the formulation made by properly selecting raw materials result in a 2.2 times improvement in the Green Star Rating. This process allows the formulator to fine tune formulations to maximise greenness and to inform the consumer about the degree amount of a given formulation that is renewable. The same approach works not only on shampoos but all formulations.

Formulation	Green Star Rating
1	3.7
2	5.5
3	8.0
4	8.2

Conclusion

The Green Star Rating System provides the formulator and consumer with a metric by which both formulations and raw materials can be evaluated. The determination allows for the consumer to pick the product with the highest Green Star Rating that provides the consumer attributes that customer demands. Inherent in this system is the belief that consumers can make educated selections of cosmetic formulations that balance the desire for green products and at the same time answer all the consumer's demands *vis-à-vis* performance.

Reference

1 US Patent Application 2009/0259409 filed in June 2008 entitled: *Process for determining the green star rating of compounds and formulations.*