| t0 (tau)   | 0          |
|--|------------|
| tf (tau)   | 0.9        |
| 1 [ipropylooh]ipropylooh=>ipropyloxy+OH>[ipropyloxy]   | 0.99999909 |
| [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
| >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
| >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl                                      |            |
| 2 >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]  | 0.73547474 |
| [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
| >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
| >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl                                      |            |
| 7 >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]  | 0.24573716 |
| [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
| >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
| >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl>[npropyl]well_1=>OH+prod_1           |            |
| 5 ->[prod_1]prod_1=>frag_1+OH>[frag_1]   | 0.18819033 |
|  |            |
| [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
| >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
| >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl>[npropyl]well_1=>OH+prod_1           |            |
| ->[prod_1]prod_1=>frag_1+OH>[frag_1]frag_1=>vinoxy+CH <sub>2</sub> O   |            |
| 6 >[vinoxy]vinoxy+O <sub>2</sub> =>CH <sub>2</sub> O+CO+OH>[CO]  | 0.18818549 |
| [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
| >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
| >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl>[npropyl]well_1=>OH+prod_1           |            |
| 4 ->[prod_1]   | 0.18815115 |
| Singa pula a haling paga a                         |            |
| [ipropylooh]ipropylooh=>ipropyloxy+OH<br>>[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|  |            |
| >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub>   |            |
| >[acetyl]acetyl(+M)=>CH <sub>3</sub> +CO(+M)>[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> | 0.13745952 |
| 3 >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]  | 0.13/43332 |
| [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
| >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
| >[acetaldehyde]CH <sub>3</sub> OO+acetaldehyde=>CH <sub>3</sub> OOH+acetyl   | 0.00040004 |
| 9 > [CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]   | 0.09049864 |

| [ipropylooh]                         | ipropylooh=>ipropyloxy+OH  |            |
|--------------------------------------|--|------------|
|                                      | 'Jipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
| >[acetaldeh                          | yde]CH <sub>3</sub> OO+acetaldehyde=>CH <sub>3</sub> OOH+acetyl  |            |
| >[acetyl]ace                         | tyl(+M)=>CH <sub>3</sub> +CO(+M)>[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> |            |
| 19 >[CH <sub>3</sub> OOH]C           | $CH_3OOH=>CH_3O+OH>[CH_3O]$  | 0.04107802 |
| [ipropylooh]                         | ipropylooh=>ipropyloxy+OH  |            |
| >[ipropyloxy                         | ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
| >[acetaldeh                          | yde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub>  |            |
| >[acetyl]ace                         | $tyl(+M) = >CH_3 + CO(+M)$   |            |
| >[CH <sub>3</sub> ]CH <sub>3</sub> O | O+CH <sub>2</sub> O=>CH <sub>3</sub> OOH+HCO> <mark>[CH<sub>3</sub>OOH]</mark> CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH   |            |
| 13 >[CH <sub>3</sub> O]              |  | 0.03870921 |
| [ipropylooh]                         | ipropylooh=>ipropyloxy+OH  |            |
| >[ipropyloxy                         | ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
| >[acetaldeh                          | yde]npropyloo+acetaldehyde=>npropylooh+acetyl  |            |
| 14 >[npropyloo                       | h]npropylooh=>npropyloxy+OH>[npropyloxy]   | 0.0320651  |
| [ipropylooh]                         | ipropylooh=>ipropyloxy+OH  |            |
| >[ipropyloxy                         | ']ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
| >[CH <sub>3</sub> ]CH <sub>3</sub> O | O+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |            |
| >[ipropyl]ipr                        | -opyloo+C <sub>3</sub> H <sub>8</sub> =>ipropylooh+ipropyl   |            |
| 16 >[ipropylool                      | n]ipropylooh=>ipropyloxy+OH>[ <mark>ipropyloxy</mark> ]  | 0.03120589 |
| [ipropylooh]                         | ipropylooh=>ipropyloxy+OH  |            |
| >[ipropyloxy                         | jipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
| >[acetaldeh                          | yde]acetaldehyde+OH=>vinoxy+H <sub>2</sub> O   |            |
| 8 >[vinoxy]vin                       | $oxy+O_2=>CH_2O+CO+OH>[CO]$  | 0.02867906 |
| [ipropylooh]                         | ipropylooh=>ipropyloxy+OH  |            |
| >[ipropyloxy                         | ']ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|                                      | yde]ipropyloo+acetaldehyde=>ipropylooh+acetyl  |            |
|                                      | n]ipropylooh=>ipropyloxy+OH>[ipropyloxy]   | 0.02567813 |
|                                      | ipropylooh=>ipropyloxy+OH  |            |
|                                      | ']ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
| - 5-                                 | O+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |            |
| >[ipropyl]ipr                        | opyloo+C <sub>3</sub> H <sub>8</sub> =>ipropylooh+ipropyl  |            |
| >[ipropylool                         | n]ipropylooh=>ipropyloxy+OH  |            |
| >[ipropyloxy                         | ']ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
| >[CH <sub>3</sub> ]CH <sub>3</sub> O | O+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |            |
| 62 >[CH <sub>3</sub> OOH]C           | CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]  | 0.02239501 |

|    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|----|---|------------|
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |            |
|    | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+O <sub>2</sub> =>CH <sub>2</sub> O+HO <sub>2</sub> |            |
|    | >[CH <sub>2</sub> O]CH <sub>3</sub> OO+CH <sub>2</sub> O=>CH <sub>3</sub> OOH+HCO   |            |
| 23 | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]   | 0.02135332 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |            |
|    | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+O <sub>2</sub> =>CH <sub>2</sub> O+HO <sub>2</sub> |            |
|    | >[CH <sub>2</sub> O]CH <sub>3</sub> CH <sub>2</sub> OO+CH <sub>2</sub> O=>CH <sub>3</sub> CH <sub>2</sub> OOH+HCO                                       |            |
| 27 | <pre>/ &gt;[CH<sub>3</sub>CH<sub>2</sub>OOH]CH<sub>3</sub>CH<sub>2</sub>OOH=&gt;ethoxy+OH&gt;[ethoxy]</pre>   | 0.02103051 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |            |
|    | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+O <sub>2</sub> =>CH <sub>2</sub> O+HO <sub>2</sub> |            |
|    | >[CH <sub>2</sub> O]npropyloo+CH <sub>2</sub> O=>npropylooh+HCO   |            |
| 31 | >[npropylooh]npropylooh=>npropyloxy+OH>[npropyloxy]   | 0.01881086 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|    | >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub>  |            |
|    | >[acetyl]acetyl(+M)=>CH <sub>3</sub> +CO(+M)  |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |            |
| 21 | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]   | 0.01863303 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |            |
|    | >[ipropyl]ipropyloo+C <sub>3</sub> H <sub>8</sub> =>ipropylooh+npropyl  |            |
| 30 | >[ipropylooh]ipropylooh=>ipropyloxy+OH>[ipropyloxy]   | 0.01820597 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |            |
|    | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+M=>CH <sub>2</sub> O+H+M                           |            |
|    | >[CH <sub>2</sub> O]CH <sub>3</sub> OO+CH <sub>2</sub> O=>CH <sub>3</sub> OOH+HCO   |            |
| 28 | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]   | 0.01679649 |
| -  |   |            |

|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|----|--|------------|
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |            |
|    | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+M=>CH <sub>2</sub> O+H+M  |            |
|    | >[CH <sub>2</sub> O]CH <sub>3</sub> CH <sub>2</sub> OO+CH <sub>2</sub> O=>CH <sub>3</sub> CH <sub>2</sub> OOH+HCO  |            |
| 40 | >[CH <sub>3</sub> CH <sub>2</sub> OOH]CH <sub>3</sub> CH <sub>2</sub> OOH=>ethoxy+OH>[ethoxy]  | 0.01621685 |
| 40 |  | 0.01021083 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[acetaldehyde]ipropyloo+acetaldehyde=>ipropylooh+acetyl   |            |
|    | >[ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
| 20 | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH             | 0.04540060 |
| 39 | >[CH <sub>3</sub> O]   | 0.01542369 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |            |
|    | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+O <sub>2</sub> =>CH <sub>2</sub> O+HO <sub>2</sub>                |            |
|    | >[CH <sub>2</sub> O]ipropyloo+CH <sub>2</sub> O=>ipropylooh+HCO  |            |
| 29 | >[ipropylooh]ipropylooh=>ipropyloxy+OH>[ipropyloxy]  | 0.01539811 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |            |
|    | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+M=>CH <sub>2</sub> O+H+M  |            |
|    | >[CH <sub>2</sub> O]npropyloo+CH <sub>2</sub> O=>npropylooh+HCO  |            |
| 41 | >[npropylooh]npropylooh=>npropyloxy+OH>[npropyloxy]  | 0.01479193 |
|    |  |            |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[acetaldehyde]npropyloo+acetaldehyde=>npropylooh+acetyl   |            |
| 22 | >[acetyl]acetyl(+M)=>CH <sub>3</sub> +CO(+M)>[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub>                                 | 0.0145054  |
| 33 | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]  | 0.0145854  |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH3+acetaldehyde  |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - |            |
|    | $->$ [C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +OH=>allyl+H <sub>2</sub> O>[allyl]allyl+HO <sub>2</sub> =>prod_2                                   |            |
| 18 | >[prod_2]prod_2=>allyloxy+OH>[allyloxy]  | 0.01408503 |
|    |  |            |

|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|----|--|------------|
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |            |
|    | >[ipropyl]ipropyloo+C <sub>3</sub> H <sub>8</sub> =>ipropylooh+npropyl   |            |
|    | >[npropyl]well_1=>OH+prod_1>[prod_1]prod_1=>frag_1+OH  |            |
|    | >[frag_1]frag_1=>vinoxy+CH <sub>2</sub> O>[vinoxy]vinoxy+O <sub>2</sub> =>CH <sub>2</sub> O+CO+OH  |            |
| 46 | >[CO]  | 0.01393757 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |            |
|    | >[ipropyl]ipropyloo+C <sub>3</sub> H <sub>8</sub> =>ipropylooh+npropyl   |            |
|    | >[npropyl]well_1=>OH+prod_1>[prod_1]prod_1=>frag_1+OH  |            |
| 45 | >[frag_1]  | 0.01393738 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |            |
|    | >[ipropyl]ipropyloo+C <sub>3</sub> H <sub>8</sub> =>ipropylooh+npropyl   |            |
| 44 | >[npropyl]well_1=>OH+prod_1>[prod_1]   | 0.01393584 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub>   |            |
|    | >[acetyl]acetylperoxy+HO <sub>2</sub> =>CH <sub>3</sub> CO <sub>3</sub> H+O <sub>2</sub>   |            |
| 10 | >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  | 0.0134568  |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |            |
|    | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+O <sub>2</sub> =>CH <sub>2</sub> O+HO <sub>2</sub>                |            |
|    | >[CH <sub>2</sub> O]CH <sub>3</sub> CH <sub>2</sub> OO+CH <sub>2</sub> O=>CH <sub>3</sub> CH <sub>2</sub> OOH+HCO  |            |
|    | >[CH <sub>3</sub> CH <sub>2</sub> OOH]CH <sub>3</sub> CH <sub>2</sub> OOH=>ethoxy+OH>[ethoxy]ethoxy=>CH <sub>3</sub> +CH <sub>2</sub> O-                               |            |
|    | ->[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH            |            |
| 66 | >[CH <sub>3</sub> O]   | 0.01224771 |
|    |  |            |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - |            |
| 12 | ->[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +HO <sub>2</sub> =>propen1ol+OH>[propen1ol]  | 0.01222806 |

|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|-----|--|------------|
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|     | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl                                      |            |
|     | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+M=>CH <sub>2</sub> O+H+M          |            |
|     | >[CH <sub>2</sub> O]ipropyloo+CH <sub>2</sub> O=>ipropylooh+HCO  |            |
| 42  | >[ipropylooh]ipropylooh=>ipropyloxy+OH>[ipropyloxy]  | 0.01201207 |
|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|     | >[acetaldehyde]ipropyloo+acetaldehyde=>ipropylooh+acetyl   |            |
|     | >[acetyl]acetyl(+M)=>CH <sub>3</sub> +CO(+M)>[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> |            |
| 50  | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]  | 0.01164393 |
|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|     | >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub>   |            |
|     | >[acetyl]H <sub>2</sub> O <sub>2</sub> +acetylperoxy=>HO <sub>2</sub> +CH <sub>3</sub> CO <sub>3</sub> H                               |            |
| 11  | >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  | 0.0111979  |
|     | <pre>[ipropylooh]ipropylooh=&gt;ipropyloxy+OH</pre>  |            |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|     | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl>[npropyl]well_1=>OH+prod_1-          |            |
|     | ->[prod_1]prod_1=>frag_1+OH>[frag_1]frag_1=>vinoxy+CH <sub>2</sub> O   |            |
|     | >[CH <sub>2</sub> O]CH <sub>3</sub> CH <sub>2</sub> OO+CH <sub>2</sub> O=>CH <sub>3</sub> CH <sub>2</sub> OOH+HCO                      |            |
| 88  | >[CH <sub>3</sub> CH <sub>2</sub> OOH]CH <sub>3</sub> CH <sub>2</sub> OOH=>ethoxy+OH>[ethoxy]  | 0.01058769 |
|     |  |            |
|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|     | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl>[npropyl]well_1=>OH+prod_1-          |            |
|     | ->[prod_1]prod_1=>frag_1+OH>[frag_1]frag_1=>vinoxy+CH <sub>2</sub> O   |            |
| 7.0 | >[CH <sub>2</sub> O]CH <sub>3</sub> OO+CH <sub>2</sub> O=>CH <sub>3</sub> OOH+HCO  | 0.01054735 |
| 70  | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]  | 0.01034733 |
|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|     | >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub>   |            |
|     | >[acetyl]acetyl(+M)=>CH <sub>3</sub> +CO(+M)   |            |
| 35  | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+acetaldehyde=>CH <sub>3</sub> OOH+acetyl   | 0.00984076 |
| 33  | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]  | 0.00304070 |

|    | [inconvlooh]inconvlooh=xinconvloon=(OL)   | 1          |
|----|---|------------|
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |            |
|    | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+M=>CH <sub>2</sub> O+H+M                               |            |
|    | >[CH <sub>2</sub> O]CH <sub>3</sub> CH <sub>2</sub> OO+CH <sub>2</sub> O=>CH <sub>3</sub> CH <sub>2</sub> OOH+HCO   |            |
|    | >[CH <sub>3</sub> CH <sub>2</sub> OOH]CH <sub>3</sub> CH <sub>2</sub> OOH=>ethoxy+OH>[ethoxy]ethoxy=>CH <sub>3</sub> +CH <sub>2</sub> O-                    |            |
|    | ->[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH |            |
| 78 | >[CH <sub>3</sub> O]  | 0.0095488  |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|    |   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl>[npropyl]well_1=>OH+prod_1-                               |            |
|    | ->[prod_1]prod_1=>frag_1+OH>[frag_1]frag_1=>vinoxy+CH <sub>2</sub> O  |            |
|    | >[CH <sub>2</sub> O]npropyloo+CH <sub>2</sub> O=>npropylooh+HCO   |            |
| 96 | >[npropylooh]npropylooh=>npropyloxy+OH>[npropyloxy]   | 0.00932816 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |            |
|    | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+O <sub>2</sub> =>CH <sub>2</sub> O+HO <sub>2</sub>     |            |
|    | >[CH <sub>2</sub> O]ipropyloo+CH <sub>2</sub> O=>ipropylooh+HCO   |            |
|    | >[ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH3+acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH  |            |
| 90 | >[CH <sub>3</sub> O]  | 0.00917882 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|    | >[ipropyloxy]ipropyloxy=>CH3+acetaldehyde   |            |
|    | >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub>  |            |
|    | >[acetyl]acetylperoxy+HO <sub>2</sub> =>CH <sub>3</sub> CO <sub>3</sub> H+O <sub>2</sub>  |            |
|    | >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH   |            |
|    | >[acetyloxy]acetyloxy+M=>CH <sub>3</sub> +CO <sub>2</sub> +M  |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH  |            |
| 34 | >[CH <sub>3</sub> O]  | 0.00846587 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl   |            |
|    | >[npropyl]npropyloo+C <sub>3</sub> H <sub>8</sub> =>npropylooh+ipropyl  |            |
| 75 | >[npropylooh]npropylooh=>npropyloxy+OH>[npropyloxy]   | 0.00812706 |
| /3 | >[iibioblioui]iibiobliooii->iibiobliox\+Oii>[iibiobliox\]   | 0.00012700 |

|   |   | 1          |
|---|---|------------|
|   | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|   | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|   | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl>[npropyl]well_1=>OH+prod_1-   |            |
|   | ->[prod_1]prod_1=>frag_1+OH>[frag_1]frag_1=>vinoxy+CH <sub>2</sub> O  |            |
|   | >[CH <sub>2</sub> O]ipropyloo+CH <sub>2</sub> O=>ipropylooh+HCO   |            |
| 9 | 1 >[ipropylooh]ipropylooh=>ipropyloxy+OH>[ipropyloxy]   | 0.00795324 |
|   | Consequence and in a second and  |            |
|   | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|   | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|   | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> = $>$ CH <sub>3</sub> OOH+ipropyl $>$ [ipropyl]ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> = $>$ CH <sub>3</sub> OOH+ipropyl $>$ [ipropyl]ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> = $>$ CH <sub>3</sub> OOH+ipropyl $>$ [ipropyl]ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyl]ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyl]ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyl]ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyl]ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyl]ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyl]ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - $>$ [ipropyloo= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - |            |
|   | $->[C3H6]C3H6+HO2=>allyl+H2O2>[allyl]allyl+HO2=>prod_2$   | 0.00707043 |
|   | 0 >[prod_2]prod_2=>allyloxy+OH>[allyloxy]   | 0.00787913 |
|   | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|   | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|   | >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub>  |            |
|   | >[acetyl]acetyl(+M)=>CH <sub>3</sub> +CO(+M)  |            |
|   | >[CH3]CH3OO+C3H8=>CH3OOH+npropyl  | 0.00722504 |
| 5 | 2 >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]   | 0.00723591 |
|   | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|   | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|   | >[acetaldehyde]CH <sub>3</sub> OO+acetaldehyde=>CH <sub>3</sub> OOH+acetyl  |            |
|   | >[acetyl]acetyl(+M)=>CH <sub>3</sub> +CO(+M)  |            |
|   | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+CH <sub>2</sub> O=>CH <sub>3</sub> OOH+HCO>[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH   |            |
| 7 | 7 >[CH <sub>3</sub> O]  | 0.00723567 |
|   | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|   | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|   | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl   |            |
|   | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+O <sub>2</sub> =>CH <sub>2</sub> O+HO <sub>2</sub>   |            |
|   | >[CH <sub>2</sub> O]CH <sub>3</sub> OO+CH <sub>2</sub> O=>CH <sub>3</sub> OOH+HCO   |            |
| 6 | 3 >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]   | 0.0071381  |
|   | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|   | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|   | >[acetaldehyde]npropyloo+acetaldehyde=>npropylooh+acetyl  |            |
|   | >[npropylooh]npropylooh=>npropyloxy+OH  |            |
|   | >[npropyloxy]npropyloxy=>C <sub>2</sub> H <sub>5</sub> +CH <sub>2</sub> O   |            |
|   | >[C <sub>2</sub> H <sub>5</sub> ]CH <sub>3</sub> CH <sub>2</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> CH <sub>2</sub> OOH+O <sub>2</sub>  |            |
| 6 | 8 >[CH <sub>3</sub> CH <sub>2</sub> OOH]CH <sub>3</sub> CH <sub>2</sub> OOH=>ethoxy+OH>[ethoxy]   | 0.00704482 |
| - |   |            |

|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|----|--|------------|
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl  |            |
|    | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+O <sub>2</sub> =>CH <sub>2</sub> O+HO <sub>2</sub>                |            |
|    | >[CH <sub>2</sub> O]CH <sub>3</sub> CH <sub>2</sub> OO+CH <sub>2</sub> O=>CH <sub>3</sub> CH <sub>2</sub> OOH+HCO  |            |
| 70 | >[CH <sub>3</sub> CH <sub>2</sub> OOH]CH <sub>3</sub> CH <sub>2</sub> OOH=>ethoxy+OH>[ethoxy]  | 0.00689832 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[acetaldehyde]CH <sub>3</sub> OO+acetaldehyde=>CH <sub>3</sub> OOH+acetyl   |            |
|    | >[acetyl]acetylperoxy+HO <sub>2</sub> =>CH <sub>3</sub> CO <sub>3</sub> H+O <sub>2</sub>   |            |
| 22 | >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  | 0.00675861 |
|    |  |            |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - |            |
| 17 | ->[C <sub>3</sub> H <sub>6</sub> ]HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> =>OH+propoxide>[propoxide]  | 0.00641717 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl  |            |
|    | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+O <sub>2</sub> =>CH <sub>2</sub> O+HO <sub>2</sub>                |            |
|    | >[CH <sub>2</sub> O]npropyloo+CH <sub>2</sub> O=>npropylooh+HCO  |            |
| 73 | >[npropylooh]npropylooh=>npropyloxy+OH>[npropyloxy]  | 0.00631319 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub>   |            |
|    | >[acetyl]H <sub>2</sub> O <sub>2</sub> +acetylperoxy=>HO <sub>2</sub> +CH <sub>3</sub> CO <sub>3</sub> H   |            |
|    | >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH  |            |
|    | >[acetyloxy]acetyloxy+M=>CH <sub>3</sub> +CO <sub>2</sub> +M   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH             |            |
| 37 | >[CH <sub>3</sub> O]   | 0.00611197 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub>   |            |
|    | >[acetyl]CH <sub>2</sub> O+acetylperoxy=>HCO+CH <sub>3</sub> CO <sub>3</sub> H   |            |
| 26 | >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  | 0.00569583 |

|     | [in novel and linear deals as in novel and OH  |             |
|-----|--|-------------|
|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |             |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |             |
|     | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl  |             |
|     | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+M=>CH <sub>2</sub> O+H+M  |             |
| 71  | >[CH <sub>2</sub> O]CH <sub>3</sub> OO+CH <sub>2</sub> O=>CH <sub>3</sub> OOH+HCO  | 0.005.00033 |
| /1  | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]  | 0.00560622  |
|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |             |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |             |
|     | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl  |             |
|     | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+M=>CH <sub>2</sub> O+H+M  |             |
|     | >[CH <sub>2</sub> O]CH <sub>3</sub> CH <sub>2</sub> OO+CH <sub>2</sub> O=>CH <sub>3</sub> CH <sub>2</sub> OOH+HCO  |             |
| 80  | >[CH <sub>3</sub> CH <sub>2</sub> OOH]CH <sub>3</sub> CH <sub>2</sub> OOH=>ethoxy+OH>[ethoxy]  | 0.00544104  |
|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |             |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |             |
|     | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl  |             |
|     | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+O <sub>2</sub> =>CH <sub>2</sub> O+HO <sub>2</sub>                |             |
|     | >[CH <sub>2</sub> O]ipropyloo+CH <sub>2</sub> O=>ipropylooh+HCO  |             |
| 72  | >[ipropylooh]ipropylooh=>ipropyloxy+OH>[ipropyloxy]  | 0.00509469  |
|     |  |             |
|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |             |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |             |
|     | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - |             |
| 32  | $->[C_3H_6]C_3H_6+OH=>allyl+H_2O>[allyl]allyl+HO_2=>allyloxy+OH>[allyloxy]$  | 0.00503292  |
|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |             |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |             |
|     | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl  |             |
|     | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+M=>CH <sub>2</sub> O+H+M  |             |
|     | >[CH <sub>2</sub> O]npropyloo+CH <sub>2</sub> O=>npropylooh+HCO  |             |
| 87  | >[npropylooh]npropylooh=>npropyloxy+OH>[npropyloxy]  | 0.00495175  |
|     | <pre>[ipropylooh]ipropylooh=&gt;ipropyloxy+OH</pre>  |             |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |             |
|     | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |             |
|     | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]C <sub>3</sub> H <sub>8</sub> +CH <sub>3</sub> O=>npropyl+CH <sub>3</sub> OH        |             |
| 27  | >[npropyl]well_1=>OH+prod_1>[prod_1]   | 0.00477189  |
| OZ. | \[ \link\ob\link\ou\] \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \  | 0.00477103  |

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[ipropylooh]ipropylooh=>ipropyloxy+OH--
    >[ipropyloxy]ipropyloxy=>CH<sub>3</sub>+acetaldehyde--
    >[CH<sub>3</sub>]CH<sub>3</sub>OO+C<sub>3</sub>H<sub>8</sub>=>CH<sub>3</sub>OOH+ipropyl--
    >[CH<sub>3</sub>OOH]CH<sub>3</sub>OOH=>CH<sub>3</sub>O+OH-->[CH<sub>3</sub>O]C<sub>3</sub>H<sub>8</sub>+CH<sub>3</sub>O=>npropyl+CH<sub>3</sub>OH--
    >[npropyl]well 1=>OH+prod 1-->[prod 1]prod 1=>frag 1+OH--
83 > [frag 1]
                                                                                                              0.00476572
    [ipropylooh]ipropylooh=>ipropyloxy+OH--
    >[ipropyloxy]ipropyloxy=>CH<sub>3</sub>+acetaldehyde--
    >[CH<sub>3</sub>]CH<sub>3</sub>OO+C<sub>3</sub>H<sub>8</sub>=>CH<sub>3</sub>OOH+ipropyl--
    >[CH<sub>3</sub>OOH]CH<sub>3</sub>OOH=>CH<sub>3</sub>O+OH-->[CH<sub>3</sub>O]C<sub>3</sub>H<sub>8</sub>+CH<sub>3</sub>O=>npropyl+CH<sub>3</sub>OH--
    >[npropyl]well 1=>OH+prod 1-->[prod 1]prod 1=>frag 1+OH--
    >[frag_1]frag_1=>vinoxy+CH<sub>2</sub>O-->[vinoxy]vinoxy+O<sub>2</sub>=>CH<sub>2</sub>O+CO+OH--
84 > [CO]
                                                                                                              0.00475205
    [ipropylooh]ipropylooh=>ipropyloxy+OH--
    >[ipropyloxy]ipropyloxy=>CH<sub>3</sub>+acetaldehyde--
    >[CH<sub>3</sub>]CH<sub>3</sub>OO+C<sub>3</sub>H<sub>8</sub>=>CH<sub>3</sub>OOH+npropyl--
    >[npropyl]npropyloo+C<sub>3</sub>H<sub>8</sub>=>npropylooh+npropyl--
69 > [npropylooh] npropylooh => npropyloxy + OH--> [npropyloxy]
                                                                                                              0.00473997
    [ipropylooh]ipropylooh=>ipropyloxy+OH--
    >[ipropyloxy]ipropyloxy=>CH<sub>3</sub>+acetaldehyde--
    >[CH<sub>3</sub>]CH<sub>3</sub>OO+C<sub>3</sub>H<sub>8</sub>=>CH<sub>3</sub>OOH+npropyl--
    >[npropyl]well 1=>HO<sub>2</sub>+prod 2-->[prod 2]prod 2=>allyloxy+OH--
55 > [allyloxy]
                                                                                                              0.00467136
    [ipropylooh]ipropylooh=>ipropyloxy+OH--
    >[ipropyloxy]ipropyloxy=>CH<sub>3</sub>+acetaldehyde--
    >[acetaldehyde]CH<sub>3</sub>OO+acetaldehyde=>CH<sub>3</sub>OOH+acetyl--
    >[acetyl]acetylperoxy+HO<sub>2</sub>=>CH<sub>3</sub>CO<sub>3</sub>H+O<sub>2</sub>--
    >[CH<sub>3</sub>CO<sub>3</sub>H]CH<sub>3</sub>CO<sub>3</sub>H=>acetyloxy+OH--
    >[acetyloxy]acetyloxy+M=>CH<sub>3</sub>+CO<sub>2</sub>+M--
    >[CH<sub>3</sub>]CH<sub>3</sub>OO+HO<sub>2</sub>=>CH<sub>3</sub>OOH+O<sub>2</sub>-->[CH<sub>3</sub>OOH]CH<sub>3</sub>OOH=>CH<sub>3</sub>O+OH--
99 > [CH<sub>3</sub>O]
                                                                                                              0.00425056
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|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|----|--|------------|
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl  |            |
|    | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]CH <sub>3</sub> O+M=>CH <sub>2</sub> O+H+M  |            |
|    | >[CH <sub>2</sub> O]ipropyloo+CH <sub>2</sub> O=>ipropylooh+HCO  |            |
| 89 | >[ipropylooh]ipropylooh=>ipropyloxy+OH>[ipropyloxy]  | 0.00396833 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[acetaldehyde]CH <sub>3</sub> OO+acetaldehyde=>CH <sub>3</sub> OOH+acetyl   |            |
|    | >[acetyl]H <sub>2</sub> O <sub>2</sub> +acetylperoxy=>HO <sub>2</sub> +CH <sub>3</sub> CO <sub>3</sub> H   |            |
| 43 | >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  | 0.00348654 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub>   |            |
|    | >[acetyl]CH <sub>2</sub> O+acetylperoxy=>HCO+CH <sub>3</sub> CO <sub>3</sub> H   |            |
|    | >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH  |            |
|    | >[acetyloxy]acetyloxy+M=>CH <sub>3</sub> +CO <sub>2</sub> +M   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH             |            |
| 98 | >[CH <sub>3</sub> O]   | 0.00329302 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - |            |
|    | ->[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +HO <sub>2</sub> =>allyl+H <sub>2</sub> O <sub>2</sub> >[allyl]allyl+HO <sub>2</sub> =>allyloxy+OH     |            |
| 49 | >[allyloxy]  | 0.00314145 |
|    |  |            |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[acetaldehyde]acetaldehyde+H=>acetyl+H <sub>2</sub>   |            |
|    | >[acetyl]acetyl(+M)=>CH <sub>3</sub> +CO(+M)>[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub>                                 |            |
| 64 | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]  | 0.00305523 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub>   |            |
|    | >[acetyl]acetyl(+M)=>CH <sub>3</sub> +CO(+M)>[CH <sub>3</sub> ]CH <sub>3</sub> +HO <sub>2</sub> =>CH <sub>3</sub> O+OH   |            |
| 56 | >[CH <sub>3</sub> O]   | 0.00298237 |

|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|----|--|------------|
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub>   |            |
|    | >[acetyl]C <sub>3</sub> H <sub>8</sub> +acetylperoxy=>ipropyl+CH <sub>3</sub> CO <sub>3</sub> H  |            |
| 51 | >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  | 0.00294338 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[acetaldehyde]acetaldehyde+acetylperoxy=>acetyl+CH <sub>3</sub> CO <sub>3</sub> H   |            |
| 24 | >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  | 0.00293333 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> -           |            |
|    | ->[C <sub>3</sub> H <sub>6</sub> ]HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> =>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide   |            |
| 25 | >[propoxide]   | 0.00283783 |
|    |  |            |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |            |
|    | >[ipropyl]O <sub>2</sub> +ipropyl=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> >[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +OH=>allyl+H <sub>2</sub> O     |            |
| 60 | >[allyl]allyl+HO <sub>2</sub> =>prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy]  | 0.00270623 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH                       |            |
| 61 | >[CH <sub>3</sub> O]   | 0.00241521 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[acetaldehyde]npropyloo+acetaldehyde=>npropylooh+acetyl   |            |
|    | >[acetyl]acetylperoxy+HO <sub>2</sub> =>CH <sub>3</sub> CO <sub>3</sub> H+O <sub>2</sub>   |            |
| 58 | >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  | 0.00238186 |
|    | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |            |
|    | >[ipropyl]O <sub>2</sub> +ipropyl=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> >[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +HO <sub>2</sub> =>propen1ol+OH |            |
| 38 | >[propen1ol]   | 0.00233744 |

|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|-----|--|------------|
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|     | >[acetaldehyde]ipropyloo+acetaldehyde=>ipropylooh+acetyl   |            |
|     | >[acetyl]acetylperoxy+HO <sub>2</sub> =>CH <sub>3</sub> CO <sub>3</sub> H+O <sub>2</sub>   |            |
| 59  | >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  | 0.00228219 |
|     | fing and a phing and a characteristic of the   |            |
|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|     | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - |            |
| 0.0 | $->[C_3H_6]H+C_3H_6=>npropyl>[npropyl]well_1=>OH+prod_1$   | 0.00222704 |
| 86  | >[prod_1]prod_1=>frag_1+OH>[frag_1]  | 0.00223704 |
|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|     | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - |            |
|     | $->[C_3H_6]H+C_3H_6=>npropyl>[npropyl]well_1=>OH+prod_1$   |            |
|     | >[prod_1]prod_1=>frag_1+OH>[frag_1]frag_1=>vinoxy+CH <sub>2</sub> O  |            |
| 93  | >[vinoxy]vinoxy+O <sub>2</sub> =>CH <sub>2</sub> O+CO+OH>[CO]  | 0.00222972 |
|     |  |            |
|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|     | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> - |            |
| 85  | ->[C <sub>3</sub> H <sub>6</sub> ]H+C <sub>3</sub> H <sub>6</sub> =>npropyl>[npropyl]well_1=>OH+prod_1>[prod_1]  | 0.00222191 |
|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|     | >[acetaldehyde]CH <sub>3</sub> OO+acetaldehyde=>CH <sub>3</sub> OOH+acetyl   |            |
|     | >[acetyl]CH <sub>2</sub> O+acetylperoxy=>HCO+CH <sub>3</sub> CO <sub>3</sub> H   |            |
| 95  | >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  | 0.00217094 |
|     |  |            |
|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|     | >[acetaldehyde]acetaldehyde+OH=>acetyl+H <sub>2</sub> O  |            |
|     | >[acetyl]acetyl(+M)=>CH <sub>3</sub> +CO(+M)>[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub>                                 |            |
| 79  | >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH>[CH <sub>3</sub> O]  | 0.00214042 |
|     | [ipropylooh]ipropylooh=>ipropyloxy+OH  |            |
|     | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |            |
|     | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl  |            |
| 36  | >[npropyl]npropyloo=>OH+propoxide>[propoxide]  | 0.00204683 |

| Spropyloxy propyloxy=>CH3+acetaldehyde-  |    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|--|----|---|------------|
| >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub> >  acetyl]C <sub>3</sub> H <sub>8</sub> +acetylperoxy=>npropyl+CH <sub>3</sub> CO <sub>3</sub> H   55   [CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]   0.00194655     [ipropylooh]ipropylooh=>ipropyloxy+OH>   [ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde>   (acetaldehyde]acetaldehyde+acetylperoxy=>acetyl+CH <sub>3</sub> CO <sub>3</sub> H>   (CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>  (acetyloxy)acetyloxy+M=>CH <sub>3</sub> +CO <sub>2</sub> +M>   (CH <sub>3</sub> CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH9   7   (CH <sub>3</sub> O)   0.0017788     [ipropylooh]ipropylooh=>ipropyloxy+OH>  [ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde>  (acetylacetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub> >  (acetylacetaldehyde+HO <sub>2</sub> =>acetyl+CH <sub>3</sub> CO <sub>3</sub> H>  (CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]   0.00159011     [ipropylooh]ipropylooh=>ipropyloxy+OH>  [ipropylooh]ipropylooh=>ipropyloxy+OH>  (acetylacetaldehyde+C>  (CH <sub>3</sub> CO <sub>3</sub> O+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl->[ipropyl]ipropyloo=>QOOH_3  (acetylacetaldehyde>  (CH <sub>3</sub> CO <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>  [ipropylooh]ipropylooh=>ipropyloxy+OH>  [ipropylooh]ipropylooh=>ipropyloxy+OH>  (aliy)ally+HO <sub>2</sub> ->prod 2->[CH <sub>3</sub> CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>  (aliy)ally+HO <sub>2</sub> ->prod 2->[prod 2]prod 2=>allyloxy+OH>  [ipropylooh]ipropylooh=>ipropyloxy+OH>  (aliy)ally+HO <sub>2</sub> ->prod 2->[CH <sub>3</sub> CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl>  (aliy)ally+HO <sub>2</sub> ->prod 2->[CH <sub>3</sub> CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl>  (aliy)ally+Popylooh]ipropylooh=>ipropyloxy+OH>  (aliy)ally+Popylooh)ipropylooh=>ipropyloxy+OH>  (aliy)ally+Popylooh=>ipropyloxy+OH>  (aliy)ally+Popylooh=  (aliy)ally+Popylooh=  (aliy)ally+Popylooh=  (aliy)ally+Popylooh=   |    |   |            |
| >[acetyl]C <sub>3</sub> H <sub>8</sub> +acetylperoxy=>npropyl+CH <sub>3</sub> CO <sub>3</sub> H 55 >[CH <sub>2</sub> CO <sub>3</sub> H]CH <sub>2</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  [ipropylooh]ipropylooh=>ipropyloxy+OH>[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde>[acetaldehyde]acetaldehyde+acetylperoxy=>acetyl+CH <sub>3</sub> CO <sub>3</sub> H>[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]acetyloxy+M=>CH <sub>3</sub> +CO <sub>2</sub> +M>[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[CH <sub>3</sub> CO]CH <sub>3</sub> CO]CO]CH <sub>3</sub> CO]CH <sub>3</sub> |    | -   |            |
| 65   \[ \text{CH}_3\text{CO}_3\text{H} \text{-\alpha} \text{costyloxy} \]   0.00194655   |    |   |            |
| [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[acetaldehyde]acetaldehyde+acetylperoxy=>acetyl+CH <sub>3</sub> CO <sub>3</sub> H >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH >[acetyloxy]acetyloxy+M=>CH <sub>3</sub> +CO <sub>2</sub> +M >[CH <sub>3</sub> OH]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH  97 >[CH <sub>3</sub> O] 0.0017788  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[acetyl]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub> >[acetyl]acetaldehyde+acetylperoxy=>acetyl+CH <sub>3</sub> CO <sub>3</sub> H  48 >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy] 0.00159011  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl->[ipropyl]ipropyloo=>QOOH_3  47 >[QOOH_3]QOOH_3=>OH+propoxide>[propoxide] 0.00158287  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+propyl >[npropyl]npropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+propyl >[npropyl]npropyloxy=>CH <sub>3</sub> +acetaldehyde >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetal  | 65 |   | 0.00104655 |
| >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[acetaldehyde]acetaldehyde+acetylperoxy=>acetyl+CH <sub>3</sub> CO <sub>3</sub> H >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH >[acetyloxy]acetyloxy+M=>CH <sub>3</sub> +CO <sub>2</sub> +M >[CH <sub>3</sub> CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH 97 >[CH <sub>3</sub> O]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub> >[acetyl]acetaldehyde+acetylperoxy=>acetyl+CH <sub>3</sub> CO <sub>3</sub> H  48 >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  [ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl->[ipropyl]ipropyloo=>QOOH_3  47 >[QOOH_3]QOOH_3=>OH+propoxide>[propoxide]  (ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   | 03 |   | 0.00194655 |
| >[acetaldehyde]acetaldehyde+acetylperoxy=>acetyl+CH <sub>3</sub> CO <sub>3</sub> H- >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH >[acetyloxy]acetyloxy+M=>CH <sub>3</sub> +CO <sub>2</sub> +M >[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH 97 >[CH <sub>3</sub> O] 0.0017788  [ipropylox]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[ipropylox]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub> >[acetyl]acetaldehyde+acetylperoxy=>acetyl+CH <sub>3</sub> CO <sub>3</sub> H 48 >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy] 0.00159011  [ipropylox]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl->[ipropyl]ipropyloo=>QOOH_3 47 >[QOOH_3]QOOH_3=>OH+propoxide>[propoxide] 0.00158287  [ipropylox]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropylox]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropylox]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide- 53 -[propoxide] 0.00143195  [ipropylox]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[ipropylox]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |    |   |            |
| >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH >[acetyloxy]acetyloxy+M=>CH <sub>3</sub> +CO <sub>2</sub> +M >[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH 97 >[CH <sub>3</sub> O] 0.0017788  [ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub> >[acetyl]acetaldehyde+acetylperoxy=>acetyl+CH <sub>3</sub> CO <sub>3</sub> H 48 >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>2</sub> =>CH <sub>3</sub> OOH+ipropyl->[ipropyl]ipropyloo=>QOOH_3 47 >[QOOH_3]QOOH_3=>OH+propoxide>[propoxide] 0.00158287  [ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[ipropyloxy]ipropylox=>CH <sub>3</sub> +acetaldehyde >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde   |    |   |            |
| >[acetyloxy]acetyloxy+M=>CH <sub>3</sub> +CO <sub>2</sub> +M >[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH 97 >[CH <sub>3</sub> O] [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub> >[acetyl]acetaldehyde+acetylperoxy=>acetyl+CH <sub>3</sub> CO <sub>3</sub> H 48 >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>QOOH_3 47 >[QOOH_3]QOOH_3=>OH+propoxide>[propoxide]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide>[propyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[ipropyloxy]ipropyloo+>ipropyloxy+OH >[ipropyloxy]ipropyloo+>ipropyloxy+OH>[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde>[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde>[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde>[ipropyloxy]ipropyloxy=  |    |   |            |
| S[CH <sub>3</sub> ]CH <sub>3</sub> OO+HO <sub>2</sub> =>CH <sub>3</sub> OOH+O <sub>2</sub> >[CH <sub>3</sub> OOH]CH <sub>3</sub> OOH=>CH <sub>3</sub> O+OH   |    |   |            |
| Section  |    |   |            |
| [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub> >[acetyl]acetaldehyde+acetylperoxy=>acetyl+CH <sub>3</sub> CO <sub>3</sub> H 48 >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ICH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>QOOH_3 47 >[QOOH_3]QOOH_3=>OH+propoxide>[propoxide]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ICH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyl]O <sub>2</sub> +ipropyl=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> >[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +HO <sub>2</sub> =>allyl+H <sub>2</sub> O <sub>2</sub> 74 >[allyl]allyl+HO <sub>2</sub> =>prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ICH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide>[propyloxy]ipropylooh=>ipropyloxy+OH>[ipropyloxy]ipropylooh=>ipropyloxy+OH>[ipropyloxy]ipropylooh=>ipropyloxy+OH>[ipropyloxy]ipropylooh=>ipropyloxy+OH>[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde>[CH <sub>3</sub> ICH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde>[CH <sub>3</sub> ICH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde>[CH <sub>3</sub> ICH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde>[CH <sub>3</sub> ICH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |    |   |            |
| >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub> >[acetyl]acetaldehyde+acetylperoxy=>acetyl+CH <sub>3</sub> CO <sub>3</sub> H  48 >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  0.00159011  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>QOOH_3 47 >[QOOH_3]QOOH_3=>OH+propoxide>[propoxide]  0.00158287  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyl]O <sub>2</sub> +ipropyl=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> >[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +HO <sub>2</sub> =>allyl+H <sub>2</sub> O <sub>2</sub> 74 >[allyl]allyl+HO <sub>2</sub> =>prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide- 53 ->[propoxide]  [ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   | 97 | >[CH <sub>3</sub> O]  | 0.0017788  |
| >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub> >[acetyl]acetaldehyde+acetylperoxy=>acetyl+CH <sub>3</sub> CO <sub>3</sub> H 48 >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OO++ipropyl>[ipropyl]ipropyloo=>QOOH_3 47 >[QOOH_3]QOOH_3=>OH+propoxide>[propoxide]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OO+H+ipropyl >[ipropyl]O <sub>2</sub> +ipropyl=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> >[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +HO <sub>2</sub> =>allyl+H <sub>2</sub> O <sub>2</sub> 74 >[allyl]allyl+HO <sub>2</sub> =>prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropylooh=>ipropyloxy+OH >[ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde>[cH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
| >[acetyl]acetaldehyde+acetylperoxy=>acetyl+CH <sub>3</sub> CO <sub>3</sub> H 48 >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>QOOH_3 47 >[QOOH_3]QOOH_3=>OH+propoxide>[propoxide]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyl]O <sub>2</sub> +ipropyl=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> >[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +HO <sub>2</sub> =>allyl+H <sub>2</sub> O <sub>2</sub> 74 >[allyl]allyl+HO <sub>2</sub> =>prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+propyl >[propyloh]ipropylooh=>ipropyloxy+OH >[ipropyloh]ipropylooh=>ipropyloxy+OH >[ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
| 48 >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ICH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>QOOH_3  47 >[QOOH_3]QOOH_3=>OH+propoxide>[propoxide]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ICH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyl]O <sub>2</sub> +ipropyl=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> >[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +HO <sub>2</sub> =>allyl+H <sub>2</sub> O <sub>2</sub> 74 >[allyl]allyl+HO <sub>2</sub> =>prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ICH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[propoxide]  [ipropyloxy]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ICH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |    | >[acetaldehyde]acetaldehyde+HO <sub>2</sub> =>acetyl+H <sub>2</sub> O <sub>2</sub>  |            |
| [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>QOOH_3 47 >[QOOH_3]QOOH_3=>OH+propoxide>[propoxide]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyl]O <sub>2</sub> +ipropyl=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> >[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +HO <sub>2</sub> =>allyl+H <sub>2</sub> O <sub>2</sub> 74 >[allyl]allyl+HO <sub>2</sub> =>prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropylooh=>ipropyloxy+OH >[ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |    | >[acetyl]acetaldehyde+acetylperoxy=>acetyl+CH <sub>3</sub> CO <sub>3</sub> H  |            |
| >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde>[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>QOOH_3   | 48 | >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]   | 0.00159011 |
| >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde>[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>QOOH_3   |    |   |            |
| >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>QOOH_3 47 >[QOOH_3]QOOH_3=>OH+propoxide>[propoxide] 0.00158287  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyl]O <sub>2</sub> +ipropyl=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> >[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +HO <sub>2</sub> =>allyl+H <sub>2</sub> O <sub>2</sub> 74 >[allyl]allyl+HO <sub>2</sub> =>prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy] 0.00152168  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide- 53 ->[propoxide] 0.00143195  [ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
| 47 >[QOOH_3]QOOH_3=>OH+propoxide>[propoxide]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyl]O <sub>2</sub> +ipropyl=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> >[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +HO <sub>2</sub> =>allyl+H <sub>2</sub> O <sub>2</sub> 74 >[allyl]allyl+HO <sub>2</sub> =>prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide- 53 ->[propoxide]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
| [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyl]O <sub>2</sub> +ipropyl=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> >[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +HO <sub>2</sub> =>allyl+H <sub>2</sub> O <sub>2</sub> 74 >[allyl]allyl+HO <sub>2</sub> =>prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy] 0.00152168  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide- 53 ->[propoxide] 0.00143195  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl>[ipropyl]ipropyloo=>QOOH_3  |            |
| >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyl]O <sub>2</sub> +ipropyl=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> >[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +HO <sub>2</sub> =>allyl+H <sub>2</sub> O <sub>2</sub> 74 >[allyl]allyl+HO <sub>2</sub> =>prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy] 0.00152168  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide- 53 ->[propoxide] 0.00143195  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   | 47 | >[QOOH_3]QOOH_3=>OH+propoxide>[propoxide]   | 0.00158287 |
| >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl >[ipropyl]O <sub>2</sub> +ipropyl=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> >[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +HO <sub>2</sub> =>allyl+H <sub>2</sub> O <sub>2</sub> 74 >[allyl]allyl+HO <sub>2</sub> =>prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy] 0.00152168  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide- 53 ->[propoxide] 0.00143195  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |    |   |            |
| $ > [CH_3]CH_3OO + C_3H_8 = > CH_3OOH + ipropyl - \\ > [ipropyl]O_2 + ipropyl = > HO_2 + C_3H_6 - > [C_3H_6]C_3H_6 + HO_2 = > allyl + H_2O_2 - \\ > [allyl]allyl + HO_2 = > prod_2 - > [prod_2]prod_2 = > allyloxy + OH > [allyloxy]                                    $  |    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
| >[ipropyl]O <sub>2</sub> +ipropyl=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> >[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +HO <sub>2</sub> =>allyl+H <sub>2</sub> O <sub>2</sub> 74 >[allyl]allyl+HO <sub>2</sub> =>prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy] 0.00152168  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide- 53 ->[propoxide] 0.00143195  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
| 74 >[allyl]allyl+HO <sub>2</sub> =>prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy] 0.00152168  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide- 53 ->[propoxide] 0.00143195  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |            |
| [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide- 53 ->[propoxide]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |    | >[ipropyl]O <sub>2</sub> +ipropyl=>HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> >[C <sub>3</sub> H <sub>6</sub> ]C <sub>3</sub> H <sub>6</sub> +HO <sub>2</sub> =>allyl+H <sub>2</sub> O <sub>2</sub> |            |
| >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide- 53 ->[propoxide] 0.00143195 [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  | 74 | >[allyl]allyl+HO <sub>2</sub> =>prod_2>[prod_2]prod_2=>allyloxy+OH>[allyloxy]   | 0.00152168 |
| >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide- 53 ->[propoxide]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
| >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide-<br>53 ->[propoxide] 0.00143195<br>[ipropylooh]ipropylooh=>ipropyloxy+OH<br>>[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde<br>>[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
| 53 ->[propoxide]  [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl   |            |
| [ipropylooh]ipropylooh=>ipropyloxy+OH >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |    | >[npropyl]npropyloo=>QOOH_2>[QOOH_2]QOOH_2=>OH+propoxide-   |            |
| >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde<br>>[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  | 53 | ->[propoxide]   | 0.00143195 |
| >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl  |    | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|  |    | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
| 54 >[ipropyl]ipropyloo=>OH+propoxide>[propoxide] 0.0014249   |    | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |            |
|  | 54 | >[ipropyl]ipropyloo=>OH+propoxide>[propoxide]   | 0.0014249  |

|          | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|----------|---|------------|
|          | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|          | >[acetaldehyde]npropyloo+acetaldehyde=>npropylooh+acetyl  |            |
|          | >[acetyl]H <sub>2</sub> O <sub>2</sub> +acetylperoxy=>HO <sub>2</sub> +CH <sub>3</sub> CO <sub>3</sub> H  |            |
| 81       | >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]   | 0.00124722 |
|          | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|          | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|          | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |            |
|          | >[ipropyl]O <sub>2</sub> +ipropyl= $>$ HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> $>$ [C <sub>3</sub> H <sub>6</sub> ]HO <sub>2</sub> +C <sub>3</sub> H <sub>6</sub> = $>$ OH+propoxide |            |
| 57       | >[propoxide]  | 0.00123391 |
|          | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|          | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|          | >[acetaldehyde]ipropyloo+acetaldehyde=>ipropylooh+acetyl  |            |
|          | >[acetyl]H <sub>2</sub> O <sub>2</sub> +acetylperoxy=>HO <sub>2</sub> +CH <sub>3</sub> CO <sub>3</sub> H  |            |
| 100      | >[CH <sub>3</sub> CO <sub>3</sub> H]CH <sub>3</sub> CO <sub>3</sub> H=>acetyloxy+OH>[acetyloxy]   | 0.00096153 |
|          | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|          | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|          | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |            |
| 67       | >[ipropyl]O <sub>2</sub> +ipropyl=>OH+propoxide>[propoxide]   | 0.00081264 |
|          | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|          | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|          | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+npropyl   |            |
|          | >[npropyl]npropyloo=>HO2+C3H6>[C3H6]C3H6+HO2=>propen1ol+OH  |            |
| 92       | >[propen1ol]  | 0.00067878 |
|          | [ipropylooh]ipropylooh=>ipropyloxy+OH   |            |
|          | >[ipropyloxy]ipropyloxy=>CH <sub>3</sub> +acetaldehyde  |            |
|          | >[CH <sub>3</sub> ]CH <sub>3</sub> OO+C <sub>3</sub> H <sub>8</sub> =>CH <sub>3</sub> OOH+ipropyl   |            |
|          | $>[ipropyl]O_2+ipropyl=>HO_2+C_3H_6>[C_3H_6]HO_2+C_3H_6=>QOOH_2$  |            |
| 94       | >[QOOH_2]QOOH_2=>OH+propoxide>[propoxide]   | 0.00055051 |
| <u> </u> |   | •          |