# Supporting Information

# A comparative Study of Two Quantum Chemical Descriptors in Predicting Toxicity of Aliphatic Compounds Towards *Tetrahymena Pyriformis*

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**Table S1.** Calculated HOMO energies, LUMO energies, ionization energies, electron affinities, electronegativities, hardness and chemical potential of aliphatic electron acceptors

| **Molecule** | **HOMO**(au) | **LUMO**(au) | **I**(eV) | **A**(eV) | **χ**(eV) | **η**(eV) | **ω**(eV) | **μ**(eV) |
|---|---|---|---|---|---|---|---|---|
| **Diols** | | | | | | | | |
| (+/-)-1,2-butanediol | -0.4267 | 0.1504 | 11.6097 | -4.0917 | 3.7590 | 15.7014 | 0.4500 | 4.0918 |
| (+/-)-1,3-butanediol | -0.4303 | 0.1491 | 11.7098 | -4.0569 | 3.8264 | 15.7667 | 0.4643 | 4.0569 |
| 1,4-butanediol | -0.4362 | 0.1573 | 11.8682 | -4.2798 | 3.7942 | 16.1479 | 0.4458 | 4.2798 |
| 1,2-pentanediol | -0.4251 | 0.1506 | 11.5678 | -4.0972 | 3.7353 | 15.6649 | 0.4453 | 4.0972 |
| 1,5-pentanediol | -0.4365 | 0.1548 | 11.8777 | -4.2115 | 3.8331 | 16.0892 | 0.4566 | 4.2115 |
| 2-methyl-2,4-pentanediol | -0.4215 | 0.1448 | 11.4690 | -3.9388 | 3.7651 | 15.4078 | 0.4600 | 3.9388 |
| (+/-)-1,2-hexanediol | -0.4247 | 0.1505 | 11.5555 | -4.0964 | 3.7296 | 15.6519 | 0.4443 | 4.0964 |
| 1,6-hexanediol | -0.4370 | 0.1564 | 11.8905 | -4.2550 | 3.8177 | 16.1455 | 0.4514 | 4.2550 |
| 1,2-decanediol | -0.4198 | 0.1507 | 11.4238 | -4.0994 | 3.6622 | 15.5232 | 0.432 | 4.0994 |
| 1,10-decanediol | -0.4280 | 0.1562 | 11.6450 | -4.2515 | 3.6968 | 15.8965 | 0.4298 | 4.2515 |
| **Halogenated alcohols** | | | | | | | | |
| 2-bromoethanol | -0.4014 | 0.1301 | 10.9220 | -3.5394 | 3.6913 | 14.4614 | 0.4711 | 3.5394 |
| 2-chloroethanol | -0.4370 | 0.1398 | 11.8918 | -3.8033 | 4.0443 | 15.6951 | 0.5211 | 3.8033 |
| 1-chloro-2-propanol | -0.4266 | 0.1364 | 11.6086 | -3.7124 | 3.9481 | 15.321 | 0.5087 | 3.7124 |
| 3-chloro-1-propanol | -0.4318 | 0.1403 | 11.7503 | -3.8177 | 3.9663 | 15.5681 | 0.5053 | 3.8177 |
| 4-chloro-1-butanol | -0.4297 | 0.1453 | 11.6932 | -3.9527 | 3.8702 | 15.6459 | 0.4787 | 3.9527 |
| 3-chloro-2,2-dimethyl-1-propanol | -0.4273 | 0.1406 | 11.6284 | -3.8264 | 3.901 | 15.4549 | 0.4923 | 3.8264 |
| 6-chloro-1-hexanol | -0.4257 | 0.1447 | 11.5841 | -3.9364 | 3.8239 | 15.5205 | 0.4711 | 3.9364 |
| 8-chloro-1-octanol | -0.4233 | 0.1448 | 11.5171 | -3.9413 | 3.7879 | 15.4584 | 0.4641 | 3.9413 |
| 6-bromo-1-hexanol | -0.3940 | 0.1348 | 10.7201 | -3.6686 | 3.5258 | 14.3887 | 0.432 | 3.6686 |
| 8-bromo-1-octanol | -0.3932 | 0.1353 | 10.6981 | -3.6806 | 3.5087 | 14.3787 | 0.4281 | 3.6806 |
| 2,3-dibromopropanol | -0.3949 | 0.1209 | 10.7468 | -3.2893 | 3.7288 | 14.0361 | 0.4953 | 3.2893 |
| **Saturated Alcohols** | | | | | | | | |
| methyl alcohol | -0.4449 | 0.1555 | 12.1054 | -4.2311 | 3.9372 | 16.3365 | 0.4744 | 4.2311 |
| ethyl alcohol | -0.4375 | 0.1547 | 11.9044 | -4.2085 | 3.8479 | 16.1128 | 0.4595 | 4.2085 |
| 1-propanol | -0.4371 | 0.1570 | 11.8943 | -4.2727 | 3.8108 | 16.167 | 0.4491 | 4.2727 |
| 2-propanol | -0.4309 | 0.1468 | 11.7261 | -3.9951 | 3.8655 | 15.7213 | 0.4752 | 3.9952 |
| 1-butanol | -0.4369 | 0.1571 | 11.8880 | -4.2754 | 3.8063 | 16.1635 | 0.4482 | 4.2754 |
| (+/-)-2-butanol | -0.4311 | 0.1503 | 11.7318 | -4.0890 | 3.8214 | 15.8209 | 0.4615 | 4.0890 |
| 2-methyl-1-propanol | -0.4356 | 0.1550 | 11.8518 | -4.2166 | 3.8176 | 16.0685 | 0.4535 | 4.2166 |
| 2-pentanol | -0.4287 | 0.1510 | 11.6641 | -4.1083 | 3.7779 | 15.7724 | 0.4524 | 4.1084 |
| 3-pentanol | -0.4211 | 0.1476 | 11.4586 | -4.0161 | 3.7213 | 15.4747 | 0.4474 | 4.0161 |
| 3-methyl-2-butanol | -0.4295 | 0.1529 | 11.6880 | -4.1603 | 3.7639 | 15.8483 | 0.4469 | 4.1603 |
| tert-amylalcohol | -0.4254 | 0.1453 | 11.5765 | -3.9524 | 3.8120 | 15.5289 | 0.4679 | 3.9524 |
| 2-methyl-1-butanol | -0.4350 | 0.1550 | 11.8366 | -4.2183 | 3.8092 | 16.0549 | 0.4519 | 4.2183 |
| 3-methyl-1-butanol | -0.4348 | 0.1526 | 11.8325 | -4.1535 | 3.8395 | 15.986 | 0.4611 | 4.1535 |
| 2,2-dimethyl-1-propanol | -0.4339 | 0.1497 | 11.8072 | -4.0722 | 3.8675 | 15.8794 | 0.4710 | 4.0722 |
| 2-methyl-2-propanol | -0.4278 | 0.1442 | 11.6415 | -3.9247 | 3.8584 | 15.5662 | 0.4782 | 3.9247 |

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|---|---|---|---|---|---|---|---|---|
| 1-hexanol | -0.4364 | 0.1569 | 11.8758 | -4.2694 | 3.8032 | 16.1452 | 0.4479 | 4.2694 |
| 3,3-dimethyl-1-butanol | -0.4351 | 0.1511 | 11.8388 | -4.1108 | 3.864 | 15.9496 | 0.4681 | 4.1108 |
| 4-methyl-1-pentanol | -0.4364 | 0.1519 | 11.8750 | -4.1339 | 3.8705 | 16.0089 | 0.4679 | 4.1339 |
| 1-heptanol | -0.4364 | 0.1568 | 11.8736 | -4.2670 | 3.8033 | 16.1406 | 0.4481 | 4.2669 |
| 2,4-dimethyl-3-pentanol | -0.4157 | 0.1496 | 11.3125 | -4.0708 | 3.6209 | 15.3833 | 0.4261 | 4.0708 |
| 1-octanol | -0.4325 | 0.1568 | 11.7680 | -4.2667 | 3.7507 | 16.0347 | 0.4387 | 4.2667 |
| 2-octanol | -0.4234 | 0.1511 | 11.5207 | -4.1103 | 3.7052 | 15.6309 | 0.4391 | 4.1102 |
| 3-octanol | -0.4177 | 0.1503 | 11.3650 | -4.0893 | 3.6379 | 15.4543 | 0.4282 | 4.0893 |
| 1-nonanol | -0.4281 | 0.1568 | 11.6497 | -4.2659 | 3.6919 | 15.9156 | 0.4282 | 4.2659 |
| 2-nonanol | -0.4210 | 0.1511 | 11.4546 | -4.1108 | 3.6719 | 15.5654 | 0.4331 | 4.1108 |
| 3-ethyl-2,2-dimethyl-3-pentanol | -0.4035 | 0.1458 | 10.9786 | -3.9668 | 3.5059 | 14.9455 | 0.4112 | 3.9668 |
| 1-decanol | -0.4246 | 0.1568 | 11.5531 | -4.2664 | 3.6433 | 15.8195 | 0.4195 | 4.2664 |
| (+/-)-4-decanol | -0.4140 | 0.1528 | 11.2649 | -4.1587 | 3.5531 | 15.4236 | 0.4093 | 4.1587 |
| 3,7-dimethyl-3-octanol | -0.4095 | 0.1440 | 11.1424 | -3.9187 | 3.6119 | 15.0611 | 0.4331 | 3.9187 |
| 1-undecanol | -0.4217 | 0.1568 | 11.4739 | -4.2662 | 3.6039 | 15.7400 | 0.4126 | 4.2662 |
| 1-dodecanol | -0.4193 | 0.1568 | 11.4083 | -4.2664 | 3.5709 | 15.6747 | 0.4068 | 4.2664 |
| 1-tridecanol | -0.4172 | 0.1568 | 11.3533 | -4.2664 | 3.5434 | 15.6198 | 0.4019 | 4.2664 |
| **Carboxylic Acids** | | | | | | | | |
| Propanoic acid | -0.4481 | 0.1524 | 12.1933 | -4.1473 | 4.023 | 16.3406 | 0.4952 | 4.1473 |
| Butyric acid | -0.4470 | 0.1500 | 12.1634 | -4.0803 | 4.0415 | 16.2437 | 0.5028 | 4.0803 |
| Valeric acid | -0.4457 | 0.1517 | 12.1283 | -4.1277 | 4.0003 | 16.2560 | 0.4922 | 4.1277 |
| Hexanoic acid | -0.4438 | 0.1519 | 12.0766 | -4.1320 | 3.9723 | 16.2086 | 0.4868 | 4.1320 |
| Heptanoic acid | -0.4414 | 0.1522 | 12.0113 | -4.1415 | 3.9349 | 16.1528 | 0.4793 | 4.1415 |
| Octanoic acid | -0.4377 | 0.1522 | 11.9098 | -4.1410 | 3.8844 | 16.0508 | 0.4700 | 4.1410 |
| Nonanoic acid | -0.4335 | 0.1522 | 11.7961 | -4.1426 | 3.8267 | 15.9387 | 0.4594 | 4.1426 |
| Decanoic acid | -0.4295 | 0.1523 | 11.6883 | -4.1432 | 3.7726 | 15.8315 | 0.4495 | 4.1432 |
| Undecanoic acid | -0.4261 | 0.1523 | 11.5939 | -4.1440 | 3.7249 | 15.7379 | 0.4408 | 4.1440 |
| iso-Butyric acid | -0.4401 | 0.1509 | 11.9743 | -4.1051 | 3.9346 | 16.0794 | 0.4814 | 4.1051 |
| Isovalerianic acid | -0.4377 | 0.1441 | 11.9095 | -3.9220 | 3.9938 | 15.8315 | 0.5038 | 3.9220 |
| Trimethylacetic acid | -0.4347 | 0.1482 | 11.8276 | -4.0327 | 3.8975 | 15.8603 | 0.4789 | 4.0327 |
| 3-Methylvaleric acid | -0.4421 | 0.1517 | 12.0301 | -4.1279 | 3.9511 | 16.1580 | 0.4831 | 4.1279 |
| 4-Methylvaleric acid | -0.4452 | 0.1499 | 12.1133 | -4.0784 | 4.0175 | 16.1918 | 0.4984 | 4.0784 |
| 2-Ethylbutyric acid | -0.4297 | 0.1478 | 11.6932 | -4.0229 | 3.8351 | 15.7161 | 0.4679 | 4.0229 |
| 2-Propylpentanoic acid | -0.4318 | 0.1547 | 11.7506 | -4.2093 | 3.7707 | 15.9599 | 0.4454 | 4.2093 |
| 2-Ethylhexanoic acid | -0.4348 | 0.1538 | 11.8306 | -4.1848 | 3.8229 | 16.0154 | 0.4563 | 4.1848 |
| Succinic acid | -0.4560 | 0.1500 | 12.4080 | -4.0803 | 4.1639 | 16.4884 | 0.5258 | 4.0803 |
| Glutaric acid | -0.4481 | 0.1425 | 12.1931 | -3.8765 | 4.1583 | 16.0696 | 0.5380 | 3.8765 |
| Adipic acid | -0.4485 | 0.1474 | 12.2053 | -4.0117 | 4.0968 | 16.2171 | 0.5175 | 4.0118 |
| Pimelic acid | -0.4454 | 0.1457 | 12.1190 | -3.9633 | 4.0779 | 16.0824 | 0.5170 | 3.9633 |
| 3,3-Dimethylglutaric acid | -0.4370 | 0.1375 | 11.8913 | -3.7426 | 4.0743 | 15.6339 | 0.5309 | 3.7426 |
| Suberic acid | -0.4433 | 0.1484 | 12.0614 | -4.0384 | 4.0115 | 16.0998 | 0.4998 | 4.0384 |
| Sebacic acid | -0.4375 | 0.1496 | 11.9041 | -4.0703 | 3.9169 | 15.9743 | 0.4802 | 4.0702 |
| 1,10-Decanedicarboxylic acid | -0.4306 | 0.1505 | 11.7174 | -4.0956 | 3.8109 | 15.813 | 0.4592 | 4.0956 |

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| Crotonic acid | -0.3840 | 0.1131 | 10.4486 | -3.0768 | 3.6859 | 13.5253 | 0.5022 | 3.0768 |
| trans-2-Pentenoic acid | -0.3827 | 0.1101 | 10.4143 | -2.9962 | 3.7090 | 13.4105 | 0.5129 | 2.9962 |
| trans-2-Hexenoic acid | -0.3814 | 0.1124 | 10.3778 | -3.0594 | 3.6592 | 13.4372 | 0.4982 | 3.0594 |
| **Halogenated acids** | | | | | | | | |
| 4-Bromobutyric acid | -0.3958 | 0.1609 | 10.7710 | -4.3780 | 3.1965 | 15.1490 | 0.3372 | 4.3780 |
| 5-Bromovaleric acid | -0.3937 | 0.1634 | 10.7133 | -4.4458 | 3.1338 | 15.1591 | 0.3239 | 4.4458 |
| 4-Chlorobutyric acid | -0.4325 | 0.1844 | 11.7691 | -5.0175 | 3.3758 | 16.7866 | 0.3394 | 5.0175 |
| 3-Chloropropionic acid | -0.4370 | 0.1792 | 11.8924 | -4.8773 | 3.5075 | 16.7697 | 0.3668 | 4.8773 |
| 5-Chlorovaleric acid | -0.4287 | 0.1875 | 11.6649 | -5.1021 | 3.2814 | 16.7670 | 0.3211 | 5.1021 |
| 2-Bromobutyric acid | -0.4056 | 0.1205 | 11.0358 | -3.2776 | 3.8791 | 14.3134 | 0.5256 | 3.2776 |
| 2-Bromoisobutyric acid | -0.3961 | 0.1550 | 10.7792 | -4.2164 | 3.2814 | 14.9955 | 0.3590 | 4.2164 |
| 2-Bromoisovaleric acid | -0.3989 | 0.1515 | 10.8554 | -4.1230 | 3.3662 | 14.9784 | 0.3782 | 4.1230 |
| 2-Bromovaleric acid | -0.4045 | 0.1208 | 11.0080 | -3.2868 | 3.8606 | 14.2949 | 0.5213 | 3.2868 |
| 2-Bromooctanoic acid | -0.4039 | 0.1213 | 10.9912 | -3.2996 | 3.8458 | 14.2908 | 0.5175 | 3.2996 |
| 2-Bromohexanoic acid | -0.4042 | 0.1210 | 10.9993 | -3.2934 | 3.8530 | 14.2927 | 0.5193 | 3.2934 |
| **Mono esters** | | | | | | | | |
| Ethyl acetate | -0.4416 | 0.1543 | 12.0159 | -4.1979 | 3.9090 | 16.2138 | 0.4712 | 4.1979 |
| Propyl acetate | -0.4407 | 0.1520 | 11.9931 | -4.1369 | 3.9281 | 16.1300 | 0.4783 | 4.1369 |
| Isopropyl acetate | -0.4397 | 0.1502 | 11.9656 | -4.0866 | 3.9395 | 16.0522 | 0.4834 | 4.0866 |
| Butyl acetate | -0.4396 | 0.1525 | 11.9620 | -4.1503 | 3.9059 | 16.1123 | 0.4734 | 4.1502 |
| Amyl acetate | -0.4388 | 0.1527 | 11.9403 | -4.1557 | 3.8923 | 16.0960 | 0.4706 | 4.1557 |
| Hexyl acetate | -0.4377 | 0.1530 | 11.9095 | -4.1639 | 3.8728 | 16.0734 | 0.4666 | 4.1639 |
| Octyl acetate | -0.4337 | 0.1532 | 11.8018 | -4.1693 | 3.8162 | 15.9711 | 0.4559 | 4.1693 |
| Decyl acetate | -0.4275 | 0.1533 | 11.6328 | -4.1715 | 3.7307 | 15.8043 | 0.4403 | 4.1715 |
| Ethyl propionate | -0.4387 | 0.1522 | 11.9376 | -4.1426 | 3.8975 | 16.0802 | 0.4723 | 4.1426 |
| Butyl propionate | -0.4367 | 0.1518 | 11.8840 | -4.1309 | 3.8765 | 16.0149 | 0.4692 | 4.1309 |
| Isobutyl propionate | -0.4381 | 0.1485 | 11.9209 | -4.0411 | 3.9399 | 15.9621 | 0.4862 | 4.0411 |
| Propyl propionate | -0.4378 | 0.1510 | 11.9125 | -4.1078 | 3.9024 | 16.0203 | 0.4753 | 4.1078 |
| tert-Butyl propionate | -0.4266 | 0.1468 | 11.6088 | -3.9938 | 3.8075 | 15.6026 | 0.4646 | 3.9938 |
| Ethyl butyrate | -0.4377 | 0.1511 | 11.9098 | -4.1113 | 3.8992 | 16.0211 | 0.4745 | 4.1113 |
| Ethyl isobutyrate | -0.4316 | 0.1483 | 11.7435 | -4.0365 | 3.8535 | 15.7800 | 0.4705 | 4.0365 |
| Ethyl valerate | -0.4365 | 0.1521 | 11.8782 | -4.1386 | 3.8698 | 16.0168 | 0.4675 | 4.1386 |
| Propyl butyrate | -0.4368 | 0.1506 | 11.8856 | -4.0975 | 3.8941 | 15.9830 | 0.4744 | 4.0974 |
| Butyl butyrate | -0.4357 | 0.1513 | 11.8562 | -4.1160 | 3.8701 | 15.9722 | 0.4689 | 4.1156 |
| Propyl valerate | -0.4357 | 0.1511 | 11.8548 | -4.1127 | 3.8711 | 15.9675 | 0.4692 | 4.1127 |
| Amyl propionate | -0.4360 | 0.1521 | 11.8630 | -4.1388 | 3.8621 | 16.0018 | 0.4661 | 4.1388 |
| Ethyl hexanoate | -0.4350 | 0.1524 | 11.8369 | -4.1462 | 3.8454 | 15.9830 | 0.4626 | 4.1462 |
| Methyl butyrate | -0.4407 | 0.1525 | 11.9914 | -4.1505 | 3.9205 | 16.1420 | 0.4761 | 4.1505 |
| Methyl valerate | -0.4395 | 0.1535 | 11.9591 | -4.1766 | 3.8912 | 16.1357 | 0.4692 | 4.1766 |
| Methyl hexanoate | -0.4378 | 0.1538 | 11.9139 | -4.1854 | 3.8643 | 16.0992 | 0.4638 | 4.1854 |
| Methyl heptanoate | -0.4360 | 0.1541 | 11.8635 | -4.1930 | 3.8353 | 16.0565 | 0.4581 | 4.1930 |
| Methyl octanoate | -0.4333 | 0.1541 | 11.7912 | -4.1927 | 3.7992 | 15.9839 | 0.4515 | 4.1927 |
| Methyl nonanoate | -0.4302 | 0.1541 | 11.7052 | -4.1938 | 3.7557 | 15.8990 | 0.4436 | 4.1938 |
| Methyl decanoate | -0.4269 | 0.1541 | 11.6176 | -4.1938 | 3.7119 | 15.8113 | 0.4357 | 4.1938 |
| Methyl undecanoate | -0.4240 | 0.1542 | 11.5362 | -4.1949 | 3.6707 | 15.7311 | 0.4283 | 4.1949 |
| Methyl formate | -0.4610 | 0.1638 | 12.5438 | -4.4575 | 4.0432 | 17.0013 | 0.4808 | 4.4575 |

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|---|---|---|---|---|---|---|---|---|
| tert-Butyl formate | -0.4417 | 0.1522 | 12.0189 | -4.1421 | 3.9384 | 16.161 | 0.4799 | 4.1421 |
| **Diesters** | | | | | | | | |
| Diethyl malonate | -0.4426 | 0.1881 | 12.0434 | -5.1184 | 3.4625 | 17.1618 | 0.3493 | 5.1184 |
| Diethyl sebacate | -0.4263 | 0.2011 | 11.5988 | -5.4724 | 3.0632 | 17.0712 | 0.2748 | 5.4724 |
| Diethyl suberate | -0.4299 | 0.2000 | 11.6986 | -5.4428 | 3.1279 | 17.1414 | 0.2854 | 5.4428 |
| Diethyl succinate | -0.4399 | 0.1896 | 11.9688 | -5.1598 | 3.4045 | 17.1286 | 0.3383 | 5.1598 |
| Dimethyl malonate | -0.4474 | 0.1856 | 12.1746 | -5.0490 | 3.5628 | 17.2236 | 0.3685 | 5.0490 |
| Dibutyl adipate | -0.4314 | 0.1988 | 11.7400 | -5.4101 | 3.1649 | 17.1501 | 0.2920 | 5.4101 |
| Dimethyl succinate | -0.4436 | 0.1872 | 12.0714 | -5.0950 | 3.4882 | 17.1665 | 0.3544 | 5.0950 |
| Diethyl adipate | -0.4338 | 0.1979 | 11.8031 | -5.3843 | 3.2094 | 17.1874 | 0.2996 | 5.3843 |
| Dimethyl brassylate | -0.4210 | 0.1998 | 11.4562 | -5.4363 | 3.0100 | 16.8924 | 0.2682 | 5.4362 |
| Dimethyl sebacate | -0.4289 | 0.1994 | 11.6717 | -5.4254 | 3.1232 | 17.0971 | 0.2853 | 5.4254 |
| Dimethyl suberate | -0.4333 | 0.1982 | 11.7917 | -5.3941 | 3.1988 | 17.1858 | 0.2977 | 5.3941 |
| Diethyl pimelate | -0.4314 | 0.2002 | 11.7397 | -5.4466 | 3.1466 | 17.1863 | 0.2880 | 5.4466 |
| Dibutyl suberate | -0.4279 | 0.2009 | 11.6447 | -5.4667 | 3.0890 | 17.1115 | 0.2788 | 5.4667 |
| Diethyl butylmalonate | -0.4351 | 0.1860 | 11.8390 | -5.0605 | 3.3893 | 16.8995 | 0.3399 | 5.0605 |
| Diethyl ethylmalonate | -0.4364 | 0.1850 | 11.8750 | -5.0341 | 3.4204 | 16.9090 | 0.3460 | 5.0341 |
| Diethyl 3-oxopimelate | -0.4087 | 0.1624 | 11.1220 | -4.4188 | 3.3516 | 15.5409 | 0.3614 | 4.4188 |
| Diethyl 4-oxopimelate | -0.4123 | 0.1614 | 11.2181 | -4.3924 | 3.4128 | 15.6105 | 0.3731 | 4.3924 |
| Diethyl methylmalonate | -0.4384 | 0.1850 | 11.9299 | -5.0343 | 3.4478 | 16.9643 | 0.3504 | 5.0343 |
| Diethyl propylmalonate | -0.4357 | 0.1857 | 11.8554 | -5.0537 | 3.4009 | 16.9090 | 0.3420 | 5.0537 |
| Dibutyl succinate | -0.4378 | 0.1907 | 11.9117 | -5.1900 | 3.3609 | 17.1017 | 0.3302 | 5.1899 |
| **Aldehyde** | | | | | | | | |
| Propionaldehyde | -0.4137 | 0.1436 | 11.2573 | -3.9064 | 3.6754 | 15.1637 | 0.4454 | 3.9064 |
| Butyraldehyde | -0.4119 | 0.1447 | 11.2086 | -3.9377 | 3.6354 | 15.1463 | 0.4363 | 3.9377 |
| Isobutyraldehyde | -0.4103 | 0.1368 | 11.1648 | -3.7233 | 3.7207 | 14.8881 | 0.4649 | 3.7233 |
| Valeraldehyde | -0.4107 | 0.1452 | 11.1756 | -3.9519 | 3.6119 | 15.1275 | 0.4312 | 3.9519 |
| 2-Methyl-butyraldehyde | -0.4085 | 0.1454 | 11.1152 | -3.9576 | 3.5788 | 15.0728 | 0.4249 | 3.9576 |
| Hexylaldehyde | -0.4093 | 0.1474 | 11.1386 | -4.0096 | 3.5645 | 15.1482 | 0.4194 | 4.0096 |
| 2-Methylvaleraldehyde | -0.4071 | 0.1464 | 11.0780 | -3.9824 | 3.5478 | 15.0603 | 0.4179 | 3.9824 |
| 2-Ethylbutyraldehyde | -0.4046 | 0.1439 | 11.0099 | -3.9149 | 3.5475 | 14.9248 | 0.4216 | 3.9149 |
| 3,3-Dimethylbutyraldehyde | -0.4072 | 0.1371 | 11.0809 | -3.7312 | 3.6749 | 14.8121 | 0.4559 | 3.7312 |
| Heptaldehyde | -0.4092 | 0.1456 | 11.1343 | -3.9614 | 3.5864 | 15.0957 | 0.4260 | 3.9614 |
| 2-Ethylhexanal | -0.4040 | 0.1455 | 10.9922 | -3.9590 | 3.5166 | 14.9512 | 0.4136 | 3.9590 |
| trans-4-Decen-1-al | -0.3536 | 0.1341 | 9.6222 | -3.6493 | 2.9864 | 13.2714 | 0.3360 | 3.6493 |
| cis-7-Decen-1-al | -0.3462 | 0.1452 | 9.4208 | -3.9522 | 2.7343 | 13.3729 | 0.2795 | 3.9522 |
| **Ketones** | | | | | | | | |
| Acetone | -0.4080 | 0.1425 | 11.1014 | -3.8765 | 3.6124 | 14.9779 | 0.4356 | 3.8765 |
| 2-Butanone | -0.4010 | 0.1402 | 10.9117 | -3.8156 | 3.5481 | 14.7272 | 0.4274 | 3.8156 |
| 2-Pentanone | -0.3996 | 0.1440 | 10.8736 | -3.9176 | 3.4780 | 14.7912 | 0.4089 | 3.9176 |
| 3-Pentanone | -0.4009 | 0.1430 | 10.9098 | -3.8920 | 3.5089 | 14.8018 | 0.4159 | 3.8920 |
| 4-Methyl-2-pentanone | -0.3985 | 0.1415 | 10.8426 | -3.8507 | 3.4960 | 14.6932 | 0.4159 | 3.8507 |
| 2-Heptanone | -0.3976 | 0.1453 | 10.8192 | -3.9532 | 3.4330 | 14.7724 | 0.3989 | 3.9532 |
| 5-Methyl-2-hexanone | -0.3979 | 0.1444 | 10.8265 | -3.9304 | 3.4481 | 14.7569 | 0.4028 | 3.9304 |
| 4-Heptanone | -0.3979 | 0.1438 | 10.8279 | -3.9122 | 3.4579 | 14.7400 | 0.4056 | 3.9121 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 2-Octanone | -0.3971 | 0.1453 | 10.8064 | -3.9546 | 3.4259 | 14.7610 | 0.3976 | 3.9546 |
| 2-Nonanone | -0.3968 | 0.1454 | 10.7969 | -3.9562 | 3.4203 | 14.7531 | 0.3965 | 3.9562 |
| 2-Decanone | -0.3965 | 0.1454 | 10.7903 | -3.9573 | 3.4165 | 14.7477 | 0.3957 | 3.9573 |
| 3-Decanone | -0.3941 | 0.1429 | 10.7228 | -3.8874 | 3.4177 | 14.6102 | 0.3997 | 3.8874 |
| 2-Undecanone | -0.3964 | 0.1455 | 10.7860 | -3.9581 | 3.4139 | 14.7441 | 0.3952 | 3.9581 |
| 2-Dodecanone | -0.3963 | 0.1455 | 10.7824 | -3.9590 | 3.4117 | 14.7414 | 0.3948 | 3.9589 |
| 7-Tridecanone | -0.3942 | 0.1453 | 10.7275 | -3.9532 | 3.3871 | 14.6807 | 0.3907 | 3.9532 |

**Table S2.** Calculated HOMO energies, LUMO energies, ionization energies, electron affinities, electronegativities, hardness, electrophilicity, chemical potential and philicity of aliphatic electron donors

| MOLECULE | HOMO | LUMO | IP(eV) | A(eV) | χ(eV) | η(eV) | ω(eV) | μ(eV) | ω+(eV) |
|---|---|---|---|---|---|---|---|---|---|
| **Amino Alcohols** | | | | | | | | | |
| 2-(methylamino)ethanol | -0.3666 | 0.1585 | 9.9767 | -4.3124 | 2.8321 | 14.2891 | 0.2807 | 4.3124 | 0.6507 |
| 4-amino-1-butanol | -0.3811 | 0.1539 | 10.3710 | -4.1878 | 3.0916 | 14.5588 | 0.3283 | 4.1878 | 0.6023 |
| 2-(ethylamino)ethanol | -0.3660 | 0.1573 | 9.9596 | -4.2811 | 2.8392 | 14.2407 | 0.2830 | 4.2811 | 0.6435 |
| 2-Propylaminoethanol | -0.3651 | 0.1584 | 9.9340 | -4.3105 | 2.8117 | 14.2445 | 0.2775 | 4.3105 | 0.6522 |
| DL-2-amino-1-pentanol | -0.3788 | 0.1516 | 10.3090 | -4.1241 | 3.0923 | 14.4328 | 0.3313 | 4.1241 | 0.5892 |
| 3-amino-2,2-dimethyl-1-propanol | -0.3787 | 0.1491 | 10.3050 | -4.0569 | 3.1240 | 14.3618 | 0.3398 | 4.0569 | 0.5730 |
| 6-amino-1-hexanol | -0.3790 | 0.1563 | 10.3120 | -4.2537 | 3.0290 | 14.5653 | 0.3150 | 4.2536 | 0.6211 |
| DL-2-amino-1-hexanol | -0.3787 | 0.1515 | 10.3040 | -4.1214 | 3.0912 | 14.4252 | 0.3312 | 4.1214 | 0.5888 |
| DL-2-amino-3-methyl-1-butanol | -0.3782 | 0.1557 | 10.2920 | -4.2368 | 3.0275 | 14.5286 | 0.3154 | 4.2368 | 0.6178 |
| 2-amino-3,3-dimethyl-butanol | -0.3774 | 0.1534 | 10.2690 | -4.1734 | 3.0479 | 14.4426 | 0.3216 | 4.1734 | 0.6030 |
| 2-amino-3-methyl-1-pentanol | -0.3777 | 0.1551 | 10.2780 | -4.2205 | 3.0290 | 14.4989 | 0.3164 | 4.2204 | 0.6143 |
| 2-amino-4-methyl-pentanol | -0.3794 | 0.1539 | 10.3230 | -4.1870 | 3.0679 | 14.5098 | 0.3243 | 4.1869 | 0.6041 |
| 2-(tert.butylamino)ethanol | -0.3603 | 0.1505 | 9.8028 | -4.0958 | 2.8535 | 13.8987 | 0.2929 | 4.0958 | 0.6035 |
| diethanolamine | -0.3697 | 0.1564 | 10.0610 | -4.2569 | 2.9021 | 14.3180 | 0.2941 | 4.2569 | 0.6328 |
| 1,3-diamino-2-hydroxy-propane | -0.3783 | 0.1543 | 10.2940 | -4.1984 | 3.0479 | 14.4927 | 0.3205 | 4.1984 | 0.6081 |
| N-methyldiethanol amine | -0.3522 | 0.1535 | 9.5841 | -4.1769 | 2.7036 | 13.7610 | 0.2656 | 4.1769 | 0.6339 |
| 3-(methylamino)-1,2-propanediol | -0.3604 | 0.1495 | 9.8072 | -4.0667 | 2.8702 | 13.8739 | 0.2969 | 4.0667 | 0.5960 |
| triethanolamine | -0.3531 | 0.1496 | 9.6080 | -4.0705 | 2.7687 | 13.6785 | 0.2802 | 4.0705 | 0.6057 |
| **Acetylenic Alcohols** | | | | | | | | | |
| 3-butyn-2-ol | -0.3956 | 0.1511 | 10.7650 | -4.1111 | 3.327 | 14.8761 | 0.3720 | 4.1111 | 0.5681 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1-pentyn-3-ol | -0.3937 | 0.1498 | 10.7130 | -4.0760 | 3.3185 | 14.7890 | 0.3723 | 4.0760 | 0.5617 |
| 2-pentyn-1-ol | -0.3666 | 0.1421 | 9.9748 | -3.8662 | 3.0543 | 13.8410 | 0.3370 | 3.8662 | 0.5400 |
| 2-penten-4-yn-1-ol | -0.3337 | 0.1306 | 9.0804 | -3.5535 | 2.7634 | 12.6339 | 0.3022 | 3.5535 | 0.4997 |
| 1-hexyn-3-ol | -0.3930 | 0.1517 | 10.6930 | -4.1290 | 3.2821 | 14.8222 | 0.3634 | 4.1290 | 0.5751 |
| 1-heptyn-3-ol | -0.3925 | 0.1520 | 10.6810 | -4.1353 | 3.2730 | 14.8165 | 0.3615 | 4.1353 | 0.5771 |
| 4-heptyn-3-ol | -0.3716 | 0.1458 | 10.1120 | -3.9663 | 3.0727 | 14.0780 | 0.3353 | 3.9663 | 0.5587 |
| 2-octyn-1-ol | -0.3656 | 0.1448 | 9.9495 | -3.9410 | 3.0043 | 13.8905 | 0.3249 | 3.9410 | 0.5591 |
| 2-nonyn-1-ol | -0.3655 | 0.1449 | 9.9468 | -3.9424 | 3.0022 | 13.8891 | 0.3245 | 3.9424 | 0.5595 |
| 2-decyn-1-ol | -0.3655 | 0.1449 | 9.9452 | -3.9434 | 3.0009 | 13.8886 | 0.3242 | 3.9434 | 0.5598 |
| 2-tridecyn-1-ol | -0.3654 | 0.1450 | 9.9430 | -3.9448 | 2.9991 | 13.8878 | 0.3238 | 3.9448 | 0.5603 |
| 4-methyl-1-pentyn-3-ol | -0.3930 | 0.1517 | 10.6930 | -4.1290 | 3.2821 | 14.8222 | 0.3634 | 4.1290 | 0.5751 |
| 4-methyl-1-heptyn-3-ol | -0.3922 | 0.1546 | 10.6710 | -4.2074 | 3.2320 | 14.8788 | 0.3510 | 4.2074 | 0.5949 |
| **Unsaturated Alcohols** | | | | | | | | | |
| 2-methyl-3-buten-2-ol | -0.3669 | 0.1495 | 9.9827 | -4.0667 | 2.9580 | 14.0494 | 0.3114 | 4.0667 | 0.5886 |
| 4-pentyn-1-ol | -0.3886 | 0.1450 | 10.5740 | -3.9454 | 3.3142 | 14.5191 | 0.3783 | 3.9454 | 0.5360 |
| 2-methyl-3-butyn-2-ol | -0.3939 | 0.1496 | 10.7190 | -4.0719 | 3.3236 | 14.7909 | 0.3734 | 4.0719 | 0.5605 |
| trans-3-hexen-1-ol | -0.3441 | 0.1567 | 9.3639 | -4.2645 | 2.5497 | 13.6285 | 0.2385 | 4.2645 | 0.6672 |
| cis-3-hexen-1-ol | -0.3400 | 0.1494 | 9.2518 | -4.0648 | 2.5935 | 13.3166 | 0.2526 | 4.0648 | 0.6204 |
| 5-hexyn-1-ol | -0.3862 | 0.1507 | 10.5090 | -4.1010 | 3.2041 | 14.6102 | 0.3513 | 4.1010 | 0.5756 |
| 3-methyl-1-pentyn-3-ol | -0.3921 | 0.1468 | 10.6710 | -3.9941 | 3.3383 | 14.6647 | 0.3800 | 3.9941 | 0.5439 |
| 4-hexen-1-ol | -0.3432 | 0.1559 | 9.3381 | -4.2414 | 2.5483 | 13.5795 | 0.2391 | 4.2414 | 0.6624 |
| 5-hexen-1-ol | -0.3608 | 0.1564 | 9.8164 | -4.2547 | 2.7808 | 14.0712 | 0.2748 | 4.2547 | 0.6433 |
| 4-pentyn-2-ol | -0.3819 | 0.1446 | 10.3930 | -3.9345 | 3.2290 | 14.3270 | 0.3639 | 3.9345 | 0.5402 |
| 5-hexyn-3-ol | -0.3931 | 0.1520 | 10.6970 | -4.1372 | 3.2798 | 14.8339 | 0.3626 | 4.1372 | 0.5769 |
| 3-heptyn-1-ol | -0.3660 | 0.1515 | 9.9588 | -4.1220 | 2.9184 | 14.0807 | 0.3024 | 4.1220 | 0.6033 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 4-heptyn-2-ol | -0.3598 | 0.1473 | 9.7906 | -4.0088 | 2.8909 | 13.7993 | 0.3028 | 4.0088 | 0.5823 |
| 3-octyn-1-ol | -0.3656 | 0.1522 | 9.9495 | -4.1413 | 2.9041 | 14.0908 | 0.2993 | 4.1413 | 0.6086 |
| 3-nonyn-1-ol | -0.3655 | 0.1527 | 9.9457 | -4.1552 | 2.8953 | 14.1008 | 0.2972 | 4.1552 | 0.6122 |
| 2-propen-1-ol | -0.3776 | 0.1506 | 10.2760 | -4.0991 | 3.0883 | 14.3749 | 0.3318 | 4.0991 | 0.5844 |
| 2-buten-1-ol | -0.3536 | 0.1519 | 9.6222 | -4.1345 | 2.7438 | 13.7566 | 0.2736 | 4.1345 | 0.6213 |
| (+/-)-3-buten-2-ol | -0.3587 | 0.1431 | 9.7601 | -3.8950 | 2.9326 | 13.6551 | 0.3149 | 3.8950 | 0.5555 |
| cis-2-buten-1,4-diol | -0.3596 | 0.1412 | 9.7860 | -3.8417 | 2.9721 | 13.6276 | 0.3241 | 3.8417 | 0.5415 |
| cis-2-penten-1-ol | -0.3586 | 0.1490 | 9.7585 | -4.0550 | 2.8517 | 13.8135 | 0.2944 | 4.0550 | 0.5952 |
| 3-penten-2-ol | -0.3514 | 0.1464 | 9.5615 | -3.9845 | 2.7885 | 13.5460 | 0.2870 | 3.9845 | 0.5860 |
| trans-2-hexen-1-ol | -0.3424 | 0.1577 | 9.3174 | -4.2898 | 2.5138 | 13.6072 | 0.2322 | 4.2898 | 0.6762 |
| 1-hexen-3-ol | -0.3741 | 0.1530 | 10.1790 | -4.1639 | 3.0077 | 14.3430 | 0.3153 | 4.1639 | 0.6044 |
| cis-2-hexen-1-ol | -0.3502 | 0.1510 | 9.5291 | -4.1100 | 2.7096 | 13.6391 | 0.2691 | 4.1099 | 0.6192 |
| trans-2-octen-1-ol | -0.3420 | 0.1577 | 9.3060 | -4.2918 | 2.5071 | 13.5977 | 0.2311 | 4.2918 | 0.6773 |
| **Amines** | | | | | | | | | |
| Propylamine | -0.3837 | 0.1586 | 10.4410 | -4.3162 | 3.0625 | 14.7575 | 0.3178 | 4.3162 | 0.6312 |
| Butylamine | -0.3833 | 0.1586 | 10.4310 | -4.3168 | 3.0569 | 14.7474 | 0.3168 | 4.3168 | 0.6318 |
| N-Methylpropylamine | -0.3619 | 0.1577 | 9.8472 | -4.2915 | 2.7779 | 14.1387 | 0.2729 | 4.2915 | 0.6513 |
| Amylamine | -0.3782 | 0.1570 | 10.2910 | -4.2713 | 3.0097 | 14.5621 | 0.3110 | 4.2713 | 0.6264 |
| N-Methylbutylamine | -0.3622 | 0.1586 | 9.8567 | -4.3146 | 2.7711 | 14.1713 | 0.2709 | 4.3146 | 0.6568 |
| Hexylamine | -0.3779 | 0.1568 | 10.2820 | -4.2678 | 3.0072 | 14.5501 | 0.3108 | 4.2678 | 0.6259 |
| Isopropylamine | -0.3834 | 0.1514 | 10.4320 | -4.1198 | 3.1561 | 14.5517 | 0.3423 | 4.1198 | 0.5832 |
| Isobutylamine | -0.3784 | 0.1501 | 10.2950 | -4.0847 | 3.1053 | 14.3800 | 0.3353 | 4.0847 | 0.5801 |
| N,N-Dimethylethylamine | -0.3405 | 0.1543 | 9.2660 | -4.1995 | 2.5332 | 13.4655 | 0.2383 | 4.1995 | 0.6549 |
| (□)-sec-Butylamine | -0.3817 | 0.1534 | 10.3870 | -4.1737 | 3.1067 | 14.5607 | 0.3314 | 4.1736 | 0.5982 |
| Isoamylamine | -0.3833 | 0.1561 | 10.4300 | -4.2482 | 3.0906 | 14.6777 | 0.3254 | 4.2482 | 0.6148 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1-Methylbutylamine | -0.3807 | 0.1539 | 10.3600 | -4.1883 | 3.0859 | 14.5485 | 0.3273 | 4.1883 | 0.6029 |
| 1-Ethylpropylamine | -0.3788 | 0.1561 | 10.3080 | -4.2488 | 3.0296 | 14.5566 | 0.3153 | 4.2488 | 0.6201 |
| 2-Methylbutylamine | -0.3826 | 0.1565 | 10.4100 | -4.2572 | 3.0762 | 14.6668 | 0.3226 | 4.2572 | 0.6178 |
| N,N-Diethylmethylamine | -0.3469 | 0.1567 | 9.4398 | -4.2629 | 2.5885 | 13.7027 | 0.2445 | 4.2629 | 0.6631 |
| tert-Butylamine | -0.3821 | 0.1462 | 10.3960 | -3.9772 | 3.2094 | 14.3732 | 0.3583 | 3.9772 | 0.5503 |
| tert-Amylamine | -0.3805 | 0.1475 | 10.3540 | -4.0123 | 3.1708 | 14.3662 | 0.3499 | 4.0123 | 0.5603 |
| (+/-)-1,2-Dimethylpropylamine | -0.3764 | 0.1537 | 10.2430 | -4.1810 | 3.0311 | 14.4241 | 0.3185 | 4.1810 | 0.6060 |
| Propargylamine | -0.3875 | 0.1533 | 10.5440 | -4.1707 | 3.1866 | 14.7145 | 0.3450 | 4.1707 | 0.5911 |
| N-Methylpropargylamine | -0.3728 | 0.1514 | 10.1430 | -4.1203 | 3.0113 | 14.2633 | 0.3179 | 4.1203 | 0.5951 |
| 1-Dimethylamino-2-propyne | -0.3597 | 0.1517 | 9.7879 | -4.1290 | 2.8294 | 13.9169 | 0.2876 | 4.1290 | 0.6125 |
| 1,1-Dimethylpropargylamine | -0.3803 | 0.1517 | 10.3490 | -4.1277 | 3.1105 | 14.4764 | 0.3342 | 4.1277 | 0.5885 |
| 2-Methoxyethylamine | -0.3870 | 0.1574 | 10.5310 | -4.2828 | 3.1240 | 14.8135 | 0.3294 | 4.2828 | 0.6191 |
| 3-Methoxypropylamine | -0.3825 | 0.1542 | 10.4090 | -4.1946 | 3.1070 | 14.6032 | 0.3305 | 4.1946 | 0.6024 |
| 3-Ethoxypropylamine | -0.3823 | 0.1542 | 10.4020 | -4.1965 | 3.1029 | 14.5988 | 0.3298 | 4.1965 | 0.6032 |

**Table S3**. Electrophilicity (ω), energy of lowest unoccupied molecular orbitals ($E_{LUMO}$), Log P, observed and calculated values of $pIGC_{50}$ for the complete set of aliphatic acceptor compounds with Tetrahymena pyriformis

| **Molecules** | **ω** | **$E_{LUMO}$** | **logP*** | **$pIGC_{50}$** | | |
|---|---|---|---|---|---|---|
| | | | | **Obs*** | **Calc**.(ω, logP) | **Calc**.(LUMO, log P) |
| **Diols** | | | | | | |
| (+/-)-1,2-butanediol | 0.4500 | 0.1504 | -0.53 | -2.0482 | -1.7563 | -1.7697 |
| (+/-)-1,3-butanediol | 0.4643 | 0.1491 | -1.38 | -2.3013 | -2.2829 | -2.2947 |
| 1,4-butanediol | 0.4458 | 0.1573 | -0.83 | -2.2365 | -1.9354 | -1.9481 |
| 1,2-pentanediol | 0.4453 | 0.1506 | 0.00 | -1.6269 | -1.4310 | -1.4429 |
| 1,5-pentanediol | 0.4566 | 0.1548 | -0.64 | -1.9344 | -1.8279 | -1.8333 |
| 2-methyl-2,4-pentanediol | 0.4600 | 0.1448 | -0.68 | -1.9531 | -1.8547 | -1.8674 |
| (+/-)-1,2-hexanediol | 0.4443 | 0.1505 | 0.53 | -1.2669 | -1.1084 | -1.1163 |
| 1,6-hexanediol | 0.4514 | 0.1564 | -0.11 | -1.4946 | -1.5022 | -1.5052 |
| 1,2-decanediol | 0.4320 | 0.1507 | 2.64 | 0.7640 | 0.1820 | 0.1840 |
| 1,10-decanediol | 0.4298 | 0.1562 | 2.01 | 0.2240 | -0.1990 | -0.1990 |
| **Halogenated alcohol** | | | | | | |
| 2-bromoethanol | 0.4711 | 0.1301 | 0.18 | -0.8457 | -1.3404 | -1.3513 |
| 2-chloroethanol | 0.5211 | 0.1398 | -0.06 | -1.4174 | -1.5224 | -1.4900 |
| 1-chloro-2-propanol | 0.5087 | 0.1364 | 0.14 | -1.4920 | -1.3919 | -1.3699 |
| 3-chloro-1-propanol | 0.5053 | 0.1403 | 0.50 | -1.3992 | -1.1708 | -1.1445 |
| 4-chloro-1-butanol | 0.4787 | 0.1453 | 0.85 | -0.7594 | -0.9390 | -0.9241 |
| 3-chloro-2,2-dimethyl-1-propanol | 0.4923 | 0.1406 | 0.81 | -0.7822 | -0.9732 | -0.9531 |
| 6-chloro-1-hexanol | 0.4711 | 0.1447 | 1.59 | -0.2726 | -0.4840 | -0.4687 |
| 8-chloro-1-octanol | 0.4641 | 0.1448 | 2.65 | 0.4878 | 0.1648 | 0.1847 |
| 6-bromo-1-hexanol | 0.4320 | 0.1348 | 1.73 | 0.0074 | -0.3706 | -0.3917 |
| 8-bromo-1-octanol | 0.4281 | 0.1353 | 2.79 | 1.0424 | 0.2759 | 0.2619 |
| 2,3-dibromopropanol | 0.4953 | 0.1209 | 0.63 | -0.4861 | -1.0846 | -1.0826 |
| **Saturated alcohol** | | | | | | |
| Methyl alcohol | 0.4744 | 0.1555 | -0.77 | -2.6656 | -1.9198 | -1.9128 |
| Ethyl alcohol | 0.4595 | 0.1547 | -0.31 | -1.9912 | -1.6295 | -1.6301 |
| 1-propanol | 0.4491 | 0.1570 | 0.25 | -1.7464 | -1.2819 | -1.2828 |
| 2-propanol | 0.4752 | 0.1468 | 0.05 | -1.8819 | -1.4223 | -1.4156 |
| 1-butanol | 0.4482 | 0.1571 | 0.88 | -1.4306 | -0.8986 | -0.8945 |
| (+/-)-2-butanol | 0.4615 | 0.1503 | 0.61 | -1.5420 | -1.0723 | -1.0673 |
| 2-methyl-1-propanol | 0.4535 | 0.1550 | 0.76 | -1.3724 | -0.9754 | -0.9705 |
| 2-pentanol | 0.4524 | 0.1510 | 1.19 | -1.1596 | -0.7134 | -0.7092 |
| 3-pentanol | 0.4474 | 0.1476 | 1.21 | -1.2437 | -0.6977 | -0.7001 |
| 3-methyl-2-butanol | 0.4469 | 0.1529 | 1.28 | -0.9959 | -0.6548 | -0.6520 |
| tert-amylalcohol | 0.4679 | 0.1453 | 0.89 | -1.1729 | -0.9068 | -0.8995 |

Continued……..

| | | | | | | |
|---|---|---|---|---|---|---|
| 2-methyl-1-butanol | 0.4519 | 0.1550 | 1.22 | -0.9528 | -0.6948 | -0.6869 |
| 3-methyl-1-butanol | 0.4611 | 0.1526 | 1.16 | -1.0359 | -0.7379 | -0.7262 |
| 2,2-dimethyl-1-propanol | 0.4710 | 0.1497 | 1.31 | -0.8702 | -0.6540 | -0.6365 |
| 2-methyl-2-propanol | 0.4782 | 0.1442 | 0.35 | -1.7911 | -1.2423 | -1.2332 |
| 1-hexanol | 0.4479 | 0.1569 | 2.03 | -0.3789 | -0.2000 | -0.1860 |
| 3,3-dimethyl-1-butanol | 0.4681 | 0.1511 | 1.62 | -0.7368 | -0.4636 | -0.4442 |
| 4-methyl-1-pentanol | 0.4679 | 0.1519 | 1.75 | -0.6372 | -0.3845 | -0.3633 |
| 1-heptanol | 0.4481 | 0.1568 | 2.72 | 0.1050 | 0.2189 | 0.2391 |
| 2,4-dimethyl-3-pentanol | 0.4261 | 0.1496 | 1.93 | -0.7052 | -0.2449 | -0.2545 |
| 1-octanol | 0.4387 | 0.1568 | 3.00 | 0.5827 | 0.3958 | 0.4116 |
| 2-octanol | 0.4391 | 0.1511 | 2.90 | 0.0011 | 0.3348 | 0.3446 |
| 3-octanol | 0.4282 | 0.1503 | 2.72 | 0.0309 | 0.2334 | 0.2329 |
| 1-nonanol | 0.4282 | 0.1568 | 3.77 | 0.8551 | 0.8711 | 0.8861 |
| 2-nonanol | 0.4331 | 0.1511 | 3.25 | 0.6183 | 0.5517 | 0.5603 |
| 3-ethyl-2,2-dimethyl-3-pentanol | 0.4112 | 0.1458 | 2.86 | -0.1691 | 0.3307 | 0.3150 |
| 1-decanol | 0.4195 | 0.1568 | 4.57 | 1.3354 | 1.3632 | 1.3790 |
| (+/-)-4-decanol | 0.4093 | 0.1528 | 3.78 | 0.8499 | 0.8909 | 0.8885 |
| 3,7-dimethyl-3-octanol | 0.4331 | 0.1440 | 3.52 | 0.3404 | 0.7157 | 0.7200 |
| 1-undecanol | 0.4126 | 0.1568 | 4.53 | 1.9547 | 1.3440 | 1.3544 |
| 1-dodecanol | 0.4068 | 0.1568 | 5.13 | 2.1612 | 1.7126 | 1.7241 |
| 1-tridecanol | 0.4019 | 0.1568 | 5.58 | 2.4497 | 1.9894 | 2.0014 |
| **Carboxylic acid** | | | | | | |
| Propanoic acid | 0.4952 | 0.1524 | 0.33 | -0.5123 | -1.2668 | -1.2378 |
| Butyric acid | 0.5028 | 0.1500 | 0.79 | -0.572 | -0.9929 | -0.9567 |
| Valeric acid | 0.4922 | 0.1517 | 1.39 | -0.2674 | -0.6208 | -0.5853 |
| Hexanoic acid | 0.4868 | 0.1519 | 1.92 | -0.2083 | -0.2950 | -0.2586 |
| Heptanoic acid | 0.4793 | 0.1522 | 2.41 | -0.1126 | 0.0081 | 0.0437 |
| Octanoic acid | 0.4700 | 0.1522 | 3.05 | 0.0807 | 0.4035 | 0.4381 |
| Nonanoic acid | 0.4594 | 0.1522 | 3.47 | 0.3509 | 0.6663 | 0.6969 |
| Decanoic acid | 0.4495 | 0.1523 | 4.09 | 0.5063 | 1.0500 | 1.0790 |
| Undecanoic acid | 0.4408 | 0.1523 | 4.53 | 0.8983 | 1.3235 | 1.3502 |
| iso-Butyric acid | 0.4814 | 0.1509 | 0.60 | -0.3334 | -1.0928 | -1.0729 |
| Isovalerianic acid | 0.5038 | 0.1441 | 1.16 | -0.3415 | -0.7689 | -0.7342 |
| Trimethylacetic acid | 0.4789 | 0.1482 | 1.47 | -0.2543 | -0.5625 | -0.5393 |
| 3-Methylvaleric acid | 0.4831 | 0.1517 | 1.75 | -0.2331 | -0.3955 | -0.3635 |
| 4-Methylvaleric acid | 0.4984 | 0.1499 | 1.75 | -0.2724 | -0.4067 | -0.3652 |
| 2-Ethylbutyric acid | 0.4679 | 0.1478 | 1.68 | -0.1523 | -0.4271 | -0.4102 |
| 2-Propylpentanoic acid | 0.4454 | 0.1547 | 2.75 | 0.0258 | 0.2391 | 0.2556 |
| 2-Ethylhexanoic acid | 0.4563 | 0.1538 | 2.64 | 0.0756 | 0.1644 | 0.1869 |
| Succinic acid | 0.5258 | 0.1500 | -0.59 | -0.9395 | -1.8477 | -1.8071 |
| Glutaric acid | 0.5380 | 0.1425 | -0.29 | -0.6387 | -1.6743 | -1.6292 |

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|---|---|---|---|---|---|---|
| Adipic acid | 0.5175 | 0.1474 | 0.08 | -0.6060 | -1.4347 | -1.3966 |
| Pimelic acid | 0.5170 | 0.1457 | 0.42 | -0.5845 | -1.2279 | -1.1887 |
| 3,3-Dimethylglutaric acid | 0.5309 | 0.1375 | 0.16 | -0.6643 | -1.3959 | -1.3566 |
| Suberic acid | 0.4998 | 0.1484 | 0.95 | -0.5116 | -0.8935 | -0.8595 |
| Sebacic acid | 0.4802 | 0.1496 | 2.01 | -0.2676 | -0.2356 | -0.2052 |
| 1,10-Decanedicarboxylic acid | 0.4592 | 0.1505 | 3.07 | -0.0863 | 0.4235 | 0.4488 |
| Crotonic acid | 0.5022 | 0.1131 | 0.72 | -0.5448 | -1.0350 | -1.0345 |
| trans-2-Pentenoic acid | 0.5129 | 0.1101 | 1.41 | -0.2774 | -0.6237 | -0.6121 |
| trans-2-Hexenoic acid | 0.4982 | 0.1124 | 1.94 | -0.1279 | -0.2911 | -0.2833 |
| **Halogenated acid** | | | | | | |
| 4-Bromobutyric acid | 0.3372 | 0.1609 | 0.68 | -0.7711 | -0.9397 | -1.0142 |
| 5-Bromovaleric acid | 0.3239 | 0.1634 | 1.21 | -0.6929 | -0.6081 | -0.6852 |
| 4-Chlorobutyric acid | 0.3394 | 0.1844 | 0.54 | -0.6773 | -1.0263 | -1.0784 |
| 3-Chloropropionic acid | 0.3668 | 0.1792 | 0.41 | -0.3321 | -1.1251 | -1.1633 |
| 5-Chlorovaleric acid | 0.3211 | 0.1875 | 1.07 | -0.2857 | -0.6911 | -0.7489 |
| 2-Bromobutyric acid | 0.5256 | 0.1205 | 1.42 | 0.1221 | -0.6268 | -0.5962 |
| 2-Bromoisobutyric acid | 0.3590 | 0.1550 | 0.86 | -0.5845 | -0.8461 | -0.9088 |
| 2-Bromoisovaleric acid | 0.3782 | 0.1515 | 1.48 | -0.5492 | -0.4835 | -0.5300 |
| 2-Bromovaleric acid | 0.5213 | 0.1208 | 1.61 | -0.0423 | -0.5083 | -0.4788 |
| 2-Bromooctanoic acid | 0.5175 | 0.1213 | 3.19 | 0.4907 | 0.4541 | 0.4953 |
| 2-Bromohexanoic acid | 0.5193 | 0.1210 | 2.14 | 0.4547 | -0.1850 | -0.1520 |
| **Mono ester** | | | | | | |
| Ethyl acetate | 0.4712 | 0.1543 | 0.73 | -1.2968 | -1.0064 | -0.9896 |
| Propyl acetate | 0.4783 | 0.1520 | 1.24 | -1.2382 | -0.7018 | -0.6774 |
| Isopropyl acetate | 0.4834 | 0.1502 | 1.02 | -1.5900 | -0.8391 | -0.8147 |
| Butyl acetate | 0.4734 | 0.1525 | 1.78 | -0.4864 | -0.3703 | -0.3442 |
| Amyl acetate | 0.4706 | 0.1527 | 2.30 | 0.1625 | -0.0525 | -0.0236 |
| Hexyl acetate | 0.4666 | 0.1530 | 2.83 | -0.0087 | 0.2724 | 0.3033 |
| Octyl acetate | 0.4559 | 0.1532 | 3.88 | 1.0570 | 0.9178 | 0.9505 |
| Decyl acetate | 0.4403 | 0.1533 | 4.94 | 1.8794 | 1.5729 | 1.6038 |
| Ethyl propionate | 0.4723 | 0.1522 | 1.21 | -0.9450 | -0.7157 | -0.6957 |
| Butyl propionate | 0.4692 | 0.1518 | 2.30 | 0.1704 | -0.0514 | -0.0244 |
| Isobutyl propionate | 0.4862 | 0.1485 | 2.17 | -0.6935 | -0.1428 | -0.1077 |
| Propyl propionate | 0.4753 | 0.1510 | 1.77 | -0.8148 | -0.3777 | -0.3518 |
| tert-Butyl propionate | 0.4646 | 0.1468 | 1.95 | -0.4095 | -0.2607 | -0.2449 |
| Ethyl butyrate | 0.4745 | 0.1511 | 1.77 | -0.4903 | -0.3772 | -0.3517 |
| Ethyl isobutyrate | 0.4705 | 0.1483 | 1.55 | -1.2709 | -0.5079 | -0.4899 |
| Ethyl valerate | 0.4675 | 0.1521 | 2.30 | -0.3580 | -0.0502 | -0.0242 |
| Propyl butyrate | 0.4744 | 0.1506 | 2.30 | -0.4138 | -0.0552 | -0.0256 |
| Butyl butyrate | 0.4689 | 0.1513 | 2.83 | 0.5157 | 0.2707 | 0.3016 |
| Propyl valerate | 0.4692 | 0.1511 | 2.83 | 0.0094 | 0.2704 | 0.3015 |

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|---|---|---|---|---|---|---|
| Amyl propionate | 0.4661 | 0.1521 | 2.83 | -0.0431 | 0.2727 | 0.3024 |
| Ethyl hexanoate | 0.4626 | 0.1524 | 2.83 | 0.0637 | 0.2753 | 0.3027 |
| Methyl butyrate | 0.4761 | 0.1525 | 1.29 | -1.2463 | -0.6698 | -0.6461 |
| Methyl valerate | 0.4692 | 0.1535 | 1.96 | -0.8448 | -0.2579 | -0.2324 |
| Methyl hexanoate | 0.4638 | 0.1538 | 2.30 | -0.5611 | -0.0475 | -0.0226 |
| Methyl heptanoate | 0.4581 | 0.1541 | 2.83 | 0.1039 | 0.2785 | 0.3043 |
| Methyl octanoate | 0.4515 | 0.1541 | 3.36 | 0.5358 | 0.6052 | 0.6309 |
| Methyl nonanoate | 0.4436 | 0.1541 | 3.88 | 1.0419 | 0.9267 | 0.9513 |
| Methyl decanoate | 0.4357 | 0.1541 | 4.41 | 1.3778 | 1.2543 | 1.2779 |
| Methyl undecanoate | 0.4283 | 0.1542 | 4.79 | 1.4248 | 1.4905 | 1.5121 |
| Methyl formate | 0.4808 | 0.1638 | 0.03 | -1.4982 | -1.4385 | -1.4120 |
| tert-Butyl formate | 0.4799 | 0.1522 | 0.97 | -1.3719 | -0.8670 | -0.8436 |
| **Di ester** | | | | | | |
| Diethyl malonate | 0.3493 | 0.1881 | 0.96 | -0.9975 | -0.7783 | -0.8161 |
| Diethyl sebacate | 0.2748 | 0.2011 | 3.90 | 1.3536 | 1.0612 | 1.0078 |
| Diethyl suberate | 0.2854 | 0.2000 | 2.84 | 0.7018 | 0.4098 | 0.3536 |
| Diethyl succinate | 0.3383 | 0.1896 | 1.19 | -0.8511 | -0.6307 | -0.6729 |
| Dimethyl malonate | 0.3685 | 0.1856 | -0.05 | -1.2869 | -1.4057 | -1.4408 |
| Dibutyl adipate | 0.2920 | 0.1988 | 3.90 | 0.7918 | 1.0488 | 1.0057 |
| Dimethyl succinate | 0.3544 | 0.1872 | 0.35 | -1.0573 | -1.1525 | -1.1928 |
| Diethyl adipate | 0.2996 | 0.1979 | 1.79 | -0.1265 | -0.2383 | -0.2954 |
| Dimethyl brassylate | 0.2682 | 0.1998 | 4.43 | 1.6536 | 1.3880 | 1.3332 |
| Dimethyl sebacate | 0.2853 | 0.1994 | 2.84 | 1.0106 | 0.4099 | 0.3530 |
| Dimethyl suberate | 0.2977 | 0.1982 | 1.79 | 0.2962 | -0.2368 | -0.2951 |
| Diethyl pimelate | 0.2880 | 0.2002 | 2.31 | 0.4069 | 0.0860 | 0.0272 |
| Dibutyl suberate | 0.2788 | 0.2009 | 4.96 | 1.6556 | 1.7021 | 1.6608 |
| Diethyl butylmalonate | 0.3399 | 0.1860 | 3.02 | 0.5566 | 0.4796 | 0.4513 |
| Diethyl ethylmalonate | 0.3460 | 0.1850 | 1.96 | -0.2422 | -0.1686 | -0.2028 |
| Diethyl 3-oxopimelate | 0.3614 | 0.1624 | 1.49 | -0.3778 | -0.4652 | -0.5136 |
| Diethyl 4-oxopimelate | 0.3731 | 0.1614 | 1.54 | -0.6378 | -0.4433 | -0.4837 |
| Diethyl methylmalonate | 0.3504 | 0.1850 | 1.44 | -0.5114 | -0.4876 | -0.5232 |
| Diethyl propylmalonate | 0.3420 | 0.1857 | 2.49 | 0.1341 | 0.1562 | 0.1245 |
| Dibutyl succinate | 0.3302 | 0.1907 | 3.60 | 0.5123 | 0.8389 | 0.8132 |
| **Aldehyde** | | | | | | |
| Propionaldehyde | 0.4454 | 0.1436 | 0.59 | -0.4855 | -1.0728 | -1.0859 |
| Butyraldehyde | 0.4363 | 0.1447 | 0.88 | -0.3805 | -0.8900 | -0.9061 |
| Isobutyraldehyde | 0.4649 | 0.1368 | 0.61 | -0.4328 | -1.0748 | -1.0799 |
| Valeraldehyde | 0.4312 | 0.1452 | 1.36 | -0.0223 | -0.5948 | -0.6099 |
| 2-Methyl-butyraldehyde | 0.4249 | 0.1454 | 1.14 | -0.3107 | -0.7238 | -0.7452 |
| Hexylaldehyde | 0.4194 | 0.1474 | 1.78 | -0.1731 | -0.3311 | -0.3491 |
| 2-Methylvaleraldehyde | 0.4179 | 0.1464 | 1.67 | -0.4745 | -0.3969 | -0.4178 |
| 2-Ethylbutyraldehyde | 0.4216 | 0.1439 | 1.67 | -0.0544 | -0.3996 | -0.4201 |

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|---|---|---|---|---|---|---|
| 3,3-Dimethylbutyraldehyde | 0.4559 | 0.1371 | 1.63 | -0.3744 | -0.4487 | -0.4511 |
| Heptaldehyde | 0.4260 | 0.1456 | 2.42 | -0.0019 | 0.0527 | 0.0436 |
| 2-Ethylhexanal | 0.4136 | 0.1455 | 2.73 | 0.1608 | 0.2501 | 0.2346 |
| trans-4-Decen-1-al | 0.3360 | 0.1341 | 4.05 | 1.2076 | 1.1080 | 1.0373 |
| cis-7-Decen-1-al | 0.2795 | 0.1452 | 3.52 | 0.9485 | 0.8270 | 0.7212 |
| **Ketones** | | | | | | |
| Acetone | 0.4356 | 0.1425 | -0.24 | -2.2036 | -1.5698 | -1.5984 |
| 2-Butanone | 0.4274 | 0.1402 | 0.29 | -1.7457 | -1.2419 | -1.2739 |
| 2-Pentanone | 0.4089 | 0.1440 | 0.91 | -1.2224 | -0.8519 | -0.8884 |
| 3-Pentanone | 0.4159 | 0.1430 | 0.85 | -1.4561 | -0.8934 | -0.9262 |
| 4-Methyl-2-pentanone | 0.4159 | 0.1415 | 1.31 | -1.2085 | -0.6141 | -0.6442 |
| 2-Heptanone | 0.3989 | 0.1453 | 1.98 | -0.4872 | -0.1948 | -0.2278 |
| 5-Methyl-2-hexanone | 0.4028 | 0.1444 | 1.88 | -0.6459 | -0.2584 | -0.2902 |
| 4-Heptanone | 0.4056 | 0.1438 | 1.91 | -0.6690 | -0.2422 | -0.2723 |
| 2-Octanone | 0.3976 | 0.1453 | 2.37 | -0.1455 | 0.0430 | 0.0126 |
| 2-Nonanone | 0.3965 | 0.1454 | 3.14 | 0.6598 | 0.5115 | 0.4871 |
| 2-Decanone | 0.3957 | 0.1454 | 3.73 | 0.5822 | 0.8703 | 0.8507 |
| 3-Decanone | 0.3997 | 0.1429 | 3.49 | 0.6265 | 0.7217 | 0.7004 |
| 2-Undecanone | 0.3952 | 0.1455 | 4.09 | 1.5346 | 1.0893 | 1.0726 |
| 2-Dodecanone | 0.3948 | 0.1455 | 4.55 | 1.6696 | 1.3690 | 1.3561 |
| 7-Tridecanone | 0.3907 | 0.1453 | 5.08 | 1.5214 | 1.6939 | 1.6825 |

*Taken from reference 46

***Table S4. Electrophilicity (ω), energy of lowest unoccupied molecular orbitals ($E_{LUMO}$), Log P, observed and calculated values of $pIGC_{50}$ for the complete set of aliphatic donor compounds with Tetrahymena pyriformis***

| **Molecules** | **ω** | **$E_{LUMO}$** | **Log P*** | **$pIGC_{50}$** | | |
|---|---|---|---|---|---|---|
| | | | | **Observed*** | **Calc.**(ω, log P) | **Calc.**(LUMO, log P) |
| **Aminoalcohols** | | | | | | |
| 2-(methylamino)ethanol | 0.2807 | 0.1585 | -0.94 | -1.8202 | -1.7571 | -1.6952 |
| 4-amino-1-butanol | 0.3283 | 0.1539 | -1.06 | -0.9752 | -1.7066 | -1.7392 |
| 2-(ethylamino)ethanol | 0.2830 | 0.1573 | -0.46 | -1.6491 | -1.4915 | -1.4331 |
| 2-Propylaminoethanol | 0.2775 | 0.1584 | 0.07 | -1.6842 | -1.2179 | -1.1541 |
| DL-2-amino-1-pentanol | 0.3313 | 0.1516 | 0.07 | -0.6718 | -1.0874 | -1.1239 |
| 3-amino-2,2-dimethyl-1-propanol | 0.3398 | 0.1491 | -0.79 | -0.9246 | -1.5325 | -1.5734 |
| 6-amino-1-hexanol | 0.3150 | 0.1563 | -0.01 | -0.9580 | -1.1703 | -1.1877 |
| DL-2-amino-1-hexanol | 0.3312 | 0.1515 | 0.60 | -0.5848 | -0.8006 | -0.8397 |
| DL-2-amino-3-methyl-1-butanol | 0.3154 | 0.1557 | -0.06 | -0.5852 | -1.1962 | -1.2118 |
| 2-amino-3,3-dimethyl-butanol | 0.3216 | 0.1534 | 0.34 | -0.7178 | -0.9647 | -0.9873 |
| 2-amino-3-methyl-1-pentanol | 0.3164 | 0.1551 | 0.47 | -0.6594 | -0.9069 | -0.9254 |
| 2-amino-4-methyl-pentanol | 0.3243 | 0.1539 | 0.47 | -0.6191 | -0.8877 | -0.9199 |
| 2-(tert.butylamino)ethanol | 0.2929 | 0.1505 | 0.41 | -1.6730 | -0.9964 | -0.9373 |
| diethanolamine | 0.2941 | 0.1564 | -1.43 | -1.7941 | -1.9898 | -1.9485 |
| 1,3-diamino-2-hydroxy-propane | 0.3205 | 0.1543 | -2.05 | -1.4275 | -2.2615 | -2.2709 |
| N-methyldiethanol amine | 0.2656 | 0.1535 | -1.04 | -1.8338 | -1.8479 | -1.7267 |
| 3-(methylamino)-1,2-propanediol | 0.2969 | 0.1495 | -1.82 | -1.5341 | -2.1942 | -2.1264 |
| triethanolamine | 0.2802 | 0.1496 | -1.00 | -1.7488 | -1.7907 | -1.6880 |
| **Acetylenic alcohols** | | | | | | |
| 3-butyn-2-ol | 0.3720 | 0.1511 | 0.14 | -0.4024 | -0.9506 | -1.0843 |
| 1-pentyn-3-ol | 0.3723 | 0.1498 | 0.67 | -1.1776 | -0.6629 | -0.7948 |
| 2-pentyn-1-ol | 0.3370 | 0.1421 | 0.89 | -0.5724 | -0.6295 | -0.6430 |
| 2-penten-4-yn-1-ol | 0.3022 | 0.1306 | -0.01 | -0.5549 | -1.2012 | -1.0741 |
| 1-hexyn-3-ol | 0.3634 | 0.1517 | 1.20 | 0.6574 | -0.3977 | -0.5197 |
| 1-heptyn-3-ol | 0.3615 | 0.1520 | 1.73 | -0.2650 | -0.1153 | -0.2370 |
| 4-heptyn-3-ol | 0.3353 | 0.1458 | 1.73 | -0.0336 | -0.1788 | -0.2096 |
| 2-octyn-1-ol | 0.3249 | 0.1448 | 2.48 | 0.1944 | 0.2020 | 0.1961 |
| 2-nonyn-1-ol | 0.3245 | 0.1449 | 3.01 | 0.6486 | 0.4880 | 0.4796 |
| 2-decyn-1-ol | 0.3242 | 0.1449 | 3.54 | 0.9855 | 0.7743 | 0.7631 |
| 2-tridecyn-1-ol | 0.3238 | 0.1450 | 5.13 | 2.3665 | 1.6343 | 1.6141 |

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|---|---|---|---|---|---|---|
| 4-methyl-1-pentyn-3-ol | 0.3634 | 0.1517 | 1.07 | -0.0267 | -0.4681 | -0.5893 |
| 4-methyl-1-heptyn-3-ol | 0.3510 | 0.1546 | 2.13 | 0.7426 | 0.0759 | -0.0346 |
| **Unsaturated alcohols** | | | | | | |
| 2-methyl-3-buten-2-ol | 0.3114 | 0.1495 | 0.52 | -1.3889 | -0.8920 | -0.8736 |
| 4-pentyn-1-ol | 0.3783 | 0.1450 | -0.01 | -1.4204 | -1.0167 | -1.1377 |
| 2-methyl-3-butyn-2-ol | 0.3734 | 0.1496 | 0.28 | -1.3114 | -0.8715 | -1.0030 |
| trans-3-hexen-1-ol | 0.2385 | 0.1567 | 1.40 | -0.7772 | -0.5924 | -0.4347 |
| cis-3-hexen-1-ol | 0.2526 | 0.1494 | 1.40 | -0.8091 | -0.5583 | -0.4022 |
| 5-hexyn-1-ol | 0.3513 | 0.1507 | 0.52 | -1.2948 | -0.7951 | -0.8792 |
| 3-methyl-1-pentyn-3-ol | 0.3800 | 0.1468 | 1.07 | -1.3226 | -0.4278 | -0.5674 |
| 4-hexen-1-ol | 0.2391 | 0.1559 | 1.40 | -0.7540 | -0.5909 | -0.4309 |
| 5-hexen-1-ol | 0.2748 | 0.1564 | 1.40 | -0.8411 | -0.5044 | -0.4331 |
| 4-pentyn-2-ol | 0.3639 | 0.1446 | 0.12 | -1.6324 | -0.9812 | -1.0663 |
| 5-hexyn-3-ol | 0.3626 | 0.1520 | 0.65 | -1.4043 | -0.6974 | -0.8155 |
| 3-heptyn-1-ol | 0.3024 | 0.1515 | 1.40 | -0.3231 | -0.4373 | -0.4115 |
| 4-heptyn-2-ol | 0.3028 | 0.1473 | 1.18 | -0.6160 | -0.5554 | -0.5109 |
| 3-octyn-1-ol | 0.2993 | 0.1522 | 1.93 | 0.0170 | -0.1580 | -0.1309 |
| 3-nonyn-1-ol | 0.2972 | 0.1527 | 2.46 | 0.3401 | 0.1241 | 0.1506 |
| 2-propen-1-ol | 0.3318 | 0.1506 | 0.17 | -1.9178 | -1.0321 | -1.0663 |
| 2-buten-1-ol | 0.2736 | 0.1519 | 0.34 | -1.4719 | -1.0811 | -0.9810 |
| (+/-)-3-buten-2-ol | 0.3149 | 0.1431 | 0.12 | -1.0529 | -1.1001 | -1.0599 |
| cis-2-buten-1,4-diol | 0.3241 | 0.1412 | -0.81 | -2.1495 | -1.5813 | -1.5491 |
| cis-2-penten-1-ol | 0.2944 | 0.1490 | 0.87 | -1.1052 | -0.7438 | -0.6844 |
| 3-penten-2-ol | 0.2870 | 0.1464 | 0.65 | -1.4010 | -0.8808 | -0.7907 |
| trans-2-hexen-1-ol | 0.2322 | 0.1577 | 1.40 | -0.4718 | -0.6077 | -0.4388 |
| 1-hexen-3-ol | 0.3153 | 0.1530 | 1.18 | -0.8113 | -0.5251 | -0.5361 |
| cis-2-hexen-1-ol | 0.2691 | 0.1510 | 1.40 | -0.7767 | -0.5180 | -0.4096 |
| trans-2-octen-1-ol | 0.2311 | 0.1577 | 2.45 | 0.3654 | -0.0418 | 0.1231 |
| **Amines** | | | | | | |
| Propylamine | 0.3178 | 0.1586 | 0.47 | -0.7075 | -0.9036 | -0.9409 |
| Butylamine | 0.3168 | 0.1586 | 0.97 | -0.5735 | -0.6352 | -0.6733 |
| N-Methylpropylamine | 0.2729 | 0.1577 | 0.84 | -0.8087 | -0.8122 | -0.7388 |
| Amylamine | 0.3110 | 0.1570 | 1.49 | -0.4848 | -0.3677 | -0.3876 |
| N-Methylbutylamine | 0.2709 | 0.1586 | 1.33 | -0.6784 | -0.5516 | -0.4803 |
| Hexylamine | 0.3108 | 0.1568 | 2.06 | -0.2197 | -0.0597 | -0.0818 |
| Isopropylamine | 0.3423 | 0.1514 | 0.26 | -0.8635 | -0.9579 | -1.0215 |
| Isobutylamine | 0.3353 | 0.1501 | 0.73 | -0.2616 | -0.7203 | -0.7641 |
| N,N-Dimethylethylamine | 0.2383 | 0.1543 | 0.70 | -0.9083 | -0.9719 | -0.7988 |
| (±)-sec-Butylamine | 0.3314 | 0.1534 | 0.74 | -0.6708 | -0.7243 | -0.7732 |
| Isoamylamine | 0.3254 | 0.1561 | 1.32 | -0.5774 | -0.4249 | -0.4748 |
| 1-Methylbutylamine | 0.3273 | 0.1539 | 1.23 | -0.6846 | -0.4690 | -0.5133 |
| 1-Ethylpropylamine | 0.3153 | 0.1561 | 1.23 | -0.8129 | -0.4982 | -0.5231 |

Continued…….

| | | | | | | |
|---|---|---|---|---|---|---|
| 2-Methylbutylamine | 0.3226 | 0.1565 | 1.32 | -0.4774 | -0.4316 | -0.4763 |
| N,N-Diethylmethylamine | 0.2445 | 0.1567 | 0.95 | -0.7559 | -0.8215 | -0.6753 |
| tert-Butylamine | 0.3583 | 0.1462 | 0.40 | -0.8973 | -0.8431 | -0.9234 |
| tert-Amylamine | 0.3499 | 0.1475 | 1.10 | -0.6978 | -0.4845 | -0.5543 |
| (+/-)-1,2-Dimethylpropylamine | 0.3185 | 0.1537 | 1.10 | -0.7095 | -0.5608 | -0.5817 |
| Propargylamine | 0.3450 | 0.1533 | -0.43 | -0.826 | -1.3247 | -1.3991 |
| N-Methylpropargylamine | 0.3179 | 0.1514 | 0.08 | -0.9818 | -1.1145 | -1.1179 |
| 1-Dimethylamino-2-propyne | 0.2876 | 0.1517 | -0.01 | -1.1451 | -1.2367 | -1.1675 |
| 1,1-Dimethylpropargylamine | 0.3342 | 0.1517 | 0.64 | -0.9104 | -0.7717 | -0.8193 |
| 2-Methoxyethylamine | 0.3294 | 0.1574 | -0.67 | -1.7903 | -1.4926 | -1.5458 |
| 3-Methoxypropylamine | 0.3305 | 0.1542 | -1.02 | -1.7725 | -1.6794 | -1.7189 |
| 3-Ethoxypropylamine | 0.3298 | 0.1542 | -0.49 | -1.7027 | -1.3943 | -1.4354 |

*Taken from reference 46