experimental training ethylbenzene 7.74% 10 × benzonitrile 5.54% cyclohexylmethanol 53.36% benzaldehyde 7.67% X anisole 11.45% 5 3-methylundecane 17.66% × chlorosulfanyl thiohypochlorite 7.3% trichlorosilane 36.72% phenoxybenzene 10.95% 0 n,n-dipropylpropan-1-amine 27.59% n,n-dibutylbutan-1-amine 24.57% phenylmethoxymethylbenzene 10.5% -5 ethoxybenzene 9.08% butylbenzene 4.76% decylbenzene 11.13% n',n'-diethylpropane-1,3-diamine 17.18% -10ethyl propanoate 5.14% diethyl propanedioate 8.05% propyl butanoate 8.43% 0.2 0.4 0.6 8.0 1.0 0.0 3-methylbutyl propanoate 10.59% dibutyl hexanedioate 1.49% dipropyl hexanedioate 5.7% 3-methylbutyl butanoate 7.23% ethyl heptanoate 13.31% butanoyl butanoate 10.61% 1,4-dibromobenzene 26.59% 1-bromo-4-methylbenzene 33.29% 1,4-xylene 1.18% methyl hexanoate 3.58% 1-bromopropane 9.21% butane 4.21% buta-1,3-diene 7.78% 3-ethyl-3-methylpentane 21.23% 3,3-diethylpentane 11.45% 3-chloroprop-1-ene 12.22% 1,2-dichloroethane 10.98% 1-iodopropane 5.31% propan-1-amine 24.11% propanenitrile 10.28% prop-2-enenitrile 4.78% ethane-1,2-diamine 7.61% prop-2-en-1-ol 7.77% prop-2-yn-1-ol 13.41% methyl formate 3.98% trimethyl(trimethylsilyloxy)silane 2.96% dimethyl-bis(trimethylsilyloxy)silane 23.66% 1,2,3,4,5,6-hexadeuteriobenzene 6.84% hexylbenzene 8.49% heptylbenzene 3.73% 1-nitropropane 7.52% 2,4-dimethylpentane 1.39% 4-methylpentan-2-one 8.44% 4-methylpentan-2-ol 12.03% 1-(dimethylamino)propan-2-ol 34.8% n-propan-2-ylpropan-2-amine 7.23% 2-propan-2-yloxypropane 4.54% propan-2-yl acetate 2.62% acetyl acetate 2.95% 5-methyloxolan-2-one 12.21% furan-2,5-dione 7.73% 1,3-xylene 3.86% 1-chloro-3-methylbenzene 25.76% ethyl 3-methylbutanoate 4.46% 2,6-dimethylheptan-4-ol 43.89% 2,6-dimethylheptan-4-one 6.84% bromocyclohexane 0.41% toluene 3.02% cyclohexanamine 12.03% nonylbenzene 9.86% 1-methylpiperazine 10.69% 4-methylmorpholine 37.62% butyl butanoate 6.92% 2-propan-2-yloxyethanol 6.59% propyl acetate 9.03% 1,3-dibromopropane 8.09% 1-bromobutane 9.77% pentane 5.24% 1-chlorobutane 9.45% butan-1-amine 10.79% propane-1,3-diamine 4.85% butane-1-thiol 6.86% ethyl formate 2.49% 1h-pyrrole 7.8% oxolane 3.53% furan 1.13% 5-methylhexan-2-one 3.06% 2-methylpropyl acetate 9.51% ethyl decanoate 3.86% methyl decanoate 3.39% heptan-2-one 13.15% 1-bromopentane 3.82% 1,4-dichlorobutane 11.99% pentan-1-amine 7.55% pentanal 8.8% 2-(ethylamino)ethanol 7.89% propyl formate 3.91% 2,6,10,15,19,23-hexamethyltetracosane 4.55% methyl octanoate 2.11% hexan-1-amine 6.01% n'-(2-aminoethyl)ethane-1,2-diamine 8.85% 1-propoxypropane 6.66% 2-acetyloxyethyl acetate 29.3% heptan-1-amine 11.94% hexanedinitrile 4.85% heptan-1-ol 4.49% heptanal 2.87% methyl dodecanoate 4.32% nonane 3.74% 1-chlorooctane 5.11% octan-1-amine 14.99% octane-1-thiol 23.77% n-butylbutan-1-amine 40.18% 1-methoxy-2-(2-methoxyethoxy)ethane 9.41% dimethoxy(dimethyl)silane 12.25% (z)-1-chloro-2,3,3,3-tetrafluoroprop-1-ene 8.4% n,n-dioctyloctan-1-amine 17.69% dimethyl pentanedioate 6.75% octyl acetate 8.06% heptyl formate 14.7% n'-[2-(2-aminoethylamino)ethyl]ethane-1,2-diamine 41.56% decan-1-ol 6.35% decanal 74.96% methyl hexadecanoate 5.86% dodec-1-ene 10.94% 1-methoxy-2-[2-(2-methoxyethoxy)ethoxy]ethane 3.34% methyl octadecanoate 5.29% methyl (z)-octadec-9-enoate 10.69% methyl (9z,12z)-octadeca-9,12-dienoate 29.35% tridecan-1-ol 18.19% 1-[2-(2-butoxyethoxy)ethoxy]butane 74.62% octadecan-1-ol 7.52% icosane 3.28% undecane 3.31% methyl icosanoate 7.31% methyl (z)-docos-13-enoate 9.77% 1-ethylnaphthalene 5.78% prop-1-ene 4.96% methoxymethane 6.87% 1,1,2,2,3,3,4,4-octafluorocyclobutane 6.14% dioctyl benzene-1,2-dicarboxylate 61.77% diphenylmethanone 18.85% cyclopentanone 6.87% n,n-diethylethanamine 3.44% diethoxymethoxyethane 19.24% bis(2-ethylhexyl) decanedioate 7.03% phenyl acetate 17.55% heptan-4-one 5.33% diethyl butanedioate 13.77% propanal 8.08% pentane-2,4-dione 13.33% propanoyl propanoate 1.36% 2,4,6-trimethyl-1,3,5-trioxane 24.59% pyrrolidine 8.95% butyl acetate 3.92% 1,4-dioxane 6.25% octan-2-ol 9.52% methyl tetradecanoate 3.56% non-1-ene 10.3% decane 3.29% nonanal 6.3% n-methylmethanamine 66.55% 1,2-dibromo-1,1,2,2-tetrafluoroethane 50.86% 2-methylprop-2-enenitrile 9.09% 1,1,2,2-tetrachloroethene 12.02% 3-methyldecane 25.6% methoxy(methoxymethoxymethoxymethoxy)methane 2.55% (e)-oct-2-ene 6.08% butan-2-ylbenzene 101.48% 2-methylbutan-1-ol 14.56% butyl 2-hydroxypropanoate 4.58% 2-piperazin-1-ylethanamine 13.31% ethyl prop-2-enoate 6.25% diethyl hexanedioate 2.49% butyl prop-2-enoate 7.45% [dimethyl(trimethylsilyloxy)silyl]oxy-dimethyl-trimethylsilyloxysilane 9.76% ethyl acetate 3.34% 1,3-diethylbenzene 22.79% oxane 18.8% heptane 3.0% n-propylpropan-1-amine 7.46% hexyl acetate 1.88% 1-butoxybutane 3.76% 1-methoxy-2-[2-[2-(2-methoxyethoxy)ethoxy]ethoxy]ethane 5.18% deuteriooxymethane 11.2% nonane-1-thiol 22.82% dichloro-methyl-phenylsilane 2.67% aziridine 20.02% 2-methylsulfanylpropane 8.94% (z)-1,2-dichloroethene 10.34% 2-methylpentadecane 21.75% 3-methylideneheptane 22.91% 2-methoxy-2-methylpropane 7.03% 1-ethoxy-1,1,2,2,3,3,4,4,4-nonafluorobutane 16.01% heptane-1-thiol 5.85% 2,5-dihydrofuran 4.69% dichloro(diethyl)silane 33.59% methyl nonanoate 3.4% 2,3-dimethyldecane 10.67% 2,3-dimethylundecane 11.93% 3-methylcyclopentan-1-one 30.49% dodecylcyclohexane 21.6% butyl 4-oxopentanoate 6.11% (e)-1,1,1,2,3,4,5,5,5-nonafluoro-4-(trifluoromethyl)pent-2-ene 11.21% 1-chloro-2-fluoro-3-nitrobenzene 34.03% octylbenzene 26.23% trimethoxysilane 14.77% trimethoxy-[3-(oxiran-2-ylmethoxy)propyl]silane 2.05% 3-chloropropyl(trimethoxy)silane 76.2% 1-propylnaphthalene 7.52% 2-chloro-1,1,1,2-tetrafluoroethane 5.84% thietane 4.77% nonylcyclohexane 1.55% 2,3-dimethylnonane 24.72% 2,2-dichloro-1,1,1-trifluoroethane 5.27% 1,1,2,2,3,3,4,4,4a,5,5,6,6,7,7,8,8,8a-octadecafluoronaphthalene 10.33% 2,3-dimethylheptane 8.55% 1,1,2,2,3,3,4,5,5,6-decafluoro-4,6-bis(trifluoromethyl)cyclohexane 5.62% 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-hexadecafluoroheptane 13.62% dichloro(phenoxy)phosphane 15.83% dichloro-phenyl-sulfanylidene-lambda5-phosphane 2.52% fluoroethane 6.95% bromo-chloro-difluoromethane 4.84% 1,2-dichloro-1,1,2-trifluoroethane 5.91% 1,1,1,2,2-pentafluoroethane 5.67% 1,1,1-trichloro-2,2,2-trifluoroethane 1.78% 1,1,1,2,2,3,3,4,4,5,5,6,6,6-tetradecafluorohexane 10.92% hexadecan-1-ol 5.2% 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-icosafluorononane 22.59% 1-methylsulfanylpropane 2.57% 1,2,3,4,5,6-hexafluorobenzene 8.28% 1,1,2,2-tetrafluoro-1-(2,2,2-trifluoroethoxy)ethane 11.92% 1,1,1-trifluoroethane 4.33% 2,2,3,3,3-pentafluoropropan-1-ol 11.96% 3,3-dichloro-1,1,1,2,2-pentafluoropropane 21.02% hexylcyclohexane 4.26% 1,1,1,2,3,3,3-heptafluoropropane 2.67% 1,1,1,3,3-pentafluoropropane 4.34% ethoxymethoxyethane 7.9% 2,2-dimethylpropane 8.28% 2,2,3-trimethylbutane 23.02% 1,3,3-trimethyl-2-oxabicyclo[2.2.2]octane 26.94% 2,6,6-trimethylbicyclo[3.1.1]heptane 36.74% 2-methyl-1,3-dioxolane 16.14% cycloheptanol 39.26% 1,3-dichloro-1,1,2,2,3-pentafluoropropane 16.2% tetranitromethane 10.16% 2-methylbut-2-ene 18.28% 1-chloro-2-methylpropane 4.43% 2-methylpropane-1-thiol 1.22% butane-2-thiol 6.39% 2,3-dimethylbuta-1,3-diene 25.26% 3-acetyloxolan-2-one 3.82% 1,1-dimethoxyethane 17.38% 2-methylfuran 18.91% pentane-1,2-diol 28.59% (1s,5r)-6,8-dioxabicyclo[3.2.1]octan-4-one 49.48% 2-methylpropylbenzene 14.09% 3-[(2s)-1-methylpyrrolidin-2-yl]pyridine 19.24% 1-chloropropane 3.36% 2,2,4-trimethylpentane 4.88% 2,2,4,4,6,6,8,8,10,10,12,12-dodecamethyl-1,3,5,7,9,11-hexaoxa-2,4,6,8,10,12-hexasilacyclododecane 8.04% 2,2,4,4,6,6,8,8,10,10-decamethyl-1,3,5,7,9,2,4,6,8,10-pentaoxapentasilecane 3.51% 2,2,4,4,6,6-hexamethyl-1,3,5,2,4,6-trioxatrisilinane 8.19% chlorocyclohexane 19.22% oxan-2-one 17.59% 2-methylpropyl formate 14.81% 1-iodobutane 9.09% 1-chlorohexane 10.69% ethyl (9z,12z)-octadeca-9,12-dienoate 13.84% 1-butylsulfanylbutane 21.48% methyl 2-methylpropanoate 3.12% 1,3-dioxo-2-benzofuran-5-carboxylic acid 10.38% methyl propanoate 8.76% 2-methylthiophene 15.24% 2,2,4,4,6,6,8,8-octamethyl-1,3,5,7,2,4,6,8-tetraoxatetrasilocane 13.34% 1-methoxypropane 23.5% tetrachloromethane 6.03% 2,3,3-trimethylpentane 3.48% heptylcyclohexane 5.6% 3,3-dimethylpentane 6.4% 2,3-dimethylpentane 2.65% 2,3,4-trimethylpentane 6.97% 2-methylcyclohexan-1-ol 8.63% 2-methylcyclohexan-1-one 61.94% pentan-3-ol 19.56% 1-methyl-4-propan-2-ylidenecyclohexene 5.58% 3-methylhexane 2.4% 3-methylpentan-1-ol 7.07% 2,4-dimethylhexane 1.42% 4-methylheptane 4.49% 3-methylheptane 2.16% heptan-3-ol 23.32% 5-chloropentan-2-one 15.28% (z)-but-2-ene 4.97% 2,2-dimethylhexane 6.09% iodobenzene 11.21% butyl pentanoate 10.39% 2-methylhexane 2.93% hexan-2-one 7.22% 2,5-dimethylhexane 3.14% 2-methylheptane 0.68% hex-1-ene 5.59% cyclohexa-1,3-diene 9.43% hept-1-ene 4.28% butyl formate 8.06% octadecane 2.69% (4r)-1-methyl-4-prop-1-en-2-ylcyclohexene 16.35% pentan-2-ol 12.87% 2-methyl-2-[(2-methylpropan-2-yl)oxy]propane 24.46% 3-ethylpentane 2.22% 3-ethylhexane 13.61% nonan-5-ol 14.5% methyl pentanoate 4.34% pentyl propanoate 8.55% (methyldisulfanyl)methane 44.29% hexan-2-ol 4.91% 1-nitrobutane 1.81% (z)-pent-2-ene 15.47% 1-iodopentane 4.58% 1-methylsulfanylbutane 2.53% pentyl acetate 9.01% hexanenitrile 5.63% 1,5-dichloropentane 6.97% methoxy(methoxymethoxy)methane 36.17% 1,2-diethoxyethane 2.17% hexyl formate 14.95% 1-(butyldisulfanyl)butane 9.81% tetradecane 3.64% pentadecane 4.53% octacosane 9.5% thiophen-2-ylmethanol 15.44% 1-iodohexane 14.43% pentyl formate 10.37% ethanol 8.27% 3-methyltridecane 26.48% (e)-pent-2-ene 14.1% 2,3,4,6,7,8,9,10-octahydropyrimido[1,2-a]azepine 53.33% 1,1,1,2,3,3-hexafluoro-2-(1,1,2,2,3,3,3-heptafluoropropoxy)-3-(1,1,2,2,2-pentafluoroethoxy)propane 6.9% methanol 11.13% propan-2-ol 10.11% propan-2-one 4.96% chloroform 8.04% heptadec-1-ene 5.12% tetramethyl silicate 10.65% 1,1,2,2-tetradeuterioethene 8.26% 1,1,1,3,3,3-hexafluoropropane 3.97% (z)-1,1,1,4,4,4-hexafluorobut-2-ene 2.75% 1-pentoxypentane 26.61% 2-methyldecane 3.01% 1-ethylsulfinylethane 31.04% 1,3,5-trimethyladamantane 7.82% propan-1-ol 10.11% butan-1-ol 6.92% pentan-1-ol 6.39% benzene 5.07% 1,1,1-trichloroethane 23.46% 1,3,5-tri(propan-2-yl)benzene 24.27% 1,3-dimethyl-1,3-diazinan-2-one 25.99% methane 5.82% bromomethane 2.1% ethane 4.53% ethene 3.85% acetylene 4.56% chloromethane 9.58% iodomethane 6.04% methanamine 5.73% formonitrile 4.96% dibromomethane 4.08% propane 4.36% ethyl 2-methylbutanoate 11.87% chloroethane 5.33% iodoethane 2.46% ethanamine 11.91% acetonitrile 7.09% acetaldehyde 12.69% ethanethiol 39.75% difluoromethane 4.89% diiodomethane 7.38% methylsulfanylmethane 15.29% oxirane 3.5% bromoform 12.64% 2-bromopropane 6.34% 2-methylpropane 4.6% 2-iodopropane 2.8% propan-2-amine 17.06% propane-2-thiol 3.06% 1,1-dichloroethane 3.49% 1,1-dichloroethene 5.71% 1,1-difluoroethane 3.82% dichloro(fluoro)methane 3.3% chloro(difluoro)methane 6.54% fluoroform 10.74% nitromethane 6.38% dichloro-methylsilane 13.23% 2-methyloxirane 4.21% bromo(trifluoro)methane 5.04% 2-methylpropane-2-thiol 39.91% 1-chloro-1,1-difluoroethane 3.47% trichloro(fluoro)methane 2.32% dichloro(difluoro)methane 4.75% tetrafluoromethane 3.67% chloro(trimethyl)silane 2.92% trichloro(methyl)silane 9.89% 2-methylbutan-2-ol 18.75% 2,2,2-trifluoroethanol 8.53% trichloro(ethenyl)silane 23.91% 3,3-dimethylbutan-2-one 9.36% [methoxy(methyl)phosphoryl]oxymethane 11.37% n,n-dimethylpropanamide 41.31% 1,1,2-trichloro-1,2,2-trifluoroethane 3.04% 1-chloro-1,1,2,2,2-pentafluoroethane 3.4% 1,1,1,2,2,2-hexafluoroethane 2.93% 1,1,1,2,2,3,3,3-octafluoropropane 6.55% 2,2,3,3-tetrafluoropropan-1-ol 9.55% 2-methylpent-1-ene 3.59% 1-cyclopropylethanone 46.39% tricyclo[5.2.1.02,6]deca-3,8-diene 13.04% 3-methylpentan-3-ol 28.66% 1-ethyladamantane 15.96% 3,5,5-trimethylcyclohex-2-en-1-one 29.6% 3,7-dimethylocta-1,6-dien-3-ol 13.6% 2-methylbutane 7.4% 2-methylbuta-1,3-diene 15.38% 2-methylpropan-1-ol 9.22% 2-methylpropanal 20.72% 2-chlorobutane 10.88% propane-1,2-diamine 7.21% butan-2-one 4.75% silane 21.81% methyl acetate 7.44% 1-nitroethane 3.42% 2,3-dimethylbutane 3.94% 1,1,2,2-tetrachloroethane 1.72% 2-nitropropane 16.91% 2,2-dimethyl-3-methylidenebicyclo[2.2.1]heptane 15.61% 2,6,6-trimethylbicyclo[3.1.1]hept-2-ene 3.87% methyl 2-methylprop-2-enoate 2.05% 1,1,1,2-tetrafluoroethane 5.76% undec-1-ene 10.51% dimethoxy(oxo)phosphanium 44.58% dec-1-ene 9.29% 1-methyl-2-nitrobenzene 5.39% 5-methyl-2-propan-2-ylcyclohexan-1-ol 23.54% 1-methylnaphthalene 5.04% 1,2,3,4,4a,5,6,7,8,8a-decahydronaphthalene 7.44% naphthalene 12.58% 2-methylnaphthalene 18.14% 3-triethoxysilylpropanenitrile 21.98% methyl docosanoate 6.18% 2-ethylnaphthalene 25.38% 1-benzothiophene 8.89% 3-methylpentane 1.62% cyclopentanol 12.55% 2-methyloxolane 7.1% oxolan-2-one 10.44% ethyl 2-methylpropanoate 0.85% 2-methylpropanoyl 2-methylpropanoate 5.22% 2-ethylbutan-1-ol 24.78% tert-butylbenzene 4.32% trichloro(phenyl)silane 54.71% 1-tert-butyl-4-methylbenzene 8.32% 2-(4-methylcyclohex-3-en-1-yl)propan-2-ol 18.51% cumene 3.04% 1-methyl-3-nitrobenzene 13.69% 2-methoxy-2-methylbutane 15.34% [dimethyl-(trimethylsilylamino)silyl]methane 6.16%